



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2021 – 12:24 PM EDT

PDB ID : 7KKD  
Title : Dihydrodipicolinate synthase (DHDPS) from C.jejuni, N84A mutant with pyruvate bound in the active site and R,R-bislysine bound at the allosteric site  
Authors : Saran, S.; Majdi Yazdi, M.; Sanders, D.A.R.  
Deposited on : 2020-10-27  
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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

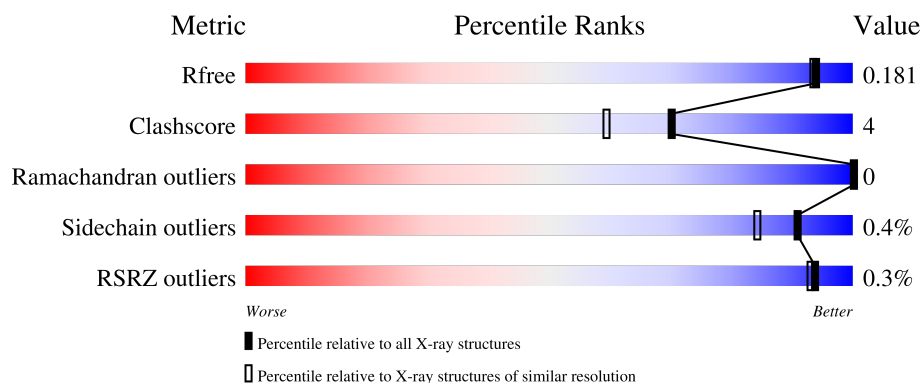
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	<div> <div>85%</div> <div>10%</div> <div>5%</div> </div>
1	B	310	<div> <div>%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	C	310	<div> <div>92%</div> <div>.</div> <div>5%</div> </div>
1	D	310	<div> <div>%</div> <div>94%</div> <div>5%</div> <div>.</div> </div>
1	E	310	<div> <div>87%</div> <div>8%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	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
5	EDO	E	303	-	-	X	X
6	PGE	E	304	-	-	X	-
6	PGE	F	305	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15889 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	1	0
			2273	1446	376	438	13			
1	B	306	Total	C	N	O	S	0	3	0
			2379	1507	404	454	14			
1	C	296	Total	C	N	O	S	0	1	0
			2278	1450	377	438	13			
1	D	306	Total	C	N	O	S	0	0	0
			2357	1495	398	450	14			
1	E	296	Total	C	N	O	S	0	1	0
			2275	1447	377	438	13			
1	F	296	Total	C	N	O	S	0	1	0
			2276	1449	379	435	13			

There are 78 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	84	ALA	ASN	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

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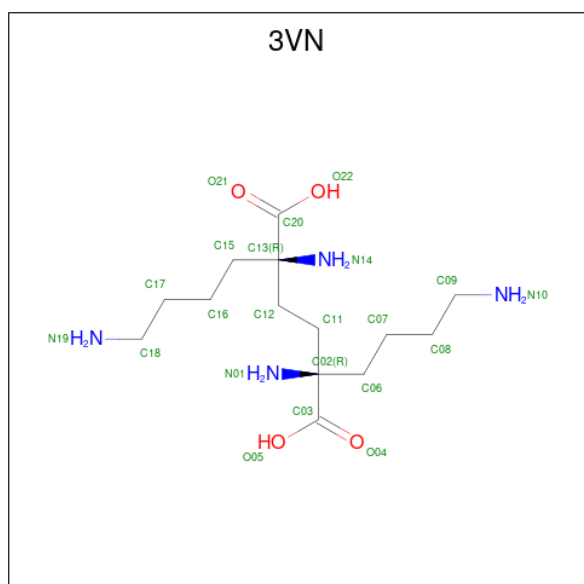
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
B	84	ALA	ASN	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	84	ALA	ASN	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	84	ALA	ASN	engineered mutation	UNP Q9PPB4
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	84	ALA	ASN	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
F	-2	HIS	-	expression tag	UNP Q9PPB4
F	-1	GLY	-	expression tag	UNP Q9PPB4
F	0	SER	-	expression tag	UNP Q9PPB4
F	84	ALA	ASN	engineered mutation	UNP Q9PPB4

- Molecule 2 is (2R,5R)-2,5-diamino-2,5-bis(4-aminobutyl)hexanedioic acid (three-letter code: 3VN) (formula: C<sub>14</sub>H<sub>30</sub>N<sub>4</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	O	
			22	14	4	4	
							0
							0

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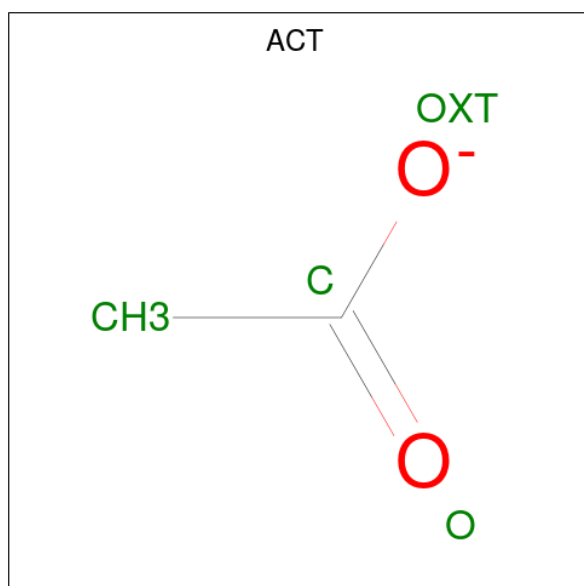
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			22	14	4	4		
2	C	1	Total	C	N	O	0	0
			22	14	4	4		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	4	Total	Mg	0	0
			4	4		
3	C	1	Total	Mg	0	0
			1	1		
3	D	2	Total	Mg	0	0
			2	2		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



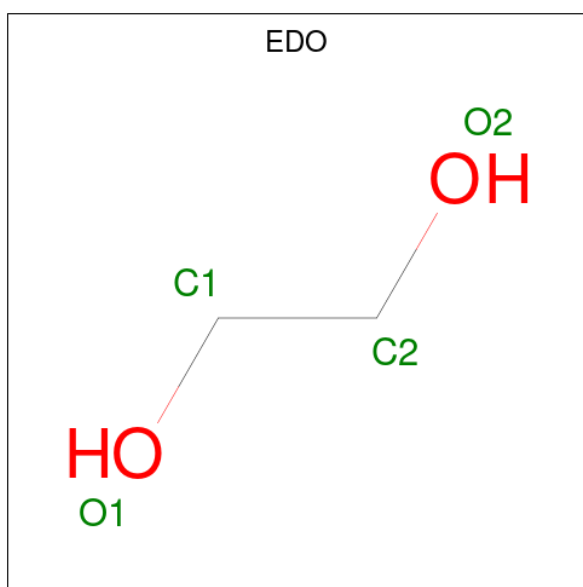
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

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

- 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		

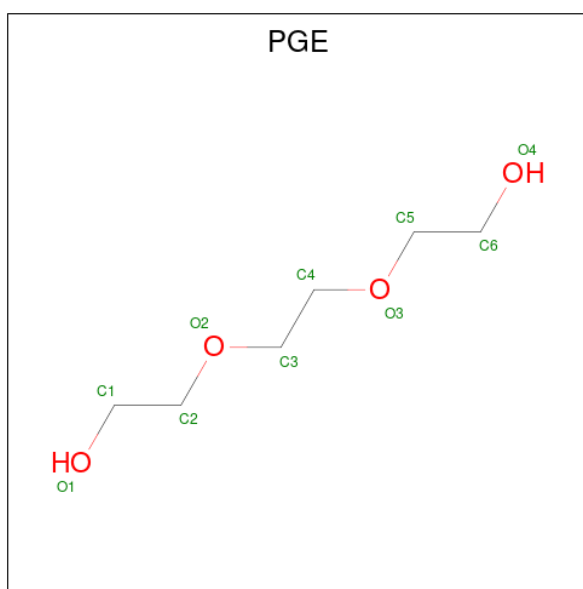
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0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

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



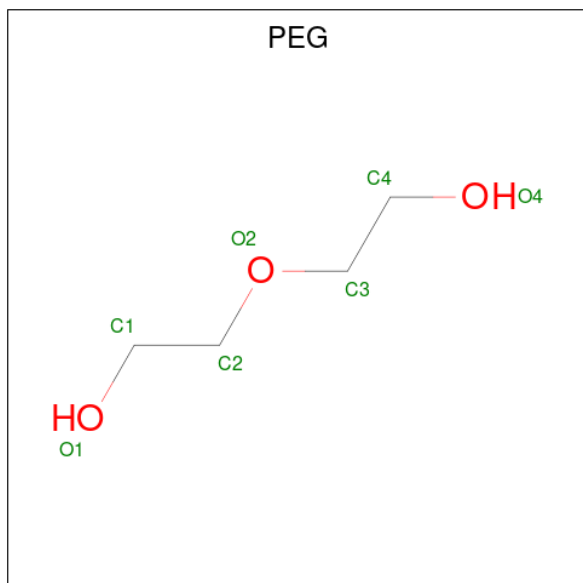
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		
6	D	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		

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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	316	Total	O	0	0
			316	316		
8	B	311	Total	O	0	0
			311	311		
8	C	343	Total	O	0	0
			343	343		
8	D	317	Total	O	0	0
			317	317		
8	E	282	Total	O	0	0
			282	282		

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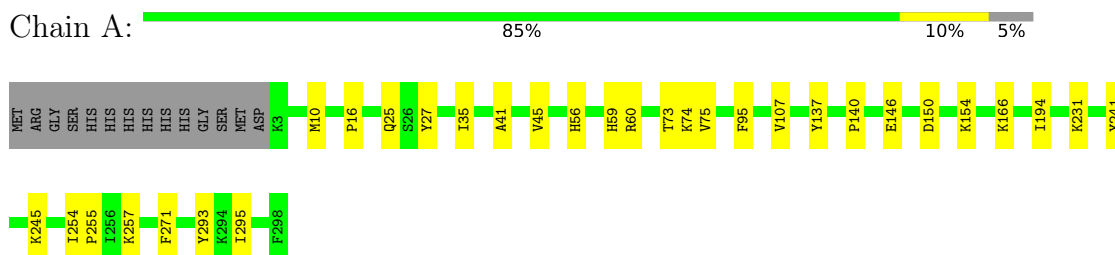
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	F	263	Total 263	O 263	0	0

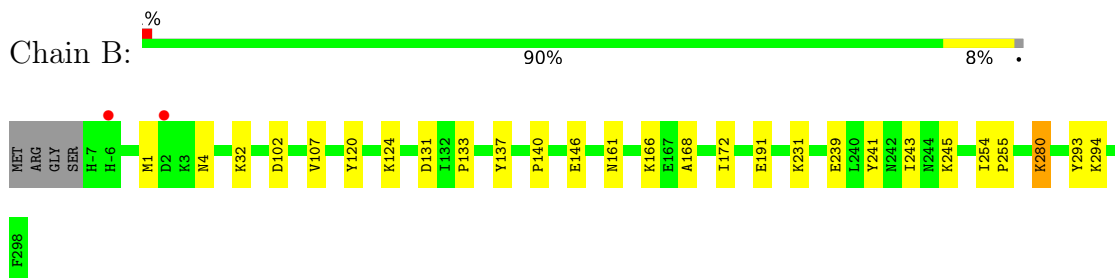
### 3 Residue-property plots

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

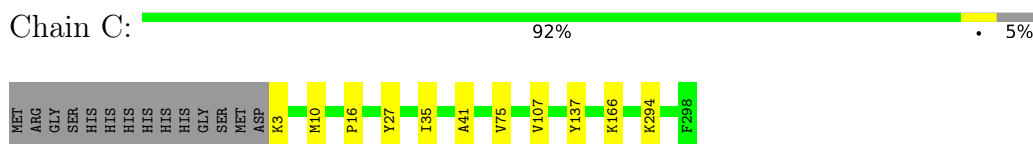
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



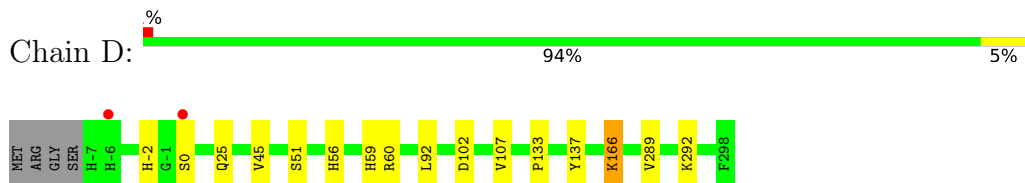
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



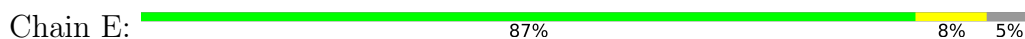
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

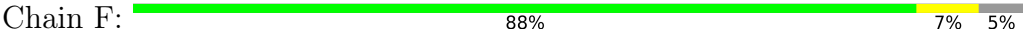


- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase





- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.55Å 225.54Å 199.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.11 – 1.60 49.11 – 1.60	Depositor EDS
% Data completeness (in resolution range)	91.9 (49.11-1.60) 88.8 (49.11-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.153 , 0.182 0.153 , 0.181	Depositor DCC
$R_{free}$ test set	11421 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.5	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15889	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: KPI, ACT, 3VN, PGE, PEG, EDO, MG

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	0.40	0/2298	0.54	0/3107
1	B	0.36	0/2411	0.53	0/3259
1	C	0.38	0/2303	0.54	0/3112
1	D	0.36	0/2385	0.56	0/3224
1	E	0.32	0/2300	0.53	0/3109
1	F	0.32	0/2302	0.52	0/3112
All	All	0.36	0/13999	0.54	0/18923

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	166	KPI	Mainchain

### 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	2273	0	2302	21	0
1	B	2379	0	2386	16	0
1	C	2278	0	2315	6	0
1	D	2357	0	2365	13	0
1	E	2275	0	2309	25	0
1	F	2276	0	2311	21	0
2	A	22	0	28	0	0
2	B	22	0	28	0	0
2	C	22	0	28	2	0
3	A	1	0	0	0	0
3	B	4	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
3	F	1	0	0	0	0
4	A	8	0	6	0	0
4	B	8	0	6	0	0
4	C	8	0	6	0	0
4	D	4	0	3	0	0
4	E	4	0	3	0	0
4	F	8	0	6	0	0
5	A	8	0	12	3	0
5	B	16	0	24	1	0
5	C	4	0	6	0	0
5	E	8	0	12	6	0
5	F	4	0	6	0	0
6	A	10	0	14	0	0
6	B	10	0	14	0	0
6	D	10	0	14	0	0
6	E	10	0	14	6	0
6	F	10	0	14	6	0
7	A	7	0	10	0	0
7	E	7	0	10	0	0
8	A	316	0	0	0	0
8	B	311	0	0	2	0
8	C	343	0	0	3	0
8	D	317	0	0	2	0
8	E	282	0	0	4	0
8	F	263	0	0	7	0
All	All	15889	0	14252	103	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 4.



All (103) 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:E:150:ASP:HB3	6:E:304:PGE:H12	1.61	0.81
1:F:150:ASP:HB3	6:F:305:PGE:H52	1.65	0.78
1:D:0:SER:HB3	8:D:407:HOH:O	1.83	0.78
1:D:-2:HIS:C	1:D:0:SER:H	1.92	0.72
1:D:-2:HIS:O	1:D:0:SER:N	2.23	0.72
1:A:295:ILE:HD12	1:A:295:ILE:N	2.06	0.71
1:E:18:LYS:NZ	8:E:401:HOH:O	2.21	0.69
1:F:3:LYS:N	8:F:401:HOH:O	2.25	0.69
1:F:154:LYS:HZ2	6:F:305:PGE:H5	1.58	0.68
1:F:113:LYS:NZ	8:F:403:HOH:O	2.28	0.64
2:C:301:3VN:N10	8:C:402:HOH:O	2.30	0.63
1:E:26:SER:CB	5:E:303:EDO:H12	2.29	0.62
1:D:289:VAL:O	1:D:292:LYS:HE3	2.00	0.61
1:E:26:SER:HB2	5:E:303:EDO:H12	1.82	0.61
1:F:154:LYS:HZ2	6:F:305:PGE:H4	1.65	0.60
1:F:280:LYS:H	1:F:280:LYS:CE	2.16	0.58
1:E:231:LYS:HG2	1:E:235:LYS:HE3	1.85	0.58
1:F:280:LYS:H	1:F:280:LYS:HE2	1.69	0.57
1:D:0:SER:O	1:D:0:SER:OG	2.22	0.56
1:F:262:LEU:HD21	1:F:283:PHE:CZ	2.41	0.56
1:A:73:THR:HB	5:A:306:EDO:H11	1.88	0.56
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.87	0.56
1:F:107:VAL:HA	1:F:137:TYR:HB3	1.87	0.55
1:B:280:LYS:HD2	8:B:591:HOH:O	2.07	0.54
1:B:161[A]:ASN:OD1	1:B:161[A]:ASN:N	2.41	0.54
1:E:154:LYS:HD2	6:E:304:PGE:H3	1.90	0.53
1:F:21:LYS:NZ	8:F:404:HOH:O	2.33	0.53
1:B:131:ASP:HA	1:B:161[B]:ASN:HD21	1.73	0.53
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.92	0.52
1:D:-2:HIS:C	1:D:0:SER:N	2.60	0.52
1:B:241:TYR:CE2	1:B:245:LYS:HG3	2.46	0.51
1:A:16:PRO:HD2	1:A:27:TYR:HD1	1.77	0.50
1:B:239:GLU:HG3	8:B:509:HOH:O	2.12	0.50
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.93	0.50
1:B:107:VAL:HA	1:B:137:TYR:HB3	1.93	0.49
1:E:252:ASN:ND2	1:E:253:PRO:HA	2.27	0.49
1:A:74:LYS:H	5:A:306:EDO:H22	1.77	0.49
1:E:292:LYS:HE2	8:E:602:HOH:O	2.13	0.48
1:C:35:ILE:HG12	1:C:75:VAL:HG21	1.95	0.48
1:E:154:LYS:HZ1	6:E:304:PGE:H1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:HIS:O	1:A:60:ARG:HG3	2.14	0.48
1:B:4:ASN:HB2	1:B:133:PRO:HG3	1.95	0.48
1:A:150:ASP:O	1:A:154:LYS:HG3	2.14	0.48
1:E:241:TYR:CE2	1:E:245:LYS:HG3	2.49	0.48
1:C:3:LYS:N	8:C:405:HOH:O	2.45	0.48
1:B:140:PRO:HG3	1:B:146:GLU:OE1	2.14	0.47
1:A:295:ILE:N	1:A:295:ILE:CD1	2.72	0.47
1:E:154:LYS:NZ	6:E:304:PGE:H1	2.29	0.47
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.95	0.47
1:C:294:LYS:HE3	8:C:661:HOH:O	2.15	0.46
1:E:292:LYS:O	1:E:292:LYS:HG2	2.15	0.46
1:F:154:LYS:NZ	6:F:305:PGE:H5	2.28	0.46
1:F:154:LYS:HD2	6:F:305:PGE:H2	1.97	0.46
1:D:292:LYS:HD2	8:D:424:HOH:O	2.15	0.46
1:A:241:TYR:CE2	1:A:245:LYS:HG3	2.51	0.46
1:B:1:MET:SD	5:B:308:EDO:H11	2.56	0.46
1:E:16:PRO:HB2	5:E:303:EDO:H22	1.98	0.46
1:E:26:SER:OG	5:E:303:EDO:H11	2.16	0.46
1:E:267:GLU:N	5:E:303:EDO:O1	2.41	0.46
1:C:16:PRO:HD2	1:C:27:TYR:HD1	1.81	0.46
1:B:168:ALA:HA	1:B:191:GLU:HG3	1.98	0.45
1:B:120:TYR:OH	1:B:124:LYS:HE3	2.16	0.45
1:F:287:GLU:O	1:F:291:LYS:HD2	2.16	0.45
1:D:45:VAL:HG21	1:D:59:HIS:CD2	2.52	0.45
6:F:305:PGE:H4	6:F:305:PGE:H22	1.77	0.45
1:F:140:PRO:HG3	1:F:146:GLU:OE1	2.17	0.45
1:F:3:LYS:N	8:F:410:HOH:O	2.50	0.45
1:F:16:PRO:HD2	1:F:27:TYR:HD1	1.81	0.45
1:E:26:SER:OG	5:E:303:EDO:C1	2.66	0.44
1:A:74:LYS:H	5:A:306:EDO:C2	2.30	0.44
1:A:60:ARG:HB3	1:A:95:PHE:CZ	2.53	0.44
1:B:32:LYS:HB3	1:B:32:LYS:HE3	1.61	0.44
1:A:10:MET:HG2	1:A:41:ALA:HB3	2.00	0.44
1:F:87[A]:HIS:HD2	8:F:630:HOH:O	2.00	0.44
1:A:45:VAL:HG21	1:A:59:HIS:CD2	2.54	0.43
1:D:56:HIS:CE1	1:D:92:LEU:HD21	2.53	0.43
1:E:25:GLN:NE2	1:E:25:GLN:H	2.16	0.43
1:A:35:ILE:HG12	1:A:75:VAL:HG21	2.01	0.43
1:E:289:VAL:HG13	8:E:514:HOH:O	2.18	0.43
2:C:301:3VN:H9	1:D:51:SER:O	2.19	0.42
1:A:257:LYS:HD3	1:A:271:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:GLU:H	1:E:57:GLU:CD	2.23	0.42
1:E:168:ALA:HA	1:E:191:GLU:HG3	2.00	0.42
1:A:140:PRO:HG3	1:A:146:GLU:OE1	2.20	0.42
1:E:280:LYS:HG2	8:E:435:HOH:O	2.19	0.42
1:A:293:TYR:O	1:A:295:ILE:CD1	2.68	0.41
1:A:231:LYS:HE3	1:A:231:LYS:HB3	1.70	0.41
1:E:117:GLN:OE1	6:E:304:PGE:H52	2.20	0.41
1:A:25:GLN:H	1:A:25:GLN:CD	2.24	0.41
1:B:243:ILE:HB	1:B:293:TYR:CE2	2.56	0.41
1:F:60:ARG:HB2	8:F:605:HOH:O	2.21	0.41
1:D:102:ASP:O	1:D:133:PRO:HD2	2.20	0.41
1:D:56:HIS:O	1:D:60:ARG:HG3	2.21	0.41
1:B:102:ASP:O	1:B:133:PRO:HD2	2.21	0.40
1:B:254:ILE:HB	1:B:255:PRO:HD3	2.02	0.40
1:E:154:LYS:CE	6:E:304:PGE:H1	2.51	0.40
1:C:10:MET:HG2	1:C:41:ALA:HB3	2.03	0.40
1:A:194:ILE:HG21	1:B:172:ILE:HG23	2.03	0.40
1:A:254:ILE:HB	1:A:255:PRO:HD3	2.02	0.40
1:F:280:LYS:HE2	1:F:280:LYS:HB2	1.96	0.40
1:E:243:ILE:HB	1:E:293:TYR:CE2	2.57	0.40
1:F:245:LYS:HD2	8:F:523:HOH:O	2.22	0.40
1:F:254:ILE:HA	1:F:271:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/310 (95%)	287 (98%)	7 (2%)	0	100	100
1	B	306/310 (99%)	299 (98%)	7 (2%)	0	100	100
1	C	294/310 (95%)	288 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	303/310 (98%)	295 (97%)	8 (3%)	0	100	100
1	E	294/310 (95%)	288 (98%)	6 (2%)	0	100	100
1	F	294/310 (95%)	287 (98%)	7 (2%)	0	100	100
All	All	1785/1860 (96%)	1744 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	245/259 (95%)	245 (100%)	0	100	100
1	B	257/259 (99%)	254 (99%)	3 (1%)	71	54
1	C	246/259 (95%)	246 (100%)	0	100	100
1	D	253/259 (98%)	252 (100%)	1 (0%)	91	84
1	E	246/259 (95%)	246 (100%)	0	100	100
1	F	245/259 (95%)	243 (99%)	2 (1%)	81	70
All	All	1492/1554 (96%)	1486 (100%)	6 (0%)	91	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	231	LYS
1	B	280	LYS
1	B	294	LYS
1	D	25	GLN
1	F	231	LYS
1	F	280	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	B	128	GLN
1	D	19	ASN
1	D	25	GLN
1	E	25	GLN
1	E	242	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	F	166	1	10,13,14	1.21	1 (10%)	6,15,17	3.10	3 (50%)
1	KPI	C	166	1	10,13,14	1.33	1 (10%)	6,15,17	2.63	2 (33%)
1	KPI	D	166	1	10,13,14	1.28	1 (10%)	6,15,17	2.36	2 (33%)
1	KPI	B	166	1	10,13,14	0.69	0	6,15,17	2.54	2 (33%)
1	KPI	A	166	1	10,13,14	0.72	0	6,15,17	2.57	2 (33%)
1	KPI	E	166	1	10,13,14	1.37	1 (10%)	6,15,17	2.00	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	F	166	1	-	0/9/14/16	-
1	KPI	C	166	1	-	0/9/14/16	-
1	KPI	D	166	1	-	0/9/14/16	-
1	KPI	B	166	1	-	0/9/14/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KPI	A	166	1	-	0/9/14/16	-
1	KPI	E	166	1	-	0/9/14/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	166	KPI	O-C	3.83	1.35	1.19
1	E	166	KPI	O-C	3.77	1.35	1.19
1	C	166	KPI	O-C	3.73	1.34	1.19
1	F	166	KPI	O-C	3.52	1.34	1.19

