



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2022 – 04:11 PM JST

PDB ID : 7DT1  
Title : The structure of Lactobacillus fermentum 4,6-alpha-Glucanotransferase  
Authors : Yang, W.K.; Yong, Y.H.; Wu, L.; Chen, S.; Zhou, J.H.; Wu, J.  
Deposited on : 2021-01-04  
Resolution : 2.43 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.25  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.25

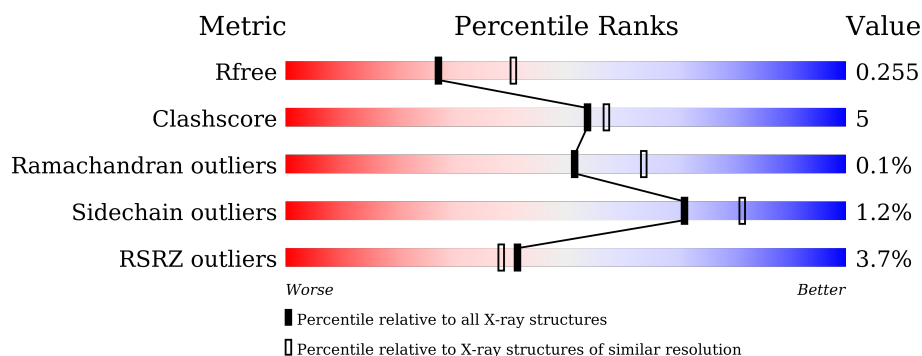
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.43 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))
$R_{free}$	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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  $\geq 3$ , 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	1047	<div> <div>3%</div> <div>72%</div> <div>9%</div> <div>19%</div> </div>
1	B	1047	<div> <div>2%</div> <div>71%</div> <div>10%</div> <div>19%</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
5	PEG	B	1129	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14678 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.

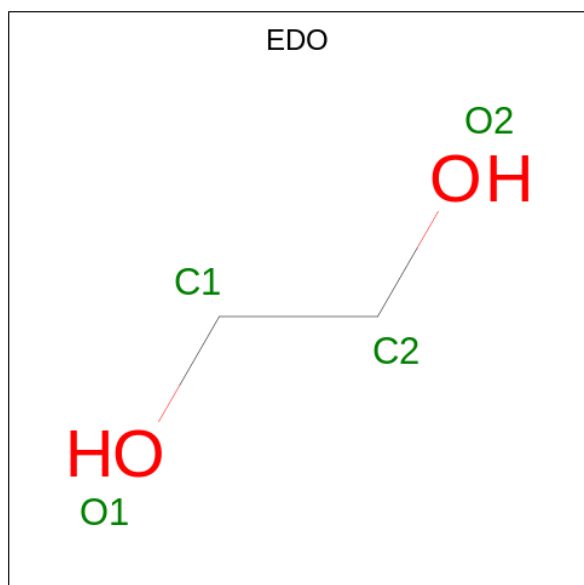
- Molecule 1 is a protein called Dextransucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	846	Total	C	N	O	S	0	1	0
			6634	4143	1117	1355	19			
1	B	845	Total	C	N	O	S	0	1	0
			6631	4142	1118	1352	19			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Ca	0	0
			5	5		
2	B	6	Total	Ca	0	0
			6	6		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).





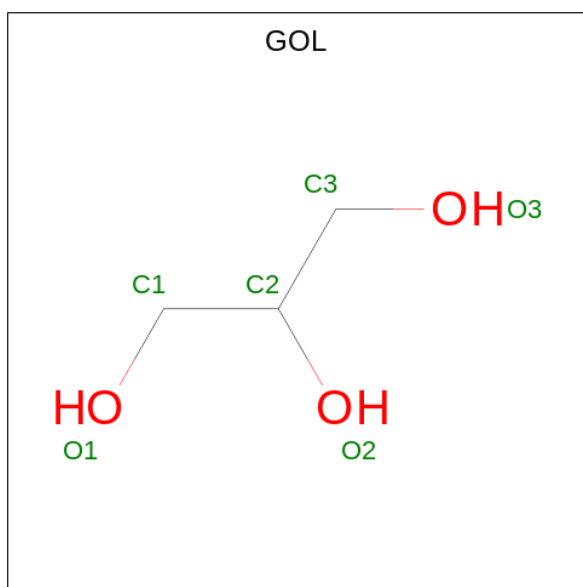
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 8 4 4	0	1
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	566	Total	O	0	0
			566	566		
6	B	590	Total	O	0	1
			591	591		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.83Å 106.08Å 106.02Å 90.00° 104.83° 90.00°	Depositor
Resolution (Å)	48.73 – 2.43 48.73 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.73-2.43) 99.8 (48.73-2.43)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.194 , 0.256 0.194 , 0.255	Depositor DCC
$R_{free}$ test set	3850 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.8	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14678	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6967e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PEG, CA, GOL, 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	0.39	0/6774	0.56	0/9221
1	B	0.41	0/6771	0.58	1/9216 (0.0%)
All	All	0.40	0/13545	0.57	1/18437 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	653	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6634	0	6269	59	0
1	B	6631	0	6271	76	0
2	A	5	0	0	0	0
2	B	6	0	0	0	0
3	A	96	0	142	7	0
3	B	64	0	96	7	0
4	A	18	0	24	2	0
4	B	18	0	23	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	14	0	20	1	0
5	B	35	0	50	8	0
6	A	566	0	0	10	0
6	B	591	0	0	14	0
All	All	14678	0	12895	140	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 5.

All (140) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ASP:OD2	1:A:638:ASN:ND2	2.18	0.75
1:A:776:GLY:O	6:A:1201:HOH:O	2.02	0.75
1:B:858:ASN:HB2	5:B:1129:PEG:H41	1.68	0.75
1:B:815:PRO:HA	5:B:1129:PEG:H11	1.71	0.72
1:B:358:ASN:H	3:B:1125:EDO:H21	1.54	0.71
1:B:679:GLY:HA2	4:B:1118:GOL:H31	1.75	0.68
1:B:637:GLN:OE1	6:B:1201:HOH:O	2.15	0.65
1:A:539:GLU:OE2	6:A:1202:HOH:O	2.14	0.64
1:B:668:ASP:O	6:B:1202:HOH:O	2.15	0.64
1:A:830:ASP:HB3	4:A:1127:GOL:H12	1.80	0.62
1:B:733:ASP:OD1	6:B:1203:HOH:O	2.16	0.62
1:A:206:ILE:HB	1:A:1019:LEU:HD11	1.81	0.61
1:B:251:ASP:OD2	1:B:255:LYS:HE2	2.01	0.60
1:B:493:ARG:NH1	6:B:1220:HOH:O	2.34	0.60
1:A:214:SER:HG	1:A:216:THR:HG1	1.50	0.59
1:B:358:ASN:N	3:B:1125:EDO:H21	2.18	0.59
1:B:715:ASN:HB3	6:B:1683:HOH:O	2.03	0.59
1:B:225:SER:HB2	1:B:231:TRP:CD2	2.38	0.58
1:B:505:TYR:HB2	1:B:529:SER:HB2	1.86	0.57
1:A:401:GLY:HA3	1:A:908:ILE:CD1	2.35	0.57
1:A:493:ARG:NH2	6:A:1221:HOH:O	2.37	0.57
1:A:672:THR:HG22	1:A:700:VAL:HG22	1.87	0.56
1:B:465:ASN:ND2	6:B:1204:HOH:O	2.17	0.56
1:A:216:THR:HG22	1:A:321:ILE:HD13	1.88	0.56
3:A:1121:EDO:H22	6:A:1298:HOH:O	2.07	0.55
1:A:214:SER:HB2	1:A:941:PHE:CE2	2.41	0.54
1:B:596:ARG:HA	3:B:1108:EDO:H22	1.90	0.54
1:B:297:ARG:NH2	6:B:1206:HOH:O	2.21	0.54
1:A:491:LEU:HD12	1:A:500:TYR:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:THR:H	1:B:276:SER:HB3	1.73	0.54
1:A:258:GLN:O	1:A:262:ASN:ND2	2.40	0.54
1:A:493:ARG:HD3	6:A:1601:HOH:O	2.07	0.54
1:B:300:ILE:O	1:B:304:VAL:HG23	2.08	0.54
1:B:859:GLU:OE2	1:B:861:TYR:HB2	2.07	0.54
1:A:328:SER:HA	3:A:1112:EDO:H12	1.89	0.53
1:A:319:ASN:O	1:A:322:THR:HB	2.08	0.53
1:B:505:TYR:CD1	1:B:529:SER:HB2	2.43	0.53
1:B:672:THR:HG22	1:B:700:VAL:HG22	1.91	0.53
1:A:636:MET:O	3:A:1121:EDO:H11	2.09	0.52
1:A:365:LYS:HE3	1:A:1013:ASN:O	2.09	0.52
1:B:558:LEU:HD12	3:B:1113:EDO:H11	1.92	0.52
1:A:599:LYS:NZ	1:A:762:PRO:O	2.43	0.51
1:B:599:LYS:HB2	1:B:604:TYR:CE1	2.45	0.51
1:B:690:ILE:HB	3:B:1116:EDO:H12	1.93	0.50
1:B:271:GLY:O	1:B:276:SER:OG	2.18	0.50
1:B:558:LEU:HD22	6:B:1723:HOH:O	2.11	0.50
1:B:352:ASP:HB3	1:B:1000:LEU:HG	1.93	0.49
5:B:1129:PEG:H21	6:B:1438:HOH:O	2.12	0.49
1:A:581:GLU:HG2	6:A:1492:HOH:O	2.12	0.49
1:B:213:ILE:HD11	1:B:1019:LEU:HG	1.93	0.49
1:A:479:TYR:HB3	1:A:499:LEU:HB2	1.95	0.49
1:B:427:LYS:H	1:B:436:ASN:HD21	1.60	0.48
1:B:326:GLU:HA	1:B:331:SER:HB3	1.96	0.48
1:A:300:ILE:O	1:A:304:VAL:HG23	2.14	0.48
3:A:1113:EDO:H11	6:A:1388:HOH:O	2.14	0.48
1:A:234:THR:HB	1:A:238:ASP:HB2	1.96	0.48
1:A:599:LYS:HE2	6:A:1215:HOH:O	2.14	0.47
1:A:862:SER:HA	1:A:908:ILE:HG13	1.96	0.47
1:A:579:LYS:HB2	1:A:582:TYR:CD2	2.50	0.47
1:A:338:SER:HA	1:A:931:ASP:OD2	2.14	0.47
1:B:857:TYR:O	5:B:1129:PEG:H32	2.14	0.47
1:A:401:GLY:HA3	1:A:908:ILE:HD13	1.96	0.47
1:A:830:ASP:OD2	3:A:1125:EDO:O1	2.30	0.46
1:A:385:ASN:HD21	4:A:1124:GOL:H2	1.79	0.46
1:A:215:TYR:CE1	1:A:1009:VAL:HG22	2.50	0.46
1:A:599:LYS:N	1:A:604:TYR:OH	2.49	0.46
1:B:251:ASP:O	1:B:255:LYS:HG3	2.16	0.46
1:B:272:LEU:HD12	1:B:299:VAL:HG21	1.98	0.46
1:B:460:ILE:HG22	1:B:466:THR:HG21	1.98	0.46
1:B:426:GLY:H	1:B:436:ASN:HD22	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:814:GLN:O	5:B:1129:PEG:H22	2.16	0.46
1:B:273:THR:HG22	1:B:276:SER:HB3	1.97	0.45
1:A:329:LYS:H	3:A:1112:EDO:H22	1.81	0.45
1:B:371:TYR:OH	1:B:915:ALA:HB3	2.16	0.45
1:B:420:TYR:CG	1:B:962:LEU:HD21	2.52	0.45
1:A:1019:LEU:HD23	1:A:1019:LEU:HA	1.83	0.45
1:A:427:LYS:HE2	1:A:427:LYS:HB3	1.51	0.45
1:B:206:ILE:HB	1:B:1019:LEU:HD11	1.99	0.45
1:B:241:PRO:HG2	1:B:244:MET:HG3	1.97	0.45
1:B:599:LYS:N	1:B:604:TYR:OH	2.50	0.45
1:A:582:TYR:HD2	6:A:1334:HOH:O	1.99	0.45
1:A:825:TYR:CZ	1:A:878:TYR:HB2	2.52	0.45
1:B:639:LYS:HE2	1:B:643:TYR:CZ	2.52	0.44
1:A:505:TYR:CD1	1:A:529:SER:HB2	2.53	0.44
5:B:1117:PEG:H12	5:B:1117:PEG:H32	1.59	0.44
1:A:420:TYR:CG	1:A:962:LEU:HD21	2.52	0.44
1:B:862:SER:OG	1:B:908:ILE:HD12	2.18	0.44
1:B:922:ASP:OD2	4:B:1124:GOL:H11	2.16	0.44
1:A:492:ASP:HB3	5:A:1132:PEG:H41	1.99	0.44
1:B:599:LYS:HD3	1:B:602:THR:OG1	2.17	0.44
1:A:225:SER:OG	1:A:227:ASP:O	2.36	0.44
1:B:732:ILE:HG13	1:B:735:GLY:H	1.83	0.44
3:A:1125:EDO:H11	6:A:1647:HOH:O	2.17	0.43
1:B:381:ARG:HA	1:B:385:ASN:O	2.18	0.43
1:B:490:MET:O	1:B:494:LYS:HG3	2.18	0.43
1:A:211:GLY:O	1:A:1018:TYR:HA	2.17	0.43
1:A:522:ILE:HG13	1:A:671:LEU:HD23	2.00	0.43
1:B:331:SER:HB2	1:B:1005:ILE:HG22	2.00	0.43
1:B:288:LYS:O	1:B:292:VAL:HG23	2.17	0.43
1:B:460:ILE:HG13	1:B:478:ILE:HD11	1.99	0.43
1:B:682:ASP:OD2	5:B:1117:PEG:H21	2.17	0.43
1:A:298:TYR:O	1:A:302:GLN:HG3	2.19	0.43
1:B:555:ARG:HA	6:B:1488:HOH:O	2.17	0.43
1:B:491:LEU:HD12	1:B:500:TYR:HB2	1.99	0.43
1:A:213:ILE:HD11	1:A:1019:LEU:HG	2.00	0.43
1:A:288:LYS:O	1:A:292:VAL:HG23	2.18	0.43
1:A:530:ILE:HG23	1:A:531:VAL:HG23	1.99	0.43
1:B:552:HIS:ND1	1:B:808:GLU:OE2	2.32	0.43
1:A:386:GLN:HG3	1:A:450:ALA:HB3	2.01	0.42
1:A:225:SER:HB2	1:A:231:TRP:CD2	2.55	0.42
1:A:272:LEU:HD12	1:A:299:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:TRP:CE2	1:A:866:ARG:HB3	2.54	0.42
1:B:267:ASN:OD1	1:B:269:ASN:HB2	2.19	0.42
1:B:579:LYS:HB2	1:B:582:TYR:CE2	2.54	0.42
1:B:642:TYR:OH	6:B:1205:HOH:O	2.19	0.42
1:B:968:GLU:HB3	5:B:1130:PEG:H32	2.01	0.42
1:A:556:LYS:HE2	1:A:556:LYS:HB3	1.89	0.42
1:A:556:LYS:HB2	1:A:812:LEU:HD12	2.01	0.42
1:A:431:TYR:HB3	1:A:885:SER:OG	2.20	0.41
1:B:319:ASN:O	1:B:322:THR:HB	2.20	0.41
1:B:823:HIS:CE1	1:B:875:LEU:HD13	2.54	0.41
1:B:853:ASN:O	3:B:1121:EDO:H12	2.20	0.41
1:B:963:GLN:NE2	6:B:1272:HOH:O	2.51	0.41
1:B:635:TYR:O	1:B:637:GLN:NE2	2.54	0.41
1:B:496:ASN:ND2	1:B:544:PRO:HD2	2.35	0.41
1:B:577:GLY:HA2	6:B:1608:HOH:O	2.20	0.41
1:A:400:VAL:O	1:A:906:GLN:HG3	2.21	0.41
1:A:859:GLU:OE2	1:A:861:TYR:HB2	2.20	0.41
1:B:308:LYS:HA	1:B:308:LYS:HD3	1.84	0.41
1:B:401:GLY:HA3	1:B:908:ILE:HG12	2.03	0.41
1:B:273:THR:HG23	1:B:276:SER:H	1.85	0.41
1:A:355:ILE:O	1:A:918:VAL:HA	2.22	0.40
1:B:533:ARG:O	1:B:663:MET:HG3	2.21	0.40
1:A:449:ASP:O	1:A:452:VAL:HG22	2.21	0.40
1:B:480:ASN:O	1:B:501:MET:HB2	2.21	0.40
1:A:666:ILE:HD11	1:A:672:THR:HG23	2.02	0.40
1:B:358:ASN:H	3:B:1125:EDO:C2	2.29	0.40
1:B:326:GLU:HG2	6:B:1596:HOH:O	2.21	0.40
1:B:393:ASP:OD1	1:B:486:GLY:HA3	2.21	0.40
1:B:679:GLY:CA	4:B:1118:GOL:H31	2.48	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	845/1047 (81%)	818 (97%)	26 (3%)	1 (0%)	51	64
1	B	844/1047 (81%)	809 (96%)	34 (4%)	1 (0%)	51	64
All	All	1689/2094 (81%)	1627 (96%)	60 (4%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	383	ILE
1	A	383	ILE

### 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	721/889 (81%)	710 (98%)	11 (2%)	65	76
1	B	720/889 (81%)	714 (99%)	6 (1%)	81	88
All	All	1441/1778 (81%)	1424 (99%)	17 (1%)	71	81

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	PRO
1	A	203	SER
1	A	322	THR
1	A	460	ILE
1	A	479	TYR
1	A	529	SER
1	A	575	SER
1	A	809	ASP
1	A	863	MET
1	A	908	ILE
1	A	952	LYS
1	B	208	ASN
1	B	248	PRO
1	B	452	VAL

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Mol	Chain	Res	Type
1	B	479	TYR
1	B	529	SER
1	B	809	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	637	GLN
1	B	637	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 11 are monoatomic - leaving 53 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	EDO	A	1119	-	3,3,3	0.52	0	2,2,2	0.27	0
3	EDO	A	1126	-	3,3,3	0.48	0	2,2,2	0.56	0
3	EDO	A	1111	-	3,3,3	0.48	0	2,2,2	0.37	0
3	EDO	A	1109	-	3,3,3	0.56	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	A	1107	-	3,3,3	0.50	0	2,2,2	0.29	0
3	EDO	A	1113	-	3,3,3	0.48	0	2,2,2	0.37	0
3	EDO	A	1117[B]	-	3,3,3	0.51	0	2,2,2	0.30	0
3	EDO	A	1120	-	3,3,3	0.44	0	2,2,2	0.43	0
3	EDO	B	1108	-	3,3,3	0.53	0	2,2,2	0.18	0
3	EDO	B	1111	-	3,3,3	0.55	0	2,2,2	0.19	0
3	EDO	B	1122	-	3,3,3	0.55	0	2,2,2	0.11	0
4	GOL	A	1127	-	5,5,5	0.31	0	5,5,5	0.53	0
3	EDO	B	1125	-	3,3,3	0.54	0	2,2,2	0.23	0
4	GOL	A	1128	-	5,5,5	0.27	0	5,5,5	0.62	0
3	EDO	A	1115	-	3,3,3	0.53	0	2,2,2	0.25	0
5	PEG	B	1129	-	6,6,6	0.49	0	5,5,5	0.30	0
3	EDO	A	1129	-	3,3,3	0.55	0	2,2,2	0.25	0
5	PEG	B	1117	-	6,6,6	0.55	0	5,5,5	0.28	0
4	GOL	B	1123	-	5,5,5	0.42	0	5,5,5	0.24	0
3	EDO	B	1121	-	3,3,3	0.59	0	2,2,2	0.16	0
3	EDO	A	1125	-	3,3,3	0.52	0	2,2,2	0.32	0
3	EDO	A	1106	-	3,3,3	0.48	0	2,2,2	0.40	0
3	EDO	A	1122	-	3,3,3	0.54	0	2,2,2	0.69	0
3	EDO	A	1108	-	3,3,3	0.48	0	2,2,2	0.39	0
3	EDO	A	1131	-	3,3,3	0.53	0	2,2,2	0.27	0
3	EDO	A	1112	-	3,3,3	0.59	0	2,2,2	0.07	0
3	EDO	B	1107	-	3,3,3	0.55	0	2,2,2	0.25	0
4	GOL	A	1124	-	5,5,5	0.31	0	5,5,5	0.45	0
3	EDO	B	1116	-	3,3,3	0.55	0	2,2,2	0.22	0
3	EDO	B	1115	-	3,3,3	0.54	0	2,2,2	0.14	0
5	PEG	B	1128	-	6,6,6	0.58	0	5,5,5	0.50	0
3	EDO	B	1110	-	3,3,3	0.55	0	2,2,2	0.20	0
3	EDO	A	1130	-	3,3,3	0.55	0	2,2,2	0.36	0
4	GOL	B	1118	-	5,5,5	0.26	0	5,5,5	0.71	0
5	PEG	A	1132	-	6,6,6	0.53	0	5,5,5	0.40	0
5	PEG	B	1130	-	6,6,6	0.52	0	5,5,5	0.33	0
3	EDO	A	1117[A]	-	3,3,3	0.50	0	2,2,2	0.25	0
3	EDO	A	1121	-	3,3,3	0.49	0	2,2,2	0.18	0
3	EDO	A	1116	-	3,3,3	0.48	0	2,2,2	0.37	0
3	EDO	B	1114	-	3,3,3	0.43	0	2,2,2	0.44	0
3	EDO	A	1123	-	3,3,3	0.48	0	2,2,2	0.38	0
3	EDO	B	1109	-	3,3,3	0.58	0	2,2,2	0.18	0
3	EDO	B	1126	-	3,3,3	0.61	0	2,2,2	0.10	0
5	PEG	A	1133	-	6,6,6	0.60	0	5,5,5	0.65	0
3	EDO	B	1113	-	3,3,3	0.53	0	2,2,2	0.44	0
3	EDO	B	1112	-	3,3,3	0.50	0	2,2,2	0.32	0
3	EDO	B	1120	-	3,3,3	0.52	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	A	1118	-	3,3,3	0.51	0	2,2,2	0.49	0
3	EDO	B	1119	-	3,3,3	0.55	0	2,2,2	0.29	0
3	EDO	A	1110	-	3,3,3	0.47	0	2,2,2	0.63	0
4	GOL	B	1124	-	5,5,5	0.44	0	5,5,5	0.27	0
3	EDO	A	1114	-	3,3,3	0.52	0	2,2,2	0.22	0
5	PEG	B	1127	-	6,6,6	0.48	0	5,5,5	0.29	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
3	EDO	A	1119	-	-	0/1/1/1	-
3	EDO	A	1126	-	-	0/1/1/1	-
3	EDO	A	1111	-	-	0/1/1/1	-
3	EDO	A	1109	-	-	1/1/1/1	-
3	EDO	A	1107	-	-	0/1/1/1	-
3	EDO	A	1113	-	-	1/1/1/1	-
3	EDO	A	1117[B]	-	-	1/1/1/1	-
3	EDO	A	1120	-	-	1/1/1/1	-
3	EDO	B	1108	-	-	0/1/1/1	-
3	EDO	B	1111	-	-	0/1/1/1	-
3	EDO	B	1122	-	-	1/1/1/1	-
4	GOL	A	1127	-	-	2/4/4/4	-
3	EDO	B	1125	-	-	1/1/1/1	-
4	GOL	A	1128	-	-	2/4/4/4	-
3	EDO	A	1115	-	-	1/1/1/1	-
5	PEG	B	1129	-	-	3/4/4/4	-
3	EDO	A	1129	-	-	1/1/1/1	-
5	PEG	B	1117	-	-	3/4/4/4	-
4	GOL	B	1123	-	-	2/4/4/4	-
3	EDO	B	1121	-	-	0/1/1/1	-
3	EDO	A	1125	-	-	1/1/1/1	-
3	EDO	A	1106	-	-	1/1/1/1	-
3	EDO	A	1122	-	-	0/1/1/1	-
3	EDO	A	1108	-	-	0/1/1/1	-
3	EDO	A	1131	-	-	1/1/1/1	-
3	EDO	A	1112	-	-	1/1/1/1	-
3	EDO	B	1107	-	-	0/1/1/1	-
4	GOL	A	1124	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	1116	-	-	1/1/1/1	-
3	EDO	B	1115	-	-	0/1/1/1	-
5	PEG	B	1128	-	-	2/4/4/4	-
3	EDO	B	1110	-	-	0/1/1/1	-
3	EDO	A	1130	-	-	0/1/1/1	-
4	GOL	B	1118	-	-	2/4/4/4	-
5	PEG	A	1132	-	-	3/4/4/4	-
5	PEG	B	1130	-	-	2/4/4/4	-
3	EDO	A	1117[A]	-	-	0/1/1/1	-
3	EDO	A	1121	-	-	1/1/1/1	-
3	EDO	A	1116	-	-	1/1/1/1	-
3	EDO	B	1114	-	-	1/1/1/1	-
3	EDO	A	1123	-	-	0/1/1/1	-
3	EDO	B	1109	-	-	0/1/1/1	-
3	EDO	B	1126	-	-	0/1/1/1	-
5	PEG	A	1133	-	-	4/4/4/4	-
3	EDO	B	1113	-	-	0/1/1/1	-
3	EDO	B	1112	-	-	1/1/1/1	-
3	EDO	B	1120	-	-	1/1/1/1	-
3	EDO	A	1118	-	-	0/1/1/1	-
3	EDO	B	1119	-	-	0/1/1/1	-
3	EDO	A	1110	-	-	0/1/1/1	-
4	GOL	B	1124	-	-	2/4/4/4	-
3	EDO	A	1114	-	-	1/1/1/1	-
5	PEG	B	1127	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1124	GOL	C1-C2-C3-O3
4	A	1127	GOL	C1-C2-C3-O3
4	A	1128	GOL	O1-C1-C2-C3
4	B	1124	GOL	C1-C2-C3-O3
5	B	1117	PEG	C1-C2-O2-C3
4	A	1127	GOL	O2-C2-C3-O3
5	A	1133	PEG	O1-C1-C2-O2

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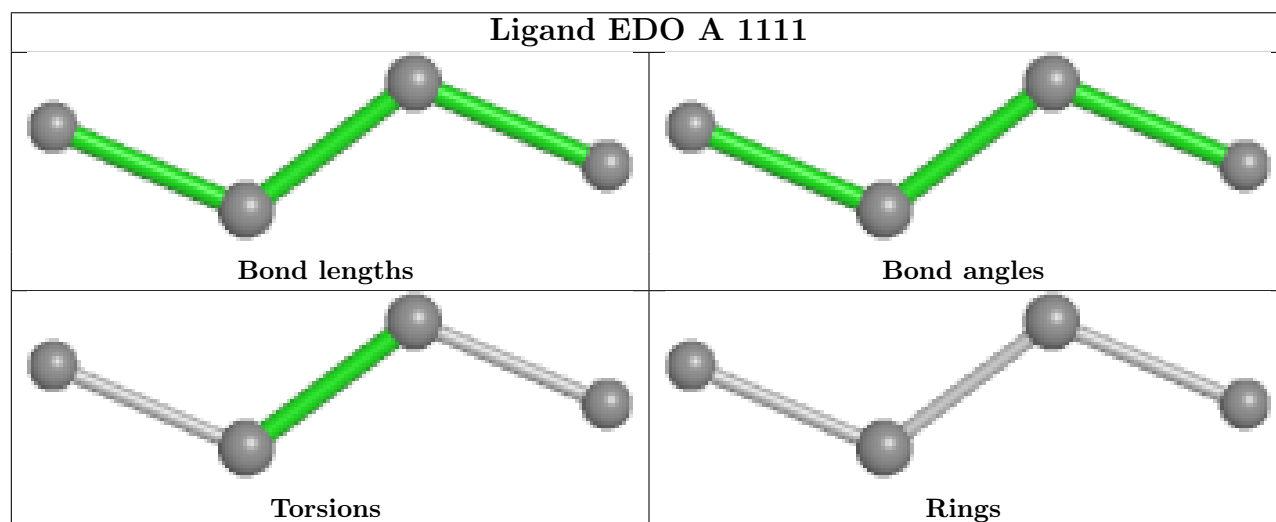
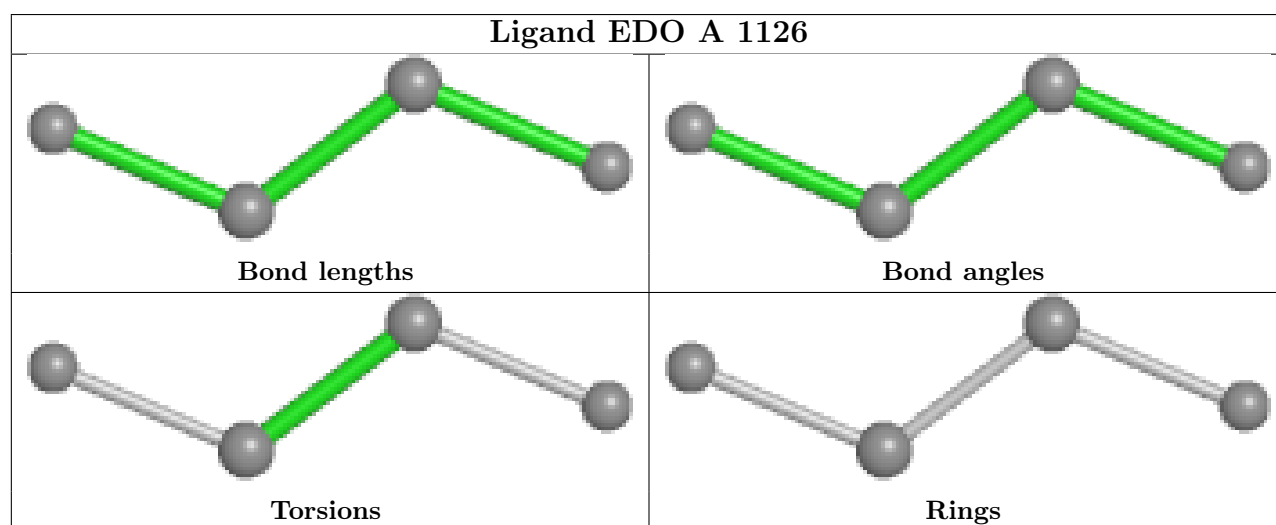
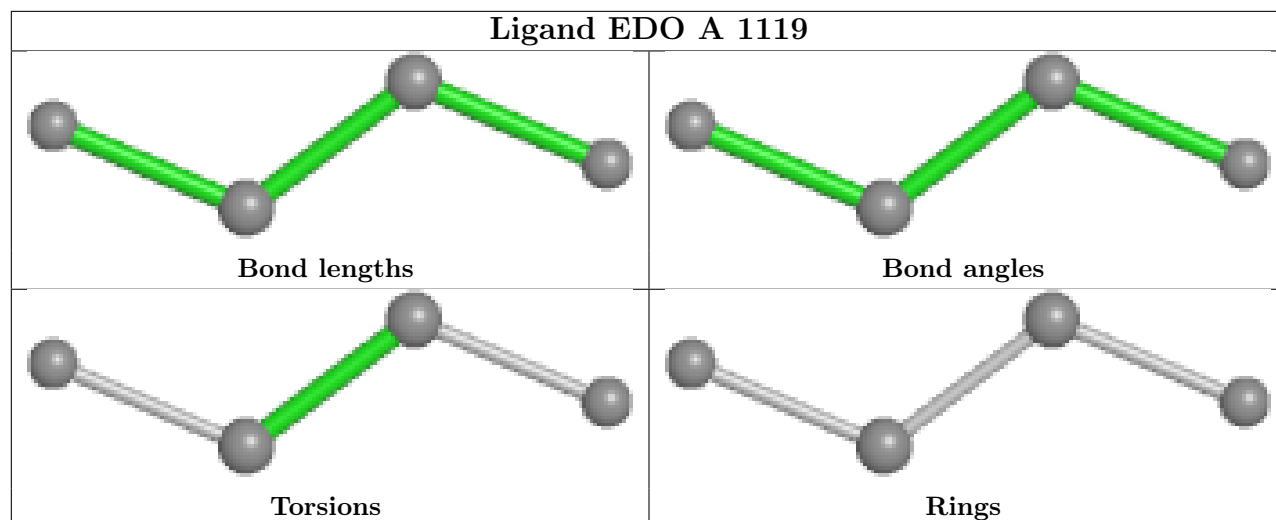
Mol	Chain	Res	Type	Atoms
5	B	1129	PEG	O1-C1-C2-O2
5	B	1129	PEG	O2-C3-C4-O4
5	B	1130	PEG	O1-C1-C2-O2
5	B	1117	PEG	O2-C3-C4-O4
4	B	1118	GOL	O1-C1-C2-C3
4	B	1123	GOL	O1-C1-C2-C3
5	B	1128	PEG	O1-C1-C2-O2
4	A	1124	GOL	O2-C2-C3-O3
4	A	1128	GOL	O1-C1-C2-O2
4	B	1124	GOL	O2-C2-C3-O3
3	A	1113	EDO	O1-C1-C2-O2
3	A	1115	EDO	O1-C1-C2-O2
3	A	1116	EDO	O1-C1-C2-O2
3	A	1120	EDO	O1-C1-C2-O2
3	A	1121	EDO	O1-C1-C2-O2
3	A	1125	EDO	O1-C1-C2-O2
3	A	1129	EDO	O1-C1-C2-O2
3	B	1112	EDO	O1-C1-C2-O2
3	B	1122	EDO	O1-C1-C2-O2
5	A	1132	PEG	O2-C3-C4-O4
4	B	1118	GOL	O1-C1-C2-O2
4	B	1123	GOL	O1-C1-C2-O2
5	A	1132	PEG	O1-C1-C2-O2
3	A	1109	EDO	O1-C1-C2-O2
5	B	1127	PEG	C1-C2-O2-C3
5	B	1128	PEG	C4-C3-O2-C2
5	A	1132	PEG	C1-C2-O2-C3
3	A	1117[B]	EDO	O1-C1-C2-O2
3	B	1125	EDO	O1-C1-C2-O2
5	A	1133	PEG	O2-C3-C4-O4
5	B	1129	PEG	C1-C2-O2-C3
5	A	1133	PEG	C1-C2-O2-C3
5	A	1133	PEG	C4-C3-O2-C2
3	A	1106	EDO	O1-C1-C2-O2
3	B	1120	EDO	O1-C1-C2-O2
3	A	1114	EDO	O1-C1-C2-O2
3	B	1116	EDO	O1-C1-C2-O2
5	B	1130	PEG	C4-C3-O2-C2
5	B	1117	PEG	O1-C1-C2-O2
3	A	1131	EDO	O1-C1-C2-O2
3	A	1112	EDO	O1-C1-C2-O2
3	B	1114	EDO	O1-C1-C2-O2

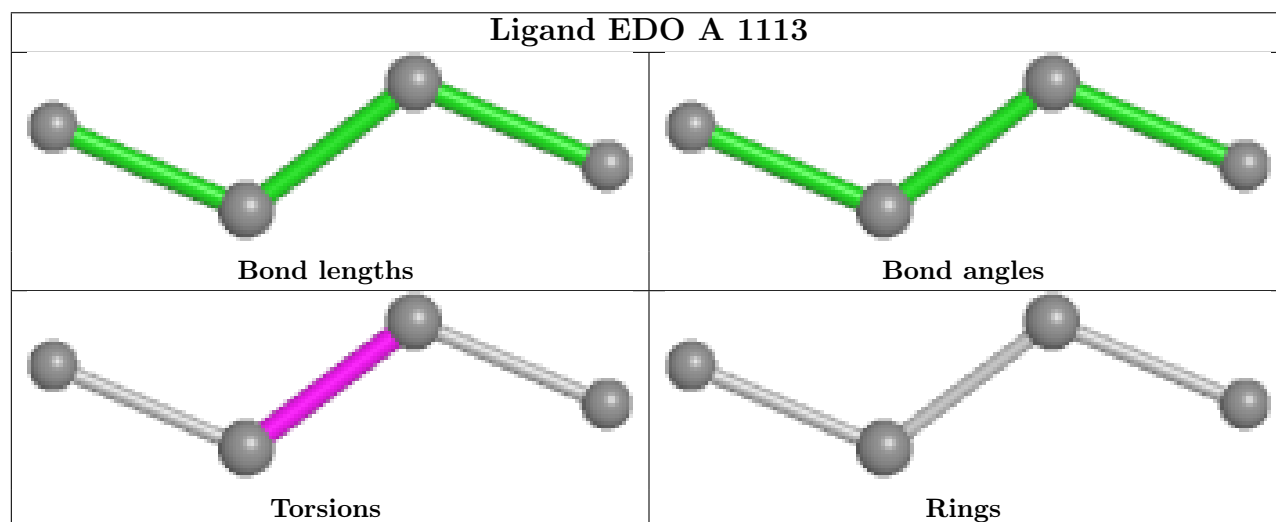
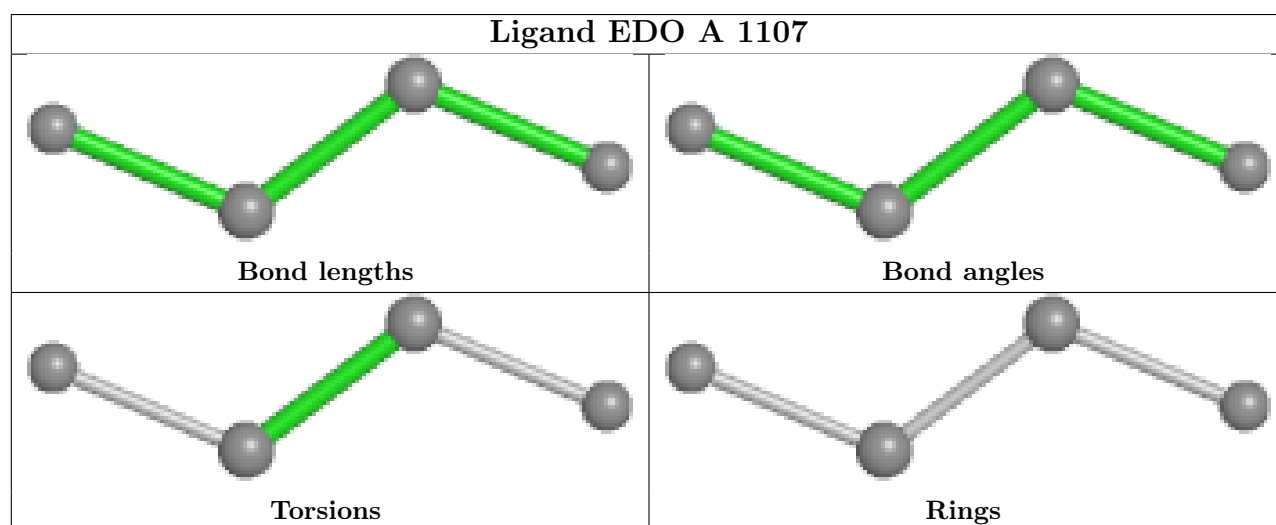
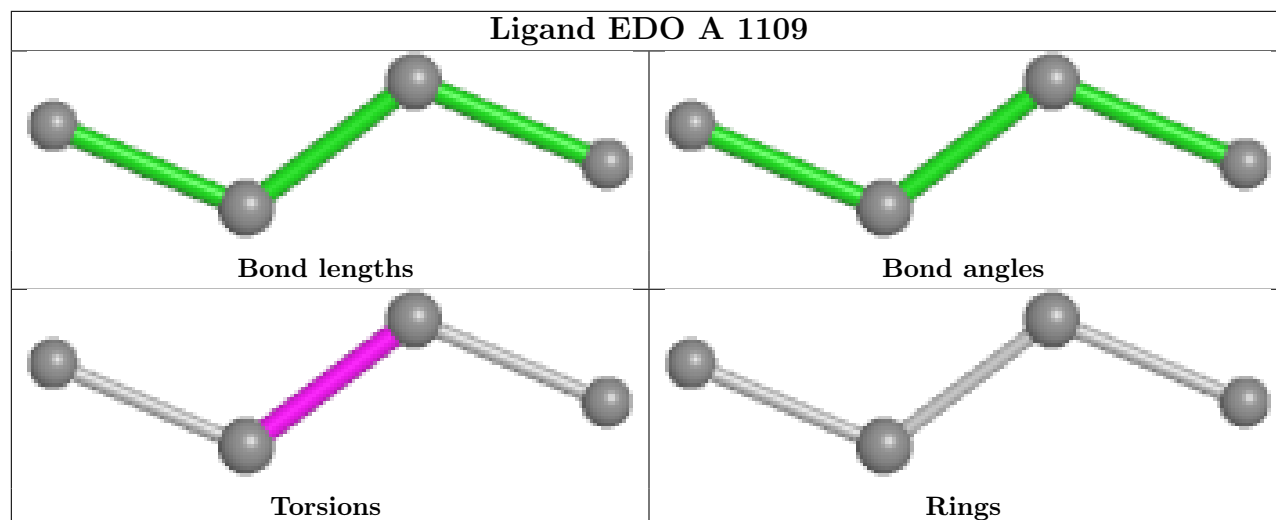
There are no ring outliers.

