



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2021 – 10:46 AM EST

PDB ID : 7KR7
Title : Dihydrodipicolinate synthase (DHDPS) from C.jejuni, H56A mutant with pyruvate bound in the active site and L-lysine at the allosteric site
Authors : Saran, S.; Sanders, D.A.R.
Deposited on : 2020-11-18
Resolution : 2.22 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

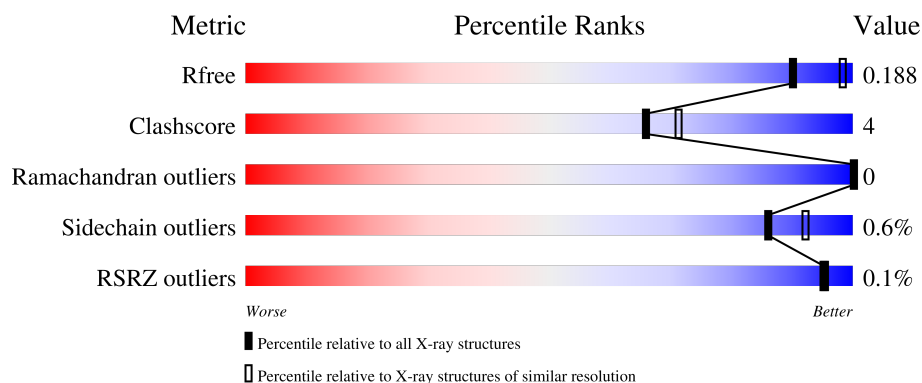
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	310	 88% 7% 5%
1	B	310	 90% 5% 5%
1	C	310	 87% 8% 5%
1	D	310	 85% 10% 5%
1	E	310	 88% 7% 5%

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Mol	Chain	Length	Quality of chain
1	F	310	 89% 7%

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	PGE	B	302	-	-	X	-
4	PGE	D	303	-	-	X	X
5	EDO	C	305	-	-	X	-
6	ACT	B	307	-	-	-	X
7	PEG	F	307	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14969 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
			2258	1435	373	437	13			
1	B	296	Total	C	N	O	S	0	0	0
			2259	1437	372	437	13			
1	C	296	Total	C	N	O	S	0	0	0
			2266	1442	375	436	13			
1	D	296	Total	C	N	O	S	0	0	0
			2255	1434	372	436	13			
1	E	296	Total	C	N	O	S	0	1	0
			2277	1449	375	440	13			
1	F	297	Total	C	N	O	S	0	0	0
			2271	1444	376	438	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	56	ALA	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

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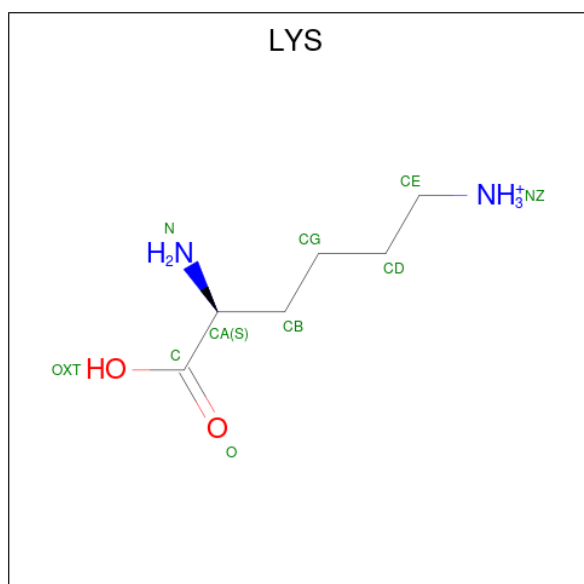
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B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
B	56	ALA	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	ALA	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	ALA	HIS	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	56	ALA	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
F	-2	HIS	-	expression tag	UNP Q9PPB4
F	-1	GLY	-	expression tag	UNP Q9PPB4
F	0	SER	-	expression tag	UNP Q9PPB4
F	56	ALA	HIS	engineered mutation	UNP Q9PPB4

- Molecule 2 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
2	A	1	Total	C	N	O	0	0
			10	6	2	2		

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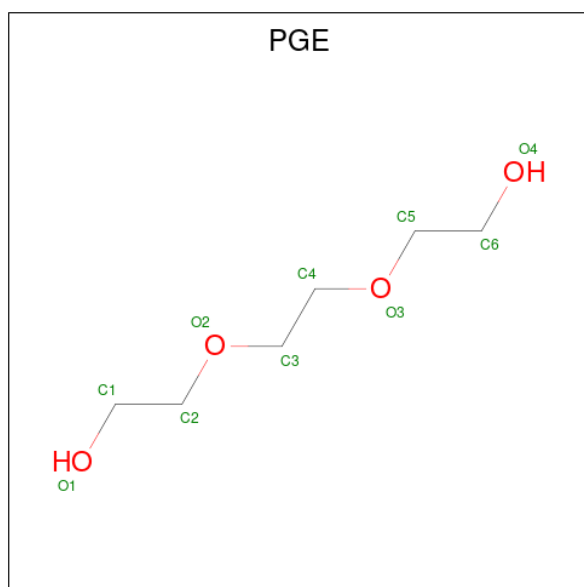
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			10	6	2	2		
2	C	1	Total	C	N	O	0	0
			10	6	2	2		
2	D	1	Total	C	N	O	0	0
			10	6	2	2		
2	E	1	Total	C	N	O	0	0
			10	6	2	2		
2	F	1	Total	C	N	O	0	0
			10	6	2	2		

- 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	C	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂) (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	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	E	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: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



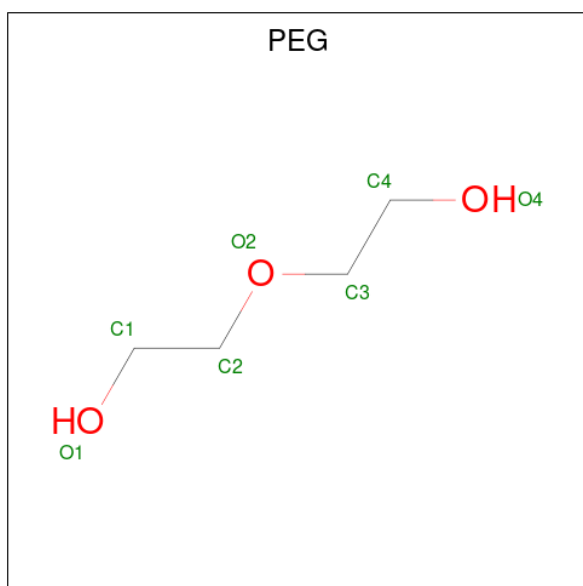
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		
6	E	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			7	4	3		
7	E	1	Total	C	O	0	0
			7	4	3		
7	F	1	Total	C	O	0	0
			7	4	3		
7	F	1	Total	C	O	0	0
			7	4	3		
7	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

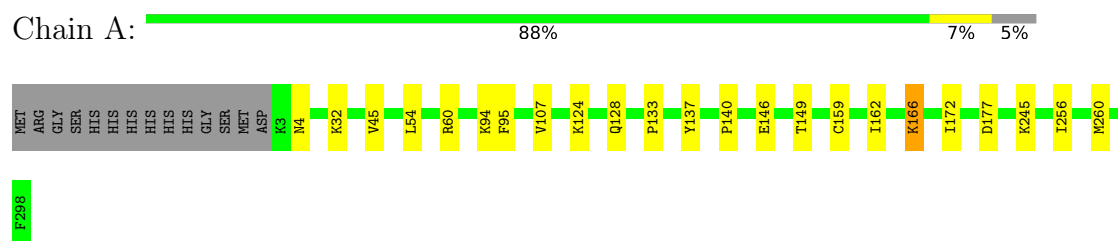
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	202	Total	O	0	0
			202	202		
9	B	192	Total	O	0	0
			192	192		
9	C	189	Total	O	0	0
			189	189		
9	D	182	Total	O	0	0
			182	182		
9	E	184	Total	O	0	0
			184	184		
9	F	194	Total	O	0	0
			194	194		

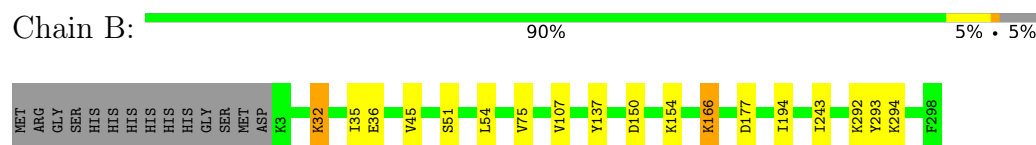
3 Residue-property plots

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.

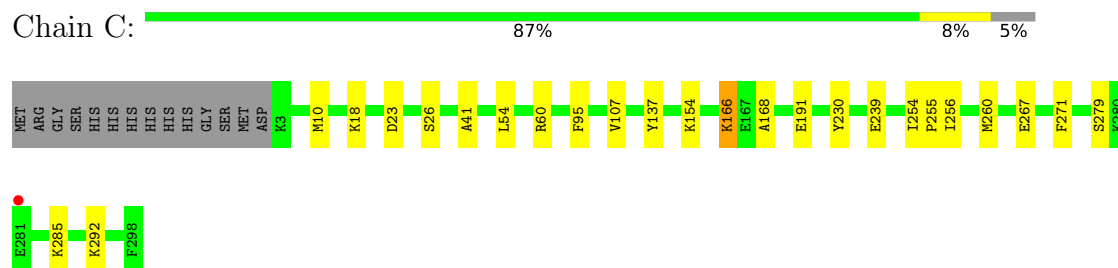
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



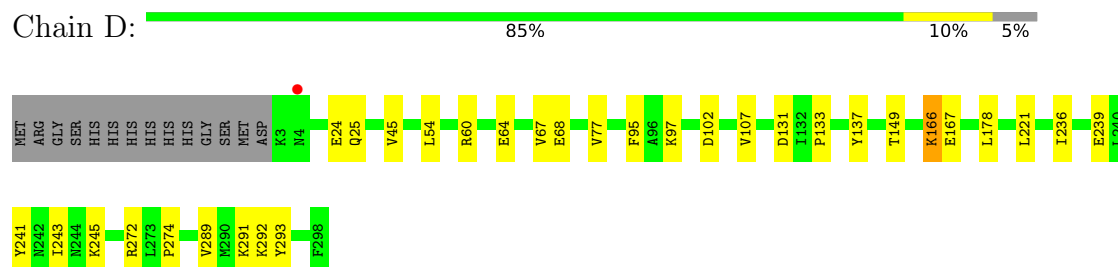
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



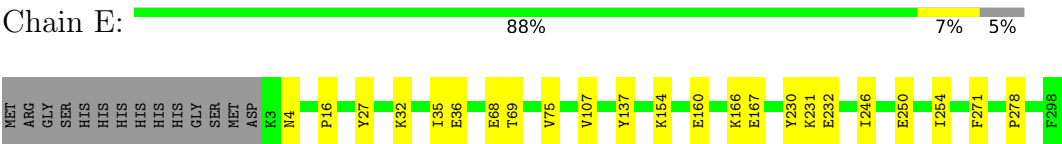
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



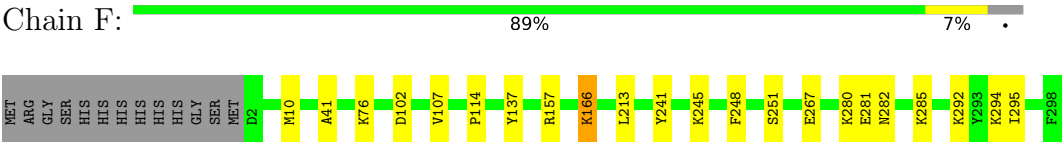
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



- 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, α , β , γ	85.80Å 231.24Å 199.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.80 – 2.22 45.80 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.80-2.22) 97.9 (45.80-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.53 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.149 , 0.189 0.152 , 0.188	Depositor DCC
R_{free} test set	4885 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14969	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PEG, GOL, KPI, PGE, MG, ACT

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	0.54	0/2281	0.63	0/3089
1	B	0.55	0/2282	0.64	0/3090
1	C	0.53	0/2289	0.61	0/3096
1	D	0.65	3/2278 (0.1%)	0.66	0/3085
1	E	0.63	1/2300 (0.0%)	0.62	0/3111
1	F	0.61	0/2294	0.62	0/3104
All	All	0.59	4/13724 (0.0%)	0.63	0/18575

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	F	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	167	GLU	CD-OE2	-5.67	1.19	1.25
1	D	24	GLU	CD-OE2	-5.57	1.19	1.25
1	D	24	GLU	CD-OE1	-5.51	1.19	1.25
1	D	167	GLU	CD-OE2	-5.21	1.20	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	KPI	Mainchain
1	B	166	KPI	Mainchain
1	F	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	2258	0	2272	17	0
1	B	2259	0	2271	16	0
1	C	2266	0	2296	27	0
1	D	2255	0	2265	21	0
1	E	2277	0	2300	14	0
1	F	2271	0	2296	17	0
2	A	10	0	12	0	0
2	B	10	0	12	1	0
2	C	10	0	12	1	0
2	D	10	0	12	0	0
2	E	10	0	12	0	0
2	F	10	0	12	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	F	1	0	0	0	0
4	A	10	0	14	0	0
4	B	10	0	14	6	0
4	C	10	0	14	5	0
4	D	20	0	28	6	0
4	E	10	0	14	3	0
5	A	8	0	12	3	0
5	B	16	0	24	1	0
5	C	8	0	12	11	0
5	E	4	0	6	0	0
5	F	4	0	6	3	0
6	A	4	0	3	0	0
6	B	4	0	3	0	0
6	C	8	0	6	0	0
6	D	4	0	3	0	0
6	E	8	0	6	0	0
6	F	8	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	7	0	10	0	0
7	E	7	0	10	0	0
7	F	21	0	29	6	0
8	B	6	0	7	0	0
9	A	202	0	0	1	0
9	B	192	0	0	2	0
9	C	189	0	0	4	0
9	D	182	0	0	1	0
9	E	184	0	0	1	0
9	F	194	0	0	1	0
All	All	14969	0	13999	112	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 (112) 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:F:251:SER:HA	7:F:307:PEG:H21	1.41	1.00
1:B:32:LYS:HE3	1:B:36:GLU:OE1	1.64	0.96
1:E:154:LYS:CE	4:E:302:PGE:H6	2.03	0.87
1:F:281:GLU:HB2	5:F:303:EDO:H12	1.58	0.85
1:E:154:LYS:CE	4:E:302:PGE:C6	2.56	0.82
1:D:289:VAL:HA	4:D:303:PGE:H12	1.62	0.81
1:C:26:SER:CB	5:C:305:EDO:H12	2.10	0.81
1:A:124:LYS:HZ3	1:A:128:GLN:NE2	1.79	0.79
1:A:124:LYS:NZ	1:A:128:GLN:NE2	2.32	0.77
1:C:26:SER:HB2	5:C:305:EDO:H12	1.66	0.77
1:C:292:LYS:HE3	5:C:304:EDO:O2	1.86	0.75
1:C:239:GLU:O	5:C:304:EDO:H11	1.87	0.73
1:E:32:LYS:O	1:E:36:GLU:HG3	1.89	0.73
4:D:303:PGE:H62	9:D:561:HOH:O	1.88	0.73
1:F:281:GLU:CB	5:F:303:EDO:H12	2.19	0.72
1:C:26:SER:OG	5:C:305:EDO:C1	2.39	0.71
1:A:124:LYS:NZ	1:A:128:GLN:HE22	1.90	0.69
1:E:154:LYS:CE	4:E:302:PGE:H62	2.23	0.67
5:C:305:EDO:H22	9:C:465:HOH:O	1.96	0.65
1:C:26:SER:OG	5:C:305:EDO:H11	1.99	0.63
1:C:154:LYS:HZ2	4:C:303:PGE:H52	1.64	0.62
1:C:26:SER:OG	5:C:305:EDO:H12	2.00	0.62
1:F:248:PHE:HD2	7:F:307:PEG:H11	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LYS:HD2	4:B:302:PGE:H52	1.83	0.61
1:D:241:TYR:OH	1:D:245:LYS:HE2	2.01	0.61
1:B:154:LYS:HE3	4:B:302:PGE:H2	1.82	0.61
1:B:150:ASP:HB3	4:B:302:PGE:H22	1.81	0.60
1:A:124:LYS:HZ1	1:A:128:GLN:HE22	1.52	0.58
1:D:64:GLU:O	1:D:68:GLU:HB2	2.04	0.57
1:C:154:LYS:HD2	4:C:303:PGE:H62	1.86	0.57
1:D:137:TYR:CD1	1:D:166:KPI:HD	2.42	0.55
1:A:4:ASN:HB3	1:A:133:PRO:HG3	1.89	0.54
1:D:292:LYS:HB2	4:D:303:PGE:H2	1.89	0.54
1:B:45:VAL:HG12	1:B:51:SER:HB3	1.91	0.53
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.88	0.53
1:D:97:LYS:HE3	1:D:131:ASP:OD1	2.09	0.53
1:F:157:ARG:O	7:F:308:PEG:H32	2.08	0.53
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.91	0.52
1:C:279:SER:HB2	9:C:560:HOH:O	2.09	0.52
1:B:107:VAL:HA	1:B:137:TYR:HB3	1.92	0.51
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.91	0.51
1:C:256:ILE:O	1:C:260:MET:HG2	2.12	0.50
5:B:304:EDO:H11	9:B:573:HOH:O	2.12	0.50
1:F:213:LEU:HD11	1:F:295:ILE:HD13	1.92	0.50
1:C:168:ALA:HA	1:C:191:GLU:HG3	1.94	0.50
1:C:239:GLU:O	5:C:304:EDO:C1	2.56	0.50
1:B:35:ILE:HG12	1:B:75:VAL:HG21	1.93	0.50
1:D:97:LYS:O	1:D:97:LYS:HG3	2.06	0.50
1:F:248:PHE:HD2	7:F:307:PEG:C1	2.25	0.50
1:F:292:LYS:HD2	9:F:547:HOH:O	2.11	0.50
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.95	0.49
1:E:4:ASN:ND2	9:E:407:HOH:O	2.42	0.49
1:B:177:ASP:OD2	9:B:401:HOH:O	2.20	0.48
1:E:35:ILE:HG12	1:E:75:VAL:HG21	1.95	0.48
1:F:241:TYR:CZ	1:F:245:LYS:HE3	2.49	0.48
1:A:177:ASP:OD2	5:A:305:EDO:H12	2.13	0.47
1:C:23:ASP:OD2	5:C:305:EDO:O2	2.26	0.47
1:A:159:CYS:HB2	1:A:162:ILE:HD12	1.97	0.47
1:C:267:GLU:H	5:C:305:EDO:H21	1.79	0.47
1:A:94:LYS:NZ	9:A:403:HOH:O	2.34	0.47
1:C:154:LYS:NZ	4:C:303:PGE:H32	2.30	0.47
1:D:97:LYS:CE	1:D:131:ASP:OD1	2.63	0.47
1:D:149:THR:HG23	1:D:178:LEU:HD23	1.97	0.46
9:C:516:HOH:O	1:D:291:LYS:HE3	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:VAL:HA	1:D:77:VAL:HG21	1.97	0.46
1:E:231:LYS:HE3	1:E:232:GLU:OE1	2.16	0.46
1:D:274:PRO:HB2	1:F:114:PRO:HB3	1.97	0.46
1:F:282:ASN:OD1	5:F:303:EDO:H11	2.16	0.46
1:B:243:ILE:HB	1:B:293:TYR:CE2	2.51	0.46
1:E:68[B]:GLU:O	1:E:69:THR:C	2.52	0.46
1:A:177:ASP:OD2	5:A:305:EDO:C1	2.64	0.45
1:C:154:LYS:HZ2	4:C:303:PGE:H32	1.81	0.45
1:B:292:LYS:HE3	1:B:293:TYR:CZ	2.51	0.45
1:C:60:ARG:HB3	1:C:95:PHE:CZ	2.51	0.45
1:E:254:ILE:HA	1:E:271:PHE:CE2	2.52	0.44
1:C:10:MET:HA	1:C:41:ALA:O	2.17	0.44
1:E:246:ILE:HD12	1:E:246:ILE:HA	1.89	0.44
1:F:294:LYS:N	1:F:294:LYS:HD3	2.32	0.44
1:C:154:LYS:HZ2	4:C:303:PGE:C5	2.28	0.44
1:A:172:ILE:HG23	1:B:194:ILE:HG21	2.00	0.44
1:C:137:TYR:CD1	1:C:166:KPI:HD	2.53	0.43
1:F:107:VAL:HA	1:F:137:TYR:HB3	2.00	0.43
1:C:254:ILE:HA	1:C:271:PHE:CE2	2.54	0.43
1:D:243:ILE:HB	1:D:293:TYR:CE2	2.54	0.43
1:B:154:LYS:CD	4:B:302:PGE:H52	2.48	0.43
1:E:250:GLU:OE1	1:E:278:PRO:HA	2.19	0.43
1:D:239:GLU:HA	4:D:303:PGE:H6	2.01	0.43
1:D:289:VAL:CA	4:D:303:PGE:H12	2.40	0.43
1:A:140:PRO:HG3	1:A:146:GLU:OE1	2.19	0.42
1:C:230:TYR:CD2	1:E:230:TYR:HD2	2.36	0.42
1:D:221:LEU:HD12	1:D:236:ILE:HG22	2.01	0.42
1:A:45:VAL:HG13	1:A:54:LEU:HD12	2.02	0.42
1:B:54:LEU:O	2:B:301:LYS:HE3	2.19	0.42
1:D:289:VAL:HG13	4:D:303:PGE:H12	2.02	0.42
1:C:254:ILE:HB	1:C:255:PRO:HD3	2.02	0.42
1:F:10:MET:HA	1:F:41:ALA:O	2.19	0.42
1:F:251:SER:HA	7:F:307:PEG:H41	2.02	0.42
1:B:154:LYS:HZ2	4:B:302:PGE:H32	1.85	0.42
1:B:294:LYS:HA	1:B:294:LYS:HD2	1.87	0.42
1:F:76:LYS:HG2	1:F:102:ASP:CG	2.39	0.42
1:B:154:LYS:NZ	4:B:302:PGE:H32	2.35	0.41
1:C:54:LEU:O	2:C:301:LYS:HE3	2.20	0.41
1:A:149:THR:HG21	5:A:305:EDO:H21	2.02	0.41
1:A:60:ARG:HB3	1:A:95:PHE:CZ	2.56	0.41
1:A:256:ILE:O	1:A:260:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LYS:HA	1:A:245:LYS:HD2	1.87	0.41
1:C:285:LYS:NZ	9:C:401:HOH:O	2.46	0.41
1:D:45:VAL:HG13	1:D:54:LEU:HD12	2.03	0.41
1:E:16:PRO:HD2	1:E:27:TYR:HD1	1.85	0.41
1:D:60:ARG:HB3	1:D:95:PHE:CZ	2.57	0.40
1:F:248:PHE:CD2	7:F:307:PEG:H11	2.51	0.40
1:D:102:ASP:O	1:D:133:PRO:HD2	2.22	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	293/310 (94%)	287 (98%)	6 (2%)	0	100	100
1	B	293/310 (94%)	289 (99%)	4 (1%)	0	100	100
1	C	293/310 (94%)	287 (98%)	6 (2%)	0	100	100
1	D	293/310 (94%)	288 (98%)	5 (2%)	0	100	100
1	E	294/310 (95%)	289 (98%)	5 (2%)	0	100	100
1	F	294/310 (95%)	290 (99%)	4 (1%)	0	100	100
All	All	1760/1860 (95%)	1730 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	243/259 (94%)	242 (100%)	1 (0%)	91	95
1	B	242/259 (93%)	241 (100%)	1 (0%)	91	95
1	C	245/259 (95%)	244 (100%)	1 (0%)	91	95
1	D	242/259 (93%)	240 (99%)	2 (1%)	81	89
1	E	245/259 (95%)	244 (100%)	1 (0%)	91	95
1	F	245/259 (95%)	242 (99%)	3 (1%)	71	82
All	All	1462/1554 (94%)	1453 (99%)	9 (1%)	86	92

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	B	32	LYS
1	C	18	LYS
1	D	25	GLN
1	D	272	ARG
1	E	160	GLU
1	F	267	GLU
1	F	280	LYS
1	F	285	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	128	GLN
1	D	4	ASN
1	E	242	ASN
1	F	4	ASN
1	F	19	ASN
1	F	25	GLN

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	A	166	1	10,13,14	1.34	1 (10%)	6,15,17	2.48	3 (50%)
1	KPI	C	166	1	10,13,14	1.32	2 (20%)	6,15,17	2.20	2 (33%)
1	KPI	B	166	1	10,13,14	1.39	1 (10%)	6,15,17	2.37	2 (33%)
1	KPI	F	166	1	10,13,14	1.45	1 (10%)	6,15,17	2.39	3 (50%)
1	KPI	E	166	1	10,13,14	1.28	2 (20%)	6,15,17	1.61	1 (16%)
1	KPI	D	166	1	10,13,14	1.28	1 (10%)	6,15,17	2.15	2 (33%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	166	KPI	O-C	4.19	1.36	1.19
1	B	166	KPI	O-C	4.01	1.35	1.19
1	A	166	KPI	O-C	3.75	1.34	1.19
1	D	166	KPI	CX2-CX1	-3.14	1.47	1.52
1	E	166	KPI	CX2-CX1	-2.74	1.47	1.52
1	C	166	KPI	CX2-CX1	-2.57	1.48	1.52
1	C	166	KPI	CA-N	-2.51	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	166	KPI	CA-N	-2.13	1.41	1.48

