



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 04:39 PM UTC

PDB ID : 7KPE / pdb_00007kpe
Title : Dihydropicolinate synthase (DHDPS) from C.jejuni, E88Q mutant with pyruvate bound in the active site and R,R-bislysine at the allosteric site
Authors : Saran, S.; Sanders, D.A.R.
Deposited on : 2020-11-11
Resolution : 2.06 Å(reported)

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

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

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

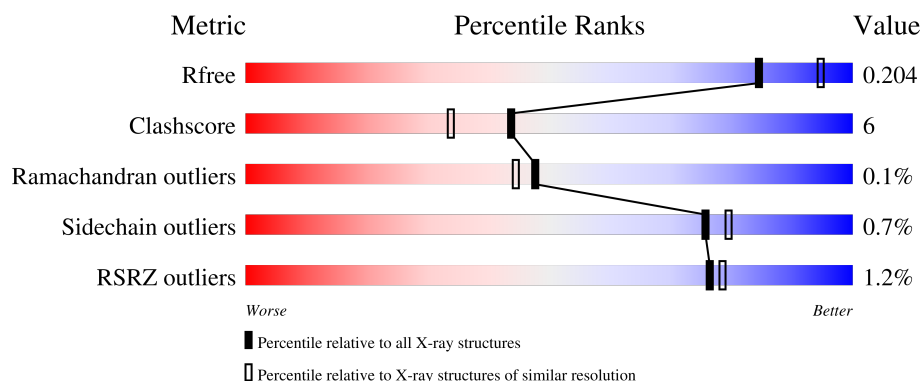
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

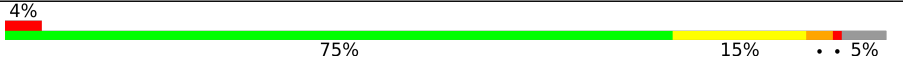
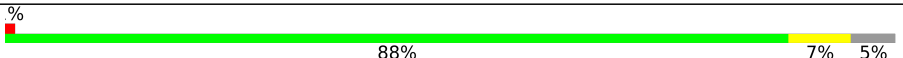
The reported resolution of this entry is 2.06 Å.

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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	% 87% 8% 5%

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
3	ACT	F	304	-	-	X	-
5	PGE	A	304	-	-	X	-
5	PGE	B	303	-	-	X	-
5	PGE	F	307	-	-	X	-
7	PEG	C	303	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14821 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
			2268	1443	376	436	13			
1	B	296	Total	C	N	O	S	0	0	0
			2275	1447	379	436	13			
1	C	296	Total	C	N	O	S	0	0	0
			2276	1447	379	437	13			
1	D	293	Total	C	N	O	S	0	0	0
			2244	1427	372	432	13			
1	E	295	Total	C	N	O	S	0	0	0
			2260	1436	375	436	13			
1	F	296	Total	C	N	O	S	0	0	0
			2259	1435	376	435	13			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9PPB4
A	-10	ARG	-	expression tag	UNP Q9PPB4
A	-9	GLY	-	expression tag	UNP Q9PPB4
A	-8	SER	-	expression tag	UNP Q9PPB4
A	-7	HIS	-	expression tag	UNP Q9PPB4
A	-6	HIS	-	expression tag	UNP Q9PPB4
A	-5	HIS	-	expression tag	UNP Q9PPB4
A	-4	HIS	-	expression tag	UNP Q9PPB4
A	-3	HIS	-	expression tag	UNP Q9PPB4
A	-2	HIS	-	expression tag	UNP Q9PPB4
A	-1	GLY	-	expression tag	UNP Q9PPB4
A	0	SER	-	expression tag	UNP Q9PPB4
A	88	GLN	GLU	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	88	GLN	GLU	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	88	GLN	GLU	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	88	GLN	GLU	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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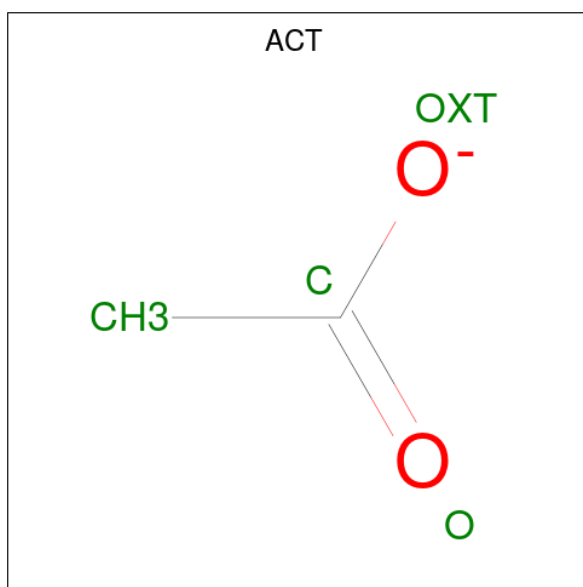
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP Q9PPB4
E	-3	HIS	-	expression tag	UNP Q9PPB4
E	-2	HIS	-	expression tag	UNP Q9PPB4
E	-1	GLY	-	expression tag	UNP Q9PPB4
E	0	SER	-	expression tag	UNP Q9PPB4
E	88	GLN	GLU	engineered 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	88	GLN	GLU	engineered mutation	UNP Q9PPB4

- Molecule 2 is MAGNESIUM ION (CCD ID: 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	1	Total Mg 1 1	0	0
2	C	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	E	1	Total Mg 1 1	0	0

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂) (labeled as "Ligand of Interest" by depositor).



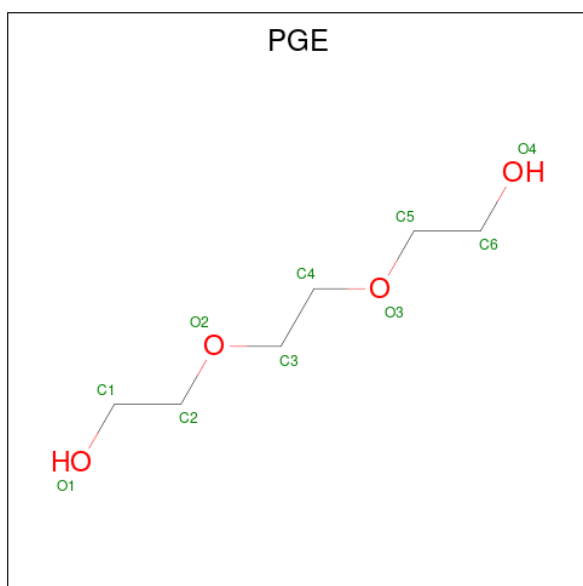
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).



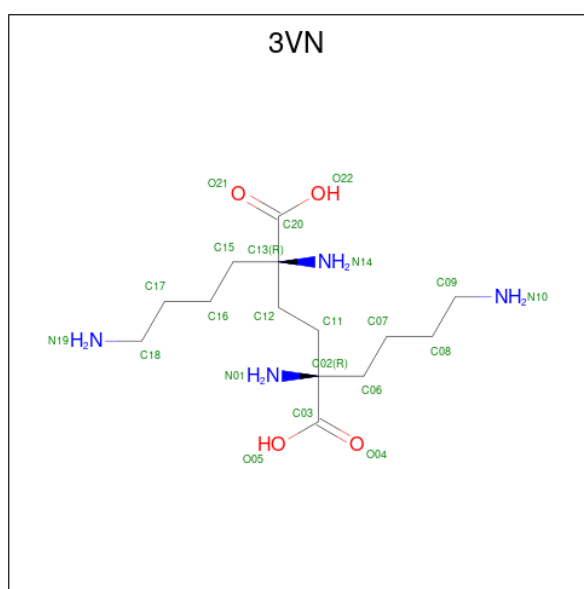
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$) (labeled as "Ligand of Interest" by depositor).



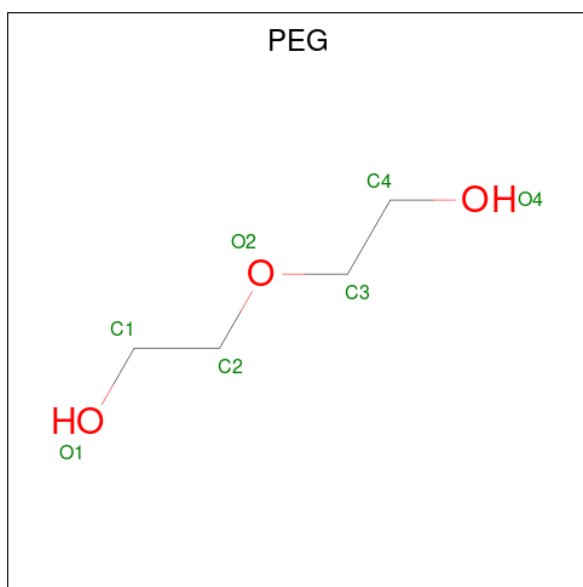
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			10	6	4		
5	E	1	Total	C	O	0	0
			10	6	4		
5	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 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).



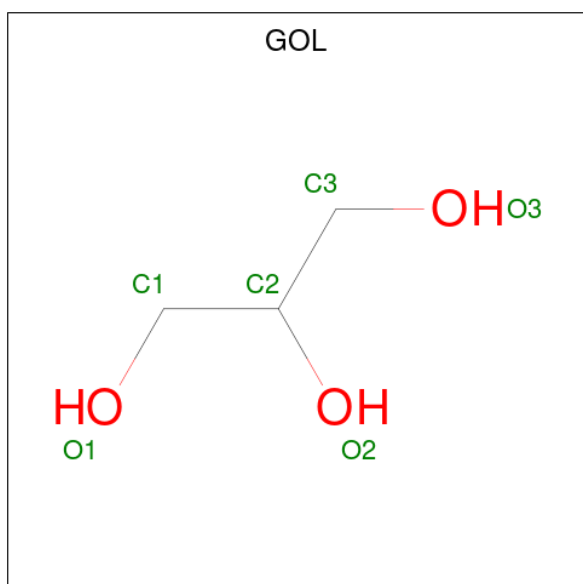
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			22	14	4	4		
6	D	1	Total	C	N	O	0	0
			22	14	4	4		
6	F	1	Total	C	N	O	0	0
			22	14	4	4		

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

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



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	206	Total	O	0	0
			206	206		
9	B	188	Total	O	0	0
			188	188		
9	C	183	Total	O	0	0
			183	183		
9	D	155	Total	O	0	0
			155	155		
9	E	171	Total	O	0	0
			171	171		
9	F	156	Total	O	0	0
			156	156		

3 Residue-property plots

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

- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain A: 



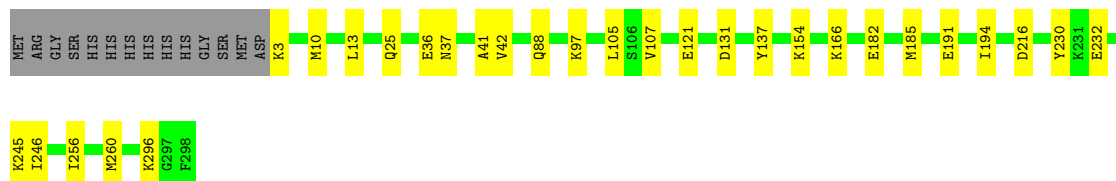
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain B: 



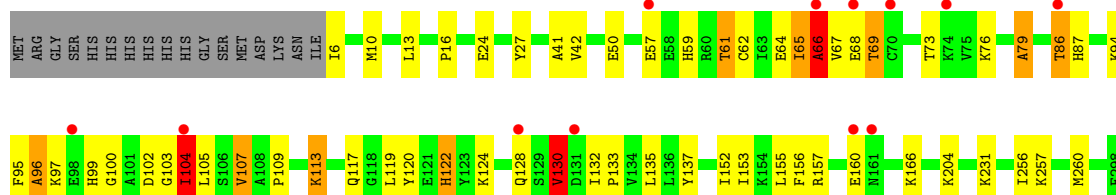
- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

Chain C: 

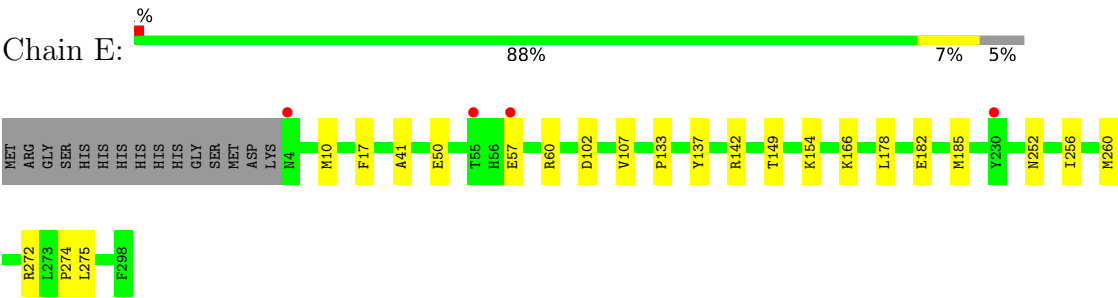


- Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase

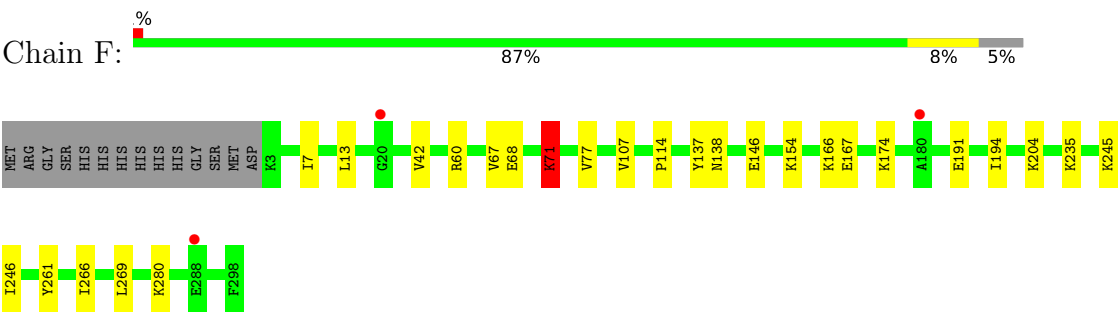
Chain D: 



● Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



● Molecule 1: 4-hydroxy-tetrahydrodipicolinate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	85.20Å 231.95Å 199.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.88 – 2.06 45.88 – 2.06	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.88-2.06) 74.4 (45.88-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.200 , 0.240 (Not available) , 0.204	Depositor DCC
R_{free} test set	6103 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.0	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	0.94	EDS
Total number of atoms	14821	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.41	1/2292 (0.0%)	0.40	0/3102
1	B	0.32	2/2299 (0.1%)	0.43	1/3109 (0.0%)
1	C	0.36	2/2300 (0.1%)	0.43	1/3109 (0.0%)
1	D	1.16	26/2268 (1.1%)	0.91	15/3070 (0.5%)
1	E	0.38	0/2284	0.48	0/3090
1	F	0.43	1/2283 (0.0%)	0.51	1/3090 (0.0%)
All	All	0.59	32/13726 (0.2%)	0.55	18/18570 (0.1%)

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

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

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	66	ALA	C-O	-6.80	1.15	1.24
1	D	95	PHE	C-O	-6.78	1.16	1.24
1	D	135	LEU	C-O	-6.63	1.16	1.24
1	D	107	VAL	C-O	-6.61	1.16	1.24
1	D	122	HIS	C-O	-6.57	1.16	1.24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	65	ILE	N-CA-C	-12.58	92.19	109.55
1	D	135	LEU	CA-C-N	8.05	132.14	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	135	LEU	C-N-CA	8.05	132.14	120.71
1	D	67	VAL	N-CA-C	-7.83	102.90	110.42
1	D	65	ILE	CA-C-O	-6.74	113.32	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	166	KPI	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2268	0	2287	29	0
1	B	2275	0	2311	20	0
1	C	2276	0	2310	29	0
1	D	2244	0	2263	45	0
1	E	2260	0	2278	16	0
1	F	2259	0	2273	37	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
3	A	4	0	3	0	0
3	C	4	0	3	1	0
3	D	4	0	3	0	0
3	E	4	0	3	0	0
3	F	12	0	9	15	0
4	A	4	0	6	0	0
4	F	8	0	12	1	0
5	A	10	0	14	11	0
5	B	10	0	14	9	0
5	E	10	0	14	5	0
5	F	10	0	14	8	0
6	B	22	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	22	0	28	3	0
6	F	22	0	28	0	0
7	C	14	0	20	13	0
7	D	7	0	10	0	0
8	F	6	0	8	2	0
9	A	206	0	0	3	0
9	B	188	0	0	1	0
9	C	183	0	0	2	0
9	D	155	0	0	2	0
9	E	171	0	0	0	0
9	F	156	0	0	2	0
All	All	14821	0	13939	169	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 6.

The worst 5 of 169 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:60:ARG:CD	3:F:304:ACT:H1	1.45	1.44
1:F:60:ARG:HD3	3:F:304:ACT:CH3	1.54	1.33
1:F:60:ARG:HH11	3:F:304:ACT:H3	1.06	1.17
1:F:60:ARG:NH1	3:F:304:ACT:H3	1.60	1.16
1:A:154:LYS:HE3	5:A:304:PGE:H2	1.31	1.08

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%)	289 (99%)	4 (1%)	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%)	289 (99%)	4 (1%)	0	100	100
1	D	290/310 (94%)	283 (98%)	6 (2%)	1 (0%)	36	30
1	E	292/310 (94%)	288 (99%)	4 (1%)	0	100	100
1	F	293/310 (94%)	288 (98%)	5 (2%)	0	100	100
All	All	1754/1860 (94%)	1726 (98%)	27 (2%)	1 (0%)	48	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	66	ALA

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	244/260 (94%)	244 (100%)	0	100	100
1	B	247/260 (95%)	247 (100%)	0	100	100
1	C	247/260 (95%)	247 (100%)	0	100	100
1	D	242/260 (93%)	235 (97%)	7 (3%)	37	33
1	E	244/260 (94%)	244 (100%)	0	100	100
1	F	243/260 (94%)	240 (99%)	3 (1%)	63	65
All	All	1467/1560 (94%)	1457 (99%)	10 (1%)	76	79

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	71	LYS
1	F	269	LEU
1	F	280	LYS
1	D	104	ILE
1	D	109	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	59	HIS
1	E	19	ASN
1	F	201	ASN
1	B	19	ASN
1	B	99	HIS

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	B	166	1	11,13,14	1.61	2 (18%)	9,15,17	3.16	4 (44%)
1	KPI	C	166	1	11,13,14	2.39	3 (27%)	9,15,17	3.68	4 (44%)
1	KPI	F	166	1	11,13,14	0.97	1 (9%)	9,15,17	3.25	4 (44%)
1	KPI	A	166	1	11,13,14	2.07	2 (18%)	9,15,17	3.72	3 (33%)
1	KPI	E	166	1	11,13,14	2.03	2 (18%)	9,15,17	3.86	4 (44%)
1	KPI	D	166	1	11,13,14	1.03	1 (9%)	9,15,17	3.27	4 (44%)

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	B	166	1	-	5/13/14/16	-
1	KPI	C	166	1	-	4/13/14/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KPI	F	166	1	-	6/13/14/16	-
1	KPI	A	166	1	-	3/13/14/16	-
1	KPI	E	166	1	-	5/13/14/16	-
1	KPI	D	166	1	-	6/13/14/16	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	KPI	O2-CX2	6.13	1.37	1.22
1	E	166	KPI	O2-CX2	5.96	1.37	1.22
1	C	166	KPI	O2-CX2	5.91	1.37	1.22
1	B	166	KPI	O-C	4.30	1.36	1.20
1	C	166	KPI	O-C	4.29	1.36	1.20

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	KPI	C1-CX1-CX2	-7.57	110.98	118.11
1	F	166	KPI	C1-CX1-CX2	-7.50	111.04	118.11
1	D	166	KPI	C1-CX1-CX2	-7.49	111.05	118.11
1	B	166	KPI	C1-CX1-CX2	-7.38	111.16	118.11
1	E	166	KPI	C1-CX1-CX2	-7.31	111.22	118.11

