Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2022 – 06:49 PM JST

PDB ID	:	7W1C
Title	:	Crystal structure of Klebsiella pneumoniae K1 capsule-specific polysaccharide lyase in a P1 crystal form
Authors	:	Tu, I.F.; Huang, K.F.; Wu, S.H.
Deposited on	:	2021-11-19
Resolution	:	1.48 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

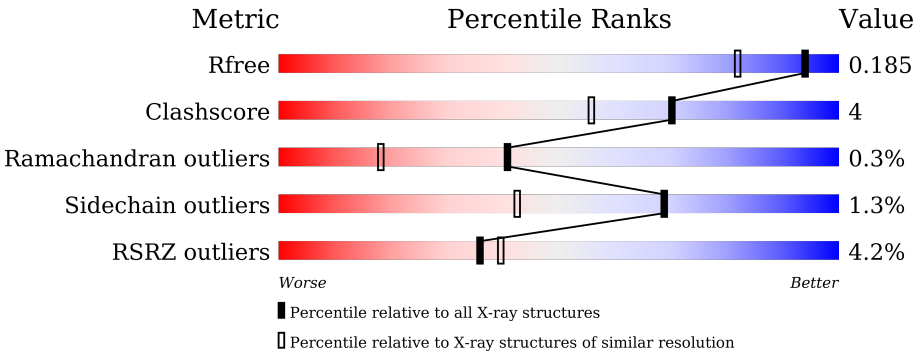
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.48 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	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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	671	3% 88% 7% ·
1	B	671	6% 85% 9% 6%
1	C	671	7% 87% 8% 5%
1	D	671	3% 84% 8% 7%
1	E	671	2% 87% 9% ·
1	F	671	4% 87% 8% · ·

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	LMR	F	707	-	-	X	-
2	LMR	F	708	-	-	X	-
3	IMD	E	704	-	-	X	-
3	IMD	F	709	-	-	X	-
4	GOL	A	803	-	X	-	-
4	GOL	B	707	-	-	X	-
4	GOL	D	704	-	X	-	-
4	GOL	F	702	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 33294 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 K1 LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	2	0
			4872	3064	842	947	19			
1	B	634	Total	C	N	O	S	0	0	0
			4793	3014	829	931	19			
1	C	640	Total	C	N	O	S	0	2	0
			4852	3054	837	942	19			
1	D	622	Total	C	N	O	S	0	0	0
			4696	2952	814	912	18			
1	E	644	Total	C	N	O	S	0	1	0
			4876	3066	843	948	19			
1	F	642	Total	C	N	O	S	0	3	0
			4878	3065	844	950	19			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
A	-18	GLY	-	expression tag	UNP A0A068Q5Q5
A	-17	SER	-	expression tag	UNP A0A068Q5Q5
A	-16	SER	-	expression tag	UNP A0A068Q5Q5
A	-15	HIS	-	expression tag	UNP A0A068Q5Q5
A	-14	HIS	-	expression tag	UNP A0A068Q5Q5
A	-13	HIS	-	expression tag	UNP A0A068Q5Q5
A	-12	HIS	-	expression tag	UNP A0A068Q5Q5
A	-11	HIS	-	expression tag	UNP A0A068Q5Q5
A	-10	HIS	-	expression tag	UNP A0A068Q5Q5
A	-9	SER	-	expression tag	UNP A0A068Q5Q5
A	-8	SER	-	expression tag	UNP A0A068Q5Q5
A	-7	GLY	-	expression tag	UNP A0A068Q5Q5
A	-6	LEU	-	expression tag	UNP A0A068Q5Q5
A	-5	VAL	-	expression tag	UNP A0A068Q5Q5
A	-4	PRO	-	expression tag	UNP A0A068Q5Q5
A	-3	ARG	-	expression tag	UNP A0A068Q5Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A068Q5Q5
A	-1	SER	-	expression tag	UNP A0A068Q5Q5
A	0	HIS	-	expression tag	UNP A0A068Q5Q5
A	213	THR	ALA	conflict	UNP A0A068Q5Q5
A	256	ILE	SER	conflict	UNP A0A068Q5Q5
A	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
A	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
B	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
B	-18	GLY	-	expression tag	UNP A0A068Q5Q5
B	-17	SER	-	expression tag	UNP A0A068Q5Q5
B	-16	SER	-	expression tag	UNP A0A068Q5Q5
B	-15	HIS	-	expression tag	UNP A0A068Q5Q5
B	-14	HIS	-	expression tag	UNP A0A068Q5Q5
B	-13	HIS	-	expression tag	UNP A0A068Q5Q5
B	-12	HIS	-	expression tag	UNP A0A068Q5Q5
B	-11	HIS	-	expression tag	UNP A0A068Q5Q5
B	-10	HIS	-	expression tag	UNP A0A068Q5Q5
B	-9	SER	-	expression tag	UNP A0A068Q5Q5
B	-8	SER	-	expression tag	UNP A0A068Q5Q5
B	-7	GLY	-	expression tag	UNP A0A068Q5Q5
B	-6	LEU	-	expression tag	UNP A0A068Q5Q5
B	-5	VAL	-	expression tag	UNP A0A068Q5Q5
B	-4	PRO	-	expression tag	UNP A0A068Q5Q5
B	-3	ARG	-	expression tag	UNP A0A068Q5Q5
B	-2	GLY	-	expression tag	UNP A0A068Q5Q5
B	-1	SER	-	expression tag	UNP A0A068Q5Q5
B	0	HIS	-	expression tag	UNP A0A068Q5Q5
B	213	THR	ALA	conflict	UNP A0A068Q5Q5
B	256	ILE	SER	conflict	UNP A0A068Q5Q5
B	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
B	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
C	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
C	-18	GLY	-	expression tag	UNP A0A068Q5Q5
C	-17	SER	-	expression tag	UNP A0A068Q5Q5
C	-16	SER	-	expression tag	UNP A0A068Q5Q5
C	-15	HIS	-	expression tag	UNP A0A068Q5Q5
C	-14	HIS	-	expression tag	UNP A0A068Q5Q5
C	-13	HIS	-	expression tag	UNP A0A068Q5Q5
C	-12	HIS	-	expression tag	UNP A0A068Q5Q5
C	-11	HIS	-	expression tag	UNP A0A068Q5Q5
C	-10	HIS	-	expression tag	UNP A0A068Q5Q5
C	-9	SER	-	expression tag	UNP A0A068Q5Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	SER	-	expression tag	UNP A0A068Q5Q5
C	-7	GLY	-	expression tag	UNP A0A068Q5Q5
C	-6	LEU	-	expression tag	UNP A0A068Q5Q5
C	-5	VAL	-	expression tag	UNP A0A068Q5Q5
C	-4	PRO	-	expression tag	UNP A0A068Q5Q5
C	-3	ARG	-	expression tag	UNP A0A068Q5Q5
C	-2	GLY	-	expression tag	UNP A0A068Q5Q5
C	-1	SER	-	expression tag	UNP A0A068Q5Q5
C	0	HIS	-	expression tag	UNP A0A068Q5Q5
C	213	THR	ALA	conflict	UNP A0A068Q5Q5
C	256	ILE	SER	conflict	UNP A0A068Q5Q5
C	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
C	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
D	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
D	-18	GLY	-	expression tag	UNP A0A068Q5Q5
D	-17	SER	-	expression tag	UNP A0A068Q5Q5
D	-16	SER	-	expression tag	UNP A0A068Q5Q5
D	-15	HIS	-	expression tag	UNP A0A068Q5Q5
D	-14	HIS	-	expression tag	UNP A0A068Q5Q5
D	-13	HIS	-	expression tag	UNP A0A068Q5Q5
D	-12	HIS	-	expression tag	UNP A0A068Q5Q5
D	-11	HIS	-	expression tag	UNP A0A068Q5Q5
D	-10	HIS	-	expression tag	UNP A0A068Q5Q5
D	-9	SER	-	expression tag	UNP A0A068Q5Q5
D	-8	SER	-	expression tag	UNP A0A068Q5Q5
D	-7	GLY	-	expression tag	UNP A0A068Q5Q5
D	-6	LEU	-	expression tag	UNP A0A068Q5Q5
D	-5	VAL	-	expression tag	UNP A0A068Q5Q5
D	-4	PRO	-	expression tag	UNP A0A068Q5Q5
D	-3	ARG	-	expression tag	UNP A0A068Q5Q5
D	-2	GLY	-	expression tag	UNP A0A068Q5Q5
D	-1	SER	-	expression tag	UNP A0A068Q5Q5
D	0	HIS	-	expression tag	UNP A0A068Q5Q5
D	213	THR	ALA	conflict	UNP A0A068Q5Q5
D	256	ILE	SER	conflict	UNP A0A068Q5Q5
D	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
D	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
E	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
E	-18	GLY	-	expression tag	UNP A0A068Q5Q5
E	-17	SER	-	expression tag	UNP A0A068Q5Q5
E	-16	SER	-	expression tag	UNP A0A068Q5Q5
E	-15	HIS	-	expression tag	UNP A0A068Q5Q5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-14	HIS	-	expression tag	UNP A0A068Q5Q5
E	-13	HIS	-	expression tag	UNP A0A068Q5Q5
E	-12	HIS	-	expression tag	UNP A0A068Q5Q5
E	-11	HIS	-	expression tag	UNP A0A068Q5Q5
E	-10	HIS	-	expression tag	UNP A0A068Q5Q5
E	-9	SER	-	expression tag	UNP A0A068Q5Q5
E	-8	SER	-	expression tag	UNP A0A068Q5Q5
E	-7	GLY	-	expression tag	UNP A0A068Q5Q5
E	-6	LEU	-	expression tag	UNP A0A068Q5Q5
E	-5	VAL	-	expression tag	UNP A0A068Q5Q5
E	-4	PRO	-	expression tag	UNP A0A068Q5Q5
E	-3	ARG	-	expression tag	UNP A0A068Q5Q5
E	-2	GLY	-	expression tag	UNP A0A068Q5Q5
E	-1	SER	-	expression tag	UNP A0A068Q5Q5
E	0	HIS	-	expression tag	UNP A0A068Q5Q5
E	213	THR	ALA	conflict	UNP A0A068Q5Q5
E	256	ILE	SER	conflict	UNP A0A068Q5Q5
E	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
E	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5
F	-19	MET	-	initiating methionine	UNP A0A068Q5Q5
F	-18	GLY	-	expression tag	UNP A0A068Q5Q5
F	-17	SER	-	expression tag	UNP A0A068Q5Q5
F	-16	SER	-	expression tag	UNP A0A068Q5Q5
F	-15	HIS	-	expression tag	UNP A0A068Q5Q5
F	-14	HIS	-	expression tag	UNP A0A068Q5Q5
F	-13	HIS	-	expression tag	UNP A0A068Q5Q5
F	-12	HIS	-	expression tag	UNP A0A068Q5Q5
F	-11	HIS	-	expression tag	UNP A0A068Q5Q5
F	-10	HIS	-	expression tag	UNP A0A068Q5Q5
F	-9	SER	-	expression tag	UNP A0A068Q5Q5
F	-8	SER	-	expression tag	UNP A0A068Q5Q5
F	-7	GLY	-	expression tag	UNP A0A068Q5Q5
F	-6	LEU	-	expression tag	UNP A0A068Q5Q5
F	-5	VAL	-	expression tag	UNP A0A068Q5Q5
F	-4	PRO	-	expression tag	UNP A0A068Q5Q5
F	-3	ARG	-	expression tag	UNP A0A068Q5Q5
F	-2	GLY	-	expression tag	UNP A0A068Q5Q5
F	-1	SER	-	expression tag	UNP A0A068Q5Q5
F	0	HIS	-	expression tag	UNP A0A068Q5Q5
F	213	THR	ALA	conflict	UNP A0A068Q5Q5
F	256	ILE	SER	conflict	UNP A0A068Q5Q5
F	391	ALA	ASP	engineered mutation	UNP A0A068Q5Q5

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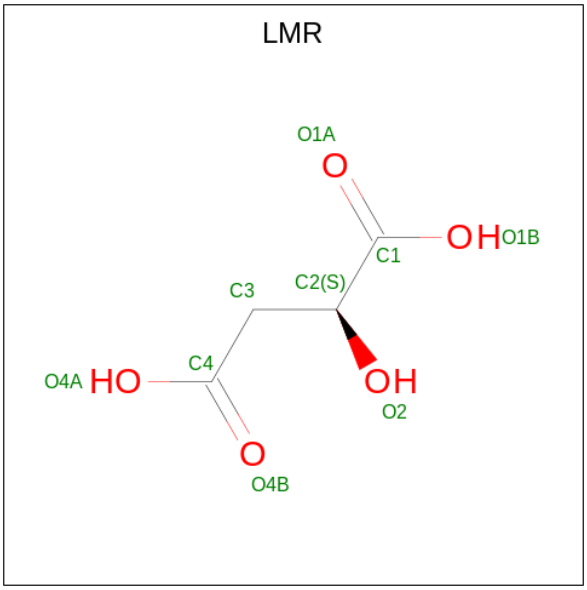
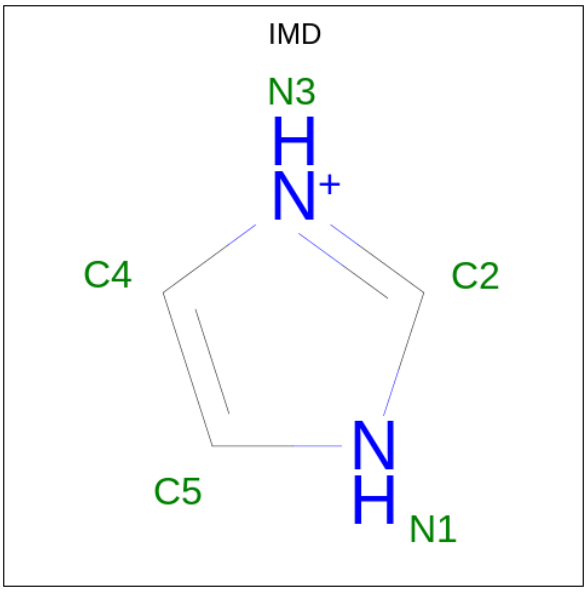
Chain	Residue	Modelled	Actual	Comment	Reference
F	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5

- Molecule 2 is (2S)-2-hydroxybutanedioic acid (three-letter code: LMR) (formula: $C_4H_6O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 4 5	0	0
2	B	1	Total C O 9 4 5	0	0
2	C	1	Total C O 9 4 5	0	0
2	D	1	Total C O 9 4 5	0	0
2	E	1	Total C O 9 4 5	0	0
2	F	1	Total C O 9 4 5	0	0
2	F	1	Total C O 9 4 5	0	0

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 5 3 2	0	0
3	A	1	Total C N 5 3 2	0	0
3	A	1	Total C N 5 3 2	0	0
3	B	1	Total C N 5 3 2	0	0
3	B	1	Total C N 5 3 2	0	0
3	B	1	Total C N 5 3 2	0	0
3	B	1	Total C N 5 3 2	0	0
3	C	1	Total C N 5 3 2	0	0
3	C	1	Total C N 5 3 2	0	0
3	C	1	Total C N 5 3 2	0	0
3	C	1	Total C N 5 3 2	0	0
3	C	1	Total C N 5 3 2	0	0
3	D	1	Total C N 5 3 2	0	0
3	D	1	Total C N 5 3 2	0	0

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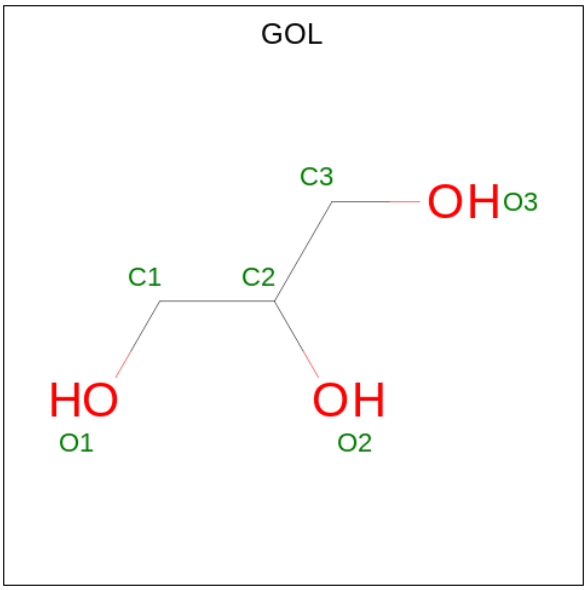
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C N 5 3 2	0	0
3	E	1	Total C N 5 3 2	0	0
3	E	1	Total C N 5 3 2	0	0
3	E	1	Total C N 5 3 2	0	0
3	E	1	Total C N 5 3 2	0	0
3	F	1	Total C N 5 3 2	0	0
3	F	1	Total C N 5 3 2	0	0
3	F	1	Total C N 5 3 2	0	0
3	F	1	Total C N 5 3 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	663	Total O 663 663	0	0
5	B	629	Total O 629 629	0	0
5	C	586	Total O 586 586	0	0

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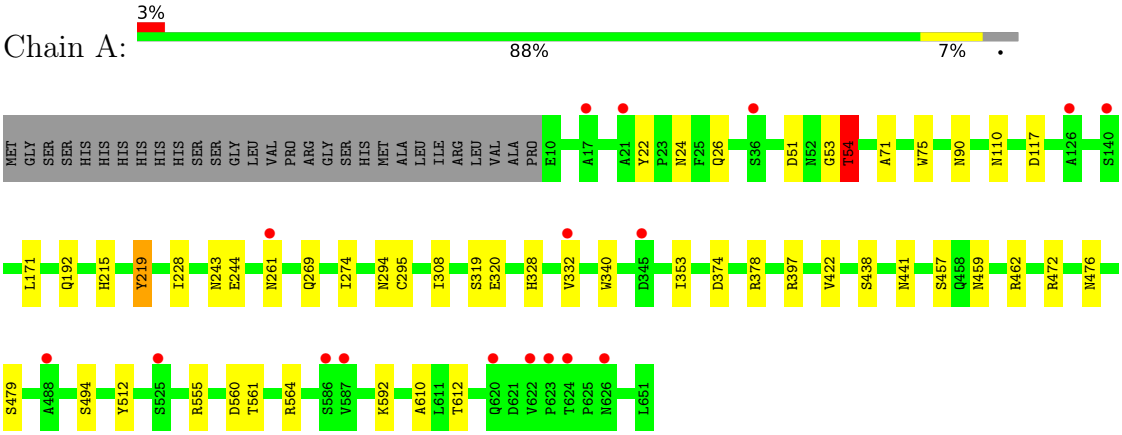
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	722	Total O 722 722	0	0
5	E	728	Total O 728 728	0	0
5	F	713	Total O 713 713	0	0

3 Residue-property plots (i)

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

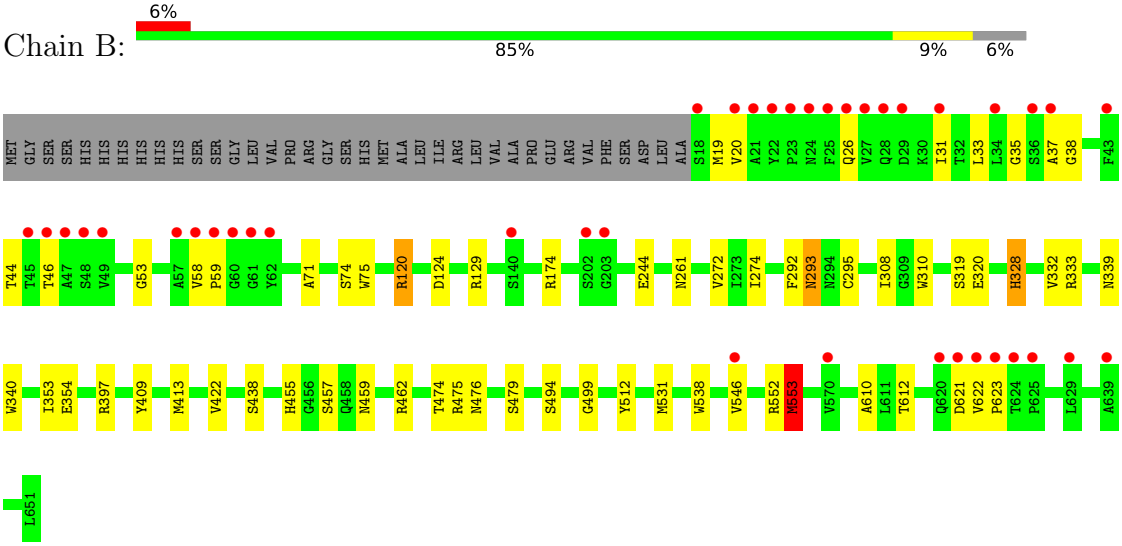
• Molecule 1: K1 LYASE

Chain A:



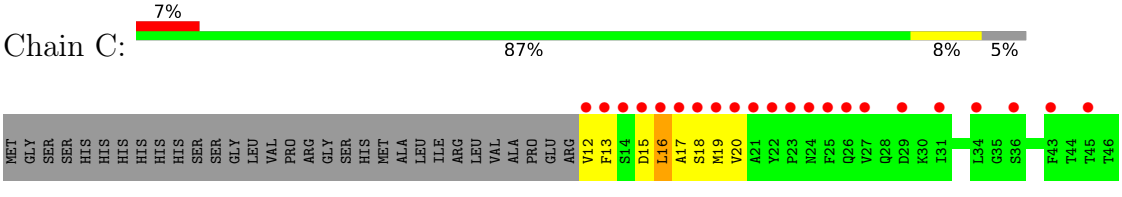
• Molecule 1: K1 LYASE

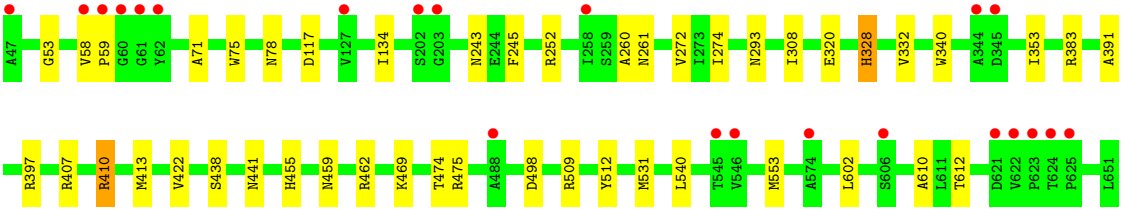
Chain B:



• Molecule 1: K1 LYASE

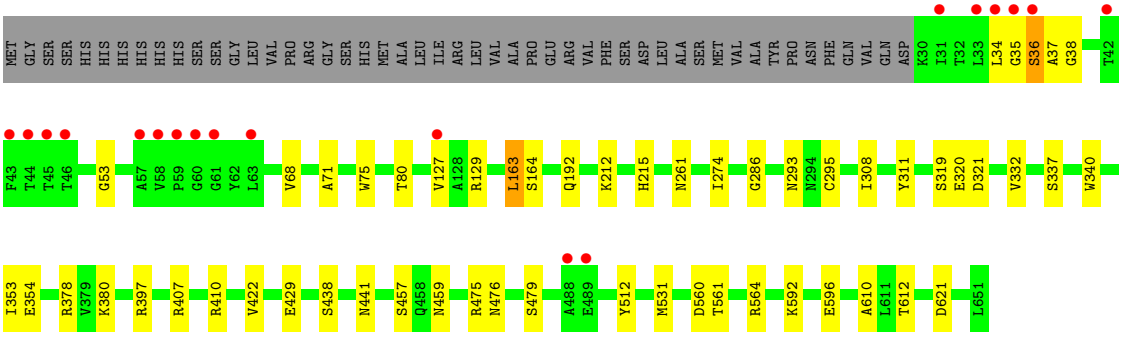
Chain C:





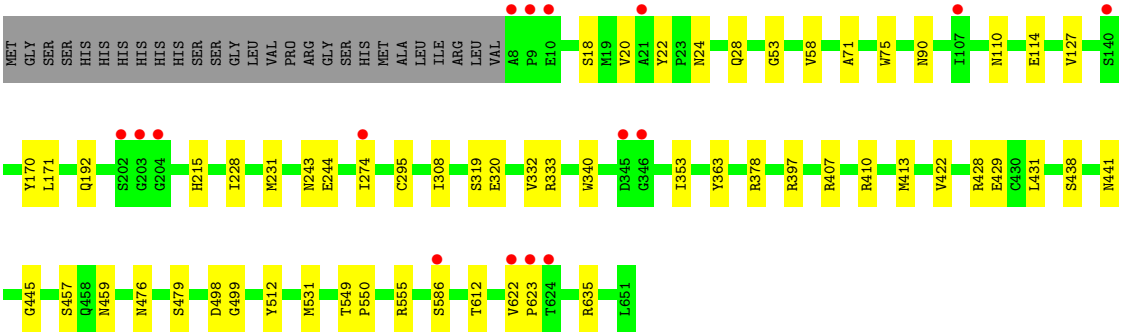
• Molecule 1: K1 LYASE

Chain D:



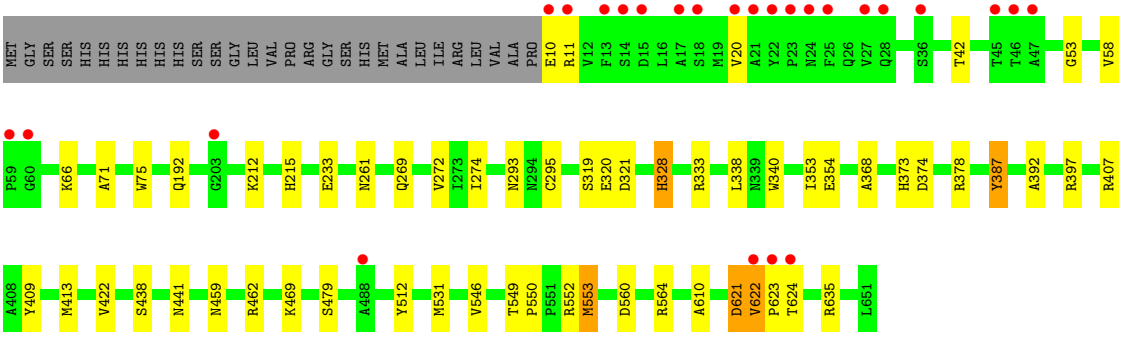
• Molecule 1: K1 LYASE

Chain E:



• Molecule 1: K1 LYASE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	90.28Å 100.57Å 125.03Å 80.50° 70.32° 83.43°	Depositor
Resolution (Å)	30.00 – 1.48 29.49 – 1.48	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.00-1.48) 96.8 (29.49-1.48)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.137 , 0.184 0.138 , 0.185	Depositor DCC
R_{free} test set	32922 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	15.8	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	33294	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMR, GOL, IMD

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	0.88	4/4976 (0.1%)	0.87	6/6774 (0.1%)
1	B	0.90	3/4896 (0.1%)	0.92	14/6666 (0.2%)
1	C	0.89	0/4959	0.89	11/6752 (0.2%)
1	D	0.90	2/4796 (0.0%)	0.89	4/6529 (0.1%)
1	E	0.90	3/4981 (0.1%)	0.89	6/6782 (0.1%)
1	F	0.94	4/4982 (0.1%)	0.92	6/6782 (0.1%)
All	All	0.90	16/29590 (0.1%)	0.90	47/40285 (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
1	D	0	1
1	F	0	1
All	All	0	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	244	GLU	CD-OE1	7.58	1.33	1.25
1	A	244	GLU	CD-OE2	7.23	1.33	1.25
1	D	596	GLU	CD-OE1	7.19	1.33	1.25
1	A	438	SER	CB-OG	-6.46	1.33	1.42
1	B	38	GLY	CA-C	6.02	1.61	1.51
1	A	219	TYR	CB-CG	5.96	1.60	1.51
1	B	494	SER	CB-OG	-5.62	1.34	1.42
1	F	354	GLU	CD-OE2	-5.40	1.19	1.25
1	F	233	GLU	CD-OE2	-5.31	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	114	GLU	CD-OE1	5.30	1.31	1.25
1	A	54	THR	CB-CG2	-5.30	1.34	1.52
1	D	429	GLU	CG-CD	5.28	1.59	1.51
1	F	387	TYR	CE1-CZ	-5.23	1.31	1.38
1	B	354	GLU	CD-OE1	-5.15	1.20	1.25
1	F	462	ARG	CD-NE	-5.07	1.37	1.46
1	E	429	GLU	CG-CD	5.02	1.59	1.51

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	553	MET	CG-SD-CE	-14.45	77.08	100.20
1	E	531	MET	CG-SD-CE	-13.60	78.44	100.20
1	C	553	MET	CG-SD-CE	-12.57	80.09	100.20
1	B	553	MET	CG-SD-CE	-10.30	83.72	100.20
1	B	462	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	C	475	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	B	475	ARG	NE-CZ-NH1	9.33	124.96	120.30
1	B	129	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	F	531	MET	CG-SD-CE	-9.07	85.69	100.20
1	D	531	MET	CG-SD-CE	-8.91	85.94	100.20
1	F	462	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	A	564	ARG	NE-CZ-NH2	-8.33	116.13	120.30
1	B	475	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	C	531	MET	CG-SD-CE	-7.76	87.78	100.20
1	D	407	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	B	531	MET	CG-SD-CE	-7.58	88.07	100.20
1	F	564	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	A	117	ASP	CB-CG-OD1	-7.28	111.75	118.30
1	C	17	ALA	N-CA-C	-7.27	91.37	111.00
1	B	462	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	B	174	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	B	120	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	C	462	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	E	378	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	C	475	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	D	564	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	E	635	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	C	410	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	C	407	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	117	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	120	ARG	NE-CZ-NH2	-5.46	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	333	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	A	555	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	124	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	C	498	ASP	CB-CG-OD1	5.34	123.11	118.30
1	E	555	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	C	383	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	E	428	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	244	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	C	252	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	129	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	292	PHE	CB-CG-CD1	5.14	124.40	120.80
1	F	560	ASP	CB-CG-OD1	5.12	122.91	118.30
1	D	475	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	462	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	F	635	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	472	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	621	ASP	Peptide
1	D	274	ILE	Peptide
1	F	621	ASP	Peptide

