wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2023 – 12:14 PM JST

PDB ID : 7YRO
Title : Crystal structure of mango fucosyltransferase 13
Authors : Okada, T.; Teramoto, T.; Ihara, H.; Ikeda, Y.; Kakuta, Y.
Deposited on : 2022-08-10
Resolution : 2.42 Å(reported)

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

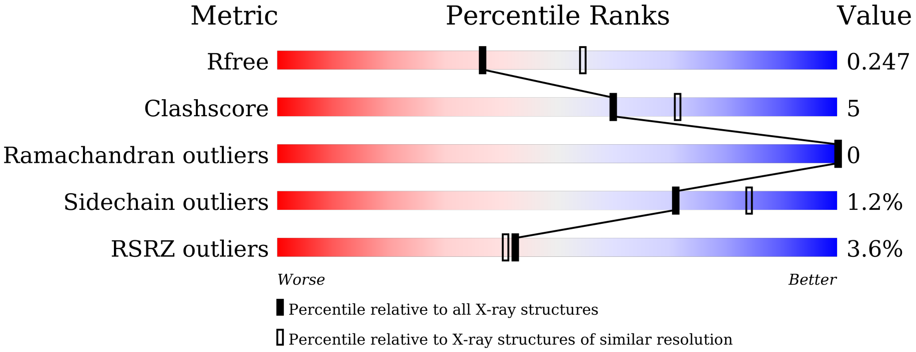
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

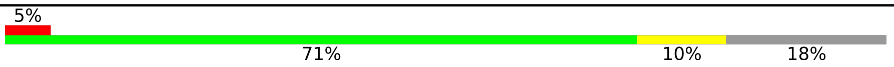
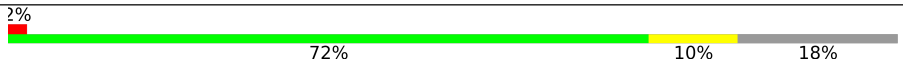
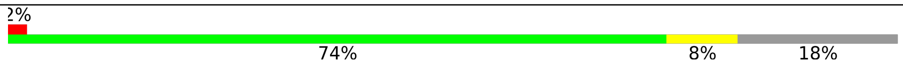
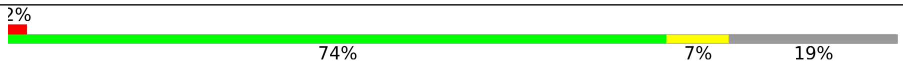
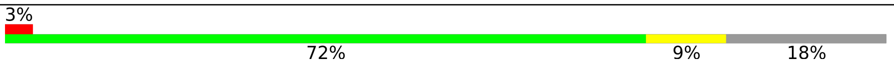
The reported resolution of this entry is 2.42 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 <=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	410	
1	B	410	
1	C	410	
1	D	410	
1	E	410	
1	F	410	

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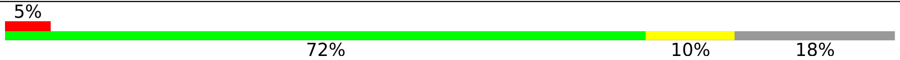
Mol	Chain	Length	Quality of chain
1	G	410	
1	H	410	

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
2	GOL	C	508	-	-	-	X

2 Entry composition

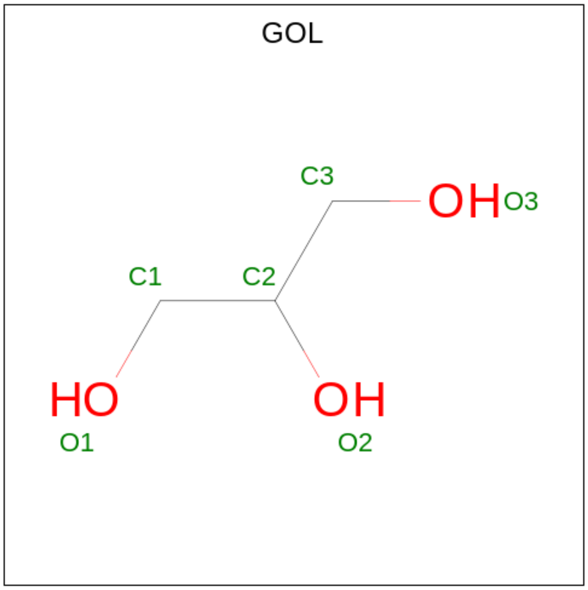
There are 7 unique types of molecules in this entry. The entry contains 21872 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	335	2629	1672	453	487	17	0	3	0
1	B	335	2656	1688	462	489	17	0	1	0
1	C	336	2638	1677	461	483	17	0	0	0
1	D	334	2638	1678	459	484	17	0	0	0
1	E	334	2656	1690	467	482	17	0	2	0
1	F	335	2648	1682	461	488	17	0	1	0
1	G	335	2639	1678	460	484	17	0	1	0
1	H	337	2605	1654	450	484	17	0	1	0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0

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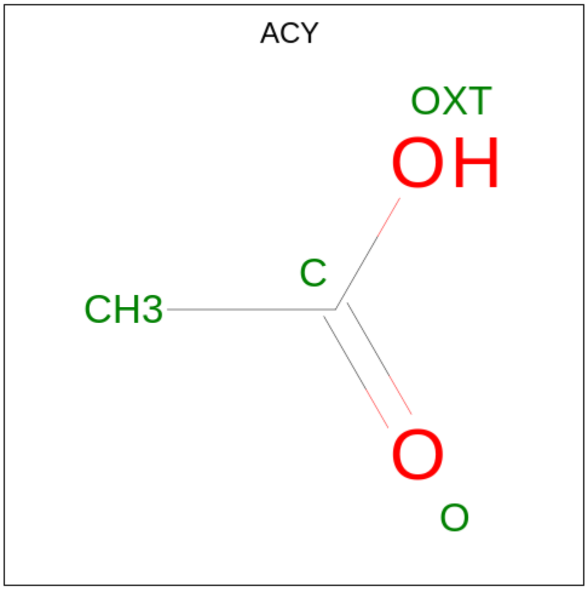
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0
2	G	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$) (labeled as "Ligand of Interest" by depositor).



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

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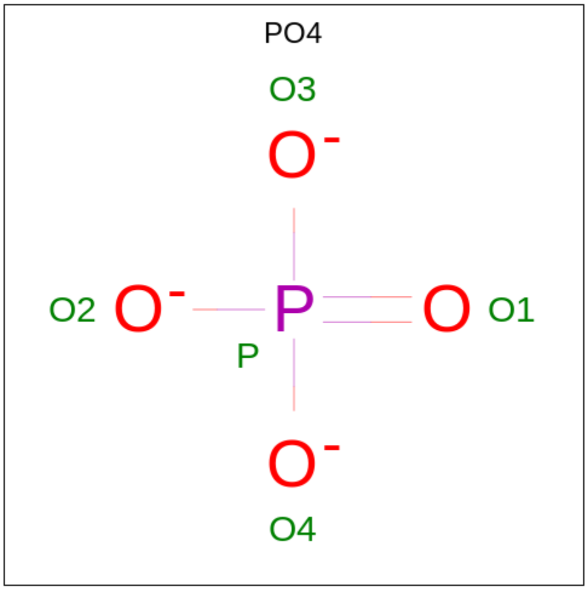
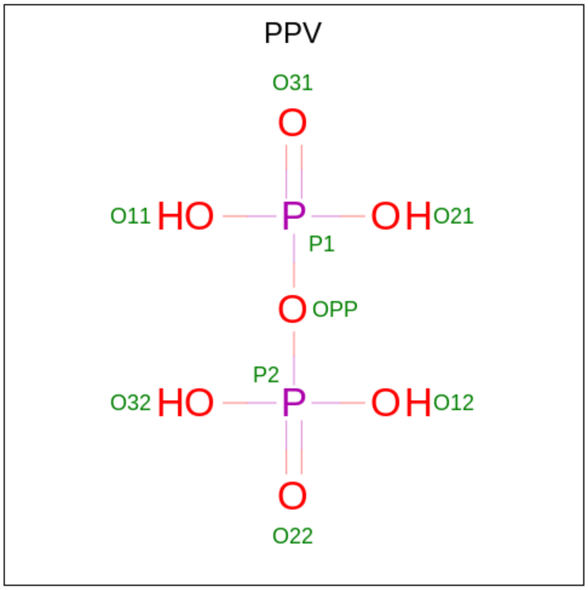
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 4 2 2	0	0
3	G	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



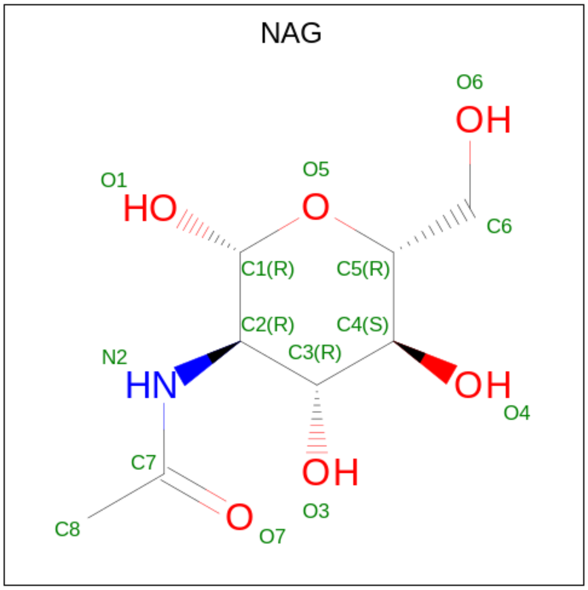
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0

- Molecule 5 is PYROPHOSPHATE (three-letter code: PPV) (formula: $H_4O_7P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O P 9 7 2	0	0
5	C	1	Total O P 9 7 2	0	0
5	D	1	Total O P 9 7 2	0	0
5	E	1	Total O P 9 7 2	0	0
5	F	1	Total O P 9 7 2	0	0
5	G	1	Total O P 9 7 2	0	0
5	H	1	Total O P 9 7 2	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	E	1	Total C N O 14 8 1 5	0	0
6	F	1	Total C N O 14 8 1 5	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	26	Total O 26 26	0	0
7	B	50	Total O 50 50	0	0
7	C	92	Total O 92 92	0	0
7	D	83	Total O 83 83	0	0
7	E	90	Total O 90 90	0	0
7	F	59	Total O 59 59	0	0
7	G	39	Total O 39 39	0	0

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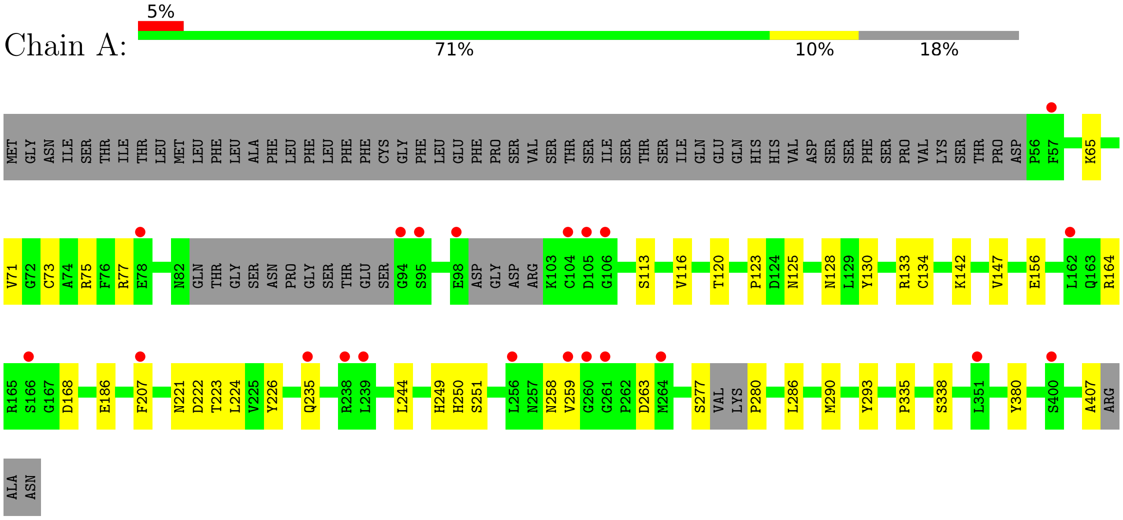
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	32	Total O 32 32	0	0

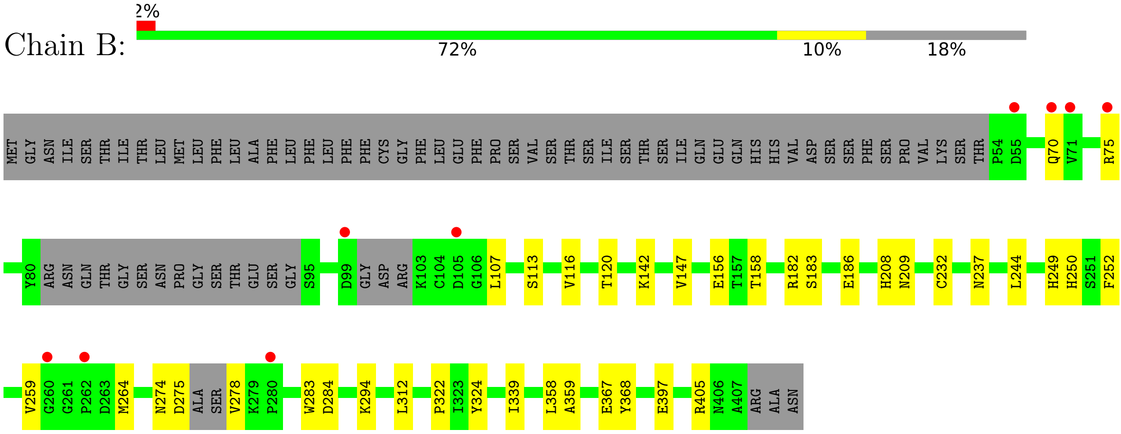
3 Residue-property plots ⓘ

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.

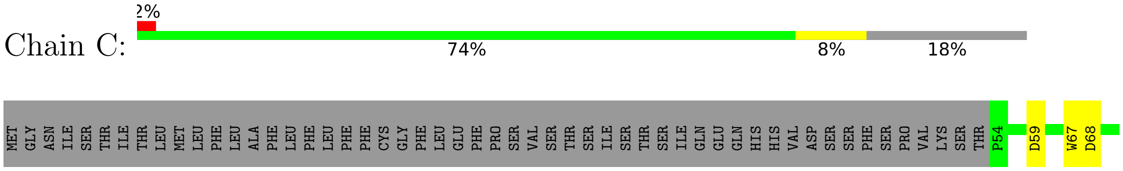
- Molecule 1: Fucosyltransferase

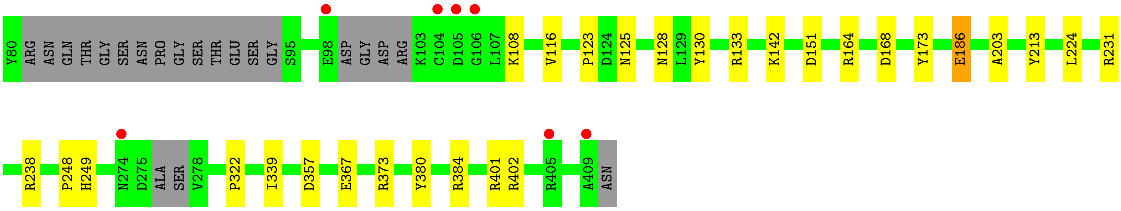


- Molecule 1: Fucosyltransferase

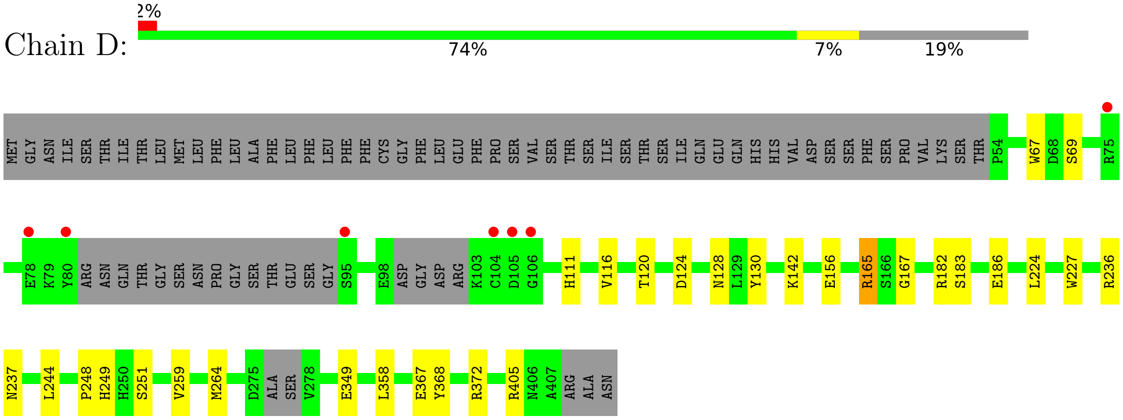


- Molecule 1: Fucosyltransferase

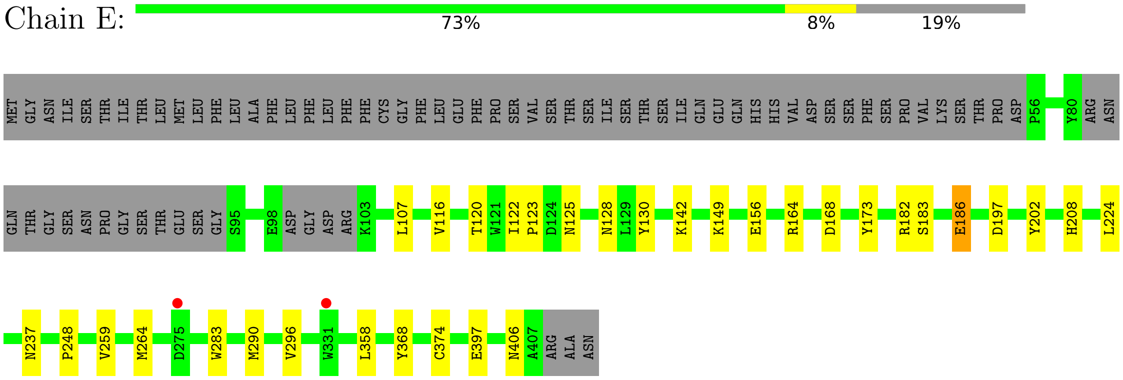




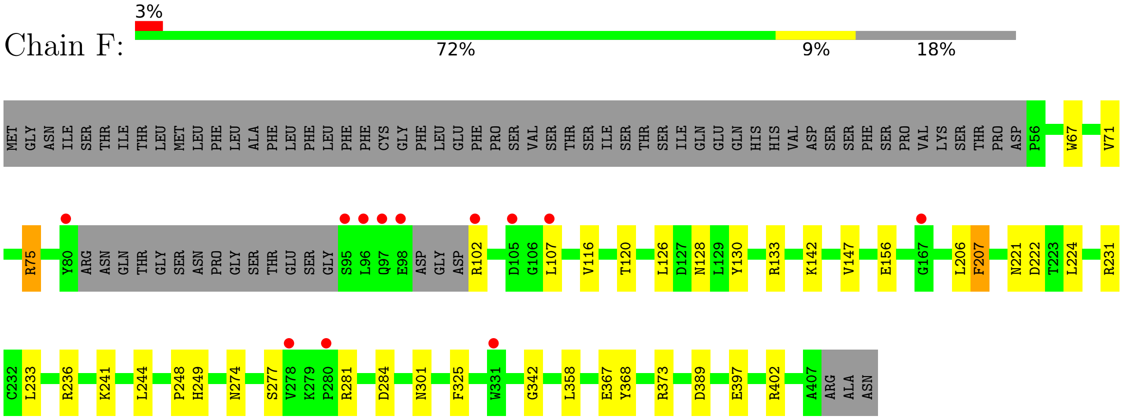
- Molecule 1: Fucosyltransferase



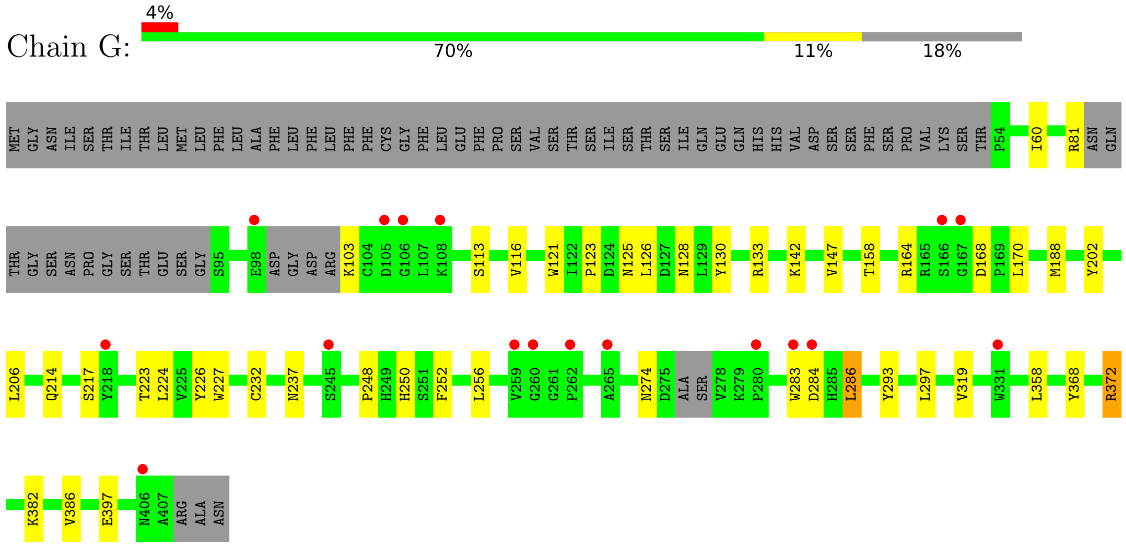
- Molecule 1: Fucosyltransferase



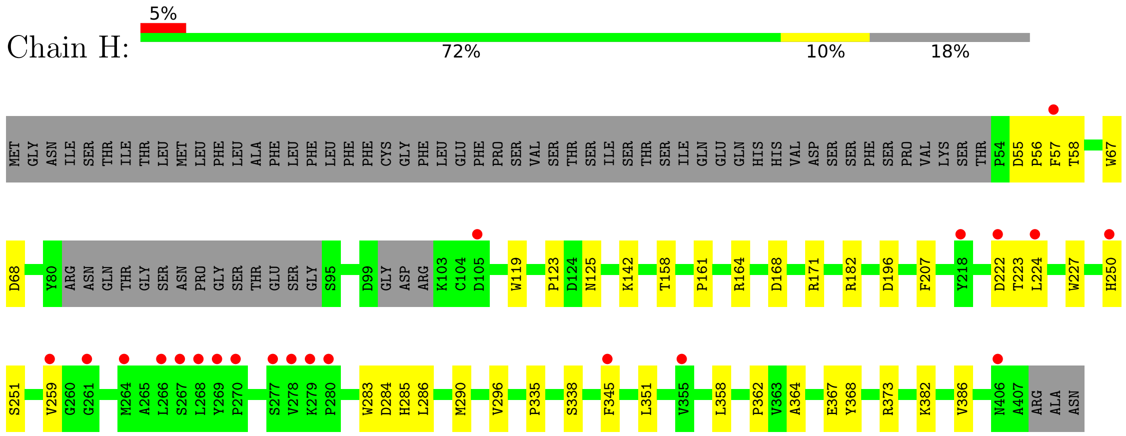
- Molecule 1: Fucosyltransferase



- Molecule 1: Fucosyltransferase



- Molecule 1: Fucosyltransferase



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.70Å 163.61Å 274.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.86 – 2.42 46.86 – 2.42	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.86-2.42) 91.7 (46.86-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.82 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.210 , 0.248 0.209 , 0.247	Depositor DCC
R_{free} test set	2000 reflections (1.34%)	wwPDB-VP
Wilson B-factor (Å^2)	43.9	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.6	EDS
L-test for twinning[2]	$< \vert L \vert > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21872	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ACY, GOL, NAG, PO4, PPV

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	0.28	0/2710	0.54	0/3691
1	B	0.27	0/2730	0.53	0/3709
1	C	0.29	0/2709	0.54	0/3683
1	D	0.29	0/2709	0.55	0/3681
1	E	0.29	0/2733	0.55	0/3711
1	F	0.27	0/2722	0.54	0/3701
1	G	0.28	0/2713	0.54	0/3689
1	H	0.28	0/2680	0.55	0/3660
All	All	0.28	0/21706	0.54	0/29525

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2629	0	2467	25	0
1	B	2656	0	2541	20	0
1	C	2638	0	2505	24	0
1	D	2638	0	2523	20	0
1	E	2656	0	2569	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2648	0	2528	28	0
1	G	2639	0	2511	24	0
1	H	2605	0	2413	28	0
2	A	6	0	8	0	0
2	B	12	0	16	0	0
2	C	36	0	48	3	0
2	D	24	0	32	2	0
2	E	18	0	24	2	0
2	F	18	0	24	1	0
2	G	6	0	8	1	0
2	H	6	0	8	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
3	C	4	0	3	0	0
3	E	4	0	3	1	0
3	F	4	0	3	1	0
3	G	4	0	3	1	0
3	H	4	0	3	1	0
4	A	5	0	0	0	0
5	B	9	0	0	0	0
5	C	9	0	0	1	0
5	D	9	0	0	1	0
5	E	9	0	0	0	0
5	F	9	0	0	2	0
5	G	9	0	0	0	0
5	H	9	0	0	0	0
6	B	14	0	13	0	0
6	C	14	0	13	1	0
6	D	14	0	13	0	0
6	E	14	0	13	0	0
6	F	14	0	13	0	0
7	A	26	0	0	0	0
7	B	50	0	0	0	0
7	C	92	0	0	3	0
7	D	83	0	0	3	0
7	E	90	0	0	2	0
7	F	59	0	0	1	0
7	G	39	0	0	0	0
7	H	32	0	0	1	0
All	All	21872	0	20311	190	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 5.

The worst 5 of 190 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:173:TYR:HB3	1:E:186:GLU:HG2	1.61	0.81
1:E:182[B]:ARG:NH2	2:E:505:GOL:O2	2.20	0.74
1:C:67:TRP:HE1	1:C:367:GLU:HG2	1.53	0.73
1:D:111:HIS:HD2	2:D:503:GOL:H12	1.54	0.70
1:B:107:LEU:HD11	1:B:397:GLU:HG3	1.74	0.70

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	330/410 (80%)	325 (98%)	5 (2%)	0	100	100
1	B	328/410 (80%)	319 (97%)	9 (3%)	0	100	100
1	C	328/410 (80%)	318 (97%)	10 (3%)	0	100	100
1	D	326/410 (80%)	315 (97%)	11 (3%)	0	100	100
1	E	330/410 (80%)	321 (97%)	9 (3%)	0	100	100
1	F	330/410 (80%)	320 (97%)	10 (3%)	0	100	100
1	G	328/410 (80%)	318 (97%)	10 (3%)	0	100	100
1	H	332/410 (81%)	320 (96%)	12 (4%)	0	100	100
All	All	2632/3280 (80%)	2556 (97%)	76 (3%)	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	280/360 (78%)	277 (99%)	3 (1%)	73	86
1	B	288/360 (80%)	285 (99%)	3 (1%)	76	87
1	C	281/360 (78%)	276 (98%)	5 (2%)	59	75
1	D	285/360 (79%)	282 (99%)	3 (1%)	73	86
1	E	288/360 (80%)	286 (99%)	2 (1%)	84	92
1	F	286/360 (79%)	283 (99%)	3 (1%)	76	87
1	G	283/360 (79%)	277 (98%)	6 (2%)	53	71
1	H	273/360 (76%)	272 (100%)	1 (0%)	91	96
All	All	2264/2880 (79%)	2238 (99%)	26 (1%)	71	86

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	186	GLU
1	F	207	PHE
1	G	372	ARG
1	F	75	ARG
1	F	241	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	HIS
1	B	163	GLN
1	B	209	ASN
1	D	70	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

41 ligands 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	$\#\|Z\| > 2$
2	GOL	C	509	-	5,5,5	0.96	0	5,5,5	0.92	0
2	GOL	B	503	-	5,5,5	0.86	0	5,5,5	1.05	0
6	NAG	E	502	1	14,14,15	0.22	0	17,19,21	0.51	0
2	GOL	E	503	-	5,5,5	0.86	0	5,5,5	1.05	0
2	GOL	F	503	-	5,5,5	0.85	0	5,5,5	1.05	0
5	PPV	H	501	-	6,8,8	0.71	0	13,13,13	1.08	1 (7%)
2	GOL	C	504	-	5,5,5	0.92	0	5,5,5	0.95	0
2	GOL	D	506	-	5,5,5	0.96	0	5,5,5	0.94	0
2	GOL	C	507	-	5,5,5	0.99	0	5,5,5	0.96	0
3	ACY	F	506	-	3,3,3	0.96	0	3,3,3	0.80	0
2	GOL	H	502	-	5,5,5	0.87	0	5,5,5	0.99	0
3	ACY	B	505	-	3,3,3	0.92	0	3,3,3	0.86	0
2	GOL	D	503	-	5,5,5	0.88	0	5,5,5	1.01	0
5	PPV	C	501	-	6,8,8	0.71	0	13,13,13	1.08	0
2	GOL	F	504	-	5,5,5	0.92	0	5,5,5	0.99	0
2	GOL	G	502	-	5,5,5	0.91	0	5,5,5	0.99	0
3	ACY	H	503	-	3,3,3	0.92	0	3,3,3	0.84	0
2	GOL	D	504	-	5,5,5	0.91	0	5,5,5	1.00	0
6	NAG	C	502	1	14,14,15	0.83	1 (7%)	17,19,21	1.46	2 (11%)
2	GOL	A	601	-	5,5,5	0.90	0	5,5,5	0.97	0
2	GOL	C	503	-	5,5,5	0.95	0	5,5,5	0.83	0
3	ACY	A	602	-	3,3,3	0.96	0	3,3,3	0.79	0
5	PPV	F	501	-	6,8,8	0.68	0	13,13,13	1.09	1 (7%)
5	PPV	D	501	-	6,8,8	0.70	0	13,13,13	1.03	1 (7%)
2	GOL	C	508	-	5,5,5	0.82	0	5,5,5	1.02	0
3	ACY	E	504	-	3,3,3	0.98	0	3,3,3	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	GOL	E	505	-	5,5,5	0.97	0	5,5,5	0.95	0
3	ACY	G	503	-	3,3,3	0.97	0	3,3,3	0.68	0
2	GOL	F	502	-	5,5,5	0.88	0	5,5,5	0.99	0
5	PPV	G	501	-	6,8,8	0.70	0	13,13,13	1.01	0
2	GOL	E	506	-	5,5,5	0.92	0	5,5,5	0.99	0
6	NAG	D	502	1	14,14,15	0.25	0	17,19,21	0.39	0
6	NAG	F	505	1	14,14,15	0.64	1 (7%)	17,19,21	0.70	0
2	GOL	B	504	-	5,5,5	0.90	0	5,5,5	0.97	0
5	PPV	B	501	-	6,8,8	0.69	0	13,13,13	1.08	0
4	PO4	A	603	-	4,4,4	0.88	0	6,6,6	0.48	0
5	PPV	E	501	-	6,8,8	0.68	0	13,13,13	1.11	1 (7%)
6	NAG	B	502	1	14,14,15	0.28	0	17,19,21	0.35	0
2	GOL	C	505	-	5,5,5	0.84	0	5,5,5	1.03	0
3	ACY	C	506	-	3,3,3	0.99	0	3,3,3	0.75	0
2	GOL	D	505	-	5,5,5	0.93	0	5,5,5	0.89	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	509	-	-	4/4/4/4	-
2	GOL	B	503	-	-	1/4/4/4	-
6	NAG	E	502	1	-	4/6/23/26	0/1/1/1
2	GOL	E	503	-	-	2/4/4/4	-
2	GOL	F	503	-	-	0/4/4/4	-
5	PPV	H	501	-	-	2/6/6/6	-
2	GOL	C	504	-	-	0/4/4/4	-
2	GOL	D	506	-	-	0/4/4/4	-
2	GOL	C	507	-	-	2/4/4/4	-
2	GOL	H	502	-	-	2/4/4/4	-
2	GOL	D	503	-	-	0/4/4/4	-
5	PPV	C	501	-	-	1/6/6/6	-
2	GOL	F	504	-	-	0/4/4/4	-
2	GOL	G	502	-	-	3/4/4/4	-
2	GOL	D	504	-	-	2/4/4/4	-
6	NAG	C	502	1	-	5/6/23/26	0/1/1/1
2	GOL	A	601	-	-	2/4/4/4	-
2	GOL	C	503	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PPV	F	501	-	-	2/6/6/6	-
5	PPV	D	501	-	-	3/6/6/6	-
2	GOL	C	508	-	-	2/4/4/4	-
2	GOL	E	505	-	-	2/4/4/4	-
2	GOL	F	502	-	-	4/4/4/4	-
5	PPV	G	501	-	-	2/6/6/6	-
2	GOL	E	506	-	-	3/4/4/4	-
6	NAG	D	502	1	-	0/6/23/26	0/1/1/1
6	NAG	F	505	1	-	4/6/23/26	0/1/1/1
2	GOL	B	504	-	-	2/4/4/4	-
5	PPV	B	501	-	-	0/6/6/6	-
5	PPV	E	501	-	-	2/6/6/6	-
6	NAG	B	502	1	-	0/6/23/26	0/1/1/1
2	GOL	C	505	-	-	0/4/4/4	-
2	GOL	D	505	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	502	NAG	C1-C2	2.55	1.56	1.52
6	F	505	NAG	O5-C1	-2.19	1.40	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	502	NAG	C2-N2-C7	4.07	128.69	122.90
6	C	502	NAG	C1-O5-C5	3.54	116.99	112.19
5	H	501	PPV	P2-OPP-P1	-2.54	124.10	132.83
5	E	501	PPV	P2-OPP-P1	-2.42	124.52	132.83
5	F	501	PPV	P2-OPP-P1	-2.25	125.10	132.83

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	503	GOL	C1-C2-C3-O3
2	C	507	GOL	C1-C2-C3-O3
2	C	508	GOL	C1-C2-C3-O3
2	C	509	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	C	509	GOL	O1-C1-C2-C3

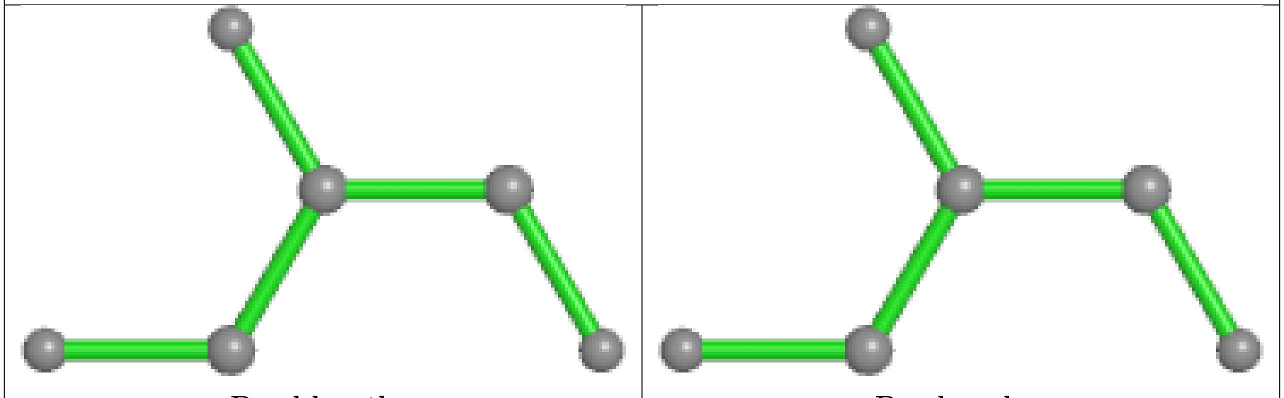
There are no ring outliers.