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	KPI	C1-CX1-CX2	-4.93	112.46	117.92
1	B	166	KPI	C1-CX1-CX2	-4.27	113.19	117.92
1	F	166	KPI	C1-CX1-CX2	-4.09	113.39	117.92
1	C	166	KPI	CE-NZ-CX1	3.97	132.46	121.77
1	D	166	KPI	C1-CX1-CX2	3.87	122.21	117.92
1	E	166	KPI	CE-NZ-CX1	3.49	131.15	121.77
1	C	166	KPI	CD-CE-NZ	-3.36	104.54	110.66
1	D	166	KPI	CE-NZ-CX1	3.03	129.92	121.77
1	F	166	KPI	C1-CX1-NZ	3.03	130.67	123.12
1	B	166	KPI	C1-CX1-NZ	3.02	130.65	123.12
1	A	166	KPI	C1-CX1-NZ	2.53	129.42	123.12
1	F	166	KPI	CE-NZ-CX1	2.06	127.31	121.77
1	A	166	KPI	CE-NZ-CX1	2.04	127.24	121.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	166	KPI	1	0
1	D	166	KPI	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 3 are monoatomic - leaving 37 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
2	LYS	E	301	-	5,9,9	0.48	0	4,10,10	0.54	0
7	PEG	E	306	-	6,6,6	0.25	0	5,5,5	1.26	1 (20%)
4	PGE	A	303	-	9,9,9	0.37	0	8,8,8	0.30	0
4	PGE	D	303	-	9,9,9	0.45	0	8,8,8	1.07	0
4	PGE	D	302	-	9,9,9	0.29	0	8,8,8	0.37	0
2	LYS	D	301	-	5,9,9	0.65	0	4,10,10	0.47	0
5	EDO	E	303	-	3,3,3	0.61	0	2,2,2	0.30	0
6	ACT	F	304	-	1,3,3	6.23	1 (100%)	0,3,3	-	-
6	ACT	C	306	-	1,3,3	7.45	1 (100%)	0,3,3	-	-
5	EDO	A	304	-	3,3,3	0.42	0	2,2,2	0.35	0
7	PEG	B	308	-	6,6,6	0.33	0	5,5,5	1.74	2 (40%)
4	PGE	E	302	-	9,9,9	0.40	0	8,8,8	0.79	0
5	EDO	A	305	-	3,3,3	0.26	0	2,2,2	0.30	0
7	PEG	F	306	-	6,6,6	0.48	0	5,5,5	0.34	0
7	PEG	F	308	-	6,6,6	0.48	0	5,5,5	1.27	1 (20%)
6	ACT	B	307	-	1,3,3	0.10	0	0,3,3	-	-
2	LYS	F	301	-	5,9,9	0.55	0	4,10,10	0.58	0
5	EDO	B	303	-	3,3,3	0.44	0	2,2,2	0.45	0
5	EDO	B	306	-	3,3,3	0.27	0	2,2,2	0.61	0
6	ACT	A	306	-	1,3,3	6.03	1 (100%)	0,3,3	-	-
2	LYS	B	301	-	5,9,9	0.37	0	4,10,10	0.51	0
7	PEG	F	307	-	6,6,6	0.68	0	5,5,5	1.17	0
6	ACT	F	305	-	1,3,3	6.70	1 (100%)	0,3,3	-	-
8	GOL	B	309	3	5,5,5	1.43	1 (20%)	5,5,5	0.58	0
6	ACT	E	304	-	1,3,3	4.72	1 (100%)	0,3,3	-	-
6	ACT	D	304	-	1,3,3	7.40	1 (100%)	0,3,3	-	-
6	ACT	E	305	-	1,3,3	6.55	1 (100%)	0,3,3	-	-
5	EDO	B	305	-	3,3,3	0.41	0	2,2,2	0.52	0
4	PGE	B	302	-	9,9,9	0.28	0	8,8,8	0.50	0
5	EDO	F	303	-	3,3,3	0.43	0	2,2,2	0.23	0
2	LYS	C	301	-	5,9,9	0.47	0	4,10,10	0.50	0
5	EDO	B	304	-	3,3,3	0.40	0	2,2,2	0.41	0
4	PGE	C	303	-	9,9,9	0.28	0	8,8,8	0.44	0
5	EDO	C	304	-	3,3,3	0.19	0	2,2,2	0.46	0
5	EDO	C	305	-	3,3,3	0.21	0	2,2,2	0.41	0
6	ACT	C	307	-	1,3,3	5.19	1 (100%)	0,3,3	-	-
2	LYS	A	301	-	5,9,9	0.49	0	4,10,10	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LYS	E	301	-	-	0/5/9/9	-
7	PEG	E	306	-	-	2/4/4/4	-
4	PGE	A	303	-	-	3/7/7/7	-
4	PGE	D	303	-	-	3/7/7/7	-
4	PGE	D	302	-	-	4/7/7/7	-
2	LYS	D	301	-	-	0/5/9/9	-
5	EDO	E	303	-	-	0/1/1/1	-
5	EDO	A	304	-	-	0/1/1/1	-
7	PEG	B	308	-	-	2/4/4/4	-
4	PGE	E	302	-	-	4/7/7/7	-
5	EDO	A	305	-	-	1/1/1/1	-
7	PEG	F	306	-	-	1/4/4/4	-
7	PEG	F	308	-	-	1/4/4/4	-
2	LYS	F	301	-	-	0/5/9/9	-
5	EDO	B	303	-	-	0/1/1/1	-
5	EDO	B	306	-	-	1/1/1/1	-
2	LYS	B	301	-	-	0/5/9/9	-
7	PEG	F	307	-	-	3/4/4/4	-
8	GOL	B	309	3	-	2/4/4/4	-
5	EDO	B	305	-	-	1/1/1/1	-
4	PGE	B	302	-	-	6/7/7/7	-
5	EDO	F	303	-	-	1/1/1/1	-
2	LYS	C	301	-	-	0/5/9/9	-
5	EDO	B	304	-	-	0/1/1/1	-
4	PGE	C	303	-	-	3/7/7/7	-
5	EDO	C	304	-	-	1/1/1/1	-
5	EDO	C	305	-	-	1/1/1/1	-
2	LYS	A	301	-	-	1/5/9/9	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	306	ACT	CH3-C	7.45	1.58	1.48
6	D	304	ACT	CH3-C	7.40	1.58	1.48
6	F	305	ACT	CH3-C	6.70	1.57	1.48
6	E	305	ACT	CH3-C	6.55	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	304	ACT	CH3-C	6.23	1.56	1.48
6	A	306	ACT	CH3-C	6.03	1.56	1.48
6	C	307	ACT	CH3-C	5.19	1.55	1.48
6	E	304	ACT	CH3-C	4.72	1.54	1.48
8	B	309	GOL	O2-C2	-2.32	1.36	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	308	PEG	O1-C1-C2	-2.62	96.63	111.81
7	E	306	PEG	O2-C3-C4	-2.13	100.72	110.07
7	F	308	PEG	O1-C1-C2	2.04	123.62	111.81
7	B	308	PEG	O2-C2-C1	-2.01	101.24	110.07

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	302	PGE	O2-C3-C4-O3
4	E	302	PGE	O2-C3-C4-O3
4	E	302	PGE	O1-C1-C2-O2
7	F	308	PEG	O2-C3-C4-O4
7	F	307	PEG	C1-C2-O2-C3
4	C	303	PGE	O2-C3-C4-O3
4	D	302	PGE	O1-C1-C2-O2
7	B	308	PEG	O1-C1-C2-O2
4	B	302	PGE	O3-C5-C6-O4
7	F	307	PEG	O2-C3-C4-O4
5	C	304	EDO	O1-C1-C2-O2
4	B	302	PGE	O1-C1-C2-O2
4	B	302	PGE	C1-C2-O2-C3
5	C	305	EDO	O1-C1-C2-O2
8	B	309	GOL	C1-C2-C3-O3
4	D	302	PGE	O3-C5-C6-O4
7	E	306	PEG	O2-C3-C4-O4
5	A	305	EDO	O1-C1-C2-O2
5	B	306	EDO	O1-C1-C2-O2
5	F	303	EDO	O1-C1-C2-O2
7	B	308	PEG	C1-C2-O2-C3
4	C	303	PGE	C1-C2-O2-C3
4	A	303	PGE	C1-C2-O2-C3
4	B	302	PGE	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
7	F	307	PEG	C4-C3-O2-C2
7	F	306	PEG	C1-C2-O2-C3
4	C	303	PGE	O1-C1-C2-O2
4	D	303	PGE	O3-C5-C6-O4
5	B	305	EDO	O1-C1-C2-O2
4	E	302	PGE	C6-C5-O3-C4
4	A	303	PGE	C6-C5-O3-C4
4	E	302	PGE	C4-C3-O2-C2
8	B	309	GOL	O2-C2-C3-O3
4	B	302	PGE	C3-C4-O3-C5
7	E	306	PEG	C1-C2-O2-C3
4	D	302	PGE	C3-C4-O3-C5
4	D	303	PGE	O2-C3-C4-O3
4	A	303	PGE	O2-C3-C4-O3
2	A	301	LYS	CG-CD-CE-NZ
4	D	303	PGE	O1-C1-C2-O2
4	B	302	PGE	O2-C3-C4-O3

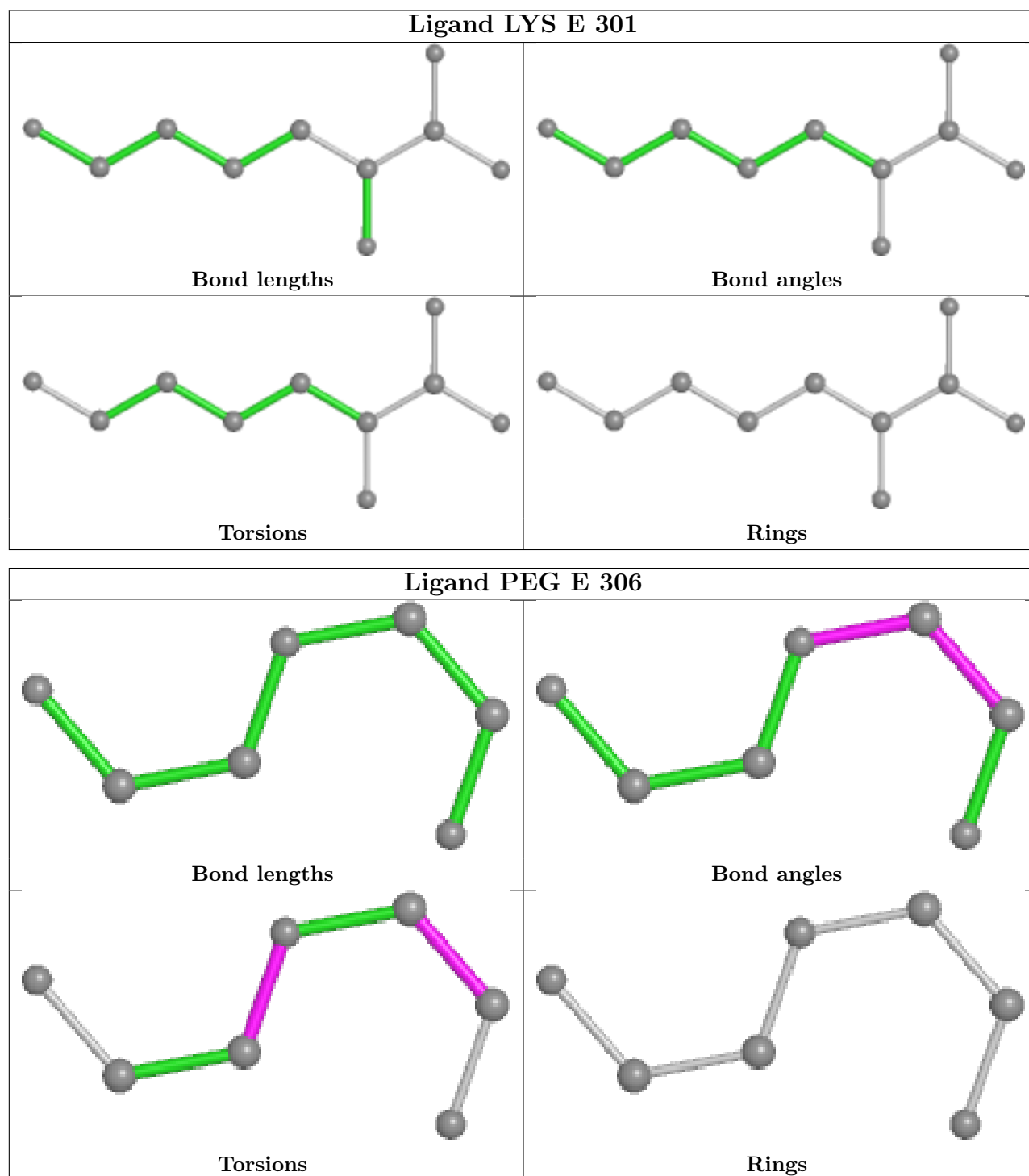
There are no ring outliers.

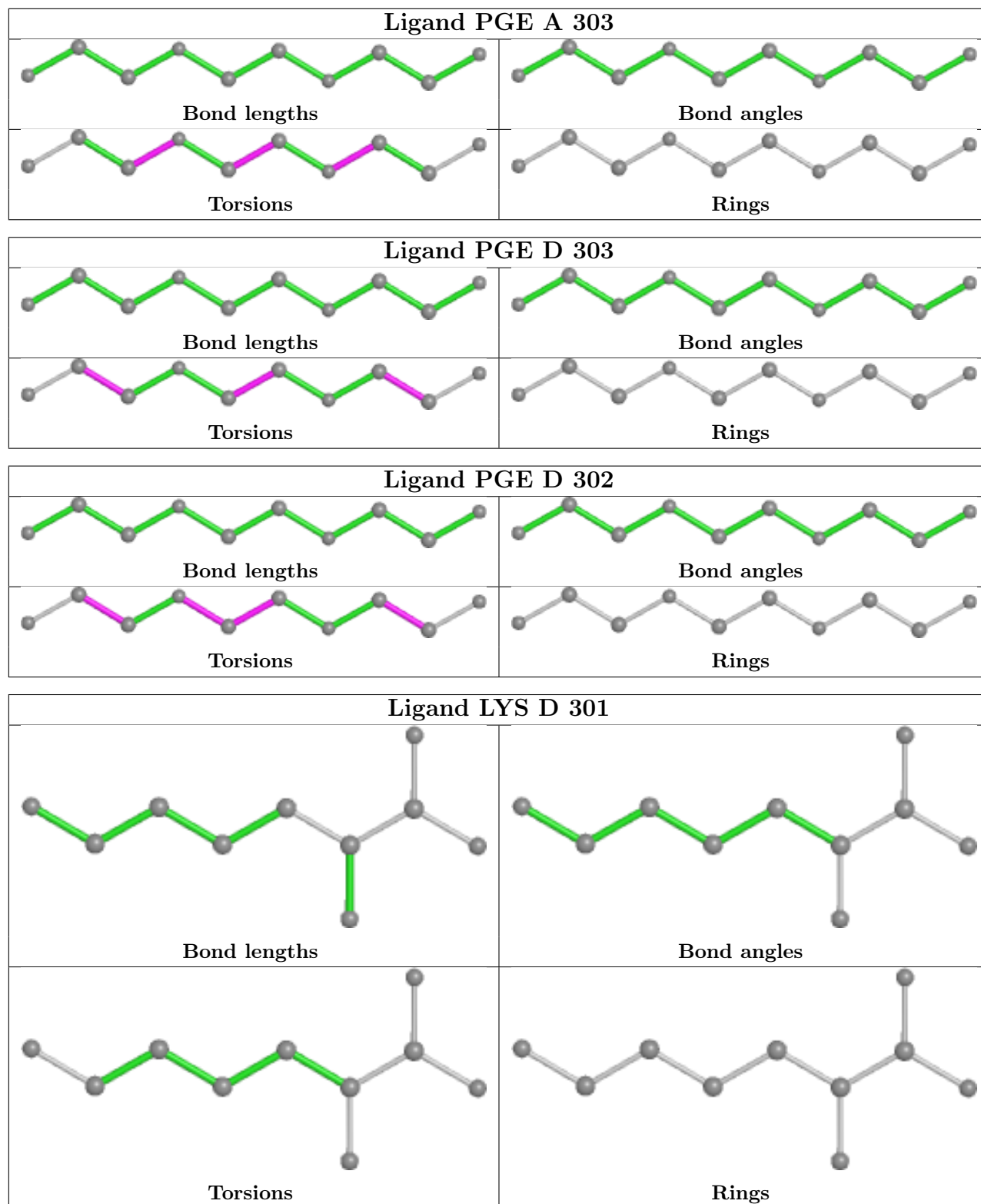
13 monomers are involved in 46 short contacts:

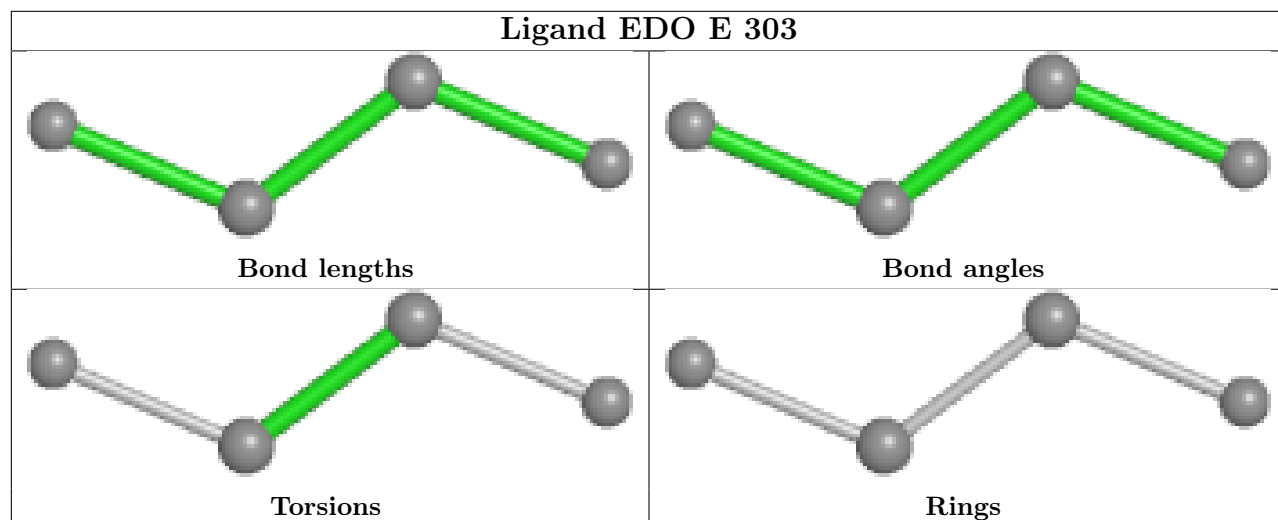
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	303	PGE	6	0
4	E	302	PGE	3	0
5	A	305	EDO	3	0
7	F	308	PEG	1	0
2	B	301	LYS	1	0
7	F	307	PEG	5	0
4	B	302	PGE	6	0
5	F	303	EDO	3	0
2	C	301	LYS	1	0
5	B	304	EDO	1	0
4	C	303	PGE	5	0
5	C	304	EDO	3	0
5	C	305	EDO	8	0

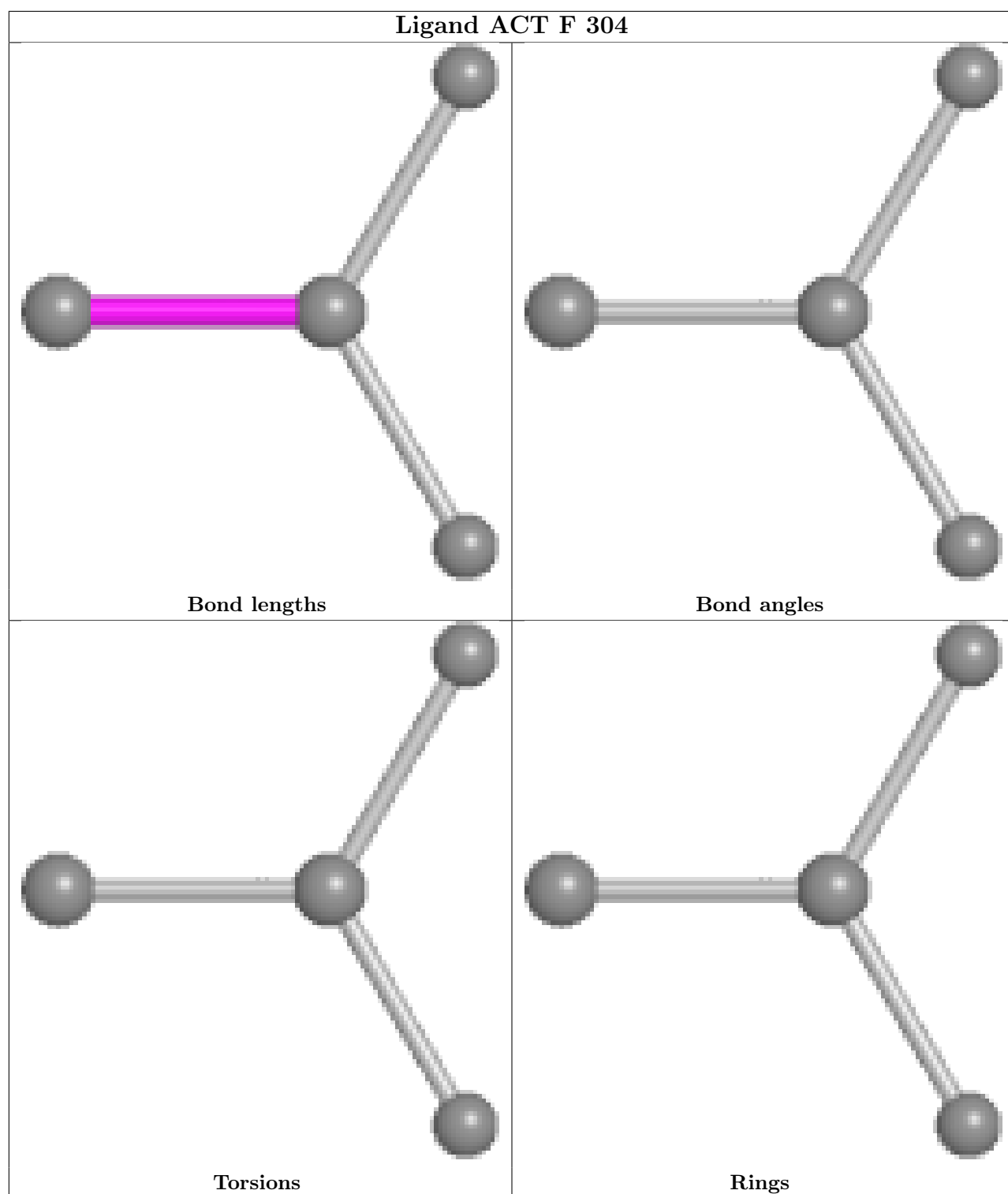
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

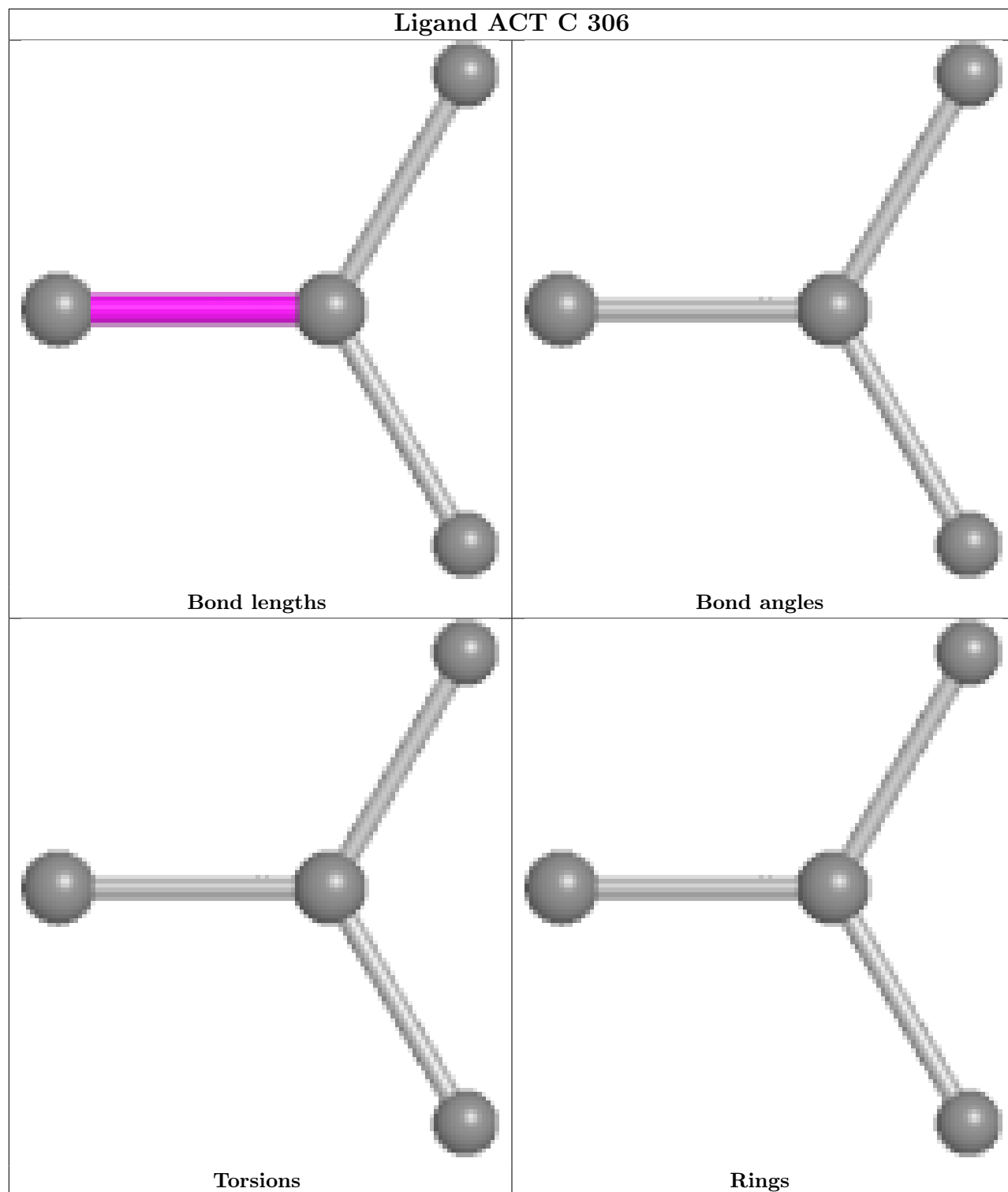
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

