



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:40 PM UTC

PDB ID : 7KXH / pdb_00007kxh
Title : Dihydrodipicolinate synthase (DHDPS) from C.jejuni with pyruvate bound in the active site and R,R-bislysine bound at the allosteric site in C2221 space group
Authors : Saran, S.; Sanders, D.A.R.
Deposited on : 2020-12-03
Resolution : 1.94 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

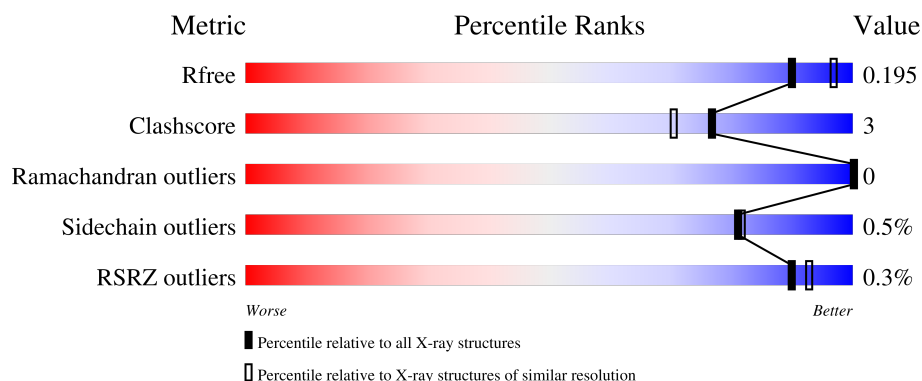
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

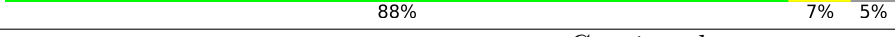
The reported resolution of this entry is 1.94 Å.

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}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	

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Mol	Chain	Length	Quality of chain
1	E	310	88% 7%5%
1	F	310	% 87% 8%•

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 14766 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 4-hydroxy-tetrahydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2278	1450	378	437	13			
1	B	296	Total	C	N	O	S	0	0	0
			2271	1444	377	437	13			
1	C	296	Total	C	N	O	S	0	0	0
			2278	1450	378	437	13			
1	D	296	Total	C	N	O	S	0	0	0
			2274	1447	377	437	13			
1	E	296	Total	C	N	O	S	0	0	0
			2279	1450	379	437	13			
1	F	297	Total	C	N	O	S	0	0	0
			2282	1451	378	440	13			

There are 72 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
B	-11	MET	-	expression tag	UNP Q9PPB4
B	-10	ARG	-	expression tag	UNP Q9PPB4
B	-9	GLY	-	expression tag	UNP Q9PPB4
B	-8	SER	-	expression tag	UNP Q9PPB4
B	-7	HIS	-	expression tag	UNP Q9PPB4

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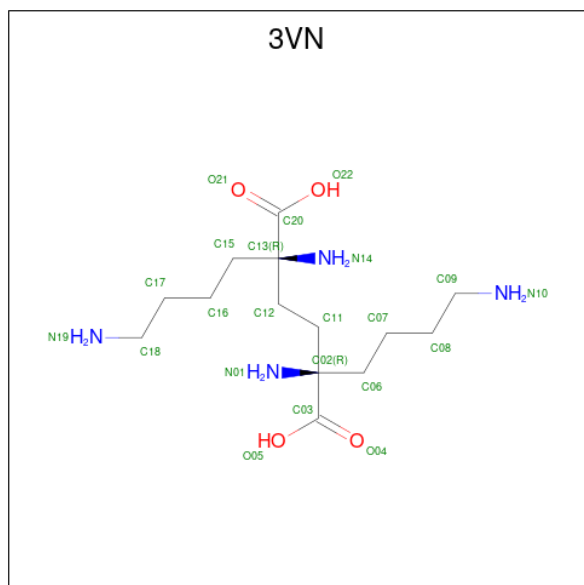
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP Q9PPB4
B	-5	HIS	-	expression tag	UNP Q9PPB4
B	-4	HIS	-	expression tag	UNP Q9PPB4
B	-3	HIS	-	expression tag	UNP Q9PPB4
B	-2	HIS	-	expression tag	UNP Q9PPB4
B	-1	GLY	-	expression tag	UNP Q9PPB4
B	0	SER	-	expression tag	UNP Q9PPB4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

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	SER	-	expression tag	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

- Molecule 2 is (2R,5R)-2,5-diamino-2,5-bis(4-aminobutyl)hexanedioic acid (CCD ID: 3VN) (formula: $C_{14}H_{30}N_4O_4$) (labeled as "Ligand of Interest" by depositor).

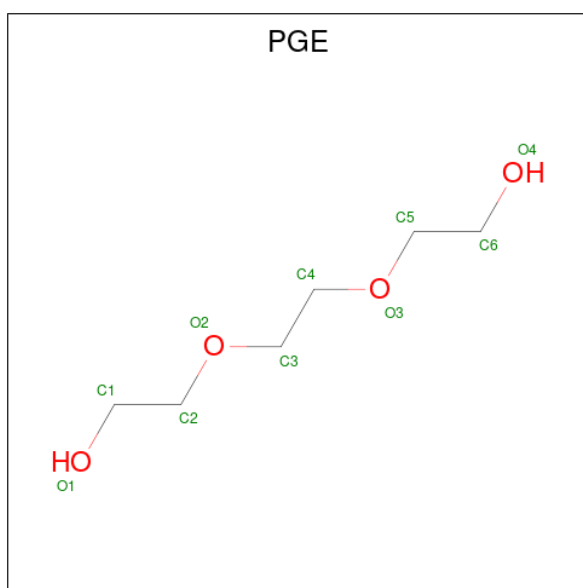


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			22	14	4	4		
2	C	1	Total	C	N	O	0	0
			22	14	4	4		
2	E	1	Total	C	N	O	0	0
			22	14	4	4		

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

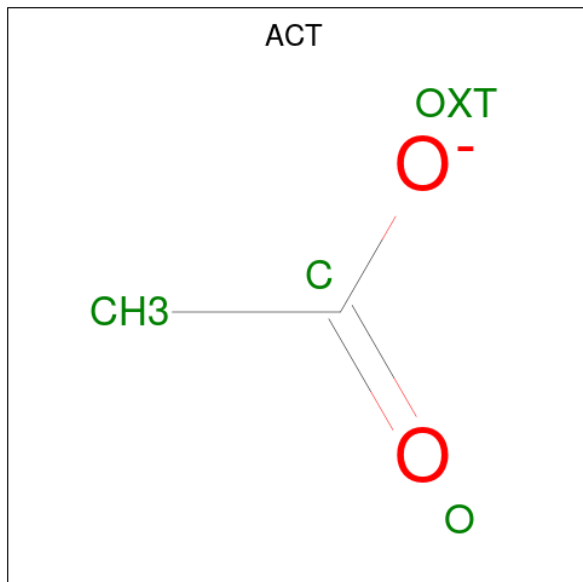
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	1	Total Mg 1 1	0	0
3	C	2	Total Mg 2 2	0	0
3	D	3	Total Mg 3 3	0	0
3	F	2	Total Mg 2 2	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$) (labeled as "Ligand of Interest" by depositor).



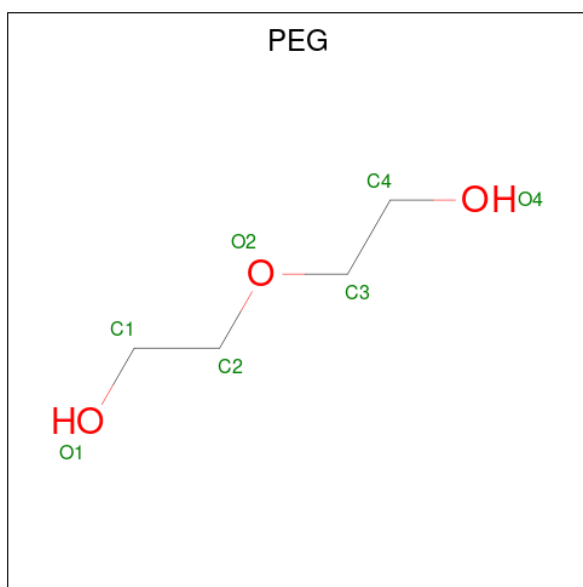
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0
4	B	1	Total C O 10 6 4	0	0
4	C	1	Total C O 10 6 4	0	0
4	D	1	Total C O 10 6 4	0	0
4	E	1	Total C O 10 6 4	0	0
4	F	1	Total C O 10 6 4	0	0

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



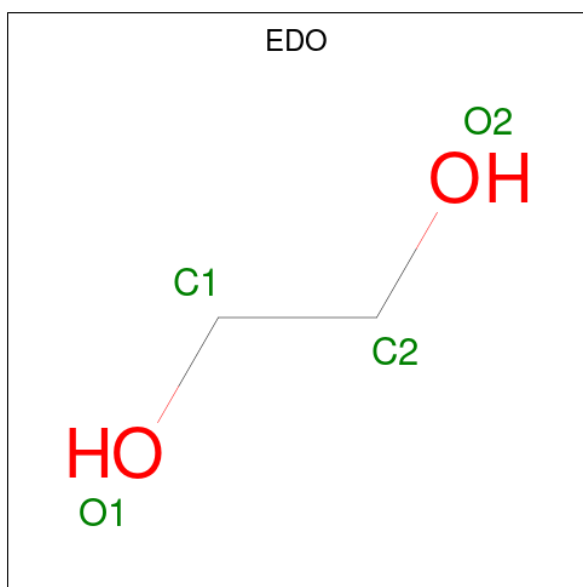
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).



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

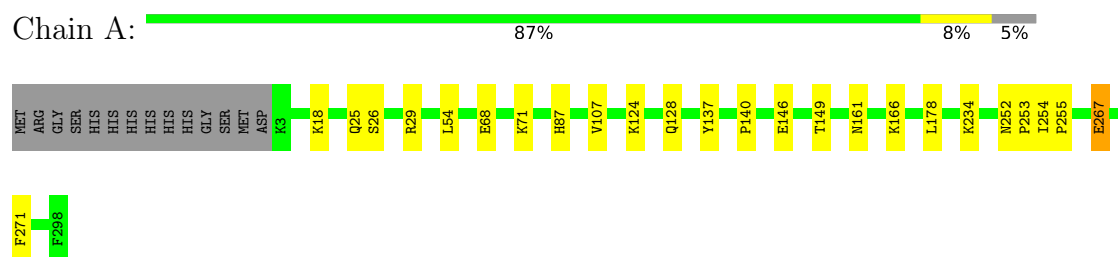
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	157	Total 157	O 157	0	0
8	B	143	Total 143	O 143	0	0
8	C	149	Total 149	O 149	0	0
8	D	137	Total 137	O 137	0	0
8	E	128	Total 128	O 128	0	0
8	F	135	Total 135	O 135	0	0

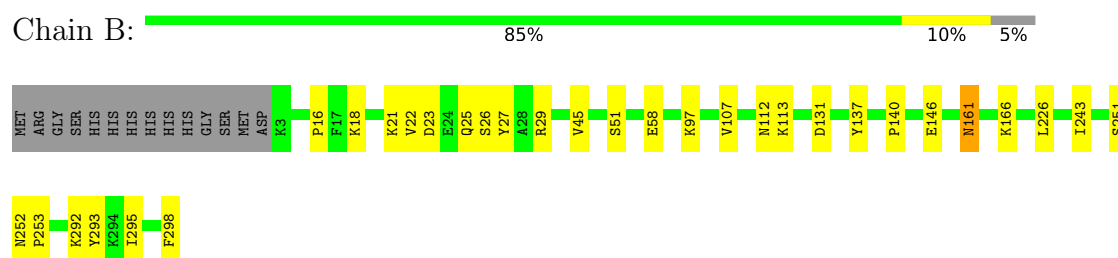
3 Residue-property plots [i](#)

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.

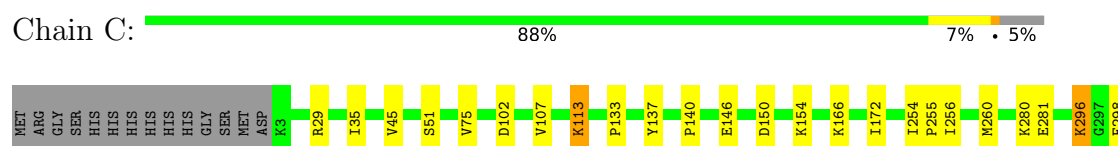
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



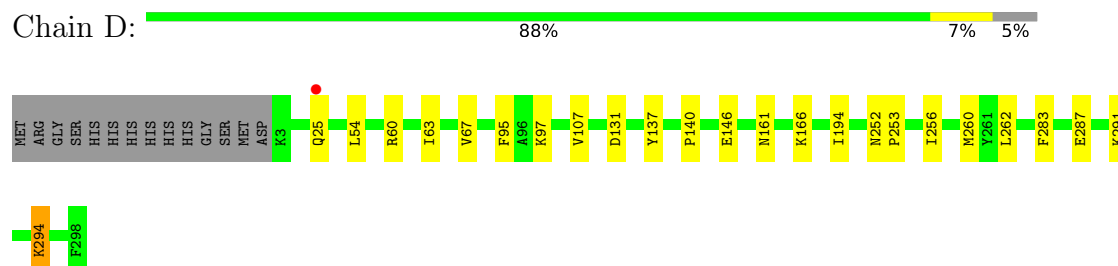
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain E:

88%

7%

5%



• Molecule 1: 4-hydroxy-tetrahydronicotinate synthase

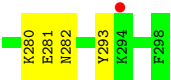
Chain F:

%

87%

8%

.



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	85.09Å 231.56Å 198.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.58 – 1.94 43.58 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.58-1.94) 94.3 (43.58-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.164 , 0.192 0.169 , 0.195	Depositor DCC
R_{free} test set	7228 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14766	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KPI, EDO, 3VN, PGE, MG, ACT, PEG

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	0.66	2/2302 (0.1%)	0.73	2/3112 (0.1%)
1	B	0.70	3/2295 (0.1%)	0.71	3/3105 (0.1%)
1	C	0.57	1/2302 (0.0%)	0.65	0/3112
1	D	0.69	2/2298 (0.1%)	0.70	1/3108 (0.0%)
1	E	0.51	0/2303	0.63	0/3113
1	F	0.59	0/2306	0.73	5/3119 (0.2%)
All	All	0.62	8/13806 (0.1%)	0.69	11/18669 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	113	LYS	C-O	-9.92	1.19	1.23
1	C	113	LYS	C-O	-7.95	1.20	1.23
1	D	294	LYS	C-O	-5.76	1.17	1.24
1	B	112	ASN	C-O	-5.70	1.16	1.24
1	A	71	LYS	C-O	-5.26	1.17	1.23
1	D	161	ASN	C-O	-5.25	1.17	1.24
1	A	26	SER	C-O	-5.17	1.18	1.24
1	B	226	LEU	C-O	-5.12	1.17	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	ILE	N-CA-C	5.87	116.56	107.99
1	F	280	LYS	CG-CD-CE	5.62	124.22	111.30
1	F	231	LYS	CB-CA-C	-5.60	102.09	110.88
1	D	25	GLN	N-CA-CB	-5.58	101.90	110.16
1	A	68	GLU	CB-CG-CD	5.45	121.86	112.60
1	B	18	LYS	CB-CG-CD	-5.43	98.82	111.30
1	F	235	LYS	CB-CG-CD	-5.39	98.90	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	ASN	N-CA-C	5.26	119.69	113.28
1	F	21	LYS	CB-CG-CD	-5.25	99.22	111.30
1	A	267	GLU	CB-CA-C	-5.12	101.32	110.70
1	F	219	SER	CB-CA-C	5.02	119.38	110.85

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	2278	0	2314	14	0
1	B	2271	0	2297	13	0
1	C	2278	0	2314	17	0
1	D	2274	0	2303	11	0
1	E	2279	0	2319	17	0
1	F	2282	0	2307	12	0
2	A	22	0	28	2	0
2	C	22	0	28	0	0
2	E	22	0	28	1	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
3	F	2	0	0	0	0
4	A	10	0	14	0	0
4	B	10	0	14	0	0
4	C	10	0	14	4	0
4	D	10	0	14	0	0
4	E	10	0	14	3	0
4	F	10	0	14	0	0
5	A	4	0	3	0	0
5	B	8	0	6	0	0
5	C	8	0	6	0	0
5	D	4	0	3	0	0
5	E	4	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	8	0	6	0	0
6	A	7	0	10	0	0
6	D	14	0	20	0	0
6	E	7	0	10	0	0
6	F	7	0	10	0	0
7	B	16	0	24	1	0
7	C	8	0	12	0	0
7	D	8	0	12	0	0
7	E	4	0	6	1	0
7	F	12	0	18	1	0
8	A	157	0	0	2	0
8	B	143	0	0	0	0
8	C	149	0	0	1	0
8	D	137	0	0	0	0
8	E	128	0	0	0	0
8	F	135	0	0	0	0
All	All	14766	0	14171	82	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 3.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:ASN:HB3	1:E:133:PRO:HG3	1.58	0.85
1:B:97:LYS:HE3	1:B:131:ASP:OD1	1.89	0.73
1:E:140:PRO:HG3	1:E:146:GLU:OE1	1.92	0.69
1:C:154:LYS:NZ	4:C:304:PGE:H3	2.07	0.69
1:C:154:LYS:HE3	4:C:304:PGE:H6	1.75	0.66
1:B:21:LYS:HE3	1:B:58:GLU:OE2	1.96	0.66
1:E:154:LYS:HZ2	4:E:302:PGE:H5	1.62	0.64
1:B:21:LYS:HE2	1:B:22:VAL:H	1.62	0.63
1:C:154:LYS:HZ2	4:C:304:PGE:H3	1.71	0.55
1:E:154:LYS:NZ	4:E:302:PGE:H5	2.22	0.54
1:E:160:GLU:O	1:E:160:GLU:HG3	2.08	0.54
1:E:142:ARG:HE	5:E:303:ACT:H1	1.74	0.53
1:C:107:VAL:HA	1:C:137:TYR:HB3	1.90	0.52
1:A:107:VAL:HA	1:A:137:TYR:HB3	1.92	0.52
1:F:107:VAL:HA	1:F:137:TYR:HB3	1.92	0.51
1:A:234:LYS:HD3	7:B:306:EDO:H12	1.92	0.51
1:F:10:MET:HG2	1:F:41:ALA:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:LYS:HG3	8:C:512:HOH:O	2.12	0.50
1:A:18:LYS:HE2	1:A:267:GLU:OE1	2.10	0.50
1:A:124:LYS:HE3	1:A:128:GLN:NE2	2.27	0.50
1:B:140:PRO:HG3	1:B:146:GLU:OE1	2.12	0.50
1:E:107:VAL:HA	1:E:137:TYR:HB3	1.94	0.50
1:D:107:VAL:HA	1:D:137:TYR:HB3	1.93	0.49
1:A:29:ARG:NH2	8:A:406:HOH:O	2.45	0.49
1:C:281:GLU:H	1:C:281:GLU:CD	2.21	0.49
1:C:29:ARG:HG2	1:C:298:PHE:CE1	2.48	0.49
1:D:63:ILE:O	1:D:67:VAL:HG23	2.14	0.48
1:D:140:PRO:HG3	1:D:146:GLU:OE1	2.14	0.48
1:A:161:ASN:OD1	1:A:161:ASN:N	2.45	0.47
1:C:45:VAL:HG12	1:C:51:SER:HB3	1.96	0.47
1:C:296:LYS:HB3	1:C:296:LYS:HE2	1.57	0.47
1:D:287:GLU:O	1:D:291:LYS:HG3	2.15	0.47
1:F:215:PRO:O	1:F:219:SER:OG	2.30	0.47
1:F:230:TYR:OH	7:F:307:EDO:H21	2.15	0.47
1:A:140:PRO:HG3	1:A:146:GLU:OE2	2.15	0.47
1:F:281:GLU:HG3	1:F:282:ASN:N	2.30	0.47
1:D:252:ASN:OD1	1:D:253:PRO:HA	2.16	0.46
1:C:102:ASP:O	1:C:133:PRO:HD2	2.15	0.45
1:E:245:LYS:HD2	1:E:245:LYS:HA	1.82	0.45
1:A:54:LEU:O	2:A:301:3VN:H9	2.16	0.45
1:E:241:TYR:CZ	1:E:245:LYS:HG3	2.52	0.45
2:A:301:3VN:H23	1:D:54:LEU:O	2.17	0.45
1:C:150:ASP:HB3	4:C:304:PGE:H62	1.99	0.45
1:F:268:SER:OG	1:F:270:GLU:HG3	2.17	0.45
1:F:221:LEU:C	1:F:221:LEU:HD23	2.41	0.45
1:A:149:THR:HG23	1:A:178:LEU:HD23	1.98	0.44
1:D:97:LYS:HE3	1:D:131:ASP:OD1	2.17	0.44
1:C:140:PRO:HG3	1:C:146:GLU:OE1	2.18	0.44
1:D:262:LEU:HD21	1:D:283:PHE:CZ	2.53	0.44
1:E:60:ARG:HB3	1:E:95:PHE:CZ	2.53	0.44
1:E:256:ILE:O	1:E:260:MET:HG2	2.18	0.44
1:B:251:SER:OG	1:C:113:LYS:HD3	2.18	0.44
1:A:254:ILE:HA	1:A:271:PHE:CE2	2.53	0.43
1:C:35:ILE:HG12	1:C:75:VAL:HG21	2.01	0.43
1:F:243:ILE:HB	1:F:293:TYR:CE1	2.53	0.43
1:E:35:ILE:HG12	1:E:75:VAL:HG21	2.01	0.43
1:E:241:TYR:CE2	1:E:245:LYS:HG3	2.52	0.43
1:E:230:TYR:OH	7:E:304:EDO:H21	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:VAL:HG12	1:B:51:SER:HB3	2.01	0.42
1:A:25:GLN:H	1:A:25:GLN:CD	2.27	0.42
1:B:29:ARG:HG2	1:B:298:PHE:CE1	2.54	0.42
1:C:256:ILE:O	1:C:260:MET:HG2	2.19	0.42
1:D:256:ILE:O	1:D:260:MET:HG2	2.19	0.42
1:A:87:HIS:HD2	8:A:545:HOH:O	2.01	0.42
1:C:254:ILE:HB	1:C:255:PRO:HD3	2.01	0.42
1:F:281:GLU:HG3	1:F:282:ASN:H	1.85	0.42
1:B:16:PRO:HD2	1:B:27:TYR:HD1	1.85	0.42
1:B:243:ILE:HB	1:B:293:TYR:CE2	2.55	0.42
1:B:23:ASP:CG	1:B:26:SER:HB3	2.44	0.42
1:C:172:ILE:HG23	1:D:194:ILE:HG21	2.02	0.42
1:F:241:TYR:CE2	1:F:245:LYS:HG3	2.55	0.42
1:E:154:LYS:NZ	4:E:302:PGE:O1	2.51	0.41
1:B:161:ASN:OD1	1:B:161:ASN:N	2.40	0.41
1:B:107:VAL:HA	1:B:137:TYR:HB3	2.03	0.41
1:D:60:ARG:HB3	1:D:95:PHE:CZ	2.55	0.41
1:E:54:LEU:O	2:E:301:3VN:H9	2.21	0.41
1:E:102:ASP:O	1:E:133:PRO:HD2	2.21	0.41
1:B:252:ASN:OD1	1:B:253:PRO:HA	2.20	0.41
1:F:149:THR:HG23	1:F:178:LEU:HD23	2.02	0.41
1:F:167:GLU:OE2	1:F:174:LYS:NZ	2.52	0.41
1:A:252:ASN:OD1	1:A:253:PRO:HA	2.21	0.40
1:A:254:ILE:HB	1:A:255:PRO:HD3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	293/310 (94%)	288 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	293/310 (94%)	289 (99%)	4 (1%)	0	100	100
1	C	293/310 (94%)	287 (98%)	6 (2%)	0	100	100
1	D	293/310 (94%)	289 (99%)	4 (1%)	0	100	100
1	E	293/310 (94%)	287 (98%)	6 (2%)	0	100	100
1	F	294/310 (95%)	290 (99%)	4 (1%)	0	100	100
All	All	1759/1860 (95%)	1730 (98%)	29 (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	247/260 (95%)	247 (100%)	0	100	100
1	B	246/260 (95%)	244 (99%)	2 (1%)	73	71
1	C	247/260 (95%)	246 (100%)	1 (0%)	84	84
1	D	246/260 (95%)	245 (100%)	1 (0%)	84	84
1	E	248/260 (95%)	247 (100%)	1 (0%)	84	84
1	F	247/260 (95%)	245 (99%)	2 (1%)	73	71
All	All	1481/1560 (95%)	1474 (100%)	7 (0%)	81	82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	25	GLN
1	B	292	LYS
1	C	296	LYS
1	D	294	LYS
1	E	21	LYS
1	F	57	GLU
1	F	97	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	229	ASN
1	B	25	GLN
1	C	25	GLN
1	D	25	GLN
1	D	37	ASN
1	E	37	ASN
1	F	201	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KPI	C	166	1	11,13,14	2.31	4 (36%)	9,15,17	3.75	4 (44%)
1	KPI	F	166	1	11,13,14	0.89	1 (9%)	9,15,17	2.94	3 (33%)
1	KPI	B	166	1	11,13,14	0.94	0	9,15,17	3.17	3 (33%)
1	KPI	E	166	1	11,13,14	1.96	2 (18%)	9,15,17	3.64	3 (33%)
1	KPI	D	166	1	11,13,14	0.74	0	9,15,17	3.41	3 (33%)
1	KPI	A	166	1	11,13,14	2.05	2 (18%)	9,15,17	3.83	3 (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	C	166	1	-	0/13/14/16	-
1	KPI	F	166	1	-	0/13/14/16	-
1	KPI	B	166	1	-	0/13/14/16	-
1	KPI	E	166	1	-	0/13/14/16	-
1	KPI	D	166	1	-	0/13/14/16	-
1	KPI	A	166	1	-	0/13/14/16	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	KPI	O2-CX2	6.10	1.37	1.22
1	E	166	KPI	O2-CX2	5.70	1.36	1.22
1	C	166	KPI	O2-CX2	5.49	1.36	1.22
1	C	166	KPI	O-C	3.96	1.35	1.20
1	E	166	KPI	O1-CX2	-2.47	1.23	1.30
1	C	166	KPI	CX2-CX1	2.39	1.52	1.49
1	C	166	KPI	O1-CX2	-2.27	1.24	1.30
1	A	166	KPI	O1-CX2	-2.15	1.24	1.30
1	F	166	KPI	O1-CX2	2.08	1.36	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	KPI	C1-CX1-CX2	-8.15	110.42	118.11
1	D	166	KPI	C1-CX1-CX2	-8.02	110.55	118.11
1	A	166	KPI	C1-CX1-CX2	-7.54	111.00	118.11
1	C	166	KPI	C1-CX1-CX2	-7.19	111.33	118.11
1	E	166	KPI	O2-CX2-CX1	-7.06	112.72	121.35
1	F	166	KPI	C1-CX1-CX2	-6.78	111.72	118.11
1	A	166	KPI	O2-CX2-CX1	-6.56	113.33	121.35
1	C	166	KPI	O2-CX2-CX1	-5.76	114.31	121.35
1	E	166	KPI	C1-CX1-CX2	-5.62	112.81	118.11
1	C	166	KPI	O1-CX2-CX1	5.42	128.05	116.50
1	E	166	KPI	O1-CX2-CX1	5.30	127.80	116.50
1	D	166	KPI	O2-CX2-CX1	5.24	127.75	121.35
1	A	166	KPI	O1-CX2-CX1	4.88	126.89	116.50
1	F	166	KPI	O2-CX2-CX1	4.59	126.95	121.35
1	B	166	KPI	O2-CX2-CX1	3.71	125.87	121.35
1	D	166	KPI	O1-CX2-O2	-2.77	117.31	123.90
1	C	166	KPI	O1-CX2-O2	-2.64	117.62	123.90
1	B	166	KPI	O1-CX2-O2	-2.38	118.22	123.90
1	F	166	KPI	O1-CX2-O2	-2.05	119.03	123.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 10 are monoatomic - leaving 35 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ACT	A	305	-	3,3,3	1.08	0	3,3,3	1.63	1 (33%)
4	PGE	E	302	-	9,9,9	0.32	0	8,8,8	0.65	0
5	ACT	C	305	-	3,3,3	1.57	1 (33%)	3,3,3	1.29	0
2	3VN	C	301	-	17,21,21	1.28	1 (5%)	18,28,28	1.49	4 (22%)
5	ACT	C	306	-	3,3,3	1.16	0	3,3,3	1.50	1 (33%)
5	ACT	D	305	-	3,3,3	1.75	1 (33%)	3,3,3	1.17	0
7	EDO	F	308	-	3,3,3	0.49	0	2,2,2	0.40	0
7	EDO	D	306	-	3,3,3	0.36	0	2,2,2	0.43	0
2	3VN	E	301	-	17,21,21	1.30	1 (5%)	18,28,28	1.50	3 (16%)
7	EDO	C	307	-	3,3,3	0.34	0	2,2,2	0.53	0
7	EDO	B	308	-	3,3,3	0.21	0	2,2,2	0.29	0
4	PGE	B	302	-	9,9,9	0.36	0	8,8,8	0.44	0
5	ACT	E	303	-	3,3,3	1.62	1 (33%)	3,3,3	1.48	0
7	EDO	C	308	-	3,3,3	0.51	0	2,2,2	0.30	0
7	EDO	F	307	-	3,3,3	0.41	0	2,2,2	0.24	0
5	ACT	F	304	-	3,3,3	1.27	0	3,3,3	1.36	0
4	PGE	A	304	-	9,9,9	0.32	0	8,8,8	0.26	0
7	EDO	B	305	-	3,3,3	0.40	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	F	306	-	3,3,3	0.41	0	2,2,2	0.54	0
7	EDO	B	307	-	3,3,3	0.27	0	2,2,2	0.83	0
4	PGE	C	304	-	9,9,9	0.30	0	8,8,8	0.55	0
4	PGE	D	304	-	9,9,9	0.29	0	8,8,8	0.47	0
6	PEG	D	309	-	6,6,6	0.31	0	5,5,5	0.37	0
7	EDO	B	306	-	3,3,3	0.49	0	2,2,2	0.25	0
7	EDO	D	307	-	3,3,3	0.21	0	2,2,2	0.60	0
6	PEG	D	308	-	6,6,6	0.47	0	5,5,5	0.46	0
6	PEG	E	305	-	6,6,6	0.49	0	5,5,5	0.26	0
5	ACT	B	304	-	3,3,3	1.15	0	3,3,3	1.47	1 (33%)
5	ACT	F	305	-	3,3,3	1.59	1 (33%)	3,3,3	1.19	0
6	PEG	A	306	-	6,6,6	0.51	0	5,5,5	0.64	0
2	3VN	A	301	-	17,21,21	1.17	1 (5%)	18,28,28	1.57	3 (16%)
5	ACT	B	303	-	3,3,3	1.46	1 (33%)	3,3,3	1.47	0
4	PGE	F	303	-	9,9,9	0.30	0	8,8,8	0.37	0
6	PEG	F	309	-	6,6,6	0.47	0	5,5,5	0.25	0
7	EDO	E	304	-	3,3,3	0.21	0	2,2,2	0.55	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
4	PGE	E	302	-	-	5/7/7/7	-
2	3VN	C	301	-	-	8/31/31/31	-
7	EDO	F	308	-	-	1/1/1/1	-
7	EDO	D	306	-	-	0/1/1/1	-
2	3VN	E	301	-	-	8/31/31/31	-
7	EDO	C	307	-	-	0/1/1/1	-
7	EDO	B	308	-	-	1/1/1/1	-
4	PGE	B	302	-	-	1/7/7/7	-
7	EDO	C	308	-	-	0/1/1/1	-
7	EDO	F	307	-	-	1/1/1/1	-
4	PGE	A	304	-	-	1/7/7/7	-
7	EDO	B	305	-	-	1/1/1/1	-
7	EDO	F	306	-	-	0/1/1/1	-
7	EDO	B	307	-	-	1/1/1/1	-
4	PGE	C	304	-	-	4/7/7/7	-
4	PGE	D	304	-	-	4/7/7/7	-
6	PEG	D	309	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	EDO	B	306	-	-	0/1/1/1	-
7	EDO	D	307	-	-	0/1/1/1	-
6	PEG	D	308	-	-	2/4/4/4	-
6	PEG	E	305	-	-	2/4/4/4	-
6	PEG	A	306	-	-	4/4/4/4	-
2	3VN	A	301	-	-	8/31/31/31	-
4	PGE	F	303	-	-	4/7/7/7	-
6	PEG	F	309	-	-	1/4/4/4	-
7	EDO	E	304	-	-	1/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	3VN	C06-C02	3.19	1.58	1.55
2	E	301	3VN	C06-C02	3.10	1.58	1.55
5	D	305	ACT	CH3-C	2.62	1.59	1.49
5	C	305	ACT	CH3-C	2.47	1.58	1.49
2	A	301	3VN	C06-C02	2.37	1.57	1.55
5	E	303	ACT	CH3-C	2.28	1.58	1.49
5	F	305	ACT	CH3-C	2.27	1.58	1.49
5	B	303	ACT	CH3-C	2.26	1.58	1.49