14 monomers are involved in 18 short contacts:

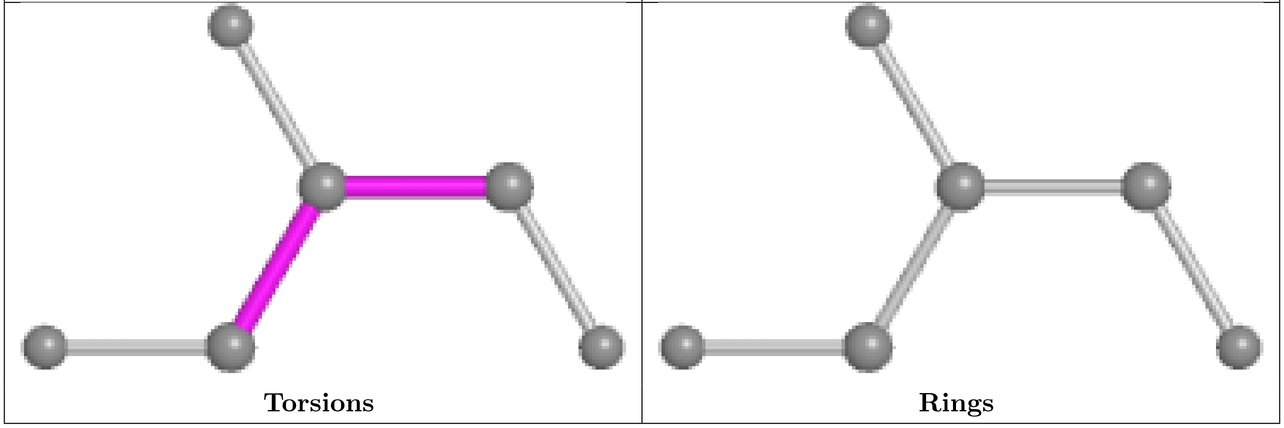
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	509	GOL	2	0
3	F	506	ACY	1	0
2	D	503	GOL	2	0
5	C	501	PPV	1	0
2	G	502	GOL	1	0
3	H	503	ACY	1	0
6	C	502	NAG	1	0
2	C	503	GOL	1	0
5	F	501	PPV	2	0
5	D	501	PPV	1	0
3	E	504	ACY	1	0
2	E	505	GOL	2	0
3	G	503	ACY	1	0
2	F	502	GOL	1	0

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 then 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 GOL C 509

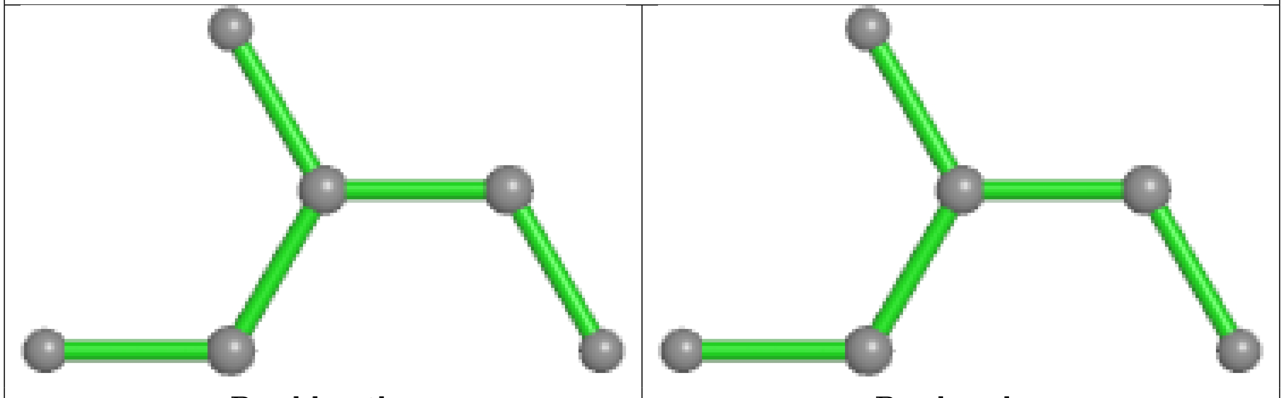


Bond lengths Bond angles

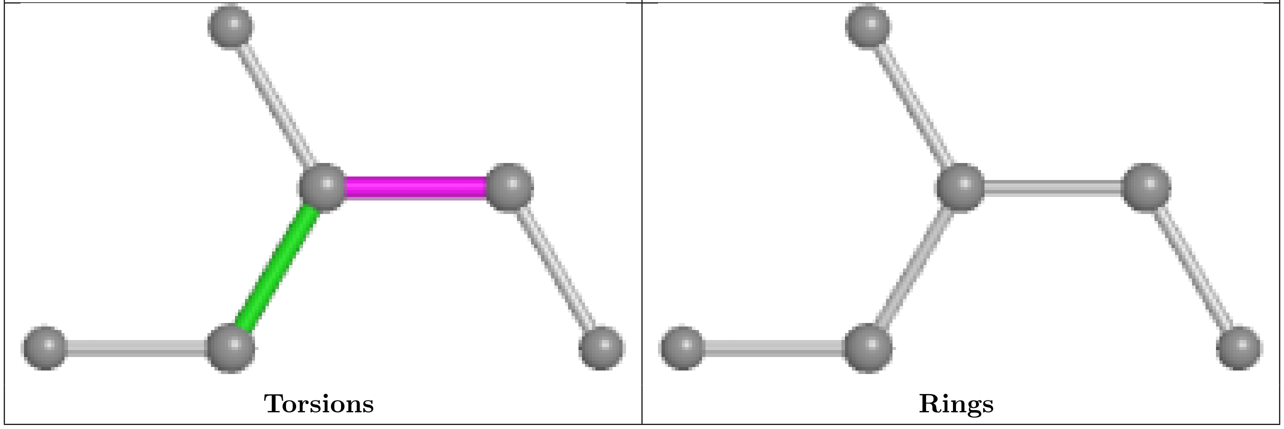


Torsions Rings

Ligand GOL B 503

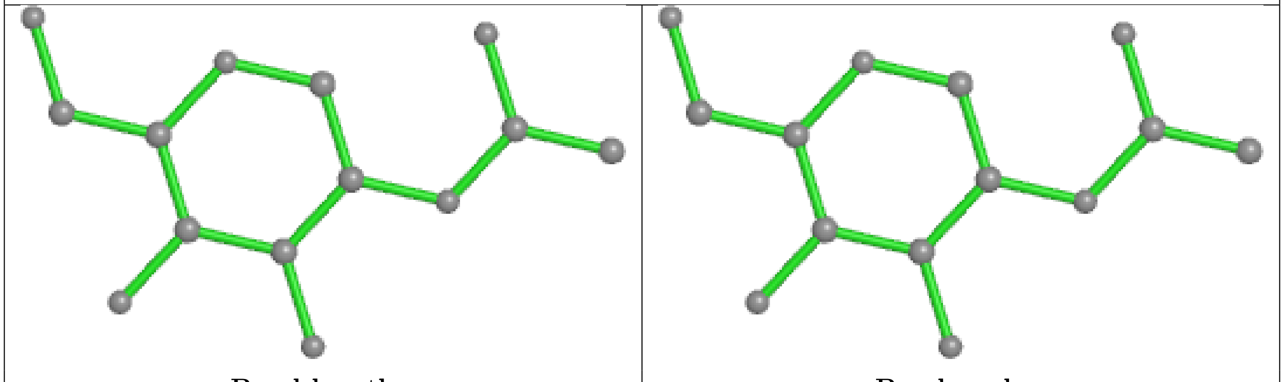


Bond lengths Bond angles



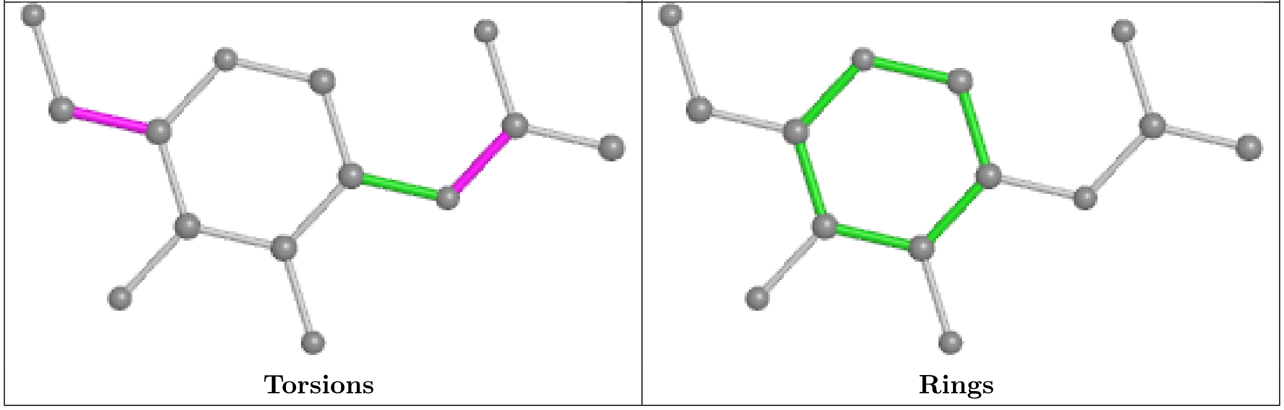
Torsions Rings

Ligand NAG E 502



Bond lengths

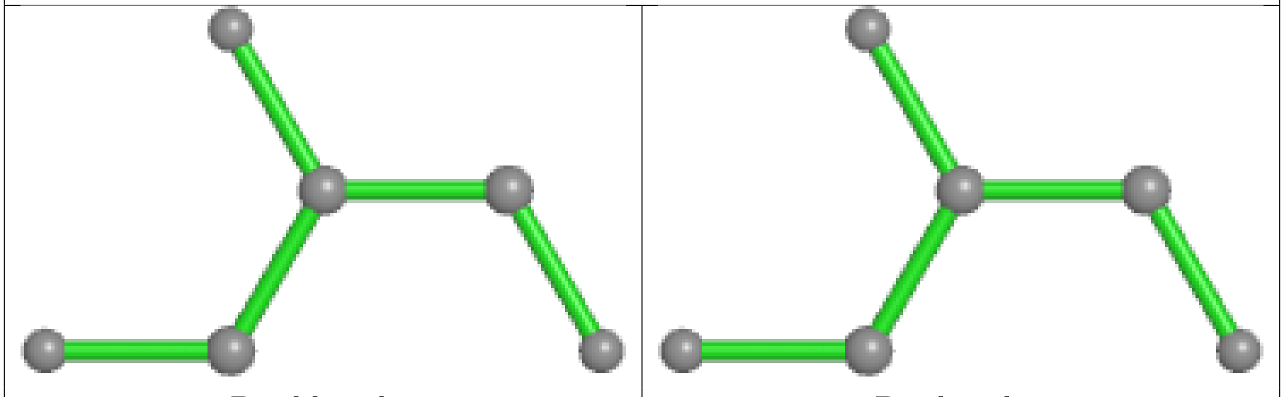
Bond angles



Torsions

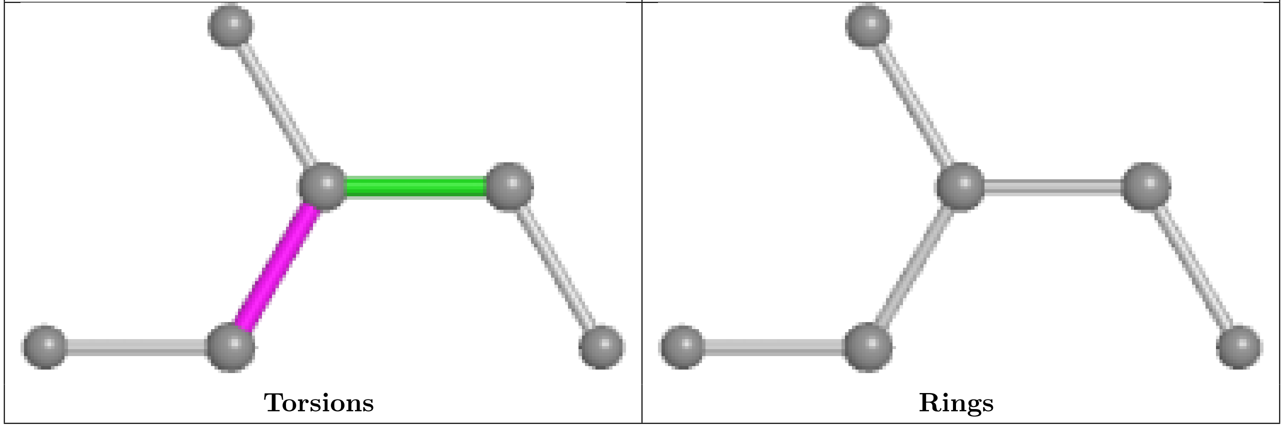
Rings

Ligand GOL E 503



Bond lengths

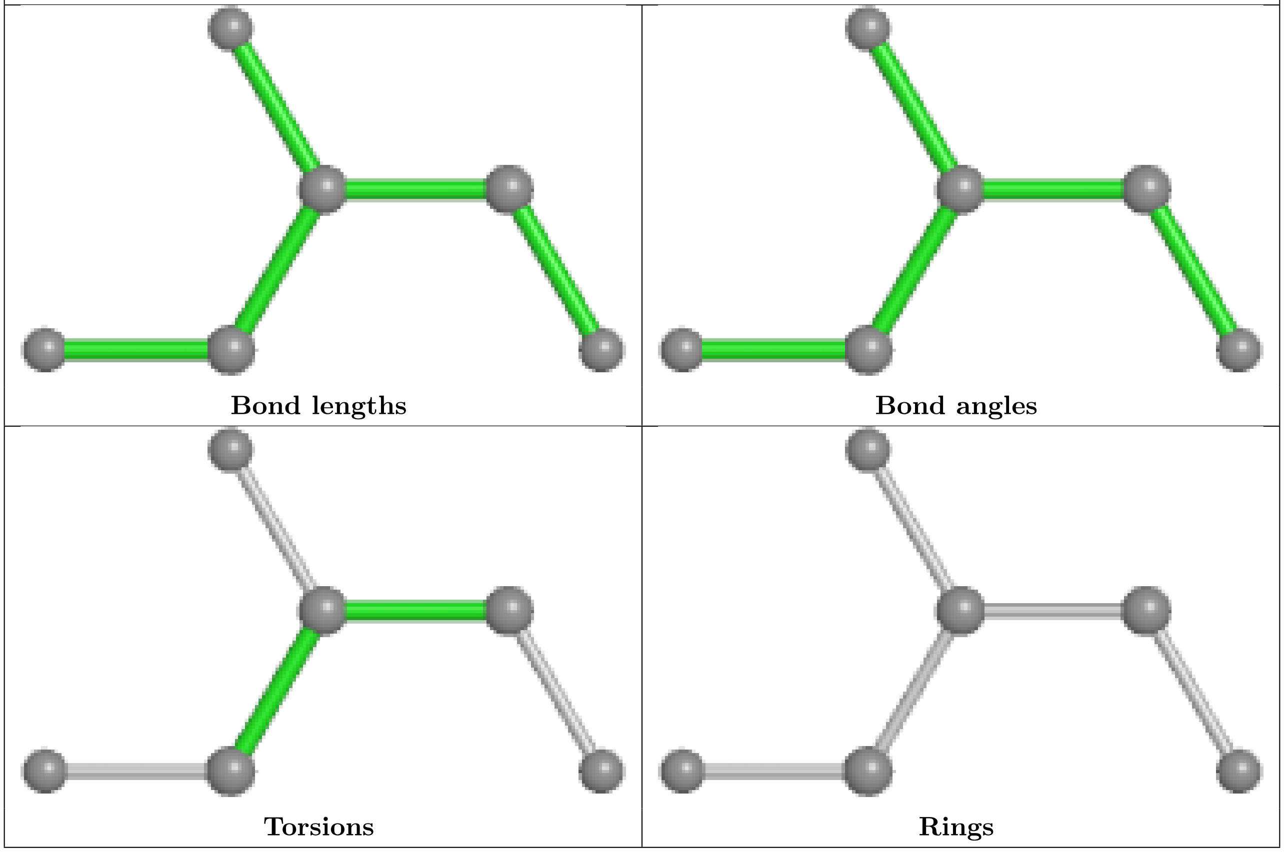
Bond angles



Torsions

Rings

Ligand GOL F 503



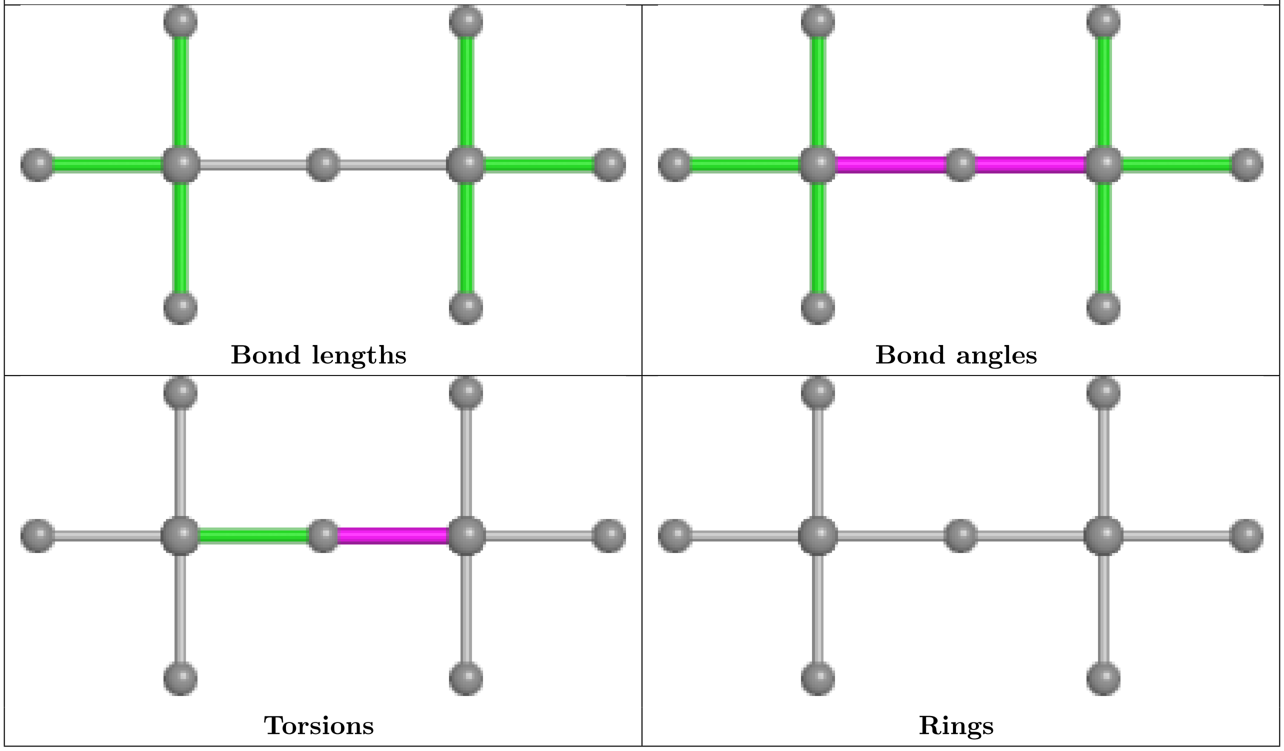
Bond lengths

Bond angles

Torsions

Rings

Ligand PPV H 501



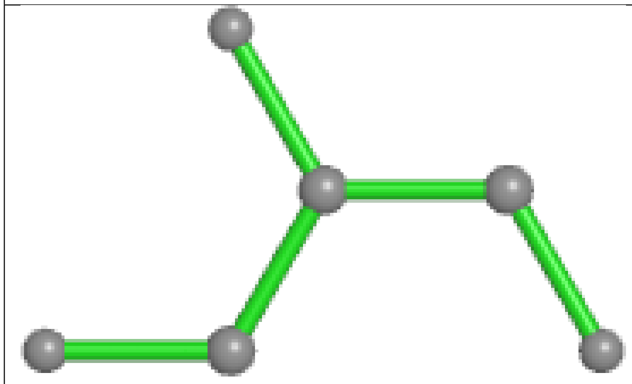
Bond lengths

Bond angles

Torsions

Rings

Ligand GOL C 504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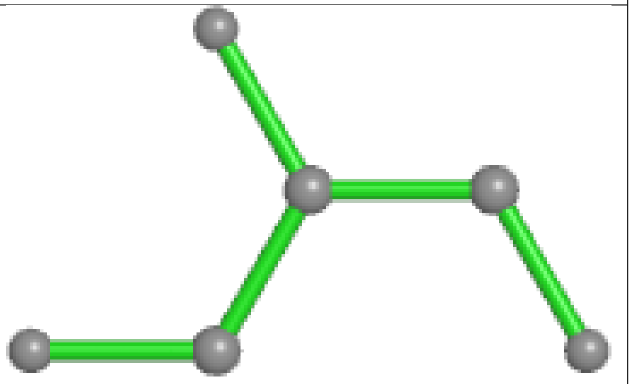
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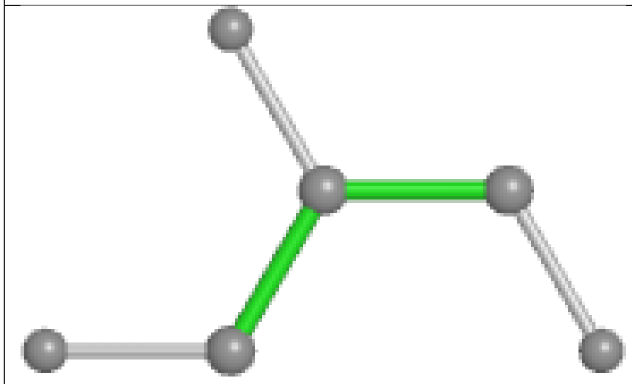
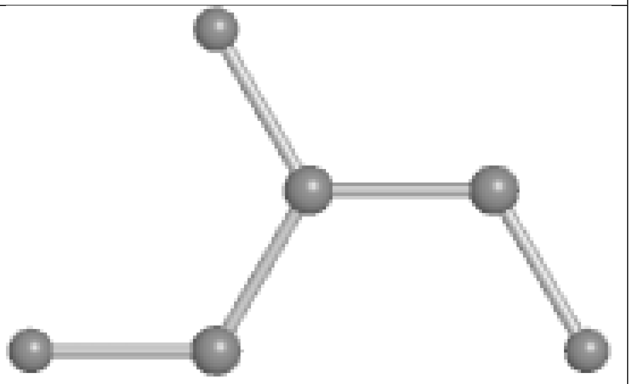
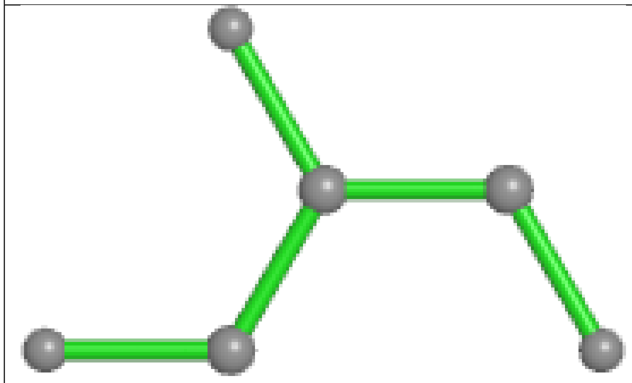
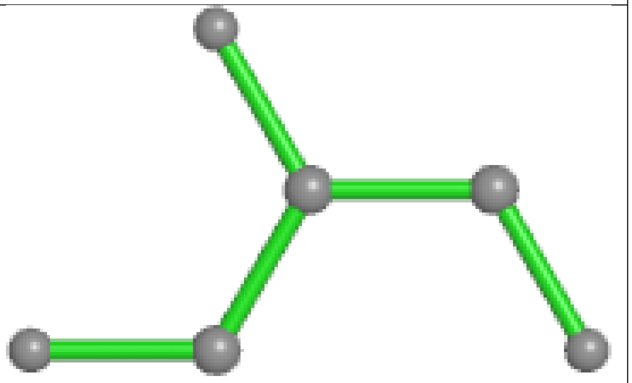
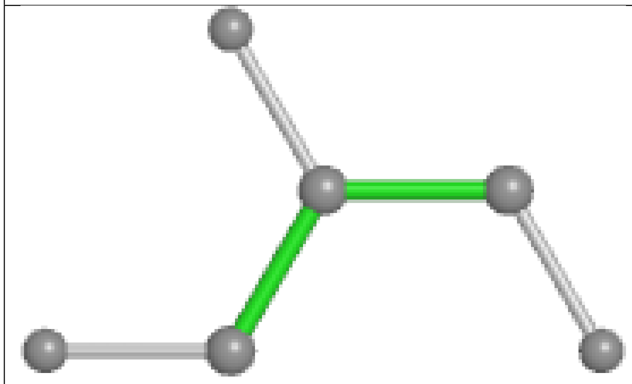

Torsions

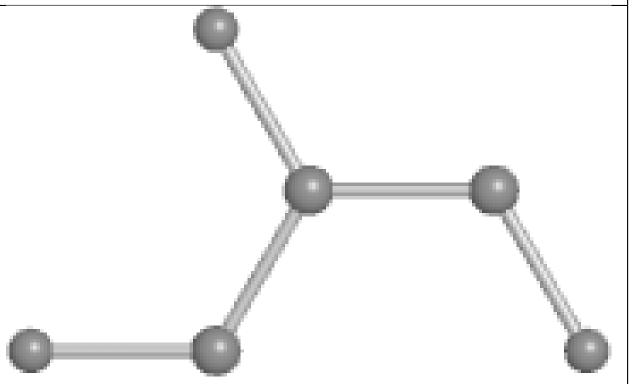

Rings

Ligand GOL D 506

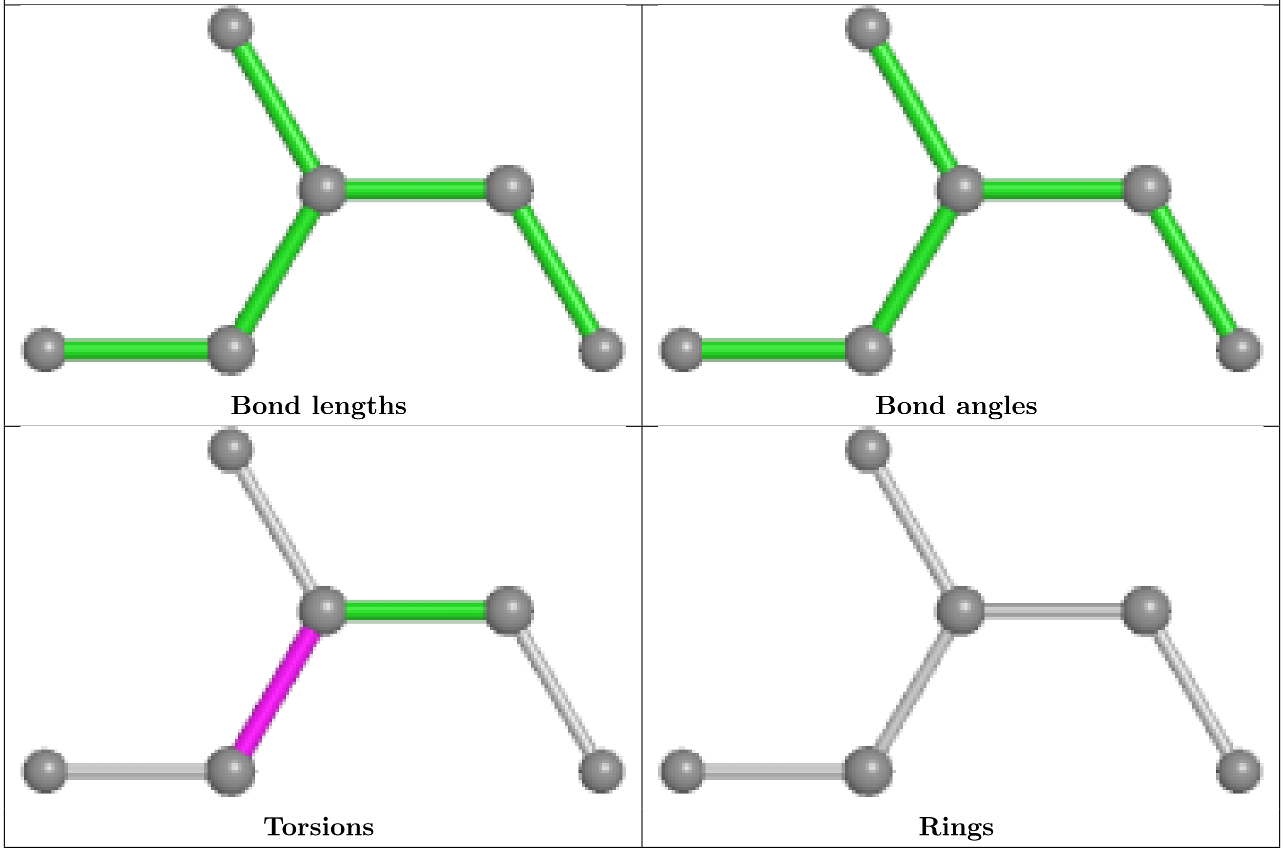

Bond lengths


Bond angles


Torsions


Rings

Ligand GOL C 507



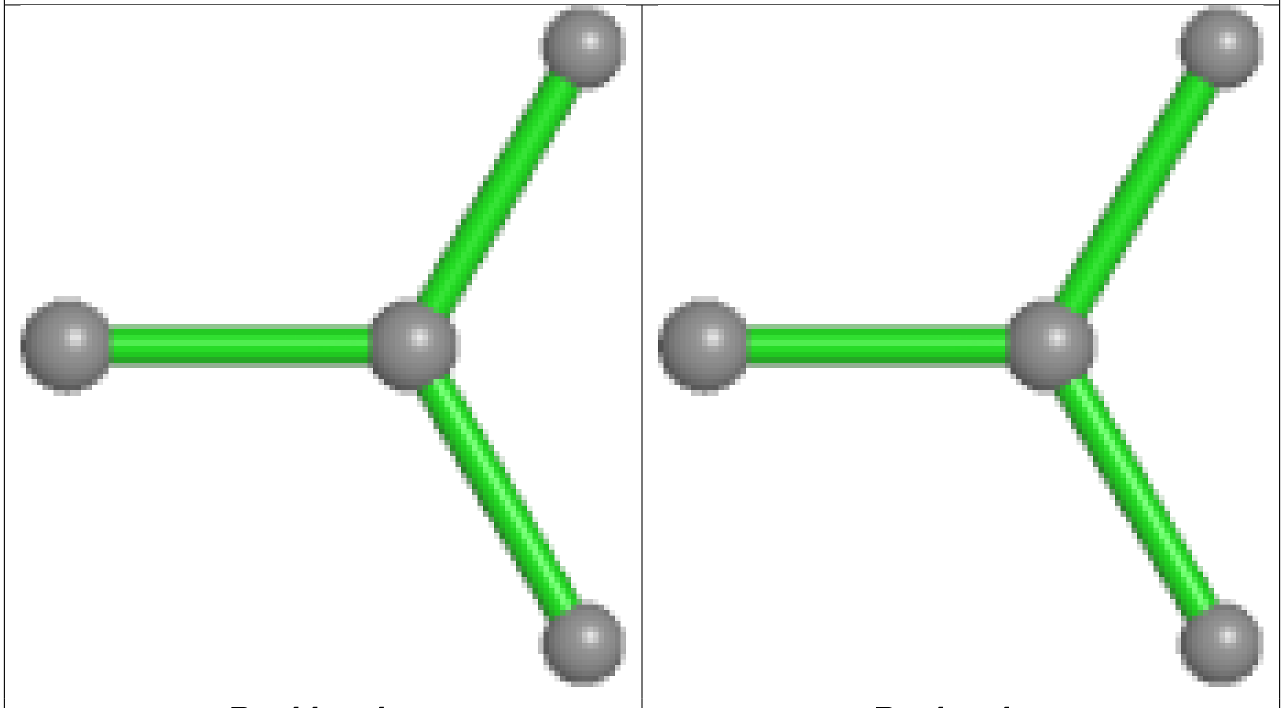
Bond lengths

Bond angles

Torsions

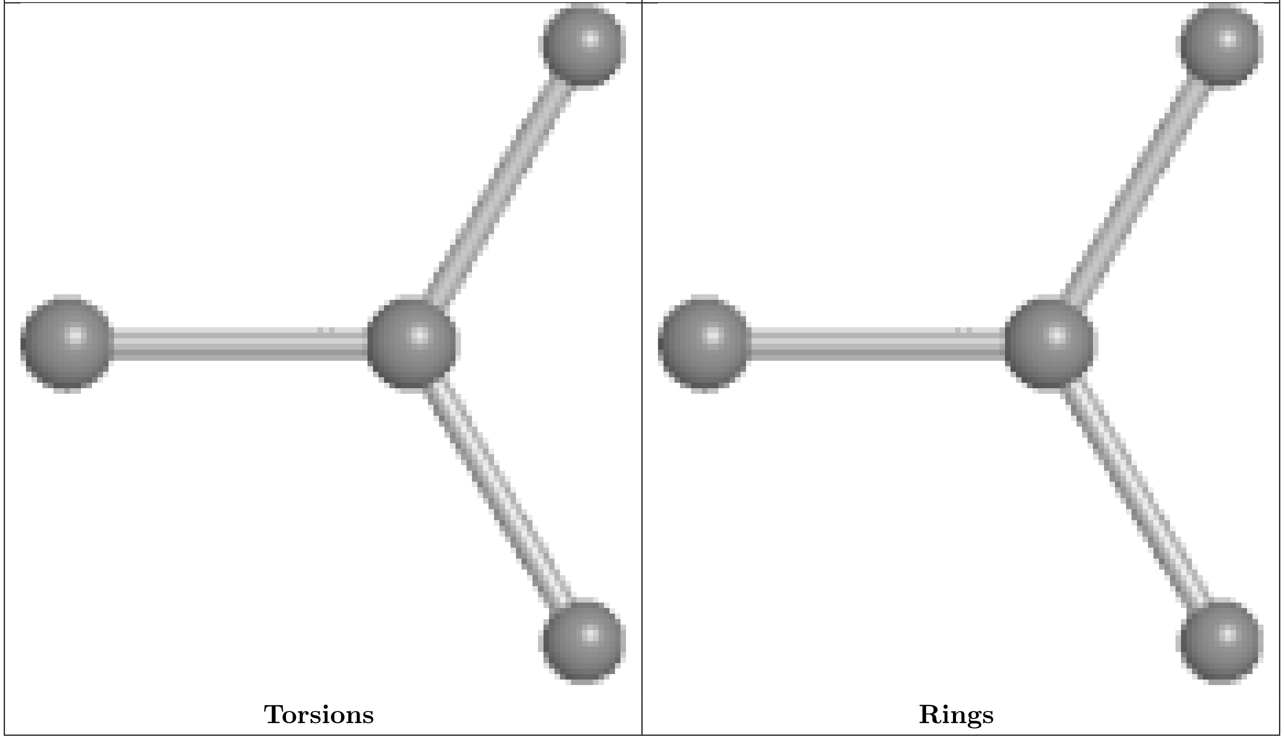
Rings

Ligand ACY F 506



Bond lengths

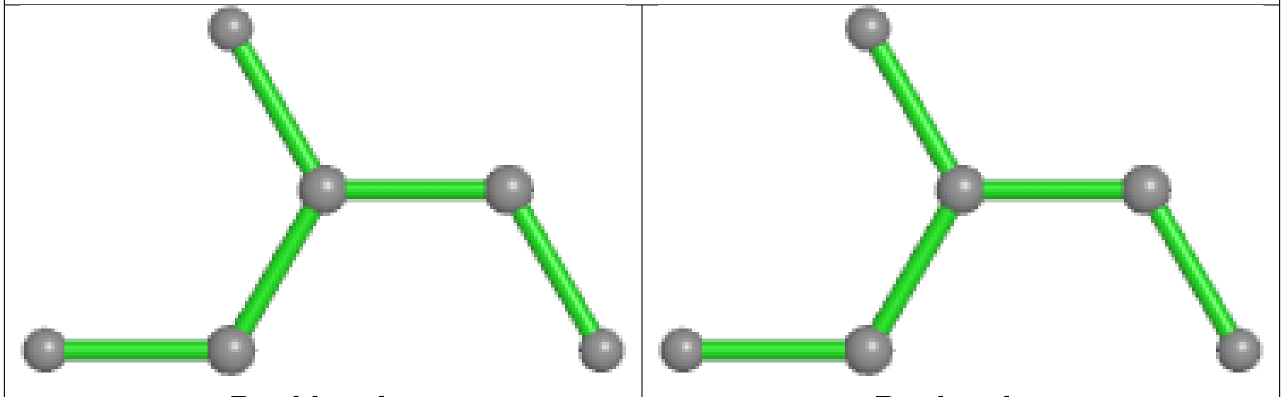
Bond angles



Torsions

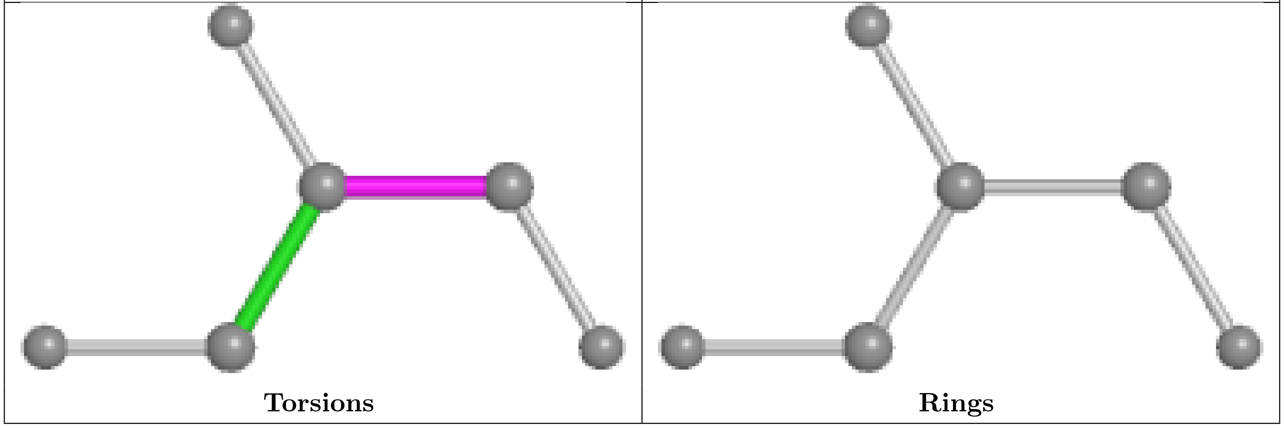
Rings

Ligand GOL H 502



Bond lengths

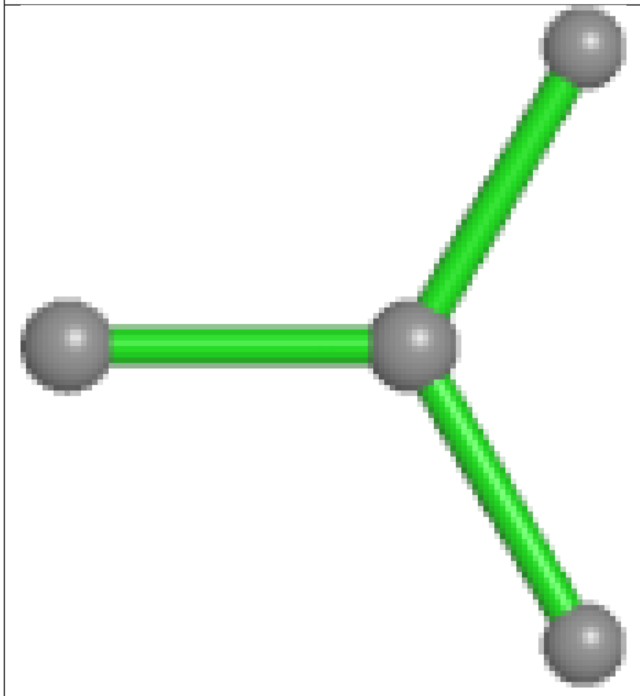
Bond angles



Torsions

Rings

Ligand ACY B 505



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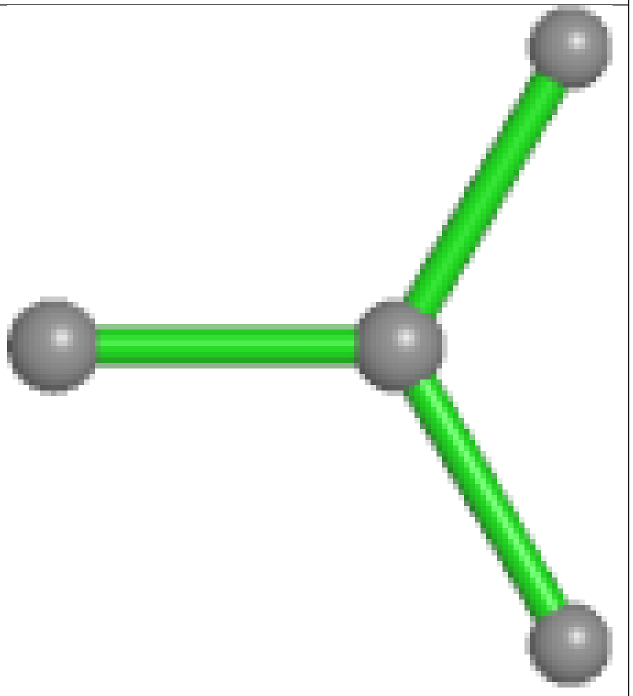

