



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 23, 2021 – 02:16 PM EST

PDB ID : 7KUZ  
Title : Dihydrodipicolinate synthase (DHDPS) from C.jejuni, H56N mutant with pyruvate bound in the active site and L-lysine bound at the allosteric site  
Authors : Saran, S.; Sanders, D.A.R.  
Deposited on : 2020-11-25  
Resolution : 2.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.23.2  
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) : 2.23.2

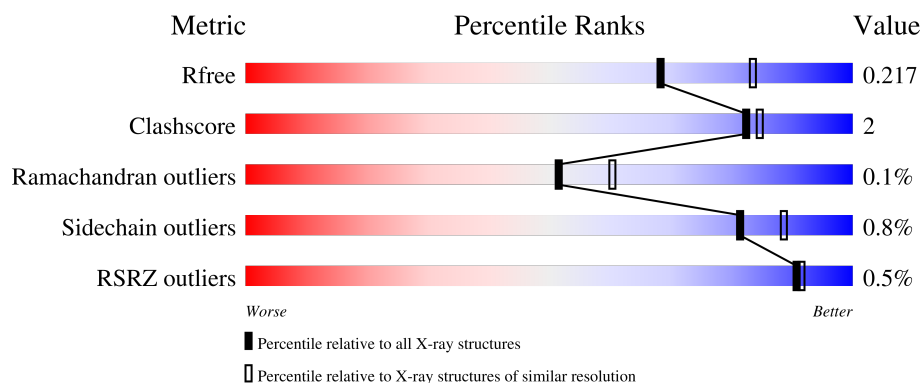
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



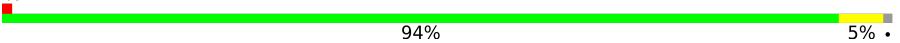


The reported resolution of this entry is 2.25 Å.

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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	310	 90% 5% • 5%
1	B	310	 91% 5% •
1	C	310	 94% 5% •
1	D	310	 92% 7% •
1	F	310	 89% 6% 5%

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Mol	Chain	Length	Quality of chain
2	E	310	

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
4	PEG	F	302	-	-	-	X
5	EDO	D	303	-	-	-	X
5	EDO	D	304	-	-	-	X
5	EDO	F	305	-	-	-	X
6	ACT	C	305	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 15196 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 4-hydroxy-tetrahydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2272	1445	377	437	13			
1	B	297	Total	C	N	O	S	0	2	0
			2282	1448	376	445	13			
1	C	306	Total	C	N	O	S	0	0	0
			2351	1489	397	451	14			
1	D	306	Total	C	N	O	S	0	0	0
			2343	1484	394	451	14			
1	F	296	Total	C	N	O	S	0	0	0
			2260	1435	374	438	13			

There are 65 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9PPB4
A	-10	ARG	-	expression tag	UNP Q9PPB4
A	-9	GLY	-	expression tag	UNP Q9PPB4
A	-8	SER	-	expression tag	UNP Q9PPB4
A	-7	HIS	-	expression tag	UNP Q9PPB4
A	-6	HIS	-	expression tag	UNP Q9PPB4
A	-5	HIS	-	expression tag	UNP Q9PPB4
A	-4	HIS	-	expression tag	UNP Q9PPB4
A	-3	HIS	-	expression tag	UNP Q9PPB4
A	-2	HIS	-	expression tag	UNP Q9PPB4
A	-1	GLY	-	expression tag	UNP Q9PPB4
A	0	SER	-	expression tag	UNP Q9PPB4
A	56	ASN	HIS	engineered mutation	UNP Q9PPB4
B	-11	MET	-	expression tag	UNP Q9PPB4
B	-10	ARG	-	expression tag	UNP Q9PPB4
B	-9	GLY	-	expression tag	UNP Q9PPB4
B	-8	SER	-	expression tag	UNP Q9PPB4
B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
B	56	ASN	HIS	engineered mutation	UNP Q9PPB4
C	-11	MET	-	expression tag	UNP Q9PPB4
C	-10	ARG	-	expression tag	UNP Q9PPB4
C	-9	GLY	-	expression tag	UNP Q9PPB4
C	-8	SER	-	expression tag	UNP Q9PPB4
C	-7	HIS	-	expression tag	UNP Q9PPB4
C	-6	HIS	-	expression tag	UNP Q9PPB4
C	-5	HIS	-	expression tag	UNP Q9PPB4
C	-4	HIS	-	expression tag	UNP Q9PPB4
C	-3	HIS	-	expression tag	UNP Q9PPB4
C	-2	HIS	-	expression tag	UNP Q9PPB4
C	-1	GLY	-	expression tag	UNP Q9PPB4
C	0	SER	-	expression tag	UNP Q9PPB4
C	56	ASN	HIS	engineered mutation	UNP Q9PPB4
D	-11	MET	-	expression tag	UNP Q9PPB4
D	-10	ARG	-	expression tag	UNP Q9PPB4
D	-9	GLY	-	expression tag	UNP Q9PPB4
D	-8	SER	-	expression tag	UNP Q9PPB4
D	-7	HIS	-	expression tag	UNP Q9PPB4
D	-6	HIS	-	expression tag	UNP Q9PPB4
D	-5	HIS	-	expression tag	UNP Q9PPB4
D	-4	HIS	-	expression tag	UNP Q9PPB4
D	-3	HIS	-	expression tag	UNP Q9PPB4
D	-2	HIS	-	expression tag	UNP Q9PPB4
D	-1	GLY	-	expression tag	UNP Q9PPB4
D	0	SER	-	expression tag	UNP Q9PPB4
D	56	ASN	HIS	engineered mutation	UNP Q9PPB4
F	-11	MET	-	expression tag	UNP Q9PPB4
F	-10	ARG	-	expression tag	UNP Q9PPB4
F	-9	GLY	-	expression tag	UNP Q9PPB4
F	-8	SER	-	expression tag	UNP Q9PPB4
F	-7	HIS	-	expression tag	UNP Q9PPB4
F	-6	HIS	-	expression tag	UNP Q9PPB4
F	-5	HIS	-	expression tag	UNP Q9PPB4
F	-4	HIS	-	expression tag	UNP Q9PPB4
F	-3	HIS	-	expression tag	UNP Q9PPB4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	HIS	-	expression tag	UNP Q9PPB4
F	-1	GLY	-	expression tag	UNP Q9PPB4
F	0	SER	-	expression tag	UNP Q9PPB4
F	56	ASN	HIS	engineered mutation	UNP Q9PPB4

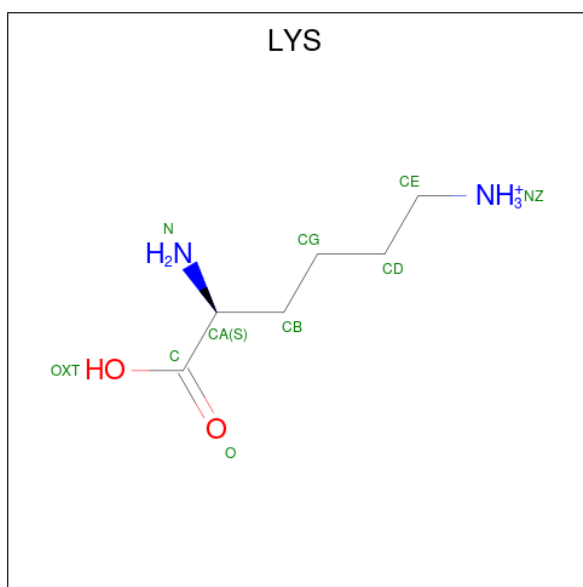
- Molecule 2 is a protein called 4-hydroxy-tetrahydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	296	Total	C	N	O	S	0	0	0
			2257	1433	375	436	13			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	MET	-	expression tag	UNP Q9PPB4
E	-10	ARG	-	expression tag	UNP Q9PPB4
E	-9	GLY	-	expression tag	UNP Q9PPB4
E	-8	SER	-	expression tag	UNP Q9PPB4
E	-7	HIS	-	expression tag	UNP Q9PPB4
E	-6	HIS	-	expression tag	UNP Q9PPB4
E	-5	HIS	-	expression tag	UNP Q9PPB4
E	-4	HIS	-	expression tag	UNP Q9PPB4
E	-3	HIS	-	expression tag	UNP Q9PPB4
E	-2	HIS	-	expression tag	UNP Q9PPB4
E	-1	GLY	-	expression tag	UNP Q9PPB4
E	0	SER	-	expression tag	UNP Q9PPB4
E	56	ASN	HIS	engineered mutation	UNP Q9PPB4

- Molecule 3 is LYSINE (three-letter code: LYS) (formula:  $C_6H_{15}N_2O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	2	2		
3	B	1	Total	C	N	O	0	0
			10	6	2	2		
3	B	1	Total	C	N	O	0	0
			10	6	2	2		
3	D	1	Total	C	N	O	0	0
			10	6	2	2		
3	E	1	Total	C	N	O	0	0
			10	6	2	2		
3	F	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 4 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
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	E	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		
4	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 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).



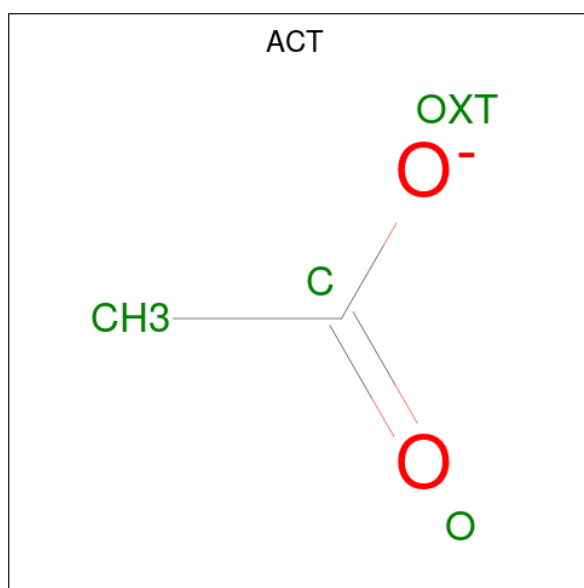
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total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

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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula:  $\text{C}_2\text{H}_3\text{O}_2$ ) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	Mg	0	0
			3	3		
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		
7	D	3	Total	Mg	0	0
			3	3		
7	E	2	Total	Mg	0	0
			2	2		
7	F	2	Total	Mg	0	0
			2	2		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		
8	A	1	Total	C	O	0	0
			10	6	4		
8	C	1	Total	C	O	0	0
			10	6	4		
8	D	1	Total	C	O	0	0
			10	6	4		
8	E	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ) (labeled as "Ligand of Interest" by depositor).





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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	198	Total	O	0	0
			198	198		
10	B	193	Total	O	0	0
			193	193		
10	C	193	Total	O	0	0
			193	193		
10	D	185	Total	O	0	0
			185	185		
10	E	186	Total	O	0	0
			186	186		
10	F	158	Total	O	0	0
			158	158		

### 3 Residue-property plots [i](#)

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

- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain A: 



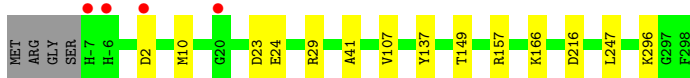
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain B: 

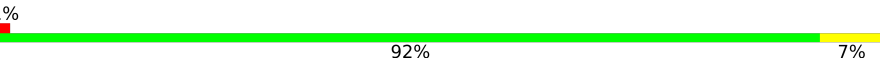


- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain C: 




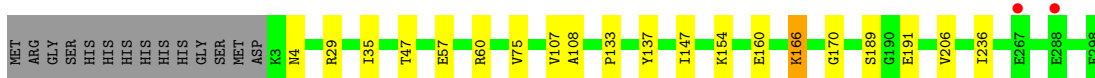
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain D: 



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain F: 



- Molecule 2: 4-hydroxy-tetrahydrodipicolinate synthase

Chain E: 

90%

5%

5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.05Å 227.33Å 202.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 2.25 49.57 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.57-2.25) 99.9 (49.57-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.25Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.177 , 0.218 0.177 , 0.217	Depositor DCC
$R_{free}$ test set	4668 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: ACT, GOL, PGE, MG, PEG, KPI, 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	0.41	0/2294	0.49	0/3102
1	B	0.49	1/2308 (0.0%)	0.54	0/3126
1	C	0.54	1/2380 (0.0%)	0.57	1/3221 (0.0%)
1	D	0.50	1/2372 (0.0%)	0.53	0/3213
1	F	0.43	0/2281	0.51	0/3089
2	E	0.40	0/2295	0.52	0/3107
All	All	0.46	3/13930 (0.0%)	0.53	1/18858 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	24	GLU	CD-OE2	-7.21	1.17	1.25
1	B	72	GLY	C-O	-5.89	1.14	1.23
1	D	160	GLU	CD-OE1	-5.72	1.19	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	23	ASP	CB-CG-OD1	8.58	126.02	118.30

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	2272	0	2307	13	0
1	B	2282	0	2285	10	0
1	C	2351	0	2350	6	0
1	D	2343	0	2325	14	0
1	F	2260	0	2271	14	0
2	E	2257	0	2276	13	0
3	A	10	0	12	0	0
3	B	20	0	24	1	0
3	D	10	0	12	1	0
3	E	10	0	12	1	0
3	F	10	0	12	0	0
4	A	7	0	10	1	0
4	B	7	0	10	0	0
4	C	14	0	20	1	0
4	E	21	0	30	1	0
4	F	21	0	30	2	0
5	A	16	0	24	4	0
5	B	20	0	28	5	0
5	C	8	0	12	1	0
5	D	16	0	24	0	0
5	E	8	0	12	2	0
5	F	16	0	24	3	0
6	A	4	0	3	0	0
6	B	16	0	12	0	0
6	C	4	0	3	0	0
6	D	4	0	3	1	0
6	E	4	0	3	0	0
6	F	4	0	3	0	0
7	A	3	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	3	0	0	0	0
7	E	2	0	0	0	0
7	F	2	0	0	0	0
8	A	20	0	28	2	0
8	C	10	0	14	0	0
8	D	10	0	14	5	0
8	E	10	0	14	1	0
9	A	6	0	8	0	0
10	A	198	0	0	1	0
10	B	193	0	0	1	0
10	C	193	0	0	0	0
10	D	185	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	E	186	0	0	2	0
10	F	158	0	0	1	0
All	All	15196	0	14215	70	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 2.

The worst 5 of 70 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:VAL:HG13	5:B:308:EDO:H21	1.51	0.93
1:A:295:ILE:H	5:A:305:EDO:H12	1.47	0.80
1:A:291:LYS:HD2	8:A:312:PGE:H6	1.72	0.71
1:F:154:LYS:HD2	4:F:304:PEG:H11	1.73	0.70
1:F:107:VAL:HA	1:F:137:TYR:HB3	1.75	0.68

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/310 (94%)	289 (99%)	4 (1%)	0	100	100
1	B	296/310 (96%)	291 (98%)	5 (2%)	0	100	100
1	C	303/310 (98%)	297 (98%)	5 (2%)	1 (0%)	41	46
1	D	303/310 (98%)	299 (99%)	4 (1%)	0	100	100
1	F	293/310 (94%)	289 (99%)	4 (1%)	0	100	100
2	E	294/310 (95%)	290 (99%)	4 (1%)	0	100	100
All	All	1782/1860 (96%)	1755 (98%)	26 (2%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2	ASP

### 5.3.2 Protein sidechains [i](#)

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	246/260 (95%)	242 (98%)	4 (2%)	62	73
1	B	246/260 (95%)	243 (99%)	3 (1%)	71	80
1	C	254/260 (98%)	253 (100%)	1 (0%)	91	94
1	D	251/260 (96%)	248 (99%)	3 (1%)	71	80
1	F	243/260 (94%)	242 (100%)	1 (0%)	91	94
2	E	245/261 (94%)	245 (100%)	0	100	100
All	All	1485/1561 (95%)	1473 (99%)	12 (1%)	81	88

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	29	ARG
1	D	106	SER
1	F	160	GLU
1	D	146	GLU
1	A	280	LYS

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

Mol	Chain	Res	Type
2	E	4	ASN
1	F	19	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.



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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
1	KPI	A	166	1	10,13,14	0.65	0	6,15,17	3.10	3 (50%)
1	KPI	F	166	1	10,13,14	0.67	0	6,15,17	3.38	3 (50%)
1	KPI	D	166	1	10,13,14	0.62	0	6,15,17	3.47	3 (50%)
1	KPI	C	166	1	10,13,14	0.64	0	6,15,17	3.08	2 (33%)
1	KPI	B	166	1	10,13,14	0.61	0	6,15,17	3.11	3 (50%)

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
1	KPI	A	166	1	-	0/9/14/16	-
1	KPI	F	166	1	-	0/9/14/16	-
1	KPI	D	166	1	-	0/9/14/16	-
1	KPI	C	166	1	-	0/9/14/16	-
1	KPI	B	166	1	-	1/9/14/16	-

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	166	KPI	C1-CX1-CX2	-6.98	110.19	117.92
1	F	166	KPI	C1-CX1-CX2	-6.45	110.78	117.92
1	B	166	KPI	C1-CX1-CX2	-6.19	111.07	117.92
1	A	166	KPI	C1-CX1-CX2	-6.18	111.08	117.92
1	C	166	KPI	C1-CX1-CX2	-6.13	111.13	117.92

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	166	KPI	C1-CX1-NZ-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	166	KPI	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 12 are monoatomic - leaving 52 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	$\# Z  > 2$
6	ACT	C	305	-	1,3,3	0.05	0	0,3,3	-	-
5	EDO	B	308	-	3,3,3	1.09	0	2,2,2	0.63	0
3	LYS	F	301	-	5,9,9	0.31	0	4,10,10	0.78	0
6	ACT	E	307	-	1,3,3	6.50	1 (100%)	0,3,3	-	-
6	ACT	B	312	-	1,3,3	6.51	1 (100%)	0,3,3	-	-
5	EDO	A	304	-	3,3,3	0.48	0	2,2,2	0.28	0
4	PEG	B	303	-	6,6,6	0.49	0	5,5,5	0.32	0
5	EDO	C	304	-	3,3,3	0.49	0	2,2,2	0.27	0
3	LYS	D	301	-	5,9,9	0.33	0	4,10,10	0.92	0
5	EDO	D	303	-	3,3,3	0.49	0	2,2,2	0.31	0
5	EDO	A	306	-	3,3,3	0.44	0	2,2,2	0.33	0
5	EDO	F	305	-	3,3,3	0.48	0	2,2,2	0.27	0
6	ACT	B	311	-	1,3,3	6.76	1 (100%)	0,3,3	-	-
8	PGE	E	310	-	9,9,9	0.32	0	8,8,8	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	GOL	A	313	-	5,5,5	0.70	0	5,5,5	0.97	0
4	PEG	C	301	-	6,6,6	0.49	0	5,5,5	0.25	0
5	EDO	B	304	-	3,3,3	0.48	0	2,2,2	0.25	0
6	ACT	B	309	-	1,3,3	6.60	1 (100%)	0,3,3	-	-
5	EDO	B	306	-	3,3,3	0.42	0	2,2,2	0.42	0
3	LYS	A	301	-	5,9,9	0.33	0	4,10,10	0.62	0
4	PEG	E	303	-	6,6,6	0.48	0	5,5,5	0.29	0
5	EDO	B	305	-	3,3,3	0.45	0	2,2,2	0.34	0
6	ACT	B	310	-	1,3,3	6.83	1 (100%)	0,3,3	-	-
4	PEG	F	303	-	6,6,6	0.50	0	5,5,5	0.23	0
4	PEG	F	304	-	6,6,6	0.47	0	5,5,5	0.25	0
3	LYS	B	302	-	5,9,9	0.29	0	4,10,10	0.69	0
5	EDO	E	306	-	3,3,3	0.42	0	2,2,2	0.38	0
4	PEG	E	304	-	6,6,6	0.48	0	5,5,5	0.30	0
5	EDO	F	306	-	3,3,3	0.46	0	2,2,2	0.30	0
3	LYS	E	301	-	5,9,9	0.28	0	4,10,10	0.53	0
8	PGE	A	312	-	9,9,9	0.35	0	8,8,8	0.20	0
6	ACT	D	306	-	1,3,3	6.69	1 (100%)	0,3,3	-	-
5	EDO	D	304	-	3,3,3	0.48	0	2,2,2	0.27	0
5	EDO	F	307	-	3,3,3	0.46	0	2,2,2	0.30	0
5	EDO	D	305	-	3,3,3	0.45	0	2,2,2	0.35	0
5	EDO	A	305	-	3,3,3	0.57	0	2,2,2	0.17	0
4	PEG	E	302	-	6,6,6	0.49	0	5,5,5	0.33	0
8	PGE	D	310	-	9,9,9	0.30	0	8,8,8	0.31	0
4	PEG	A	302	-	6,6,6	0.59	0	5,5,5	1.86	1 (20%)
4	PEG	C	302	-	6,6,6	0.49	0	5,5,5	0.21	0
4	PEG	F	302	-	6,6,6	0.49	0	5,5,5	0.24	0
3	LYS	B	301	-	5,9,9	0.36	0	4,10,10	0.45	0
5	EDO	A	303	-	3,3,3	0.46	0	2,2,2	0.30	0
5	EDO	E	305	-	3,3,3	0.50	0	2,2,2	0.23	0
5	EDO	F	308	-	3,3,3	0.47	0	2,2,2	0.29	0
8	PGE	C	307	-	9,9,9	0.32	0	8,8,8	0.28	0
5	EDO	B	307	-	3,3,3	0.46	0	2,2,2	0.31	0
5	EDO	D	302	-	3,3,3	0.48	0	2,2,2	0.27	0
8	PGE	A	311	-	9,9,9	0.29	0	8,8,8	0.27	0
6	ACT	F	309	-	1,3,3	6.88	1 (100%)	0,3,3	-	-
6	ACT	A	307	-	1,3,3	6.47	1 (100%)	0,3,3	-	-
5	EDO	C	303	-	3,3,3	0.52	0	2,2,2	0.23	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
5	EDO	B	308	-	-	1/1/1/1	-
3	LYS	F	301	-	-	4/5/9/9	-
5	EDO	A	304	-	-	1/1/1/1	-
4	PEG	B	303	-	-	3/4/4/4	-
5	EDO	C	304	-	-	0/1/1/1	-
3	LYS	D	301	-	-	2/5/9/9	-
5	EDO	D	303	-	-	0/1/1/1	-
5	EDO	A	306	-	-	0/1/1/1	-
5	EDO	F	305	-	-	0/1/1/1	-
8	PGE	E	310	-	-	5/7/7/7	-
9	GOL	A	313	-	-	4/4/4/4	-
4	PEG	C	301	-	-	2/4/4/4	-
5	EDO	B	304	-	-	0/1/1/1	-
5	EDO	B	306	-	-	1/1/1/1	-
3	LYS	A	301	-	-	1/5/9/9	-
4	PEG	E	303	-	-	1/4/4/4	-
5	EDO	B	305	-	-	0/1/1/1	-
4	PEG	F	303	-	-	0/4/4/4	-
4	PEG	F	304	-	-	3/4/4/4	-
3	LYS	B	302	-	-	3/5/9/9	-
5	EDO	E	306	-	-	1/1/1/1	-
4	PEG	E	304	-	-	2/4/4/4	-
5	EDO	F	306	-	-	0/1/1/1	-
3	LYS	E	301	-	-	2/5/9/9	-
8	PGE	A	312	-	-	4/7/7/7	-
5	EDO	D	304	-	-	0/1/1/1	-
5	EDO	F	307	-	-	0/1/1/1	-
5	EDO	D	305	-	-	1/1/1/1	-
5	EDO	A	305	-	-	1/1/1/1	-
4	PEG	E	302	-	-	3/4/4/4	-
8	PGE	D	310	-	-	4/7/7/7	-
4	PEG	A	302	-	-	2/4/4/4	-
4	PEG	C	302	-	-	0/4/4/4	-
4	PEG	F	302	-	-	1/4/4/4	-
3	LYS	B	301	-	-	0/5/9/9	-
5	EDO	A	303	-	-	0/1/1/1	-
5	EDO	E	305	-	-	0/1/1/1	-
5	EDO	F	308	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PGE	C	307	-	-	2/7/7/7	-
5	EDO	B	307	-	-	0/1/1/1	-
5	EDO	D	302	-	-	0/1/1/1	-
8	PGE	A	311	-	-	5/7/7/7	-
5	EDO	C	303	-	-	1/1/1/1	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	309	ACT	CH3-C	6.88	1.57	1.48
6	B	310	ACT	CH3-C	6.83	1.57	1.48
6	B	311	ACT	CH3-C	6.76	1.57	1.48
6	D	306	ACT	CH3-C	6.69	1.57	1.48
6	B	309	ACT	CH3-C	6.60	1.57	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	302	PEG	O1-C1-C2	-3.46	91.75	111.81

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	LYS	N-CA-CB-CG
3	B	302	LYS	C-CA-CB-CG
3	D	301	LYS	C-CA-CB-CG
3	F	301	LYS	N-CA-CB-CG
3	F	301	LYS	C-CA-CB-CG

There are no ring outliers.

20 monomers are involved in 32 short contacts:

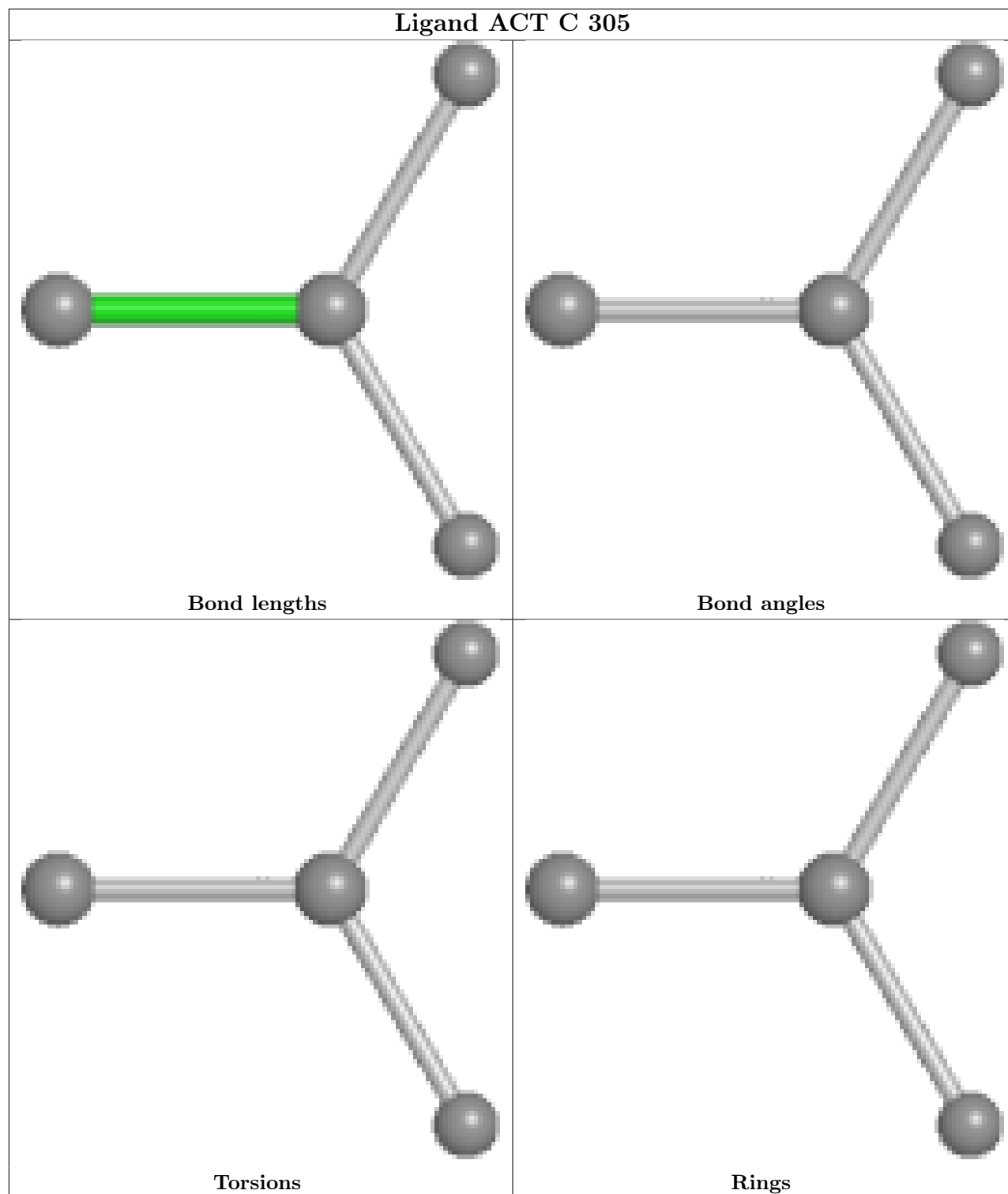
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	308	EDO	3	0
3	D	301	LYS	1	0
5	A	306	EDO	1	0
8	E	310	PGE	1	0
5	B	306	EDO	2	0
4	F	304	PEG	1	0

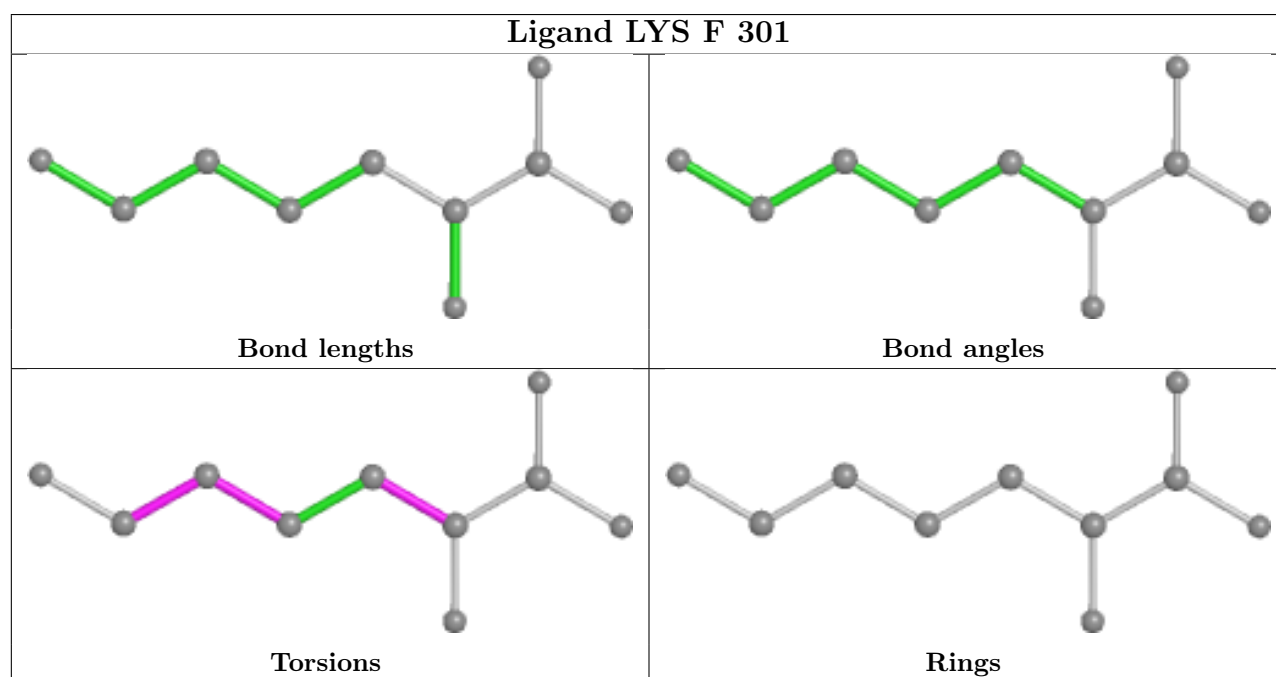
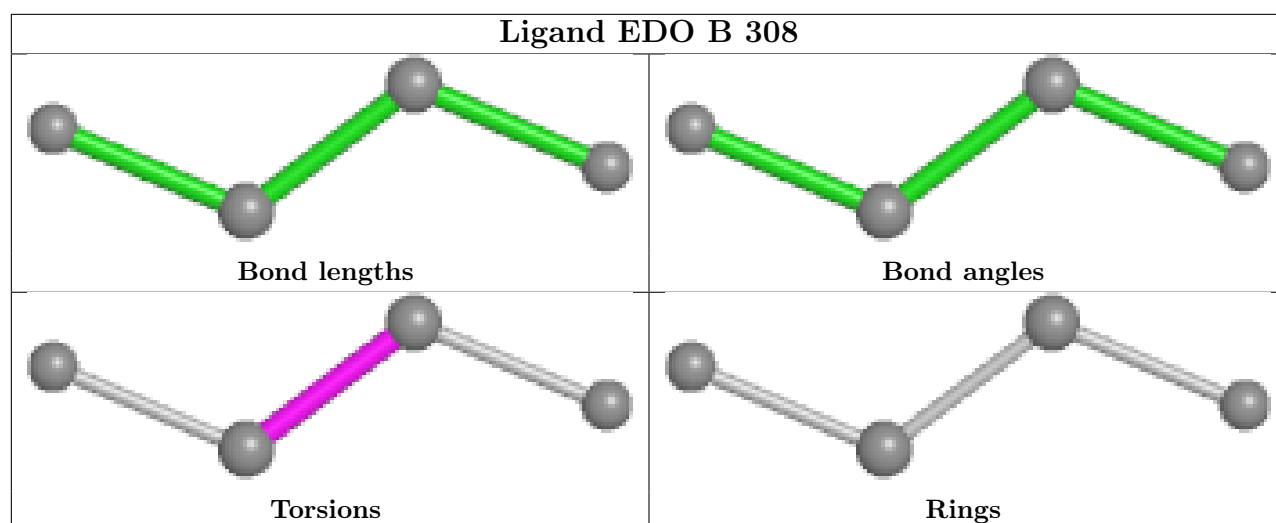
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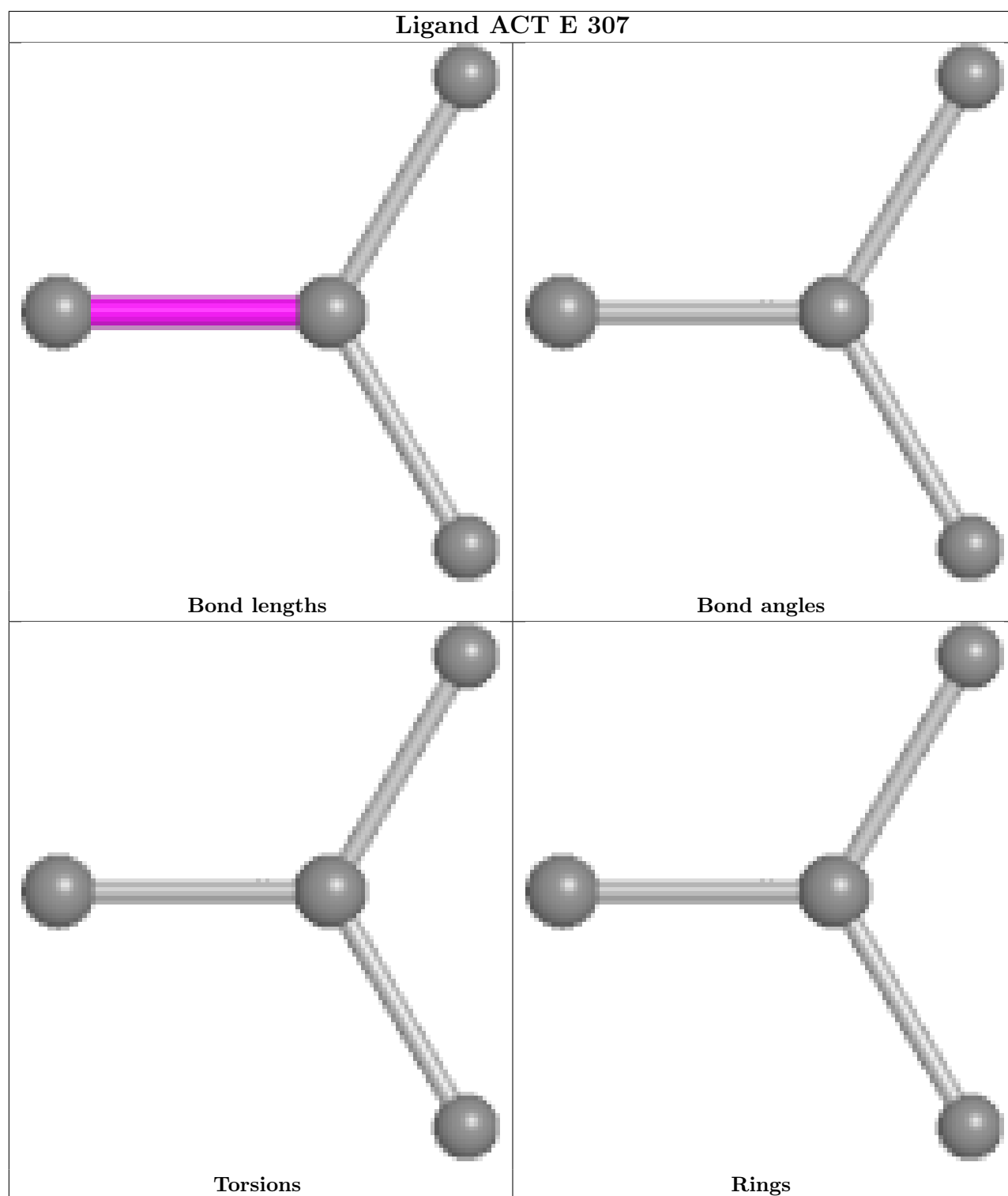
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	LYS	1	0
5	E	306	EDO	2	0
4	E	304	PEG	1	0
5	F	306	EDO	3	0
3	E	301	LYS	1	0
8	A	312	PGE	1	0
6	D	306	ACT	1	0
5	A	305	EDO	3	0
8	D	310	PGE	5	0
4	A	302	PEG	1	0
4	C	302	PEG	1	0
4	F	302	PEG	1	0
8	A	311	PGE	1	0
5	C	303	EDO	1	0

