



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 29, 2021 – 10:20 AM EST

PDB ID : 7KX1  
Title : Dihydrodipicolinate synthase (DHDPS) from C.jejuni, Y110F mutant with pyruvate bound in the active in C2221 space group  
Authors : Saran, S.; Sanders, D.A.R.  
Deposited on : 2020-12-02  
Resolution : 2.04 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

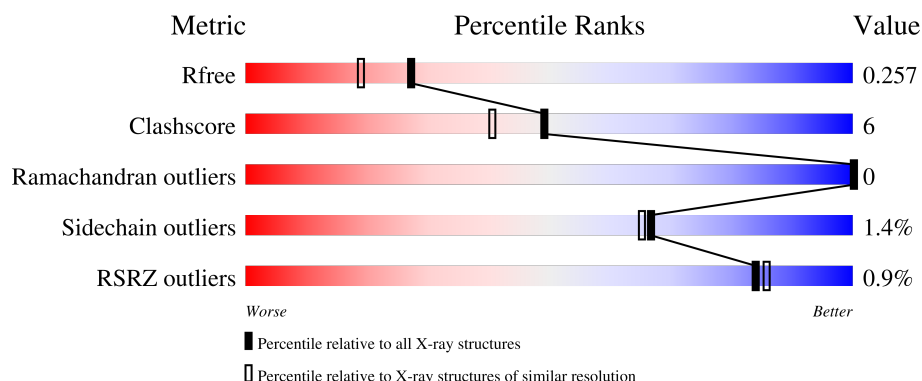
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.04 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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>2%</div> <div>83% 13% 5%</div> </div>
1	B	310	<div> <div>2%</div> <div>82% 13% 5%</div> </div>
1	C	310	<div> <div>82% 14% 5%</div> </div>
1	D	310	<div> <div>2%</div> <div>85% 9% 5%</div> </div>
1	E	310	<div> <div>2%</div> <div>83% 12% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	310	<div><div><div>%</div><div><div></div><div>82%</div><div>13%</div><div>.</div></div></div></div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	C	303	-	-	X	-
5	ACT	B	304	-	-	X	-
6	PEG	C	302	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14350 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
			2266	1443	374	436	13			
1	B	296	Total	C	N	O	S	0	0	0
			2274	1447	378	436	13			
1	C	296	Total	C	N	O	S	0	0	0
			2273	1447	377	436	13			
1	D	296	Total	C	N	O	S	0	0	0
			2273	1446	378	436	13			
1	E	296	Total	C	N	O	S	0	0	0
			2272	1447	376	436	13			
1	F	297	Total	C	N	O	S	0	0	0
			2286	1454	380	439	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	110	PHE	TYR	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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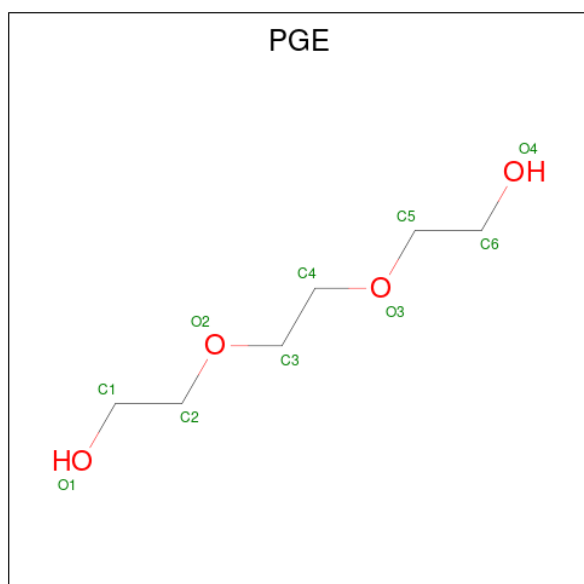
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
B	110	PHE	TYR	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	110	PHE	TYR	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	110	PHE	TYR	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	110	PHE	TYR	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	110	PHE	TYR	engineered mutation	UNP Q9PPB4

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



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

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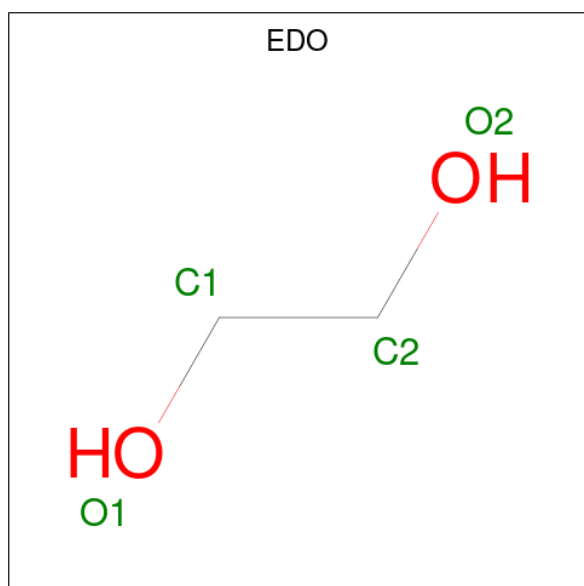
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		
2	D	1	Total	C	O	0	0
			10	6	4		
2	E	1	Total	C	O	0	0
			10	6	4		
2	F	1	Total	C	O	0	0
			10	6	4		

- 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	1	Total	Mg	0	0
			1	1		

- Molecule 4 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).



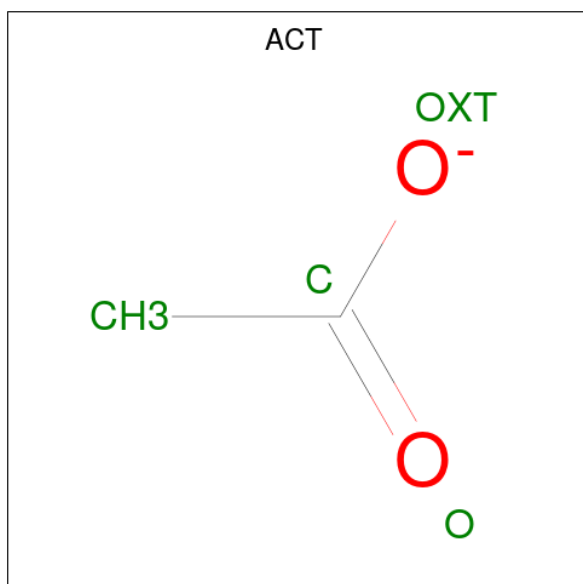
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

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

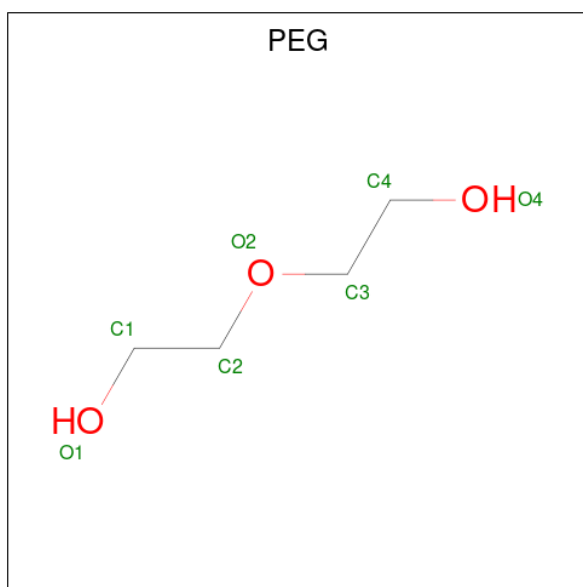
- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 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
6	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	114	Total	O	0	0
			114	114		
7	B	104	Total	O	0	0
			104	104		
7	C	93	Total	O	0	0
			93	93		
7	D	103	Total	O	0	0
			103	103		
7	E	95	Total	O	0	0
			95	95		
7	F	92	Total	O	0	0
			92	92		

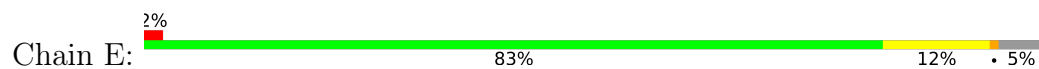


- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

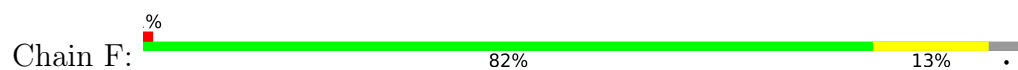




• Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



• 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, $\alpha$ , $\beta$ , $\gamma$	83.81Å 230.10Å 199.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.85 – 2.04 45.85 – 2.04	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.85-2.04) 82.5 (45.85-2.04)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.29 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.213 , 0.254 0.220 , 0.257	Depositor DCC
$R_{free}$ test set	6133 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14350	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, PEG, EDO, ACT, KPI, 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	0.45	0/2290	0.58	0/3098
1	B	0.50	0/2298	0.54	0/3107
1	C	0.45	0/2297	0.54	0/3106
1	D	0.44	0/2297	0.49	0/3105
1	E	0.41	0/2296	0.52	0/3104
1	F	0.41	0/2310	0.56	0/3122
All	All	0.44	0/13788	0.54	0/18642

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	B	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	166	KPI	Mainchain
1	D	166	KPI	Mainchain
1	E	166	KPI	Mainchain

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Mol	Chain	Res	Type	Group
1	F	166	KPI	Mainchain

## 5.2 Too-close contacts ⓘ

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	2266	0	2288	26	0
1	B	2274	0	2307	29	0
1	C	2273	0	2303	40	1
1	D	2273	0	2306	20	0
1	E	2272	0	2307	28	0
1	F	2286	0	2323	26	0
2	A	10	0	14	3	0
2	B	10	0	14	1	0
2	C	10	0	14	5	0
2	D	10	0	14	0	0
2	E	10	0	14	3	0
2	F	10	0	14	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	8	0	12	1	0
4	C	4	0	6	6	0
4	D	4	0	6	2	0
4	F	4	0	6	1	0
5	B	4	0	3	3	0
5	C	4	0	3	0	0
5	E	4	0	3	0	0
5	F	4	0	3	1	0
6	C	7	0	10	7	0
7	A	114	0	0	1	0
7	B	104	0	0	4	0
7	C	93	0	0	0	0
7	D	103	0	0	1	0
7	E	95	0	0	2	0
7	F	92	0	0	4	0
All	All	14350	0	13970	164	1

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 6.