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	166	KPI	C1-CX1-CX2	-6.23	111.02	117.92
1	A	166	KPI	C1-CX1-CX2	-5.10	112.27	117.92
1	C	166	KPI	C1-CX1-CX2	-5.08	112.30	117.92
1	B	166	KPI	C1-CX1-CX2	-4.94	112.45	117.92
1	D	166	KPI	C1-CX1-CX2	-4.59	112.84	117.92
1	F	166	KPI	C1-CX1-NZ	3.27	131.27	123.12
1	E	166	KPI	C1-CX1-NZ	3.21	131.12	123.12
1	C	166	KPI	C1-CX1-NZ	3.03	130.69	123.12
1	B	166	KPI	C1-CX1-NZ	2.98	130.55	123.12
1	D	166	KPI	C1-CX1-NZ	2.86	130.25	123.12
1	A	166	KPI	C1-CX1-NZ	2.78	130.05	123.12
1	E	166	KPI	C1-CX1-CX2	-2.74	114.88	117.92
1	E	166	KPI	CE-NZ-CX1	2.16	127.58	121.77
1	F	166	KPI	CE-NZ-CX1	2.07	127.33	121.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 39 ligands modelled in this entry, 9 are monoatomic - leaving 30 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
5	EDO	B	310	-	3,3,3	0.37	0	2,2,2	1.23	0
5	EDO	B	309	-	3,3,3	0.46	0	2,2,2	0.28	0
5	EDO	C	305	-	3,3,3	0.44	0	2,2,2	0.38	0
4	ACT	C	304	-	1,3,3	6.54	1 (100%)	0,3,3	-	-
6	PGE	E	304	-	9,9,9	0.27	0	8,8,8	0.39	0
5	EDO	A	306	-	3,3,3	0.29	0	2,2,2	0.66	0
6	PGE	B	312	-	9,9,9	0.25	0	8,8,8	0.30	0
7	PEG	A	308	-	6,6,6	0.51	0	5,5,5	0.26	0
7	PEG	E	305	-	6,6,6	0.46	0	5,5,5	0.36	0
4	ACT	B	307	-	1,3,3	6.12	1 (100%)	0,3,3	-	-
2	3VN	B	301	-	15,21,21	1.26	1 (6%)	12,28,28	1.60	3 (25%)
2	3VN	A	301	-	15,21,21	1.19	1 (6%)	12,28,28	1.75	5 (41%)
4	ACT	A	303	-	1,3,3	5.95	1 (100%)	0,3,3	-	-
4	ACT	C	303	-	1,3,3	6.06	1 (100%)	0,3,3	-	-
6	PGE	D	304	-	9,9,9	0.29	0	8,8,8	0.25	0
6	PGE	F	305	-	9,9,9	0.28	0	8,8,8	0.50	0
4	ACT	F	302	-	1,3,3	7.10	1 (100%)	0,3,3	-	-
4	ACT	D	303	-	1,3,3	7.16	1 (100%)	0,3,3	-	-
4	ACT	A	304	-	1,3,3	5.82	1 (100%)	0,3,3	-	-
5	EDO	B	311	3	3,3,3	0.36	0	2,2,2	0.42	0
5	EDO	B	308	-	3,3,3	0.40	0	2,2,2	0.49	0
2	3VN	C	301	-	15,21,21	1.21	1 (6%)	12,28,28	1.59	2 (16%)
4	ACT	F	303	-	1,3,3	6.13	1 (100%)	0,3,3	-	-
5	EDO	E	303	-	3,3,3	0.41	0	2,2,2	0.67	0
4	ACT	B	306	-	1,3,3	6.51	1 (100%)	0,3,3	-	-
6	PGE	A	307	-	9,9,9	0.33	0	8,8,8	0.18	0
5	EDO	A	305	-	3,3,3	0.52	0	2,2,2	0.21	0
5	EDO	E	302	-	3,3,3	0.44	0	2,2,2	0.43	0
5	EDO	F	304	-	3,3,3	0.56	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ACT	E	301	-	1,3,3	3.20	1 (100%)	0,3,3	-	-

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	310	-	-	1/1/1/1	-
5	EDO	B	309	-	-	1/1/1/1	-
5	EDO	C	305	-	-	1/1/1/1	-
6	PGE	E	304	-	-	3/7/7/7	-
5	EDO	A	306	-	-	0/1/1/1	-
6	PGE	B	312	-	-	1/7/7/7	-
7	PEG	A	308	-	-	3/4/4/4	-
7	PEG	E	305	-	-	2/4/4/4	-
2	3VN	B	301	-	-	0/19/31/31	-
2	3VN	A	301	-	-	1/19/31/31	-
6	PGE	D	304	-	-	0/7/7/7	-
6	PGE	F	305	-	-	4/7/7/7	-
5	EDO	B	311	3	-	0/1/1/1	-
5	EDO	B	308	-	-	1/1/1/1	-
2	3VN	C	301	-	-	2/19/31/31	-
5	EDO	E	303	-	-	1/1/1/1	-
6	PGE	A	307	-	-	0/7/7/7	-
5	EDO	A	305	-	-	1/1/1/1	-
5	EDO	E	302	-	-	0/1/1/1	-
5	EDO	F	304	-	-	0/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	303	ACT	CH3-C	7.16	1.57	1.48
4	F	302	ACT	CH3-C	7.10	1.57	1.48
4	C	304	ACT	CH3-C	6.54	1.57	1.48
4	B	306	ACT	CH3-C	6.51	1.57	1.48
4	F	303	ACT	CH3-C	6.13	1.56	1.48
4	B	307	ACT	CH3-C	6.12	1.56	1.48
4	C	303	ACT	CH3-C	6.06	1.56	1.48
4	A	303	ACT	CH3-C	5.95	1.56	1.48
4	A	304	ACT	CH3-C	5.82	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	301	ACT	CH3-C	3.20	1.52	1.48
2	B	301	3VN	C06-C02	2.90	1.58	1.55
2	A	301	3VN	C06-C02	2.83	1.58	1.55
2	C	301	3VN	C06-C02	2.55	1.57	1.55

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	3VN	C11-C12-C13	-3.12	109.68	115.19
2	C	301	3VN	C11-C12-C13	-2.85	110.15	115.19
2	A	301	3VN	C12-C11-C02	-2.53	110.72	115.19
2	B	301	3VN	C12-C11-C02	-2.43	110.91	115.19
2	B	301	3VN	C11-C02-C06	-2.42	106.84	111.94
2	A	301	3VN	C11-C02-C06	-2.32	107.06	111.94
2	B	301	3VN	C11-C12-C13	-2.26	111.20	115.19
2	A	301	3VN	C15-C13-C12	-2.16	107.38	111.94
2	C	301	3VN	C12-C11-C02	-2.12	111.45	115.19
2	A	301	3VN	C15-C16-C17	-2.07	107.03	113.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	304	PGE	O2-C3-C4-O3
7	A	308	PEG	O1-C1-C2-O2
6	E	304	PGE	O3-C5-C6-O4
7	A	308	PEG	O2-C3-C4-O4
5	A	305	EDO	O1-C1-C2-O2
5	B	309	EDO	O1-C1-C2-O2
5	B	310	EDO	O1-C1-C2-O2
2	C	301	3VN	C07-C08-C09-N10
6	F	305	PGE	O3-C5-C6-O4
7	A	308	PEG	C1-C2-O2-C3
6	B	312	PGE	C1-C2-O2-C3
7	E	305	PEG	C1-C2-O2-C3
6	F	305	PGE	C3-C4-O3-C5
5	E	303	EDO	O1-C1-C2-O2
6	E	304	PGE	C3-C4-O3-C5
2	C	301	3VN	C06-C07-C08-C09
5	C	305	EDO	O1-C1-C2-O2
7	E	305	PEG	O1-C1-C2-O2
2	A	301	3VN	C16-C17-C18-N19

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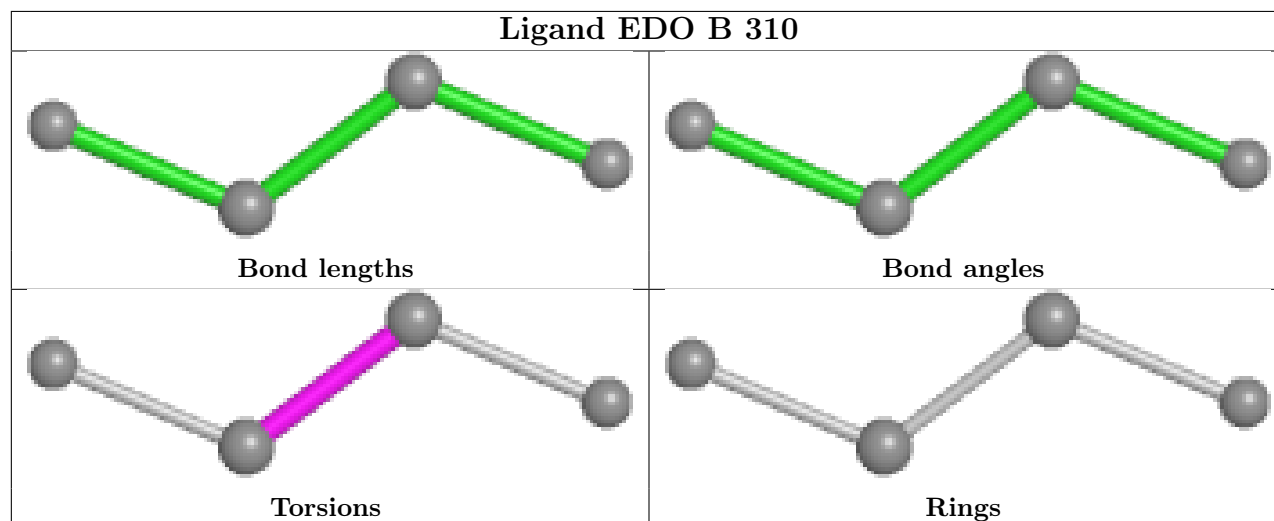
Mol	Chain	Res	Type	Atoms
5	B	308	EDO	O1-C1-C2-O2
6	F	305	PGE	C4-C3-O2-C2
6	F	305	PGE	O2-C3-C4-O3

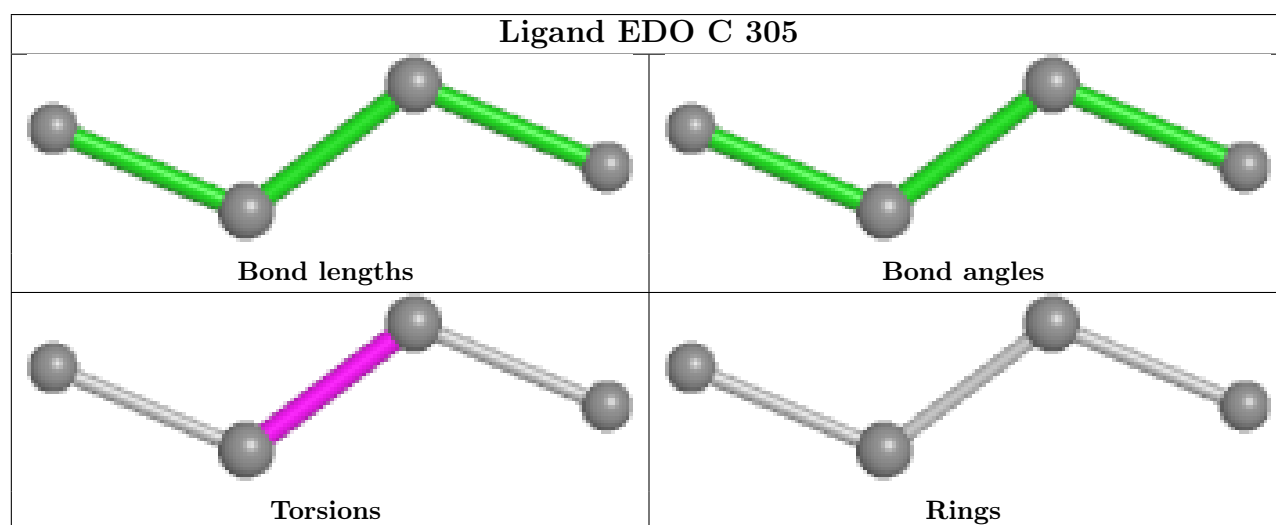
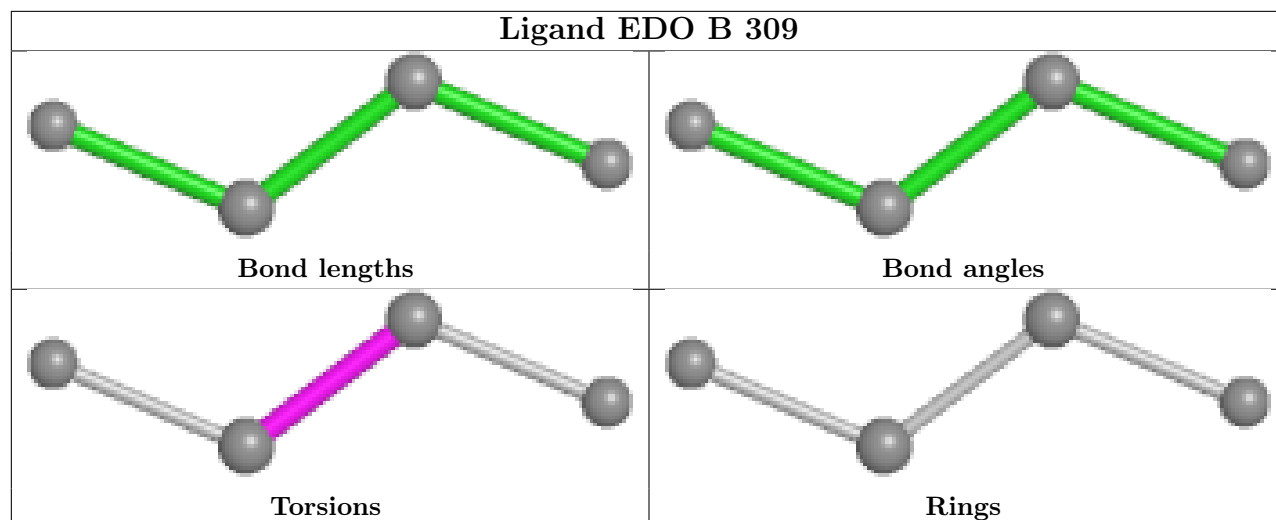
There are no ring outliers.

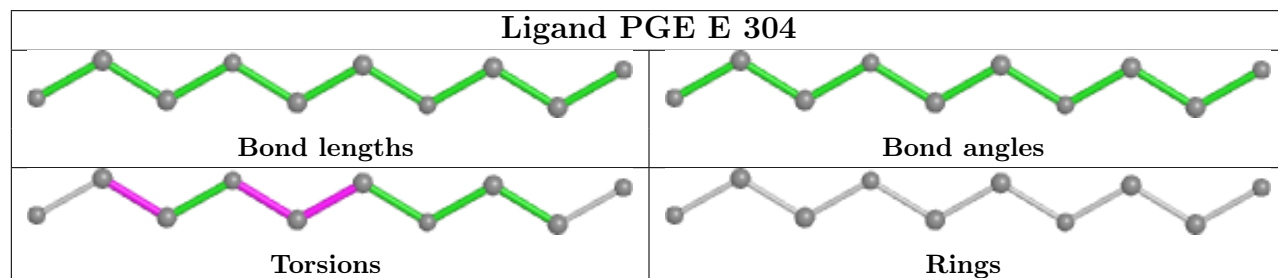
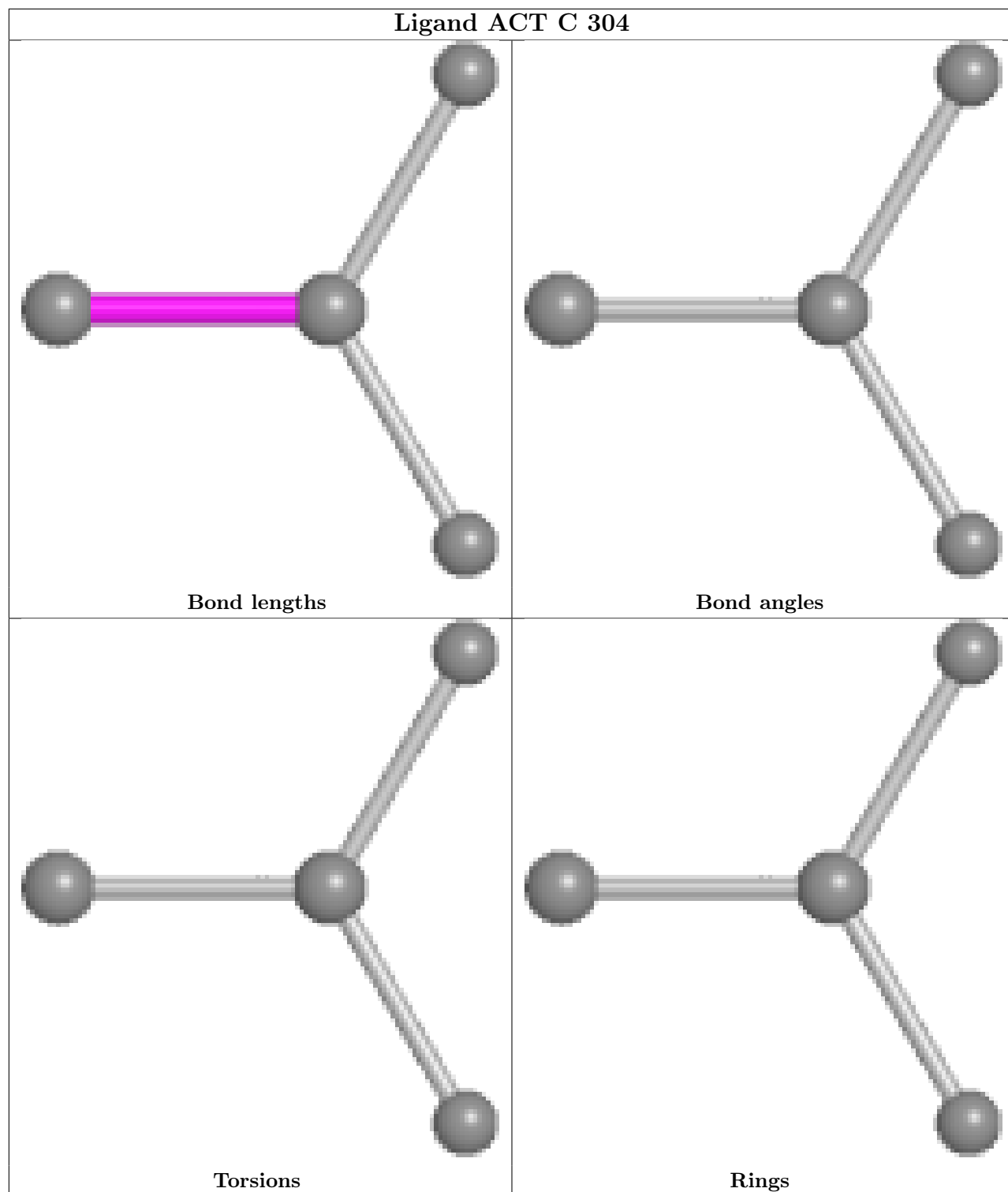
6 monomers are involved in 24 short contacts:

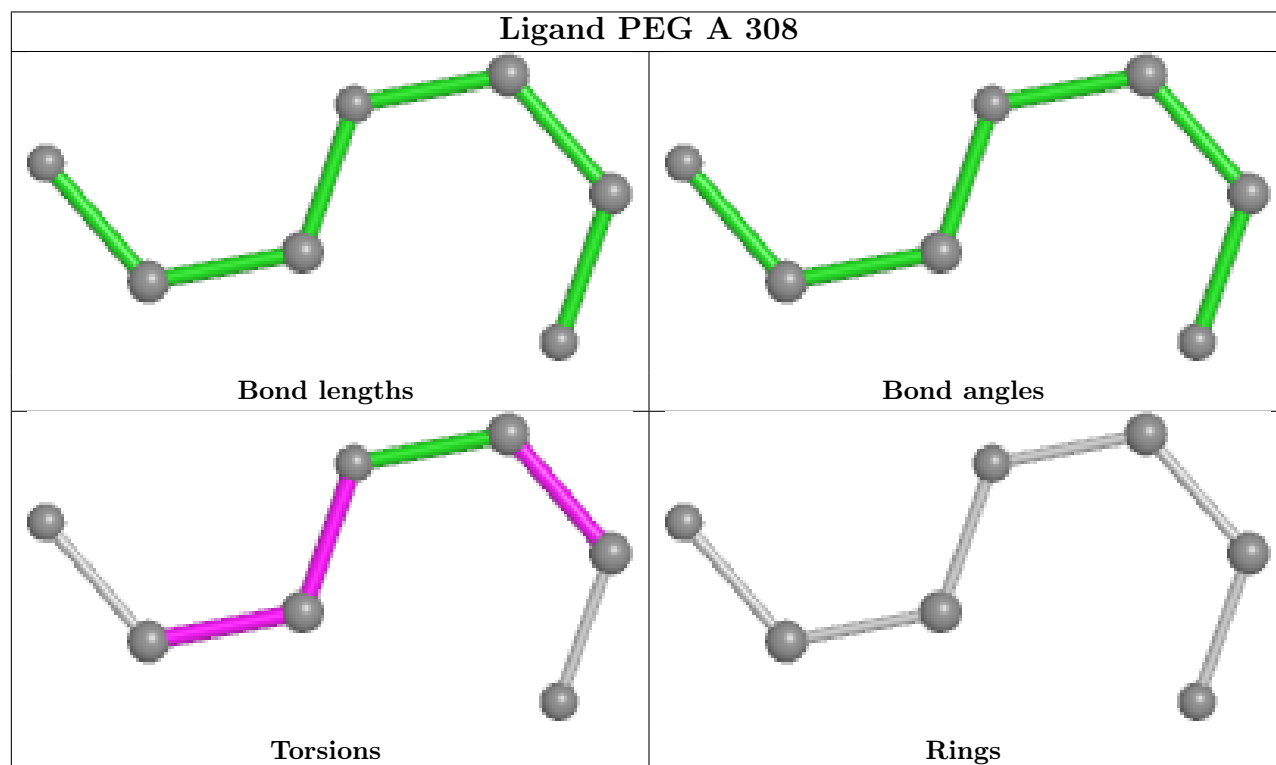
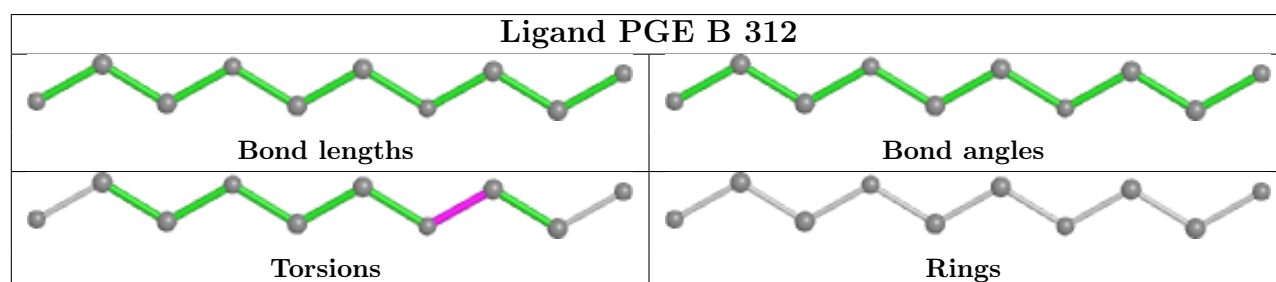
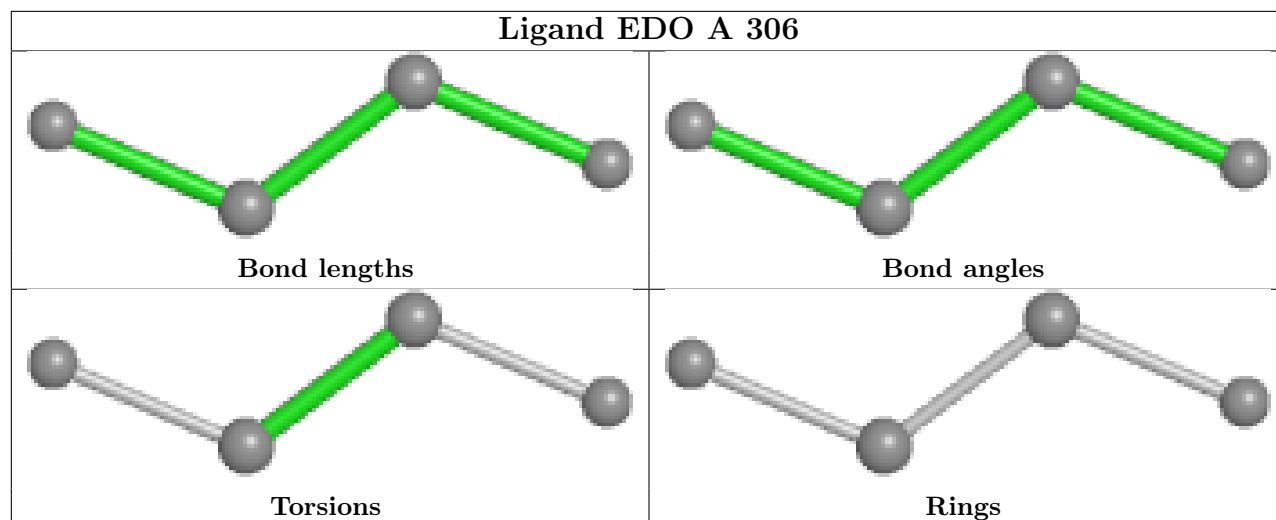
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	304	PGE	6	0
5	A	306	EDO	3	0
6	F	305	PGE	6	0
5	B	308	EDO	1	0
2	C	301	3VN	2	0
5	E	303	EDO	6	0