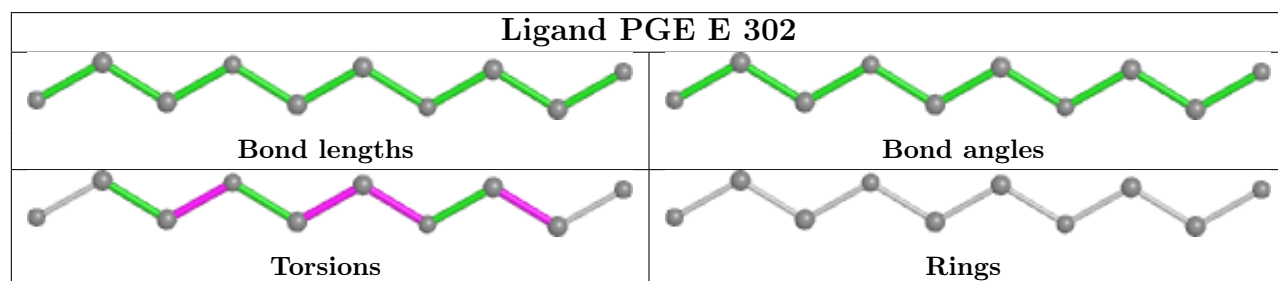
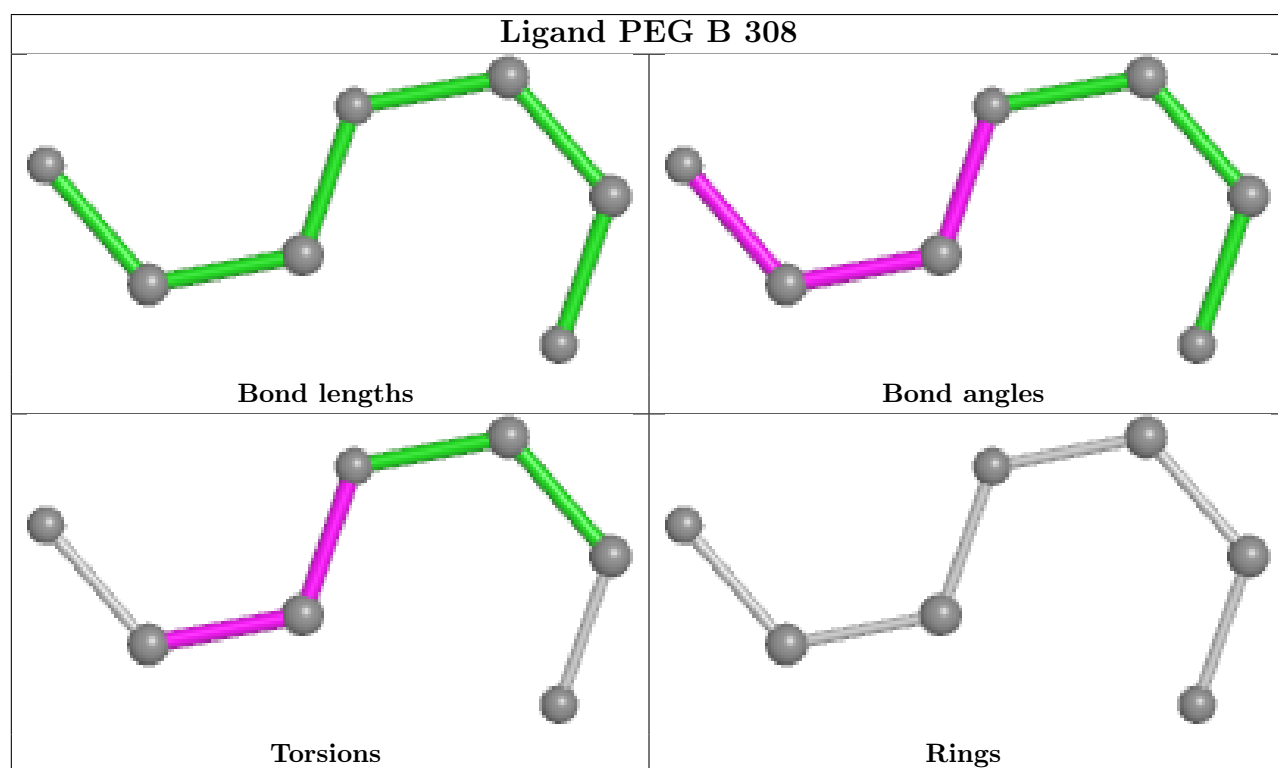
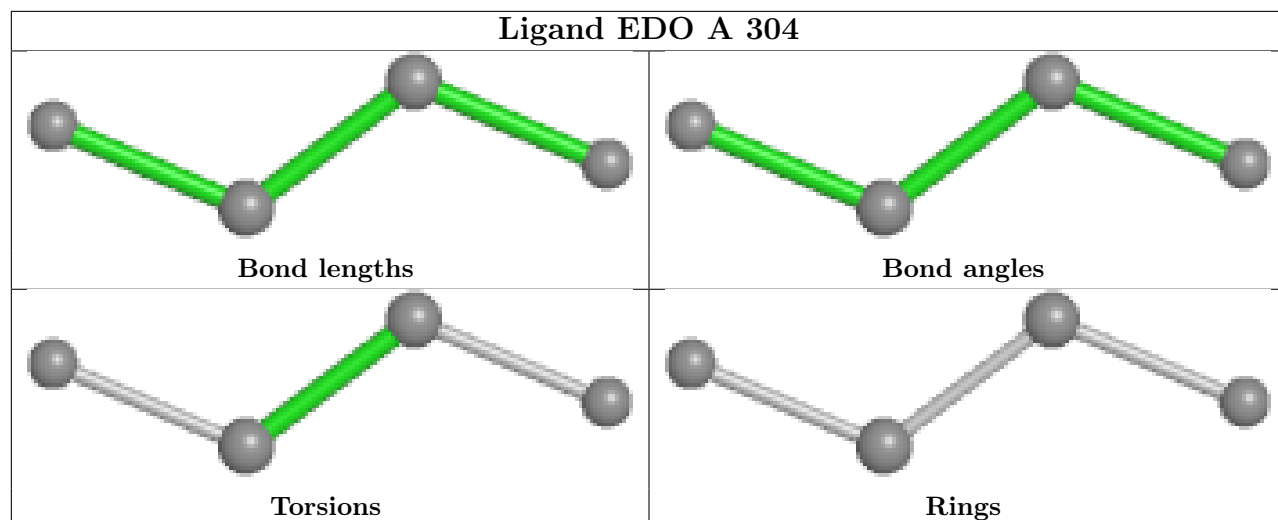


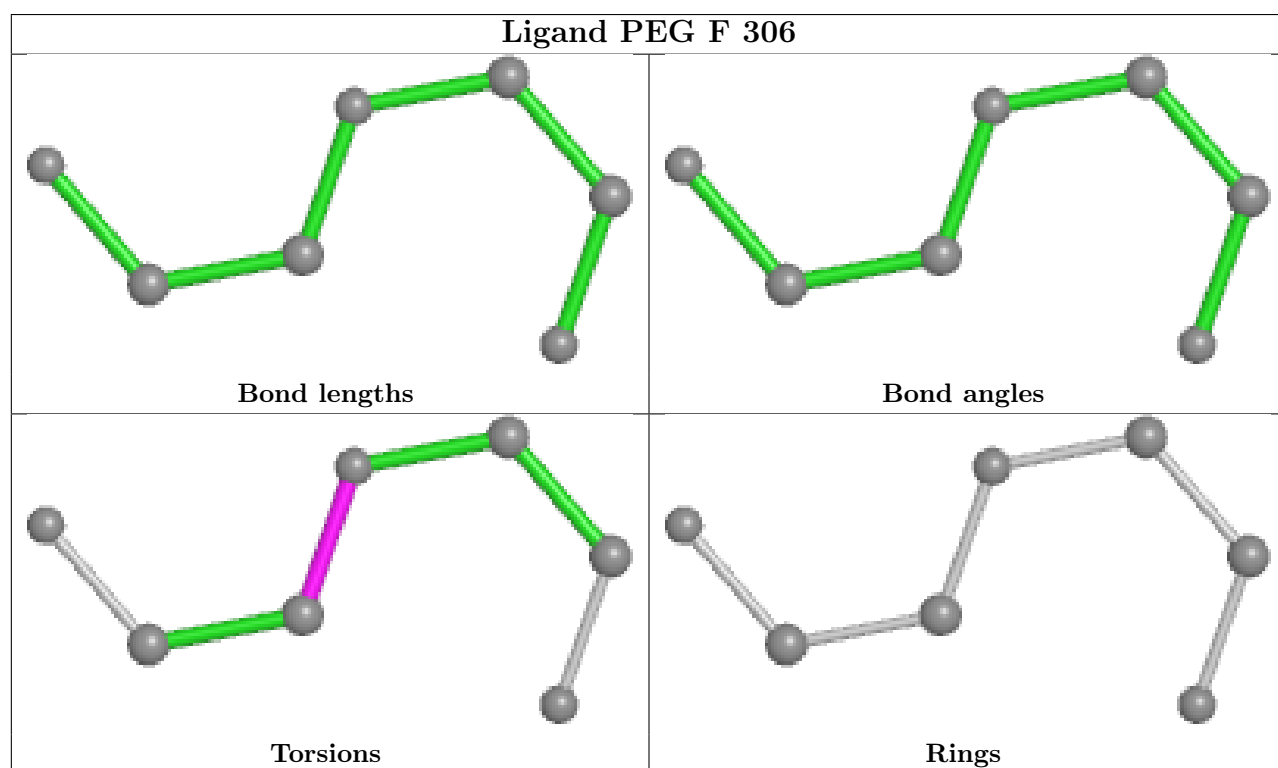
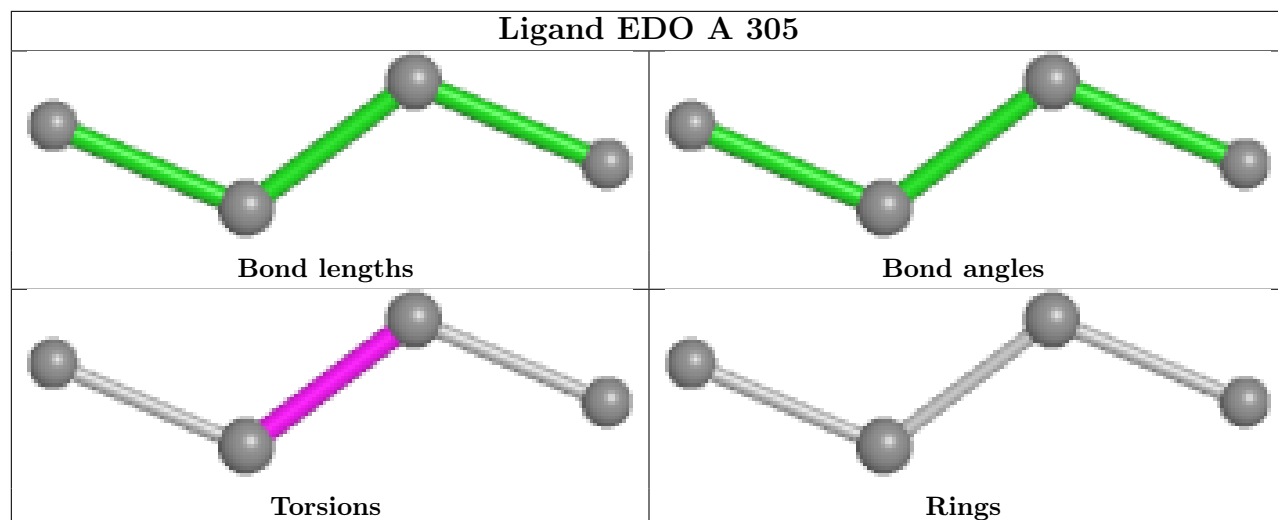