The worst 5 of 164 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LYS:CE	2:A:301:PGE:H6	1.57	1.35
1:D:169:SER:HB2	4:D:302:EDO:H12	1.20	1.15
1:A:154:LYS:CE	2:A:301:PGE:C6	2.31	1.08
1:C:202:GLY:O	6:C:302:PEG:H42	1.57	1.03
1:C:154:LYS:CE	2:C:301:PGE:H52	1.95	0.96

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:GLU:OE1	1:C:288:GLU:OE1[3_455]	2.08	0.12

## 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%)	286 (98%)	7 (2%)	0	100	100
1	B	293/310 (94%)	284 (97%)	9 (3%)	0	100	100
1	C	293/310 (94%)	285 (97%)	8 (3%)	0	100	100
1	D	293/310 (94%)	285 (97%)	8 (3%)	0	100	100
1	E	293/310 (94%)	285 (97%)	8 (3%)	0	100	100
1	F	294/310 (95%)	286 (97%)	8 (3%)	0	100	100
All	All	1759/1860 (95%)	1711 (97%)	48 (3%)	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	244/260 (94%)	239 (98%)	5 (2%)	55	50
1	B	247/260 (95%)	245 (99%)	2 (1%)	81	82
1	C	246/260 (95%)	241 (98%)	5 (2%)	55	50
1	D	247/260 (95%)	244 (99%)	3 (1%)	71	70
1	E	247/260 (95%)	243 (98%)	4 (2%)	62	59
1	F	249/260 (96%)	248 (100%)	1 (0%)	91	91
All	All	1480/1560 (95%)	1460 (99%)	20 (1%)	67	65

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	161	ASN
1	E	249	CYS
1	F	292	LYS
1	E	268	SER
1	B	280	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	E	4	ASN
1	E	59	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	0.67	0	6,15,17	3.03	3 (50%)
1	KPI	C	166	1	10,13,14	0.59	0	6,15,17	2.97	3 (50%)
1	KPI	E	166	1	10,13,14	1.38	1 (10%)	6,15,17	3.26	3 (50%)
1	KPI	B	166	1	10,13,14	1.42	1 (10%)	6,15,17	2.83	3 (50%)
1	KPI	F	166	1	10,13,14	1.31	1 (10%)	6,15,17	2.95	3 (50%)
1	KPI	D	166	1	10,13,14	1.39	1 (10%)	6,15,17	2.87	3 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KPI	A	166	1	-	0/9/14/16	-
1	KPI	C	166	1	-	0/9/14/16	-
1	KPI	E	166	1	-	1/9/14/16	-
1	KPI	B	166	1	-	1/9/14/16	-
1	KPI	F	166	1	-	0/9/14/16	-
1	KPI	D	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	B	166	KPI	O-C	4.20	1.36	1.19
1	D	166	KPI	O-C	4.14	1.36	1.19
1	E	166	KPI	O-C	4.11	1.36	1.19
1	F	166	KPI	O-C	3.85	1.35	1.19

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	166	KPI	C1-CX1-CX2	-6.00	111.28	117.92
1	A	166	KPI	C1-CX1-CX2	-5.95	111.33	117.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	166	KPI	C1-CX1-CX2	-5.76	111.54	117.92
1	C	166	KPI	C1-CX1-CX2	-5.73	111.57	117.92
1	B	166	KPI	C1-CX1-CX2	-5.53	111.80	117.92

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	166	KPI	C-CA-CB-CG
1	E	166	KPI	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	ACT	E	302	-	1,3,3	1.03	0	0,3,3	-	-
2	PGE	B	301	-	9,9,9	0.33	0	8,8,8	0.18	0
4	EDO	B	303	-	3,3,3	0.23	0	2,2,2	0.40	0
5	ACT	B	304	-	1,3,3	0.57	0	0,3,3	-	-
2	PGE	D	301	-	9,9,9	0.34	0	8,8,8	0.22	0
4	EDO	B	302	-	3,3,3	0.22	0	2,2,2	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	C	303	-	3,3,3	0.30	0	2,2,2	1.40	0
4	EDO	F	302	-	3,3,3	0.45	0	2,2,2	0.44	0
4	EDO	D	302	-	3,3,3	0.27	0	2,2,2	0.68	0
2	PGE	F	301	-	9,9,9	0.27	0	8,8,8	0.48	0
2	PGE	E	301	-	9,9,9	0.30	0	8,8,8	0.25	0
2	PGE	A	301	-	9,9,9	0.33	0	8,8,8	0.41	0
2	PGE	C	301	-	9,9,9	0.46	0	8,8,8	0.76	0
5	ACT	C	304	-	1,3,3	1.67	0	0,3,3	-	-
5	ACT	F	303	-	1,3,3	0.79	0	0,3,3	-	-
6	PEG	C	302	-	6,6,6	0.25	0	5,5,5	1.01	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	PGE	B	301	-	-	5/7/7/7	-
4	EDO	B	303	-	-	1/1/1/1	-
2	PGE	D	301	-	-	4/7/7/7	-
4	EDO	B	302	-	-	0/1/1/1	-
4	EDO	C	303	-	-	0/1/1/1	-
4	EDO	F	302	-	-	1/1/1/1	-
4	EDO	D	302	-	-	1/1/1/1	-
2	PGE	F	301	-	-	3/7/7/7	-
2	PGE	E	301	-	-	4/7/7/7	-
2	PGE	A	301	-	-	2/7/7/7	-
2	PGE	C	301	-	-	2/7/7/7	-
6	PEG	C	302	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	PGE	O3-C5-C6-O4
2	E	301	PGE	O2-C3-C4-O3
2	F	301	PGE	O2-C3-C4-O3

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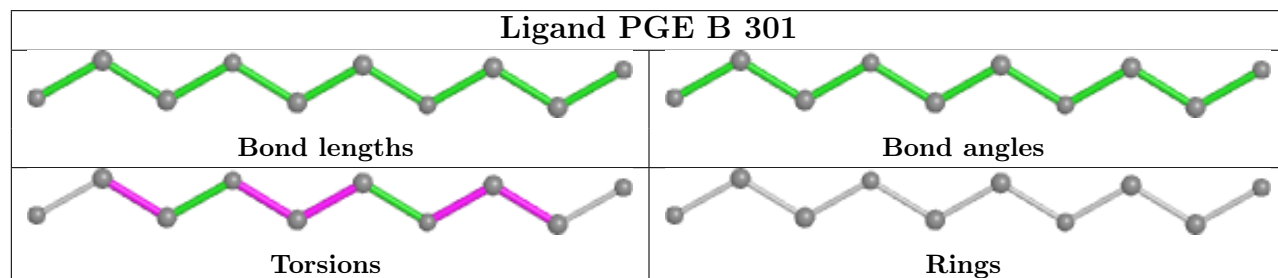
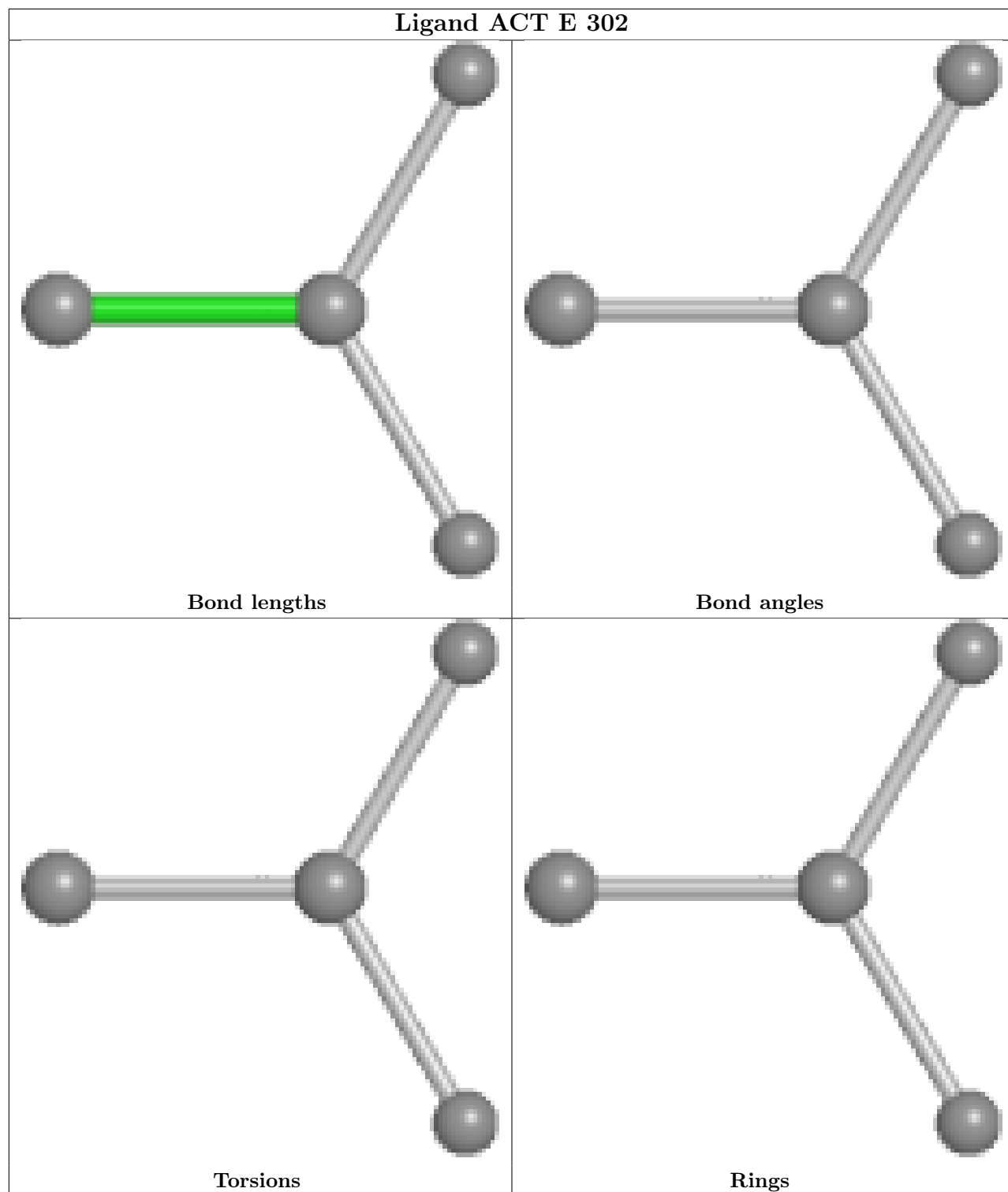
Mol	Chain	Res	Type	Atoms
2	B	301	PGE	O1-C1-C2-O2
2	E	301	PGE	O3-C5-C6-O4

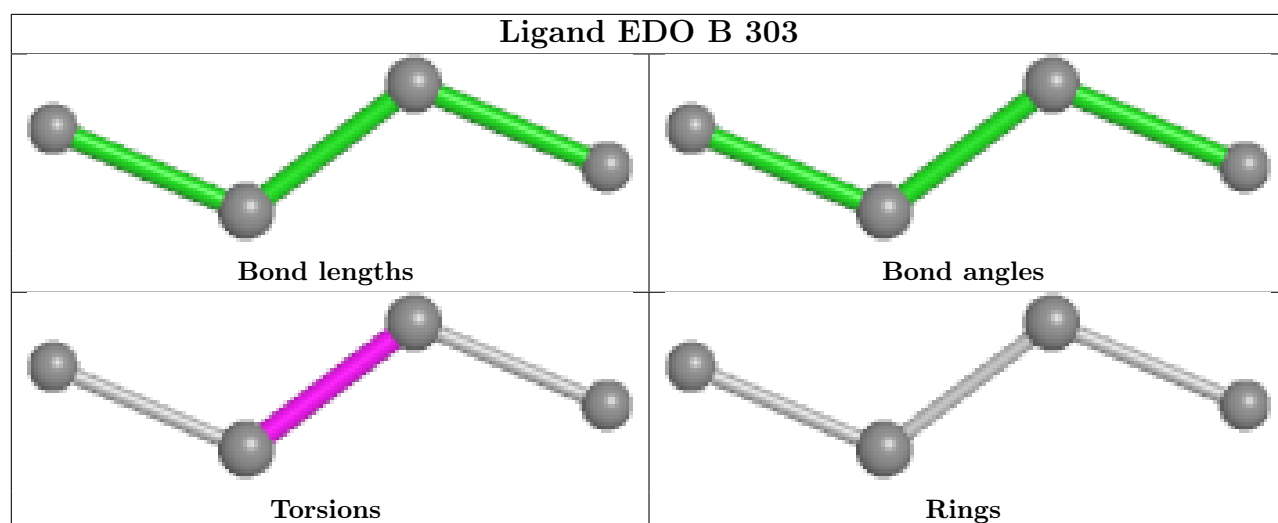
There are no ring outliers.