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	4872	0	4726	29	0
1	B	4793	0	4650	36	0
1	C	4852	0	4711	31	0
1	D	4696	0	4562	35	0
1	E	4876	0	4728	33	0
1	F	4878	0	4725	47	0
2	A	9	0	4	0	0
2	B	9	0	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	9	0	4	0	0
2	D	9	0	4	0	0
2	E	9	0	4	0	0
2	F	18	0	8	8	0
3	A	15	0	15	0	0
3	B	20	0	20	5	0
3	C	25	0	25	2	0
3	D	15	0	15	0	0
3	E	20	0	20	10	0
3	F	20	0	20	7	0
4	A	12	0	16	0	0
4	B	18	0	23	5	0
4	C	24	0	32	1	0
4	D	18	0	24	2	0
4	E	18	0	24	0	0
4	F	18	0	24	0	0
5	A	663	0	0	6	0
5	B	629	0	0	6	1
5	C	586	0	0	4	0
5	D	722	0	0	3	0
5	E	728	0	0	5	0
5	F	713	0	0	7	1
All	All	33294	0	28388	206	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (206) 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)
2:F:707:LMR:C2	2:F:708:LMR:O2	1.69	1.40
2:F:707:LMR:H2	2:F:708:LMR:O2	1.21	1.34
2:F:707:LMR:C2	2:F:708:LMR:HO2	1.66	0.83
1:C:16:LEU:O	1:C:20:VAL:HG22	1.82	0.80
2:F:707:LMR:O2	2:F:708:LMR:O2	1.85	0.79
3:E:704:IMD:H4	1:F:378:ARG:HG2	1.67	0.76
1:E:192:GLN:HE22	1:E:215:HIS:H	1.36	0.74
3:B:706:IMD:H5	5:B:1039:HOH:O	1.87	0.74
3:E:704:IMD:C4	1:F:378:ARG:HG2	2.18	0.73
1:F:192:GLN:HE22	1:F:215:HIS:H	1.35	0.73
1:A:192:GLN:HE22	1:A:215:HIS:H	1.34	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:TRP:HE1	4:B:707:GOL:H31	1.55	0.70
1:F:373:HIS:HE1	2:F:708:LMR:O4B	1.75	0.70
1:B:35:GLY:O	1:B:37:ALA:N	2.22	0.68
1:D:80:THR:HG23	5:D:1309:HOH:O	1.92	0.68
1:F:333:ARG:HH21	2:F:707:LMR:H2	1.59	0.68
1:D:192:GLN:HE22	1:D:215:HIS:H	1.43	0.67
3:F:705:IMD:H5	5:F:1091:HOH:O	1.97	0.65
1:F:622:VAL:HB	1:F:623:PRO:CD	2.27	0.64
1:C:15:ASP:O	1:C:16:LEU:CB	2.46	0.63
3:B:704:IMD:H2	5:B:1021:HOH:O	1.97	0.63
1:F:622:VAL:HG23	1:F:624:THR:H	1.63	0.62
1:D:127:VAL:HG11	1:D:129:ARG:NH2	2.14	0.62
3:E:704:IMD:H4	1:F:378:ARG:NE	2.14	0.62
3:E:704:IMD:H4	1:F:378:ARG:CG	2.28	0.62
1:C:243:ASN:HB3	1:C:274[A]:ILE:HG23	1.83	0.61
1:A:269:GLN:HG2	5:A:1517:HOH:O	2.00	0.61
1:D:286:GLY:HA2	4:D:705:GOL:H32	1.81	0.61
1:C:58:VAL:HG22	1:C:59:PRO:HD2	1.82	0.60
3:E:704:IMD:H4	1:F:378:ARG:HE	1.64	0.60
1:D:378:ARG:HE	3:F:709:IMD:H2	1.67	0.60
1:A:378:ARG:HE	3:C:805:IMD:H2	1.66	0.60
1:E:171:LEU:CD2	1:E:228:ILE:HD13	2.32	0.60
1:D:410:ARG:HH22	1:E:215:HIS:HD2	1.51	0.59
1:D:354:GLU:OE2	1:F:387:TYR:OH	2.18	0.58
3:E:704:IMD:C4	1:F:378:ARG:HE	2.17	0.58
1:D:35:GLY:HA3	1:D:36:SER:HB3	1.85	0.57
1:F:622:VAL:HB	1:F:623:PRO:HD2	1.86	0.57
1:B:310:TRP:NE1	4:B:707:GOL:H31	2.18	0.57
1:D:212:LYS:NZ	1:D:321:ASP:OD2	2.31	0.57
1:E:171:LEU:CD2	1:E:228:ILE:CD1	2.82	0.57
3:E:704:IMD:H4	1:F:378:ARG:CD	2.35	0.57
1:D:35:GLY:CA	1:D:36:SER:CB	2.83	0.56
1:C:15:ASP:O	1:C:16:LEU:HB2	2.05	0.55
1:F:413:MET:HE2	5:F:948:HOH:O	2.05	0.55
1:B:310:TRP:HE1	4:B:707:GOL:C3	2.19	0.55
1:B:413:MET:HE2	5:B:937:HOH:O	2.05	0.55
3:F:703:IMD:H2	5:F:1040:HOH:O	2.06	0.55
5:D:1053:HOH:O	1:F:328:HIS:HD2	1.89	0.54
1:D:378:ARG:HE	3:F:709:IMD:C2	2.19	0.54
1:E:171:LEU:HD23	1:E:228:ILE:HD13	1.89	0.54
1:D:378:ARG:NE	3:F:709:IMD:H2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ASN:HB3	1:A:274:ILE:HG23	1.91	0.53
1:C:397:ARG:HA	1:C:422:VAL:HG21	1.90	0.53
1:A:171:LEU:CD2	1:A:228:ILE:CD1	2.87	0.53
1:F:397:ARG:HA	1:F:422:VAL:HG21	1.89	0.53
1:C:15:ASP:OD1	1:C:18:SER:HB2	2.08	0.53
1:A:610:ALA:HA	1:B:612:THR:HB	1.91	0.53
1:D:308:ILE:HB	1:D:332:VAL:HG12	1.90	0.52
1:E:586:SER:HB2	5:E:1004:HOH:O	2.08	0.52
1:A:494[B]:SER:OG	5:A:901:HOH:O	2.13	0.52
1:D:80:THR:HG22	5:D:1143:HOH:O	2.08	0.52
1:A:219:TYR:OH	1:D:621:ASP:OD1	2.20	0.52
1:F:71:ALA:HA	1:F:75:TRP:CZ3	2.44	0.52
1:E:71:ALA:HA	1:E:75:TRP:CZ3	2.44	0.51
1:F:621:ASP:HB3	1:F:622:VAL:HG22	1.92	0.51
1:B:37:ALA:HB1	1:B:74:SER:O	2.11	0.51
1:D:410:ARG:HH22	1:E:215:HIS:CD2	2.28	0.51
1:A:261:ASN:HD21	1:A:294:ASN:HD22	1.58	0.51
1:E:410:ARG:HH22	1:F:215:HIS:CD2	2.29	0.51
1:B:19:MET:CE	1:B:33:LEU:HB2	2.40	0.50
1:F:469:LYS:HE2	5:F:1165:HOH:O	2.10	0.50
1:B:20:VAL:HA	1:B:58:VAL:HG12	1.93	0.50
1:E:170:TYR:CD1	1:E:231:MET:HG3	2.47	0.50
1:B:44:THR:OG1	1:B:46:THR:HG22	2.11	0.50
1:A:612:THR:HB	1:C:610:ALA:HA	1.93	0.50
1:C:15:ASP:OD1	1:C:18:SER:CB	2.59	0.50
1:D:560:ASP:OD1	1:D:561:THR:HG23	2.12	0.50
1:A:328:HIS:HD2	5:B:1134:HOH:O	1.95	0.50
1:E:397:ARG:HA	1:E:422:VAL:HG21	1.94	0.50
1:B:409:TYR:CE2	3:B:708:IMD:H2	2.47	0.49
1:E:295:CYS:O	1:E:319:SER:HA	2.12	0.49
5:A:1201:HOH:O	1:C:328:HIS:HD2	1.95	0.49
1:A:51:ASP:OD2	1:A:54:THR:HG22	2.12	0.49
1:D:35:GLY:CA	1:D:36:SER:HB3	2.43	0.48
1:D:295:CYS:O	1:D:319:SER:HA	2.14	0.48
1:A:592:LYS:HG2	1:C:602:LEU:HD13	1.94	0.48
1:C:71:ALA:HA	1:C:75:TRP:CZ3	2.49	0.48
1:C:117:ASP:OD1	3:C:804:IMD:H5	2.14	0.48
4:C:802:GOL:H12	5:C:1067:HOH:O	2.14	0.47
1:D:610:ALA:HA	1:E:612:THR:HB	1.96	0.47
1:E:171:LEU:HD23	1:E:228:ILE:CD1	2.42	0.47
1:E:410:ARG:HH22	1:F:215:HIS:HD2	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:ASN:HB3	1:E:274:ILE:HG23	1.96	0.47
2:F:707:LMR:C2	2:F:708:LMR:C2	2.85	0.47
1:D:457:SER:O	1:D:476:ASN:HA	2.15	0.46
1:E:308:ILE:HB	1:E:332:VAL:HG12	1.97	0.46
1:E:363:TYR:OH	1:F:215:HIS:HE1	1.98	0.46
1:F:413:MET:CE	5:F:1377:HOH:O	2.64	0.46
1:A:560:ASP:OD1	1:A:561:THR:HG23	2.15	0.46
1:D:397:ARG:HA	1:D:422:VAL:HG21	1.96	0.46
1:C:455:HIS:HA	1:C:474:THR:O	2.14	0.46
1:E:22:TYR:CZ	1:E:24:ASN:HB2	2.51	0.46
1:F:413:MET:HE3	5:F:1377:HOH:O	2.16	0.46
1:D:71:ALA:HA	1:D:75:TRP:CZ3	2.50	0.46
1:E:170:TYR:HD1	5:E:1351:HOH:O	1.98	0.46
3:E:704:IMD:C5	1:F:378:ARG:HE	2.29	0.46
1:B:499:GLY:O	1:C:469:LYS:HE2	2.16	0.45
1:B:552:ARG:C	1:B:553:MET:HG2	2.36	0.45
1:A:215:HIS:HD2	1:C:410:ARG:HH22	1.65	0.45
1:C:13:PHE:CD2	1:C:19:MET:HA	2.51	0.45
1:E:22:TYR:CE2	1:E:24:ASN:HB2	2.51	0.45
2:F:707:LMR:O2	2:F:708:LMR:C2	2.64	0.45
1:C:509:ARG:HD2	1:C:540:LEU:HB2	1.98	0.45
1:C:308:ILE:HB	1:C:332:VAL:HG12	1.99	0.45
1:E:320:GLU:HA	1:E:353:ILE:O	2.16	0.45
1:A:215:HIS:CD2	1:C:410:ARG:HH22	2.35	0.44
1:A:308:ILE:HB	1:A:332:VAL:HG12	2.00	0.44
1:F:20:VAL:HA	1:F:58:VAL:HG12	1.98	0.44
1:A:71:ALA:HA	1:A:75:TRP:CZ3	2.53	0.44
1:B:272:VAL:HG12	1:B:274:ILE:HG13	2.00	0.44
1:D:163:LEU:C	1:D:163:LEU:HD12	2.38	0.44
1:B:35:GLY:C	1:B:37:ALA:H	2.16	0.44
1:B:610:ALA:HA	1:C:612:THR:HB	2.00	0.44
1:F:374:ASP:HA	1:F:397:ARG:O	2.17	0.44
1:B:71:ALA:HA	1:B:75:TRP:CZ3	2.53	0.44
1:B:339:ASN:HD21	4:B:707:GOL:C3	2.31	0.44
1:D:612:THR:HB	1:F:610:ALA:HA	1.99	0.44
1:B:457:SER:O	1:B:476:ASN:HA	2.17	0.44
1:C:16:LEU:O	1:C:16:LEU:HG	2.18	0.43
1:E:622:VAL:HG23	1:E:623:PRO:HA	1.98	0.43
3:E:704:IMD:C2	5:E:1317:HOH:O	2.66	0.43
1:B:308:ILE:HB	1:B:332:VAL:HG12	1.99	0.43
1:C:261:ASN:HA	1:C:293:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:ALA:HA	1:C:413:MET:HE2	1.99	0.43
1:F:622:VAL:CB	1:F:623:PRO:CD	2.96	0.43
1:A:459:ASN:HA	1:A:479:SER:O	2.18	0.43
1:B:409:TYR:HE2	3:B:708:IMD:H2	1.83	0.43
1:B:261:ASN:HA	1:B:293:ASN:O	2.17	0.43
3:B:708:IMD:H4	5:C:992:HOH:O	2.17	0.43
1:D:320:GLU:HA	1:D:353:ILE:O	2.19	0.43
1:F:269:GLN:NE2	5:F:814:HOH:O	2.50	0.43
1:F:552:ARG:C	1:F:553:MET:HG2	2.35	0.43
1:A:54:THR:CG2	5:A:1454:HOH:O	2.66	0.43
1:D:261:ASN:HA	1:D:293:ASN:O	2.18	0.43
1:A:54:THR:HG23	5:A:1454:HOH:O	2.19	0.43
1:B:397:ARG:HA	1:B:422:VAL:HG21	1.99	0.43
3:E:704:IMD:C4	1:F:378:ARG:CG	2.92	0.43
1:D:378:ARG:HG2	3:F:709:IMD:C2	2.49	0.43
1:E:457:SER:H	1:E:476:ASN:HD22	1.66	0.43
1:B:320:GLU:HA	1:B:353:ILE:O	2.17	0.43
1:B:333:ARG:HH21	2:B:703:LMR:H3A	1.83	0.43
1:A:374:ASP:HA	1:A:397:ARG:O	2.18	0.42
1:B:328:HIS:HD2	5:C:1177:HOH:O	2.02	0.42
1:B:295:CYS:O	1:B:319:SER:HA	2.19	0.42
1:C:438:SER:HA	1:C:459:ASN:O	2.19	0.42
1:F:459:ASN:HA	1:F:479:SER:O	2.20	0.42
1:B:35:GLY:C	1:B:37:ALA:N	2.71	0.42
1:F:295:CYS:O	1:F:319:SER:HA	2.19	0.42
1:E:20:VAL:HA	1:E:58:VAL:HG12	2.01	0.42
1:E:459:ASN:HA	1:E:479:SER:O	2.20	0.42
1:A:320:GLU:HA	1:A:353:ILE:O	2.18	0.42
1:C:272:VAL:HG12	1:C:274[B]:ILE:HG13	2.02	0.42
1:D:286:GLY:HA2	4:D:705:GOL:C3	2.48	0.42
1:B:58:VAL:O	1:B:59:PRO:C	2.53	0.42
1:C:12:VAL:HG12	1:C:13:PHE:N	2.35	0.42
1:E:499:GLY:O	1:F:469:LYS:HE3	2.20	0.42
1:F:212:LYS:NZ	1:F:321:ASP:OD2	2.33	0.42
1:F:438:SER:HA	1:F:459:ASN:O	2.20	0.42
1:F:549:THR:HA	1:F:550:PRO:HD3	1.89	0.42
1:D:459:ASN:HA	1:D:479:SER:O	2.19	0.42
1:F:409:TYR:HE2	3:F:709:IMD:C2	2.32	0.42
1:A:295:CYS:O	1:A:319:SER:HA	2.20	0.42
1:C:413:MET:CE	5:C:1382:HOH:O	2.68	0.42
1:F:368:ALA:HA	1:F:392:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASN:HA	1:A:110:ASN:O	2.20	0.41
1:A:561:THR:HG22	5:A:1426:HOH:O	2.19	0.41
1:B:413:MET:HE3	5:B:1309:HOH:O	2.20	0.41
1:B:459:ASN:HA	1:B:479:SER:O	2.20	0.41
1:E:498:ASP:OD1	5:E:801:HOH:O	2.21	0.41
1:F:320:GLU:HA	1:F:353:ILE:O	2.20	0.41
1:D:36:SER:C	1:D:38:GLY:H	2.23	0.41
1:F:338:LEU:O	1:F:373:HIS:HD2	2.03	0.41
1:A:22:TYR:CZ	1:A:24:ASN:HB2	2.55	0.41
1:A:397:ARG:HA	1:A:422:VAL:HG21	2.02	0.41
1:A:457:SER:O	1:A:476:ASN:HA	2.20	0.41
1:D:380:LYS:HE3	1:F:407:ARG:HD3	2.02	0.41
1:B:438:SER:HA	1:B:459:ASN:O	2.20	0.41
1:E:438:SER:HA	1:E:459:ASN:O	2.21	0.41
1:C:134:ILE:O	1:C:260:ALA:HA	2.21	0.41
1:D:438:SER:HA	1:D:459:ASN:O	2.21	0.41
1:B:339:ASN:HD21	4:B:707:GOL:H32	1.85	0.41
1:C:320:GLU:HA	1:C:353:ILE:O	2.20	0.41
1:D:163:LEU:HD12	1:D:163:LEU:O	2.20	0.41
1:F:272:VAL:HG12	1:F:274:ILE:HG13	2.03	0.41
1:B:455:HIS:HA	1:B:474:THR:O	2.20	0.41
1:E:90:ASN:HA	1:E:110:ASN:O	2.21	0.41
1:F:261:ASN:HA	1:F:293:ASN:O	2.20	0.41
1:B:538:TRP:CH2	1:B:553:MET:CE	3.04	0.40
1:E:413:MET:CE	5:E:1391:HOH:O	2.69	0.40
1:E:407:ARG:HA	1:E:431:LEU:O	2.22	0.40
1:B:413:MET:CE	5:B:1309:HOH:O	2.69	0.40
1:D:311:TYR:CD2	1:D:337:SER:HB3	2.57	0.40
1:C:245:PHE:CE1	1:C:274[A]:ILE:CD1	3.04	0.40
1:E:549:THR:HA	1:E:550:PRO:HD3	1.98	0.40
1:F:42:THR:CG2	1:F:66:LYS:HD3	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:900:HOH:O	5:F:1443:HOH:O[1_664]	1.93	0.27

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	642/671 (96%)	618 (96%)	23 (4%)	1 (0%)	47	23
1	B	632/671 (94%)	605 (96%)	25 (4%)	2 (0%)	41	18
1	C	640/671 (95%)	612 (96%)	26 (4%)	2 (0%)	41	18
1	D	620/671 (92%)	594 (96%)	23 (4%)	3 (0%)	29	9
1	E	643/671 (96%)	617 (96%)	24 (4%)	2 (0%)	41	18
1	F	643/671 (96%)	619 (96%)	22 (3%)	2 (0%)	41	18
All	All	3820/4026 (95%)	3665 (96%)	143 (4%)	12 (0%)	41	18

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	622	VAL
1	D	36	SER
1	B	623	PRO
1	D	37	ALA
1	E	53	GLY
1	B	53	GLY
1	C	53	GLY
1	D	53	GLY
1	F	53	GLY
1	A	53	GLY
1	C	16	LEU
1	E	445	GLY

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	522/544 (96%)	517 (99%)	5 (1%)	76	54
1	B	513/544 (94%)	503 (98%)	10 (2%)	57	26
1	C	520/544 (96%)	515 (99%)	5 (1%)	76	54
1	D	502/544 (92%)	494 (98%)	8 (2%)	62	34
1	E	522/544 (96%)	516 (99%)	6 (1%)	73	50
1	F	523/544 (96%)	516 (99%)	7 (1%)	69	42
All	All	3102/3264 (95%)	3061 (99%)	41 (1%)	69	42

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	54	THR
1	A	340	TRP
1	A	441	ASN
1	A	512	TYR
1	B	26	GLN
1	B	31	ILE
1	B	120	ARG
1	B	293	ASN
1	B	328	HIS
1	B	340	TRP
1	B	512	TYR
1	B	546	VAL
1	B	553	MET
1	B	622	VAL
1	C	78	ASN
1	C	328	HIS
1	C	340	TRP
1	C	441	ASN
1	C	512	TYR
1	D	34	LEU
1	D	68	VAL
1	D	163	LEU
1	D	164	SER
1	D	340	TRP
1	D	441	ASN
1	D	512	TYR
1	D	592	LYS

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Mol	Chain	Res	Type
1	E	18	SER
1	E	28	GLN
1	E	127	VAL
1	E	340	TRP
1	E	441	ASN
1	E	512	TYR
1	F	10	GLU
1	F	11	ARG
1	F	328	HIS
1	F	340	TRP
1	F	441	ASN
1	F	512	TYR
1	F	546	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	A	215	HIS
1	A	261	ASN
1	A	328	HIS
1	A	441	ASN
1	B	110	ASN
1	B	234	ASN
1	B	293	ASN
1	B	328	HIS
1	B	458	GLN
1	B	577	ASN
1	C	90	ASN
1	C	110	ASN
1	C	234	ASN
1	C	328	HIS
1	C	441	ASN
1	D	192	GLN
1	D	441	ASN
1	D	577	ASN
1	D	620	GLN
1	E	28	GLN
1	E	90	ASN
1	E	110	ASN
1	E	192	GLN
1	E	215	HIS

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Mol	Chain	Res	Type
1	E	234	ASN
1	E	367	GLN
1	E	441	ASN
1	E	476	ASN
1	F	192	GLN
1	F	215	HIS
1	F	328	HIS
1	F	373	HIS
1	F	441	ASN
1	F	458	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

48 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	$\#\|Z\| > 2$
4	GOL	E	703	-	5,5,5	2.08	2 (40%)	5,5,5	1.77	1 (20%)
3	IMD	C	805	-	3,5,5	0.73	0	4,5,5	0.52	0
4	GOL	C	801	-	5,5,5	0.99	0	5,5,5	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	F	706	-	5,5,5	1.75	1 (20%)	5,5,5	1.20	0
3	IMD	E	708	-	3,5,5	0.77	0	4,5,5	0.83	0
2	LMR	E	707	-	2,8,8	2.94	1 (50%)	3,10,10	1.86	1 (33%)
2	LMR	B	703	-	2,8,8	3.69	2 (100%)	3,10,10	3.46	2 (66%)
4	GOL	A	806	-	5,5,5	0.22	0	5,5,5	0.78	0
3	IMD	C	810	-	3,5,5	0.57	0	4,5,5	0.22	0
3	IMD	E	704	-	3,5,5	0.91	0	4,5,5	0.97	0
3	IMD	B	708	-	3,5,5	0.53	0	4,5,5	0.63	0
3	IMD	B	705	-	3,5,5	0.56	0	4,5,5	0.85	0
3	IMD	A	805	-	3,5,5	0.61	0	4,5,5	0.70	0
4	GOL	B	707	-	5,5,5	1.28	0	5,5,5	1.42	1 (20%)
4	GOL	F	702	-	5,5,5	1.41	1 (20%)	5,5,5	1.71	2 (40%)
3	IMD	E	702	-	3,5,5	0.59	0	4,5,5	0.54	0
3	IMD	E	705	-	3,5,5	0.57	0	4,5,5	0.72	0
4	GOL	C	802	-	5,5,5	2.08	1 (20%)	5,5,5	1.35	1 (20%)
3	IMD	C	804	-	3,5,5	0.65	0	4,5,5	0.77	0
4	GOL	D	707	-	5,5,5	0.40	0	5,5,5	0.44	0
4	GOL	B	701	-	5,5,5	0.24	0	5,5,5	0.63	0
4	GOL	E	706	-	5,5,5	0.93	0	5,5,5	0.72	0
4	GOL	B	702	-	5,5,5	1.17	0	5,5,5	1.00	0
3	IMD	F	705	-	3,5,5	0.90	0	4,5,5	0.65	0
3	IMD	C	806	-	3,5,5	0.51	0	4,5,5	0.93	0
3	IMD	A	804	-	3,5,5	0.56	0	4,5,5	0.32	0
2	LMR	D	702	-	2,8,8	1.01	0	3,10,10	1.56	1 (33%)
4	GOL	C	803	-	5,5,5	0.53	0	5,5,5	0.87	0
4	GOL	A	803	-	5,5,5	1.08	0	5,5,5	1.80	2 (40%)
3	IMD	F	703	-	3,5,5	0.42	0	4,5,5	0.45	0
3	IMD	B	706	-	3,5,5	1.00	0	4,5,5	0.52	0
3	IMD	D	706	-	3,5,5	0.61	0	4,5,5	0.72	0
4	GOL	D	705	-	5,5,5	2.80	4 (80%)	5,5,5	1.32	1 (20%)
3	IMD	B	704	-	3,5,5	0.70	0	4,5,5	0.46	0
3	IMD	F	709	-	3,5,5	0.66	0	4,5,5	0.45	0
4	GOL	F	701	-	5,5,5	0.75	0	5,5,5	0.74	0
3	IMD	D	701	-	3,5,5	0.55	0	4,5,5	0.26	0
4	GOL	C	807	-	5,5,5	0.40	0	5,5,5	1.06	0
4	GOL	E	701	-	5,5,5	0.54	0	5,5,5	0.20	0
3	IMD	F	704	-	3,5,5	0.74	0	4,5,5	0.68	0
2	LMR	F	707	-	2,8,8	1.74	1 (50%)	3,10,10	4.06	1 (33%)
2	LMR	A	801	-	2,8,8	0.85	0	3,10,10	1.92	1 (33%)
2	LMR	F	708	-	2,8,8	1.57	0	3,10,10	2.94	3 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	IMD	A	802	-	3,5,5	0.53	0	4,5,5	0.48	0
4	GOL	D	704	-	5,5,5	0.67	0	5,5,5	1.70	2 (40%)
2	LMR	C	809	-	2,8,8	0.72	0	3,10,10	2.73	3 (100%)
3	IMD	D	703	-	3,5,5	0.80	0	4,5,5	0.47	0
3	IMD	C	808	-	3,5,5	0.72	0	4,5,5	0.35	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	GOL	E	703	-	-	2/4/4/4	-
4	GOL	F	706	-	-	2/4/4/4	-
4	GOL	C	801	-	-	2/4/4/4	-
3	IMD	C	805	-	-	-	0/1/1/1
3	IMD	E	708	-	-	-	0/1/1/1
2	LMR	E	707	-	-	0/2/8/8	-
2	LMR	B	703	-	-	0/2/8/8	-
4	GOL	A	806	-	-	2/4/4/4	-
3	IMD	C	810	-	-	-	0/1/1/1
3	IMD	E	704	-	-	-	0/1/1/1
4	GOL	B	707	-	-	2/4/4/4	-
3	IMD	B	705	-	-	-	0/1/1/1
3	IMD	A	805	-	-	-	0/1/1/1
3	IMD	B	708	-	-	-	0/1/1/1
4	GOL	F	702	-	-	4/4/4/4	-
4	GOL	C	802	-	-	2/4/4/4	-
3	IMD	E	702	-	-	-	0/1/1/1
3	IMD	E	705	-	-	-	0/1/1/1
3	IMD	C	804	-	-	-	0/1/1/1
4	GOL	D	707	-	-	0/4/4/4	-
4	GOL	B	701	-	-	0/4/4/4	-
4	GOL	E	706	-	-	0/4/4/4	-
4	GOL	B	702	-	-	2/4/4/4	-
3	IMD	F	705	-	-	-	0/1/1/1
3	IMD	A	804	-	-	-	0/1/1/1
3	IMD	C	806	-	-	-	0/1/1/1
2	LMR	D	702	-	-	2/2/8/8	-
4	GOL	C	803	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	803	-	-	4/4/4/4	-
3	IMD	F	703	-	-	-	0/1/1/1
4	GOL	D	705	-	-	0/4/4/4	-
3	IMD	B	706	-	-	-	0/1/1/1
3	IMD	D	706	-	-	-	0/1/1/1
3	IMD	B	704	-	-	-	0/1/1/1
3	IMD	F	709	-	-	-	0/1/1/1
4	GOL	F	701	-	-	2/4/4/4	-
3	IMD	D	701	-	-	-	0/1/1/1
4	GOL	C	807	-	-	0/4/4/4	-
4	GOL	E	701	-	-	2/4/4/4	-
3	IMD	F	704	-	-	-	0/1/1/1
2	LMR	F	707	-	-	1/2/8/8	-
2	LMR	A	801	-	-	0/2/8/8	-
2	LMR	F	708	-	-	0/2/8/8	-
3	IMD	A	802	-	-	-	0/1/1/1
4	GOL	D	704	-	-	4/4/4/4	-
2	LMR	C	809	-	-	0/2/8/8	-
3	IMD	D	703	-	-	-	0/1/1/1
3	IMD	C	808	-	-	-	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	703	LMR	C3-C2	4.74	1.59	1.53
2	E	707	LMR	C3-C2	-4.05	1.47	1.53
4	C	802	GOL	O2-C2	3.76	1.54	1.43
4	E	703	GOL	O2-C2	3.72	1.54	1.43
4	F	706	GOL	C1-C2	3.34	1.65	1.51
4	D	705	GOL	O1-C1	3.31	1.56	1.42
4	D	705	GOL	O3-C3	3.15	1.55	1.42
4	D	705	GOL	C1-C2	3.08	1.64	1.51
4	D	705	GOL	O2-C2	2.85	1.51	1.43
4	E	703	GOL	C1-C2	2.37	1.61	1.51
4	F	702	GOL	O2-C2	2.31	1.50	1.43
2	B	703	LMR	O2-C2	-2.19	1.37	1.42
2	F	707	LMR	C3-C2	-2.14	1.50	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	707	LMR	C3-C2-C1	6.83	119.79	111.10
2	B	703	LMR	C3-C2-C1	-4.70	105.12	111.10
2	B	703	LMR	O2-C2-C3	3.45	116.08	108.50
2	F	708	LMR	O2-C2-C3	3.18	115.48	108.50
2	C	809	LMR	O2-C2-C3	3.08	115.27	108.50
2	F	708	LMR	C3-C2-C1	-3.06	107.20	111.10
4	B	707	GOL	C3-C2-C1	-2.91	100.38	111.70
4	E	703	GOL	O3-C3-C2	2.86	123.90	110.20
4	A	803	GOL	O3-C3-C2	-2.76	96.96	110.20
4	F	702	GOL	O2-C2-C1	2.73	121.16	109.12
2	C	809	LMR	C3-C2-C1	2.73	114.57	111.10
4	D	704	GOL	O3-C3-C2	-2.55	97.96	110.20
2	F	708	LMR	O2-C2-C1	-2.53	104.05	111.66
4	C	802	GOL	O2-C2-C1	2.41	119.73	109.12
2	D	702	LMR	O2-C2-C3	2.37	113.71	108.50
2	C	809	LMR	O2-C2-C1	-2.34	104.63	111.66
4	D	704	GOL	C3-C2-C1	2.20	120.26	111.70
4	F	702	GOL	O1-C1-C2	2.19	120.72	110.20
2	A	801	LMR	O2-C2-C3	2.14	113.21	108.50
4	D	705	GOL	O3-C3-C2	2.08	120.18	110.20
2	E	707	LMR	O2-C2-C1	-2.05	105.50	111.66
4	A	803	GOL	C3-C2-C1	2.05	119.66	111.70

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	707	LMR	C1-C2-C3-C4
4	A	803	GOL	C1-C2-C3-O3
4	A	803	GOL	O2-C2-C3-O3
4	A	806	GOL	C1-C2-C3-O3
4	B	702	GOL	C1-C2-C3-O3
4	B	702	GOL	O2-C2-C3-O3
4	C	801	GOL	O1-C1-C2-C3
4	D	704	GOL	C1-C2-C3-O3
4	D	704	GOL	O2-C2-C3-O3
4	E	701	GOL	C1-C2-C3-O3
4	E	703	GOL	C1-C2-C3-O3
4	F	701	GOL	C1-C2-C3-O3
4	F	702	GOL	O1-C1-C2-C3
4	F	702	GOL	C1-C2-C3-O3
4	F	706	GOL	O1-C1-C2-C3
4	F	706	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	803	GOL	O1-C1-C2-C3
4	B	707	GOL	O1-C1-C2-C3
4	C	802	GOL	C1-C2-C3-O3
4	D	704	GOL	O1-C1-C2-C3
4	A	806	GOL	O2-C2-C3-O3
4	C	801	GOL	O1-C1-C2-O2
4	C	802	GOL	O2-C2-C3-O3
4	E	701	GOL	O2-C2-C3-O3
4	F	701	GOL	O2-C2-C3-O3
4	F	702	GOL	O1-C1-C2-O2
4	F	702	GOL	O2-C2-C3-O3
4	E	703	GOL	O2-C2-C3-O3
2	D	702	LMR	C1-C2-C3-C4
4	D	704	GOL	O1-C1-C2-O2
2	D	702	LMR	O2-C2-C3-C4
4	A	803	GOL	O1-C1-C2-O2
4	B	707	GOL	O1-C1-C2-O2

There are no ring outliers.

