



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2021 – 12:32 PM EDT

PDB ID : 7KKG
Title : Dihydrodipicolinate synthase (DHDPS) from C.jejuni, N84D mutant with pyruvate bound in the active site and L-lysine bound at the allosteric site
Authors : Saran, S.; Majdi Yazdi, M.; Sanders, D.A.R.
Deposited on : 2020-10-27
Resolution : 1.64 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

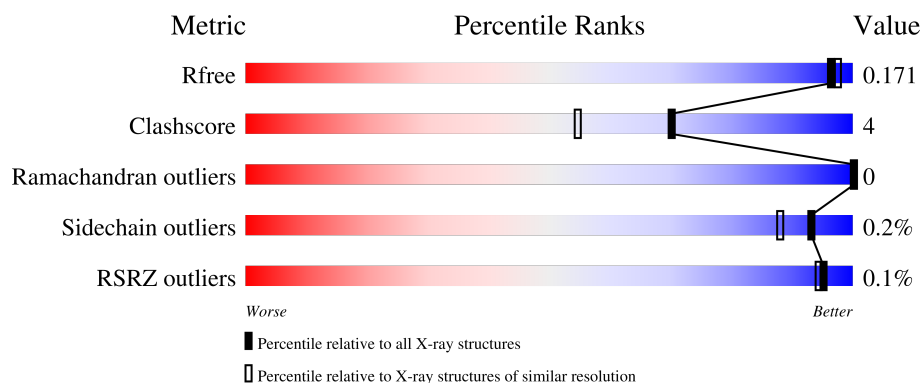
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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	
1	B	310	
1	C	310	
1	D	310	
1	E	310	

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Mol	Chain	Length	Quality of chain
1	F	310	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PG4	D	304	-	-	X	-
5	PEG	E	304	-	-	X	-
6	PGE	F	305	-	-	X	-
7	EDO	E	305	-	-	X	-
7	EDO	F	307	-	-	X	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 16387 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	297	Total	C	N	O	S	0	4	0
			2300	1459	384	444	13			
1	B	306	Total	C	N	O	S	0	4	0
			2374	1502	402	456	14			
1	C	295	Total	C	N	O	S	0	4	0
			2285	1449	380	443	13			
1	D	306	Total	C	N	O	S	0	5	0
			2380	1504	405	457	14			
1	E	296	Total	C	N	O	S	0	4	0
			2292	1455	383	441	13			
1	F	296	Total	C	N	O	S	0	5	0
			2295	1455	383	444	13			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9PPB4
A	-10	ARG	-	expression tag	UNP Q9PPB4
A	-9	GLY	-	expression tag	UNP Q9PPB4
A	-8	SER	-	expression tag	UNP Q9PPB4
A	-7	HIS	-	expression tag	UNP Q9PPB4
A	-6	HIS	-	expression tag	UNP Q9PPB4
A	-5	HIS	-	expression tag	UNP Q9PPB4
A	-4	HIS	-	expression tag	UNP Q9PPB4
A	-3	HIS	-	expression tag	UNP Q9PPB4
A	-2	HIS	-	expression tag	UNP Q9PPB4
A	-1	GLY	-	expression tag	UNP Q9PPB4
A	0	SER	-	expression tag	UNP Q9PPB4
A	84	ASP	ASN	engineered mutation	UNP Q9PPB4
B	-11	MET	-	expression tag	UNP Q9PPB4
B	-10	ARG	-	expression tag	UNP Q9PPB4
B	-9	GLY	-	expression tag	UNP Q9PPB4
B	-8	SER	-	expression tag	UNP Q9PPB4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP Q9PPB4
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4
B	84	ASP	ASN	engineered mutation	UNP Q9PPB4
C	-11	MET	-	expression tag	UNP Q9PPB4
C	-10	ARG	-	expression tag	UNP Q9PPB4
C	-9	GLY	-	expression tag	UNP Q9PPB4
C	-8	SER	-	expression tag	UNP Q9PPB4
C	-7	HIS	-	expression tag	UNP Q9PPB4
C	-6	HIS	-	expression tag	UNP Q9PPB4
C	-5	HIS	-	expression tag	UNP Q9PPB4
C	-4	HIS	-	expression tag	UNP Q9PPB4
C	-3	HIS	-	expression tag	UNP Q9PPB4
C	-2	HIS	-	expression tag	UNP Q9PPB4
C	-1	GLY	-	expression tag	UNP Q9PPB4
C	0	SER	-	expression tag	UNP Q9PPB4
C	84	ASP	ASN	engineered mutation	UNP Q9PPB4
D	-11	MET	-	expression tag	UNP Q9PPB4
D	-10	ARG	-	expression tag	UNP Q9PPB4
D	-9	GLY	-	expression tag	UNP Q9PPB4
D	-8	SER	-	expression tag	UNP Q9PPB4
D	-7	HIS	-	expression tag	UNP Q9PPB4
D	-6	HIS	-	expression tag	UNP Q9PPB4
D	-5	HIS	-	expression tag	UNP Q9PPB4
D	-4	HIS	-	expression tag	UNP Q9PPB4
D	-3	HIS	-	expression tag	UNP Q9PPB4
D	-2	HIS	-	expression tag	UNP Q9PPB4
D	-1	GLY	-	expression tag	UNP Q9PPB4
D	0	SER	-	expression tag	UNP Q9PPB4
D	84	ASP	ASN	engineered mutation	UNP Q9PPB4
E	-11	MET	-	expression tag	UNP Q9PPB4
E	-10	ARG	-	expression tag	UNP Q9PPB4
E	-9	GLY	-	expression tag	UNP Q9PPB4
E	-8	SER	-	expression tag	UNP Q9PPB4
E	-7	HIS	-	expression tag	UNP Q9PPB4
E	-6	HIS	-	expression tag	UNP Q9PPB4
E	-5	HIS	-	expression tag	UNP Q9PPB4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q9PPB4
E	-3	HIS	-	expression tag	UNP Q9PPB4
E	-2	HIS	-	expression tag	UNP Q9PPB4
E	-1	GLY	-	expression tag	UNP Q9PPB4
E	0	SER	-	expression tag	UNP Q9PPB4
E	84	ASP	ASN	engineered mutation	UNP Q9PPB4
F	-11	MET	-	expression tag	UNP Q9PPB4
F	-10	ARG	-	expression tag	UNP Q9PPB4
F	-9	GLY	-	expression tag	UNP Q9PPB4
F	-8	SER	-	expression tag	UNP Q9PPB4
F	-7	HIS	-	expression tag	UNP Q9PPB4
F	-6	HIS	-	expression tag	UNP Q9PPB4
F	-5	HIS	-	expression tag	UNP Q9PPB4
F	-4	HIS	-	expression tag	UNP Q9PPB4
F	-3	HIS	-	expression tag	UNP Q9PPB4
F	-2	HIS	-	expression tag	UNP Q9PPB4
F	-1	GLY	-	expression tag	UNP Q9PPB4
F	0	SER	-	expression tag	UNP Q9PPB4
F	84	ASP	ASN	engineered mutation	UNP Q9PPB4

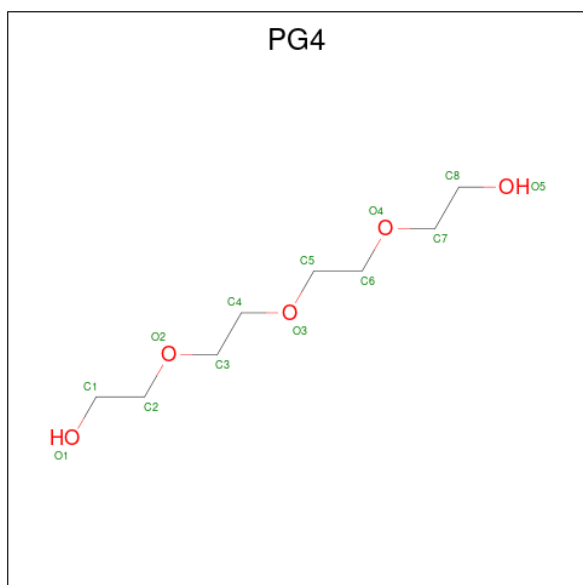
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	4	Total Mg 4 4	0	0
2	C	8	Total Mg 8 8	0	0
2	D	3	Total Mg 3 3	0	0
2	E	2	Total Mg 2 2	0	0
2	F	3	Total Mg 3 3	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	C	2	Total	Na	0	0
			2	2		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



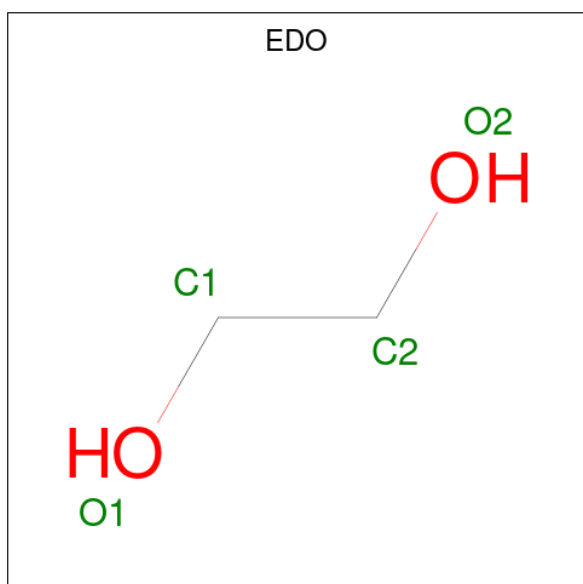
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		
5	E	1	Total	C	O	0	0
			7	4	3		
5	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄) (labeled as "Ligand of Interest" by depositor).



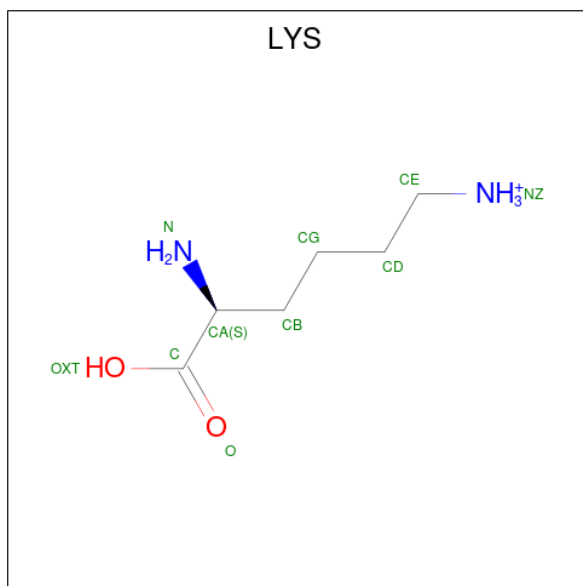
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 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
8	A	1	Total C N O 10 6 2 2	0	0
8	B	1	Total C N O 10 6 2 2	0	0

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

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



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

- Molecule 10 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
10	F	1	Total	C	O	0	0
			4	2	2		
10	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	409	Total	O	0	0
			409	409		
11	B	389	Total	O	0	0
			389	389		
11	C	376	Total	O	0	0
			376	376		
11	D	378	Total	O	0	0
			378	378		
11	E	334	Total	O	0	0
			334	334		
11	F	313	Total	O	0	0
			313	313		

3 Residue-property plots [i](#)

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

- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain A: 



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain B: 



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain C: 



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain D: 




- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain E: 



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	85.67Å 225.73Å 200.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.88 – 1.64 49.27 – 1.64	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.88-1.64) 98.8 (49.27-1.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.34 (at 1.64Å)	Xtriage
Refinement program	PHENIX dev_2398	Depositor
R, R_{free}	0.138 , 0.169 0.140 , 0.171	Depositor DCC
R_{free} test set	11683 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	12.2	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16387	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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, PG4, NA, GOL, KPI, MG, PGE, PEG, 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	0.60	0/2344	0.71	0/3166
1	B	0.56	0/2425	0.71	0/3276
1	C	0.59	0/2330	0.70	0/3148
1	D	0.67	0/2435	0.76	2/3289 (0.1%)
1	E	0.55	0/2336	0.69	0/3155
1	F	0.59	0/2344	0.71	0/3166
All	All	0.59	0/14214	0.71	2/19200 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	216	ASP	CB-CG-OD1	11.52	128.67	118.30
1	D	216	ASP	CB-CG-OD2	-5.68	113.18	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2300	0	2340	15	0
1	B	2374	0	2386	13	0
1	C	2285	0	2309	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2380	0	2393	16	0
1	E	2292	0	2336	18	0
1	F	2295	0	2331	27	0
2	A	1	0	0	0	0
2	B	4	0	0	0	0
2	C	8	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
2	F	3	0	0	0	0
3	A	1	0	0	0	0
3	C	2	0	0	0	0
4	A	13	0	18	3	0
4	B	13	0	18	0	0
4	D	13	0	18	10	0
5	A	7	0	10	0	0
5	B	7	0	10	0	0
5	C	7	0	10	0	0
5	D	7	0	10	0	0
5	E	14	0	20	4	0
5	F	7	0	10	0	0
6	A	10	0	14	1	0
6	C	20	0	28	2	0
6	F	10	0	14	7	0
7	A	8	0	12	2	0
7	C	8	0	12	4	0
7	E	12	0	18	9	0
7	F	8	0	10	12	0
8	A	10	0	12	0	0
8	B	10	0	12	0	0
8	C	10	0	12	0	0
8	D	10	0	12	0	0
8	E	10	0	12	0	0
8	F	10	0	12	0	0
9	B	6	0	8	1	0
10	F	8	0	6	0	0
11	A	409	0	0	3	0
11	B	389	0	0	2	0
11	C	376	0	0	3	0
11	D	378	0	0	3	0
11	E	334	0	0	3	0
11	F	313	0	0	3	0
All	All	16387	0	14413	104	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 (104) 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:46:GLY:H	7:F:307:EDO:H12	1.13	1.10
1:F:12:ALA:HA	7:F:307:EDO:H22	1.42	0.98
1:D:154:LYS:HZ2	4:D:304:PG4:H41	1.31	0.94
1:F:46:GLY:H	7:F:307:EDO:C1	1.82	0.92
1:F:46:GLY:N	7:F:307:EDO:H12	1.88	0.87
1:F:154:LYS:HZ2	6:F:305:PGE:H32	1.43	0.81
1:F:12:ALA:CA	7:F:307:EDO:H22	2.11	0.79
1:B:142:ARG:HD3	1:E:113[B]:LYS:HE3	1.69	0.74
1:A:166:KPI:H1A	11:A:528:HOH:O	1.87	0.74
1:B:166:KPI:H1A	11:B:455:HOH:O	1.87	0.74
7:E:305:EDO:H11	11:E:450:HOH:O	1.90	0.71
1:A:150:ASP:HB3	11:A:715:HOH:O	1.89	0.71
1:E:113[B]:LYS:HE2	11:E:464:HOH:O	1.90	0.71
1:E:267:GLU:HB3	7:E:305:EDO:H12	1.73	0.70
1:F:43:VAL:O	7:F:307:EDO:H11	1.93	0.69
1:F:166:KPI:H1A	11:F:438:HOH:O	1.94	0.68
1:D:154:LYS:NZ	4:D:304:PG4:H62	2.09	0.68
1:D:166:KPI:H1A	11:D:516:HOH:O	1.92	0.68
1:E:154:LYS:HZ1	5:E:304:PEG:H12	1.58	0.67
1:B:142:ARG:HD3	1:E:113[B]:LYS:CE	2.25	0.66
1:E:154:LYS:HZ2	5:E:304:PEG:H32	1.61	0.66
1:A:113[B]:LYS:NZ	11:A:401:HOH:O	2.29	0.65
1:F:43:VAL:HG12	7:F:307:EDO:O2	1.96	0.65
1:C:94:LYS:HE2	1:C:129:SER:HB2	1.79	0.65
1:D:154:LYS:HZ2	4:D:304:PG4:C4	2.08	0.64
1:C:245:LYS:HG3	7:C:314:EDO:H22	1.80	0.62
1:C:65:ILE:HA	7:C:315:EDO:H12	1.82	0.62
1:C:142[B]:ARG:NE	11:C:403:HOH:O	2.33	0.62
1:B:76:LYS:HE3	11:B:646:HOH:O	2.00	0.61
1:A:292:LYS:HZ1	4:A:303:PG4:H11	1.68	0.58
1:C:150:ASP:HB3	6:C:313:PGE:H62	1.85	0.57
1:F:154:LYS:HZ2	6:F:305:PGE:H1	1.68	0.57
1:F:43:VAL:O	7:F:307:EDO:C1	2.53	0.56
1:E:32:LYS:HE3	1:E:36:GLU:OE2	2.06	0.56
1:D:154:LYS:HZ3	4:D:304:PG4:H62	1.72	0.55
1:F:12:ALA:HB1	7:F:307:EDO:H21	1.88	0.55
1:A:21:LYS:HZ2	7:A:307:EDO:H21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:ASN:HB3	11:C:401:HOH:O	2.06	0.55
1:E:166:KPI:H1A	11:E:476:HOH:O	2.05	0.55
1:D:94:LYS:HE2	1:D:129:SER:HB2	1.89	0.54
1:F:154:LYS:NZ	6:F:305:PGE:H52	2.24	0.53
1:C:245:LYS:CG	7:C:314:EDO:H22	2.39	0.53
1:A:292:LYS:HE2	4:A:303:PG4:H32	1.91	0.53
1:E:154:LYS:NZ	5:E:304:PEG:H12	2.25	0.52
1:D:154:LYS:HD2	4:D:304:PG4:H42	1.92	0.52
1:D:154:LYS:NZ	4:D:304:PG4:H22	2.25	0.52
1:F:154:LYS:NZ	6:F:305:PGE:H1	2.25	0.51
1:A:21:LYS:NZ	7:A:307:EDO:H21	2.25	0.51
1:E:26:SER:CB	7:E:305:EDO:H21	2.41	0.51
1:D:154:LYS:HZ2	4:D:304:PG4:H62	1.76	0.51
1:D:151:THR:OG1	4:D:304:PG4:H31	2.11	0.50
1:C:241:TYR:OH	7:C:314:EDO:H21	2.12	0.50
1:F:154:LYS:HD2	6:F:305:PGE:H5	1.94	0.50
1:F:142[B]:ARG:HD2	11:F:414:HOH:O	2.11	0.49
1:F:94:LYS:HE2	1:F:129:SER:HB2	1.94	0.49
1:F:45:VAL:N	7:F:307:EDO:H12	2.28	0.49
1:F:235:LYS:HG2	11:F:646:HOH:O	2.13	0.48
1:F:32:LYS:NZ	1:F:36:GLU:OE2	2.38	0.48
1:B:4:ASN:HB2	1:B:133:PRO:HG3	1.96	0.48
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.96	0.48
1:E:292:LYS:HD3	7:E:307:EDO:H22	1.97	0.47
1:C:124:LYS:HE2	1:C:128:GLN:HE22	1.79	0.47
1:C:232[B]:GLU:CD	11:C:401:HOH:O	2.52	0.47
1:B:45:VAL:HG12	1:B:51[B]:SER:HB2	1.95	0.47
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.96	0.47
1:A:45:VAL:HG12	1:A:51[B]:SER:HB2	1.97	0.46
1:D:45:VAL:HG12	1:D:51[B]:SER:HB2	1.98	0.46
1:C:124:LYS:HE2	1:C:128:GLN:NE2	2.31	0.45
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.98	0.45
1:F:107:VAL:HA	1:F:137:TYR:HB3	1.97	0.45
1:A:254:ILE:HB	1:A:255:PRO:HD3	1.98	0.45
1:D:-7:HIS:N	11:D:414:HOH:O	2.48	0.45
1:D:74:LYS:HD3	11:D:405:HOH:O	2.16	0.44
1:B:294:LYS:HG2	9:B:308:GOL:H31	2.00	0.44
1:E:26:SER:OG	7:E:305:EDO:H21	2.16	0.44
1:E:267:GLU:H	7:E:305:EDO:C2	2.30	0.44
1:E:242:ASN:CB	7:E:307:EDO:H21	2.47	0.44
1:A:252:ASN:ND2	1:A:253:PRO:HA	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:LYS:HZ2	4:D:304:PG4:H22	1.82	0.44
1:F:57[B]:GLU:OE1	7:F:306:EDO:H11	2.18	0.44
1:E:242:ASN:HB3	7:E:307:EDO:H21	2.01	0.43
1:B:35:ILE:HG12	1:B:75:VAL:HG21	2.01	0.43
1:B:39:ILE:HD12	1:B:39:ILE:HG23	1.75	0.43
1:B:120:TYR:CE2	1:B:124:LYS:HE2	2.53	0.43
1:E:181:HIS:CD2	7:E:306:EDO:H11	2.54	0.43
1:F:43:VAL:CG1	7:F:307:EDO:O2	2.64	0.43
1:C:45:VAL:HG12	1:C:51[B]:SER:HB2	2.01	0.43
1:E:154:LYS:NZ	5:E:304:PEG:H32	2.31	0.43
1:A:292:LYS:NZ	4:A:303:PG4:H11	2.32	0.42
1:C:161:ASN:OD1	1:C:161:ASN:N	2.49	0.42
1:F:150:ASP:HB3	6:F:305:PGE:H12	2.02	0.42
1:B:107:VAL:HA	1:B:137:TYR:HB3	2.02	0.42
1:C:154:LYS:NZ	6:C:313:PGE:H6	2.35	0.41
1:F:140:PRO:HG3	1:F:146:GLU:OE1	2.20	0.41
4:D:304:PG4:H41	4:D:304:PG4:H22	1.74	0.41
1:F:154:LYS:NZ	6:F:305:PGE:H32	2.23	0.41
1:A:39:ILE:HD12	1:A:39:ILE:HG23	1.80	0.41
1:D:216:ASP:OD2	1:D:296:LYS:HE2	2.21	0.41
1:B:254:ILE:HB	1:B:255:PRO:HD3	2.02	0.40
1:A:278:PRO:O	6:A:305:PGE:H6	2.22	0.40
1:A:137:TYR:CD1	1:A:166:KPI:HD	2.57	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	298/310 (96%)	293 (98%)	5 (2%)	0	100	100
1	B	307/310 (99%)	301 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	296/310 (96%)	291 (98%)	5 (2%)	0	100	100
1	D	308/310 (99%)	300 (97%)	8 (3%)	0	100	100
1	E	297/310 (96%)	291 (98%)	6 (2%)	0	100	100
1	F	298/310 (96%)	292 (98%)	6 (2%)	0	100	100
All	All	1804/1860 (97%)	1768 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	253/260 (97%)	253 (100%)	0	100	100
1	B	261/260 (100%)	260 (100%)	1 (0%)	91	84
1	C	251/260 (96%)	251 (100%)	0	100	100
1	D	262/260 (101%)	262 (100%)	0	100	100
1	E	252/260 (97%)	252 (100%)	0	100	100
1	F	253/260 (97%)	251 (99%)	2 (1%)	81	68
All	All	1532/1560 (98%)	1529 (100%)	3 (0%)	93	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	47	THR
1	F	47	THR
1	F	97	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	KPI	F	166	1	10,13,14	1.02	0	6,15,17	3.14	2 (33%)
1	KPI	C	166	1	10,13,14	2.60	4 (40%)	6,15,17	3.67	2 (33%)
1	KPI	D	166	1	10,13,14	1.29	1 (10%)	6,15,17	2.86	2 (33%)
1	KPI	B	166	1	10,13,14	1.41	2 (20%)	6,15,17	2.68	2 (33%)
1	KPI	E	166	1	10,13,14	1.41	2 (20%)	6,15,17	2.98	2 (33%)
1	KPI	A	166	1	10,13,14	1.25	1 (10%)	6,15,17	2.50	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	F	166	1	-	0/9/14/16	-
1	KPI	C	166	1	-	1/9/14/16	-
1	KPI	D	166	1	-	0/9/14/16	-
1	KPI	B	166	1	-	0/9/14/16	-
1	KPI	E	166	1	-	0/9/14/16	-
1	KPI	A	166	1	-	0/9/14/16	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	KPI	CX2-CX1	5.60	1.60	1.52
1	C	166	KPI	C1-CX1	4.74	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	166	KPI	C1-CX1	3.25	1.56	1.50
1	B	166	KPI	C1-CX1	3.22	1.56	1.50
1	E	166	KPI	C1-CX1	3.05	1.56	1.50
1	A	166	KPI	C1-CX1	3.01	1.56	1.50
1	C	166	KPI	CX1-NZ	-2.24	1.23	1.29
1	C	166	KPI	CA-N	-2.21	1.41	1.48
1	B	166	KPI	CA-N	-2.15	1.41	1.48
1	E	166	KPI	CA-N	-2.11	1.41	1.48

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	166	KPI	C1-CX1-CX2	7.30	126.01	117.92
1	B	166	KPI	CE-NZ-CX1	5.99	137.88	121.77
1	F	166	KPI	CE-NZ-CX1	5.93	137.71	121.77
1	E	166	KPI	CE-NZ-CX1	5.66	137.00	121.77
1	A	166	KPI	CE-NZ-CX1	5.52	136.62	121.77
1	D	166	KPI	CE-NZ-CX1	5.13	135.57	121.77
1	C	166	KPI	CE-NZ-CX1	4.90	134.96	121.77
1	F	166	KPI	C1-CX1-CX2	-4.73	112.68	117.92
1	D	166	KPI	C1-CX1-CX2	-4.48	112.96	117.92
1	E	166	KPI	C1-CX1-CX2	-4.36	113.09	117.92
1	B	166	KPI	C1-CX1-CX2	-2.40	115.26	117.92
1	A	166	KPI	C1-CX1-CX2	-2.09	115.61	117.92

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	166	KPI	CD-CE-NZ-CX1

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	166	KPI	1	0
1	D	166	KPI	1	0
1	B	166	KPI	1	0
1	E	166	KPI	1	0
1	A	166	KPI	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 24 are monoatomic - leaving 32 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	$\# Z > 2$
10	ACT	F	310	-	1,3,3	1.28	0	0,3,3	-	-
8	LYS	A	308	-	5,9,9	0.97	0	4,10,10	0.70	0
5	PEG	D	305	-	6,6,6	0.46	0	5,5,5	0.43	0
5	PEG	F	304	-	6,6,6	0.48	0	5,5,5	0.34	0
4	PG4	D	304	-	12,12,12	0.49	0	11,11,11	0.79	0
6	PGE	C	312	-	9,9,9	0.30	0	8,8,8	0.23	0
10	ACT	F	309	-	1,3,3	1.39	0	0,3,3	-	-
8	LYS	D	306	-	5,9,9	0.68	0	4,10,10	0.78	0
7	EDO	E	305	-	3,3,3	0.37	0	2,2,2	0.13	0
7	EDO	F	307	-	3,3,3	1.41	0	2,2,2	1.40	0
4	PG4	A	303	-	12,12,12	0.54	0	11,11,11	0.37	0
6	PGE	A	305	-	9,9,9	0.33	0	8,8,8	0.36	0
6	PGE	F	305	-	9,9,9	0.30	0	8,8,8	0.55	0
5	PEG	B	306	-	6,6,6	0.48	0	5,5,5	0.32	0
8	LYS	C	316	-	5,9,9	0.89	0	4,10,10	0.82	0
8	LYS	F	308	-	5,9,9	0.69	0	4,10,10	0.59	0
5	PEG	A	304	-	6,6,6	0.48	0	5,5,5	0.62	0
6	PGE	C	313	-	9,9,9	0.35	0	8,8,8	0.51	0
7	EDO	E	306	-	3,3,3	0.47	0	2,2,2	0.33	0
4	PG4	B	305	-	12,12,12	0.49	0	11,11,11	0.31	0
8	LYS	E	308	-	5,9,9	0.54	0	4,10,10	0.99	0
7	EDO	C	315	-	3,3,3	0.53	0	2,2,2	0.24	0
5	PEG	E	304	-	6,6,6	0.48	0	5,5,5	0.48	0
8	LYS	B	307	-	5,9,9	0.81	0	4,10,10	0.75	0
9	GOL	B	308	-	5,5,5	0.33	0	5,5,5	0.34	0
7	EDO	C	314	-	3,3,3	0.36	0	2,2,2	0.73	0
5	PEG	C	311	-	6,6,6	0.46	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	A	307	-	3,3,3	0.31	0	2,2,2	0.55	0
7	EDO	F	306	-	3,3,3	0.39	0	2,2,2	0.45	0
7	EDO	E	307	-	3,3,3	0.26	0	2,2,2	0.59	0
5	PEG	E	303	-	6,6,6	0.48	0	5,5,5	0.35	0
7	EDO	A	306	-	3,3,3	0.60	0	2,2,2	0.63	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
8	LYS	A	308	-	-	0/5/9/9	-
5	PEG	D	305	-	-	1/4/4/4	-
5	PEG	F	304	-	-	2/4/4/4	-
4	PG4	D	304	-	-	7/10/10/10	-
6	PGE	C	312	-	-	2/7/7/7	-
8	LYS	D	306	-	-	0/5/9/9	-
7	EDO	E	305	-	-	1/1/1/1	-
7	EDO	F	307	-	-	1/1/1/1	-
4	PG4	A	303	-	-	2/10/10/10	-
6	PGE	A	305	-	-	5/7/7/7	-
6	PGE	F	305	-	-	4/7/7/7	-
5	PEG	B	306	-	-	1/4/4/4	-
8	LYS	C	316	-	-	0/5/9/9	-
8	LYS	F	308	-	-	0/5/9/9	-
5	PEG	A	304	-	-	1/4/4/4	-
6	PGE	C	313	-	-	2/7/7/7	-
7	EDO	E	306	-	-	1/1/1/1	-
4	PG4	B	305	-	-	2/10/10/10	-
8	LYS	E	308	-	-	0/5/9/9	-
7	EDO	C	315	-	-	1/1/1/1	-
5	PEG	E	304	-	-	3/4/4/4	-
8	LYS	B	307	-	-	0/5/9/9	-
9	GOL	B	308	-	-	4/4/4/4	-
7	EDO	C	314	-	-	0/1/1/1	-
5	PEG	C	311	-	-	3/4/4/4	-
7	EDO	A	307	-	-	0/1/1/1	-
7	EDO	F	306	-	-	1/1/1/1	-
7	EDO	E	307	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	E	303	-	-	1/4/4/4	-
7	EDO	A	306	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	308	GOL	O1-C1-C2-C3
6	A	305	PGE	C3-C4-O3-C5
6	A	305	PGE	O2-C3-C4-O3
6	C	313	PGE	O3-C5-C6-O4
7	E	306	EDO	O1-C1-C2-O2
5	A	304	PEG	O1-C1-C2-O2
5	E	304	PEG	O1-C1-C2-O2
5	F	304	PEG	O1-C1-C2-O2
5	F	304	PEG	O2-C3-C4-O4
6	A	305	PGE	O1-C1-C2-O2
9	B	308	GOL	C1-C2-C3-O3
5	E	303	PEG	O2-C3-C4-O4
6	C	312	PGE	O3-C5-C6-O4
4	A	303	PG4	O2-C3-C4-O3
9	B	308	GOL	O1-C1-C2-O2
7	C	315	EDO	O1-C1-C2-O2
7	E	305	EDO	O1-C1-C2-O2
7	F	307	EDO	O1-C1-C2-O2
5	E	304	PEG	O2-C3-C4-O4
9	B	308	GOL	O2-C2-C3-O3
5	D	305	PEG	O1-C1-C2-O2
7	E	307	EDO	O1-C1-C2-O2
7	F	306	EDO	O1-C1-C2-O2
5	E	304	PEG	C1-C2-O2-C3
6	C	312	PGE	C6-C5-O3-C4
6	A	305	PGE	C1-C2-O2-C3
4	D	304	PG4	C6-C5-O3-C4
5	C	311	PEG	C1-C2-O2-C3
4	A	303	PG4	C1-C2-O2-C3
4	D	304	PG4	O4-C7-C8-O5
6	C	313	PGE	C1-C2-O2-C3
6	F	305	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
6	F	305	PGE	C3-C4-O3-C5
6	F	305	PGE	C1-C2-O2-C3
4	B	305	PG4	C8-C7-O4-C6
4	D	304	PG4	C8-C7-O4-C6
5	C	311	PEG	C4-C3-O2-C2
5	C	311	PEG	O1-C1-C2-O2
4	D	304	PG4	O3-C5-C6-O4
6	F	305	PGE	O2-C3-C4-O3
4	D	304	PG4	C4-C3-O2-C2
4	D	304	PG4	O1-C1-C2-O2
6	A	305	PGE	O3-C5-C6-O4
4	B	305	PG4	O1-C1-C2-O2
5	B	306	PEG	O1-C1-C2-O2
4	D	304	PG4	O2-C3-C4-O3