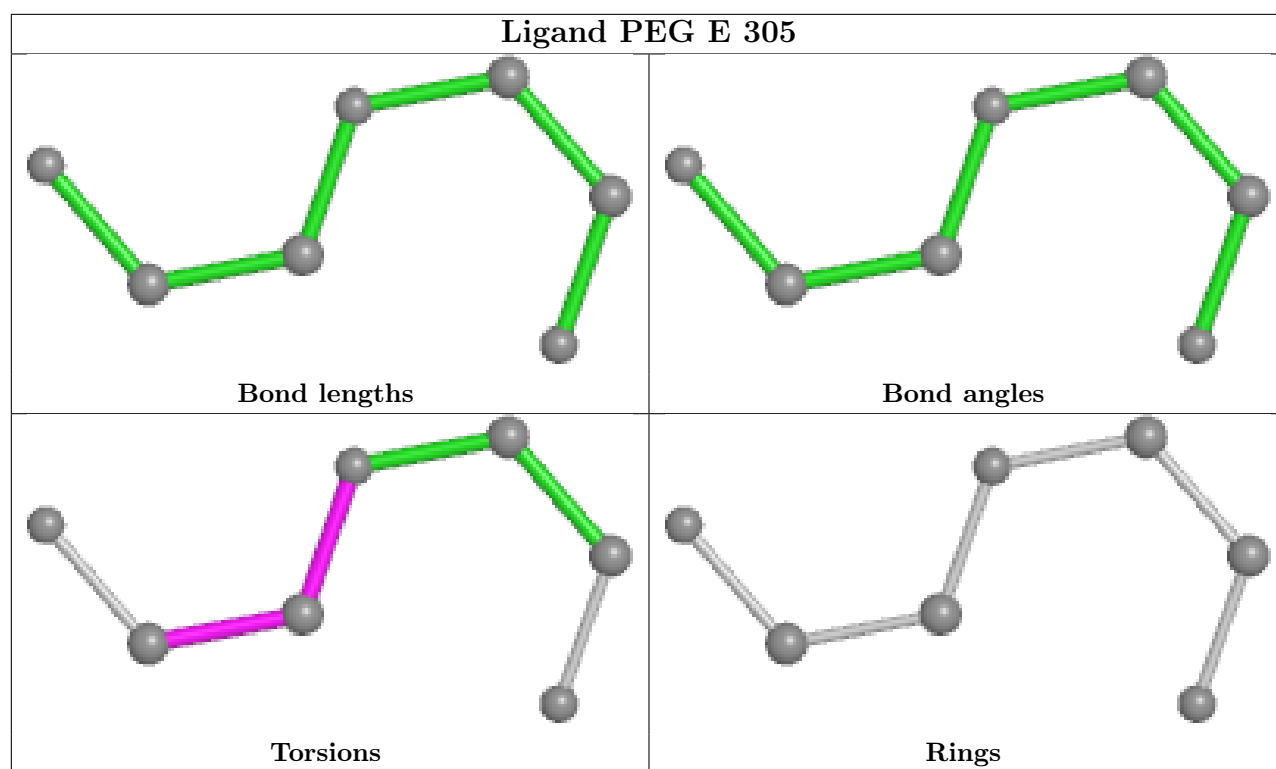
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

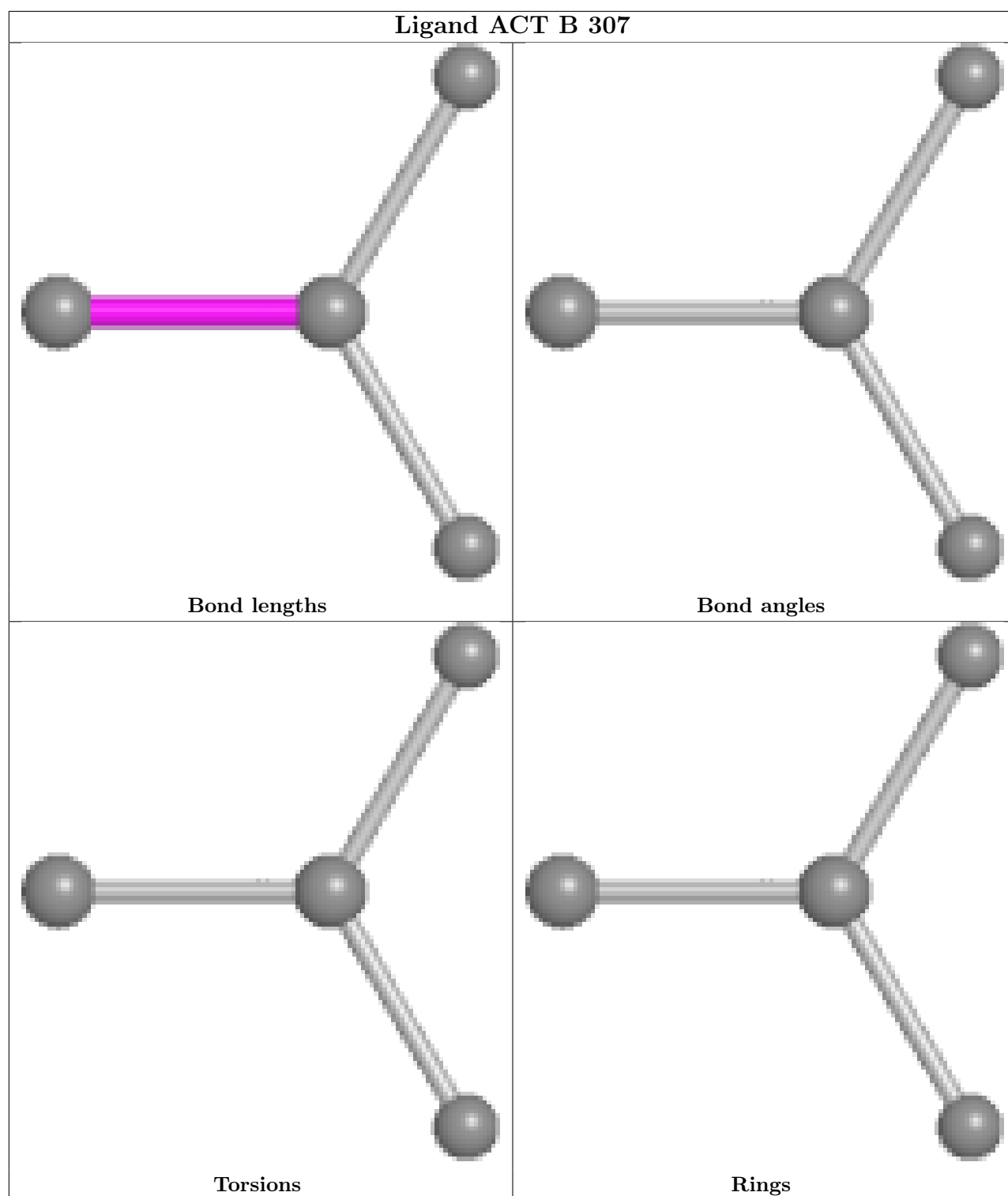




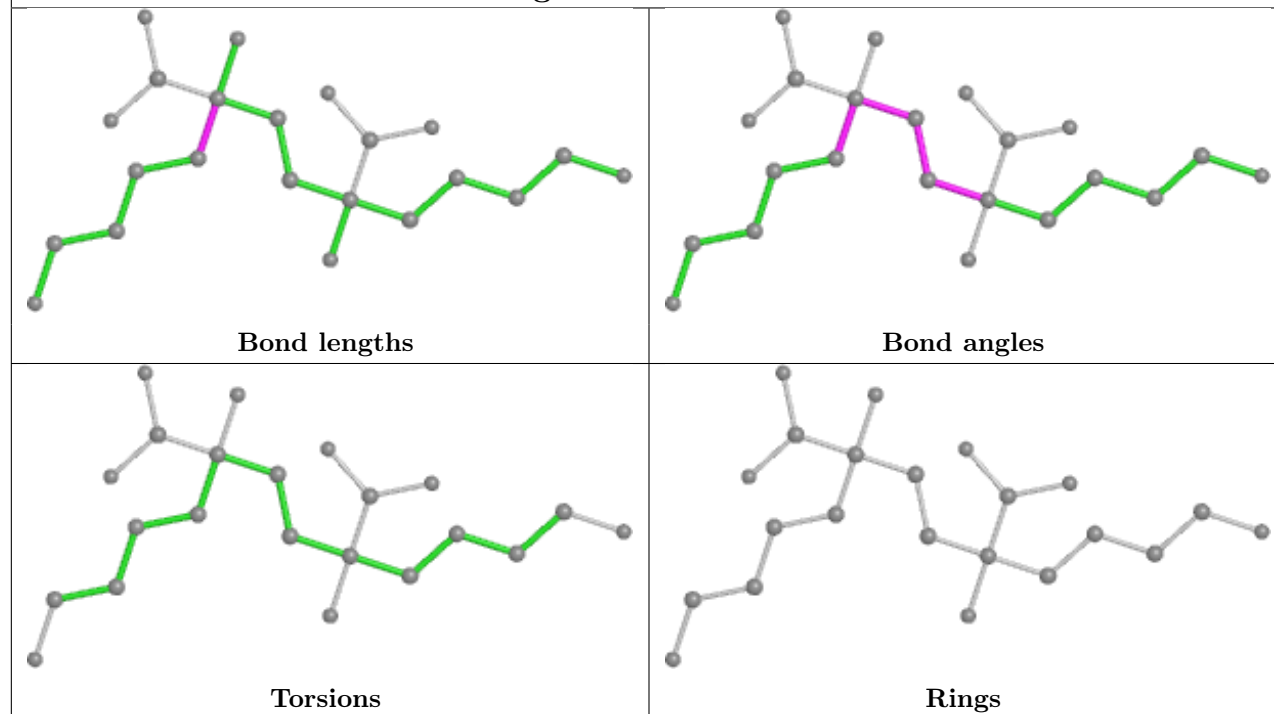




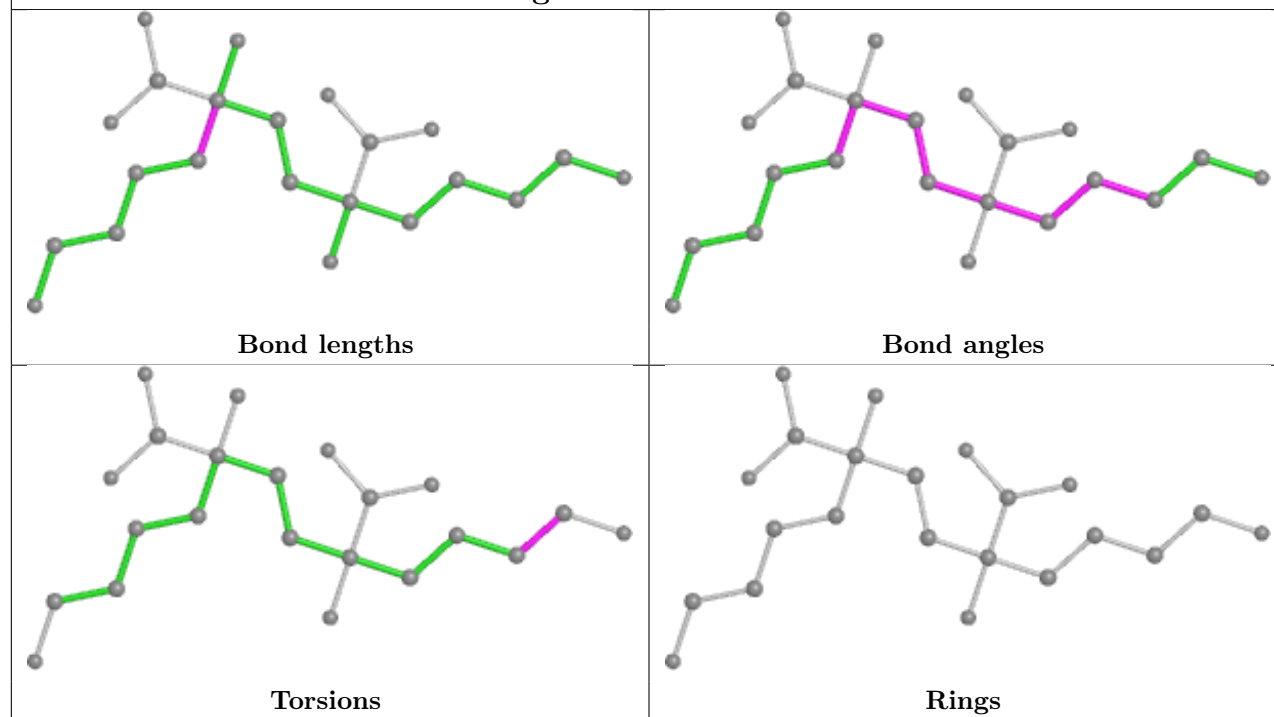




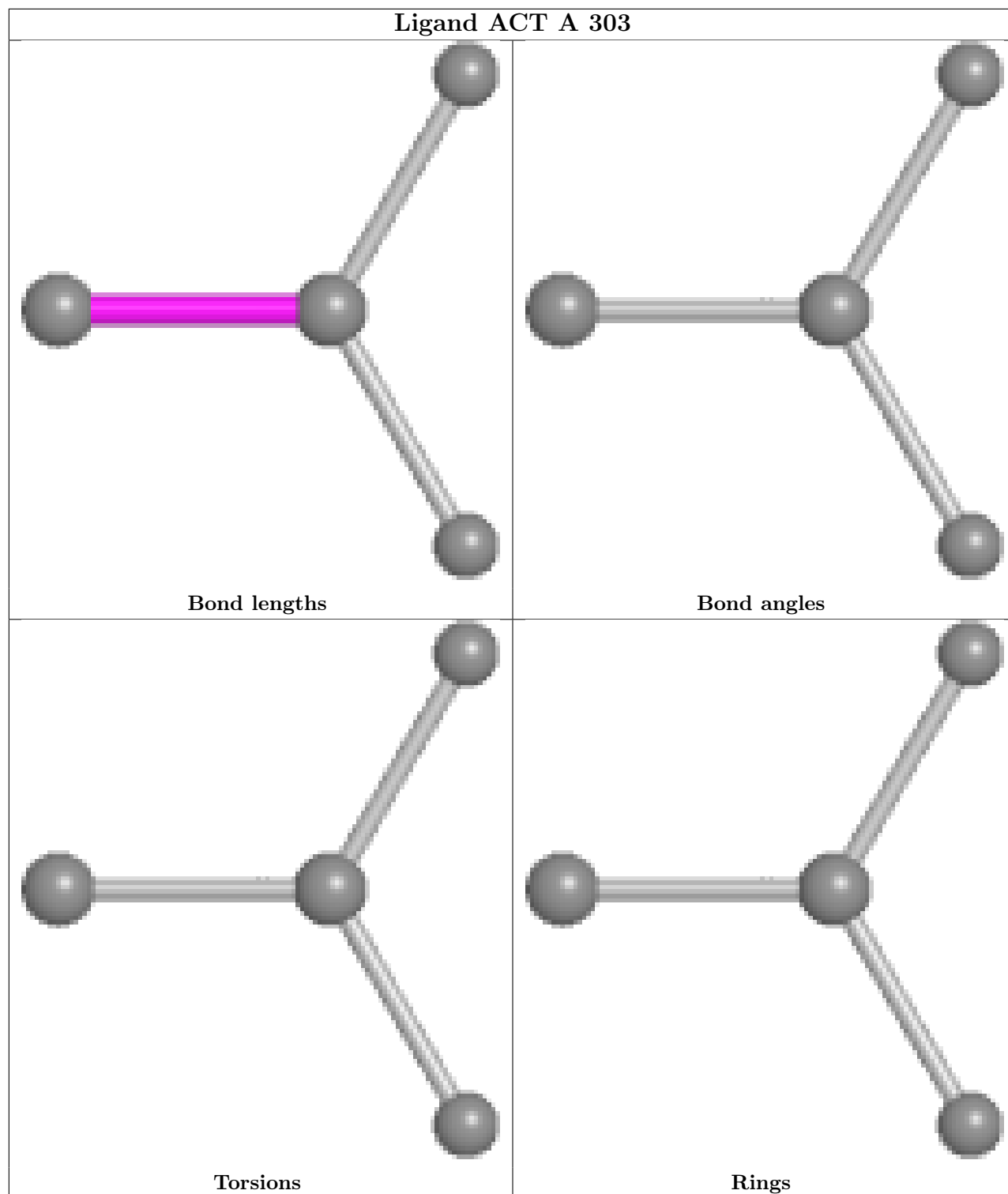
## Ligand 3VN B 301

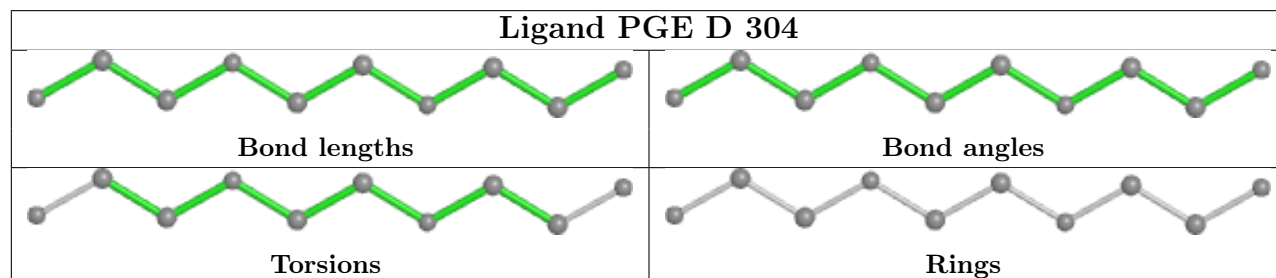
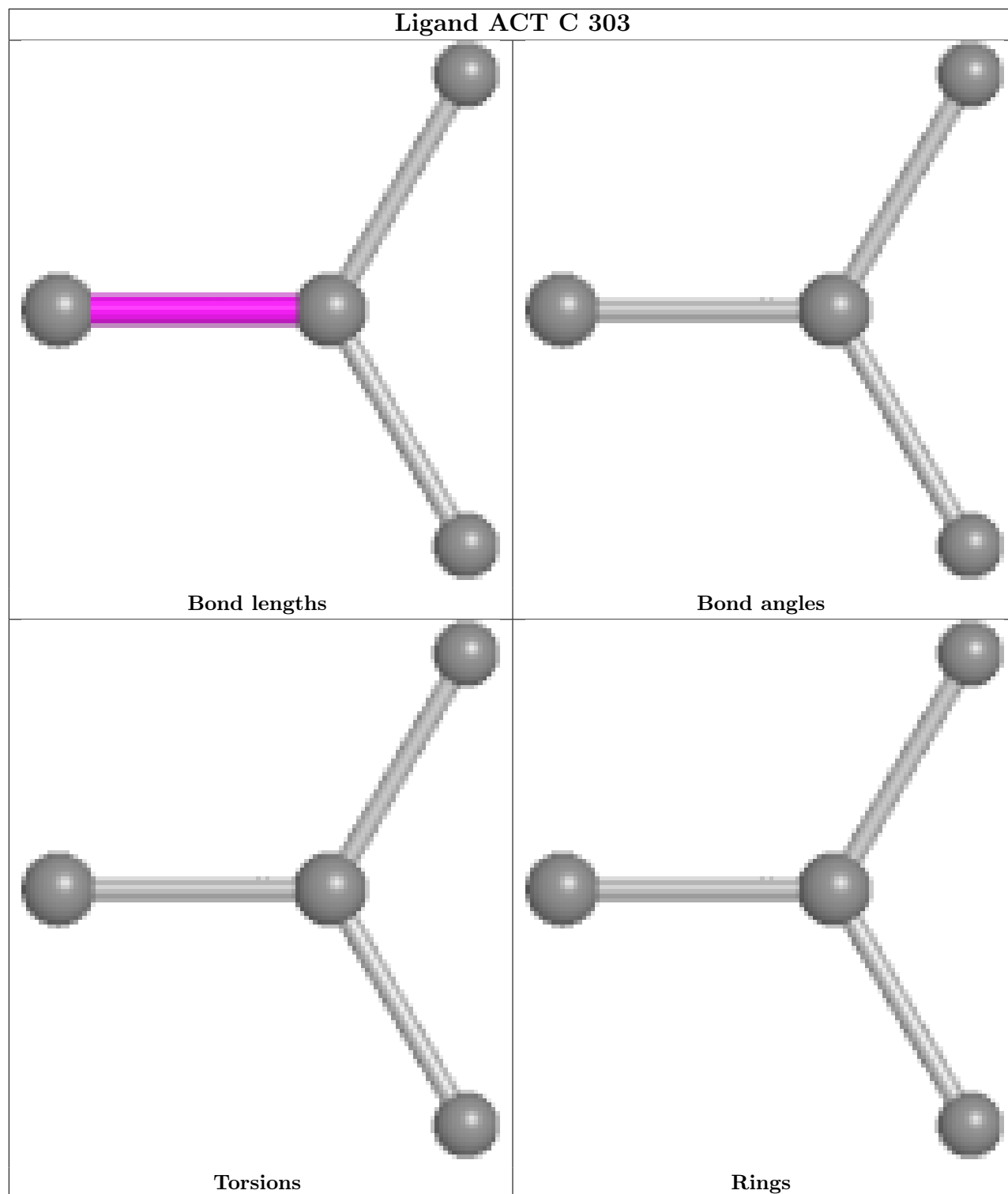


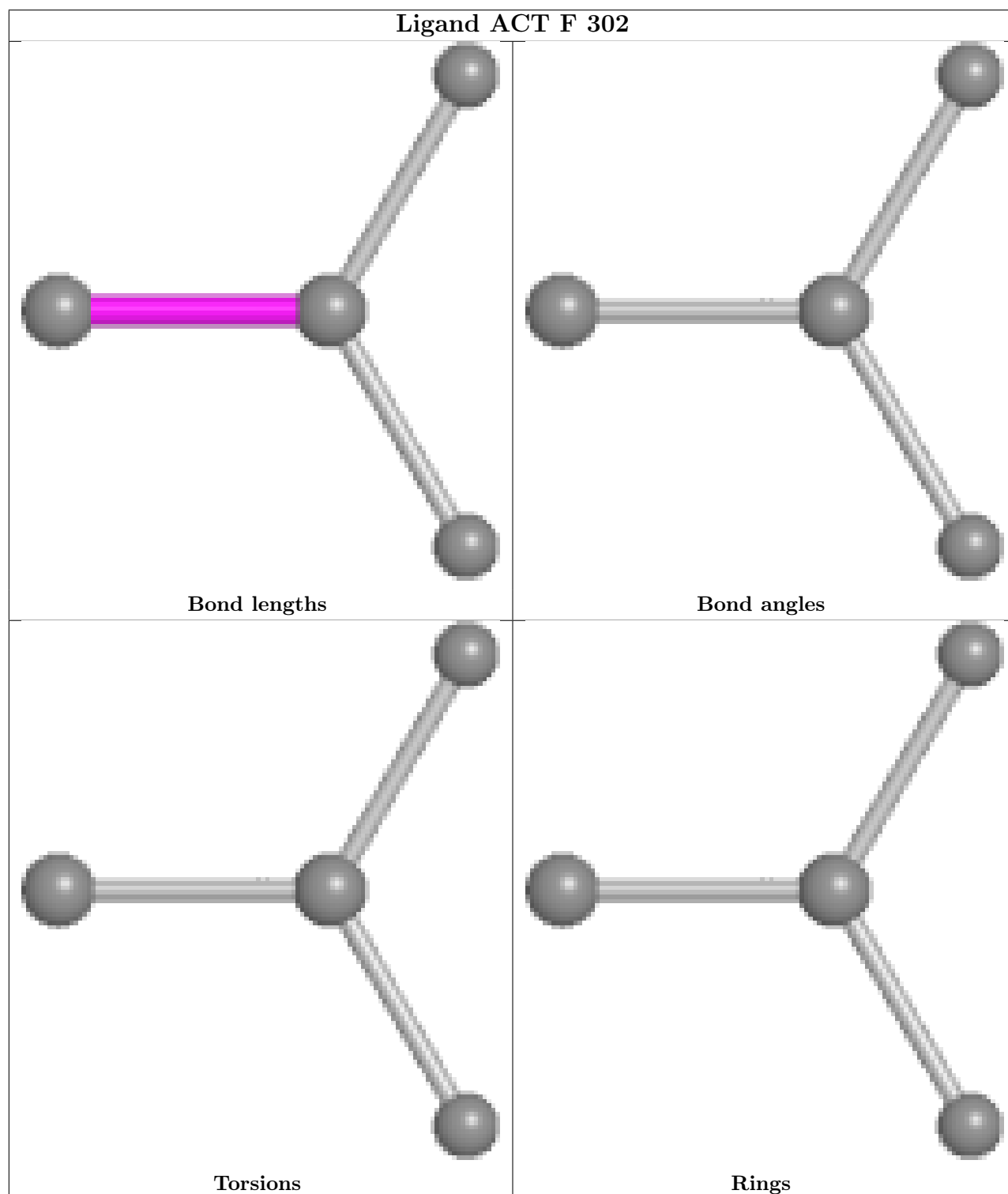
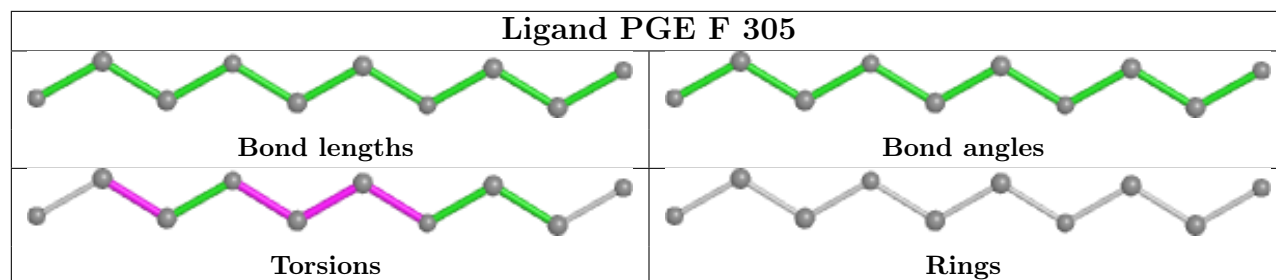
## Ligand 3VN A 301