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	3VN	C06-C02-C11	-2.52	106.69	111.99
2	A	301	3VN	C15-C13-C12	-2.46	106.83	111.99
2	C	301	3VN	O22-C20-C13	2.37	120.02	113.69
2	C	301	3VN	C06-C02-C11	-2.33	107.11	111.99
2	E	301	3VN	C06-C02-C11	-2.31	107.13	111.99
2	E	301	3VN	O22-C20-C13	2.26	119.72	113.69
2	C	301	3VN	O05-C03-C02	2.22	119.61	113.69
2	C	301	3VN	C15-C13-C12	-2.15	107.49	111.99
2	E	301	3VN	O05-C03-C02	2.11	119.32	113.69
2	A	301	3VN	C16-C15-C13	-2.07	111.50	115.16
5	A	305	ACT	OXT-C-O	2.01	129.48	122.03
5	B	304	ACT	OXT-C-O	2.01	129.48	122.03
5	C	306	ACT	OXT-C-O	2.00	129.45	122.03

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	301	3VN	C12-C13-C20-O21
2	E	301	3VN	C12-C13-C20-O22
4	C	304	PGE	O1-C1-C2-O2
4	F	303	PGE	O1-C1-C2-O2
6	D	308	PEG	O1-C1-C2-O2
6	F	309	PEG	O1-C1-C2-O2
4	C	304	PGE	O2-C3-C4-O3
7	E	304	EDO	O1-C1-C2-O2
4	D	304	PGE	O3-C5-C6-O4
6	A	306	PEG	O1-C1-C2-O2
6	D	308	PEG	O2-C3-C4-O4
6	D	309	PEG	O1-C1-C2-O2
4	E	302	PGE	O3-C5-C6-O4
6	E	305	PEG	O1-C1-C2-O2
4	E	302	PGE	O2-C3-C4-O3
7	B	308	EDO	O1-C1-C2-O2
4	E	302	PGE	C3-C4-O3-C5
4	C	304	PGE	O3-C5-C6-O4
7	B	307	EDO	O1-C1-C2-O2
4	D	304	PGE	O2-C3-C4-O3
6	A	306	PEG	O2-C3-C4-O4
4	D	304	PGE	C3-C4-O3-C5
4	E	302	PGE	C1-C2-O2-C3
4	F	303	PGE	C3-C4-O3-C5
4	F	303	PGE	C6-C5-O3-C4
4	E	302	PGE	C4-C3-O2-C2
6	E	305	PEG	C1-C2-O2-C3
2	A	301	3VN	C11-C02-C03-O04
2	A	301	3VN	C11-C02-C03-O05
2	A	301	3VN	C12-C13-C20-O21
2	A	301	3VN	C12-C13-C20-O22
2	C	301	3VN	C11-C02-C03-O04
2	C	301	3VN	C11-C02-C03-O05
2	C	301	3VN	C12-C13-C20-O21
2	C	301	3VN	C12-C13-C20-O22
2	E	301	3VN	C11-C02-C03-O04
2	E	301	3VN	C11-C02-C03-O05
2	E	301	3VN	C15-C13-C20-O21
2	E	301	3VN	C15-C13-C20-O22
6	A	306	PEG	C1-C2-O2-C3
4	F	303	PGE	O2-C3-C4-O3
7	F	308	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	304	PGE	C1-C2-O2-C3
7	F	307	EDO	O1-C1-C2-O2
6	A	306	PEG	C4-C3-O2-C2
4	B	302	PGE	O3-C5-C6-O4
4	C	304	PGE	C1-C2-O2-C3
2	A	301	3VN	C06-C02-C03-O04
2	A	301	3VN	C06-C02-C03-O05
2	A	301	3VN	C15-C13-C20-O21
2	A	301	3VN	C15-C13-C20-O22
2	C	301	3VN	C06-C02-C03-O04
2	C	301	3VN	C06-C02-C03-O05
2	C	301	3VN	C15-C13-C20-O21
2	C	301	3VN	C15-C13-C20-O22
2	E	301	3VN	C06-C02-C03-O04
2	E	301	3VN	C06-C02-C03-O05
4	D	304	PGE	C4-C3-O2-C2
7	B	305	EDO	O1-C1-C2-O2

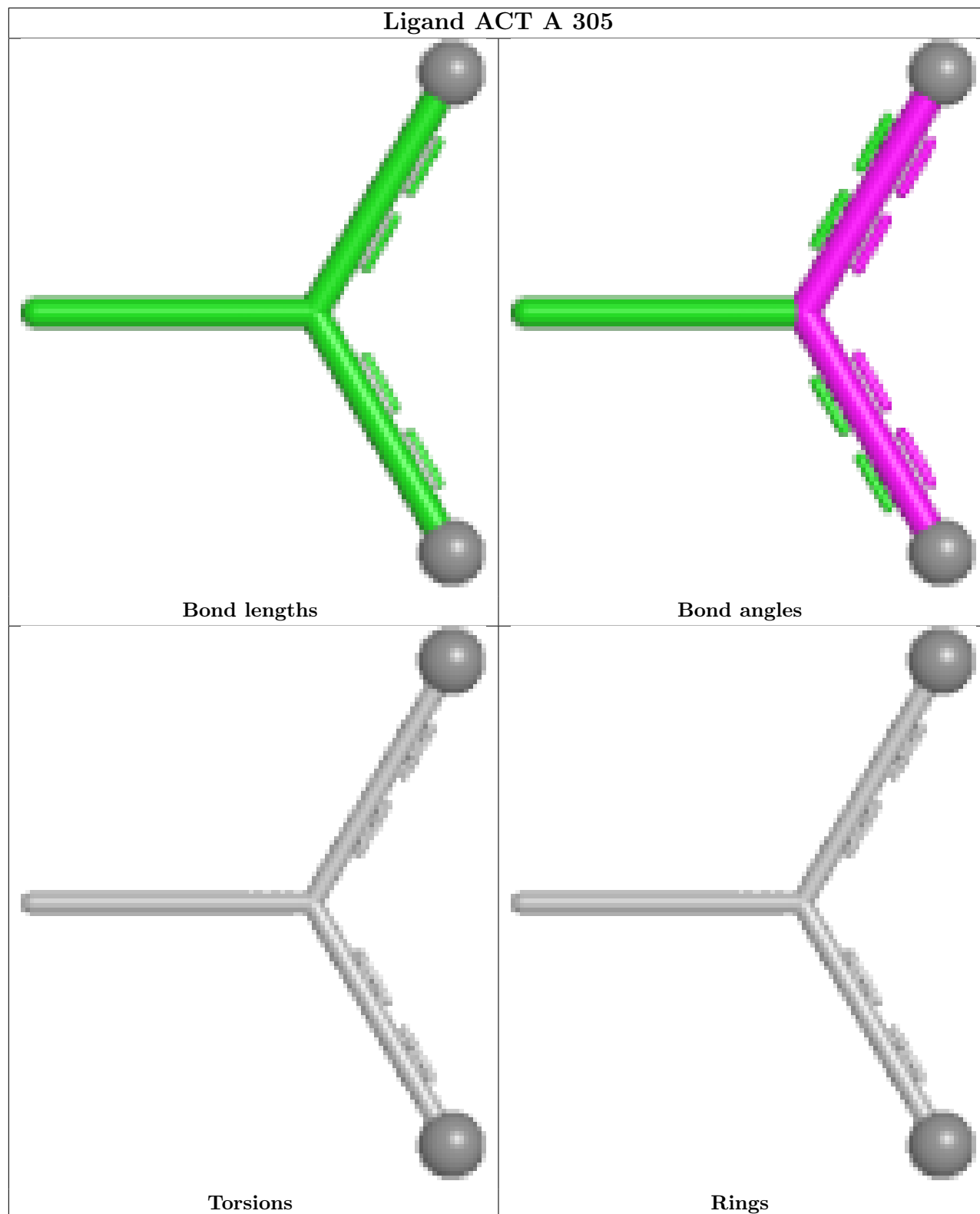
There are no ring outliers.

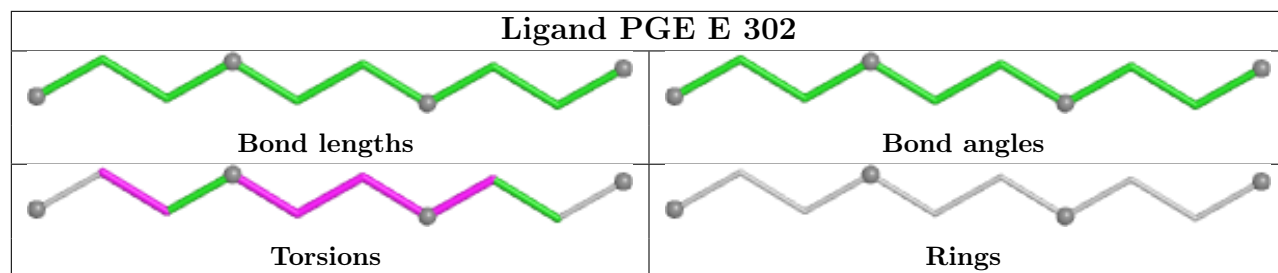
8 monomers are involved in 14 short contacts:

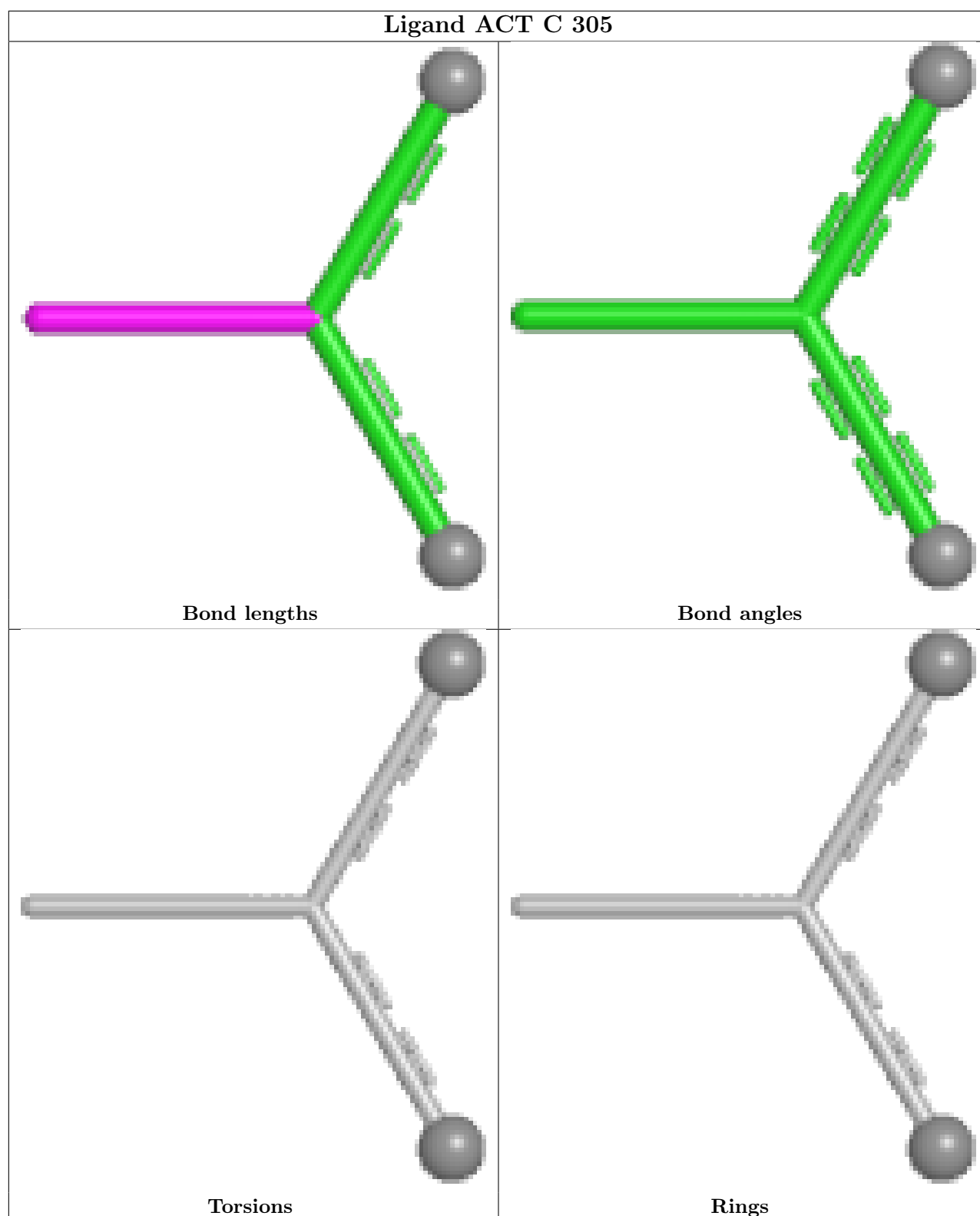
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	302	PGE	3	0
2	E	301	3VN	1	0
5	E	303	ACT	1	0
7	F	307	EDO	1	0
4	C	304	PGE	4	0
7	B	306	EDO	1	0
2	A	301	3VN	2	0
7	E	304	EDO	1	0

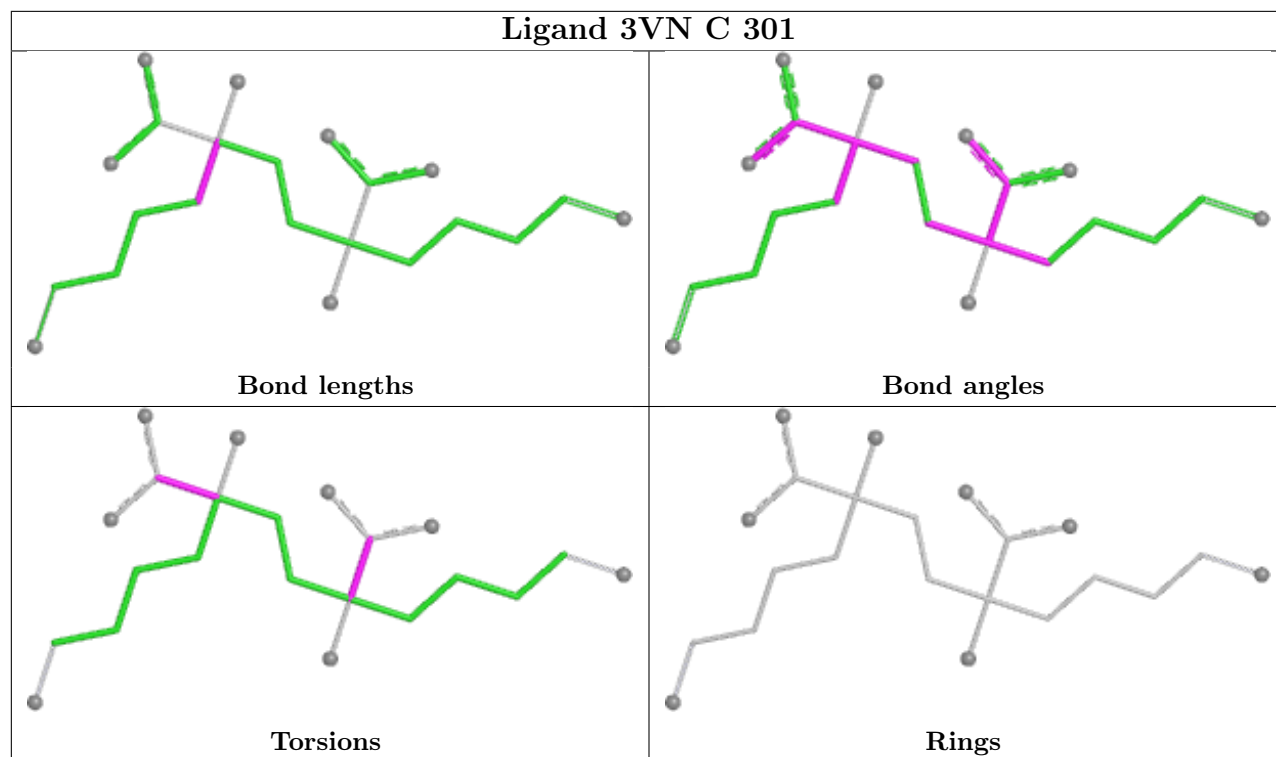
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

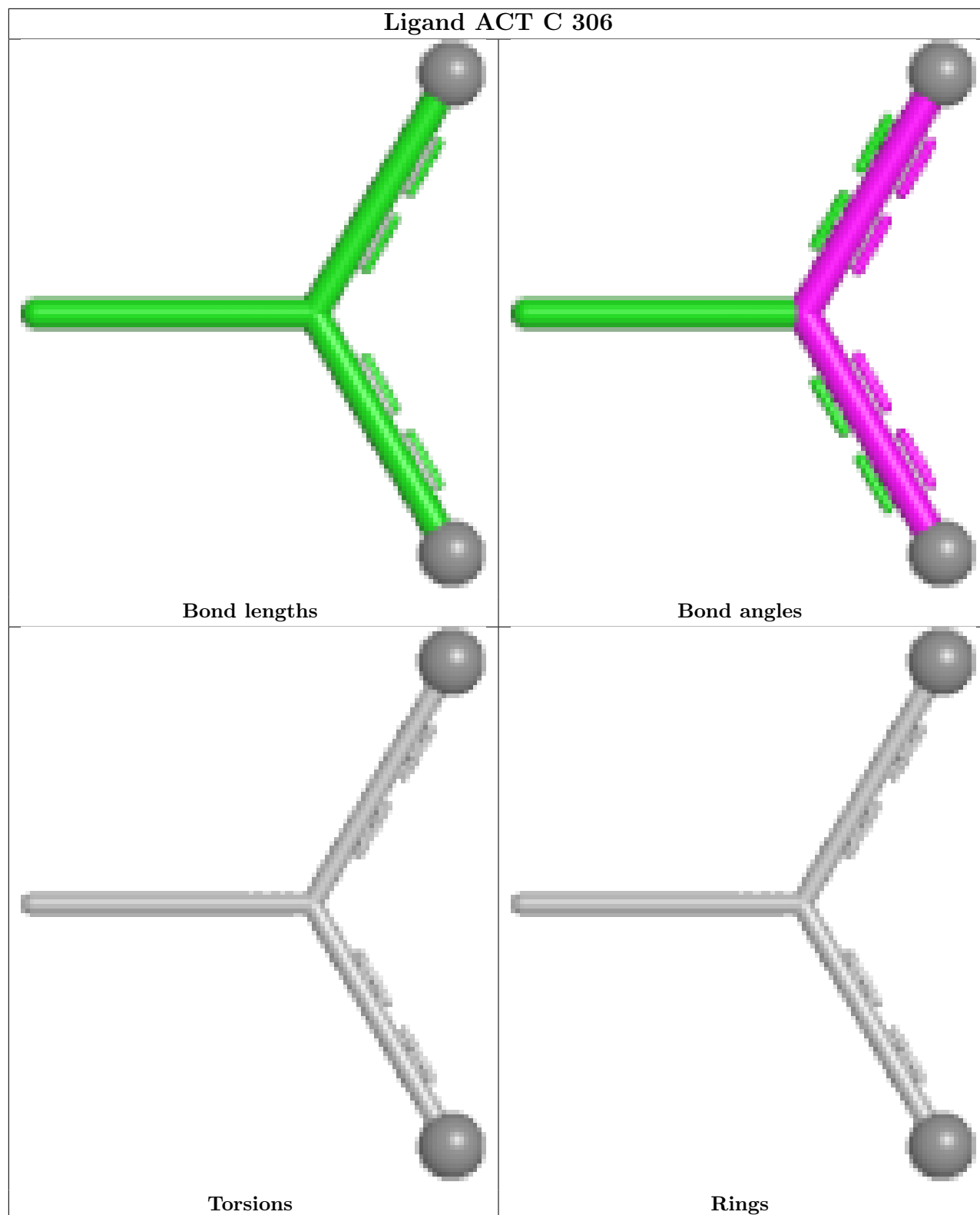
equivalents in the CSD to analyse the geometry.