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	166	KPI	NZ-CX1-CX2-O1
1	A	166	KPI	NZ-CX1-CX2-O2
1	B	166	KPI	NZ-CX1-CX2-O1
1	B	166	KPI	NZ-CX1-CX2-O2
1	B	166	KPI	C1-CX1-CX2-O1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 28 ligands modelled in this entry, 7 are monoatomic - leaving 21 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$
3	ACT	F	302	-	3,3,3	1.26	1 (33%)	3,3,3	0.92	0
5	PGE	A	304	-	9,9,9	0.55	0	8,8,8	1.24	1 (12%)
3	ACT	E	302	-	3,3,3	0.97	0	3,3,3	1.79	1 (33%)
4	EDO	F	306	-	3,3,3	0.55	0	2,2,2	0.75	0
3	ACT	F	304	-	3,3,3	1.09	0	3,3,3	0.59	0
7	PEG	D	304	-	6,6,6	0.33	0	5,5,5	0.58	0
6	3VN	B	301	-	17,21,21	1.30	1 (5%)	18,28,28	1.44	4 (22%)
6	3VN	F	301	-	17,21,21	1.22	1 (5%)	18,28,28	1.75	4 (22%)
7	PEG	C	304	-	6,6,6	0.50	0	5,5,5	1.13	1 (20%)
3	ACT	D	305	-	3,3,3	1.05	0	3,3,3	1.21	0
5	PGE	E	303	-	9,9,9	0.38	0	8,8,8	0.44	0
3	ACT	C	305	-	3,3,3	1.27	1 (33%)	3,3,3	0.20	0
4	EDO	A	303	-	3,3,3	0.24	0	2,2,2	0.46	0
5	PGE	F	307	-	9,9,9	0.37	0	8,8,8	0.72	0
7	PEG	C	303	-	6,6,6	0.32	0	5,5,5	0.81	0
8	GOL	F	308	-	5,5,5	0.45	0	5,5,5	0.84	0
6	3VN	D	301	-	17,21,21	1.27	1 (5%)	18,28,28	1.50	4 (22%)
5	PGE	B	303	-	9,9,9	0.42	0	8,8,8	0.72	0
3	ACT	A	302	-	3,3,3	1.19	0	3,3,3	0.57	0
4	EDO	F	305	-	3,3,3	0.60	0	2,2,2	0.16	0
3	ACT	F	303	-	3,3,3	0.84	0	3,3,3	1.10	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	EDO	A	303	-	-	1/1/1/1	-
5	PGE	A	304	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PEG	D	304	-	-	3/4/4/4	-
6	3VN	B	301	-	-	10/31/31/31	-
6	3VN	F	301	-	-	9/31/31/31	-
4	EDO	F	306	-	-	1/1/1/1	-
5	PGE	F	307	-	-	3/7/7/7	-
7	PEG	C	304	-	-	2/4/4/4	-
4	EDO	F	305	-	-	0/1/1/1	-
7	PEG	C	303	-	-	2/4/4/4	-
8	GOL	F	308	-	-	3/4/4/4	-
6	3VN	D	301	-	-	11/31/31/31	-
5	PGE	B	303	-	-	3/7/7/7	-
5	PGE	E	303	-	-	5/7/7/7	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	301	3VN	C06-C02	2.58	1.57	1.55
6	D	301	3VN	C06-C02	2.50	1.57	1.55
6	F	301	3VN	C06-C02	2.32	1.57	1.55
3	C	305	ACT	OXT-C	-2.09	1.21	1.30
3	F	302	ACT	OXT-C	-2.05	1.21	1.30

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	301	3VN	C16-C15-C13	-3.36	109.20	115.16
6	F	301	3VN	C07-C06-C02	-2.92	109.98	115.16
6	F	301	3VN	O22-C20-C13	2.77	121.08	113.69
6	D	301	3VN	C07-C06-C02	-2.74	110.31	115.16
6	F	301	3VN	O05-C03-C02	2.66	120.79	113.69

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	301	3VN	C11-C02-C03-O04
6	B	301	3VN	C11-C02-C03-O05
6	B	301	3VN	C12-C13-C20-O21
6	B	301	3VN	C12-C13-C20-O22

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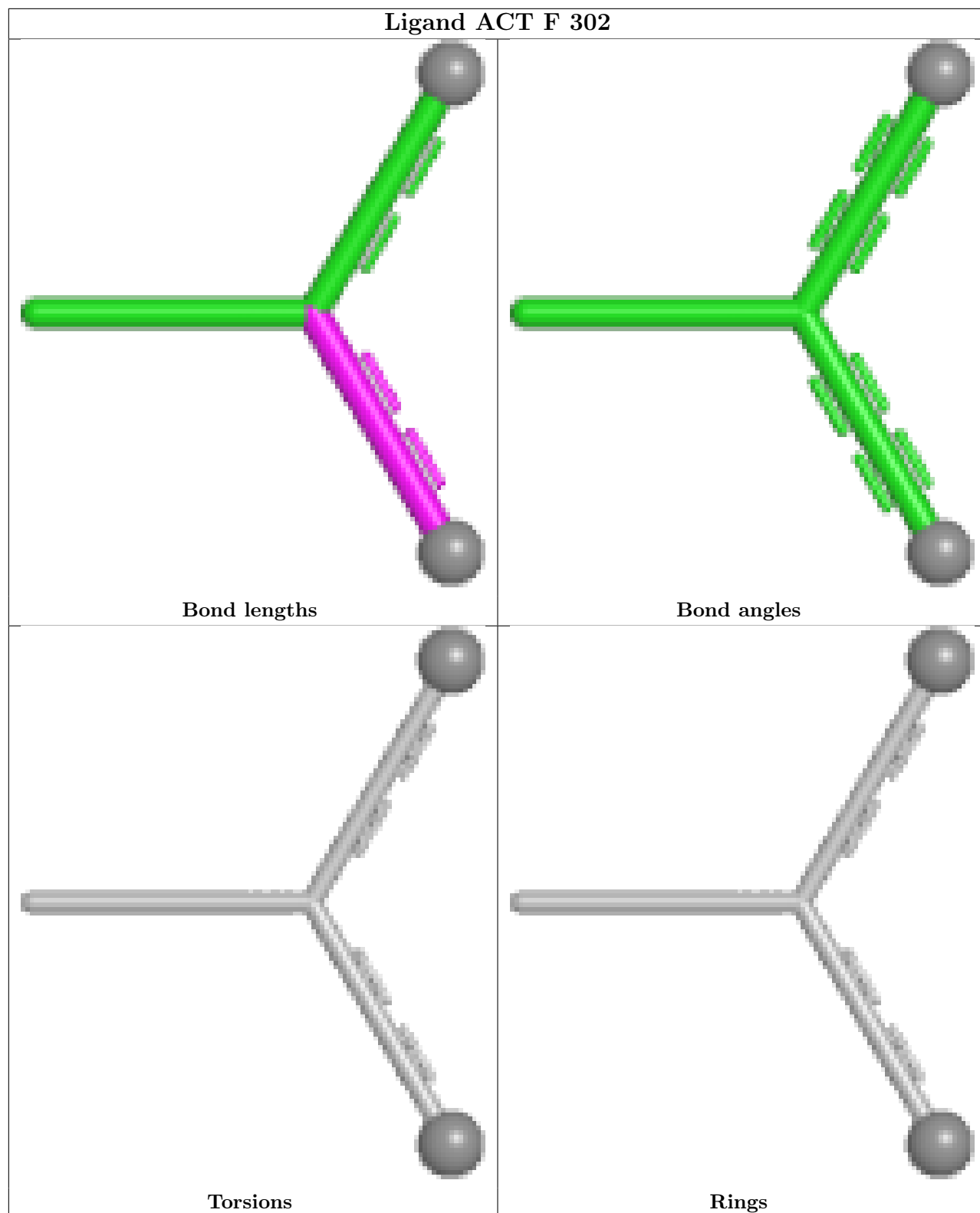
Mol	Chain	Res	Type	Atoms
6	D	301	3VN	C11-C02-C03-O04

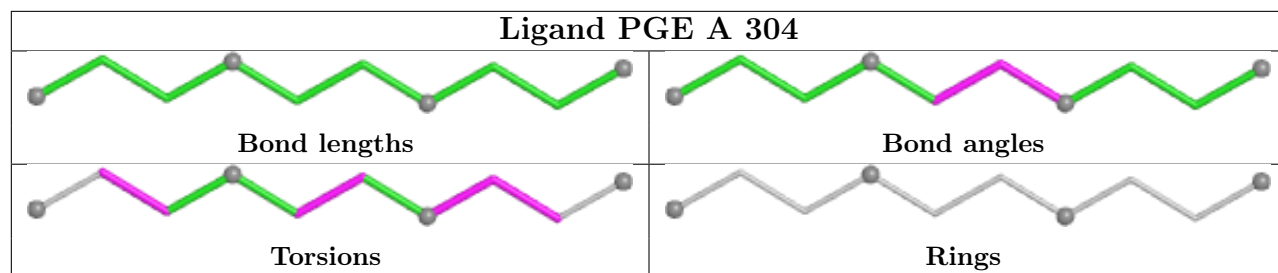
There are no ring outliers.

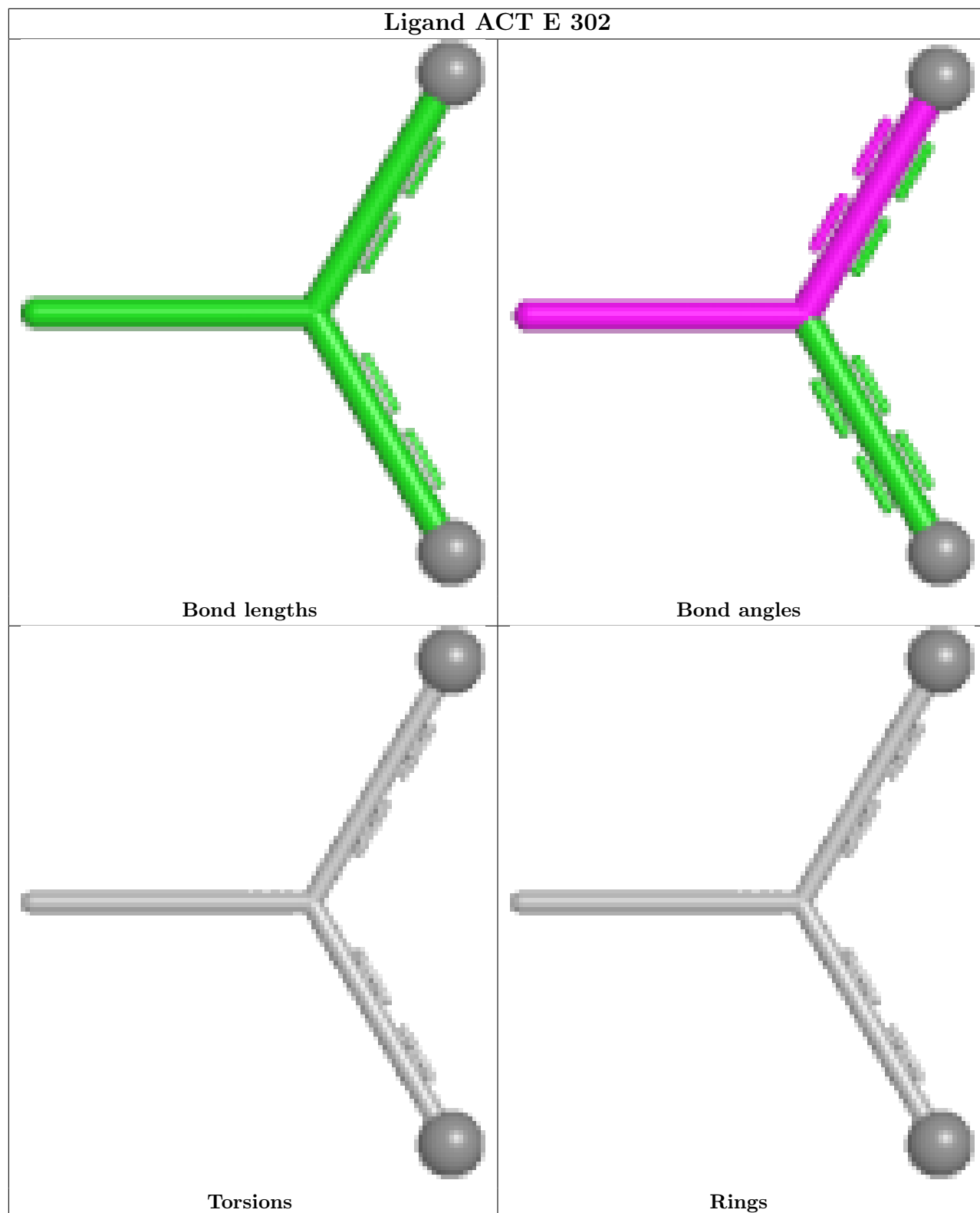
12 monomers are involved in 68 short contacts:

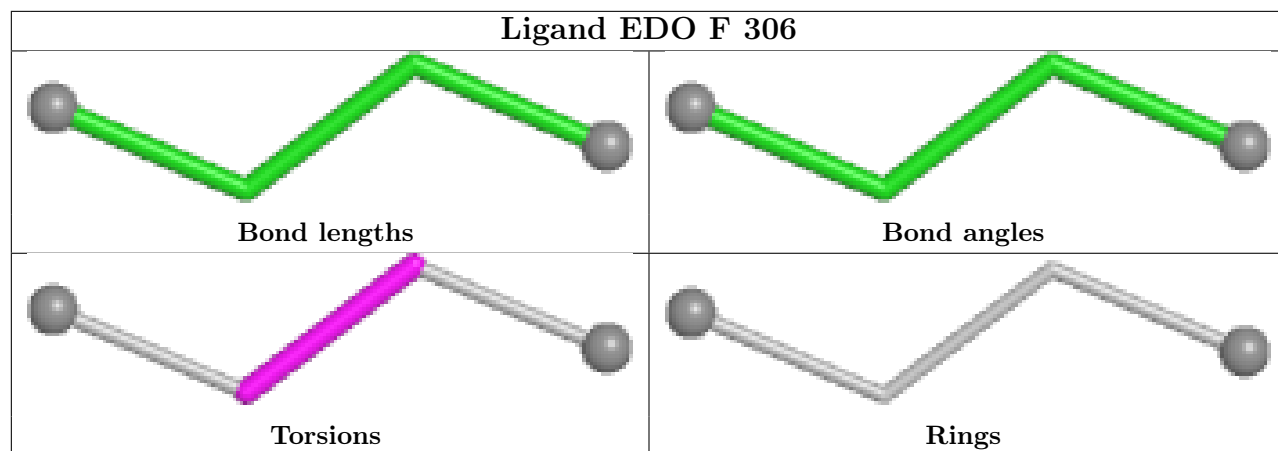
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	304	PGE	11	0
4	F	306	EDO	1	0
3	F	304	ACT	14	0
7	C	304	PEG	1	0
5	E	303	PGE	5	0
3	C	305	ACT	1	0
5	F	307	PGE	8	0
7	C	303	PEG	12	0
8	F	308	GOL	2	0
6	D	301	3VN	3	0
5	B	303	PGE	9	0
3	F	303	ACT	1	0

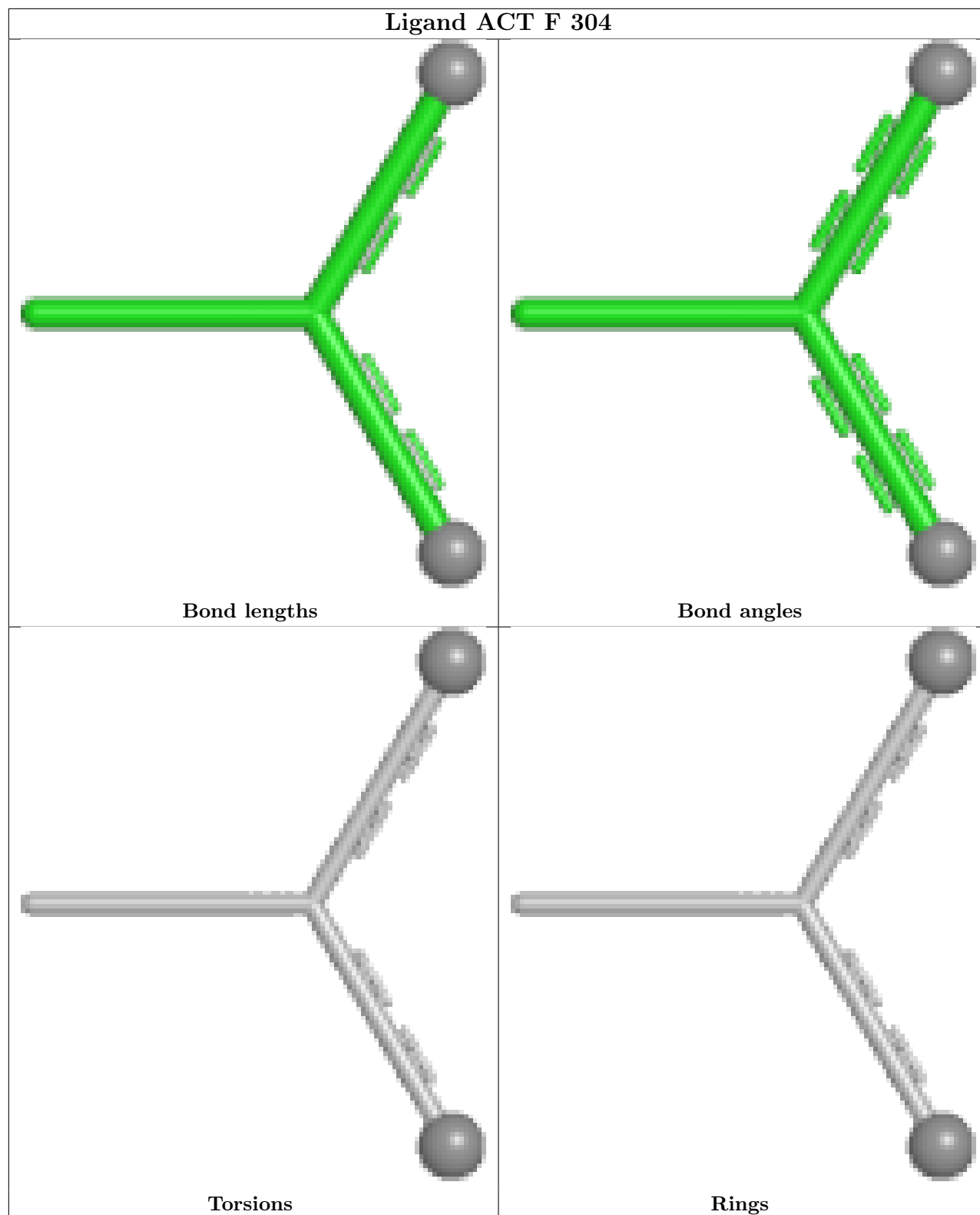
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