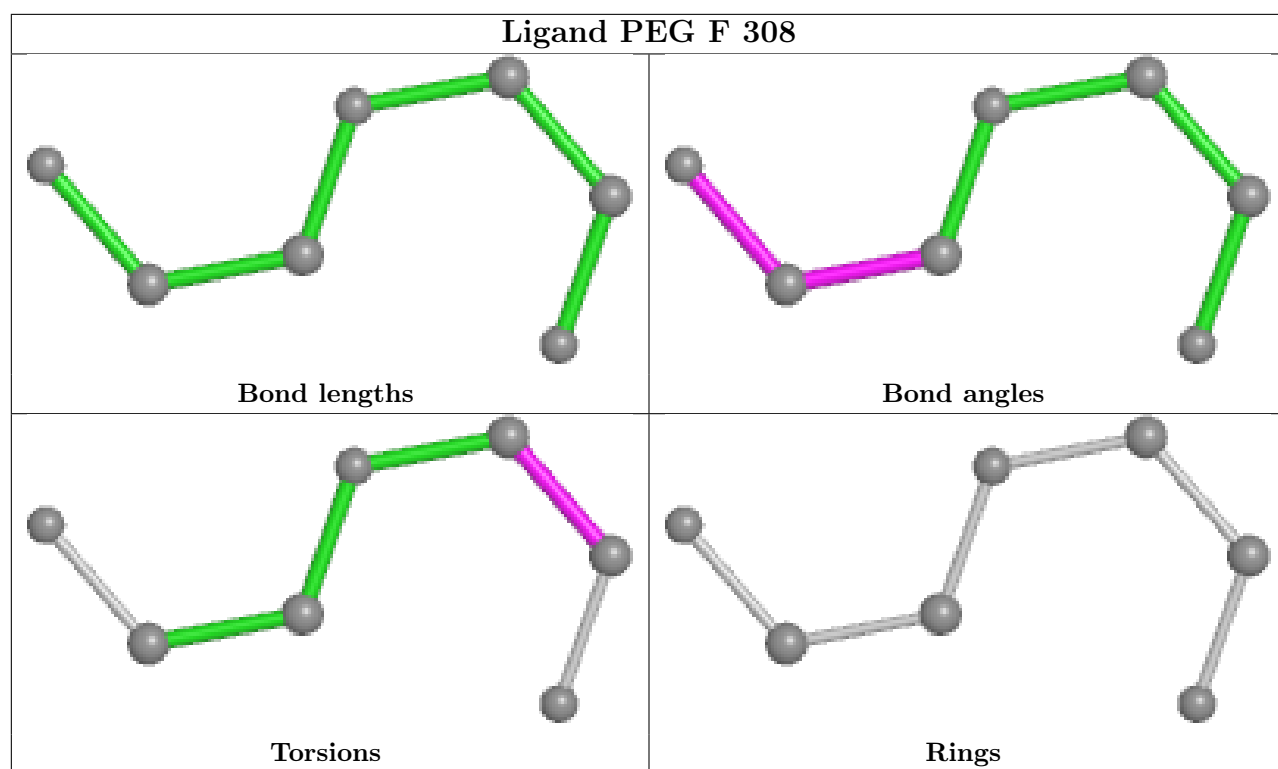


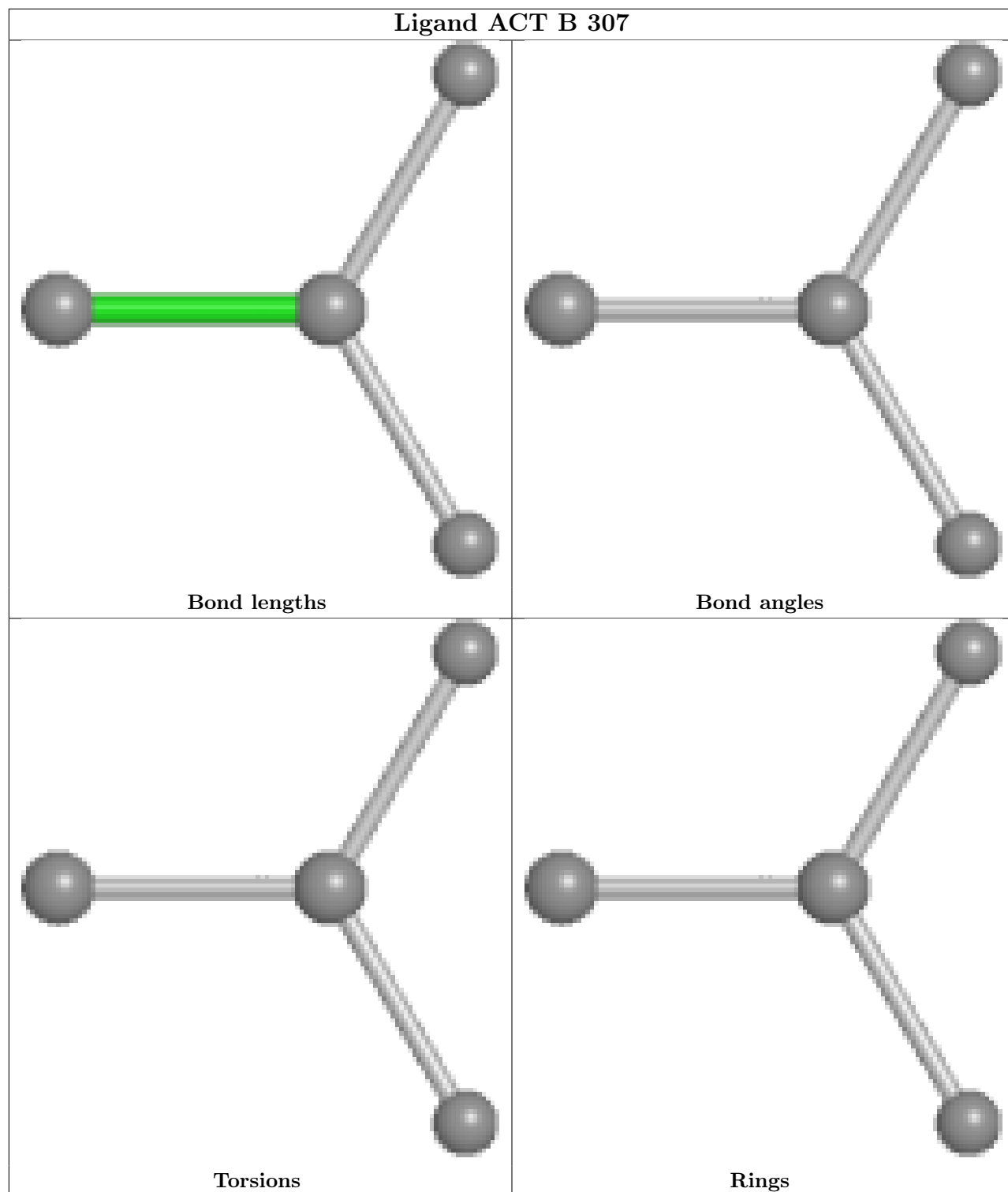




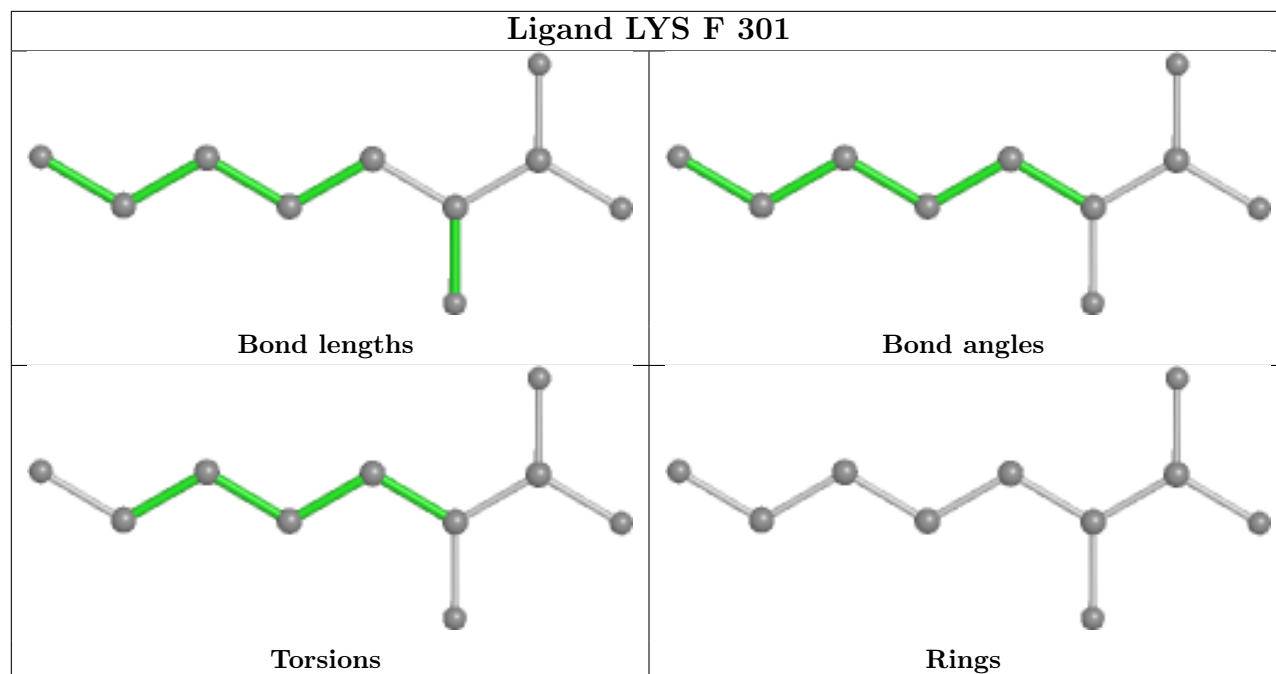




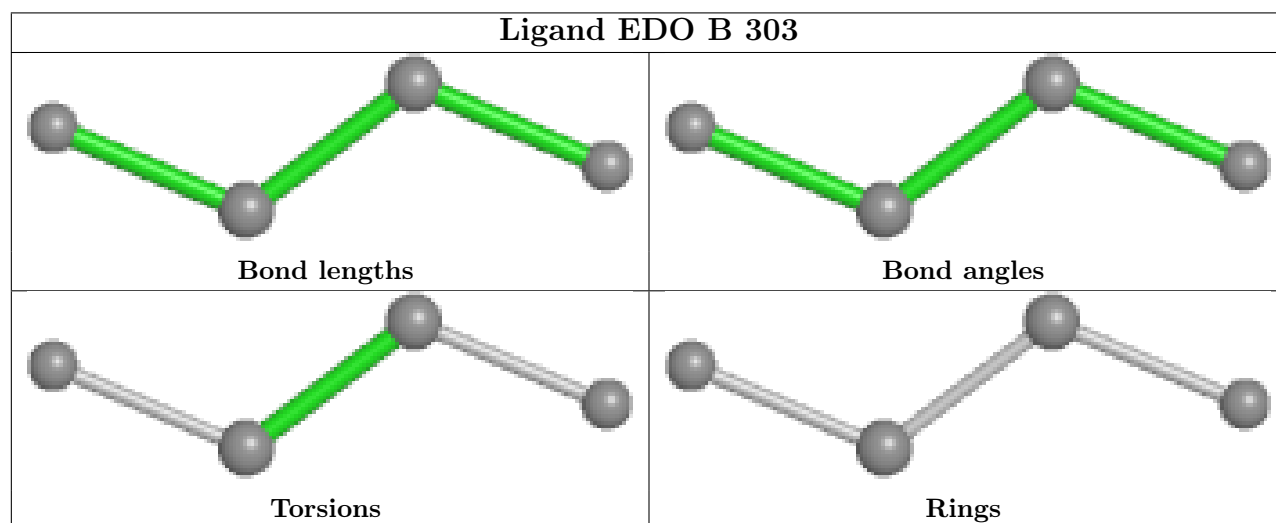




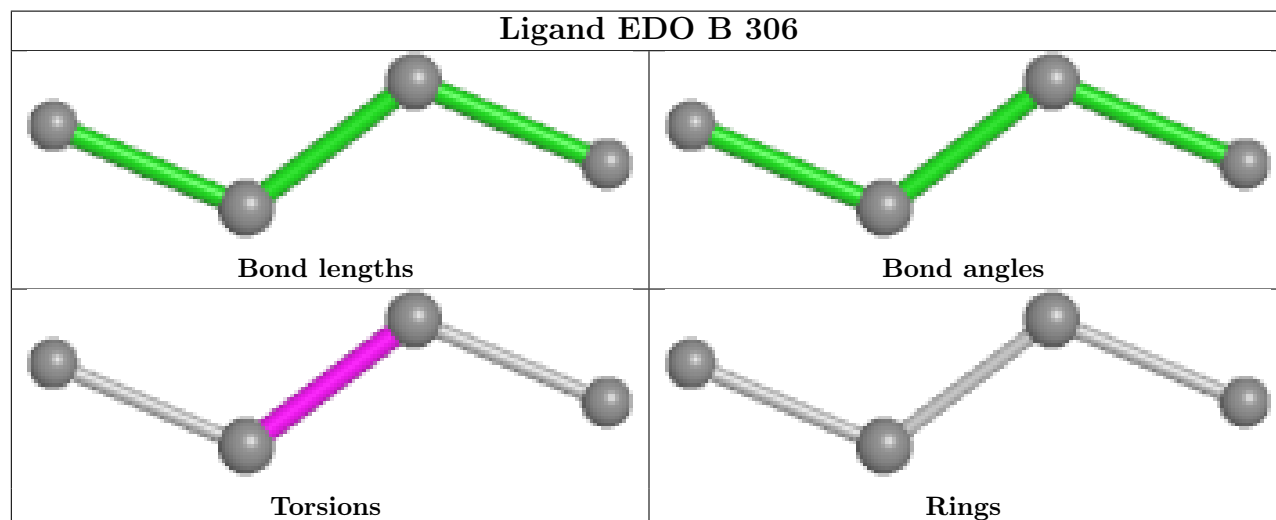
Ligand LYS F 301

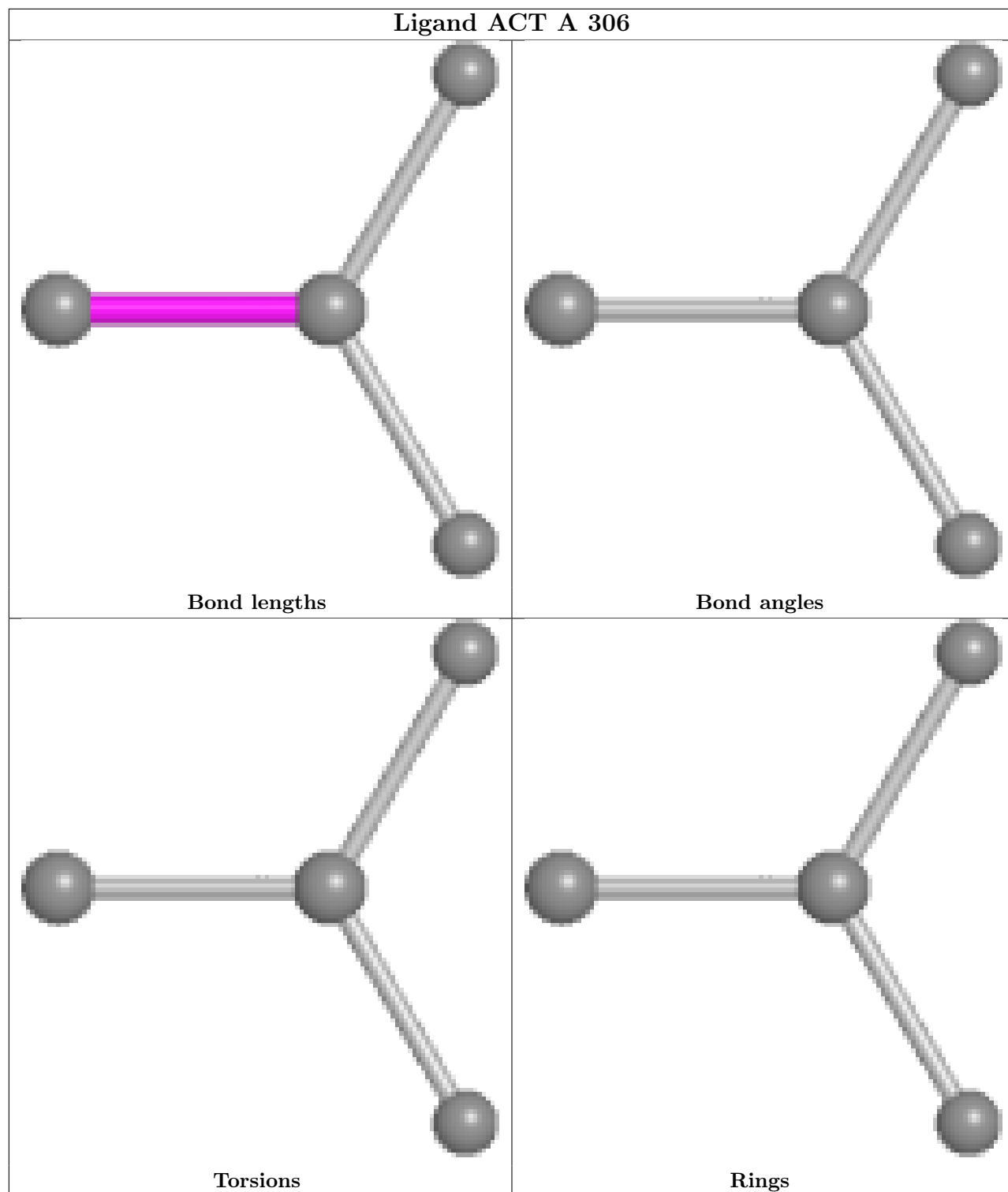


Ligand EDO B 303

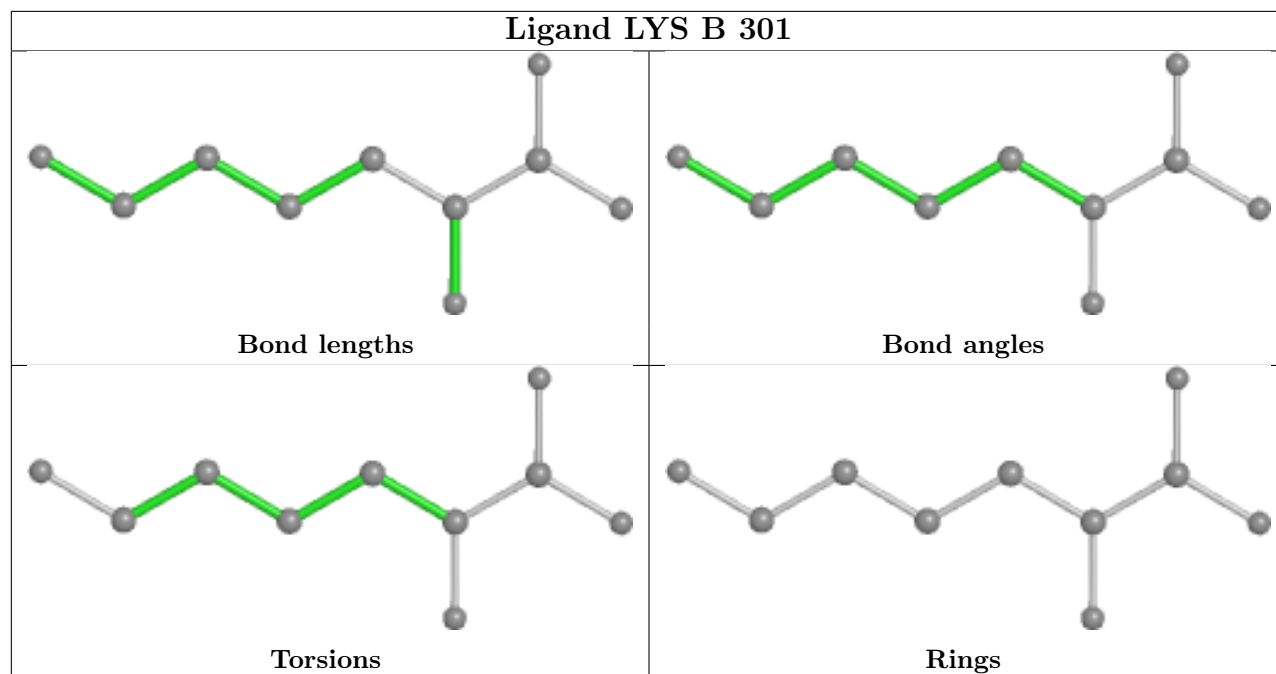


Ligand EDO B 306

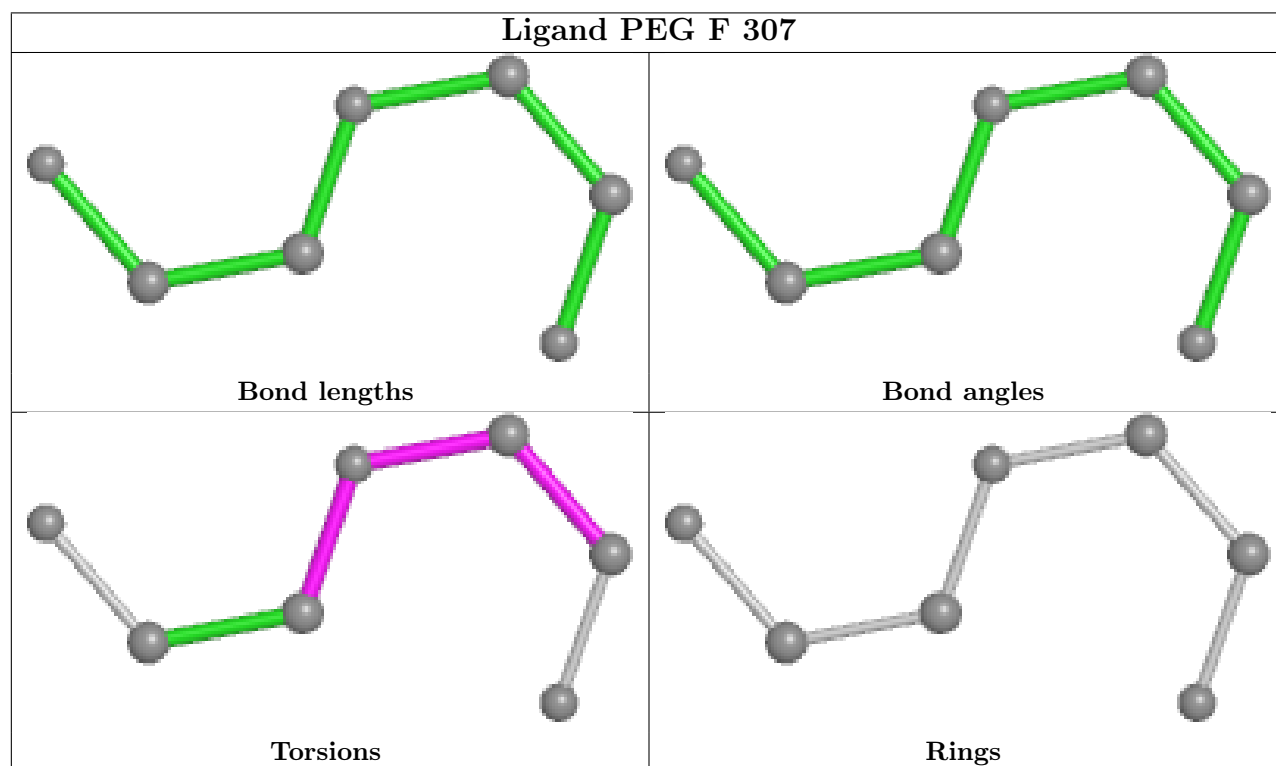


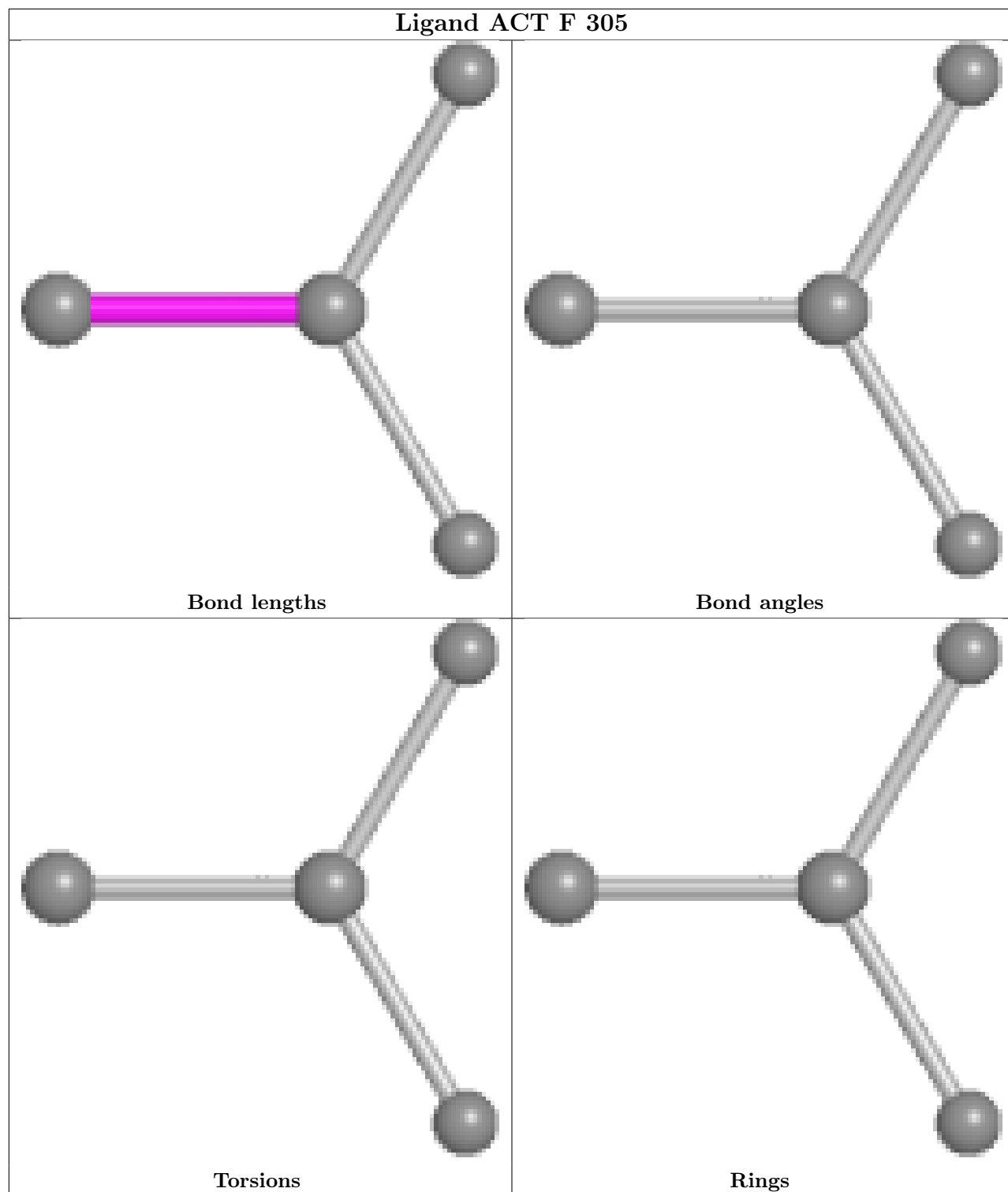


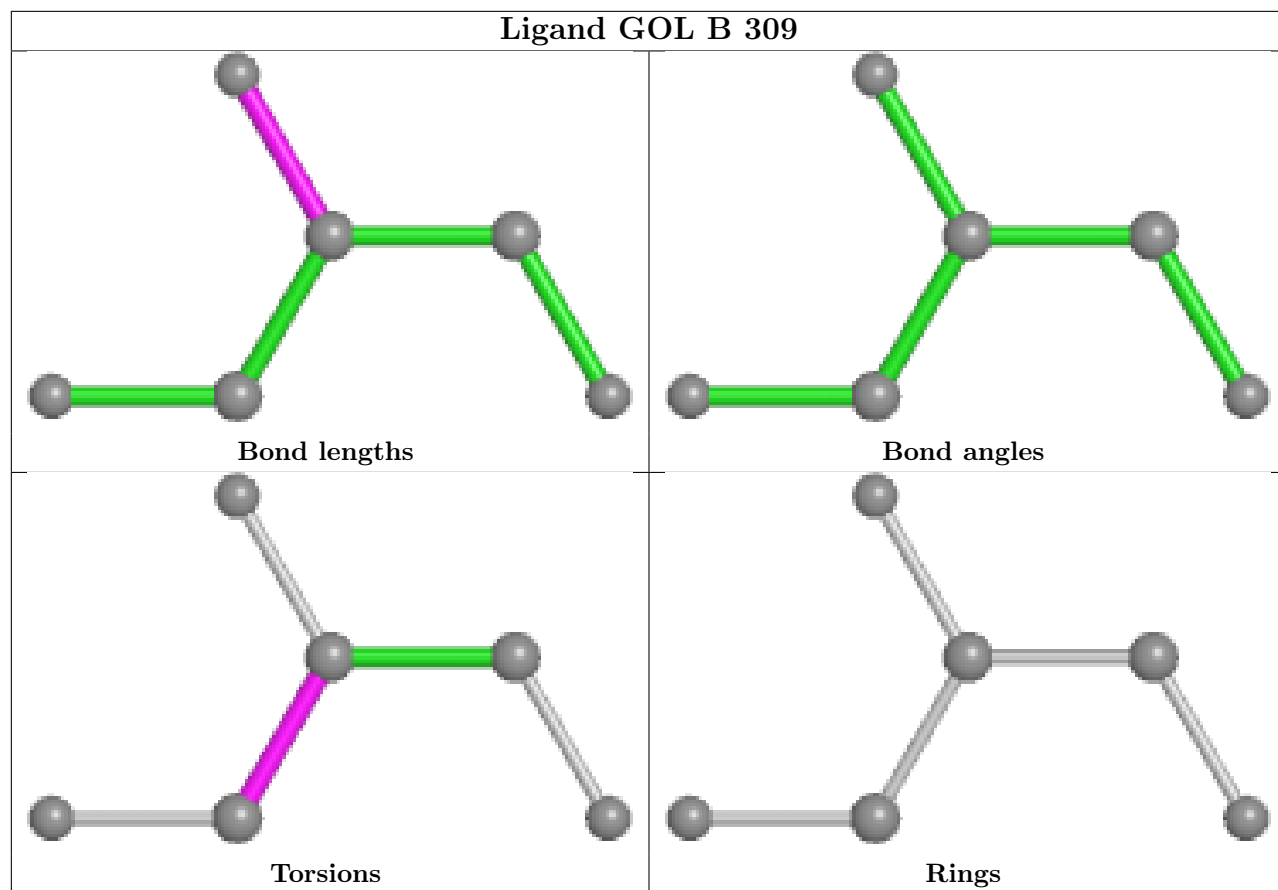
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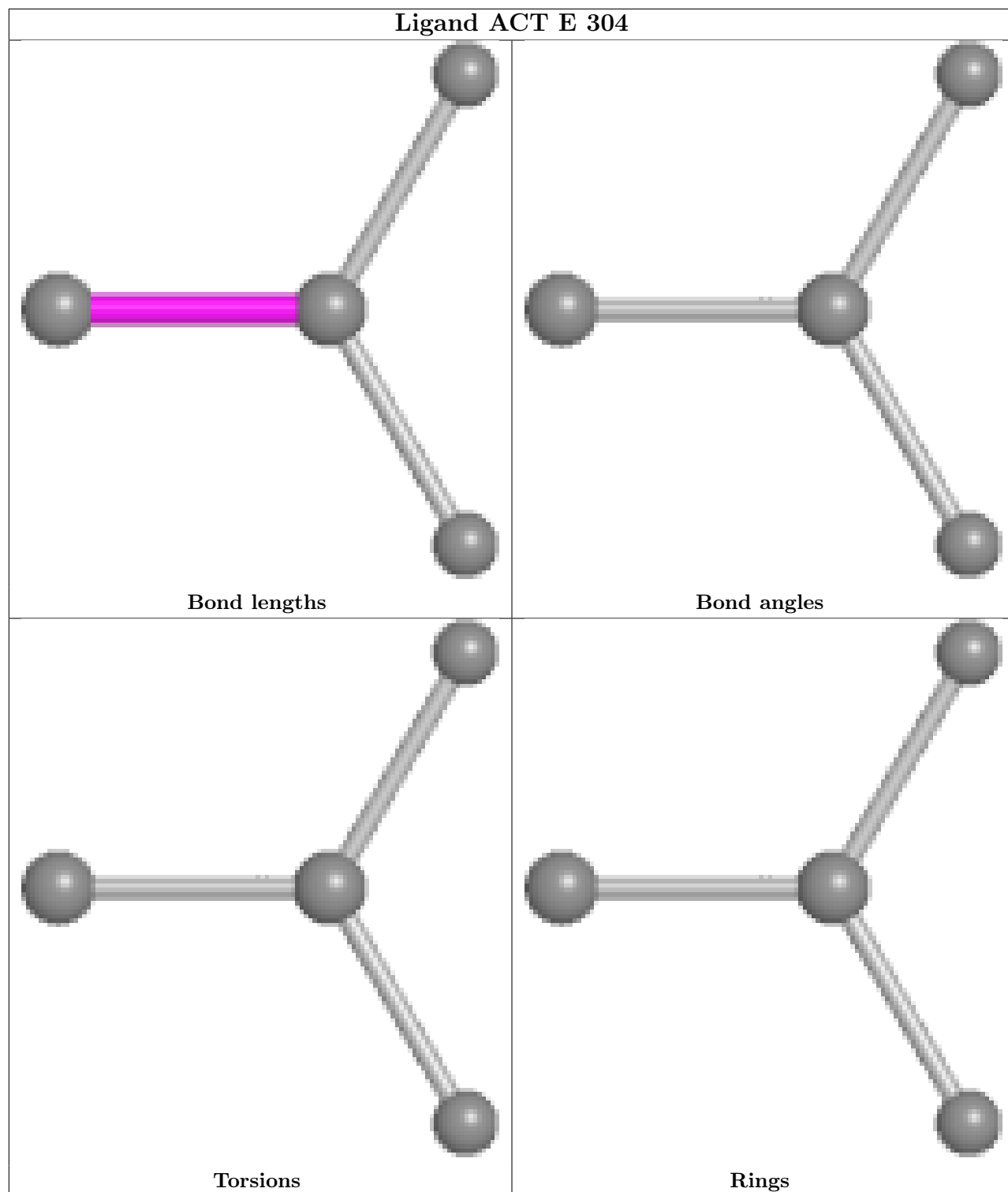


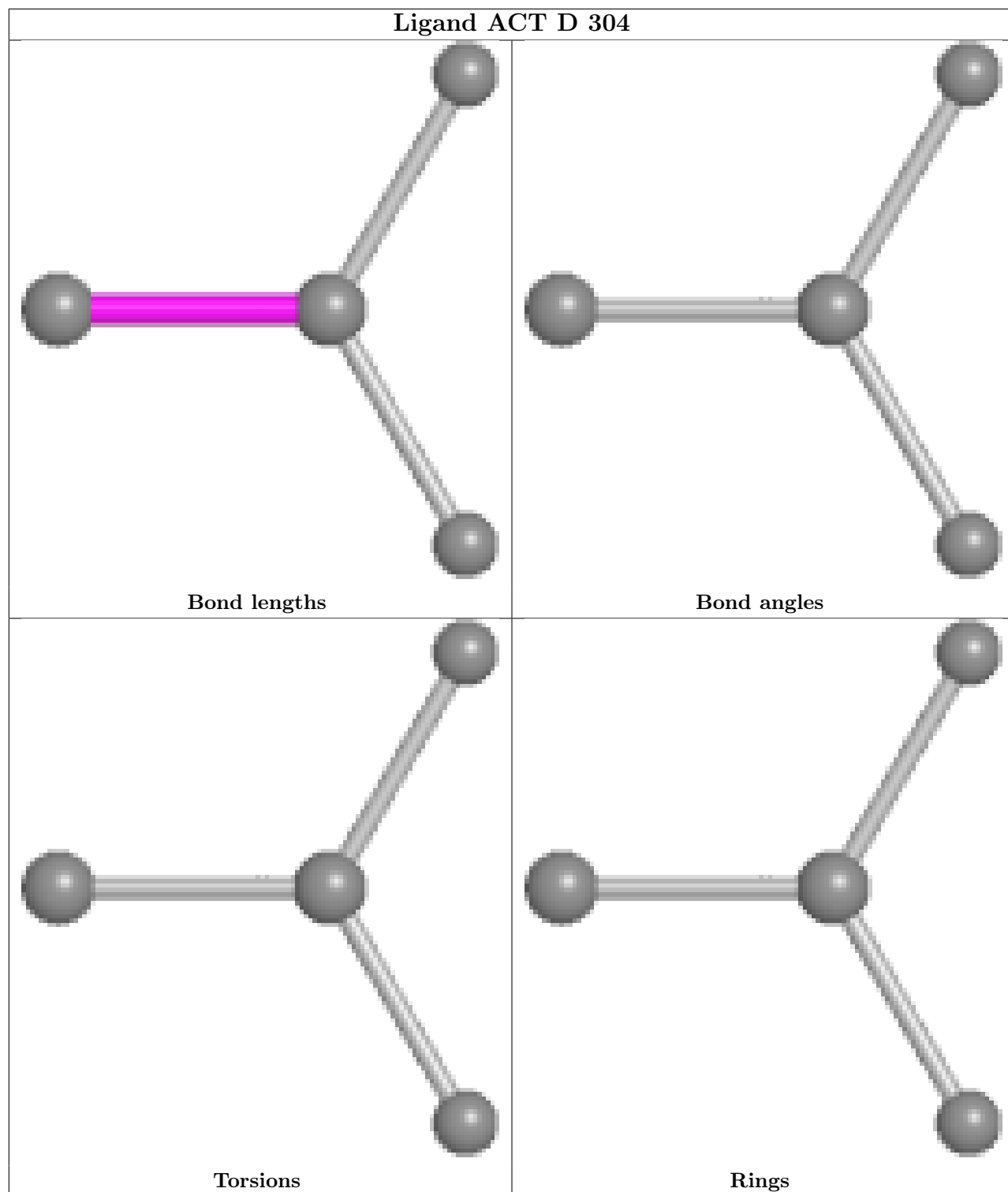
Ligand PEG F 307

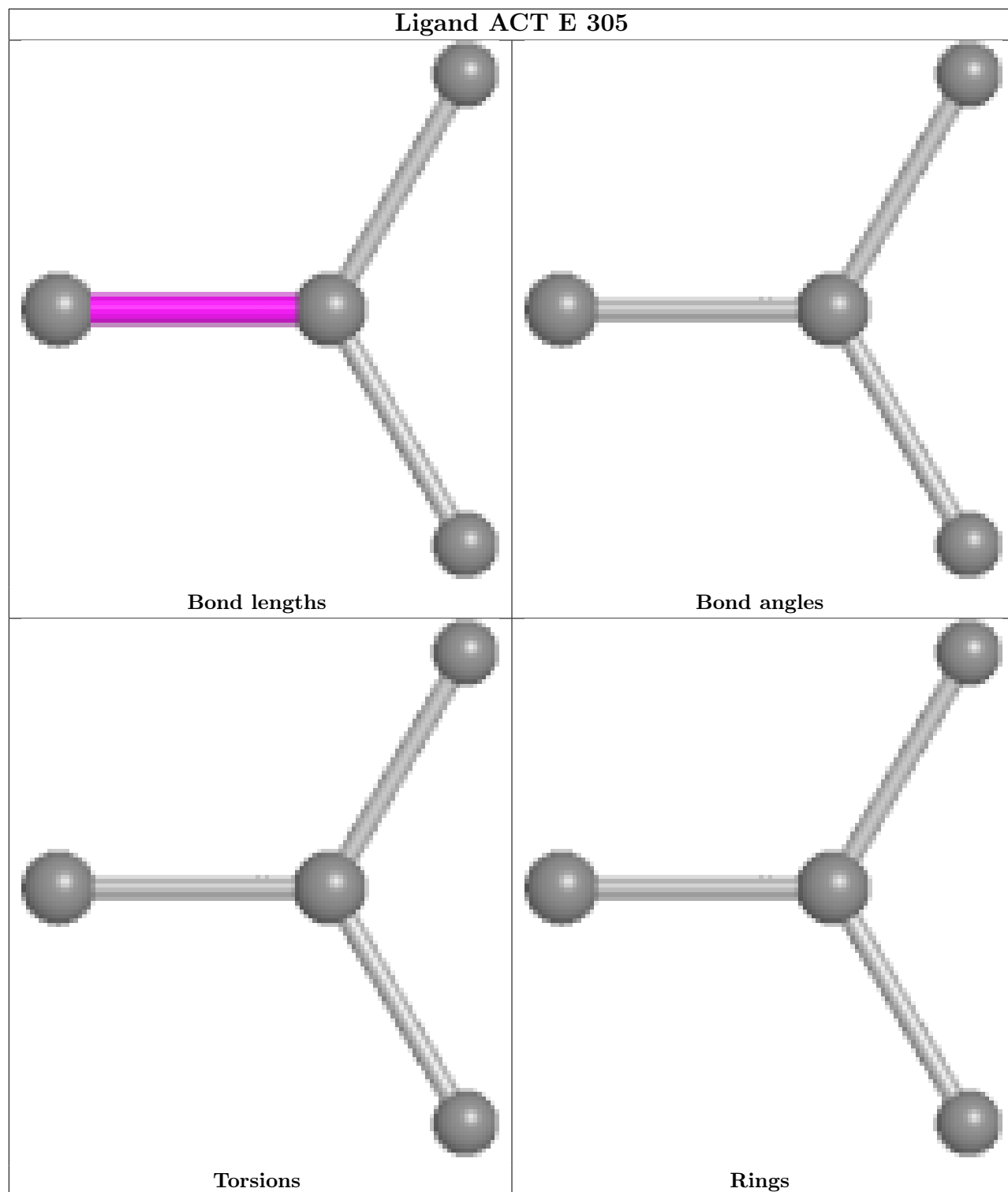


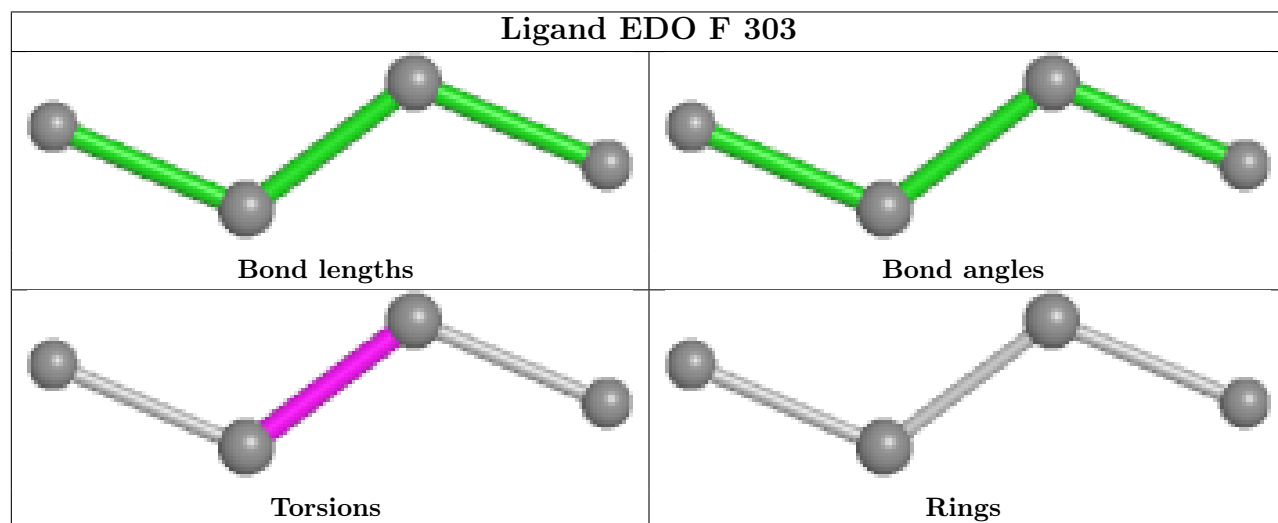
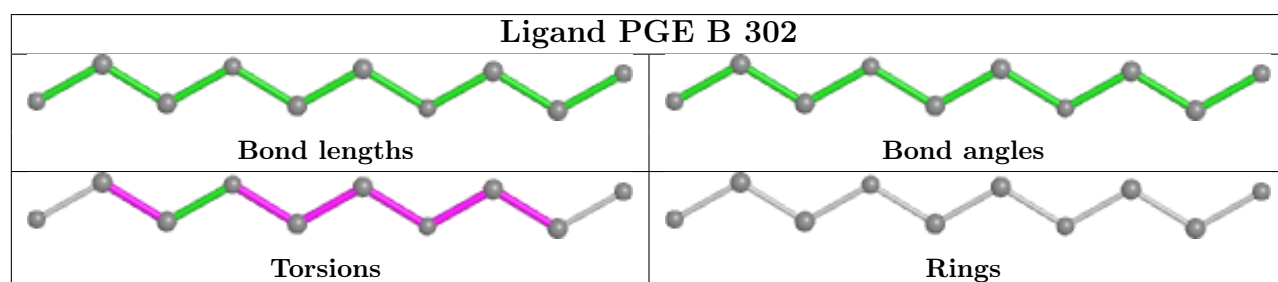
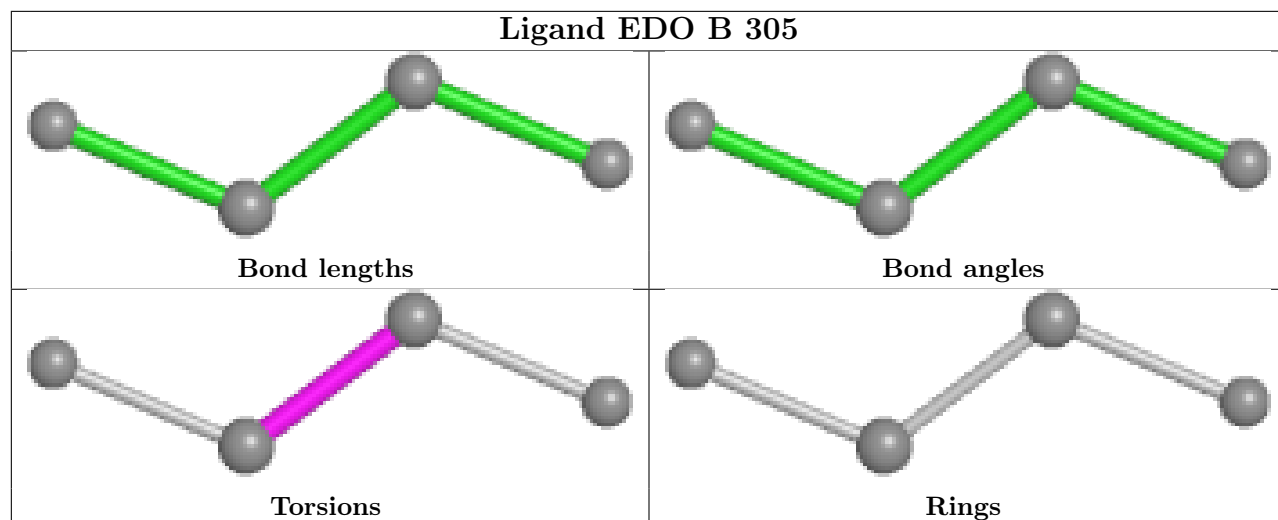