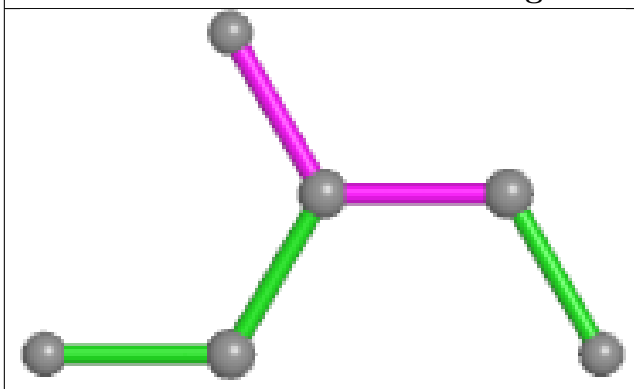
15 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	805	IMD	1	0
2	B	703	LMR	1	0
3	E	704	IMD	10	0
3	B	708	IMD	3	0
4	B	707	GOL	5	0
4	C	802	GOL	1	0
3	C	804	IMD	1	0
3	F	705	IMD	1	0
3	F	703	IMD	1	0
3	B	706	IMD	1	0
4	D	705	GOL	2	0
3	B	704	IMD	1	0
3	F	709	IMD	5	0
2	F	707	LMR	7	0
2	F	708	LMR	7	0

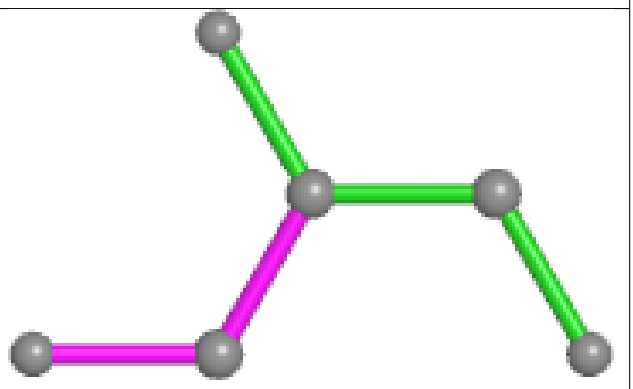
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

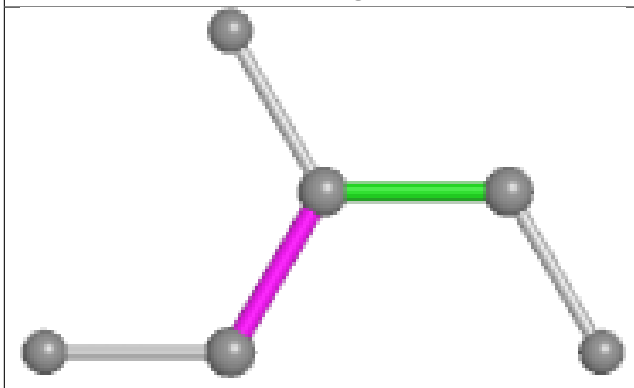
Ligand GOL E 703



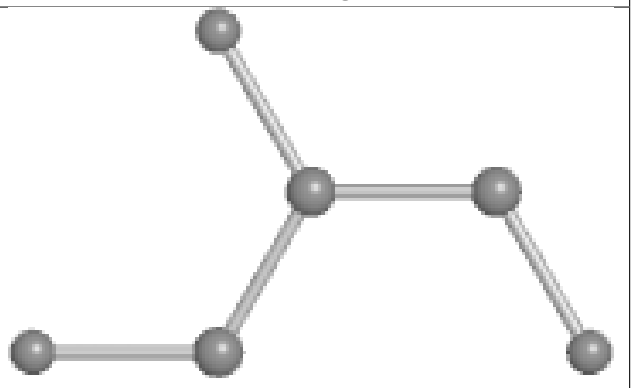
Bond lengths



Bond angles

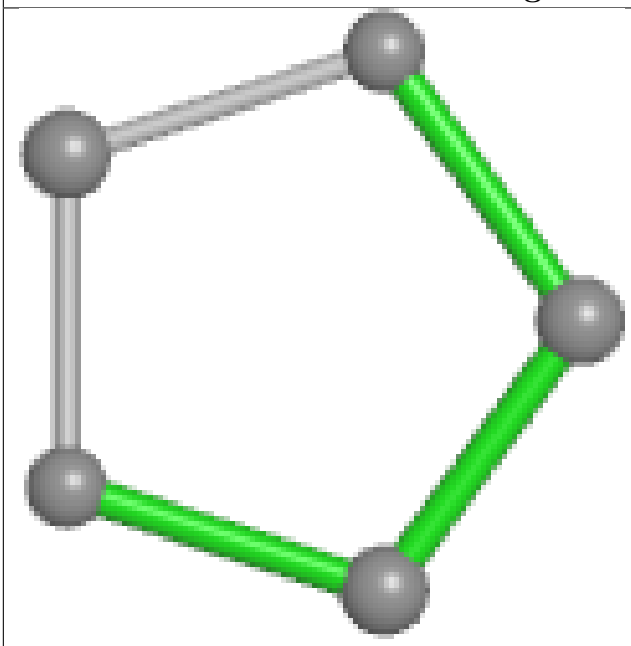


Torsions



Rings

Ligand IMD C 805



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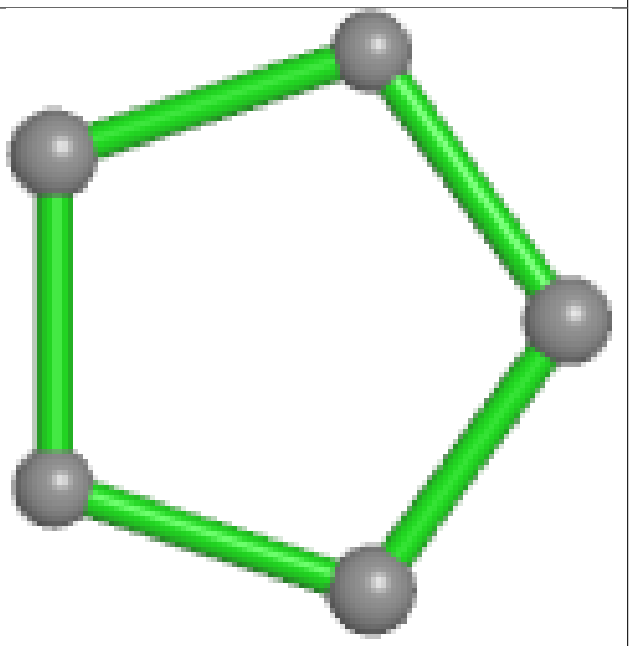

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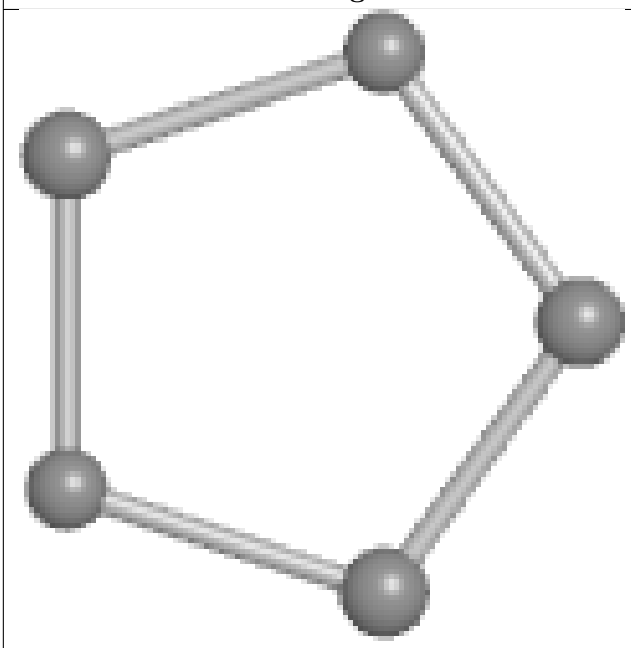

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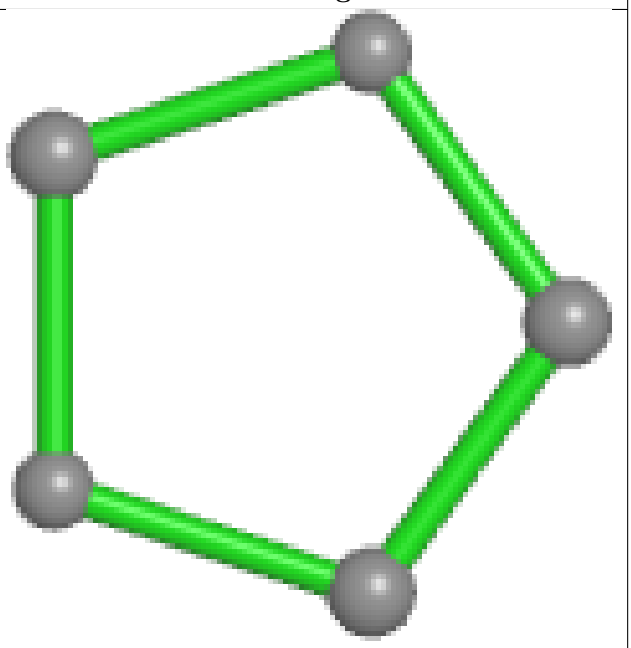
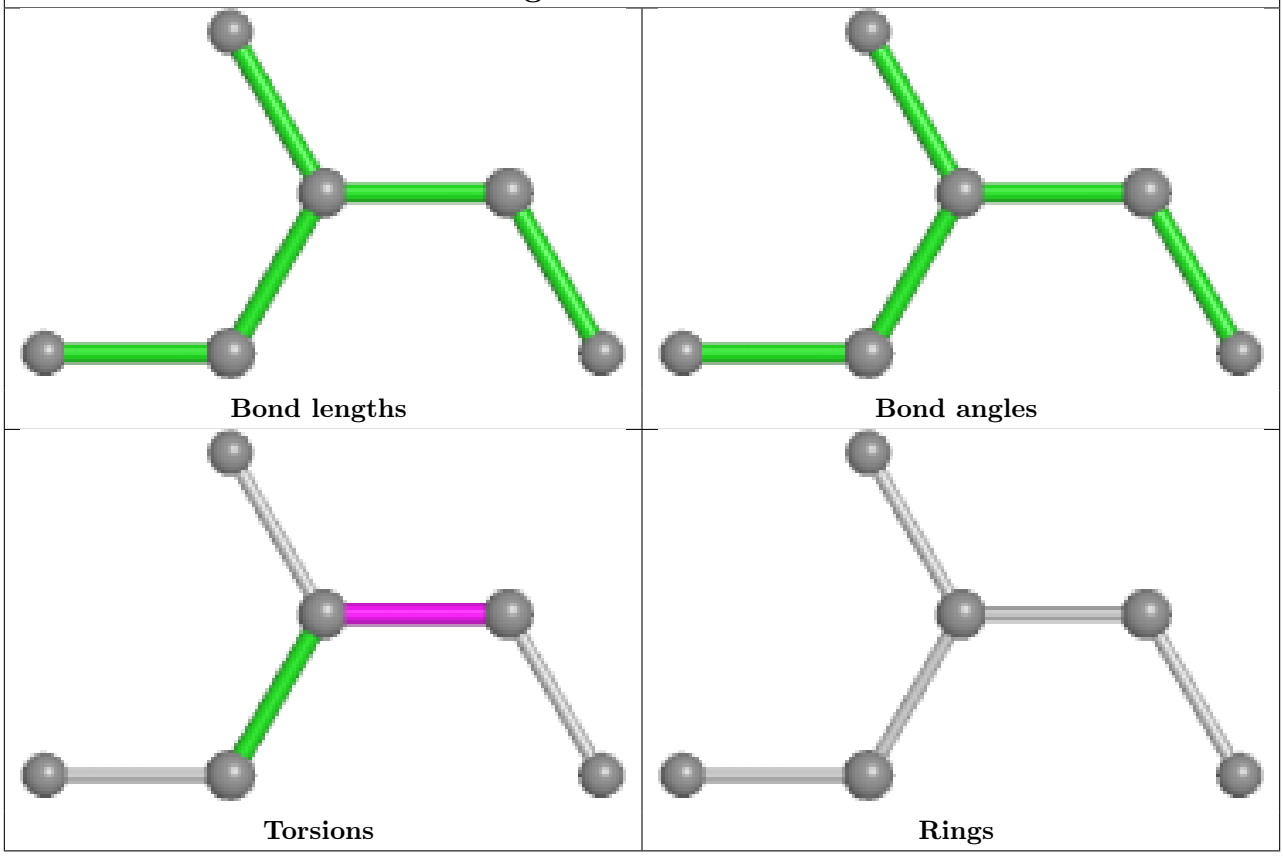


Rings

Ligand GOL C 801



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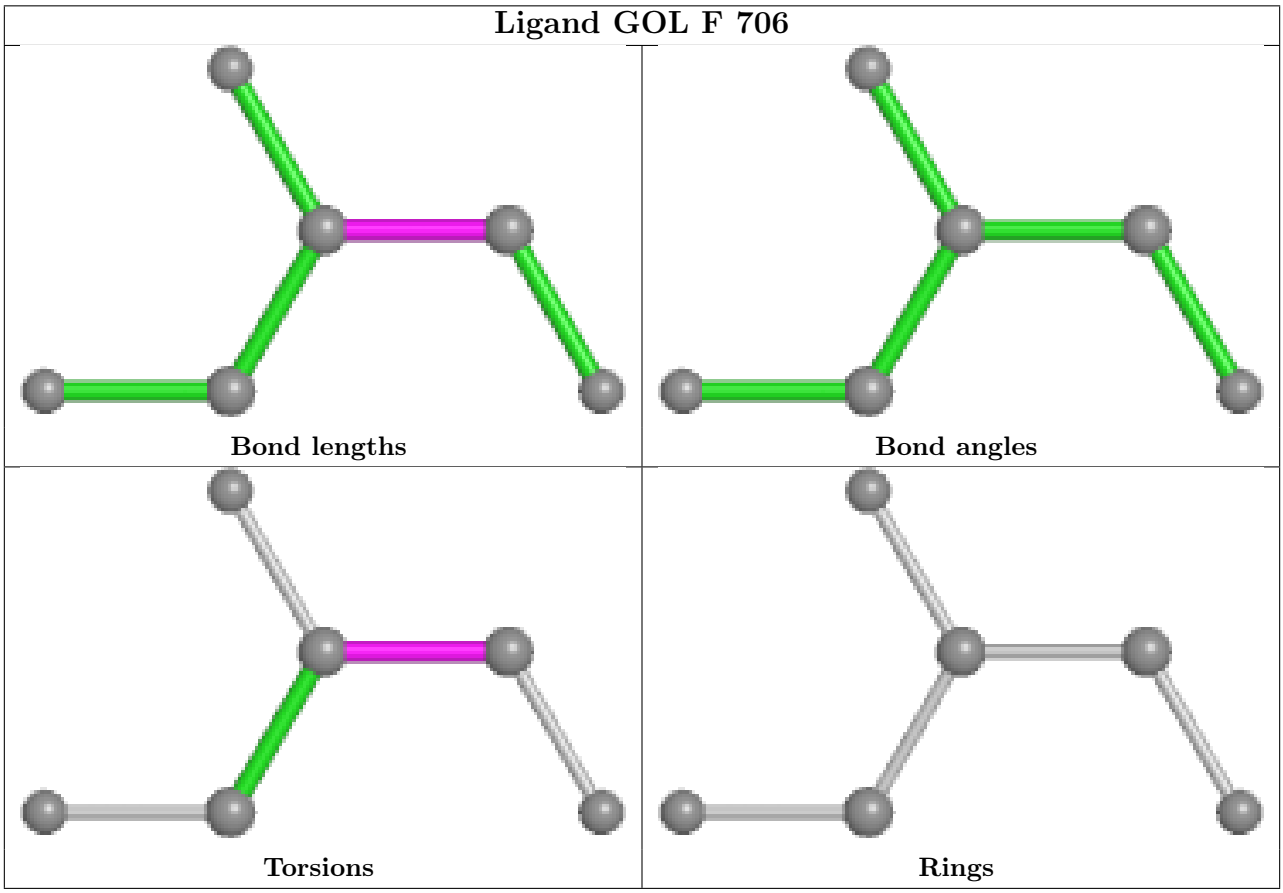

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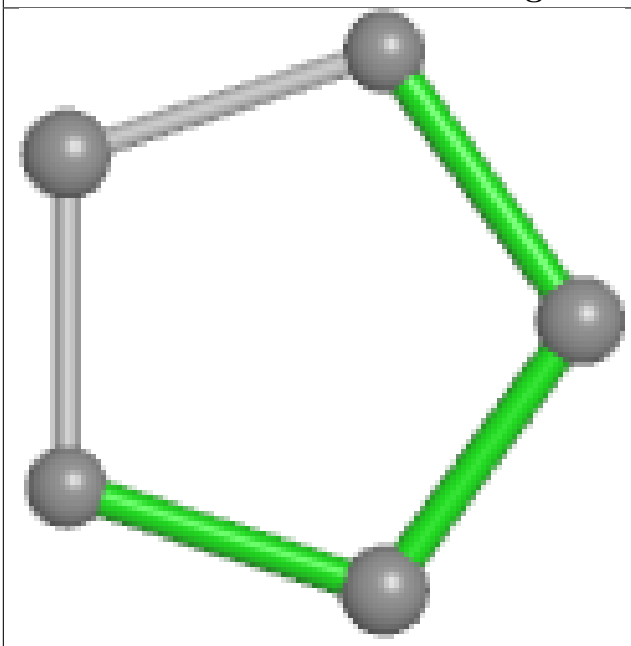

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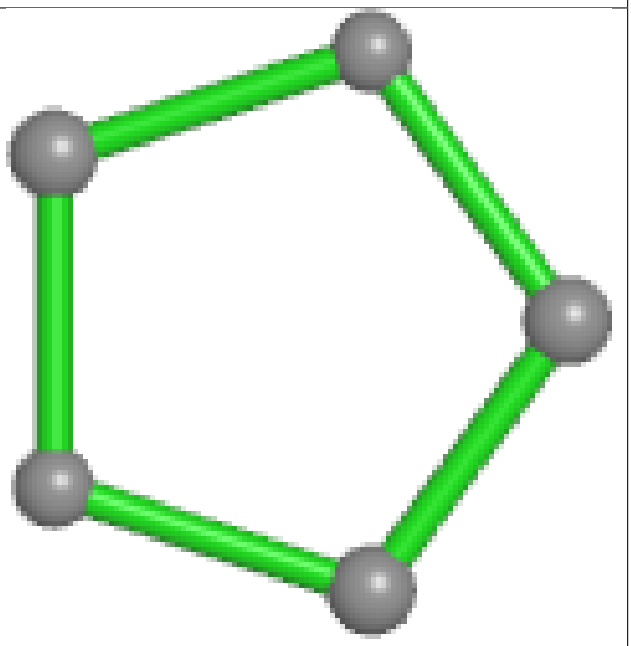
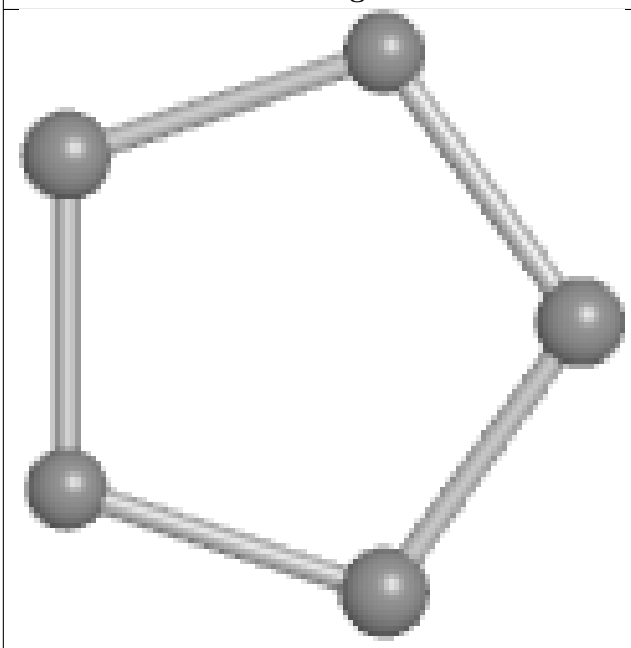


Bond angles



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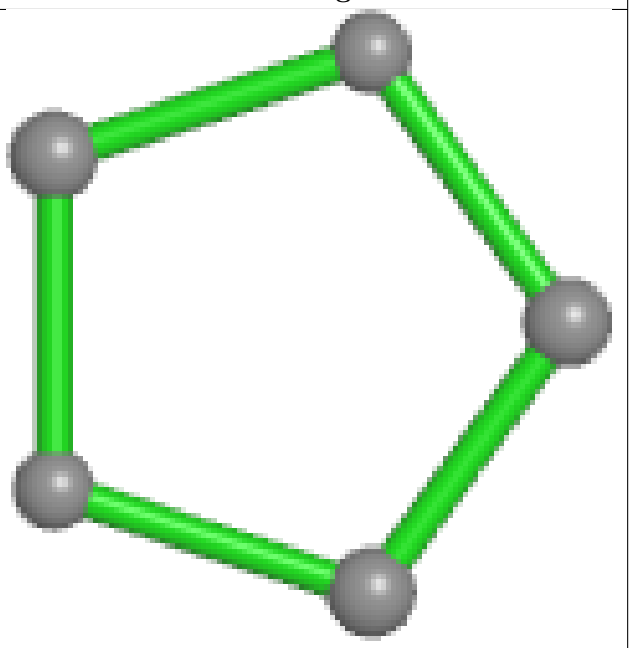
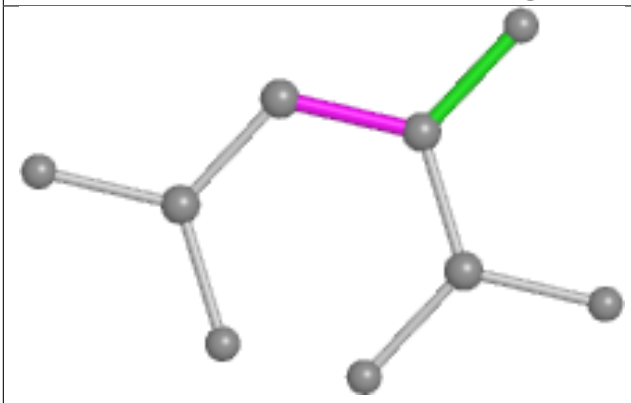


Rings

Ligand LMR E 707



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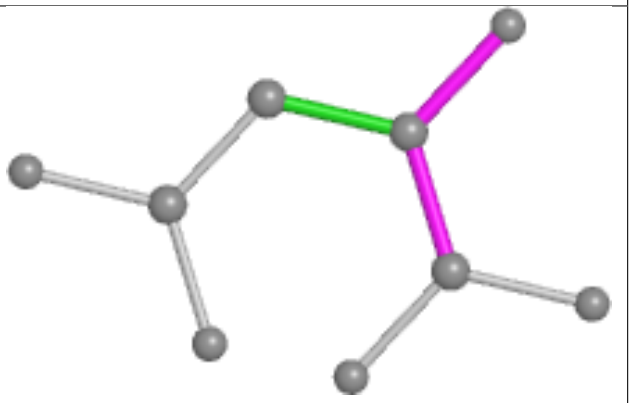

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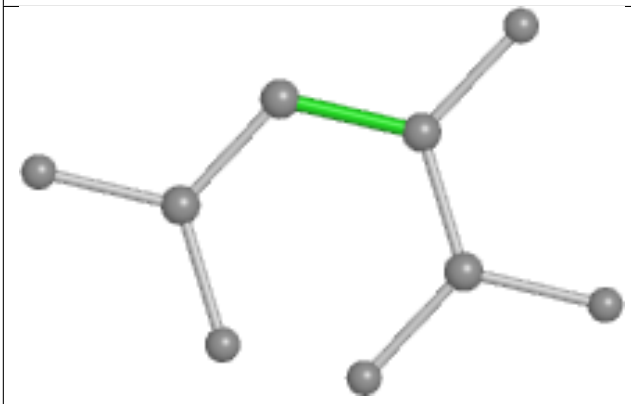

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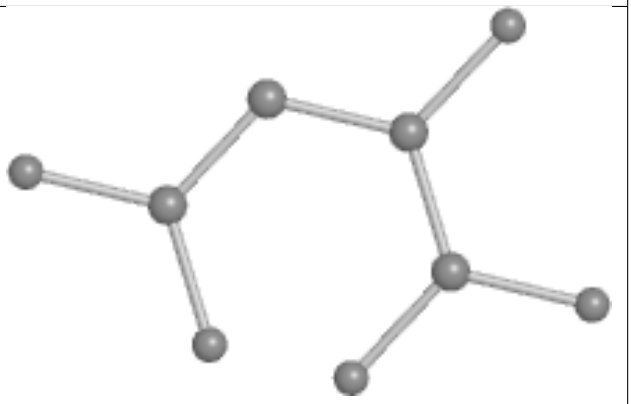
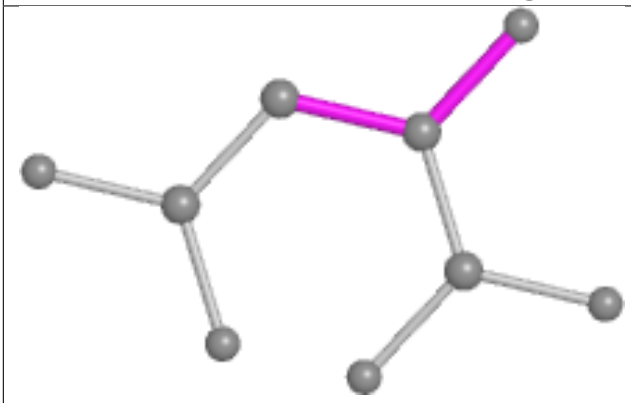


Rings

Ligand LMR B 703



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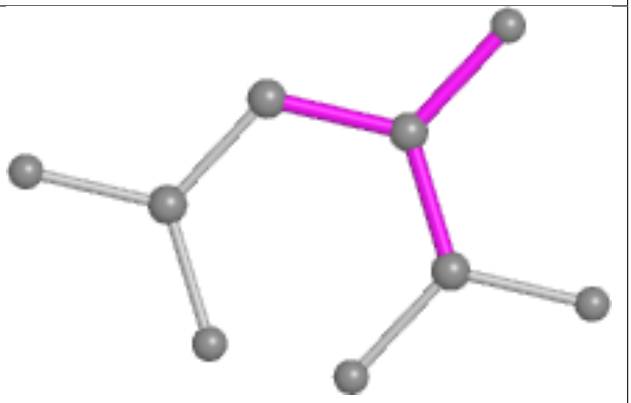

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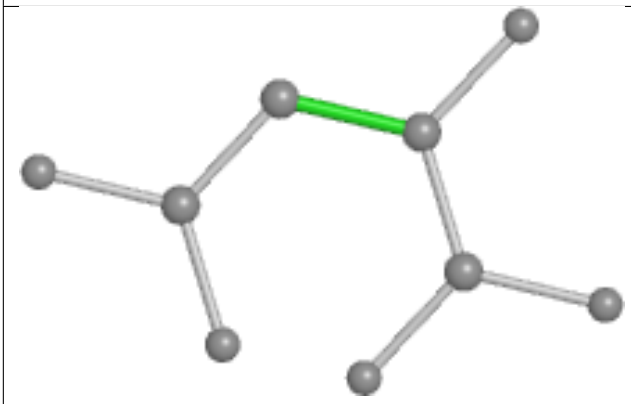

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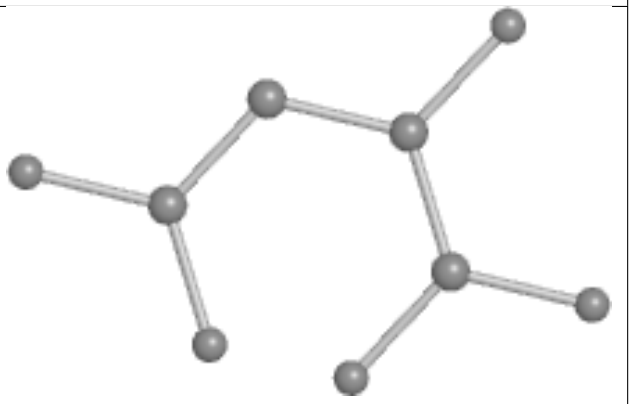
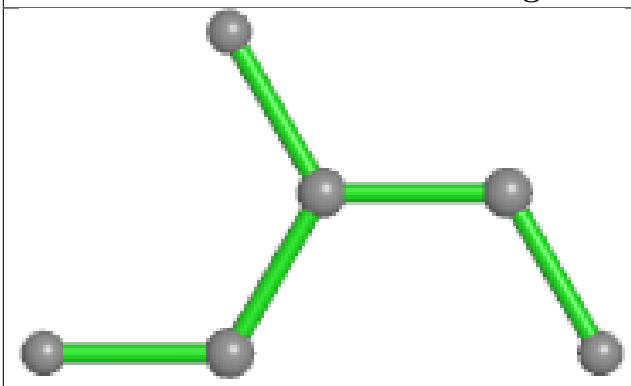