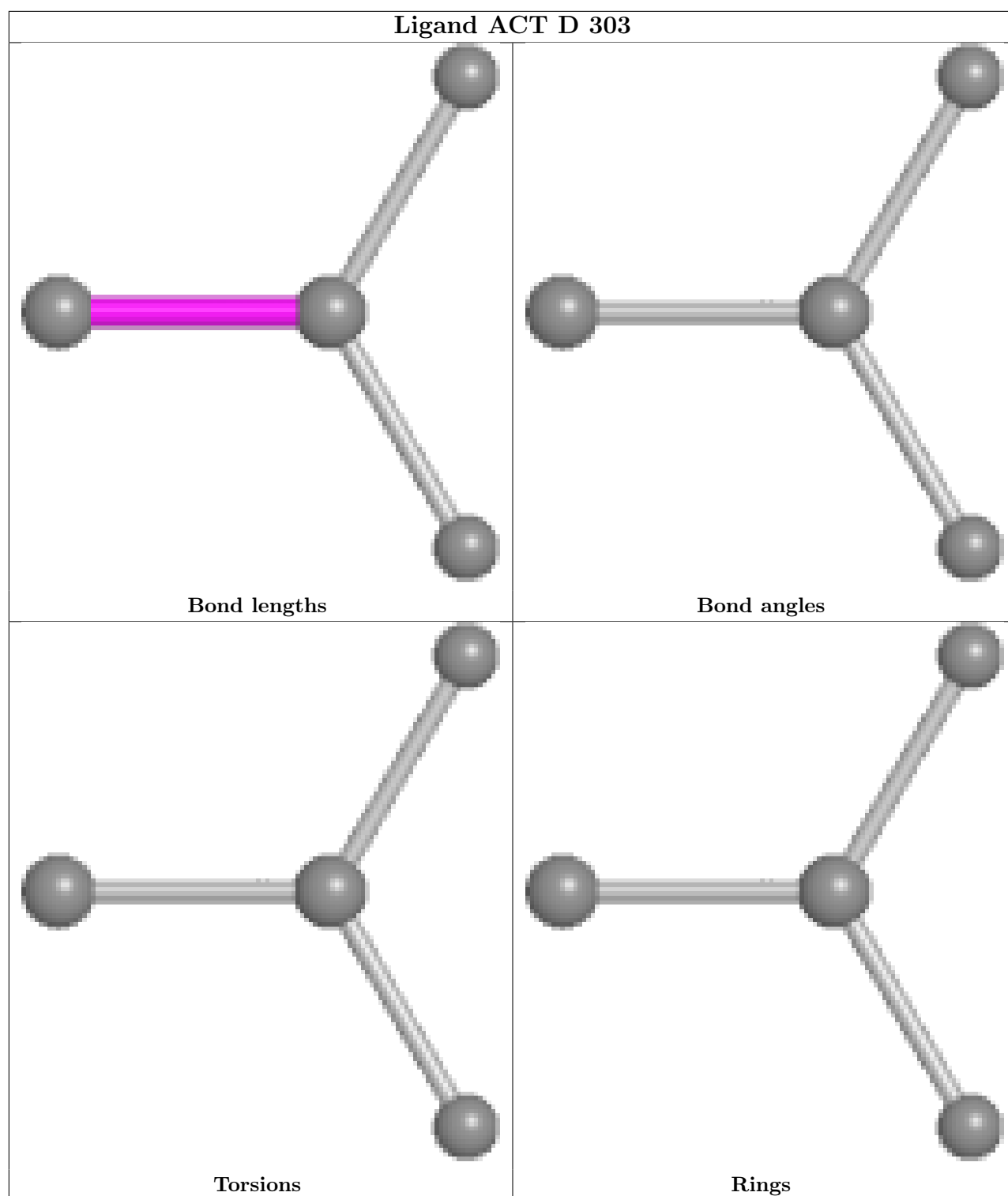


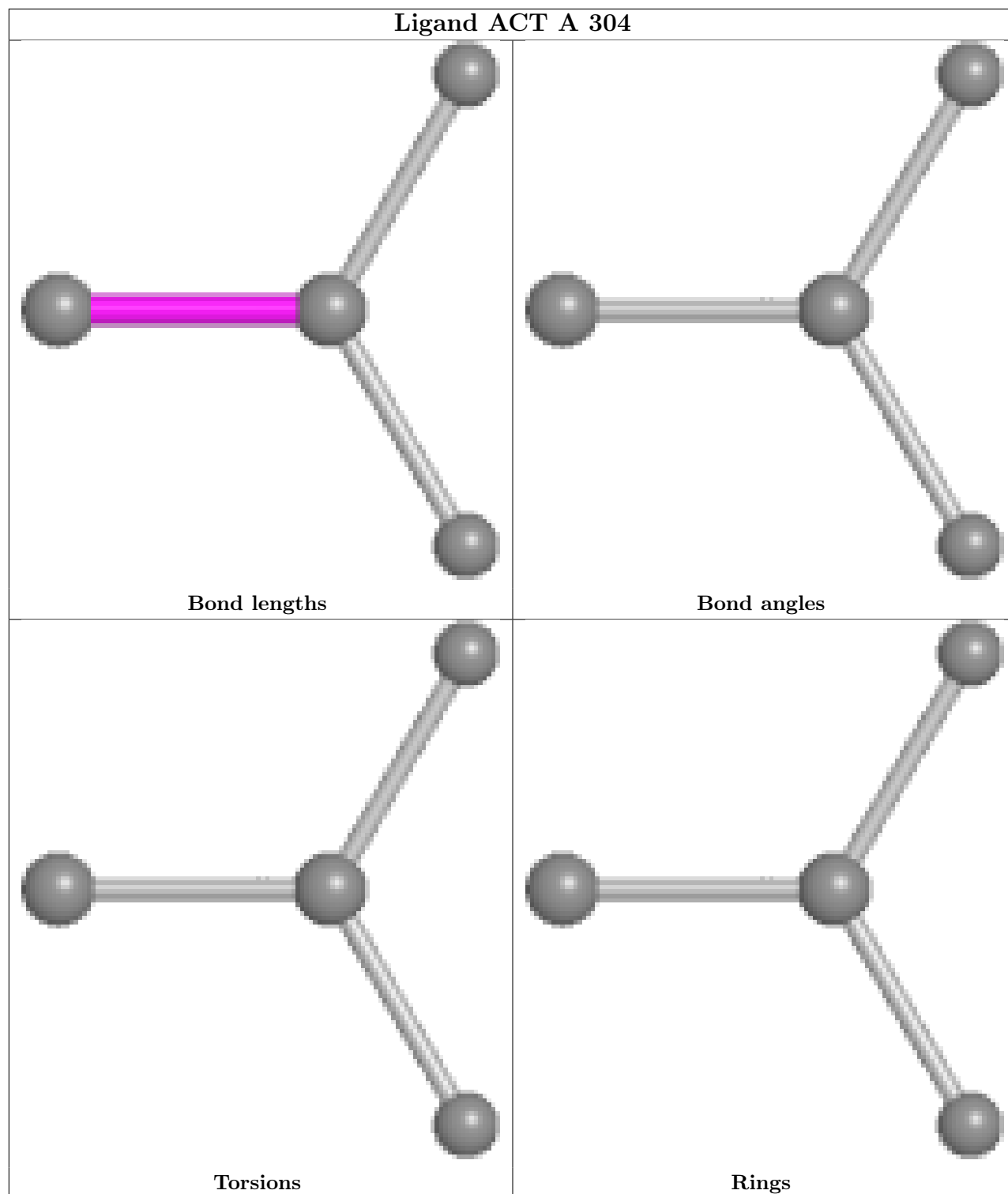


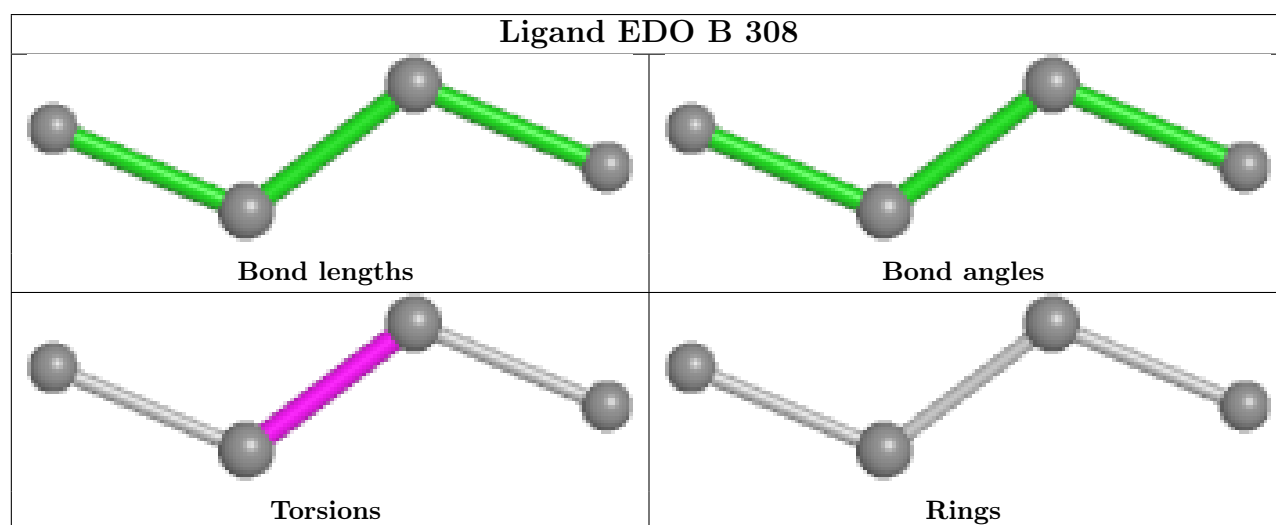
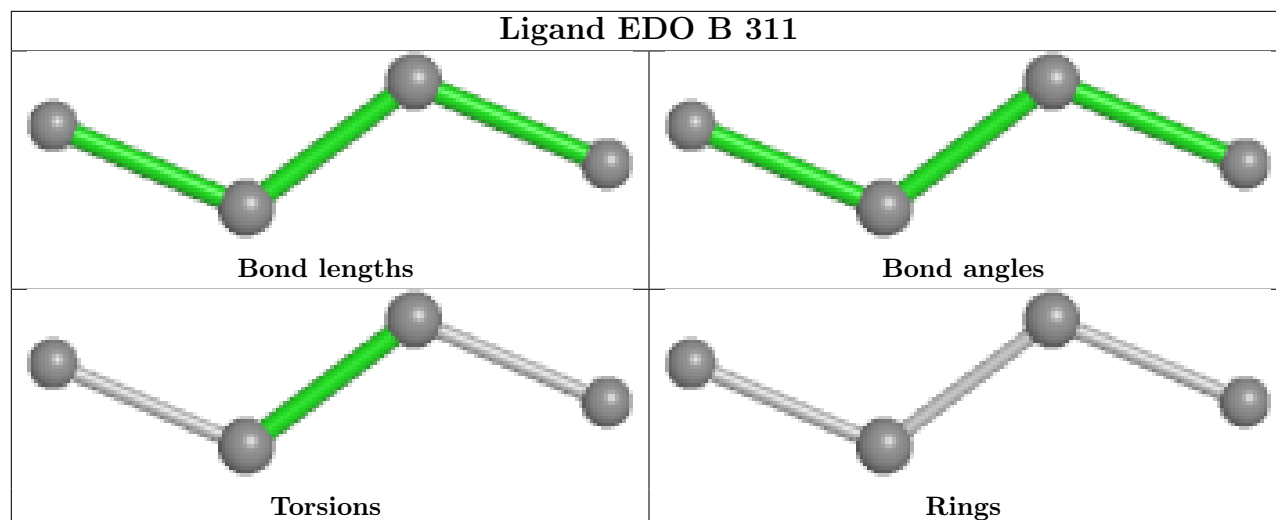


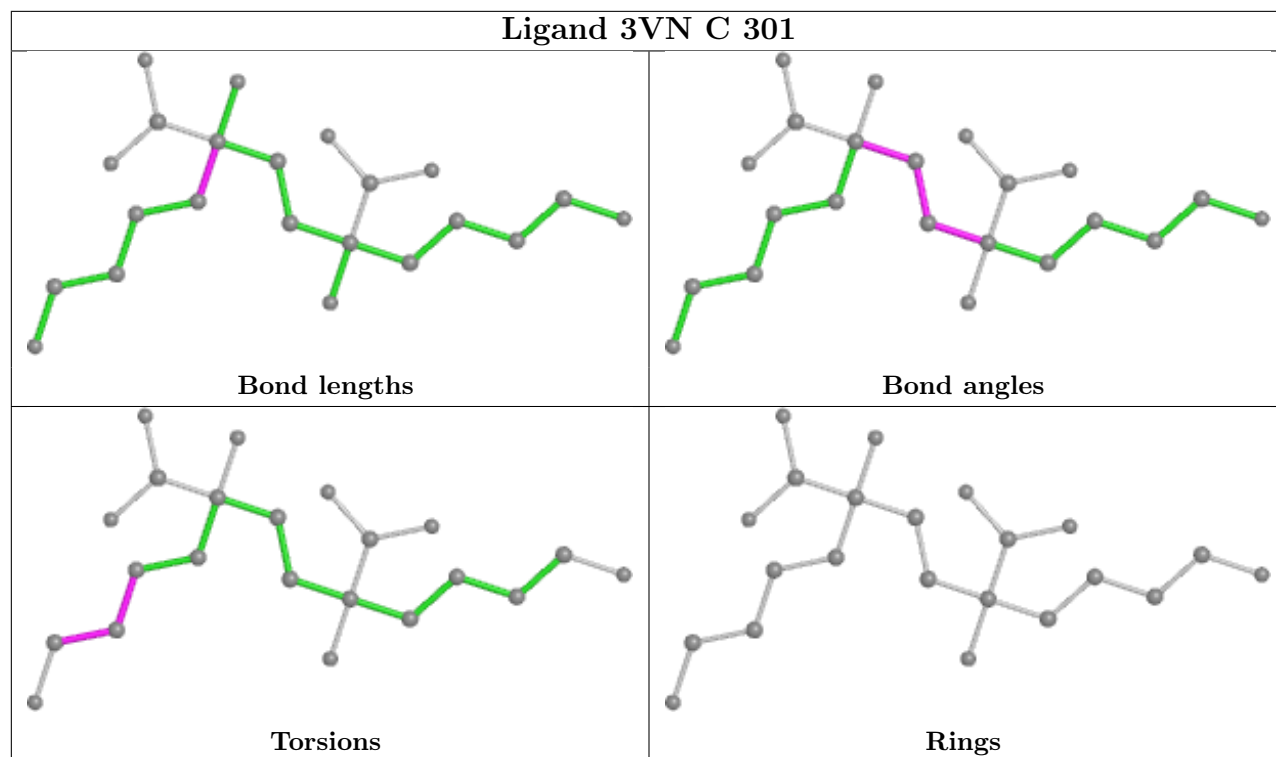


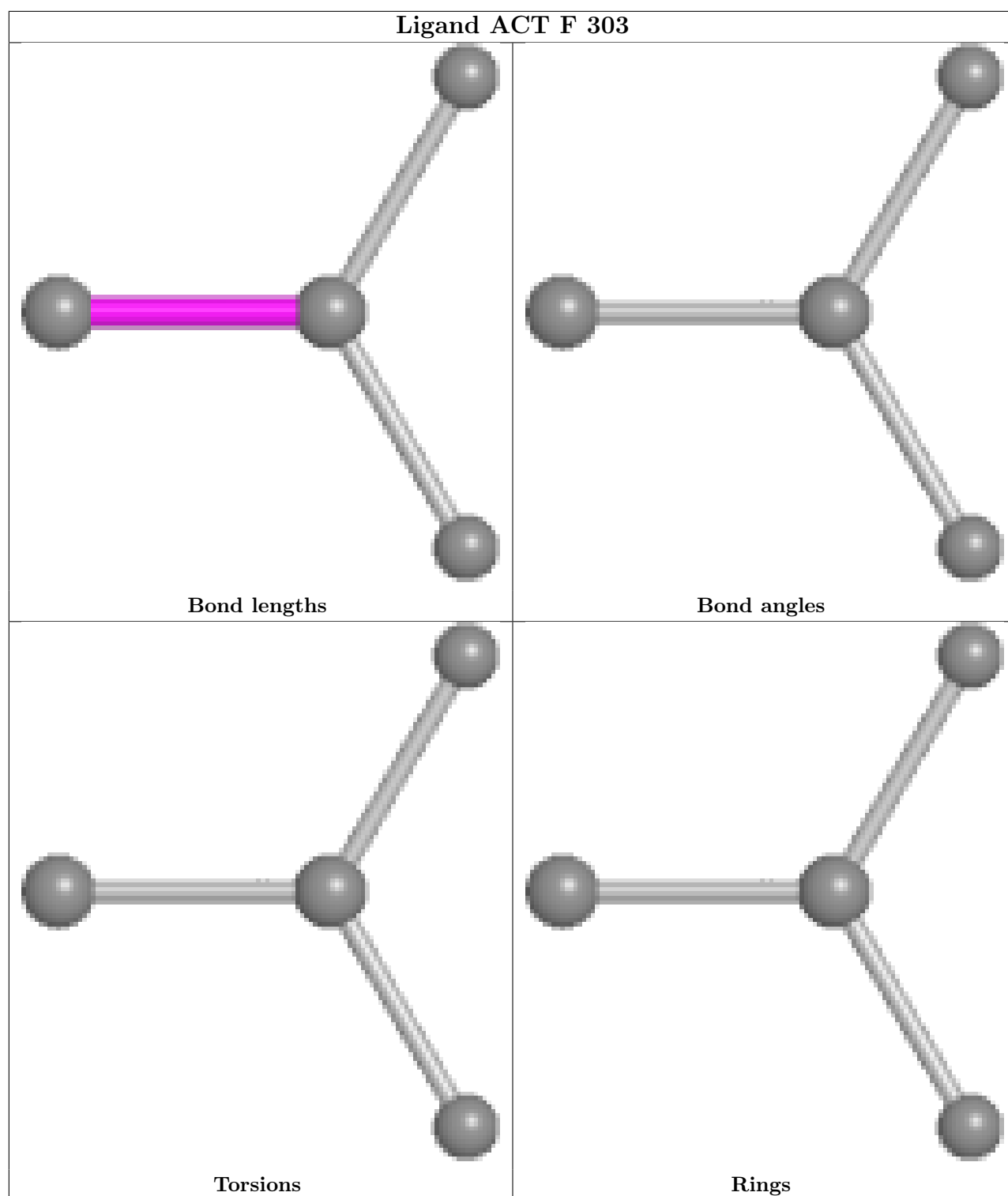




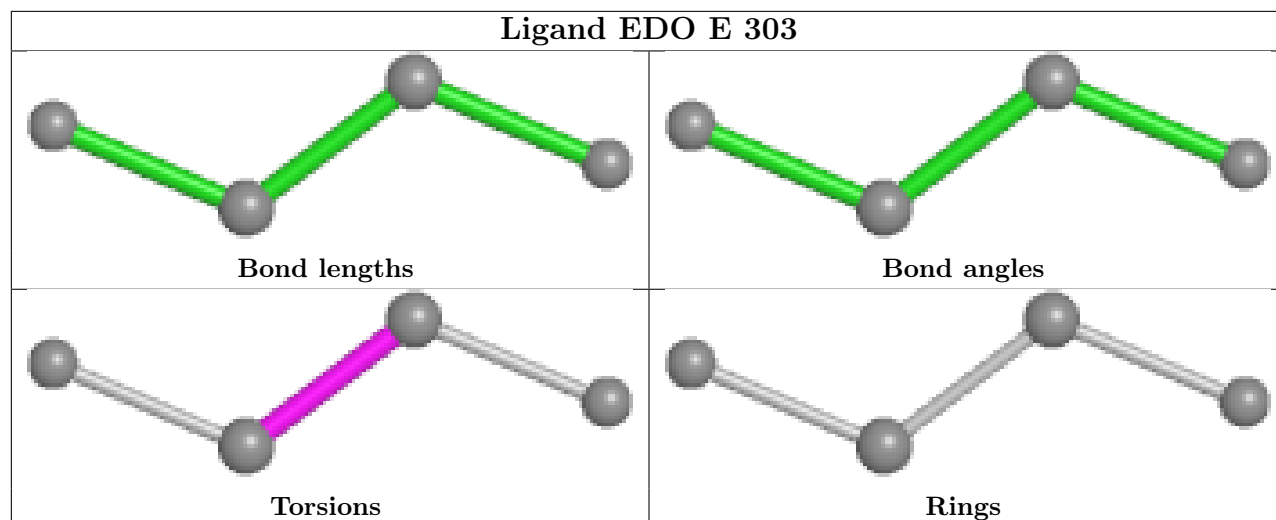


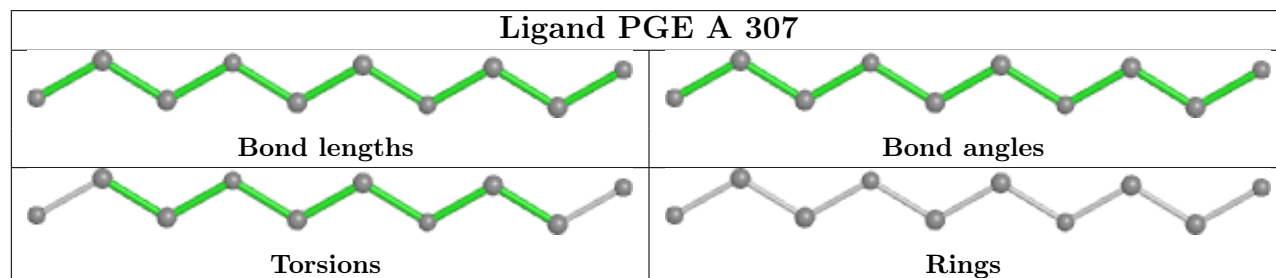
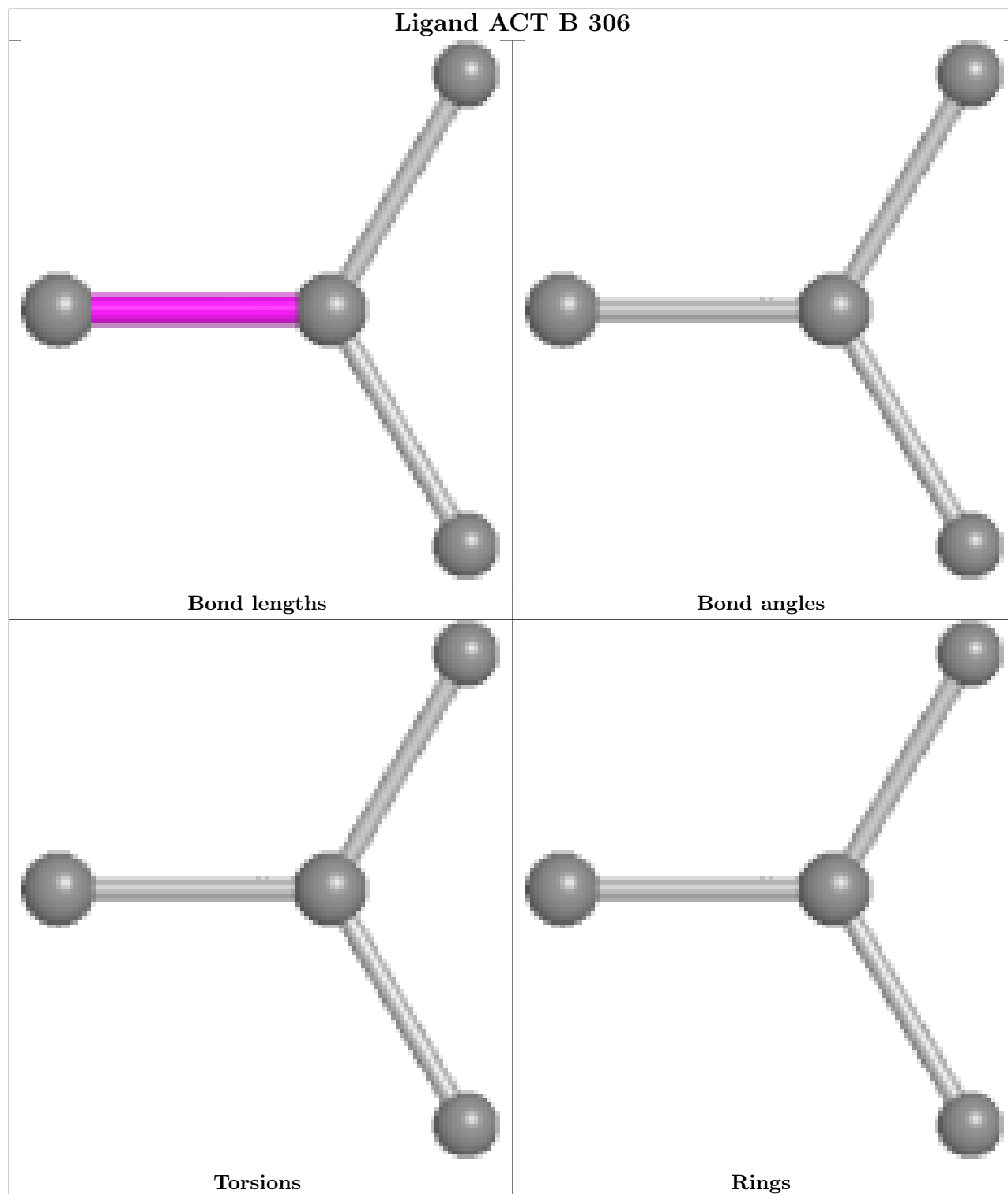