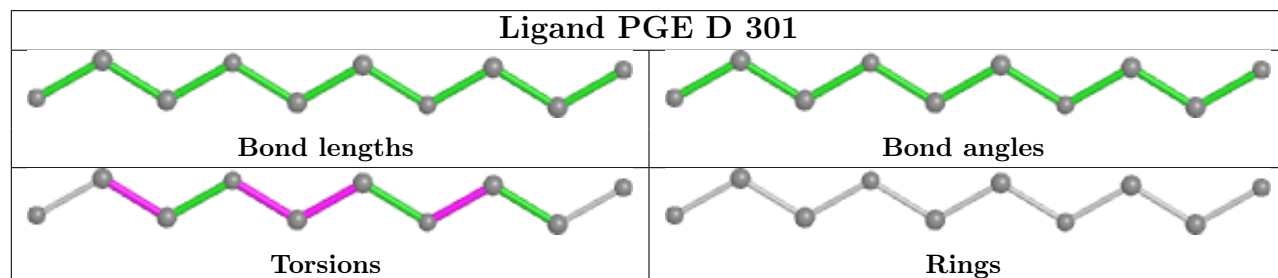
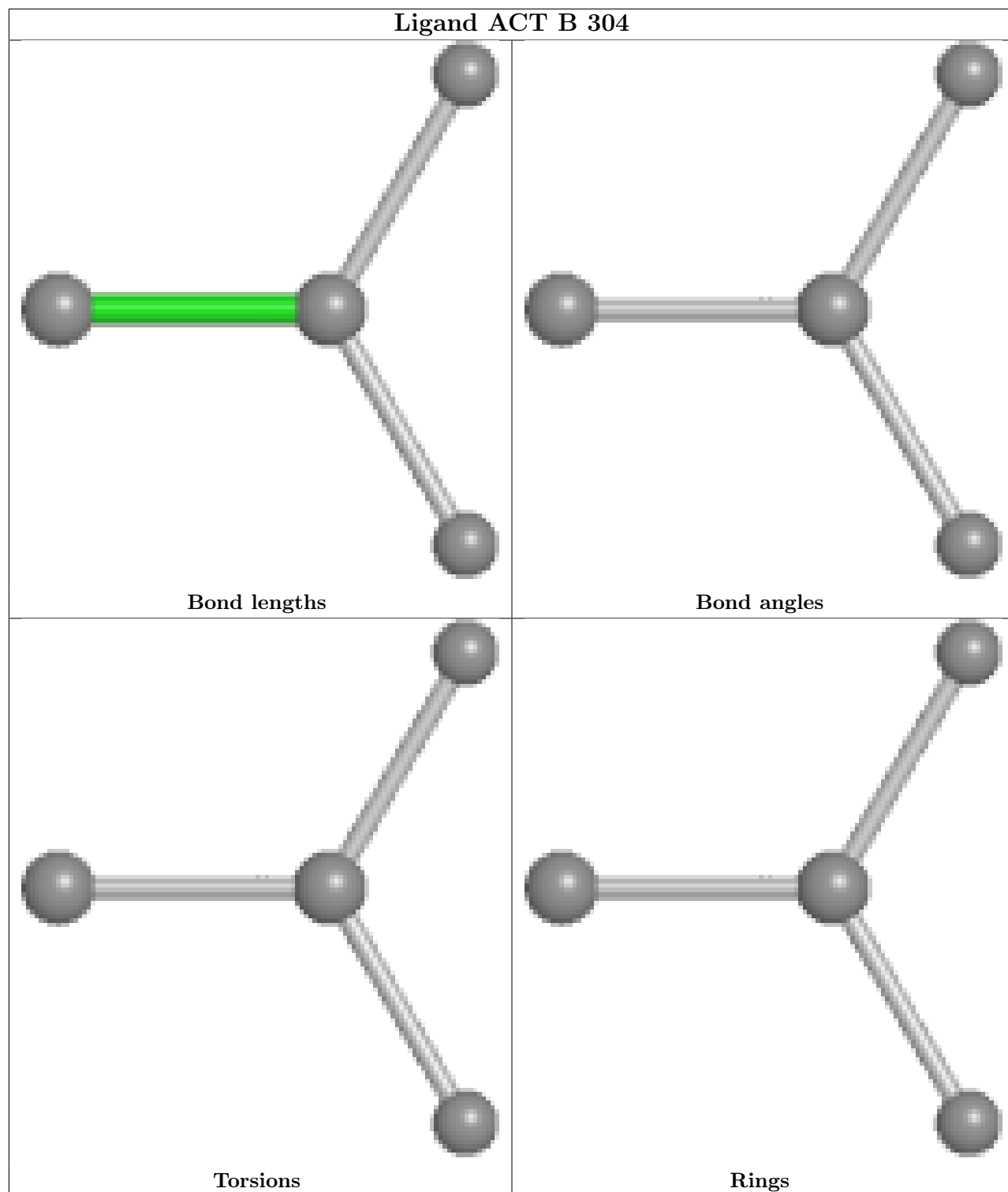
11 monomers are involved in 33 short contacts:

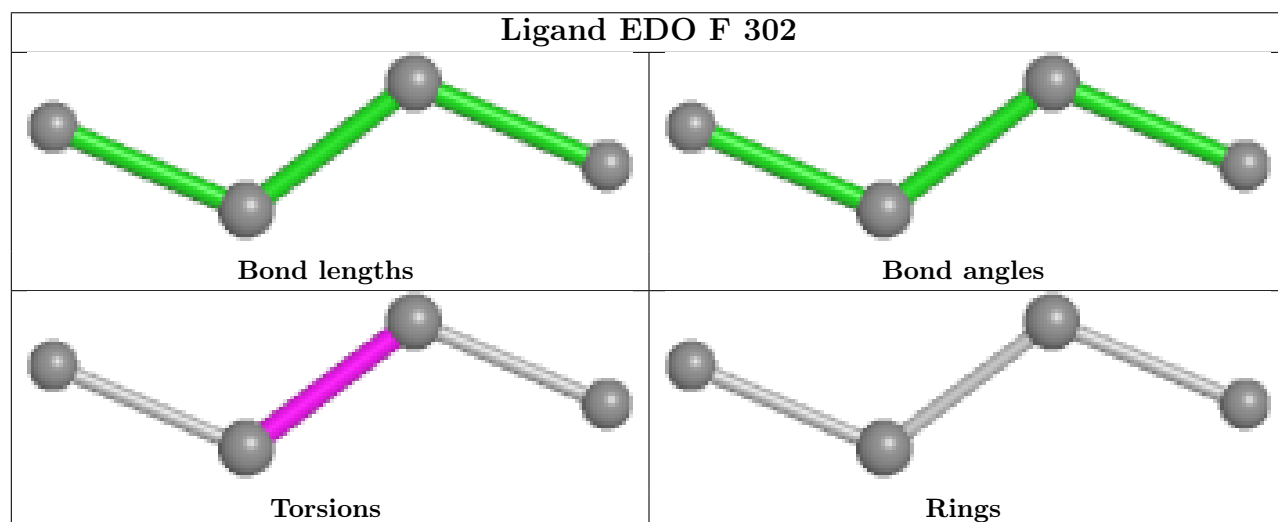
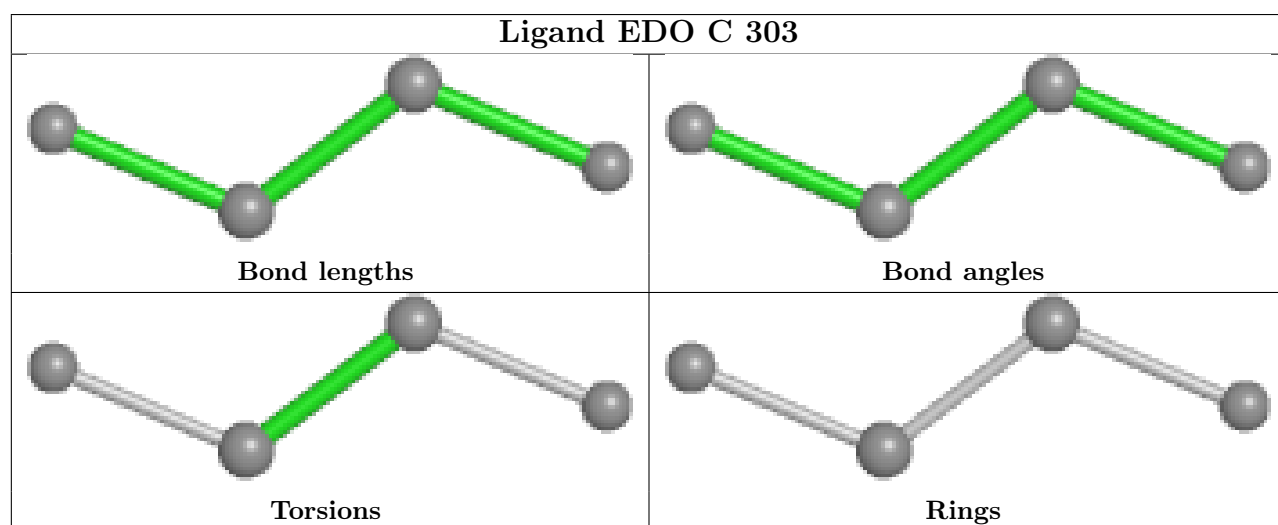
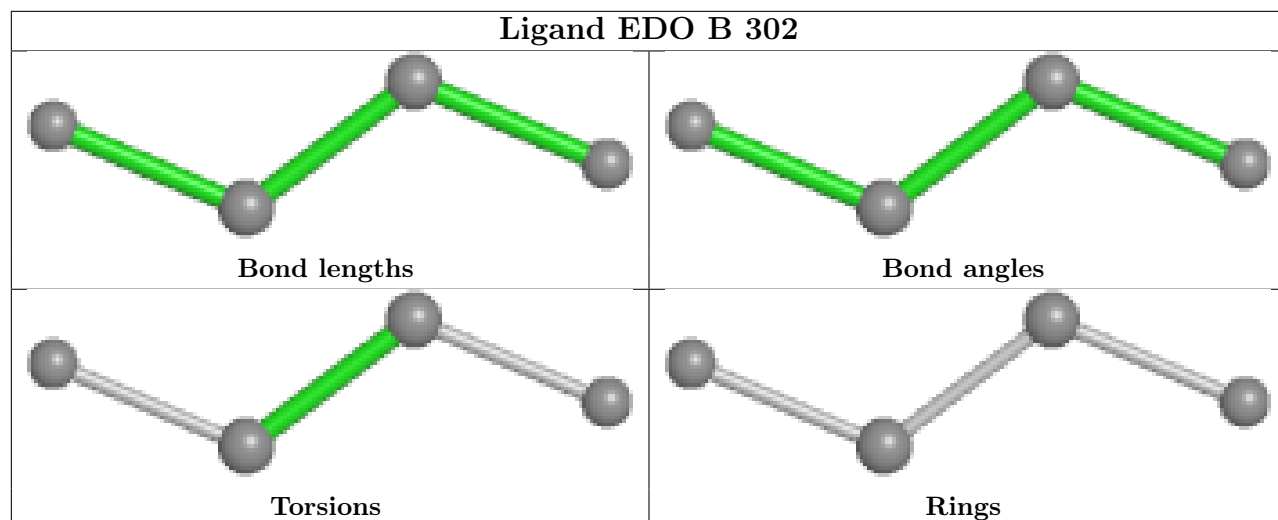
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	PGE	1	0
5	B	304	ACT	3	0
4	B	302	EDO	1	0
4	C	303	EDO	6	0
4	F	302	EDO	1	0
4	D	302	EDO	2	0
2	E	301	PGE	3	0
2	A	301	PGE	3	0
2	C	301	PGE	5	0
5	F	303	ACT	1	0
6	C	302	PEG	7	0