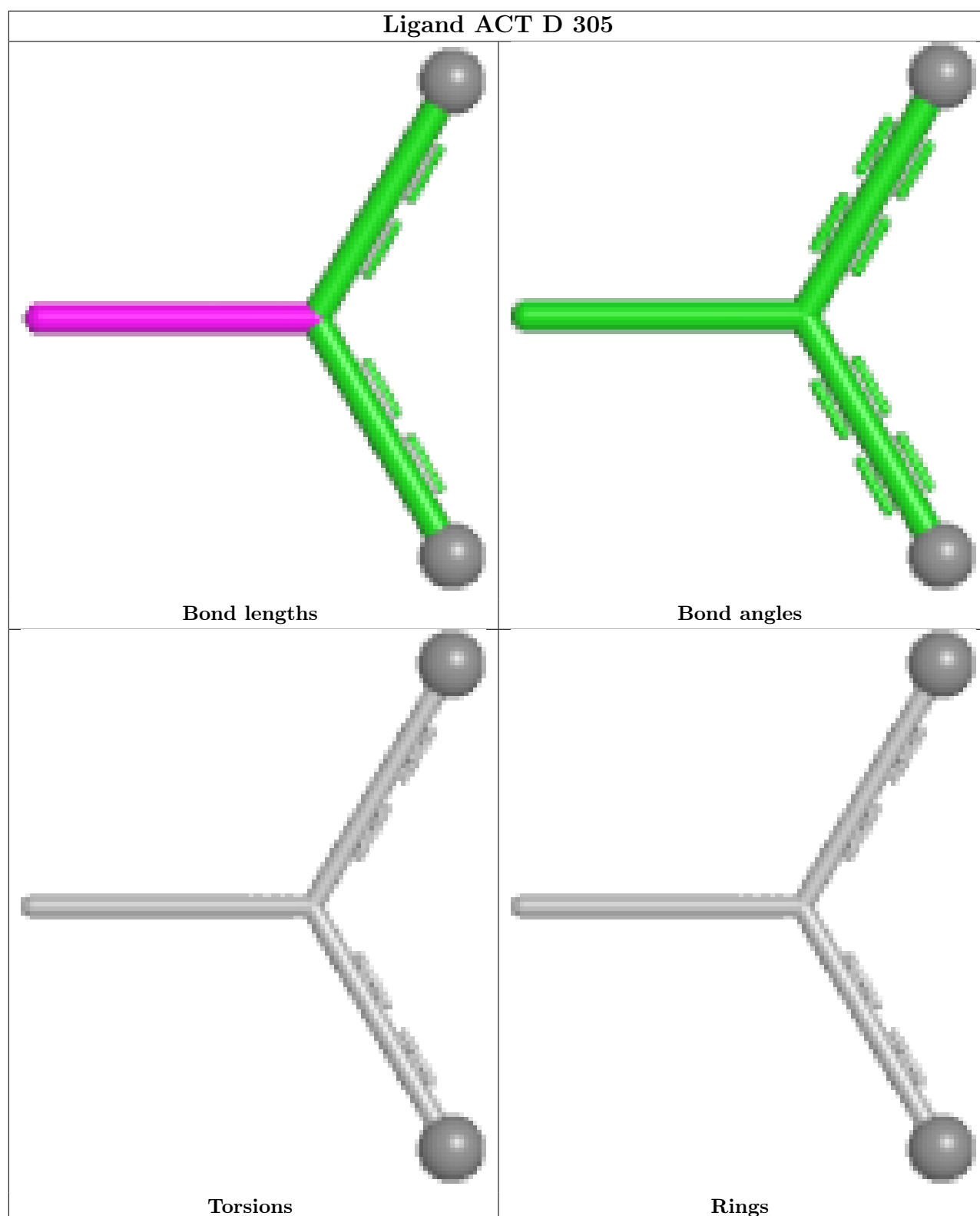




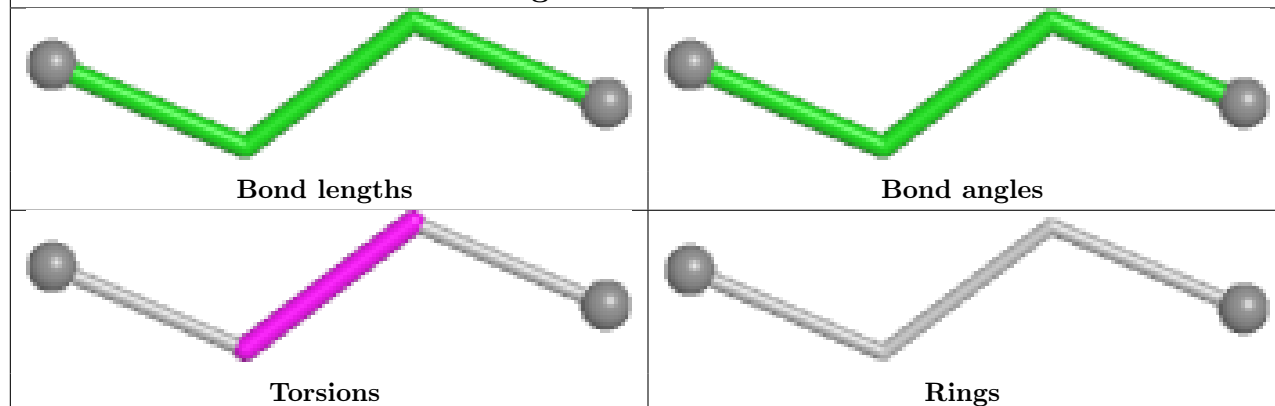




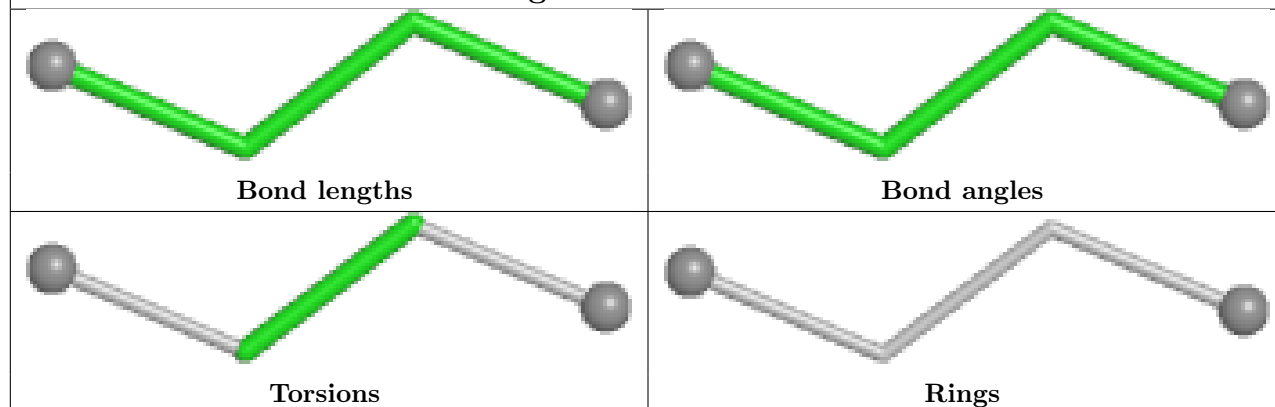




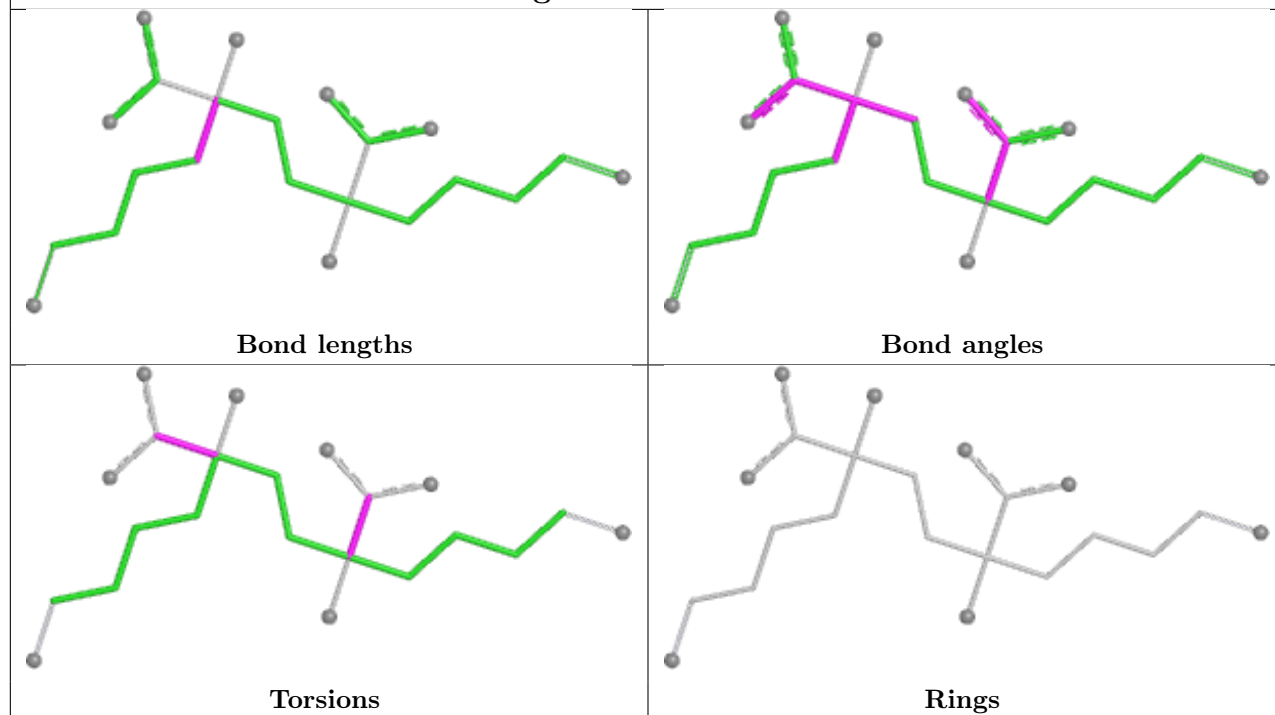
Ligand EDO F 308

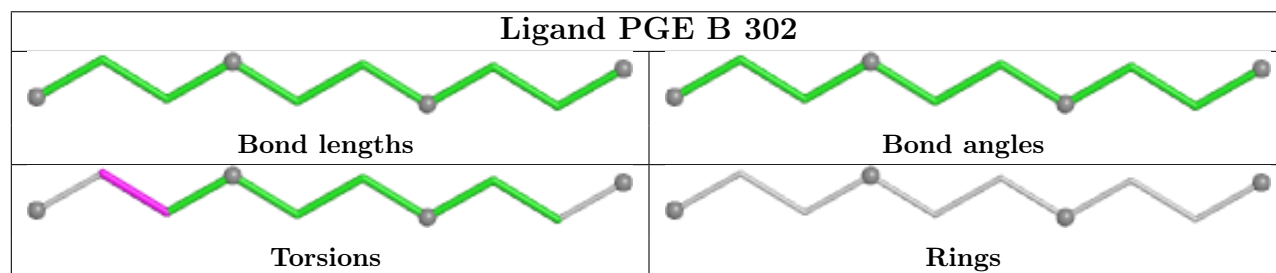
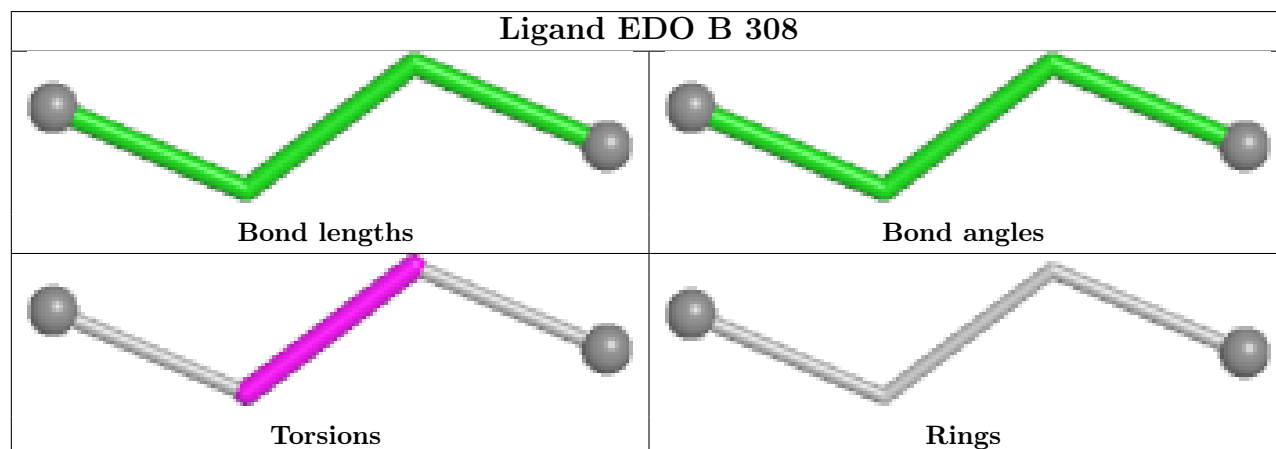
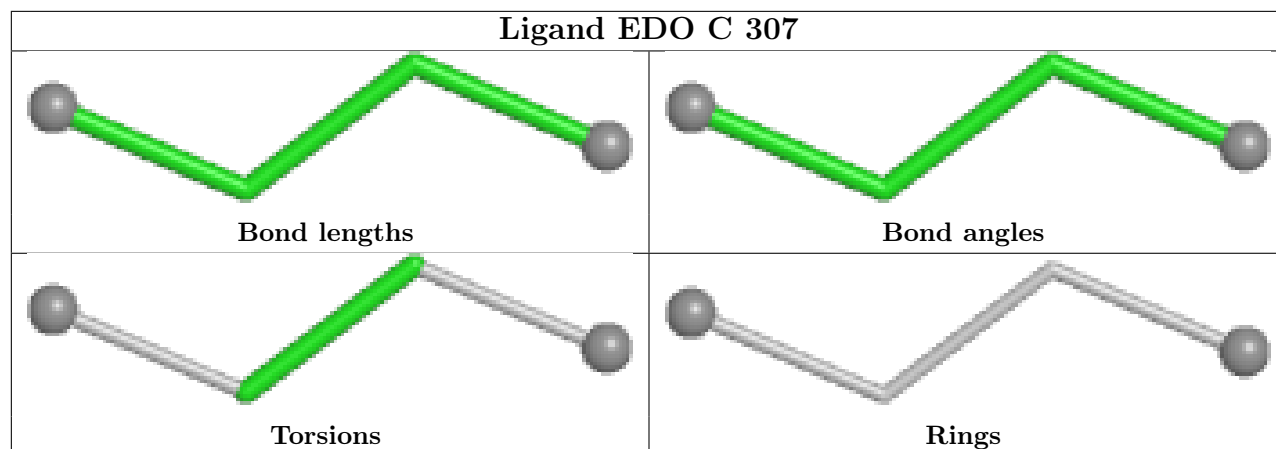


Ligand EDO D 306

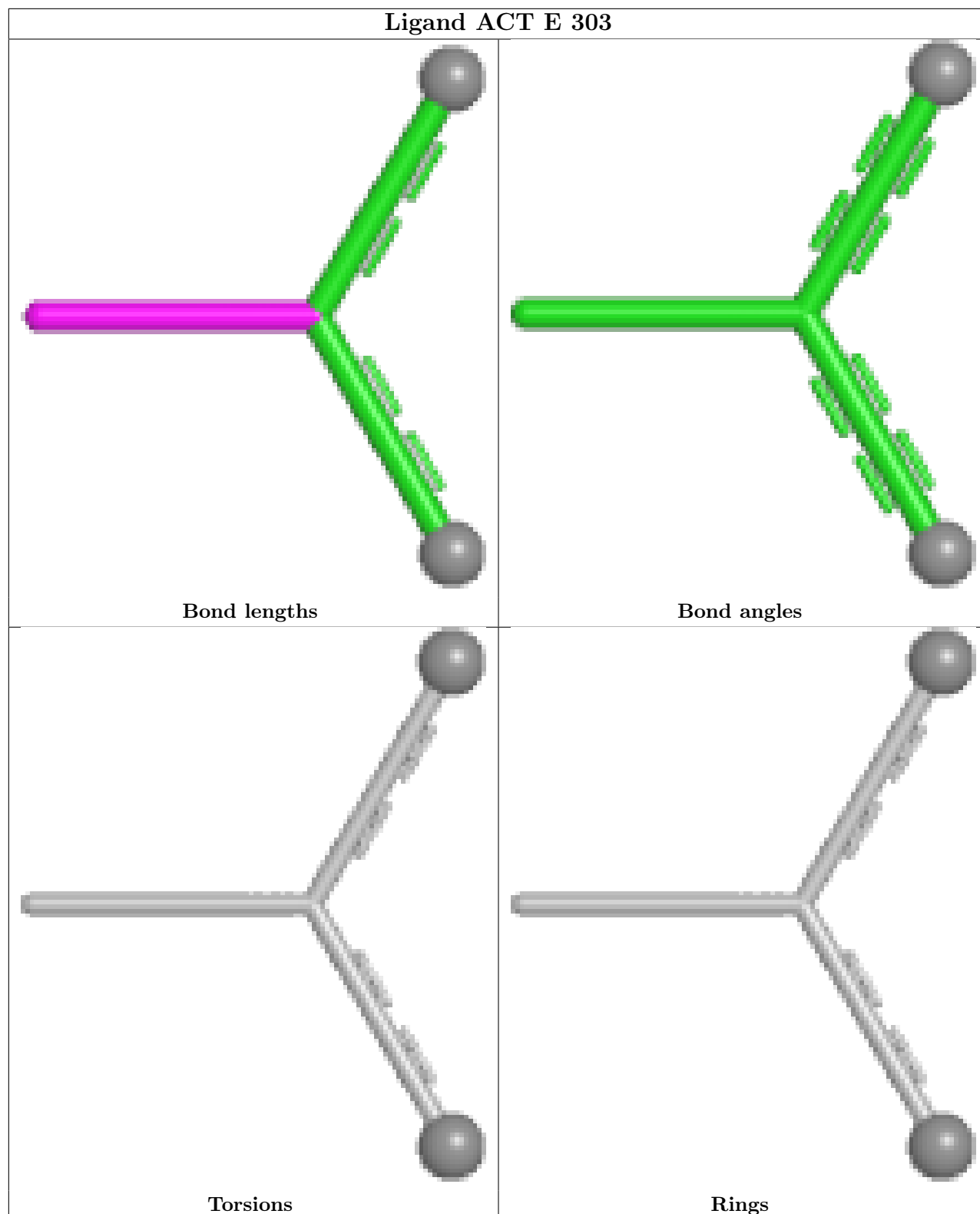


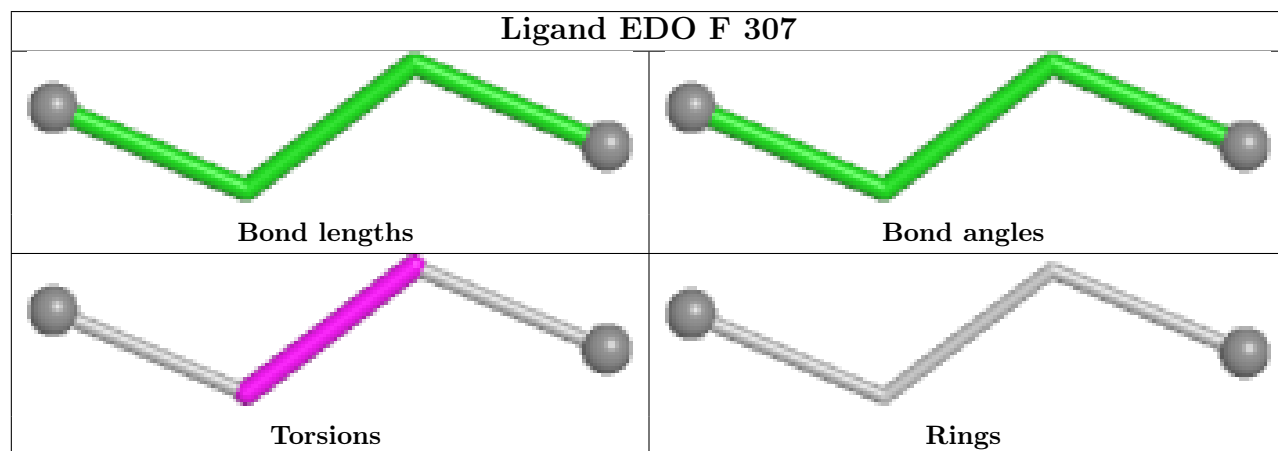
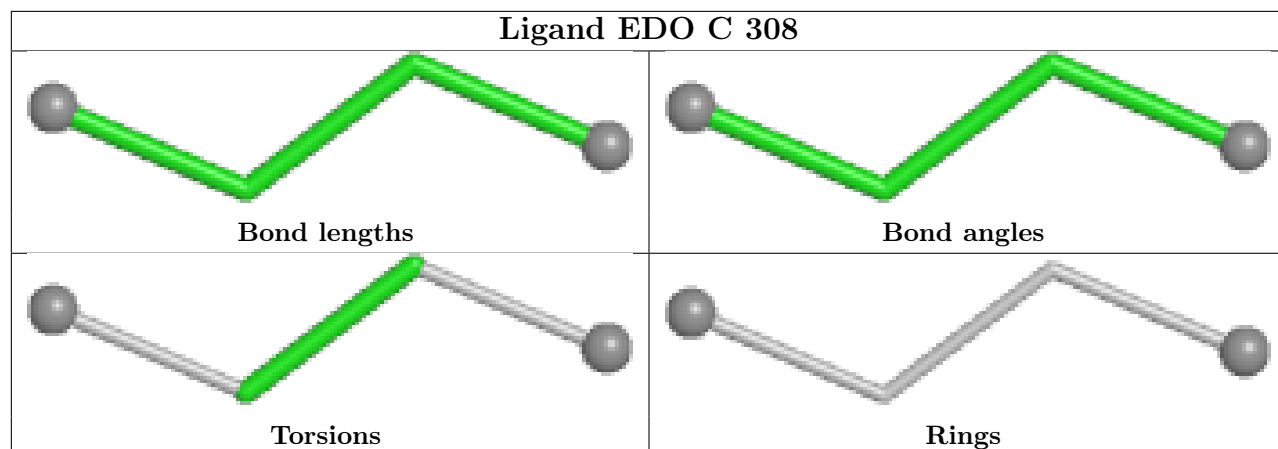
Ligand 3VN E 301

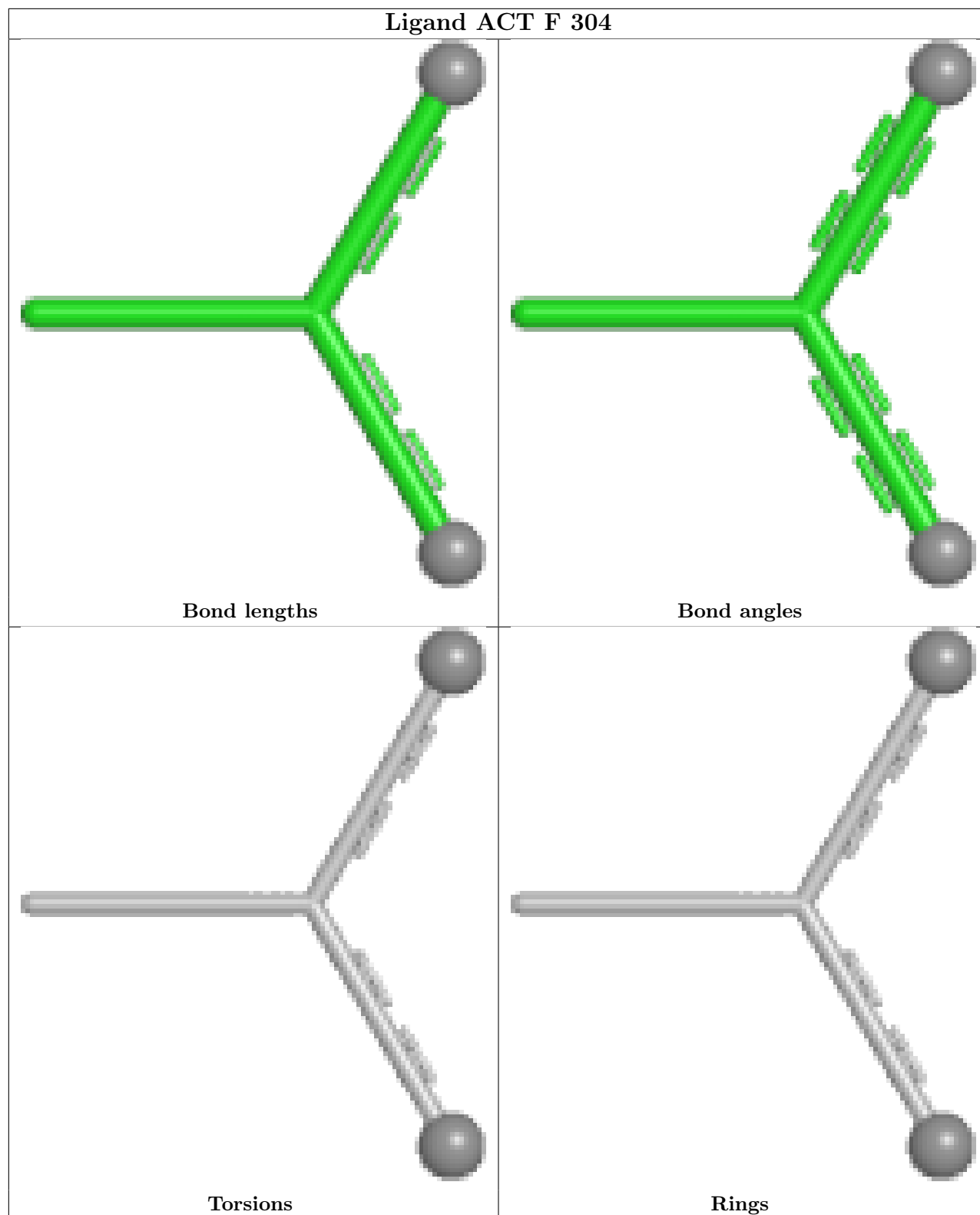


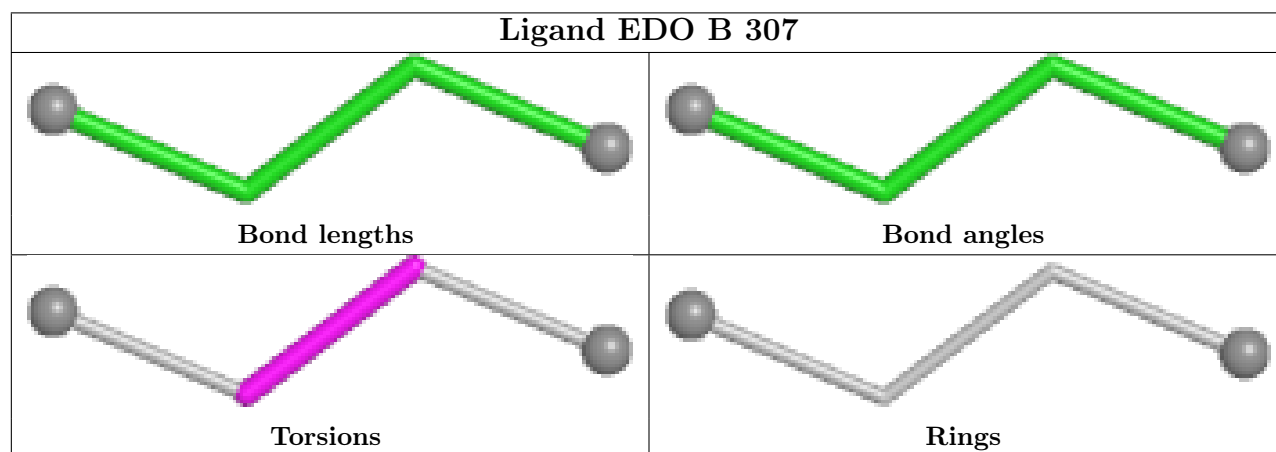
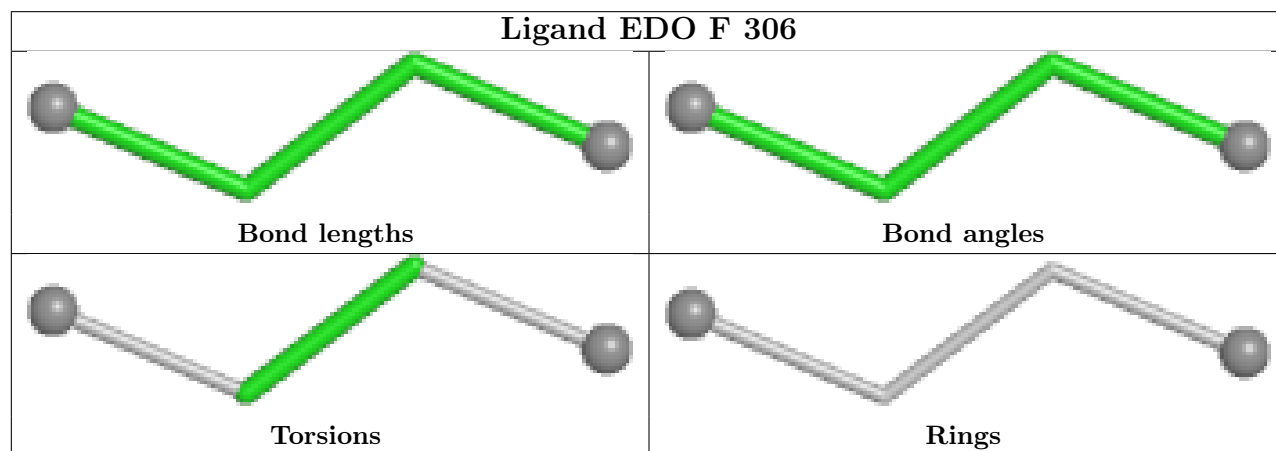
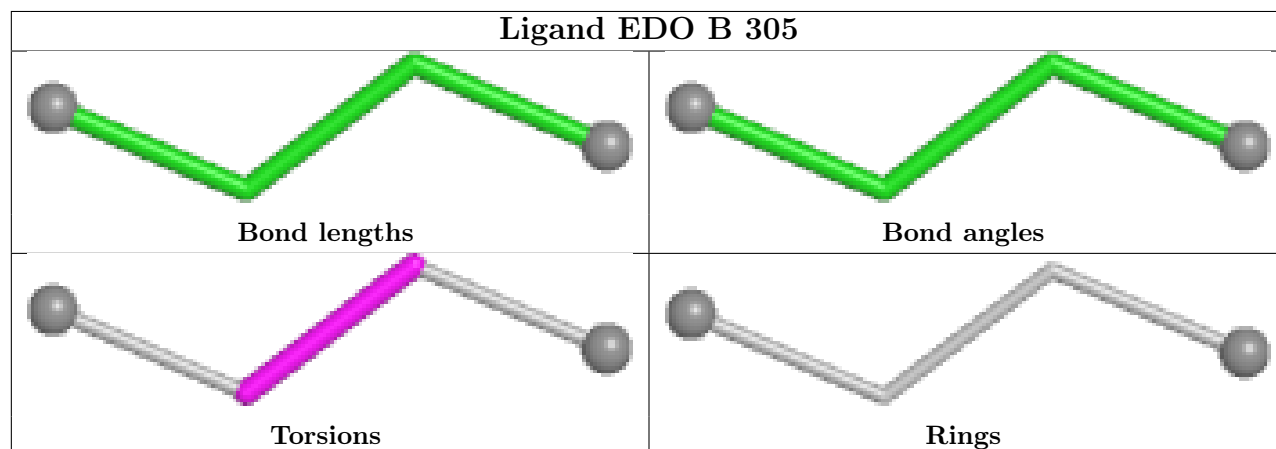
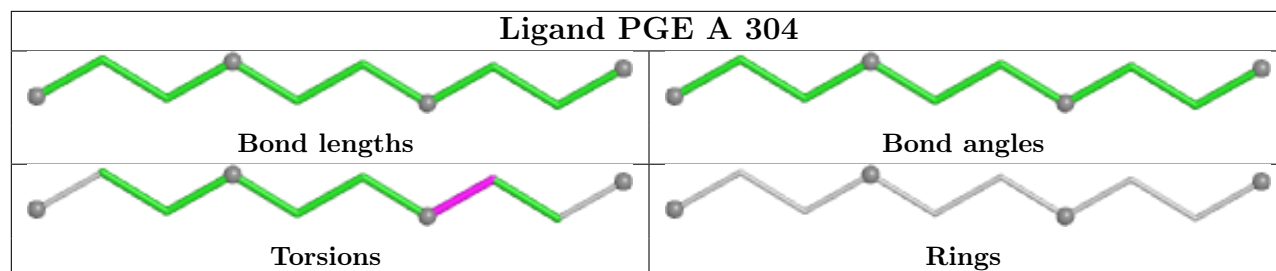