Rings

Ligand GOL A 806



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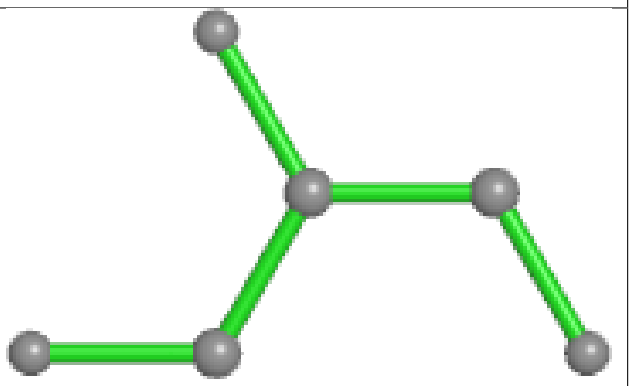
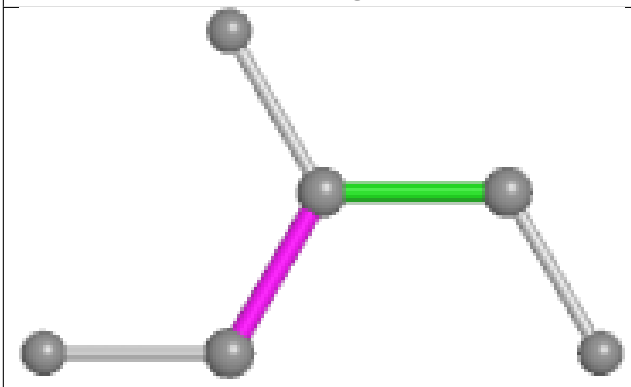


Bond angles



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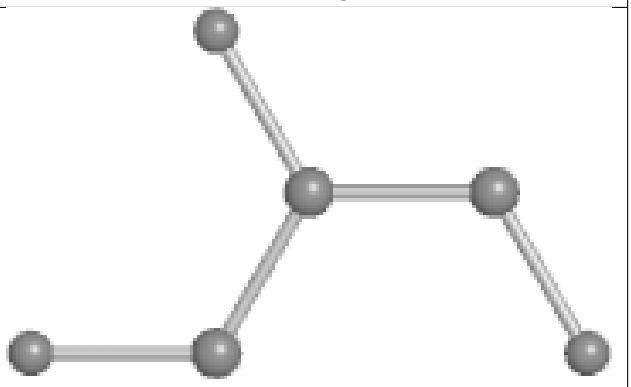
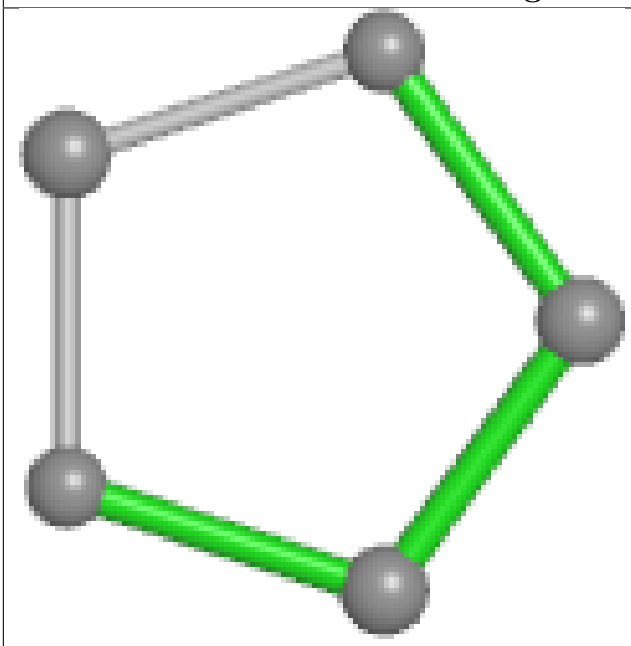


Rings

Ligand IMD C 810



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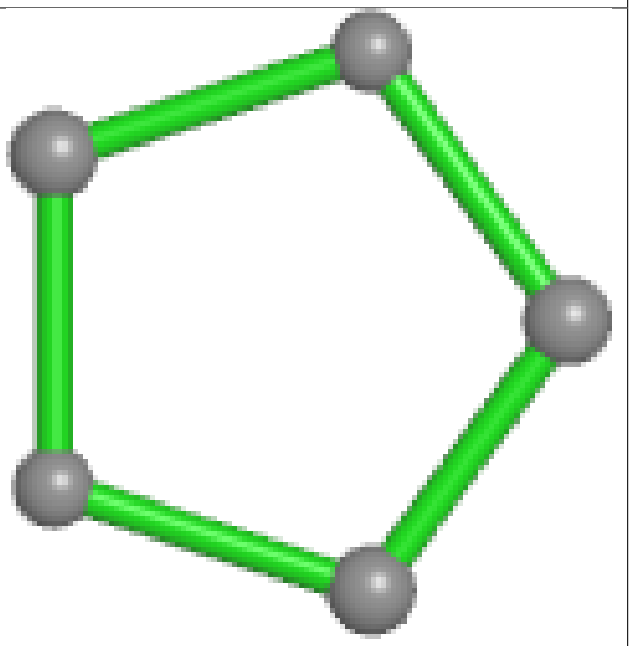

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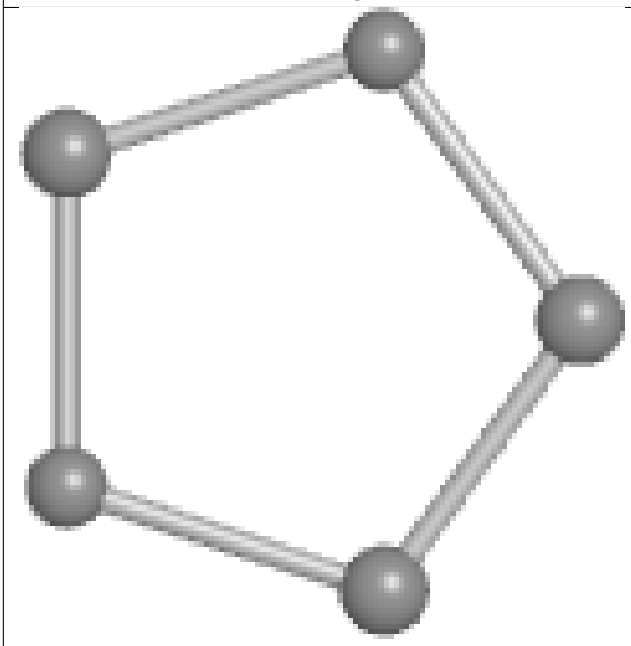

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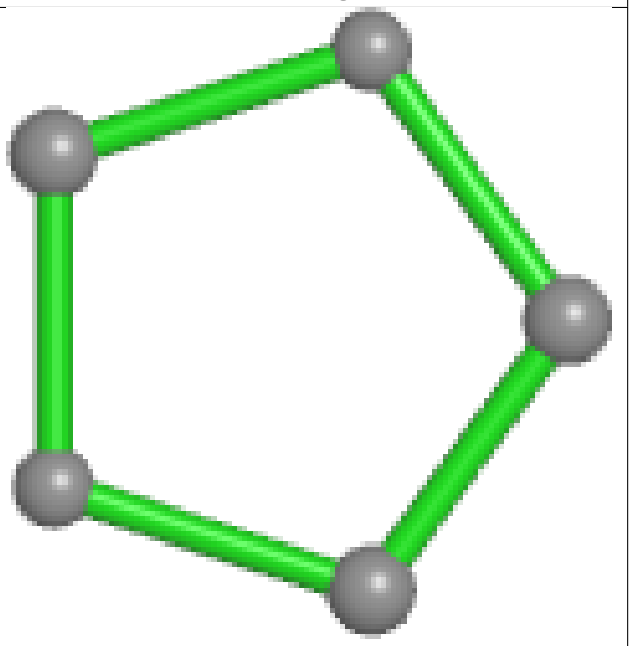
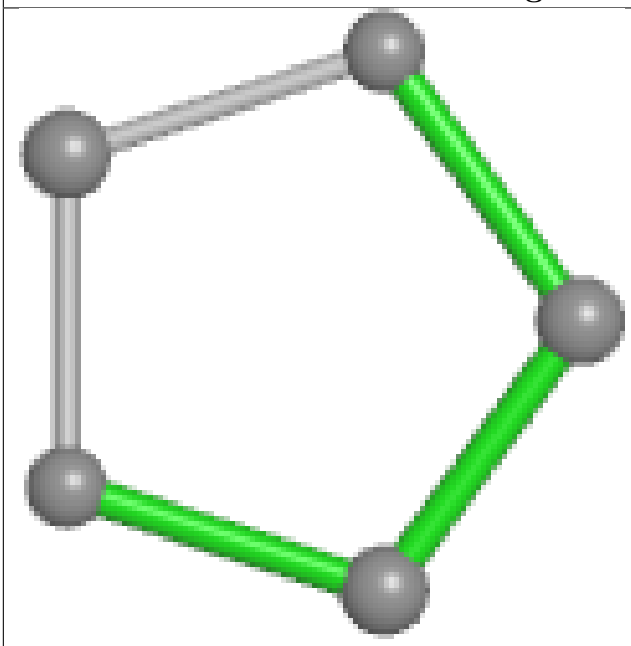


Rings

Ligand IMD E 704



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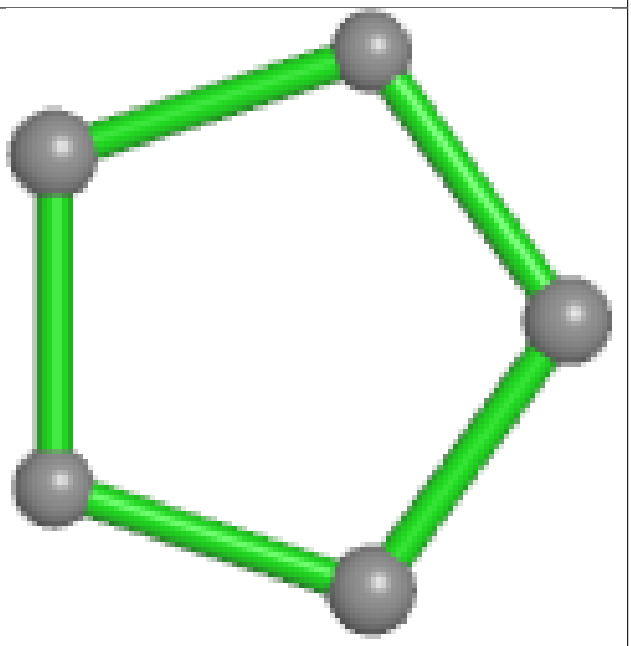
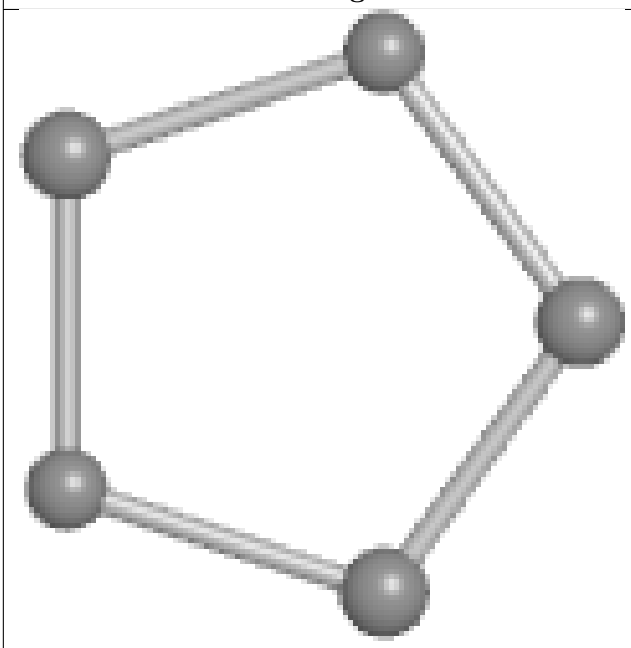


Bond angles



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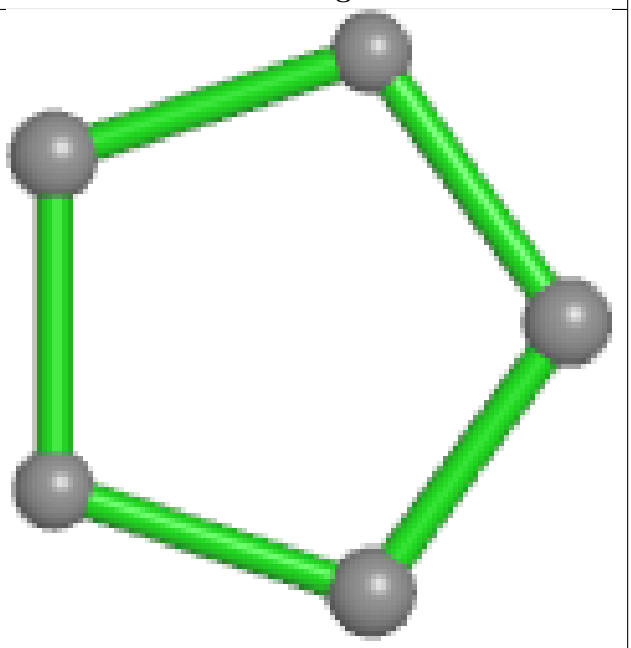
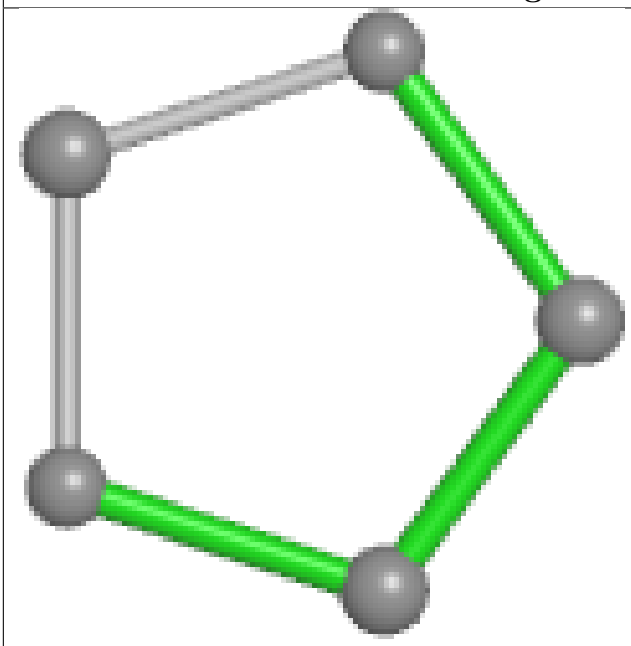


Rings

Ligand IMD B 708



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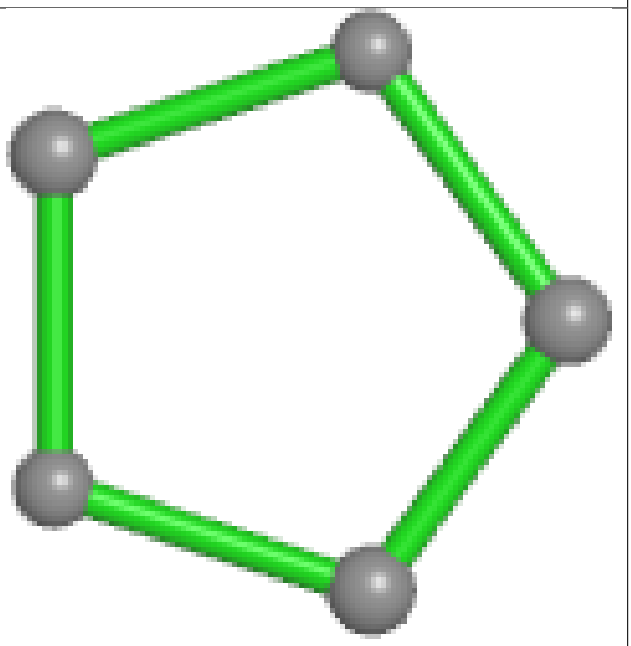
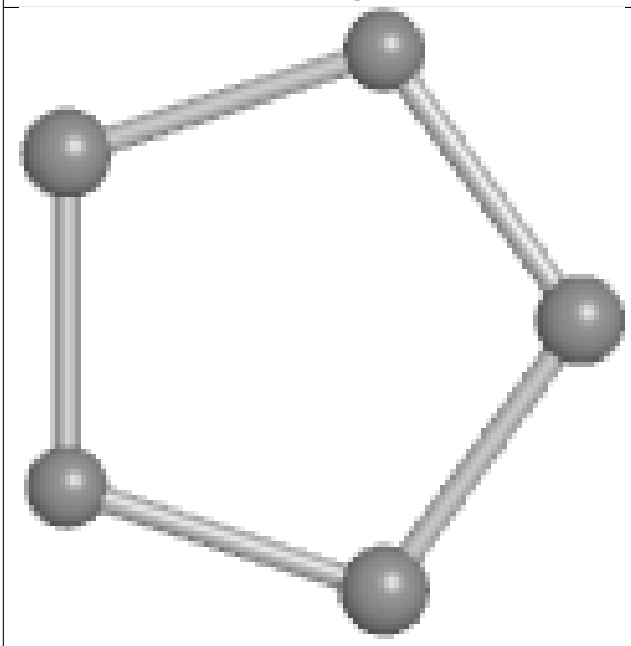


Bond angles



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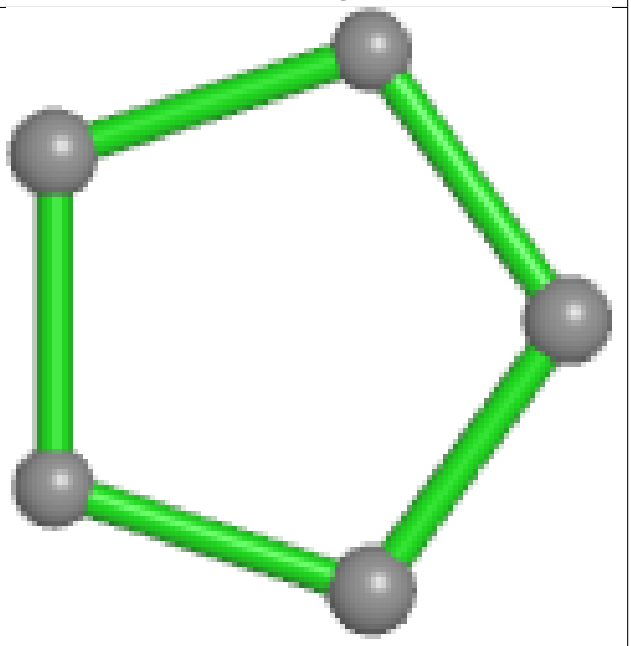
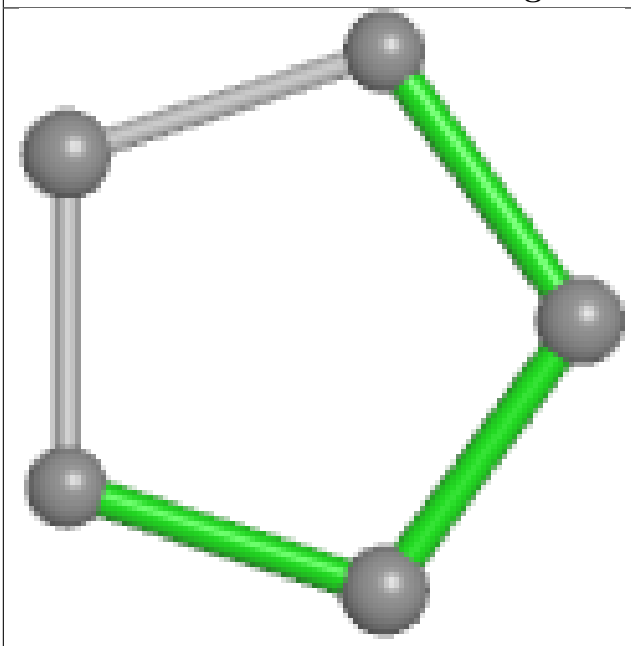
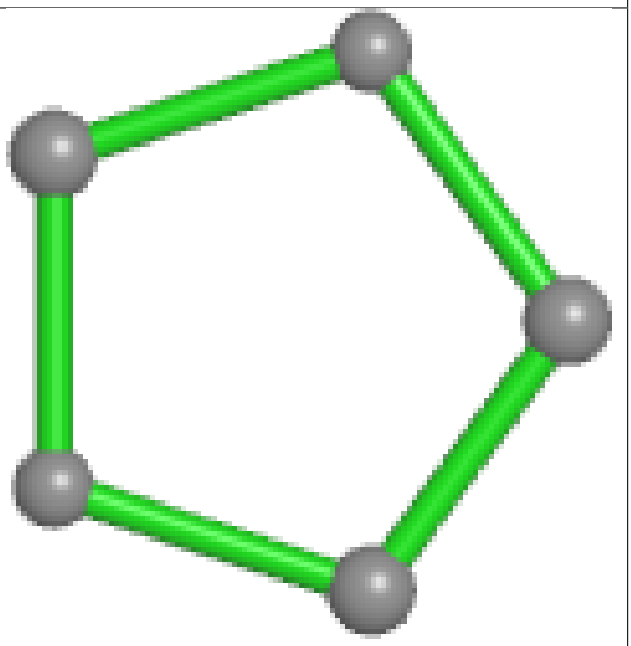


Rings

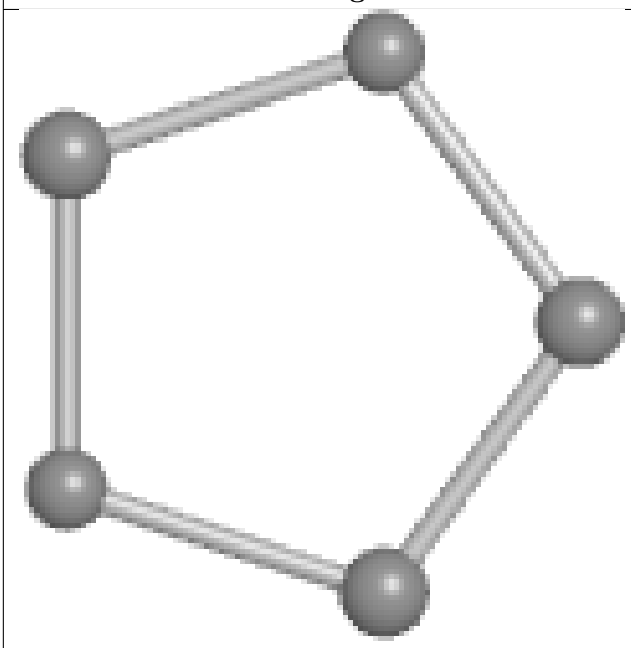
Ligand IMD B 705



Bond lengths



Bond angles



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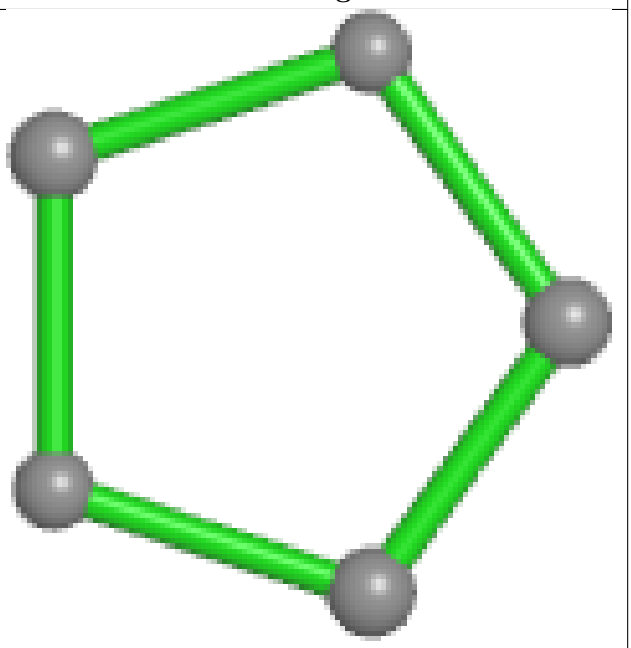
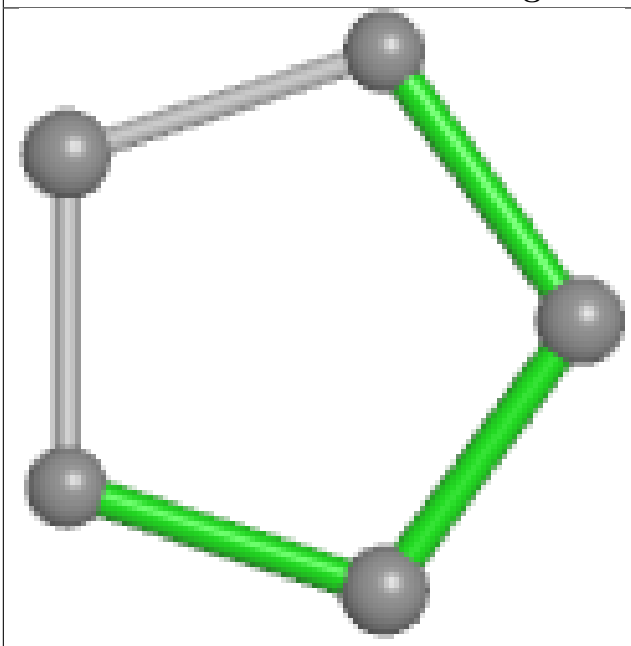
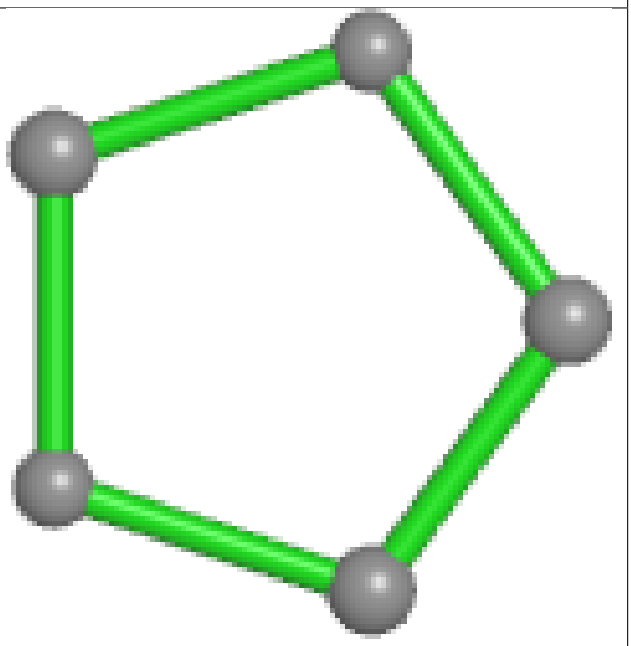