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

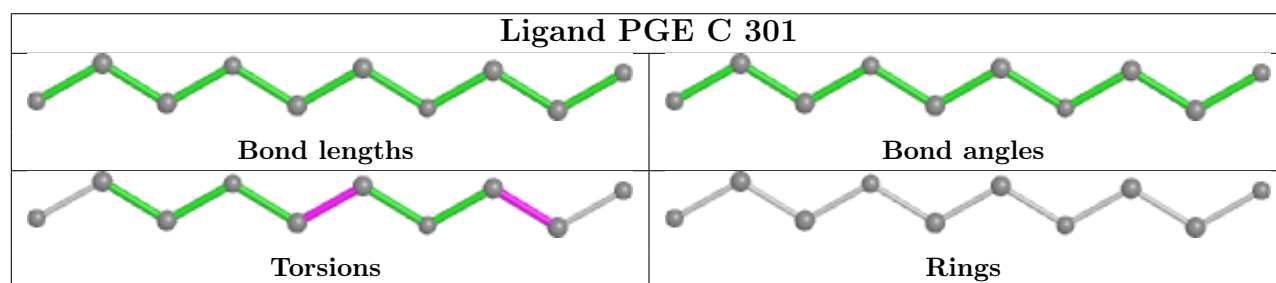
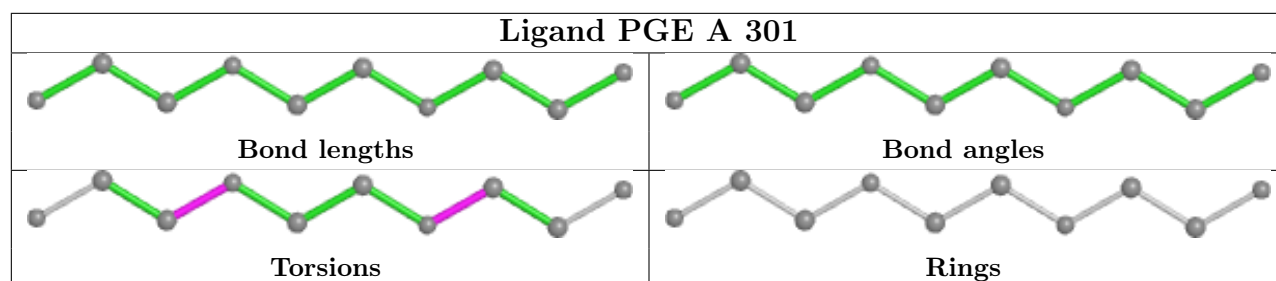
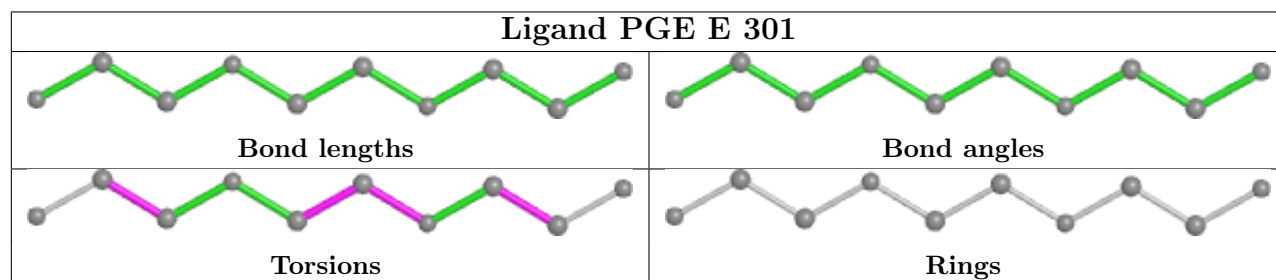
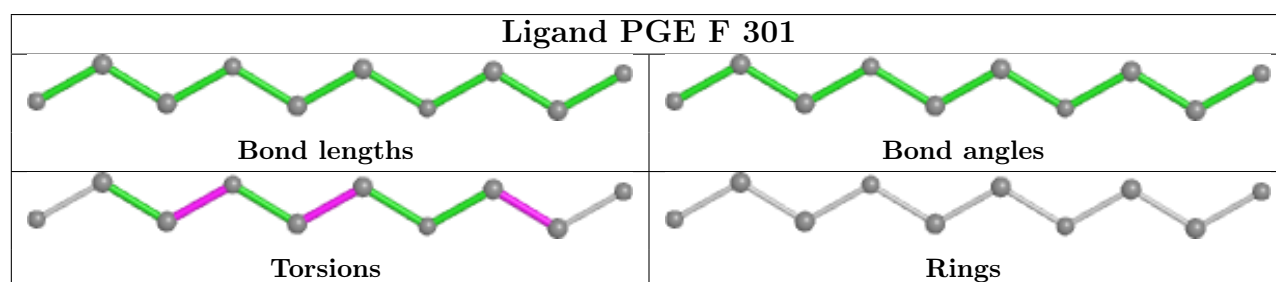
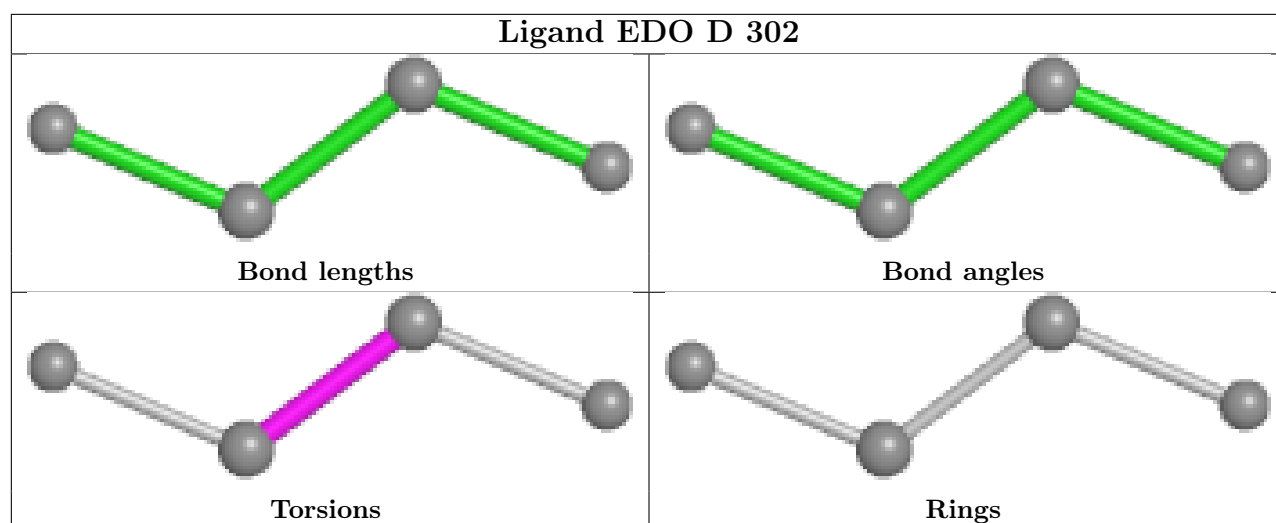