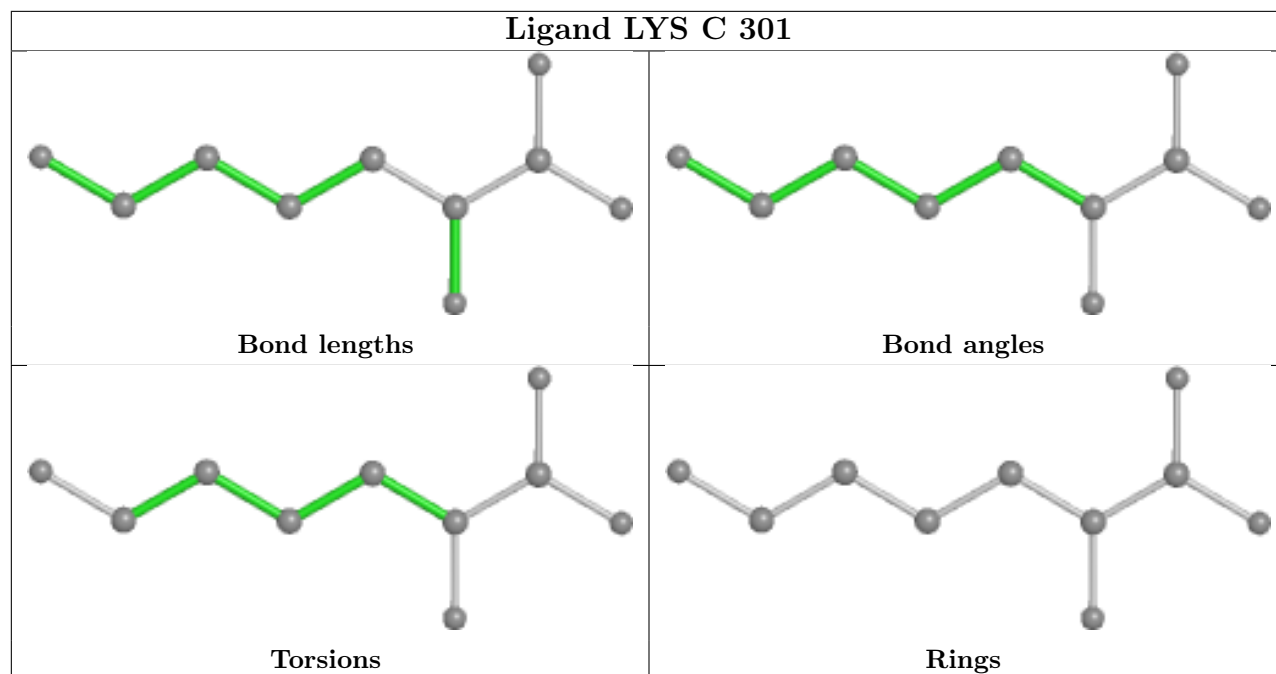




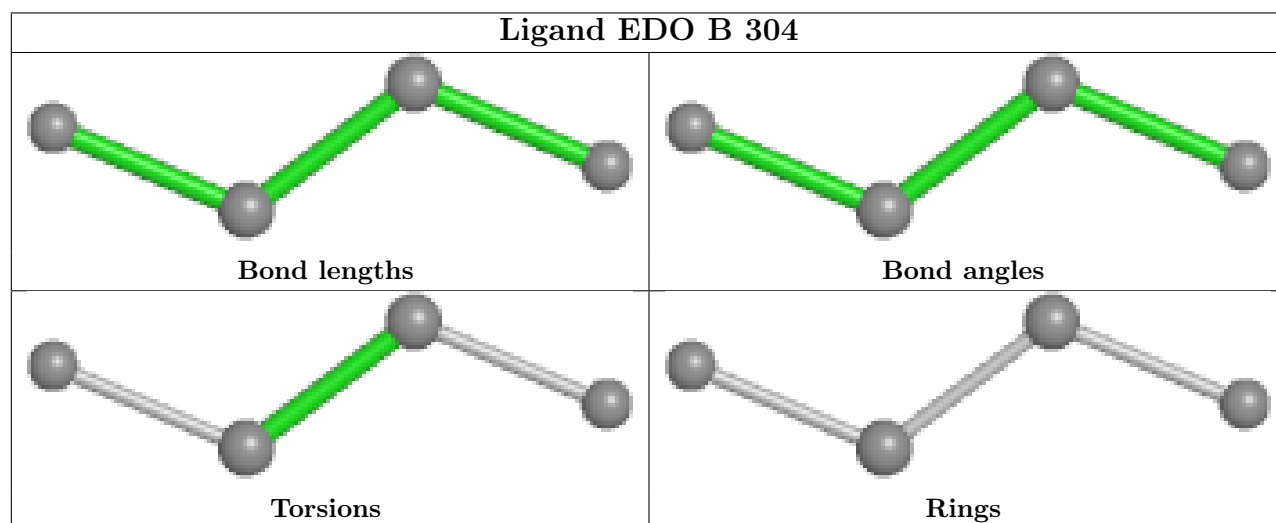




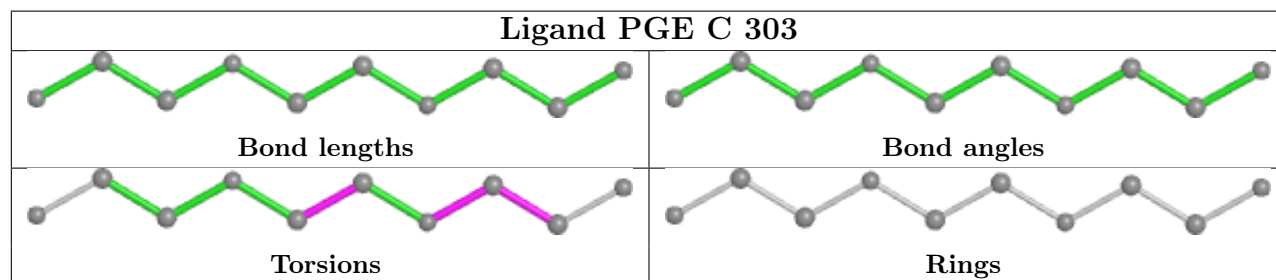
Ligand LYS C 301

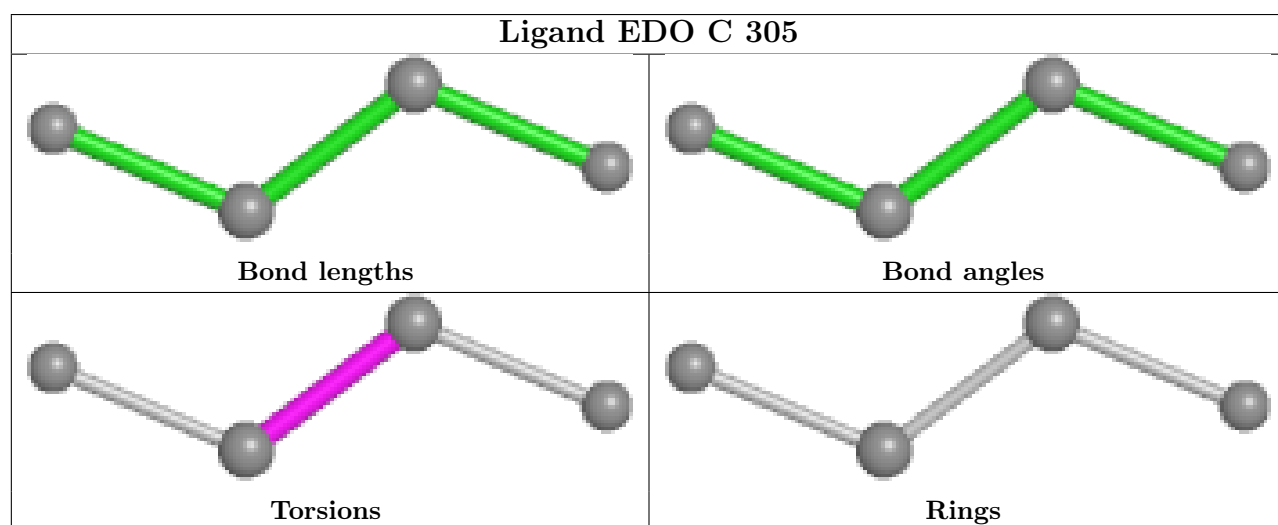
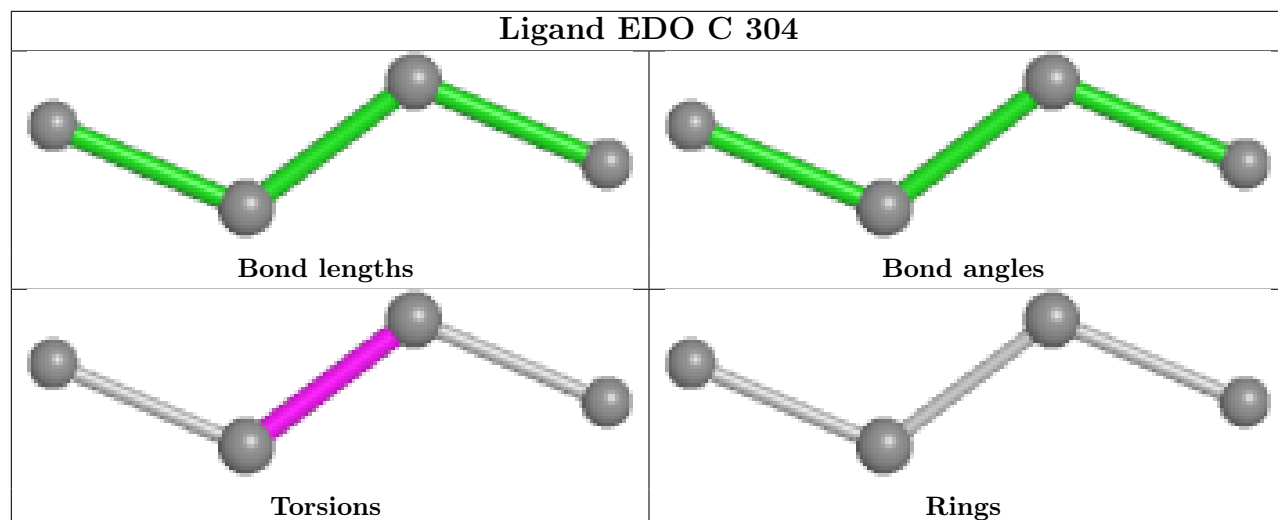


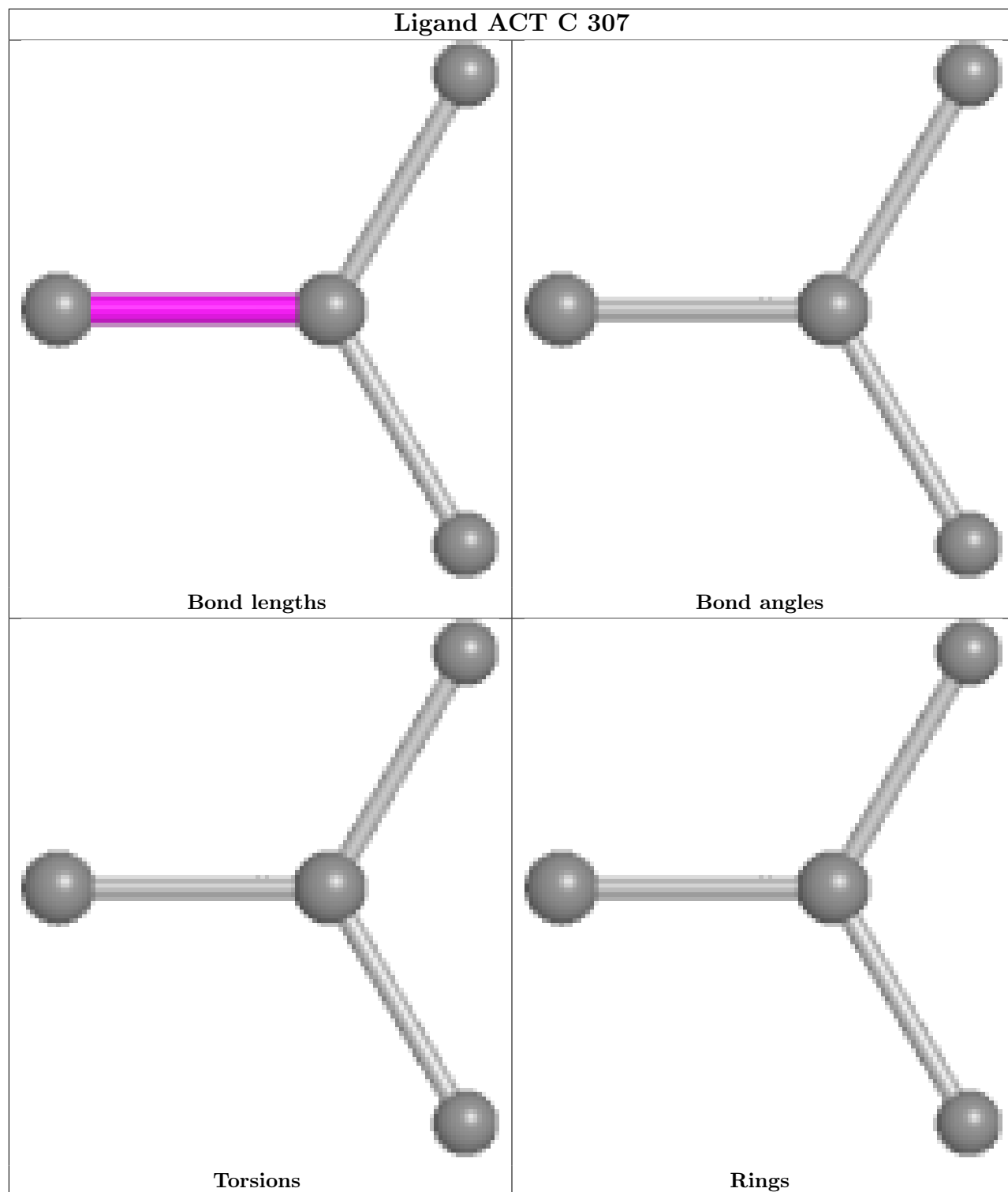
Ligand EDO B 304

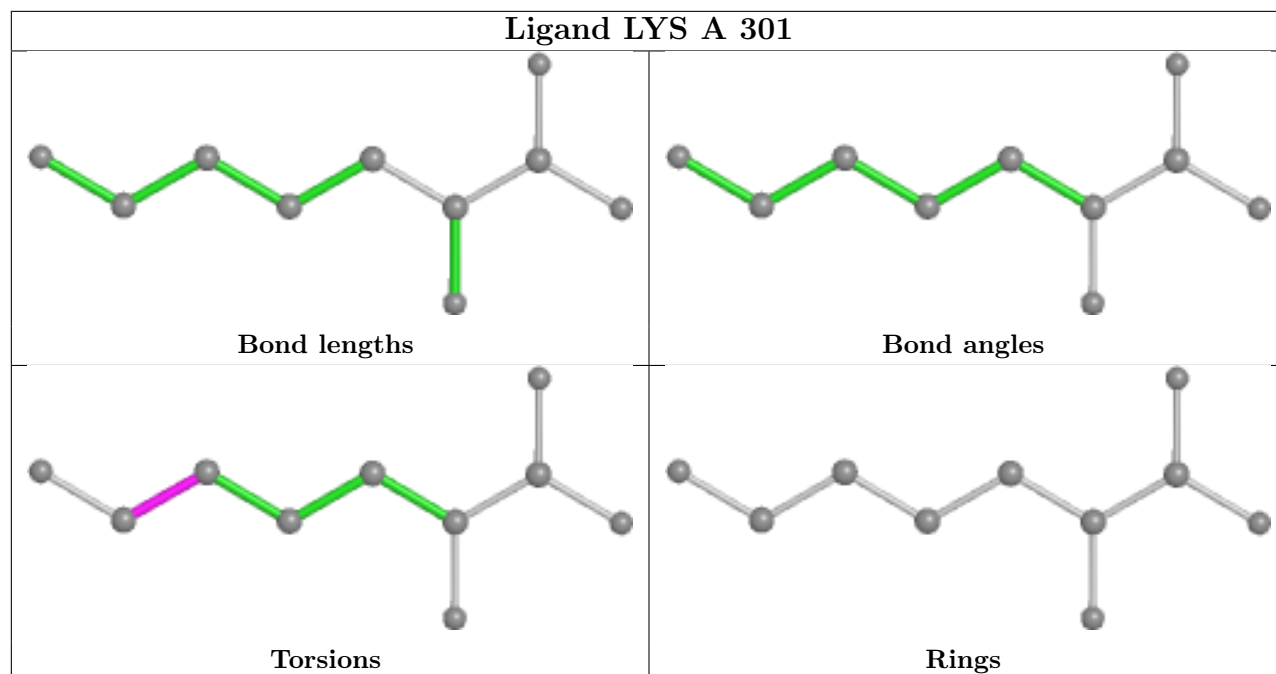


Ligand PGE C 303









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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	295/310 (95%)	-0.73	0	100 100	16, 22, 38, 56	0
1	B	295/310 (95%)	-0.79	0	100 100	16, 22, 38, 53	0
1	C	295/310 (95%)	-0.69	1 (0%)	94 93	16, 22, 40, 53	0
1	D	295/310 (95%)	-0.75	1 (0%)	94 93	16, 24, 41, 64	0
1	E	295/310 (95%)	-0.69	0	100 100	16, 23, 42, 56	0
1	F	296/310 (95%)	-0.68	0	100 100	15, 23, 43, 63	0
All	All	1771/1860 (95%)	-0.72	2 (0%)	95 95	15, 22, 40, 64	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	ASN	2.2
1	C	281	GLU	2.0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KPI	D	166	14/15	0.88	0.14	18,23,28,31	0
1	KPI	C	166	14/15	0.94	0.14	16,21,28,34	0
1	KPI	A	166	14/15	0.95	0.12	16,18,27,28	0
1	KPI	B	166	14/15	0.95	0.10	15,18,28,34	0
1	KPI	E	166	14/15	0.95	0.11	16,21,26,27	0
1	KPI	F	166	14/15	0.96	0.10	14,17,27,28	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ACT	F	305	4/4	0.70	0.25	54,55,55,56	0
4	PGE	D	303	10/10	0.74	0.55	20,20,20,20	0
7	PEG	F	308	7/7	0.75	0.34	20,20,20,20	0
5	EDO	B	305	4/4	0.76	0.14	55,55,55,56	0
6	ACT	B	307	4/4	0.76	0.55	20,20,20,20	0
6	ACT	C	306	4/4	0.78	0.23	41,42,43,46	0
3	MG	A	302	1/1	0.80	0.16	41,41,41,41	0
7	PEG	F	307	7/7	0.81	0.42	20,20,20,20	0
8	GOL	B	309	6/6	0.81	0.17	34,37,38,39	0
6	ACT	E	304	4/4	0.83	0.21	56,56,57,59	0
6	ACT	D	304	4/4	0.85	0.16	53,55,55,55	0
5	EDO	C	304	4/4	0.88	0.38	20,20,20,20	0
7	PEG	B	308	7/7	0.88	0.42	20,20,20,20	0
7	PEG	F	306	7/7	0.88	0.14	47,49,54,54	0
4	PGE	C	303	10/10	0.89	0.20	41,47,50,53	0
5	EDO	B	303	4/4	0.89	0.16	49,49,50,50	0
5	EDO	F	303	4/4	0.89	0.44	20,20,20,20	0
7	PEG	E	306	7/7	0.89	0.34	20,20,20,20	0
4	PGE	D	302	10/10	0.90	0.14	43,46,49,51	0
4	PGE	A	303	10/10	0.90	0.18	43,45,49,51	0
6	ACT	C	307	4/4	0.90	0.21	47,50,52,52	0
5	EDO	B	306	4/4	0.91	0.47	20,20,20,20	0
4	PGE	B	302	10/10	0.91	0.12	39,45,60,62	0
5	EDO	A	304	4/4	0.91	0.11	49,49,50,51	0
6	ACT	A	306	4/4	0.91	0.13	47,48,49,51	0
6	ACT	F	304	4/4	0.92	0.24	50,50,51,51	0
5	EDO	A	305	4/4	0.92	0.35	20,20,20,20	0
5	EDO	C	305	4/4	0.92	0.59	20,20,20,20	0
5	EDO	B	304	4/4	0.92	0.15	50,52,54,56	0
4	PGE	E	302	10/10	0.93	0.17	41,44,49,53	0
6	ACT	E	305	4/4	0.93	0.13	55,56,57,57	0
2	LYS	A	301	10/10	0.95	0.13	16,22,23,23	0

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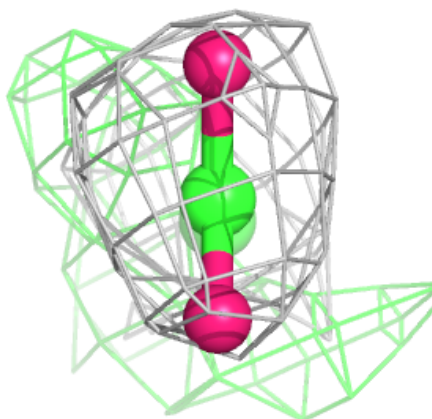
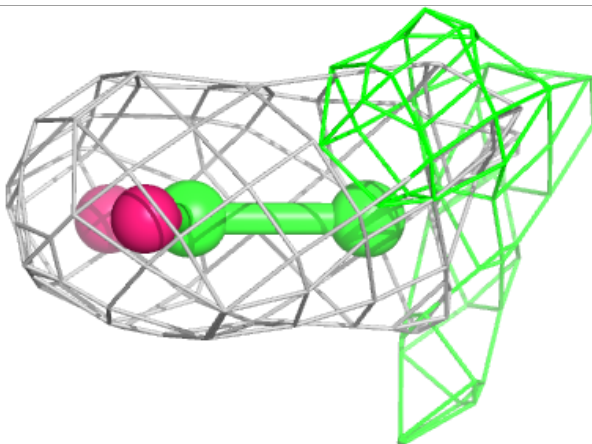
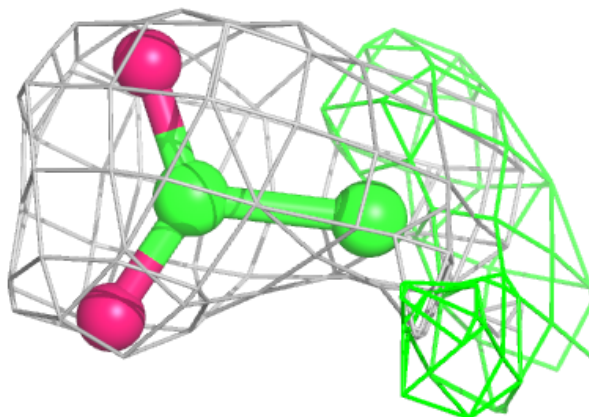
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	LYS	F	301	10/10	0.96	0.11	16,18,21,22	0
2	LYS	C	301	10/10	0.96	0.12	17,20,21,22	0
2	LYS	E	301	10/10	0.97	0.10	16,19,22,23	0
5	EDO	E	303	4/4	0.97	0.07	18,21,24,26	0
2	LYS	D	301	10/10	0.97	0.09	15,19,24,26	0
2	LYS	B	301	10/10	0.98	0.11	14,18,22,23	0
3	MG	C	302	1/1	0.99	0.18	11,11,11,11	0
3	MG	F	302	1/1	1.00	0.15	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.