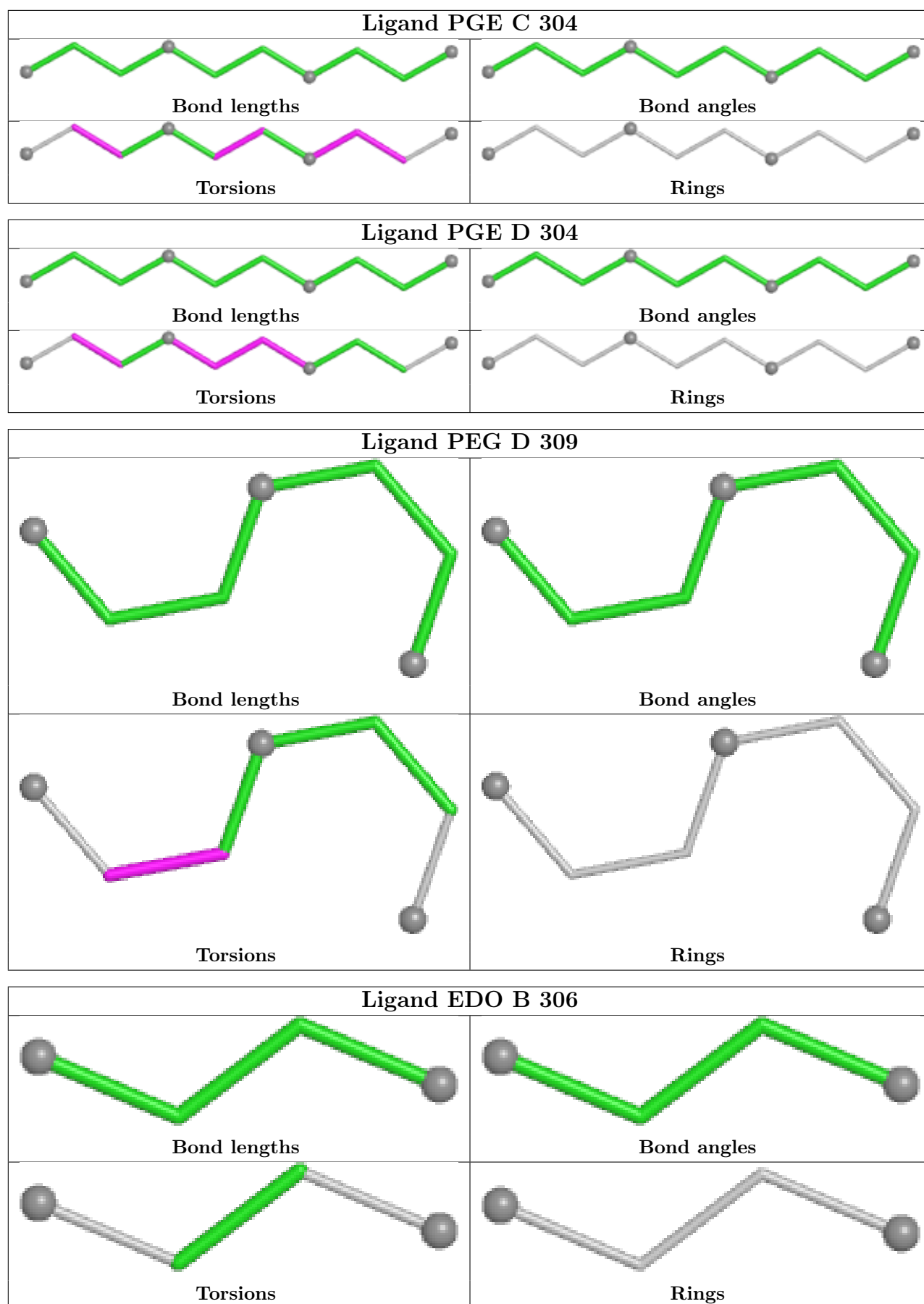
Ligand ACT E 303

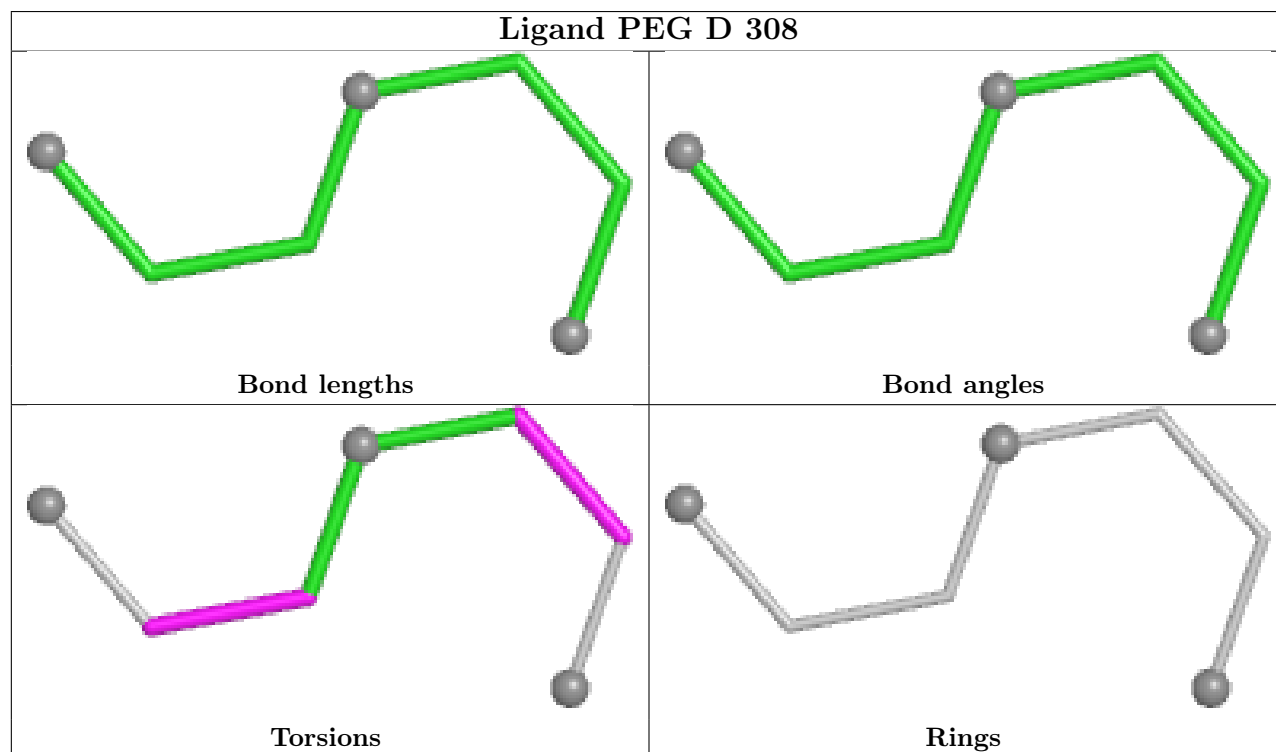
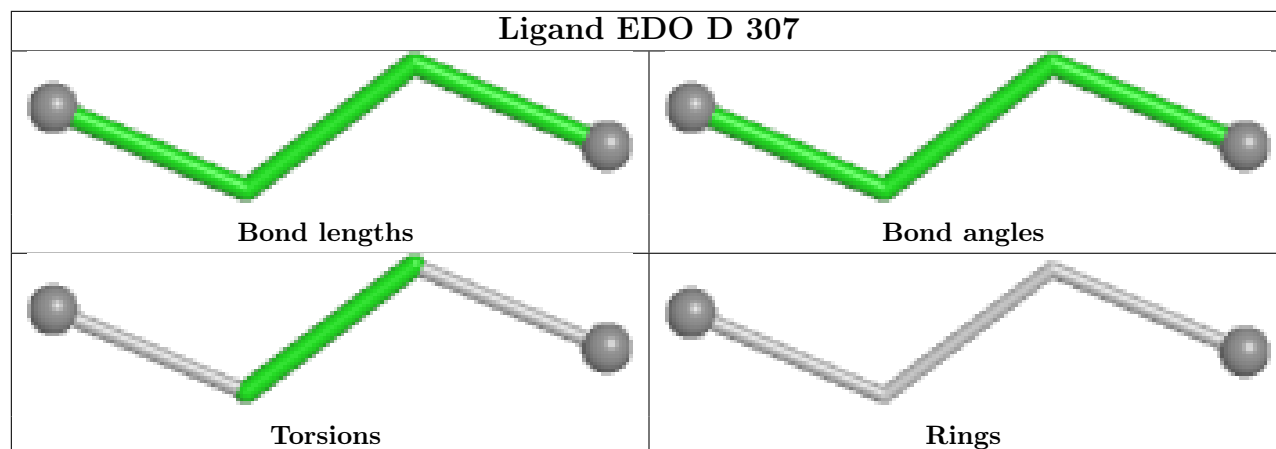


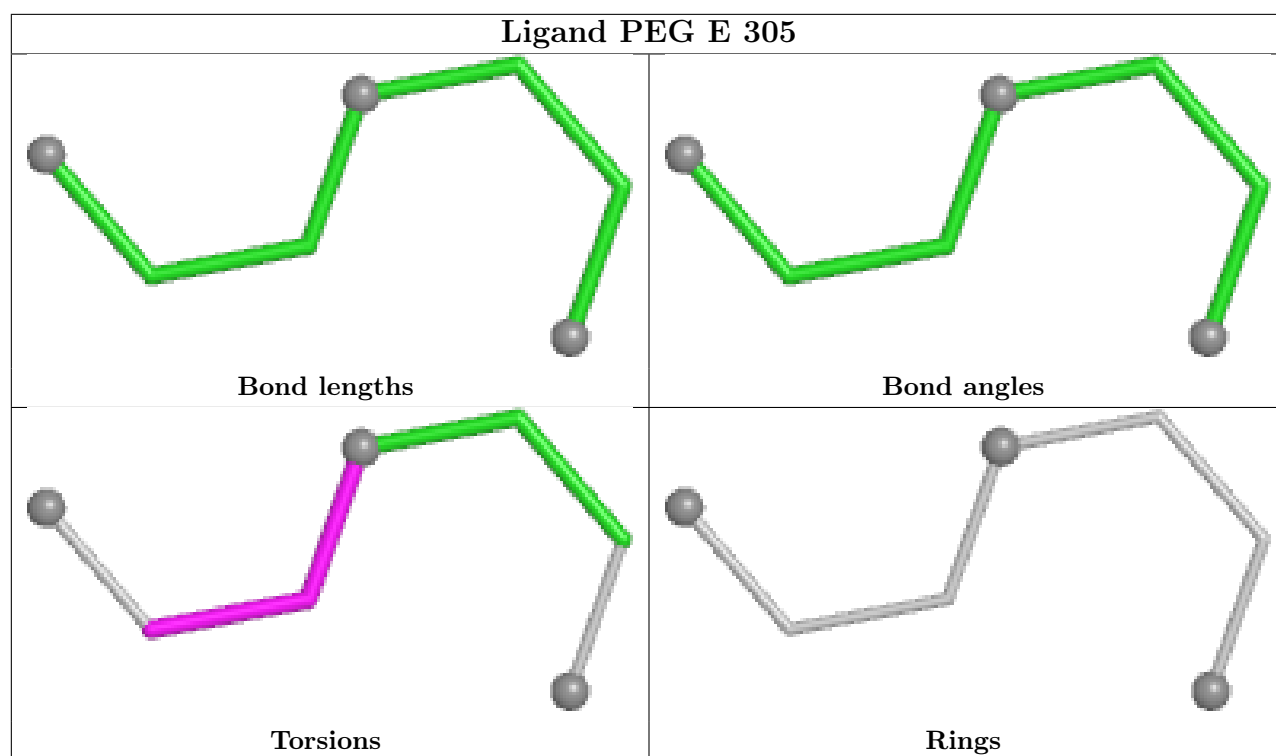


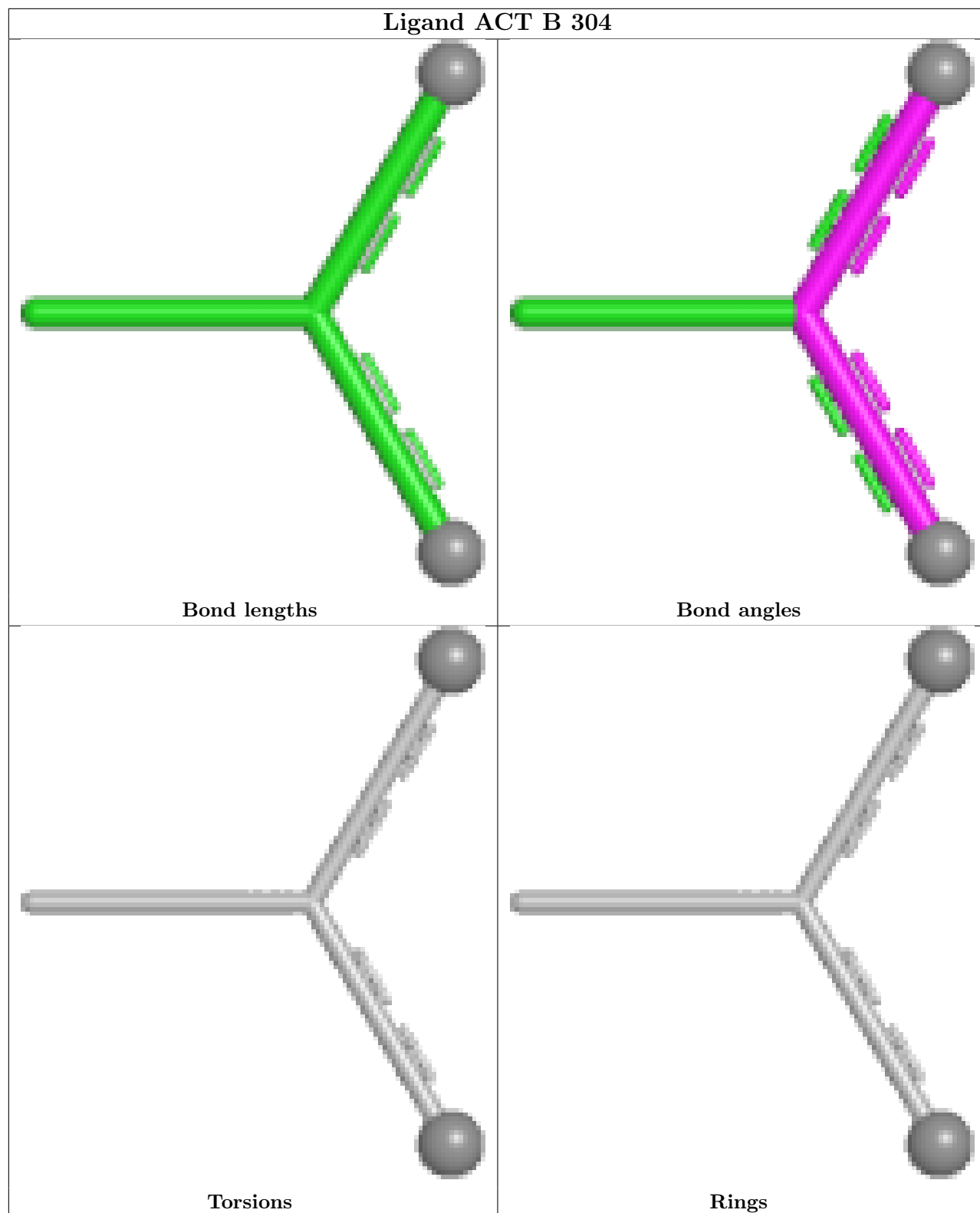


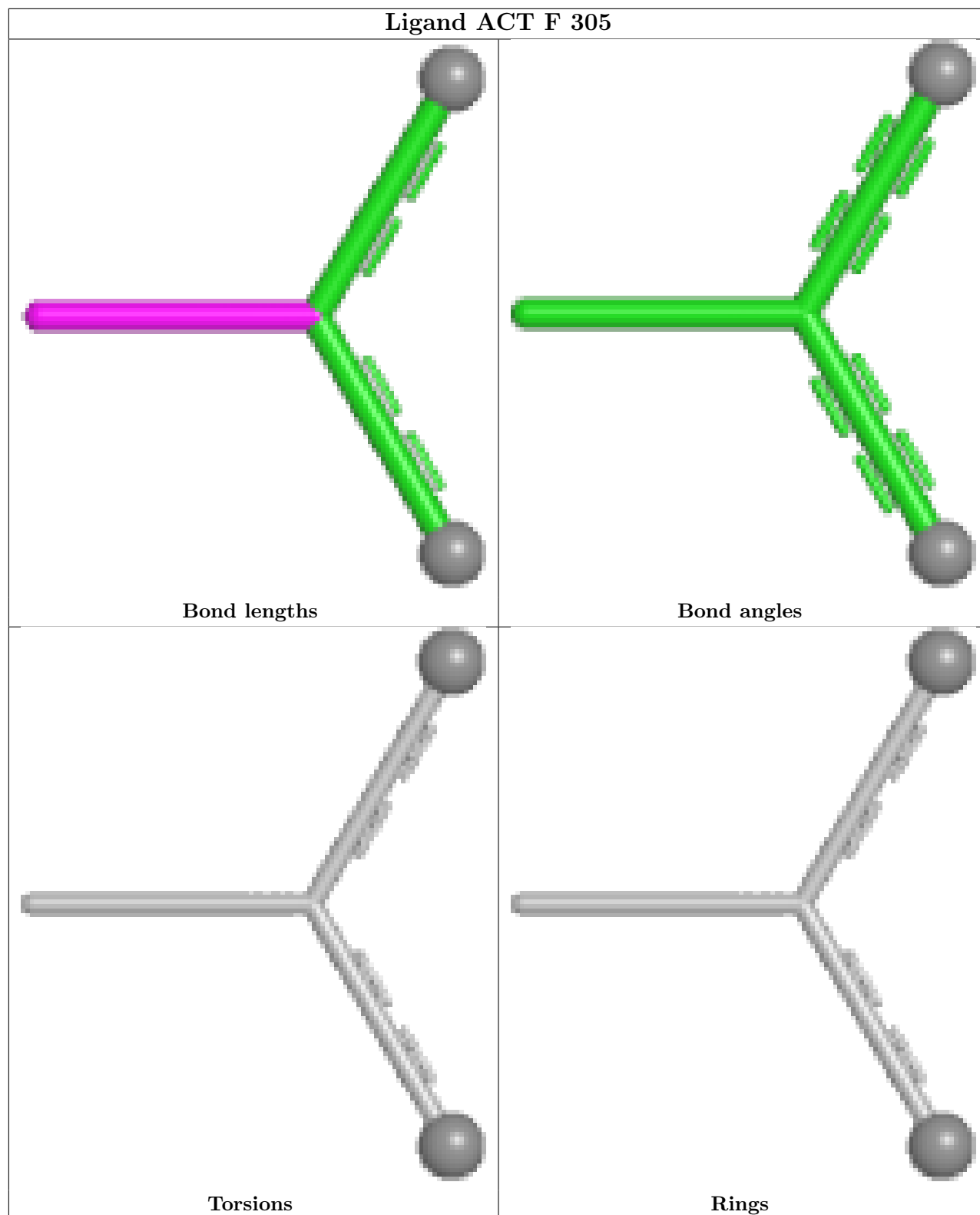


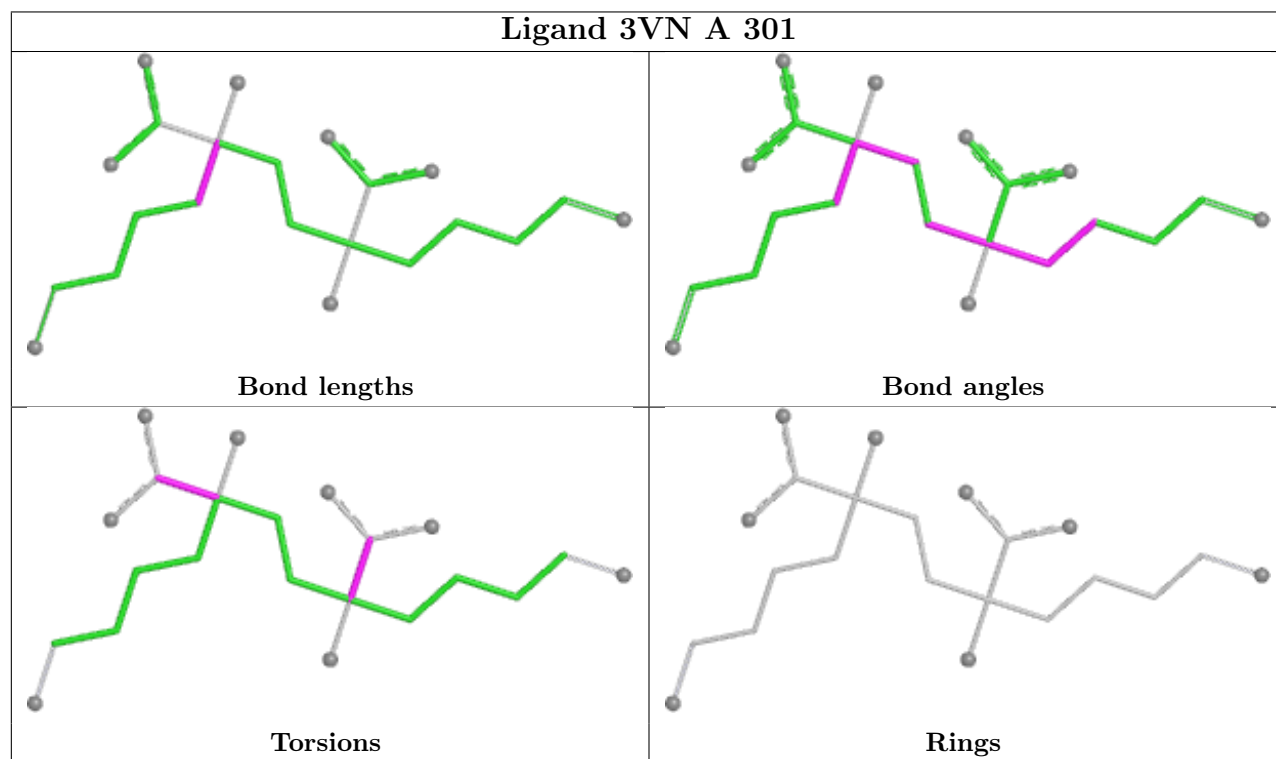
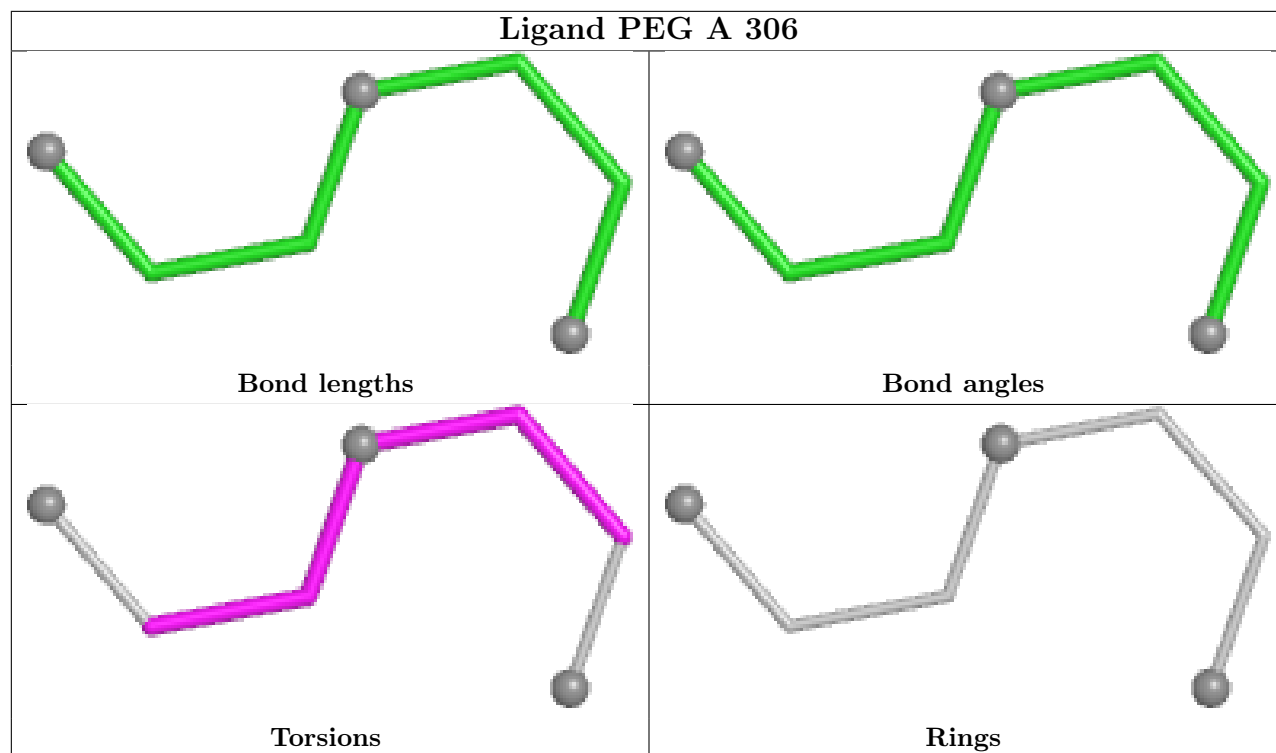