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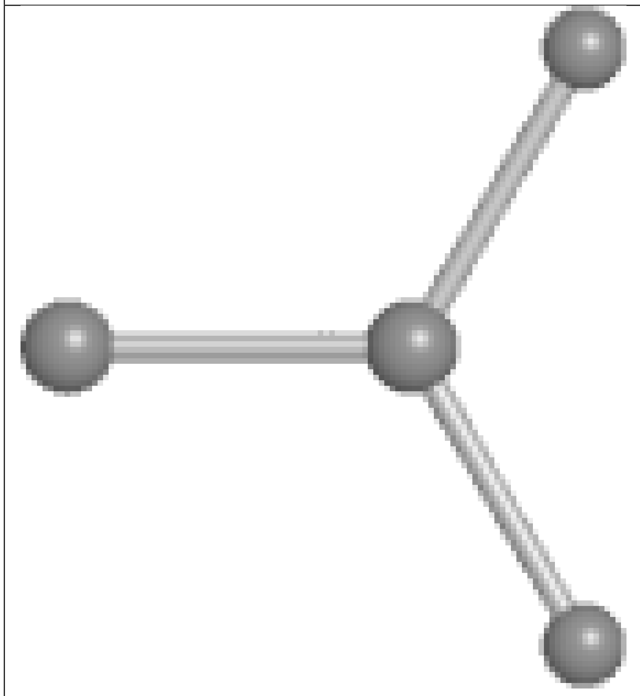
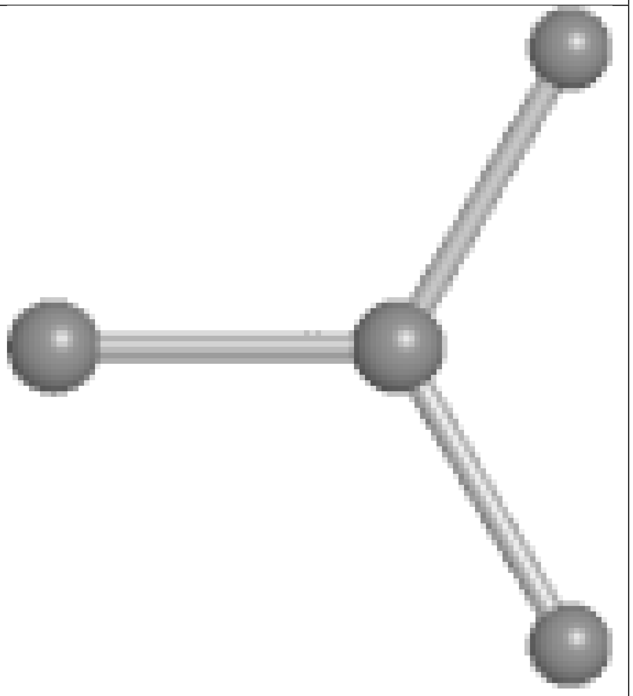
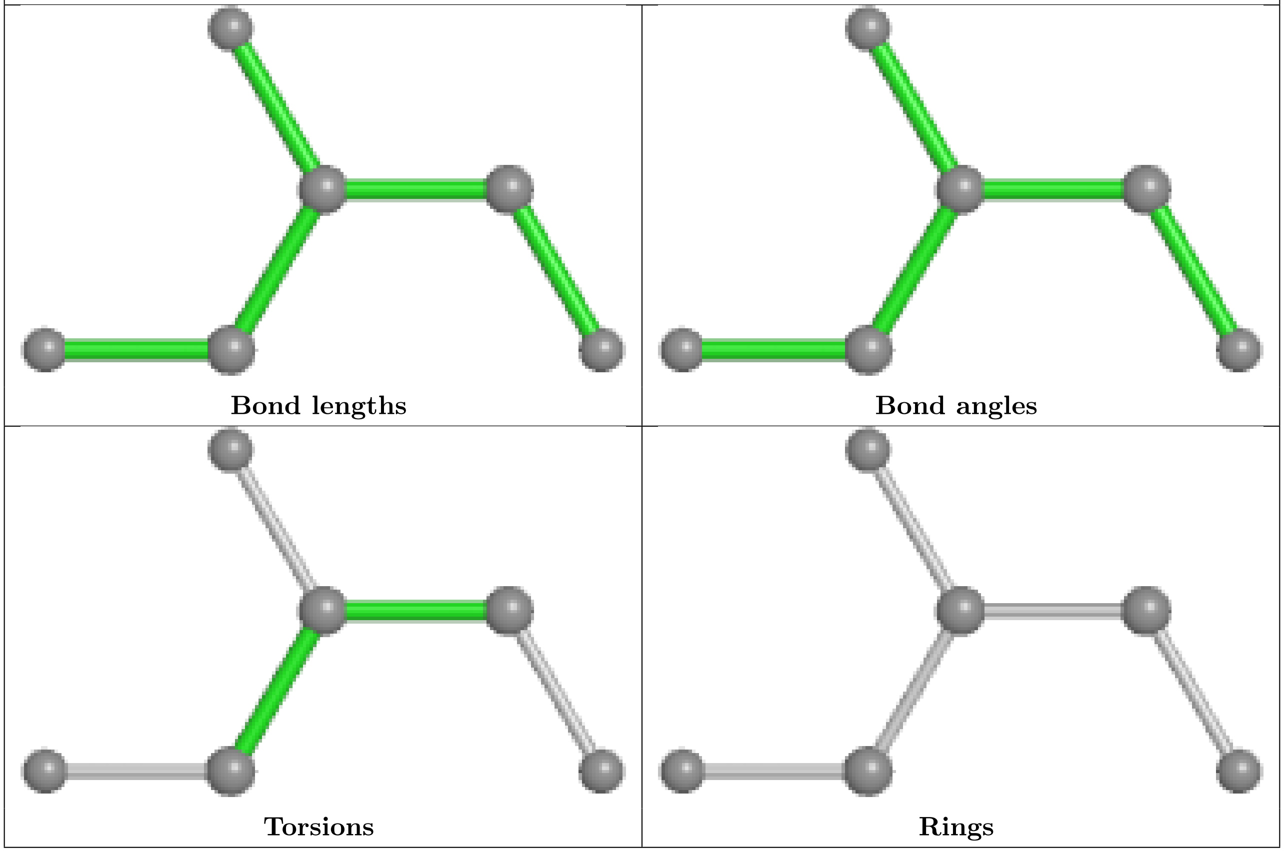