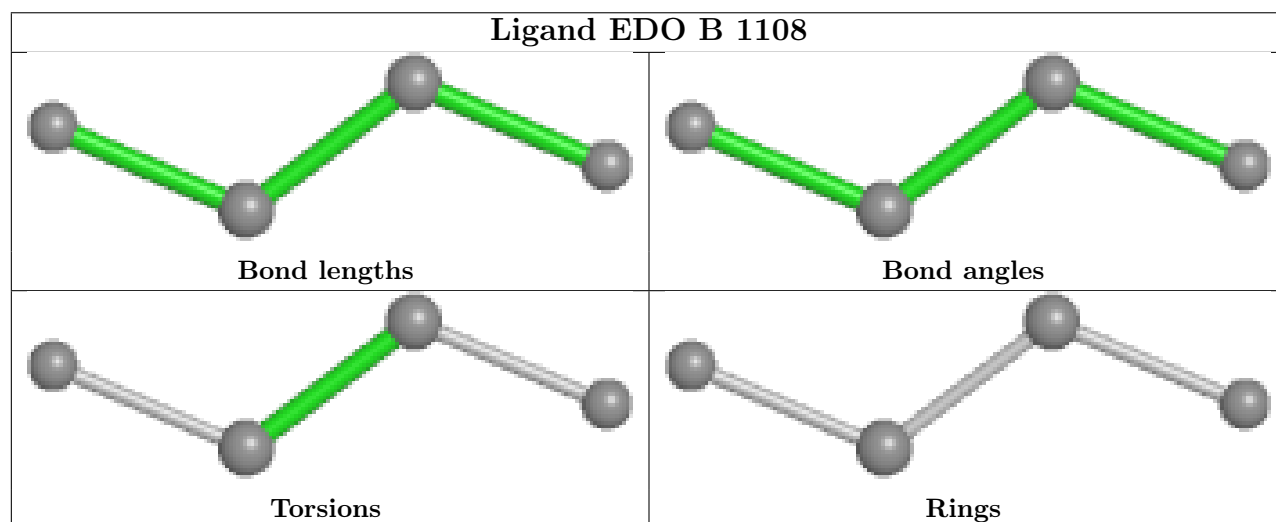
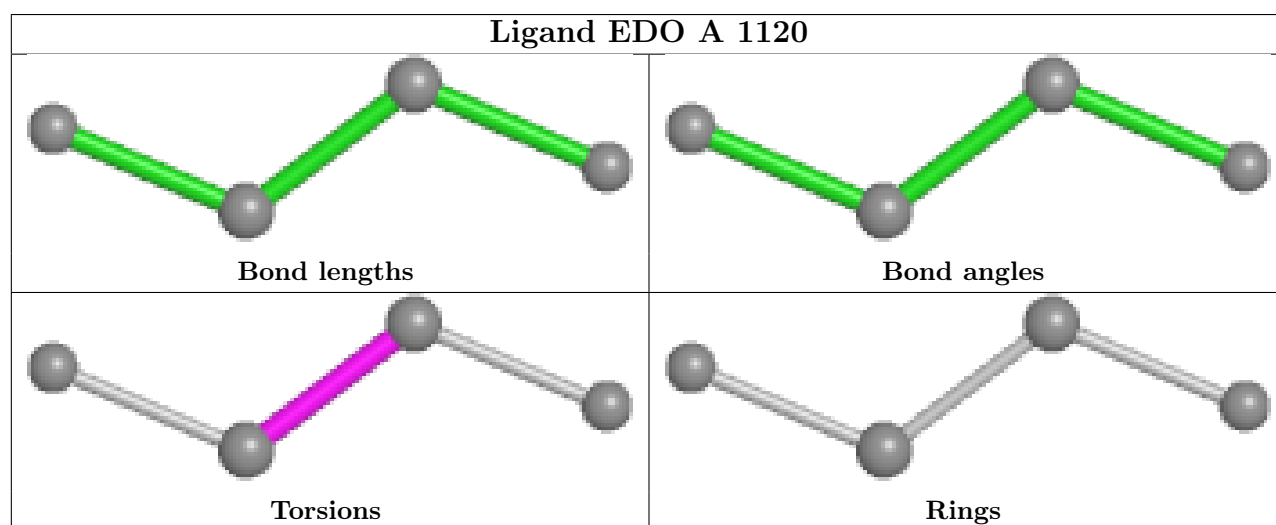
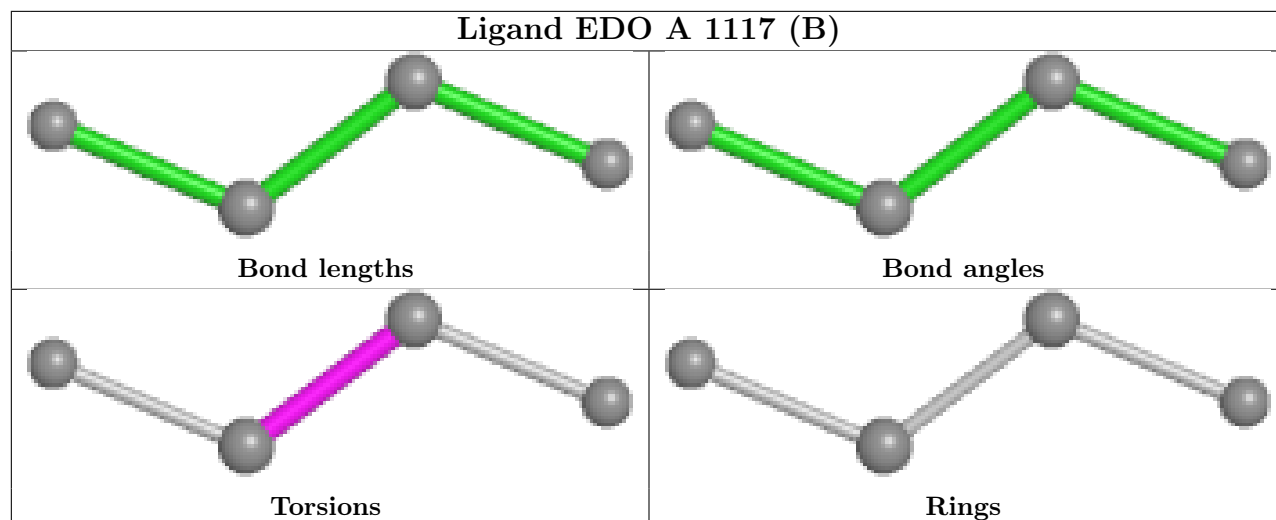
17 monomers are involved in 28 short contacts:

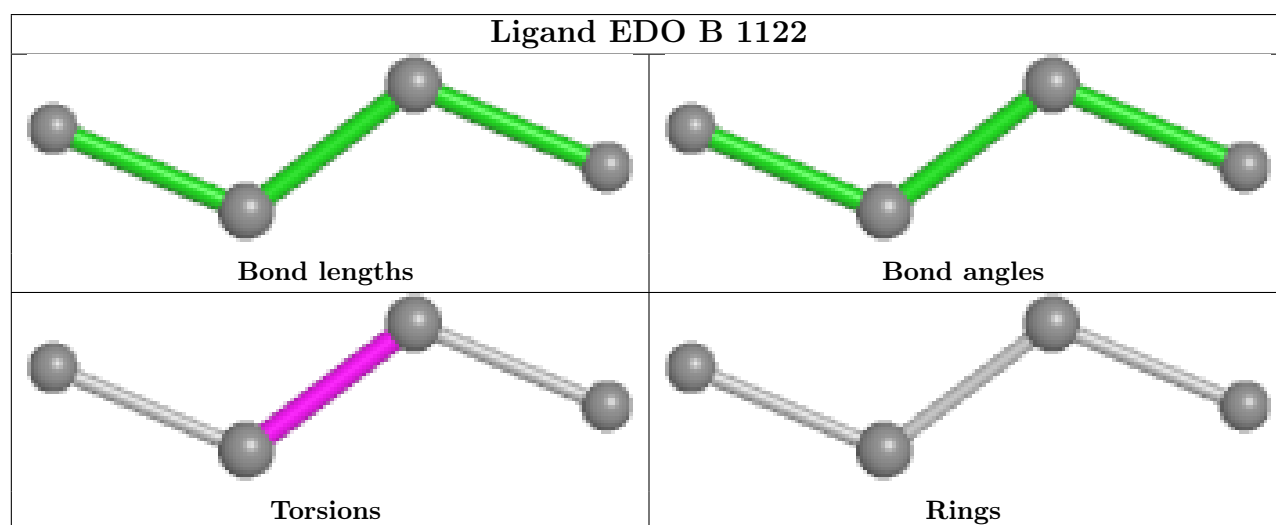
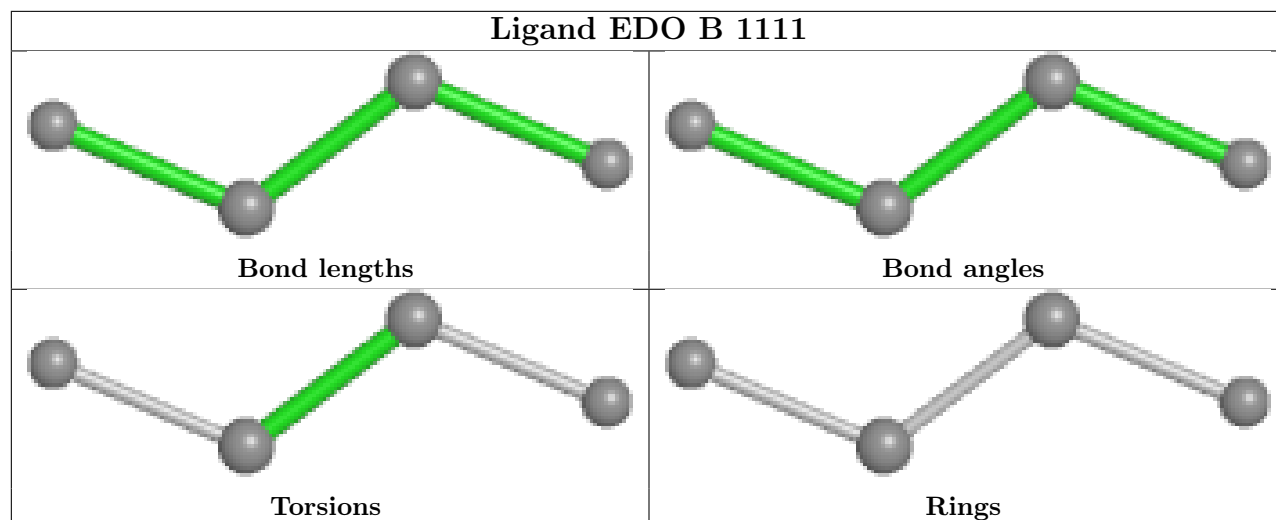
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1113	EDO	1	0
3	B	1108	EDO	1	0
4	A	1127	GOL	1	0
3	B	1125	EDO	3	0
5	B	1129	PEG	5	0
5	B	1117	PEG	2	0
3	B	1121	EDO	1	0
3	A	1125	EDO	2	0
3	A	1112	EDO	2	0
4	A	1124	GOL	1	0
3	B	1116	EDO	1	0
4	B	1118	GOL	2	0
5	A	1132	PEG	1	0
5	B	1130	PEG	1	0
3	A	1121	EDO	2	0
3	B	1113	EDO	1	0
4	B	1124	GOL	1	0

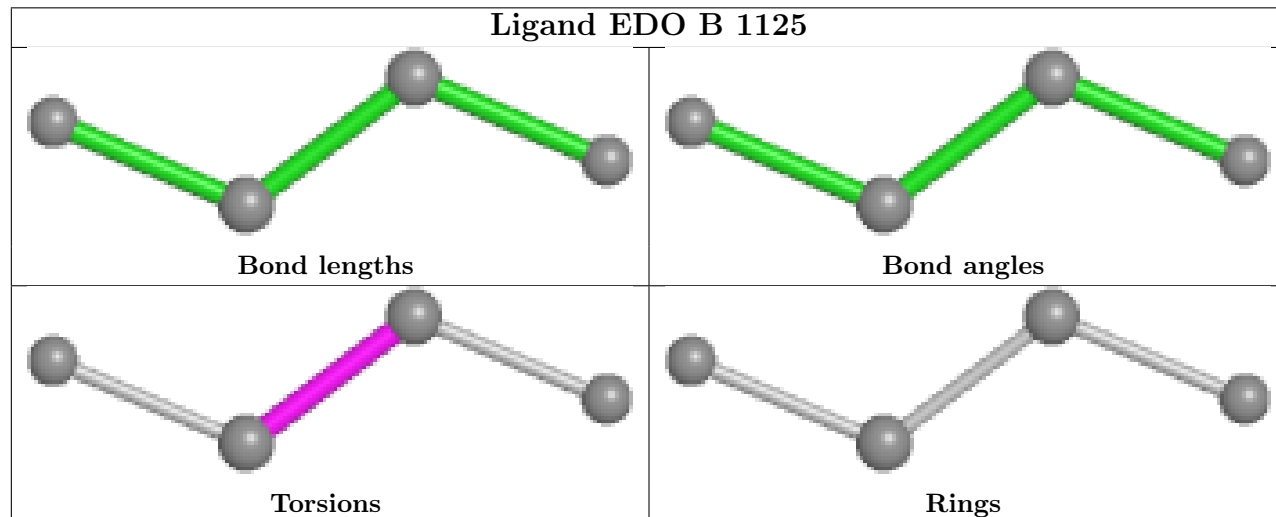
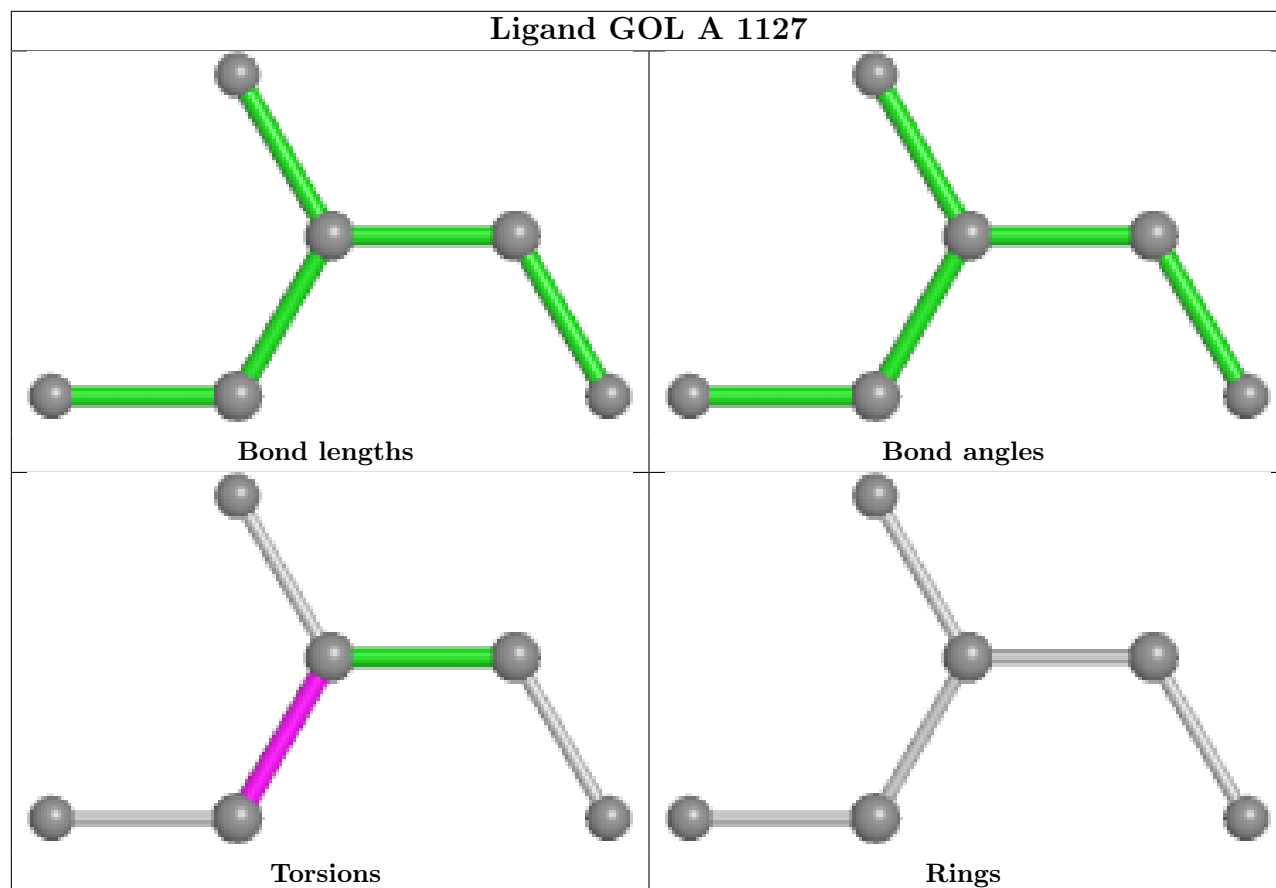
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



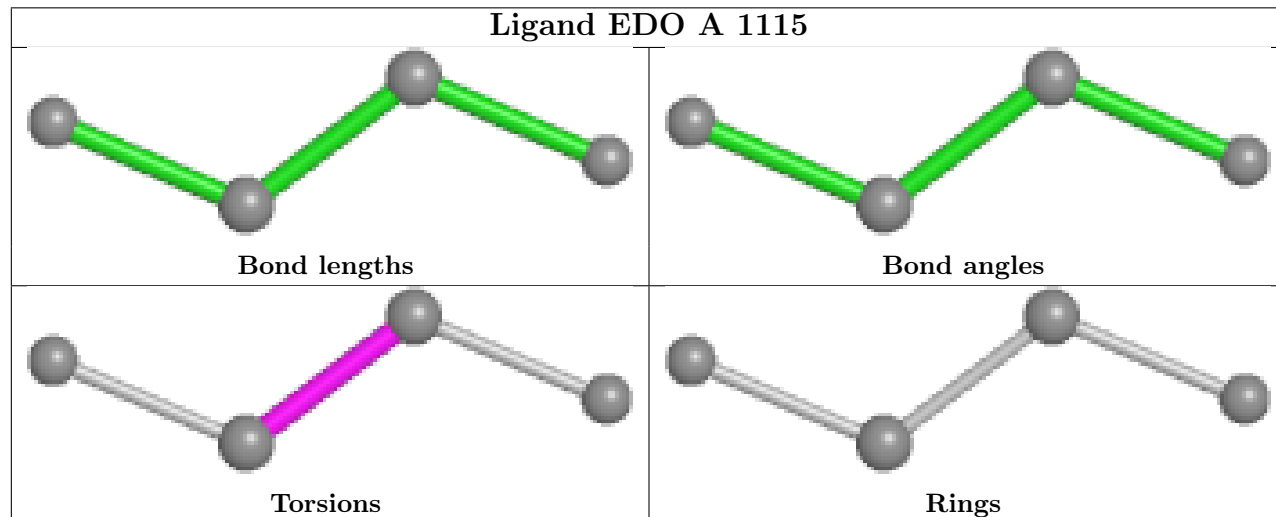
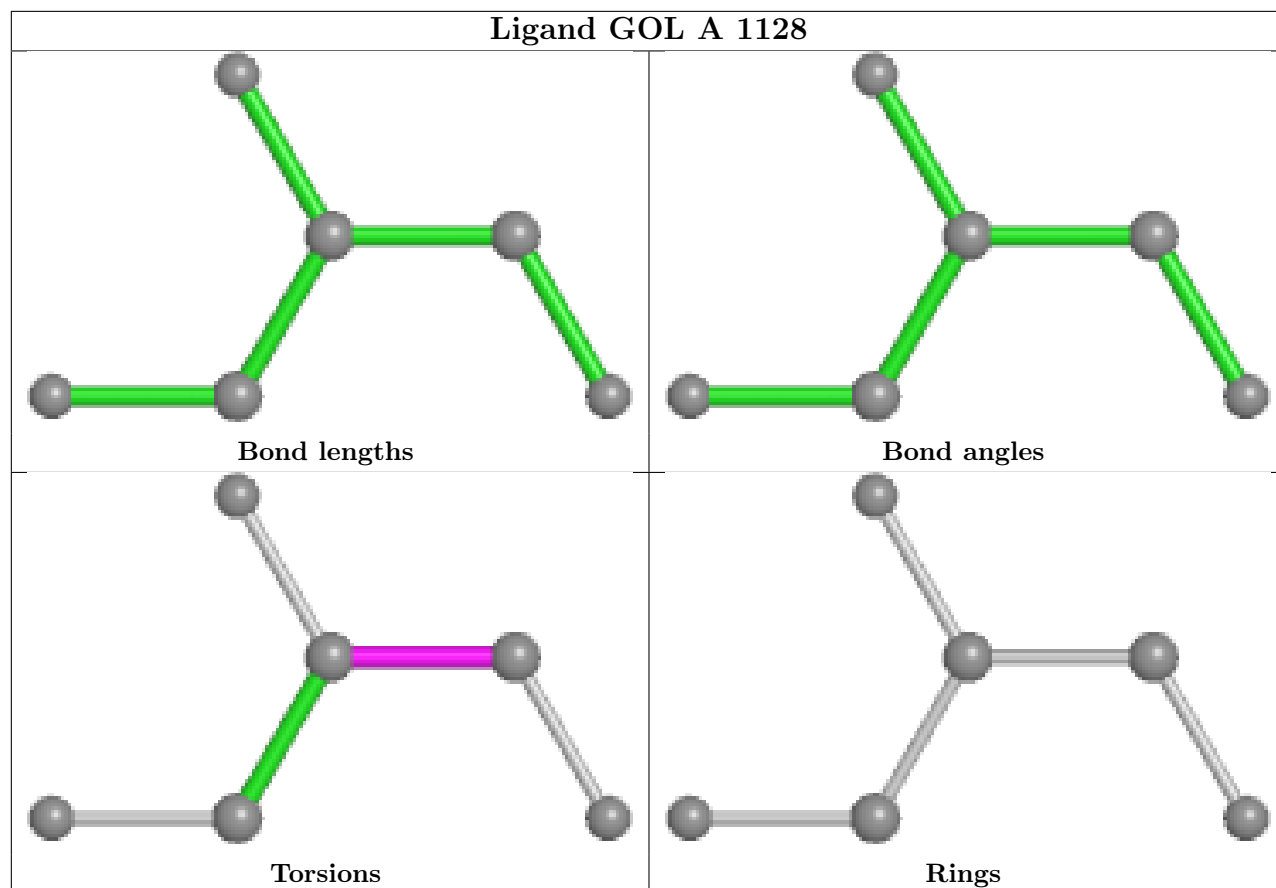


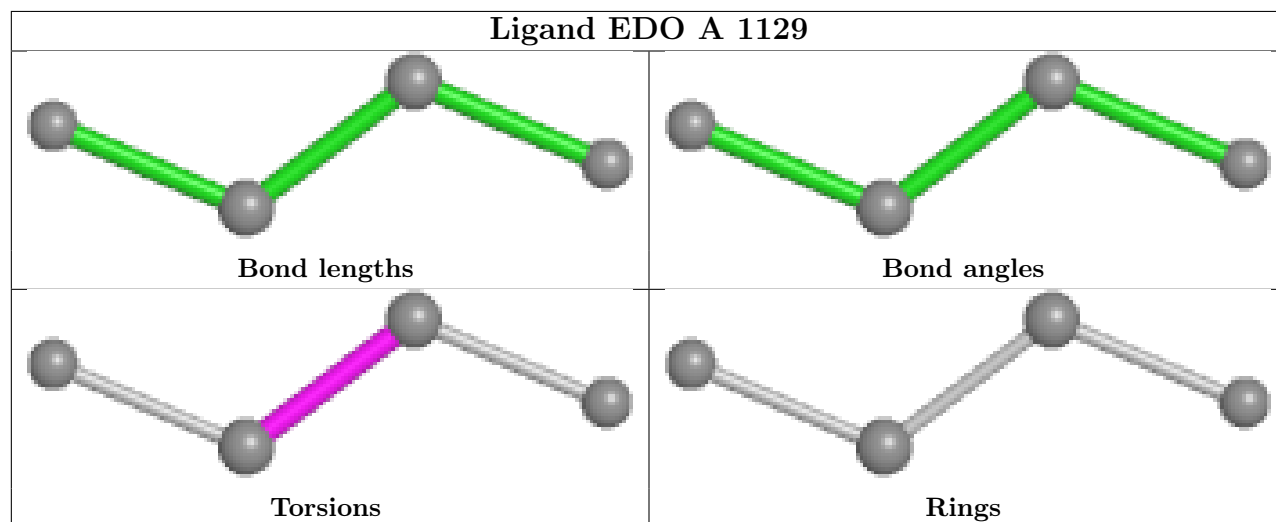
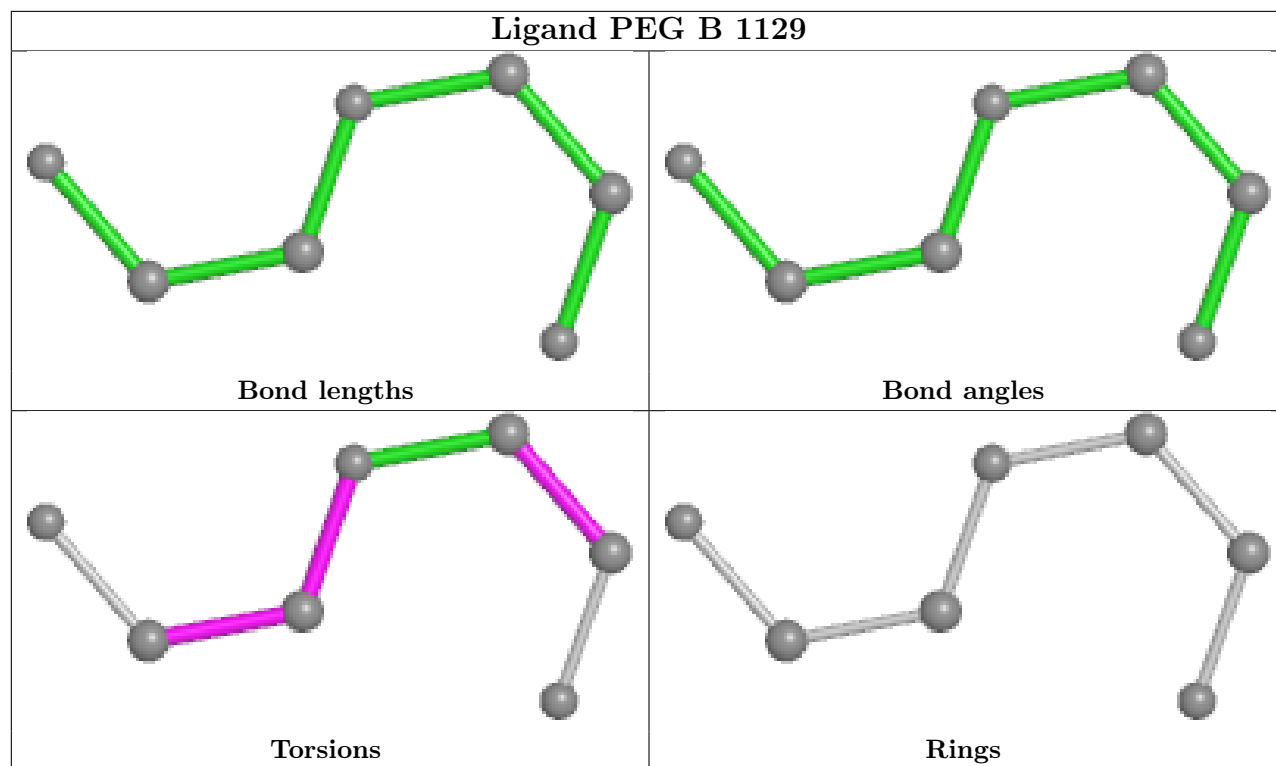


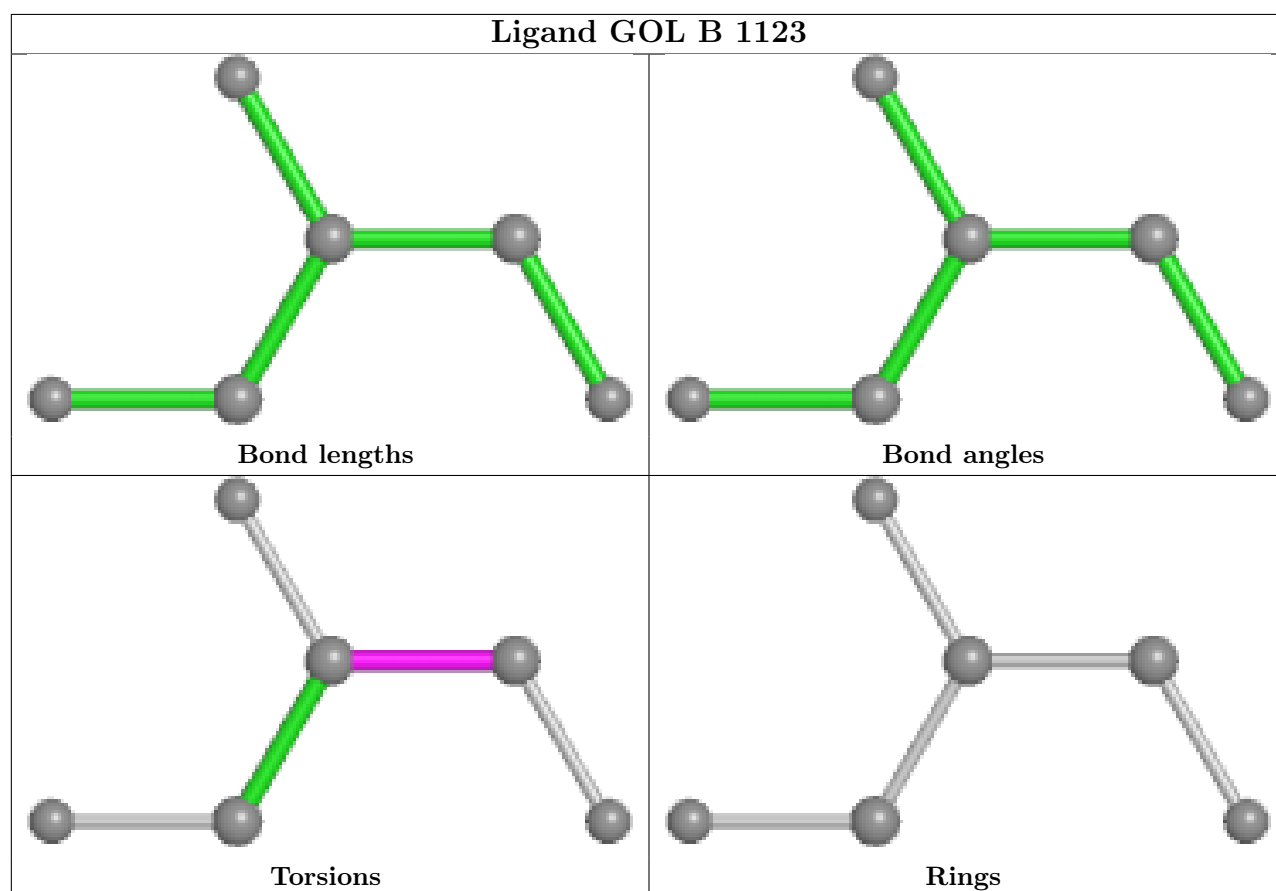
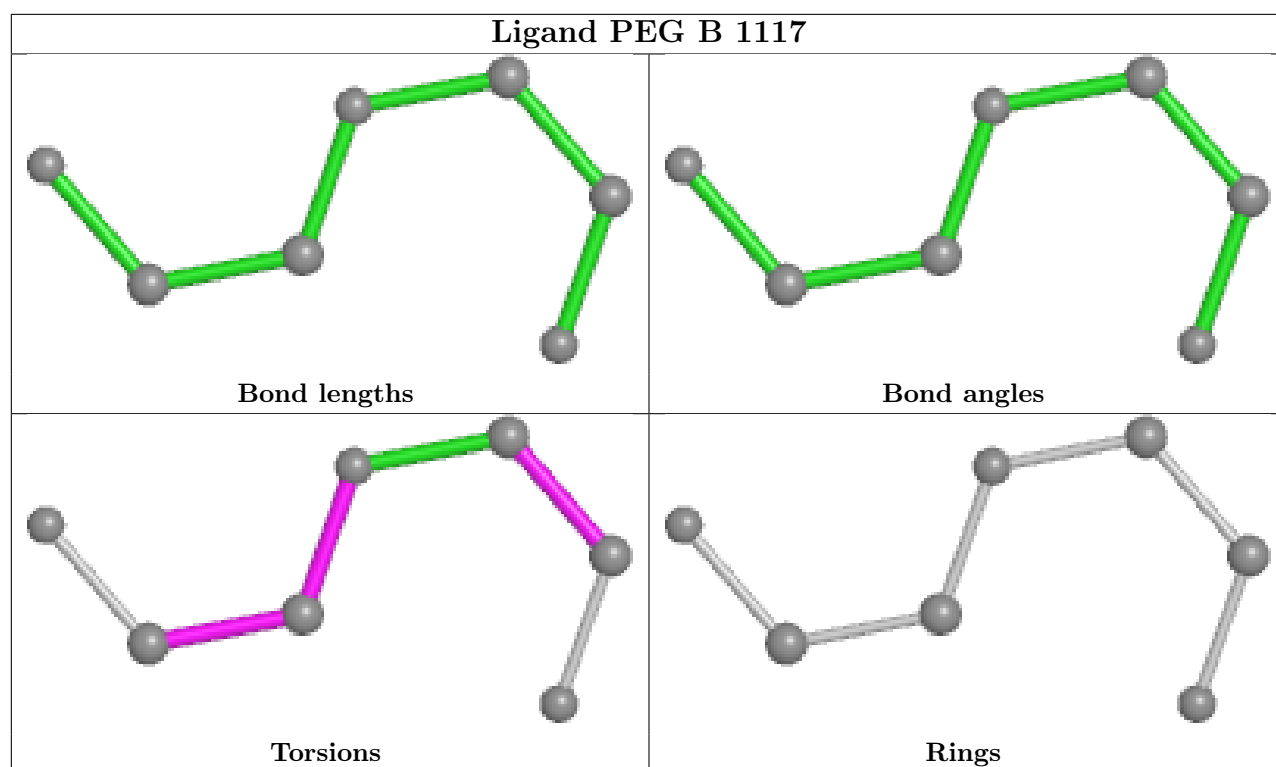