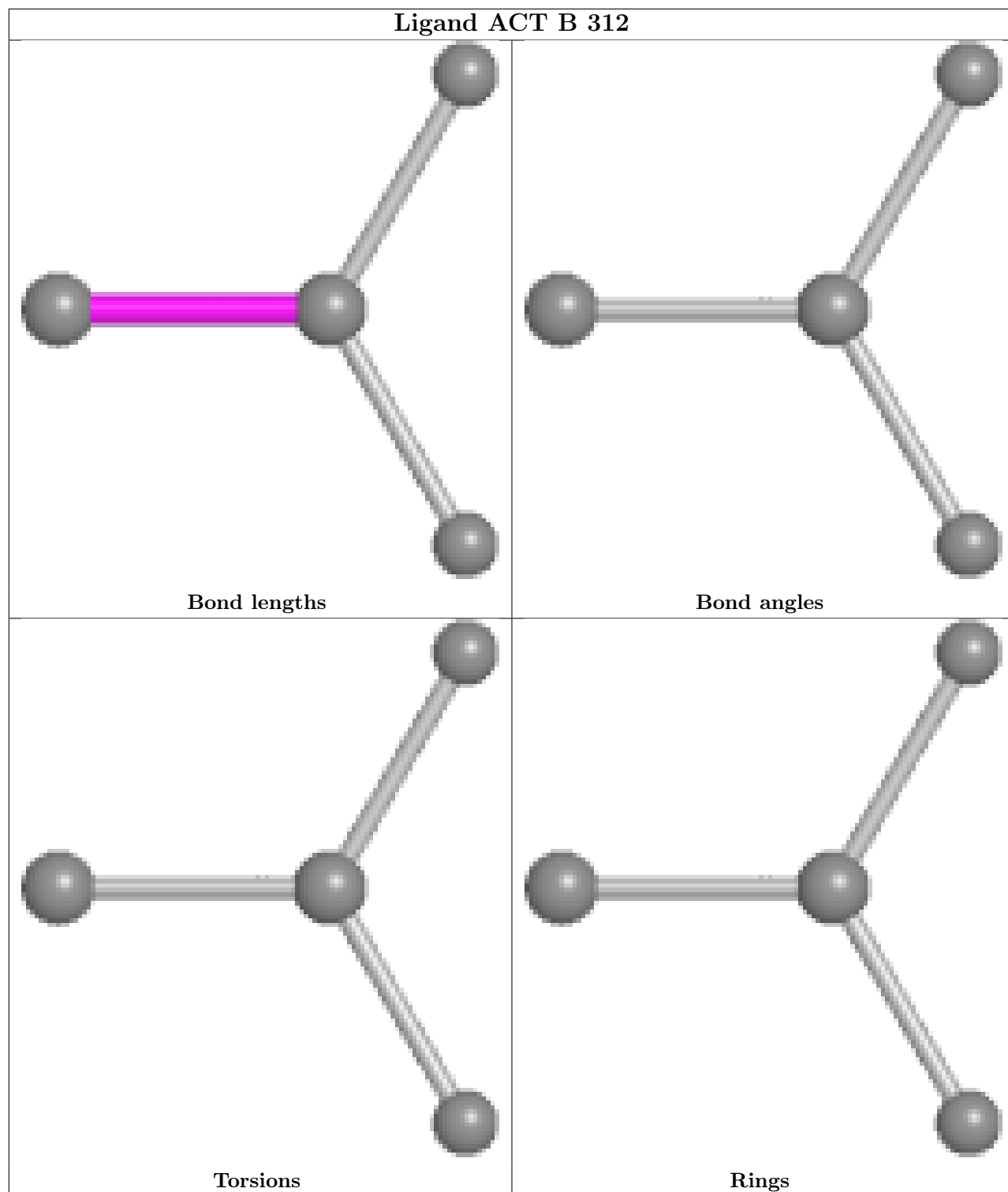
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

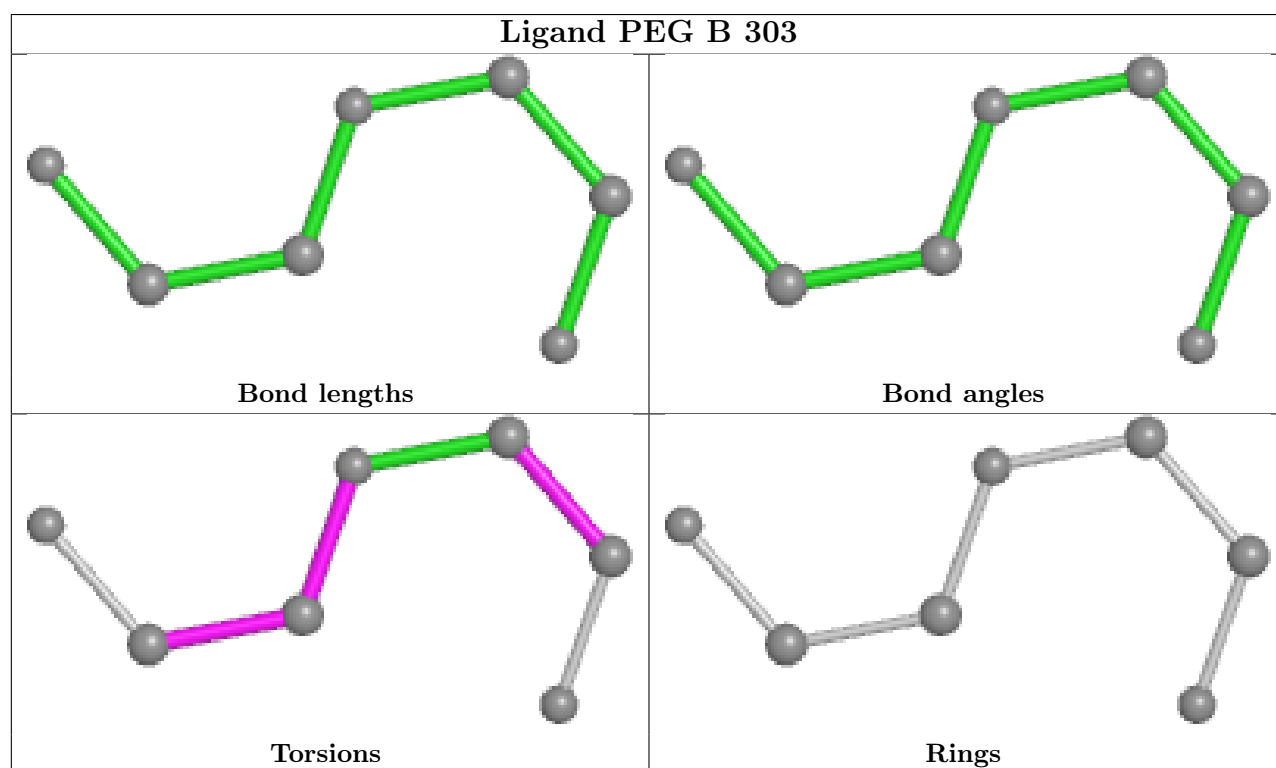
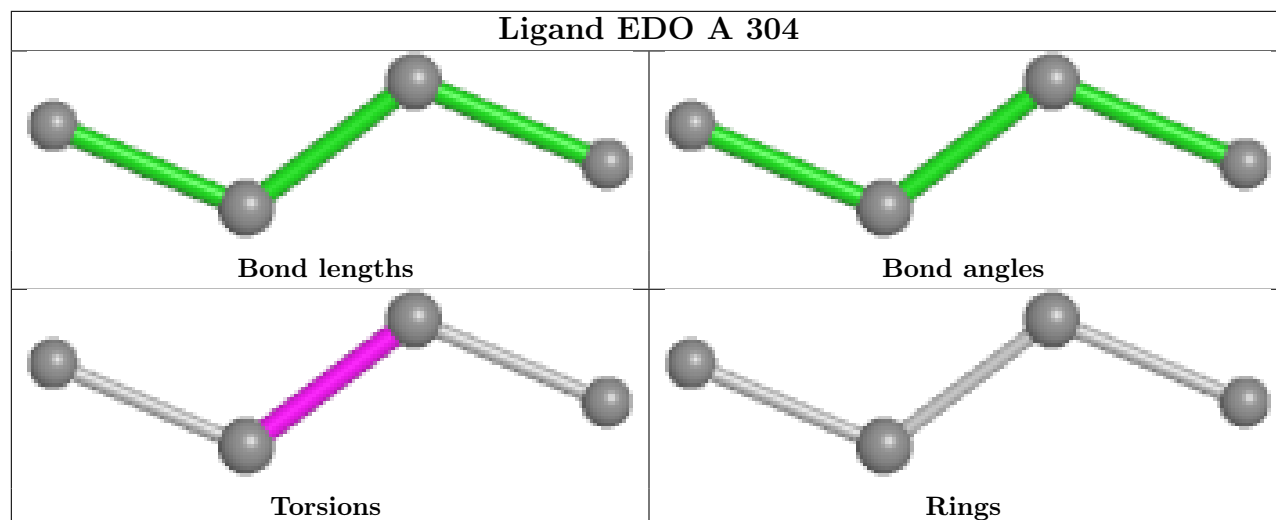


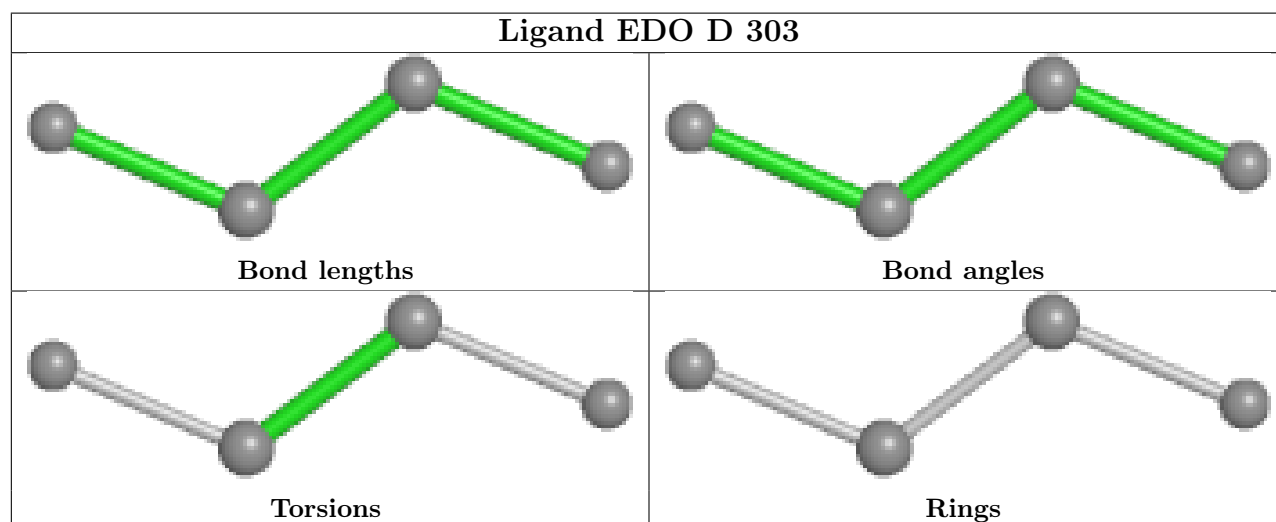
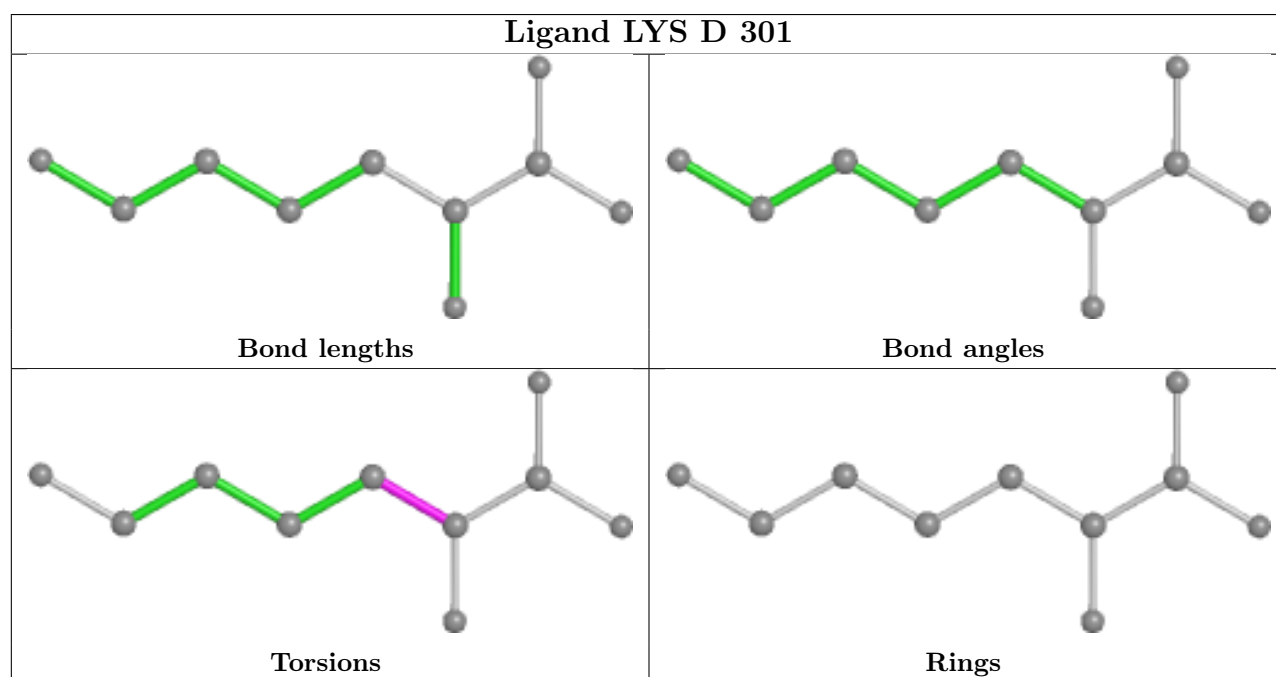
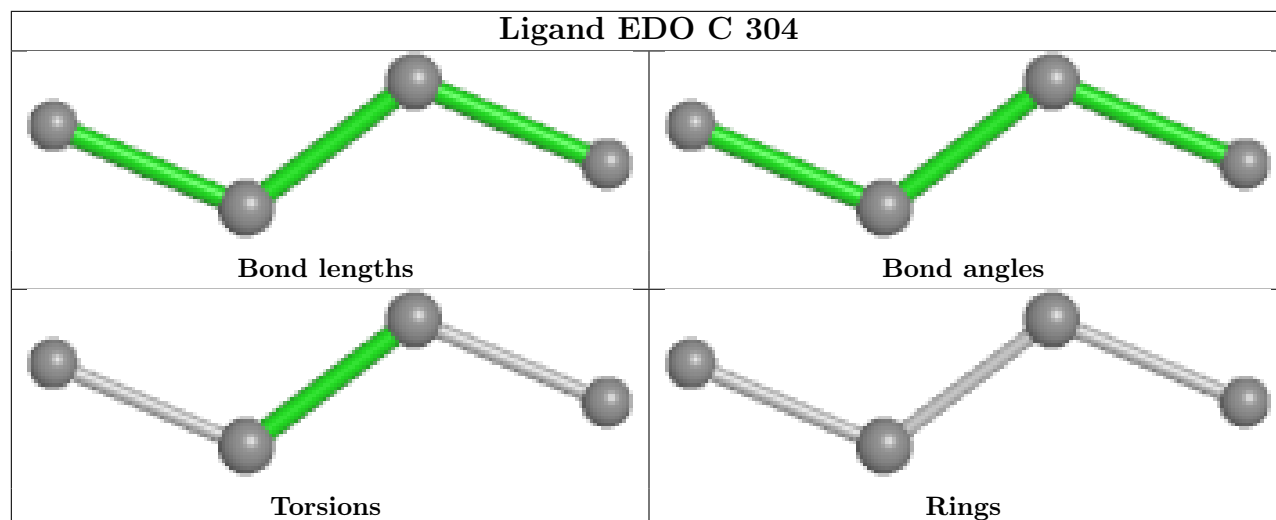


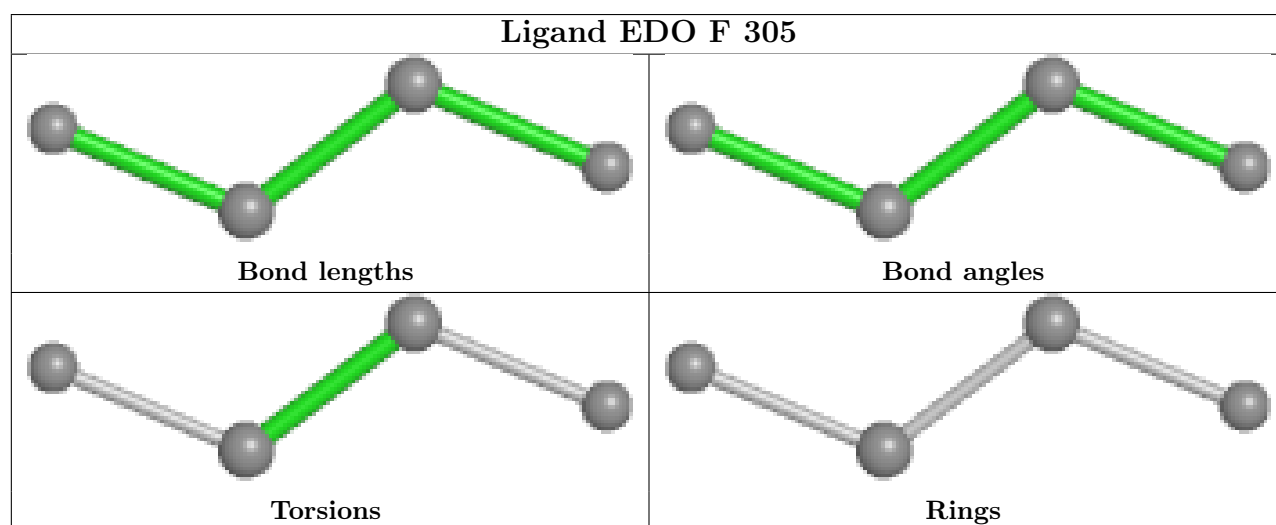
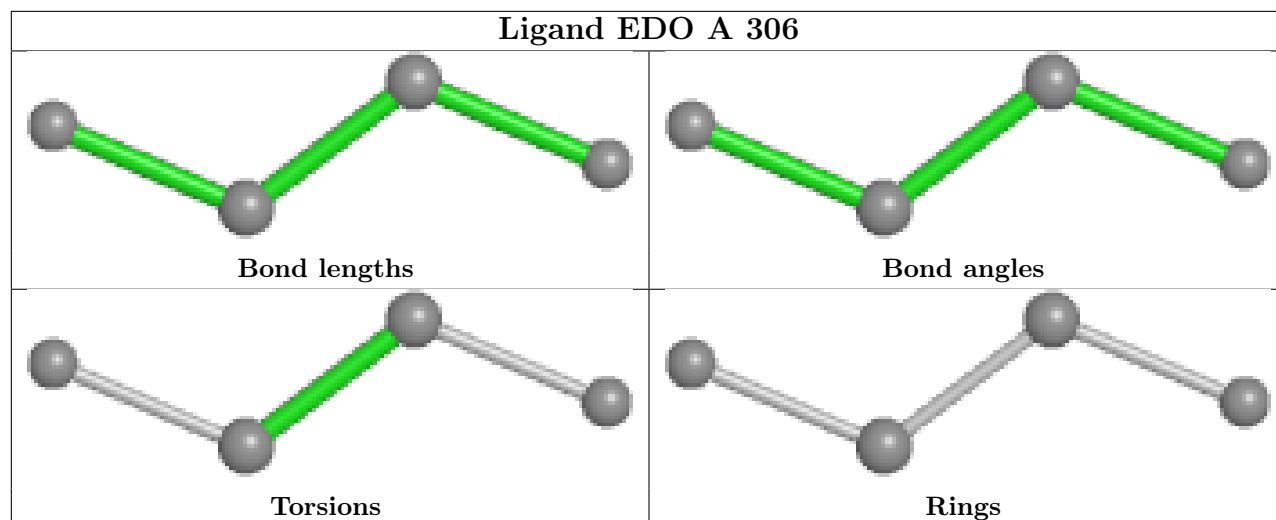


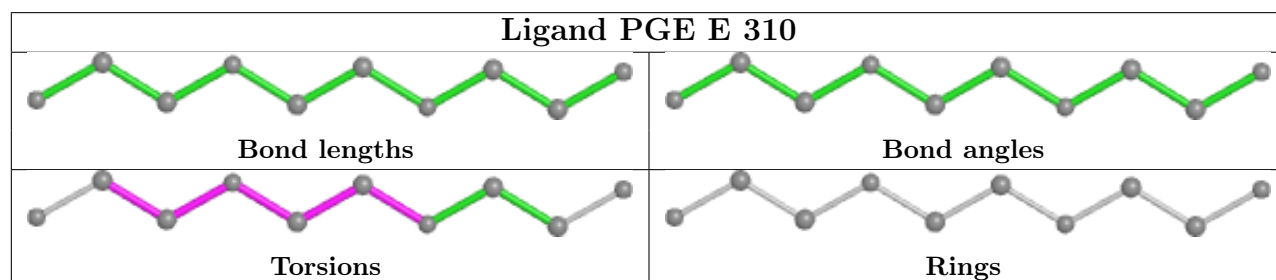
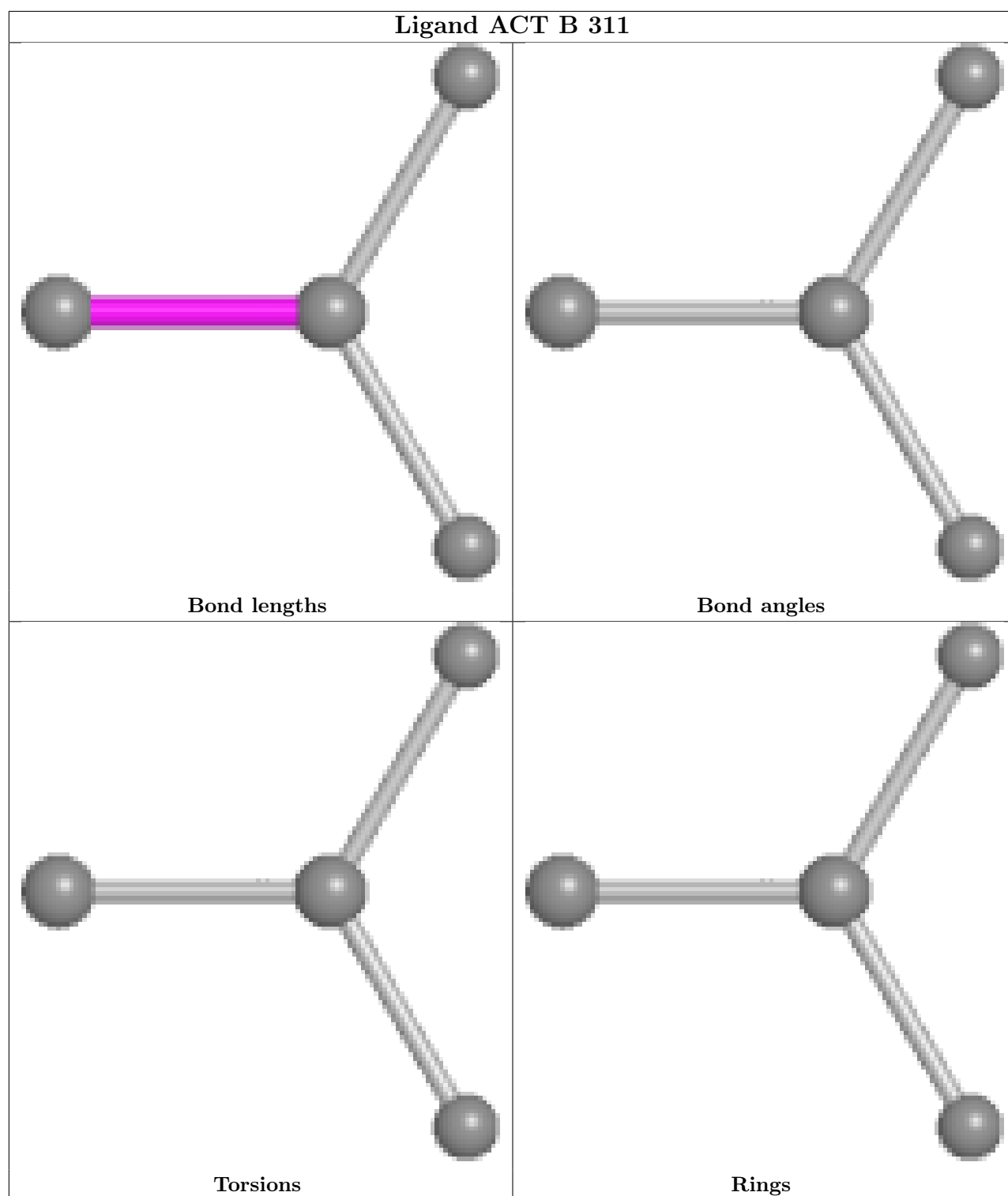


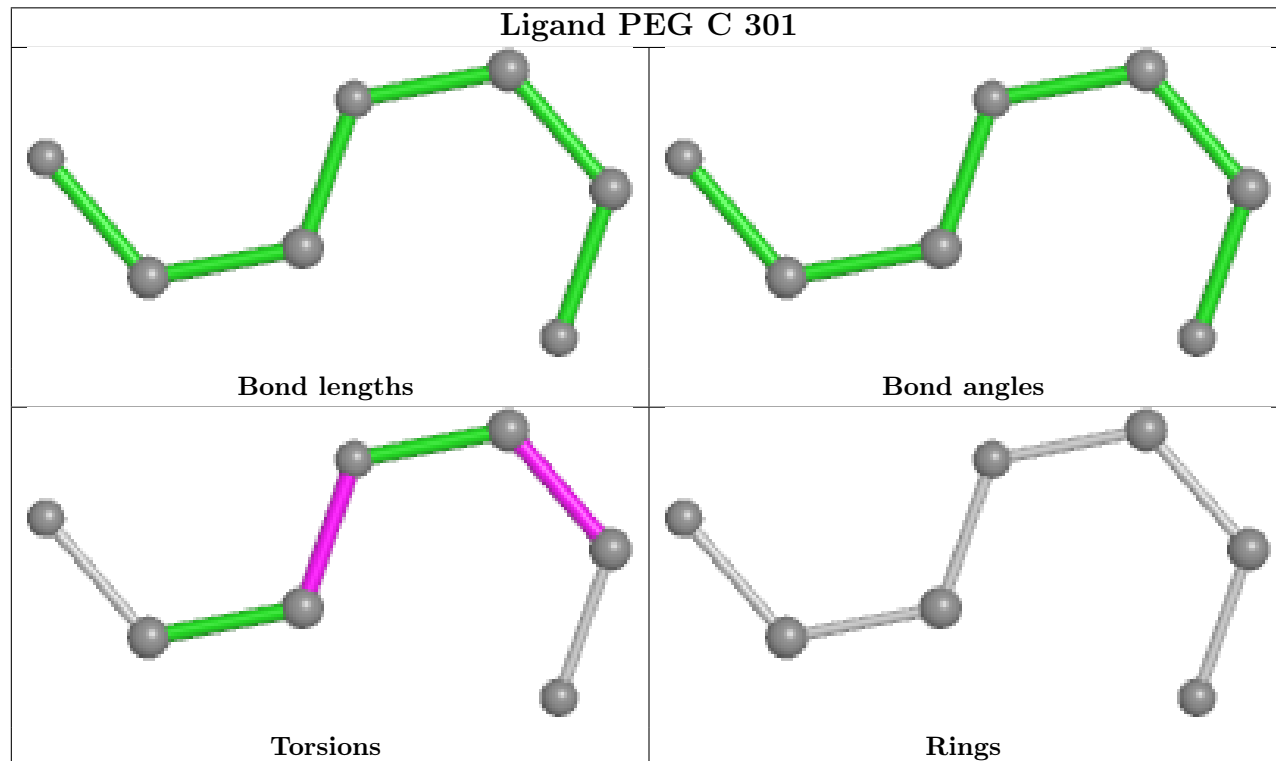
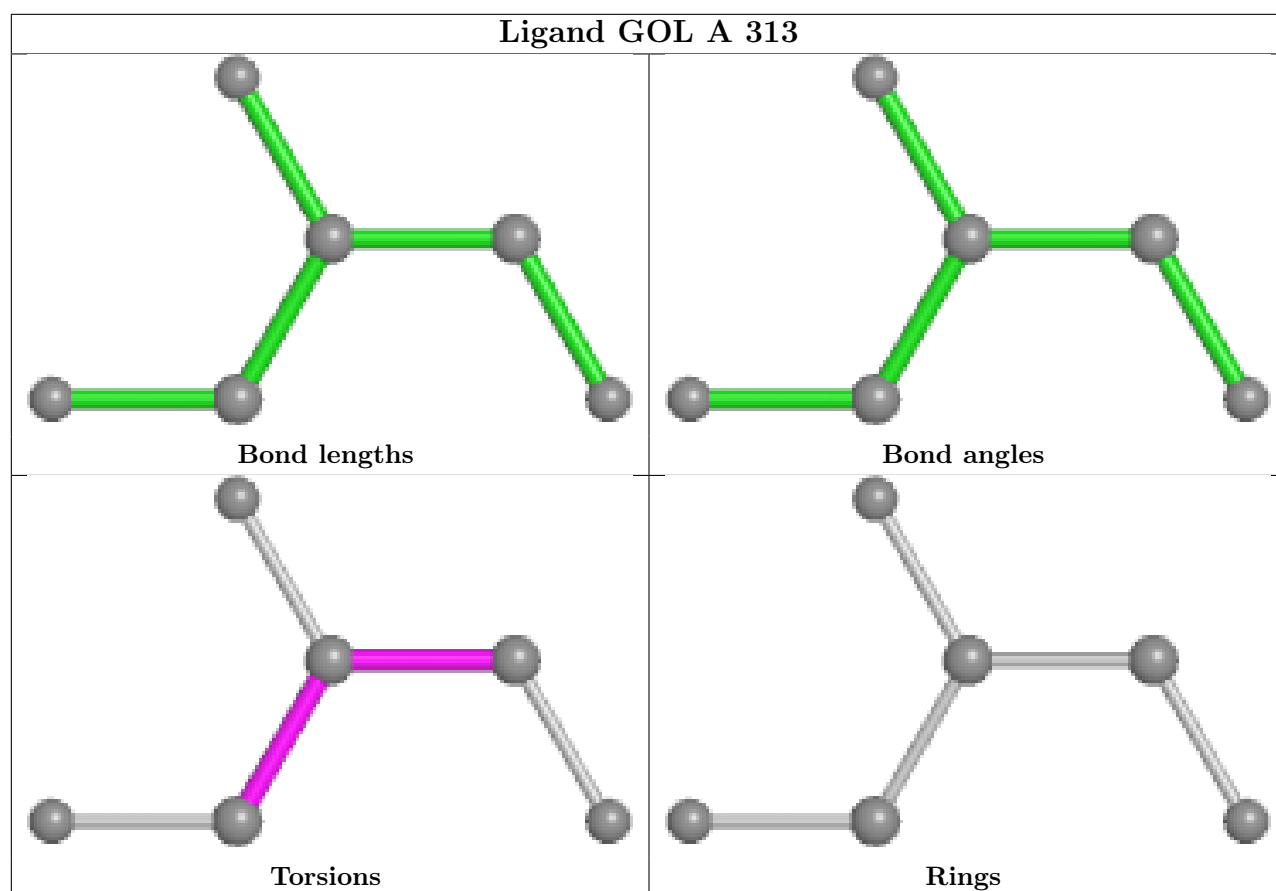


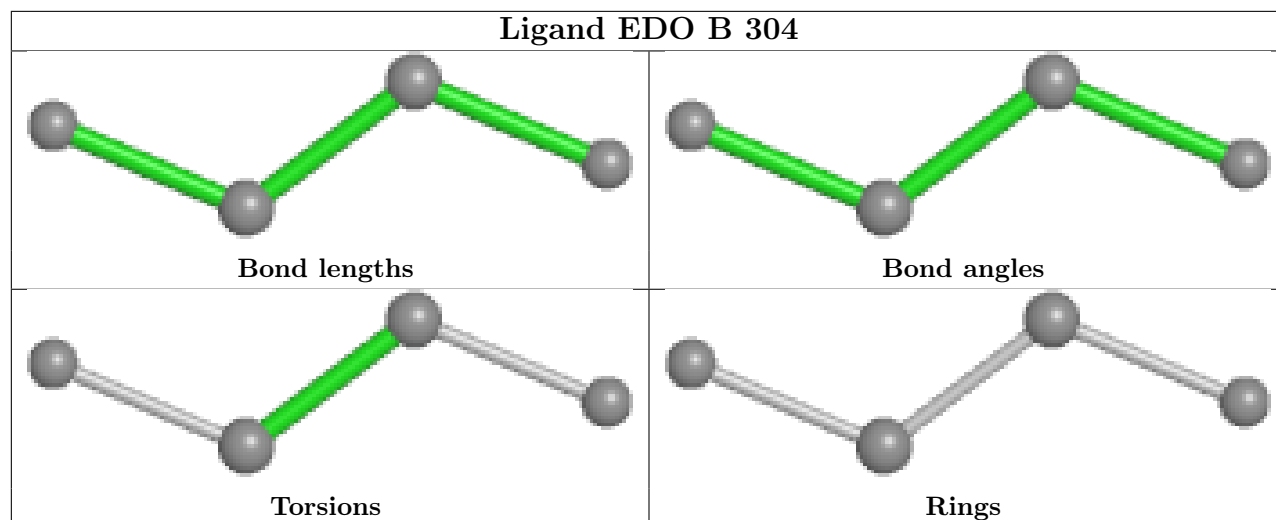




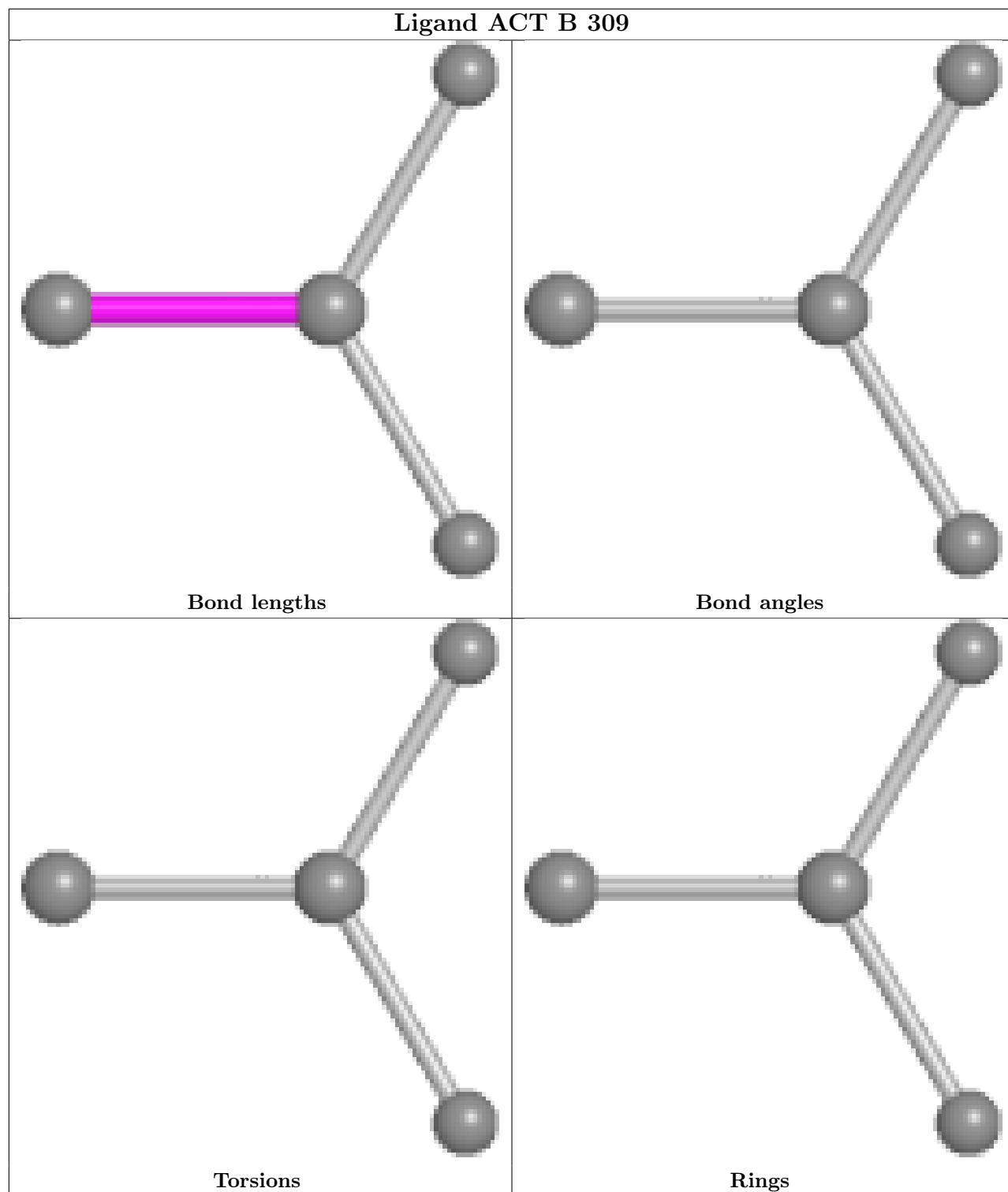


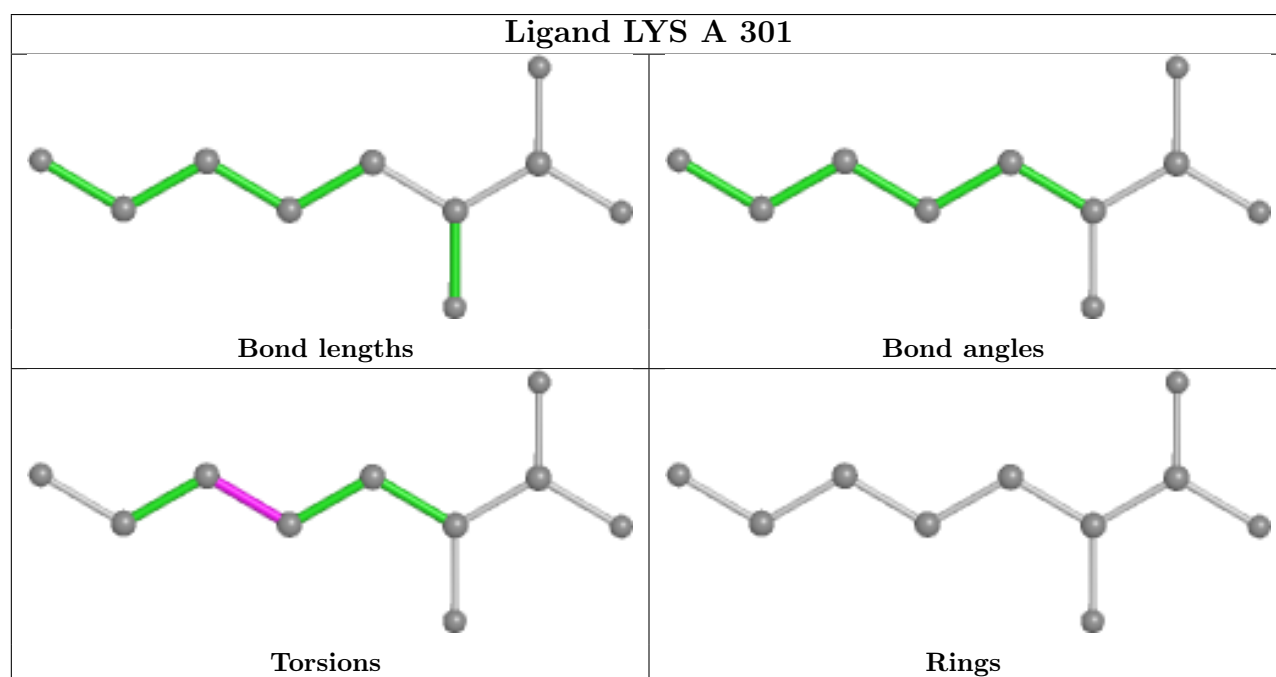
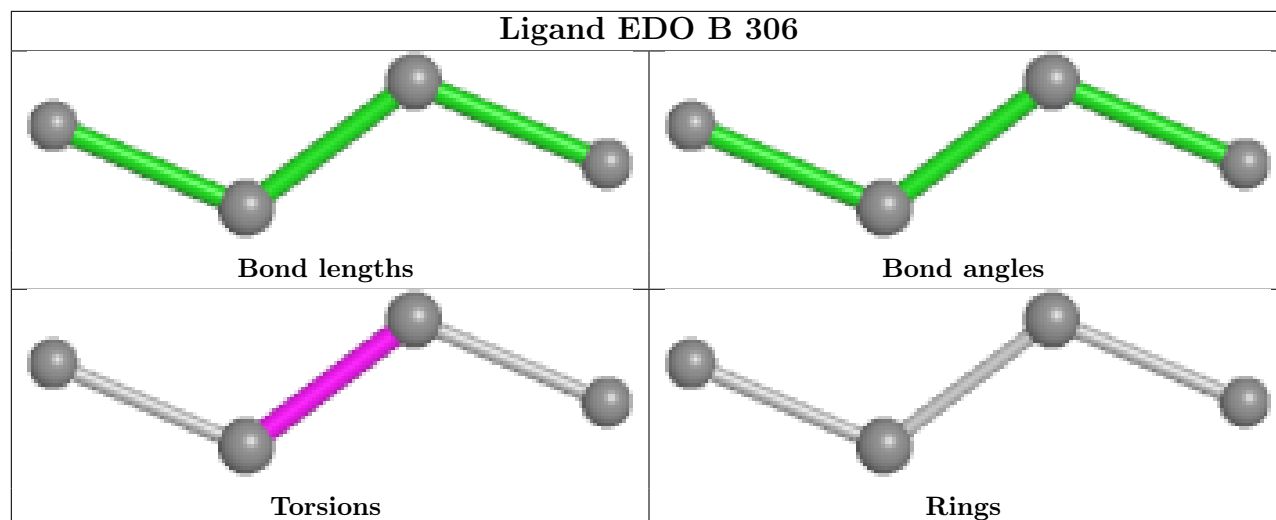