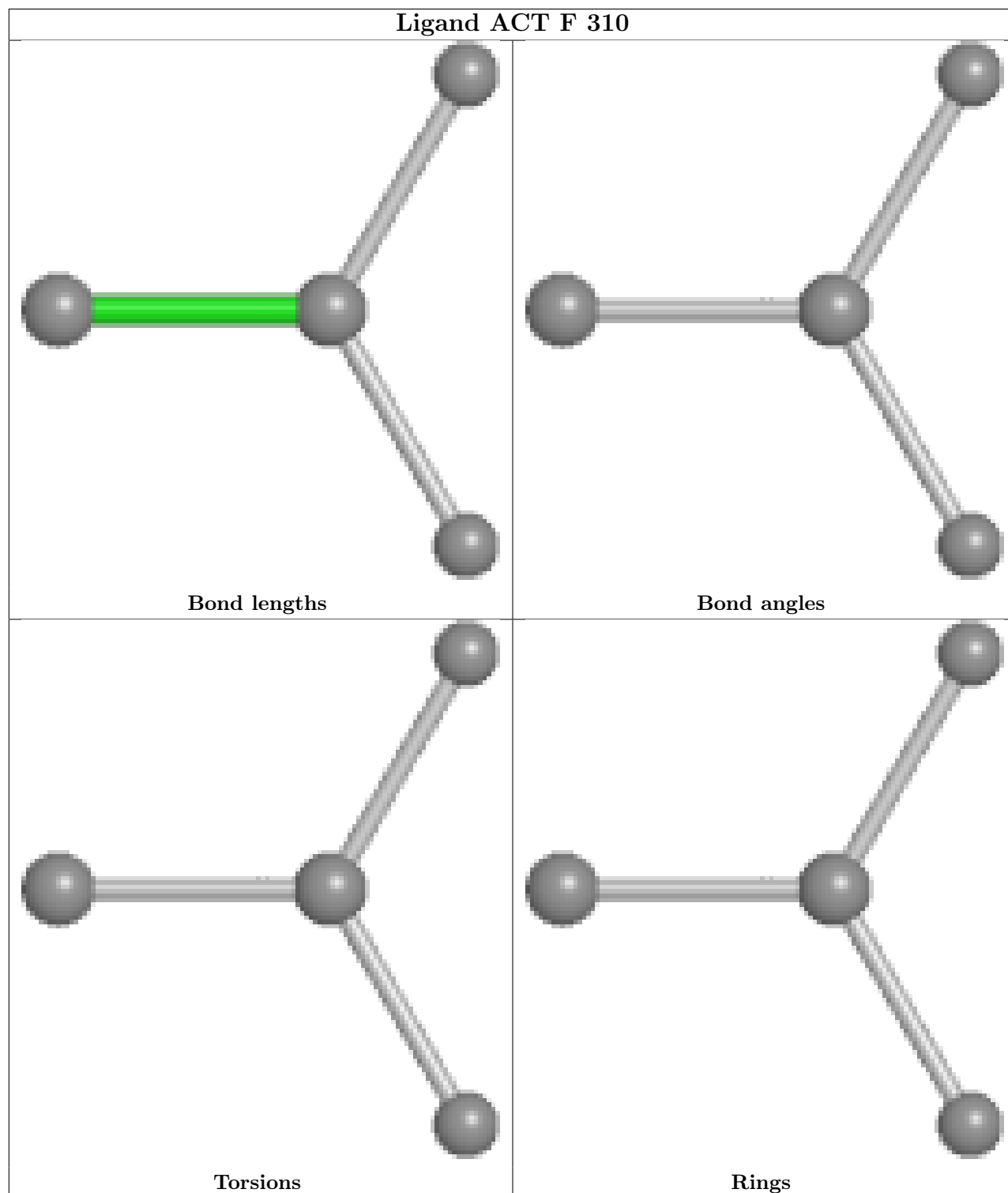
There are no ring outliers.

15 monomers are involved in 55 short contacts:

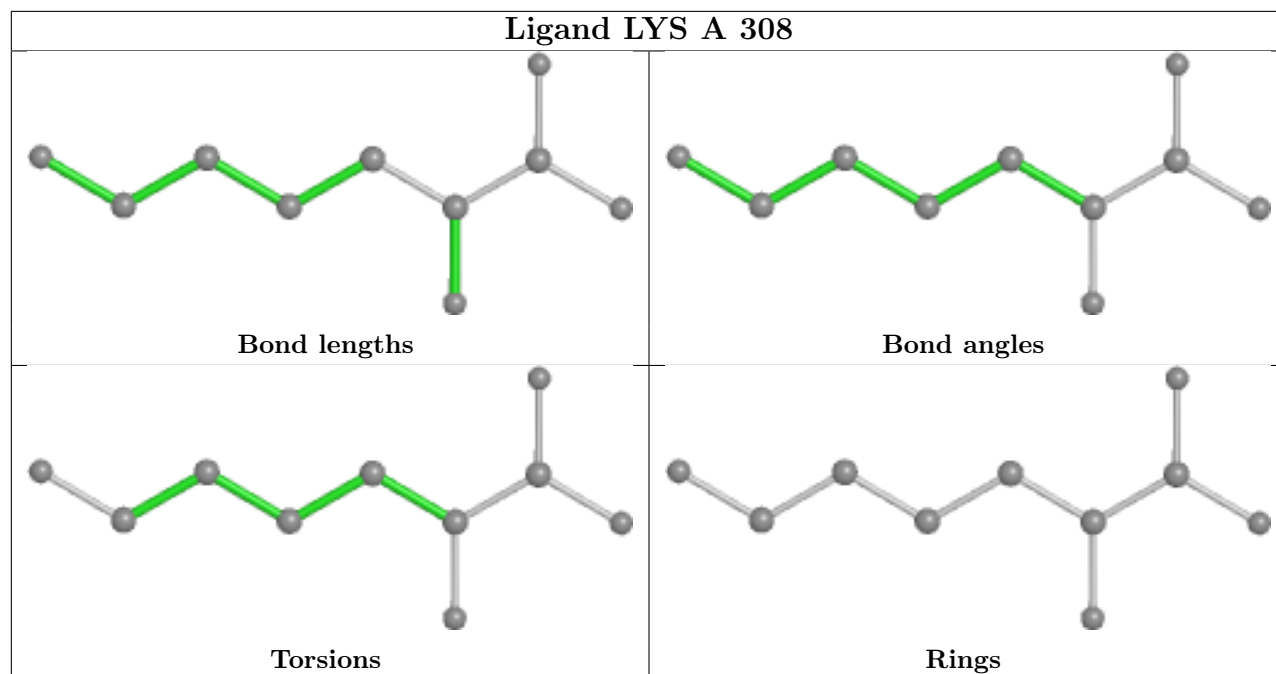
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	304	PG4	10	0
7	E	305	EDO	5	0
7	F	307	EDO	11	0
4	A	303	PG4	3	0
6	A	305	PGE	1	0
6	F	305	PGE	7	0
6	C	313	PGE	2	0
7	E	306	EDO	1	0
7	C	315	EDO	1	0
5	E	304	PEG	4	0
9	B	308	GOL	1	0
7	C	314	EDO	3	0
7	A	307	EDO	2	0
7	F	306	EDO	1	0
7	E	307	EDO	3	0

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

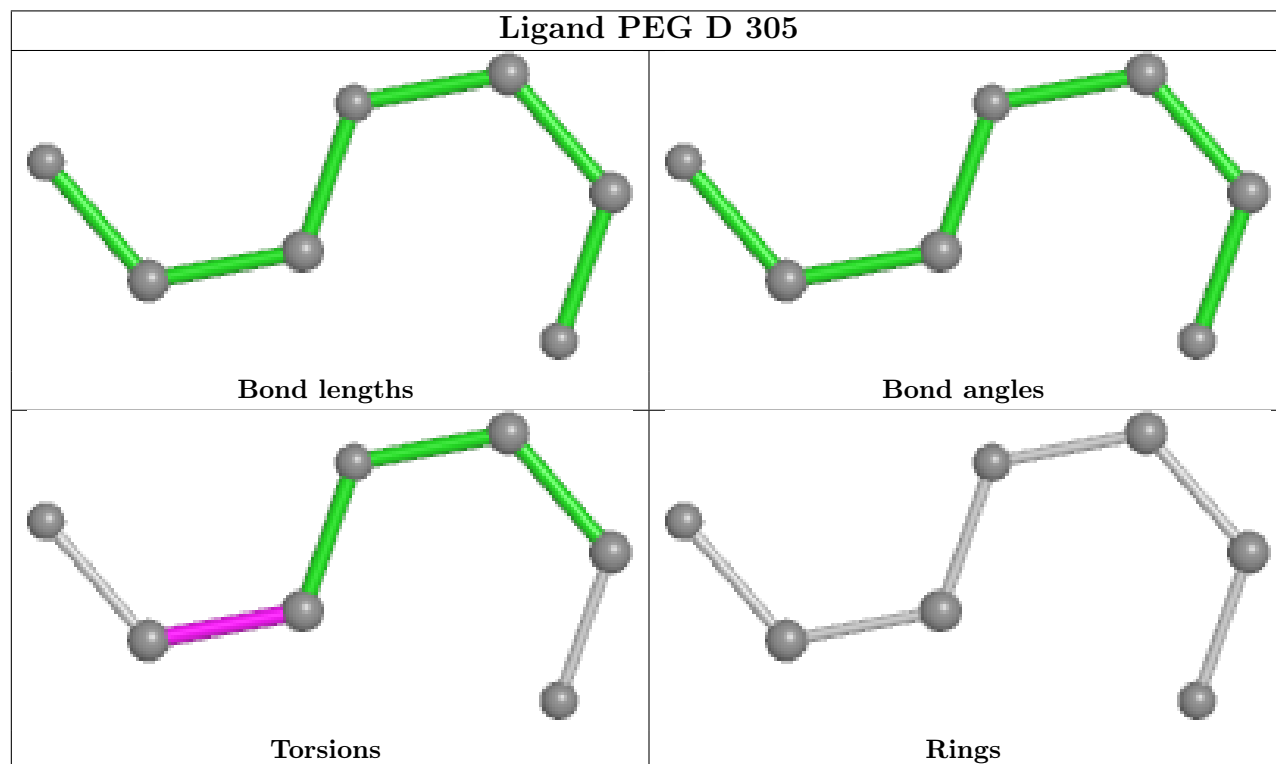
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

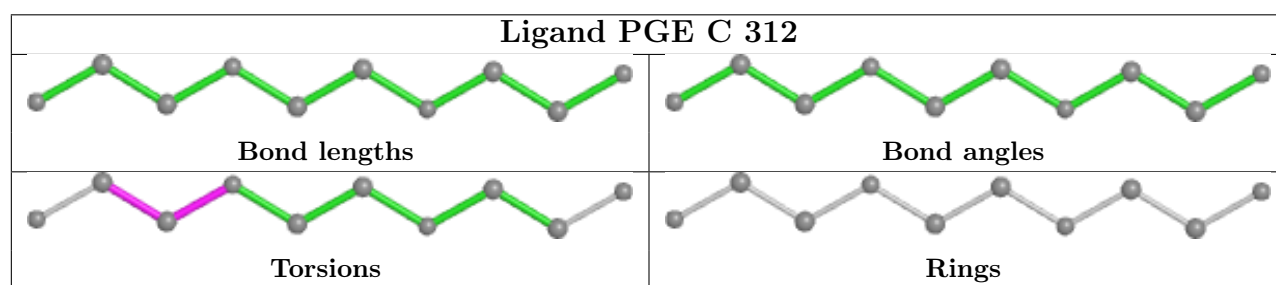
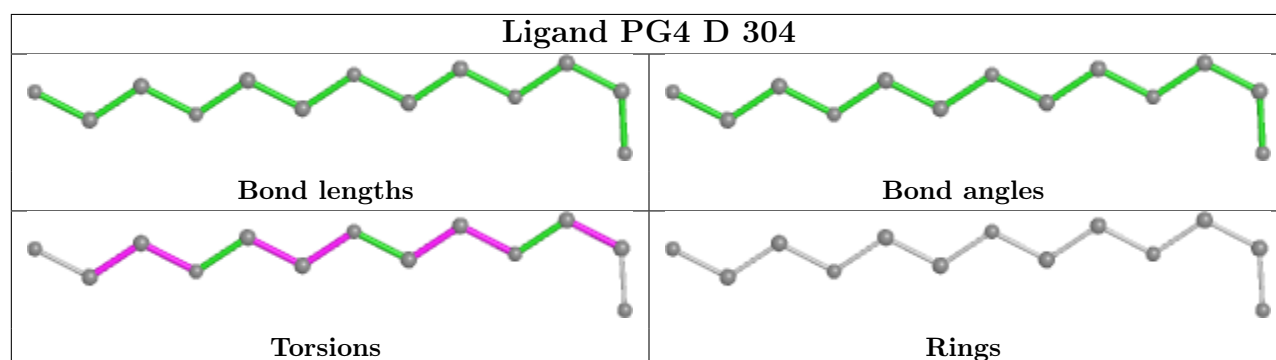
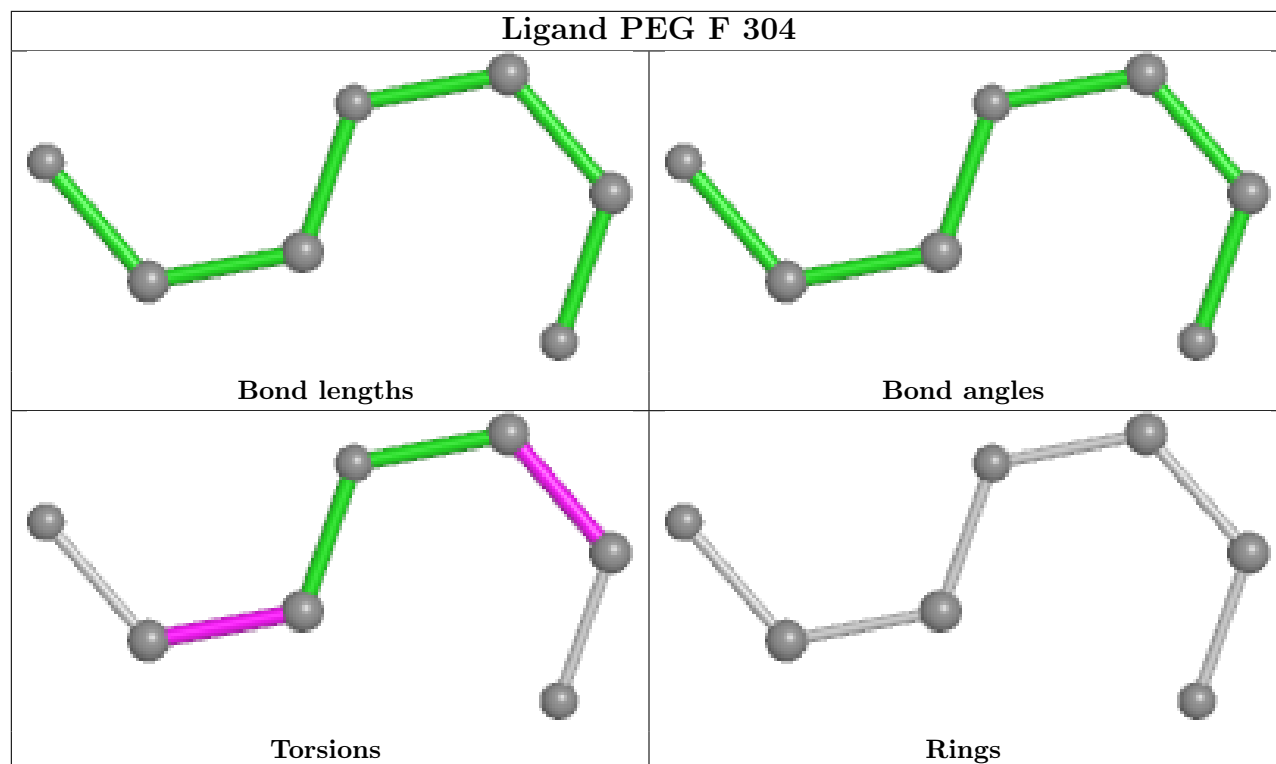