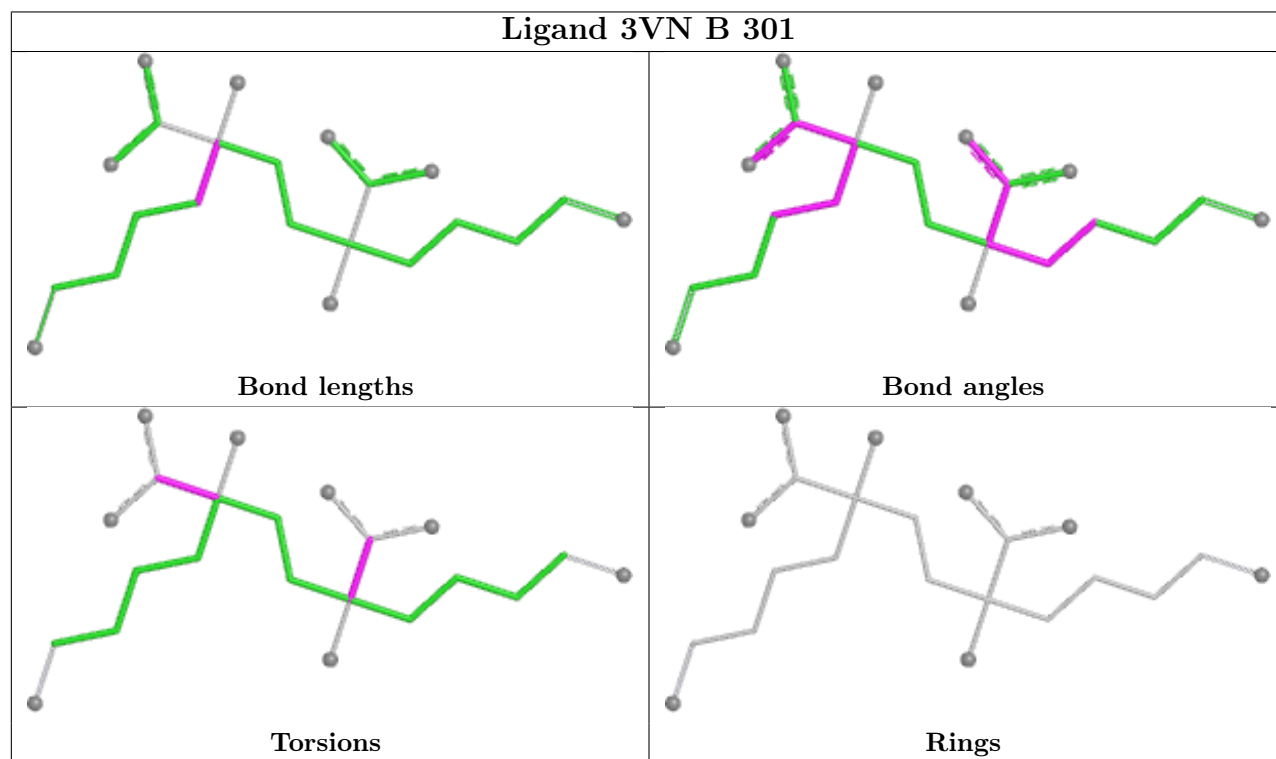
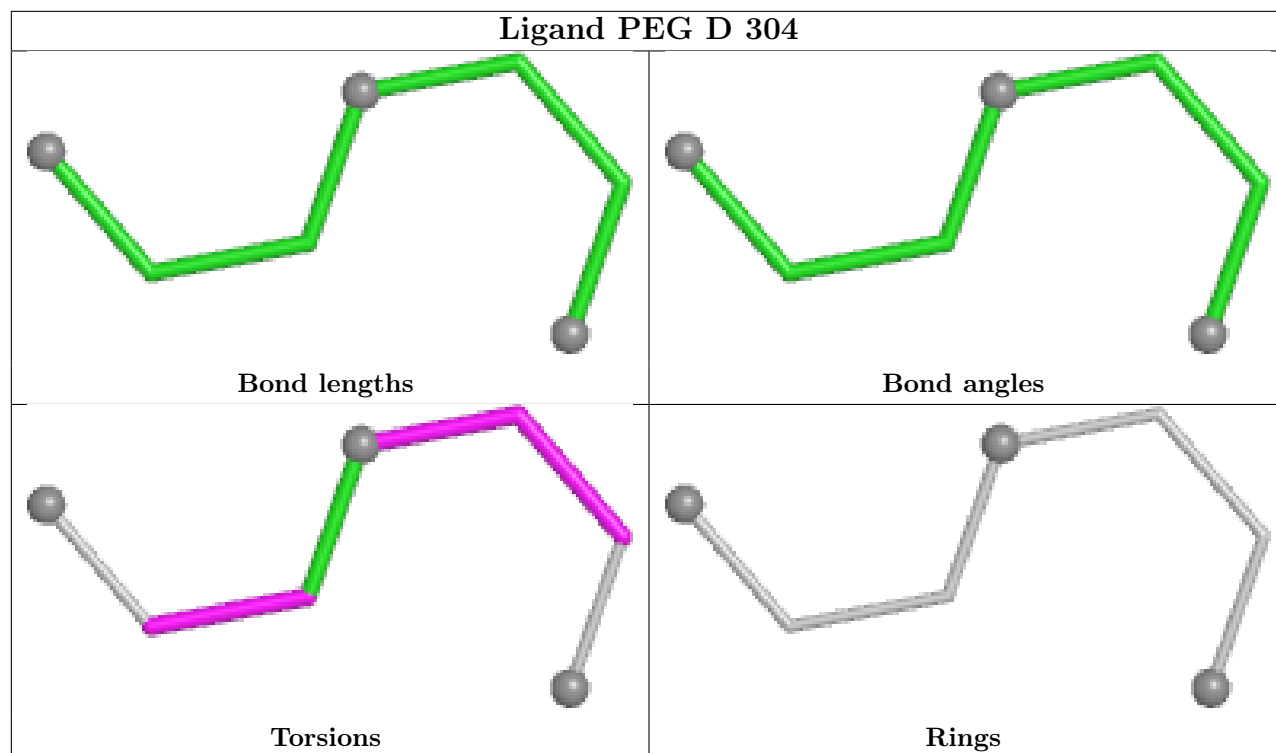




