



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2026 – 02:32 PM JST

PDB ID : 26JL / pdb_000026jl
Title : Crystal structure of the AAA+ domain of Vibrio cholerae FlrA
Authors : Dasgupta, J.; Sen, U.; Das, R.
Deposited on : 2026-05-01
Resolution : 3.20 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

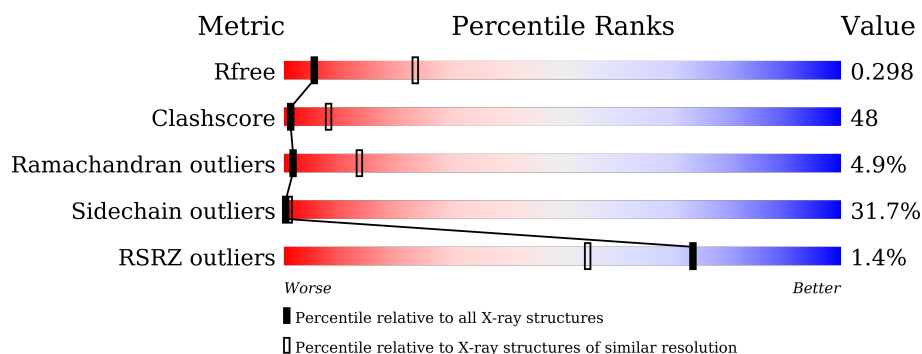
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	259	<div> <div>2%</div> <div>15% 58% 23% 5%</div> </div>
1	B	259	<div> <div>%</div> <div>18% 56% 21% 5%</div> </div>
1	C	259	<div> <div>2%</div> <div>16% 55% 25% .</div> </div>
1	D	259	<div> <div>%</div> <div>19% 53% 25% .</div> </div>
1	E	259	<div> <div>2%</div> <div>18% 53% 25% 5%</div> </div>
1	F	259	<div> <div>%</div> <div>18% 51% 27% 5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	B	440	-	X	-	-
2	EDO	C	404	-	-	X	-
2	EDO	D	405	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13833 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 Flagellar regulatory protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2035	1276	367	377	15			
1	B	259	Total	C	N	O	S	0	0	0
			2035	1276	367	377	15			
1	C	259	Total	C	N	O	S	0	0	0
			2035	1276	367	377	15			
1	D	259	Total	C	N	O	S	0	0	0
			2035	1276	367	377	15			
1	E	259	Total	C	N	O	S	0	0	0
			2035	1276	367	377	15			
1	F	259	Total	C	N	O	S	0	0	0
			2035	1276	367	377	15			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	-	expression tag	UNP A0A0H3AM86
A	128	SER	-	expression tag	UNP A0A0H3AM86
A	129	GLY	-	expression tag	UNP A0A0H3AM86
A	130	LEU	-	expression tag	UNP A0A0H3AM86
A	131	VAL	-	expression tag	UNP A0A0H3AM86
A	132	PRO	-	expression tag	UNP A0A0H3AM86
A	133	ARG	-	expression tag	UNP A0A0H3AM86
A	134	GLY	-	expression tag	UNP A0A0H3AM86
A	135	SER	-	expression tag	UNP A0A0H3AM86
A	136	HIS	-	expression tag	UNP A0A0H3AM86
A	137	MET	-	expression tag	UNP A0A0H3AM86
B	127	ALA	-	expression tag	UNP A0A0H3AM86
B	128	SER	-	expression tag	UNP A0A0H3AM86
B	129	GLY	-	expression tag	UNP A0A0H3AM86
B	130	LEU	-	expression tag	UNP A0A0H3AM86
B	131	VAL	-	expression tag	UNP A0A0H3AM86
B	132	PRO	-	expression tag	UNP A0A0H3AM86

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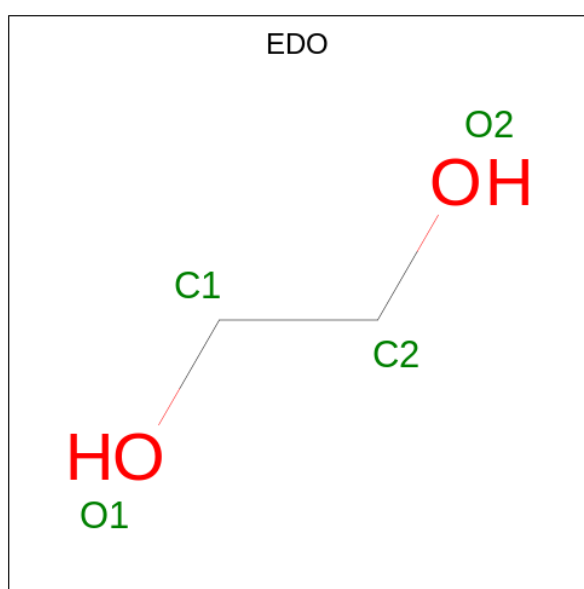
Chain	Residue	Modelled	Actual	Comment	Reference
B	133	ARG	-	expression tag	UNP A0A0H3AM86
B	134	GLY	-	expression tag	UNP A0A0H3AM86
B	135	SER	-	expression tag	UNP A0A0H3AM86
B	136	HIS	-	expression tag	UNP A0A0H3AM86
B	137	MET	-	expression tag	UNP A0A0H3AM86
C	127	ALA	-	expression tag	UNP A0A0H3AM86
C	128	SER	-	expression tag	UNP A0A0H3AM86
C	129	GLY	-	expression tag	UNP A0A0H3AM86
C	130	LEU	-	expression tag	UNP A0A0H3AM86
C	131	VAL	-	expression tag	UNP A0A0H3AM86
C	132	PRO	-	expression tag	UNP A0A0H3AM86
C	133	ARG	-	expression tag	UNP A0A0H3AM86
C	134	GLY	-	expression tag	UNP A0A0H3AM86
C	135	SER	-	expression tag	UNP A0A0H3AM86
C	136	HIS	-	expression tag	UNP A0A0H3AM86
C	137	MET	-	expression tag	UNP A0A0H3AM86
D	127	ALA	-	expression tag	UNP A0A0H3AM86
D	128	SER	-	expression tag	UNP A0A0H3AM86
D	129	GLY	-	expression tag	UNP A0A0H3AM86
D	130	LEU	-	expression tag	UNP A0A0H3AM86
D	131	VAL	-	expression tag	UNP A0A0H3AM86
D	132	PRO	-	expression tag	UNP A0A0H3AM86
D	133	ARG	-	expression tag	UNP A0A0H3AM86
D	134	GLY	-	expression tag	UNP A0A0H3AM86
D	135	SER	-	expression tag	UNP A0A0H3AM86
D	136	HIS	-	expression tag	UNP A0A0H3AM86
D	137	MET	-	expression tag	UNP A0A0H3AM86
E	127	ALA	-	expression tag	UNP A0A0H3AM86
E	128	SER	-	expression tag	UNP A0A0H3AM86
E	129	GLY	-	expression tag	UNP A0A0H3AM86
E	130	LEU	-	expression tag	UNP A0A0H3AM86
E	131	VAL	-	expression tag	UNP A0A0H3AM86
E	132	PRO	-	expression tag	UNP A0A0H3AM86
E	133	ARG	-	expression tag	UNP A0A0H3AM86
E	134	GLY	-	expression tag	UNP A0A0H3AM86
E	135	SER	-	expression tag	UNP A0A0H3AM86
E	136	HIS	-	expression tag	UNP A0A0H3AM86
E	137	MET	-	expression tag	UNP A0A0H3AM86
F	127	ALA	-	expression tag	UNP A0A0H3AM86
F	128	SER	-	expression tag	UNP A0A0H3AM86
F	129	GLY	-	expression tag	UNP A0A0H3AM86
F	130	LEU	-	expression tag	UNP A0A0H3AM86

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Chain	Residue	Modelled	Actual	Comment	Reference
F	131	VAL	-	expression tag	UNP A0A0H3AM86
F	132	PRO	-	expression tag	UNP A0A0H3AM86
F	133	ARG	-	expression tag	UNP A0A0H3AM86
F	134	GLY	-	expression tag	UNP A0A0H3AM86
F	135	SER	-	expression tag	UNP A0A0H3AM86
F	136	HIS	-	expression tag	UNP A0A0H3AM86
F	137	MET	-	expression tag	UNP A0A0H3AM86

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



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

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

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

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

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

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

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

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

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

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

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

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[illegible]

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

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

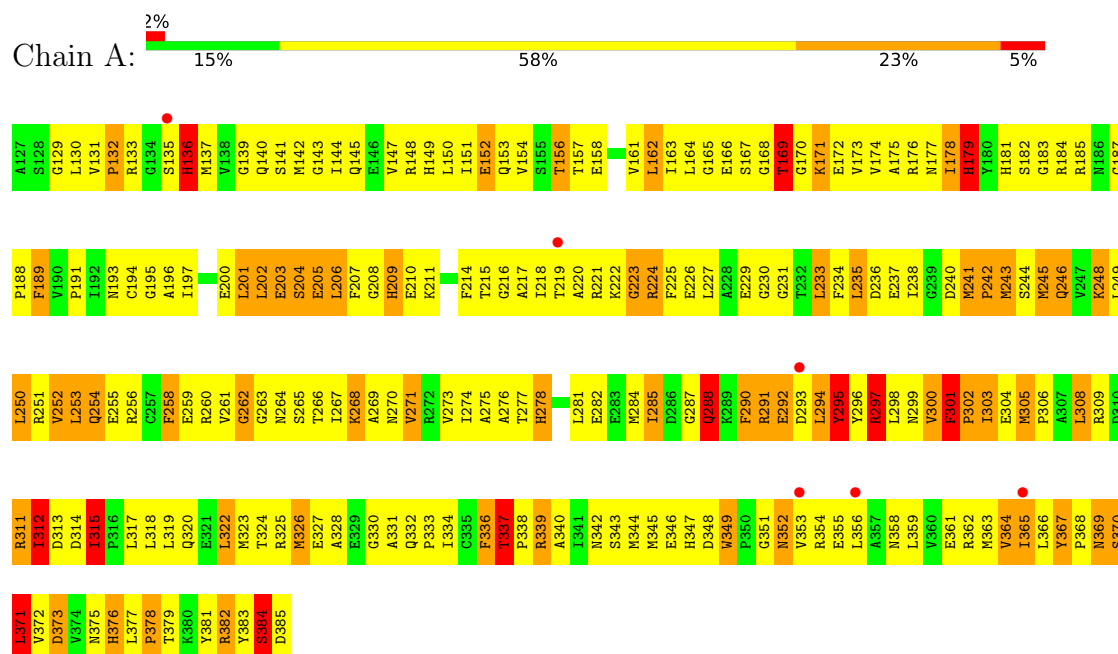
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	96	Total	O	0	0
			96	96		
3	B	91	Total	O	0	0
			91	91		
3	C	100	Total	O	0	0
			100	100		
3	D	98	Total	O	0	0
			98	98		
3	E	97	Total	O	0	0
			97	97		
3	F	101	Total	O	0	0
			101	101		

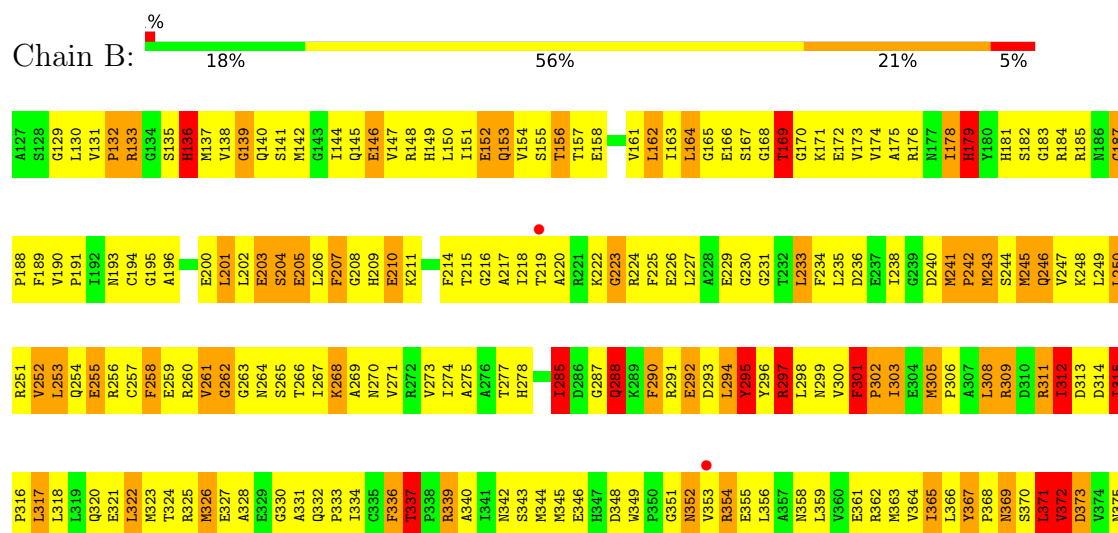
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Flagellar regulatory protein A

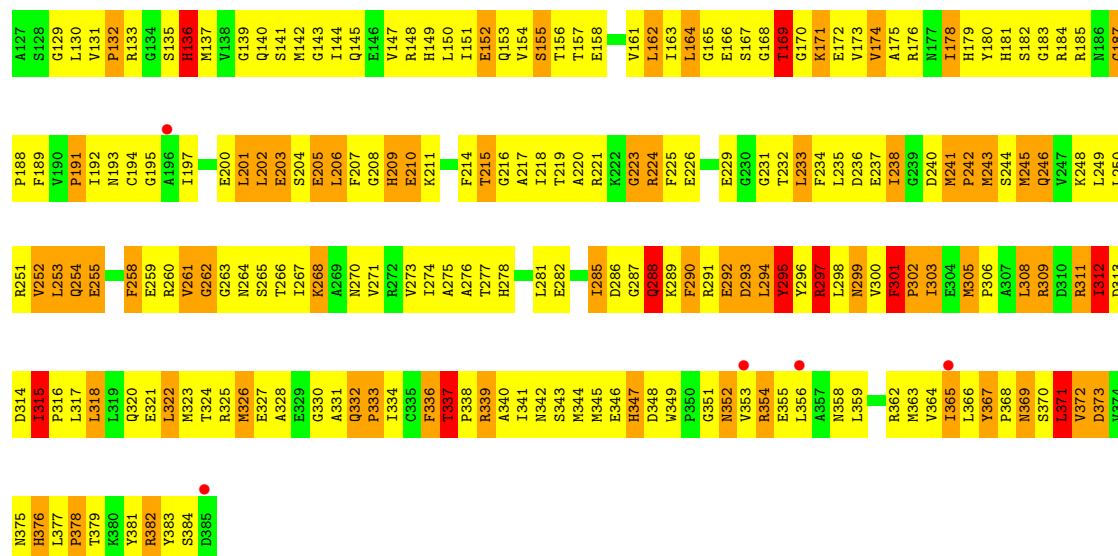
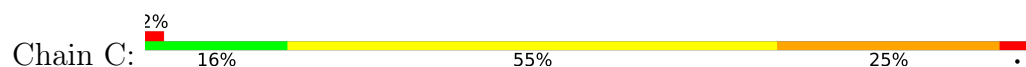


• Molecule 1: Flagellar regulatory protein A

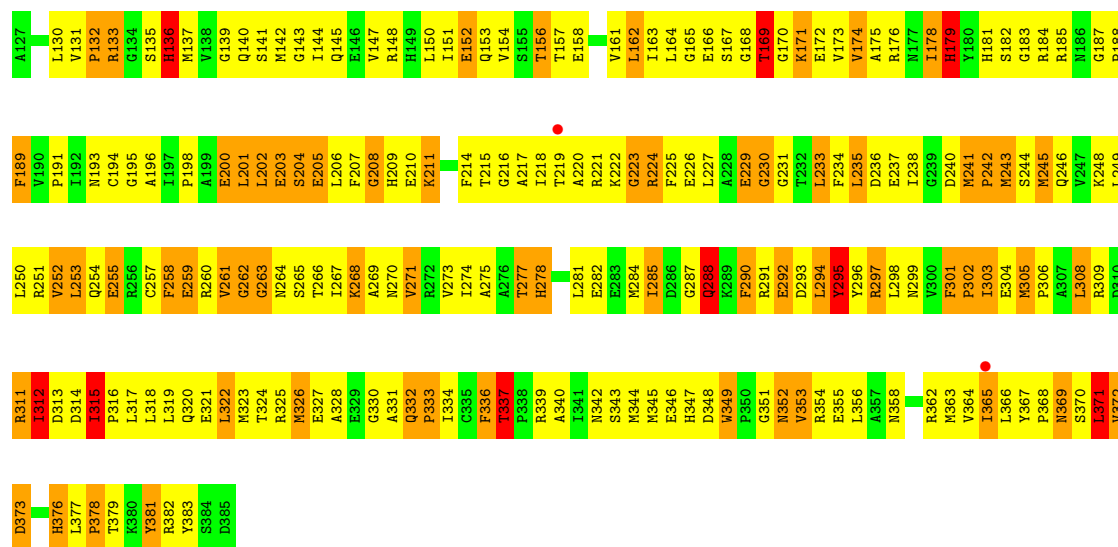
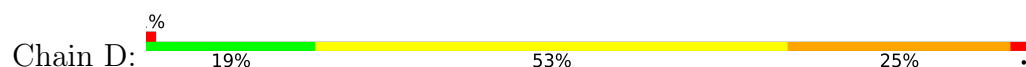


H376
L377
P378
T379
K380
Y381
R382
S384
D385

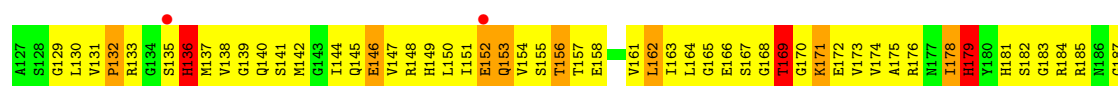
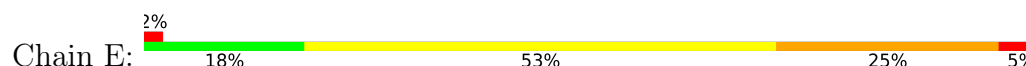
• Molecule 1: Flagellar regulatory protein A

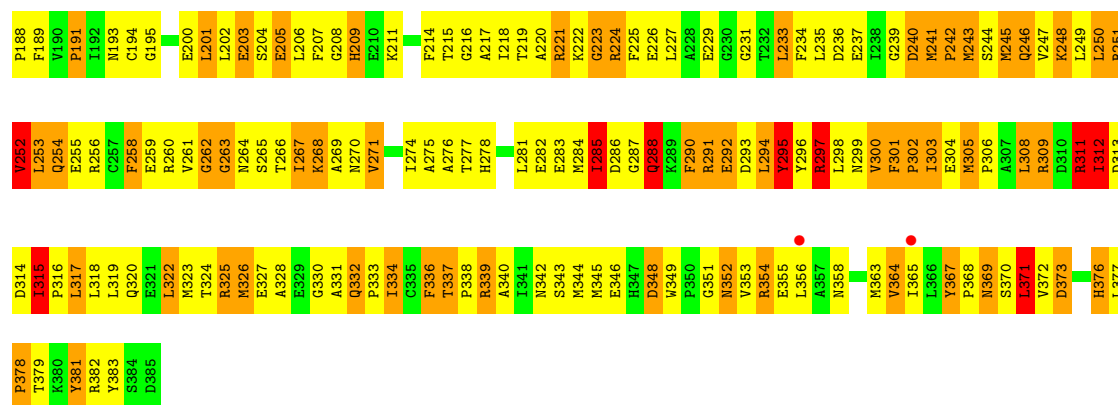


• Molecule 1: Flagellar regulatory protein A

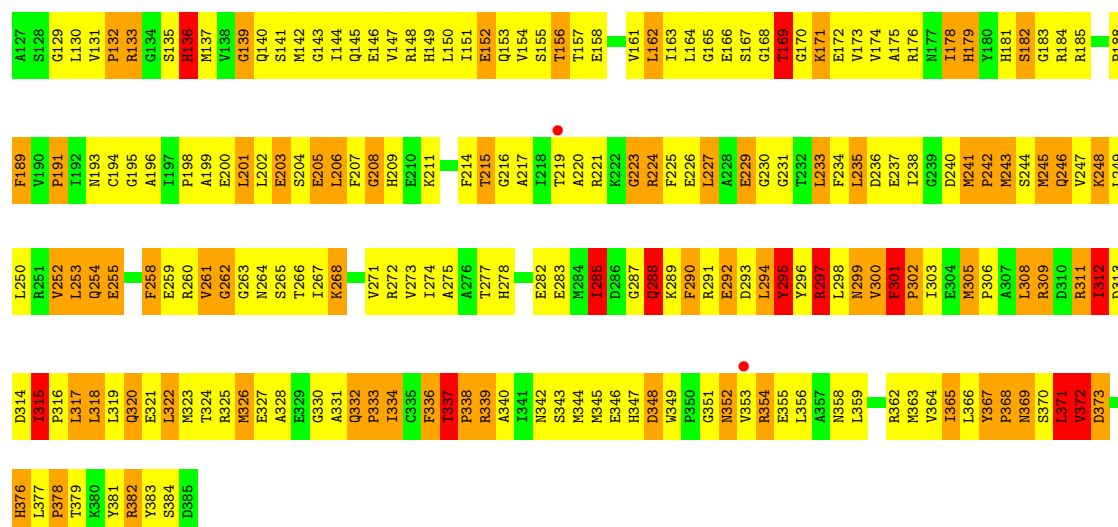
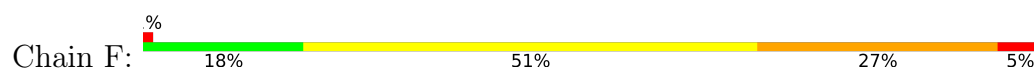


• Molecule 1: Flagellar regulatory protein A





● Molecule 1: Flagellar regulatory protein A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	101.17Å 101.17Å 49.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	9.98 – 3.20 9.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (9.98-3.20) 99.2 (9.98-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.220 , 0.295 0.261 , 0.298	Depositor DCC
R_{free} test set	2047 reflections (6.64%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.499 for h+k,-h,l 0.499 for -k,h+k,l 0.499 for k,-h-k,l 0.499 for -h-k,h,l 0.499 for -h,-k,l 0.418 for h,-h-k,-l 0.418 for -h-k,k,-l 0.418 for k,h,-l 0.418 for -k,-h,-l 0.418 for -h,h+k,-l 0.418 for h+k,-k,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	13833	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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: EDO

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	0.94	1/2072 (0.0%)	1.55	45/2798 (1.6%)
1	B	0.95	2/2072 (0.1%)	1.56	38/2798 (1.4%)
1	C	0.98	4/2072 (0.2%)	1.59	38/2798 (1.4%)
1	D	0.93	1/2072 (0.0%)	1.56	38/2798 (1.4%)
1	E	0.97	2/2072 (0.1%)	1.57	45/2798 (1.6%)
1	F	0.93	1/2072 (0.0%)	1.61	51/2798 (1.8%)
All	All	0.95	11/12432 (0.1%)	1.57	255/16788 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	7
1	C	0	4
1	D	0	5
1	E	0	6
1	F	0	6
All	All	0	32

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	347	HIS	CG-CD2	-7.40	1.27	1.35
1	C	209	HIS	CG-CD2	-7.06	1.28	1.35
1	C	352	ASN	CA-C	-6.33	1.50	1.53
1	E	352	ASN	CA-C	-6.30	1.50	1.53
1	B	352	ASN	CA-C	-6.20	1.50	1.53
1	F	352	ASN	CA-C	-5.80	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	353	VAL	CA-CB	5.42	1.60	1.54
1	B	337	THR	CA-C	5.22	1.57	1.52
1	C	337	THR	CA-C	5.20	1.57	1.52
1	A	278	HIS	CG-CD2	5.17	1.41	1.35
1	E	267	ILE	CA-C	5.02	1.58	1.52

All (255) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	262	GLY	N-CA-C	11.75	126.83	112.73
1	B	351	GLY	N-CA-C	-10.45	92.55	111.25
1	E	351	GLY	N-CA-C	-10.32	91.20	112.04
1	F	351	GLY	N-CA-C	-10.26	93.02	112.51
1	B	262	GLY	N-CA-C	10.01	124.74	112.73
1	C	262	GLY	N-CA-C	9.87	125.40	112.77
1	D	262	GLY	N-CA-C	9.78	124.46	112.73
1	F	336	PHE	N-CA-C	9.66	124.03	109.63
1	E	262	GLY	N-CA-C	9.48	124.10	112.73
1	F	293	ASP	N-CA-C	9.24	121.11	111.14
1	C	336	PHE	N-CA-C	9.19	123.33	109.63
1	C	351	GLY	N-CA-C	-9.19	93.48	112.04
1	A	337	THR	N-CA-C	9.17	125.22	109.82
1	C	293	ASP	N-CA-C	9.16	121.03	111.14
1	C	332	GLN	CA-C-N	9.09	131.20	119.84
1	C	332	GLN	C-N-CA	9.09	131.20	119.84
1	B	294	LEU	N-CA-C	9.04	124.11	108.02
1	D	337	THR	N-CA-C	8.98	123.85	110.10
1	E	336	PHE	N-CA-C	8.77	122.70	109.63
1	D	336	PHE	N-CA-C	8.73	122.64	109.63
1	D	294	LEU	N-CA-C	8.71	122.62	108.34
1	E	293	ASP	N-CA-C	8.62	120.45	111.14
1	A	262	GLY	N-CA-C	8.58	123.03	112.73
1	C	337	THR	N-CA-C	8.56	123.98	109.09
1	E	294	LEU	N-CA-C	8.55	123.24	108.02
1	B	337	THR	N-CA-C	8.51	123.91	109.09
1	E	337	THR	N-CA-C	8.51	124.11	109.82
1	B	312	ILE	N-CA-C	8.48	119.28	110.72
1	C	157	THR	N-CA-C	8.47	122.58	109.96
1	B	336	PHE	N-CA-C	8.42	122.18	109.63
1	A	336	PHE	N-CA-C	8.38	122.12	109.63
1	B	330	GLY	N-CA-C	-8.38	93.33	113.18
1	A	293	ASP	N-CA-C	8.35	120.16	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	157	THR	N-CA-C	8.26	122.26	109.96
1	A	294	LEU	N-CA-C	8.09	122.42	108.02
1	C	371	LEU	N-CA-C	8.04	122.87	112.26
1	D	208	GLY	N-CA-C	8.02	123.22	110.87
1	E	312	ILE	N-CA-C	7.92	118.72	110.72
1	D	293	ASP	N-CA-C	7.90	119.67	111.14
1	C	370	SER	N-CA-C	7.80	118.99	108.23
1	B	293	ASP	N-CA-C	7.79	119.55	111.14
1	F	337	THR	N-CA-C	7.75	122.84	109.82
1	B	301	PHE	CA-C-N	7.74	129.51	119.84
1	B	301	PHE	C-N-CA	7.74	129.51	119.84
1	F	312	ILE	N-CA-C	7.74	118.53	110.72
1	C	294	LEU	N-CA-C	7.72	121.77	108.02
1	D	376	HIS	N-CA-C	7.70	121.93	112.54
1	F	332	GLN	CA-C-N	7.67	129.43	119.84
1	F	332	GLN	C-N-CA	7.67	129.43	119.84
1	B	371	LEU	N-CA-C	7.66	122.38	112.26
1	C	246	GLN	N-CA-C	7.66	119.53	111.03
1	F	170	GLY	N-CA-C	-7.61	95.14	113.18
1	E	322	LEU	N-CA-C	7.60	119.56	111.28
1	E	373	ASP	N-CA-C	-7.57	97.86	109.14
1	F	294	LEU	N-CA-C	7.47	121.32	108.02
1	D	330	GLY	N-CA-C	-7.45	95.52	113.18
1	B	373	ASP	N-CA-C	-7.43	98.06	109.14
1	D	312	ILE	N-CA-C	7.41	118.21	110.72
1	B	157	THR	N-CA-C	7.40	121.12	110.10
1	E	330	GLY	N-CA-C	-7.37	95.71	113.18
1	D	301	PHE	CA-C-N	7.32	128.99	119.84
1	D	301	PHE	C-N-CA	7.32	128.99	119.84
1	D	157	THR	N-CA-C	7.29	120.96	110.10
1	B	170	GLY	N-CA-C	-7.27	95.95	113.18
1	C	322	LEU	N-CA-C	7.25	119.18	111.28
1	F	246	GLN	N-CA-C	7.23	118.95	111.14
1	F	322	LEU	N-CA-C	7.23	119.16	111.28
1	A	312	ILE	N-CA-C	7.21	118.00	110.72
1	A	330	GLY	N-CA-C	-7.20	96.11	113.18
1	F	376	HIS	N-CA-C	7.11	120.07	111.82
1	C	170	GLY	N-CA-C	-7.10	96.36	113.18
1	A	170	GLY	N-CA-C	-7.09	96.37	113.18
1	F	330	GLY	N-CA-C	-7.08	96.40	113.18
1	D	170	GLY	N-CA-C	-7.08	96.41	113.18
1	A	384	SER	N-CA-C	7.04	119.81	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	THR	N-CA-C	7.01	120.55	110.10
1	E	378	PRO	N-CA-C	7.00	121.67	110.40
1	C	330	GLY	N-CA-C	-7.00	96.59	113.18
1	F	295	TYR	N-CA-C	-6.99	102.05	110.44
1	E	170	GLY	N-CA-C	-6.96	96.68	113.18
1	D	370	SER	N-CA-C	6.90	117.76	108.23
1	F	157	THR	N-CA-C	6.90	120.38	110.10
1	D	371	LEU	N-CA-C	6.89	121.36	112.26
1	D	315	ILE	CA-C-N	-6.88	112.54	119.56
1	D	315	ILE	C-N-CA	-6.88	112.54	119.56
1	D	322	LEU	N-CA-C	6.80	118.69	111.28
1	F	378	PRO	N-CA-C	6.75	121.27	110.40
1	A	352	ASN	CB-CA-C	-6.71	107.03	115.89
1	A	373	ASP	N-CA-C	-6.69	99.18	109.14
1	E	252	VAL	N-CA-C	-6.60	107.06	113.53
1	E	247	VAL	N-CA-C	-6.60	104.91	111.77
1	A	209	HIS	N-CA-C	6.59	119.36	108.49
1	E	295	TYR	N-CA-C	-6.59	102.53	110.44
1	C	312	ILE	N-CA-C	6.58	117.37	110.72
1	F	373	ASP	N-CA-C	-6.58	99.34	109.14
1	A	370	SER	N-CA-C	6.53	117.24	108.23
1	C	373	ASP	N-CA-C	-6.51	99.44	109.14
1	E	187	GLY	CA-C-N	-6.49	113.84	120.85
1	E	187	GLY	C-N-CA	-6.49	113.84	120.85
1	E	246	GLN	N-CA-C	6.49	118.23	111.03
1	A	301	PHE	CA-C-N	6.48	127.94	119.84
1	A	301	PHE	C-N-CA	6.48	127.94	119.84
1	B	322	LEU	N-CA-C	6.44	118.30	111.28
1	D	143	GLY	N-CA-C	6.43	121.01	112.77
1	F	289	LYS	N-CA-C	-6.39	104.74	112.54
1	D	352	ASN	CB-CA-C	-6.38	107.47	115.89
1	B	378	PRO	N-CA-C	6.34	120.61	110.40
1	F	301	PHE	CA-C-N	6.31	127.72	119.84
1	F	301	PHE	C-N-CA	6.31	127.72	119.84
1	B	295	TYR	N-CA-C	-6.30	102.88	110.44
1	A	376	HIS	N-CA-C	6.29	120.68	112.89
1	C	143	GLY	N-CA-C	6.28	120.09	112.49
1	A	378	PRO	N-CA-C	6.25	120.46	110.40
1	C	315	ILE	CB-CA-C	-6.23	107.75	114.35
1	B	179	HIS	N-CA-C	-6.22	104.41	111.07
1	E	376	HIS	N-CA-C	6.19	120.09	112.54
1	C	209	HIS	N-CA-C	6.18	118.69	108.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	301	PHE	CA-C-N	6.16	127.54	119.84
1	C	301	PHE	C-N-CA	6.16	127.54	119.84
1	A	322	LEU	N-CA-C	6.16	117.99	111.28
1	F	368	PRO	CA-C-O	-6.16	114.46	121.11
1	F	189	PHE	CA-C-N	-6.13	117.52	122.85
1	F	189	PHE	C-N-CA	-6.13	117.52	122.85
1	B	258	PHE	N-CA-C	6.10	118.23	109.14
1	A	367	TYR	CA-C-N	-6.09	111.51	120.46
1	A	367	TYR	C-N-CA	-6.09	111.51	120.46
1	B	247	VAL	N-CA-C	-6.07	105.46	111.77
1	A	295	TYR	N-CA-C	-6.03	103.20	110.44
1	B	246	GLN	N-CA-C	6.03	117.72	111.03
1	C	376	HIS	N-CA-C	6.02	120.36	112.89
1	C	295	TYR	N-CA-C	-6.01	103.22	110.44
1	C	354	ARG	N-CA-C	6.00	117.62	111.14
1	A	246	GLN	N-CA-C	5.99	117.50	110.97
1	E	352	ASN	CA-C-O	5.99	121.41	117.94
1	C	289	LYS	N-CA-C	-5.96	105.26	112.54
1	D	222	LYS	N-CA-C	-5.96	97.50	107.99
1	E	258	PHE	N-CA-C	5.96	118.02	109.14
1	A	189	PHE	CA-C-N	-5.95	117.67	122.85
1	A	189	PHE	C-N-CA	-5.95	117.67	122.85
1	F	223	GLY	N-CA-C	-5.94	99.09	113.18
1	A	222	LYS	N-CA-C	-5.94	97.53	107.99
1	C	129	GLY	N-CA-C	-5.94	99.11	113.18
1	C	223	GLY	N-CA-C	-5.92	99.14	113.18
1	A	315	ILE	CA-C-N	-5.88	113.56	119.56
1	A	315	ILE	C-N-CA	-5.88	113.56	119.56
1	D	187	GLY	CA-C-N	-5.86	114.52	120.85
1	D	187	GLY	C-N-CA	-5.86	114.52	120.85
1	C	299	ASN	N-CA-C	5.86	119.74	112.59
1	D	258	PHE	N-CA-C	5.80	117.79	109.14
1	C	378	PRO	N-CA-C	5.80	119.73	110.40
1	F	370	SER	N-CA-C	5.80	116.23	108.23
1	E	222	LYS	N-CA-C	-5.79	97.80	107.99
1	B	376	HIS	N-CA-C	5.79	120.06	112.89
1	A	187	GLY	CA-C-N	-5.78	114.61	120.85
1	A	187	GLY	C-N-CA	-5.78	114.61	120.85
1	C	337	THR	CA-C-N	-5.77	112.62	119.84
1	C	337	THR	C-N-CA	-5.77	112.62	119.84
1	F	354	ARG	N-CA-C	5.77	117.37	111.14
1	A	371	LEU	N-CA-C	5.74	119.84	112.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	223	GLY	N-CA-C	-5.73	99.59	113.18
1	B	139	GLY	N-CA-C	5.73	121.74	111.03
1	A	179	HIS	N-CA-C	-5.71	104.25	111.11
1	F	371	LEU	N-CA-C	5.71	119.80	112.26
1	E	248	LYS	N-CA-C	-5.67	106.32	113.18
1	F	129	GLY	N-CA-C	-5.65	99.80	113.18
1	E	370	SER	N-CA-C	5.64	116.02	108.23
1	F	368	PRO	O-C-N	5.63	126.73	122.73
1	D	211	LYS	N-CA-C	5.63	117.79	110.53
1	D	373	ASP	N-CA-C	-5.63	100.75	109.14
1	B	223	GLY	N-CA-C	-5.61	99.88	113.18
1	C	258	PHE	N-CA-C	5.58	117.45	109.14
1	F	351	GLY	CA-C-N	-5.56	117.18	123.13
1	F	351	GLY	C-N-CA	-5.56	117.18	123.13
1	D	378	PRO	N-CA-C	5.54	119.32	110.40
1	E	315	ILE	CA-C-N	-5.54	113.19	119.28
1	E	315	ILE	C-N-CA	-5.54	113.19	119.28
1	B	294	LEU	CB-CA-C	-5.53	102.28	110.62
1	D	259	GLU	N-CA-C	5.53	117.91	108.90
1	D	179	HIS	N-CA-C	-5.52	105.16	111.07
1	F	315	ILE	CA-C-N	-5.52	113.21	119.28
1	F	315	ILE	C-N-CA	-5.52	113.21	119.28
1	D	189	PHE	CA-C-N	-5.51	118.06	122.85
1	D	189	PHE	C-N-CA	-5.51	118.06	122.85
1	E	179	HIS	N-CA-C	-5.48	104.53	111.11
1	F	258	PHE	N-CA-C	5.48	117.31	109.14
1	C	294	LEU	CB-CA-C	-5.47	102.35	110.62
1	E	371	LEU	N-CA-C	5.47	119.48	112.26
1	E	364	VAL	N-CA-C	5.46	119.68	112.04
1	F	334	ILE	CB-CA-C	-5.45	102.36	111.29
1	E	291	ARG	NE-CZ-NH2	5.44	124.09	119.20
1	F	294	LEU	CB-CA-C	-5.43	102.42	110.62
1	F	299	ASN	N-CA-C	5.43	119.22	112.59
1	F	139	GLY	N-CA-C	5.42	121.16	111.03
1	E	294	LEU	CB-CA-C	-5.41	102.45	110.62
1	A	223	GLY	N-CA-C	-5.40	100.38	113.18
1	B	370	SER	N-CA-C	5.40	115.68	108.23
1	D	295	TYR	N-CA-C	-5.39	103.97	110.44
1	B	222	LYS	N-CA-C	-5.39	98.50	107.99
1	A	258	PHE	N-CA-C	5.38	117.16	109.14
1	F	367	TYR	CA-C-N	-5.38	113.79	120.79
1	F	367	TYR	C-N-CA	-5.38	113.79	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	223	GLY	N-CA-C	-5.38	100.43	113.18
1	A	197	ILE	CA-C-N	-5.37	115.05	120.21
1	A	197	ILE	C-N-CA	-5.37	115.05	120.21
1	B	190	VAL	CA-C-N	5.37	126.55	119.84
1	B	190	VAL	C-N-CA	5.37	126.55	119.84
1	B	315	ILE	CA-C-N	-5.35	113.40	119.28
1	B	315	ILE	C-N-CA	-5.35	113.40	119.28
1	D	331	ALA	N-CA-C	5.33	119.78	113.28
1	E	354	ARG	N-CA-C	5.33	116.90	111.14
1	B	367	TYR	CA-C-N	-5.31	112.65	120.46
1	B	367	TYR	C-N-CA	-5.31	112.65	120.46
1	B	187	GLY	N-CA-C	-5.29	101.54	112.34
1	E	334	ILE	N-CA-C	5.29	114.98	108.53
1	F	367	TYR	CB-CA-C	-5.29	104.29	111.21
1	E	221	ARG	CA-C-N	-5.27	114.66	122.41
1	E	221	ARG	C-N-CA	-5.27	114.66	122.41
1	D	229	GLU	N-CA-C	5.25	117.31	110.43
1	D	230	GLY	N-CA-C	-5.24	108.01	115.30
1	A	143	GLY	N-CA-C	5.23	119.46	112.77
1	B	354	ARG	N-CA-C	5.20	116.76	111.14
1	C	315	ILE	CA-C-N	-5.20	113.56	119.28
1	C	315	ILE	C-N-CA	-5.20	113.56	119.28
1	E	367	TYR	CA-C-N	-5.17	112.86	120.46
1	E	367	TYR	C-N-CA	-5.17	112.86	120.46
1	B	129	GLY	N-CA-C	-5.17	100.94	113.18
1	E	351	GLY	CA-C-N	-5.17	117.46	123.04
1	E	351	GLY	C-N-CA	-5.17	117.46	123.04
1	F	337	THR	CA-C-N	-5.16	113.38	119.84
1	F	337	THR	C-N-CA	-5.16	113.38	119.84
1	A	129	GLY	N-CA-C	-5.16	100.95	113.18
1	A	248	LYS	N-CA-C	-5.14	106.96	113.18
1	F	229	GLU	N-CA-C	5.13	116.92	110.24
1	F	255	GLU	N-CA-C	-5.11	107.18	113.41
1	A	294	LEU	CB-CA-C	-5.11	102.91	110.62
1	F	247	VAL	N-CA-C	-5.09	106.47	111.77
1	E	129	GLY	N-CA-C	-5.09	101.12	113.18
1	E	300	VAL	CB-CA-C	-5.08	105.47	111.97
1	A	349	TRP	N-CA-C	5.07	121.01	109.81
1	C	367	TYR	CB-CA-C	-5.07	104.57	111.21
1	A	331	ALA	N-CA-C	5.06	119.45	113.28
1	D	349	TRP	N-CA-C	5.06	120.99	109.81
1	D	278	HIS	N-CA-C	-5.05	106.70	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	300	VAL	CB-CA-C	-5.05	105.50	111.97
1	A	300	VAL	CB-CA-C	-5.05	105.51	111.97
1	E	209	HIS	N-CA-C	5.04	116.81	108.49
1	F	208	GLY	N-CA-C	5.04	125.13	113.18
1	C	187	GLY	N-CA-C	-5.04	102.07	112.34
1	A	364	VAL	N-CA-C	5.03	119.09	112.04
1	B	383	TYR	N-CA-C	-5.03	106.56	113.30
1	A	319	LEU	N-CA-C	-5.03	105.89	112.23
1	F	368	PRO	CB-CA-C	-5.02	107.65	111.87
1	F	143	GLY	N-CA-C	5.01	119.18	112.77
1	B	352	ASN	CB-CA-C	-5.00	109.87	117.07
1	E	311	ARG	N-CA-C	-5.00	105.66	112.26

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	THR	Peptide
1	A	223	GLY	Peptide
1	A	294	LEU	Peptide
1	A	297	ARG	Peptide
1	B	133	ARG	Peptide
1	B	153	GLN	Peptide
1	B	169	THR	Peptide
1	B	223	GLY	Peptide
1	B	285	ILE	Peptide
1	B	294	LEU	Peptide
1	B	297	ARG	Peptide
1	C	169	THR	Peptide
1	C	223	GLY	Peptide
1	C	294	LEU	Peptide
1	C	297	ARG	Peptide
1	D	133	ARG	Peptide
1	D	169	THR	Peptide
1	D	223	GLY	Peptide
1	D	294	LEU	Peptide
1	D	297	ARG	Peptide
1	E	153	GLN	Peptide
1	E	169	THR	Peptide
1	E	223	GLY	Peptide
1	E	285	ILE	Peptide
1	E	294	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	E	297	ARG	Peptide
1	F	133	ARG	Peptide
1	F	169	THR	Peptide
1	F	223	GLY	Peptide
1	F	285	ILE	Peptide
1	F	294	LEU	Peptide
1	F	297	ARG	Peptide

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	2035	0	2036	217	0
1	B	2035	0	2036	217	0
1	C	2035	0	2036	232	0
1	D	2035	0	2036	218	0
1	E	2035	0	2036	209	0
1	F	2035	0	2036	219	0
2	A	172	0	258	8	0
2	B	188	0	281	8	0
2	C	152	0	228	9	0
2	D	156	0	234	9	0
2	E	192	0	288	8	0
2	F	180	0	270	5	0
3	A	96	0	0	18	0
3	B	91	0	0	16	0
3	C	100	0	0	20	0
3	D	98	0	0	18	0
3	E	97	0	0	16	0
3	F	101	0	0	18	0
All	All	13833	0	13775	1294	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 48.

All (1294) 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:154:VAL:HG21	1:B:181:HIS:HB3	1.30	1.10
1:F:154:VAL:HG21	1:F:181:HIS:HB3	1.33	1.10
1:C:208:GLY:HA3	1:C:260:ARG:HG3	1.08	1.08
1:F:208:GLY:HA3	1:F:260:ARG:HG3	1.10	1.07
1:D:208:GLY:HA3	1:D:260:ARG:HG3	1.10	1.06
1:B:208:GLY:HA3	1:B:260:ARG:HG3	1.10	1.05
1:E:208:GLY:HA3	1:E:260:ARG:HG3	1.09	1.05
1:D:154:VAL:HG21	1:D:181:HIS:HB3	1.38	1.05
1:A:208:GLY:HA3	1:A:260:ARG:HG3	1.07	1.04
1:C:211:LYS:HG3	1:C:216:GLY:HA2	1.39	1.02
1:E:154:VAL:HG21	1:E:181:HIS:HB3	1.39	1.01
1:F:211:LYS:HG3	1:F:216:GLY:HA2	1.42	1.00
1:A:154:VAL:HG21	1:A:181:HIS:HB3	1.40	1.00
1:A:211:LYS:HG3	1:A:216:GLY:HA2	1.40	1.00
1:C:154:VAL:HG21	1:C:181:HIS:HB3	1.39	0.99
1:E:211:LYS:HG3	1:E:216:GLY:HA2	1.45	0.94
1:E:251:ARG:NH2	1:F:196:ALA:O	2.02	0.93
1:A:158:GLU:OE1	3:A:501:HOH:O	1.89	0.91
1:F:147:VAL:HG23	1:F:303:ILE:HD11	1.51	0.91
1:D:315:ILE:HA	1:D:318:LEU:HB2	1.54	0.90
1:F:167:SER:OG	1:F:354:ARG:NH2	2.05	0.90
1:E:315:ILE:HA	1:E:318:LEU:HB2	1.53	0.89
1:C:147:VAL:HG23	1:C:303:ILE:HD11	1.55	0.89
1:F:154:VAL:HG11	1:F:178:ILE:HD11	1.54	0.89
1:B:211:LYS:HG3	1:B:216:GLY:HA2	1.56	0.88
1:B:339:ARG:NH1	3:B:502:HOH:O	2.06	0.88
1:F:201:LEU:HB2	1:F:204:SER:HB2	1.54	0.88
1:E:201:LEU:HB2	1:E:204:SER:HB2	1.56	0.87
1:A:315:ILE:HA	1:A:318:LEU:HB2	1.57	0.87
1:F:364:VAL:O	1:F:368:PRO:HG3	1.75	0.86
1:B:208:GLY:HA3	1:B:260:ARG:CG	2.02	0.86
1:A:262:GLY:O	1:A:264:ASN:N	2.08	0.86
1:B:158:GLU:OE1	3:B:501:HOH:O	1.93	0.86
1:E:251:ARG:HG3	1:E:251:ARG:HH21	1.40	0.86
1:B:315:ILE:HA	1:B:318:LEU:HB2	1.56	0.85
1:D:147:VAL:HG23	1:D:303:ILE:HD11	1.57	0.85
1:F:209:HIS:CE1	1:F:217:ALA:HB1	2.12	0.85
1:D:211:LYS:HG3	1:D:216:GLY:HA2	1.58	0.85
1:C:158:GLU:OE1	3:C:502:HOH:O	1.95	0.85
1:E:169:THR:HB	1:E:305:MET:HB2	1.59	0.84
1:C:327:GLU:OE2	3:C:501:HOH:O	1.95	0.84
1:C:169:THR:HB	1:C:305:MET:HB2	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:SER:OG	1:D:354:ARG:NH2	2.10	0.84
1:E:167:SER:OG	1:E:354:ARG:NH2	2.11	0.84
1:D:208:GLY:HA3	1:D:260:ARG:CG	2.03	0.84
1:D:262:GLY:O	1:D:264:ASN:N	2.10	0.84
1:E:243:MET:HE2	1:E:244:SER:HA	1.59	0.84
1:C:167:SER:OG	1:C:354:ARG:NH2	2.10	0.84
1:D:209:HIS:CE1	1:D:217:ALA:HB1	2.12	0.84
1:F:327:GLU:OE2	3:F:501:HOH:O	1.95	0.83
1:D:201:LEU:HD13	1:D:205:GLU:HB3	1.61	0.83
1:C:201:LEU:HB2	1:C:204:SER:HB2	1.59	0.82
1:E:339:ARG:NH1	3:E:504:HOH:O	2.11	0.82
1:F:169:THR:HB	1:F:305:MET:HB2	1.58	0.82
1:C:336:PHE:HE1	1:C:377:LEU:HD21	1.45	0.82
1:B:209:HIS:CE1	1:B:217:ALA:HB1	2.13	0.82
1:A:167:SER:OG	1:A:354:ARG:NH2	2.13	0.81
1:E:185:ARG:NH1	3:E:506:HOH:O	2.12	0.81
1:E:262:GLY:O	1:E:264:ASN:N	2.13	0.81
1:A:201:LEU:HD13	1:A:205:GLU:HB3	1.60	0.81
1:B:203:GLU:OE1	1:B:248:LYS:NZ	2.12	0.81
1:E:209:HIS:CE1	1:E:217:ALA:HB1	2.15	0.81
1:B:262:GLY:O	1:B:264:ASN:N	2.13	0.81
1:A:208:GLY:HA3	1:A:260:ARG:CG	2.01	0.81
1:C:339:ARG:NH1	3:C:506:HOH:O	2.13	0.81
1:D:169:THR:HB	1:D:305:MET:HB2	1.63	0.81
1:F:158:GLU:OE1	3:F:502:HOH:O	1.98	0.81
1:A:243:MET:HE2	1:A:244:SER:HA	1.64	0.80
1:D:364:VAL:O	1:D:368:PRO:HG3	1.81	0.80
1:E:188:PRO:HD2	1:E:231:GLY:HA3	1.60	0.80
1:D:183:GLY:HA2	1:D:185:ARG:HE	1.45	0.80
1:A:148:ARG:O	1:A:152:GLU:N	2.15	0.79
1:C:262:GLY:O	1:C:264:ASN:N	2.12	0.79
1:B:142:MET:SD	1:B:142:MET:N	2.55	0.79
1:F:262:GLY:O	1:F:264:ASN:N	2.14	0.79
1:D:308:LEU:HA	1:D:311:ARG:HB2	1.65	0.79
1:D:339:ARG:NH1	3:D:504:HOH:O	2.15	0.79
1:B:167:SER:OG	1:B:354:ARG:NH2	2.14	0.79
1:D:158:GLU:OE1	3:D:501:HOH:O	2.00	0.79
1:D:148:ARG:O	1:D:152:GLU:N	2.14	0.78
1:D:363:MET:HE2	1:D:367:TYR:HB2	1.66	0.78
1:A:147:VAL:HG23	1:A:303:ILE:HD11	1.64	0.78
1:F:148:ARG:HA	1:F:151:ILE:HB	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:415:EDO:H12	2:F:416:EDO:H12	1.65	0.78
1:F:148:ARG:O	1:F:152:GLU:N	2.14	0.77
1:A:201:LEU:HB2	1:A:204:SER:HB2	1.66	0.77
1:D:142:MET:SD	1:D:142:MET:N	2.58	0.77
1:A:148:ARG:HA	1:A:151:ILE:HB	1.66	0.77
1:A:363:MET:HE2	1:A:367:TYR:HB2	1.67	0.77
1:D:188:PRO:HD2	1:D:231:GLY:HA3	1.65	0.77
1:F:363:MET:HE2	1:F:367:TYR:HB2	1.67	0.76
1:E:158:GLU:OE1	3:E:501:HOH:O	2.02	0.76
1:C:237:GLU:OE2	3:C:503:HOH:O	2.03	0.76
1:C:208:GLY:HA3	1:C:260:ARG:CG	2.04	0.76
1:E:147:VAL:HG23	1:E:303:ILE:HD11	1.66	0.76
1:A:308:LEU:HA	1:A:311:ARG:HB2	1.67	0.76
1:F:188:PRO:HD2	1:F:231:GLY:HA3	1.68	0.76
1:A:209:HIS:CE1	1:A:217:ALA:HB1	2.20	0.76
1:C:183:GLY:HA2	1:C:185:ARG:HE	1.51	0.76
1:E:151:ILE:O	1:E:154:VAL:N	2.19	0.75
1:C:209:HIS:CE1	1:C:217:ALA:HB1	2.21	0.75
1:A:297:ARG:NH2	3:A:506:HOH:O	2.19	0.75
1:E:202:LEU:HB3	1:E:245:MET:SD	2.26	0.75
1:B:201:LEU:HD13	1:B:205:GLU:HB3	1.68	0.74
1:C:364:VAL:HG13	1:C:368:PRO:HB3	1.69	0.74
1:D:202:LEU:HB3	1:D:245:MET:SD	2.28	0.74
1:A:346:GLU:O	3:A:502:HOH:O	2.04	0.74
1:C:296:TYR:OH	3:C:504:HOH:O	2.05	0.74
1:C:168:GLY:H	1:C:171:LYS:HG2	1.53	0.74
1:D:148:ARG:HA	1:D:151:ILE:HB	1.68	0.74
1:F:185:ARG:NH1	3:F:511:HOH:O	2.21	0.74
1:C:148:ARG:HA	1:C:151:ILE:HB	1.69	0.73
1:E:135:SER:OG	3:E:502:HOH:O	2.05	0.73
1:E:327:GLU:OE2	3:E:503:HOH:O	2.06	0.73
1:B:178:ILE:HG12	1:B:182:SER:OG	1.89	0.73
1:E:297:ARG:NH2	3:E:510:HOH:O	2.20	0.73
1:F:339:ARG:NH1	3:F:510:HOH:O	2.20	0.73
1:A:208:GLY:CA	1:A:260:ARG:HG3	2.02	0.73
1:A:142:MET:SD	1:A:142:MET:N	2.61	0.73
1:A:168:GLY:H	1:A:171:LYS:HG2	1.52	0.73
1:A:362:ARG:HB3	1:F:300:VAL:O	1.87	0.73
1:C:315:ILE:HA	1:C:318:LEU:HB2	1.69	0.73
1:F:202:LEU:HB3	1:F:245:MET:SD	2.27	0.73
1:A:183:GLY:HA2	1:A:185:ARG:HE	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:ILE:O	1:C:154:VAL:N	2.22	0.73
1:D:172:GLU:HG2	1:D:175:ALA:HB3	1.71	0.73
1:D:243:MET:SD	1:D:291:ARG:NH2	2.61	0.73
1:E:178:ILE:O	1:E:182:SER:HB2	1.89	0.73
1:E:208:GLY:HA3	1:E:260:ARG:CG	2.04	0.73
1:B:364:VAL:HG13	1:B:368:PRO:HB3	1.70	0.72
1:B:364:VAL:O	1:B:368:PRO:HG3	1.88	0.72
1:E:363:MET:HE2	1:E:367:TYR:HB2	1.68	0.72
1:C:238:ILE:HD11	1:C:275:ALA:HB1	1.71	0.72
1:F:336:PHE:HE1	1:F:377:LEU:HD21	1.53	0.72
1:F:183:GLY:HA2	1:F:185:ARG:HE	1.53	0.72
1:B:144:ILE:HD12	1:B:147:VAL:HG11	1.72	0.72
1:B:172:GLU:HG3	1:B:234:PHE:CE2	2.25	0.72
1:B:202:LEU:HB3	1:B:245:MET:SD	2.29	0.72
1:D:185:ARG:NH1	3:D:510:HOH:O	2.23	0.72
1:A:151:ILE:O	1:A:154:VAL:N	2.22	0.72
1:B:375:ASN:O	3:B:503:HOH:O	2.08	0.72
1:B:169:THR:HB	1:B:305:MET:HB2	1.71	0.71
1:B:363:MET:HE2	1:B:367:TYR:HB2	1.73	0.71
1:C:346:GLU:O	3:C:505:HOH:O	2.06	0.71
1:D:315:ILE:O	1:D:318:LEU:N	2.22	0.71
1:E:168:GLY:H	1:E:171:LYS:HG2	1.55	0.71
1:E:242:PRO:O	1:E:246:GLN:HG3	1.90	0.71
1:F:346:GLU:O	3:F:503:HOH:O	2.06	0.71
1:A:161:VAL:HB	1:A:274:ILE:HG23	1.72	0.71
1:F:296:TYR:OH	3:F:504:HOH:O	2.08	0.71
1:D:327:GLU:OE2	3:D:502:HOH:O	2.08	0.71
1:A:209:HIS:O	1:A:209:HIS:ND1	2.22	0.71
2:D:410:EDO:H12	2:D:411:EDO:H12	1.73	0.71
1:C:148:ARG:O	1:C:152:GLU:N	2.20	0.71
1:B:188:PRO:HD2	1:B:231:GLY:HA3	1.71	0.71
1:D:337:THR:HG21	1:D:373:ASP:HA	1.70	0.71
1:E:183:GLY:HA2	1:E:185:ARG:HE	1.53	0.71
1:A:339:ARG:NH1	3:A:508:HOH:O	2.22	0.71
1:B:183:GLY:HA2	1:B:185:ARG:HE	1.55	0.71
1:B:185:ARG:NH1	3:B:508:HOH:O	2.22	0.71
1:C:337:THR:HG21	1:C:373:ASP:HA	1.73	0.71
1:E:179:HIS:ND1	1:E:184:ARG:O	2.23	0.71
1:B:337:THR:HG21	1:B:373:ASP:HA	1.73	0.70
1:E:368:PRO:O	1:E:369:ASN:HB2	1.89	0.70
1:A:368:PRO:O	1:A:369:ASN:HB2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:PHE:CE1	1:C:377:LEU:HD21	2.26	0.70
1:D:242:PRO:O	1:D:246:GLN:HG3	1.92	0.70
1:E:312:ILE:HG13	1:E:345:MET:HG3	1.72	0.70
1:C:300:VAL:O	1:D:362:ARG:HB3	1.92	0.70
1:D:179:HIS:ND1	1:D:184:ARG:O	2.25	0.70
1:F:368:PRO:O	1:F:369:ASN:HB2	1.91	0.70
1:E:336:PHE:HE1	1:E:377:LEU:HD21	1.56	0.70
1:C:185:ARG:NH1	3:C:513:HOH:O	2.24	0.70
1:A:172:GLU:HG2	1:A:175:ALA:HB3	1.73	0.70
1:E:144:ILE:HD12	1:E:147:VAL:HG11	1.74	0.70
1:B:242:PRO:O	1:B:246:GLN:HG3	1.91	0.70
1:A:178:ILE:O	1:A:182:SER:HB2	1.92	0.70
1:A:315:ILE:O	1:A:318:LEU:N	2.24	0.69
1:A:340:ALA:O	1:A:343:SER:N	2.23	0.69
1:B:346:GLU:O	3:B:504:HOH:O	2.09	0.69
1:D:151:ILE:O	1:D:154:VAL:N	2.25	0.69
1:F:297:ARG:NH2	3:F:513:HOH:O	2.24	0.69
1:D:340:ALA:O	1:D:343:SER:N	2.24	0.69
1:C:178:ILE:HG12	1:C:182:SER:OG	1.93	0.69
1:A:375:ASN:O	3:A:503:HOH:O	2.09	0.69
1:C:297:ARG:NH2	3:C:515:HOH:O	2.25	0.69
1:B:308:LEU:HA	1:B:311:ARG:HB2	1.75	0.69
1:F:151:ILE:O	1:F:154:VAL:N	2.26	0.69
1:D:178:ILE:O	1:D:182:SER:HB2	1.93	0.69
1:D:336:PHE:HE1	1:D:377:LEU:HD21	1.56	0.69
1:E:315:ILE:O	1:E:318:LEU:N	2.26	0.69
1:A:168:GLY:O	1:A:353:VAL:HB	1.93	0.69
1:D:161:VAL:HB	1:D:274:ILE:HG23	1.73	0.69
1:D:297:ARG:NH2	3:D:511:HOH:O	2.25	0.68
1:C:201:LEU:HD13	1:C:205:GLU:HB3	1.73	0.68
1:A:202:LEU:HB3	1:A:245:MET:SD	2.33	0.68
1:C:178:ILE:O	1:C:182:SER:HB2	1.93	0.68
1:D:166:GLU:O	1:D:169:THR:OG1	2.09	0.68
1:E:340:ALA:O	1:E:343:SER:N	2.26	0.68
1:F:154:VAL:CG1	1:F:178:ILE:HD11	2.23	0.68
1:F:166:GLU:O	1:F:169:THR:OG1	2.10	0.68
1:B:147:VAL:HG23	1:B:303:ILE:HD11	1.75	0.68
1:E:308:LEU:HA	1:E:311:ARG:HB2	1.74	0.68
1:A:185:ARG:NH1	3:A:509:HOH:O	2.26	0.68
1:F:237:GLU:OE2	3:F:505:HOH:O	2.11	0.68
1:C:315:ILE:O	1:C:318:LEU:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:GLU:O	3:E:505:HOH:O	2.12	0.68
1:F:336:PHE:CE1	1:F:377:LEU:HD21	2.29	0.68
1:F:209:HIS:O	1:F:209:HIS:ND1	2.26	0.68
1:D:346:GLU:O	3:D:503:HOH:O	2.11	0.68
1:A:178:ILE:HG12	1:A:182:SER:OG	1.94	0.68
1:C:209:HIS:O	1:C:209:HIS:ND1	2.26	0.68
1:E:364:VAL:O	1:E:368:PRO:HG3	1.94	0.68
1:A:205:GLU:O	1:A:224:ARG:HG2	1.94	0.67
1:B:151:ILE:O	1:B:154:VAL:N	2.27	0.67
1:D:168:GLY:O	1:D:353:VAL:HB	1.93	0.67
1:E:270:ASN:ND2	2:E:413:EDO:O2	2.27	0.67
1:B:327:GLU:OE2	3:B:505:HOH:O	2.12	0.67
1:B:368:PRO:O	1:B:369:ASN:HB2	1.93	0.67
1:D:144:ILE:HD12	1:D:147:VAL:HG11	1.75	0.67
1:E:148:ARG:O	1:E:152:GLU:N	2.23	0.67
1:B:243:MET:HE2	1:B:244:SER:HA	1.77	0.67
1:B:297:ARG:NH2	3:B:510:HOH:O	2.25	0.67
1:C:332:GLN:NE2	3:C:511:HOH:O	2.20	0.67
1:E:300:VAL:O	1:F:362:ARG:HB3	1.95	0.67
1:A:290:PHE:O	1:A:292:GLU:N	2.26	0.67
1:B:336:PHE:HE1	1:B:377:LEU:HD21	1.59	0.66
1:E:337:THR:HG21	1:E:373:ASP:HA	1.78	0.66
1:F:137:MET:O	3:F:506:HOH:O	2.13	0.66
1:B:179:HIS:ND1	1:B:184:ARG:O	2.29	0.66
1:D:194:CYS:SG	1:D:241:MET:HG3	2.36	0.66
1:A:282:GLU:HA	1:A:285:ILE:HG13	1.76	0.66
1:E:201:LEU:HD13	1:E:205:GLU:HB3	1.75	0.66
1:F:308:LEU:HA	1:F:311:ARG:HB2	1.77	0.66
1:B:178:ILE:O	1:B:182:SER:HB2	1.94	0.66
1:C:308:LEU:HA	1:C:311:ARG:HB2	1.76	0.66
1:A:327:GLU:OE2	3:A:504:HOH:O	2.13	0.66
1:A:364:VAL:O	1:A:368:PRO:HG3	1.96	0.66
2:A:443:EDO:H11	2:F:436:EDO:H21	1.77	0.66
1:D:234:PHE:CD1	1:D:274:ILE:HB	2.30	0.66
1:E:148:ARG:HA	1:E:151:ILE:HB	1.77	0.66
1:E:178:ILE:HG12	1:E:182:SER:OG	1.96	0.66
1:A:166:GLU:O	1:A:169:THR:OG1	2.14	0.66
1:F:337:THR:OG1	1:F:372:VAL:O	2.05	0.66
1:E:137:MET:O	3:E:507:HOH:O	2.13	0.65
1:F:151:ILE:O	1:F:154:VAL:HG13	1.95	0.65
1:C:202:LEU:HB3	1:C:245:MET:SD	2.35	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:GLU:OE1	1:D:248:LYS:NZ	2.20	0.65
1:B:334:ILE:CG2	1:B:368:PRO:HA	2.26	0.65
2:A:407:EDO:H12	2:A:408:EDO:H12	1.78	0.65
1:C:195:GLY:HA2	1:C:240:ASP:HB3	1.77	0.65
1:B:270:ASN:ND2	2:B:412:EDO:O2	2.29	0.65
1:C:270:ASN:ND2	2:C:412:EDO:O2	2.29	0.65
1:C:363:MET:HE2	1:C:367:TYR:HB2	1.78	0.65
1:A:300:VAL:O	1:B:362:ARG:HB3	1.97	0.65
1:D:336:PHE:CE1	1:D:377:LEU:HD21	2.31	0.65
1:F:344:MET:HE3	1:F:359:LEU:HD23	1.78	0.65
1:F:382:ARG:O	3:F:507:HOH:O	2.14	0.65
1:A:179:HIS:ND1	1:A:184:ARG:O	2.30	0.65
1:B:300:VAL:O	1:C:362:ARG:HB3	1.97	0.65
1:E:348:ASP:OD1	3:E:505:HOH:O	2.15	0.65
1:B:168:GLY:O	1:B:353:VAL:HB	1.96	0.65
1:E:168:GLY:O	1:E:353:VAL:HB	1.97	0.65
1:F:201:LEU:O	1:F:204:SER:N	2.29	0.65
1:F:315:ILE:O	1:F:318:LEU:N	2.29	0.65
1:B:167:SER:O	1:B:352:ASN:HB2	1.97	0.64
1:B:312:ILE:HG13	1:B:345:MET:HG3	1.78	0.64
1:B:336:PHE:CE1	1:B:377:LEU:HD21	2.32	0.64
1:C:295:TYR:C	1:C:299:ASN:HB2	2.22	0.64
1:C:348:ASP:OD1	3:C:505:HOH:O	2.15	0.64
1:B:195:GLY:HA2	1:B:240:ASP:HB3	1.77	0.64
1:D:368:PRO:O	1:D:369:ASN:HB2	1.97	0.64
1:E:146:GLU:HG3	1:E:146:GLU:O	1.97	0.64
1:E:176:ARG:HH11	1:E:189:PHE:HD2	1.45	0.64
1:F:211:LYS:CG	1:F:216:GLY:HA2	2.22	0.64
1:A:144:ILE:HD13	1:A:311:ARG:HH21	1.63	0.64
1:B:315:ILE:O	1:B:318:LEU:N	2.30	0.64
1:F:147:VAL:HG22	1:F:151:ILE:HG13	1.80	0.64
1:F:168:GLY:H	1:F:171:LYS:HG2	1.62	0.64
1:A:141:SER:HB2	1:A:144:ILE:HG22	1.78	0.64
1:E:301:PHE:CE2	1:F:365:ILE:HG21	2.33	0.64
1:F:250:LEU:HD11	1:F:254:GLN:HE21	1.62	0.64
1:F:337:THR:HG21	1:F:373:ASP:HA	1.80	0.64
1:B:172:GLU:HG2	1:B:175:ALA:HB3	1.80	0.64
1:C:201:LEU:O	1:C:204:SER:N	2.28	0.64
1:E:142:MET:SD	1:E:142:MET:N	2.70	0.64
1:F:151:ILE:HD13	2:F:410:EDO:H11	1.79	0.64
1:F:208:GLY:HA3	1:F:260:ARG:CG	2.06	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:MET:CE	1:B:142:MET:H	2.11	0.64
1:B:151:ILE:HD13	2:B:404:EDO:H11	1.80	0.63
1:B:340:ALA:O	1:B:343:SER:N	2.31	0.63
1:C:166:GLU:O	1:C:169:THR:OG1	2.14	0.63
1:D:178:ILE:HG12	1:D:182:SER:OG	1.98	0.63
1:A:147:VAL:HG22	1:A:151:ILE:HG13	1.79	0.63
1:D:142:MET:H	1:D:142:MET:CE	2.12	0.63
1:F:195:GLY:HA2	1:F:240:ASP:HB3	1.79	0.63
1:E:172:GLU:HG3	1:E:234:PHE:CE2	2.32	0.63
1:D:270:ASN:ND2	2:D:413:EDO:O2	2.31	0.63
1:D:325:ARG:HG3	2:D:411:EDO:H22	1.79	0.63
1:F:161:VAL:HB	1:F:274:ILE:HG23	1.79	0.63
1:D:312:ILE:HD11	1:D:345:MET:O	1.98	0.63
1:E:221:ARG:NH1	3:E:508:HOH:O	2.18	0.63
1:E:325:ARG:HG3	2:E:410:EDO:H22	1.81	0.63
1:C:205:GLU:O	1:C:224:ARG:HG2	1.99	0.63
1:D:203:GLU:HA	1:D:207:PHE:CD1	2.34	0.63
1:F:215:THR:HG22	2:F:444:EDO:H22	1.81	0.63
1:C:135:SER:OG	3:C:507:HOH:O	2.14	0.63
1:C:282:GLU:HA	1:C:285:ILE:HG13	1.81	0.63
1:D:282:GLU:HA	1:D:285:ILE:HG13	1.79	0.63
1:D:168:GLY:HA2	1:D:171:LYS:HE2	1.79	0.62
1:E:166:GLU:O	1:E:169:THR:OG1	2.17	0.62
1:E:336:PHE:CE1	1:E:377:LEU:HD21	2.34	0.62
1:B:348:ASP:OD1	3:B:504:HOH:O	2.16	0.62
1:E:205:GLU:O	1:E:224:ARG:HG2	1.99	0.62
1:F:290:PHE:O	1:F:292:GLU:N	2.29	0.62
1:B:168:GLY:HA2	1:B:171:LYS:HE2	1.82	0.62
1:B:295:TYR:C	1:B:299:ASN:HB2	2.25	0.62
1:D:234:PHE:HD1	1:D:274:ILE:HB	1.64	0.62
1:A:244:SER:O	1:A:248:LYS:HD3	2.00	0.62
1:C:364:VAL:O	1:C:368:PRO:HG3	2.00	0.62
1:A:207:PHE:CE1	1:A:245:MET:HE1	2.34	0.62
1:D:211:LYS:CG	1:D:216:GLY:HA2	2.29	0.62
1:E:203:GLU:OE1	1:E:248:LYS:NZ	2.23	0.62
1:A:287:GLY:O	1:A:288:GLN:HB2	2.00	0.62
1:A:211:LYS:CG	1:A:216:GLY:HA2	2.23	0.61
1:B:146:GLU:HG3	1:B:146:GLU:O	1.99	0.61
1:F:219:THR:O	1:F:219:THR:OG1	2.17	0.61
1:C:194:CYS:SG	1:C:241:MET:HG3	2.39	0.61
1:E:211:LYS:CG	1:E:216:GLY:HA2	2.23	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:VAL:HB	1:B:274:ILE:HG23	1.80	0.61
1:C:142:MET:SD	1:C:142:MET:N	2.73	0.61
1:F:168:GLY:O	1:F:353:VAL:HB	2.00	0.61
1:A:169:THR:HB	1:A:305:MET:HB2	1.82	0.61
1:C:172:GLU:HG3	1:C:234:PHE:CE2	2.36	0.61
1:F:205:GLU:O	1:F:224:ARG:HG2	2.01	0.61
1:A:295:TYR:C	1:A:299:ASN:HB2	2.25	0.61
1:D:178:ILE:HD12	2:D:405:EDO:O2	2.00	0.61
1:D:349:TRP:CH2	1:D:356:LEU:HD23	2.36	0.61
1:F:315:ILE:HA	1:F:318:LEU:HB2	1.82	0.61
1:A:349:TRP:CH2	1:A:356:LEU:HD23	2.36	0.61
1:B:208:GLY:CA	1:B:260:ARG:HG3	2.05	0.61
1:C:211:LYS:CG	1:C:216:GLY:HA2	2.23	0.61
1:C:368:PRO:O	1:C:369:ASN:HB2	2.00	0.61
1:B:151:ILE:O	1:B:154:VAL:HG22	2.01	0.61
1:C:334:ILE:HG22	1:C:368:PRO:HA	1.83	0.61
1:A:178:ILE:HD12	2:A:402:EDO:O2	2.01	0.61
1:B:301:PHE:CE2	1:C:365:ILE:HG21	2.35	0.61
1:C:168:GLY:O	1:C:353:VAL:HB	2.01	0.61
1:D:147:VAL:HG22	1:D:151:ILE:HG13	1.82	0.61
1:A:344:MET:O	1:A:349:TRP:NE1	2.27	0.60
1:D:201:LEU:O	1:D:204:SER:N	2.32	0.60
1:E:201:LEU:O	1:E:204:SER:N	2.27	0.60
1:F:178:ILE:HG13	1:F:182:SER:OG	2.01	0.60
1:B:176:ARG:HH11	1:B:189:PHE:HD2	1.50	0.60
1:B:337:THR:OG1	1:B:372:VAL:O	2.07	0.60
1:C:337:THR:OG1	1:C:372:VAL:O	2.10	0.60
1:A:201:LEU:O	1:A:204:SER:N	2.26	0.60
1:A:337:THR:HG21	1:A:373:ASP:HA	1.82	0.60
1:F:295:TYR:C	1:F:299:ASN:HB2	2.26	0.60
1:C:178:ILE:HD12	2:C:404:EDO:O2	2.00	0.60
1:C:224:ARG:C	1:C:225:PHE:HD1	2.10	0.60
1:C:312:ILE:HD11	1:C:345:MET:O	2.01	0.60
1:E:167:SER:O	1:E:352:ASN:HB2	2.01	0.60
1:A:337:THR:OG1	1:A:372:VAL:O	2.11	0.60
1:C:205:GLU:HG2	1:C:206:LEU:HD23	1.84	0.60
1:E:268:LYS:HB2	3:E:547:HOH:O	2.02	0.60
1:A:242:PRO:O	1:A:246:GLN:HG3	2.02	0.60
1:C:151:ILE:HD13	2:C:404:EDO:H11	1.83	0.60
1:D:252:VAL:HG13	1:D:258:PHE:HB3	1.84	0.60
1:E:151:ILE:HD13	2:E:404:EDO:H11	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ARG:HG3	2:A:408:EDO:H22	1.84	0.60
1:C:179:HIS:ND1	1:C:184:ARG:O	2.30	0.60
1:E:195:GLY:HA2	1:E:240:ASP:HB3	1.83	0.60
1:F:364:VAL:HG13	1:F:368:PRO:HB3	1.84	0.60
1:D:163:ILE:HA	1:D:303:ILE:O	2.02	0.59
1:E:193:ASN:OD1	1:E:236:ASP:HB3	2.02	0.59
1:A:204:SER:HA	1:A:208:GLY:O	2.01	0.59
1:E:262:GLY:C	1:E:264:ASN:H	2.10	0.59
2:E:409:EDO:H12	2:E:410:EDO:H12	1.83	0.59
1:F:142:MET:SD	1:F:142:MET:N	2.75	0.59
1:A:334:ILE:HG22	1:A:369:ASN:H	1.67	0.59
1:B:194:CYS:SG	1:B:241:MET:HG3	2.43	0.59
1:B:250:LEU:HD23	1:B:251:ARG:HG2	1.83	0.59
1:C:206:LEU:O	1:C:225:PHE:HB2	2.02	0.59
1:D:295:TYR:C	1:D:299:ASN:HB2	2.26	0.59
1:B:201:LEU:O	1:B:204:SER:N	2.29	0.59
1:B:211:LYS:CG	1:B:216:GLY:HA2	2.31	0.59
1:C:340:ALA:O	1:C:343:SER:N	2.36	0.59
1:A:347:HIS:HB3	1:A:349:TRP:NE1	2.18	0.59
1:E:209:HIS:ND1	1:E:209:HIS:O	2.35	0.59
1:F:150:LEU:HD22	1:F:301:PHE:HZ	1.67	0.59
1:A:318:LEU:O	1:A:322:LEU:HG	2.03	0.59
1:D:243:MET:HE2	1:D:244:SER:HA	1.84	0.59
1:F:144:ILE:HD12	1:F:147:VAL:HG11	1.83	0.59
1:C:144:ILE:HD12	1:C:147:VAL:HG11	1.85	0.59
1:E:161:VAL:HB	1:E:274:ILE:HG23	1.84	0.59
1:E:178:ILE:HD12	2:E:404:EDO:O2	2.03	0.59
1:A:203:GLU:HA	1:A:207:PHE:CD1	2.37	0.59
1:B:162:LEU:HD21	1:B:298:LEU:HD13	1.85	0.59
1:C:161:VAL:HB	1:C:274:ILE:HG23	1.85	0.59
1:E:139:GLY:HA2	1:E:314:ASP:OD1	2.03	0.59
1:E:334:ILE:HG22	1:E:368:PRO:HA	1.85	0.59
1:F:141:SER:HB2	1:F:144:ILE:HG22	1.84	0.58
1:A:249:LEU:HA	1:A:252:VAL:HG23	1.84	0.58
1:B:371:LEU:HD12	1:B:371:LEU:H	1.68	0.58
1:C:290:PHE:O	1:C:292:GLU:N	2.31	0.58
1:A:163:ILE:HA	1:A:303:ILE:O	2.02	0.58
1:B:325:ARG:HG3	2:B:410:EDO:H22	1.85	0.58
1:E:295:TYR:C	1:E:299:ASN:HB2	2.28	0.58
1:A:151:ILE:O	1:A:154:VAL:HG13	2.03	0.58
1:A:312:ILE:HG13	1:A:345:MET:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:PHE:CE1	1:A:377:LEU:HD21	2.38	0.58
1:F:176:ARG:HH11	1:F:189:PHE:HD2	1.51	0.58
1:E:233:LEU:O	1:E:274:ILE:N	2.37	0.58
1:A:336:PHE:HE1	1:A:377:LEU:HD21	1.68	0.58
1:B:163:ILE:HA	1:B:303:ILE:O	2.02	0.58
1:C:131:VAL:HG22	1:C:132:PRO:O	2.03	0.58
1:C:176:ARG:HG2	1:C:189:PHE:CE2	2.39	0.58
1:C:193:ASN:OD1	1:C:236:ASP:HB3	2.04	0.58
1:D:142:MET:H	1:D:142:MET:HE2	1.67	0.58
1:A:262:GLY:C	1:A:264:ASN:H	2.09	0.58
1:A:291:ARG:NH2	1:B:240:ASP:OD1	2.37	0.58
2:B:409:EDO:H12	2:B:410:EDO:H12	1.85	0.58
1:C:326:MET:HG3	1:C:326:MET:O	2.03	0.58
1:D:267:ILE:HG22	1:D:268:LYS:H	1.69	0.58
1:D:337:THR:OG1	1:D:372:VAL:O	2.14	0.58
1:E:244:SER:O	1:E:248:LYS:HD3	2.04	0.58
1:F:135:SER:OG	3:F:509:HOH:O	2.17	0.58
1:F:204:SER:HA	1:F:208:GLY:O	2.04	0.58
1:B:224:ARG:C	1:B:225:PHE:HD1	2.12	0.57
1:C:176:ARG:HH11	1:C:189:PHE:HD2	1.51	0.57
1:D:224:ARG:C	1:D:225:PHE:HD1	2.12	0.57
1:D:277:THR:HB	1:D:281:LEU:HD21	1.86	0.57
1:F:249:LEU:HA	1:F:252:VAL:HG23	1.86	0.57
1:D:287:GLY:O	1:D:288:GLN:HB2	2.03	0.57
1:E:151:ILE:O	1:E:154:VAL:HG13	2.04	0.57
1:A:172:GLU:HG3	1:A:234:PHE:CZ	2.39	0.57
1:B:291:ARG:NH2	1:C:240:ASP:OD1	2.38	0.57
1:C:136:HIS:CE1	1:C:176:ARG:HB2	2.38	0.57
1:E:290:PHE:N	1:E:290:PHE:CD1	2.72	0.57
1:B:290:PHE:CD1	1:B:290:PHE:N	2.71	0.57
1:C:167:SER:O	1:C:352:ASN:HB2	2.04	0.57
1:D:204:SER:HA	1:D:208:GLY:O	2.04	0.57
1:D:347:HIS:HB3	1:D:349:TRP:NE1	2.20	0.57
1:E:287:GLY:O	1:E:288:GLN:HB2	2.04	0.57
1:F:203:GLU:OE1	1:F:248:LYS:NZ	2.34	0.57
1:A:349:TRP:HZ3	1:A:355:GLU:HB3	1.69	0.57
1:B:148:ARG:O	1:B:152:GLU:N	2.30	0.57
1:B:151:ILE:O	1:B:154:VAL:HG13	2.04	0.57
1:C:371:LEU:HD12	1:C:371:LEU:H	1.70	0.57
1:D:136:HIS:CE1	1:D:176:ARG:HB2	2.40	0.57
1:A:252:VAL:HG13	1:A:258:PHE:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:PHE:CE2	1:B:365:ILE:HG21	2.39	0.57
1:C:139:GLY:HA2	1:C:314:ASP:OD1	2.05	0.57
1:A:151:ILE:HD13	2:A:402:EDO:H11	1.86	0.57
1:A:220:ALA:HB1	1:A:260:ARG:NH2	2.19	0.57
1:E:163:ILE:HA	1:E:303:ILE:O	2.05	0.57
1:E:204:SER:HA	1:E:208:GLY:O	2.05	0.57
1:D:151:ILE:HD13	2:D:405:EDO:H11	1.85	0.57
1:D:205:GLU:O	1:D:224:ARG:HG2	2.04	0.57
1:B:322:LEU:O	1:B:325:ARG:HB2	2.04	0.57
1:B:326:MET:O	1:B:326:MET:HG3	2.04	0.57
1:C:168:GLY:N	1:C:171:LYS:HG2	2.18	0.57
1:C:375:ASN:O	3:C:509:HOH:O	2.18	0.57
1:D:210:GLU:HB2	1:D:220:ALA:HB2	1.87	0.57
1:E:224:ARG:C	1:E:225:PHE:HD1	2.13	0.57
1:B:139:GLY:HA2	1:B:314:ASP:OD1	2.05	0.56
1:C:250:LEU:HD11	1:C:254:GLN:HE21	1.70	0.56
1:D:312:ILE:HG13	1:D:345:MET:HG3	1.87	0.56
1:F:176:ARG:HG2	1:F:189:PHE:CE2	2.40	0.56
1:A:139:GLY:HA2	1:A:314:ASP:OD1	2.04	0.56
1:B:148:ARG:HA	1:B:151:ILE:HB	1.85	0.56
1:B:238:ILE:HD11	1:B:275:ALA:HB1	1.86	0.56
1:B:262:GLY:C	1:B:264:ASN:H	2.12	0.56
1:A:370:SER:HB3	1:A:371:LEU:HD12	1.87	0.56
1:B:142:MET:H	1:B:142:MET:HE2	1.70	0.56
1:F:322:LEU:O	1:F:325:ARG:HB2	2.05	0.56
1:D:176:ARG:HH11	1:D:189:PHE:HD2	1.52	0.56
1:E:162:LEU:HD21	1:E:298:LEU:HD13	1.87	0.56
1:B:168:GLY:H	1:B:171:LYS:HG3	1.70	0.56
1:B:205:GLU:O	1:B:224:ARG:HG2	2.04	0.56
1:B:314:ASP:O	1:B:317:LEU:HG	2.05	0.56
2:C:409:EDO:H12	2:C:410:EDO:H12	1.86	0.56
1:C:249:LEU:HA	1:C:252:VAL:HG23	1.86	0.56
1:C:349:TRP:CH2	1:C:356:LEU:HD23	2.40	0.56
1:D:139:GLY:HA2	1:D:314:ASP:OD1	2.06	0.56
1:F:220:ALA:HB1	1:F:260:ARG:NH2	2.21	0.56
1:D:326:MET:O	1:D:326:MET:HG3	2.06	0.56
1:C:291:ARG:NH2	1:D:240:ASP:OD1	2.39	0.56
1:E:334:ILE:CG2	1:E:368:PRO:HA	2.36	0.56
1:A:312:ILE:HD11	1:A:345:MET:O	2.06	0.56
1:B:147:VAL:HG22	1:B:151:ILE:HG13	1.88	0.56
1:B:168:GLY:H	1:B:171:LYS:CG	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:GLY:HA2	1:D:240:ASP:HB3	1.88	0.56
1:F:139:GLY:HA2	1:F:314:ASP:OD1	2.05	0.56
1:D:342:ASN:O	1:D:345:MET:HB3	2.05	0.55
1:E:290:PHE:O	1:E:292:GLU:N	2.33	0.55
1:A:290:PHE:CD1	1:A:290:PHE:N	2.74	0.55
1:C:151:ILE:O	1:C:154:VAL:HG13	2.06	0.55
1:D:135:SER:O	1:D:136:HIS:HB2	2.04	0.55
1:F:312:ILE:HD11	1:F:345:MET:O	2.05	0.55
1:A:194:CYS:SG	1:A:241:MET:HG3	2.46	0.55
1:A:334:ILE:CG2	1:A:368:PRO:HA	2.36	0.55
1:D:349:TRP:HZ3	1:D:355:GLU:HB3	1.70	0.55
1:F:224:ARG:C	1:F:225:PHE:HD1	2.13	0.55
1:A:195:GLY:HA2	1:A:240:ASP:HB3	1.88	0.55
1:B:135:SER:O	1:B:136:HIS:HB2	2.06	0.55
1:C:301:PHE:CE1	1:D:365:ILE:HD13	2.42	0.55
1:D:141:SER:HB2	1:D:144:ILE:HG22	1.88	0.55
1:A:162:LEU:HG	1:A:298:LEU:HD22	1.88	0.55
1:D:151:ILE:O	1:D:154:VAL:HG13	2.07	0.55
1:D:233:LEU:HD22	1:D:234:PHE:N	2.22	0.55
1:D:318:LEU:O	1:D:322:LEU:HG	2.07	0.55
1:F:136:HIS:CE1	1:F:176:ARG:HB2	2.42	0.55
1:F:340:ALA:O	1:F:343:SER:N	2.40	0.55
1:D:168:GLY:HA2	1:D:171:LYS:HG3	1.89	0.55
1:D:220:ALA:HB1	1:D:260:ARG:NH2	2.22	0.55
1:A:270:ASN:ND2	2:A:410:EDO:O2	2.39	0.55
1:A:326:MET:HG3	1:A:326:MET:O	2.07	0.55
1:B:290:PHE:O	1:B:292:GLU:N	2.34	0.55
1:E:311:ARG:NH1	1:E:318:LEU:HD11	2.22	0.55
1:E:337:THR:OG1	1:E:372:VAL:O	2.08	0.55
1:B:201:LEU:HB2	1:B:204:SER:HB3	1.89	0.55
1:D:290:PHE:O	1:D:292:GLU:N	2.36	0.55
1:A:168:GLY:H	1:A:171:LYS:CG	2.20	0.55
1:C:322:LEU:O	1:C:325:ARG:HB2	2.07	0.55
1:D:238:ILE:HD11	1:D:275:ALA:HB1	1.89	0.55
1:B:178:ILE:HD12	2:B:404:EDO:O2	2.06	0.54
1:F:199:ALA:HA	1:F:202:LEU:HD23	1.88	0.54
1:F:242:PRO:O	1:F:246:GLN:HB2	2.07	0.54
1:F:152:GLU:HA	1:F:152:GLU:OE2	2.08	0.54
1:F:234:PHE:HE2	1:F:236:ASP:HB2	1.72	0.54
1:A:135:SER:O	1:A:136:HIS:HB2	2.06	0.54
1:B:372:VAL:CG2	1:B:376:HIS:HB2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:VAL:HG22	1:C:151:ILE:HG13	1.90	0.54
1:D:322:LEU:O	1:D:325:ARG:HB2	2.07	0.54
1:A:136:HIS:CE1	1:A:176:ARG:HB2	2.43	0.54
1:A:154:VAL:HG12	1:A:178:ILE:HD11	1.89	0.54
1:A:372:VAL:CG2	1:A:376:HIS:HB2	2.38	0.54
1:B:287:GLY:O	1:B:288:GLN:HB2	2.07	0.54
1:C:233:LEU:O	1:C:274:ILE:N	2.41	0.54
1:A:142:MET:H	1:A:142:MET:CE	2.20	0.54
1:A:371:LEU:HD12	1:A:371:LEU:H	1.72	0.54
2:A:412:EDO:H12	3:A:526:HOH:O	2.08	0.54
1:B:331:ALA:HB1	2:B:420:EDO:H22	1.89	0.54
1:C:262:GLY:C	1:C:264:ASN:H	2.10	0.54
1:D:221:ARG:NH1	3:D:505:HOH:O	2.16	0.54
1:D:237:GLU:OE2	3:D:506:HOH:O	2.18	0.54
1:D:285:ILE:HG23	1:D:290:PHE:HB2	1.89	0.54
1:E:326:MET:O	1:E:326:MET:HG3	2.06	0.54
1:D:209:HIS:O	1:D:220:ALA:HA	2.07	0.54
1:E:342:ASN:O	1:E:345:MET:HB3	2.08	0.54
1:A:131:VAL:HG22	1:A:132:PRO:O	2.08	0.54
1:B:334:ILE:HG22	1:B:369:ASN:H	1.72	0.54
1:D:290:PHE:CD1	1:D:290:PHE:N	2.74	0.54
1:F:287:GLY:O	1:F:288:GLN:HB2	2.08	0.54
1:B:147:VAL:HG23	1:B:303:ILE:CD1	2.38	0.54
1:C:137:MET:O	3:C:510:HOH:O	2.18	0.54
1:C:206:LEU:HD13	1:C:225:PHE:CZ	2.43	0.54
1:C:334:ILE:CG2	1:C:368:PRO:HA	2.38	0.54
1:E:314:ASP:O	1:E:317:LEU:HG	2.08	0.54
1:F:262:GLY:C	1:F:264:ASN:H	2.12	0.54
1:F:167:SER:O	1:F:352:ASN:HB2	2.08	0.53
1:F:326:MET:HG3	1:F:326:MET:O	2.07	0.53
1:B:249:LEU:HA	1:B:252:VAL:HG23	1.90	0.53
1:D:156:THR:HA	1:D:182:SER:O	2.08	0.53
1:C:142:MET:HE2	1:C:142:MET:H	1.74	0.53
1:E:131:VAL:HG22	1:E:132:PRO:O	2.07	0.53
1:B:150:LEU:HD22	1:B:301:PHE:HZ	1.73	0.53
1:C:287:GLY:O	1:C:288:GLN:HB2	2.08	0.53
1:D:176:ARG:HG2	1:D:189:PHE:CE2	2.43	0.53
1:D:207:PHE:HE2	1:D:252:VAL:HG21	1.74	0.53
1:E:172:GLU:HG2	1:E:175:ALA:HB3	1.89	0.53
1:B:209:HIS:O	1:B:209:HIS:ND1	2.40	0.53
1:C:332:GLN:HB2	1:C:368:PRO:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:VAL:HG22	1:E:151:ILE:HG13	1.90	0.53
1:F:312:ILE:HG13	1:F:345:MET:HG3	1.90	0.53
1:A:176:ARG:HH11	1:A:189:PHE:HD2	1.56	0.53
1:B:131:VAL:HG22	1:B:132:PRO:O	2.09	0.53
1:D:140:GLN:O	1:D:140:GLN:HG2	2.09	0.53
1:D:268:LYS:HB2	3:D:548:HOH:O	2.07	0.53
1:F:282:GLU:HA	1:F:285:ILE:HG13	1.90	0.53
1:C:312:ILE:HG13	1:C:345:MET:HG3	1.91	0.53
1:B:220:ALA:HB1	1:B:260:ARG:NH2	2.24	0.53
1:C:184:ARG:HB3	1:C:231:GLY:HA2	1.90	0.53
1:D:262:GLY:C	1:D:264:ASN:H	2.08	0.53
1:C:219:THR:O	1:C:219:THR:OG1	2.21	0.53
1:D:344:MET:O	1:D:349:TRP:NE1	2.30	0.53
1:B:156:THR:HA	1:B:182:SER:O	2.09	0.53
1:E:220:ALA:HB1	1:E:260:ARG:NH2	2.24	0.53
1:B:318:LEU:O	1:B:322:LEU:HG	2.09	0.52
1:C:210:GLU:HB2	1:C:220:ALA:HB2	1.91	0.52
1:D:152:GLU:OE2	1:D:152:GLU:HA	2.10	0.52
1:D:205:GLU:HG2	1:D:206:LEU:HD23	1.91	0.52
1:F:206:LEU:O	1:F:225:PHE:HB2	2.09	0.52
1:A:235:LEU:HD12	1:A:275:ALA:HB2	1.91	0.52
1:B:252:VAL:HG13	1:B:258:PHE:HB3	1.90	0.52
1:C:172:GLU:OE1	1:C:191:PRO:HB3	2.08	0.52
2:D:415:EDO:H12	3:D:538:HOH:O	2.09	0.52
1:E:135:SER:O	1:E:136:HIS:HB2	2.09	0.52
1:E:267:ILE:HG22	1:E:268:LYS:H	1.75	0.52
1:E:318:LEU:O	1:E:322:LEU:HG	2.09	0.52
1:F:144:ILE:HD13	1:F:311:ARG:HH21	1.74	0.52
1:F:326:MET:O	1:F:327:GLU:HG2	2.09	0.52
1:A:250:LEU:HD11	1:A:254:GLN:HE21	1.74	0.52
1:D:193:ASN:OD1	1:D:236:ASP:HB3	2.08	0.52
1:D:244:SER:O	1:D:248:LYS:HD3	2.10	0.52
1:D:251:ARG:HH11	1:D:255:GLU:CD	2.17	0.52
1:B:233:LEU:HD22	1:B:234:PHE:N	2.24	0.52
1:E:136:HIS:CE1	1:E:176:ARG:HB2	2.44	0.52
1:F:193:ASN:OD1	1:F:236:ASP:HB3	2.10	0.52
1:A:149:HIS:ND1	1:B:366:LEU:HD11	2.25	0.52
1:A:250:LEU:HD23	1:A:251:ARG:HG2	1.91	0.52
1:B:154:VAL:CG1	1:B:178:ILE:HD11	2.39	0.52
1:C:144:ILE:HD13	1:C:311:ARG:HH21	1.74	0.52
1:E:194:CYS:SG	1:E:241:MET:HG3	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:MET:O	3:B:507:HOH:O	2.19	0.52
1:C:162:LEU:HD12	1:C:299:ASN:OD1	2.08	0.52
1:C:163:ILE:HA	1:C:303:ILE:O	2.09	0.52
1:A:234:PHE:CD1	1:A:274:ILE:HB	2.44	0.52
1:B:144:ILE:HD13	1:B:311:ARG:HH21	1.74	0.52
2:C:414:EDO:H12	3:C:531:HOH:O	2.09	0.52
1:E:206:LEU:O	1:E:225:PHE:HB2	2.09	0.52
1:F:168:GLY:N	1:F:171:LYS:HG2	2.25	0.52
1:B:179:HIS:O	1:B:185:ARG:HG2	2.10	0.52
1:B:233:LEU:HD22	1:B:234:PHE:H	1.75	0.52
1:B:251:ARG:NH1	1:B:255:GLU:OE1	2.30	0.52
1:F:337:THR:HG22	1:F:338:PRO:N	2.25	0.52
1:C:281:LEU:HD12	1:C:295:TYR:HE1	1.75	0.52
1:C:301:PHE:CE2	1:D:365:ILE:HG21	2.45	0.52
1:C:349:TRP:CZ3	1:C:356:LEU:HD23	2.44	0.52
1:F:131:VAL:HG22	1:F:132:PRO:O	2.09	0.52
1:F:163:ILE:HA	1:F:303:ILE:O	2.10	0.52
1:F:179:HIS:ND1	1:F:184:ARG:O	2.43	0.52
1:B:207:PHE:CE1	1:B:245:MET:HE1	2.45	0.52
1:C:140:GLN:OE1	1:C:313:ASP:OD2	2.28	0.52
1:C:204:SER:HA	1:C:208:GLY:O	2.09	0.52
1:A:207:PHE:HE2	1:A:252:VAL:CG2	2.23	0.51
1:C:290:PHE:CD1	1:C:290:PHE:N	2.78	0.51
1:E:281:LEU:HD12	1:E:295:TYR:HE1	1.74	0.51
1:A:165:GLY:O	1:A:278:HIS:CG	2.62	0.51
1:A:224:ARG:C	1:A:225:PHE:HD1	2.18	0.51
1:E:203:GLU:HA	1:E:207:PHE:CD1	2.45	0.51
1:D:371:LEU:H	1:D:371:LEU:HD12	1.75	0.51
1:E:162:LEU:HD12	1:E:299:ASN:OD1	2.11	0.51
1:E:176:ARG:NH1	1:E:189:PHE:HD2	2.07	0.51
1:F:290:PHE:N	1:F:290:PHE:CD1	2.78	0.51
1:F:308:LEU:HA	1:F:311:ARG:CB	2.40	0.51
1:B:165:GLY:O	1:B:278:HIS:CG	2.63	0.51
1:B:193:ASN:OD1	1:B:236:ASP:HB3	2.11	0.51
1:B:285:ILE:HD13	1:B:290:PHE:HB2	1.91	0.51
1:F:358:ASN:O	1:F:362:ARG:HG2	2.11	0.51
1:D:165:GLY:O	1:D:278:HIS:CG	2.64	0.51
1:B:150:LEU:HD22	1:B:301:PHE:CZ	2.45	0.51
1:B:176:ARG:NH1	1:B:189:PHE:HD2	2.07	0.51
1:C:140:GLN:HG2	1:C:140:GLN:O	2.11	0.51
1:B:150:LEU:HD12	1:B:303:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ASN:O	1:B:345:MET:HB3	2.11	0.51
1:D:209:HIS:O	1:D:209:HIS:ND1	2.44	0.51
1:F:172:GLU:OE1	1:F:191:PRO:HB3	2.11	0.51
1:D:235:LEU:HD12	1:D:275:ALA:HB2	1.92	0.51
1:F:140:GLN:O	1:F:140:GLN:HG2	2.11	0.51
1:F:331:ALA:O	1:F:332:GLN:HG3	2.10	0.51
1:B:311:ARG:NH1	1:B:318:LEU:HD11	2.26	0.51
1:C:168:GLY:CA	1:C:171:LYS:HG2	2.41	0.51
1:D:137:MET:O	3:D:507:HOH:O	2.19	0.51
1:F:137:MET:HB2	3:F:553:HOH:O	2.10	0.51
1:A:144:ILE:HD12	1:A:147:VAL:HG11	1.92	0.51
1:A:240:ASP:OD1	1:F:291:ARG:NH2	2.43	0.51
1:A:243:MET:HE2	1:A:244:SER:CA	2.39	0.51
1:A:322:LEU:O	1:A:325:ARG:HB2	2.10	0.51
1:C:176:ARG:HG2	1:C:189:PHE:HE2	1.74	0.51
1:E:154:VAL:HG12	1:E:178:ILE:HD11	1.93	0.51
1:E:249:LEU:HA	1:E:252:VAL:HG23	1.92	0.51
1:E:334:ILE:HG22	1:E:369:ASN:H	1.75	0.51
1:A:206:LEU:O	1:A:225:PHE:HB2	2.11	0.50
1:A:219:THR:O	1:A:219:THR:OG1	2.23	0.50
1:B:267:ILE:HG22	1:B:268:LYS:H	1.75	0.50
1:C:179:HIS:O	1:C:185:ARG:HG2	2.11	0.50
1:D:131:VAL:HG22	1:D:132:PRO:O	2.10	0.50
1:B:140:GLN:O	1:B:140:GLN:HG2	2.11	0.50
1:C:331:ALA:HB1	2:C:419:EDO:H22	1.92	0.50
1:E:147:VAL:HG23	1:E:303:ILE:CD1	2.37	0.50
1:F:142:MET:HE2	1:F:142:MET:H	1.76	0.50
1:F:178:ILE:O	1:F:182:SER:OG	2.26	0.50
1:F:285:ILE:HG23	1:F:290:PHE:HB2	1.93	0.50
1:A:147:VAL:HG23	1:A:303:ILE:CD1	2.37	0.50
1:B:207:PHE:CD1	1:B:207:PHE:N	2.79	0.50
1:B:301:PHE:HE2	1:C:365:ILE:HG21	1.76	0.50
1:C:165:GLY:O	1:C:278:HIS:CG	2.64	0.50
1:C:242:PRO:O	1:C:246:GLN:HB2	2.11	0.50
1:C:275:ALA:HB3	1:C:298:LEU:HD21	1.94	0.50
1:E:152:GLU:OE2	1:E:152:GLU:HA	2.12	0.50
1:B:164:LEU:HD23	1:B:295:TYR:OH	2.11	0.50
1:C:162:LEU:HD21	1:C:298:LEU:HD13	1.92	0.50
1:D:349:TRP:CZ3	1:D:355:GLU:HB3	2.47	0.50
1:F:252:VAL:HG13	1:F:258:PHE:HB3	1.94	0.50
1:A:229:GLU:HA	1:A:271:VAL:CG1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ILE:HD11	1:B:345:MET:O	2.12	0.50
1:B:344:MET:HE3	1:B:359:LEU:HD23	1.93	0.50
1:D:219:THR:O	1:D:219:THR:OG1	2.22	0.50
1:E:165:GLY:O	1:E:278:HIS:CG	2.64	0.50
1:F:201:LEU:HD13	1:F:205:GLU:HB3	1.94	0.50
1:B:244:SER:O	1:B:248:LYS:HD3	2.12	0.50
1:C:204:SER:C	1:C:206:LEU:H	2.20	0.50
1:C:214:PHE:C	1:C:216:GLY:H	2.19	0.50
1:A:308:LEU:HA	1:A:311:ARG:CB	2.41	0.50
1:C:154:VAL:CG2	1:C:181:HIS:HB3	2.28	0.50
1:F:150:LEU:HD22	1:F:301:PHE:CZ	2.47	0.50
1:F:214:PHE:O	1:F:216:GLY:N	2.45	0.50
1:F:315:ILE:HA	1:F:318:LEU:CB	2.41	0.50
1:F:371:LEU:H	1:F:371:LEU:HD12	1.76	0.50
1:C:136:HIS:HE1	1:C:176:ARG:HB2	1.75	0.49
1:E:251:ARG:NH2	1:E:251:ARG:HG3	2.18	0.49
1:E:251:ARG:HH21	1:E:251:ARG:CG	2.18	0.49
1:F:207:PHE:CE1	1:F:245:MET:HE1	2.47	0.49
1:A:162:LEU:HD21	1:A:298:LEU:HD13	1.93	0.49
1:B:219:THR:O	1:B:219:THR:OG1	2.30	0.49
1:C:152:GLU:OE2	1:C:152:GLU:HA	2.11	0.49
1:C:154:VAL:HG12	1:C:178:ILE:HD11	1.94	0.49
1:D:168:GLY:H	1:D:171:LYS:CG	2.25	0.49
1:B:268:LYS:HB2	3:B:550:HOH:O	2.11	0.49
1:D:326:MET:O	1:D:327:GLU:HG2	2.13	0.49
1:E:337:THR:HB	1:E:340:ALA:HB3	1.94	0.49
1:F:168:GLY:CA	1:F:171:LYS:HG2	2.42	0.49
1:F:321:GLU:O	1:F:325:ARG:HD3	2.12	0.49
1:B:230:GLY:HA3	3:B:562:HOH:O	2.12	0.49
1:A:285:ILE:HG23	1:A:290:PHE:HB2	1.94	0.49
1:B:206:LEU:O	1:B:225:PHE:HB2	2.11	0.49
1:E:252:VAL:HG13	1:E:258:PHE:HB3	1.94	0.49
1:F:172:GLU:HG2	1:F:175:ALA:HB3	1.94	0.49
1:A:142:MET:H	1:A:142:MET:HE2	1.77	0.49
1:C:142:MET:H	1:C:142:MET:CE	2.25	0.49
1:D:207:PHE:HE2	1:D:252:VAL:CG2	2.25	0.49
1:E:297:ARG:HG3	1:E:297:ARG:O	2.12	0.49
1:F:162:LEU:HG	1:F:298:LEU:HD22	1.92	0.49
1:A:150:LEU:HD12	1:A:303:ILE:HD12	1.93	0.49
1:C:220:ALA:HB1	1:C:260:ARG:NH2	2.27	0.49
1:C:355:GLU:O	1:C:358:ASN:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:PHE:HE2	1:E:252:VAL:CG2	2.26	0.49
1:E:290:PHE:N	1:E:290:PHE:HD1	2.11	0.49
1:B:204:SER:HA	1:B:208:GLY:O	2.12	0.49
1:C:141:SER:O	1:C:145:GLN:HG3	2.13	0.49
1:C:243:MET:HE2	1:C:244:SER:HA	1.95	0.49
1:F:221:ARG:NH1	3:F:508:HOH:O	2.16	0.49
1:F:319:LEU:HA	1:F:322:LEU:HG	1.95	0.49
1:F:355:GLU:O	1:F:358:ASN:HB3	2.13	0.49
1:B:332:GLN:NE2	3:B:514:HOH:O	2.35	0.49
1:D:233:LEU:HD22	1:D:234:PHE:H	1.76	0.49
1:E:312:ILE:HD11	1:E:345:MET:O	2.13	0.49
1:F:162:LEU:HD12	1:F:299:ASN:OD1	2.13	0.49
1:A:214:PHE:C	1:A:216:GLY:H	2.20	0.49
1:B:326:MET:O	1:B:327:GLU:HG2	2.13	0.49
1:C:344:MET:HE3	1:C:359:LEU:HD23	1.94	0.49
1:E:249:LEU:O	1:E:253:LEU:HG	2.13	0.49
1:B:176:ARG:HG2	1:B:189:PHE:CE2	2.48	0.48
1:B:246:GLN:O	1:B:249:LEU:HB2	2.13	0.48
1:B:267:ILE:HG22	1:B:268:LYS:N	2.27	0.48
1:C:321:GLU:O	1:C:325:ARG:HD3	2.13	0.48
1:B:152:GLU:OE2	1:B:152:GLU:HA	2.12	0.48
1:B:249:LEU:O	1:B:253:LEU:HG	2.12	0.48
1:B:349:TRP:CH2	1:B:356:LEU:HD23	2.48	0.48
1:C:372:VAL:CG2	1:C:376:HIS:HB2	2.42	0.48
1:D:334:ILE:HG22	1:D:369:ASN:H	1.78	0.48
1:F:349:TRP:CZ3	1:F:356:LEU:HD23	2.49	0.48
1:A:251:ARG:HD2	1:B:196:ALA:O	2.13	0.48
1:C:209:HIS:O	1:C:220:ALA:HA	2.13	0.48
1:C:251:ARG:HH11	1:C:255:GLU:CD	2.19	0.48
1:C:342:ASN:O	1:C:345:MET:HB3	2.13	0.48
1:D:267:ILE:HG22	1:D:268:LYS:N	2.28	0.48
1:E:214:PHE:O	1:E:216:GLY:N	2.47	0.48
1:F:243:MET:SD	1:F:291:ARG:NH2	2.82	0.48
1:D:135:SER:OG	3:D:508:HOH:O	2.20	0.48
1:D:172:GLU:HG3	1:D:234:PHE:CZ	2.48	0.48
1:E:172:GLU:OE1	1:E:191:PRO:HB3	2.13	0.48
1:B:207:PHE:HD1	1:B:207:PHE:H	1.61	0.48
1:B:243:MET:HA	1:B:246:GLN:HB2	1.96	0.48
1:C:326:MET:O	1:C:327:GLU:HG2	2.13	0.48
1:F:249:LEU:O	1:F:253:LEU:HG	2.13	0.48
1:F:349:TRP:CH2	1:F:356:LEU:HD23	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ILE:O	1:C:147:VAL:HG12	2.14	0.48
1:A:342:ASN:O	1:A:345:MET:HB3	2.14	0.48
1:C:150:LEU:HD12	1:C:303:ILE:HD12	1.96	0.48
1:D:281:LEU:O	1:D:284:MET:N	2.47	0.48
1:F:214:PHE:C	1:F:216:GLY:H	2.22	0.48
1:F:233:LEU:O	1:F:274:ILE:N	2.47	0.48
1:B:291:ARG:O	1:B:292:GLU:HB2	2.14	0.48
1:B:309:ARG:HG2	1:B:348:ASP:HA	1.96	0.48
1:C:207:PHE:CE1	1:C:245:MET:HE1	2.49	0.48
1:D:257:CYS:HB3	1:D:267:ILE:O	2.14	0.48
1:A:204:SER:C	1:A:206:LEU:H	2.20	0.48
1:B:256:ARG:HG2	1:B:269:ALA:O	2.14	0.48
2:B:414:EDO:H12	3:B:527:HOH:O	2.13	0.48
1:C:214:PHE:O	1:C:216:GLY:N	2.47	0.48
1:C:347:HIS:HB3	1:C:349:TRP:NE1	2.29	0.48
1:D:308:LEU:HA	1:D:311:ARG:H	1.78	0.48
1:D:348:ASP:OD1	3:D:503:HOH:O	2.20	0.48
1:E:144:ILE:HD13	1:E:311:ARG:HH21	1.78	0.48
1:E:149:HIS:ND1	1:F:366:LEU:HD11	2.28	0.48
1:F:156:THR:HA	1:F:182:SER:O	2.12	0.48
1:D:136:HIS:HE1	1:D:176:ARG:HB2	1.78	0.48
1:D:298:LEU:HA	1:D:298:LEU:HD23	1.72	0.48
1:D:315:ILE:O	1:D:319:LEU:N	2.41	0.48
1:E:168:GLY:H	1:E:171:LYS:CG	2.24	0.48
1:E:349:TRP:CH2	1:E:356:LEU:HD23	2.48	0.48
1:F:342:ASN:O	1:F:345:MET:HB3	2.13	0.48
1:A:249:LEU:HG	1:A:253:LEU:HD11	1.95	0.47
1:A:355:GLU:O	1:A:358:ASN:HB3	2.14	0.47
1:C:309:ARG:HG2	1:C:348:ASP:HA	1.95	0.47
1:D:150:LEU:HD12	1:D:303:ILE:HD12	1.96	0.47
1:E:229:GLU:HA	1:E:271:VAL:CG1	2.44	0.47
1:F:140:GLN:OE1	1:F:313:ASP:OD2	2.32	0.47
1:F:165:GLY:O	1:F:278:HIS:CG	2.67	0.47
1:A:193:ASN:OD1	1:A:236:ASP:HB3	2.13	0.47
1:B:203:GLU:H	1:B:203:GLU:HG2	1.44	0.47
1:D:378:PRO:O	1:D:382:ARG:HB2	2.13	0.47
1:F:206:LEU:HD13	1:F:225:PHE:CZ	2.49	0.47
1:A:140:GLN:O	1:A:140:GLN:HG2	2.13	0.47
1:A:207:PHE:HE2	1:A:252:VAL:HG21	1.79	0.47
1:A:308:LEU:HA	1:A:311:ARG:H	1.79	0.47
1:C:149:HIS:ND1	1:D:366:LEU:HD11	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:GLY:H	1:D:171:LYS:HG2	1.80	0.47
1:E:204:SER:C	1:E:206:LEU:H	2.20	0.47
1:B:204:SER:C	1:B:206:LEU:H	2.21	0.47
1:C:162:LEU:HD13	1:C:164:LEU:HD11	1.95	0.47
1:D:355:GLU:O	1:D:358:ASN:HB3	2.14	0.47
1:E:204:SER:C	1:E:206:LEU:N	2.72	0.47
1:F:140:GLN:C	1:F:145:GLN:HE21	2.23	0.47
1:A:137:MET:O	3:A:507:HOH:O	2.20	0.47
1:C:164:LEU:HD23	1:C:295:TYR:OH	2.15	0.47
1:E:151:ILE:O	1:E:154:VAL:HG22	2.15	0.47
1:E:154:VAL:CG1	1:E:178:ILE:HD11	2.44	0.47
1:E:322:LEU:O	1:E:325:ARG:HB2	2.14	0.47
1:E:378:PRO:O	1:E:382:ARG:HB2	2.13	0.47
1:F:235:LEU:HD12	1:F:275:ALA:HB2	1.96	0.47
1:F:309:ARG:HG2	1:F:348:ASP:HA	1.97	0.47
1:F:334:ILE:HG22	1:F:368:PRO:HA	1.97	0.47
1:D:211:LYS:CD	1:D:216:GLY:HA2	2.44	0.47
1:E:142:MET:CE	1:E:142:MET:H	2.26	0.47
1:E:142:MET:H	1:E:142:MET:HE2	1.78	0.47
1:E:301:PHE:CE1	1:F:365:ILE:HD13	2.50	0.47
1:F:267:ILE:HG22	1:F:268:LYS:H	1.79	0.47
1:A:156:THR:HA	1:A:182:SER:O	2.14	0.47
1:A:267:ILE:HG22	1:A:268:LYS:H	1.79	0.47
1:A:348:ASP:OD1	3:A:502:HOH:O	2.20	0.47
1:A:365:ILE:HG21	1:F:301:PHE:CE2	2.50	0.47
1:B:137:MET:HB2	3:B:563:HOH:O	2.13	0.47
1:C:155:SER:OG	3:C:512:HOH:O	2.20	0.47
1:C:238:ILE:HG13	1:C:276:ALA:O	2.15	0.47
1:D:154:VAL:HG12	1:D:178:ILE:HD11	1.97	0.47
1:D:162:LEU:HD21	1:D:298:LEU:HD13	1.96	0.47
1:E:179:HIS:O	1:E:185:ARG:HG2	2.14	0.47
1:F:142:MET:H	1:F:142:MET:CE	2.28	0.47
1:F:198:PRO:O	1:F:202:LEU:HD21	2.14	0.47
1:A:382:ARG:NH2	3:A:503:HOH:O	2.47	0.47
1:B:141:SER:O	1:B:145:GLN:HG3	2.15	0.47
1:C:150:LEU:HD22	1:C:301:PHE:HZ	1.80	0.47
1:E:355:GLU:O	1:E:358:ASN:HB3	2.14	0.47
1:A:172:GLU:HG3	1:A:234:PHE:CE1	2.50	0.47
1:A:358:ASN:O	1:A:362:ARG:HG2	2.15	0.47
1:B:251:ARG:HH11	1:B:255:GLU:CD	2.19	0.47
1:B:296:TYR:CG	1:B:297:ARG:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:PHE:CE1	1:D:245:MET:HE1	2.50	0.47
1:E:349:TRP:CZ3	1:E:356:LEU:HD23	2.50	0.47
1:C:254:GLN:NE2	3:C:504:HOH:O	2.41	0.46
1:C:337:THR:HG22	1:C:338:PRO:N	2.29	0.46
1:F:141:SER:O	1:F:145:GLN:HG3	2.15	0.46
1:F:184:ARG:HB3	1:F:231:GLY:HA2	1.97	0.46
1:F:207:PHE:HE2	1:F:252:VAL:CG2	2.28	0.46
1:B:296:TYR:O	1:B:299:ASN:N	2.48	0.46
1:C:188:PRO:HD2	1:C:231:GLY:HA3	1.98	0.46
1:A:311:ARG:NH1	1:A:318:LEU:HD11	2.30	0.46
1:B:151:ILE:CD1	2:B:404:EDO:H11	2.45	0.46
1:F:325:ARG:HD2	1:F:325:ARG:HA	1.64	0.46
1:A:209:HIS:O	1:A:220:ALA:HA	2.16	0.46
1:B:355:GLU:O	1:B:358:ASN:HB3	2.16	0.46
1:D:140:GLN:C	1:D:145:GLN:HE21	2.24	0.46
1:E:207:PHE:CD1	1:E:207:PHE:N	2.83	0.46
1:E:249:LEU:HG	1:E:253:LEU:HD11	1.98	0.46
1:E:283:GLU:O	1:E:287:GLY:N	2.47	0.46
1:E:326:MET:O	1:E:327:GLU:HG2	2.16	0.46
1:A:144:ILE:HD13	1:A:311:ARG:NH2	2.29	0.46
1:A:176:ARG:NH1	1:A:189:PHE:HD2	2.14	0.46
1:A:214:PHE:O	1:A:216:GLY:N	2.49	0.46
1:A:230:GLY:HA3	3:A:568:HOH:O	2.16	0.46
1:A:234:PHE:HD1	1:A:274:ILE:HB	1.81	0.46
1:B:154:VAL:HG12	1:B:178:ILE:HD11	1.97	0.46
1:B:331:ALA:C	1:B:332:GLN:HG3	2.41	0.46
1:C:168:GLY:HA2	1:C:171:LYS:HG2	1.98	0.46
1:D:141:SER:O	1:D:145:GLN:HG3	2.16	0.46
1:F:275:ALA:HB3	1:F:298:LEU:HD21	1.97	0.46
1:A:147:VAL:O	1:A:151:ILE:N	2.46	0.46
1:A:233:LEU:HD22	1:A:234:PHE:N	2.30	0.46
1:B:352:ASN:HB3	1:B:353:VAL:H	1.46	0.46
1:C:204:SER:C	1:C:206:LEU:N	2.74	0.46
1:D:172:GLU:CG	1:D:175:ALA:HB3	2.44	0.46
1:E:178:ILE:HB	2:E:404:EDO:H21	1.96	0.46
1:E:250:LEU:O	1:E:254:GLN:N	2.33	0.46
1:F:372:VAL:CG2	1:F:376:HIS:HB2	2.46	0.46
1:A:352:ASN:HB3	1:A:353:VAL:H	1.48	0.46
1:D:308:LEU:HA	1:D:311:ARG:CB	2.41	0.46
1:E:137:MET:HB2	3:E:566:HOH:O	2.16	0.46
1:F:205:GLU:HG2	1:F:206:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:GLU:HB2	1:A:220:ALA:HB2	1.98	0.46
1:A:366:LEU:HD11	1:F:149:HIS:ND1	2.31	0.46
1:C:246:GLN:O	1:C:249:LEU:HB2	2.16	0.46
1:E:291:ARG:NH2	1:F:240:ASP:OD1	2.49	0.46
1:B:147:VAL:O	1:B:150:LEU:HB2	2.16	0.46
1:E:156:THR:HA	1:E:182:SER:O	2.15	0.46
1:E:299:ASN:OD1	1:E:302:PRO:HB3	2.16	0.46
1:F:176:ARG:NH1	1:F:189:PHE:HD2	2.14	0.46
1:A:301:PHE:CE1	1:B:365:ILE:HD13	2.51	0.45
1:B:140:GLN:OE1	1:B:313:ASP:OD2	2.33	0.45
1:B:172:GLU:CG	1:B:175:ALA:HB3	2.46	0.45
1:C:140:GLN:C	1:C:145:GLN:HE21	2.24	0.45
1:C:245:MET:HE2	1:C:248:LYS:HE2	1.97	0.45
1:C:296:TYR:CG	1:C:297:ARG:N	2.84	0.45
1:D:230:GLY:HA3	3:D:563:HOH:O	2.16	0.45
1:D:337:THR:HB	1:D:340:ALA:HB3	1.98	0.45
1:E:163:ILE:HG13	1:E:303:ILE:HG23	1.98	0.45
1:F:150:LEU:HD12	1:F:303:ILE:HD12	1.98	0.45
1:F:203:GLU:HA	1:F:207:PHE:CD1	2.52	0.45
1:B:233:LEU:O	1:B:274:ILE:N	2.50	0.45
1:B:349:TRP:CZ3	1:B:356:LEU:HD23	2.51	0.45
1:D:372:VAL:CG2	1:D:376:HIS:HB2	2.47	0.45
1:E:214:PHE:C	1:E:216:GLY:H	2.24	0.45
1:E:371:LEU:HD12	1:E:371:LEU:H	1.81	0.45
1:F:204:SER:C	1:F:206:LEU:H	2.22	0.45
1:A:137:MET:HB2	3:A:560:HOH:O	2.15	0.45
1:A:201:LEU:HB2	1:A:204:SER:CB	2.44	0.45
1:A:204:SER:C	1:A:206:LEU:N	2.74	0.45
1:D:233:LEU:O	1:D:273:VAL:HA	2.16	0.45
1:D:351:GLY:HA3	1:D:355:GLU:HB2	1.98	0.45
1:E:246:GLN:O	1:E:249:LEU:HB2	2.17	0.45
1:A:152:GLU:OE2	1:A:152:GLU:HA	2.16	0.45
1:A:349:TRP:CZ3	1:A:355:GLU:HB3	2.49	0.45
1:C:364:VAL:CG1	1:C:368:PRO:HB3	2.44	0.45
1:F:194:CYS:SG	1:F:241:MET:HG3	2.57	0.45
1:A:203:GLU:OE1	1:A:248:LYS:NZ	2.32	0.45
1:A:296:TYR:O	1:A:299:ASN:N	2.50	0.45
1:C:150:LEU:HD22	1:C:301:PHE:CZ	2.51	0.45
1:C:267:ILE:HG22	1:C:268:LYS:H	1.82	0.45
1:F:176:ARG:HG2	1:F:189:PHE:HE2	1.81	0.45
1:A:334:ILE:HG22	1:A:368:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:LEU:HA	1:B:311:ARG:CB	2.44	0.45
1:D:174:VAL:HG21	1:D:305:MET:SD	2.57	0.45
1:D:207:PHE:CD1	1:D:207:PHE:N	2.85	0.45
1:D:296:TYR:CG	1:D:297:ARG:N	2.85	0.45
1:A:184:ARG:HB3	1:A:231:GLY:HA2	1.99	0.45
1:A:301:PHE:HA	1:A:302:PRO:HD3	1.76	0.45
1:F:268:LYS:HB2	3:F:547:HOH:O	2.15	0.45
1:F:337:THR:HB	1:F:340:ALA:HB3	1.99	0.45
1:B:290:PHE:N	1:B:290:PHE:HD1	2.14	0.45
1:D:176:ARG:NH1	1:D:189:PHE:HD2	2.15	0.45
1:D:198:PRO:HB2	1:D:200:GLU:HG3	1.98	0.45
1:F:207:PHE:CD1	1:F:207:PHE:N	2.85	0.45
1:A:290:PHE:N	1:A:290:PHE:HD1	2.15	0.45
1:D:162:LEU:HD12	1:D:299:ASN:OD1	2.17	0.45
1:E:256:ARG:HG2	1:E:269:ALA:O	2.17	0.45
2:E:415:EDO:H12	3:E:524:HOH:O	2.16	0.45
1:F:147:VAL:O	1:F:151:ILE:N	2.47	0.45
1:F:283:GLU:O	1:F:287:GLY:N	2.48	0.45
1:B:166:GLU:O	1:B:169:THR:OG1	2.23	0.45
1:C:151:ILE:O	1:C:154:VAL:HG22	2.17	0.45
1:A:136:HIS:HE1	1:A:176:ARG:HB2	1.80	0.44
1:B:204:SER:C	1:B:206:LEU:N	2.75	0.44
1:C:309:ARG:CG	1:C:348:ASP:HA	2.48	0.44
1:D:211:LYS:HD2	1:D:216:GLY:HA2	1.97	0.44
1:D:358:ASN:O	1:D:362:ARG:HG2	2.17	0.44
1:A:326:MET:O	1:A:327:GLU:HG2	2.17	0.44
1:B:172:GLU:HG3	1:B:234:PHE:CZ	2.51	0.44
1:B:258:PHE:CE1	1:B:269:ALA:HB2	2.51	0.44
1:C:176:ARG:NH1	1:C:189:PHE:HD2	2.14	0.44
1:C:179:HIS:HE1	1:C:187:GLY:O	2.00	0.44
1:C:207:PHE:CD1	1:C:207:PHE:N	2.85	0.44
1:F:238:ILE:HD11	1:F:275:ALA:HB1	1.99	0.44
1:B:201:LEU:HB2	1:B:204:SER:CB	2.47	0.44
1:C:249:LEU:O	1:C:253:LEU:HG	2.17	0.44
1:C:325:ARG:HG3	2:C:410:EDO:H22	1.99	0.44
1:F:158:GLU:HA	1:F:272:ARG:HG2	2.00	0.44
1:A:151:ILE:O	1:A:154:VAL:HG22	2.18	0.44
1:A:179:HIS:O	1:A:185:ARG:HG2	2.18	0.44
1:B:151:ILE:O	1:B:152:GLU:C	2.58	0.44
1:B:214:PHE:O	1:B:216:GLY:N	2.46	0.44
1:C:297:ARG:O	1:C:297:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:ILE:O	1:D:316:PRO:C	2.59	0.44
1:D:315:ILE:HG13	1:D:316:PRO:N	2.33	0.44
1:D:364:VAL:HG13	1:D:368:PRO:HB3	2.00	0.44
1:E:193:ASN:CG	1:E:236:ASP:HB3	2.41	0.44
1:C:171:LYS:H	1:C:171:LYS:HG3	1.46	0.44
1:C:189:PHE:HD1	1:C:232:THR:HG1	1.66	0.44
1:D:325:ARG:HA	1:D:325:ARG:HD2	1.79	0.44
1:E:282:GLU:O	1:E:286:ASP:N	2.36	0.44
1:F:209:HIS:O	1:F:220:ALA:HA	2.18	0.44
1:F:297:ARG:O	1:F:297:ARG:HG3	2.17	0.44
1:A:206:LEU:HD13	1:A:225:PHE:CZ	2.52	0.44
1:B:163:ILE:HG13	1:B:303:ILE:HG23	2.00	0.44
1:B:210:GLU:HA	1:B:217:ALA:O	2.17	0.44
1:C:333:PRO:O	1:C:369:ASN:N	2.50	0.44
1:D:168:GLY:CA	1:D:171:LYS:HG3	2.47	0.44
1:D:321:GLU:O	1:D:325:ARG:HD3	2.18	0.44
1:E:141:SER:O	1:E:145:GLN:HG3	2.17	0.44
1:C:202:LEU:HD22	1:C:202:LEU:HA	1.86	0.44
1:D:194:CYS:N	1:D:236:ASP:O	2.49	0.44
1:E:202:LEU:O	1:E:206:LEU:HD12	2.18	0.44
1:E:301:PHE:HA	1:E:302:PRO:HD3	1.82	0.44
1:E:319:LEU:HA	1:E:322:LEU:HG	1.99	0.44
1:A:168:GLY:HA2	1:A:171:LYS:HE2	2.00	0.44
1:E:150:LEU:HD22	1:E:301:PHE:HZ	1.83	0.44
1:E:206:LEU:HD22	1:E:225:PHE:CE1	2.53	0.44
1:E:296:TYR:CG	1:E:297:ARG:N	2.85	0.44
1:E:378:PRO:HD2	1:E:381:TYR:CE1	2.53	0.44
1:B:138:VAL:HG22	1:B:317:LEU:HD12	1.99	0.44
1:B:144:ILE:C	1:B:147:VAL:HG12	2.43	0.44
1:C:137:MET:HB2	3:C:548:HOH:O	2.17	0.44
1:C:144:ILE:HD12	1:C:147:VAL:CG1	2.47	0.44
1:C:285:ILE:HG23	1:C:290:PHE:HB2	2.00	0.44
1:E:207:PHE:CE1	1:E:245:MET:HE1	2.52	0.44
1:A:205:GLU:HG2	1:A:206:LEU:HD23	1.99	0.43
1:A:365:ILE:HD13	1:F:301:PHE:CE1	2.52	0.43
1:B:149:HIS:ND1	1:C:366:LEU:HD11	2.33	0.43
1:B:297:ARG:HG3	1:B:297:ARG:O	2.18	0.43
1:F:243:MET:HE2	1:F:244:SER:HA	2.00	0.43
1:A:349:TRP:CZ3	1:A:356:LEU:HD23	2.53	0.43
1:A:371:LEU:H	1:A:371:LEU:CD1	2.30	0.43
1:B:154:VAL:O	1:B:156:THR:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:SER:O	1:C:248:LYS:HD3	2.18	0.43
1:E:219:THR:O	1:E:219:THR:OG1	2.31	0.43
1:A:344:MET:HE3	1:A:359:LEU:HD23	2.00	0.43
1:B:138:VAL:HG22	1:B:317:LEU:CD1	2.48	0.43
1:C:178:ILE:HB	2:C:404:EDO:H21	1.99	0.43
1:C:378:PRO:O	1:C:382:ARG:HB2	2.18	0.43
1:D:137:MET:HB2	3:D:551:HOH:O	2.17	0.43
1:D:202:LEU:O	1:D:207:PHE:HE1	2.01	0.43
1:E:164:LEU:HB2	1:E:304:GLU:HG2	2.01	0.43
1:E:224:ARG:HG2	1:E:224:ARG:H	1.65	0.43
1:E:275:ALA:HB3	1:E:298:LEU:HD21	1.99	0.43
1:F:151:ILE:O	1:F:154:VAL:HG22	2.19	0.43
1:A:151:ILE:O	1:A:152:GLU:C	2.62	0.43
1:A:207:PHE:CD1	1:A:207:PHE:N	2.87	0.43
1:A:268:LYS:HB2	3:A:546:HOH:O	2.17	0.43
1:B:136:HIS:CE1	1:B:176:ARG:HB2	2.53	0.43
1:C:162:LEU:O	1:C:302:PRO:HA	2.18	0.43
1:D:203:GLU:H	1:D:203:GLU:HG2	1.62	0.43
1:D:249:LEU:O	1:D:253:LEU:HG	2.19	0.43
1:E:176:ARG:HG2	1:E:189:PHE:CE2	2.53	0.43
1:D:140:GLN:OE1	1:D:313:ASP:OD2	2.37	0.43
1:D:340:ALA:O	1:D:343:SER:OG	2.23	0.43
1:E:151:ILE:O	1:E:152:GLU:C	2.59	0.43
1:E:305:MET:HG3	3:E:531:HOH:O	2.18	0.43
1:F:168:GLY:HA2	1:F:171:LYS:HG2	2.01	0.43
1:F:230:GLY:HA3	3:F:564:HOH:O	2.18	0.43
1:B:243:MET:SD	1:B:291:ARG:NH2	2.91	0.43
1:B:288:GLN:NE2	3:B:517:HOH:O	2.47	0.43
1:B:349:TRP:CZ3	1:B:355:GLU:HB3	2.54	0.43
1:C:172:GLU:HG3	1:C:234:PHE:CD2	2.53	0.43
1:C:180:TYR:O	1:C:185:ARG:NE	2.52	0.43
1:C:221:ARG:NH1	3:C:508:HOH:O	2.17	0.43
1:D:166:GLU:H	1:D:166:GLU:HG3	1.63	0.43
1:D:229:GLU:HA	1:D:271:VAL:CG1	2.48	0.43
1:F:144:ILE:HD12	1:F:147:VAL:CG1	2.48	0.43
1:A:178:ILE:HB	2:A:402:EDO:H21	2.01	0.43
1:B:207:PHE:CZ	1:B:245:MET:HE1	2.54	0.43
1:B:214:PHE:C	1:B:216:GLY:H	2.26	0.43
1:B:224:ARG:O	1:B:225:PHE:HD1	2.00	0.43
1:B:233:LEU:O	1:B:273:VAL:HA	2.19	0.43
1:B:308:LEU:HA	1:B:311:ARG:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ILE:HG22	1:C:202:LEU:HD21	2.01	0.43
1:C:341:ILE:O	1:C:345:MET:N	2.51	0.43
1:A:256:ARG:HG2	1:A:269:ALA:O	2.19	0.43
1:A:337:THR:HB	1:A:340:ALA:HB3	2.01	0.43
1:A:378:PRO:O	1:A:382:ARG:HB2	2.19	0.43
1:B:301:PHE:HA	1:B:302:PRO:HD3	1.72	0.43
1:C:172:GLU:HG2	1:C:175:ALA:HB3	2.01	0.43
1:D:178:ILE:HB	2:D:405:EDO:H21	1.99	0.43
1:E:236:ASP:HA	1:E:276:ALA:HB3	2.01	0.43
1:E:288:GLN:NE2	3:E:515:HOH:O	2.43	0.43
1:E:308:LEU:H	1:E:308:LEU:HG	1.60	0.43
1:F:227:LEU:HD23	1:F:227:LEU:HA	1.82	0.43
1:F:315:ILE:O	1:F:316:PRO:C	2.61	0.43
1:F:378:PRO:O	1:F:382:ARG:HB2	2.19	0.43
1:C:273:VAL:HG12	1:C:274:ILE:N	2.34	0.43
1:C:298:LEU:HD23	1:C:298:LEU:HA	1.81	0.43
1:D:296:TYR:O	1:D:299:ASN:N	2.52	0.43
1:E:372:VAL:CG2	1:E:376:HIS:HB2	2.48	0.43
1:F:172:GLU:HG3	1:F:234:PHE:CE1	2.53	0.43
1:F:296:TYR:CG	1:F:297:ARG:N	2.86	0.43
1:A:196:ALA:HB1	1:F:250:LEU:HD23	2.01	0.43
1:A:221:ARG:NH1	3:A:510:HOH:O	2.27	0.43
1:B:250:LEU:HD23	1:B:251:ARG:CG	2.46	0.43
1:E:267:ILE:HG22	1:E:268:LYS:N	2.34	0.43
1:E:308:LEU:HA	1:E:311:ARG:H	1.84	0.43
1:B:315:ILE:HG13	1:B:316:PRO:N	2.32	0.42
1:D:144:ILE:HD12	1:D:147:VAL:CG1	2.44	0.42
1:D:214:PHE:O	1:D:216:GLY:N	2.52	0.42
1:E:205:GLU:HG3	1:E:224:ARG:HE	1.84	0.42
1:F:136:HIS:HE1	1:F:176:ARG:HB2	1.82	0.42
1:F:291:ARG:O	1:F:292:GLU:HB2	2.19	0.42
1:A:141:SER:O	1:A:145:GLN:HG3	2.19	0.42
1:A:354:ARG:HD2	3:A:519:HOH:O	2.18	0.42
1:D:162:LEU:HG	1:D:298:LEU:HD22	2.00	0.42
1:E:315:ILE:O	1:E:316:PRO:C	2.62	0.42
1:F:235:LEU:HG	1:F:274:ILE:O	2.20	0.42
1:F:298:LEU:HD23	1:F:298:LEU:HA	1.77	0.42
1:F:317:LEU:O	1:F:320:GLN:N	2.52	0.42
1:A:148:ARG:O	1:A:151:ILE:N	2.51	0.42
1:A:163:ILE:O	1:A:276:ALA:HA	2.18	0.42
1:E:237:GLU:C	1:E:239:GLY:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:ILE:O	1:F:147:VAL:HG12	2.20	0.42
1:A:176:ARG:HG2	1:A:189:PHE:CE2	2.54	0.42
1:A:233:LEU:O	1:A:274:ILE:N	2.52	0.42
1:B:275:ALA:HB3	1:B:298:LEU:HD21	2.02	0.42
1:D:204:SER:C	1:D:206:LEU:H	2.26	0.42
1:E:140:GLN:OE1	1:E:313:ASP:OD2	2.36	0.42
1:E:147:VAL:O	1:E:151:ILE:N	2.48	0.42
1:F:204:SER:C	1:F:206:LEU:N	2.75	0.42
1:F:250:LEU:HD11	3:F:504:HOH:O	2.18	0.42
1:F:254:GLN:NE2	3:F:504:HOH:O	2.47	0.42
1:A:241:MET:HG2	3:A:572:HOH:O	2.19	0.42
1:A:243:MET:HA	1:A:246:GLN:HB2	2.02	0.42
1:B:164:LEU:HD12	1:B:164:LEU:N	2.34	0.42
1:C:203:GLU:HA	1:C:207:PHE:CD1	2.54	0.42
1:D:258:PHE:CE1	1:D:269:ALA:HB2	2.55	0.42
1:C:135:SER:O	1:C:136:HIS:HB2	2.18	0.42
1:C:174:VAL:CG2	1:C:305:MET:SD	3.08	0.42
1:C:291:ARG:HG3	1:C:293:ASP:OD1	2.20	0.42
1:D:260:ARG:HG2	1:D:261:VAL:N	2.35	0.42
1:D:337:THR:CG2	1:D:373:ASP:HA	2.45	0.42
1:E:166:GLU:H	1:E:166:GLU:HG3	1.68	0.42
1:F:315:ILE:O	1:F:319:LEU:N	2.47	0.42
1:F:325:ARG:HG3	2:F:416:EDO:H22	2.01	0.42
1:A:203:GLU:H	1:A:203:GLU:HG2	1.48	0.42
1:A:296:TYR:CG	1:A:297:ARG:N	2.88	0.42
1:B:296:TYR:C	1:B:299:ASN:H	2.27	0.42
1:C:203:GLU:OE1	1:C:248:LYS:NZ	2.40	0.42
1:C:225:PHE:CE1	1:C:233:LEU:HD11	2.55	0.42
1:C:337:THR:HB	1:C:340:ALA:HB3	2.01	0.42
1:D:201:LEU:HB2	1:D:204:SER:HB3	2.02	0.42
1:D:291:ARG:O	1:D:292:GLU:HB2	2.19	0.42
1:D:378:PRO:HD2	1:D:381:TYR:HE1	1.85	0.42
2:D:413:EDO:H12	3:D:523:HOH:O	2.19	0.42
1:F:295:TYR:O	1:F:299:ASN:HB2	2.20	0.42
1:F:348:ASP:OD1	3:F:503:HOH:O	2.21	0.42
1:A:148:ARG:HG3	1:A:149:HIS:N	2.34	0.42
1:A:295:TYR:O	1:A:299:ASN:HB2	2.20	0.42
1:A:365:ILE:HD13	1:F:301:PHE:CZ	2.55	0.42
1:C:151:ILE:CD1	2:C:404:EDO:H11	2.47	0.42
1:C:229:GLU:HA	1:C:271:VAL:CG1	2.50	0.42
1:C:260:ARG:HG2	1:C:261:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:LEU:HD13	1:E:164:LEU:HD11	2.01	0.42
1:E:203:GLU:H	1:E:203:GLU:HG2	1.48	0.42
1:E:209:HIS:O	1:E:220:ALA:HA	2.20	0.42
1:E:344:MET:O	1:E:349:TRP:NE1	2.44	0.42
1:A:238:ILE:HD11	1:A:275:ALA:HB1	2.02	0.42
1:A:370:SER:HB3	1:A:371:LEU:H	1.62	0.42
1:C:166:GLU:H	1:C:166:GLU:HG3	1.64	0.42
1:C:358:ASN:O	1:C:362:ARG:HG2	2.20	0.42
1:D:332:GLN:HE21	1:D:332:GLN:HB2	1.50	0.42
1:C:315:ILE:O	1:C:316:PRO:C	2.63	0.42
1:C:347:HIS:ND1	1:C:348:ASP:N	2.68	0.42
1:E:281:LEU:HD12	1:E:295:TYR:CE1	2.54	0.42
1:F:162:LEU:HD21	1:F:298:LEU:HD13	2.02	0.42
1:A:281:LEU:O	1:A:285:ILE:N	2.49	0.41
1:A:291:ARG:O	1:A:292:GLU:HB2	2.20	0.41
1:C:332:GLN:NE2	1:C:368:PRO:HG2	2.34	0.41
1:D:151:ILE:O	1:D:152:GLU:C	2.62	0.41
1:D:164:LEU:O	1:D:304:GLU:HB3	2.20	0.41
1:D:352:ASN:HB3	1:D:353:VAL:H	1.57	0.41
1:E:211:LYS:CD	1:E:216:GLY:HA2	2.50	0.41
1:F:273:VAL:HG12	1:F:274:ILE:N	2.35	0.41
1:A:188:PRO:HD2	1:A:231:GLY:HA3	2.02	0.41
1:B:257:CYS:HB3	1:B:267:ILE:O	2.20	0.41
1:B:344:MET:O	1:B:349:TRP:NE1	2.50	0.41
1:C:295:TYR:O	1:C:299:ASN:HB2	2.19	0.41
1:E:298:LEU:HA	1:E:298:LEU:HD23	1.74	0.41
1:E:309:ARG:HG2	1:E:348:ASP:HA	2.02	0.41
1:F:148:ARG:O	1:F:151:ILE:N	2.54	0.41
1:F:317:LEU:H	1:F:317:LEU:HG	1.45	0.41
1:F:347:HIS:ND1	1:F:348:ASP:N	2.66	0.41
1:A:135:SER:O	1:A:177:ASN:ND2	2.52	0.41
1:A:297:ARG:O	1:A:297:ARG:HG3	2.20	0.41
1:B:154:VAL:HG11	1:B:178:ILE:HD11	2.03	0.41
1:B:203:GLU:HA	1:B:207:PHE:CD1	2.56	0.41
1:C:268:LYS:HB2	3:C:547:HOH:O	2.19	0.41
1:C:325:ARG:HD2	1:C:325:ARG:HA	1.65	0.41
1:D:152:GLU:C	1:D:154:VAL:H	2.28	0.41
1:D:243:MET:HA	1:D:246:GLN:HB2	2.02	0.41
1:F:151:ILE:O	1:F:152:GLU:C	2.62	0.41
1:F:229:GLU:H	1:F:229:GLU:HG3	1.65	0.41
1:A:281:LEU:O	1:A:284:MET:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ILE:HD13	1:C:311:ARG:NH2	2.34	0.41
1:C:147:VAL:O	1:C:151:ILE:N	2.48	0.41
1:E:209:HIS:ND1	1:E:219:THR:O	2.53	0.41
1:A:233:LEU:HD22	1:A:234:PHE:H	1.85	0.41
1:A:351:GLY:HA3	1:A:355:GLU:HB2	2.01	0.41
1:B:334:ILE:HG22	1:B:368:PRO:HA	2.00	0.41
1:C:151:ILE:O	1:C:152:GLU:C	2.62	0.41
1:C:192:ILE:HG23	3:C:588:HOH:O	2.20	0.41
1:C:197:ILE:CG2	1:C:202:LEU:HD21	2.50	0.41
1:D:179:HIS:O	1:D:185:ARG:HG2	2.20	0.41
1:D:315:ILE:HD12	1:D:319:LEU:HD21	2.01	0.41
1:E:144:ILE:C	1:E:147:VAL:HG12	2.44	0.41
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.73	0.41
1:B:295:TYR:O	1:B:299:ASN:HB2	2.20	0.41
1:C:334:ILE:C	1:C:334:ILE:HD12	2.45	0.41
1:F:146:GLU:O	1:F:146:GLU:HG3	2.21	0.41
1:F:267:ILE:HG22	1:F:268:LYS:N	2.35	0.41
1:B:359:LEU:HD13	1:B:381:TYR:CZ	2.56	0.41
1:D:147:VAL:HG23	1:D:303:ILE:CD1	2.40	0.41
1:E:162:LEU:HG	1:E:298:LEU:O	2.21	0.41
1:E:263:GLY:O	1:E:264:ASN:HB2	2.21	0.41
1:E:282:GLU:HA	1:E:285:ILE:HG13	2.01	0.41
1:F:309:ARG:CG	1:F:348:ASP:HA	2.51	0.41
1:F:312:ILE:HG13	1:F:345:MET:CG	2.50	0.41
1:A:164:LEU:O	1:A:304:GLU:HB3	2.21	0.41
1:A:337:THR:HG22	1:A:338:PRO:N	2.36	0.41
1:C:174:VAL:HG22	1:C:305:MET:SD	2.60	0.41
1:D:151:ILE:CD1	2:D:405:EDO:H11	2.49	0.41
1:D:251:ARG:NH1	1:D:255:GLU:OE1	2.36	0.41
1:E:162:LEU:O	1:E:302:PRO:HA	2.21	0.41
1:E:337:THR:HG22	1:E:338:PRO:N	2.35	0.41
1:F:179:HIS:O	1:F:185:ARG:HG2	2.20	0.41
1:A:144:ILE:HD12	1:A:147:VAL:CG1	2.50	0.41
1:A:181:HIS:CE1	3:A:542:HOH:O	2.74	0.41
1:A:273:VAL:HG12	1:A:274:ILE:N	2.36	0.41
1:B:179:HIS:HE1	1:B:187:GLY:O	2.04	0.41
1:C:250:LEU:HD23	1:D:196:ALA:HB1	2.03	0.41
1:C:252:VAL:HG13	1:C:258:PHE:HB3	2.03	0.41
1:C:260:ARG:HD2	1:C:267:ILE:HD11	2.03	0.41
1:C:267:ILE:HG22	1:C:268:LYS:N	2.36	0.41
1:C:337:THR:HG21	1:C:373:ASP:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:TRP:CZ3	1:C:355:GLU:HB3	2.56	0.41
1:D:151:ILE:O	1:D:154:VAL:HG22	2.21	0.41
1:D:299:ASN:OD1	1:D:302:PRO:HB3	2.21	0.41
1:E:138:VAL:HG22	1:E:317:LEU:CD1	2.51	0.41
1:E:140:GLN:O	1:E:140:GLN:HG2	2.20	0.41
1:E:150:LEU:HD22	1:E:301:PHE:CZ	2.56	0.41
1:E:162:LEU:HD23	1:E:162:LEU:HA	1.83	0.41
1:E:270:ASN:HB3	3:E:577:HOH:O	2.21	0.41
1:E:281:LEU:O	1:E:284:MET:N	2.54	0.41
1:E:332:GLN:HE21	1:E:332:GLN:HB2	1.47	0.41
1:E:352:ASN:HB3	1:E:353:VAL:H	1.47	0.41
1:F:195:GLY:HA3	1:F:237:GLU:HB3	2.03	0.41
1:F:347:HIS:HB3	1:F:349:TRP:NE1	2.36	0.41
1:B:229:GLU:HA	1:B:271:VAL:CG1	2.51	0.41
1:C:162:LEU:HD23	1:C:162:LEU:HA	1.94	0.41
1:C:352:ASN:HB3	1:C:353:VAL:H	1.54	0.41
1:D:200:GLU:HG3	1:D:200:GLU:H	1.65	0.41
1:E:291:ARG:O	1:E:292:GLU:HB2	2.21	0.41
1:E:331:ALA:HB1	2:E:422:EDO:H22	2.03	0.41
1:F:301:PHE:HA	1:F:302:PRO:HD3	1.78	0.41
1:A:202:LEU:HD22	1:A:202:LEU:HA	1.91	0.40
1:A:384:SER:O	1:A:385:ASP:C	2.64	0.40
1:B:148:ARG:O	1:B:151:ILE:N	2.54	0.40
1:B:202:LEU:O	1:B:206:LEU:HD12	2.21	0.40
1:B:321:GLU:C	1:B:325:ARG:HD3	2.46	0.40
1:D:281:LEU:O	1:D:285:ILE:N	2.49	0.40
1:D:371:LEU:H	1:D:371:LEU:CD1	2.35	0.40
1:F:179:HIS:CE1	1:F:184:ARG:O	2.74	0.40
1:F:193:ASN:CG	1:F:236:ASP:HB3	2.46	0.40
1:F:308:LEU:HA	1:F:311:ARG:H	1.86	0.40
1:B:181:HIS:CE1	3:B:545:HOH:O	2.74	0.40
1:C:301:PHE:CZ	1:D:365:ILE:HD13	2.57	0.40
1:D:175:ALA:O	1:D:189:PHE:CE1	2.74	0.40
1:D:176:ARG:HG2	1:D:189:PHE:HE2	1.86	0.40
1:D:206:LEU:O	1:D:225:PHE:HB2	2.21	0.40
1:E:211:LYS:HD2	1:E:216:GLY:HA2	2.02	0.40
1:F:162:LEU:O	1:F:302:PRO:HA	2.20	0.40
1:F:260:ARG:HG2	1:F:261:VAL:N	2.36	0.40
1:A:144:ILE:O	1:A:147:VAL:HG12	2.21	0.40
1:B:224:ARG:HG2	1:B:224:ARG:H	1.60	0.40
1:B:273:VAL:HG12	1:B:274:ILE:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ASN:OD1	1:B:302:PRO:HB3	2.21	0.40
1:C:147:VAL:HG23	1:C:303:ILE:CD1	2.39	0.40
1:D:250:LEU:HD11	3:D:512:HOH:O	2.21	0.40
1:E:229:GLU:HA	1:E:271:VAL:HG11	2.04	0.40
1:F:207:PHE:HE2	1:F:252:VAL:HG22	1.87	0.40
1:F:211:LYS:CD	1:F:216:GLY:HA2	2.51	0.40
1:B:210:GLU:HG2	1:B:261:VAL:HG21	2.03	0.40
1:C:218:ILE:HD12	1:C:218:ILE:H	1.85	0.40
1:C:308:LEU:HA	1:C:311:ARG:CB	2.48	0.40
1:D:263:GLY:O	1:D:264:ASN:HB2	2.22	0.40
1:D:333:PRO:O	1:D:369:ASN:N	2.54	0.40
1:D:337:THR:HG21	1:D:373:ASP:OD1	2.21	0.40
1:F:234:PHE:CD1	1:F:274:ILE:HB	2.56	0.40
1:F:332:GLN:HA	1:F:333:PRO:HD3	1.77	0.40
1:A:195:GLY:HA3	1:A:237:GLU:O	2.22	0.40
1:C:148:ARG:O	1:C:151:ILE:N	2.55	0.40
1:C:312:ILE:HG13	1:C:345:MET:CG	2.52	0.40
1:C:347:HIS:HB3	1:C:349:TRP:CE2	2.57	0.40
1:D:144:ILE:HD13	1:D:311:ARG:HH21	1.85	0.40
1:D:203:GLU:HG3	3:D:567:HOH:O	2.21	0.40
1:D:204:SER:C	1:D:206:LEU:N	2.79	0.40
1:D:281:LEU:HD12	1:D:295:TYR:HE1	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	257/259 (99%)	213 (83%)	32 (12%)	12 (5%)	2	14
1	B	257/259 (99%)	215 (84%)	29 (11%)	13 (5%)	1	13
1	C	257/259 (99%)	214 (83%)	31 (12%)	12 (5%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	257/259 (99%)	214 (83%)	31 (12%)	12 (5%)	2	14
1	E	257/259 (99%)	215 (84%)	30 (12%)	12 (5%)	2	14
1	F	257/259 (99%)	217 (84%)	25 (10%)	15 (6%)	1	10
All	All	1542/1554 (99%)	1288 (84%)	178 (12%)	76 (5%)	1	13