Torsions



Rings

Ligand GOL D 503



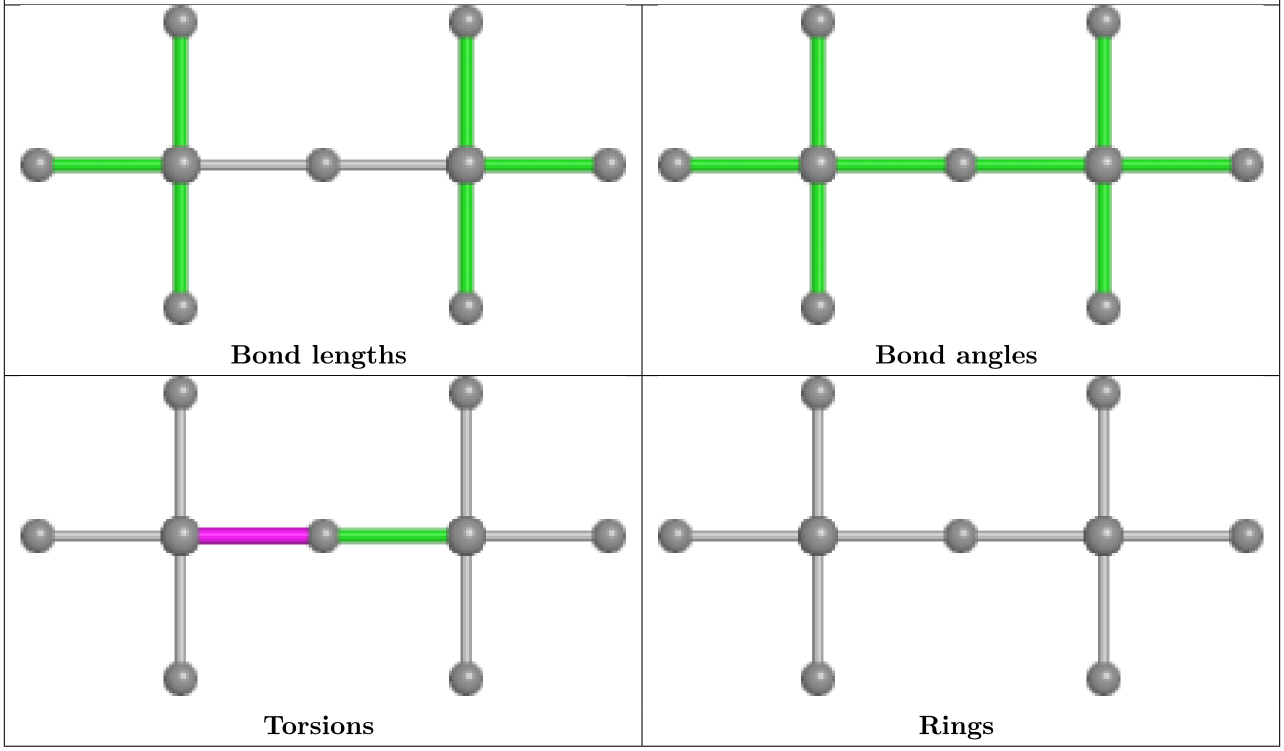
Bond lengths

Bond angles

Torsions

Rings

Ligand PPV C 501



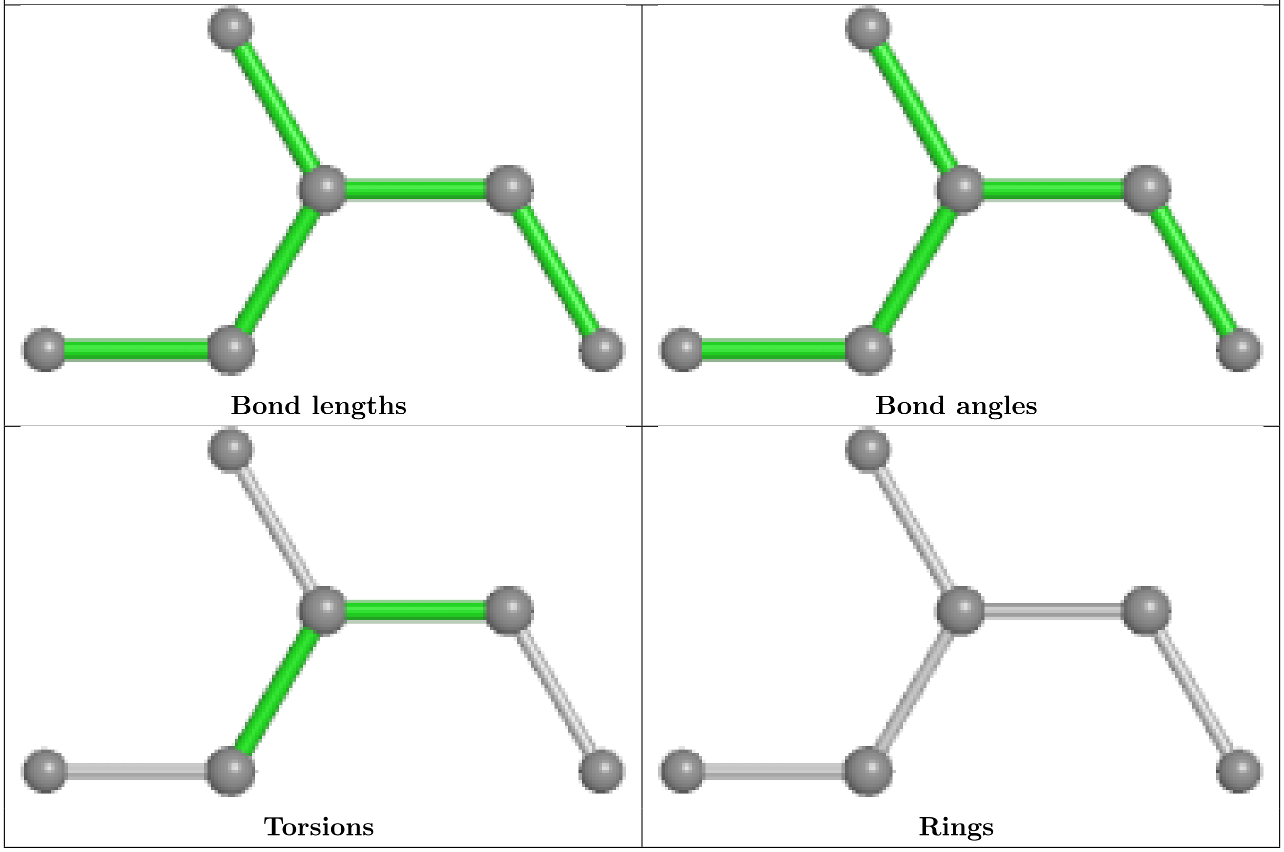
Bond lengths

Bond angles

Torsions

Rings

Ligand GOL F 504



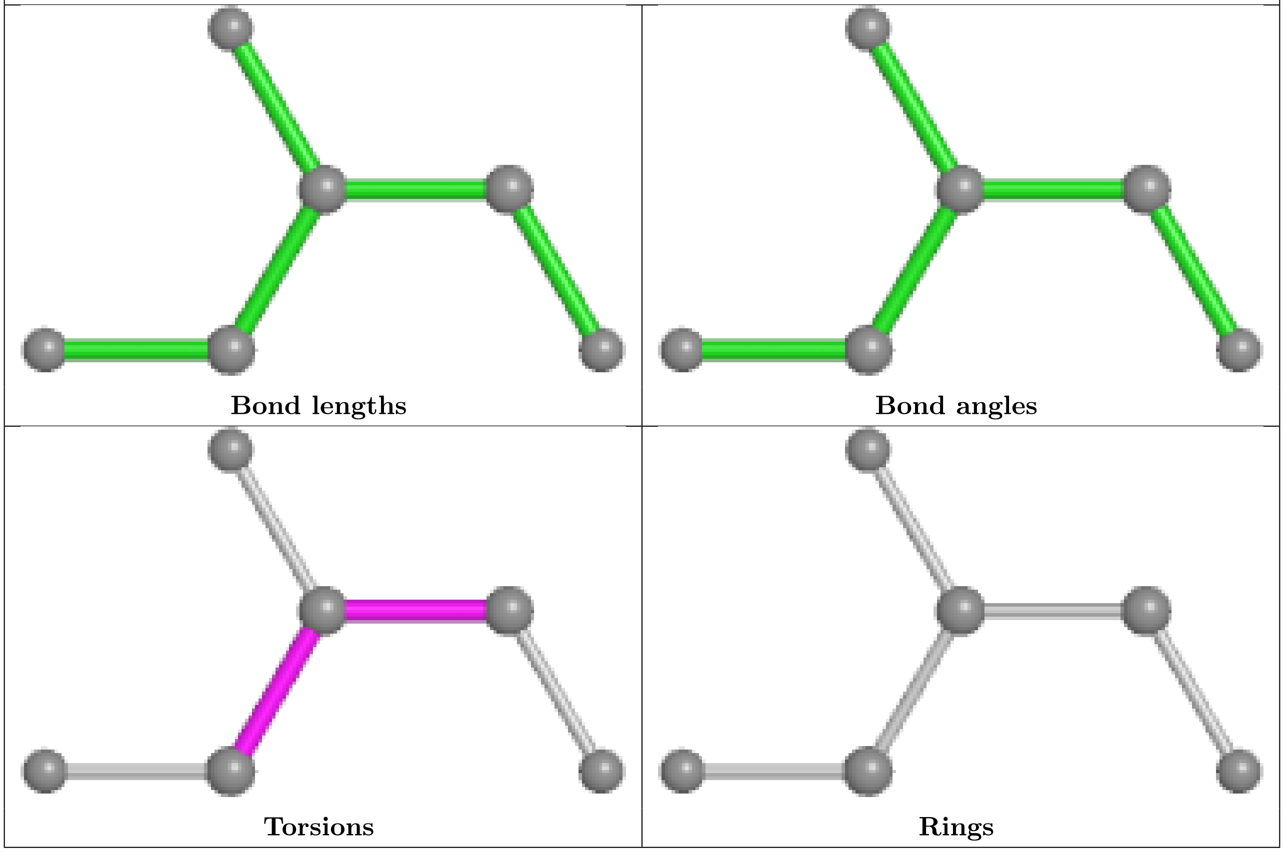
Bond lengths

Bond angles

Torsions

Rings

Ligand GOL G 502



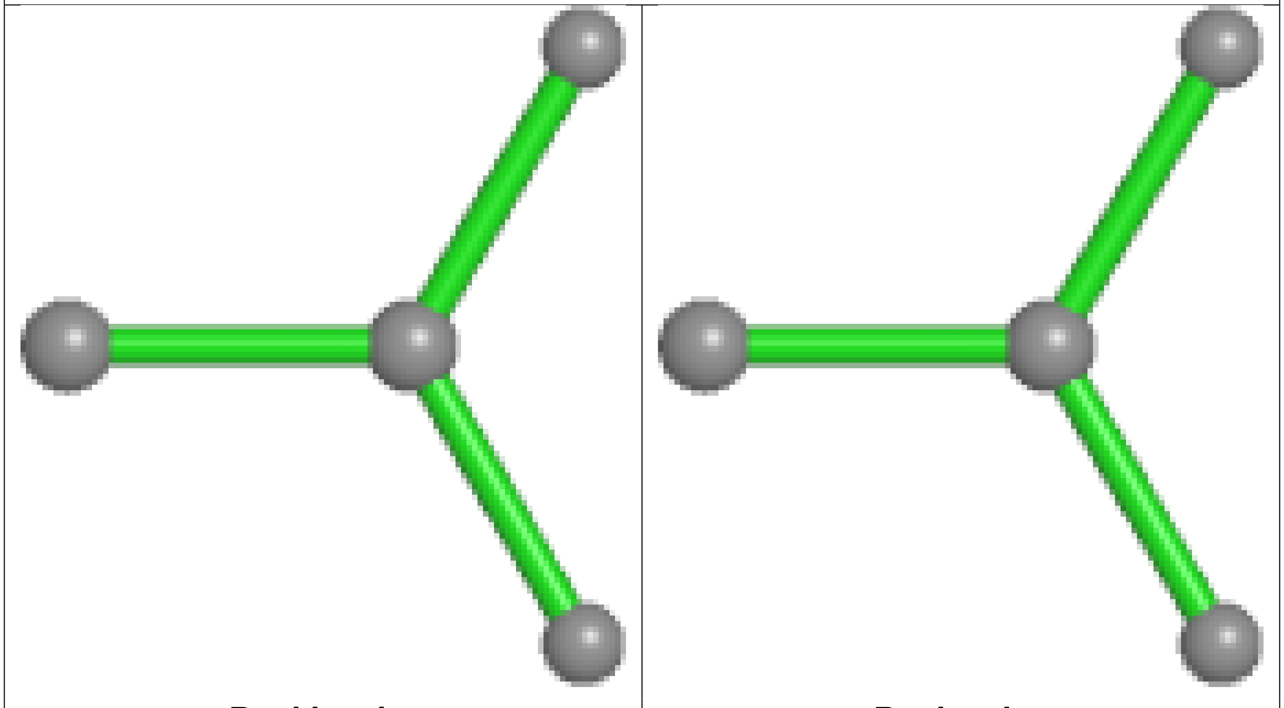
Bond lengths

Bond angles

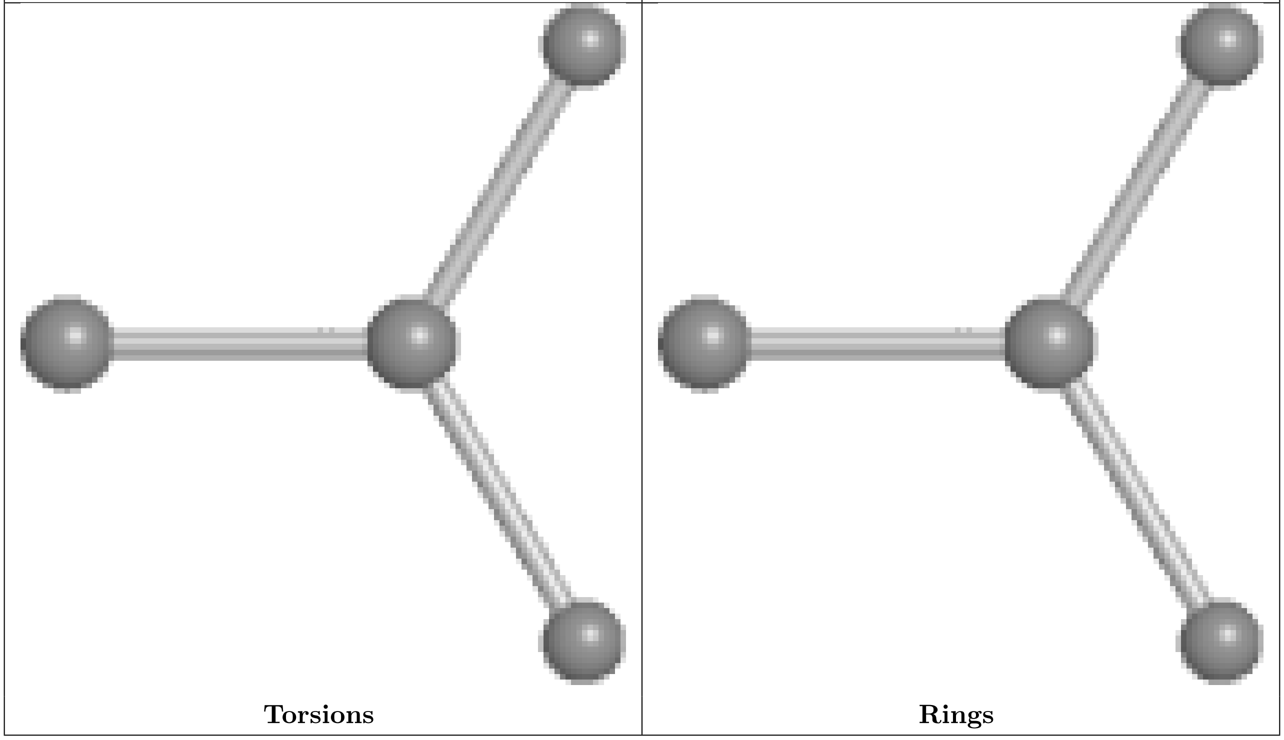
Torsions

Rings

Ligand ACY H 503

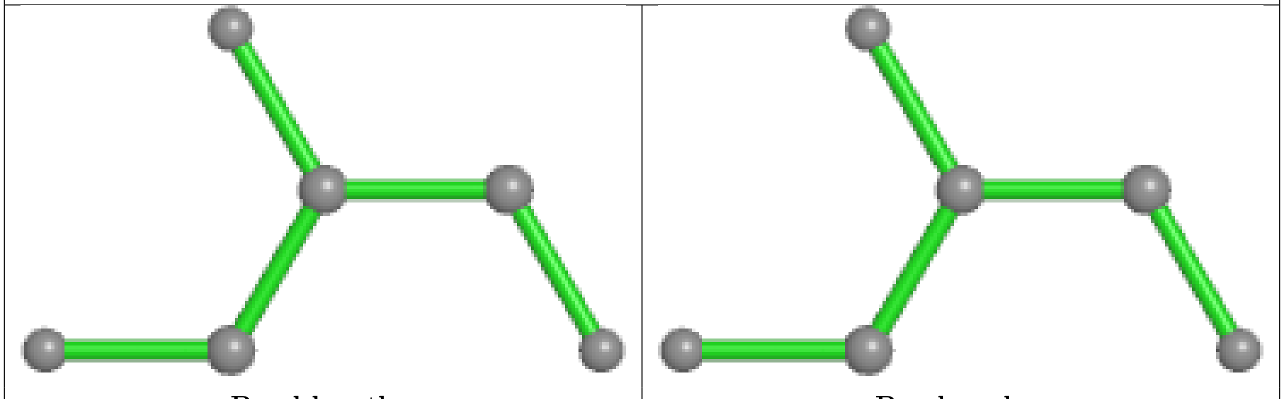


Bond lengths **Bond angles**



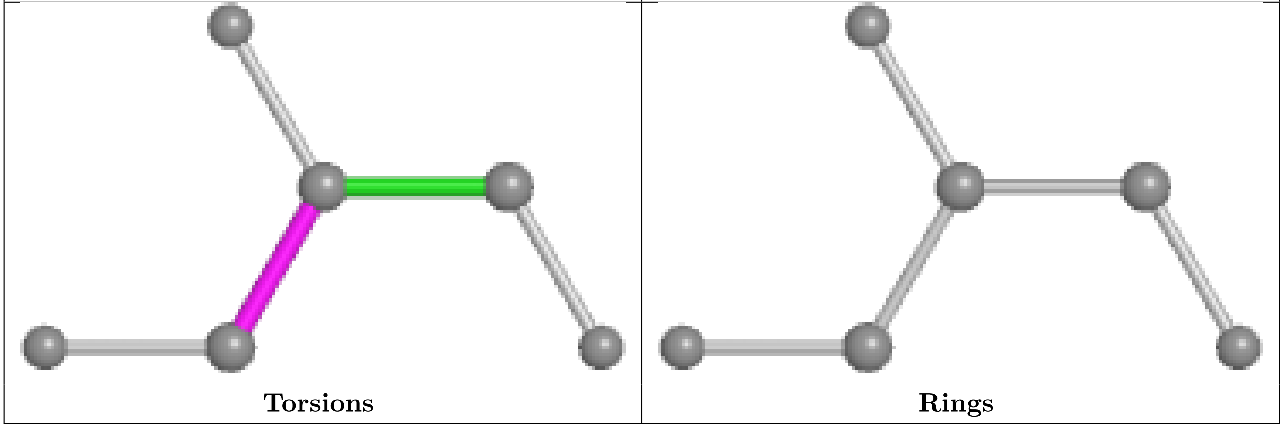
Torsions **Rings**

Ligand GOL D 504



Bond lengths

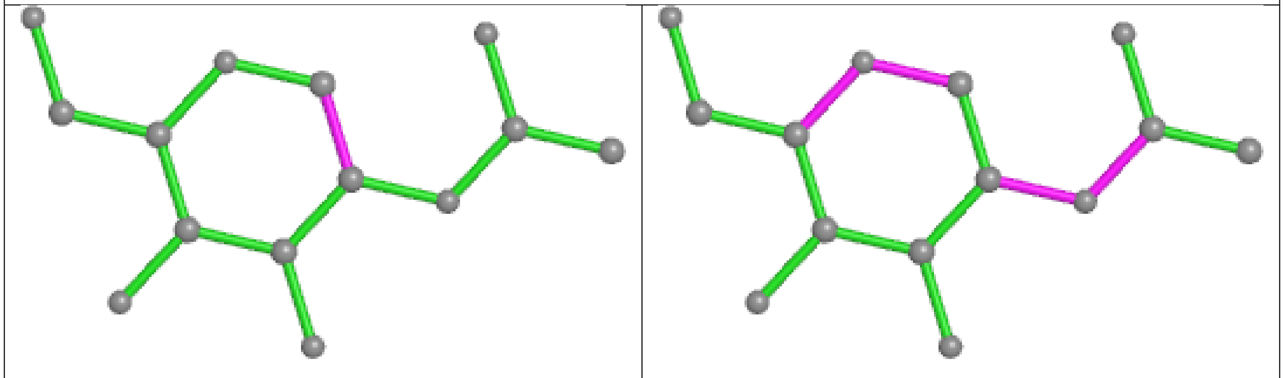
Bond angles



Torsions

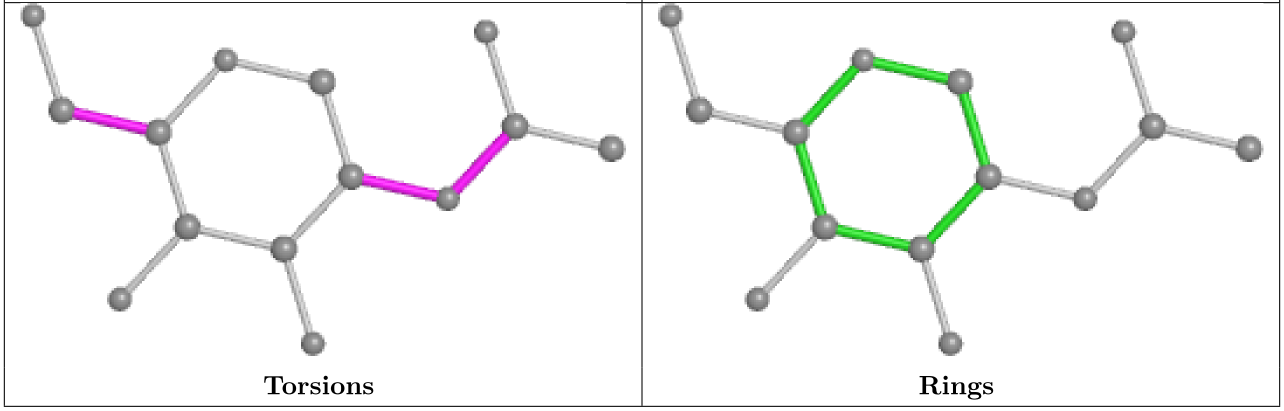
Rings

Ligand NAG C 502



Bond lengths

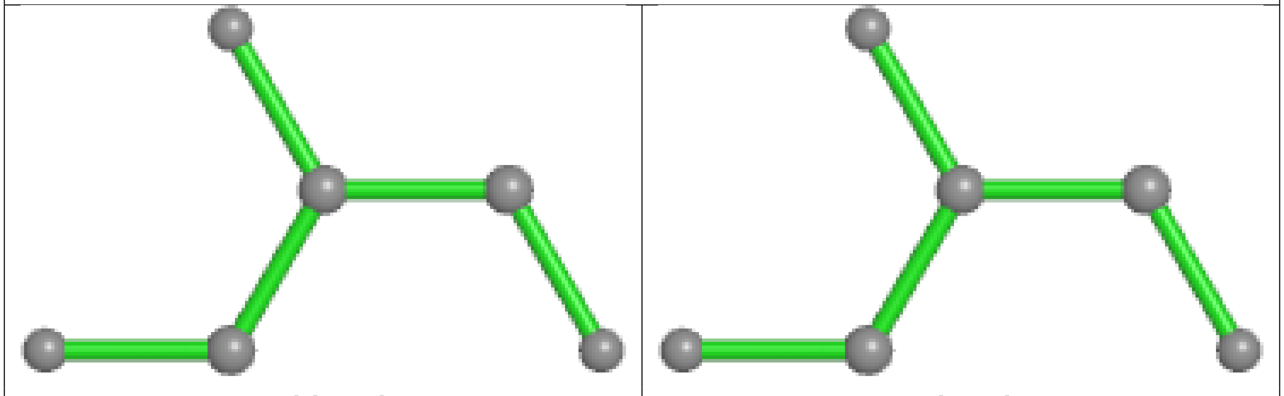
Bond angles



Torsions

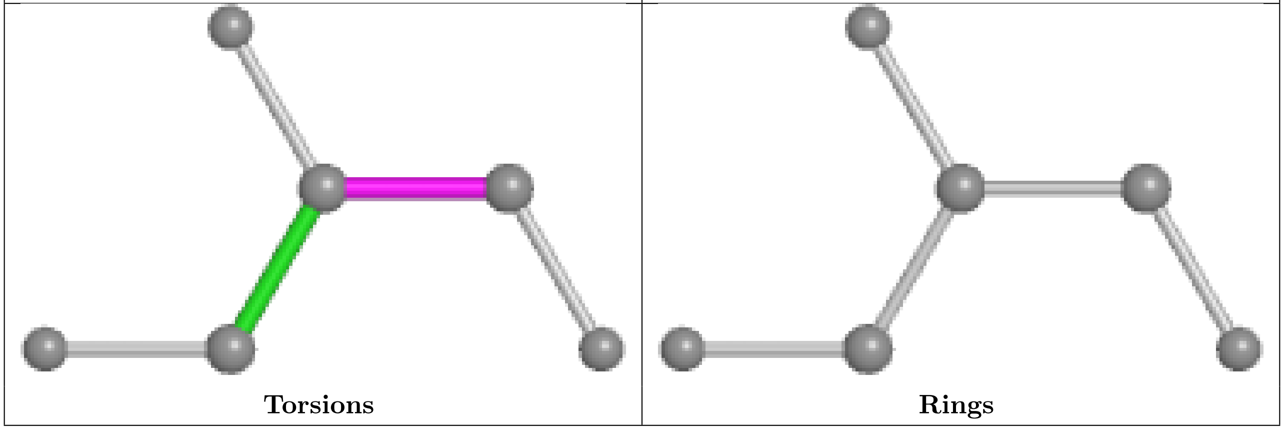
Rings

Ligand GOL A 601



Bond lengths

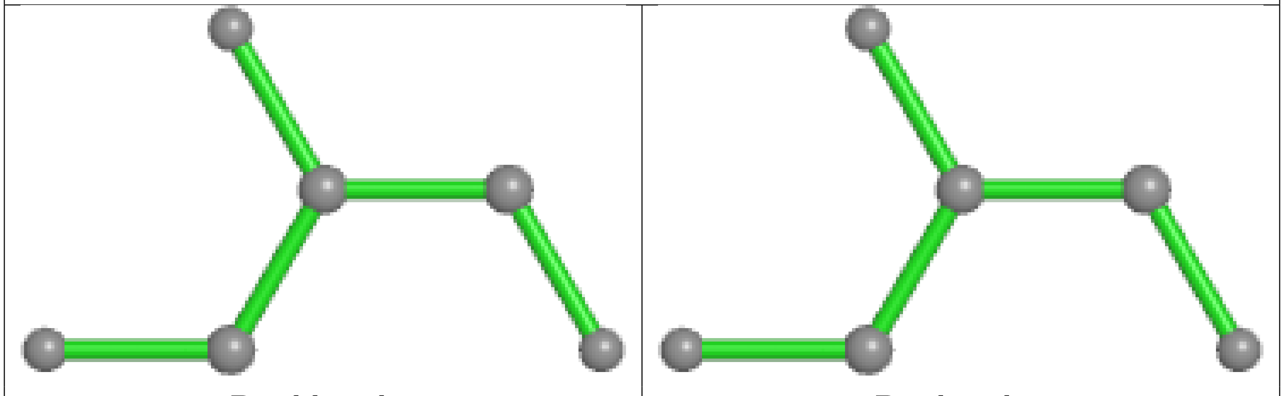
Bond angles



Torsions

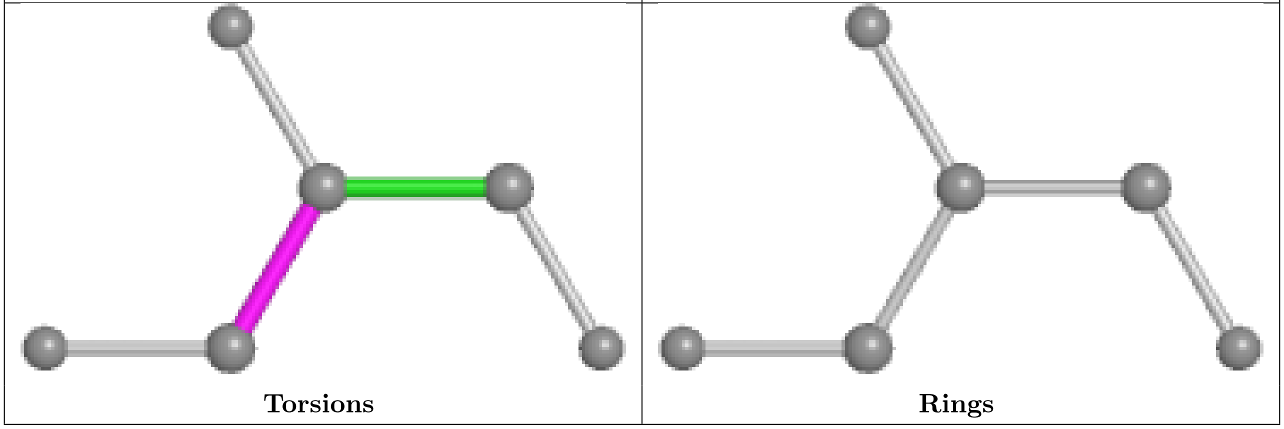
Rings

Ligand GOL C 503



Bond lengths

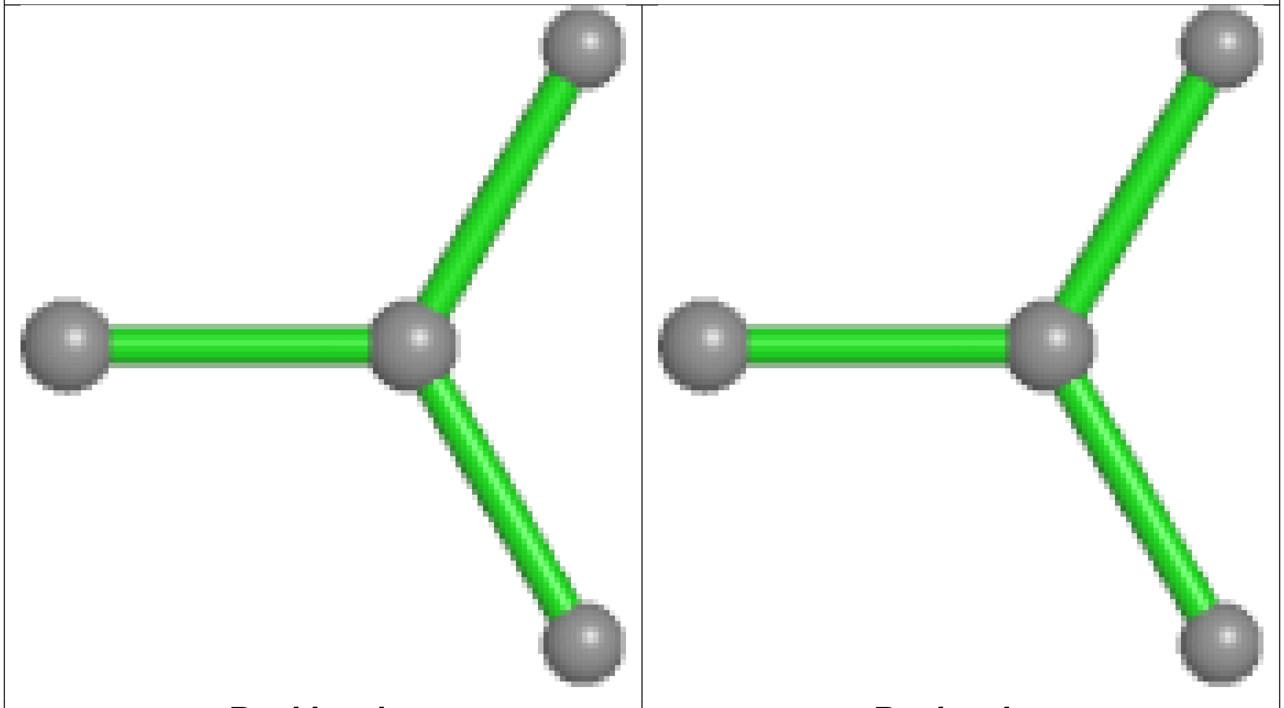
Bond angles



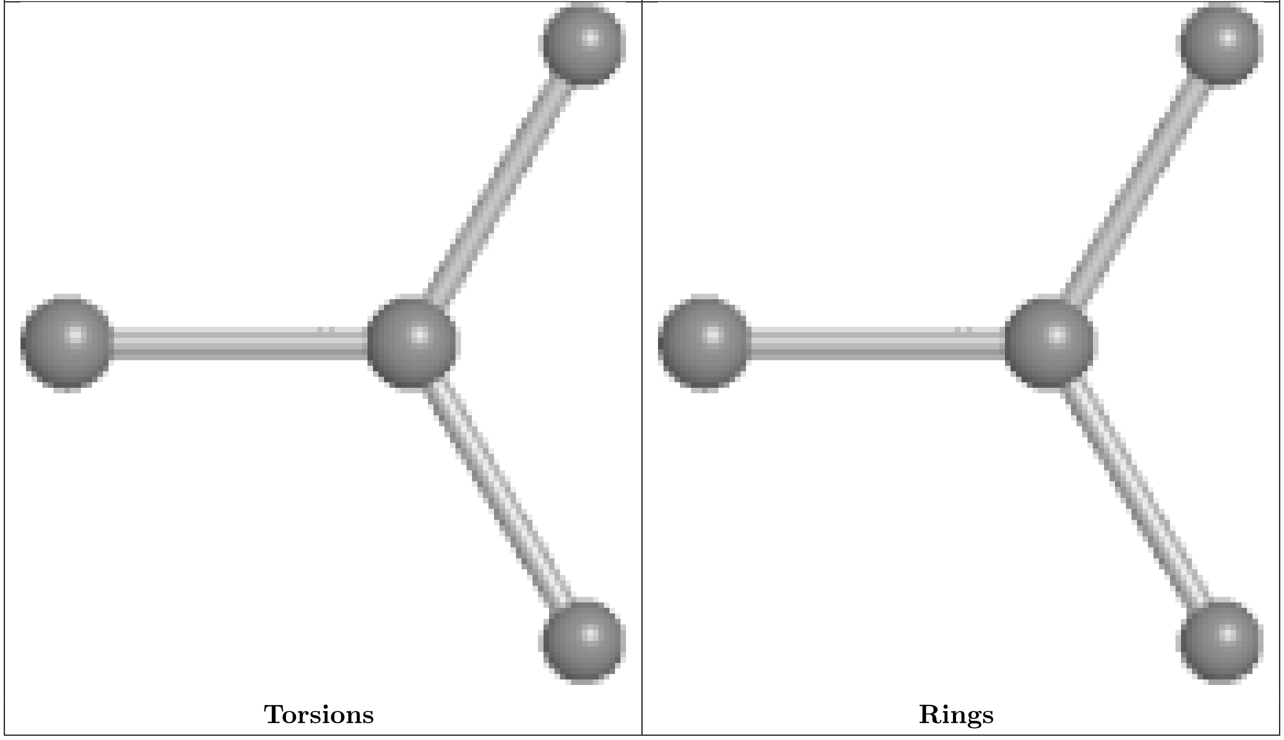
Torsions

Rings

Ligand ACY A 602

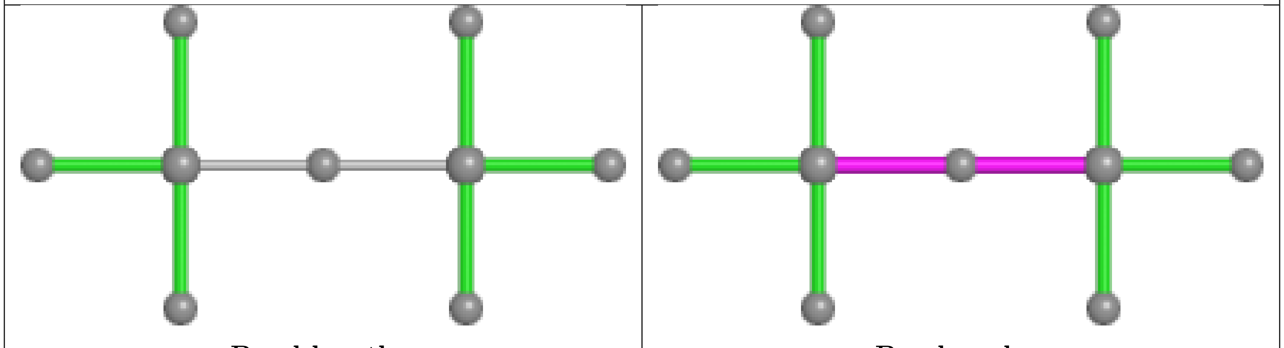


Bond lengths **Bond angles**

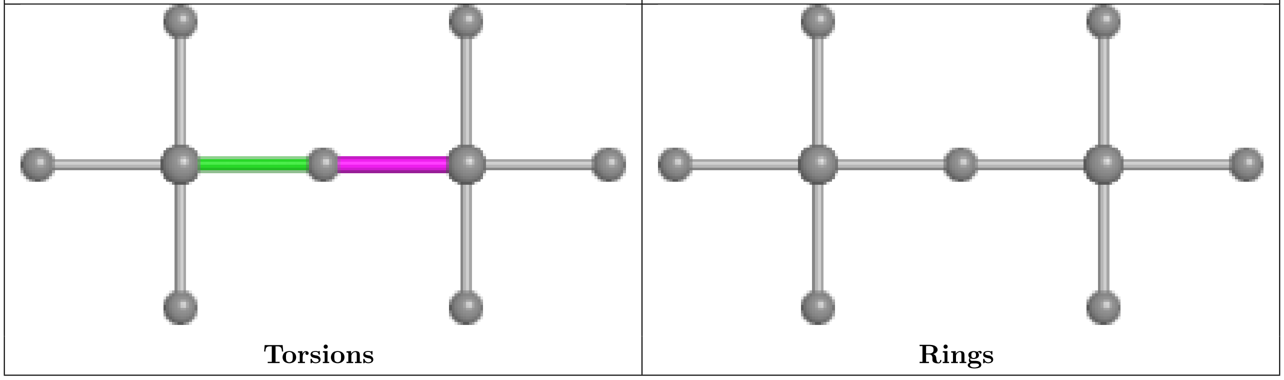


Torsions **Rings**

Ligand PPV F 501

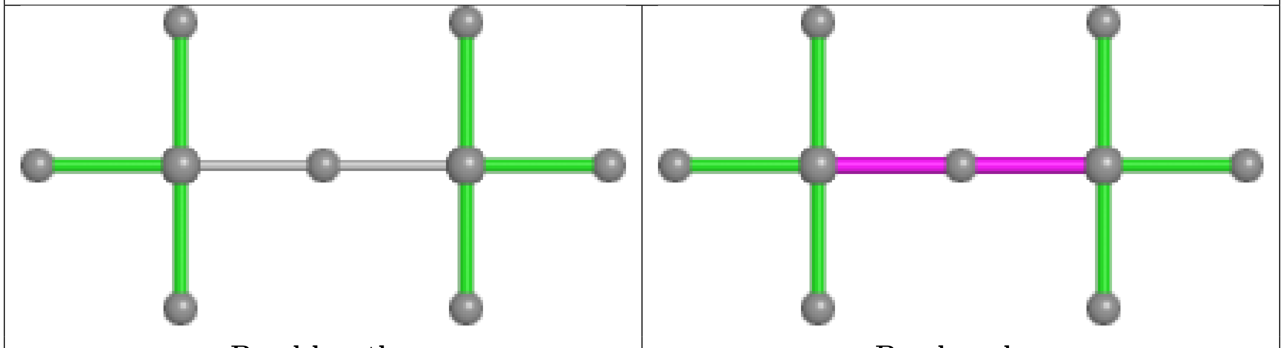


Bond lengths Bond angles

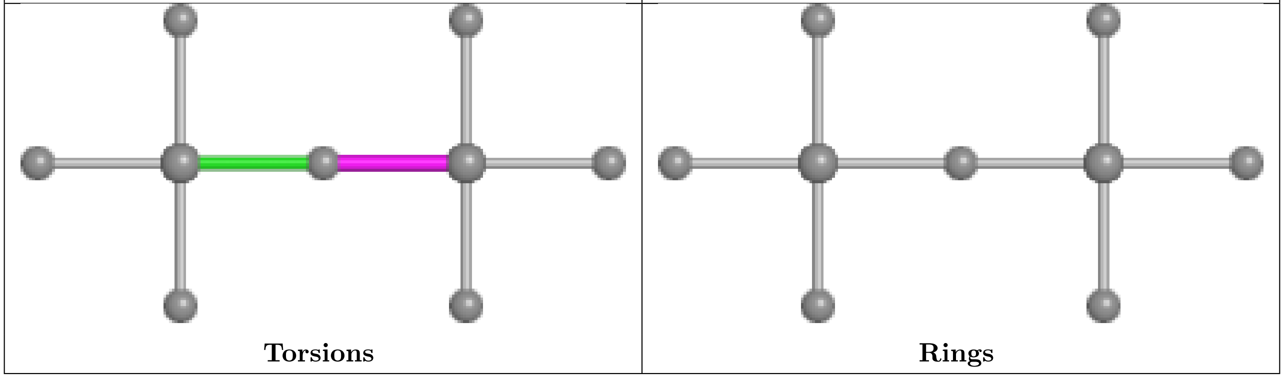


Torsions Rings

Ligand PPV D 501

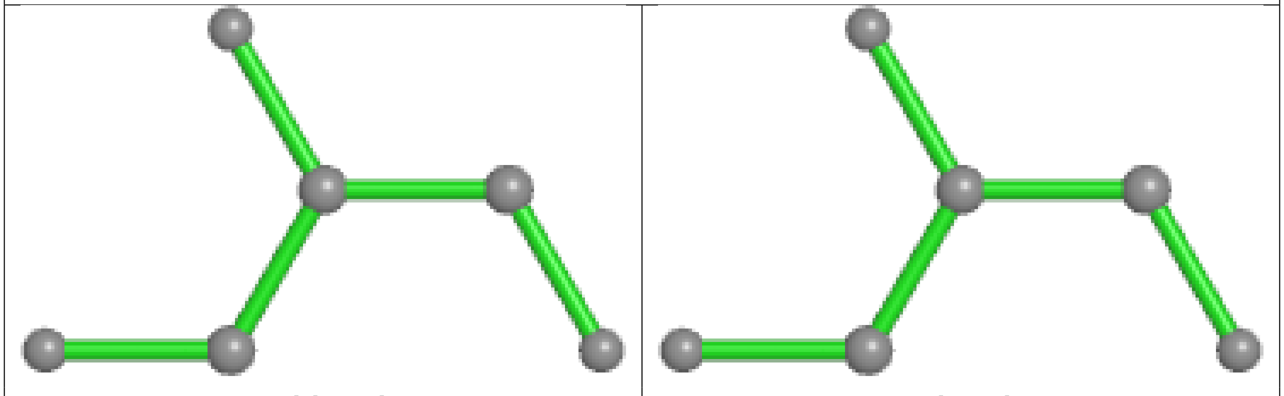


Bond lengths Bond angles

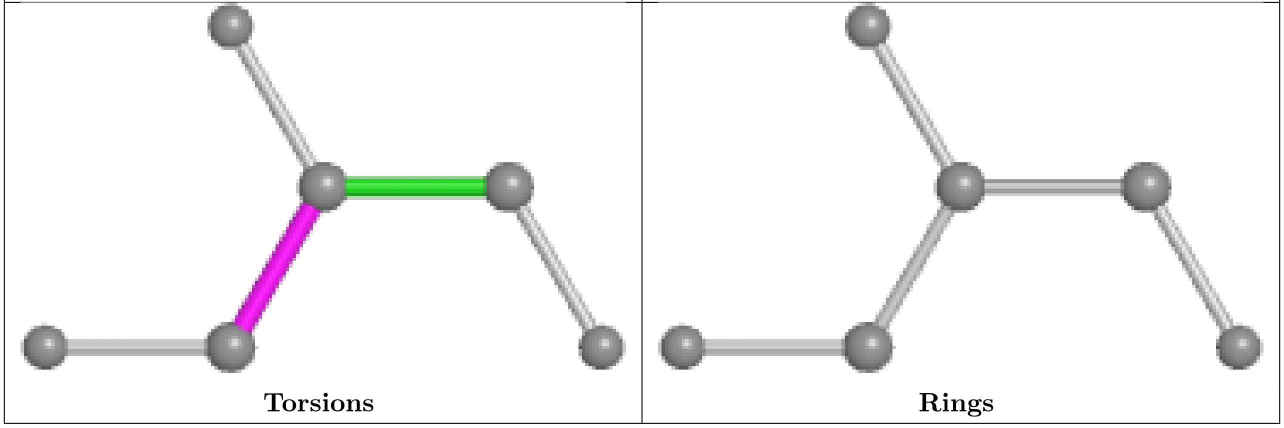


Torsions Rings

Ligand GOL C 508

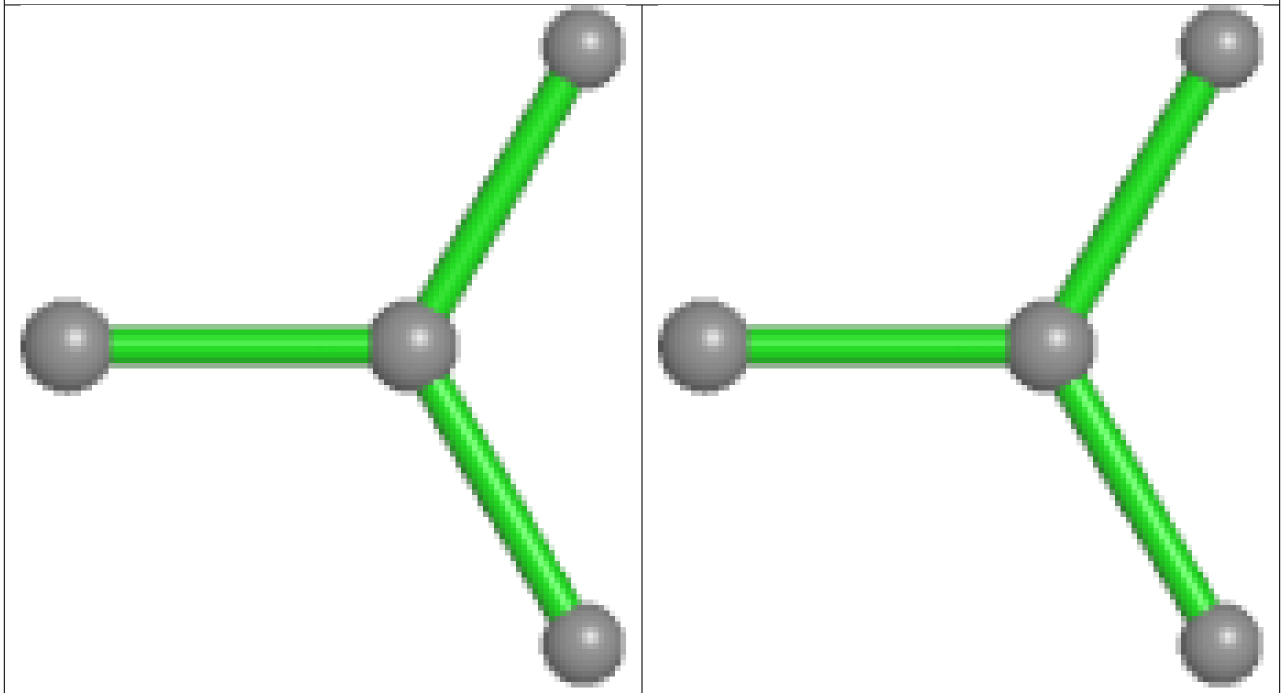


Bond lengths Bond angles



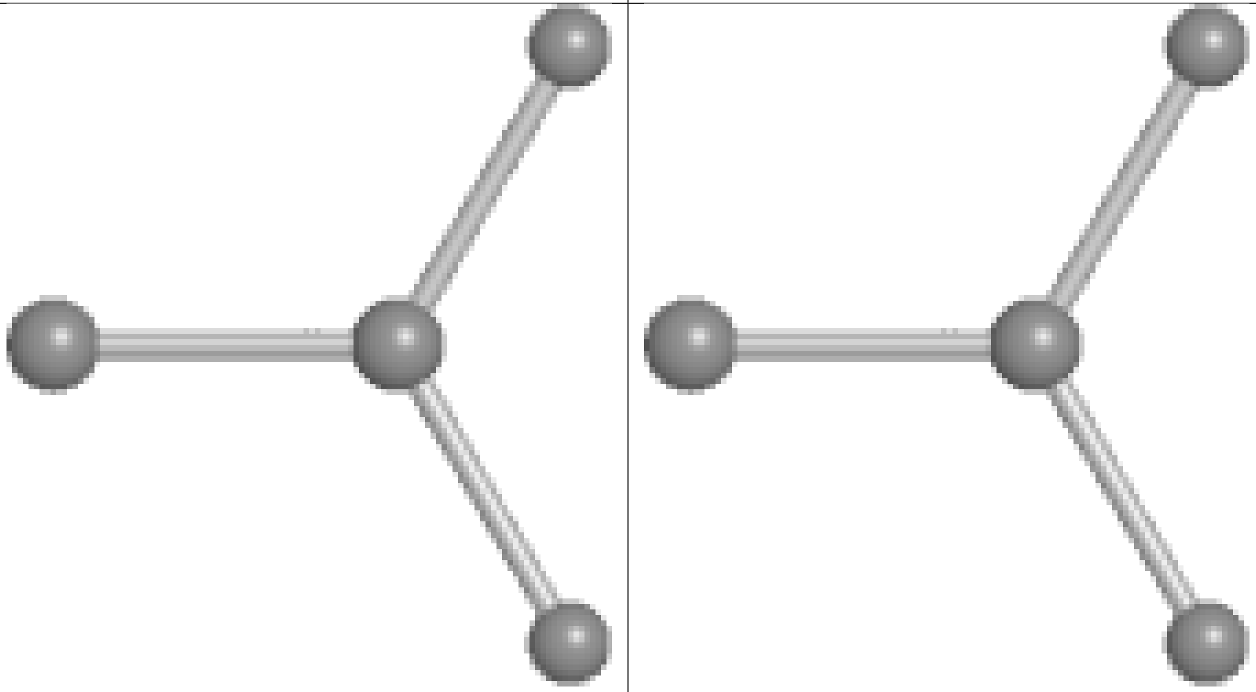
Torsions Rings

Ligand ACY E 504



Bond lengths

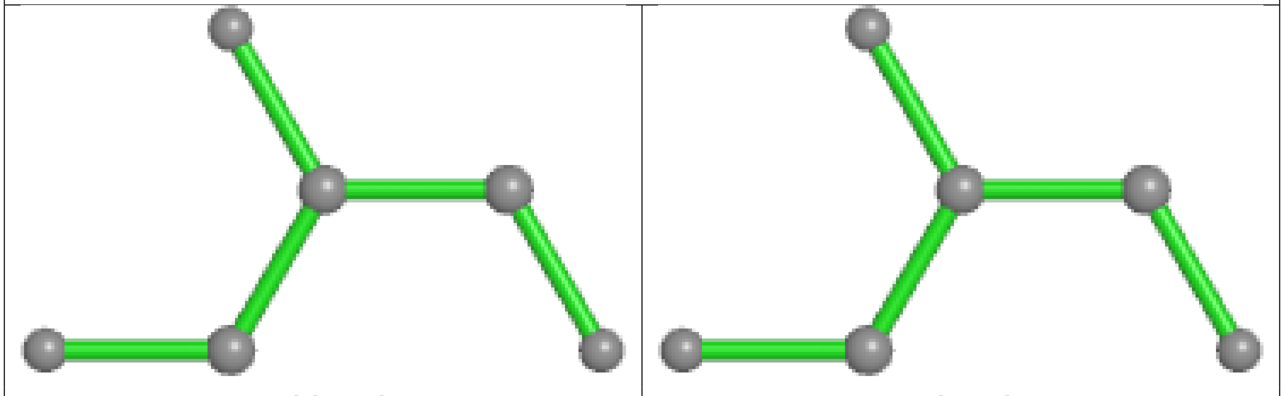
Bond angles



Torsions

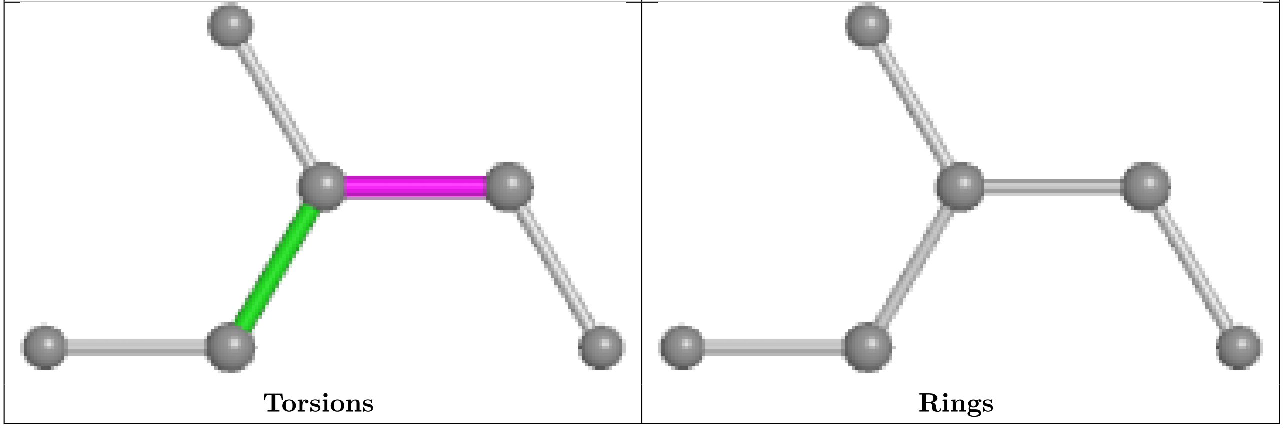
Rings

Ligand GOL E 505



Bond lengths

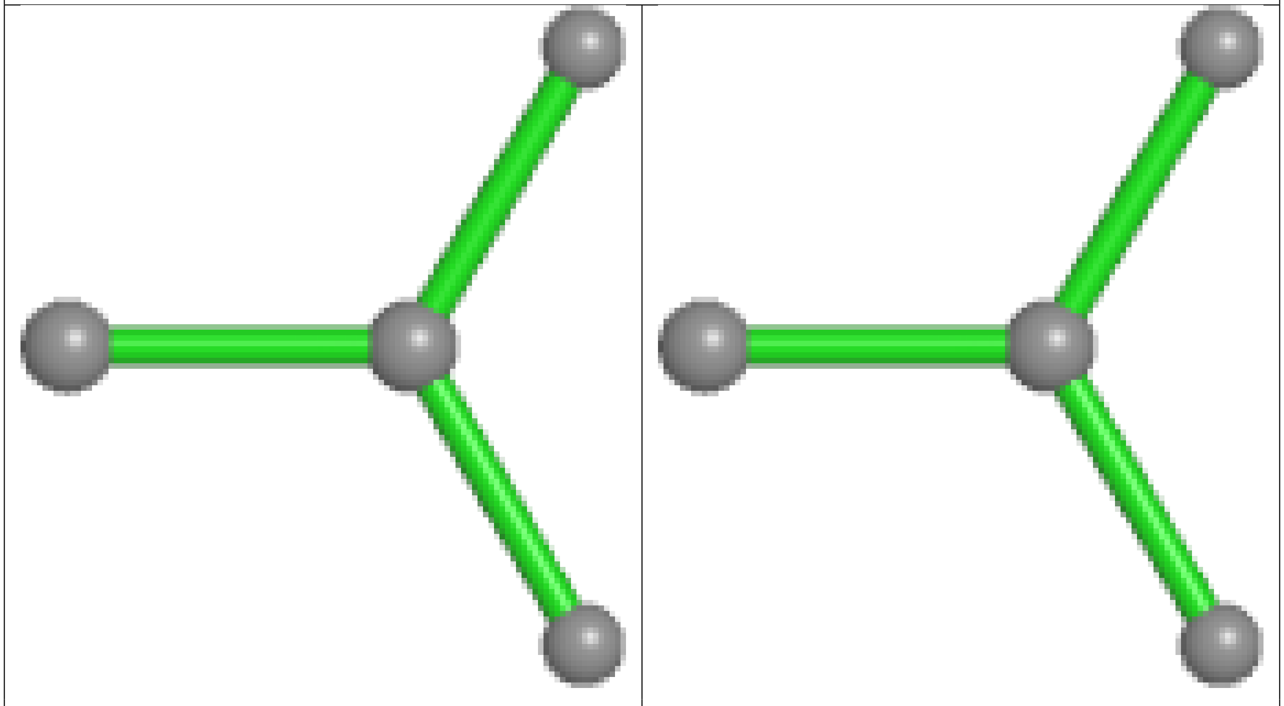
Bond angles



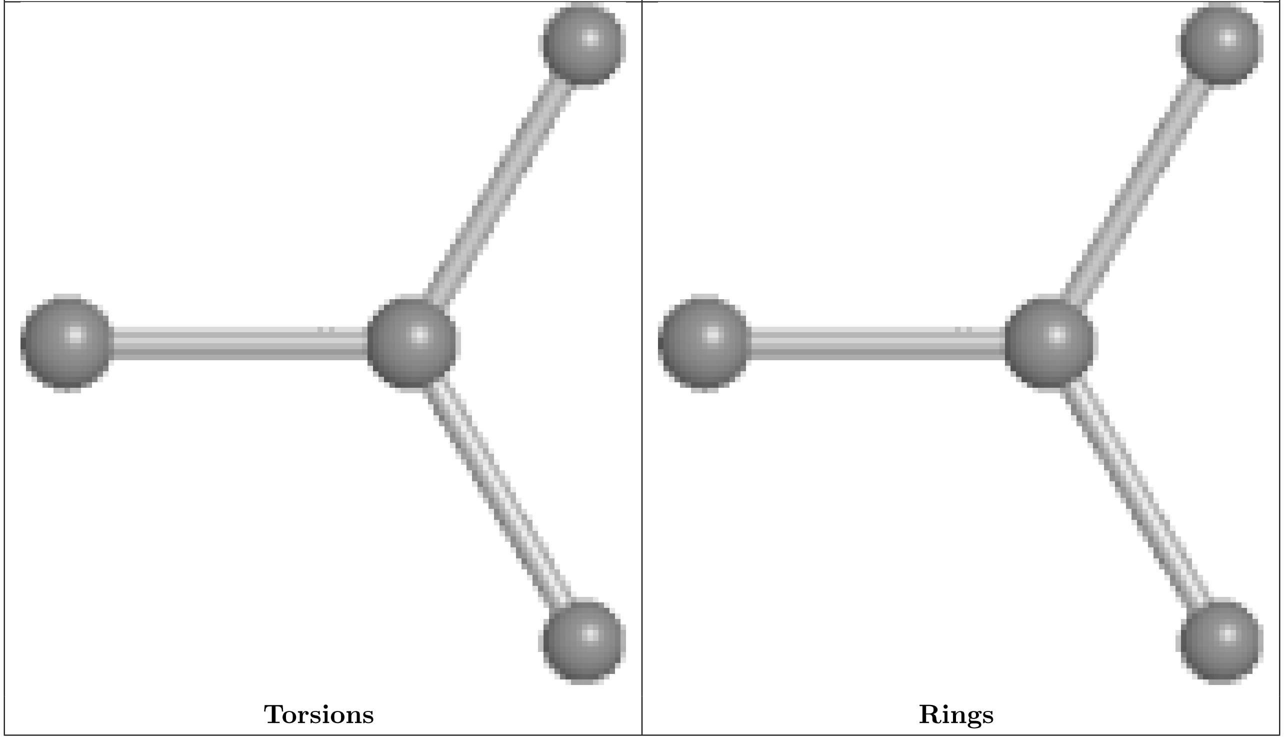
Torsions

Rings

Ligand ACY G 503

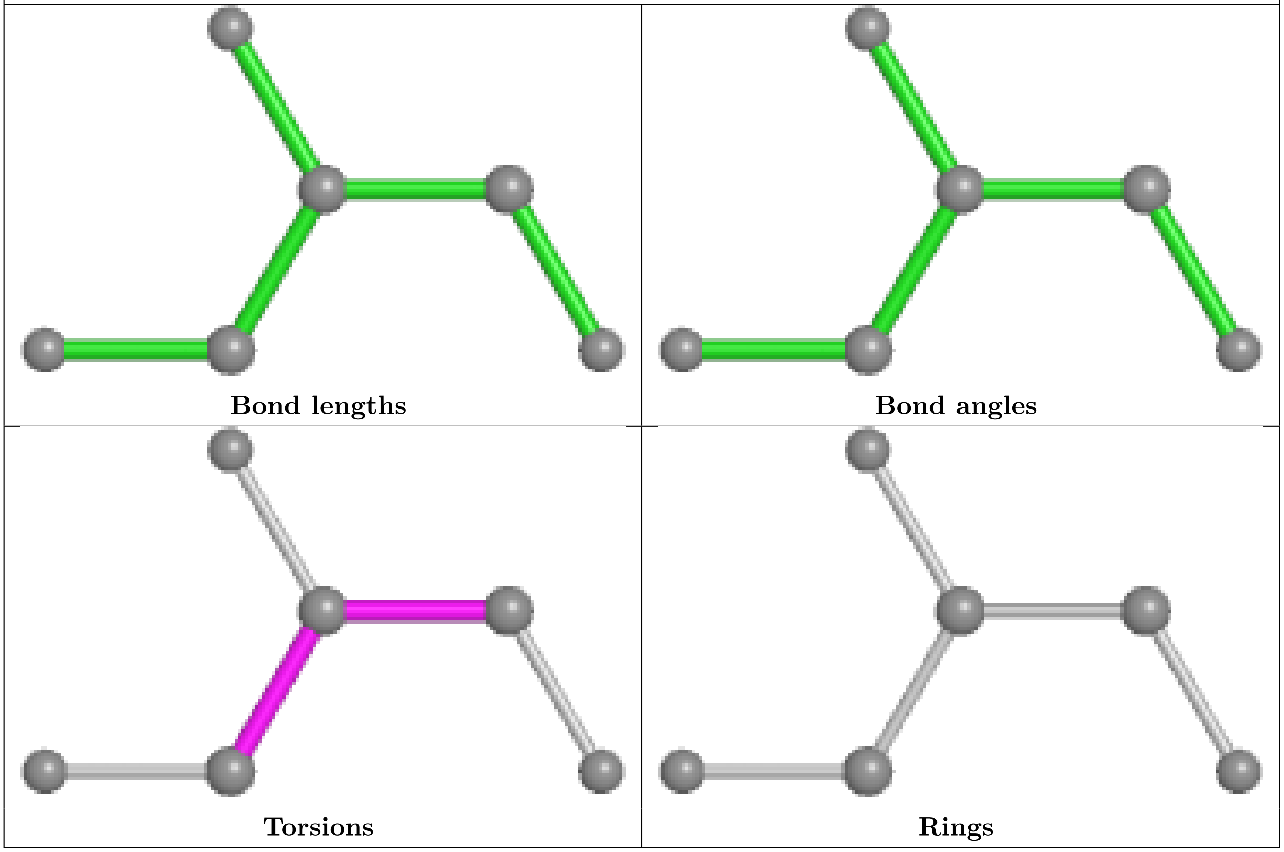


Bond lengths **Bond angles**



Torsions **Rings**

Ligand GOL F 502



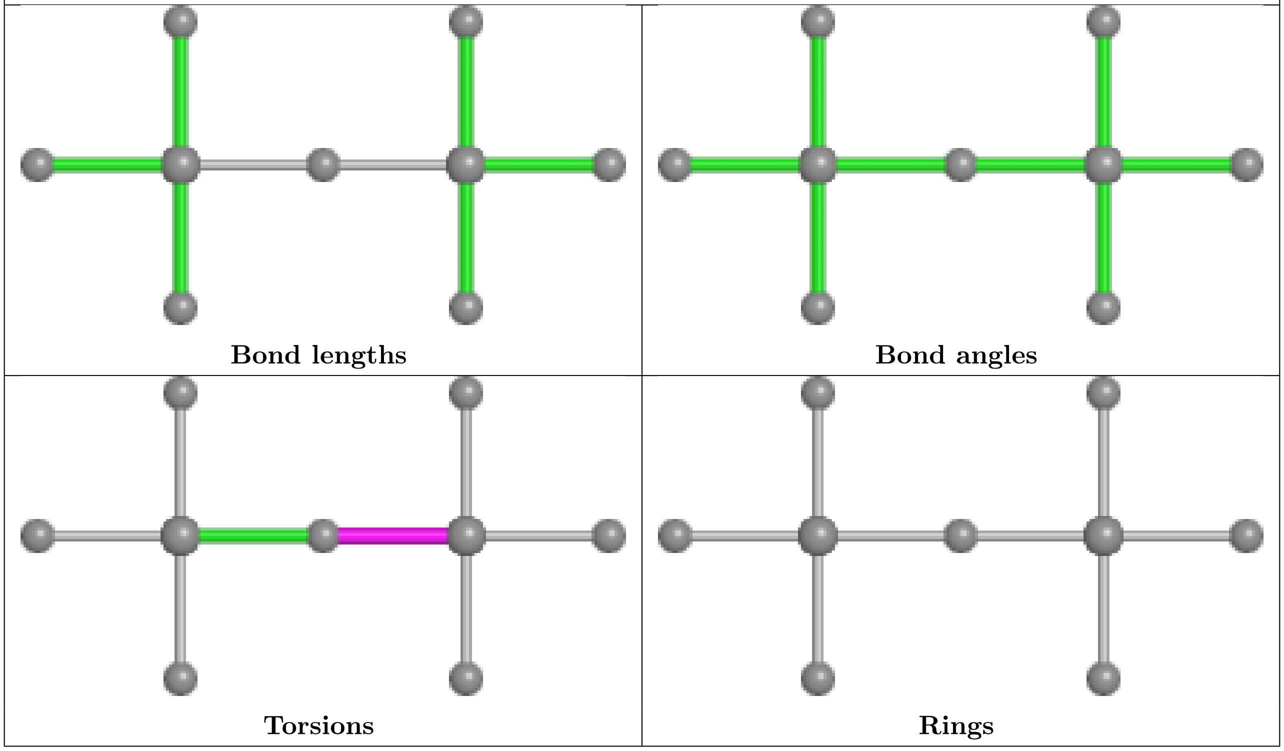
Bond lengths

Bond angles

Torsions

Rings

Ligand PPV G 501



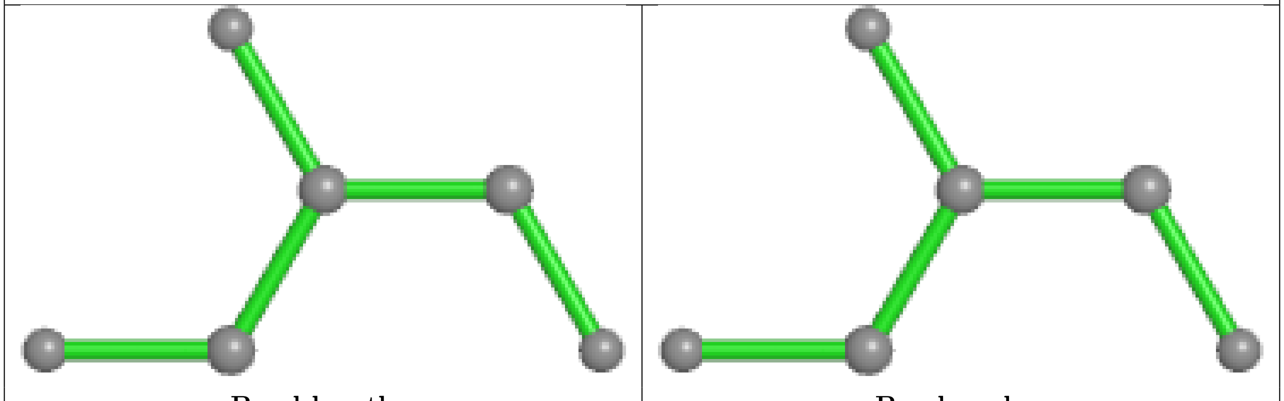
Bond lengths

Bond angles

Torsions

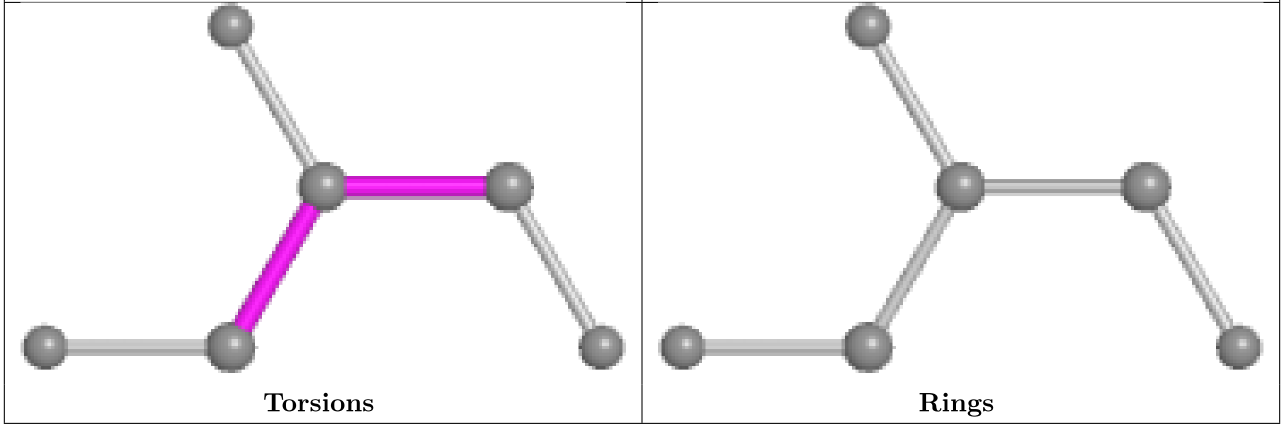
Rings

Ligand GOL E 506



Bond lengths

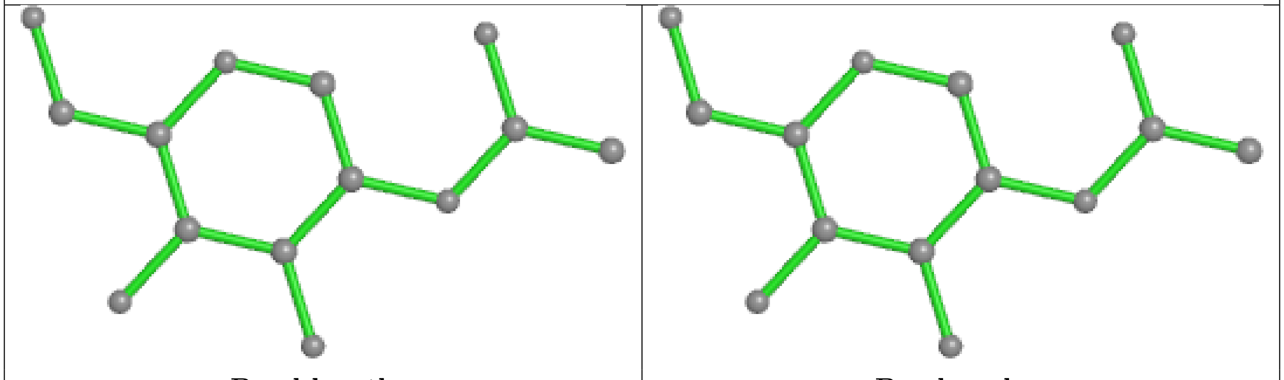
Bond angles



Torsions

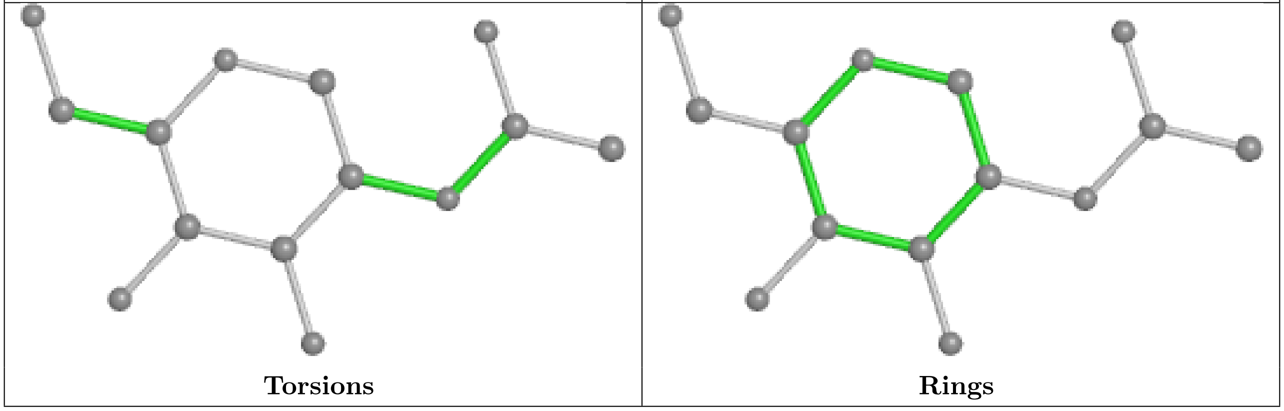
Rings

Ligand NAG D 502



Bond lengths

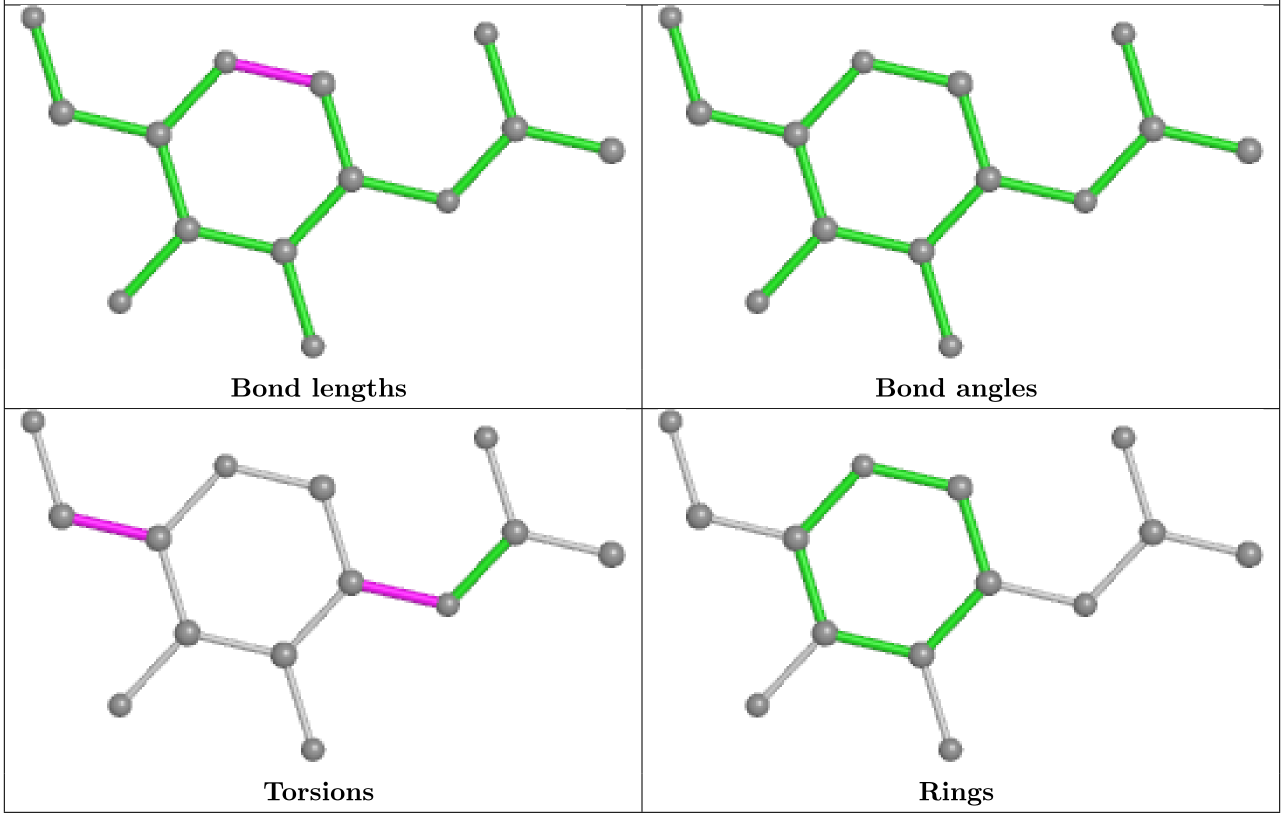
Bond angles



Torsions

Rings

Ligand NAG F 505



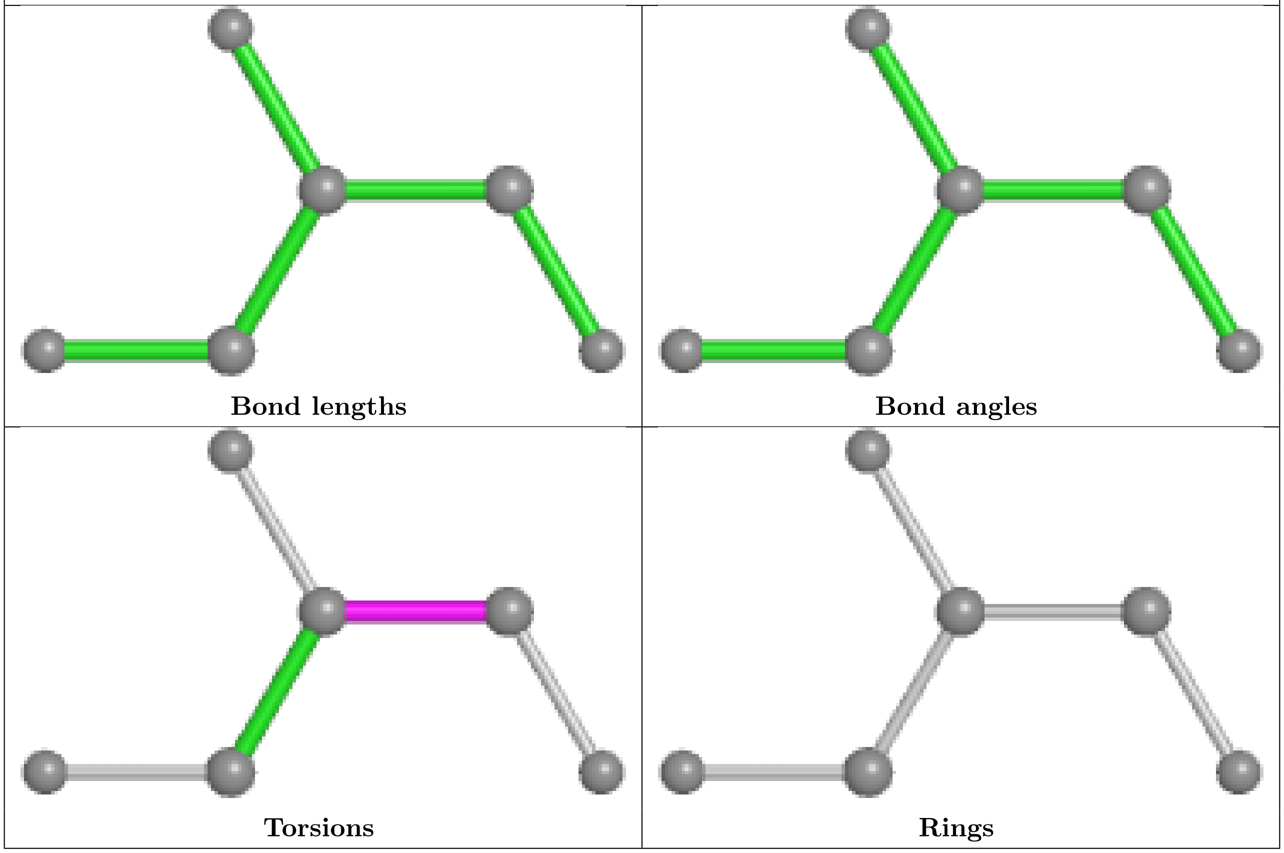
Bond lengths

Bond angles

Torsions

Rings

Ligand GOL B 504



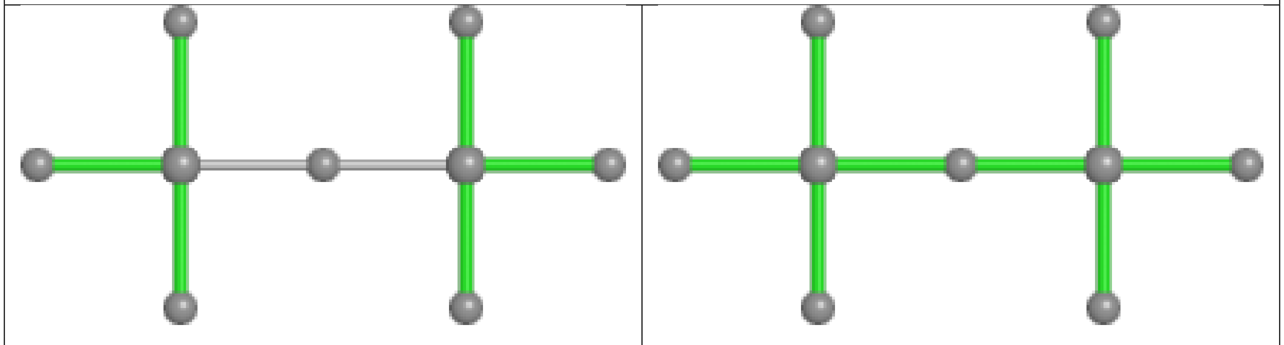
Bond lengths

Bond angles

Torsions

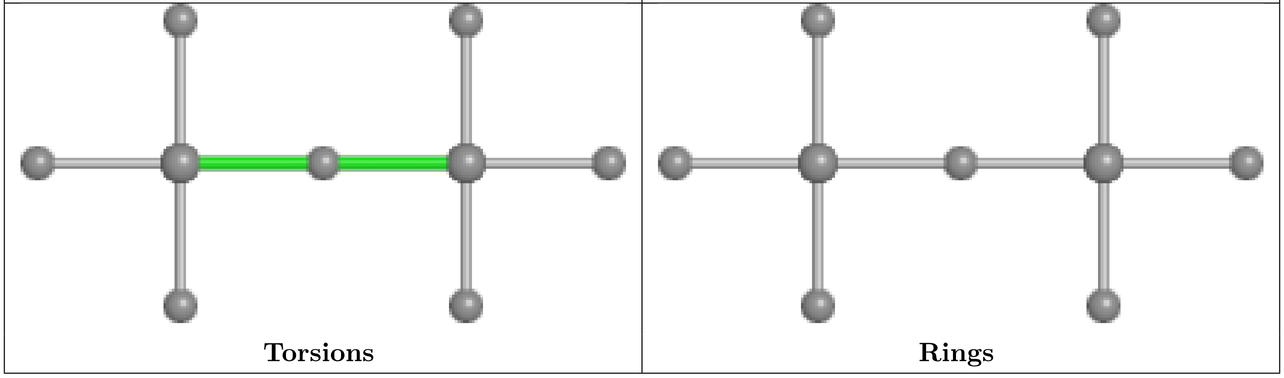
Rings

Ligand PPV B 501



Bond lengths

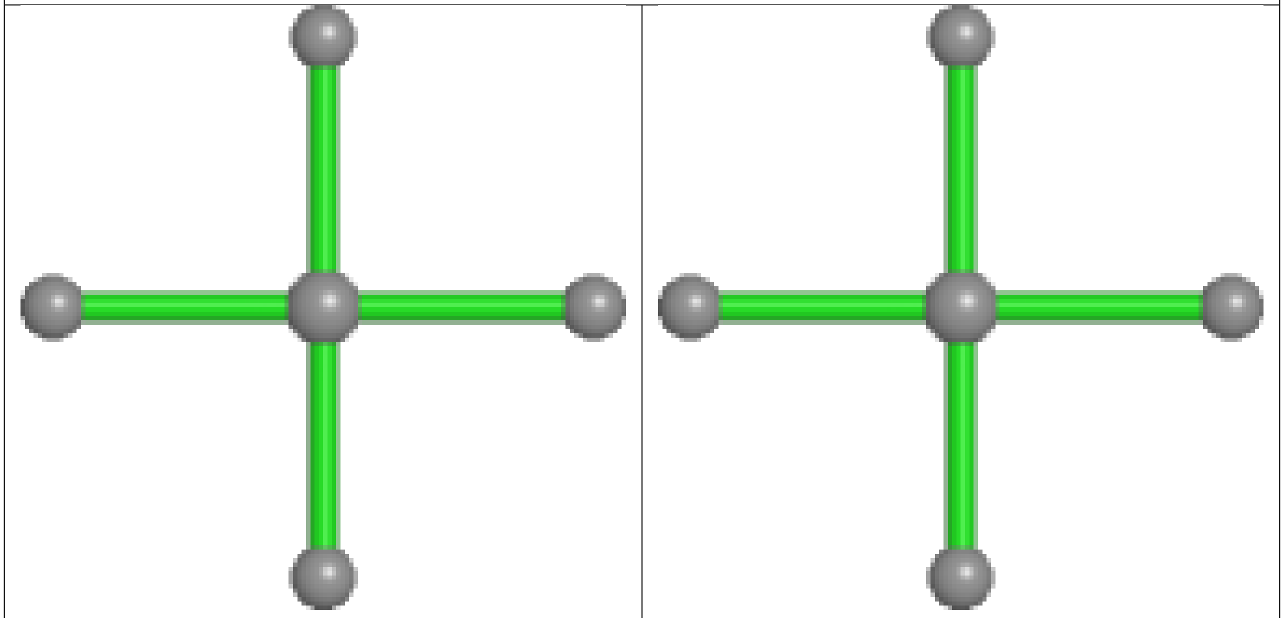
Bond angles



Torsions

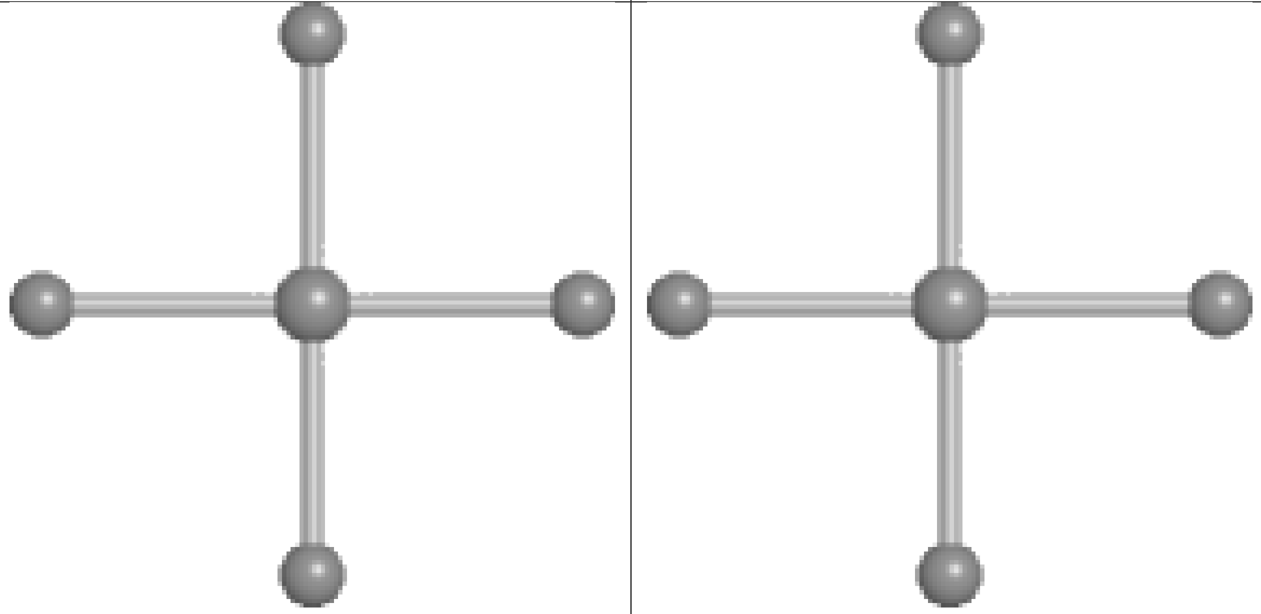
Rings

Ligand PO4 A 603



Bond lengths

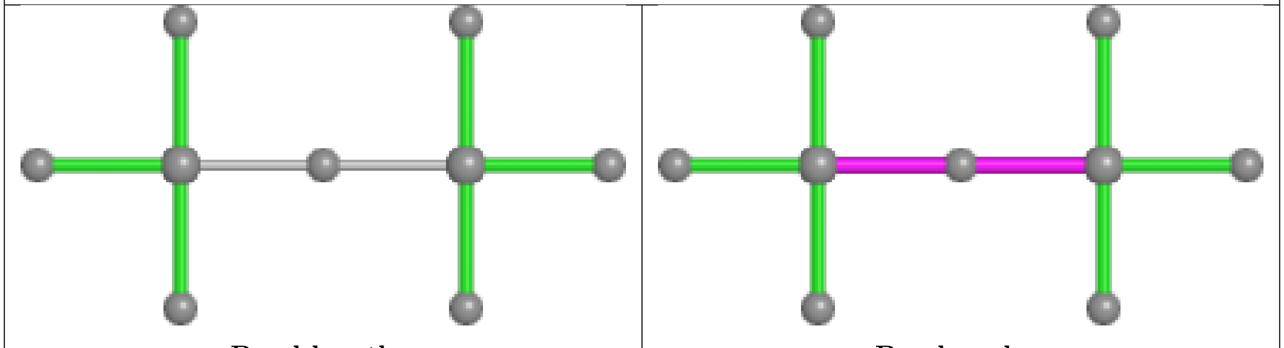
Bond angles



Torsions

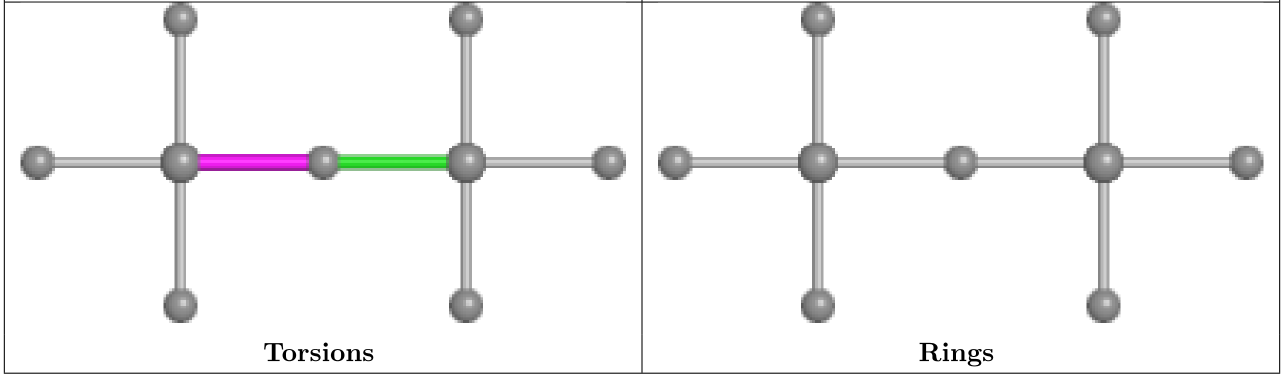