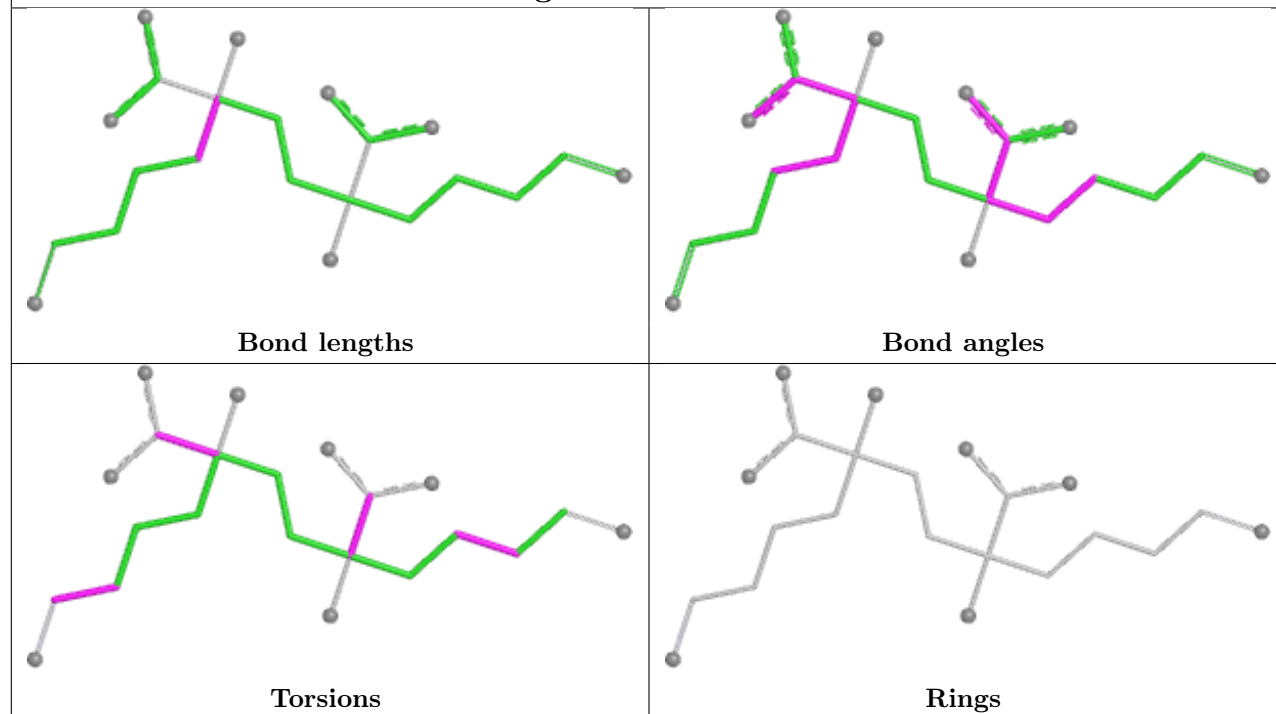




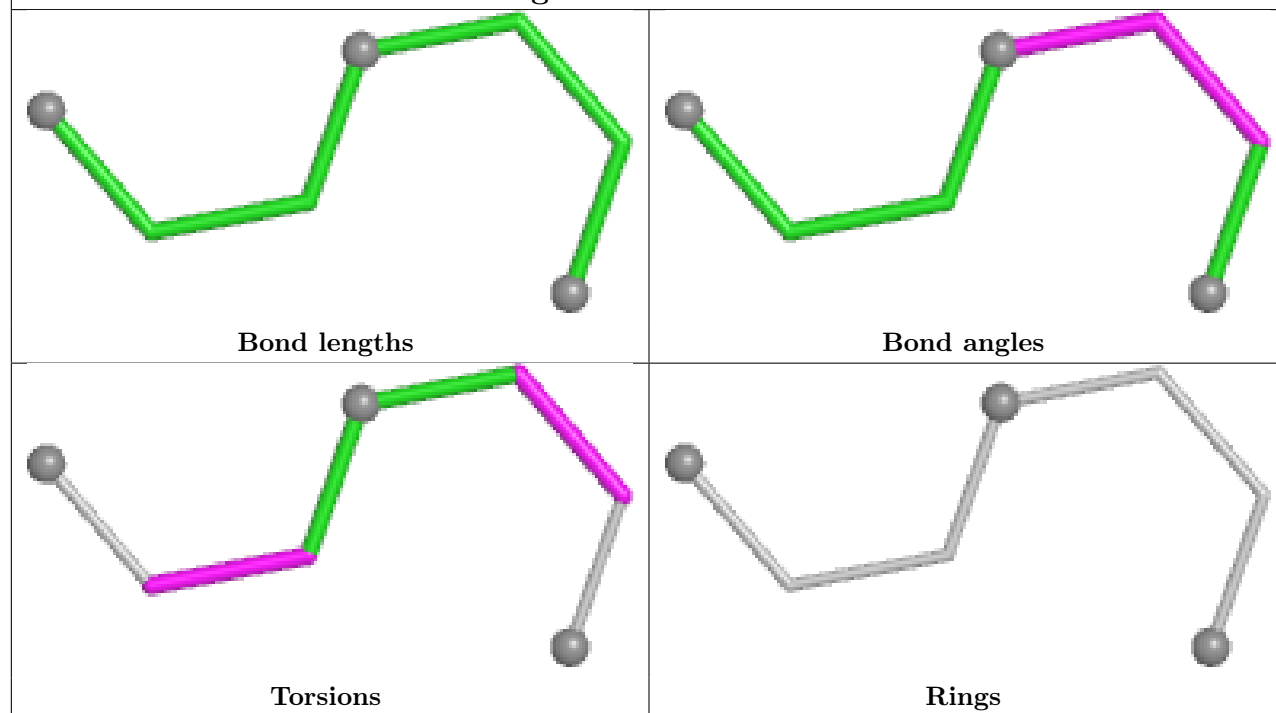


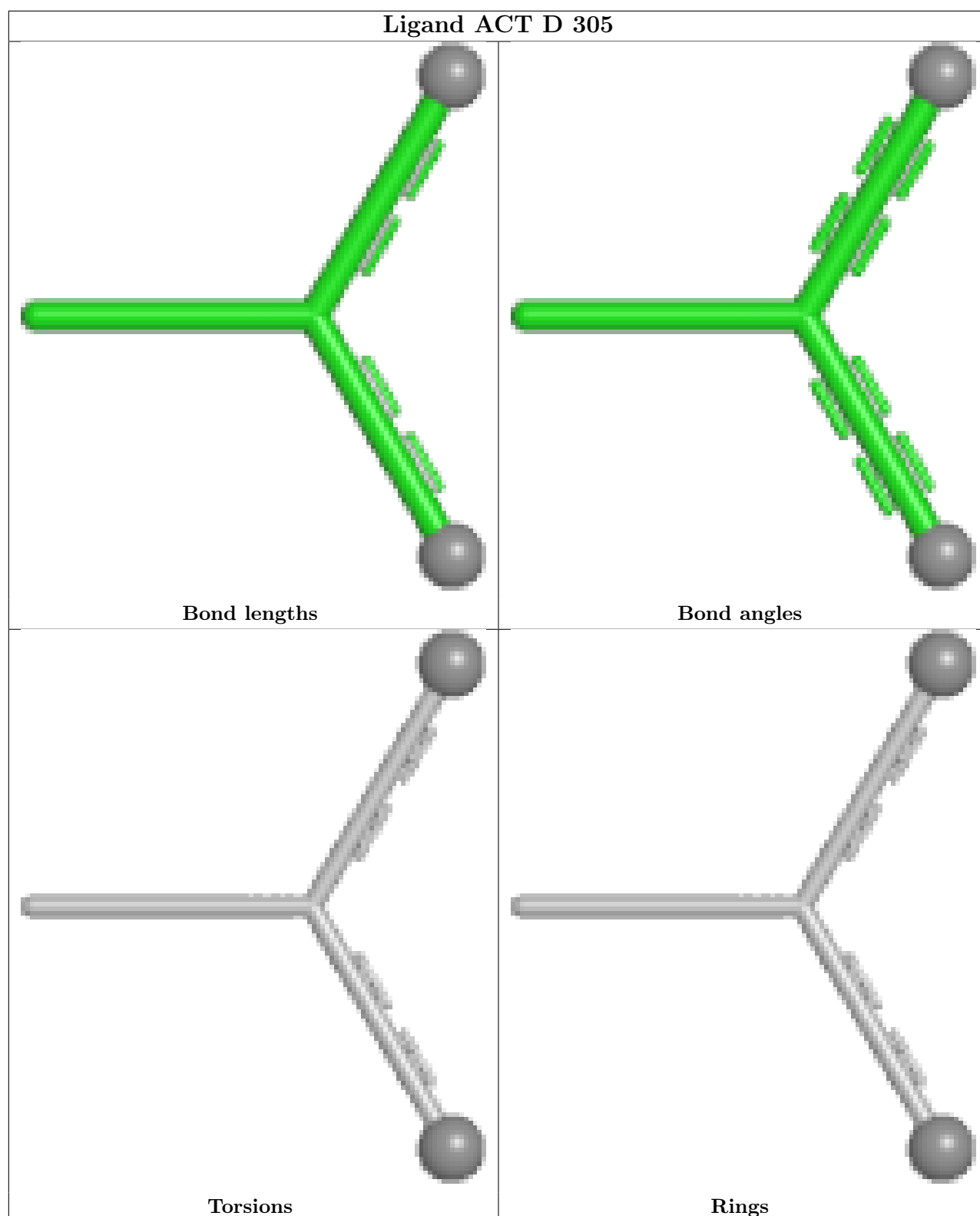


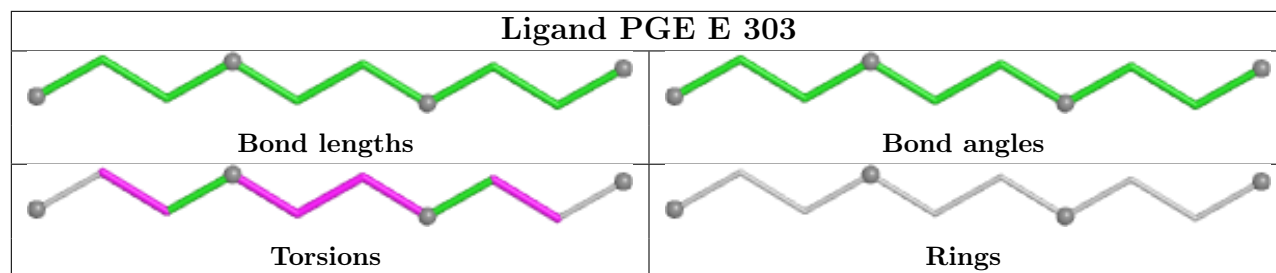
Ligand 3VN F 301

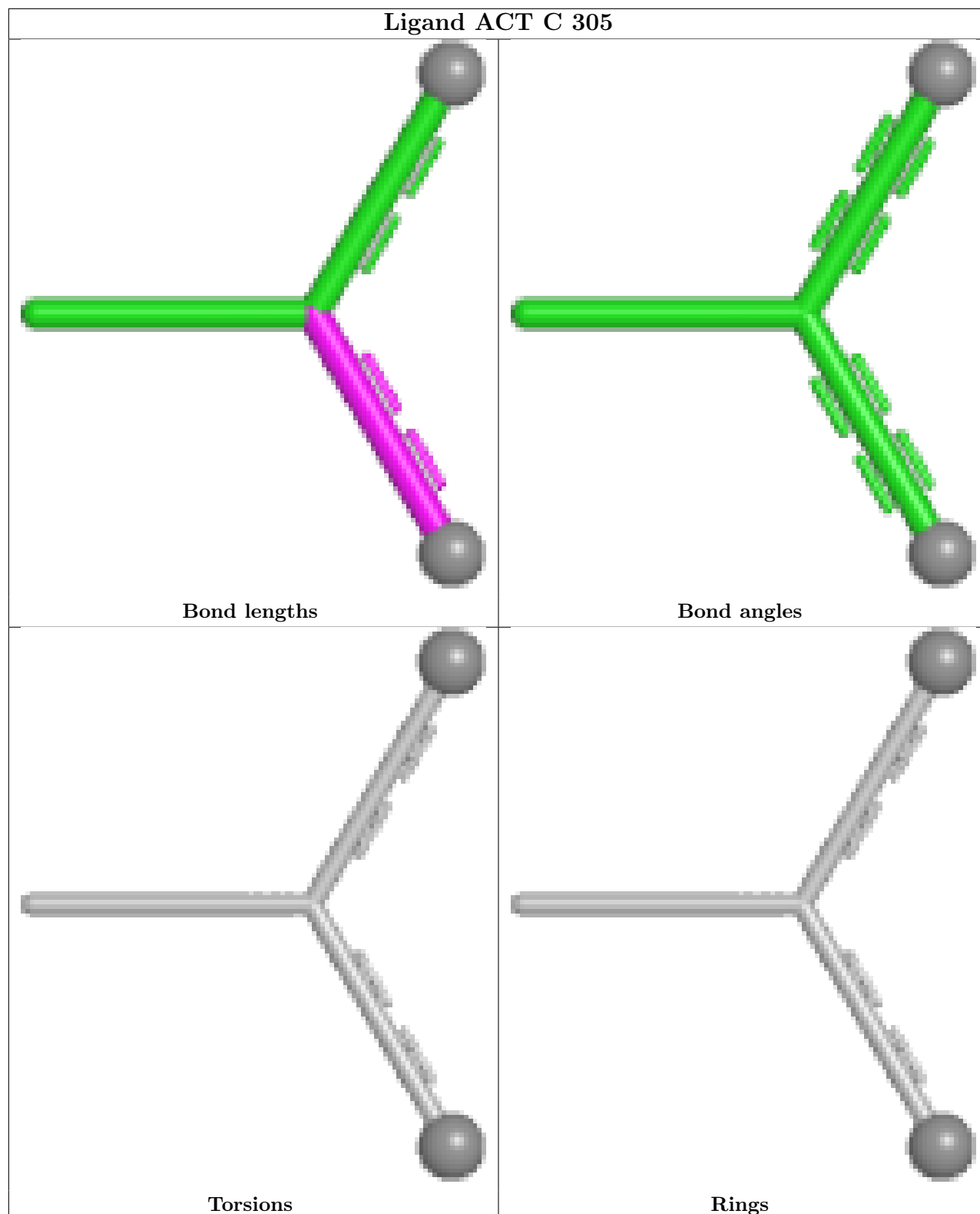


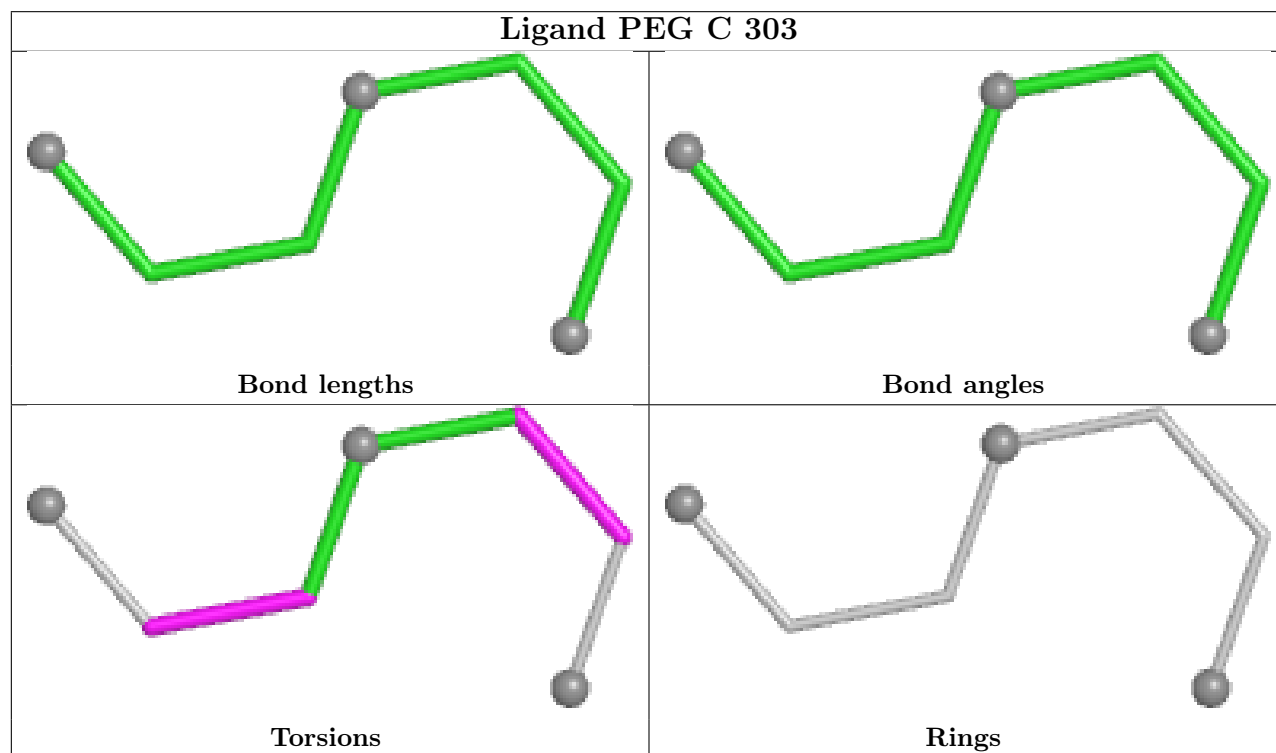
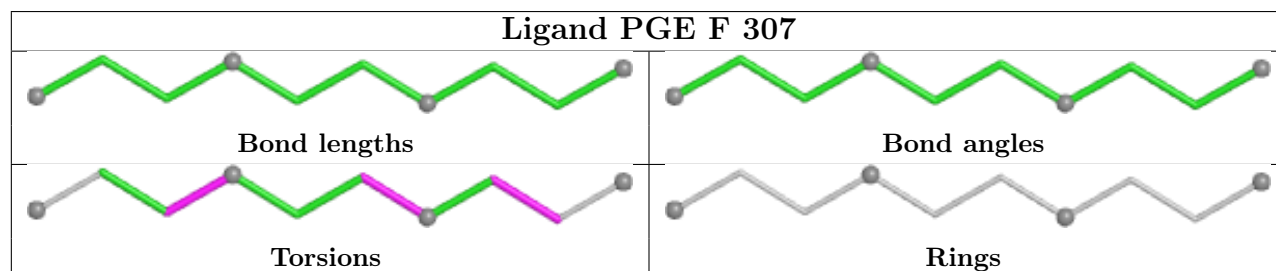
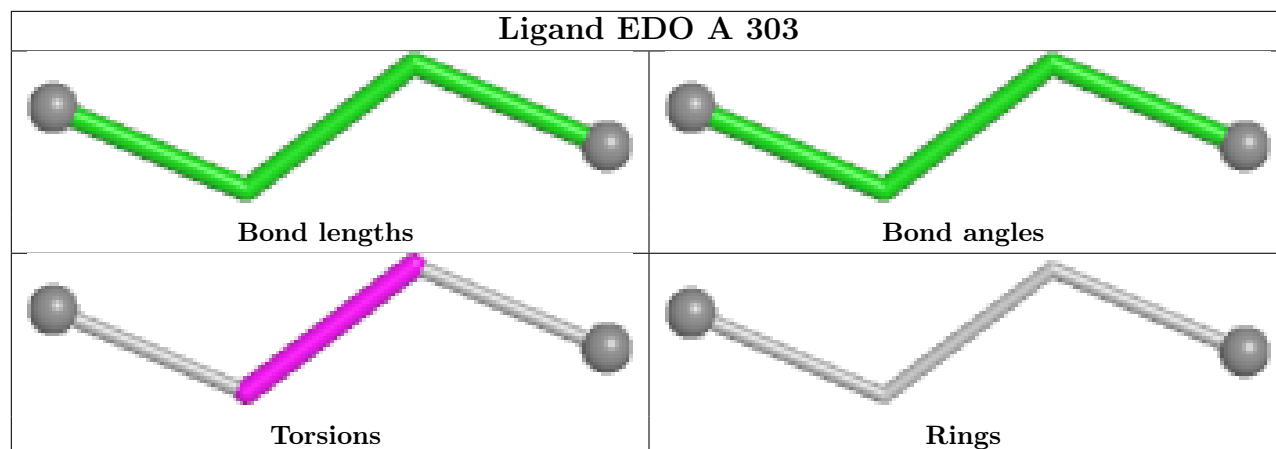
Ligand PEG C 304

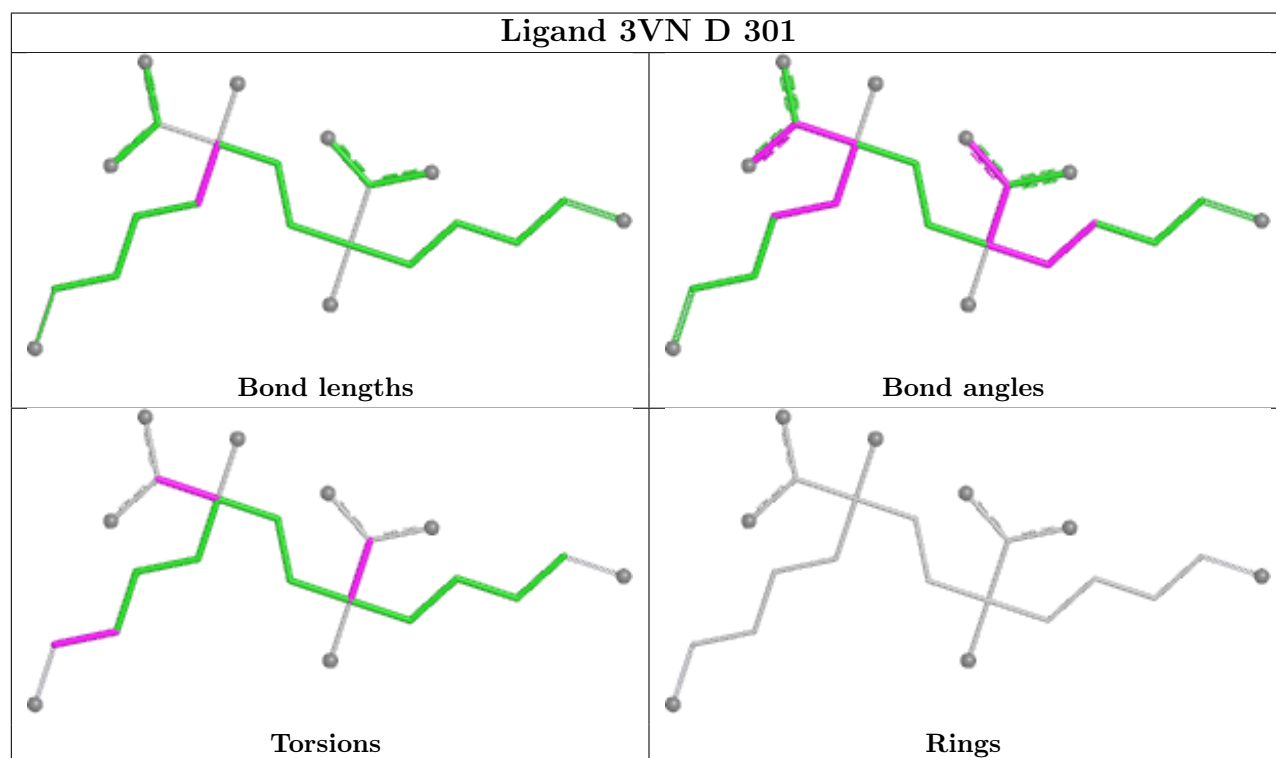
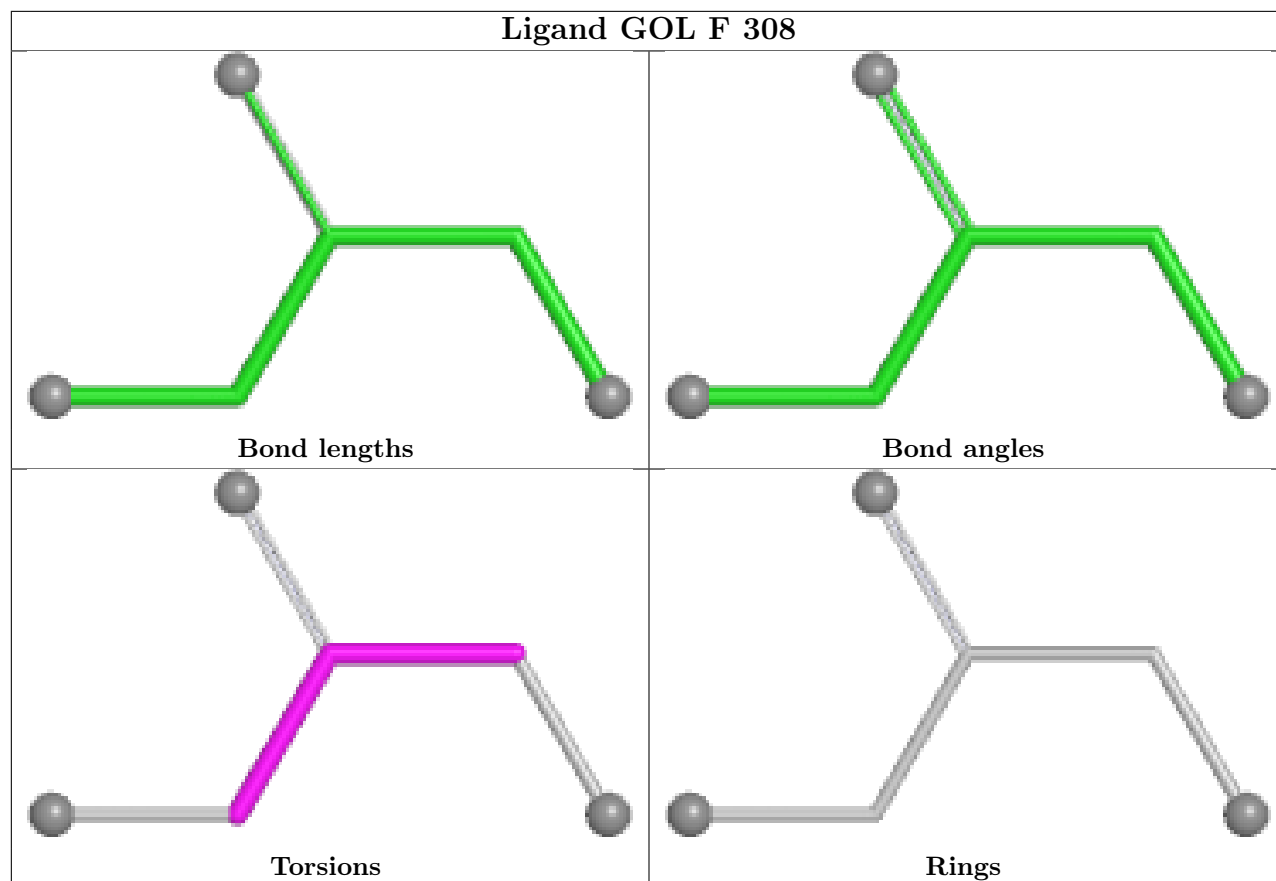