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	PRO
1	A	263	GLY
1	A	288	GLN
1	A	328	ALA
1	B	263	GLY
1	B	288	GLN
1	B	328	ALA
1	C	191	PRO
1	C	263	GLY
1	C	288	GLN
1	C	328	ALA
1	D	191	PRO
1	D	263	GLY
1	D	288	GLN
1	D	328	ALA
1	D	333	PRO
1	E	191	PRO
1	E	263	GLY
1	E	288	GLN
1	E	328	ALA
1	F	191	PRO
1	F	263	GLY
1	F	288	GLN
1	F	328	ALA
1	A	136	HIS
1	A	333	PRO
1	A	369	ASN
1	B	136	HIS
1	B	215	THR
1	B	333	PRO
1	B	369	ASN
1	C	369	ASN
1	D	136	HIS

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Mol	Chain	Res	Type
1	E	136	HIS
1	E	215	THR
1	E	333	PRO
1	E	369	ASN
1	F	215	THR
1	F	369	ASN
1	A	132	PRO
1	A	215	THR
1	A	242	PRO
1	A	302	PRO
1	A	306	PRO
1	B	191	PRO
1	B	306	PRO
1	C	132	PRO
1	C	136	HIS
1	C	242	PRO
1	C	302	PRO
1	D	132	PRO
1	D	215	THR
1	D	242	PRO
1	D	306	PRO
1	D	369	ASN
1	E	132	PRO
1	E	242	PRO
1	E	302	PRO
1	E	306	PRO
1	F	132	PRO
1	F	136	HIS
1	F	242	PRO
1	F	306	PRO
1	B	132	PRO
1	B	242	PRO
1	C	215	THR
1	C	306	PRO
1	F	302	PRO
1	F	339	ARG
1	F	372	VAL
1	B	302	PRO
1	B	372	VAL
1	D	302	PRO
1	F	333	PRO
1	F	338	PRO

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Mol	Chain	Res	Type
1	C	333	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	220/220 (100%)	147 (67%)	73 (33%)	0	1
1	B	220/220 (100%)	150 (68%)	70 (32%)	0	1
1	C	220/220 (100%)	149 (68%)	71 (32%)	0	1
1	D	220/220 (100%)	155 (70%)	65 (30%)	0	1
1	E	220/220 (100%)	150 (68%)	70 (32%)	0	1
1	F	220/220 (100%)	150 (68%)	70 (32%)	0	1
All	All	1320/1320 (100%)	901 (68%)	419 (32%)	0	1

All (419) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	LEU
1	A	133	ARG
1	A	136	HIS
1	A	152	GLU
1	A	153	GLN
1	A	156	THR
1	A	162	LEU
1	A	169	THR
1	A	171	LYS
1	A	173	VAL
1	A	174	VAL
1	A	178	ILE
1	A	179	HIS
1	A	200	GLU
1	A	201	LEU
1	A	202	LEU
1	A	203	GLU

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Mol	Chain	Res	Type
1	A	204	SER
1	A	205	GLU
1	A	206	LEU
1	A	218	ILE
1	A	224	ARG
1	A	226	GLU
1	A	227	LEU
1	A	233	LEU
1	A	235	LEU
1	A	241	MET
1	A	243	MET
1	A	245	MET
1	A	250	LEU
1	A	252	VAL
1	A	253	LEU
1	A	254	GLN
1	A	255	GLU
1	A	259	GLU
1	A	261	VAL
1	A	265	SER
1	A	266	THR
1	A	268	LYS
1	A	271	VAL
1	A	277	THR
1	A	285	ILE
1	A	288	GLN
1	A	290	PHE
1	A	291	ARG
1	A	292	GLU
1	A	295	TYR
1	A	297	ARG
1	A	301	PHE
1	A	303	ILE
1	A	305	MET
1	A	308	LEU
1	A	309	ARG
1	A	311	ARG
1	A	312	ILE
1	A	313	ASP
1	A	315	ILE
1	A	317	LEU
1	A	320	GLN

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Mol	Chain	Res	Type
1	A	323	MET
1	A	324	THR
1	A	326	MET
1	A	332	GLN
1	A	337	THR
1	A	339	ARG
1	A	361	GLU
1	A	365	ILE
1	A	371	LEU
1	A	379	THR
1	A	381	TYR
1	A	382	ARG
1	A	383	TYR
1	A	384	SER
1	B	130	LEU
1	B	133	ARG
1	B	136	HIS
1	B	146	GLU
1	B	152	GLU
1	B	153	GLN
1	B	155	SER
1	B	156	THR
1	B	162	LEU
1	B	164	LEU
1	B	169	THR
1	B	173	VAL
1	B	174	VAL
1	B	178	ILE
1	B	179	HIS
1	B	200	GLU
1	B	201	LEU
1	B	203	GLU
1	B	204	SER
1	B	205	GLU
1	B	207	PHE
1	B	210	GLU
1	B	218	ILE
1	B	226	GLU
1	B	227	LEU
1	B	233	LEU
1	B	235	LEU
1	B	241	MET

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Mol	Chain	Res	Type
1	B	243	MET
1	B	245	MET
1	B	250	LEU
1	B	252	VAL
1	B	253	LEU
1	B	254	GLN
1	B	255	GLU
1	B	259	GLU
1	B	261	VAL
1	B	265	SER
1	B	266	THR
1	B	268	LYS
1	B	277	THR
1	B	285	ILE
1	B	288	GLN
1	B	290	PHE
1	B	292	GLU
1	B	295	TYR
1	B	297	ARG
1	B	301	PHE
1	B	303	ILE
1	B	305	MET
1	B	308	LEU
1	B	309	ARG
1	B	311	ARG
1	B	312	ILE
1	B	315	ILE
1	B	317	LEU
1	B	320	GLN
1	B	323	MET
1	B	324	THR
1	B	326	MET
1	B	337	THR
1	B	339	ARG
1	B	361	GLU
1	B	365	ILE
1	B	371	LEU
1	B	372	VAL
1	B	379	THR
1	B	381	TYR
1	B	382	ARG
1	B	383	TYR

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Mol	Chain	Res	Type
1	C	130	LEU
1	C	133	ARG
1	C	136	HIS
1	C	152	GLU
1	C	153	GLN
1	C	155	SER
1	C	156	THR
1	C	162	LEU
1	C	164	LEU
1	C	169	THR
1	C	171	LYS
1	C	173	VAL
1	C	174	VAL
1	C	178	ILE
1	C	200	GLU
1	C	201	LEU
1	C	202	LEU
1	C	203	GLU
1	C	205	GLU
1	C	206	LEU
1	C	210	GLU
1	C	215	THR
1	C	224	ARG
1	C	226	GLU
1	C	233	LEU
1	C	235	LEU
1	C	238	ILE
1	C	241	MET
1	C	243	MET
1	C	245	MET
1	C	252	VAL
1	C	253	LEU
1	C	254	GLN
1	C	255	GLU
1	C	259	GLU
1	C	261	VAL
1	C	265	SER
1	C	266	THR
1	C	268	LYS
1	C	277	THR
1	C	285	ILE
1	C	286	ASP

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Mol	Chain	Res	Type
1	C	288	GLN
1	C	290	PHE
1	C	292	GLU
1	C	295	TYR
1	C	297	ARG
1	C	301	PHE
1	C	303	ILE
1	C	305	MET
1	C	308	LEU
1	C	309	ARG
1	C	311	ARG
1	C	312	ILE
1	C	315	ILE
1	C	317	LEU
1	C	318	LEU
1	C	320	GLN
1	C	323	MET
1	C	324	THR
1	C	326	MET
1	C	337	THR
1	C	339	ARG
1	C	365	ILE
1	C	371	LEU
1	C	372	VAL
1	C	379	THR
1	C	381	TYR
1	C	382	ARG
1	C	383	TYR
1	C	384	SER
1	D	130	LEU
1	D	133	ARG
1	D	136	HIS
1	D	152	GLU
1	D	153	GLN
1	D	156	THR
1	D	162	LEU
1	D	169	THR
1	D	171	LYS
1	D	173	VAL
1	D	174	VAL
1	D	178	ILE
1	D	179	HIS

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Mol	Chain	Res	Type
1	D	200	GLU
1	D	201	LEU
1	D	202	LEU
1	D	203	GLU
1	D	204	SER
1	D	205	GLU
1	D	218	ILE
1	D	224	ARG
1	D	226	GLU
1	D	227	LEU
1	D	233	LEU
1	D	235	LEU
1	D	241	MET
1	D	243	MET
1	D	245	MET
1	D	252	VAL
1	D	253	LEU
1	D	254	GLN
1	D	255	GLU
1	D	259	GLU
1	D	261	VAL
1	D	265	SER
1	D	266	THR
1	D	268	LYS
1	D	271	VAL
1	D	277	THR
1	D	285	ILE
1	D	288	GLN
1	D	290	PHE
1	D	292	GLU
1	D	295	TYR
1	D	301	PHE
1	D	303	ILE
1	D	305	MET
1	D	308	LEU
1	D	309	ARG
1	D	311	ARG
1	D	312	ILE
1	D	315	ILE
1	D	317	LEU
1	D	320	GLN
1	D	323	MET

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Mol	Chain	Res	Type
1	D	324	THR
1	D	326	MET
1	D	332	GLN
1	D	337	THR
1	D	365	ILE
1	D	371	LEU
1	D	372	VAL
1	D	379	THR
1	D	381	TYR
1	D	383	TYR
1	E	130	LEU
1	E	133	ARG
1	E	136	HIS
1	E	146	GLU
1	E	152	GLU
1	E	153	GLN
1	E	155	SER
1	E	156	THR
1	E	162	LEU
1	E	169	THR
1	E	171	LYS
1	E	173	VAL
1	E	174	VAL
1	E	178	ILE
1	E	179	HIS
1	E	200	GLU
1	E	201	LEU
1	E	203	GLU
1	E	205	GLU
1	E	218	ILE
1	E	224	ARG
1	E	226	GLU
1	E	227	LEU
1	E	233	LEU
1	E	235	LEU
1	E	240	ASP
1	E	241	MET
1	E	243	MET
1	E	245	MET
1	E	250	LEU
1	E	251	ARG
1	E	252	VAL

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Mol	Chain	Res	Type
1	E	253	LEU
1	E	254	GLN
1	E	255	GLU
1	E	259	GLU
1	E	261	VAL
1	E	265	SER
1	E	266	THR
1	E	268	LYS
1	E	271	VAL
1	E	277	THR
1	E	285	ILE
1	E	288	GLN
1	E	290	PHE
1	E	292	GLU
1	E	295	TYR
1	E	297	ARG
1	E	301	PHE
1	E	303	ILE
1	E	305	MET
1	E	308	LEU
1	E	309	ARG
1	E	311	ARG
1	E	312	ILE
1	E	315	ILE
1	E	317	LEU
1	E	320	GLN
1	E	323	MET
1	E	324	THR
1	E	325	ARG
1	E	326	MET
1	E	332	GLN
1	E	339	ARG
1	E	348	ASP
1	E	365	ILE
1	E	371	LEU
1	E	379	THR
1	E	381	TYR
1	E	383	TYR
1	F	130	LEU
1	F	133	ARG
1	F	136	HIS
1	F	152	GLU

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Mol	Chain	Res	Type
1	F	153	GLN
1	F	155	SER
1	F	156	THR
1	F	162	LEU
1	F	164	LEU
1	F	169	THR
1	F	171	LYS
1	F	173	VAL
1	F	174	VAL
1	F	178	ILE
1	F	179	HIS
1	F	182	SER
1	F	200	GLU
1	F	201	LEU
1	F	203	GLU
1	F	205	GLU
1	F	206	LEU
1	F	224	ARG
1	F	226	GLU
1	F	227	LEU
1	F	233	LEU
1	F	235	LEU
1	F	241	MET
1	F	243	MET
1	F	245	MET
1	F	248	LYS
1	F	252	VAL
1	F	253	LEU
1	F	254	GLN
1	F	255	GLU
1	F	259	GLU
1	F	261	VAL
1	F	265	SER
1	F	266	THR
1	F	268	LYS
1	F	271	VAL
1	F	277	THR
1	F	285	ILE
1	F	288	GLN
1	F	290	PHE
1	F	292	GLU
1	F	295	TYR

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Mol	Chain	Res	Type
1	F	297	ARG
1	F	301	PHE
1	F	305	MET
1	F	308	LEU
1	F	309	ARG
1	F	311	ARG
1	F	312	ILE
1	F	315	ILE
1	F	317	LEU
1	F	318	LEU
1	F	320	GLN
1	F	323	MET
1	F	324	THR
1	F	326	MET
1	F	337	THR
1	F	348	ASP
1	F	365	ILE
1	F	371	LEU
1	F	372	VAL
1	F	379	THR
1	F	381	TYR
1	F	382	ARG
1	F	383	TYR
1	F	384	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	HIS
1	A	160	ASN
1	A	177	ASN
1	A	181	HIS
1	A	254	GLN
1	A	264	ASN
1	A	270	ASN
1	A	288	GLN
1	A	332	GLN
1	B	136	HIS
1	B	145	GLN
1	B	181	HIS
1	B	264	ASN
1	B	270	ASN

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Mol	Chain	Res	Type
1	B	288	GLN
1	C	136	HIS
1	C	145	GLN
1	C	160	ASN
1	C	177	ASN
1	C	181	HIS
1	C	254	GLN
1	C	264	ASN
1	C	270	ASN
1	C	288	GLN
1	C	332	GLN
1	D	136	HIS
1	D	140	GLN
1	D	145	GLN
1	D	160	ASN
1	D	177	ASN
1	D	181	HIS
1	D	254	GLN
1	D	270	ASN
1	D	332	GLN
1	E	136	HIS
1	E	140	GLN
1	E	145	GLN
1	E	160	ASN
1	E	177	ASN
1	E	181	HIS
1	E	264	ASN
1	E	270	ASN
1	E	288	GLN
1	E	332	GLN
1	F	136	HIS
1	F	145	GLN
1	F	153	GLN
1	F	160	ASN
1	F	177	ASN
1	F	181	HIS
1	F	254	GLN
1	F	270	ASN
1	F	332	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 ⓘ

260 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	$\# Z > 2$
2	EDO	F	405	-	3,3,3	0.42	0	2,2,2	0.37	0
2	EDO	F	428	-	3,3,3	0.55	0	2,2,2	0.17	0
2	EDO	E	434	-	3,3,3	0.77	0	2,2,2	0.30	0
2	EDO	B	447	-	3,3,3	0.42	0	2,2,2	0.37	0
2	EDO	F	444	-	3,3,3	0.42	0	2,2,2	0.40	0
2	EDO	E	445	-	3,3,3	0.55	0	2,2,2	0.21	0
2	EDO	A	440	-	3,3,3	0.49	0	2,2,2	0.30	0
2	EDO	B	408	-	3,3,3	0.56	0	2,2,2	0.02	0
2	EDO	F	423	-	3,3,3	0.64	0	2,2,2	0.24	0
2	EDO	B	443	-	3,3,3	0.50	0	2,2,2	0.21	0
2	EDO	A	438	-	3,3,3	0.42	0	2,2,2	0.40	0
2	EDO	A	408	-	3,3,3	0.46	0	2,2,2	0.74	0
2	EDO	C	419	-	3,3,3	0.52	0	2,2,2	0.18	0
2	EDO	A	416	-	3,3,3	0.48	0	2,2,2	0.26	0
2	EDO	A	423	-	3,3,3	0.58	0	2,2,2	0.13	0
2	EDO	E	402	-	3,3,3	0.44	0	2,2,2	0.37	0
2	EDO	C	436	-	3,3,3	0.45	0	2,2,2	0.47	0
2	EDO	E	426	-	3,3,3	0.44	0	2,2,2	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	F	419	-	3,3,3	0.50	0	2,2,2	0.15	0
2	EDO	A	424	-	3,3,3	0.44	0	2,2,2	0.53	0
2	EDO	D	433	-	3,3,3	0.41	0	2,2,2	0.40	0
2	EDO	B	445	-	3,3,3	0.58	0	2,2,2	0.11	0
2	EDO	E	431	-	3,3,3	0.49	0	2,2,2	0.28	0
2	EDO	F	413	-	3,3,3	0.54	0	2,2,2	0.12	0
2	EDO	A	413	-	3,3,3	0.61	0	2,2,2	0.18	0
2	EDO	D	417	-	3,3,3	0.54	0	2,2,2	0.19	0
2	EDO	E	432	-	3,3,3	0.38	0	2,2,2	0.44	0
2	EDO	A	418	-	3,3,3	0.54	0	2,2,2	0.20	0
2	EDO	B	435	-	3,3,3	0.38	0	2,2,2	0.50	0
2	EDO	C	408	-	3,3,3	0.48	0	2,2,2	0.27	0
2	EDO	C	438	-	3,3,3	0.58	0	2,2,2	0.40	0
2	EDO	E	403	-	3,3,3	0.48	0	2,2,2	0.29	0
2	EDO	E	436	-	3,3,3	0.44	0	2,2,2	0.47	0
2	EDO	E	437	-	3,3,3	0.52	0	2,2,2	0.17	0
2	EDO	C	424	-	3,3,3	0.54	0	2,2,2	0.21	0
2	EDO	E	447	-	3,3,3	0.52	0	2,2,2	0.23	0
2	EDO	A	412	-	3,3,3	0.43	0	2,2,2	0.41	0
2	EDO	C	413	-	3,3,3	0.49	0	2,2,2	0.14	0
2	EDO	B	430	-	3,3,3	0.57	0	2,2,2	0.08	0
2	EDO	E	420	-	3,3,3	0.43	0	2,2,2	0.50	0
2	EDO	D	410	-	3,3,3	0.37	0	2,2,2	0.54	0
2	EDO	E	413	-	3,3,3	0.46	0	2,2,2	0.39	0
2	EDO	E	438	-	3,3,3	0.72	0	2,2,2	0.15	0
2	EDO	E	418	-	3,3,3	0.58	0	2,2,2	0.08	0
2	EDO	F	414	-	3,3,3	0.42	0	2,2,2	0.33	0
2	EDO	A	427	-	3,3,3	0.37	0	2,2,2	0.54	0
2	EDO	C	410	-	3,3,3	0.49	0	2,2,2	0.65	0
2	EDO	F	436	-	3,3,3	0.56	0	2,2,2	0.26	0
2	EDO	A	431	-	3,3,3	0.49	0	2,2,2	0.28	0
2	EDO	C	430	-	3,3,3	0.50	0	2,2,2	0.16	0
2	EDO	F	416	-	3,3,3	0.40	0	2,2,2	0.83	0
2	EDO	D	439	-	3,3,3	0.53	0	2,2,2	0.30	0
2	EDO	E	446	-	3,3,3	0.54	0	2,2,2	0.17	0
2	EDO	F	422	-	3,3,3	0.58	0	2,2,2	0.14	0
2	EDO	B	428	-	3,3,3	0.45	0	2,2,2	0.28	0
2	EDO	A	422	-	3,3,3	0.45	0	2,2,2	0.40	0
2	EDO	E	444	-	3,3,3	0.51	0	2,2,2	0.19	0
2	EDO	B	444	-	3,3,3	0.52	0	2,2,2	0.26	0
2	EDO	A	409	-	3,3,3	0.40	0	2,2,2	0.33	0
2	EDO	C	416	-	3,3,3	0.59	0	2,2,2	0.26	0
2	EDO	C	431	-	3,3,3	0.48	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	429	-	3,3,3	0.47	0	2,2,2	0.27	0
2	EDO	F	438	-	3,3,3	0.49	0	2,2,2	0.10	0
2	EDO	D	422	-	3,3,3	0.52	0	2,2,2	0.12	0
2	EDO	A	437	-	3,3,3	0.51	0	2,2,2	0.20	0
2	EDO	C	422	-	3,3,3	0.39	0	2,2,2	0.68	0
2	EDO	C	432	-	3,3,3	0.55	0	2,2,2	0.18	0
2	EDO	D	428	-	3,3,3	0.47	0	2,2,2	0.31	0
2	EDO	C	425	-	3,3,3	0.43	0	2,2,2	0.47	0
2	EDO	C	429	-	3,3,3	0.65	0	2,2,2	0.42	0
2	EDO	C	437	-	3,3,3	0.57	0	2,2,2	0.09	0
2	EDO	C	412	-	3,3,3	0.46	0	2,2,2	0.41	0
2	EDO	B	404	-	3,3,3	0.42	0	2,2,2	0.44	0
2	EDO	B	431	-	3,3,3	0.50	0	2,2,2	0.19	0
2	EDO	F	442	-	3,3,3	0.51	0	2,2,2	0.32	0
2	EDO	B	438	-	3,3,3	0.54	0	2,2,2	0.07	0
2	EDO	B	422	-	3,3,3	0.53	0	2,2,2	0.24	0
2	EDO	F	410	-	3,3,3	0.43	0	2,2,2	0.41	0
2	EDO	F	441	-	3,3,3	0.49	0	2,2,2	0.29	0
2	EDO	A	404	-	3,3,3	0.61	0	2,2,2	0.11	0
2	EDO	A	410	-	3,3,3	0.46	0	2,2,2	0.48	0
2	EDO	B	409	-	3,3,3	0.32	0	2,2,2	0.65	0
2	EDO	B	423	-	3,3,3	0.44	0	2,2,2	0.57	0
2	EDO	D	416	-	3,3,3	0.65	0	2,2,2	0.25	0
2	EDO	D	411	-	3,3,3	0.45	0	2,2,2	0.77	0
2	EDO	E	401	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	D	406	-	3,3,3	0.56	0	2,2,2	0.19	0
2	EDO	B	442	-	3,3,3	0.47	0	2,2,2	0.30	0
2	EDO	C	427	-	3,3,3	0.45	0	2,2,2	0.36	0
2	EDO	D	404	-	3,3,3	0.50	0	2,2,2	0.24	0
2	EDO	E	435	-	3,3,3	0.49	0	2,2,2	0.21	0
2	EDO	B	418	-	3,3,3	0.48	0	2,2,2	0.27	0
2	EDO	C	404	-	3,3,3	0.41	0	2,2,2	0.50	0
2	EDO	F	408	-	3,3,3	0.53	0	2,2,2	0.24	0
2	EDO	A	426	-	3,3,3	0.47	0	2,2,2	0.47	0
2	EDO	F	439	-	3,3,3	0.59	0	2,2,2	0.12	0
2	EDO	A	402	-	3,3,3	0.39	0	2,2,2	0.51	0
2	EDO	D	438	-	3,3,3	0.47	0	2,2,2	0.16	0
2	EDO	E	414	-	3,3,3	0.60	0	2,2,2	0.11	0
2	EDO	A	443	-	3,3,3	0.55	0	2,2,2	0.12	0
2	EDO	F	404	-	3,3,3	0.71	0	2,2,2	0.17	0
2	EDO	D	423	-	3,3,3	0.57	0	2,2,2	0.20	0
2	EDO	F	418	-	3,3,3	0.50	0	2,2,2	0.32	0
2	EDO	F	443	-	3,3,3	0.50	0	2,2,2	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	F	432	-	3,3,3	0.44	0	2,2,2	0.53	0
2	EDO	A	421	-	3,3,3	0.43	0	2,2,2	0.60	0
2	EDO	A	430	-	3,3,3	0.44	0	2,2,2	0.50	0
2	EDO	A	432	-	3,3,3	0.76	0	2,2,2	0.26	0
2	EDO	F	403	-	3,3,3	0.56	0	2,2,2	0.09	0
2	EDO	E	440	-	3,3,3	0.48	0	2,2,2	0.15	0
2	EDO	D	402	-	3,3,3	0.51	0	2,2,2	0.25	0
2	EDO	E	411	-	3,3,3	0.50	0	2,2,2	0.27	0
2	EDO	E	415	-	3,3,3	0.52	0	2,2,2	0.26	0
2	EDO	C	402	-	3,3,3	0.55	0	2,2,2	0.14	0
2	EDO	F	412	-	3,3,3	0.52	0	2,2,2	0.18	0
2	EDO	B	439	-	3,3,3	0.46	0	2,2,2	0.21	0
2	EDO	B	424	-	3,3,3	0.44	0	2,2,2	0.43	0
2	EDO	A	417	-	3,3,3	0.41	0	2,2,2	0.41	0
2	EDO	F	417	-	3,3,3	0.42	0	2,2,2	0.29	0
2	EDO	B	413	-	3,3,3	0.60	0	2,2,2	0.05	0
2	EDO	F	401	-	3,3,3	0.44	0	2,2,2	0.32	0
2	EDO	B	433	-	3,3,3	0.56	0	2,2,2	0.11	0
2	EDO	F	420	-	3,3,3	0.47	0	2,2,2	0.31	0
2	EDO	A	439	-	3,3,3	0.58	0	2,2,2	0.06	0
2	EDO	D	427	-	3,3,3	0.43	0	2,2,2	0.54	0
2	EDO	E	433	-	3,3,3	0.55	0	2,2,2	0.04	0
2	EDO	F	434	-	3,3,3	0.47	0	2,2,2	0.22	0
2	EDO	B	426	-	3,3,3	0.48	0	2,2,2	0.46	0
2	EDO	B	402	-	3,3,3	0.53	0	2,2,2	0.29	0
2	EDO	E	441	-	3,3,3	0.39	0	2,2,2	0.66	0
2	EDO	C	421	-	3,3,3	0.59	0	2,2,2	0.18	0
2	EDO	A	403	-	3,3,3	0.53	0	2,2,2	0.35	0
2	EDO	D	425	-	3,3,3	0.43	0	2,2,2	0.41	0
2	EDO	E	409	-	3,3,3	0.33	0	2,2,2	0.67	0
2	EDO	F	425	-	3,3,3	0.46	0	2,2,2	0.33	0
2	EDO	B	432	-	3,3,3	0.49	0	2,2,2	0.41	0
2	EDO	D	429	-	3,3,3	0.46	0	2,2,2	0.33	0
2	EDO	E	408	-	3,3,3	0.56	0	2,2,2	0.05	0
2	EDO	E	439	-	3,3,3	0.39	0	2,2,2	0.48	0
2	EDO	F	402	-	3,3,3	0.44	0	2,2,2	0.31	0
2	EDO	B	403	-	3,3,3	0.51	0	2,2,2	0.28	0
2	EDO	D	436	-	3,3,3	0.52	0	2,2,2	0.18	0
2	EDO	C	423	-	3,3,3	0.45	0	2,2,2	0.41	0
2	EDO	E	427	-	3,3,3	0.64	0	2,2,2	0.01	0
2	EDO	D	403	-	3,3,3	0.52	0	2,2,2	0.04	0
2	EDO	E	442	-	3,3,3	0.52	0	2,2,2	0.18	0
2	EDO	B	427	-	3,3,3	0.46	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	412	-	3,3,3	0.45	0	2,2,2	0.44	0
2	EDO	E	443	-	3,3,3	0.54	0	2,2,2	0.27	0
2	EDO	F	424	-	3,3,3	0.46	0	2,2,2	0.28	0
2	EDO	C	426	-	3,3,3	0.46	0	2,2,2	0.29	0
2	EDO	A	435	-	3,3,3	0.55	0	2,2,2	0.14	0
2	EDO	E	419	-	3,3,3	0.54	0	2,2,2	0.15	0
2	EDO	B	420	-	3,3,3	0.50	0	2,2,2	0.26	0
2	EDO	D	407	-	3,3,3	0.59	0	2,2,2	0.08	0
2	EDO	E	425	-	3,3,3	0.42	0	2,2,2	0.66	0
2	EDO	D	413	-	3,3,3	0.44	0	2,2,2	0.50	0
2	EDO	A	420	-	3,3,3	0.59	0	2,2,2	0.16	0
2	EDO	F	421	-	3,3,3	0.59	0	2,2,2	0.18	0
2	EDO	B	429	-	3,3,3	0.38	0	2,2,2	0.49	0
2	EDO	A	442	-	3,3,3	0.42	0	2,2,2	0.57	0
2	EDO	A	414	-	3,3,3	0.53	0	2,2,2	0.17	0
2	EDO	B	415	-	3,3,3	0.55	0	2,2,2	0.01	0
2	EDO	D	434	-	3,3,3	0.46	0	2,2,2	0.42	0
2	EDO	F	415	-	3,3,3	0.33	0	2,2,2	0.55	0
2	EDO	B	446	-	3,3,3	0.50	0	2,2,2	0.35	0
2	EDO	B	416	-	3,3,3	0.59	0	2,2,2	0.07	0
2	EDO	A	415	-	3,3,3	0.55	0	2,2,2	0.08	0
2	EDO	E	416	-	3,3,3	0.61	0	2,2,2	0.16	0
2	EDO	D	408	-	3,3,3	0.52	0	2,2,2	0.17	0
2	EDO	D	430	-	3,3,3	0.34	0	2,2,2	0.64	0
2	EDO	E	428	-	3,3,3	0.49	0	2,2,2	0.21	0
2	EDO	D	424	-	3,3,3	0.43	0	2,2,2	0.63	0
2	EDO	C	403	-	3,3,3	0.50	0	2,2,2	0.30	0
2	EDO	E	404	-	3,3,3	0.33	0	2,2,2	0.71	0
2	EDO	C	411	-	3,3,3	0.49	0	2,2,2	0.21	0
2	EDO	C	417	-	3,3,3	0.54	0	2,2,2	0.14	0
2	EDO	B	441	-	3,3,3	0.49	0	2,2,2	0.37	0
2	EDO	C	409	-	3,3,3	0.35	0	2,2,2	0.67	0
2	EDO	B	419	-	3,3,3	0.50	0	2,2,2	0.28	0
2	EDO	B	405	-	3,3,3	0.47	0	2,2,2	0.27	0
2	EDO	A	441	-	3,3,3	0.35	0	2,2,2	0.59	0
2	EDO	B	414	-	3,3,3	0.49	0	2,2,2	0.28	0
2	EDO	F	409	-	3,3,3	0.51	0	2,2,2	0.33	0
2	EDO	A	419	-	3,3,3	0.56	0	2,2,2	0.02	0
2	EDO	E	424	-	3,3,3	0.63	0	2,2,2	0.07	0
2	EDO	B	407	-	3,3,3	0.57	0	2,2,2	0.17	0
2	EDO	F	431	-	3,3,3	0.48	0	2,2,2	0.26	0
2	EDO	F	437	-	3,3,3	0.40	0	2,2,2	0.68	0
2	EDO	E	406	-	3,3,3	0.58	0	2,2,2	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	F	407	-	3,3,3	0.56	0	2,2,2	0.24	0
2	EDO	C	420	-	3,3,3	0.52	0	2,2,2	0.18	0
2	EDO	A	407	-	3,3,3	0.37	0	2,2,2	0.56	0
2	EDO	D	415	-	3,3,3	0.38	0	2,2,2	0.49	0
2	EDO	E	412	-	3,3,3	0.43	0	2,2,2	0.26	0
2	EDO	F	433	-	3,3,3	0.43	0	2,2,2	0.35	0
2	EDO	B	401	-	3,3,3	0.56	0	2,2,2	0.16	0
2	EDO	B	417	-	3,3,3	0.53	0	2,2,2	0.10	0
2	EDO	C	414	-	3,3,3	0.43	0	2,2,2	0.36	0
2	EDO	A	433	-	3,3,3	0.42	0	2,2,2	0.46	0
2	EDO	A	401	-	3,3,3	0.53	0	2,2,2	0.30	0
2	EDO	C	415	-	3,3,3	0.61	0	2,2,2	0.16	0
2	EDO	D	432	-	3,3,3	0.47	0	2,2,2	0.36	0
2	EDO	F	430	-	3,3,3	0.45	0	2,2,2	0.43	0
2	EDO	F	411	-	3,3,3	0.46	0	2,2,2	0.40	0
2	EDO	B	406	-	3,3,3	0.61	0	2,2,2	0.05	0
2	EDO	A	411	-	3,3,3	0.56	0	2,2,2	0.13	0
2	EDO	F	406	-	3,3,3	0.57	0	2,2,2	0.17	0
2	EDO	B	440	-	3,3,3	2.11	2 (66%)	2,2,2	1.17	0
2	EDO	F	445	-	3,3,3	0.51	0	2,2,2	0.25	0
2	EDO	D	401	-	3,3,3	0.56	0	2,2,2	0.20	0
2	EDO	D	412	-	3,3,3	0.46	0	2,2,2	0.15	0
2	EDO	E	417	-	3,3,3	0.56	0	2,2,2	0.18	0
2	EDO	D	420	-	3,3,3	0.54	0	2,2,2	0.09	0
2	EDO	E	423	-	3,3,3	0.55	0	2,2,2	0.10	0
2	EDO	D	414	-	3,3,3	0.51	0	2,2,2	0.16	0
2	EDO	A	425	-	3,3,3	0.46	0	2,2,2	0.31	0
2	EDO	E	429	-	3,3,3	0.42	0	2,2,2	0.54	0
2	EDO	A	434	-	3,3,3	0.59	0	2,2,2	0.15	0
2	EDO	E	410	-	3,3,3	0.42	0	2,2,2	0.75	0
2	EDO	B	411	-	3,3,3	0.43	0	2,2,2	0.26	0
2	EDO	C	407	-	3,3,3	0.47	0	2,2,2	0.31	0
2	EDO	F	427	-	3,3,3	0.53	0	2,2,2	0.14	0
2	EDO	D	409	-	3,3,3	0.51	0	2,2,2	0.20	0
2	EDO	C	434	-	3,3,3	0.46	0	2,2,2	0.28	0
2	EDO	B	421	-	3,3,3	0.51	0	2,2,2	0.19	0
2	EDO	D	405	-	3,3,3	0.39	0	2,2,2	0.46	0
2	EDO	F	426	-	3,3,3	0.49	0	2,2,2	0.24	0
2	EDO	C	433	-	3,3,3	0.80	0	2,2,2	0.29	0
2	EDO	D	418	-	3,3,3	0.56	0	2,2,2	0.15	0
2	EDO	F	440	-	3,3,3	0.49	0	2,2,2	0.20	0
2	EDO	D	437	-	3,3,3	0.58	0	2,2,2	0.25	0
2	EDO	E	407	-	3,3,3	0.49	0	2,2,2	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	428	-	3,3,3	0.59	0	2,2,2	0.08	0
2	EDO	C	401	-	3,3,3	0.60	0	2,2,2	0.24	0
2	EDO	B	436	-	3,3,3	0.53	0	2,2,2	0.20	0
2	EDO	C	435	-	3,3,3	0.44	0	2,2,2	0.43	0
2	EDO	D	421	-	3,3,3	0.51	0	2,2,2	0.25	0
2	EDO	F	429	-	3,3,3	0.42	0	2,2,2	0.64	0
2	EDO	F	435	-	3,3,3	0.33	0	2,2,2	0.56	0
2	EDO	D	435	-	3,3,3	0.59	0	2,2,2	0.17	0
2	EDO	B	425	-	3,3,3	0.53	0	2,2,2	0.24	0
2	EDO	A	436	-	3,3,3	0.43	0	2,2,2	0.39	0
2	EDO	E	422	-	3,3,3	0.46	0	2,2,2	0.31	0
2	EDO	C	406	-	3,3,3	0.54	0	2,2,2	0.05	0
2	EDO	D	431	-	3,3,3	0.68	0	2,2,2	0.49	0
2	EDO	E	405	-	3,3,3	0.52	0	2,2,2	0.22	0
2	EDO	D	419	-	3,3,3	0.61	0	2,2,2	0.04	0
2	EDO	E	430	-	3,3,3	0.44	0	2,2,2	0.33	0
2	EDO	C	428	-	3,3,3	0.34	0	2,2,2	0.56	0
2	EDO	E	421	-	3,3,3	0.44	0	2,2,2	0.33	0
2	EDO	A	405	-	3,3,3	0.57	0	2,2,2	0.03	0
2	EDO	A	406	-	3,3,3	0.47	0	2,2,2	0.24	0
2	EDO	B	434	-	3,3,3	0.73	0	2,2,2	0.20	0
2	EDO	B	437	-	3,3,3	0.52	0	2,2,2	0.13	0
2	EDO	D	426	-	3,3,3	0.56	0	2,2,2	0.12	0
2	EDO	C	405	-	3,3,3	0.53	0	2,2,2	0.25	0
2	EDO	C	418	-	3,3,3	0.47	0	2,2,2	0.33	0
2	EDO	E	448	-	3,3,3	0.26	0	2,2,2	0.84	0
2	EDO	B	410	-	3,3,3	0.51	0	2,2,2	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	F	405	-	-	0/1/1/1	-
2	EDO	F	428	-	-	0/1/1/1	-
2	EDO	E	434	-	-	0/1/1/1	-
2	EDO	B	447	-	-	1/1/1/1	-
2	EDO	F	444	-	-	0/1/1/1	-
2	EDO	E	445	-	-	1/1/1/1	-
2	EDO	A	440	-	-	0/1/1/1	-
2	EDO	B	408	-	-	1/1/1/1	-
2	EDO	F	423	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	443	-	-	1/1/1/1	-
2	EDO	A	438	-	-	1/1/1/1	-
2	EDO	A	408	-	-	0/1/1/1	-
2	EDO	C	419	-	-	0/1/1/1	-
2	EDO	A	416	-	-	1/1/1/1	-
2	EDO	A	423	-	-	1/1/1/1	-
2	EDO	E	402	-	-	1/1/1/1	-
2	EDO	C	436	-	-	0/1/1/1	-
2	EDO	E	426	-	-	0/1/1/1	-
2	EDO	F	419	-	-	0/1/1/1	-
2	EDO	A	424	-	-	1/1/1/1	-
2	EDO	D	433	-	-	1/1/1/1	-
2	EDO	B	445	-	-	1/1/1/1	-
2	EDO	E	431	-	-	0/1/1/1	-
2	EDO	F	413	-	-	0/1/1/1	-
2	EDO	A	413	-	-	0/1/1/1	-
2	EDO	D	417	-	-	0/1/1/1	-
2	EDO	E	432	-	-	1/1/1/1	-
2	EDO	A	418	-	-	1/1/1/1	-
2	EDO	B	435	-	-	0/1/1/1	-
2	EDO	C	408	-	-	1/1/1/1	-
2	EDO	C	438	-	-	0/1/1/1	-
2	EDO	E	403	-	-	1/1/1/1	-
2	EDO	E	436	-	-	0/1/1/1	-
2	EDO	E	437	-	-	1/1/1/1	-
2	EDO	C	424	-	-	1/1/1/1	-
2	EDO	E	447	-	-	1/1/1/1	-
2	EDO	A	412	-	-	0/1/1/1	-
2	EDO	C	413	-	-	1/1/1/1	-
2	EDO	B	430	-	-	0/1/1/1	-
2	EDO	E	420	-	-	1/1/1/1	-
2	EDO	D	410	-	-	0/1/1/1	-
2	EDO	E	413	-	-	0/1/1/1	-
2	EDO	E	438	-	-	1/1/1/1	-
2	EDO	E	418	-	-	1/1/1/1	-
2	EDO	F	414	-	-	1/1/1/1	-
2	EDO	A	427	-	-	1/1/1/1	-
2	EDO	C	410	-	-	0/1/1/1	-
2	EDO	F	436	-	-	1/1/1/1	-
2	EDO	A	431	-	-	1/1/1/1	-
2	EDO	C	430	-	-	0/1/1/1	-
2	EDO	F	416	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	439	-	-	1/1/1/1	-
2	EDO	E	446	-	-	1/1/1/1	-
2	EDO	F	422	-	-	0/1/1/1	-
2	EDO	B	428	-	-	0/1/1/1	-
2	EDO	A	422	-	-	0/1/1/1	-
2	EDO	E	444	-	-	1/1/1/1	-
2	EDO	B	444	-	-	1/1/1/1	-
2	EDO	A	409	-	-	0/1/1/1	-
2	EDO	C	416	-	-	1/1/1/1	-
2	EDO	C	431	-	-	1/1/1/1	-
2	EDO	A	429	-	-	0/1/1/1	-
2	EDO	F	438	-	-	1/1/1/1	-
2	EDO	D	422	-	-	0/1/1/1	-
2	EDO	A	437	-	-	0/1/1/1	-
2	EDO	C	422	-	-	1/1/1/1	-
2	EDO	C	432	-	-	1/1/1/1	-
2	EDO	D	428	-	-	1/1/1/1	-
2	EDO	C	425	-	-	1/1/1/1	-
2	EDO	C	429	-	-	1/1/1/1	-
2	EDO	C	437	-	-	1/1/1/1	-
2	EDO	C	412	-	-	0/1/1/1	-
2	EDO	B	404	-	-	1/1/1/1	-
2	EDO	B	431	-	-	1/1/1/1	-
2	EDO	F	442	-	-	1/1/1/1	-
2	EDO	B	438	-	-	1/1/1/1	-
2	EDO	B	422	-	-	0/1/1/1	-
2	EDO	F	410	-	-	0/1/1/1	-
2	EDO	F	441	-	-	0/1/1/1	-
2	EDO	A	404	-	-	0/1/1/1	-
2	EDO	A	410	-	-	0/1/1/1	-
2	EDO	B	409	-	-	0/1/1/1	-
2	EDO	B	423	-	-	1/1/1/1	-
2	EDO	D	416	-	-	0/1/1/1	-
2	EDO	D	411	-	-	1/1/1/1	-
2	EDO	E	401	-	-	1/1/1/1	-
2	EDO	D	406	-	-	0/1/1/1	-
2	EDO	B	442	-	-	1/1/1/1	-
2	EDO	C	427	-	-	1/1/1/1	-
2	EDO	D	404	-	-	0/1/1/1	-
2	EDO	E	435	-	-	0/1/1/1	-
2	EDO	B	418	-	-	1/1/1/1	-
2	EDO	C	404	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	F	408	-	-	0/1/1/1	-
2	EDO	A	426	-	-	0/1/1/1	-
2	EDO	F	439	-	-	0/1/1/1	-
2	EDO	A	402	-	-	1/1/1/1	-
2	EDO	D	438	-	-	0/1/1/1	-
2	EDO	E	414	-	-	1/1/1/1	-
2	EDO	A	443	-	-	1/1/1/1	-
2	EDO	F	404	-	-	0/1/1/1	-
2	EDO	D	423	-	-	0/1/1/1	-
2	EDO	F	418	-	-	0/1/1/1	-
2	EDO	F	443	-	-	1/1/1/1	-
2	EDO	F	432	-	-	1/1/1/1	-
2	EDO	A	421	-	-	1/1/1/1	-
2	EDO	A	430	-	-	1/1/1/1	-
2	EDO	A	432	-	-	1/1/1/1	-
2	EDO	F	403	-	-	1/1/1/1	-
2	EDO	E	440	-	-	1/1/1/1	-
2	EDO	D	402	-	-	0/1/1/1	-
2	EDO	E	411	-	-	1/1/1/1	-
2	EDO	E	415	-	-	0/1/1/1	-
2	EDO	C	402	-	-	0/1/1/1	-
2	EDO	F	412	-	-	0/1/1/1	-
2	EDO	B	439	-	-	1/1/1/1	-
2	EDO	B	424	-	-	0/1/1/1	-
2	EDO	A	417	-	-	1/1/1/1	-
2	EDO	F	417	-	-	0/1/1/1	-
2	EDO	B	413	-	-	0/1/1/1	-
2	EDO	F	401	-	-	0/1/1/1	-
2	EDO	B	433	-	-	1/1/1/1	-
2	EDO	F	420	-	-	0/1/1/1	-
2	EDO	A	439	-	-	0/1/1/1	-
2	EDO	D	427	-	-	1/1/1/1	-
2	EDO	E	433	-	-	0/1/1/1	-
2	EDO	F	434	-	-	0/1/1/1	-
2	EDO	B	426	-	-	1/1/1/1	-
2	EDO	B	402	-	-	0/1/1/1	-
2	EDO	E	441	-	-	1/1/1/1	-
2	EDO	C	421	-	-	0/1/1/1	-
2	EDO	A	403	-	-	0/1/1/1	-
2	EDO	D	425	-	-	0/1/1/1	-
2	EDO	E	409	-	-	0/1/1/1	-
2	EDO	F	425	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	432	-	-	0/1/1/1	-
2	EDO	D	429	-	-	0/1/1/1	-
2	EDO	E	408	-	-	1/1/1/1	-
2	EDO	E	439	-	-	1/1/1/1	-
2	EDO	F	402	-	-	1/1/1/1	-
2	EDO	B	403	-	-	1/1/1/1	-
2	EDO	D	436	-	-	0/1/1/1	-
2	EDO	C	423	-	-	1/1/1/1	-
2	EDO	E	427	-	-	1/1/1/1	-
2	EDO	D	403	-	-	1/1/1/1	-
2	EDO	E	442	-	-	0/1/1/1	-
2	EDO	B	427	-	-	1/1/1/1	-
2	EDO	B	412	-	-	0/1/1/1	-
2	EDO	E	443	-	-	1/1/1/1	-
2	EDO	F	424	-	-	0/1/1/1	-
2	EDO	C	426	-	-	1/1/1/1	-
2	EDO	A	435	-	-	0/1/1/1	-
2	EDO	E	419	-	-	1/1/1/1	-
2	EDO	B	420	-	-	0/1/1/1	-
2	EDO	D	407	-	-	0/1/1/1	-
2	EDO	E	425	-	-	1/1/1/1	-
2	EDO	D	413	-	-	0/1/1/1	-
2	EDO	A	420	-	-	0/1/1/1	-
2	EDO	F	421	-	-	0/1/1/1	-
2	EDO	B	429	-	-	1/1/1/1	-
2	EDO	A	442	-	-	1/1/1/1	-
2	EDO	A	414	-	-	0/1/1/1	-
2	EDO	B	415	-	-	0/1/1/1	-
2	EDO	D	434	-	-	0/1/1/1	-
2	EDO	F	415	-	-	0/1/1/1	-
2	EDO	B	446	-	-	0/1/1/1	-
2	EDO	B	416	-	-	1/1/1/1	-
2	EDO	A	415	-	-	1/1/1/1	-
2	EDO	E	416	-	-	1/1/1/1	-
2	EDO	D	408	-	-	0/1/1/1	-
2	EDO	D	430	-	-	1/1/1/1	-
2	EDO	E	428	-	-	1/1/1/1	-
2	EDO	D	424	-	-	1/1/1/1	-
2	EDO	C	403	-	-	0/1/1/1	-
2	EDO	E	404	-	-	1/1/1/1	-
2	EDO	C	411	-	-	0/1/1/1	-
2	EDO	C	417	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	441	-	-	1/1/1/1	-
2	EDO	C	409	-	-	1/1/1/1	-
2	EDO	B	419	-	-	1/1/1/1	-
2	EDO	B	405	-	-	1/1/1/1	-
2	EDO	A	441	-	-	1/1/1/1	-
2	EDO	B	414	-	-	0/1/1/1	-
2	EDO	F	409	-	-	0/1/1/1	-
2	EDO	A	419	-	-	0/1/1/1	-
2	EDO	E	424	-	-	0/1/1/1	-
2	EDO	B	407	-	-	0/1/1/1	-
2	EDO	F	431	-	-	1/1/1/1	-
2	EDO	F	437	-	-	1/1/1/1	-
2	EDO	E	406	-	-	0/1/1/1	-
2	EDO	F	407	-	-	0/1/1/1	-
2	EDO	C	420	-	-	0/1/1/1	-
2	EDO	A	407	-	-	0/1/1/1	-
2	EDO	D	415	-	-	0/1/1/1	-
2	EDO	E	412	-	-	1/1/1/1	-
2	EDO	F	433	-	-	0/1/1/1	-
2	EDO	B	401	-	-	0/1/1/1	-
2	EDO	B	417	-	-	1/1/1/1	-
2	EDO	C	414	-	-	0/1/1/1	-
2	EDO	A	433	-	-	0/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	C	415	-	-	1/1/1/1	-
2	EDO	D	432	-	-	0/1/1/1	-
2	EDO	F	430	-	-	1/1/1/1	-
2	EDO	F	411	-	-	0/1/1/1	-
2	EDO	B	406	-	-	0/1/1/1	-
2	EDO	A	411	-	-	1/1/1/1	-
2	EDO	F	406	-	-	1/1/1/1	-
2	EDO	B	440	-	-	1/1/1/1	-
2	EDO	F	445	-	-	0/1/1/1	-
2	EDO	D	401	-	-	0/1/1/1	-
2	EDO	D	412	-	-	0/1/1/1	-
2	EDO	E	417	-	-	0/1/1/1	-
2	EDO	D	420	-	-	1/1/1/1	-
2	EDO	E	423	-	-	0/1/1/1	-
2	EDO	D	414	-	-	1/1/1/1	-
2	EDO	A	425	-	-	1/1/1/1	-
2	EDO	E	429	-	-	1/1/1/1	-
2	EDO	A	434	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	E	410	-	-	0/1/1/1	-
2	EDO	B	411	-	-	0/1/1/1	-
2	EDO	C	407	-	-	0/1/1/1	-
2	EDO	F	427	-	-	1/1/1/1	-
2	EDO	D	409	-	-	1/1/1/1	-
2	EDO	C	434	-	-	1/1/1/1	-
2	EDO	B	421	-	-	0/1/1/1	-
2	EDO	D	405	-	-	1/1/1/1	-
2	EDO	F	426	-	-	1/1/1/1	-
2	EDO	C	433	-	-	0/1/1/1	-
2	EDO	D	418	-	-	0/1/1/1	-
2	EDO	F	440	-	-	1/1/1/1	-
2	EDO	D	437	-	-	0/1/1/1	-
2	EDO	E	407	-	-	0/1/1/1	-
2	EDO	A	428	-	-	0/1/1/1	-
2	EDO	C	401	-	-	0/1/1/1	-
2	EDO	B	436	-	-	1/1/1/1	-
2	EDO	C	435	-	-	1/1/1/1	-
2	EDO	D	421	-	-	1/1/1/1	-
2	EDO	F	429	-	-	1/1/1/1	-
2	EDO	F	435	-	-	1/1/1/1	-
2	EDO	D	435	-	-	1/1/1/1	-
2	EDO	B	425	-	-	1/1/1/1	-
2	EDO	A	436	-	-	1/1/1/1	-
2	EDO	E	422	-	-	0/1/1/1	-
2	EDO	C	406	-	-	1/1/1/1	-
2	EDO	D	431	-	-	1/1/1/1	-
2	EDO	E	405	-	-	0/1/1/1	-
2	EDO	D	419	-	-	0/1/1/1	-
2	EDO	E	430	-	-	0/1/1/1	-
2	EDO	C	428	-	-	1/1/1/1	-
2	EDO	E	421	-	-	1/1/1/1	-
2	EDO	A	405	-	-	0/1/1/1	-
2	EDO	A	406	-	-	1/1/1/1	-
2	EDO	B	434	-	-	1/1/1/1	-
2	EDO	B	437	-	-	1/1/1/1	-
2	EDO	D	426	-	-	1/1/1/1	-
2	EDO	C	405	-	-	0/1/1/1	-
2	EDO	C	418	-	-	1/1/1/1	-
2	EDO	E	448	-	-	1/1/1/1	-
2	EDO	B	410	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	440	EDO	O1-C1	-2.82	1.27	1.42
2	B	440	EDO	O2-C2	2.27	1.53	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (134) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	429	EDO	O1-C1-C2-O2
2	E	444	EDO	O1-C1-C2-O2
2	A	406	EDO	O1-C1-C2-O2
2	A	417	EDO	O1-C1-C2-O2
2	A	421	EDO	O1-C1-C2-O2
2	A	424	EDO	O1-C1-C2-O2
2	A	431	EDO	O1-C1-C2-O2
2	A	434	EDO	O1-C1-C2-O2
2	A	442	EDO	O1-C1-C2-O2
2	B	408	EDO	O1-C1-C2-O2
2	B	418	EDO	O1-C1-C2-O2
2	B	419	EDO	O1-C1-C2-O2
2	B	426	EDO	O1-C1-C2-O2
2	B	429	EDO	O1-C1-C2-O2
2	B	433	EDO	O1-C1-C2-O2
2	B	438	EDO	O1-C1-C2-O2
2	C	408	EDO	O1-C1-C2-O2
2	C	418	EDO	O1-C1-C2-O2
2	C	422	EDO	O1-C1-C2-O2
2	C	428	EDO	O1-C1-C2-O2
2	C	432	EDO	O1-C1-C2-O2
2	C	437	EDO	O1-C1-C2-O2
2	D	409	EDO	O1-C1-C2-O2
2	D	414	EDO	O1-C1-C2-O2
2	D	424	EDO	O1-C1-C2-O2
2	D	427	EDO	O1-C1-C2-O2
2	D	439	EDO	O1-C1-C2-O2
2	E	402	EDO	O1-C1-C2-O2
2	E	408	EDO	O1-C1-C2-O2
2	E	418	EDO	O1-C1-C2-O2
2	E	421	EDO	O1-C1-C2-O2
2	E	425	EDO	O1-C1-C2-O2
2	E	428	EDO	O1-C1-C2-O2
2	E	429	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	E	437	EDO	O1-C1-C2-O2
2	E	441	EDO	O1-C1-C2-O2
2	E	447	EDO	O1-C1-C2-O2
2	E	448	EDO	O1-C1-C2-O2
2	F	402	EDO	O1-C1-C2-O2
2	F	403	EDO	O1-C1-C2-O2
2	F	414	EDO	O1-C1-C2-O2
2	F	425	EDO	O1-C1-C2-O2
2	F	429	EDO	O1-C1-C2-O2
2	F	432	EDO	O1-C1-C2-O2
2	F	435	EDO	O1-C1-C2-O2
2	F	438	EDO	O1-C1-C2-O2
2	F	442	EDO	O1-C1-C2-O2
2	A	443	EDO	O1-C1-C2-O2
2	D	420	EDO	O1-C1-C2-O2
2	E	432	EDO	O1-C1-C2-O2
2	E	443	EDO	O1-C1-C2-O2
2	E	445	EDO	O1-C1-C2-O2
2	F	443	EDO	O1-C1-C2-O2
2	A	416	EDO	O1-C1-C2-O2
2	B	423	EDO	O1-C1-C2-O2
2	B	445	EDO	O1-C1-C2-O2
2	C	435	EDO	O1-C1-C2-O2
2	D	403	EDO	O1-C1-C2-O2
2	D	426	EDO	O1-C1-C2-O2
2	E	427	EDO	O1-C1-C2-O2
2	E	440	EDO	O1-C1-C2-O2
2	A	411	EDO	O1-C1-C2-O2
2	A	427	EDO	O1-C1-C2-O2
2	A	430	EDO	O1-C1-C2-O2
2	A	438	EDO	O1-C1-C2-O2
2	B	441	EDO	O1-C1-C2-O2
2	B	444	EDO	O1-C1-C2-O2
2	C	425	EDO	O1-C1-C2-O2
2	E	419	EDO	O1-C1-C2-O2
2	A	441	EDO	O1-C1-C2-O2
2	B	405	EDO	O1-C1-C2-O2
2	B	425	EDO	O1-C1-C2-O2
2	B	439	EDO	O1-C1-C2-O2
2	B	440	EDO	O1-C1-C2-O2
2	B	442	EDO	O1-C1-C2-O2
2	B	447	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	C	424	EDO	O1-C1-C2-O2
2	C	431	EDO	O1-C1-C2-O2
2	D	431	EDO	O1-C1-C2-O2
2	E	446	EDO	O1-C1-C2-O2
2	F	431	EDO	O1-C1-C2-O2
2	F	436	EDO	O1-C1-C2-O2
2	B	404	EDO	O1-C1-C2-O2
2	B	427	EDO	O1-C1-C2-O2
2	B	443	EDO	O1-C1-C2-O2
2	C	406	EDO	O1-C1-C2-O2
2	E	401	EDO	O1-C1-C2-O2
2	E	414	EDO	O1-C1-C2-O2
2	F	406	EDO	O1-C1-C2-O2
2	F	440	EDO	O1-C1-C2-O2
2	A	423	EDO	O1-C1-C2-O2
2	B	417	EDO	O1-C1-C2-O2
2	C	404	EDO	O1-C1-C2-O2
2	C	416	EDO	O1-C1-C2-O2
2	C	417	EDO	O1-C1-C2-O2
2	E	404	EDO	O1-C1-C2-O2
2	F	426	EDO	O1-C1-C2-O2
2	A	402	EDO	O1-C1-C2-O2
2	A	415	EDO	O1-C1-C2-O2
2	A	418	EDO	O1-C1-C2-O2
2	A	425	EDO	O1-C1-C2-O2
2	A	436	EDO	O1-C1-C2-O2
2	B	403	EDO	O1-C1-C2-O2
2	B	416	EDO	O1-C1-C2-O2
2	B	434	EDO	O1-C1-C2-O2
2	B	436	EDO	O1-C1-C2-O2
2	B	437	EDO	O1-C1-C2-O2
2	C	409	EDO	O1-C1-C2-O2
2	C	413	EDO	O1-C1-C2-O2
2	C	415	EDO	O1-C1-C2-O2
2	C	423	EDO	O1-C1-C2-O2
2	C	426	EDO	O1-C1-C2-O2
2	C	434	EDO	O1-C1-C2-O2
2	D	405	EDO	O1-C1-C2-O2
2	D	421	EDO	O1-C1-C2-O2
2	D	428	EDO	O1-C1-C2-O2
2	D	435	EDO	O1-C1-C2-O2
2	E	403	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	E	412	EDO	O1-C1-C2-O2
2	E	416	EDO	O1-C1-C2-O2
2	E	420	EDO	O1-C1-C2-O2
2	E	438	EDO	O1-C1-C2-O2
2	E	439	EDO	O1-C1-C2-O2
2	F	423	EDO	O1-C1-C2-O2
2	F	427	EDO	O1-C1-C2-O2
2	F	430	EDO	O1-C1-C2-O2
2	F	437	EDO	O1-C1-C2-O2
2	A	432	EDO	O1-C1-C2-O2
2	B	431	EDO	O1-C1-C2-O2
2	C	427	EDO	O1-C1-C2-O2
2	D	411	EDO	O1-C1-C2-O2
2	D	430	EDO	O1-C1-C2-O2
2	D	433	EDO	O1-C1-C2-O2
2	E	411	EDO	O1-C1-C2-O2

There are no ring outliers.

34 monomers are involved in 46 short contacts:

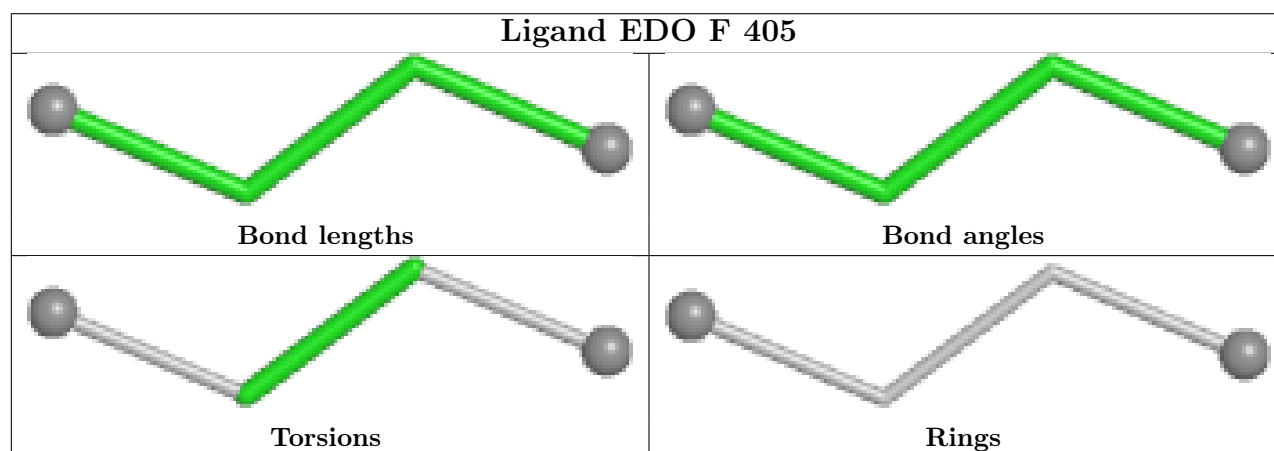
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	444	EDO	1	0
2	A	408	EDO	2	0
2	C	419	EDO	1	0
2	A	412	EDO	1	0
2	D	410	EDO	1	0
2	E	413	EDO	1	0
2	C	410	EDO	2	0
2	F	436	EDO	1	0
2	F	416	EDO	2	0
2	C	412	EDO	1	0
2	B	404	EDO	3	0
2	F	410	EDO	1	0
2	A	410	EDO	1	0
2	B	409	EDO	1	0
2	D	411	EDO	2	0
2	C	404	EDO	4	0
2	A	402	EDO	3	0
2	A	443	EDO	1	0
2	E	415	EDO	1	0
2	E	409	EDO	1	0
2	B	412	EDO	1	0

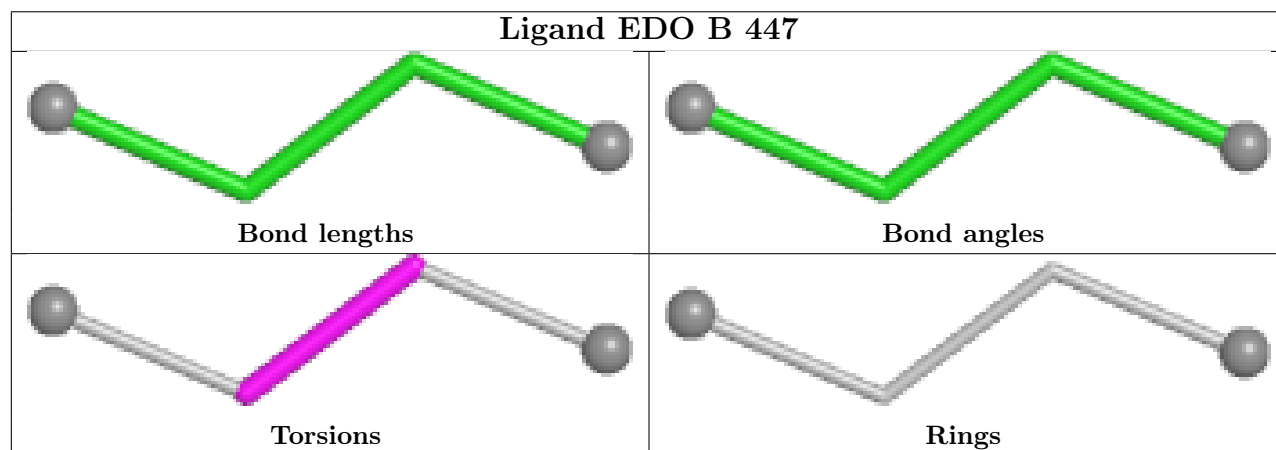
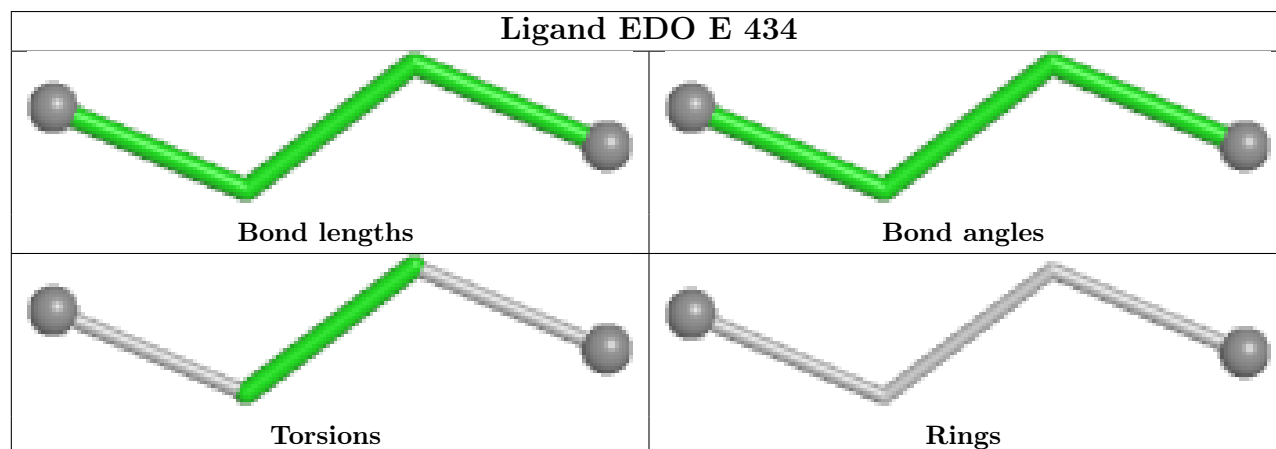
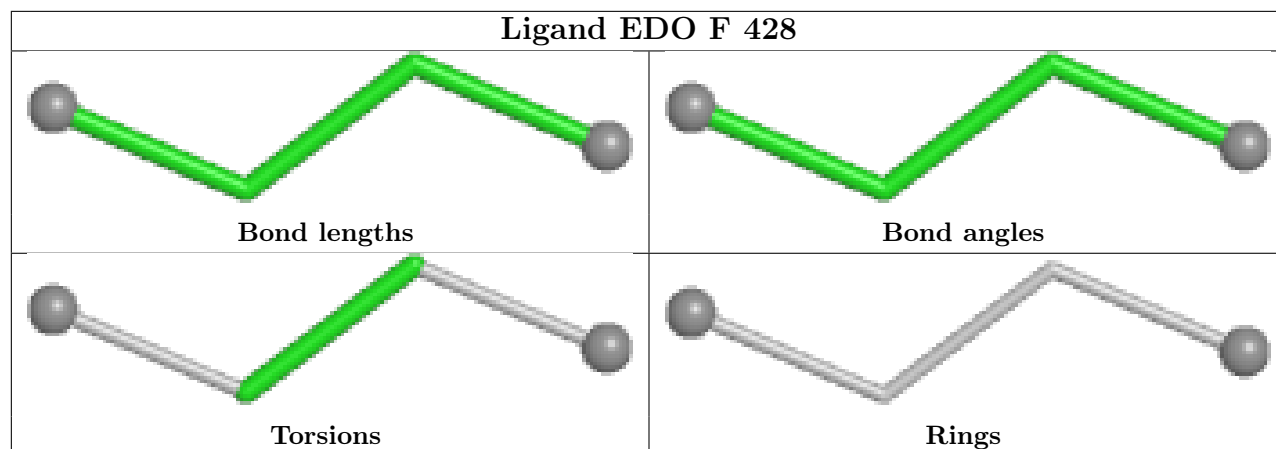
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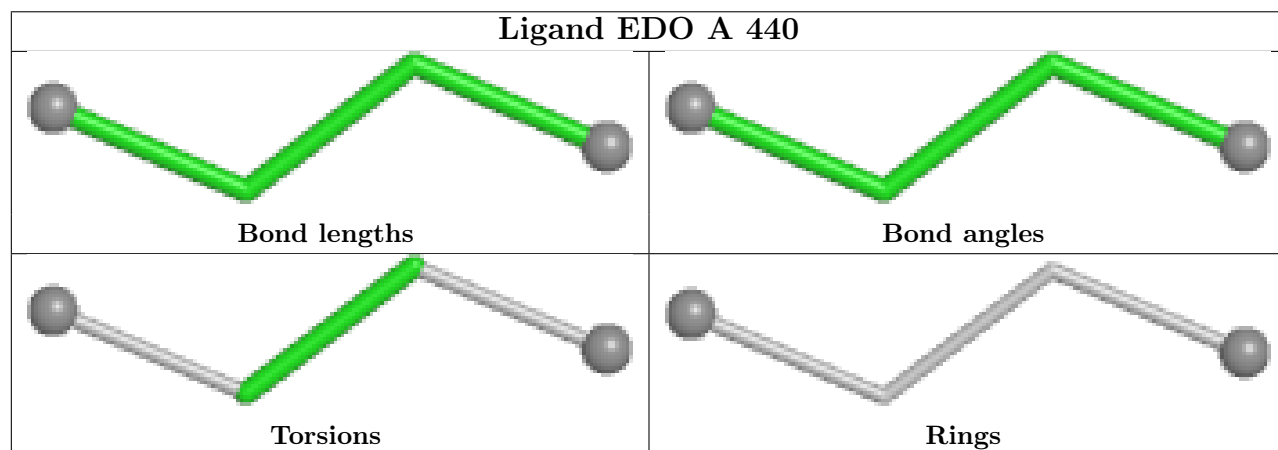
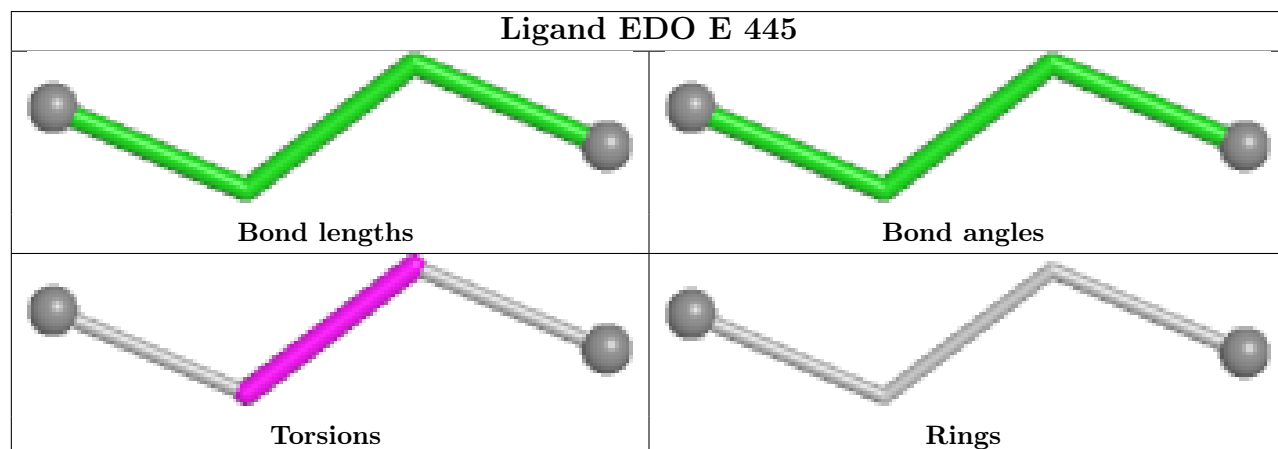
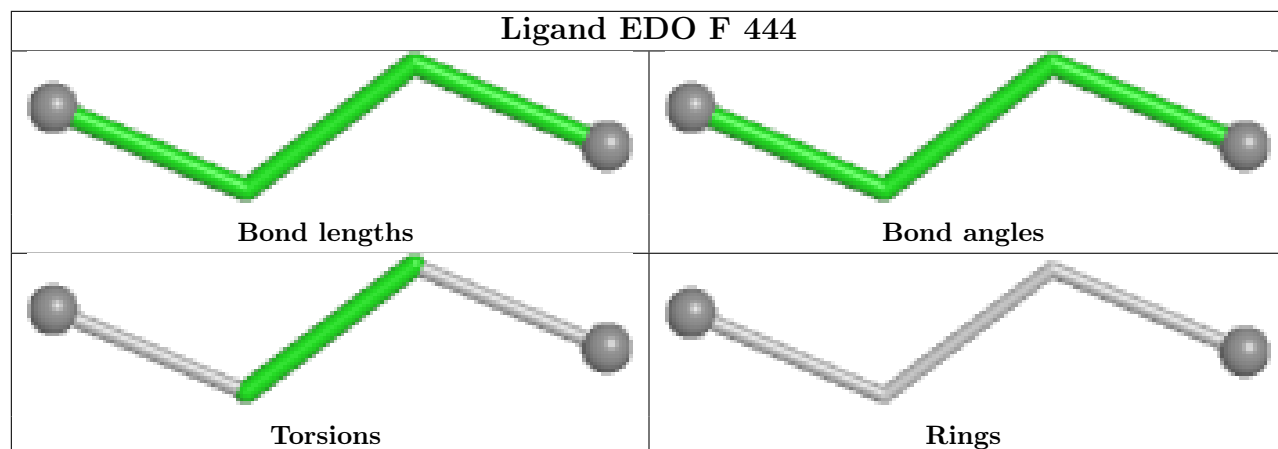
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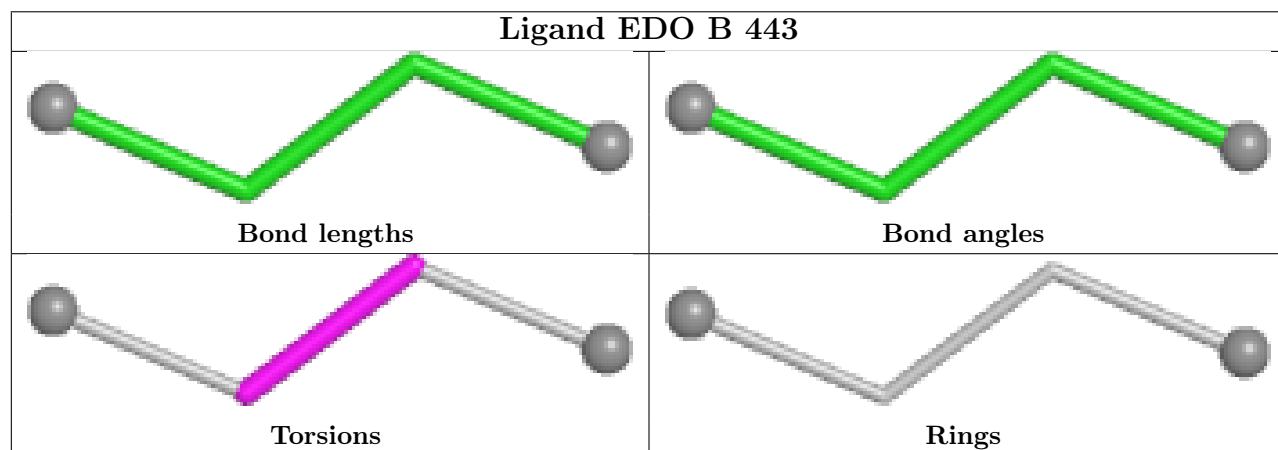
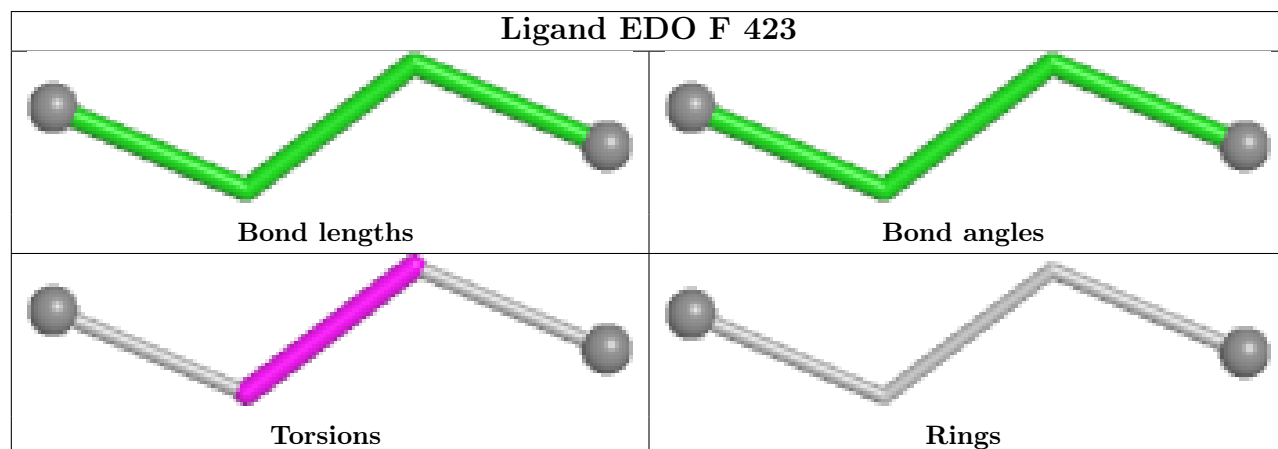
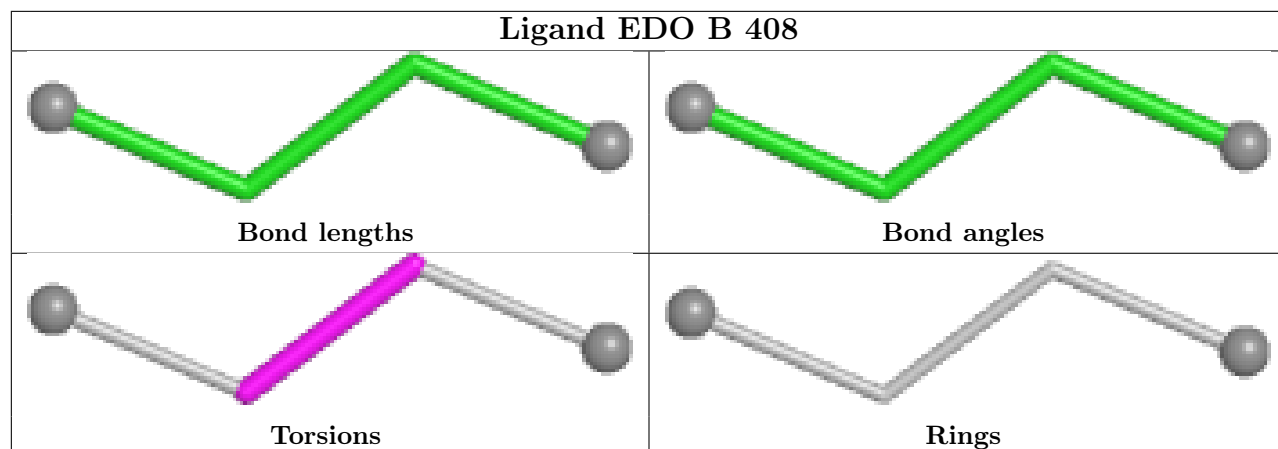
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	420	EDO	1	0
2	D	413	EDO	2	0
2	F	415	EDO	1	0
2	E	404	EDO	3	0
2	C	409	EDO	1	0
2	B	414	EDO	1	0
2	A	407	EDO	1	0
2	D	415	EDO	1	0
2	C	414	EDO	1	0
2	E	410	EDO	2	0
2	D	405	EDO	4	0
2	E	422	EDO	1	0
2	B	410	EDO	2	0

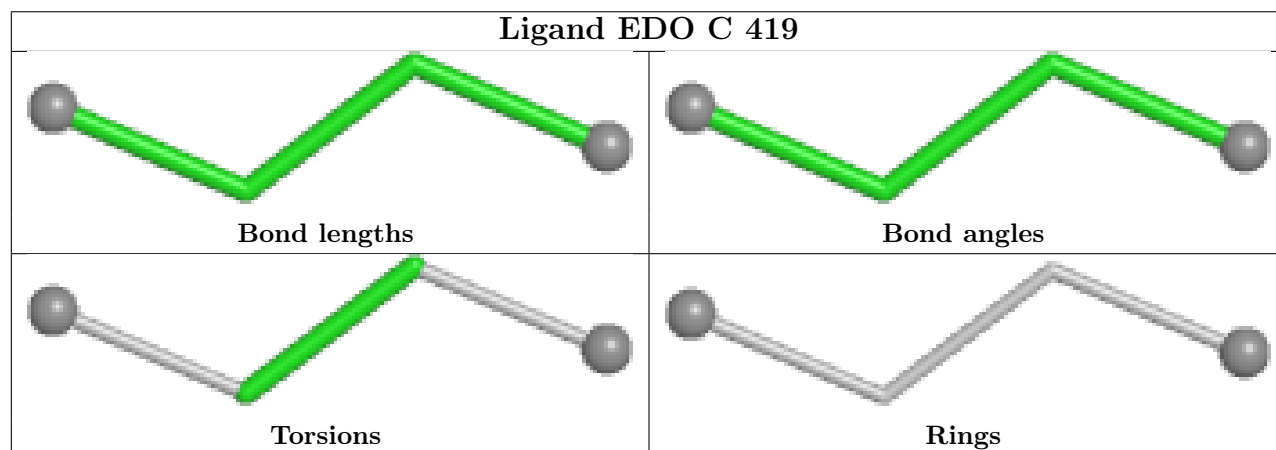
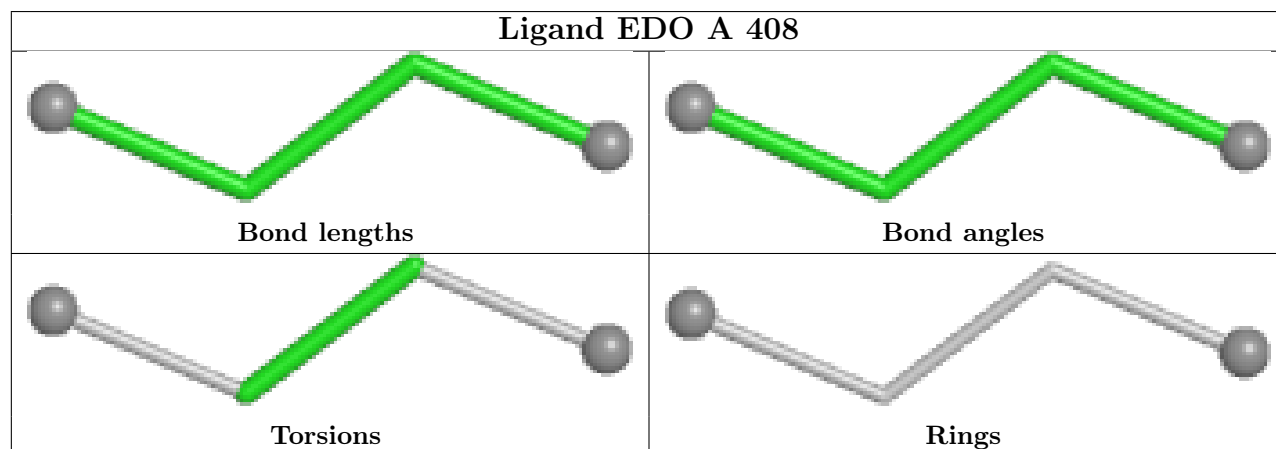
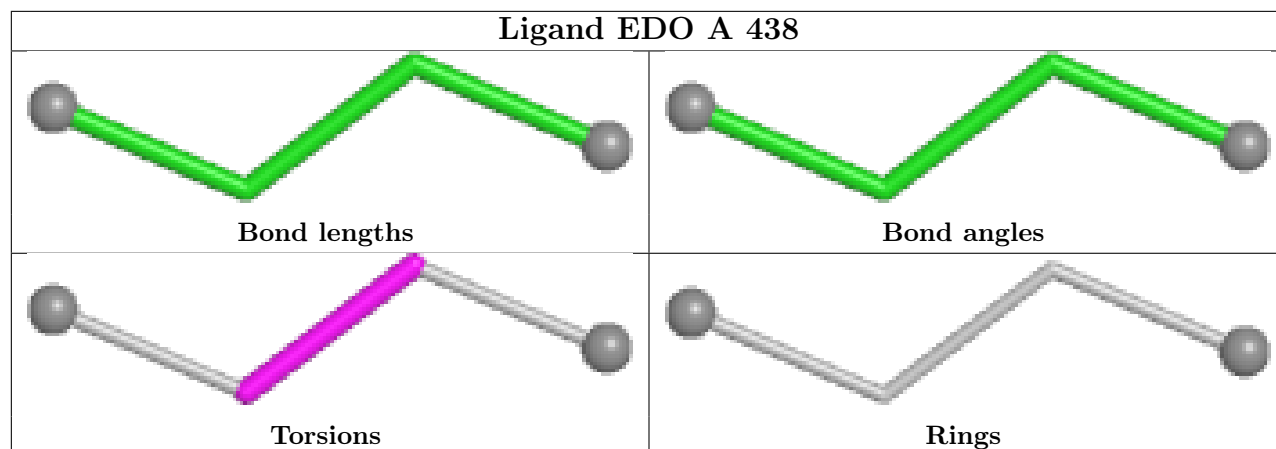
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

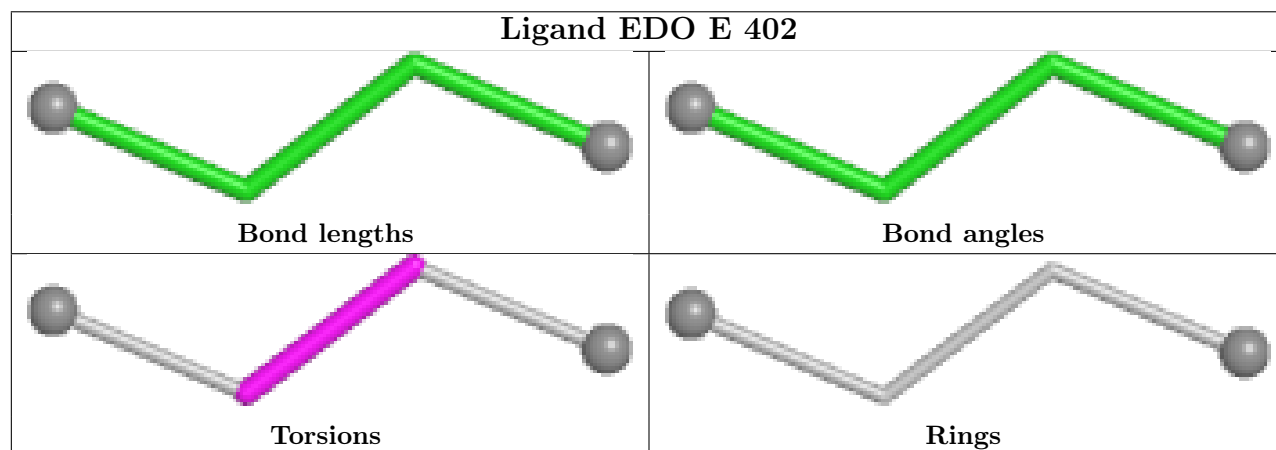
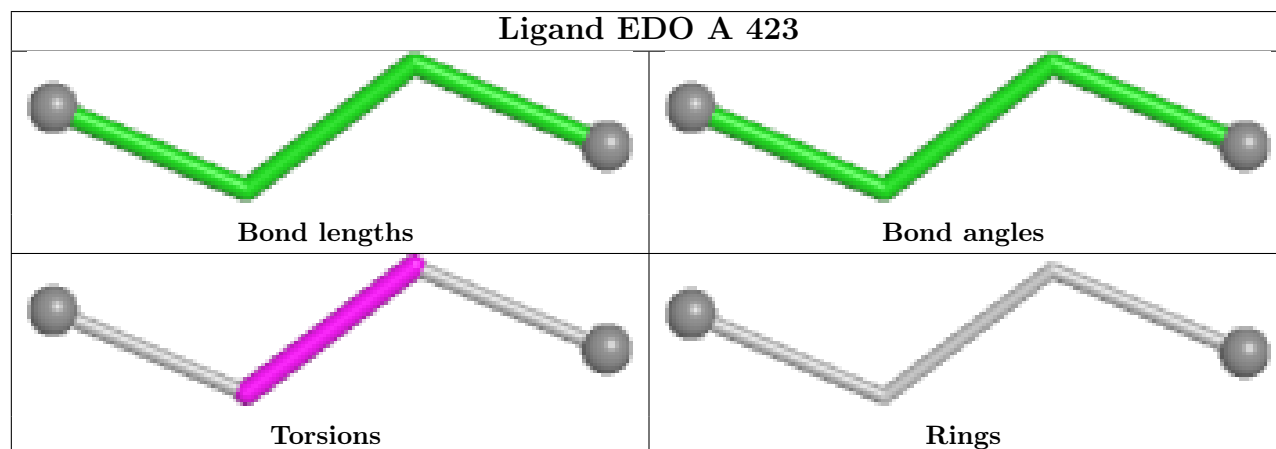
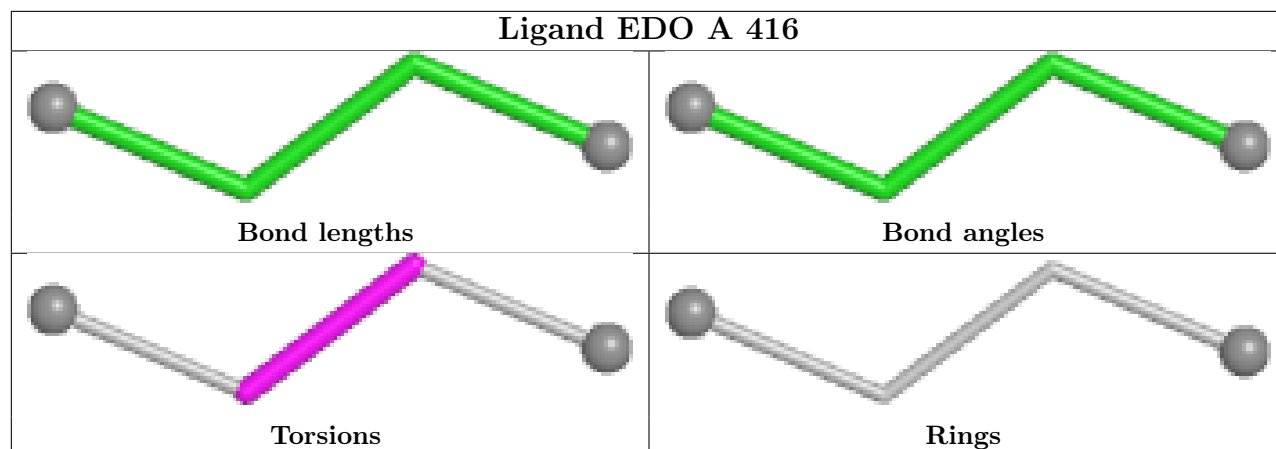


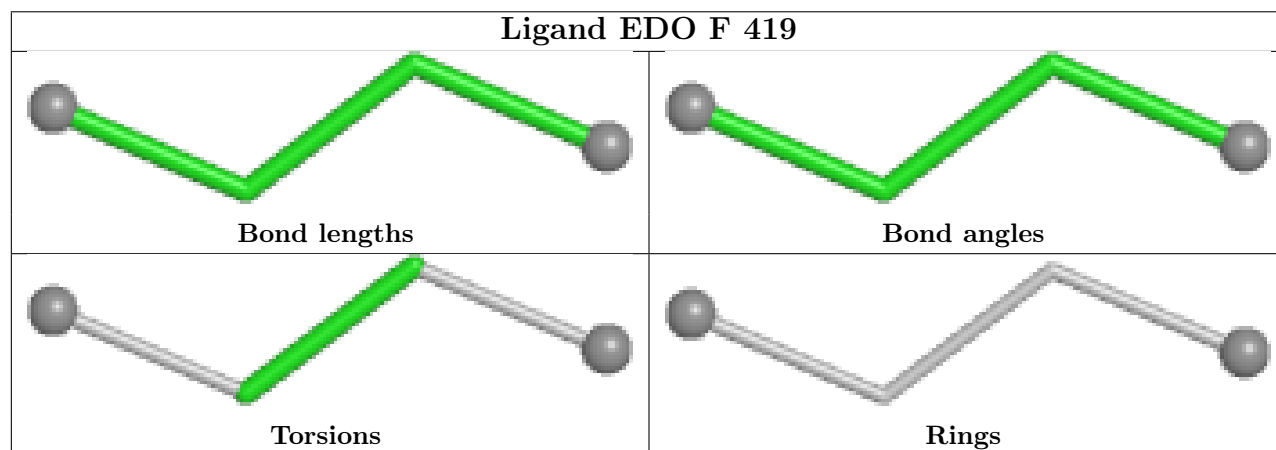
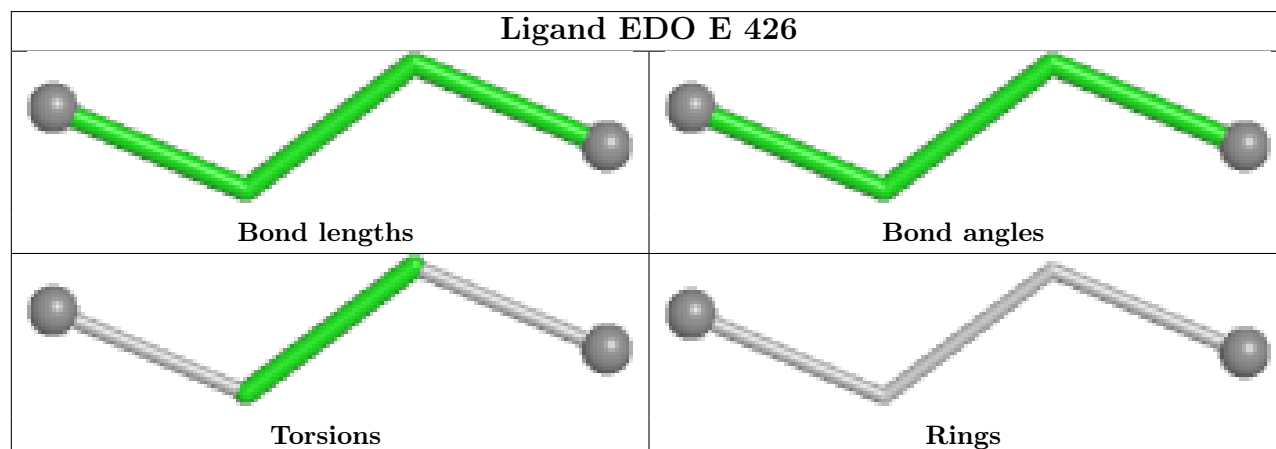
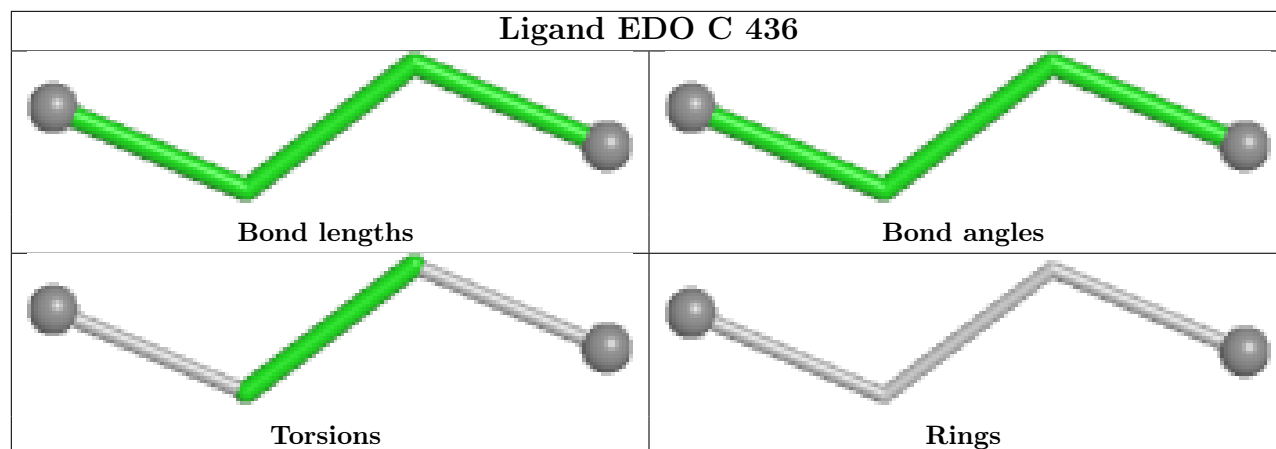


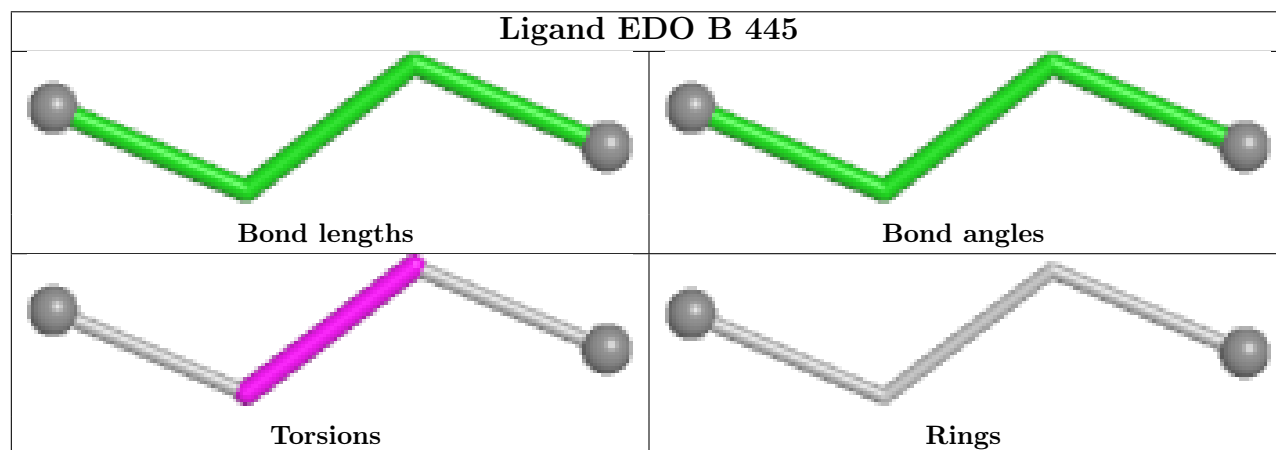
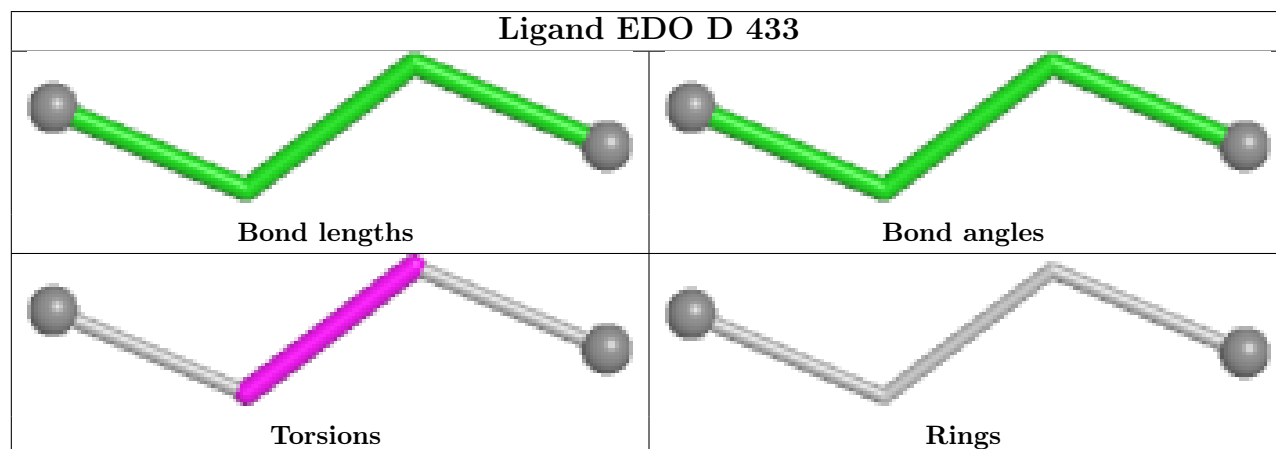
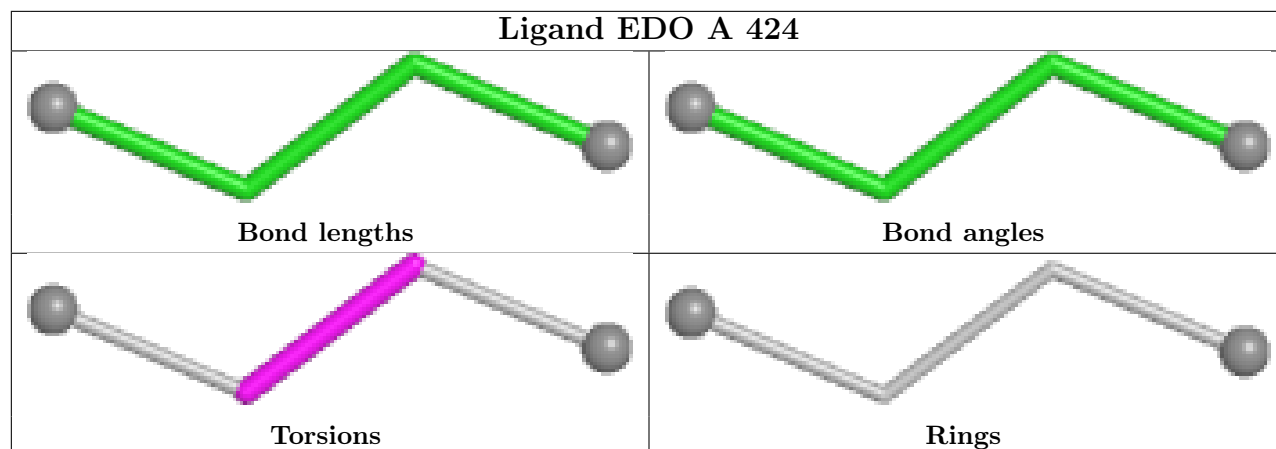


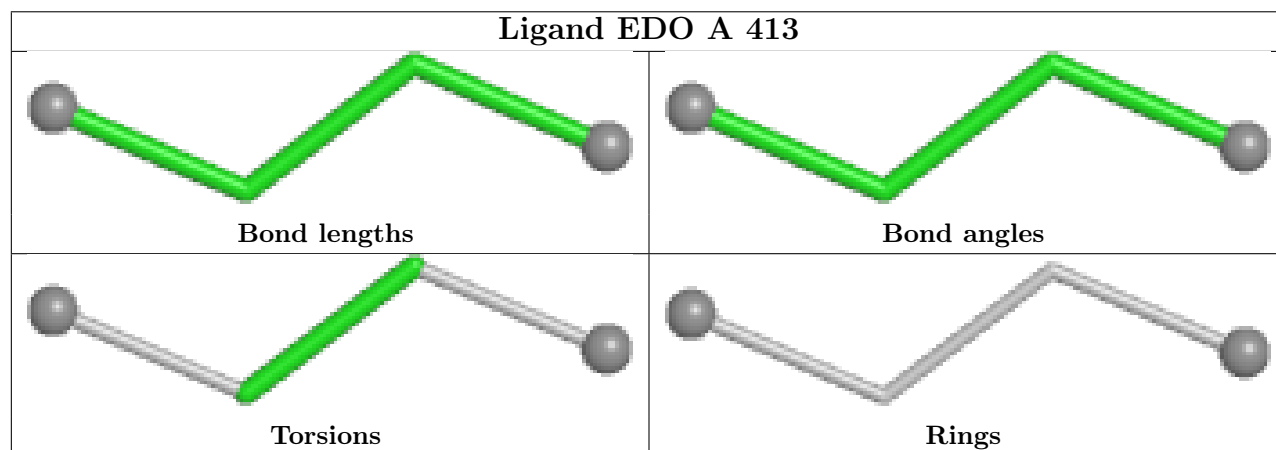
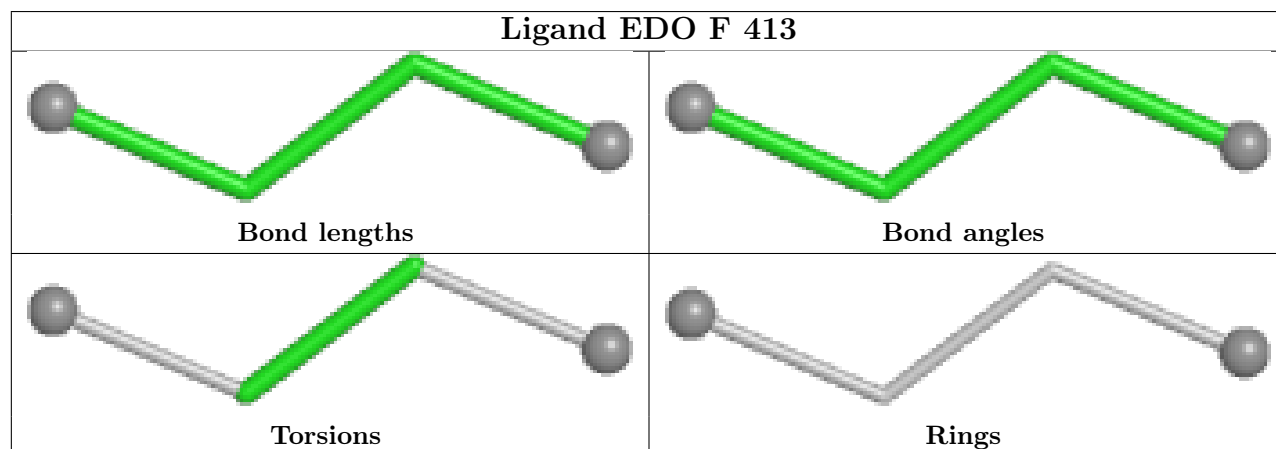
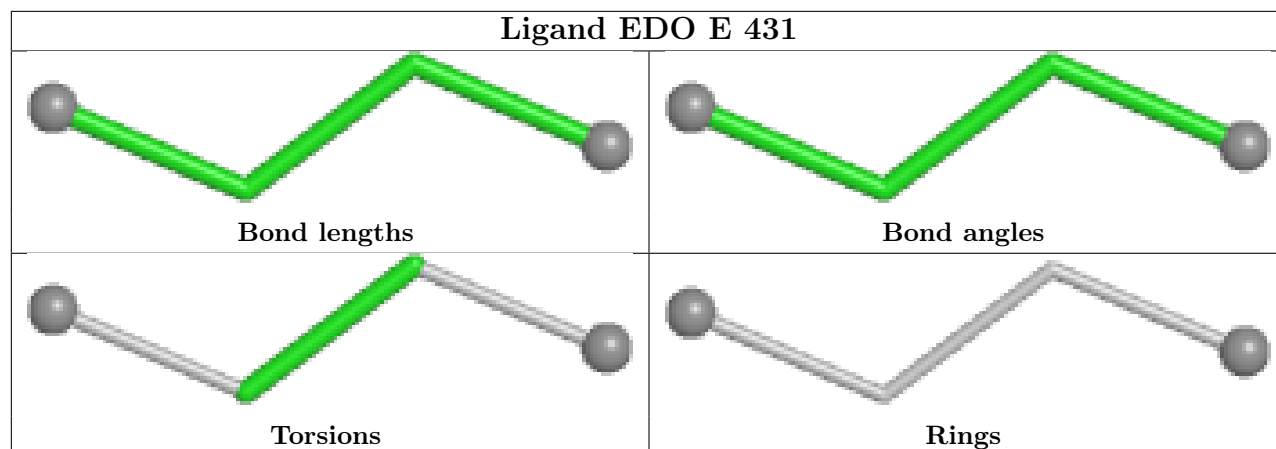


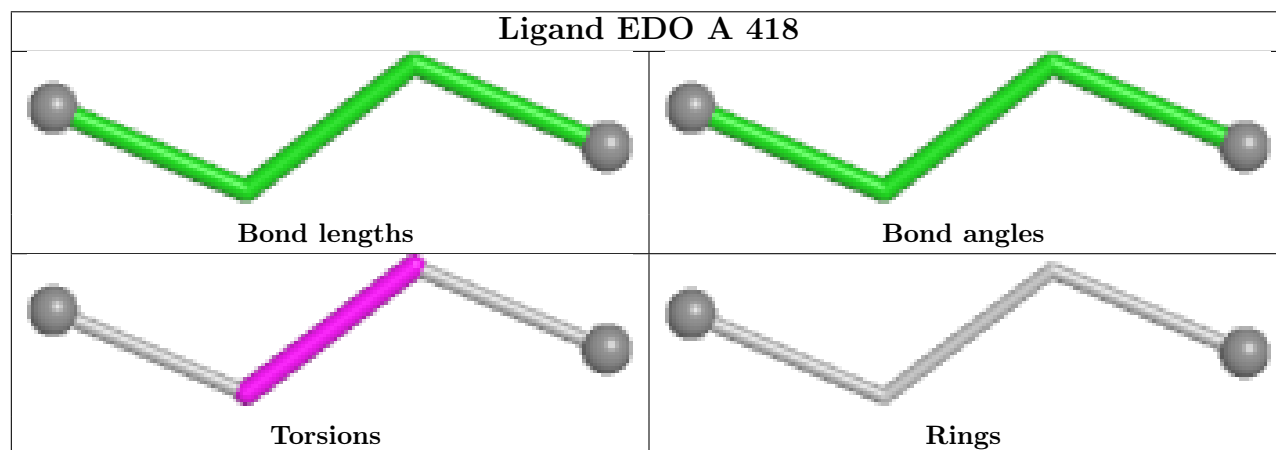
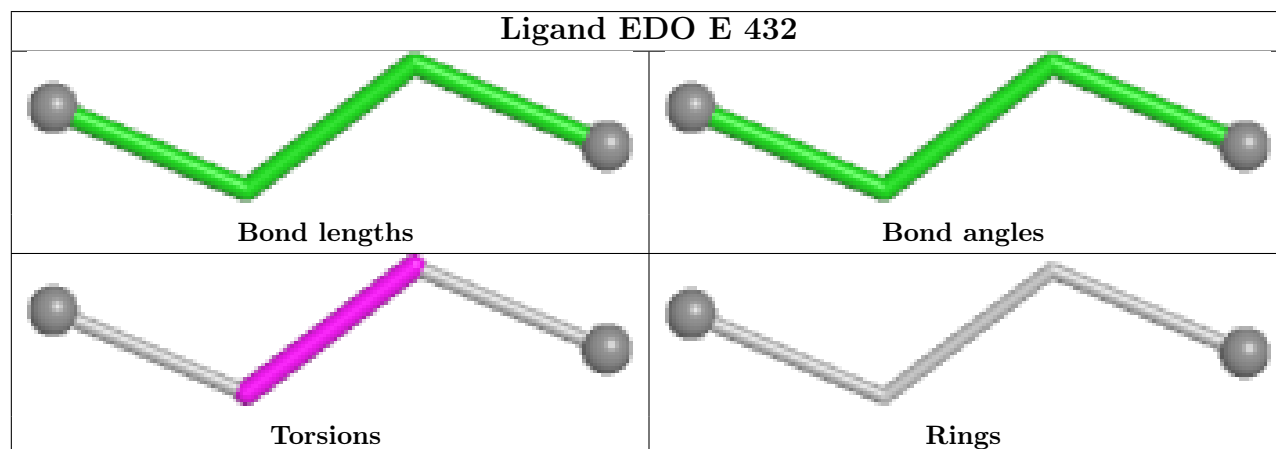
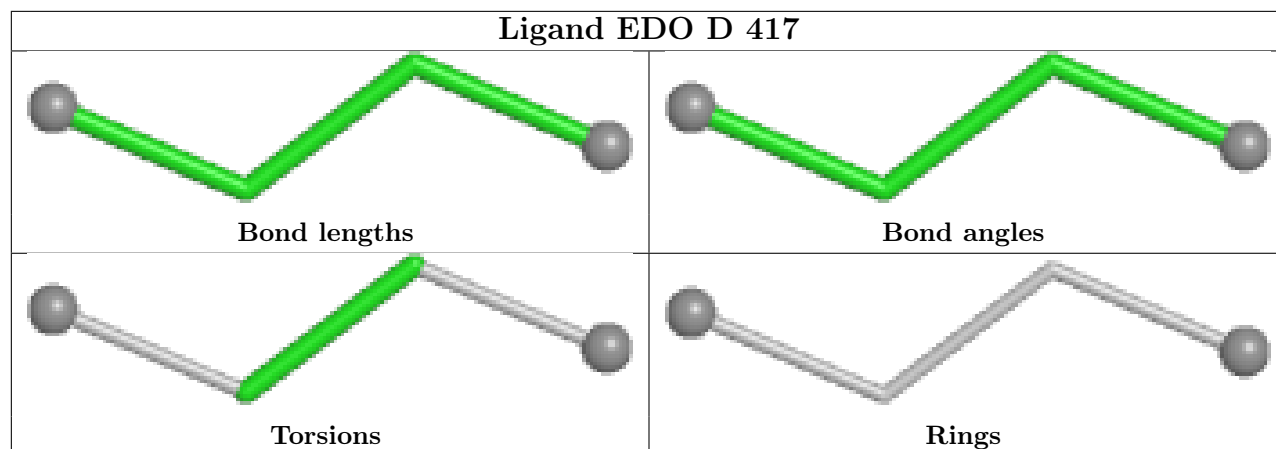


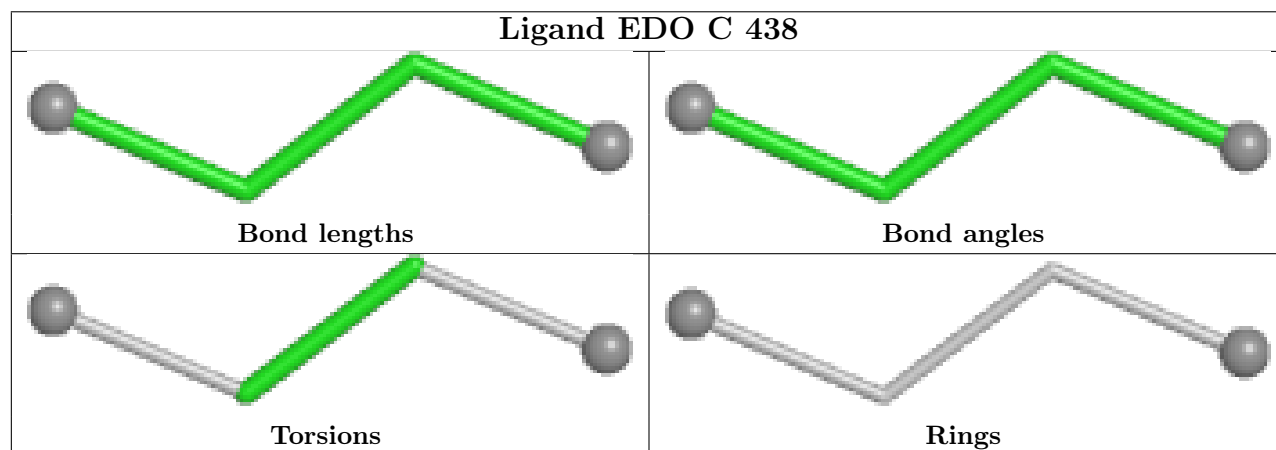
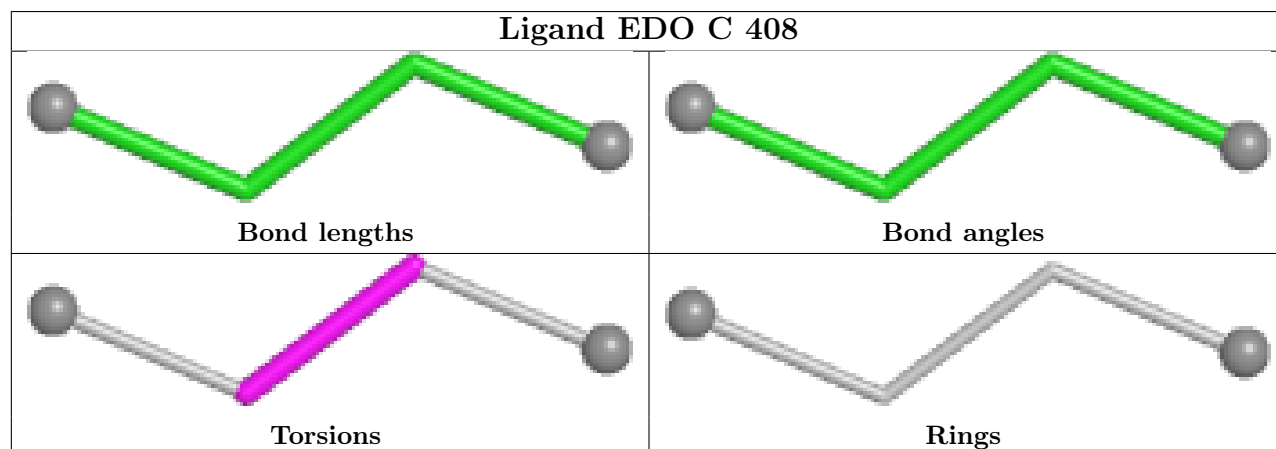
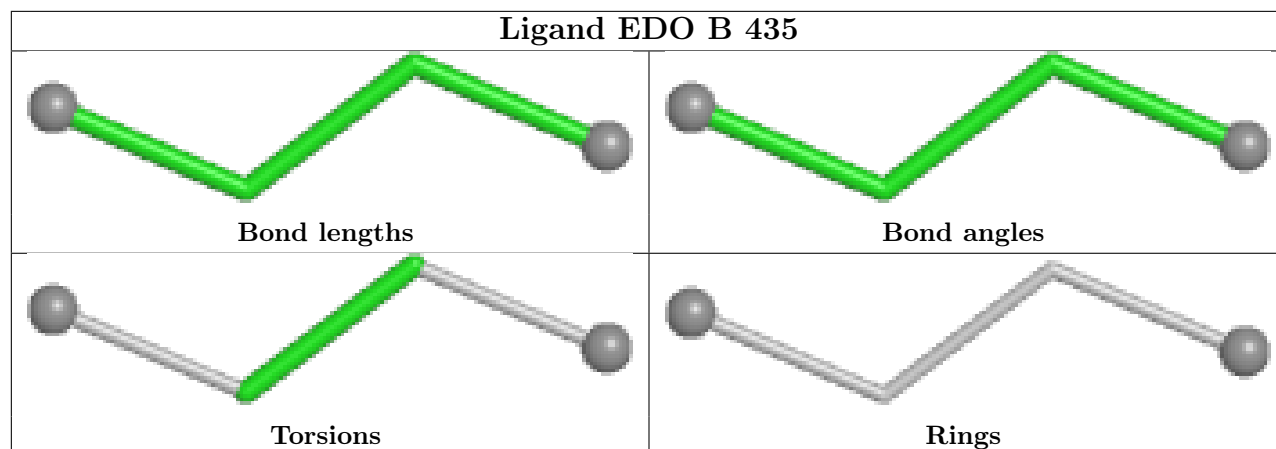


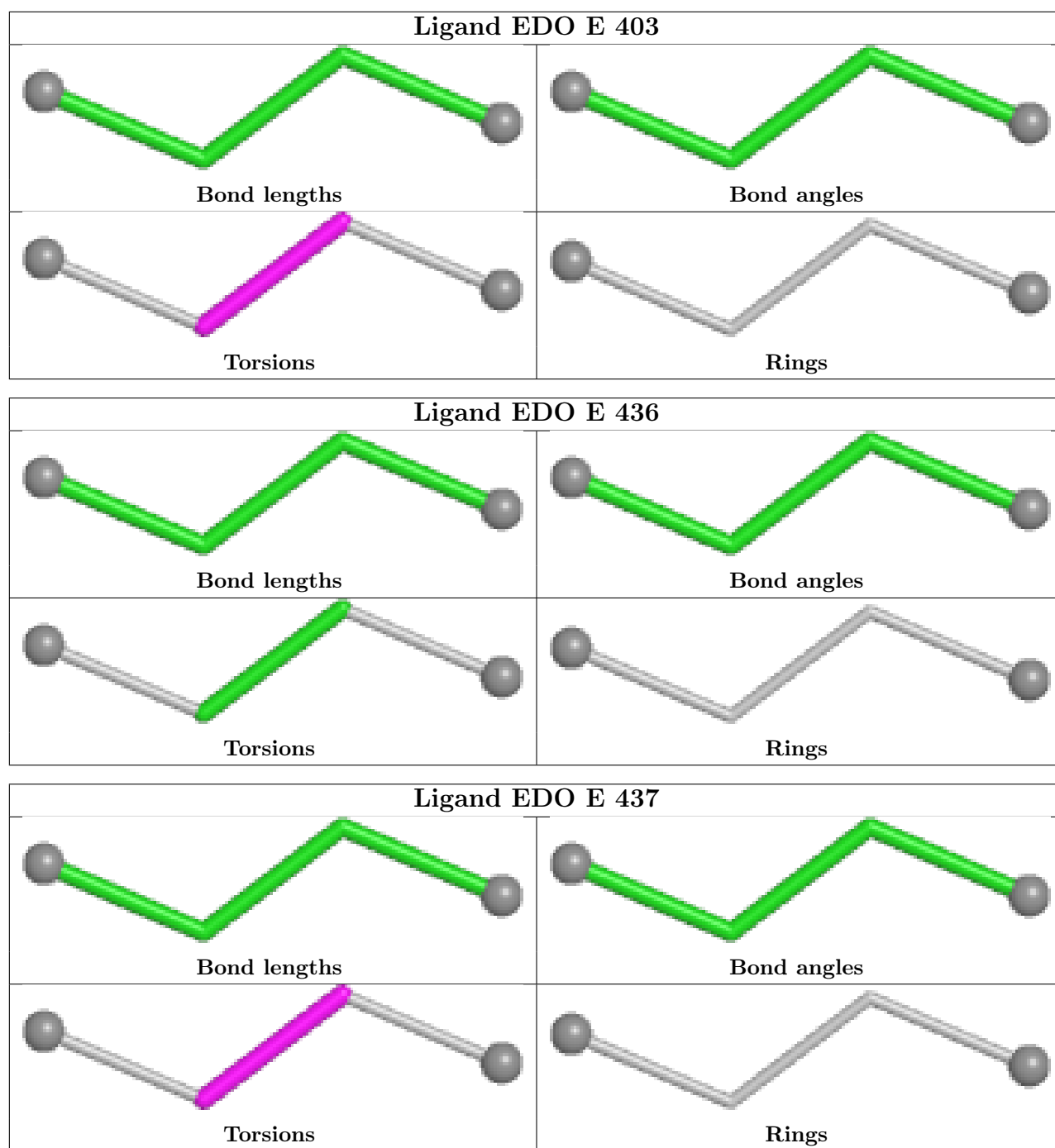


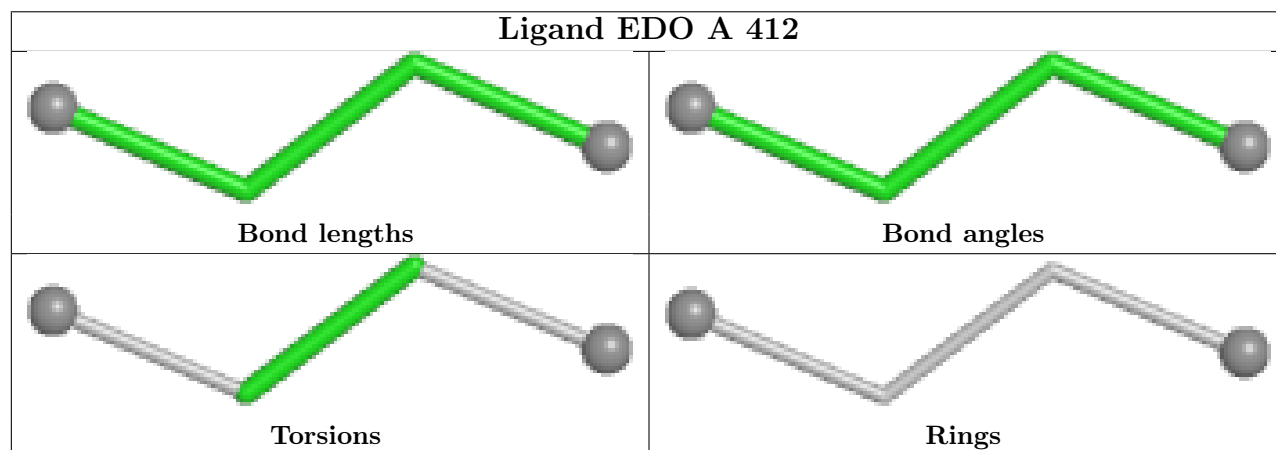
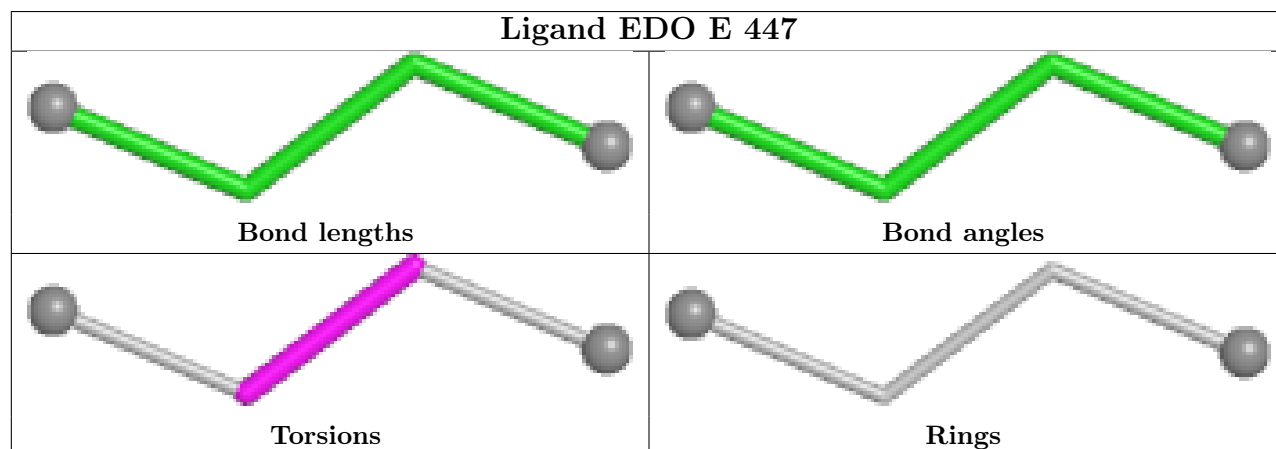
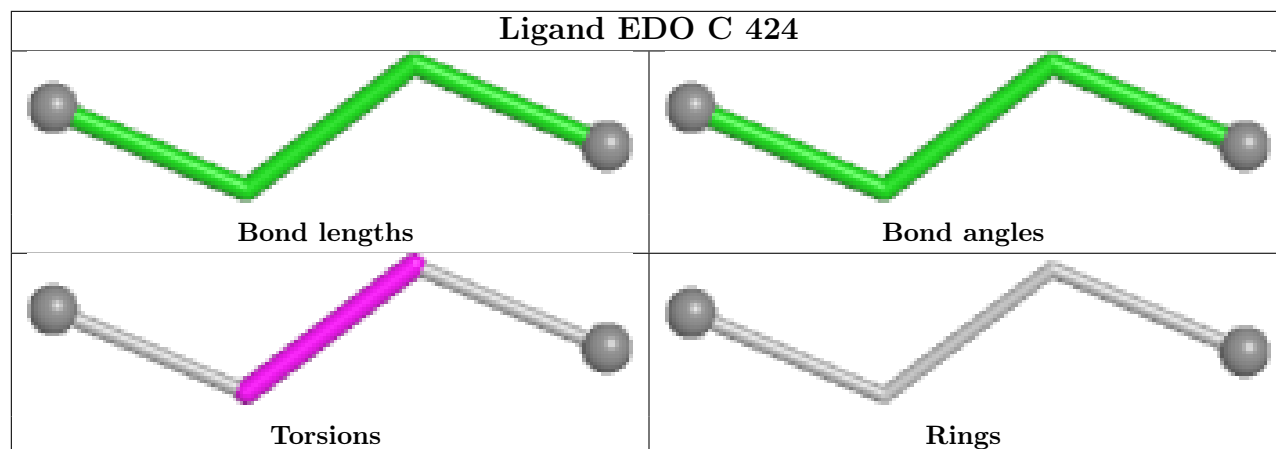


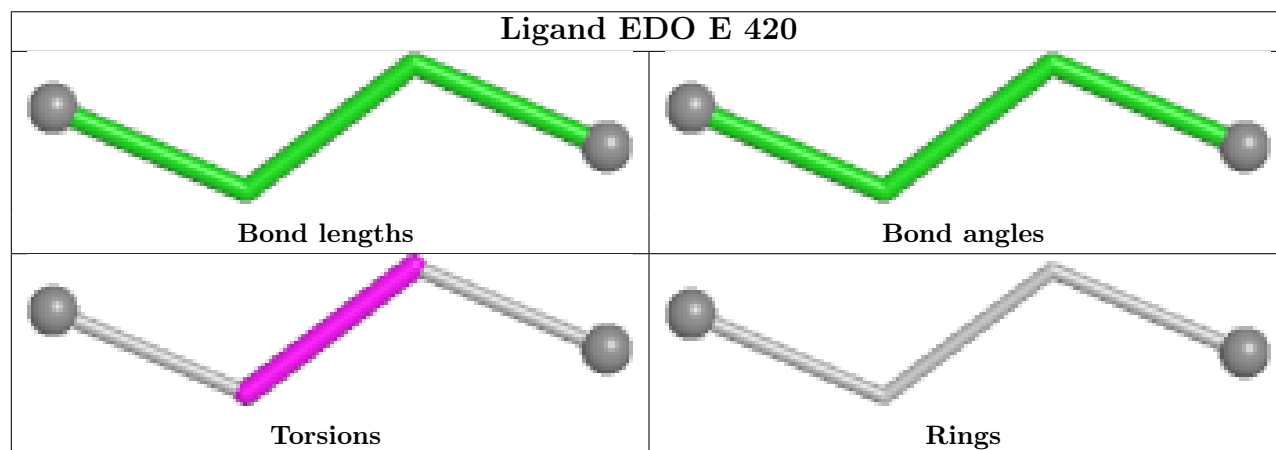
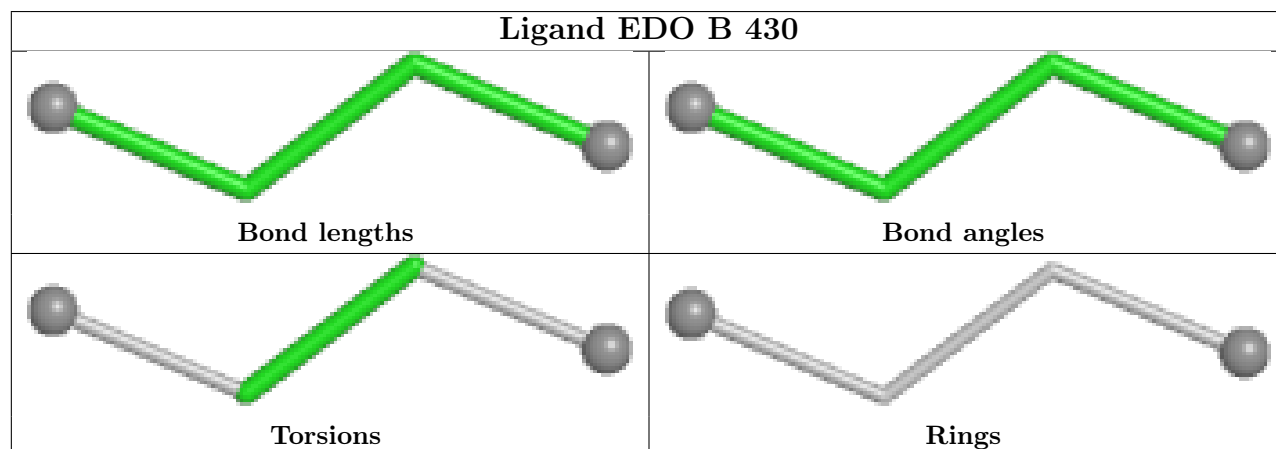
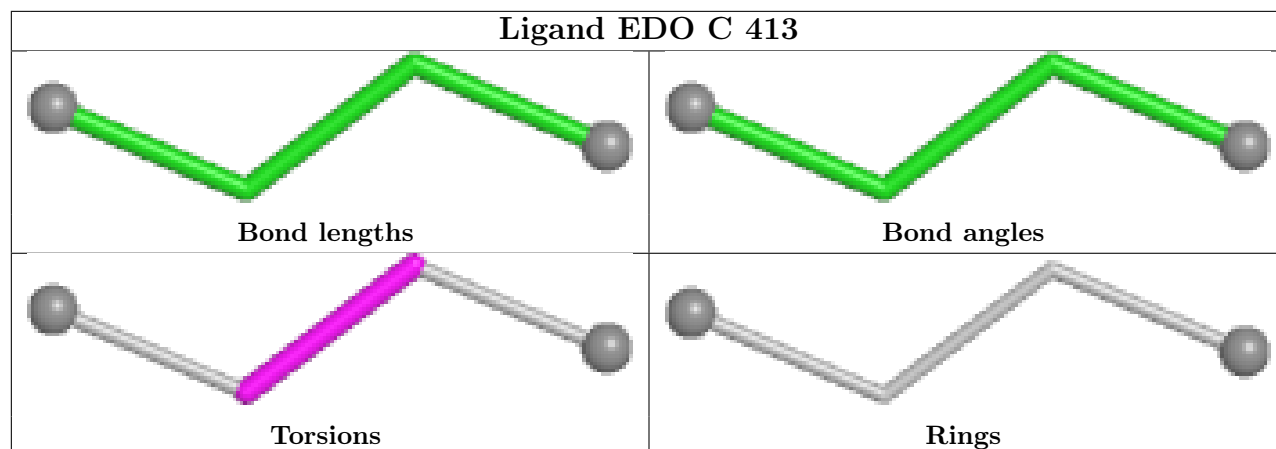


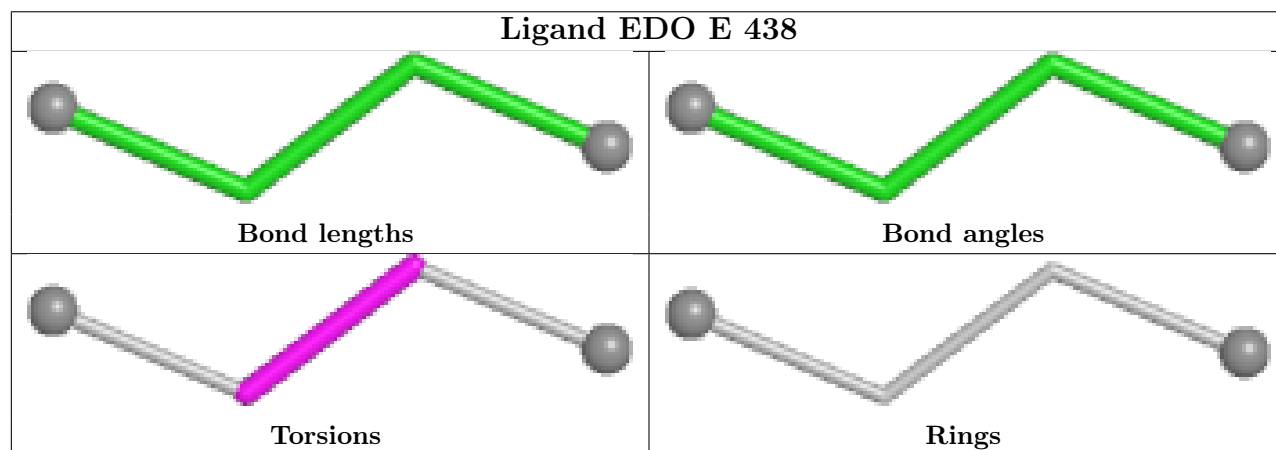
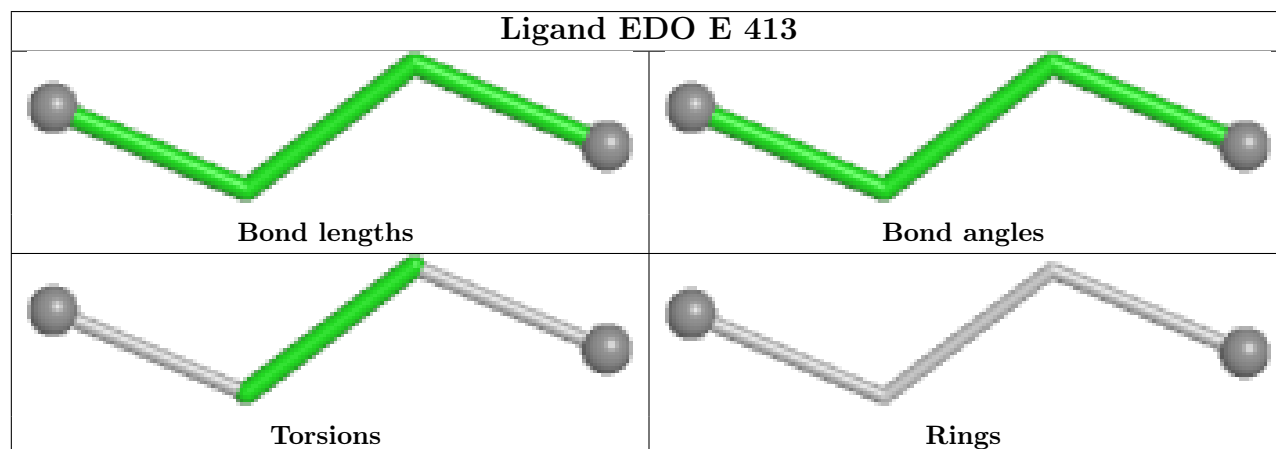
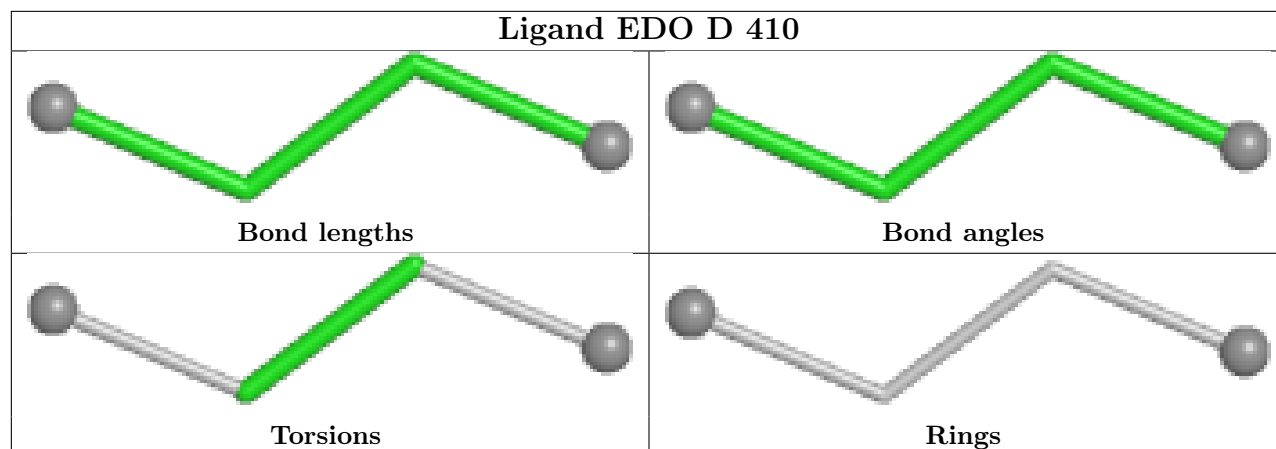