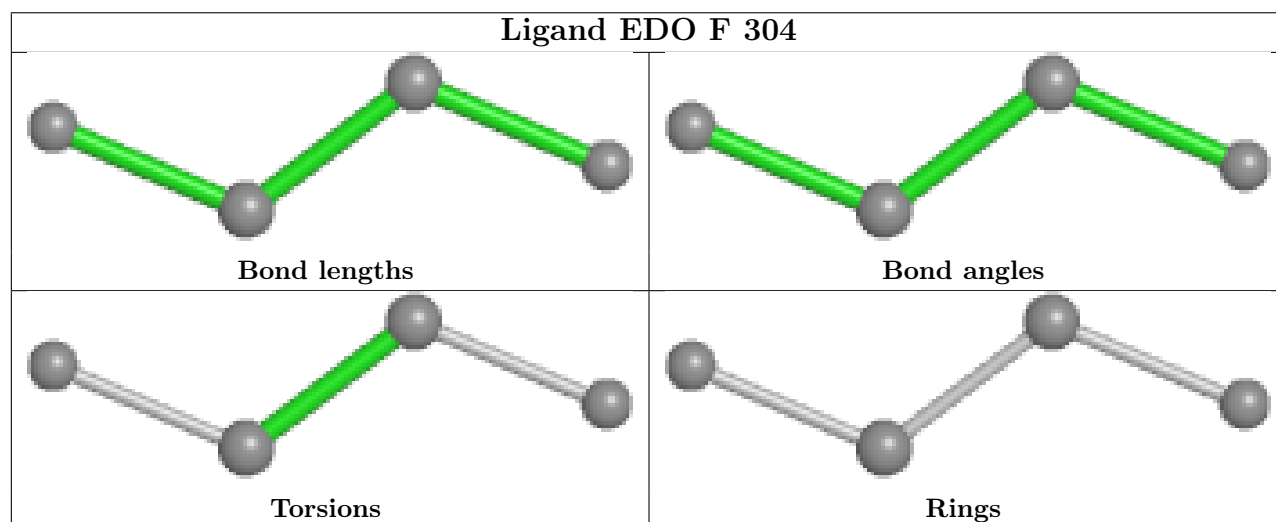
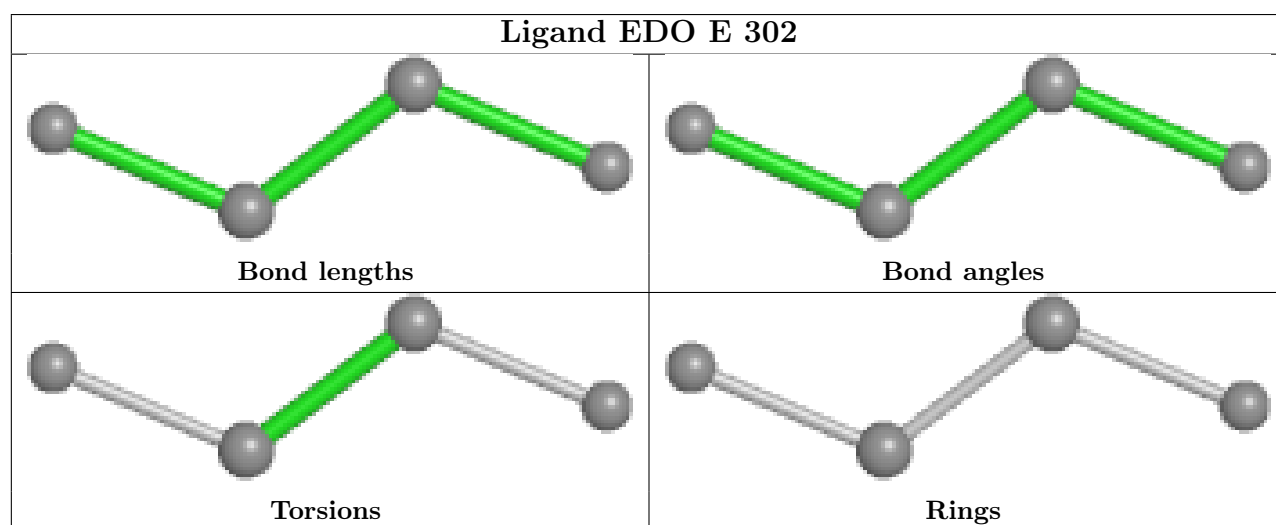
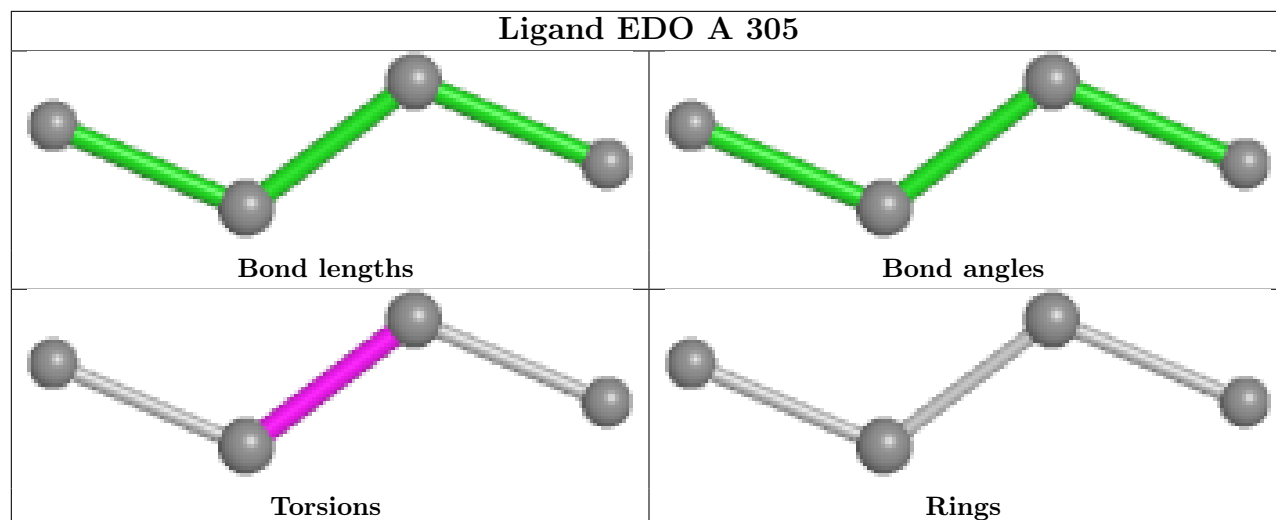


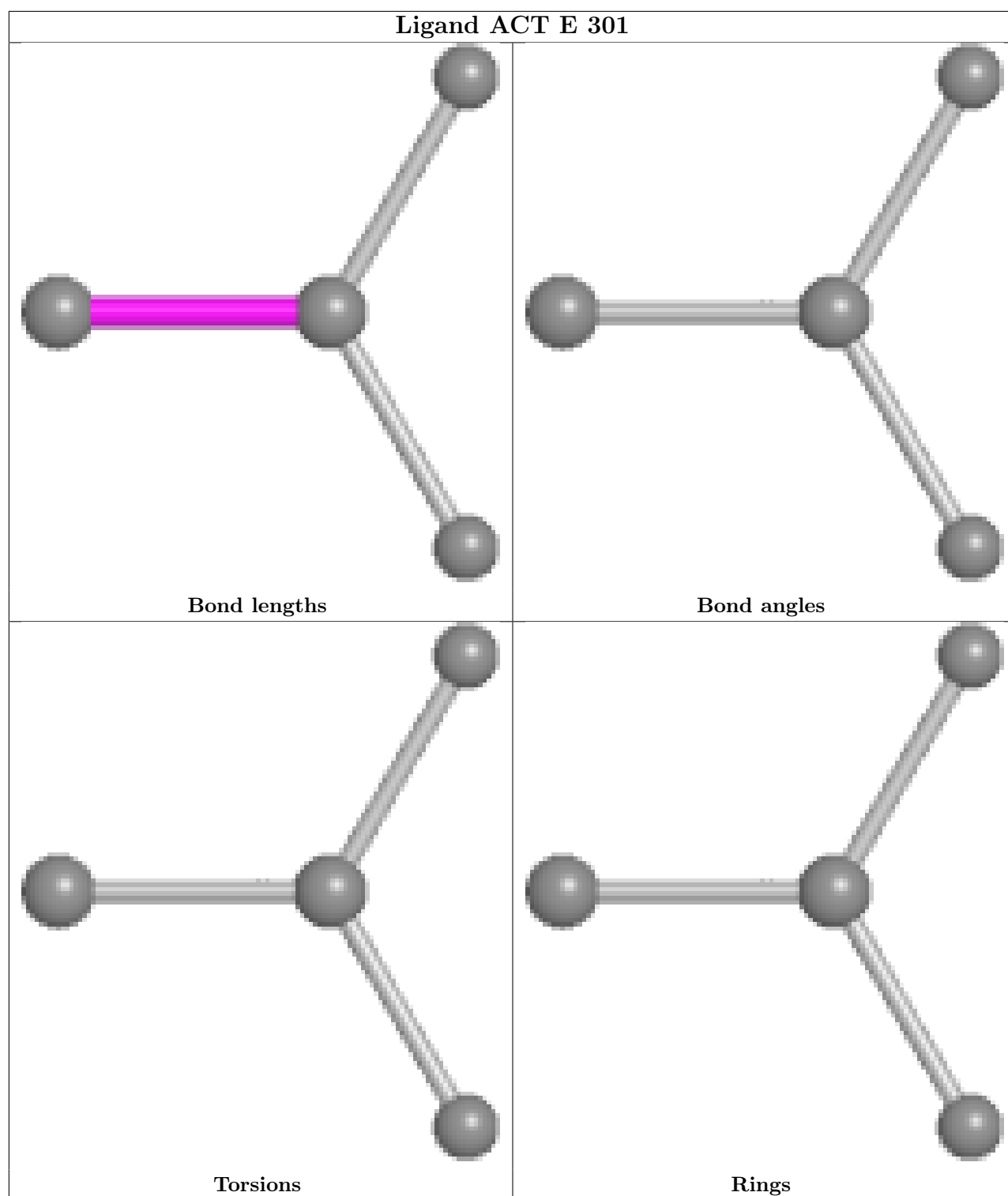












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [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%)	-0.44	0 100 100	10, 14, 29, 41	0
1	B	305/310 (98%)	-0.47	2 (0%) 87 87	10, 14, 31, 49	0
1	C	295/310 (95%)	-0.53	0 100 100	10, 13, 27, 43	0
1	D	305/310 (98%)	-0.46	2 (0%) 87 87	10, 15, 32, 46	0
1	E	295/310 (95%)	-0.45	0 100 100	11, 16, 31, 41	0
1	F	295/310 (95%)	-0.35	1 (0%) 94 93	11, 17, 36, 47	0
All	All	1790/1860 (96%)	-0.45	5 (0%) 94 93	10, 15, 32, 49	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	0	SER	4.7
1	B	-6[A]	HIS	2.7
1	F	95	PHE	2.7
1	B	2	ASP	2.2
1	D	-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	B	166	14/15	0.93	0.09	8,11,21,22	0
1	KPI	D	166	14/15	0.95	0.08	10,11,19,19	0
1	KPI	E	166	14/15	0.95	0.09	9,12,20,22	0
1	KPI	F	166	14/15	0.95	0.10	11,14,19,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KPI	C	166	14/15	0.96	0.09	9,11,18,22	0
1	KPI	A	166	14/15	0.96	0.10	9,11,22,23	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
3	MG	B	305	1/1	0.44	0.19	22,22,22,22	0
2	3VN	C	301	22/22	0.52	0.23	43,51,57,58	0
2	3VN	A	301	22/22	0.55	0.26	41,55,63,63	0
7	PEG	E	305	7/7	0.64	0.24	56,57,60,61	0
5	EDO	B	310	4/4	0.69	0.20	45,48,49,54	0
5	EDO	E	303	4/4	0.71	0.51	20,20,20,20	0
2	3VN	B	301	22/22	0.73	0.21	29,36,40,43	0
7	PEG	A	308	7/7	0.75	0.21	43,48,59,63	0
4	ACT	C	303	4/4	0.81	0.16	46,47,51,51	0
6	PGE	E	304	10/10	0.83	0.14	32,42,46,48	0
4	ACT	E	301	4/4	0.83	0.15	17,31,32,41	0
6	PGE	A	307	10/10	0.83	0.13	31,37,43,48	0
6	PGE	B	312	10/10	0.84	0.13	32,36,42,44	0
4	ACT	A	303	4/4	0.85	0.14	34,41,43,48	0
5	EDO	C	305	4/4	0.85	0.19	45,46,47,49	0
5	EDO	E	302	4/4	0.85	0.09	45,45,45,48	0
5	EDO	A	306	4/4	0.86	0.25	34,36,38,43	0
4	ACT	F	302	4/4	0.87	0.12	33,34,34,36	0
6	PGE	F	305	10/10	0.88	0.15	31,37,44,46	0
5	EDO	B	309	4/4	0.88	0.14	43,43,45,47	0
4	ACT	B	306	4/4	0.88	0.12	38,44,46,46	0
4	ACT	F	303	4/4	0.89	0.15	33,41,42,42	0
5	EDO	B	311	4/4	0.90	0.26	28,38,39,53	0
4	ACT	A	304	4/4	0.90	0.12	26,34,35,36	0
5	EDO	B	308	4/4	0.90	0.14	27,41,45,46	0
3	MG	D	302	1/1	0.90	0.12	37,37,37,37	0

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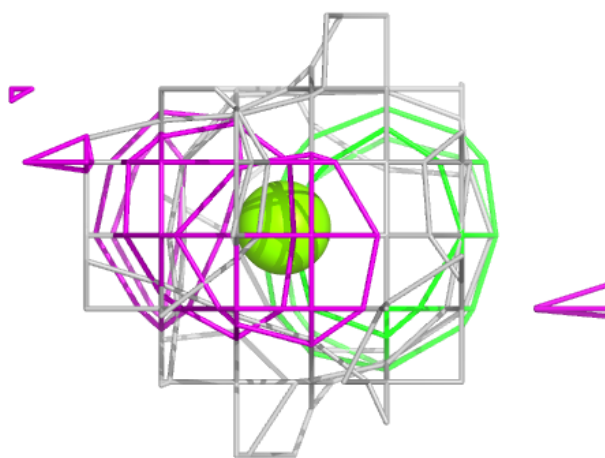
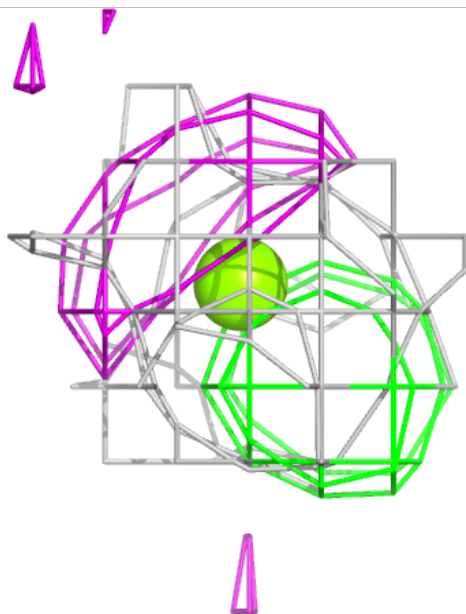
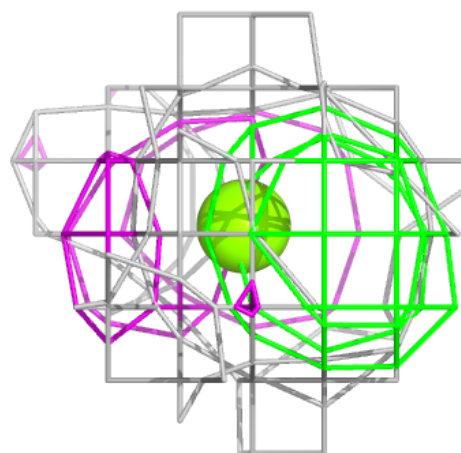
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	A	305	4/4	0.90	0.13	19,29,30,34	0
4	ACT	C	304	4/4	0.91	0.11	38,45,48,49	0
4	ACT	D	303	4/4	0.92	0.11	22,27,28,30	0
6	PGE	D	304	10/10	0.92	0.10	32,34,41,44	0
4	ACT	B	307	4/4	0.93	0.09	21,26,28,32	0
3	MG	F	301	1/1	0.94	0.21	23,23,23,23	0
3	MG	B	304	1/1	0.95	0.08	39,39,39,39	0
3	MG	B	303	1/1	0.96	0.08	32,32,32,32	0
3	MG	C	302	1/1	0.97	0.09	35,35,35,35	0
5	EDO	F	304	4/4	0.98	0.07	14,15,16,16	0
3	MG	D	301	1/1	0.99	0.12	14,14,14,14	0
3	MG	A	302	1/1	0.99	0.14	15,15,15,15	0
3	MG	B	302	1/1	0.99	0.07	14,14,14,14	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.



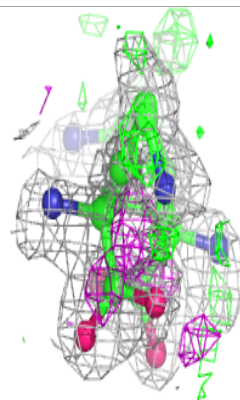
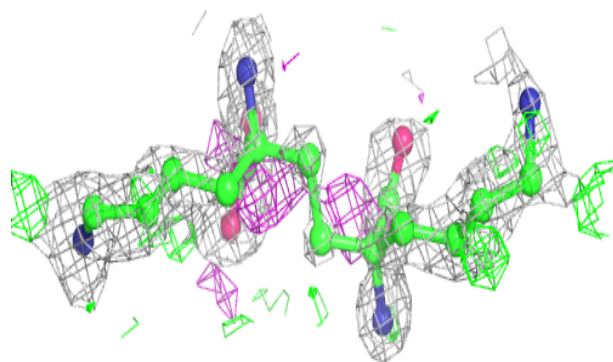
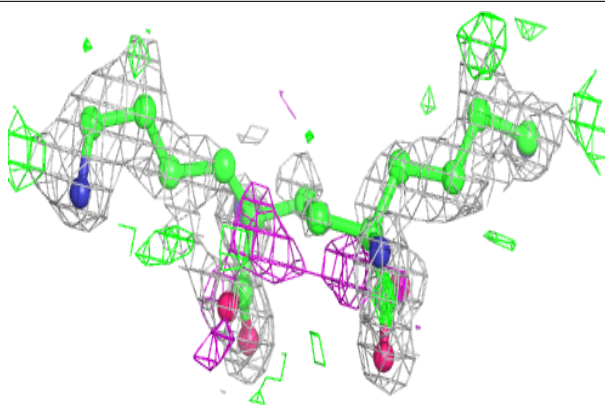
**Electron density around MG B 305:**

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and green (positive)

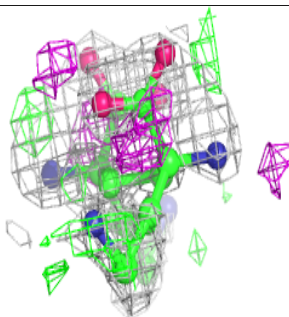
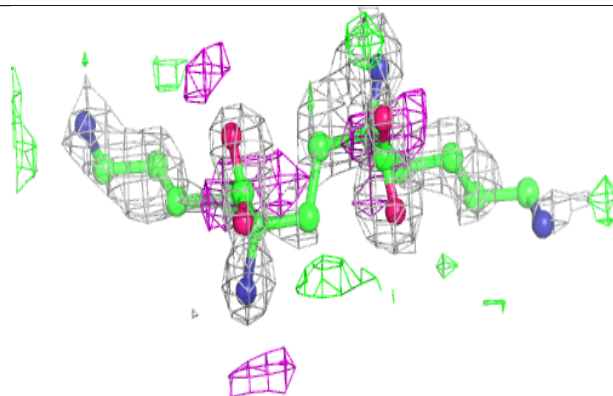
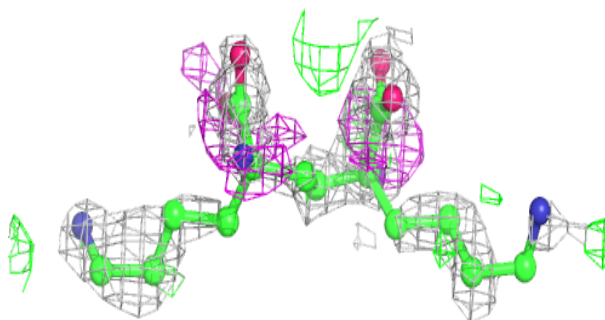


**Electron density around 3VN C 301:**

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and green (positive)

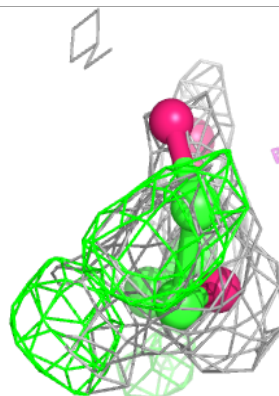
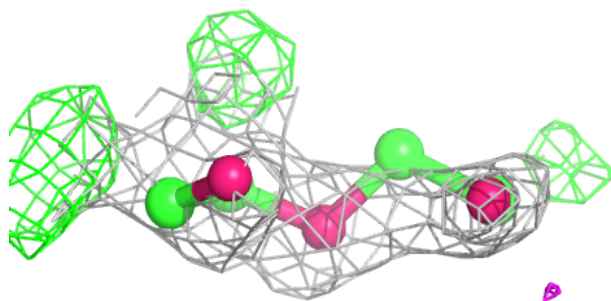
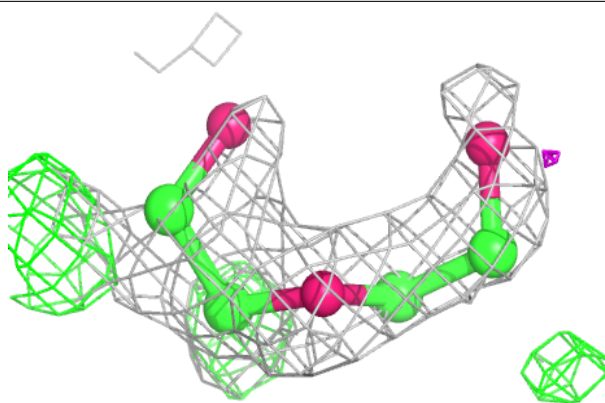
**Electron density around 3VN A 301:**