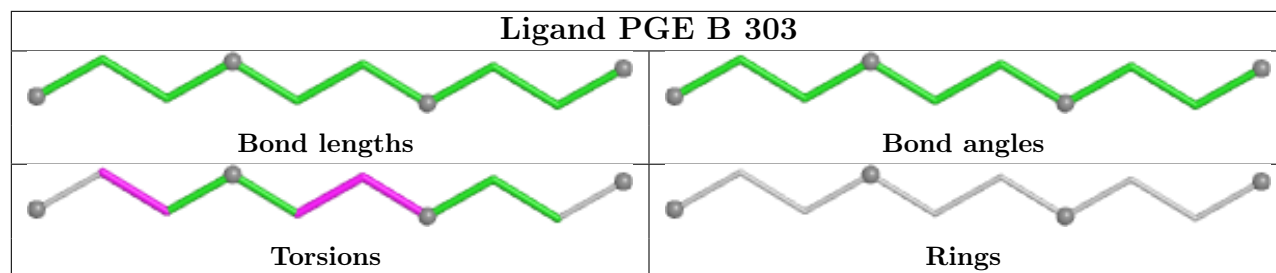


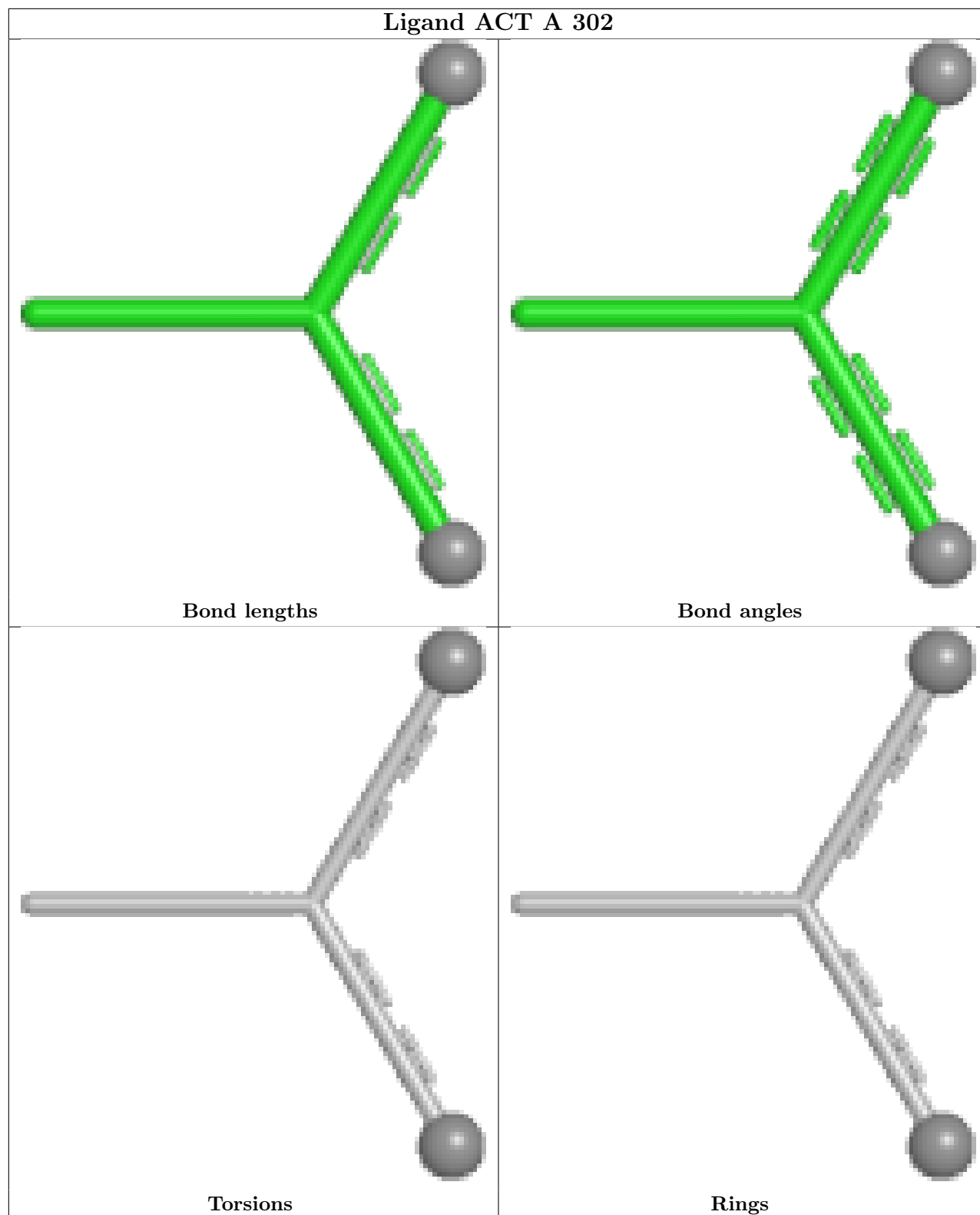


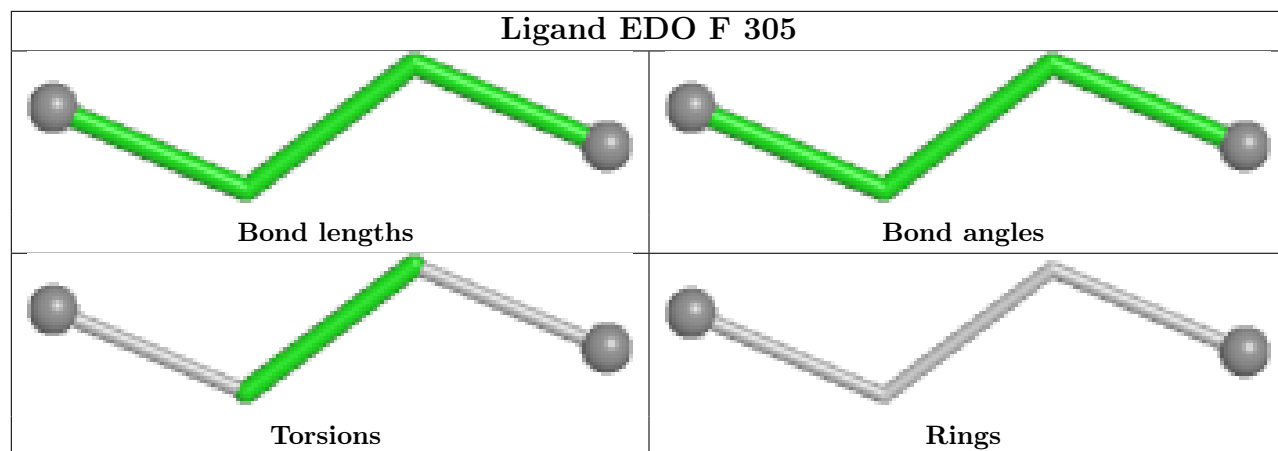


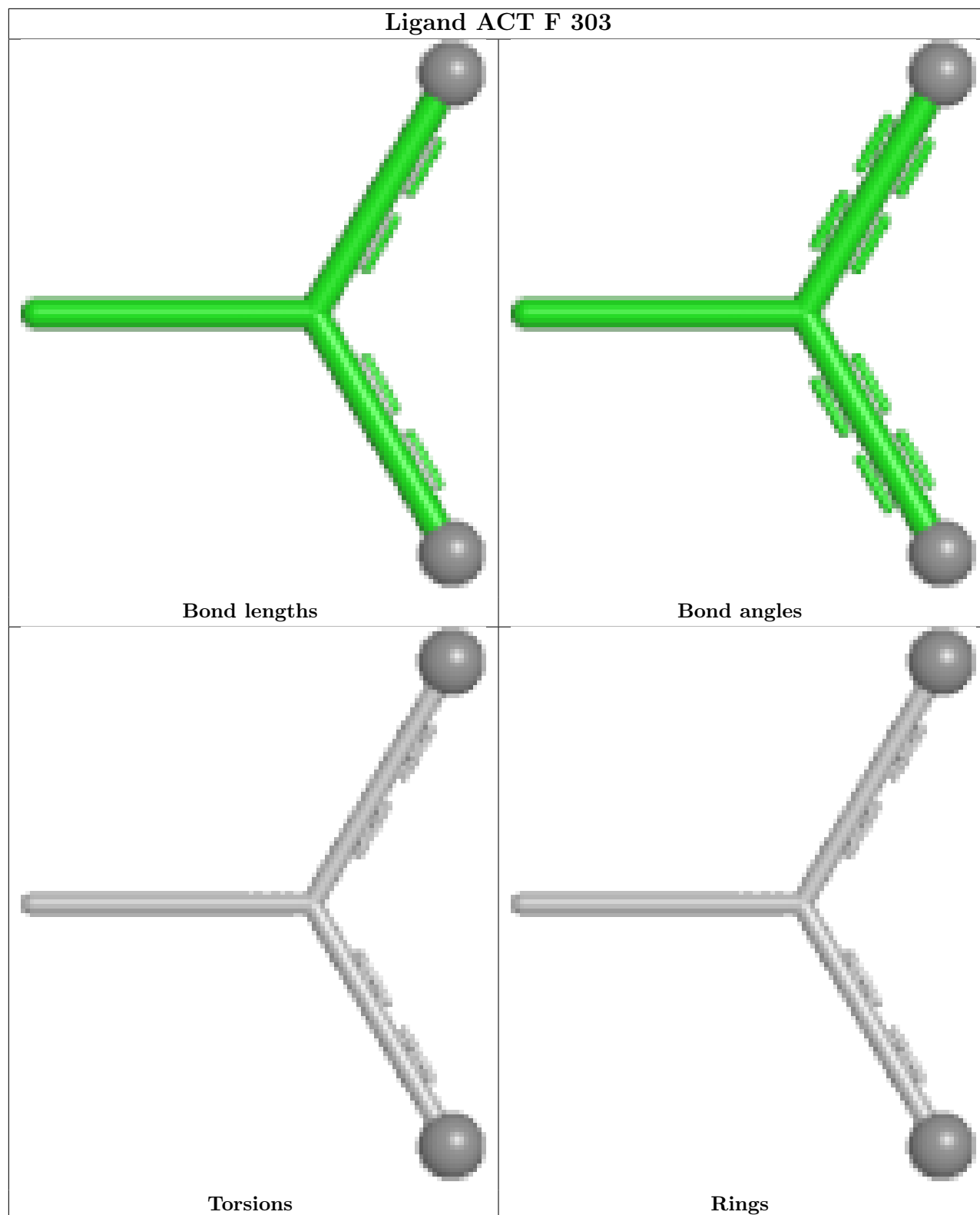












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.04	0 100 100	21, 27, 38, 49	0
1	B	295/310 (95%)	-0.02	3 (1%) 79 82	22, 27, 40, 46	0
1	C	295/310 (95%)	-0.00	0 100 100	21, 27, 38, 51	0
1	D	292/310 (94%)	0.22	12 (4%) 41 42	22, 27, 38, 48	0
1	E	294/310 (94%)	0.14	4 (1%) 73 75	22, 31, 43, 51	0
1	F	295/310 (95%)	0.19	3 (1%) 79 82	22, 31, 47, 54	0
All	All	1766/1860 (94%)	0.08	22 (1%) 76 78	21, 28, 42, 54	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	57	GLU	4.4
1	D	66	ALA	4.2
1	D	68	GLU	3.5
1	F	288	GLU	3.0
1	D	104	ILE	3.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KPI	A	166	14/15	0.87	0.12	22,24,38,42	0
1	KPI	E	166	14/15	0.87	0.11	24,27,36,39	0
1	KPI	C	166	14/15	0.89	0.11	21,23,35,37	0
1	KPI	B	166	14/15	0.90	0.10	20,23,32,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	KPI	D	166	14/15	0.91	0.10	21,26,37,42	0
1	KPI	F	166	14/15	0.93	0.12	22,27,41,43	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
3	ACT	E	302	4/4	0.47	0.28	20,20,20,20	0
8	GOL	F	308	6/6	0.50	0.25	20,20,20,20	0
2	MG	A	301	1/1	0.57	0.14	30,30,30,30	0
3	ACT	F	303	4/4	0.59	0.26	20,20,20,20	0
3	ACT	F	302	4/4	0.63	0.30	20,20,20,20	0
3	ACT	D	305	4/4	0.68	0.22	20,20,20,20	0
3	ACT	A	302	4/4	0.70	0.29	20,20,20,20	0
5	PGE	F	307	10/10	0.73	0.24	20,20,20,20	0
3	ACT	C	305	4/4	0.73	0.23	20,20,20,20	0
7	PEG	C	304	7/7	0.75	0.30	20,20,20,20	0
5	PGE	B	303	10/10	0.77	0.19	20,20,20,20	0
2	MG	C	302	1/1	0.78	0.25	30,30,30,30	0
5	PGE	A	304	10/10	0.78	0.18	20,20,20,20	0
5	PGE	E	303	10/10	0.79	0.19	20,20,20,20	0
3	ACT	F	304	4/4	0.79	0.25	20,20,20,20	0
2	MG	D	303	1/1	0.83	0.21	30,30,30,30	0
7	PEG	C	303	7/7	0.83	0.15	20,20,20,20	0
7	PEG	D	304	7/7	0.86	0.16	20,20,20,20	0
4	EDO	A	303	4/4	0.86	0.15	20,20,20,20	0
6	3VN	F	301	22/22	0.87	0.24	53,65,69,71	0
2	MG	E	301	1/1	0.88	0.13	30,30,30,30	0
2	MG	C	301	1/1	0.88	0.10	30,30,30,30	0
4	EDO	F	306	4/4	0.89	0.17	20,20,20,20	0
6	3VN	D	301	22/22	0.90	0.14	30,39,50,52	0
2	MG	B	302	1/1	0.91	0.08	30,30,30,30	0
6	3VN	B	301	22/22	0.94	0.10	28,34,38,42	0

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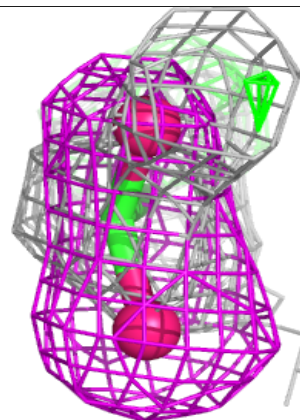
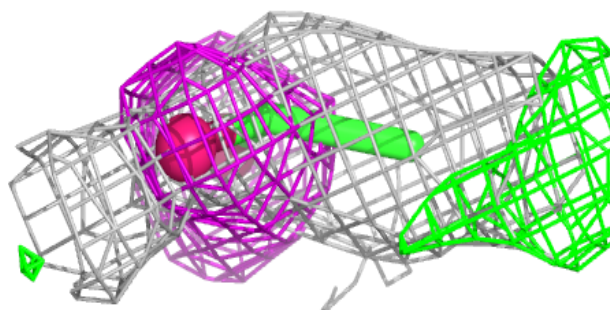
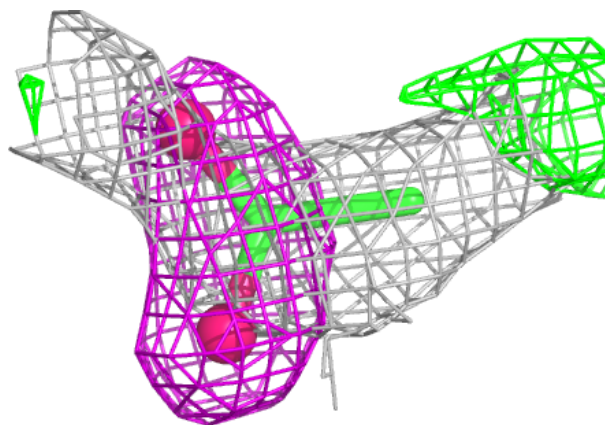
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	D	302	1/1	0.97	0.21	30,30,30,30	0
4	EDO	F	305	4/4	0.97	0.09	20,20,20,20	0

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

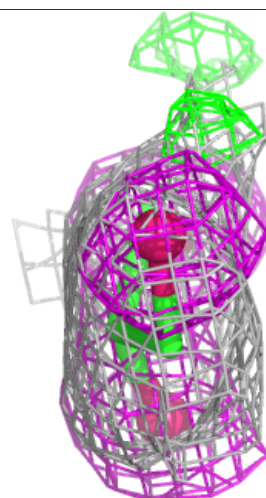
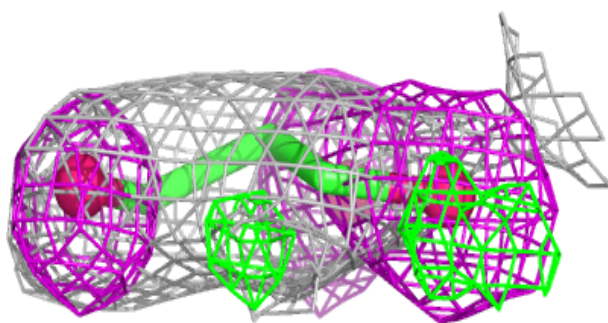
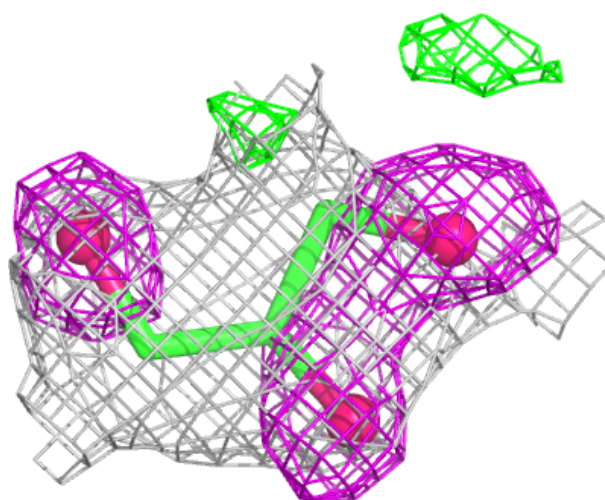
Electron density around ACT E 302:

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



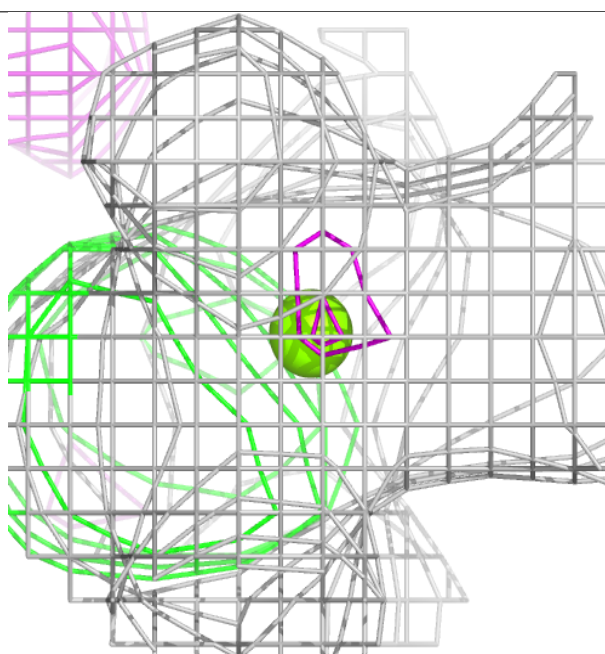
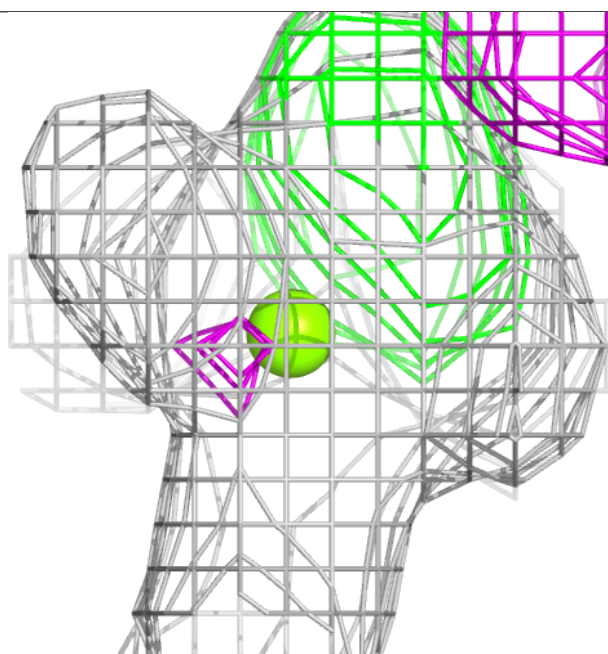
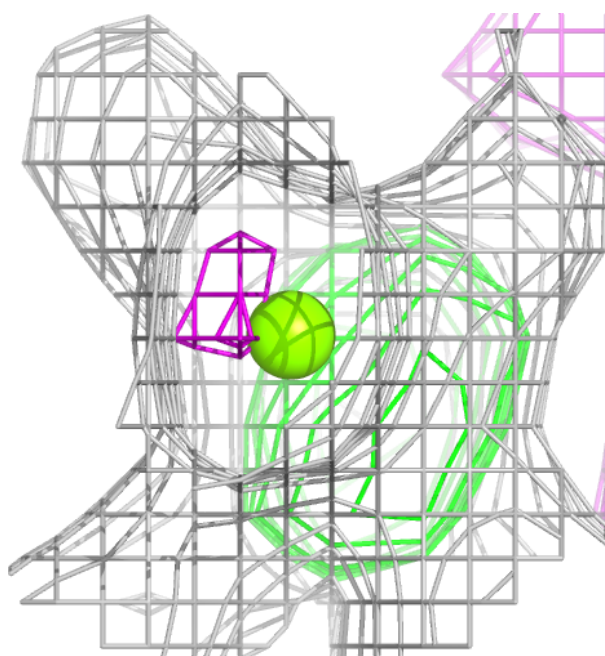
Electron density around GOL F 308:

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



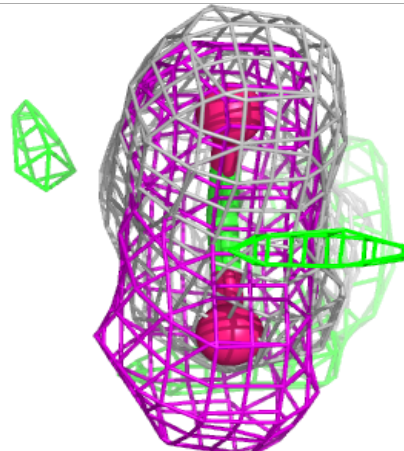
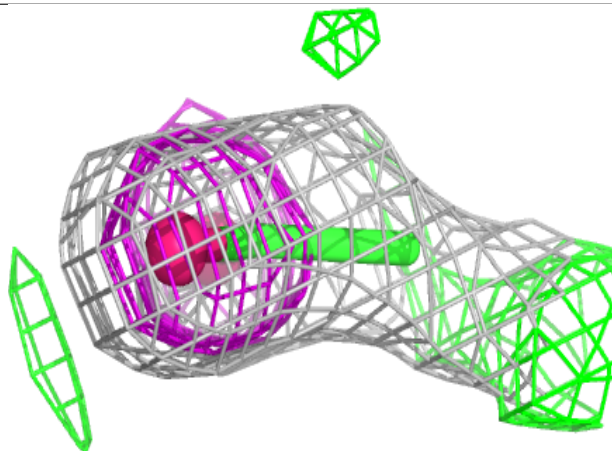
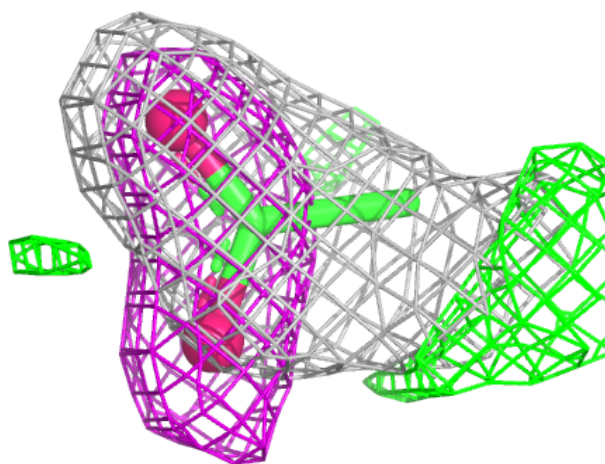
Electron density around MG A 301:

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and green (positive)



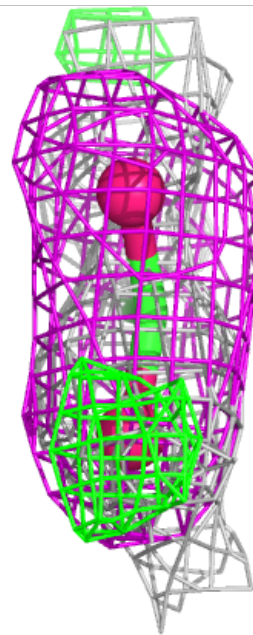
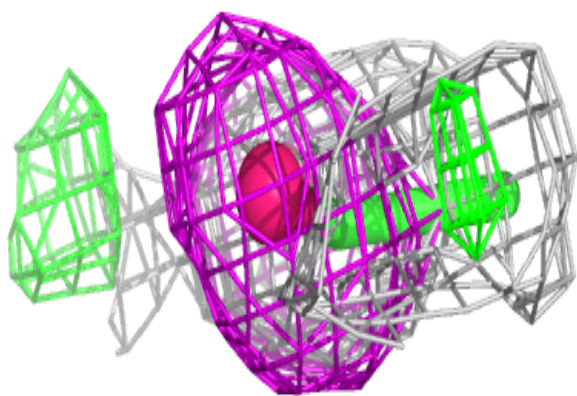
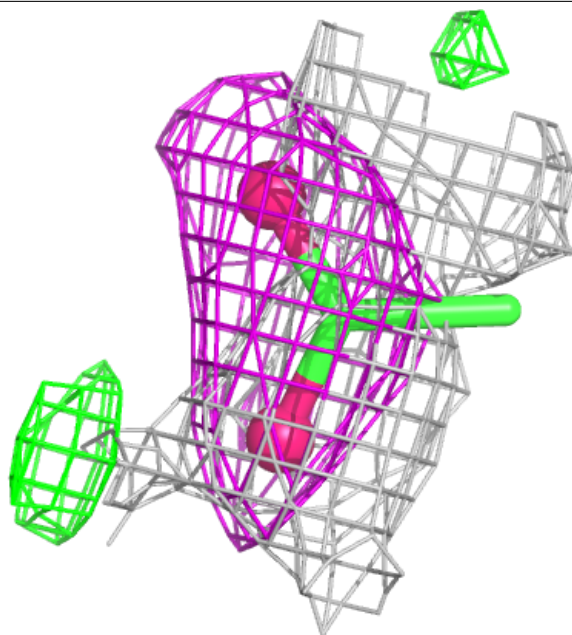
Electron density around ACT F 303:

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and green (positive)