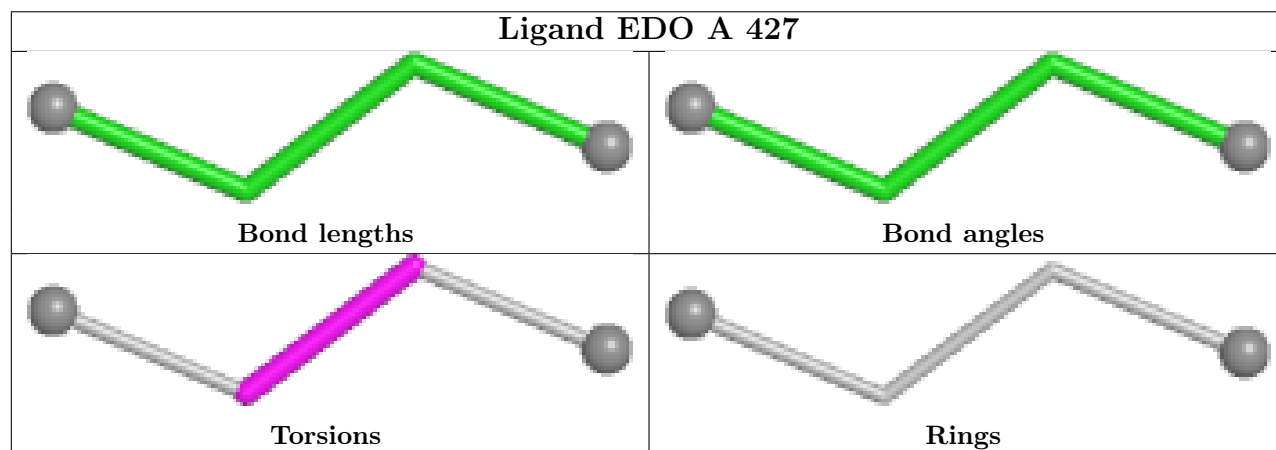
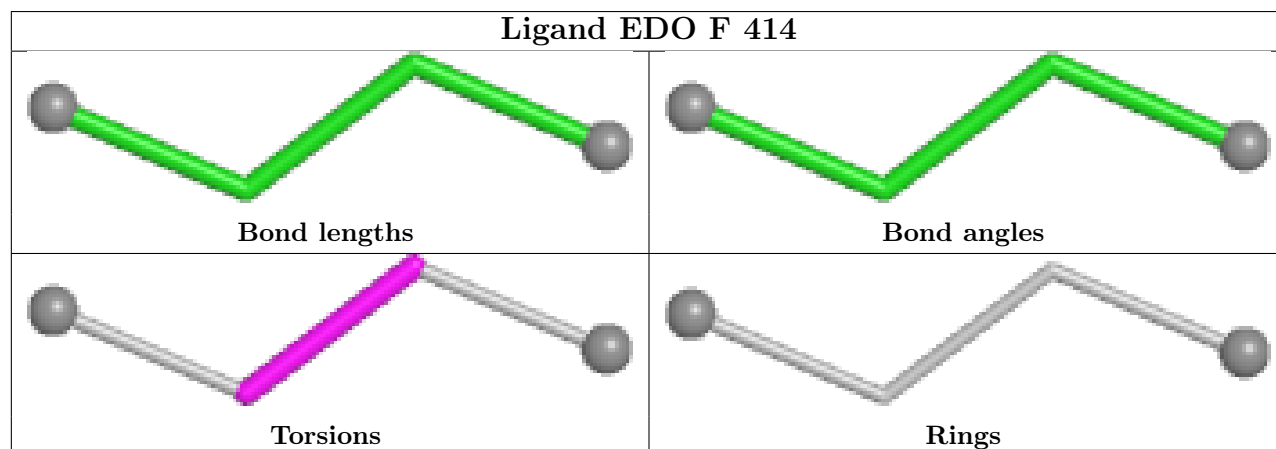
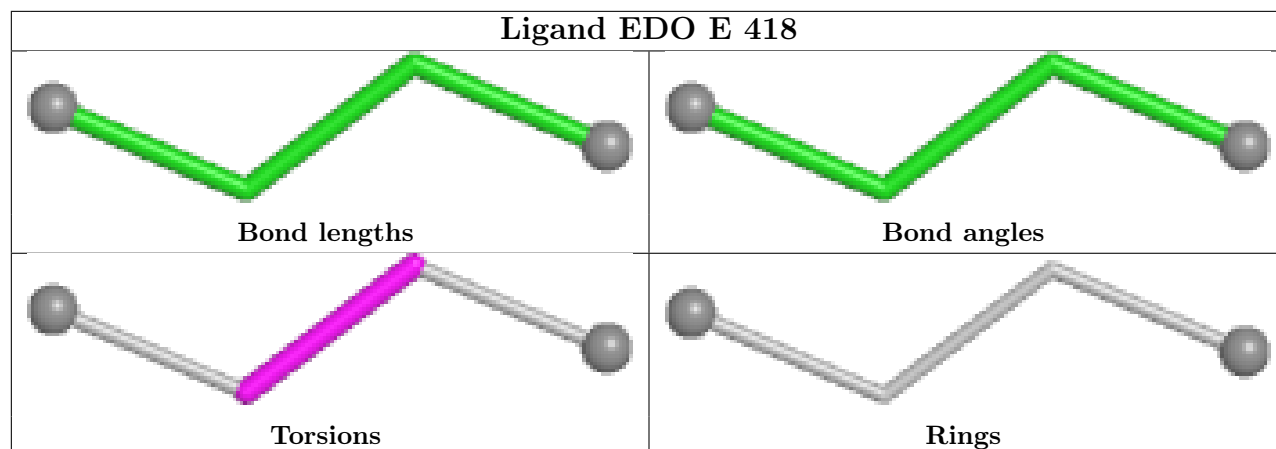


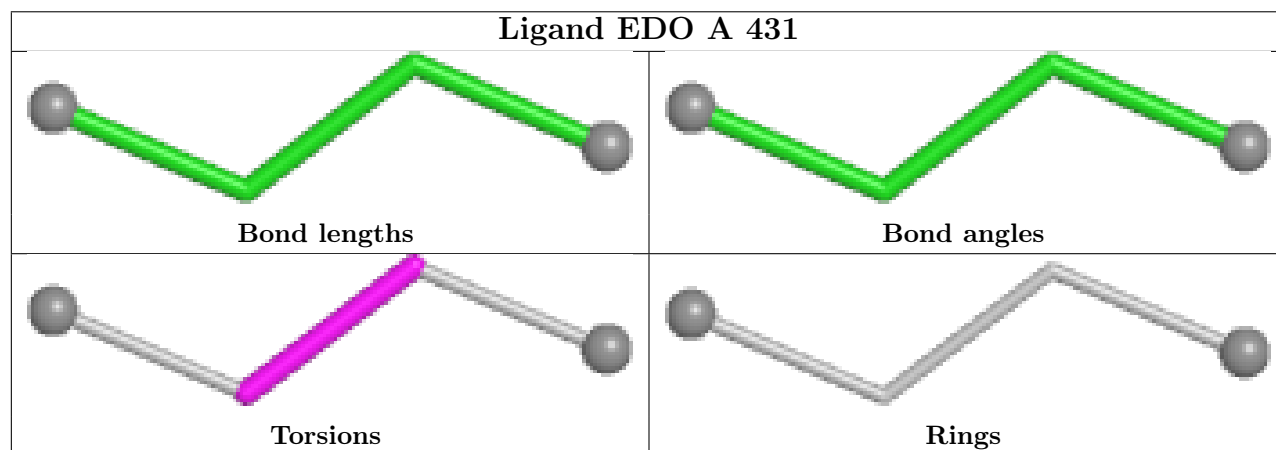
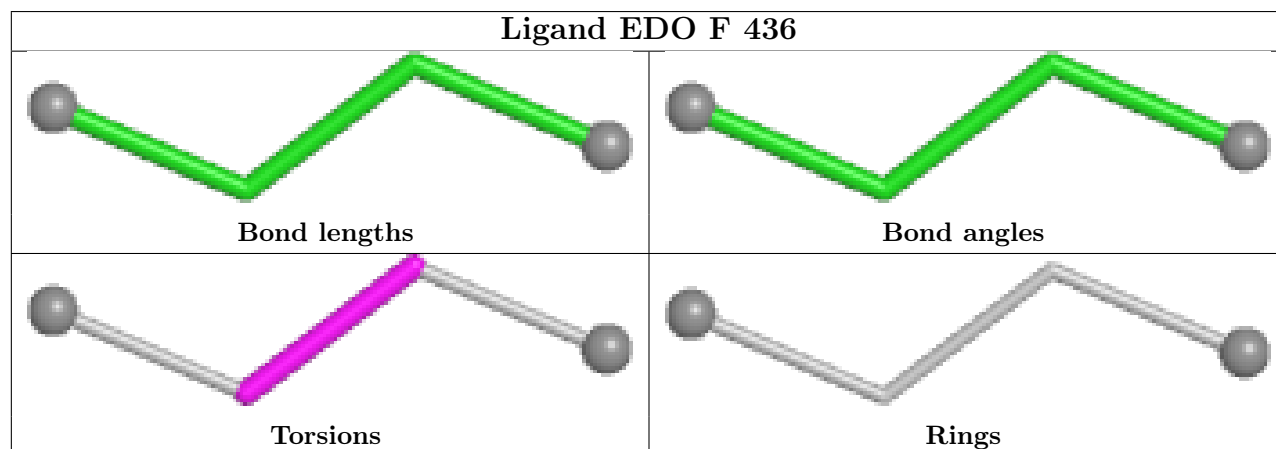
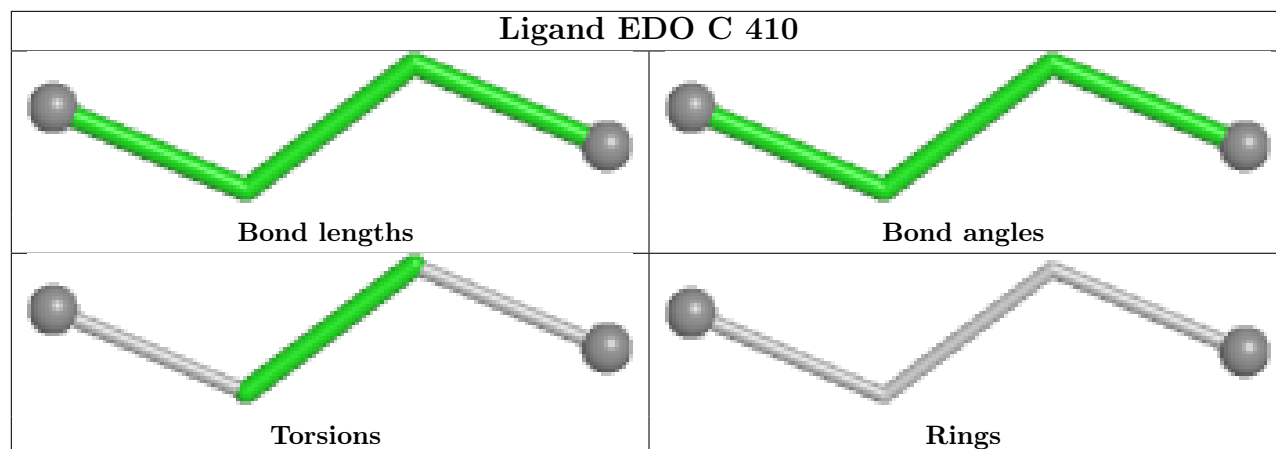


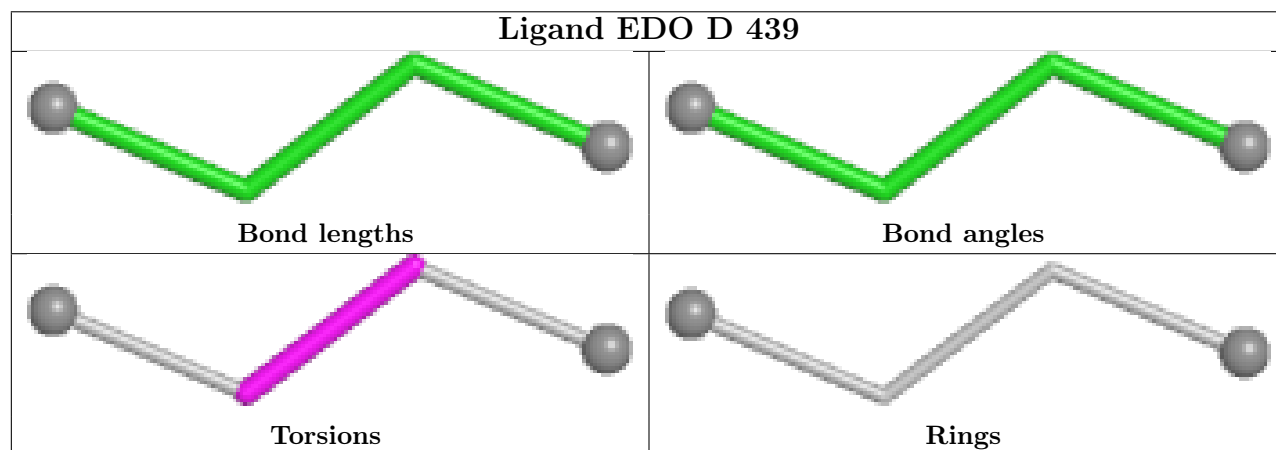
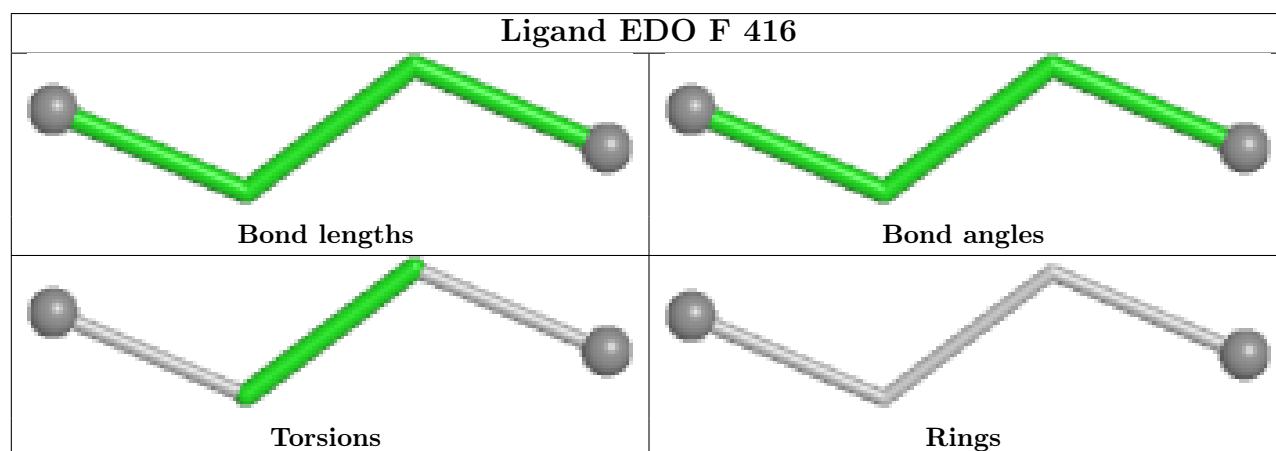
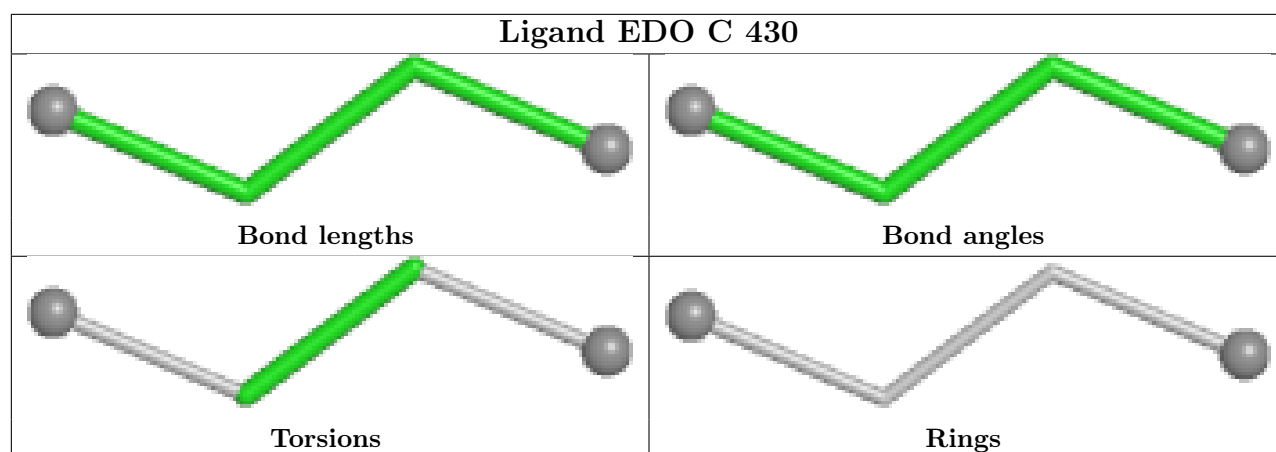


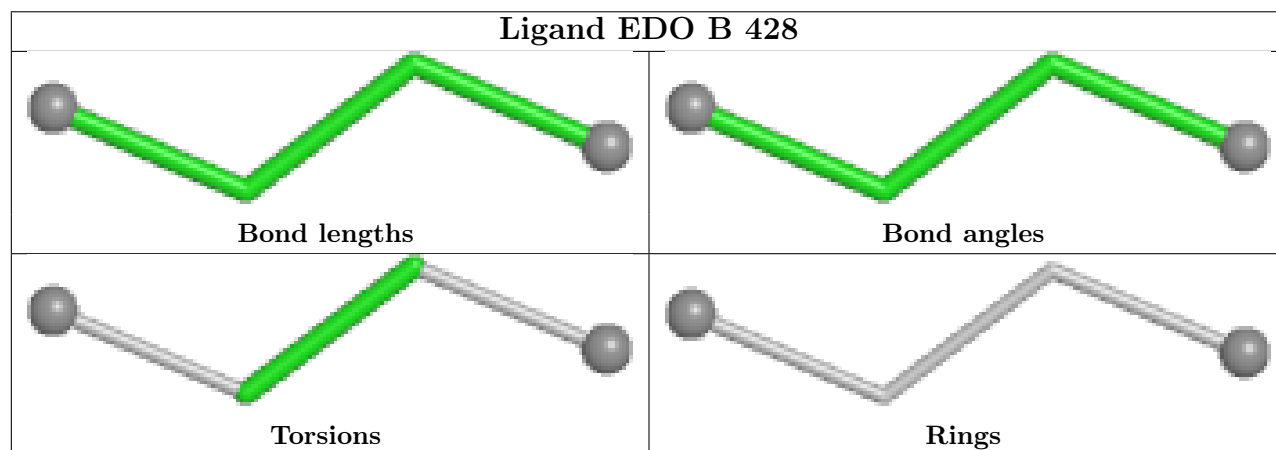
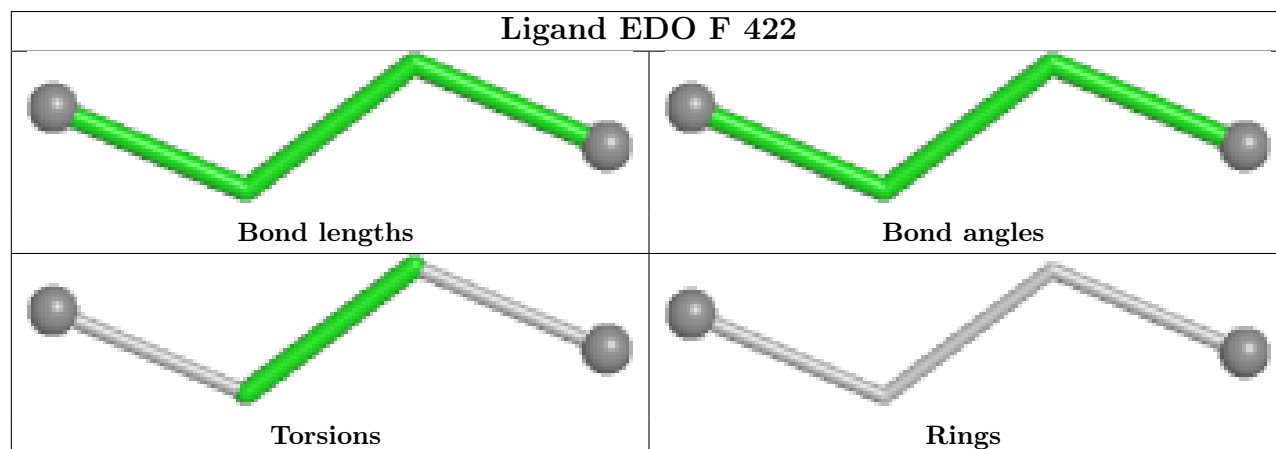
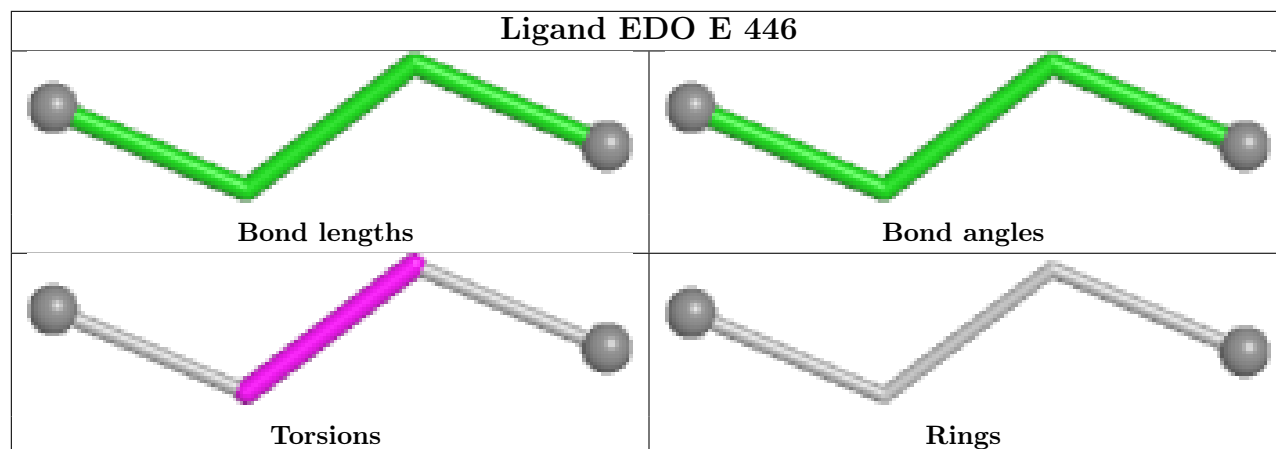


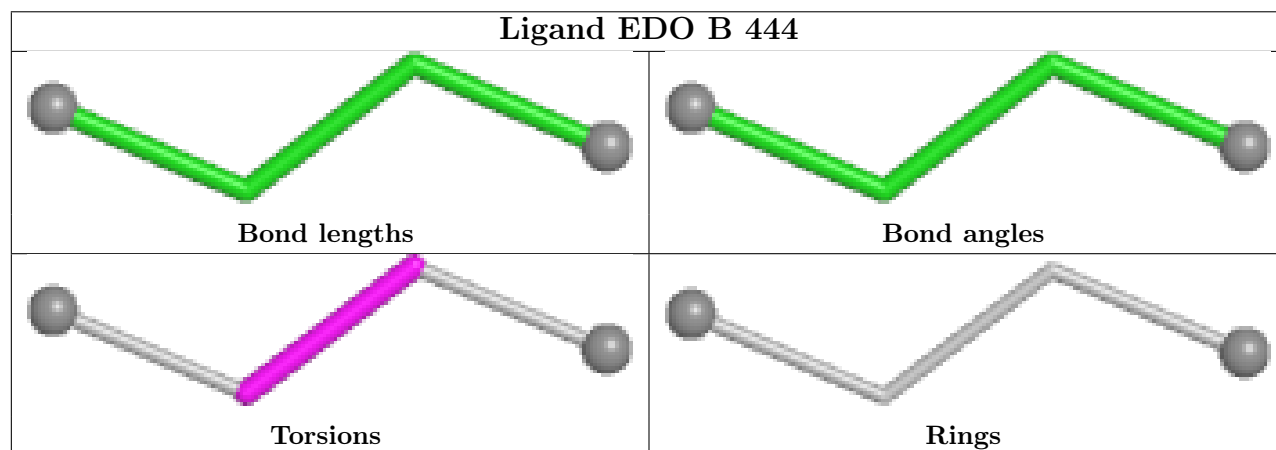
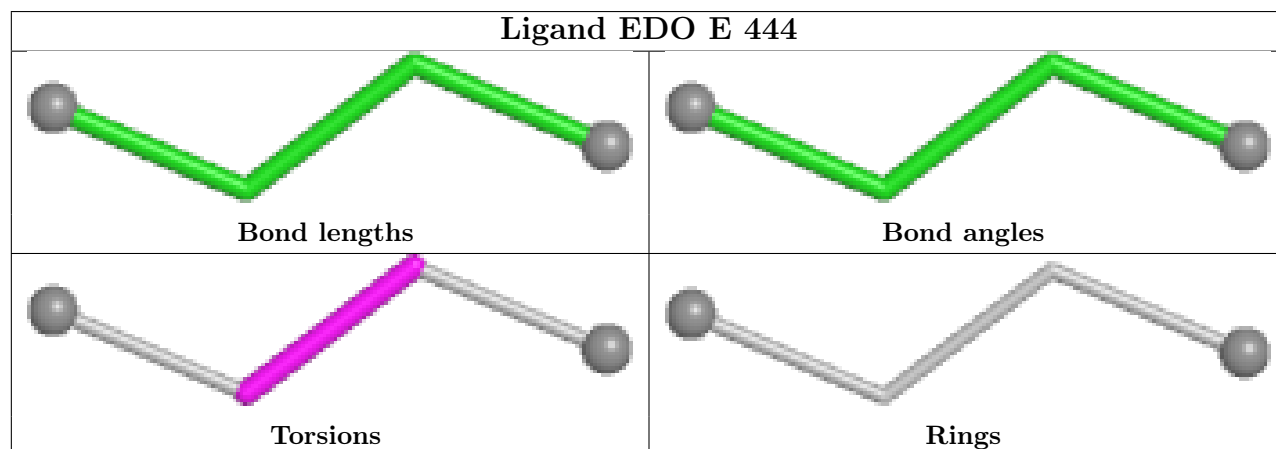
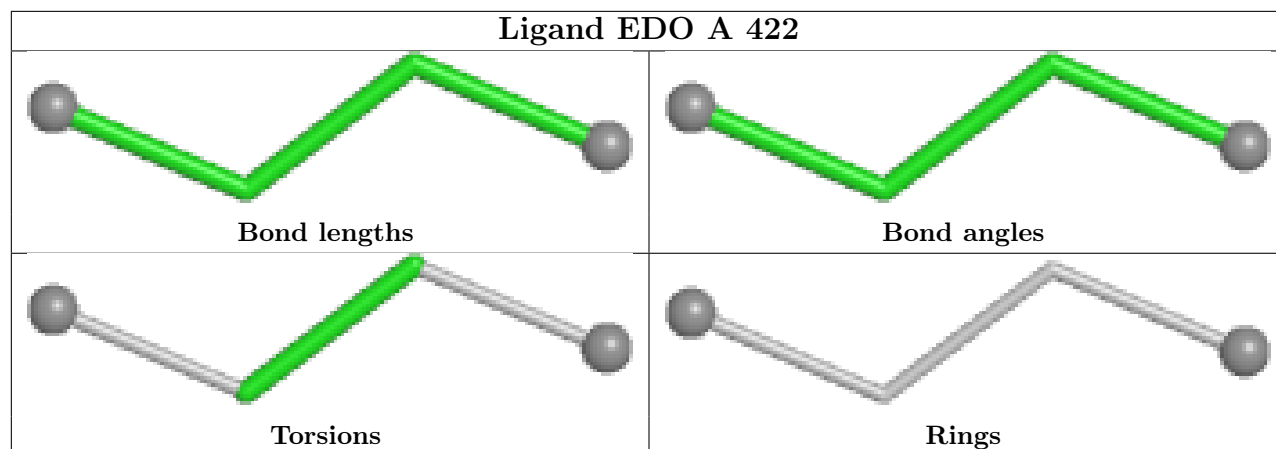


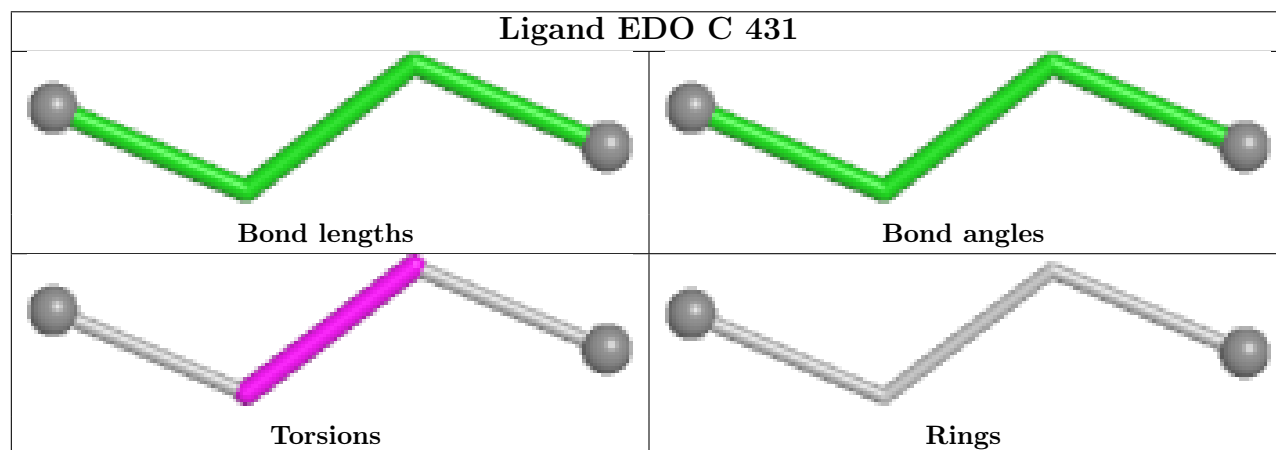
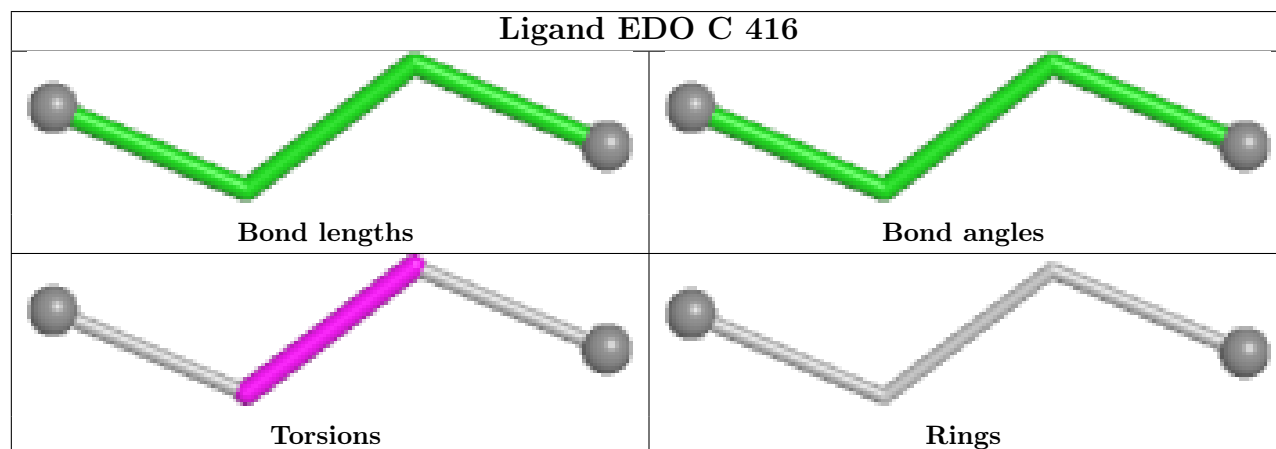
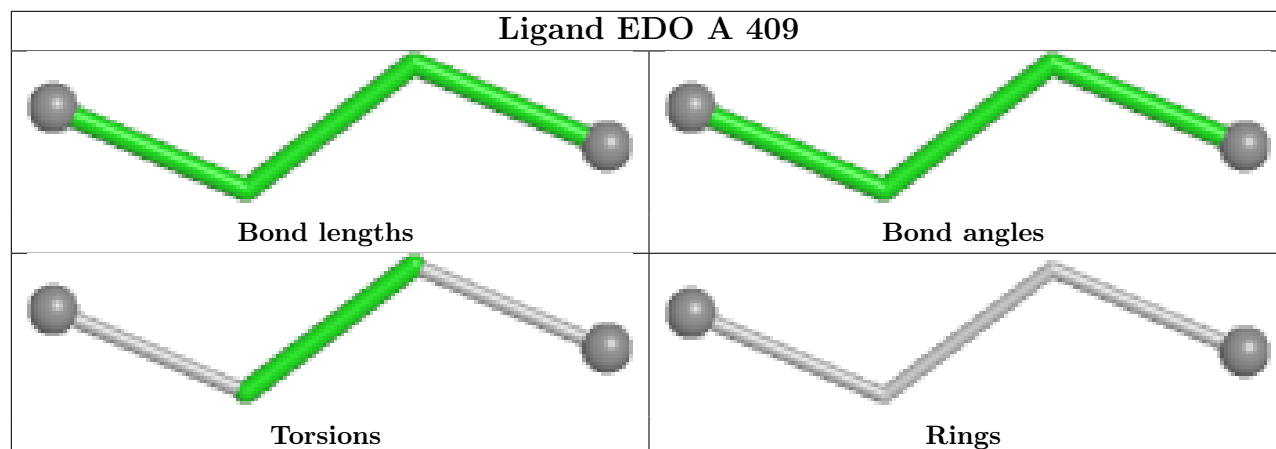


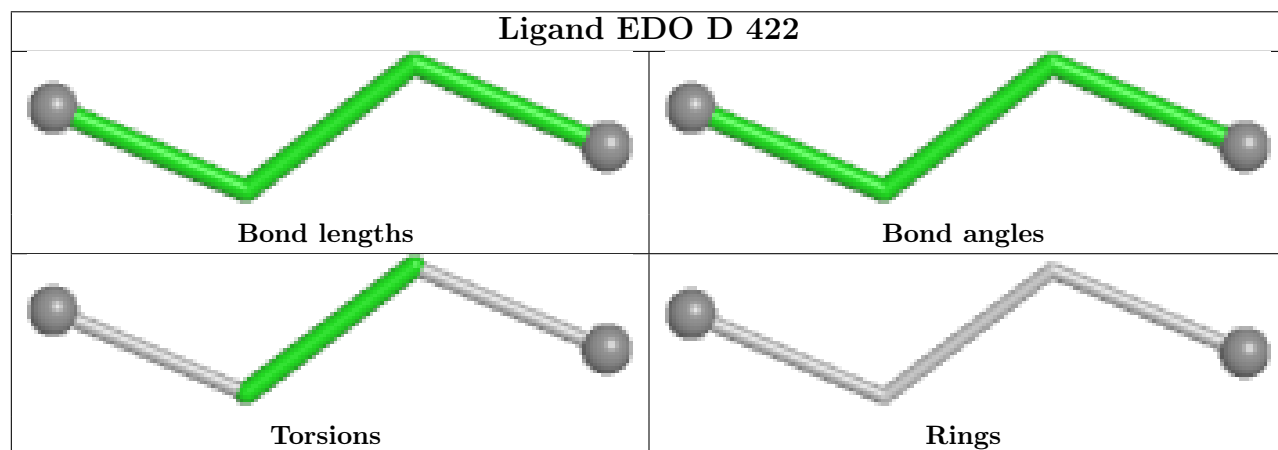
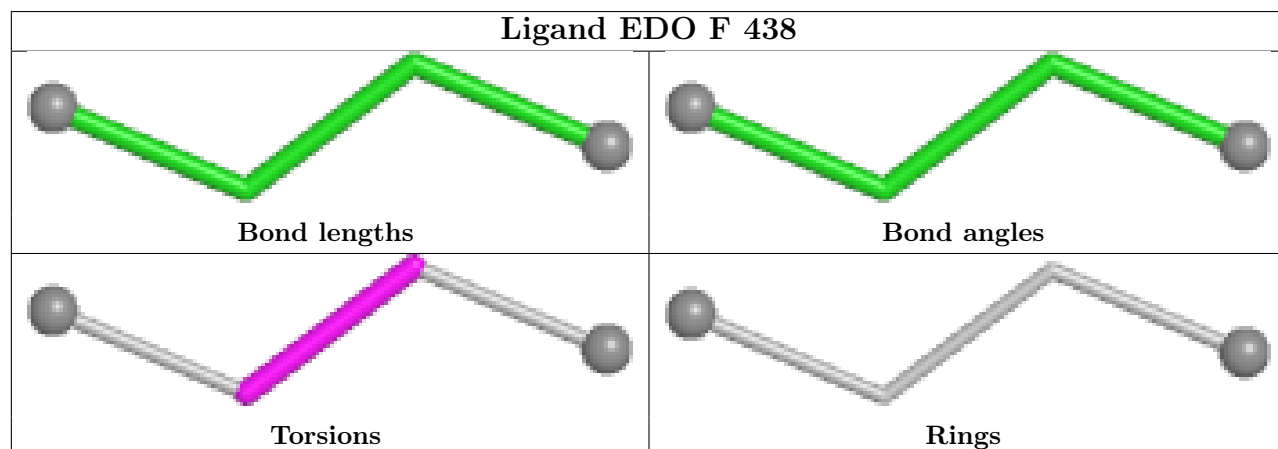
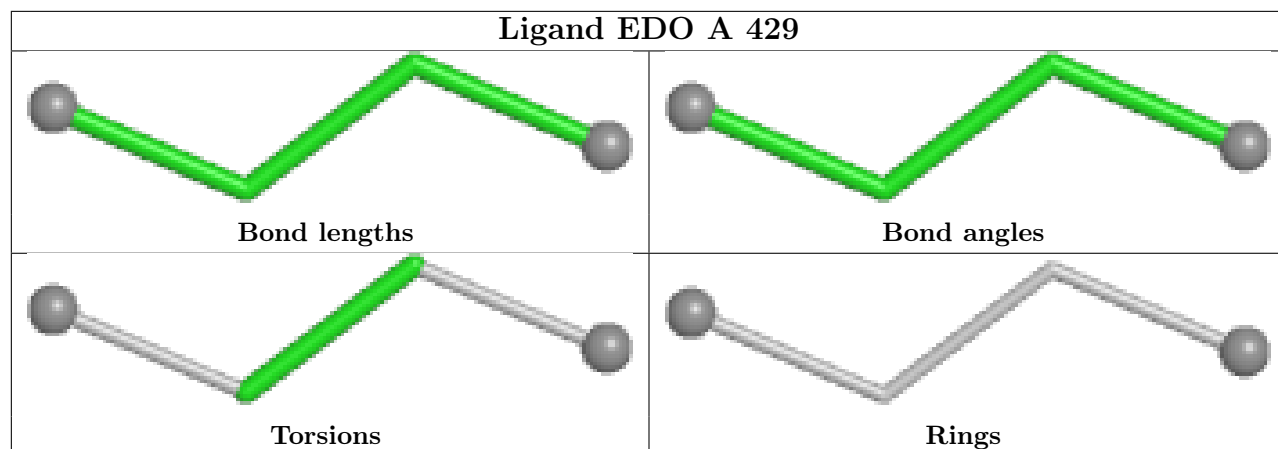


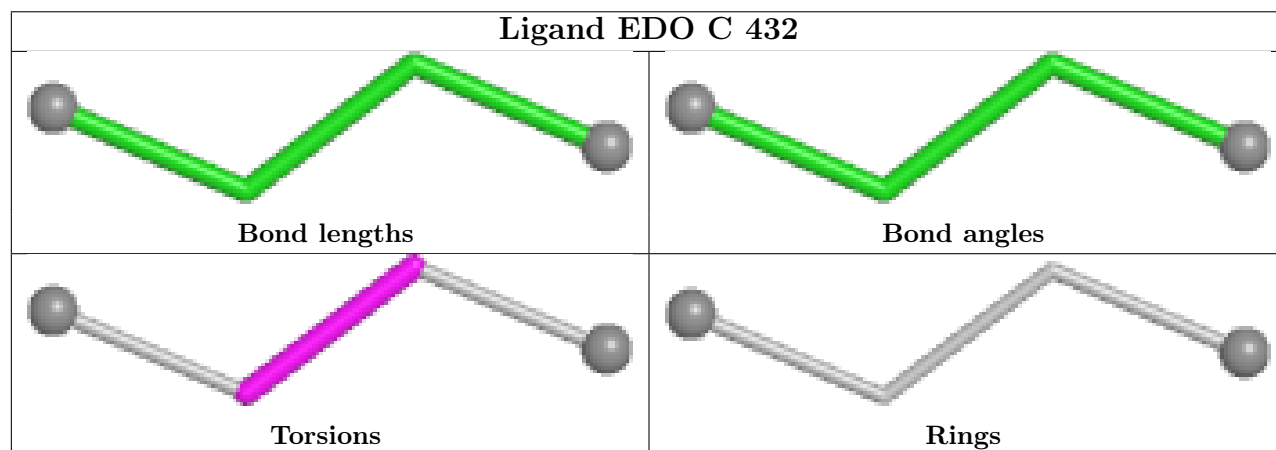
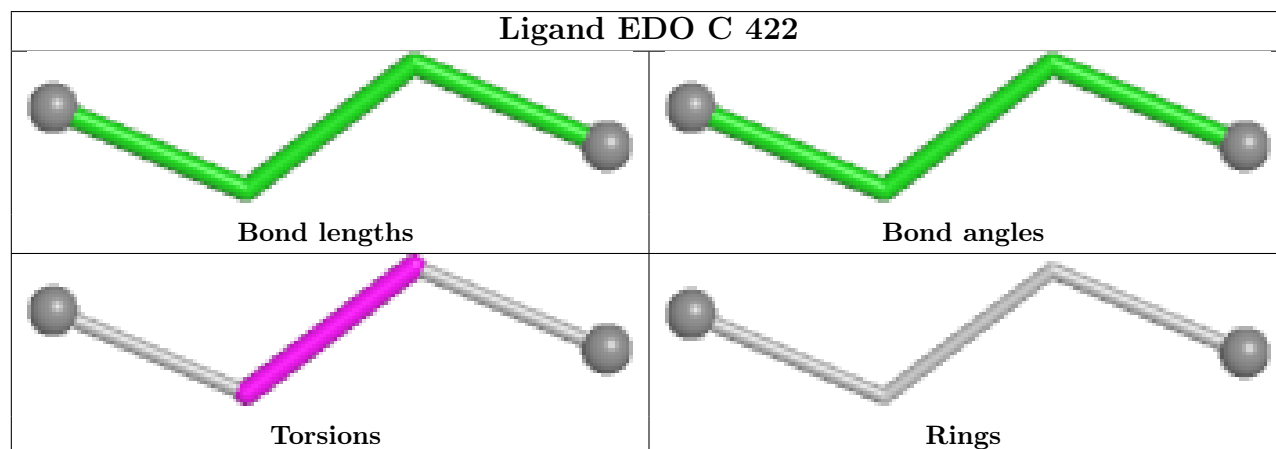
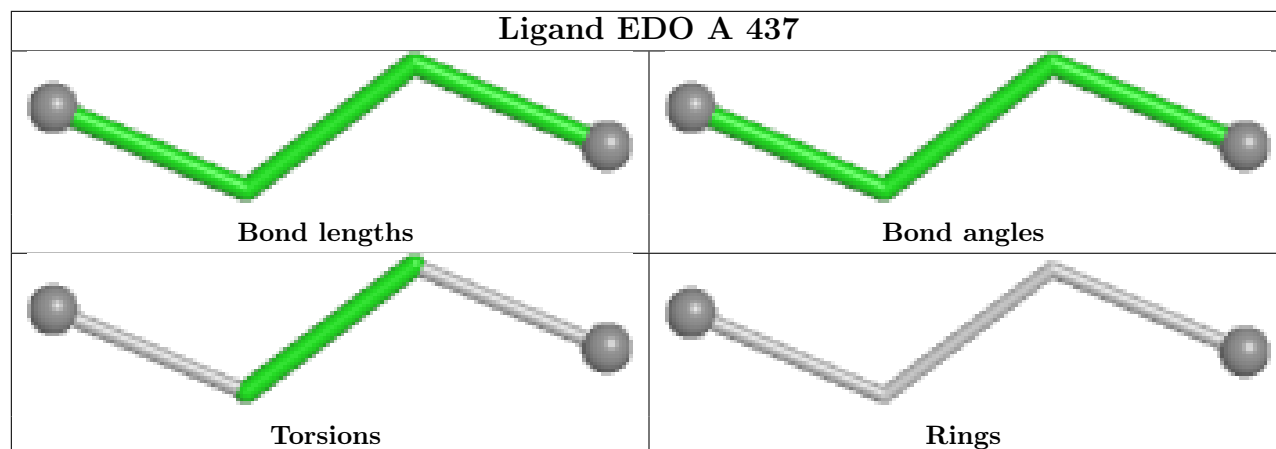


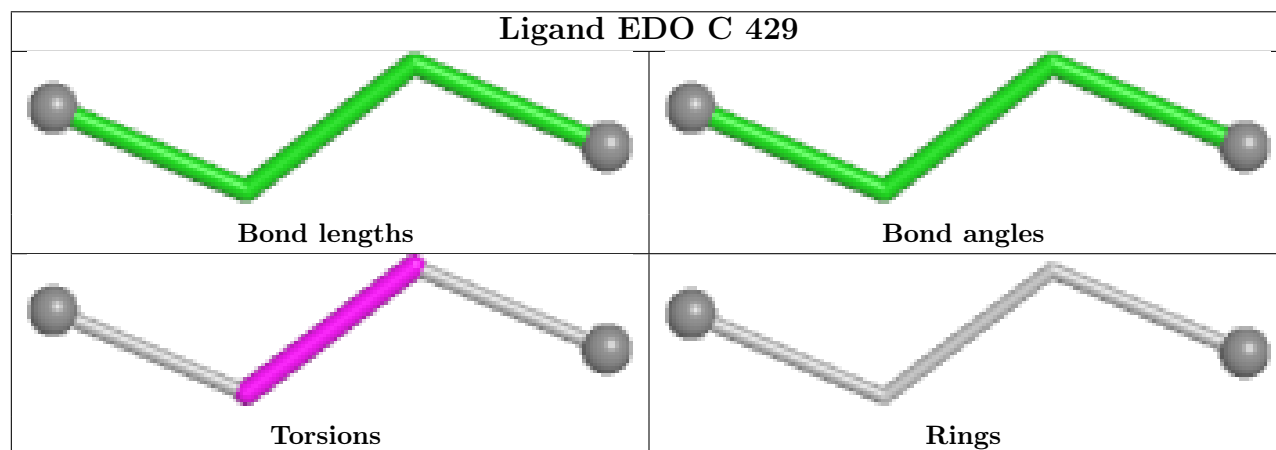
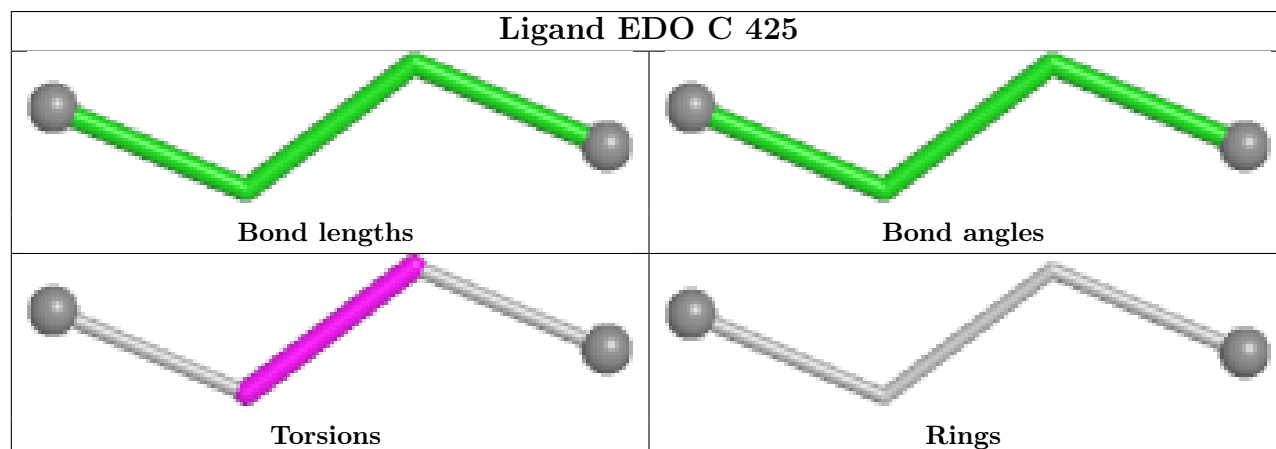
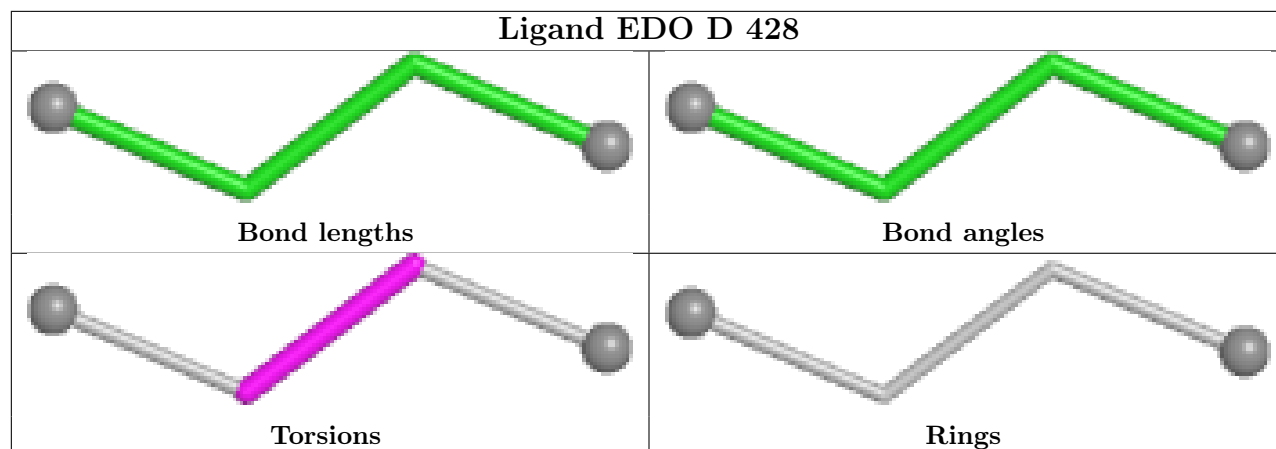


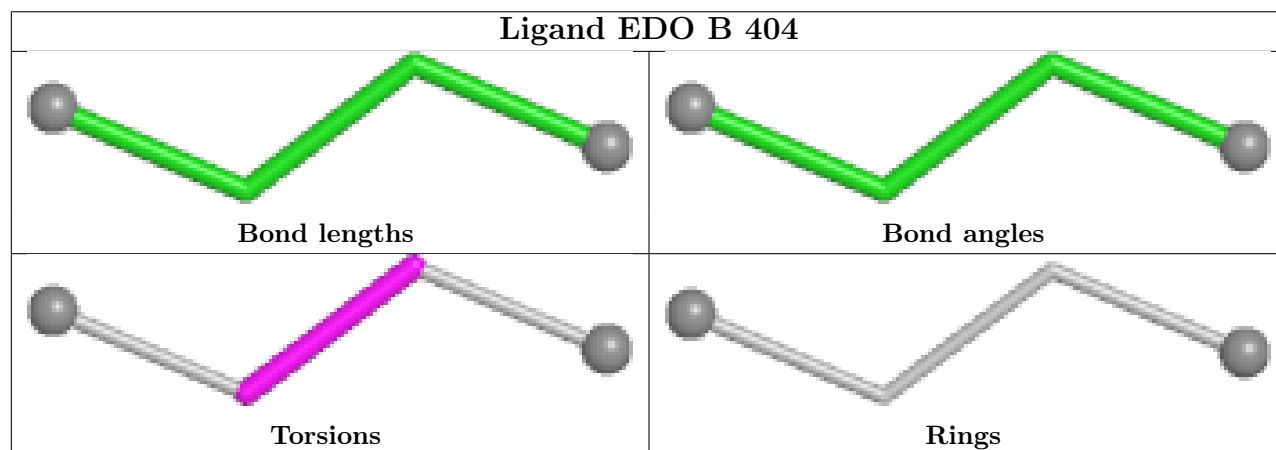
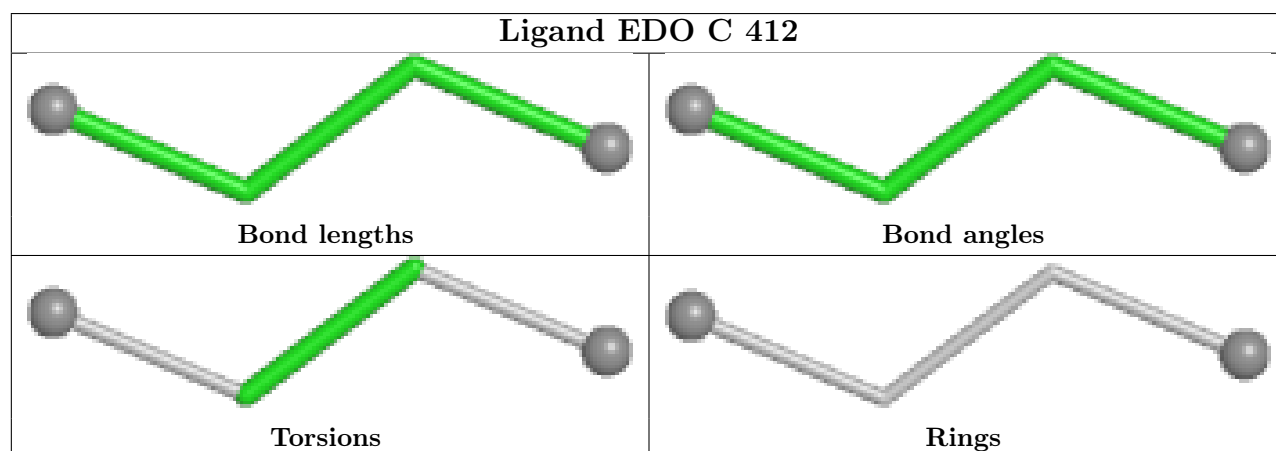
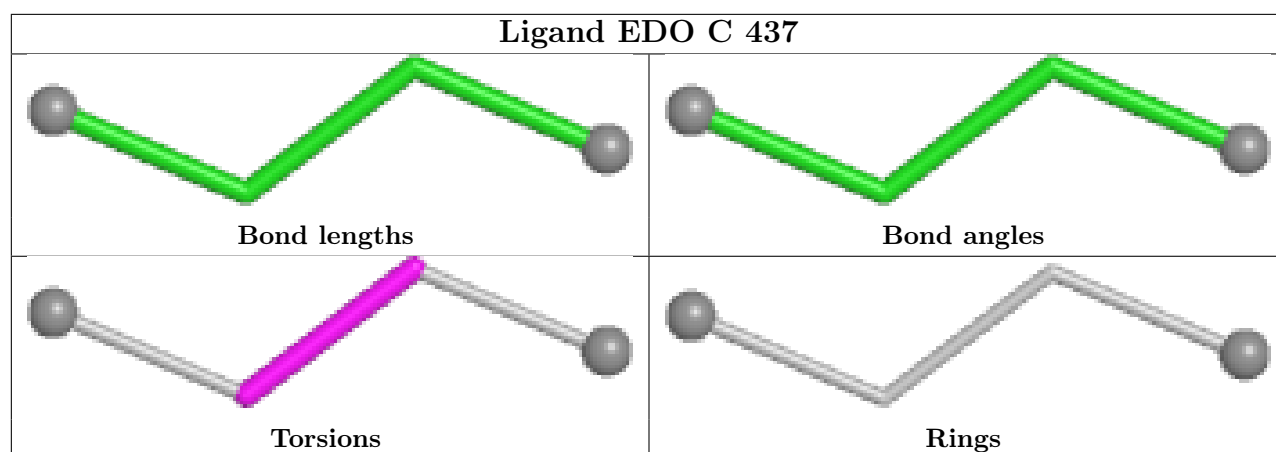


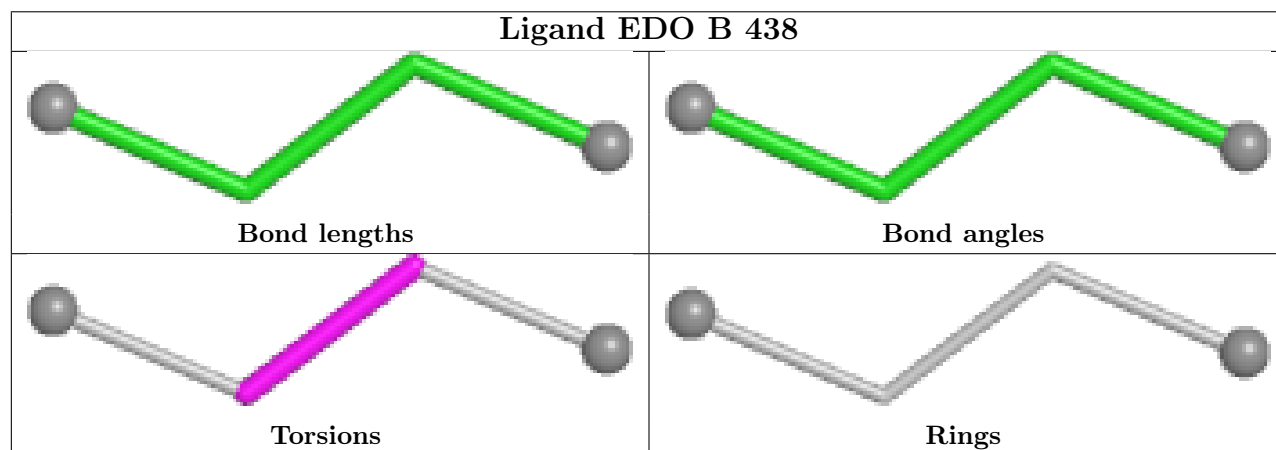
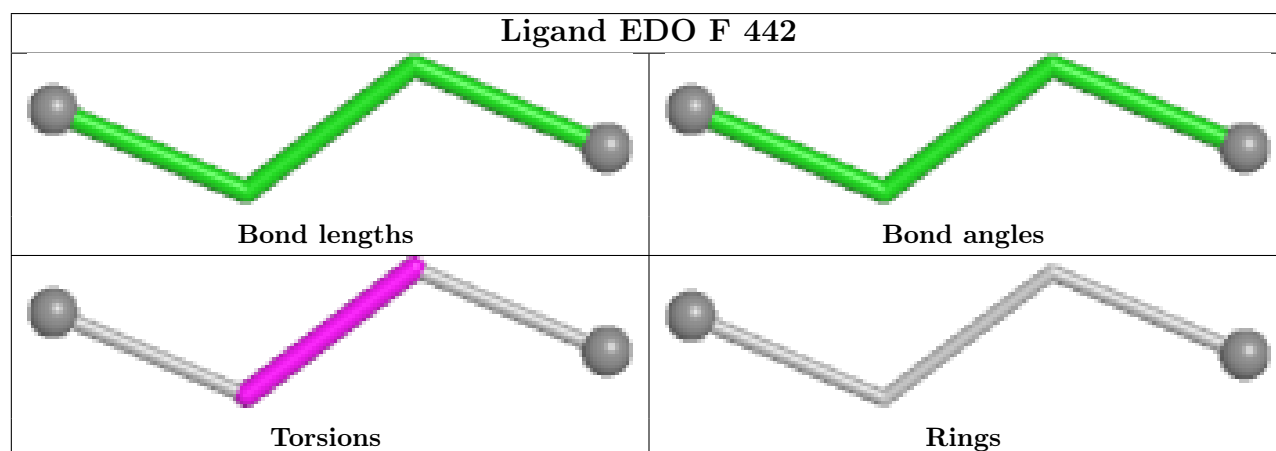
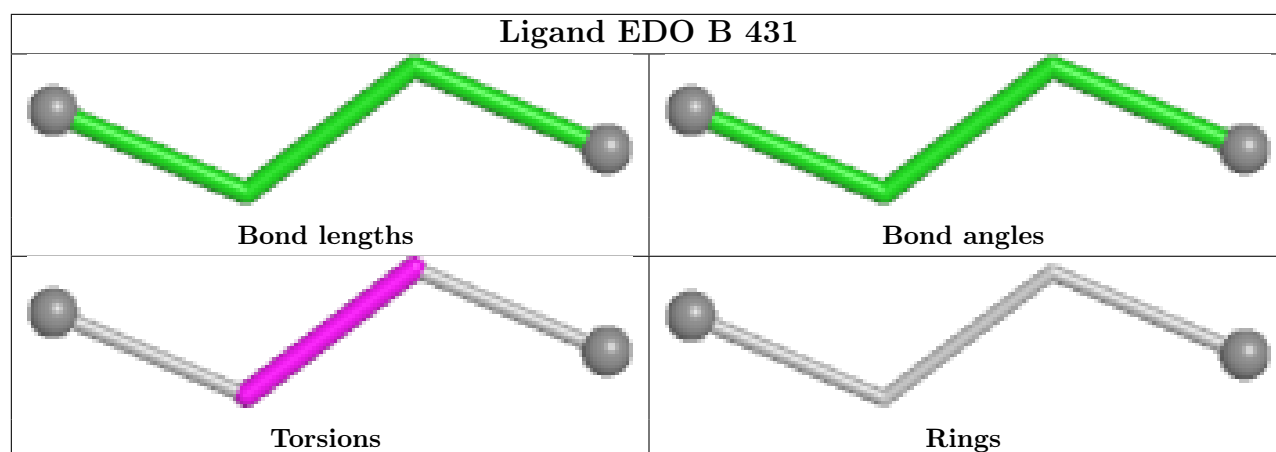


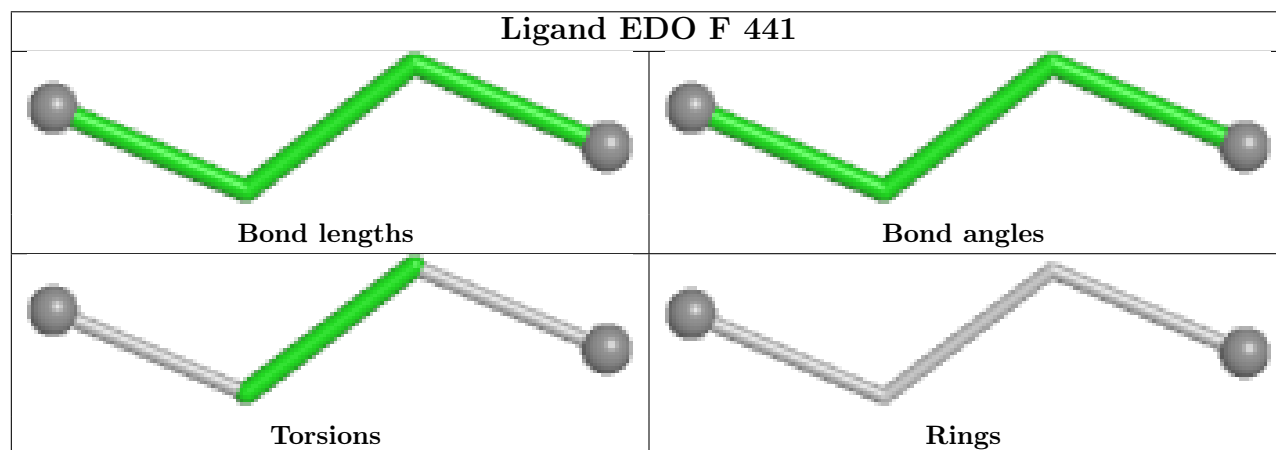
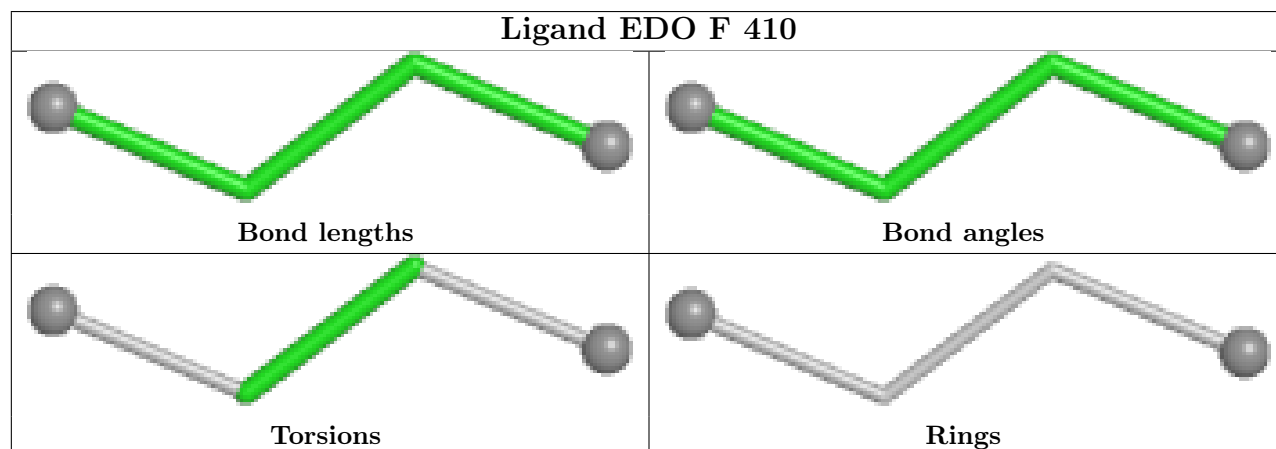
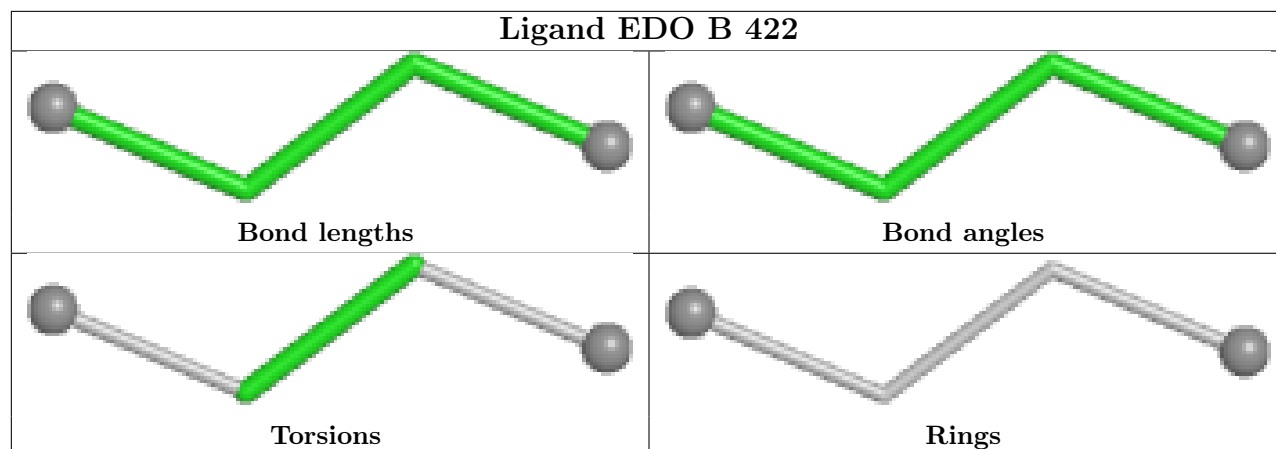


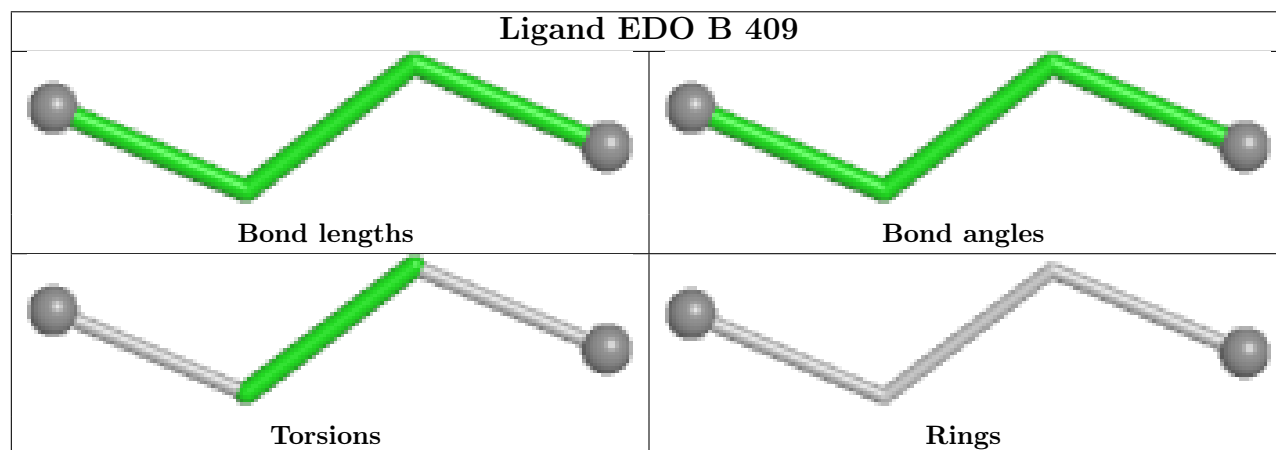
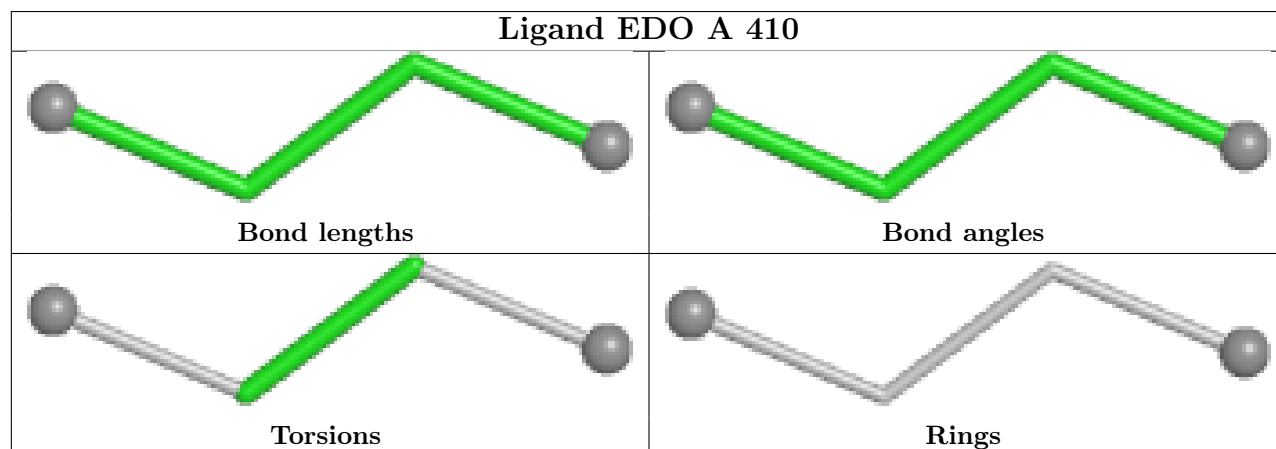
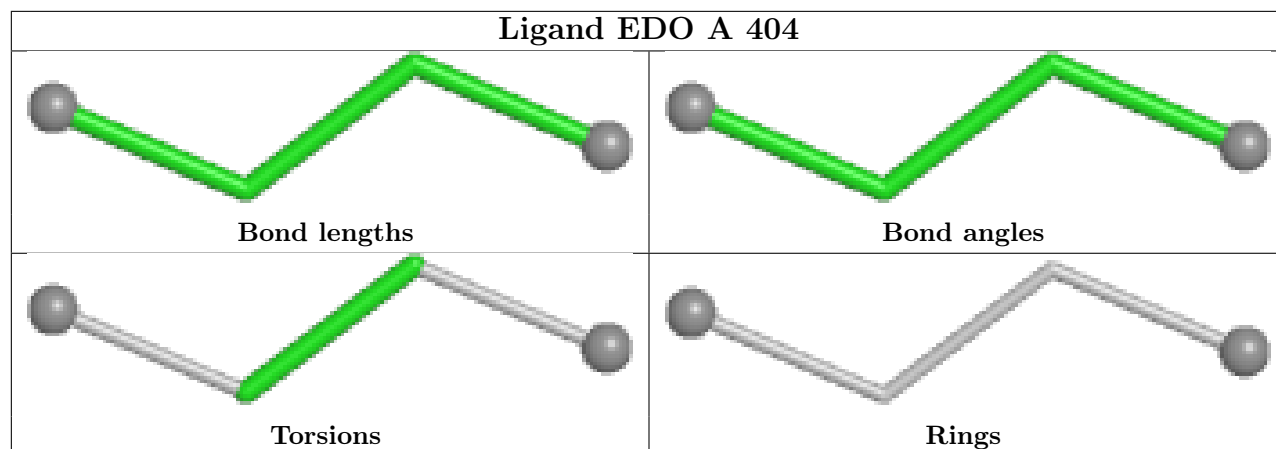


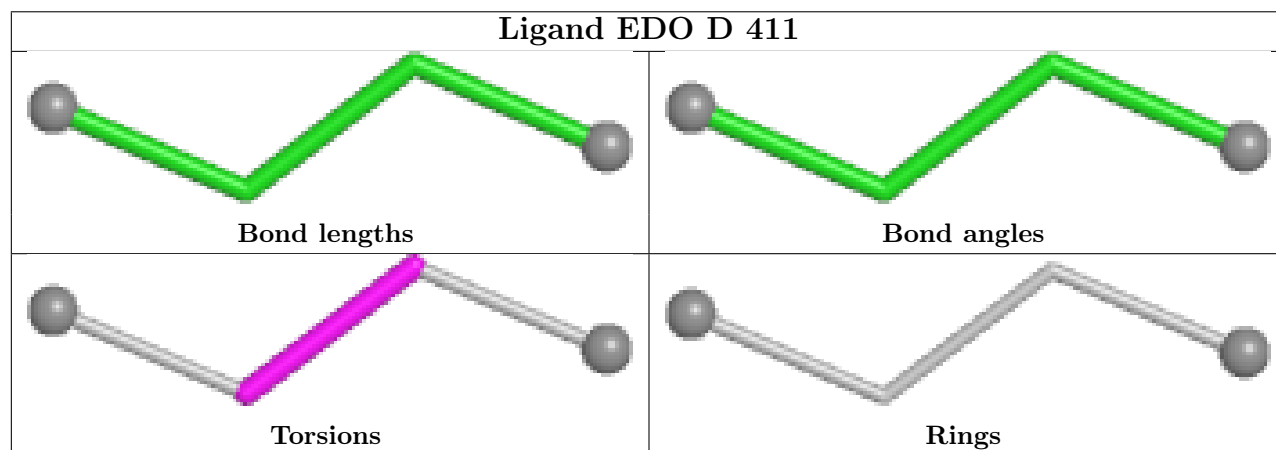
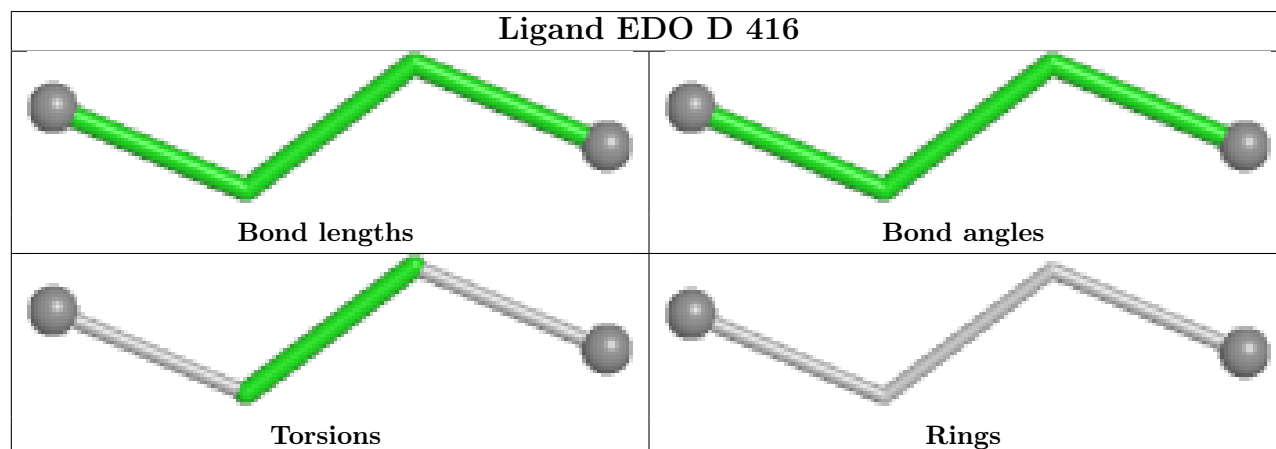
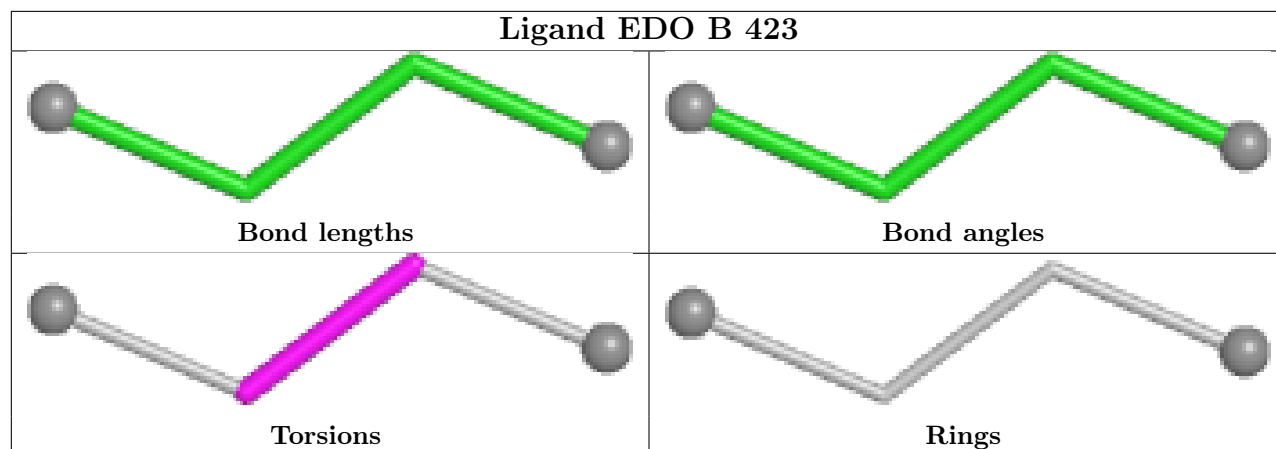


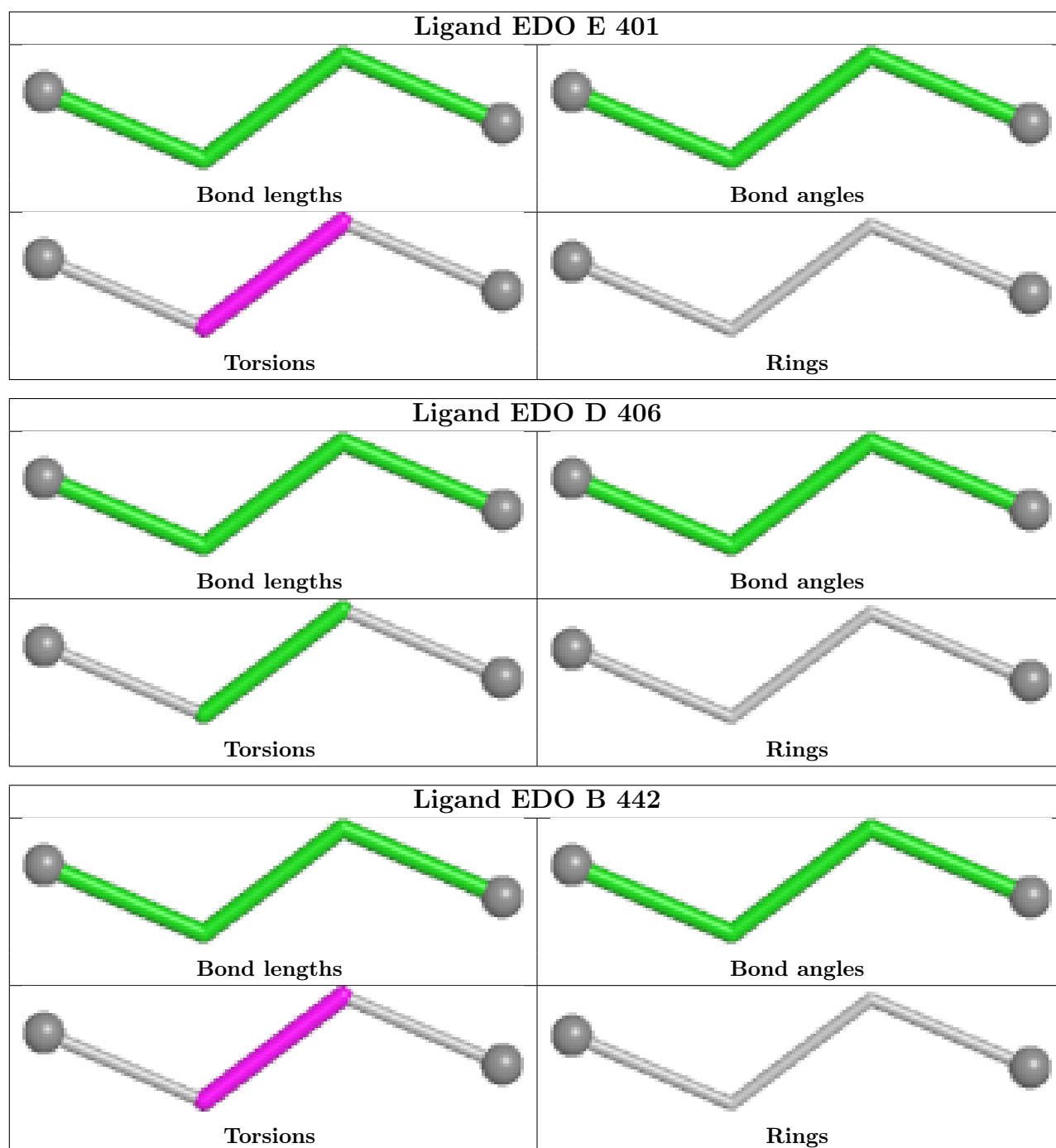


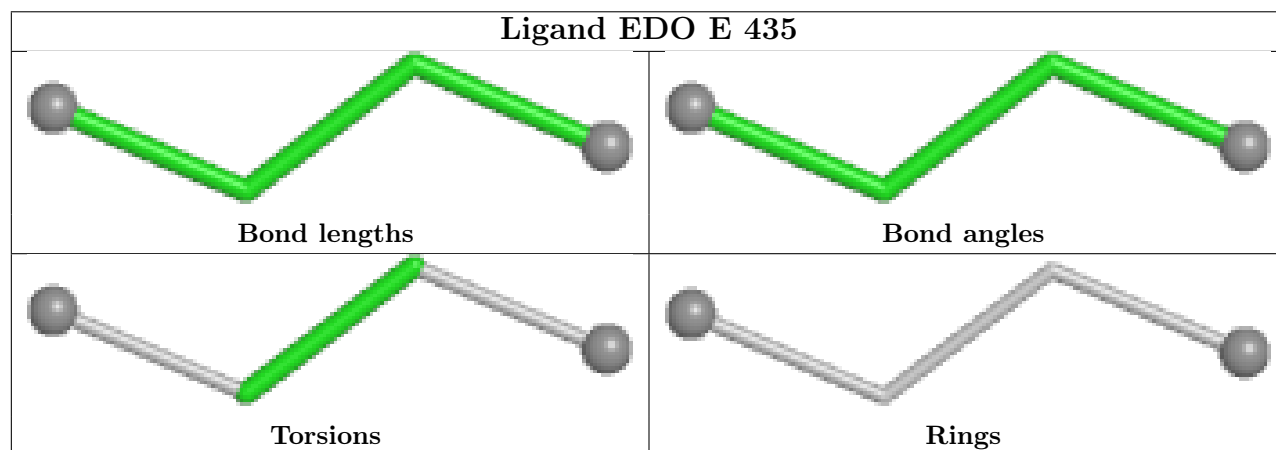
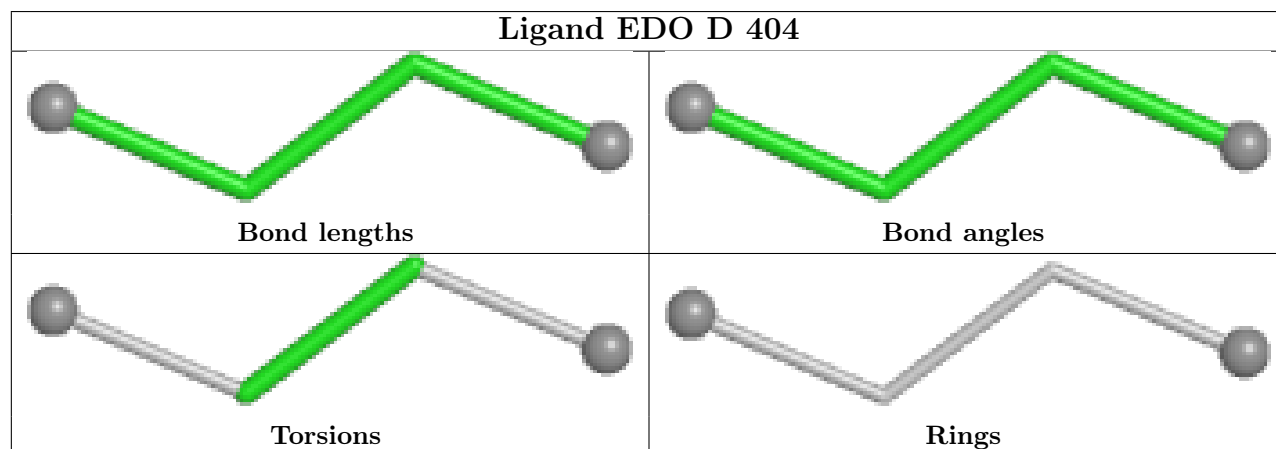
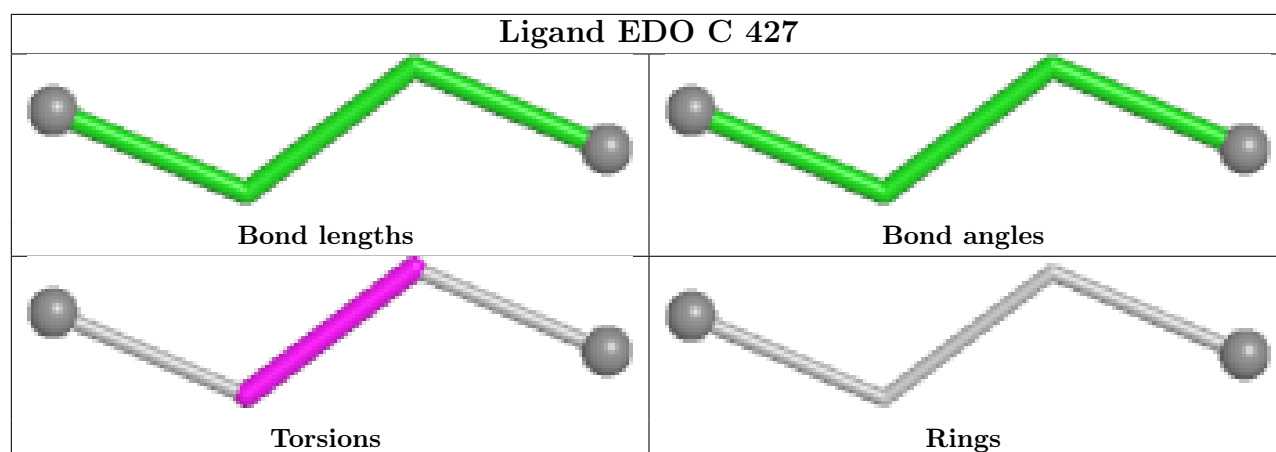


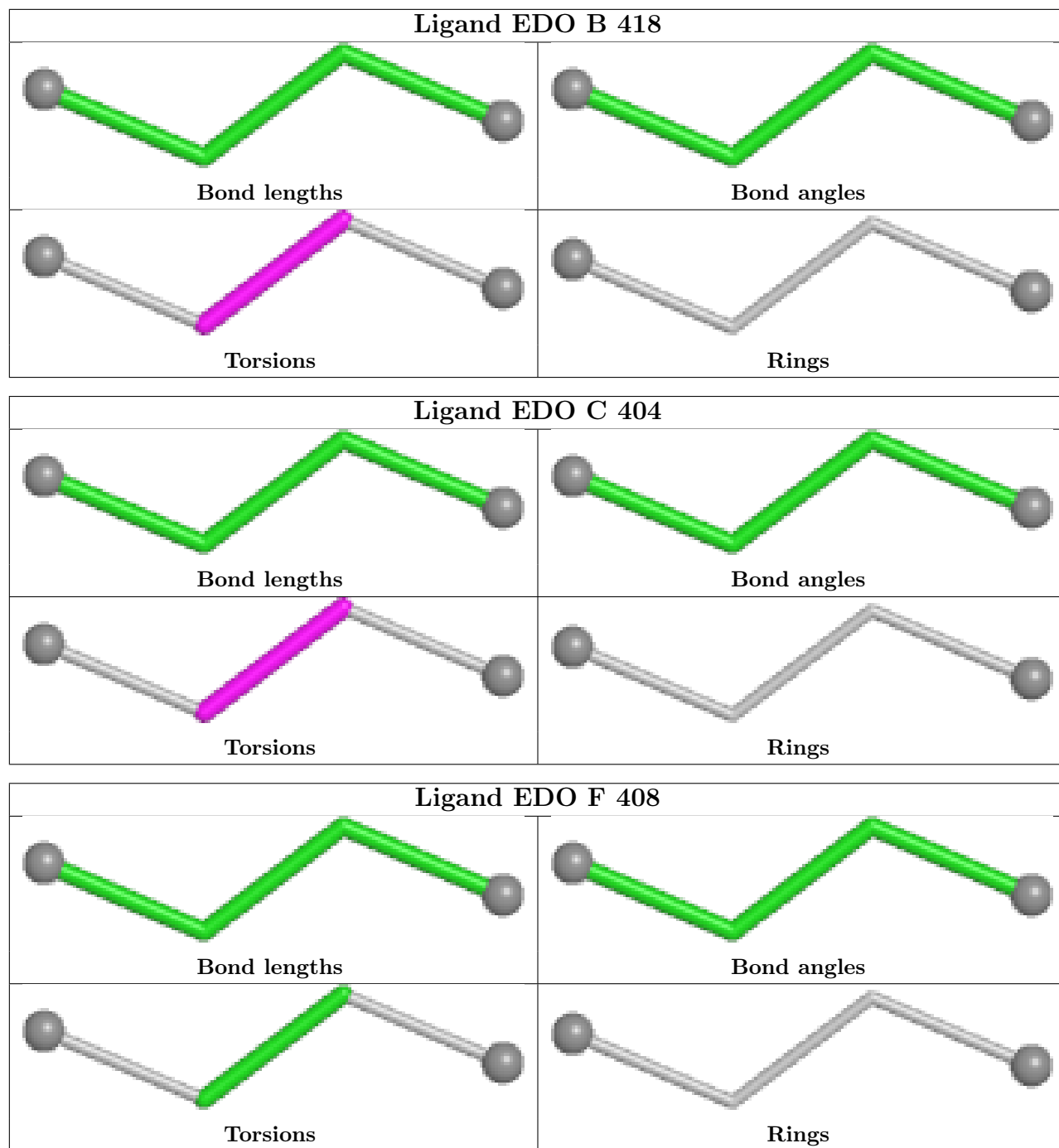


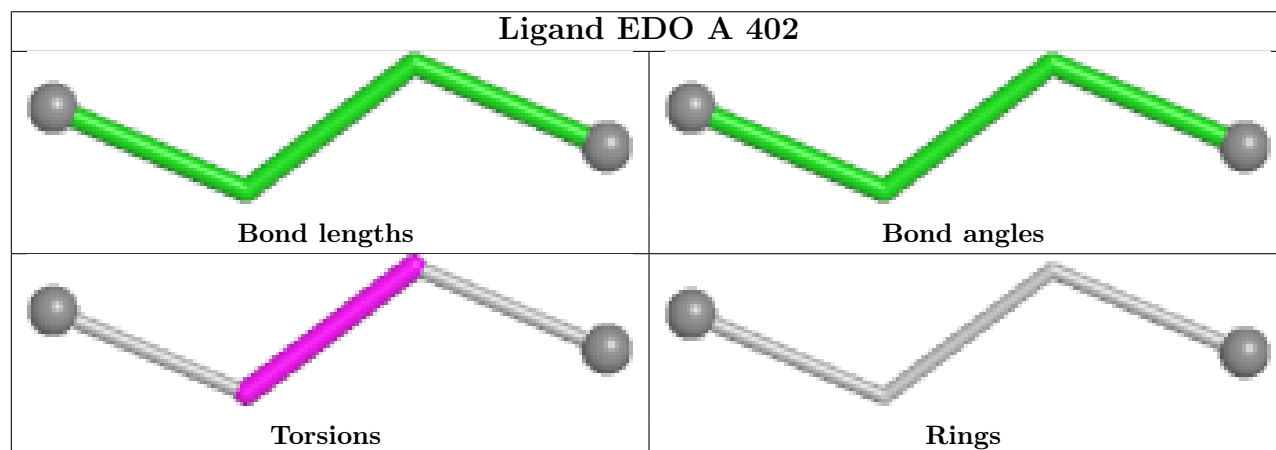
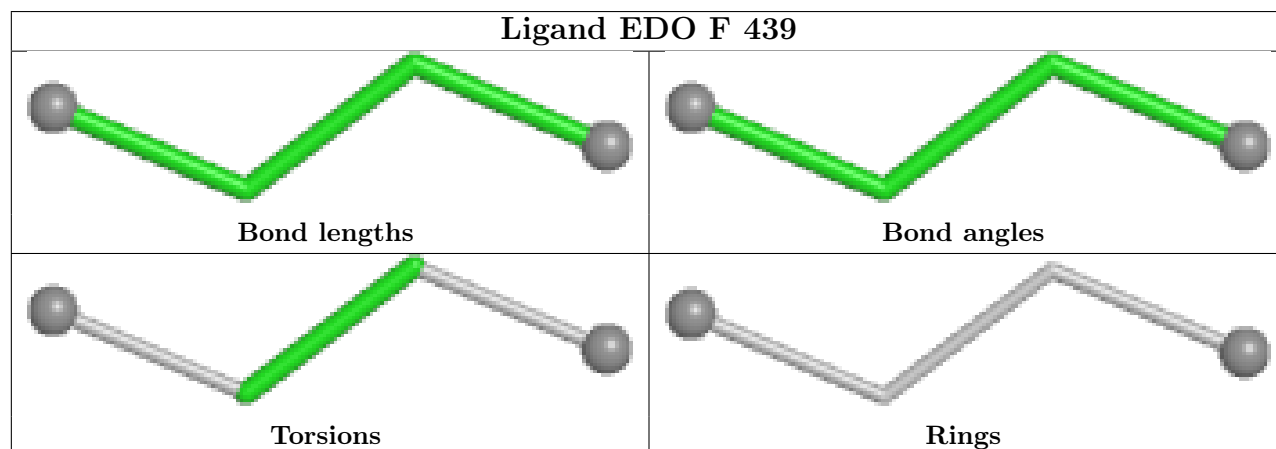
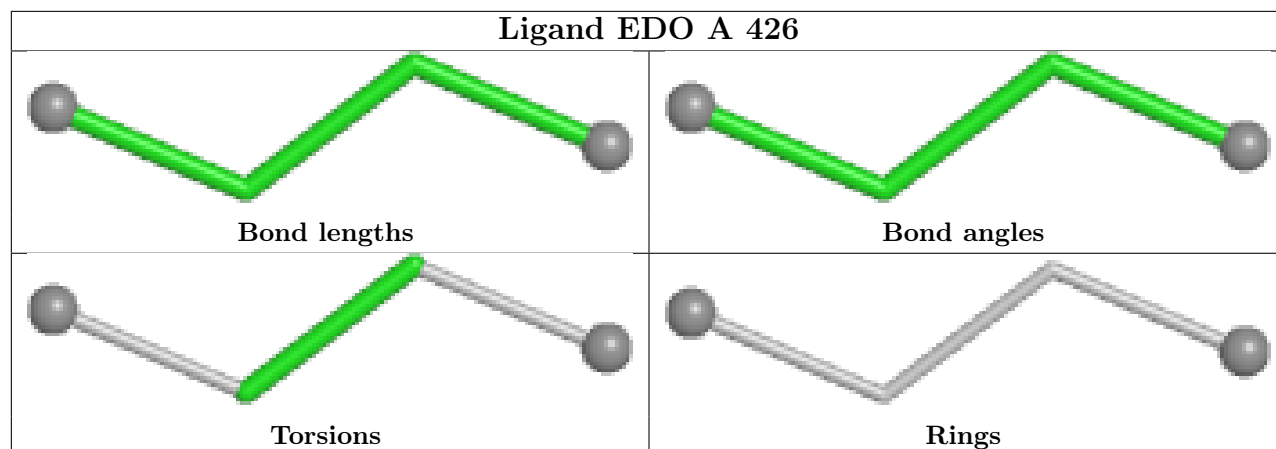


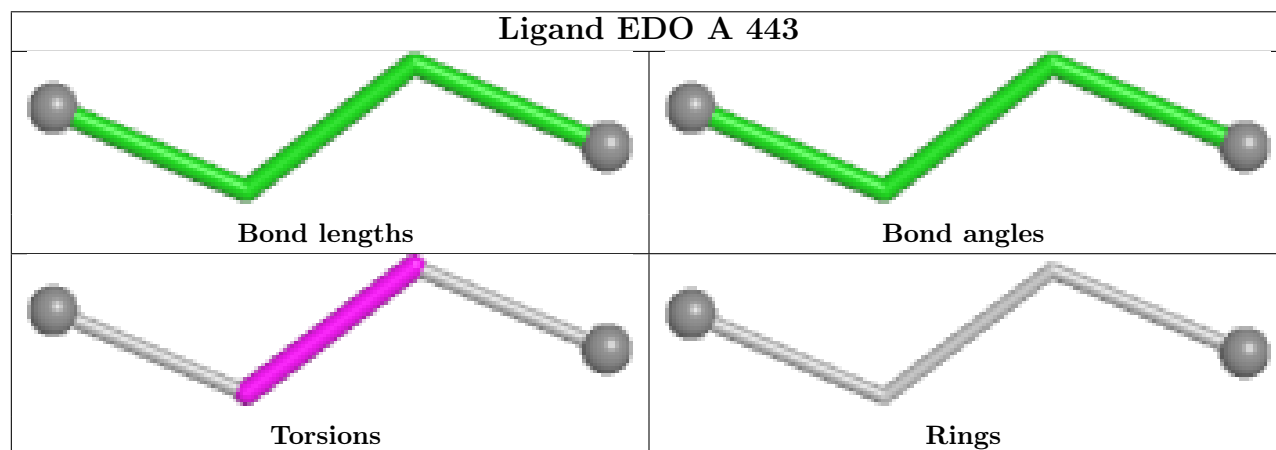
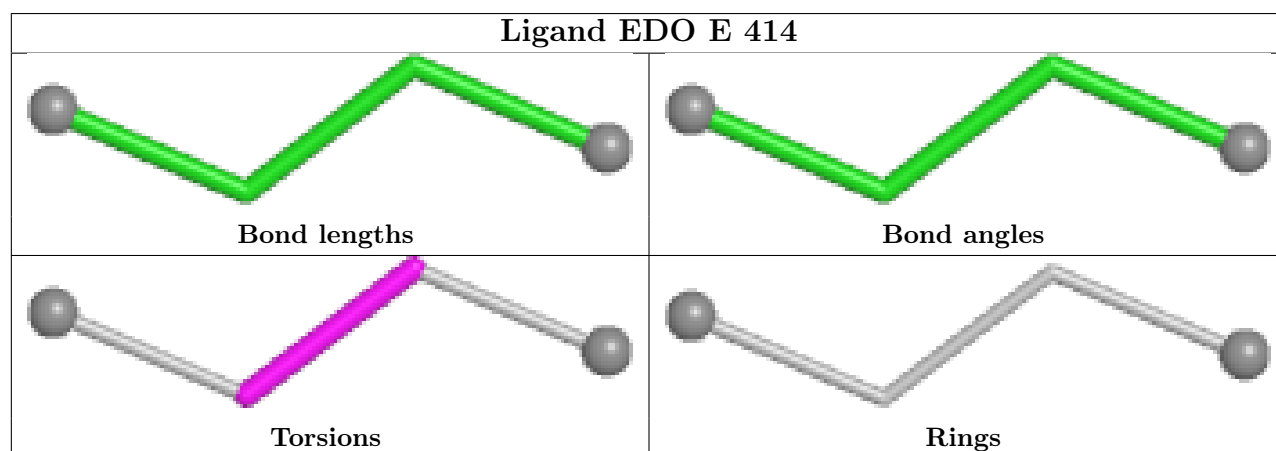
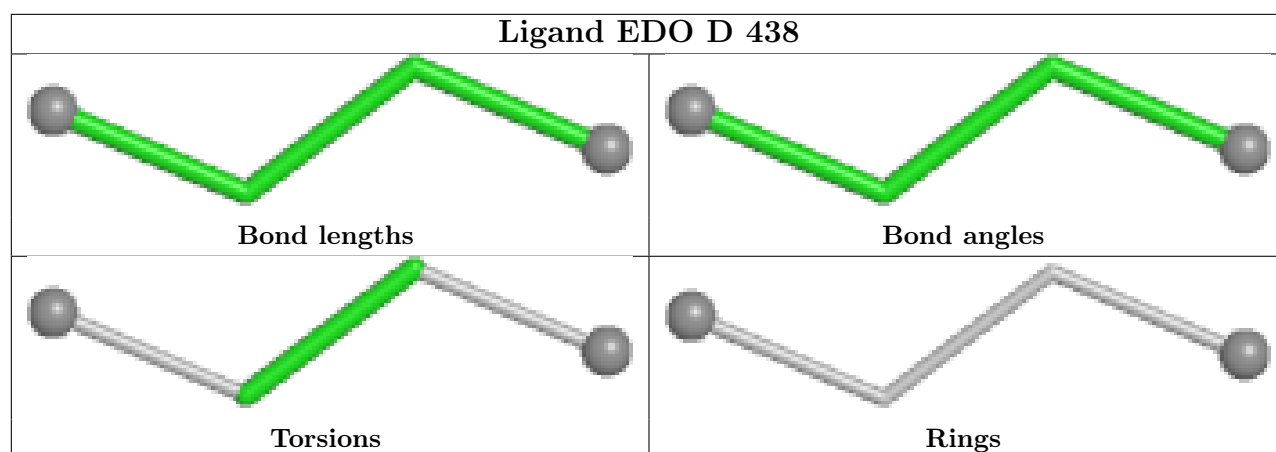


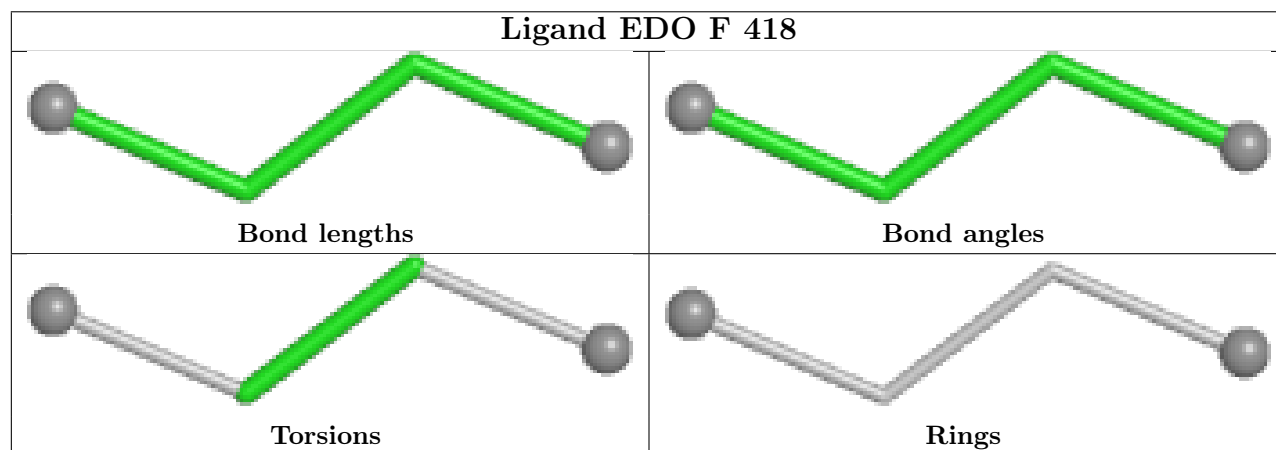
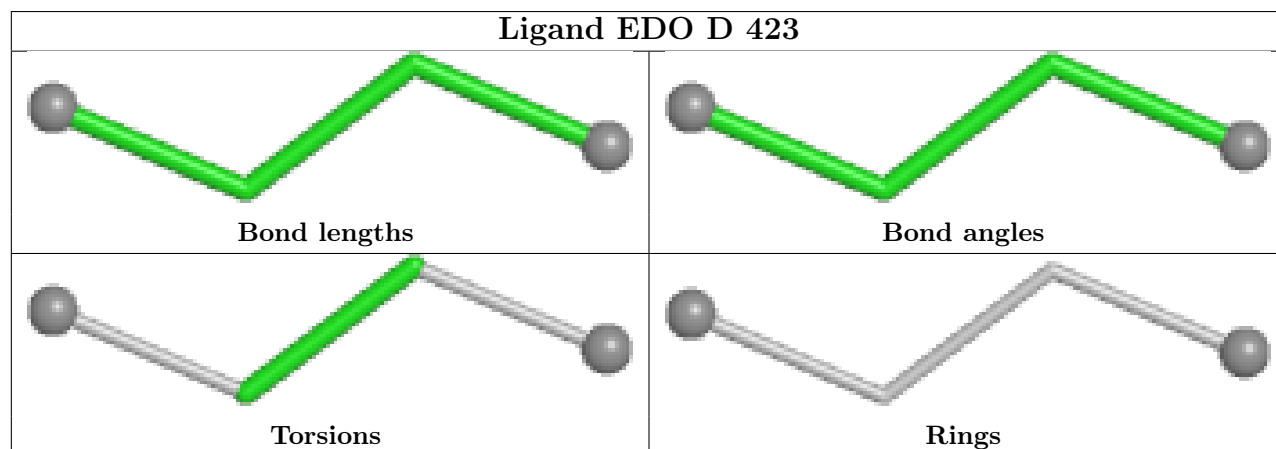
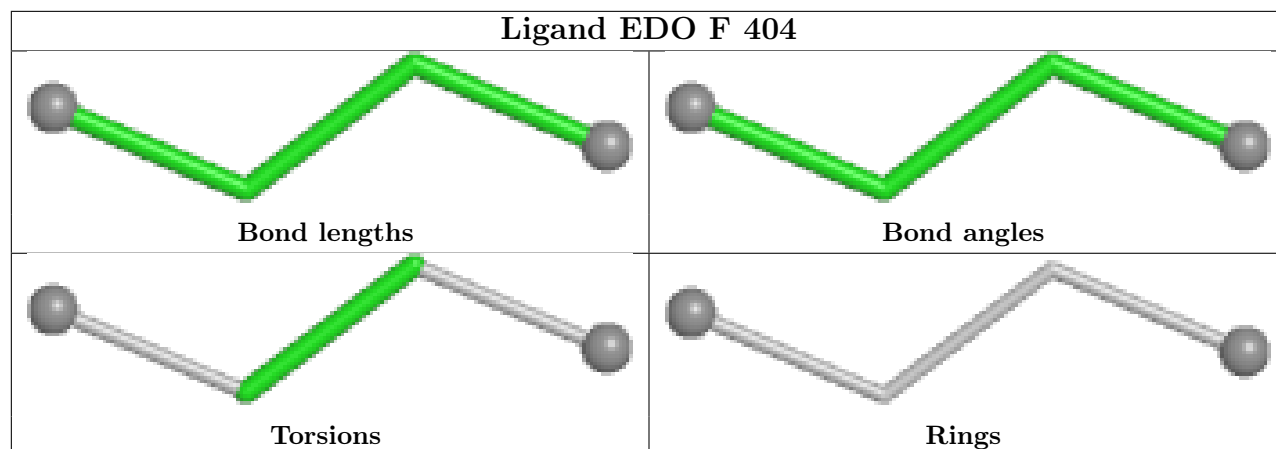


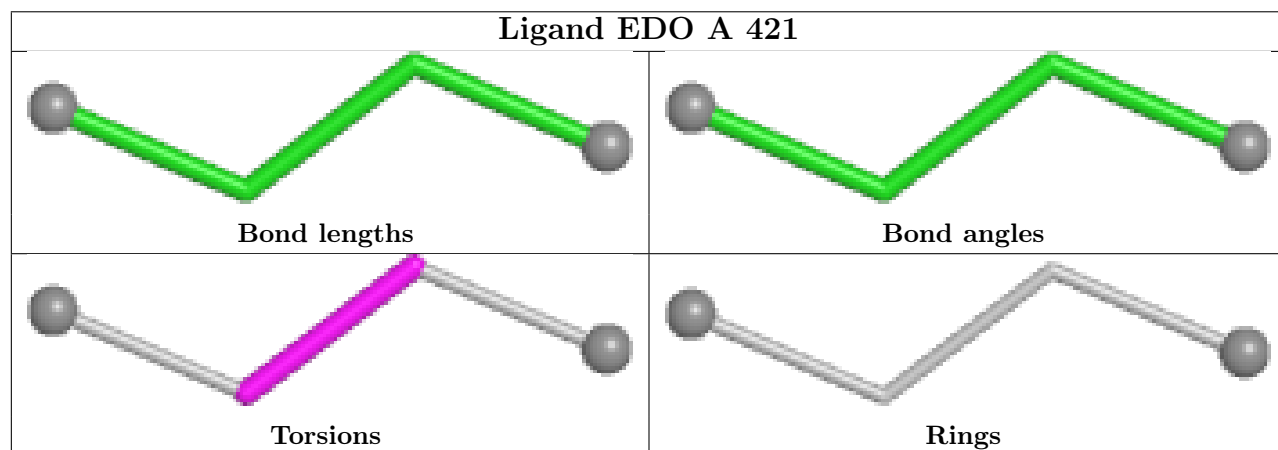
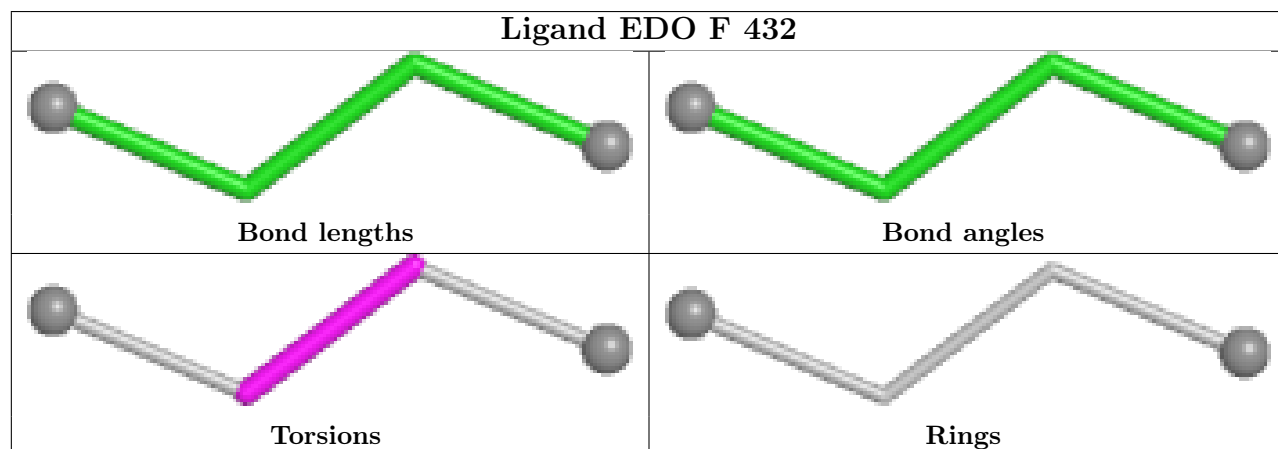
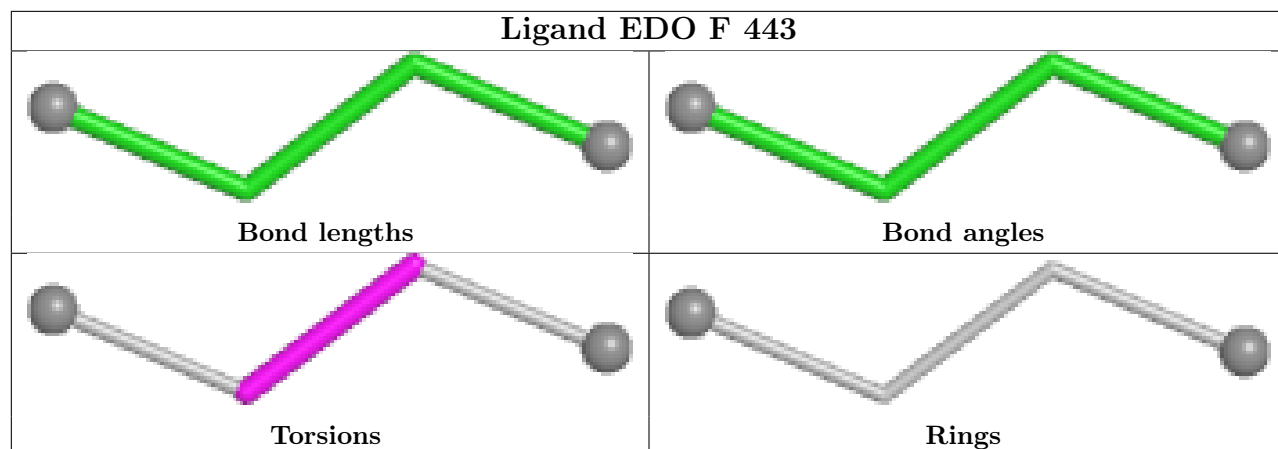


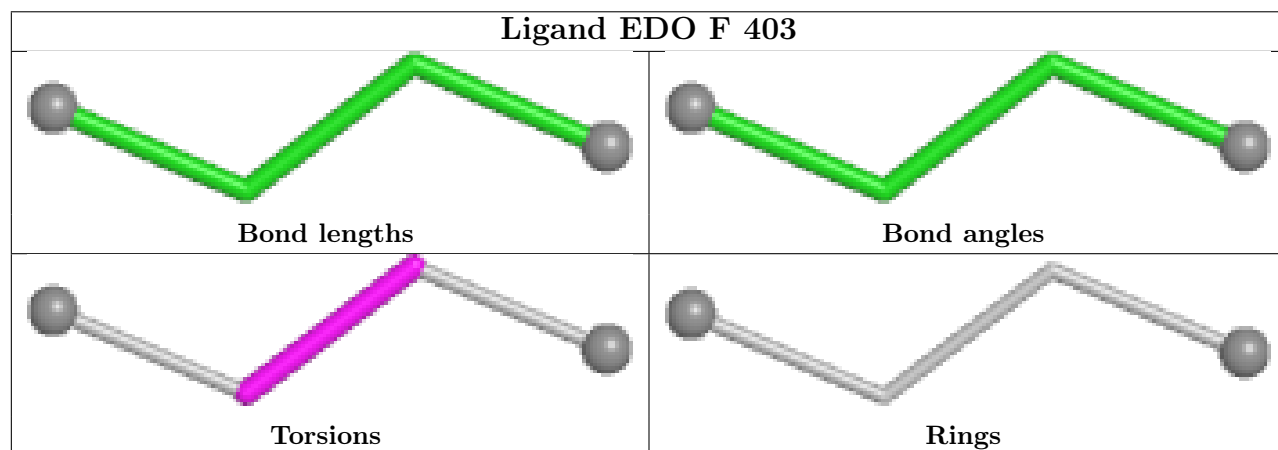
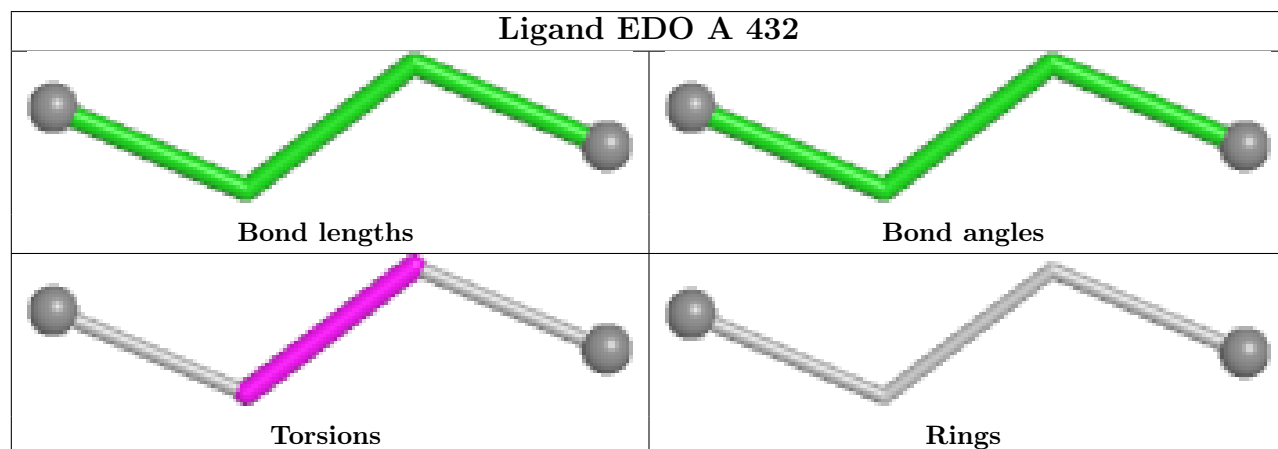
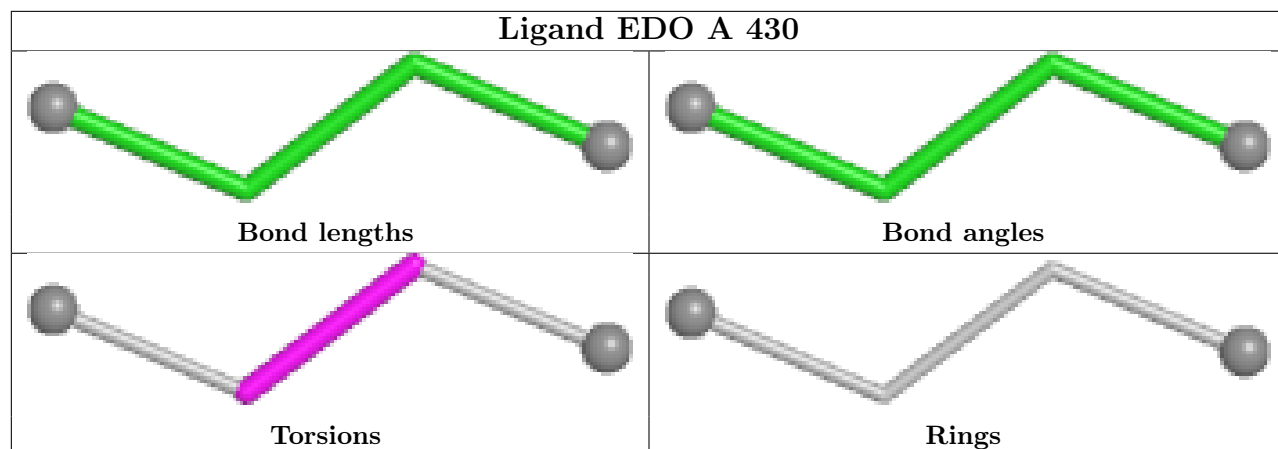


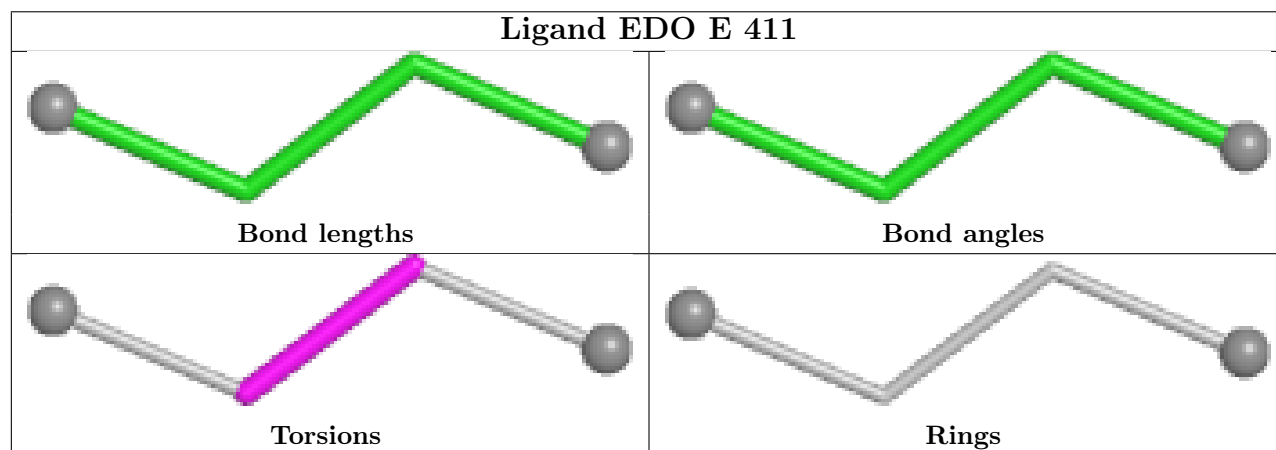
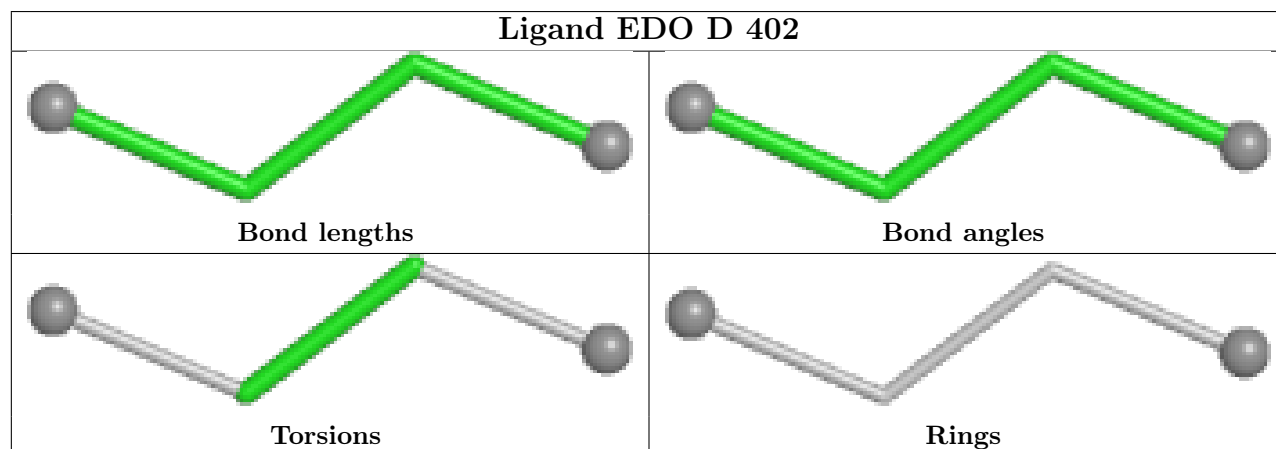
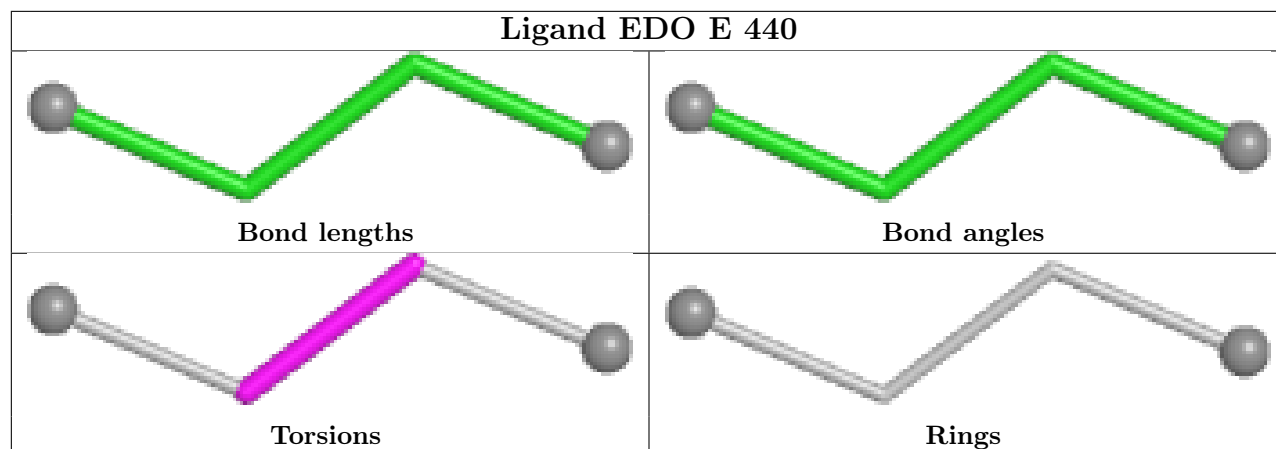


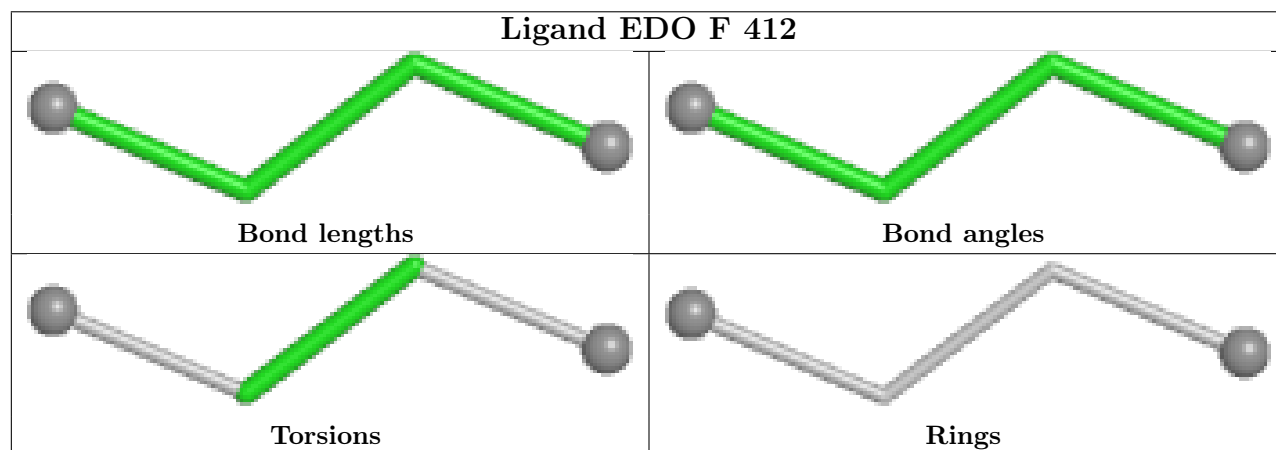
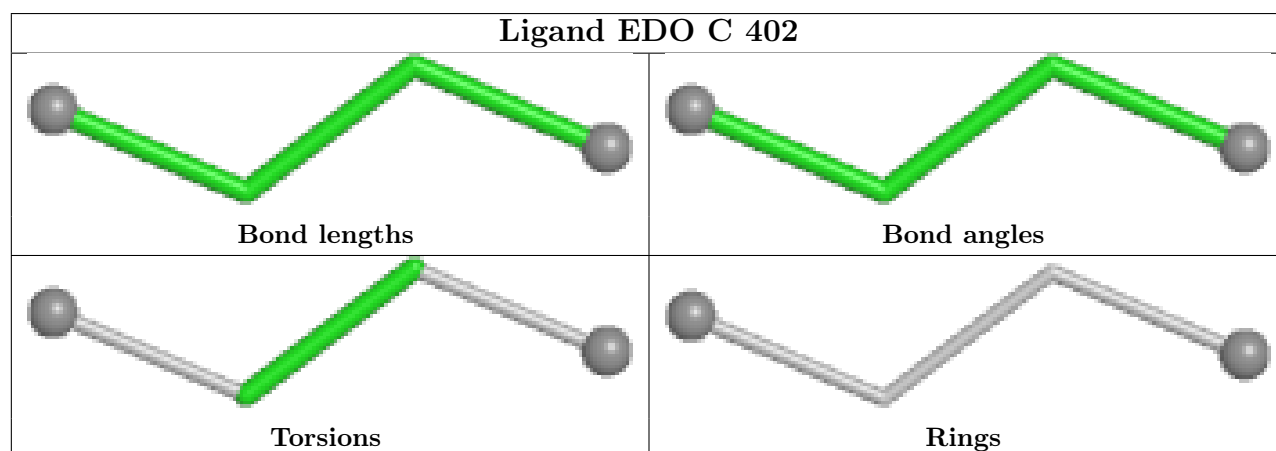
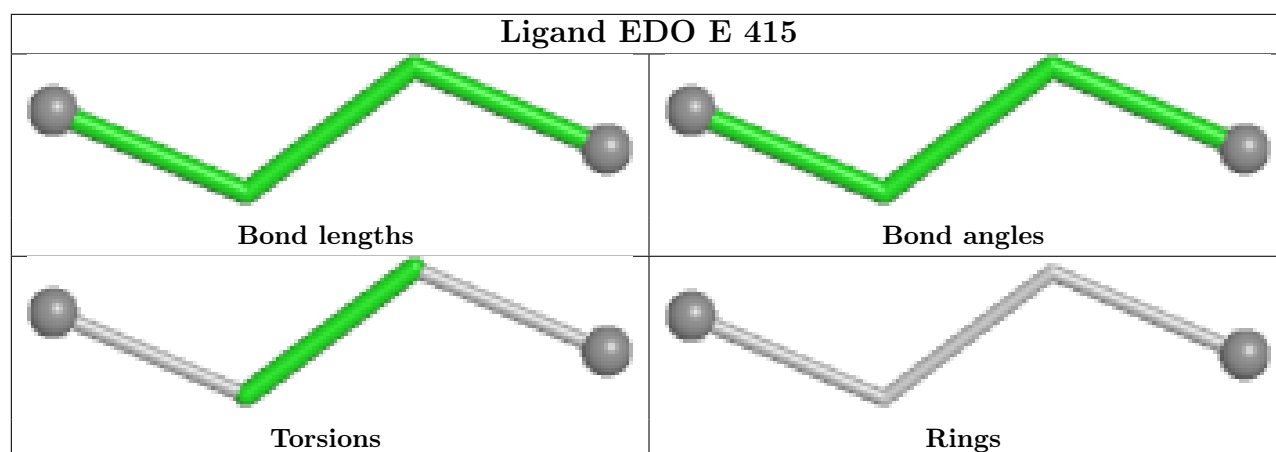


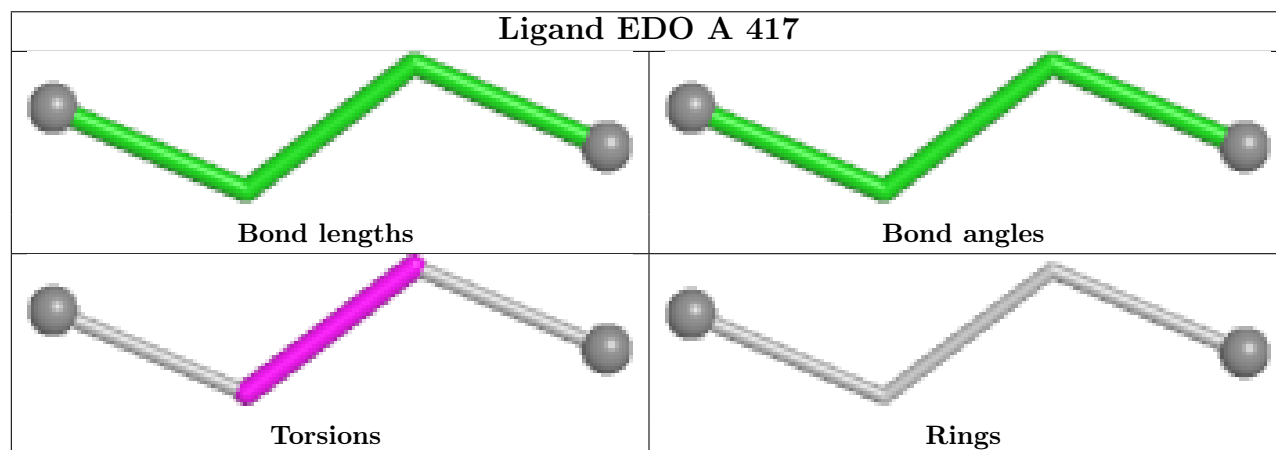
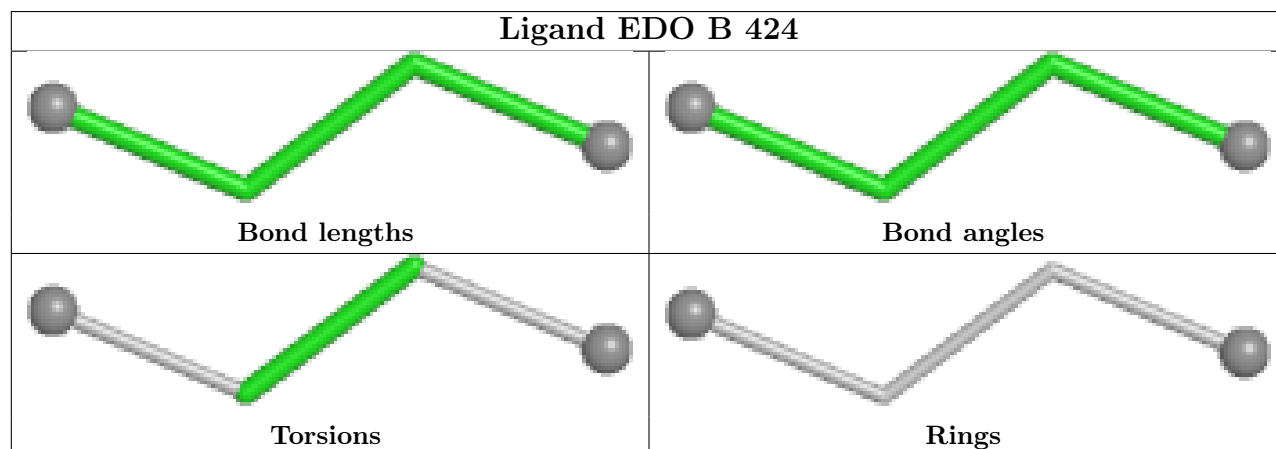
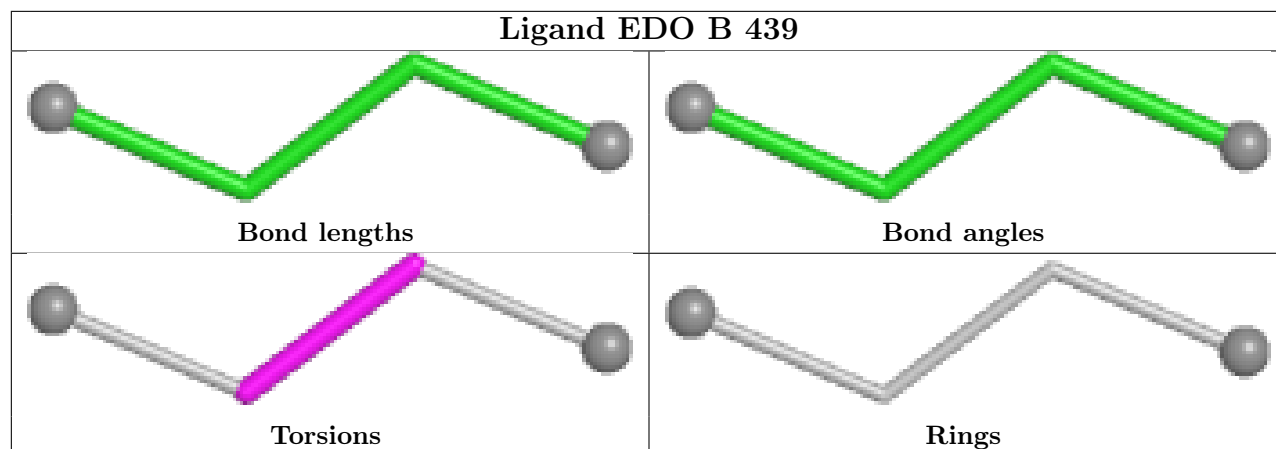