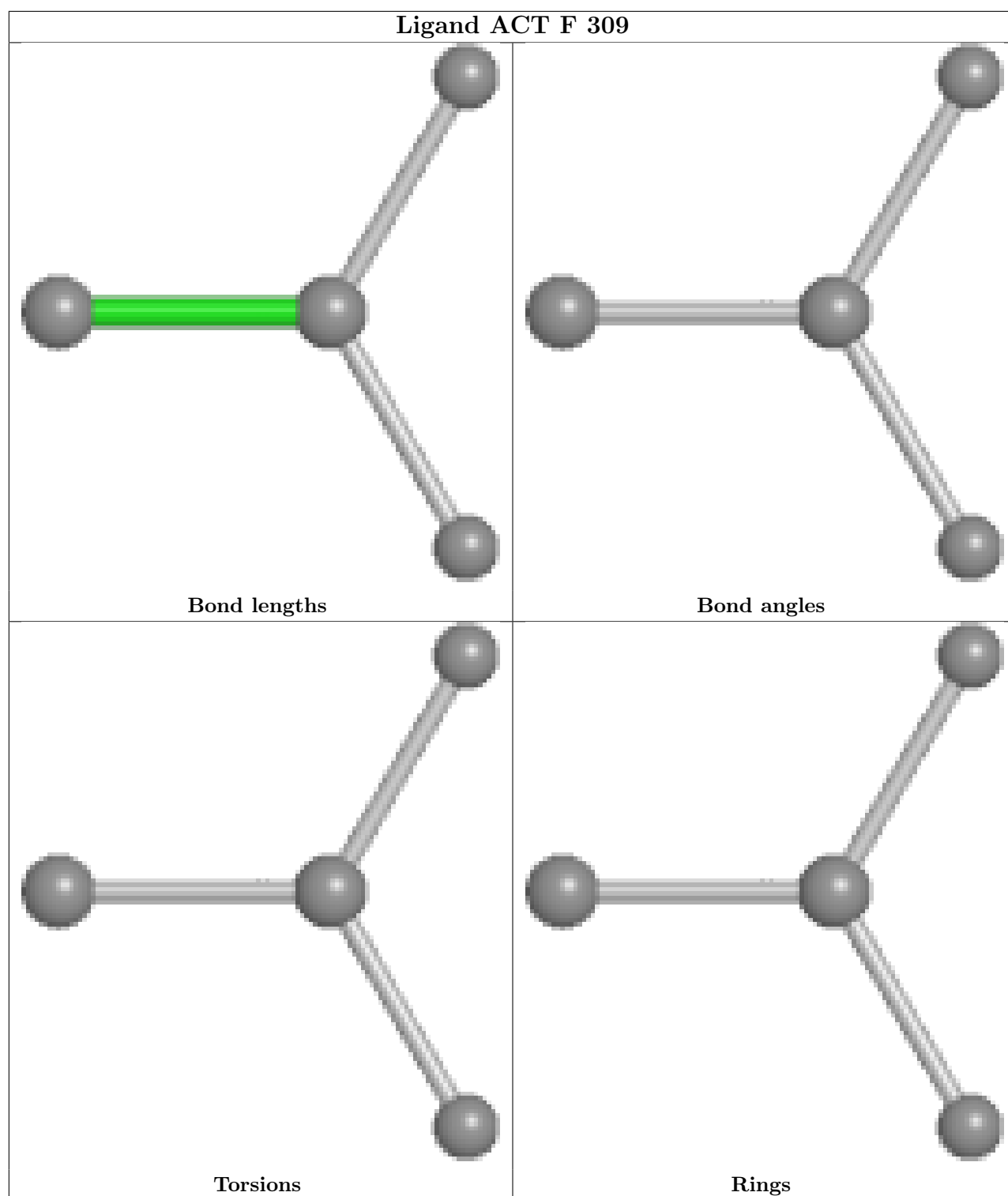
Ligand LYS A 308



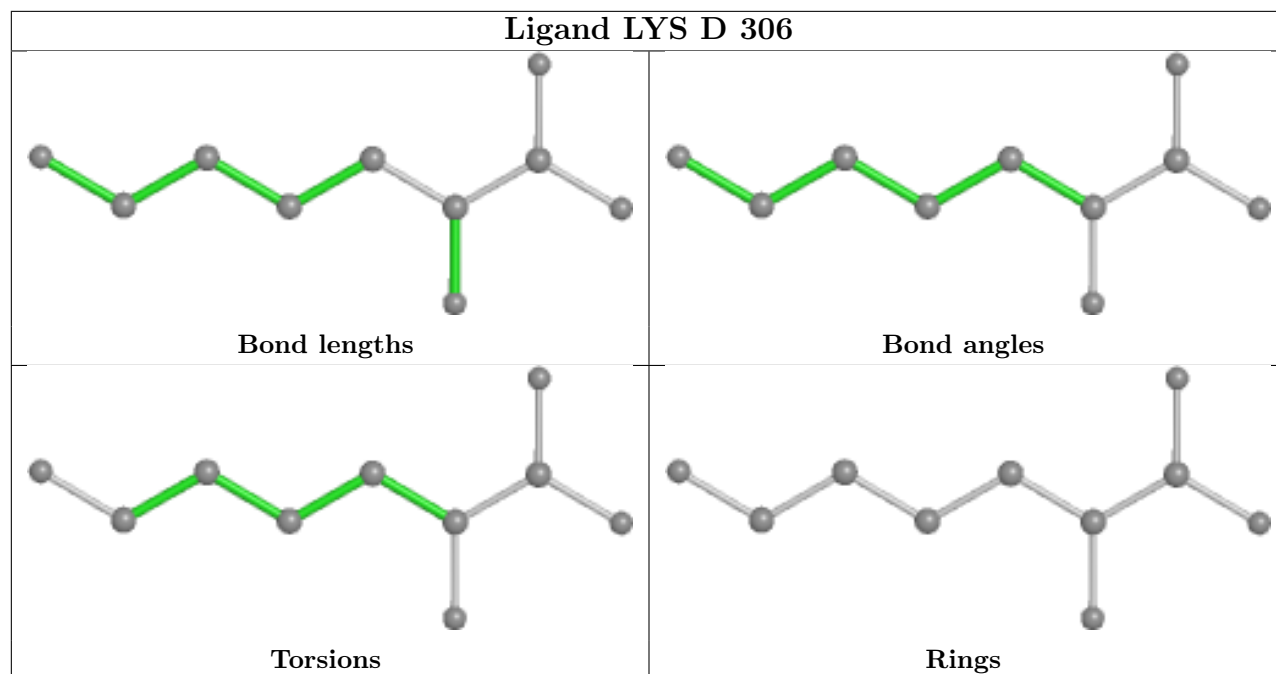
Ligand PEG D 305



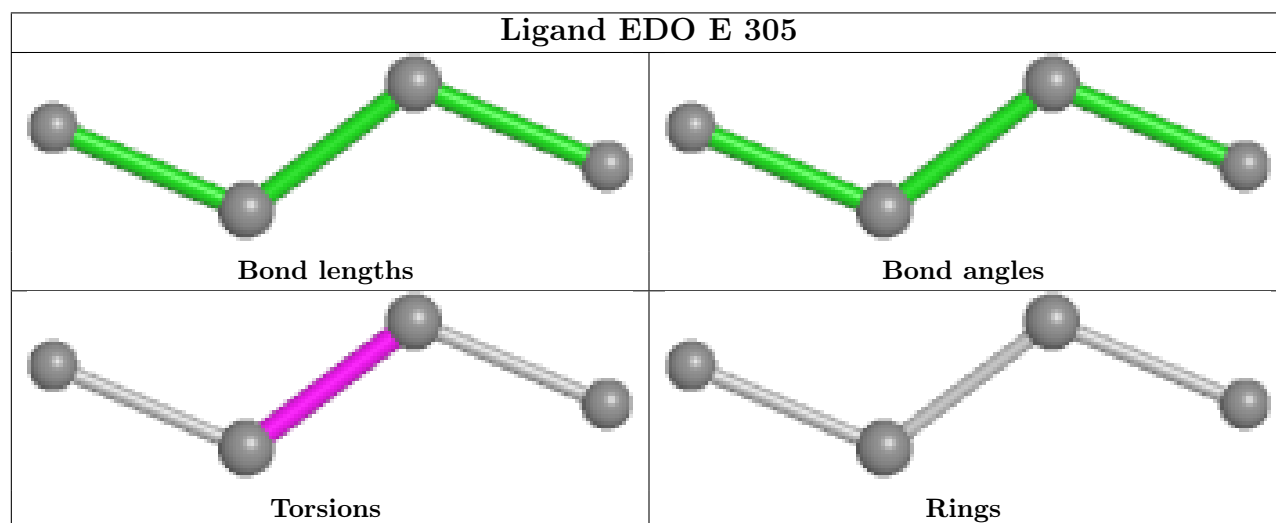




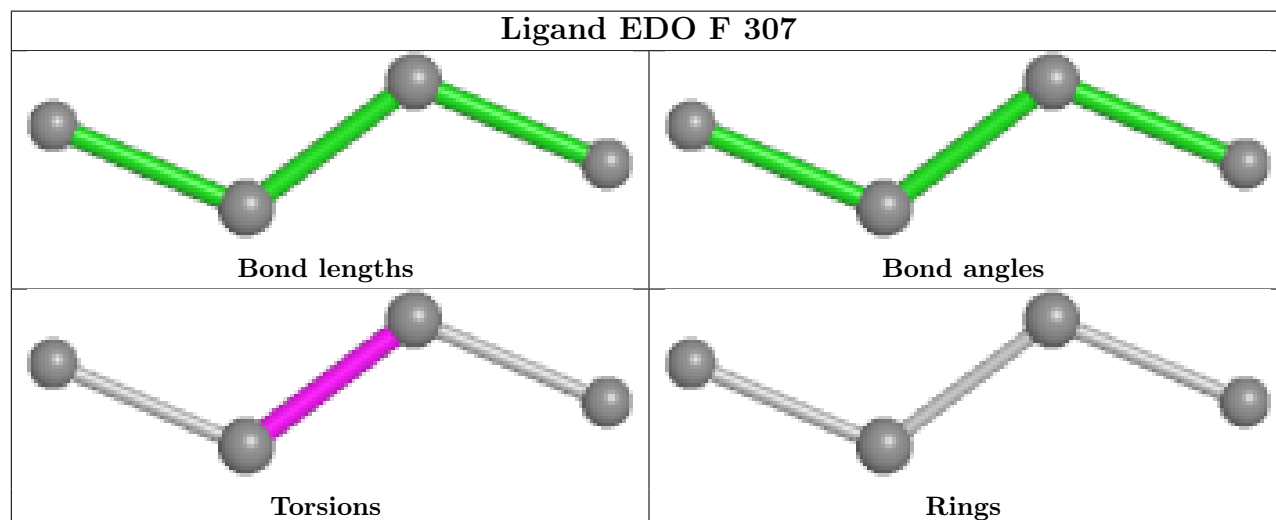
Ligand LYS D 306

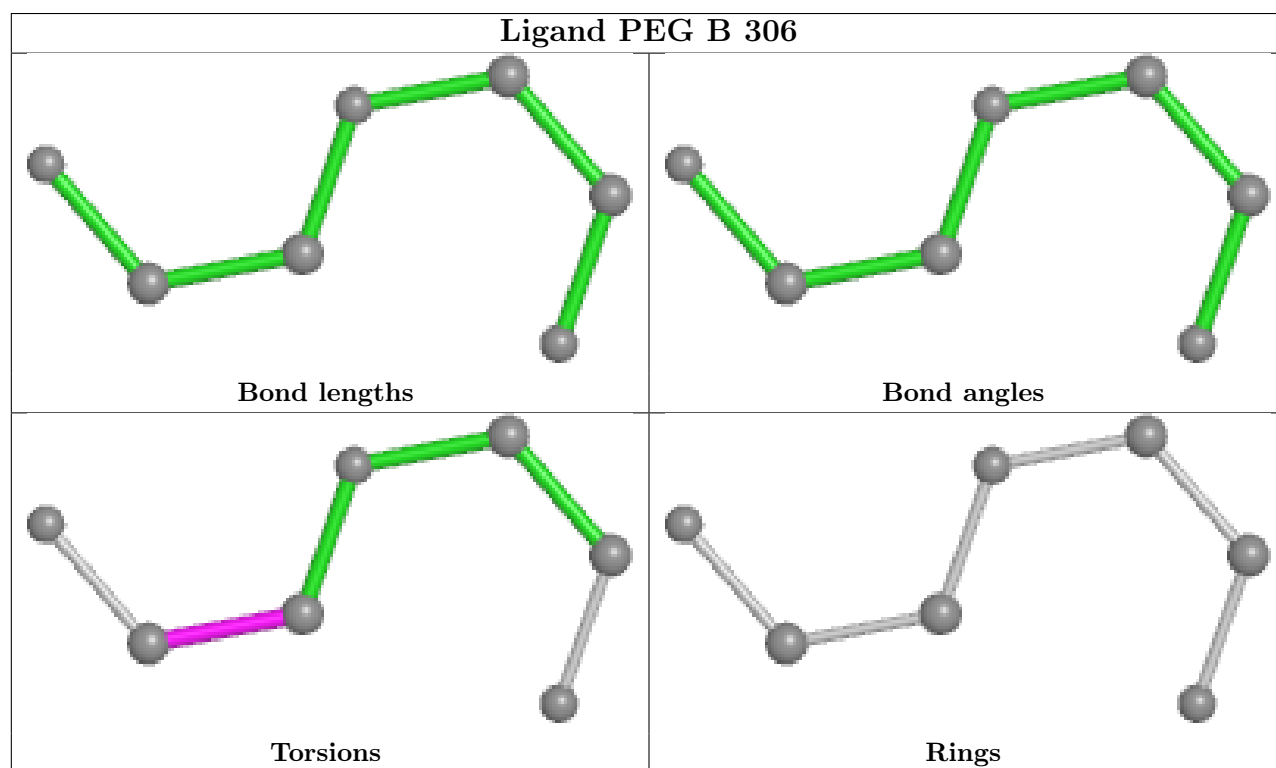
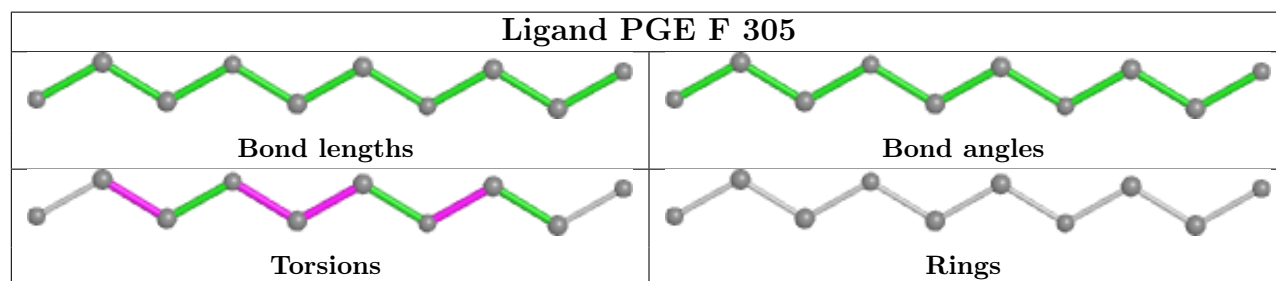
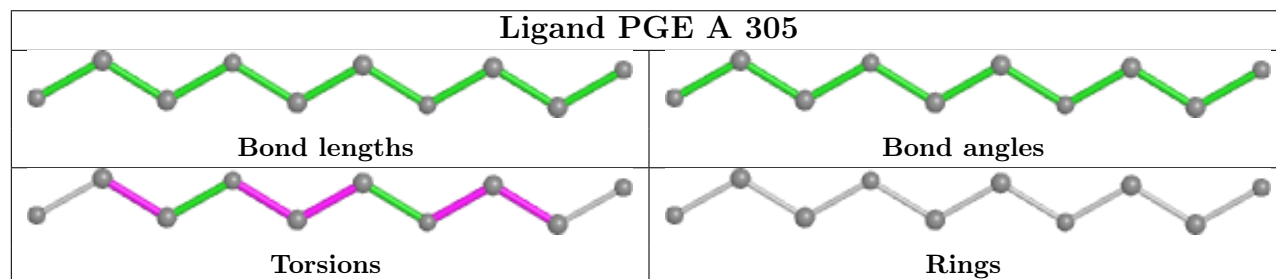
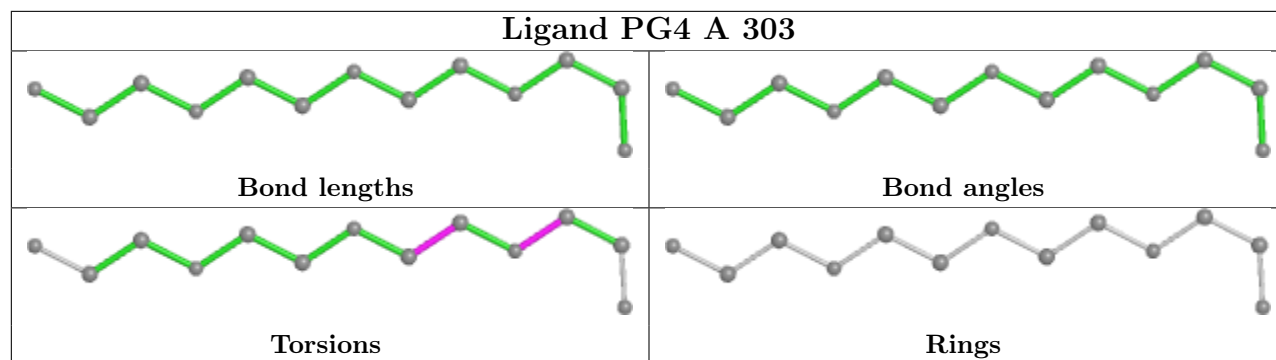


Ligand EDO E 305

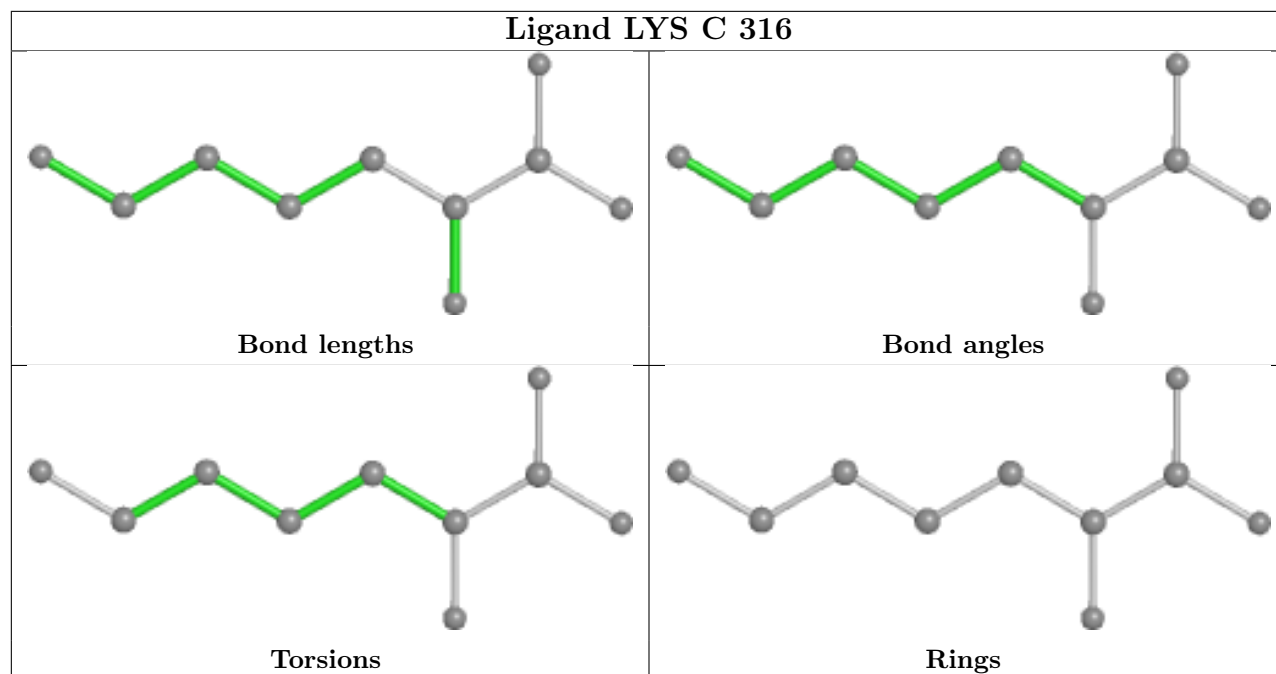


Ligand EDO F 307

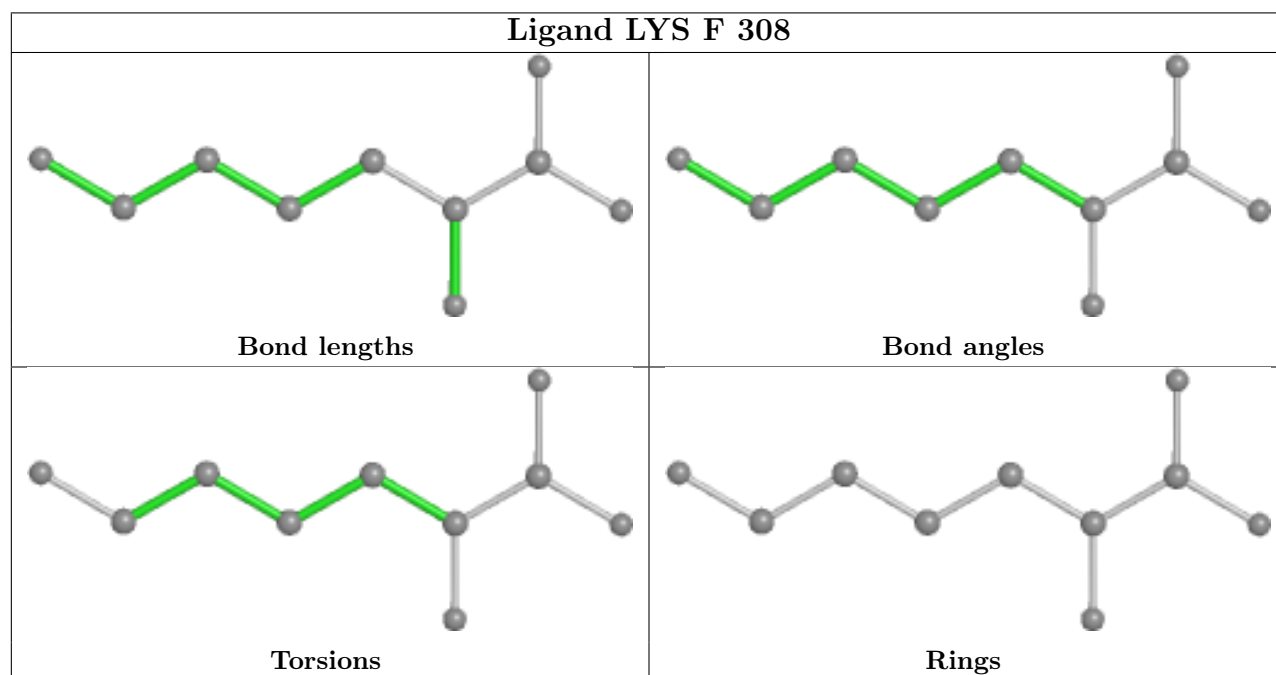


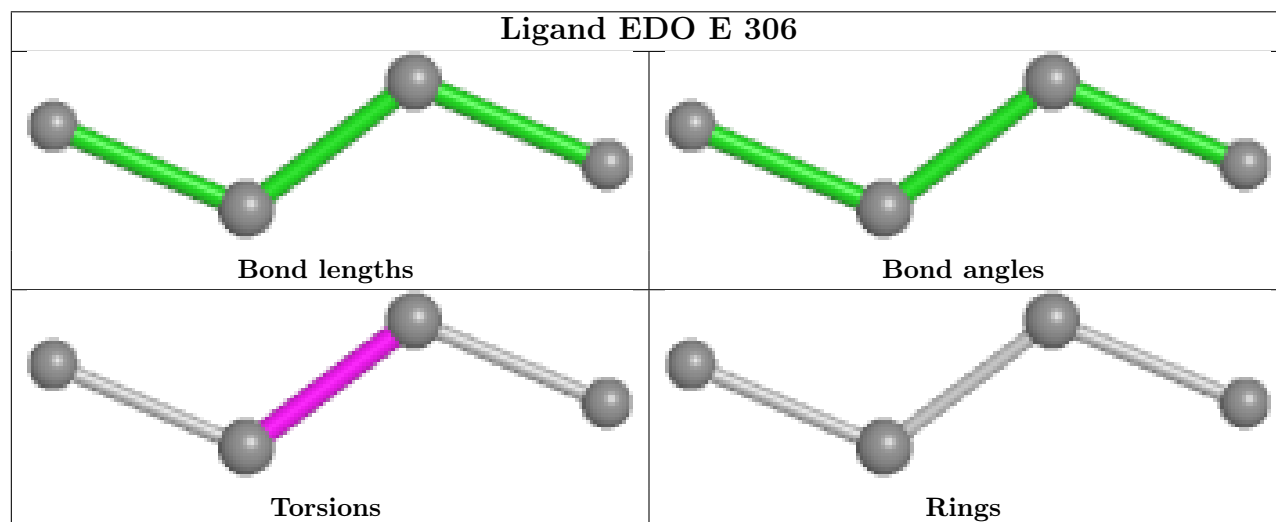
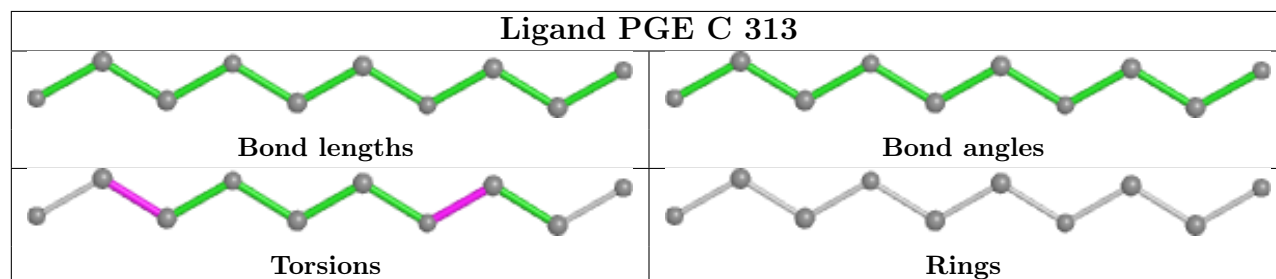
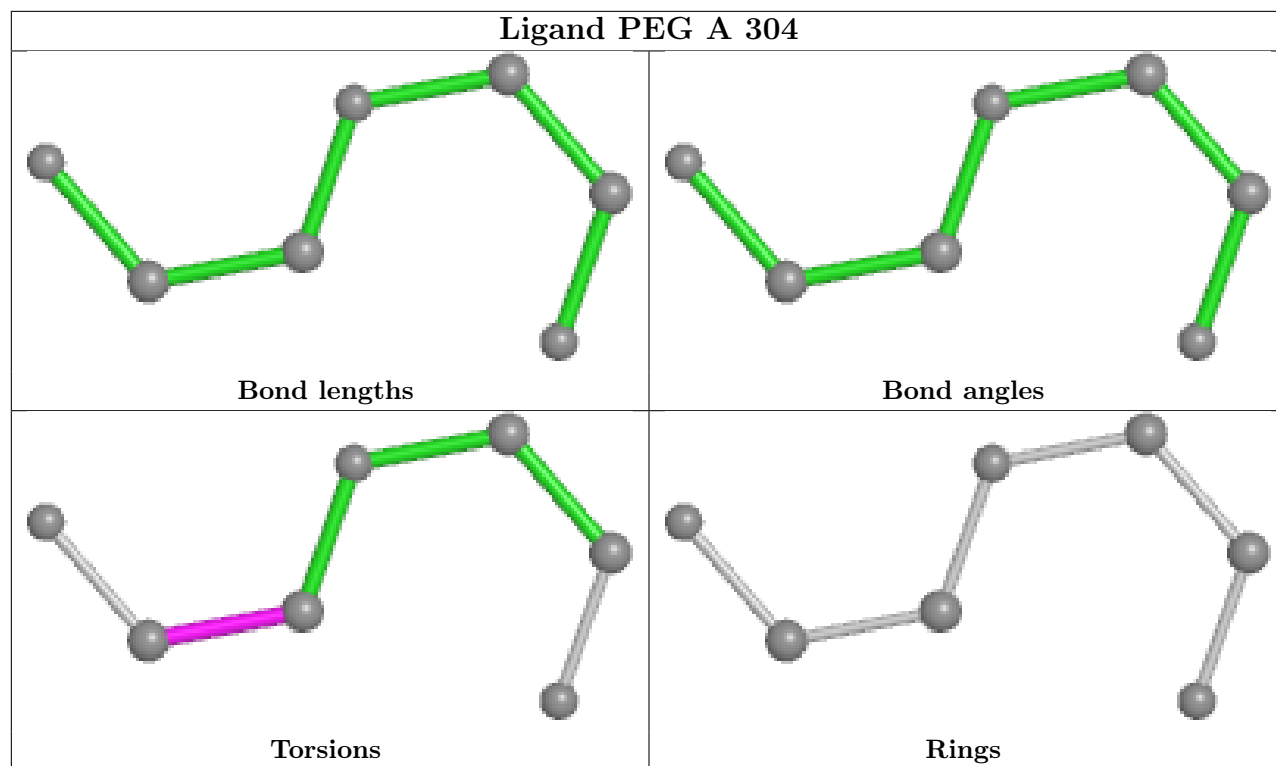


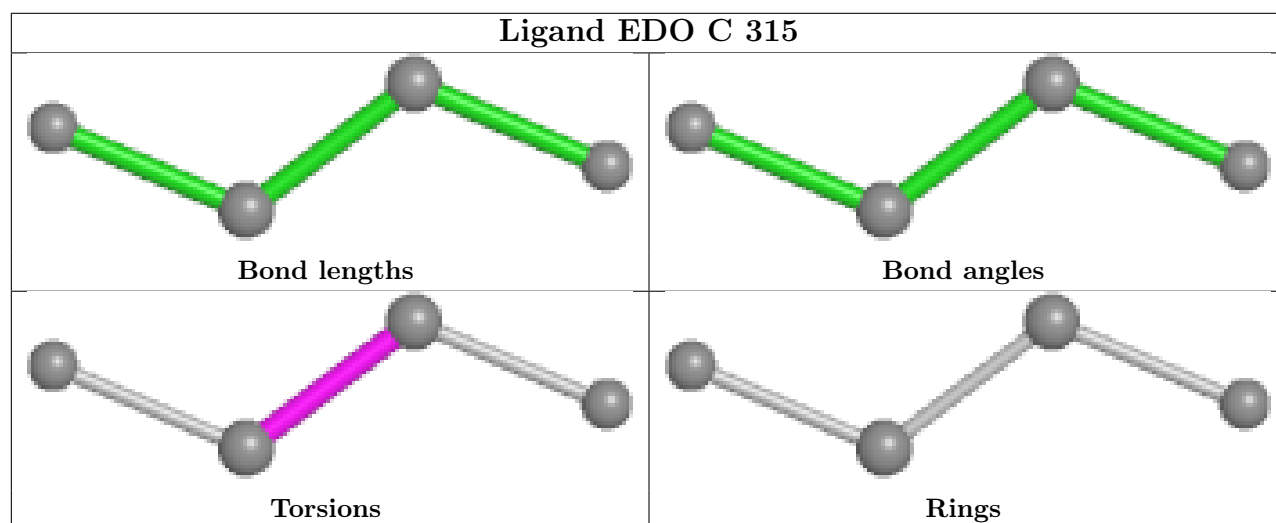
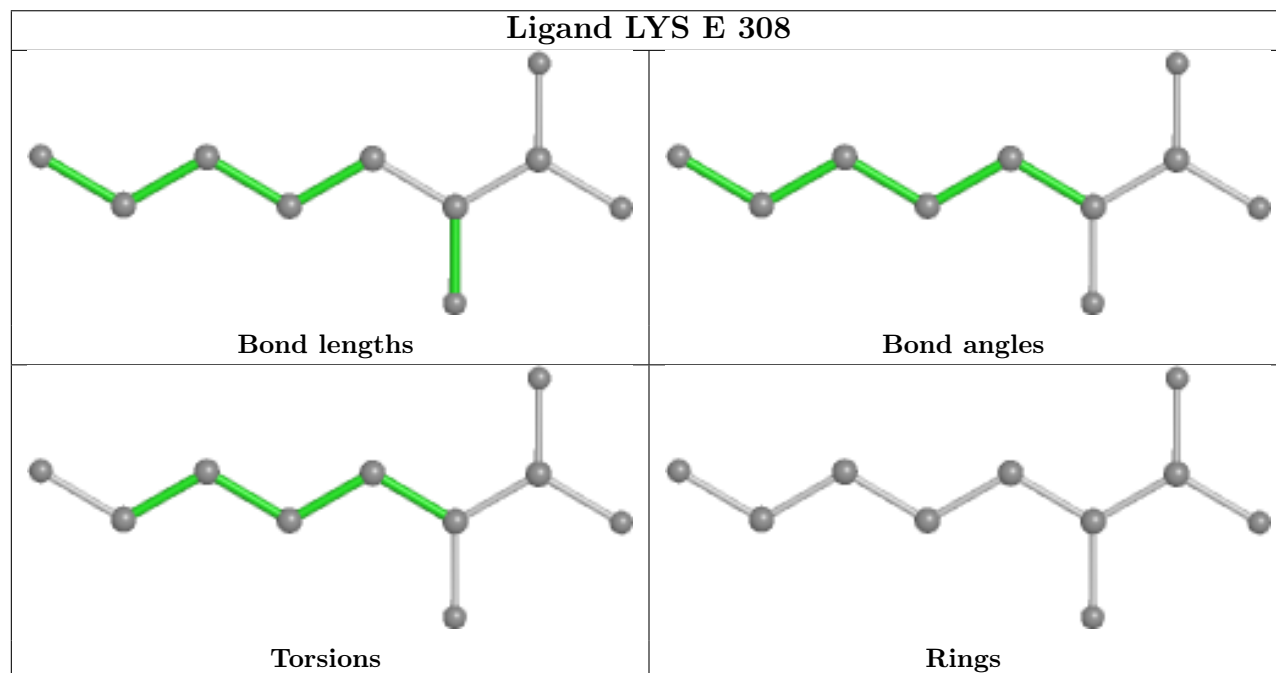
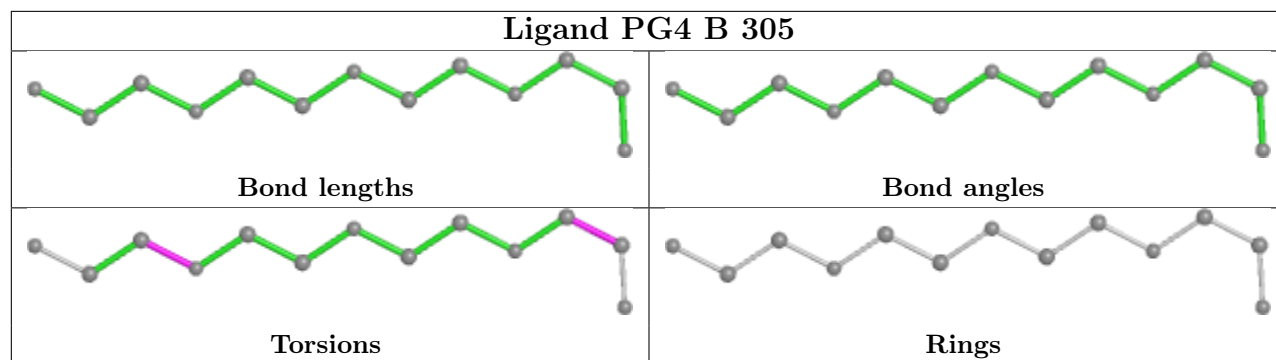
Ligand LYS C 316

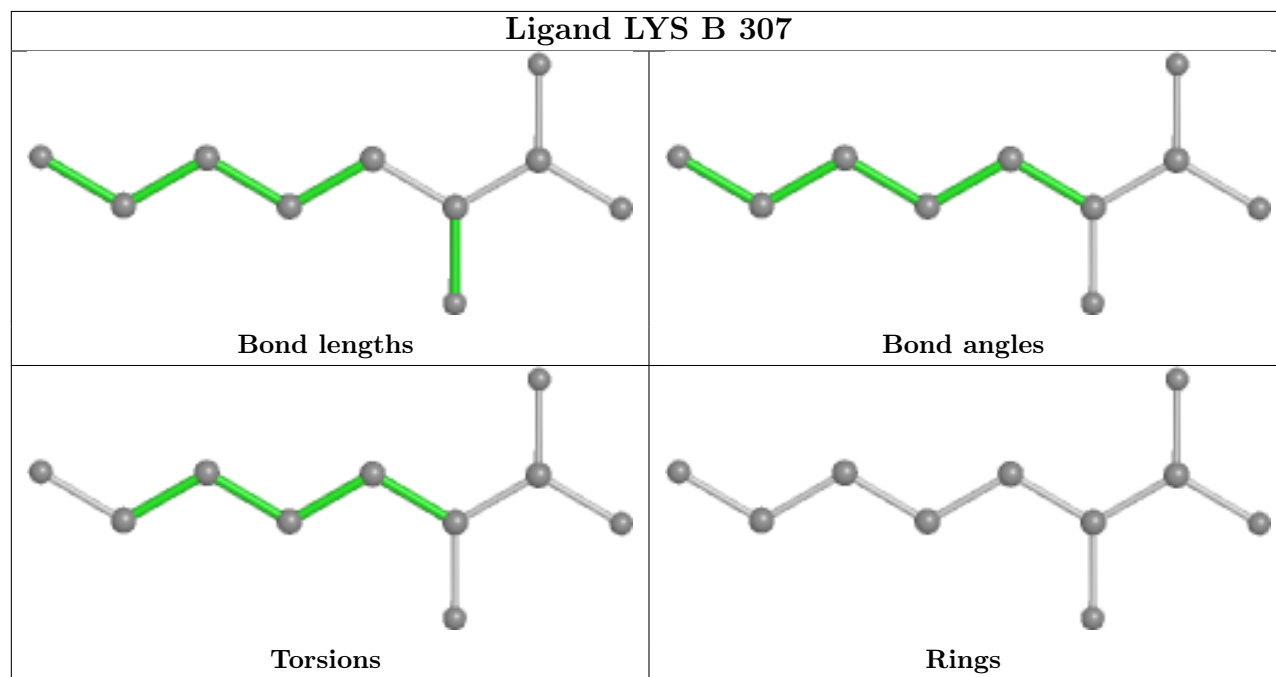
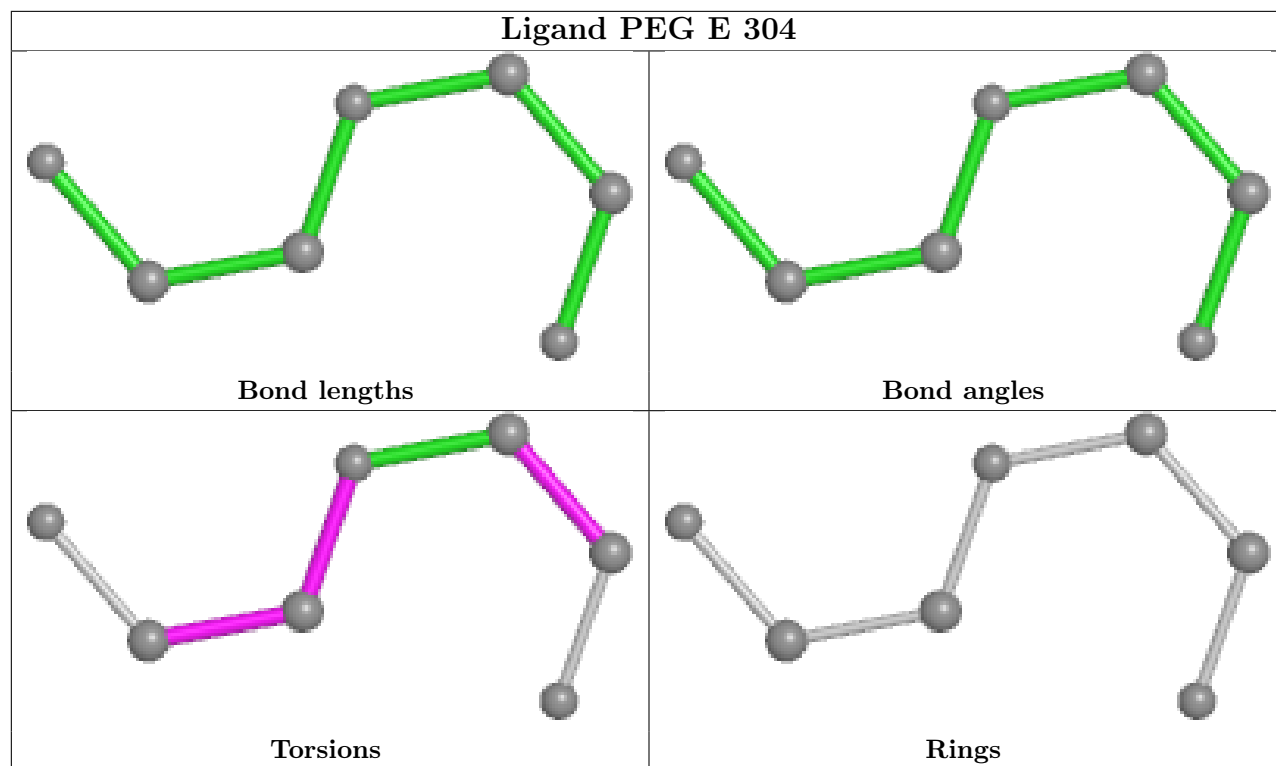