Rings

Ligand PPV E 501



Bond lengths

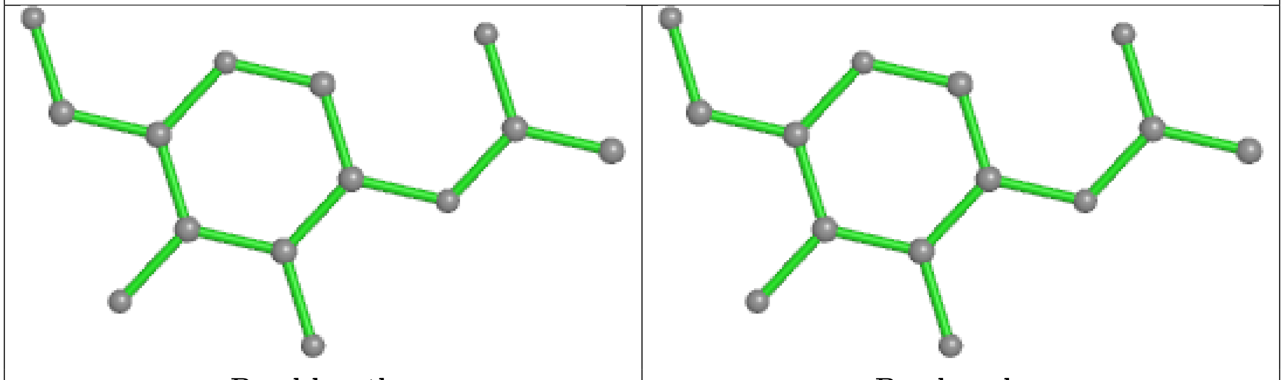
Bond angles



Torsions

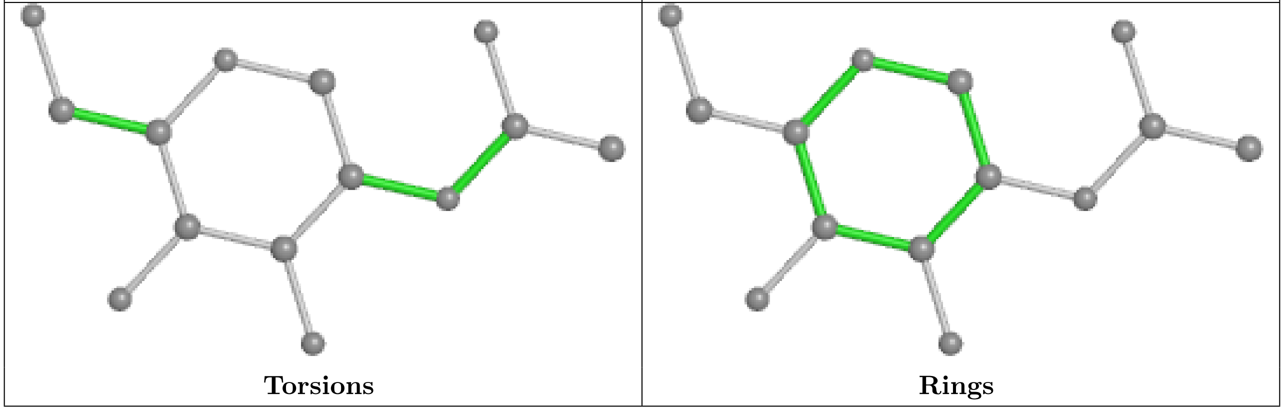
Rings

Ligand NAG B 502



Bond lengths

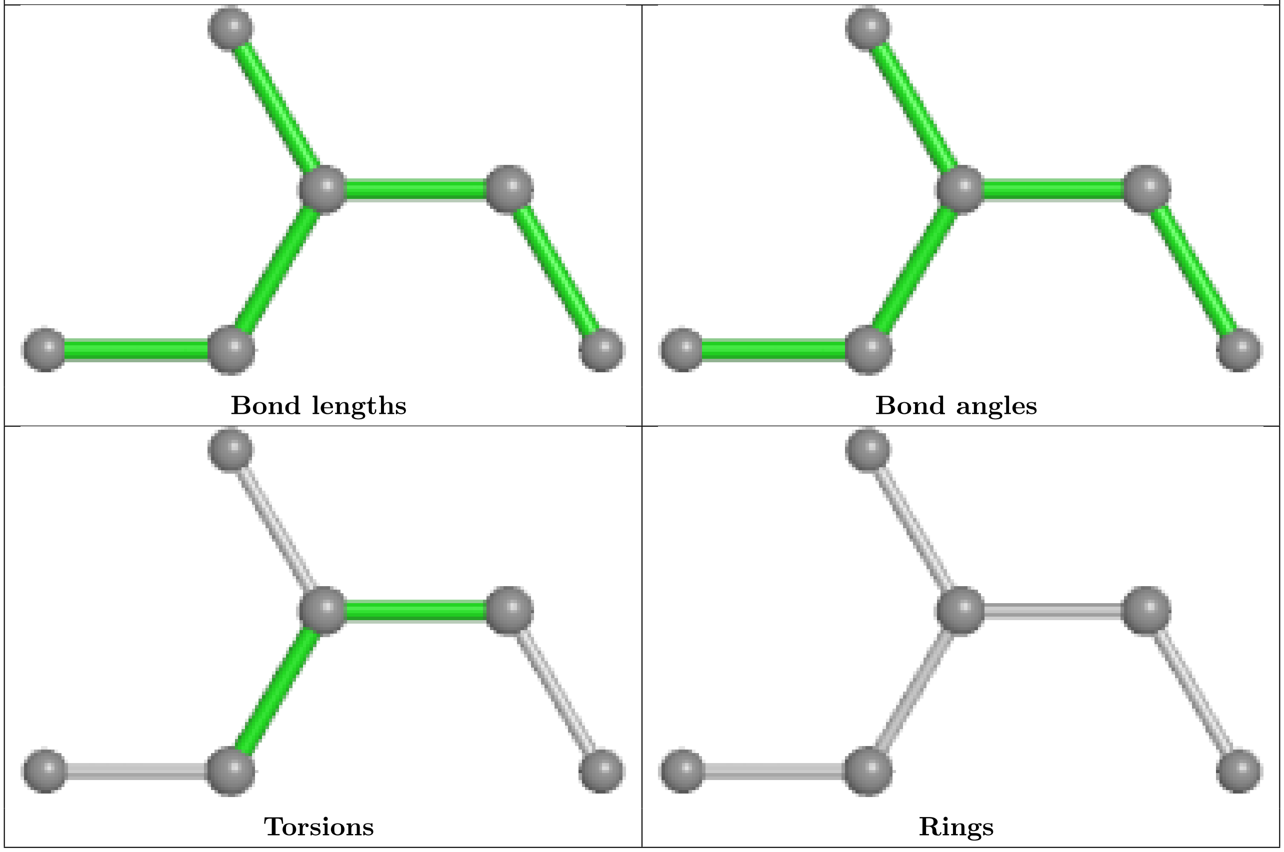
Bond angles



Torsions

Rings

Ligand GOL C 505



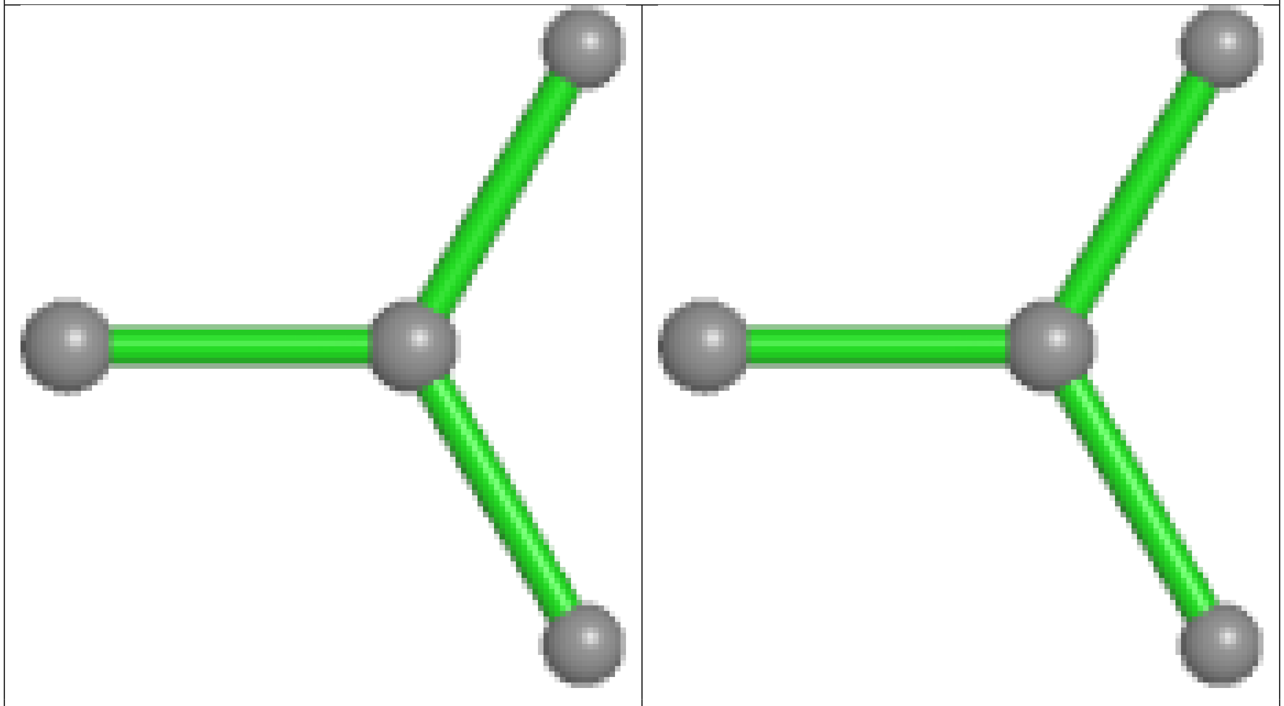
Bond lengths

Bond angles

Torsions

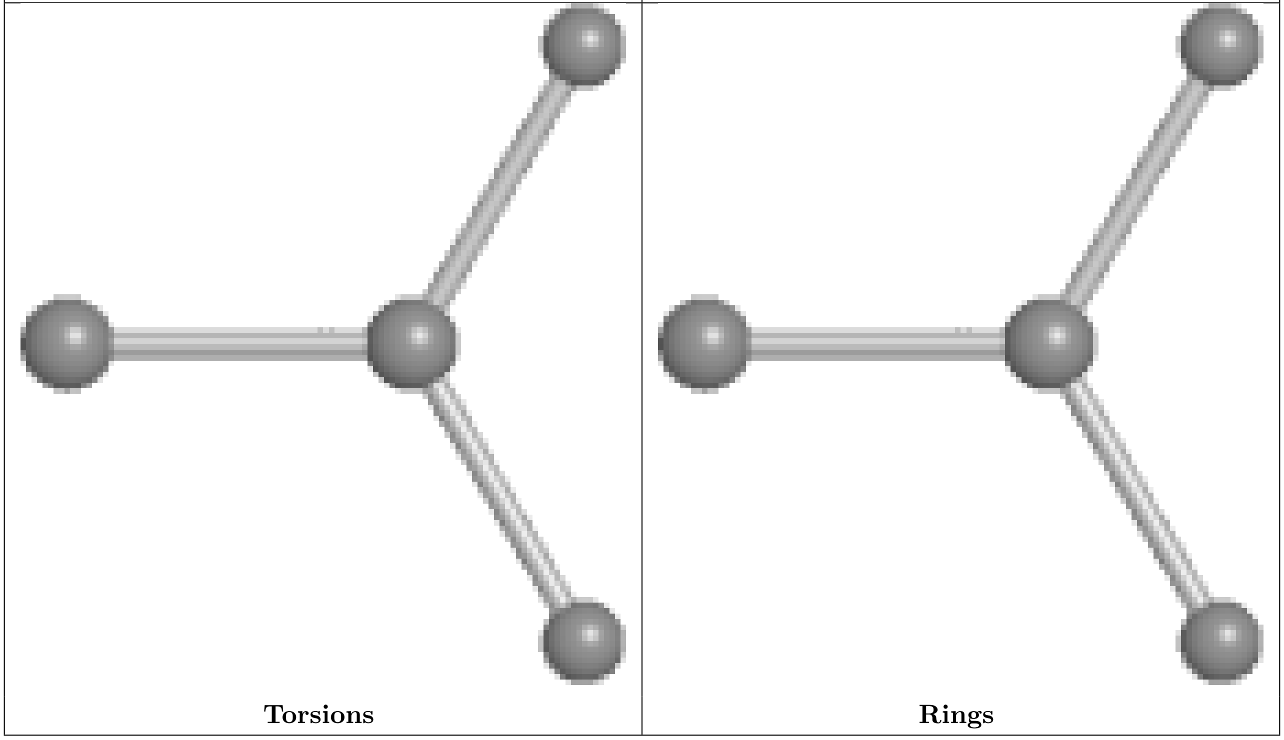
Rings

Ligand ACY C 506



Bond lengths

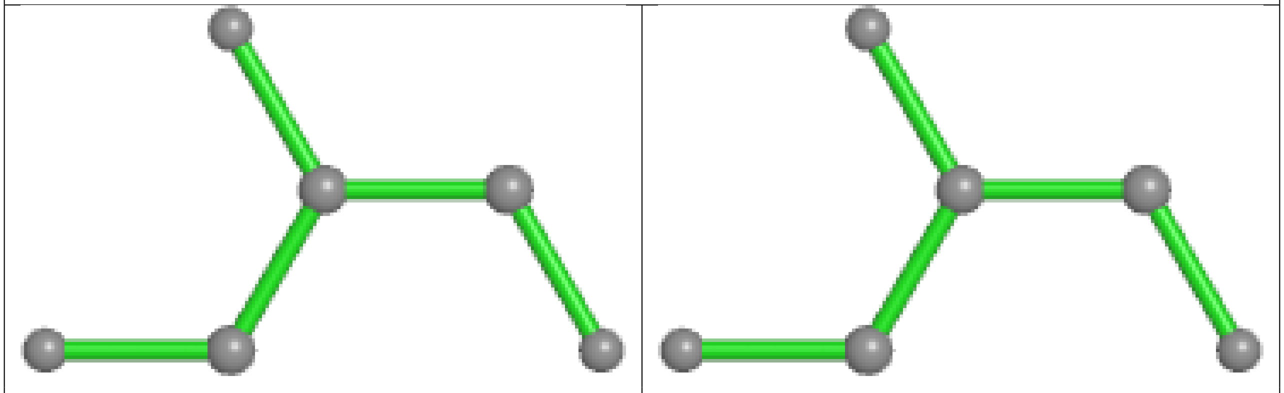
Bond angles



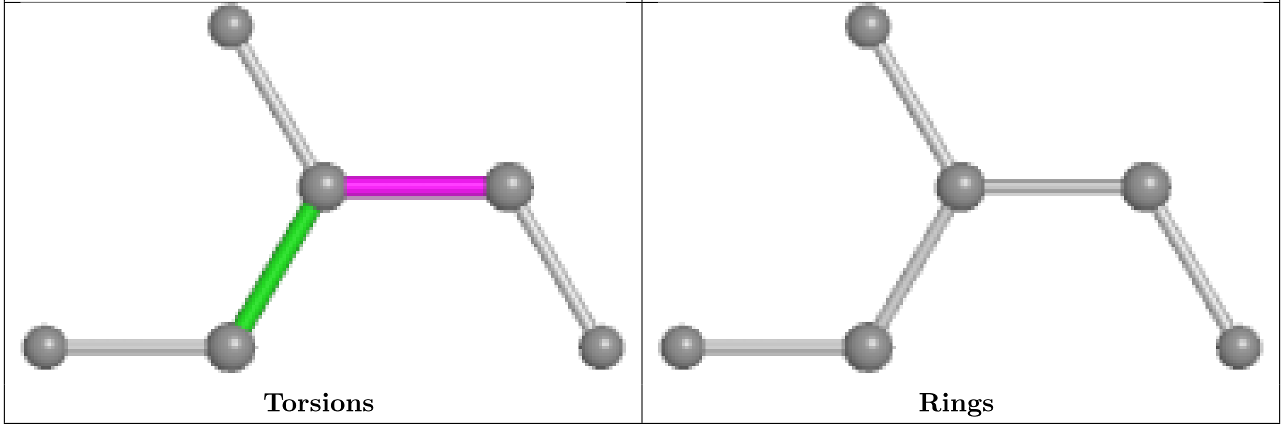
Torsions

Rings

Ligand GOL D 505



Bond lengths **Bond angles**



Torsions **Rings**

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	335/410 (81%)	0.26	21 (6%)	20	18	50, 69, 93, 110	0
1	B	335/410 (81%)	0.01	9 (2%)	54	52	41, 59, 83, 106	0
1	C	336/410 (81%)	-0.09	7 (2%)	63	60	37, 47, 78, 100	0
1	D	334/410 (81%)	-0.10	7 (2%)	63	60	33, 49, 76, 127	0
1	E	334/410 (81%)	-0.22	2 (0%)	89	88	31, 45, 75, 120	0
1	F	335/410 (81%)	-0.17	12 (3%)	42	41	36, 50, 78, 101	0
1	G	335/410 (81%)	0.11	17 (5%)	28	26	42, 59, 84, 113	0
1	H	337/410 (82%)	0.30	21 (6%)	20	19	41, 67, 93, 121	0
All	All	2681/3280 (81%)	0.01	96 (3%)	42	41	31, 55, 87, 127	0

The worst 5 of 96 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	278	VAL	8.7
1	H	266	LEU	4.9
1	A	105	ASP	4.8
1	C	105	ASP	4.5
1	H	279	LYS	4.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	C	502	14/15	0.55	0.31	84,95,101,103	0
6	NAG	F	505	14/15	0.60	0.26	98,110,115,117	0
2	GOL	C	508	6/6	0.73	0.42	63,67,73,74	0
4	PO4	A	603	5/5	0.74	0.33	90,96,104,111	0
5	PPV	G	501	9/9	0.74	0.29	91,97,111,111	0
6	NAG	D	502	14/15	0.78	0.21	57,75,85,87	0
3	ACY	F	506	4/4	0.80	0.45	61,66,70,71	0
2	GOL	E	505	6/6	0.81	0.17	59,63,64,65	0
5	PPV	F	501	9/9	0.81	0.31	74,92,106,106	0
6	NAG	B	502	14/15	0.82	0.26	75,94,103,113	0
2	GOL	B	504	6/6	0.84	0.20	57,73,74,76	0
2	GOL	E	506	6/6	0.85	0.25	61,63,68,68	0
5	PPV	E	501	9/9	0.85	0.26	59,73,85,93	0
3	ACY	A	602	4/4	0.86	0.15	63,70,71,72	0
2	GOL	C	503	6/6	0.86	0.25	54,61,66,67	0
3	ACY	B	505	4/4	0.87	0.20	53,60,68,74	0
2	GOL	D	503	6/6	0.87	0.21	55,64,67,70	0
2	GOL	D	506	6/6	0.88	0.19	50,54,61,62	0
5	PPV	D	501	9/9	0.88	0.38	69,83,90,102	0
6	NAG	E	502	14/15	0.88	0.19	78,88,95,95	0
2	GOL	D	505	6/6	0.88	0.20	46,49,52,72	0
3	ACY	H	503	4/4	0.89	0.20	60,62,64,66	0
3	ACY	C	506	4/4	0.89	0.18	43,54,57,61	0
5	PPV	C	501	9/9	0.89	0.35	67,86,93,99	0
2	GOL	F	502	6/6	0.90	0.20	51,63,63,69	0
5	PPV	B	501	9/9	0.90	0.30	73,92,98,105	0
2	GOL	A	601	6/6	0.90	0.17	62,68,75,87	0
2	GOL	E	503	6/6	0.91	0.19	41,46,58,65	0
3	ACY	E	504	4/4	0.91	0.12	39,47,54,54	0
5	PPV	H	501	9/9	0.91	0.28	88,105,108,122	0
2	GOL	C	504	6/6	0.91	0.18	49,52,58,61	0
3	ACY	G	503	4/4	0.92	0.18	52,58,62,69	0
2	GOL	F	503	6/6	0.92	0.12	52,57,64,69	0
2	GOL	C	509	6/6	0.92	0.15	45,53,57,60	0
2	GOL	C	505	6/6	0.93	0.20	54,59,62,69	0
2	GOL	C	507	6/6	0.93	0.24	59,60,63,72	0
2	GOL	B	503	6/6	0.93	0.15	51,55,59,67	0

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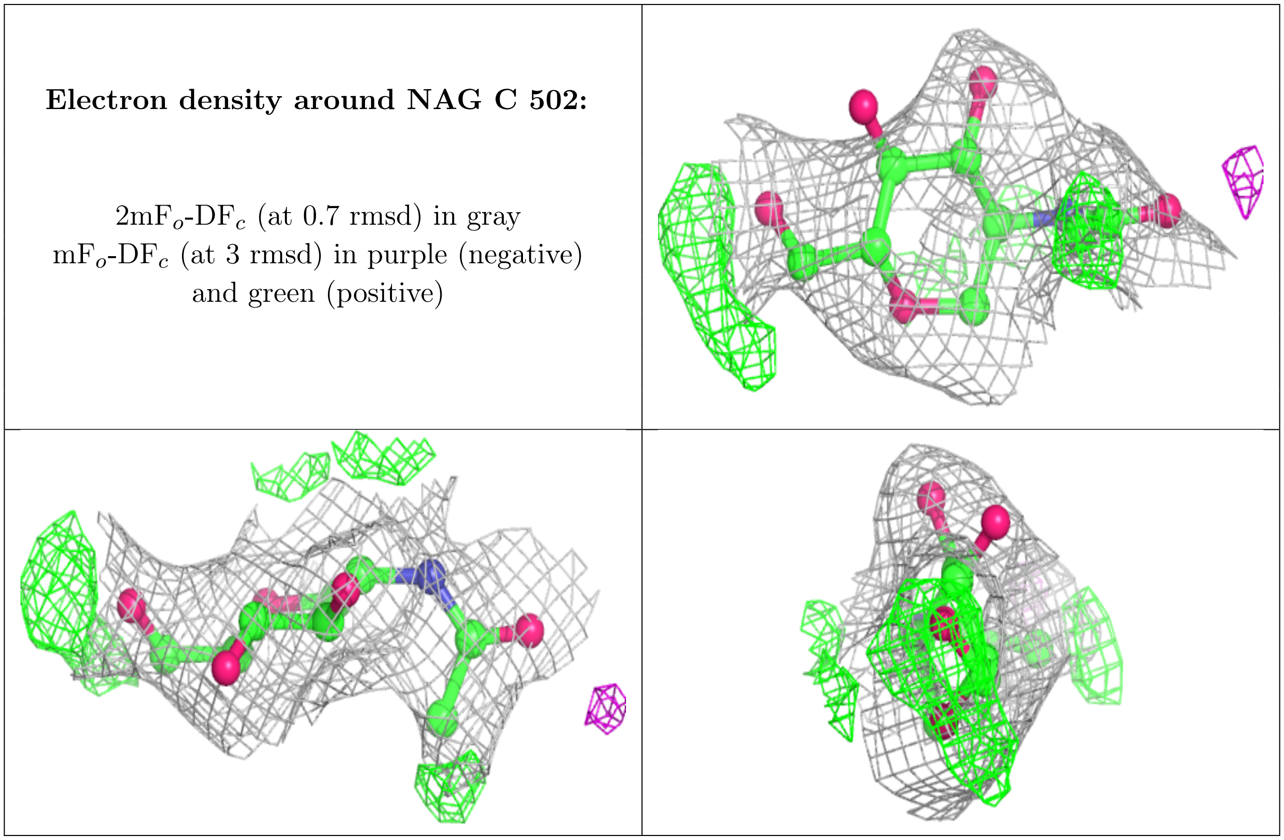
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	H	502	6/6	0.93	0.12	52,60,65,76	0
2	GOL	D	504	6/6	0.94	0.17	54,58,62,70	0
2	GOL	F	504	6/6	0.94	0.10	47,51,54,64	0
2	GOL	G	502	6/6	0.94	0.20	48,51,57,65	0

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.