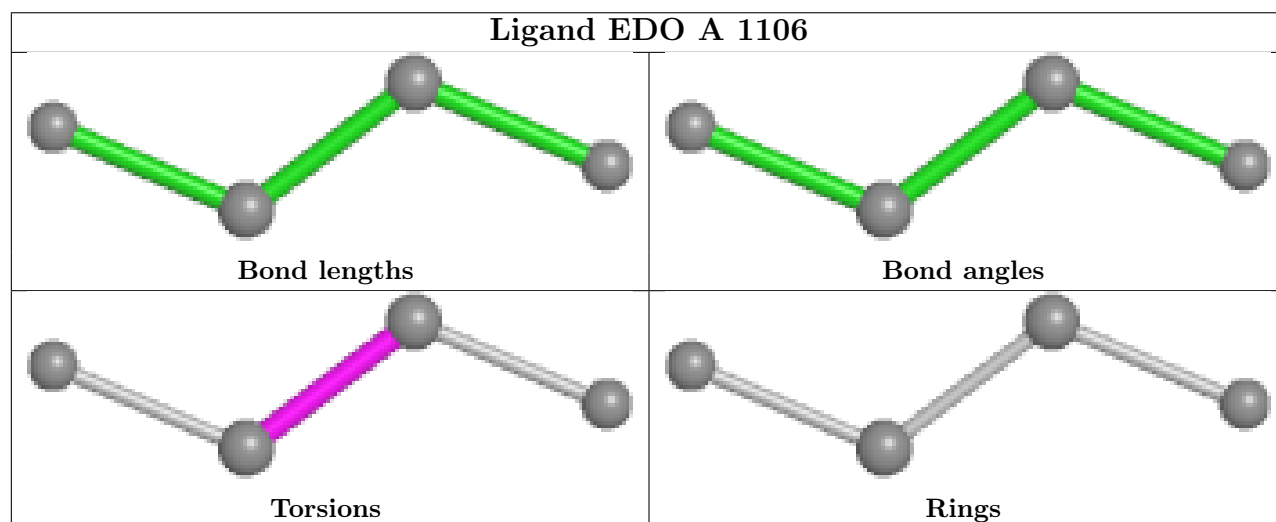
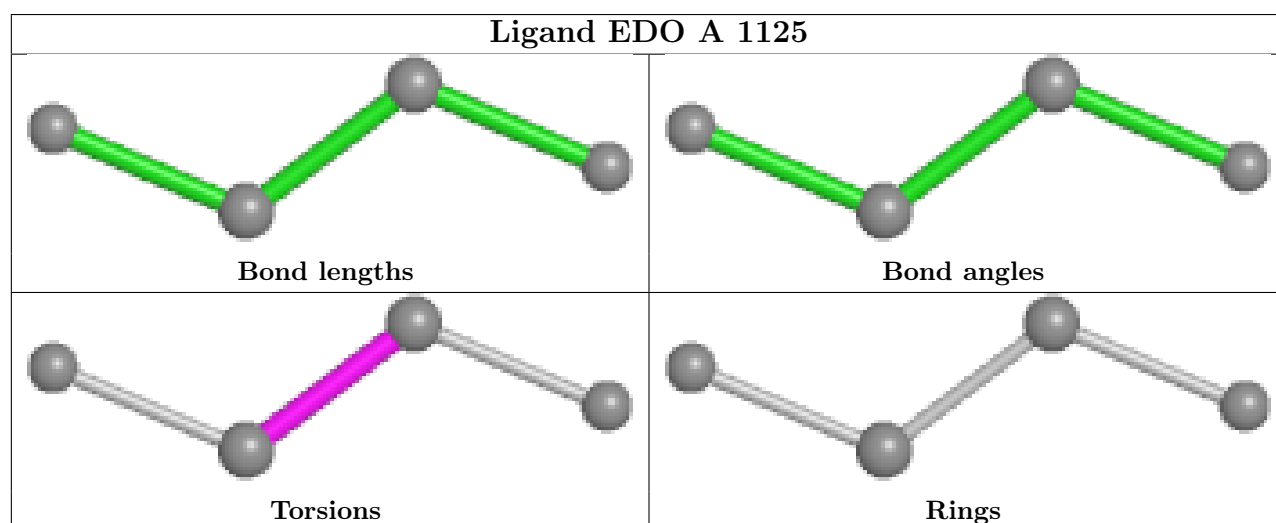
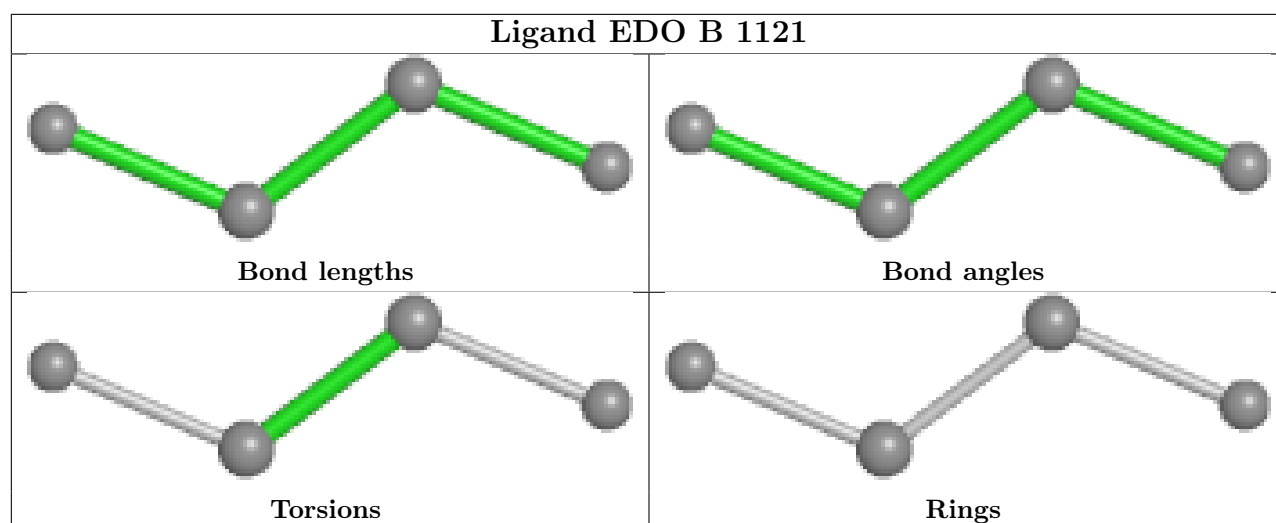


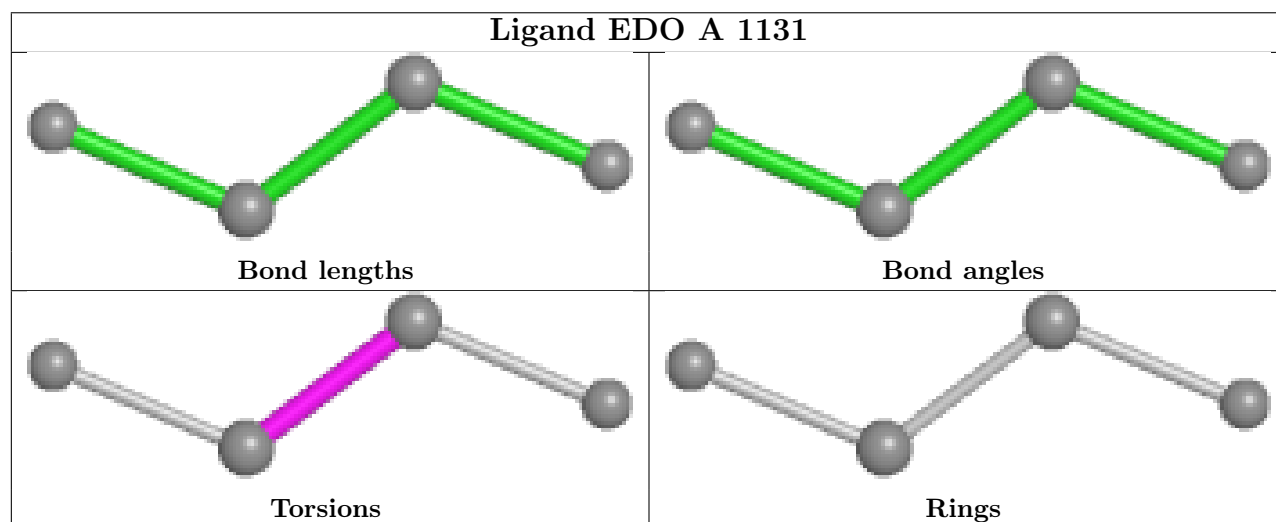
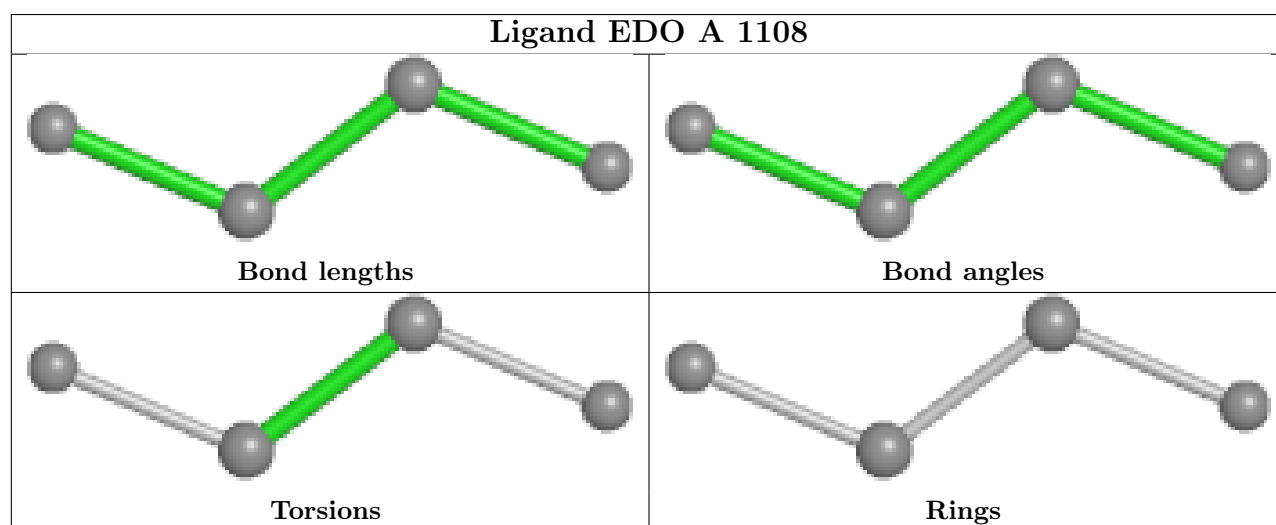
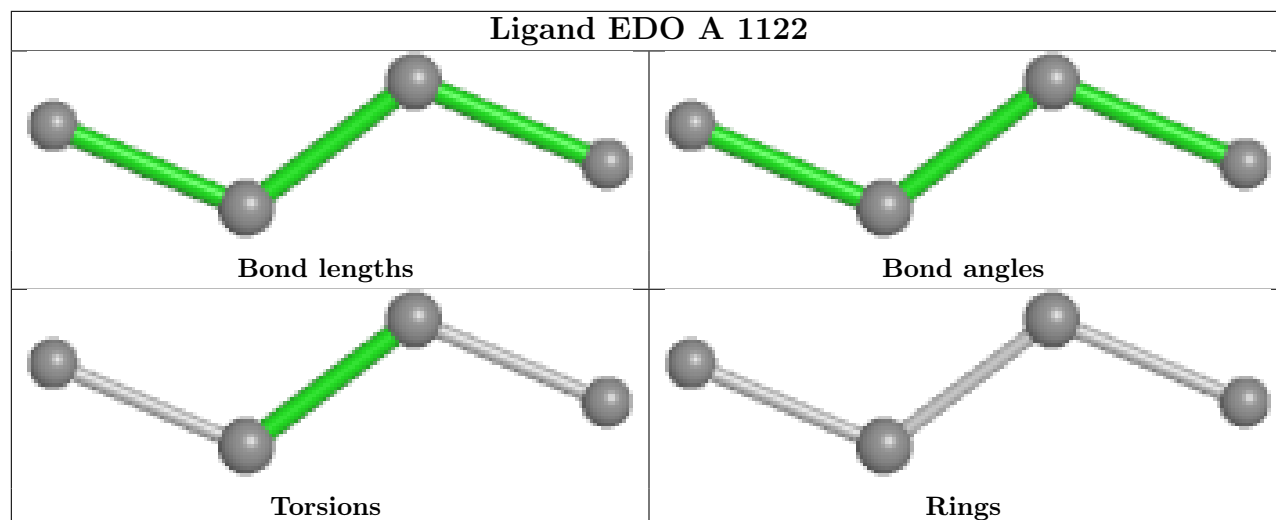


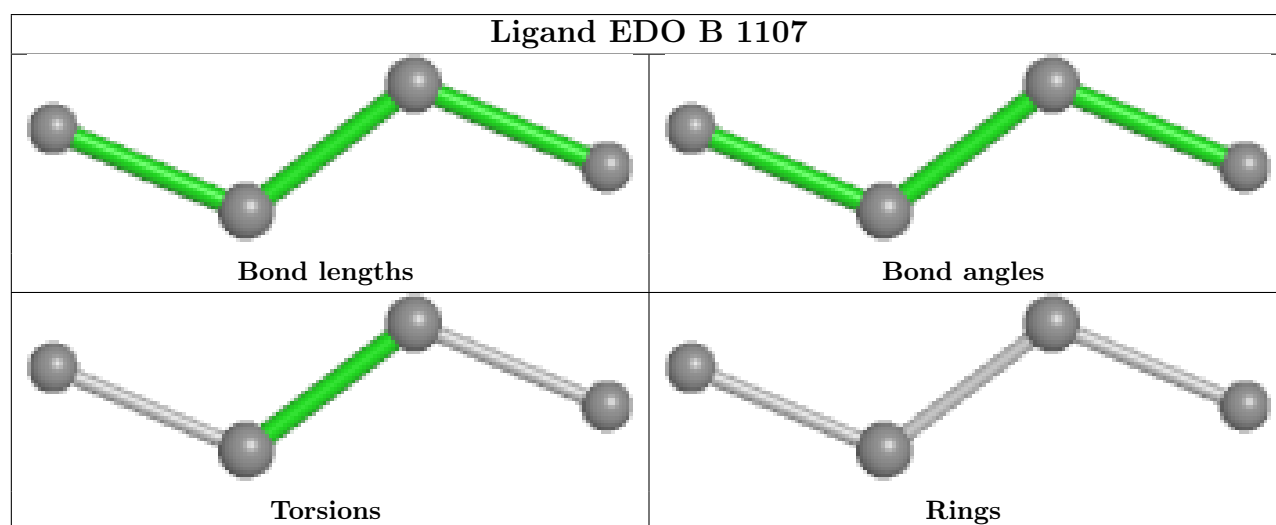
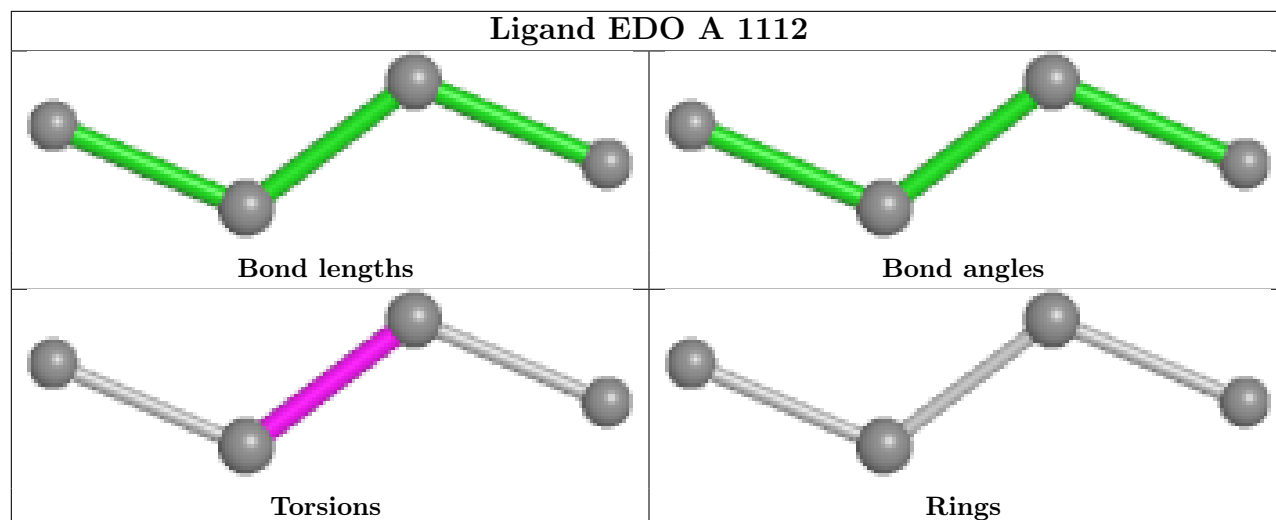


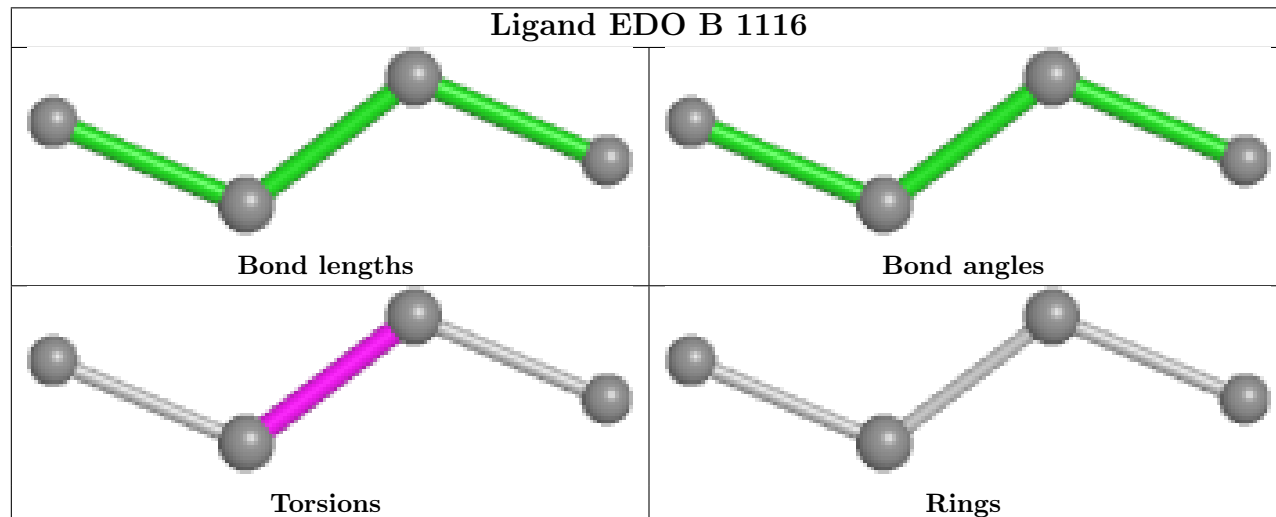
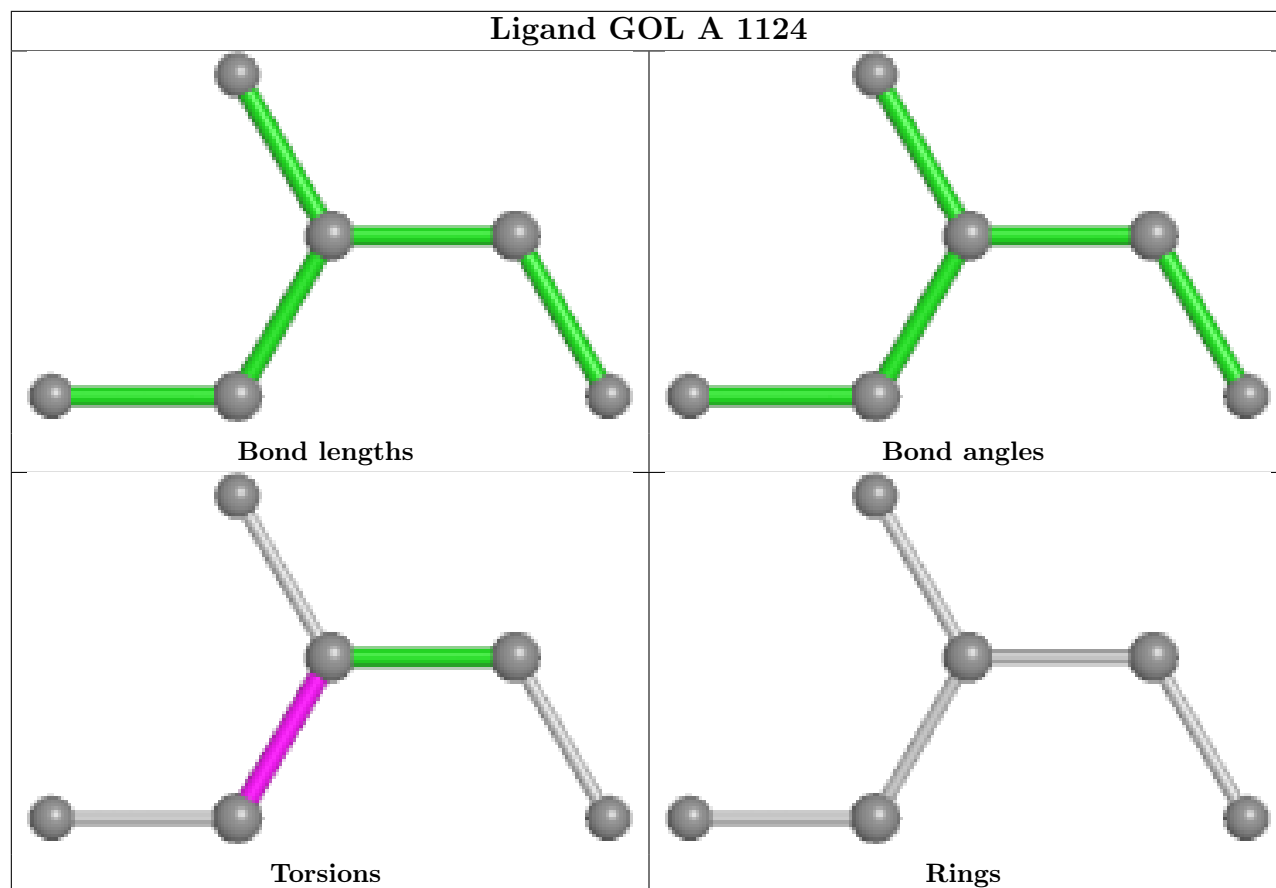


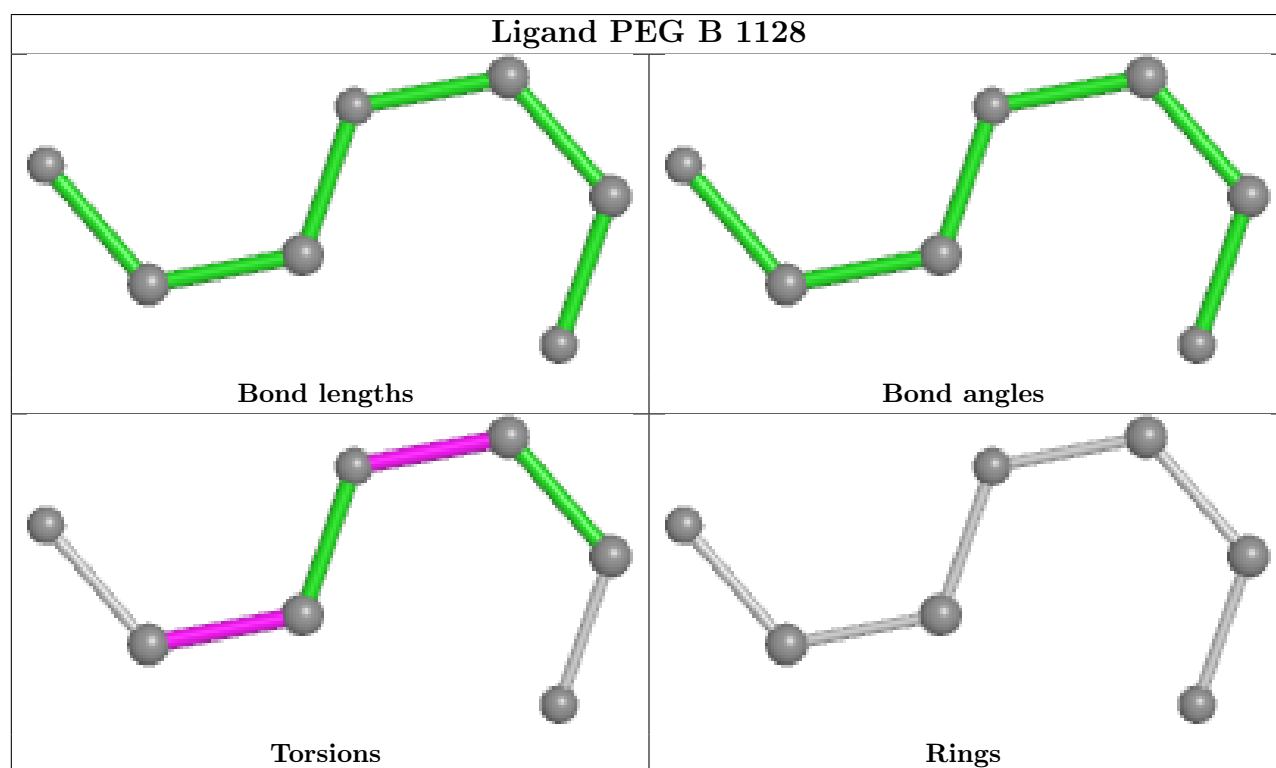
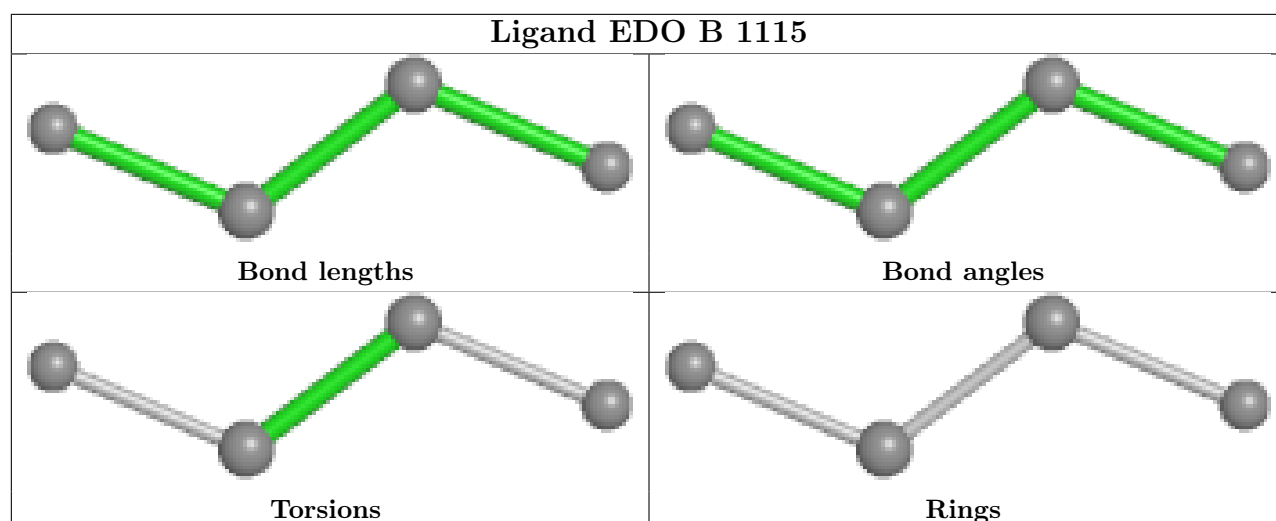




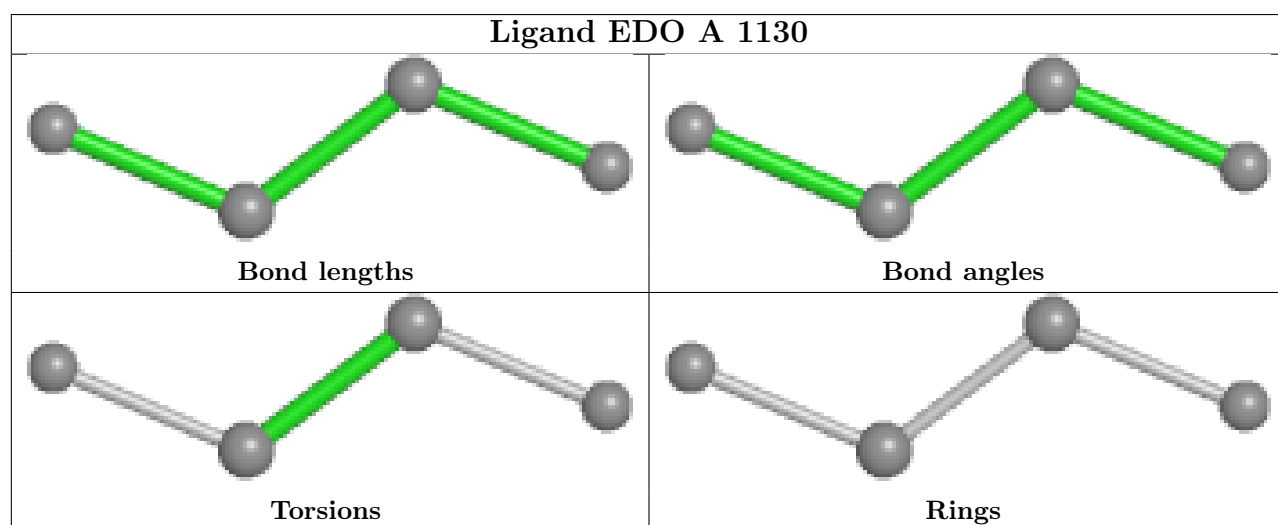
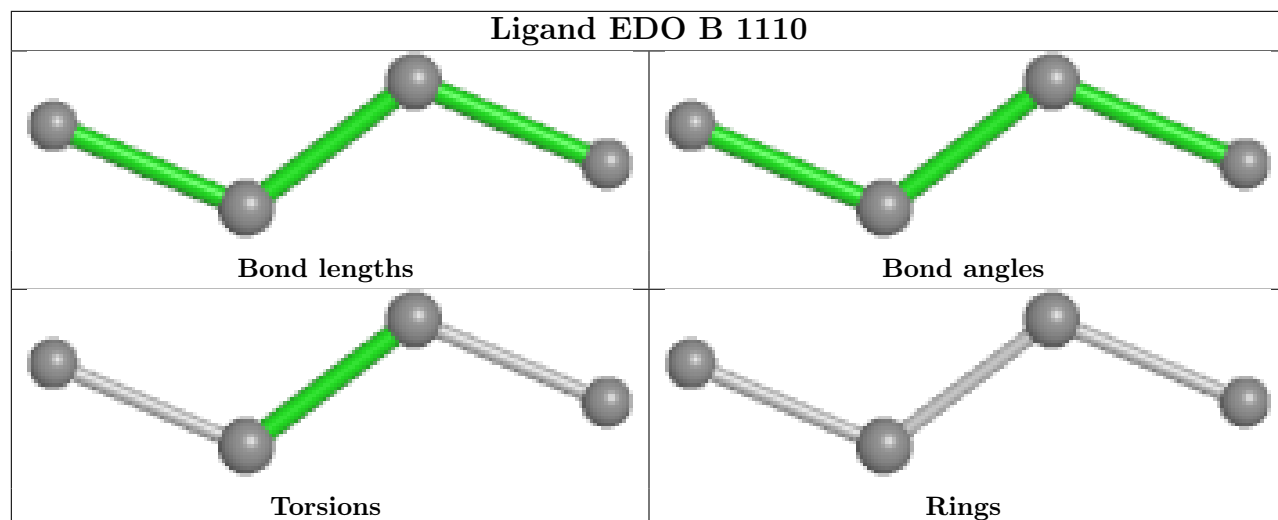


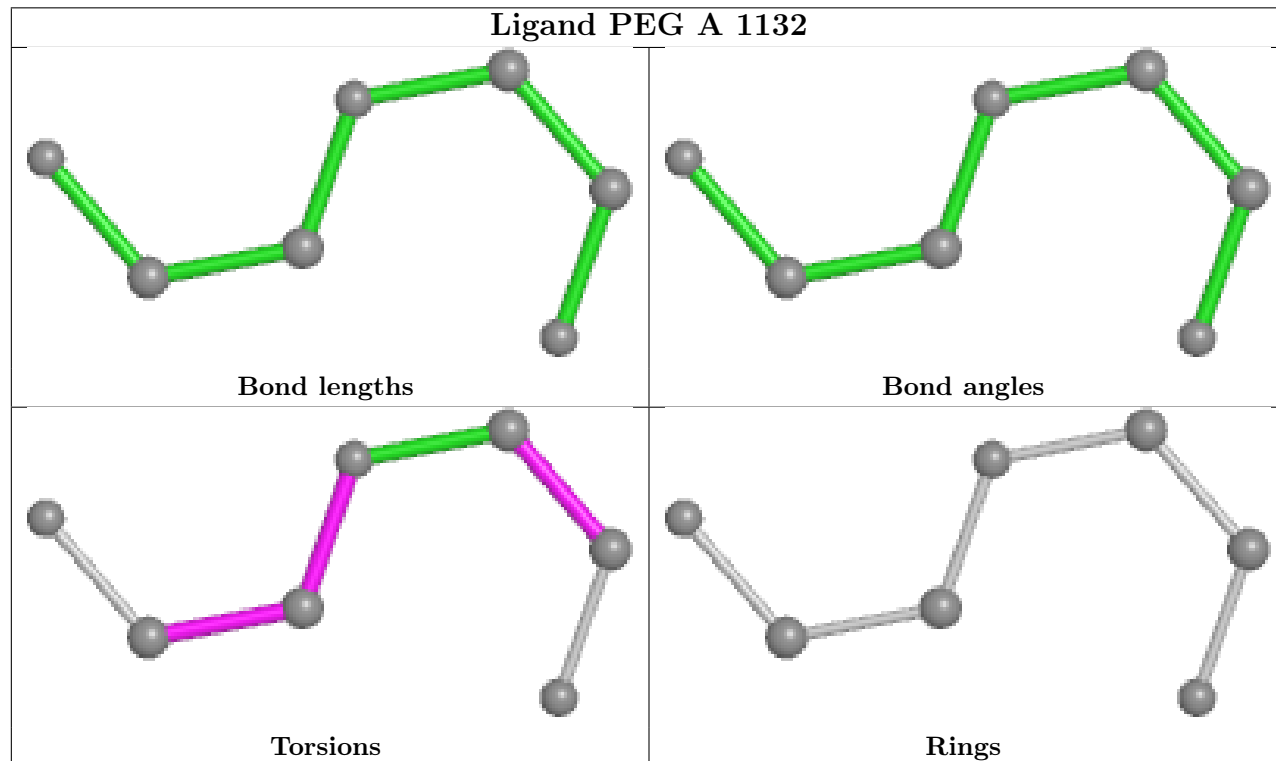
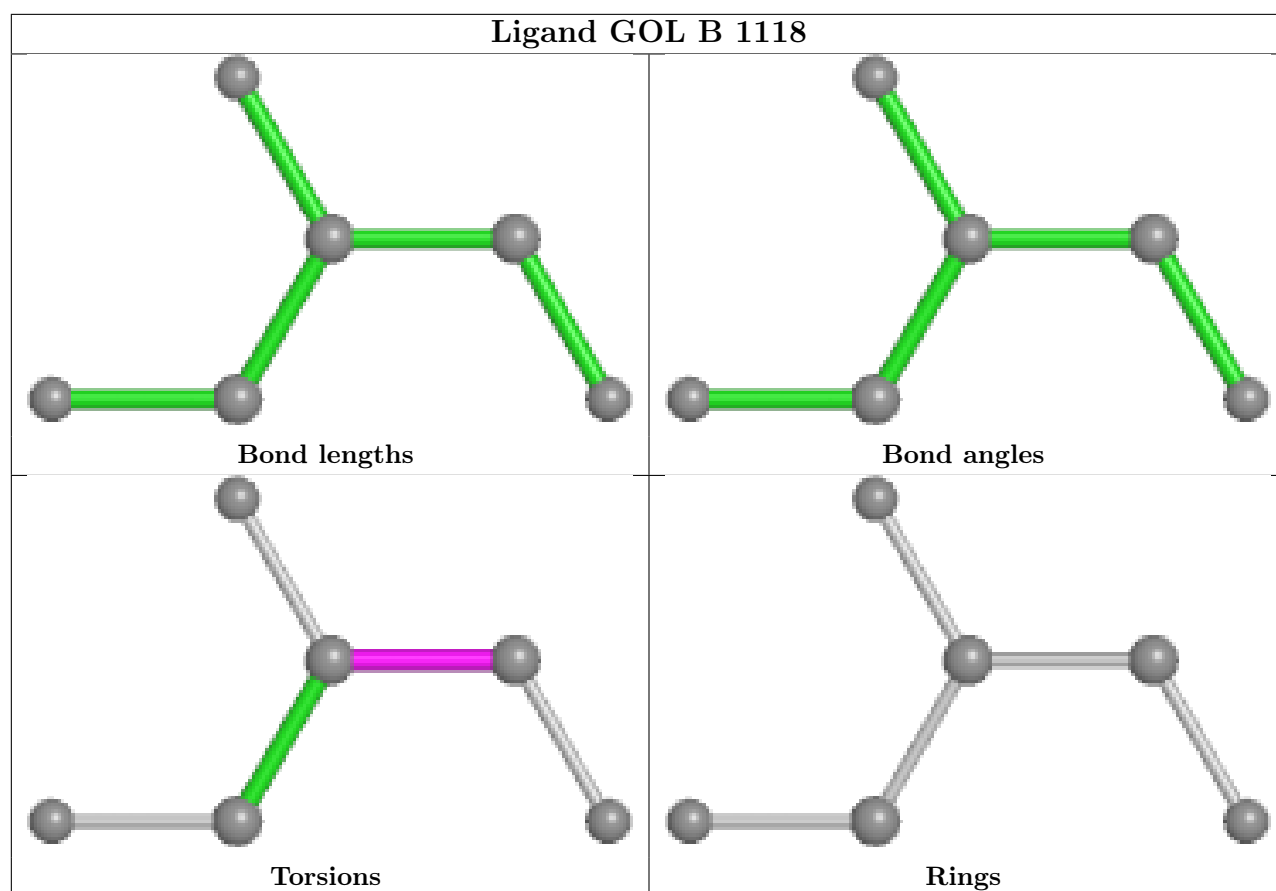