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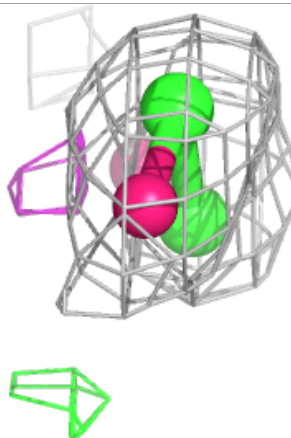
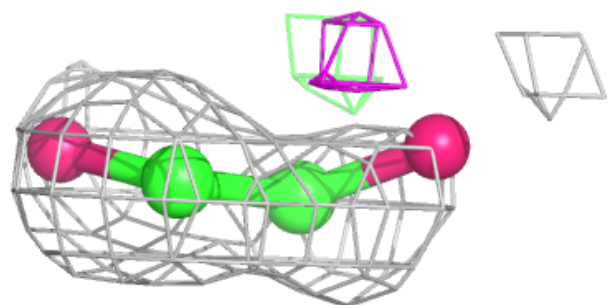
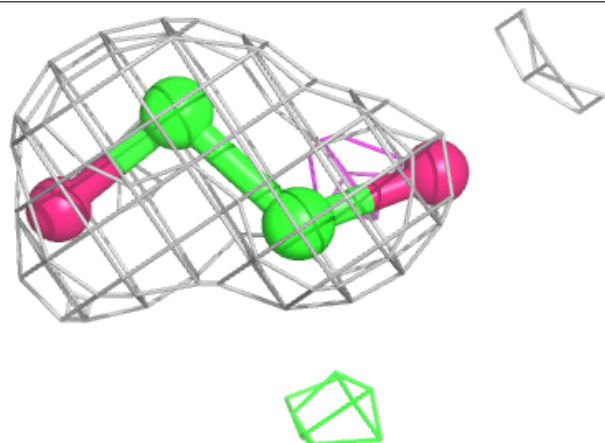


**Electron density around PEG E 305:**

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and green (positive)

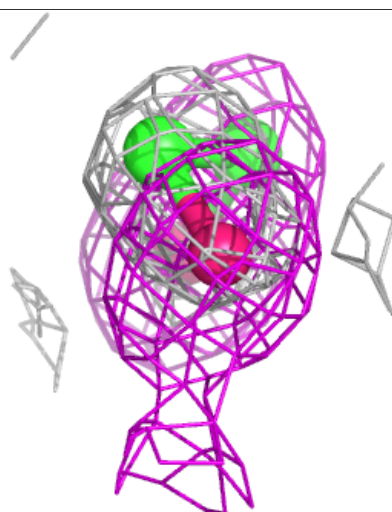
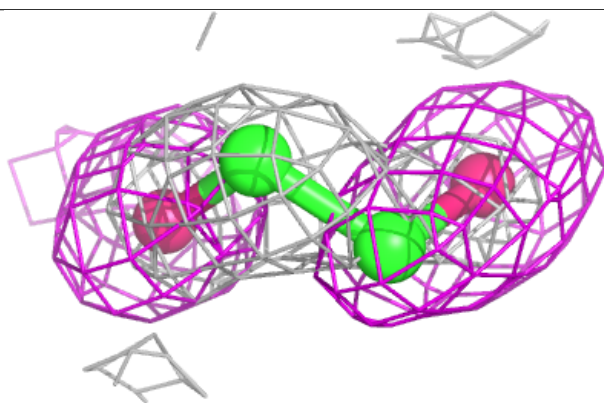
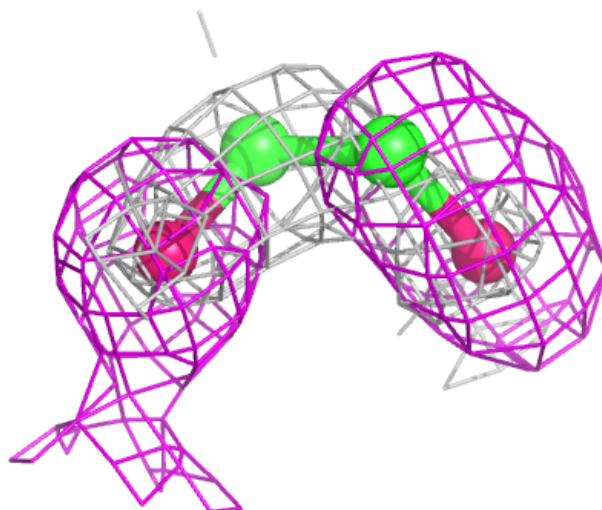
**Electron density around EDO B 310:**

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



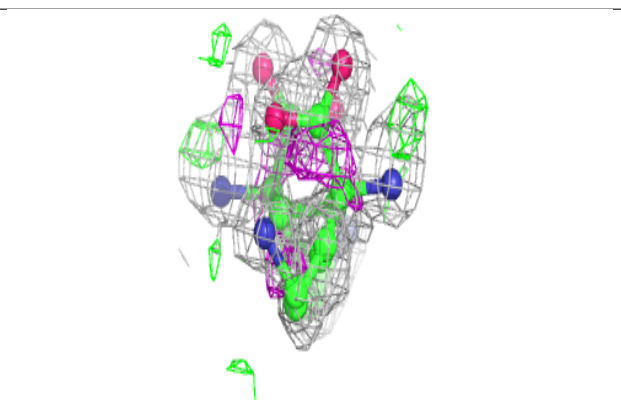
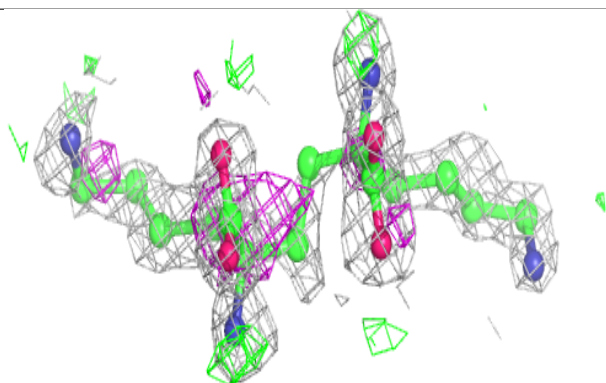
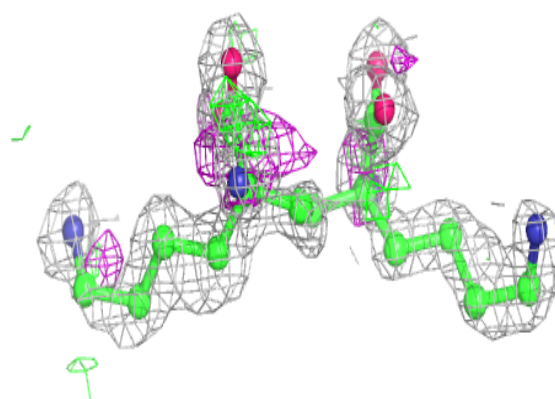
**Electron density around EDO E 303:**

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

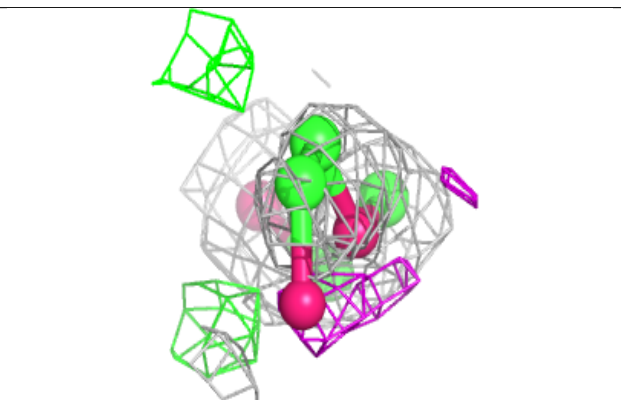
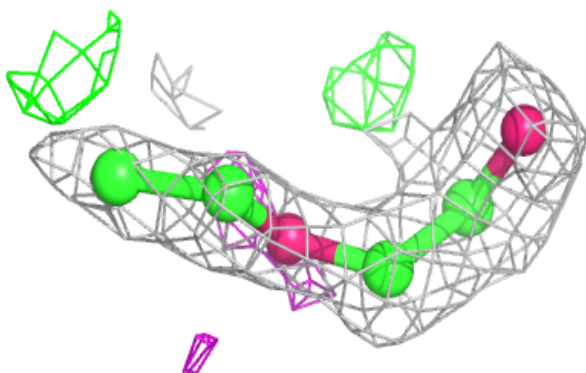
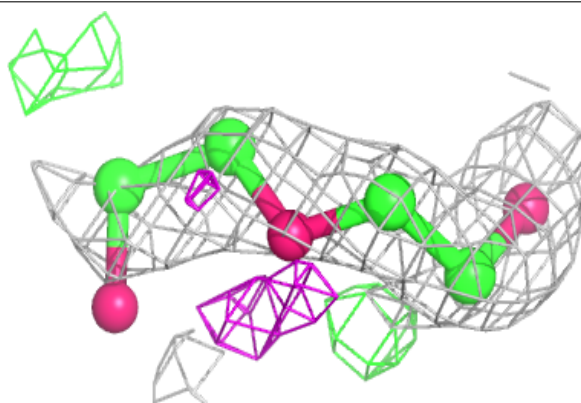


**Electron density around 3VN B 301:**

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

**Electron density around PEG A 308:**

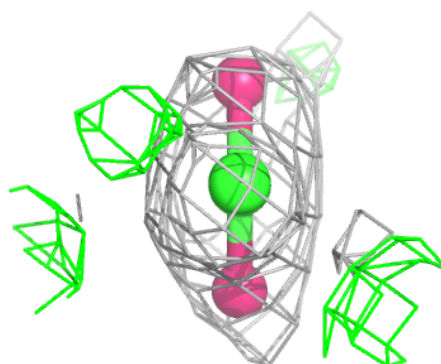
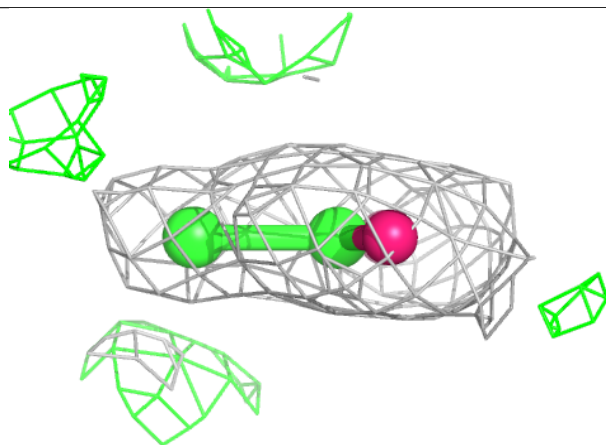
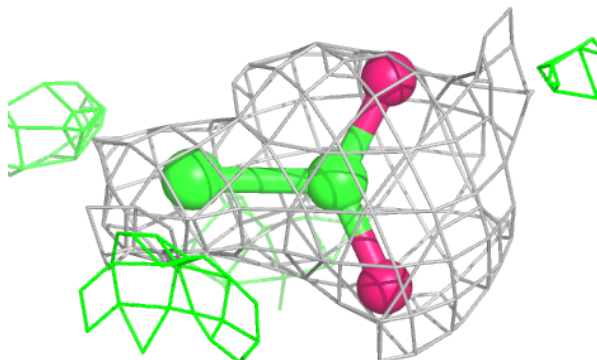
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



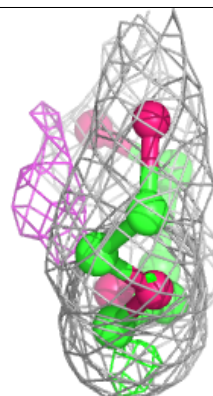
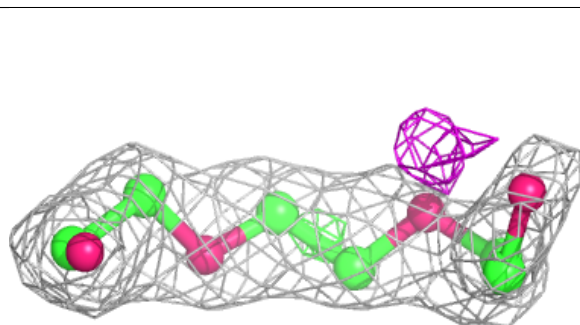
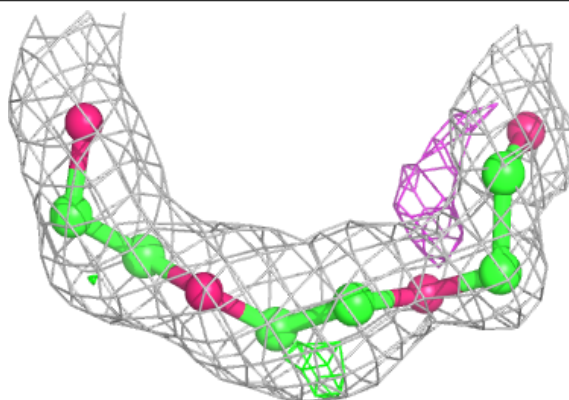


**Electron density around ACT C 303:**

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

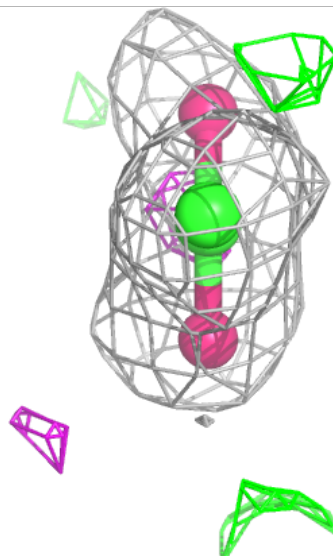
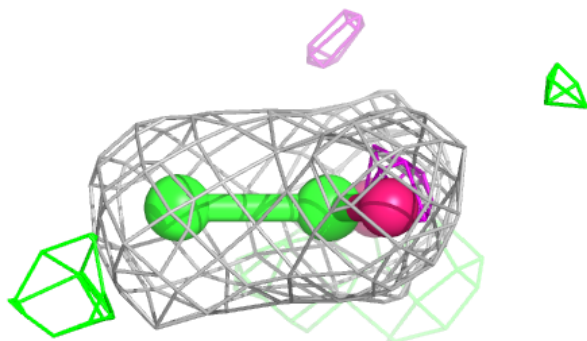
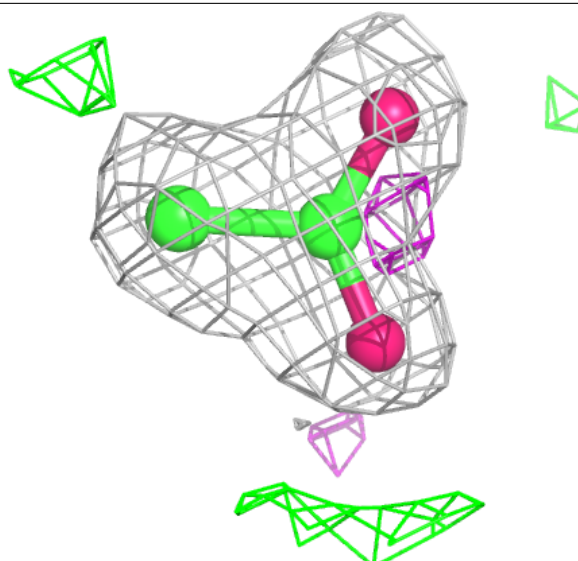
**Electron density around PGE E 304:**

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



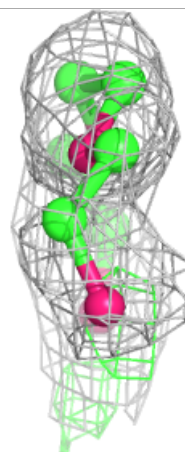
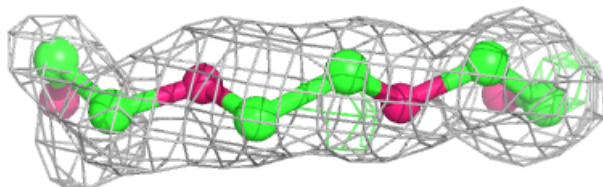
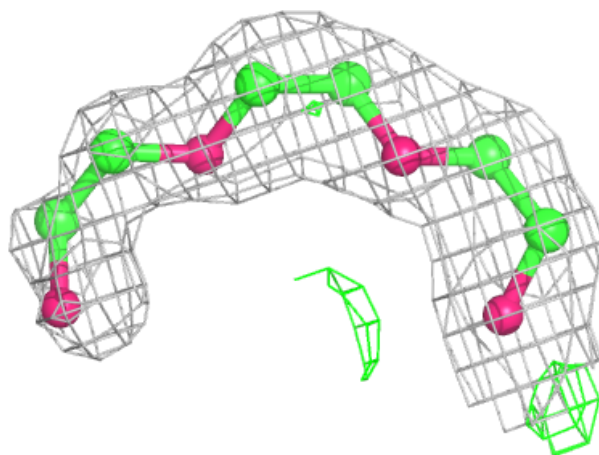
**Electron density around ACT E 301:**

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



**Electron density around PGE A 307:**

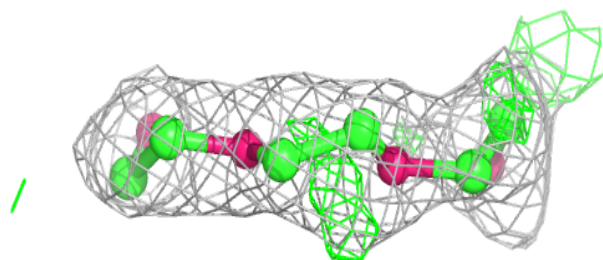
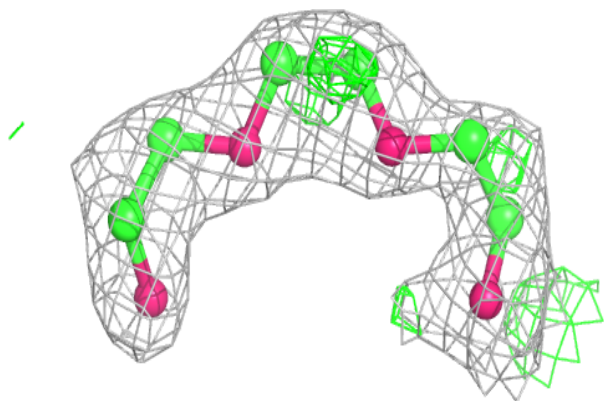
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





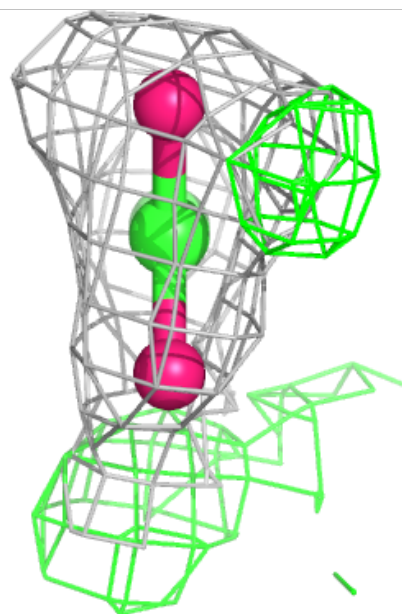
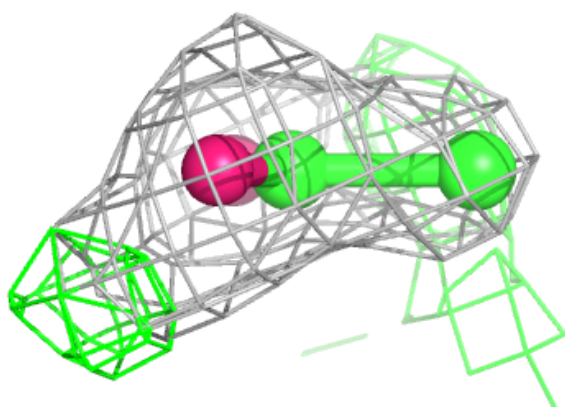
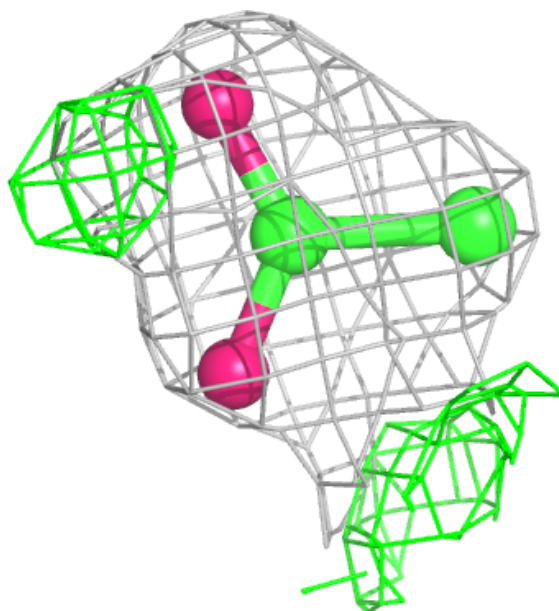
**Electron density around PGE B 312:**

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



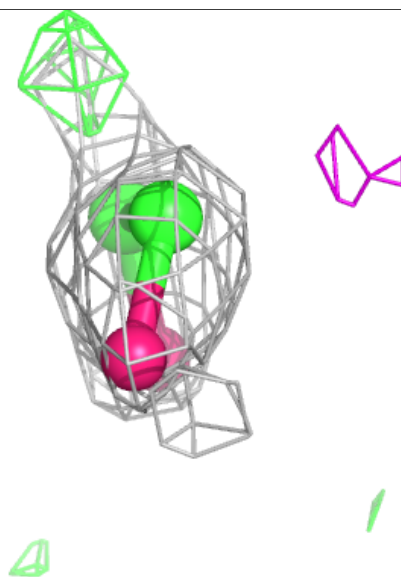
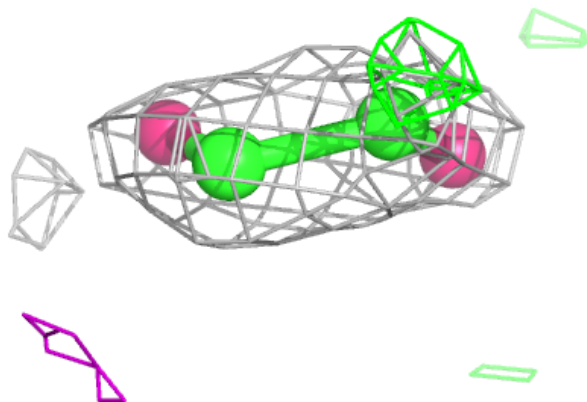
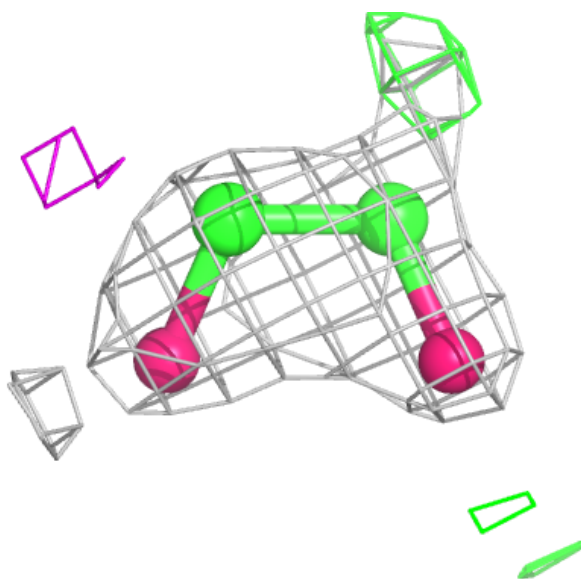
**Electron density around ACT A 303:**

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



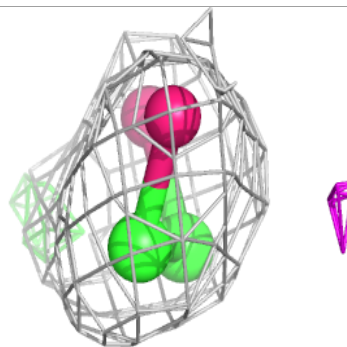
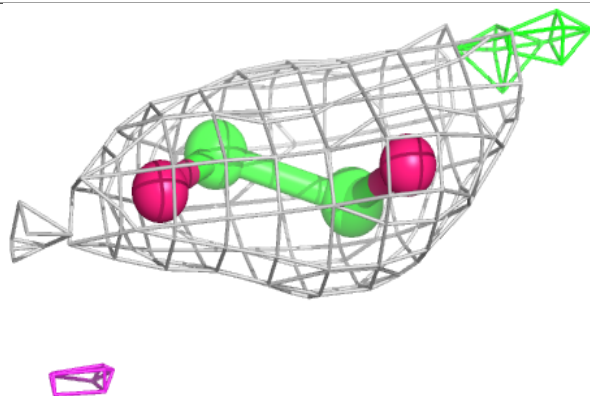
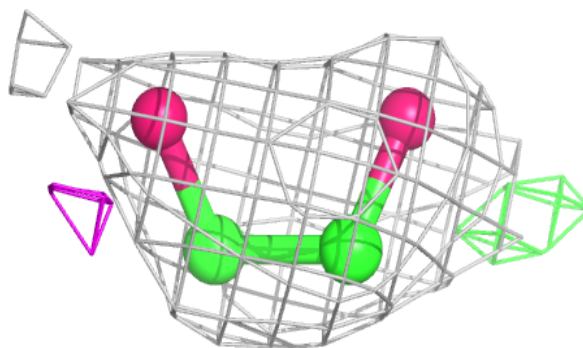
**Electron density around EDO C 305:**