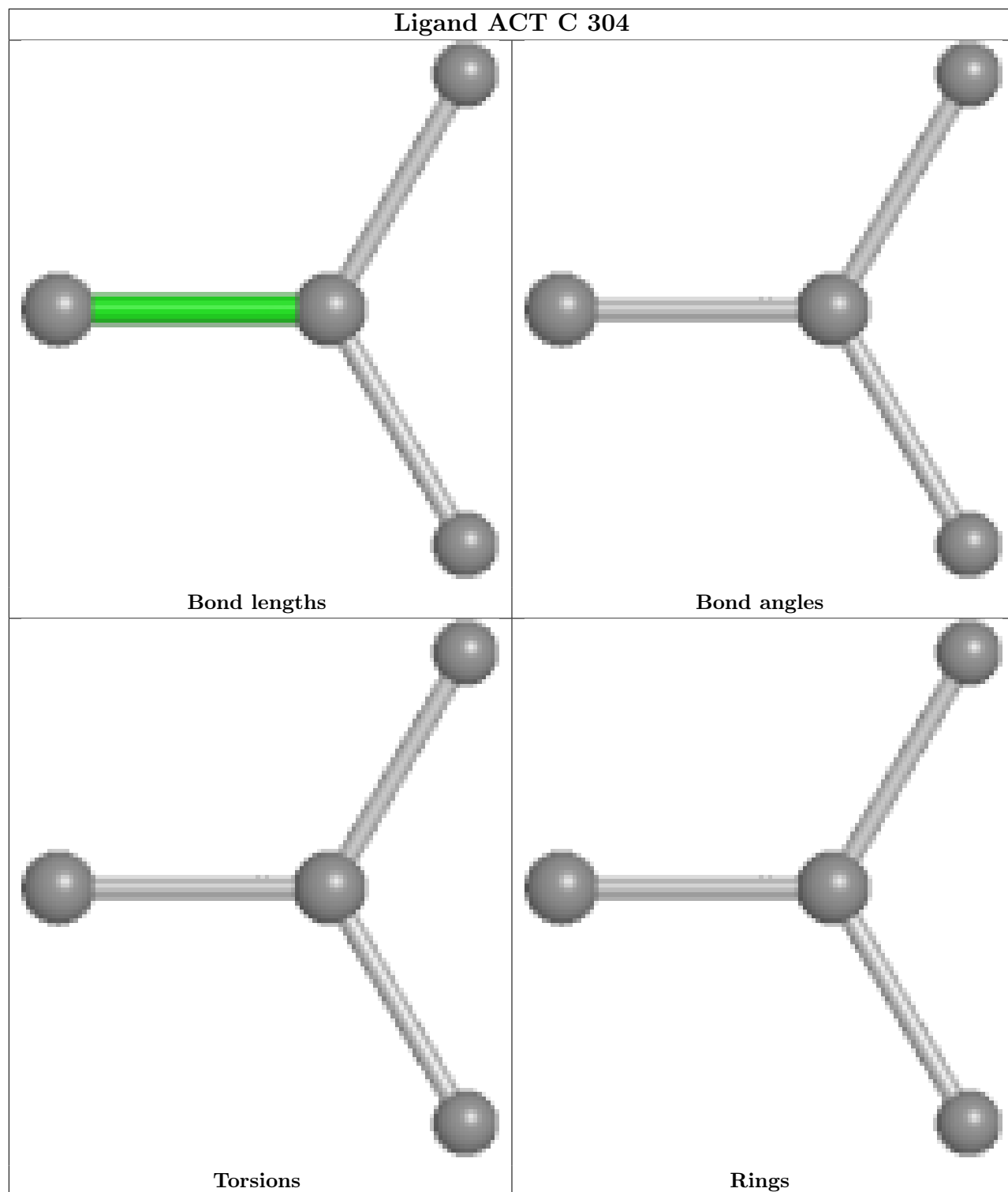


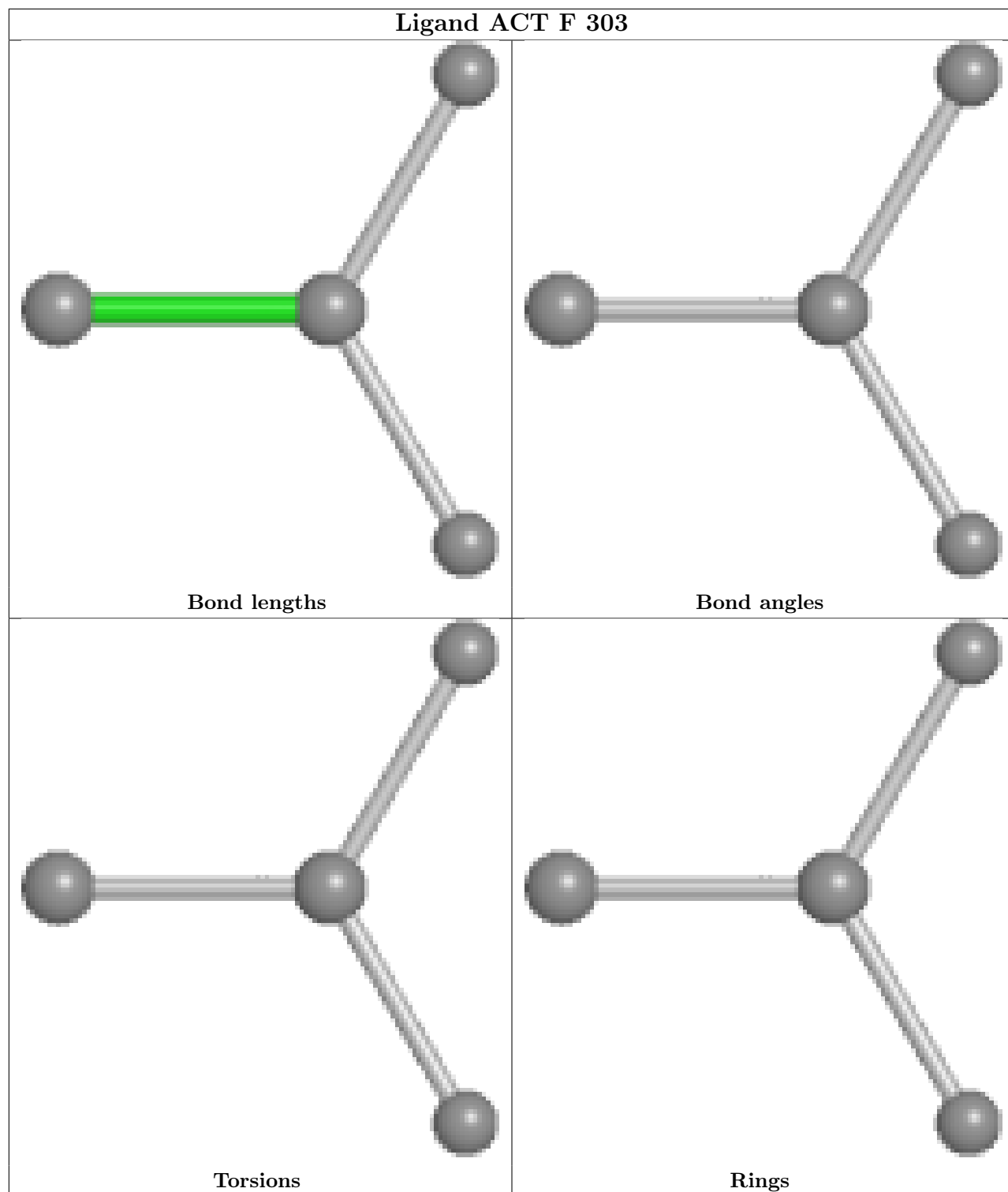


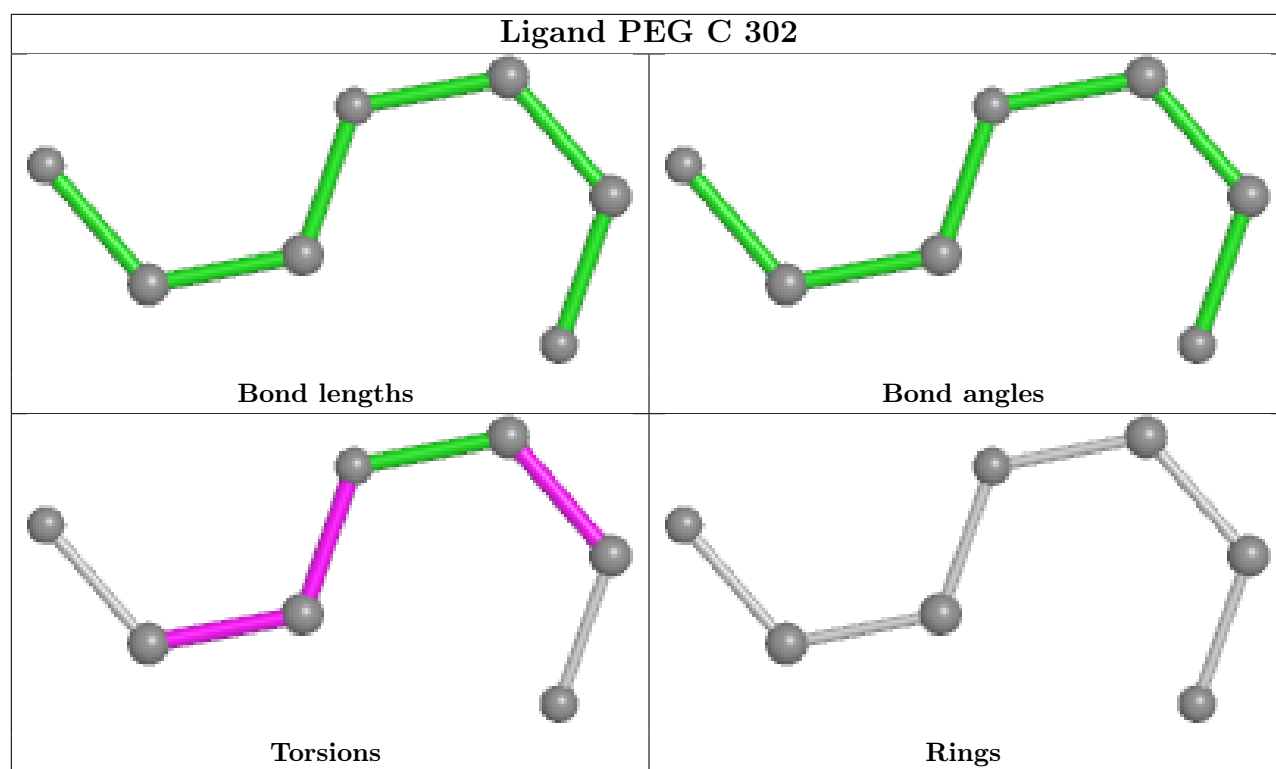












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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%)	-0.20	3 (1%) 82 84	30, 41, 61, 76	0
1	B	295/310 (95%)	-0.13	2 (0%) 87 89	31, 42, 61, 75	0
1	C	295/310 (95%)	-0.09	1 (0%) 94 94	33, 42, 61, 72	0
1	D	295/310 (95%)	-0.20	2 (0%) 87 89	34, 44, 61, 73	0
1	E	295/310 (95%)	-0.19	5 (1%) 70 73	34, 45, 63, 83	0
1	F	296/310 (95%)	-0.07	3 (1%) 82 84	32, 45, 64, 79	0
All	All	1771/1860 (95%)	-0.15	16 (0%) 84 86	30, 43, 62, 83	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	129	SER	2.8
1	E	87	HIS	2.7
1	F	98	GLU	2.6
1	B	98	GLU	2.6
1	A	267	GLU	2.6

### 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	D	166	14/15	0.83	0.17	37,44,65,69	0
1	KPI	C	166	14/15	0.85	0.18	35,39,63,68	0
1	KPI	A	166	14/15	0.86	0.17	30,39,62,63	0
1	KPI	F	166	14/15	0.87	0.16	33,42,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KPI	E	166	14/15	0.89	0.13	39,42,63,64	0
1	KPI	B	166	14/15	0.89	0.15	29,40,61,61	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

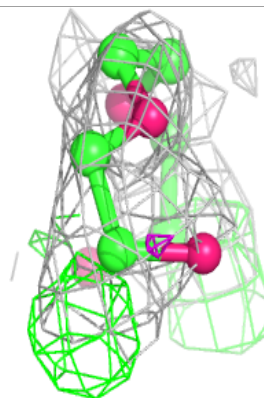
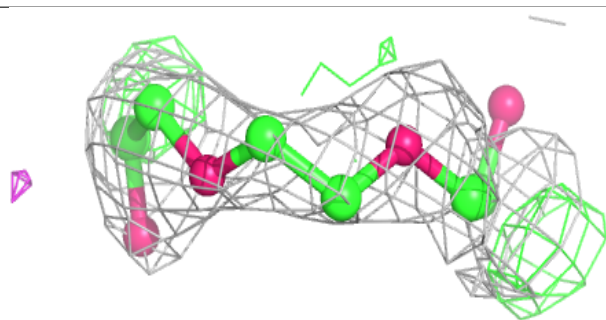
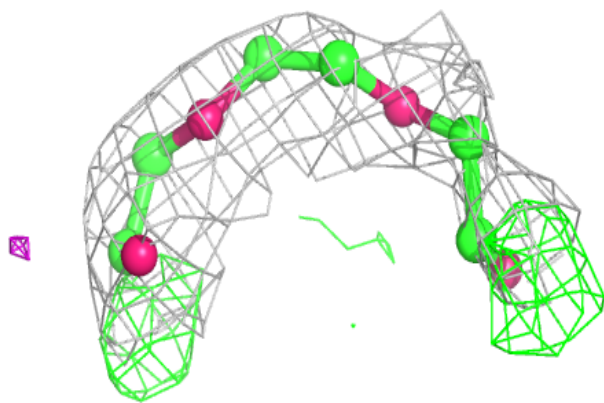
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	PGE	F	301	10/10	0.74	0.29	65,70,74,78	0
5	ACT	F	303	4/4	0.75	0.38	20,20,20,20	0
2	PGE	D	301	10/10	0.77	0.20	57,60,64,65	0
2	PGE	E	301	10/10	0.80	0.15	53,55,60,60	0
2	PGE	C	301	10/10	0.84	0.13	49,50,56,57	0
2	PGE	B	301	10/10	0.85	0.12	48,51,57,60	0
5	ACT	C	304	4/4	0.86	0.33	20,20,20,20	0
6	PEG	C	302	7/7	0.86	0.49	20,20,20,20	0
4	EDO	C	303	4/4	0.87	0.32	20,20,20,20	0
5	ACT	E	302	4/4	0.88	0.47	20,20,20,20	0
2	PGE	A	301	10/10	0.89	0.15	51,53,54,55	0
4	EDO	B	303	4/4	0.90	0.36	20,20,20,20	0
5	ACT	B	304	4/4	0.90	0.38	20,20,20,20	0
4	EDO	F	302	4/4	0.91	0.30	20,20,20,20	0
3	MG	A	302	1/1	0.92	0.25	30,30,30,30	0
4	EDO	D	302	4/4	0.92	0.39	20,20,20,20	0
4	EDO	B	302	4/4	0.94	0.29	20,20,20,20	0
3	MG	B	305	1/1	0.96	0.08	30,30,30,30	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.

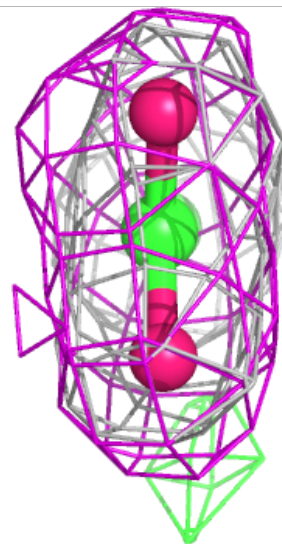
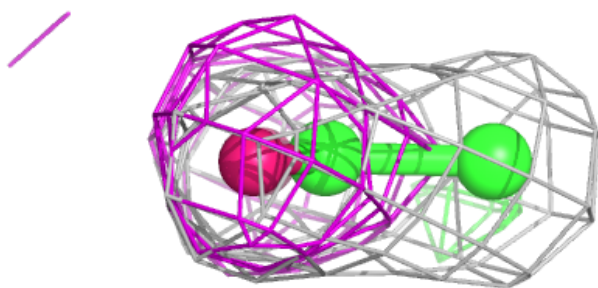
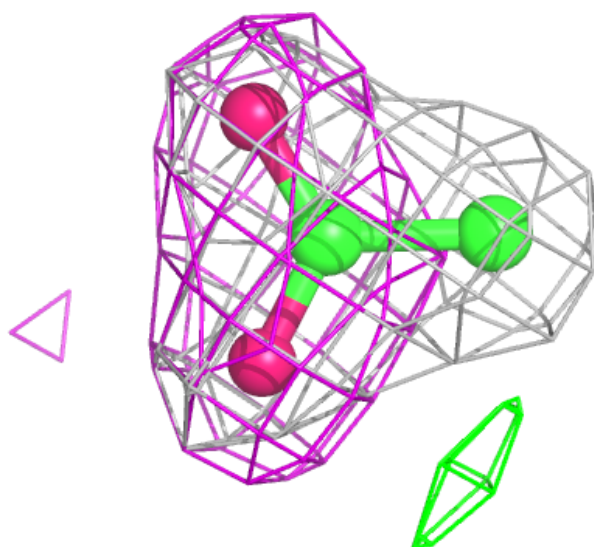
**Electron density around PGE F 301:**