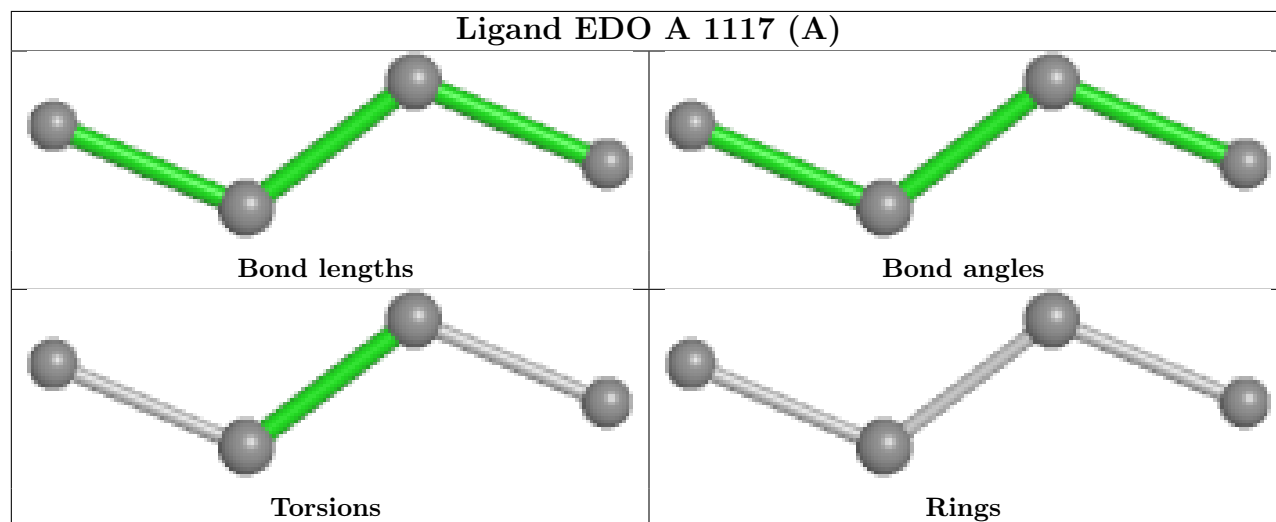
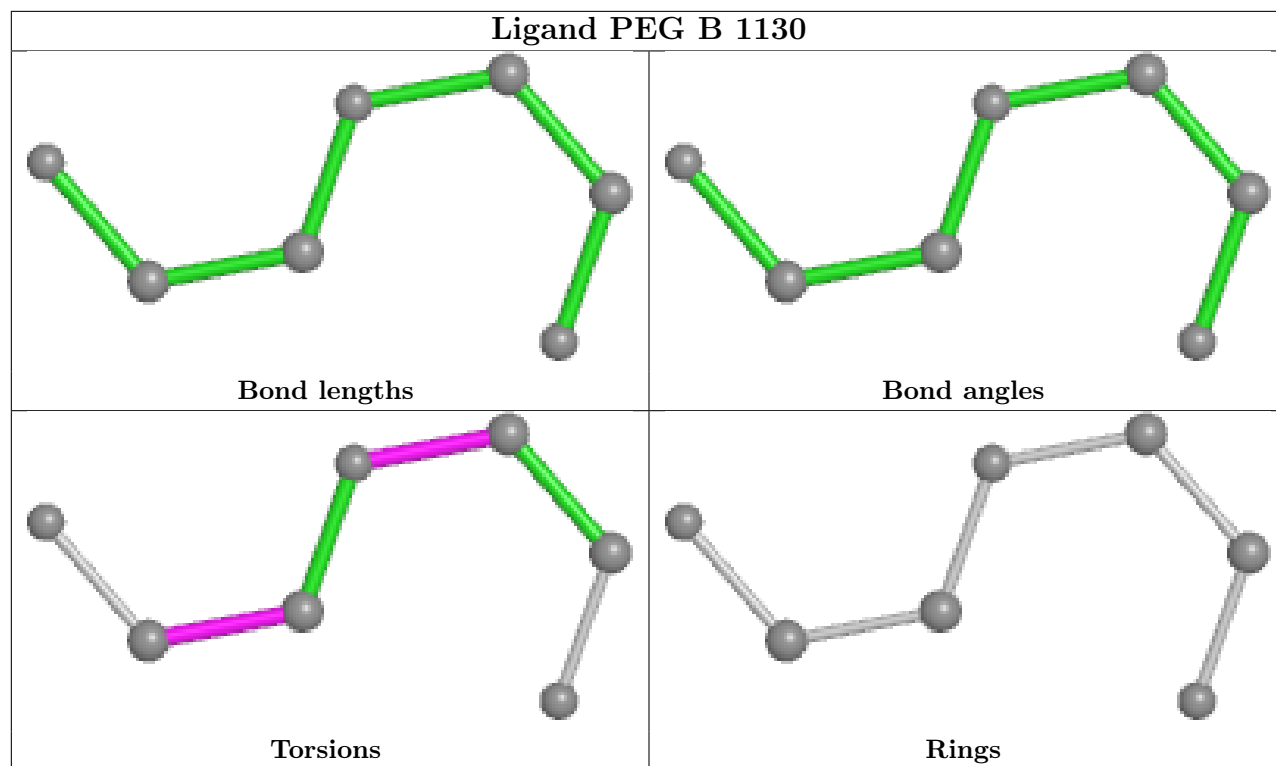


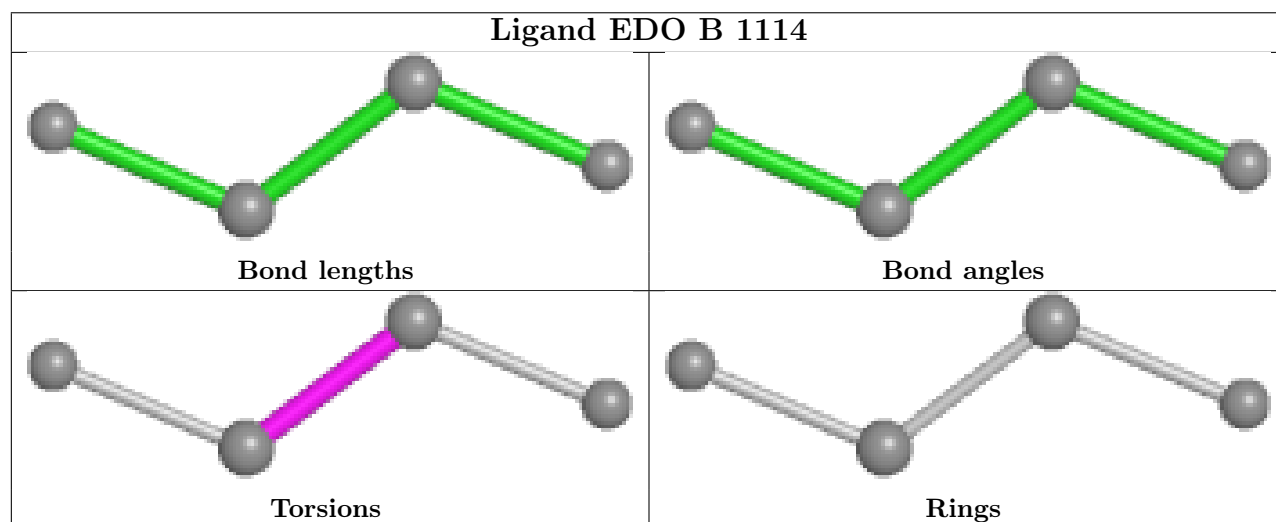
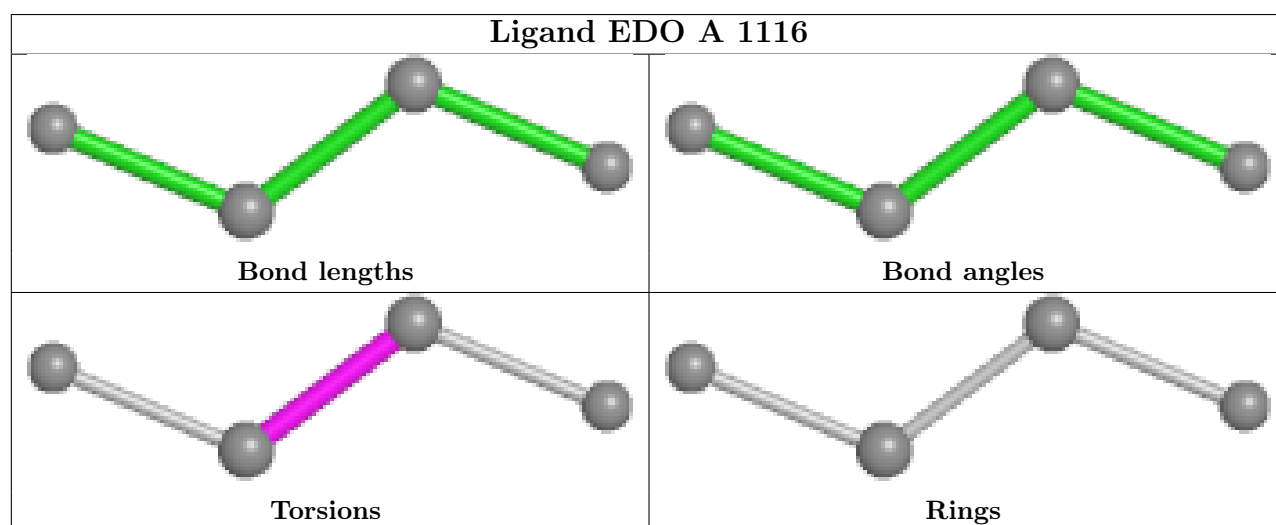
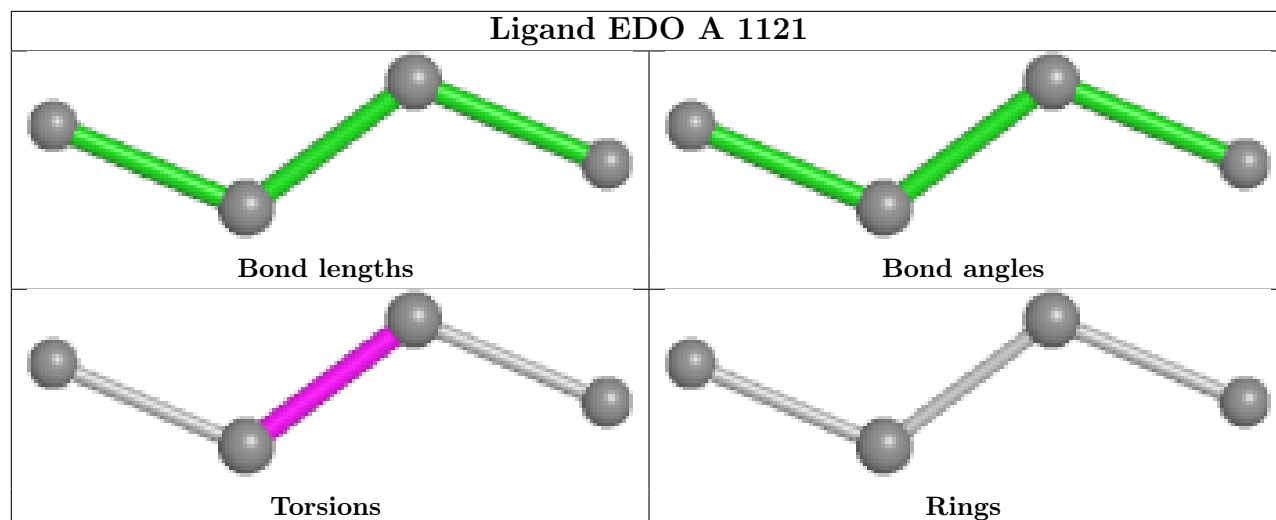


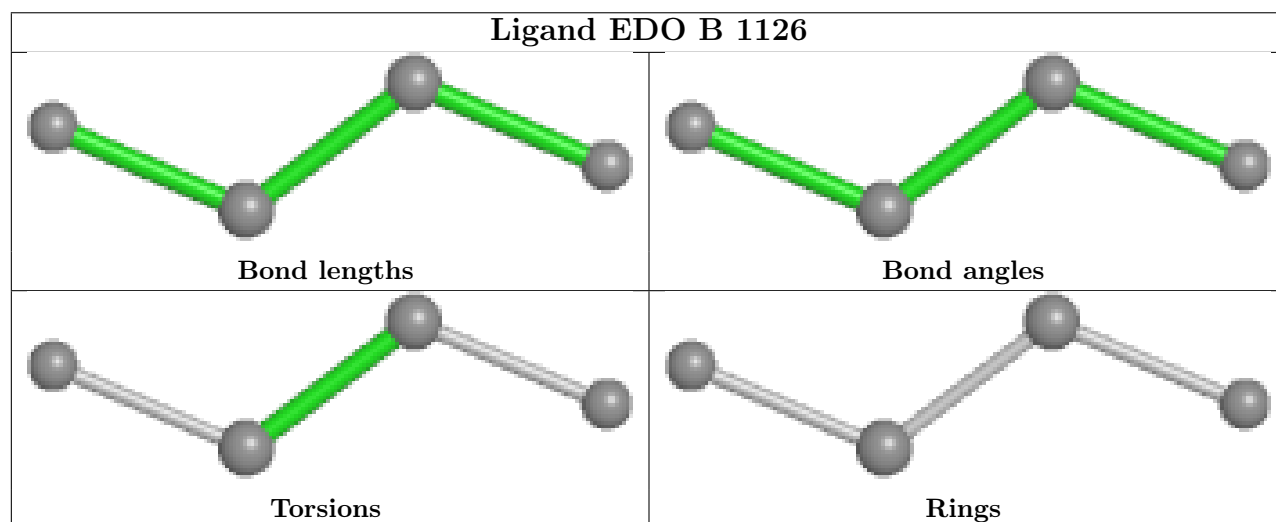
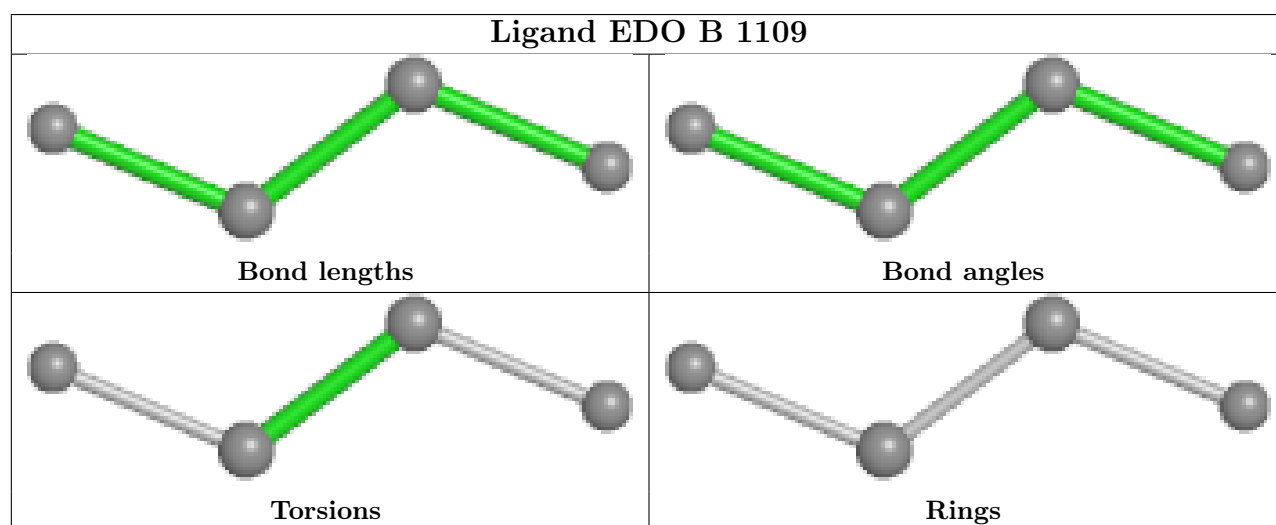
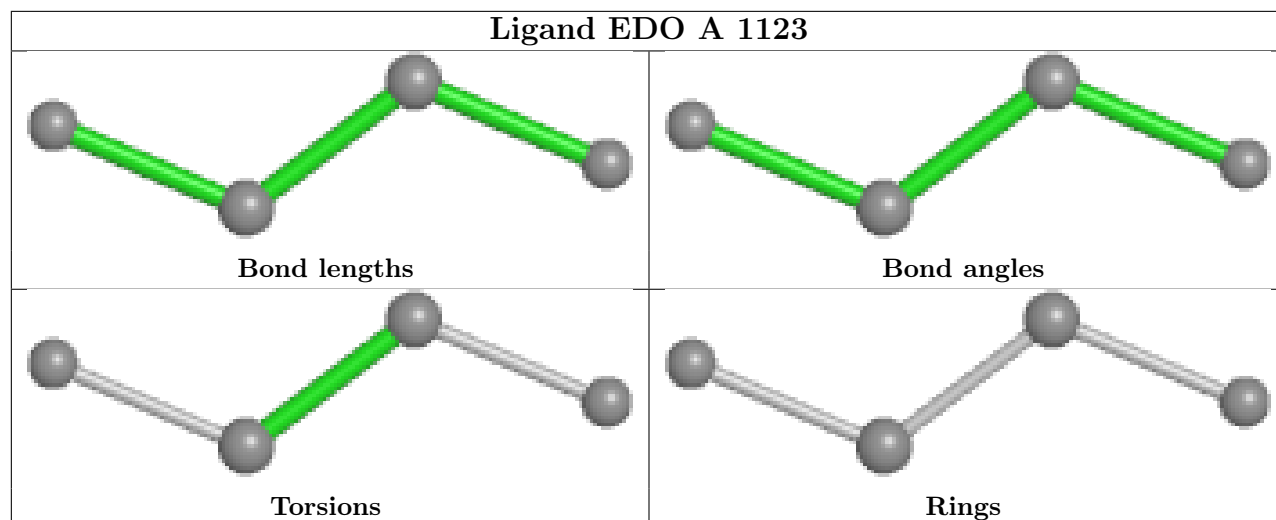


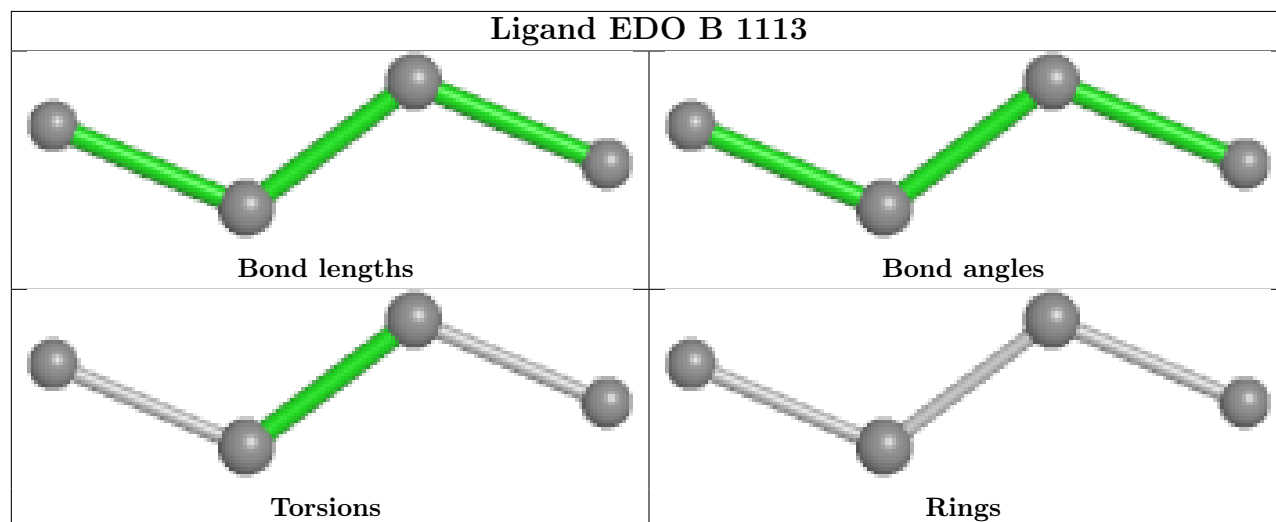
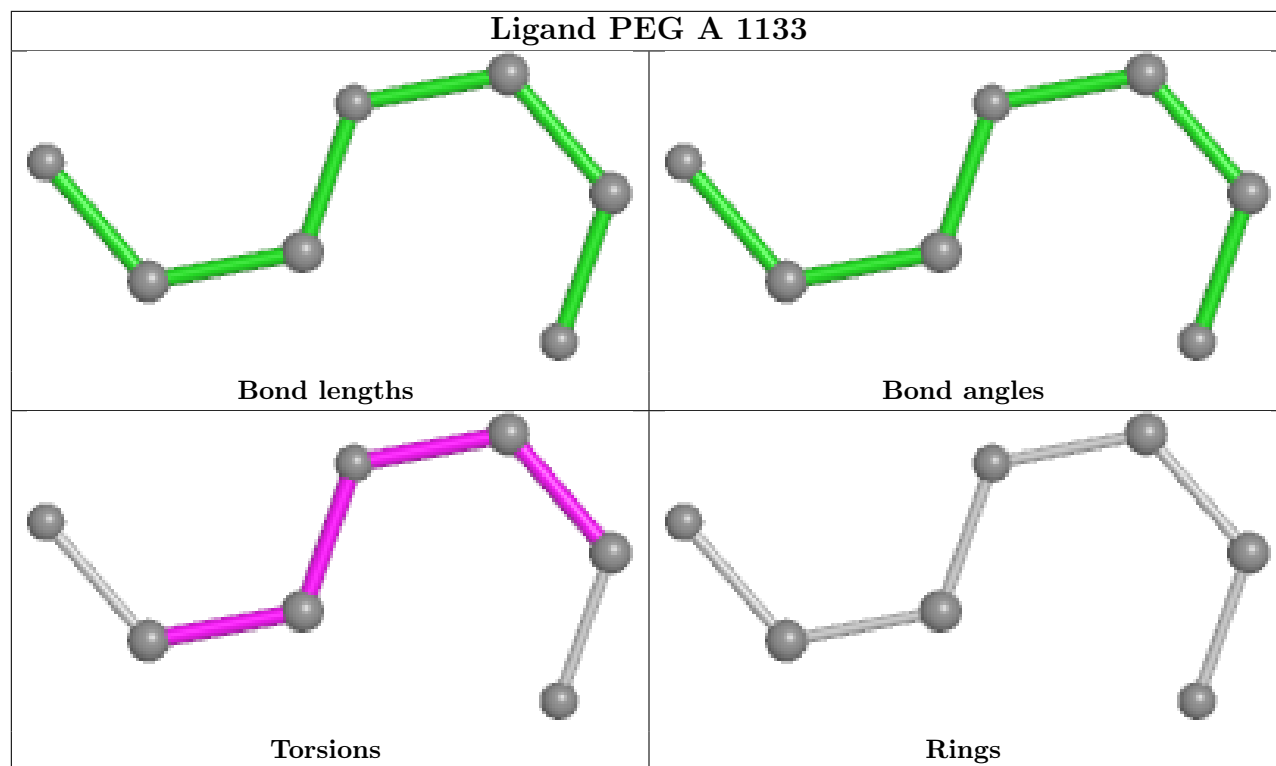


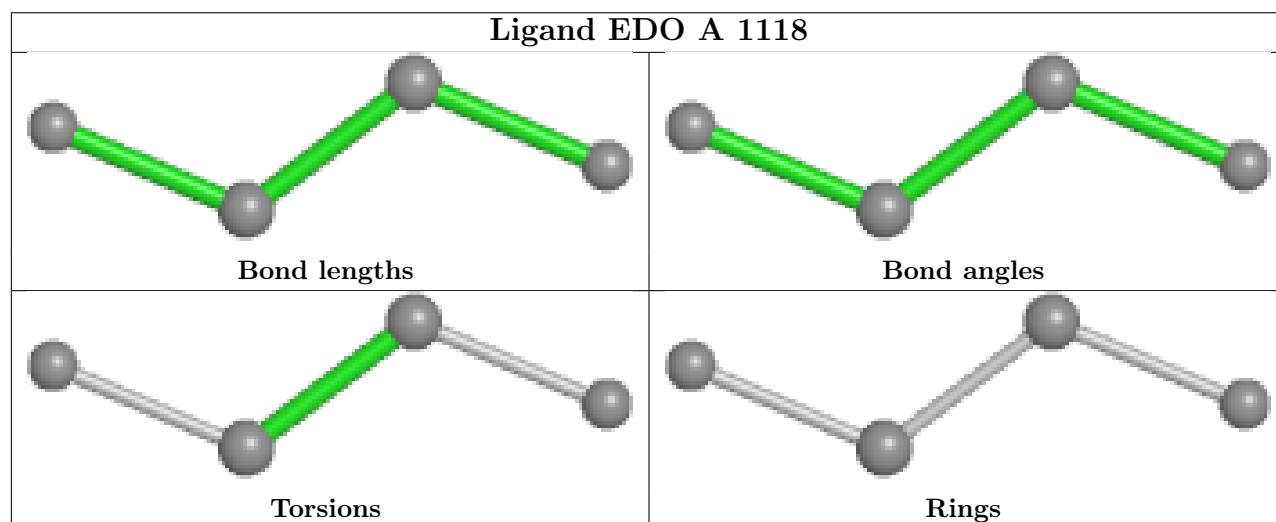
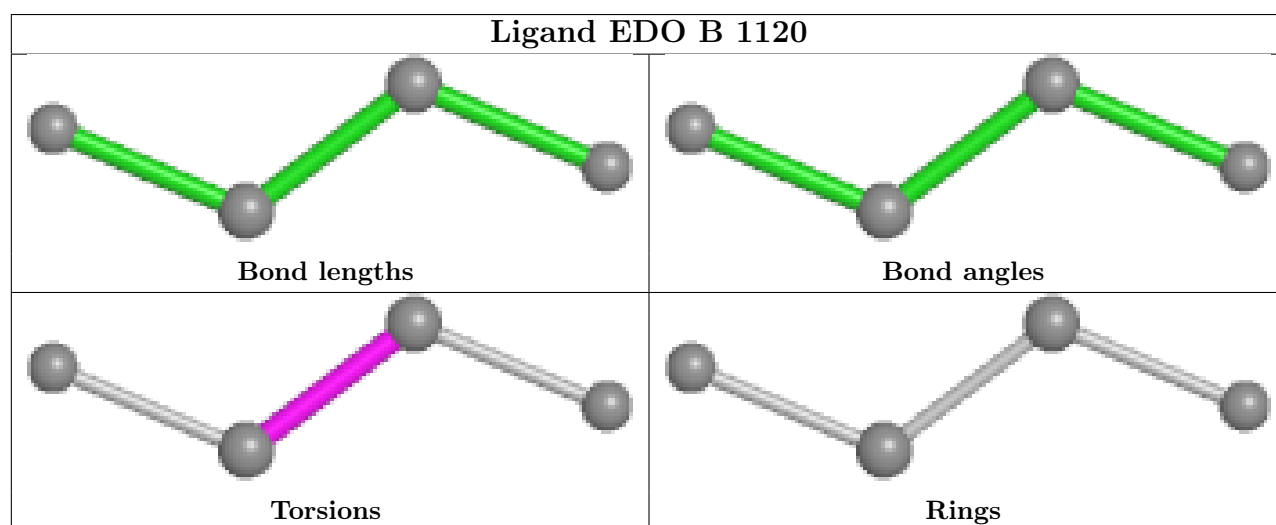
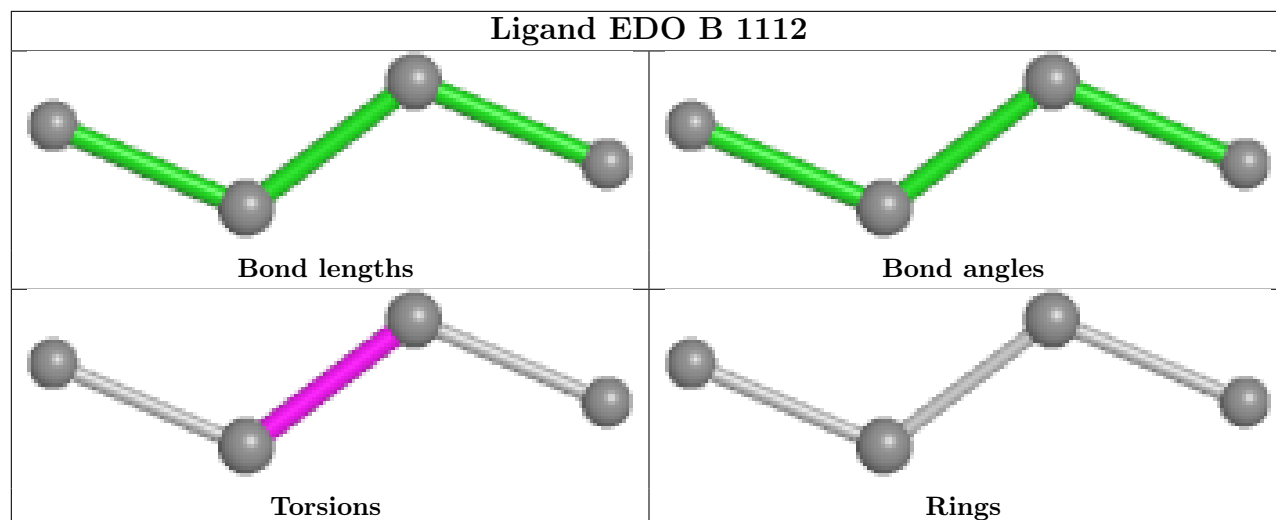


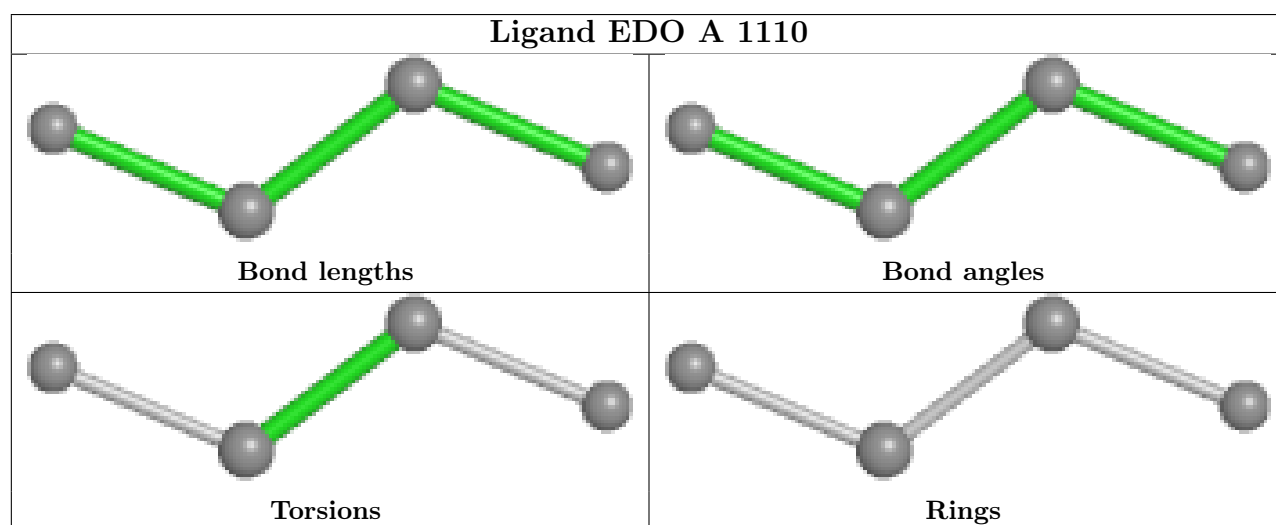
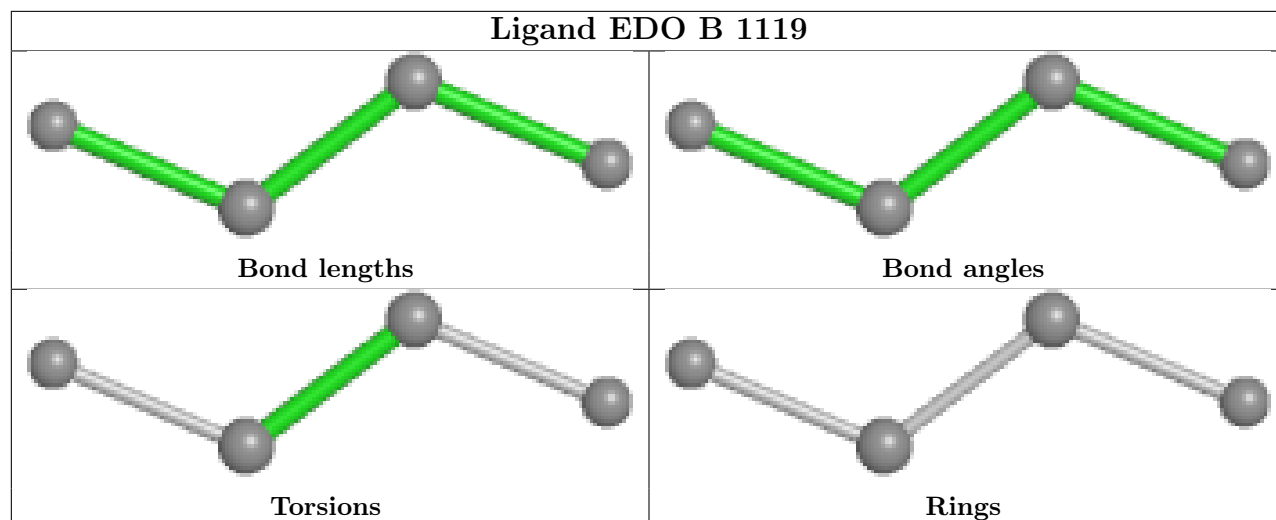




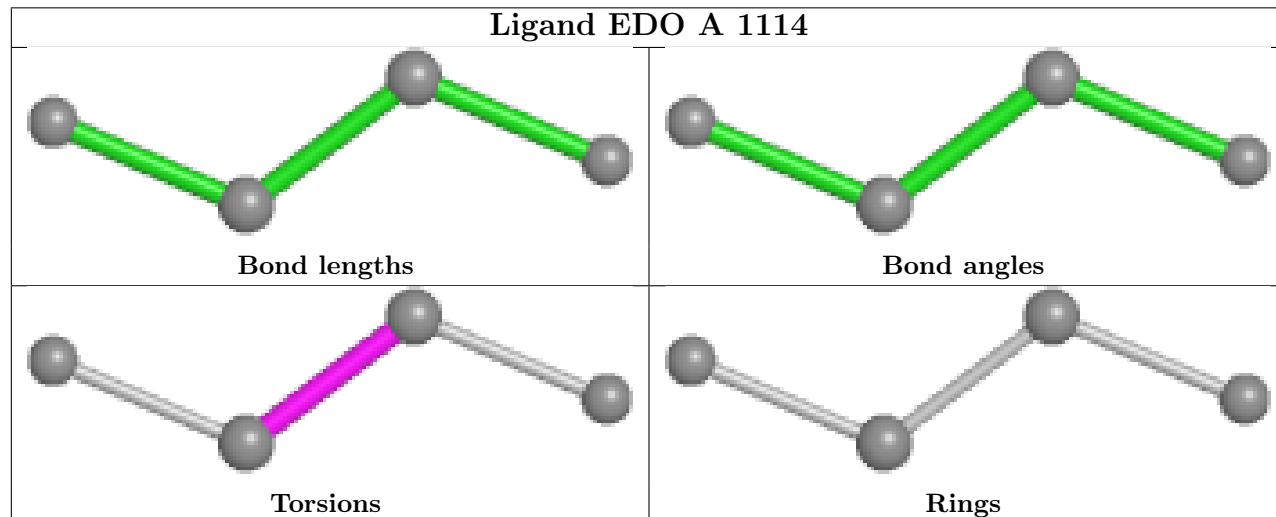
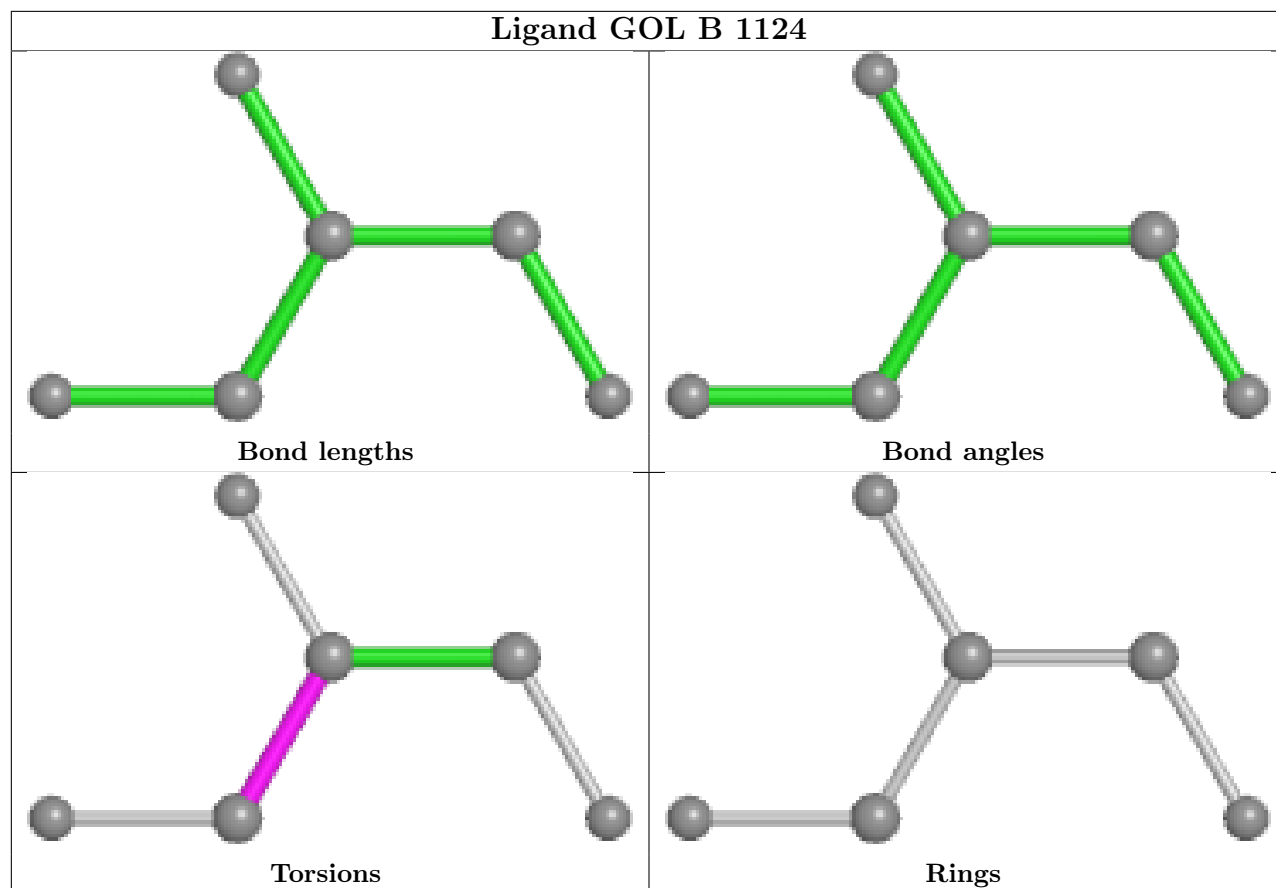