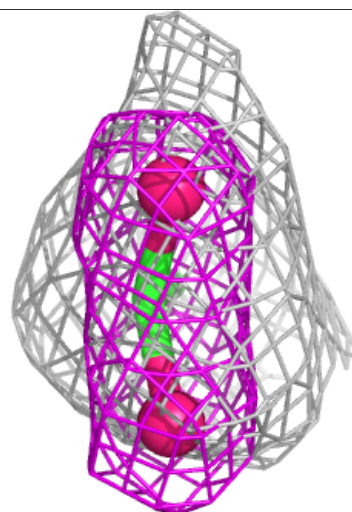
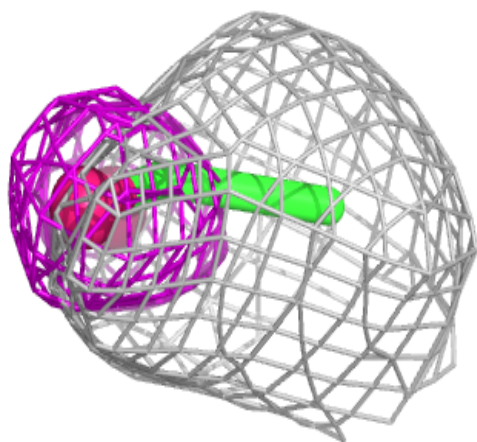
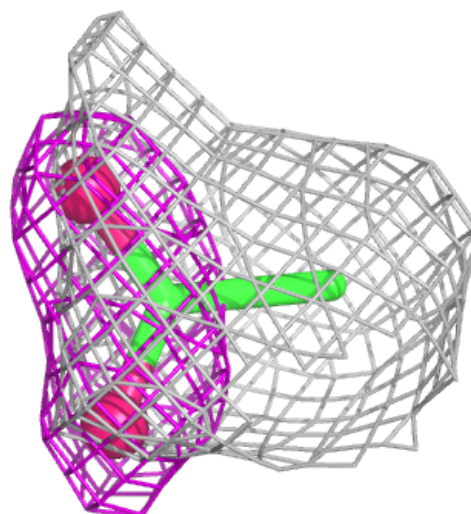
Electron density around ACT F 302:

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and green (positive)



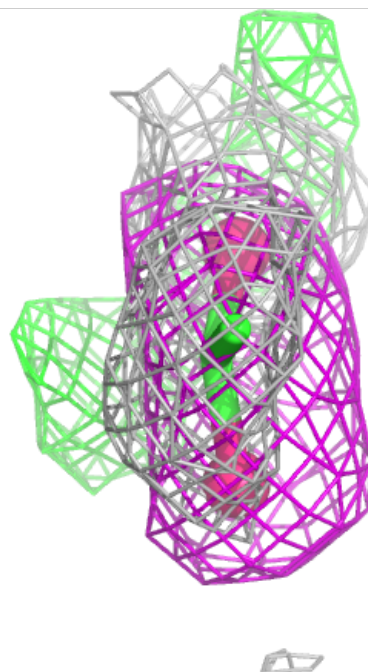
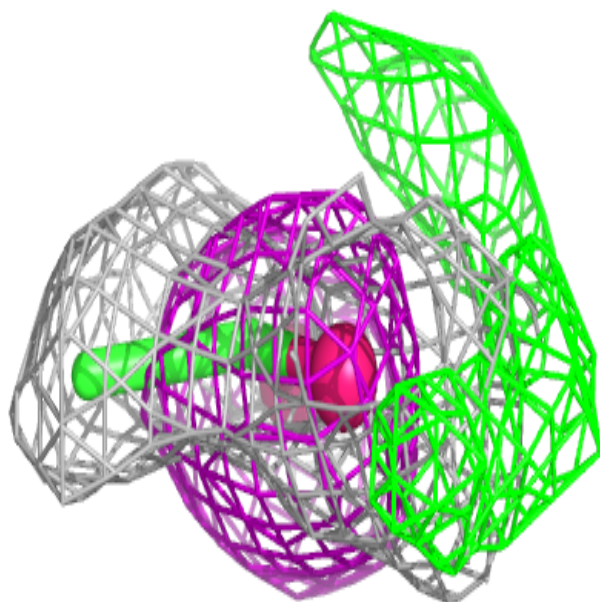
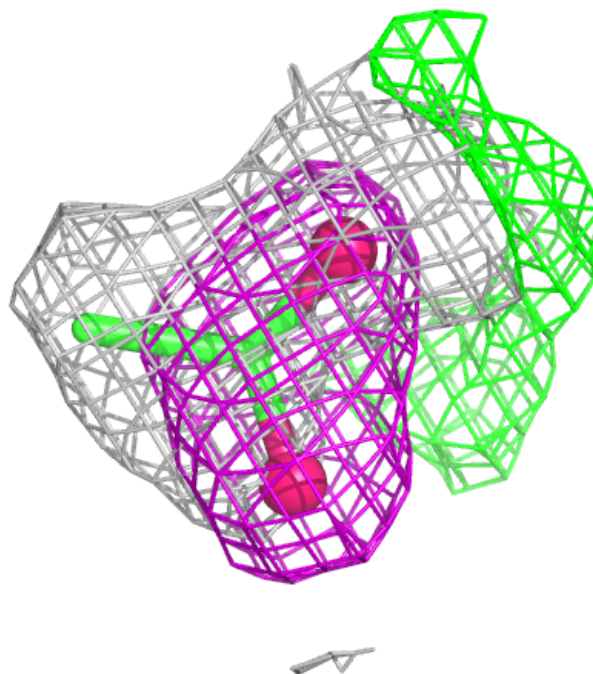
Electron density around ACT D 305:

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and green (positive)



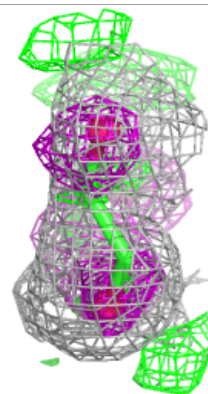
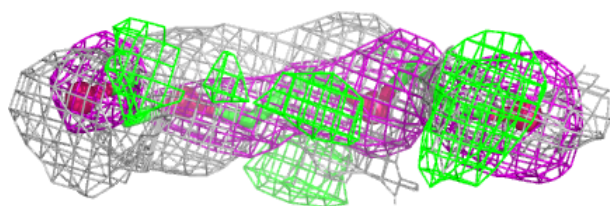
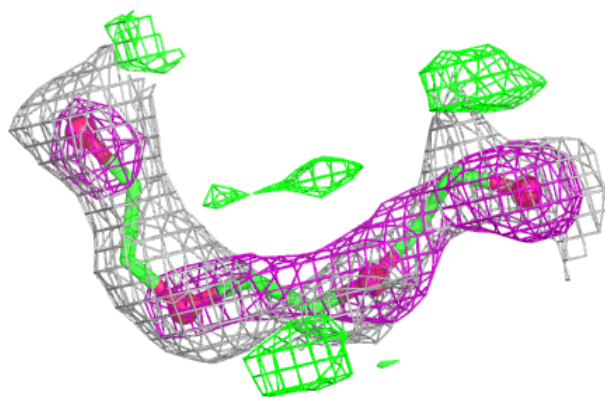
Electron density around ACT A 302:

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



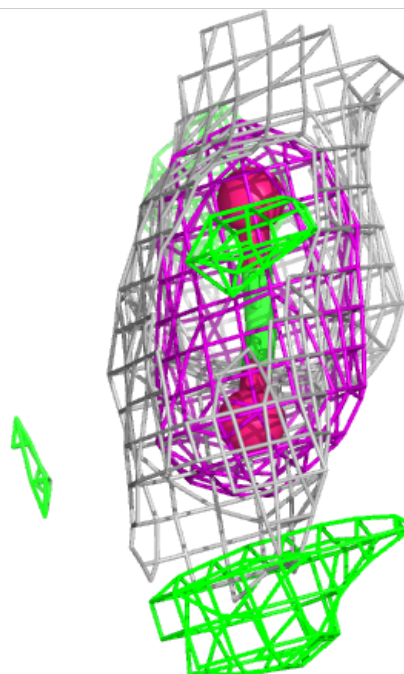
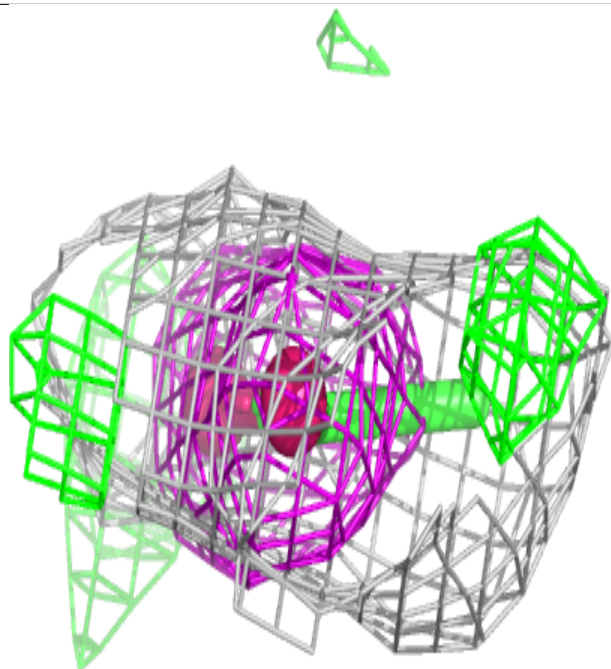
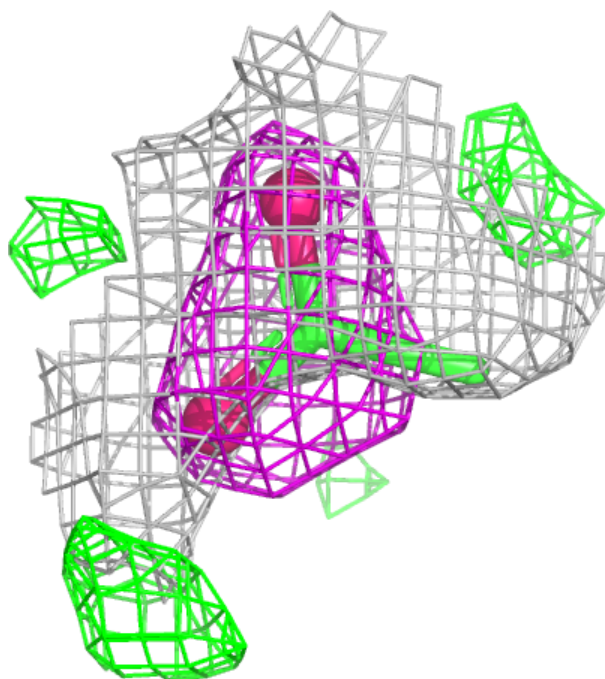
Electron density around PGE F 307:

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and green (positive)



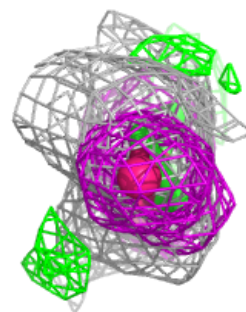
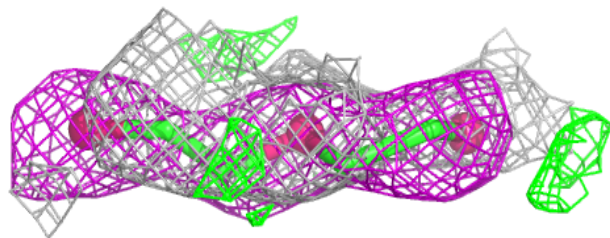
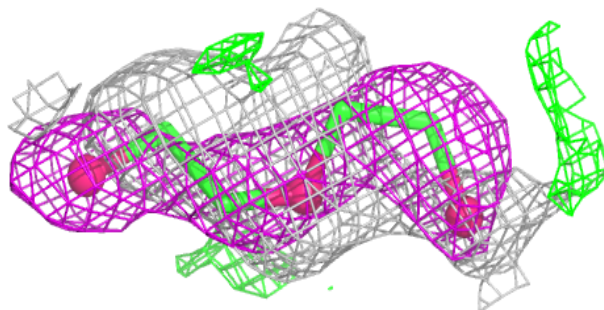
Electron density around ACT C 305:

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and green (positive)

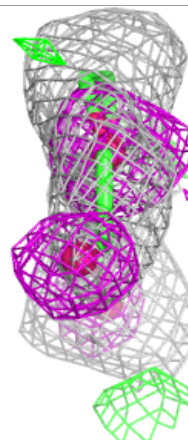
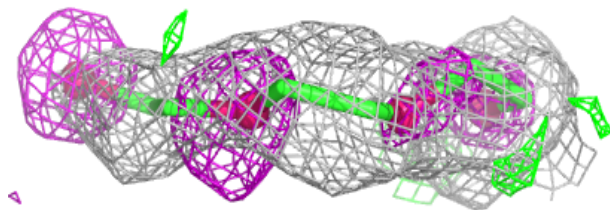
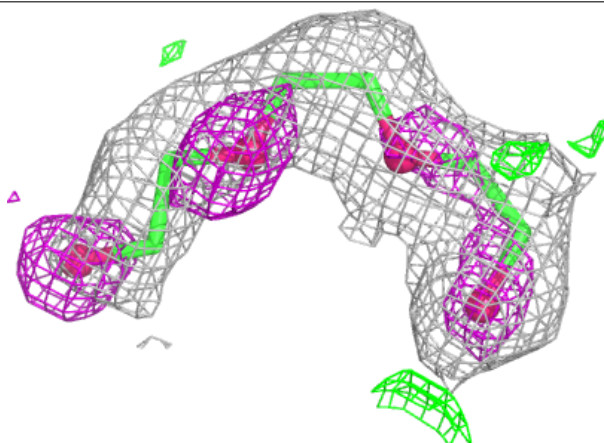


Electron density around PEG C 304:

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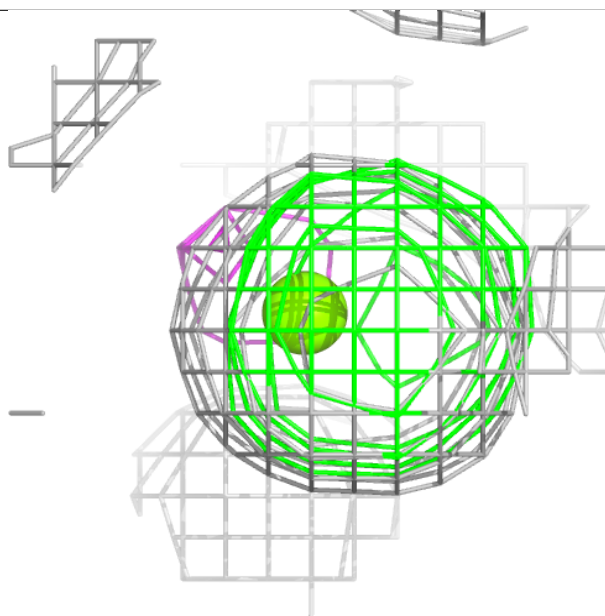
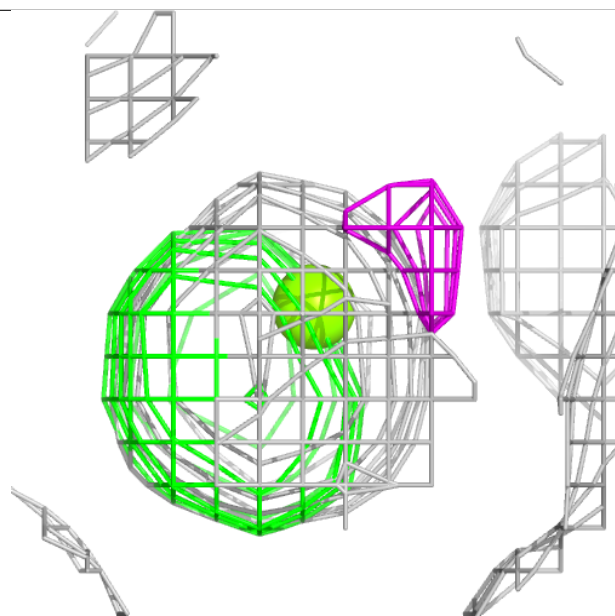
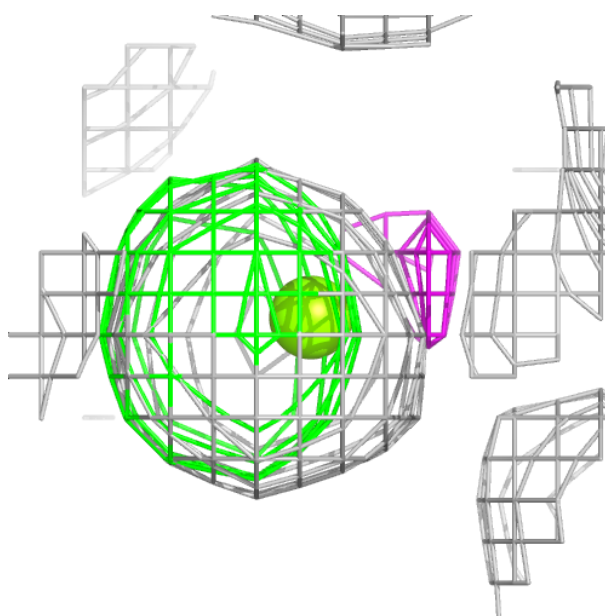
**Electron density around PGE B 303:**

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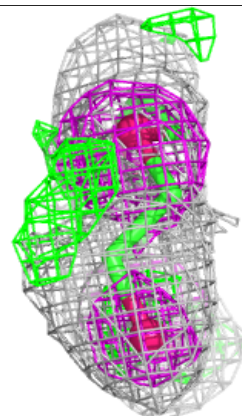
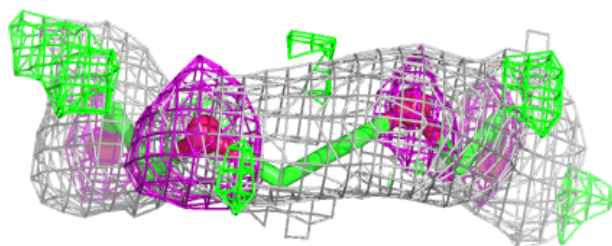
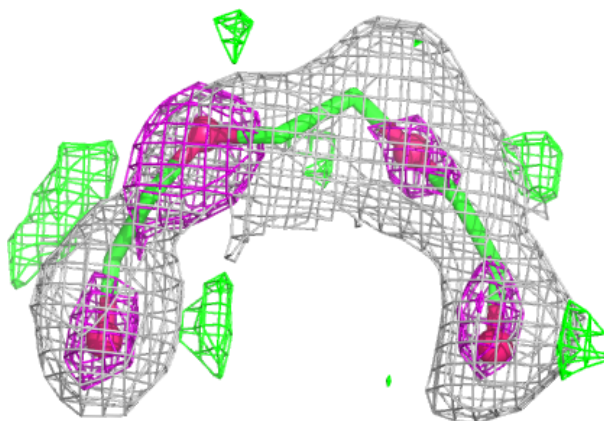
Electron density around MG C 302:

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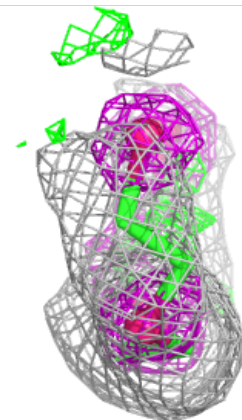
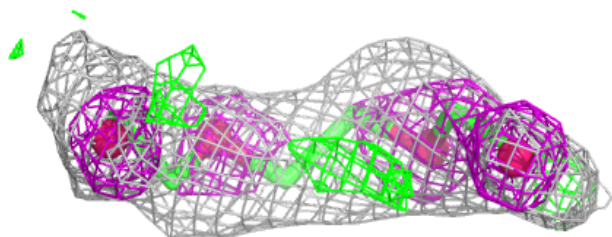
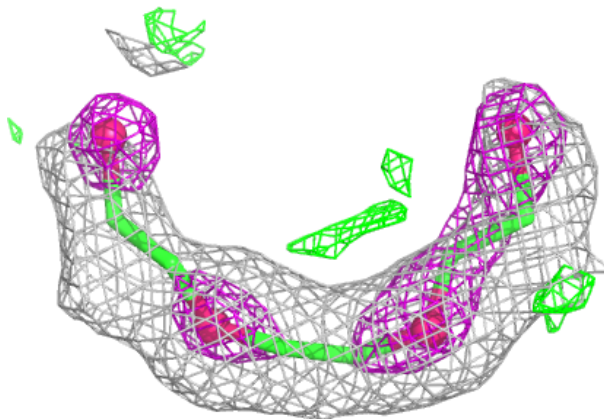