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



**Electron density around ACT F 303:**

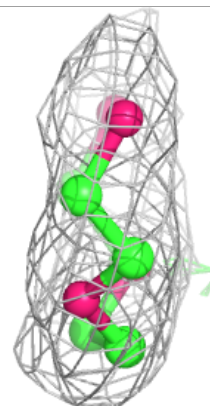
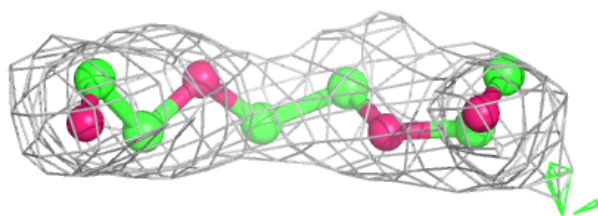
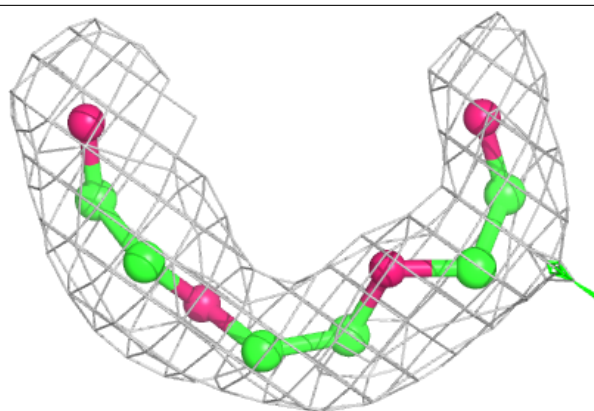
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



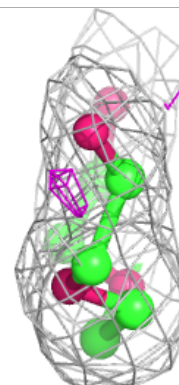
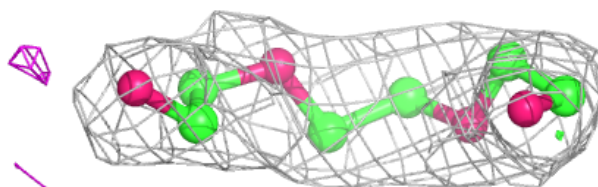
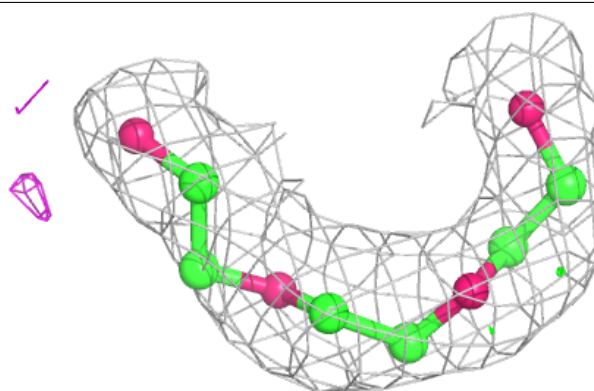


**Electron density around PGE D 301:**

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

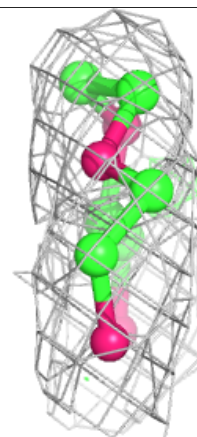
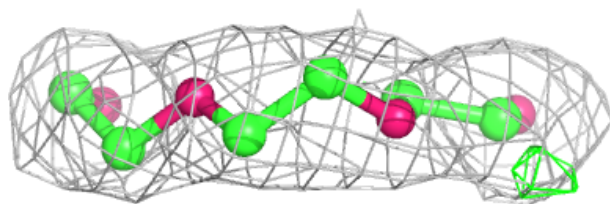
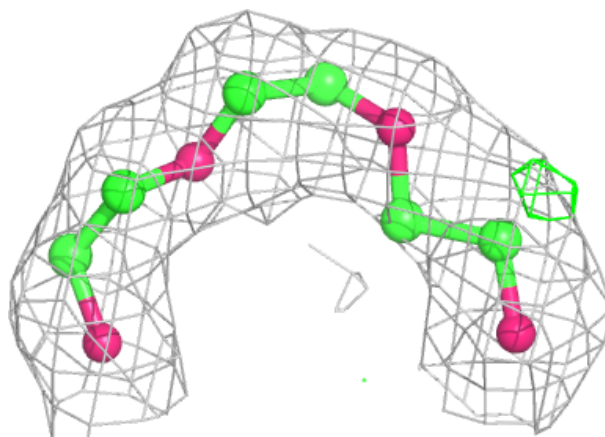
**Electron density around PGE E 301:**

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and green (positive)

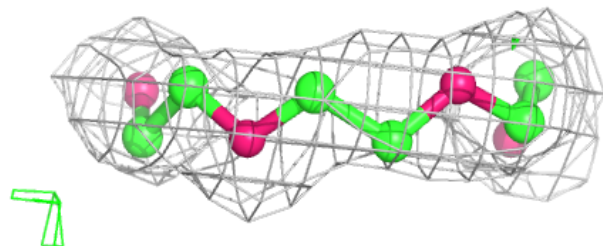
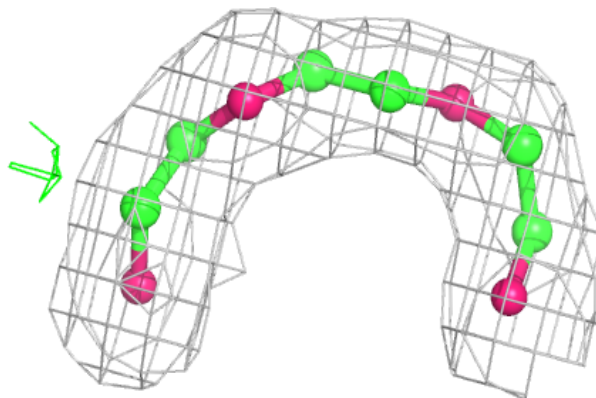


**Electron density around PGE C 301:**

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and green (positive)

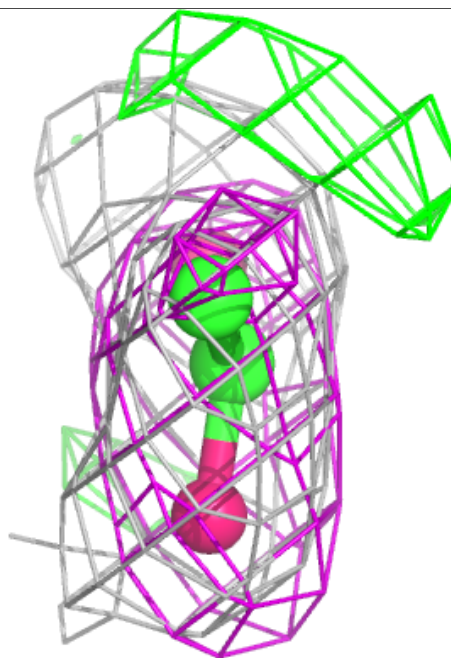
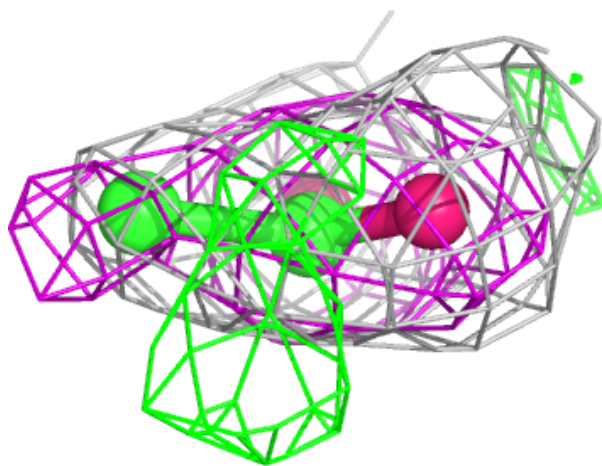
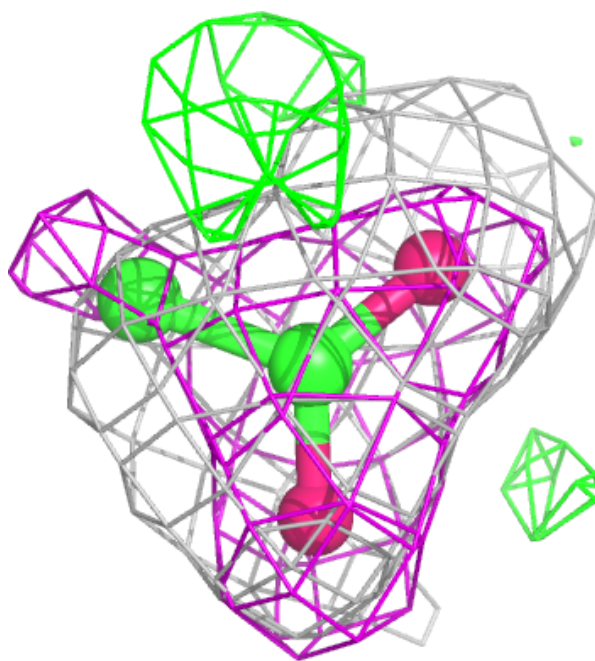
**Electron density around PGE B 301:**

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



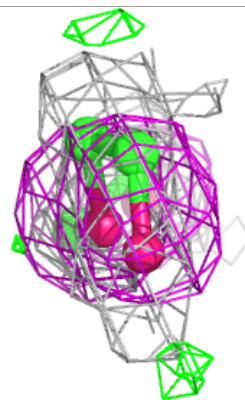
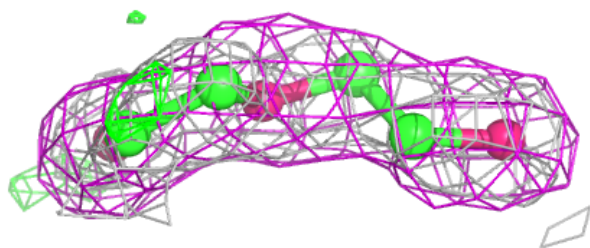
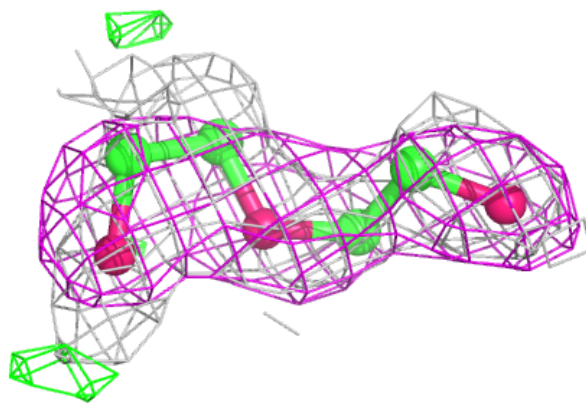
**Electron density around ACT C 304:**