Rings

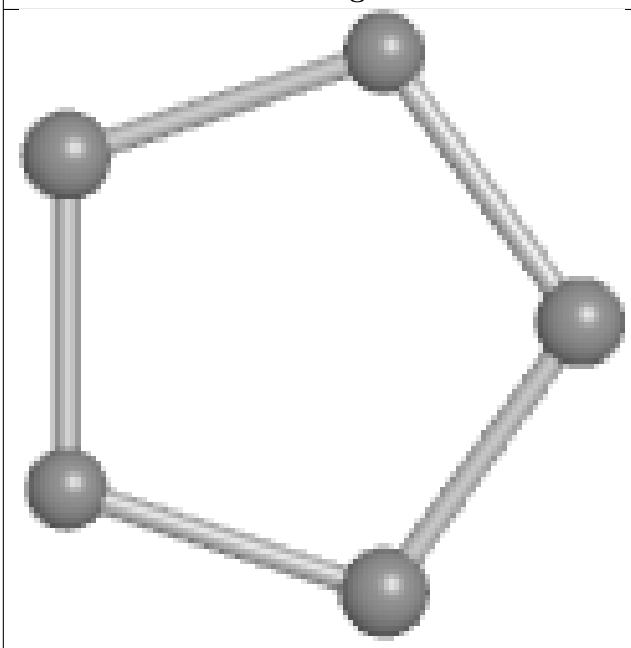
Ligand IMD A 805



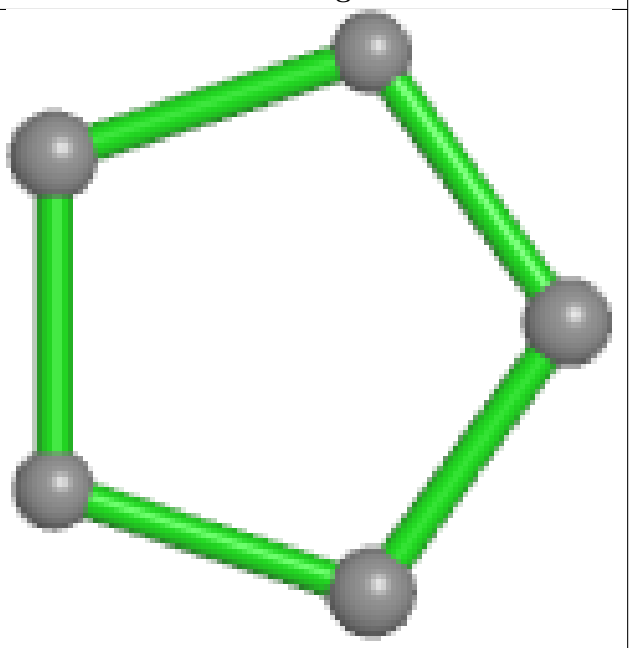
Bond lengths



Bond angles

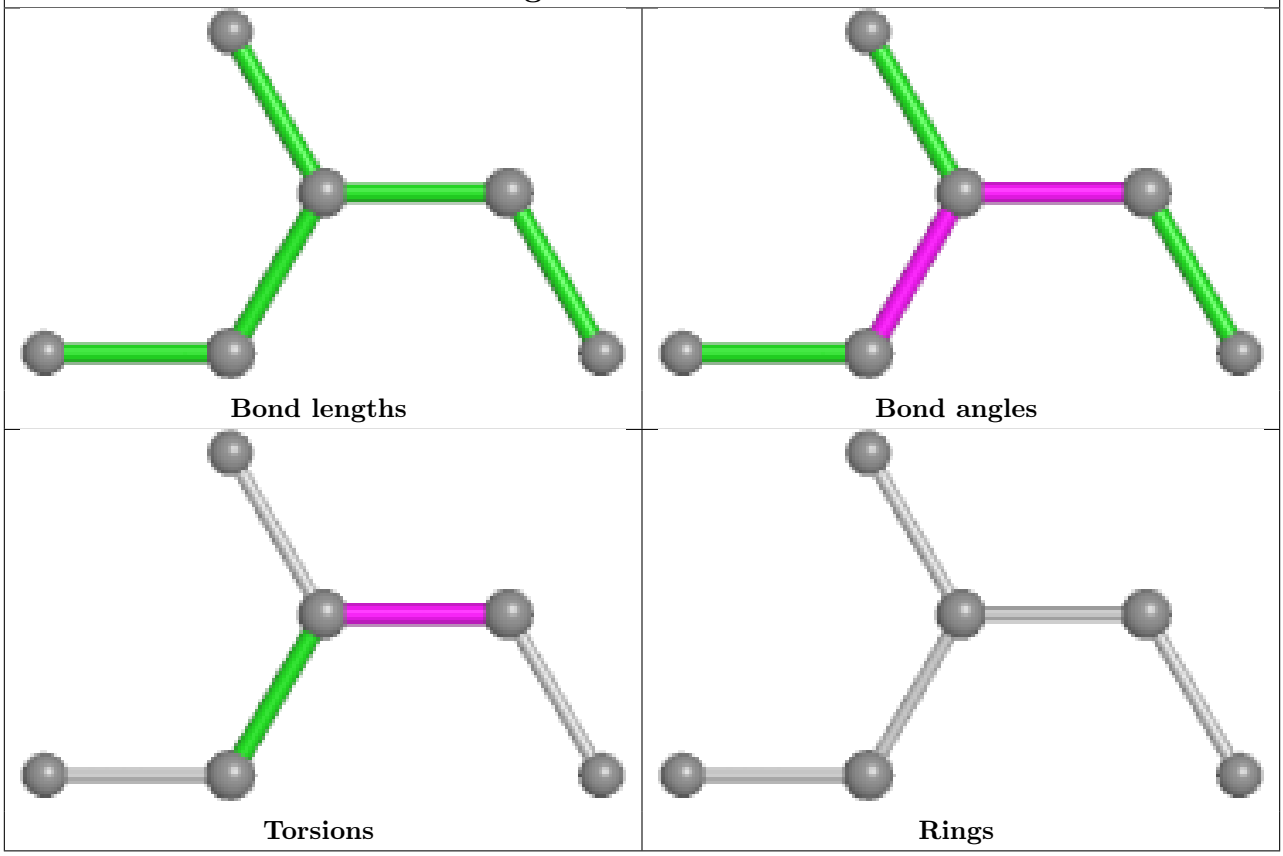


Torsions

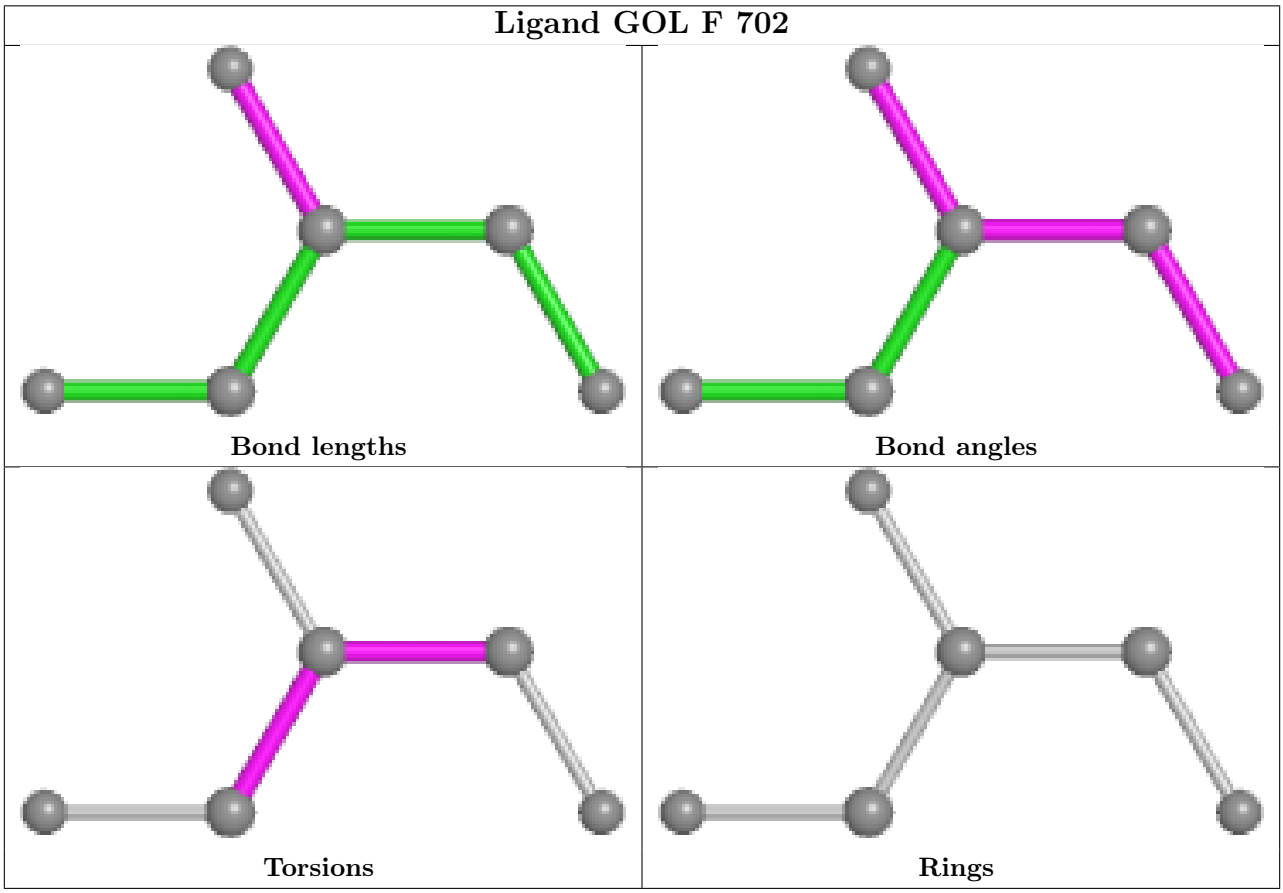


Rings

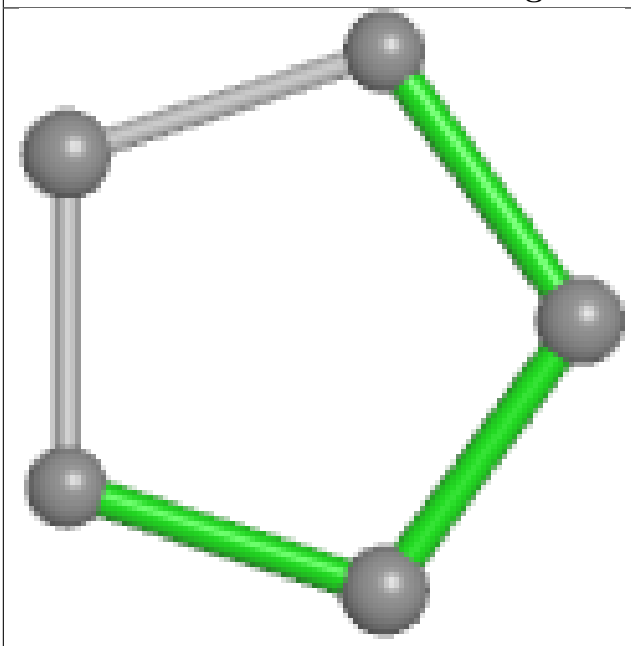
Ligand GOL B 707



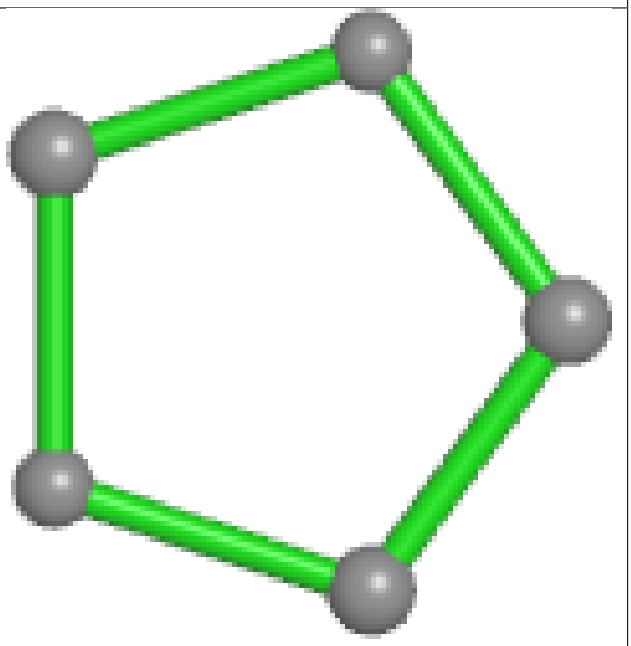
Ligand GOL F 702



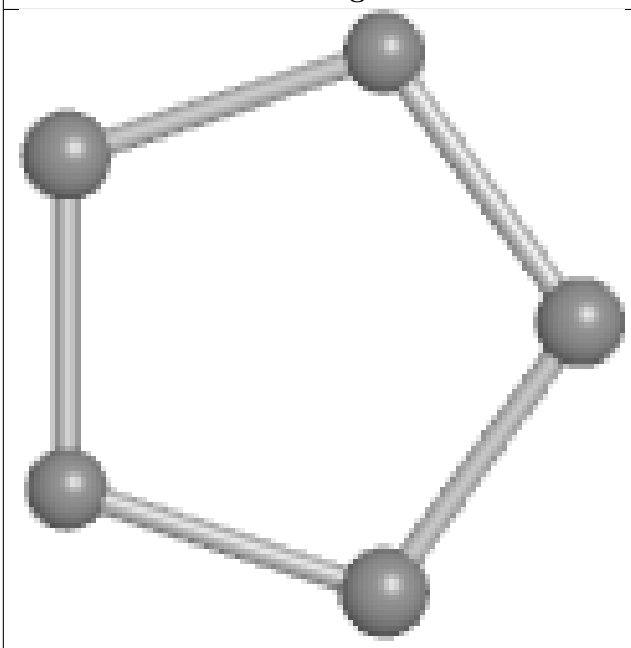
Ligand IMD E 702



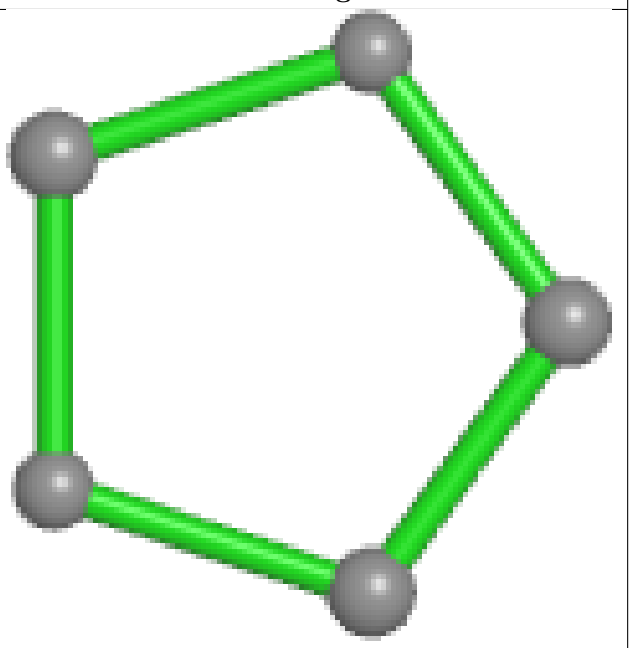
Bond lengths



Bond angles

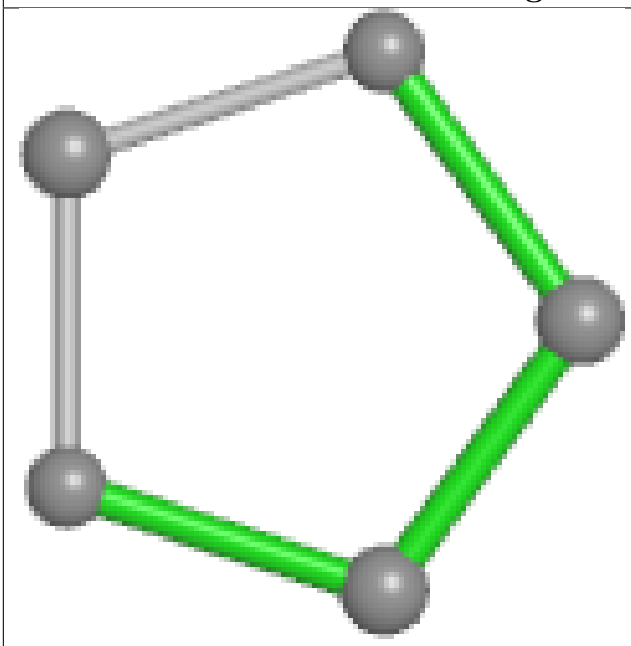


Torsions

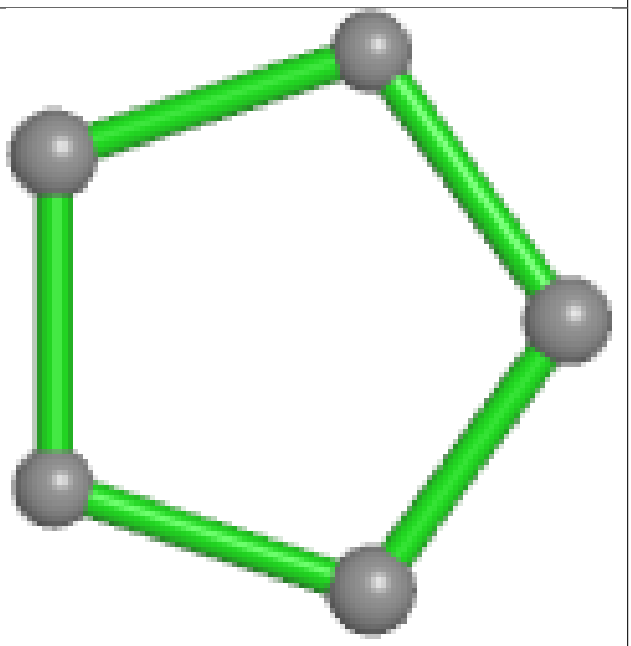


Rings

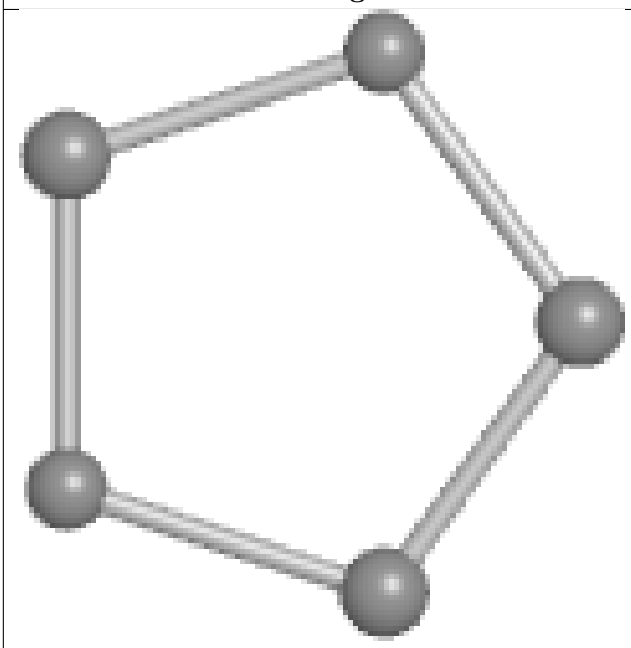
Ligand IMD E 705



Bond lengths



Bond angles



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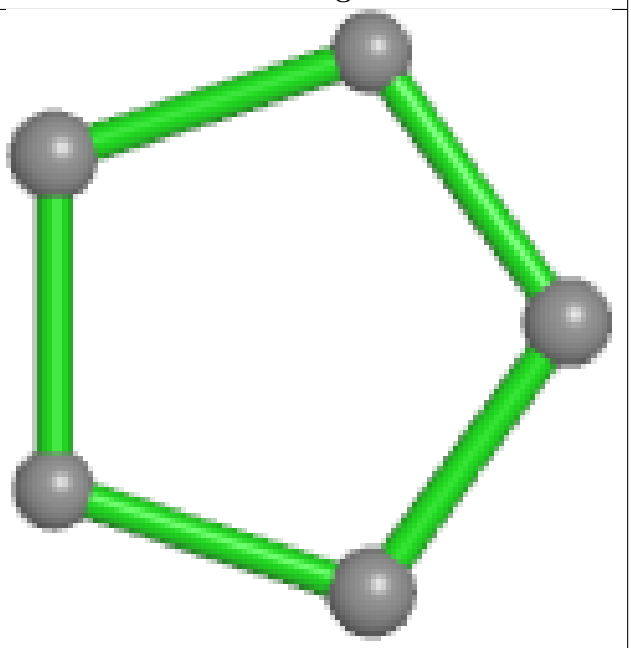
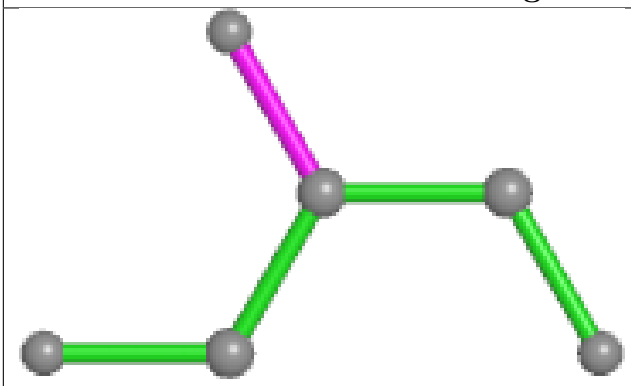
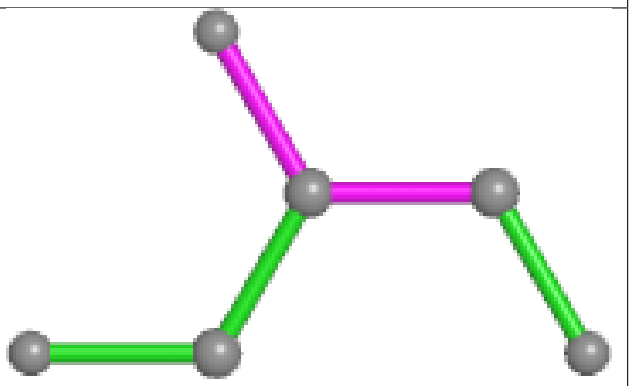


Rings

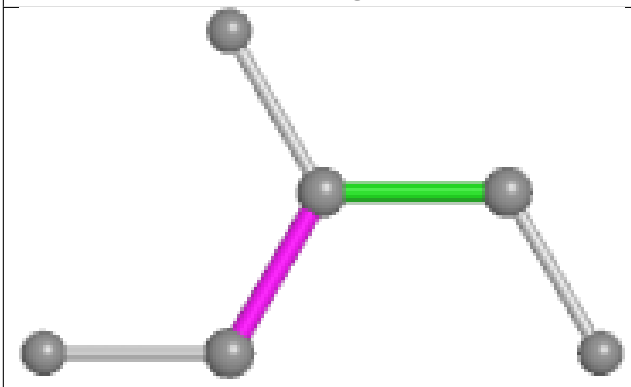
Ligand GOL C 802



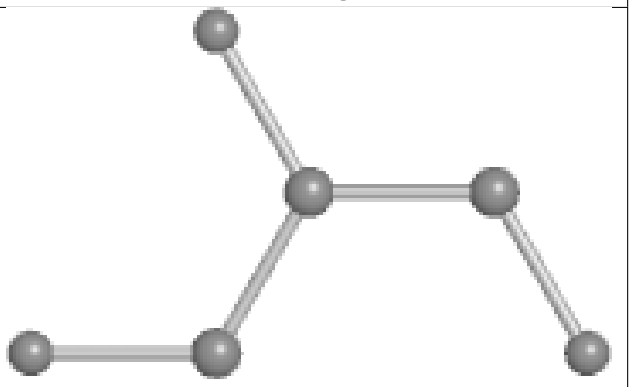
Bond lengths



Bond angles

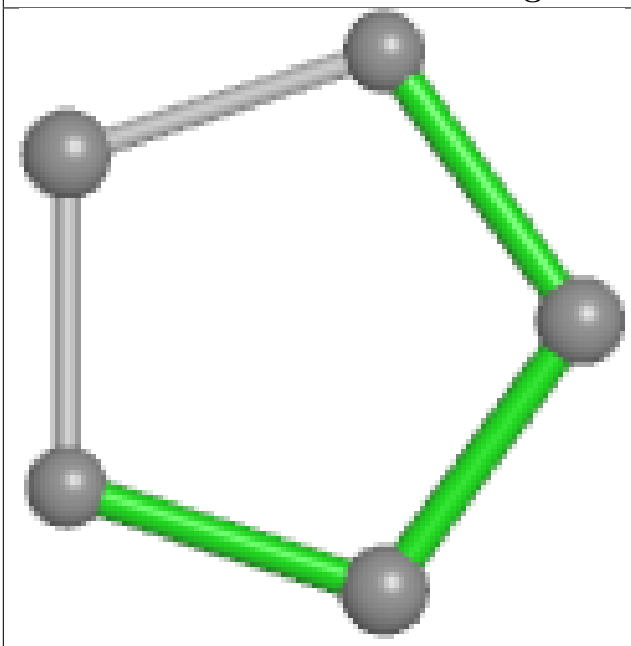


Torsions

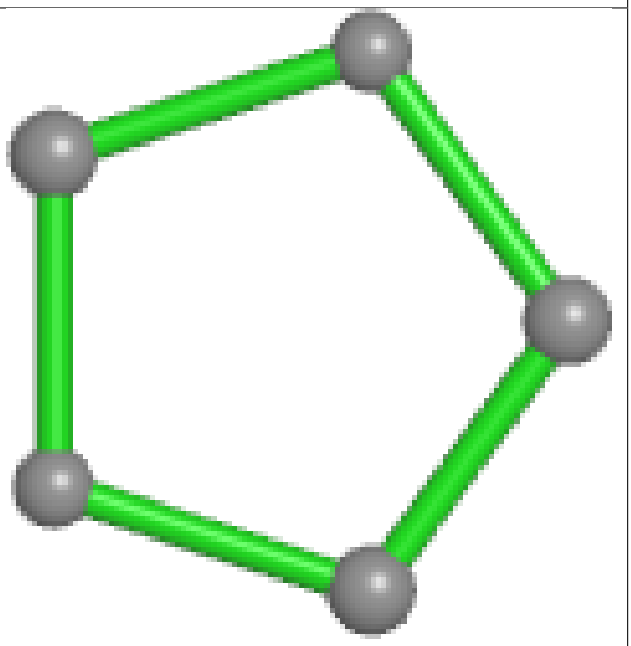


Rings

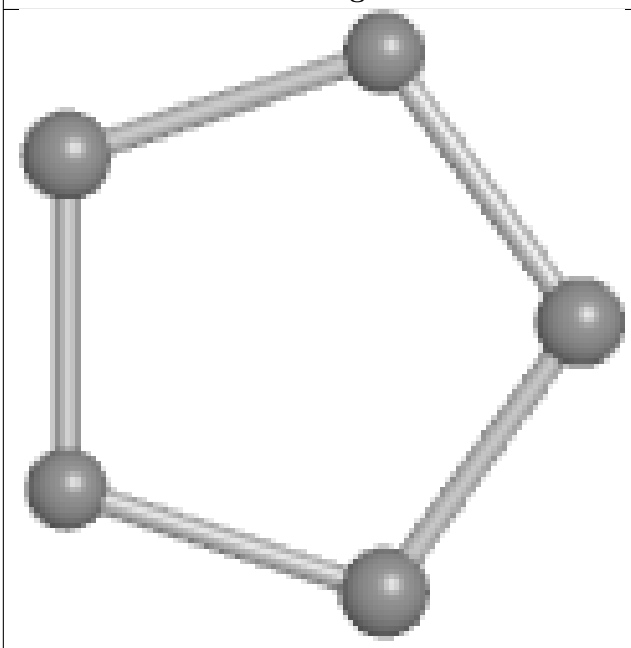
Ligand IMD C 804



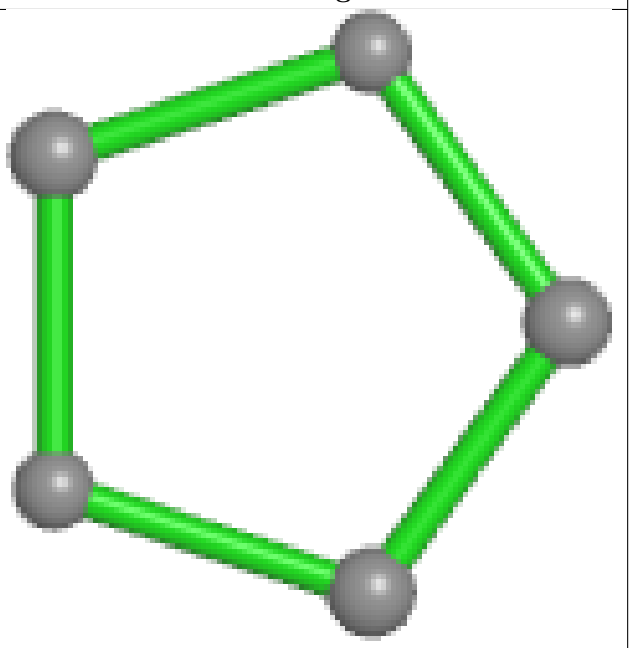
Bond lengths



Bond angles

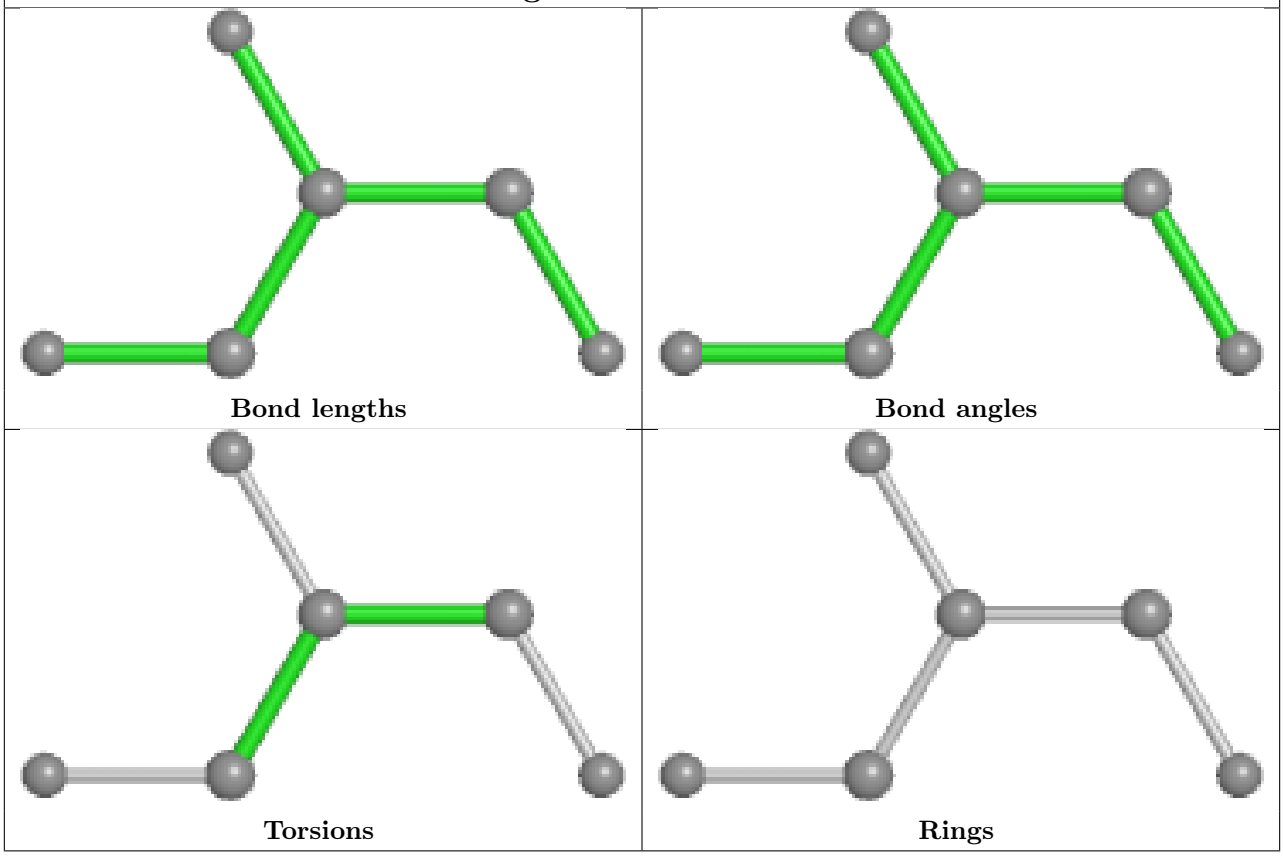


Torsions



Rings

Ligand GOL D 707



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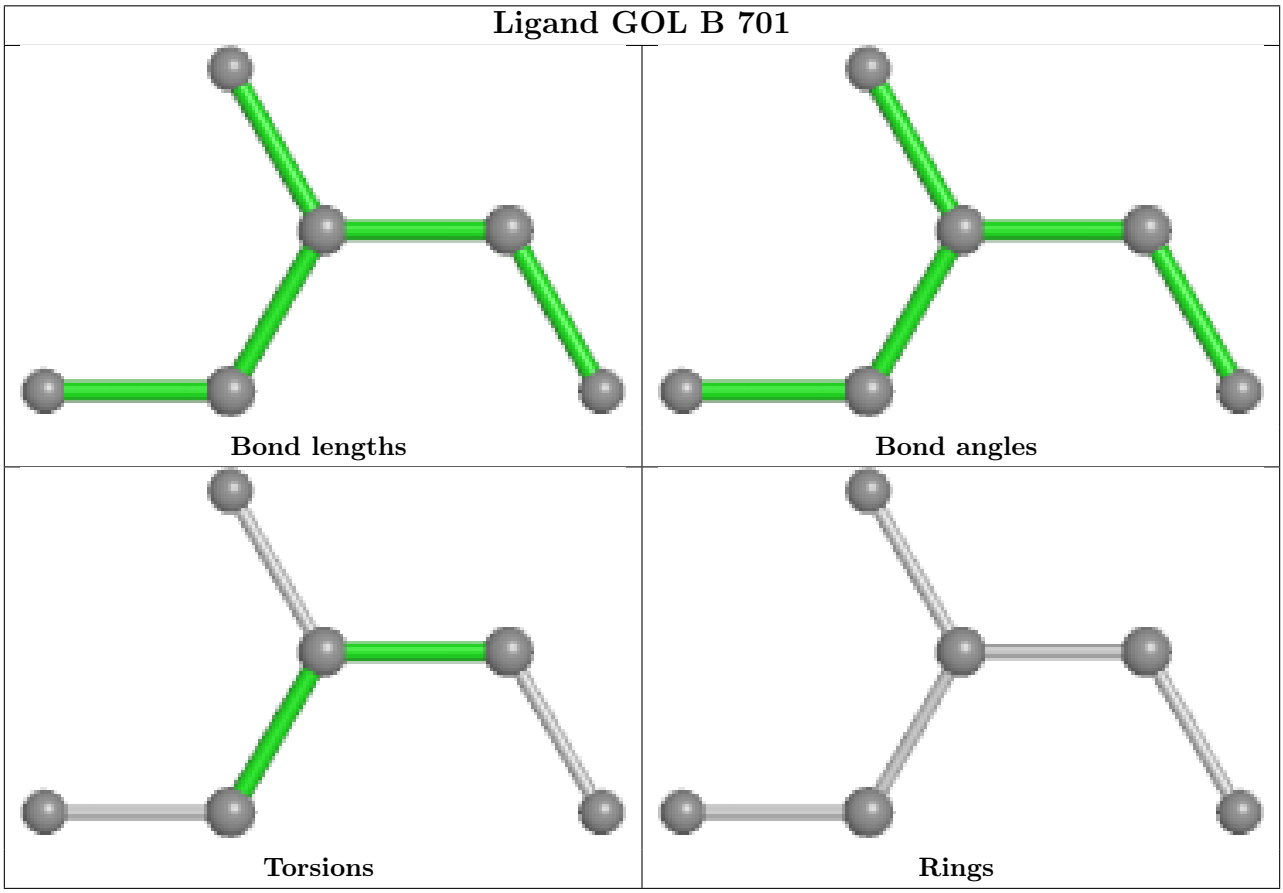