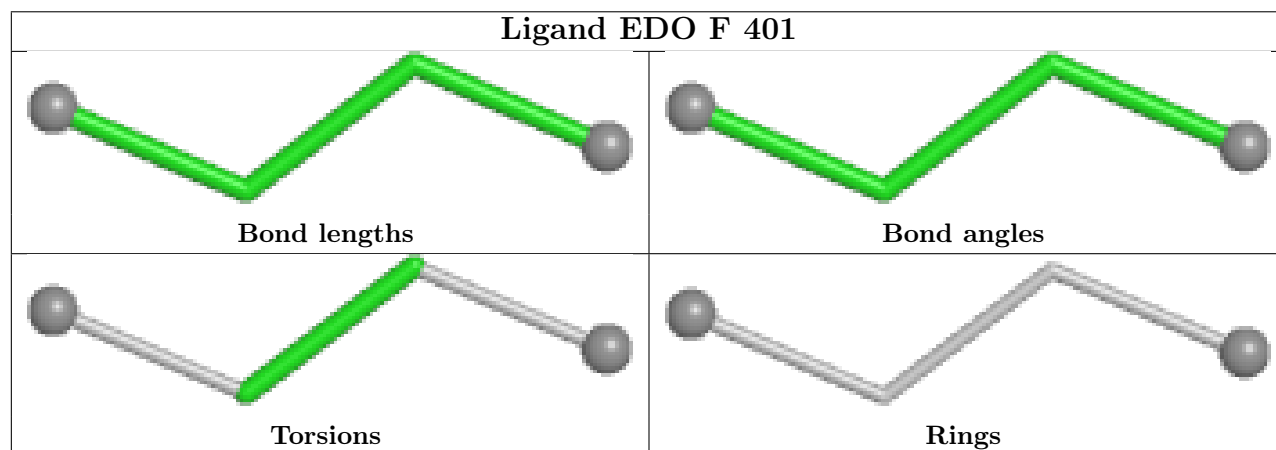
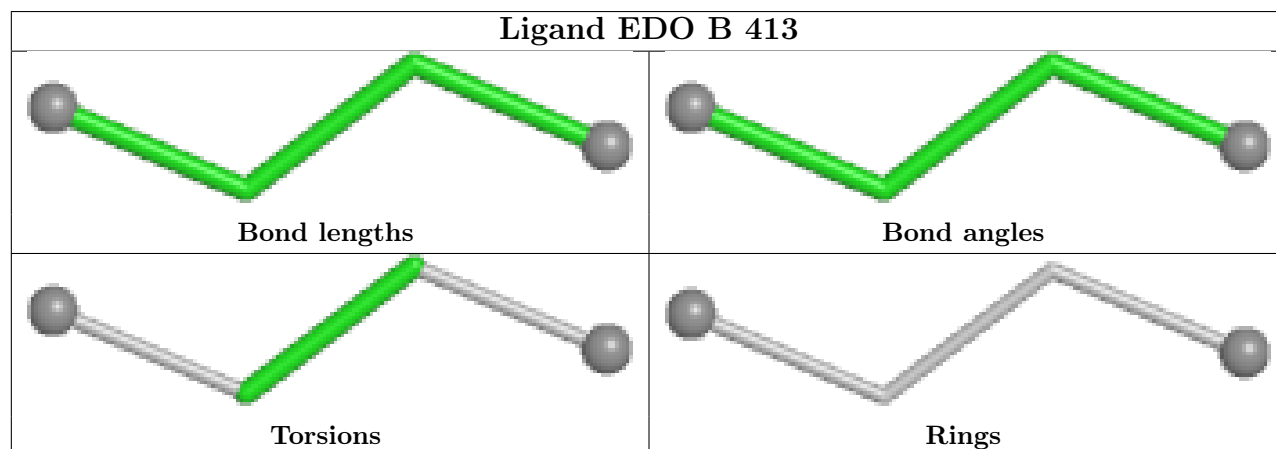
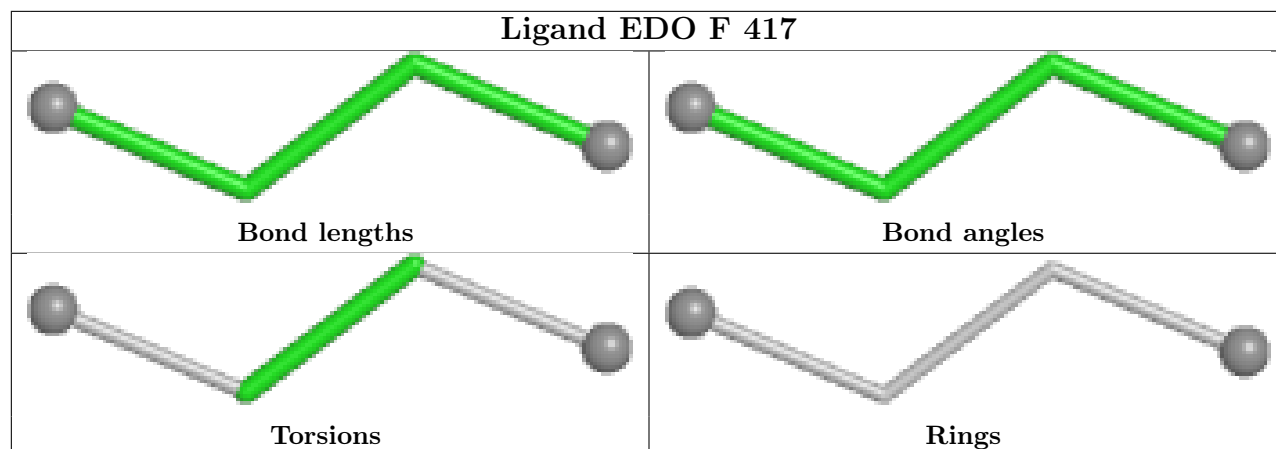


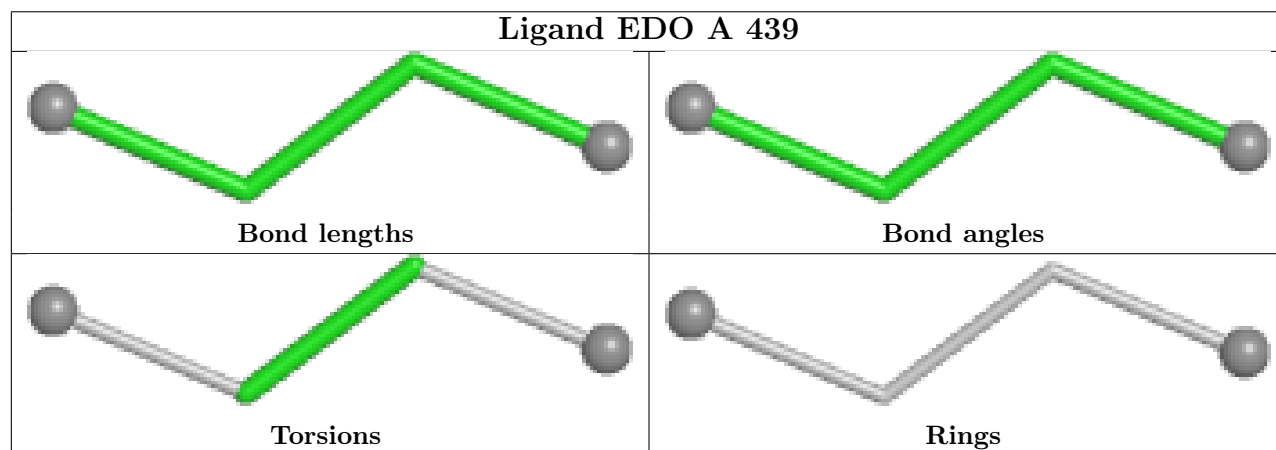
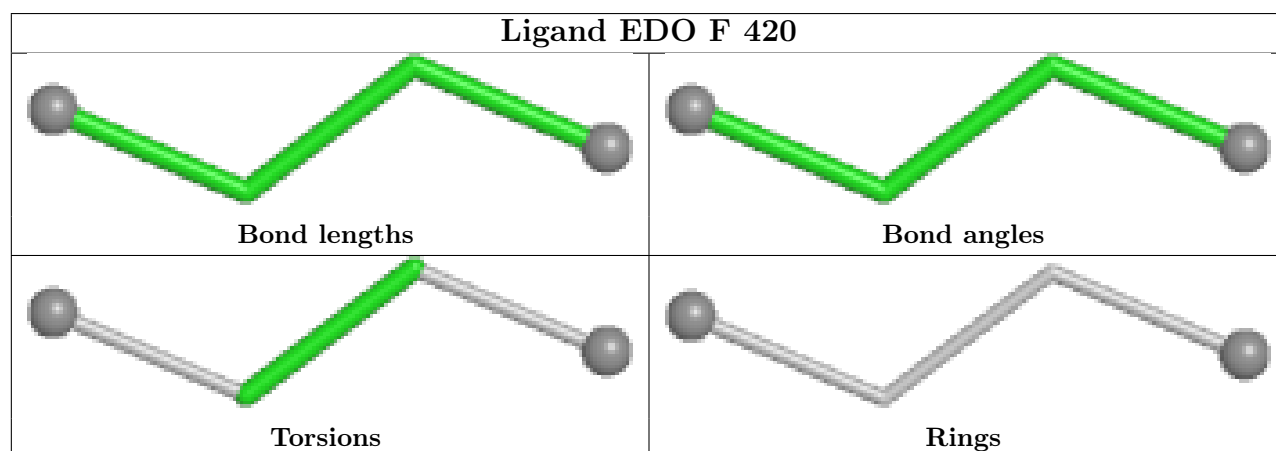
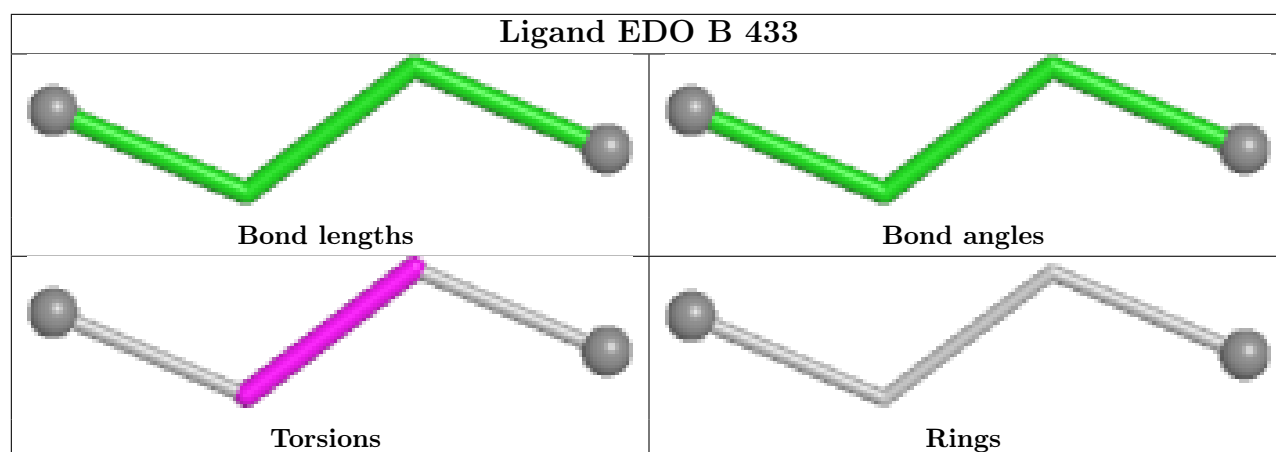


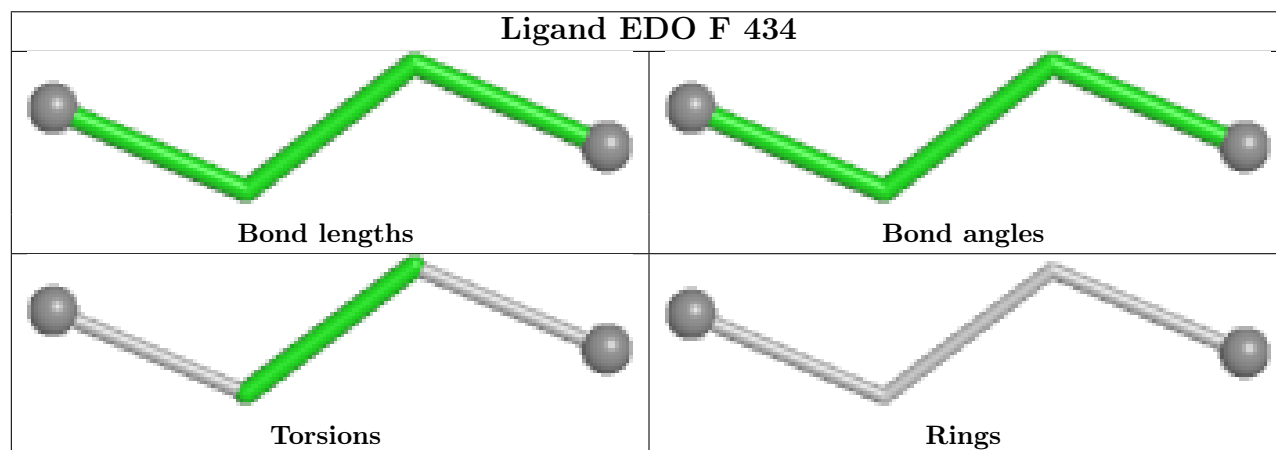
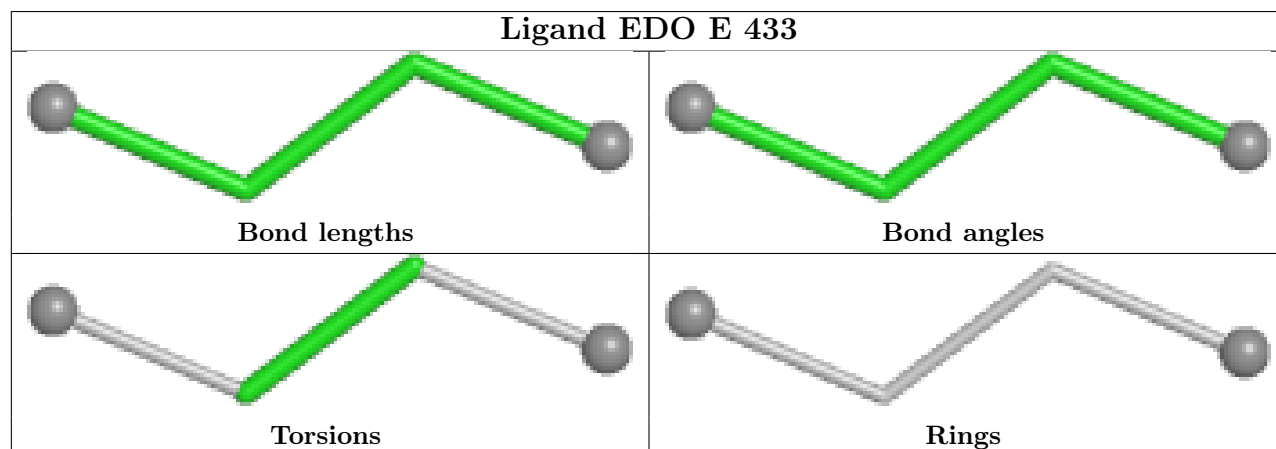
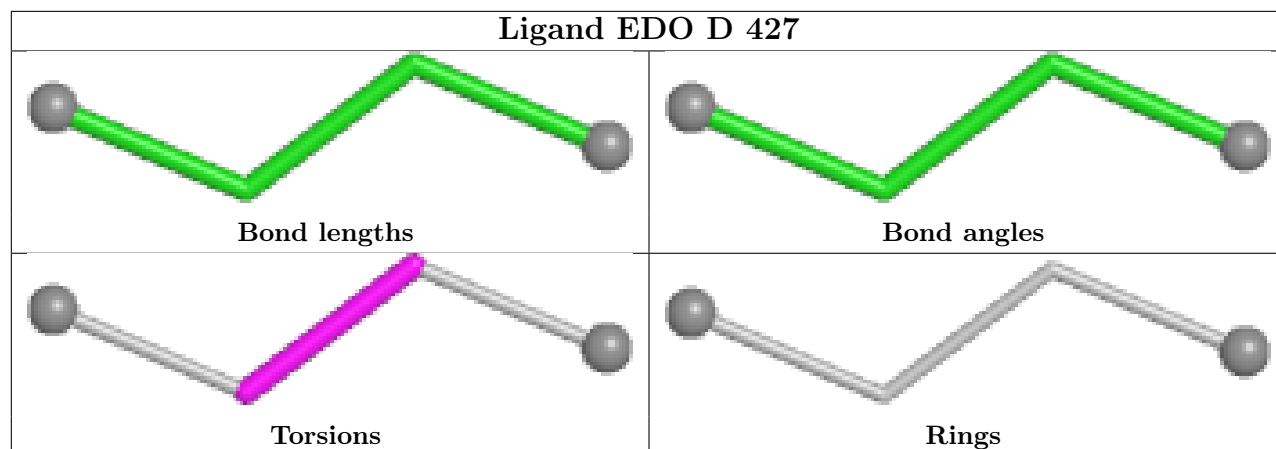


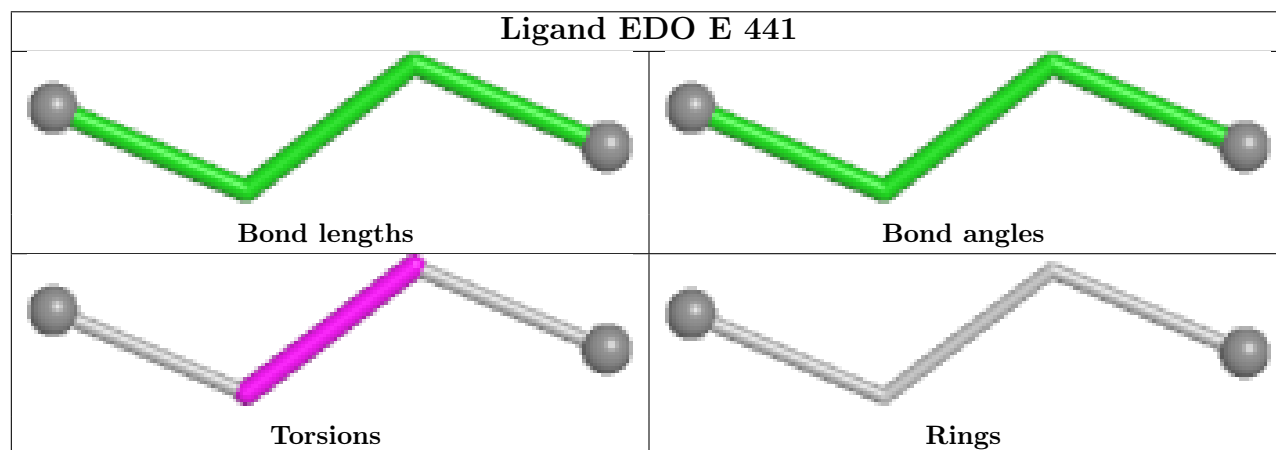
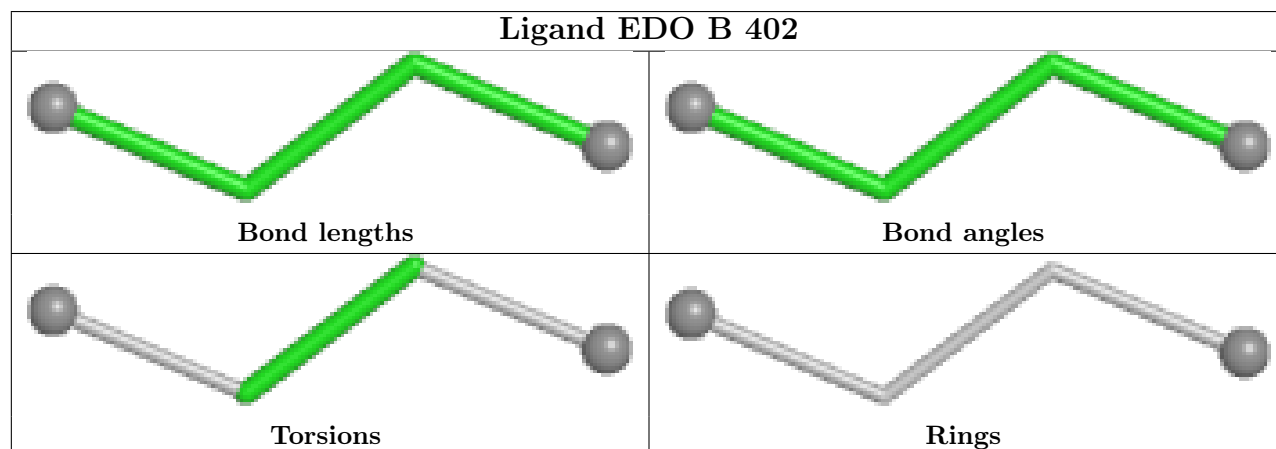
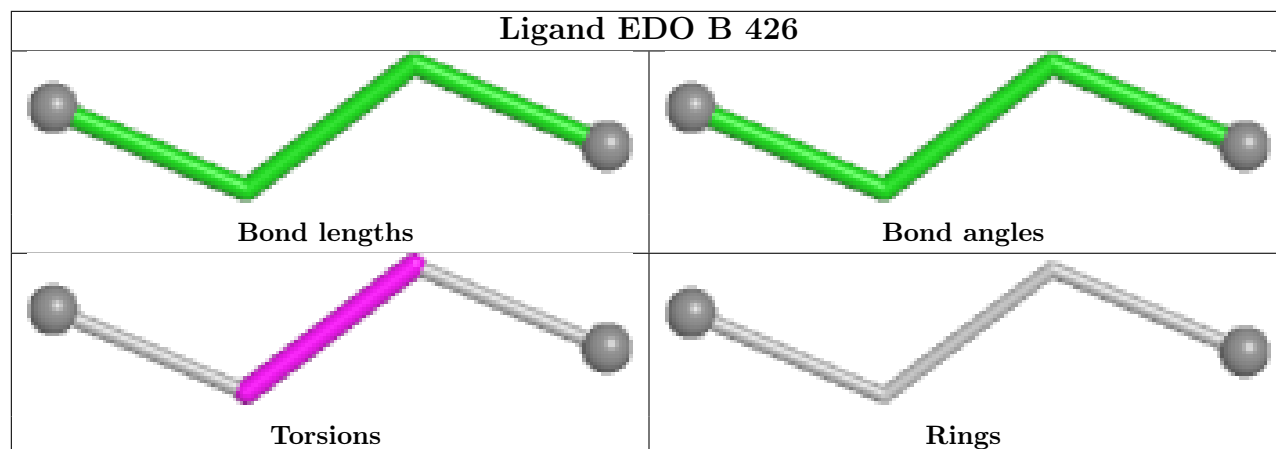


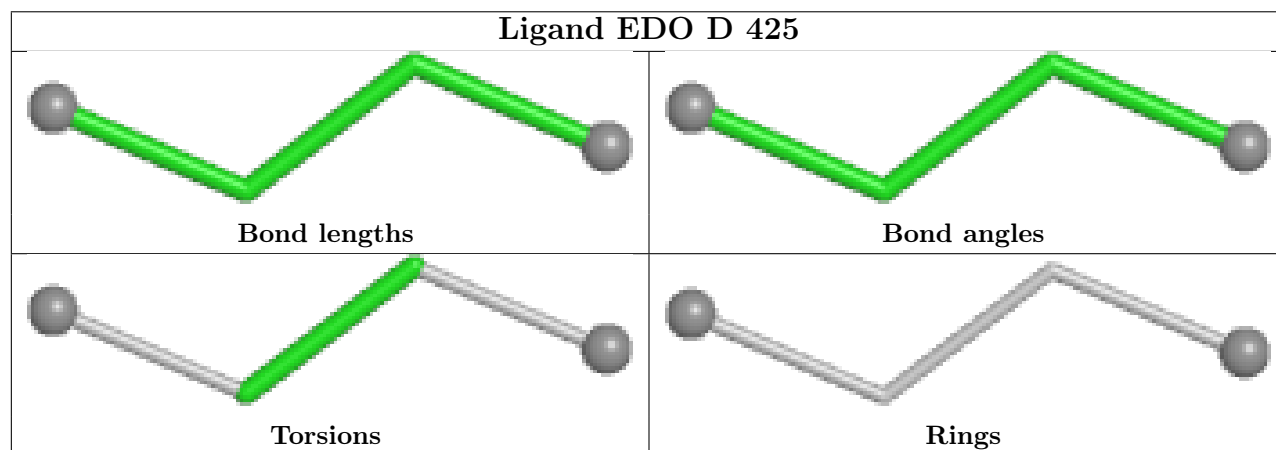
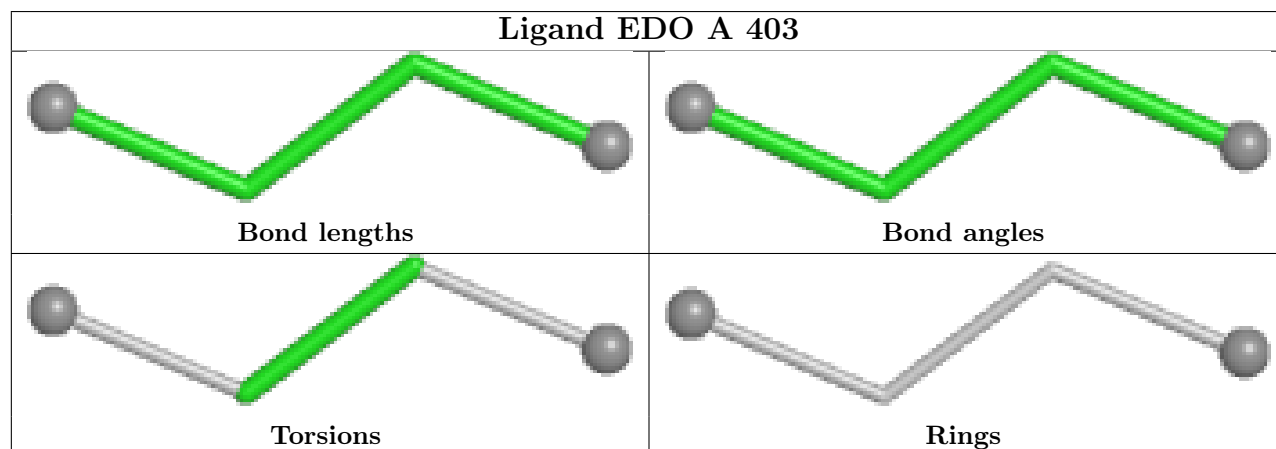
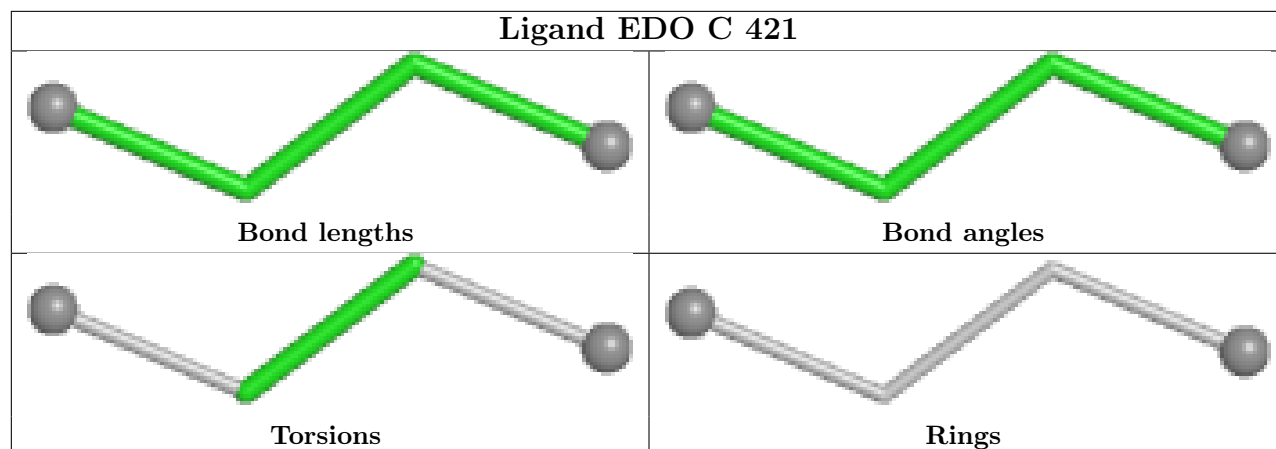


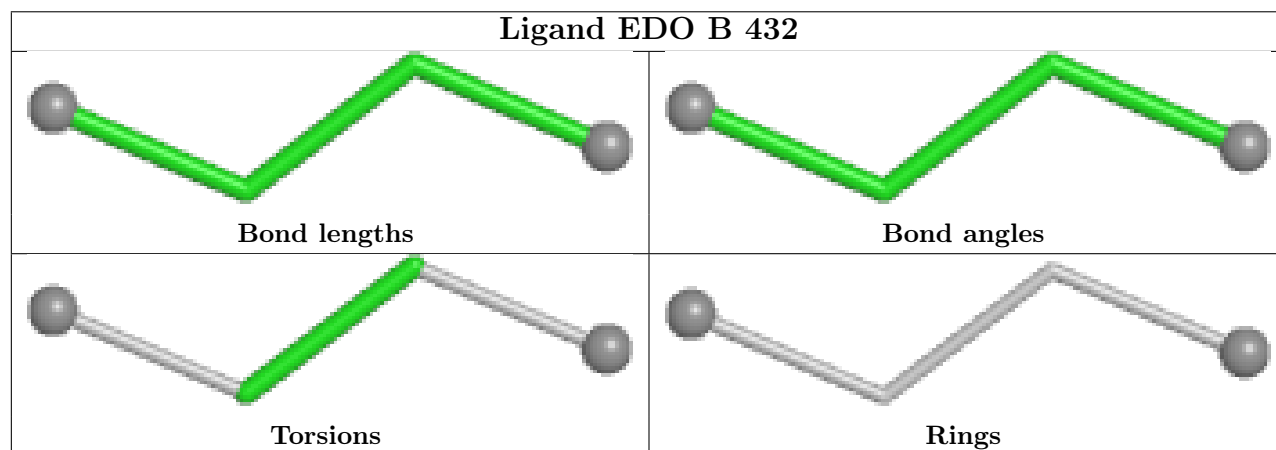
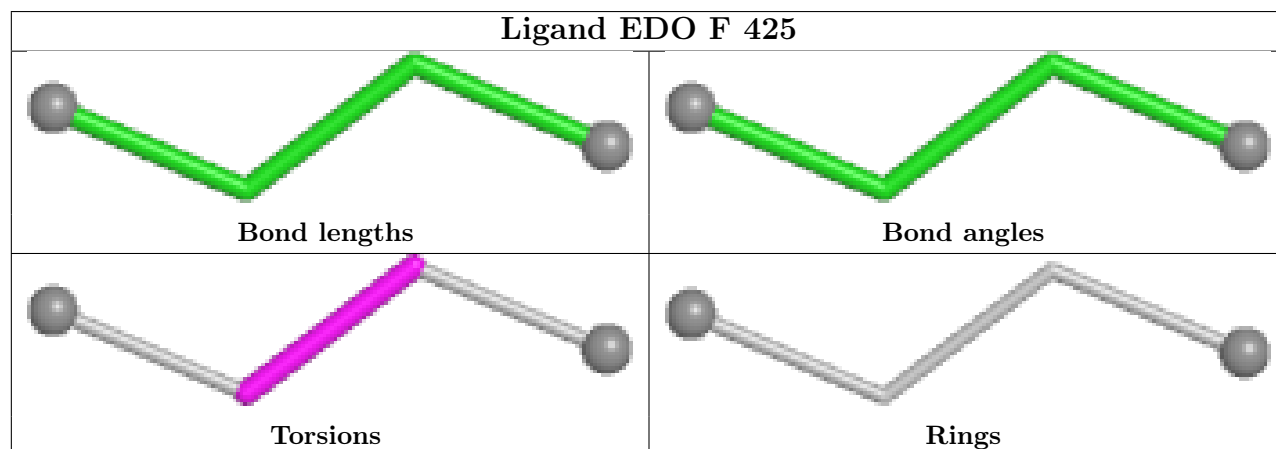
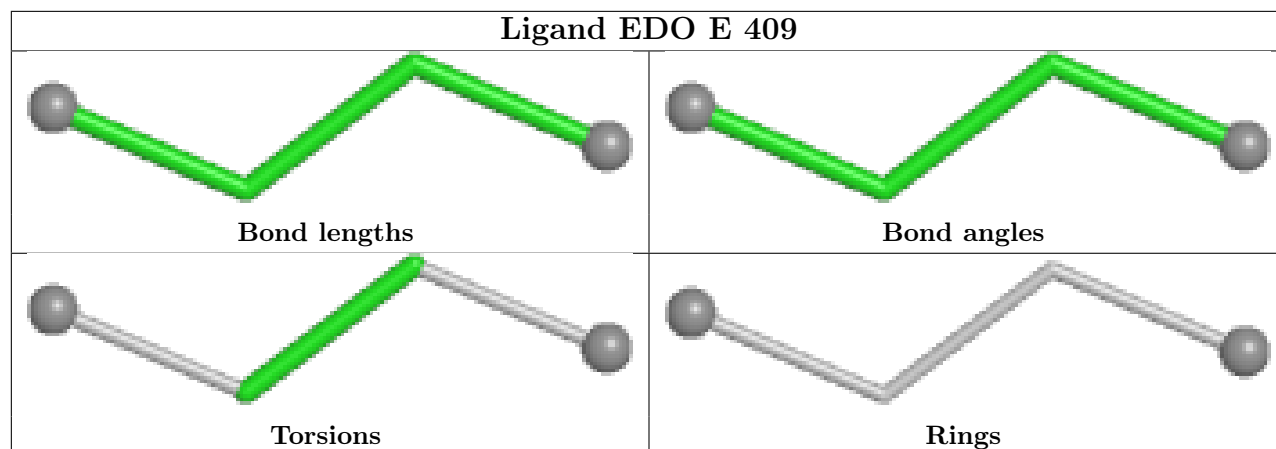


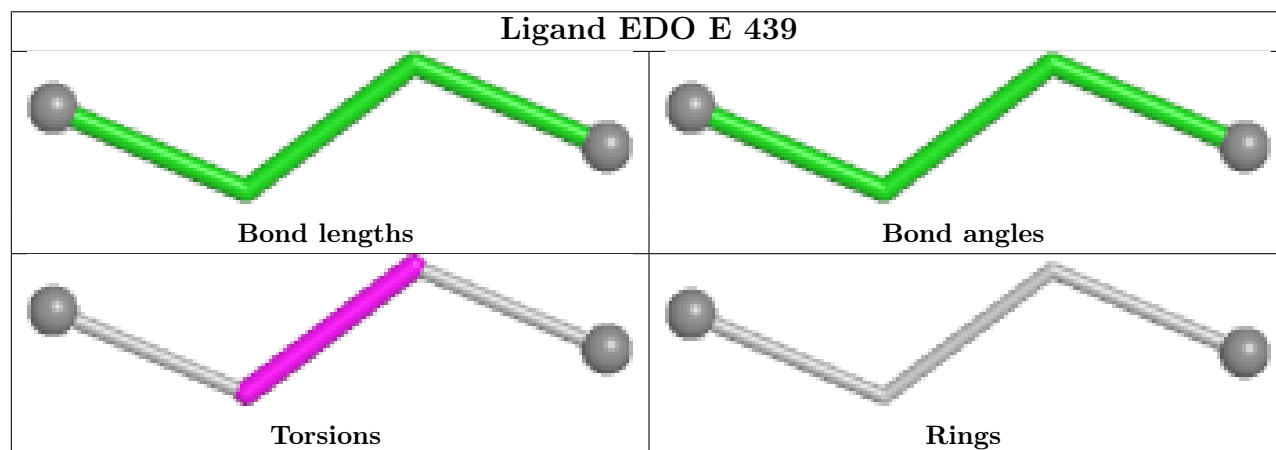
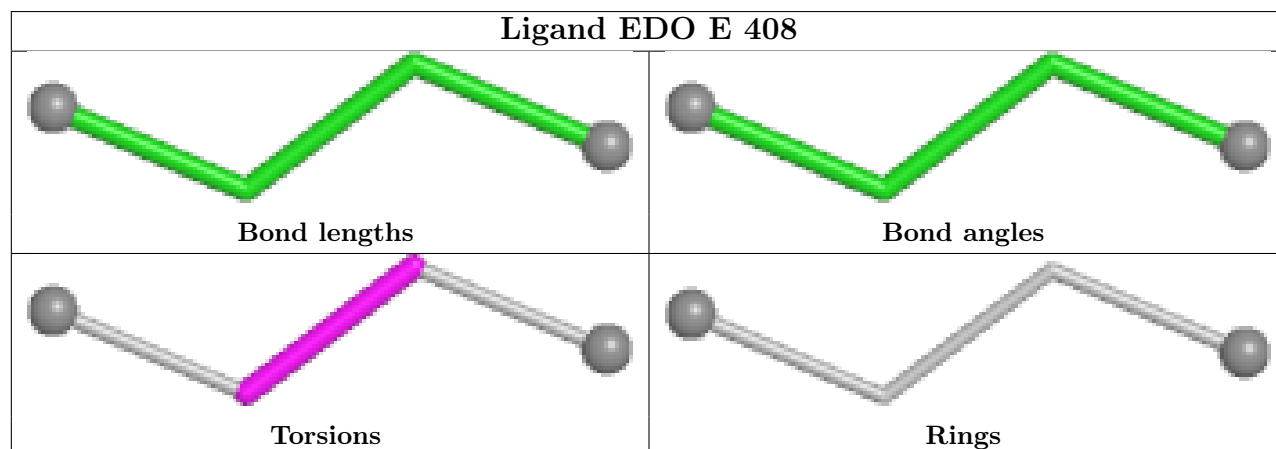
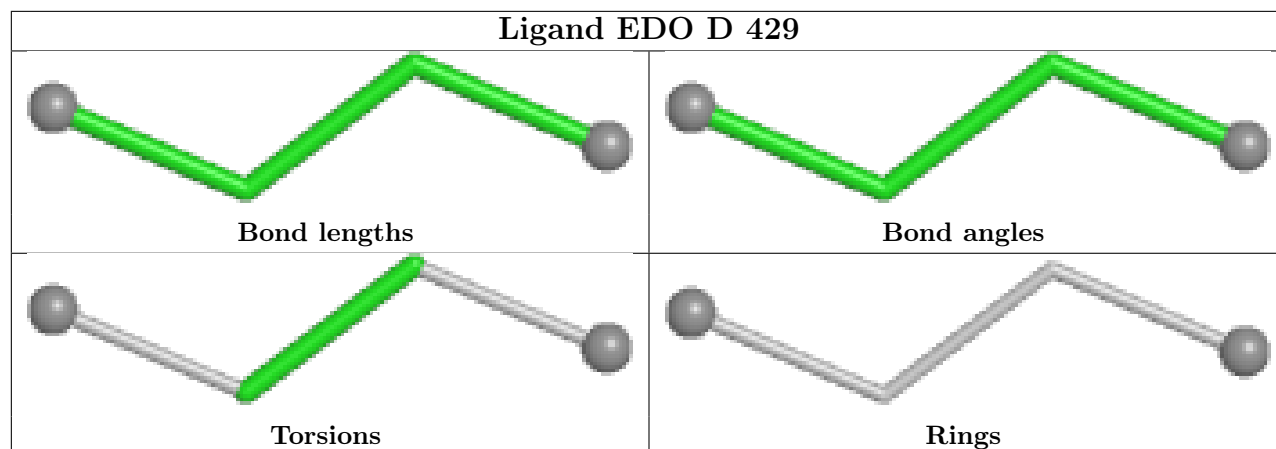


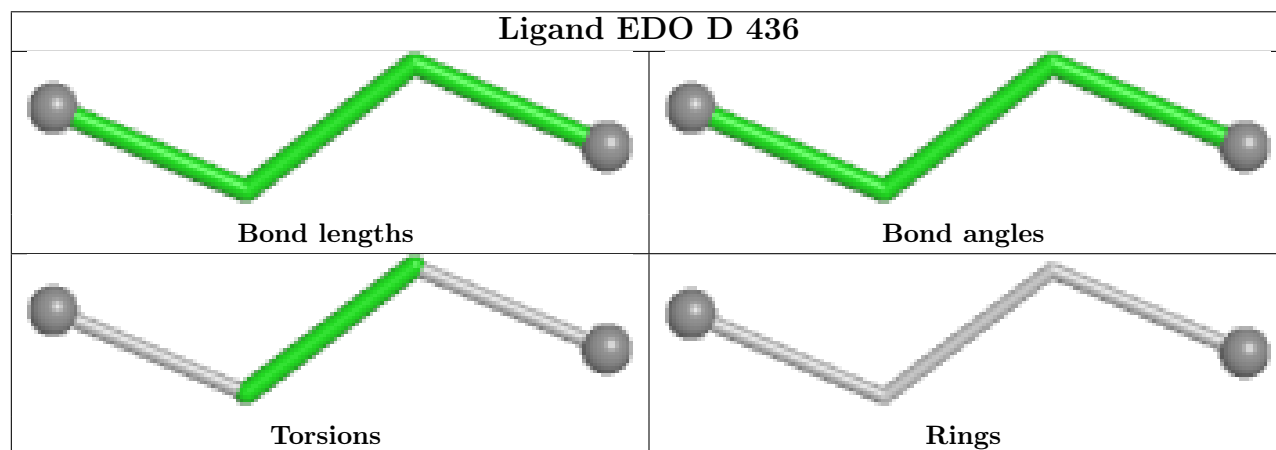
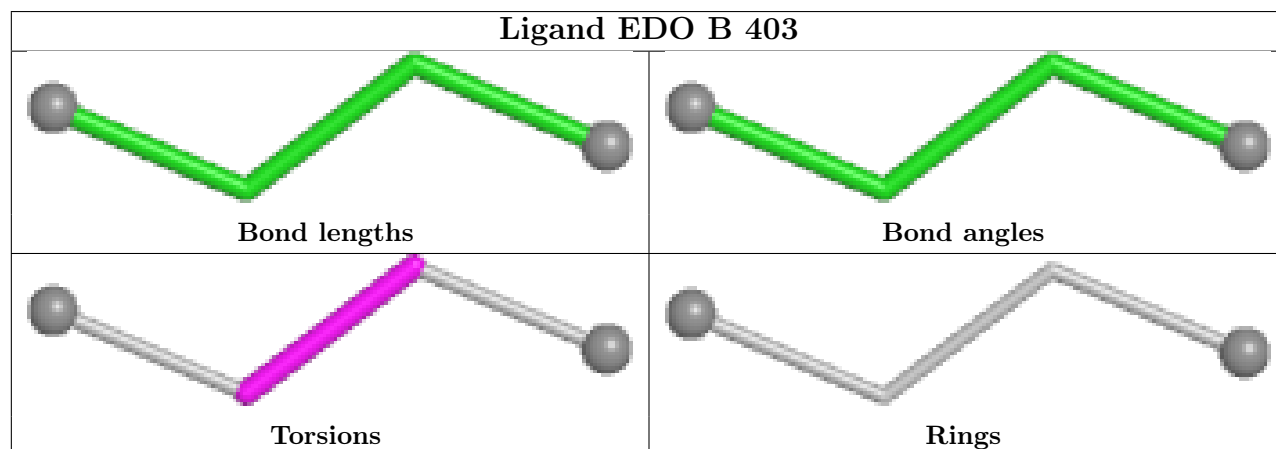
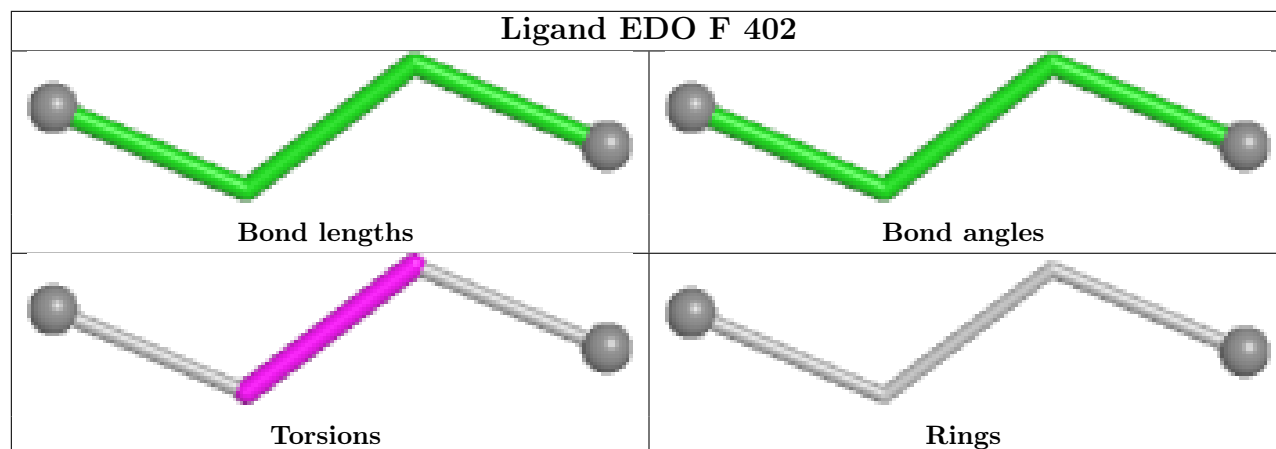


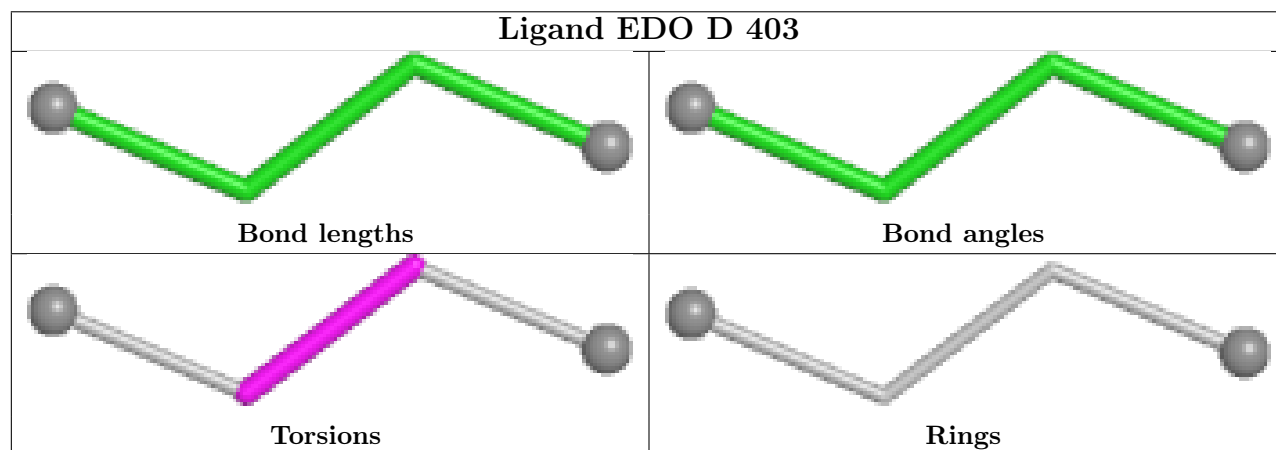
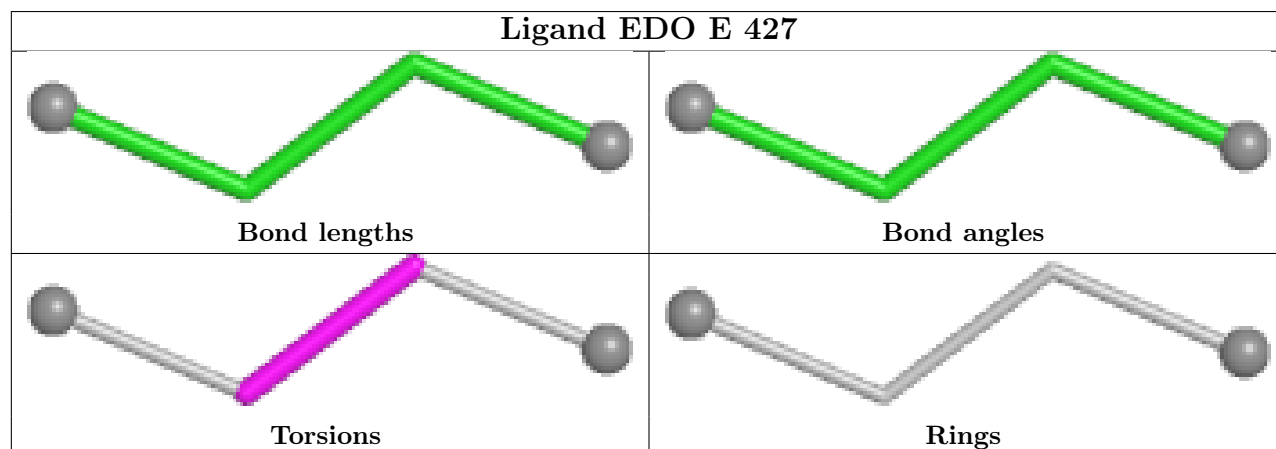
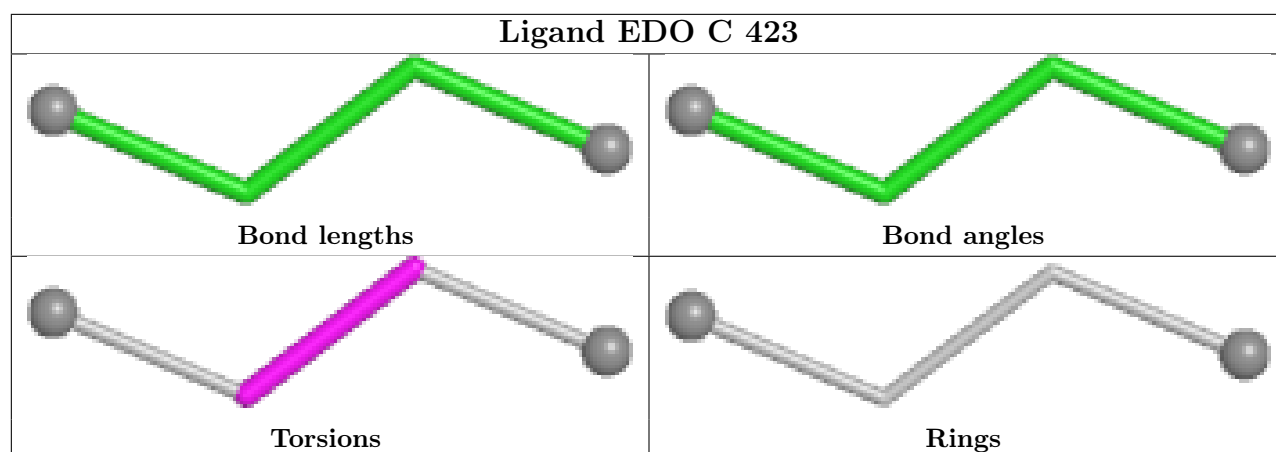


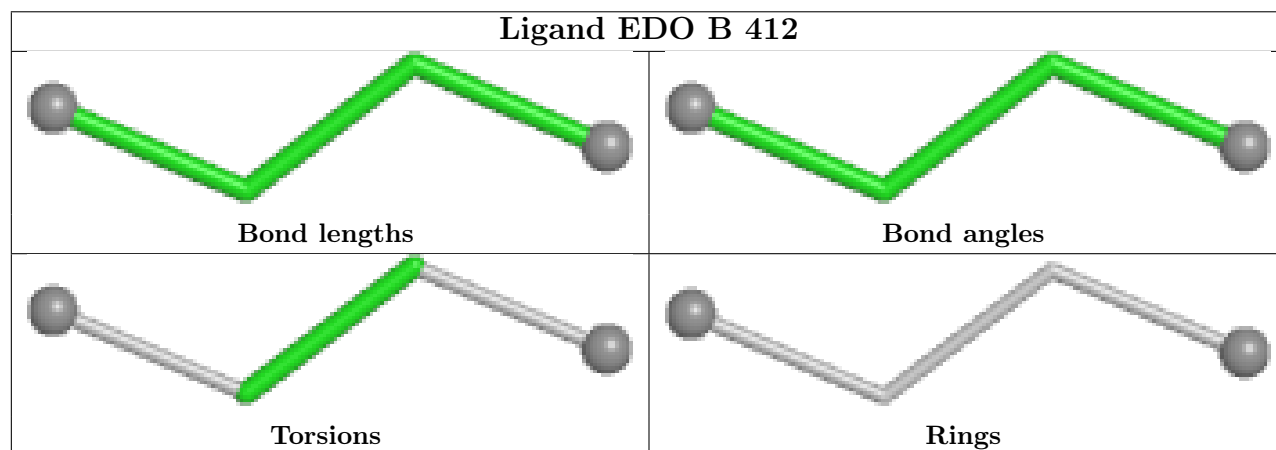
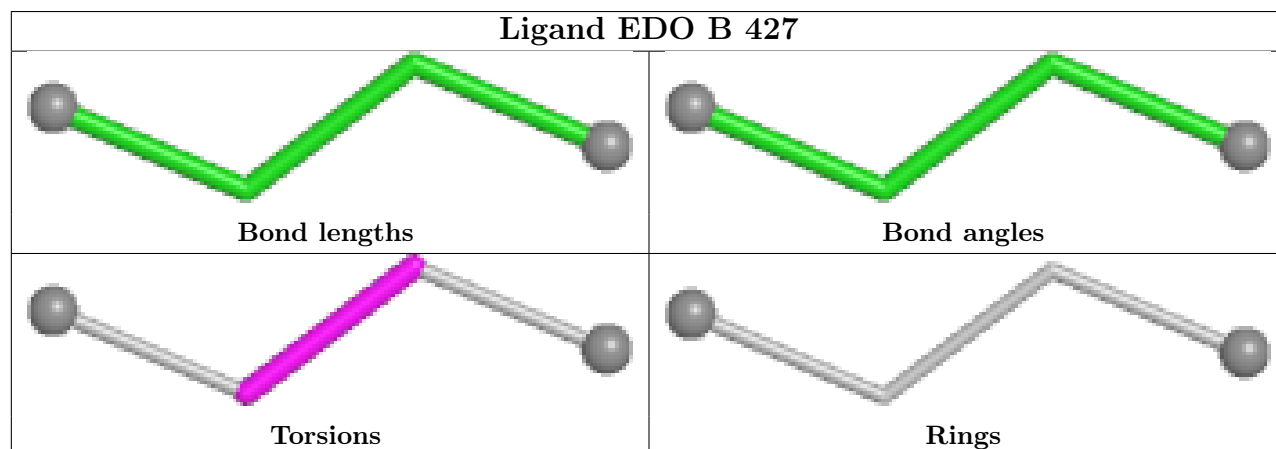
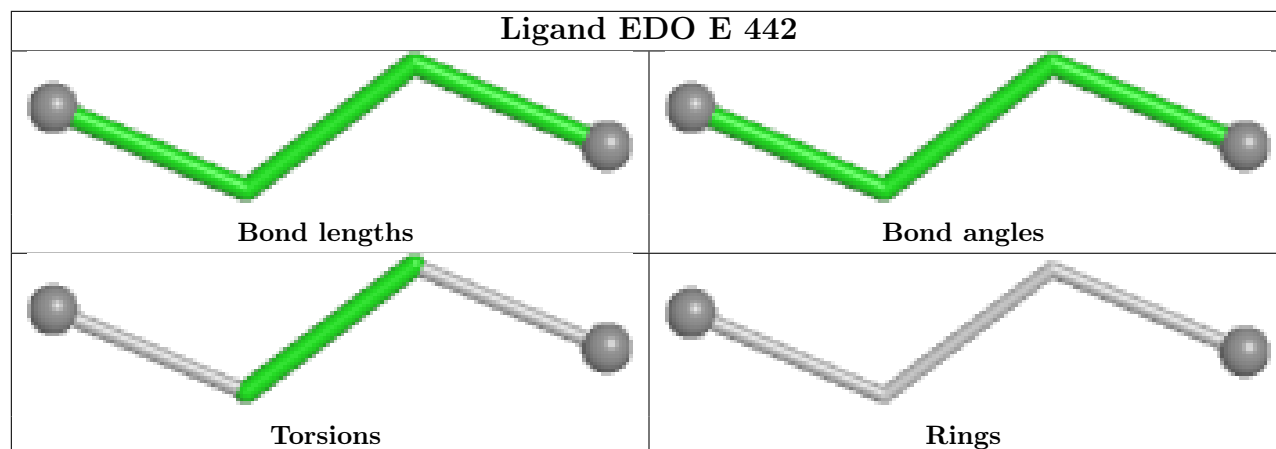


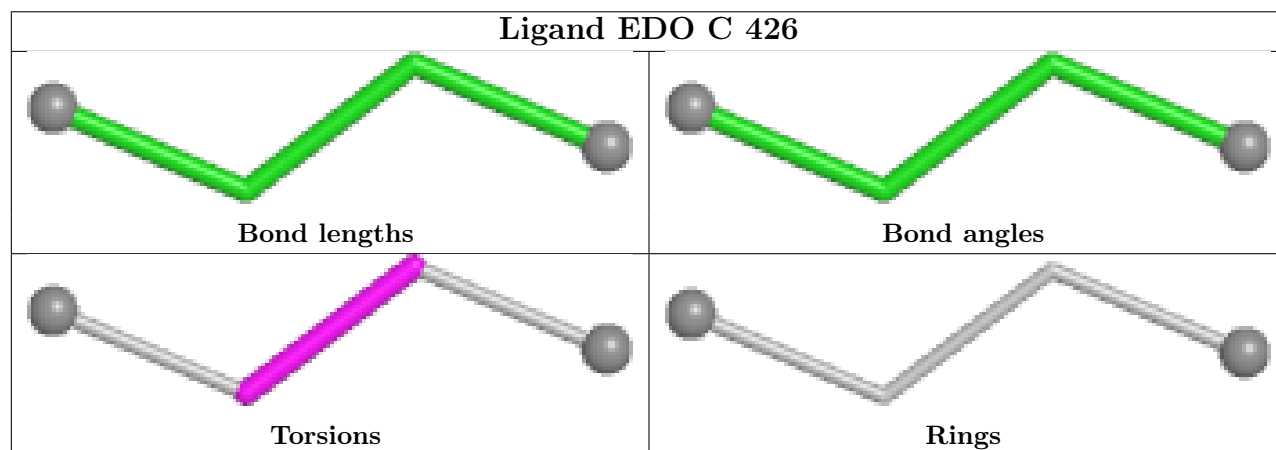
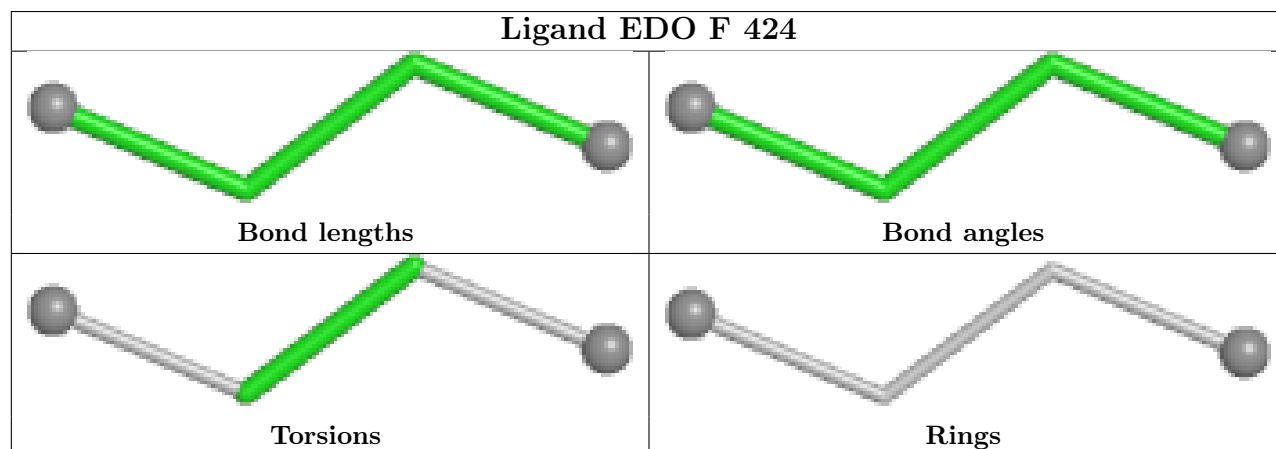
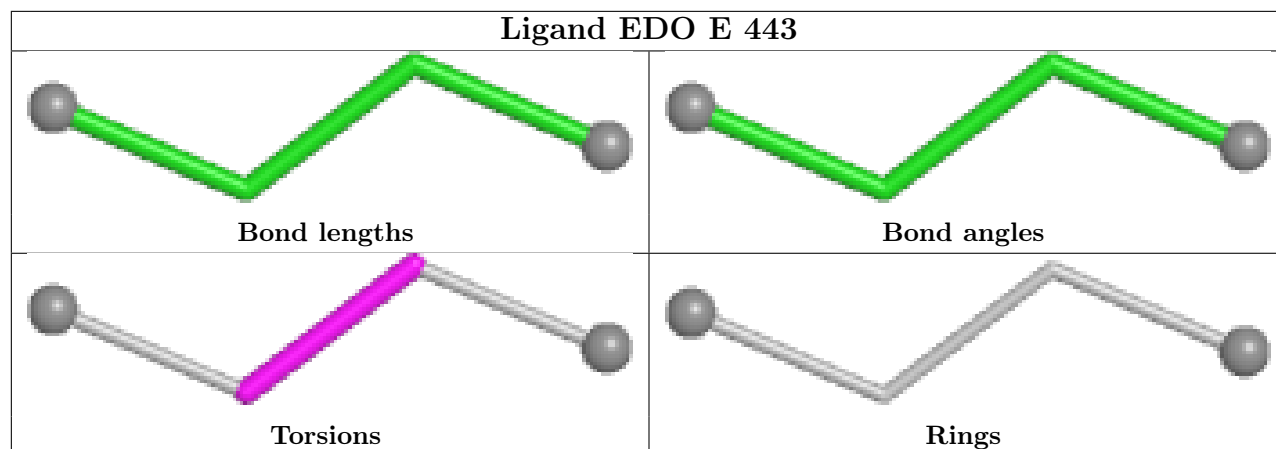


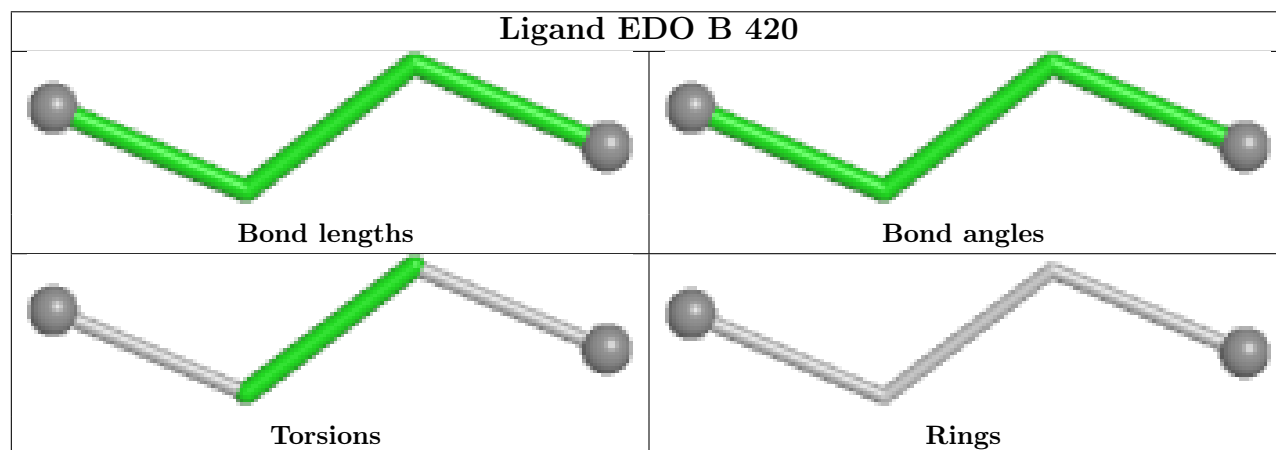
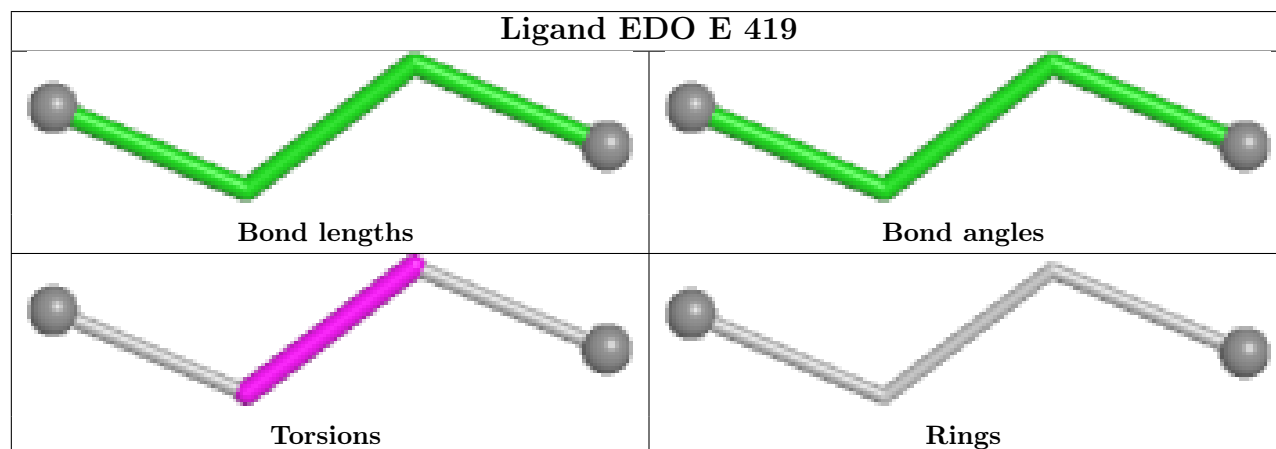
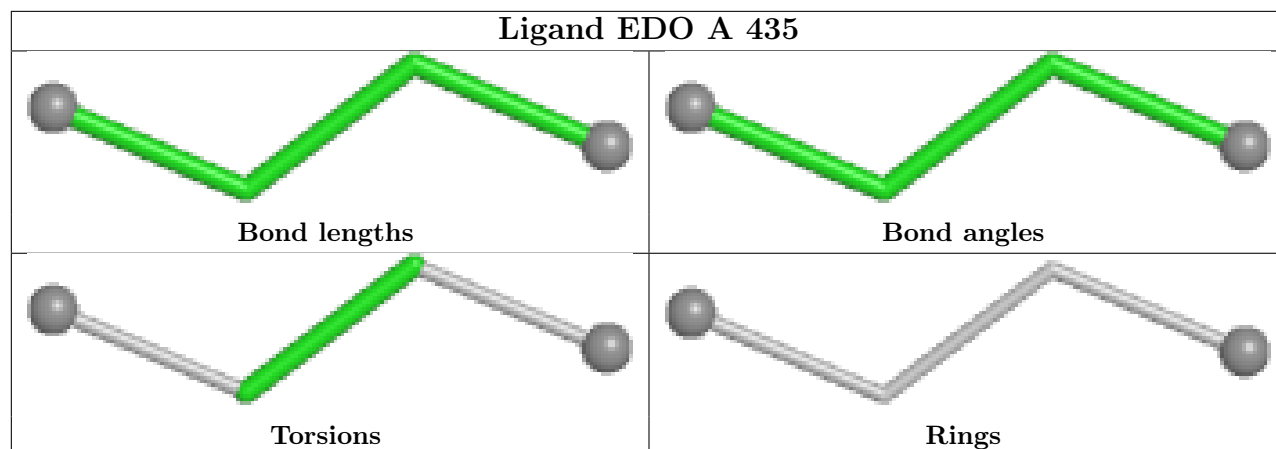


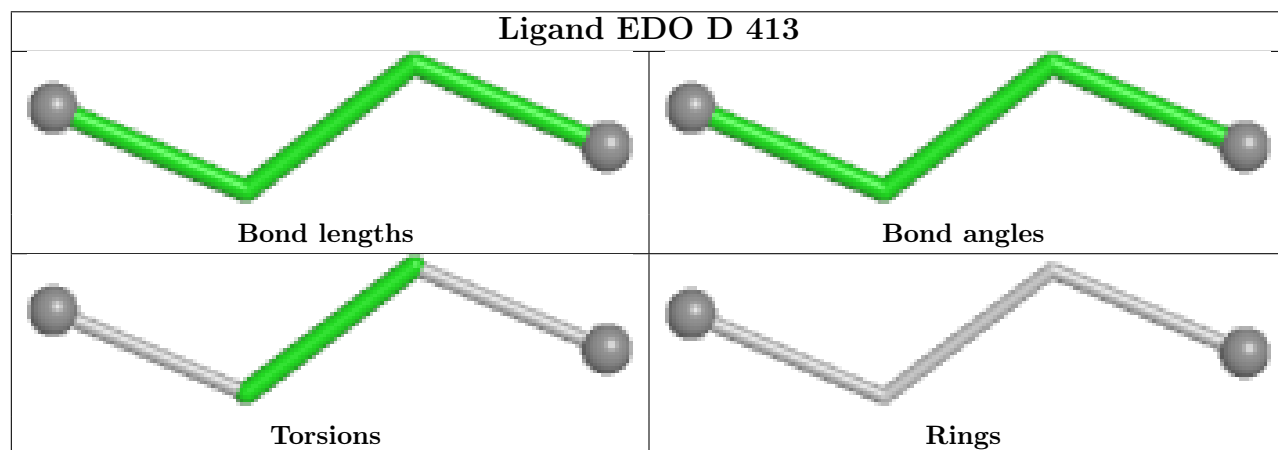
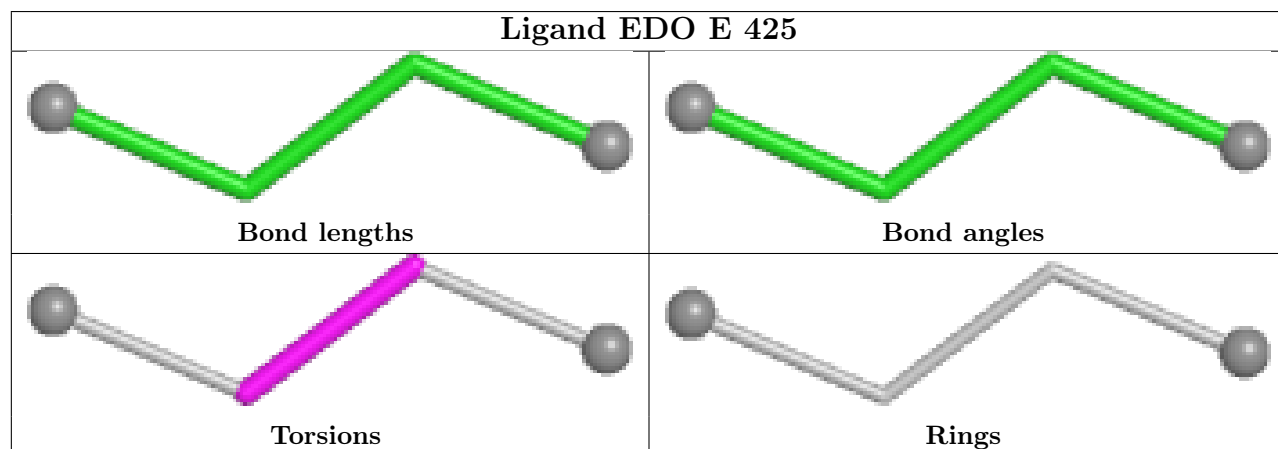
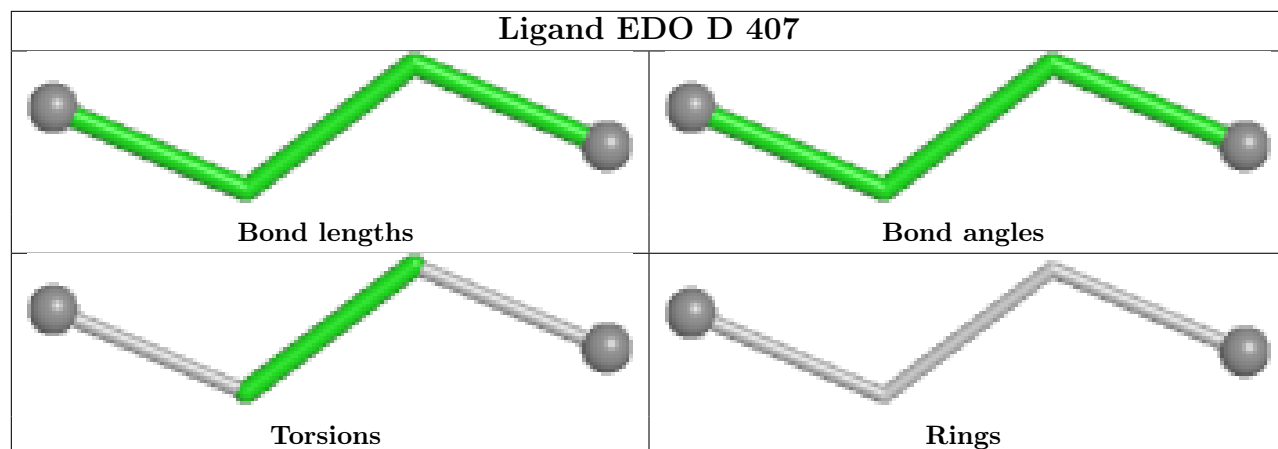


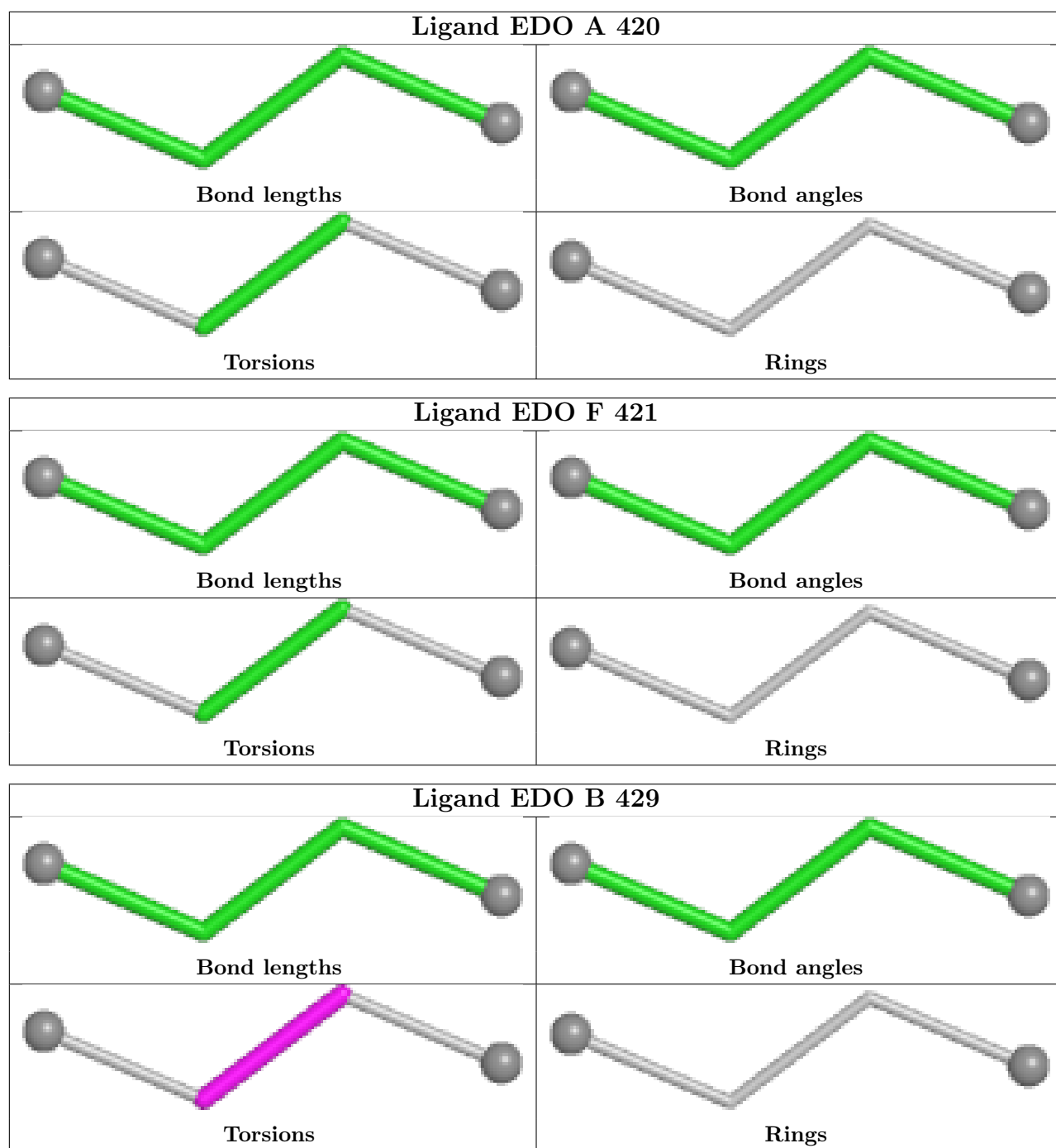


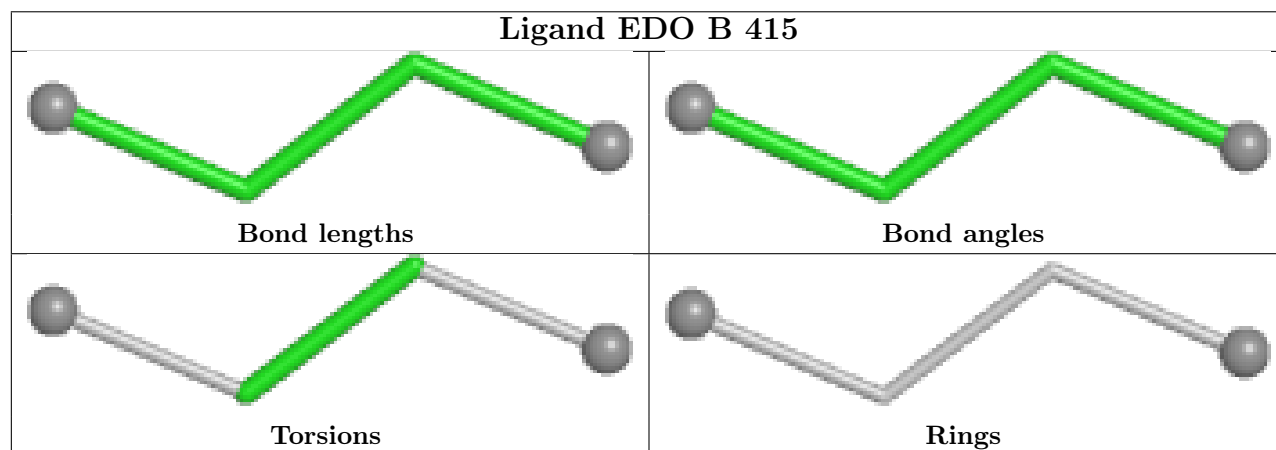
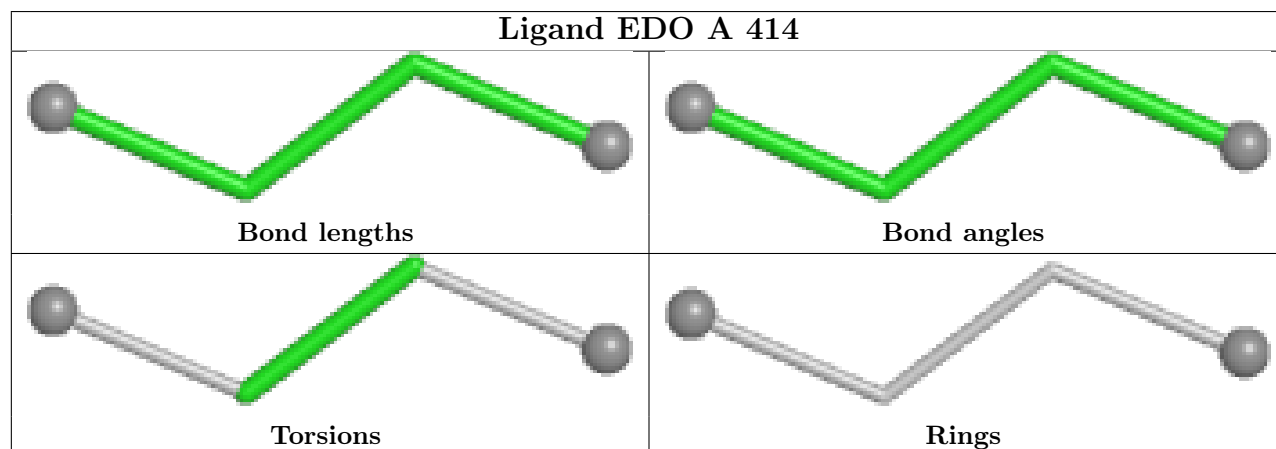
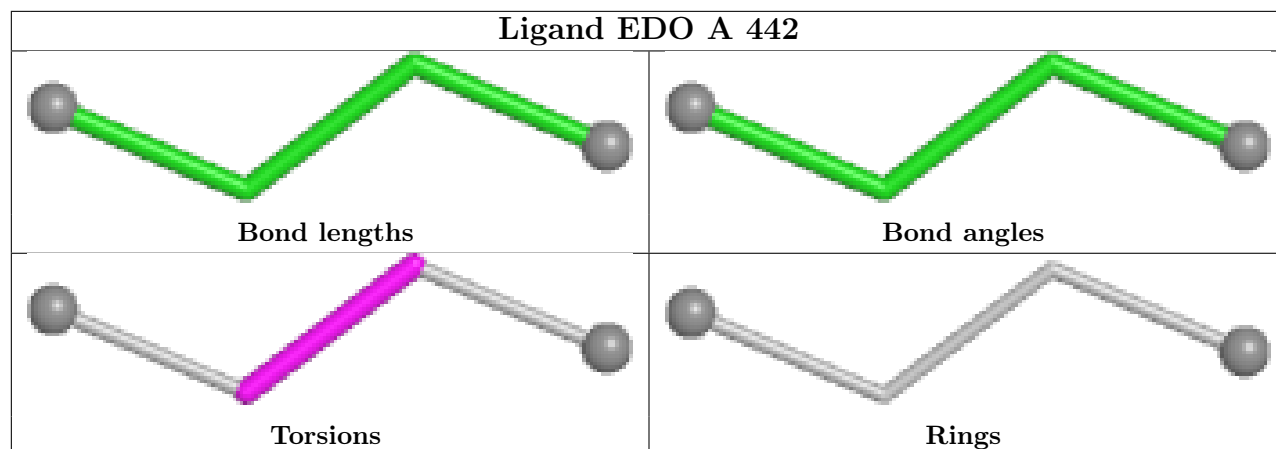


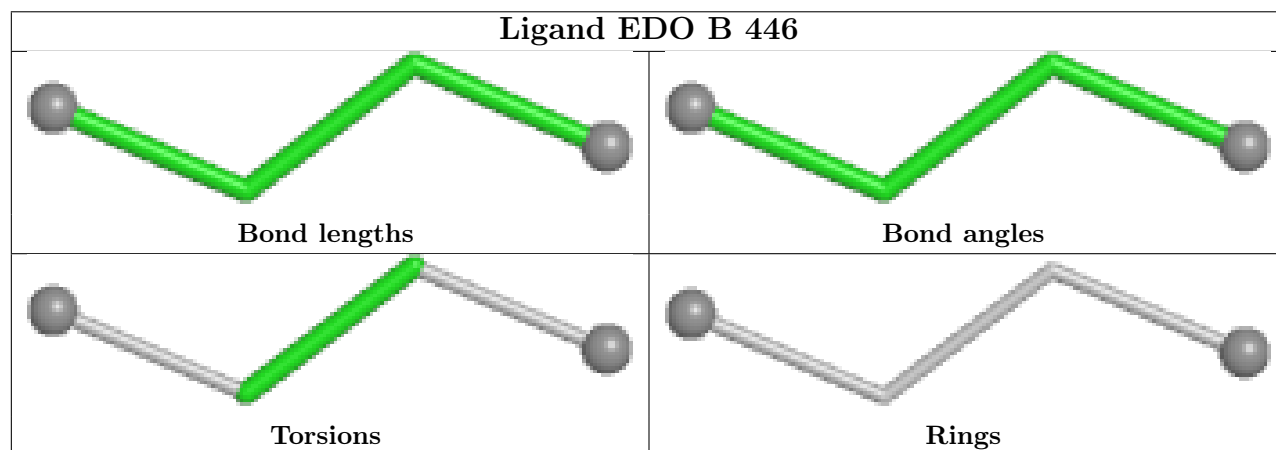
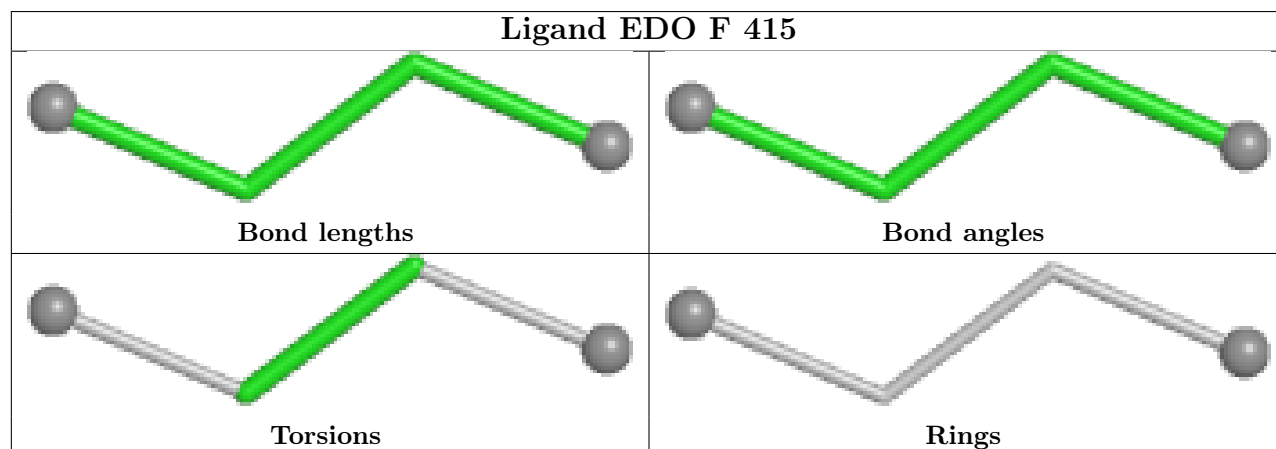
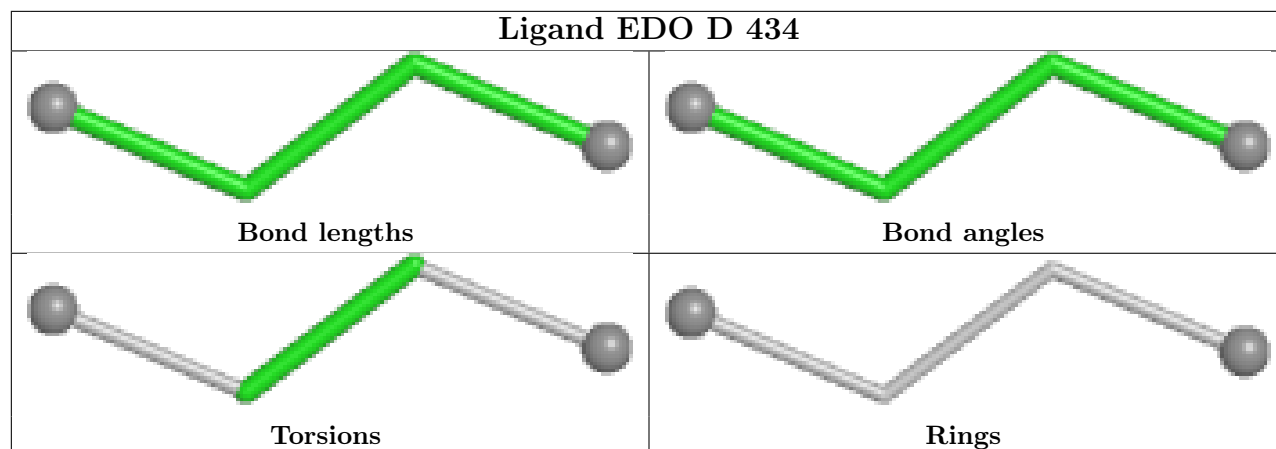


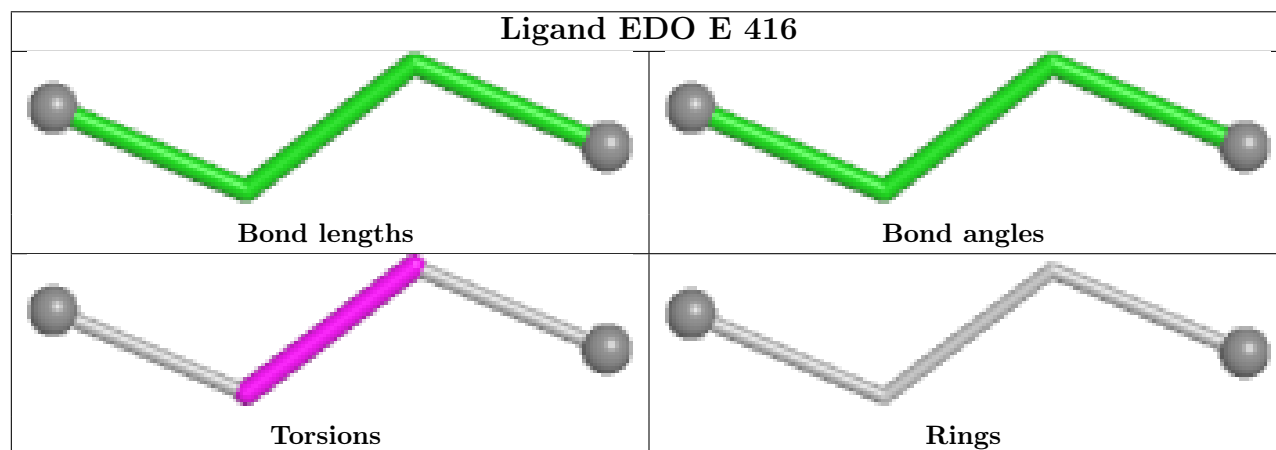
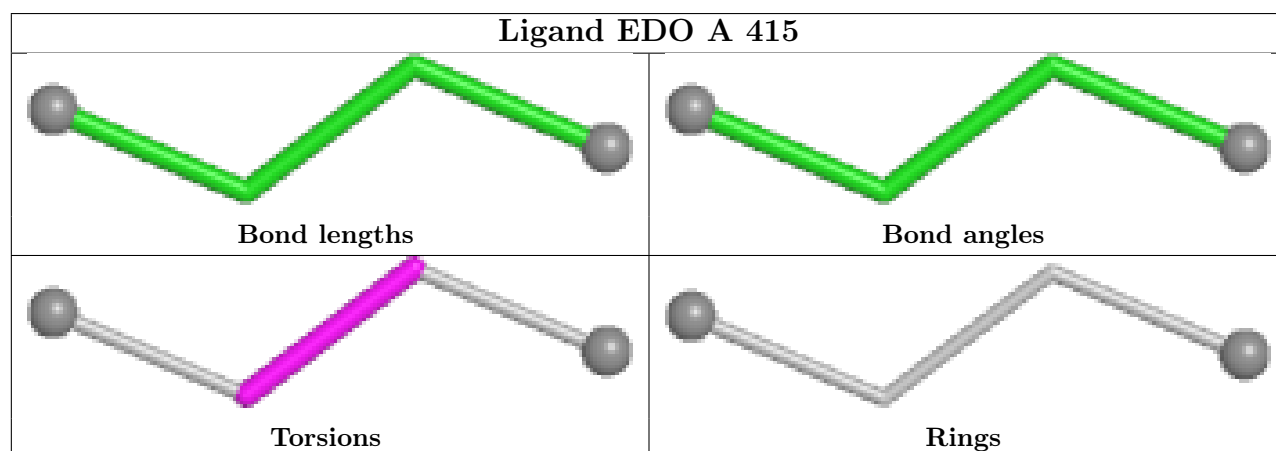
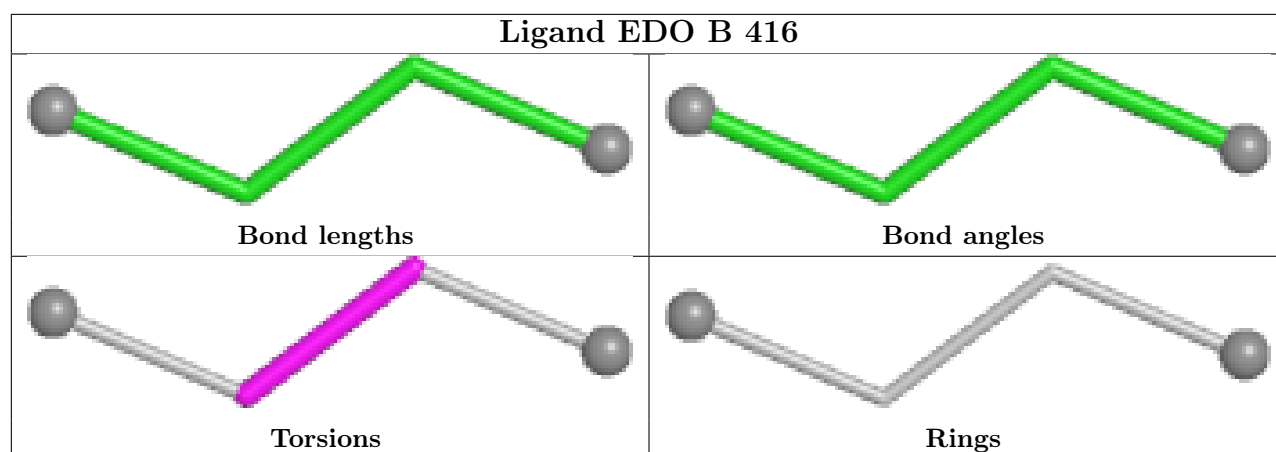


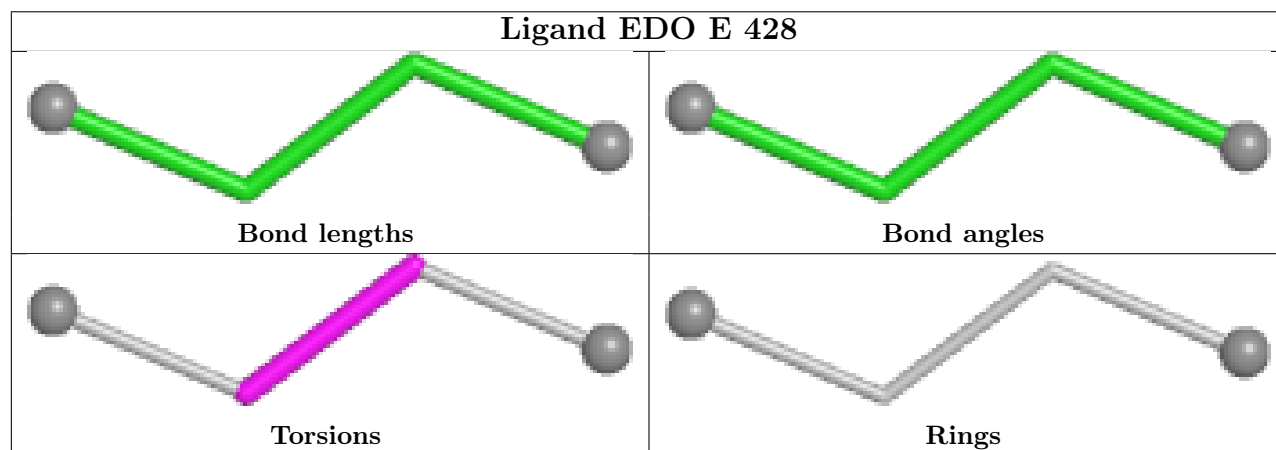
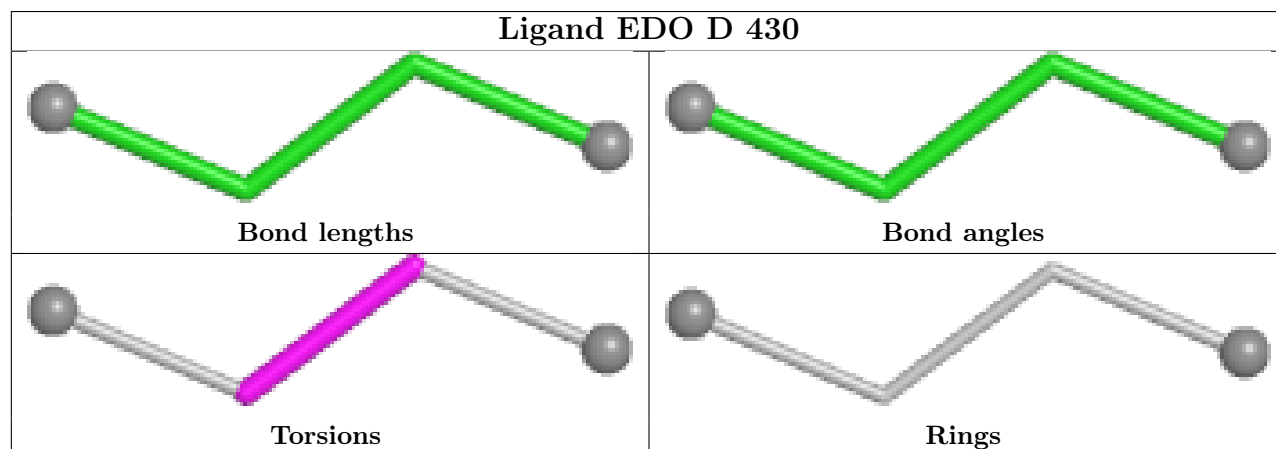
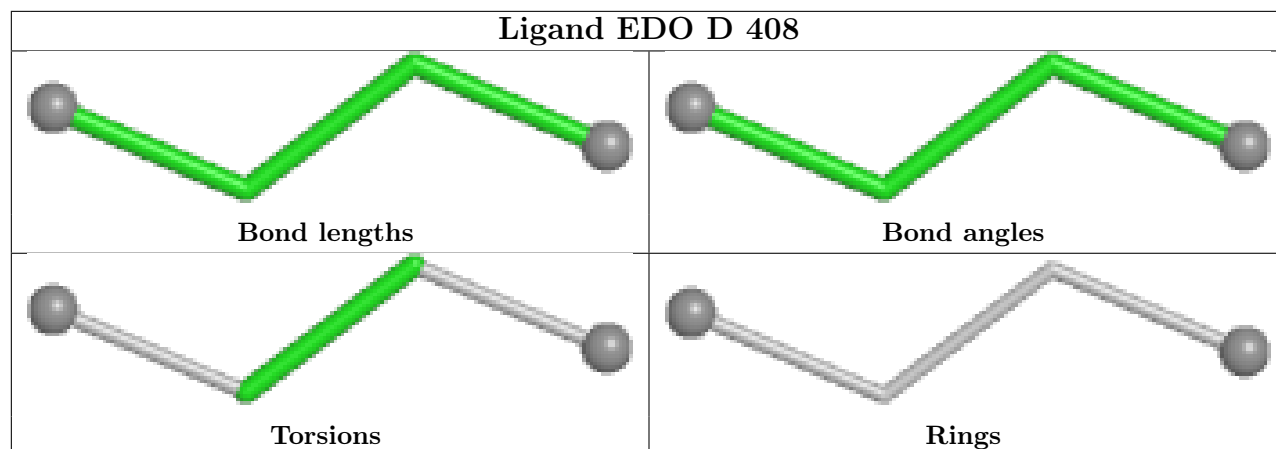


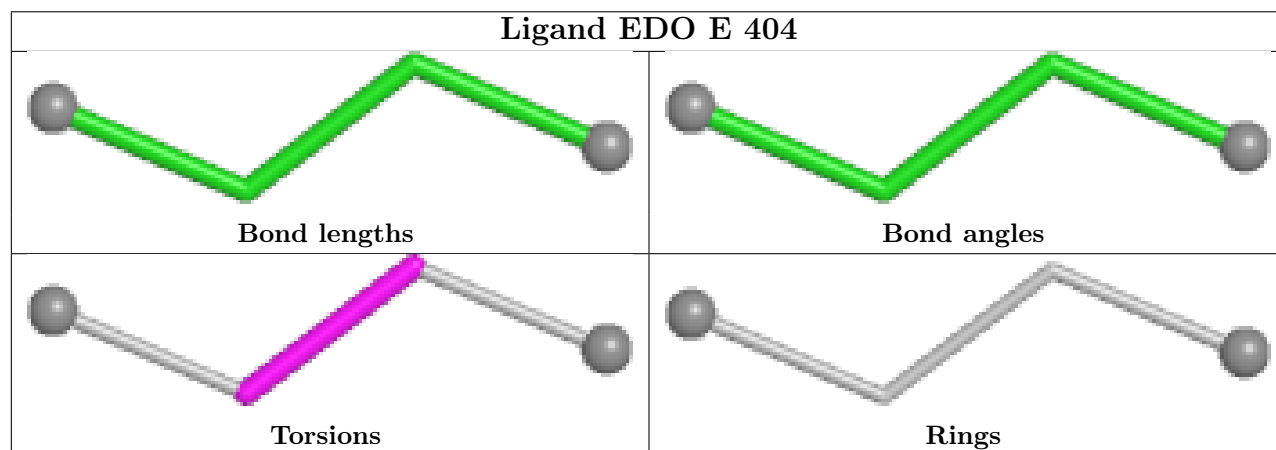
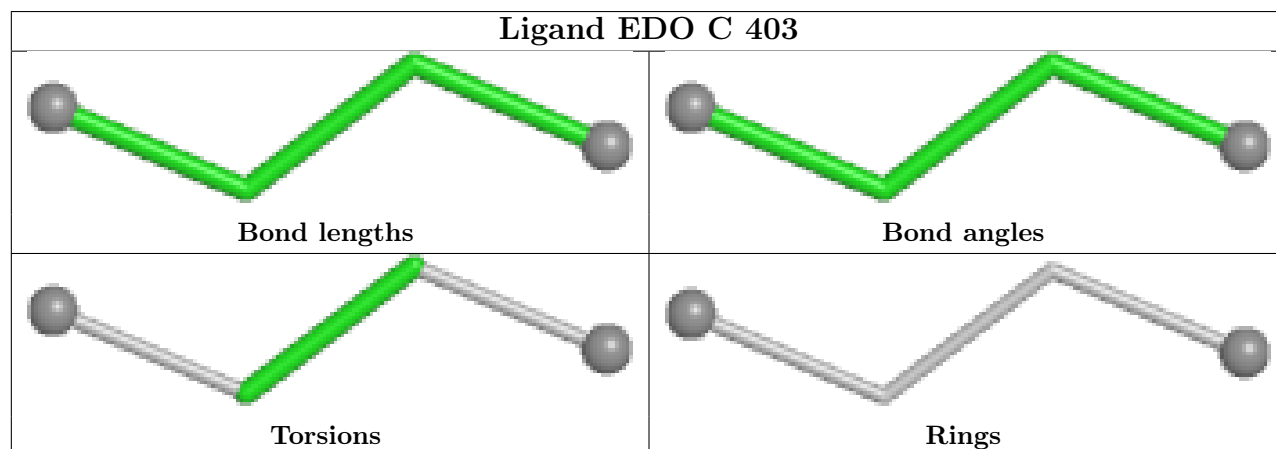
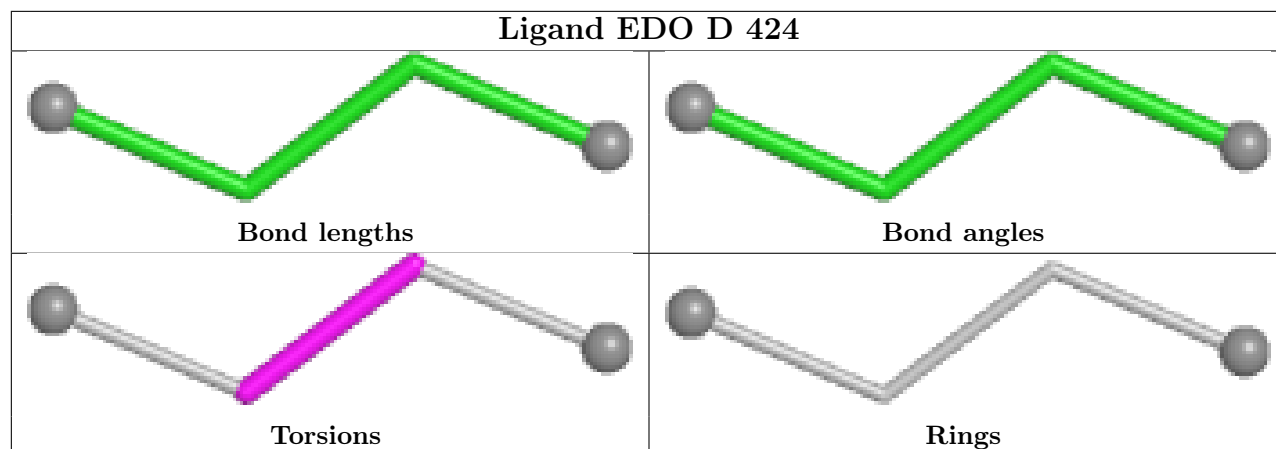


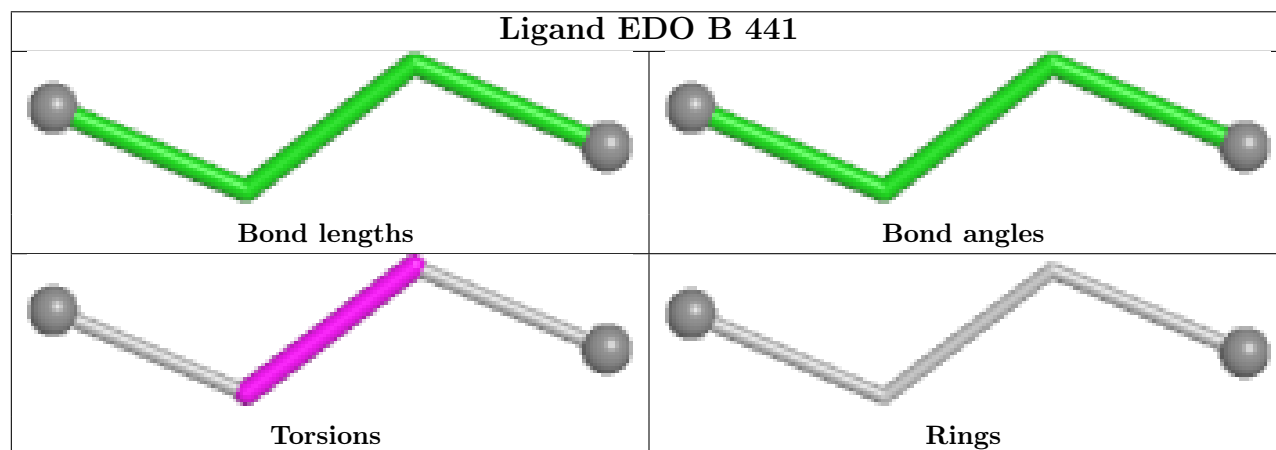
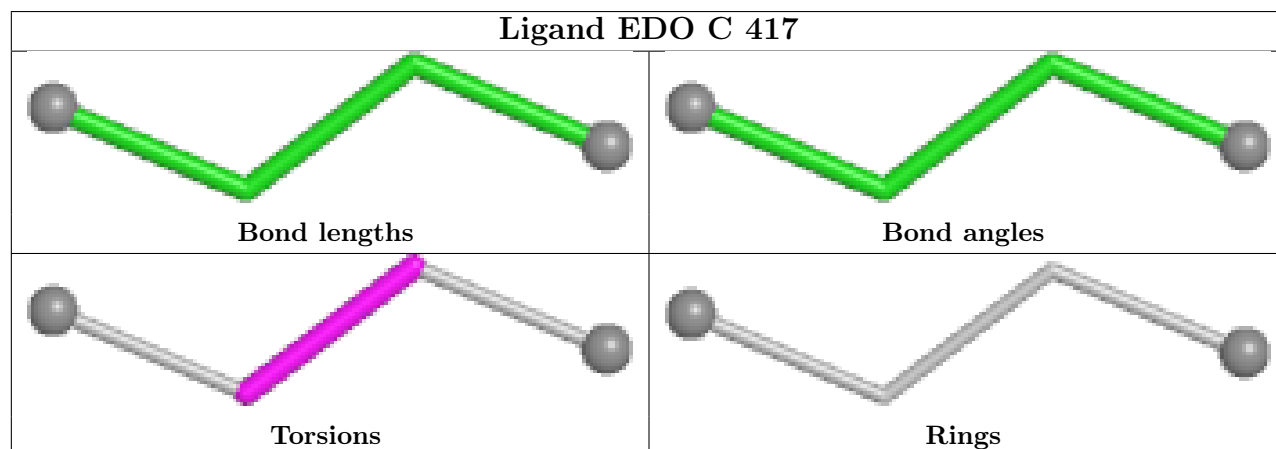
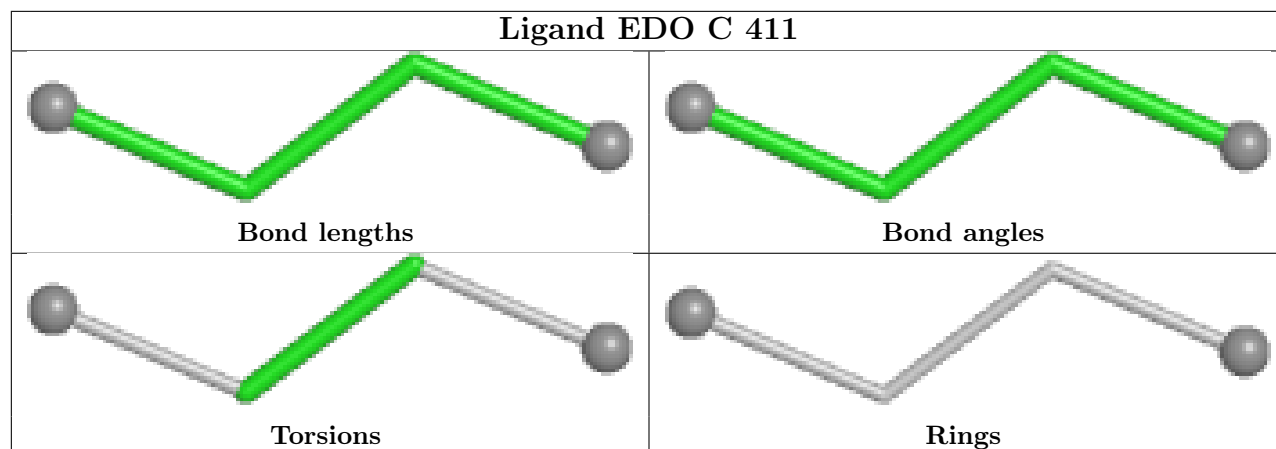


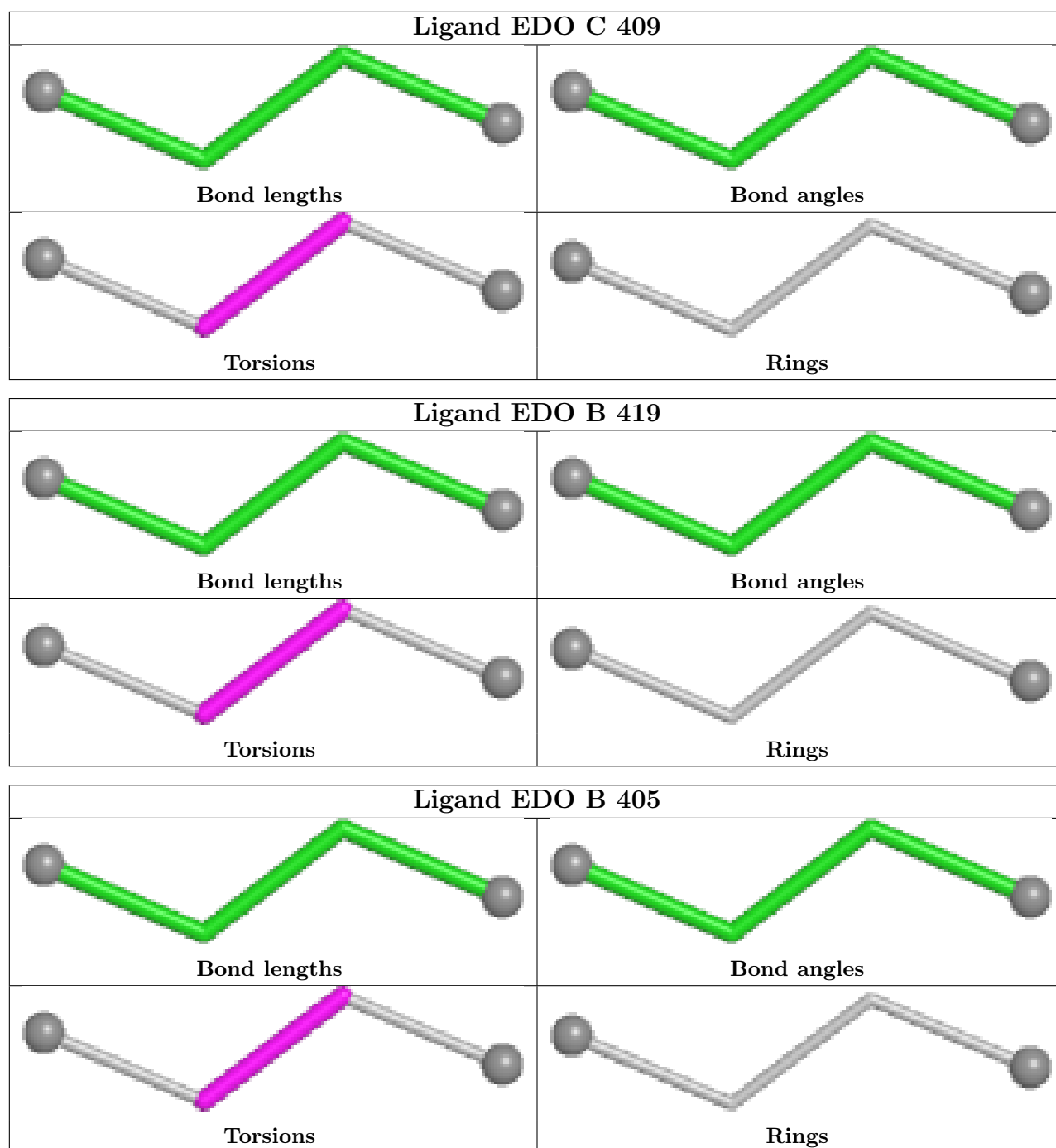


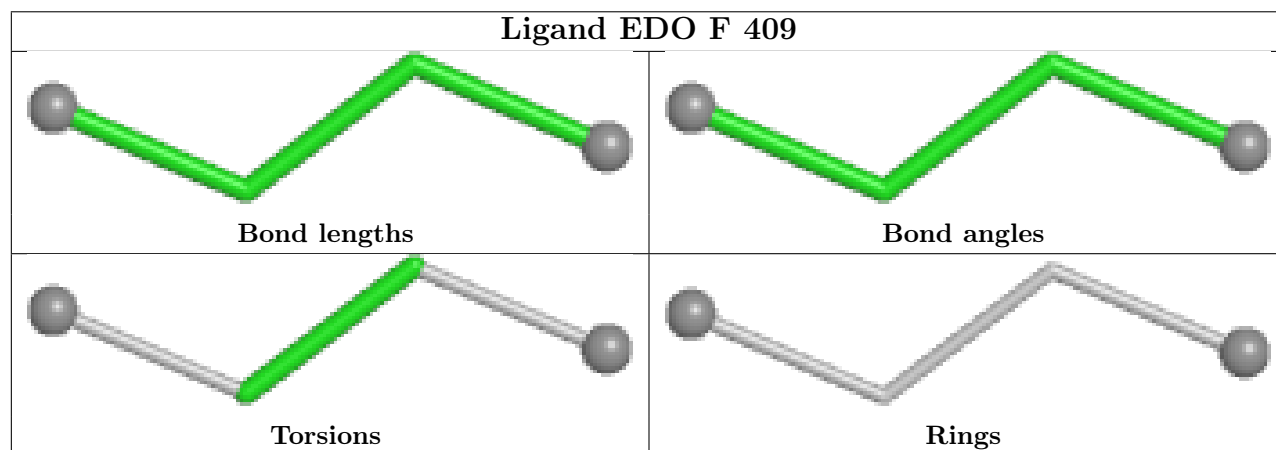
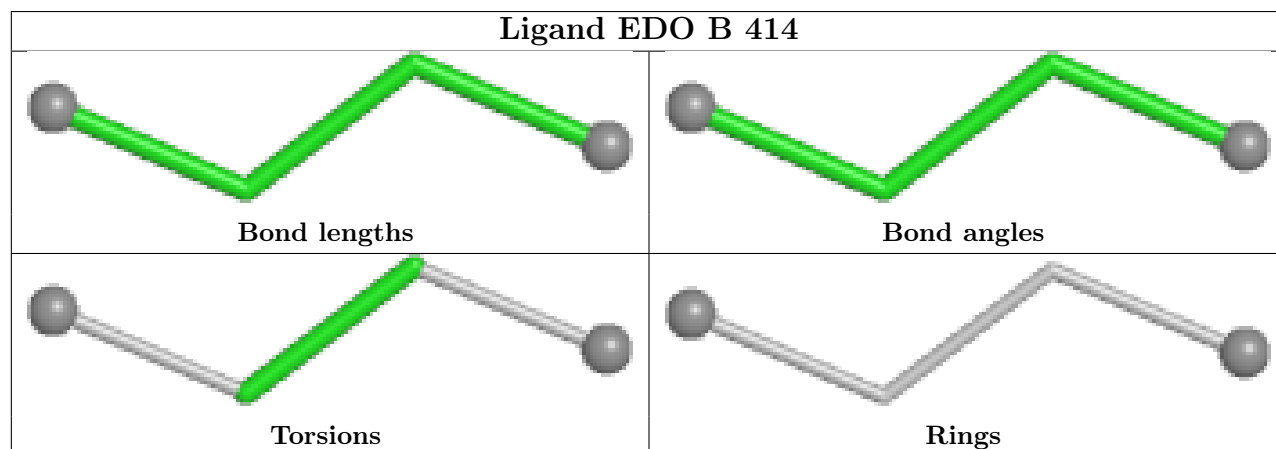
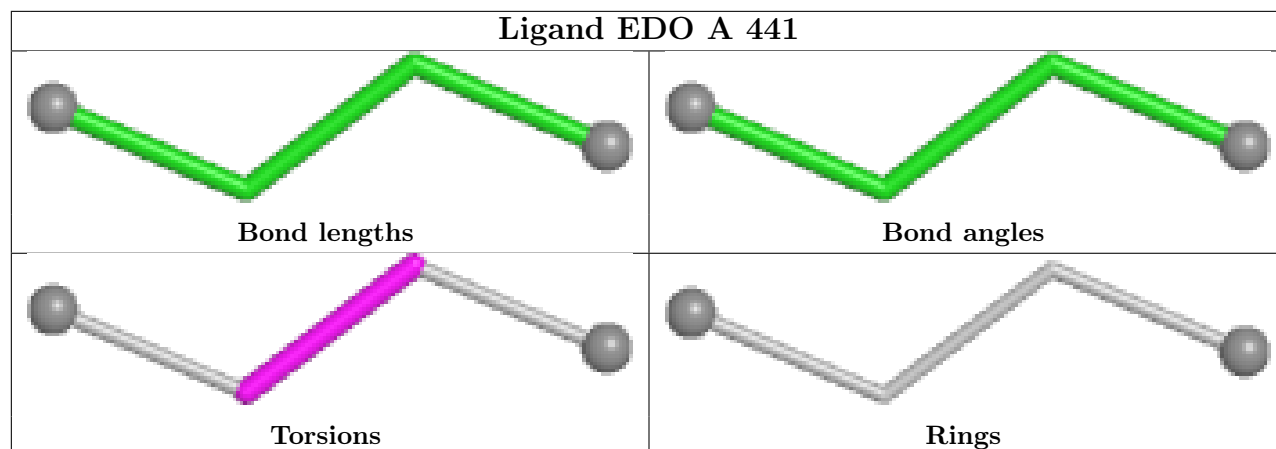


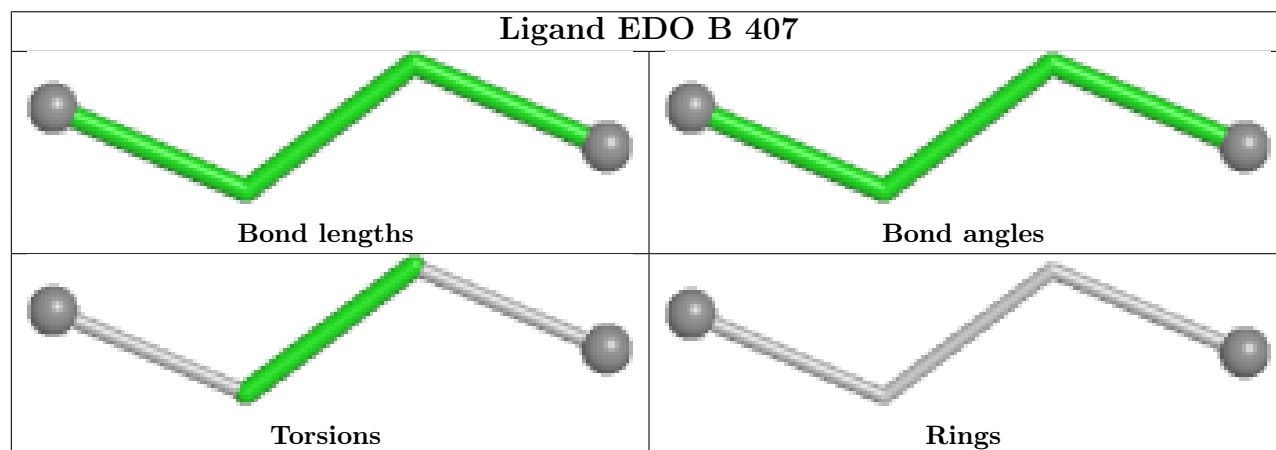
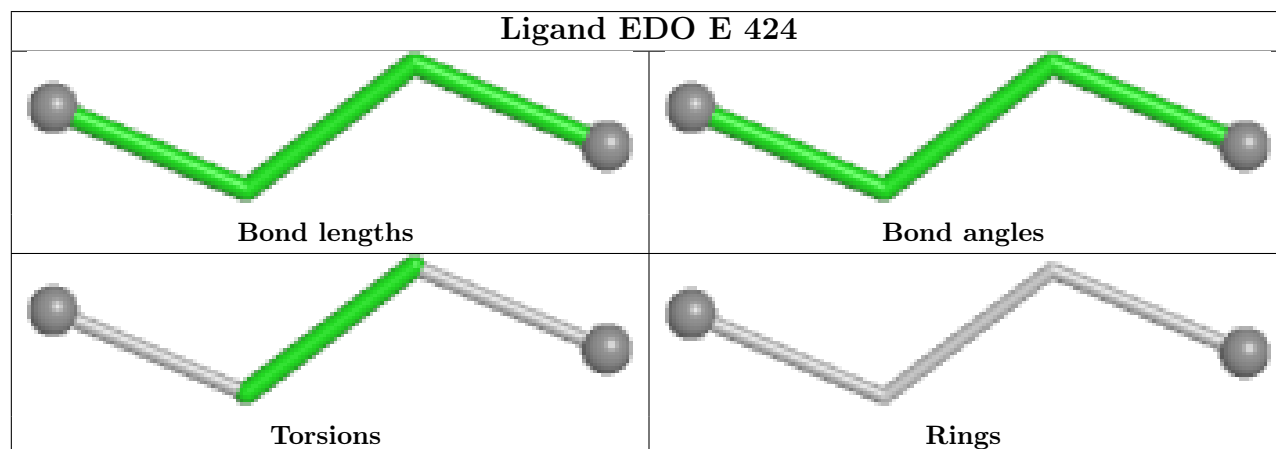
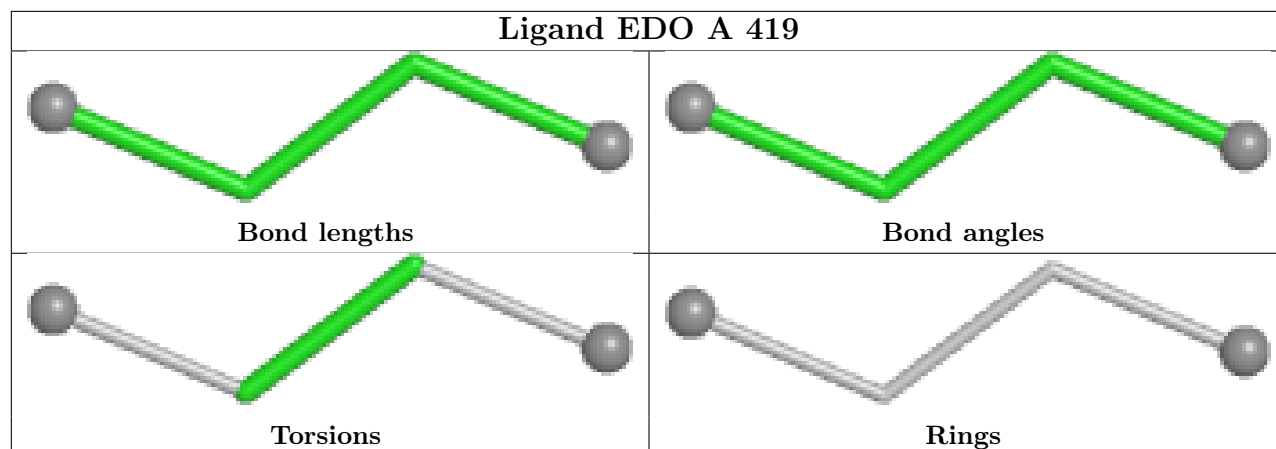


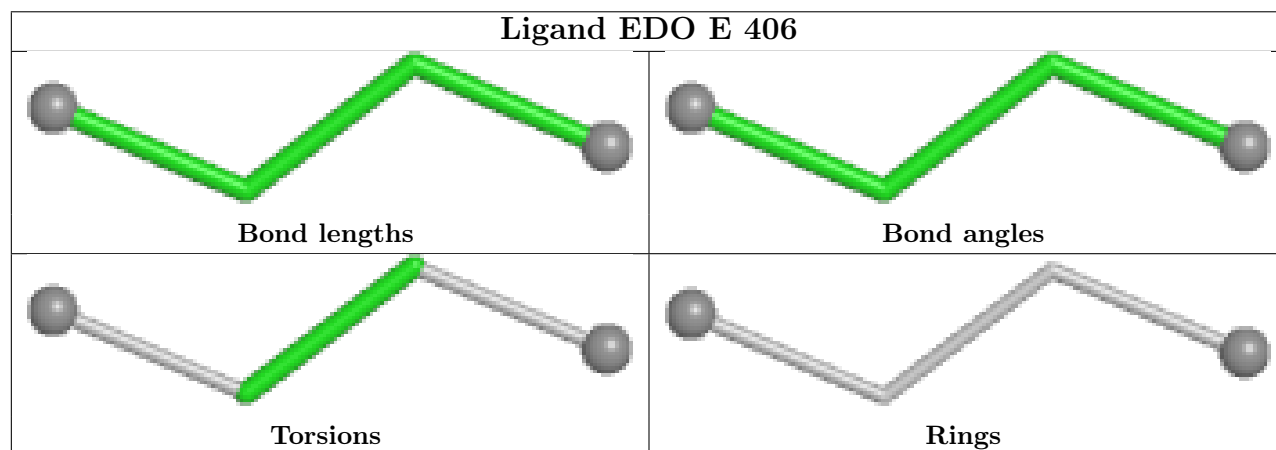
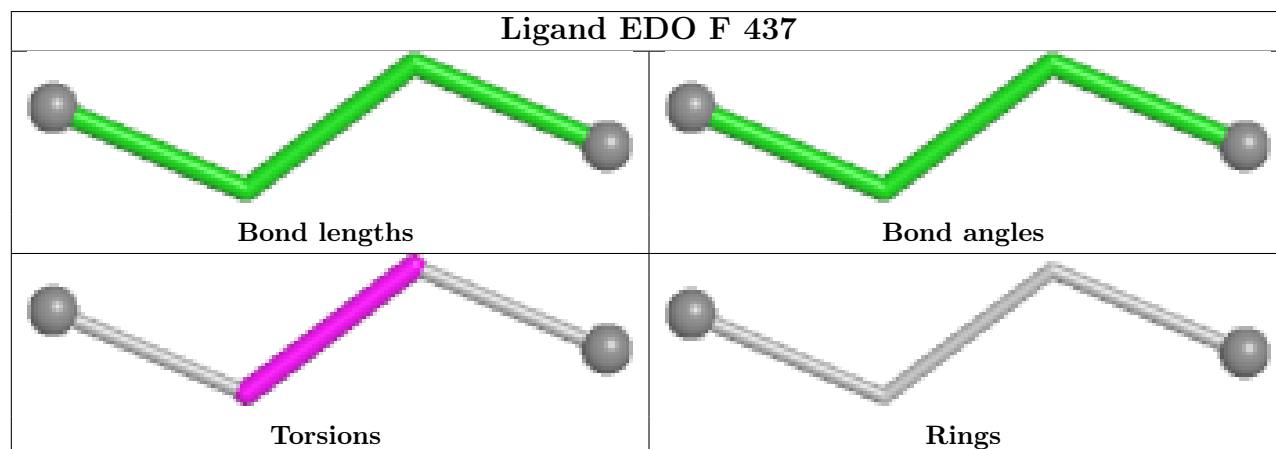
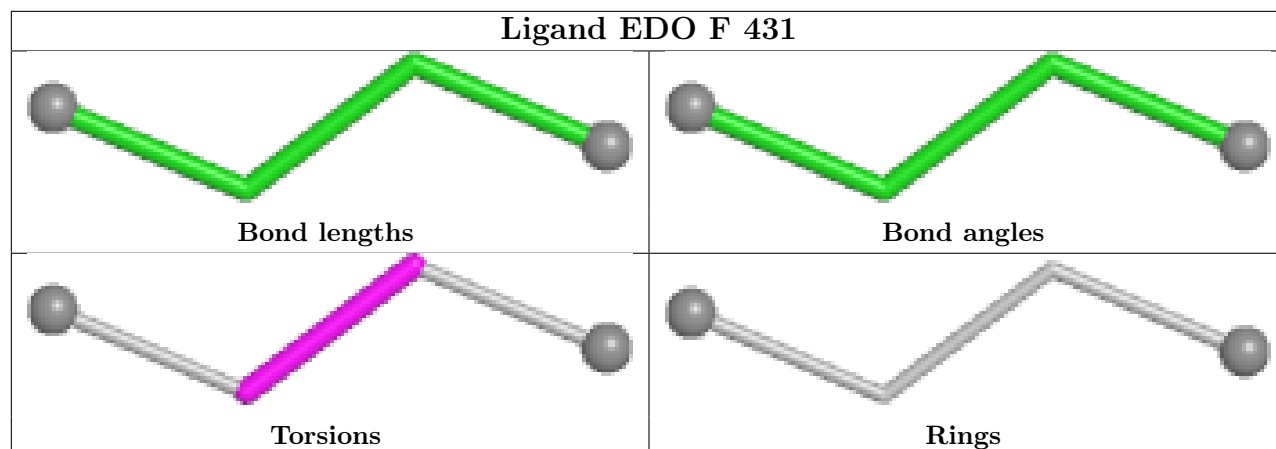


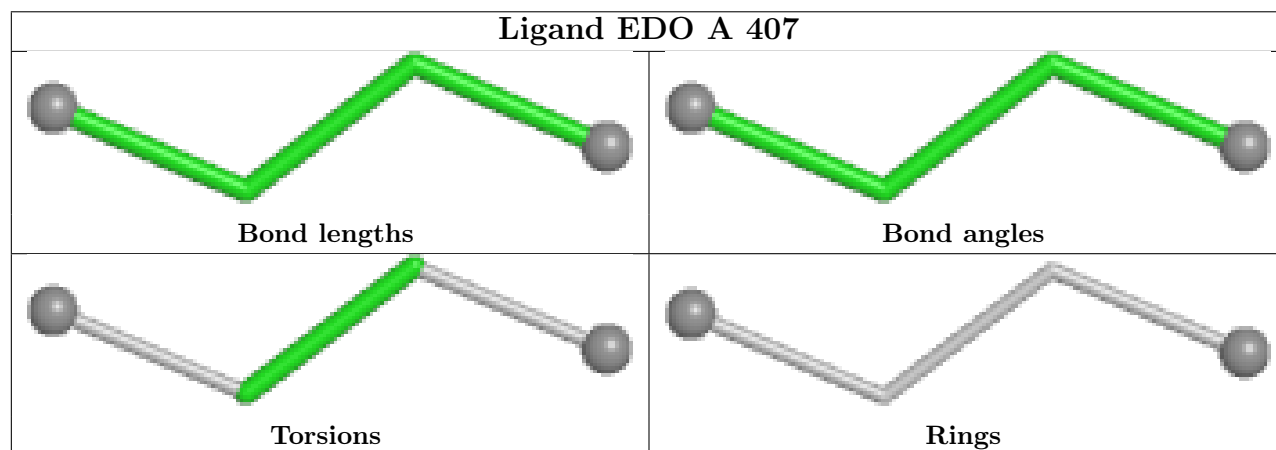
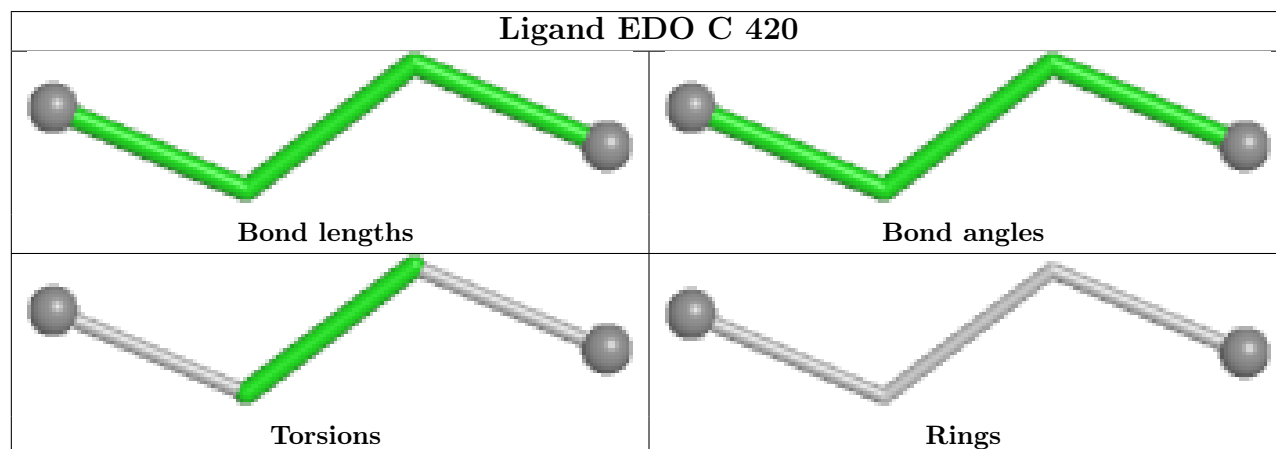
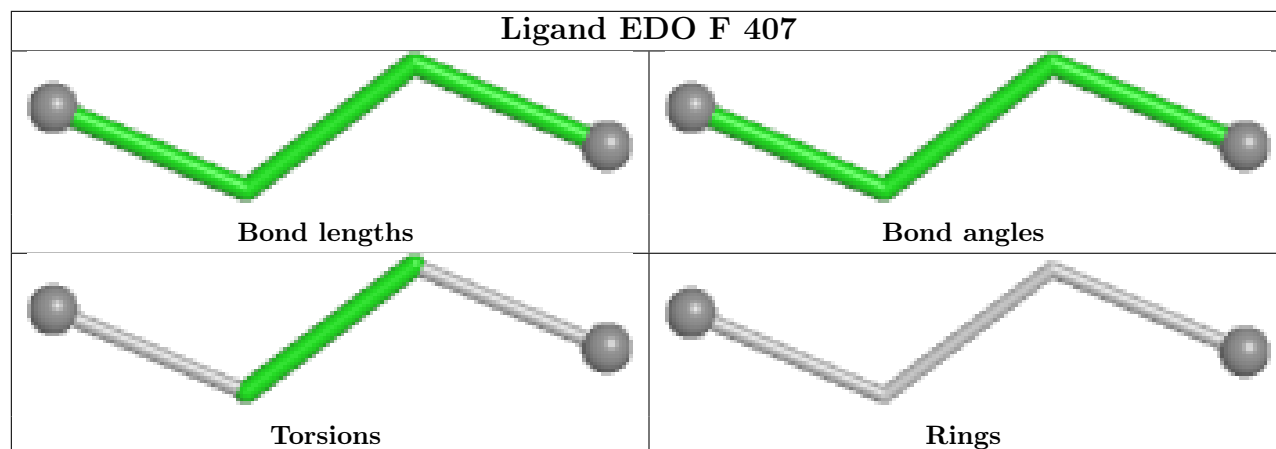


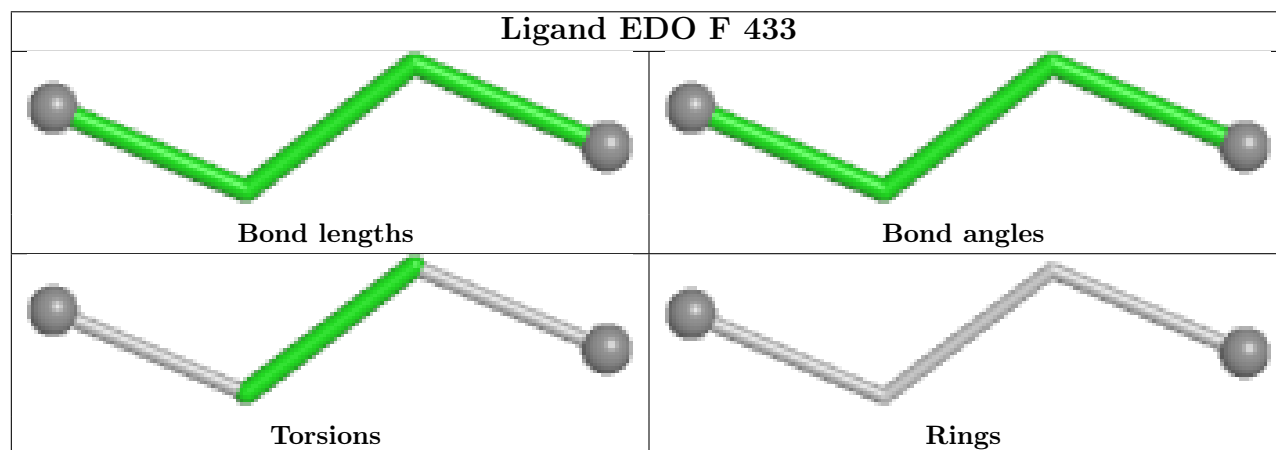
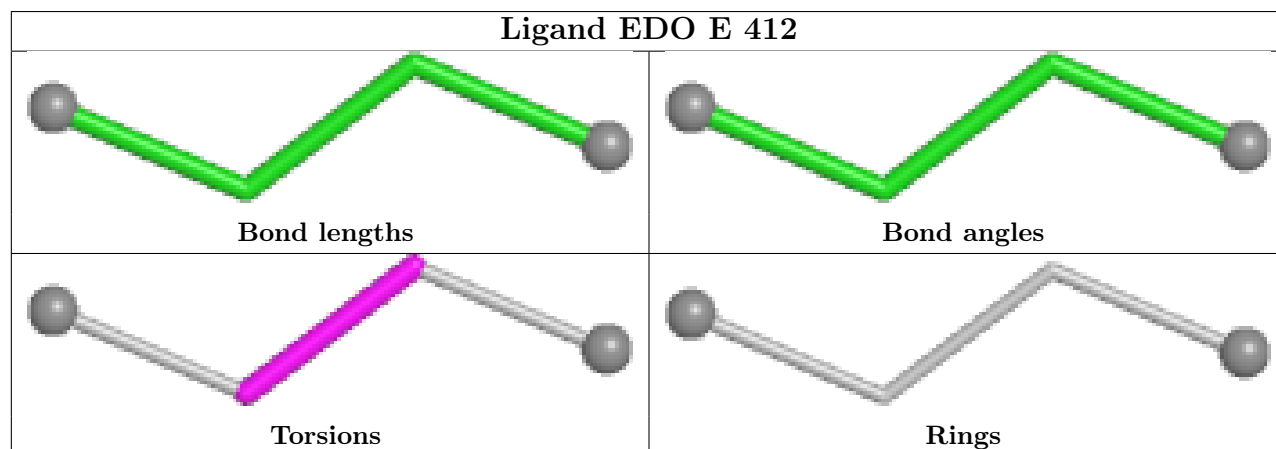
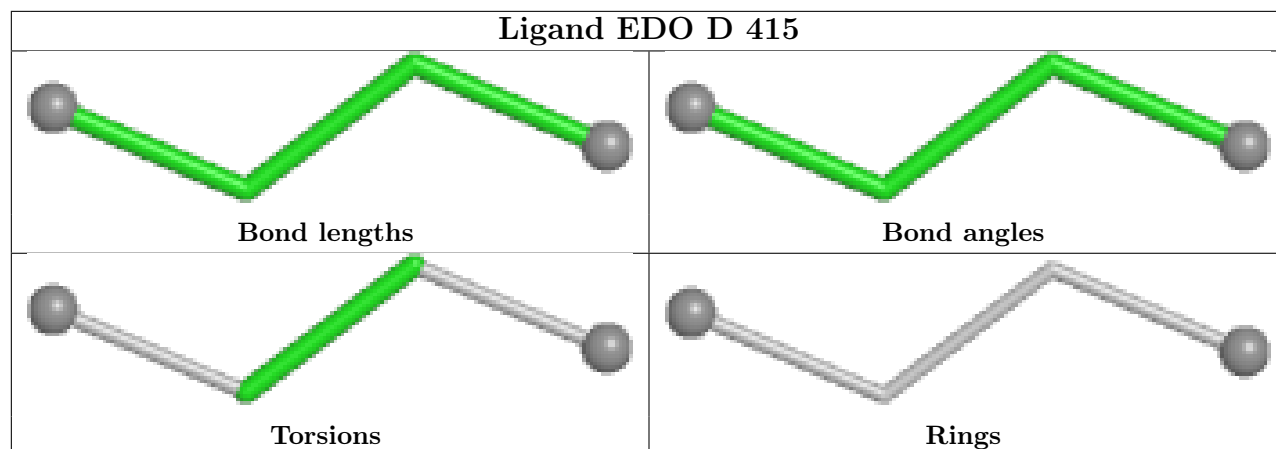