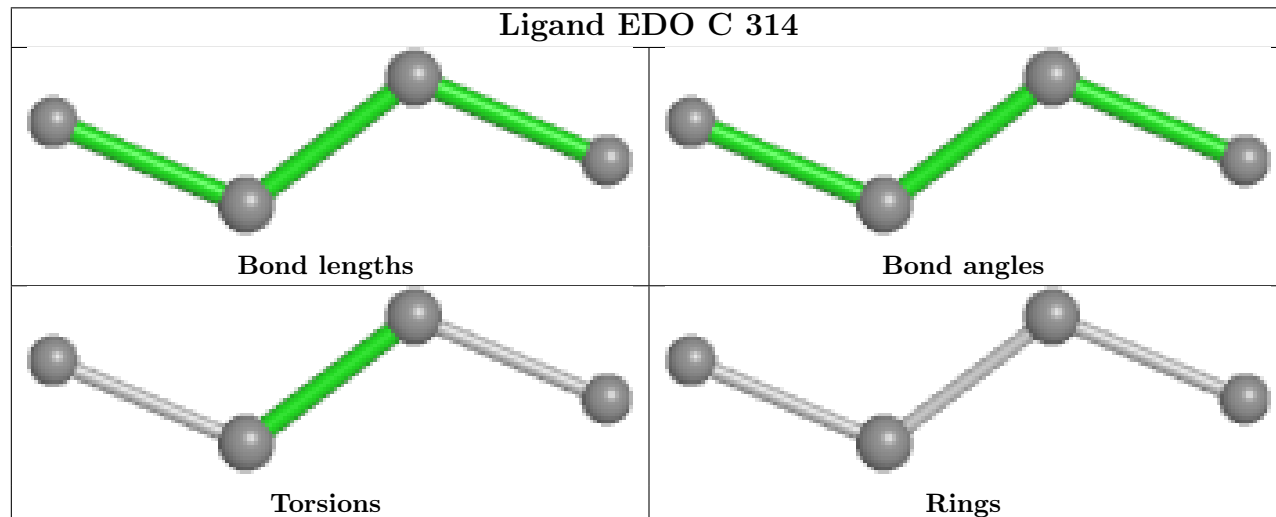
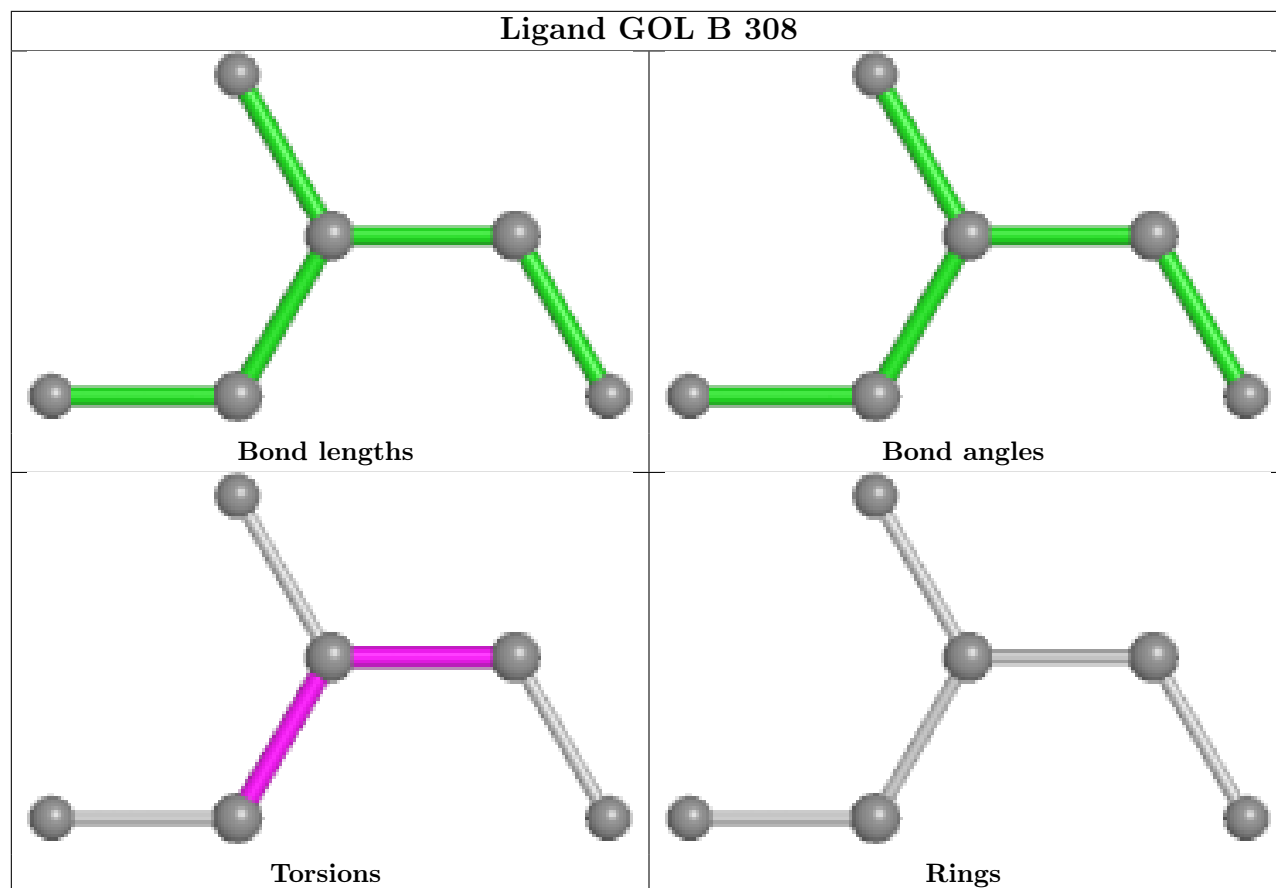
Ligand LYS F 308

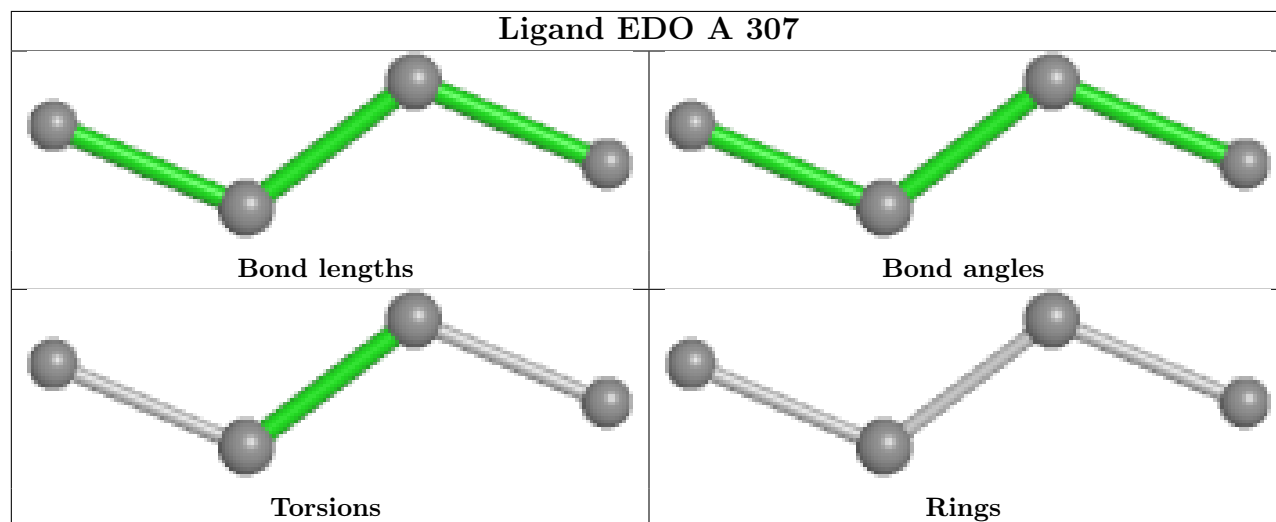
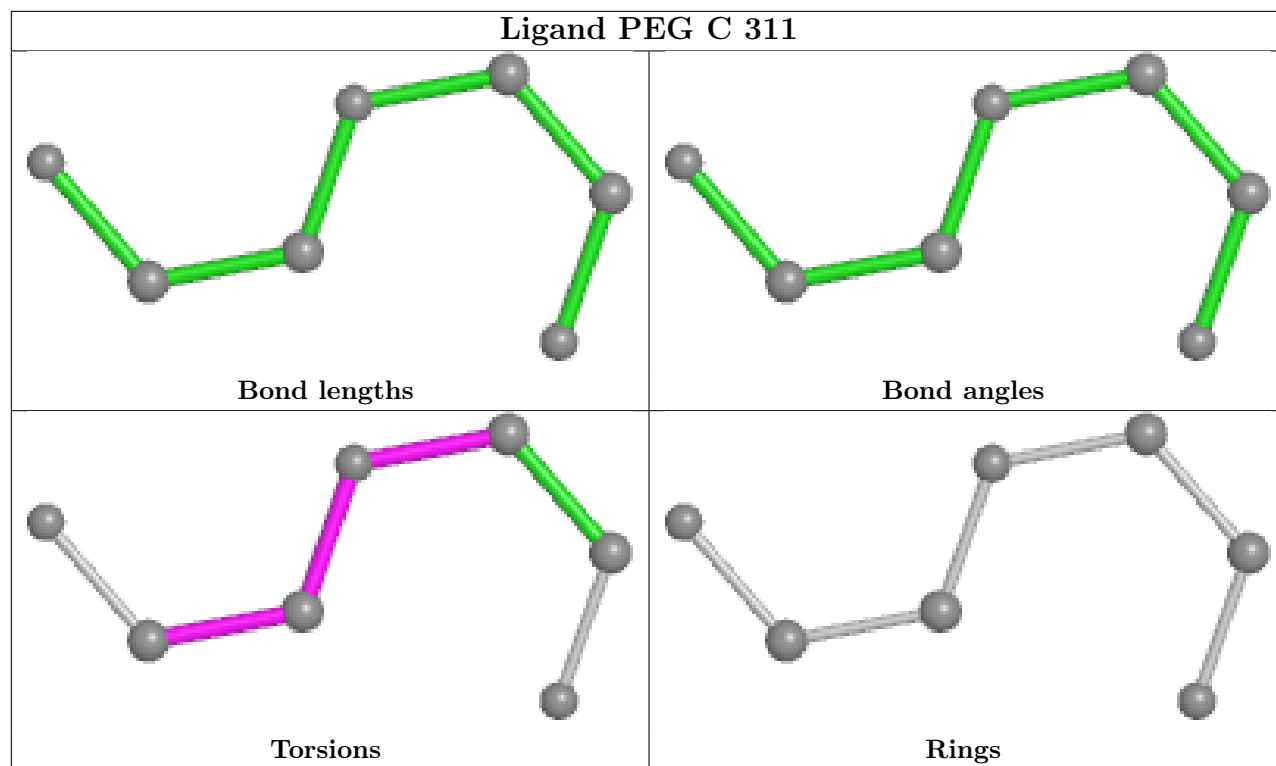


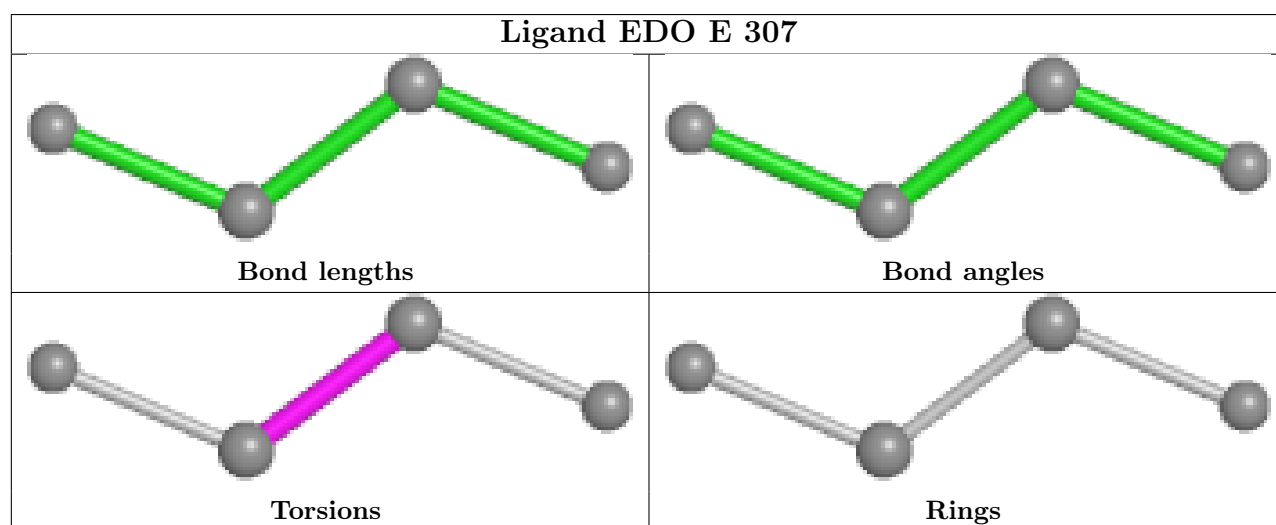
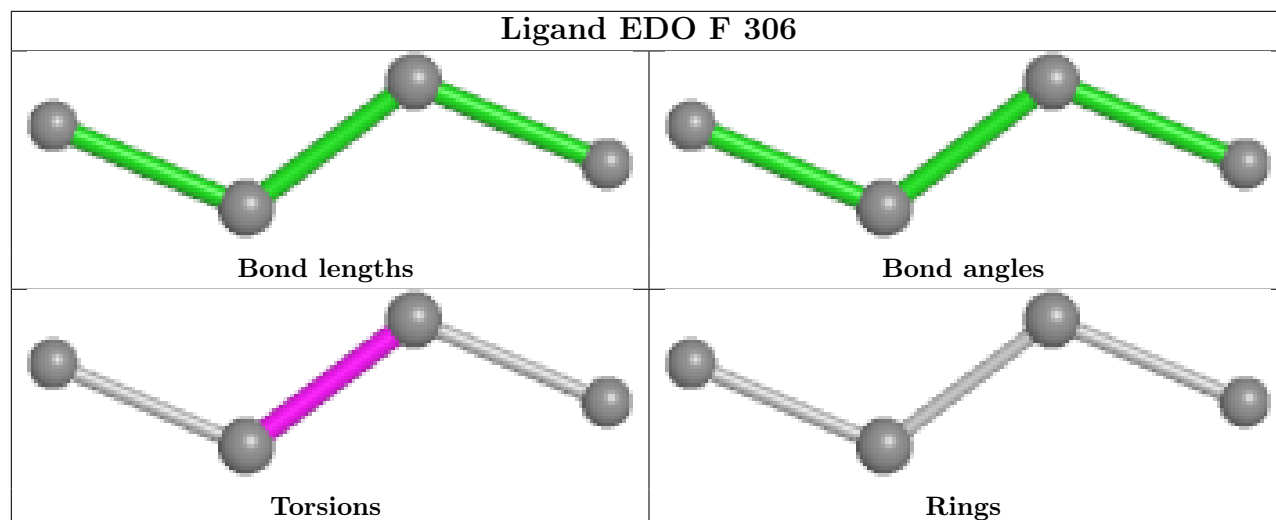


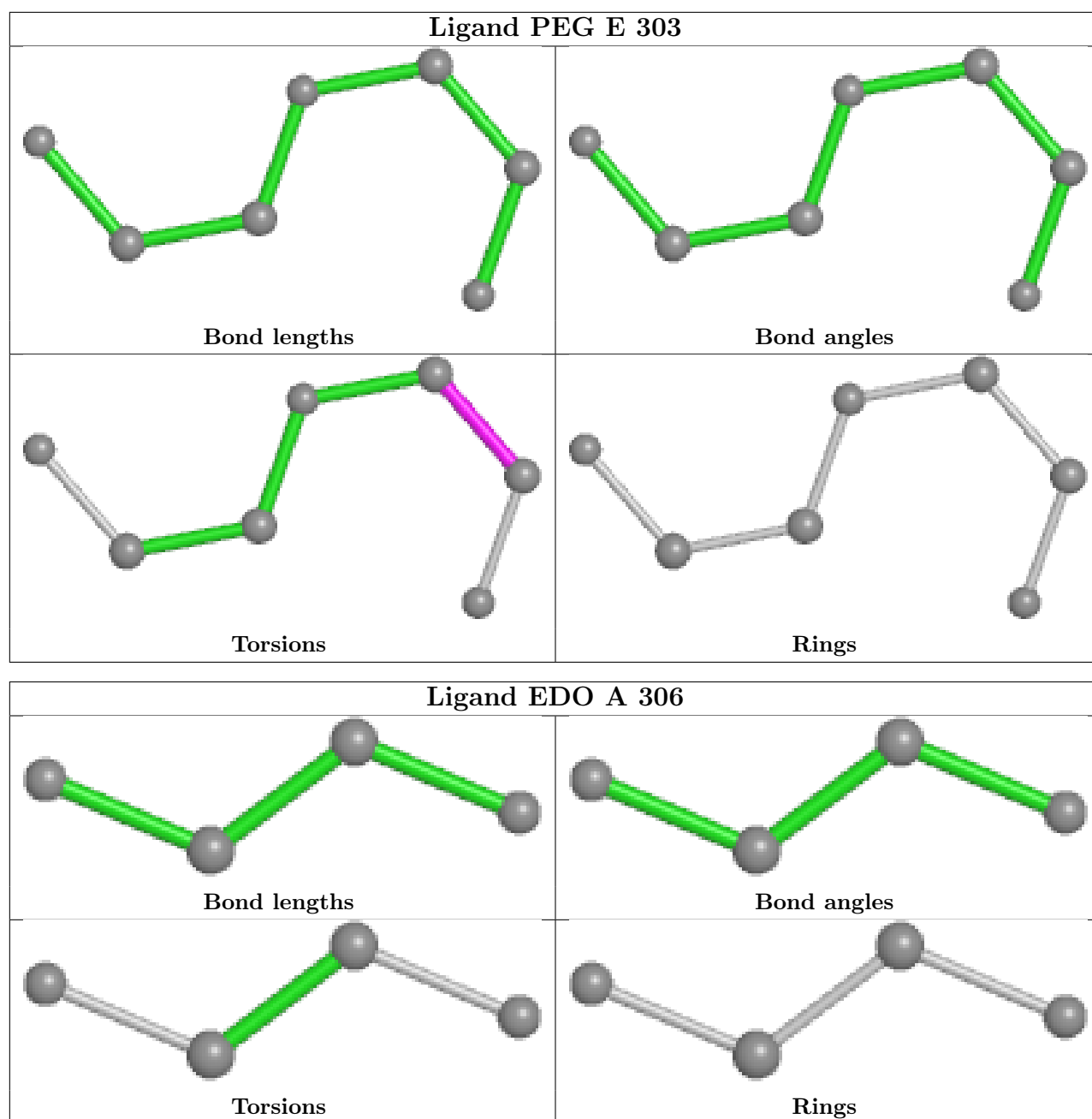












5.7 Other polymers [i](#)

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	296/310 (95%)	-0.71	0 100 100	7, 10, 21, 41	0
1	B	305/310 (98%)	-0.68	1 (0%) 94 94	7, 11, 24, 58	0
1	C	294/310 (94%)	-0.65	0 100 100	7, 11, 21, 35	0
1	D	305/310 (98%)	-0.66	0 100 100	8, 11, 25, 39	0
1	E	295/310 (95%)	-0.61	0 100 100	8, 12, 25, 37	0
1	F	295/310 (95%)	-0.57	0 100 100	8, 12, 26, 40	0
All	All	1790/1860 (96%)	-0.65	1 (0%) 95 94	7, 11, 24, 58	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ASP	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, 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	B	166	14/15	0.61	0.26	20,20,20,20	0
1	KPI	D	166	14/15	0.63	0.25	20,20,20,20	0
1	KPI	C	166	14/15	0.64	0.28	20,20,20,20	0
1	KPI	F	166	14/15	0.65	0.25	20,20,20,20	0
1	KPI	E	166	14/15	0.67	0.25	20,20,20,20	0
1	KPI	A	166	14/15	0.68	0.25	20,20,20,20	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	PGE	A	305	10/10	0.77	0.20	35,45,49,53	0
7	EDO	F	307	4/4	0.78	0.59	20,20,20,20	0
5	PEG	E	303	7/7	0.82	0.18	26,36,49,50	0
5	PEG	B	306	7/7	0.83	0.16	27,38,45,47	0
2	MG	C	307	1/1	0.84	0.11	40,40,40,40	0
5	PEG	A	304	7/7	0.84	0.12	26,41,44,46	0
6	PGE	C	313	10/10	0.84	0.17	31,34,47,59	0
2	MG	B	303	1/1	0.84	0.14	41,41,41,41	0
2	MG	C	304	1/1	0.85	0.12	39,39,39,39	0
7	EDO	C	314	4/4	0.86	0.18	26,27,30,48	0
7	EDO	E	306	4/4	0.86	0.23	32,34,36,46	0
5	PEG	F	304	7/7	0.86	0.13	29,38,52,54	0
7	EDO	A	307	4/4	0.88	0.35	36,42,42,47	0
2	MG	C	306	1/1	0.88	0.19	35,35,35,35	0
7	EDO	C	315	4/4	0.89	0.21	28,29,37,44	0
2	MG	C	303	1/1	0.89	0.18	43,43,43,43	0
5	PEG	C	311	7/7	0.89	0.11	28,37,44,46	0
7	EDO	E	307	4/4	0.90	0.36	33,36,37,41	0
2	MG	D	303	1/1	0.90	0.16	35,35,35,35	0
7	EDO	F	306	4/4	0.91	0.25	43,44,45,49	0
7	EDO	E	305	4/4	0.91	0.36	19,36,38,40	0
9	GOL	B	308	6/6	0.91	0.18	39,40,47,50	0
6	PGE	F	305	10/10	0.92	0.15	23,32,44,52	0
2	MG	C	302	1/1	0.92	0.13	36,36,36,36	0
10	ACT	F	310	4/4	0.92	0.15	21,25,31,36	0
5	PEG	D	305	7/7	0.93	0.12	25,41,54,64	0
5	PEG	E	304	7/7	0.93	0.09	25,33,36,44	0
4	PG4	D	304	13/13	0.94	0.09	15,29,42,42	0
7	EDO	A	306	4/4	0.94	0.09	14,14,14,15	0
6	PGE	C	312	10/10	0.94	0.13	22,27,36,43	0
10	ACT	F	309	4/4	0.94	0.21	25,26,33,56	0
4	PG4	A	303	13/13	0.94	0.12	21,28,47,51	0

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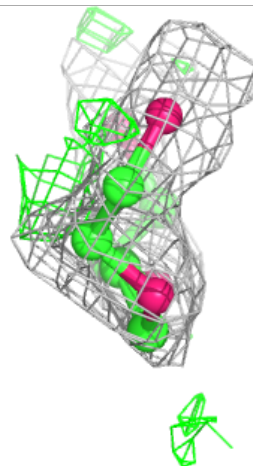
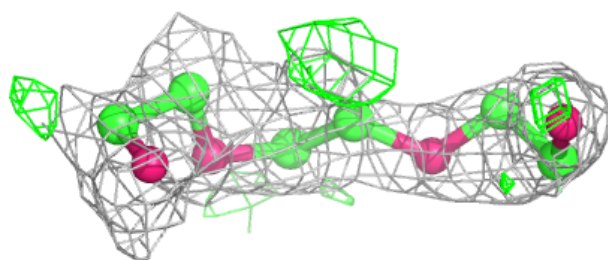
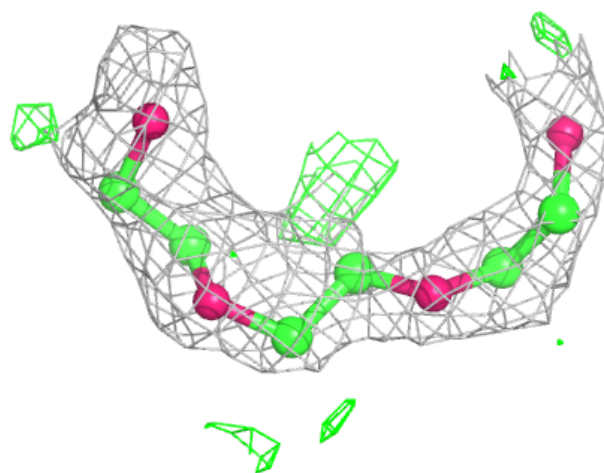
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	E	302	1/1	0.95	0.21	41,41,41,41	0
4	PG4	B	305	13/13	0.95	0.12	22,25,40,43	0
8	LYS	B	307	10/10	0.96	0.07	6,9,11,12	0
2	MG	C	308	1/1	0.96	0.25	38,38,38,38	0
8	LYS	C	316	10/10	0.97	0.08	8,9,10,10	0
3	NA	A	302	1/1	0.97	0.10	29,29,29,29	0
8	LYS	A	308	10/10	0.97	0.07	7,9,9,10	0
3	NA	C	309	1/1	0.97	0.05	25,25,25,25	0
8	LYS	E	308	10/10	0.98	0.07	7,9,11,12	0
8	LYS	F	308	10/10	0.98	0.08	7,9,10,10	0
2	MG	B	302	1/1	0.98	0.07	10,10,10,10	0
3	NA	C	310	1/1	0.98	0.08	26,26,26,26	0
8	LYS	D	306	10/10	0.98	0.06	7,8,10,13	0
2	MG	C	301	1/1	0.99	0.09	11,11,11,11	0
2	MG	D	301	1/1	0.99	0.08	17,17,17,17	0
2	MG	D	302	1/1	0.99	0.10	9,9,9,9	0
2	MG	B	301	1/1	0.99	0.12	9,9,9,9	0
2	MG	B	304	1/1	0.99	0.27	22,22,22,22	0
2	MG	F	302	1/1	0.99	0.19	17,17,17,17	0
2	MG	F	303	1/1	0.99	0.03	22,22,22,22	0
2	MG	E	301	1/1	1.00	0.15	9,9,9,9	0
2	MG	A	301	1/1	1.00	0.14	8,8,8,8	0
2	MG	F	301	1/1	1.00	0.16	10,10,10,10	0
2	MG	C	305	1/1	1.00	0.11	9,9,9,9	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.