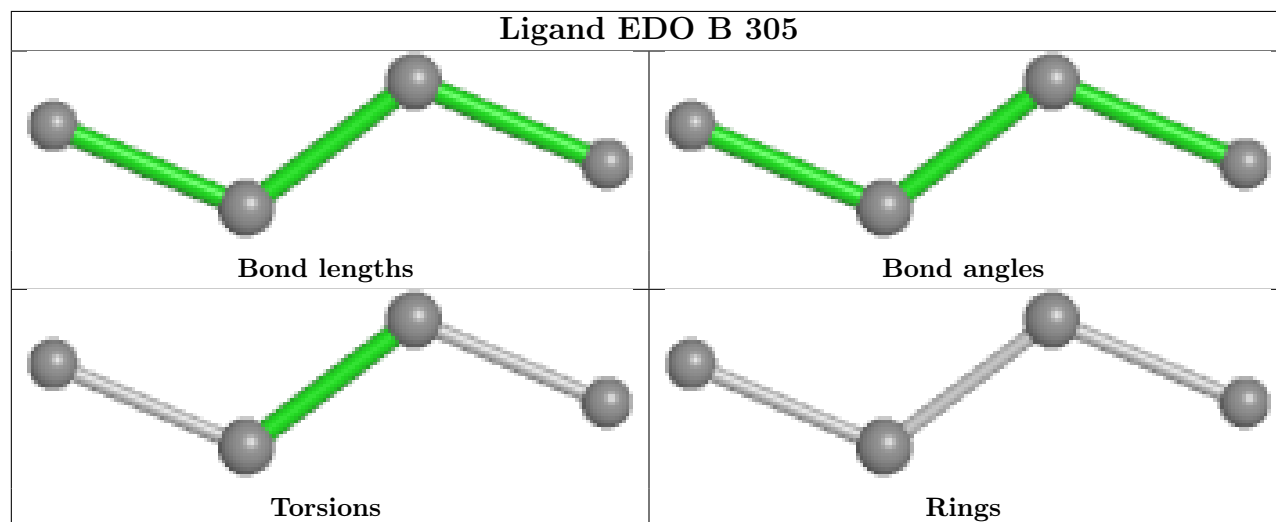
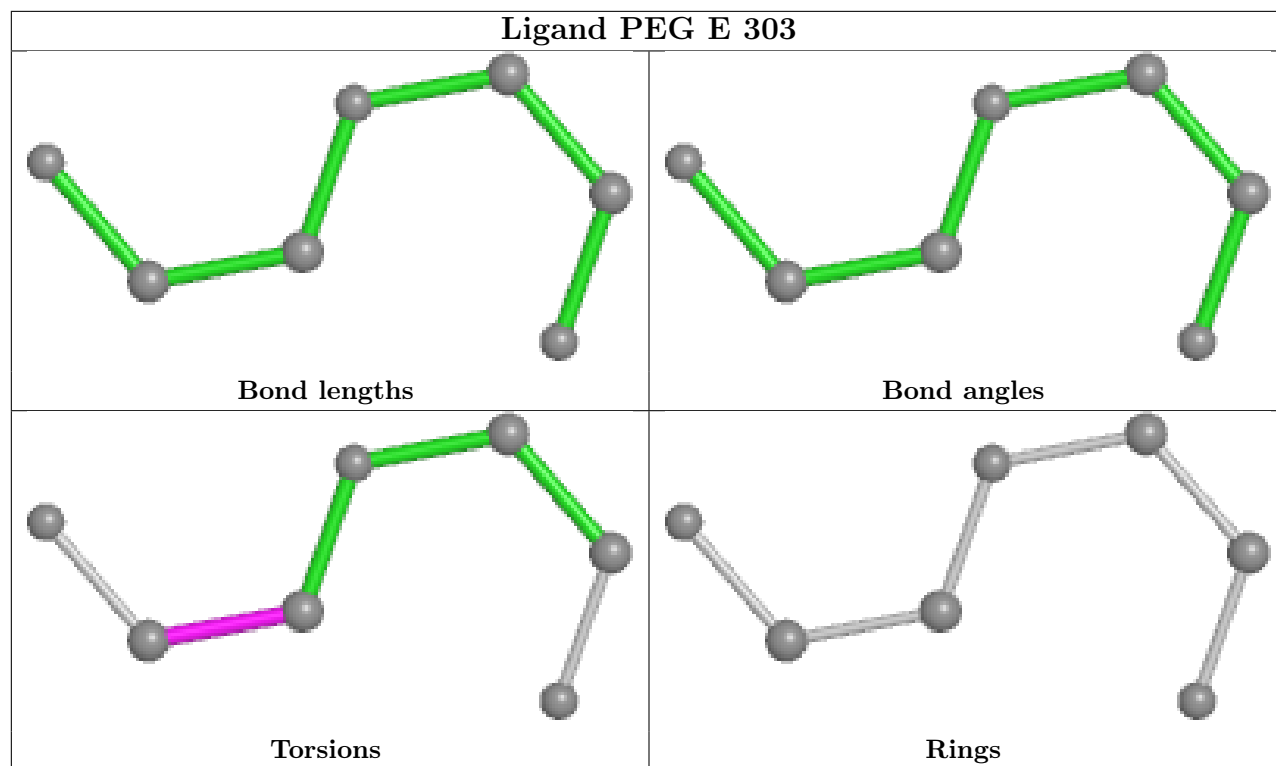


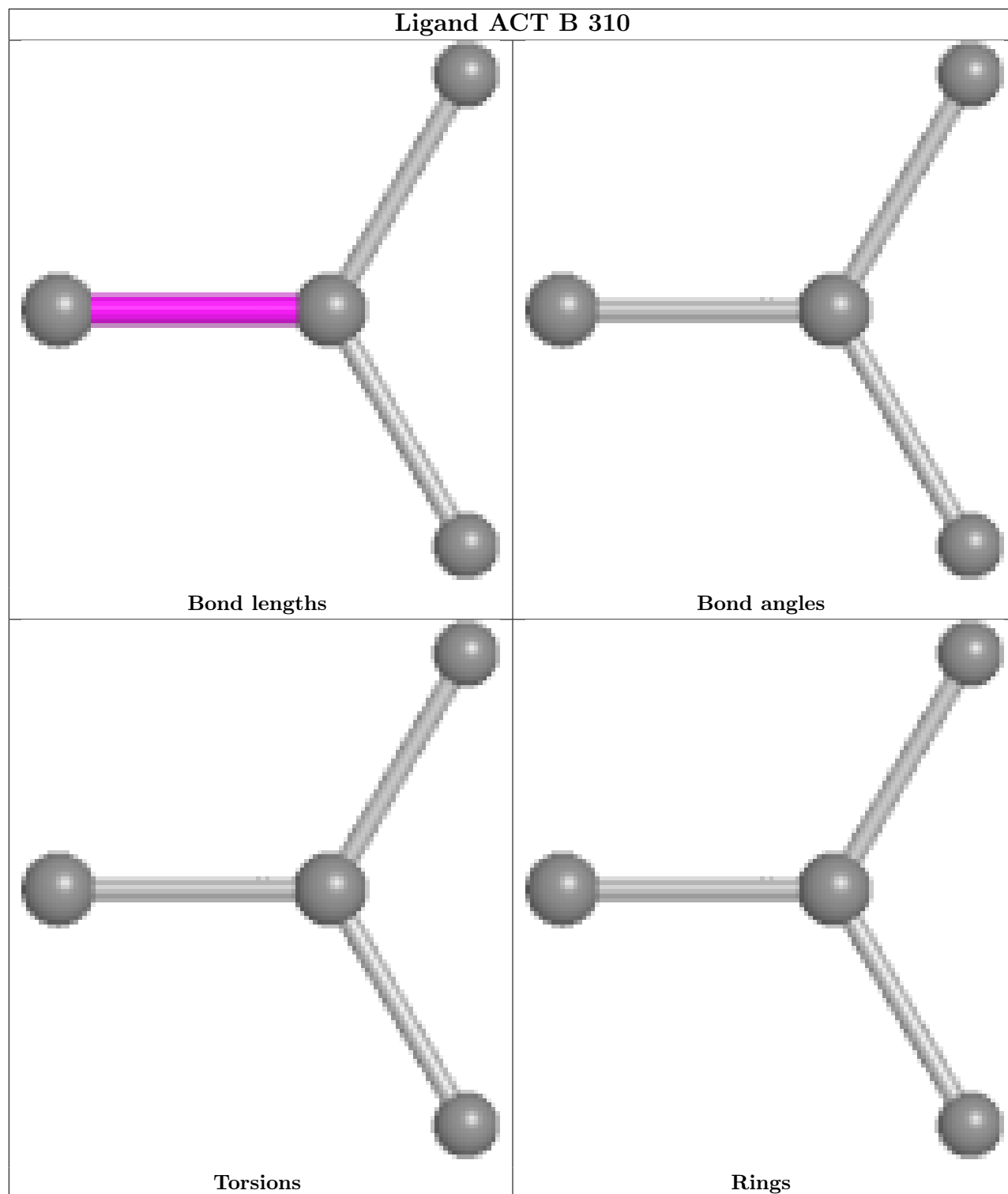


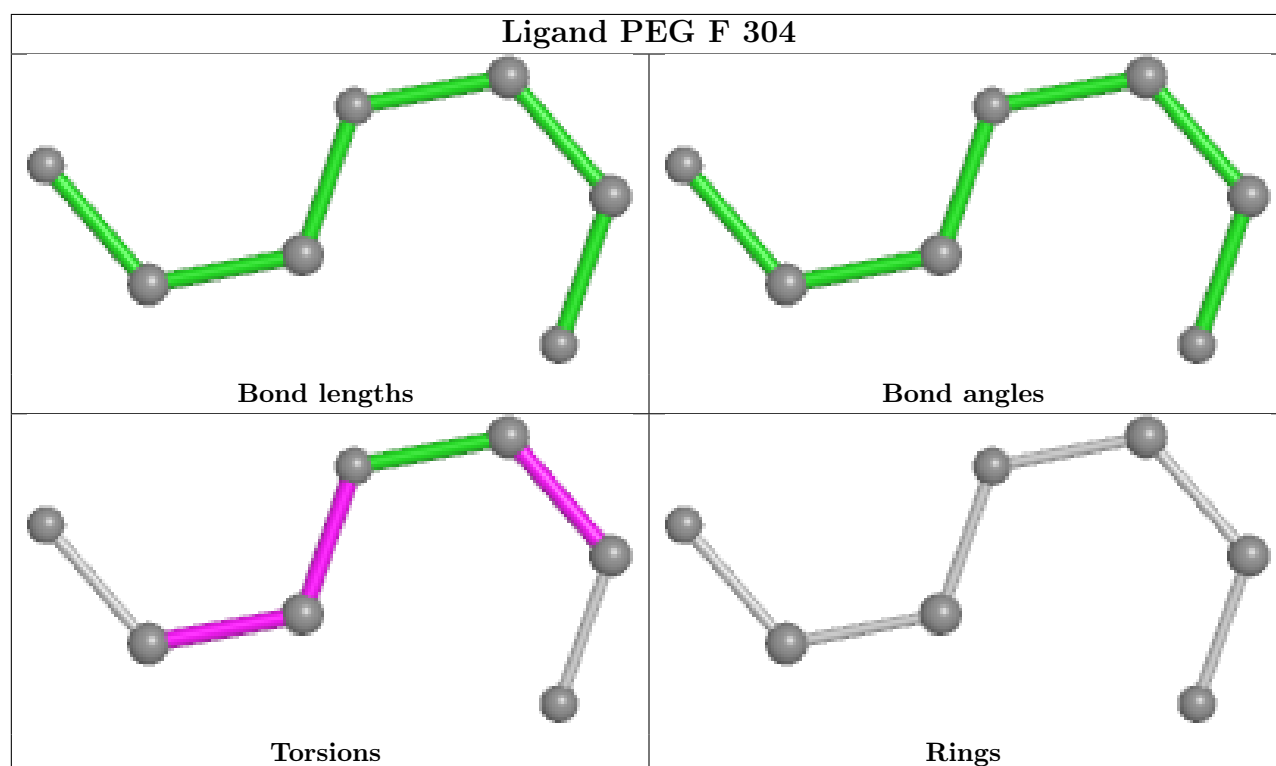
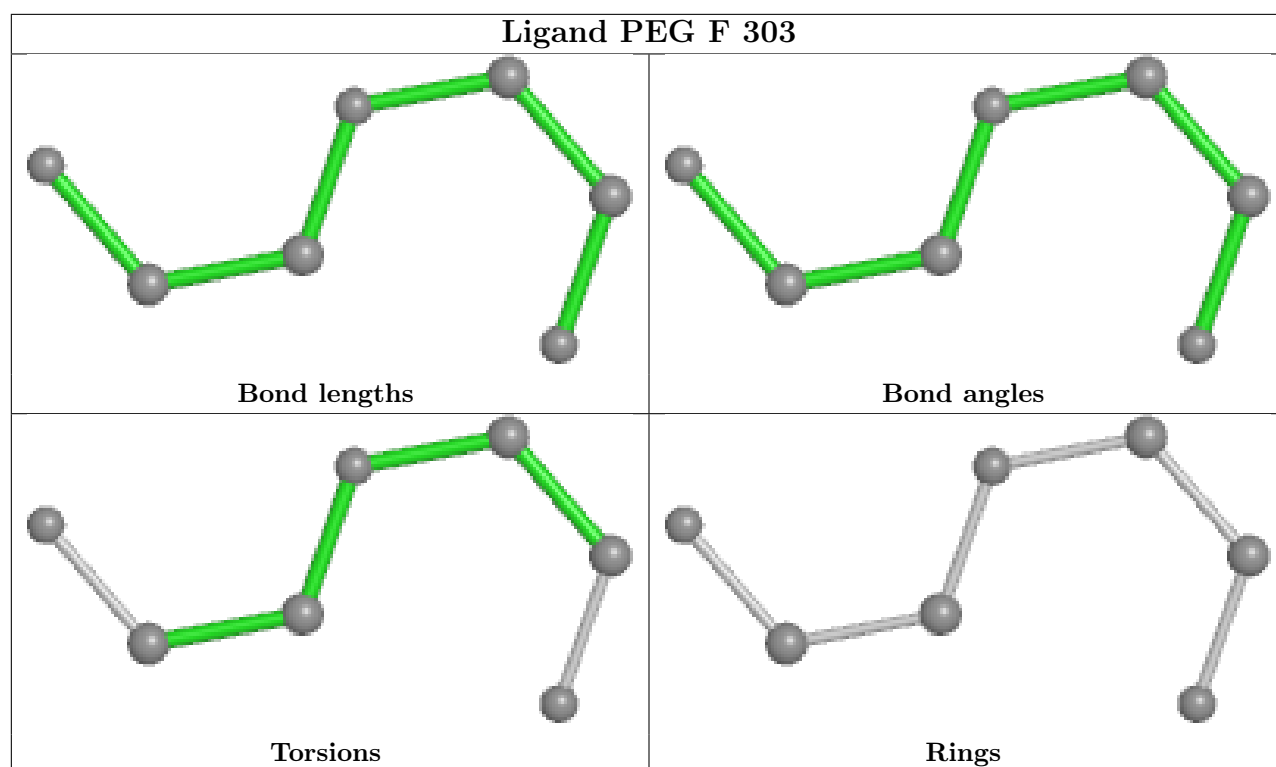




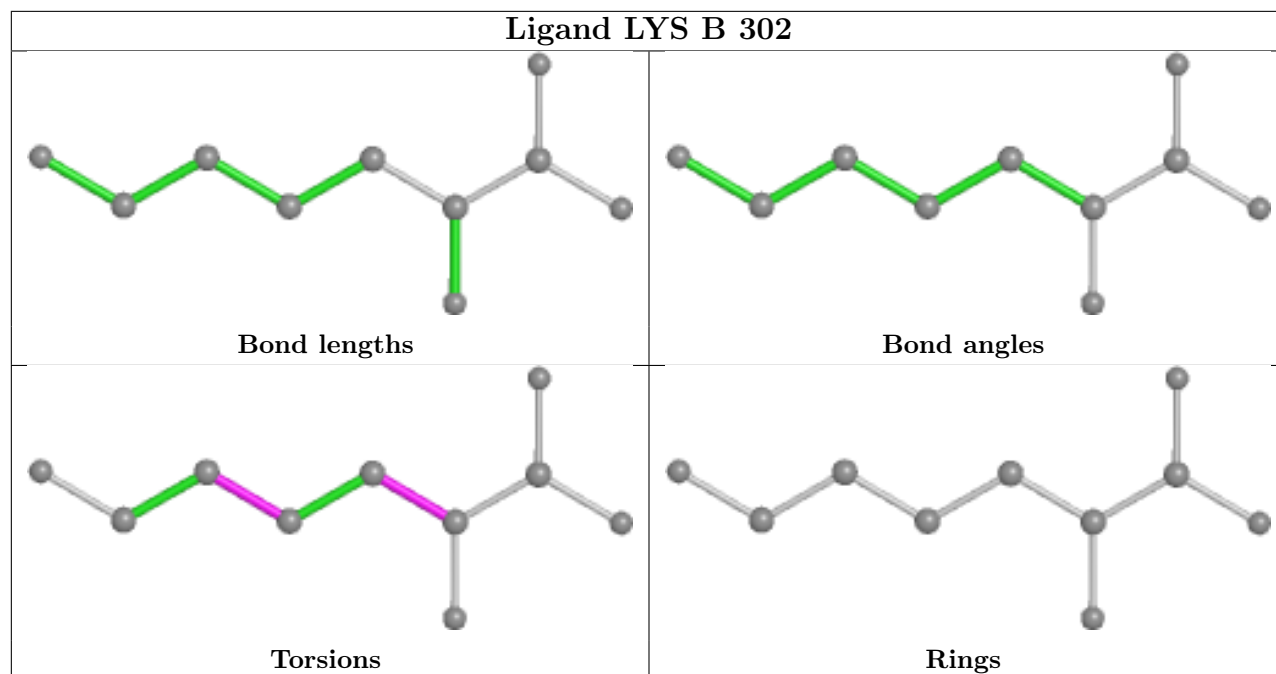




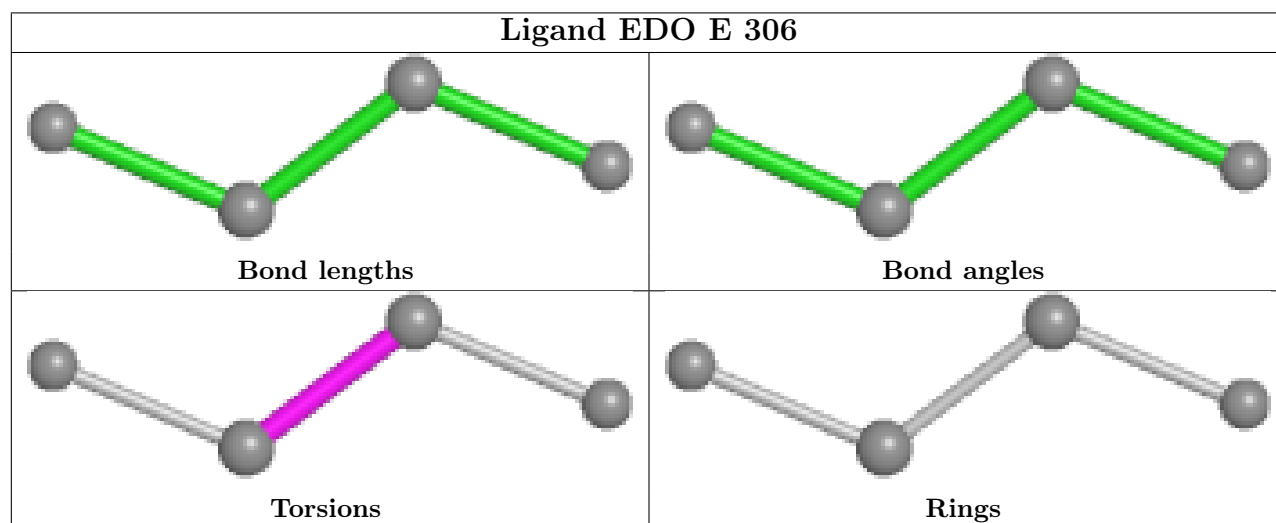


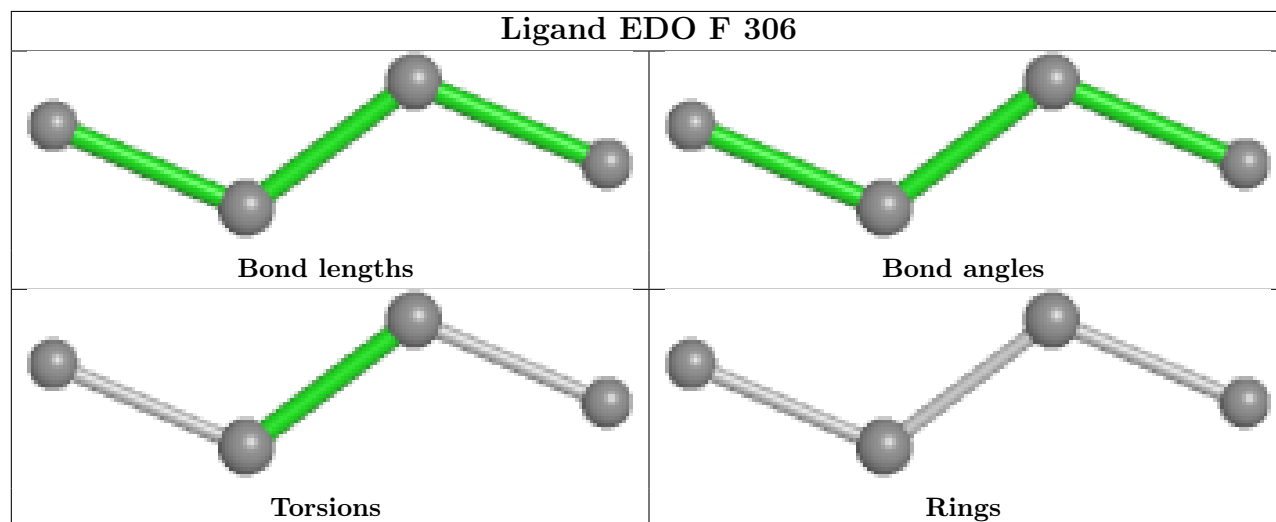
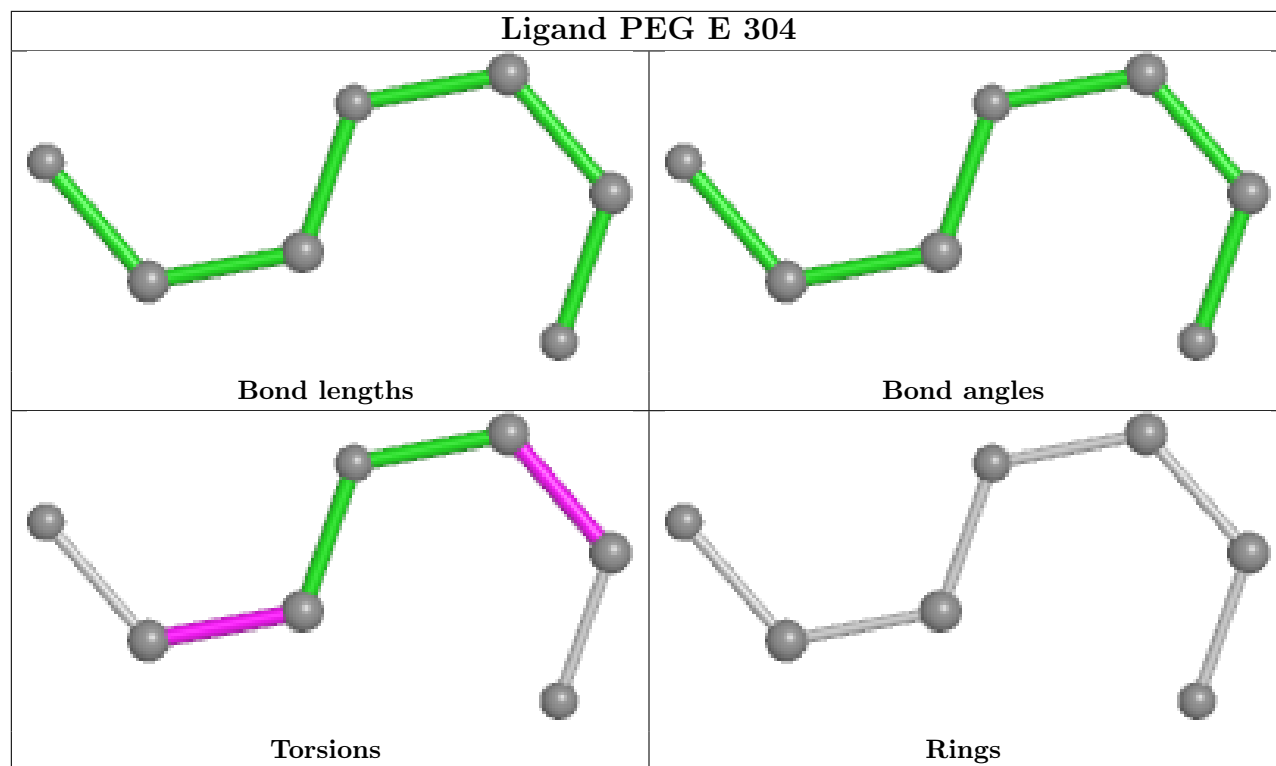


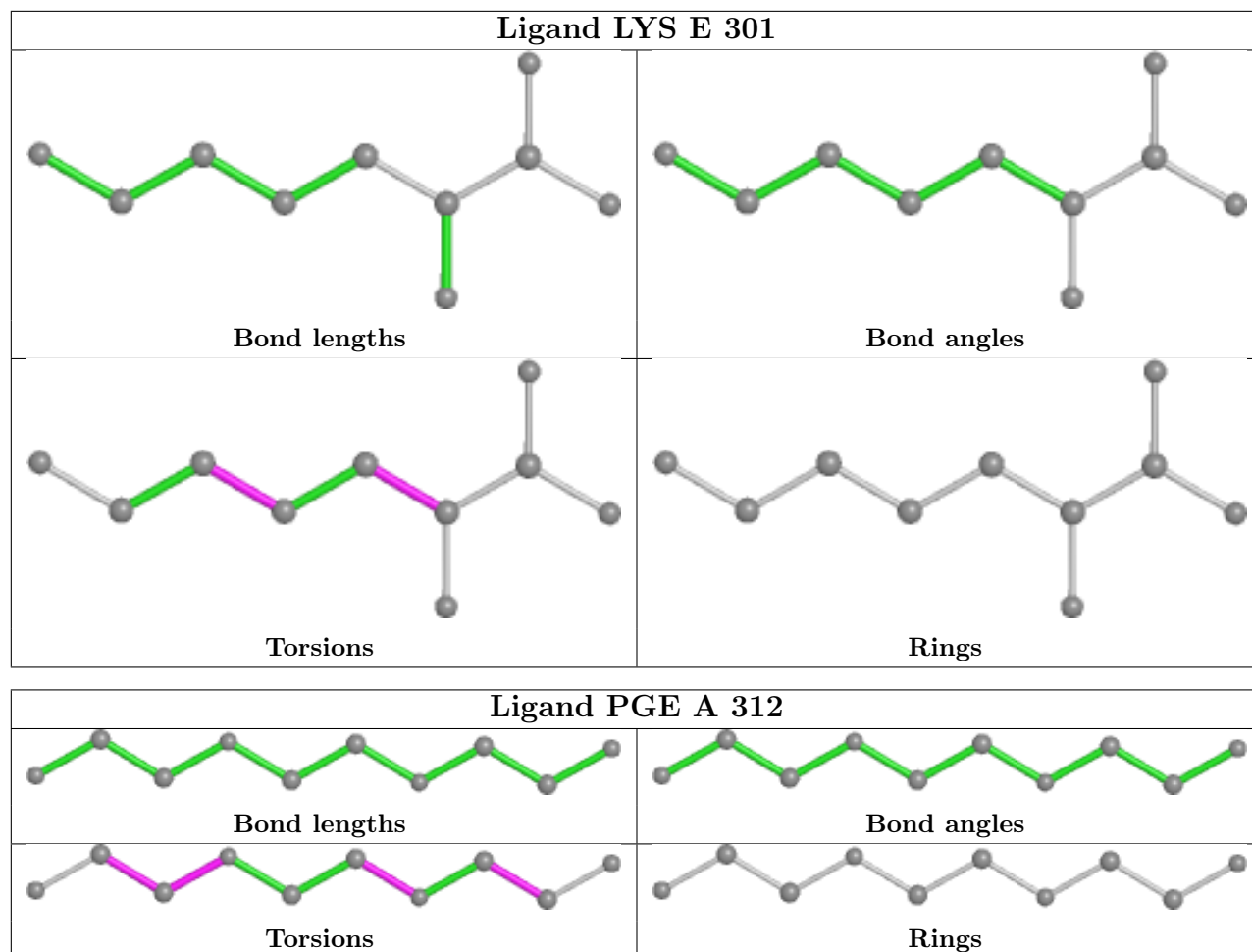
## Ligand LYS B 302



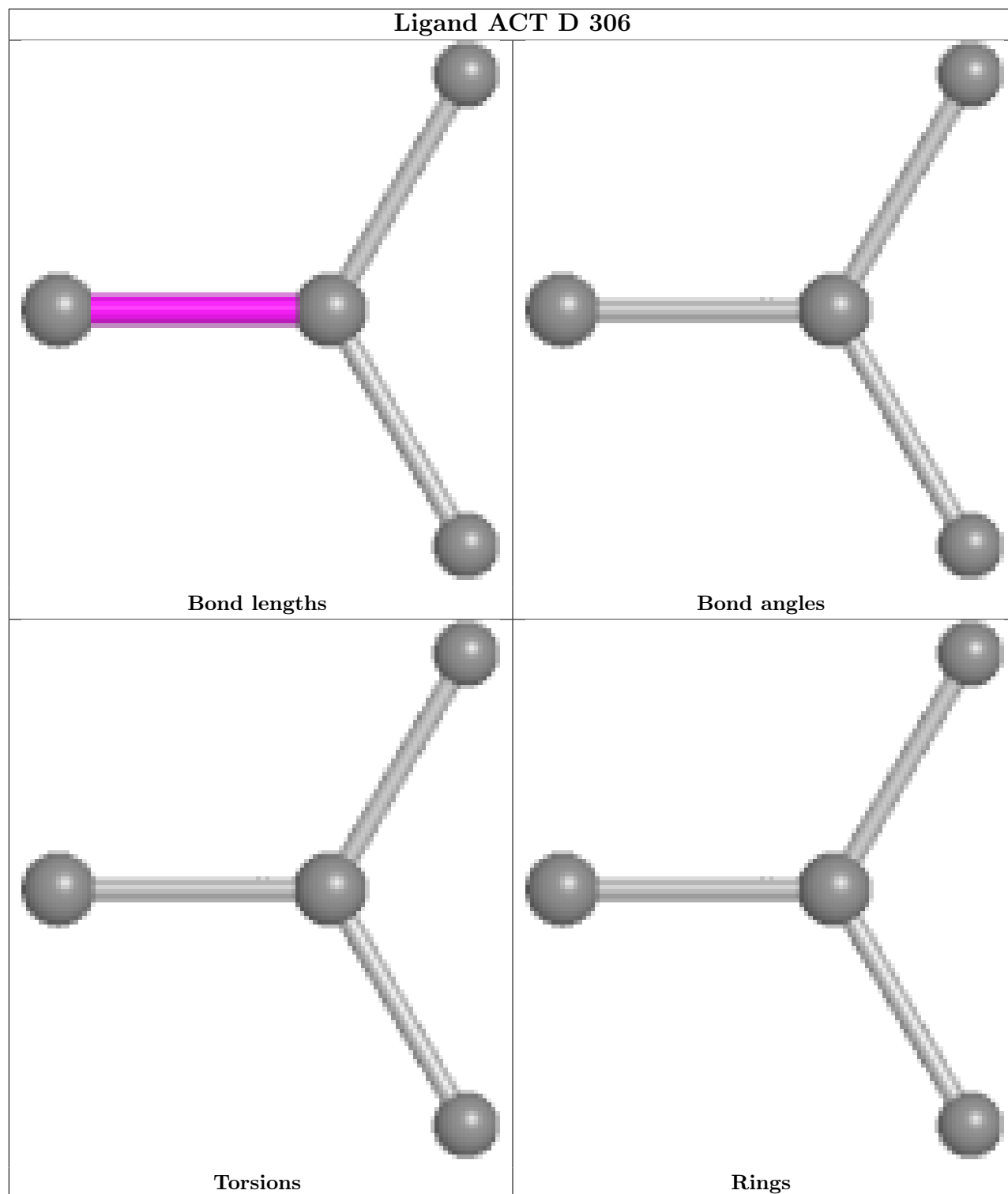
## Ligand EDO E 306

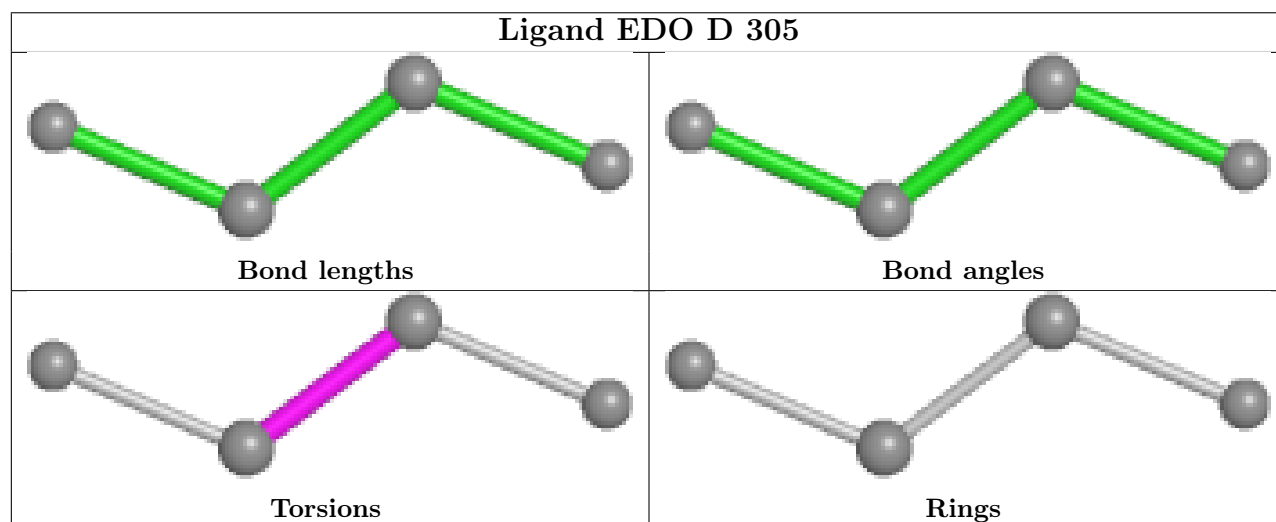
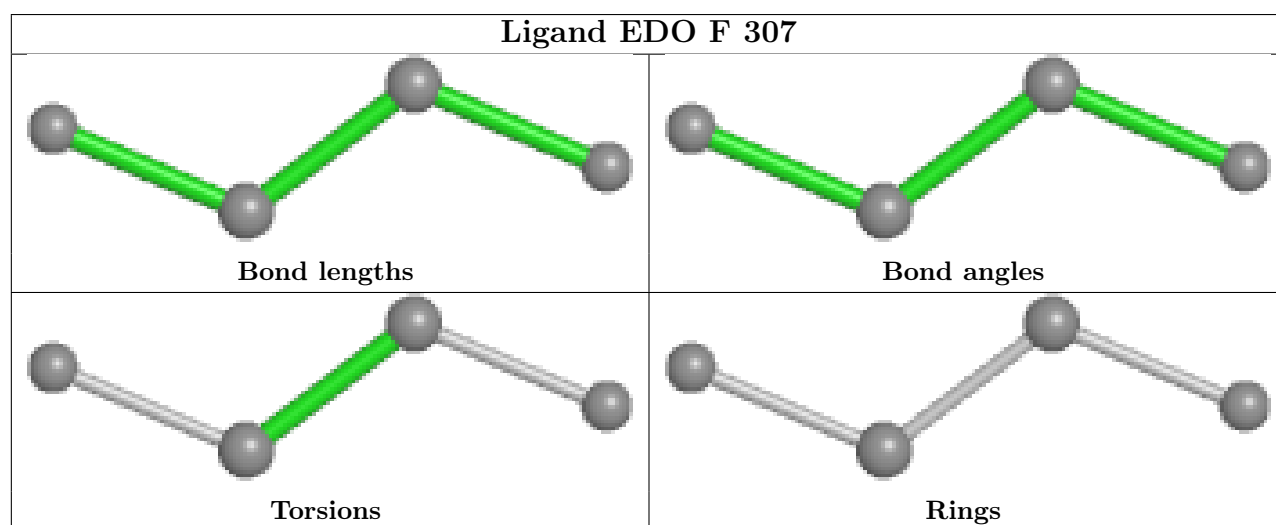
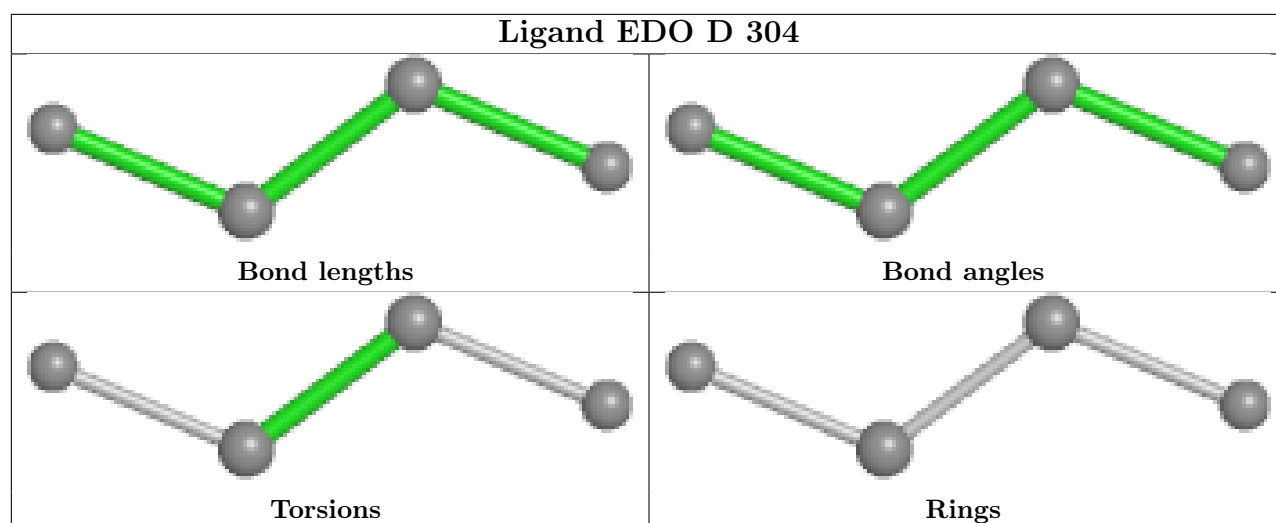