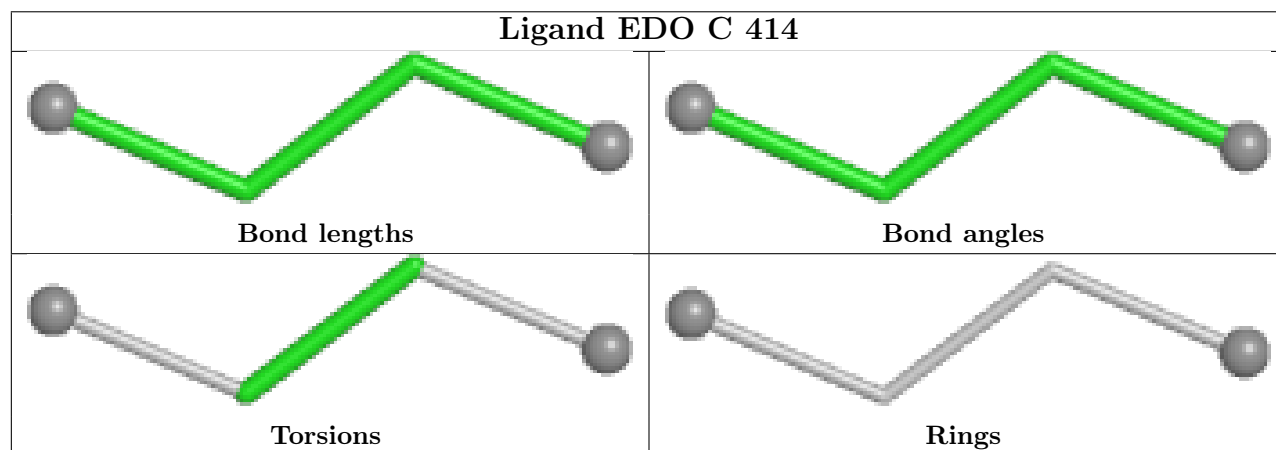
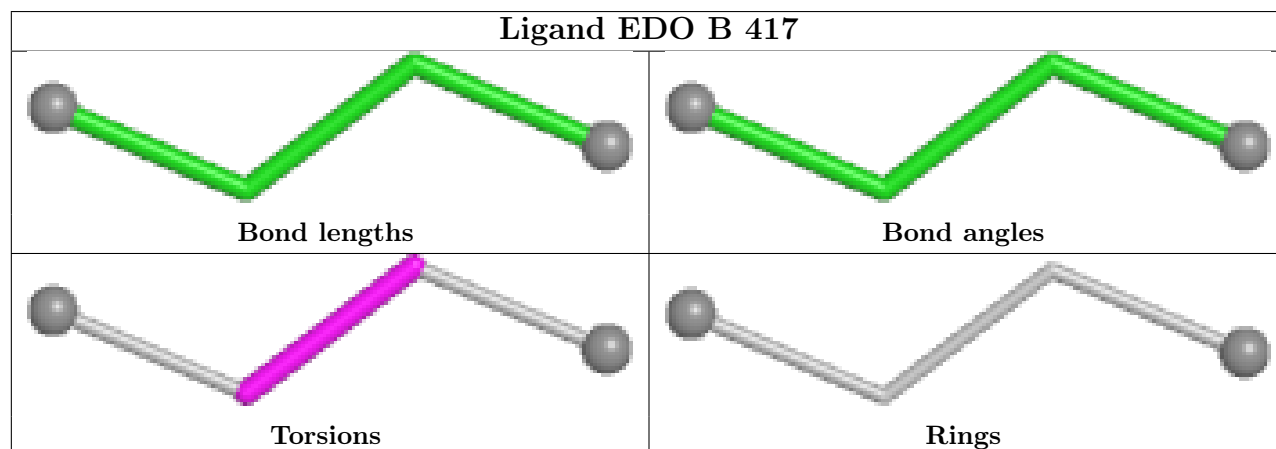
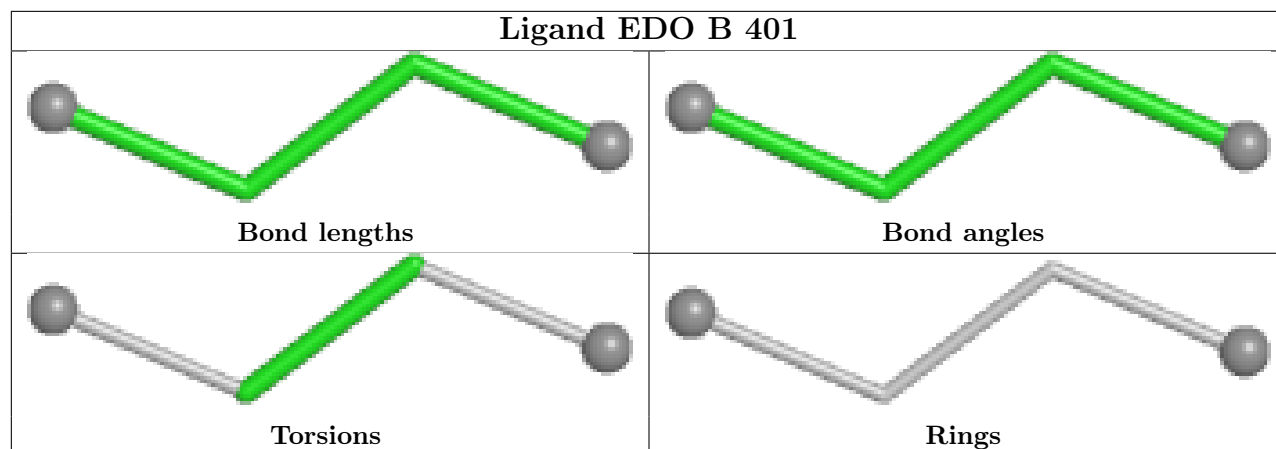


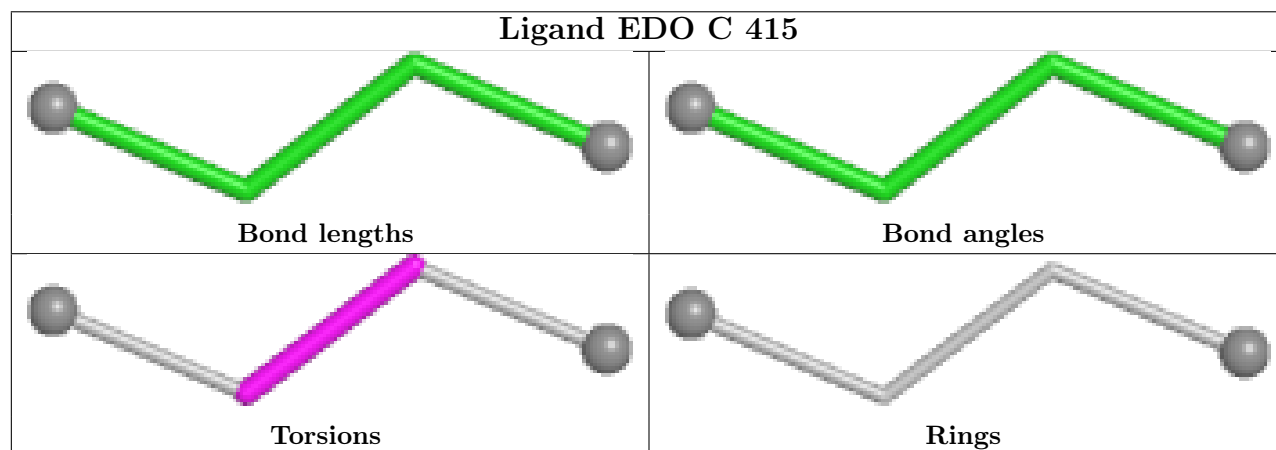
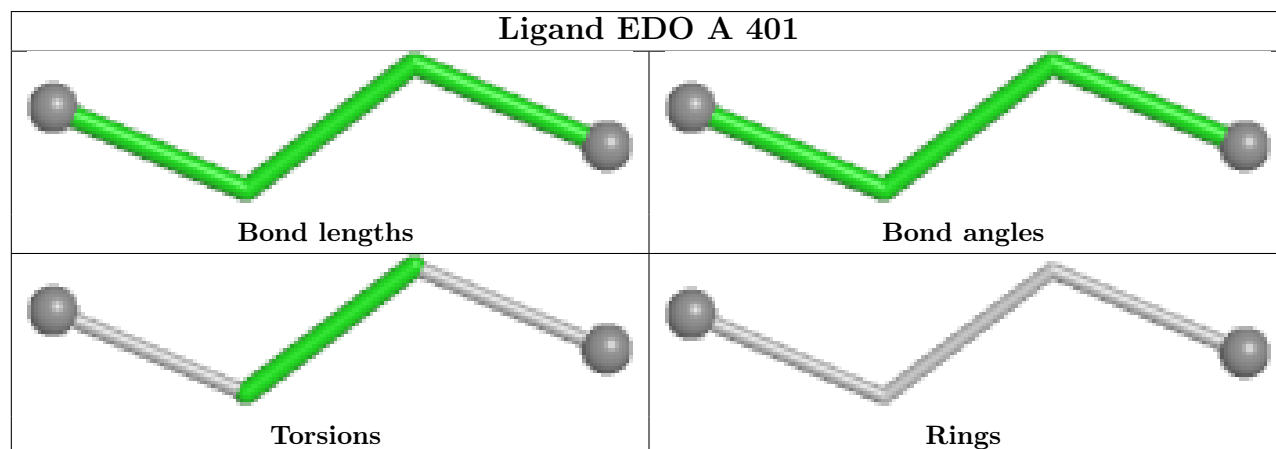
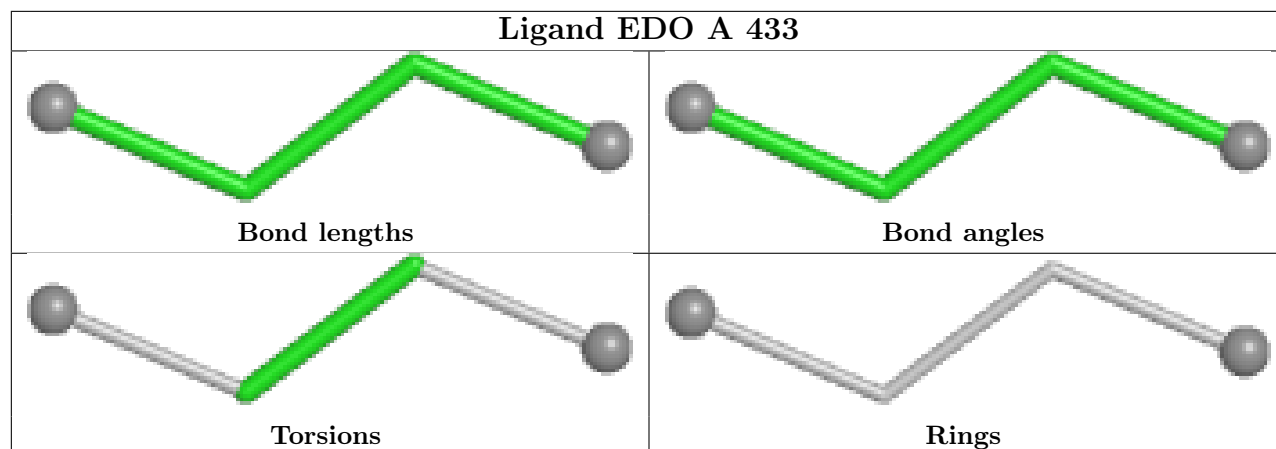


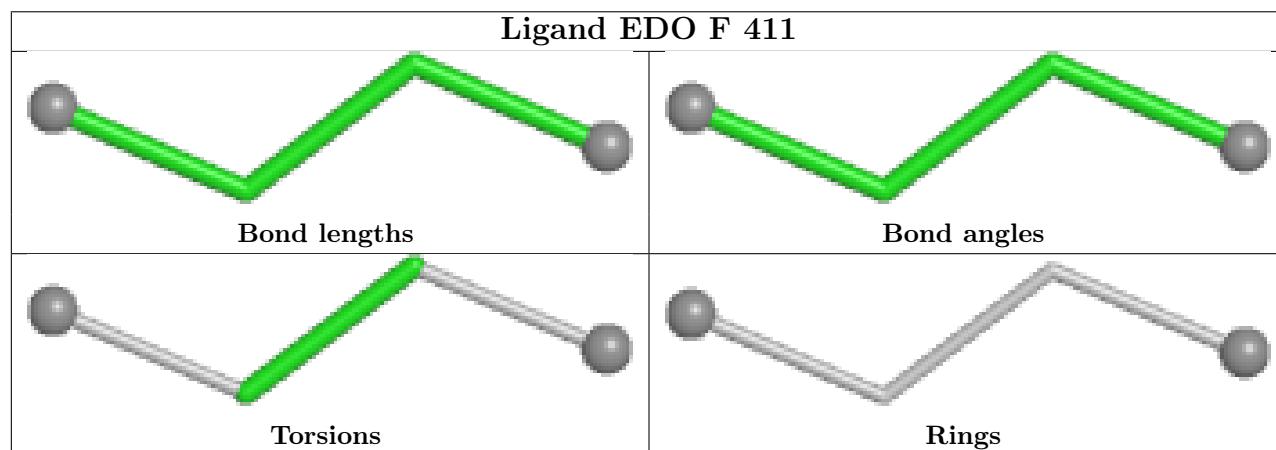
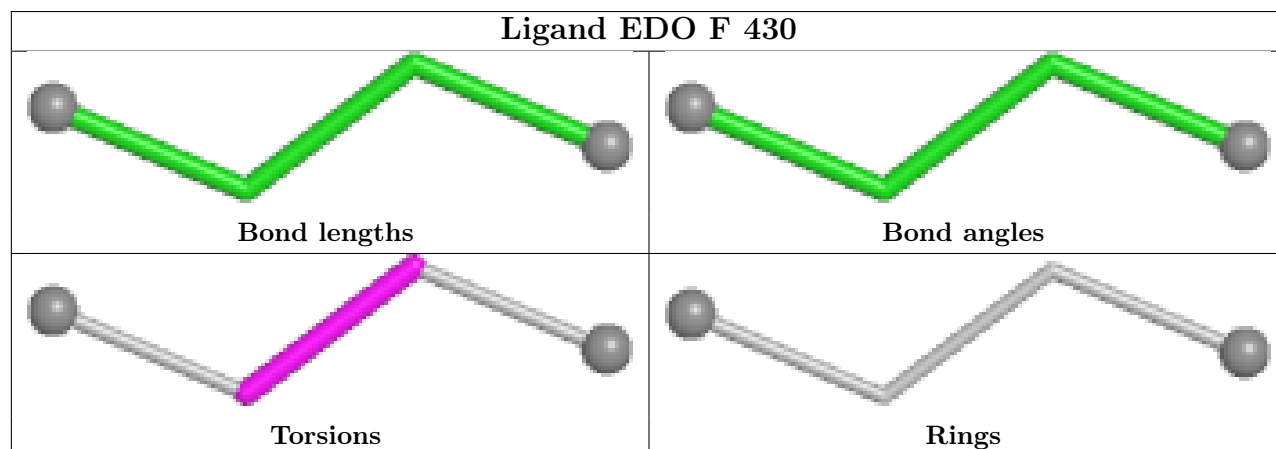
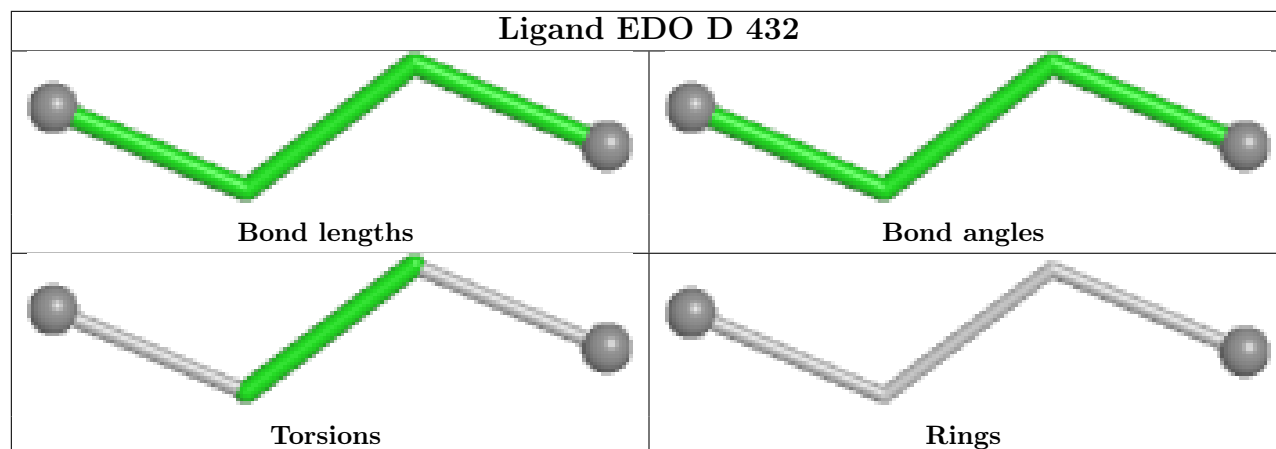


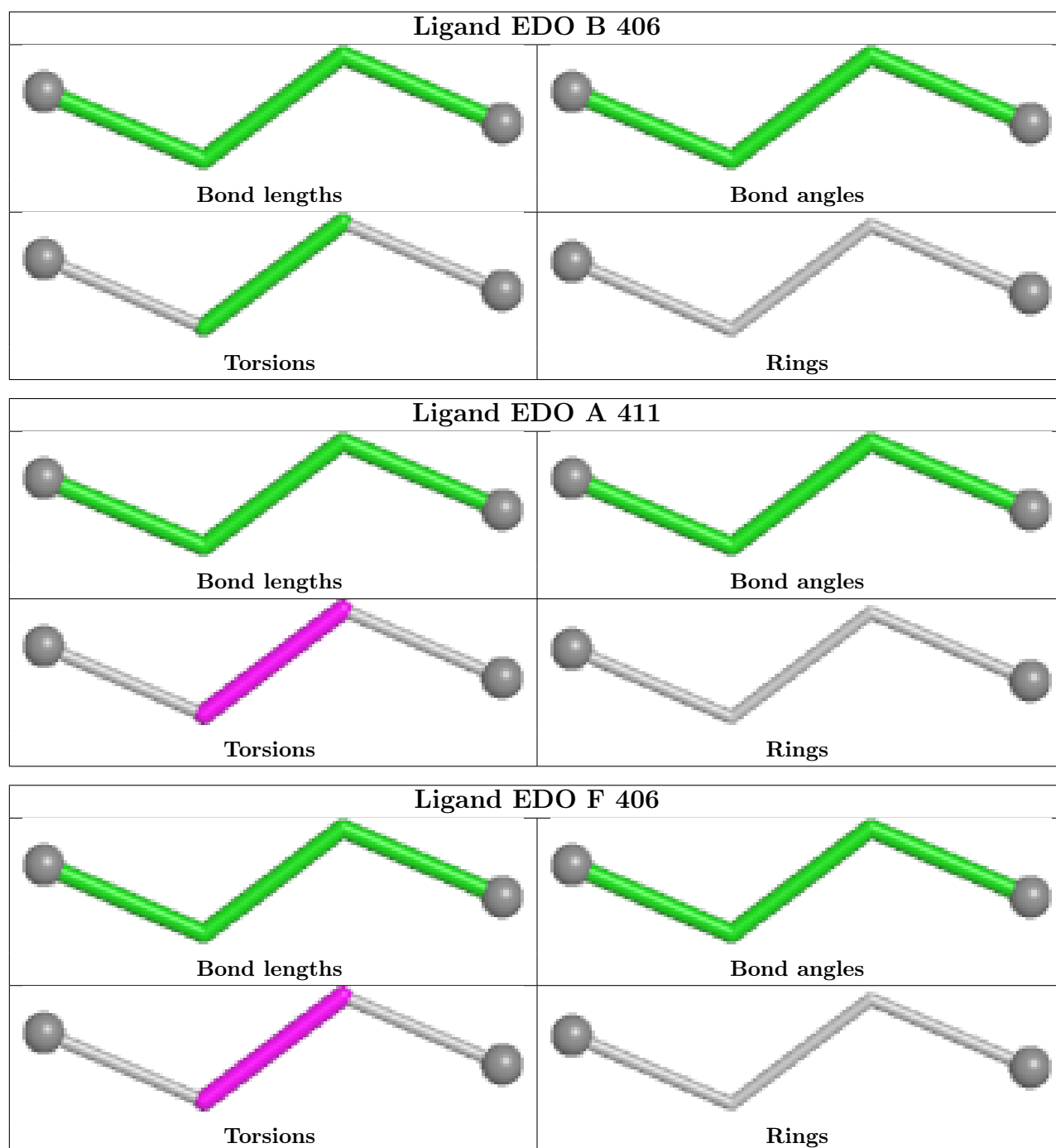


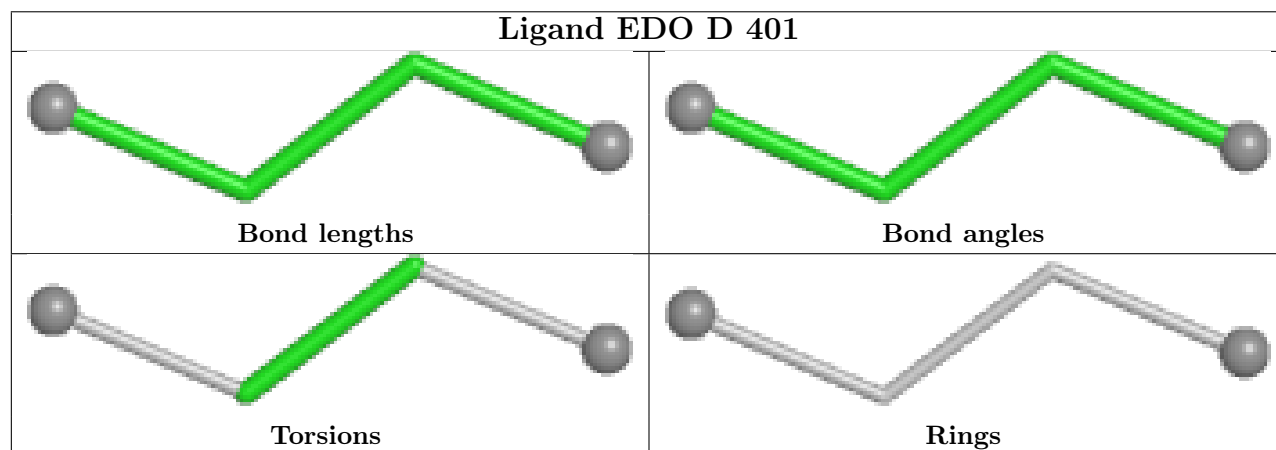
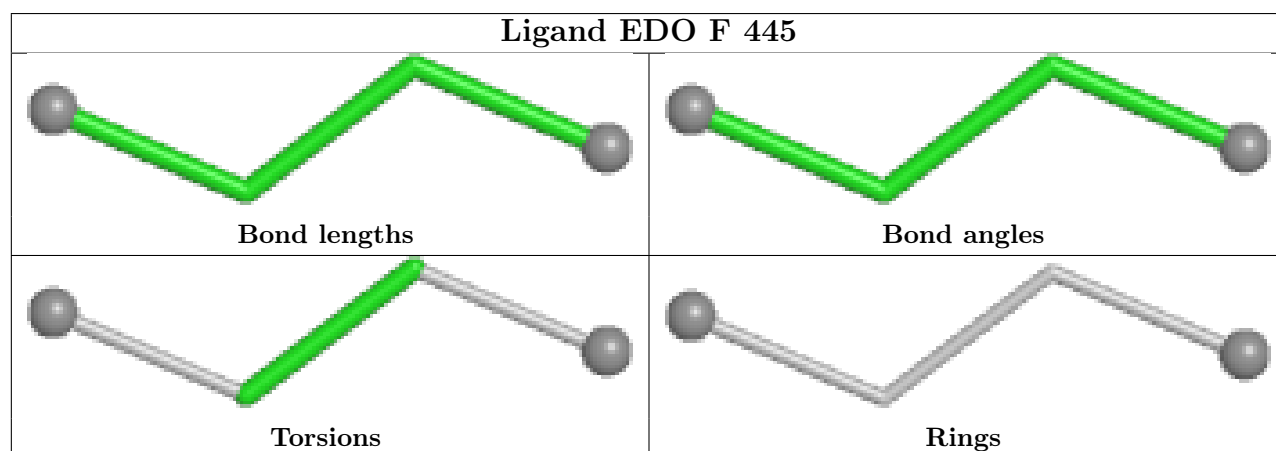
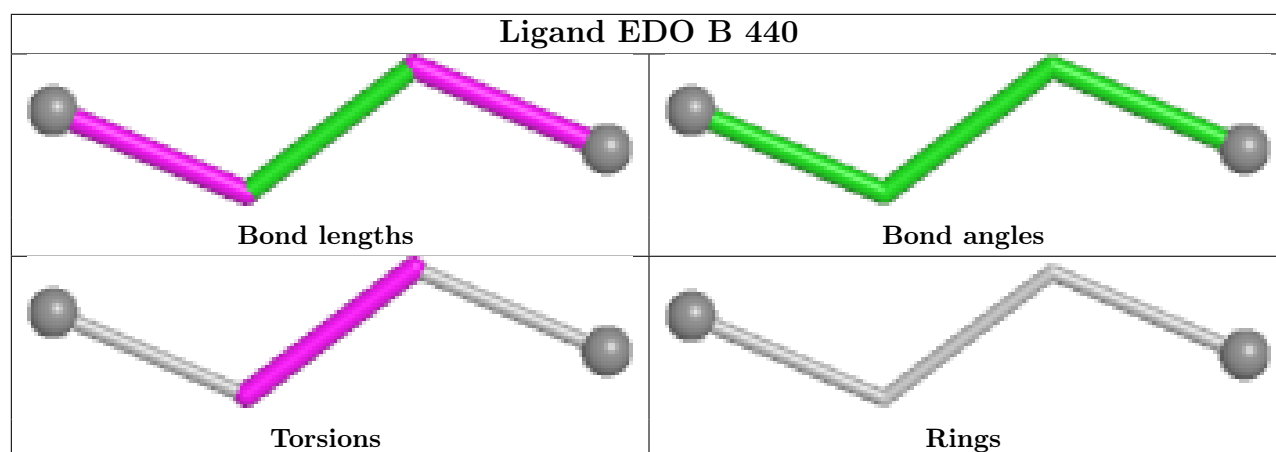


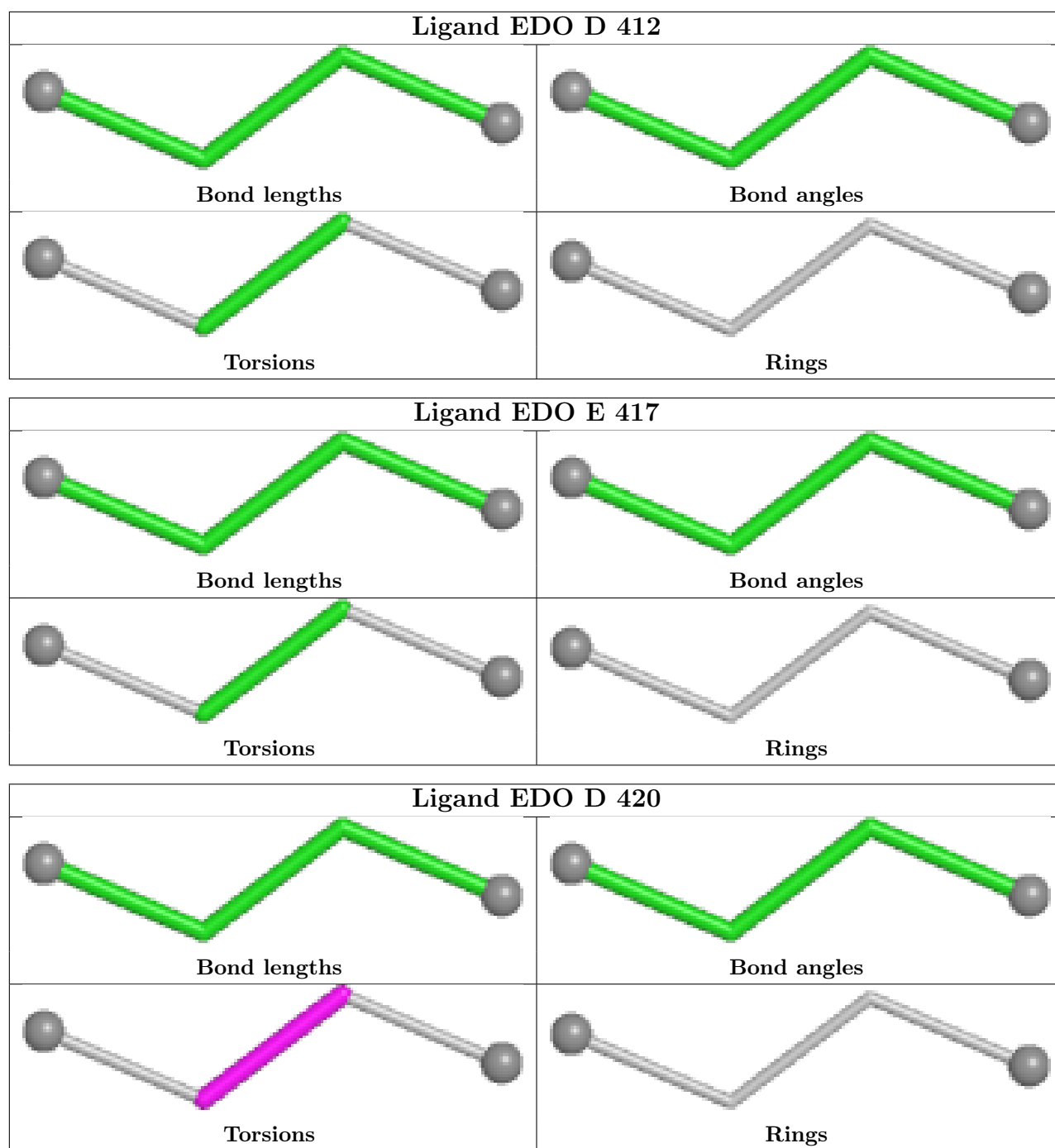


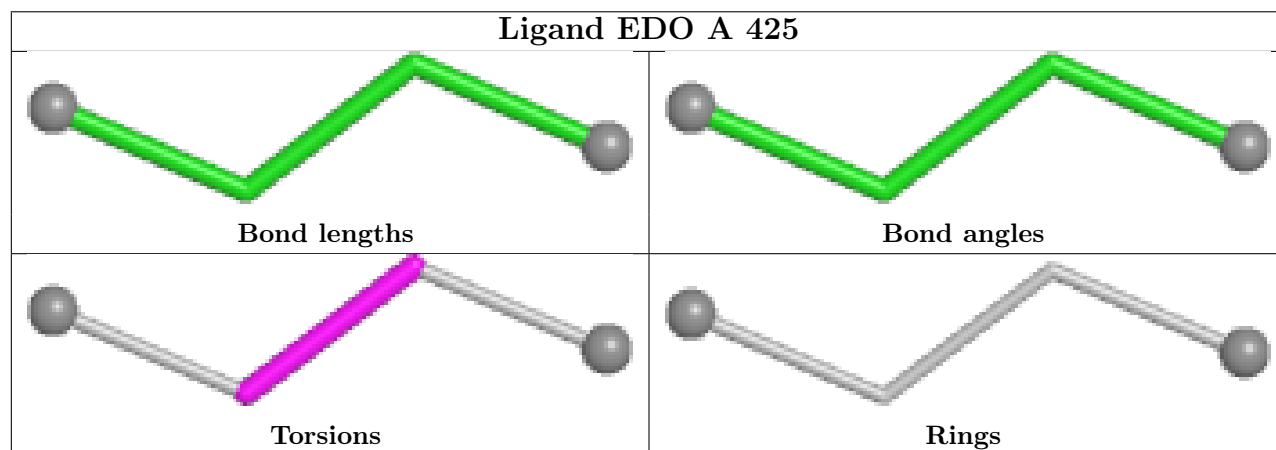
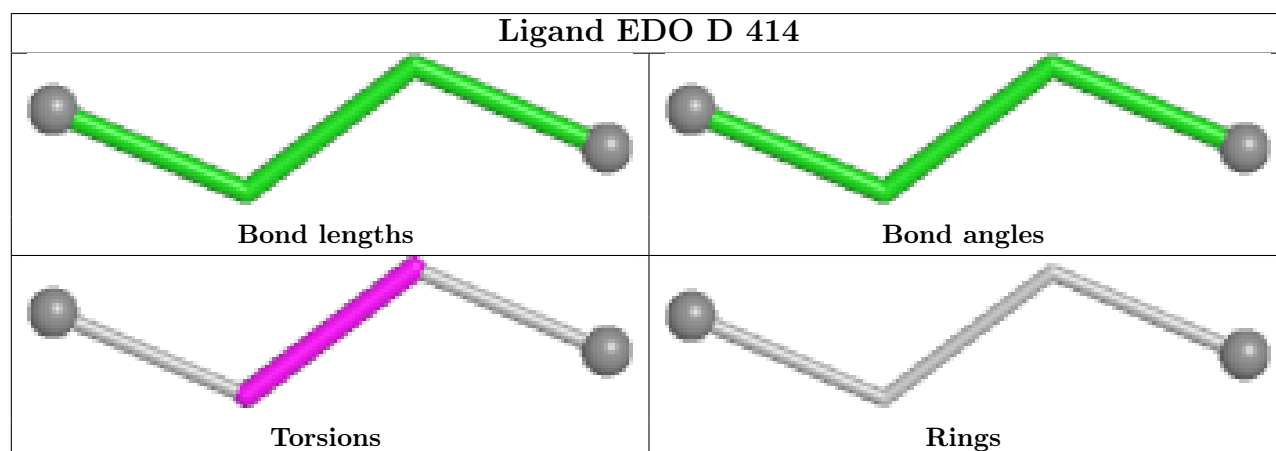
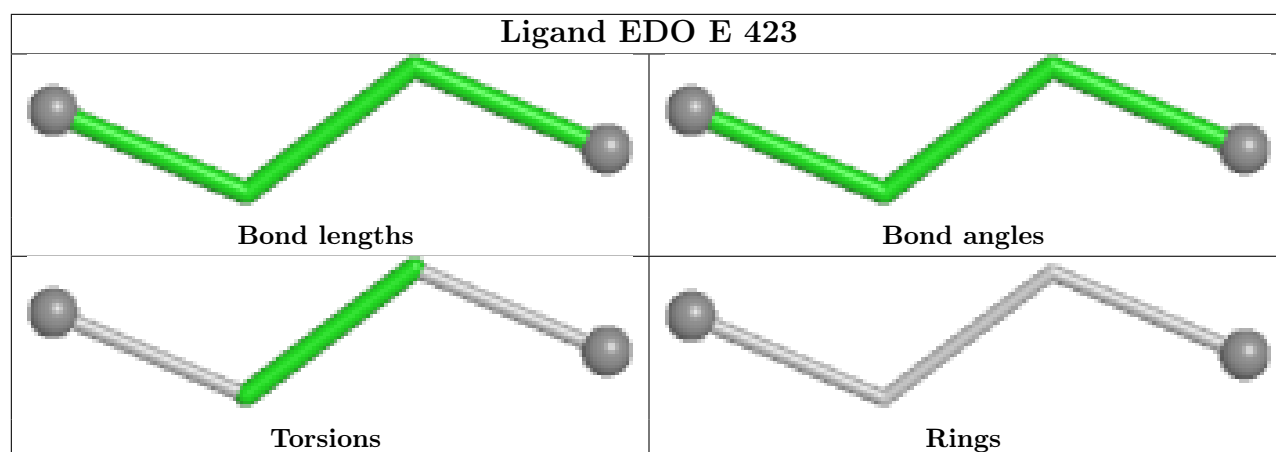


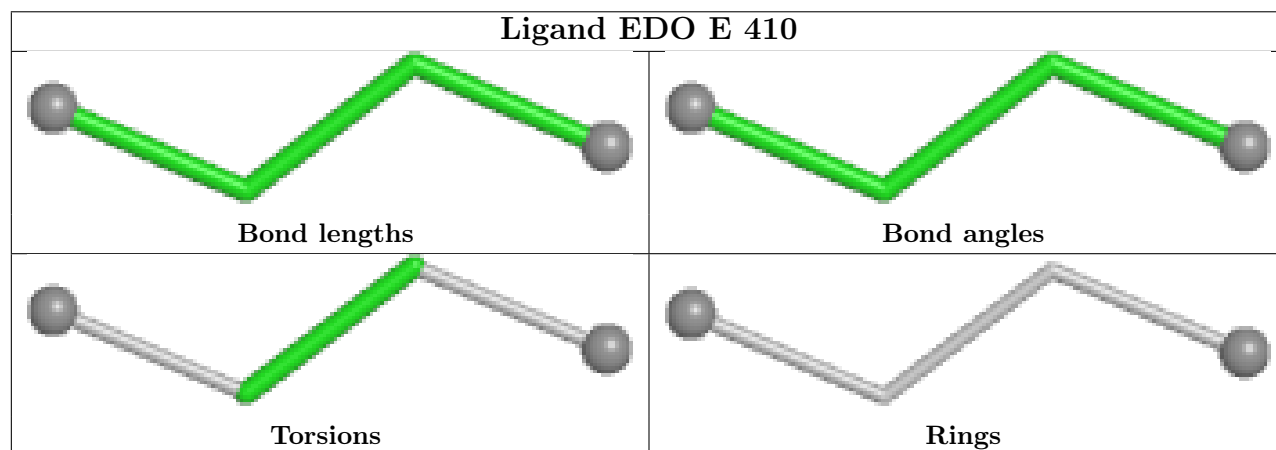
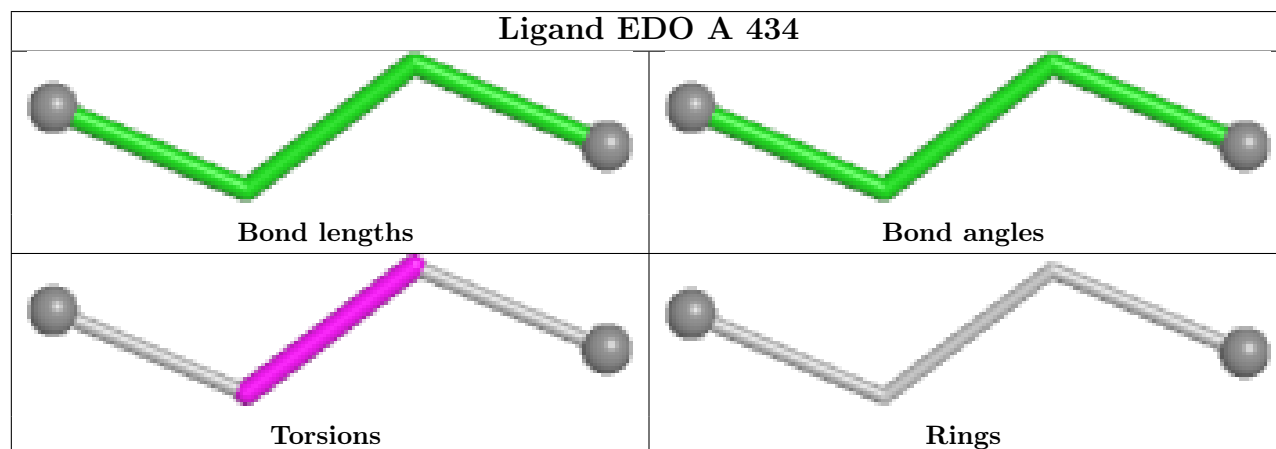
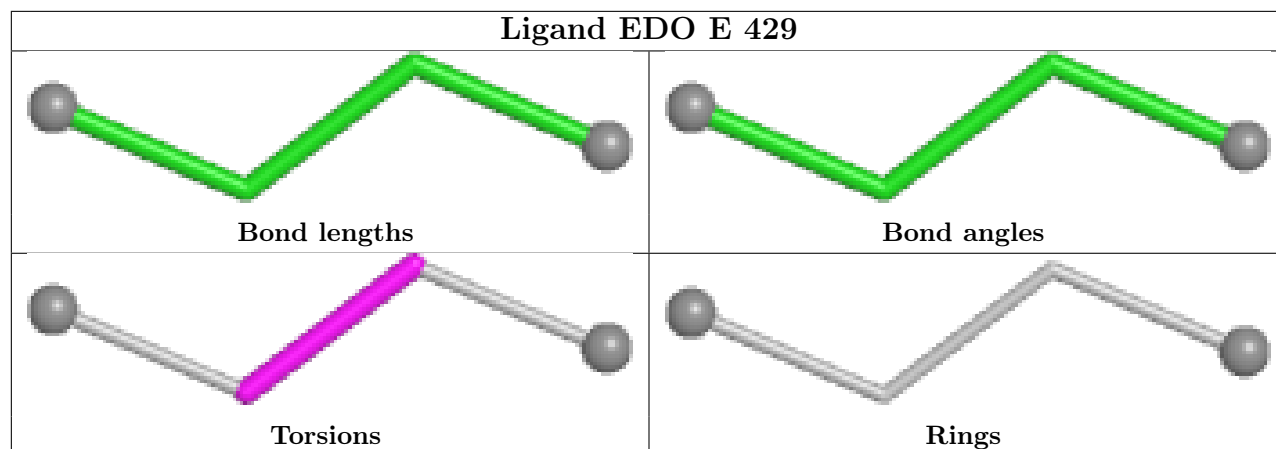


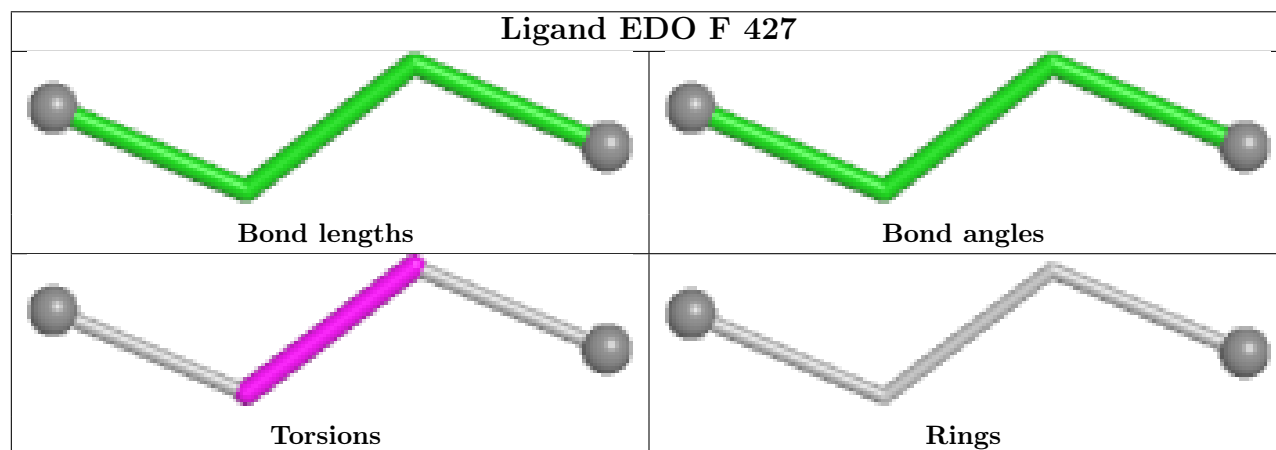
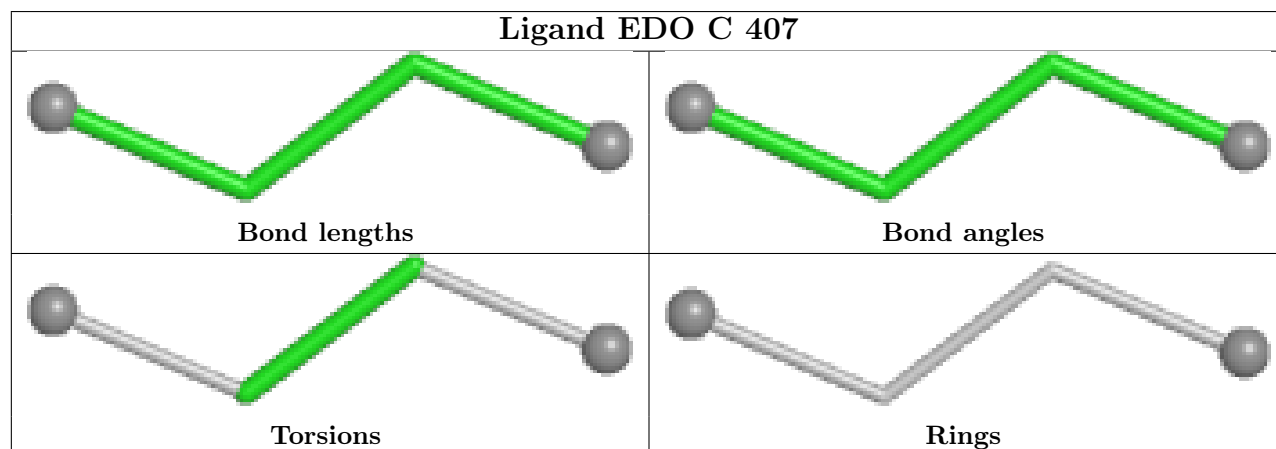
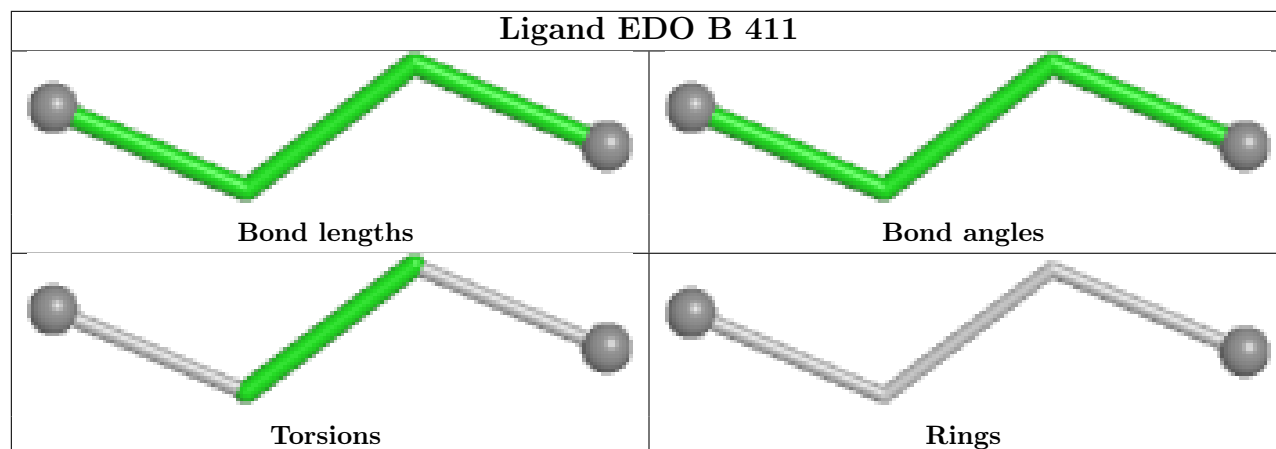


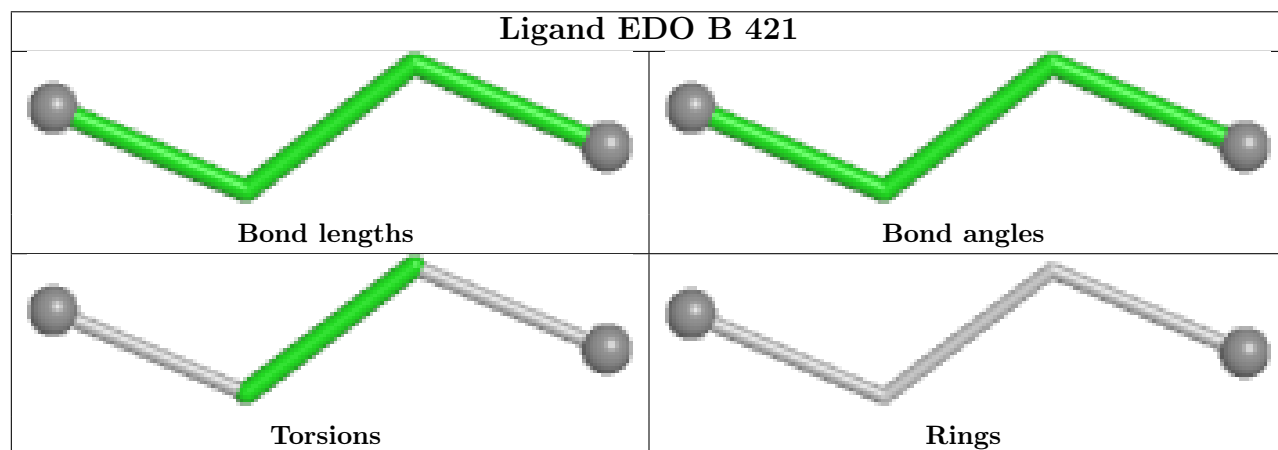
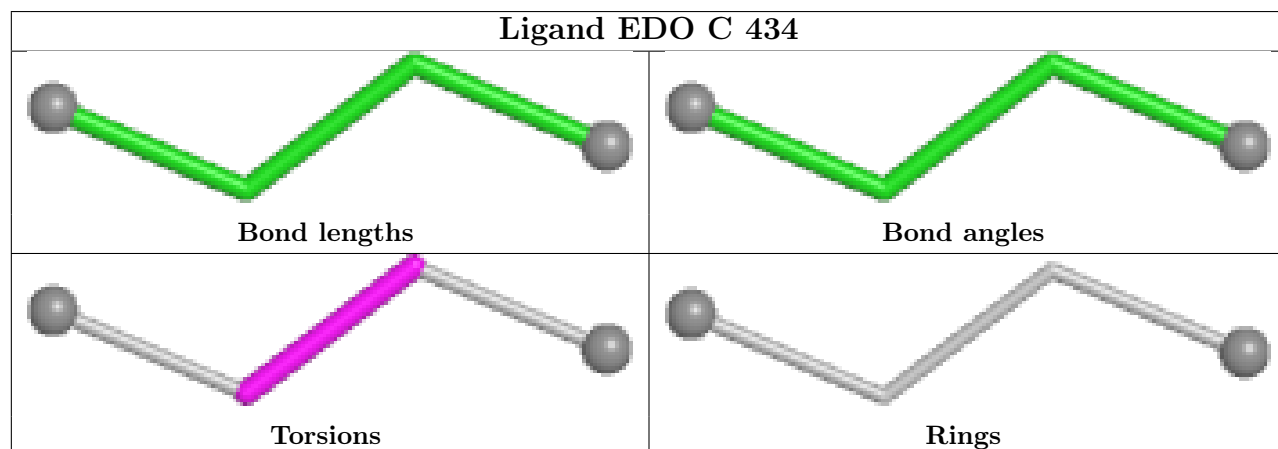
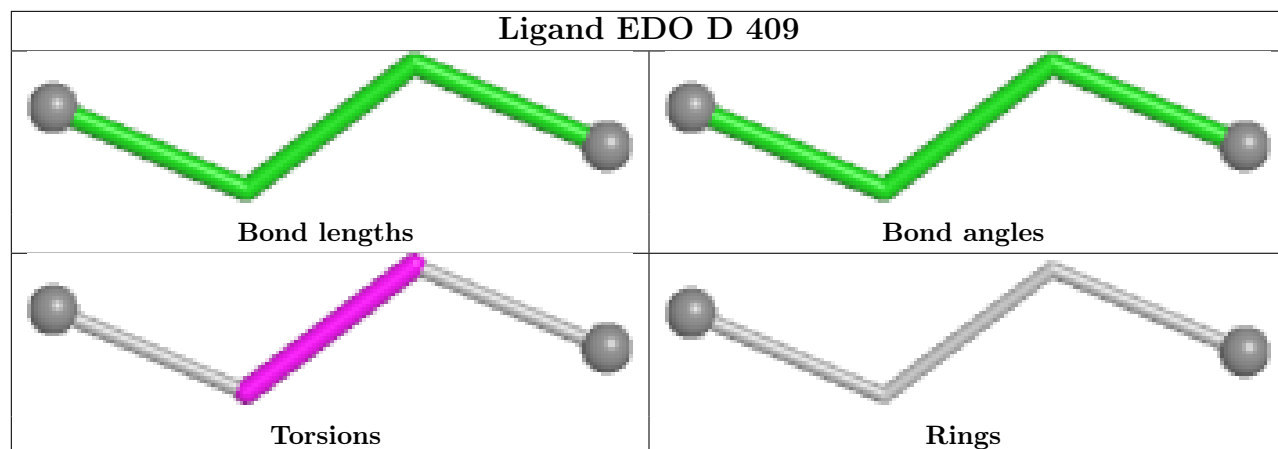


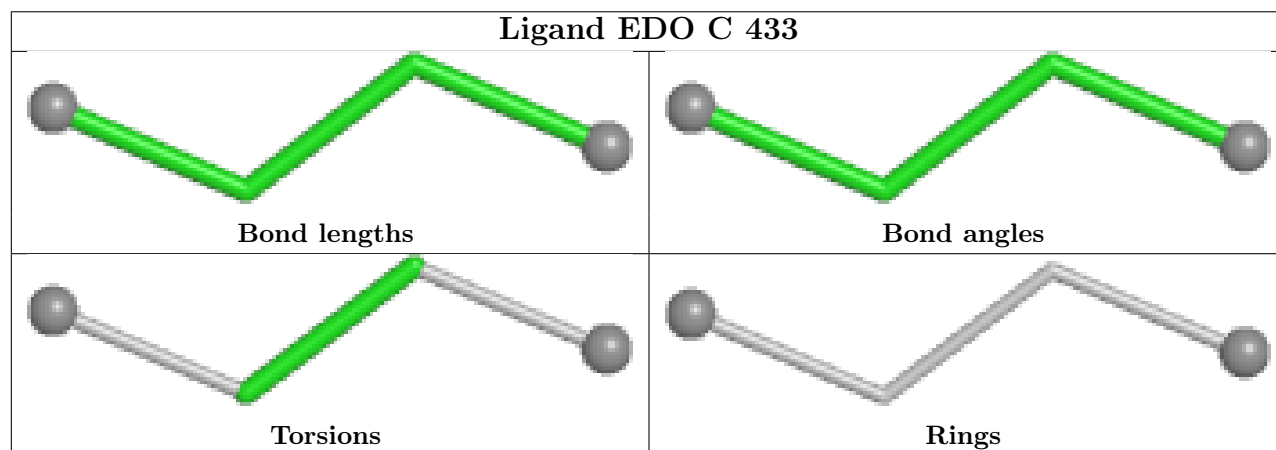
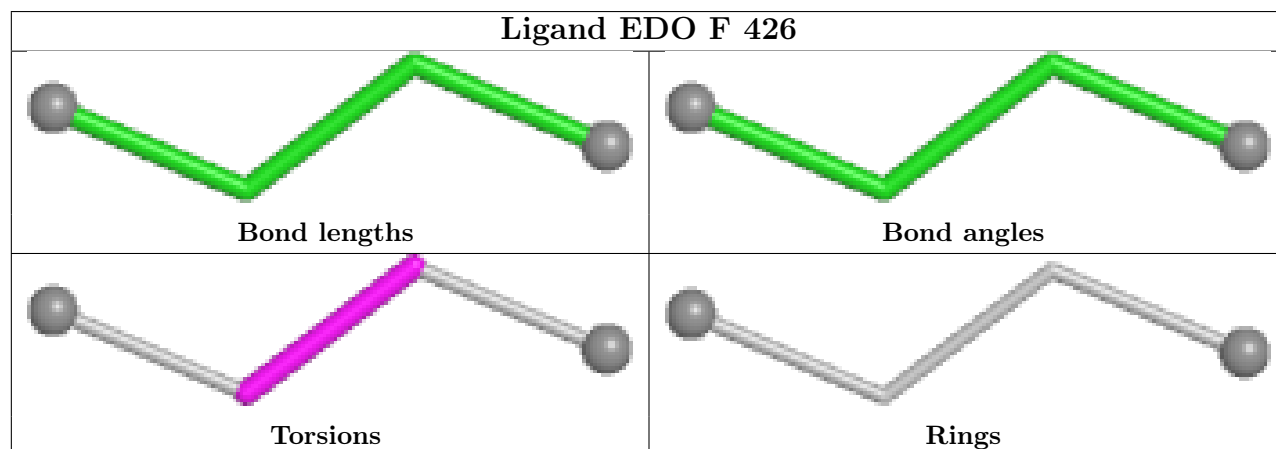
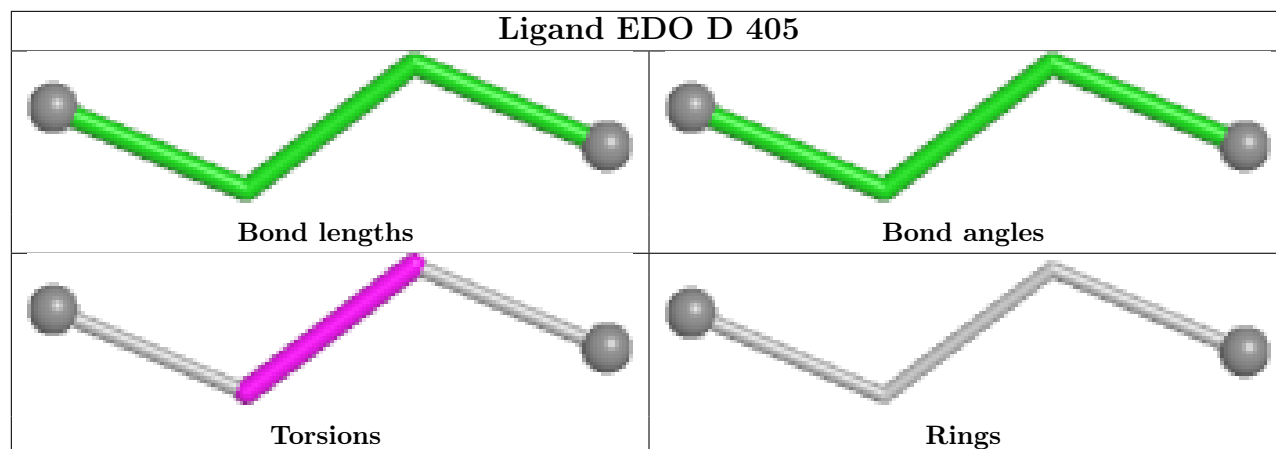


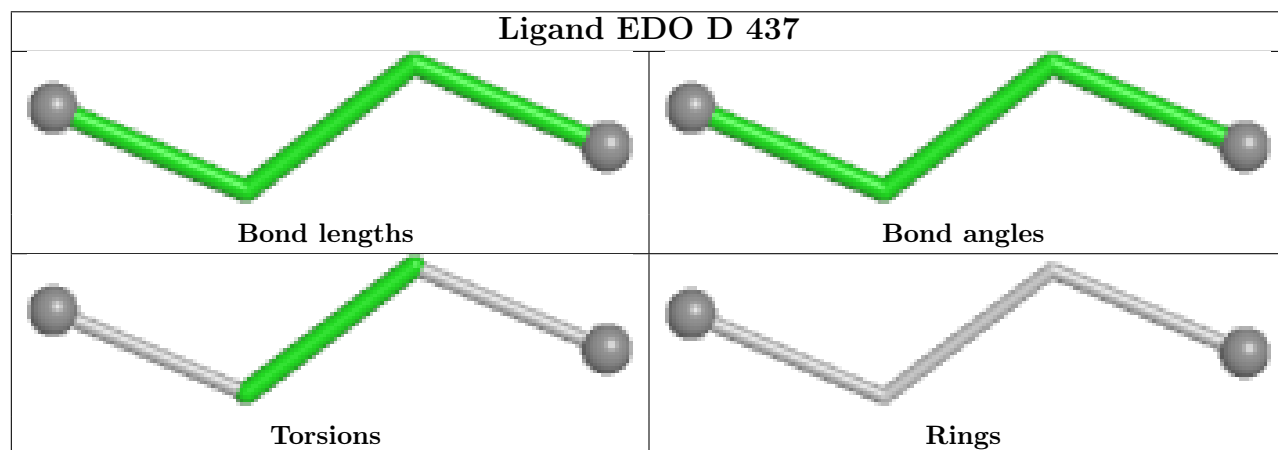
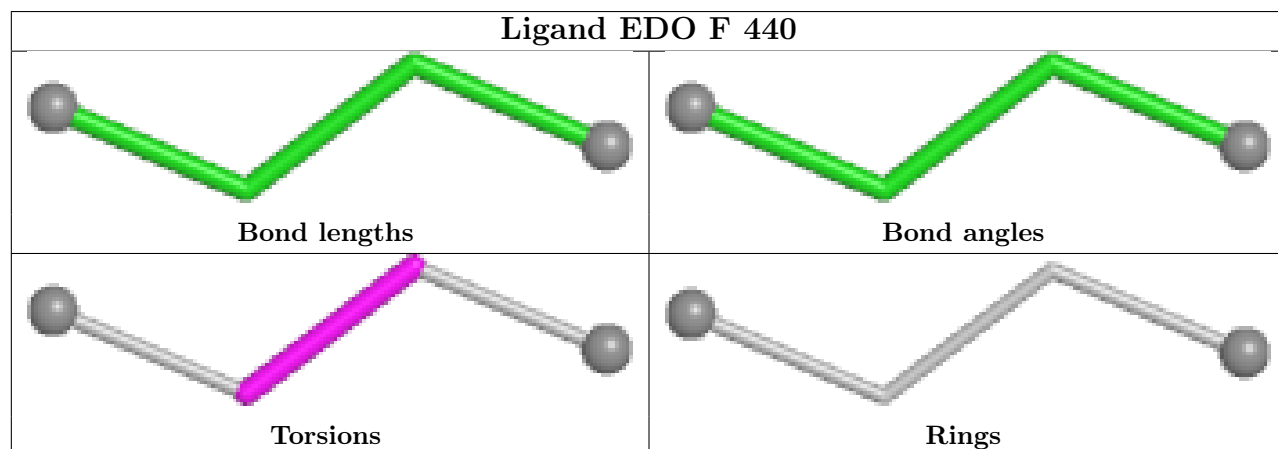
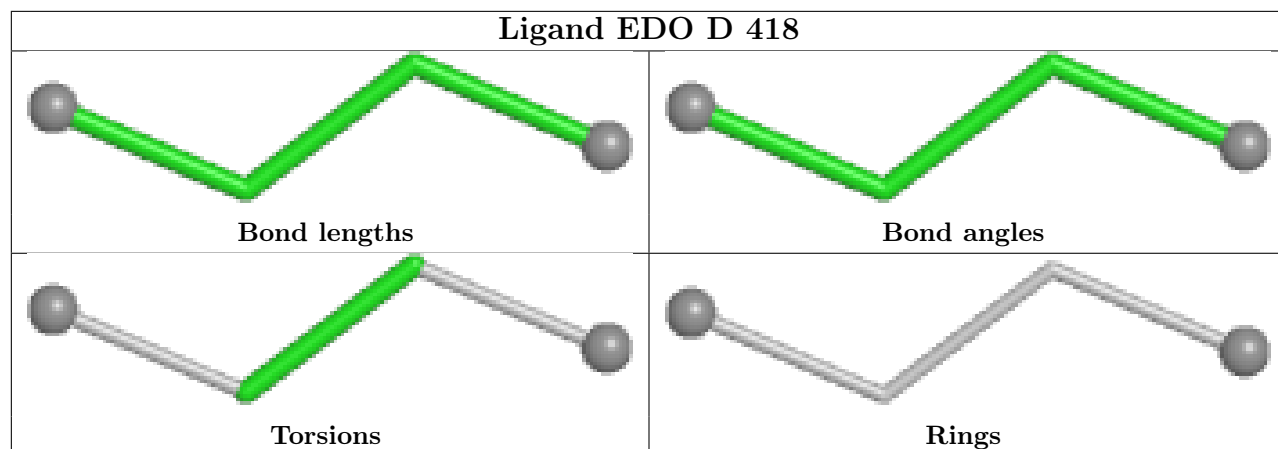


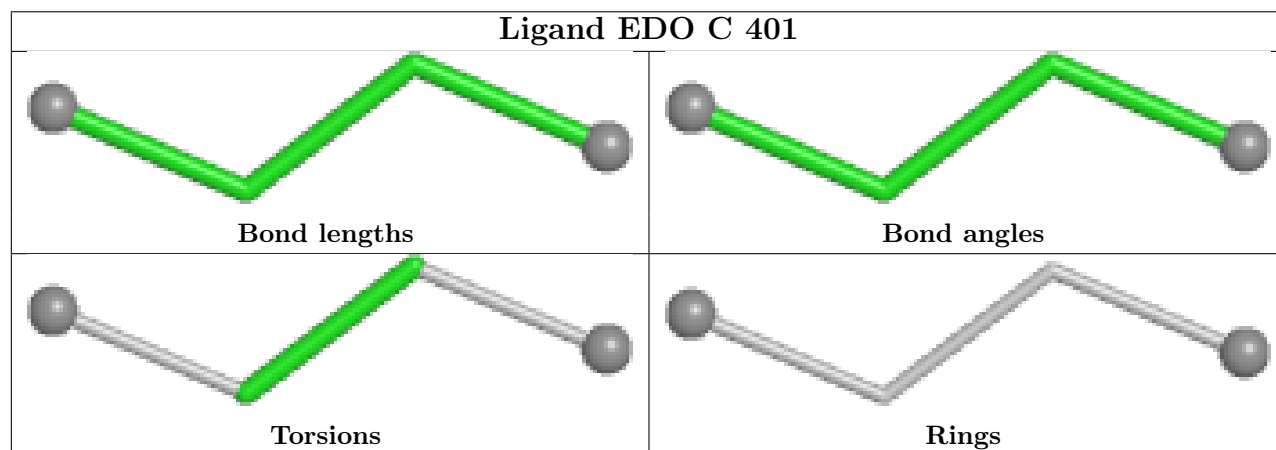
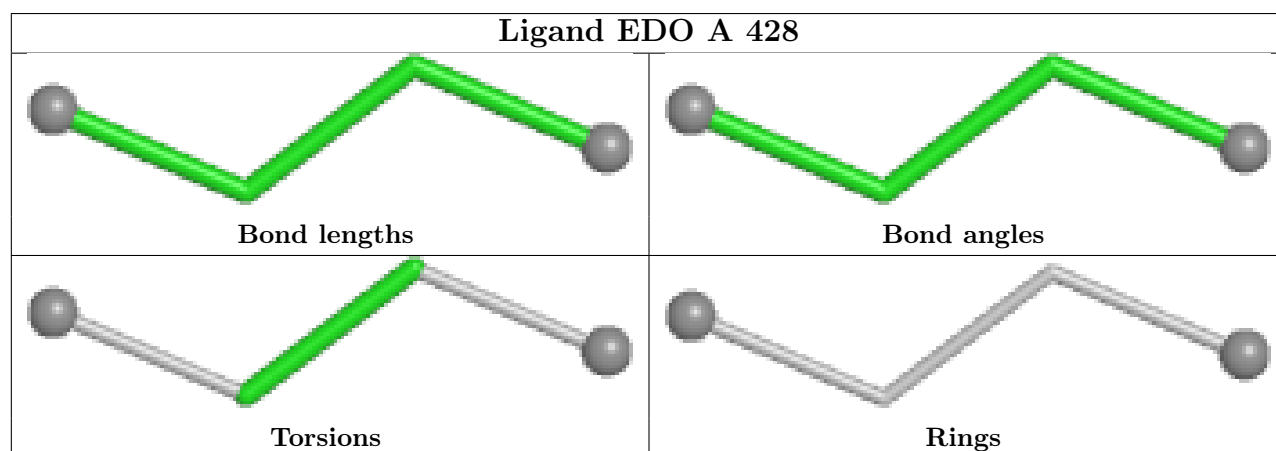
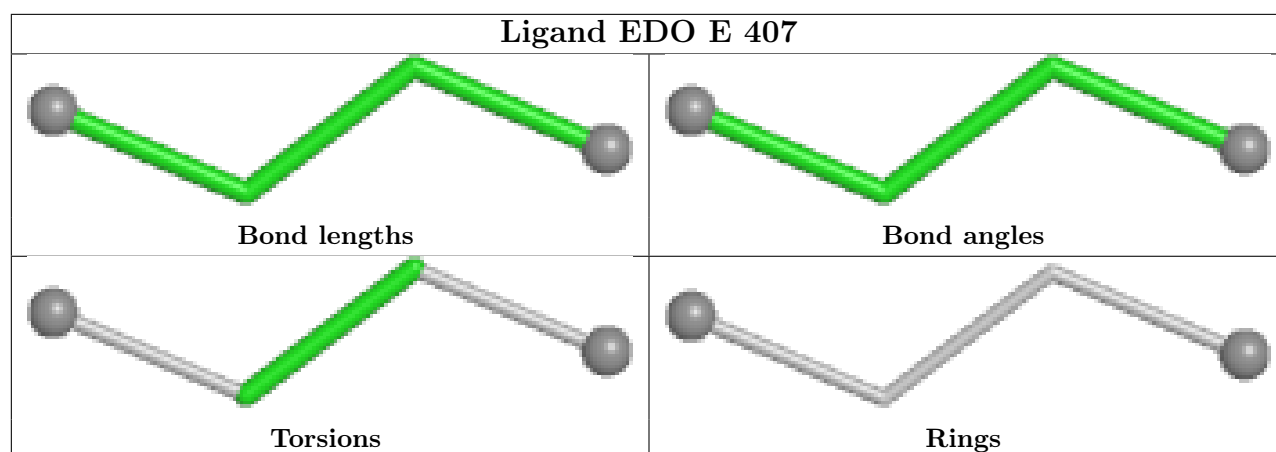


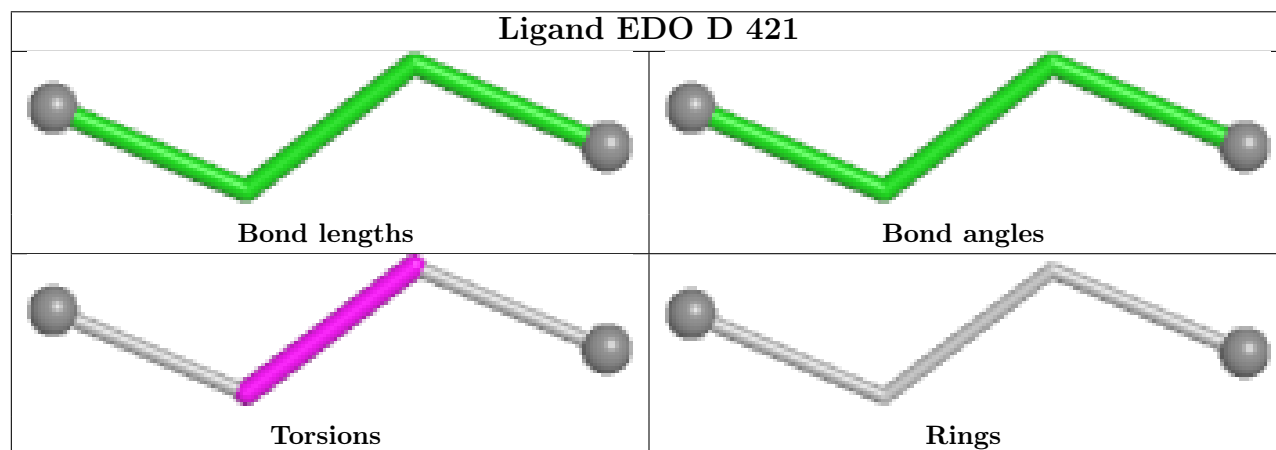
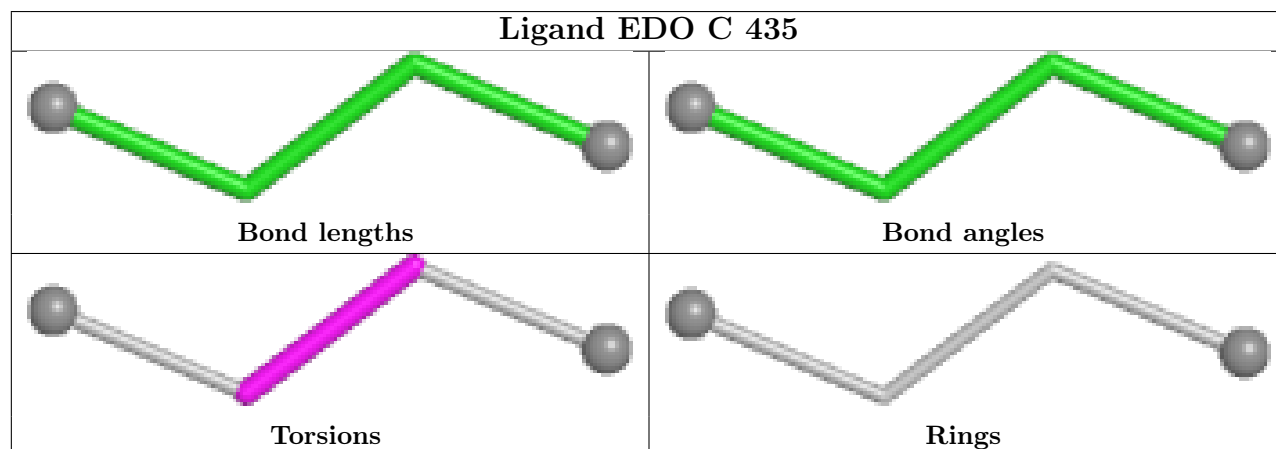
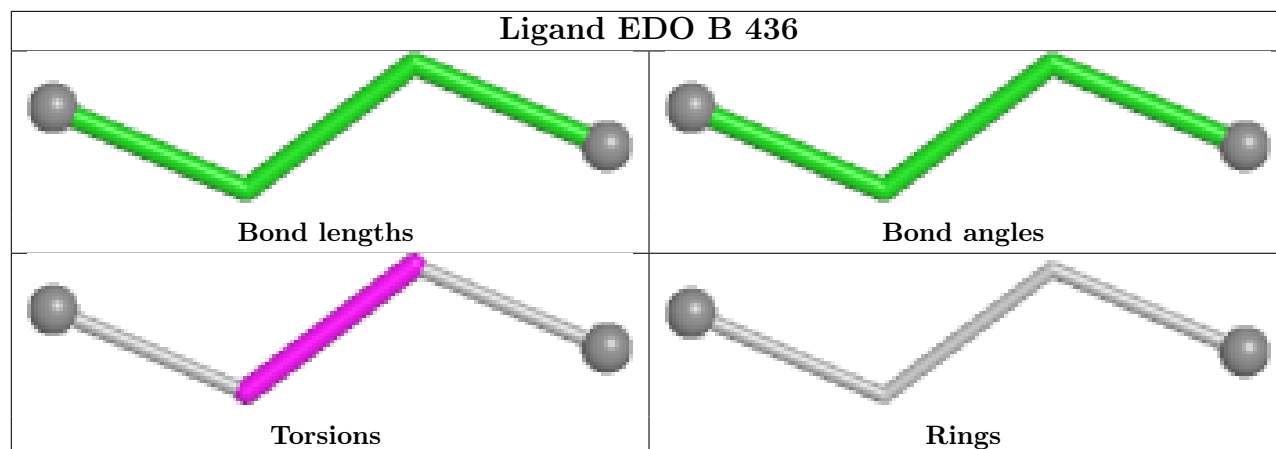


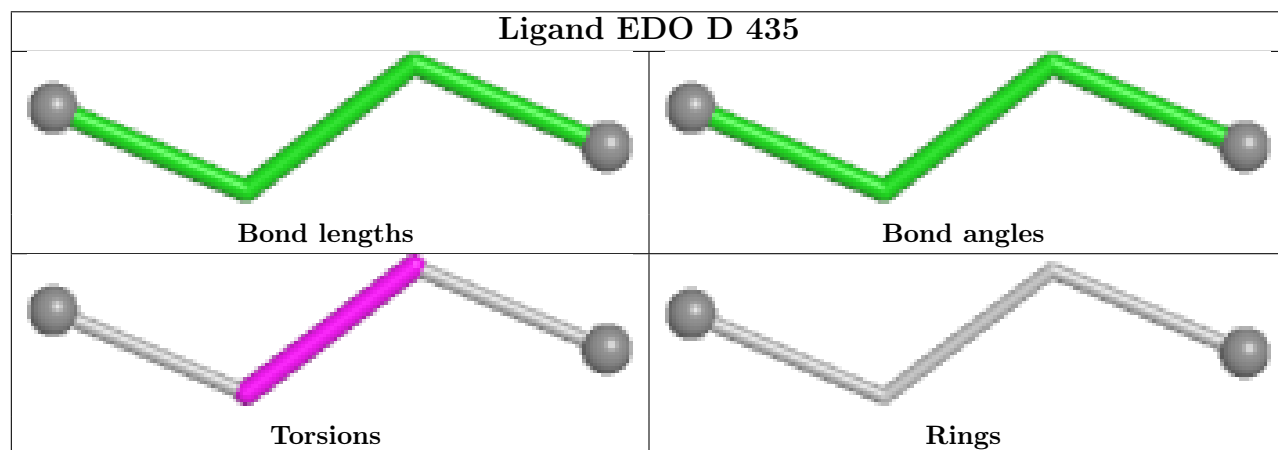
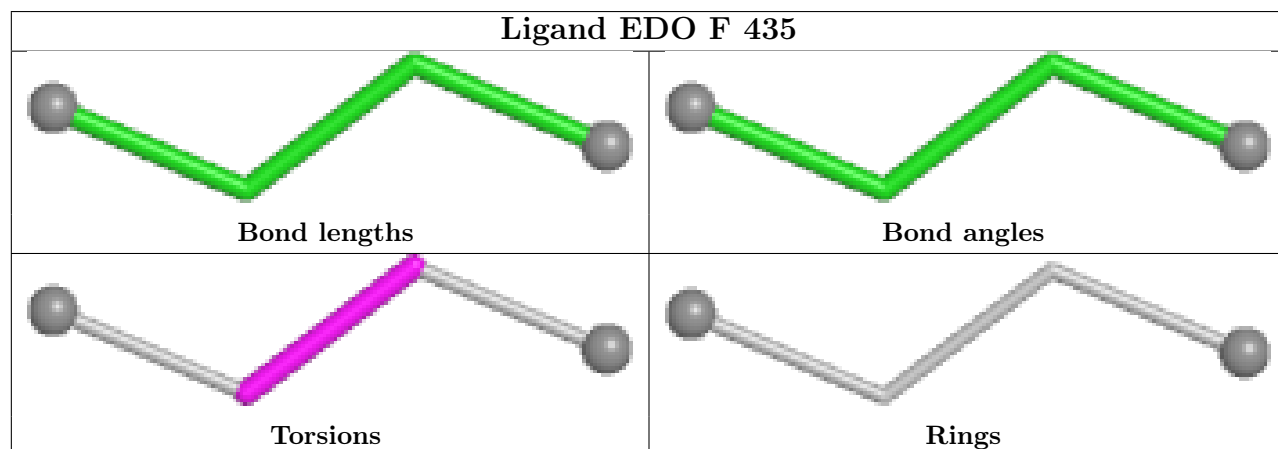
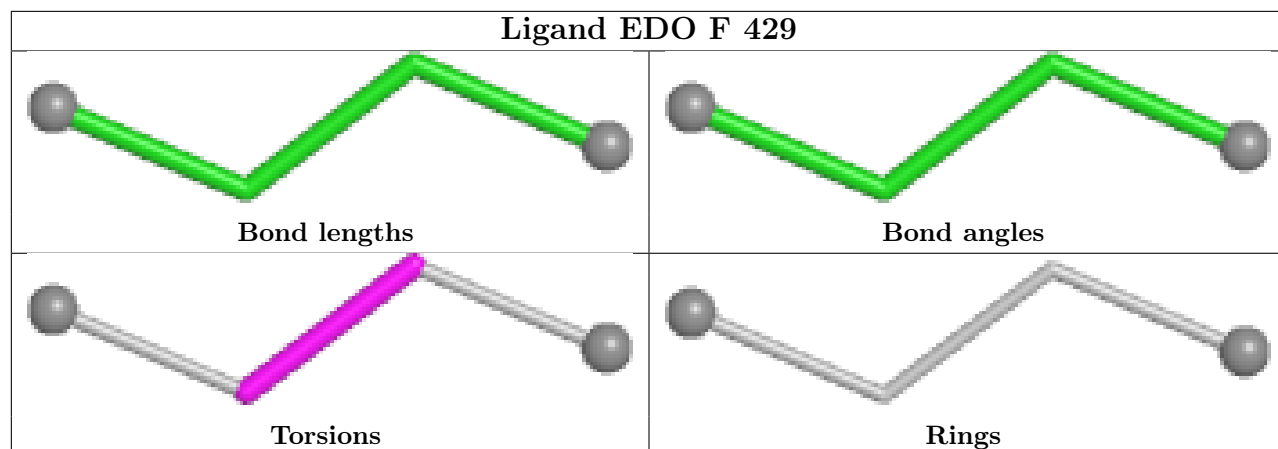


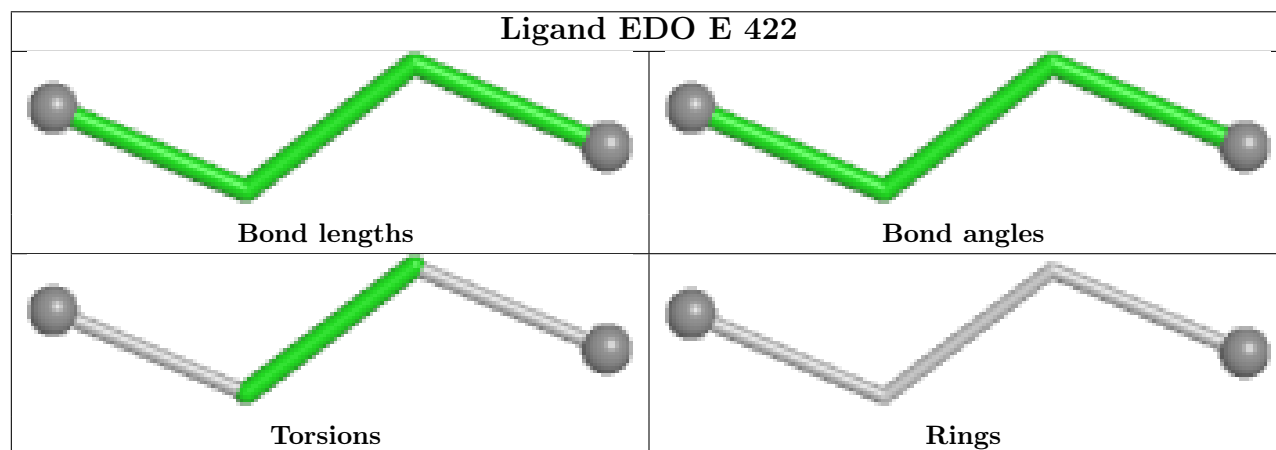
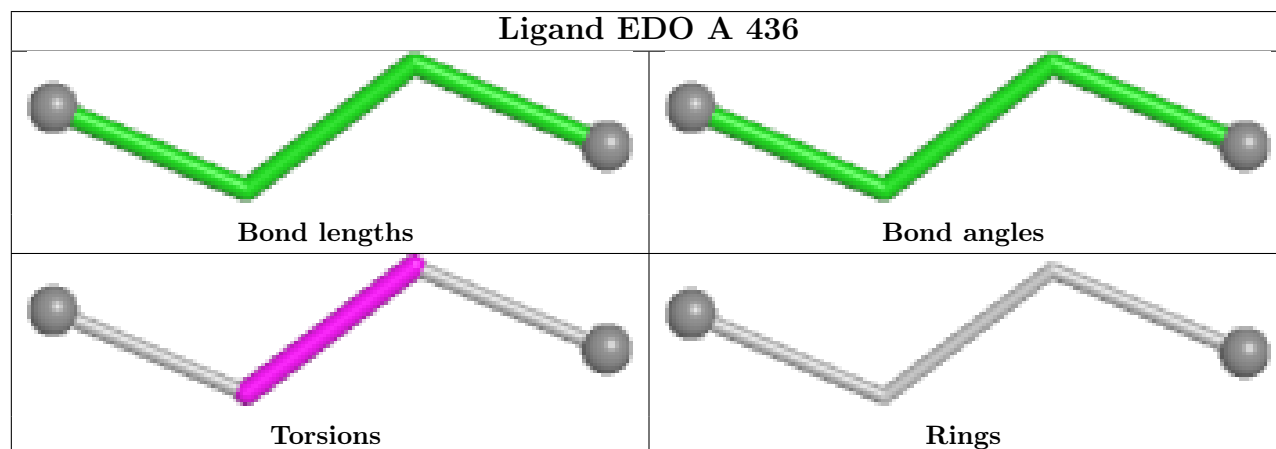
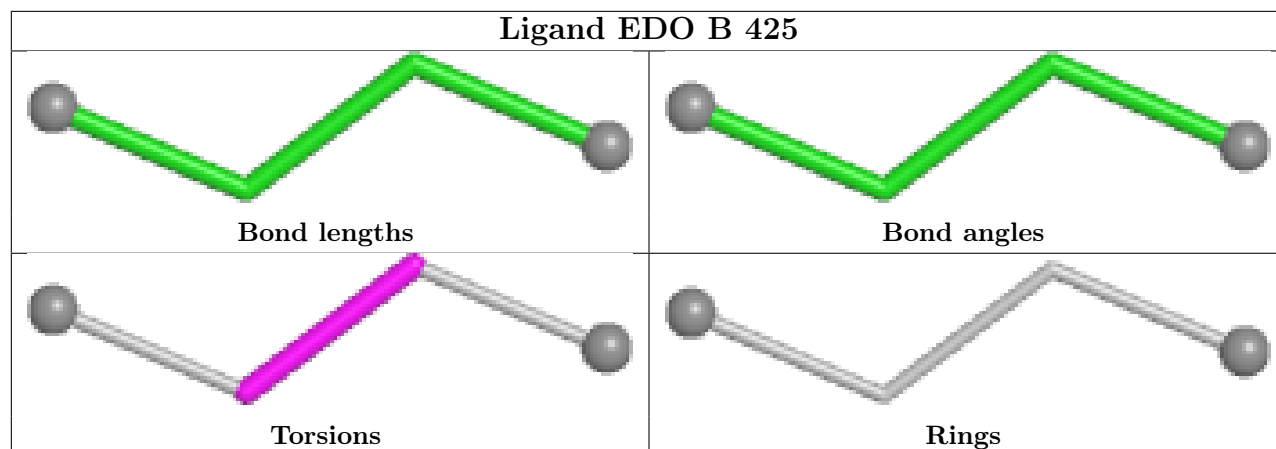


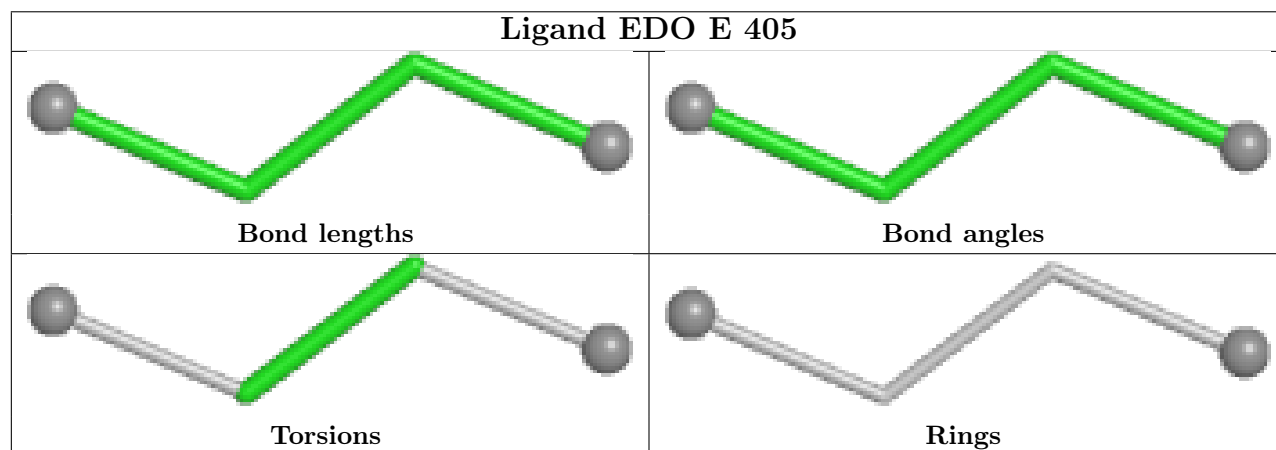
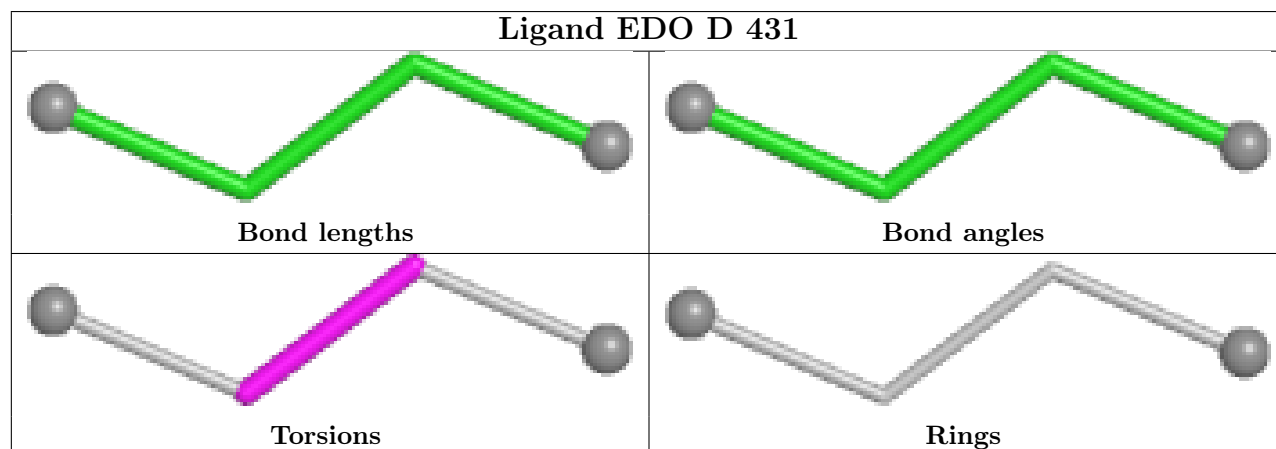
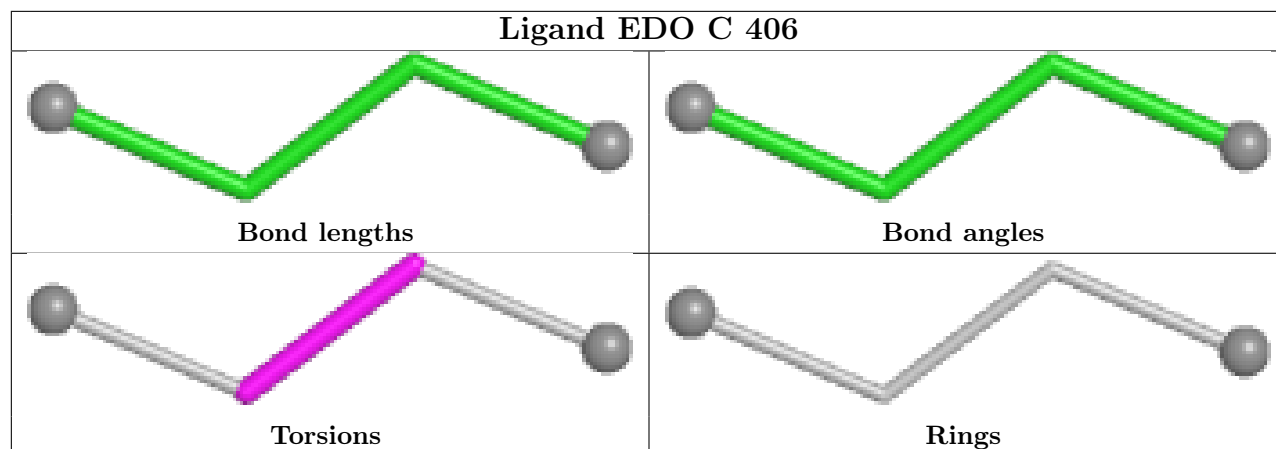


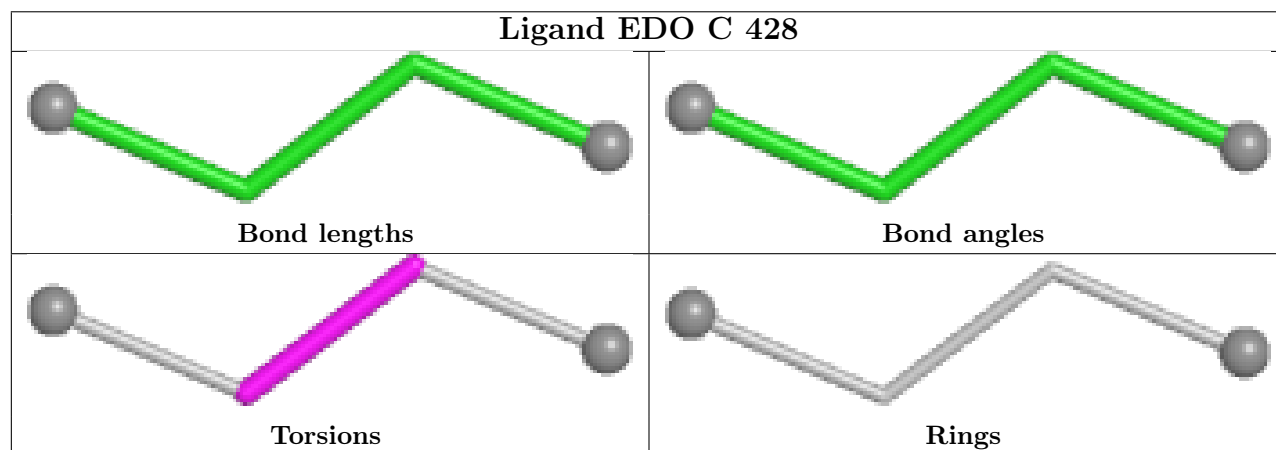
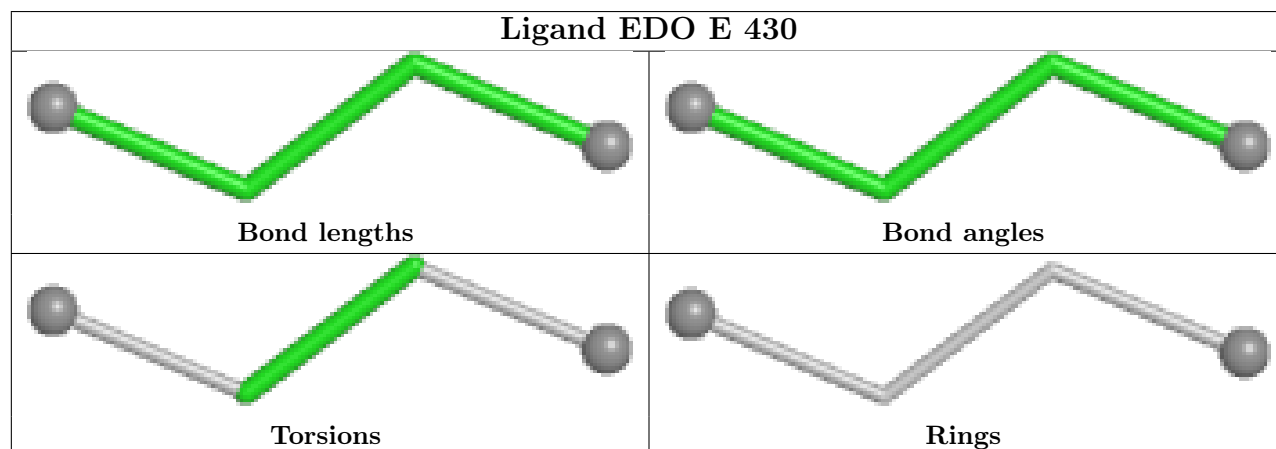
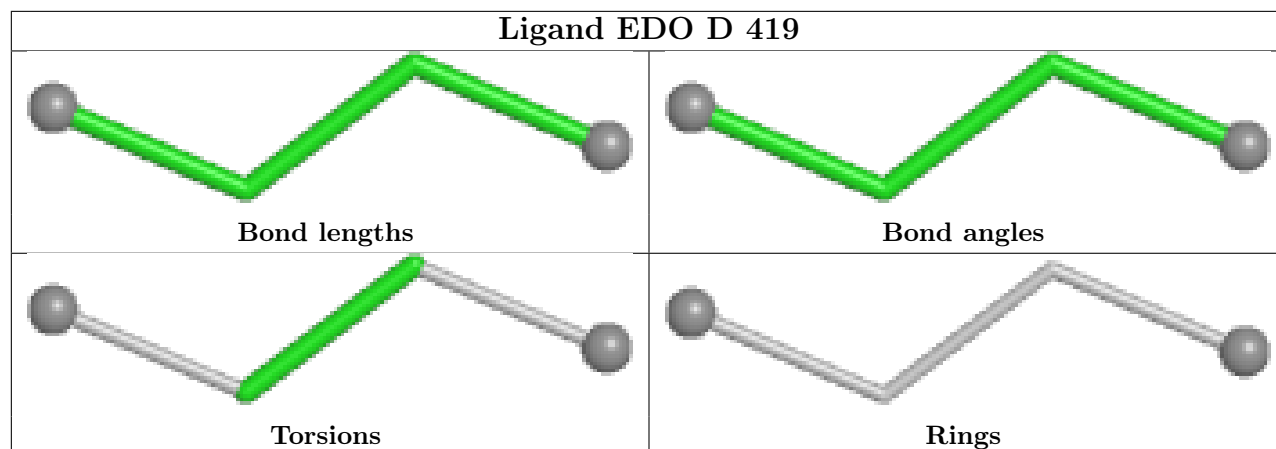


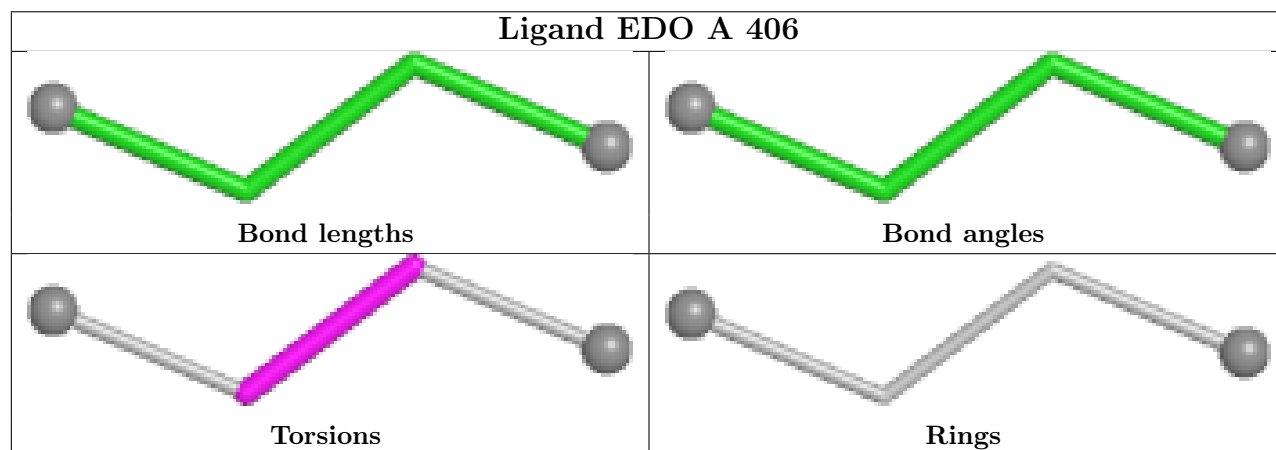
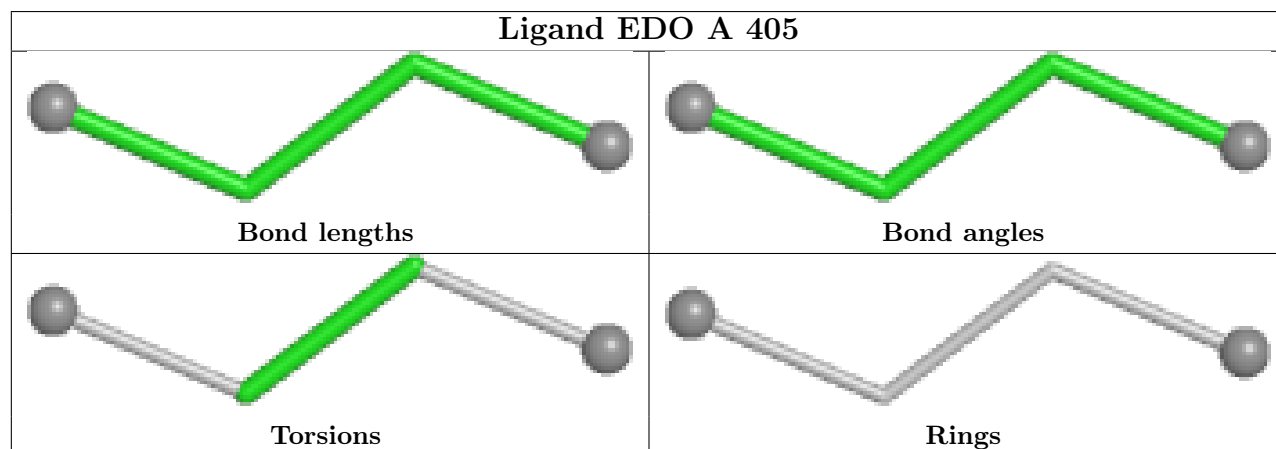
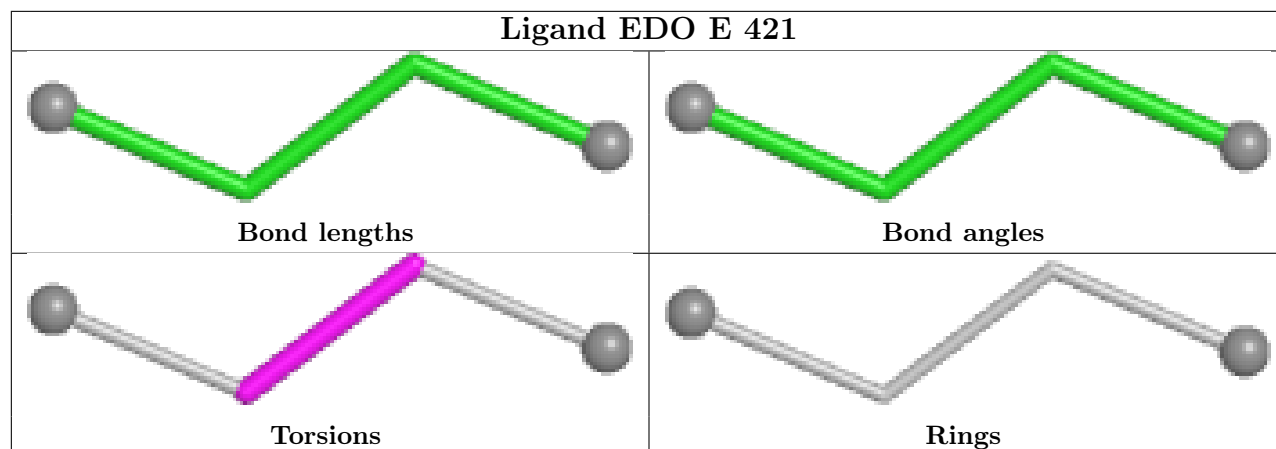


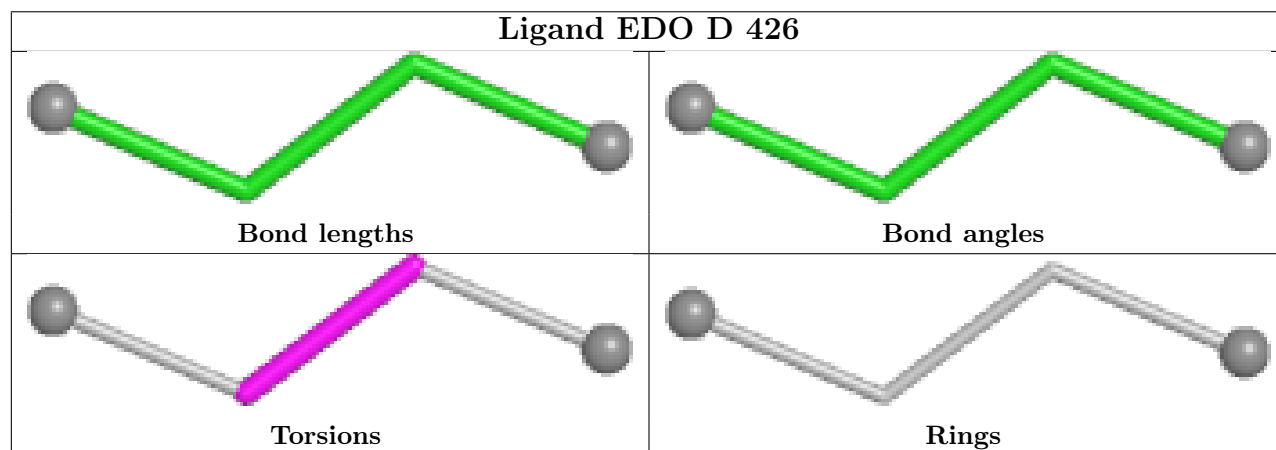
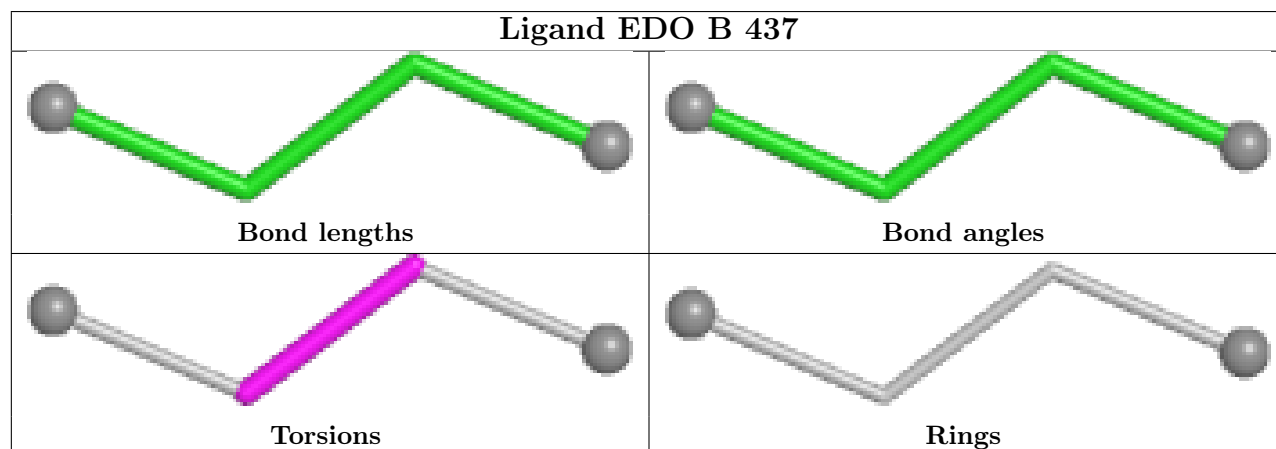
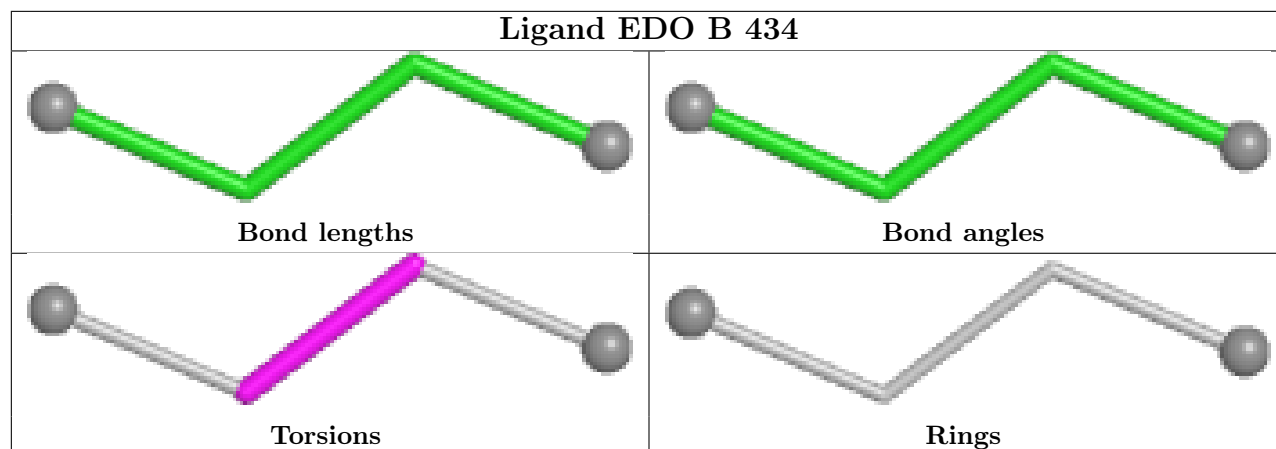


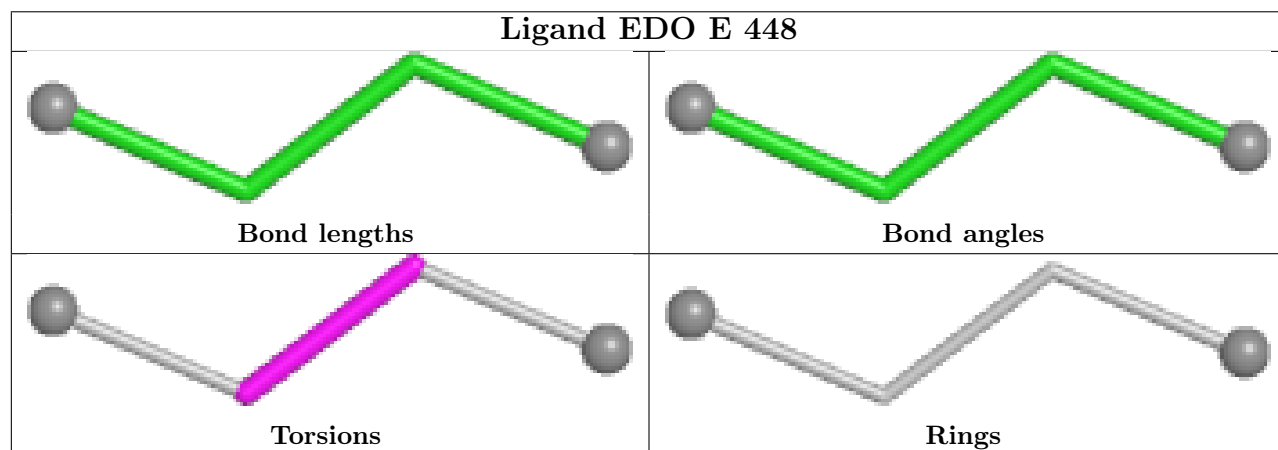
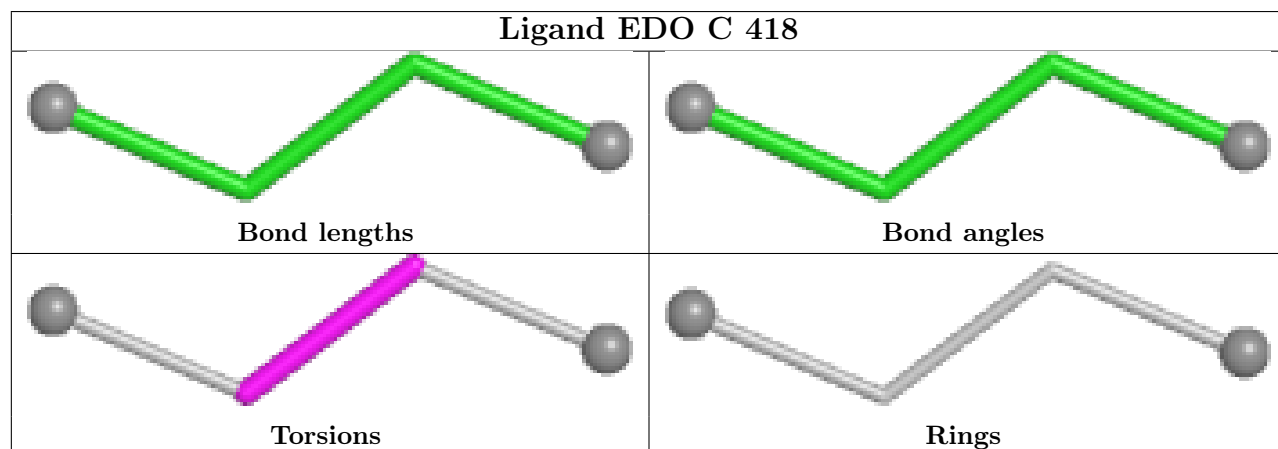
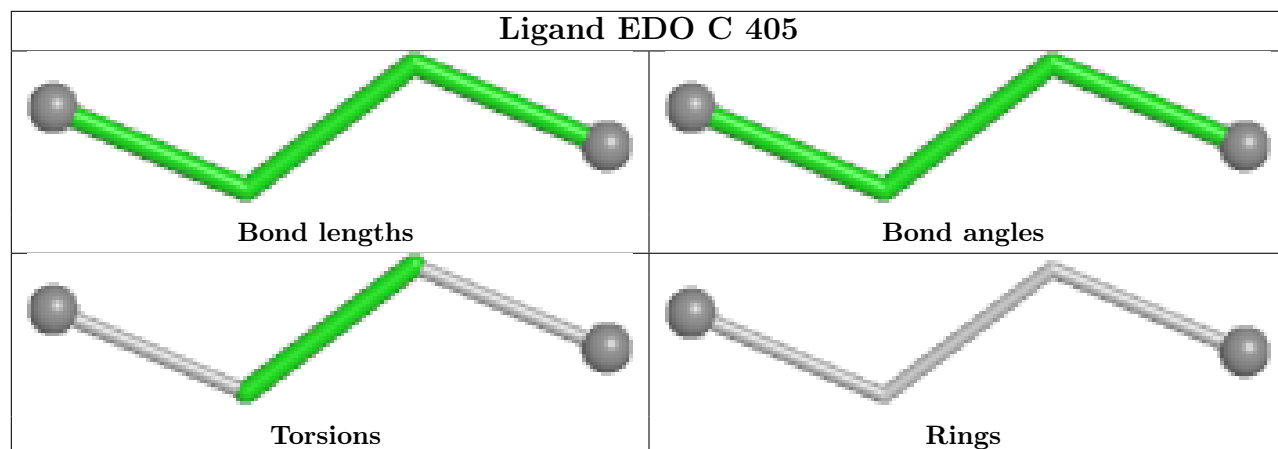


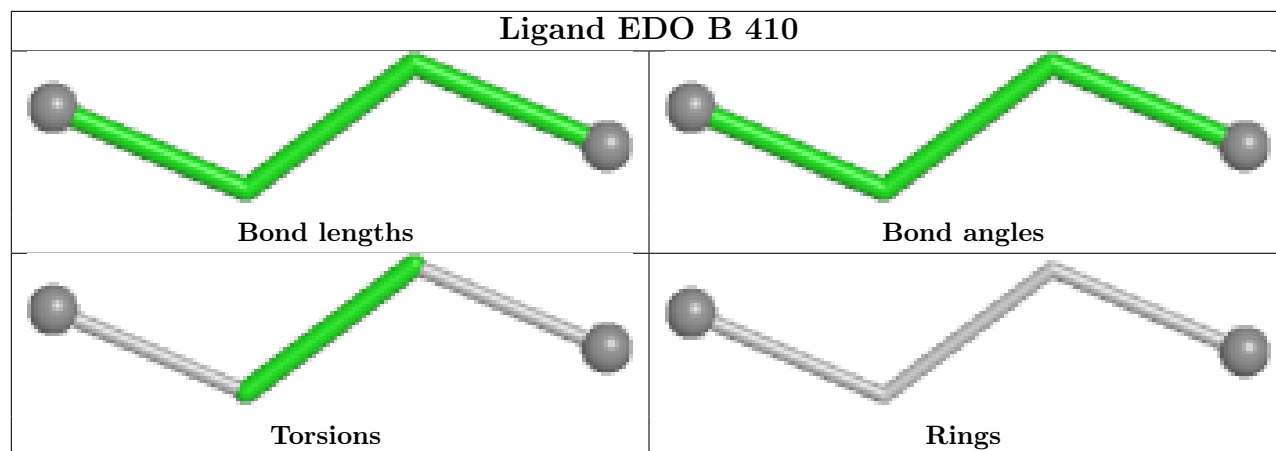












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	259/259 (100%)	-0.58	6 (2%) 61 41	13, 32, 52, 74	0
1	B	259/259 (100%)	-0.59	2 (0%) 82 67	15, 32, 51, 73	0
1	C	259/259 (100%)	-0.51	5 (1%) 66 46	13, 32, 53, 71	0
1	D	259/259 (100%)	-0.59	2 (0%) 82 67	13, 31, 52, 73	0
1	E	259/259 (100%)	-0.56	4 (1%) 72 52	14, 32, 52, 73	0
1	F	259/259 (100%)	-0.59	2 (0%) 82 67	12, 32, 51, 71	0
All	All	1554/1554 (100%)	-0.57	21 (1%) 73 54	12, 32, 52, 74	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	219	THR	4.3
1	A	353	VAL	3.6
1	C	353	VAL	3.6
1	D	365	ILE	3.4
1	F	353	VAL	3.4
1	C	365	ILE	2.9
1	B	219	THR	2.8
1	A	219	THR	2.8
1	A	365	ILE	2.8
1	B	353	VAL	2.6
1	E	365	ILE	2.5
1	C	196	ALA	2.5
1	D	219	THR	2.5
1	E	135	SER	2.3
1	E	152	GLU	2.2
1	E	356	LEU	2.2
1	A	293	ASP	2.1
1	C	385	ASP	2.1
1	A	356	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	135	SER	2.1
1	C	356	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	E	446	4/4	0.89	0.16	48,48,48,48	0
2	EDO	C	427	4/4	0.90	0.26	26,26,26,26	0
2	EDO	E	431	4/4	0.90	0.29	26,26,26,26	0
2	EDO	B	428	4/4	0.90	0.20	22,22,22,22	0
2	EDO	F	444	4/4	0.91	0.09	37,37,37,37	0
2	EDO	A	426	4/4	0.92	0.30	27,27,27,27	0
2	EDO	E	445	4/4	0.92	0.33	40,40,40,40	0
2	EDO	B	441	4/4	0.92	0.09	54,54,54,54	0
2	EDO	F	418	4/4	0.92	0.06	19,25,34,34	0
2	EDO	F	434	4/4	0.92	0.29	25,25,25,25	0
2	EDO	B	414	4/4	0.92	0.07	15,20,23,24	0
2	EDO	A	443	4/4	0.93	0.06	41,41,41,41	0
2	EDO	E	432	4/4	0.93	0.20	32,32,32,32	0
2	EDO	B	403	4/4	0.93	0.17	7,8,11,16	0
2	EDO	A	423	4/4	0.93	0.06	17,17,17,17	0
2	EDO	C	436	4/4	0.93	0.11	36,36,36,36	0
2	EDO	D	425	4/4	0.93	0.09	72,72,72,72	0
2	EDO	E	426	4/4	0.93	0.08	70,70,70,70	0
2	EDO	D	403	4/4	0.94	0.24	54,61,66,68	0
2	EDO	D	420	4/4	0.94	0.13	61,68,73,75	0
2	EDO	A	428	4/4	0.94	0.09	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	D	429	4/4	0.94	0.17	20,20,20,20	0
2	EDO	B	434	4/4	0.94	0.09	26,26,26,26	0
2	EDO	B	437	4/4	0.94	0.10	23,23,23,23	0
2	EDO	A	401	4/4	0.94	0.28	4,6,9,14	0
2	EDO	E	433	4/4	0.94	0.09	39,39,39,39	0
2	EDO	B	446	4/4	0.94	0.14	56,56,56,56	0
2	EDO	C	403	4/4	0.94	0.20	5,7,10,15	0
2	EDO	F	403	4/4	0.94	0.05	29,29,29,29	0
2	EDO	F	404	4/4	0.94	0.09	21,21,21,21	0
2	EDO	A	416	4/4	0.94	0.07	42,49,54,56	0
2	EDO	C	433	4/4	0.94	0.09	21,21,21,21	0
2	EDO	F	443	4/4	0.94	0.30	37,37,37,37	0
2	EDO	A	427	4/4	0.94	0.27	37,37,37,37	0
2	EDO	F	445	4/4	0.94	0.07	46,46,46,46	0
2	EDO	B	426	4/4	0.95	0.10	11,11,11,11	0
2	EDO	E	441	4/4	0.95	0.16	35,35,35,35	0
2	EDO	D	404	4/4	0.95	0.22	6,8,11,15	0
2	EDO	C	418	4/4	0.95	0.06	24,27,28,29	0
2	EDO	B	438	4/4	0.95	0.21	37,37,37,37	0
2	EDO	C	432	4/4	0.95	0.05	34,34,34,34	0
2	EDO	F	406	4/4	0.95	0.06	22,22,22,22	0
2	EDO	D	439	4/4	0.95	0.05	40,40,40,40	0
2	EDO	F	420	4/4	0.95	0.06	13,18,21,22	0
2	EDO	F	424	4/4	0.95	0.06	42,50,55,56	0
2	EDO	A	431	4/4	0.95	0.05	30,30,30,30	0
2	EDO	F	436	4/4	0.95	0.13	38,38,38,38	0
2	EDO	F	440	4/4	0.95	0.09	26,26,26,26	0
2	EDO	F	442	4/4	0.95	0.12	34,34,34,34	0
2	EDO	E	429	4/4	0.95	0.10	11,11,11,11	0
2	EDO	A	421	4/4	0.95	0.06	21,21,21,21	0
2	EDO	D	402	4/4	0.95	0.11	17,23,26,26	0
2	EDO	D	424	4/4	0.96	0.07	23,23,23,23	0
2	EDO	A	440	4/4	0.96	0.12	19,19,19,19	0
2	EDO	D	426	4/4	0.96	0.05	19,19,19,19	0
2	EDO	B	444	4/4	0.96	0.10	30,30,30,30	0
2	EDO	D	432	4/4	0.96	0.07	39,39,39,39	0
2	EDO	D	433	4/4	0.96	0.08	22,22,22,22	0
2	EDO	D	435	4/4	0.96	0.04	34,34,34,34	0
2	EDO	D	436	4/4	0.96	0.08	36,36,36,36	0
2	EDO	A	442	4/4	0.96	0.10	28,28,28,28	0
2	EDO	E	403	4/4	0.96	0.24	4,6,9,14	0
2	EDO	E	404	4/4	0.96	0.10	15,19,19,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	E	411	4/4	0.96	0.06	13,28,35,40	0
2	EDO	E	413	4/4	0.96	0.05	18,24,33,33	0
2	EDO	E	419	4/4	0.96	0.06	42,50,54,56	0
2	EDO	E	421	4/4	0.96	0.05	19,21,23,24	0
2	EDO	B	447	4/4	0.96	0.05	32,32,32,32	0
2	EDO	E	428	4/4	0.96	0.04	32,32,32,32	0
2	EDO	C	402	4/4	0.96	0.08	14,19,22,23	0
2	EDO	A	417	4/4	0.96	0.05	13,16,17,18	0
2	EDO	A	412	4/4	0.96	0.06	10,15,17,19	0
2	EDO	C	420	4/4	0.96	0.09	15,15,15,15	0
2	EDO	E	434	4/4	0.96	0.08	20,20,20,20	0
2	EDO	C	424	4/4	0.96	0.04	30,30,30,30	0
2	EDO	E	443	4/4	0.96	0.11	18,18,18,18	0
2	EDO	C	425	4/4	0.96	0.08	15,15,15,15	0
2	EDO	A	422	4/4	0.96	0.07	73,73,73,73	0
2	EDO	C	428	4/4	0.96	0.18	37,37,37,37	0
2	EDO	B	424	4/4	0.96	0.08	68,68,68,68	0
2	EDO	A	403	4/4	0.96	0.10	19,21,23,28	0
2	EDO	F	408	4/4	0.96	0.10	9,15,18,18	0
2	EDO	F	409	4/4	0.96	0.14	7,9,12,17	0
2	EDO	F	416	4/4	0.96	0.13	2,3,4,22	0
2	EDO	C	434	4/4	0.96	0.07	35,35,35,35	0
2	EDO	A	434	4/4	0.96	0.05	19,19,19,19	0
2	EDO	C	438	4/4	0.96	0.08	40,40,40,40	0
2	EDO	F	425	4/4	0.96	0.07	24,26,28,29	0
2	EDO	F	427	4/4	0.96	0.09	18,18,18,18	0
2	EDO	F	429	4/4	0.96	0.07	26,26,26,26	0
2	EDO	F	430	4/4	0.96	0.05	58,58,58,58	0
2	EDO	B	430	4/4	0.96	0.09	30,30,30,30	0
2	EDO	A	436	4/4	0.96	0.07	40,40,40,40	0
2	EDO	F	439	4/4	0.96	0.07	24,24,24,24	0
2	EDO	A	438	4/4	0.96	0.06	30,30,30,30	0
2	EDO	F	441	4/4	0.96	0.11	55,55,55,55	0
2	EDO	D	406	4/4	0.96	0.11	29,31,33,37	0
2	EDO	D	407	4/4	0.96	0.07	4,17,20,28	0
2	EDO	A	439	4/4	0.96	0.09	30,30,30,30	0
2	EDO	D	422	4/4	0.96	0.08	18,18,18,18	0
2	EDO	D	434	4/4	0.97	0.08	38,38,38,38	0
2	EDO	B	405	4/4	0.97	0.09	21,23,25,30	0
2	EDO	C	406	4/4	0.97	0.06	5,17,20,28	0
2	EDO	C	410	4/4	0.97	0.12	4,5,5,24	0
2	EDO	E	401	4/4	0.97	0.04	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	E	402	4/4	0.97	0.05	26,28,30,31	0
2	EDO	C	414	4/4	0.97	0.05	14,19,21,23	0
2	EDO	B	410	4/4	0.97	0.12	3,4,4,23	0
2	EDO	E	406	4/4	0.97	0.04	8,21,23,31	0
2	EDO	E	410	4/4	0.97	0.12	5,6,6,24	0
2	EDO	B	412	4/4	0.97	0.03	16,22,31,31	0
2	EDO	C	422	4/4	0.97	0.07	18,18,18,18	0
2	EDO	A	429	4/4	0.97	0.05	14,28,35,41	0
2	EDO	B	417	4/4	0.97	0.04	2,2,3,8	0
2	EDO	E	423	4/4	0.97	0.08	14,14,14,14	0
2	EDO	E	425	4/4	0.97	0.06	21,21,21,21	0
2	EDO	B	418	4/4	0.97	0.05	53,61,66,67	0
2	EDO	E	427	4/4	0.97	0.04	20,20,20,20	0
2	EDO	B	419	4/4	0.97	0.04	18,21,22,23	0
2	EDO	C	429	4/4	0.97	0.10	33,33,33,33	0
2	EDO	C	431	4/4	0.97	0.05	27,28,31,36	0
2	EDO	B	423	4/4	0.97	0.06	22,22,22,22	0
2	EDO	A	407	4/4	0.97	0.12	6,7,14,17	0
2	EDO	A	432	4/4	0.97	0.08	15,15,15,15	0
2	EDO	E	437	4/4	0.97	0.04	20,20,20,20	0
2	EDO	E	438	4/4	0.97	0.11	26,26,26,26	0
2	EDO	E	439	4/4	0.97	0.09	31,31,31,31	0
2	EDO	C	435	4/4	0.97	0.06	31,36,40,40	0
2	EDO	A	433	4/4	0.97	0.07	33,33,33,33	0
2	EDO	C	437	4/4	0.97	0.15	43,43,43,43	0
2	EDO	B	429	4/4	0.97	0.17	36,36,36,36	0
2	EDO	E	447	4/4	0.97	0.05	42,42,42,42	0
2	EDO	D	401	4/4	0.97	0.05	4,5,5,6	0
2	EDO	A	419	4/4	0.97	0.09	16,16,16,16	0
2	EDO	B	431	4/4	0.97	0.06	11,25,32,38	0
2	EDO	F	407	4/4	0.97	0.05	6,6,9,11	0
2	EDO	A	408	4/4	0.97	0.14	4,5,6,24	0
2	EDO	B	435	4/4	0.97	0.05	26,26,26,26	0
2	EDO	F	411	4/4	0.97	0.10	22,24,26,30	0
2	EDO	A	410	4/4	0.97	0.05	17,24,32,32	0
2	EDO	D	408	4/4	0.97	0.07	13,14,17,18	0
2	EDO	D	411	4/4	0.97	0.12	5,6,6,24	0
2	EDO	D	415	4/4	0.97	0.05	8,13,15,17	0
2	EDO	D	418	4/4	0.97	0.06	4,5,5,10	0
2	EDO	D	419	4/4	0.97	0.06	7,7,10,11	0
2	EDO	A	411	4/4	0.97	0.05	16,19,23,27	0
2	EDO	B	439	4/4	0.97	0.05	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	F	431	4/4	0.97	0.04	14,14,14,14	0
2	EDO	F	432	4/4	0.97	0.09	15,15,15,15	0
2	EDO	A	424	4/4	0.97	0.06	15,15,15,15	0
2	EDO	F	435	4/4	0.97	0.18	31,31,31,31	0
2	EDO	B	442	4/4	0.97	0.05	32,32,32,32	0
2	EDO	F	437	4/4	0.97	0.07	21,21,21,21	0
2	EDO	F	438	4/4	0.97	0.07	48,48,48,48	0
2	EDO	A	404	4/4	0.97	0.06	10,22,25,33	0
2	EDO	D	427	4/4	0.97	0.09	14,14,14,14	0
2	EDO	A	413	4/4	0.97	0.10	10,11,14,16	0
2	EDO	D	430	4/4	0.97	0.23	36,36,36,36	0
2	EDO	D	431	4/4	0.97	0.12	39,39,39,39	0
2	EDO	B	402	4/4	0.97	0.07	19,24,28,28	0
2	EDO	A	406	4/4	0.97	0.06	6,9,12,13	0
2	EDO	E	414	4/4	0.98	0.05	21,24,28,32	0
2	EDO	E	415	4/4	0.98	0.05	15,20,22,24	0
2	EDO	E	416	4/4	0.98	0.10	11,12,15,17	0
2	EDO	E	417	4/4	0.98	0.05	39,41,47,50	0
2	EDO	E	418	4/4	0.98	0.03	4,4,4,9	0
2	EDO	B	421	4/4	0.98	0.07	15,15,15,15	0
2	EDO	E	420	4/4	0.98	0.05	22,23,26,31	0
2	EDO	B	445	4/4	0.98	0.07	38,38,38,38	0
2	EDO	E	422	4/4	0.98	0.07	12,17,33,40	0
2	EDO	A	402	4/4	0.98	0.07	13,16,17,34	0
2	EDO	B	406	4/4	0.98	0.06	7,20,23,31	0
2	EDO	C	401	4/4	0.98	0.04	6,6,9,11	0
2	EDO	B	425	4/4	0.98	0.04	21,21,21,21	0
2	EDO	B	407	4/4	0.98	0.06	9,11,14,15	0
2	EDO	C	404	4/4	0.98	0.07	12,16,17,34	0
2	EDO	E	430	4/4	0.98	0.08	70,70,70,70	0
2	EDO	C	405	4/4	0.98	0.10	18,20,22,26	0
2	EDO	D	410	4/4	0.98	0.11	7,8,15,18	0
2	EDO	B	427	4/4	0.98	0.07	74,74,74,74	0
2	EDO	D	412	4/4	0.98	0.05	8,9,11,12	0
2	EDO	E	435	4/4	0.98	0.05	10,24,31,37	0
2	EDO	D	413	4/4	0.98	0.03	17,23,32,32	0
2	EDO	C	407	4/4	0.98	0.07	14,15,19,20	0
2	EDO	D	416	4/4	0.98	0.10	13,14,17,19	0
2	EDO	C	408	4/4	0.98	0.07	8,11,13,15	0
2	EDO	E	442	4/4	0.98	0.04	33,33,33,33	0
2	EDO	C	409	4/4	0.98	0.09	7,8,15,18	0
2	EDO	E	444	4/4	0.98	0.05	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	B	408	4/4	0.98	0.07	5,8,10,12	0
2	EDO	D	421	4/4	0.98	0.07	13,18,34,41	0
2	EDO	C	411	4/4	0.98	0.04	3,5,8,9	0
2	EDO	F	402	4/4	0.98	0.04	27,27,30,35	0
2	EDO	C	412	4/4	0.98	0.04	19,25,34,34	0
2	EDO	B	409	4/4	0.98	0.10	5,6,13,16	0
2	EDO	F	405	4/4	0.98	0.04	35,35,35,35	0
2	EDO	C	415	4/4	0.98	0.11	9,10,13,15	0
2	EDO	C	417	4/4	0.98	0.04	4,4,4,9	0
2	EDO	D	428	4/4	0.98	0.06	74,74,74,74	0
2	EDO	A	430	4/4	0.98	0.05	27,27,30,35	0
2	EDO	C	419	4/4	0.98	0.06	11,16,32,39	0
2	EDO	F	412	4/4	0.98	0.06	6,19,22,30	0
2	EDO	F	413	4/4	0.98	0.06	18,19,23,24	0
2	EDO	F	415	4/4	0.98	0.11	5,6,14,16	0
2	EDO	A	435	4/4	0.98	0.04	2,2,5,7	0
2	EDO	B	432	4/4	0.98	0.04	25,25,28,33	0
2	EDO	F	419	4/4	0.98	0.06	19,22,26,30	0
2	EDO	C	423	4/4	0.98	0.04	62,62,62,62	0
2	EDO	F	421	4/4	0.98	0.11	14,15,18,20	0
2	EDO	F	423	4/4	0.98	0.03	2,2,2,7	0
2	EDO	B	433	4/4	0.98	0.03	34,34,34,34	0
2	EDO	B	413	4/4	0.98	0.07	17,19,24,28	0
2	EDO	F	426	4/4	0.98	0.07	12,17,33,40	0
2	EDO	C	426	4/4	0.98	0.07	66,66,66,66	0
2	EDO	D	437	4/4	0.98	0.08	38,38,38,38	0
2	EDO	D	438	4/4	0.98	0.04	32,32,32,32	0
2	EDO	A	405	4/4	0.98	0.07	16,17,21,22	0
2	EDO	B	436	4/4	0.98	0.04	20,20,20,20	0
2	EDO	F	433	4/4	0.98	0.08	65,65,65,65	0
2	EDO	B	415	4/4	0.98	0.10	9,10,13,15	0
2	EDO	B	416	4/4	0.98	0.07	43,44,50,53	0
2	EDO	B	401	4/4	0.98	0.05	7,7,10,12	0
2	EDO	E	405	4/4	0.98	0.10	18,20,22,26	0
2	EDO	B	440	4/4	0.98	0.07	34,34,34,34	0
2	EDO	E	407	4/4	0.98	0.07	13,14,18,19	0
2	EDO	E	408	4/4	0.98	0.06	5,8,11,12	0
2	EDO	E	409	4/4	0.98	0.10	5,6,13,16	0
2	EDO	A	437	4/4	0.98	0.04	24,24,24,24	0
2	EDO	A	425	4/4	0.98	0.06	70,70,70,70	0
2	EDO	E	412	4/4	0.98	0.03	1,2,4,7	0
2	EDO	B	443	4/4	0.98	0.07	39,39,39,39	0

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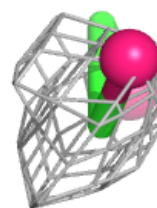
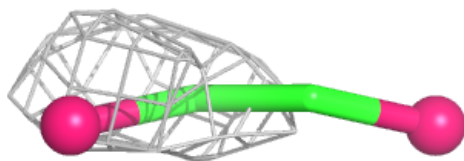
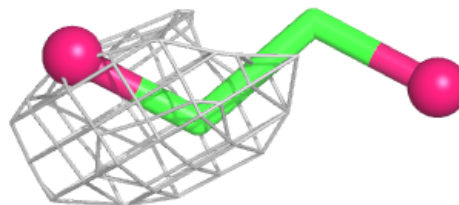
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	F	417	4/4	0.99	0.05	5,5,7,10	0
2	EDO	B	411	4/4	0.99	0.03	2,3,4,5	0
2	EDO	E	440	4/4	0.99	0.04	16,16,16,16	0
2	EDO	C	413	4/4	0.99	0.04	11,14,18,22	0
2	EDO	B	420	4/4	0.99	0.05	10,15,31,38	0
2	EDO	F	422	4/4	0.99	0.05	38,39,45,49	0
2	EDO	B	404	4/4	0.99	0.08	16,19,20,37	0
2	EDO	D	423	4/4	0.99	0.03	16,16,16,16	0
2	EDO	D	405	4/4	0.99	0.09	12,15,16,33	0
2	EDO	E	424	4/4	0.99	0.04	19,19,19,19	0
2	EDO	C	416	4/4	0.99	0.05	45,46,52,56	0
2	EDO	F	428	4/4	0.99	0.03	13,13,13,13	0
2	EDO	E	448	4/4	0.99	0.04	29,29,29,29	0
2	EDO	F	401	4/4	0.99	0.04	12,26,33,39	0
2	EDO	C	430	4/4	0.99	0.04	11,25,32,38	0
2	EDO	B	422	4/4	0.99	0.04	18,18,18,18	0
2	EDO	D	409	4/4	0.99	0.07	7,10,13,14	0
2	EDO	A	441	4/4	0.99	0.04	17,17,17,17	0
2	EDO	A	409	4/4	0.99	0.04	3,4,5,6	0
2	EDO	A	414	4/4	0.99	0.06	36,37,44,47	0
2	EDO	C	421	4/4	0.99	0.04	18,18,18,18	0
2	EDO	D	414	4/4	0.99	0.05	12,14,19,23	0
2	EDO	F	410	4/4	0.99	0.05	14,18,19,36	0
2	EDO	A	418	4/4	0.99	0.06	13,18,34,41	0
2	EDO	A	415	4/4	0.99	0.04	3,3,3,8	0
2	EDO	E	436	4/4	0.99	0.04	20,20,23,28	0
2	EDO	F	414	4/4	0.99	0.06	5,8,11,12	0
2	EDO	D	417	4/4	0.99	0.07	36,37,43,46	0
2	EDO	A	420	4/4	0.99	0.04	20,20,20,20	0

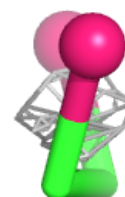
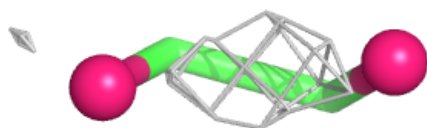
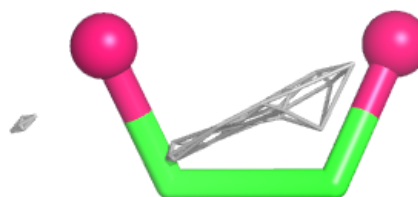
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EDO E 446:

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

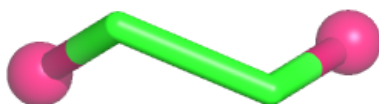
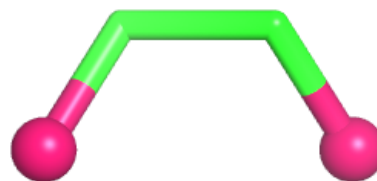
**Electron density around EDO C 427:**

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

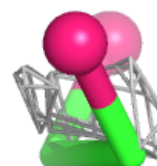
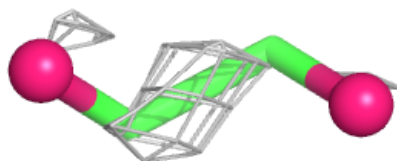
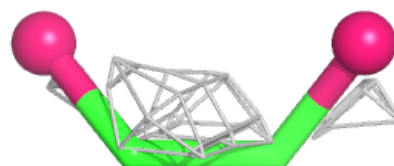


Electron density around EDO E 431:

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

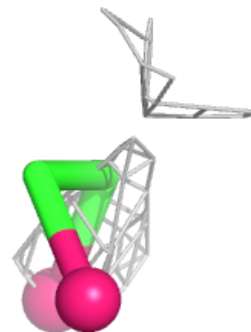
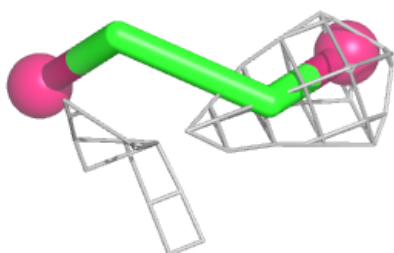
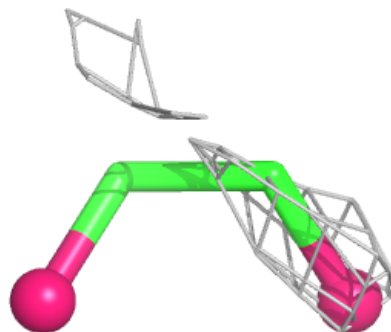
**Electron density around EDO B 428:**

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

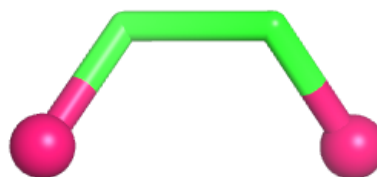


Electron density around EDO F 444:

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

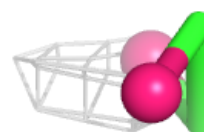
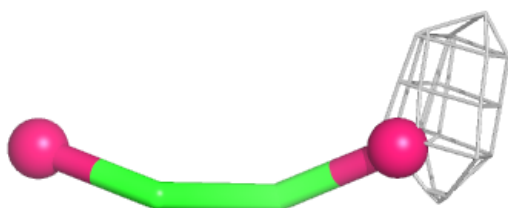
**Electron density around EDO A 426:**

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

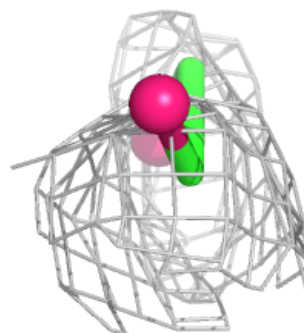
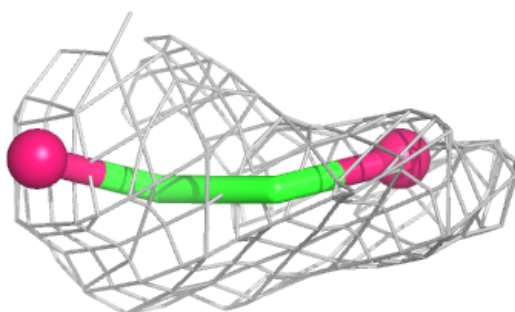
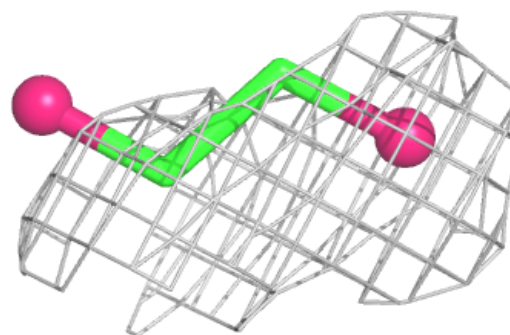


Electron density around EDO E 445:

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

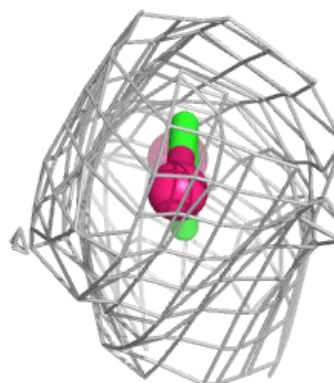
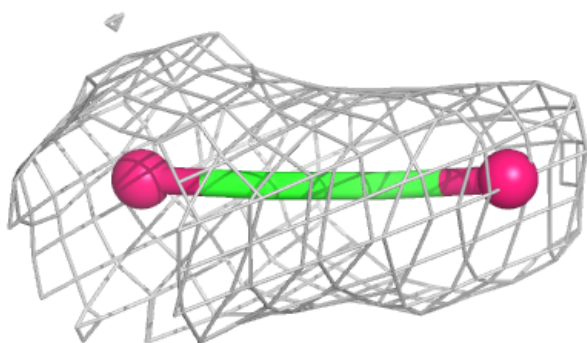
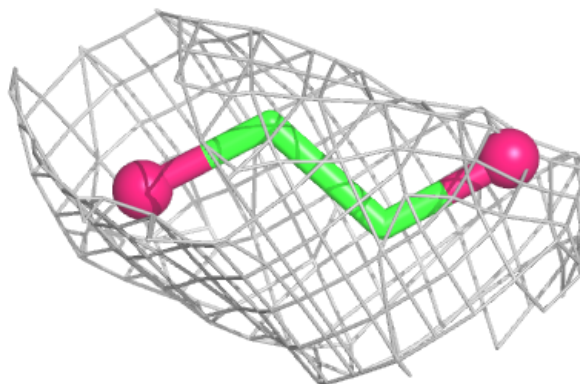
**Electron density around EDO B 441:**