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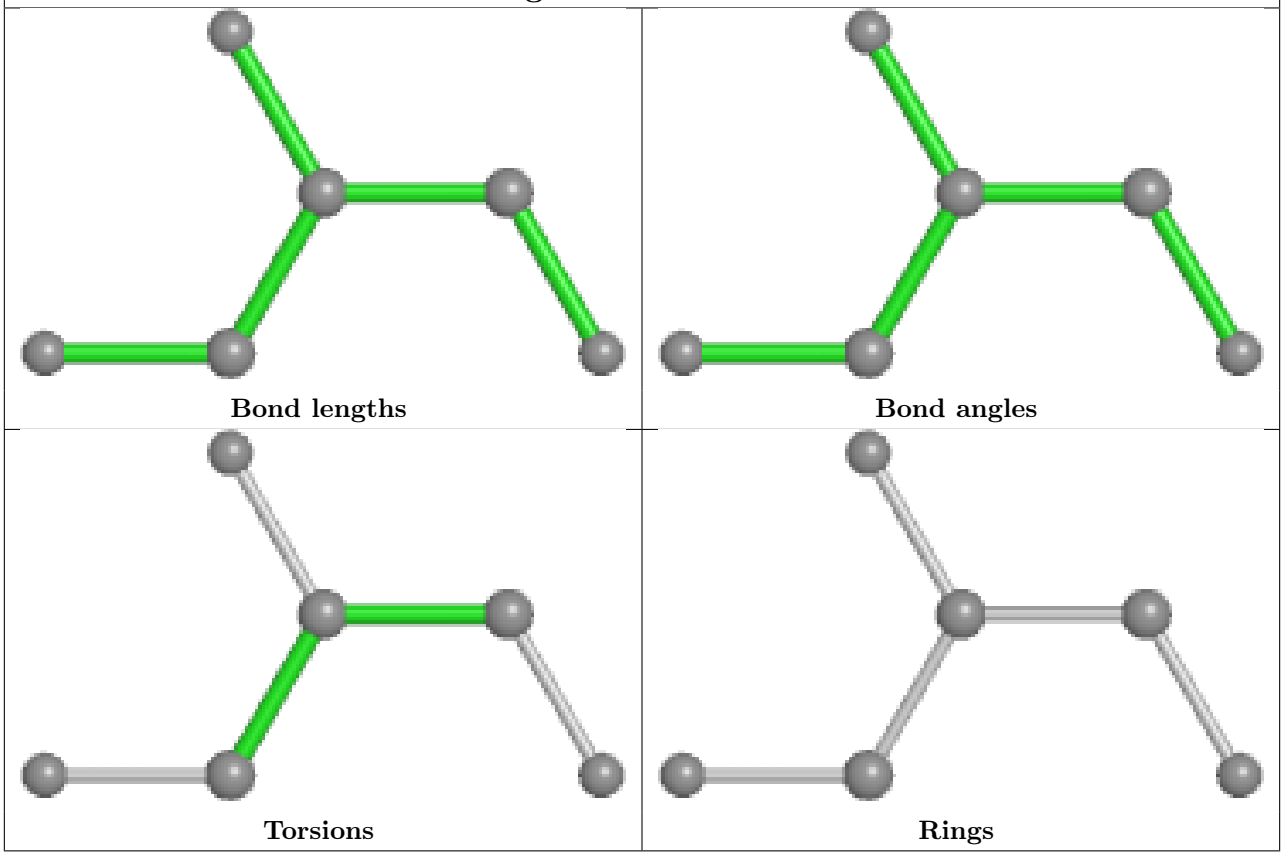

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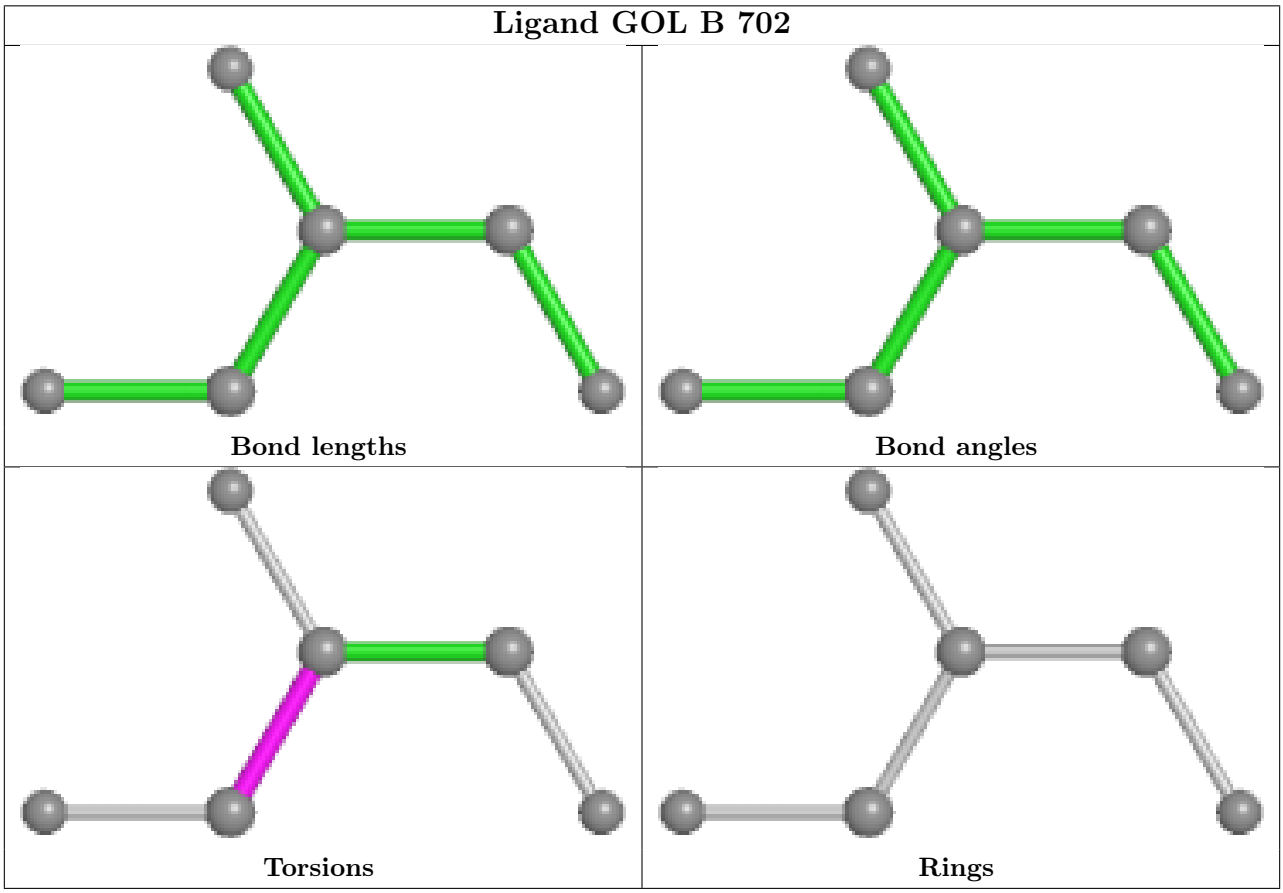
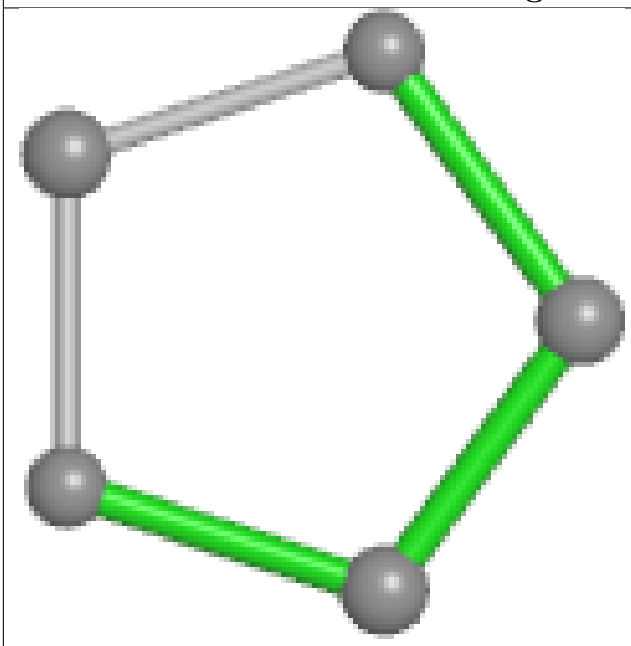
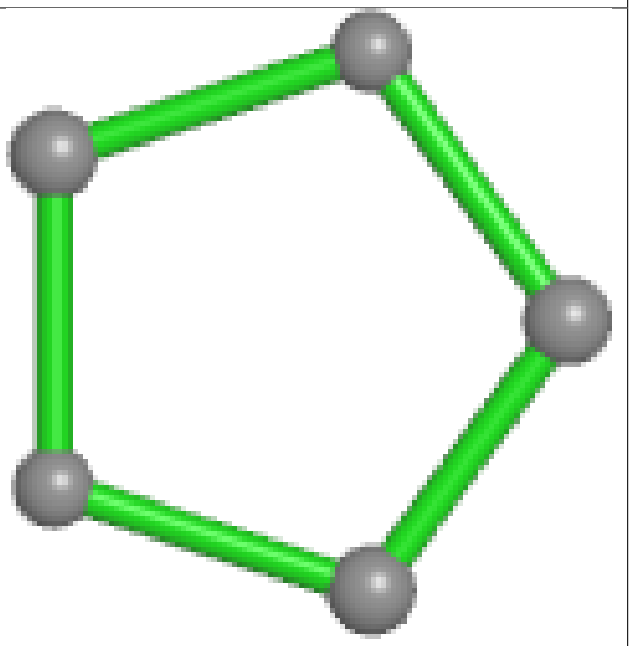


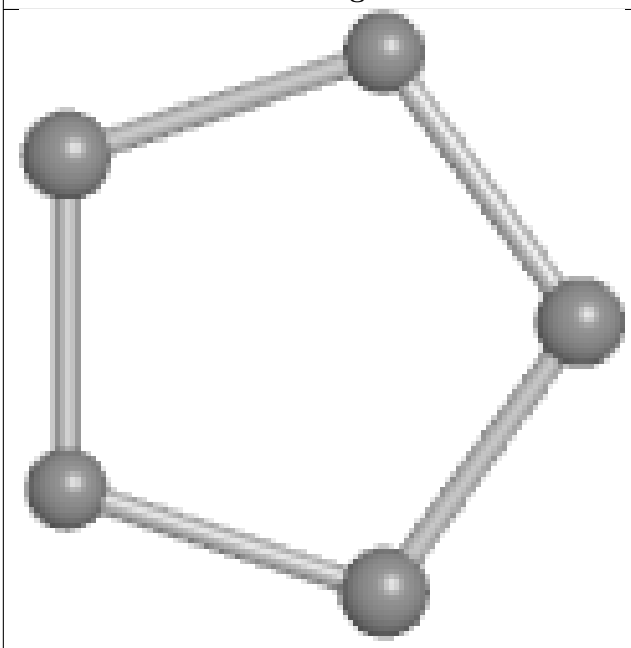
Ligand IMD F 705



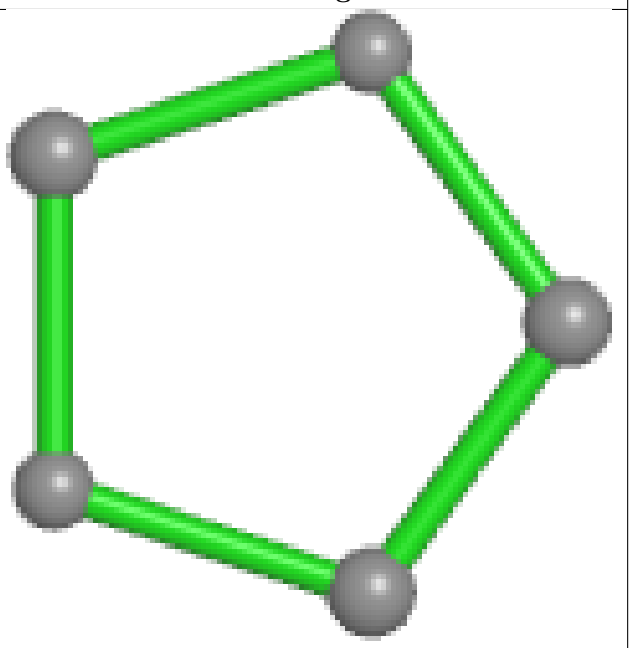
Bond lengths



Bond angles

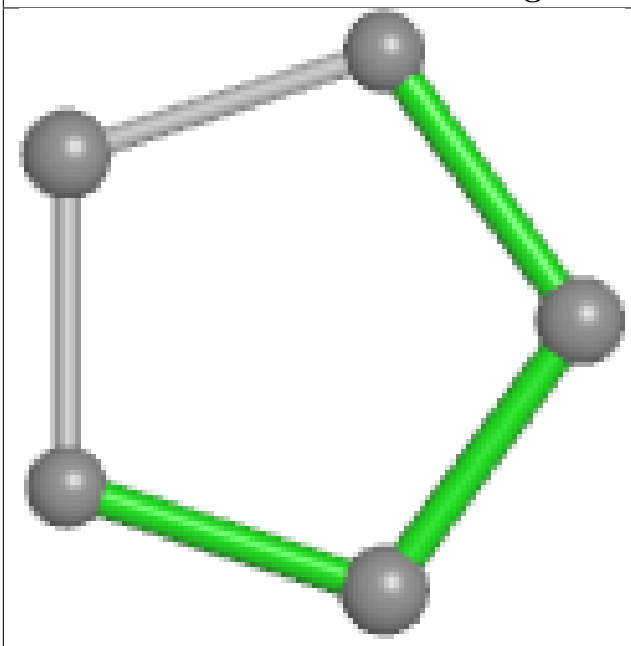


Torsions



Rings

Ligand IMD C 806



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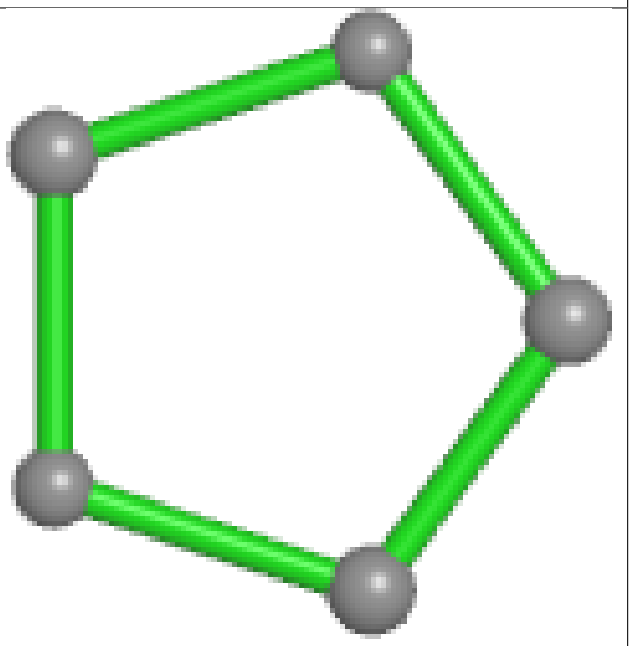
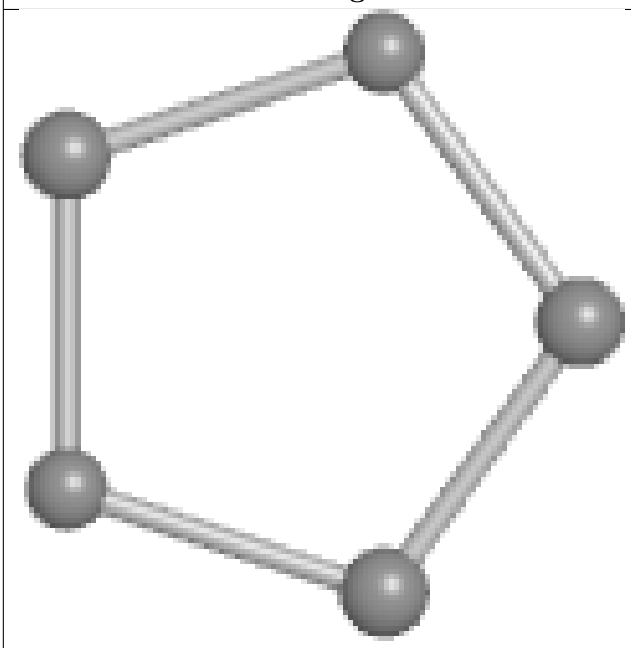
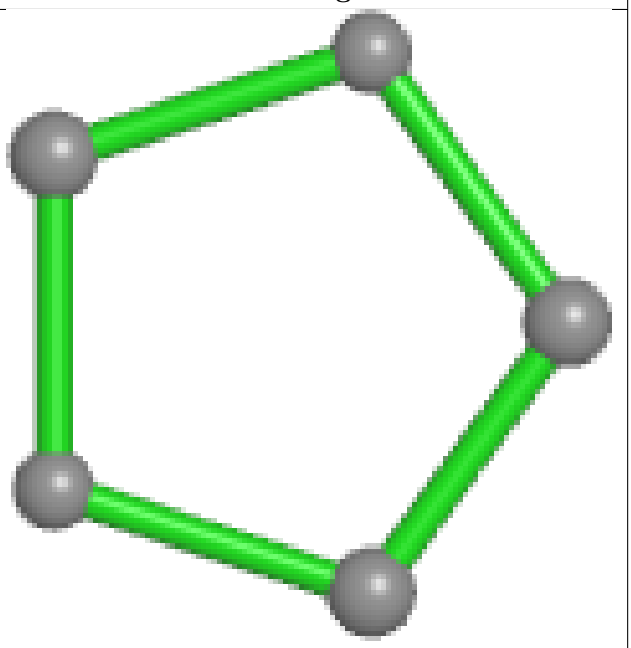