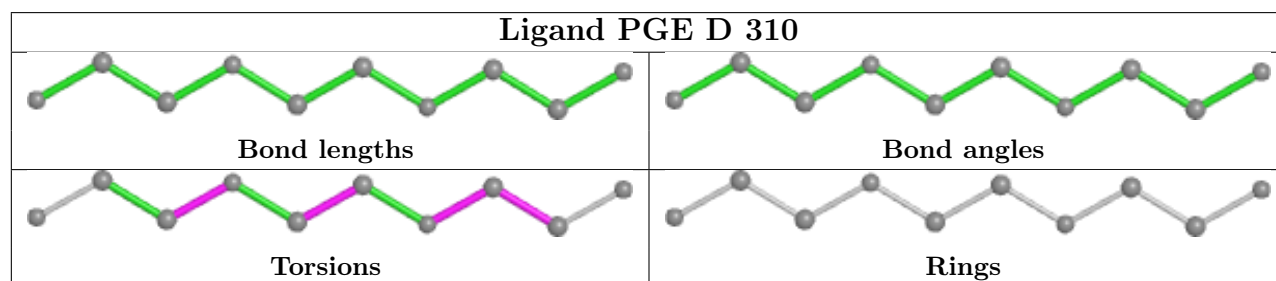
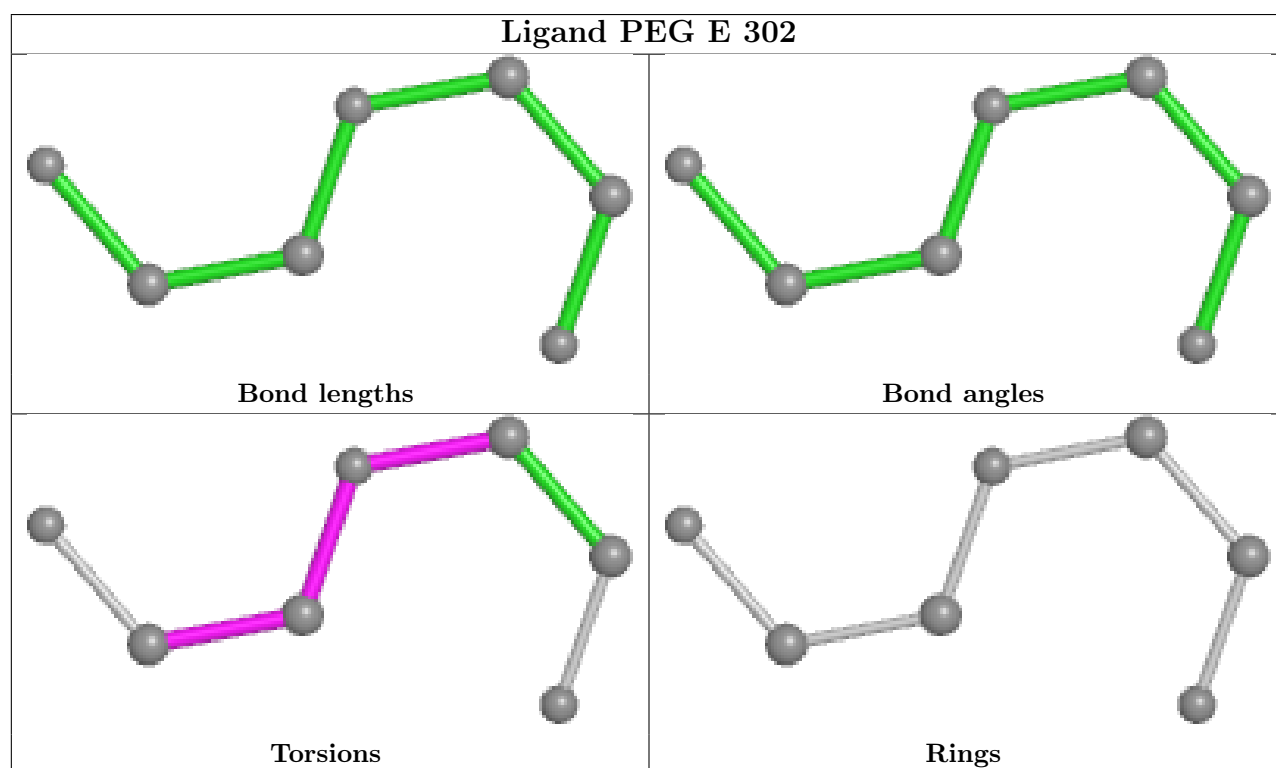
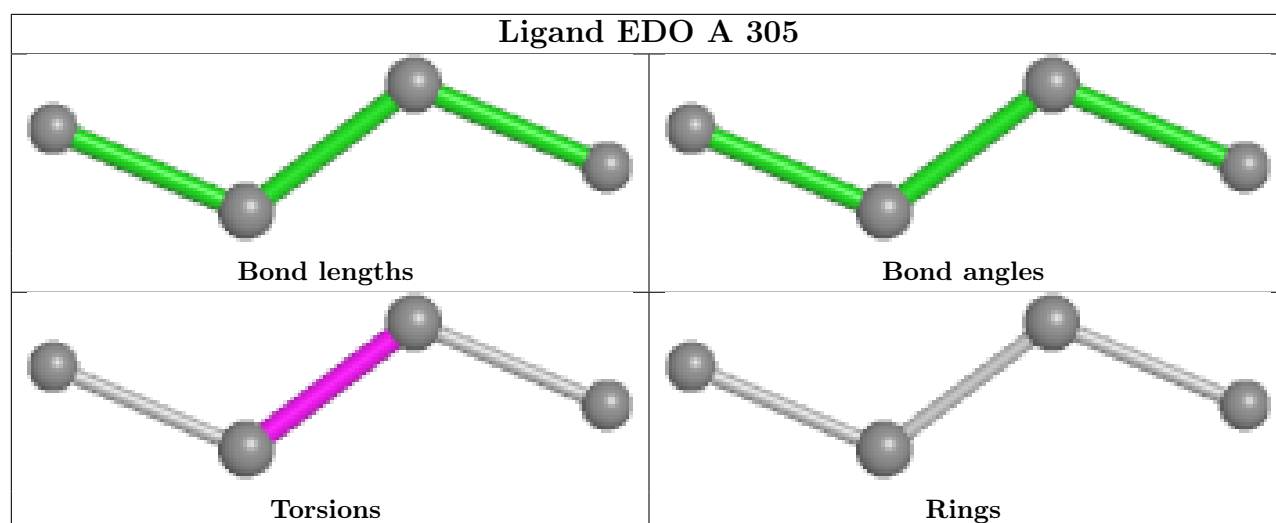


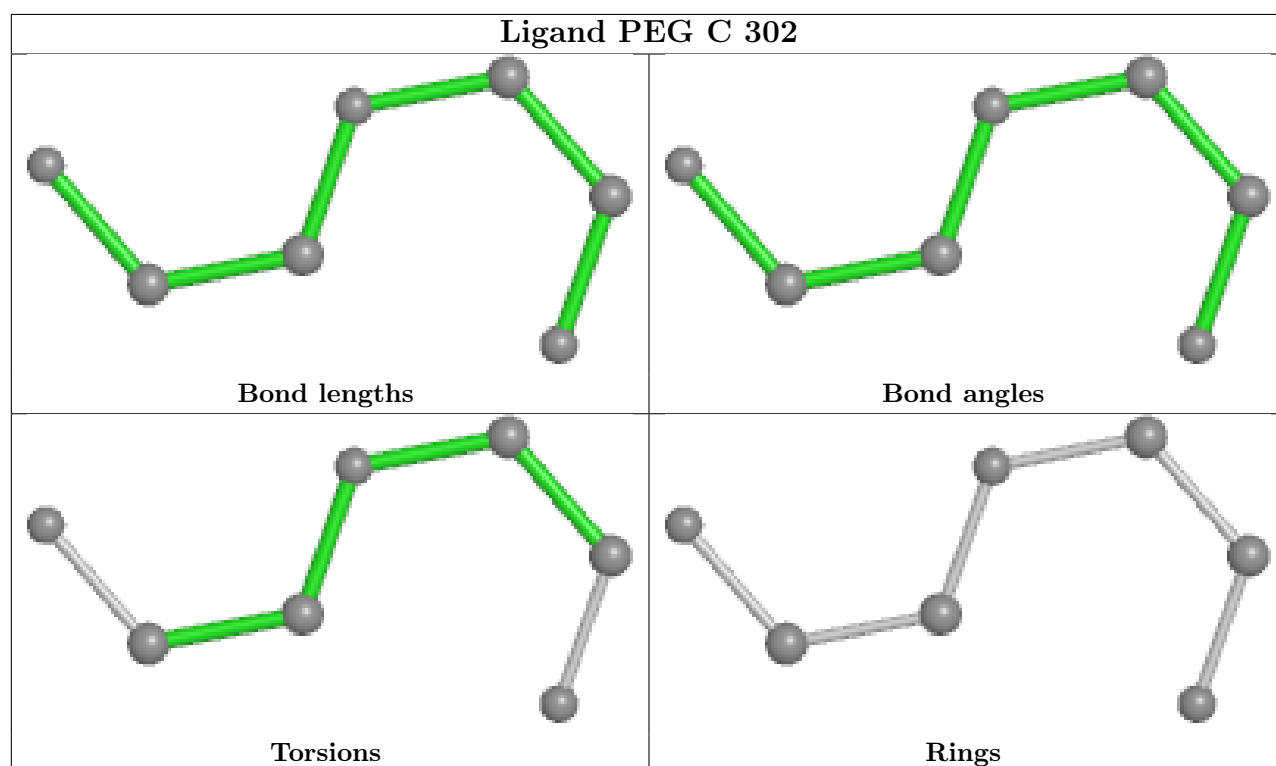
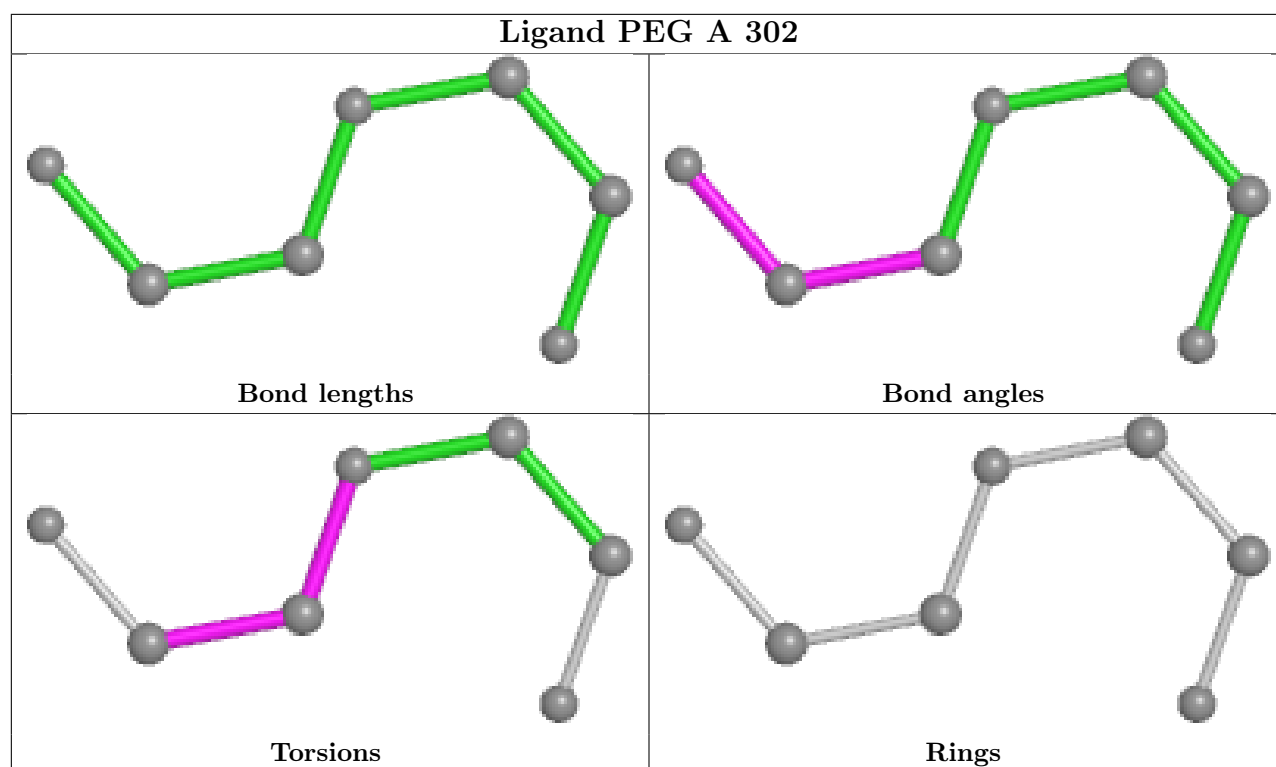


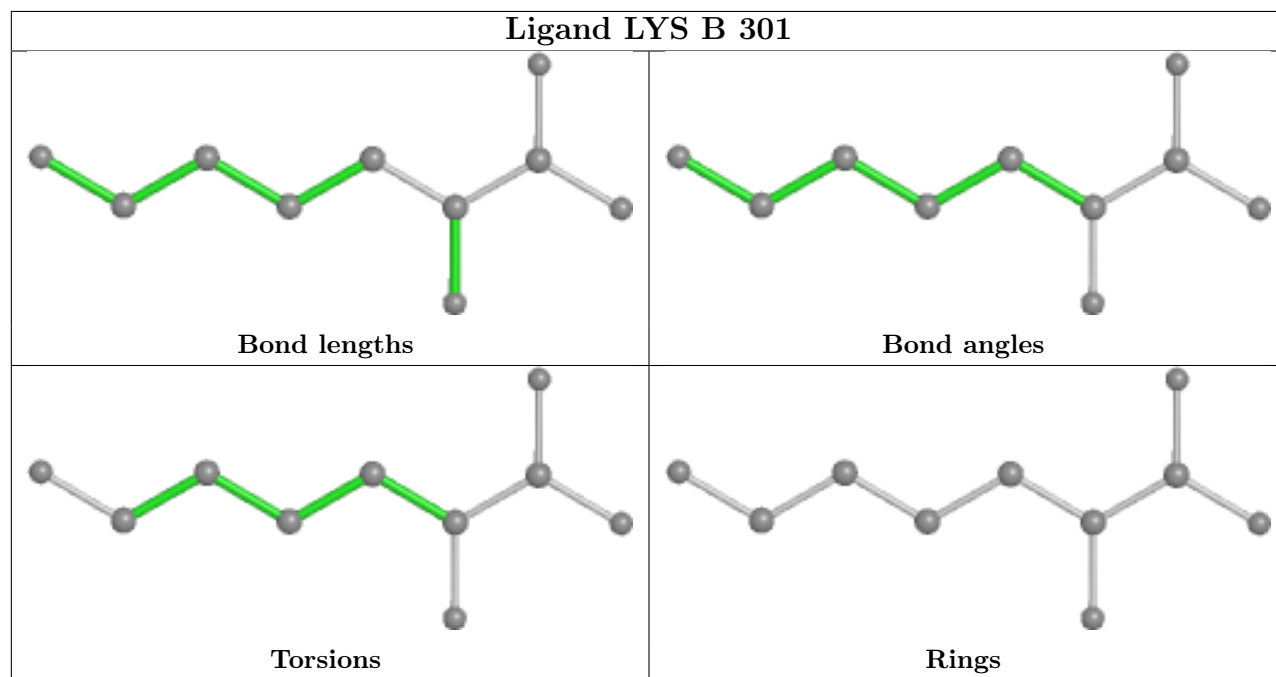
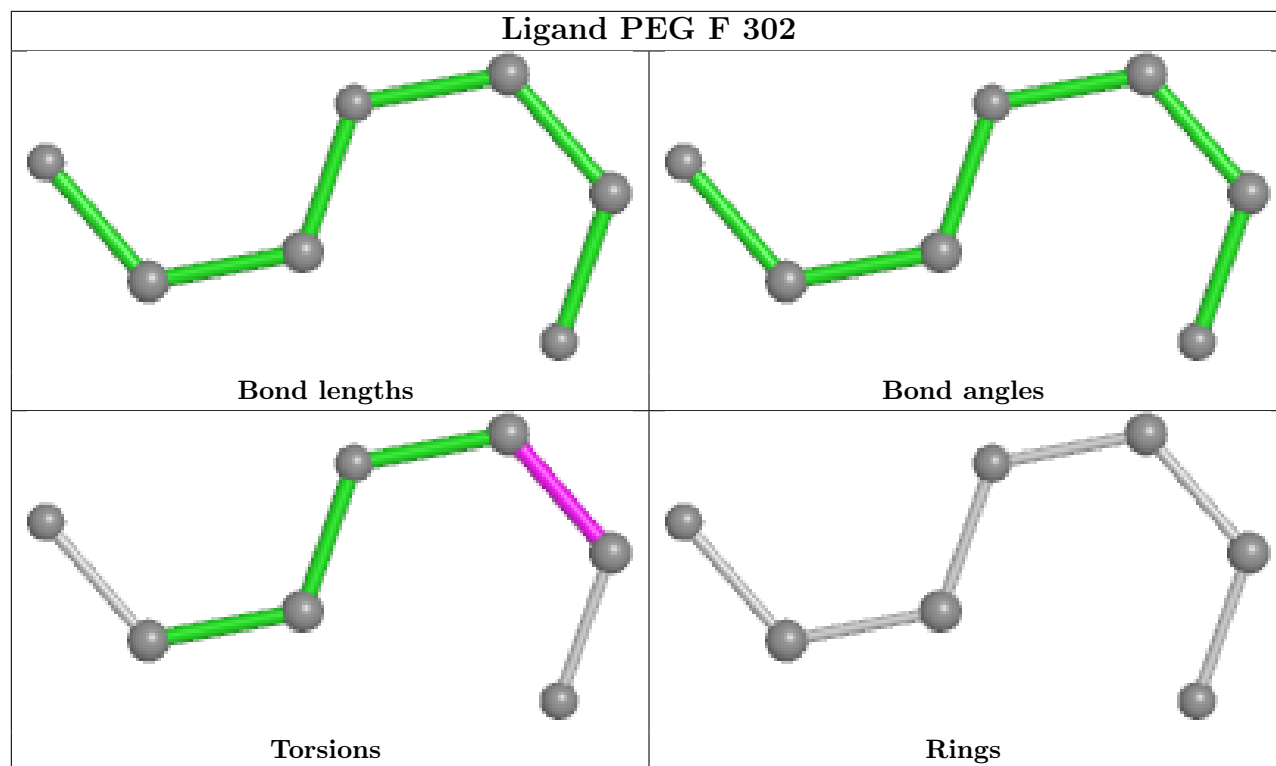


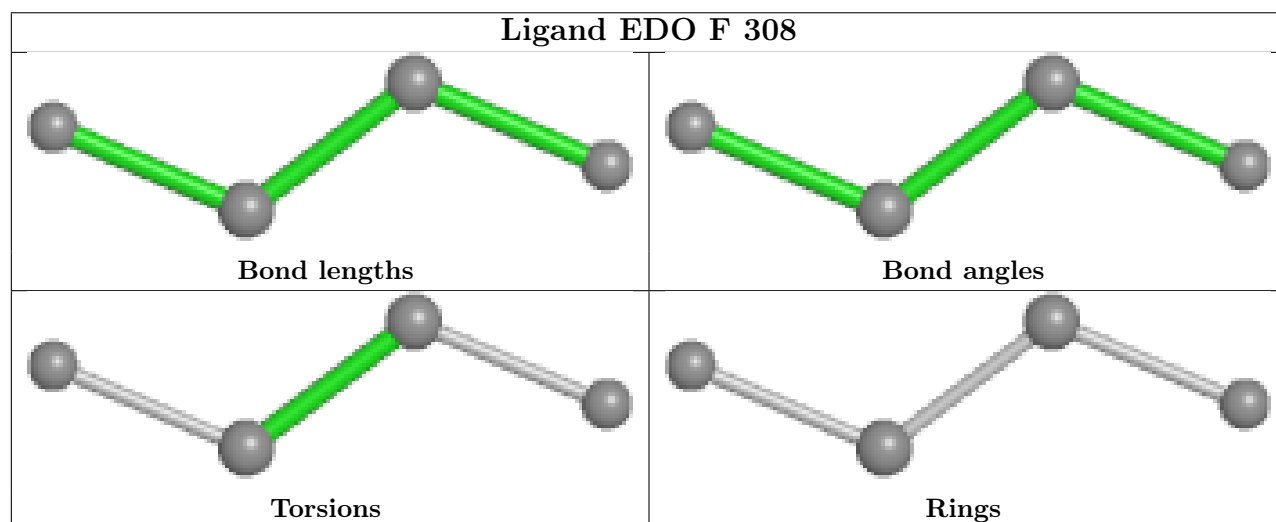
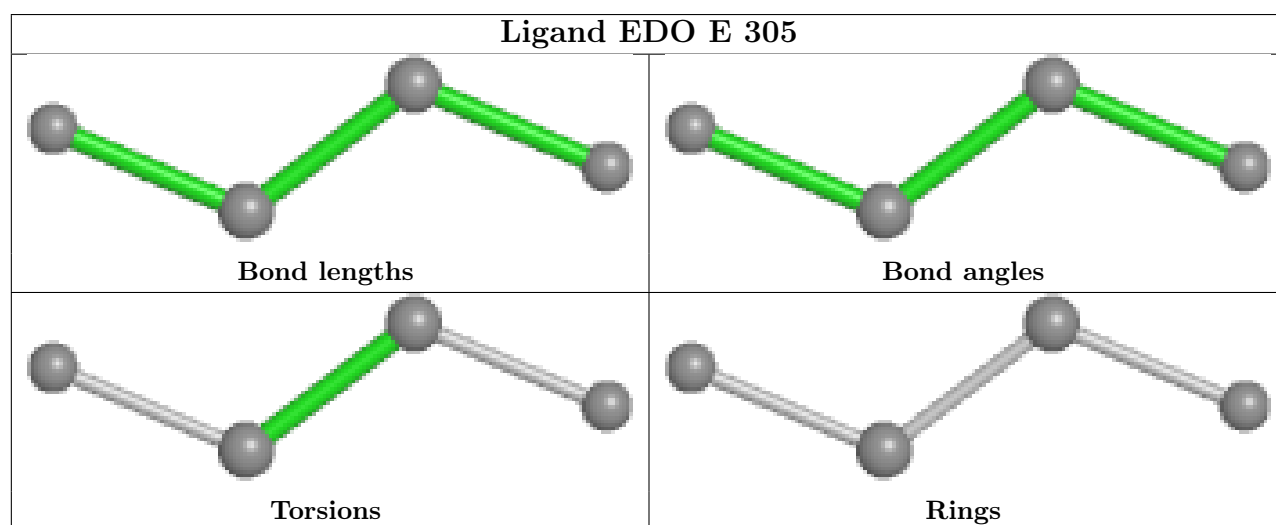
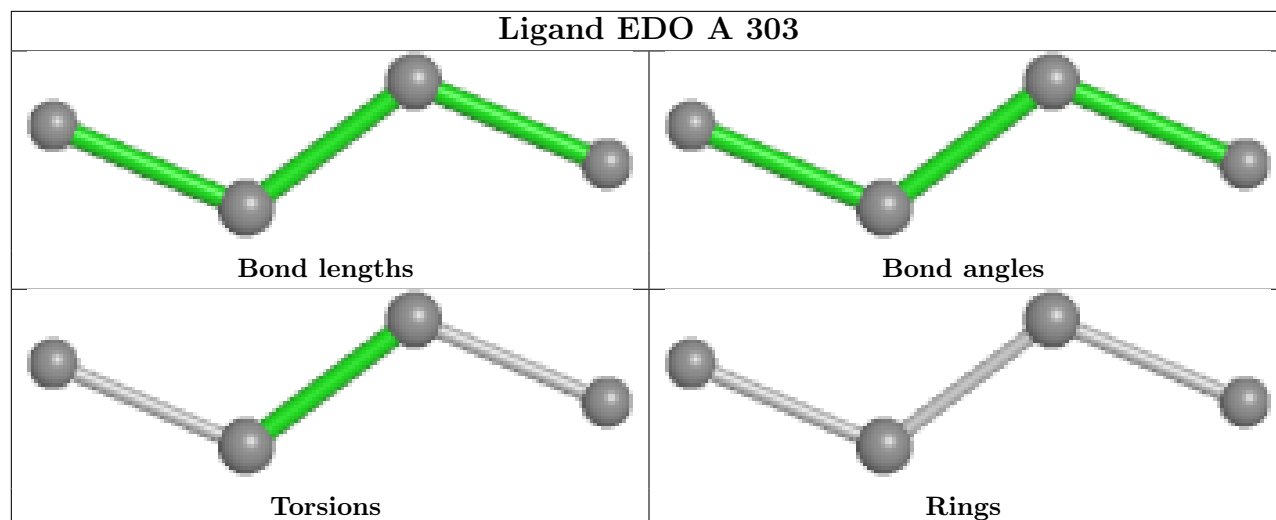


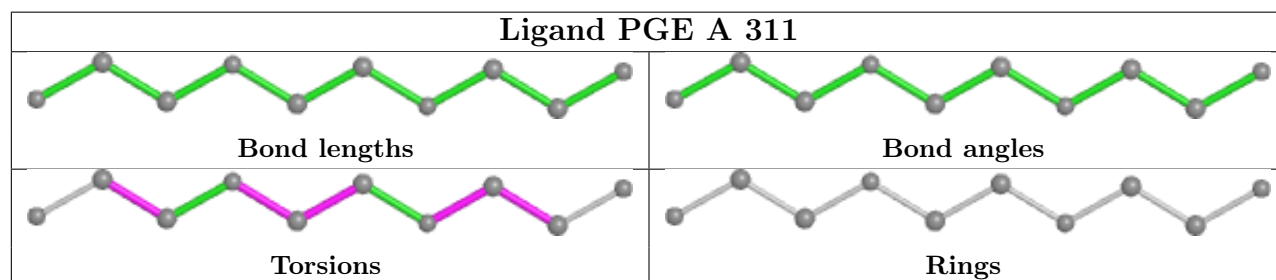
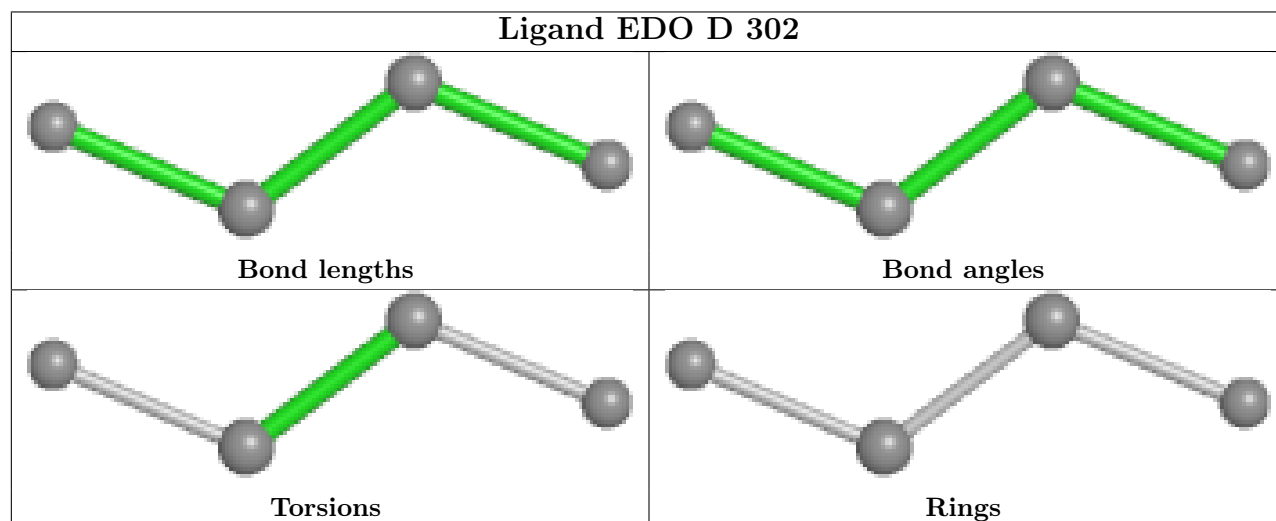
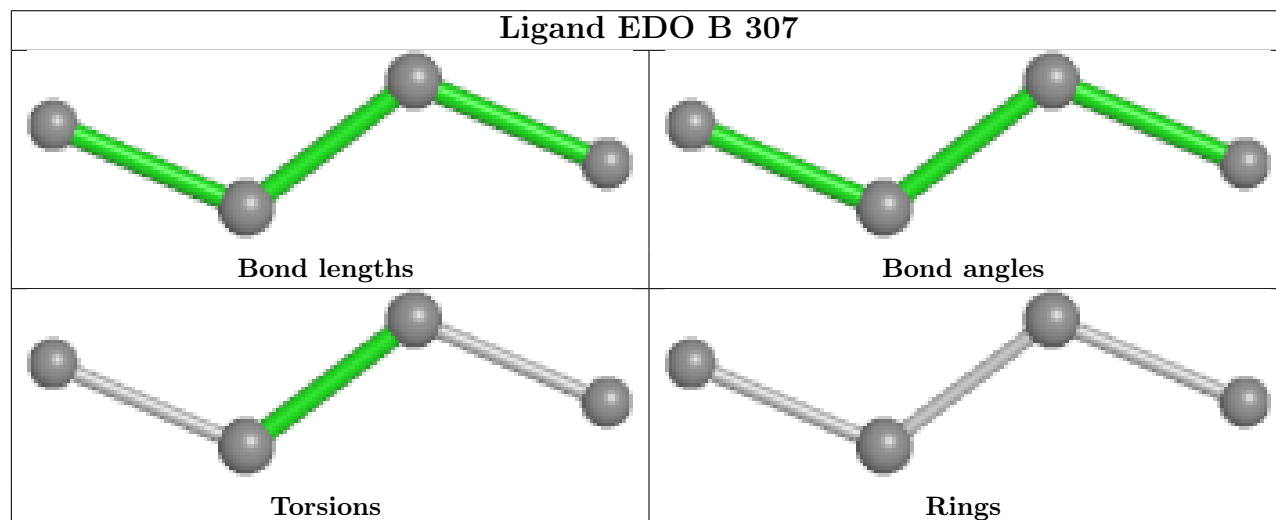
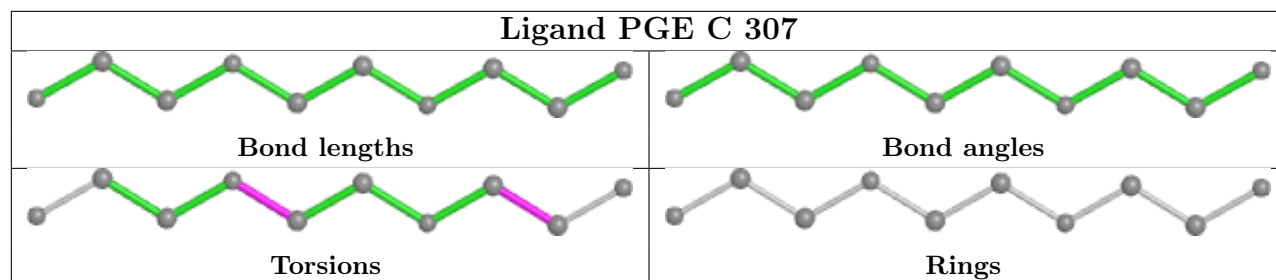