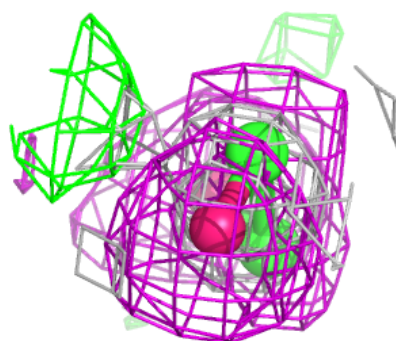
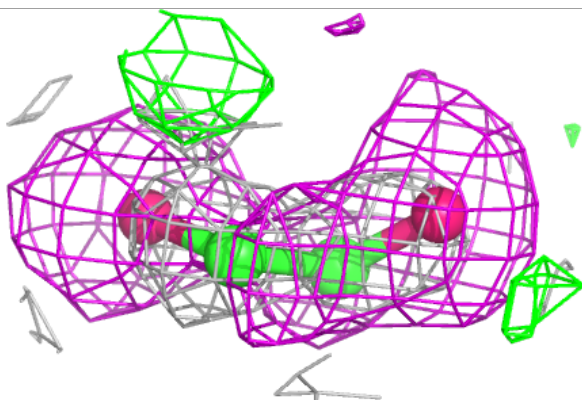
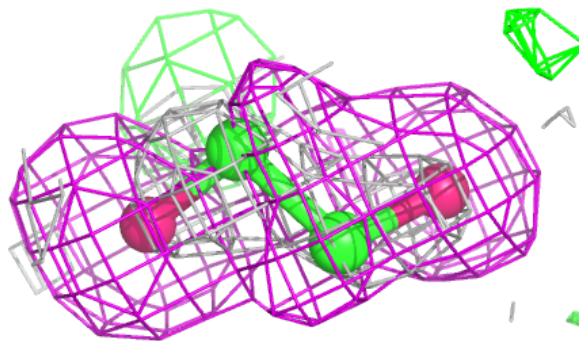
Electron density around PGE A 305:

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

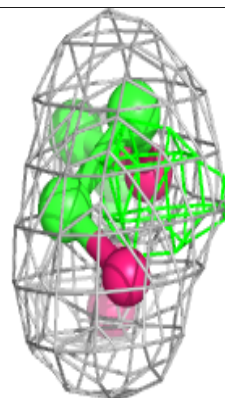
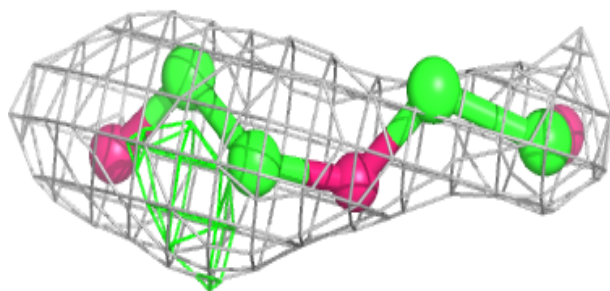
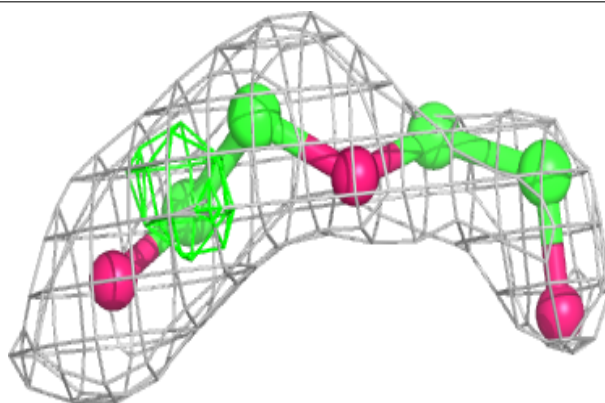


Electron density around EDO F 307:

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

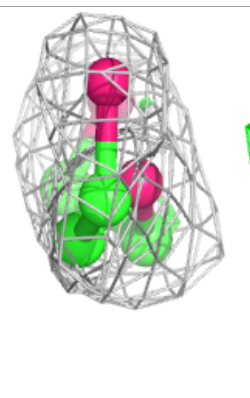
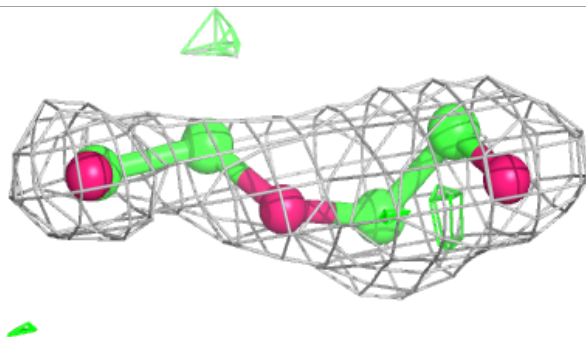
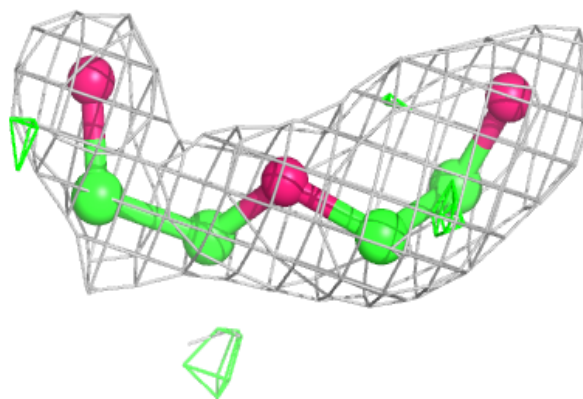
**Electron density around PEG E 303:**

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



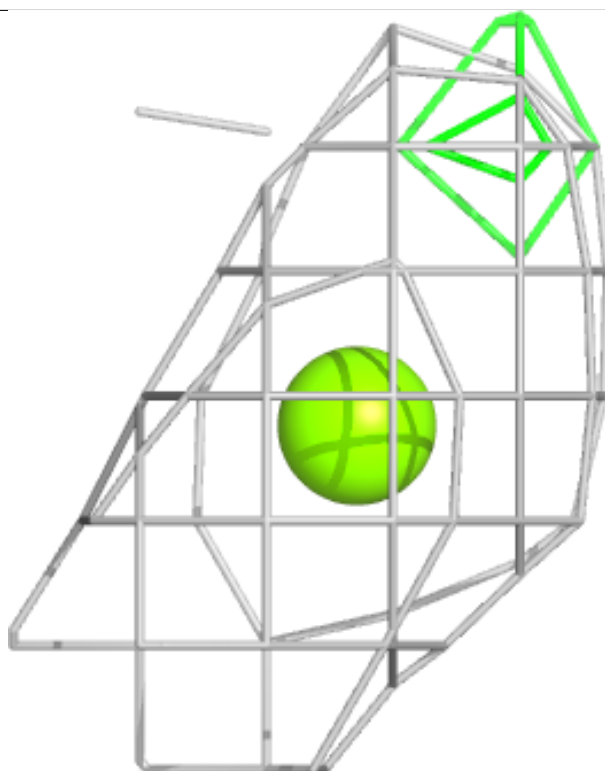
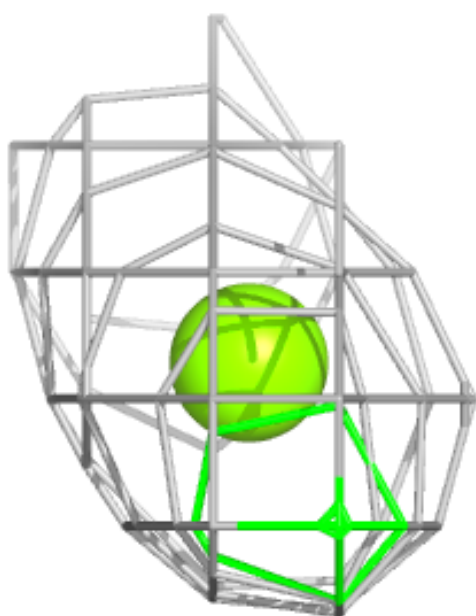
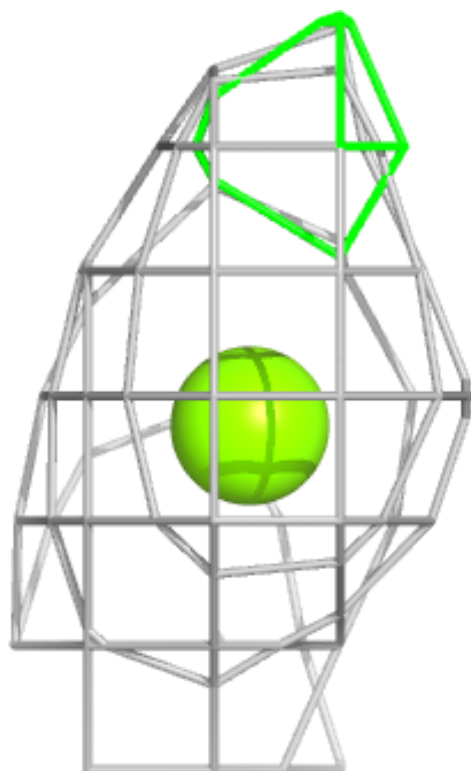
Electron density around PEG B 306:

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



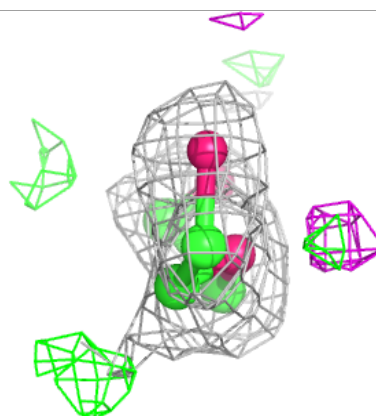
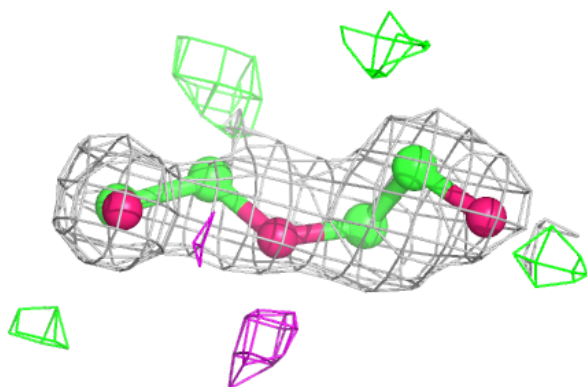
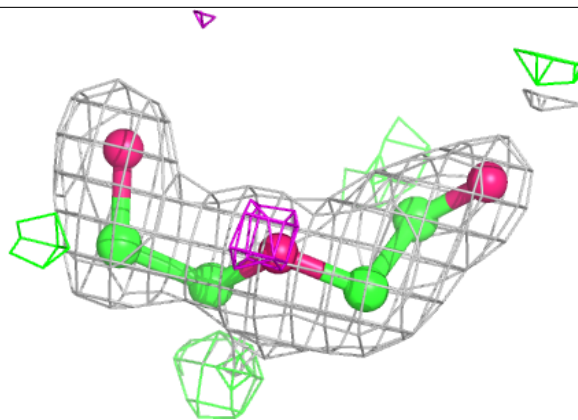
Electron density around MG C 307:

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

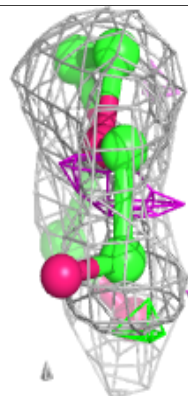
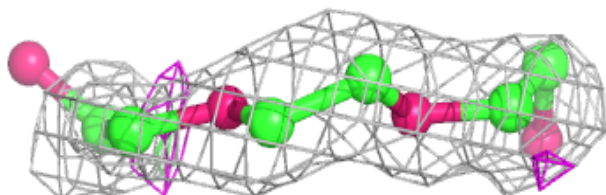
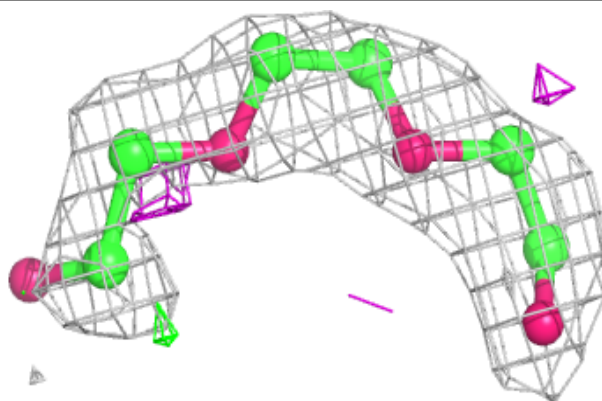


Electron density around PEG A 304:

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

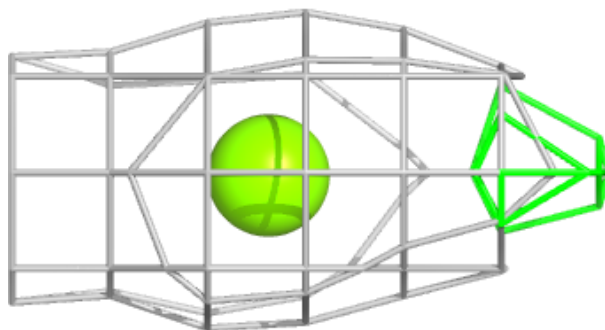
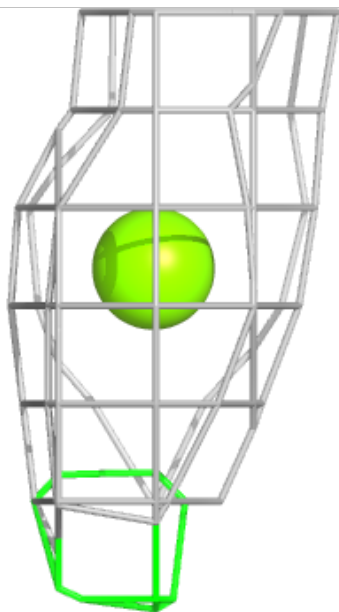
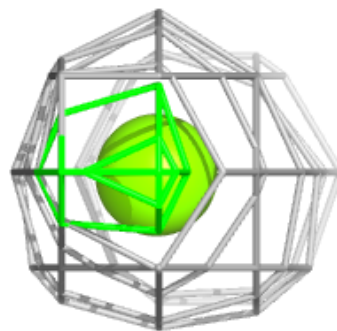
**Electron density around PGE C 313:**

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



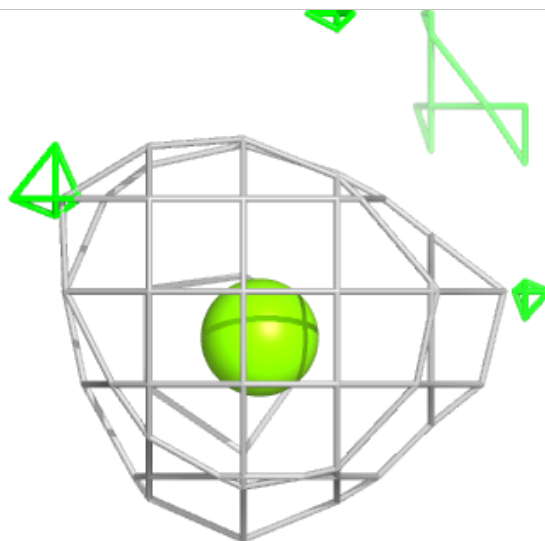
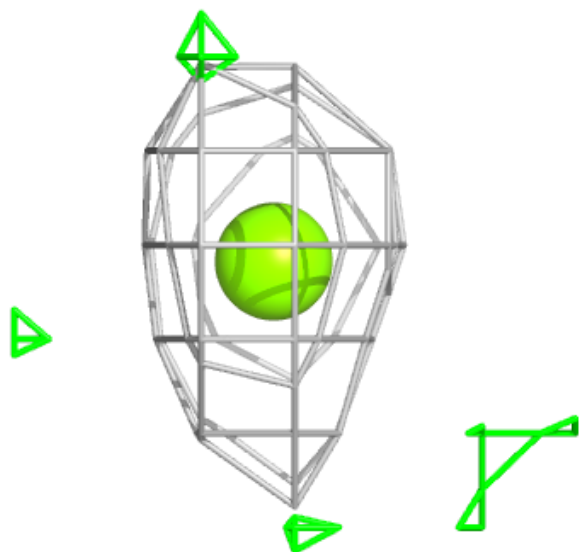
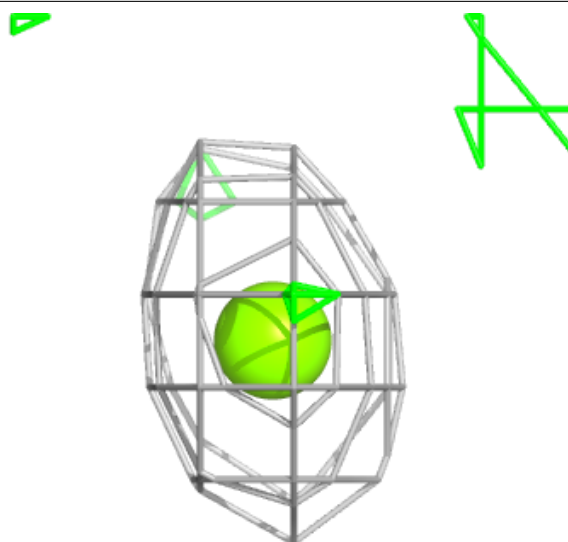
Electron density around MG B 303:

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



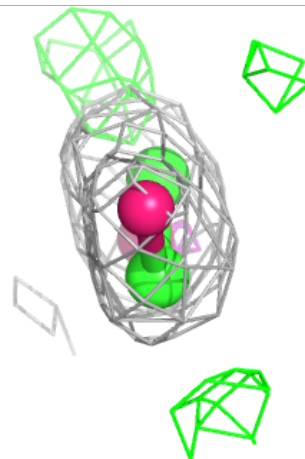
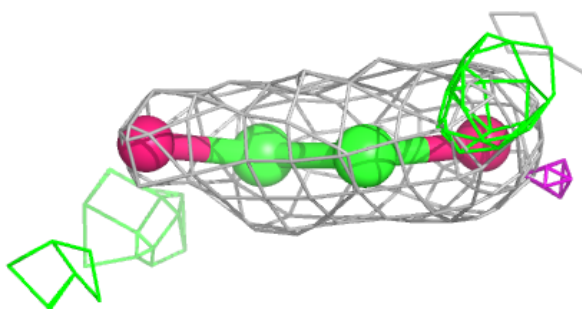
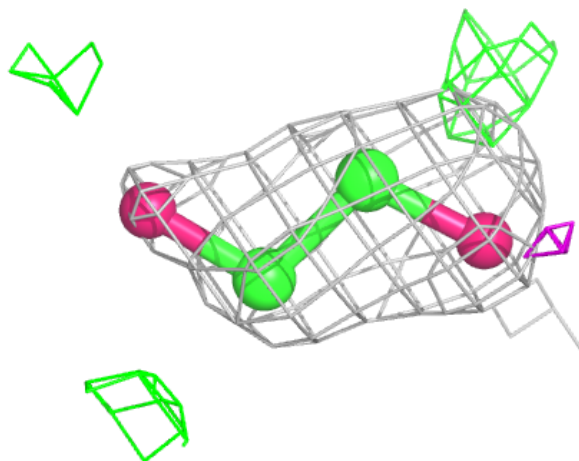
Electron density around MG C 304:

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



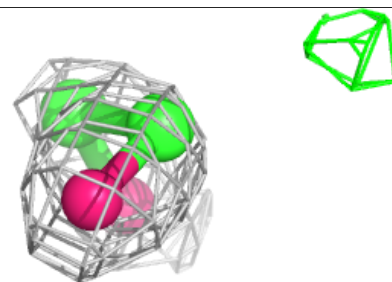
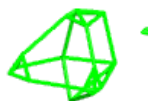
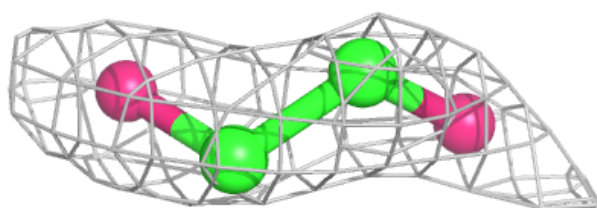
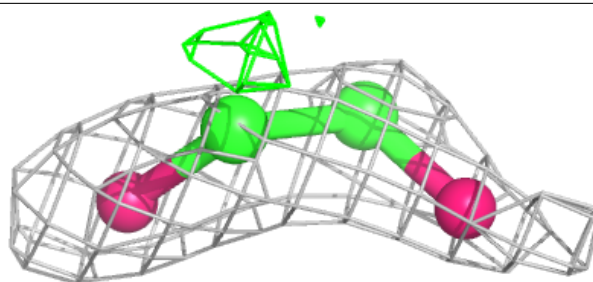
Electron density around EDO C 314:

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

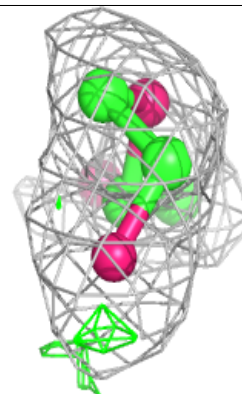
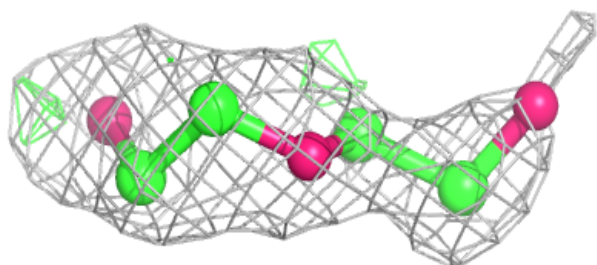
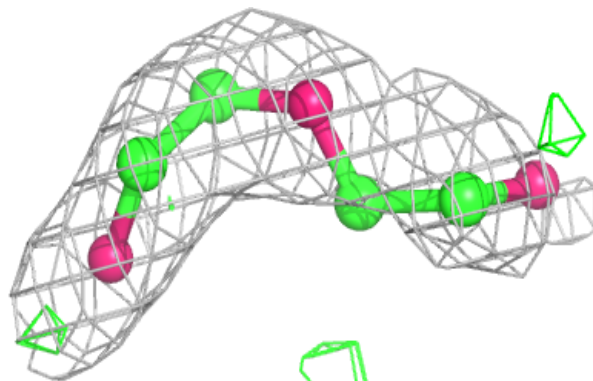


Electron density around EDO E 306:

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

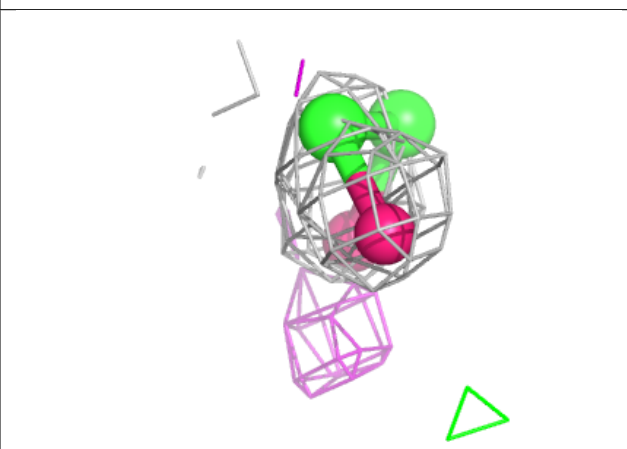
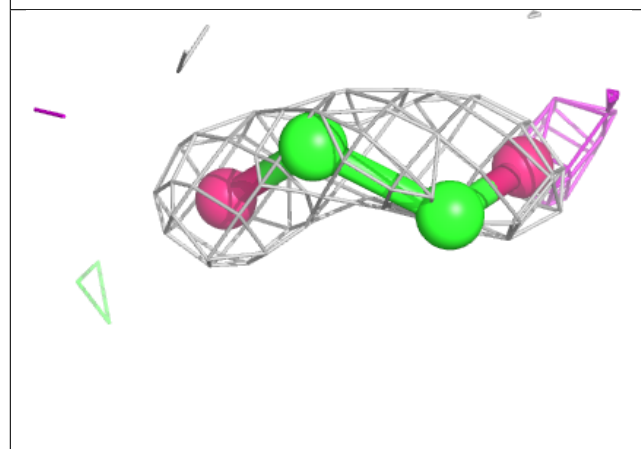
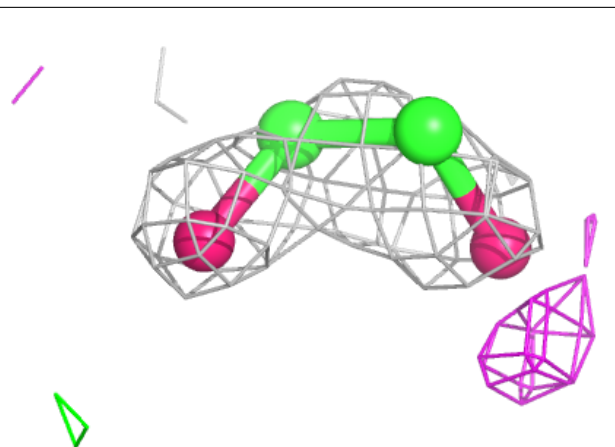
**Electron density around PEG F 304:**

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



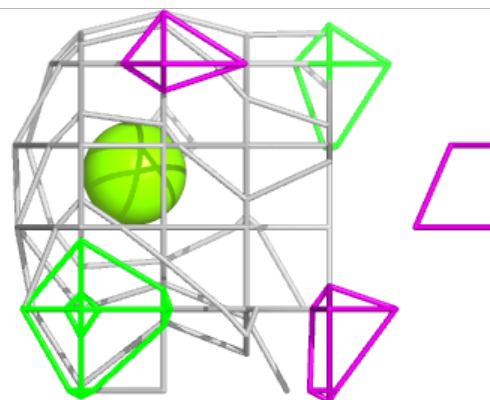
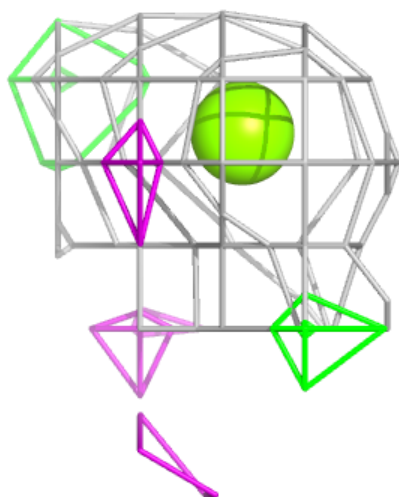
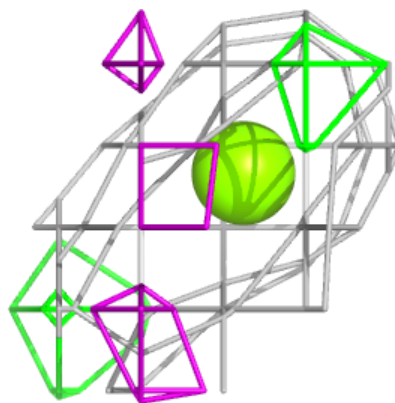
Electron density around EDO A 307:

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



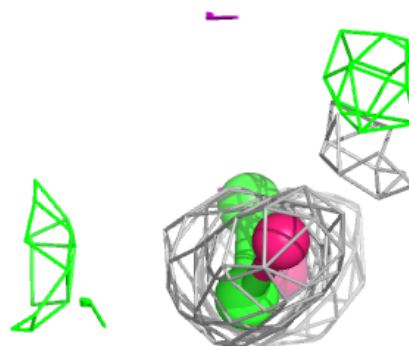
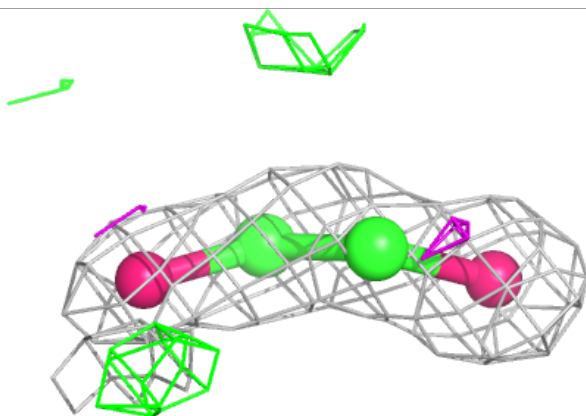
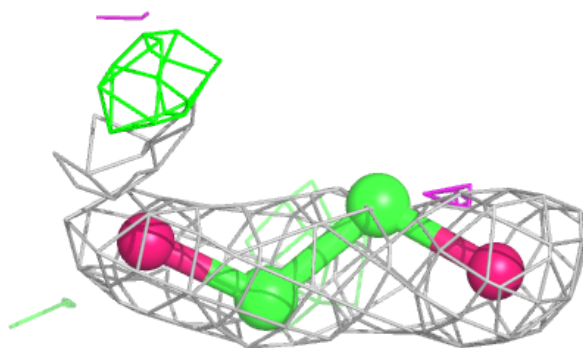
Electron density around MG C 306:

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



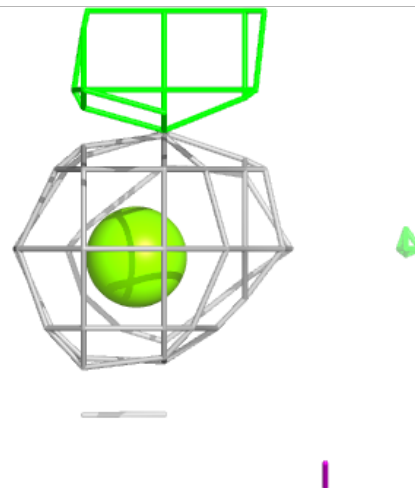
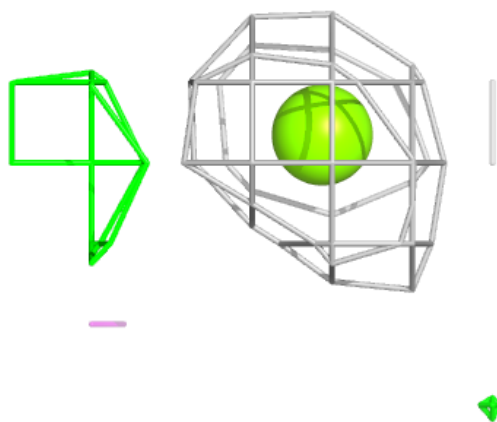
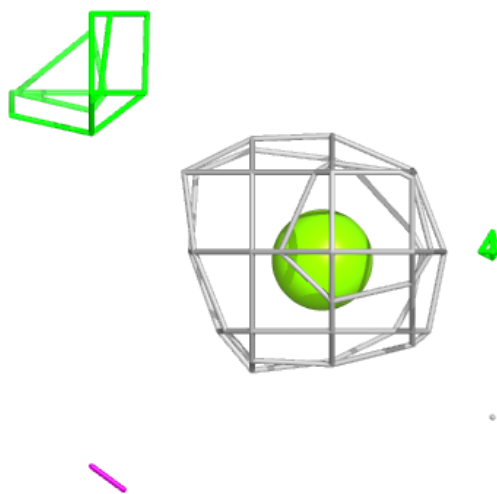
Electron density around EDO C 315:

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



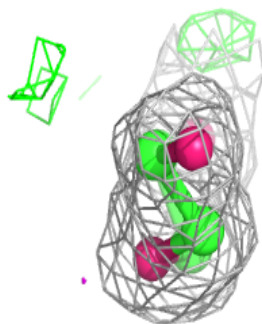
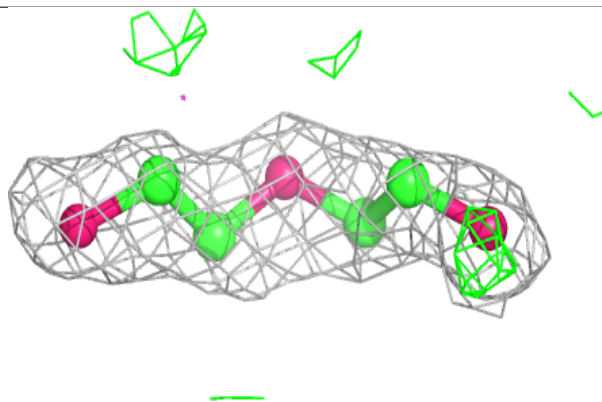
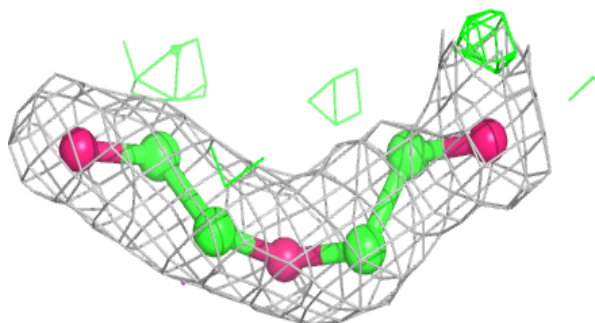
Electron density around MG C 303:

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

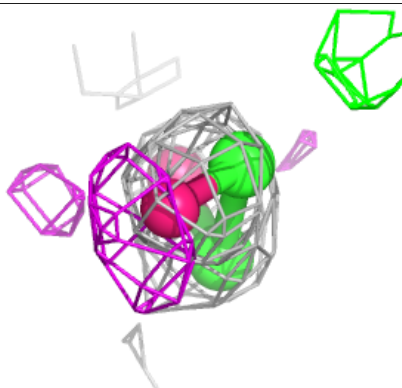
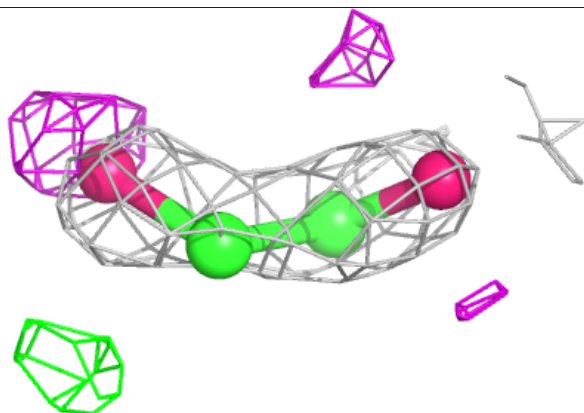
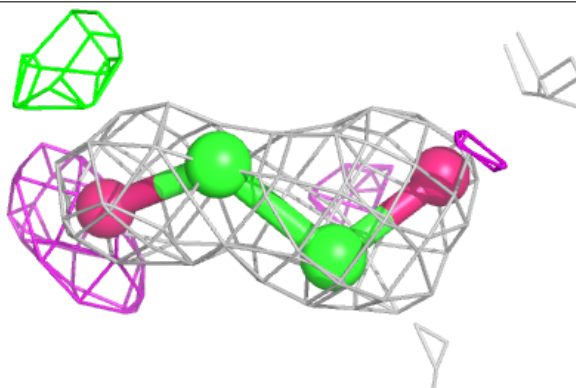