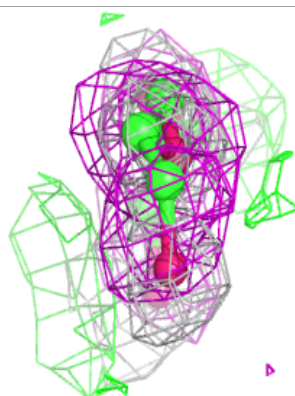
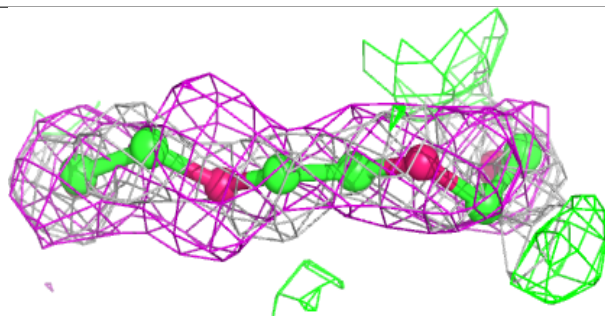
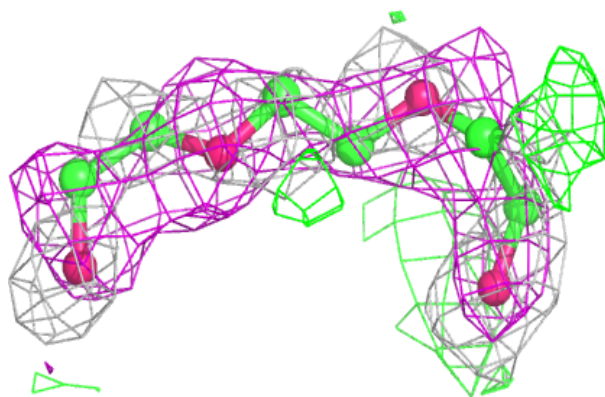
Electron density around ACT F 305:

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

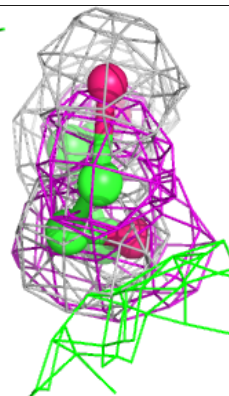
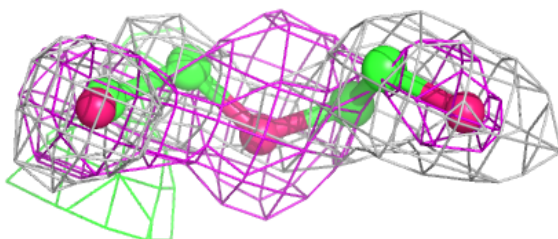
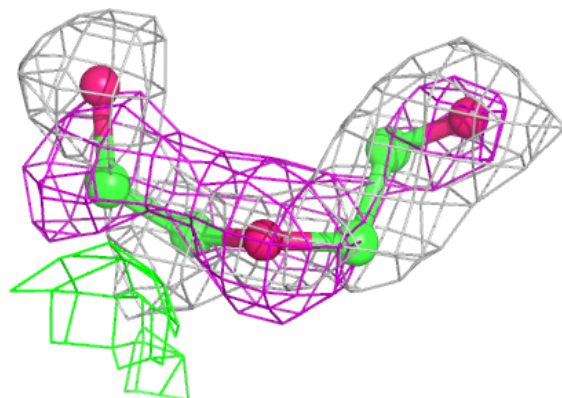


Electron density around PGE D 303:

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

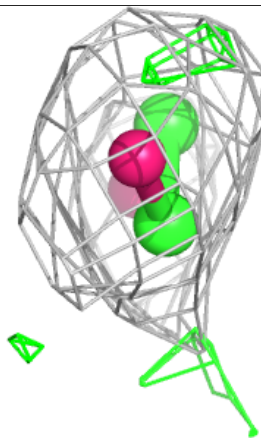
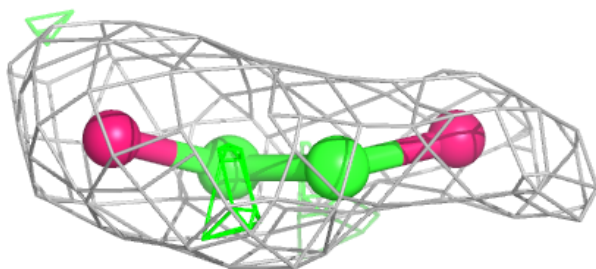
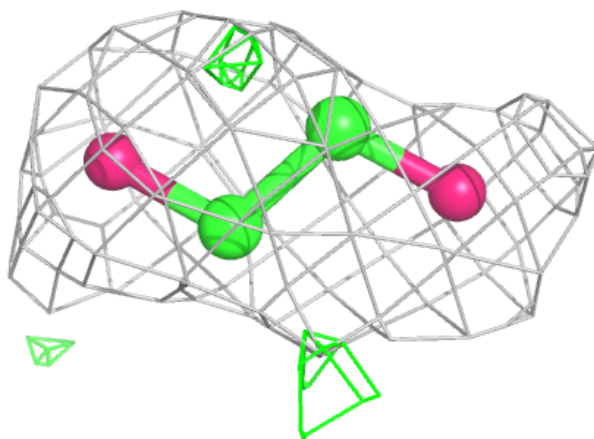
**Electron density around PEG F 308:**

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



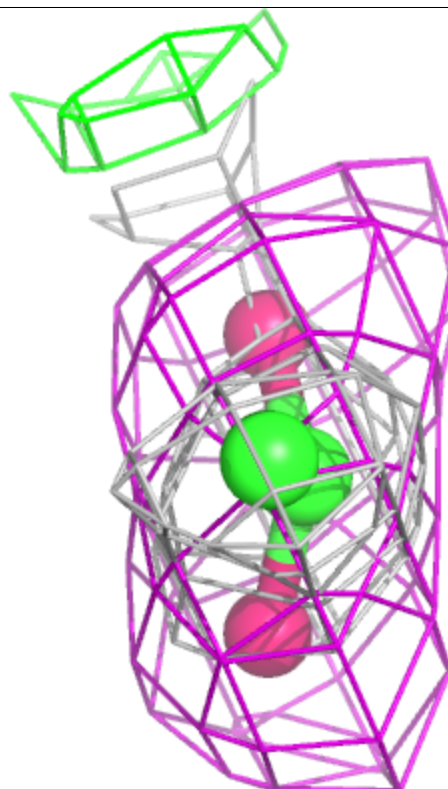
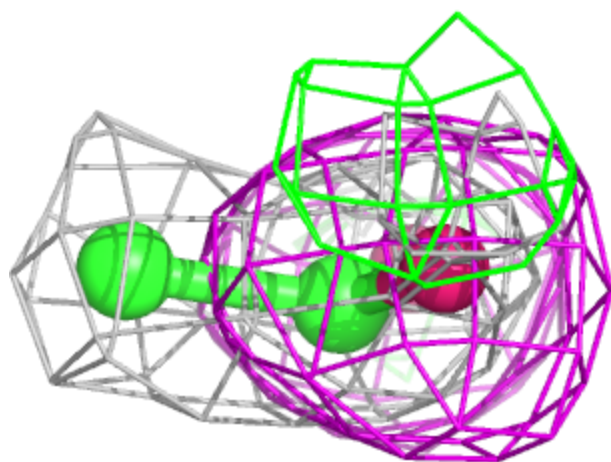
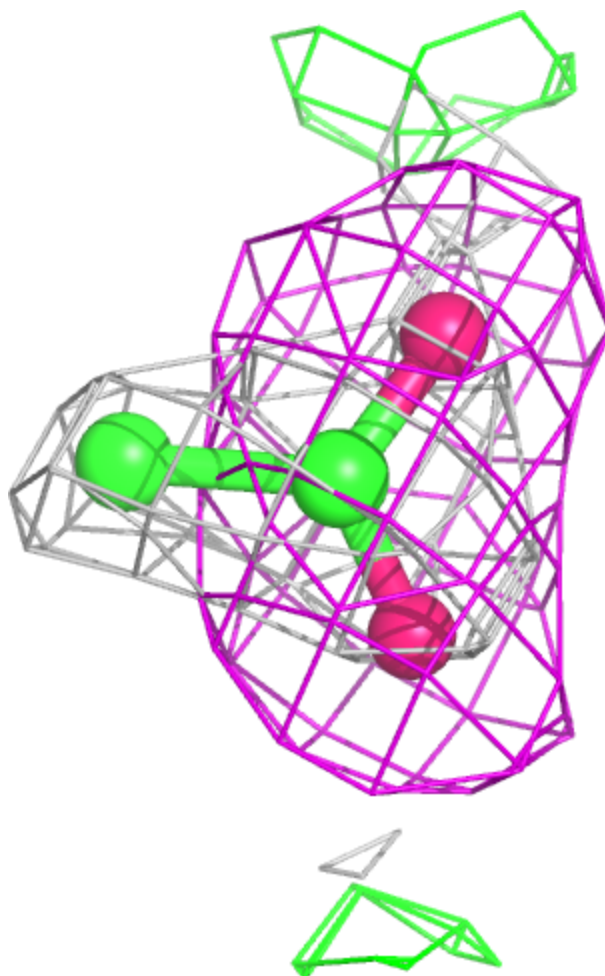
Electron density around EDO B 305:

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



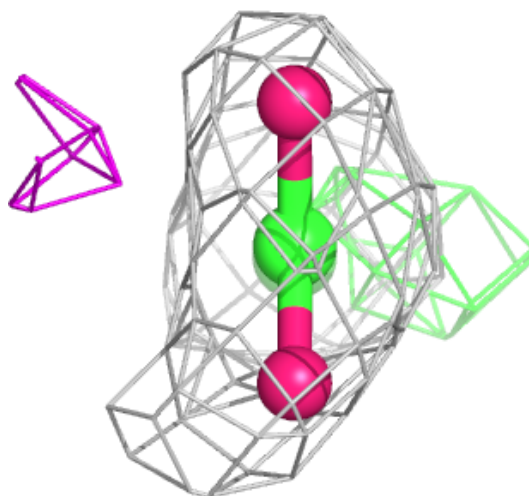
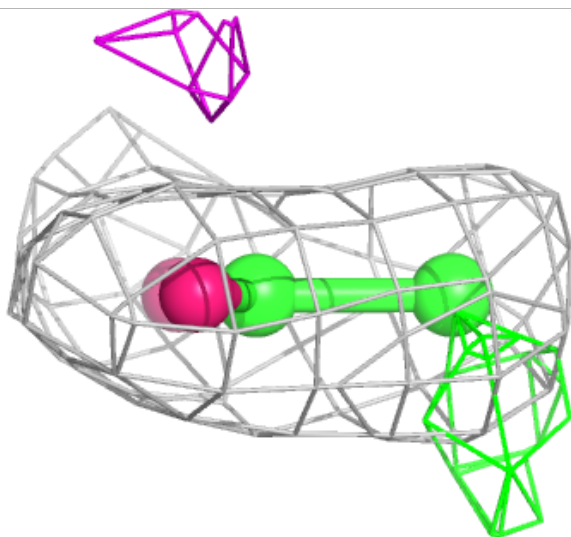
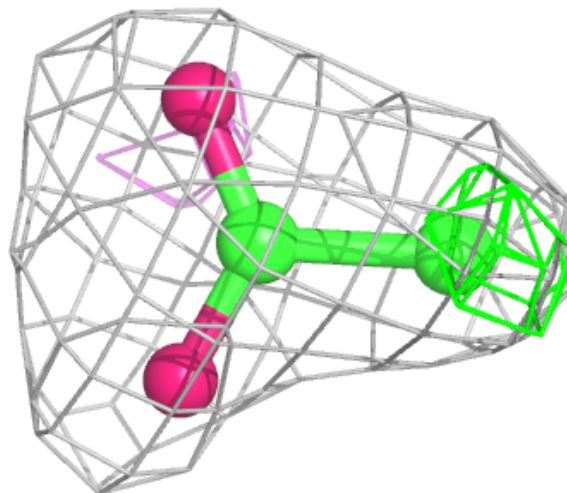
Electron density around ACT B 307:

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



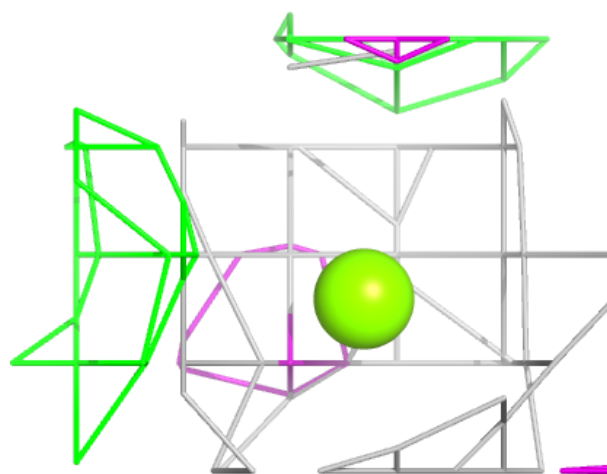
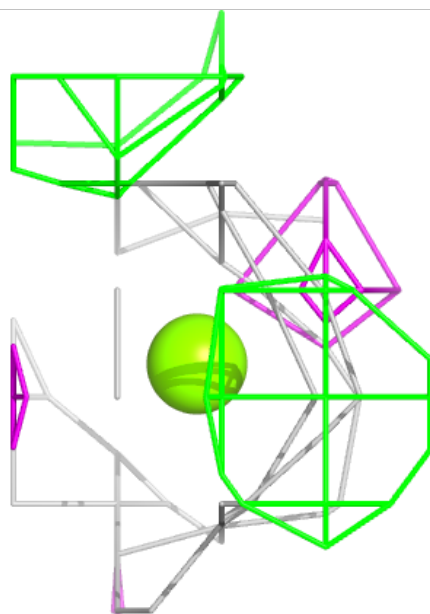
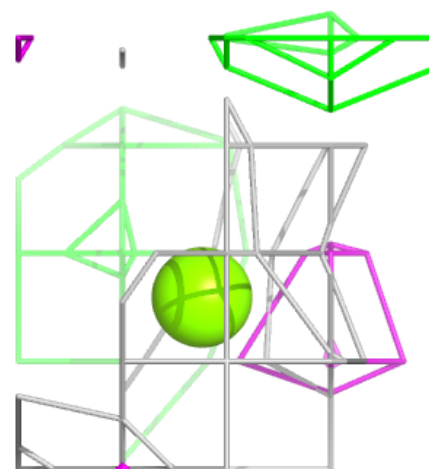
Electron density around ACT C 306:

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



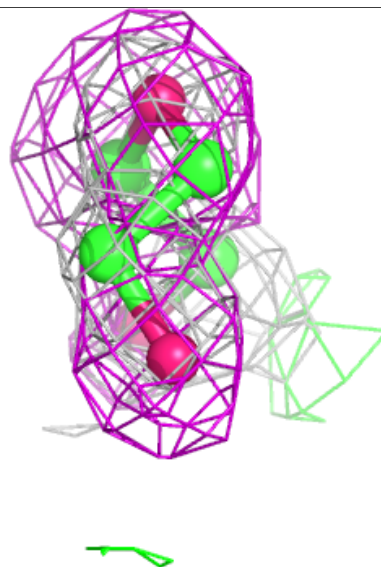
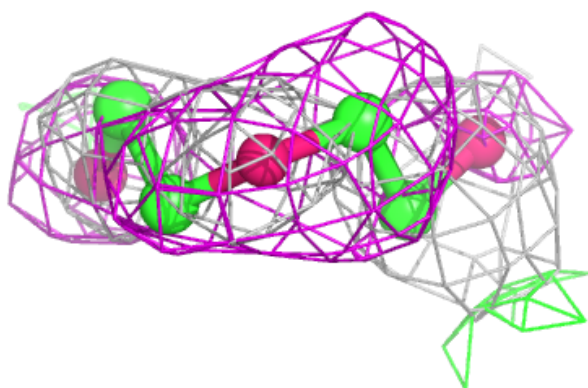
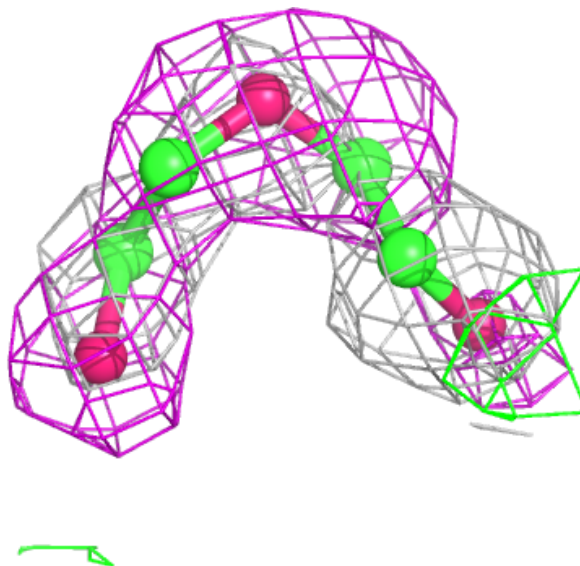
Electron density around MG A 302:

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



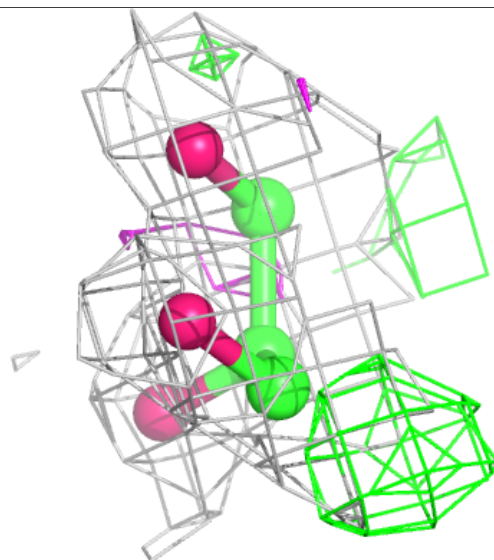
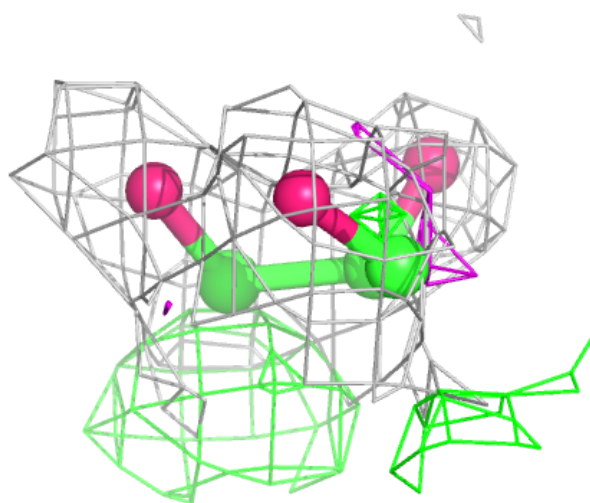
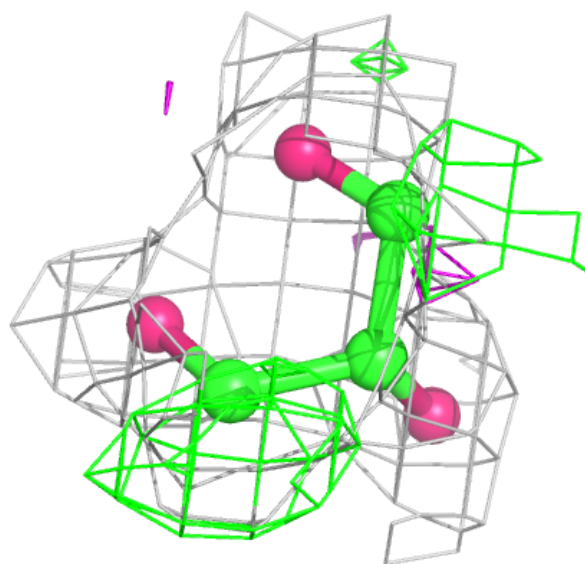
Electron density around PEG F 307:

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



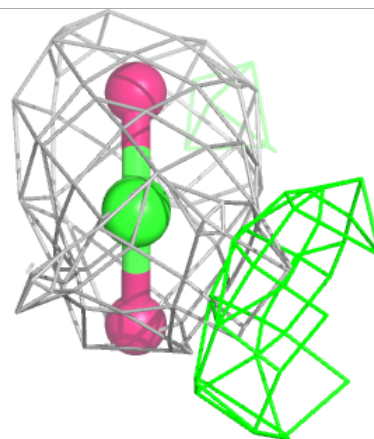
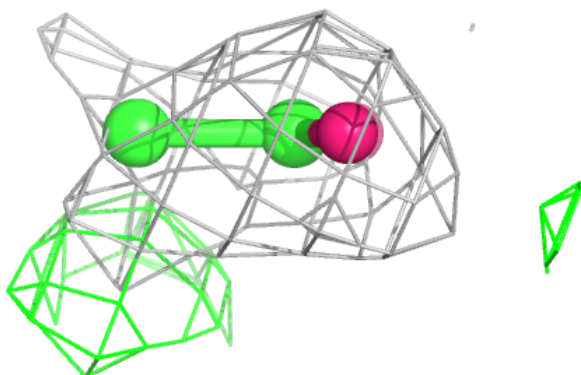
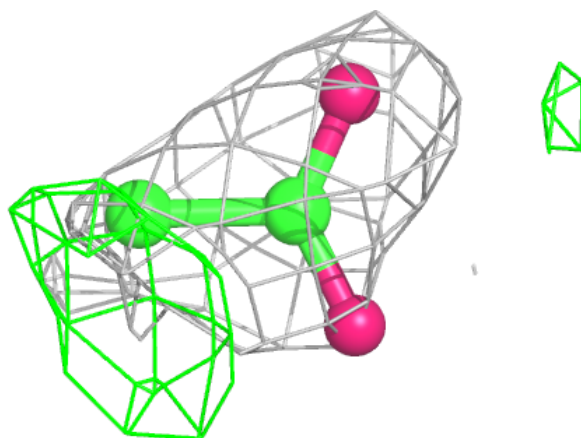
Electron density around GOL B 309:

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



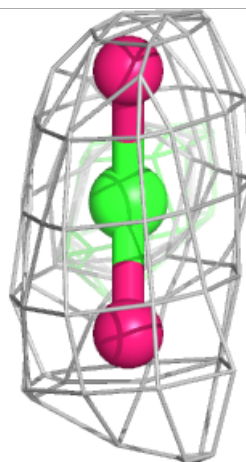
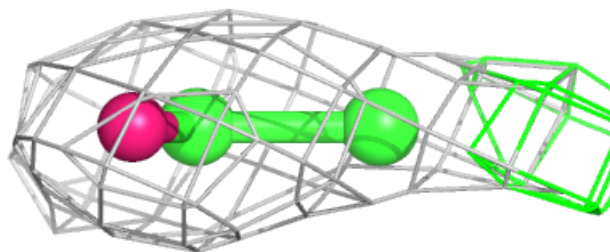
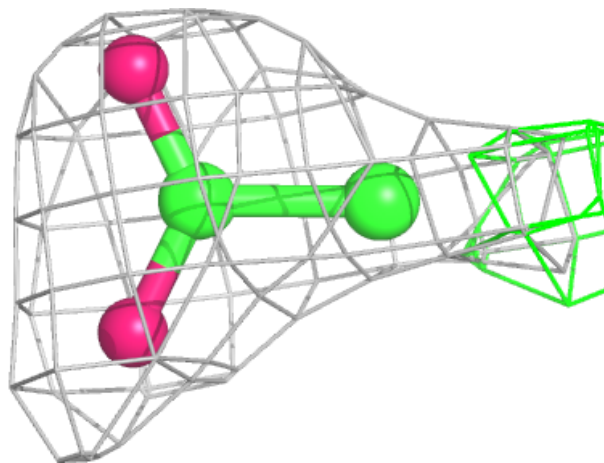
Electron density around ACT E 304:

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



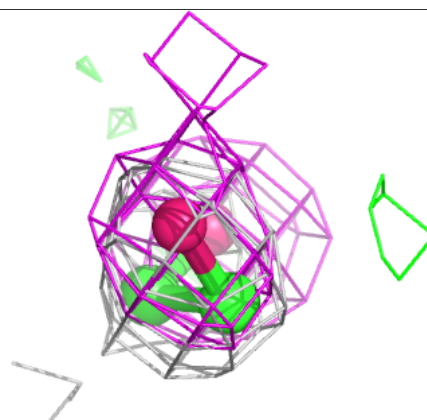
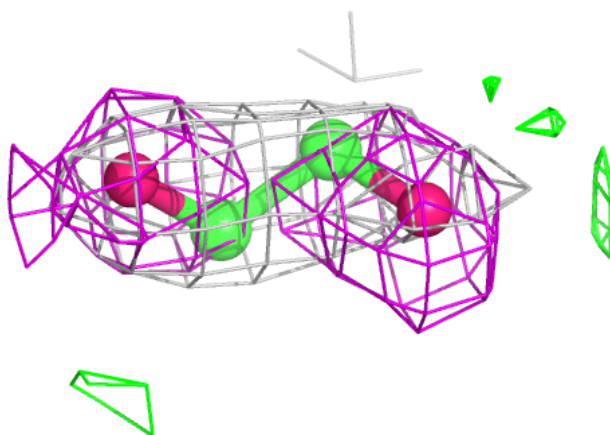
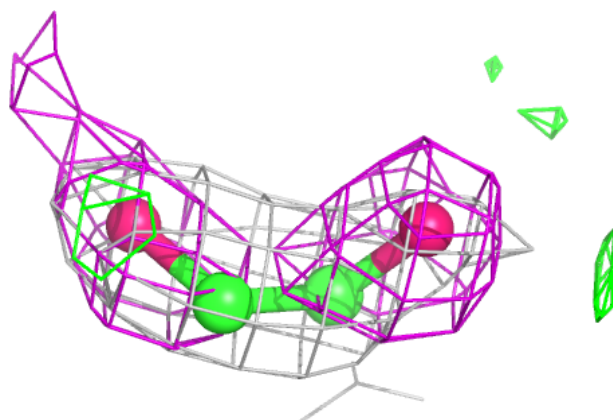
Electron density around ACT D 304:

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



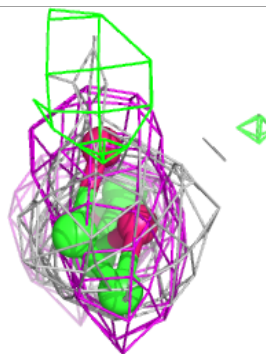
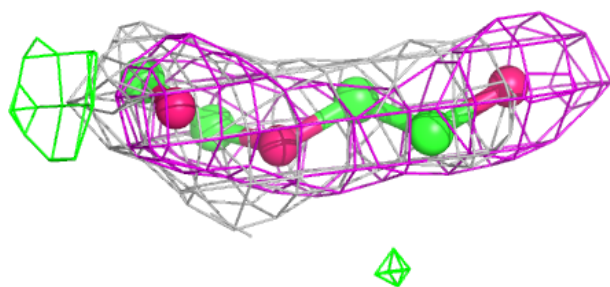
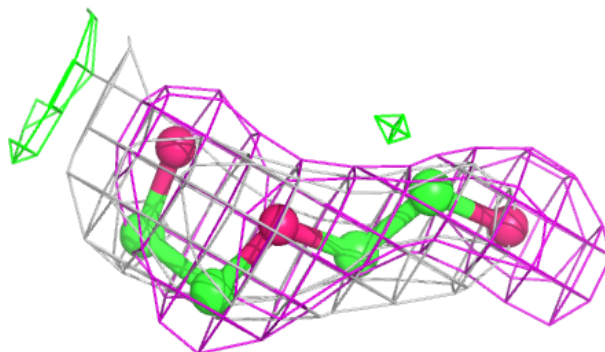
Electron density around EDO C 304:

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

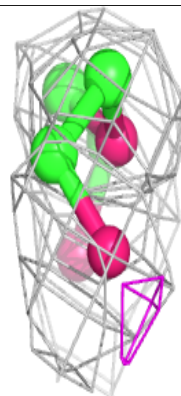
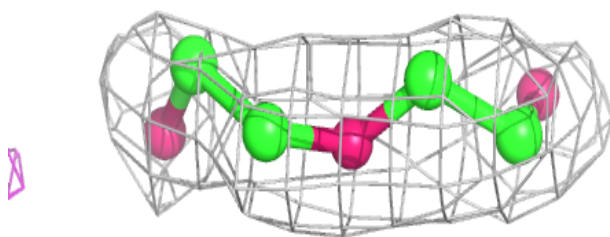
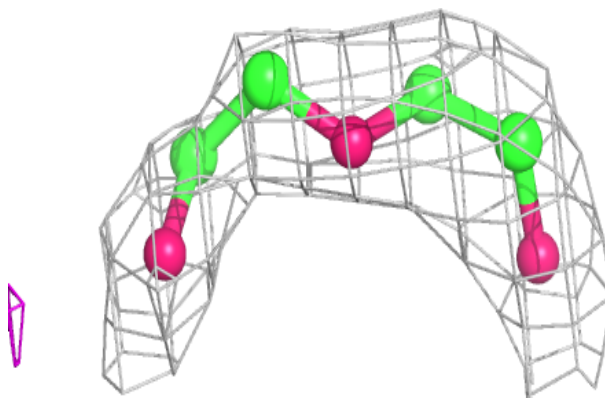