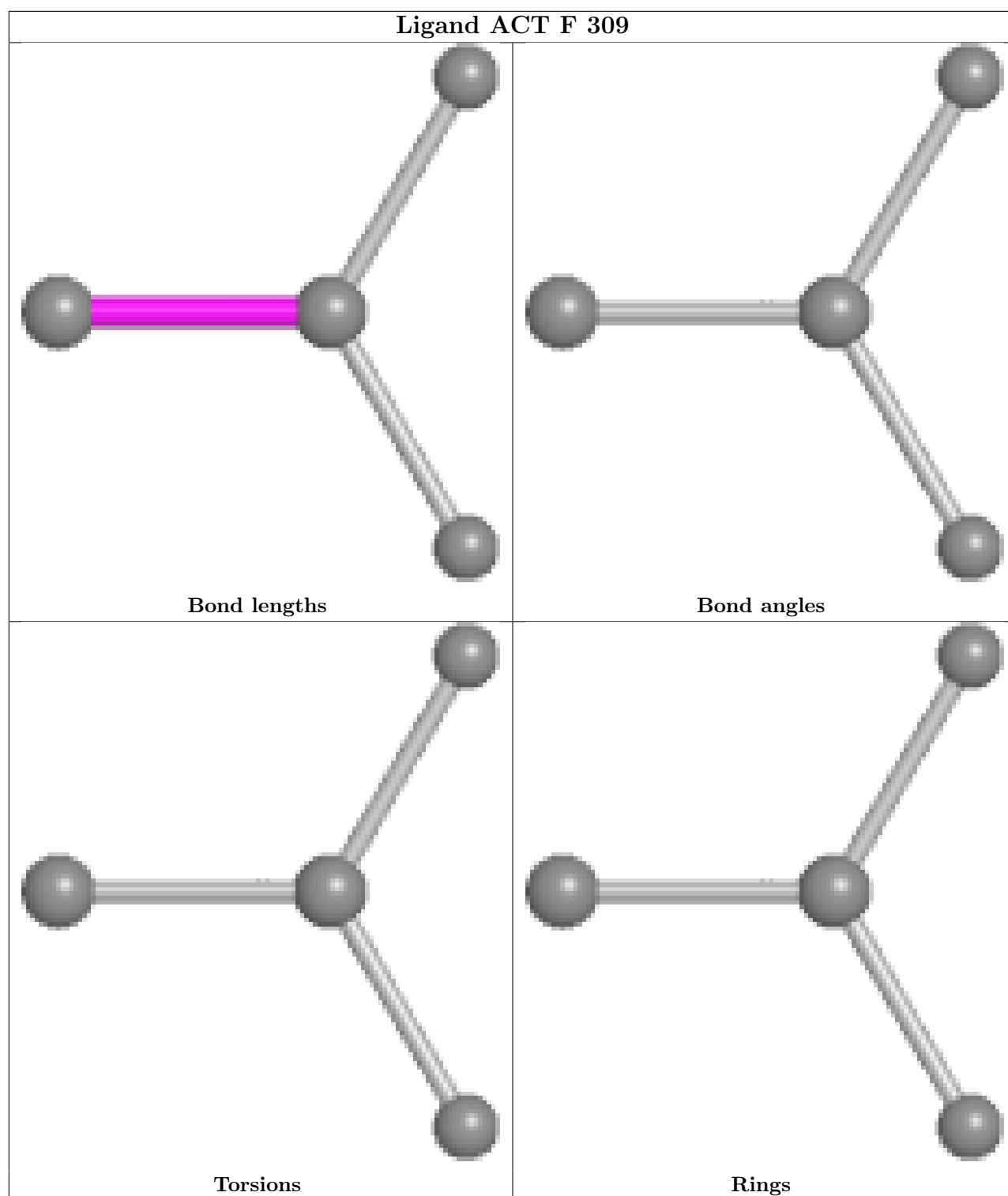




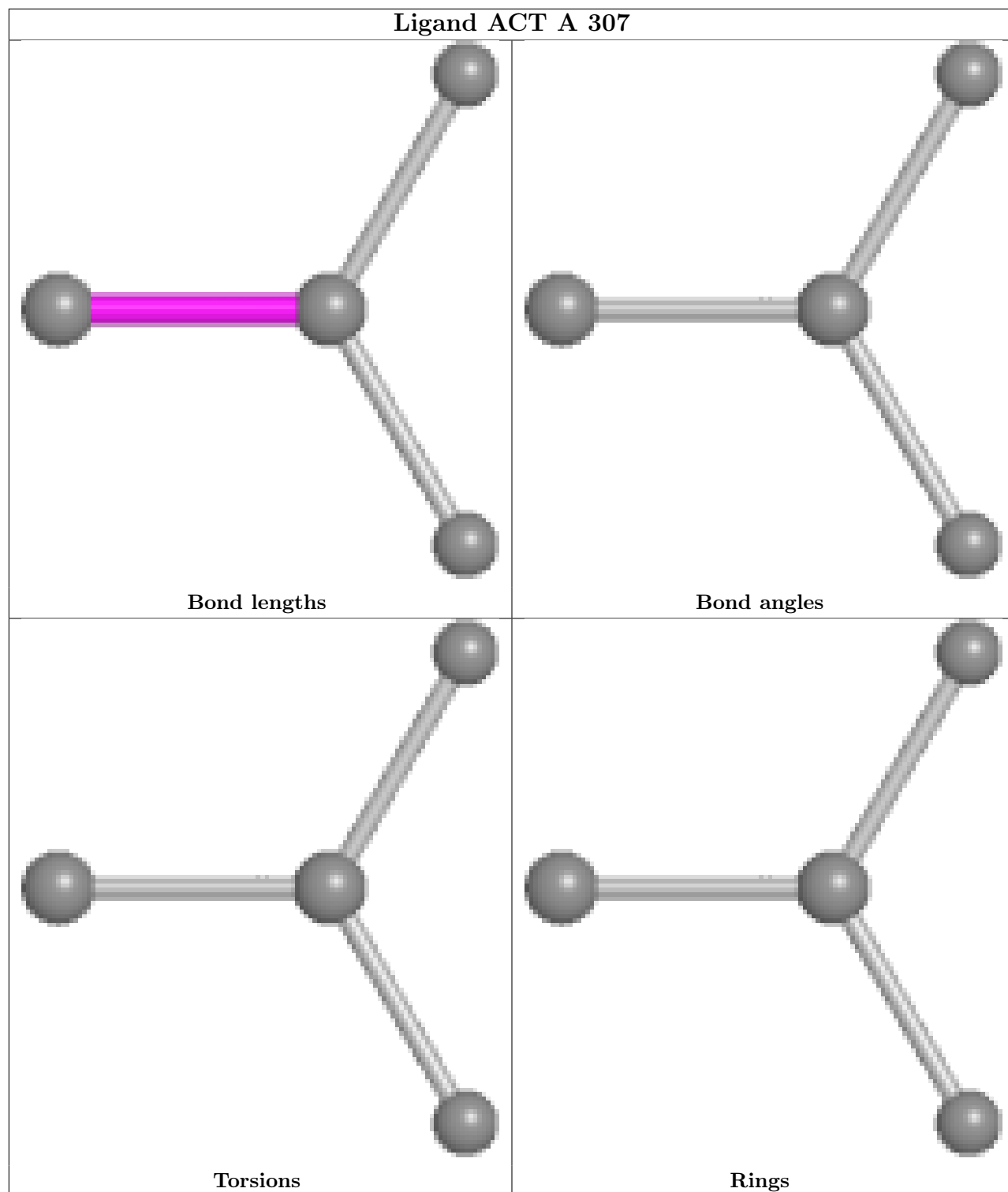


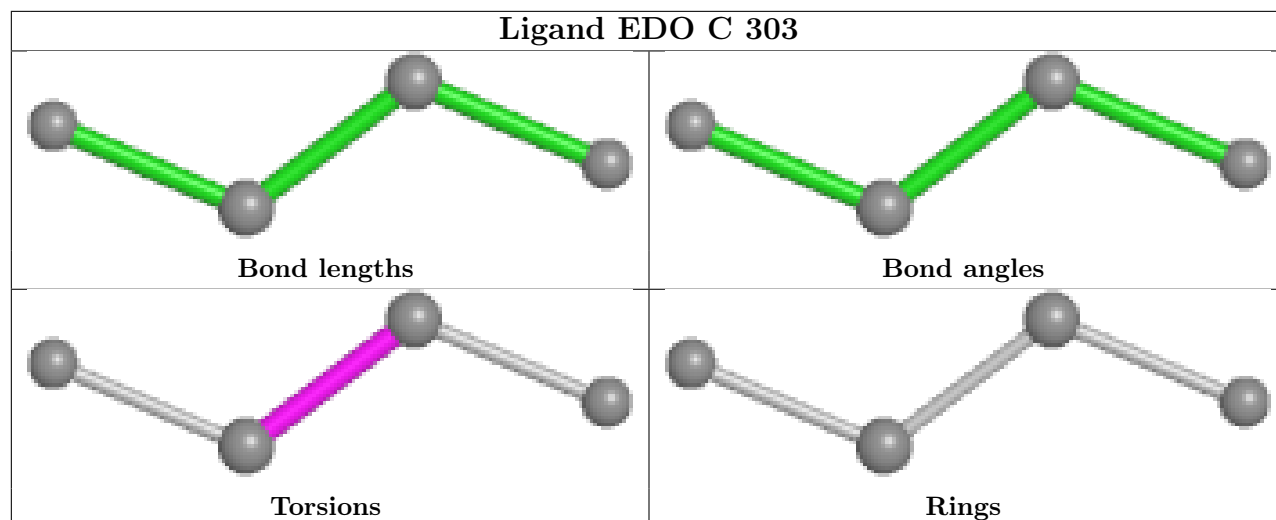












## 5.7 Other polymers [i](#)

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	295/310 (95%)	-0.32	0 100 100	11, 17, 30, 51	0
1	B	296/310 (95%)	-0.35	1 (0%) 94 94	12, 17, 30, 54	0
1	C	305/310 (98%)	-0.32	4 (1%) 77 79	12, 18, 34, 58	0
1	D	305/310 (98%)	-0.31	2 (0%) 87 88	12, 18, 32, 47	0
1	F	295/310 (95%)	-0.21	2 (0%) 87 88	13, 19, 35, 50	0
2	E	296/310 (95%)	-0.28	0 100 100	14, 19, 33, 56	0
All	All	1792/1860 (96%)	-0.30	9 (0%) 91 91	11, 18, 33, 58	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ASP	3.5
1	C	20	GLY	2.7
1	F	288	GLU	2.4
1	D	-6	HIS	2.2
1	C	-6	HIS	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(Å <sup>2</sup> )	Q<0.9
1	KPI	A	166	14/15	0.78	0.22	13,20,26,27	0
1	KPI	D	166	14/15	0.78	0.18	12,15,25,25	0
1	KPI	F	166	14/15	0.80	0.21	16,21,29,31	0
1	KPI	C	166	14/15	0.81	0.19	14,21,32,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KPI	B	166	14/15	0.83	0.18	13,19,29,30	0

### 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
5	EDO	D	303	4/4	0.35	0.58	62,63,63,63	0
5	EDO	D	304	4/4	0.35	0.52	66,66,66,66	0
5	EDO	F	305	4/4	0.47	0.54	66,66,66,66	0
6	ACT	F	309	4/4	0.47	0.33	61,61,62,62	0
4	PEG	F	302	7/7	0.50	0.62	63,63,64,64	0
4	PEG	C	302	7/7	0.55	0.40	63,63,63,64	0
5	EDO	A	305	4/4	0.55	0.35	34,35,35,36	0
5	EDO	F	306	4/4	0.59	0.34	57,57,57,57	0
4	PEG	C	301	7/7	0.62	0.34	60,60,63,63	0
8	PGE	A	312	10/10	0.62	0.26	49,50,51,51	0
5	EDO	A	303	4/4	0.65	0.22	55,55,55,55	0
5	EDO	C	303	4/4	0.65	0.36	40,40,42,42	0
9	GOL	A	313	6/6	0.65	0.21	31,32,33,33	0
5	EDO	B	307	4/4	0.66	0.29	52,52,52,52	0
4	PEG	E	303	7/7	0.70	0.30	41,43,46,47	0
4	PEG	F	303	7/7	0.71	0.27	64,64,64,65	0
6	ACT	B	310	4/4	0.72	0.34	61,61,61,62	0
6	ACT	B	311	4/4	0.73	0.31	47,48,48,48	0
6	ACT	C	305	4/4	0.74	0.42	20,20,20,20	0
8	PGE	E	310	10/10	0.75	0.35	57,58,59,59	0
5	EDO	D	302	4/4	0.80	0.23	41,41,41,41	0
4	PEG	E	302	7/7	0.80	0.23	49,49,49,49	0
5	EDO	B	305	4/4	0.81	0.21	42,42,43,43	0
6	ACT	B	312	4/4	0.82	0.27	58,58,58,59	0
5	EDO	F	308	4/4	0.82	0.39	45,45,45,45	0
5	EDO	E	306	4/4	0.83	0.20	45,45,45,45	0
5	EDO	A	306	4/4	0.83	0.25	42,42,42,42	0

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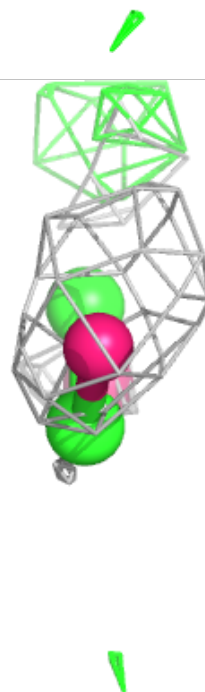
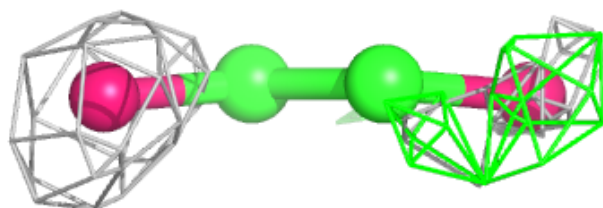
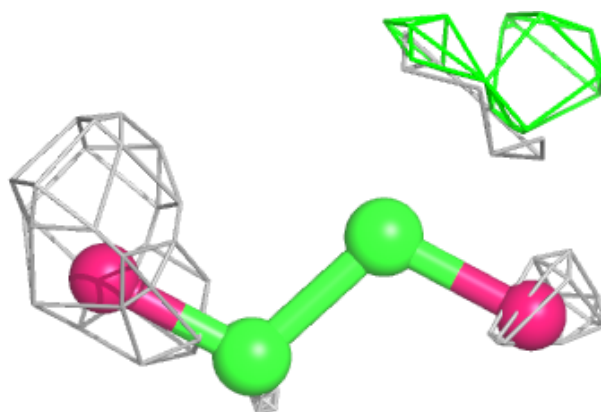
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	D	305	4/4	0.83	0.18	33,34,35,35	0
5	EDO	C	304	4/4	0.84	0.18	26,28,28,29	0
5	EDO	A	304	4/4	0.85	0.24	42,42,42,43	0
6	ACT	D	306	4/4	0.85	0.37	49,49,49,50	0
3	LYS	F	301	10/10	0.86	0.21	16,18,29,32	0
5	EDO	B	306	4/4	0.86	0.44	44,44,45,45	0
6	ACT	A	307	4/4	0.87	0.28	51,51,51,51	0
5	EDO	F	307	4/4	0.87	0.16	52,52,52,52	0
4	PEG	B	303	7/7	0.88	0.17	41,42,44,45	0
3	LYS	D	301	10/10	0.88	0.17	19,21,24,24	0
6	ACT	B	309	4/4	0.88	0.20	52,53,53,53	0
3	LYS	A	301	10/10	0.89	0.20	20,22,23,23	0
8	PGE	D	310	10/10	0.89	0.20	33,37,44,46	0
3	LYS	E	301	10/10	0.89	0.18	18,20,34,35	0
8	PGE	A	311	10/10	0.89	0.18	39,40,41,41	0
8	PGE	C	307	10/10	0.90	0.15	34,35,37,38	0
4	PEG	E	304	7/7	0.90	0.17	38,39,43,46	0
3	LYS	B	301	10/10	0.90	0.14	17,18,18,19	0
5	EDO	E	305	4/4	0.90	0.22	45,45,45,45	0
4	PEG	F	304	7/7	0.91	0.17	36,37,39,41	0
7	MG	A	308	1/1	0.91	0.07	21,21,21,21	0
7	MG	D	309	1/1	0.91	0.16	39,39,39,39	0
7	MG	E	309	1/1	0.91	0.08	48,48,48,48	0
5	EDO	B	304	4/4	0.91	0.18	39,39,39,39	0
6	ACT	E	307	4/4	0.92	0.13	50,50,50,50	0
4	PEG	A	302	7/7	0.94	0.30	20,20,20,20	0
5	EDO	B	308	4/4	0.94	0.41	20,20,20,20	0
3	LYS	B	302	10/10	0.95	0.14	15,17,19,20	0
7	MG	A	310	1/1	0.97	0.07	28,28,28,28	0
7	MG	C	306	1/1	0.97	0.18	17,17,17,17	0
7	MG	D	307	1/1	0.98	0.19	12,12,12,12	0
7	MG	D	308	1/1	0.98	0.14	29,29,29,29	0
7	MG	F	311	1/1	0.98	0.11	30,30,30,30	0
7	MG	B	313	1/1	0.99	0.16	16,16,16,16	0
7	MG	F	310	1/1	0.99	0.19	13,13,13,13	0
7	MG	E	308	1/1	0.99	0.14	10,10,10,10	0
7	MG	A	309	1/1	1.00	0.13	11,11,11,11	0

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

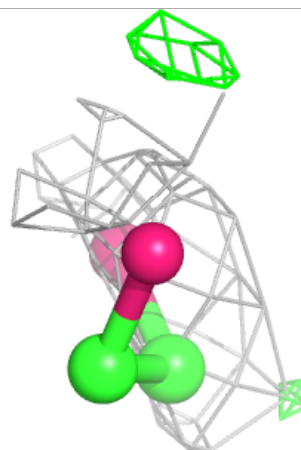
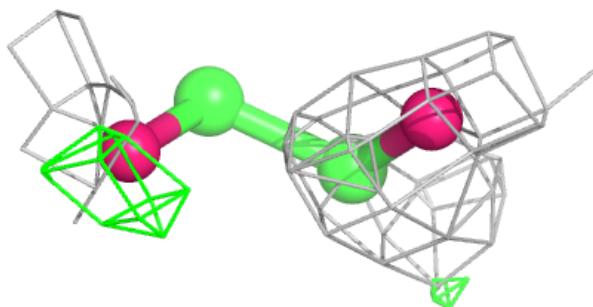
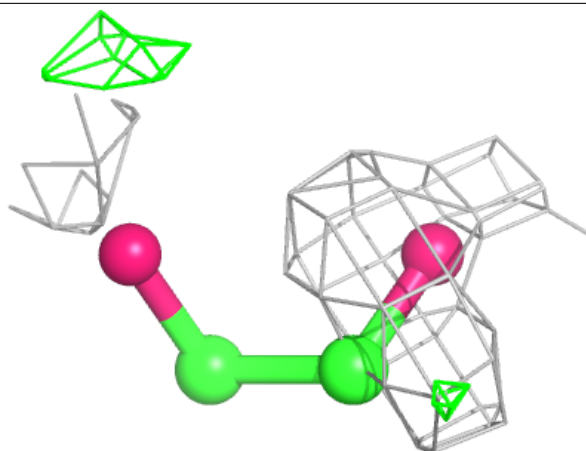
**Electron density around EDO D 303:**

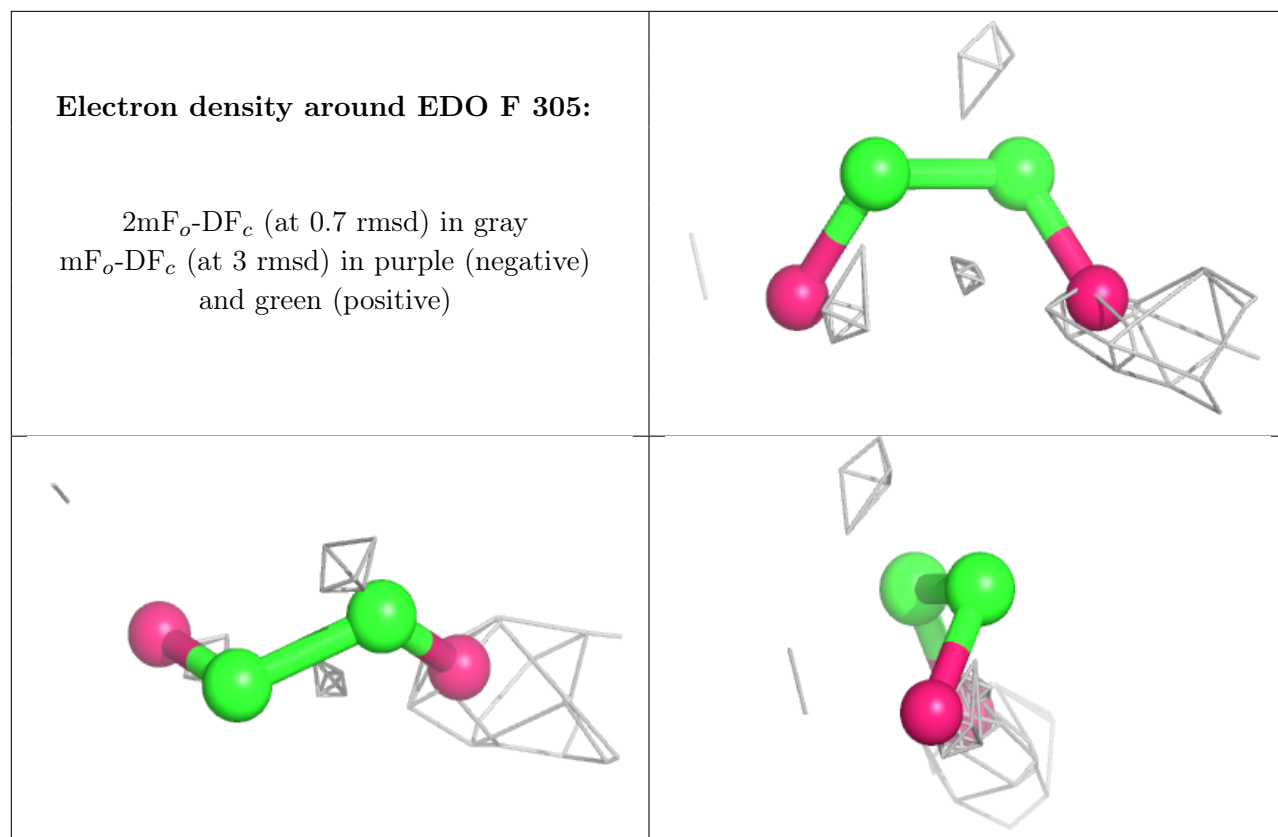
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around EDO D 304:**

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

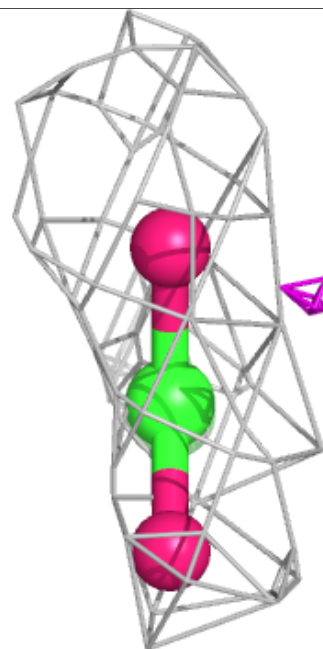
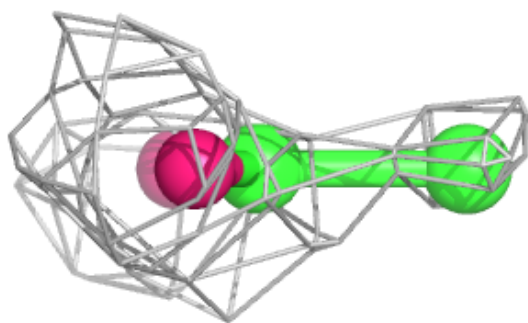
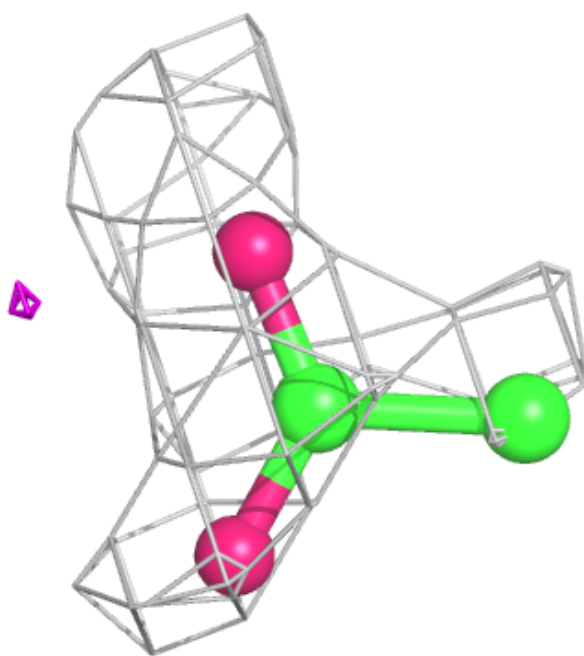






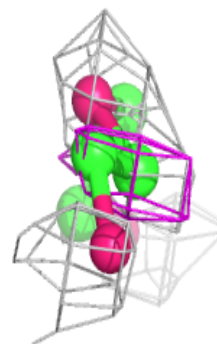
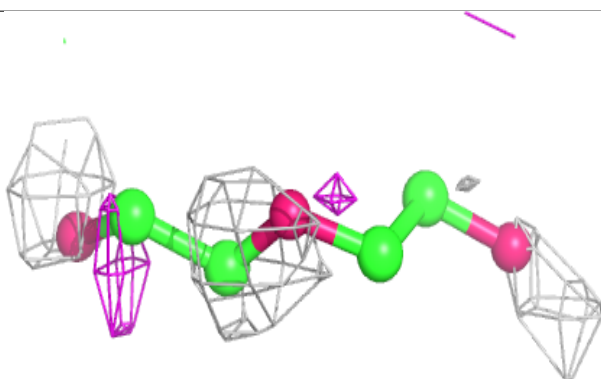
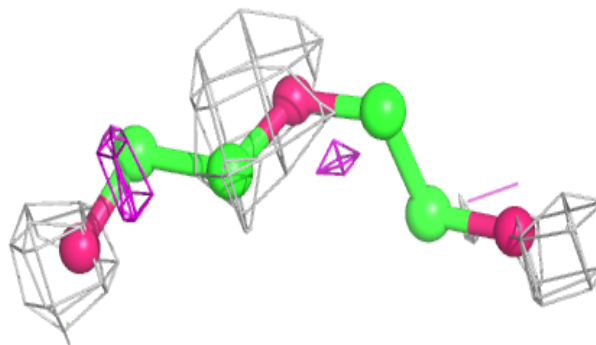
**Electron density around ACT F 309:**

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

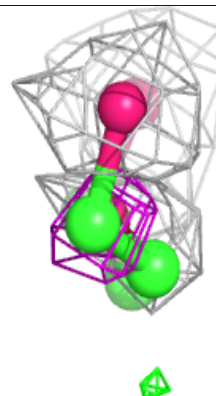
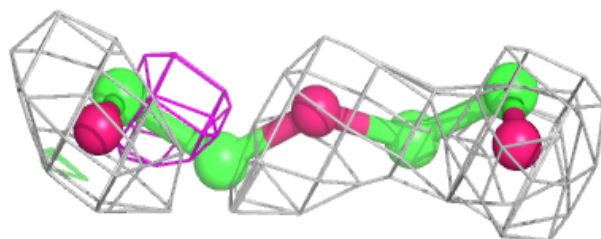
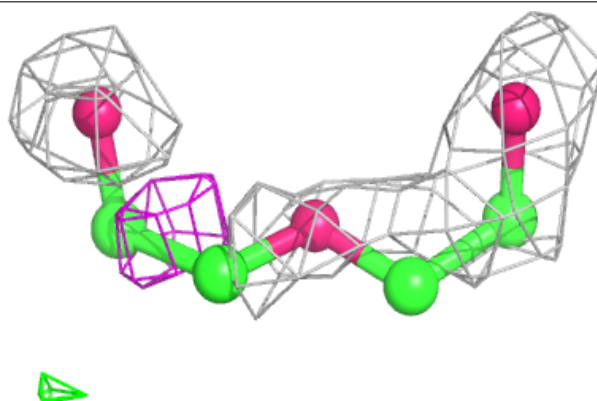


**Electron density around PEG F 302:**

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

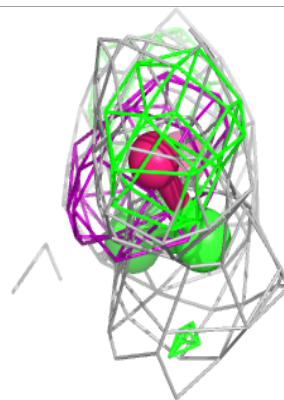
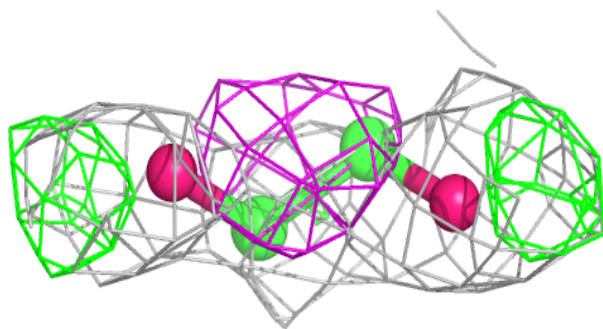
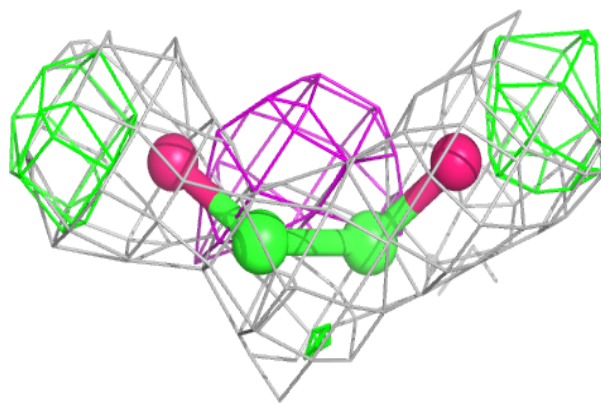
**Electron density around PEG C 302:**

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

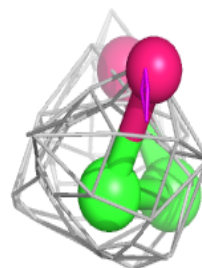
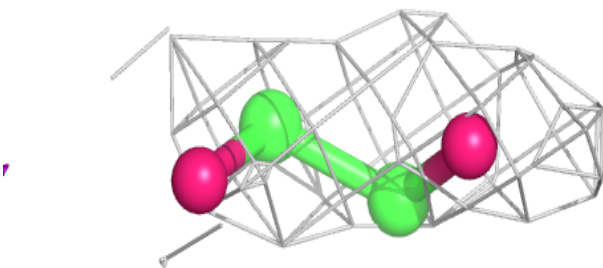
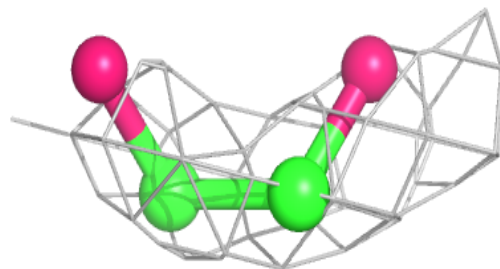


**Electron density around EDO A 305:**

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

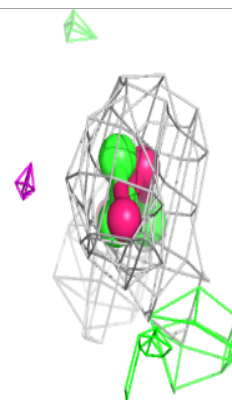
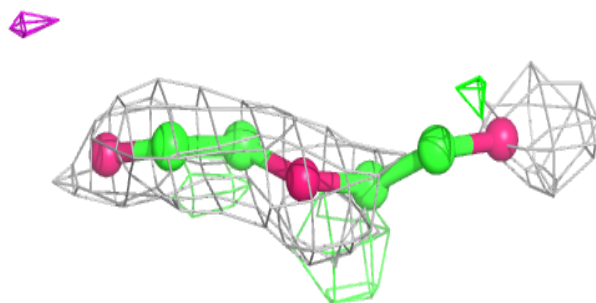
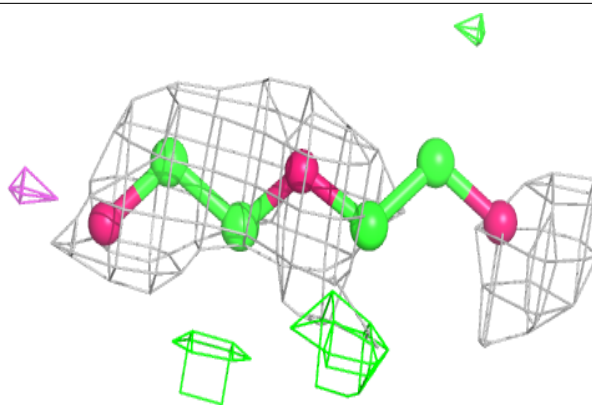
**Electron density around EDO F 306:**

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

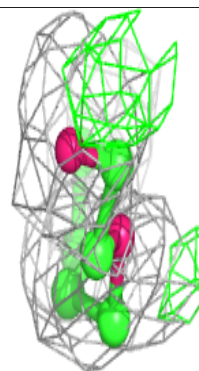
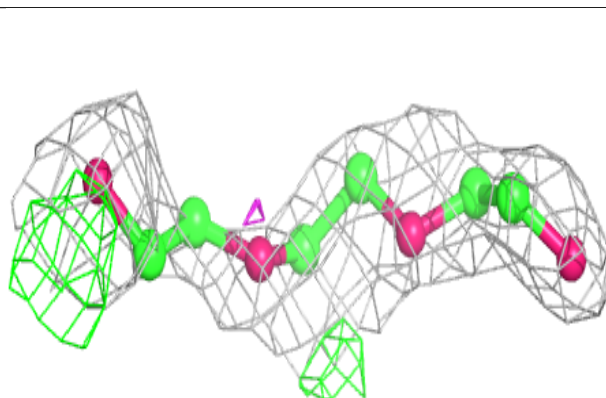
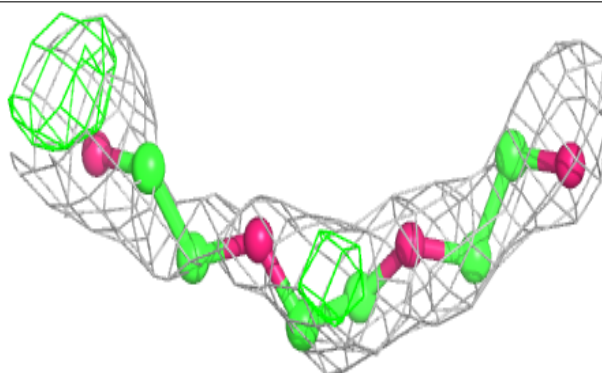


**Electron density around PEG C 301:**

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

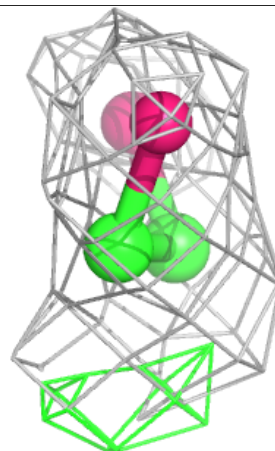
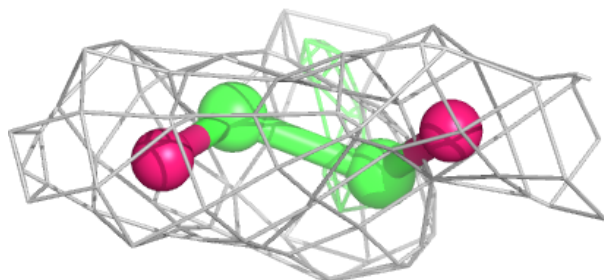
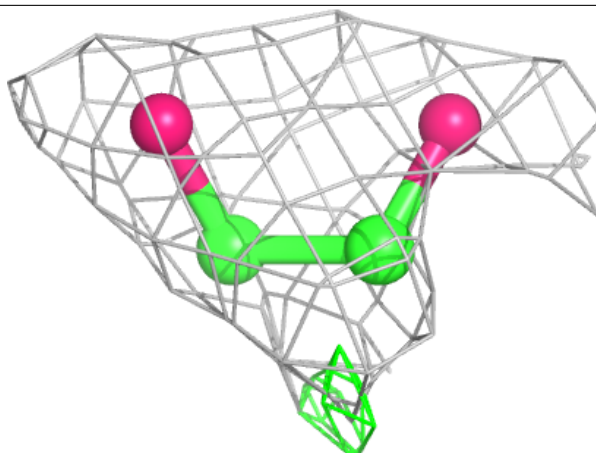
**Electron density around PGE A 312:**

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

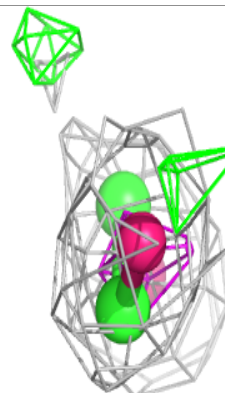
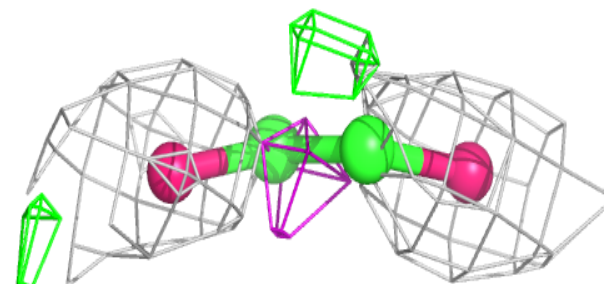
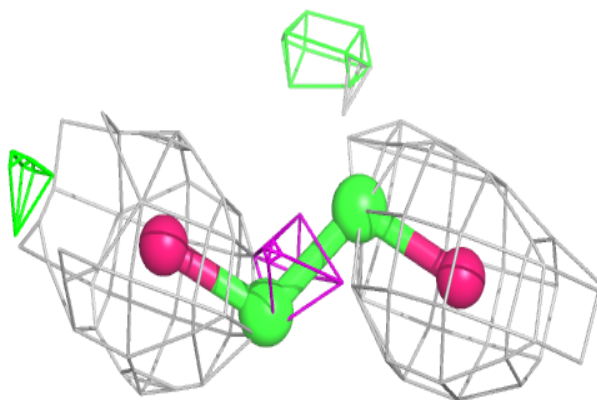


**Electron density around EDO A 303:**

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

**Electron density around EDO C 303:**

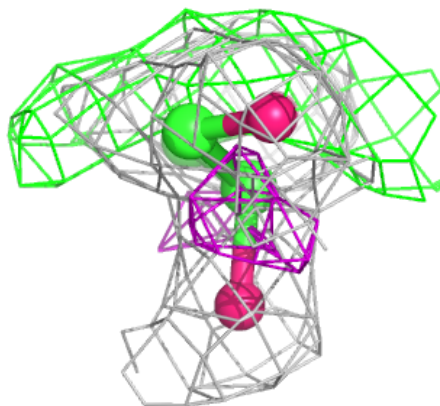
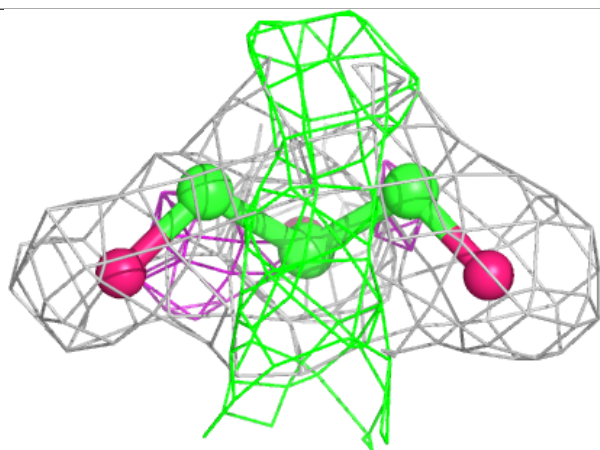
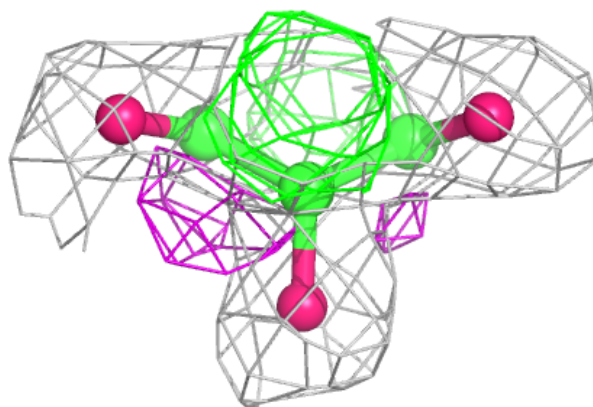
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