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

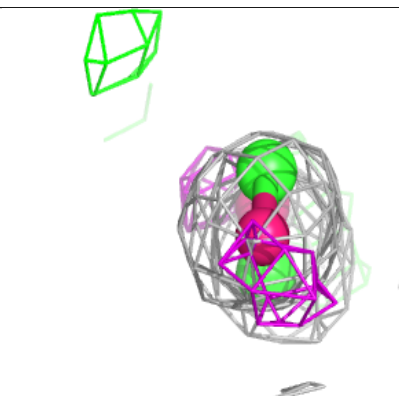
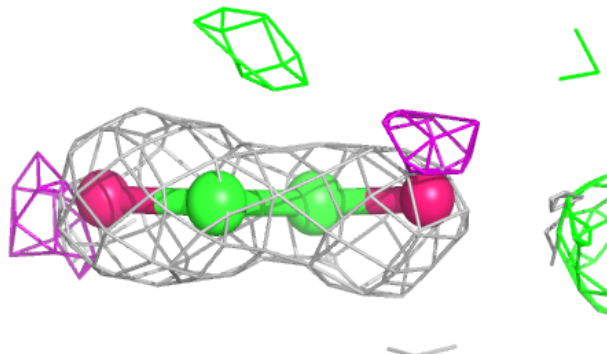
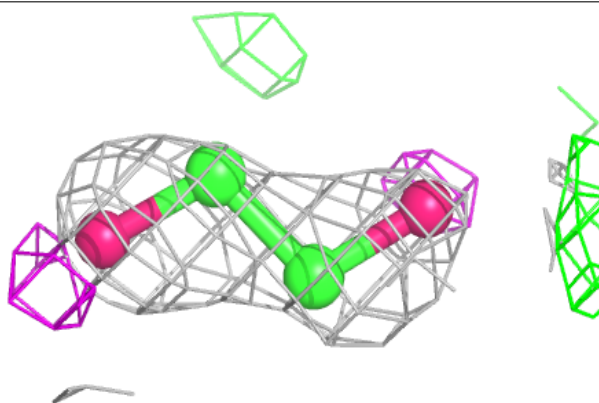


**Electron density around EDO E 302:**

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

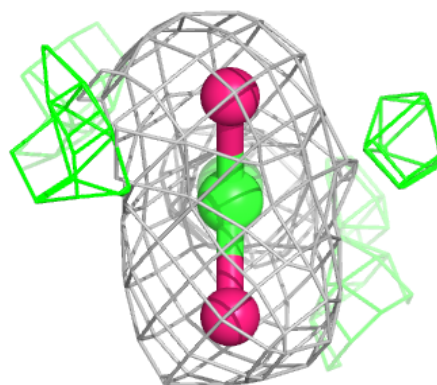
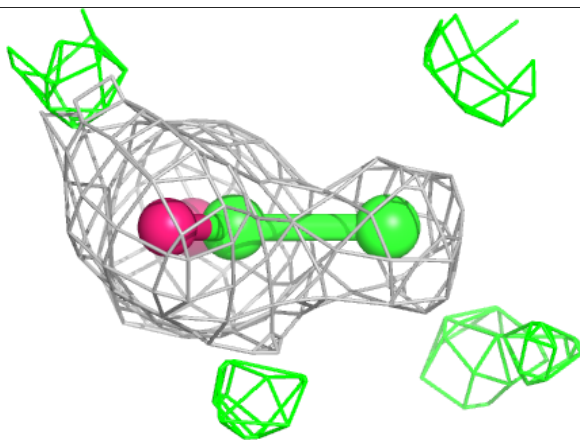
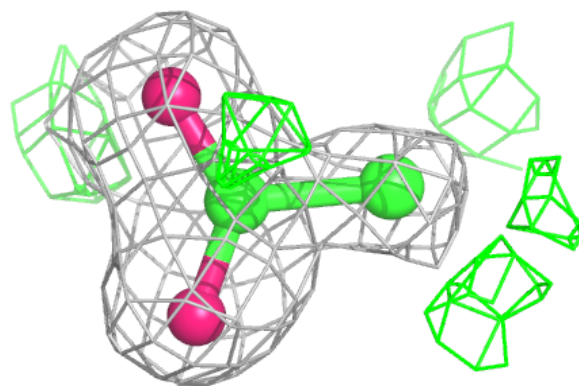
**Electron density around EDO A 306:**

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



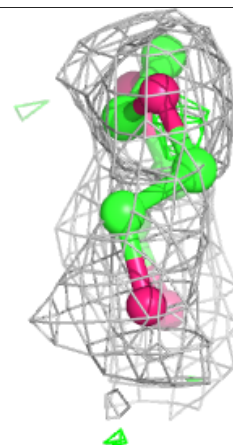
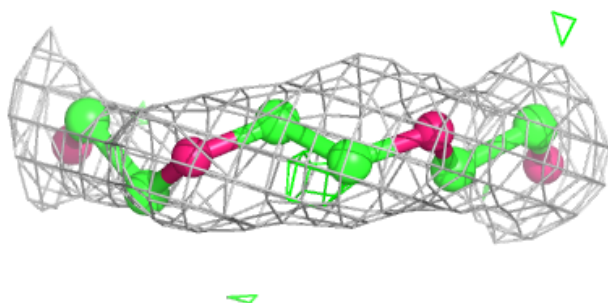
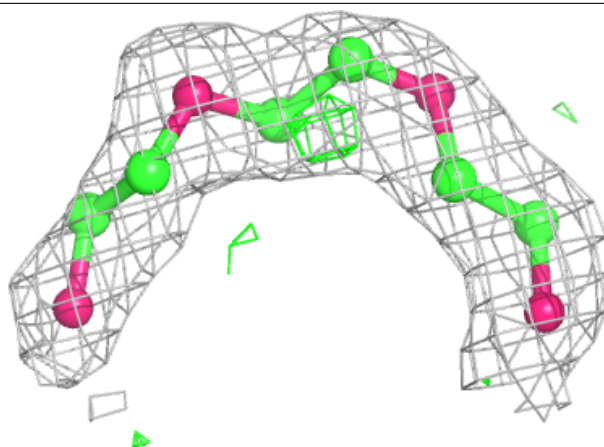
**Electron density around ACT F 302:**

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



**Electron density around PGE F 305:**

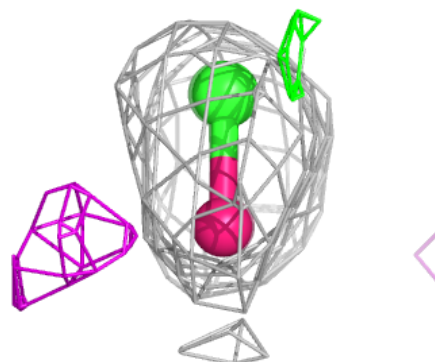
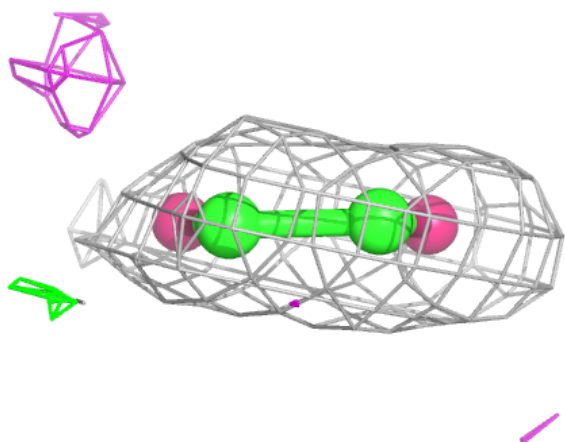
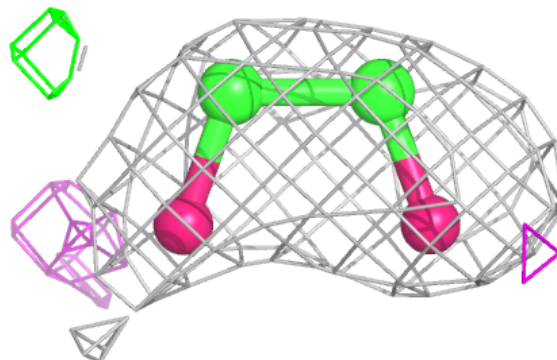
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





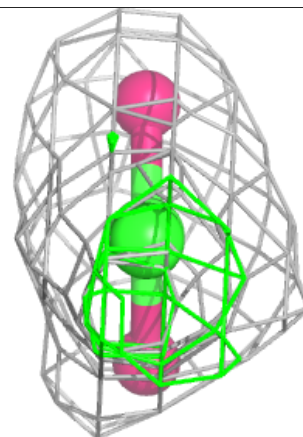
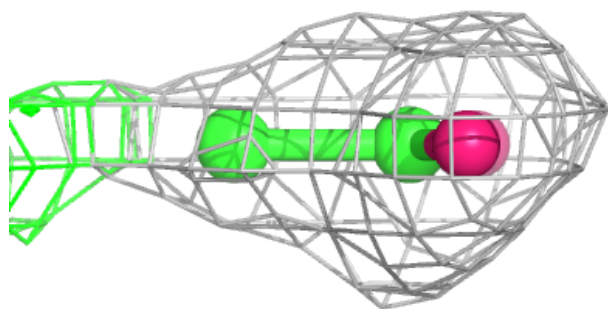
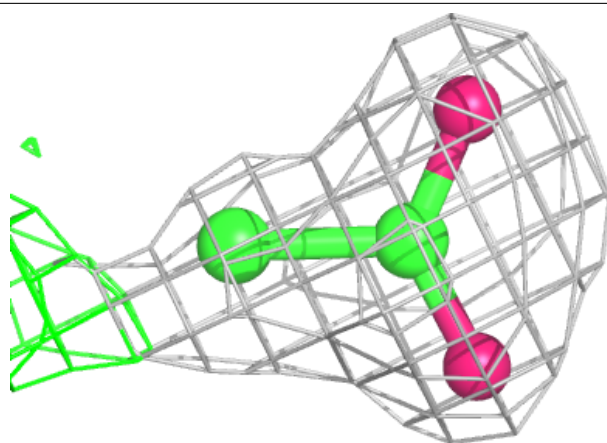
**Electron density around EDO B 309:**

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



**Electron density around ACT B 306:**

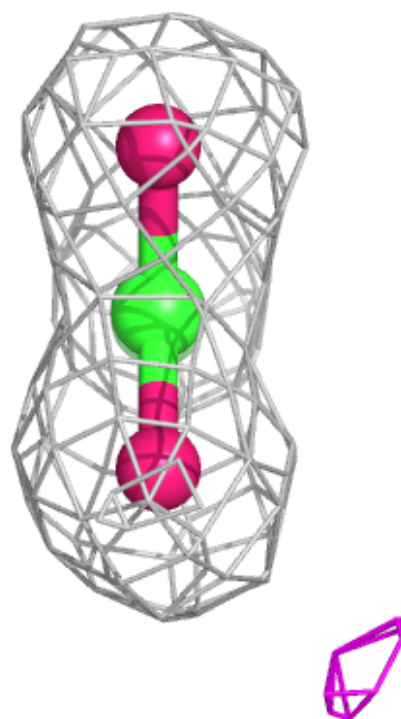
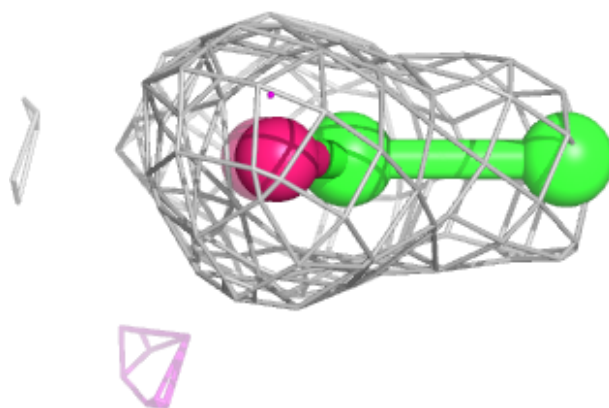
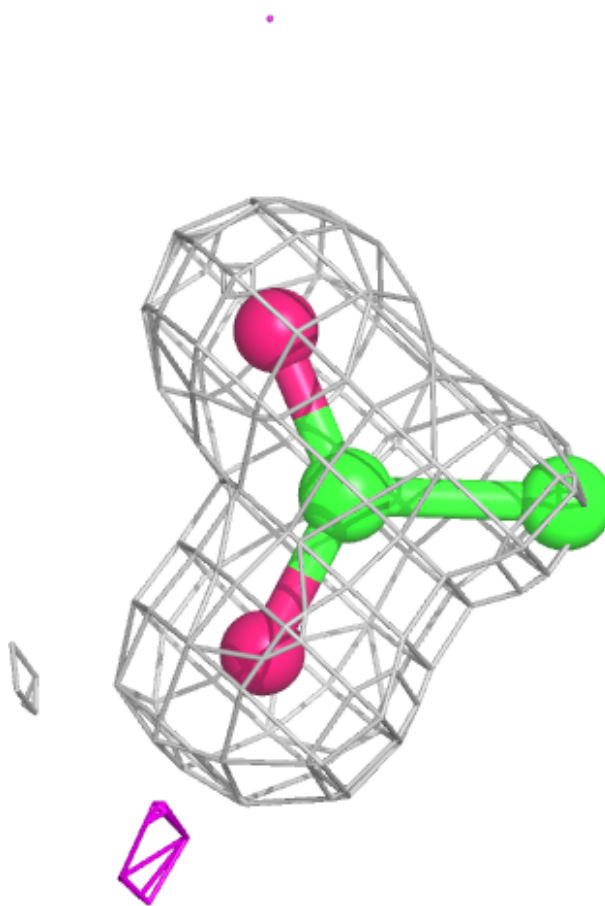
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





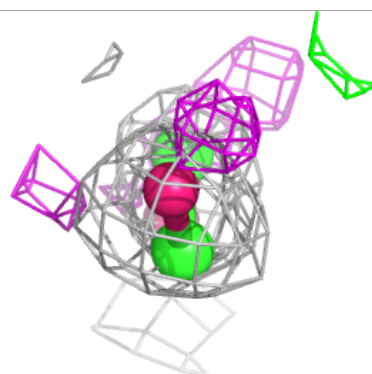
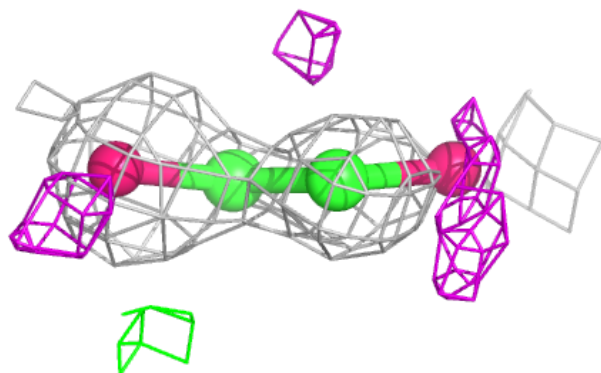
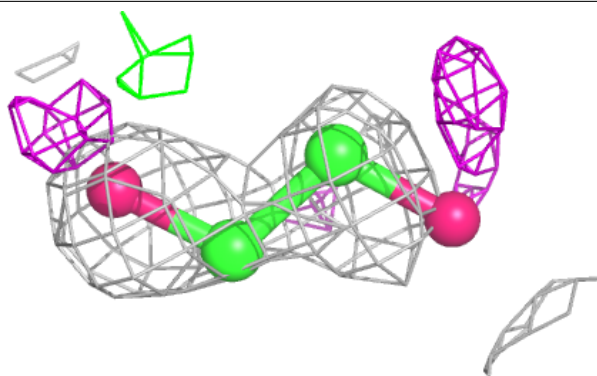
**Electron density around ACT F 303:**

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

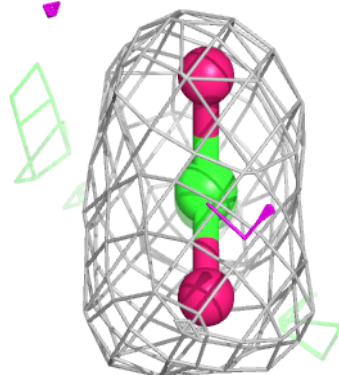
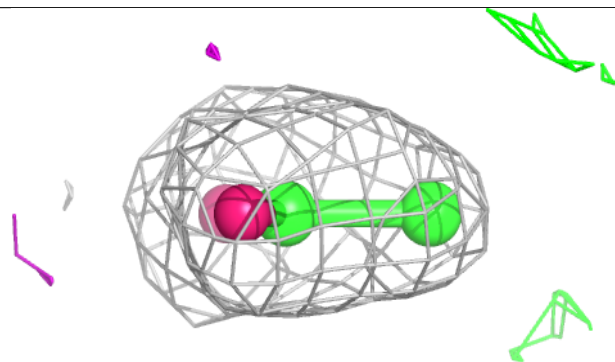
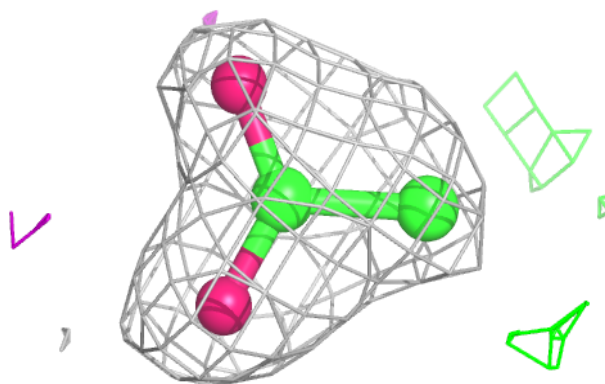


**Electron density around EDO B 311:**

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

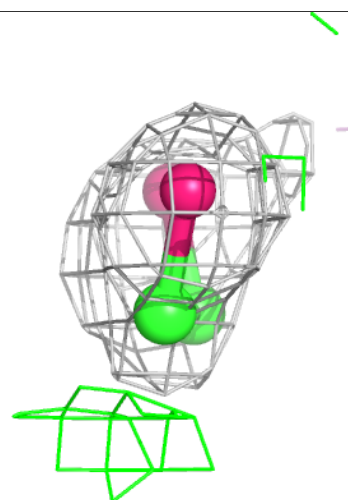
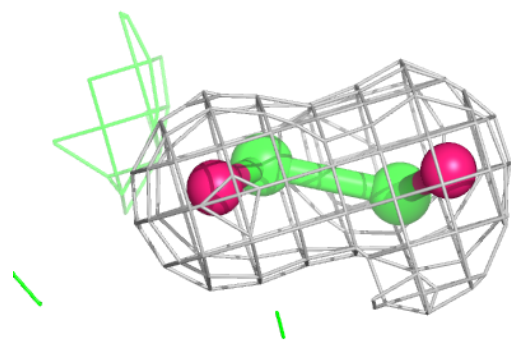
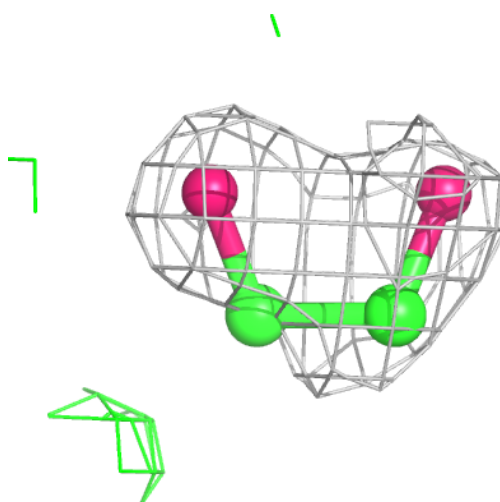
**Electron density around ACT A 304:**

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



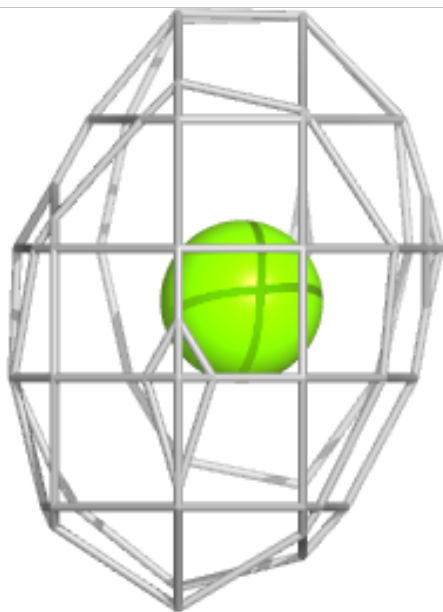
**Electron density around EDO B 308:**

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



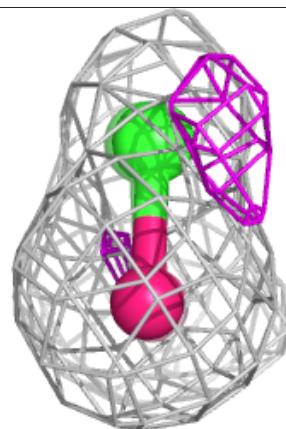
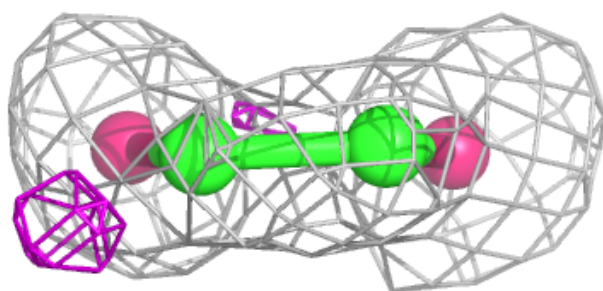
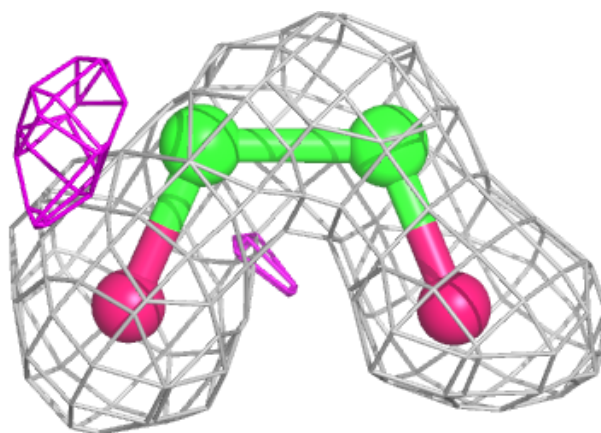
**Electron density around MG D 302:**

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



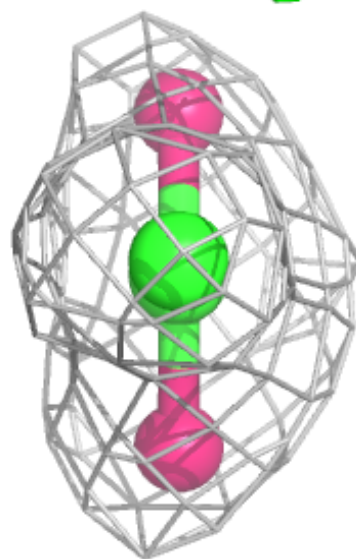
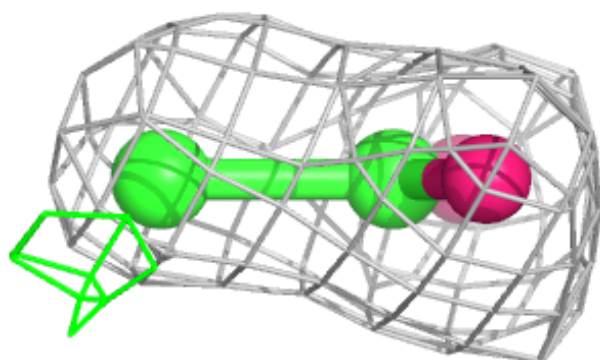
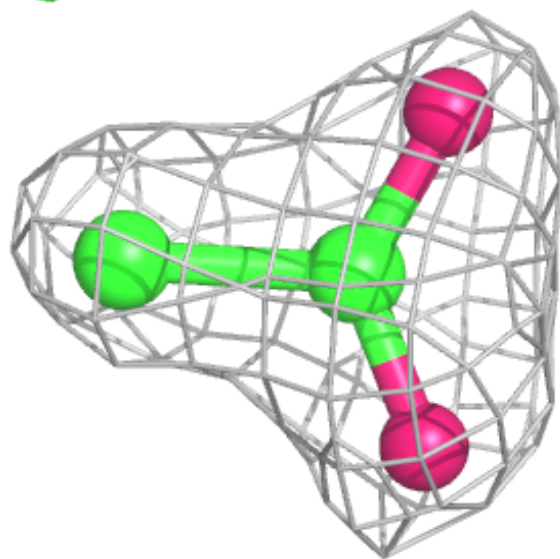
**Electron density around EDO A 305:**

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



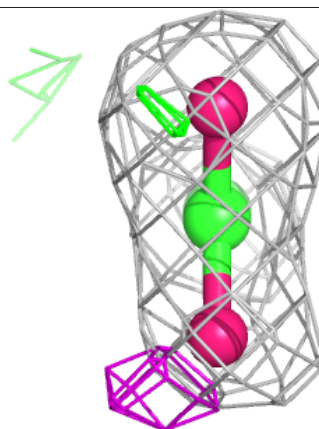
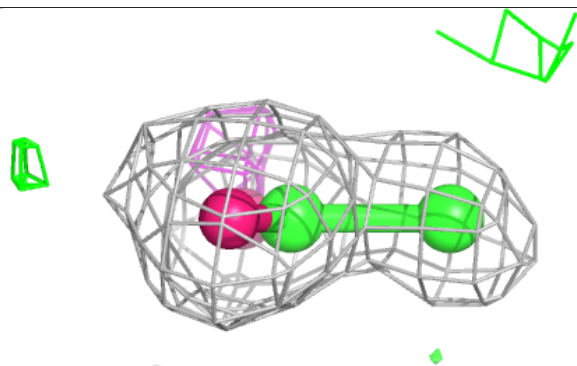
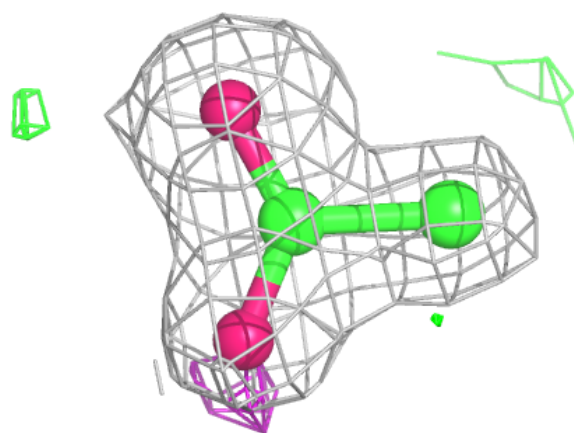
**Electron density around ACT C 304:**