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

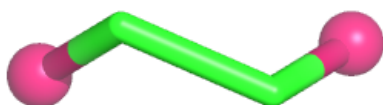
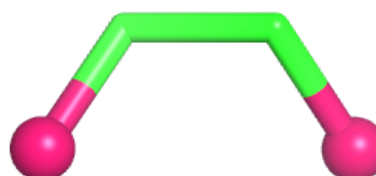


Electron density around EDO F 418:

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

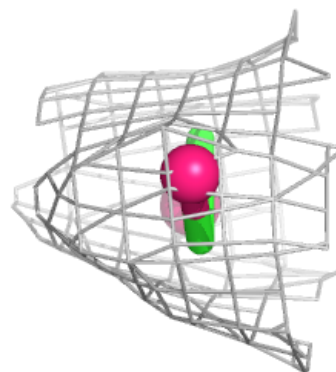
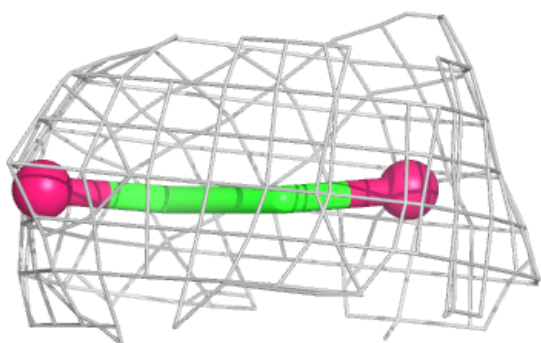
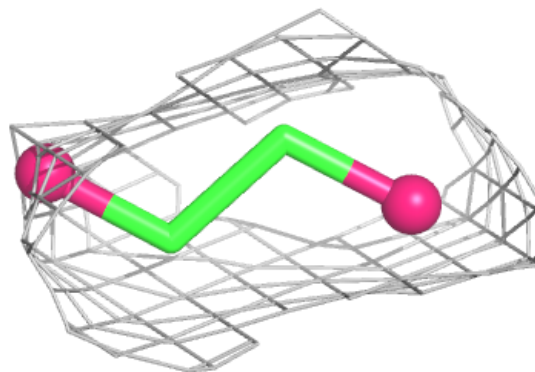
**Electron density around EDO F 434:**

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

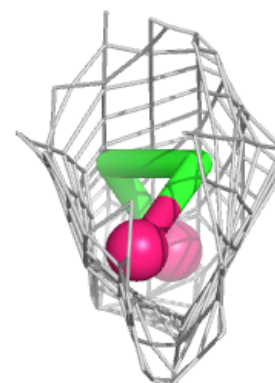
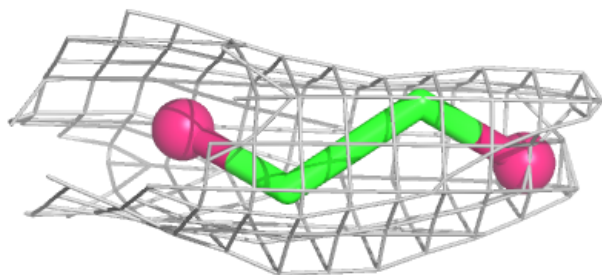
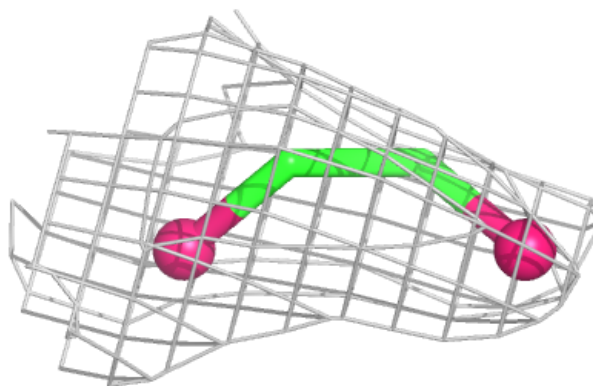


Electron density around EDO B 414:

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

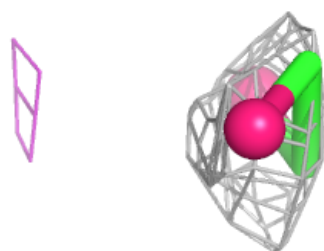
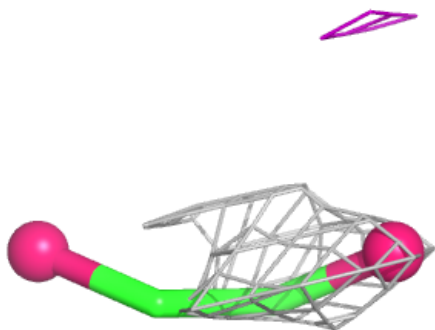
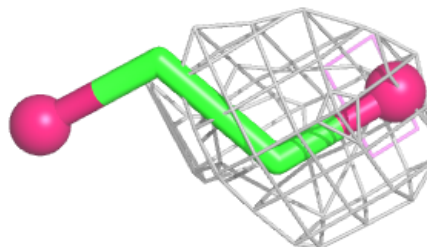
**Electron density around EDO A 443:**

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

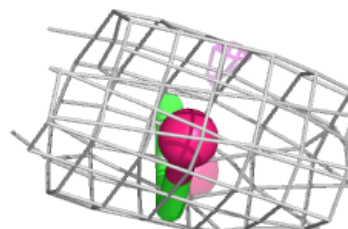
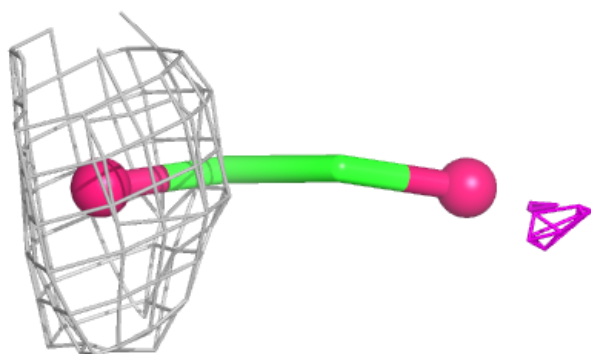
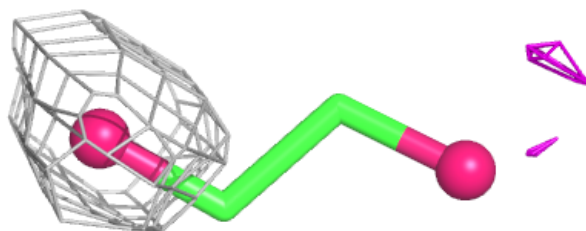


Electron density around EDO E 432:

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

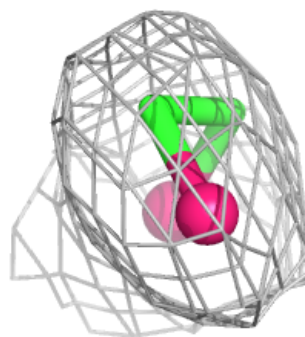
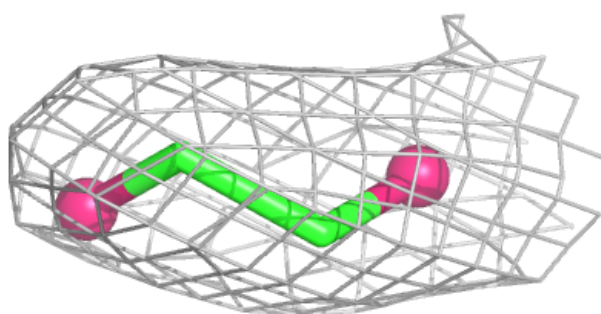
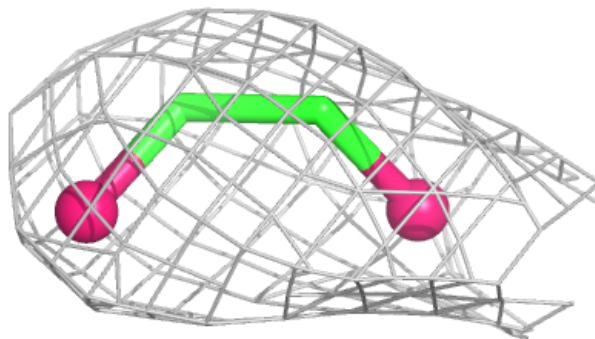
**Electron density around EDO B 403:**

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

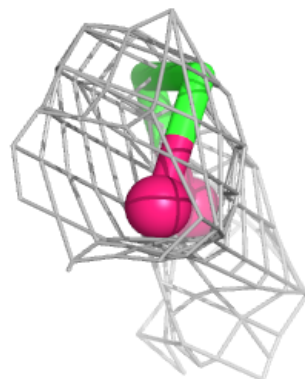
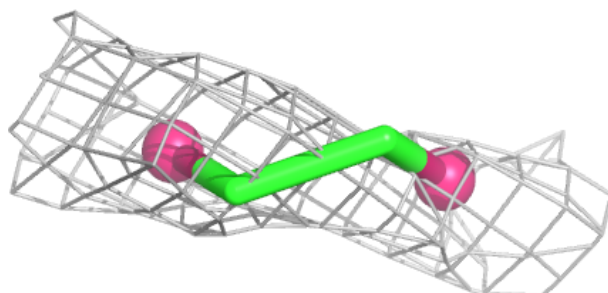
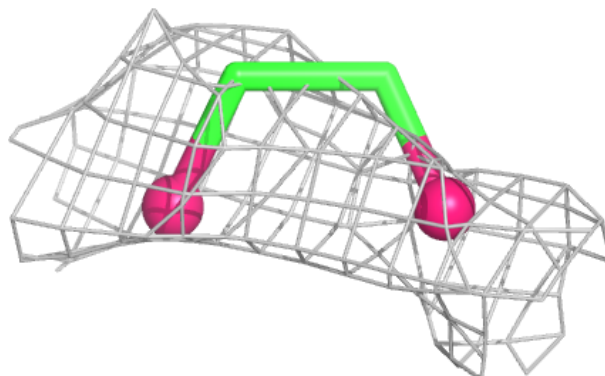


Electron density around EDO A 423:

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

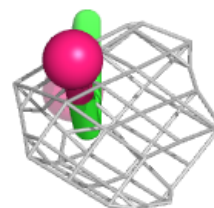
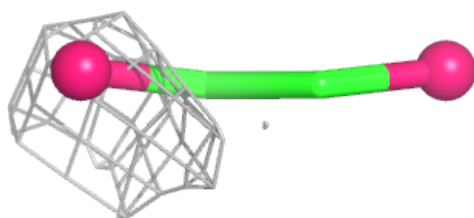
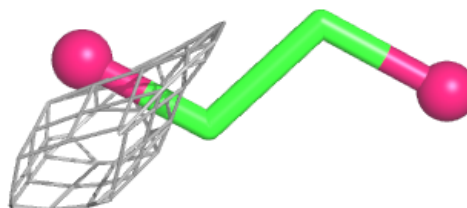
**Electron density around EDO C 436:**

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

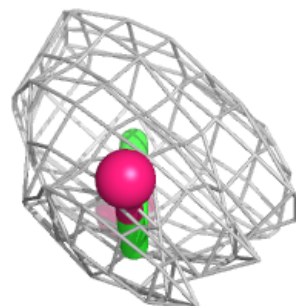
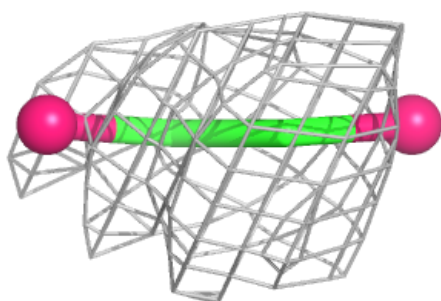
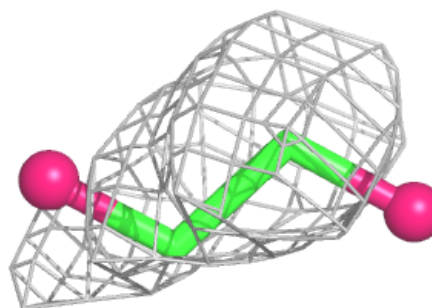


Electron density around EDO D 425:

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

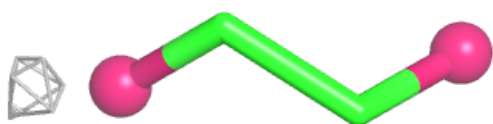
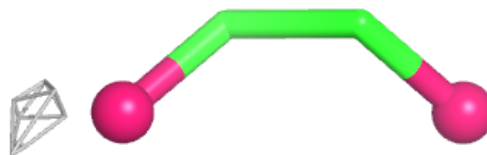
**Electron density around EDO E 426:**

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

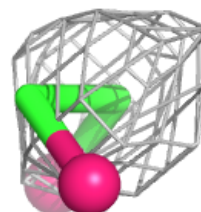
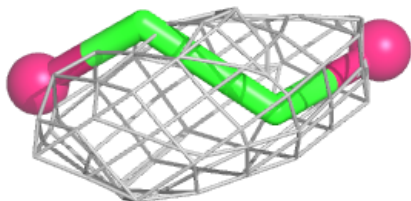
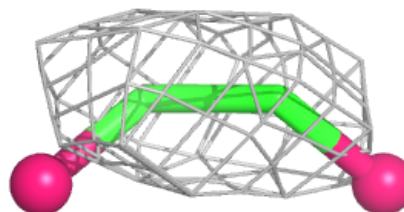


Electron density around EDO D 403:

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

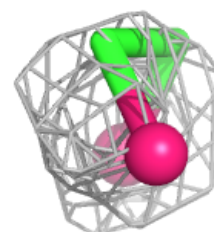
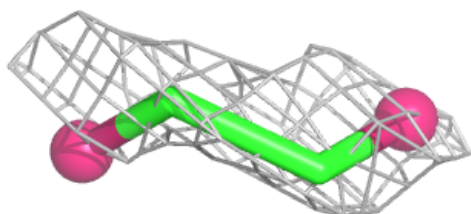
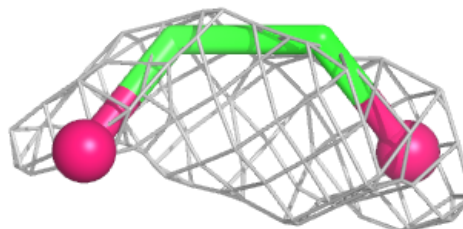
**Electron density around EDO D 420:**

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

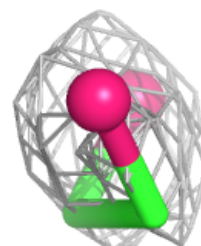
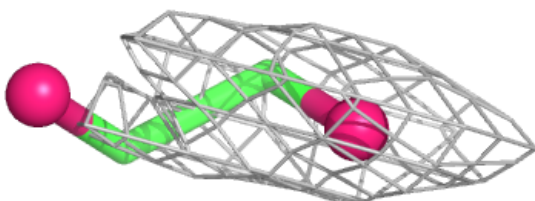
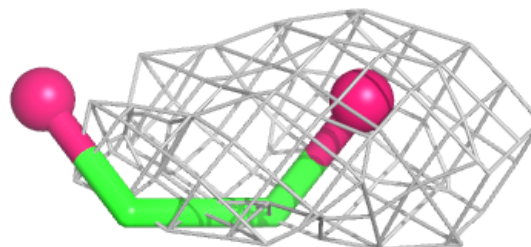


Electron density around EDO A 428:

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

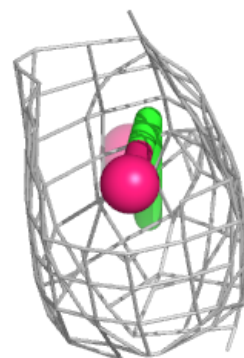
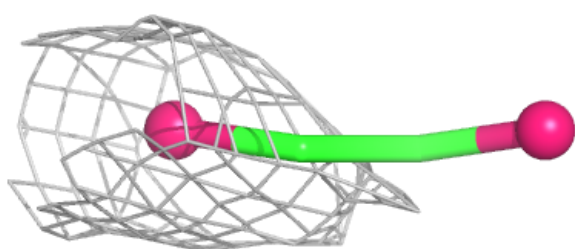
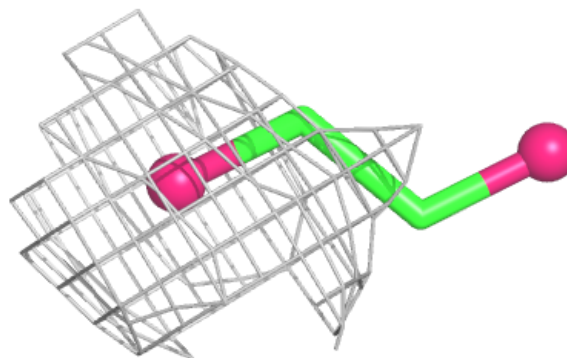
**Electron density around EDO D 429:**

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

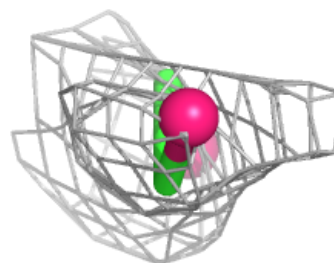
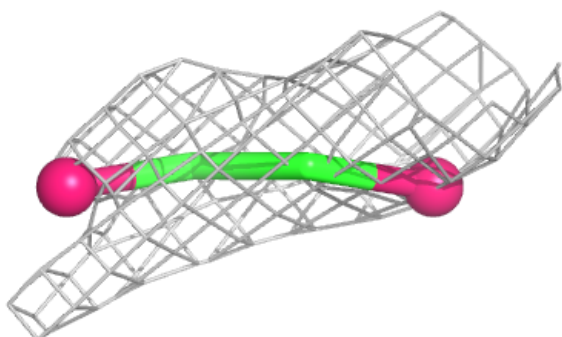
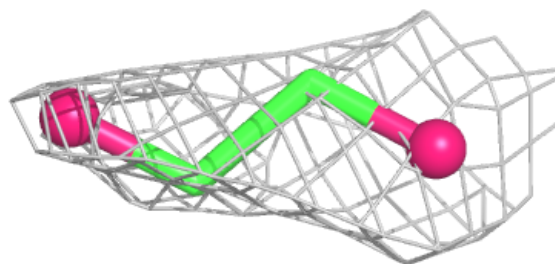


Electron density around EDO B 434:

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

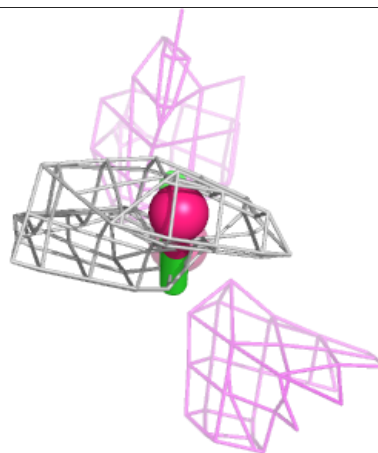
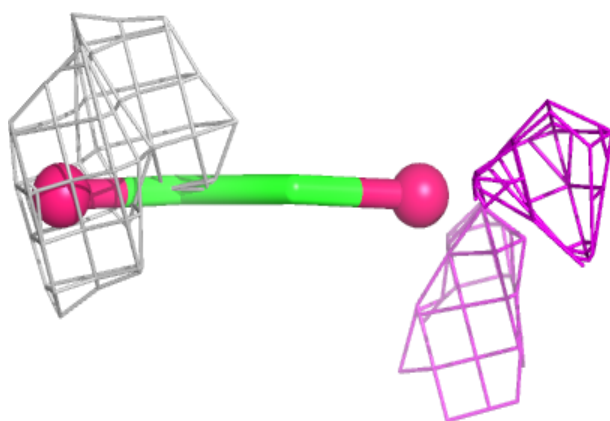
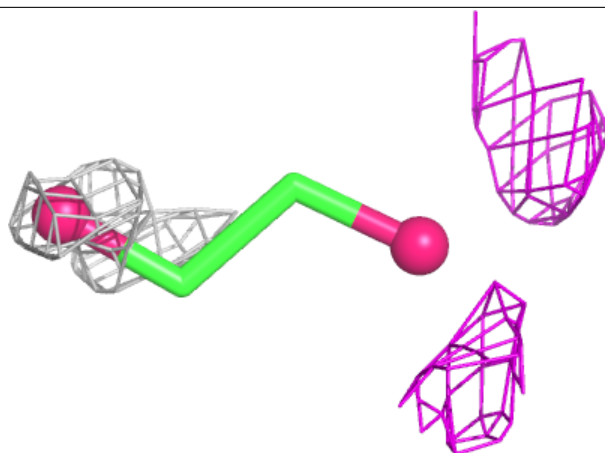
**Electron density around EDO B 437:**

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



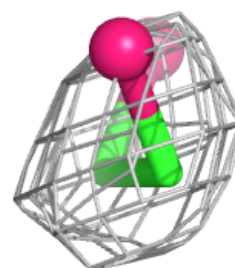
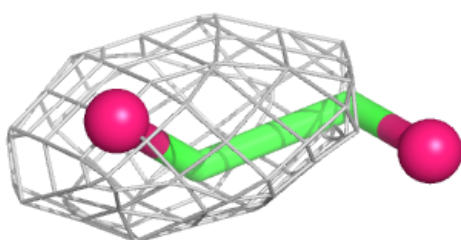
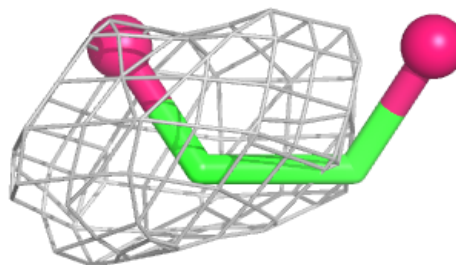
Electron density around EDO A 401:

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

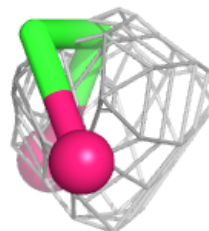
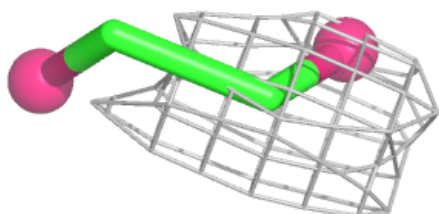
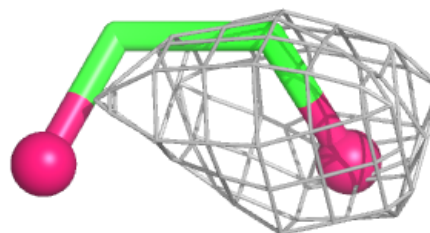


Electron density around EDO E 433:

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

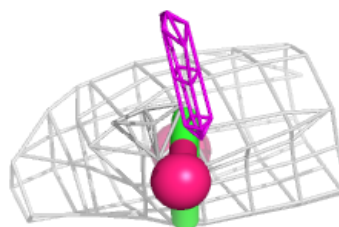
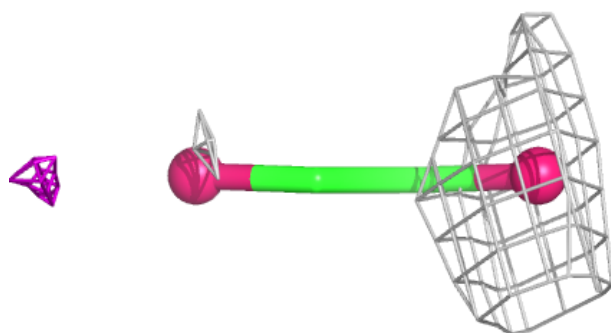
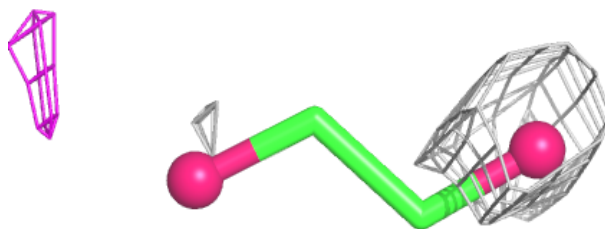
**Electron density around EDO B 446:**

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

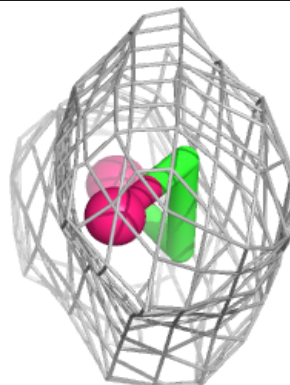
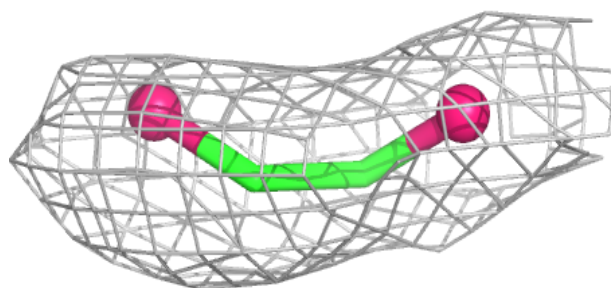
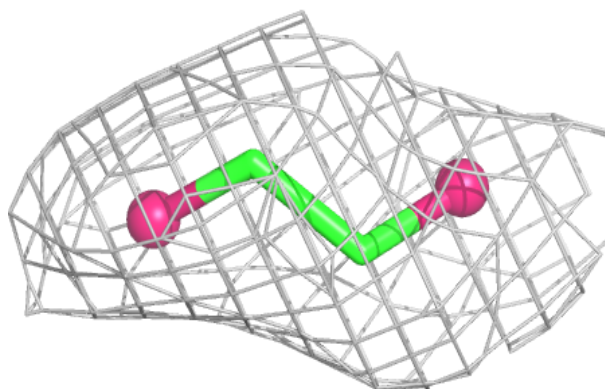


Electron density around EDO C 403:

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

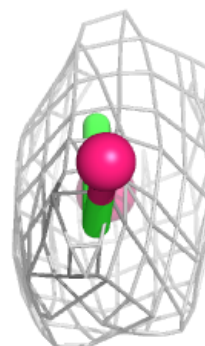
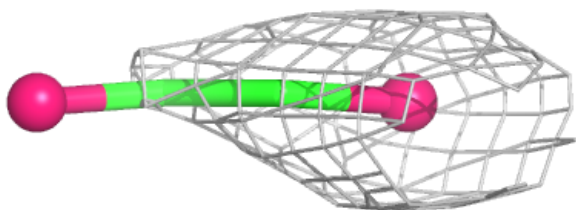
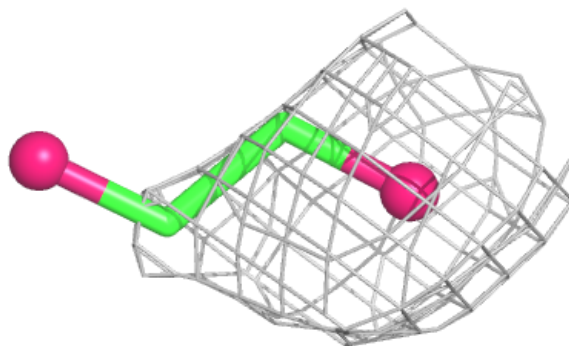
**Electron density around EDO F 403:**

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

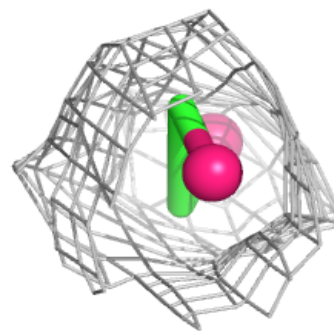
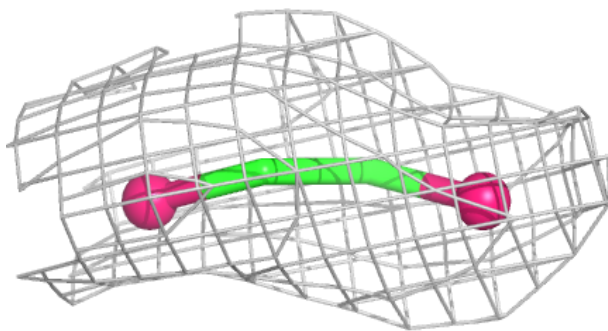
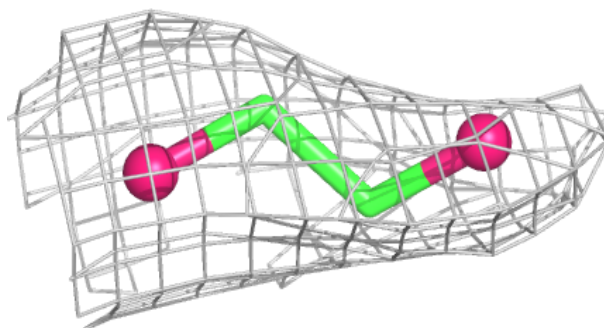


Electron density around EDO F 404:

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

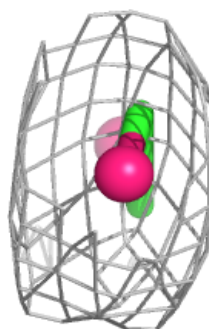
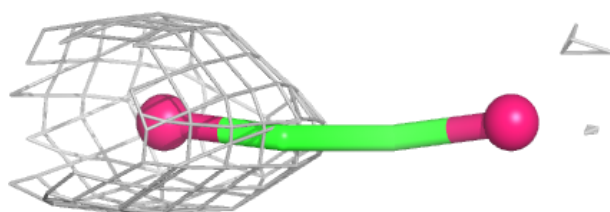
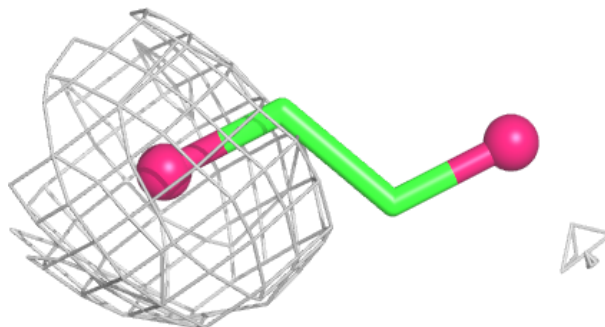
**Electron density around EDO A 416:**

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



Electron density around EDO C 433:

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

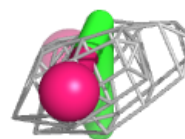
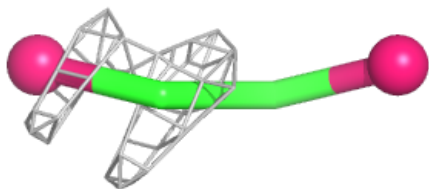
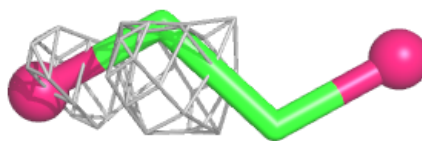
**Electron density around EDO F 443:**

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

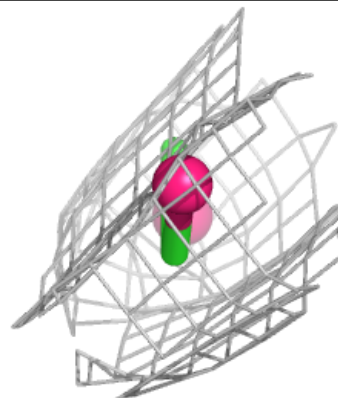
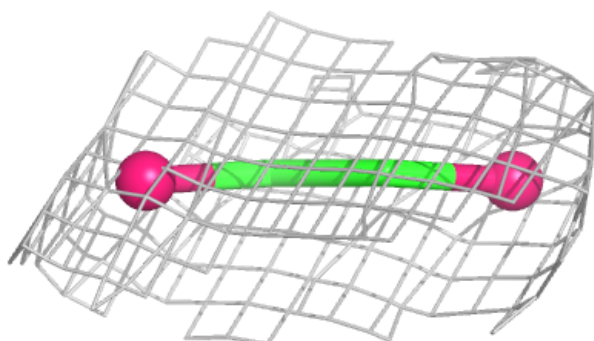
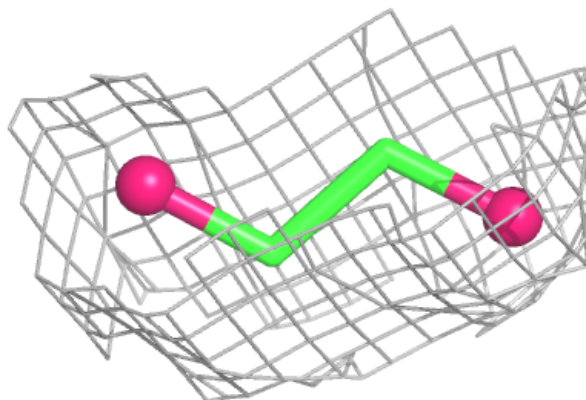


Electron density around EDO A 427:

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

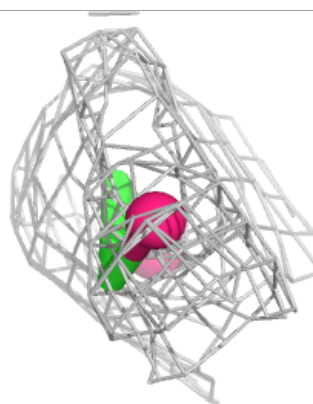
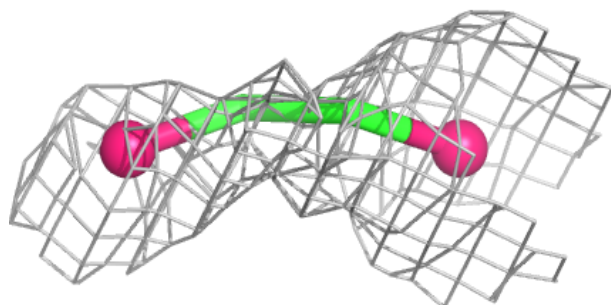
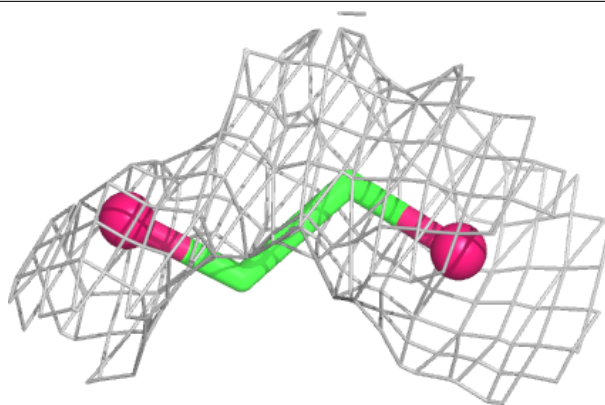
**Electron density around EDO F 445:**

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

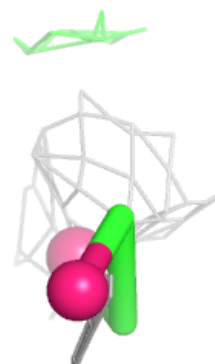
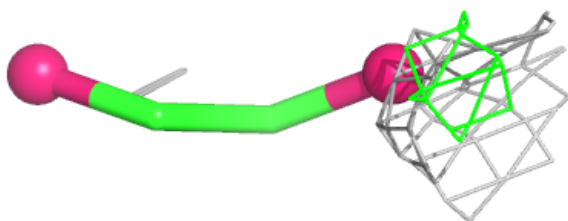
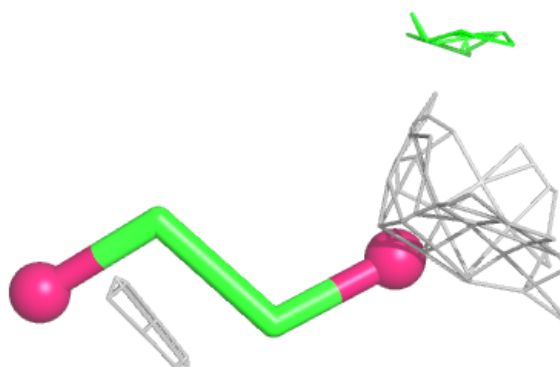


Electron density around EDO B 426:

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

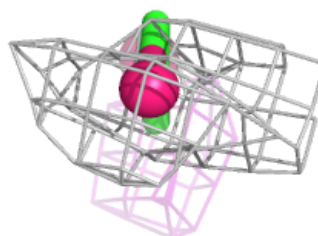
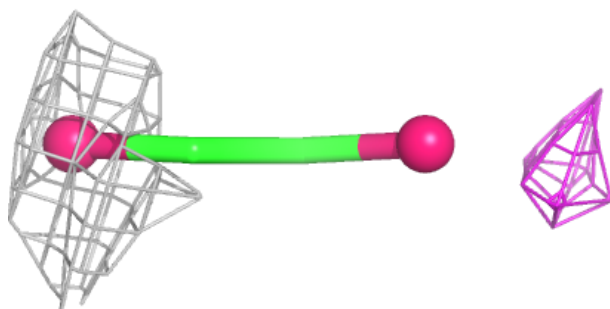
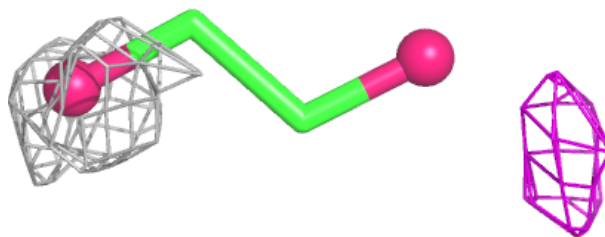
**Electron density around EDO E 441:**

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

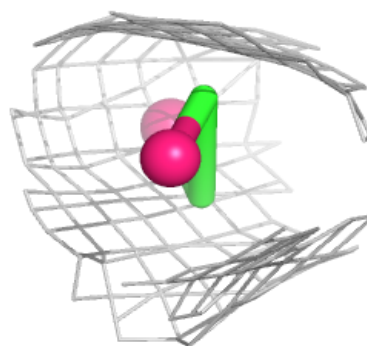
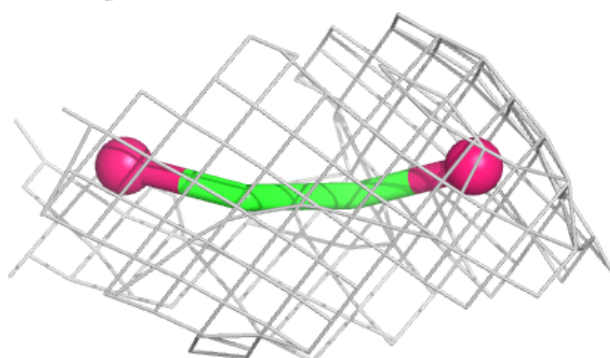
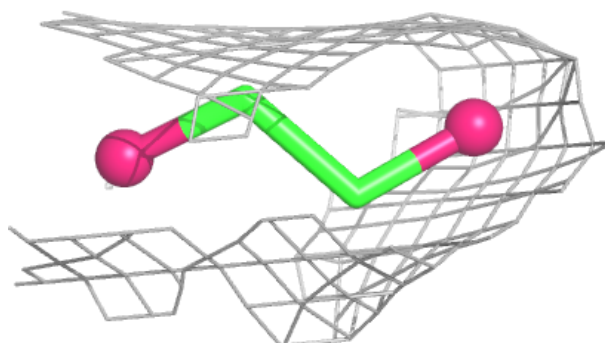


Electron density around EDO D 404:

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

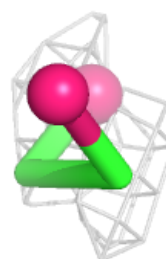
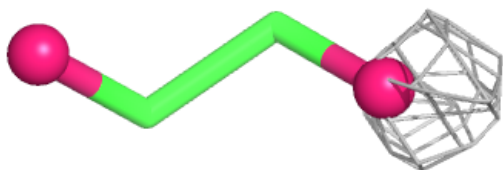
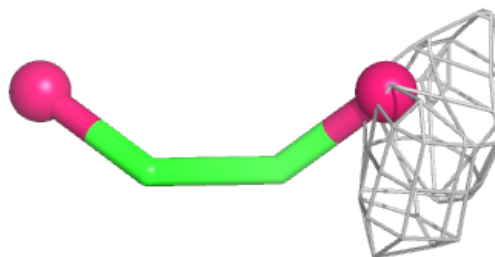
**Electron density around EDO C 418:**

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

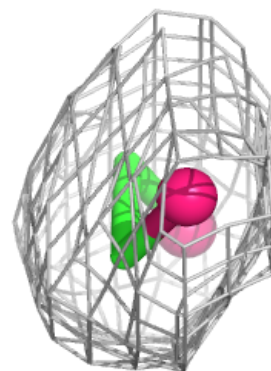
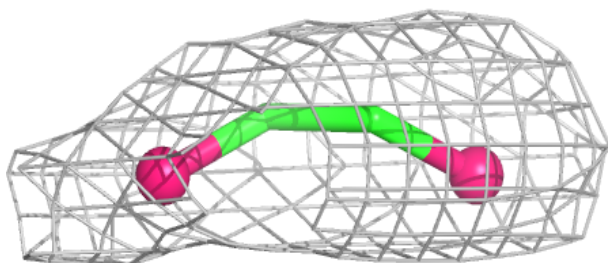
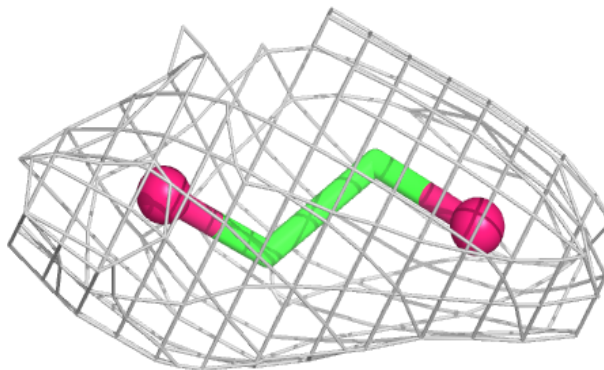


Electron density around EDO B 438:

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

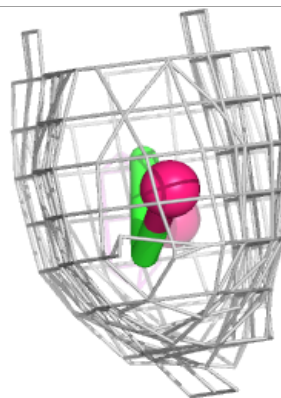
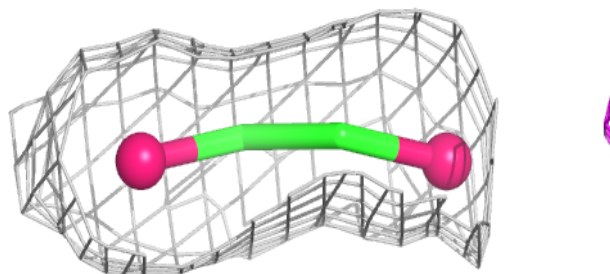
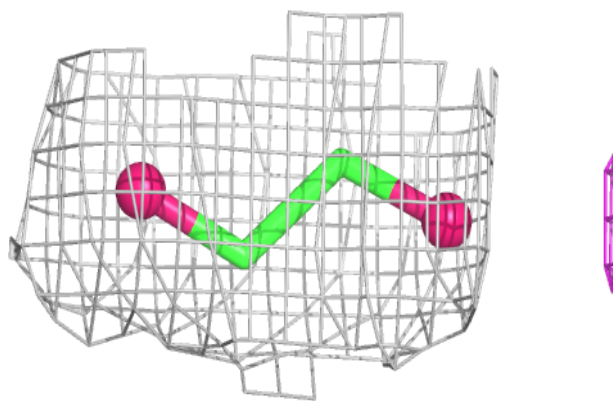
**Electron density around EDO C 432:**

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

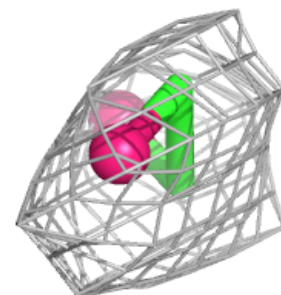
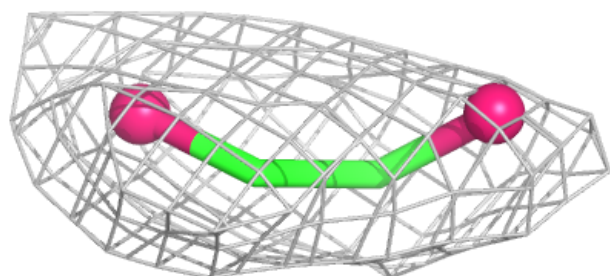
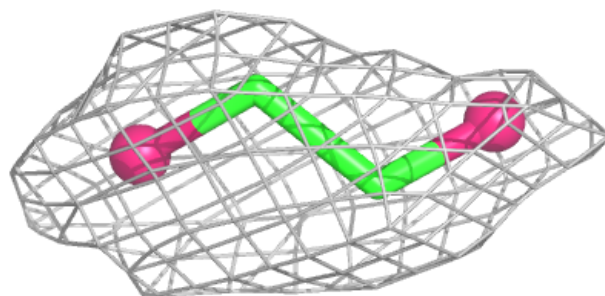


Electron density around EDO F 406:

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

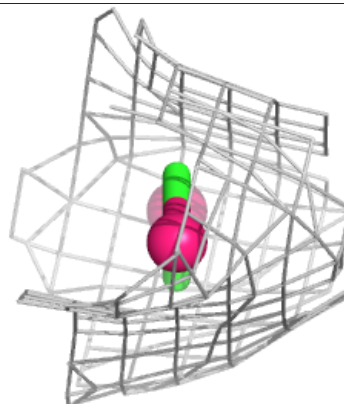
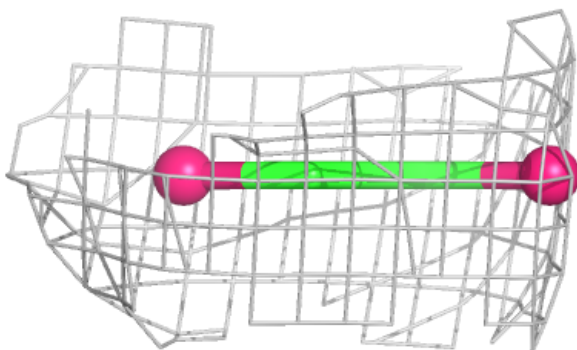
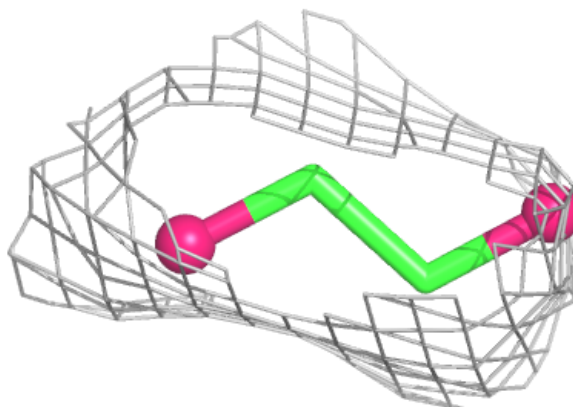
**Electron density around EDO D 439:**

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

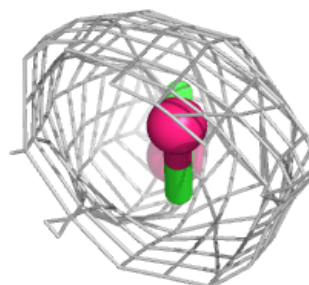
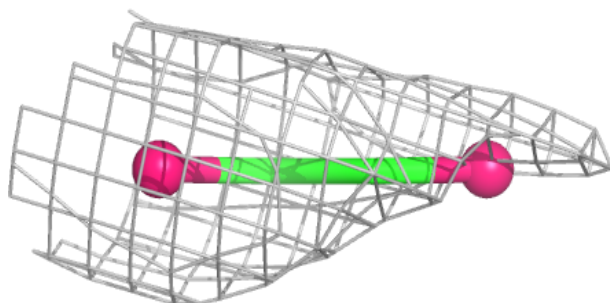
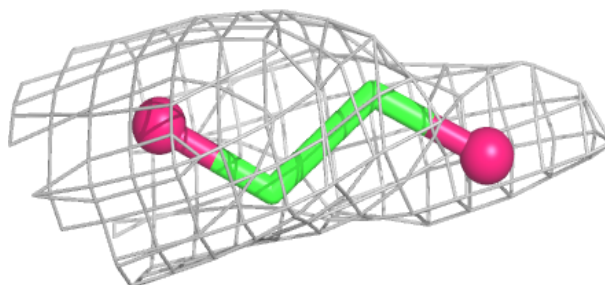


Electron density around EDO F 420:

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

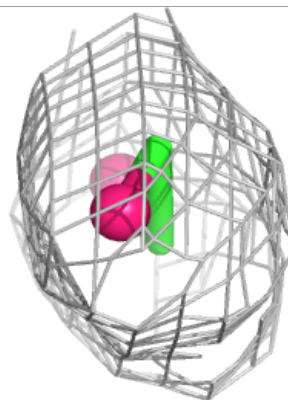
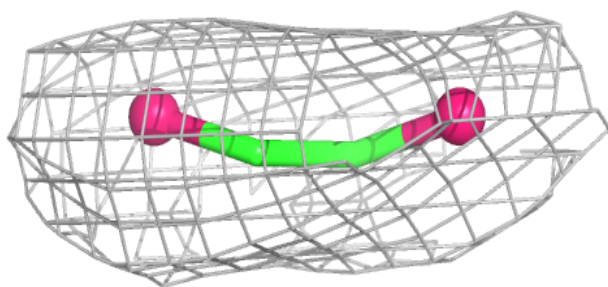
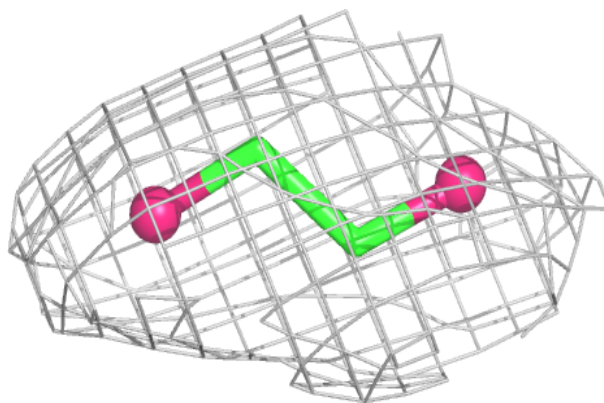
**Electron density around EDO F 424:**

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

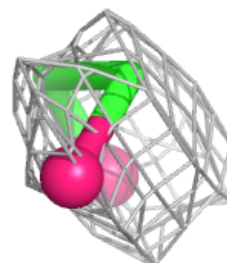
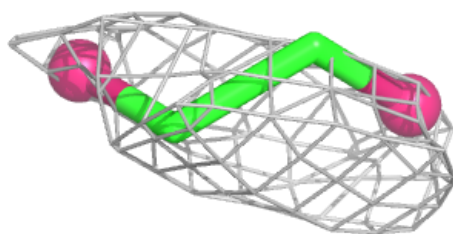
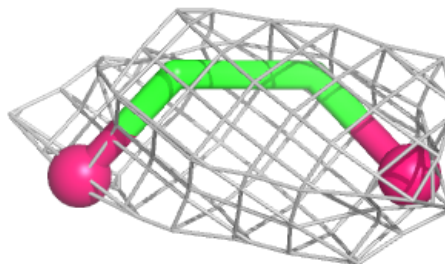


Electron density around EDO A 431:

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

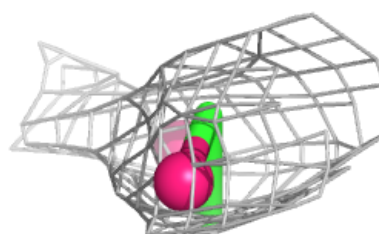
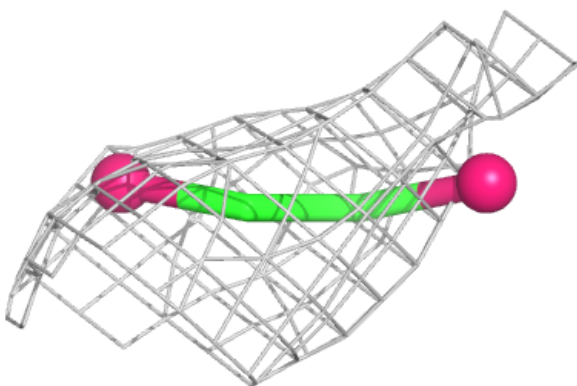
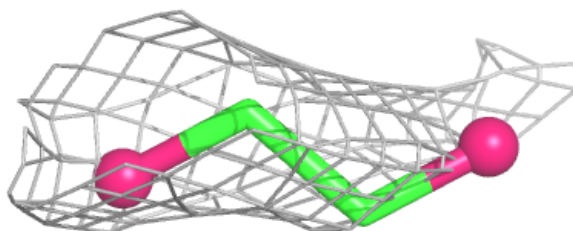
**Electron density around EDO F 436:**

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

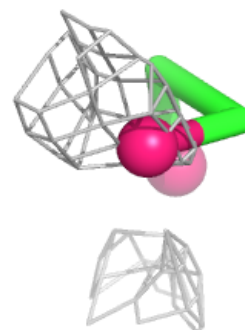
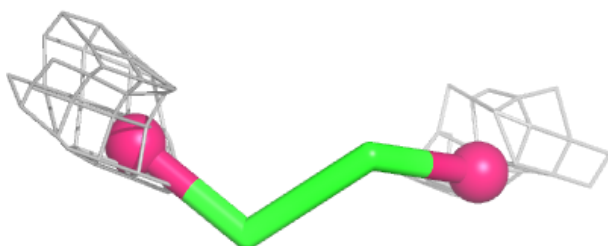
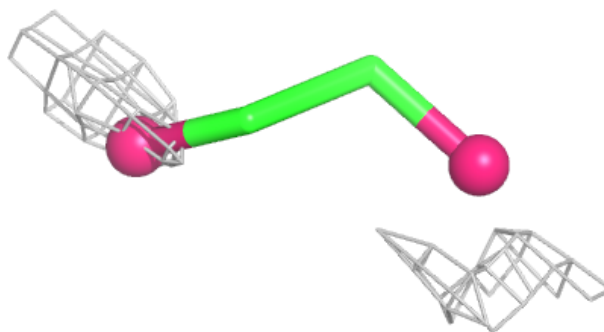


Electron density around EDO F 440:

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

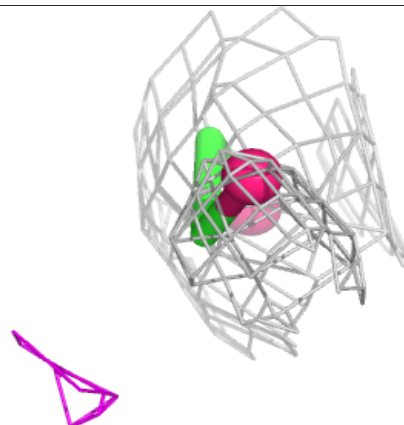
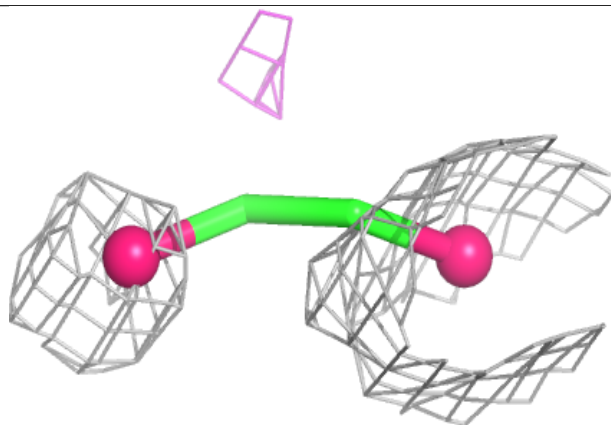
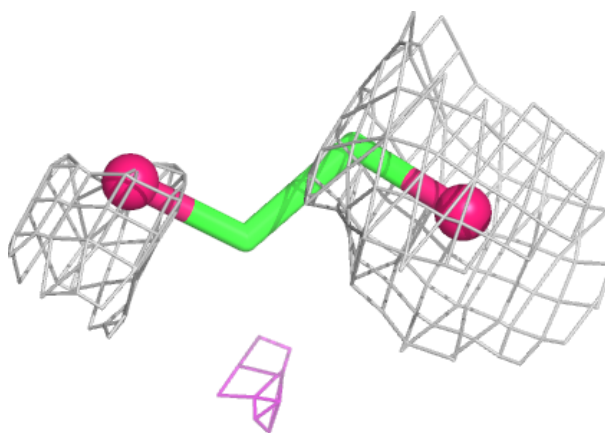
**Electron density around EDO F 442:**

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

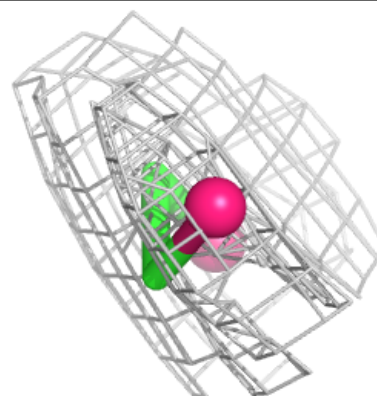
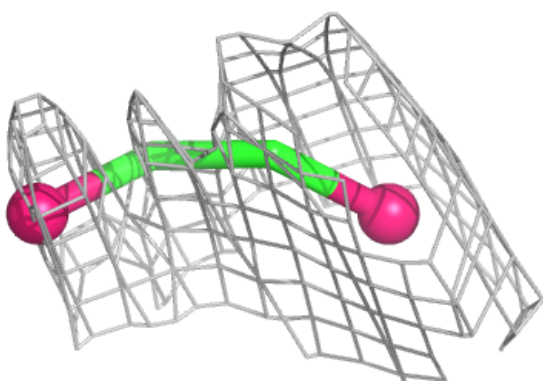
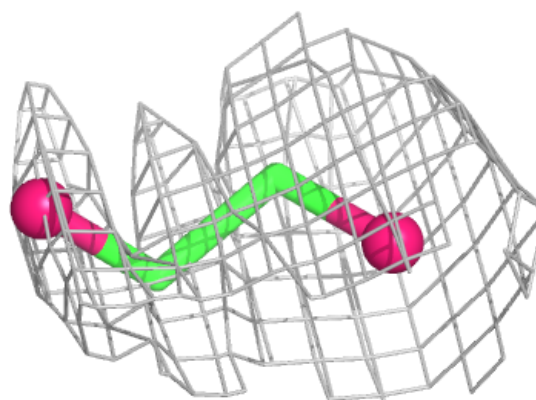


Electron density around EDO E 429:

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

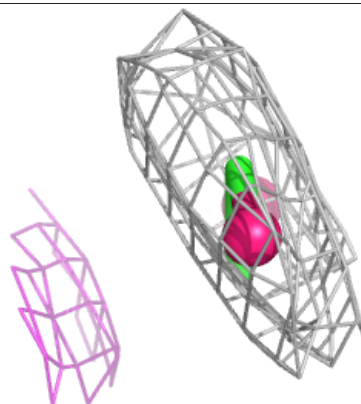
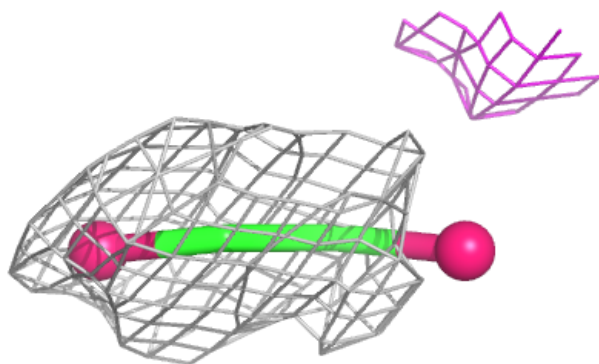
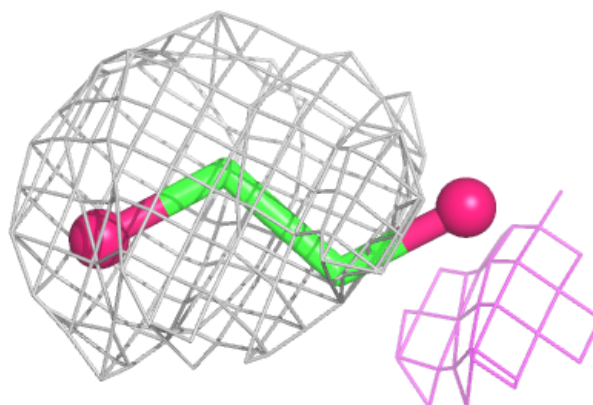
**Electron density around EDO A 421:**

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

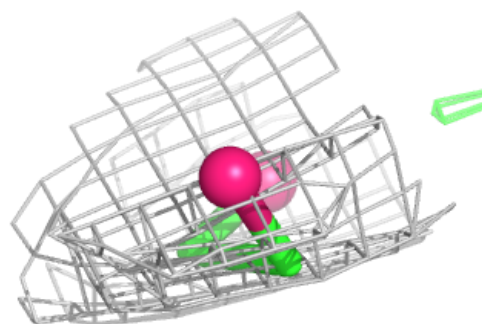
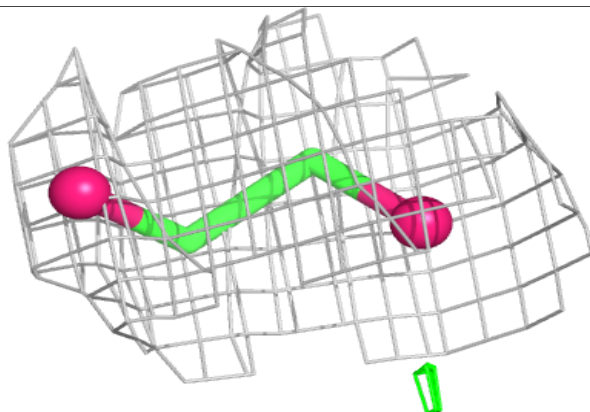
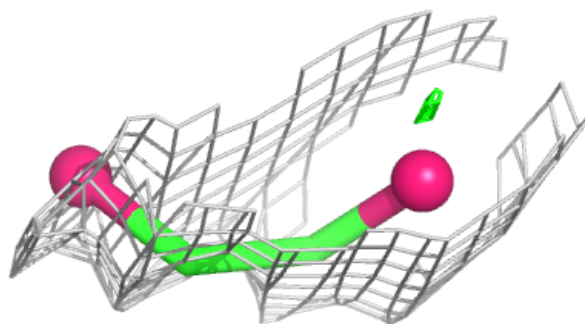


Electron density around EDO D 402:

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

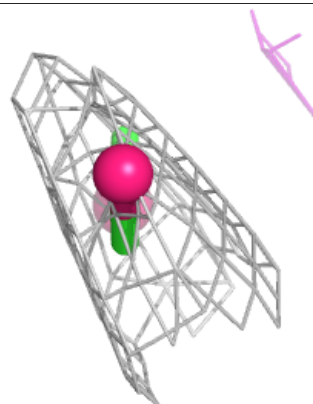
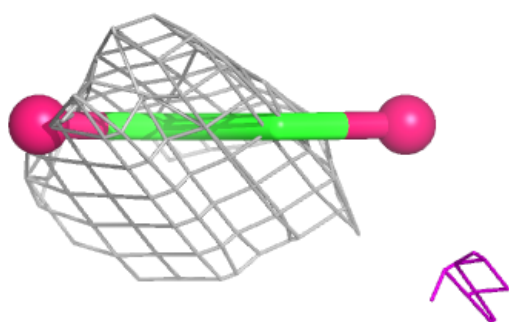
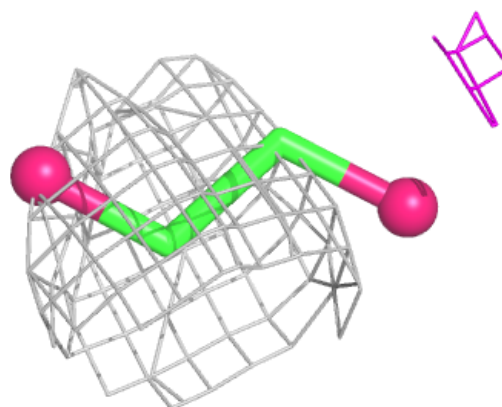
**Electron density around EDO D 424:**

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

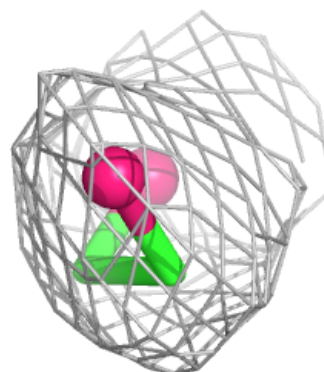
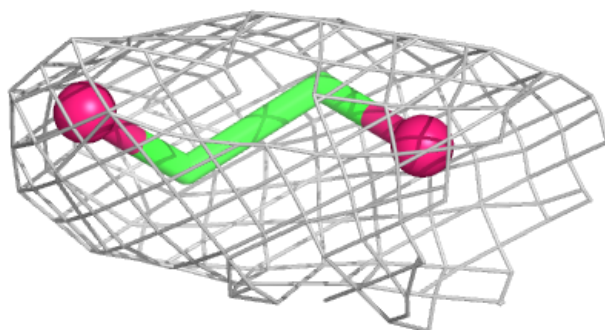
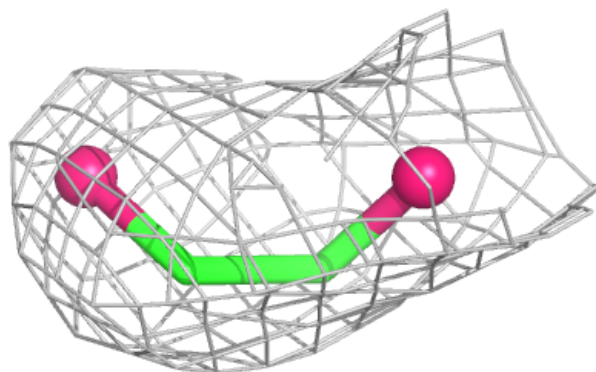


Electron density around EDO A 440:

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

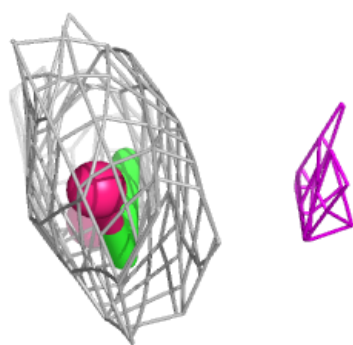
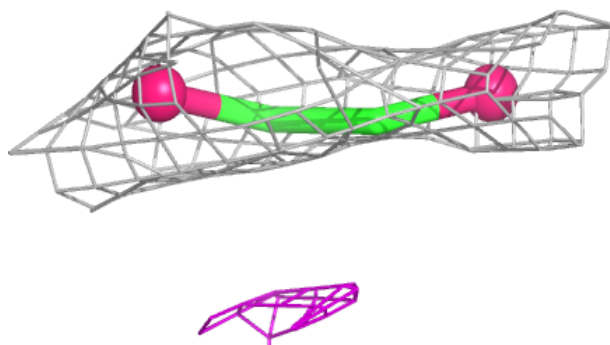
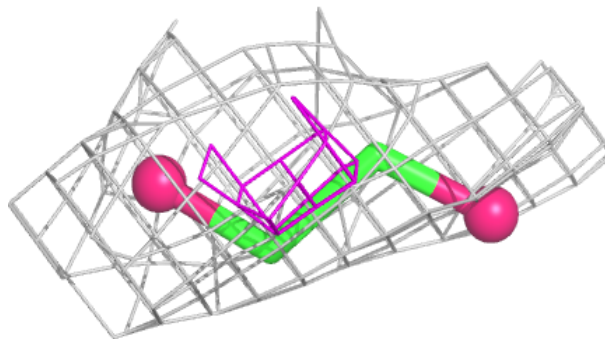
**Electron density around EDO D 426:**

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

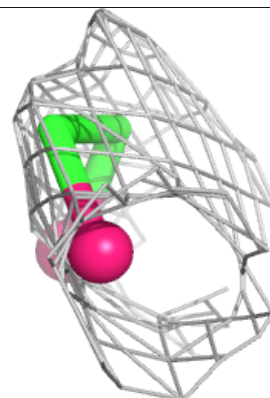
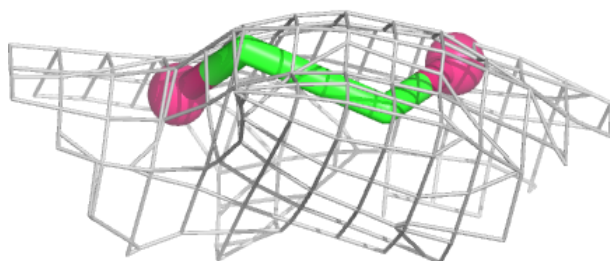


Electron density around EDO B 444:

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

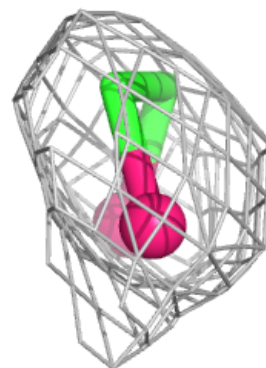
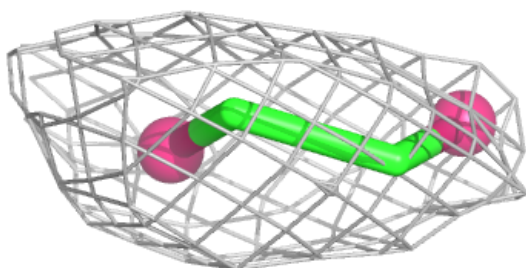
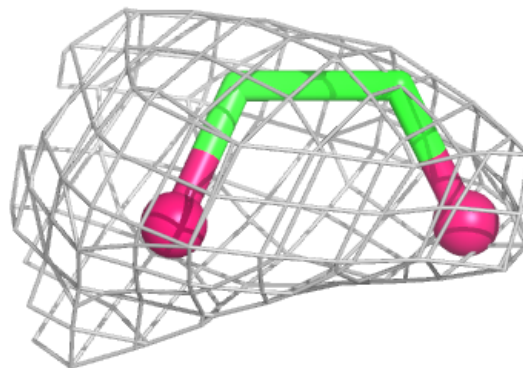
**Electron density around EDO D 432:**

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

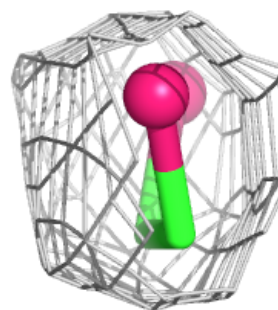
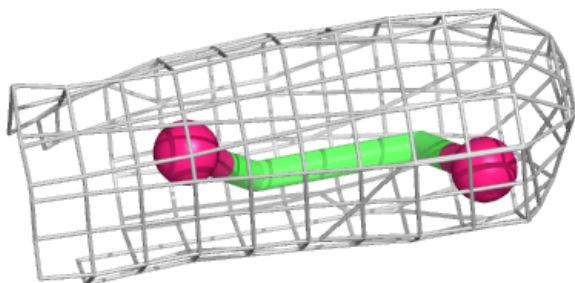
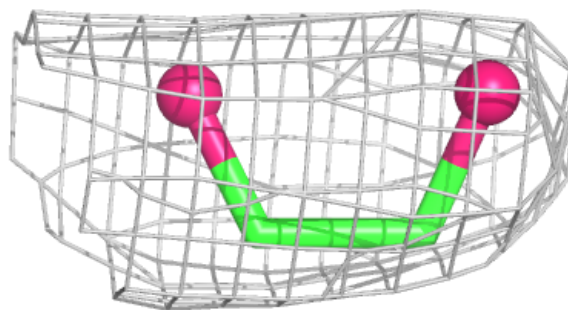


Electron density around EDO D 433:

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

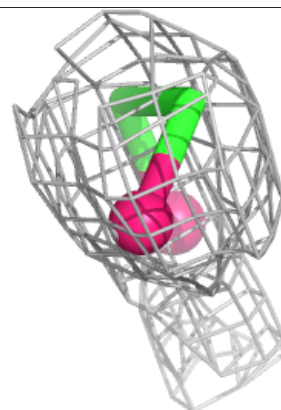
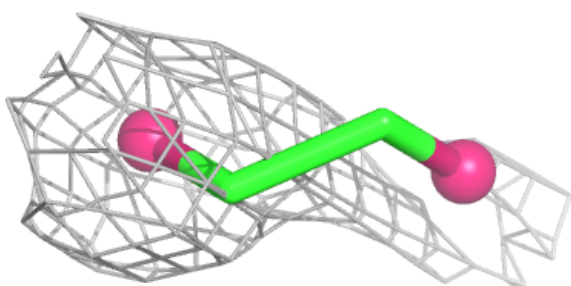
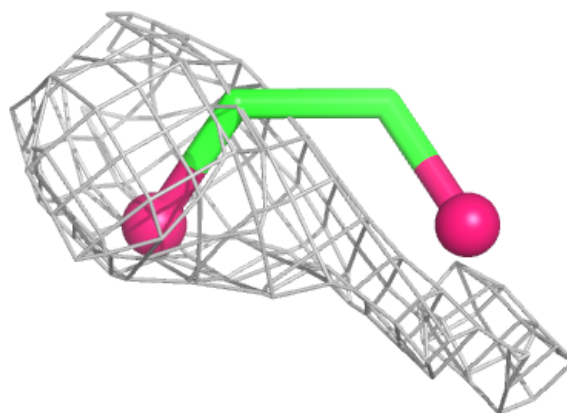
**Electron density around EDO D 435:**

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

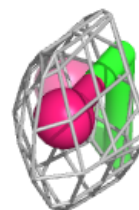
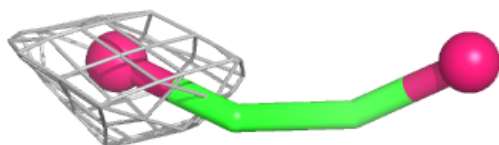
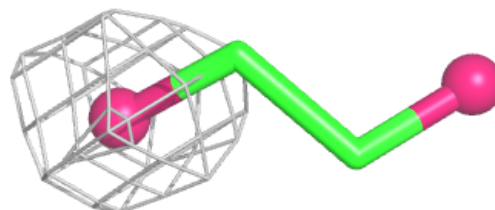


Electron density around EDO D 436:

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

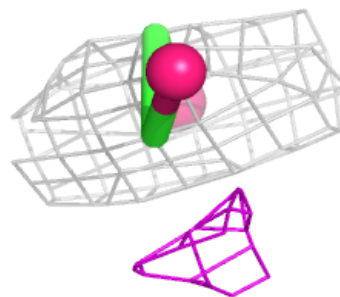
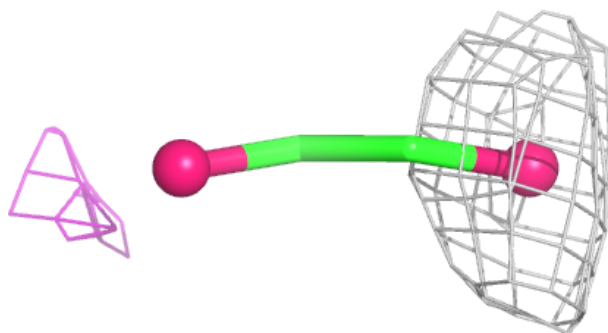
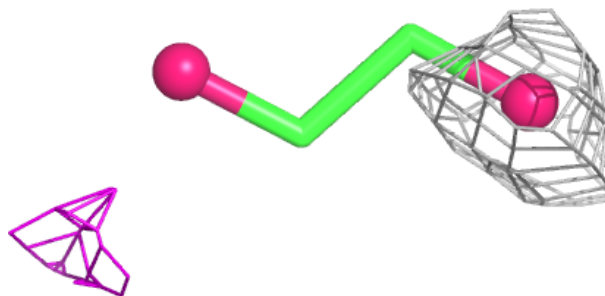
**Electron density around EDO A 442:**

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

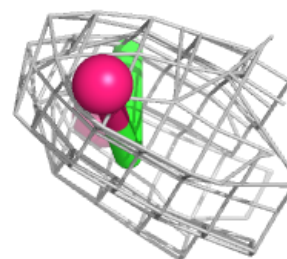
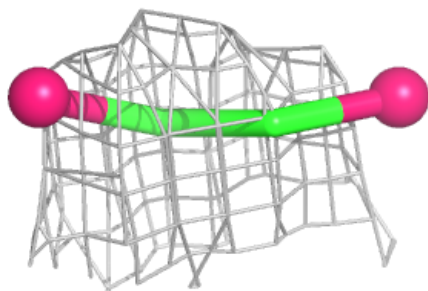
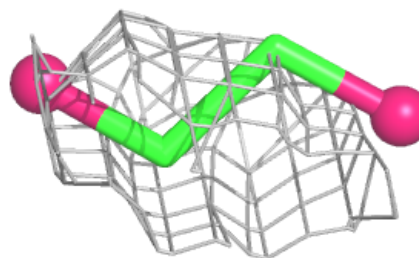


Electron density around EDO E 403:

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

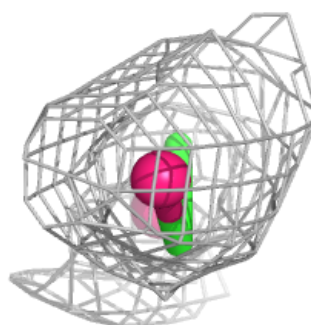
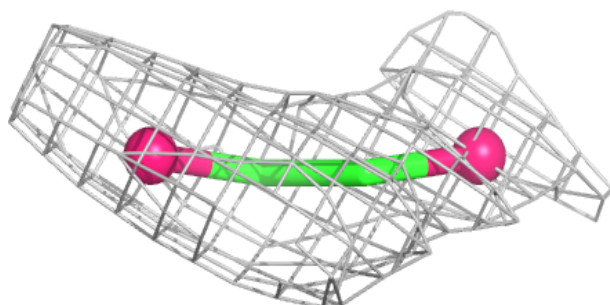
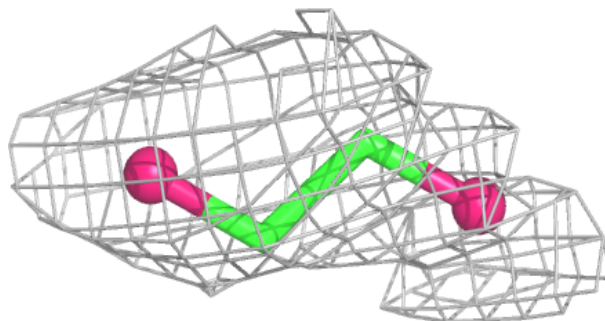
**Electron density around EDO E 404:**

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

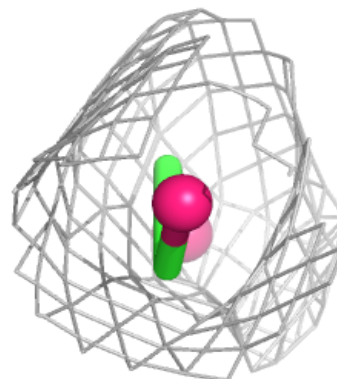
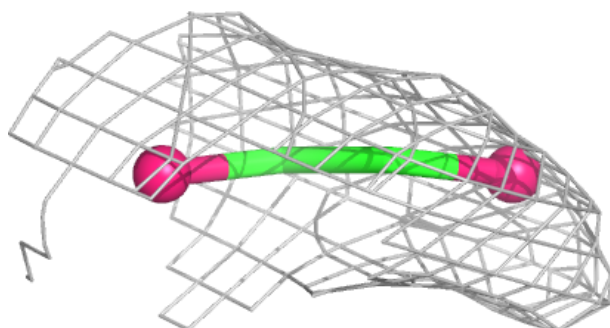
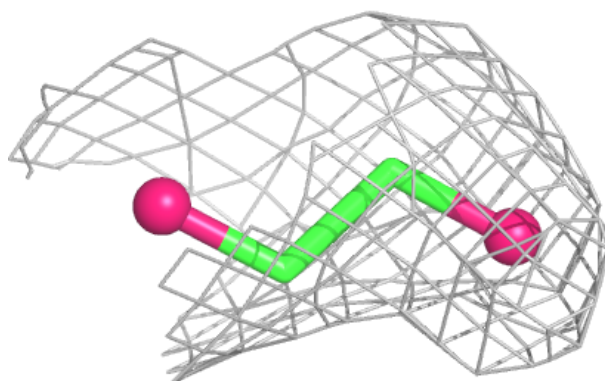


Electron density around EDO E 411:

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

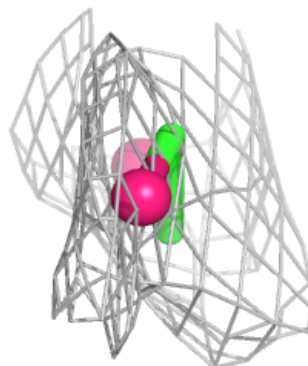
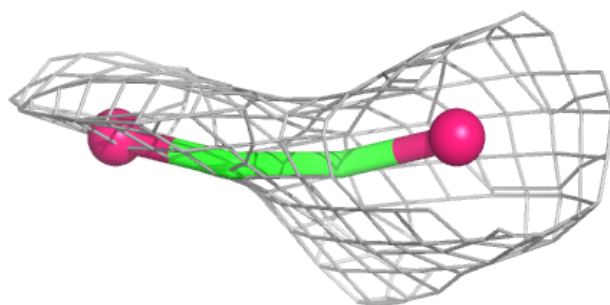
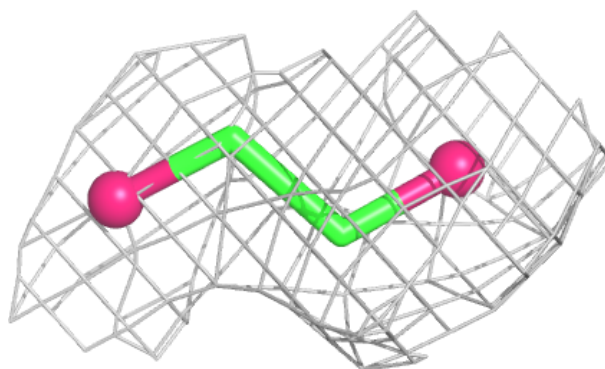
**Electron density around EDO E 413:**

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

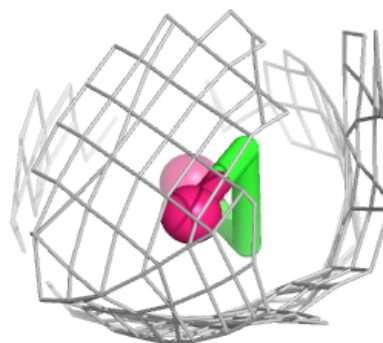
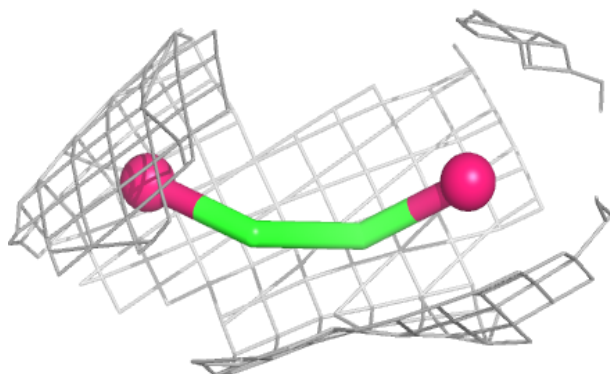
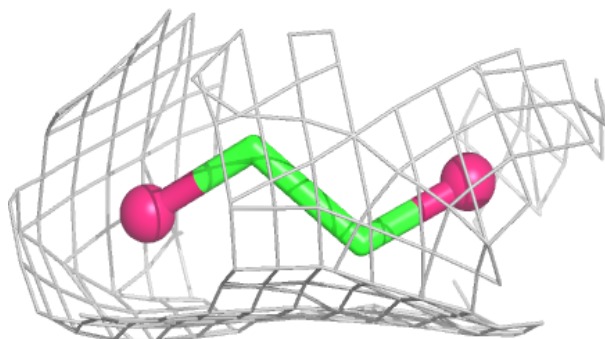


Electron density around EDO E 419:

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

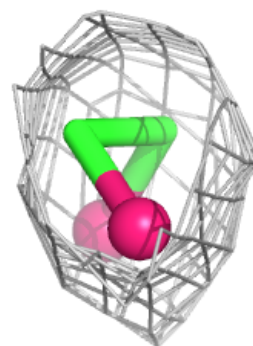
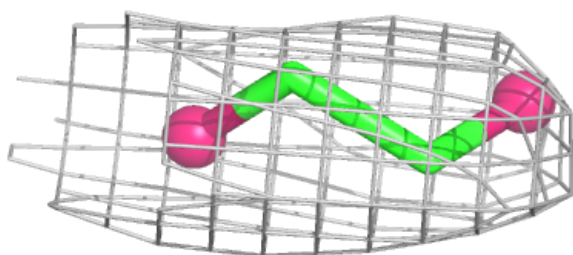
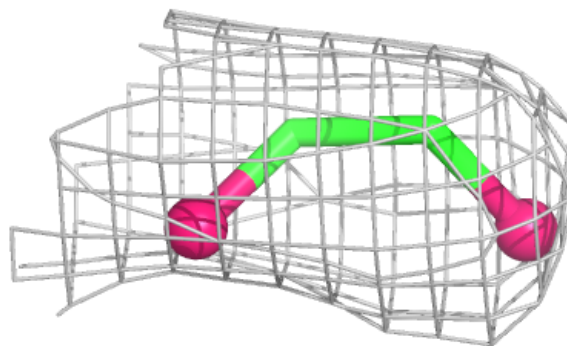
**Electron density around EDO E 421:**

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

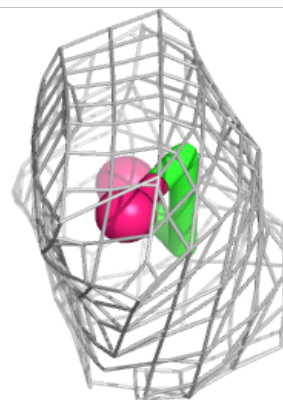
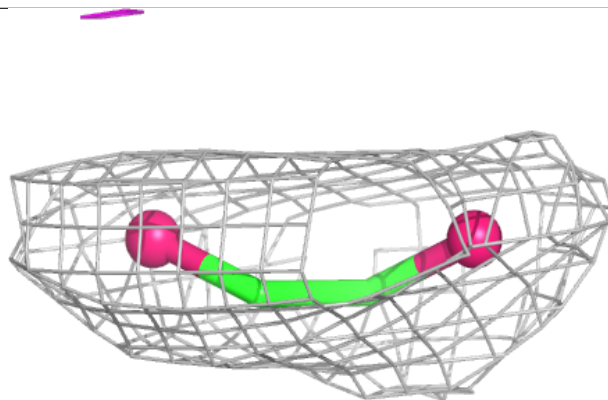
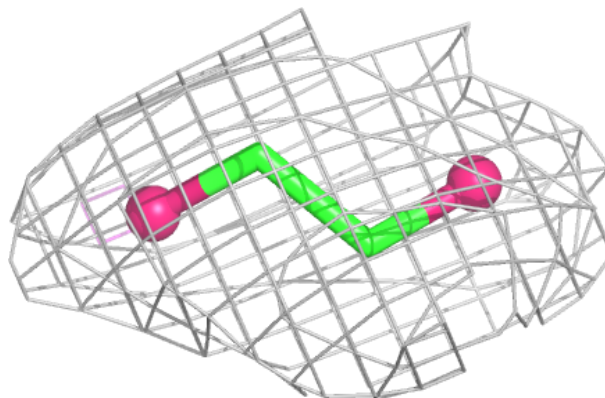


Electron density around EDO B 447:

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

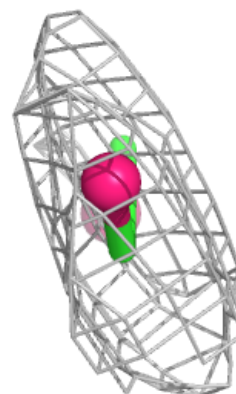
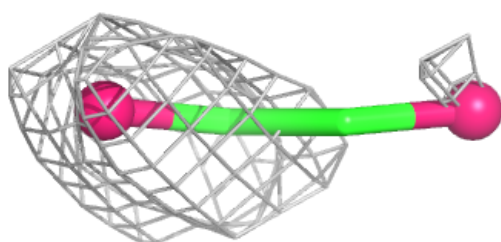
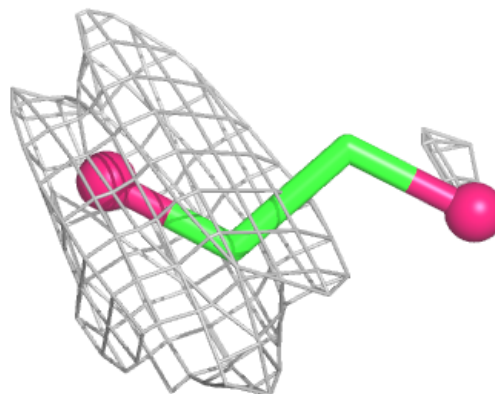
**Electron density around EDO E 428:**

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

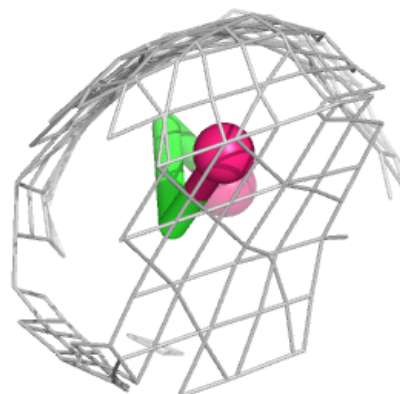
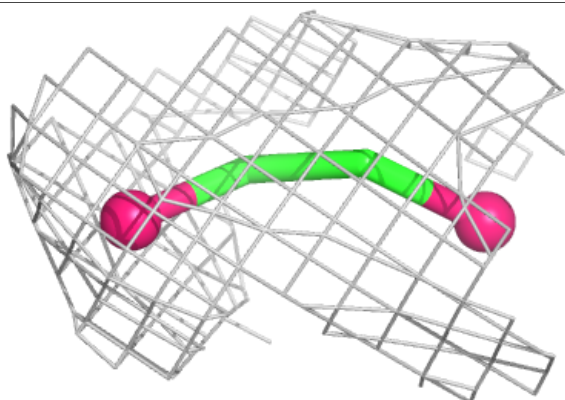
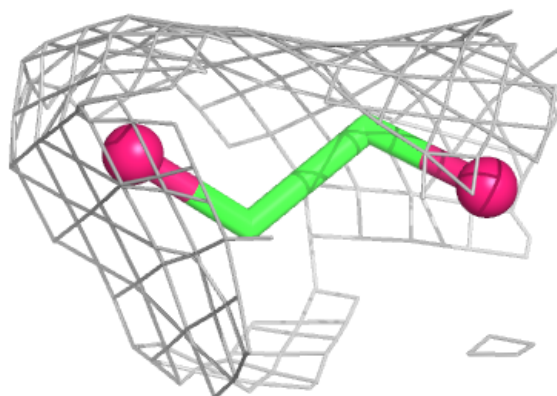


Electron density around EDO C 402:

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

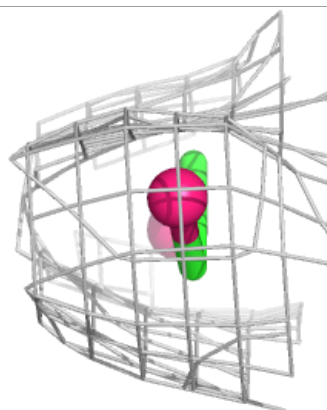
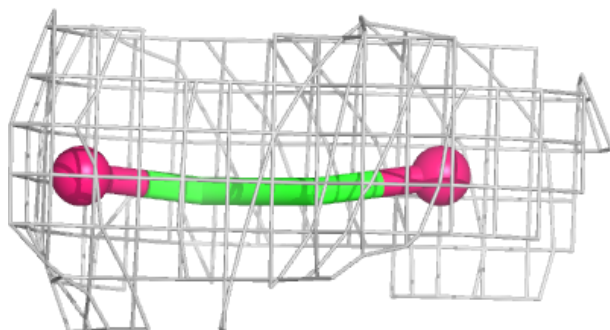
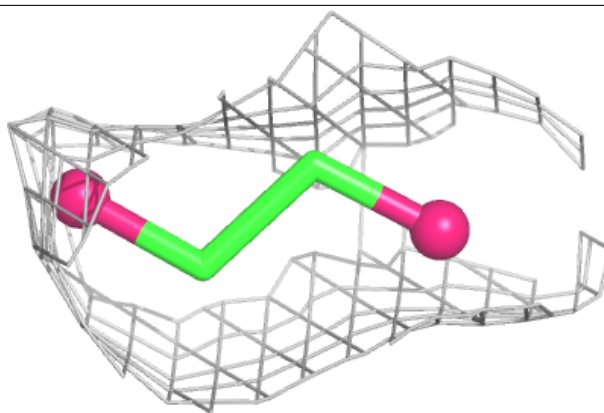
**Electron density around EDO A 417:**

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

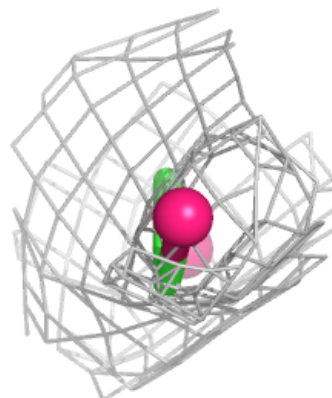
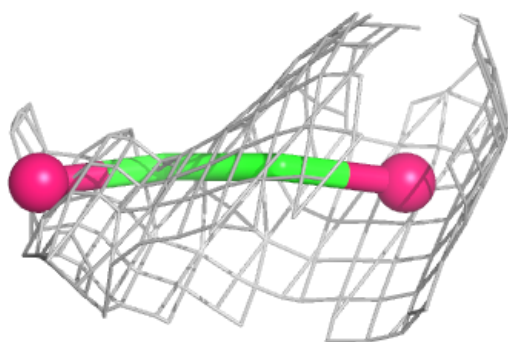
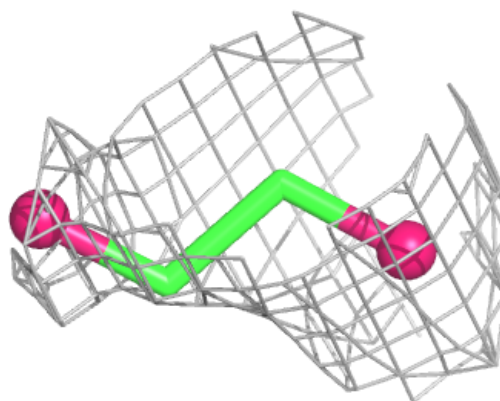


Electron density around EDO A 412:

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

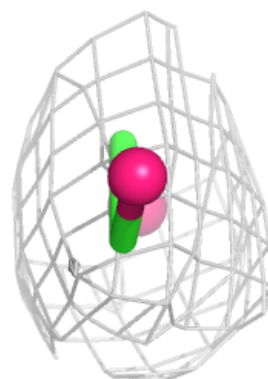
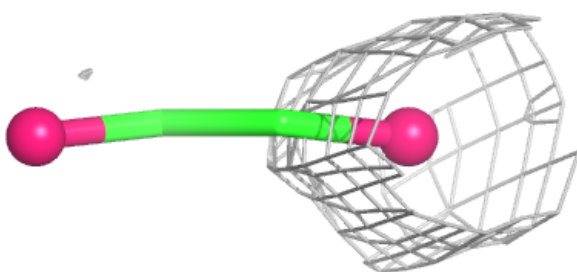
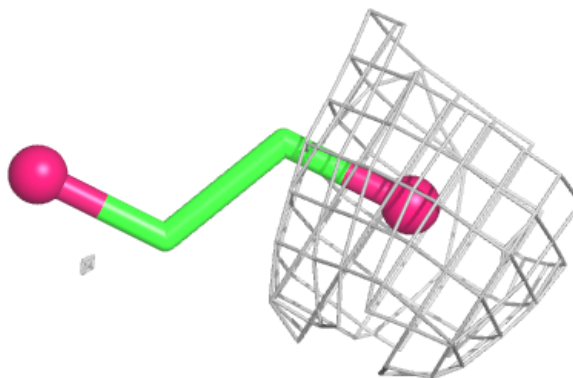
**Electron density around EDO C 420:**

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

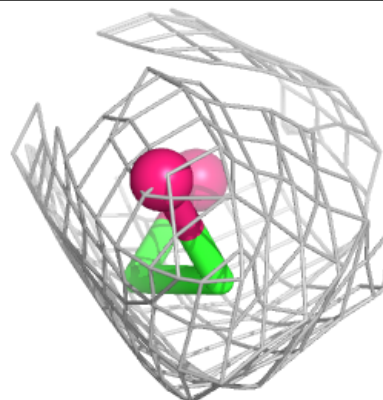
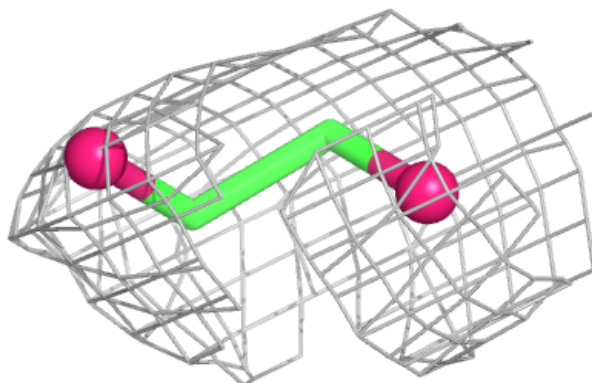
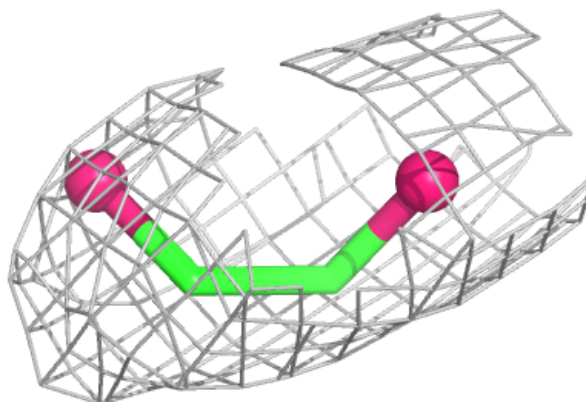


Electron density around EDO E 434:

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

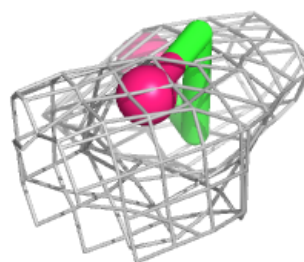
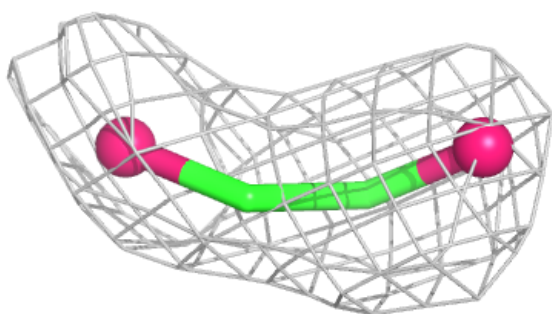
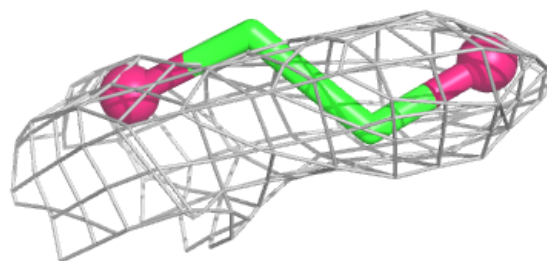
**Electron density around EDO C 424:**

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

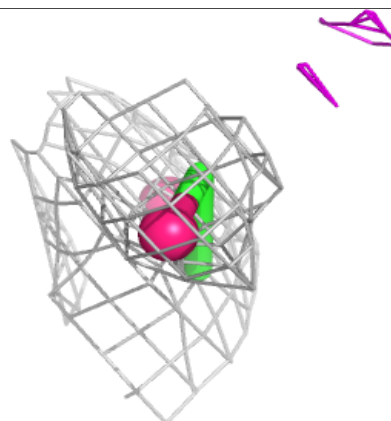
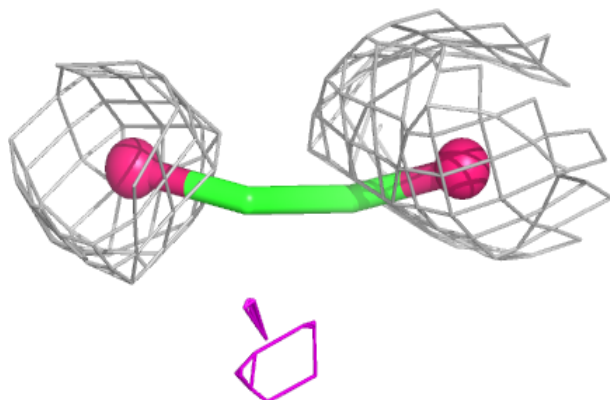
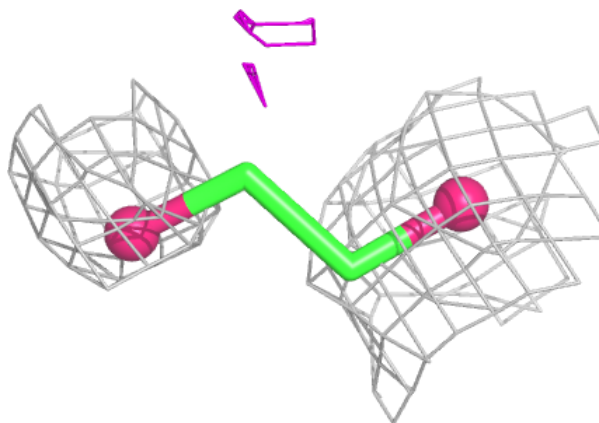


Electron density around EDO E 443:

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

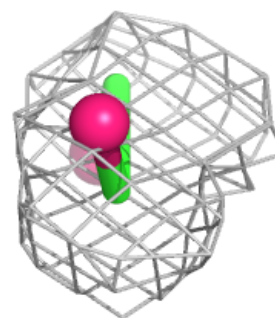
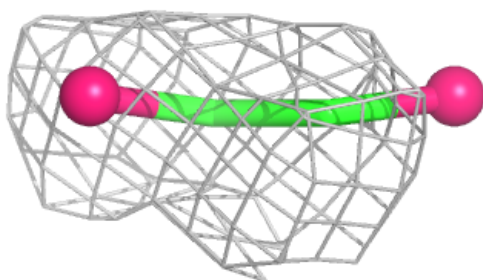
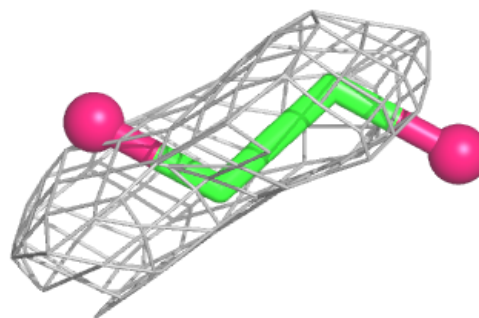
**Electron density around EDO C 425:**

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

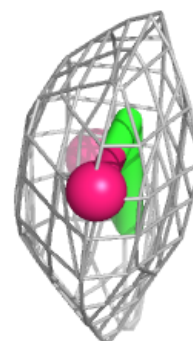
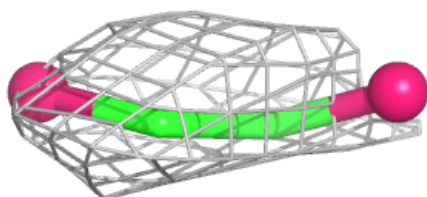
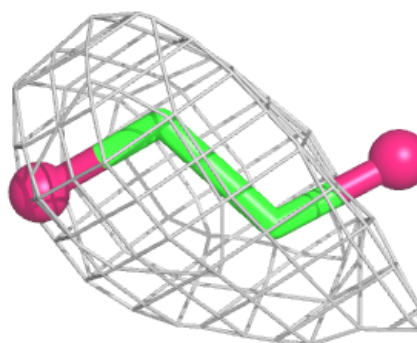


Electron density around EDO A 422:

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

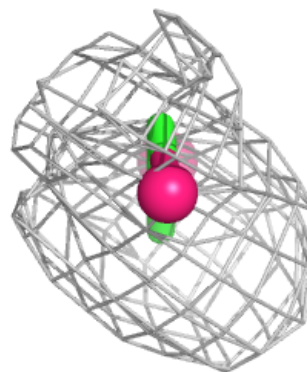
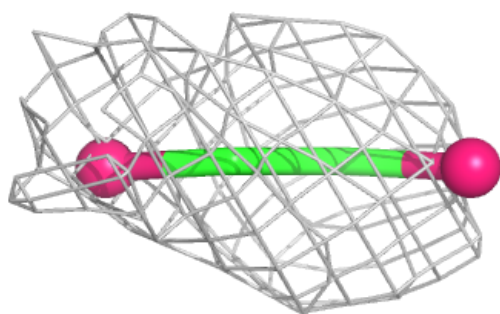
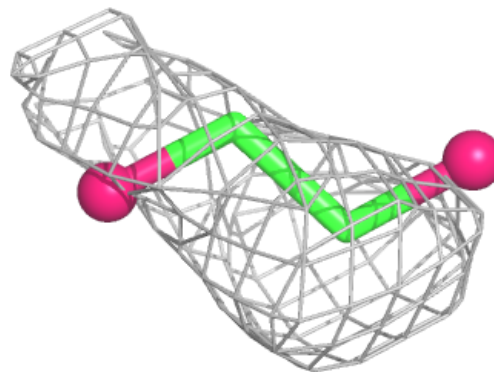
**Electron density around EDO C 428:**

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



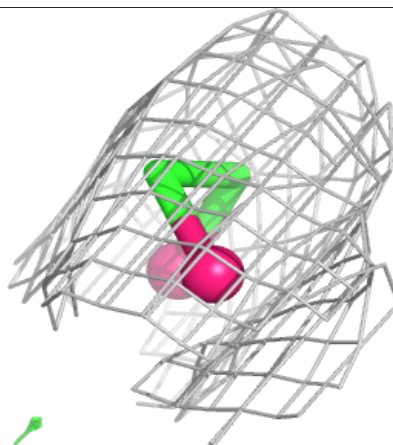
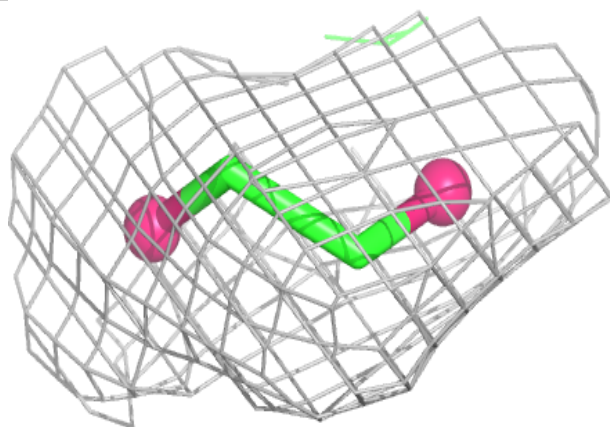
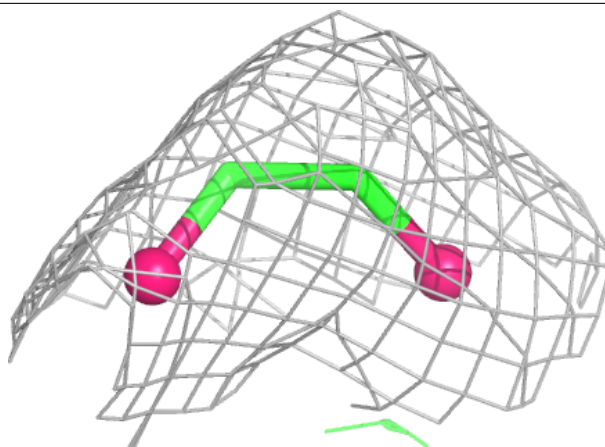
Electron density around EDO B 424:

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



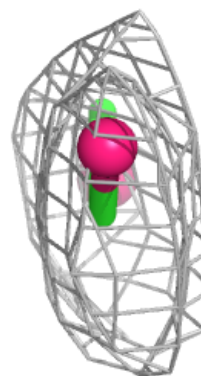
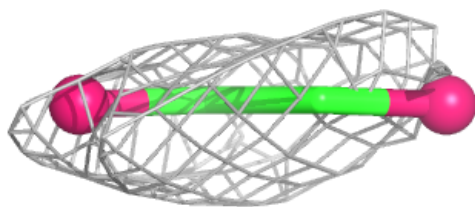
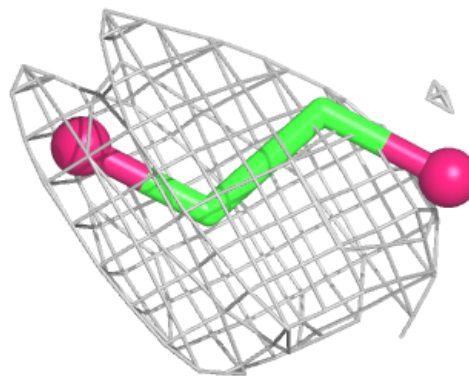
Electron density around EDO A 403:

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

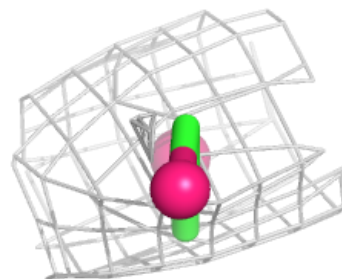
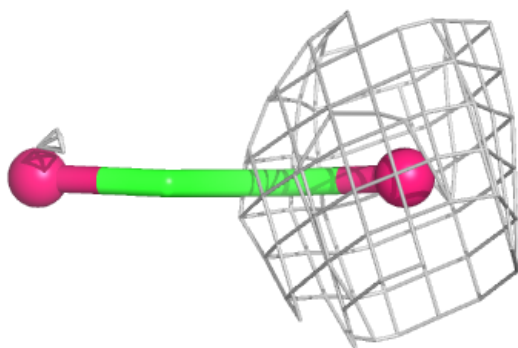
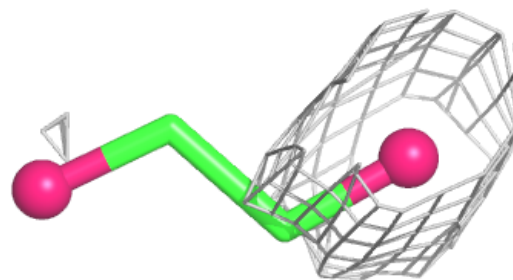


Electron density around EDO F 408:

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

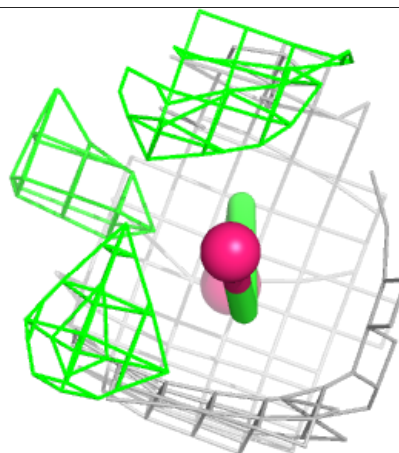
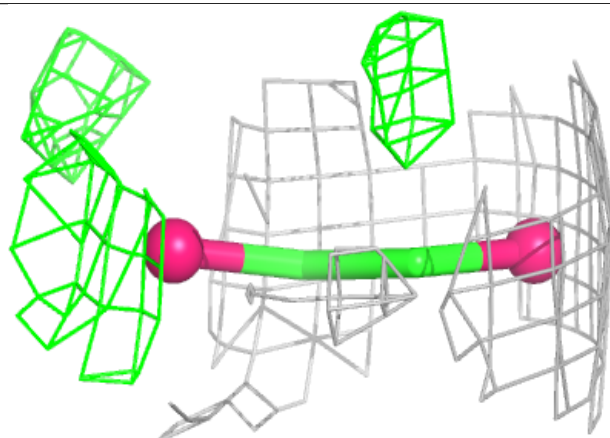
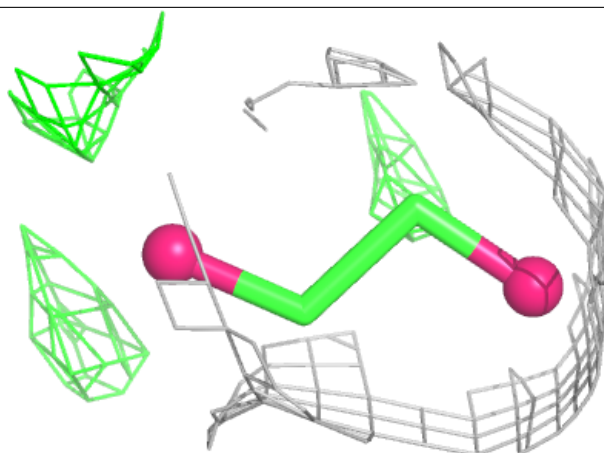
**Electron density around EDO F 409:**

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

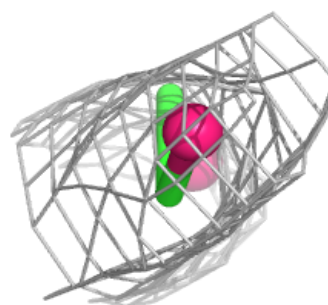
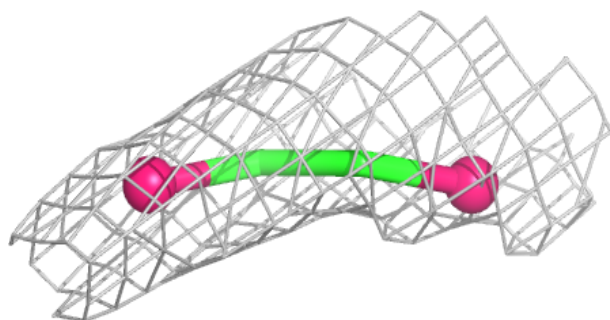
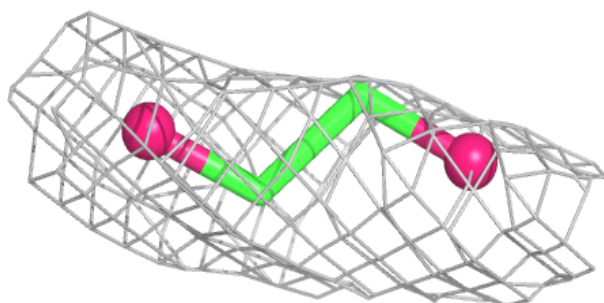


Electron density around EDO F 416:

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

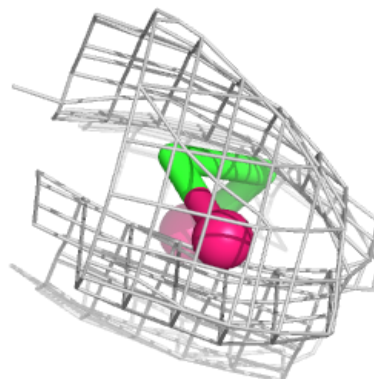
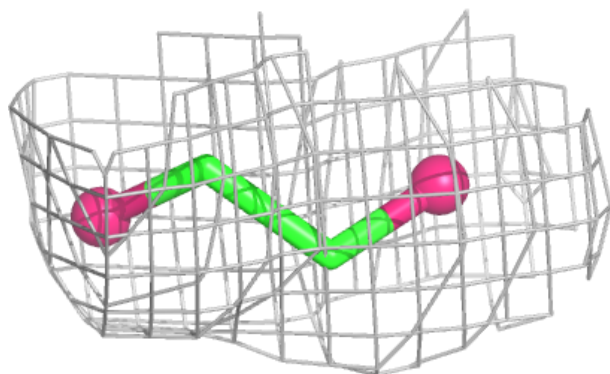
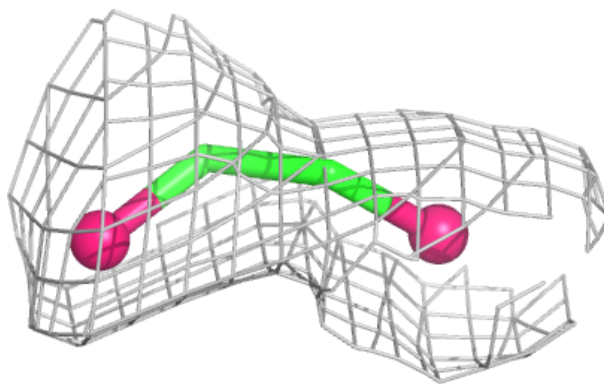
**Electron density around EDO C 434:**

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

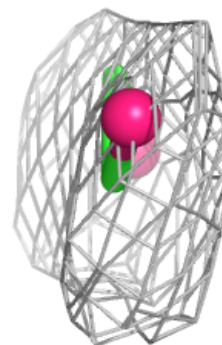
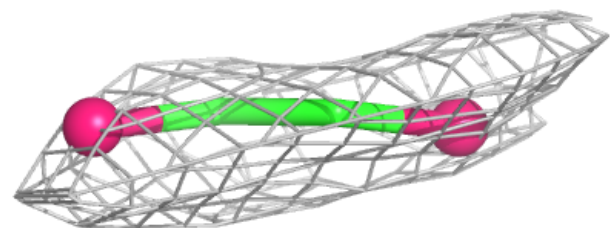
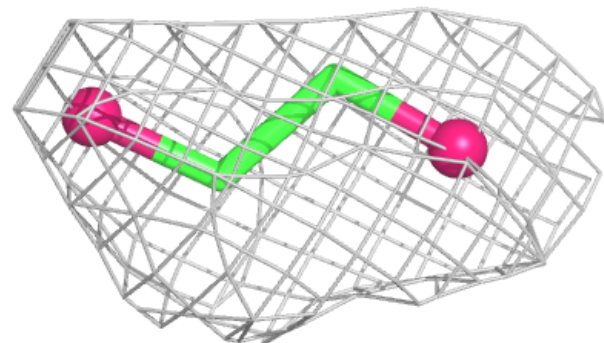


Electron density around EDO A 434:

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

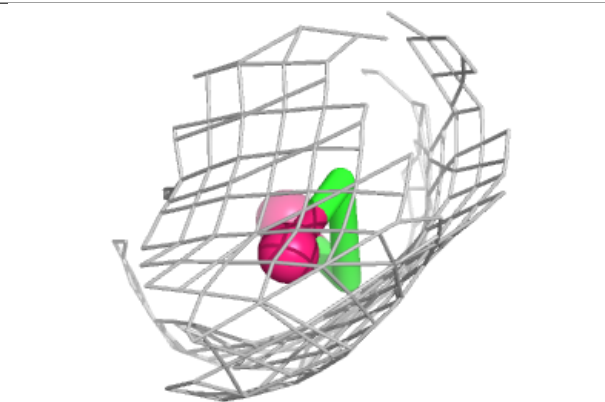
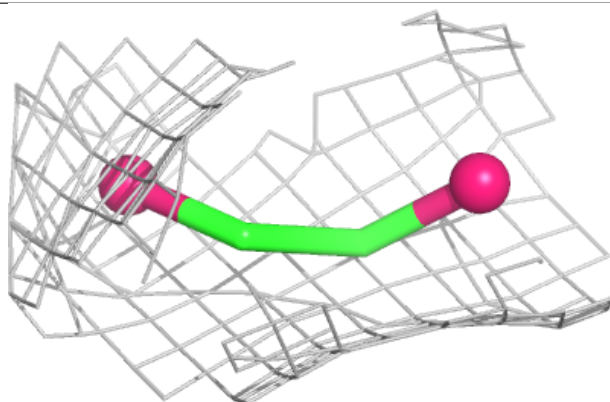
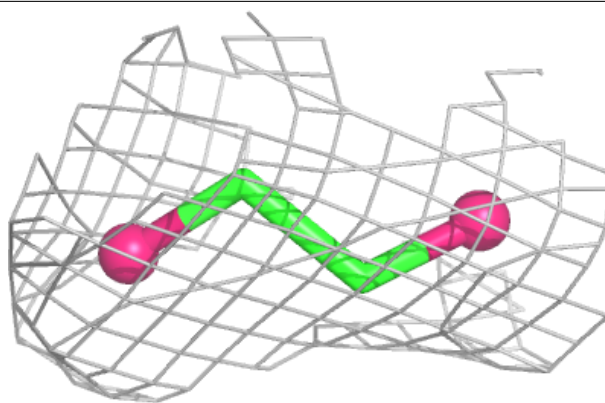
**Electron density around EDO C 438:**

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

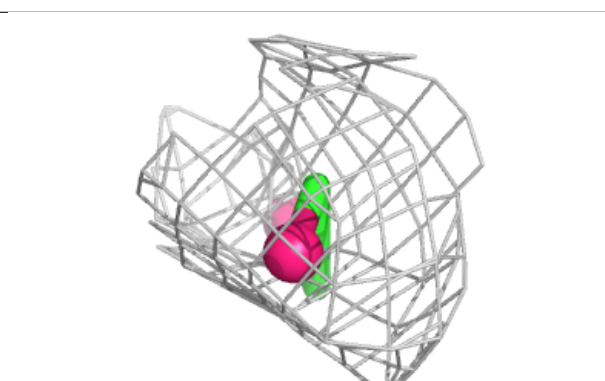
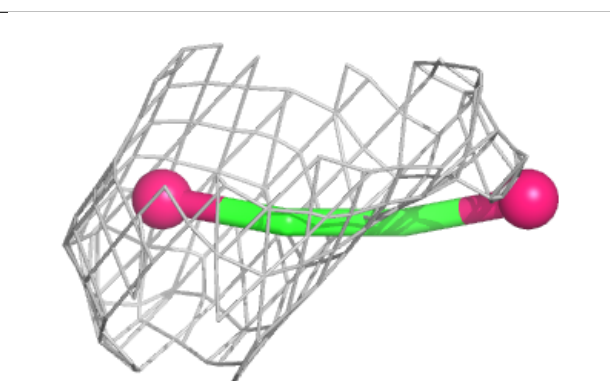
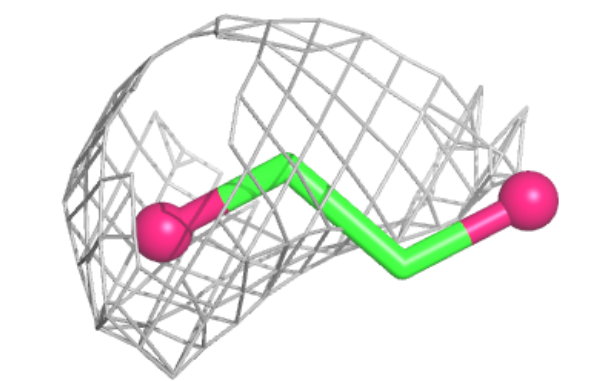


Electron density around EDO F 425:

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

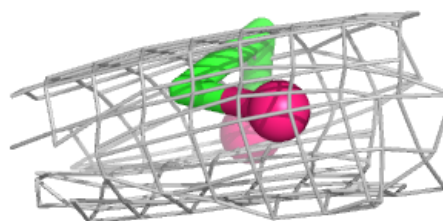
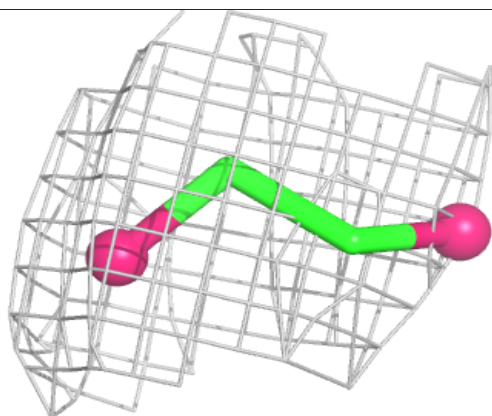
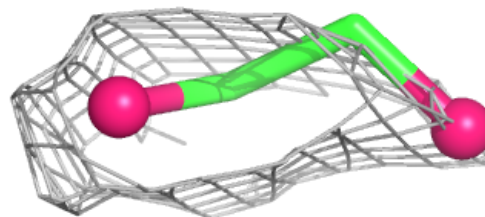
**Electron density around EDO F 427:**

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

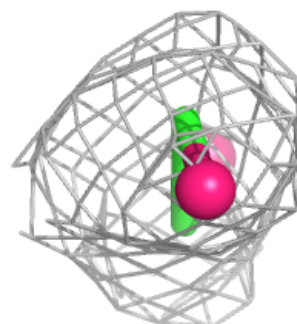
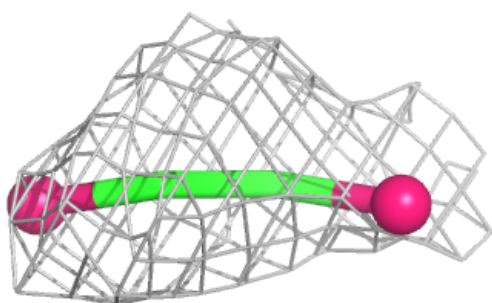
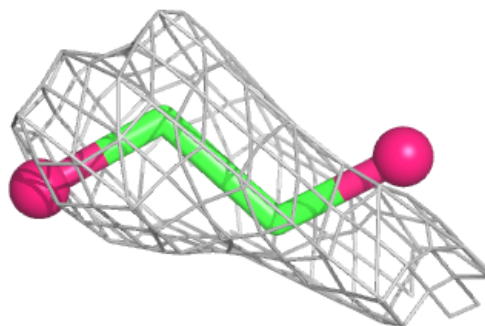


Electron density around EDO F 429:

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

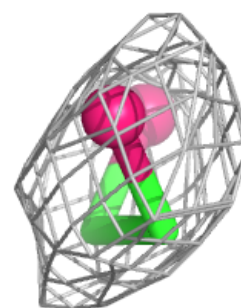
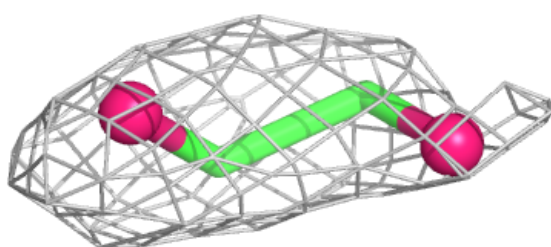
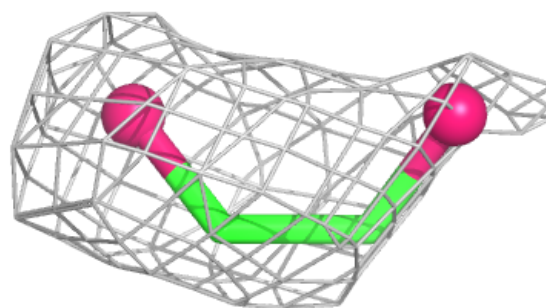
**Electron density around EDO F 430:**

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

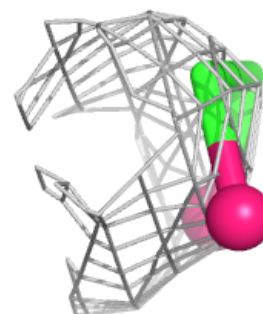
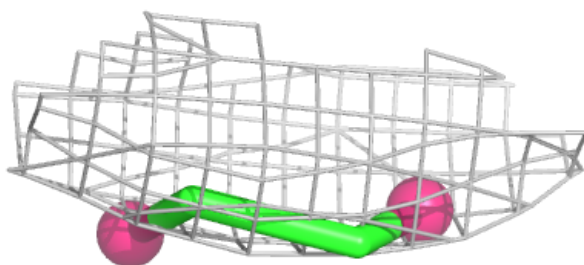
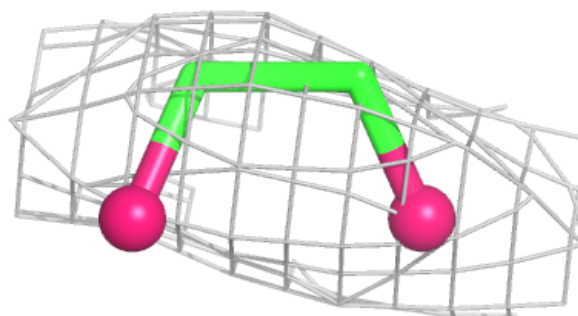


Electron density around EDO B 430:

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

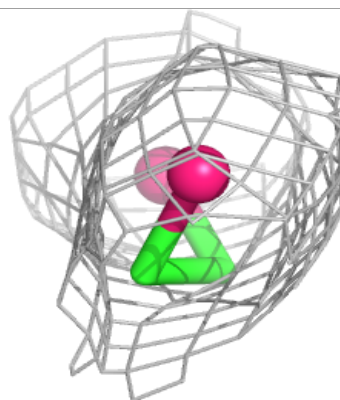
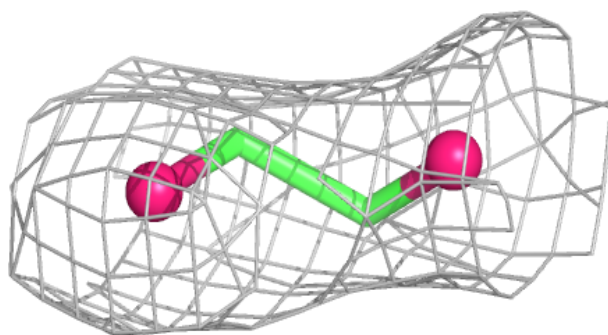
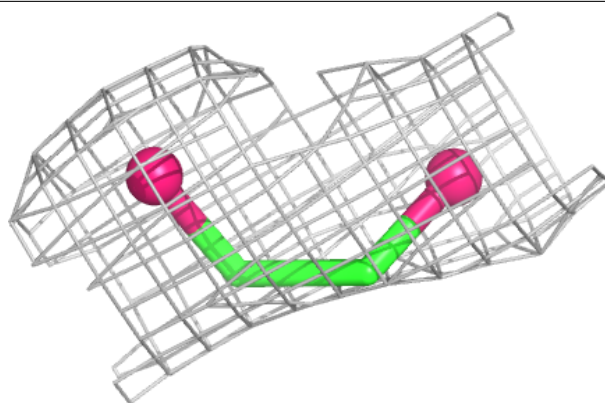
**Electron density around EDO A 436:**

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

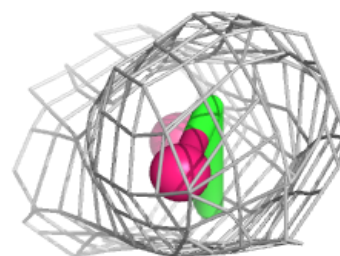
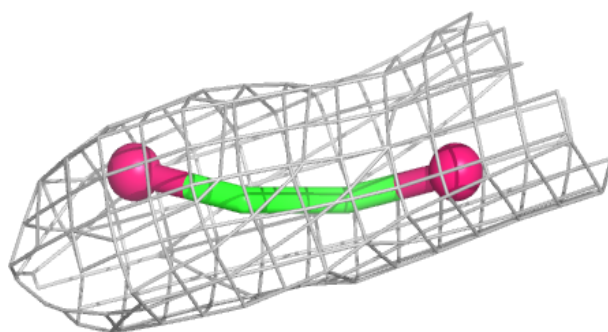
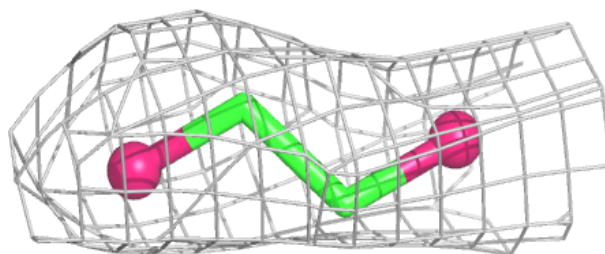


Electron density around EDO F 439:

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

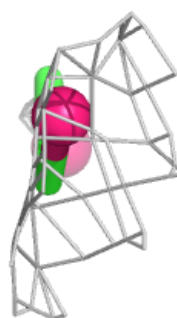
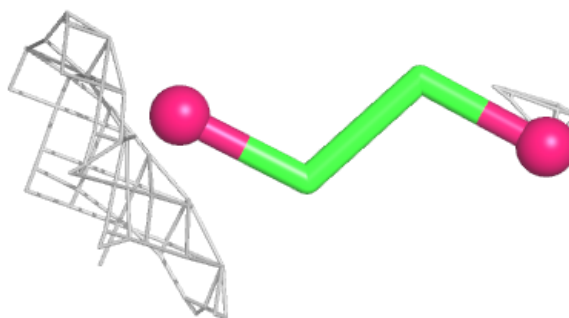
**Electron density around EDO A 438:**

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



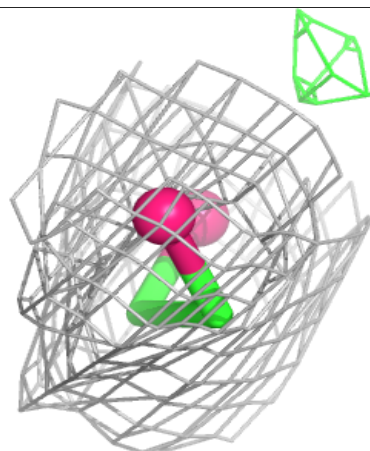
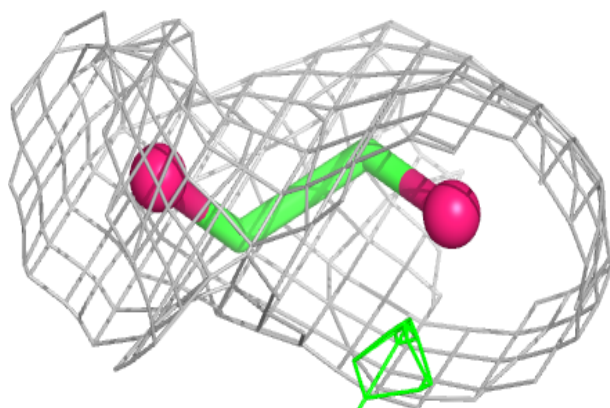
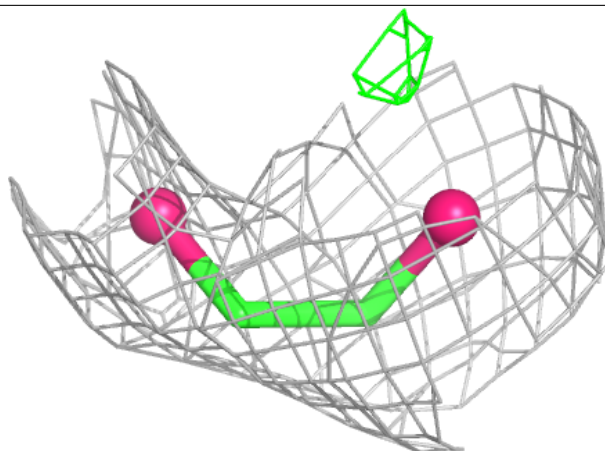
Electron density around EDO F 441:

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

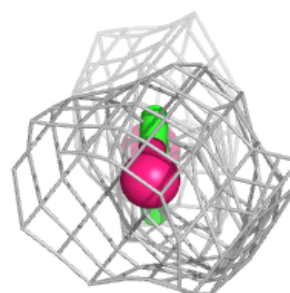
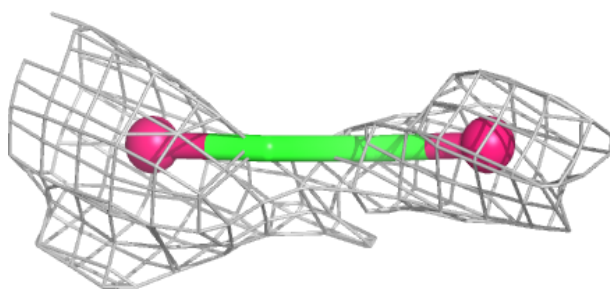
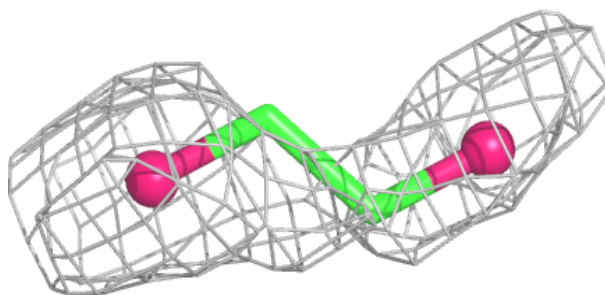


Electron density around EDO D 406:

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

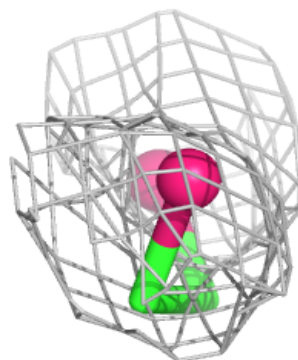
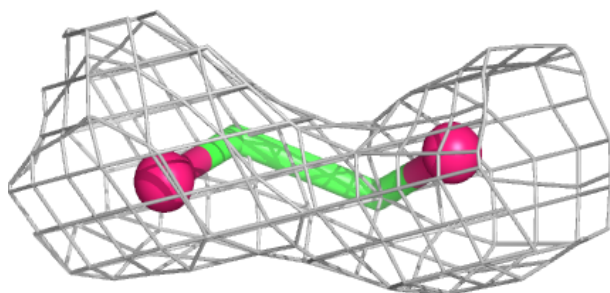
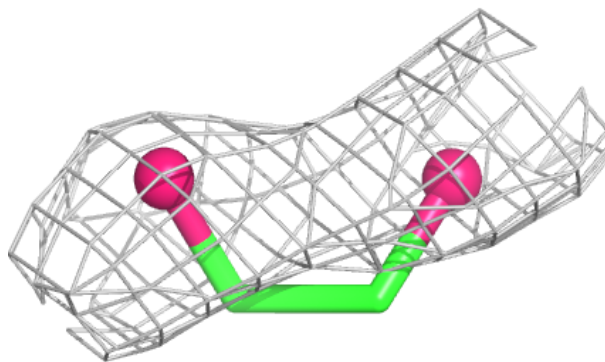
**Electron density around EDO D 407:**

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

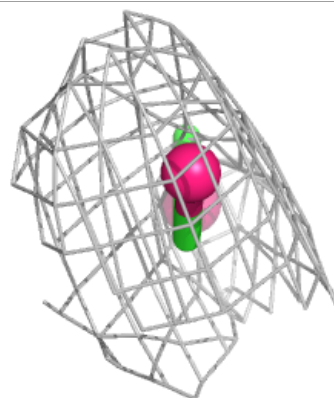
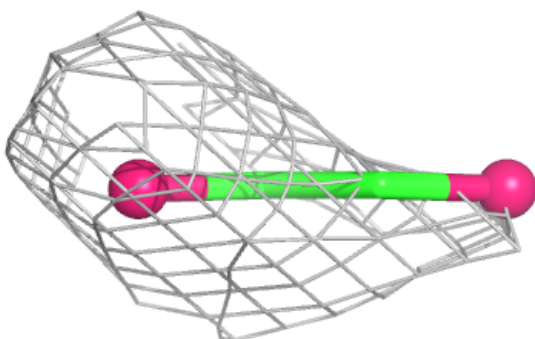
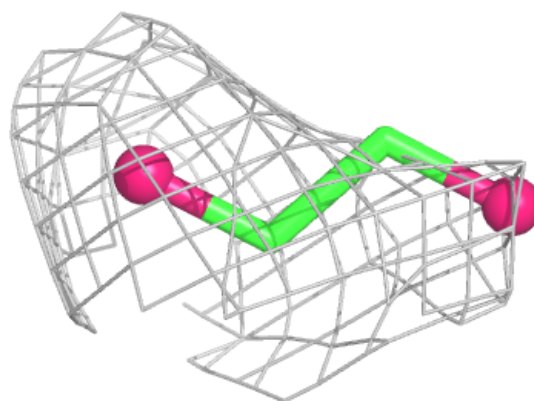


Electron density around EDO A 439:

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

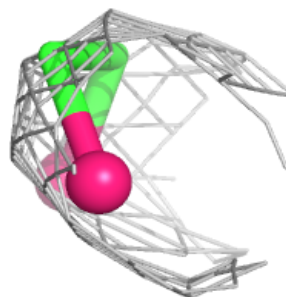
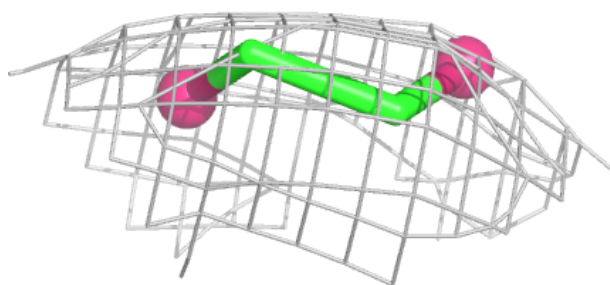
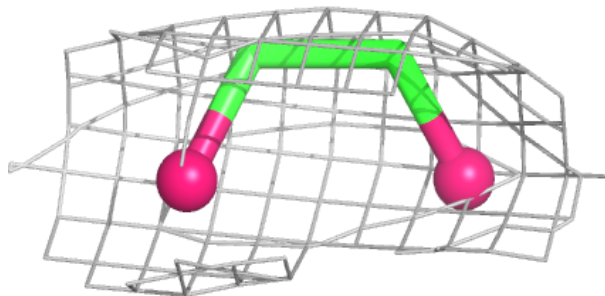
**Electron density around EDO D 422:**