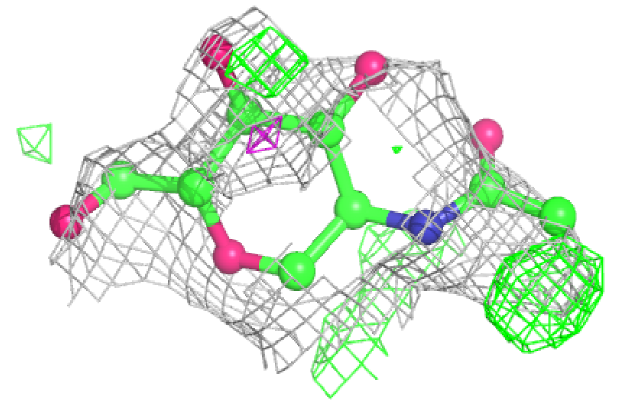


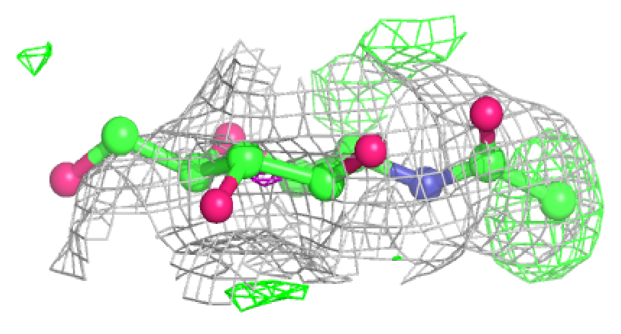
Electron density around NAG C 502:

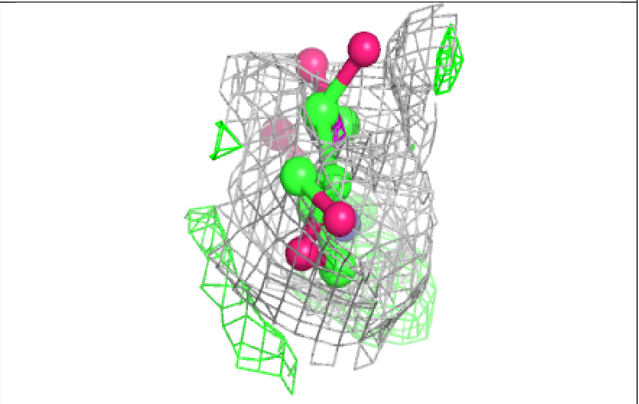
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

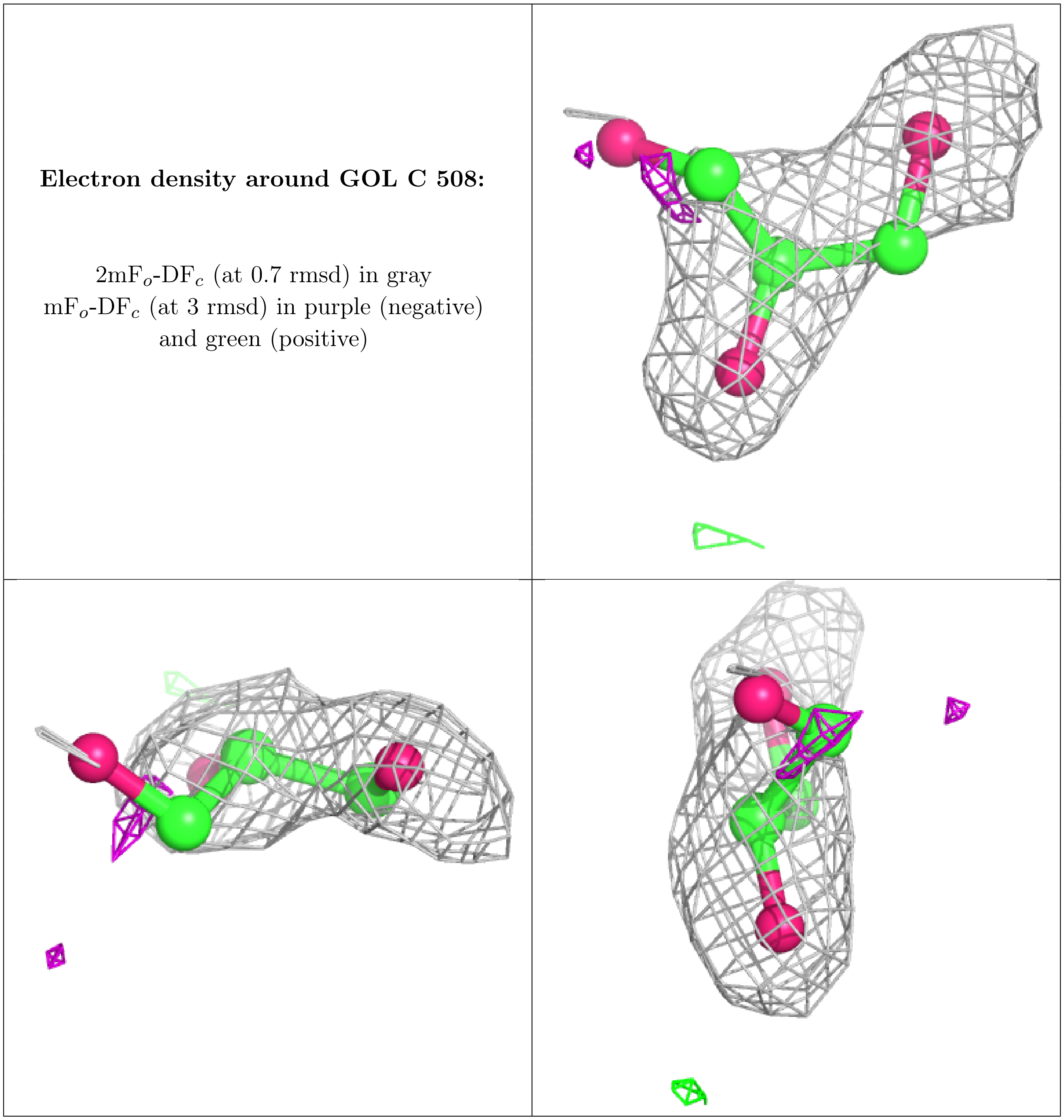
Electron density around NAG F 505:

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







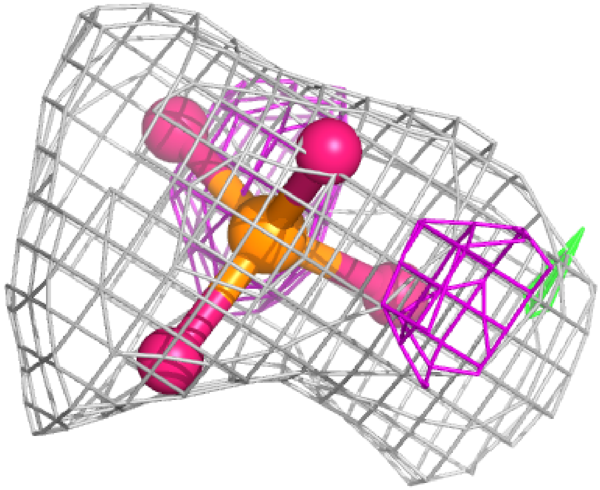


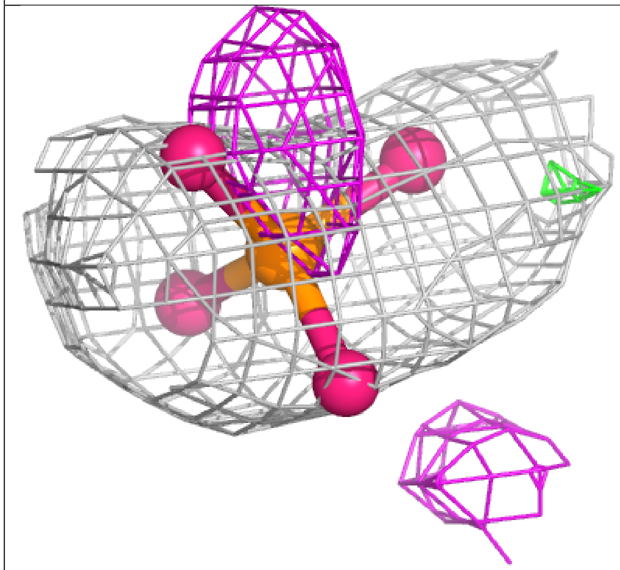
Electron density around GOL C 508:

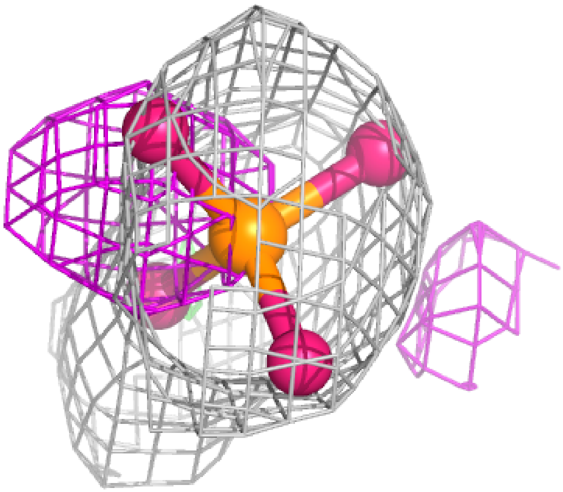
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around PO4 A 603:

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

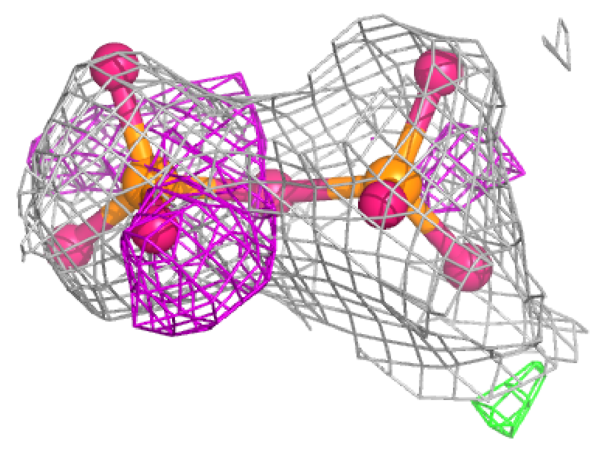


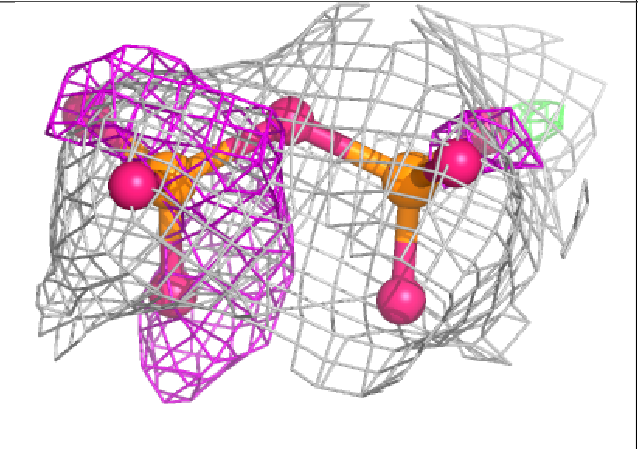


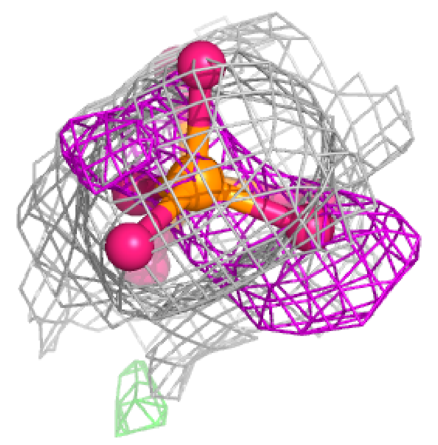


Electron density around PPV G 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

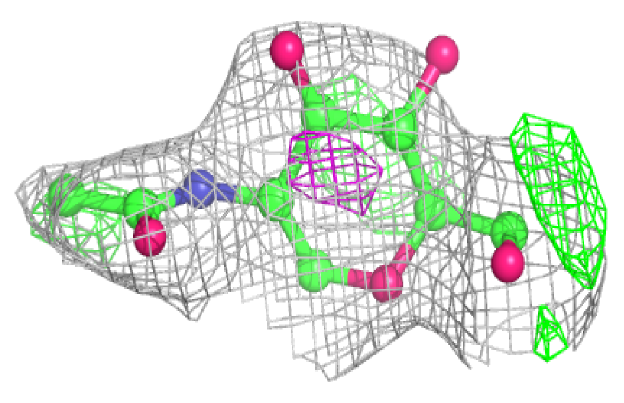


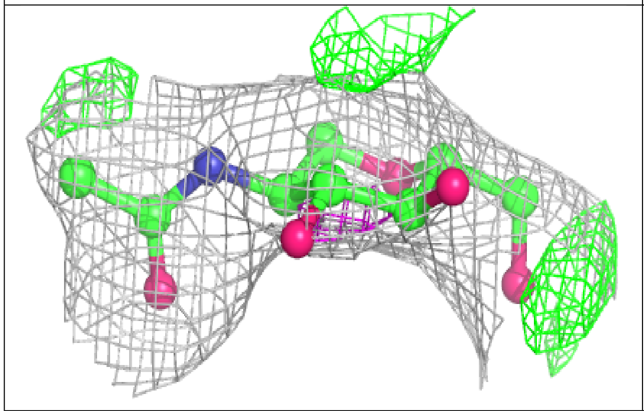


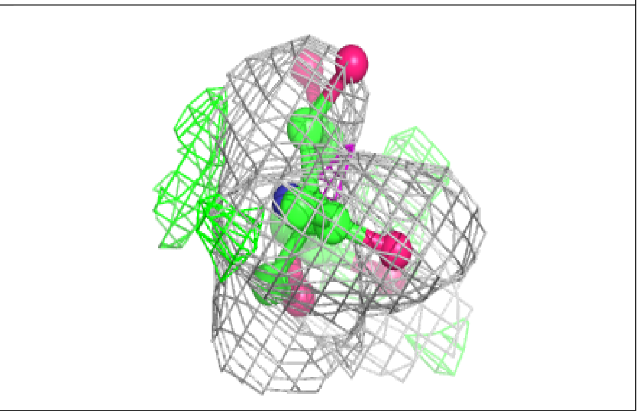


Electron density around NAG D 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

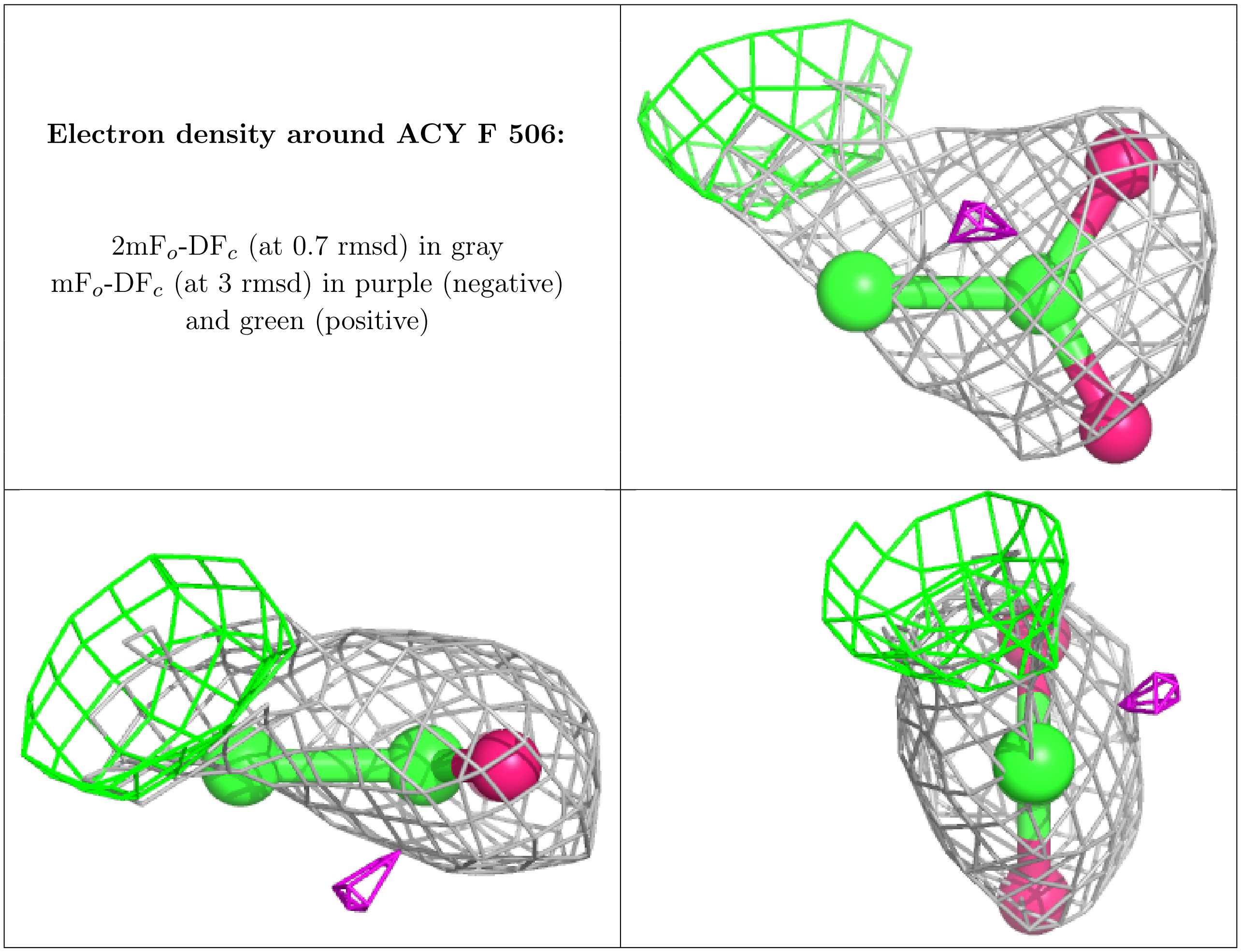






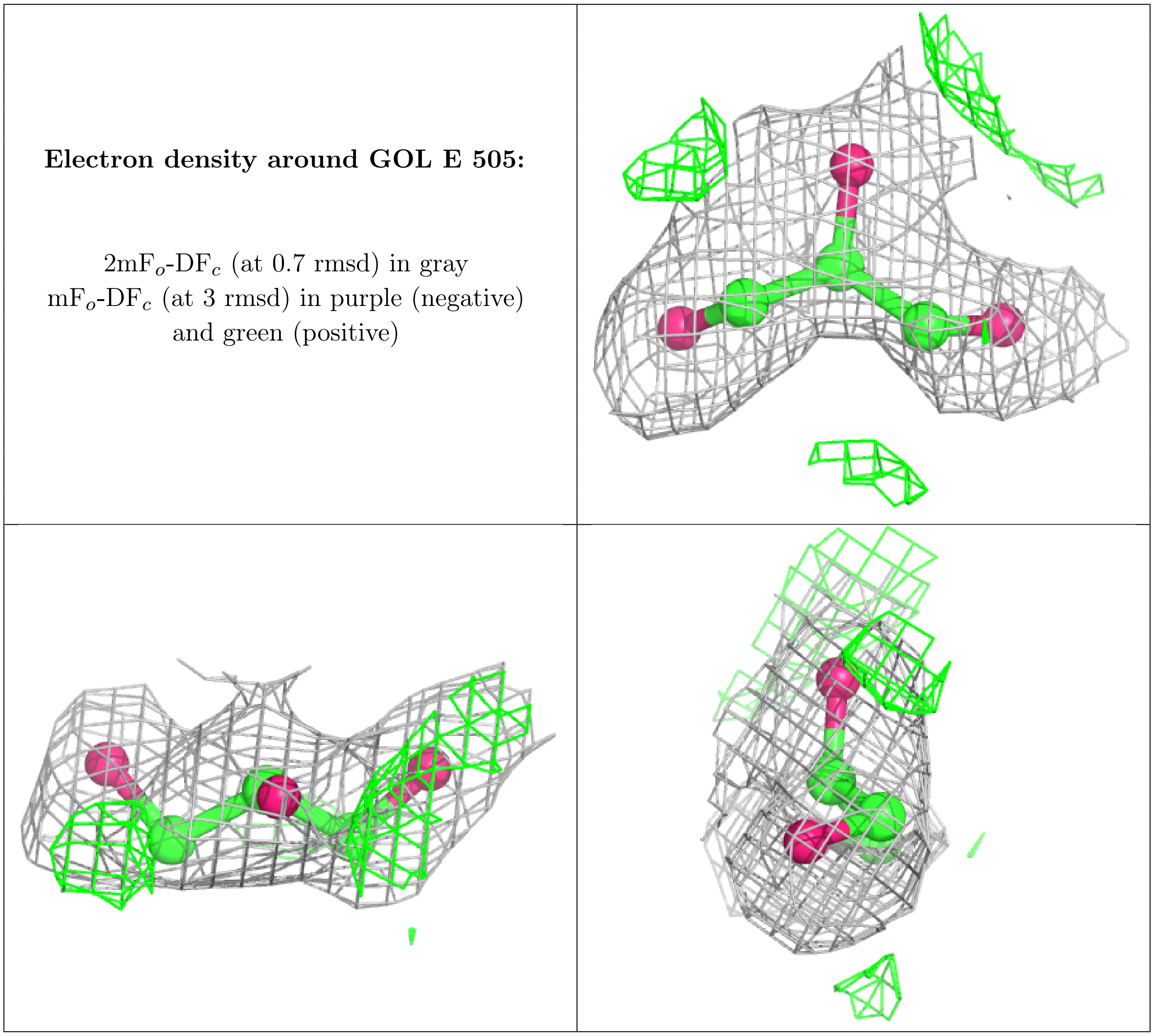
Electron density around ACY F 506:

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



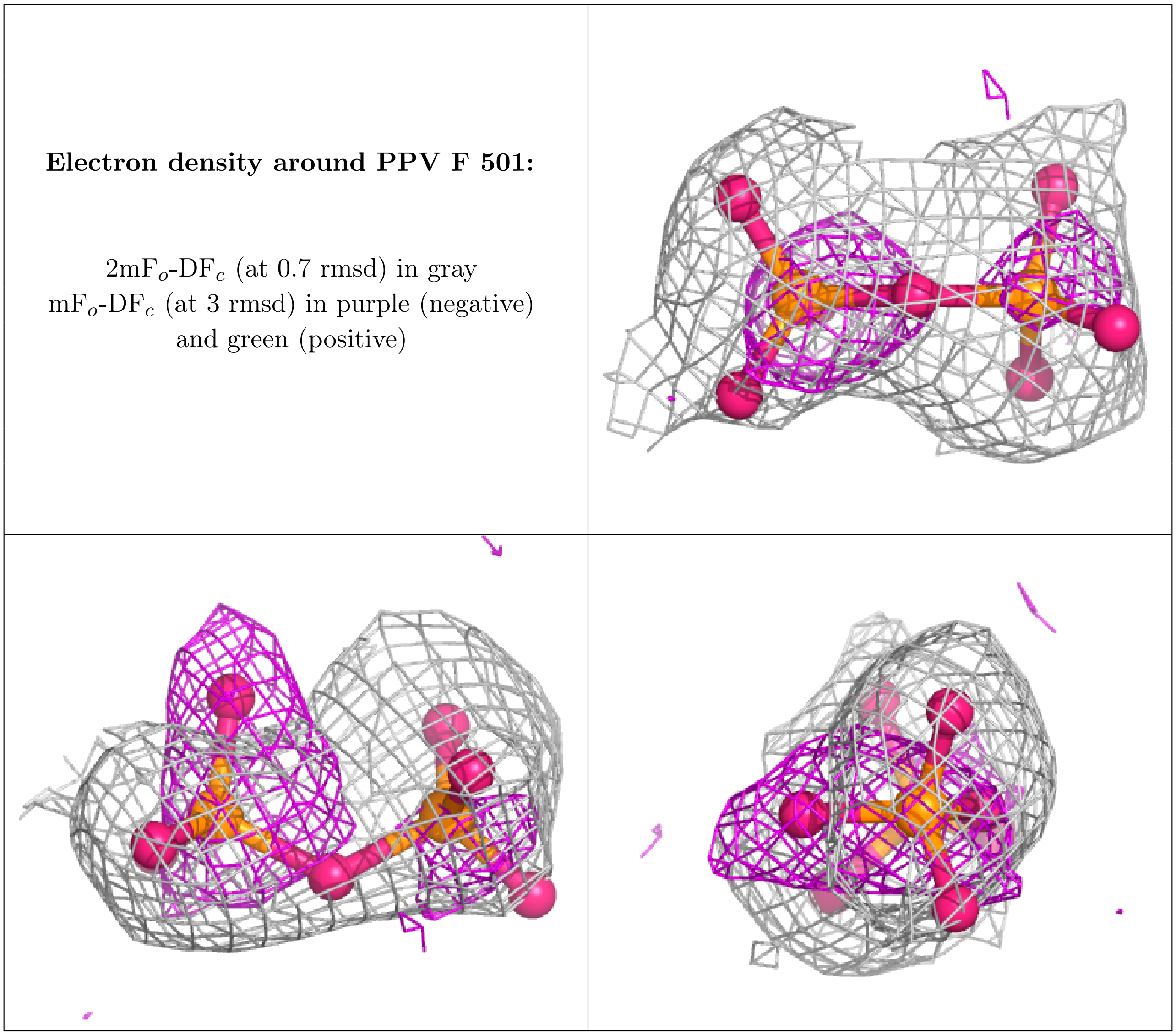
Electron density around GOL E 505:

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



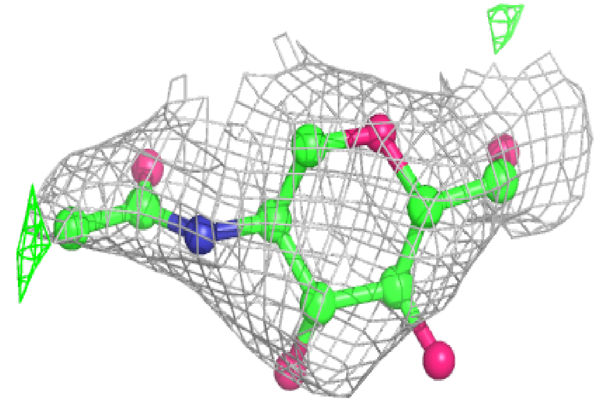
Electron density around PPV F 501:

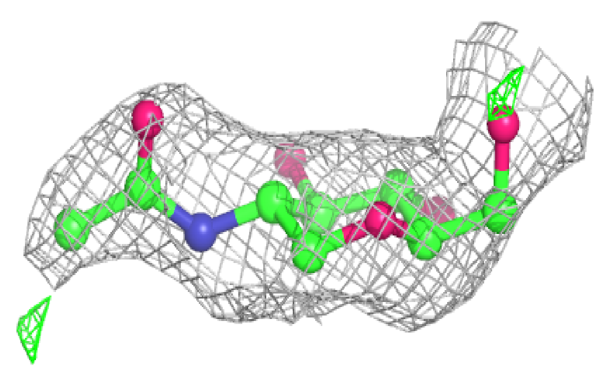
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

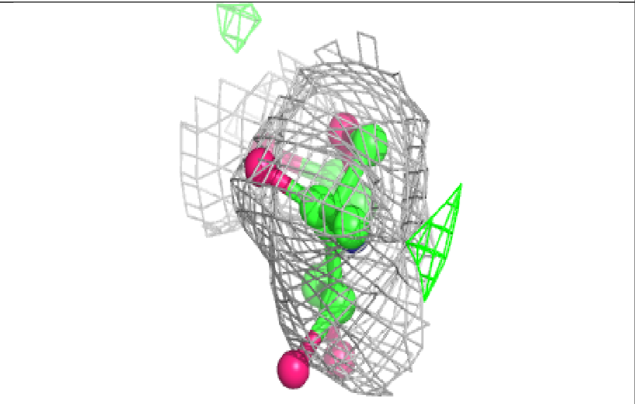


Electron density around NAG B 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

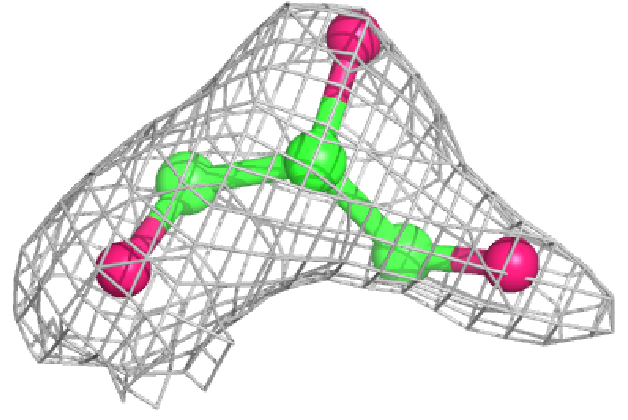


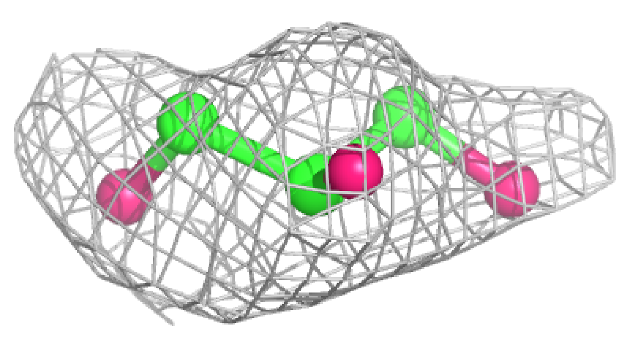


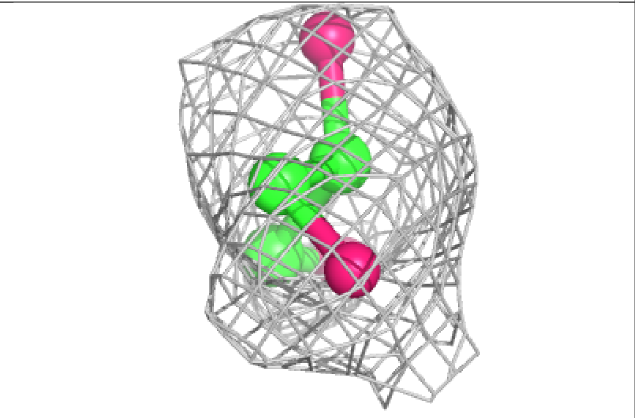


Electron density around GOL B 504:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

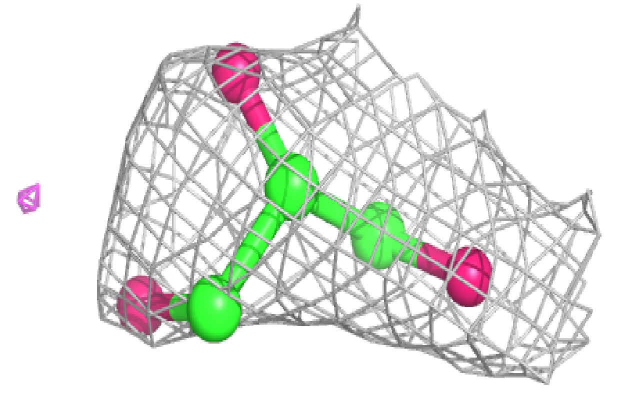


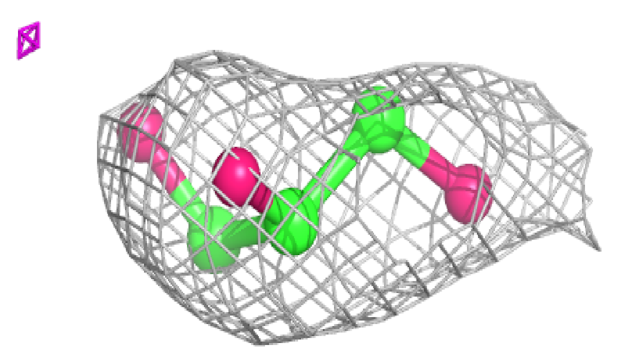


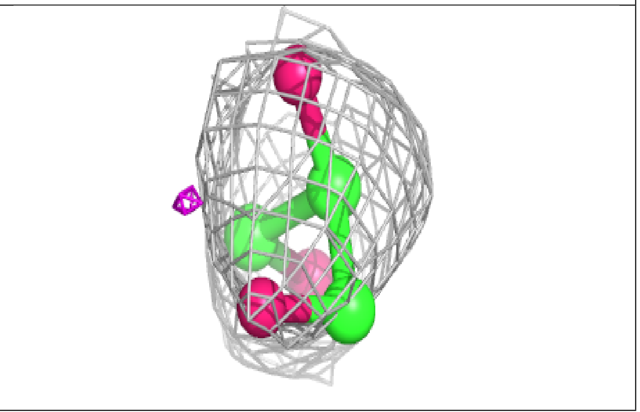


Electron density around GOL E 506:

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

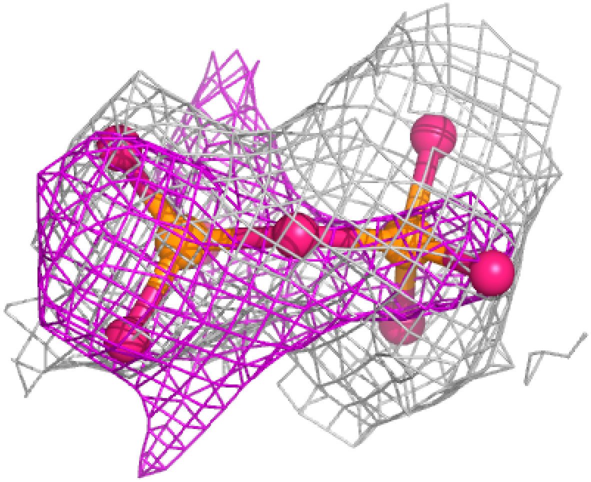


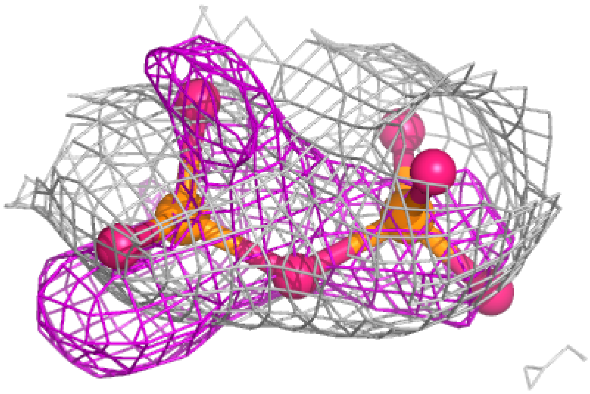


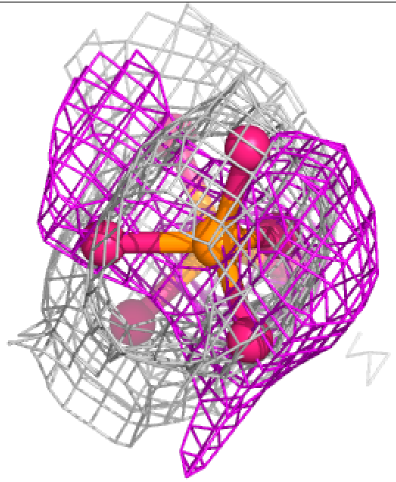


Electron density around PPV E 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