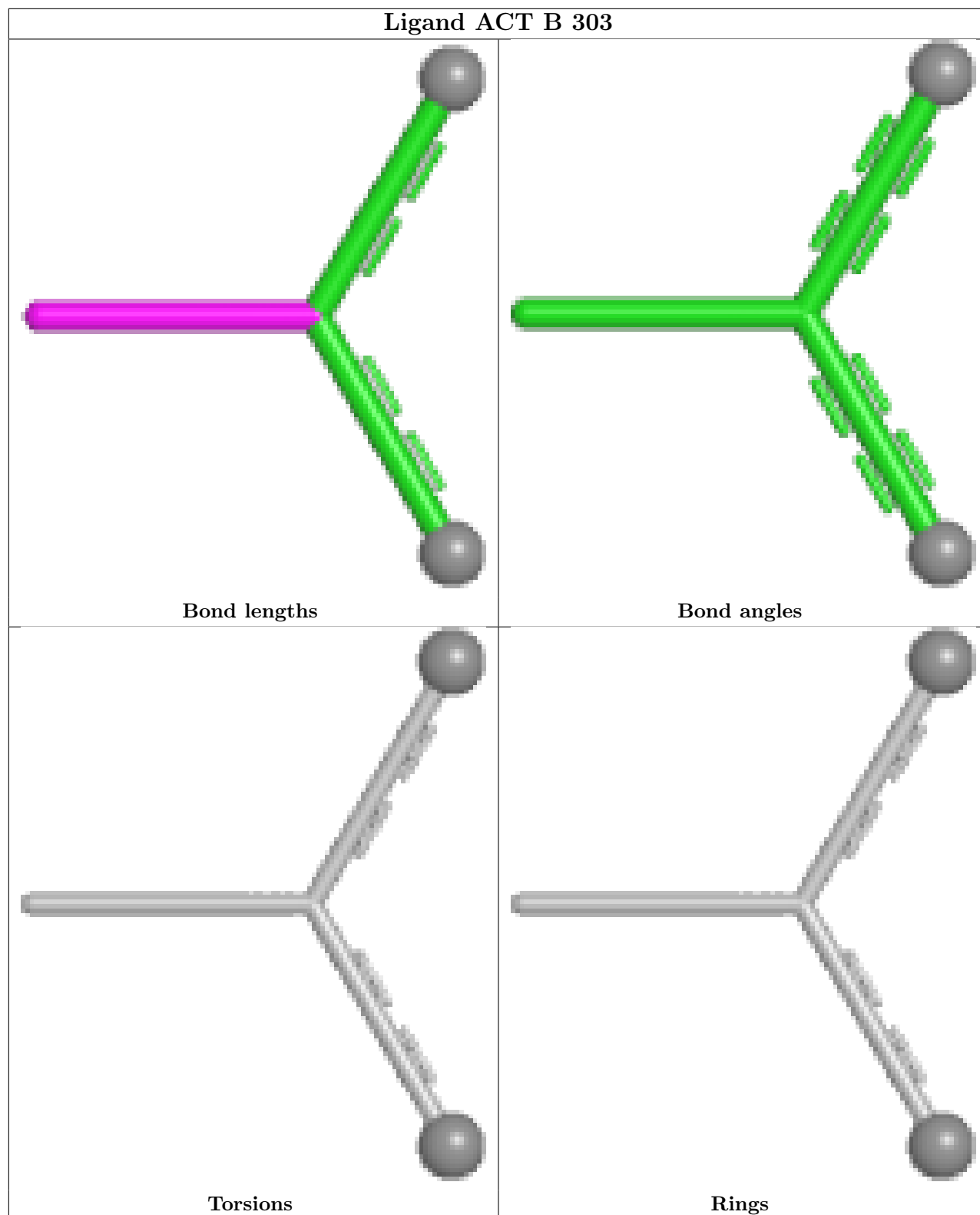


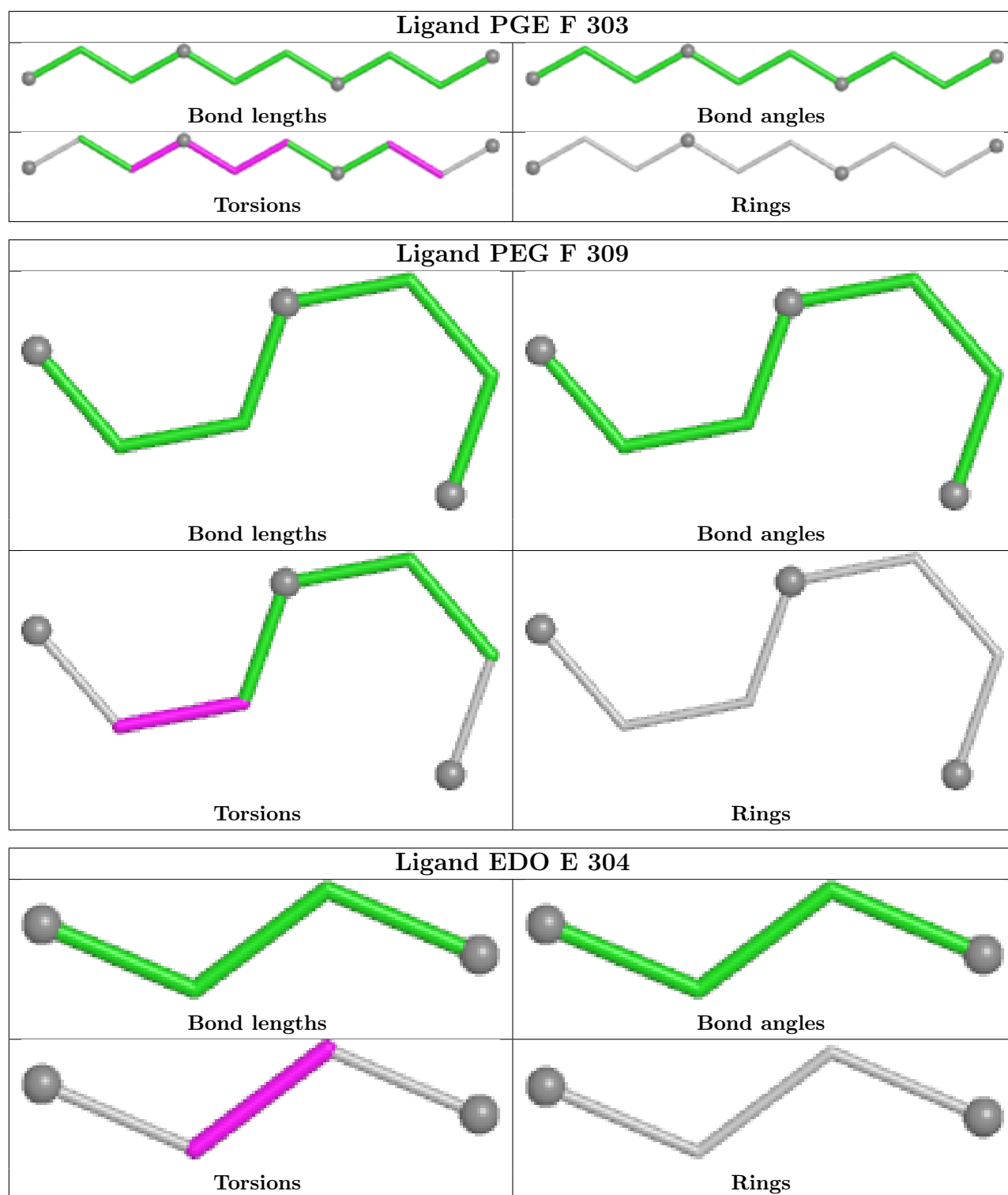












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	295/310 (95%)	-0.28	0	100 100	25, 32, 50, 67	0
1	B	295/310 (95%)	-0.31	0	100 100	25, 31, 48, 57	0
1	C	295/310 (95%)	-0.28	0	100 100	26, 32, 49, 58	0
1	D	295/310 (95%)	-0.25	1 (0%)	90 93	27, 33, 52, 62	0
1	E	295/310 (95%)	-0.14	1 (0%)	90 93	26, 36, 53, 66	0
1	F	296/310 (95%)	-0.05	3 (1%)	79 84	25, 36, 61, 73	0
All	All	1771/1860 (95%)	-0.22	5 (0%)	90 93	25, 33, 52, 73	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	4	ASN	3.1
1	D	25	GLN	2.9
1	F	294	LYS	2.6
1	F	2	ASP	2.4
1	F	227	ASP	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KPI	D	166	14/15	0.93	0.07	24,28,34,37	0
1	KPI	E	166	14/15	0.94	0.07	28,31,38,42	0
1	KPI	C	166	14/15	0.95	0.07	25,29,33,34	0
1	KPI	B	166	14/15	0.96	0.06	24,26,35,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	KPI	A	166	14/15	0.96	0.06	24,27,32,37	0
1	KPI	F	166	14/15	0.96	0.06	25,28,37,39	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
7	EDO	B	307	4/4	0.69	0.28	20,20,20,20	0
5	ACT	F	305	4/4	0.70	0.17	58,61,62,62	0
5	ACT	F	304	4/4	0.70	0.22	67,67,68,70	0
7	EDO	C	307	4/4	0.72	0.21	54,56,57,59	0
7	EDO	E	304	4/4	0.74	0.27	20,20,20,20	0
5	ACT	D	305	4/4	0.75	0.24	61,61,63,68	0
6	PEG	D	308	7/7	0.77	0.20	64,66,68,69	0
7	EDO	D	307	4/4	0.78	0.29	20,20,20,20	0
7	EDO	B	305	4/4	0.78	0.17	70,70,71,73	0
5	ACT	E	303	4/4	0.80	0.23	67,72,73,75	0
6	PEG	A	306	7/7	0.80	0.25	20,20,20,20	0
3	MG	F	302	1/1	0.82	0.22	66,66,66,66	0
5	ACT	B	303	4/4	0.83	0.17	50,55,57,57	0
4	PGE	E	302	10/10	0.83	0.18	57,58,65,67	0
5	ACT	C	305	4/4	0.85	0.16	60,62,63,63	0
7	EDO	B	306	4/4	0.85	0.15	52,53,53,56	0
6	PEG	F	309	7/7	0.85	0.14	59,64,70,72	0
6	PEG	E	305	7/7	0.86	0.13	67,68,69,70	0
6	PEG	D	309	7/7	0.86	0.29	20,20,20,20	0
7	EDO	F	306	4/4	0.86	0.17	56,61,63,64	0
4	PGE	C	304	10/10	0.87	0.16	58,61,65,67	0
4	PGE	F	303	10/10	0.87	0.13	52,59,60,60	0
7	EDO	F	308	4/4	0.87	0.25	20,20,20,20	0
7	EDO	D	306	4/4	0.88	0.14	57,58,58,60	0
3	MG	D	303	1/1	0.89	0.22	60,60,60,60	0
7	EDO	B	308	4/4	0.89	0.34	20,20,20,20	0

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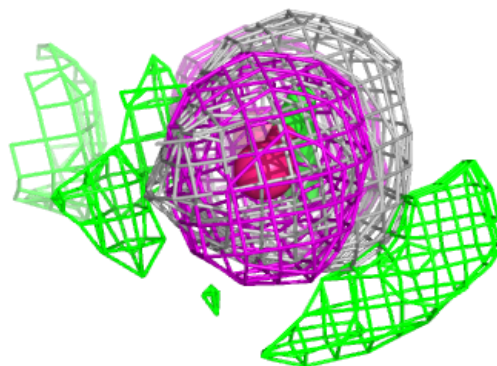
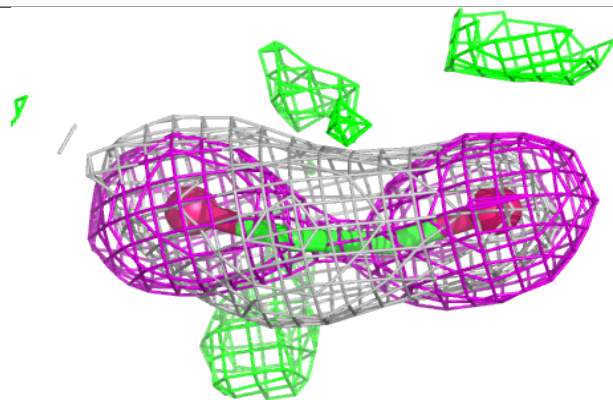
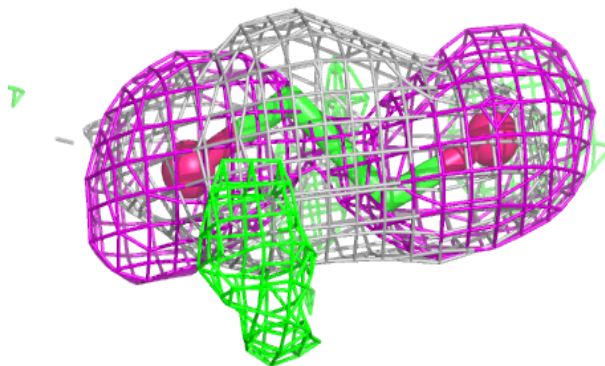
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	3VN	A	301	22/22	0.89	0.24	38,71,78,78	0
2	3VN	C	301	22/22	0.89	0.25	40,72,77,78	0
5	ACT	A	305	4/4	0.90	0.14	44,51,52,56	0
4	PGE	B	302	10/10	0.90	0.12	50,53,56,57	0
7	EDO	F	307	4/4	0.91	0.12	58,61,64,67	0
2	3VN	E	301	22/22	0.91	0.17	42,50,70,72	0
4	PGE	D	304	10/10	0.92	0.11	52,54,61,64	0
4	PGE	A	304	10/10	0.92	0.11	51,55,60,61	0
5	ACT	B	304	4/4	0.93	0.10	61,61,62,62	0
7	EDO	C	308	4/4	0.93	0.12	44,49,51,54	0
3	MG	A	303	1/1	0.93	0.25	30,30,30,30	0
3	MG	C	303	1/1	0.93	0.19	69,69,69,69	0
5	ACT	C	306	4/4	0.95	0.12	65,65,65,67	0
3	MG	B	301	1/1	0.95	0.04	33,33,33,33	0
3	MG	D	301	1/1	0.96	0.19	56,56,56,56	0
3	MG	C	302	1/1	0.98	0.09	27,27,27,27	0
3	MG	D	302	1/1	0.98	0.13	31,31,31,31	0
3	MG	A	302	1/1	0.98	0.03	31,31,31,31	0
3	MG	F	301	1/1	0.99	0.06	31,31,31,31	0

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

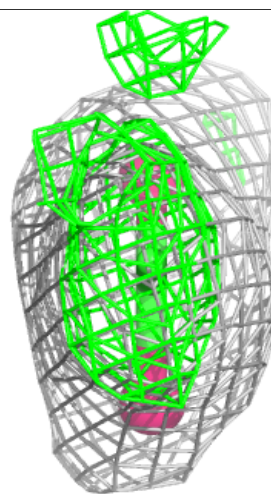
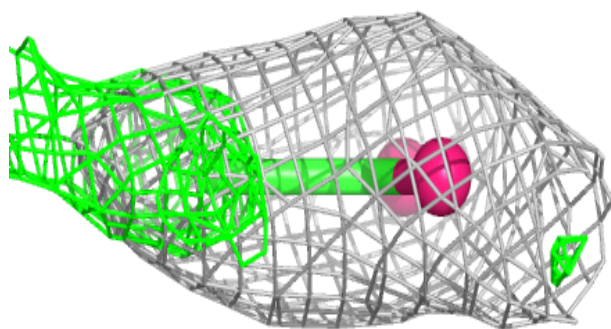
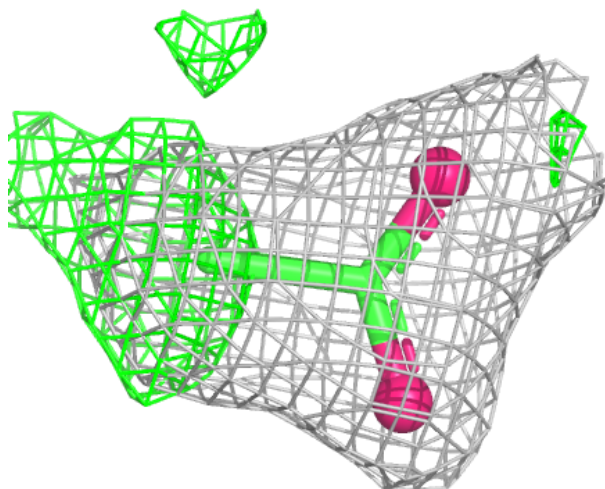
Electron density around EDO B 307:

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



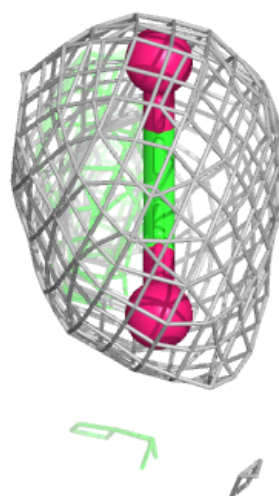
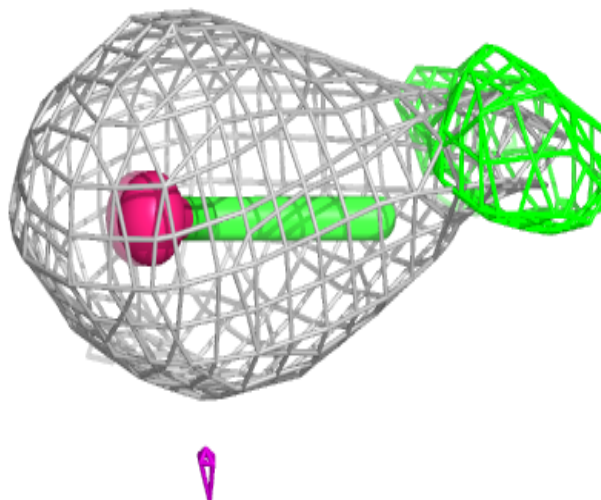
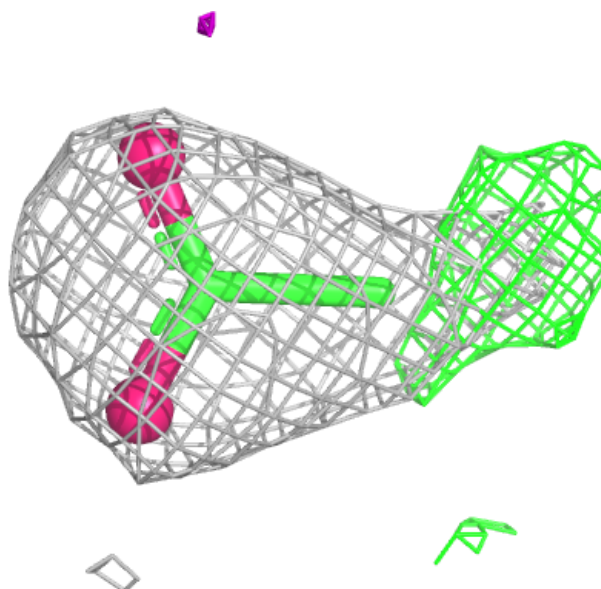
Electron density around ACT F 305:

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



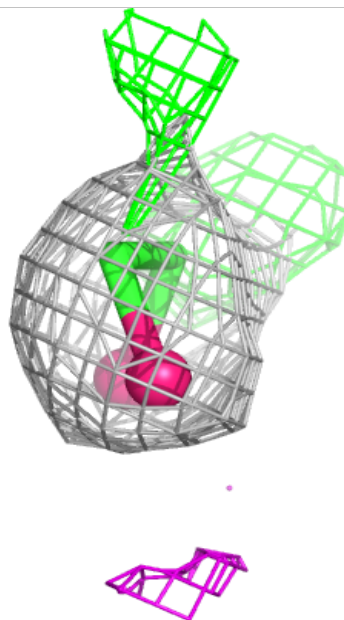
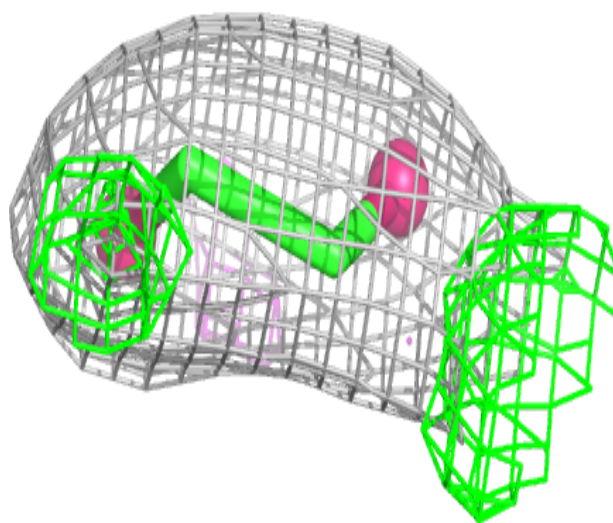
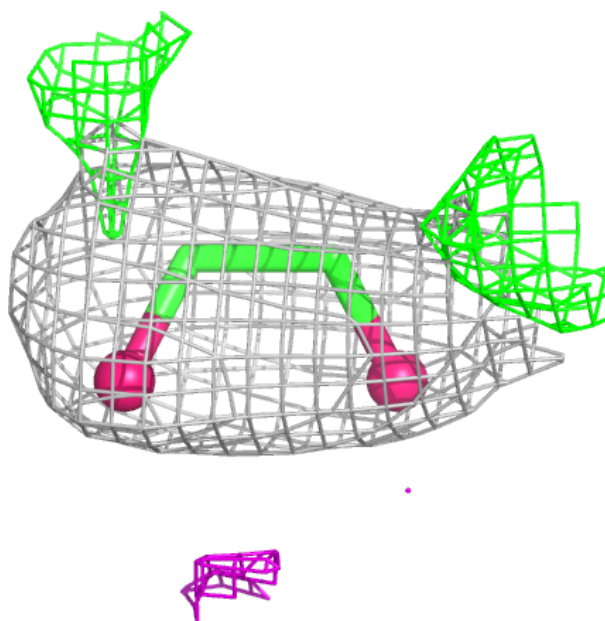
Electron density around ACT F 304:

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



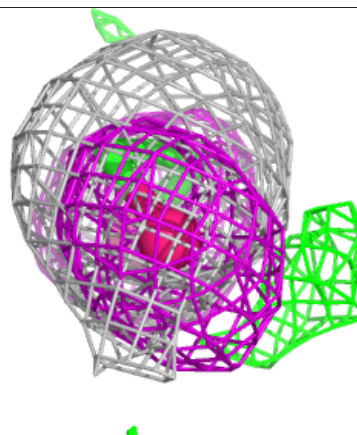
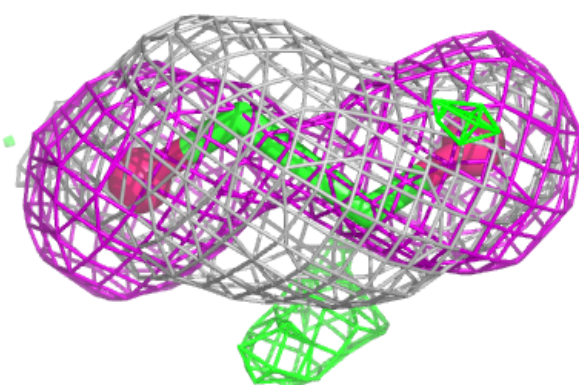
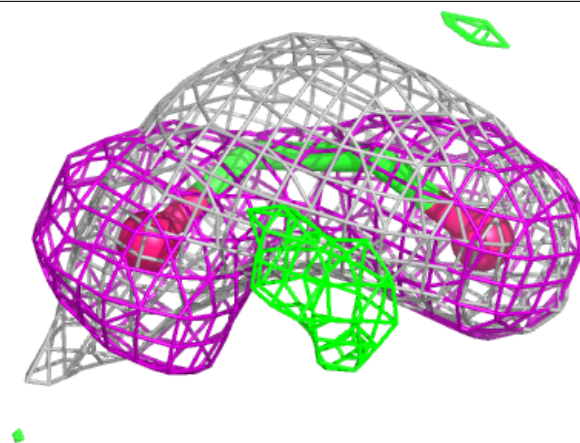
Electron density around EDO C 307:

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



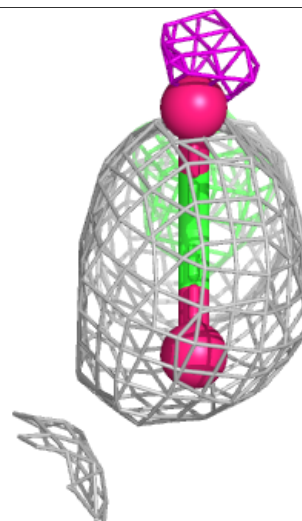
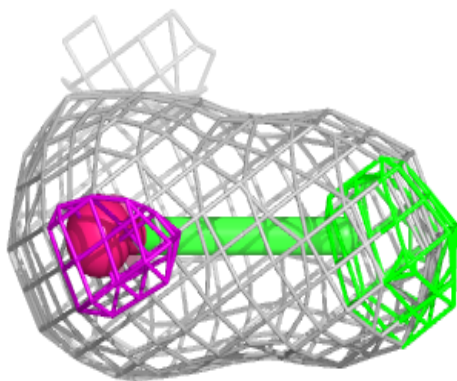
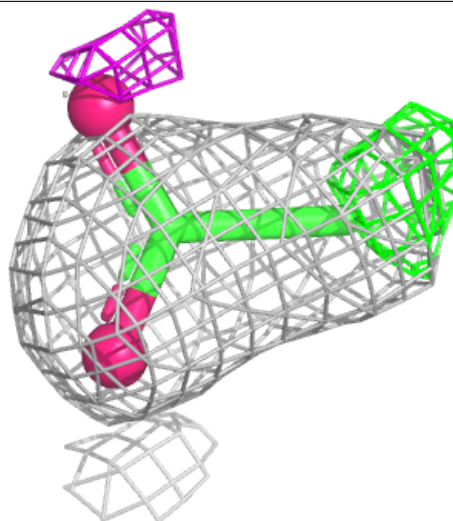
Electron density around EDO E 304:

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



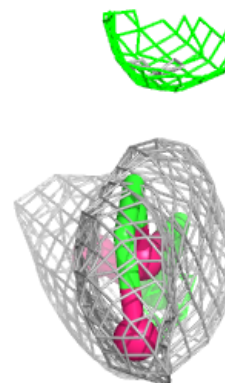
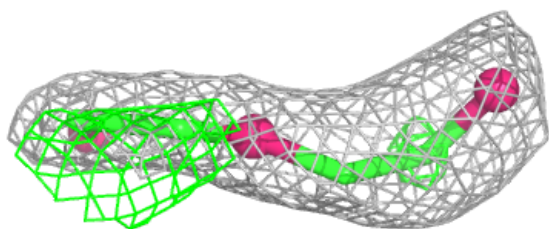
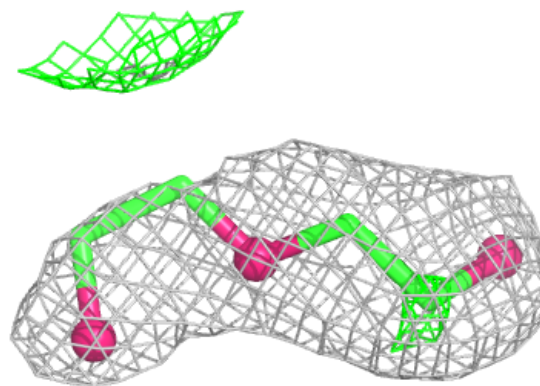
Electron density around ACT D 305:

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

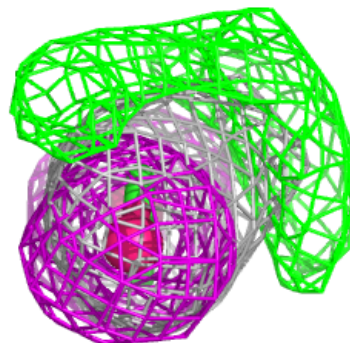
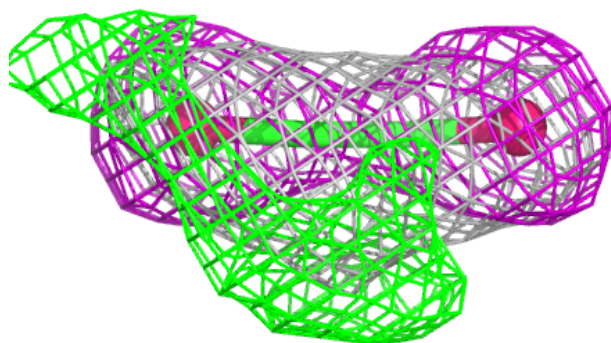
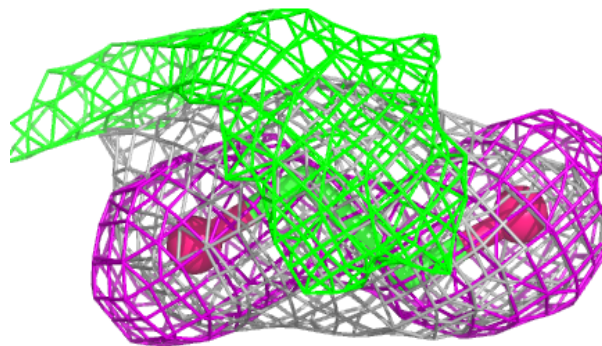


Electron density around PEG D 308:

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

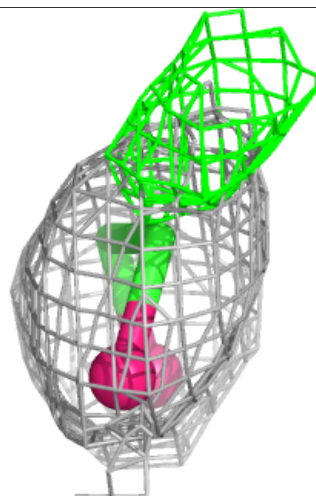
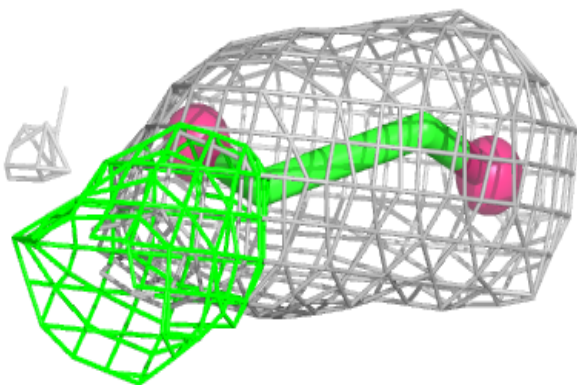
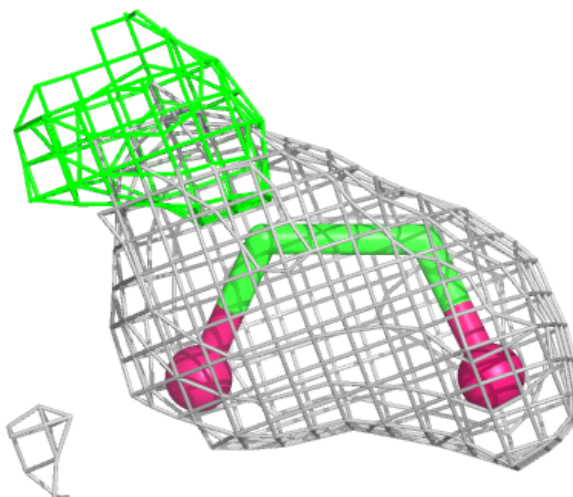
**Electron density around EDO D 307:**

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



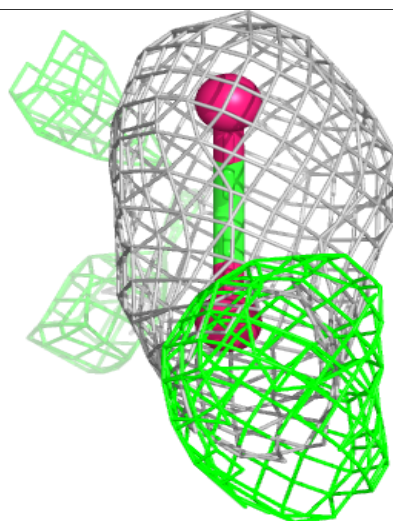
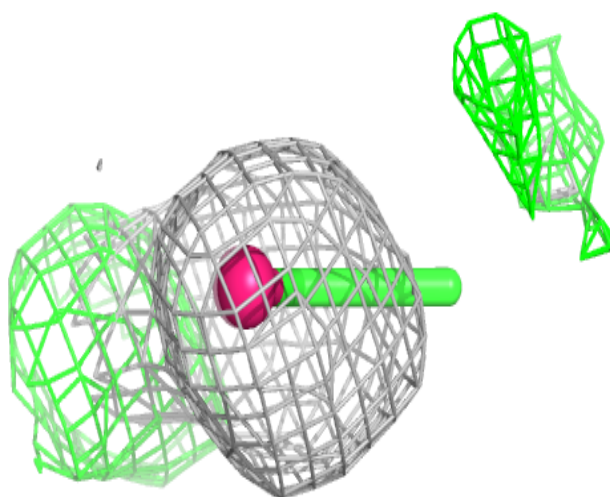
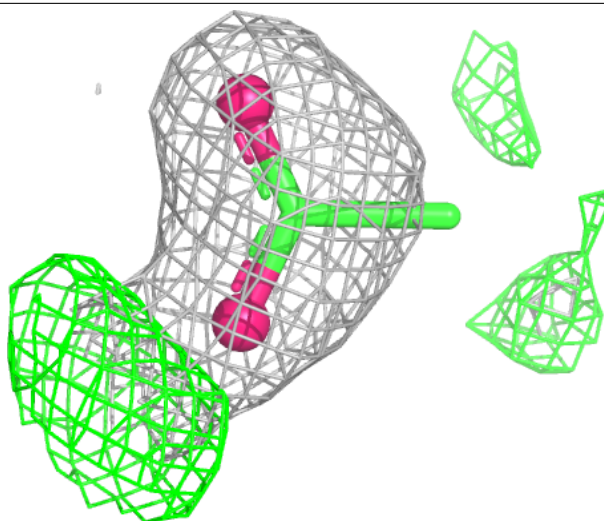
Electron density around EDO B 305:

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



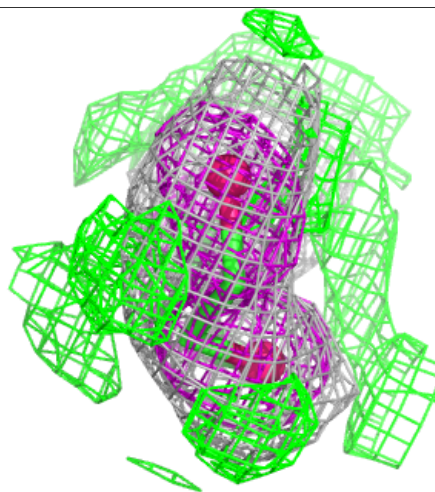
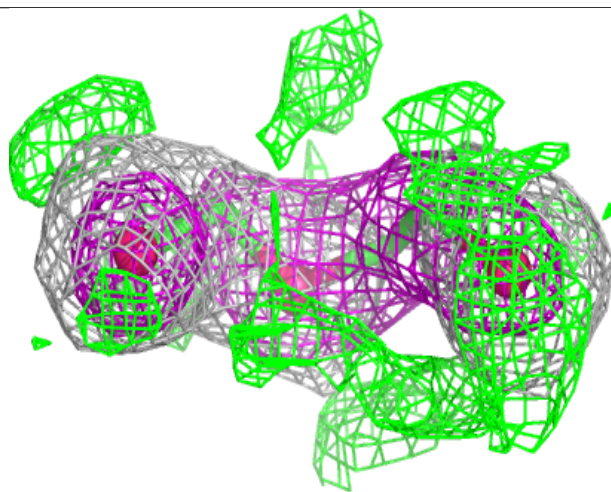
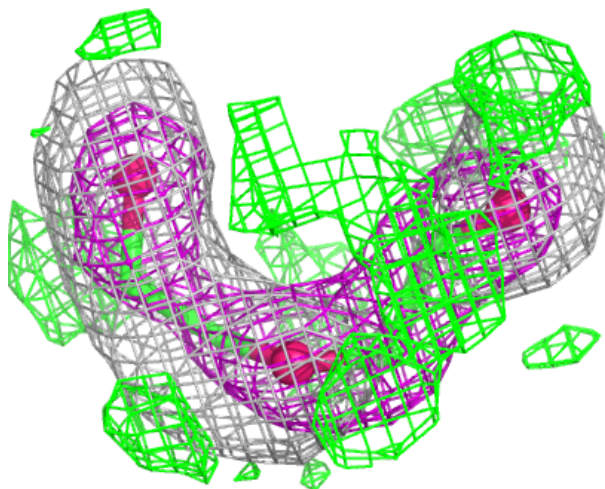
Electron density around ACT E 303:

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



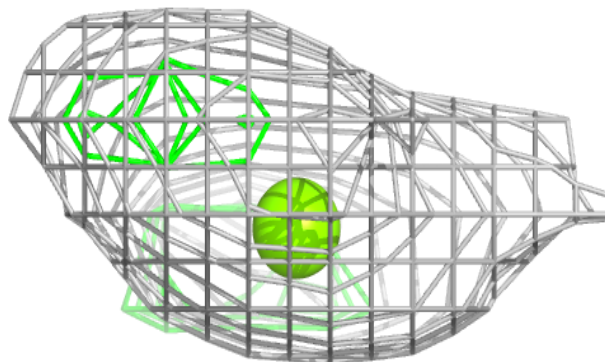
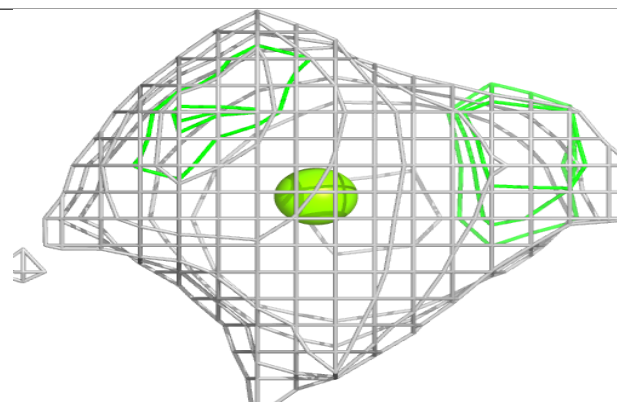
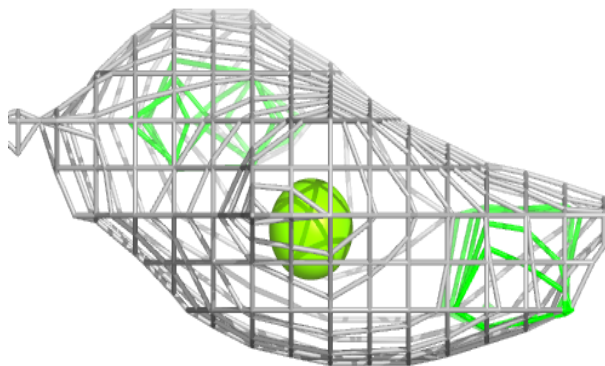
Electron density around PEG A 306:

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



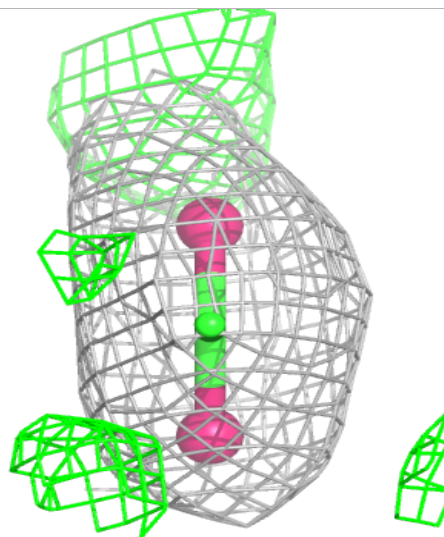
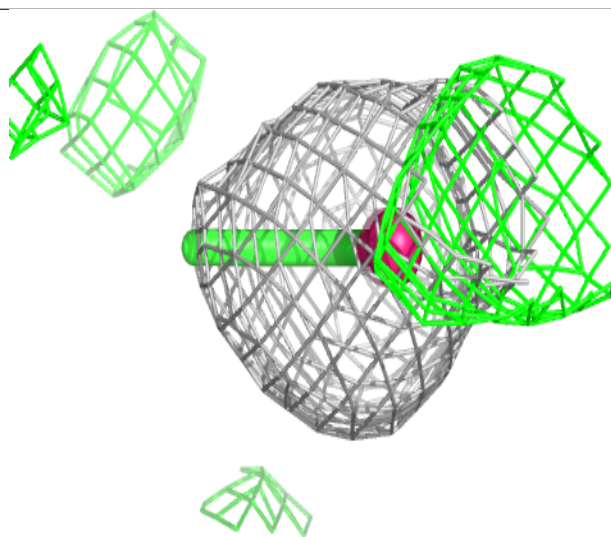
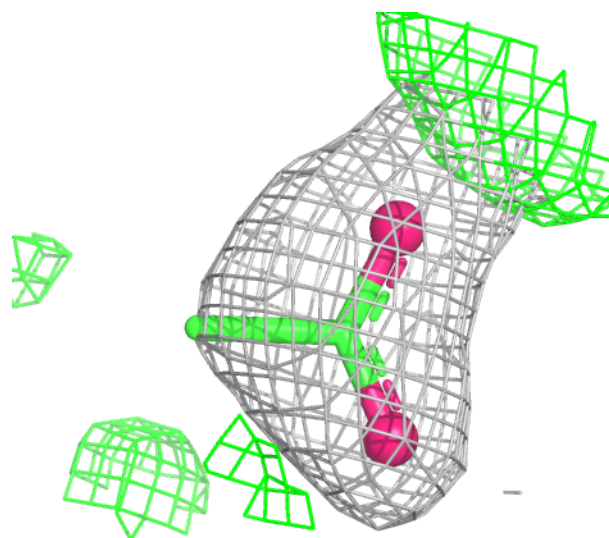
Electron density around MG F 302:

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



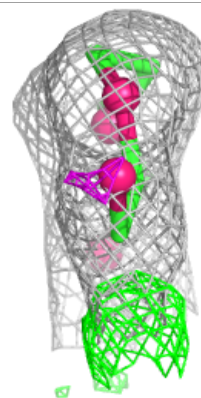
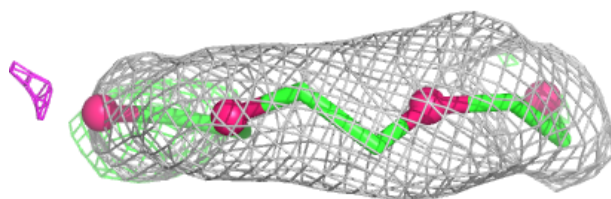
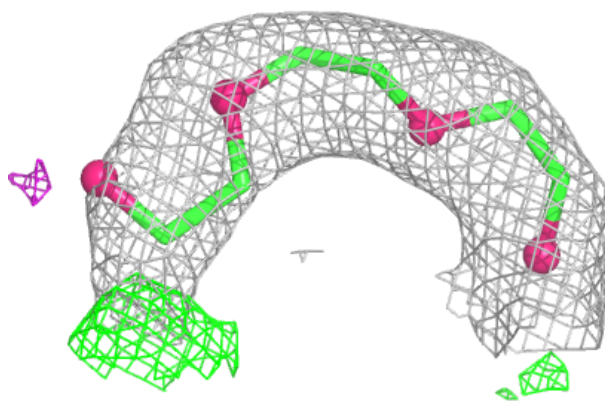
Electron density around ACT B 303:

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



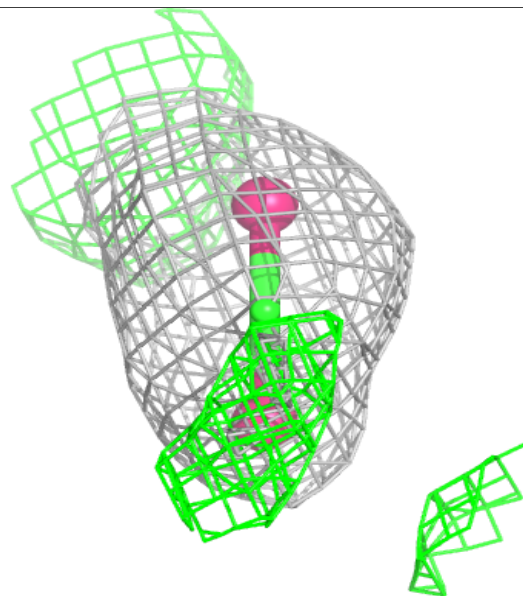
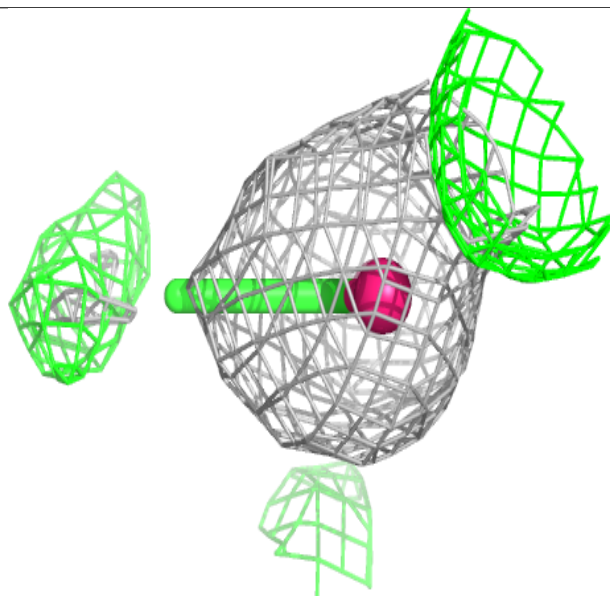
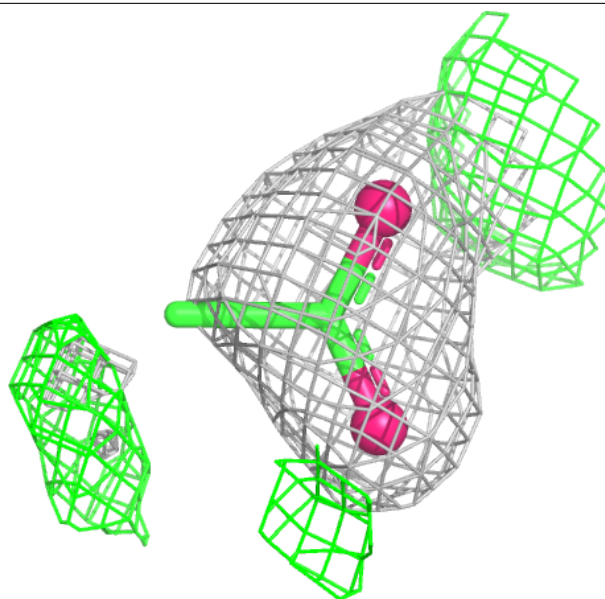
Electron density around PGE E 302:

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



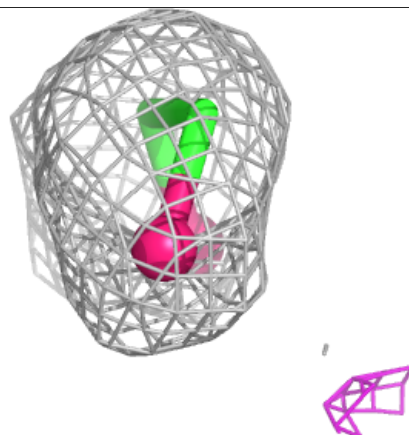
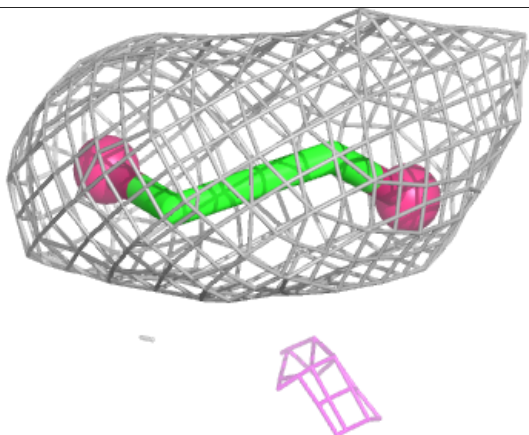
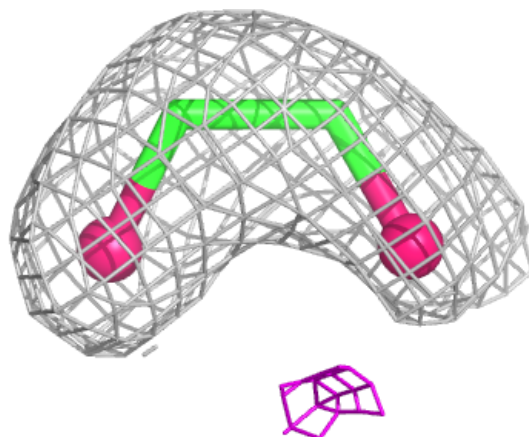
Electron density around ACT C 305:

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

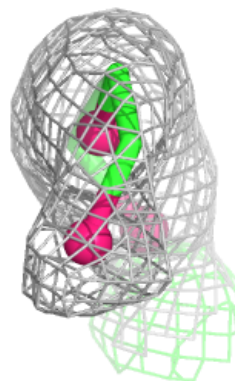
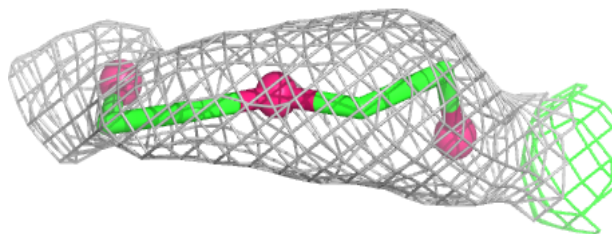
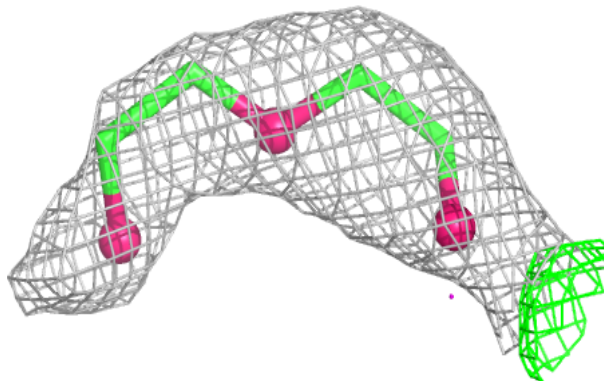


Electron density around EDO B 306:

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

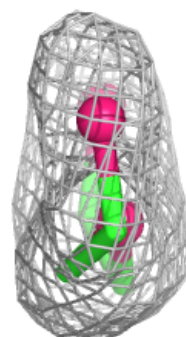
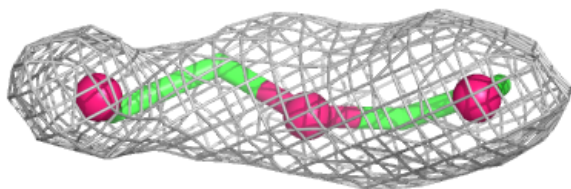
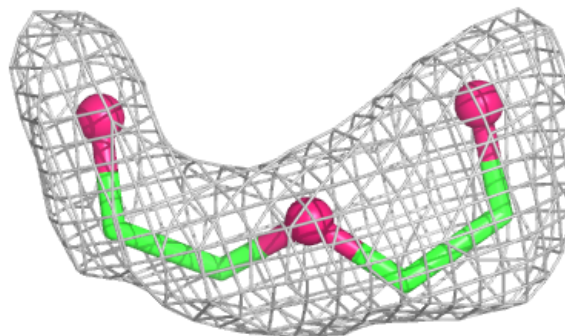
**Electron density around PEG F 309:**

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

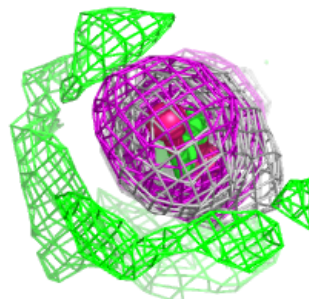
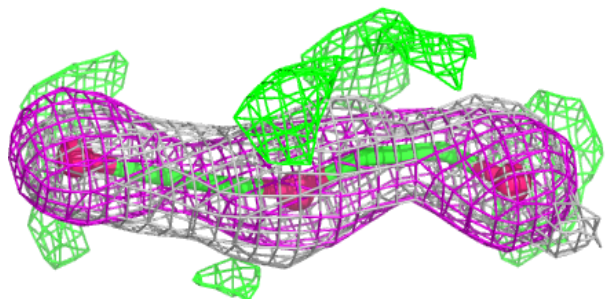
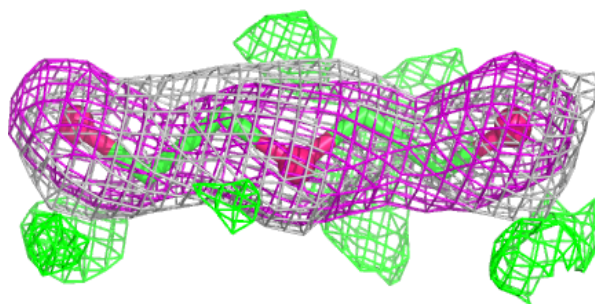


Electron density around PEG E 305:

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

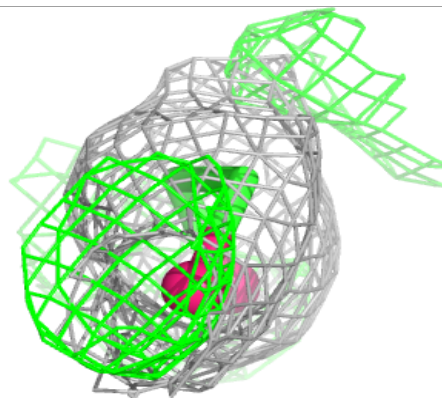
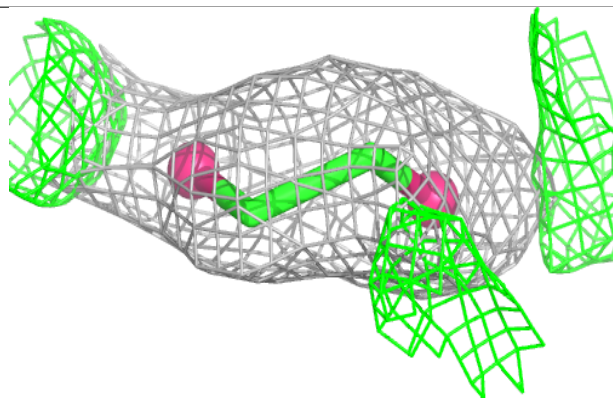
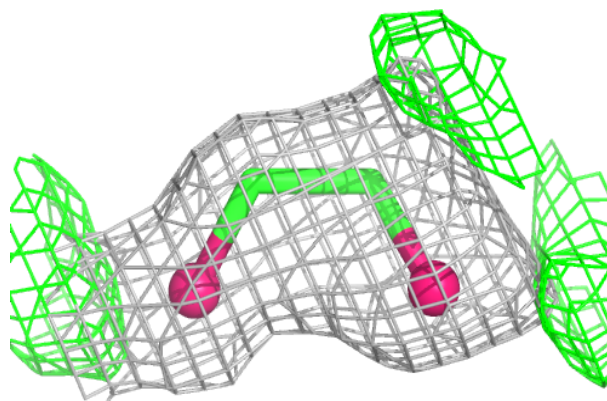
**Electron density around PEG D 309:**

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



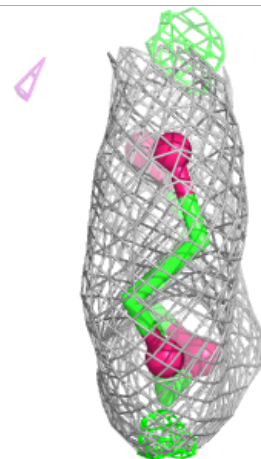
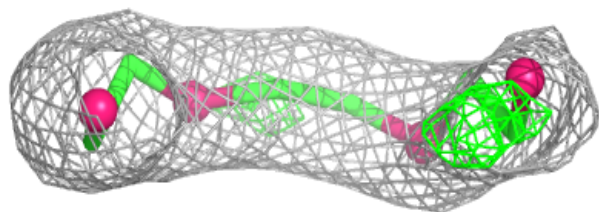
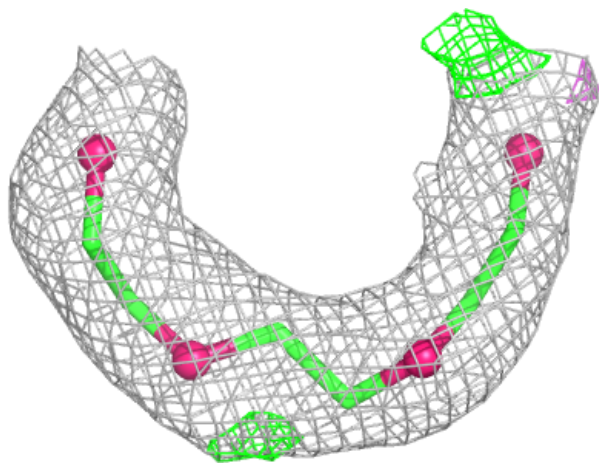
Electron density around EDO F 306:

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



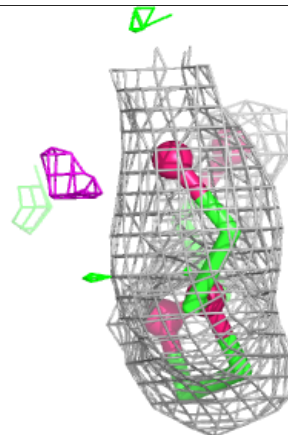
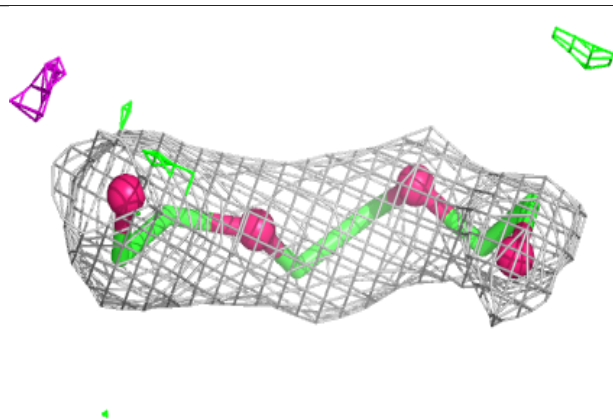
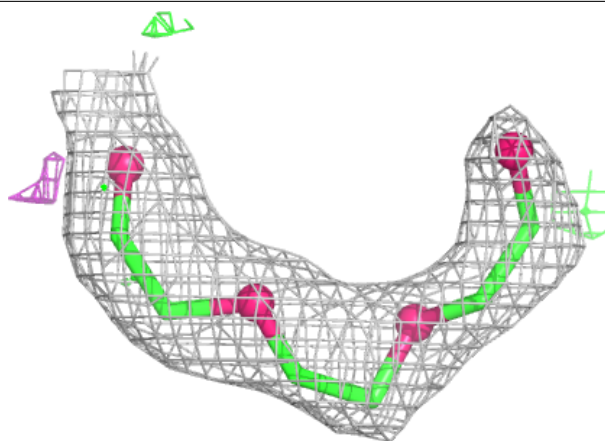
Electron density around PGE C 304:

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



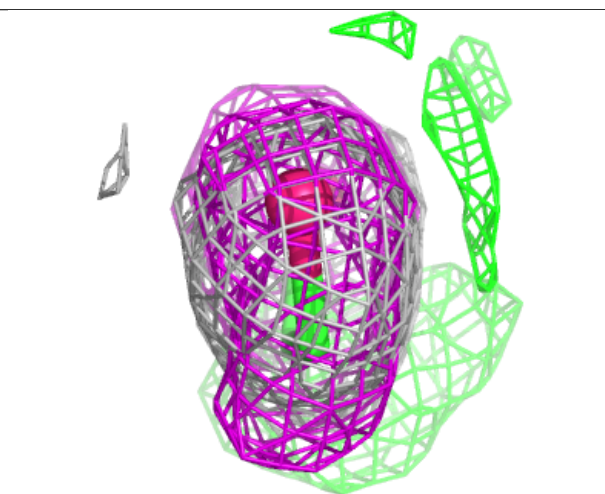
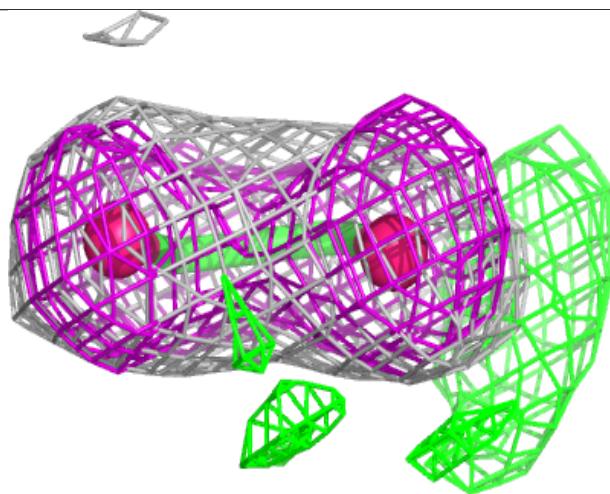
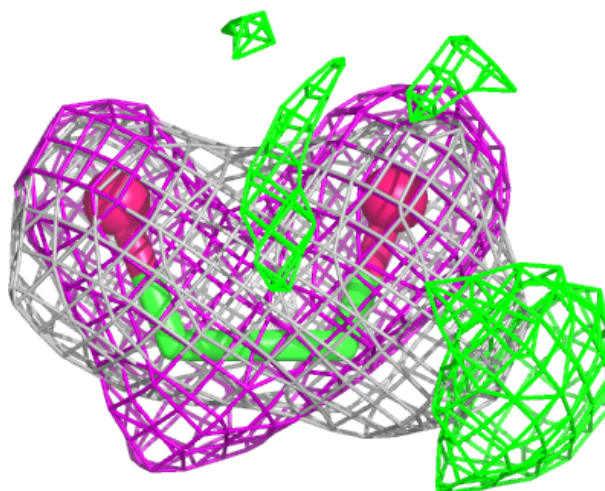
Electron density around PGE F 303:

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



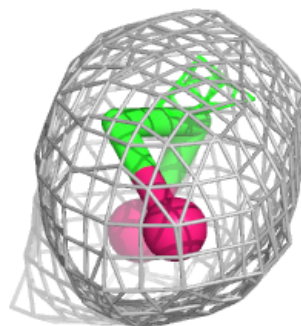
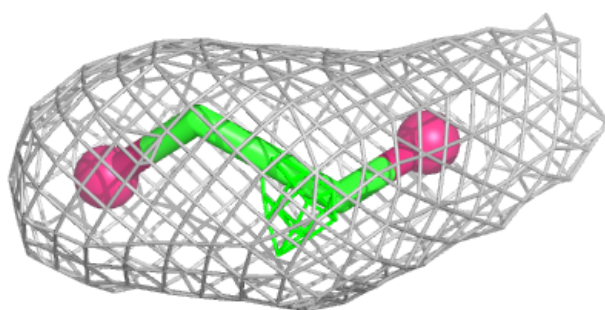
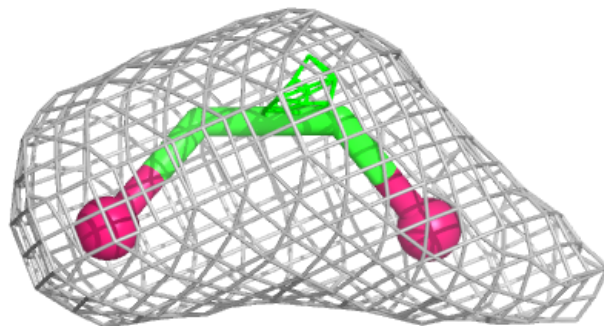
Electron density around EDO F 308:

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



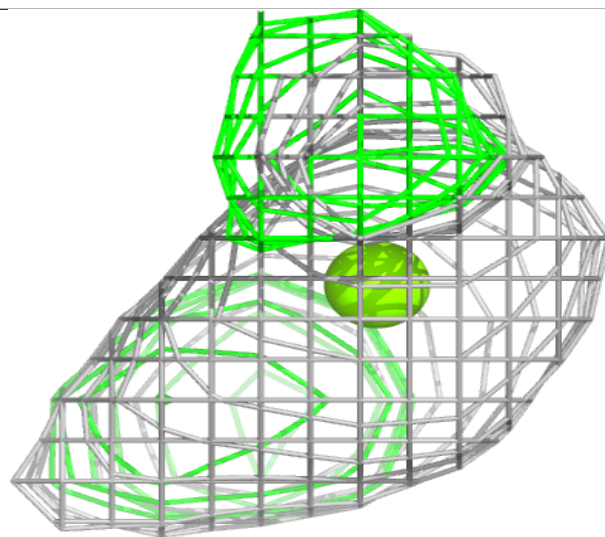
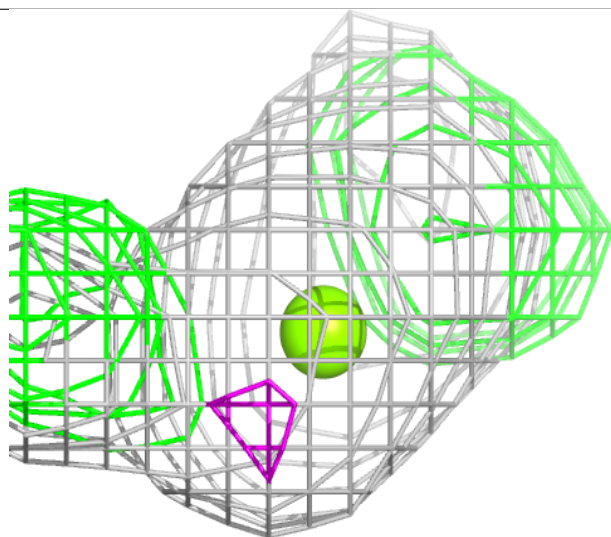
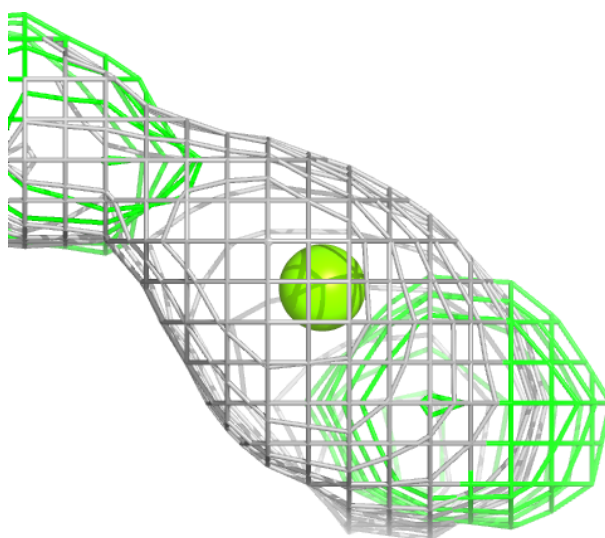
Electron density around EDO D 306:

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



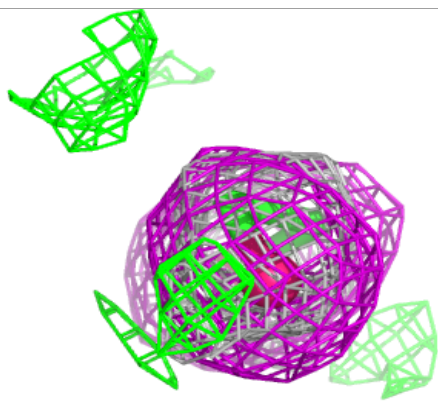
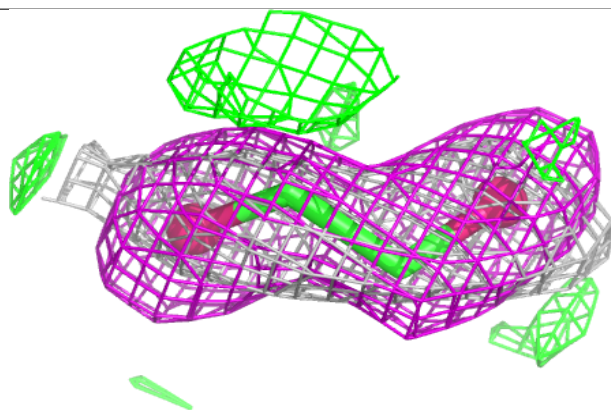
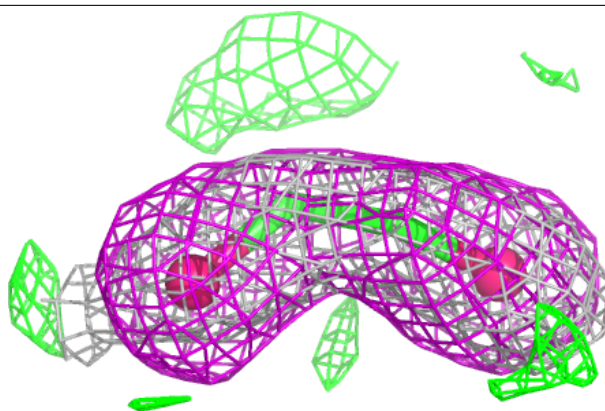
Electron density around MG D 303:

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

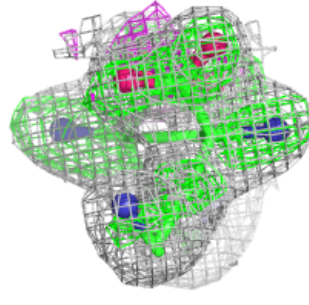
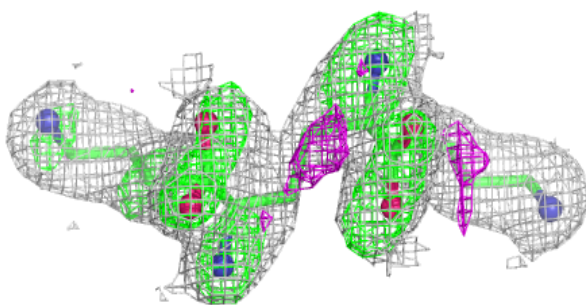
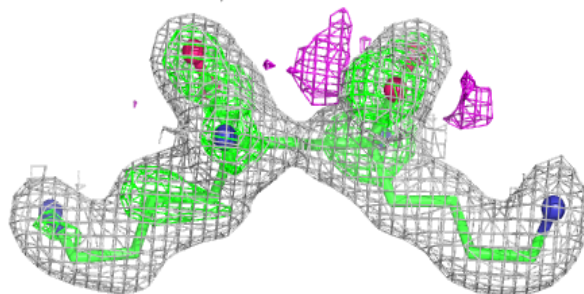


Electron density around EDO B 308:

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

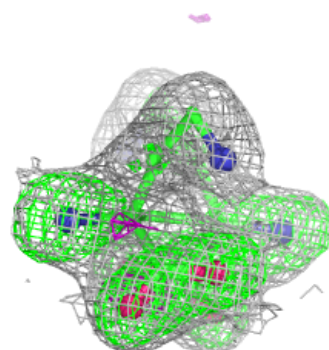
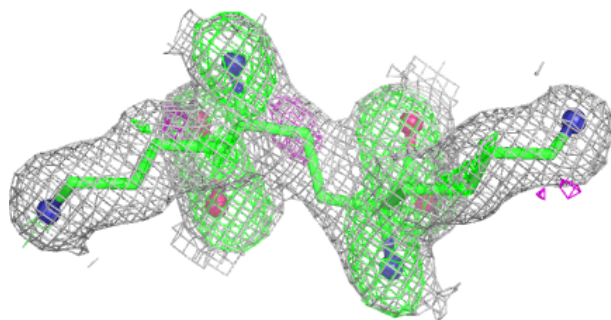
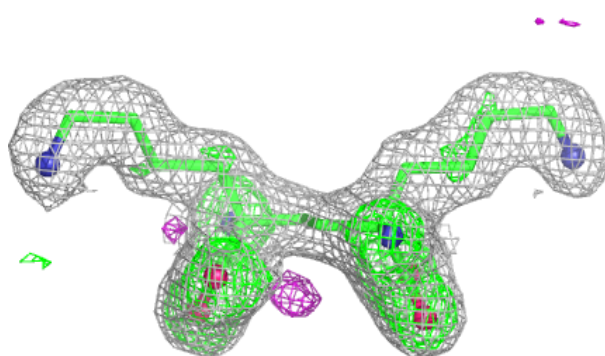
**Electron density around 3VN A 301:**

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



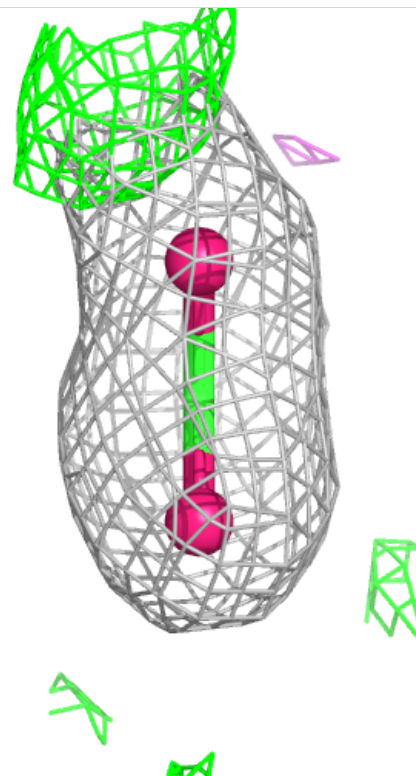
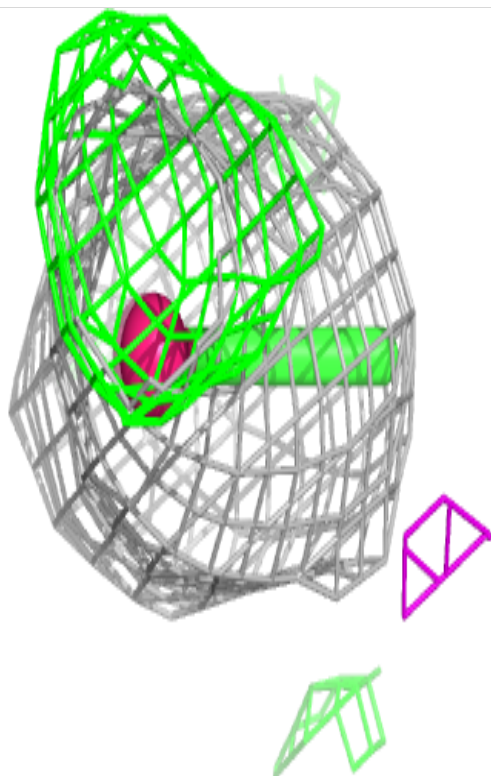
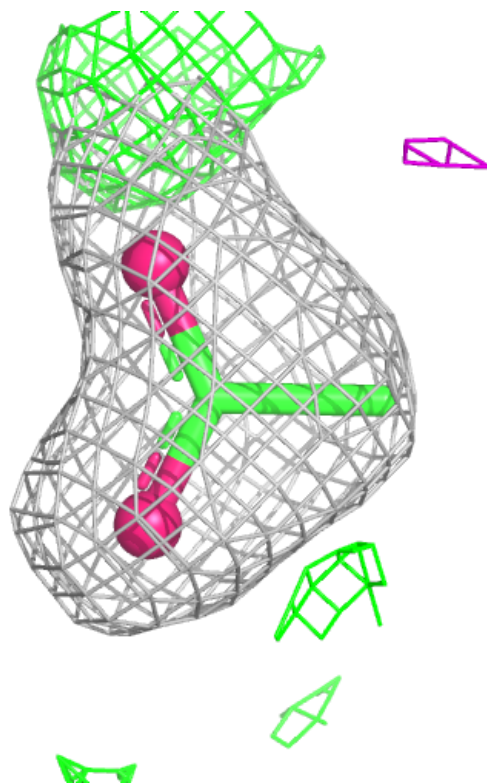
Electron density around 3VN C 301:

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



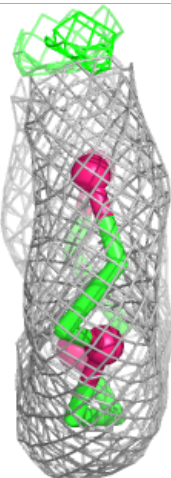
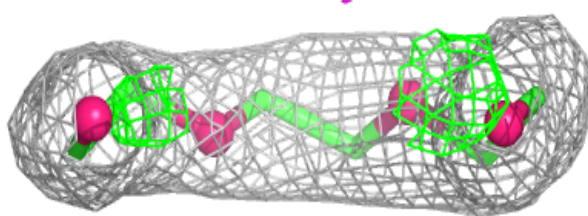
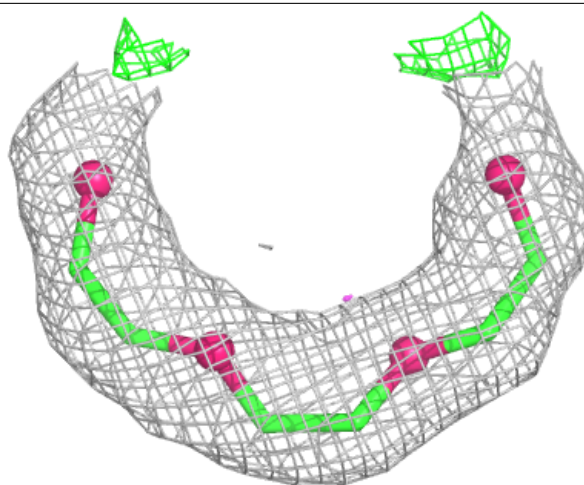
Electron density around ACT A 305:

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



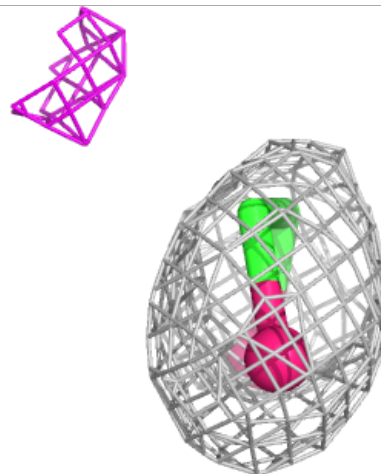
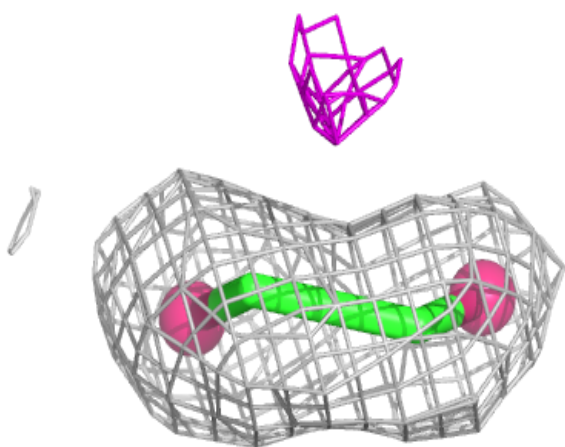
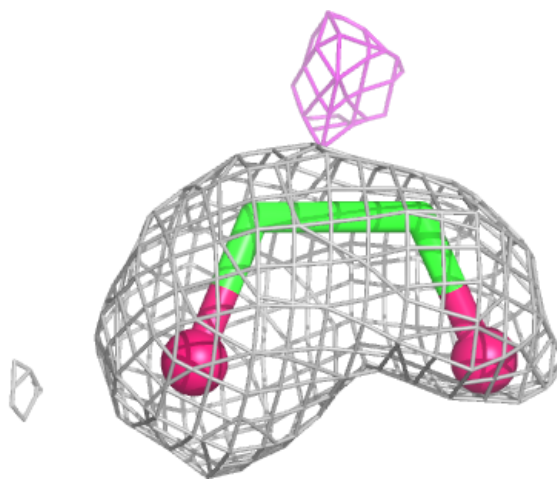
Electron density around PGE B 302:

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



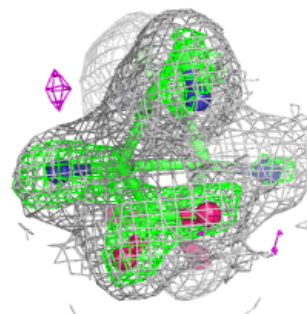
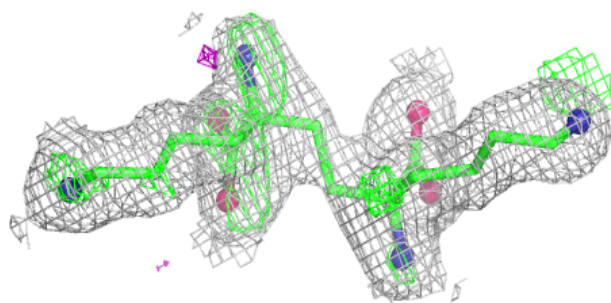
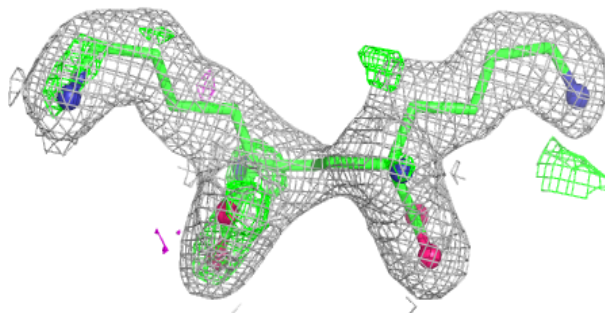
Electron density around EDO F 307:

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

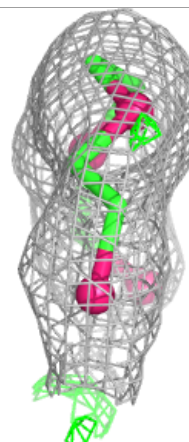
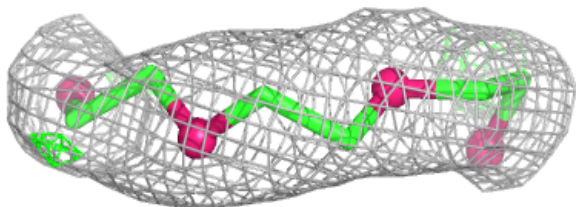
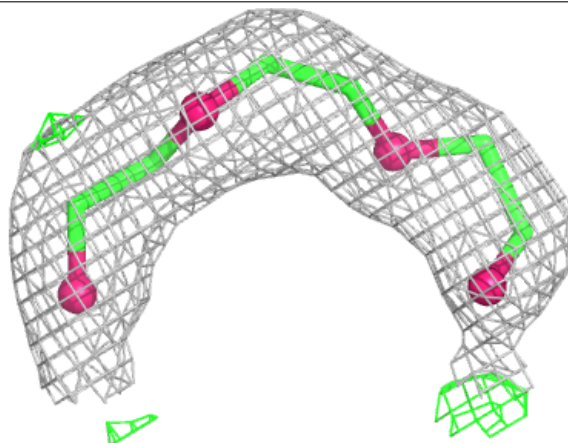


Electron density around 3VN E 301:

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

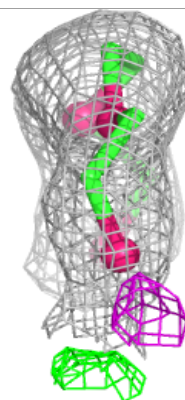
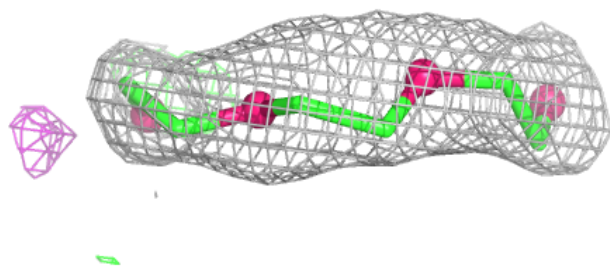
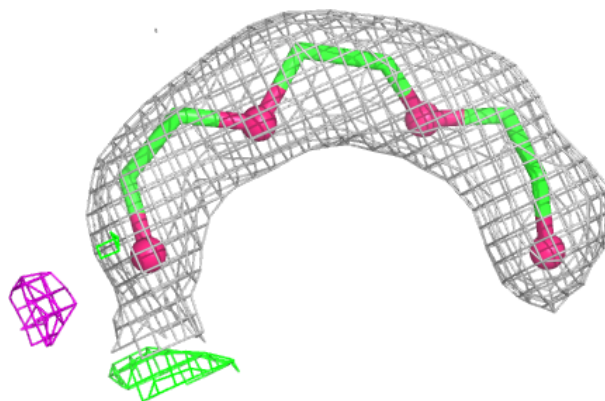
**Electron density around PGE D 304:**

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



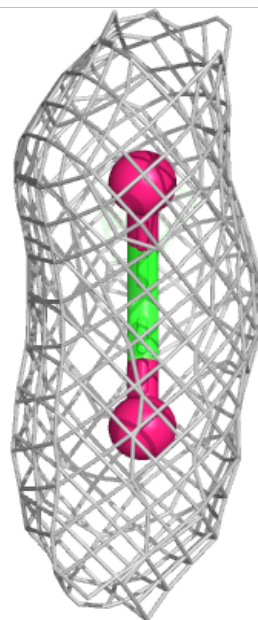
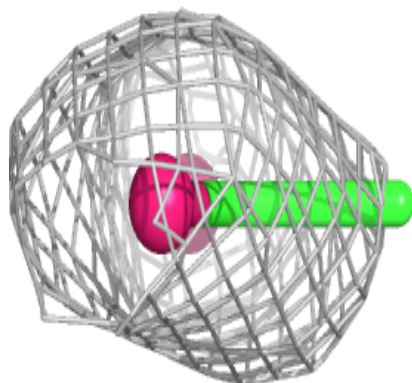
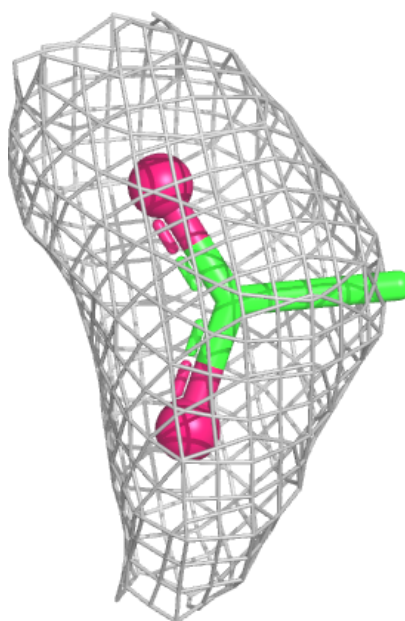
Electron density around PGE A 304:

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



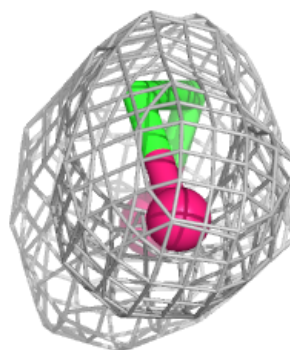
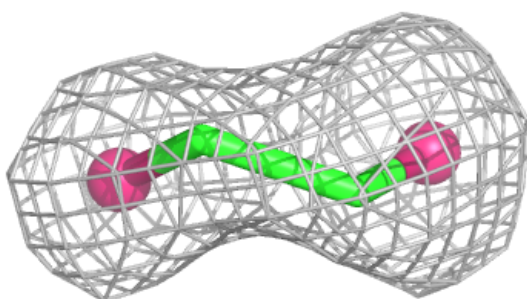
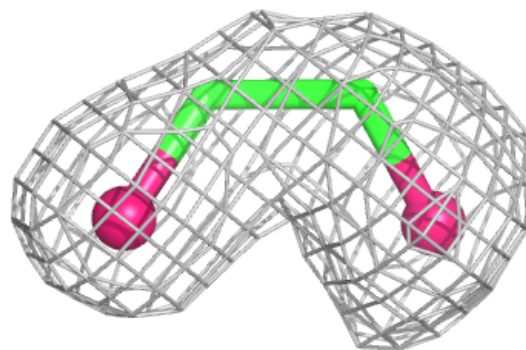
Electron density around ACT B 304:

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



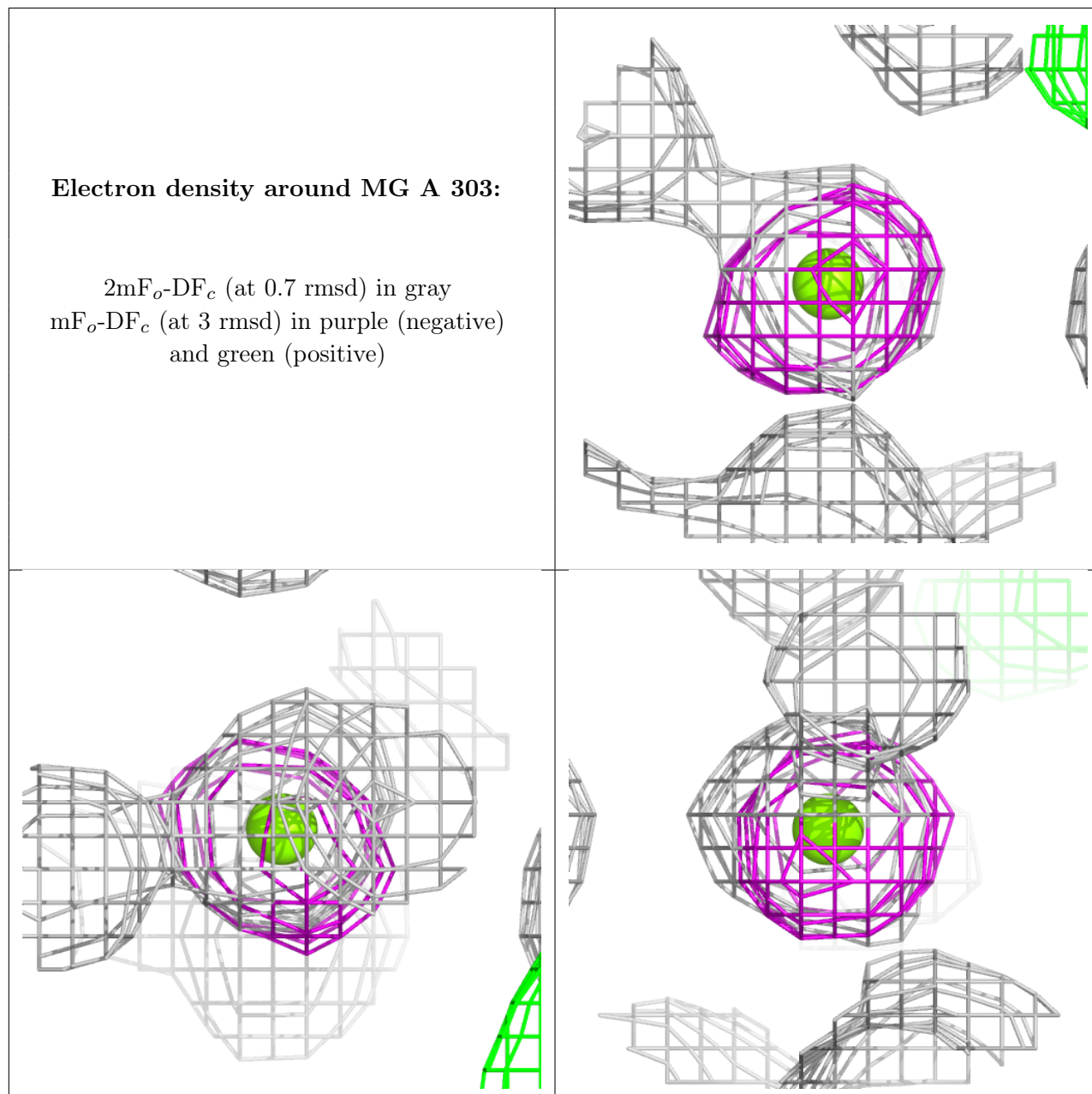
Electron density around EDO C 308:

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



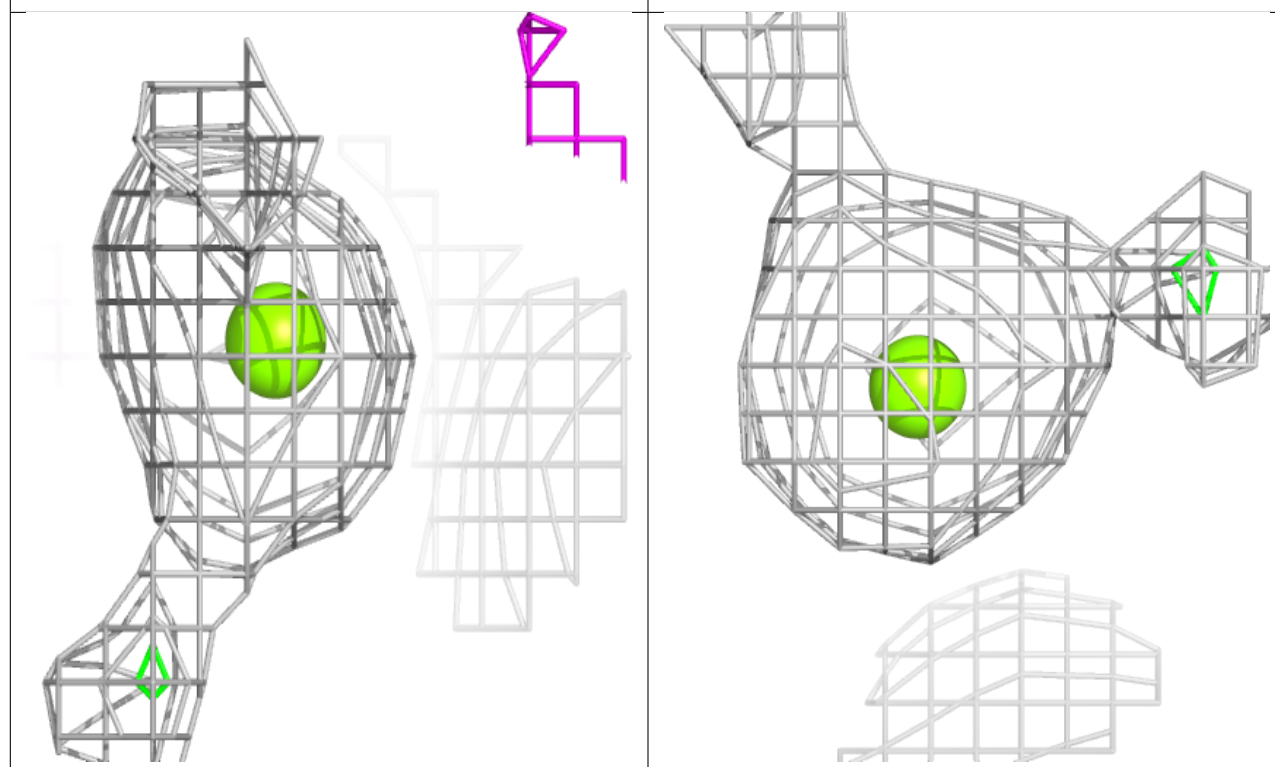
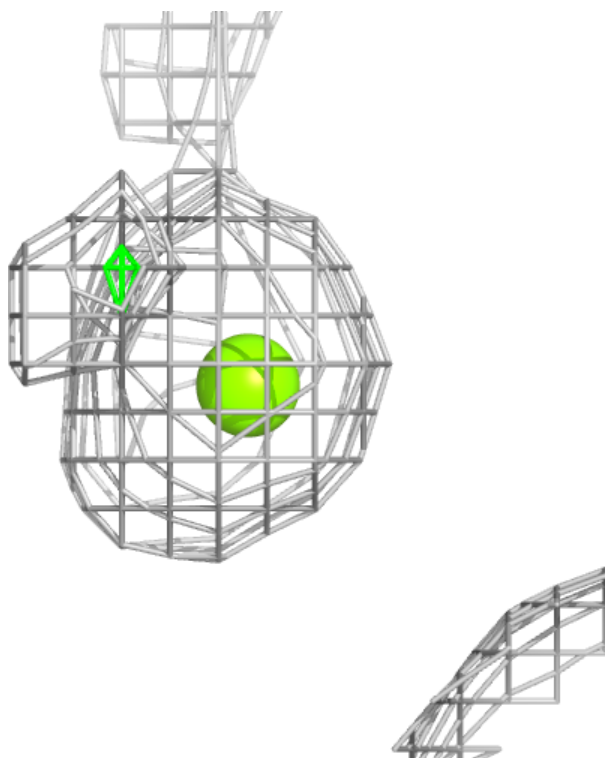
Electron density around MG A 303:

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



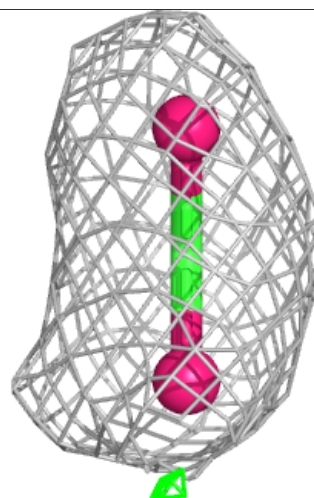
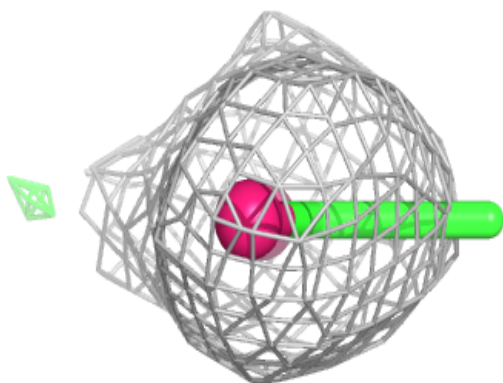
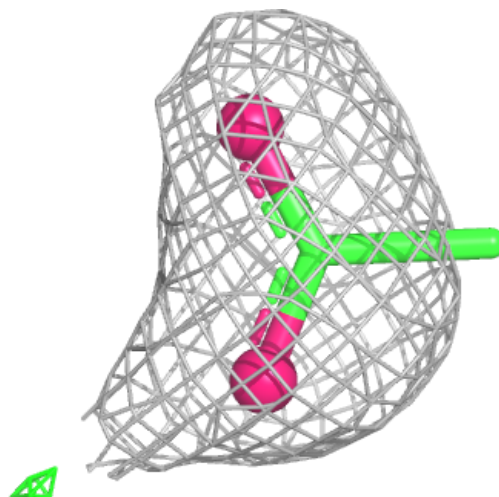
Electron density around MG C 303:

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



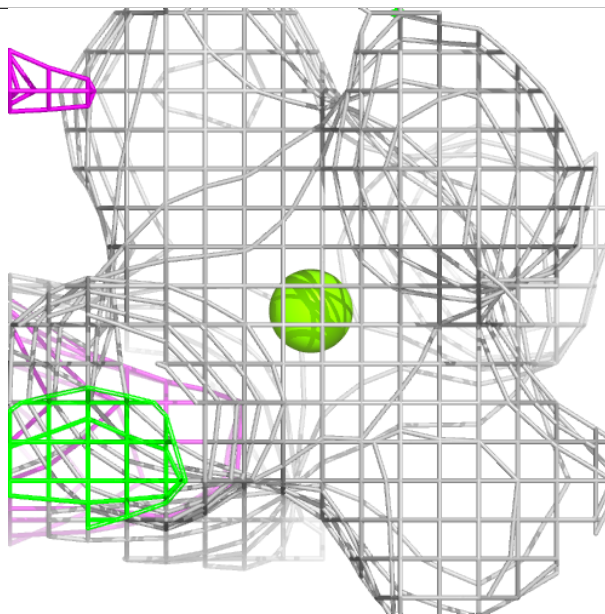
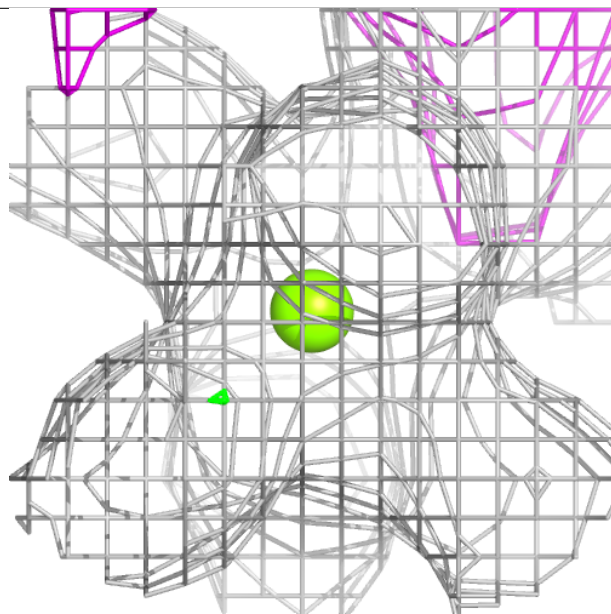
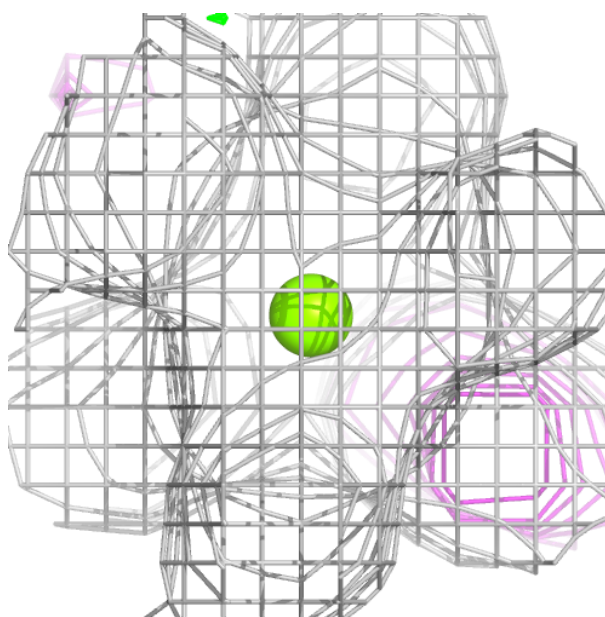
Electron density around ACT C 306:

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



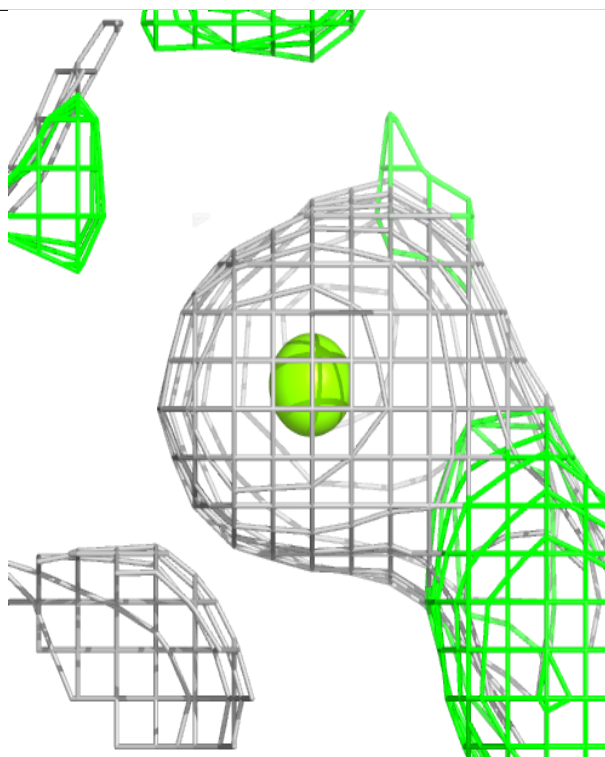
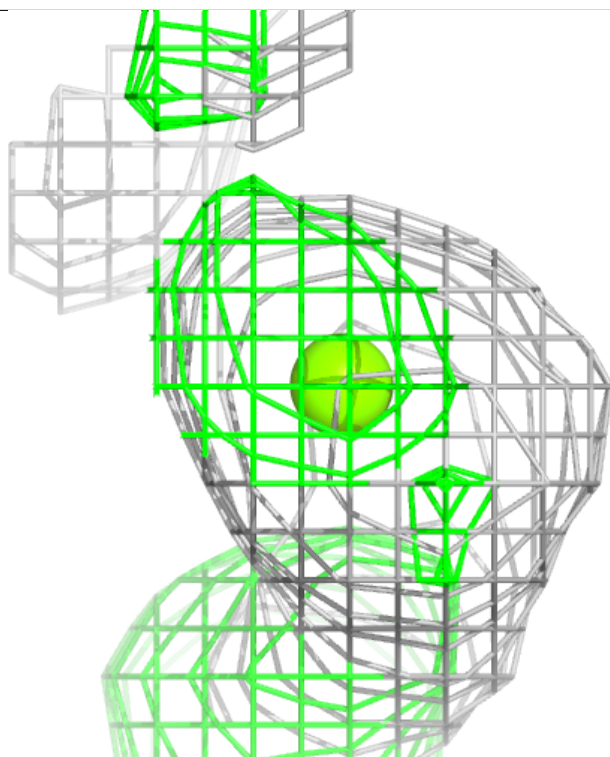
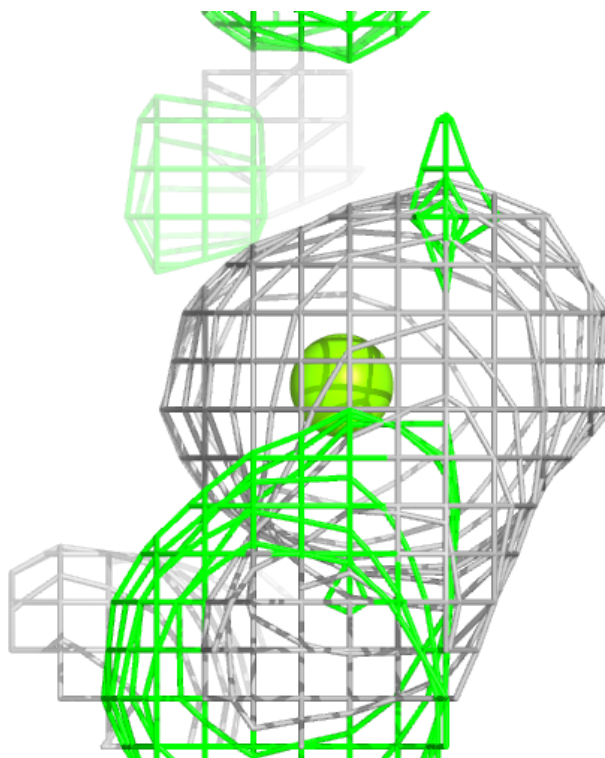
Electron density around MG B 301:

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



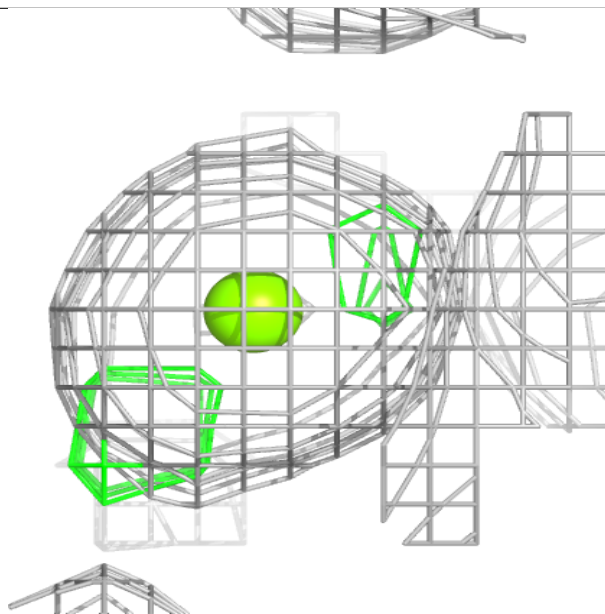
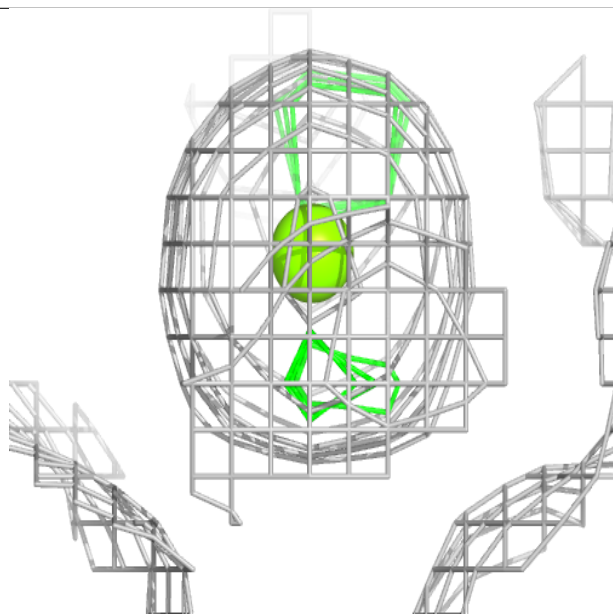
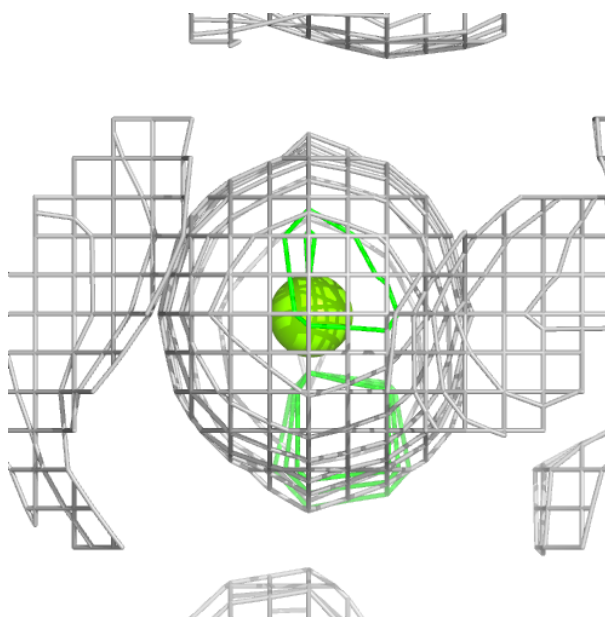
Electron density around MG D 301:

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



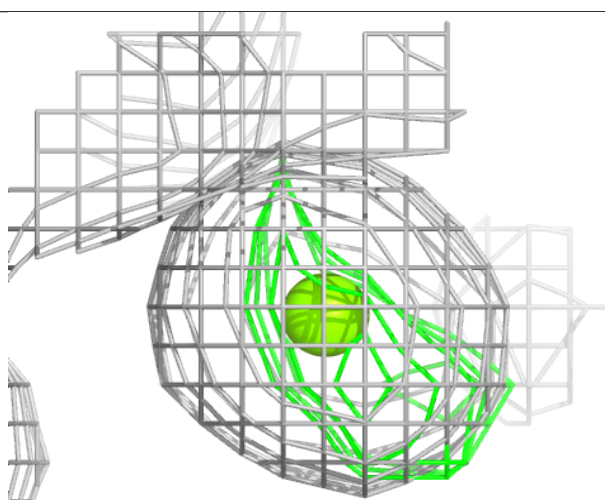
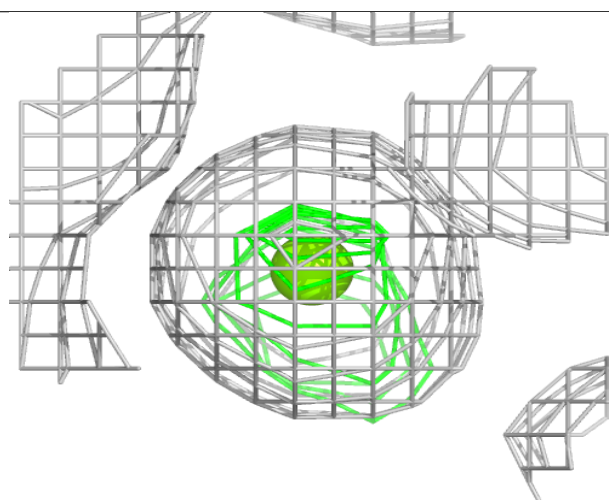
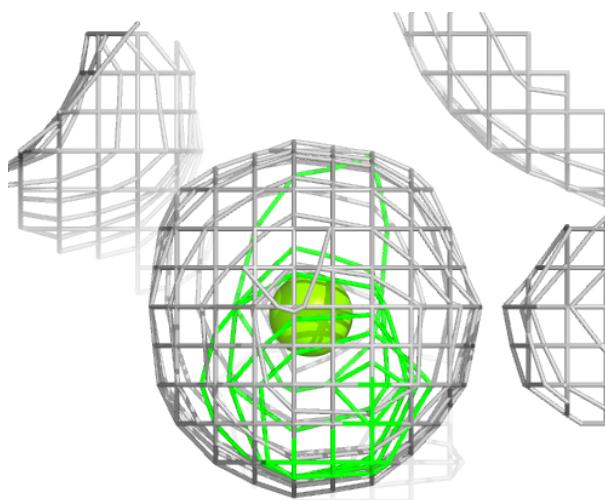
Electron density around MG C 302:

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



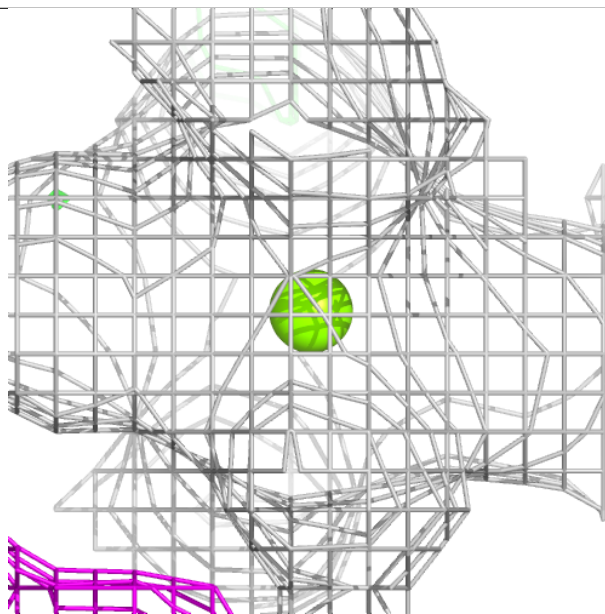
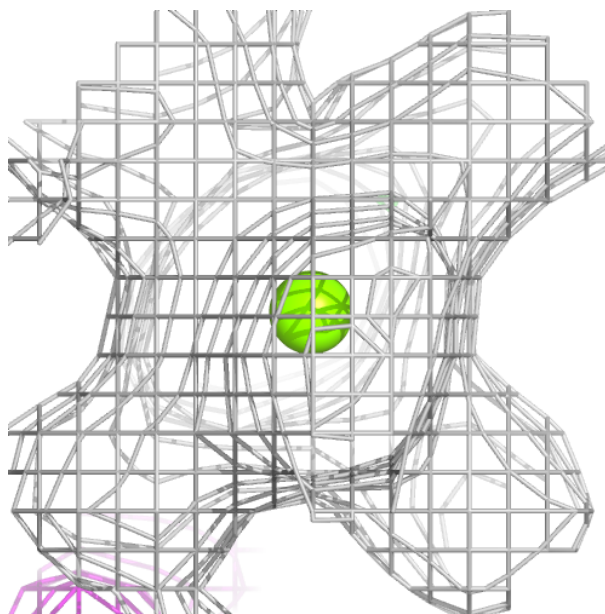
Electron density around MG D 302:

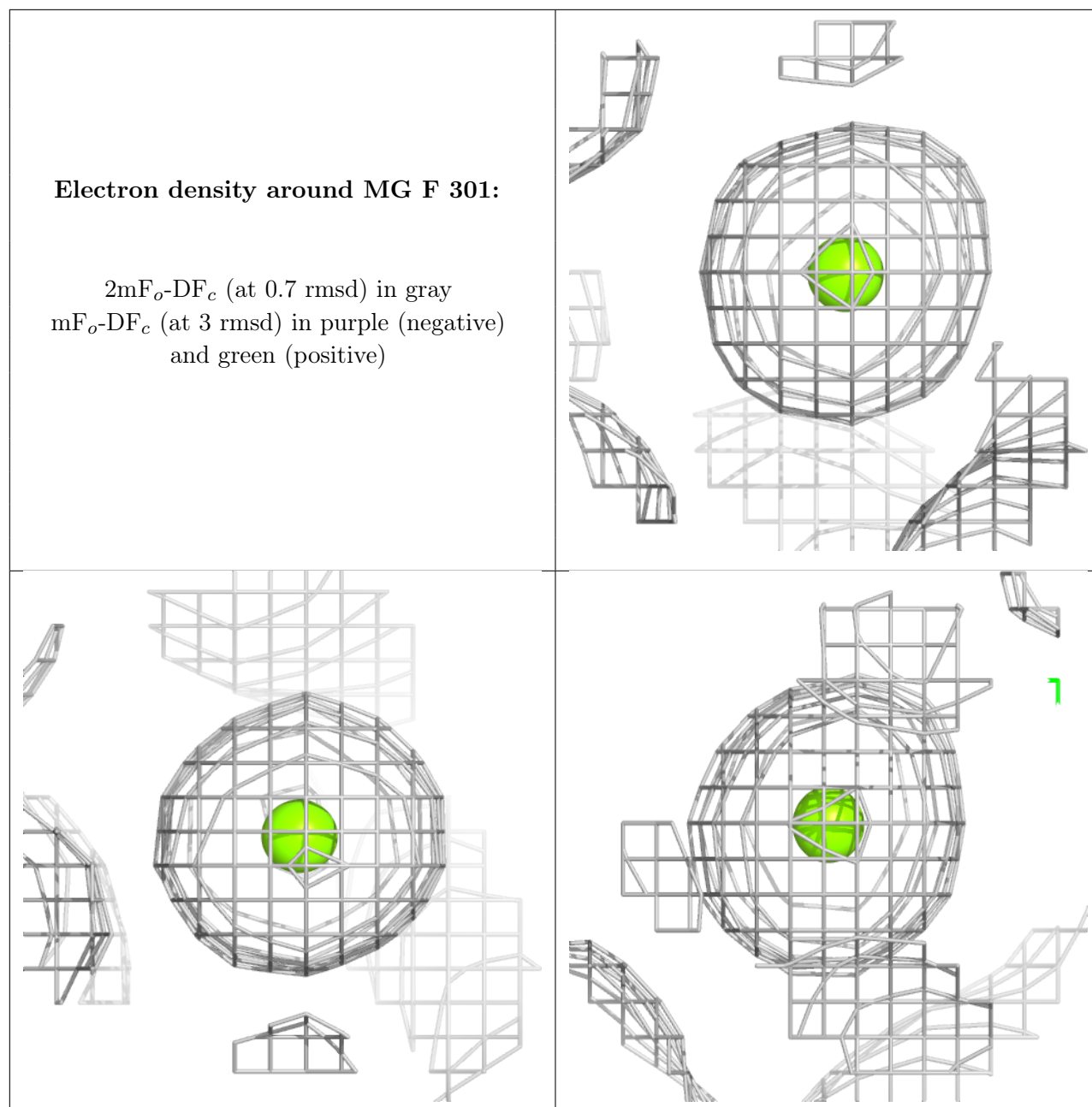
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.