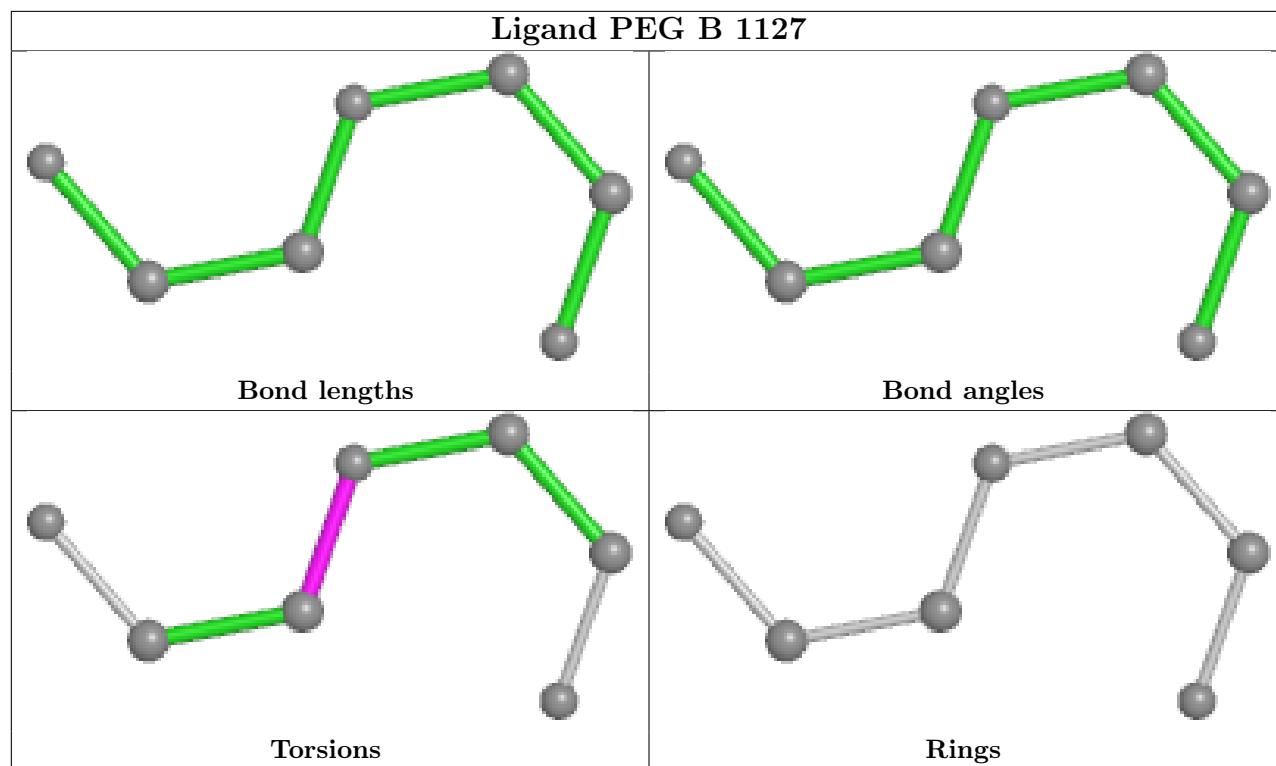












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	846/1047 (80%)	0.01	36 (4%) 35 32	11, 25, 58, 80	0
1	B	845/1047 (80%)	-0.05	26 (3%) 49 45	14, 24, 53, 71	0
All	All	1691/2094 (80%)	-0.02	62 (3%) 41 38	11, 25, 56, 80	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1022	SER	4.4
1	A	271	GLY	4.4
1	A	266	GLU	4.4
1	A	273	THR	4.3
1	A	1022	SER	4.2
1	B	228	GLY	3.9
1	A	272	LEU	3.8
1	B	306	ALA	3.6
1	A	192	GLY	3.6
1	A	222	TYR	3.5
1	A	285	ALA	3.4
1	A	270	TYR	3.4
1	A	280	LEU	3.3
1	A	269	ASN	3.2
1	A	687	MET	3.2
1	B	305	VAL	3.1
1	B	270	TYR	3.0
1	A	267	ASN	2.9
1	B	1023	ASN	2.9
1	A	279	ASP	2.9
1	A	261	VAL	2.9
1	A	298	TYR	2.9
1	A	305	VAL	2.8
1	B	279	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	192	GLY	2.7
1	A	303	HIS	2.7
1	A	232	TYR	2.7
1	A	308	LYS	2.7
1	A	284	THR	2.6
1	A	191	ALA	2.6
1	A	307	ALA	2.6
1	A	265	TYR	2.6
1	B	265	TYR	2.5
1	A	268	SER	2.5
1	A	315	ASN	2.4
1	B	264	GLY	2.4
1	A	274	ALA	2.4
1	A	711	THR	2.4
1	B	275	GLY	2.4
1	B	277	VAL	2.4
1	B	304	VAL	2.4
1	A	264	GLY	2.3
1	B	222	TYR	2.3
1	B	267	ASN	2.3
1	A	296	LEU	2.3
1	B	687	MET	2.3
1	B	285	ALA	2.3
1	B	266	GLU	2.3
1	A	257	ILE	2.2
1	A	278	LYS	2.2
1	B	194	TRP	2.2
1	B	818	THR	2.2
1	B	193	PRO	2.2
1	B	269	ASN	2.2
1	B	268	SER	2.2
1	A	260	PHE	2.1
1	B	260	PHE	2.1
1	B	1028	ASN	2.1
1	A	299	VAL	2.1
1	A	743	ILE	2.0
1	B	232	TYR	2.0
1	A	1021	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	B	1124	6/6	0.58	0.33	44,48,55,71	0
3	EDO	A	1122	4/4	0.60	0.34	43,58,58,60	0
3	EDO	A	1106	4/4	0.64	0.23	58,58,61,64	0
3	EDO	B	1119	4/4	0.74	0.23	45,46,47,49	0
3	EDO	A	1125	4/4	0.74	0.25	44,49,51,54	0
5	PEG	B	1127	7/7	0.77	0.31	45,52,56,59	0
5	PEG	A	1132	7/7	0.79	0.27	39,47,52,54	0
3	EDO	B	1107	4/4	0.80	0.30	38,42,43,47	0
5	PEG	B	1117	7/7	0.81	0.48	32,43,48,54	0
3	EDO	B	1114	4/4	0.81	0.23	43,43,50,51	0
5	PEG	B	1128	7/7	0.81	0.27	32,40,44,47	0
3	EDO	A	1112	4/4	0.82	0.34	35,39,39,45	0
3	EDO	A	1115	4/4	0.83	0.26	30,34,37,53	0
5	PEG	A	1133	7/7	0.83	0.26	38,42,48,51	0
3	EDO	A	1130	4/4	0.83	0.29	37,39,40,42	0
4	GOL	A	1127	6/6	0.83	0.27	39,44,50,50	0
2	CA	B	1105	1/1	0.83	0.12	60,60,60,60	0
5	PEG	B	1130	7/7	0.83	0.18	40,44,48,49	0
3	EDO	A	1114	4/4	0.84	0.24	37,38,39,42	0
4	GOL	B	1123	6/6	0.84	0.27	30,34,37,38	0
3	EDO	A	1109	4/4	0.84	0.23	38,40,46,47	0
4	GOL	A	1124	6/6	0.85	0.38	32,42,45,45	0
3	EDO	B	1109	4/4	0.85	0.19	37,40,41,41	0
3	EDO	B	1125	4/4	0.86	0.31	28,33,36,37	0
3	EDO	A	1108	4/4	0.86	0.37	39,41,44,47	0
3	EDO	B	1120	4/4	0.86	0.30	37,38,47,49	0
4	GOL	A	1128	6/6	0.86	0.28	36,39,41,42	0
3	EDO	A	1131	4/4	0.87	0.22	35,37,39,44	0
3	EDO	A	1110	4/4	0.87	0.16	31,37,41,43	0
3	EDO	B	1121	4/4	0.87	0.18	40,43,44,45	0
3	EDO	A	1113	4/4	0.87	0.22	38,40,42,48	0
3	EDO	A	1118	4/4	0.87	0.18	32,39,40,45	0

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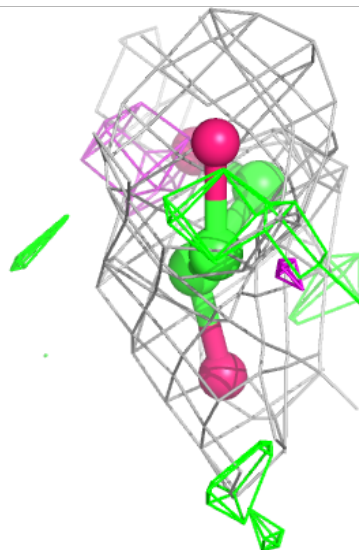
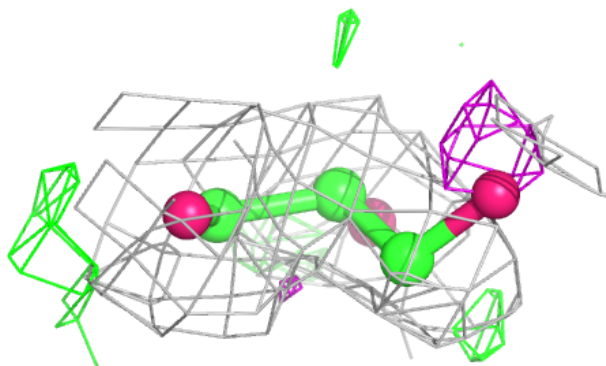
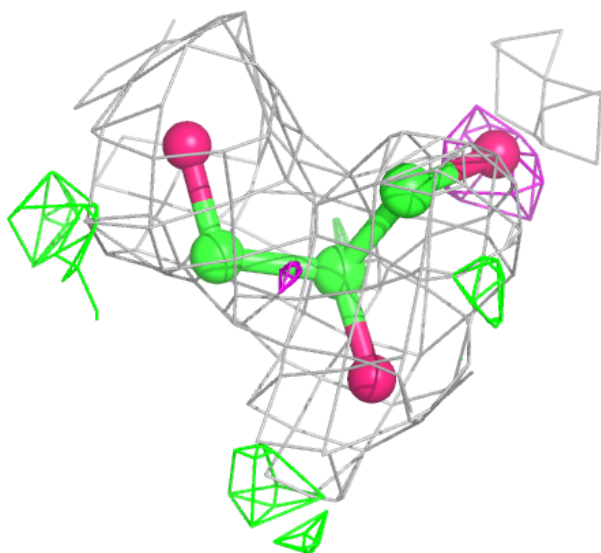
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	1110	4/4	0.88	0.28	41,47,48,51	0
3	EDO	B	1112	4/4	0.88	0.25	46,51,53,54	0
2	CA	B	1106	1/1	0.88	0.08	58,58,58,58	0
3	EDO	B	1122	4/4	0.88	0.14	37,39,42,42	0
3	EDO	A	1107	4/4	0.89	0.24	38,38,44,45	0
3	EDO	B	1111	4/4	0.90	0.23	38,40,40,49	0
3	EDO	A	1129	4/4	0.90	0.17	36,41,42,45	0
2	CA	A	1105	1/1	0.90	0.07	63,63,63,63	0
3	EDO	B	1115	4/4	0.90	0.29	40,42,42,48	0
3	EDO	A	1119	4/4	0.90	0.27	46,47,47,47	0
3	EDO	A	1126	4/4	0.91	0.17	29,34,34,41	0
3	EDO	A	1111	4/4	0.91	0.25	54,54,58,58	0
3	EDO	B	1126	4/4	0.91	0.18	33,34,35,40	0
4	GOL	B	1118	6/6	0.91	0.35	39,41,48,52	0
3	EDO	A	1123	4/4	0.92	0.22	28,28,34,36	0
3	EDO	B	1108	4/4	0.92	0.35	39,39,45,45	0
3	EDO	B	1113	4/4	0.92	0.17	37,39,44,46	0
3	EDO	A	1116	4/4	0.92	0.15	55,55,55,58	0
2	CA	B	1103	1/1	0.92	0.06	44,44,44,44	0
5	PEG	B	1129	7/7	0.92	0.39	32,34,44,45	0
3	EDO	B	1116	4/4	0.92	0.33	31,31,33,41	0
3	EDO	A	1117[A]	4/4	0.93	0.18	32,34,34,36	4
3	EDO	A	1117[B]	4/4	0.93	0.18	33,34,35,37	4
3	EDO	A	1120	4/4	0.93	0.15	43,44,47,47	0
2	CA	A	1104	1/1	0.94	0.08	47,47,47,47	0
2	CA	A	1102	1/1	0.95	0.09	38,38,38,38	0
2	CA	B	1104	1/1	0.95	0.12	61,61,61,61	0
2	CA	A	1103	1/1	0.96	0.15	62,62,62,62	0
2	CA	B	1102	1/1	0.97	0.10	36,36,36,36	0
3	EDO	A	1121	4/4	0.97	0.13	33,39,39,43	0
2	CA	A	1101	1/1	0.99	0.06	21,21,21,21	0
2	CA	B	1101	1/1	0.99	0.07	18,18,18,18	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.

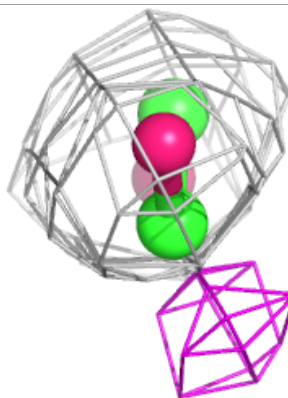
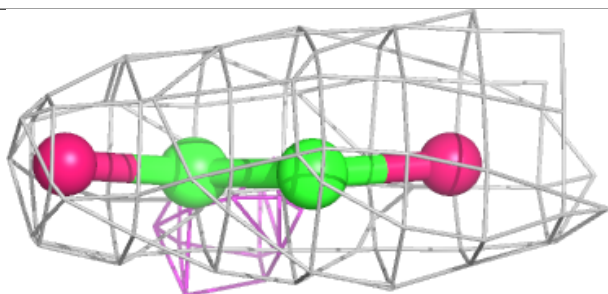
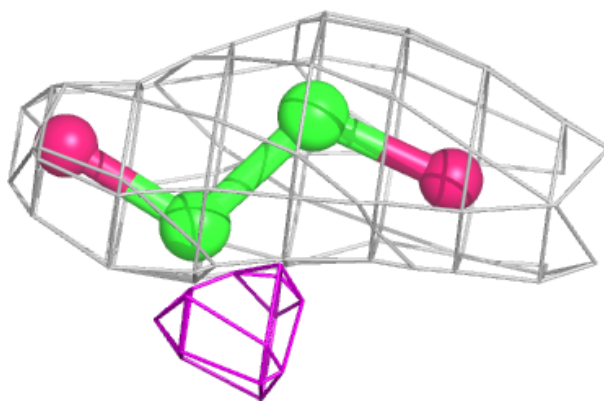
**Electron density around GOL B 1124:**

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



**Electron density around EDO A 1122:**

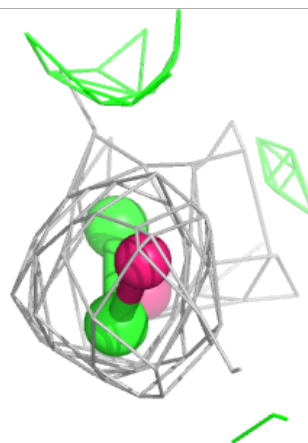
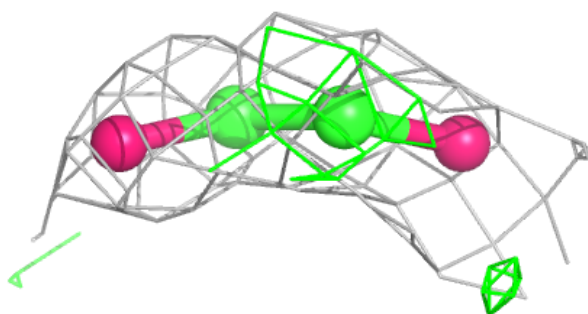
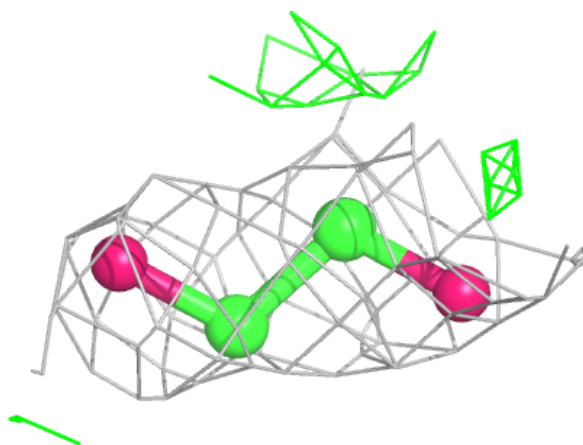
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





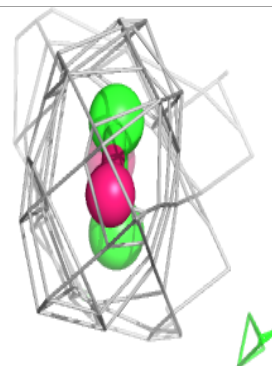
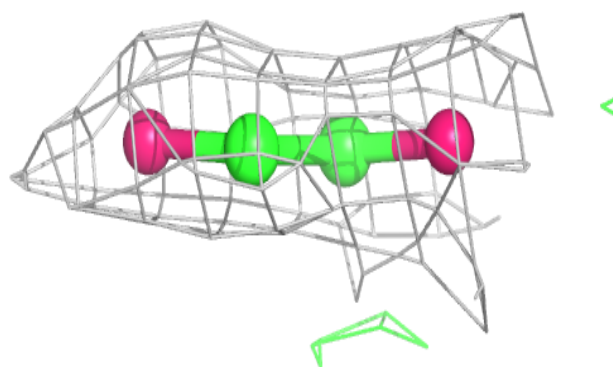
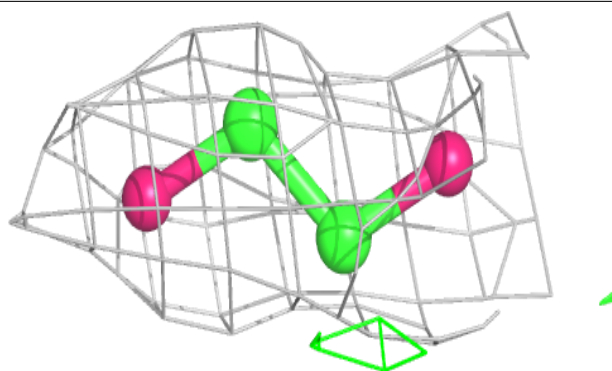
**Electron density around EDO A 1106:**

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

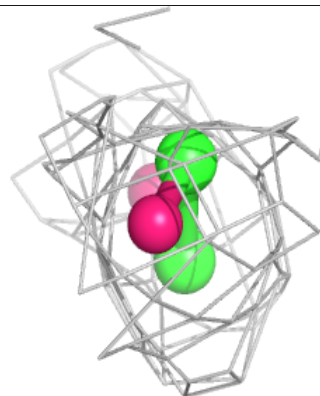
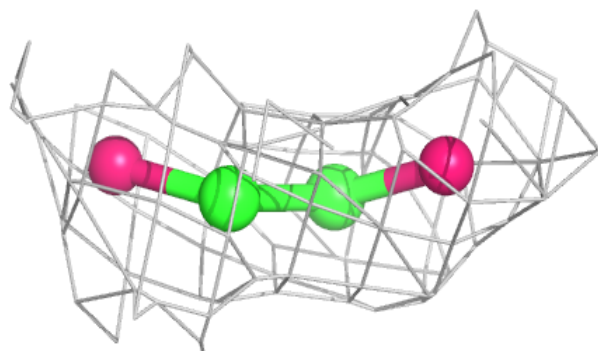
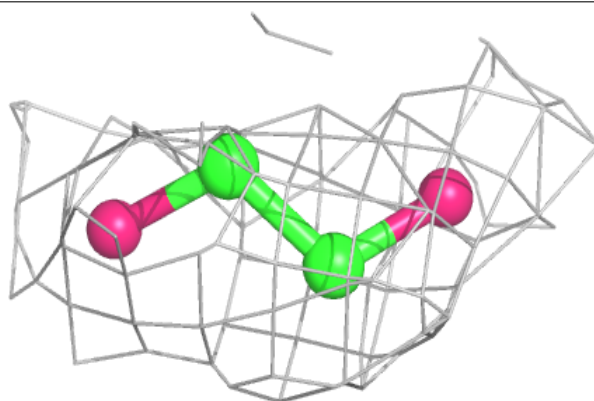


**Electron density around EDO B 1119:**

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

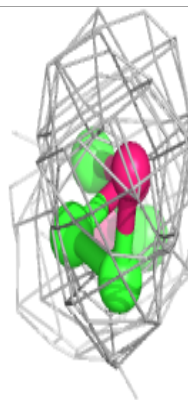
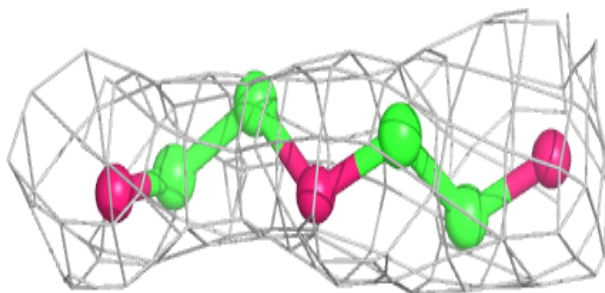
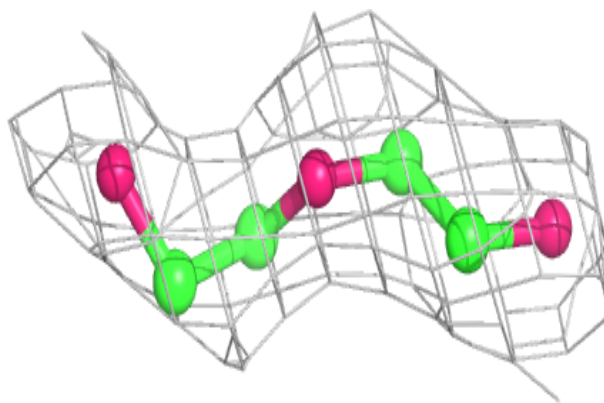
**Electron density around EDO A 1125:**

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

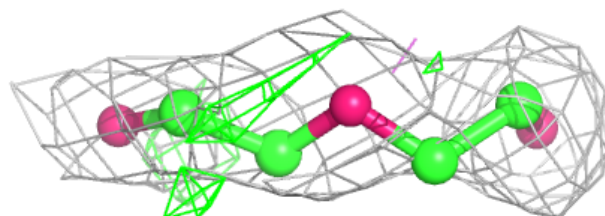
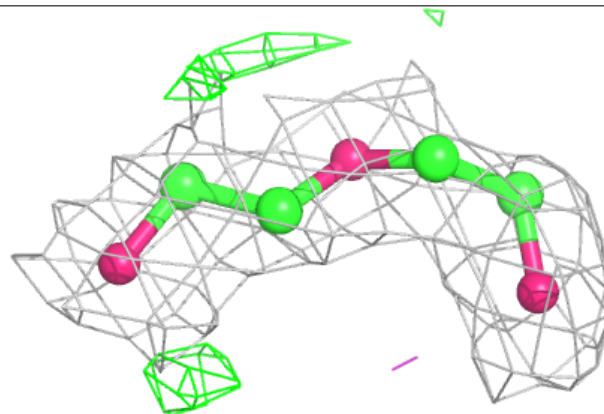


**Electron density around PEG B 1127:**

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

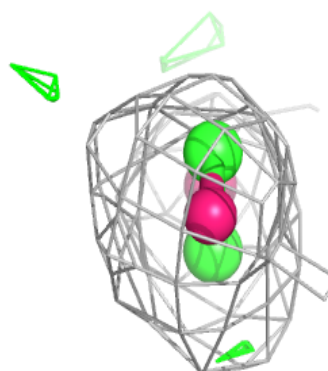
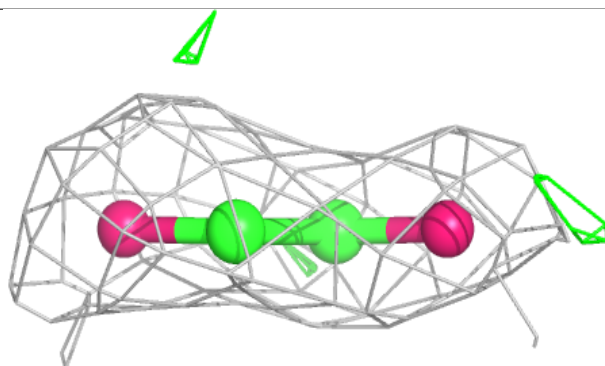
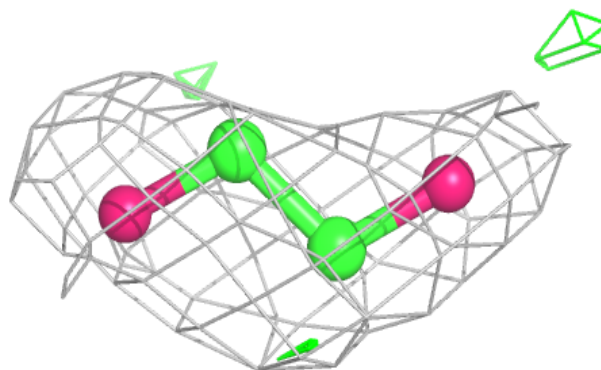
**Electron density around PEG A 1132:**

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

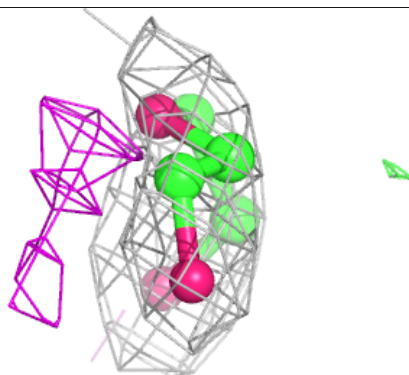
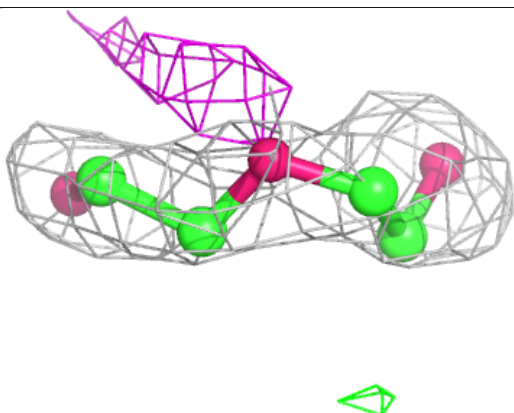
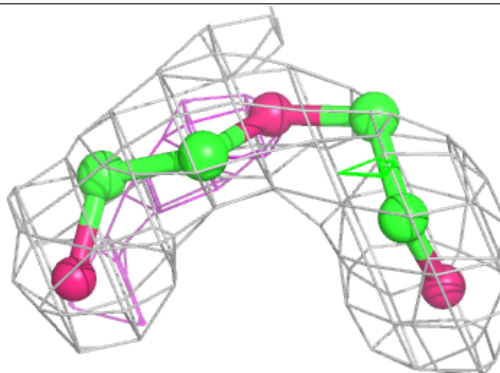


**Electron density around EDO B 1107:**

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

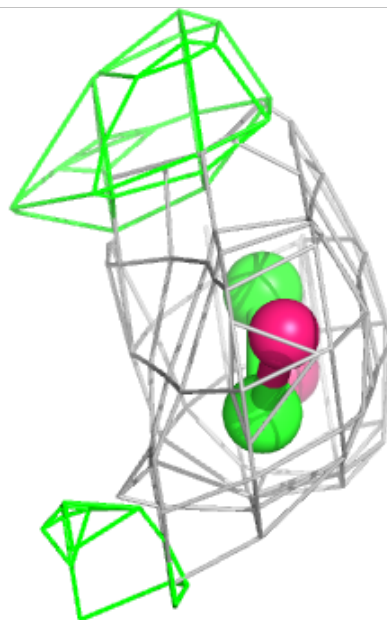
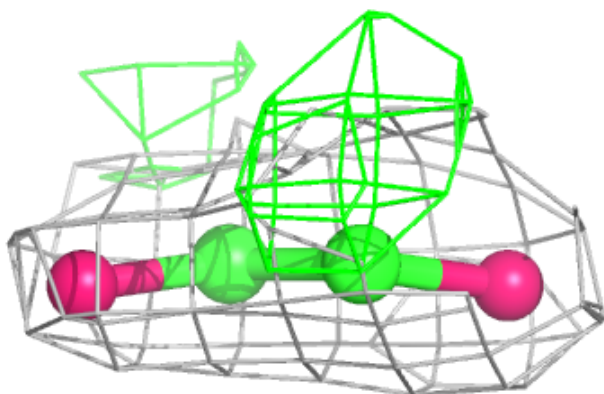
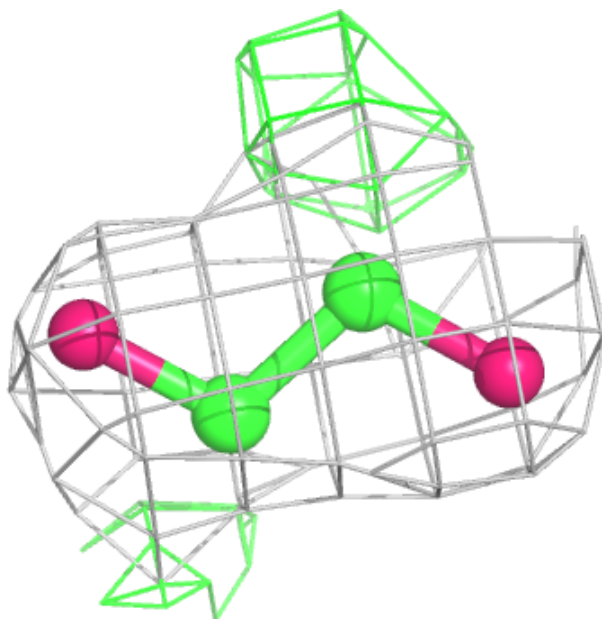
**Electron density around PEG B 1117:**

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



**Electron density around EDO B 1114:**

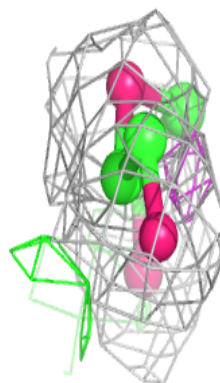
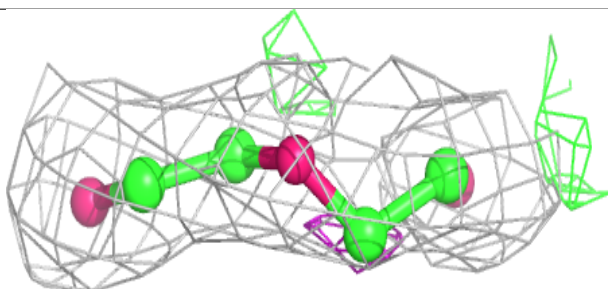
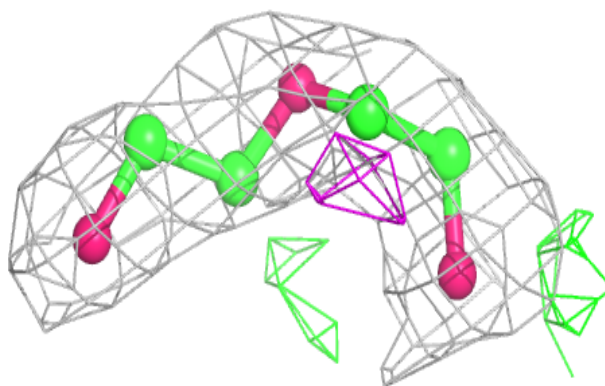
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



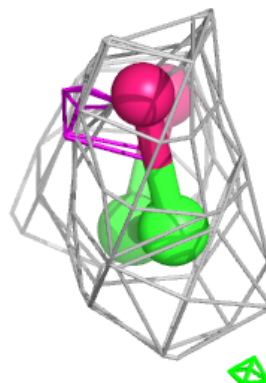
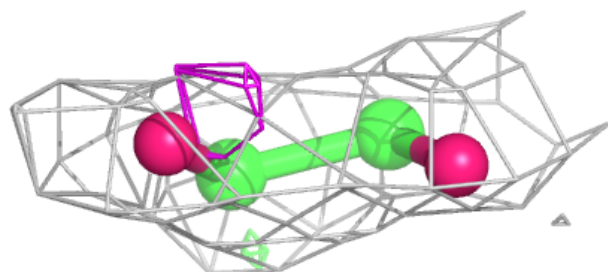
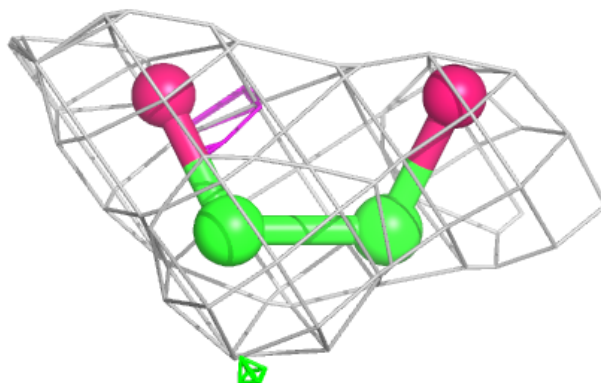


**Electron density around PEG B 1128:**

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

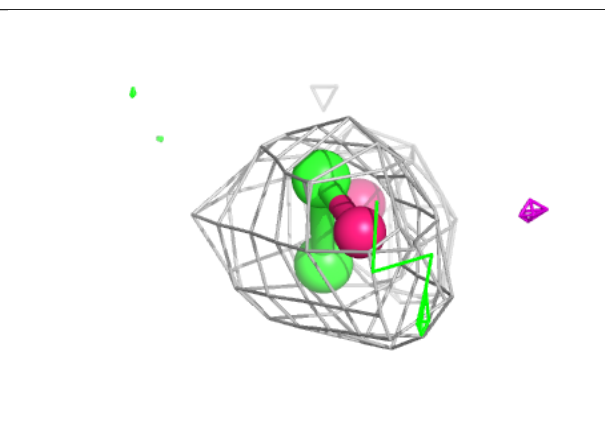
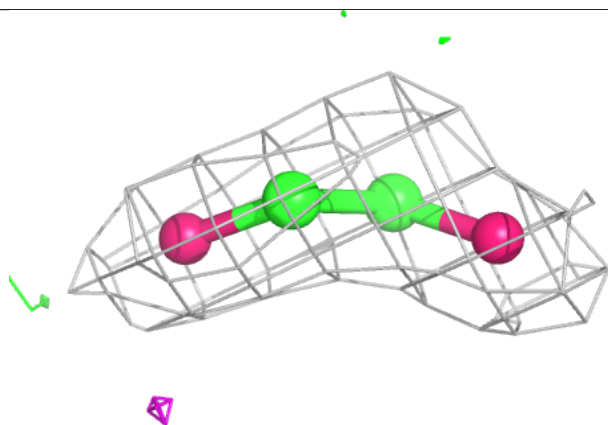
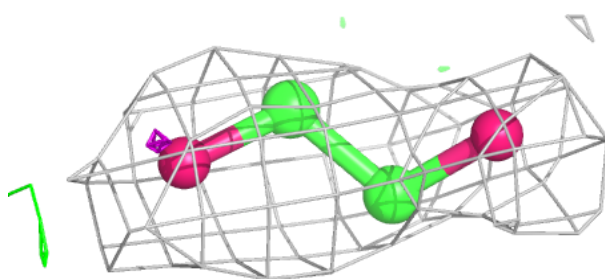
**Electron density around EDO A 1112:**

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

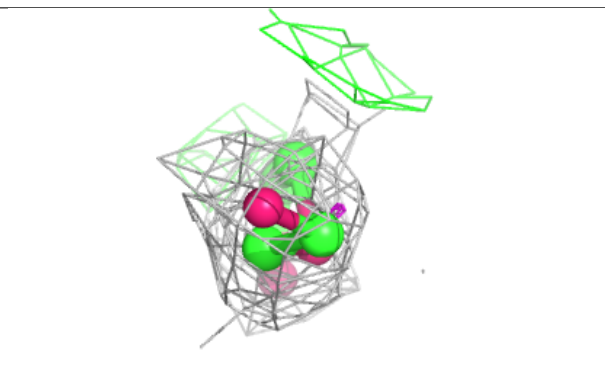
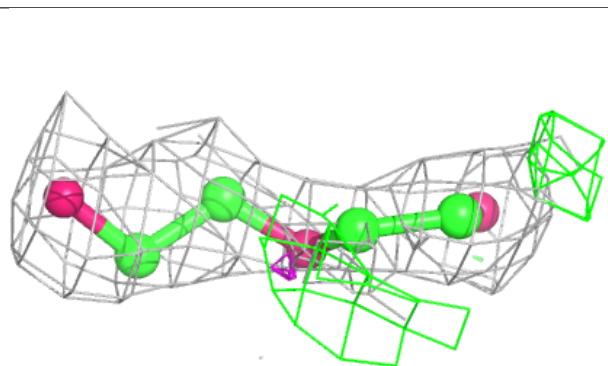
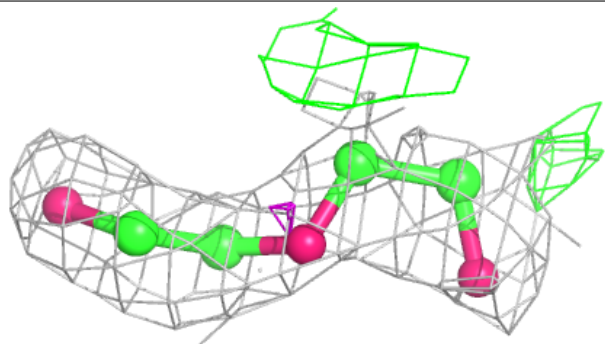


**Electron density around EDO A 1115:**

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

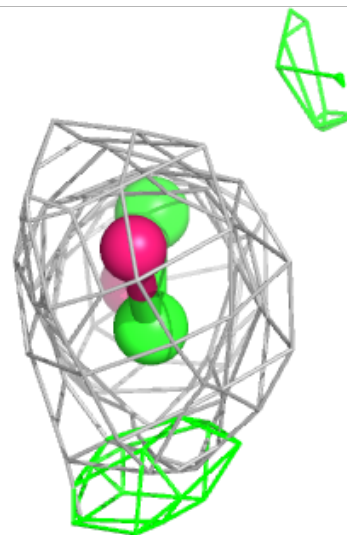
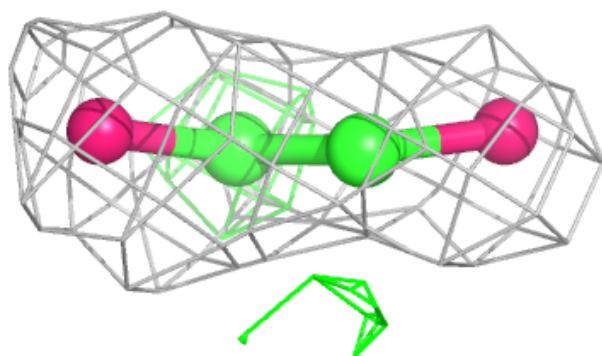
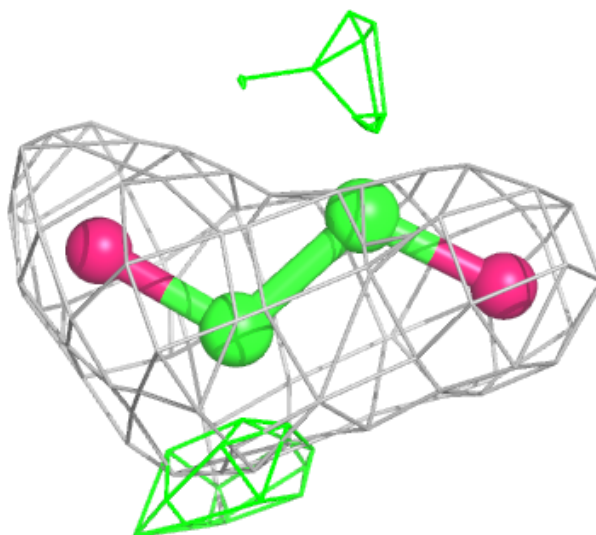
**Electron density around PEG A 1133:**