Electron density around PGE A 304:

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

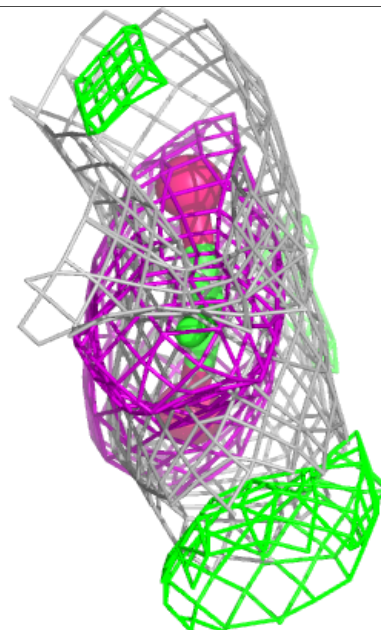
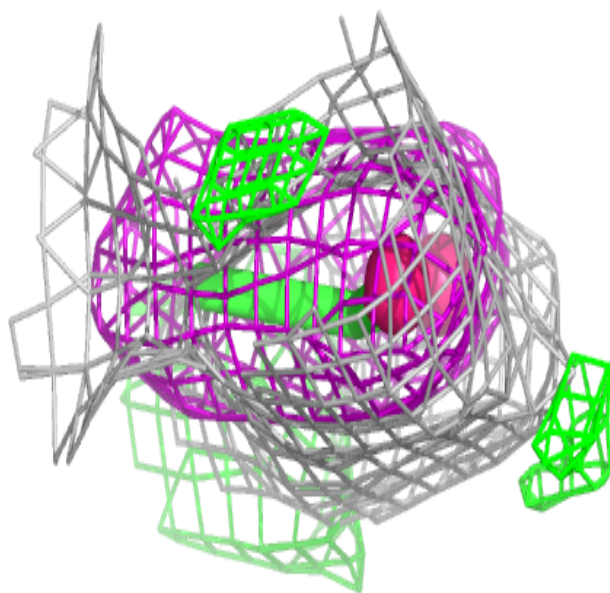
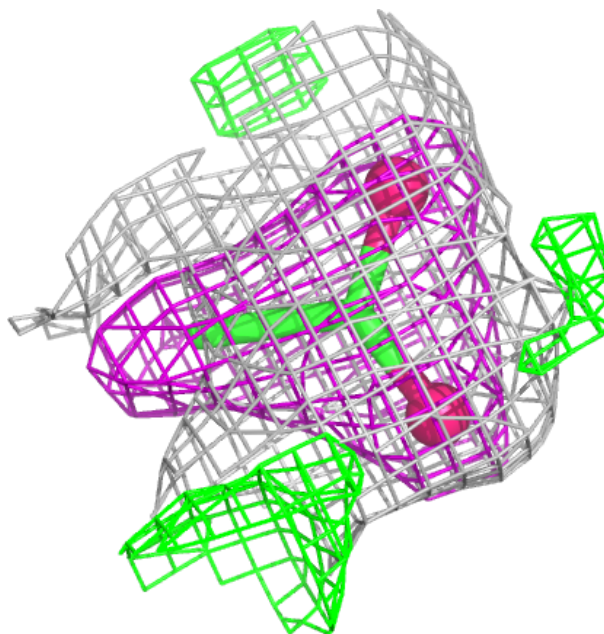
**Electron density around PGE E 303:**

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and green (positive)



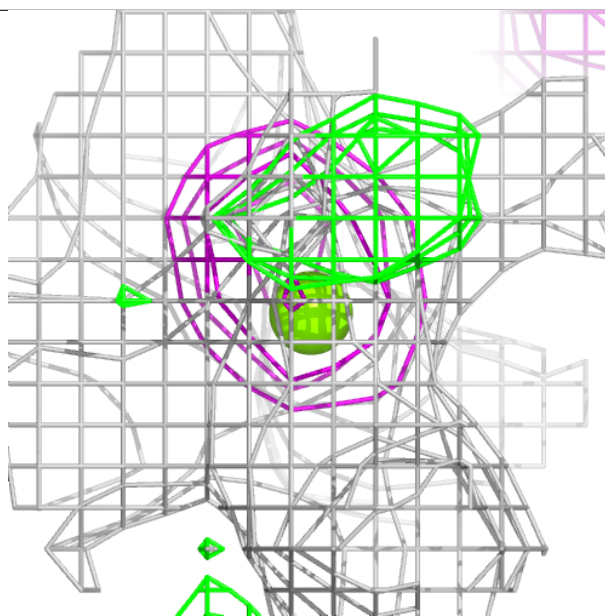
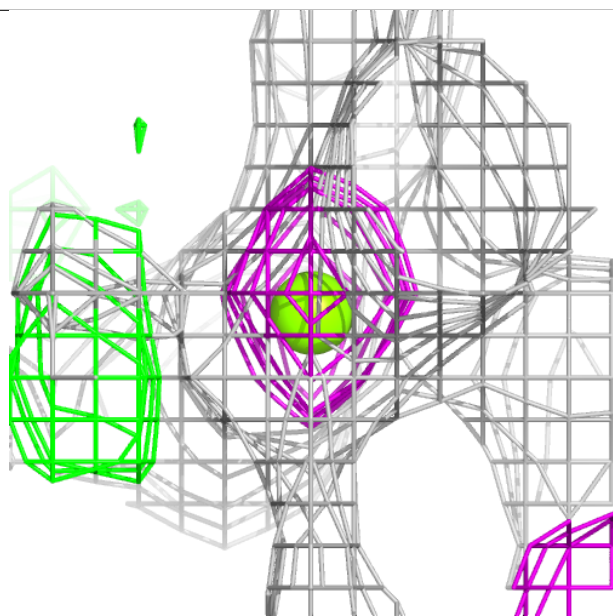
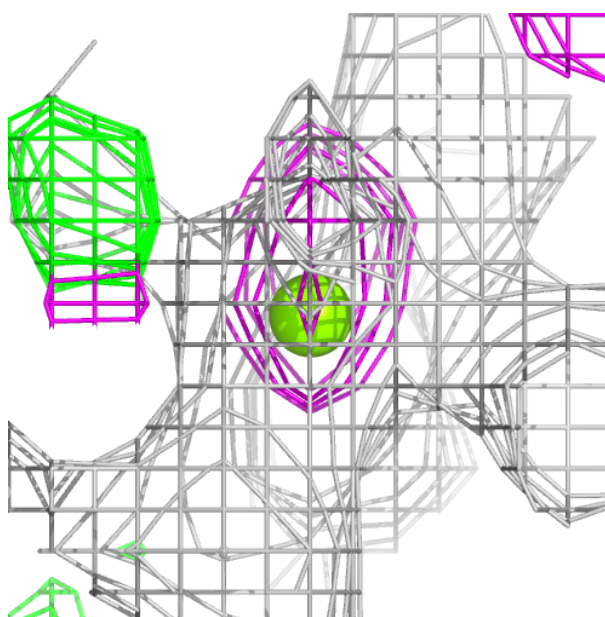
Electron density around ACT F 304:

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and green (positive)



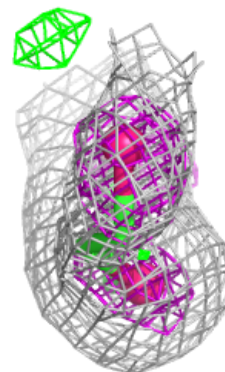
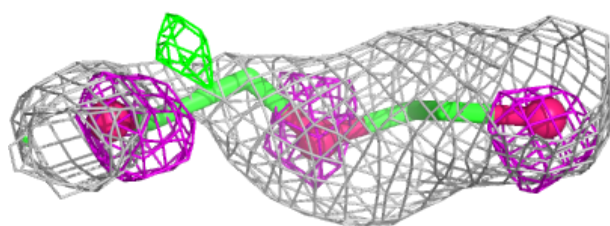
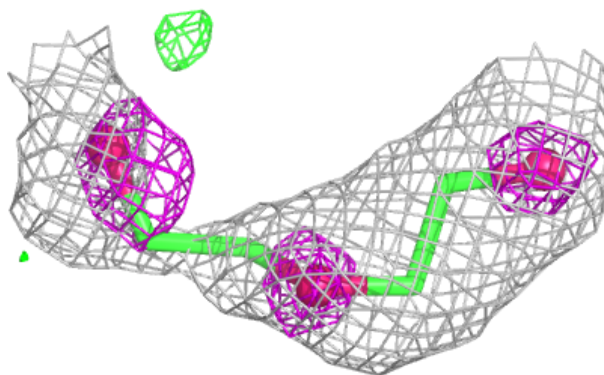
Electron density around MG D 303:

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and green (positive)

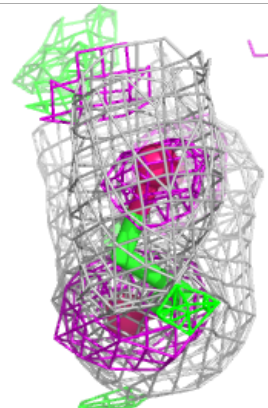
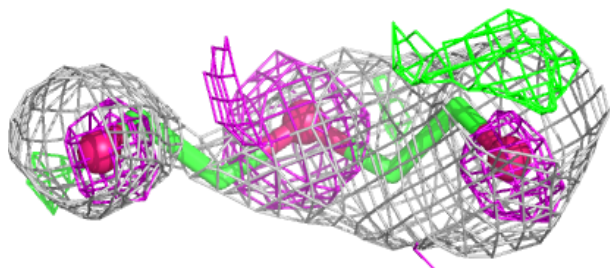
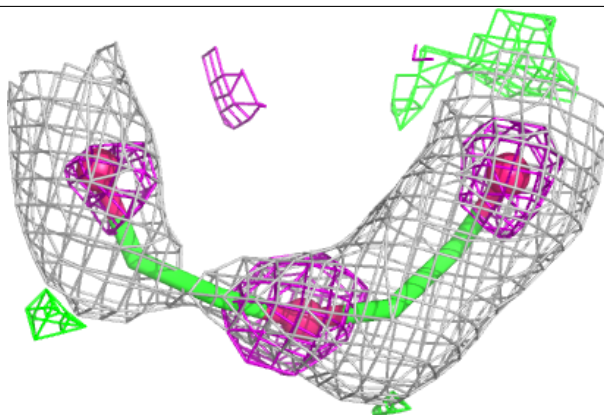


Electron density around PEG C 303:

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and green (positive)

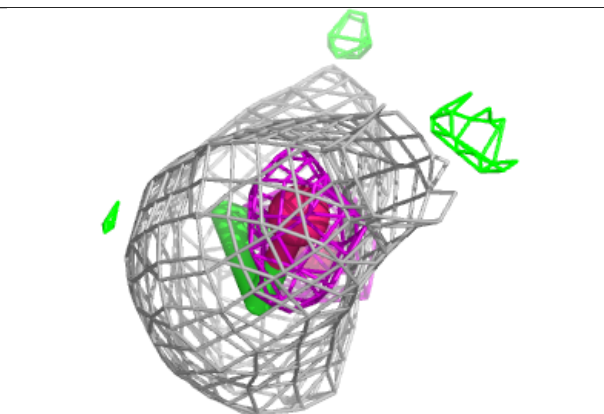
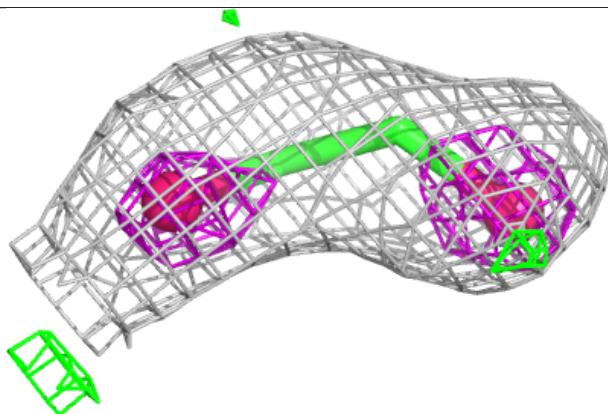
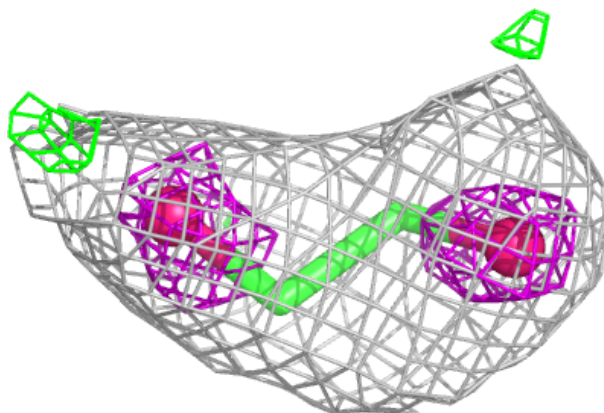
**Electron density around PEG D 304:**

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and green (positive)

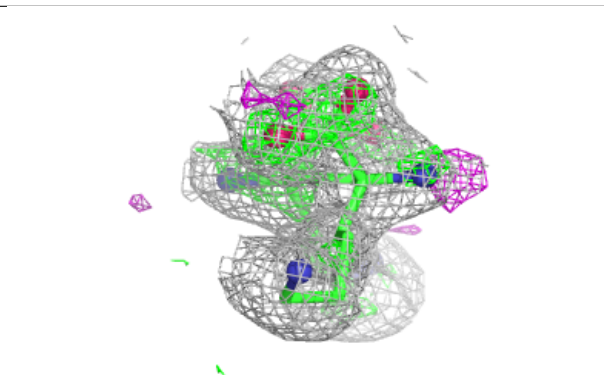
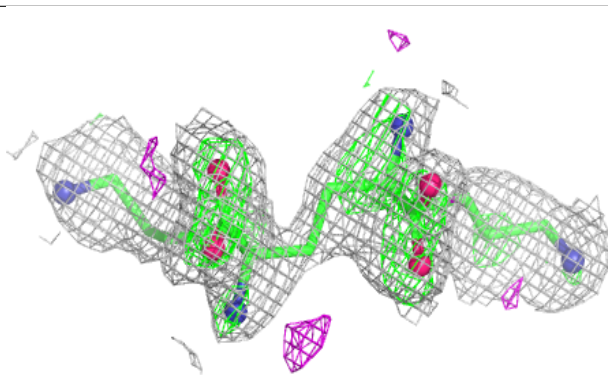
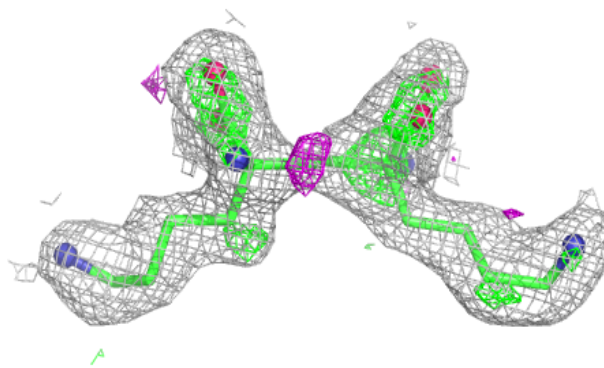


Electron density around EDO A 303:

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and green (positive)

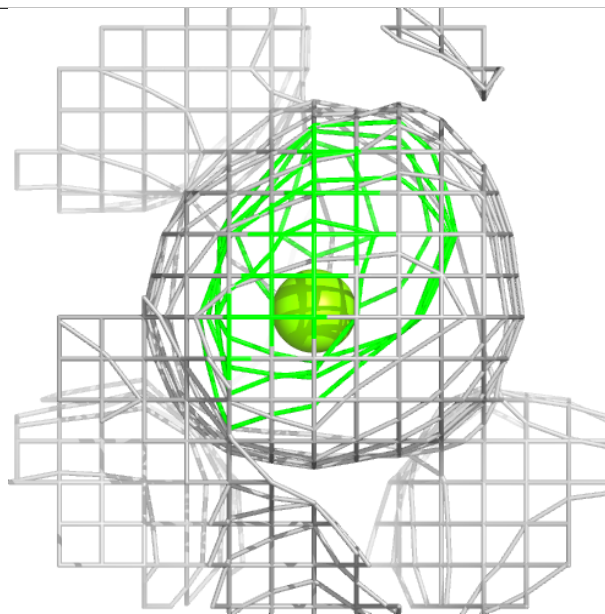
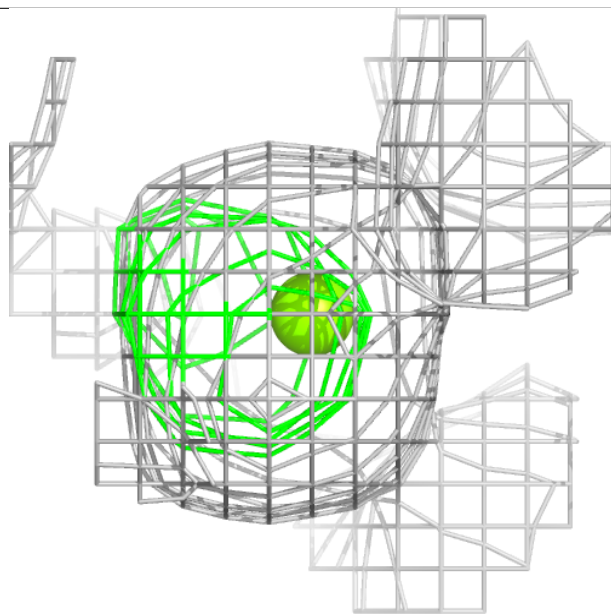
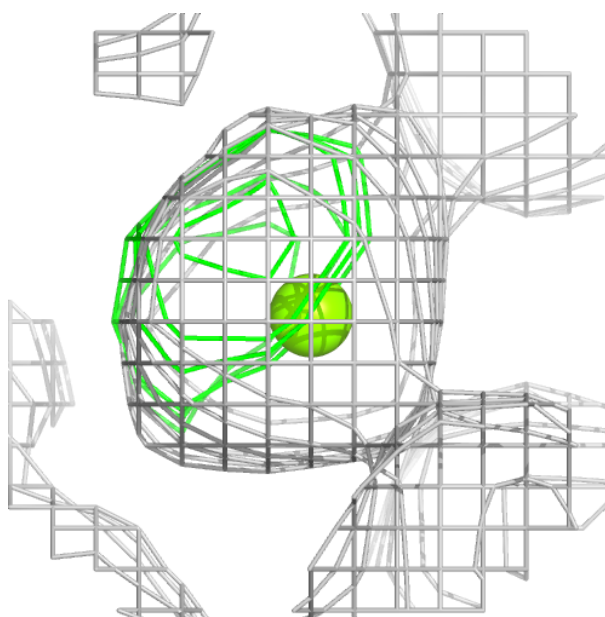
**Electron density around 3VN F 301:**

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and green (positive)