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



**Electron density around PEG C 302:**

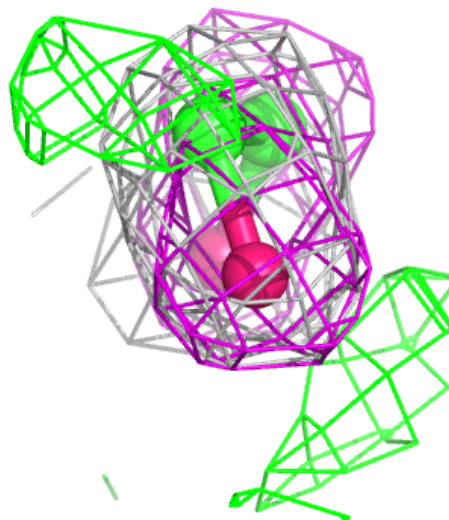
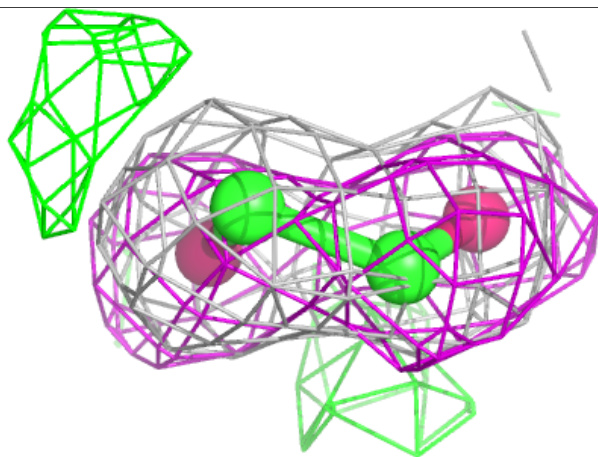
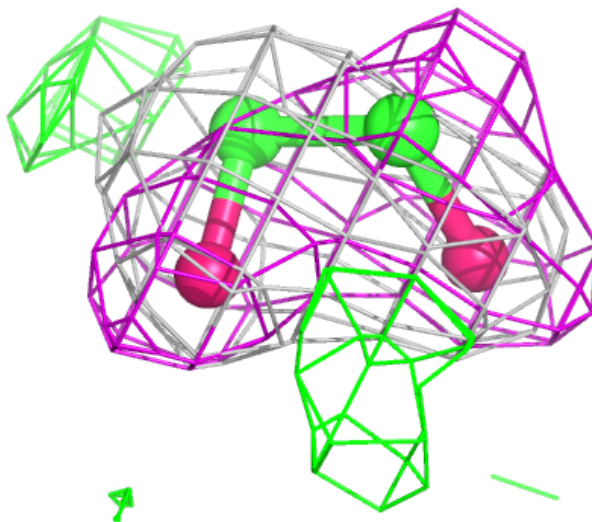
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





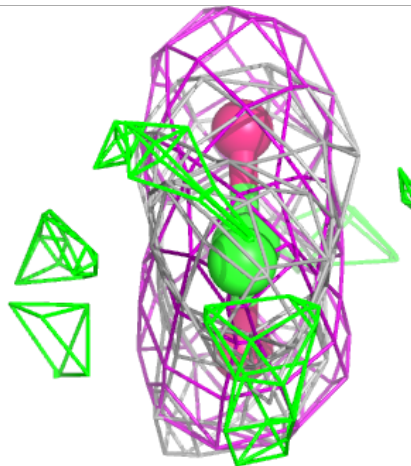
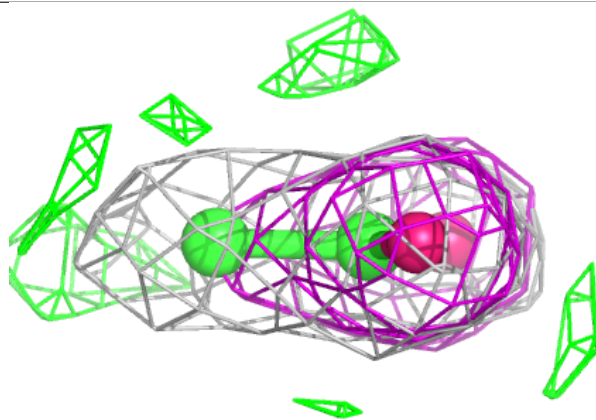
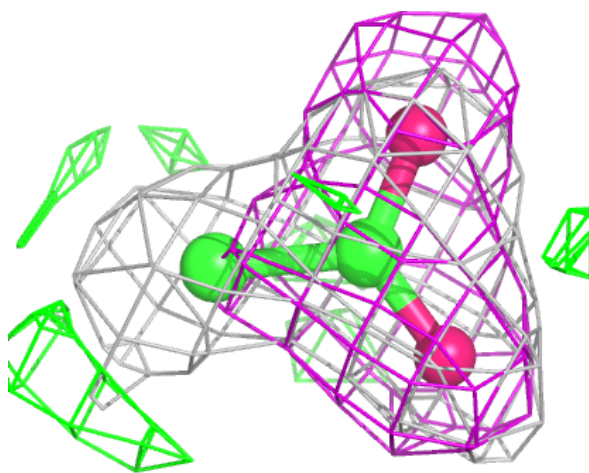
**Electron density around EDO C 303:**

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



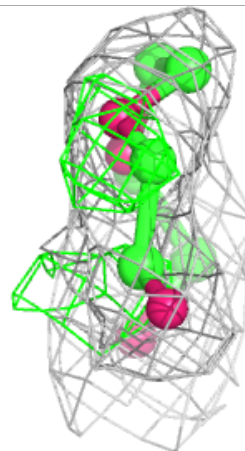
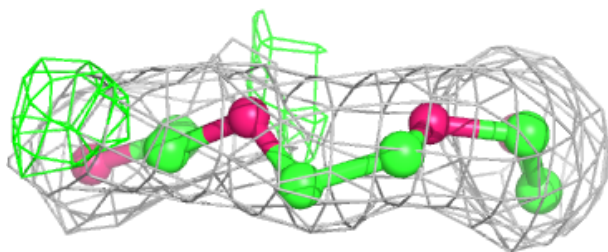
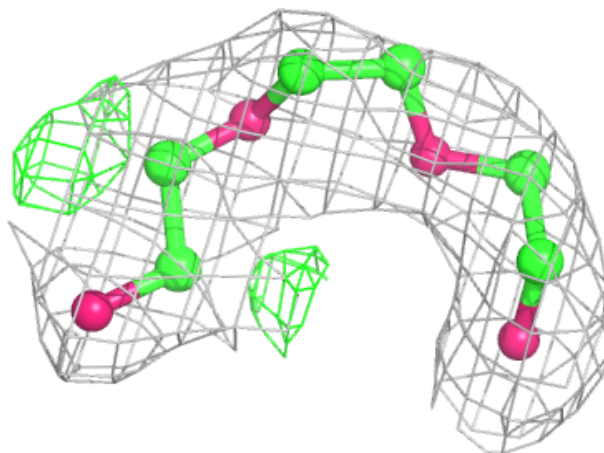
**Electron density around ACT E 302:**

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



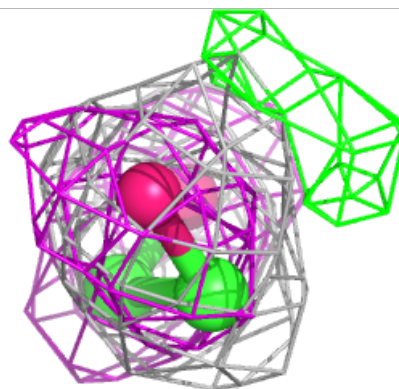
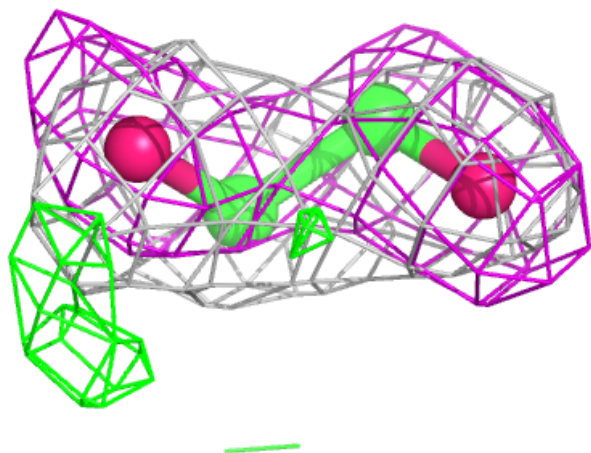
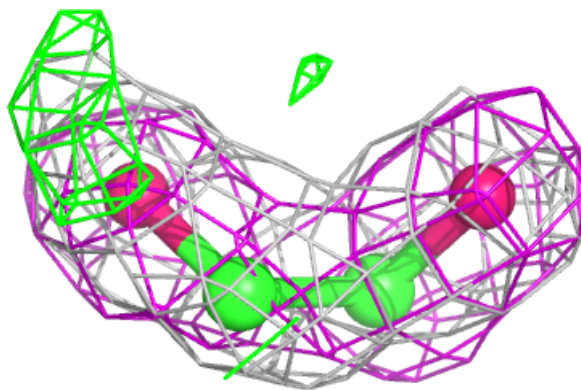
**Electron density around PGE A 301:**

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



**Electron density around EDO B 303:**

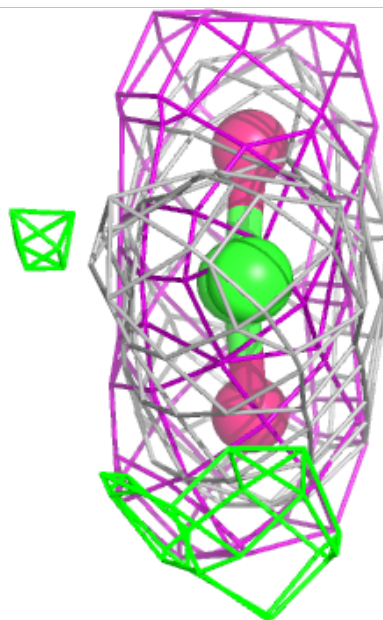
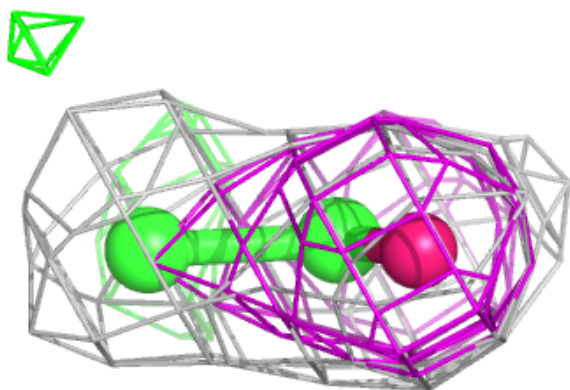
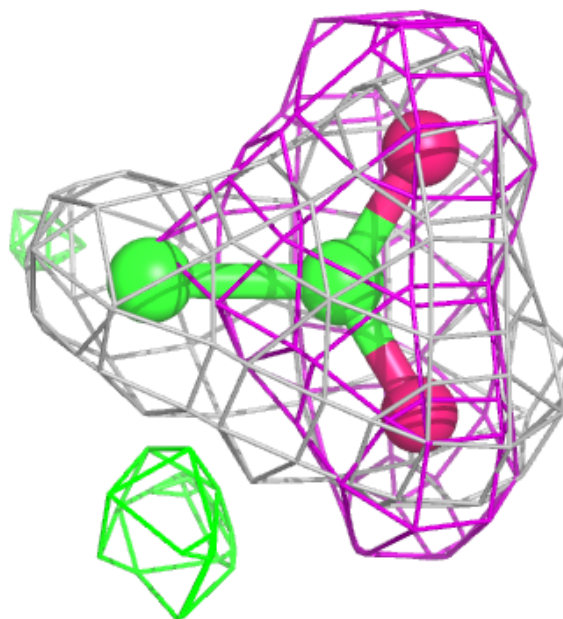
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