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



**Electron density around EDO A 1130:**

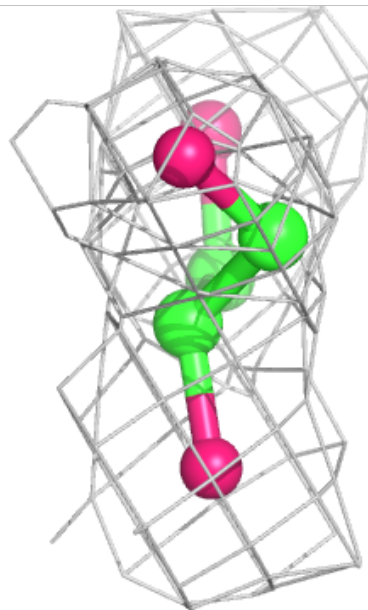
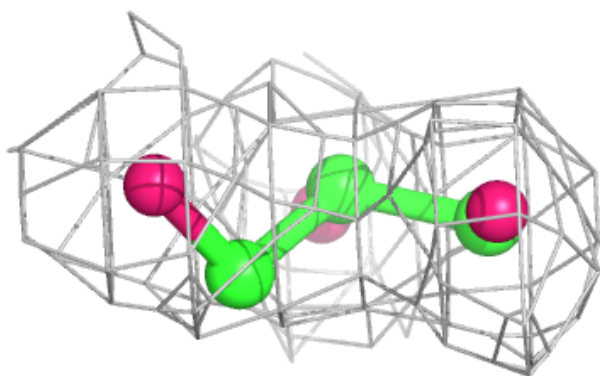
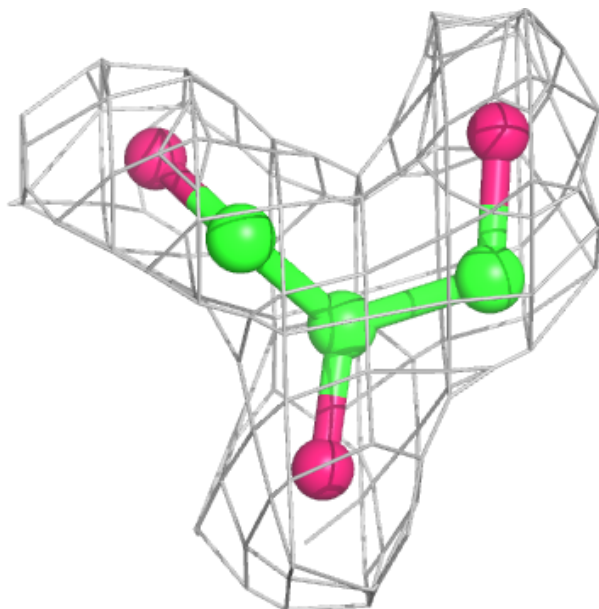
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





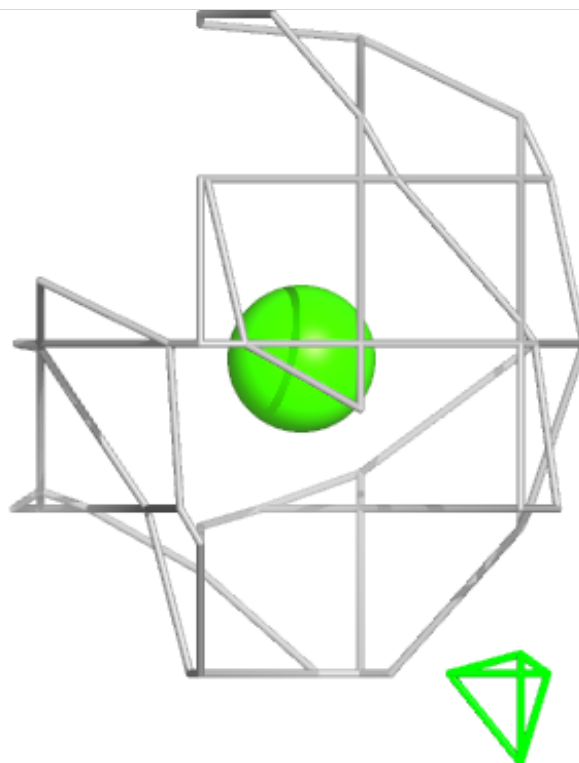
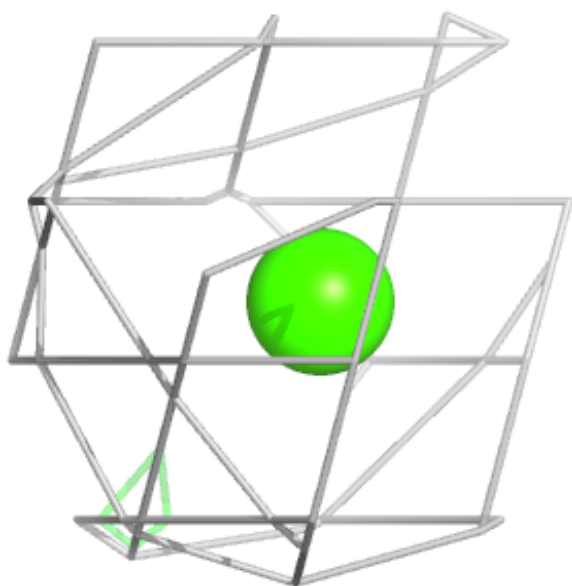
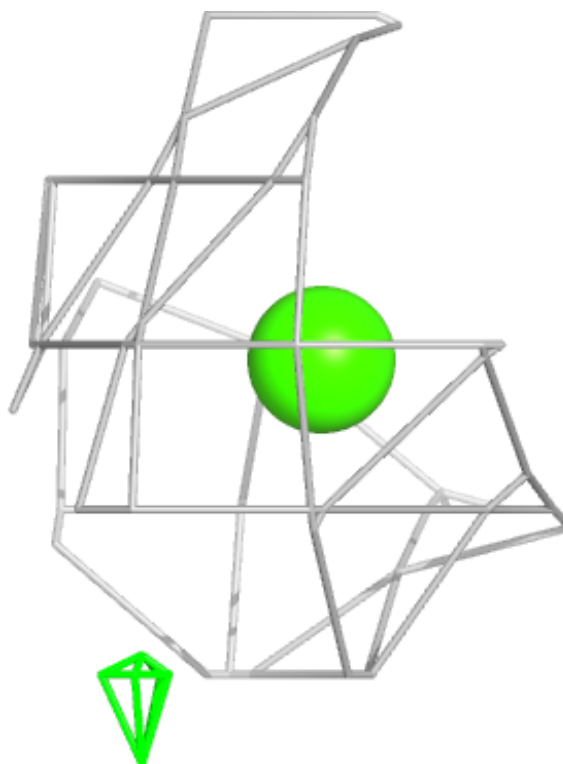
**Electron density around GOL A 1127:**

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



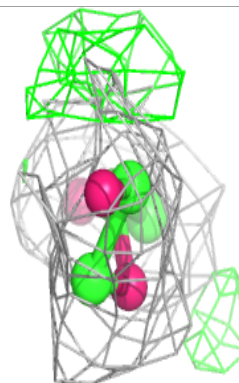
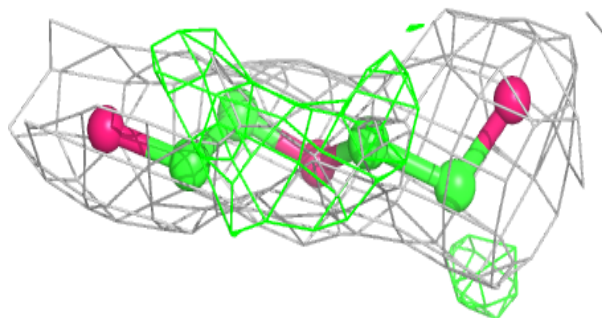
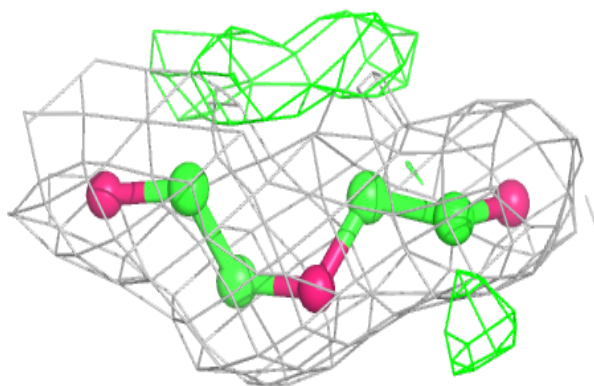
**Electron density around CA B 1105:**

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

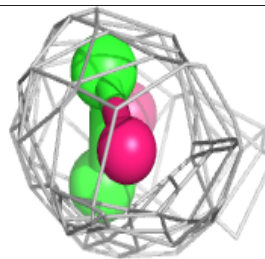
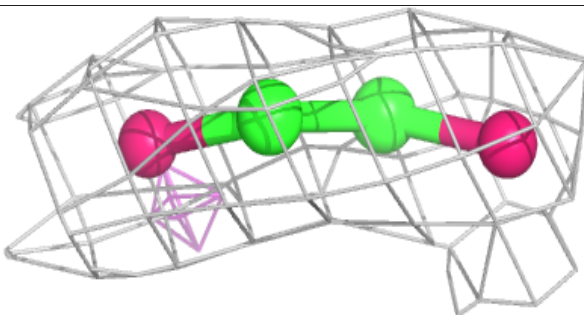
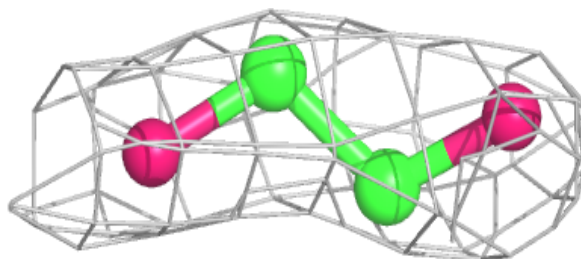


**Electron density around PEG B 1130:**

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

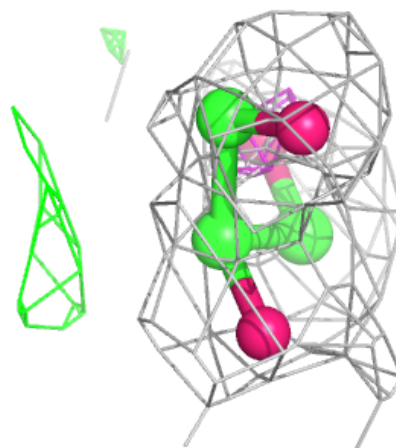
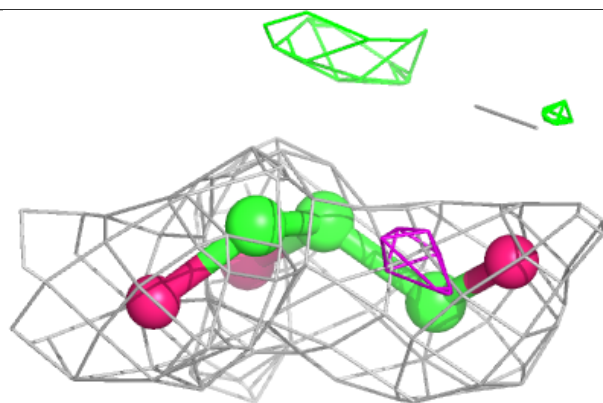
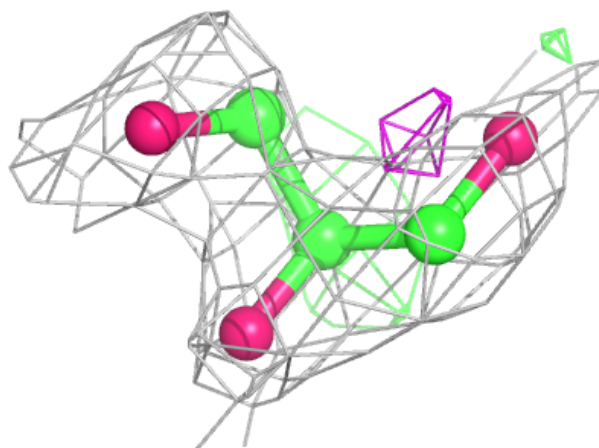
**Electron density around EDO A 1114:**

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



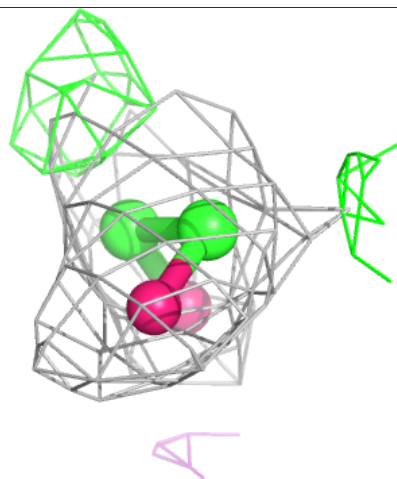
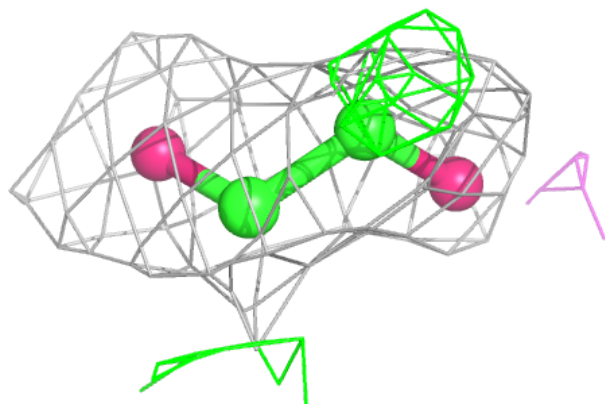
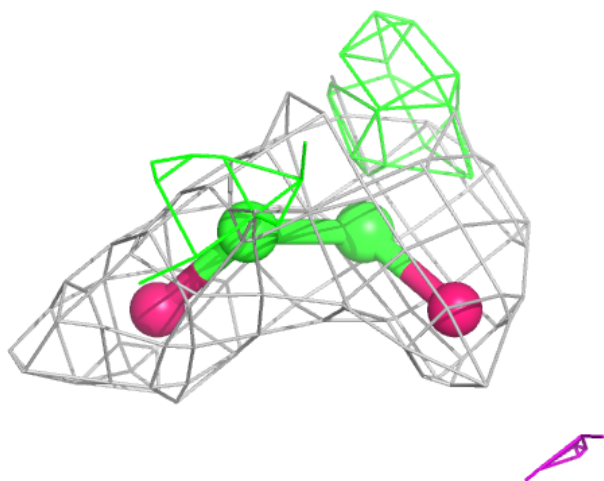
**Electron density around GOL B 1123:**

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



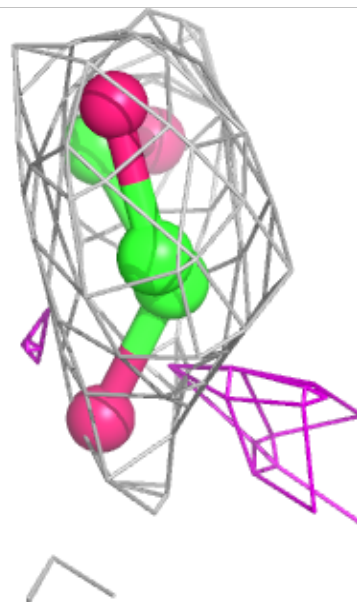
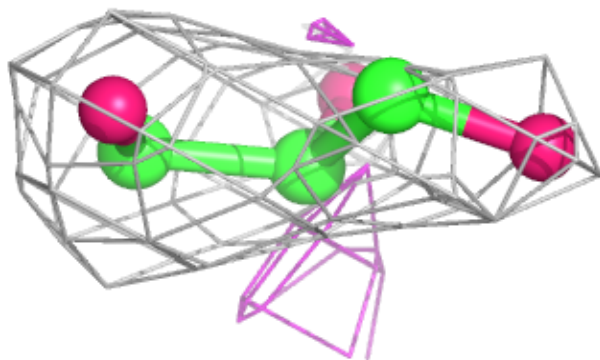
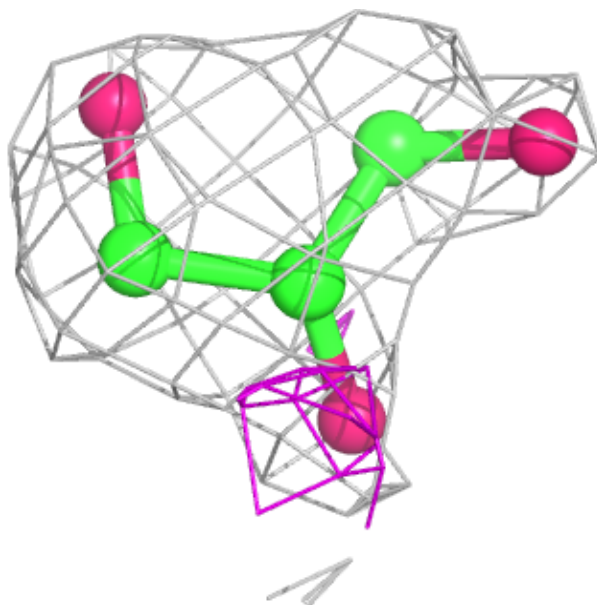
**Electron density around EDO A 1109:**

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



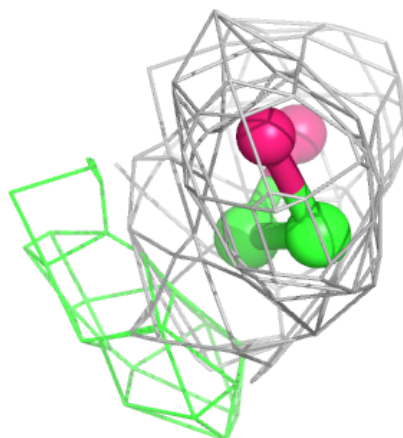
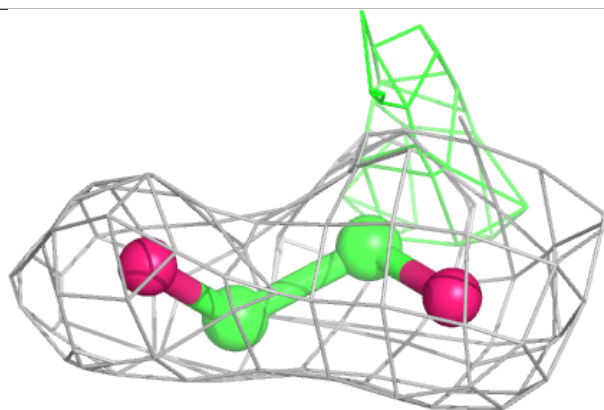
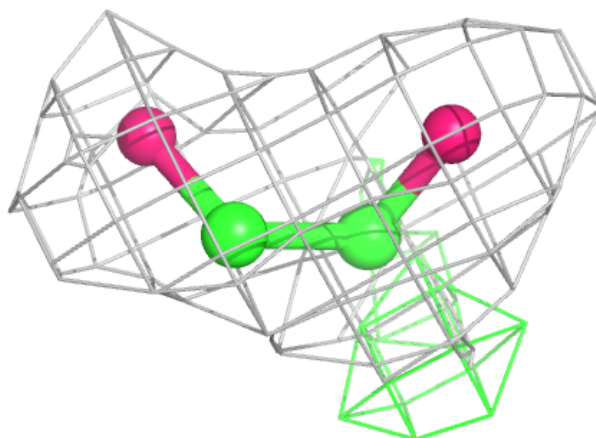
**Electron density around GOL A 1124:**

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



**Electron density around EDO B 1109:**

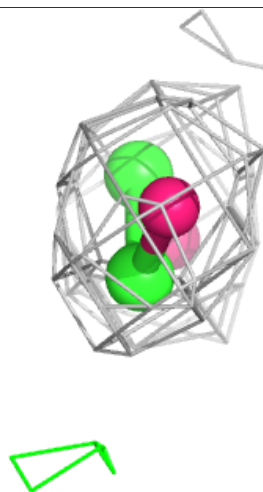
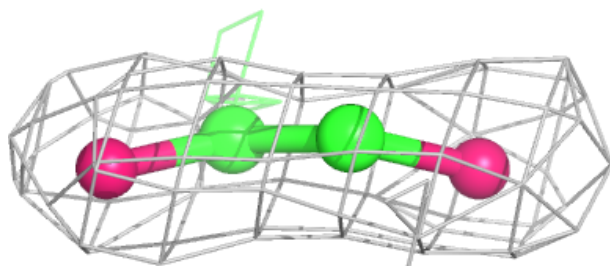
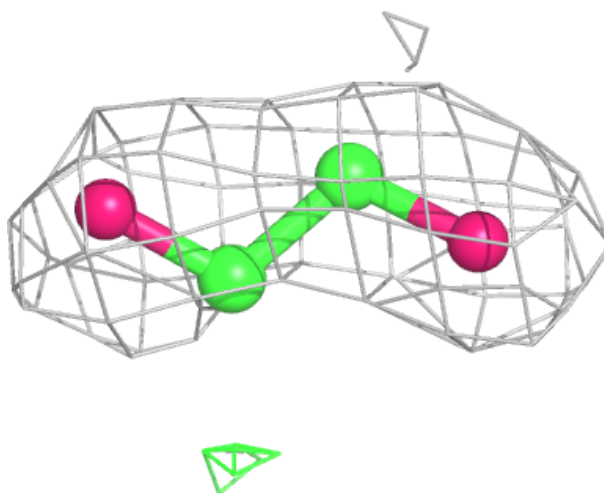
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around EDO B 1125:**

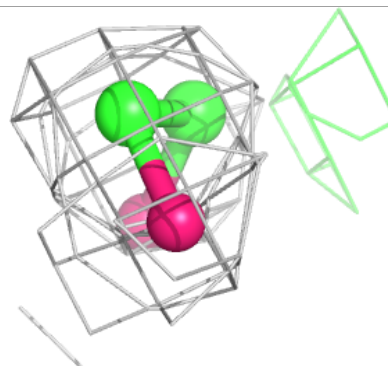
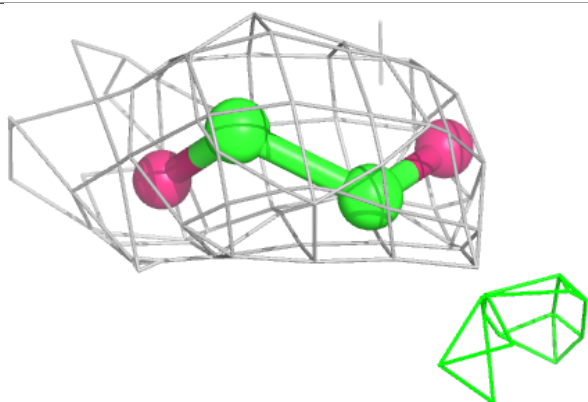
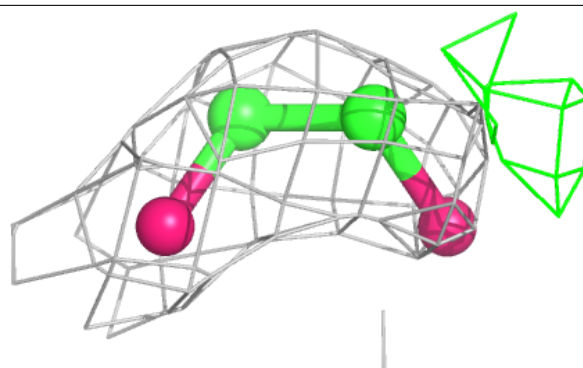
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



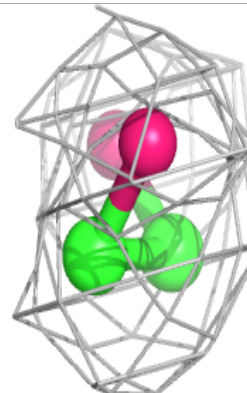
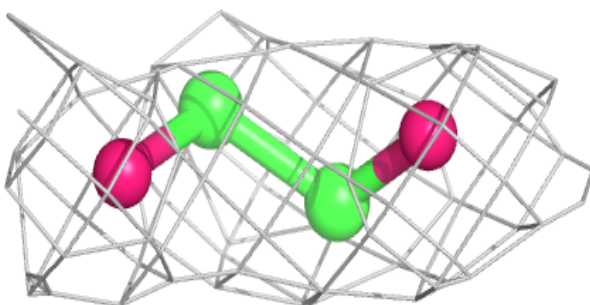
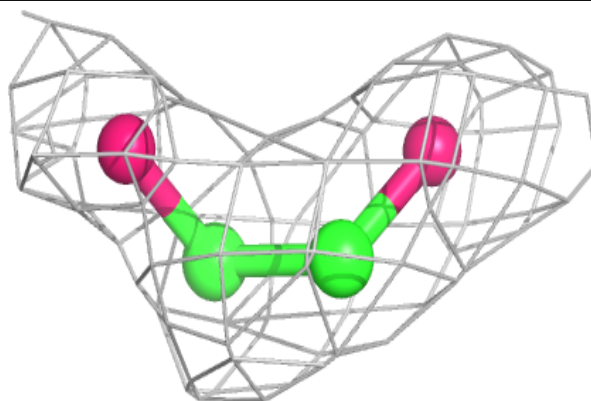


**Electron density around EDO A 1108:**

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

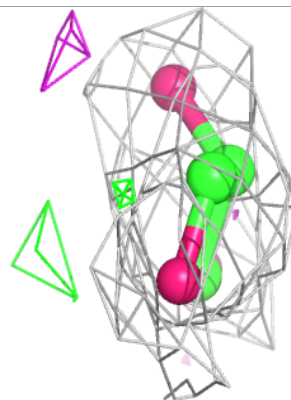
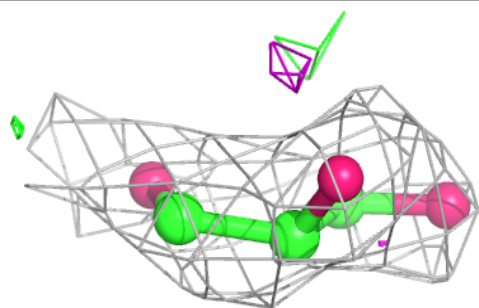
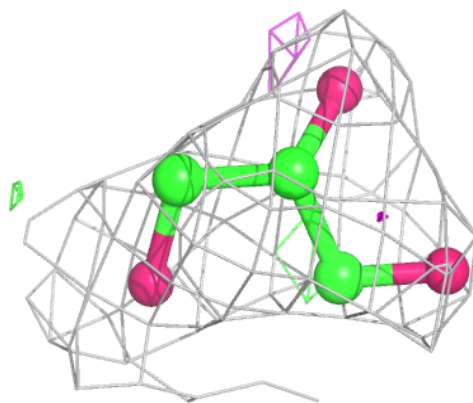
**Electron density around EDO B 1120:**

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



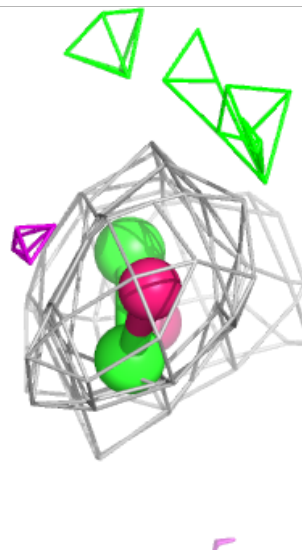
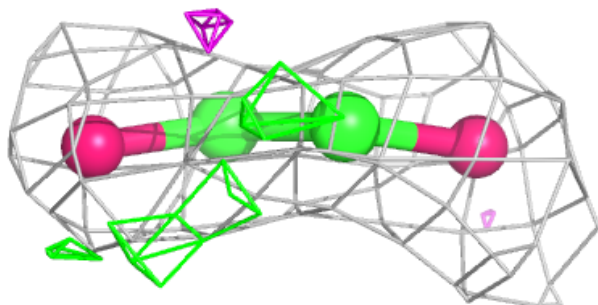
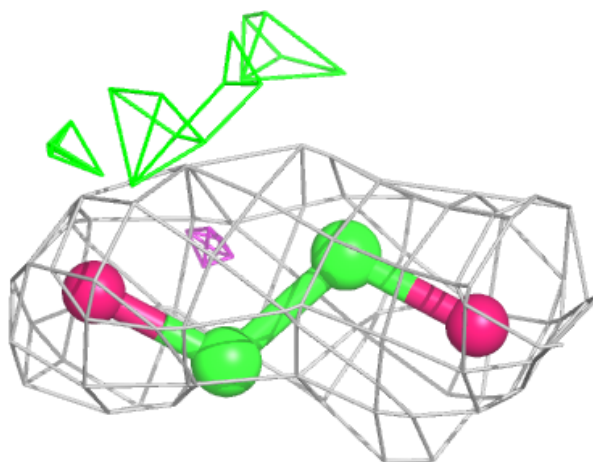
**Electron density around GOL A 1128:**

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



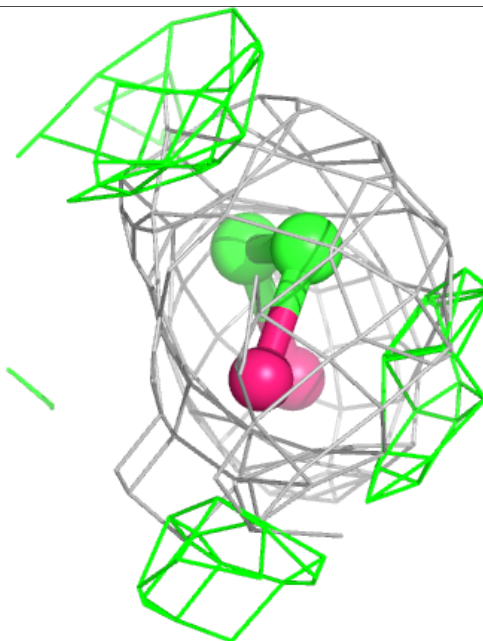
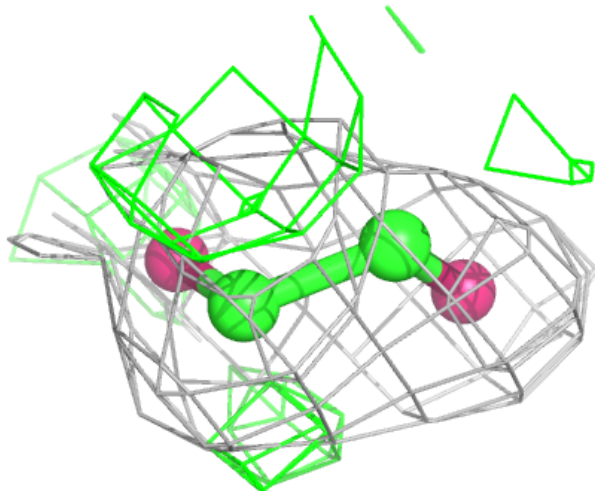
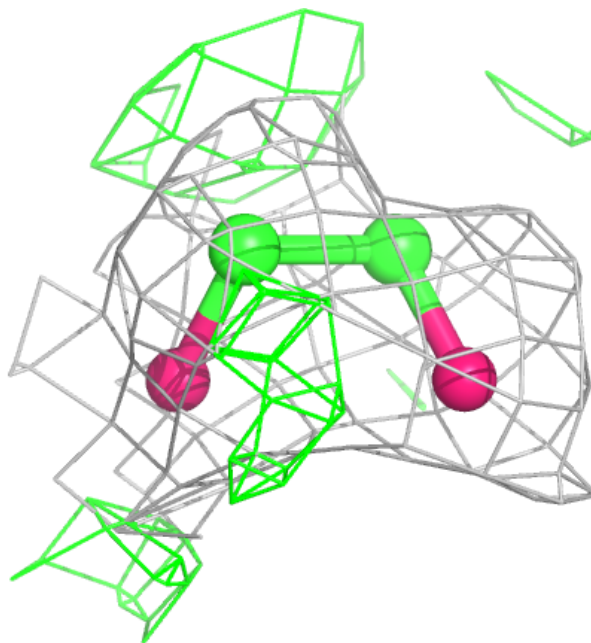
**Electron density around EDO A 1131:**

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



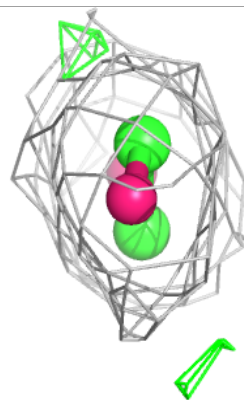
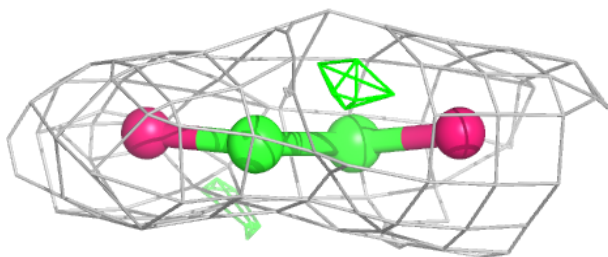
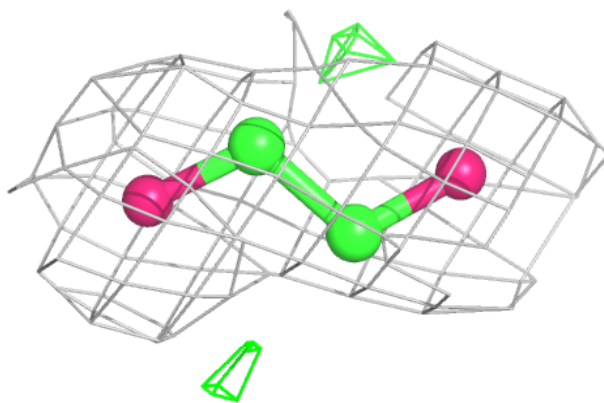
**Electron density around EDO A 1110:**

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

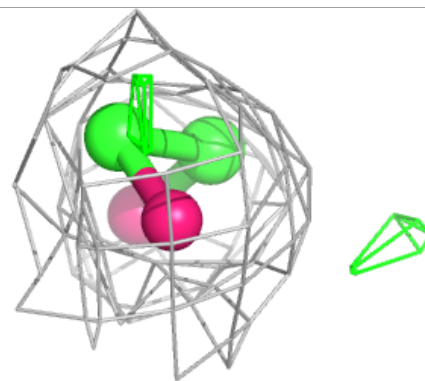
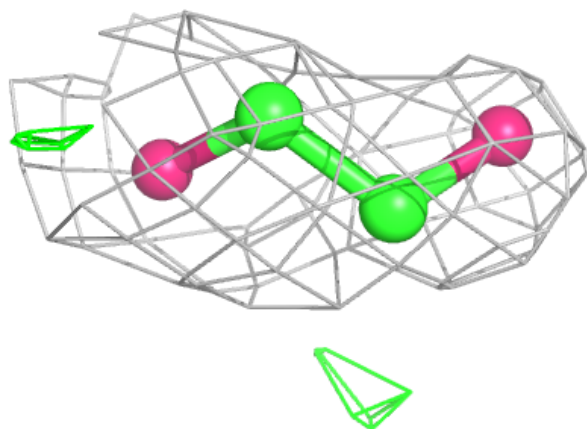
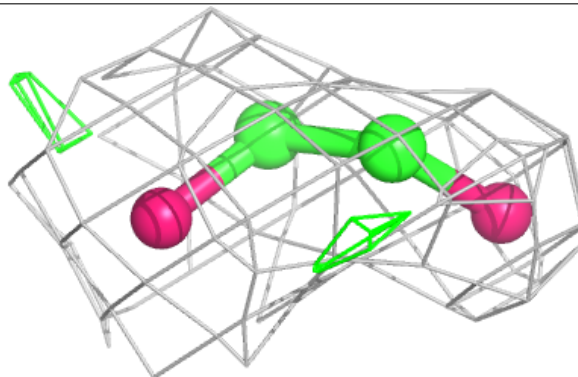


**Electron density around EDO B 1121:**

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

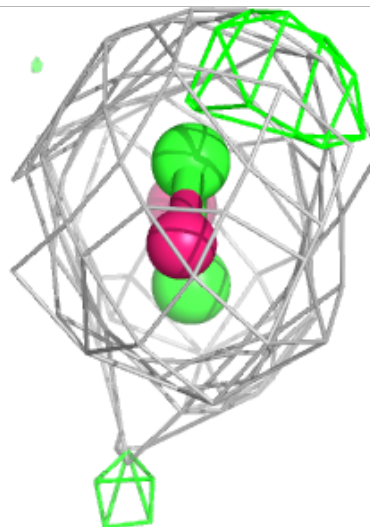
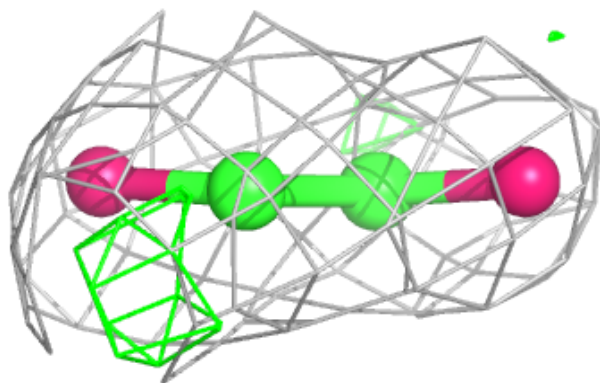
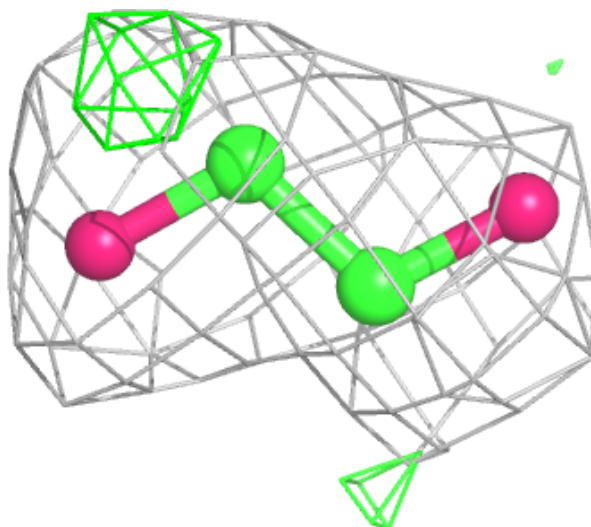
**Electron density around EDO A 1113:**