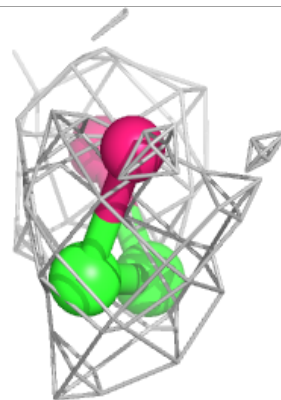
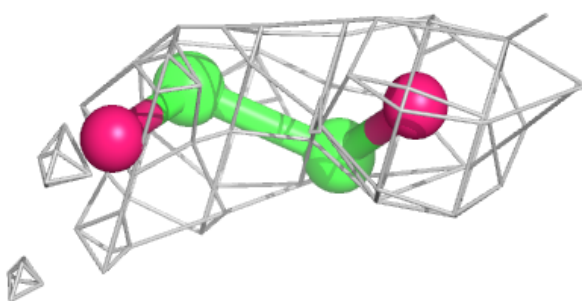
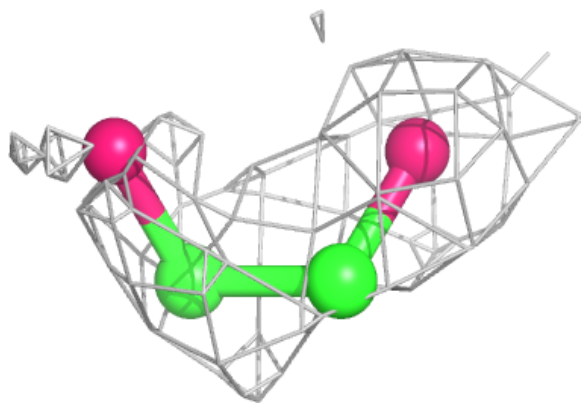
**Electron density around GOL A 313:**

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

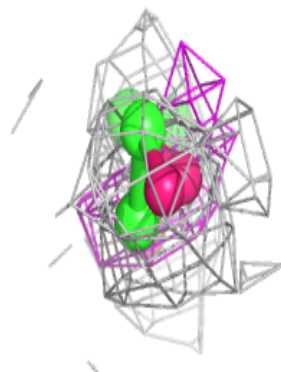
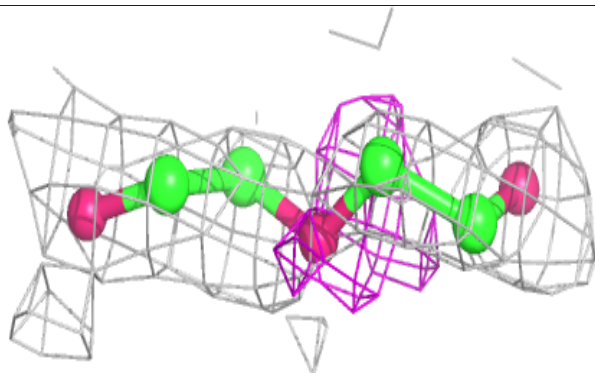
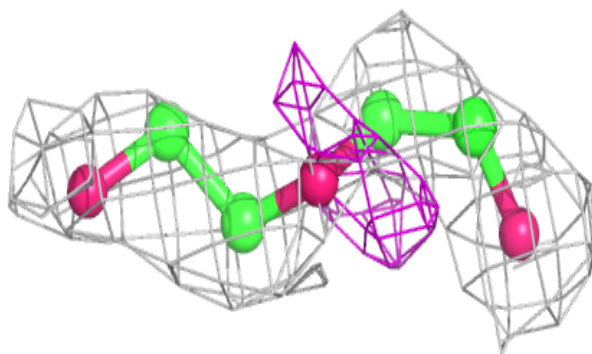


**Electron density around EDO B 307:**

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

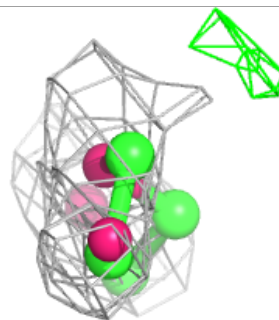
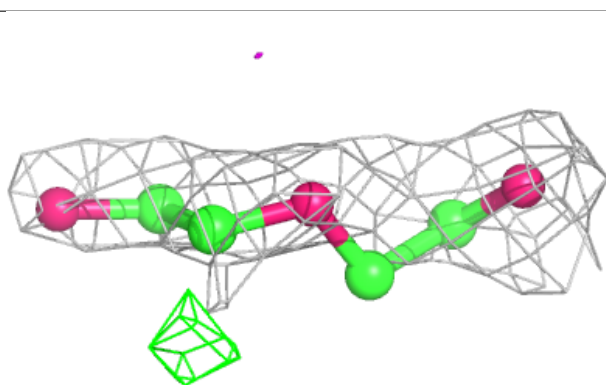
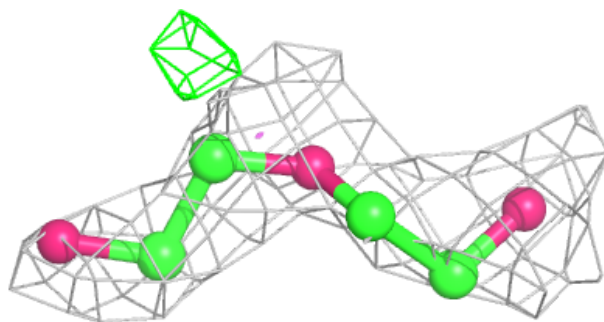
**Electron density around PEG E 303:**

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



**Electron density around PEG F 303:**

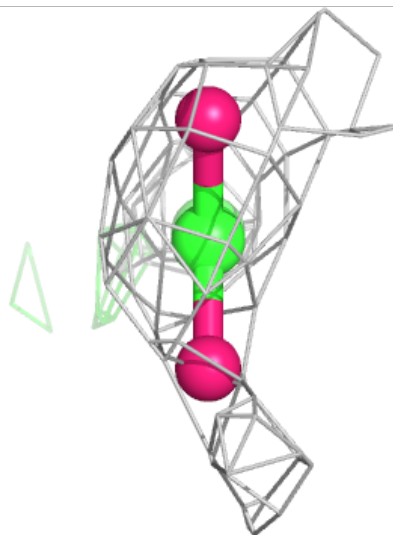
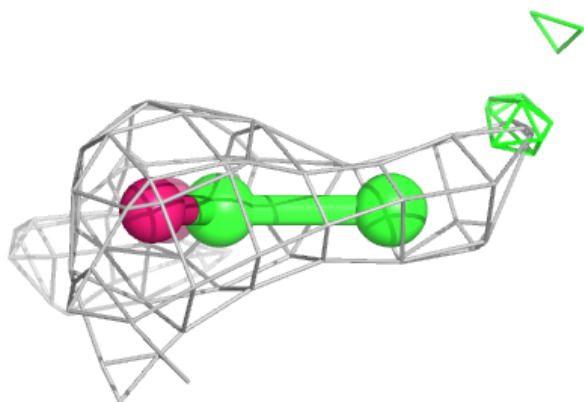
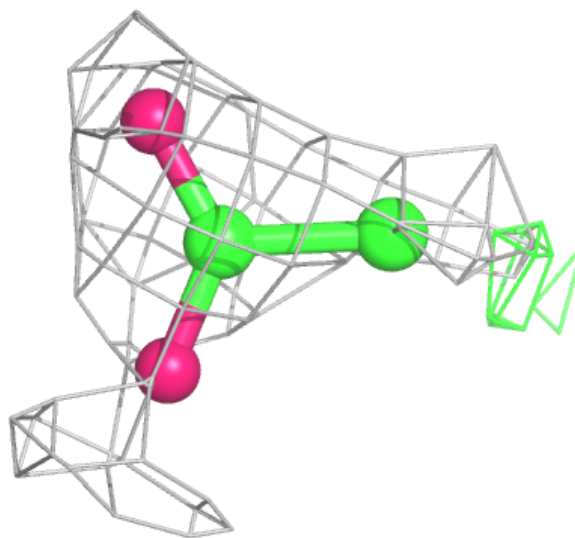
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





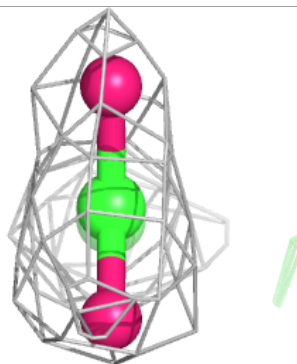
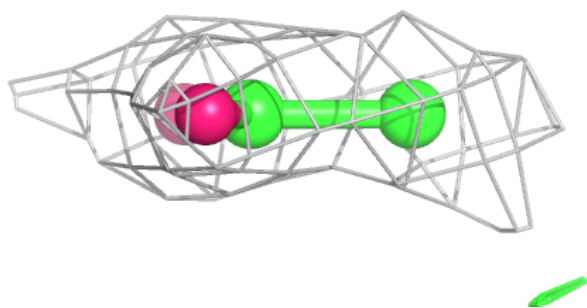
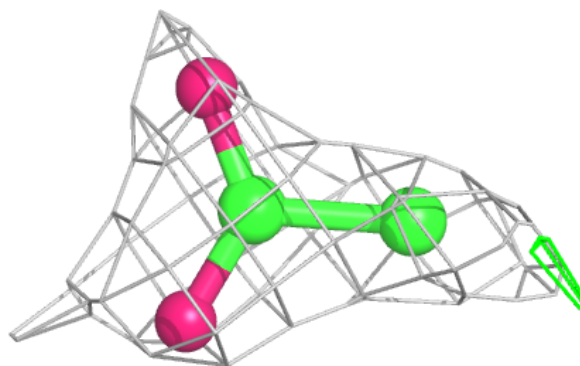
**Electron density around ACT B 310:**

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



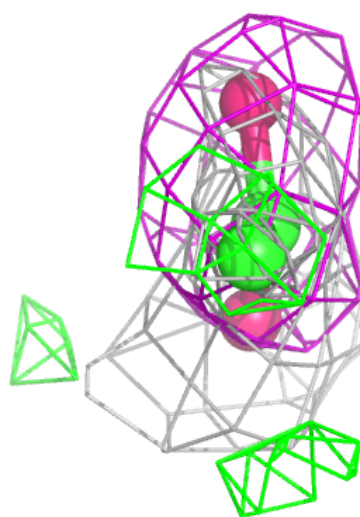
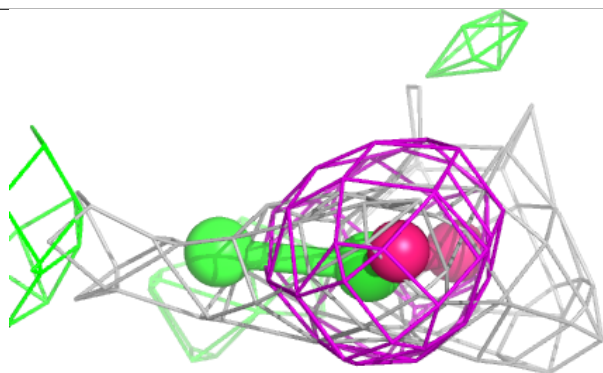
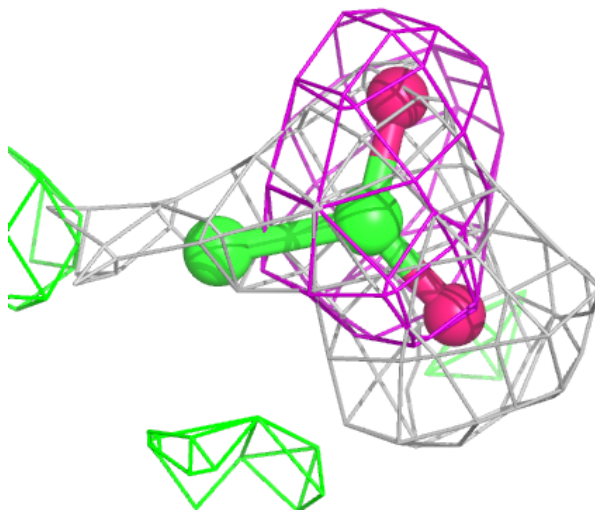
**Electron density around ACT B 311:**

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



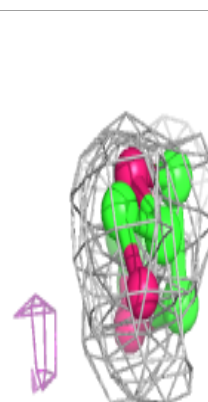
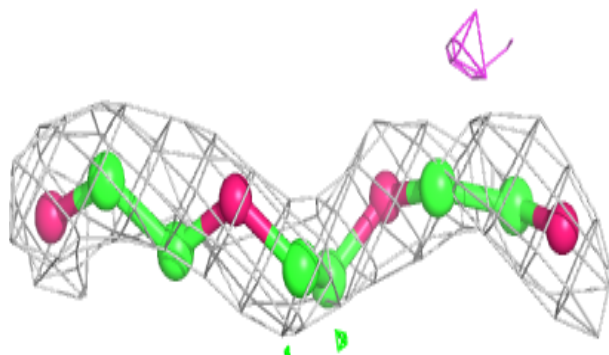
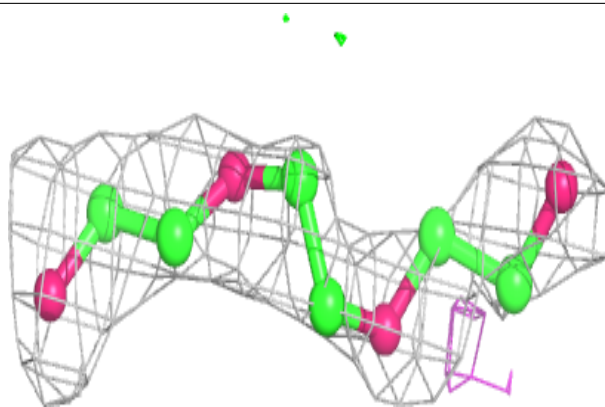
**Electron density around ACT C 305:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

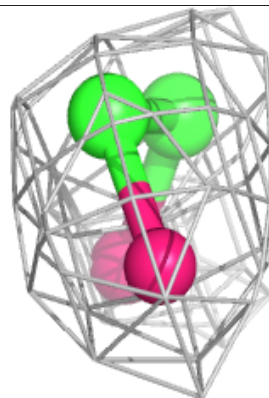
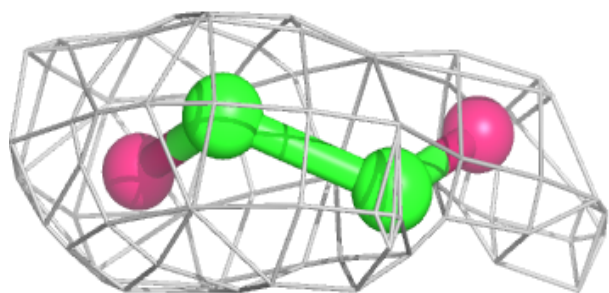
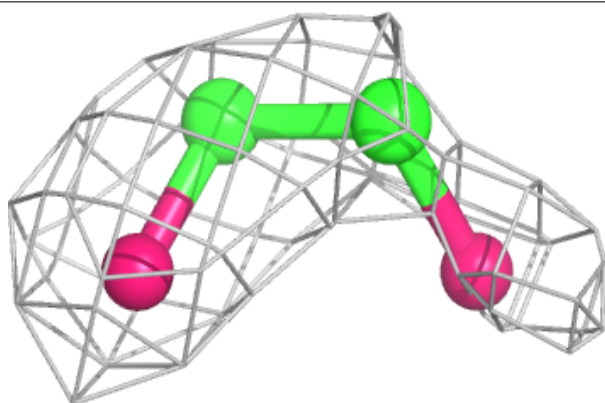


**Electron density around PGE E 310:**

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

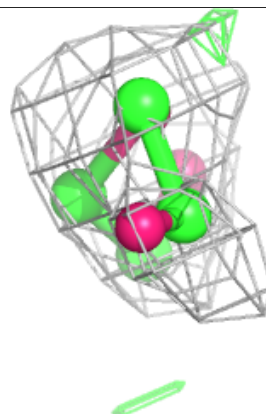
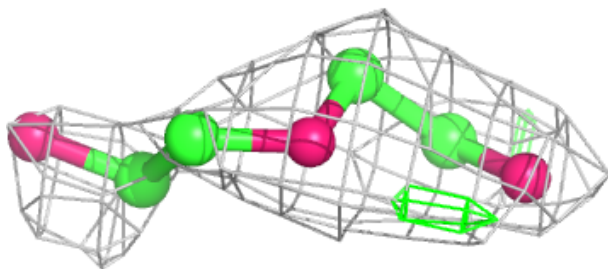
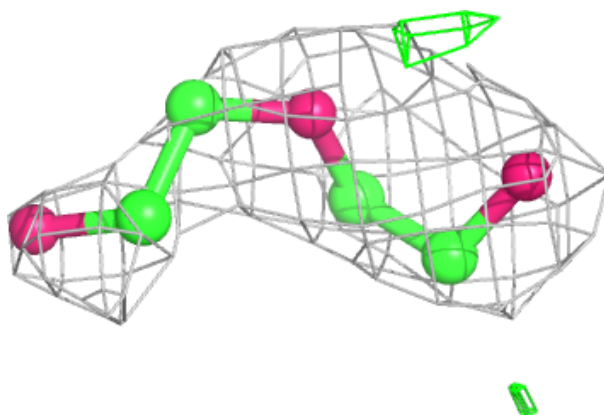
**Electron density around EDO D 302:**

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

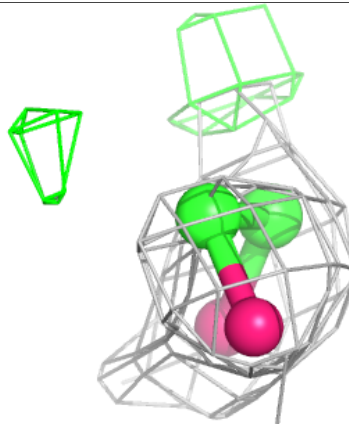
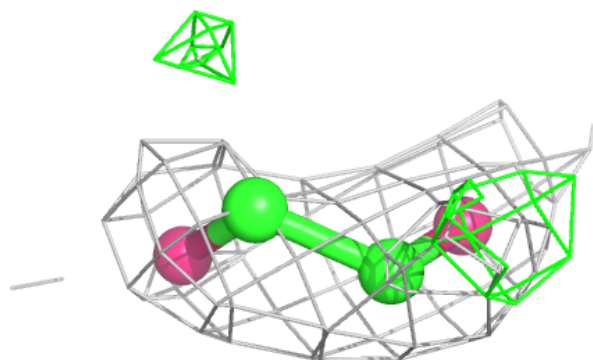
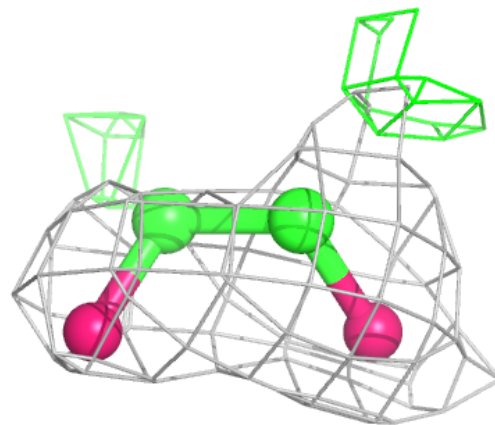


**Electron density around PEG E 302:**

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

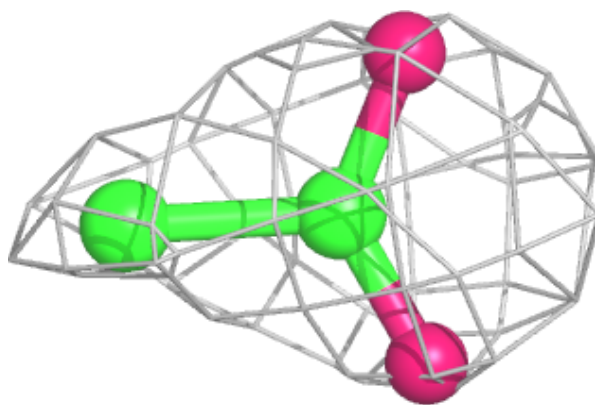
**Electron density around EDO B 305:**

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

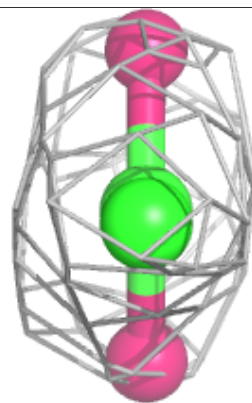
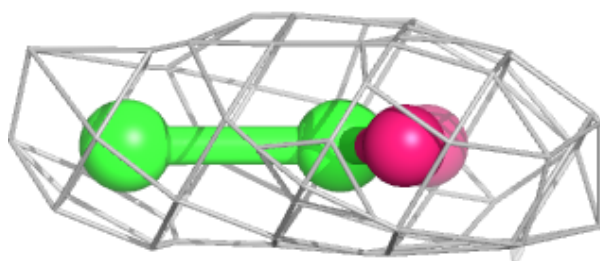


**Electron density around ACT B 312:**

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



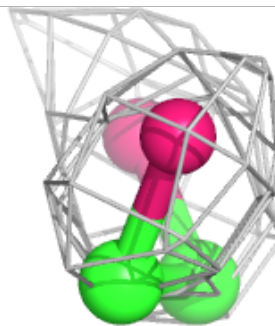
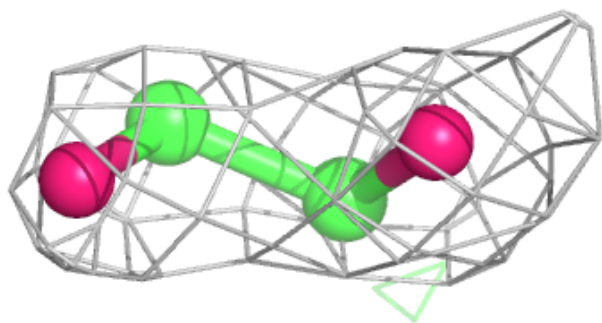
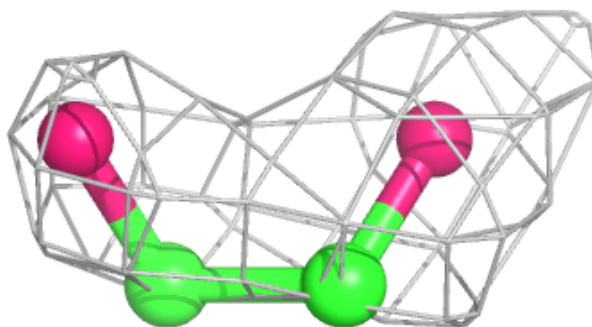
b



c

**Electron density around EDO F 308:**

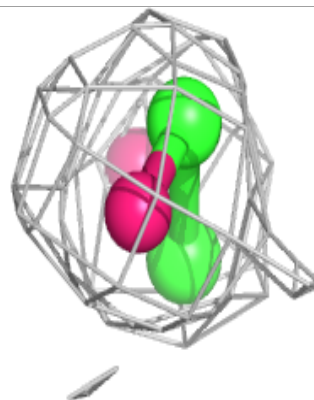
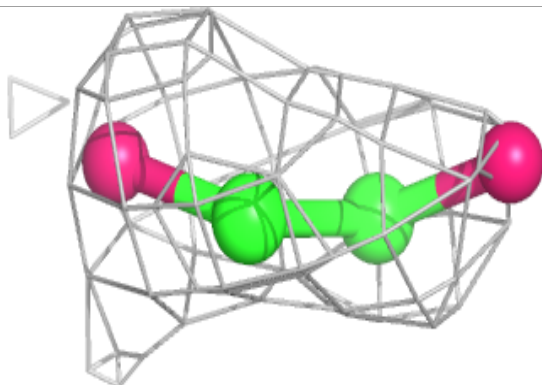
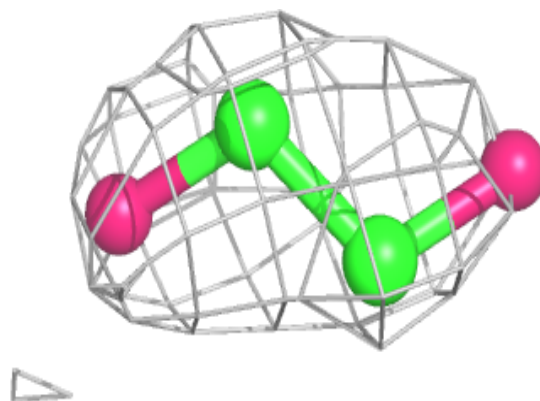
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



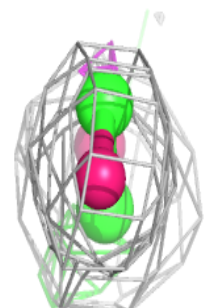
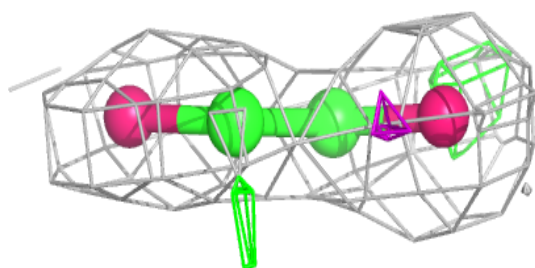
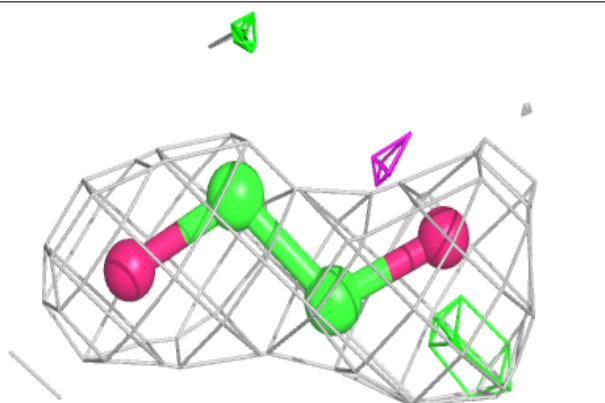


**Electron density around EDO E 306:**

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

**Electron density around EDO A 306:**

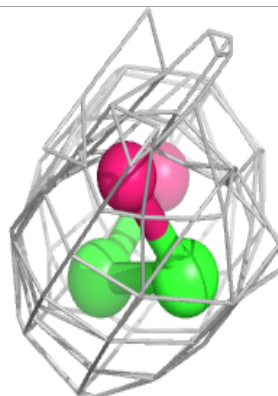
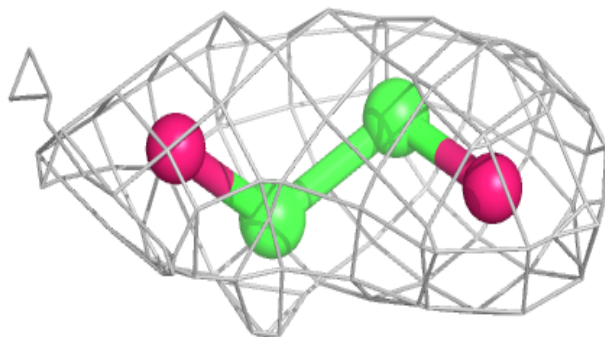
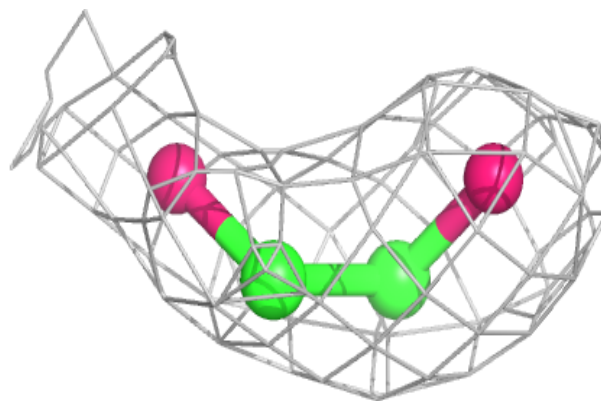
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





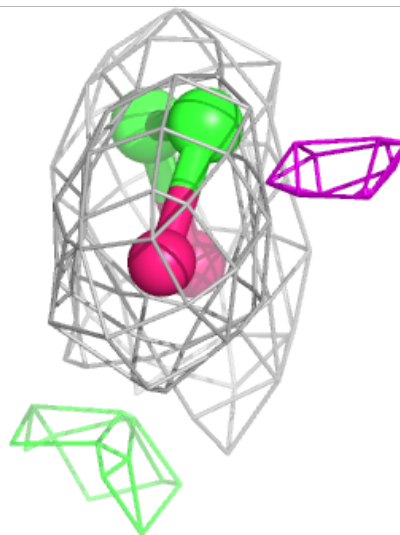
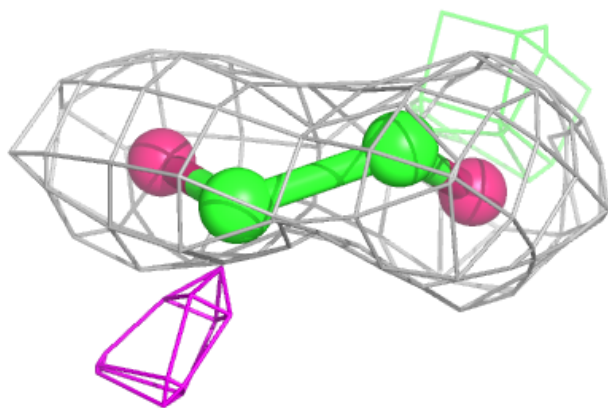
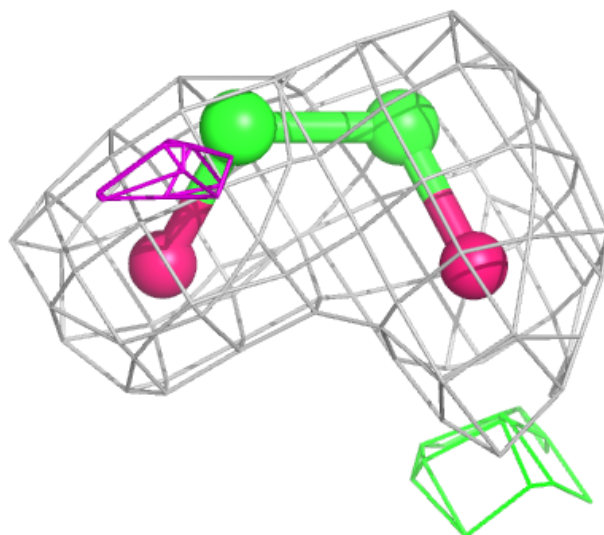
**Electron density around EDO D 305:**

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



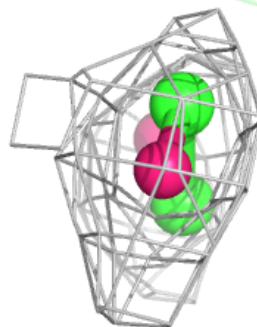
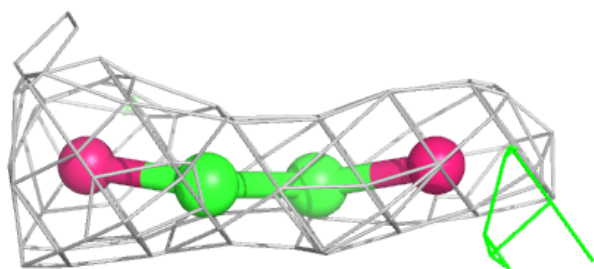
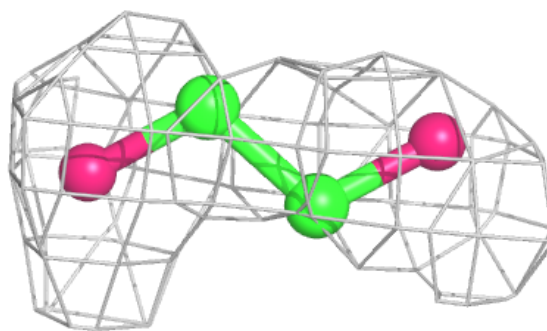
**Electron density around EDO C 304:**

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



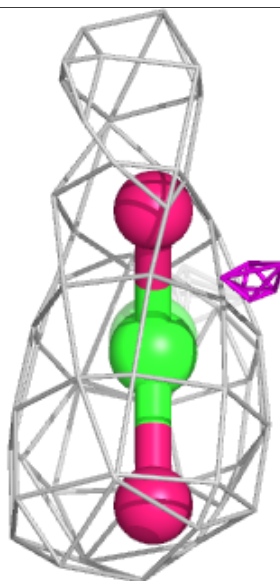
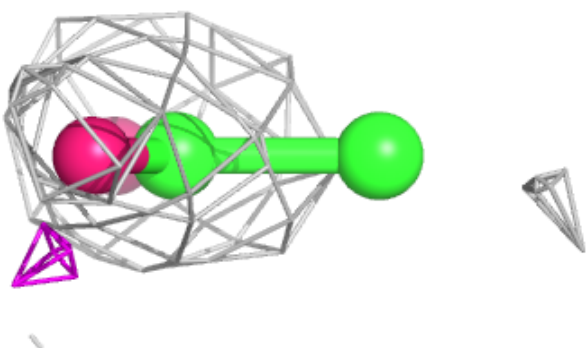
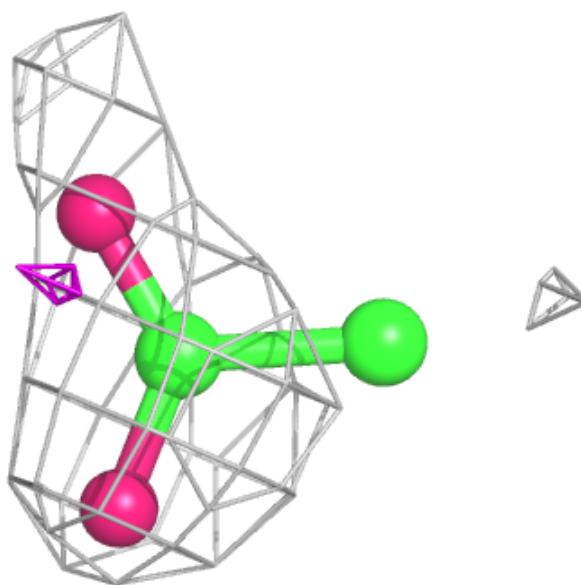
**Electron density around EDO A 304:**

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



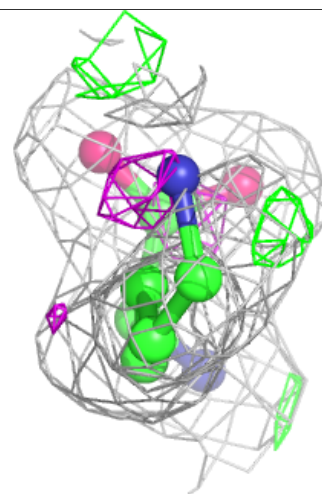
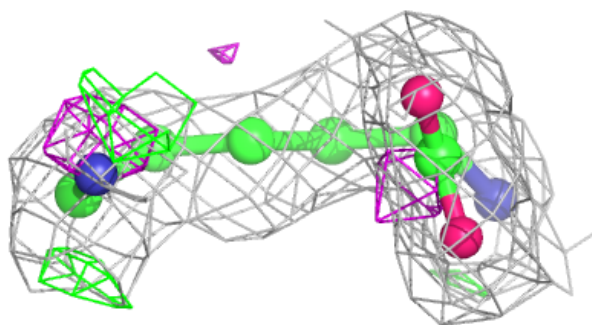
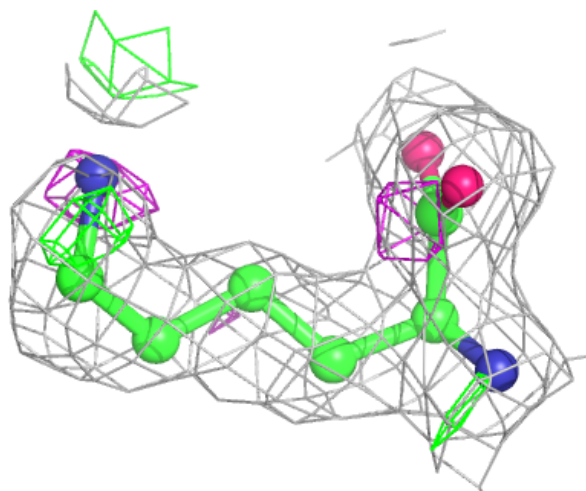
**Electron density around ACT D 306:**