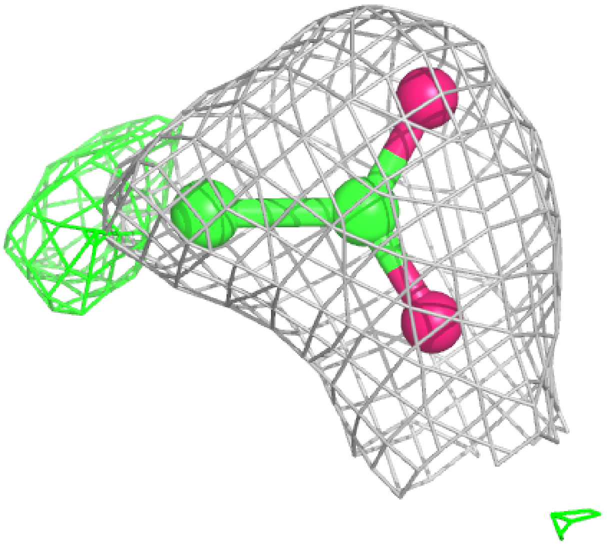


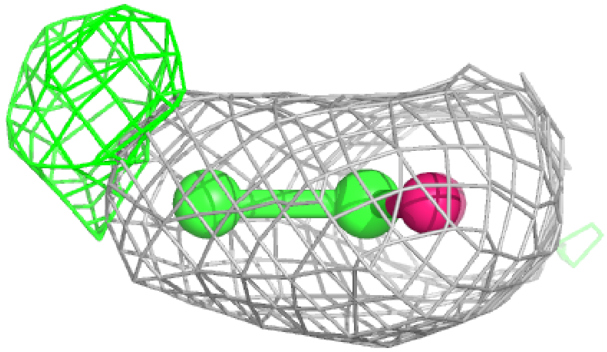


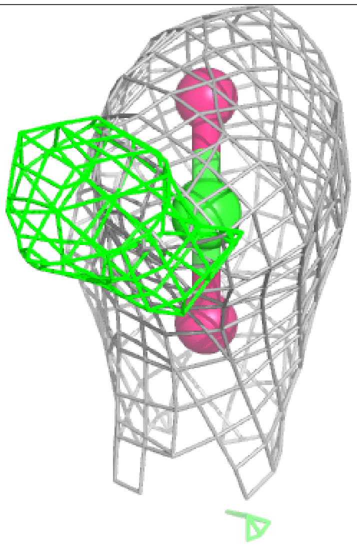


Electron density around ACY A 602:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

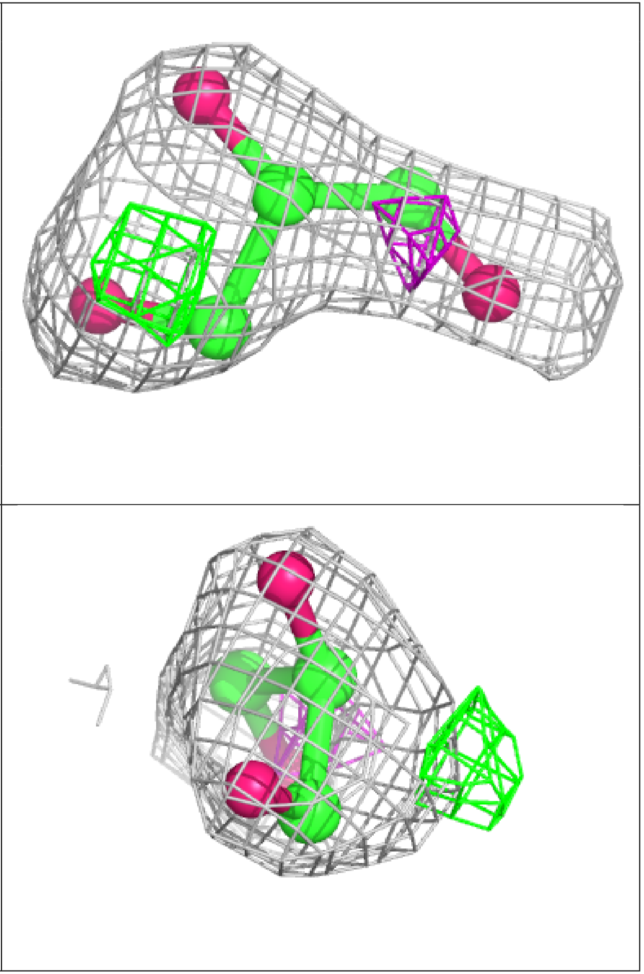


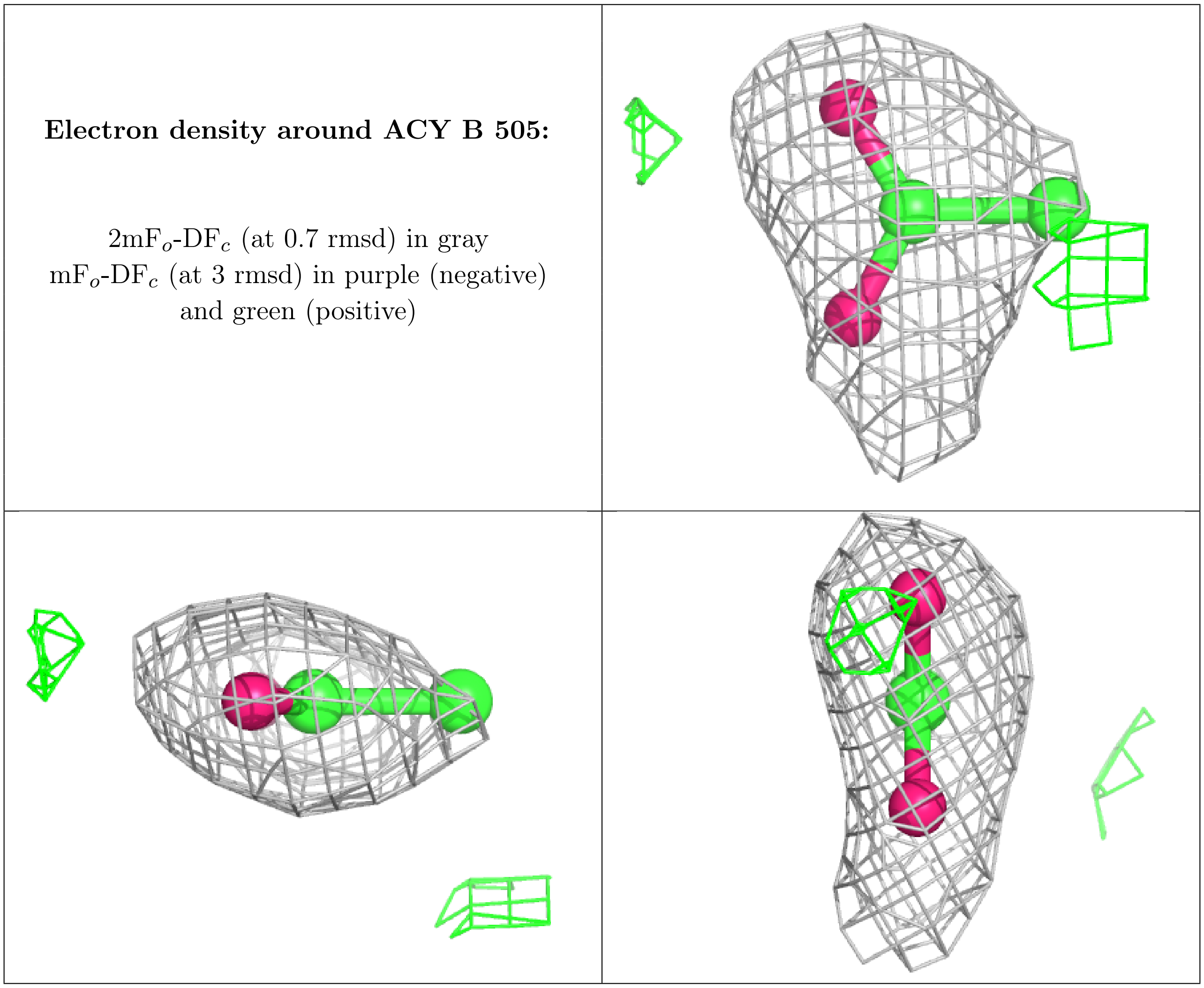




Electron density around GOL C 503:

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



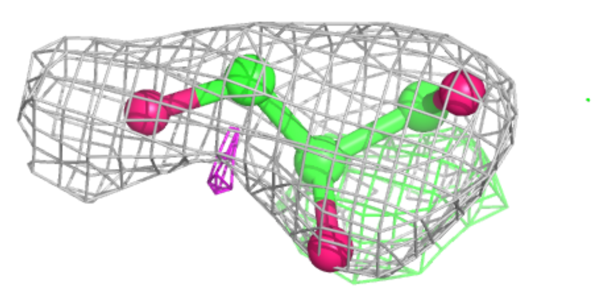


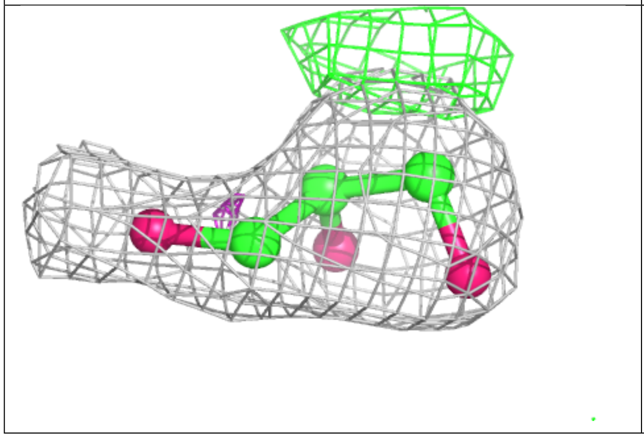
Electron density around ACY B 505:

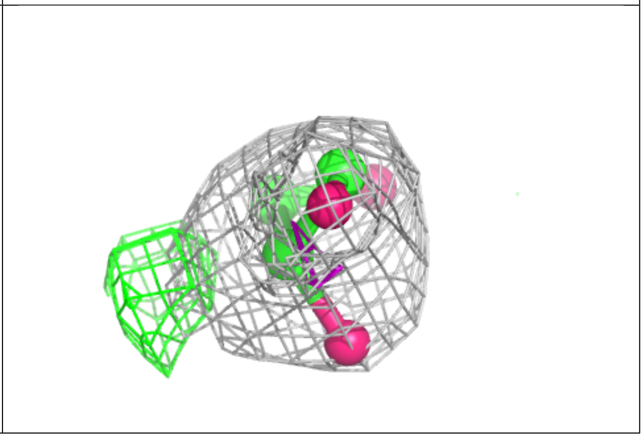
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around GOL D 503:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

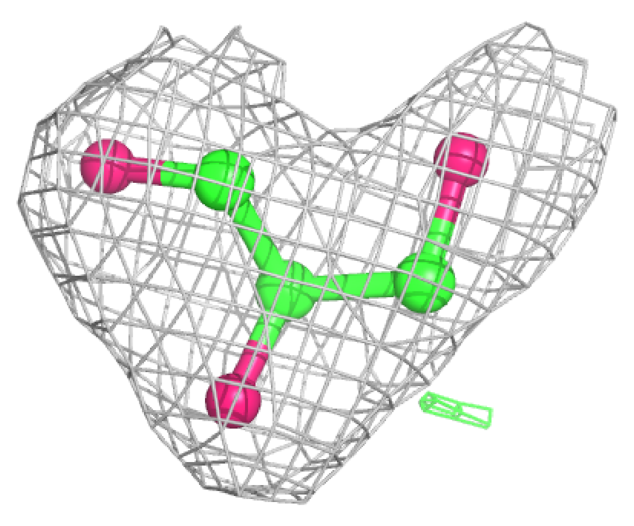


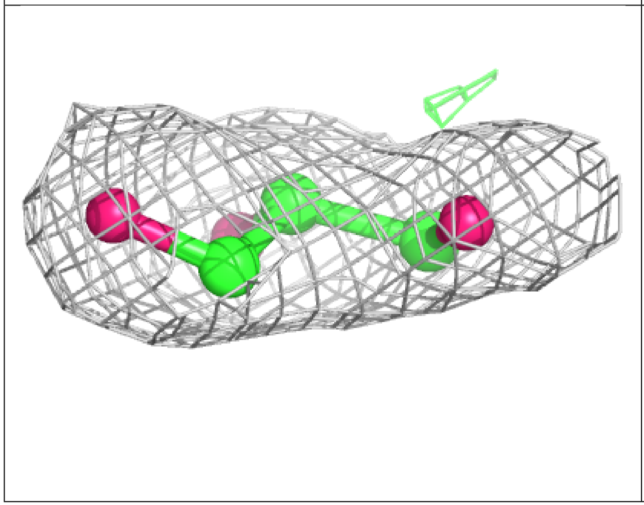


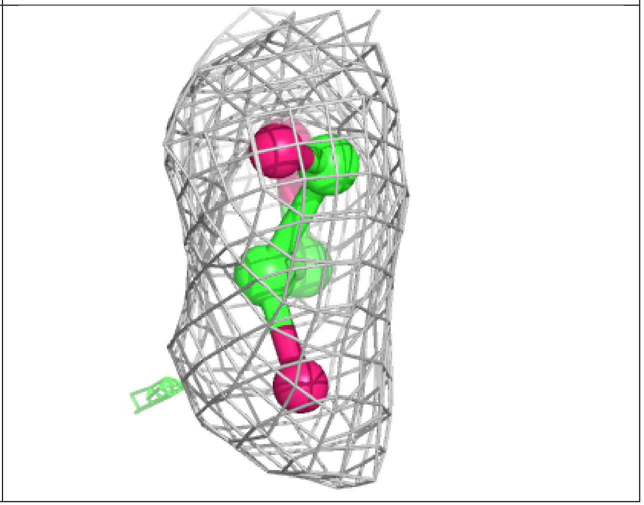


Electron density around GOL D 506:

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

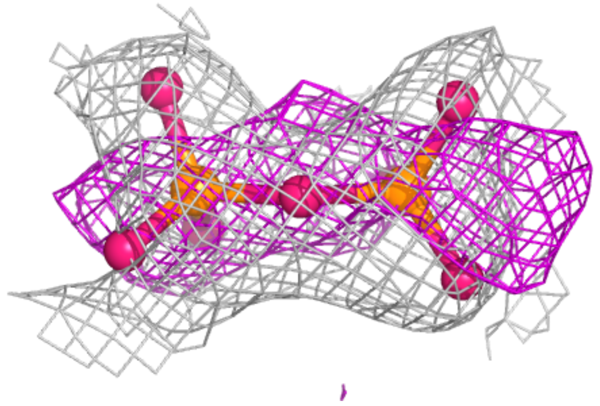


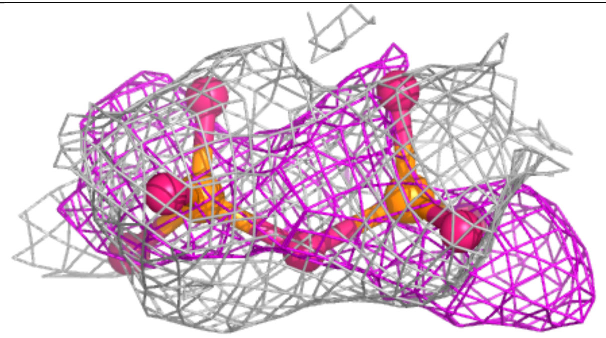


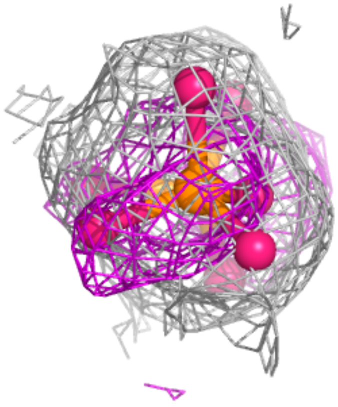


Electron density around PPV D 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

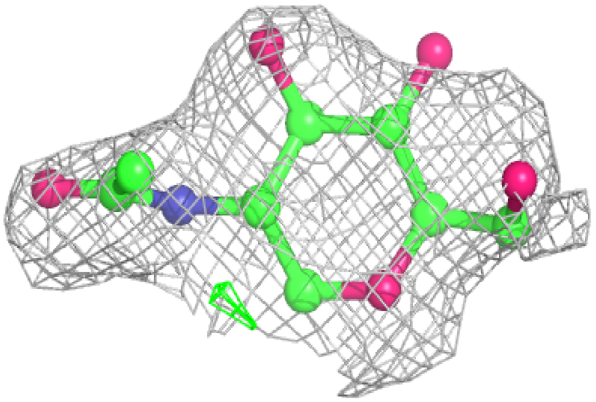


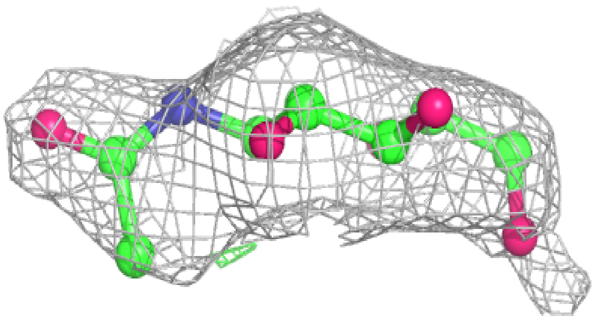


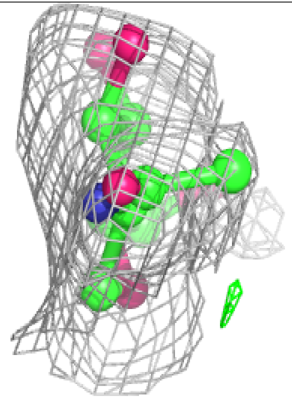


Electron density around NAG E 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

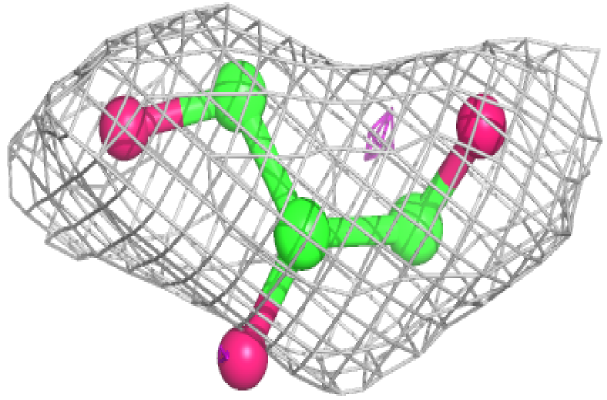


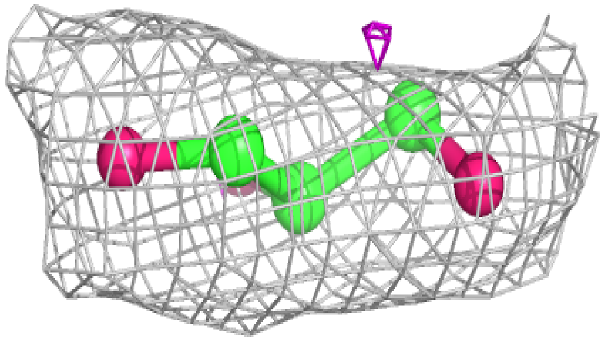


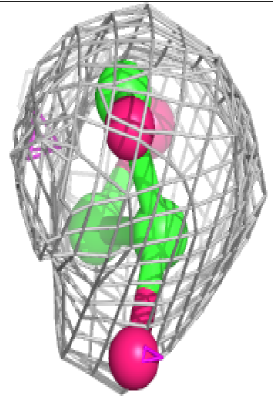


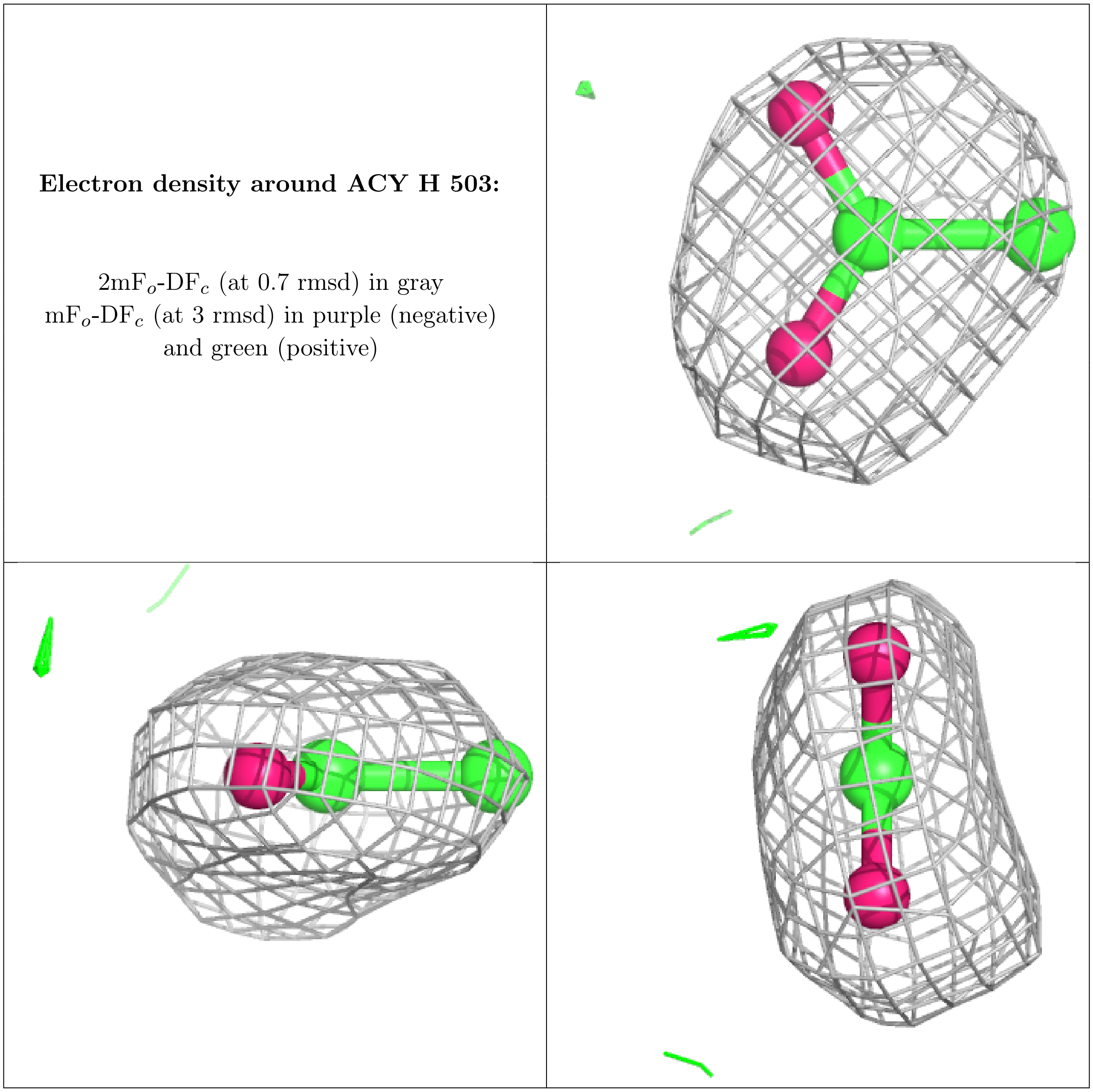
Electron density around GOL D 505:

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







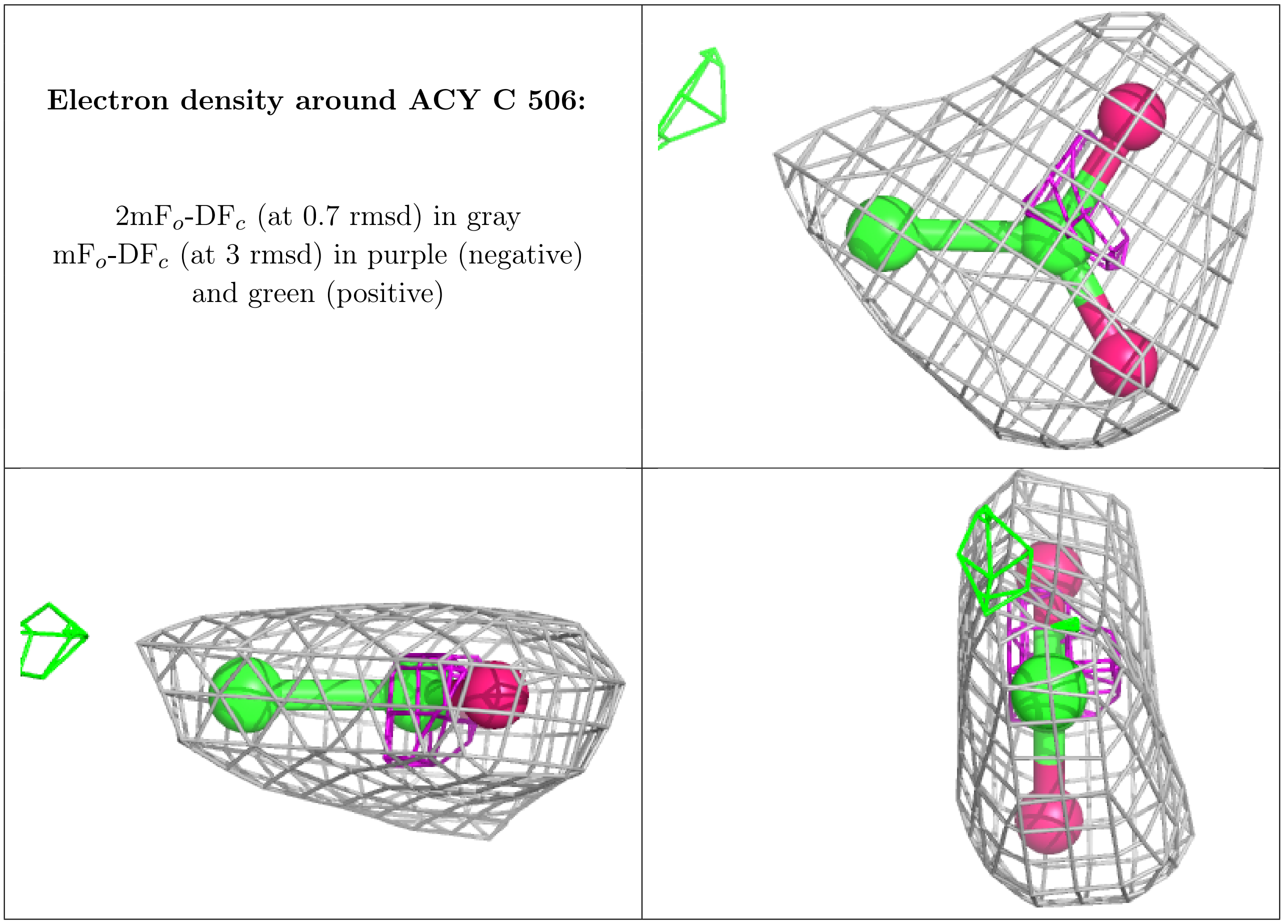


Electron density around ACY H 503:

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

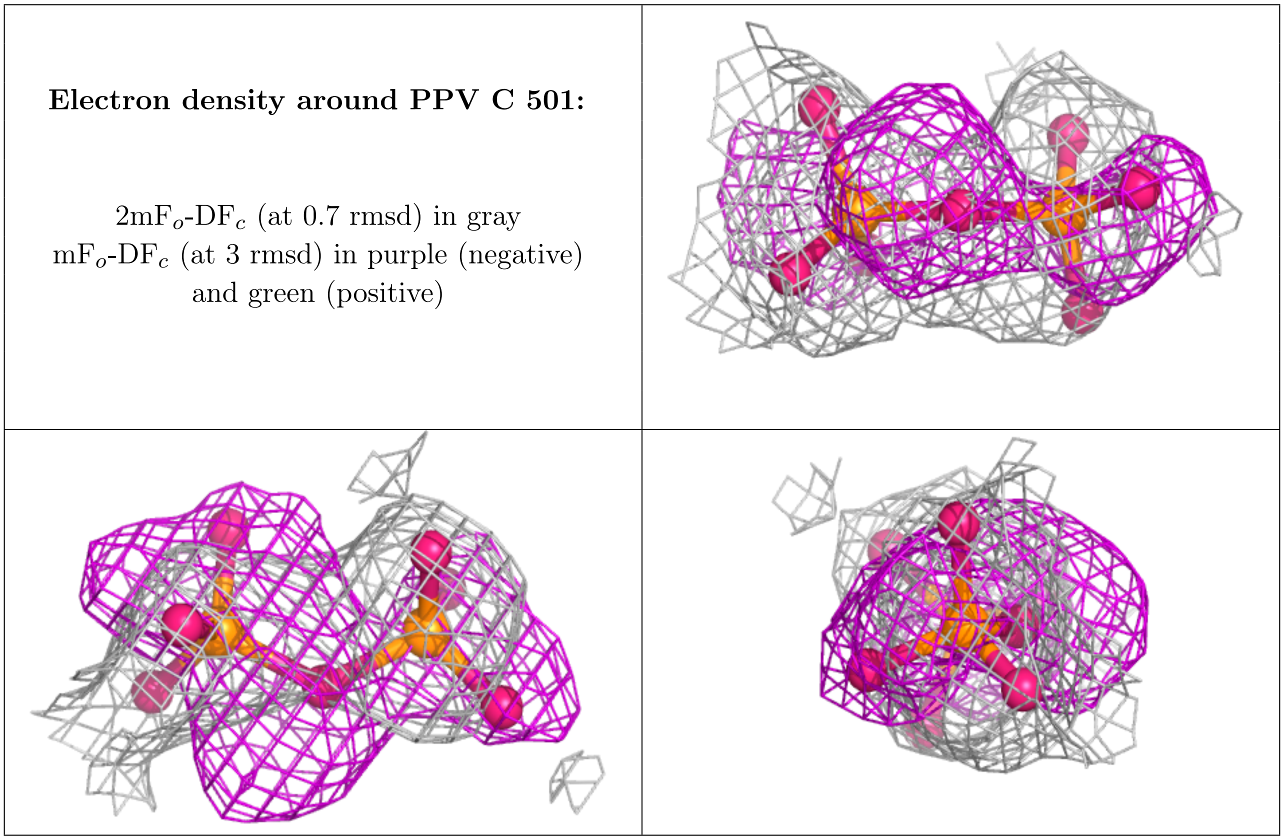
Electron density around ACY C 506:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



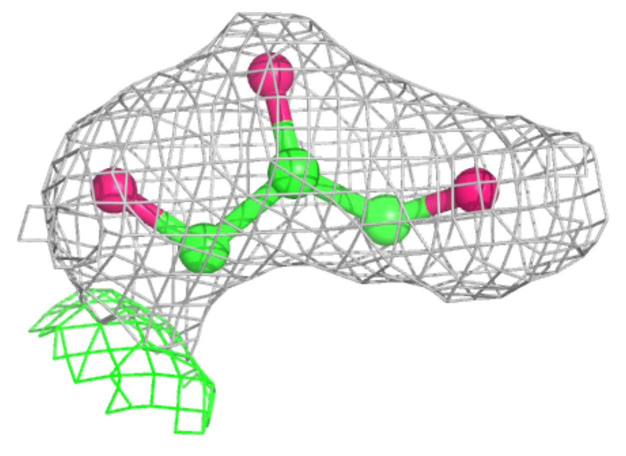
Electron density around PPV C 501:

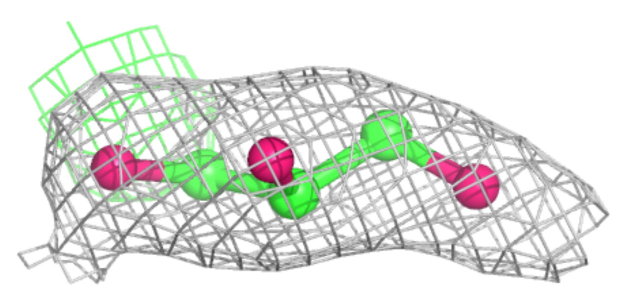
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

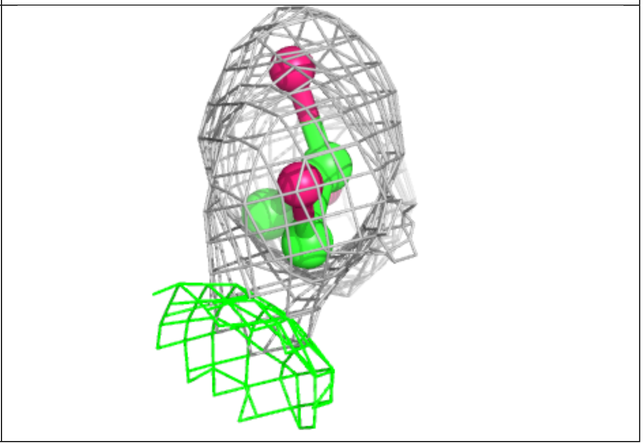


Electron density around GOL F 502:

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

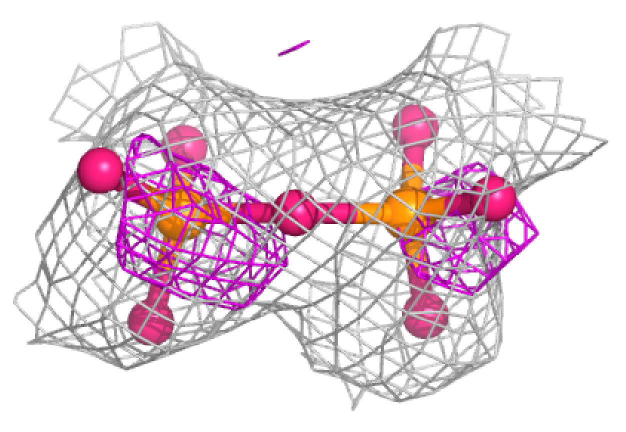


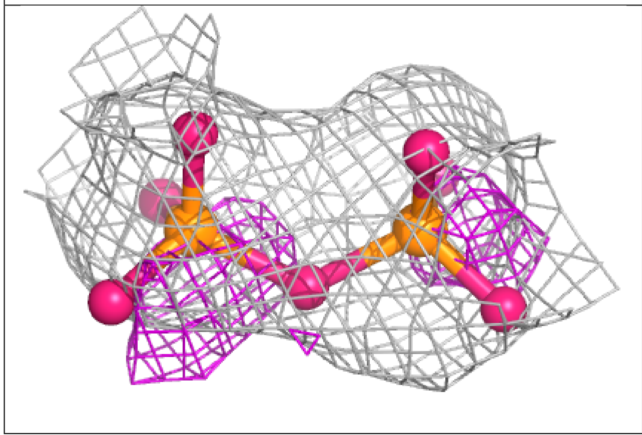


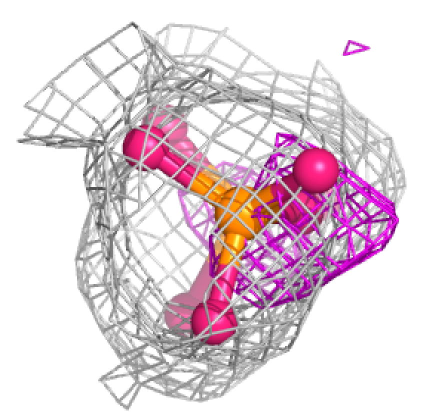


Electron density around PPV B 501:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

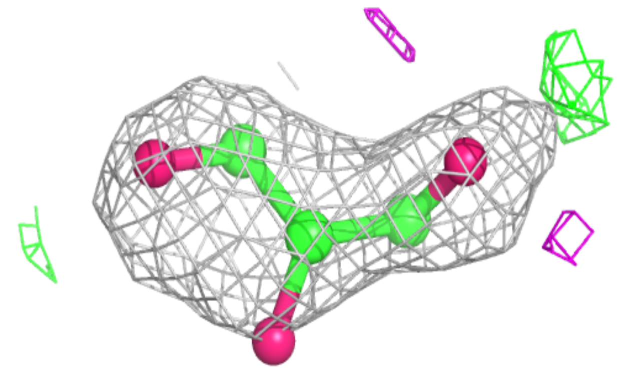


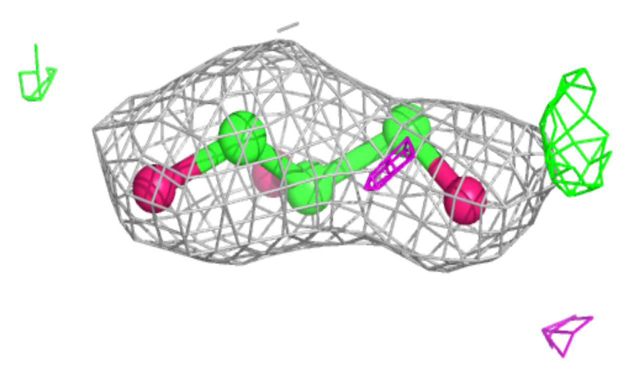


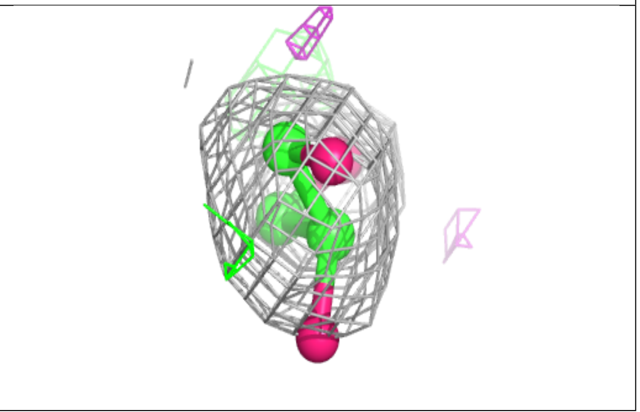


Electron density around GOL A 601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

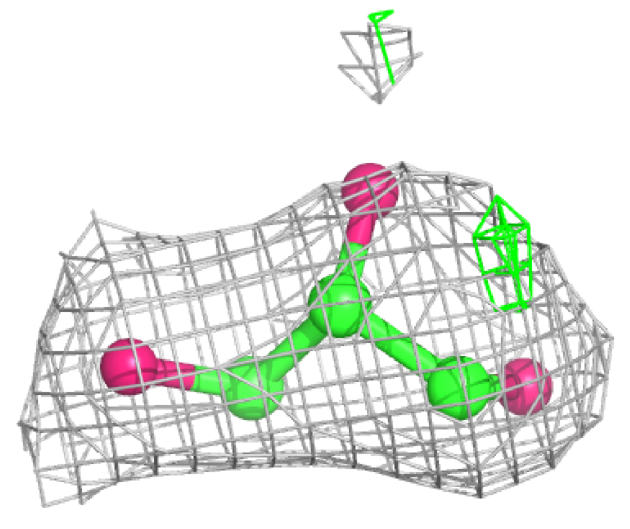


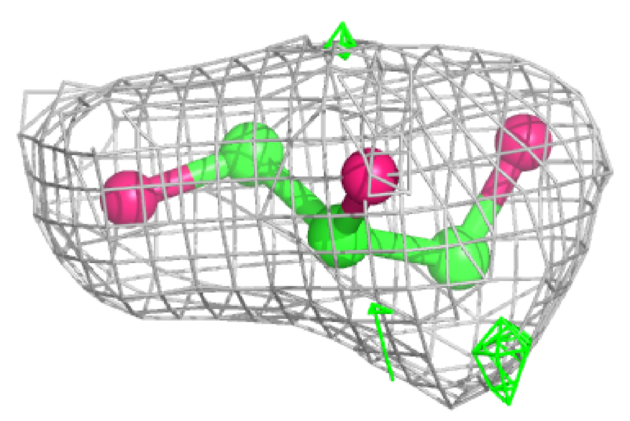


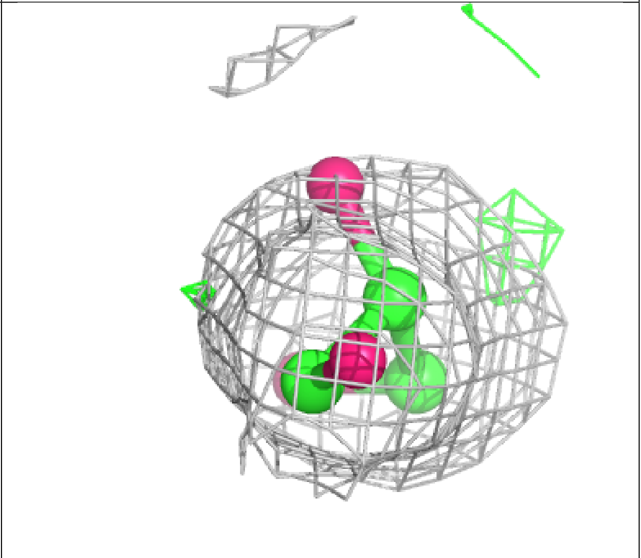


Electron density around GOL E 503:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