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

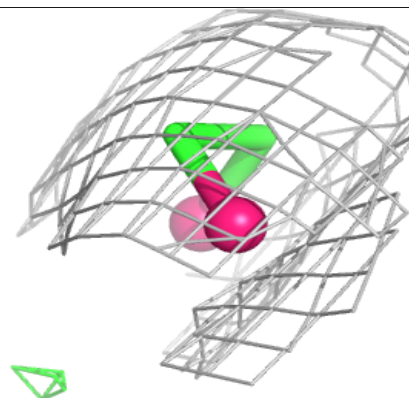
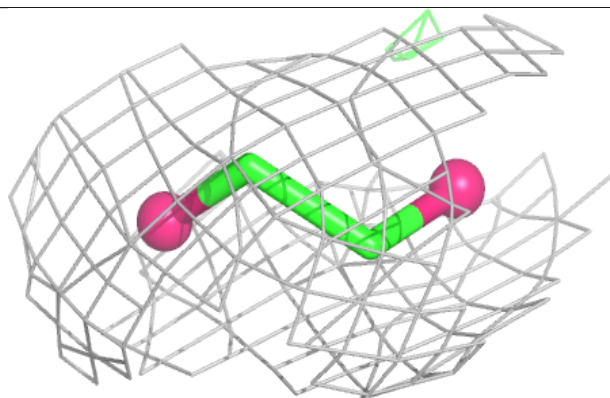
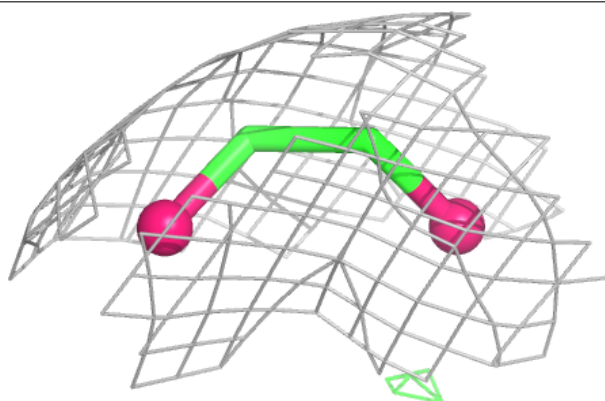


Electron density around EDO D 434:

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

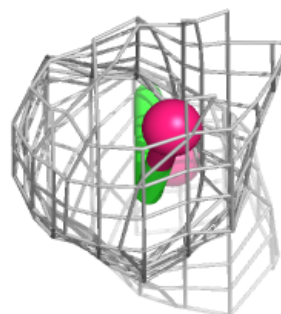
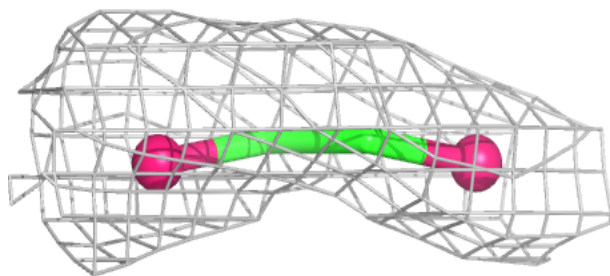
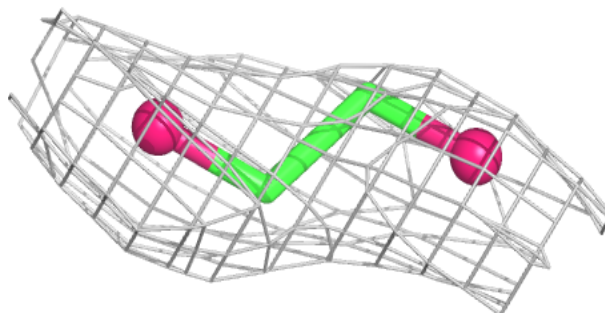
**Electron density around EDO B 405:**

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

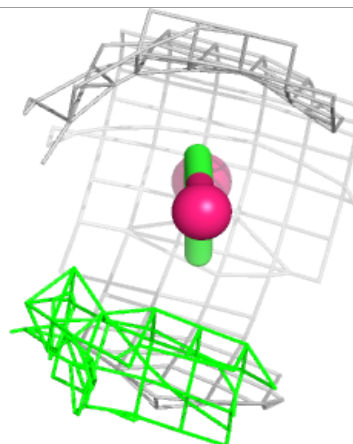
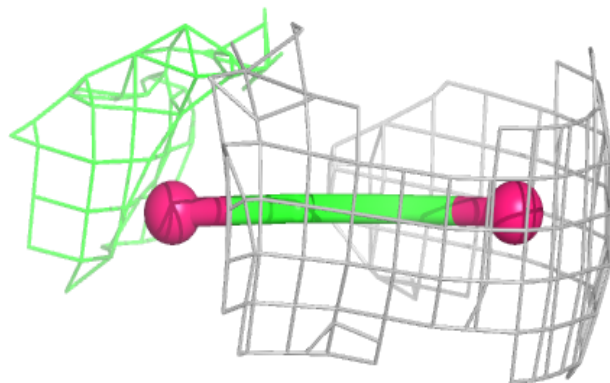
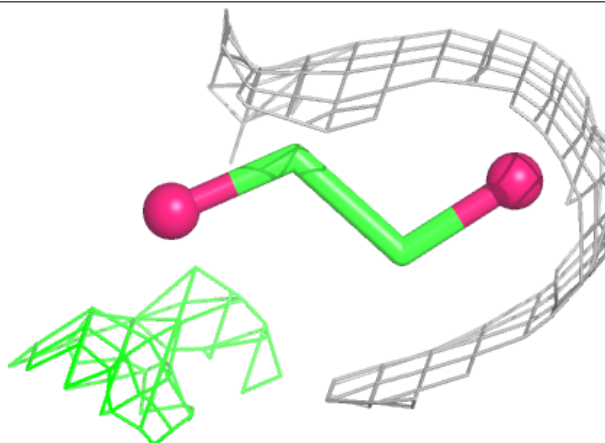


Electron density around EDO C 406:

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

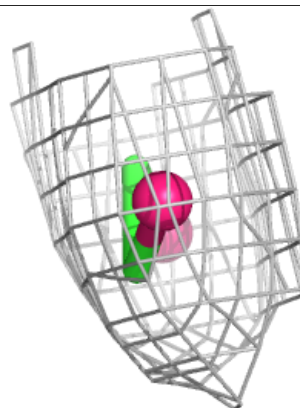
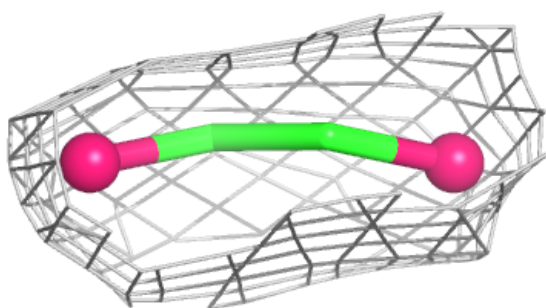
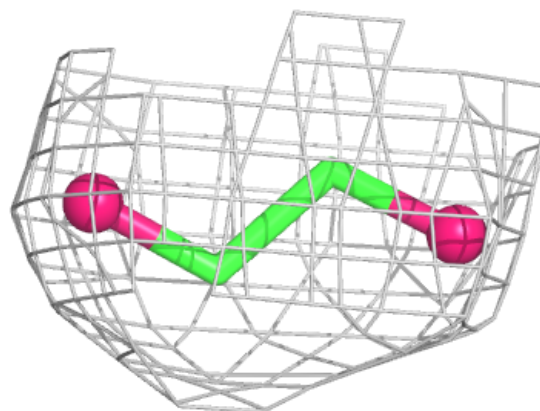
**Electron density around EDO C 410:**

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

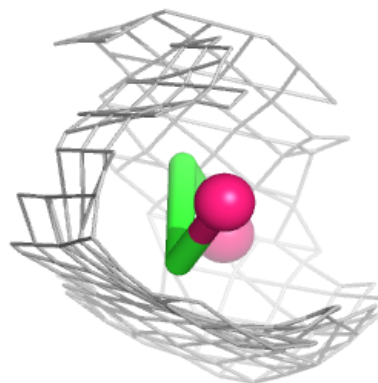
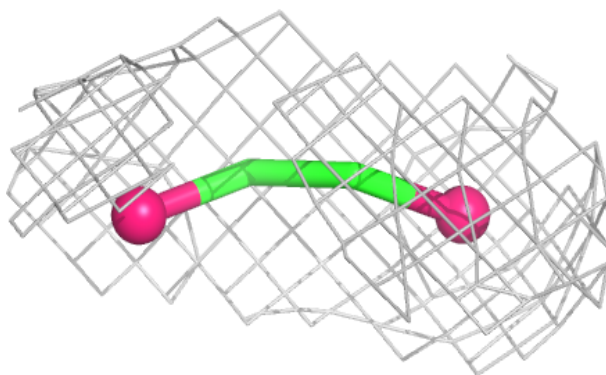
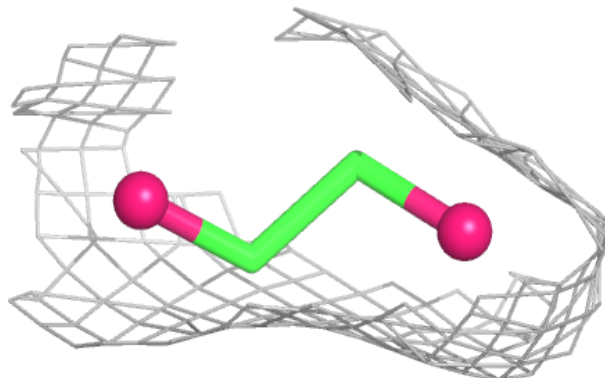


Electron density around EDO E 401:

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

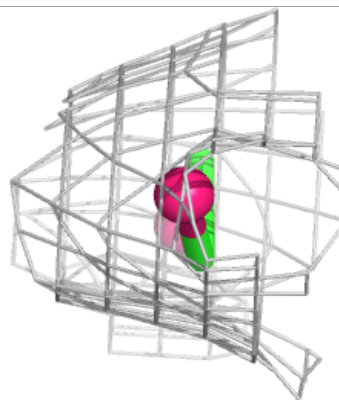
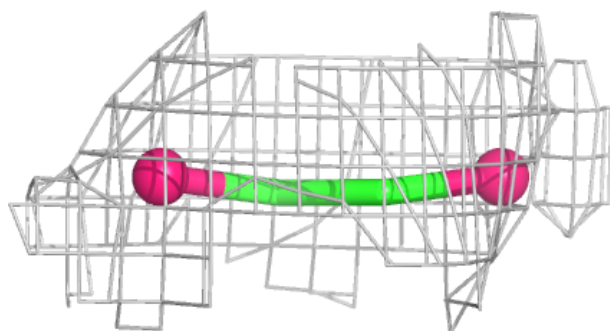
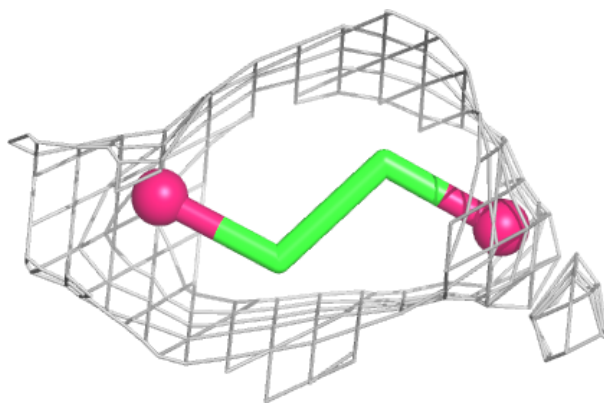
**Electron density around EDO E 402:**

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

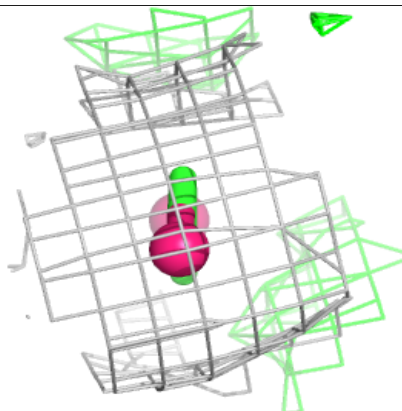
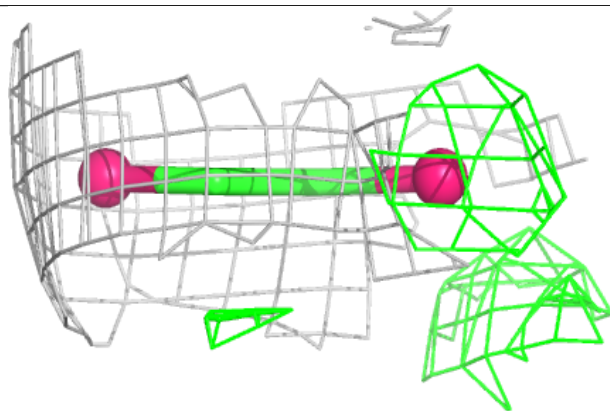
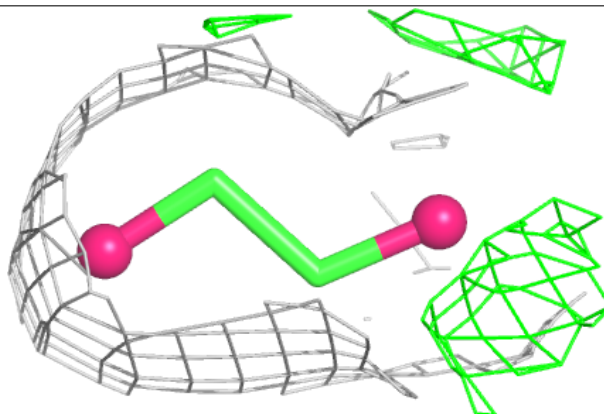


Electron density around EDO C 414:

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

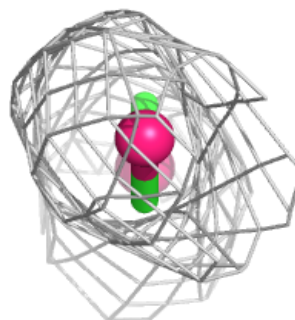
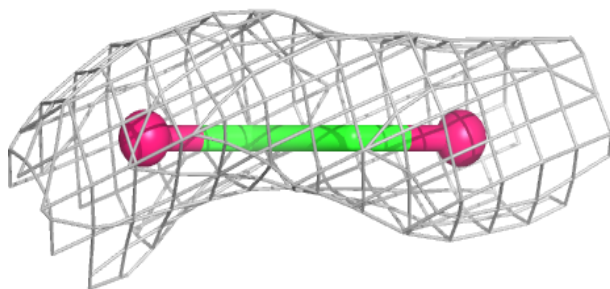
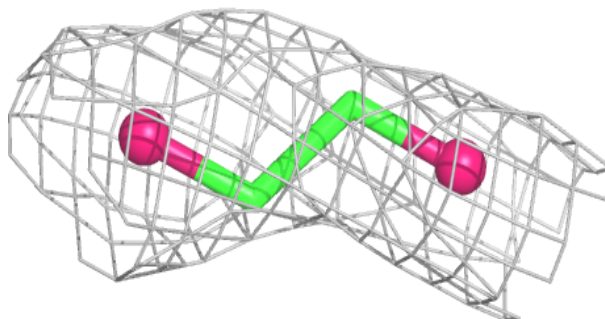
**Electron density around EDO B 410:**

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

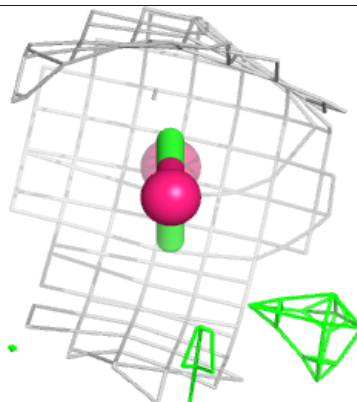
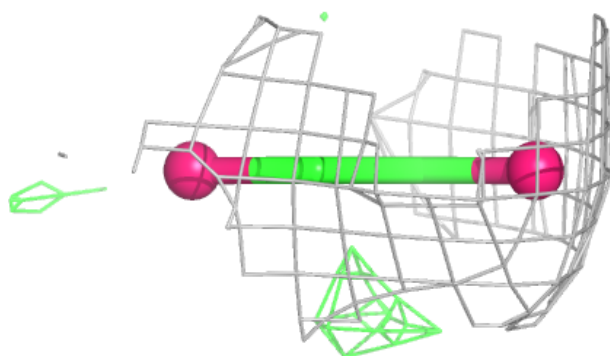
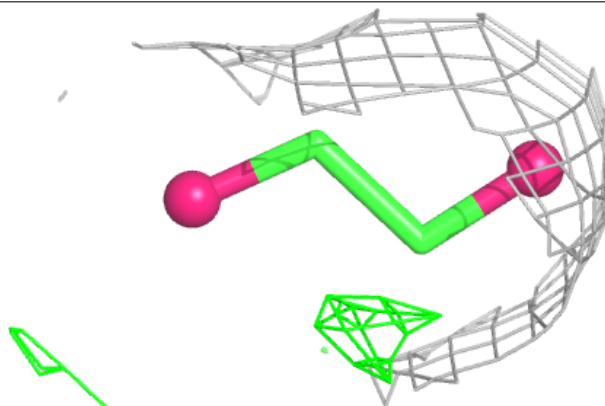


Electron density around EDO E 406:

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

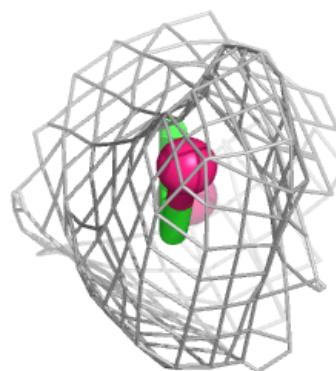
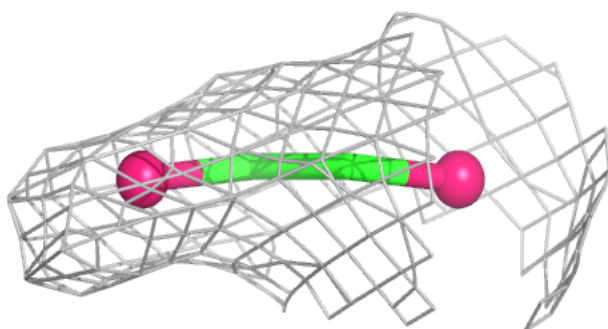
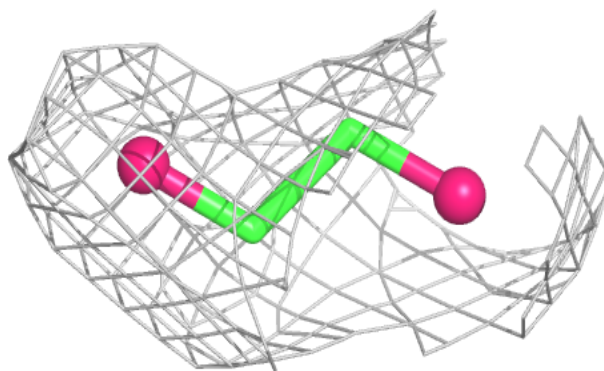
**Electron density around EDO E 410:**

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

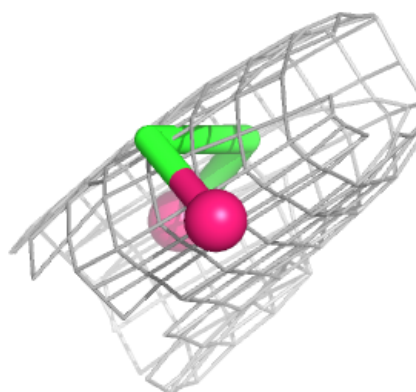
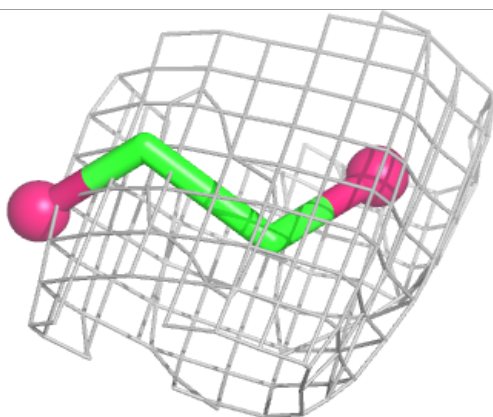
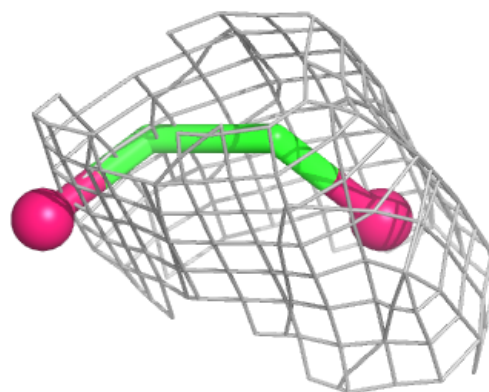


Electron density around EDO B 412:

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

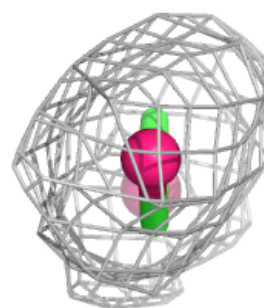
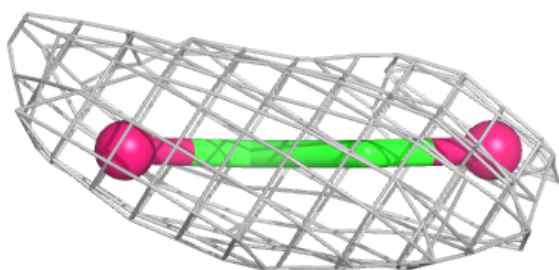
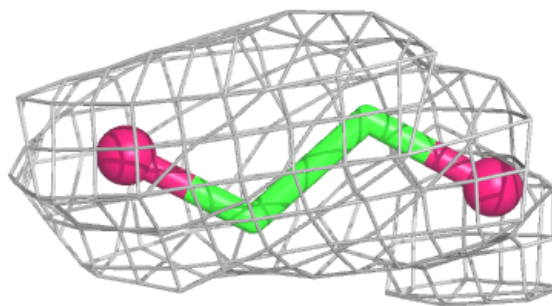
**Electron density around EDO C 422:**

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

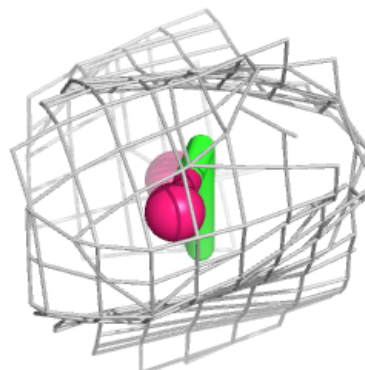
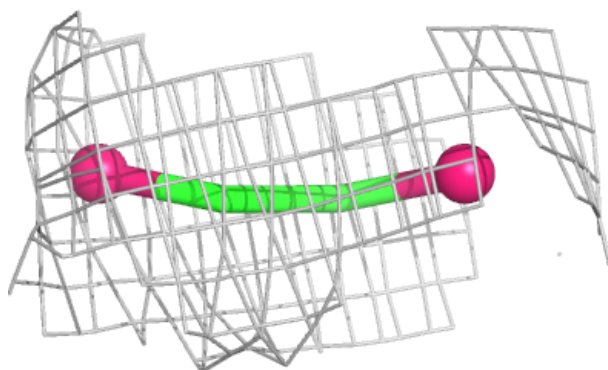
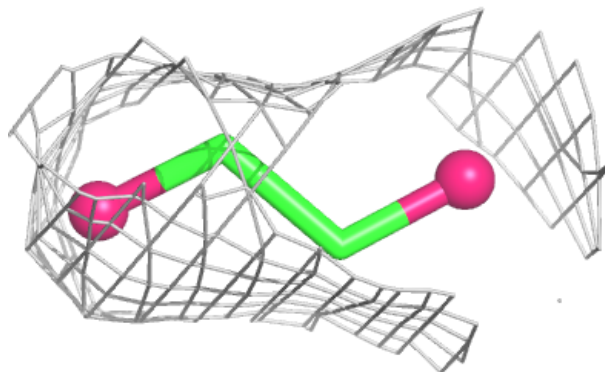


Electron density around EDO A 429:

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

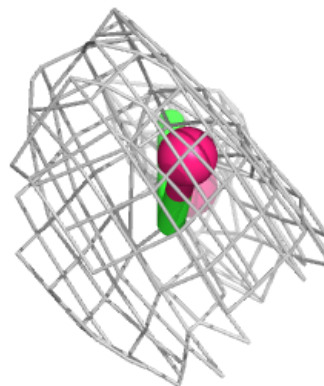
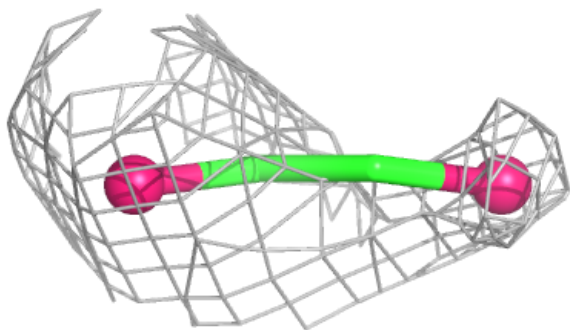
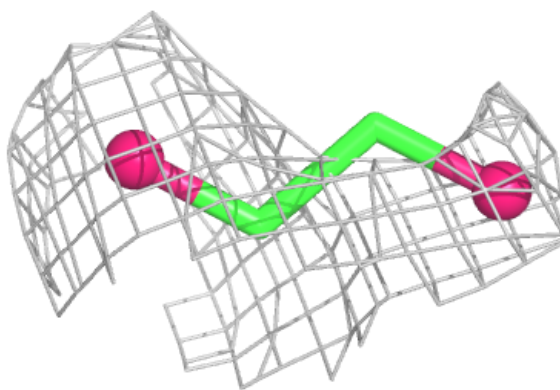
**Electron density around EDO B 417:**

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

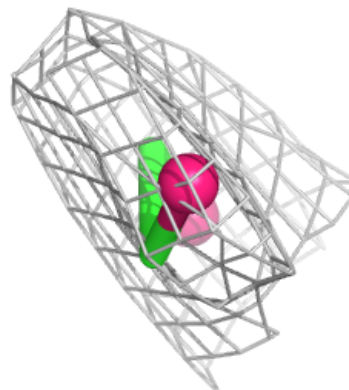
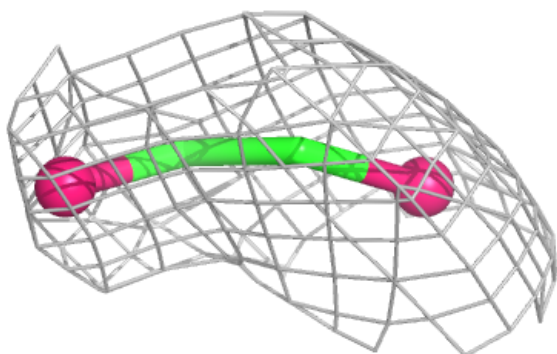
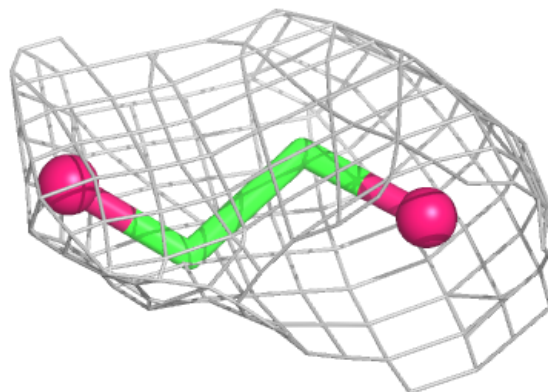


Electron density around EDO E 423:

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

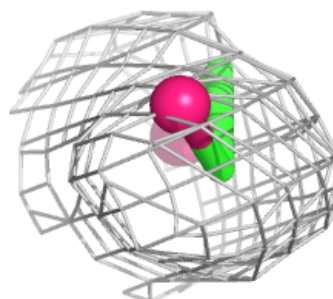
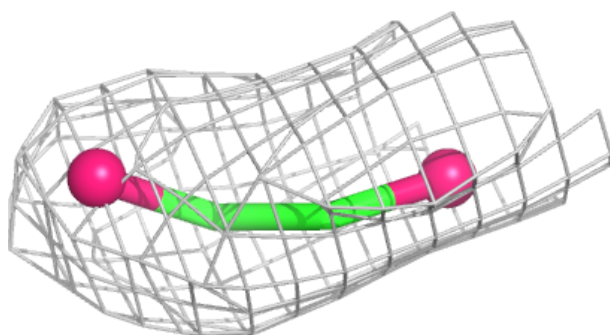
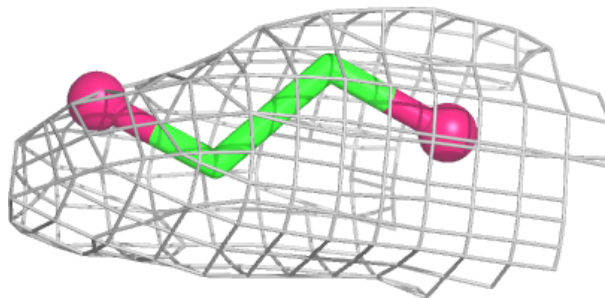
**Electron density around EDO E 425:**

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

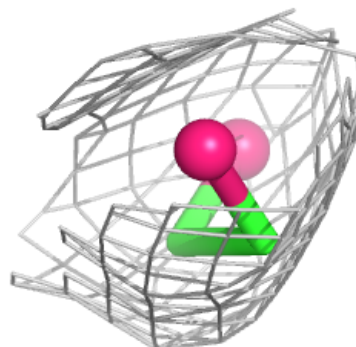
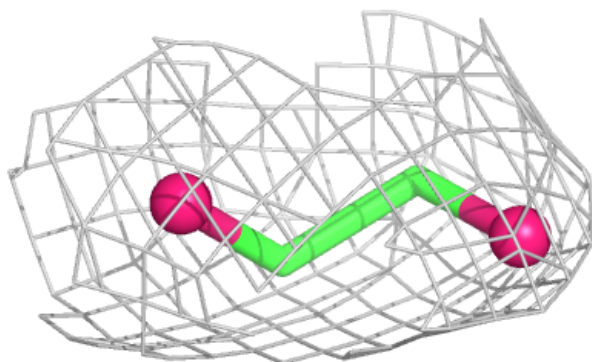
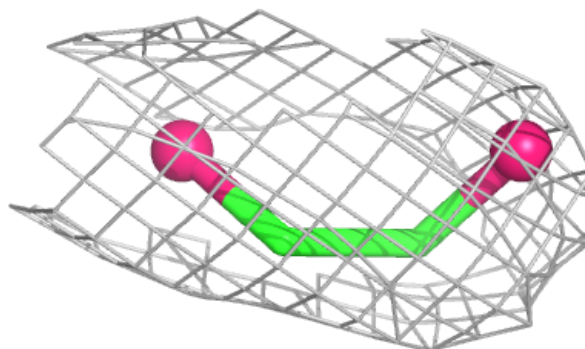


Electron density around EDO B 418:

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

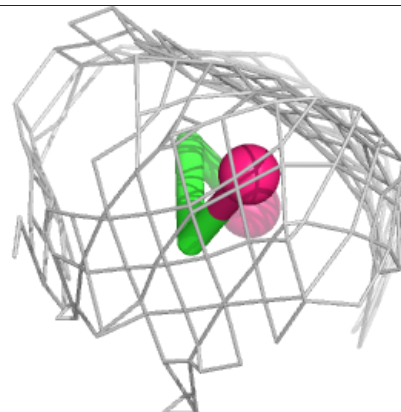
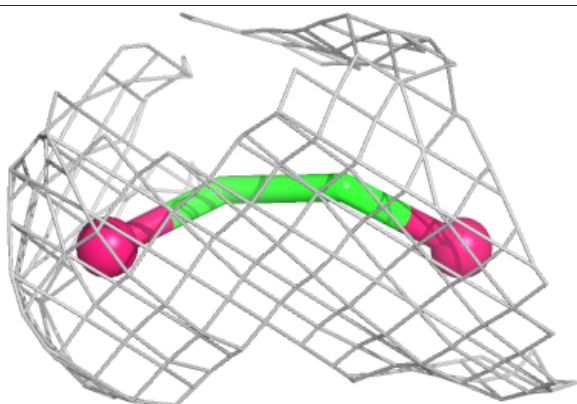
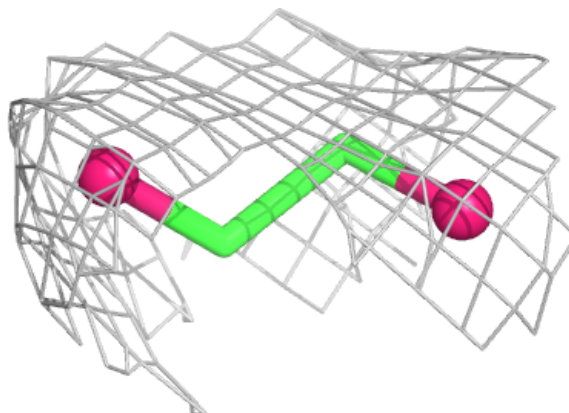
**Electron density around EDO E 427:**

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

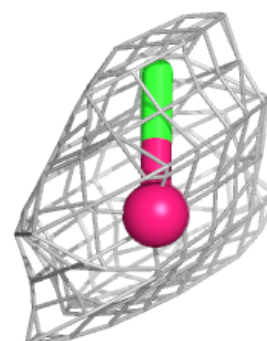
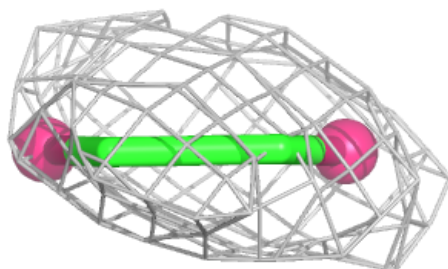
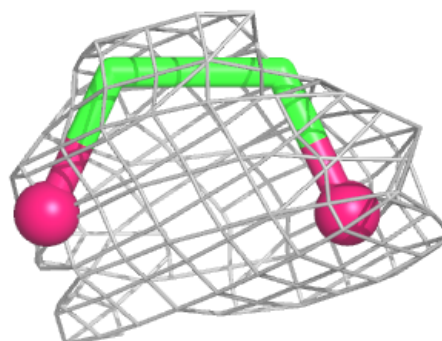


Electron density around EDO B 419:

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

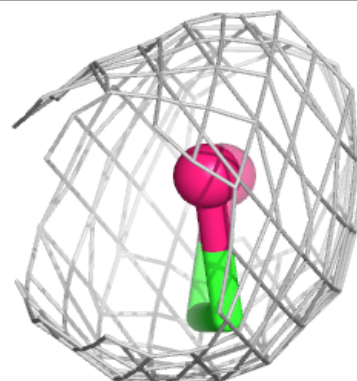
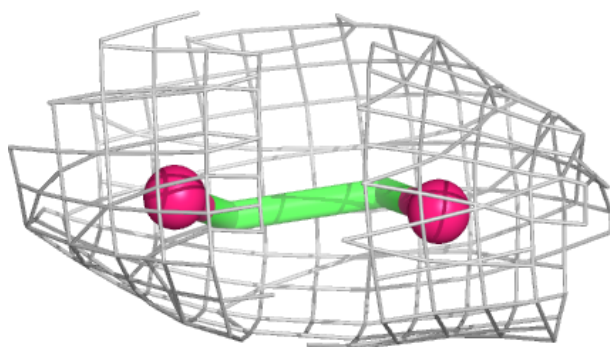
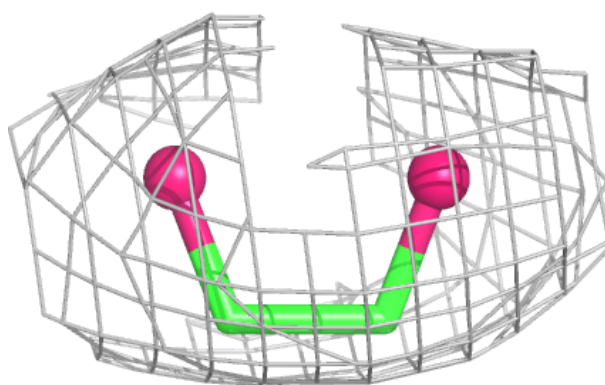
**Electron density around EDO C 429:**

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

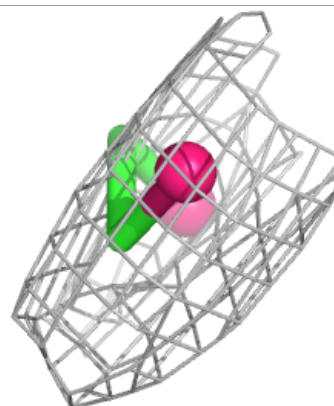
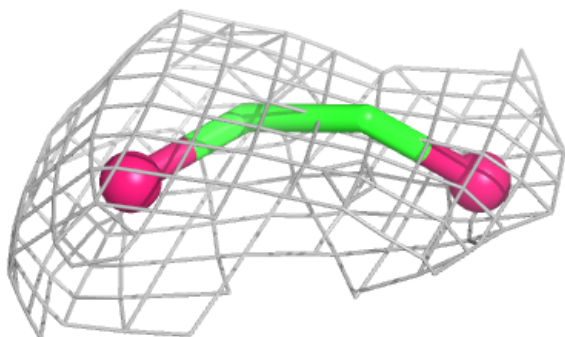
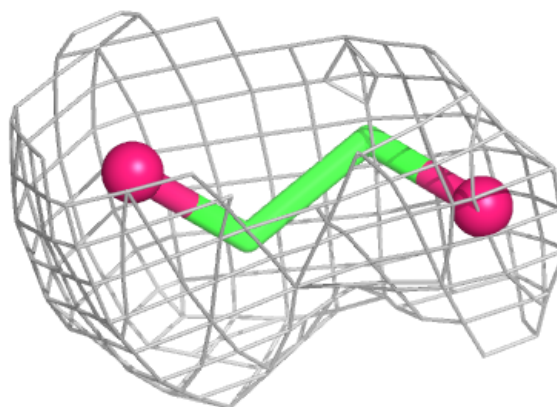


Electron density around EDO C 431:

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

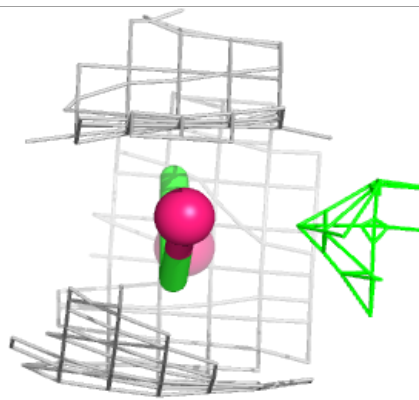
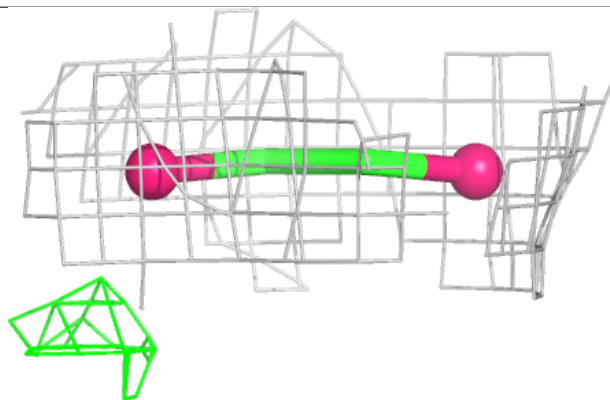
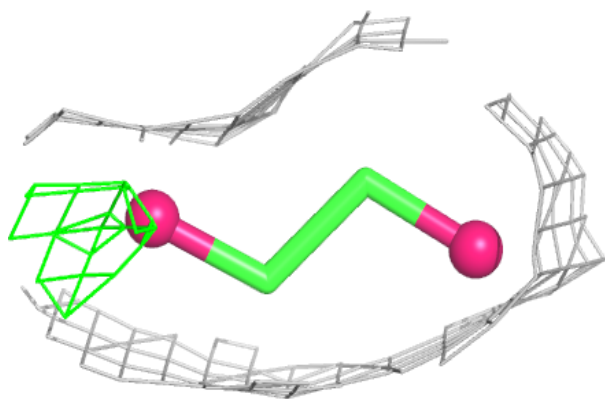
**Electron density around EDO B 423:**

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

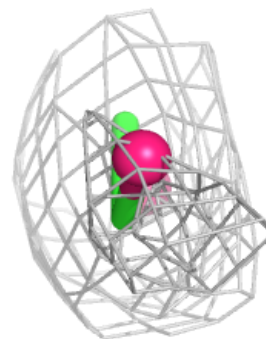
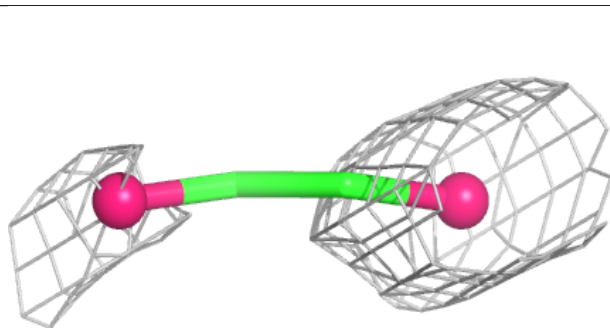
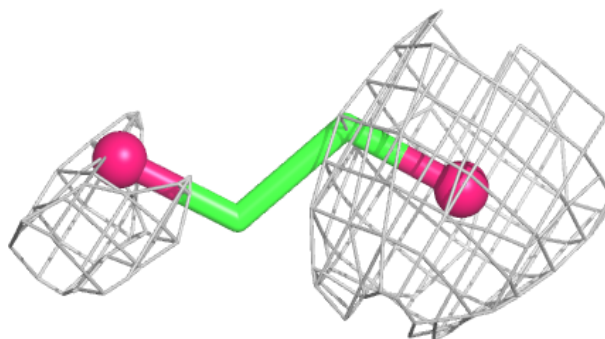


Electron density around EDO A 407:

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

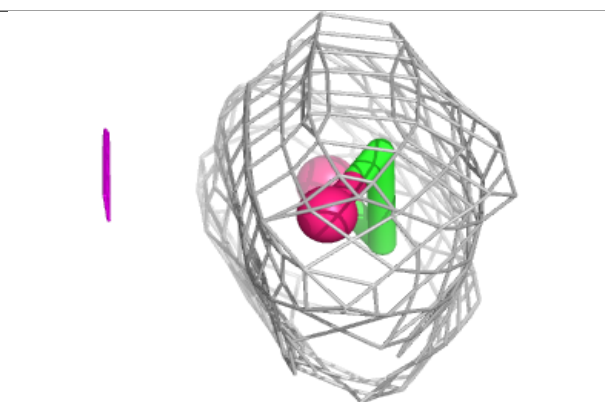
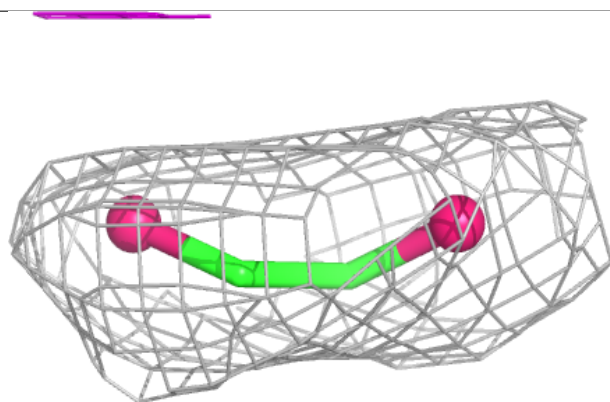
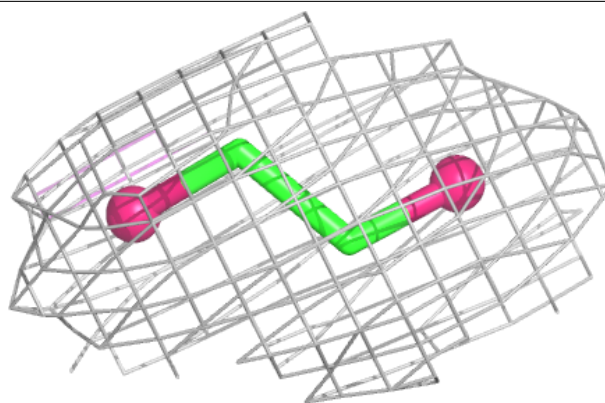
**Electron density around EDO A 432:**

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

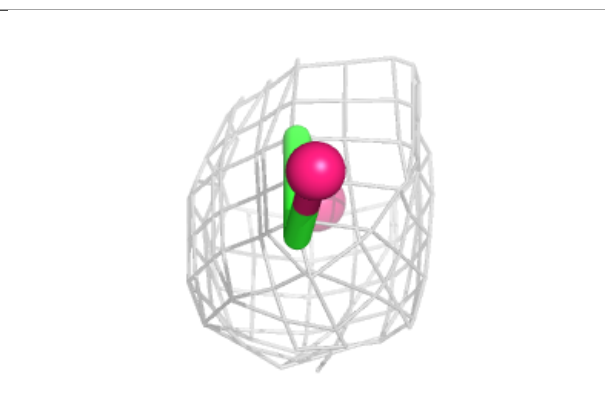
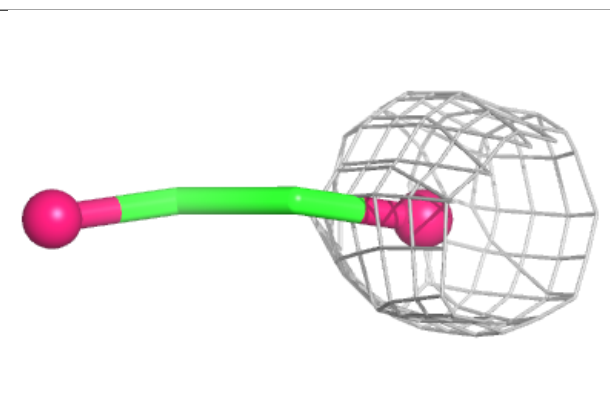
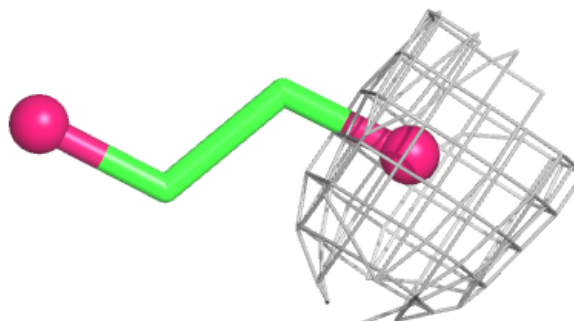


Electron density around EDO E 437:

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

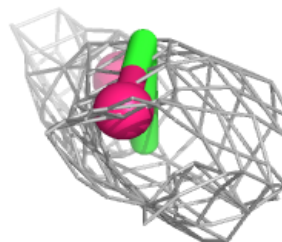
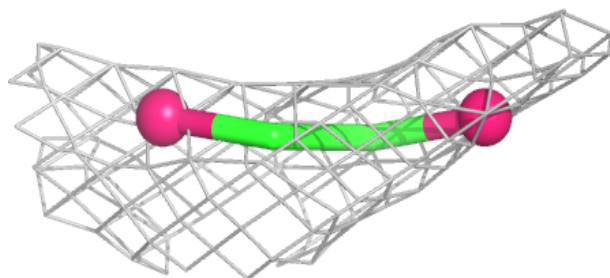
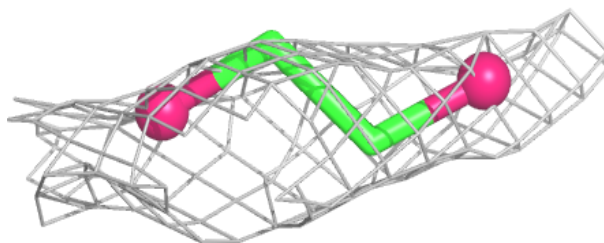
**Electron density around EDO E 438:**

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

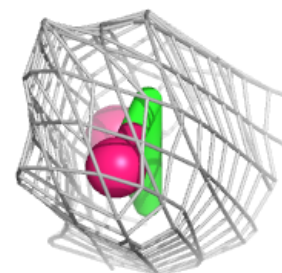
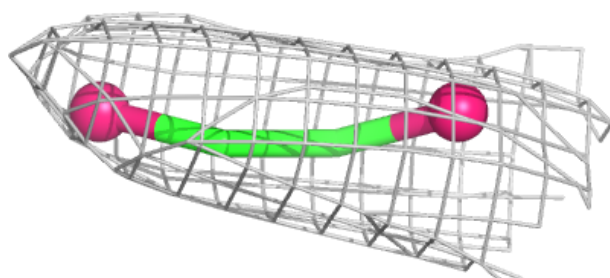
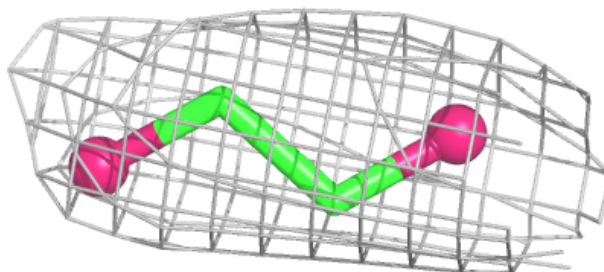


Electron density around EDO E 439:

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

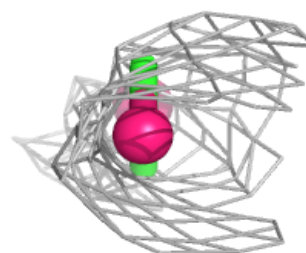
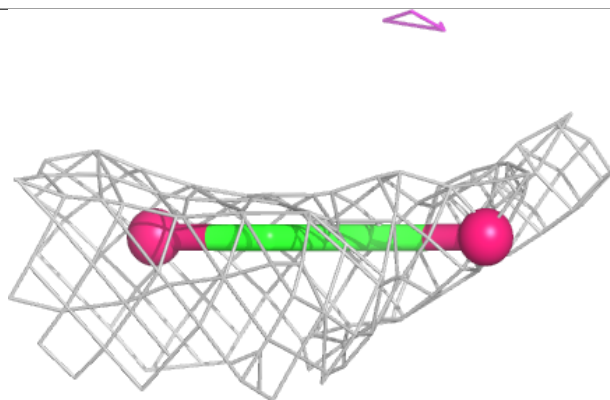
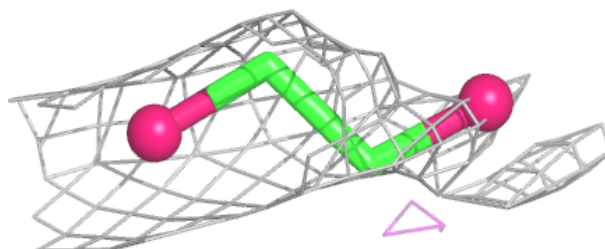
**Electron density around EDO C 435:**

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

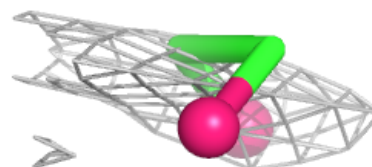
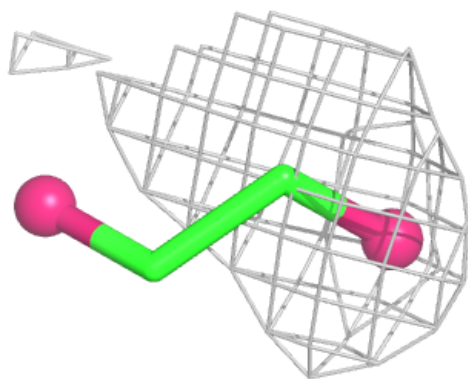
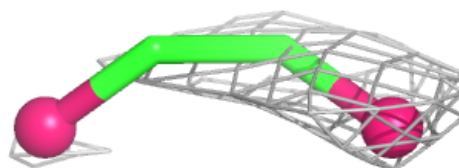


Electron density around EDO A 433:

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

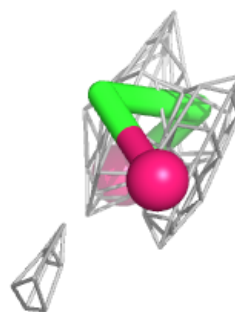
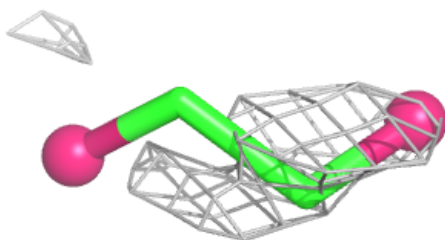
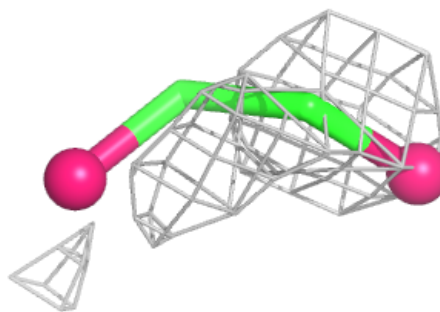
**Electron density around EDO C 437:**

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



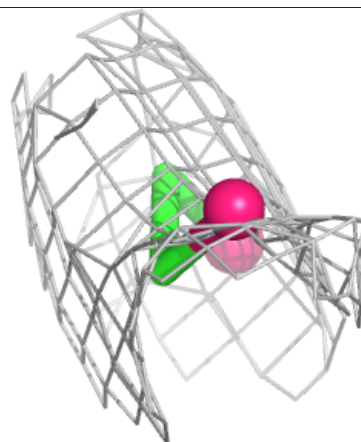
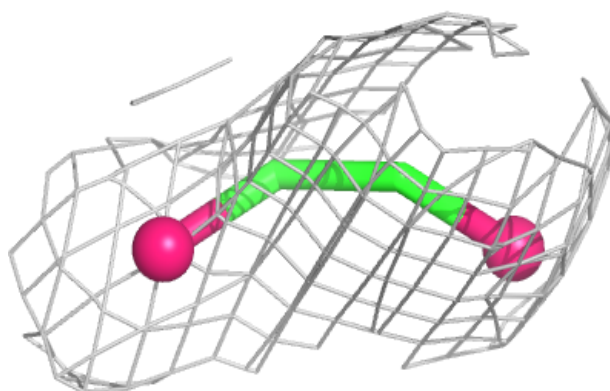
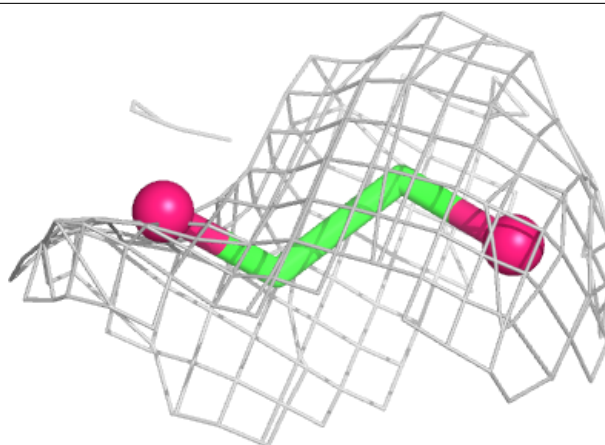
Electron density around EDO B 429:

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

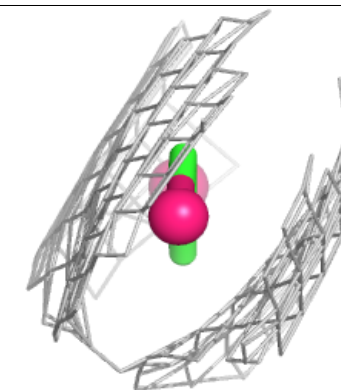
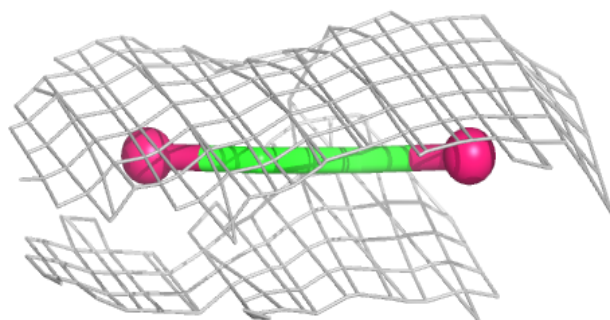
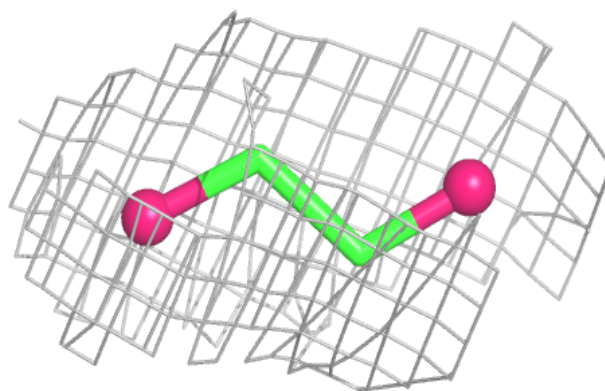


Electron density around EDO E 447:

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

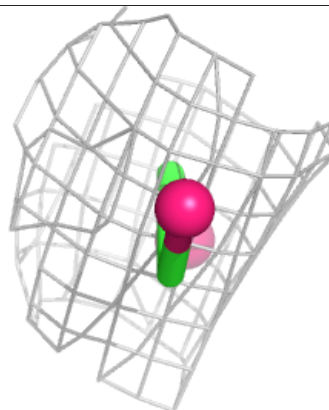
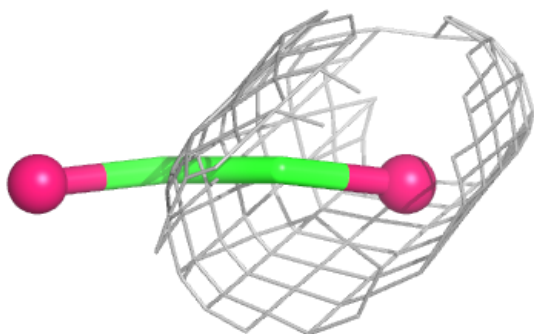
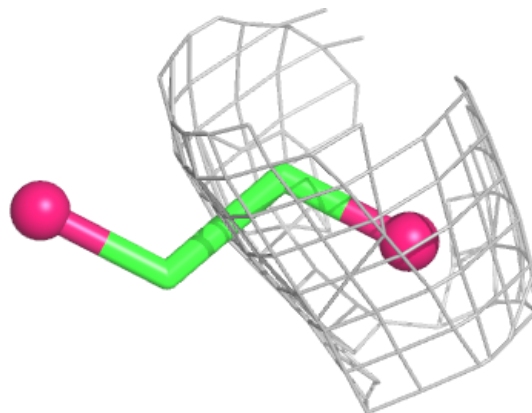
**Electron density around EDO D 401:**

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

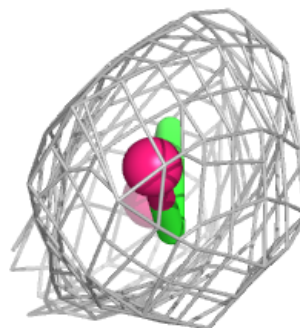
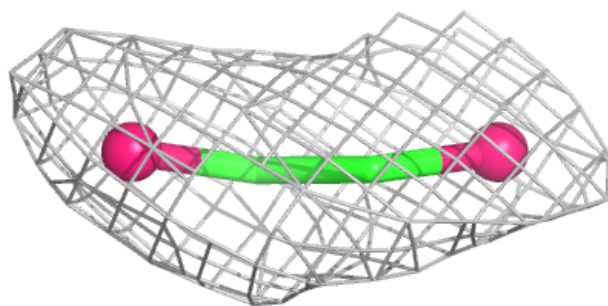
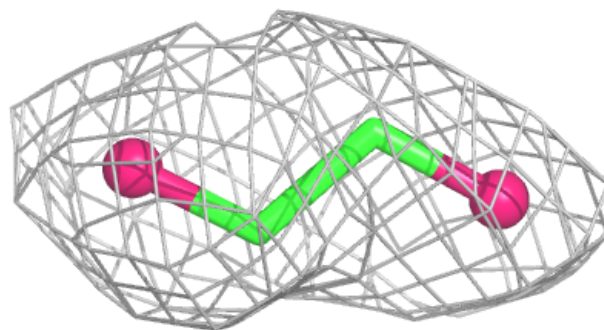


Electron density around EDO A 419:

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

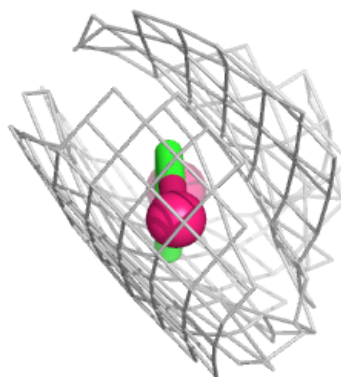
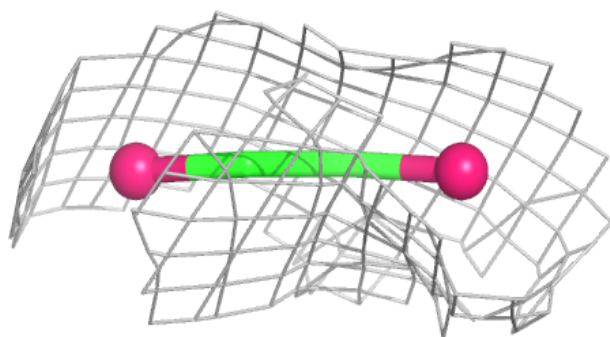
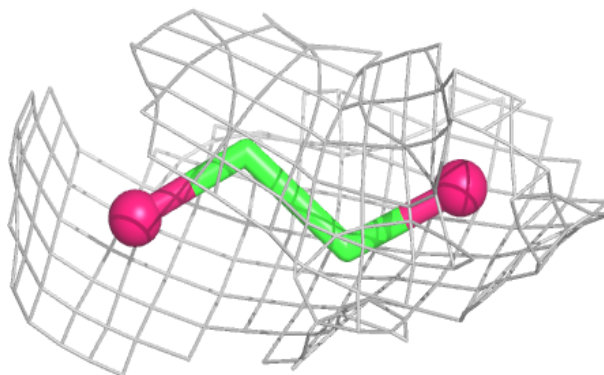
**Electron density around EDO B 431:**

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

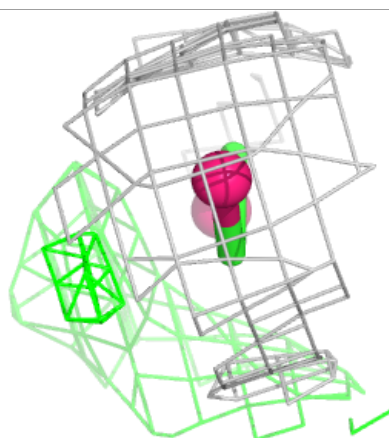
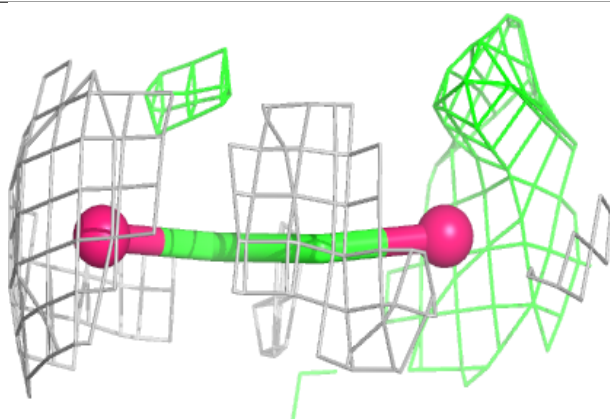
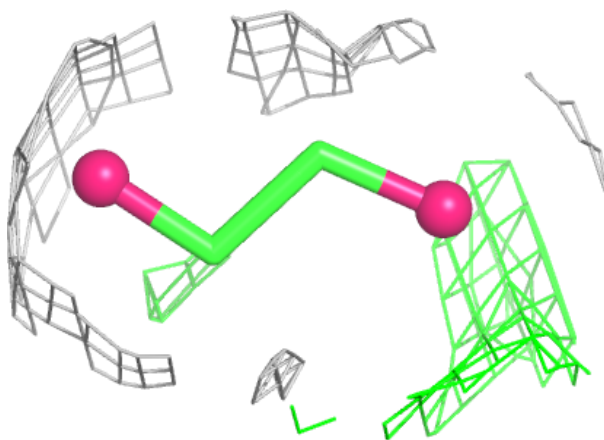


Electron density around EDO F 407:

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

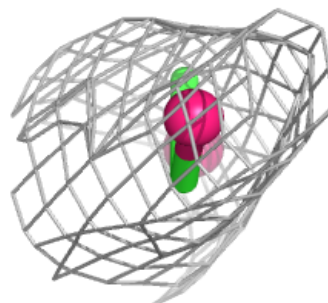
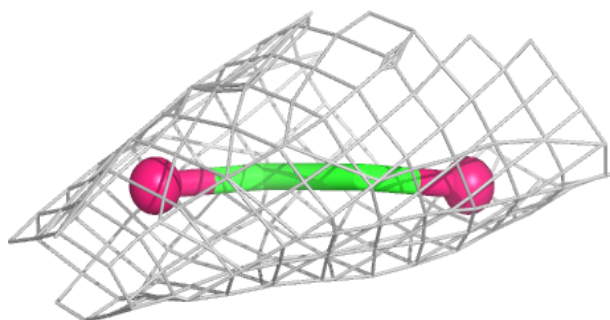
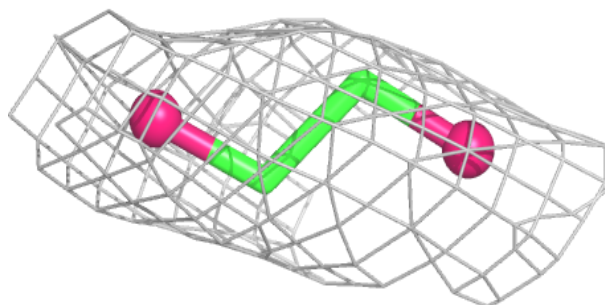
**Electron density around EDO A 408:**

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



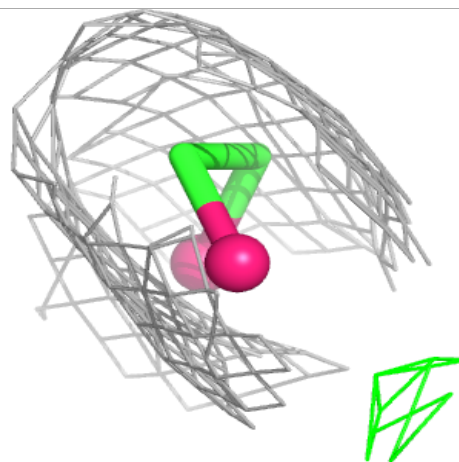
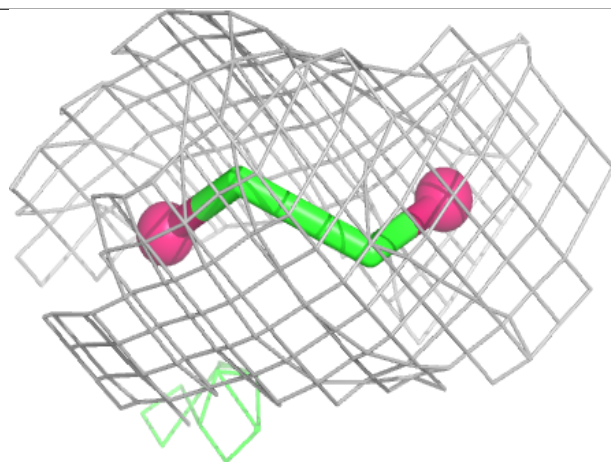
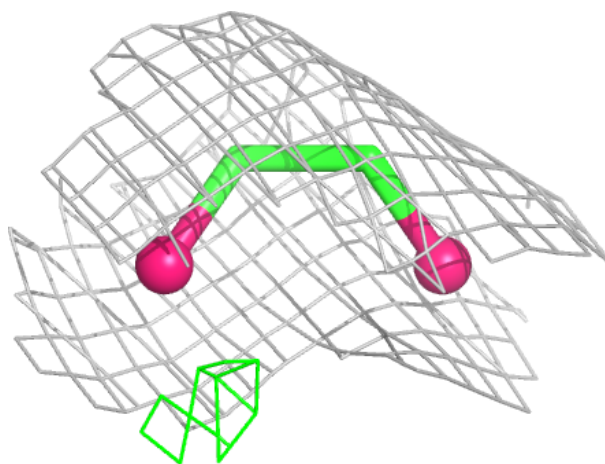
Electron density around EDO B 435:

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



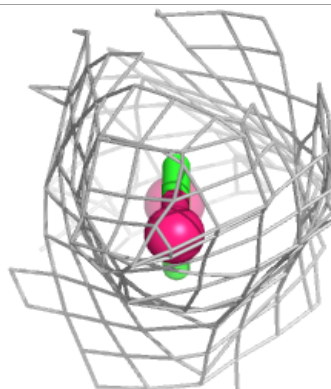
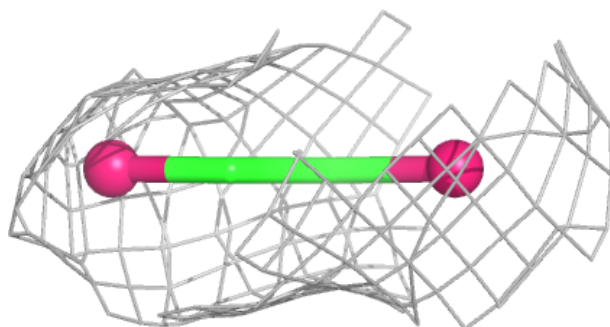
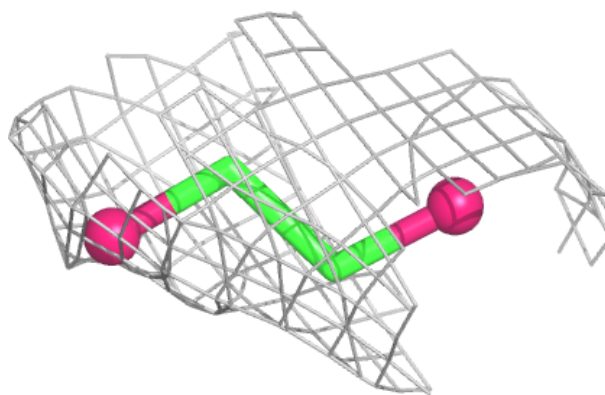
Electron density around EDO F 411:

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

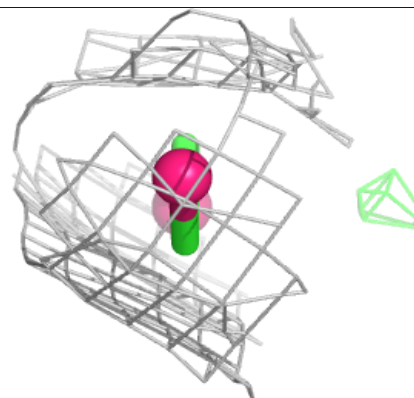
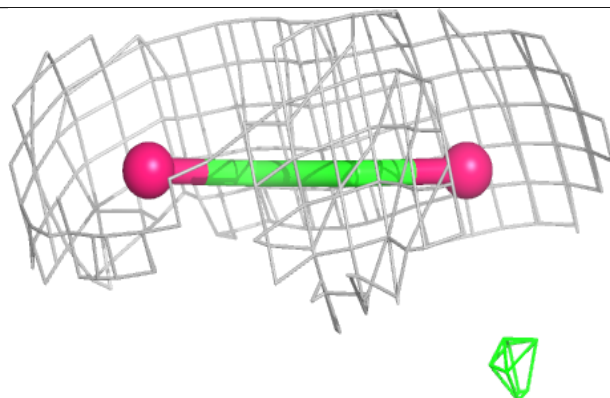
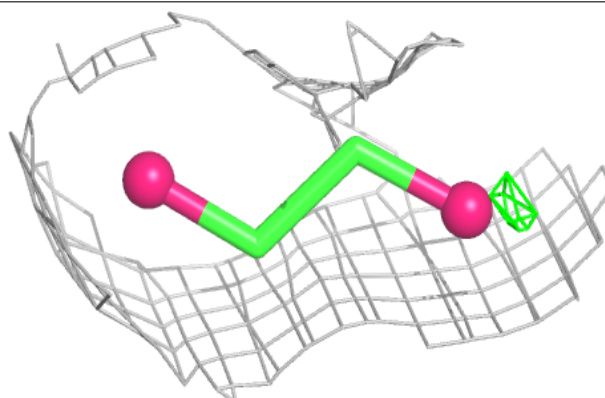


Electron density around EDO A 410:

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

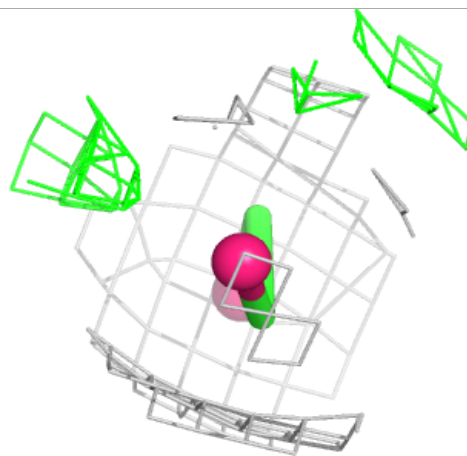
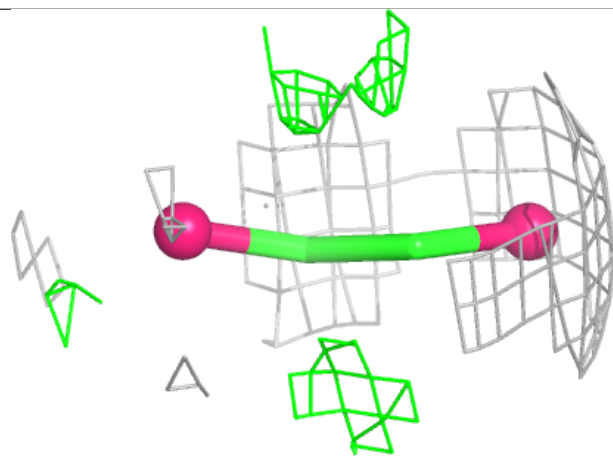
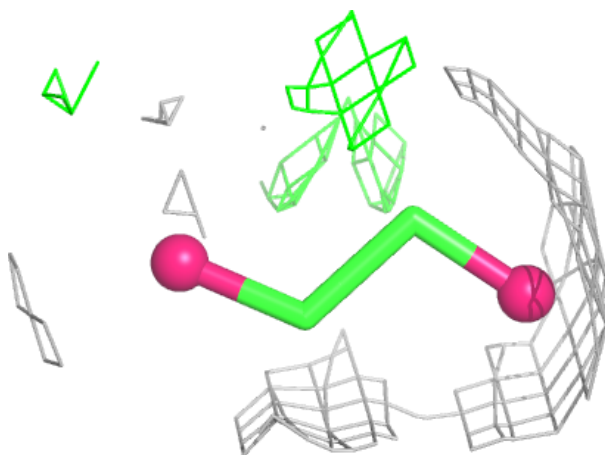
**Electron density around EDO D 408:**

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



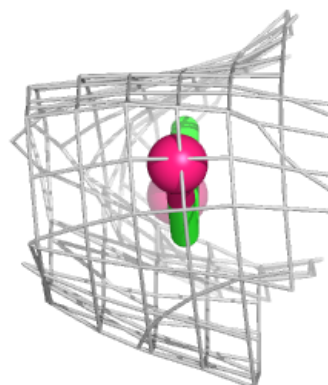
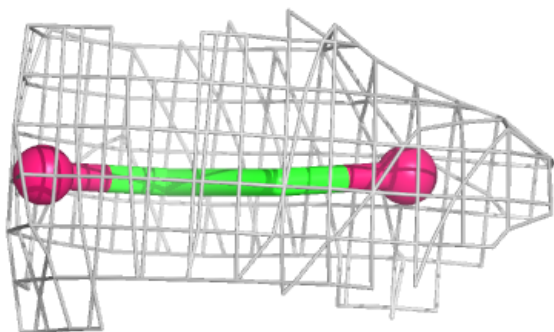
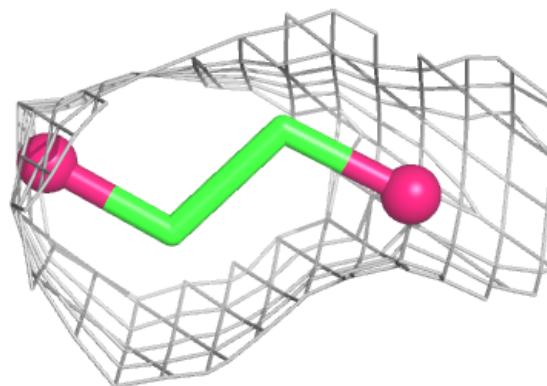
Electron density around EDO D 411:

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

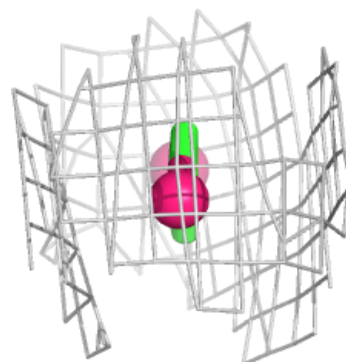
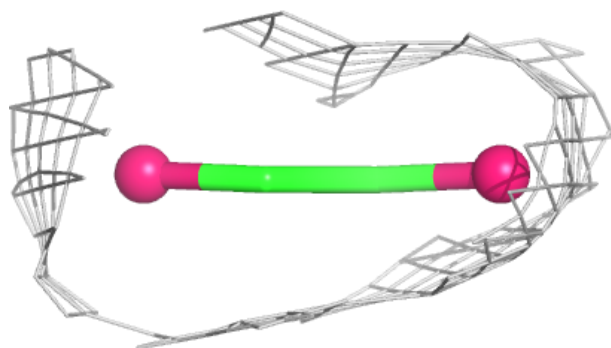
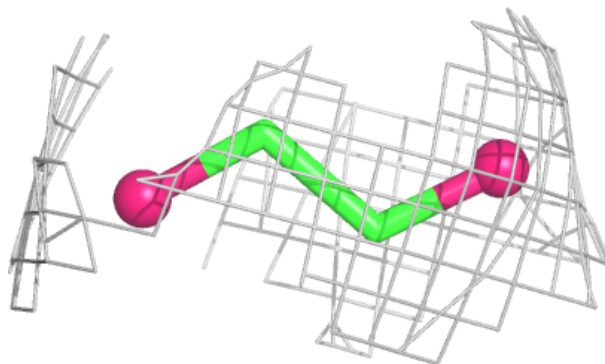


Electron density around EDO D 415:

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

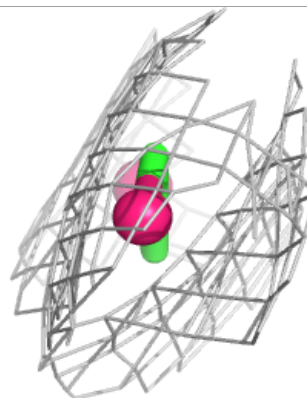
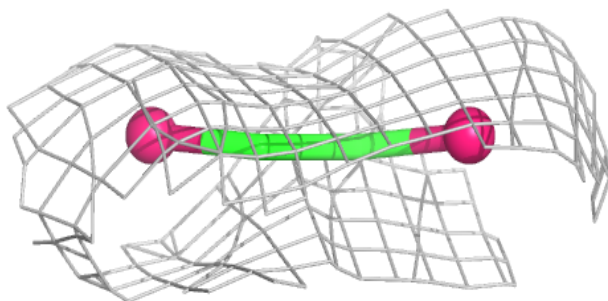
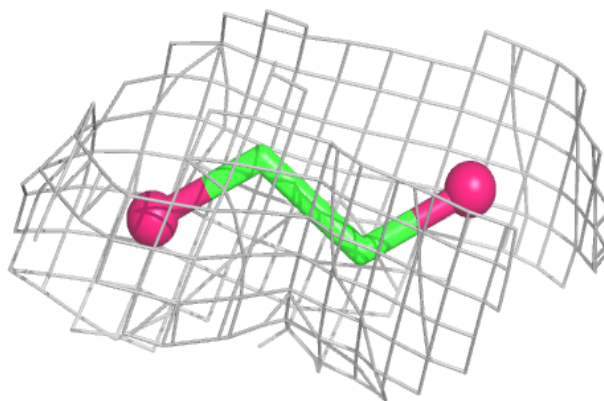
**Electron density around EDO D 418:**

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

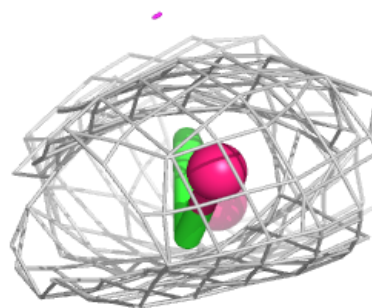
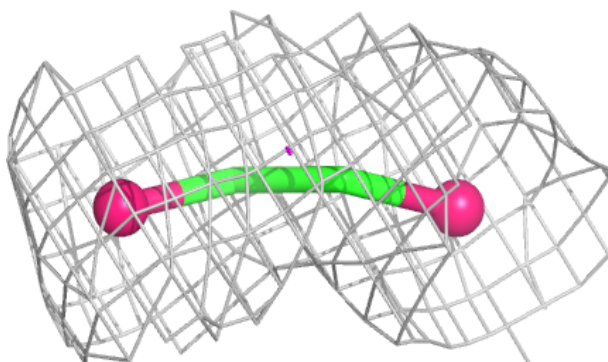
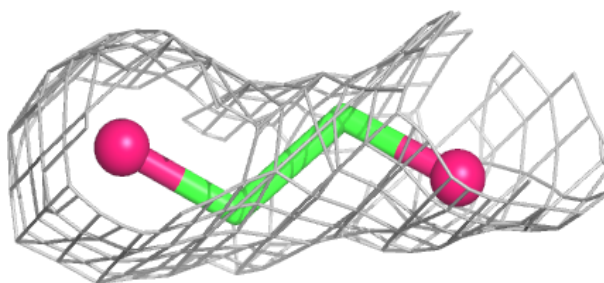


Electron density around EDO D 419:

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

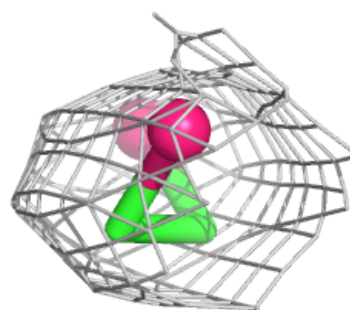
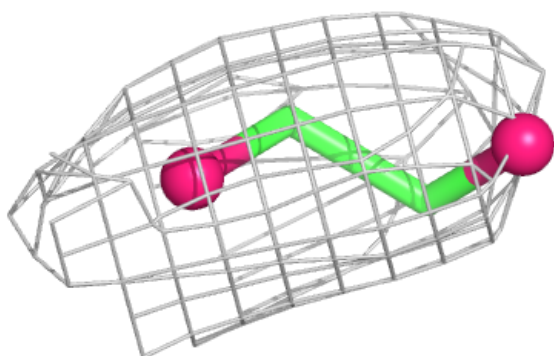
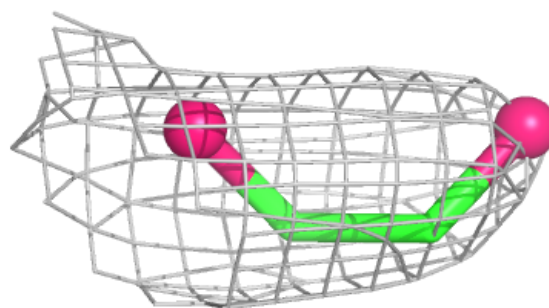
**Electron density around EDO A 411:**

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

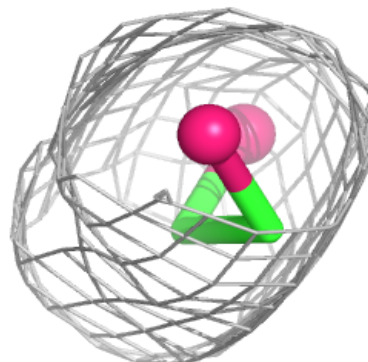
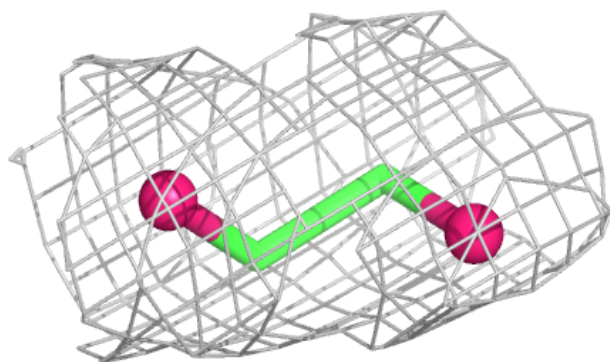
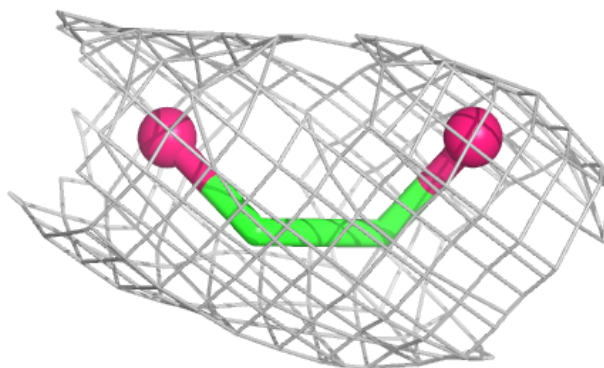


Electron density around EDO B 439:

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

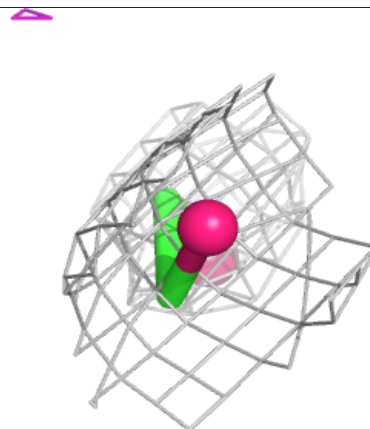
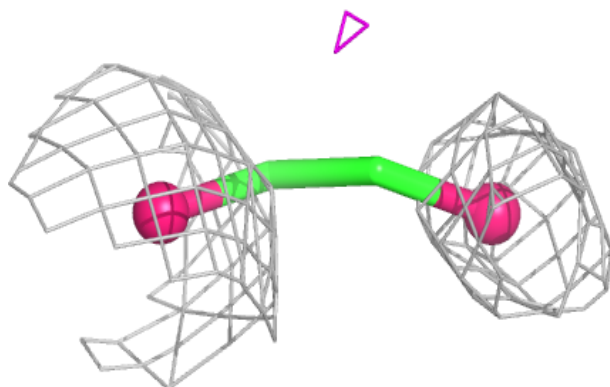
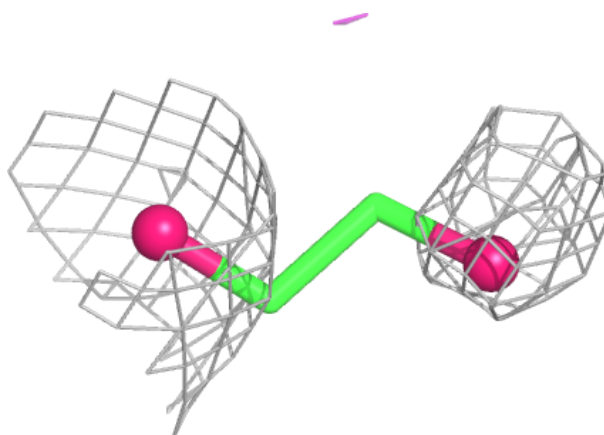
**Electron density around EDO F 431:**

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



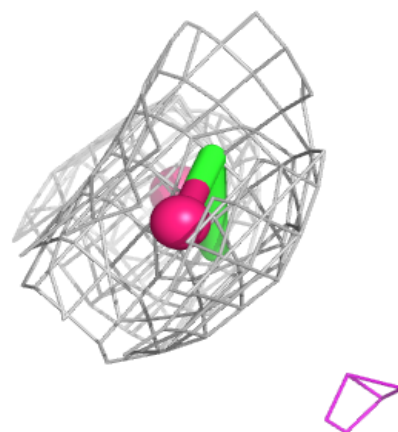
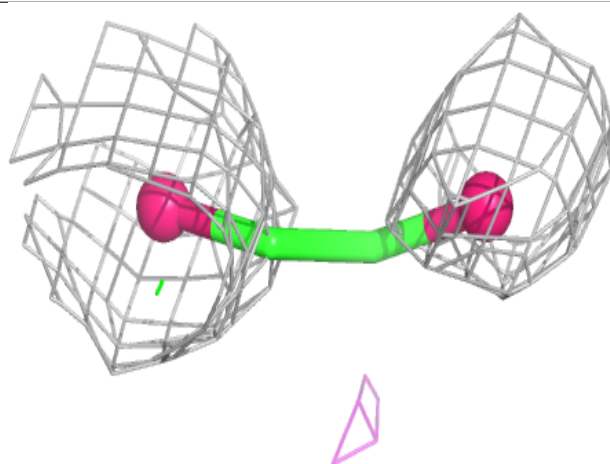
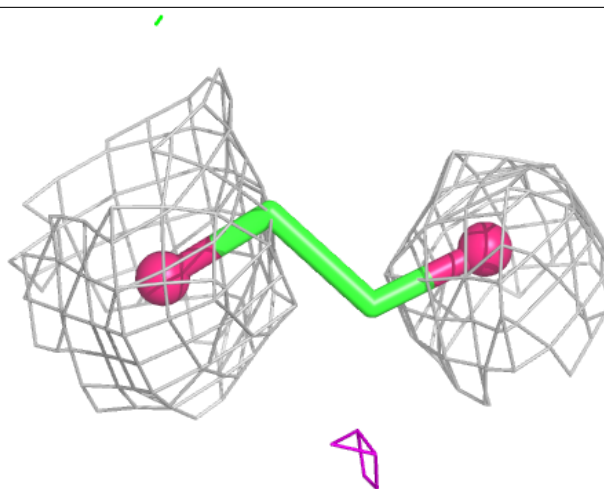
Electron density around EDO F 432:

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



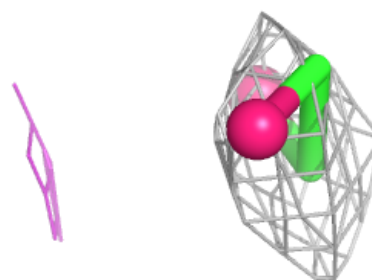
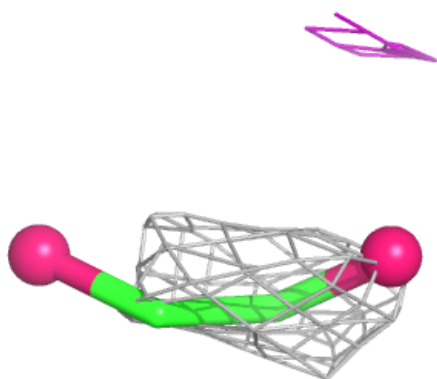
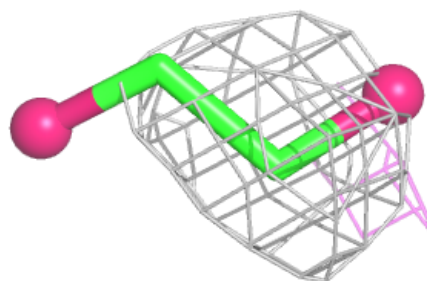
Electron density around EDO A 424:

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

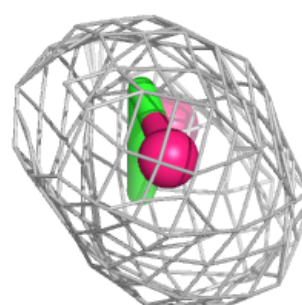
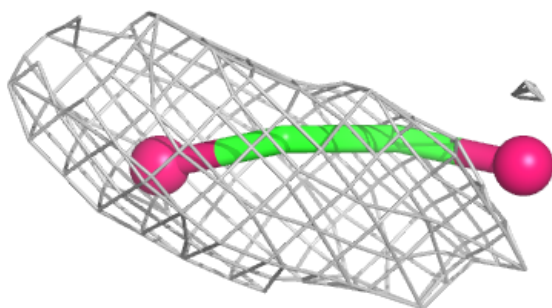
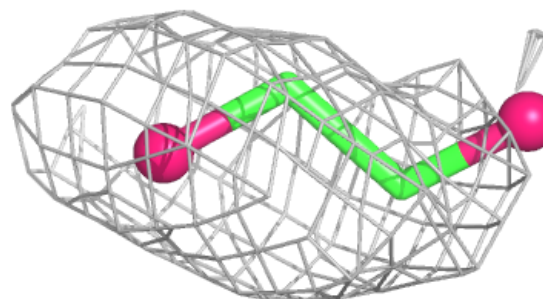


Electron density around EDO F 435:

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

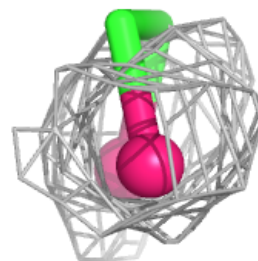
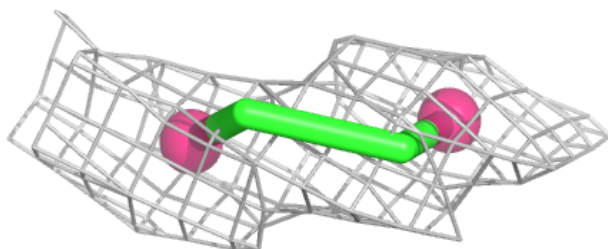
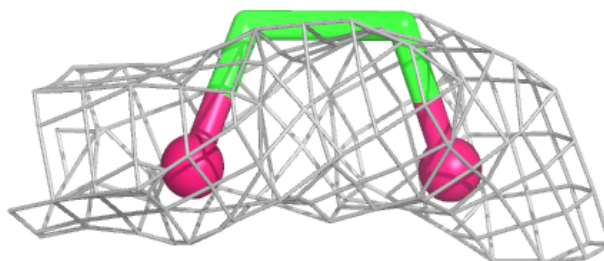
**Electron density around EDO B 442:**

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

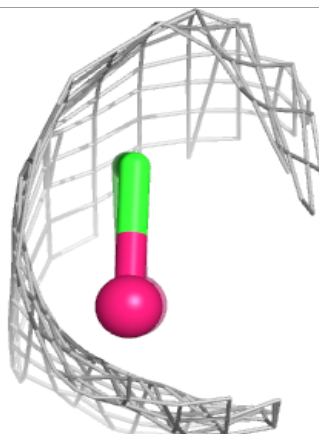
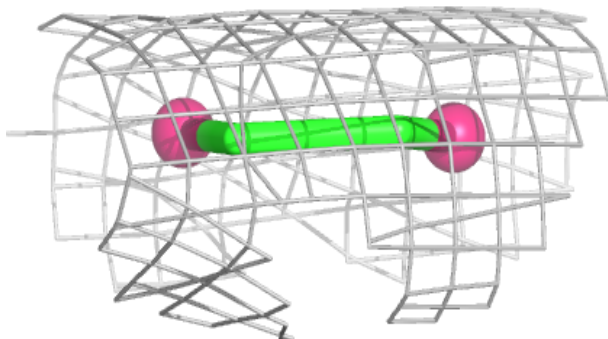
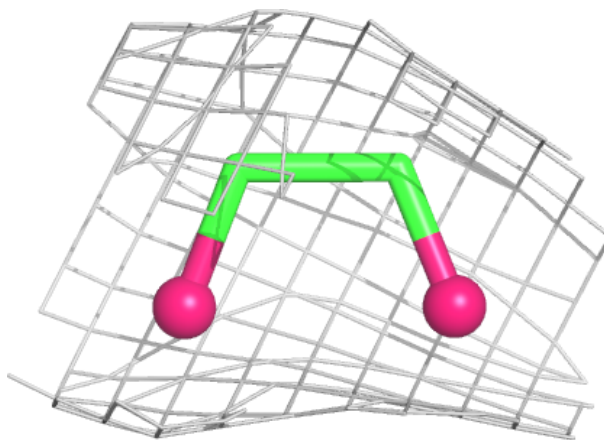


Electron density around EDO F 437:

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

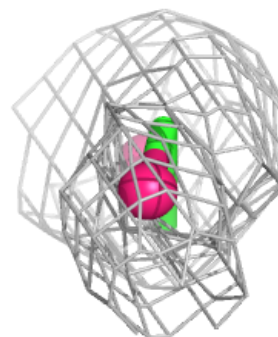
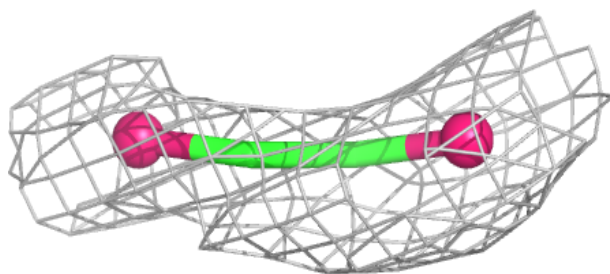
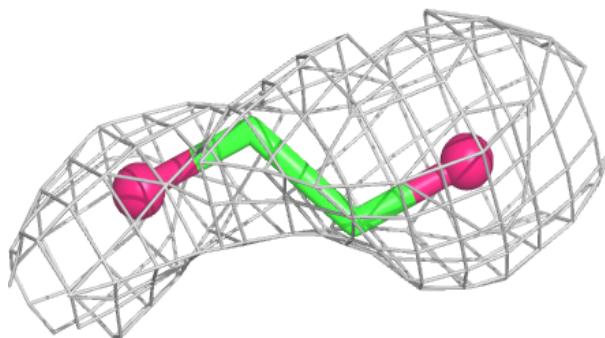
**Electron density around EDO F 438:**

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

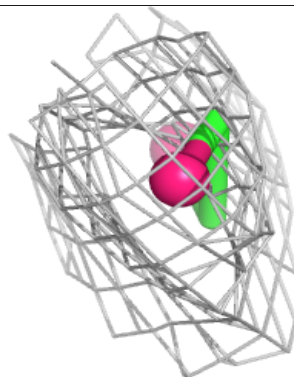
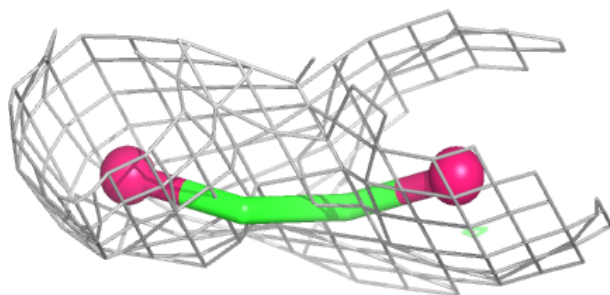
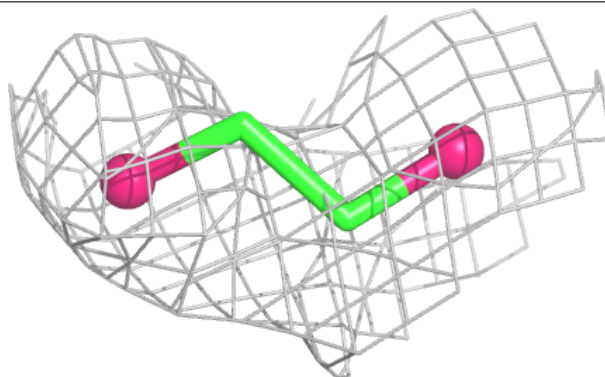


Electron density around EDO A 404:

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

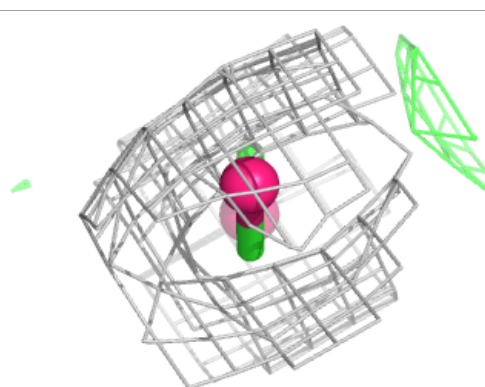
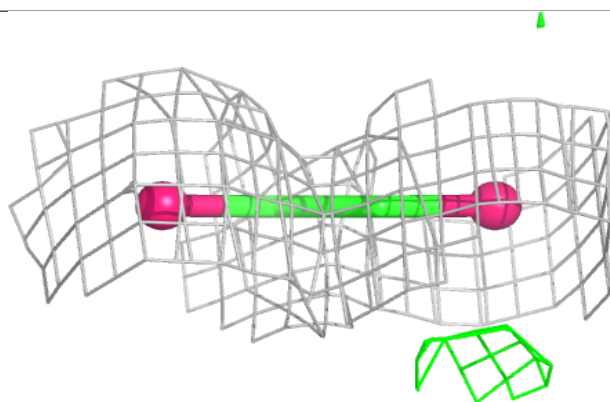
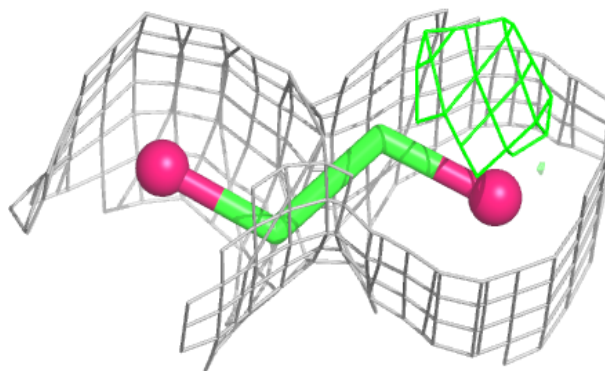
**Electron density around EDO D 427:**

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

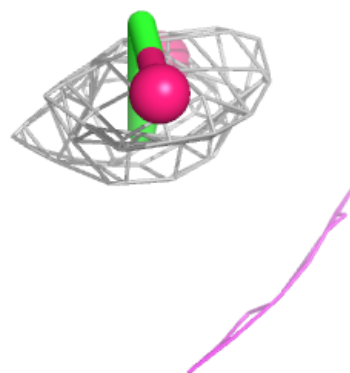
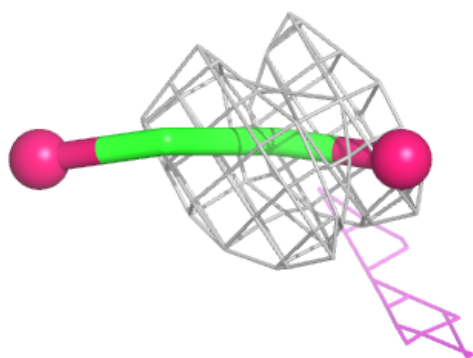
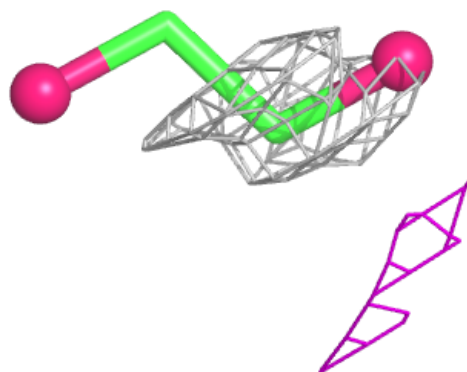


Electron density around EDO A 413:

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

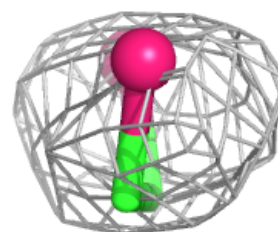
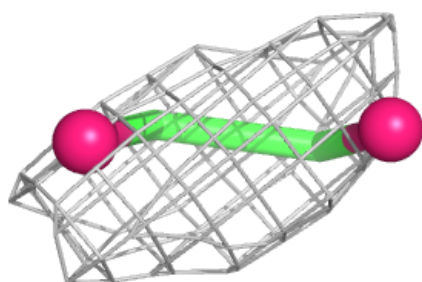
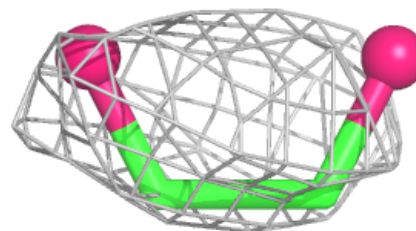
**Electron density around EDO D 430:**

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

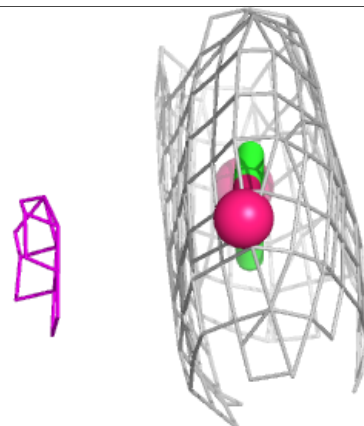
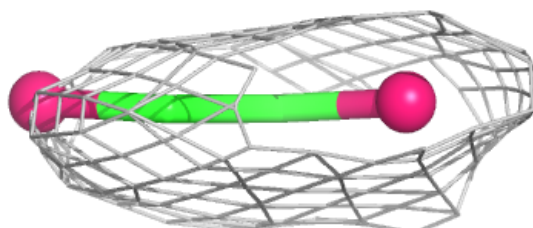
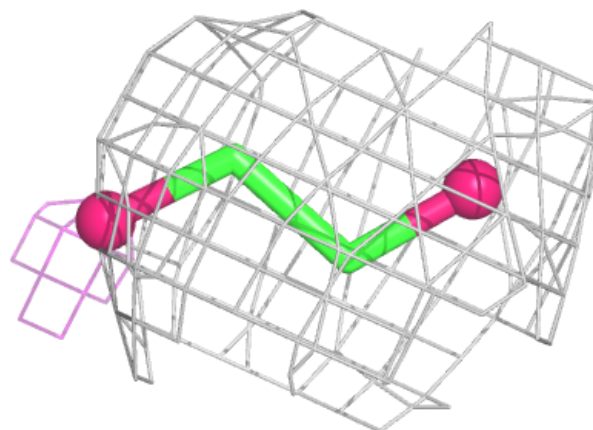


Electron density around EDO D 431:

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

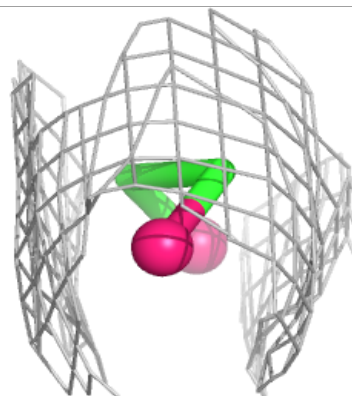
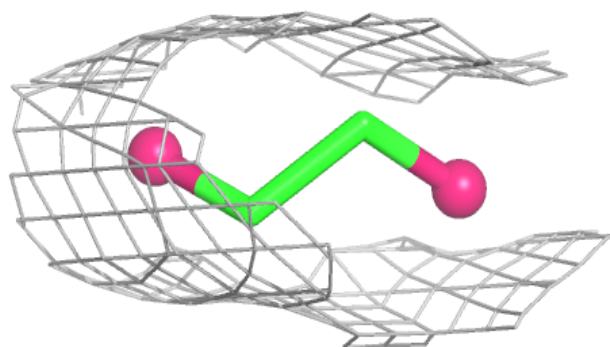
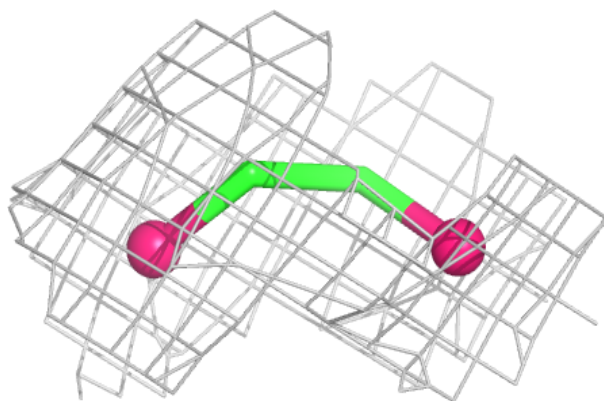
**Electron density around EDO B 402:**

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

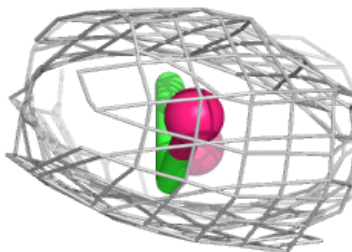
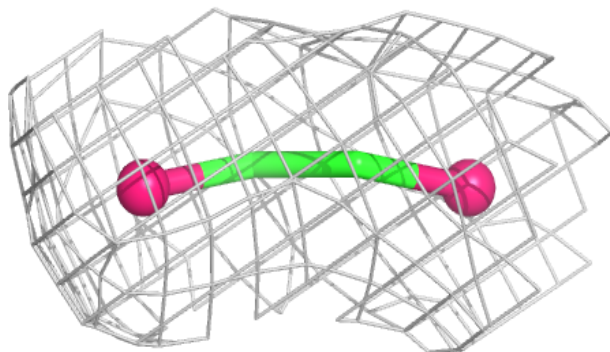
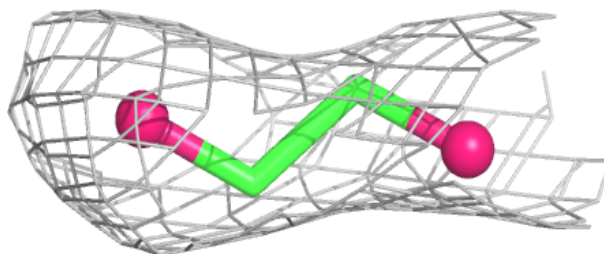


Electron density around EDO A 406:

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

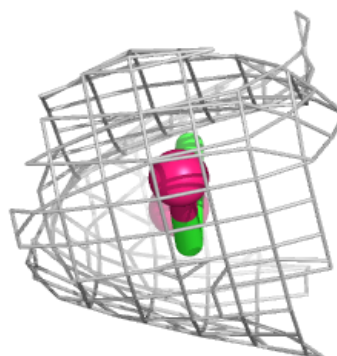
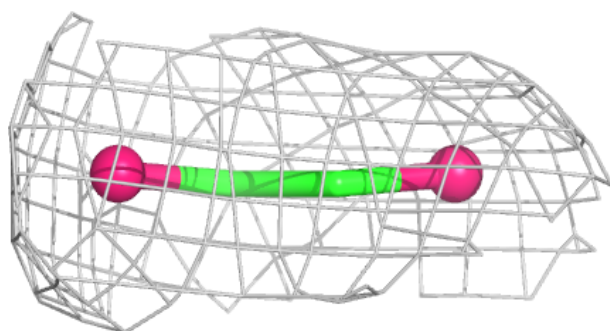
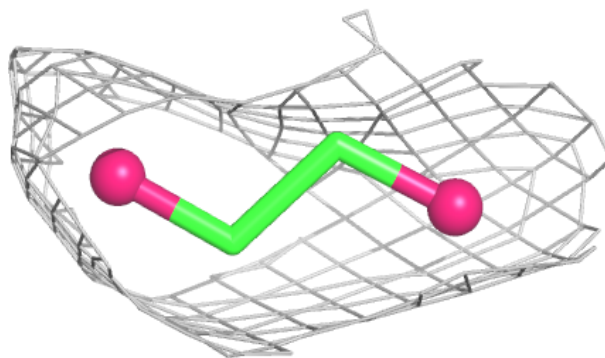
**Electron density around EDO E 414:**

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

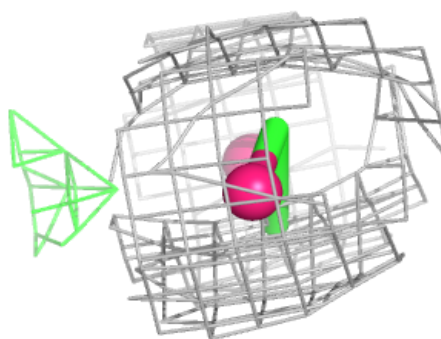
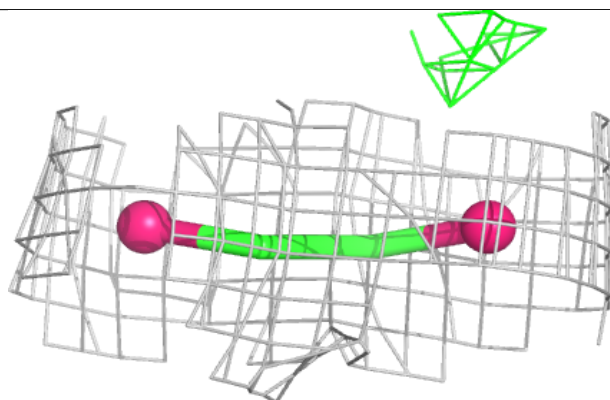
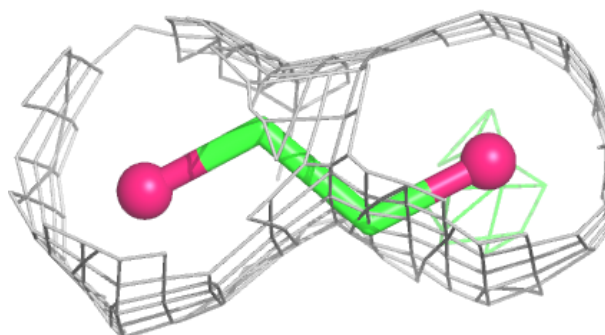


Electron density around EDO E 415:

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

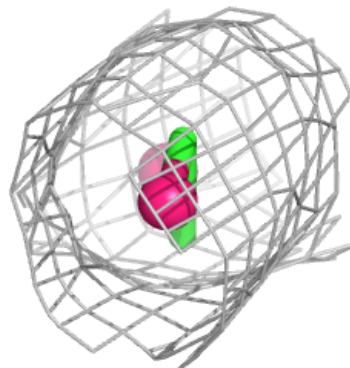
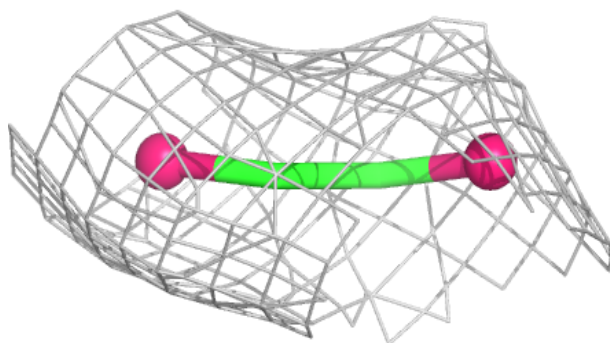
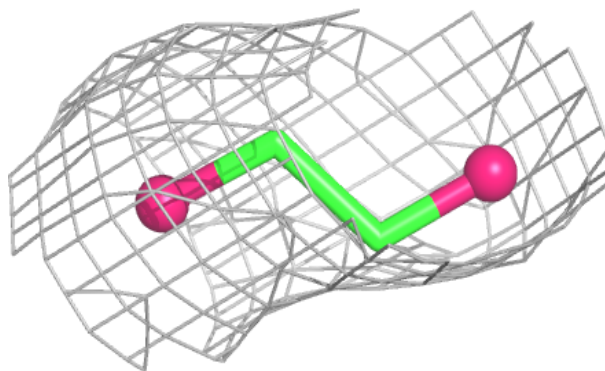
**Electron density around EDO E 416:**

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

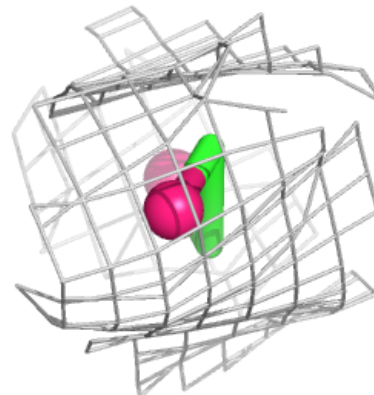
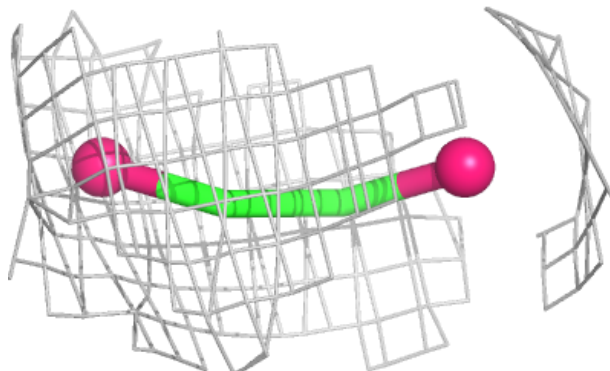
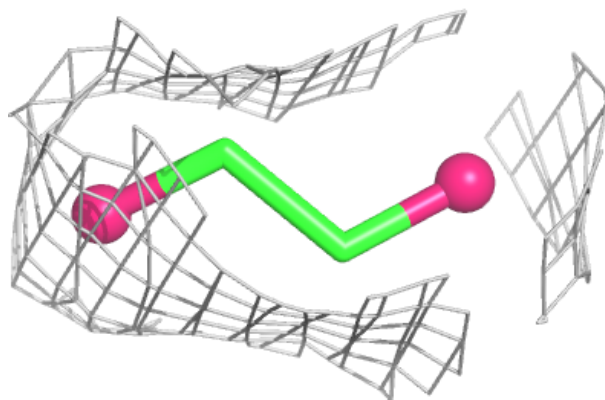


Electron density around EDO E 417:

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

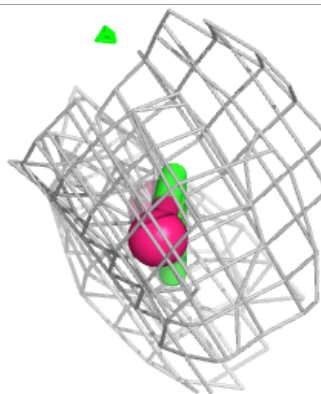
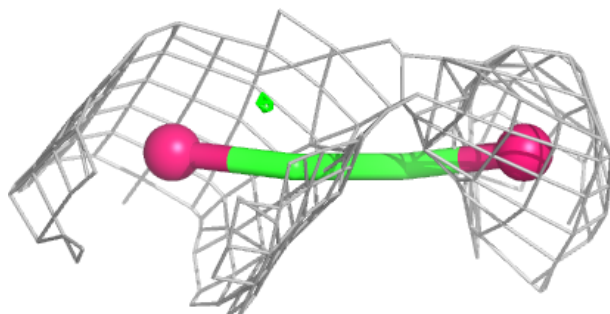
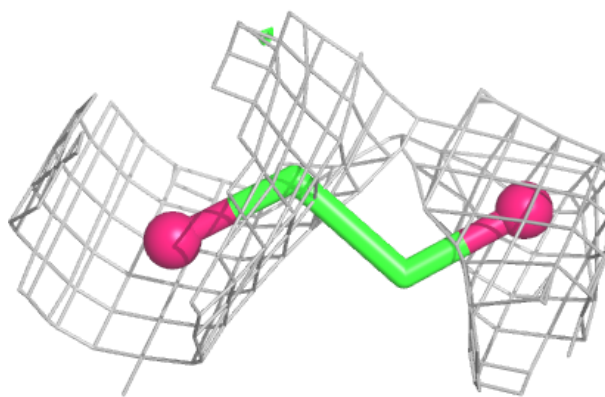
**Electron density around EDO E 418:**

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

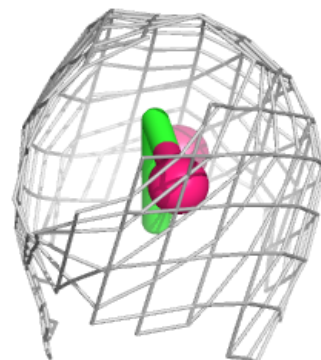
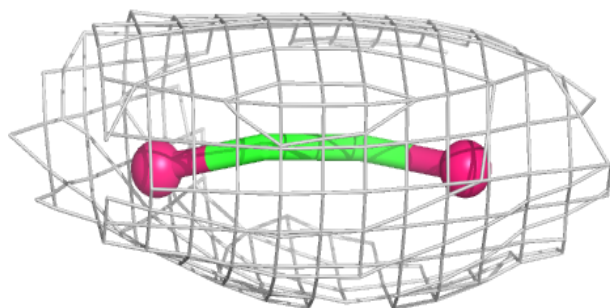
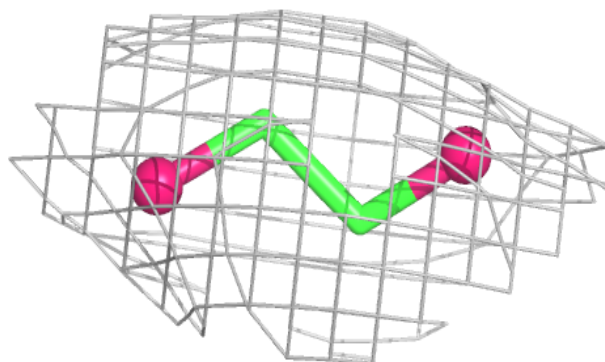


Electron density around EDO B 421:

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

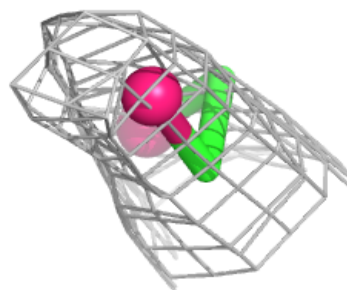
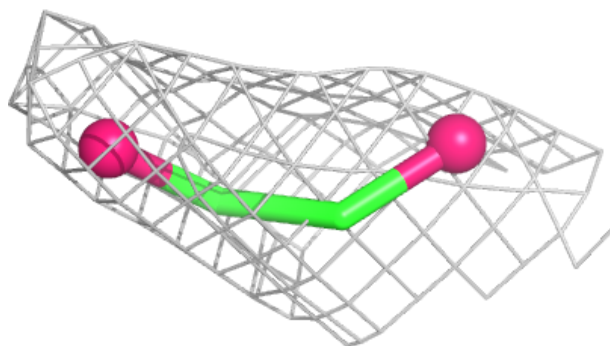
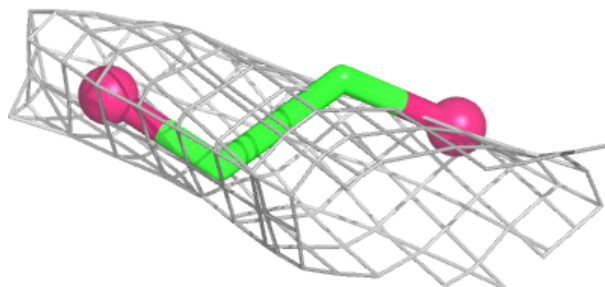
**Electron density around EDO E 420:**

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

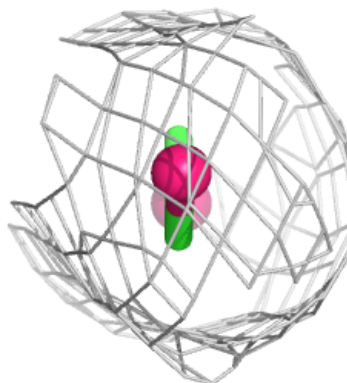
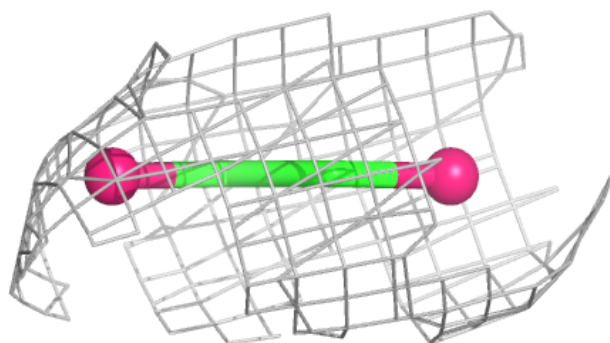
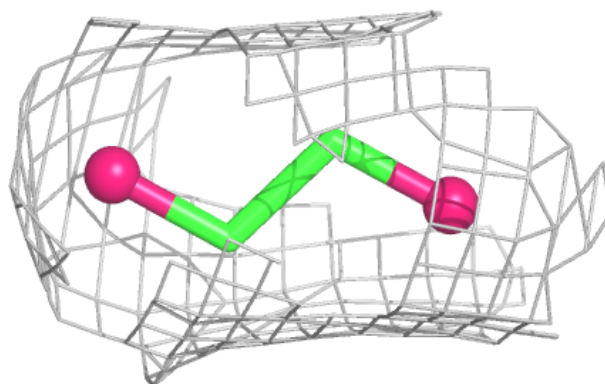


Electron density around EDO B 445:

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

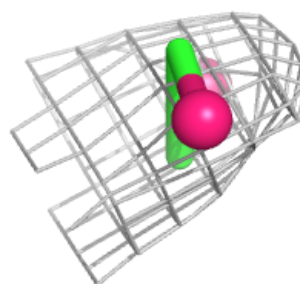
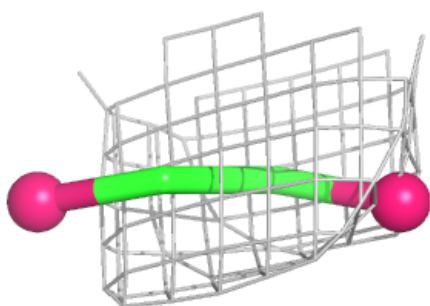
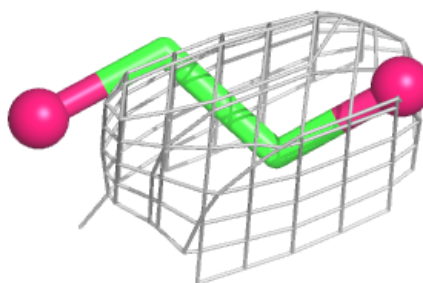
**Electron density around EDO E 422:**

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

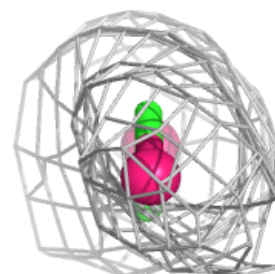
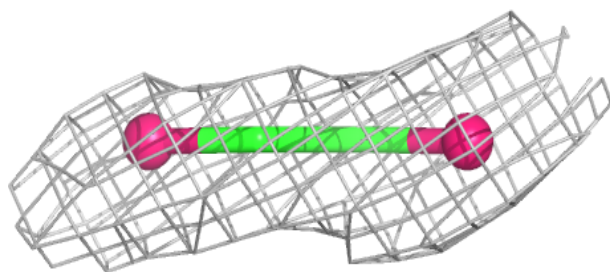
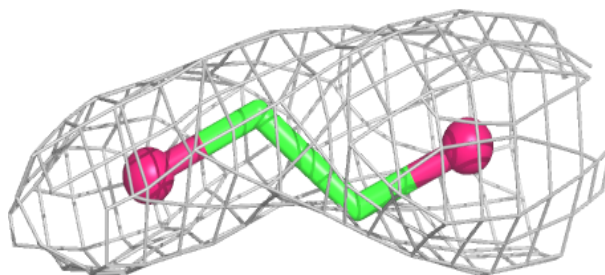


Electron density around EDO A 402:

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

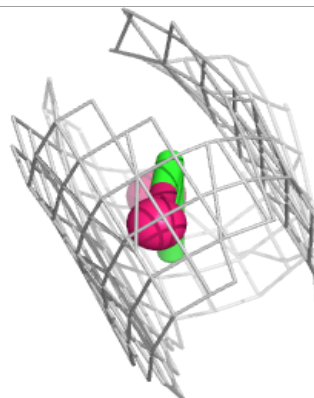
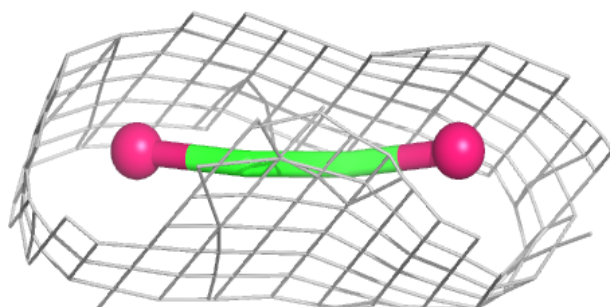
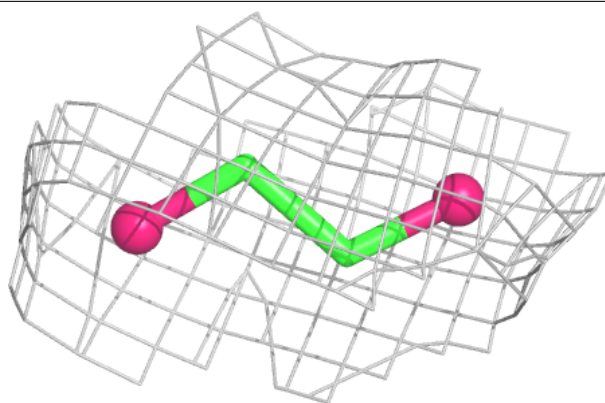
**Electron density around EDO B 406:**

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

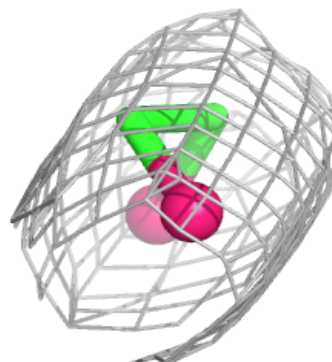
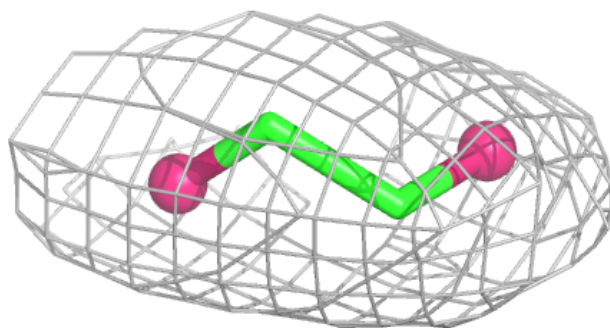
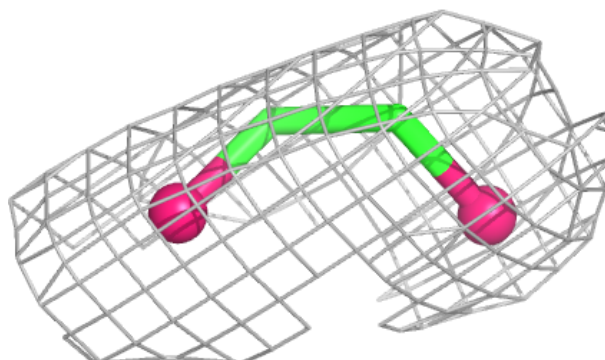


Electron density around EDO C 401:

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

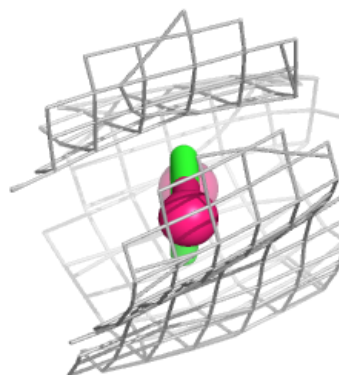
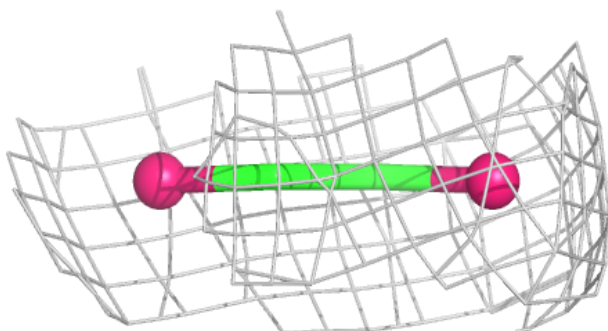
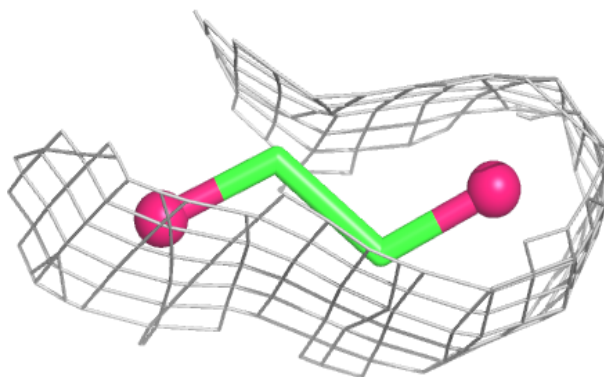
**Electron density around EDO B 425:**

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

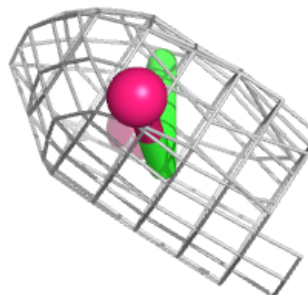
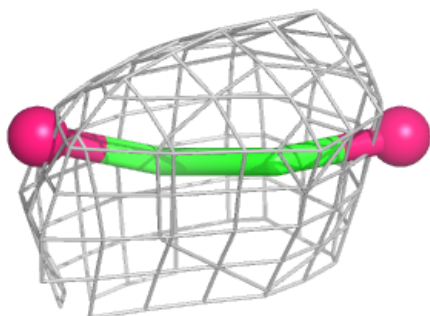
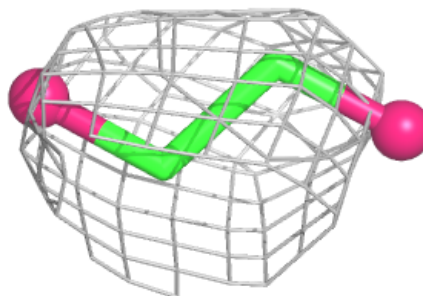


Electron density around EDO B 407:

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

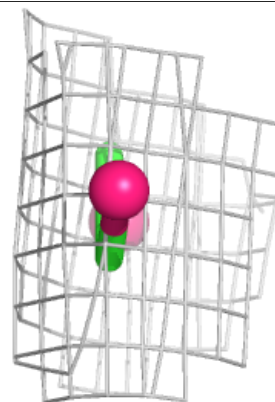
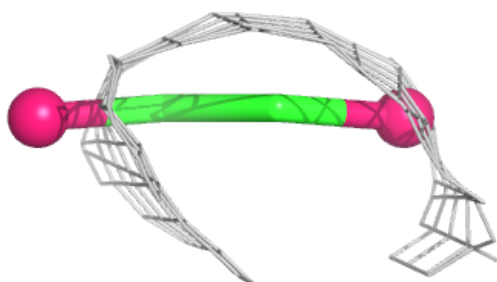
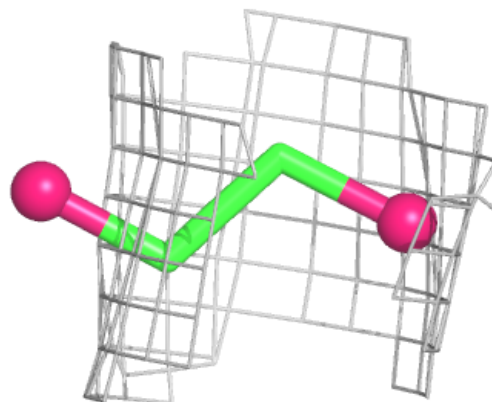
**Electron density around EDO C 404:**

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

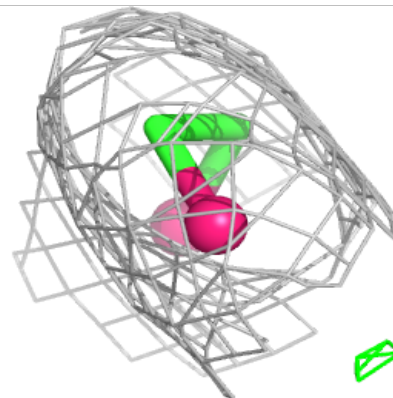
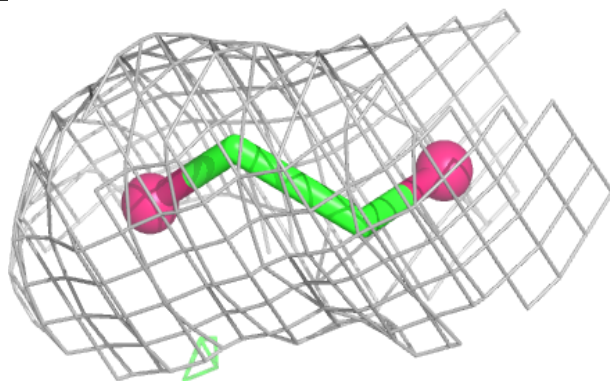
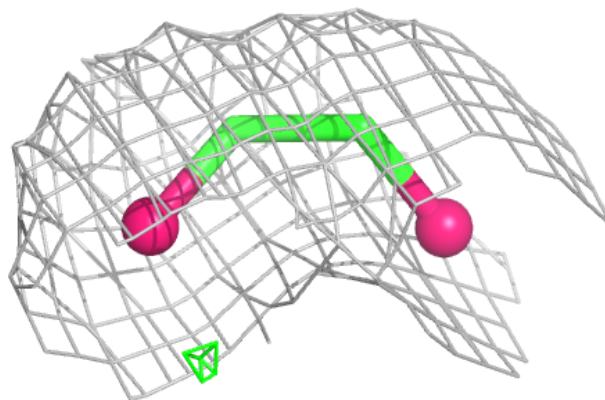


Electron density around EDO E 430:

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

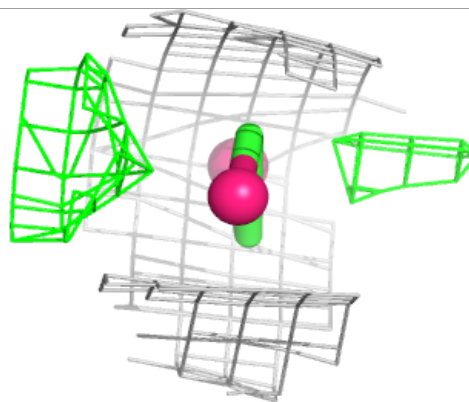
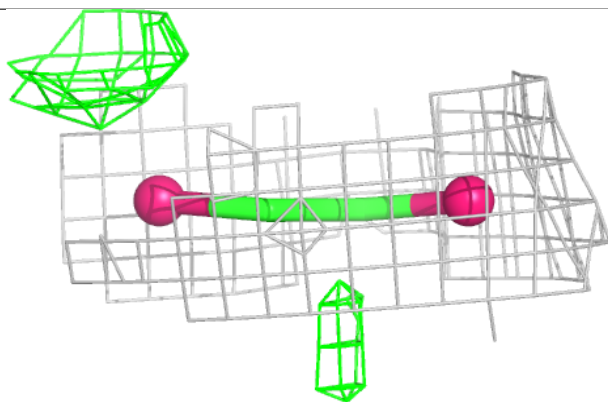
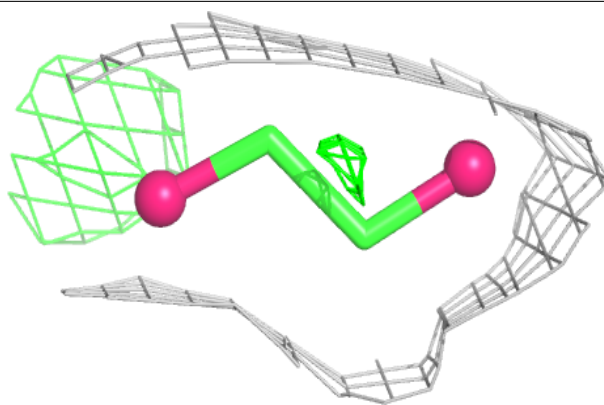
**Electron density around EDO C 405:**

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

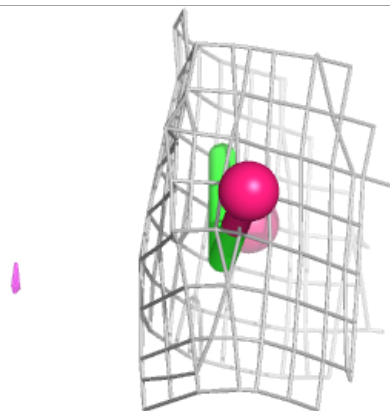
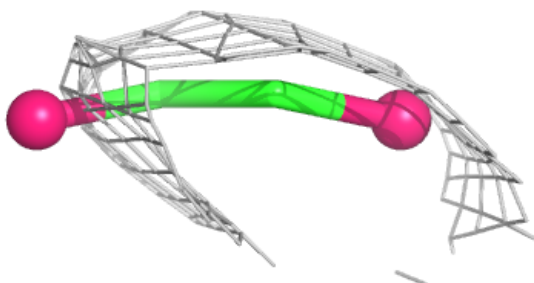
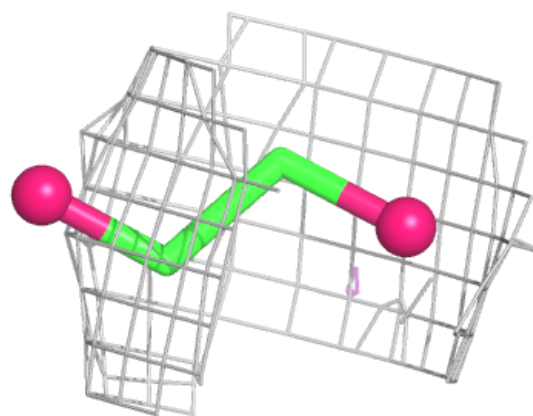


Electron density around EDO D 410:

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

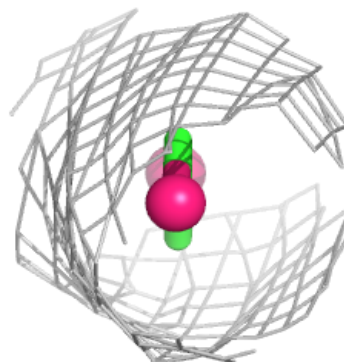
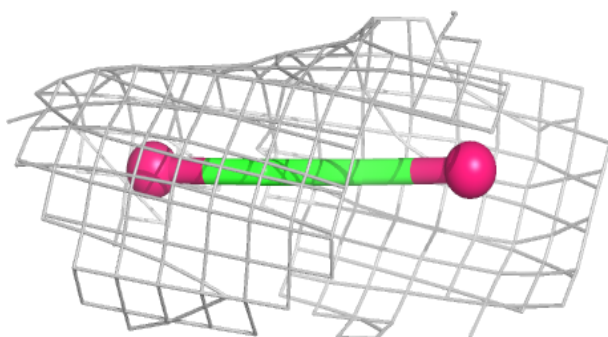
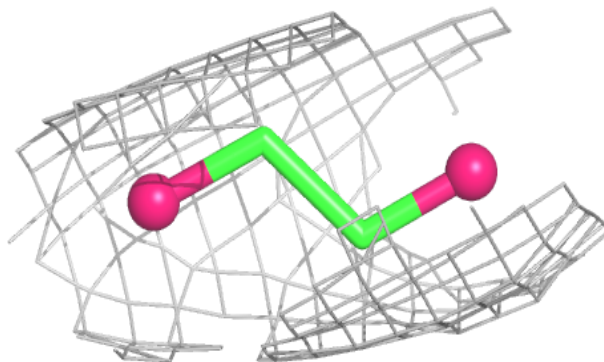
**Electron density around EDO B 427:**

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

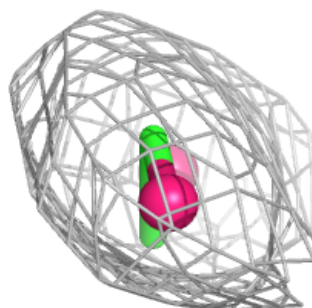
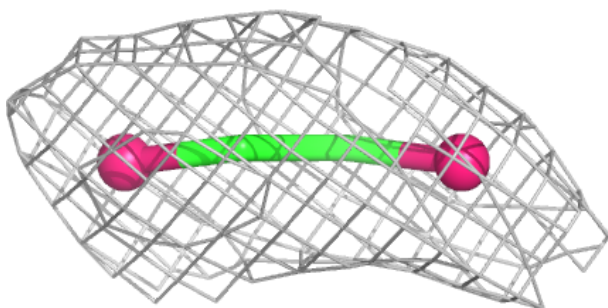
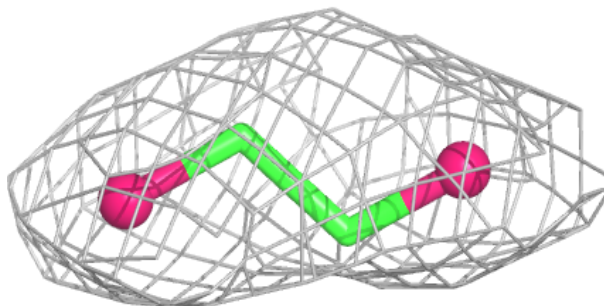


Electron density around EDO D 412:

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

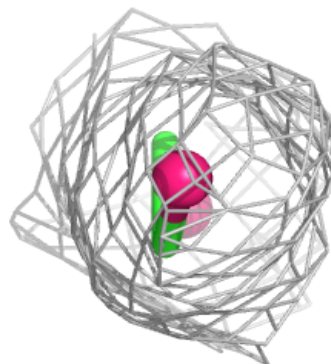
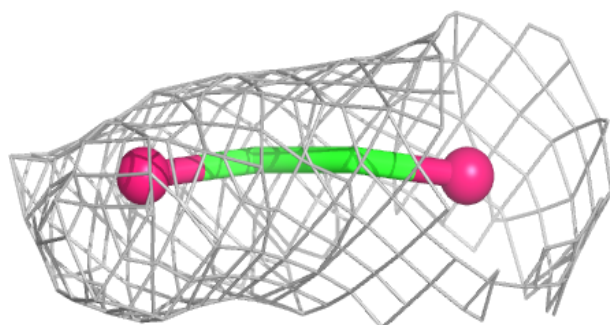
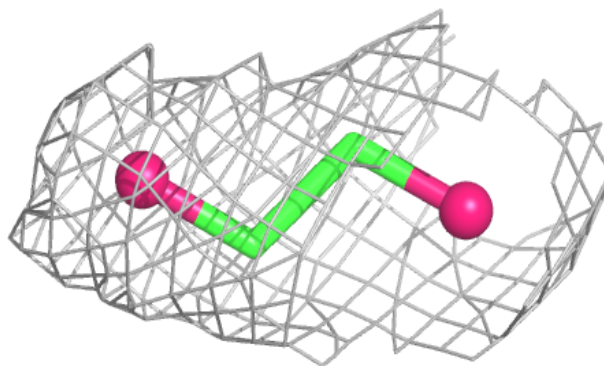
**Electron density around EDO E 435:**

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

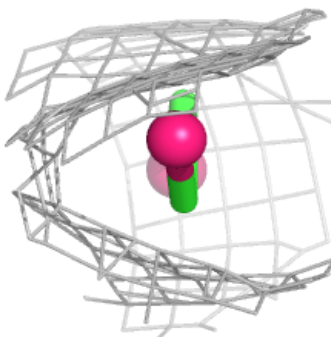
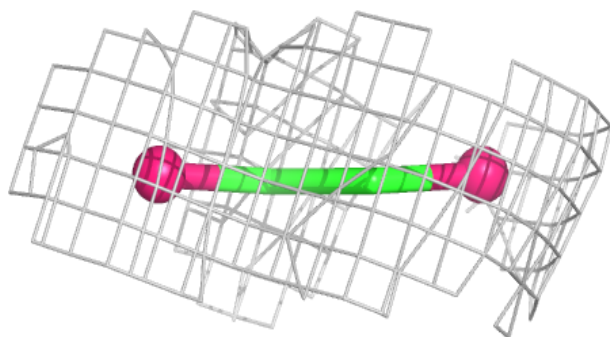
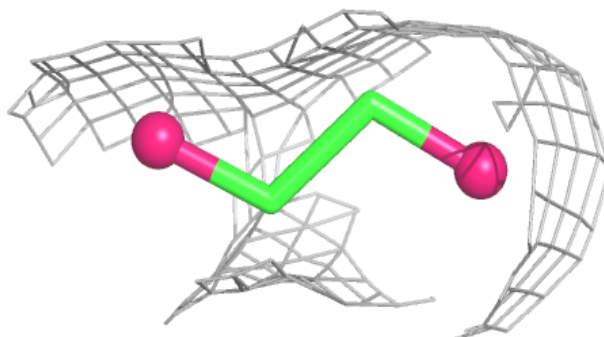


Electron density around EDO D 413:

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

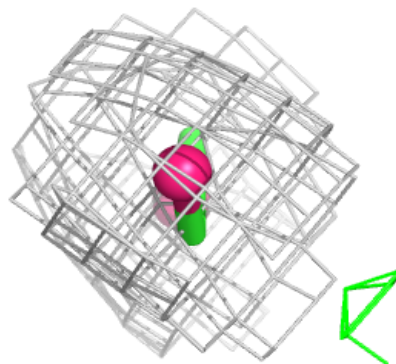
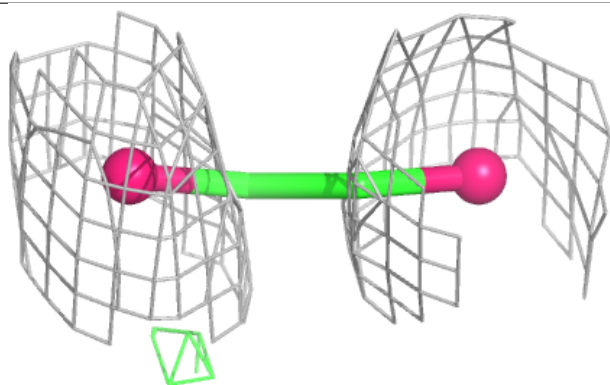
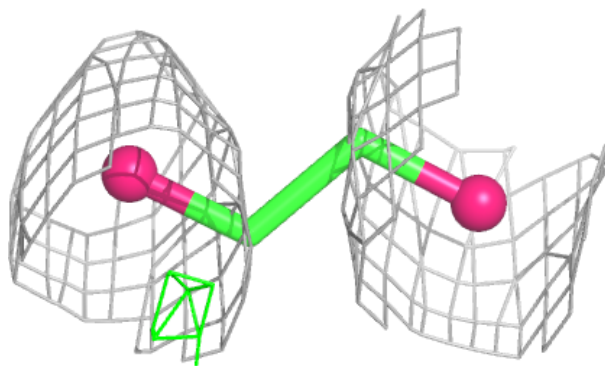
**Electron density around EDO C 407:**

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

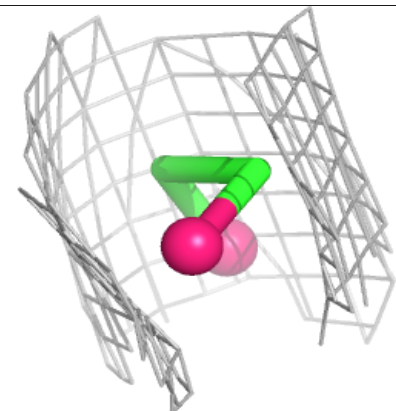
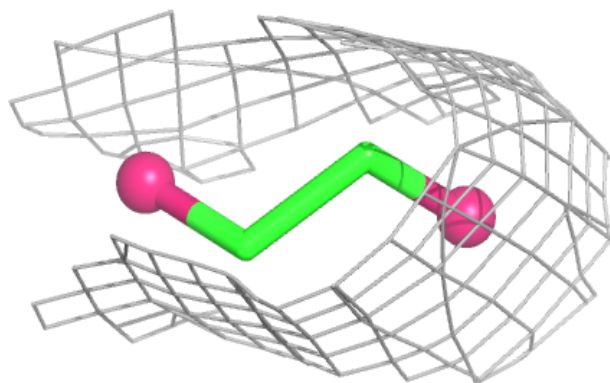
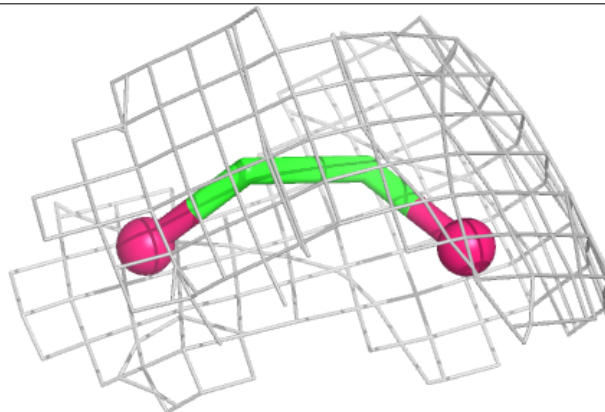


Electron density around EDO D 416:

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

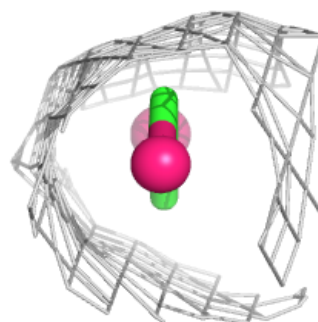
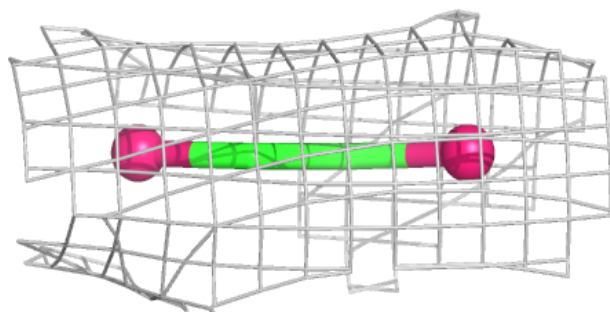
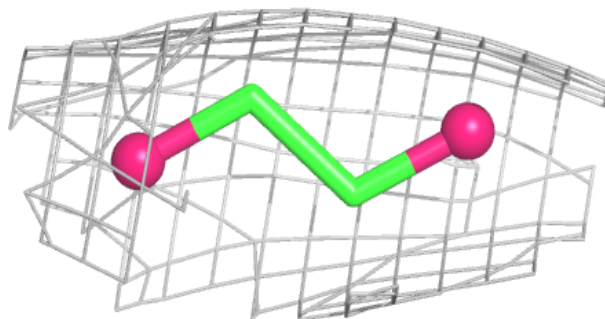
**Electron density around EDO C 408:**

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

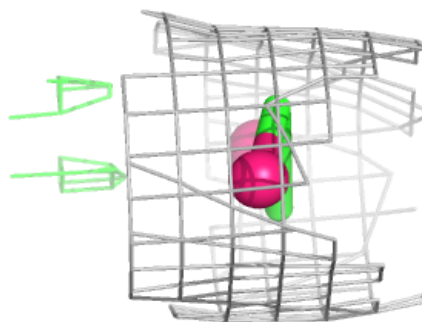
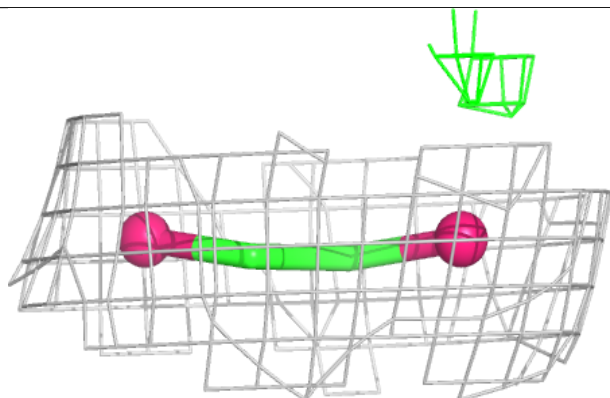
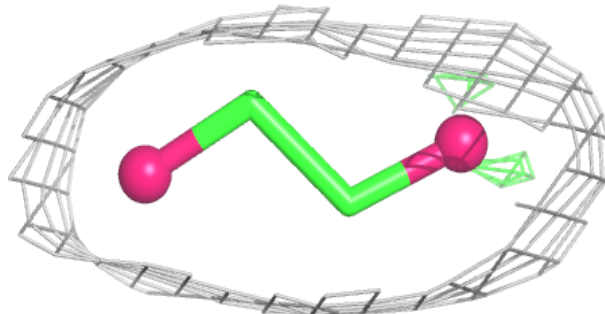


Electron density around EDO E 442:

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

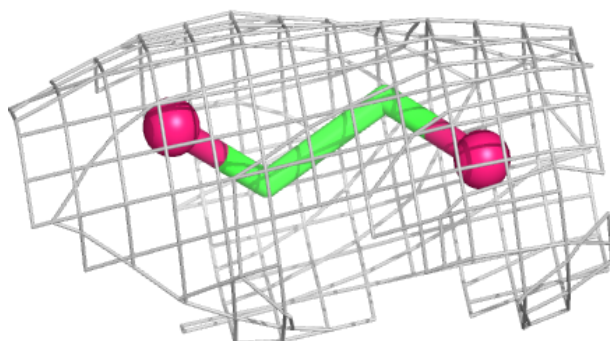
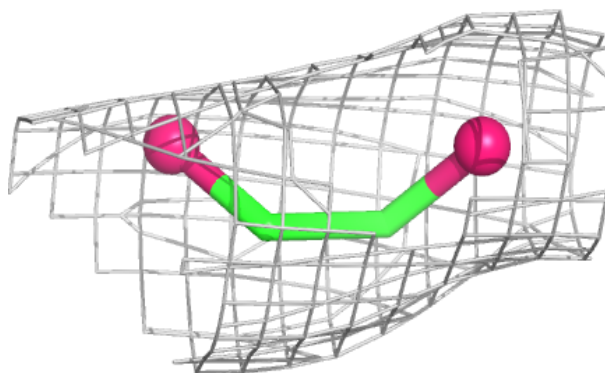
**Electron density around EDO C 409:**

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

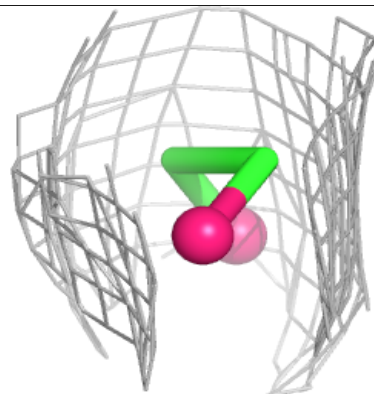
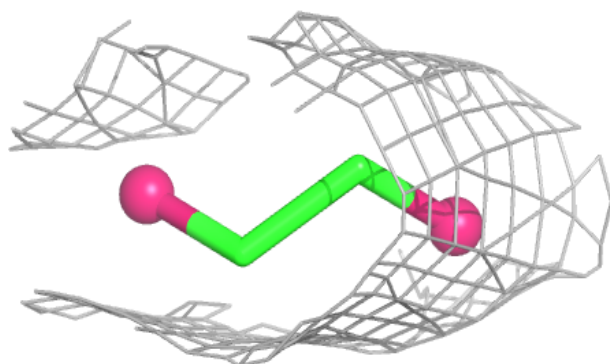
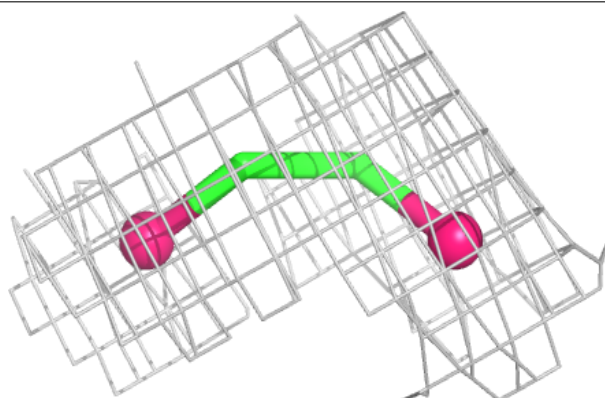


Electron density around EDO E 444:

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

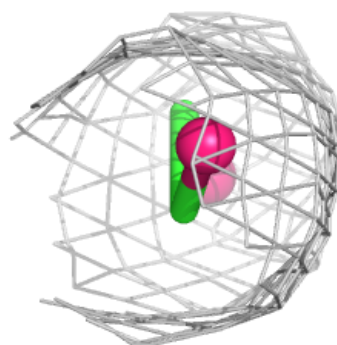
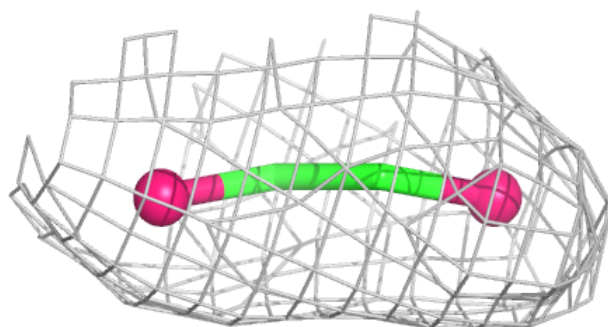
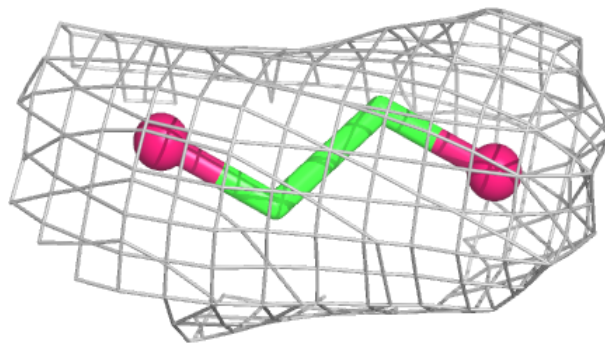
**Electron density around EDO B 408:**

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

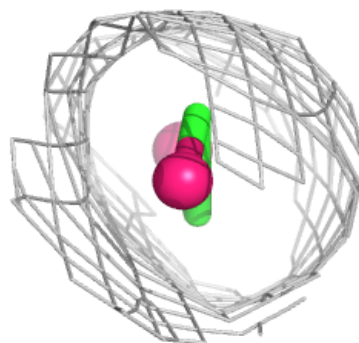
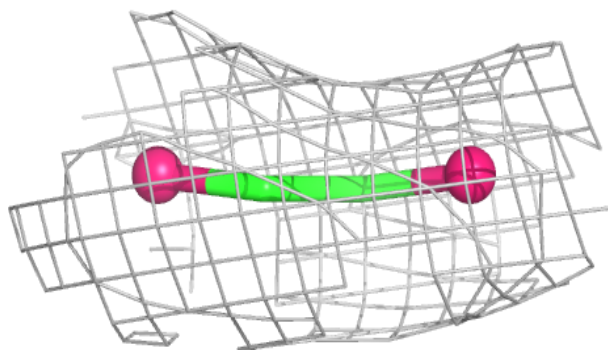
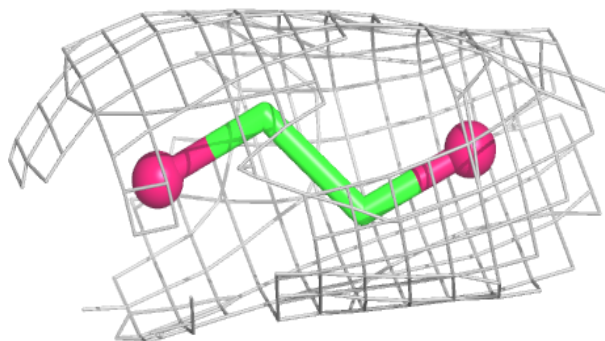


Electron density around EDO D 421:

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

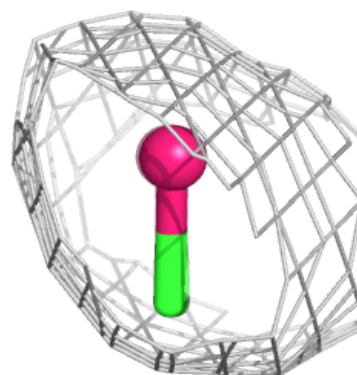
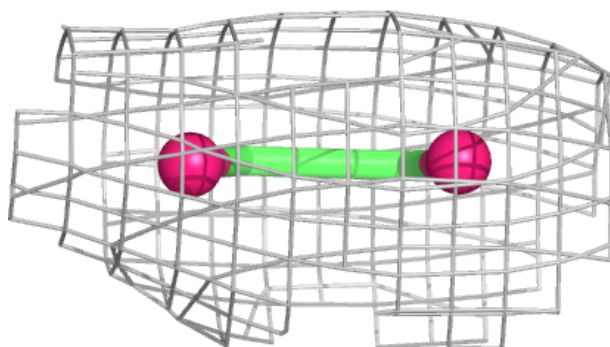
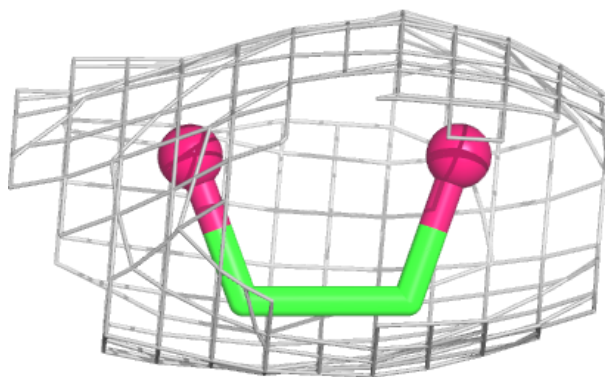
**Electron density around EDO C 411:**

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

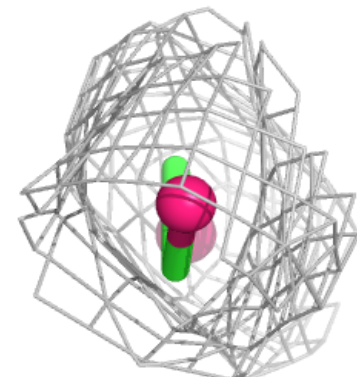
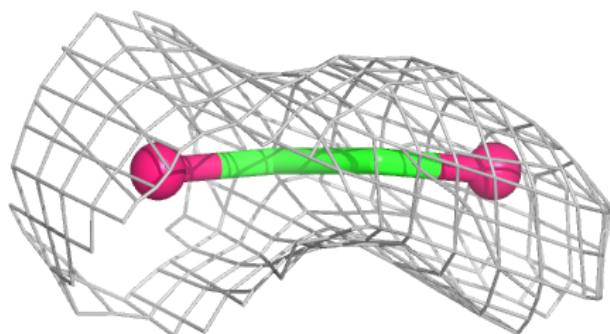
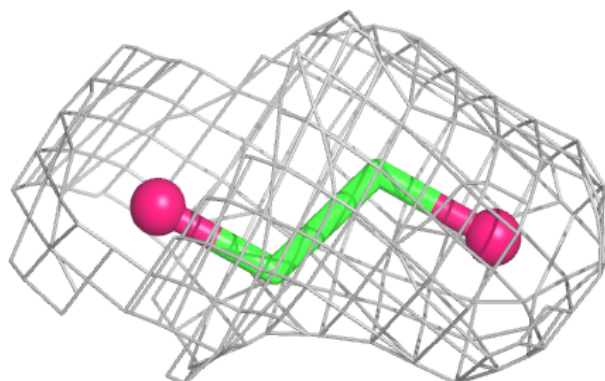


Electron density around EDO F 402:

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

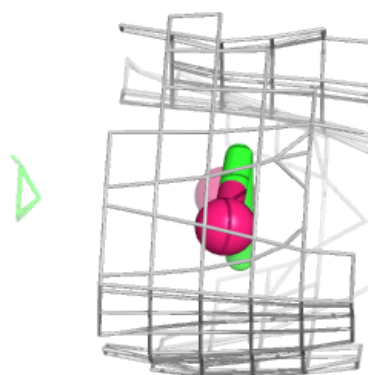
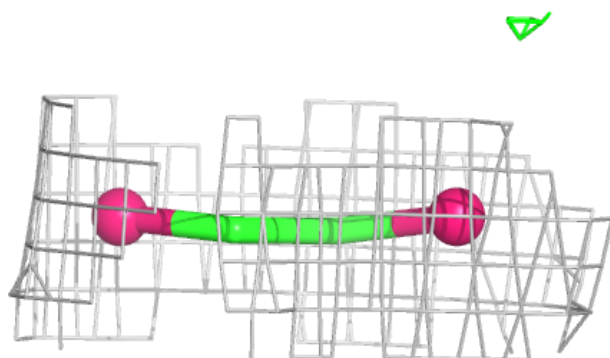
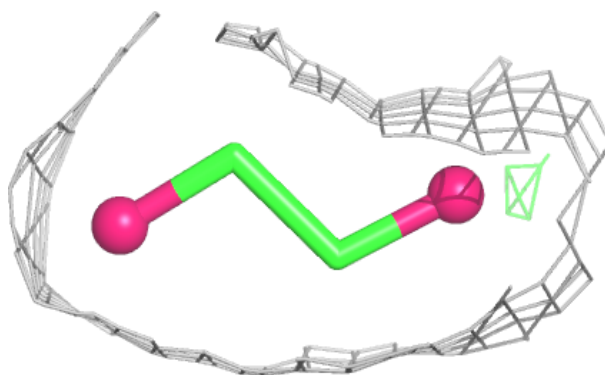
**Electron density around EDO C 412:**

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

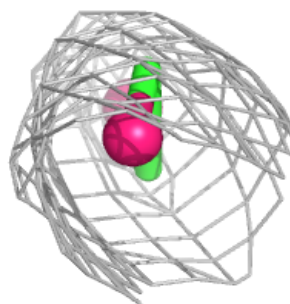
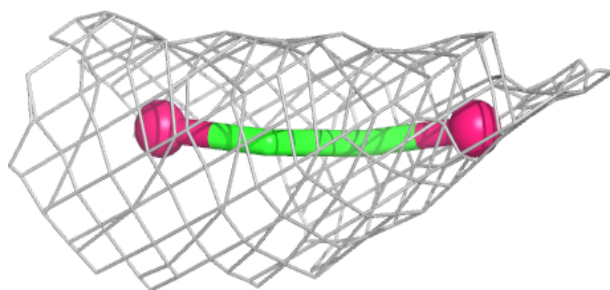
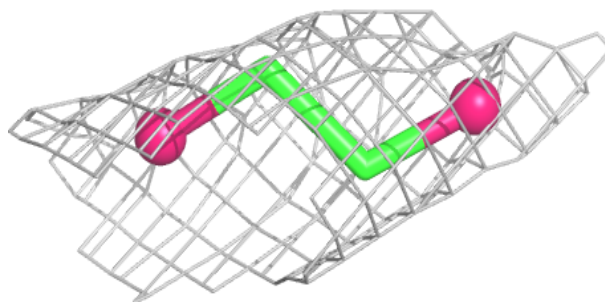


Electron density around EDO B 409:

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

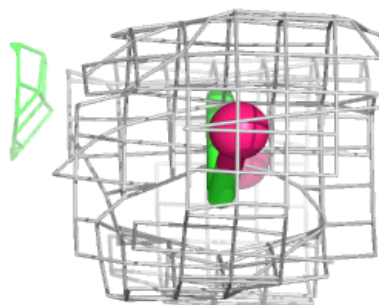
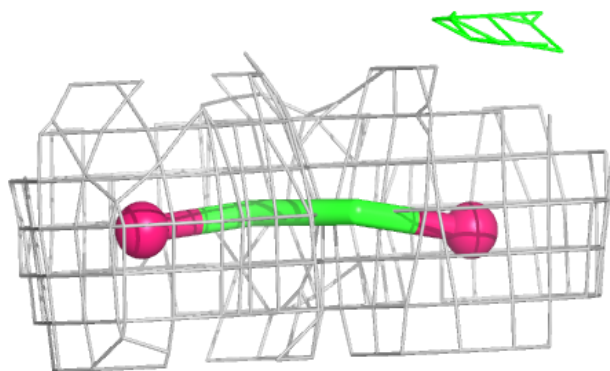
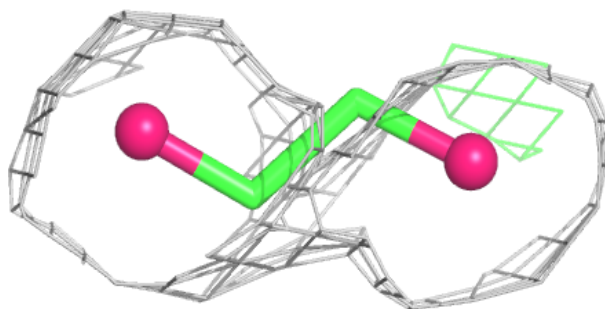
**Electron density around EDO F 405:**

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

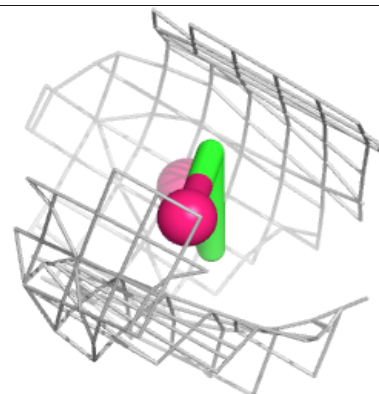
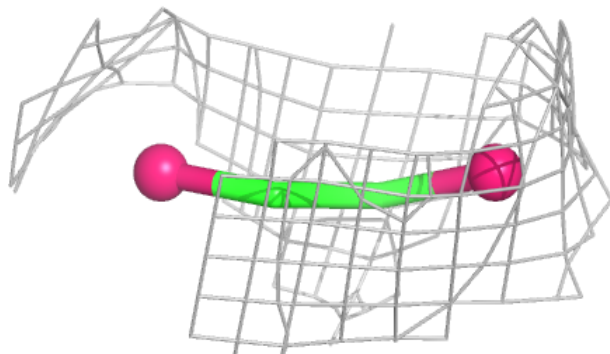
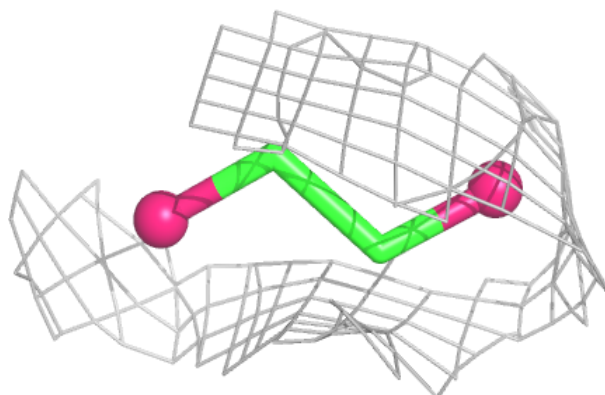


Electron density around EDO C 415:

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

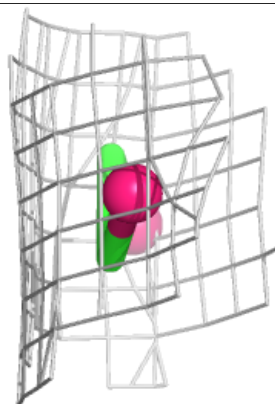
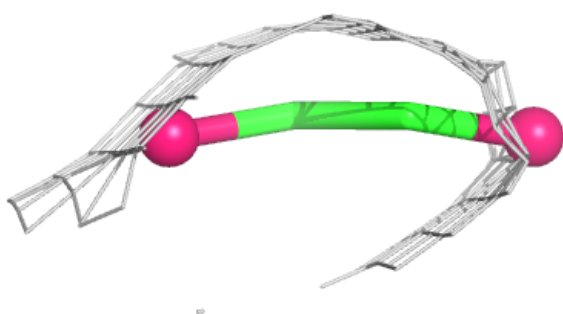
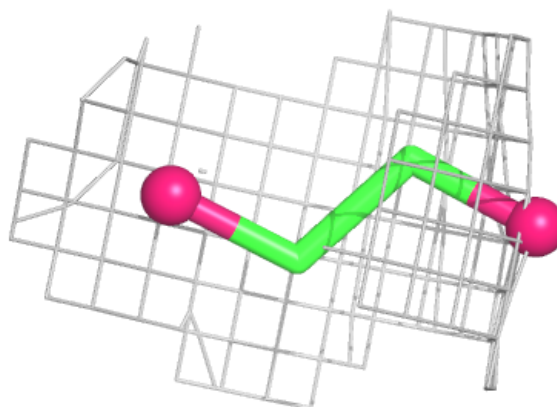
**Electron density around EDO C 417:**

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

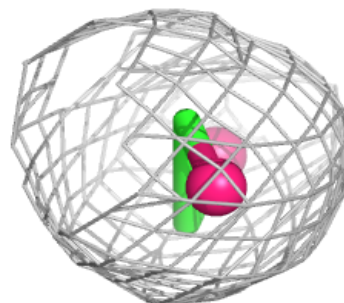
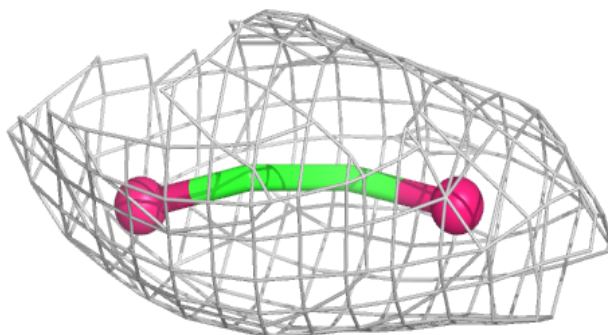
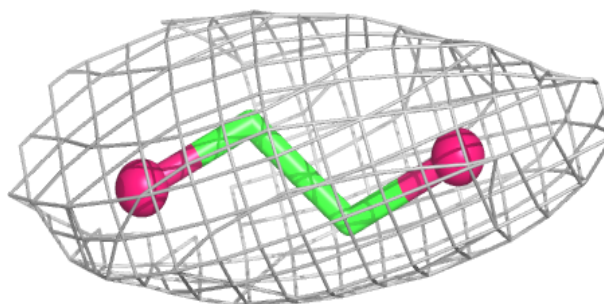


Electron density around EDO D 428:

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

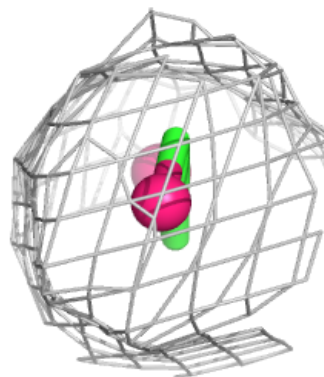
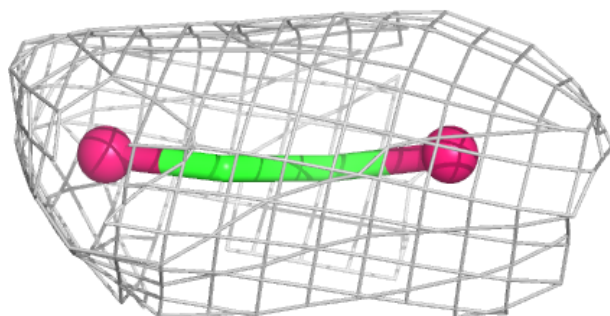
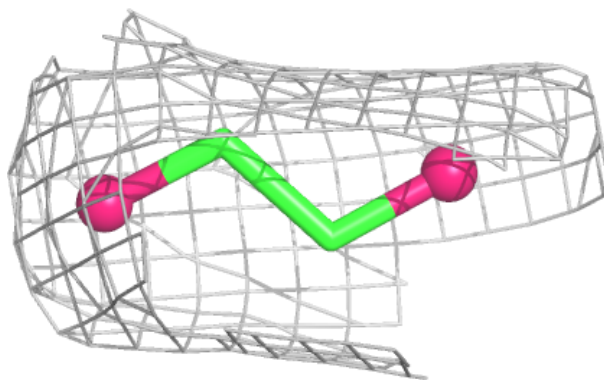
**Electron density around EDO A 430:**

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

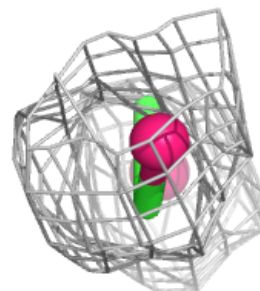
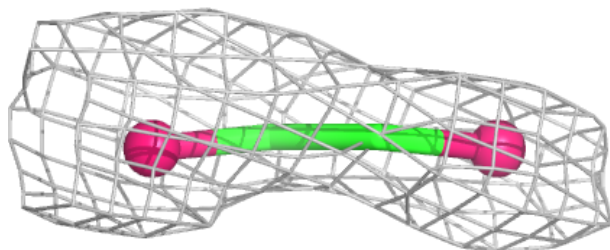
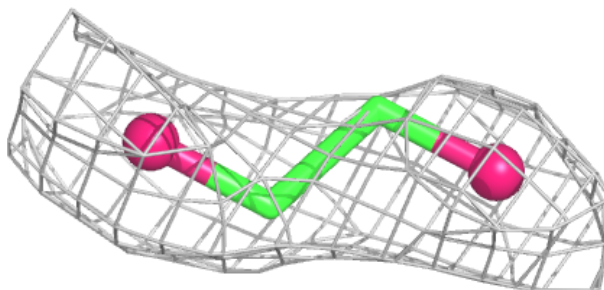


Electron density around EDO C 419:

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

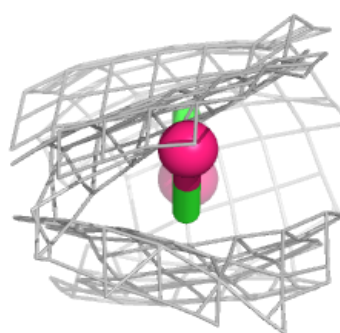
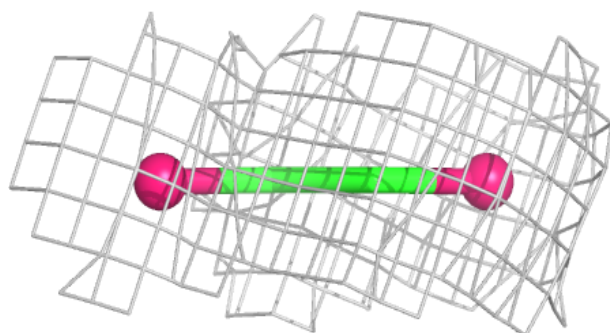
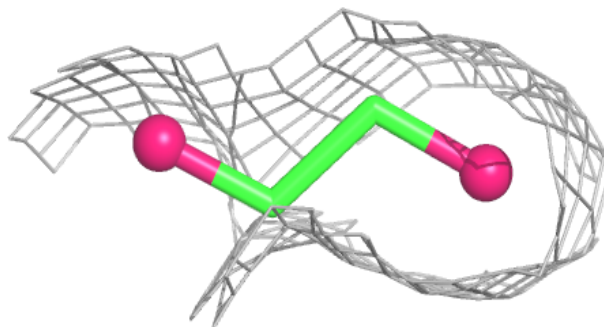
**Electron density around EDO F 412:**

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

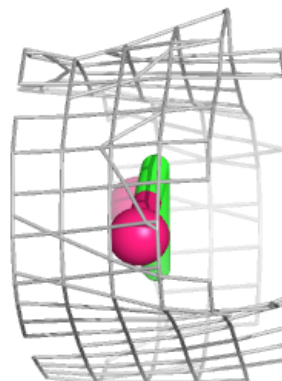
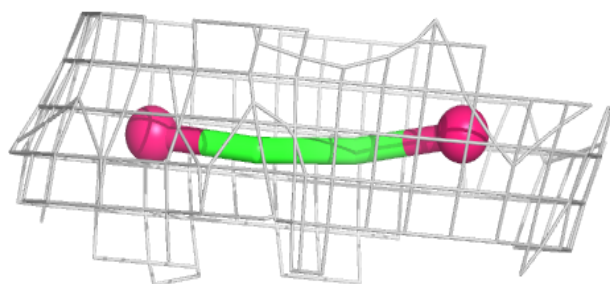
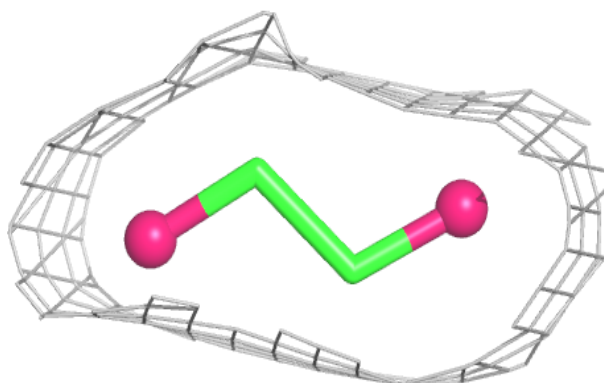


Electron density around EDO F 413:

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

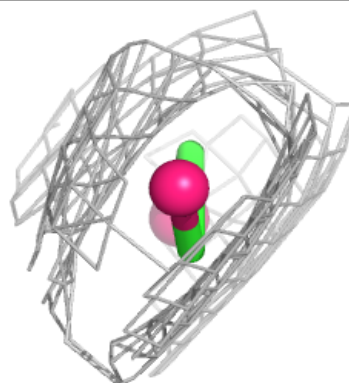
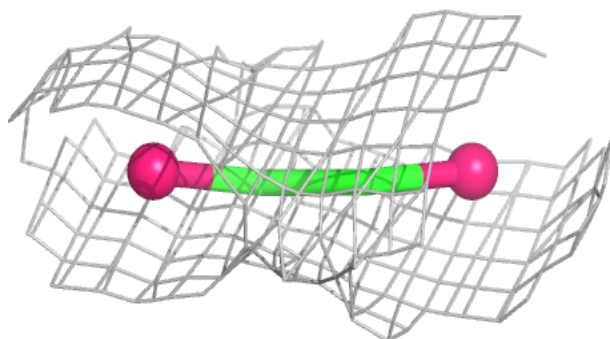
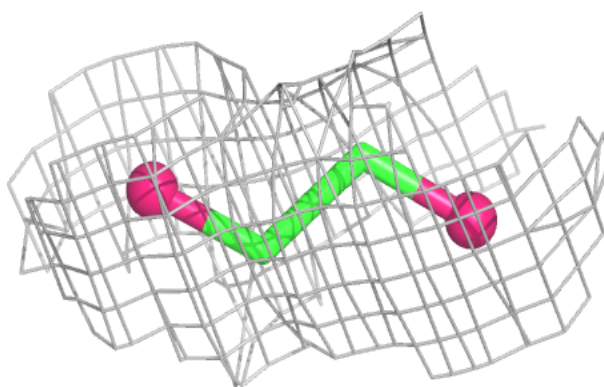
**Electron density around EDO F 415:**

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

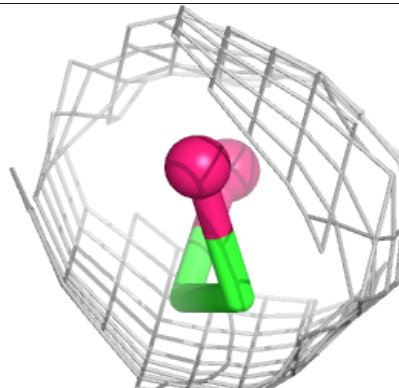
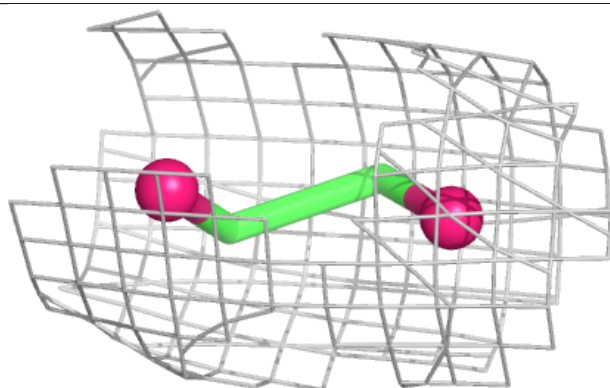
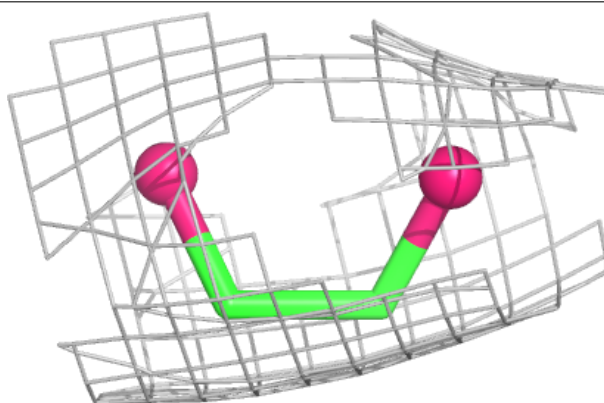


Electron density around EDO A 435:

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

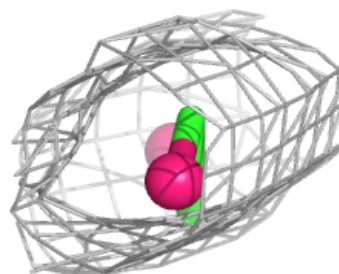
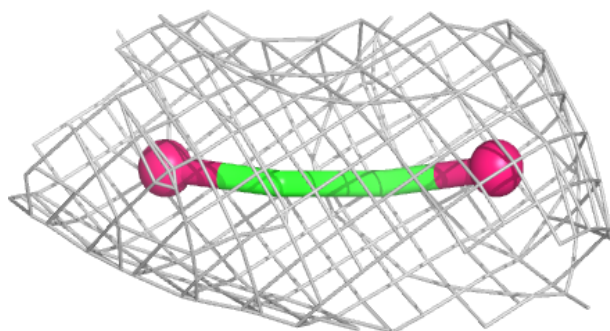
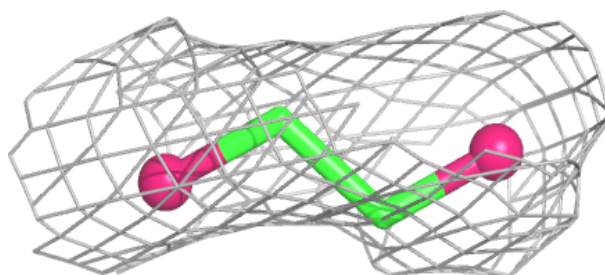
**Electron density around EDO B 432:**

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

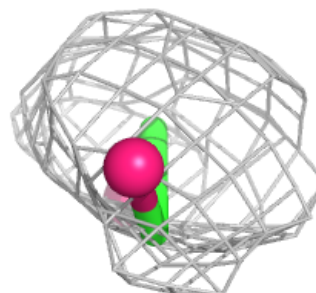
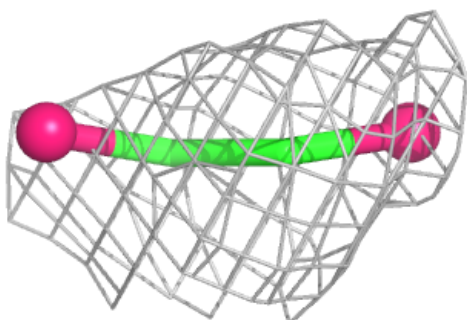
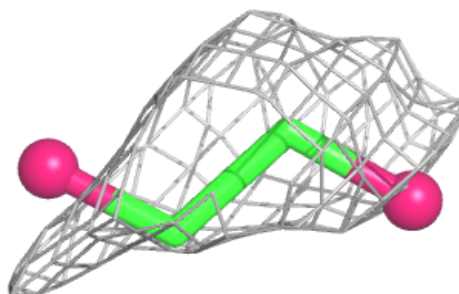


Electron density around EDO F 419:

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

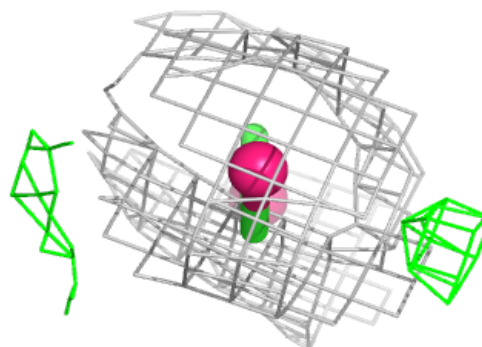
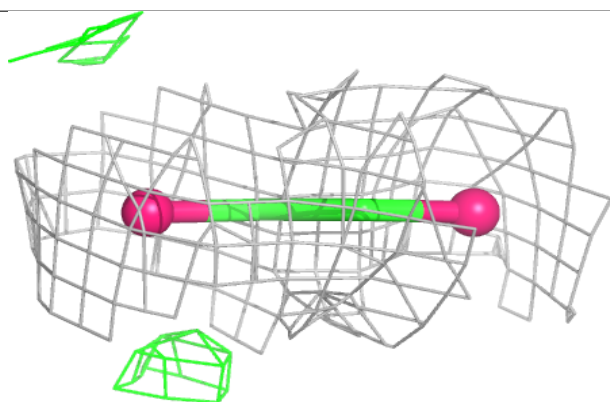
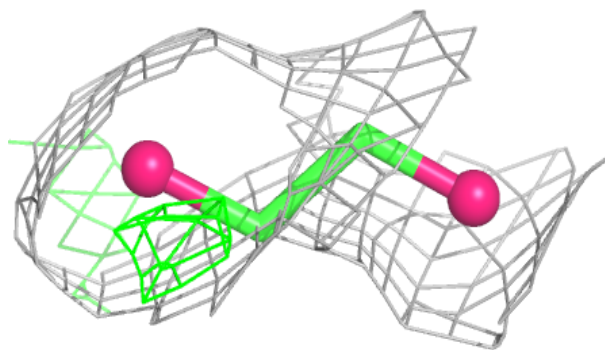
**Electron density around EDO C 423:**

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

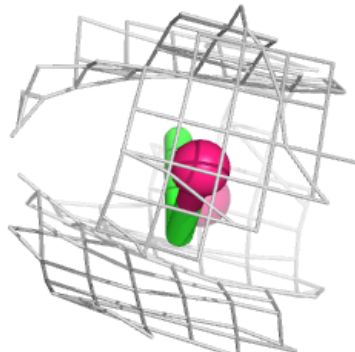
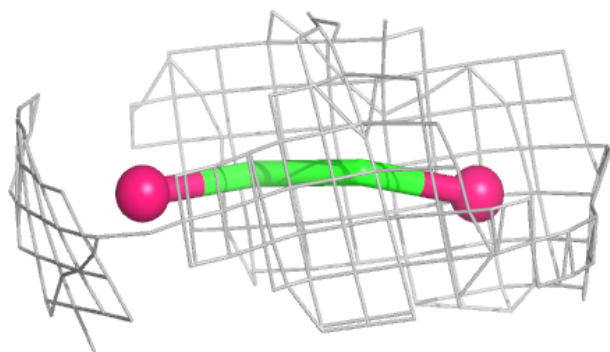
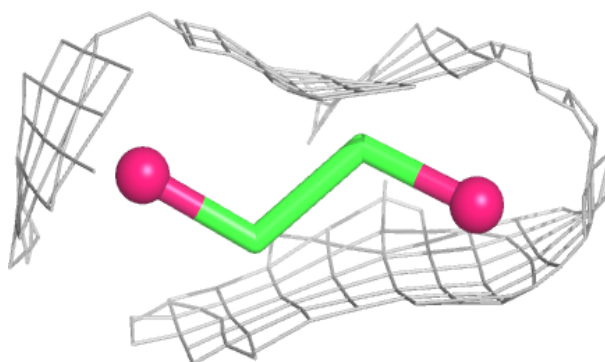


Electron density around EDO F 421:

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

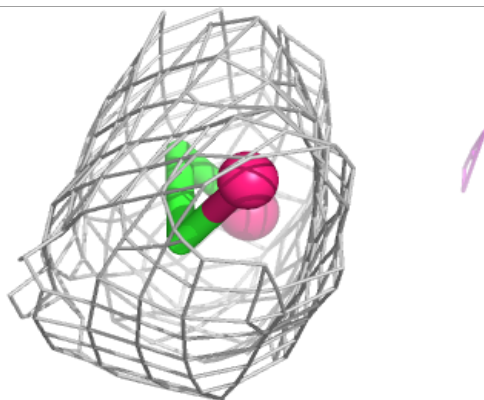
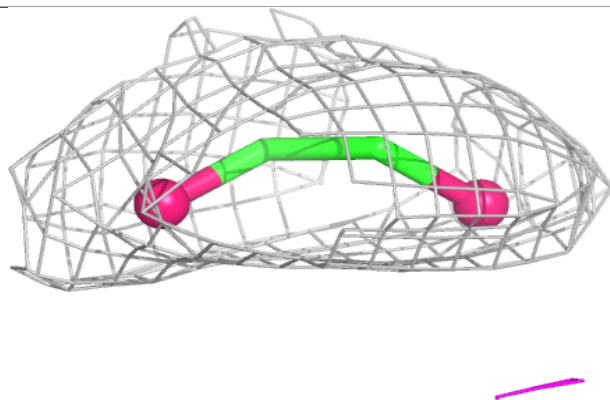
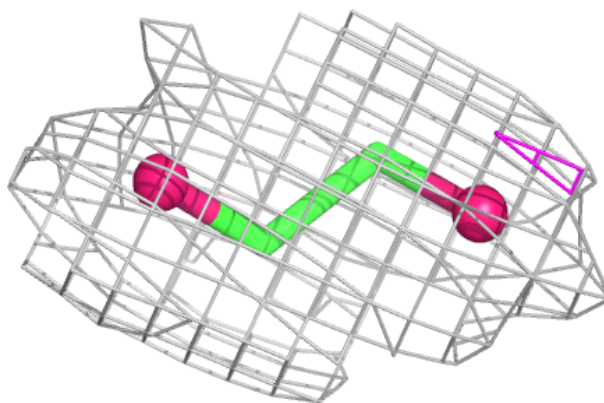
**Electron density around EDO F 423:**

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

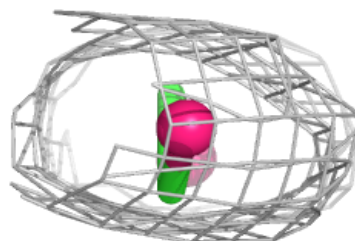
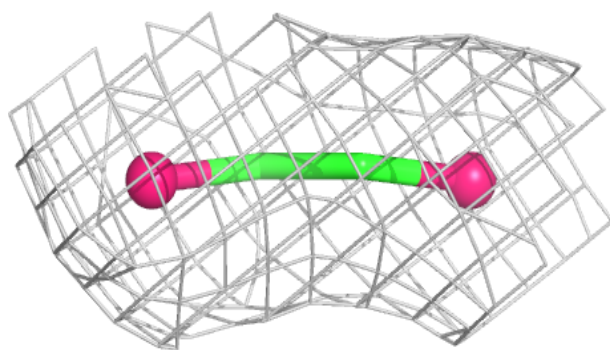
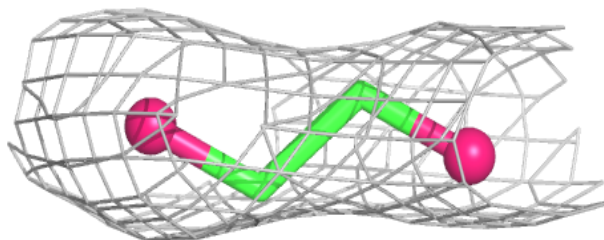


Electron density around EDO B 433:

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

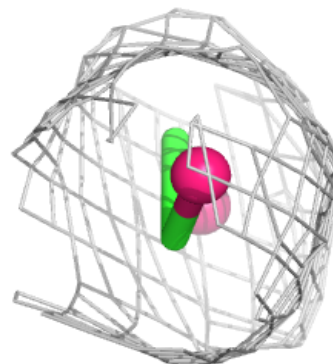
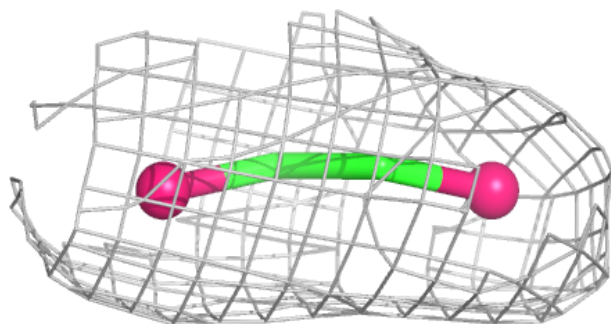
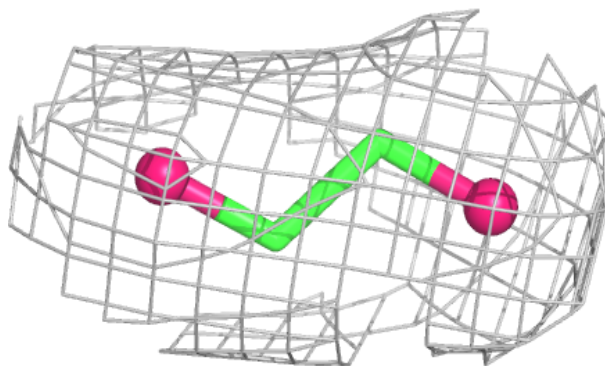
**Electron density around EDO B 413:**

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

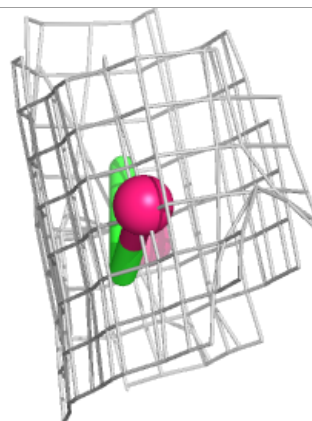
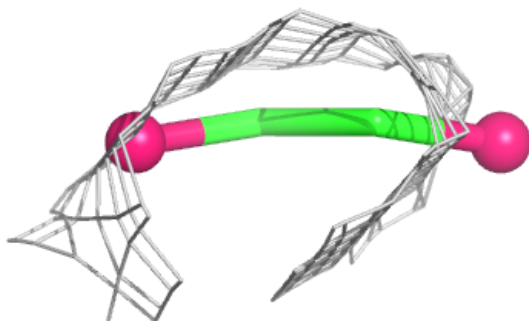
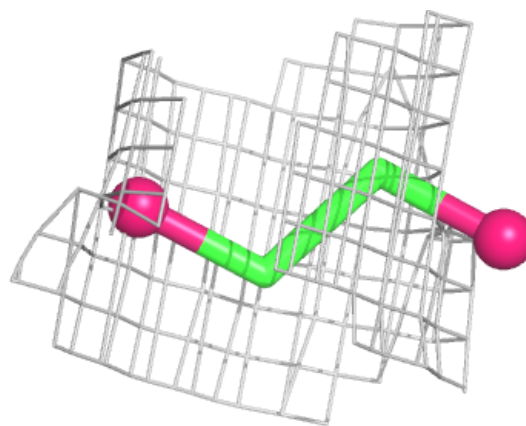


Electron density around EDO F 426:

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

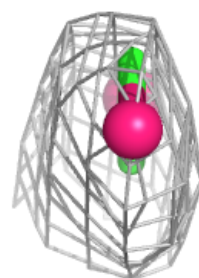
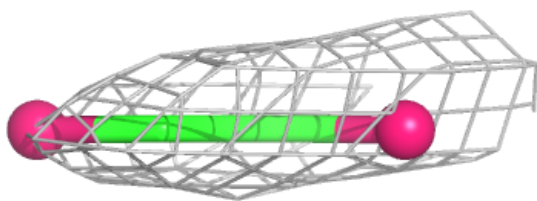
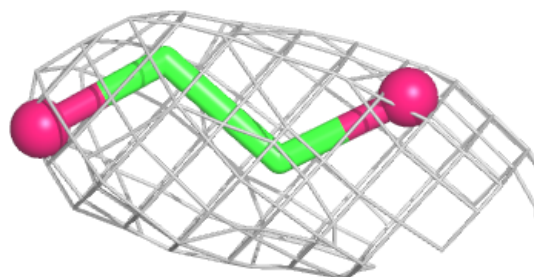
**Electron density around EDO C 426:**

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

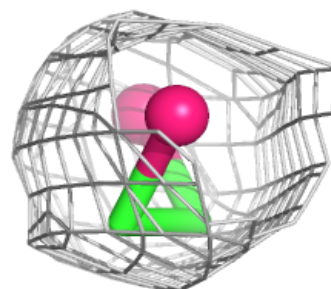
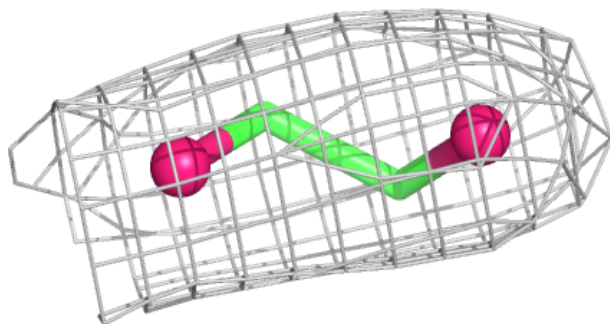
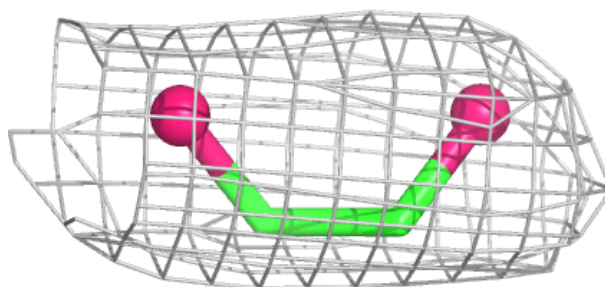


Electron density around EDO D 437:

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

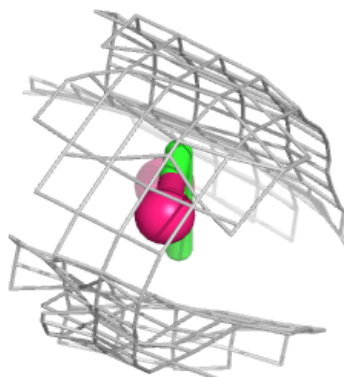
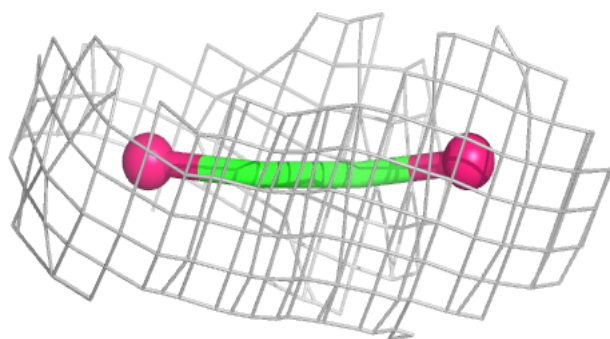
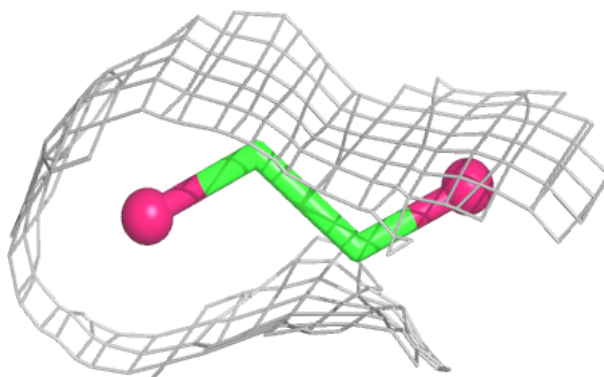
**Electron density around EDO D 438:**

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

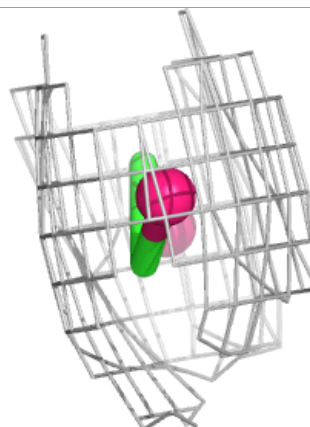
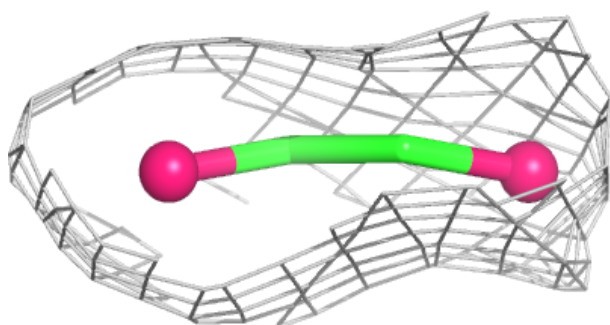
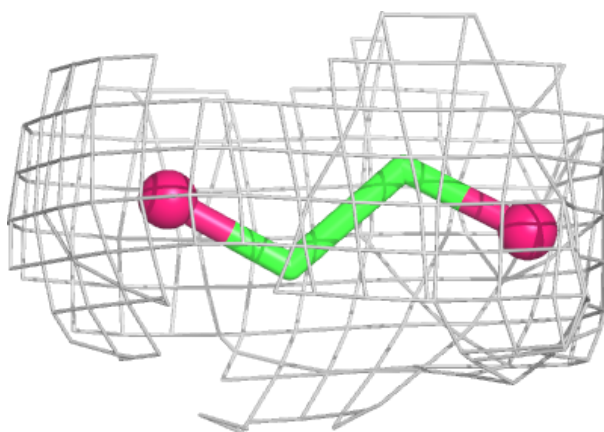


Electron density around EDO A 405:

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

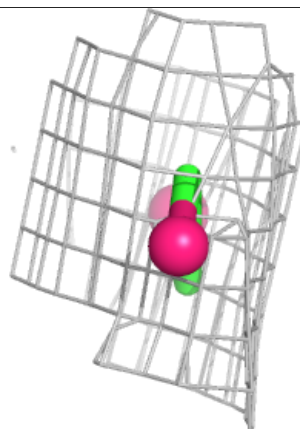
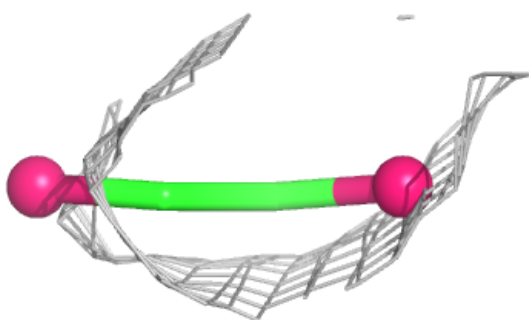
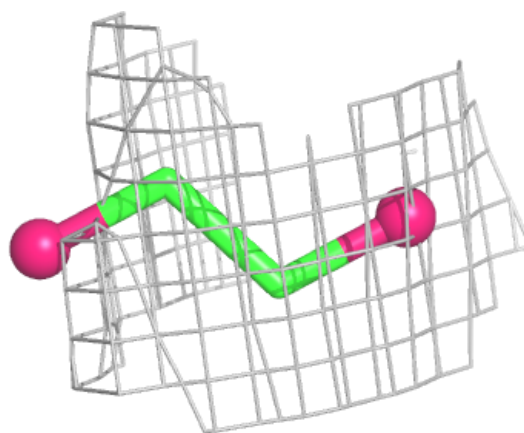
**Electron density around EDO B 436:**

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

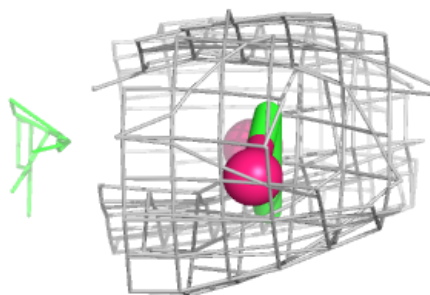
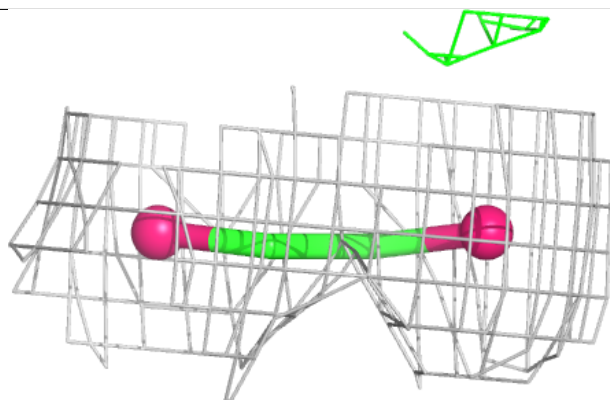
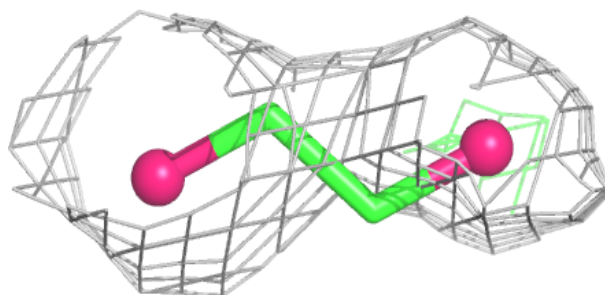


Electron density around EDO F 433:

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

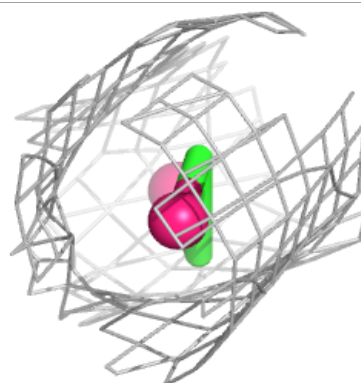
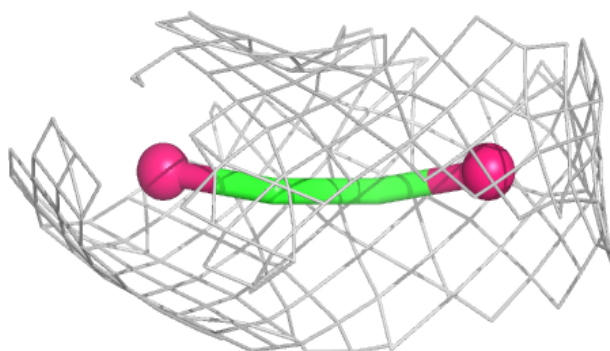
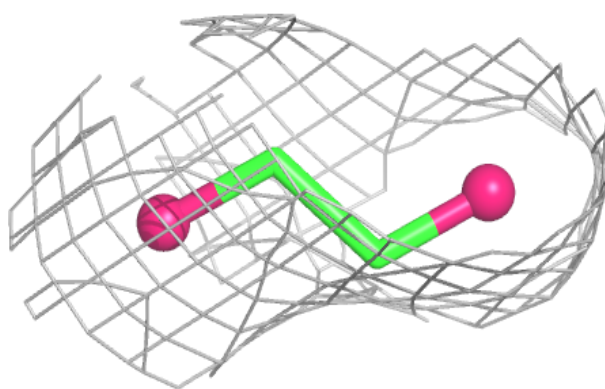
**Electron density around EDO B 415:**

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

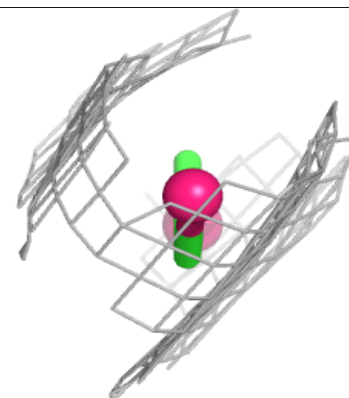
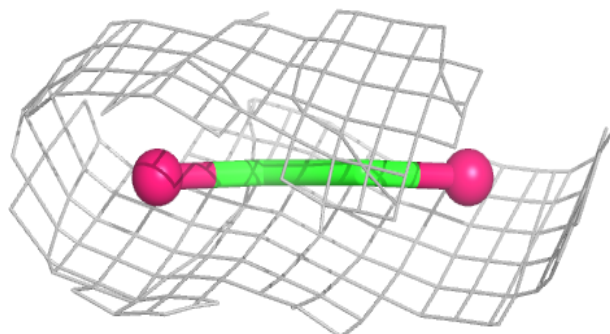
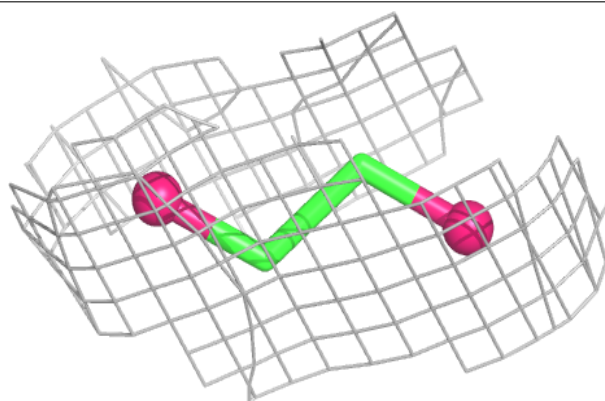


Electron density around EDO B 416:

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

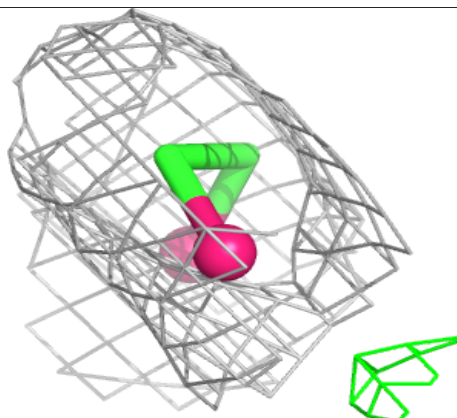
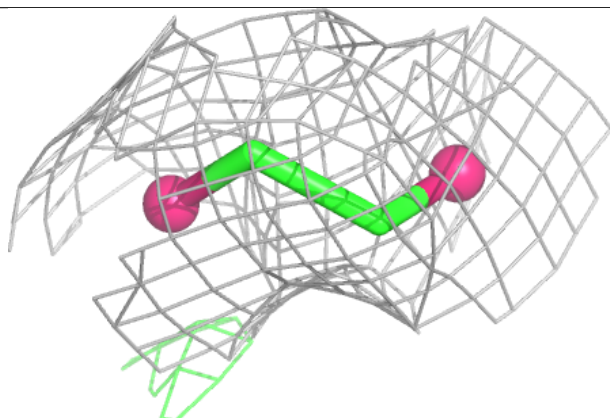
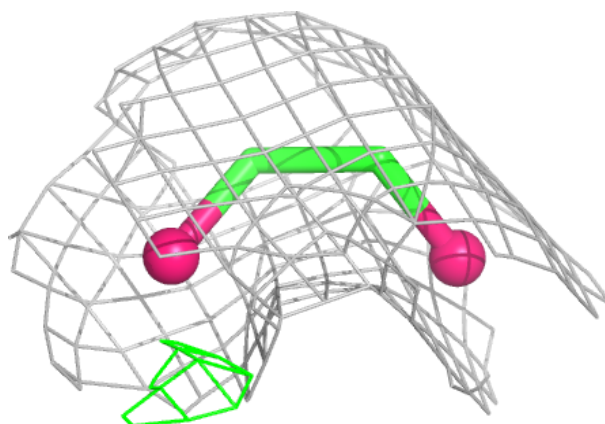
**Electron density around EDO B 401:**

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

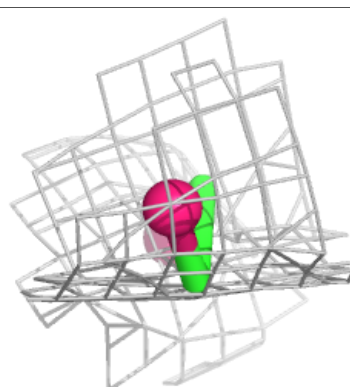
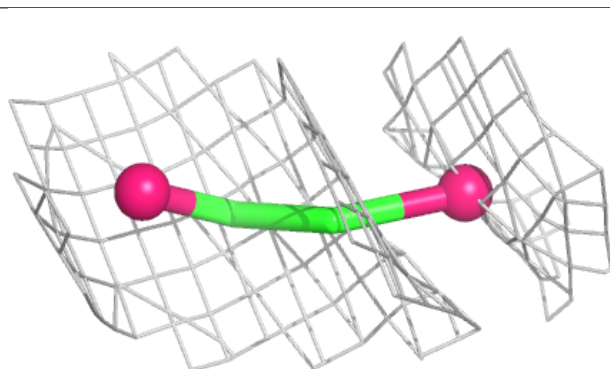
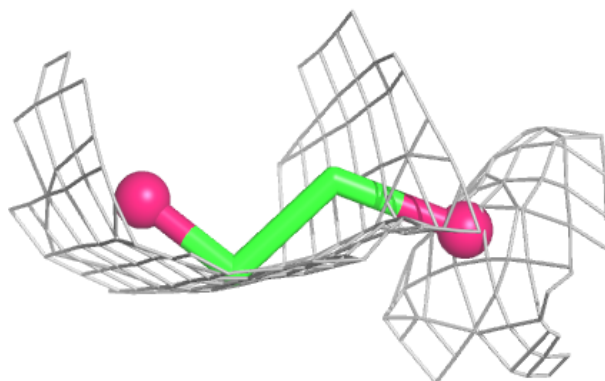


Electron density around EDO E 405:

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

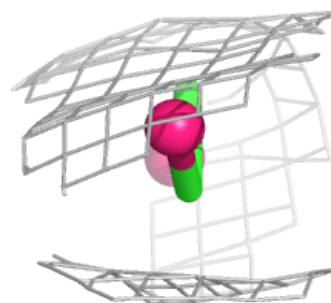
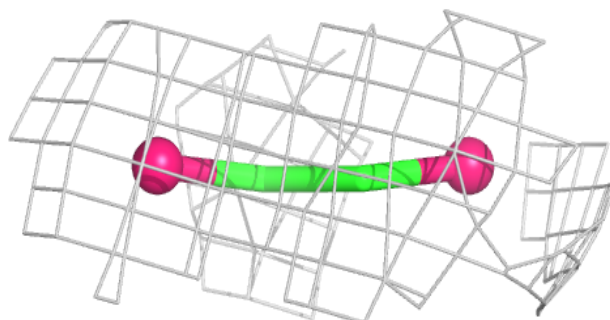
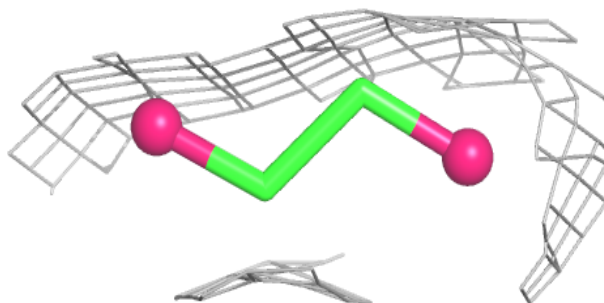
**Electron density around EDO B 440:**

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

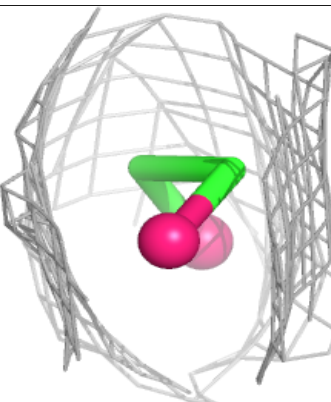
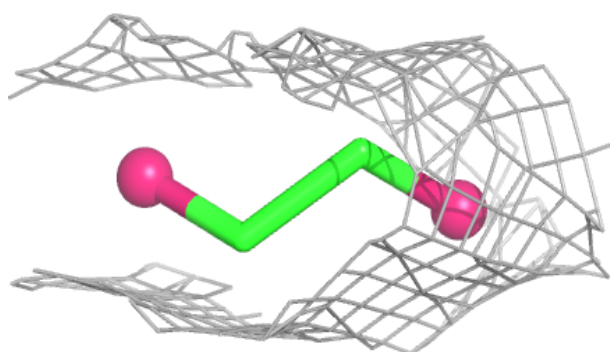
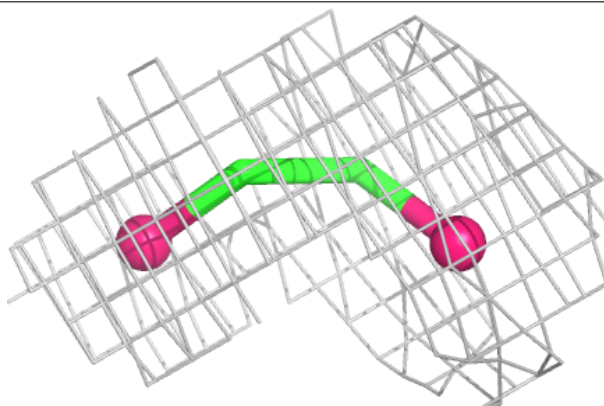


Electron density around EDO E 407:

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

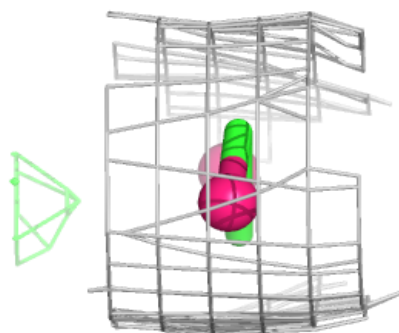
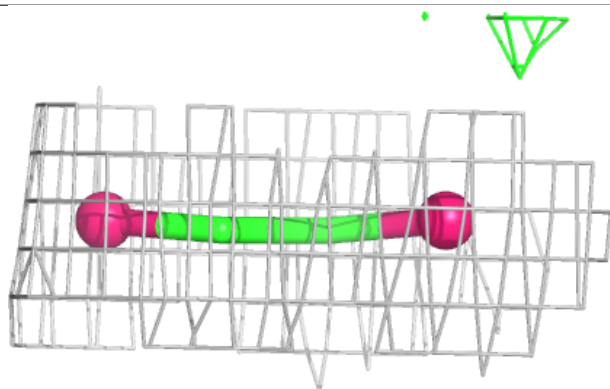
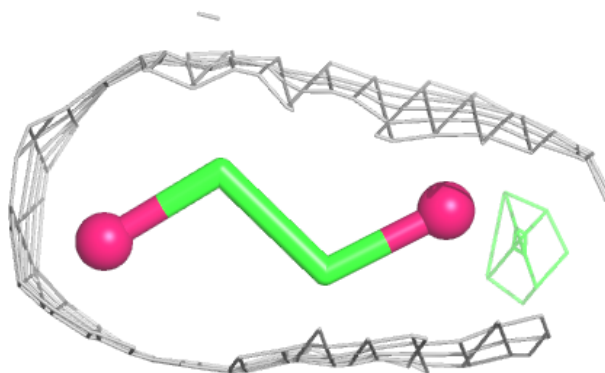
**Electron density around EDO E 408:**

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



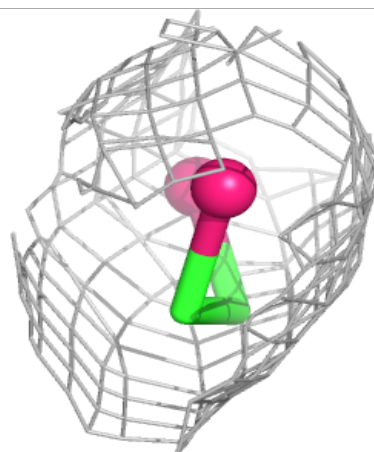
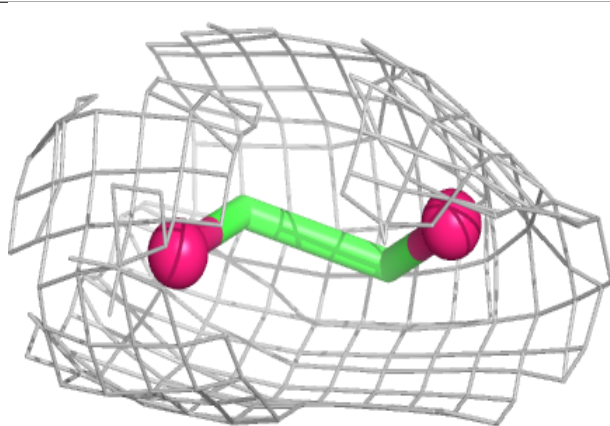
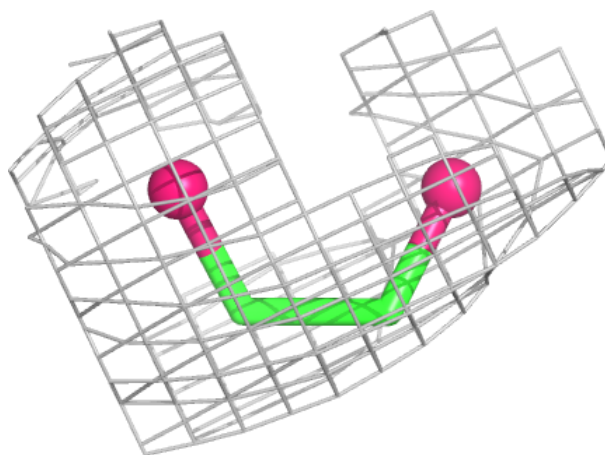
Electron density around EDO E 409:

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



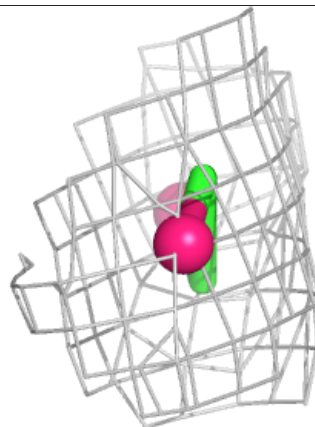
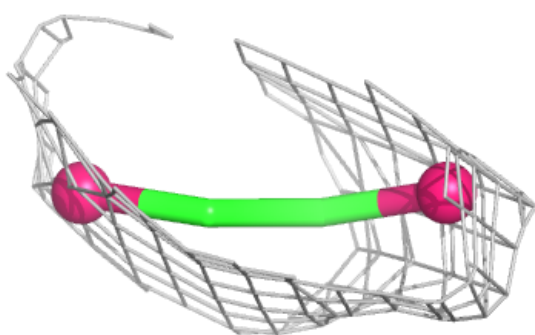
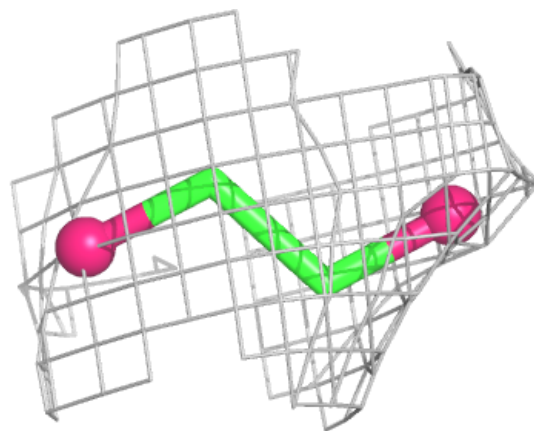
Electron density around EDO A 437:

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

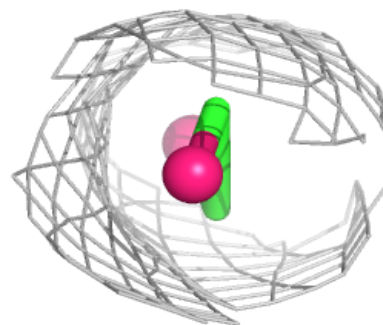
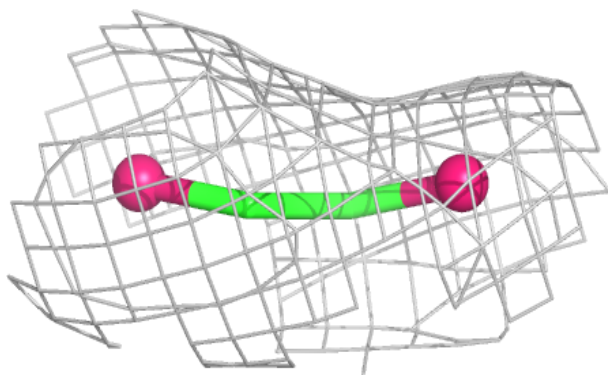
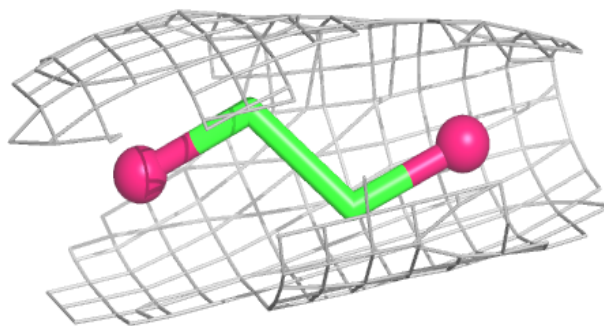


Electron density around EDO A 425:

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

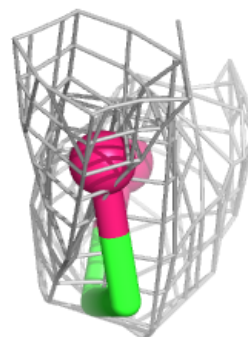
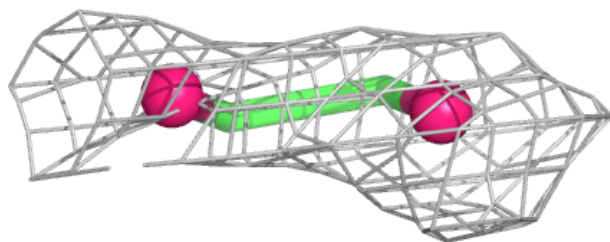
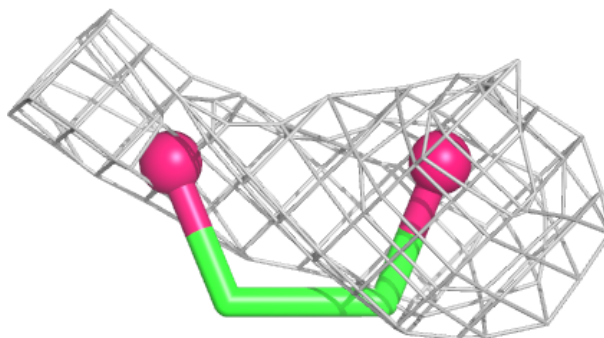
**Electron density around EDO E 412:**

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

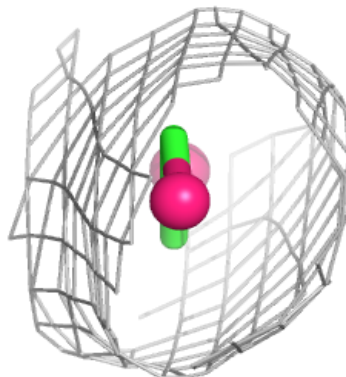
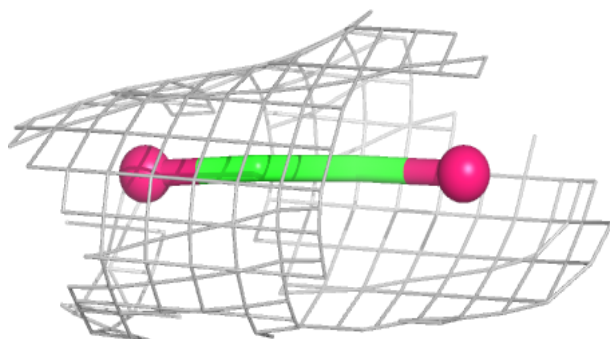
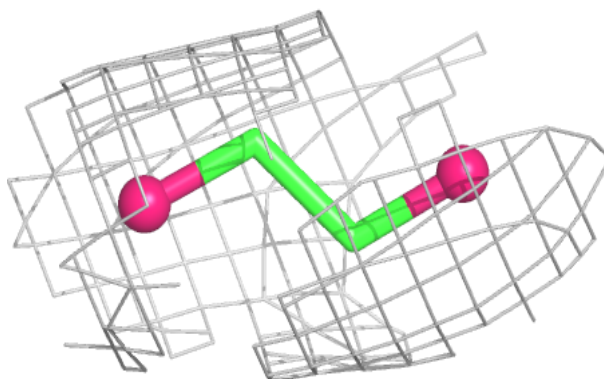


Electron density around EDO B 443:

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

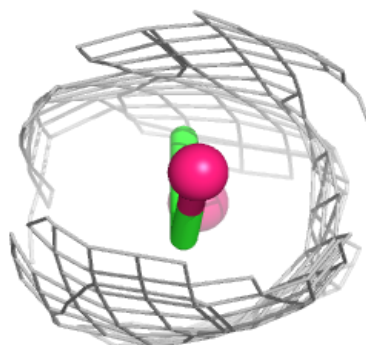
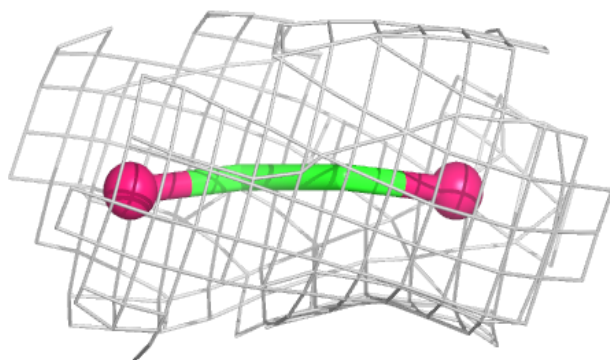
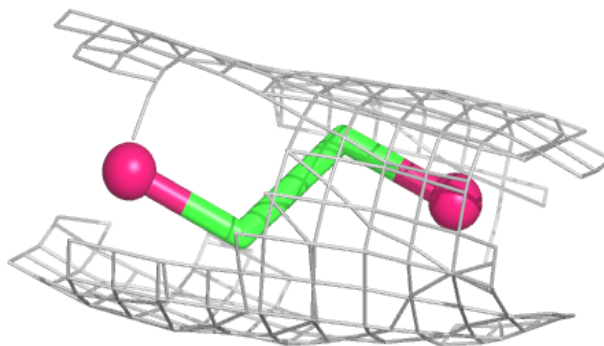
**Electron density around EDO F 417:**

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

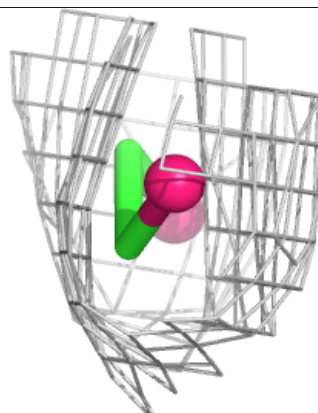
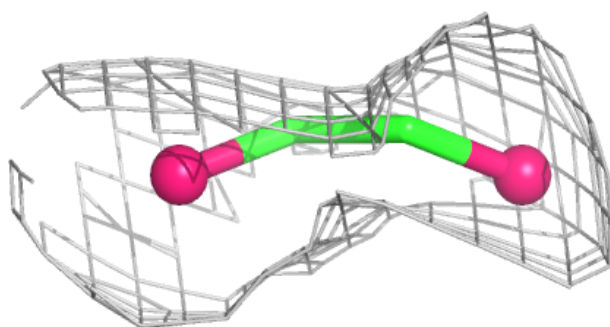
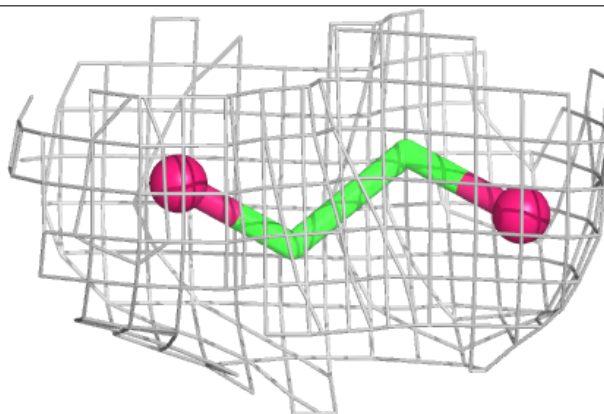


Electron density around EDO B 411:

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

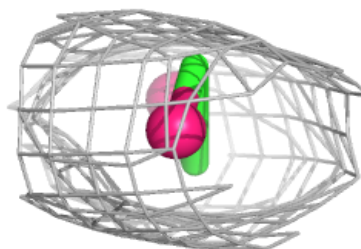
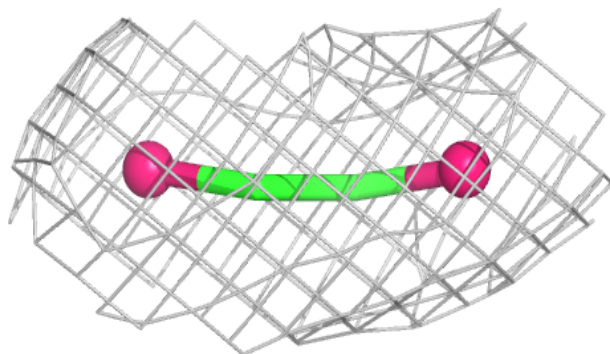
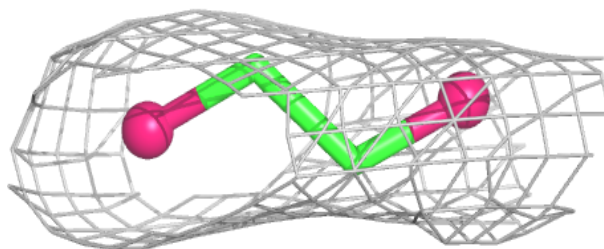
**Electron density around EDO E 440:**

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

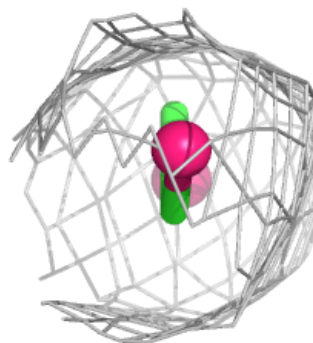
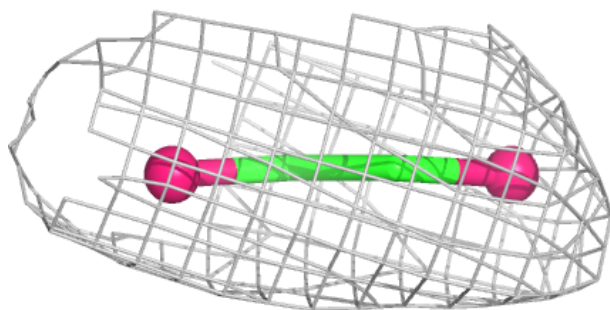
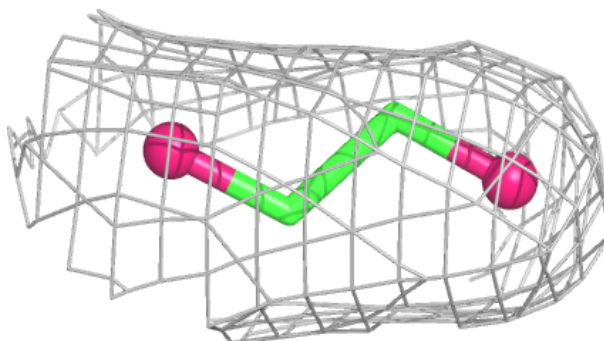


Electron density around EDO C 413:

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

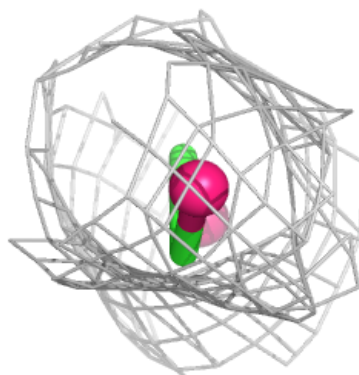
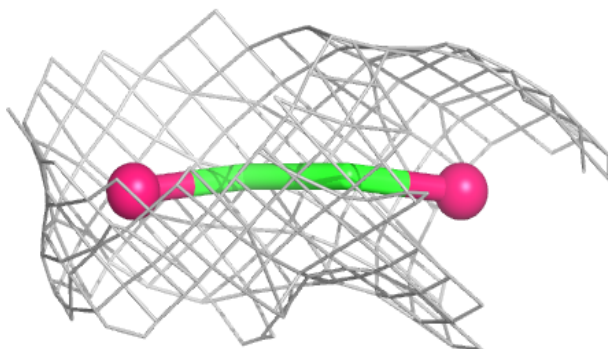
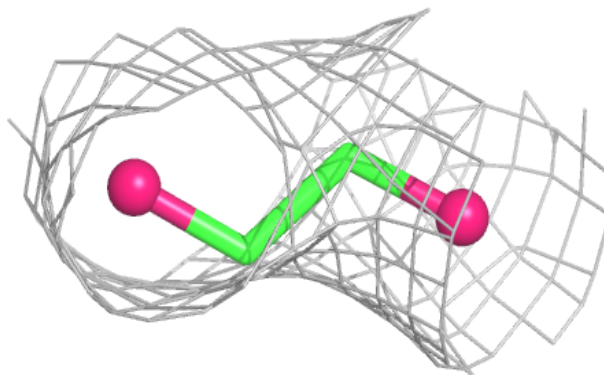
**Electron density around EDO B 420:**

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

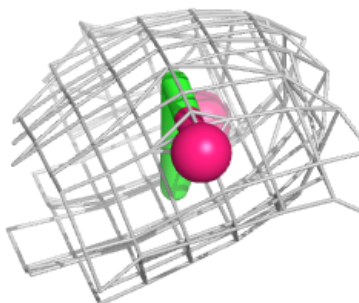
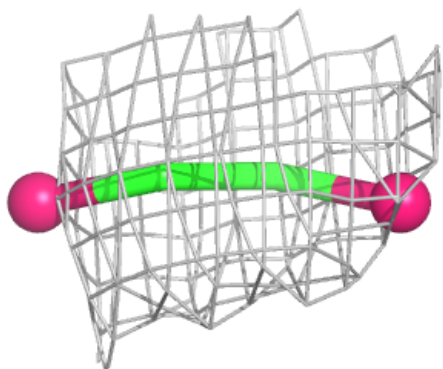
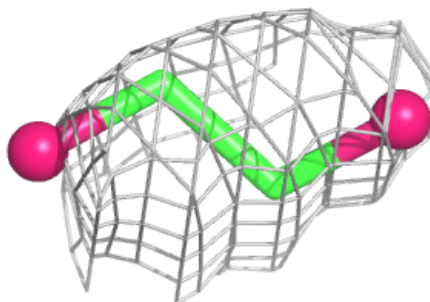


Electron density around EDO F 422:

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

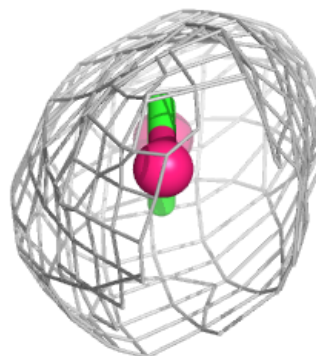
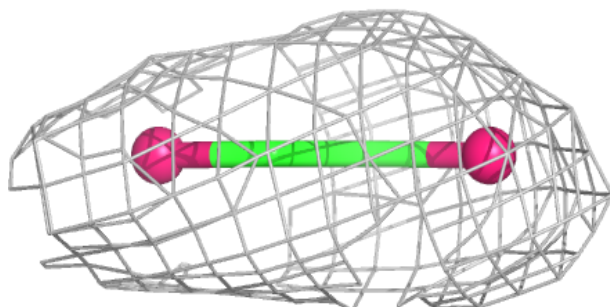
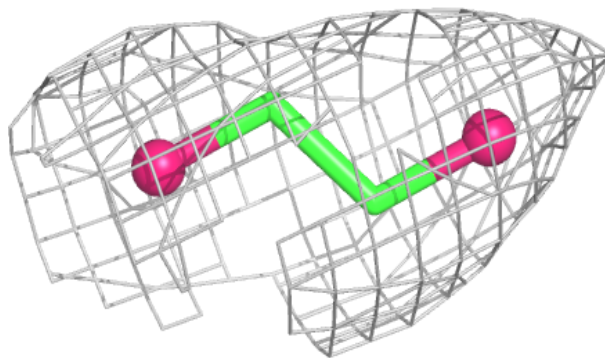
**Electron density around EDO B 404:**

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

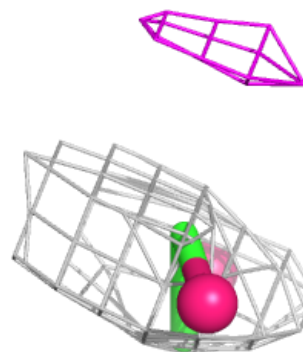
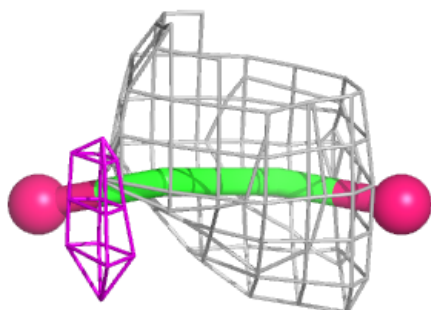
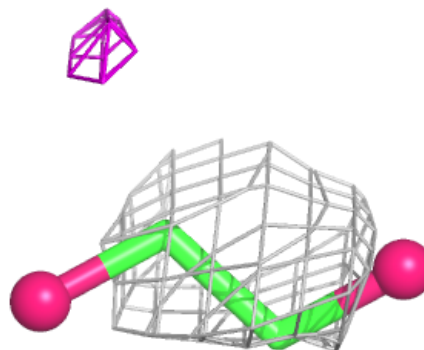


Electron density around EDO D 423:

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

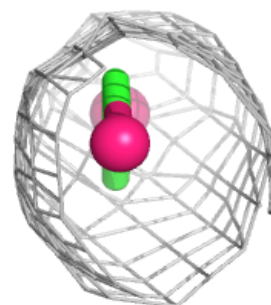
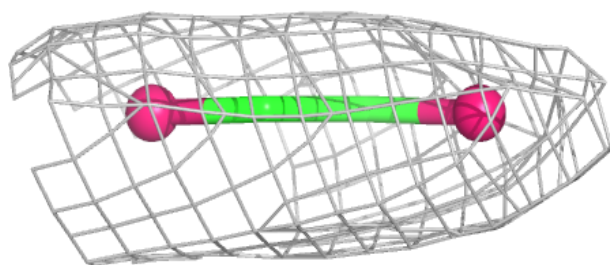
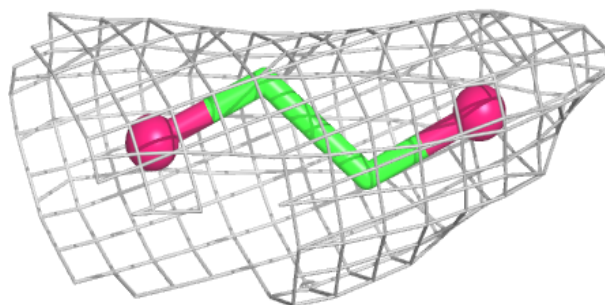
**Electron density around EDO D 405:**

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

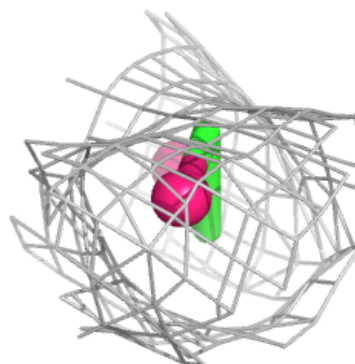
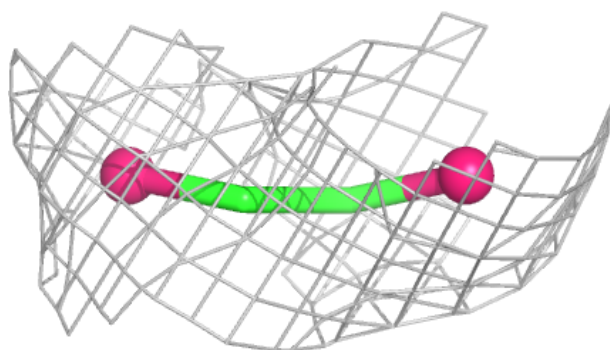
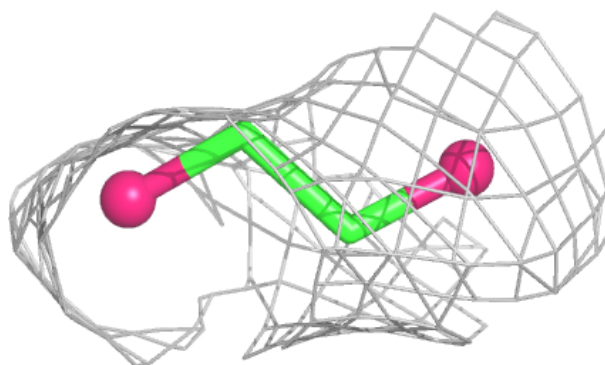


Electron density around EDO E 424:

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

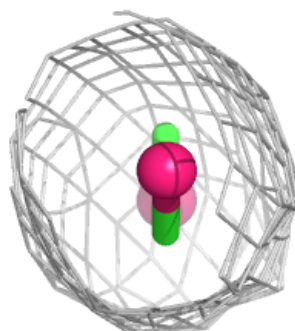
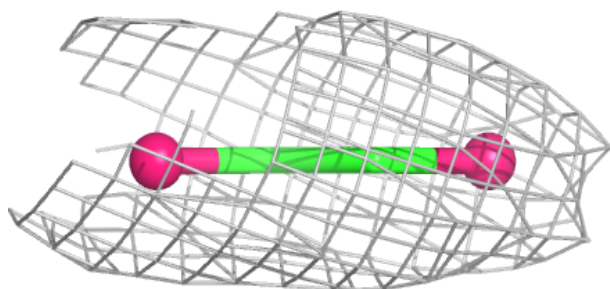
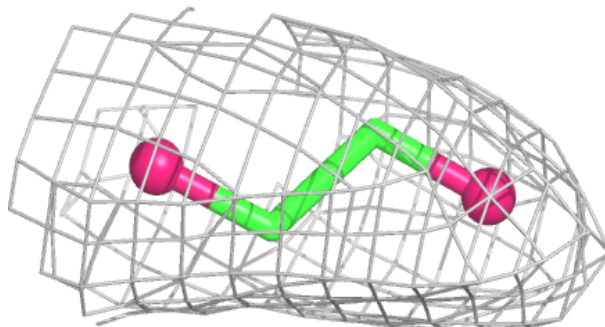
**Electron density around EDO C 416:**

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

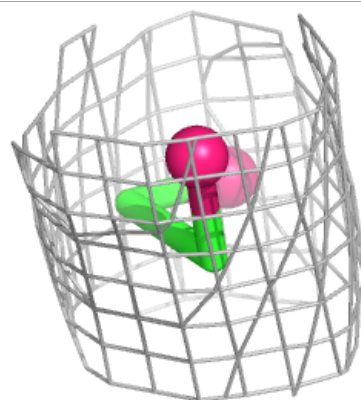
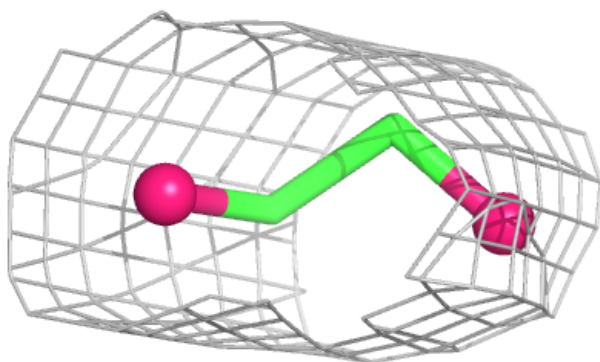
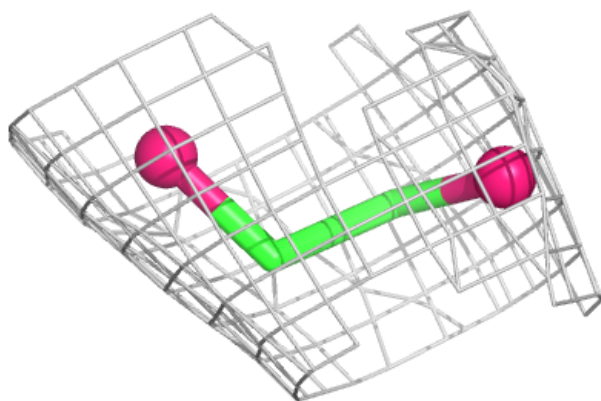


Electron density around EDO F 428:

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

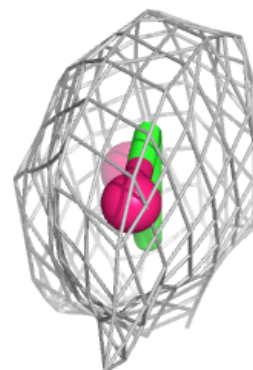
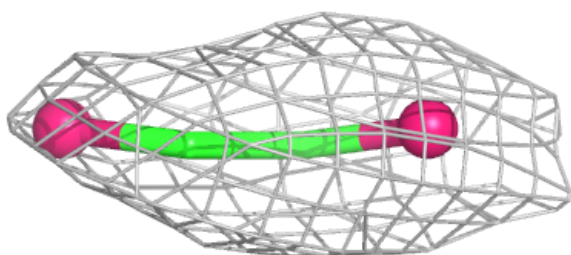
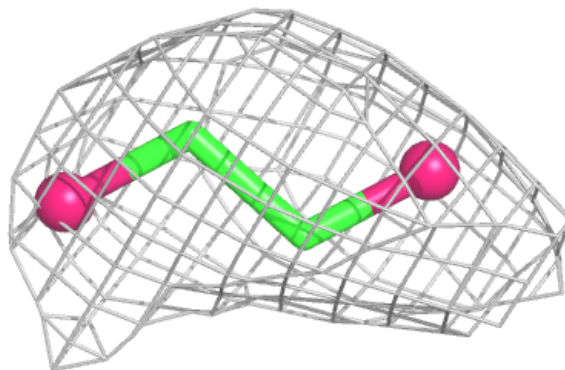
**Electron density around EDO E 448:**

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

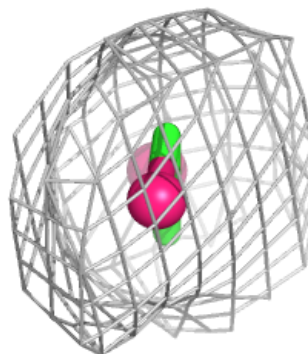
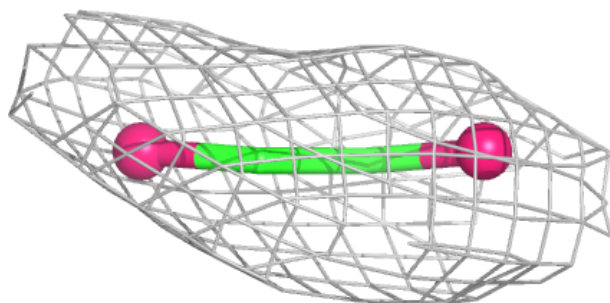
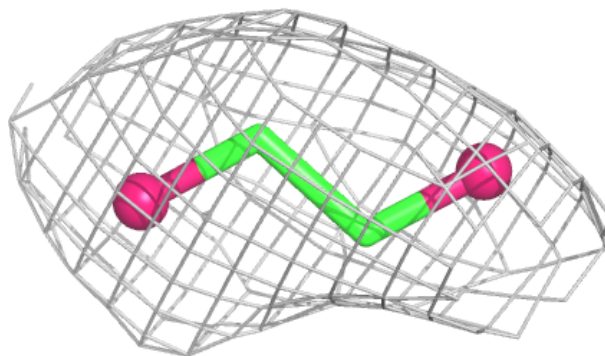


Electron density around EDO F 401:

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

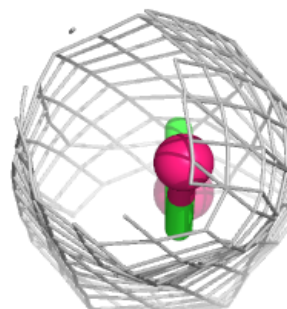
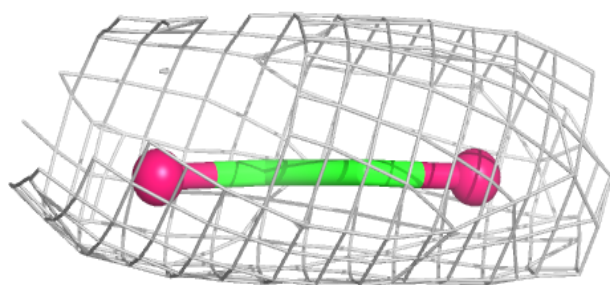
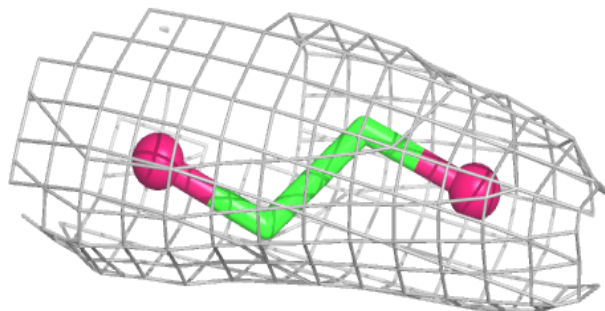
**Electron density around EDO C 430:**

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

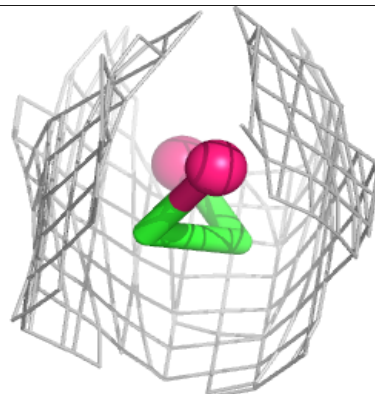
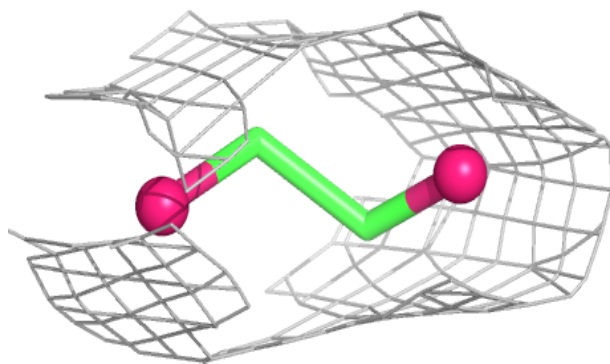
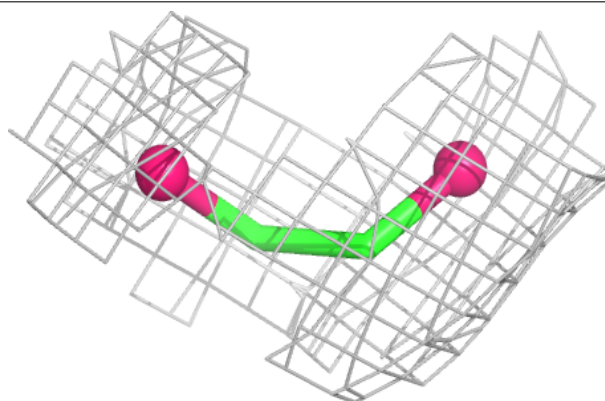


Electron density around EDO B 422:

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

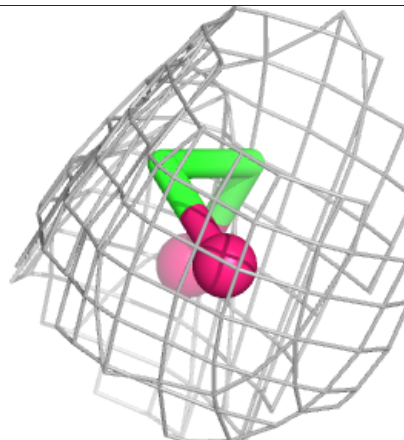
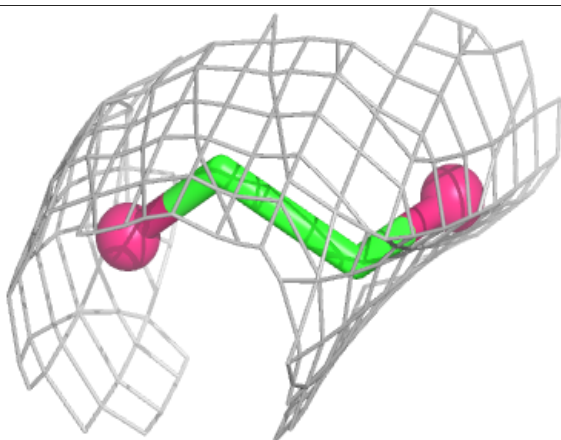
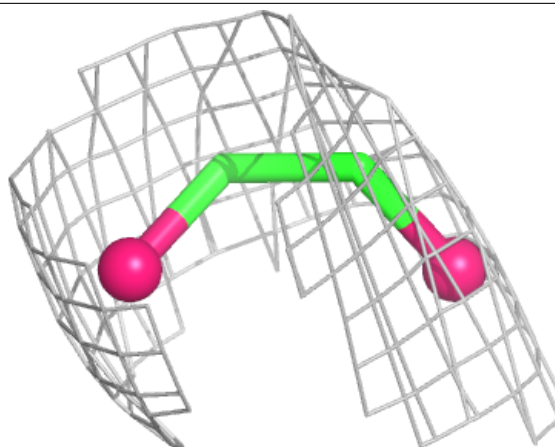
**Electron density around EDO D 409:**

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

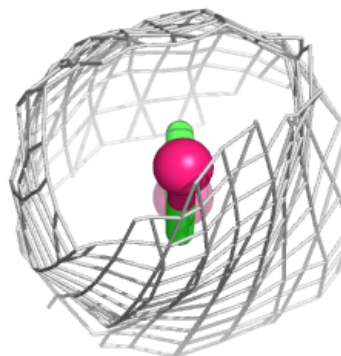
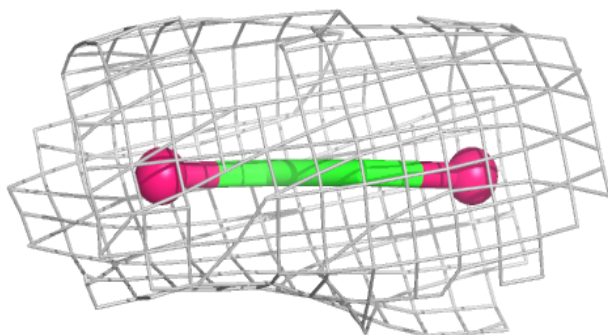
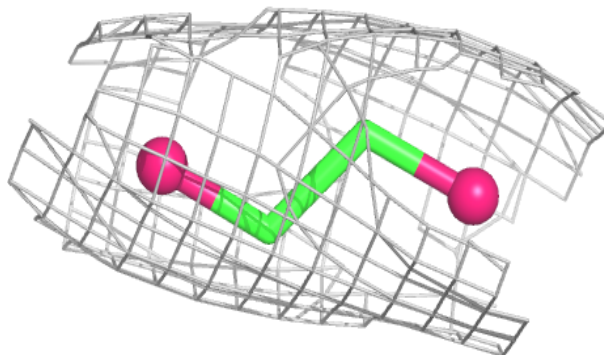


Electron density around EDO A 441:

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

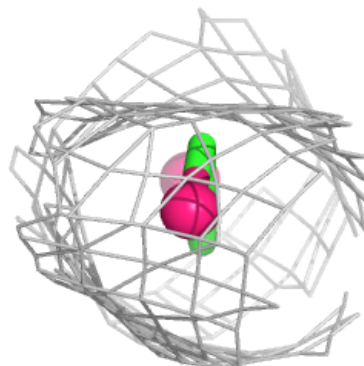
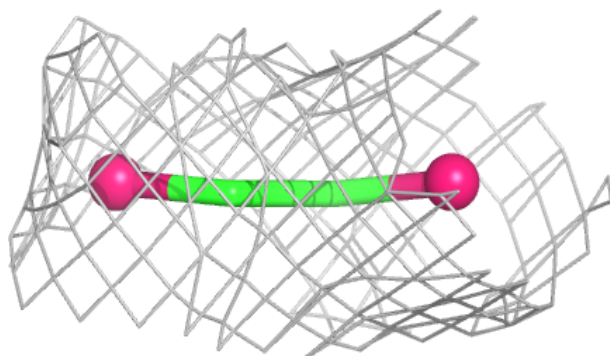
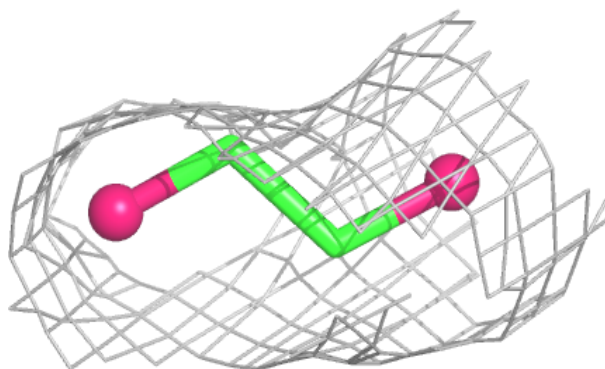
**Electron density around EDO A 409:**

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

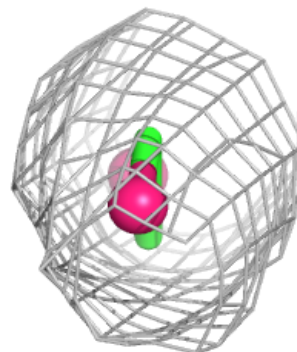
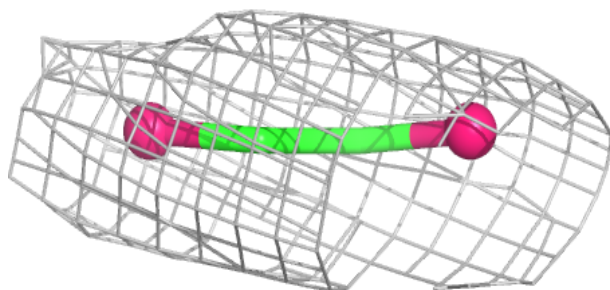
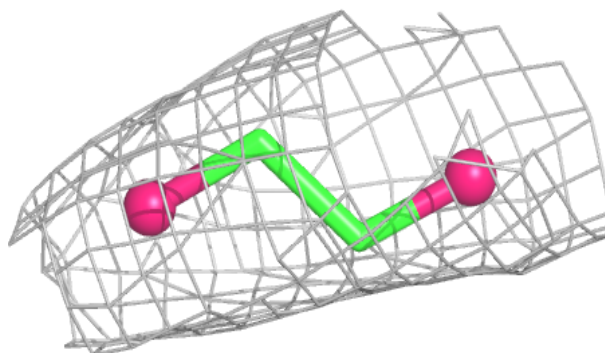


Electron density around EDO A 414:

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

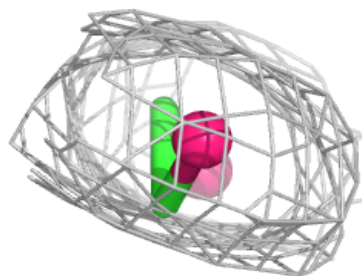
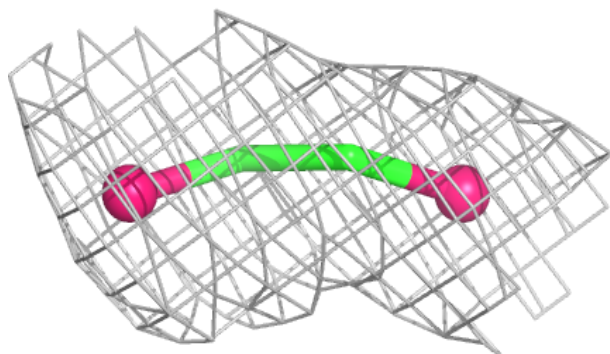
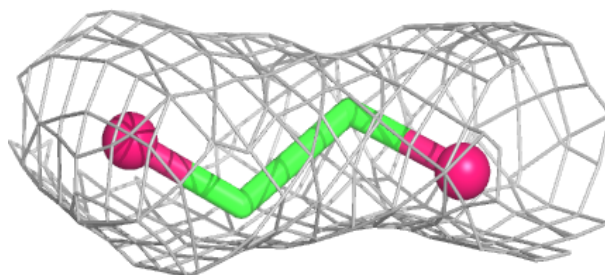
**Electron density around EDO C 421:**

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

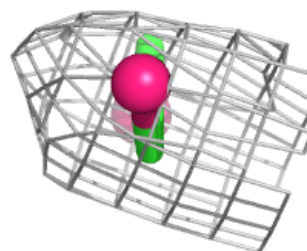
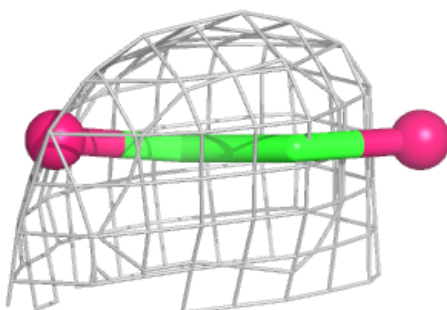
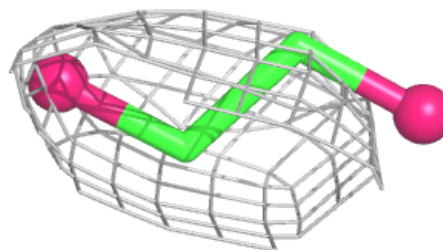


Electron density around EDO D 414:

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

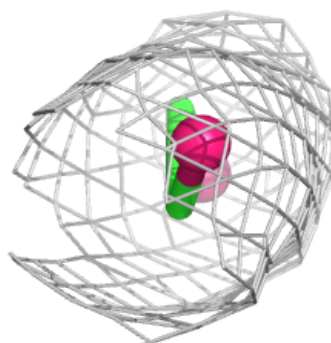
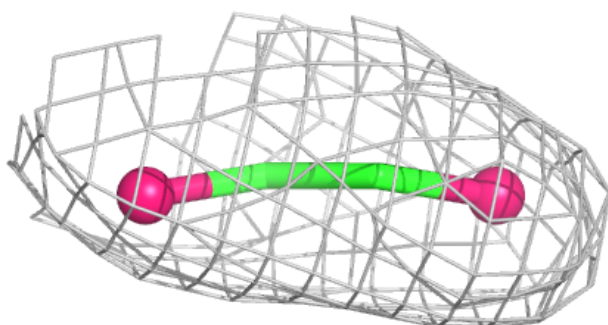
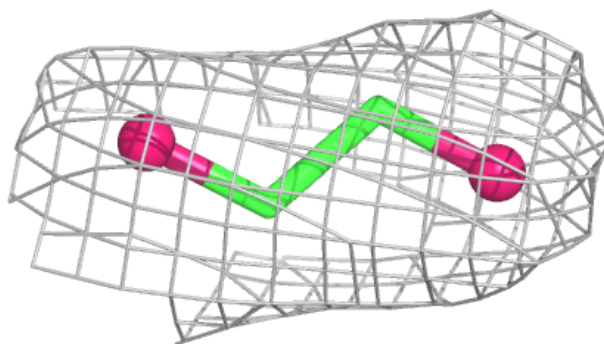
**Electron density around EDO F 410:**

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

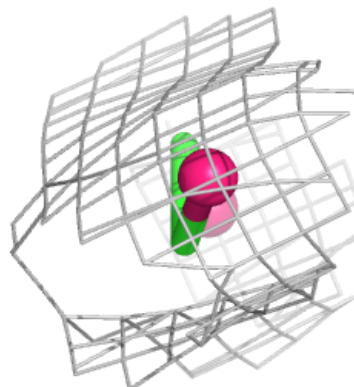
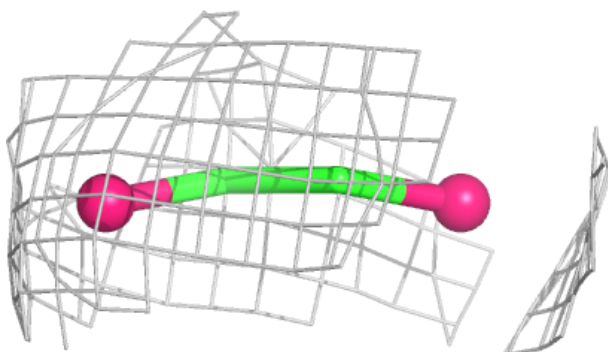
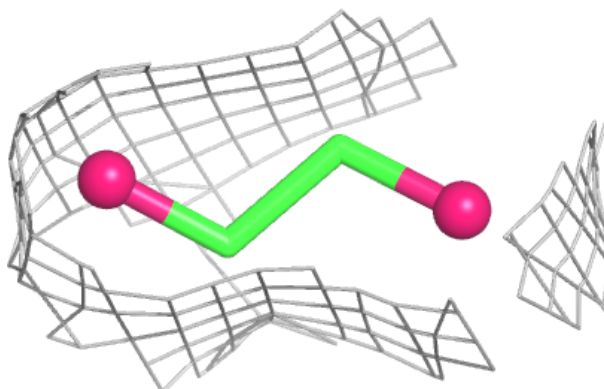


Electron density around EDO A 418:

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

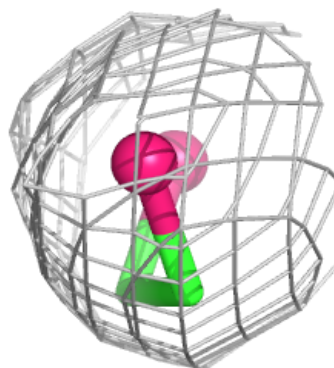
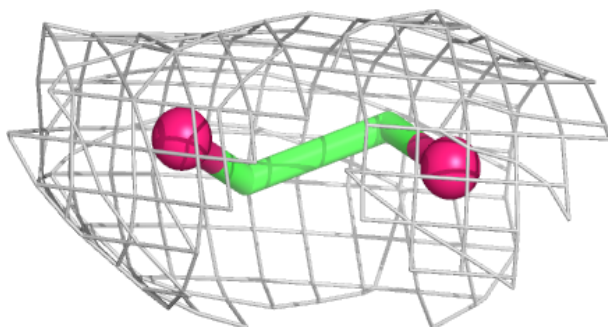
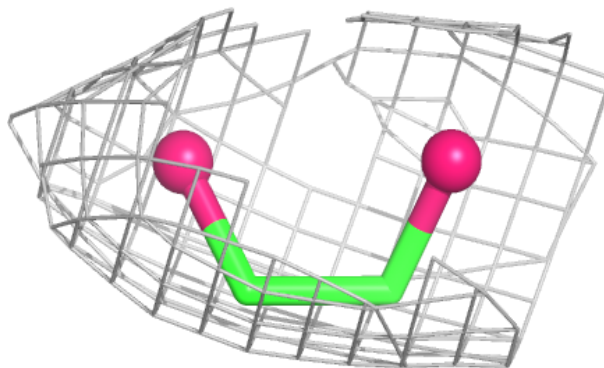
**Electron density around EDO A 415:**

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

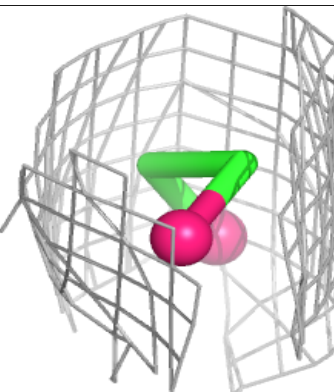
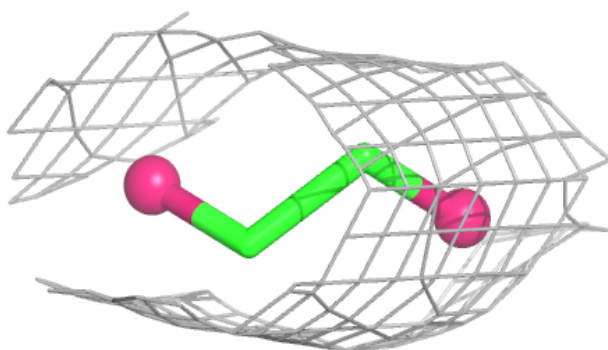
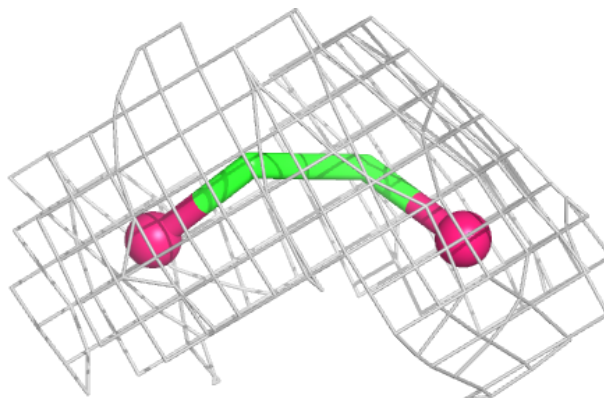


Electron density around EDO E 436:

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

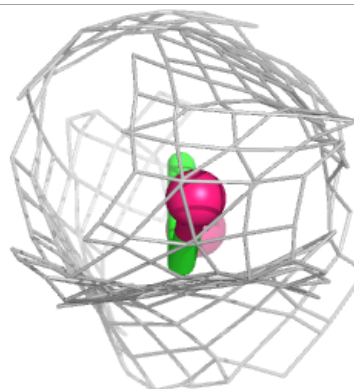
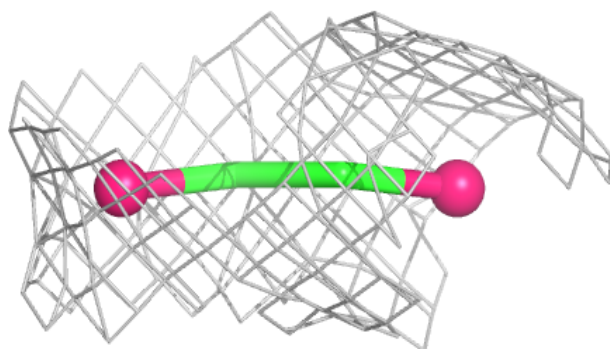
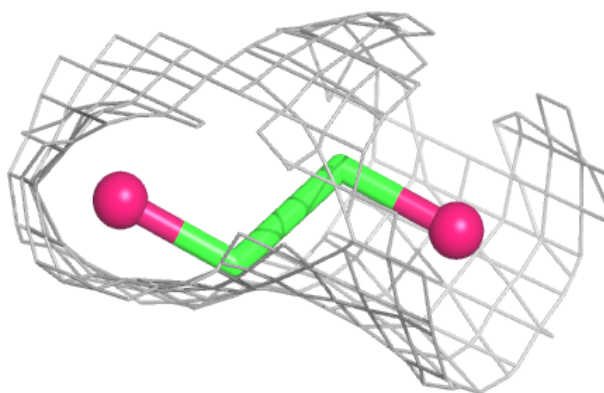
**Electron density around EDO F 414:**

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

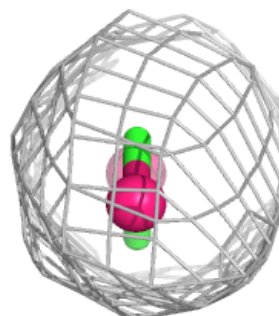
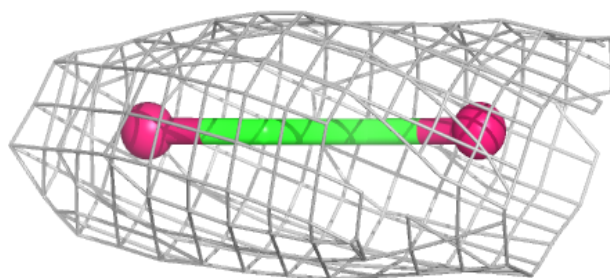
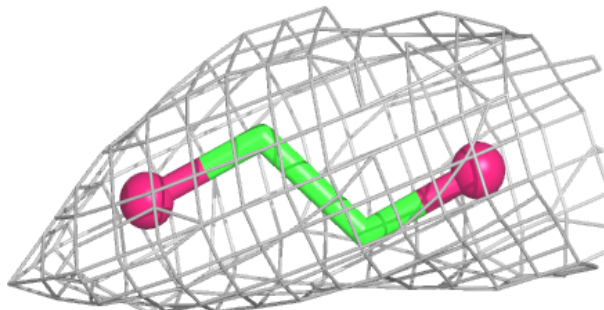


Electron density around EDO D 417:

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

**Electron density around EDO A 420:**

$2mF_o-DF_c$ (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.