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



**Electron density around ACT D 303:**

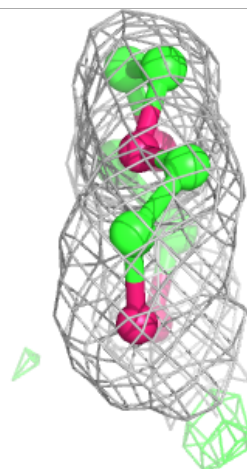
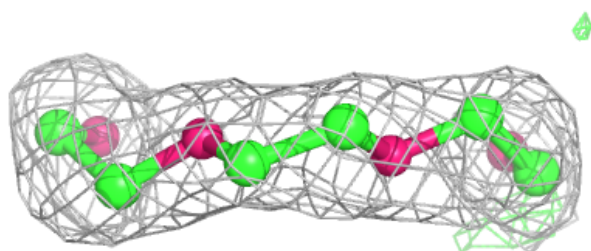
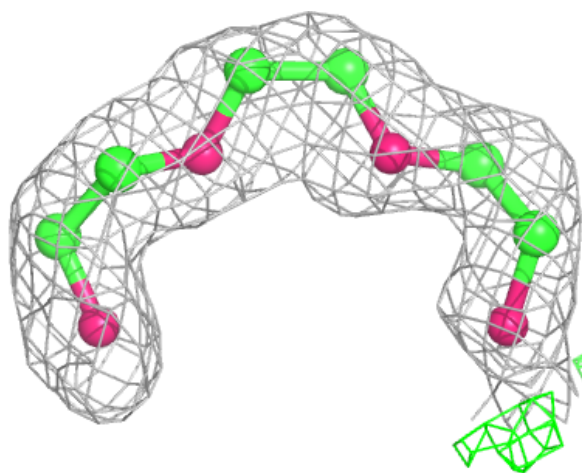
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around PGE D 304:**

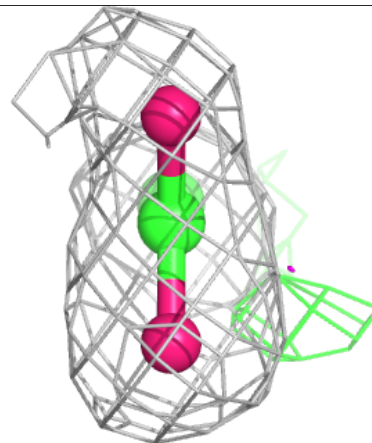
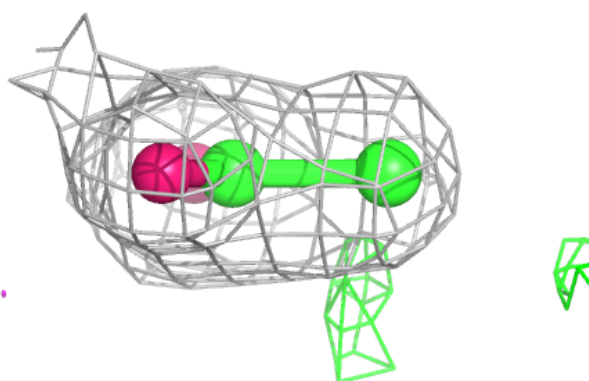
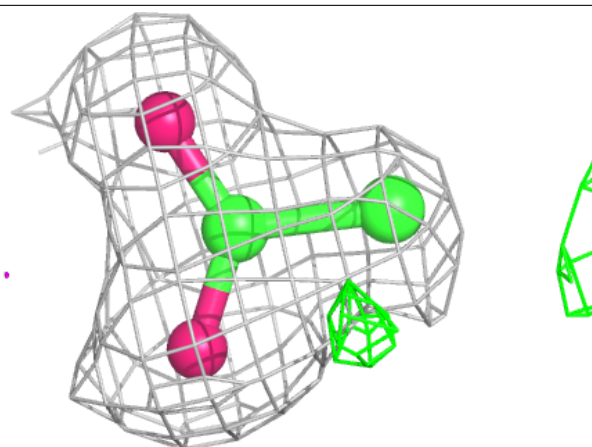
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





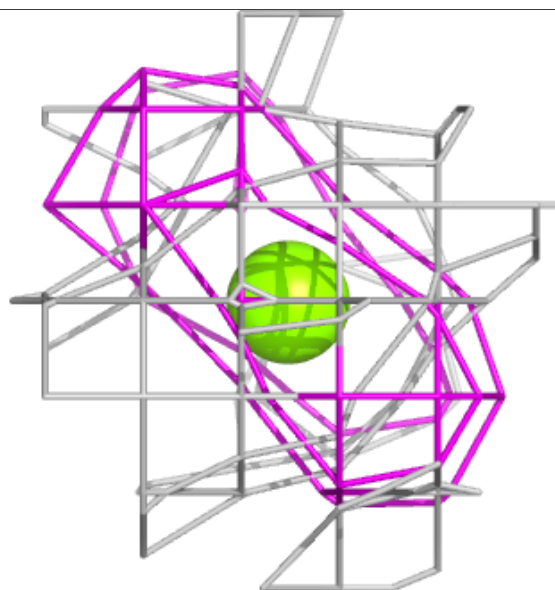
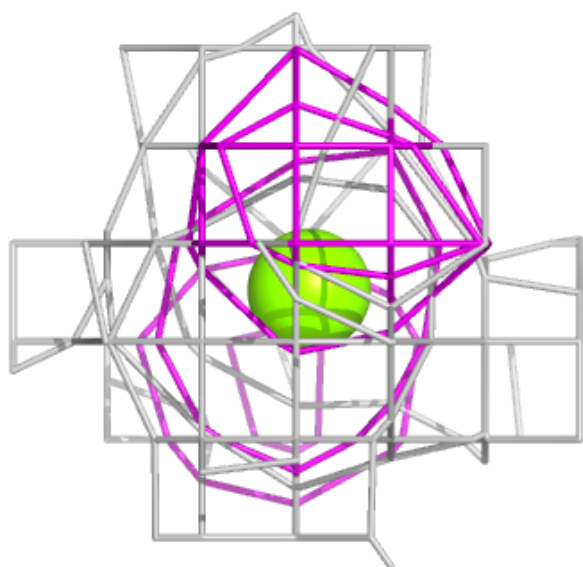
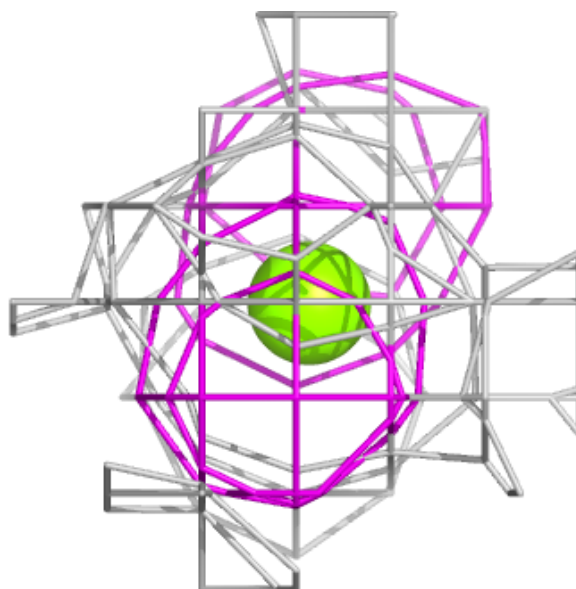
**Electron density around ACT B 307:**

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



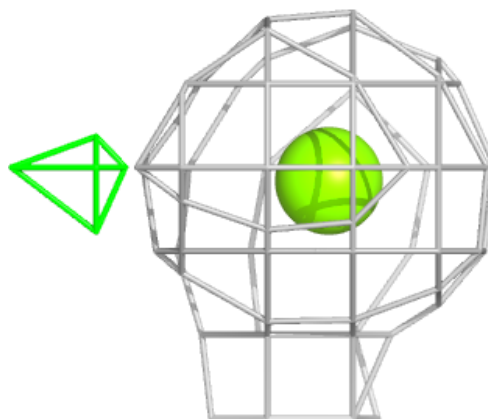
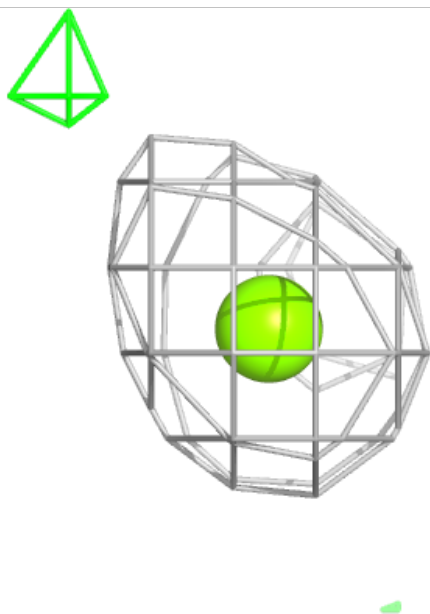
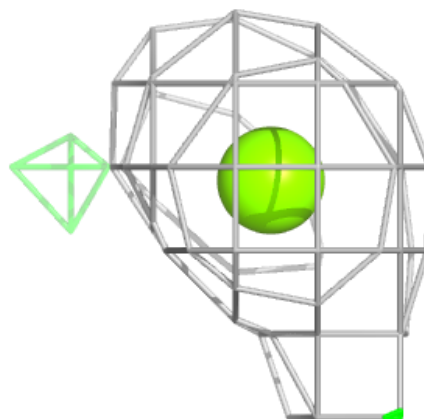
**Electron density around MG F 301:**

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



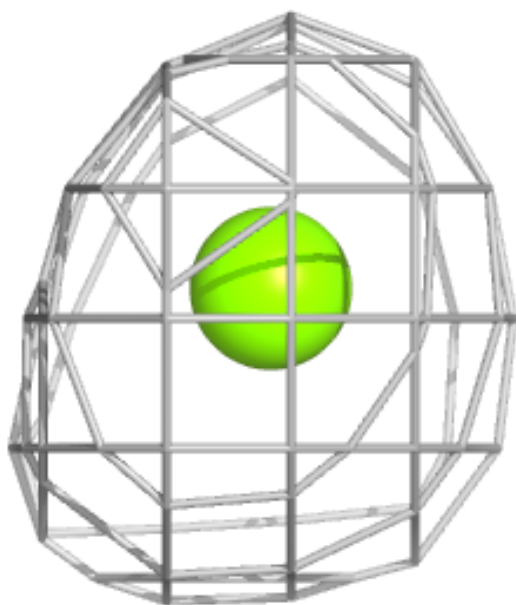
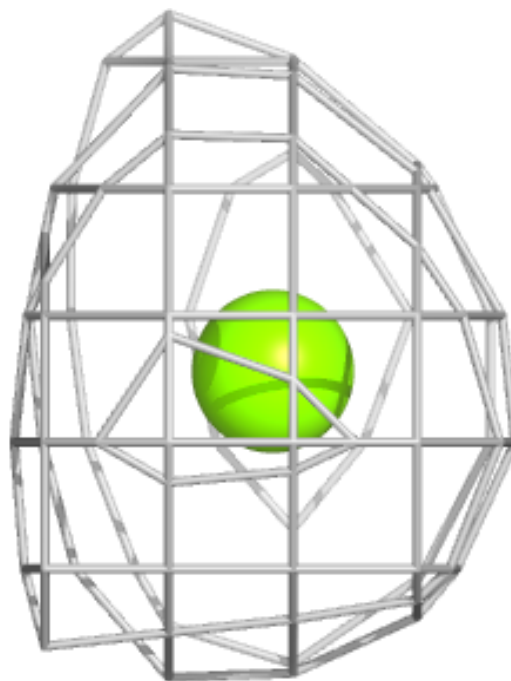
**Electron density around MG B 304:**

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



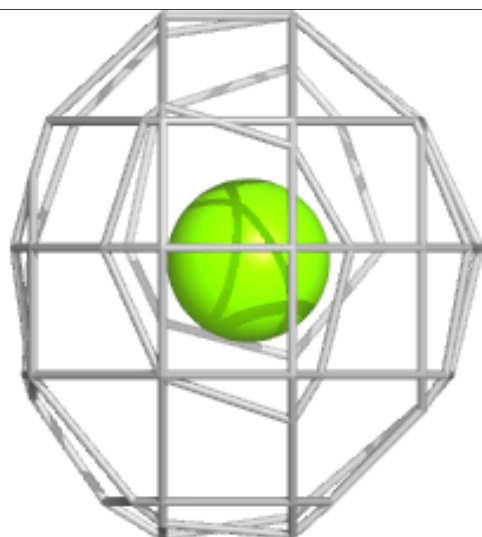
**Electron density around MG B 303:**

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



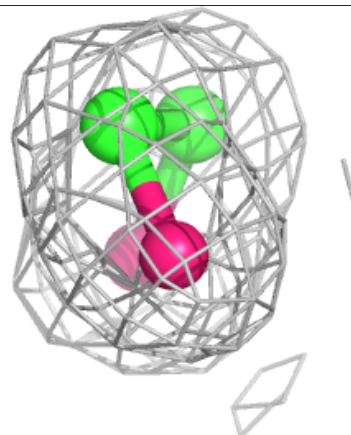
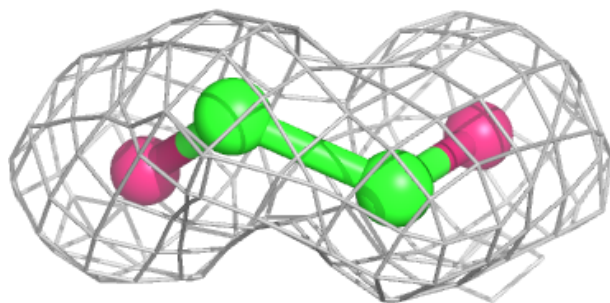
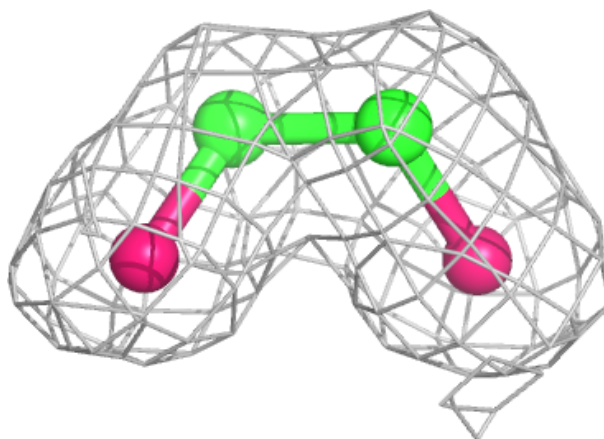
**Electron density around MG C 302:**

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



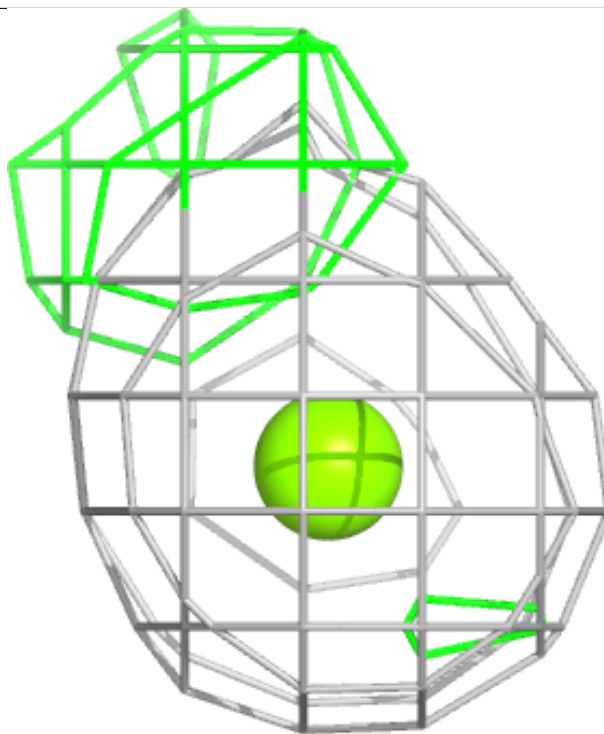
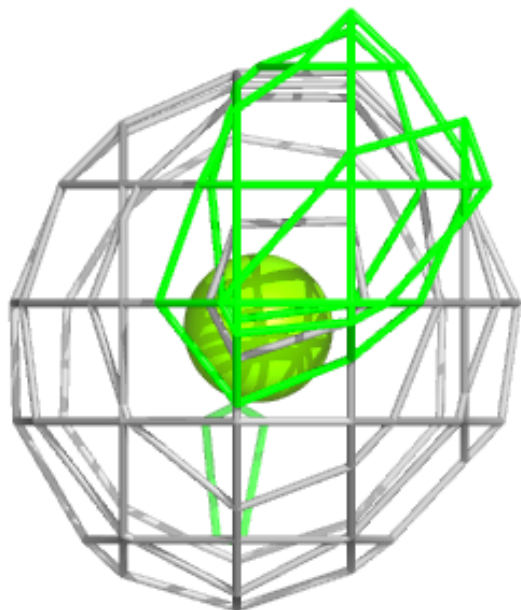
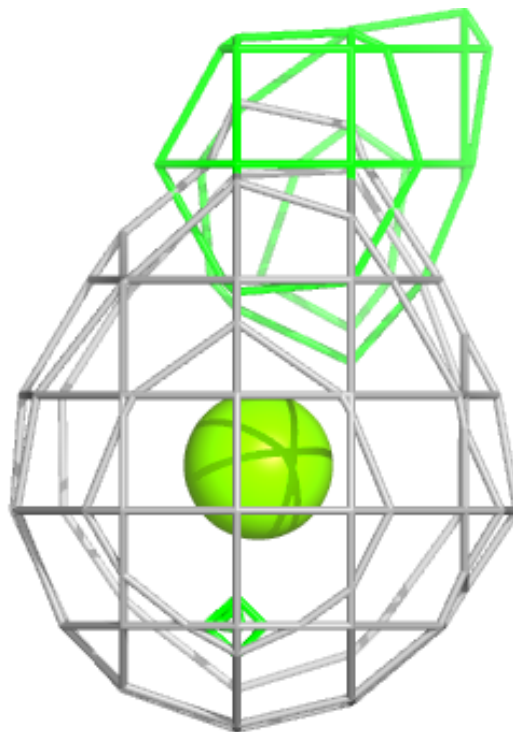
**Electron density around EDO F 304:**

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



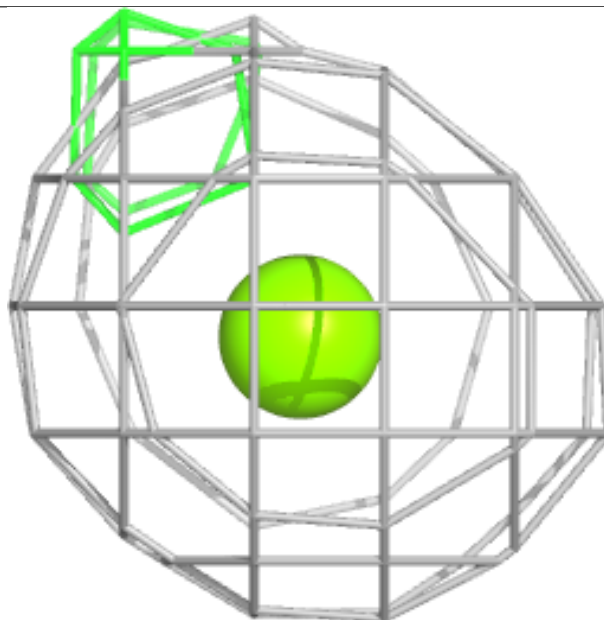
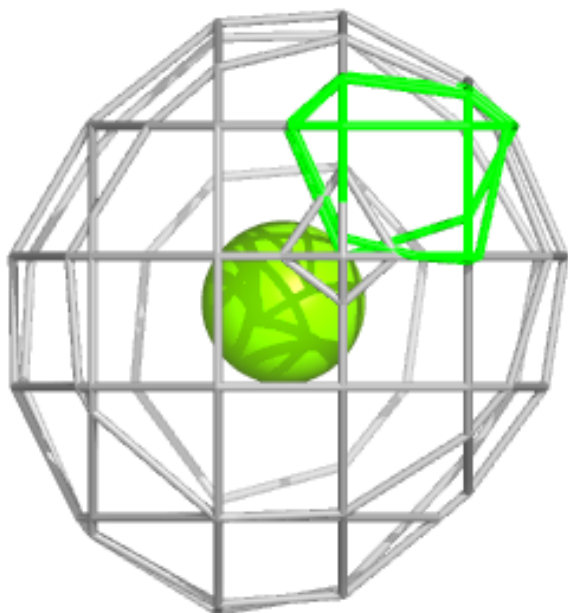
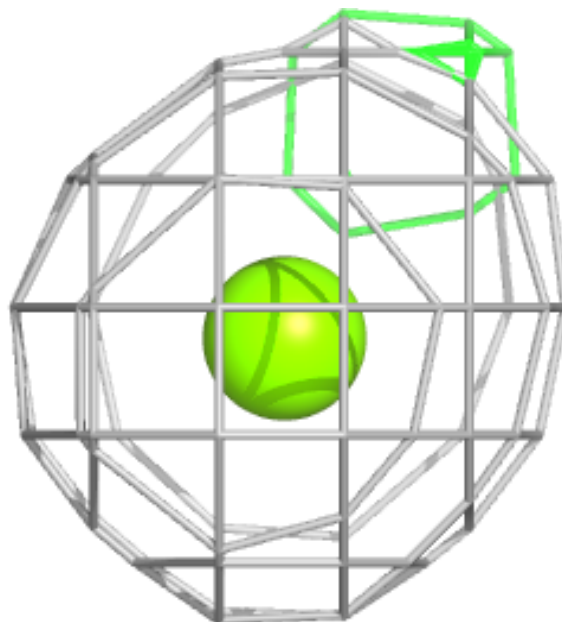
**Electron density around MG D 301:**

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



**Electron density around MG A 302:**

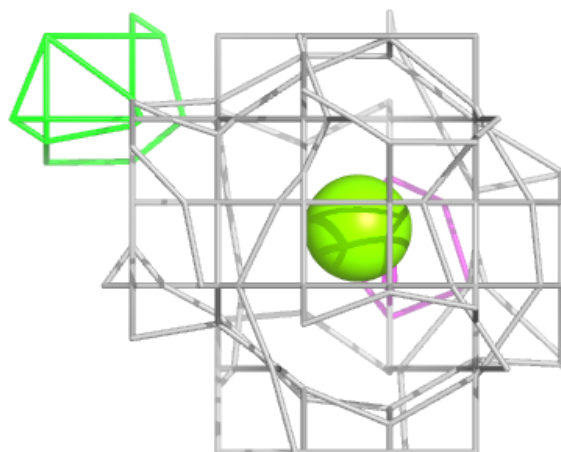
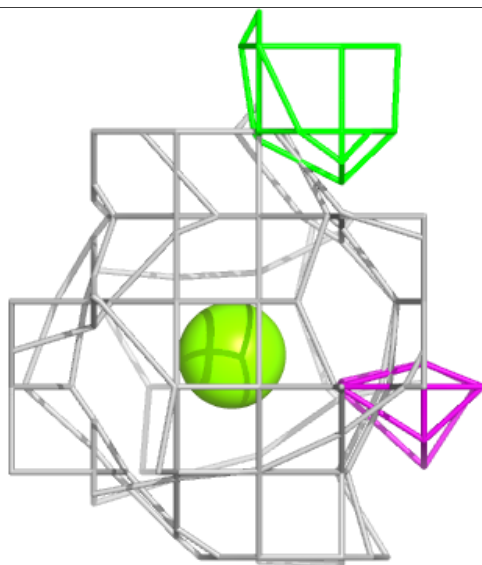
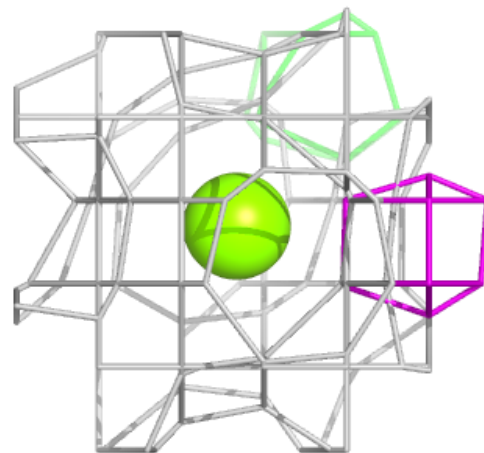
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MG 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.