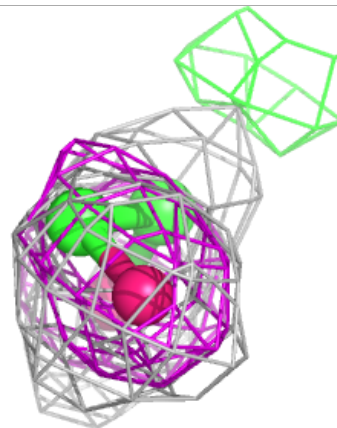
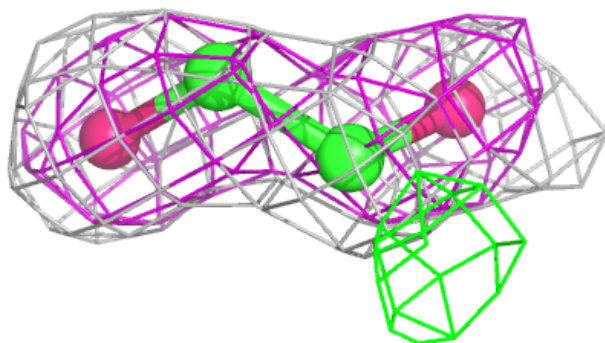
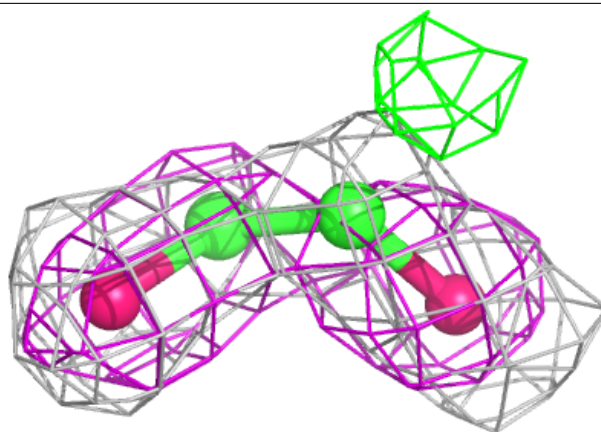
**Electron density around ACT B 304:**

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



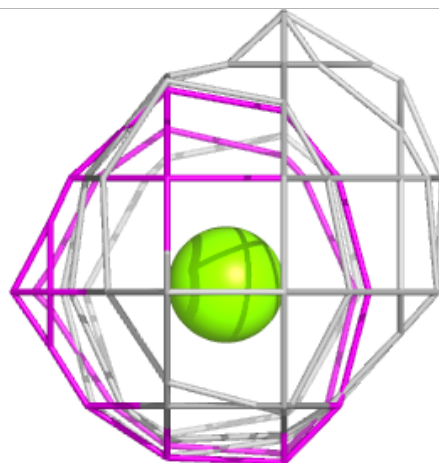
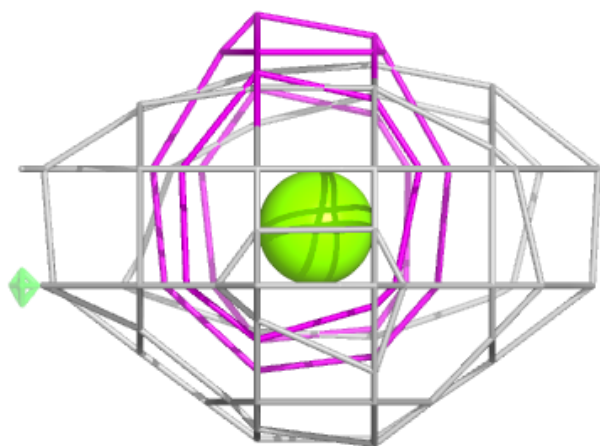
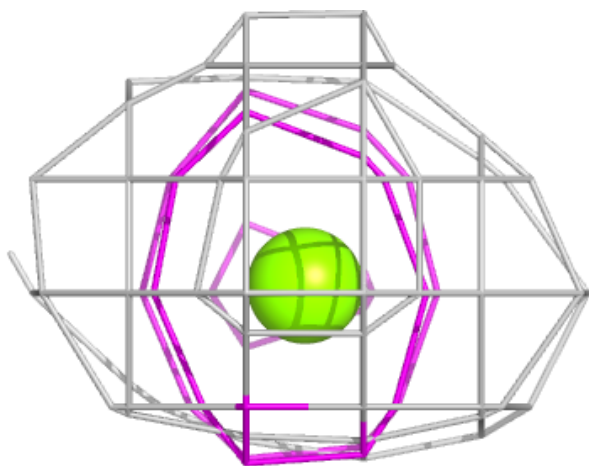
**Electron density around EDO F 302:**

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



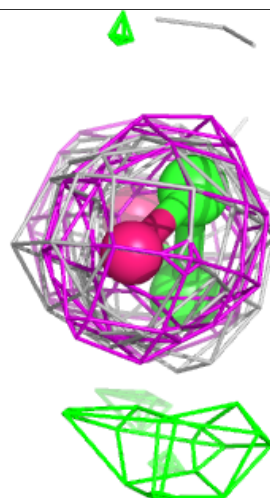
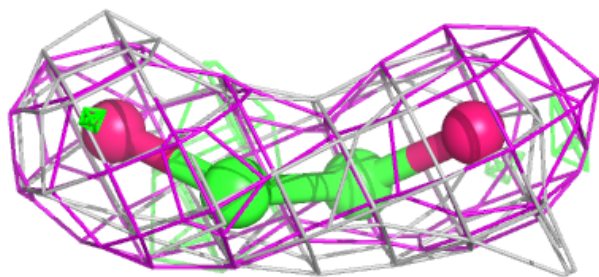
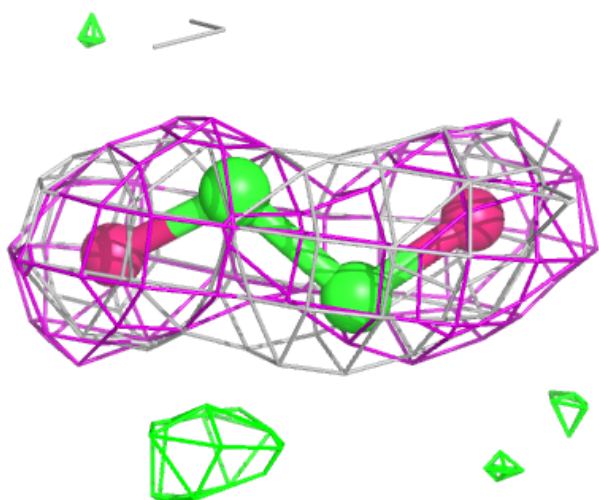
**Electron density around MG A 302:**

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



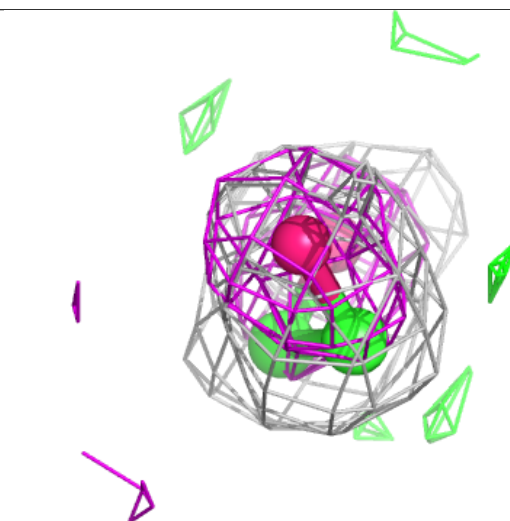
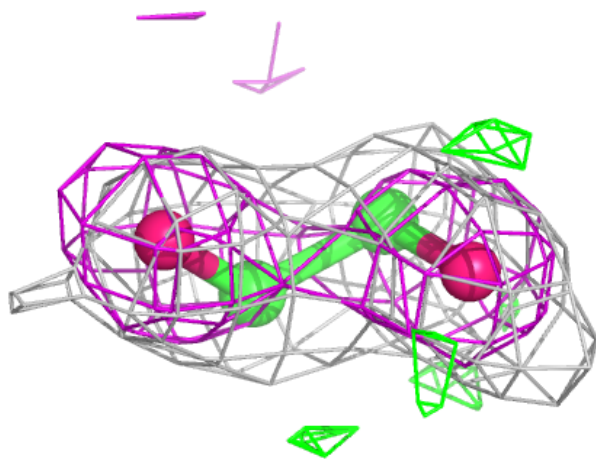
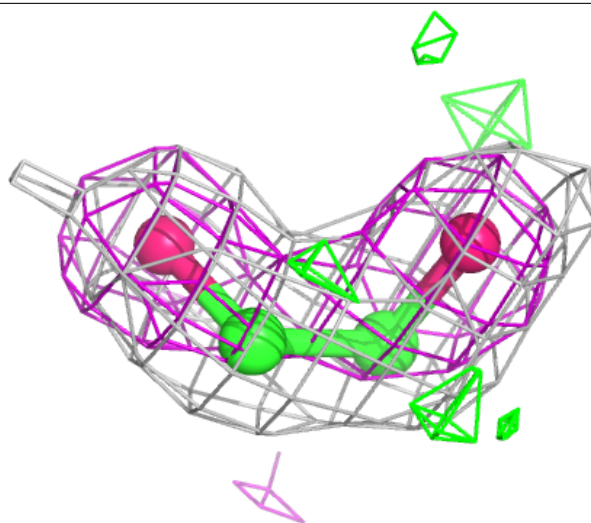
**Electron density around EDO D 302:**

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



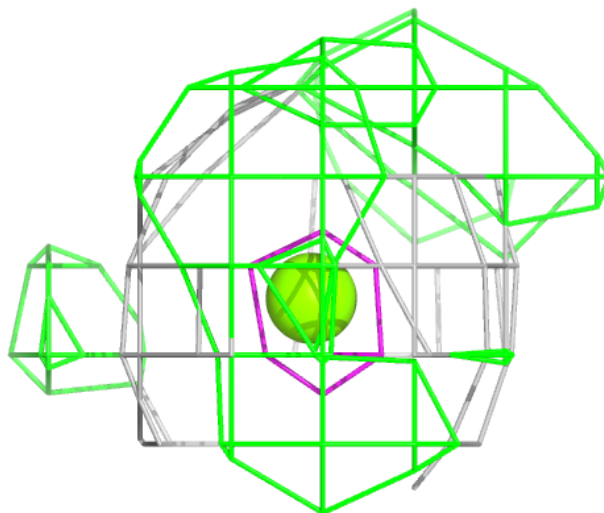
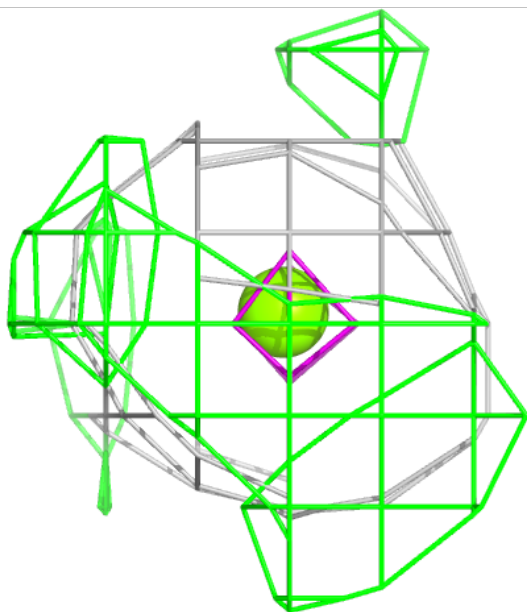
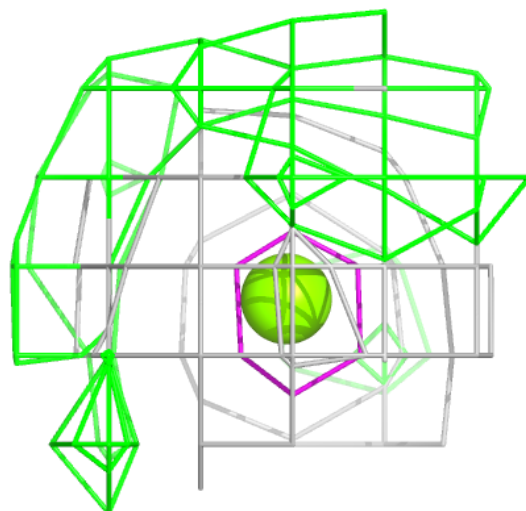
**Electron density around EDO B 302:**

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



**Electron density around MG 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.