Bond angles

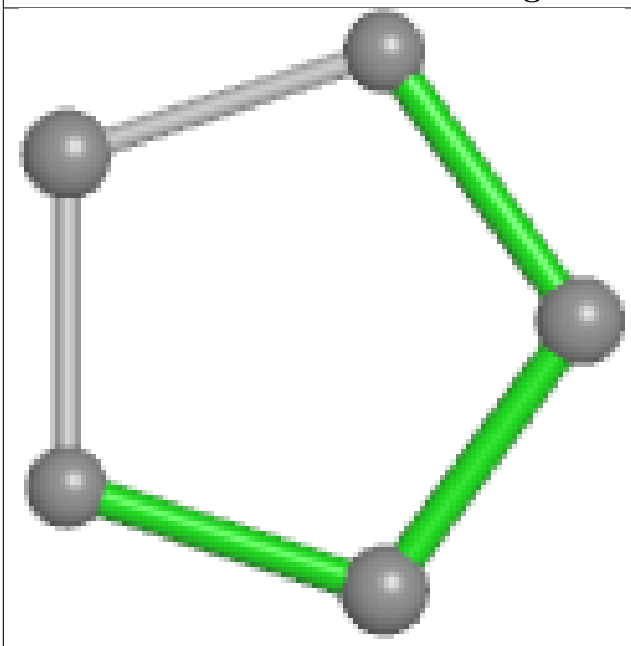


Torsions

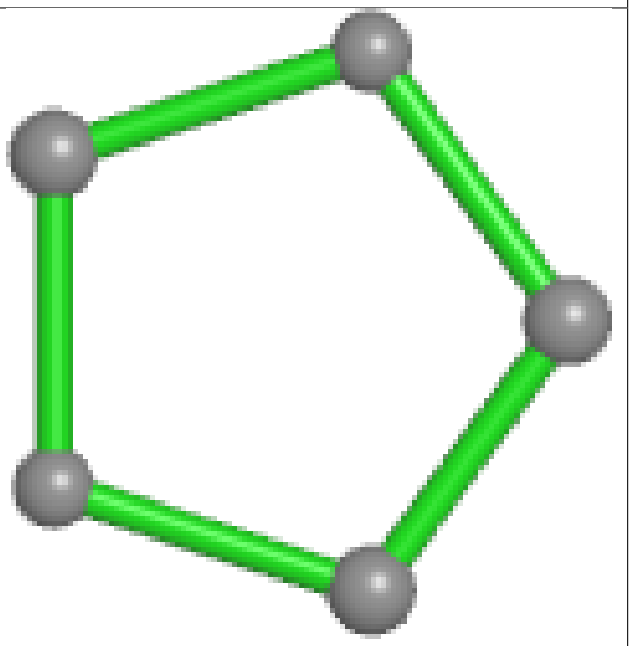


Rings

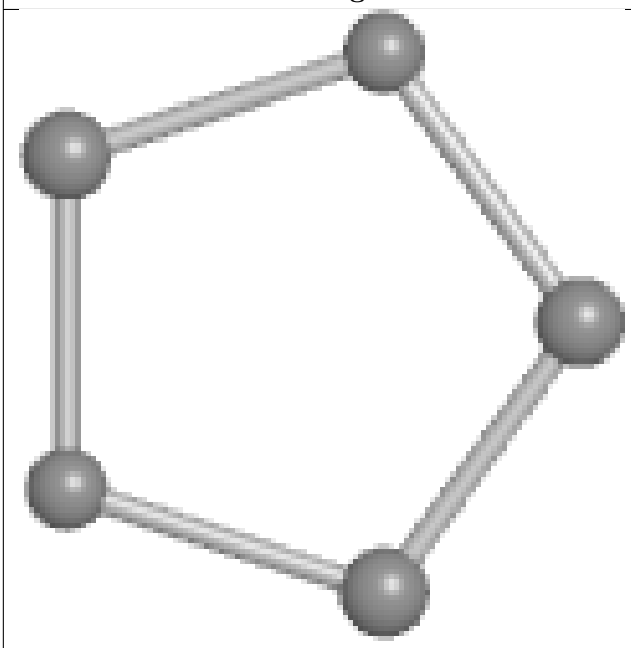
Ligand IMD A 804



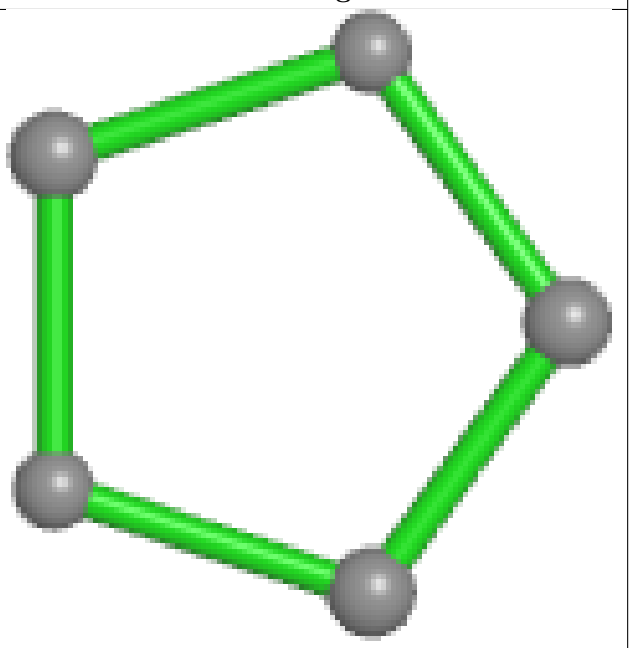
Bond lengths



Bond angles

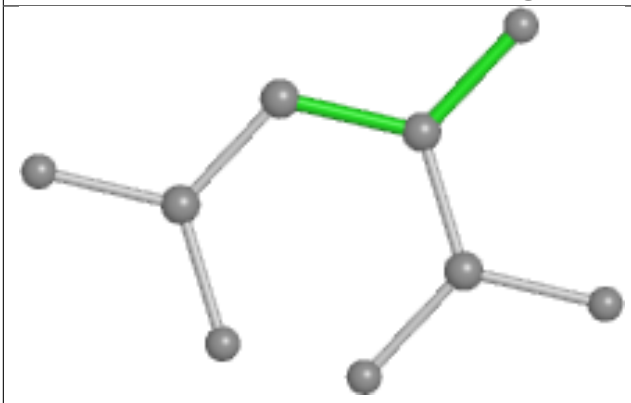


Torsions

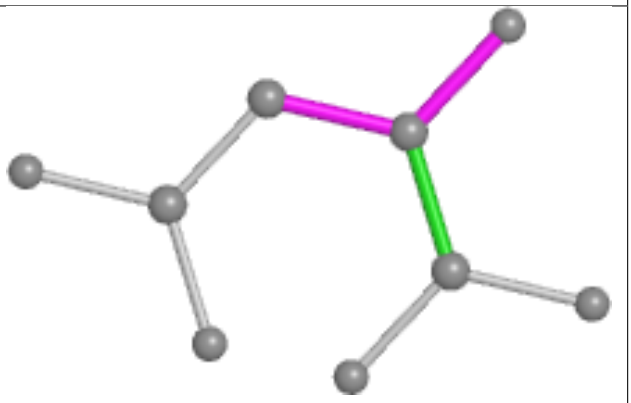


Rings

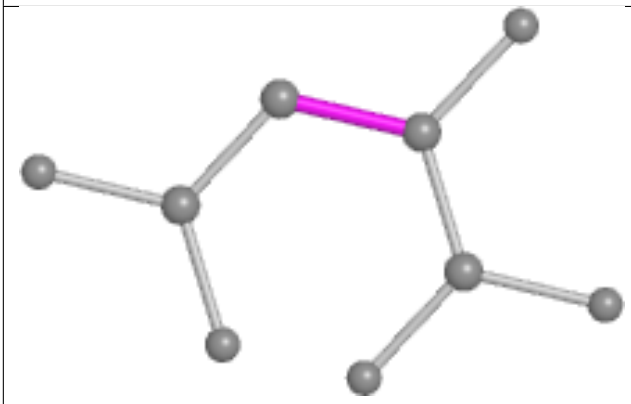
Ligand LMR D 702



Bond lengths



Bond angles



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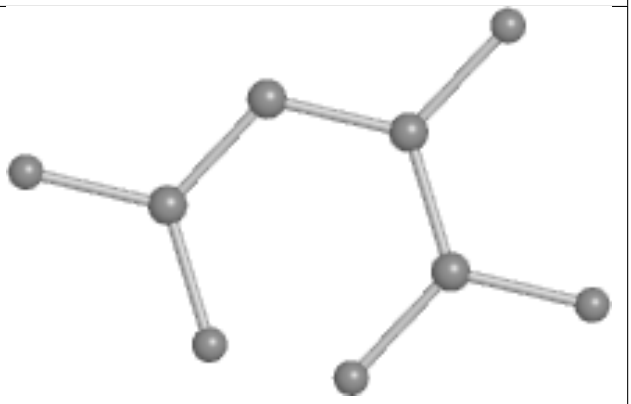
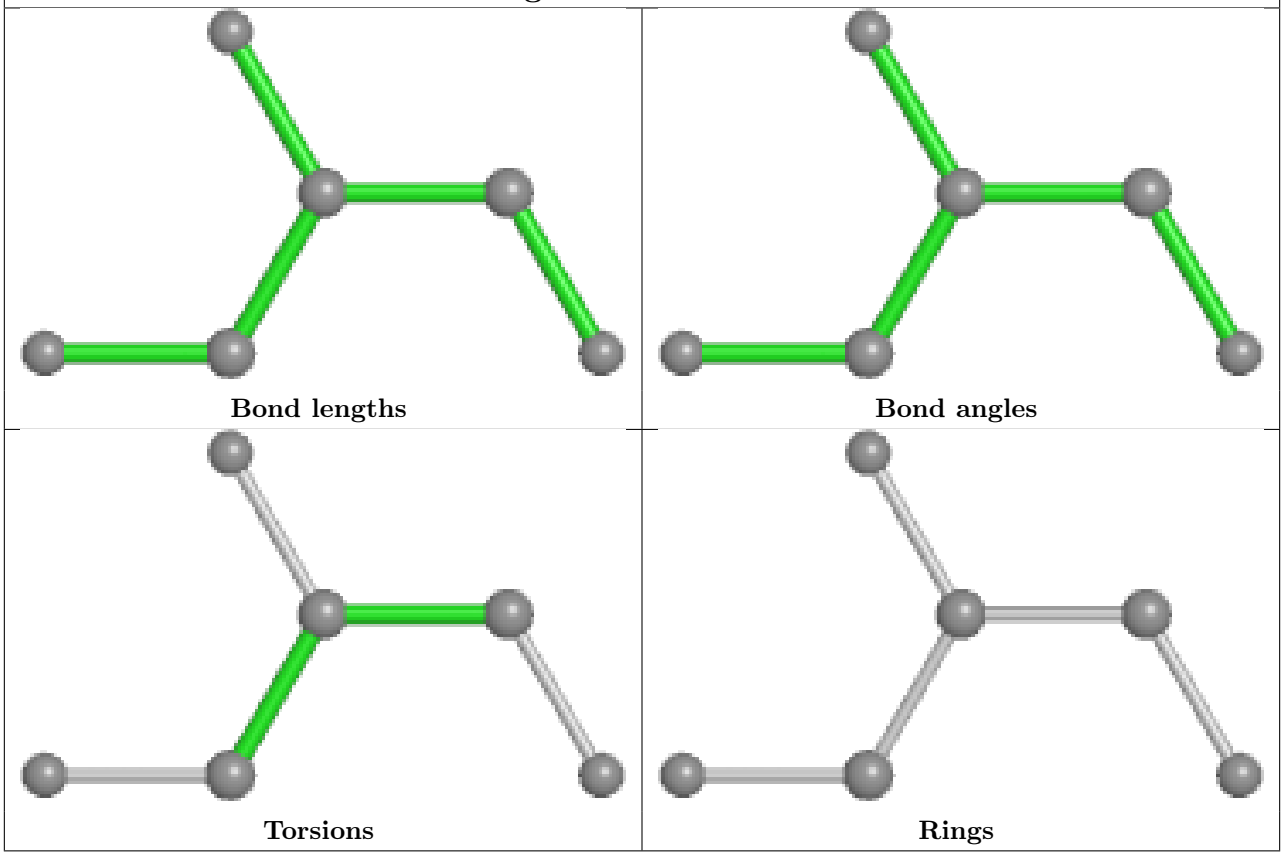
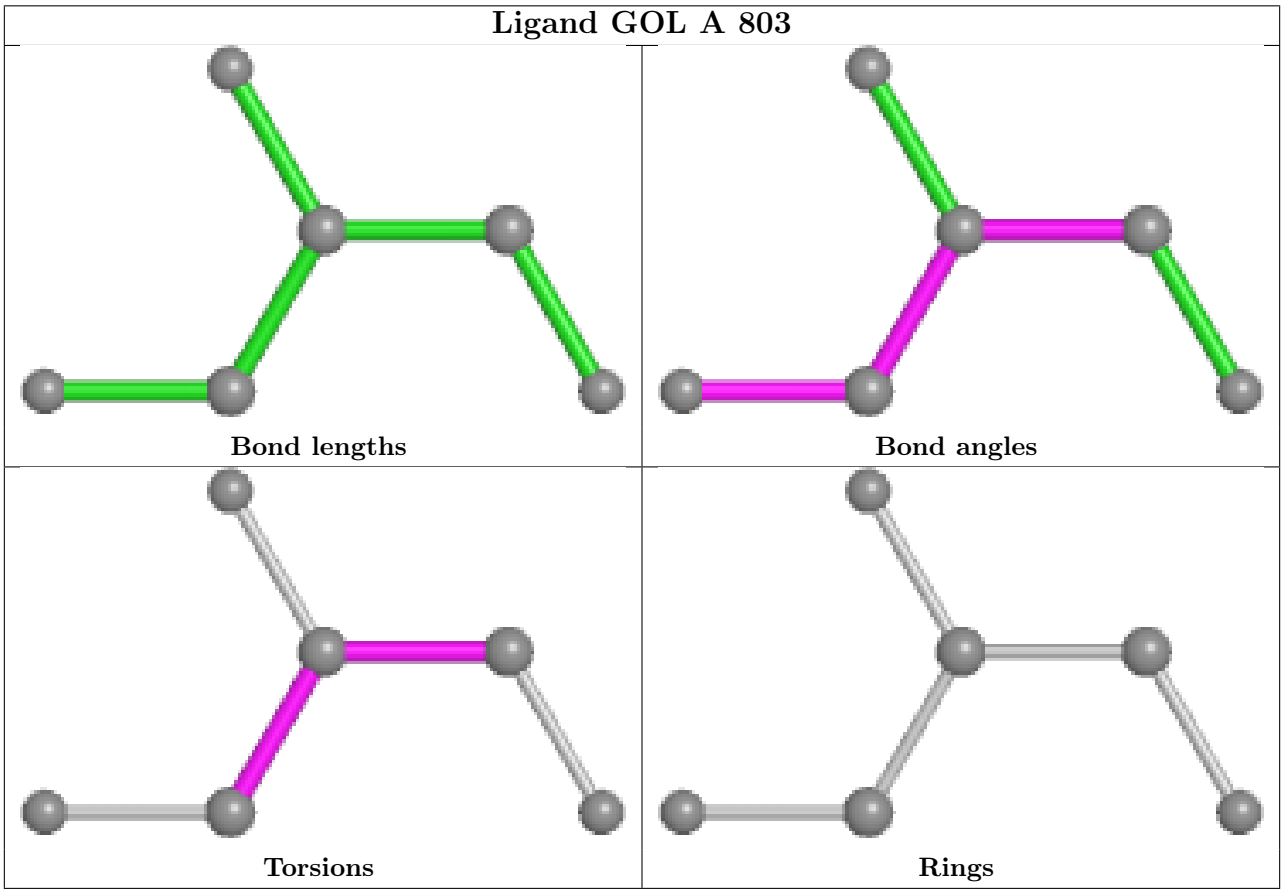


Rings

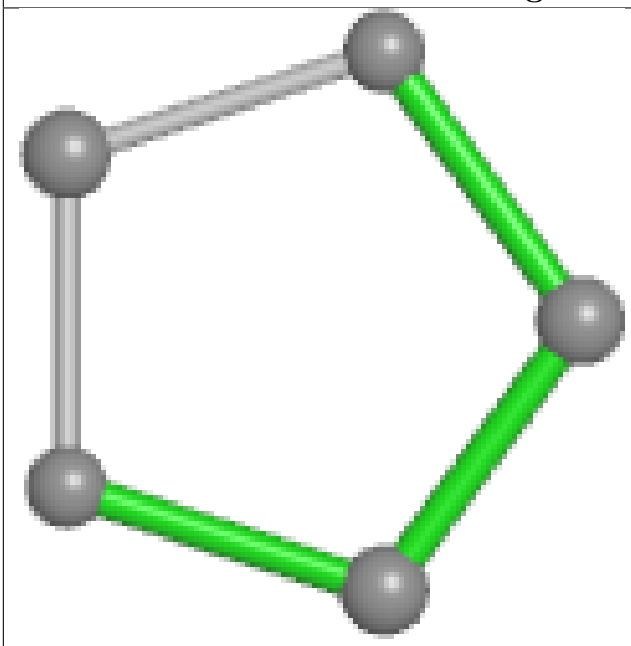
Ligand GOL C 803



Ligand GOL A 803



Ligand IMD F 703



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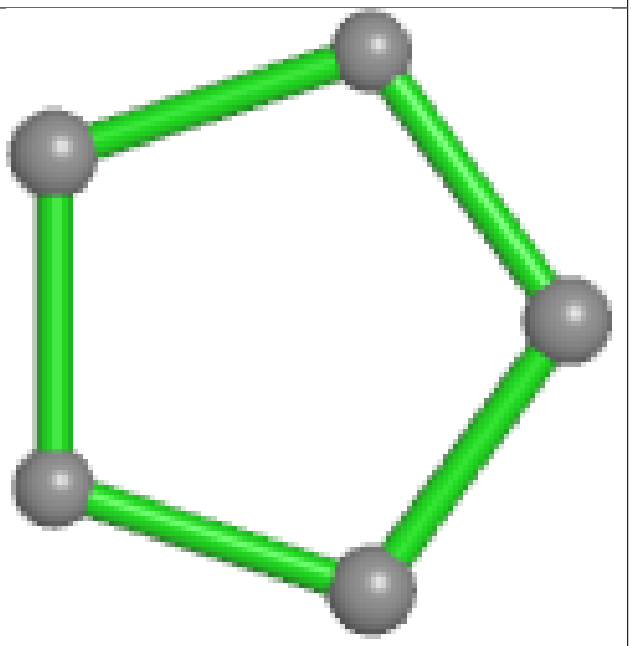
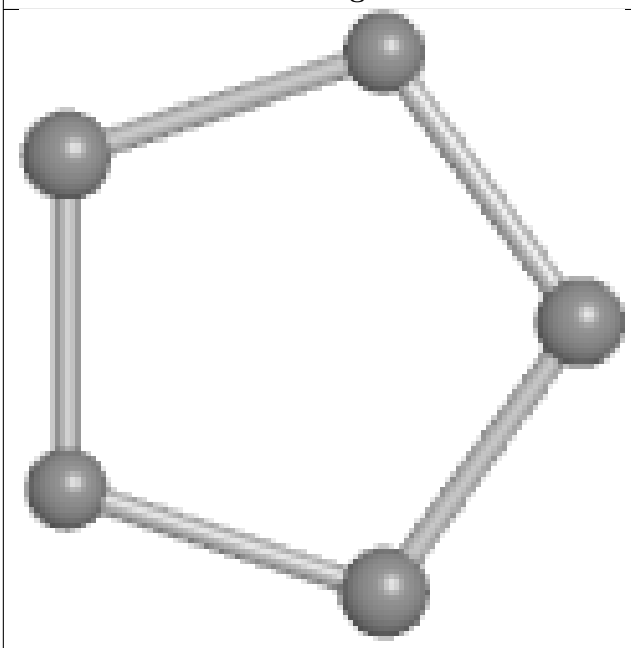


Bond angles



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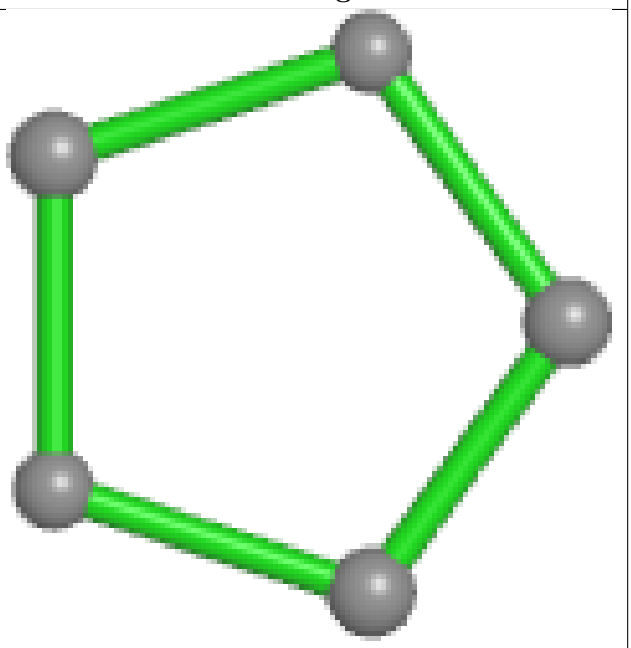
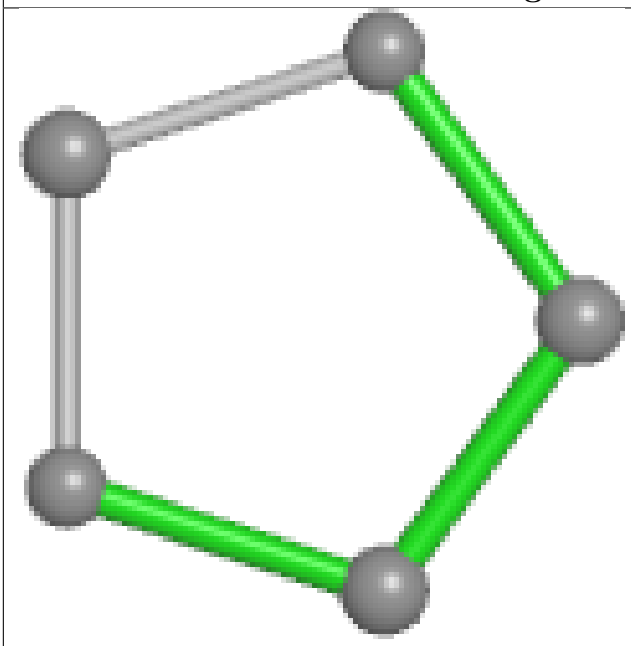


Rings

Ligand IMD B 706



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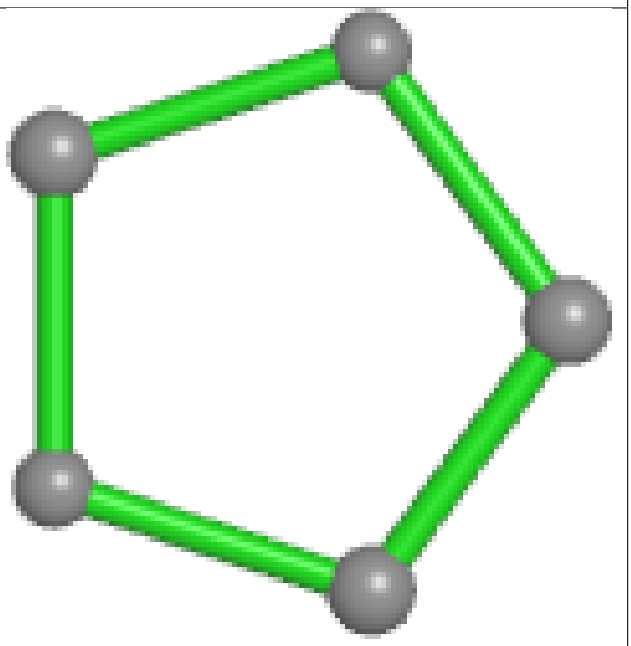
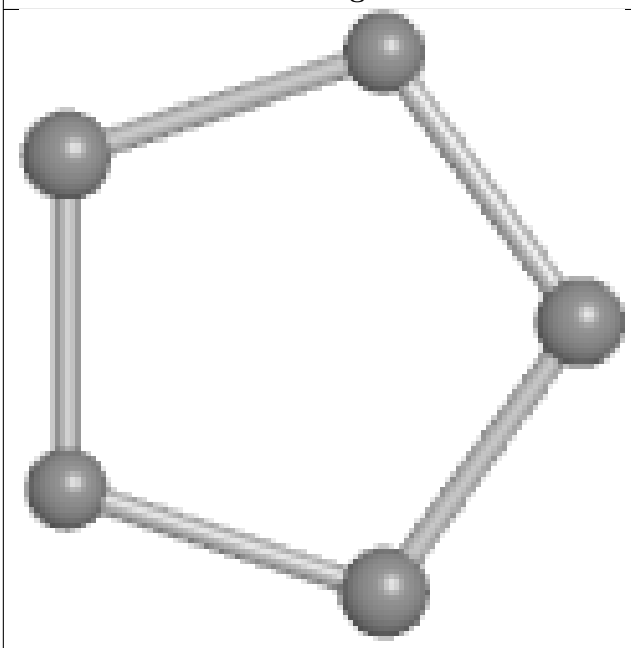


Bond angles



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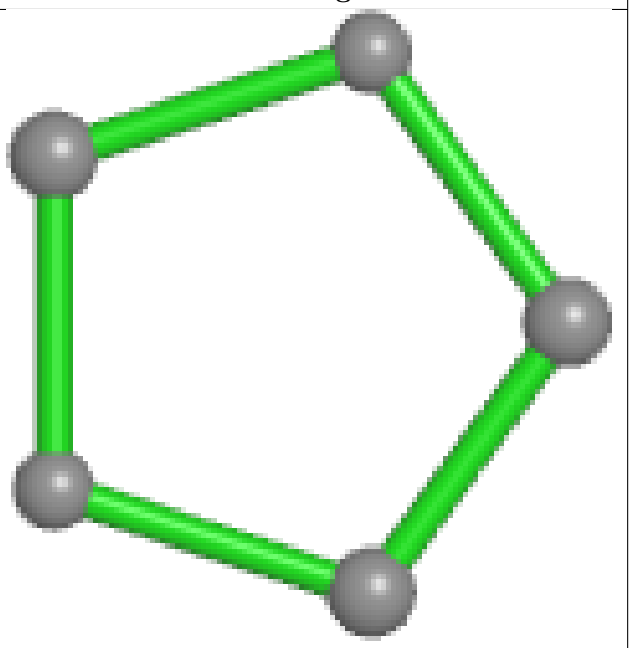
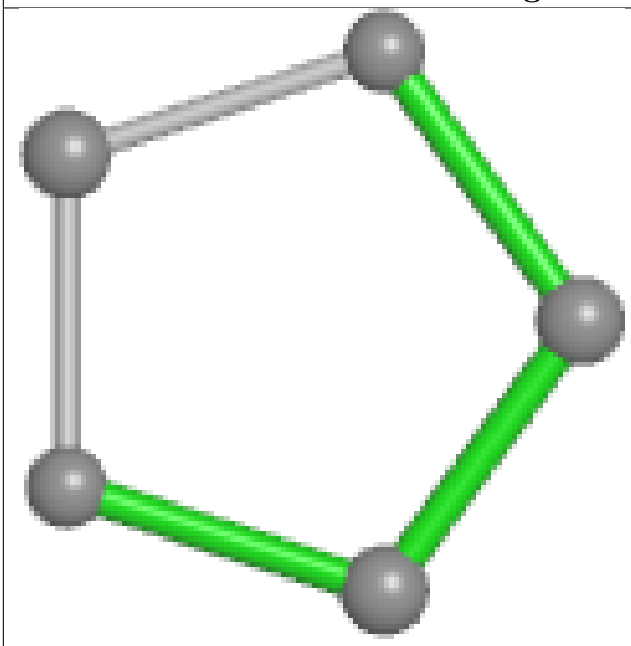
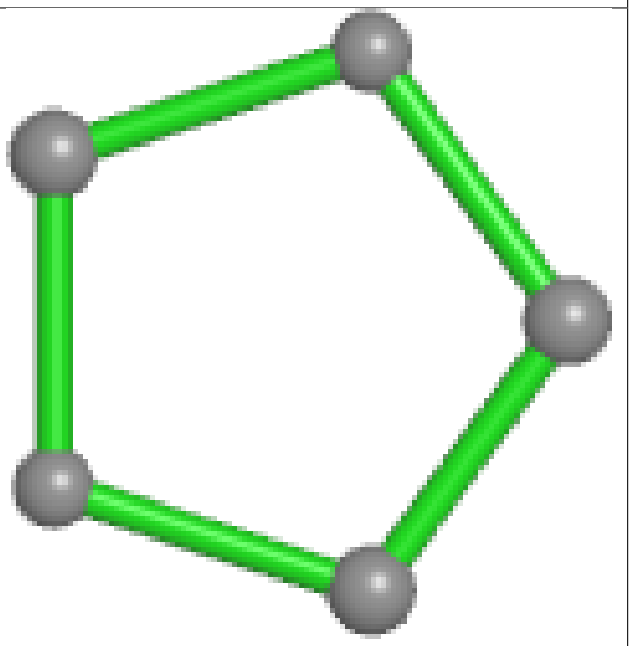


Rings

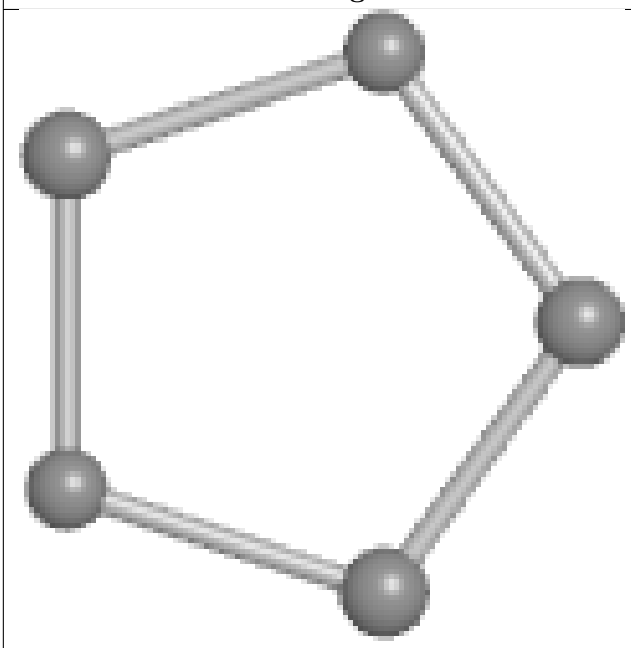
Ligand IMD D 706



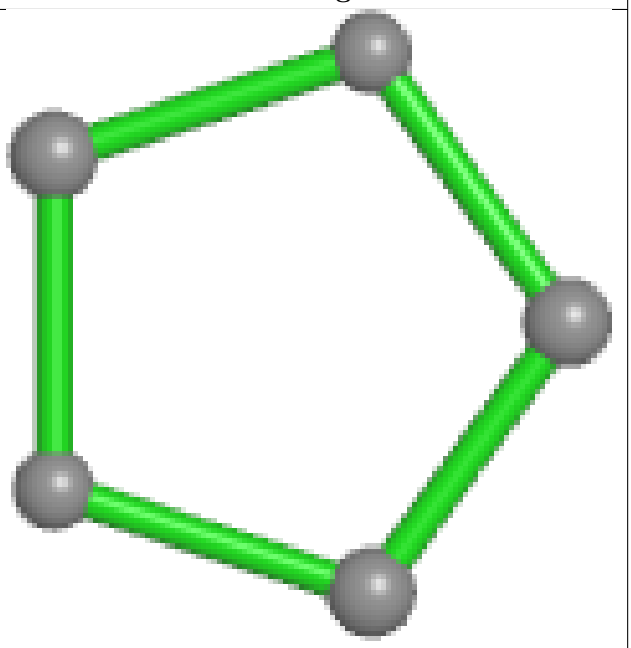
Bond lengths



Bond angles

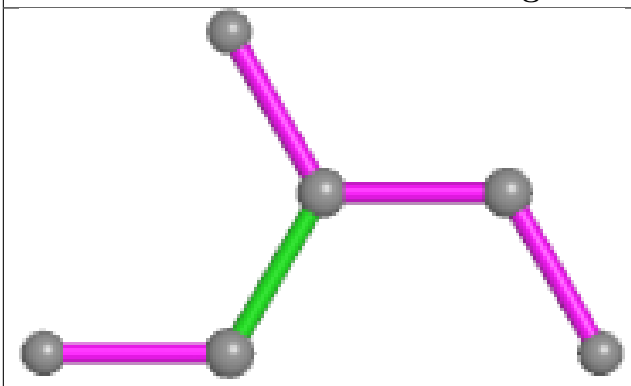


Torsions

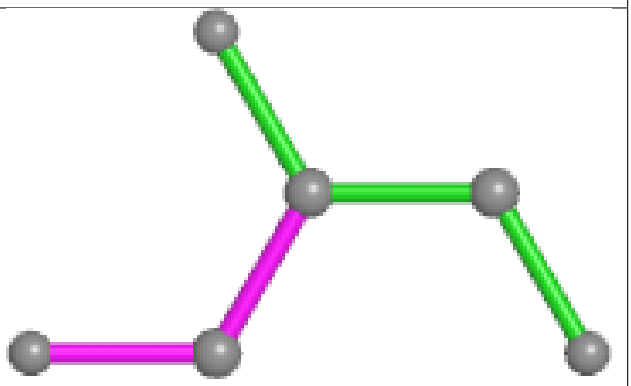


Rings

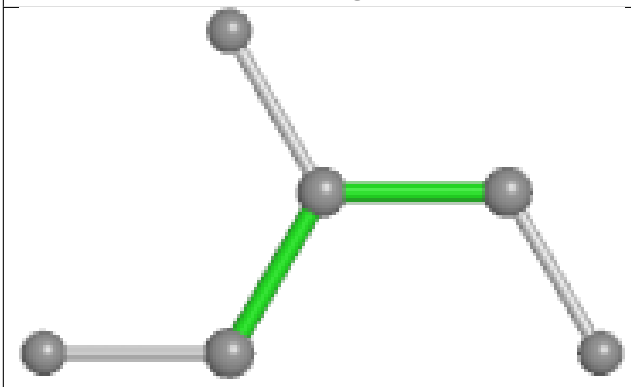
Ligand GOL D 705



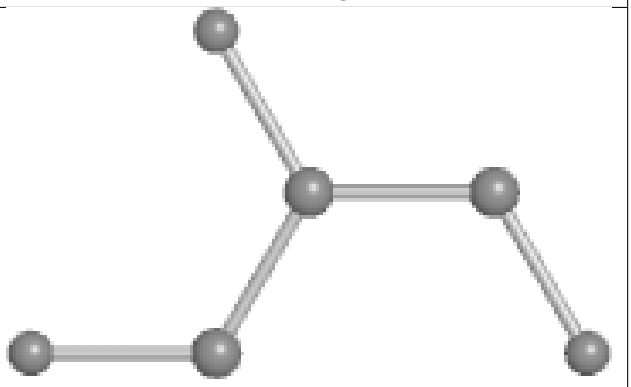
Bond lengths



Bond angles

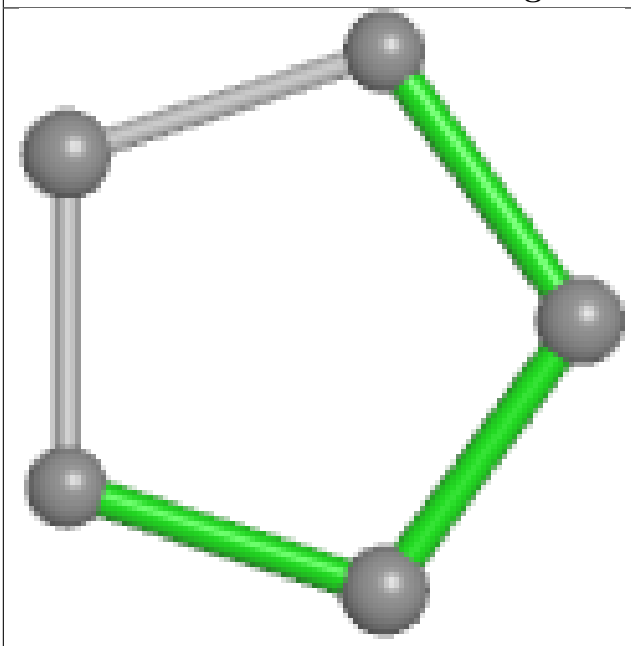


Torsions



Rings

Ligand IMD B 704



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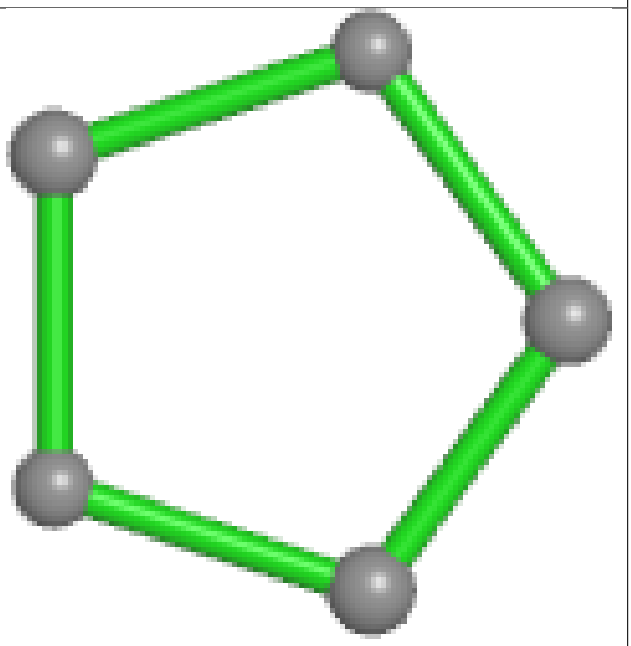
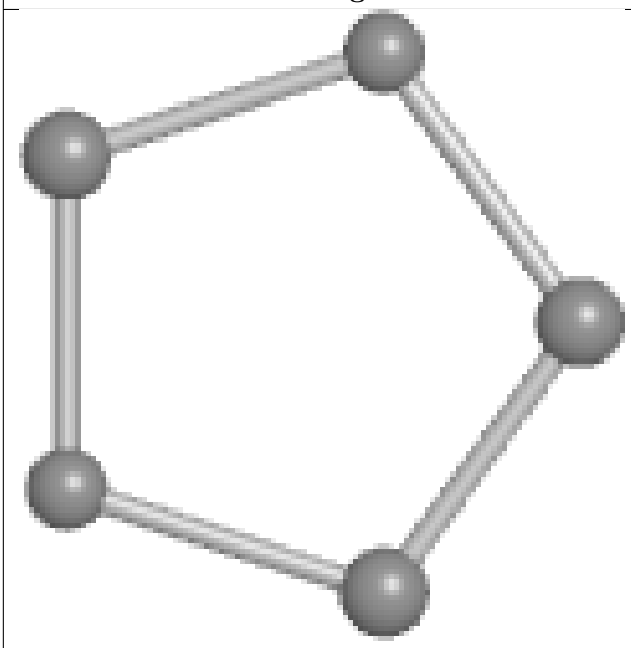