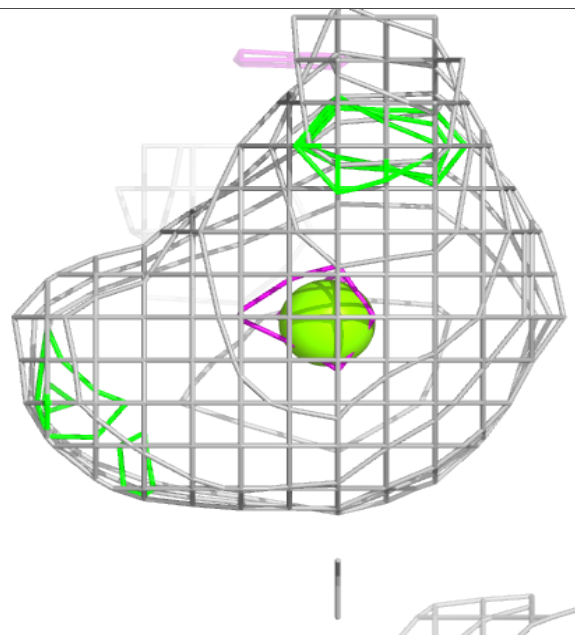
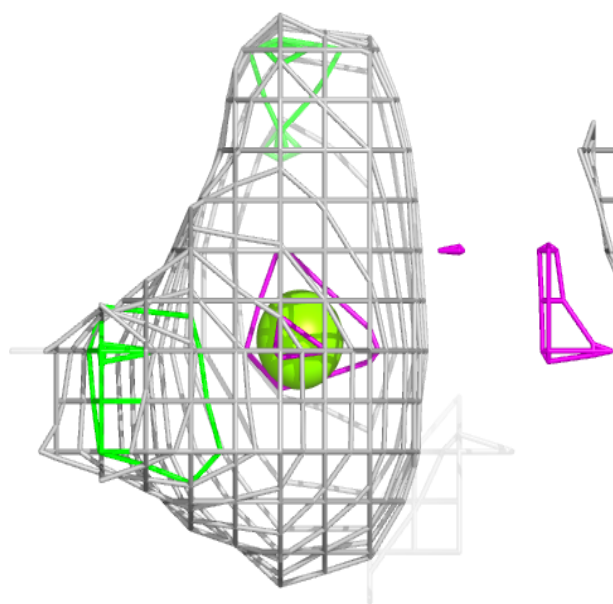
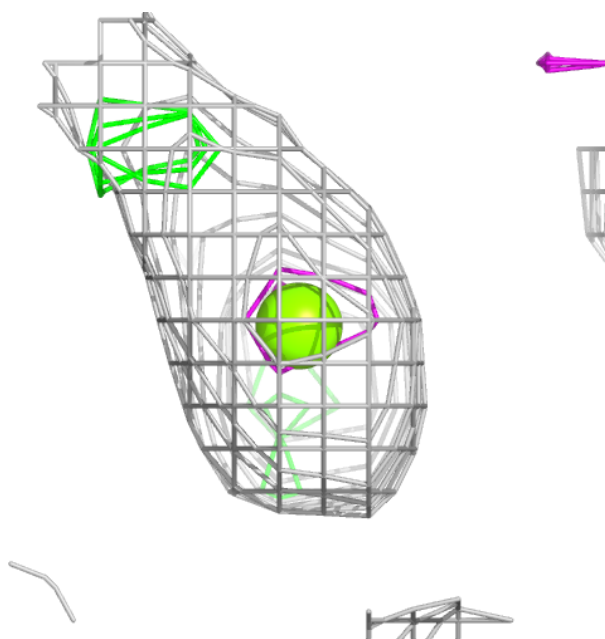
Electron density around MG E 301:

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and green (positive)



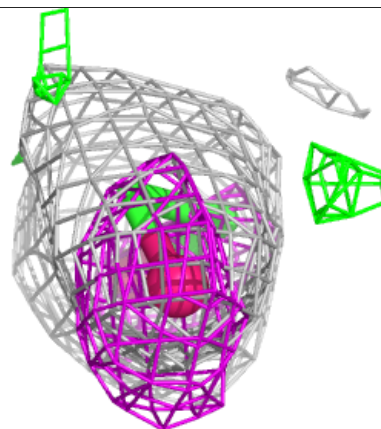
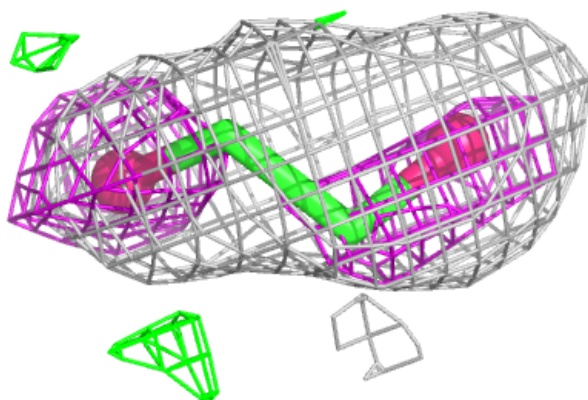
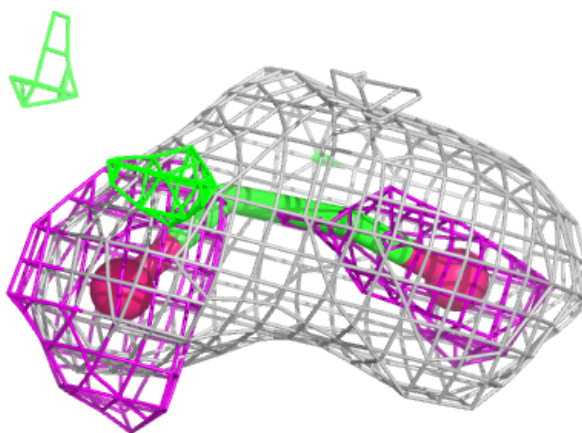
Electron density around MG C 301:

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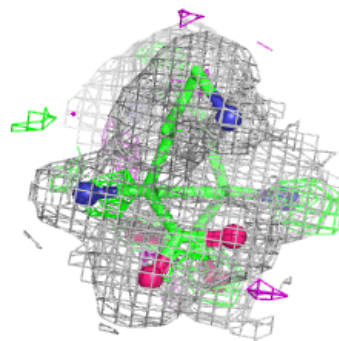
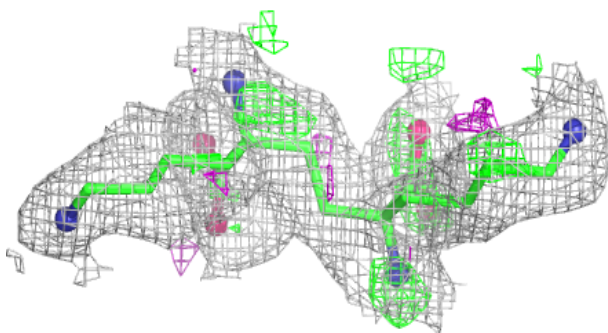
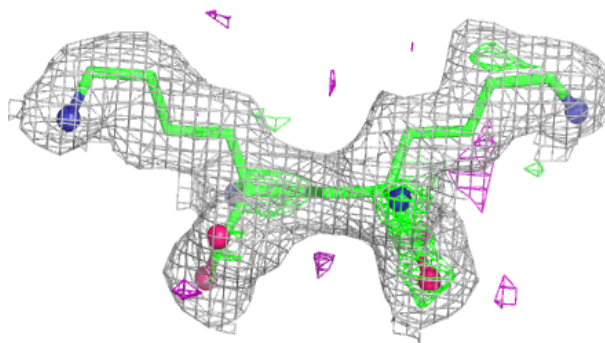


Electron density around EDO F 306:

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and green (positive)

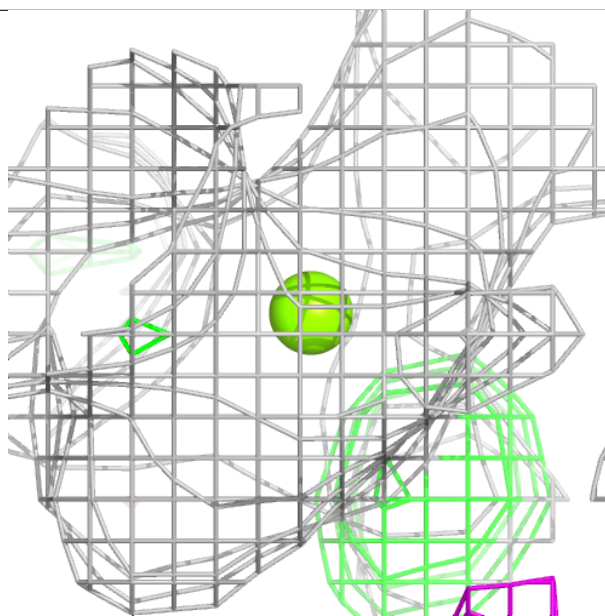
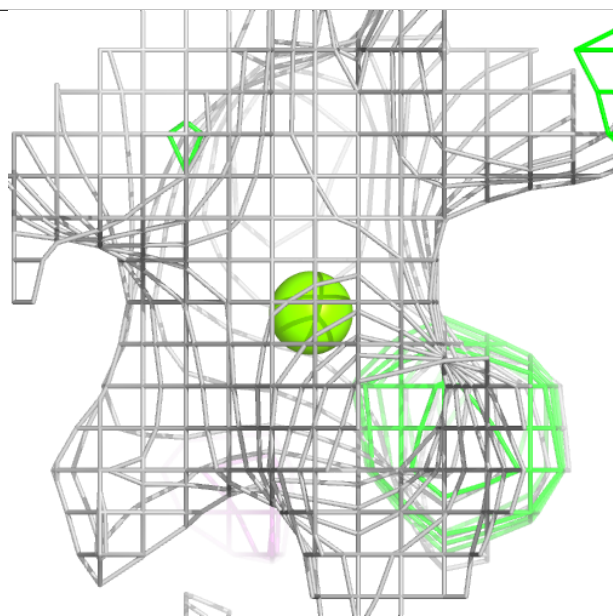
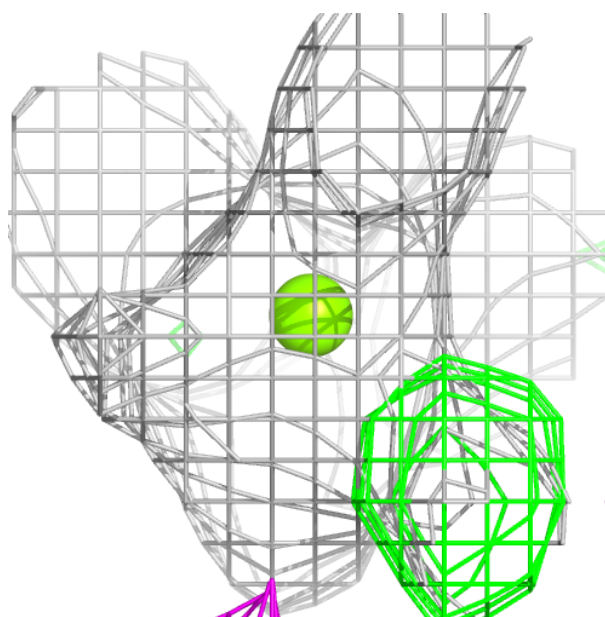
**Electron density around 3VN D 301:**

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



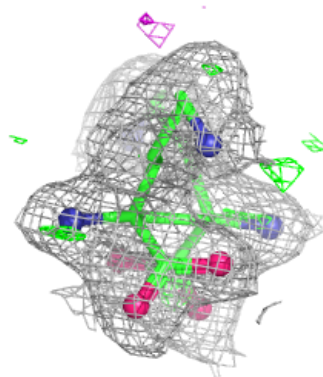
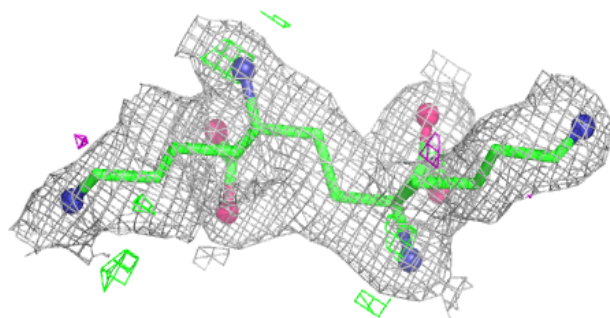
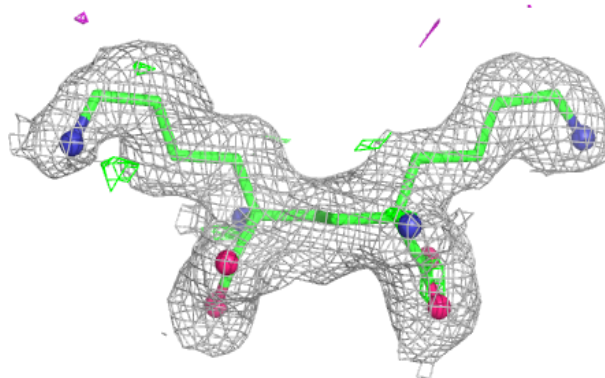
Electron density around MG B 302:

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



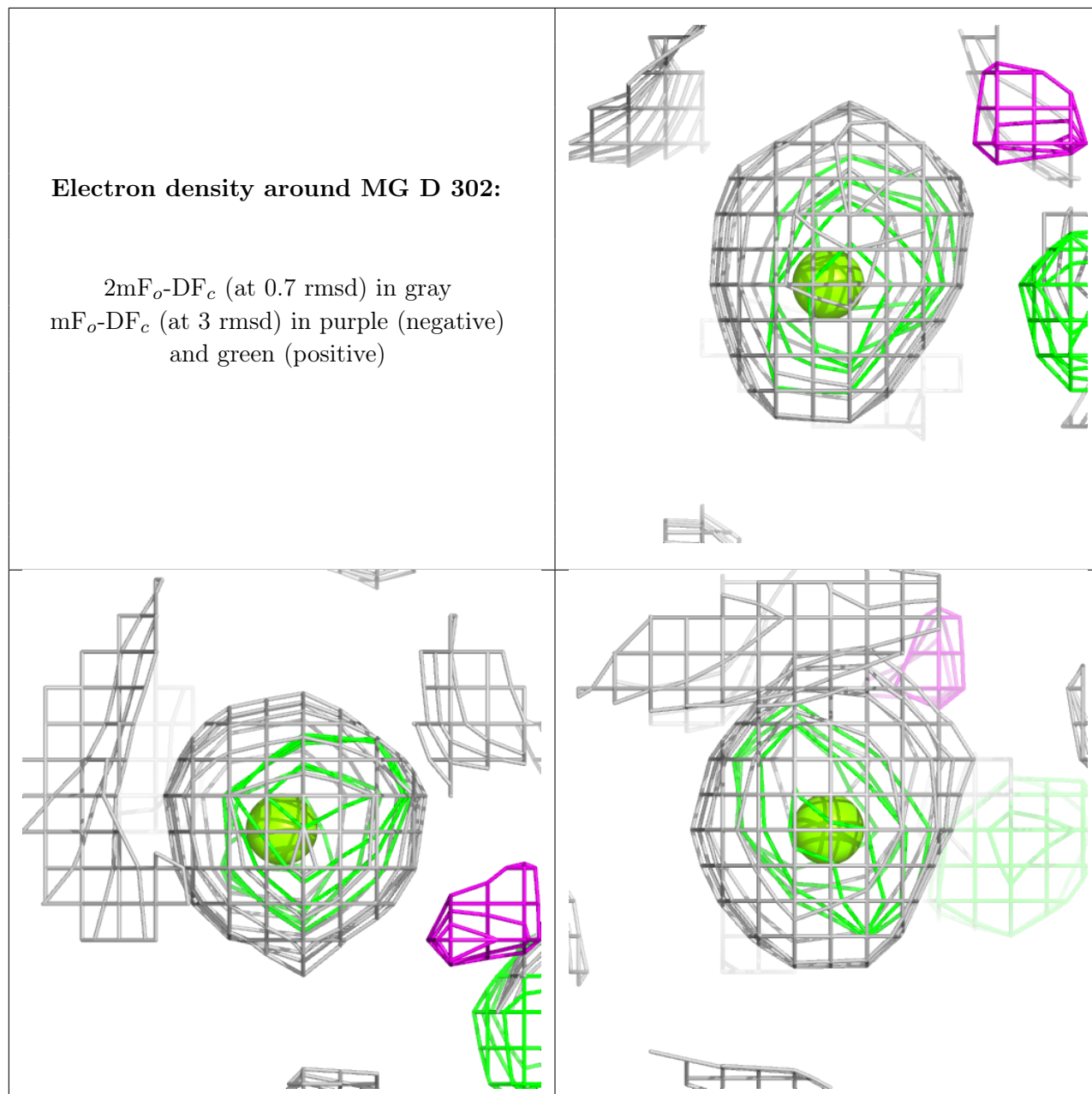
Electron density around 3VN B 301:

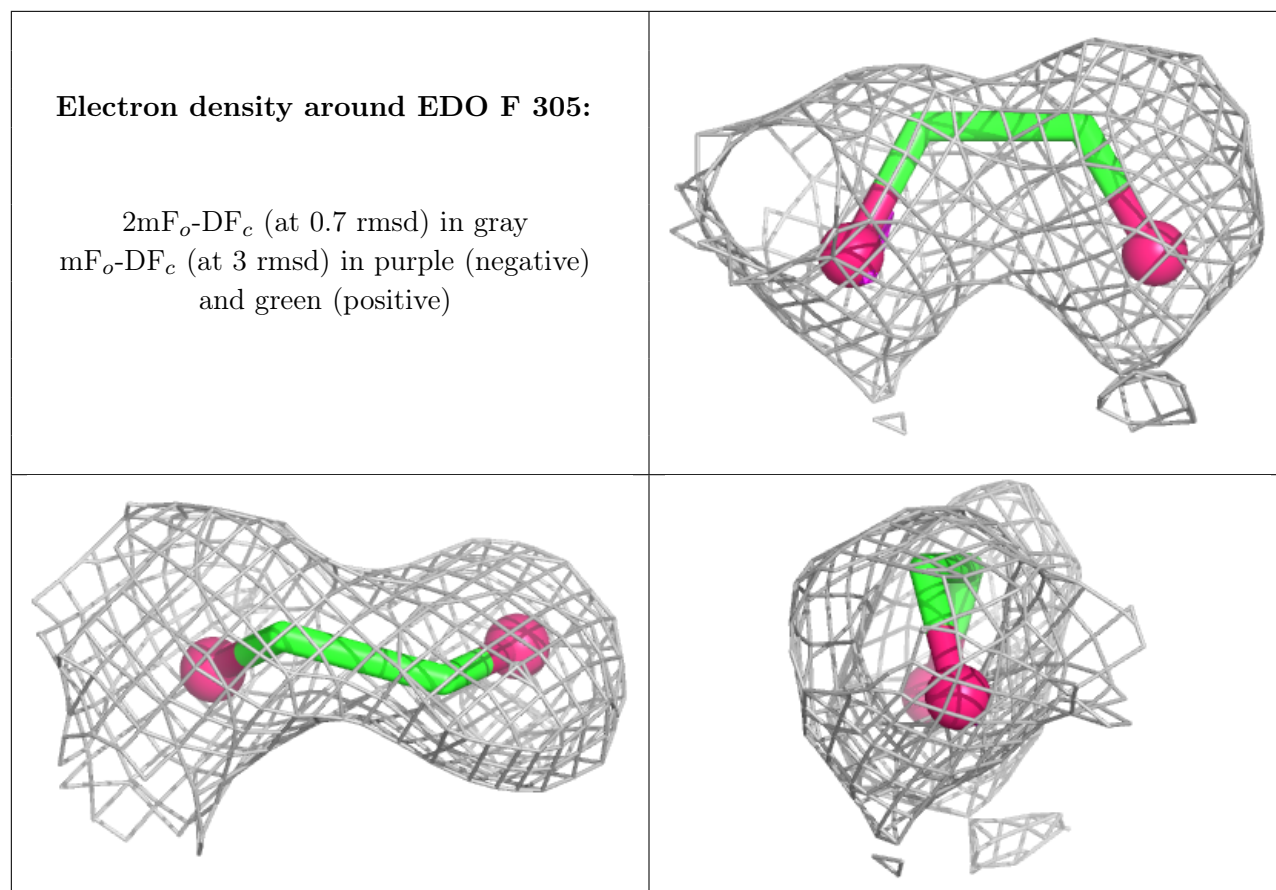
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.