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



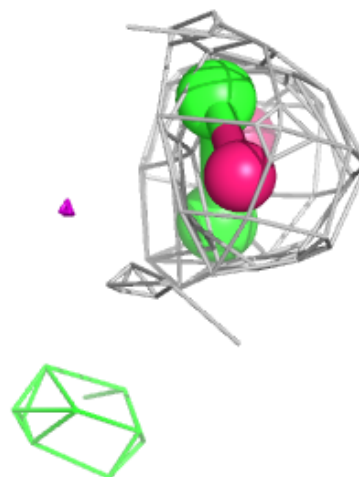
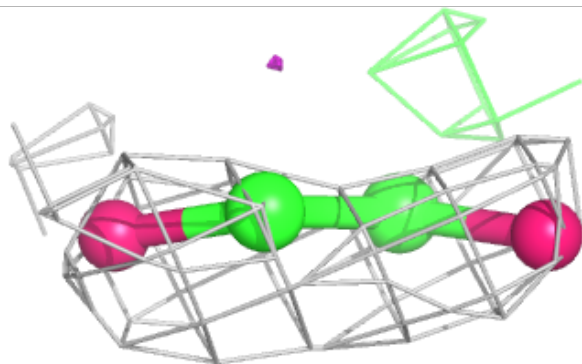
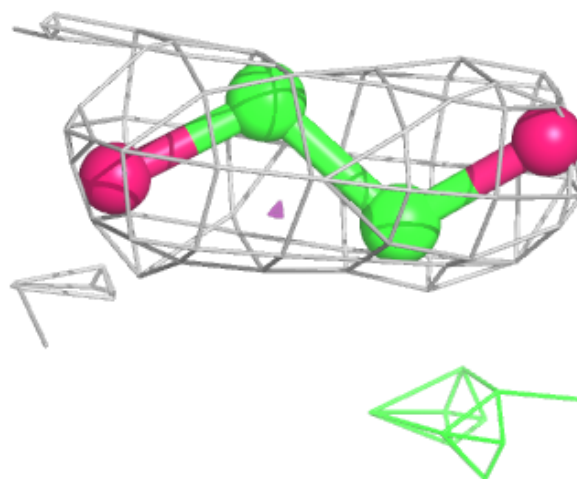
**Electron density around LYS F 301:**

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



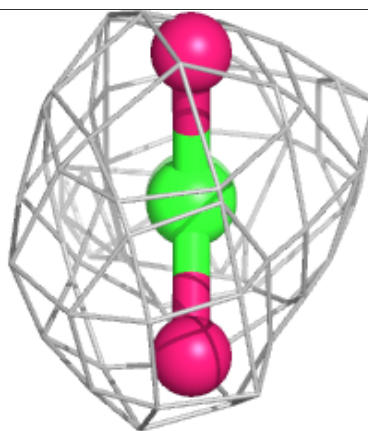
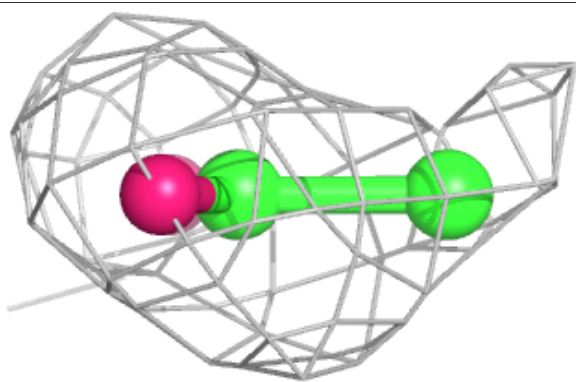
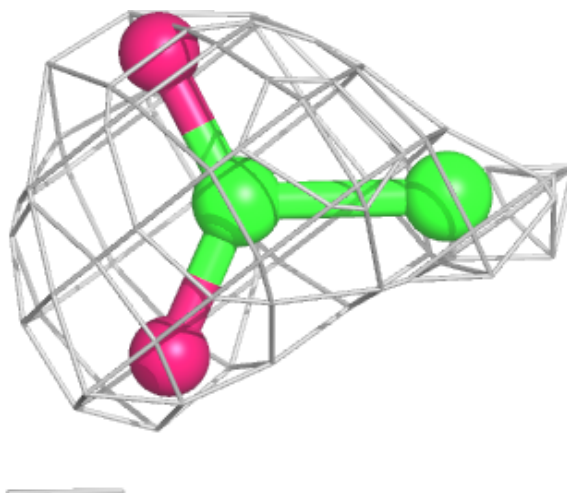
**Electron density around EDO B 306:**

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



**Electron density around ACT A 307:**

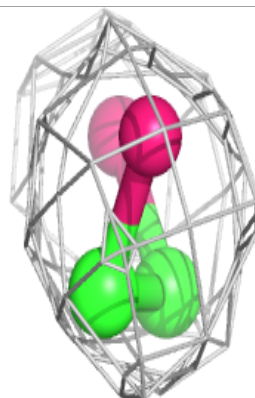
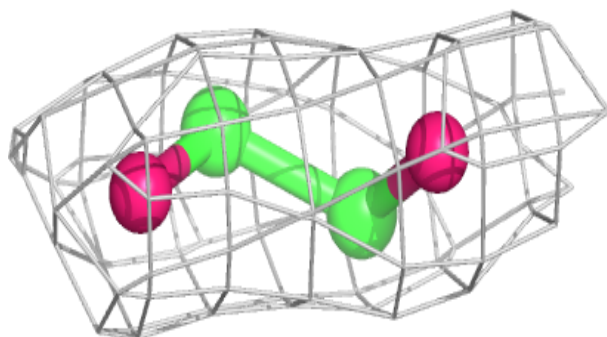
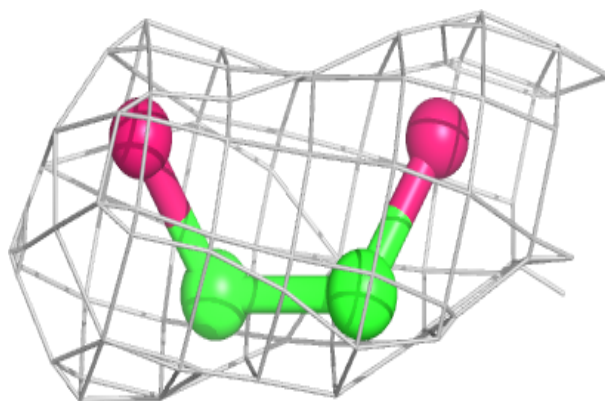
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



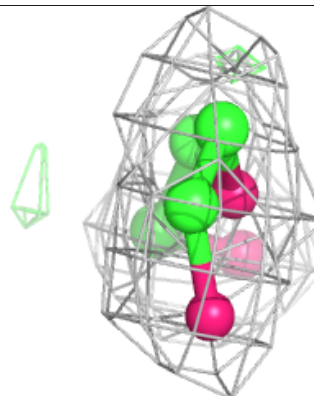
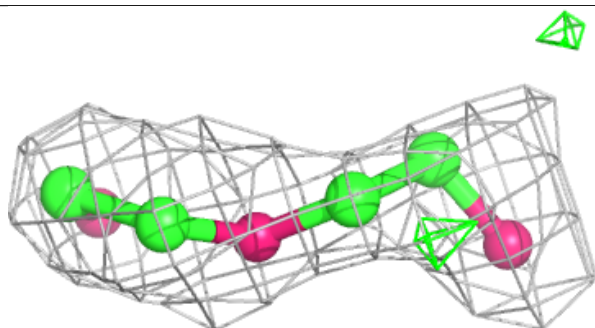
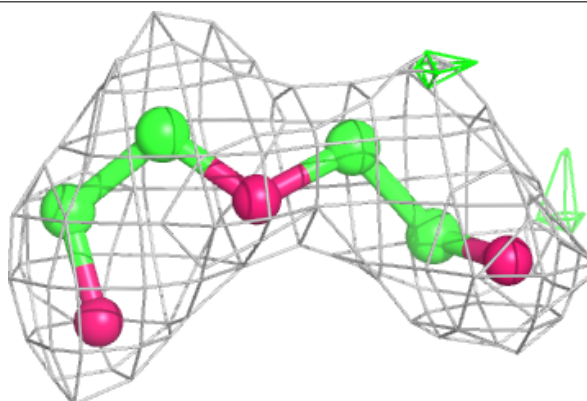


**Electron density around EDO F 307:**

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

**Electron density around PEG B 303:**

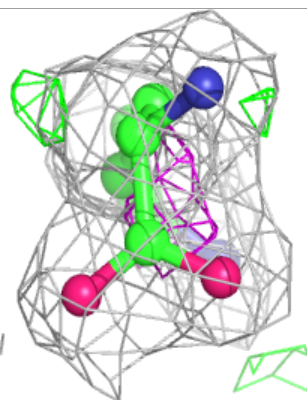
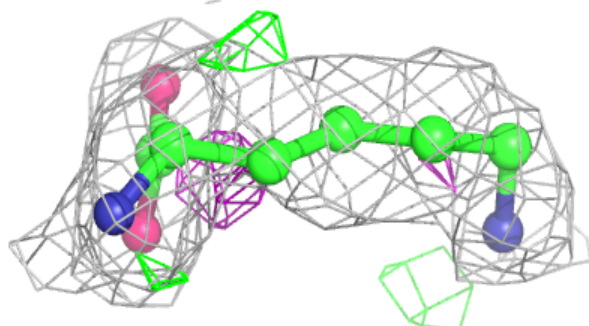
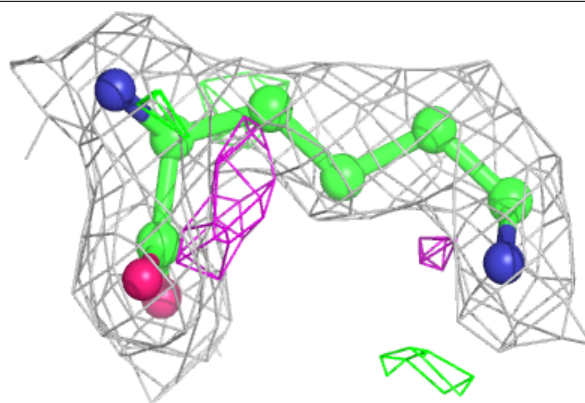
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



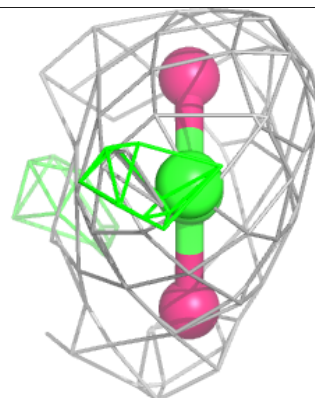
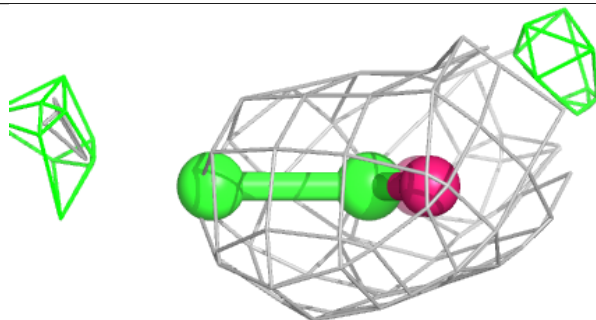
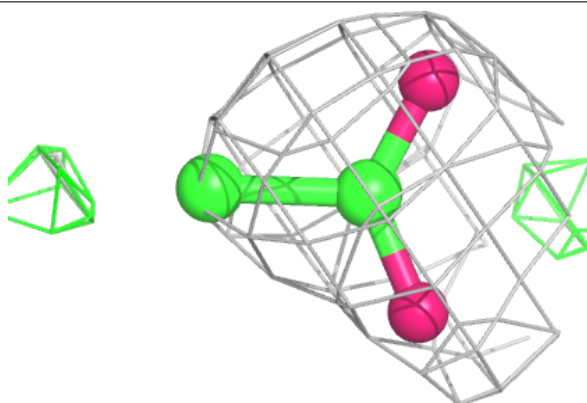


**Electron density around LYS D 301:**

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

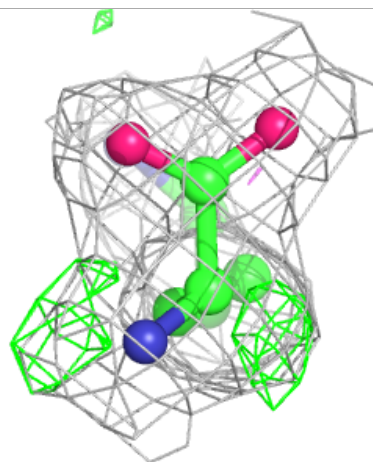
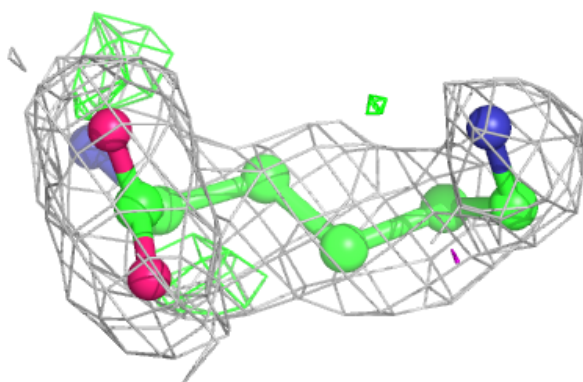
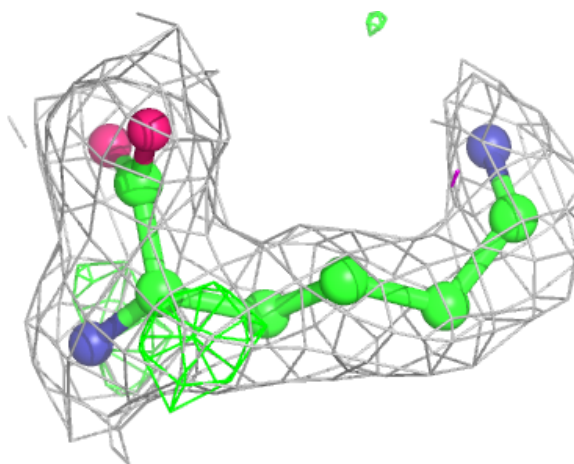
**Electron density around ACT B 309:**

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



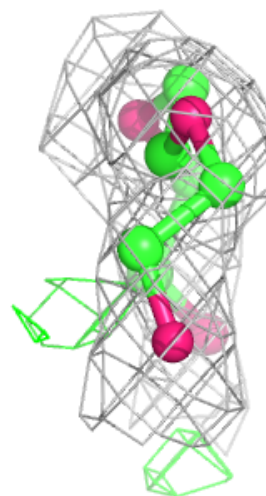
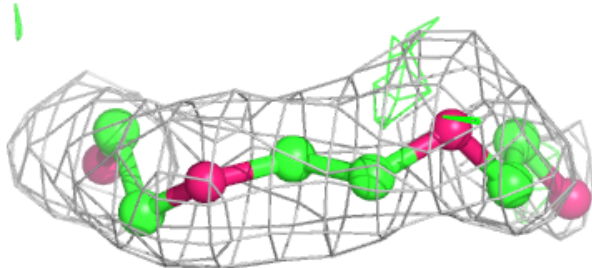
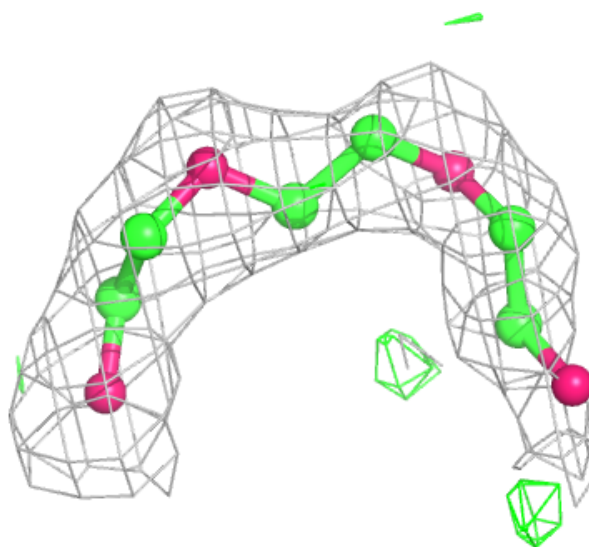
**Electron density around LYS A 301:**

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



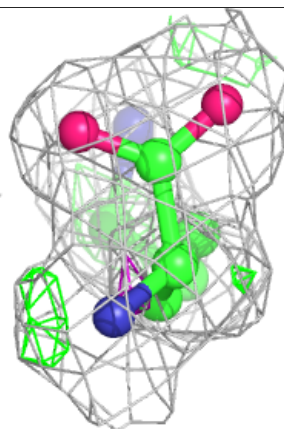
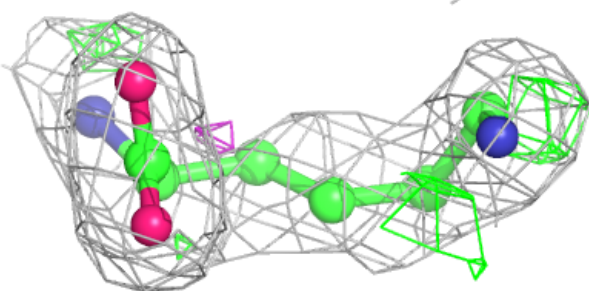
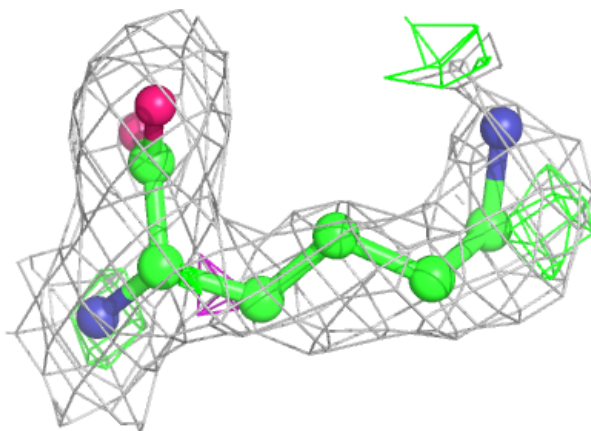
**Electron density around PGE D 310:**

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



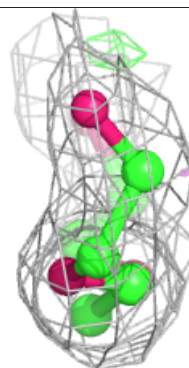
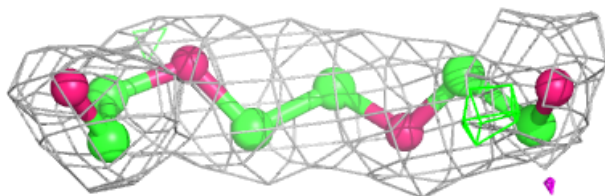
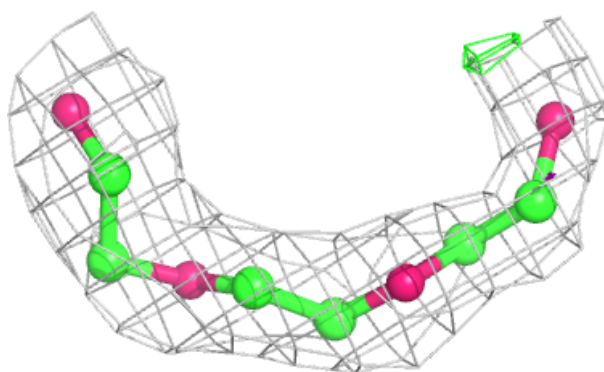
**Electron density around LYS E 301:**

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



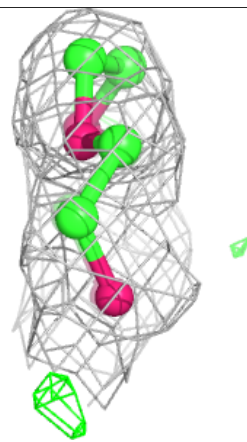
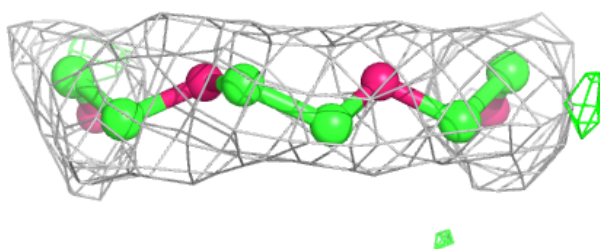
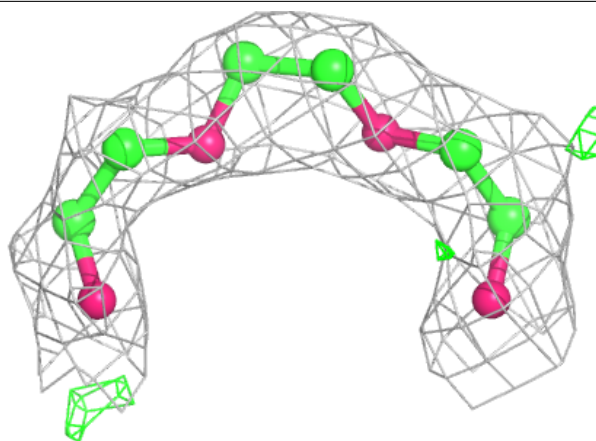
**Electron density around PGE A 311:**

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

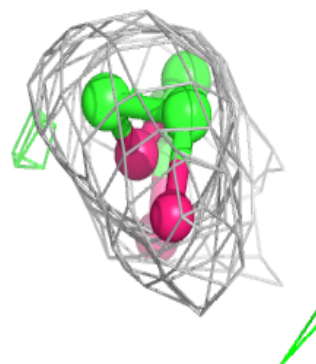
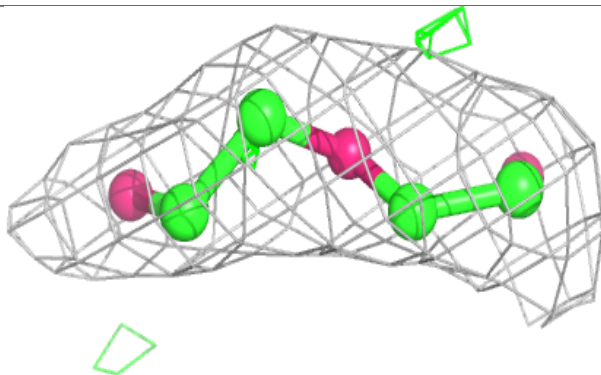
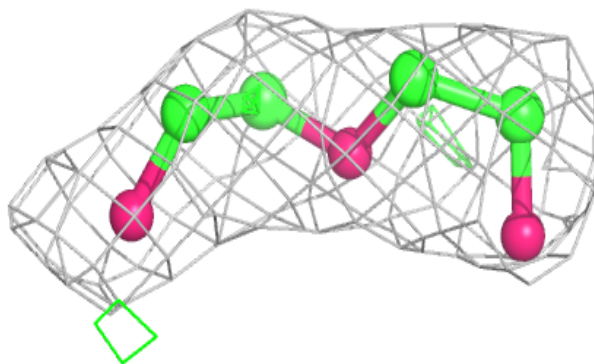


**Electron density around PGE C 307:**

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

**Electron density around PEG E 304:**

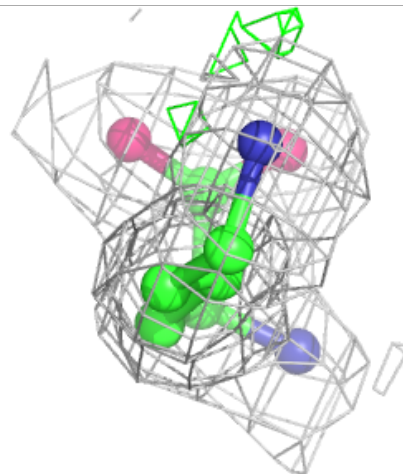
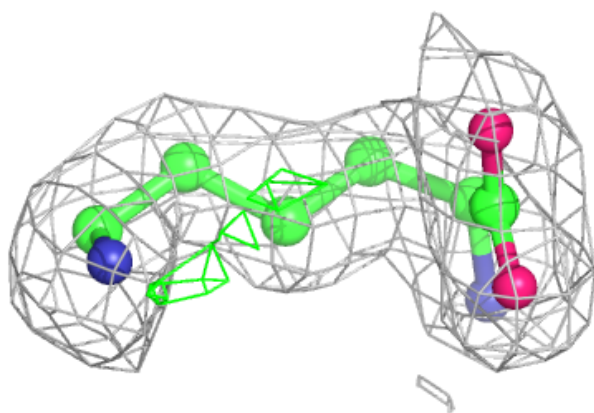
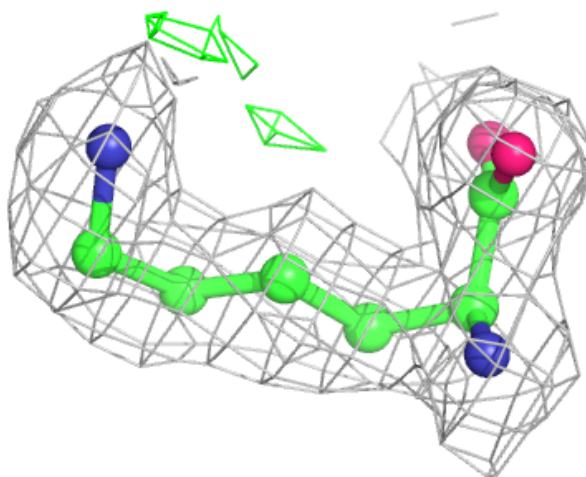
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





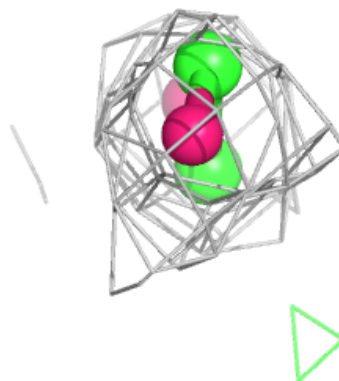
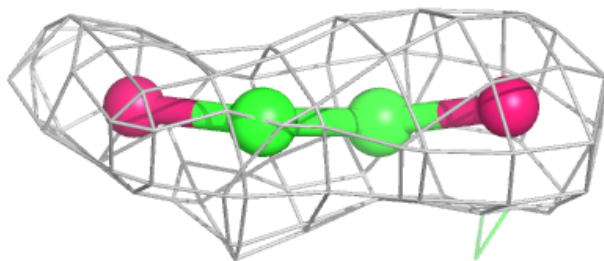
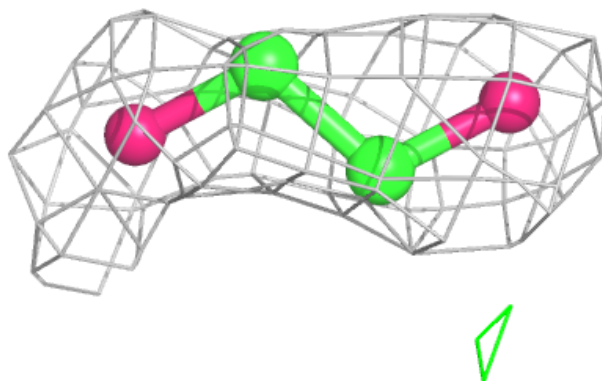
**Electron density around LYS B 301:**

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



**Electron density around EDO E 305:**

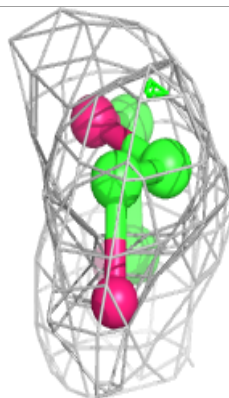
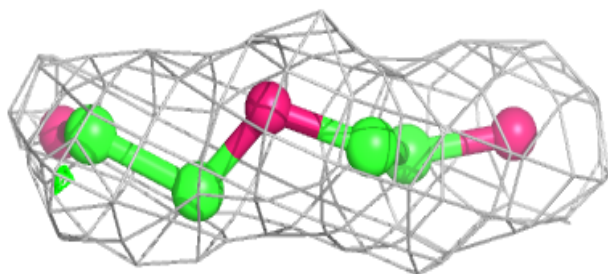
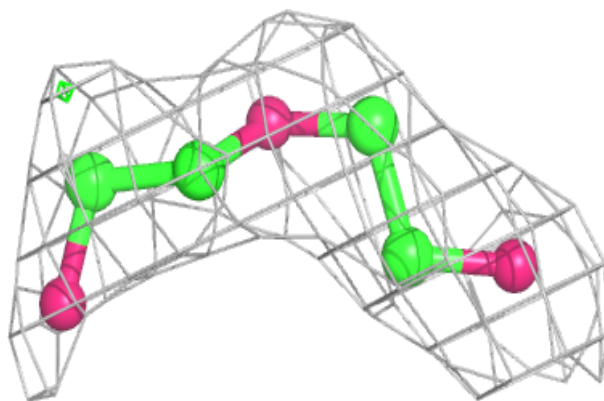
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





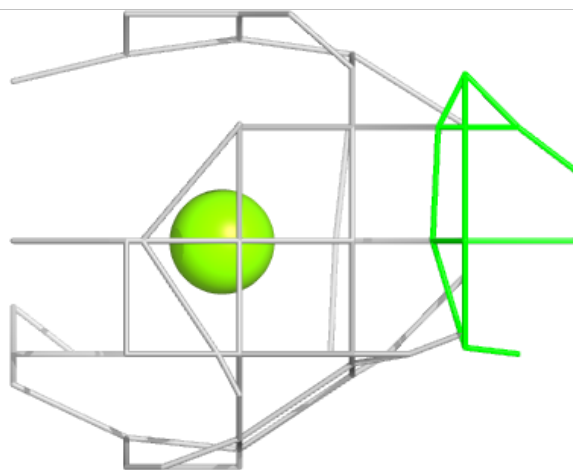
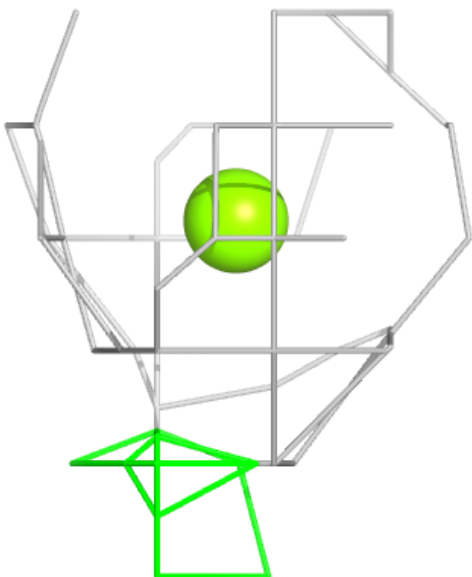
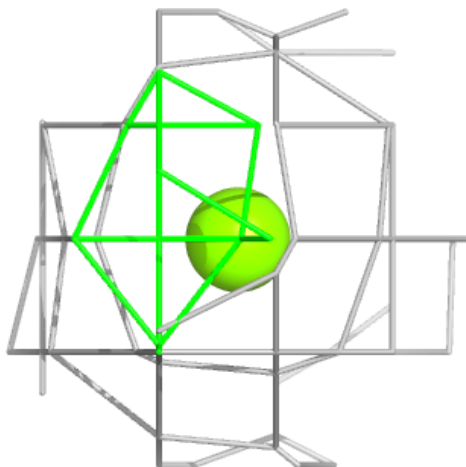
**Electron density around PEG F 304:**

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



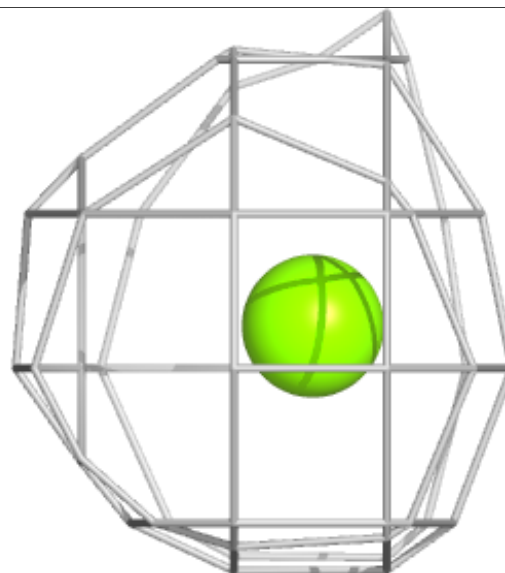
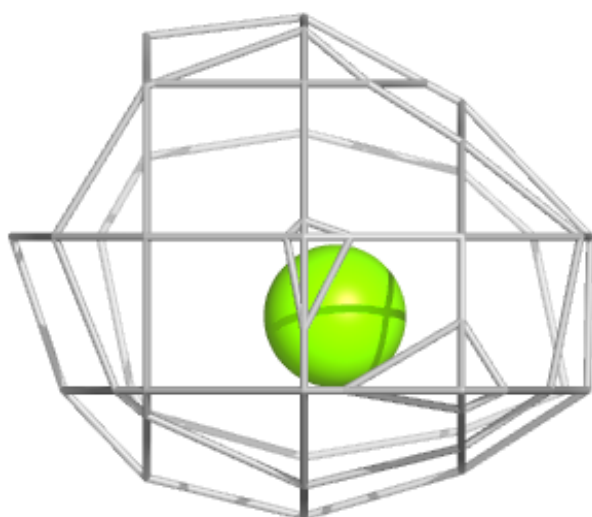
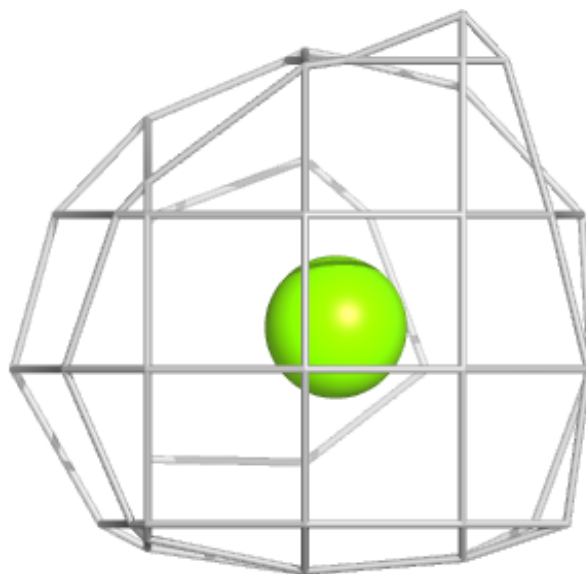
**Electron density around MG A 308:**

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



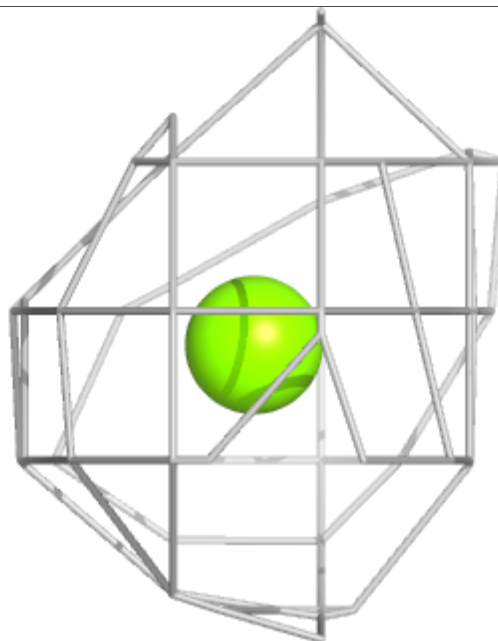
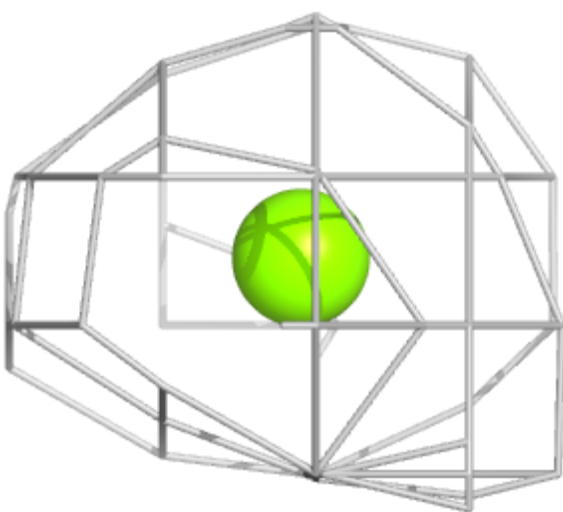
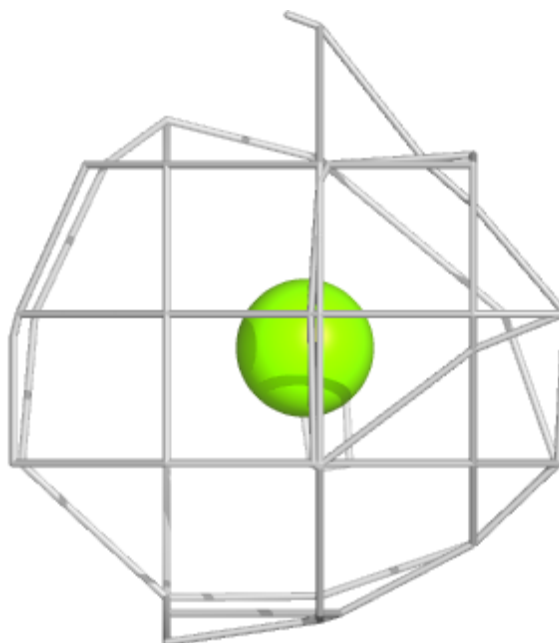
**Electron density around MG D 309:**

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



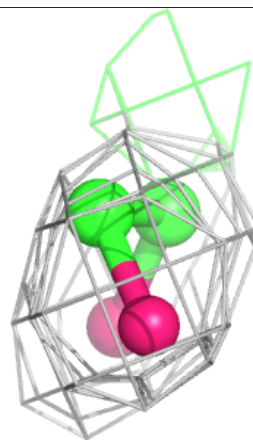
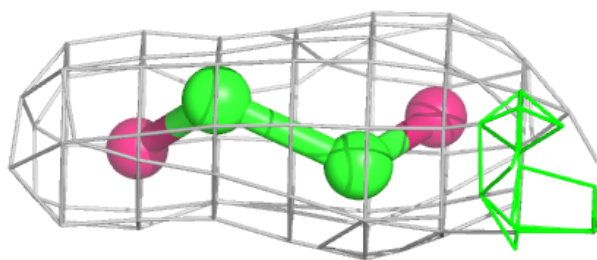
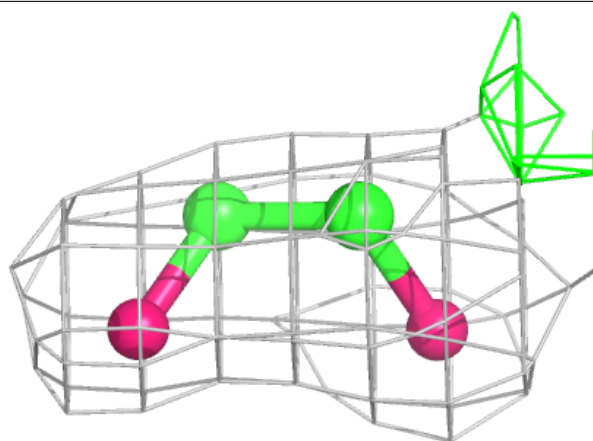
**Electron density around MG E 309:**