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



**Electron density around EDO A 1118:**

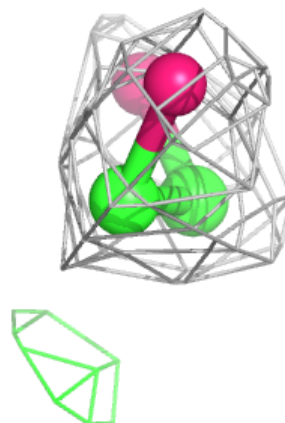
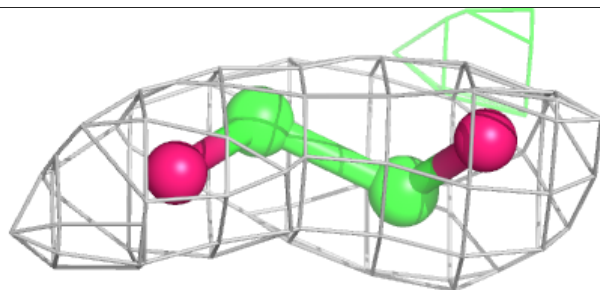
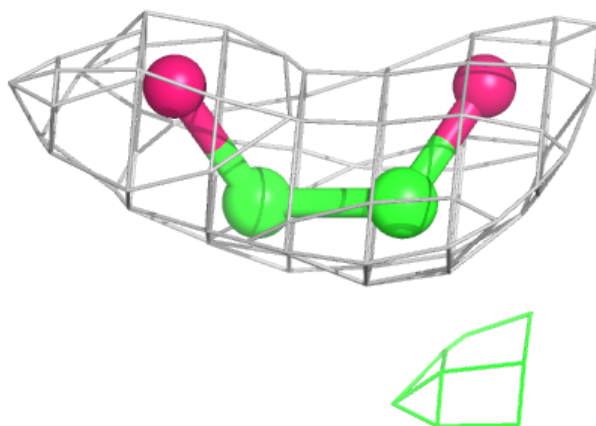
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



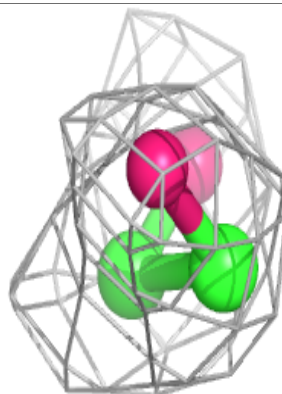
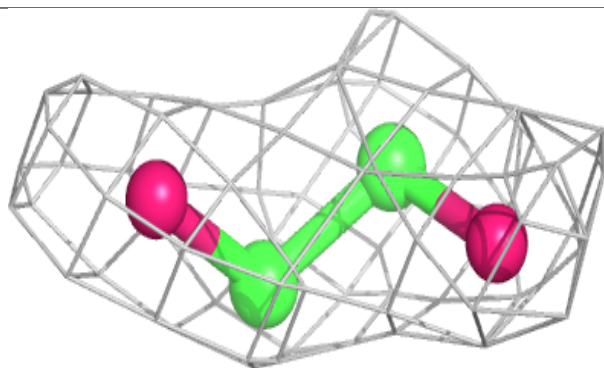
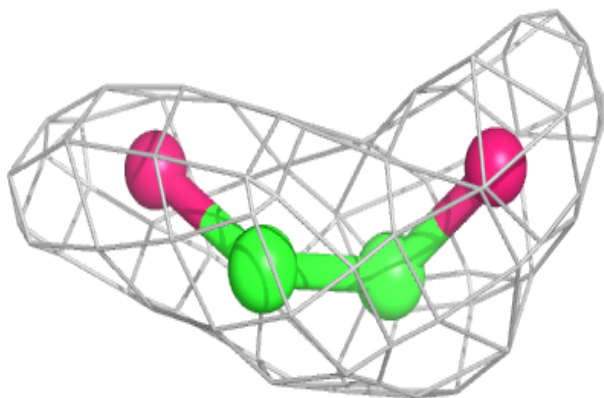


**Electron density around EDO B 1110:**

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

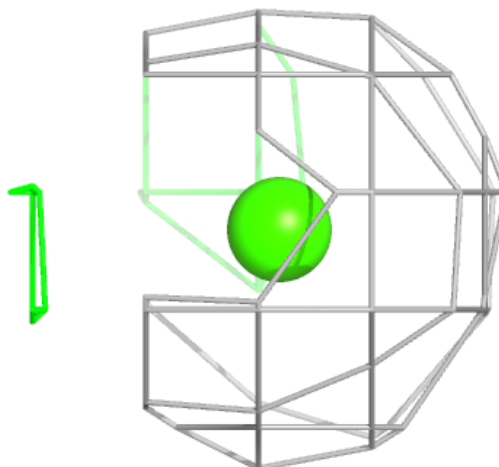
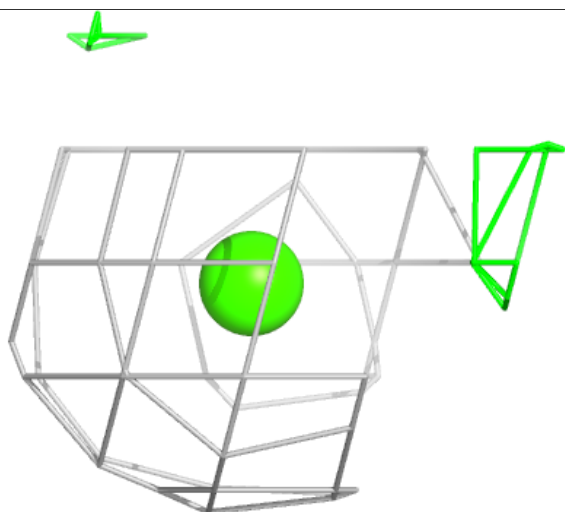
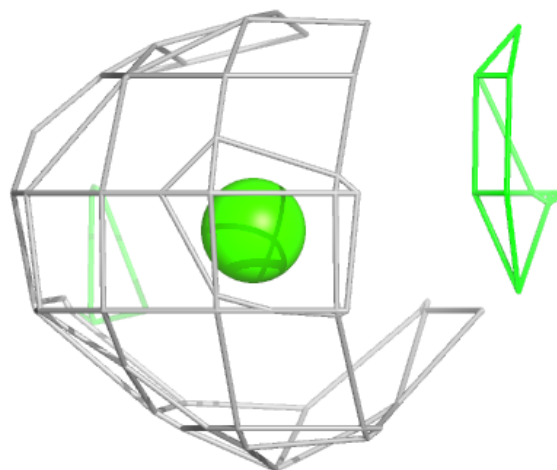
**Electron density around EDO B 1112:**

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



**Electron density around CA B 1106:**

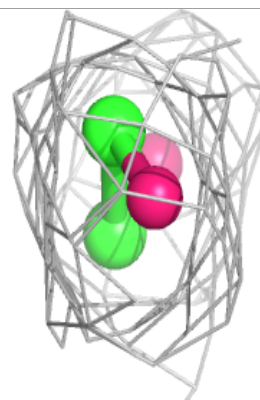
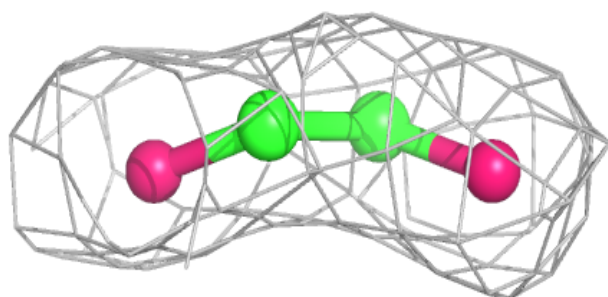
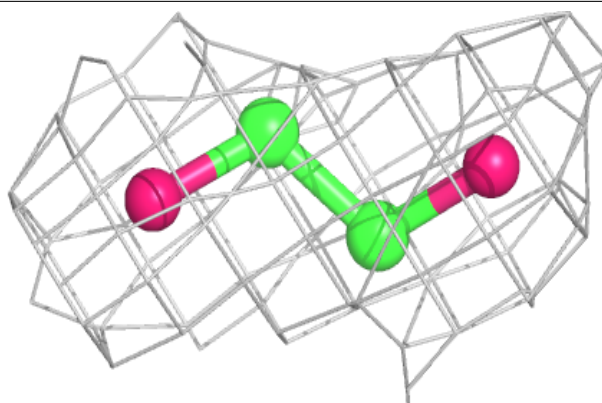
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





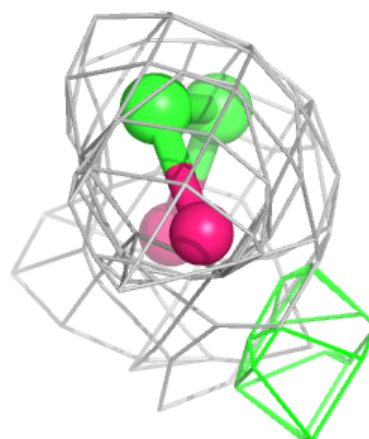
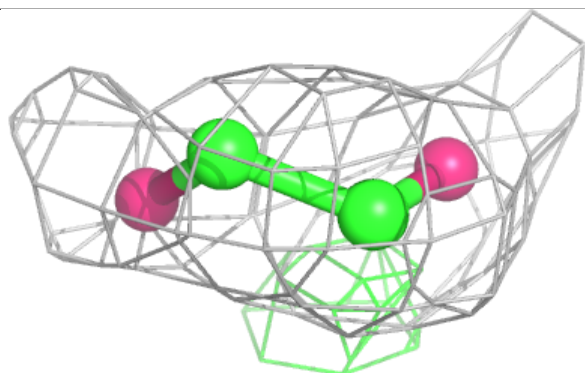
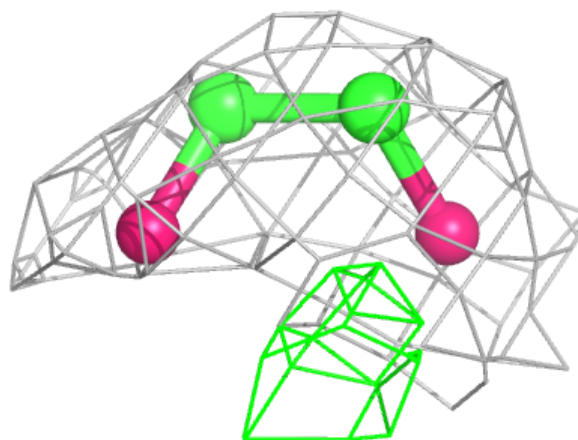
**Electron density around EDO B 1122:**

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



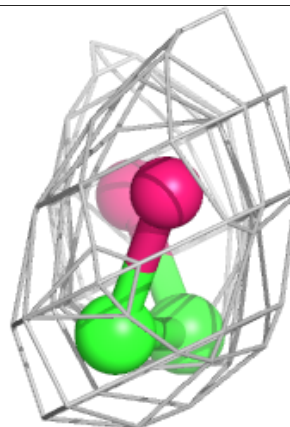
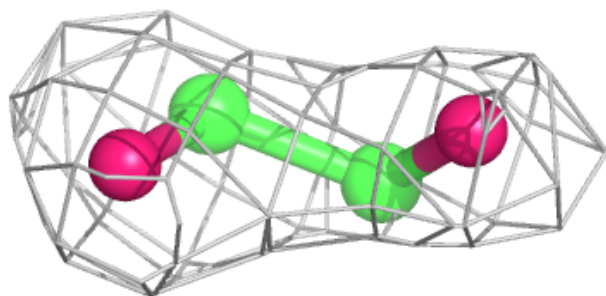
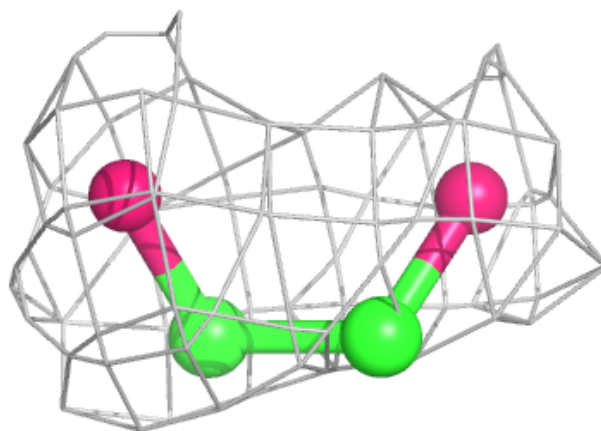
**Electron density around EDO A 1107:**

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



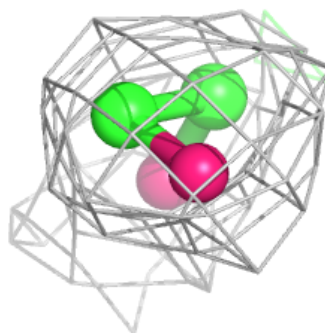
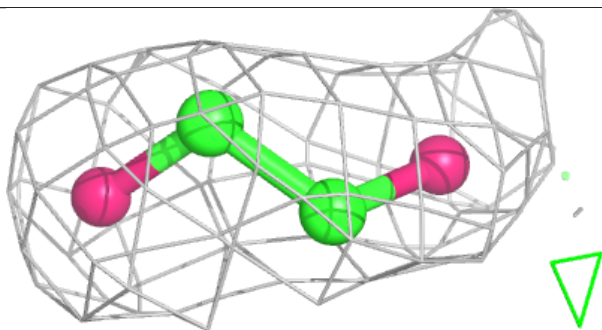
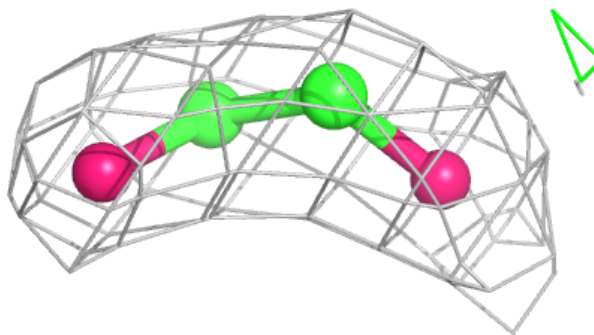
**Electron density around EDO B 1111:**

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



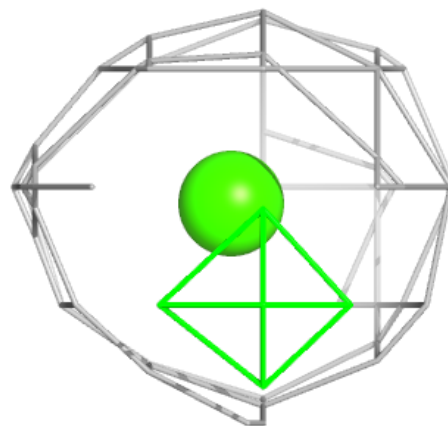
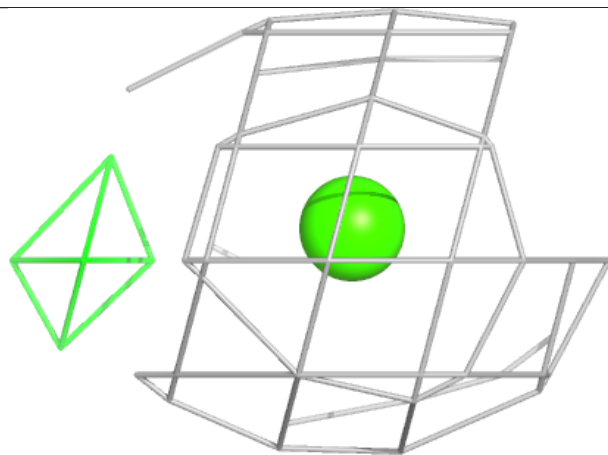
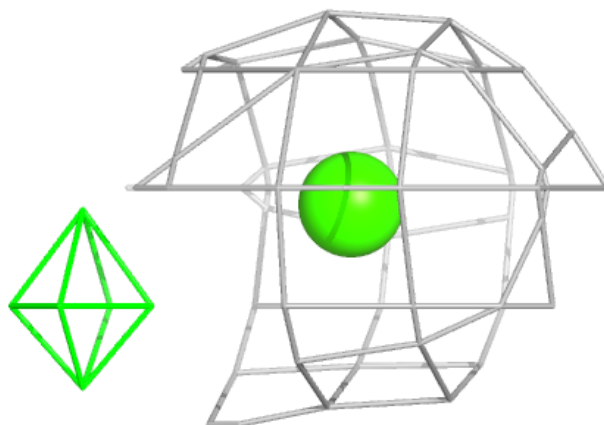
**Electron density around EDO A 1129:**

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



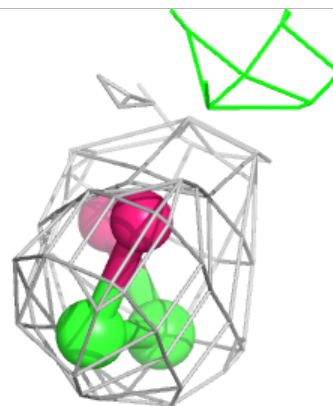
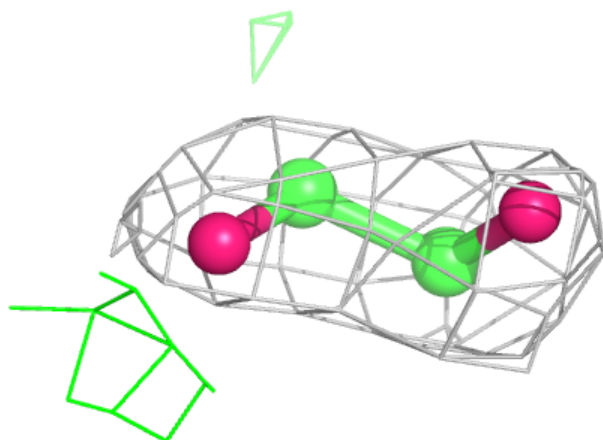
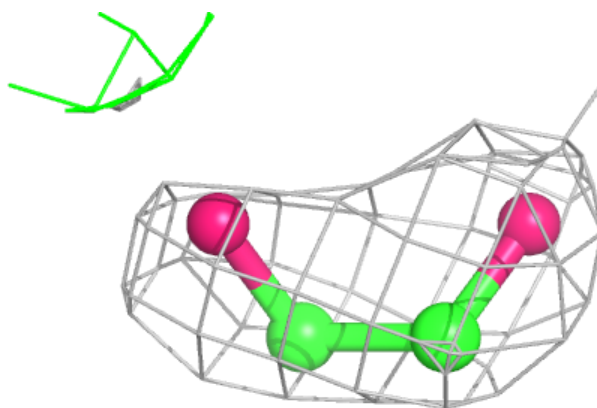
**Electron density around CA A 1105:**

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



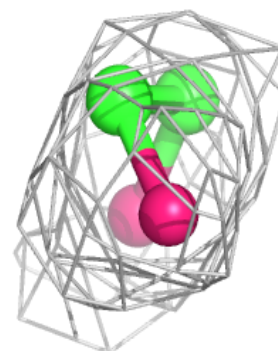
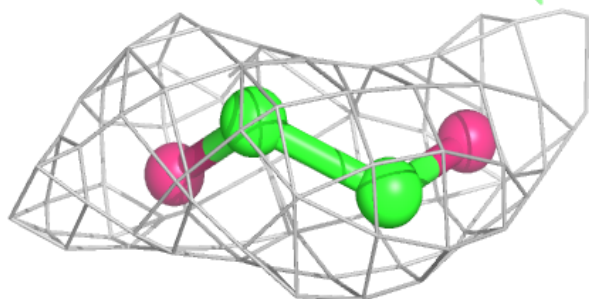
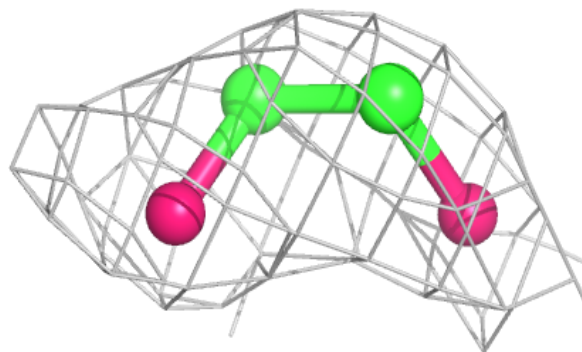
**Electron density around EDO B 1115:**

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



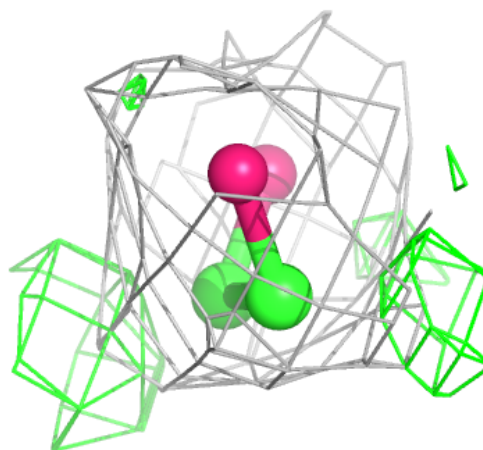
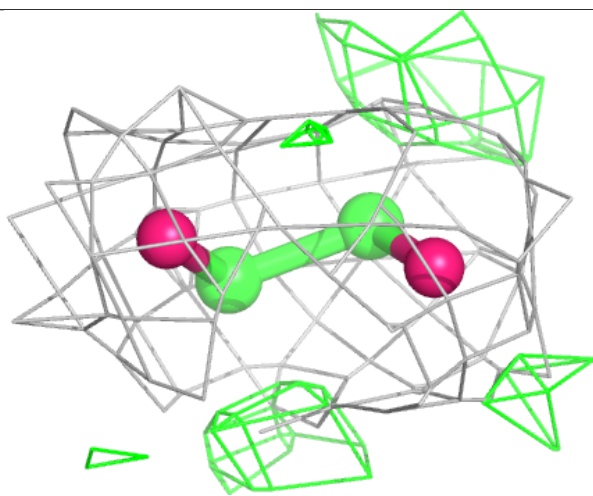
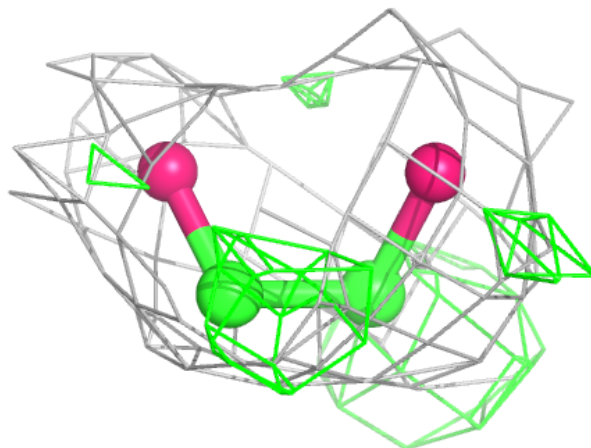
**Electron density around EDO A 1119:**

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



**Electron density around EDO A 1126:**

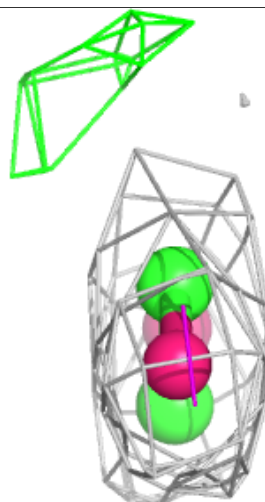
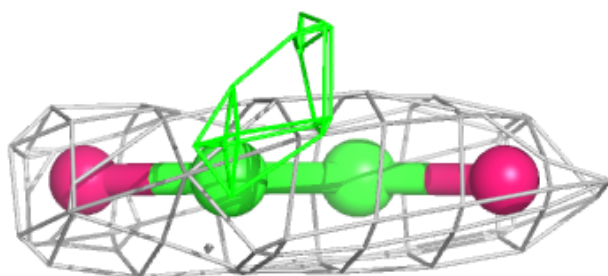
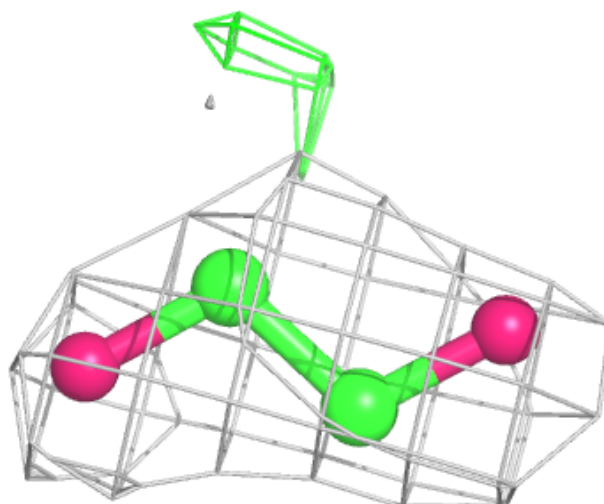
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





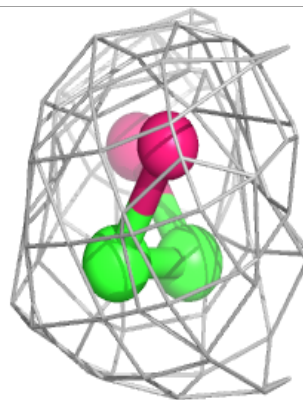
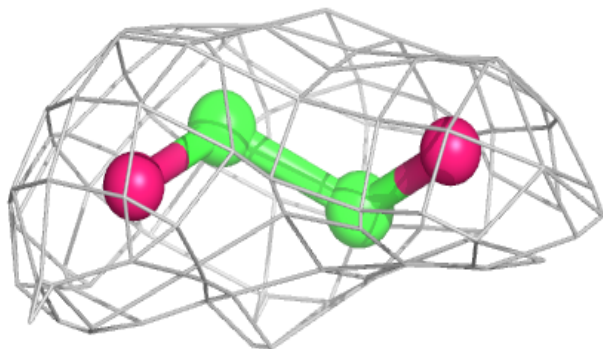
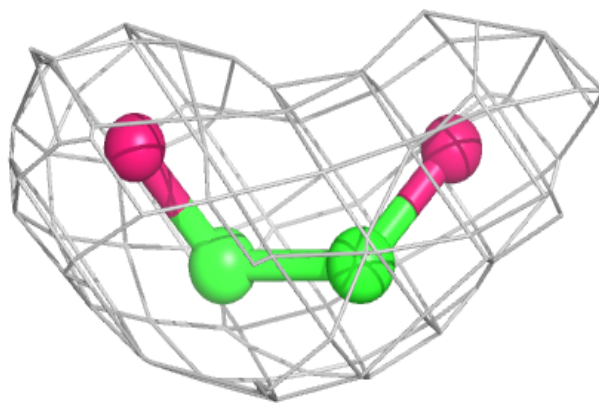
**Electron density around EDO A 1111:**

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



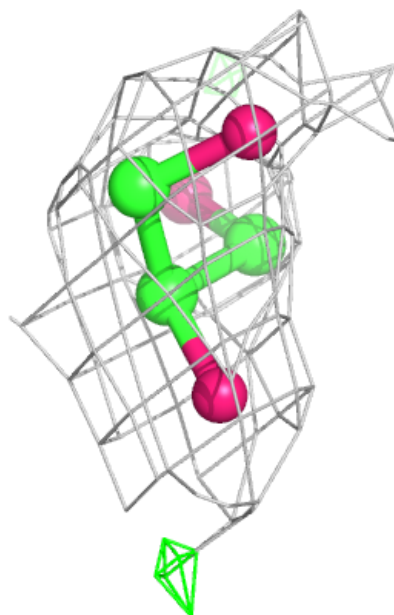
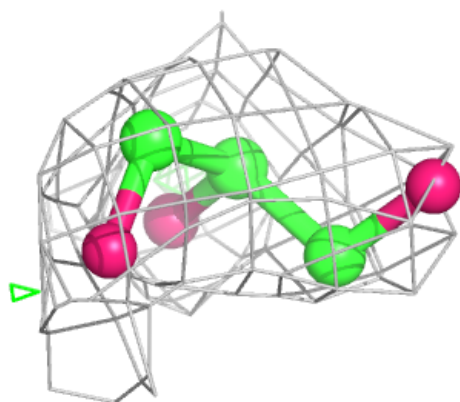
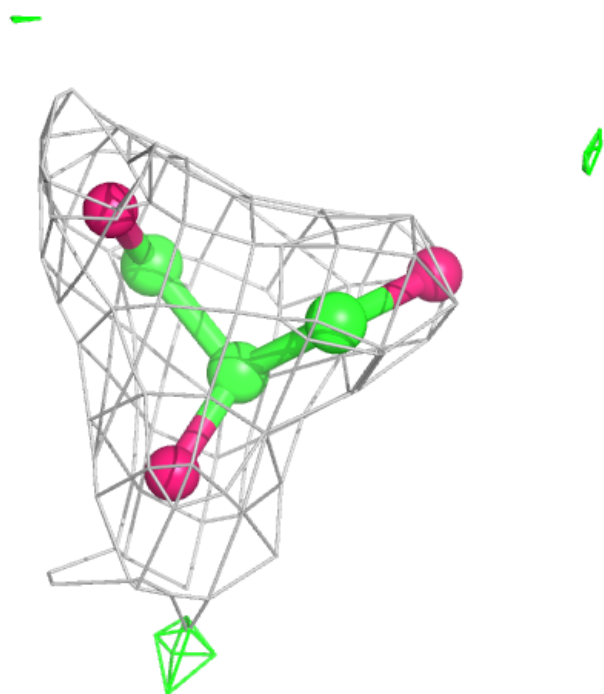
**Electron density around EDO B 1126:**

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



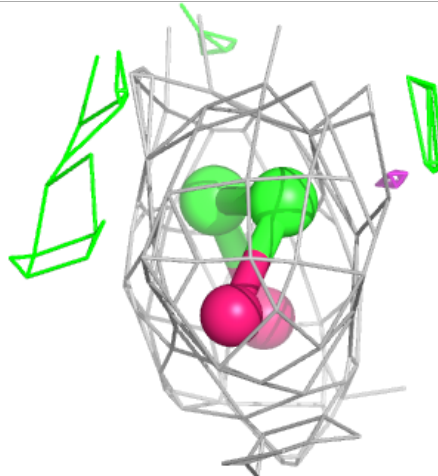
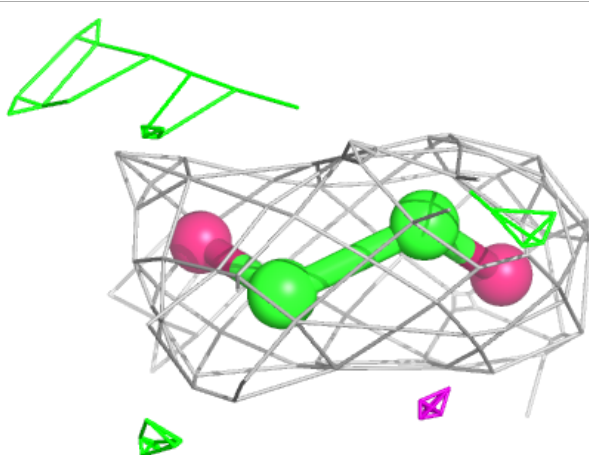
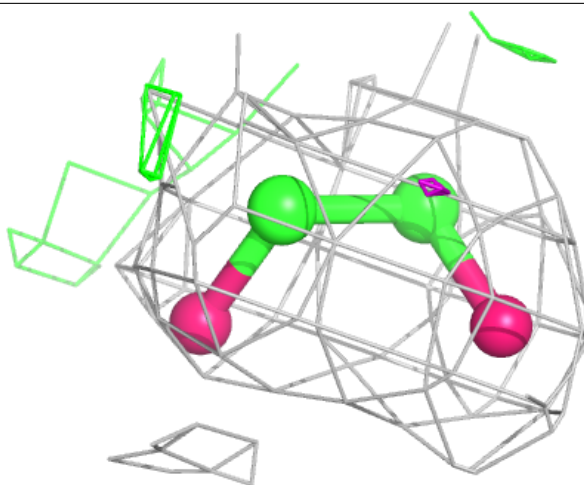
**Electron density around GOL B 1118:**

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



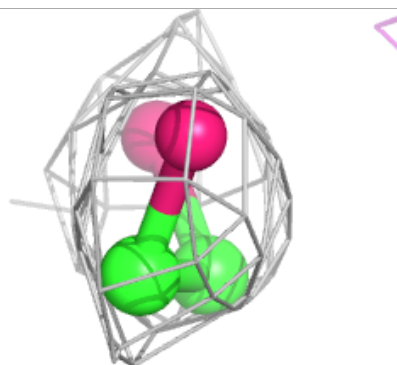
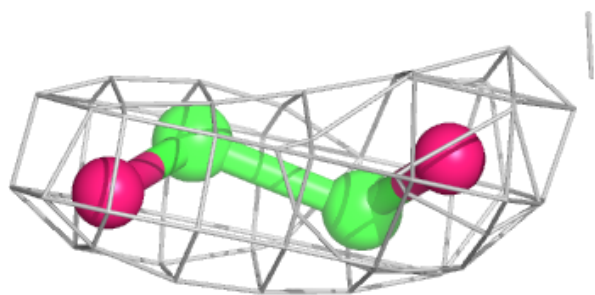
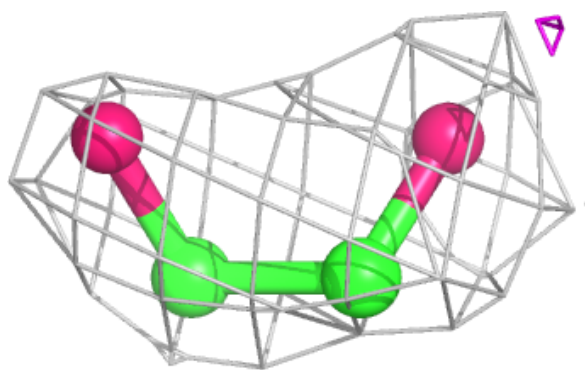
**Electron density around EDO A 1123:**

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



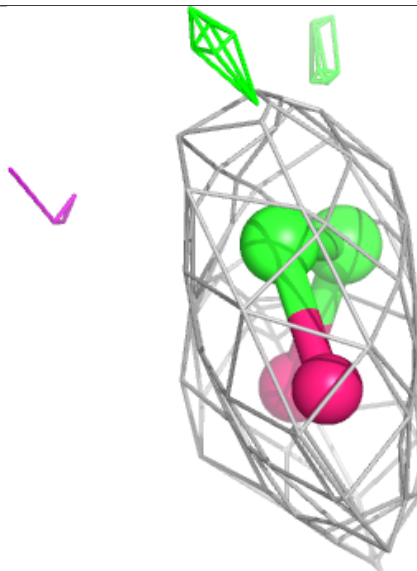
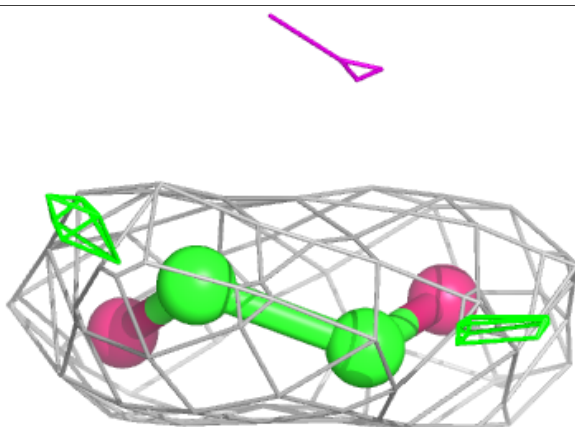
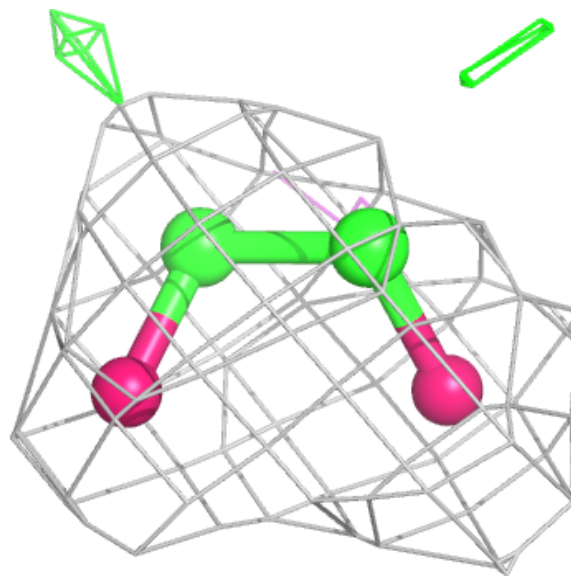
**Electron density around EDO B 1108:**

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



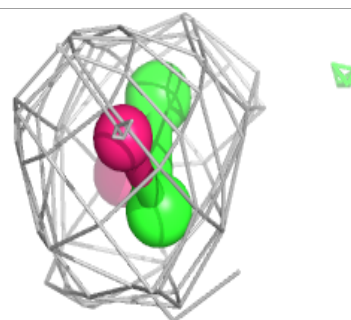
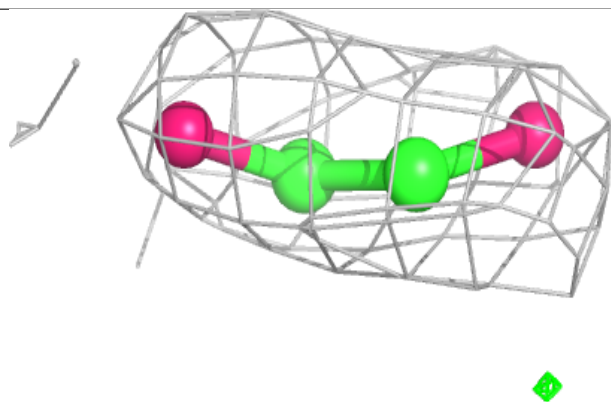
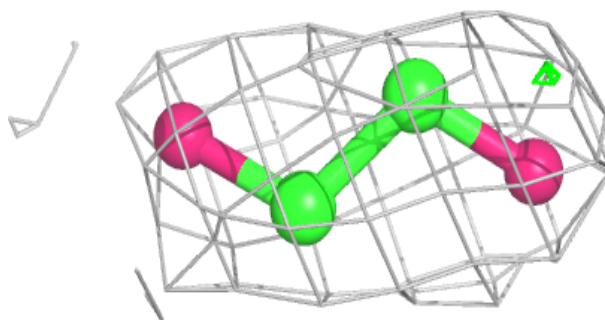
**Electron density around EDO B 1113:**