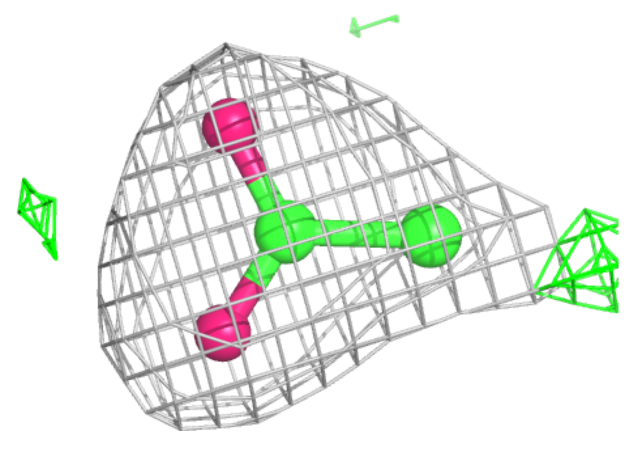


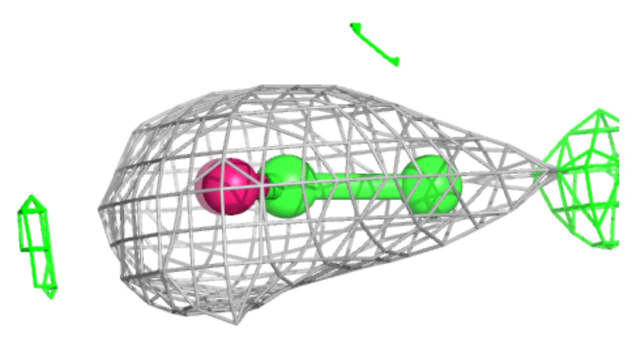


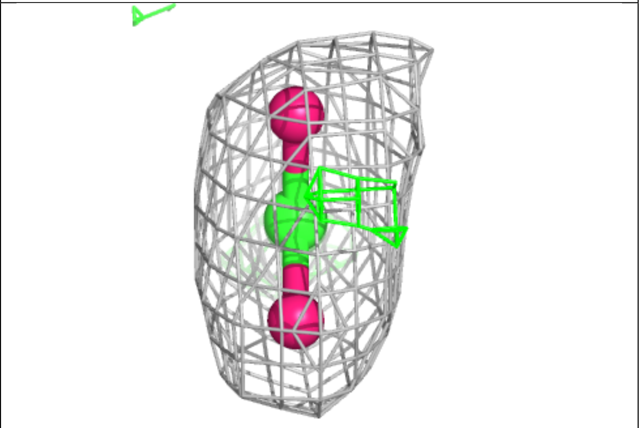


Electron density around ACY E 504:

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

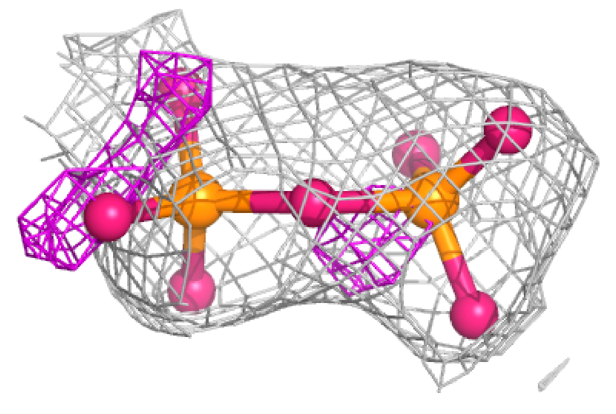


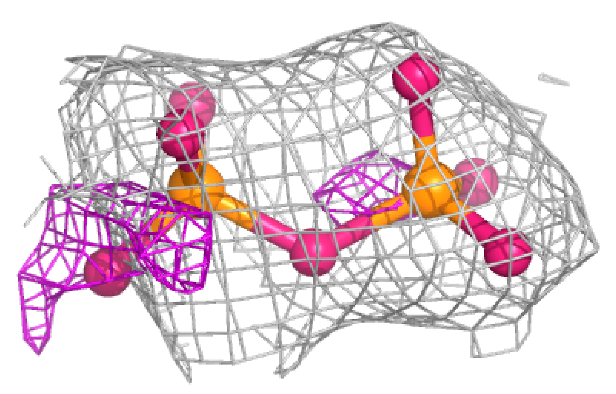


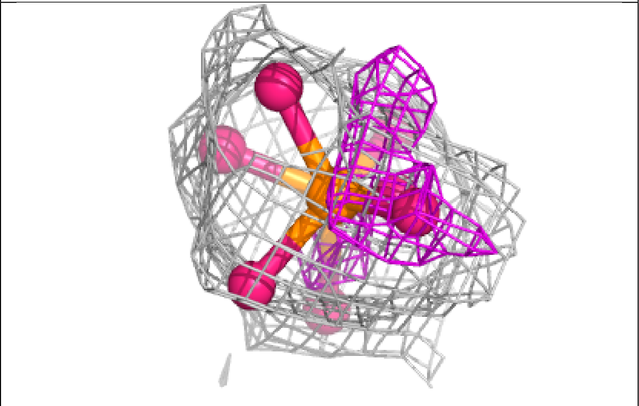


Electron density around PPV H 501:

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

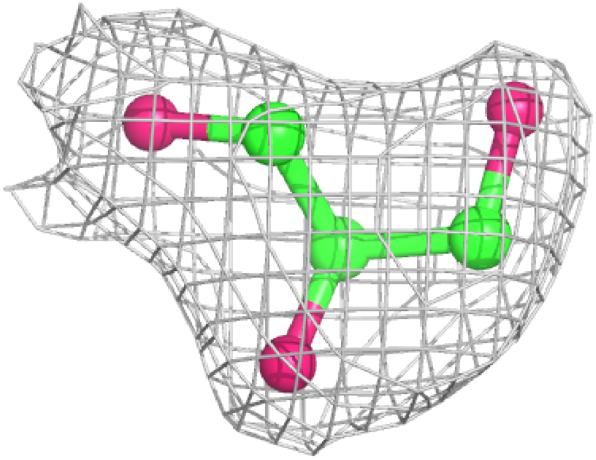


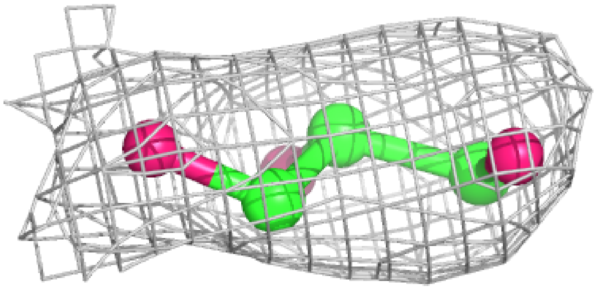


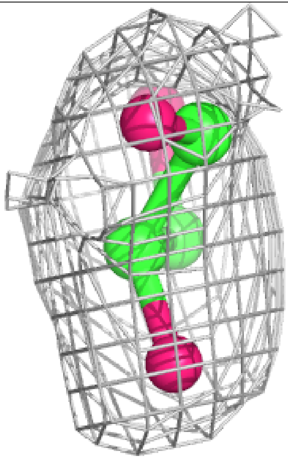


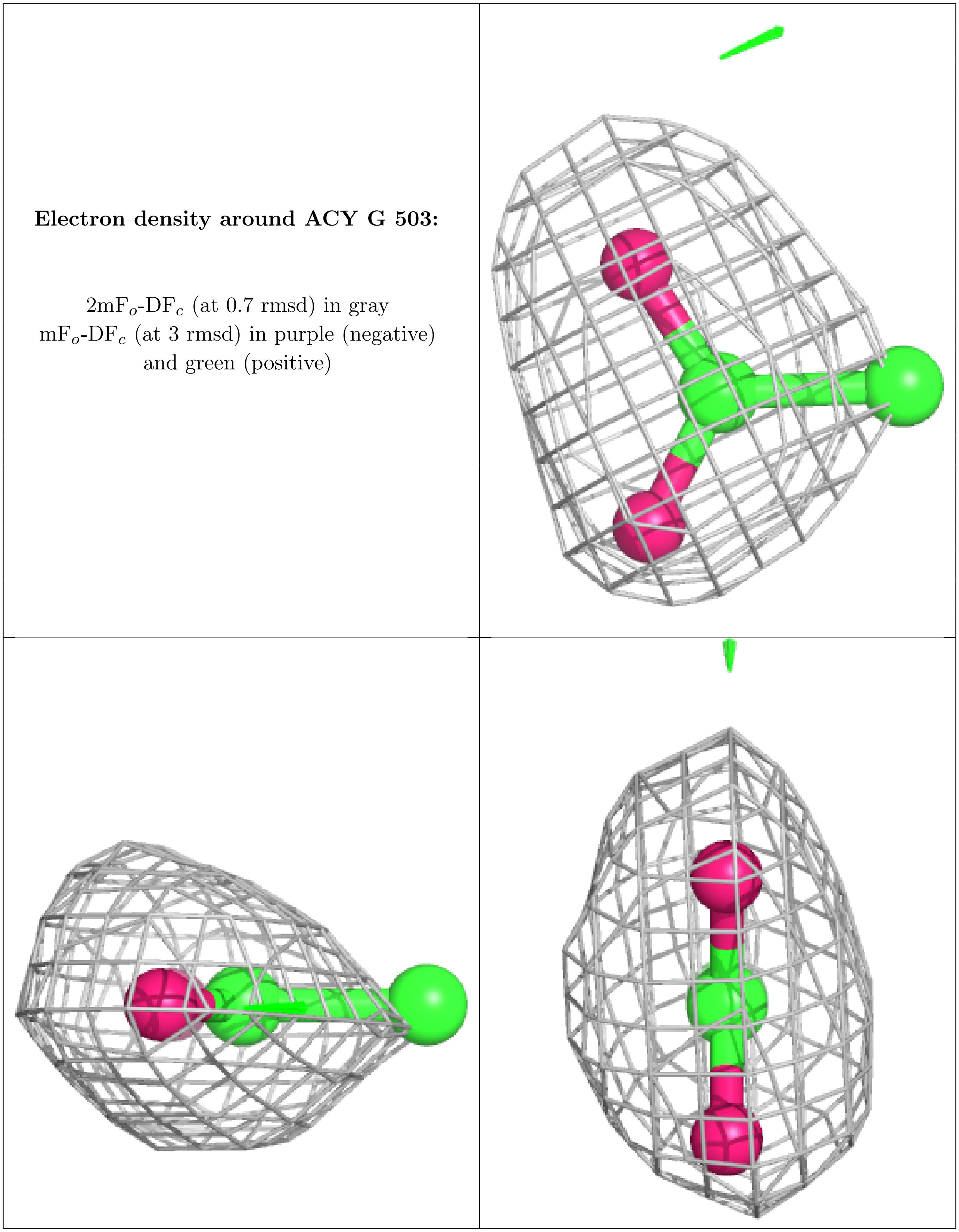
Electron density around GOL C 504:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







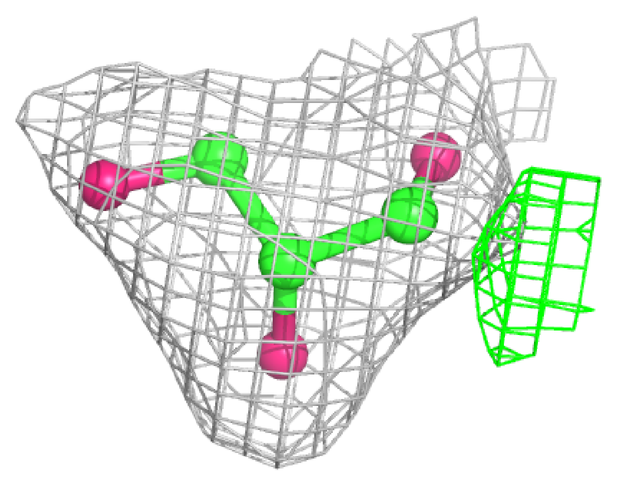


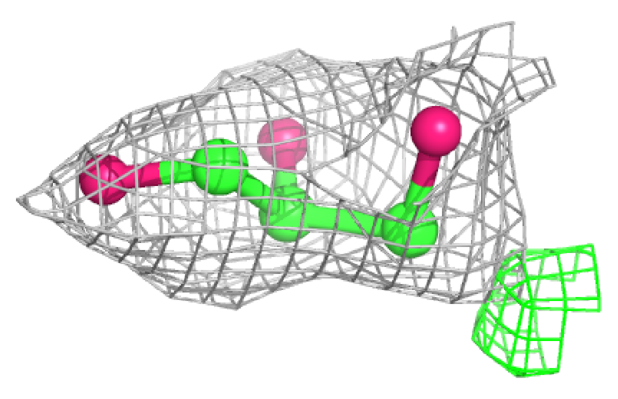
Electron density around ACY G 503:

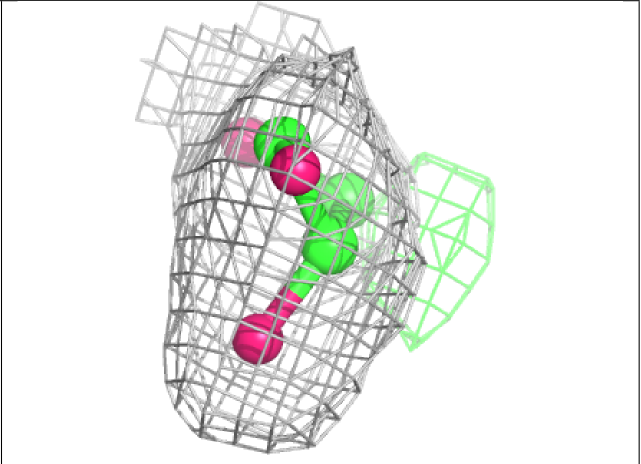
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

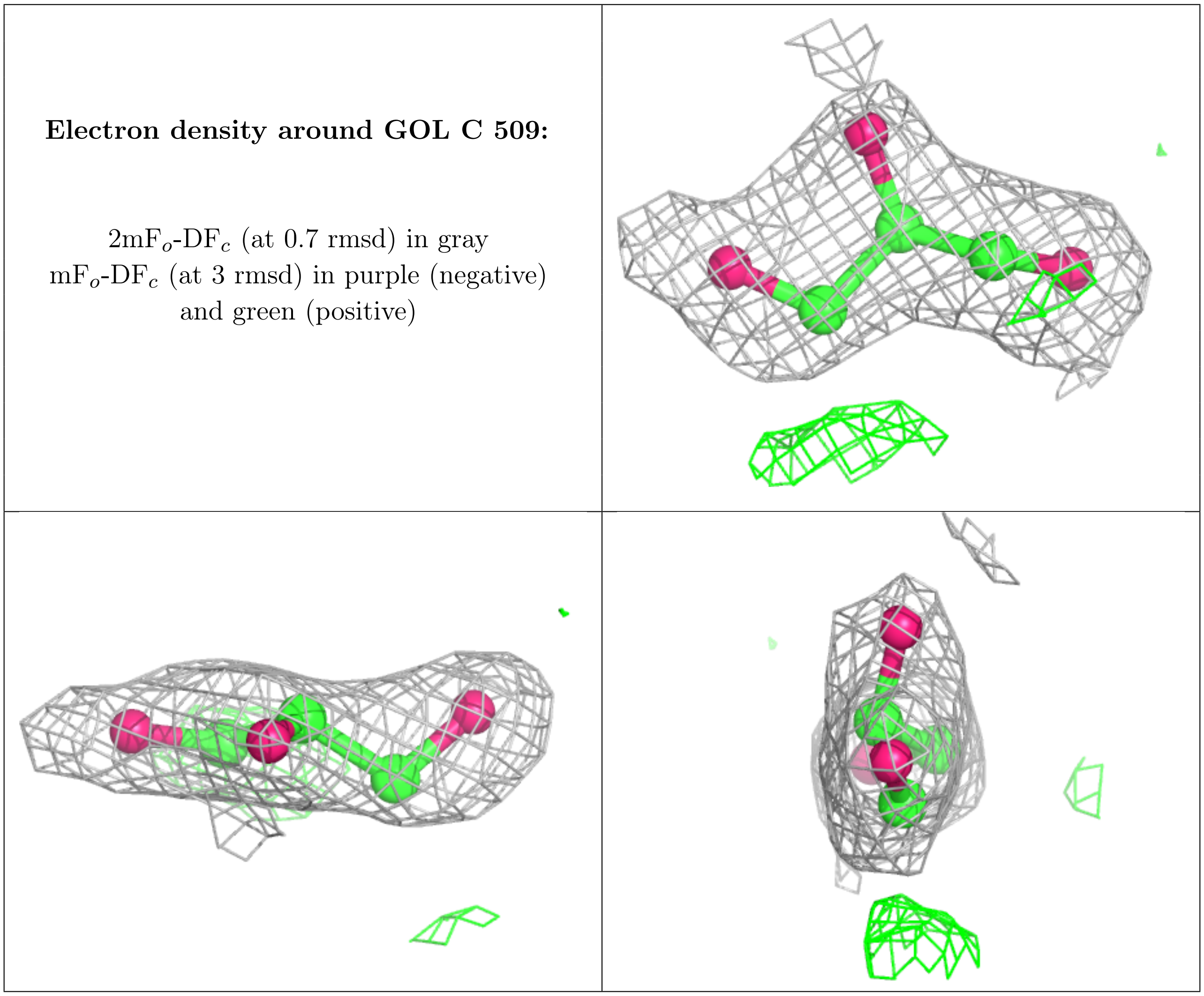
Electron density around GOL F 503:

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







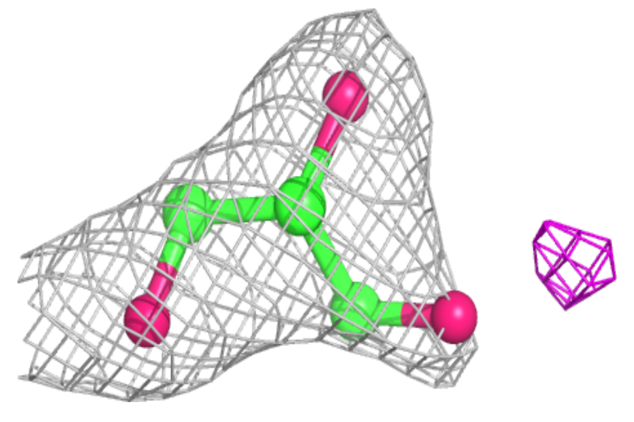


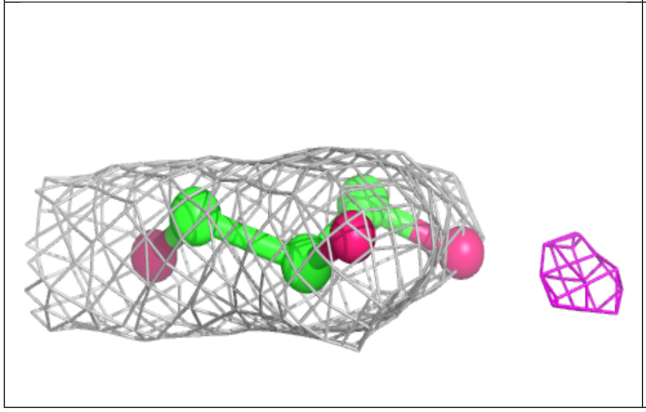
Electron density around GOL C 509:

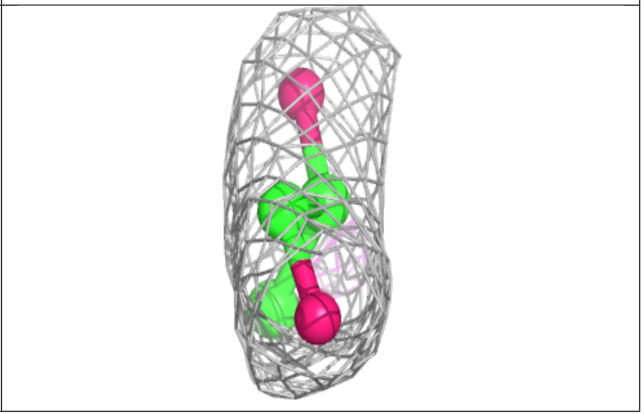
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around GOL C 505:

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

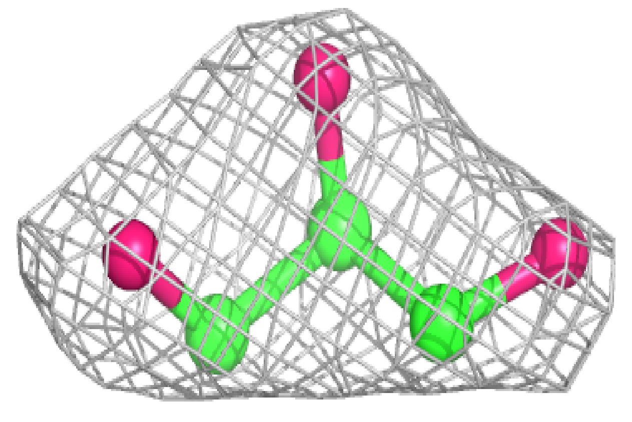


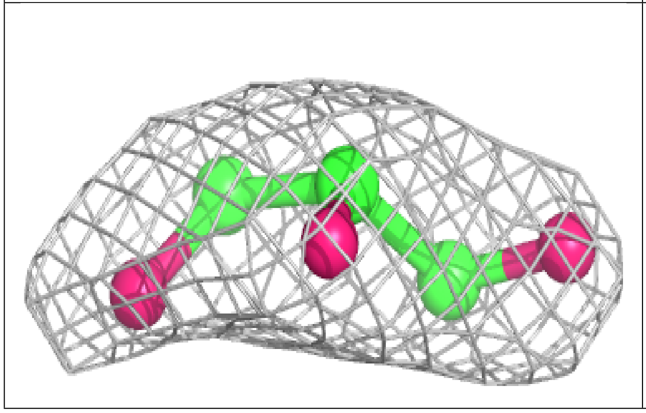


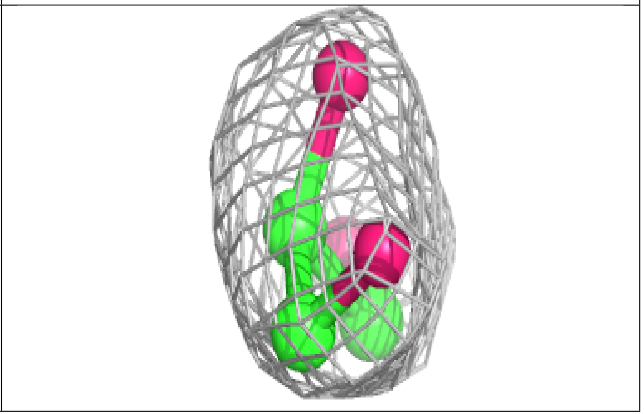


Electron density around GOL C 507:

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

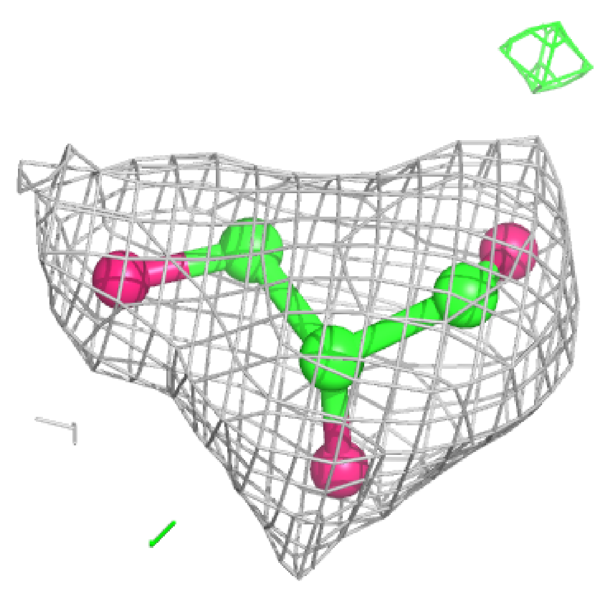


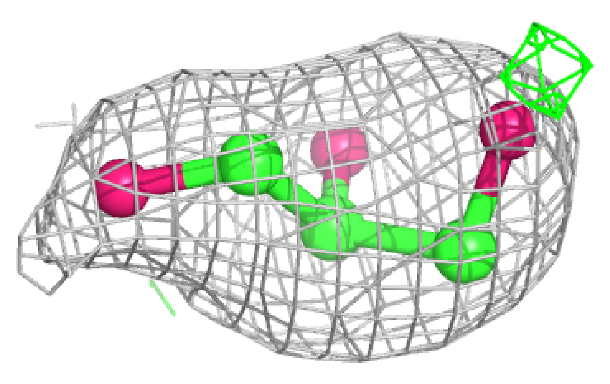


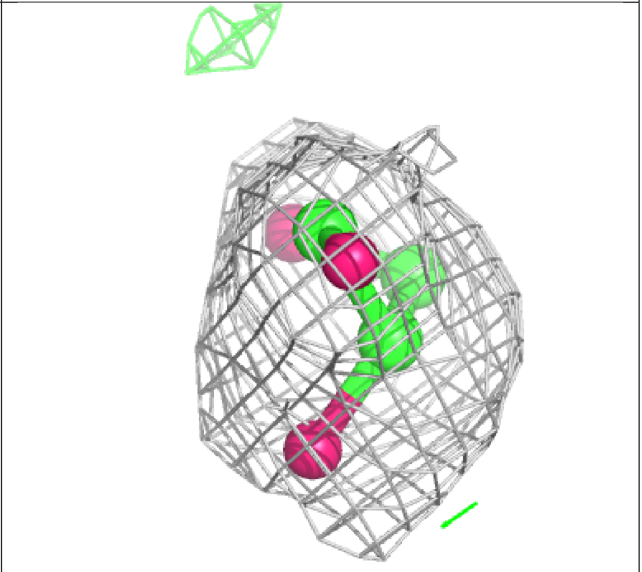


Electron density around GOL B 503:

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

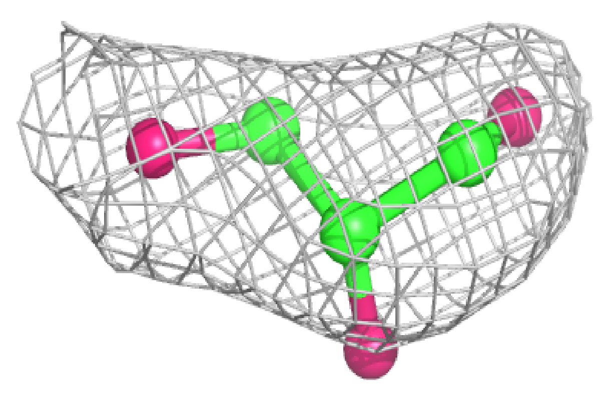


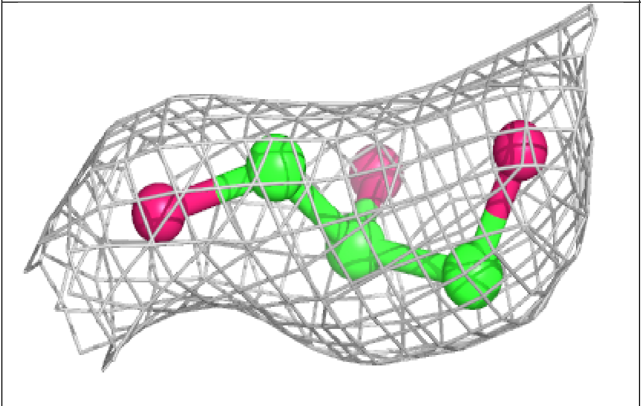


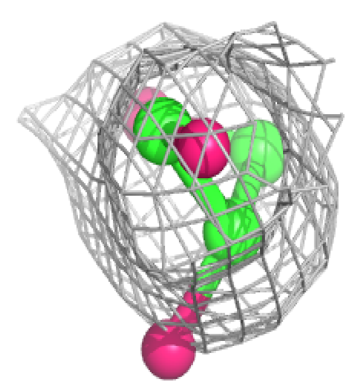


Electron density around GOL H 502:

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

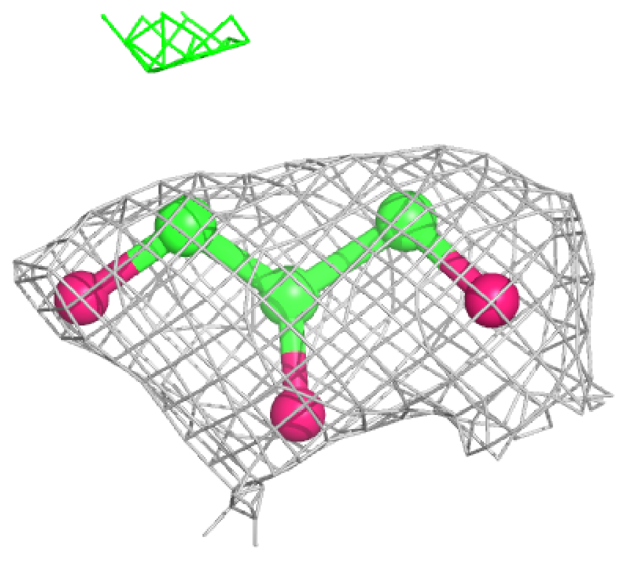


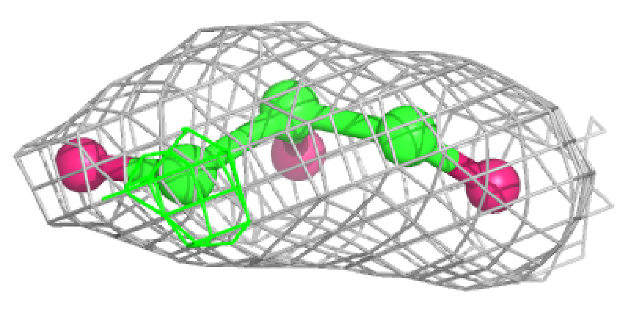


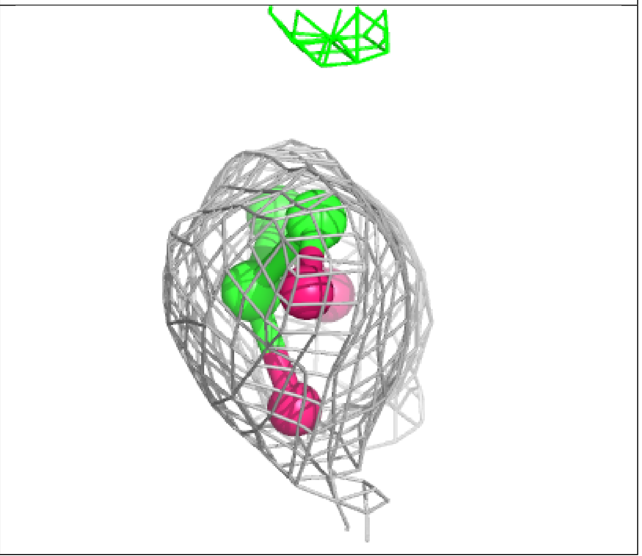


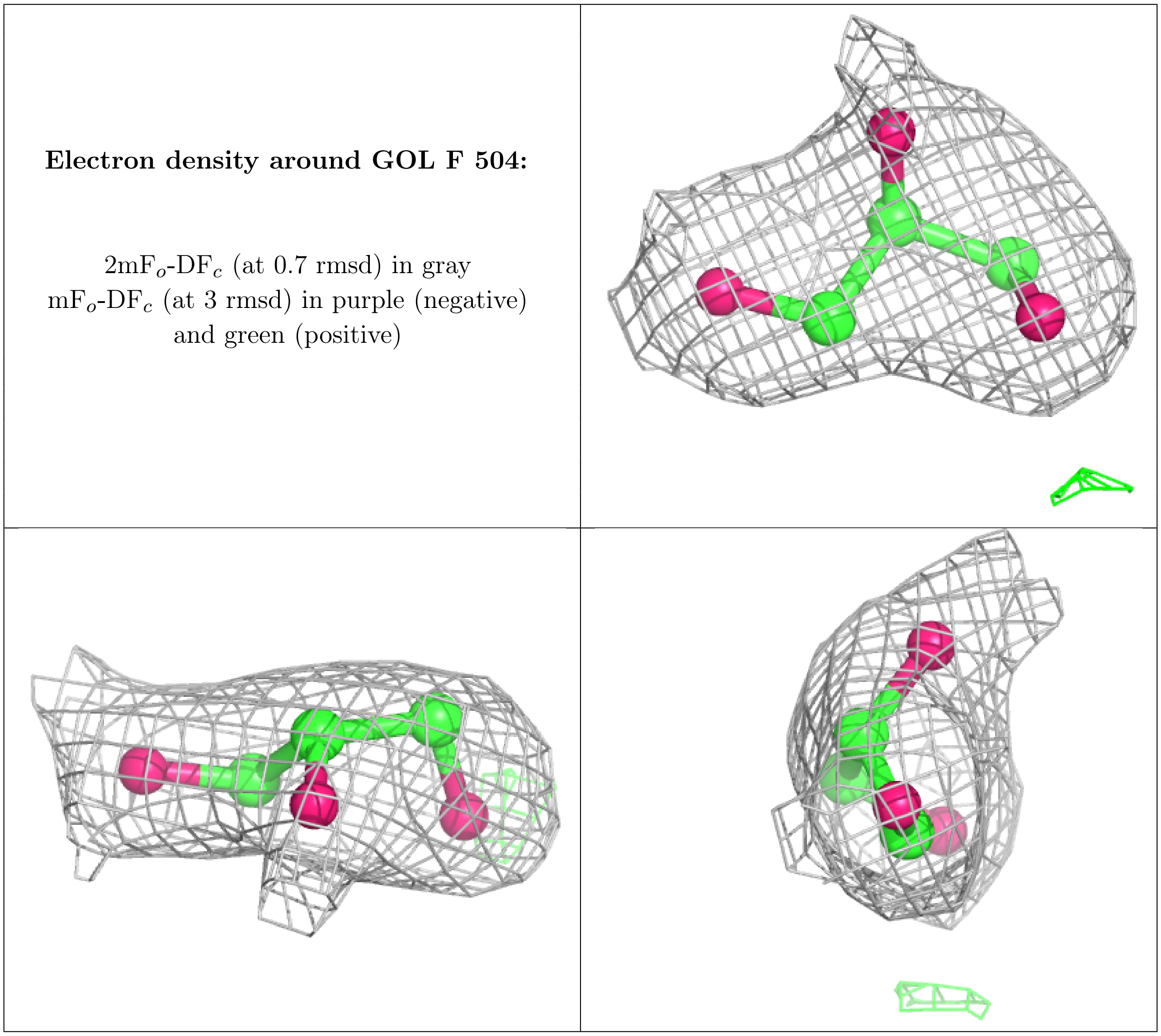
Electron density around GOL D 504:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



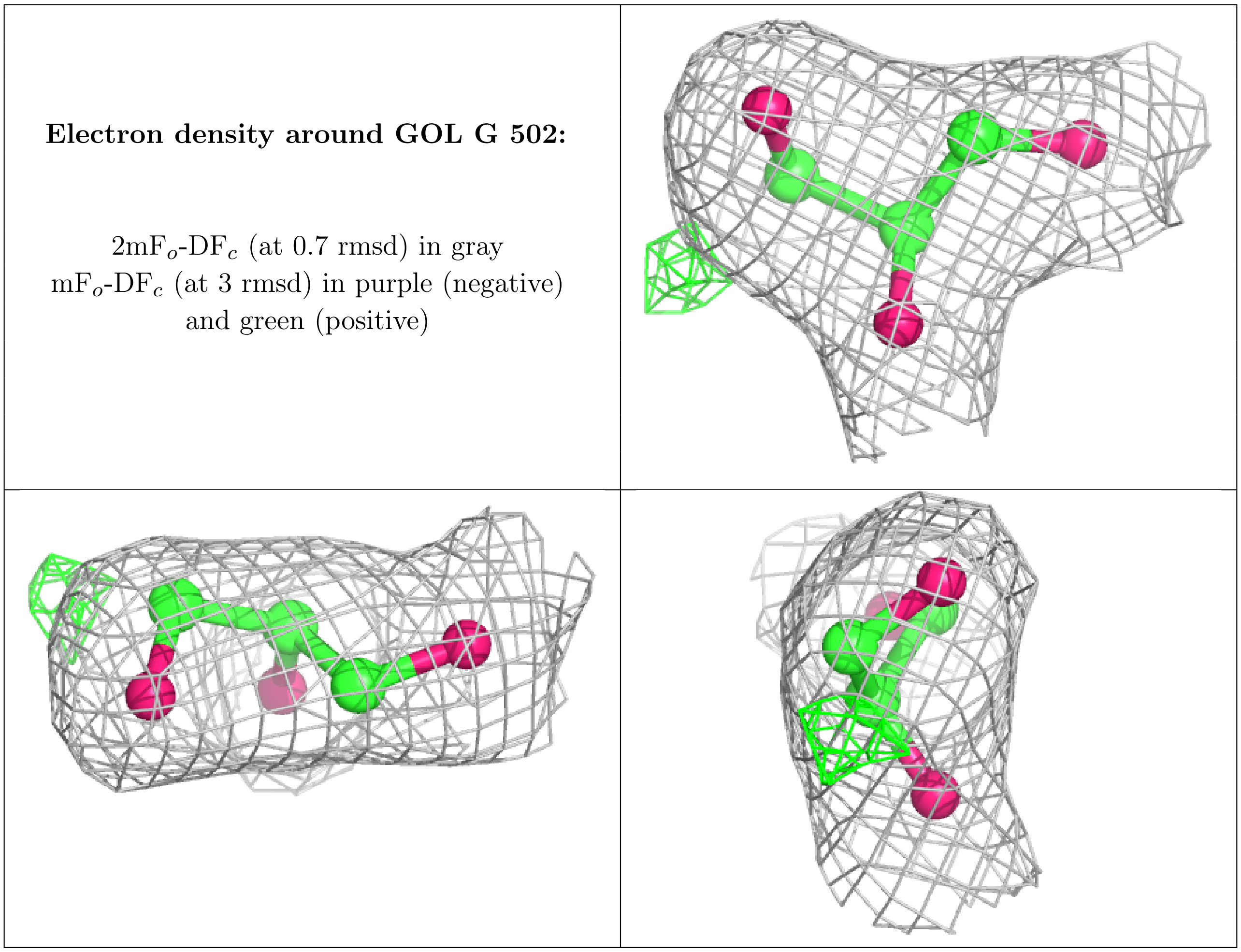






Electron density around GOL F 504:

$2mF_o$-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 G 502:

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.