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



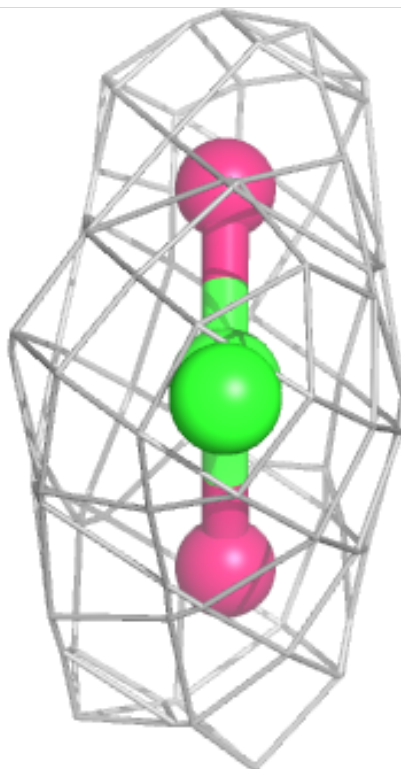
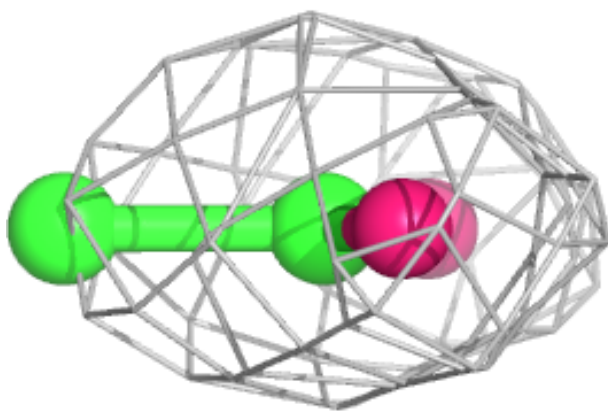
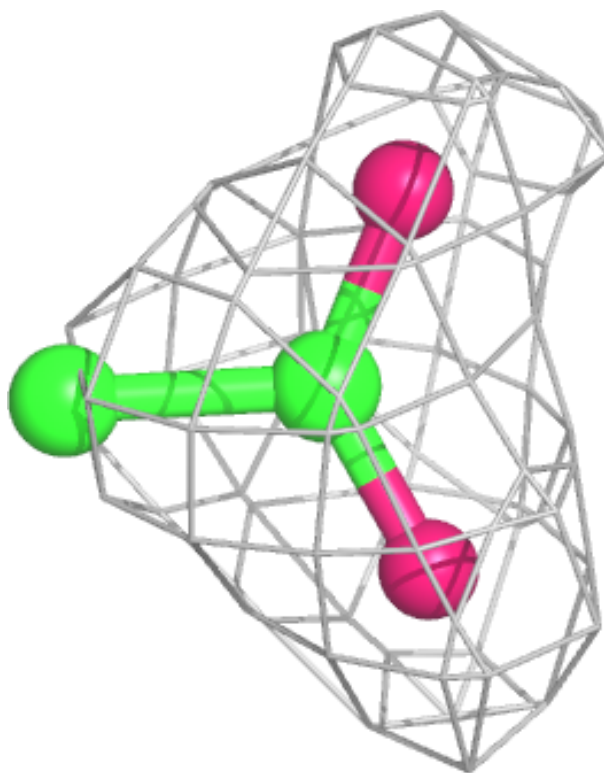
**Electron density around EDO B 304:**

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



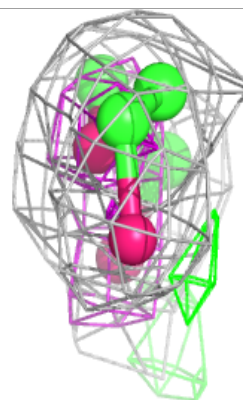
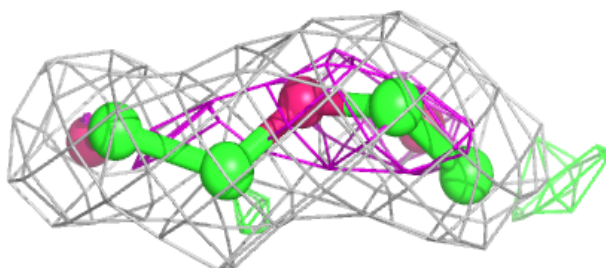
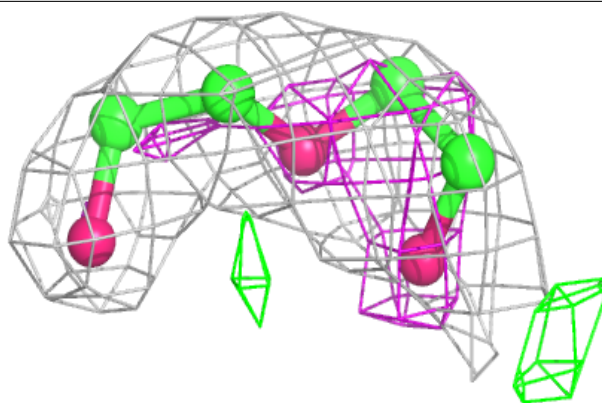
**Electron density around ACT E 307:**

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



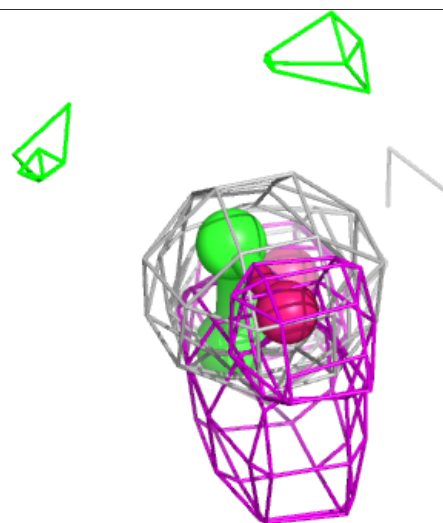
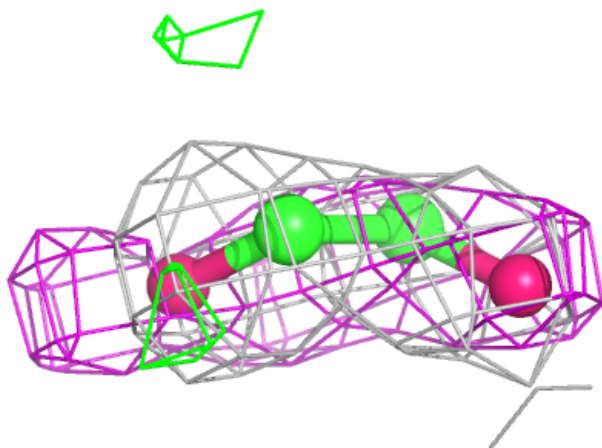
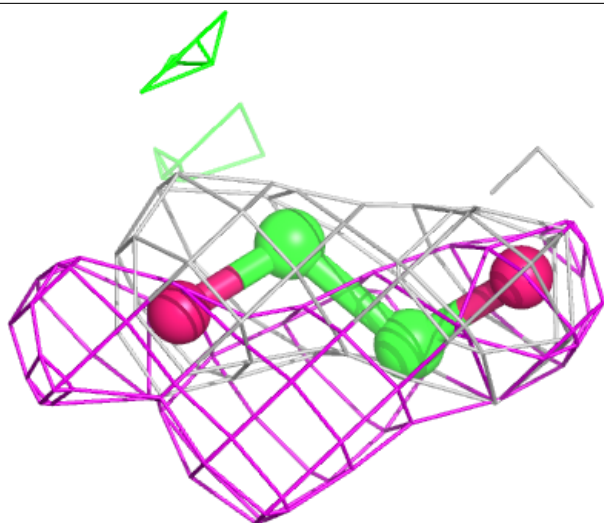
**Electron density around PEG A 302:**

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



**Electron density around EDO B 308:**

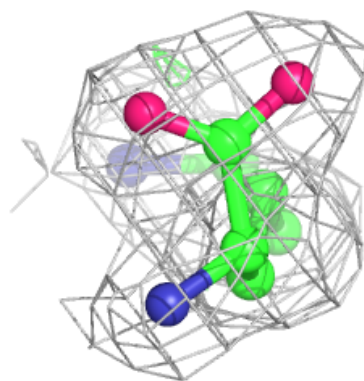
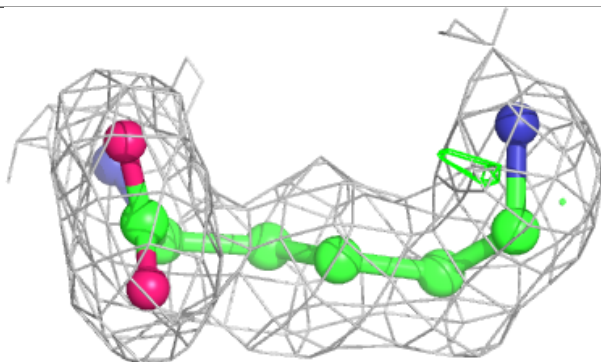
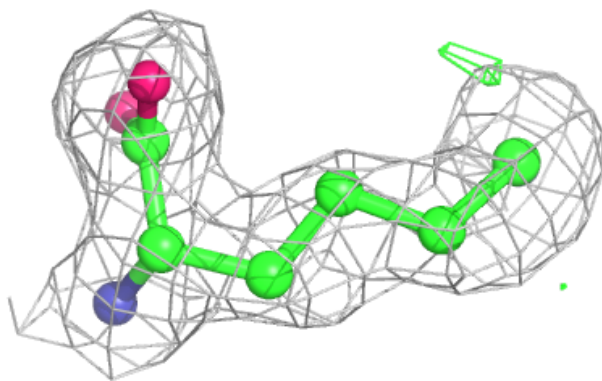
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





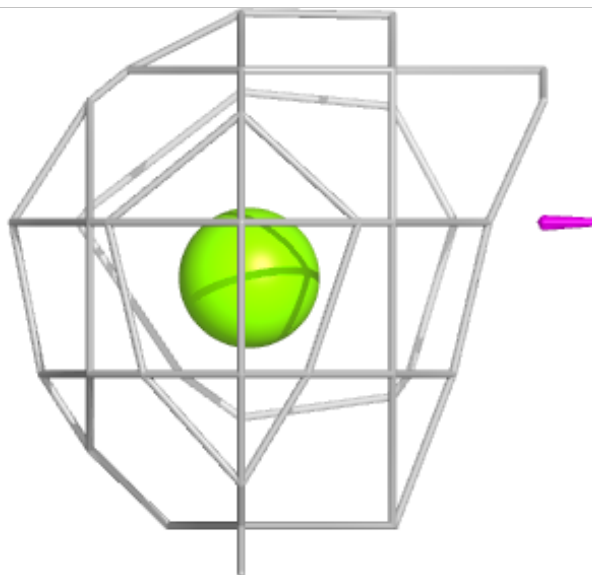
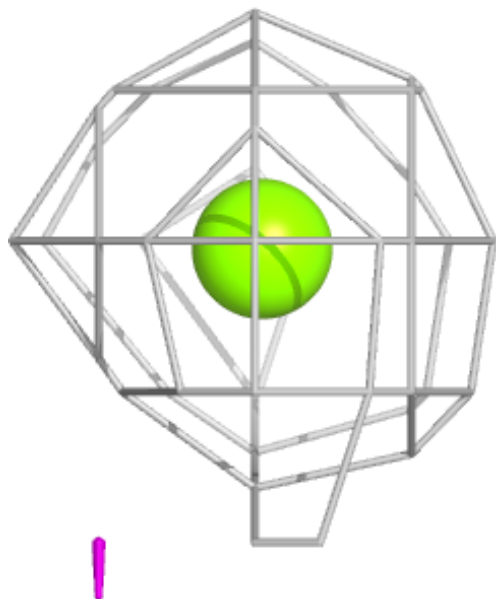
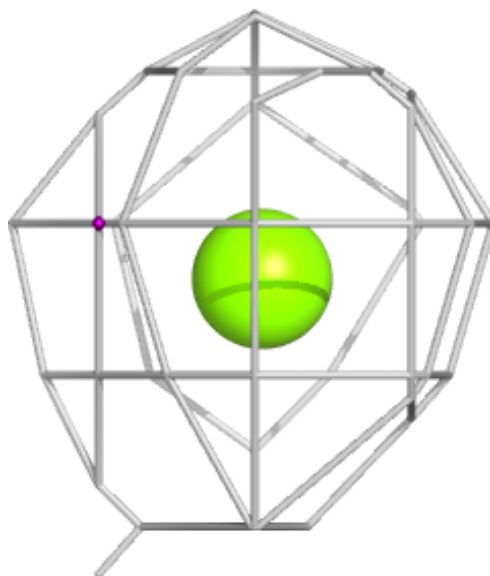
**Electron density around LYS B 302:**

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



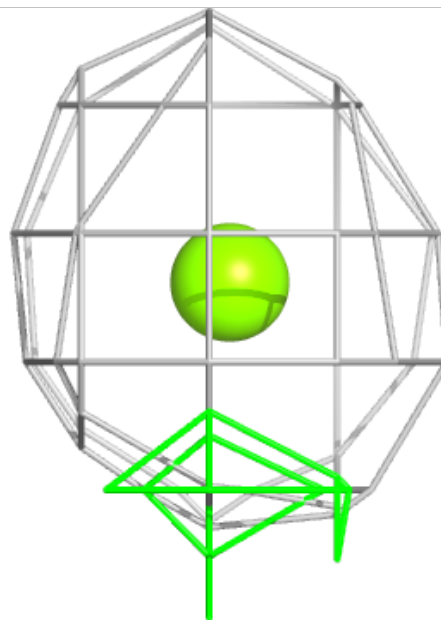
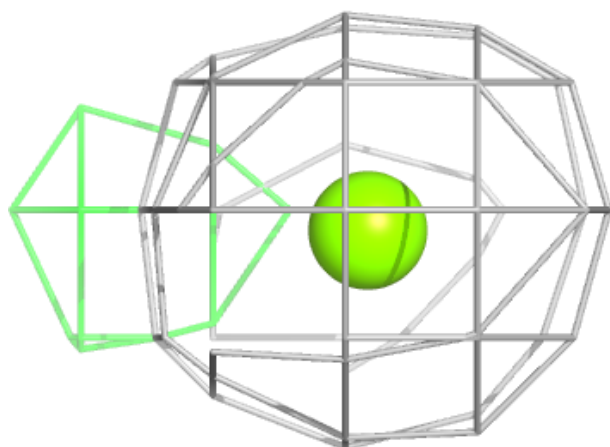
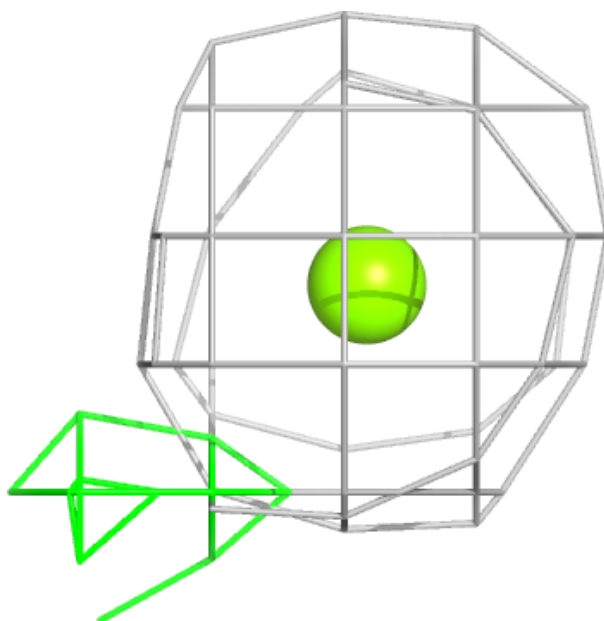
**Electron density around MG A 310:**

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



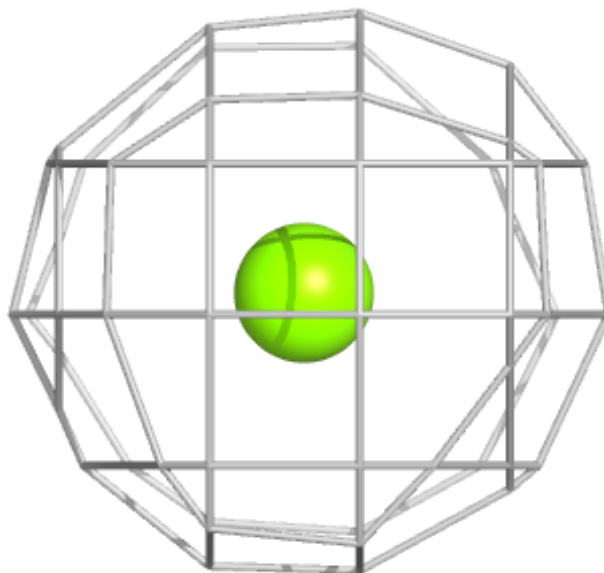
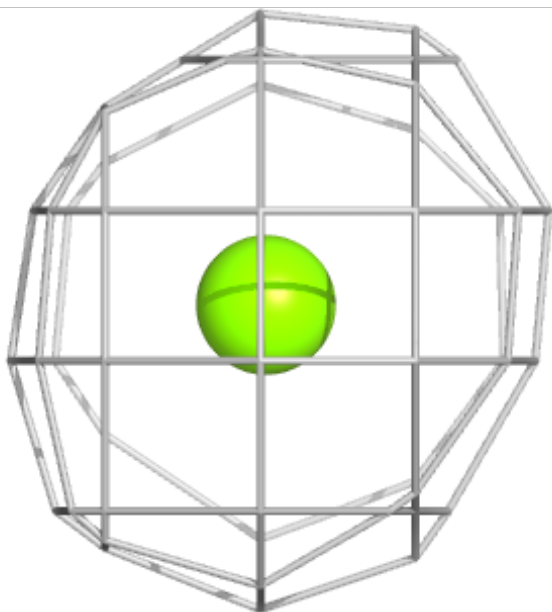
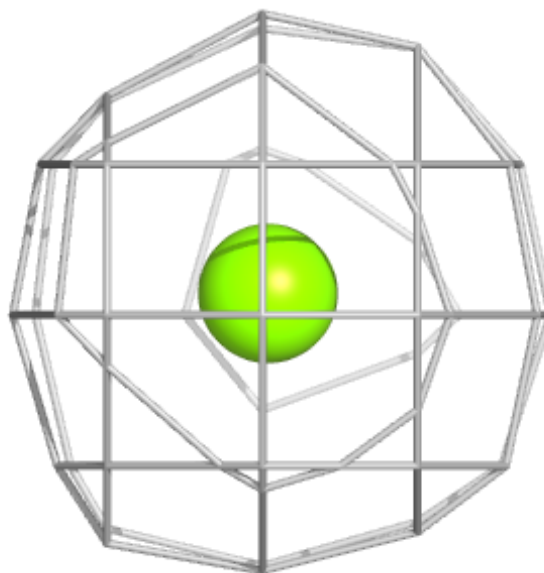
**Electron density around MG C 306:**

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



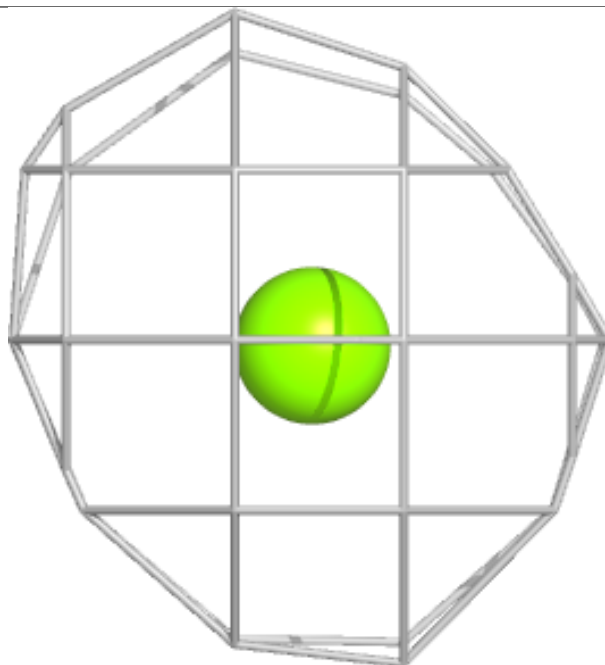
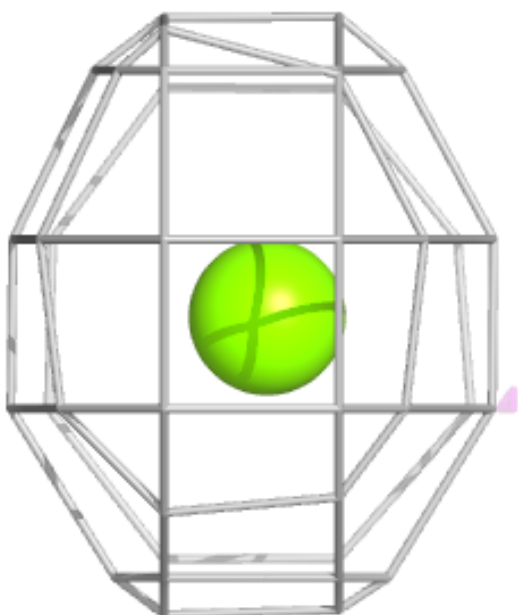
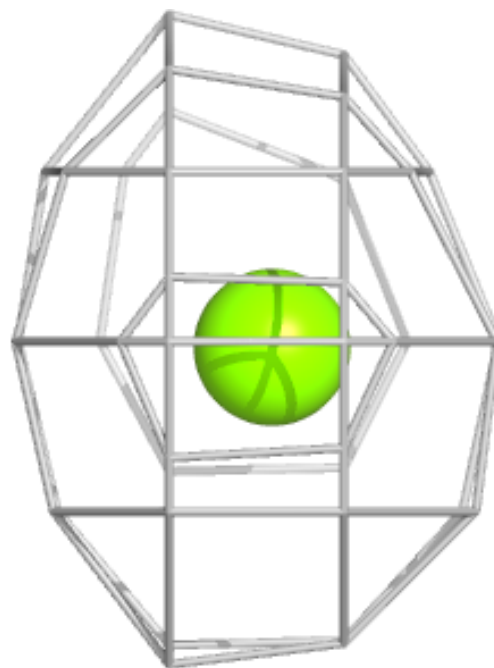
**Electron density around MG D 307:**

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



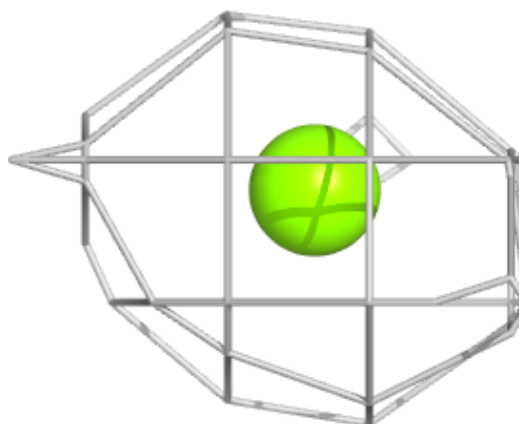
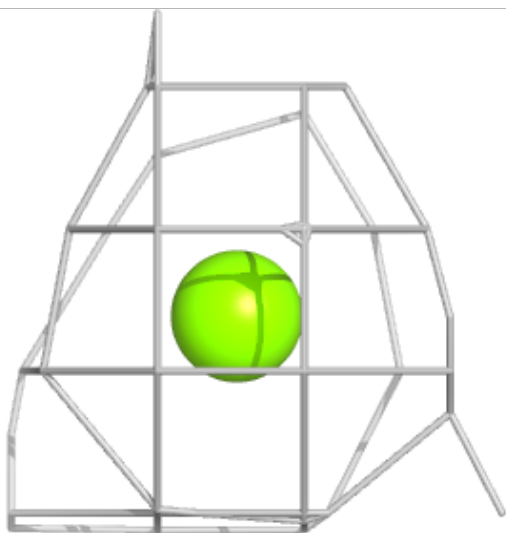
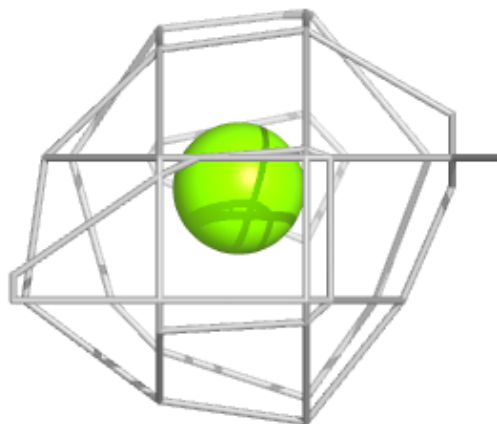
**Electron density around MG D 308:**

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



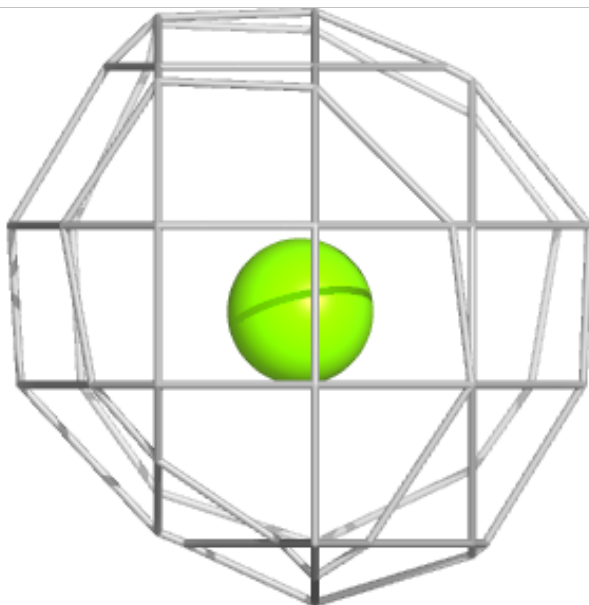
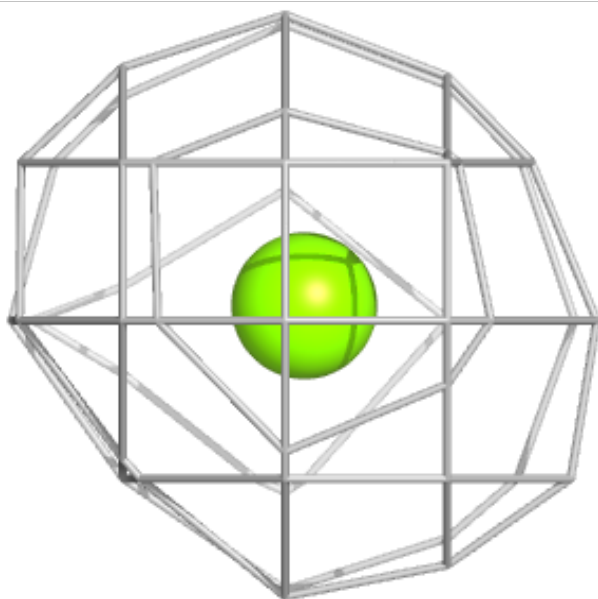
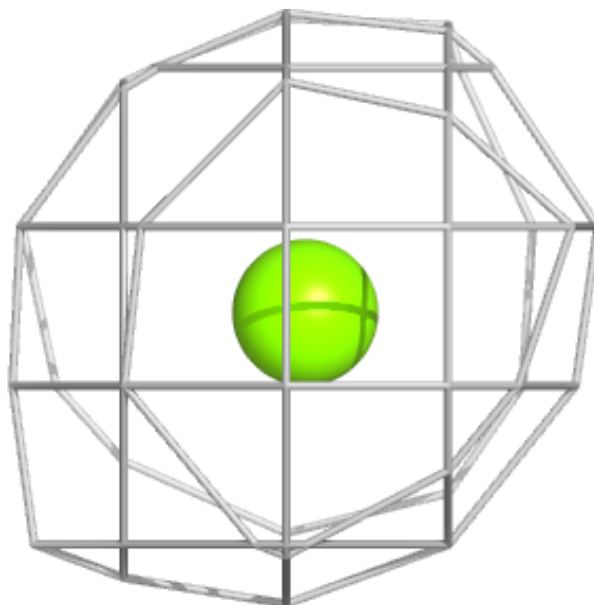
**Electron density around MG F 311:**

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



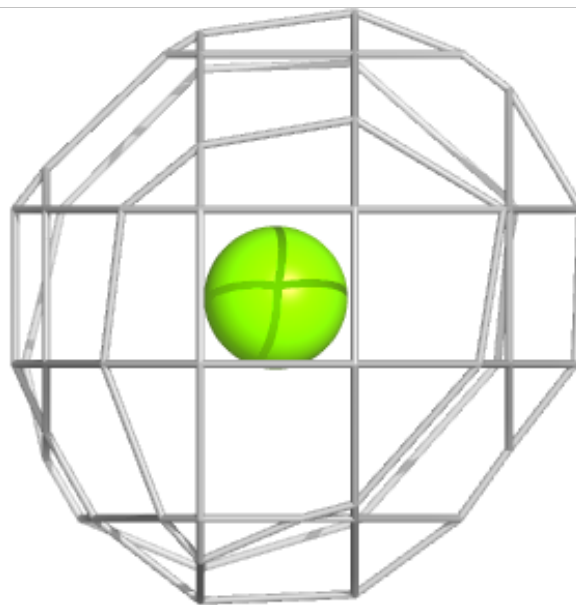
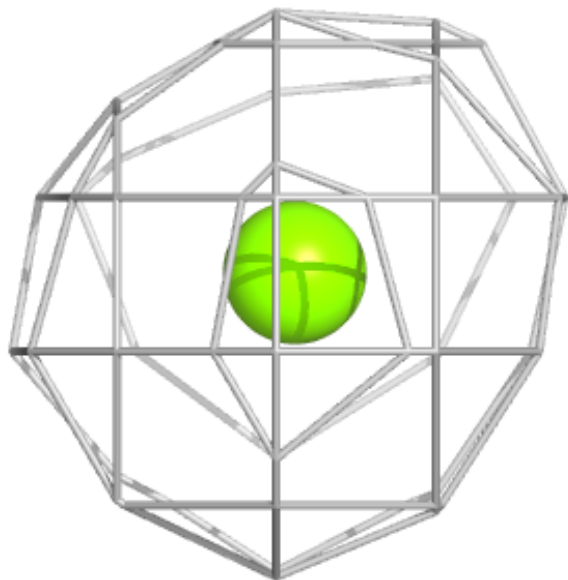
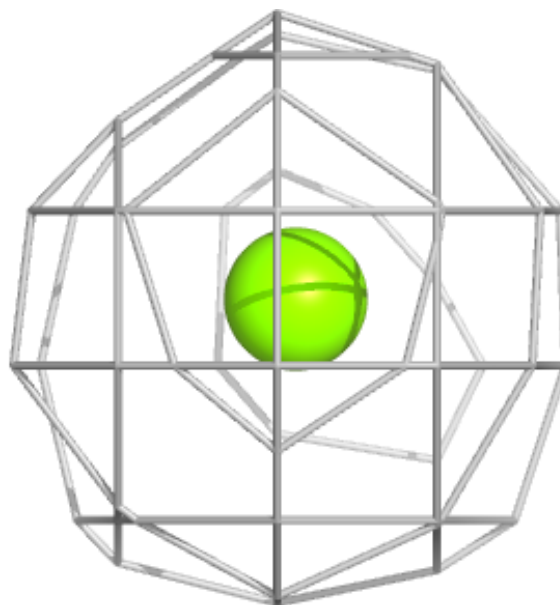
**Electron density around MG B 313:**

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



**Electron density around MG F 310:**

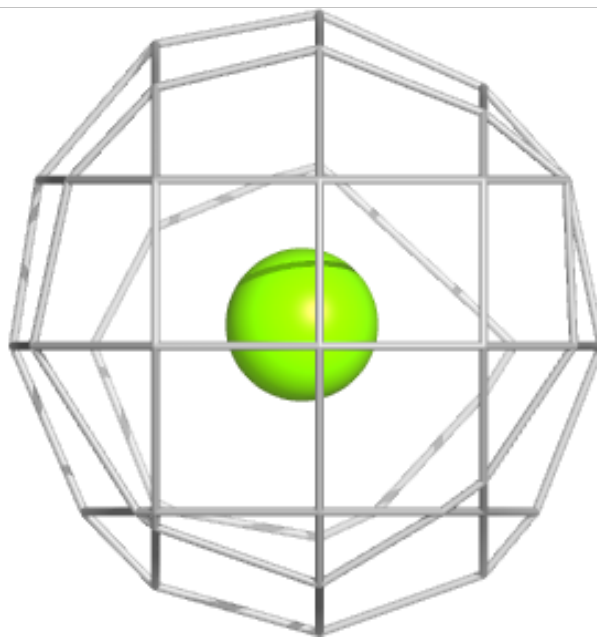
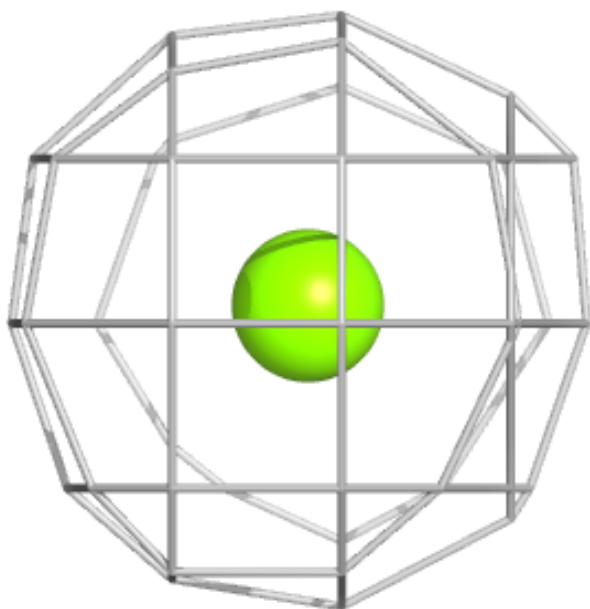
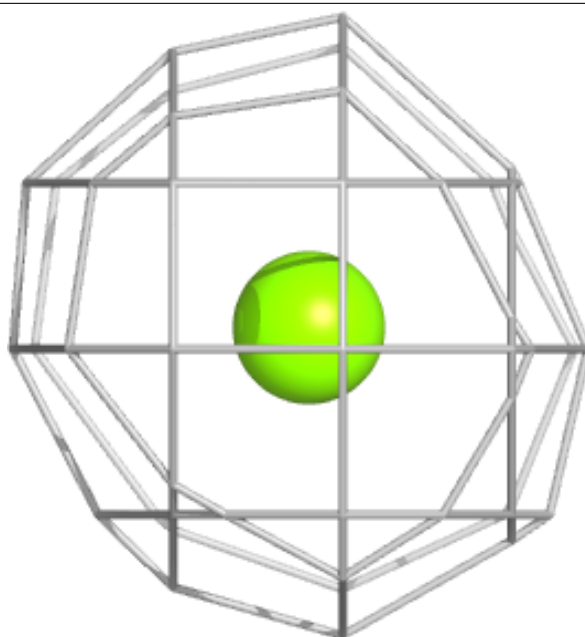
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





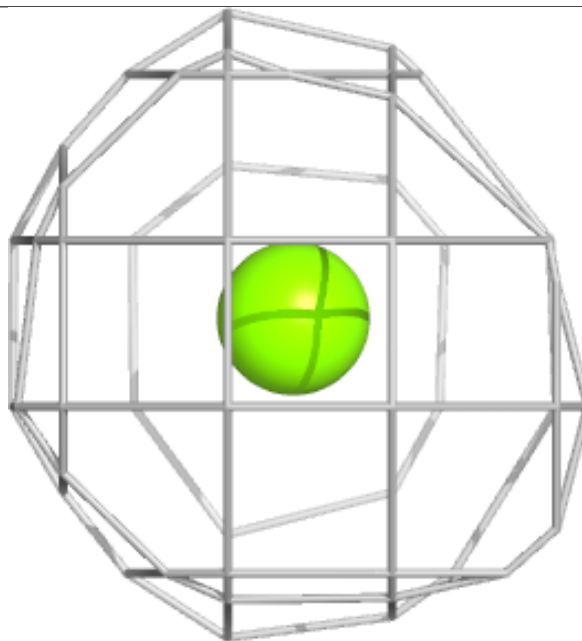
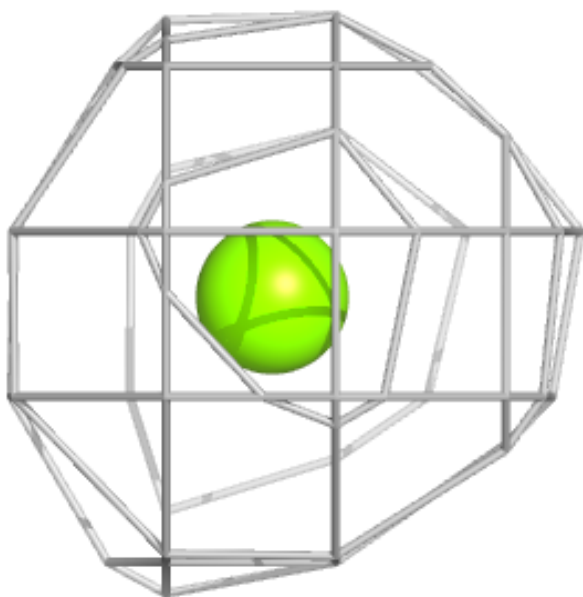
**Electron density around MG E 308:**

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



**Electron density around MG A 309:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.