Electron density around PEG C 311:

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

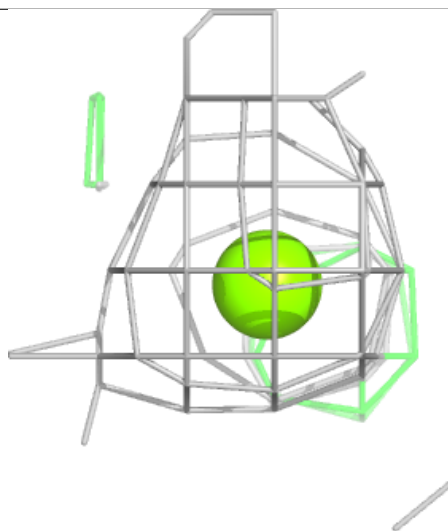
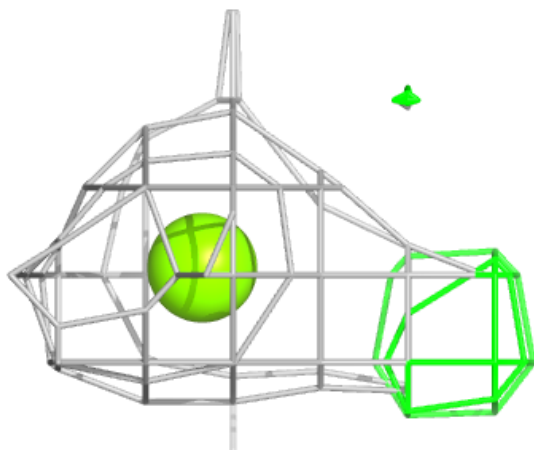
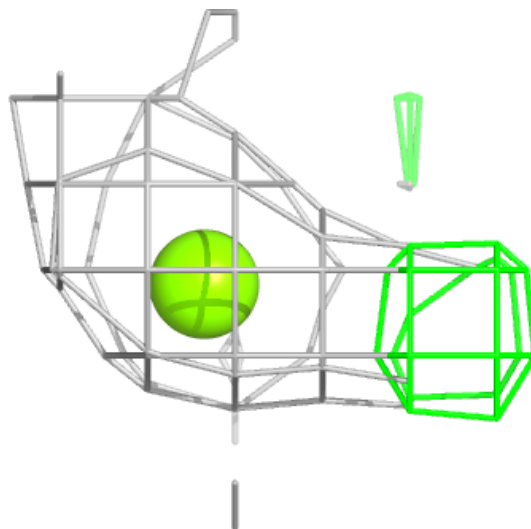
**Electron density around EDO E 307:**

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



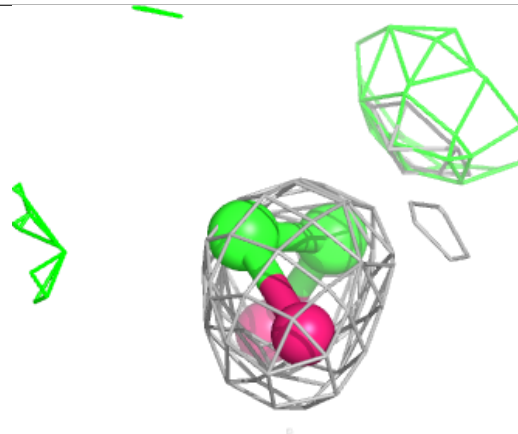
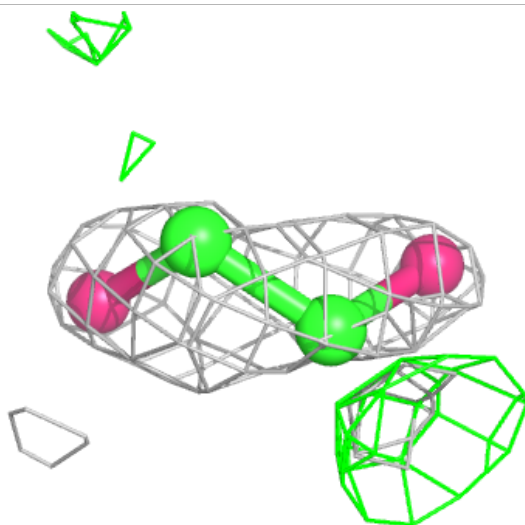
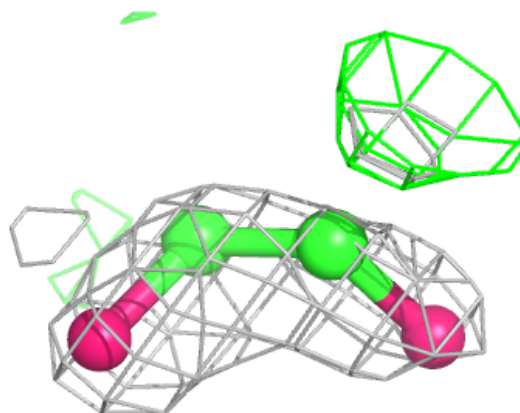
Electron density around MG D 303:

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



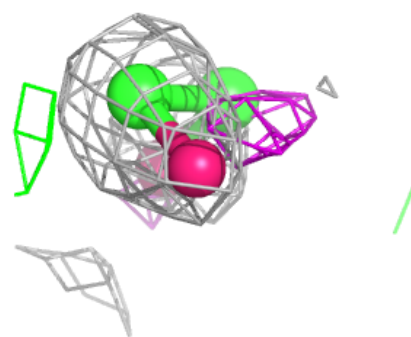
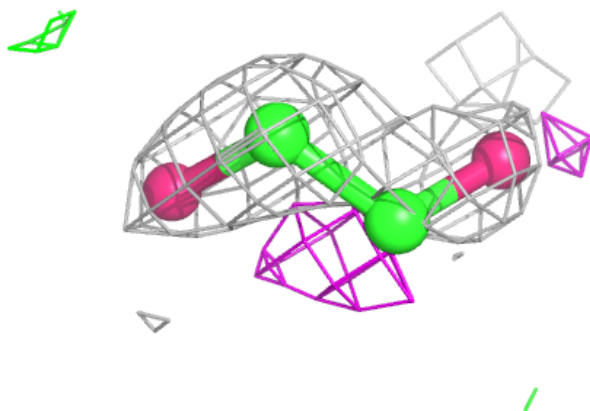
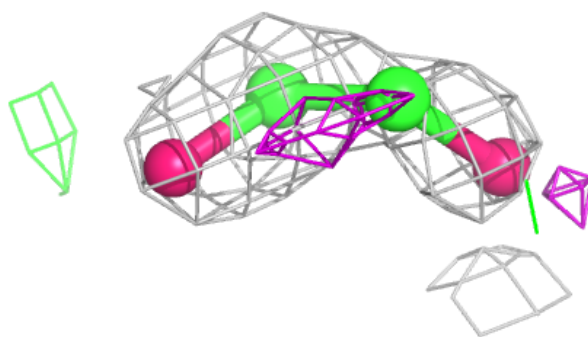
Electron density around EDO F 306:

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

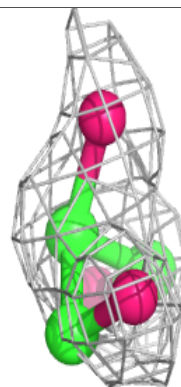
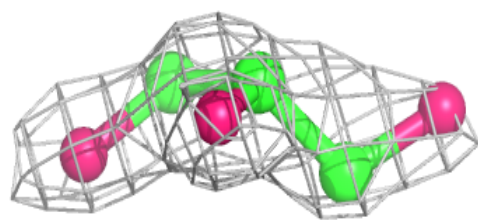
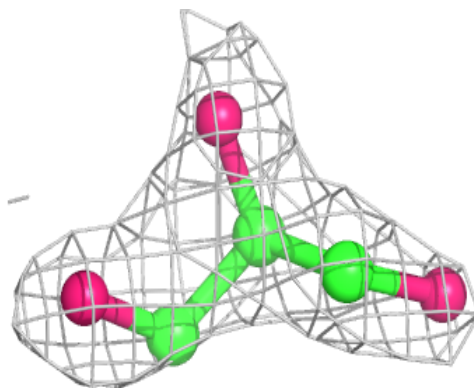


Electron density around EDO E 305:

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

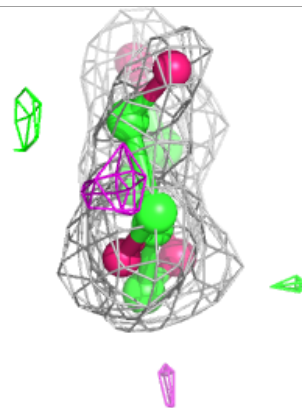
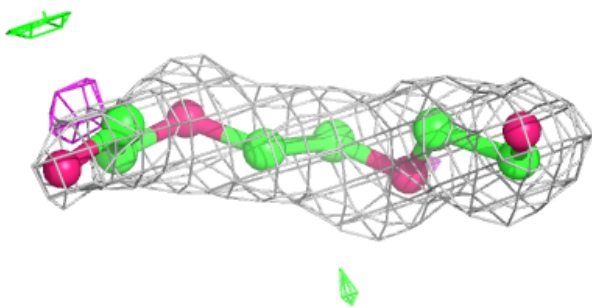
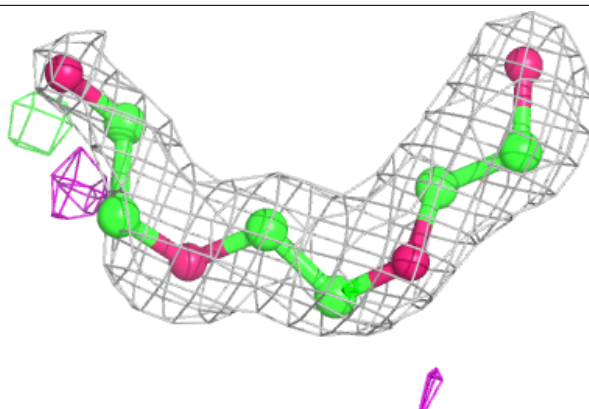
**Electron density around GOL B 308:**

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



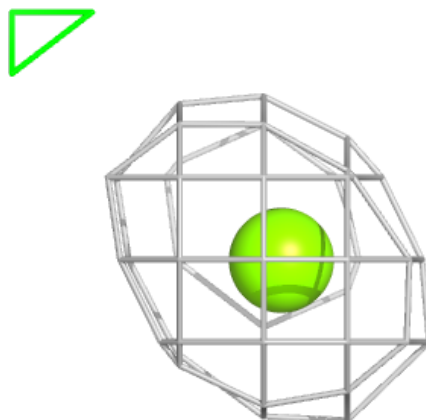
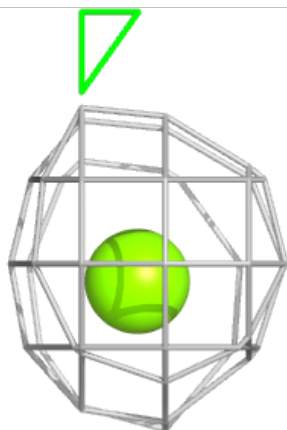
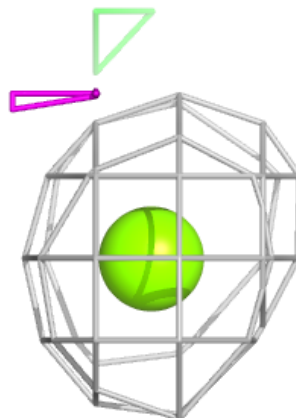
Electron density around PGE F 305:

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



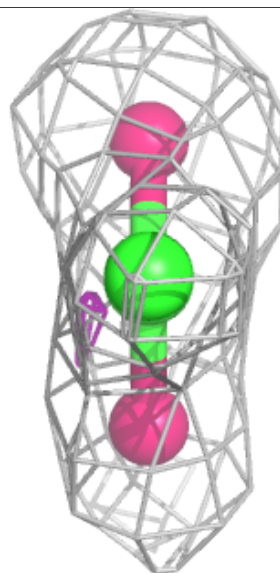
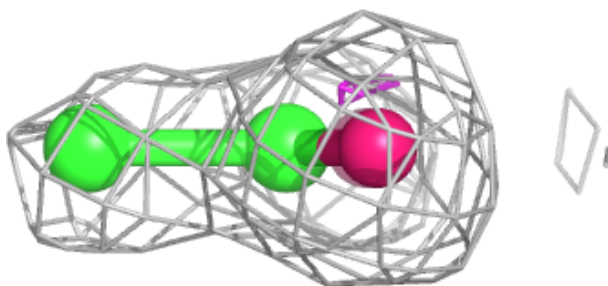
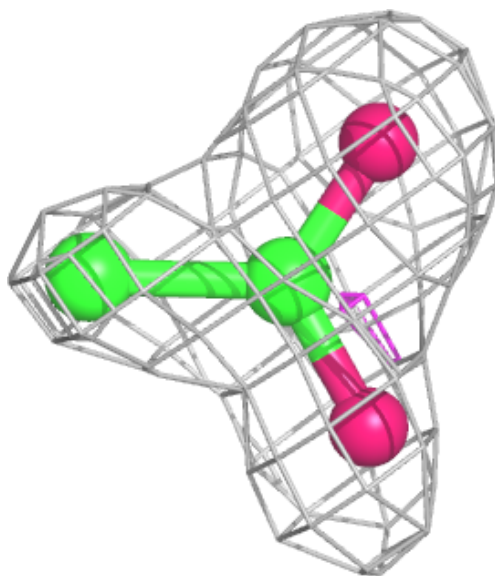
Electron density around MG C 302:

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



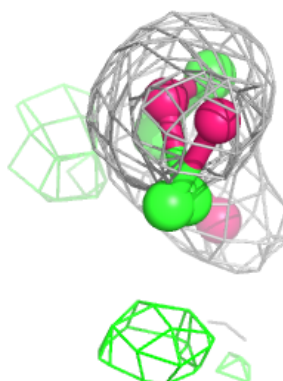
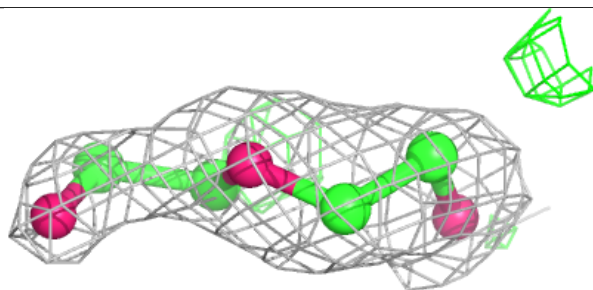
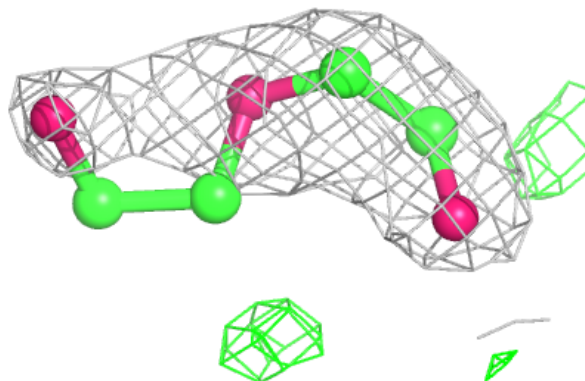
Electron density around ACT F 310:

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

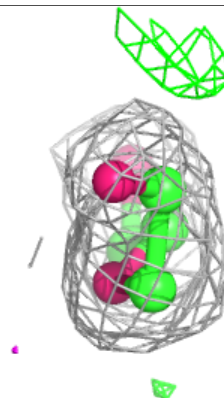
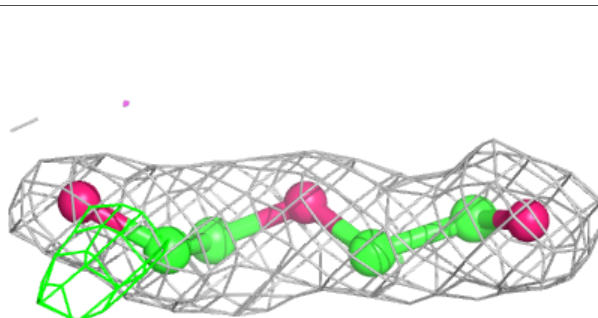
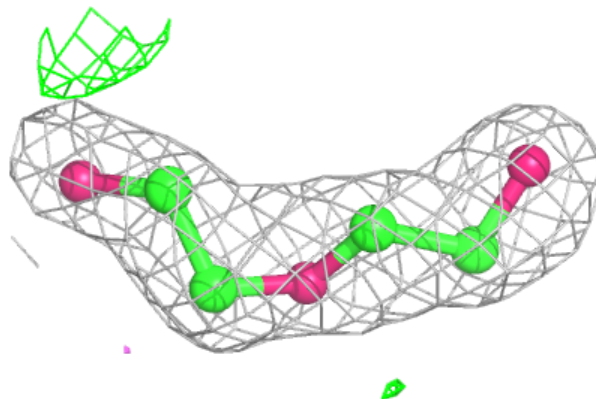


Electron density around PEG D 305:

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

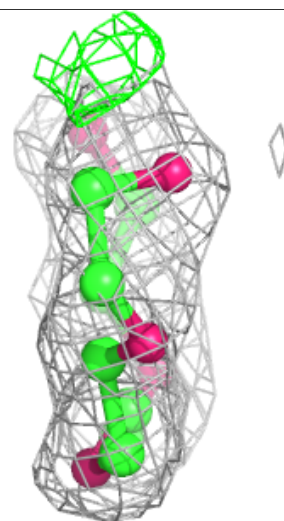
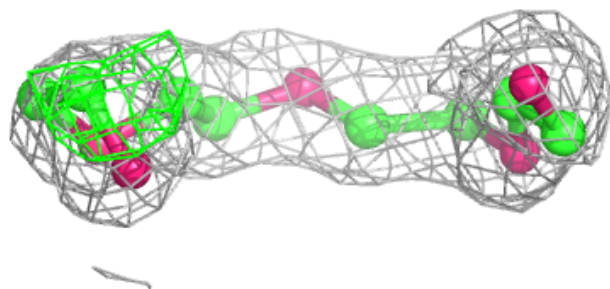
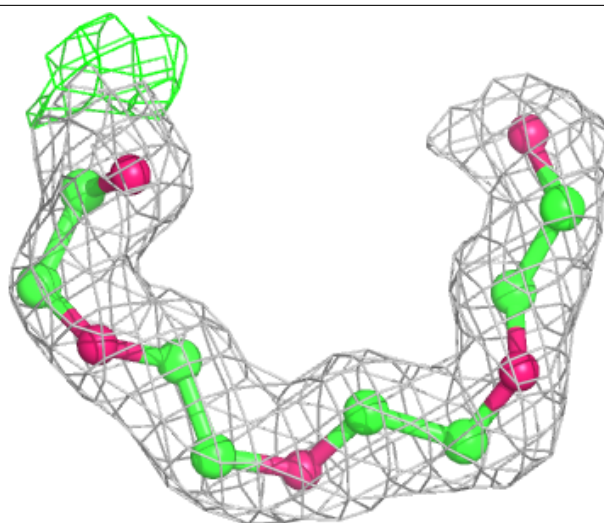
**Electron density around PEG E 304:**

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



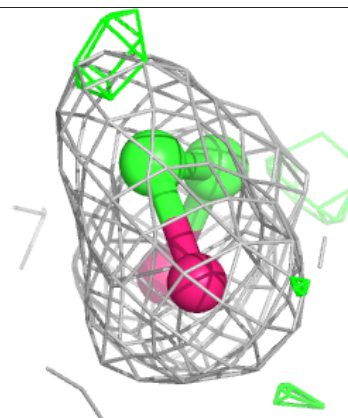
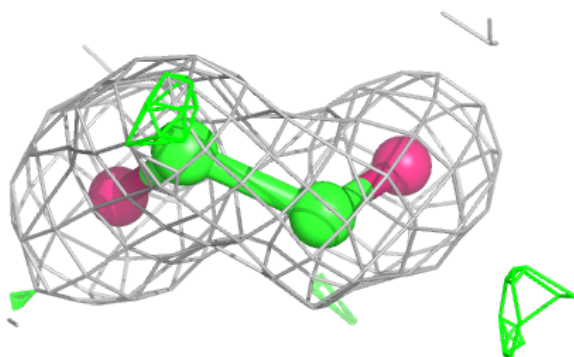
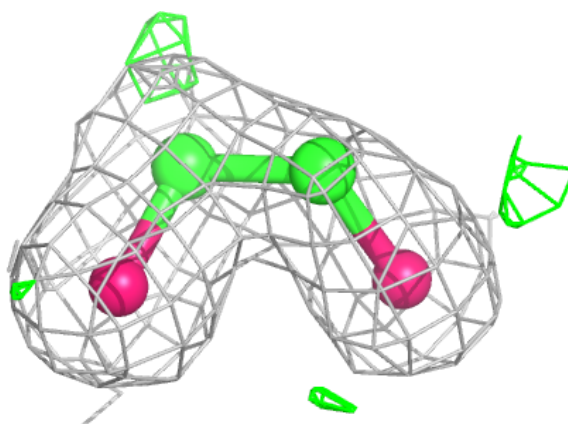
Electron density around PG4 D 304:

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



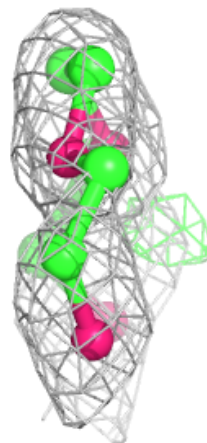
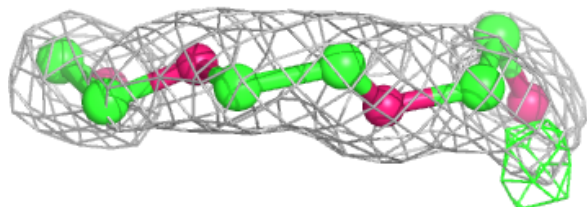
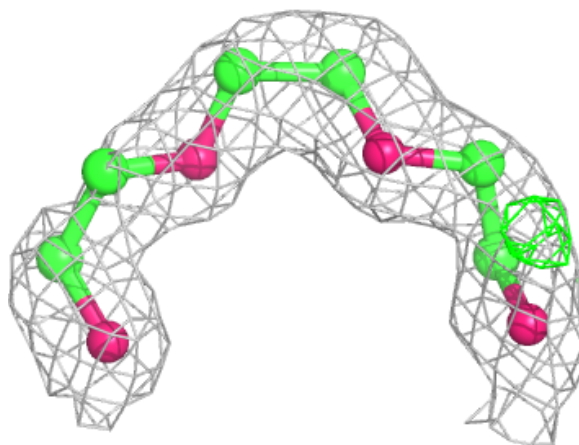
Electron density around EDO A 306:

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



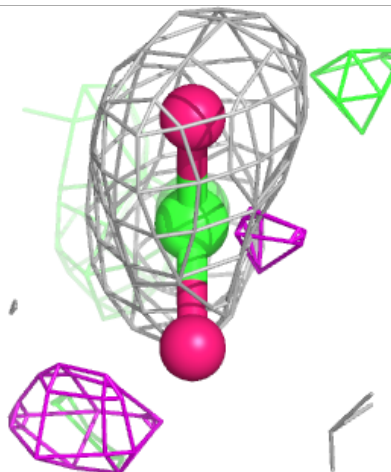
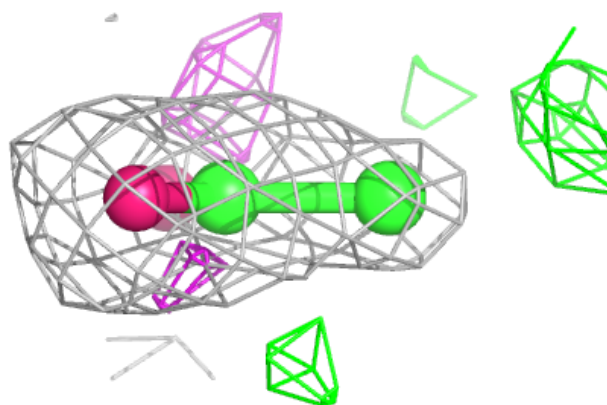
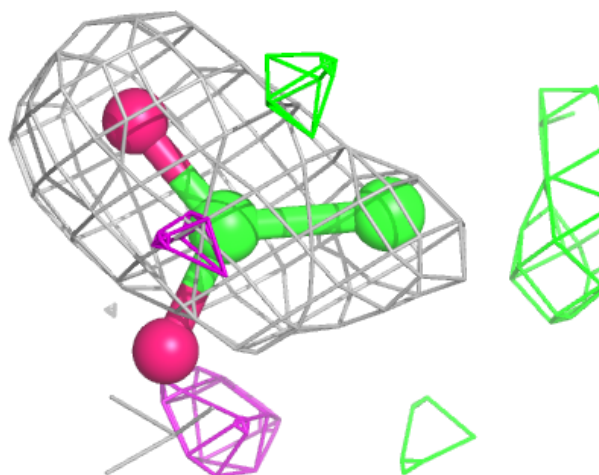
Electron density around PGE C 312:

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



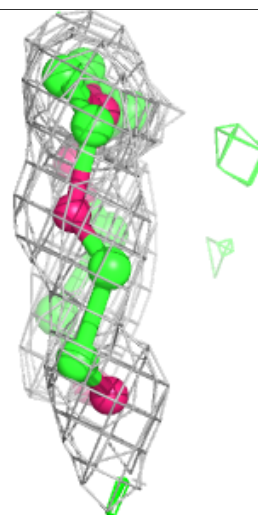
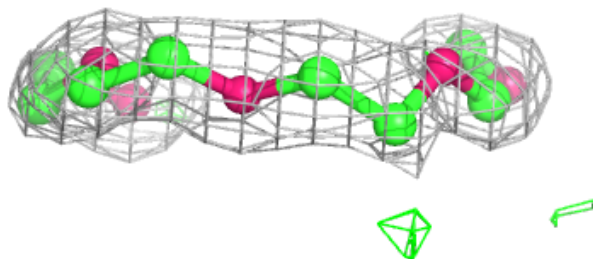
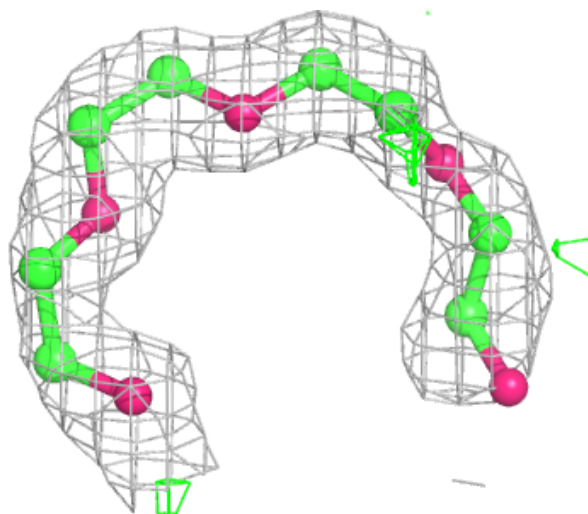
Electron density around ACT F 309:

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



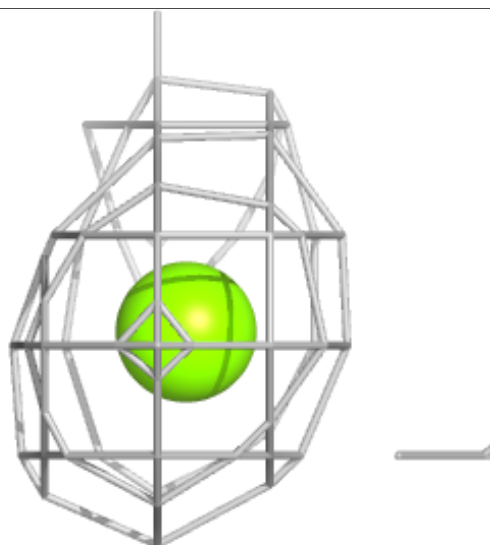
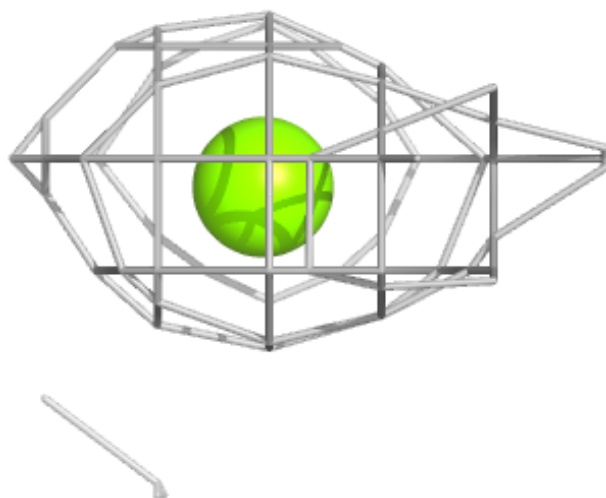
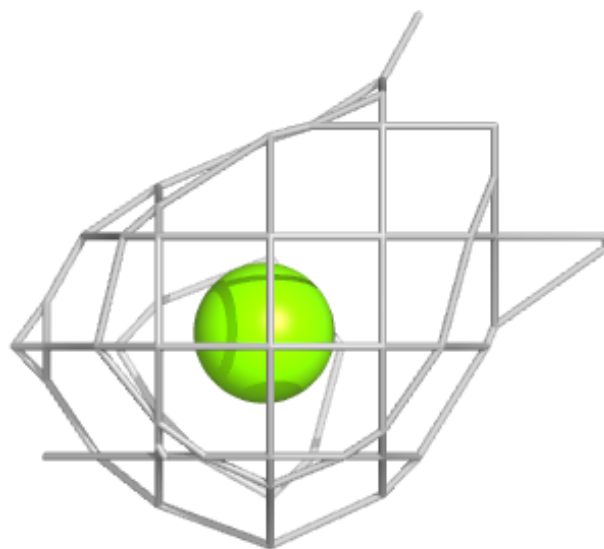
Electron density around PG4 A 303:

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



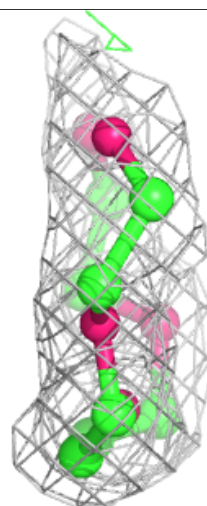
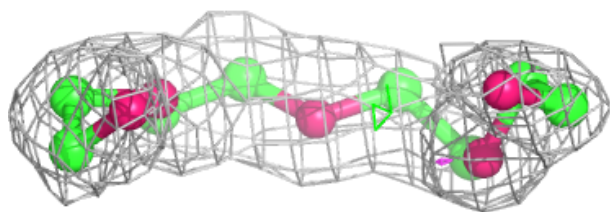
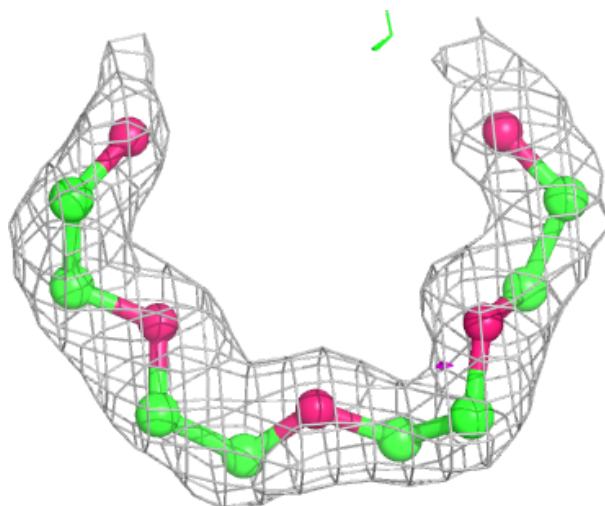
Electron density around MG E 302:

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



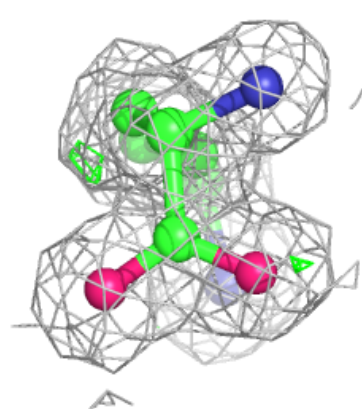
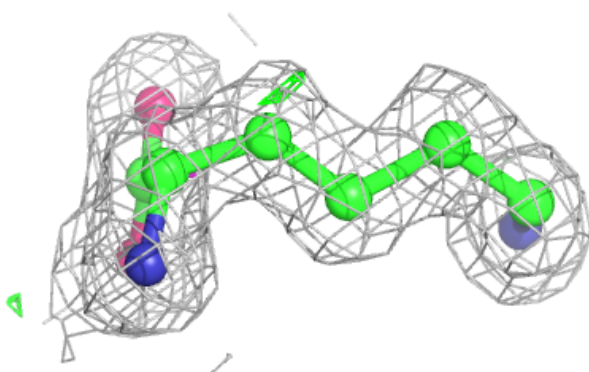
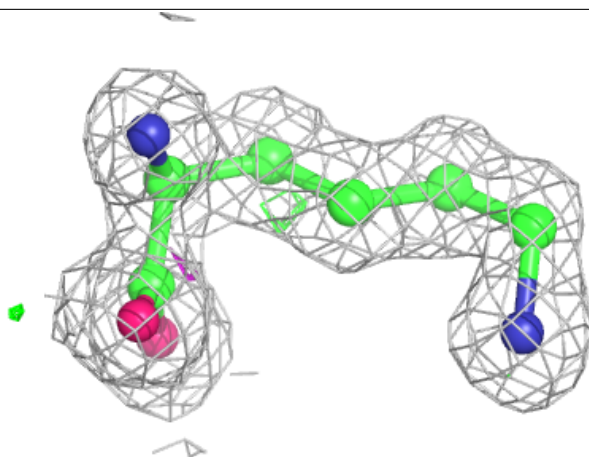
Electron density around PG4 B 305:

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



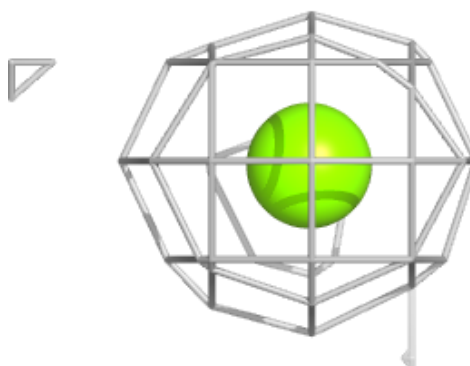
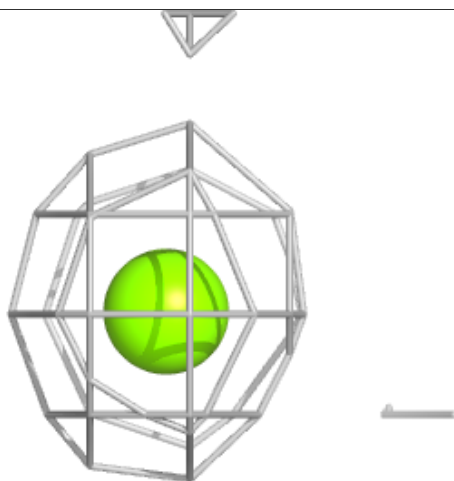
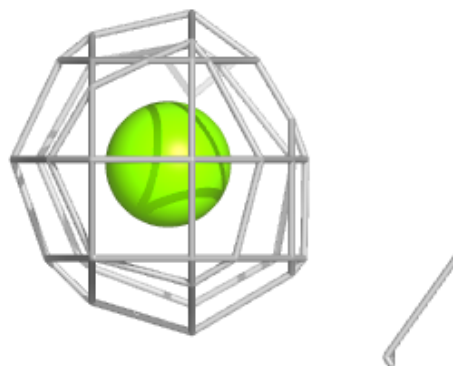
Electron density around LYS B 307:

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



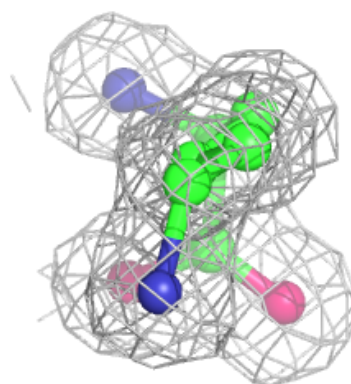
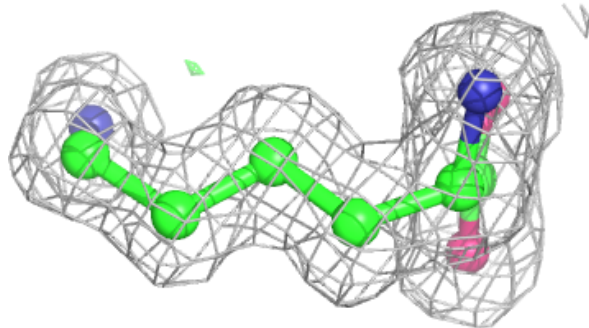
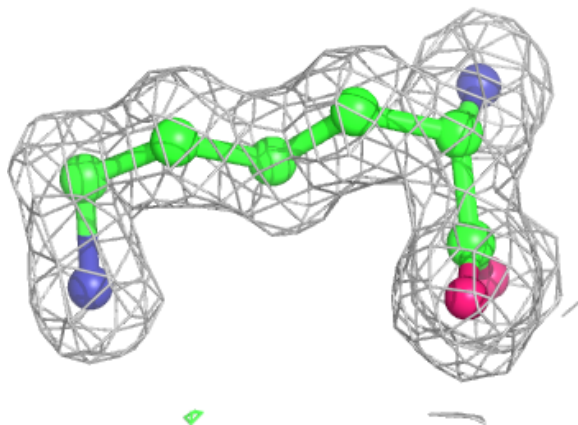
Electron density around MG C 308:

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



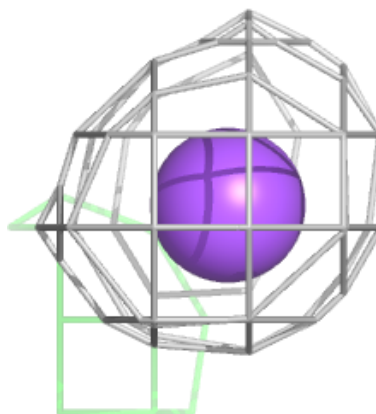
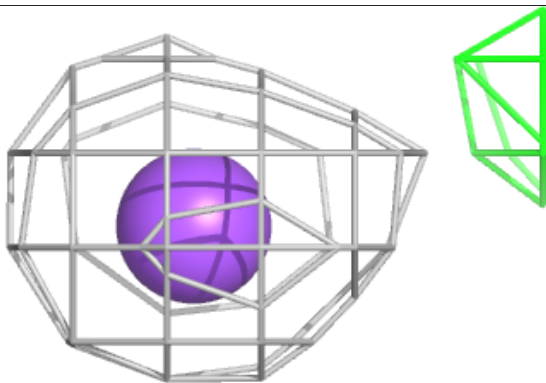
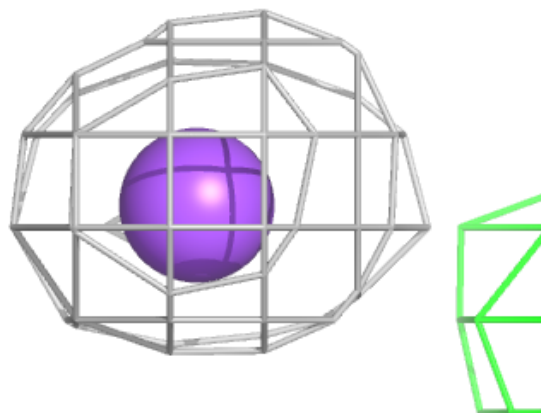
Electron density around LYS C 316:

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



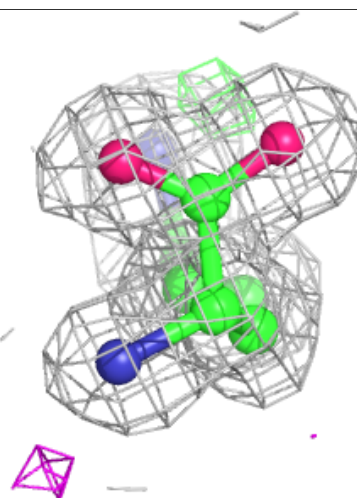
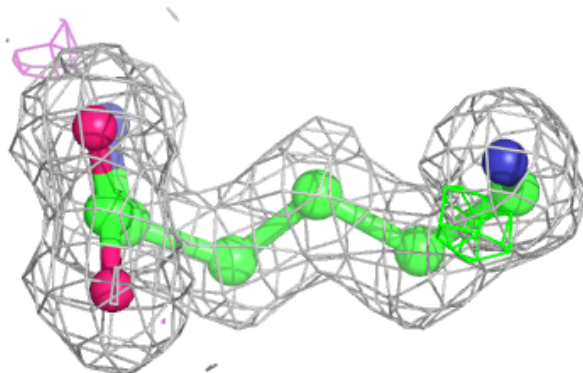
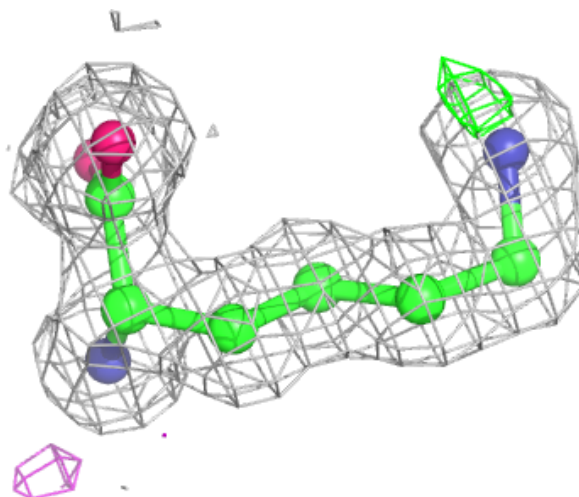
Electron density around NA A 302:

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



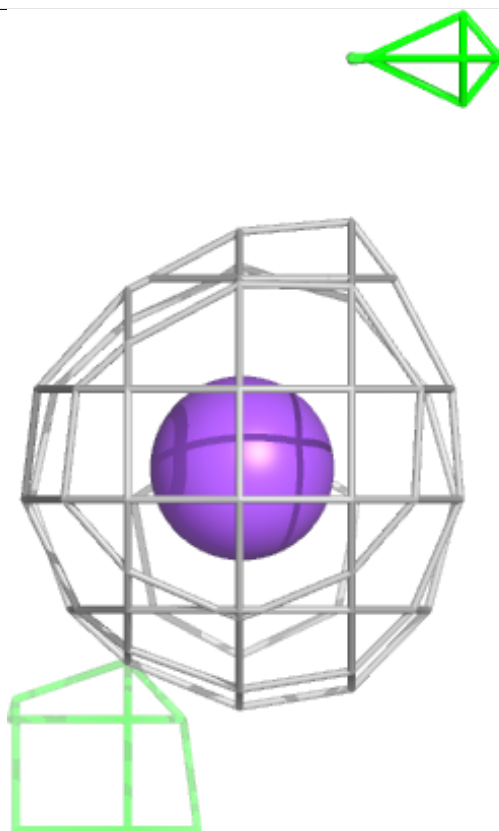
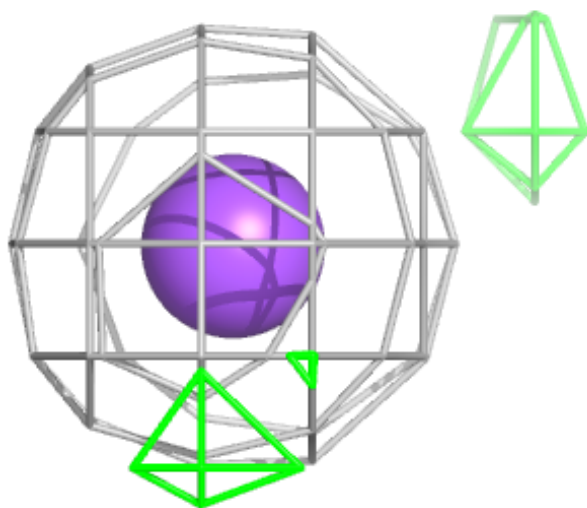
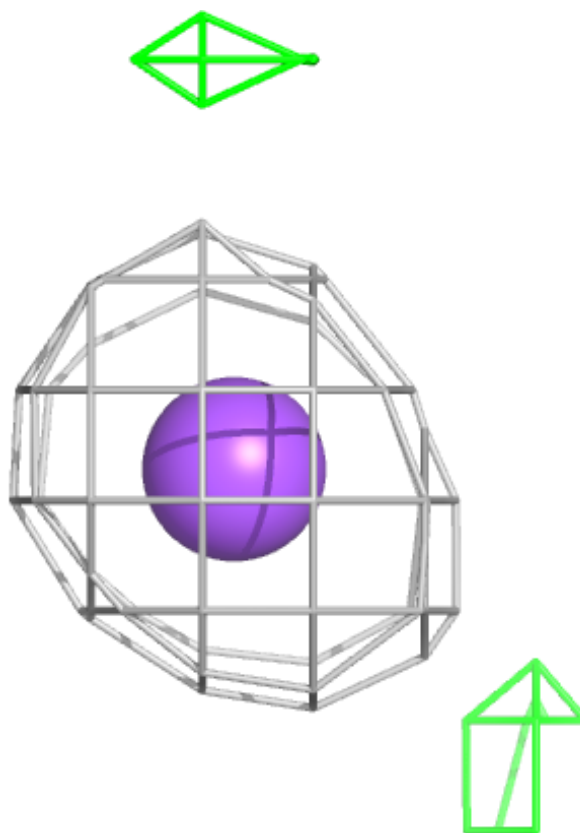
Electron density around LYS A 308:

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



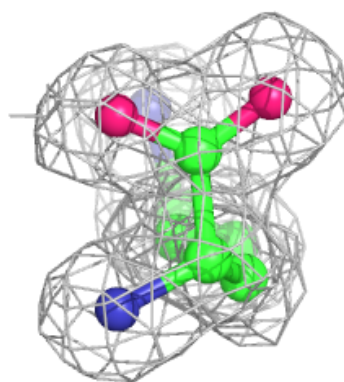
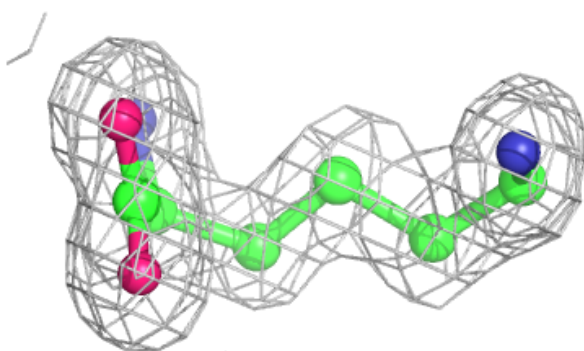
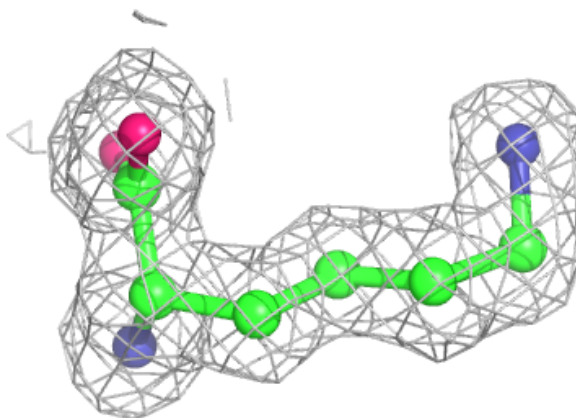
Electron density around NA C 309:

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



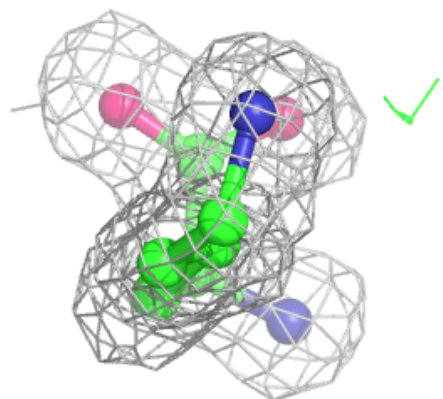
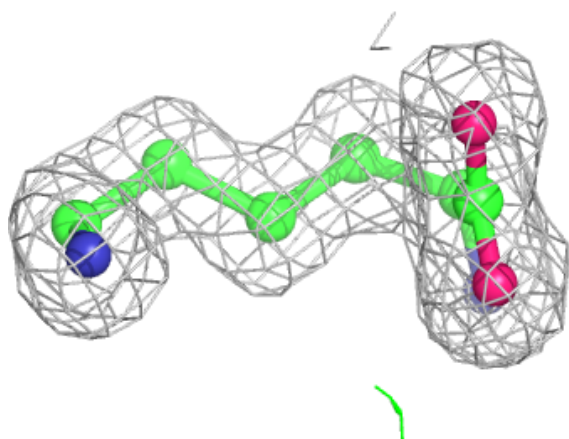
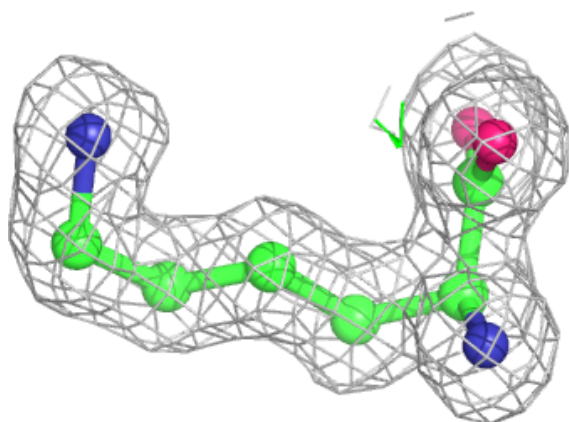
Electron density around LYS E 308:

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



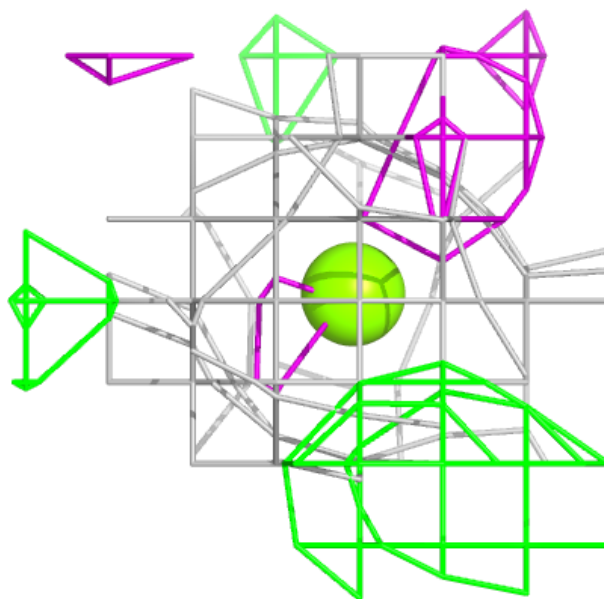
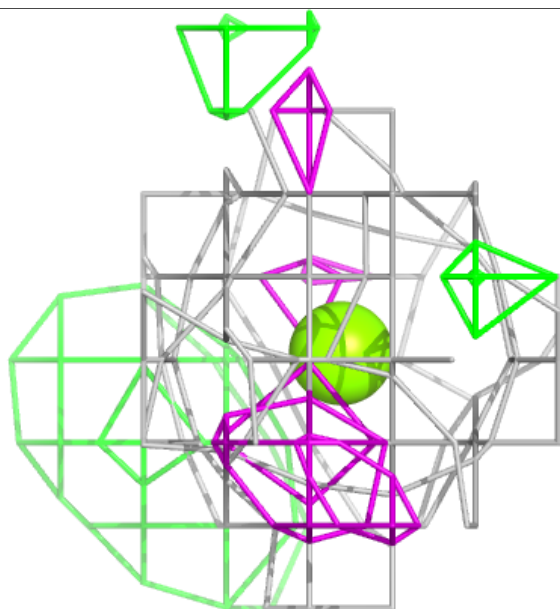
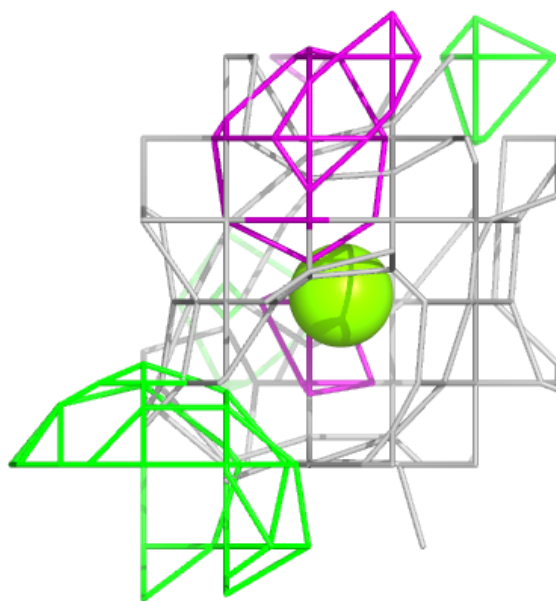
Electron density around LYS F 308:

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



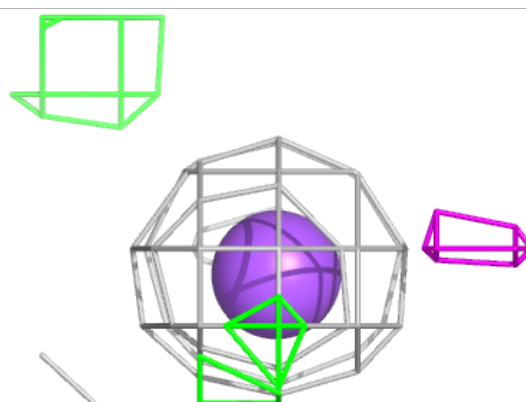
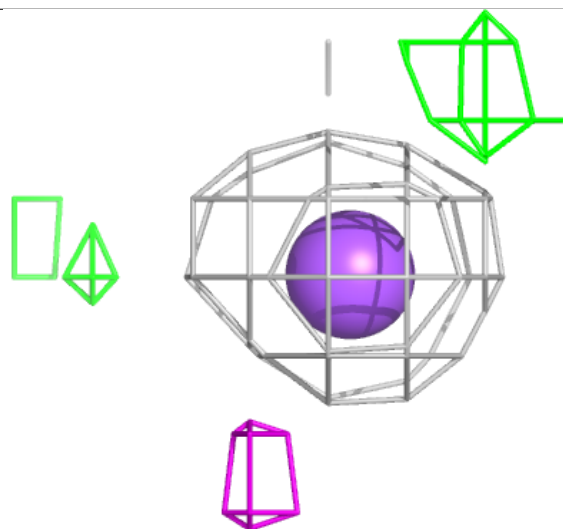
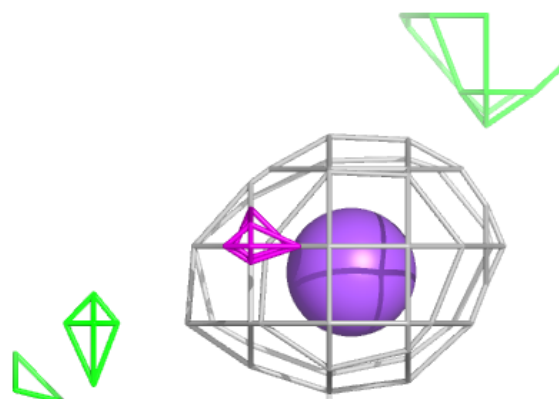
Electron density around MG B 302:

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



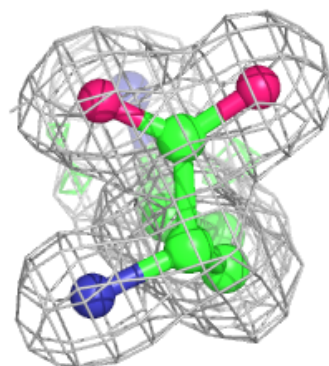
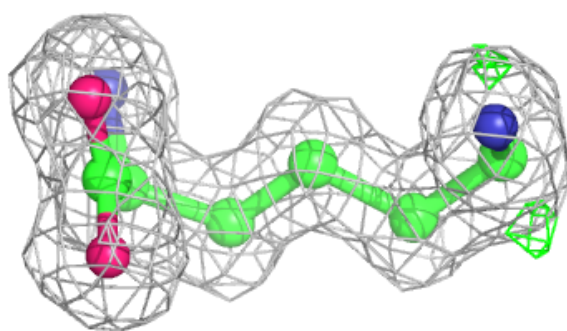
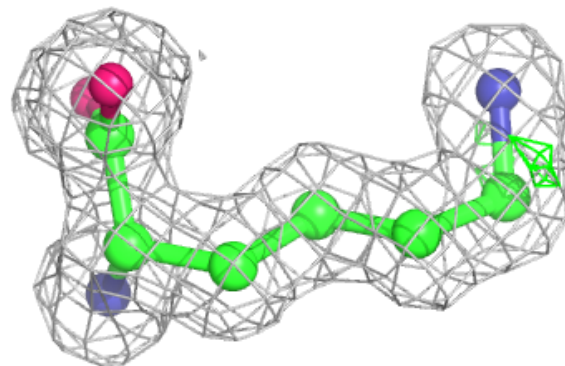
Electron density around NA C 310:

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



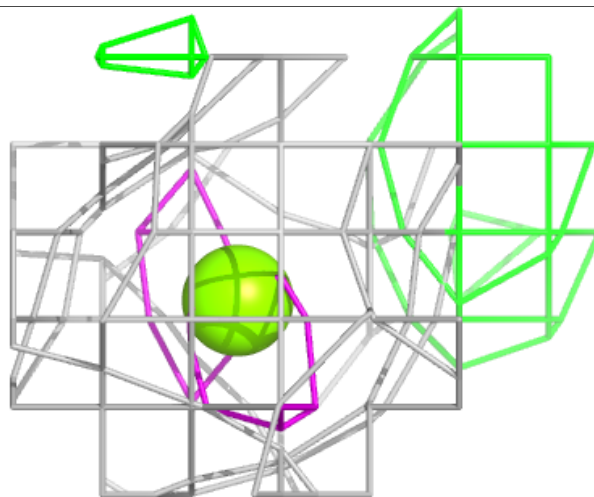
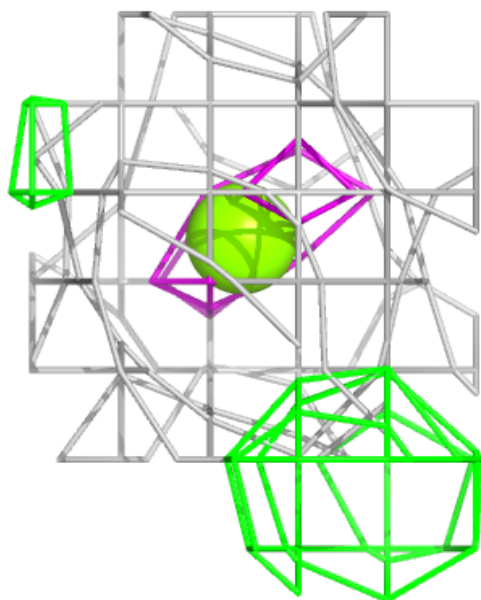
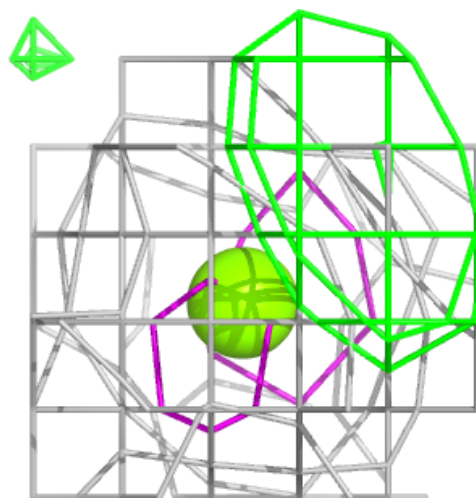
Electron density around LYS D 306:

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



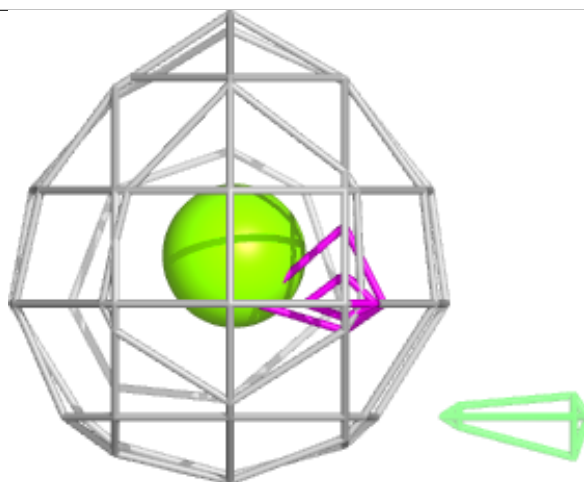
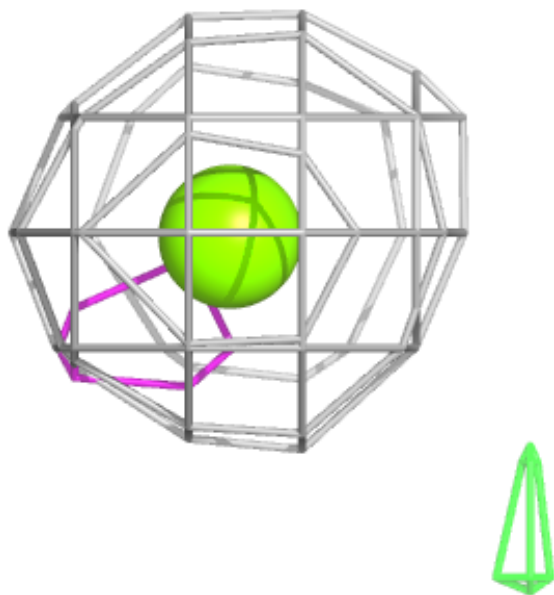
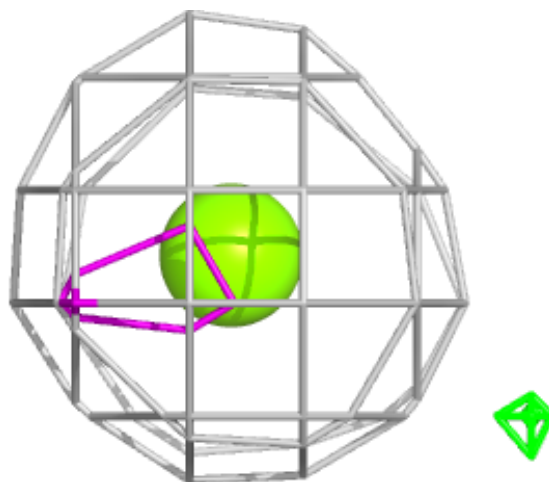
Electron density around MG C 301:

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



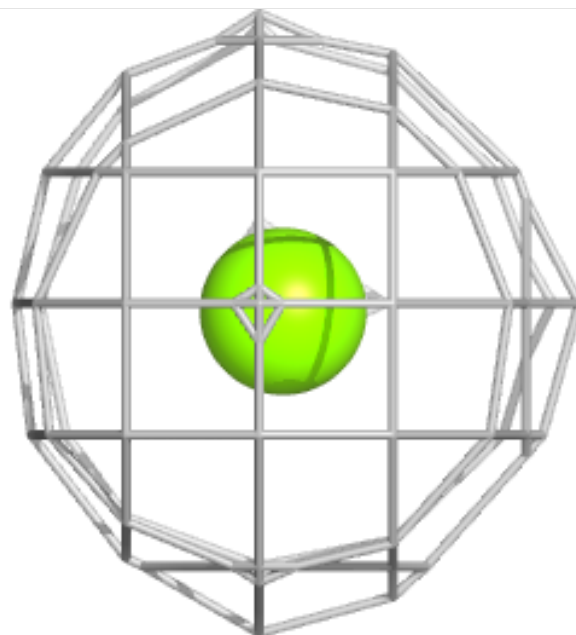
Electron density around MG D 301:

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



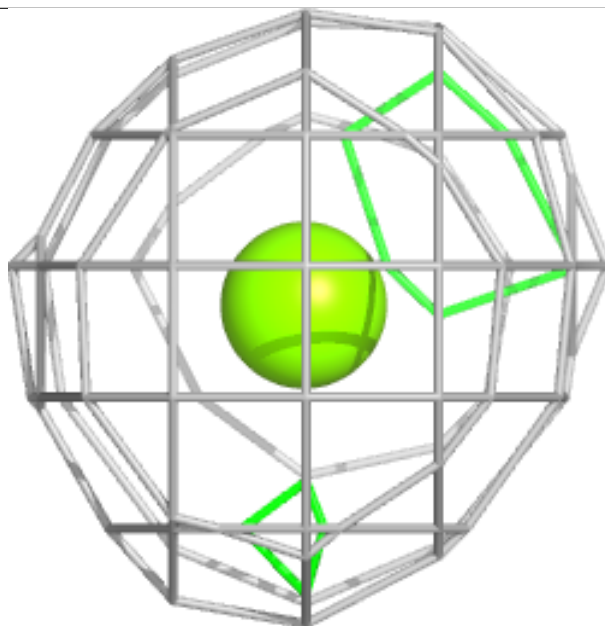
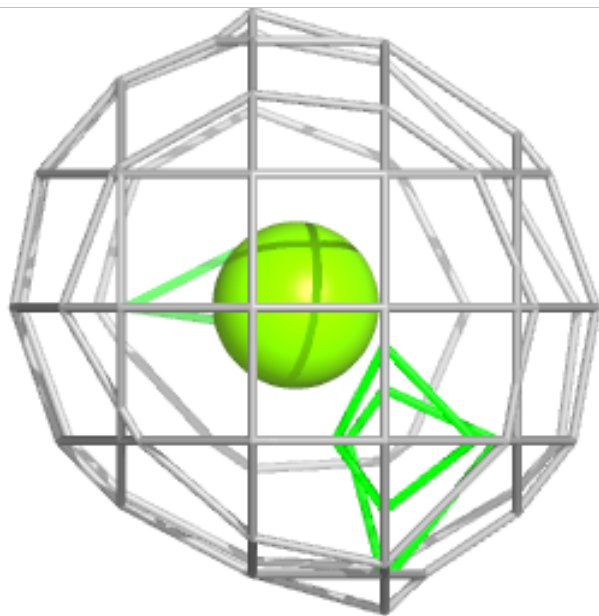
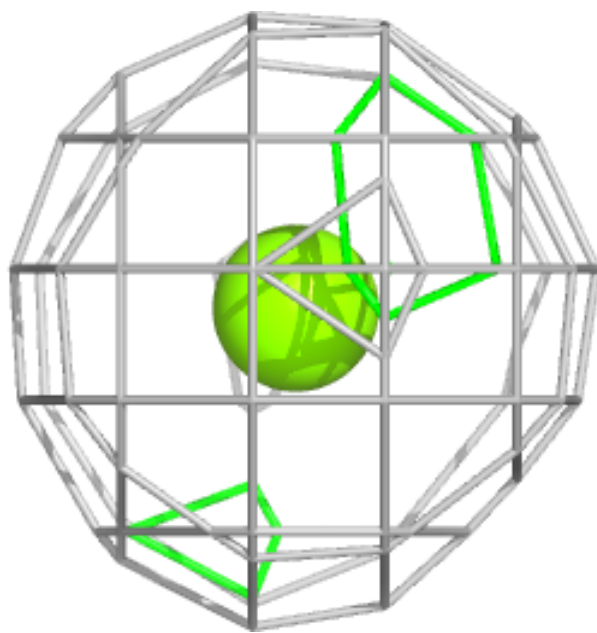
Electron density around MG D 302:

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



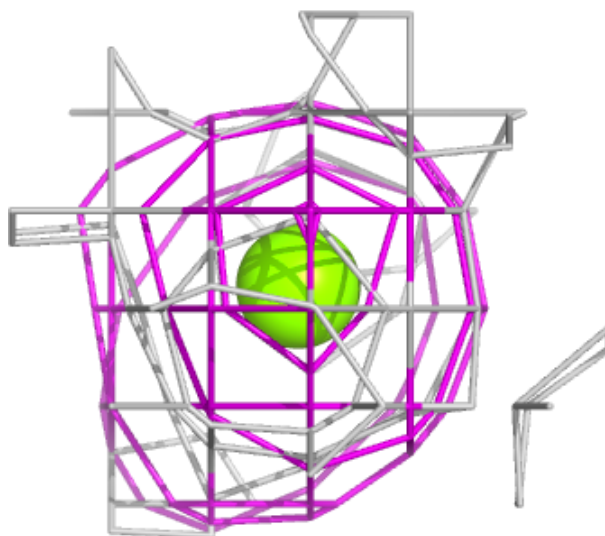
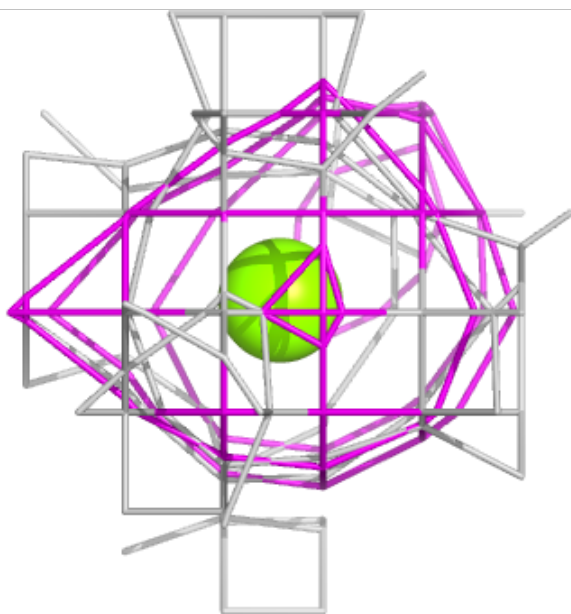
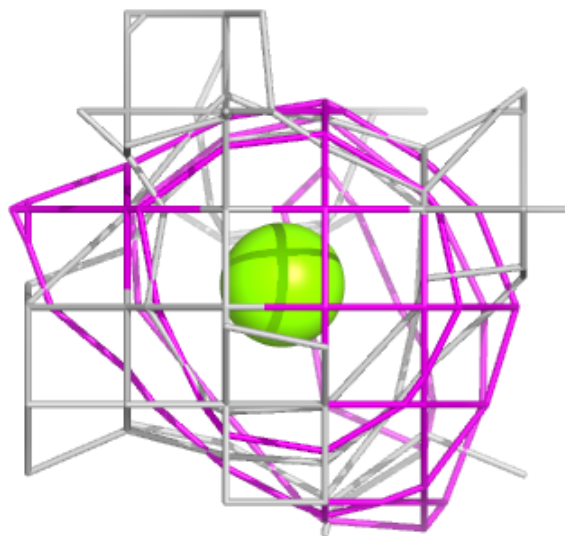
Electron density around MG B 301:

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



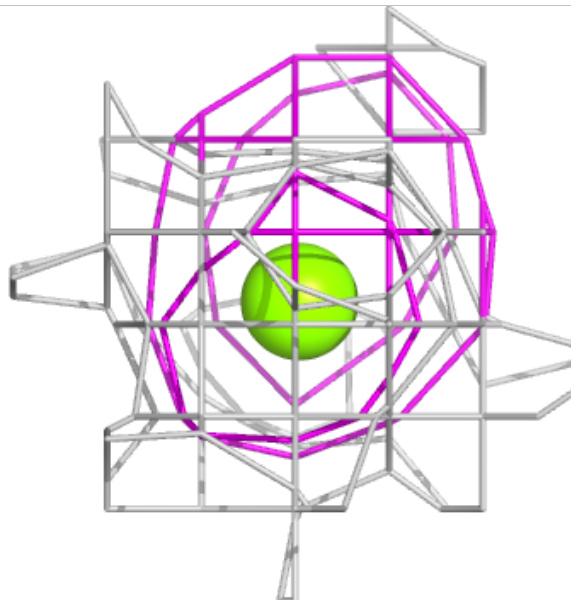
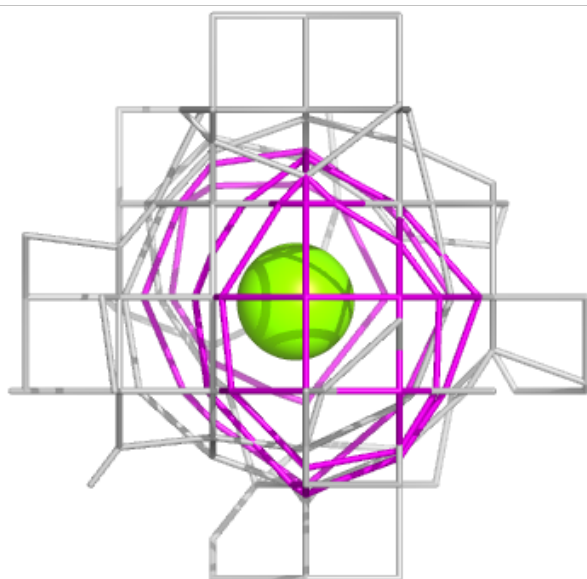
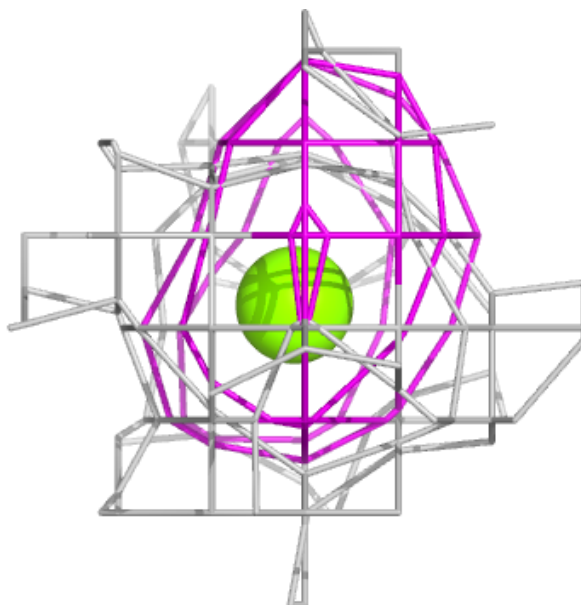
Electron density around MG B 304:

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



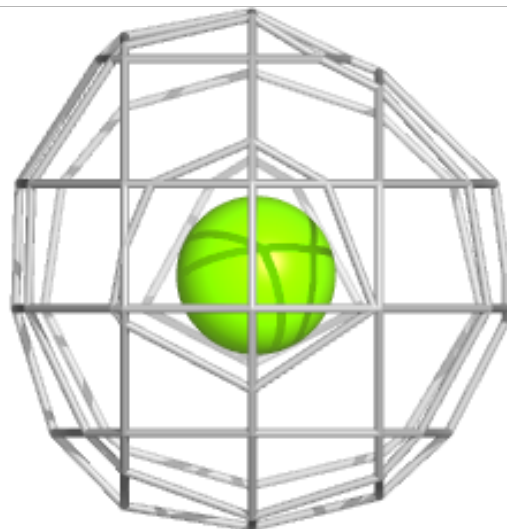
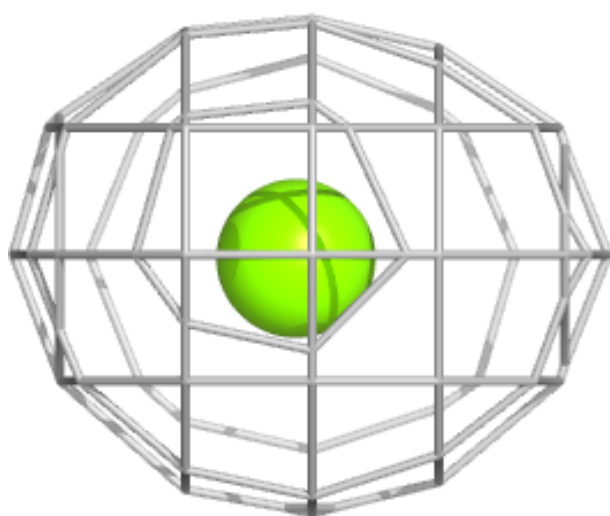
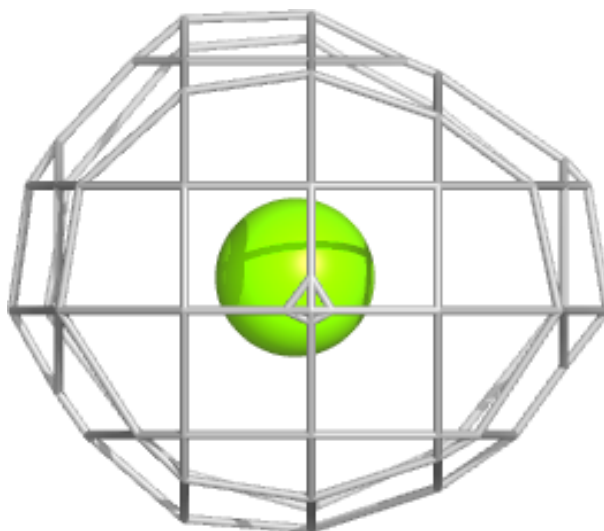
Electron density around MG F 302:

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



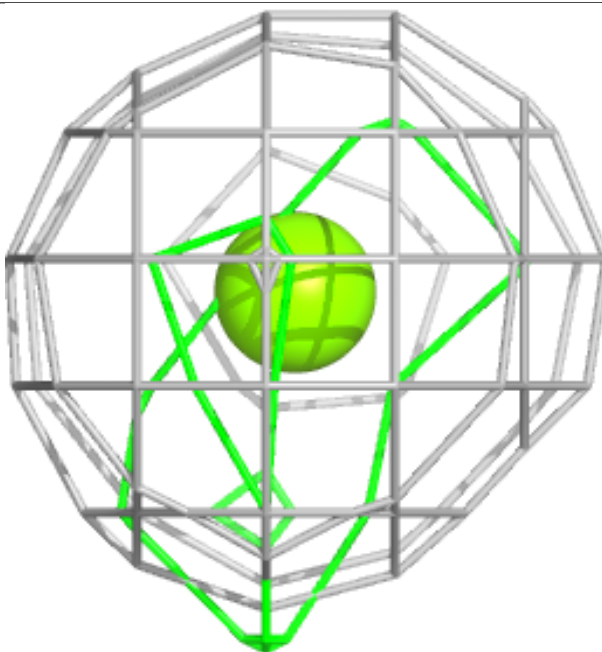
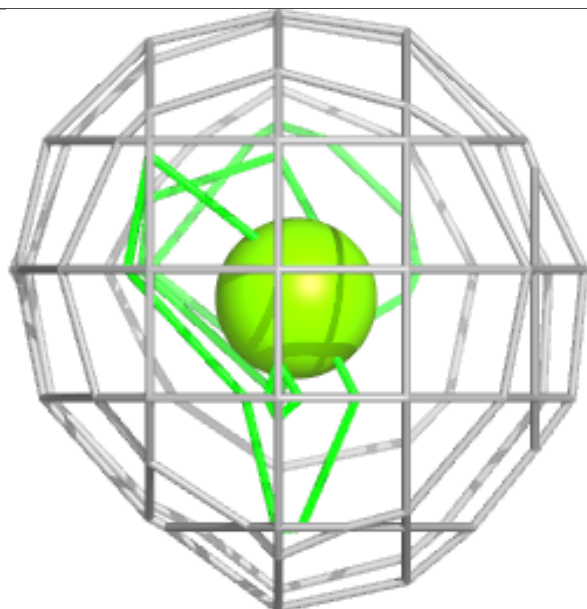
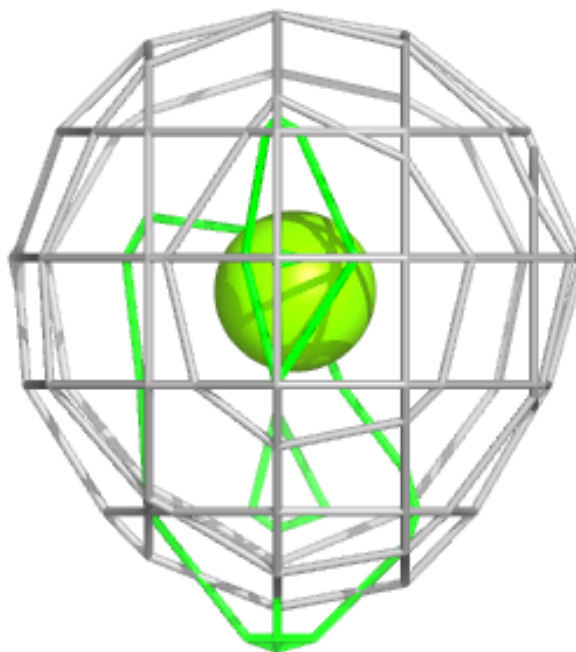
Electron density around MG F 303:

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



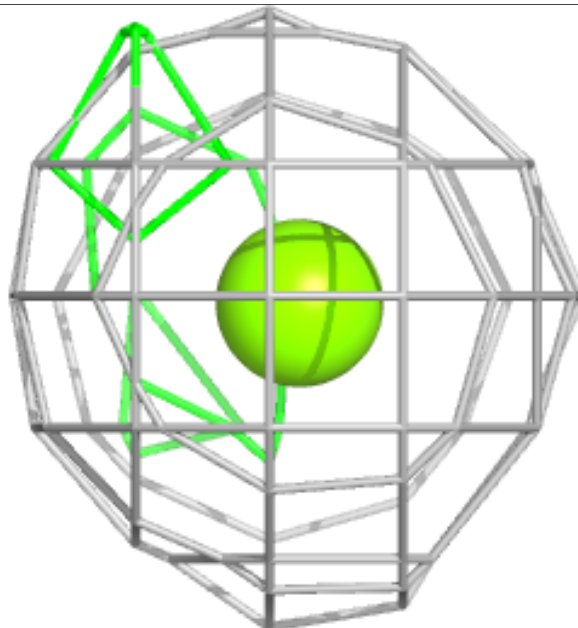
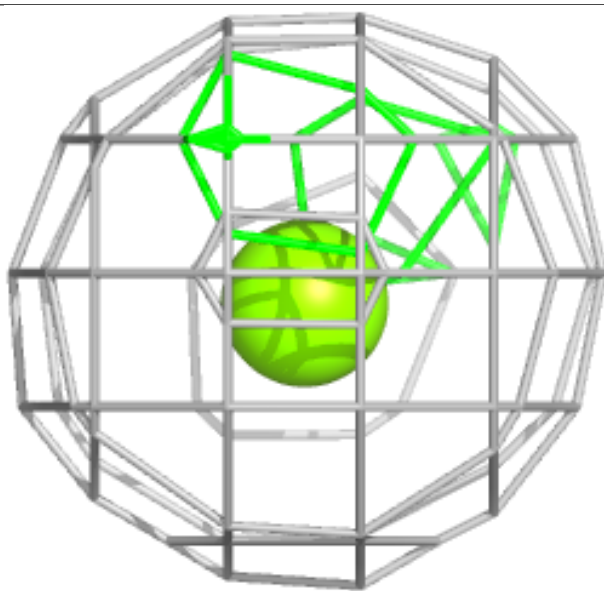
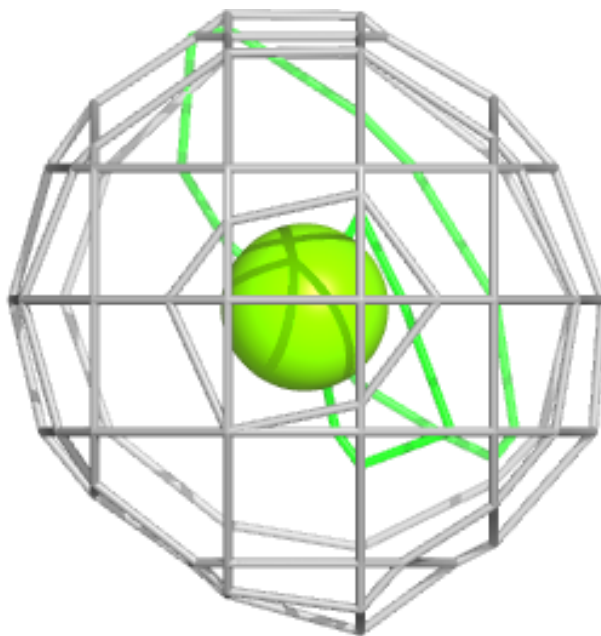
Electron density around MG E 301:

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



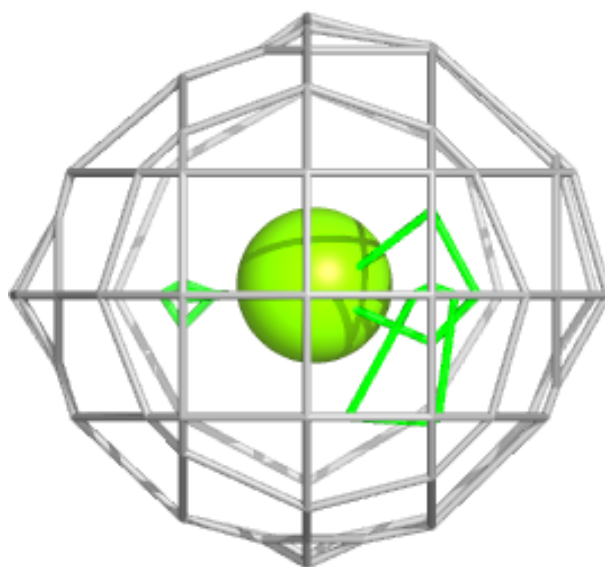
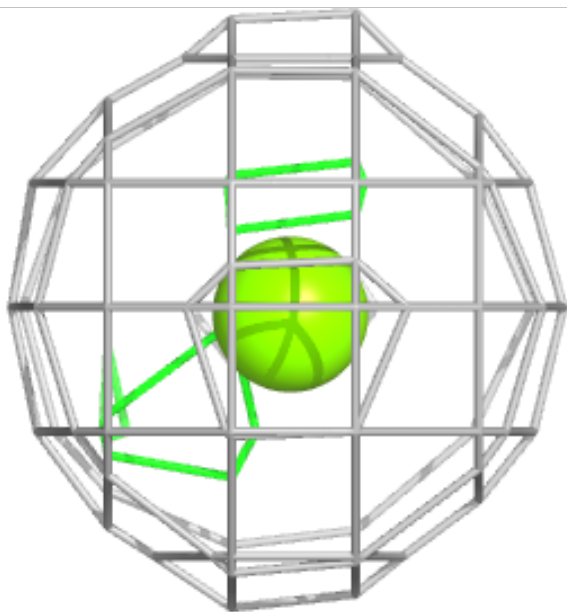
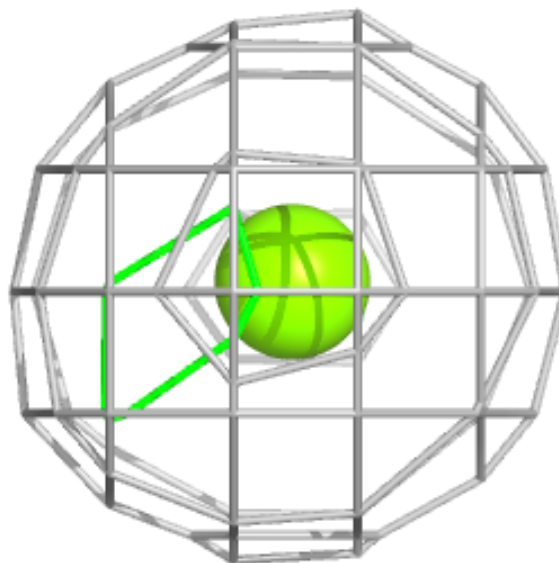
Electron density around MG A 301:

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



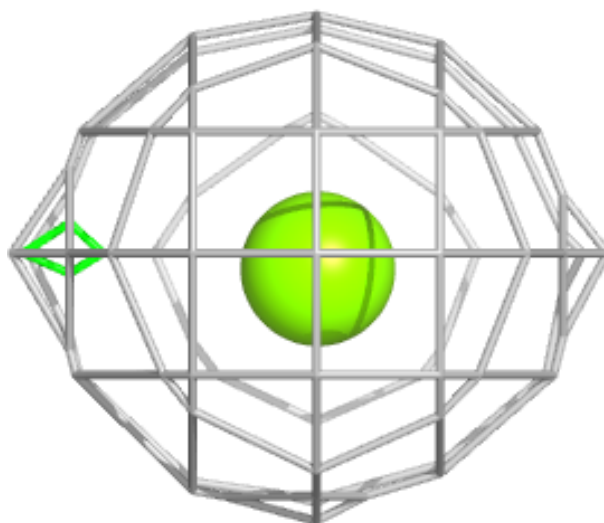
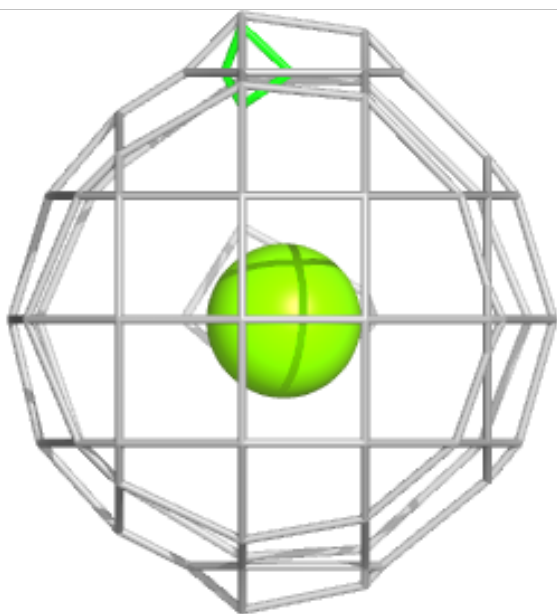
Electron density around MG F 301:

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



Electron density around MG 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.