Electron density around PEG B 308:

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

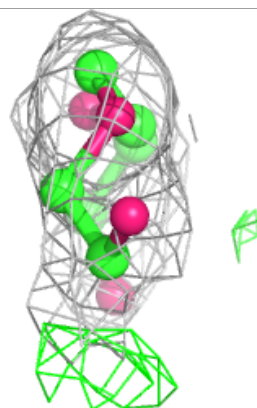
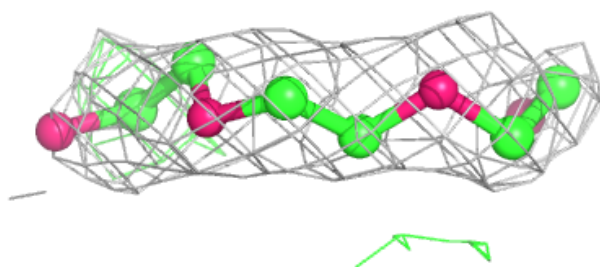
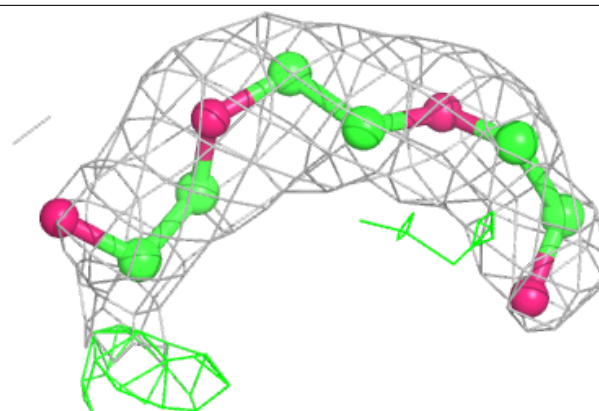
**Electron density around PEG F 306:**

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

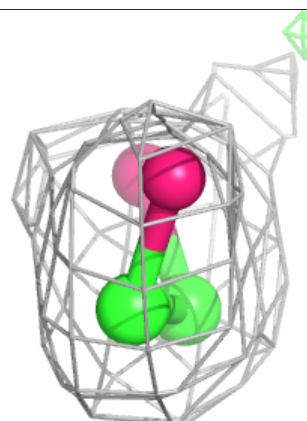
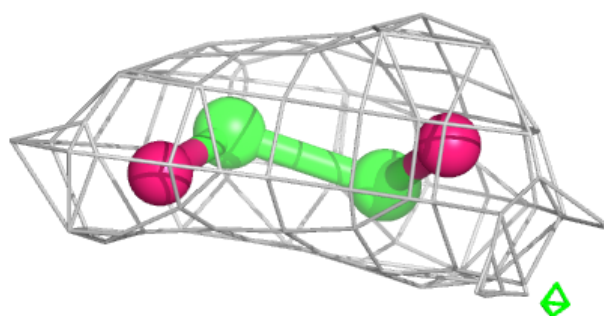
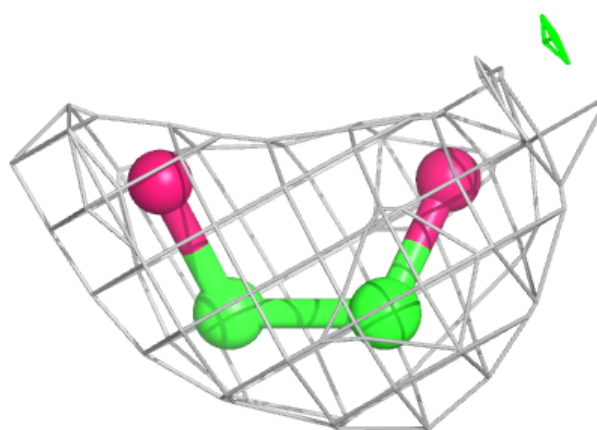


Electron density around PGE C 303:

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

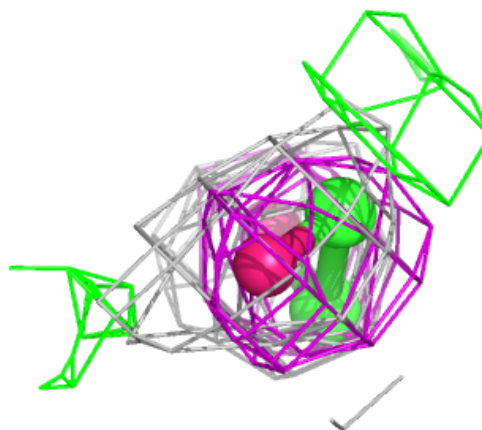
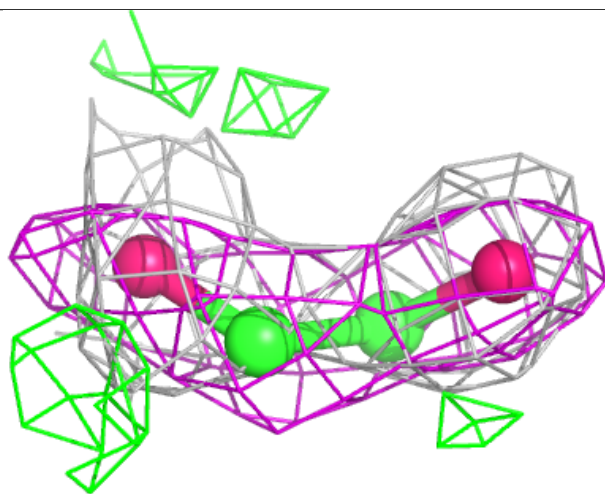
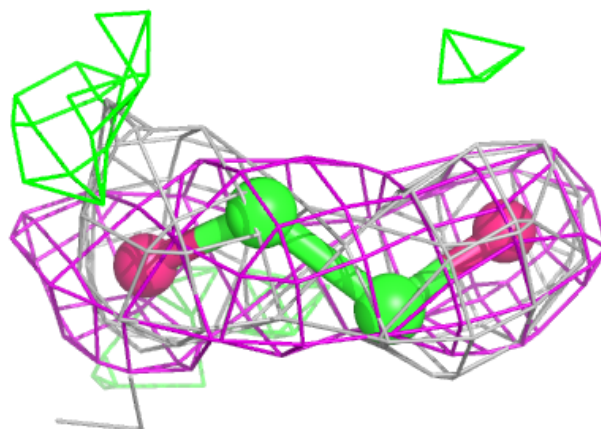
**Electron density around EDO B 303:**

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



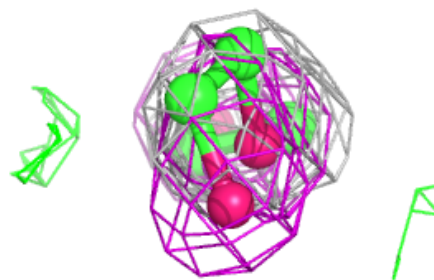
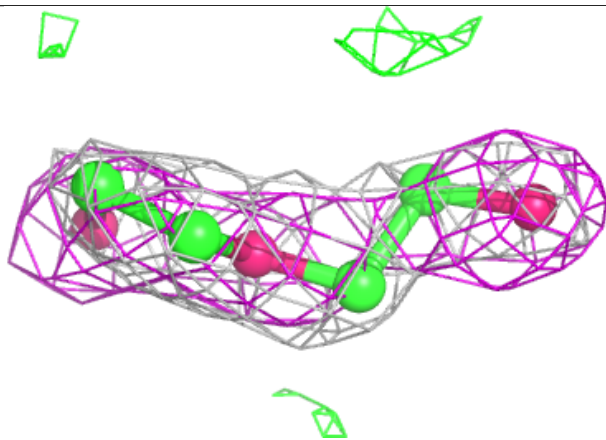
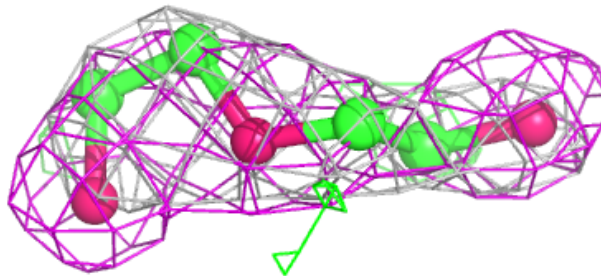
Electron density around EDO F 303:

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



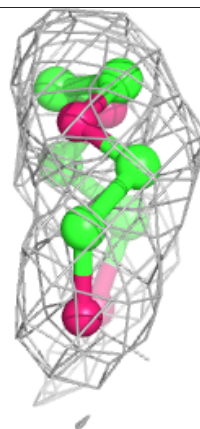
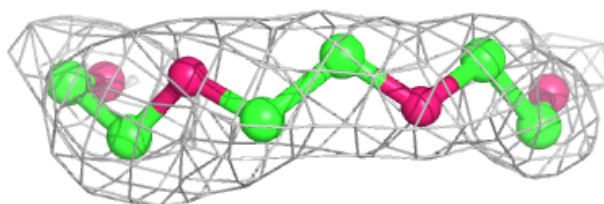
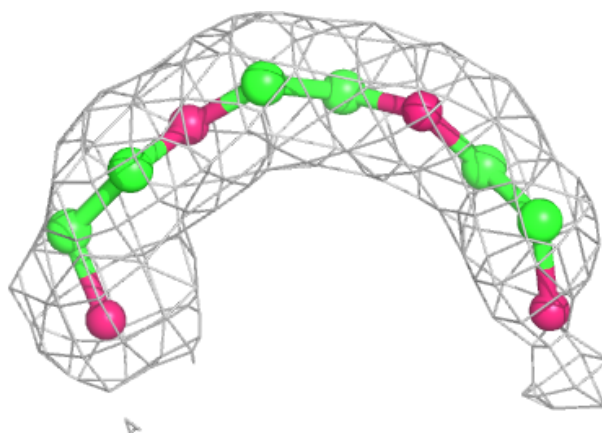
Electron density around PEG E 306:

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

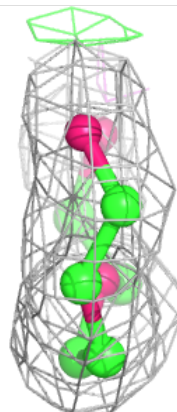
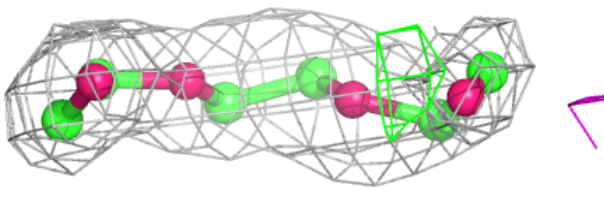
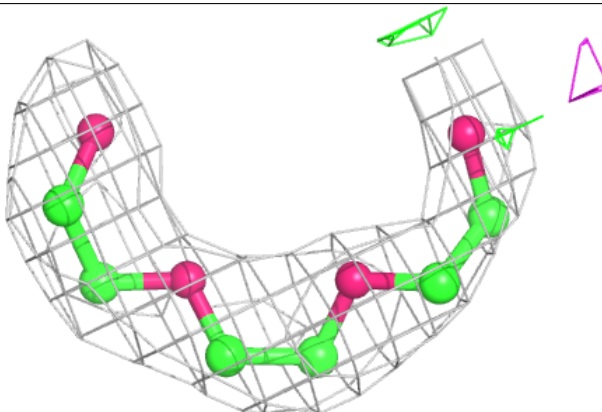


Electron density around PGE D 302:

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

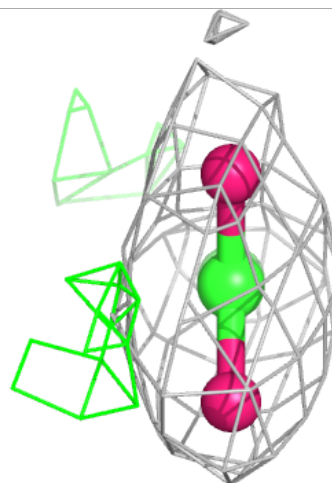
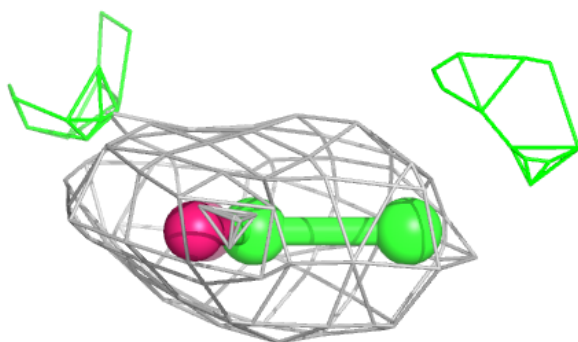
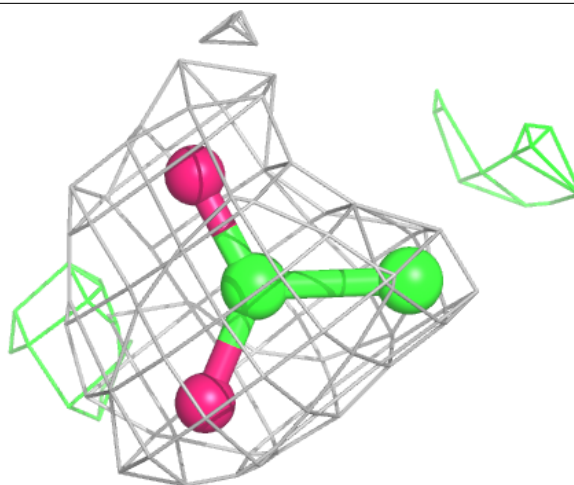
**Electron density around PGE A 303:**

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



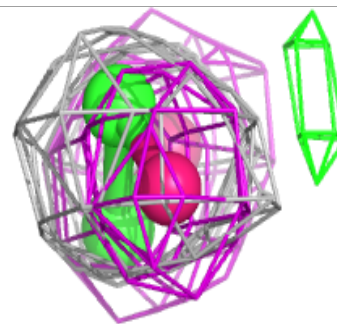
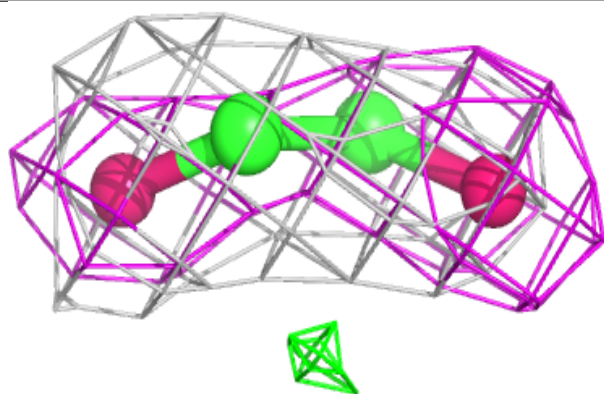
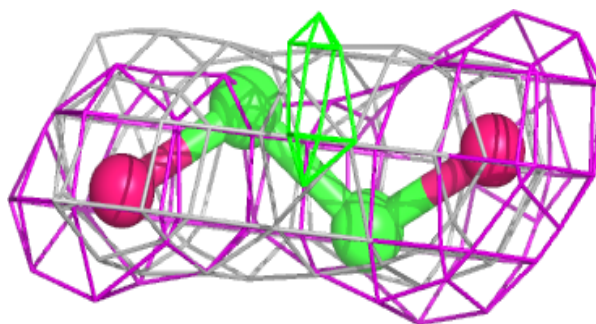
Electron density around ACT C 307:

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



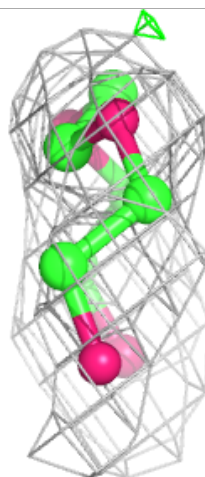
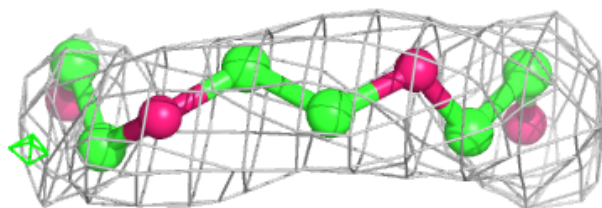
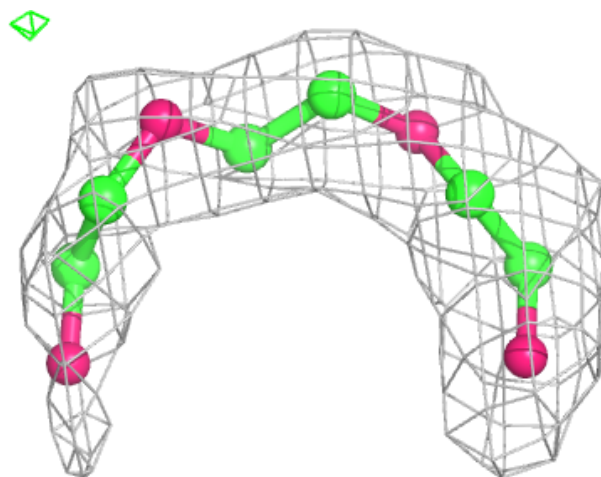
Electron density around EDO B 306:

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



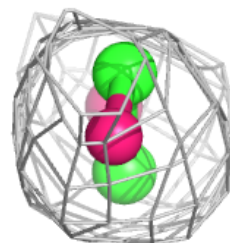
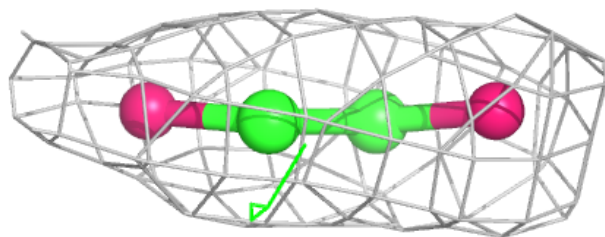
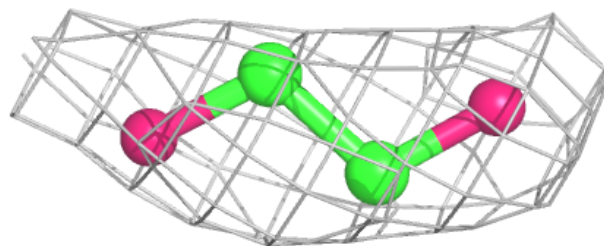
Electron density around PGE B 302:

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



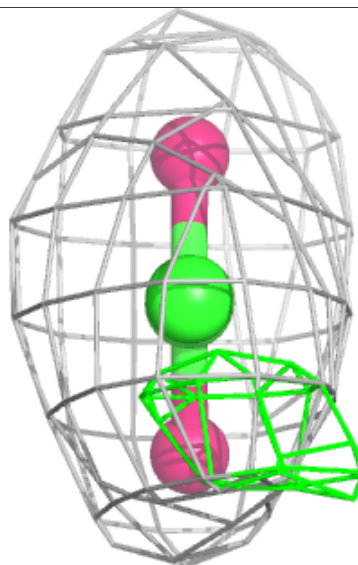
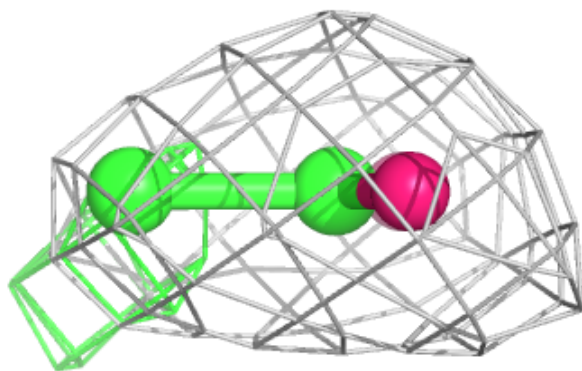
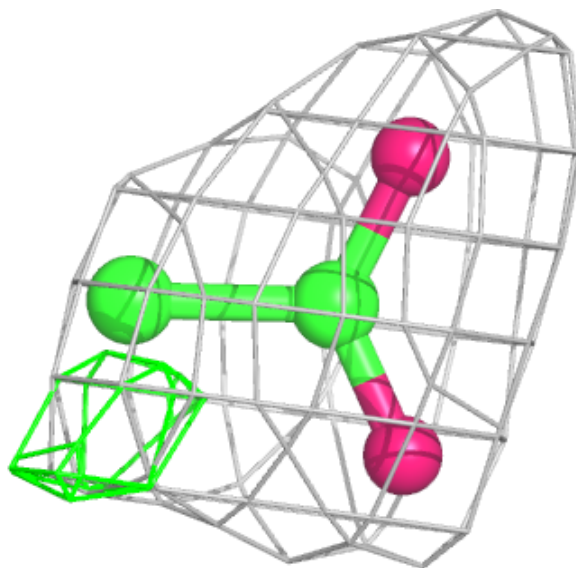
Electron density around EDO A 304:

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



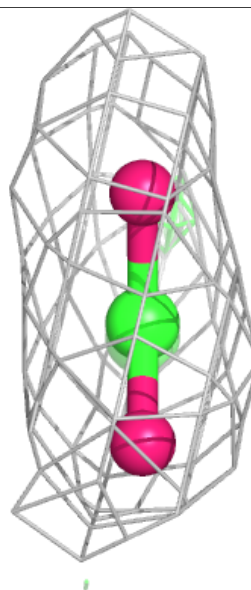
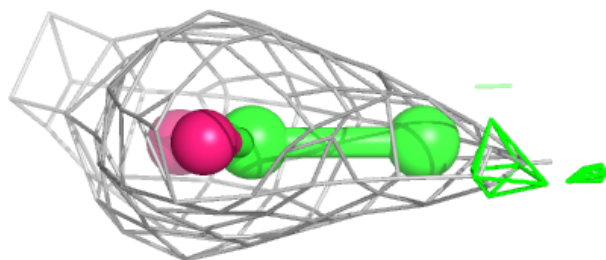
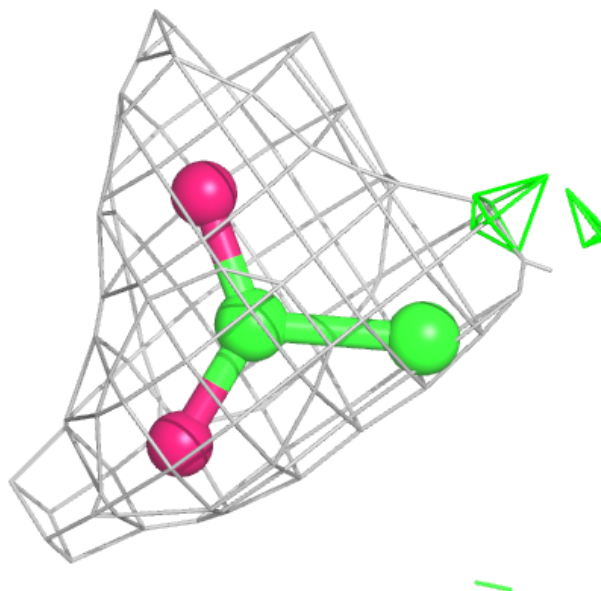
Electron density around ACT A 306:

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



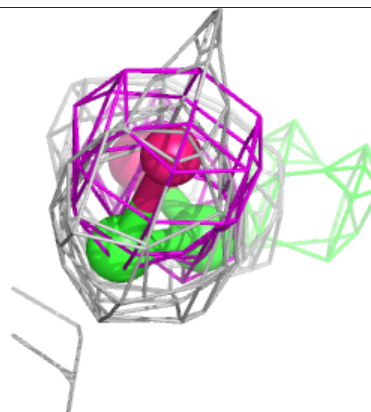
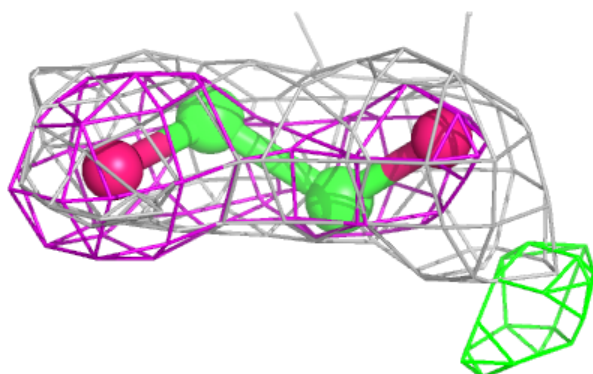
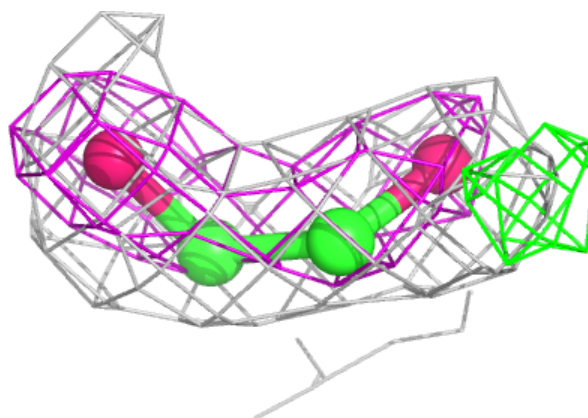
Electron density around ACT F 304:

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



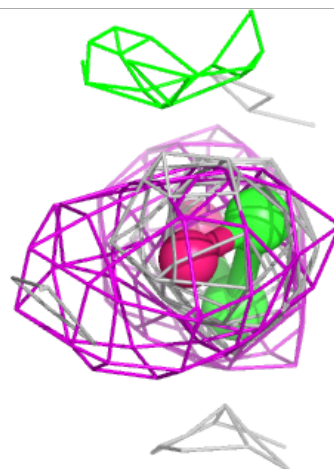
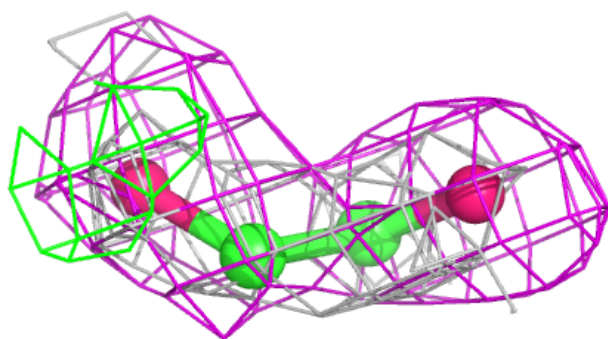
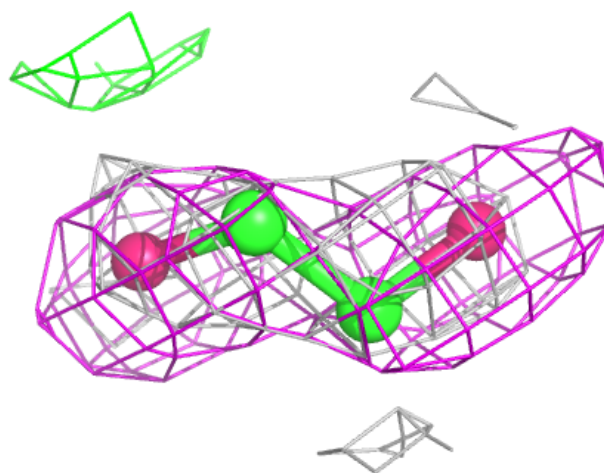
Electron density around EDO A 305:

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



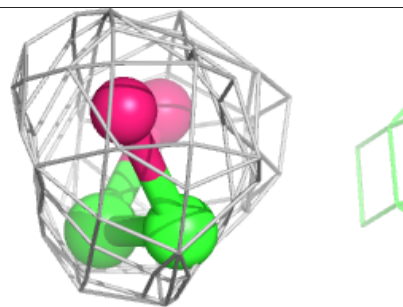
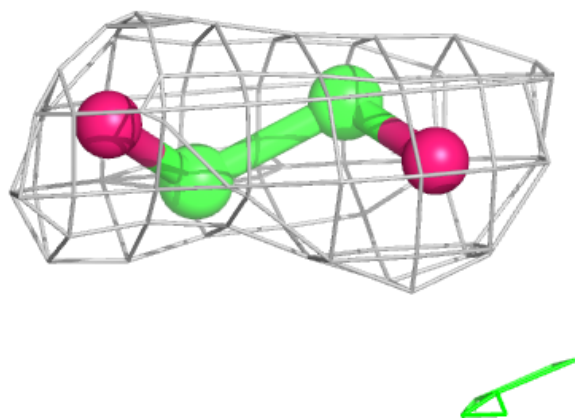
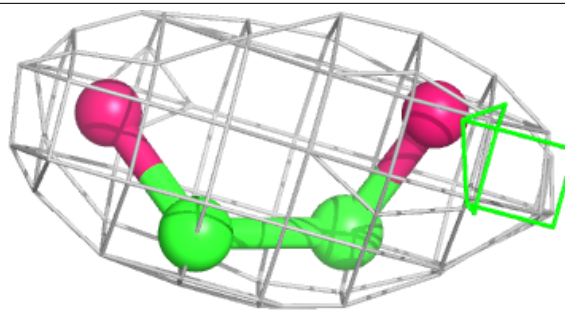
Electron density around EDO C 305:

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



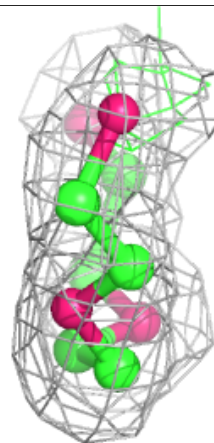
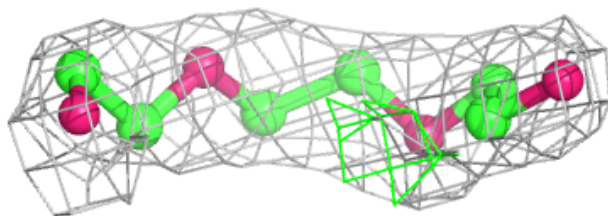
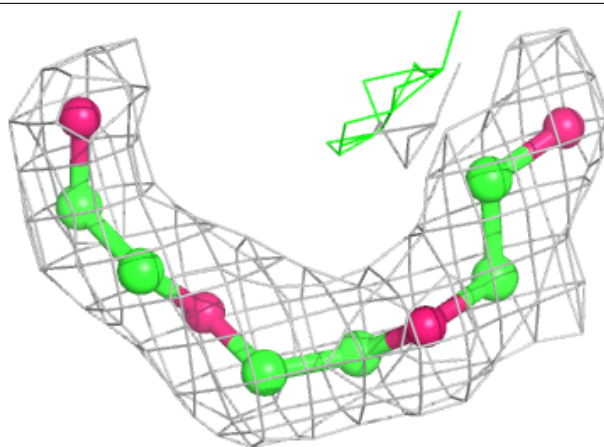
Electron density around EDO B 304:

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



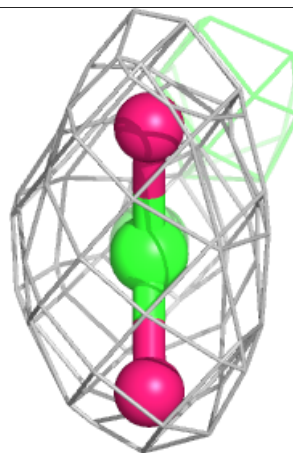
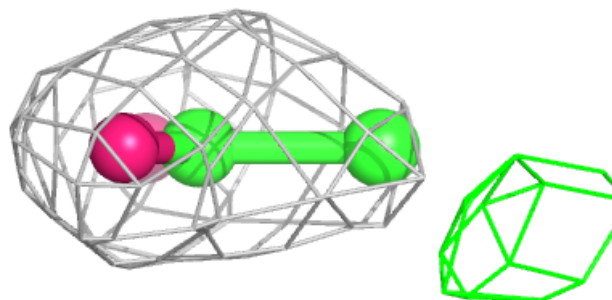
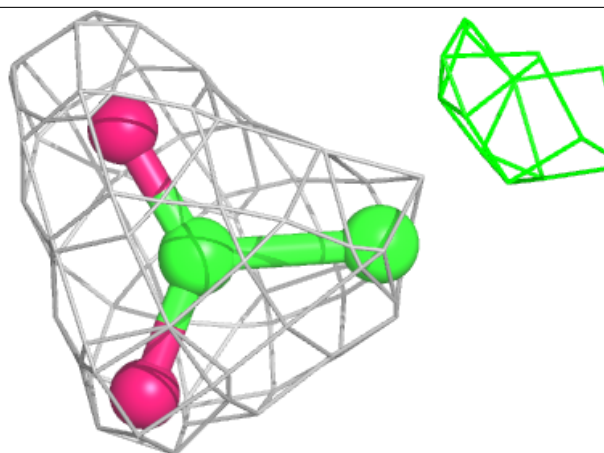
Electron density around PGE E 302:

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



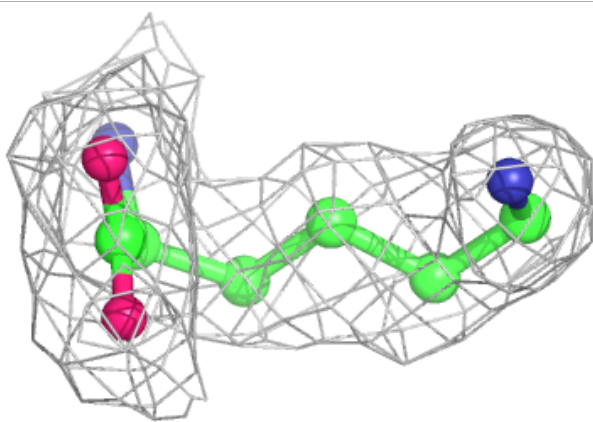
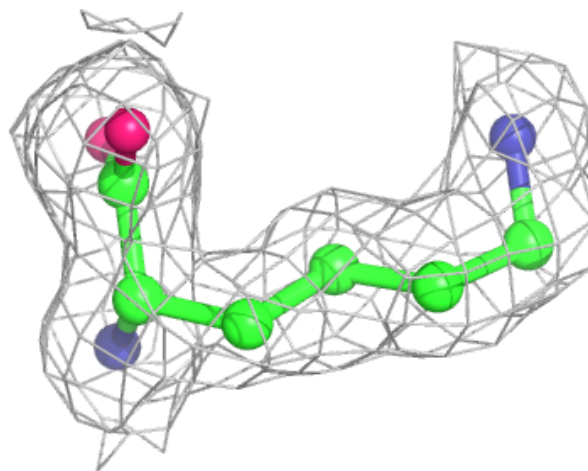
Electron density around ACT E 305:

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



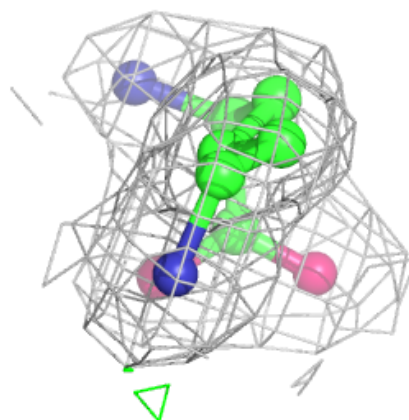
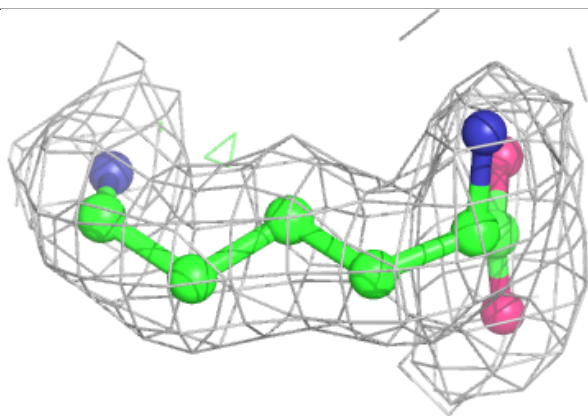
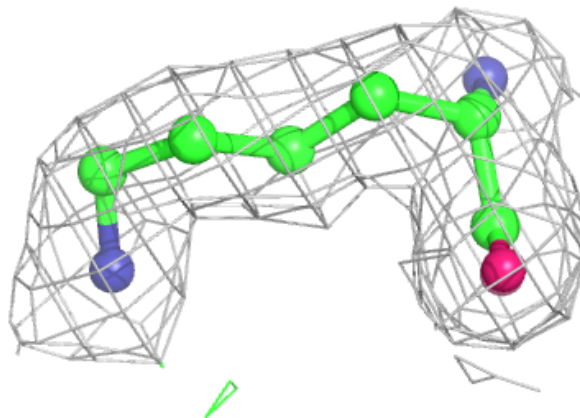
Electron density around LYS A 301:

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



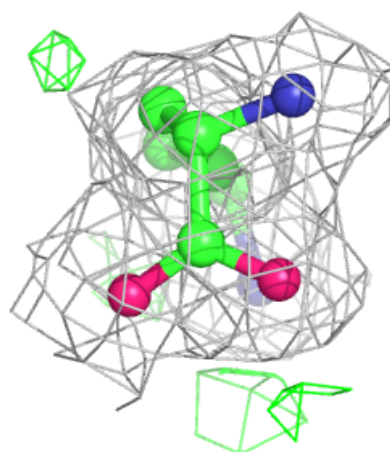
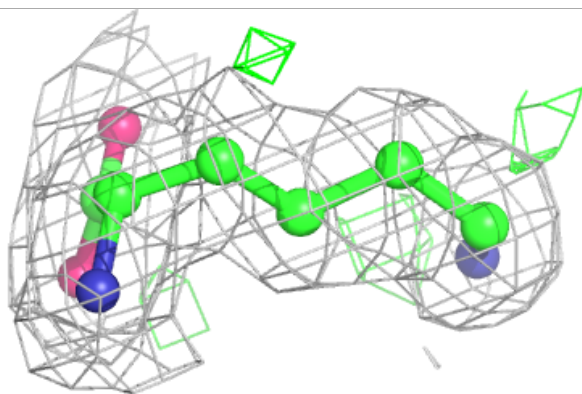
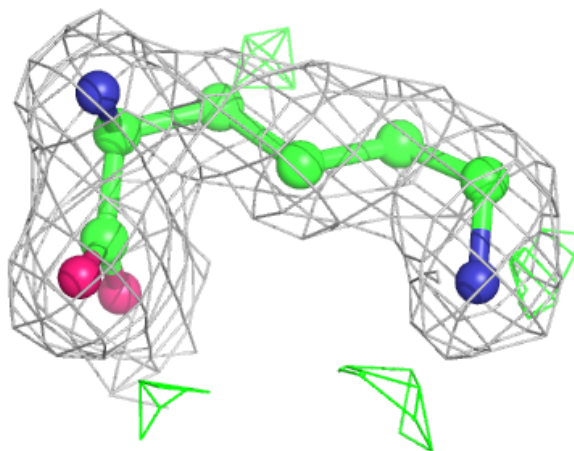
Electron density around LYS F 301:

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



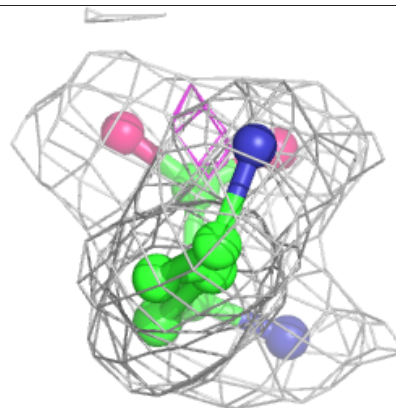
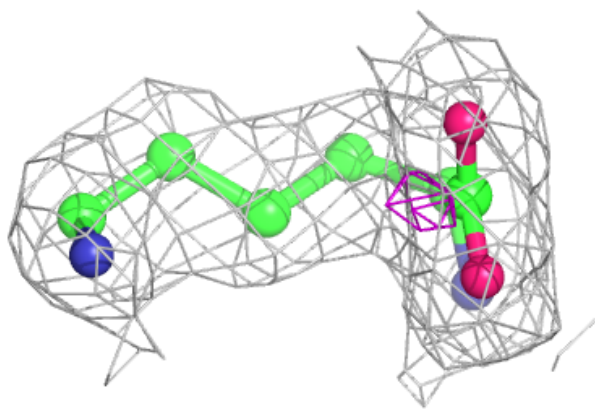
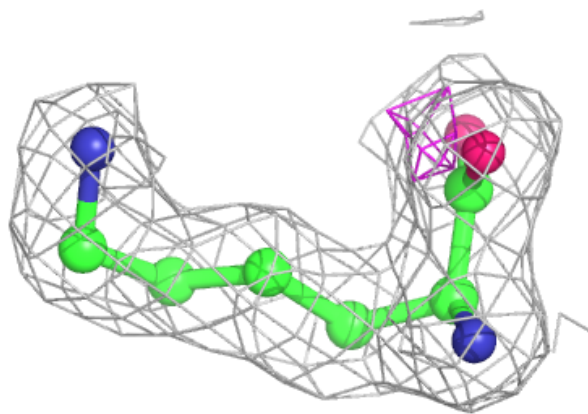
Electron density around LYS C 301:

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



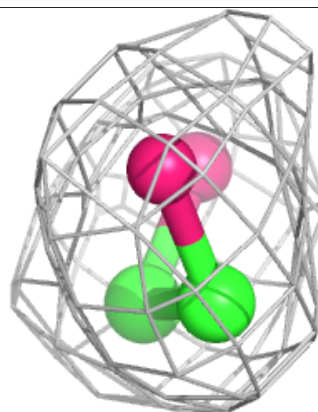
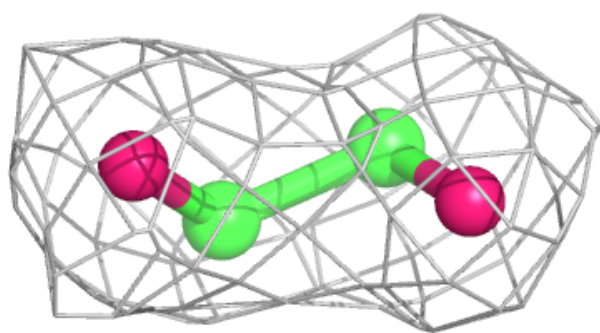
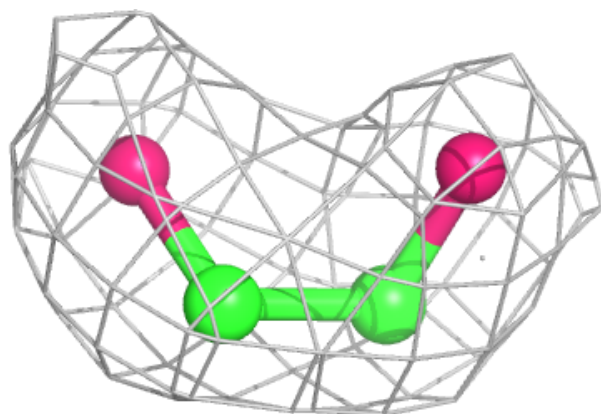
Electron density around LYS E 301:

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



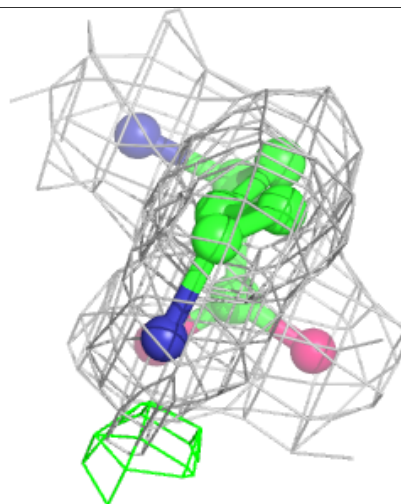
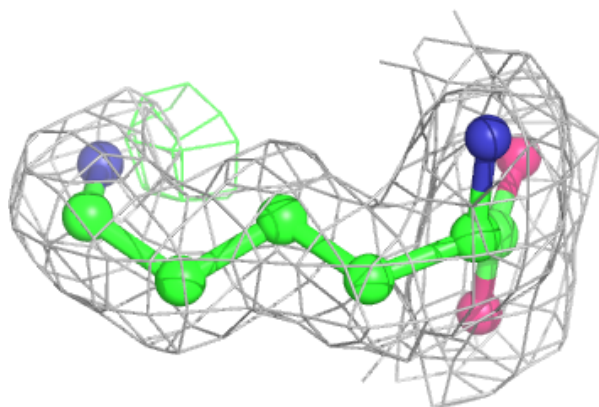
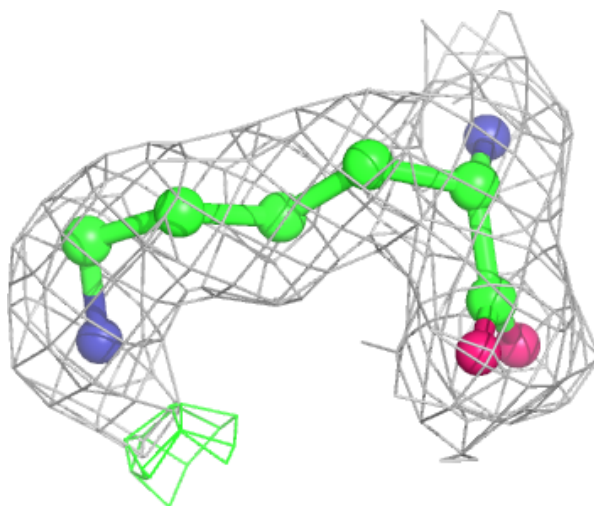
Electron density around EDO E 303:

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



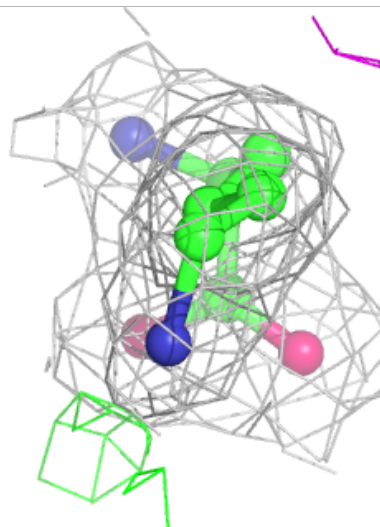
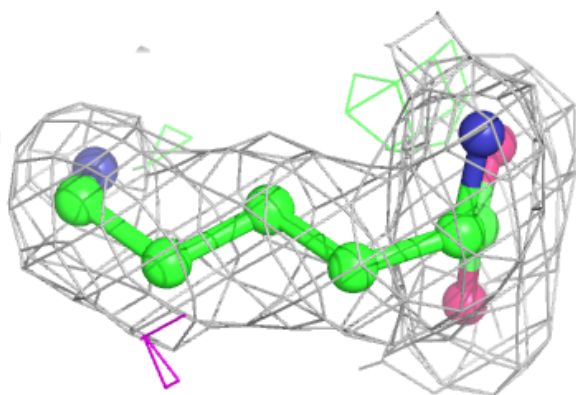
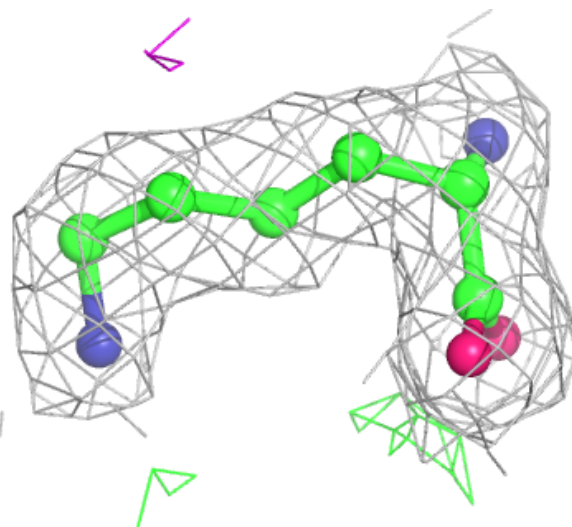
Electron density around LYS D 301:

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



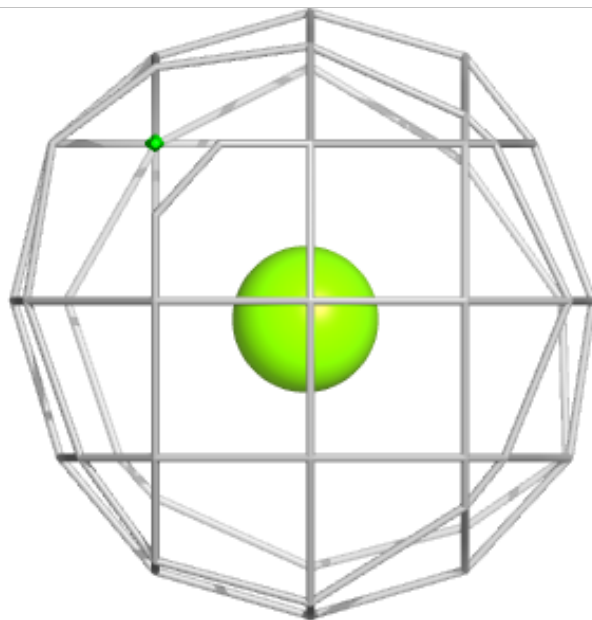
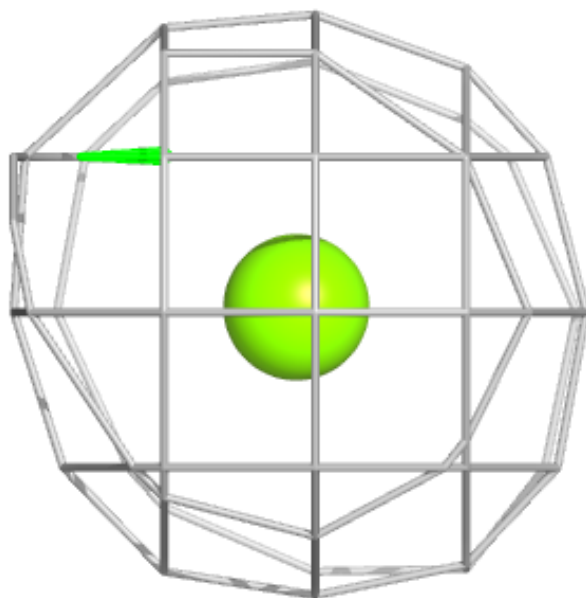
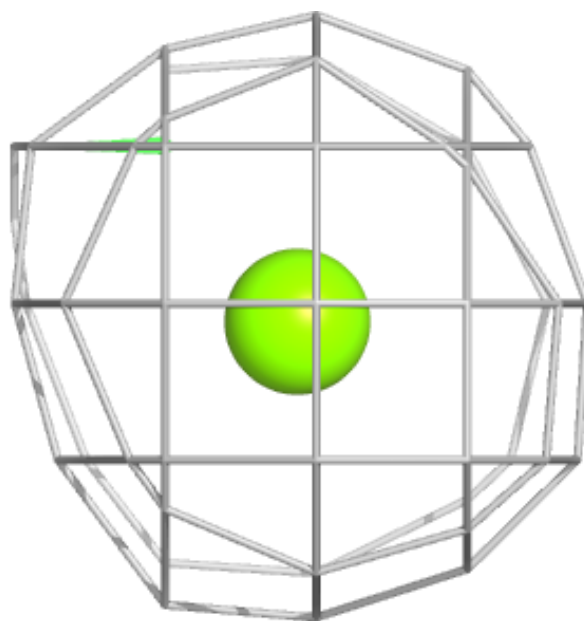
Electron density around LYS B 301:

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



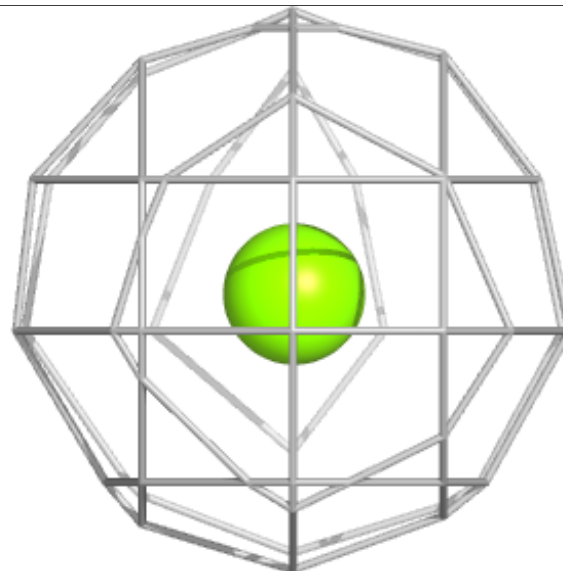
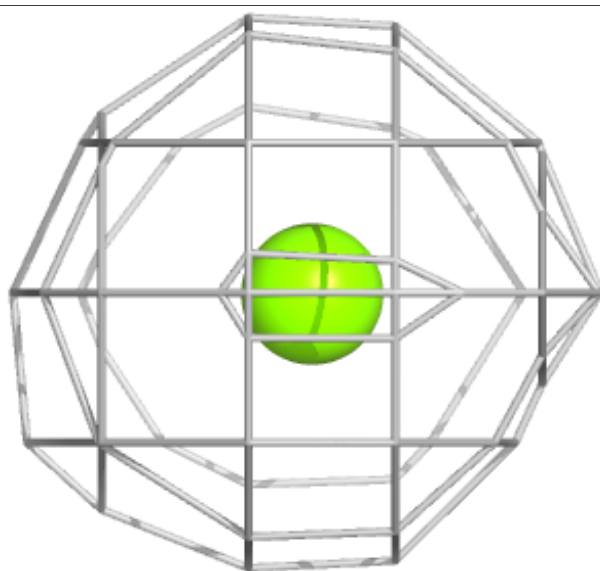
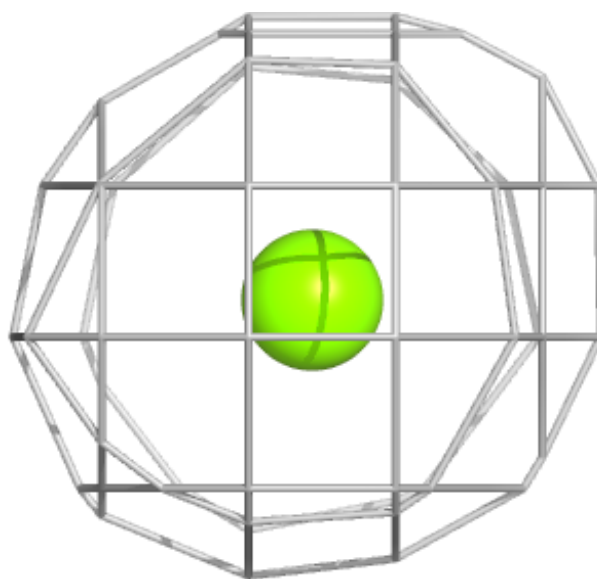
Electron density around MG C 302:

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



Electron density around MG 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.