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



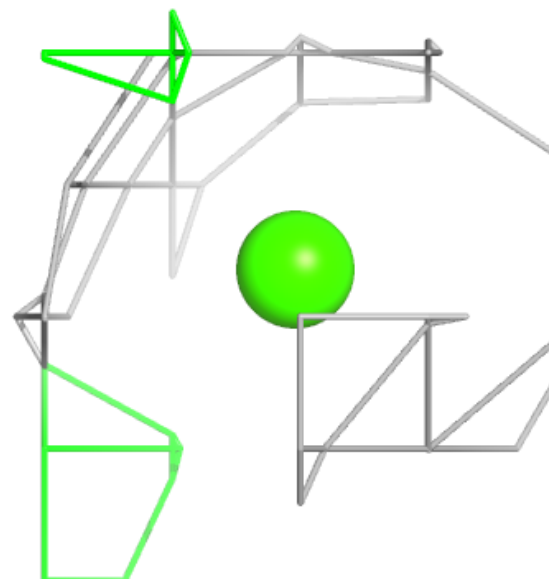
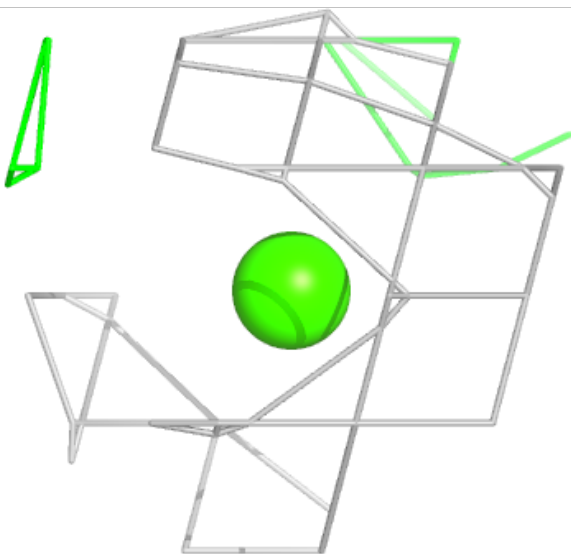
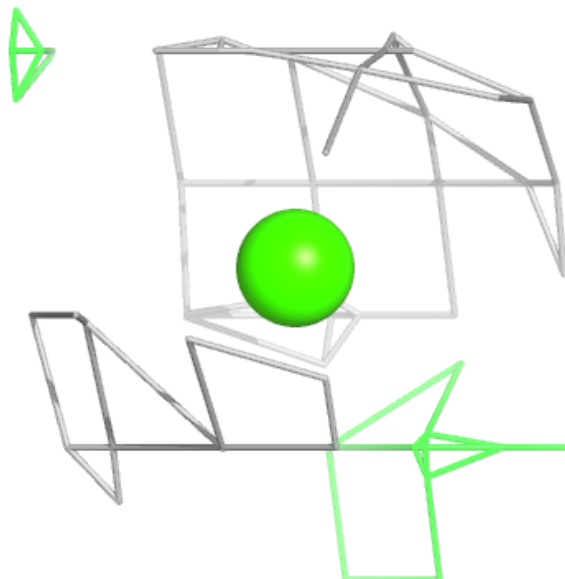
**Electron density around EDO A 1116:**

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



**Electron density around CA B 1103:**

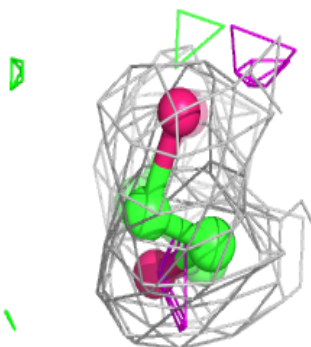
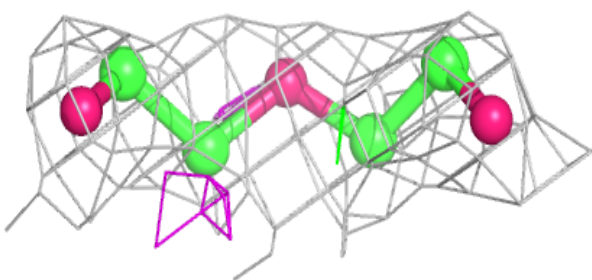
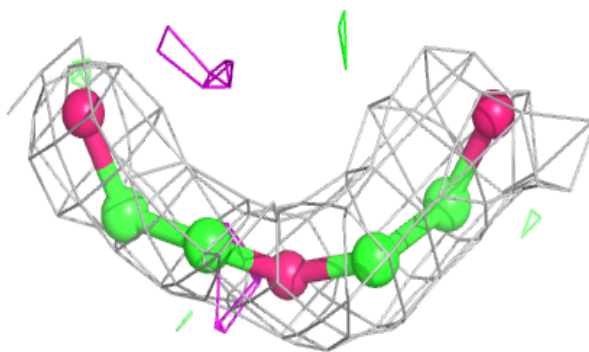
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



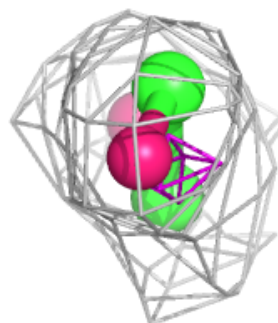
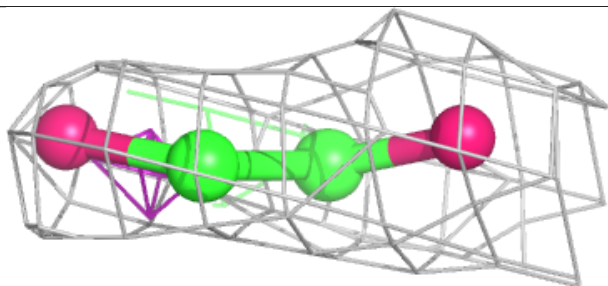
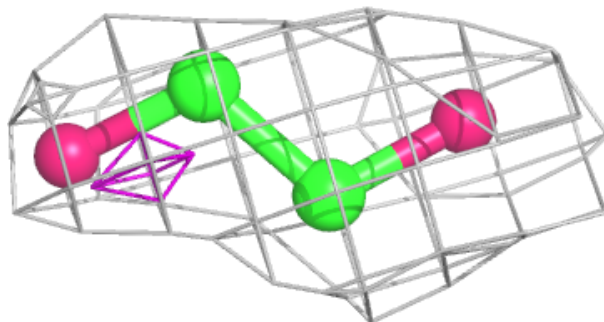


**Electron density around PEG B 1129:**

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

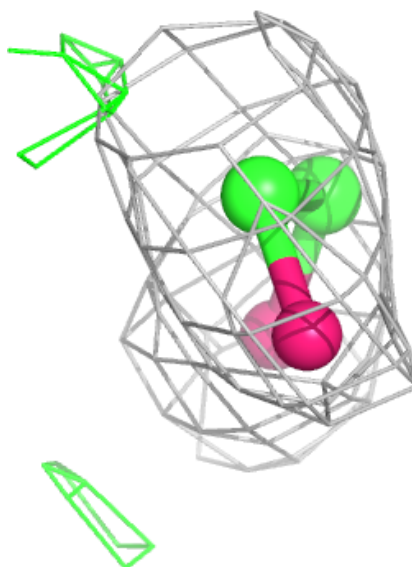
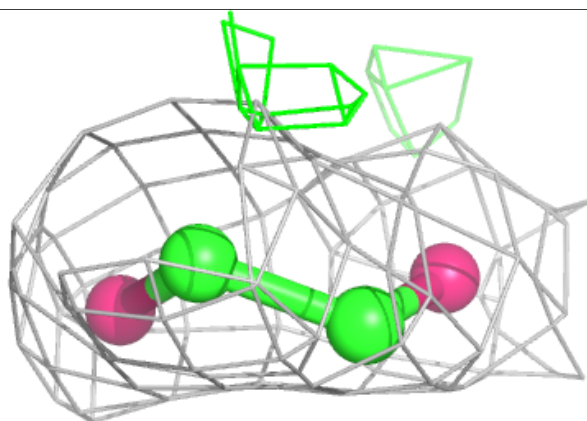
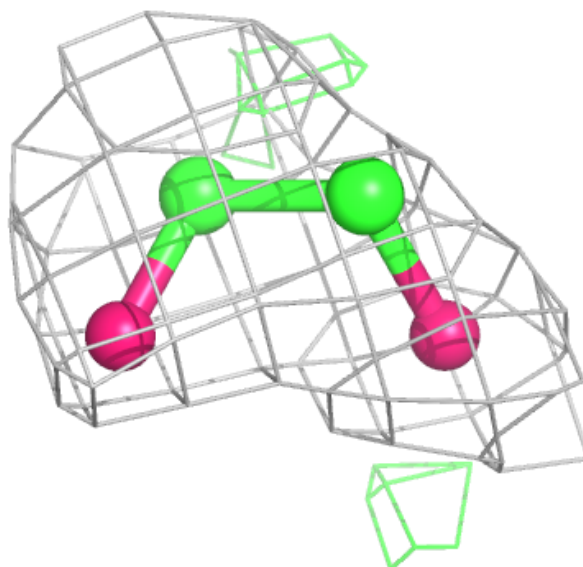
**Electron density around EDO B 1116:**

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



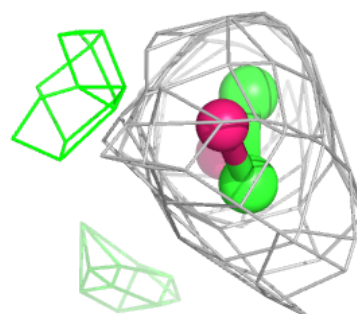
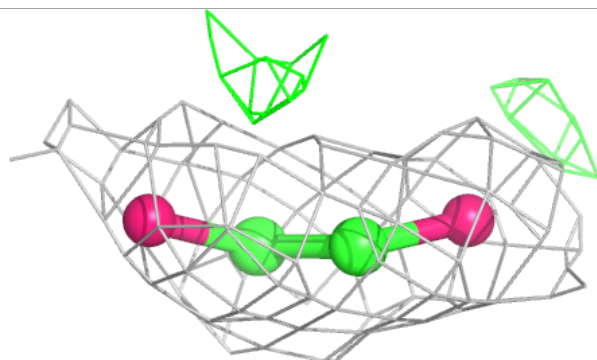
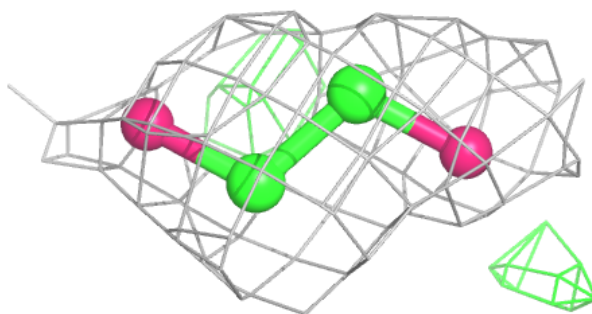
**Electron density around EDO A 1117 (A):**

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

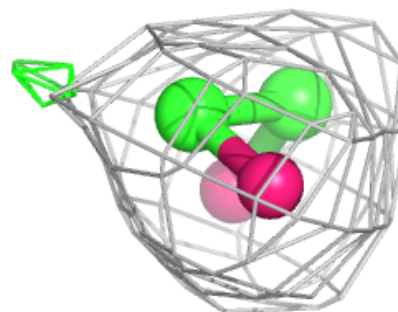
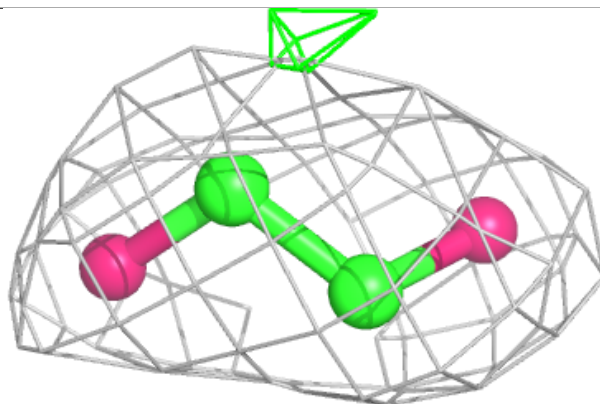
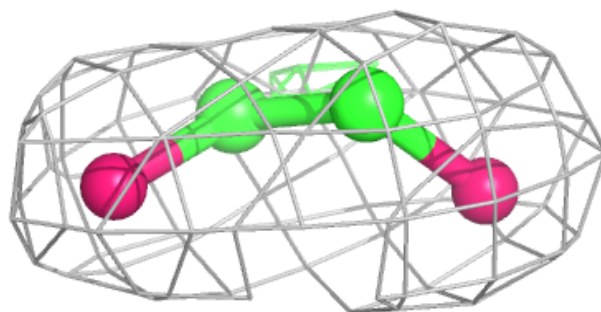


**Electron density around EDO A 1117 (B):**

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

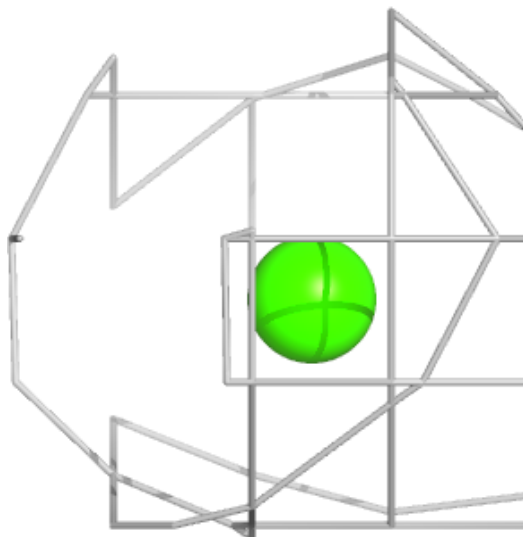
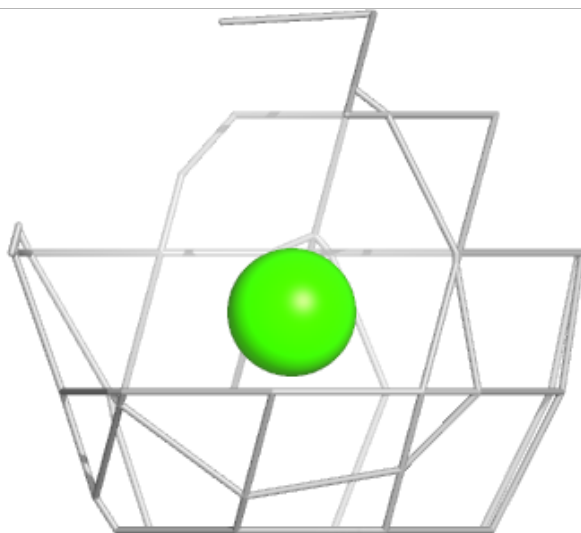
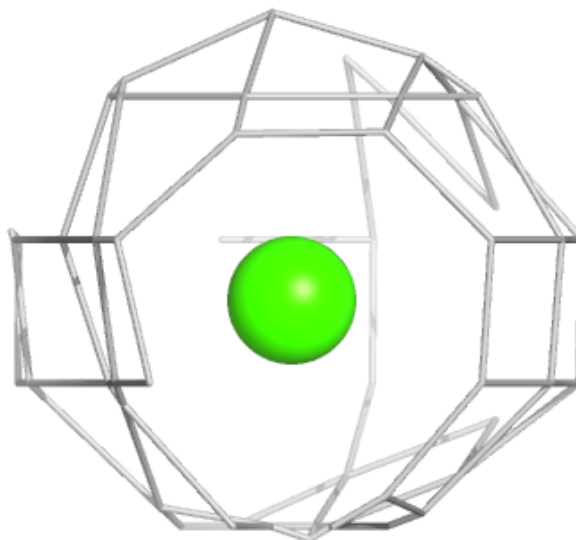
**Electron density around EDO A 1120:**

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



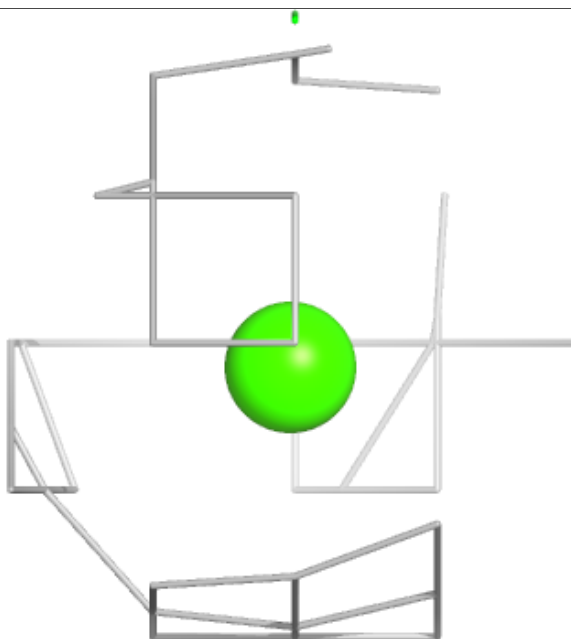
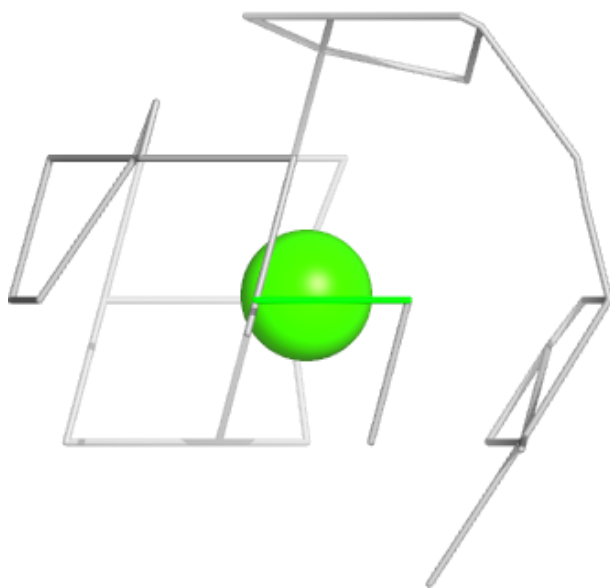
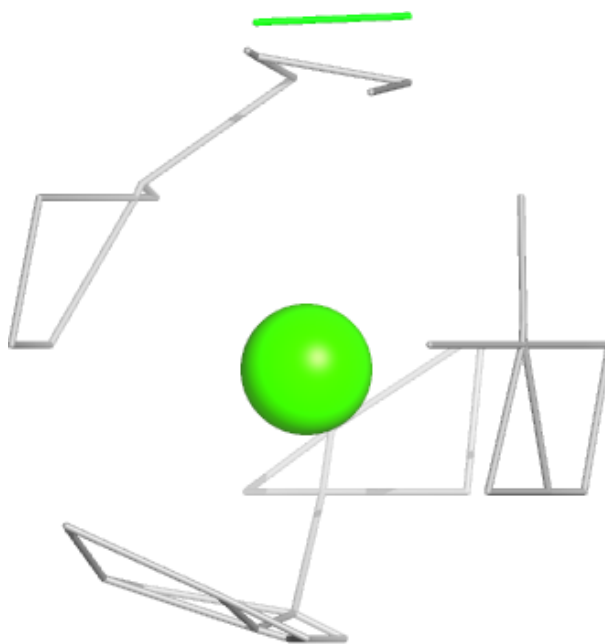
**Electron density around CA A 1104:**

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



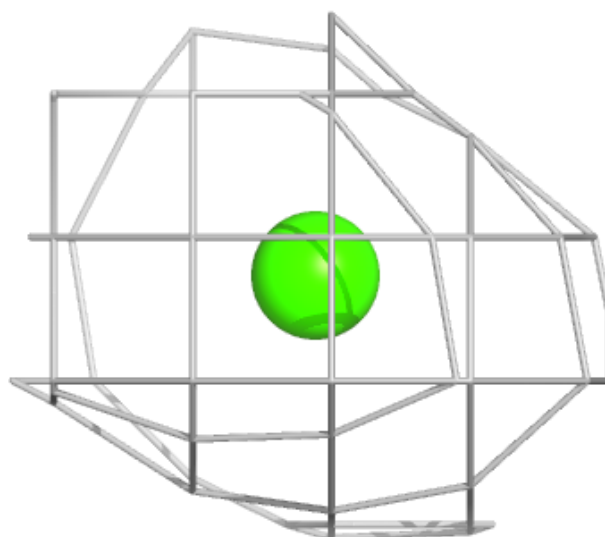
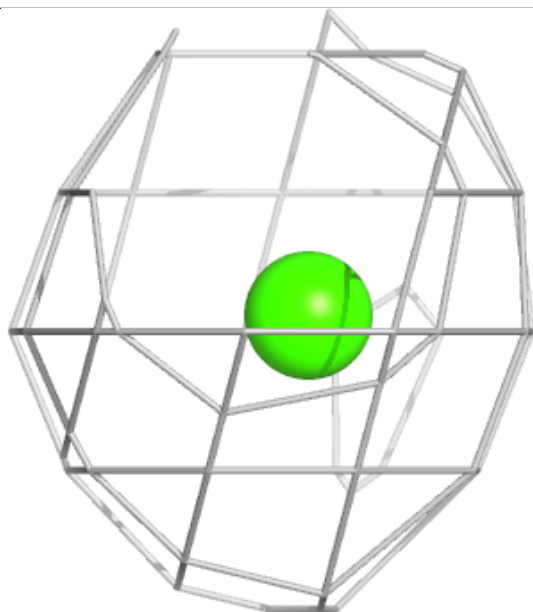
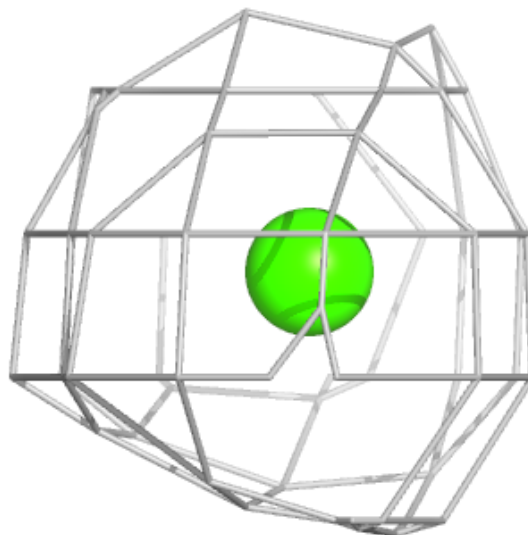
**Electron density around CA A 1102:**

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



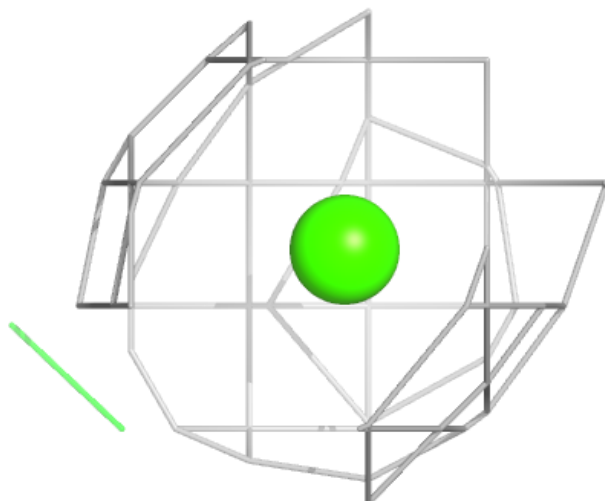
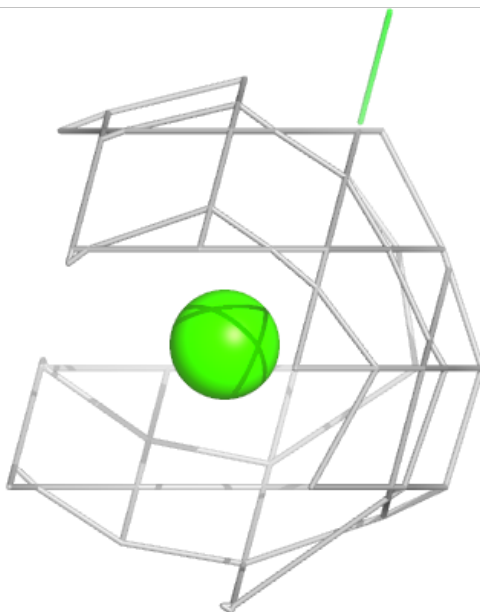
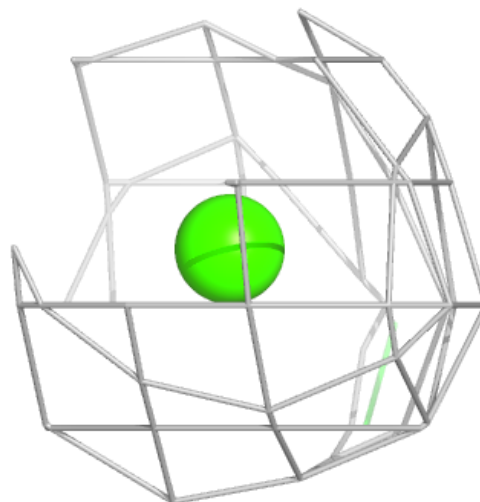
**Electron density around CA B 1104:**

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



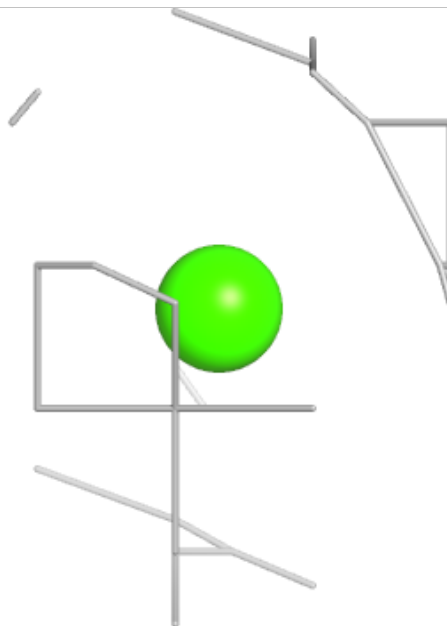
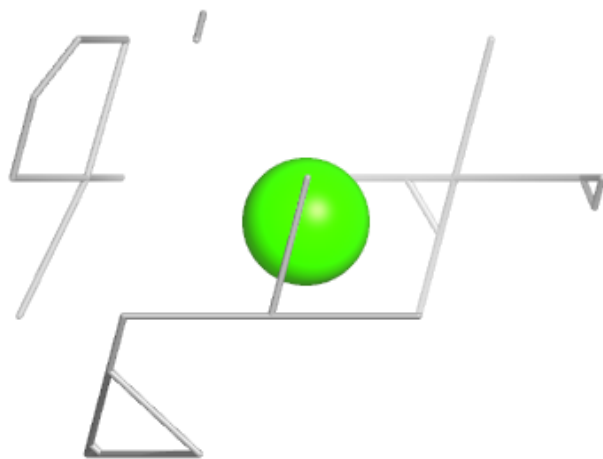
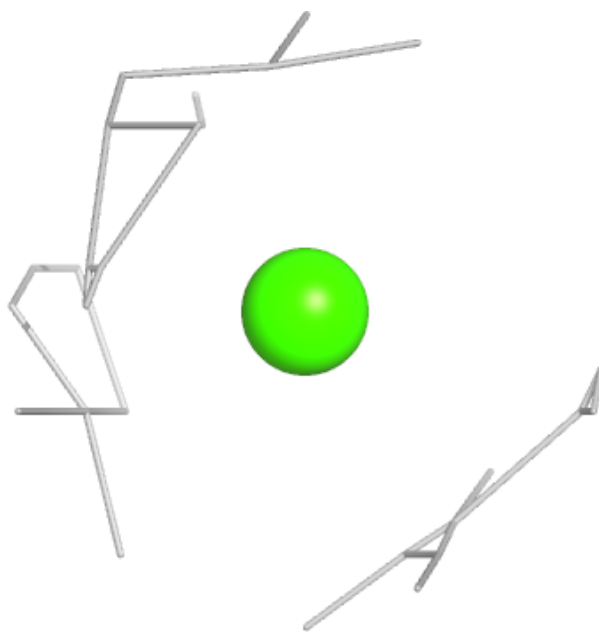
**Electron density around CA A 1103:**

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



**Electron density around CA B 1102:**

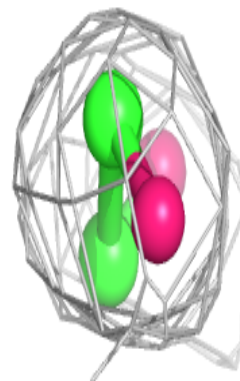
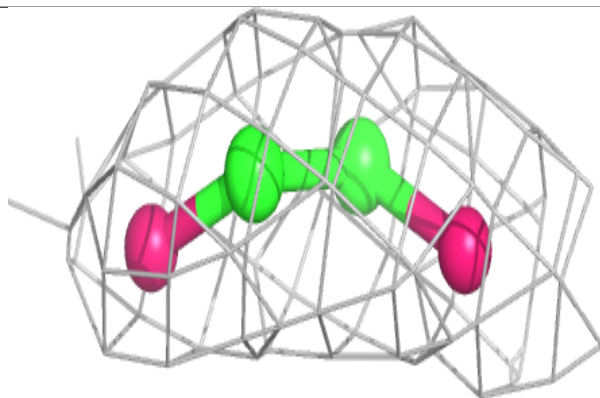
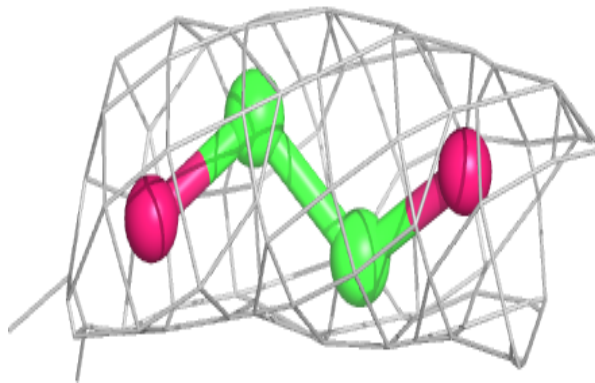
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





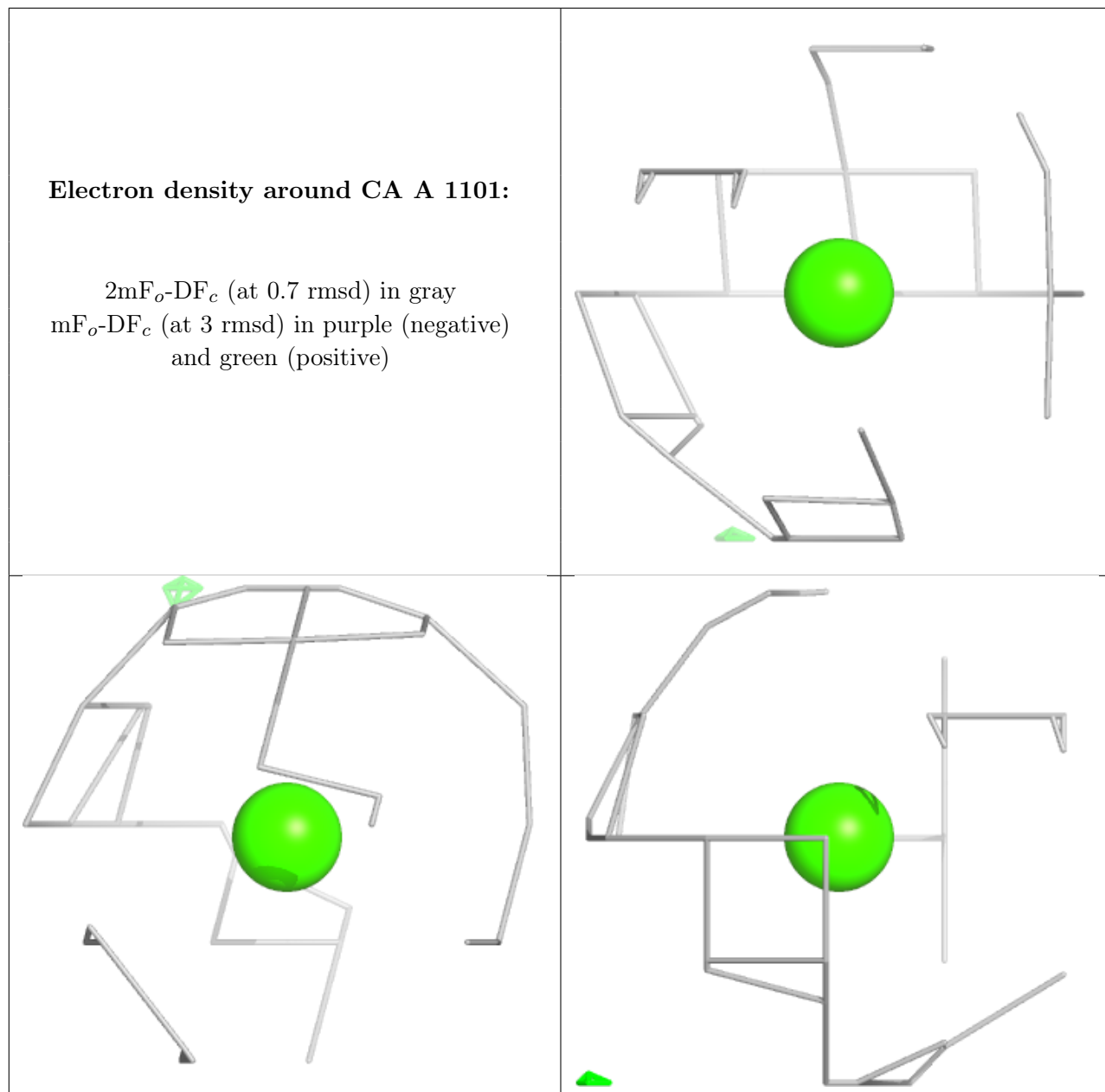
**Electron density around EDO A 1121:**

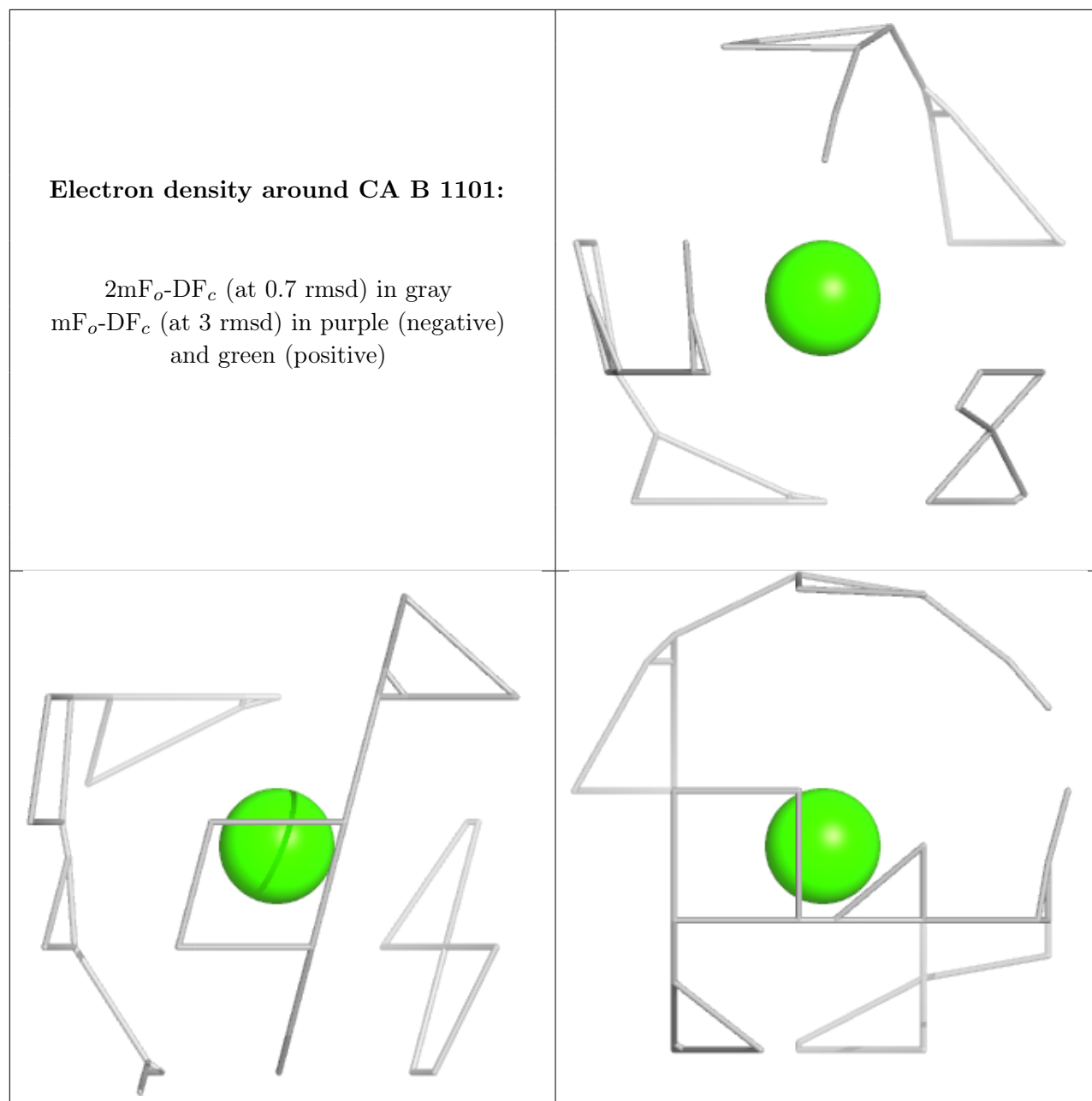
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CA A 1101:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.