Bond angles



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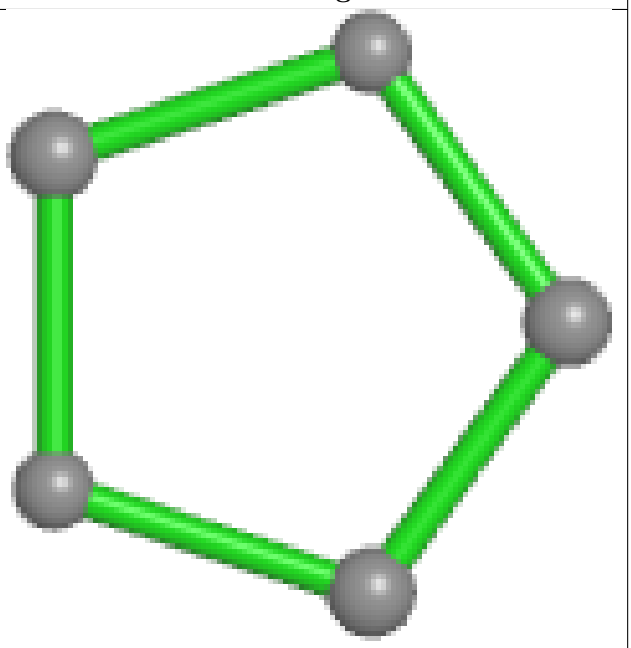
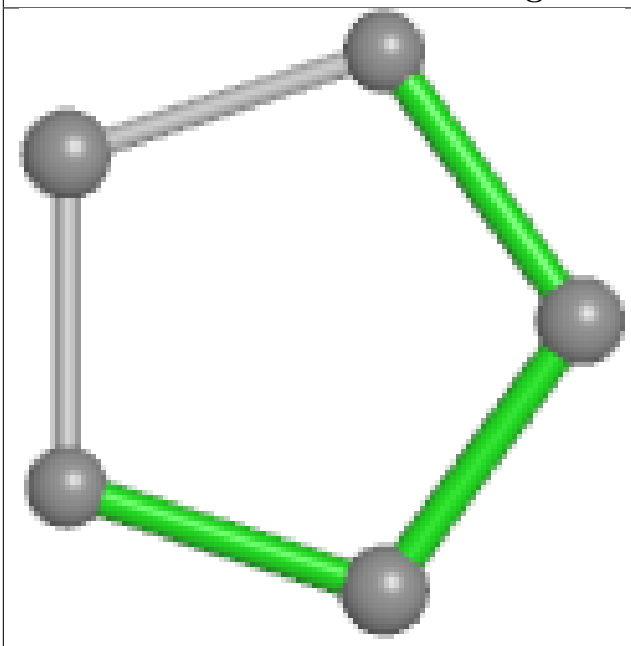


Rings

Ligand IMD F 709



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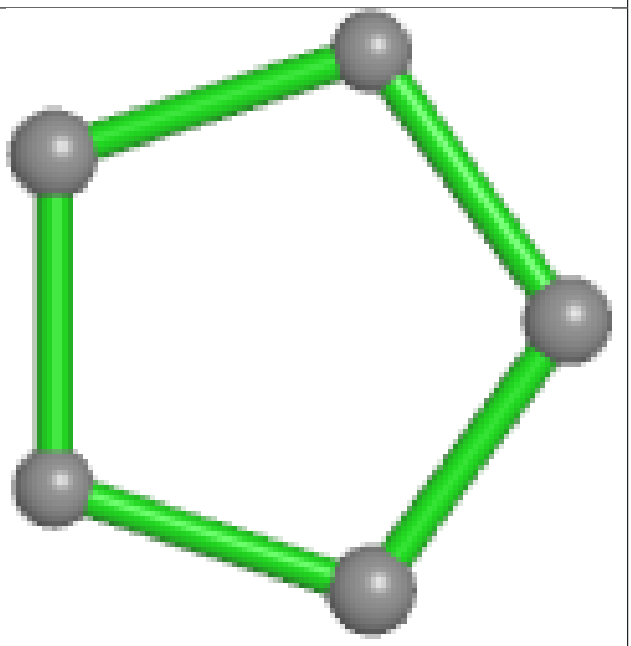
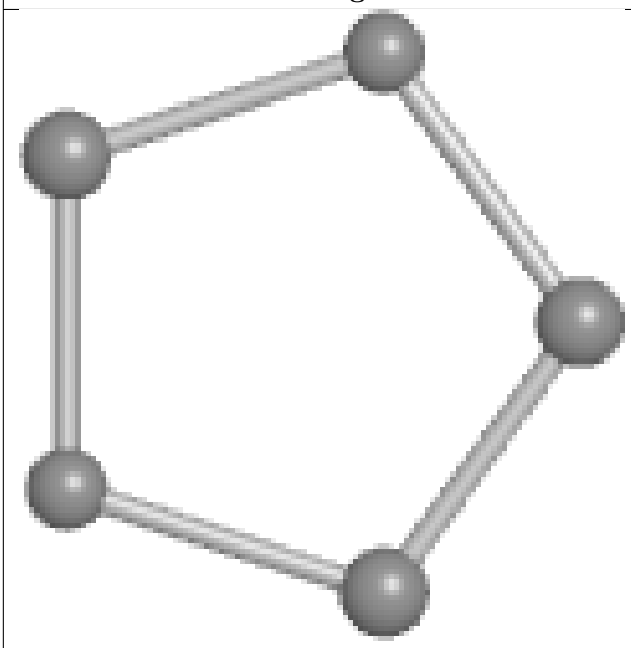
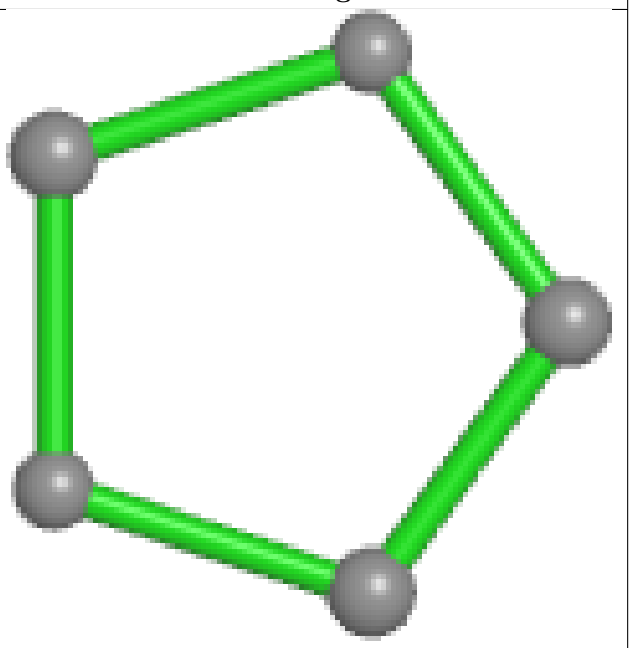


Bond angles

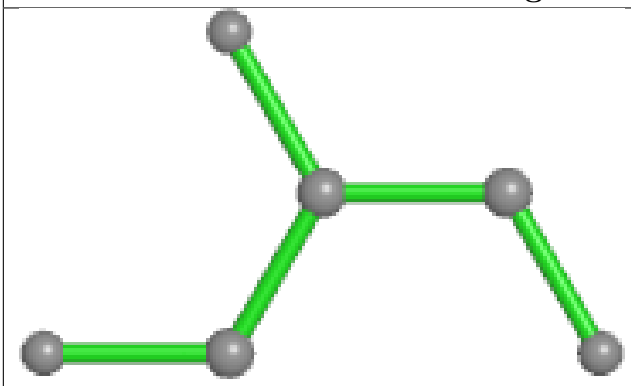


Torsions



Rings

Ligand GOL F 701



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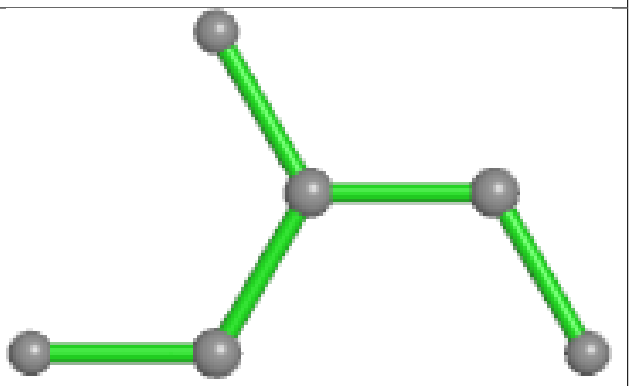
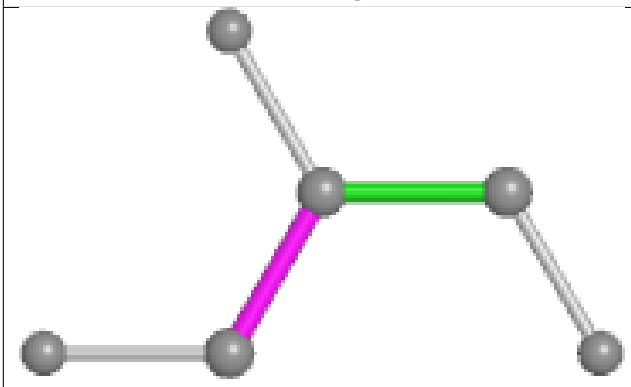
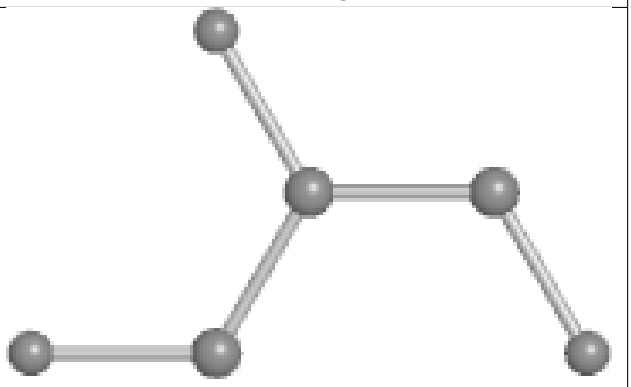


Bond angles

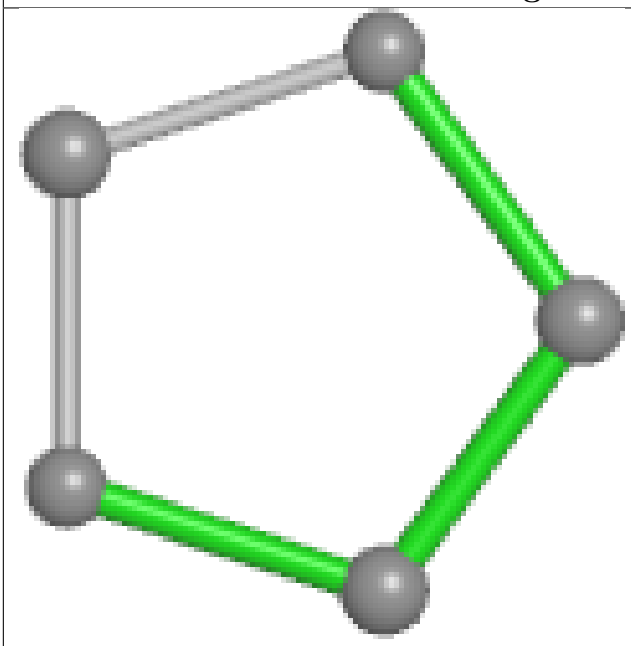


Torsions



Rings

Ligand IMD D 701



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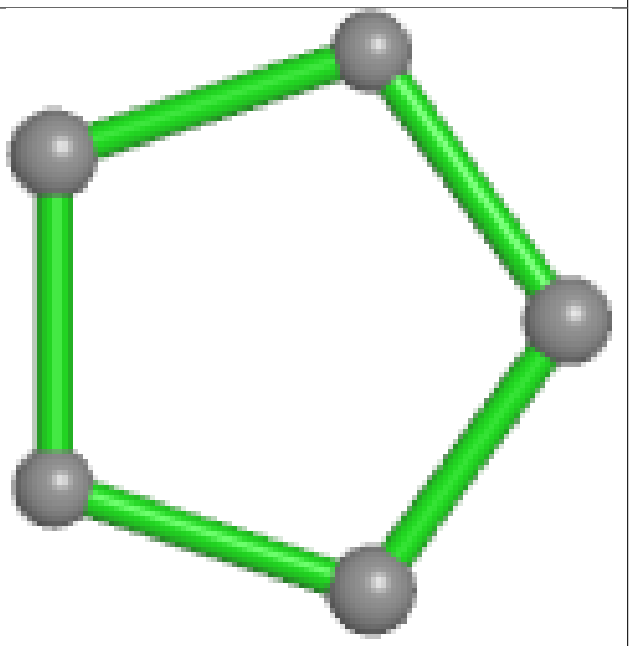
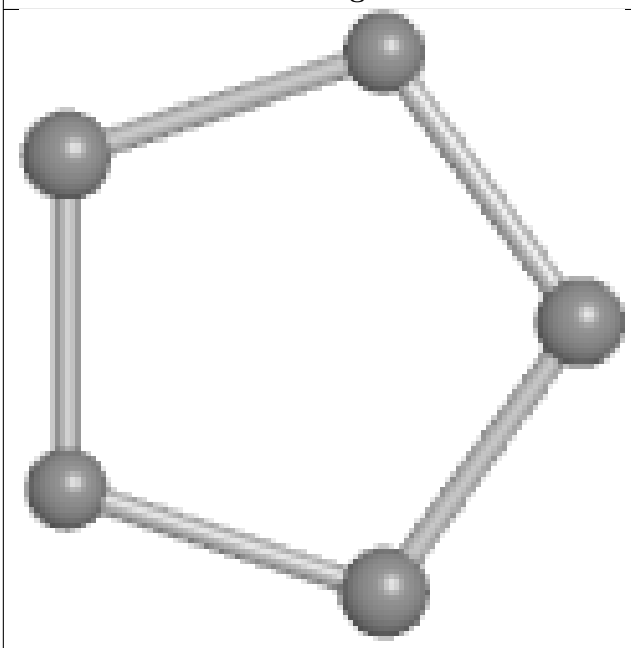


Bond angles



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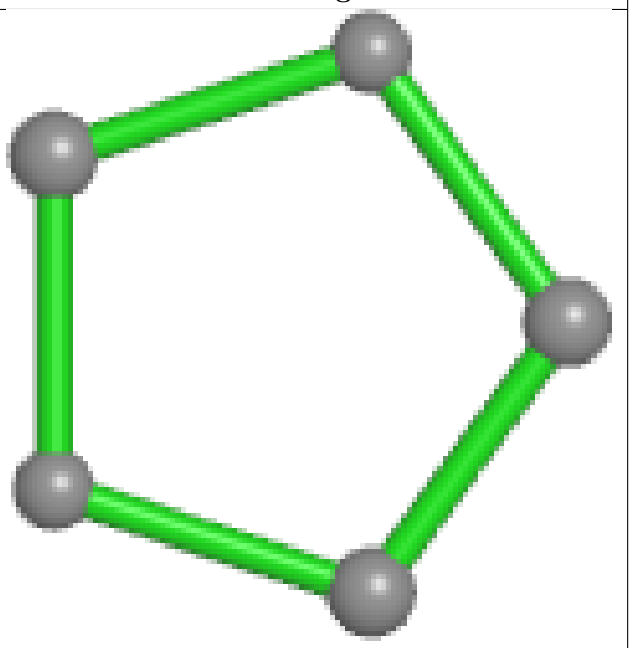
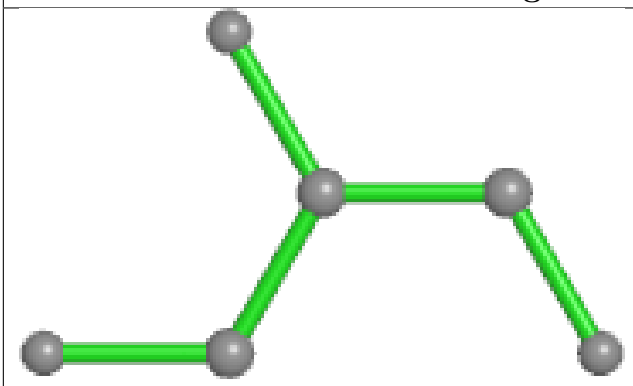


Rings

Ligand GOL C 807



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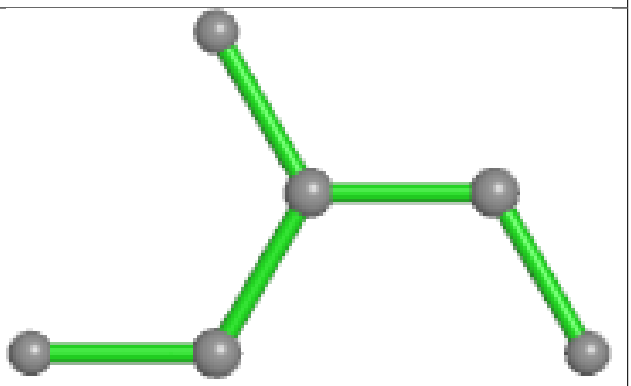
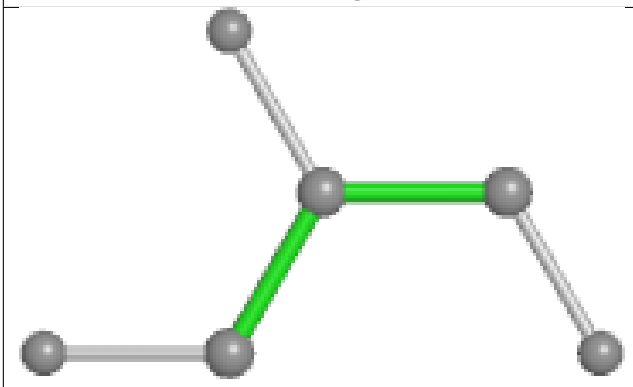


Bond angles



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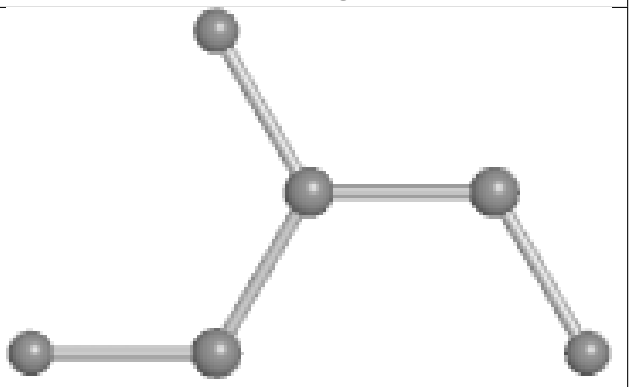
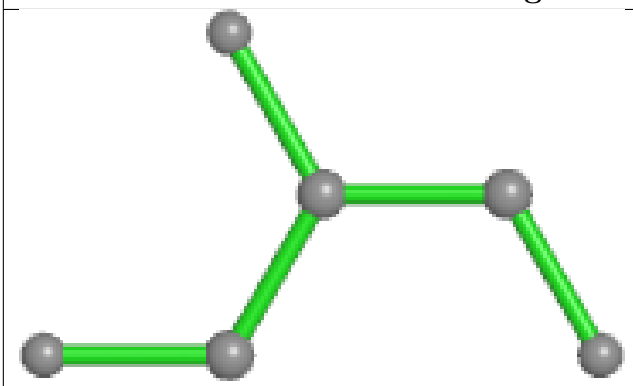


Rings

Ligand GOL E 701



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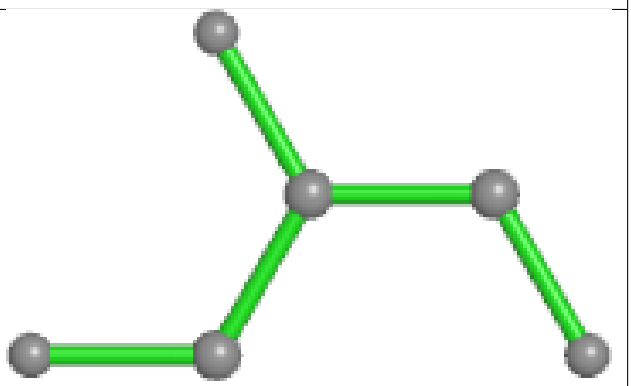
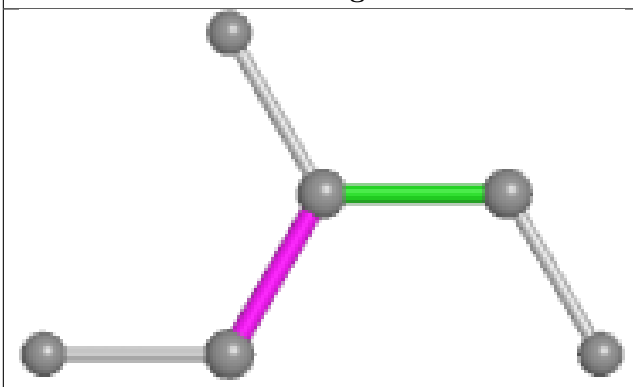


Bond angles



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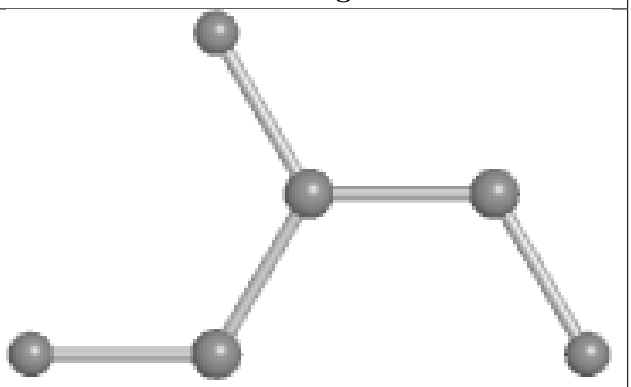
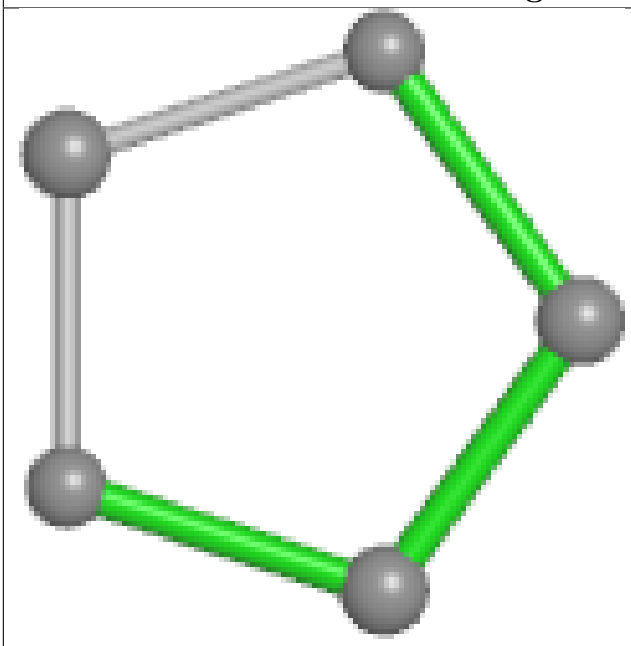


Rings

Ligand IMD F 704



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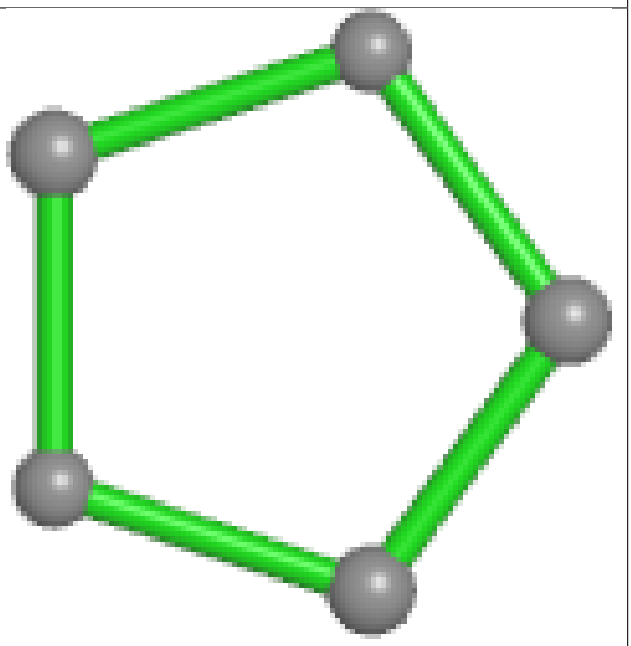

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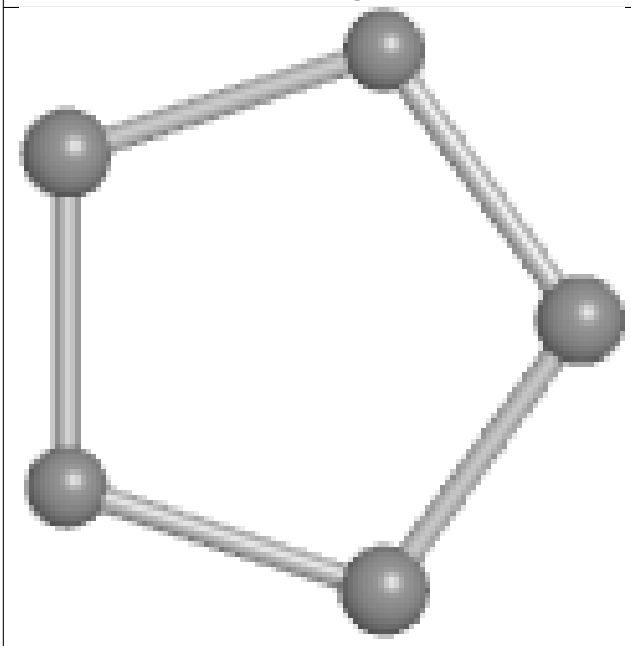

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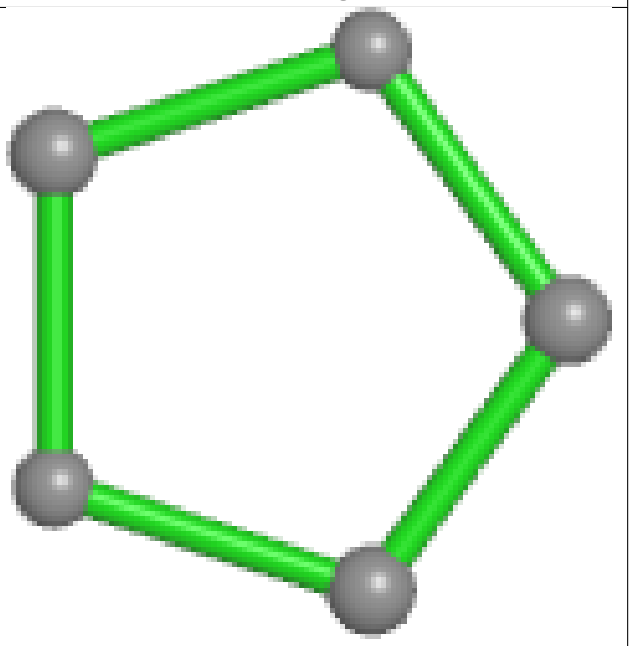
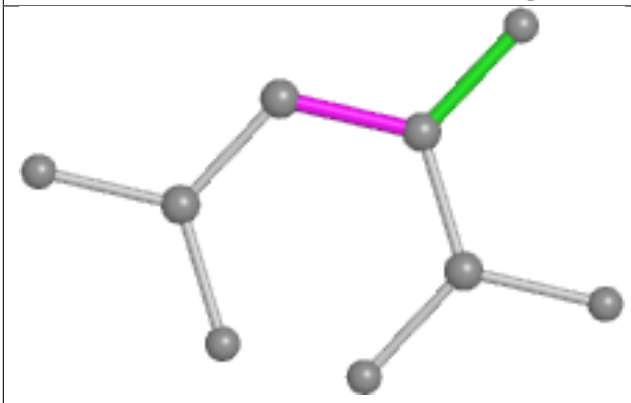


Rings

Ligand LMR F 707



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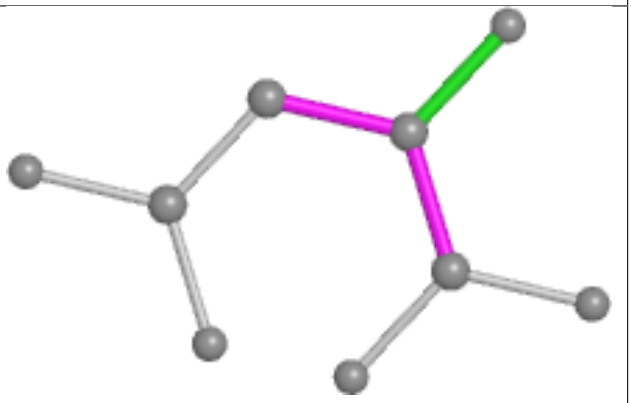
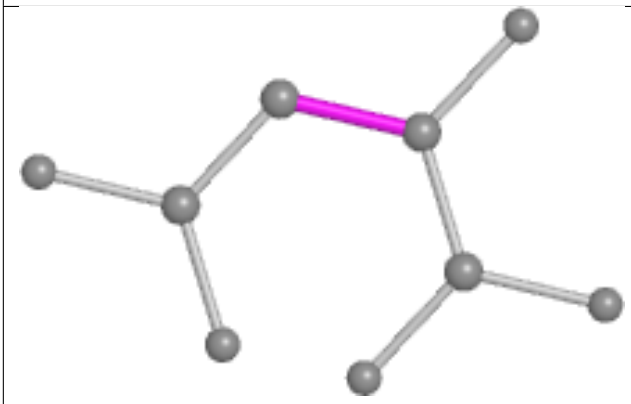
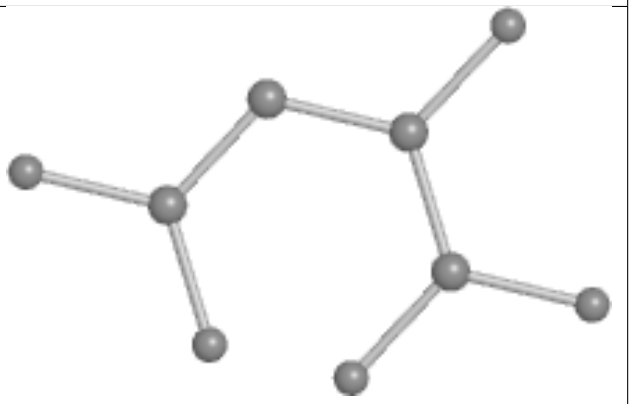


Bond angles

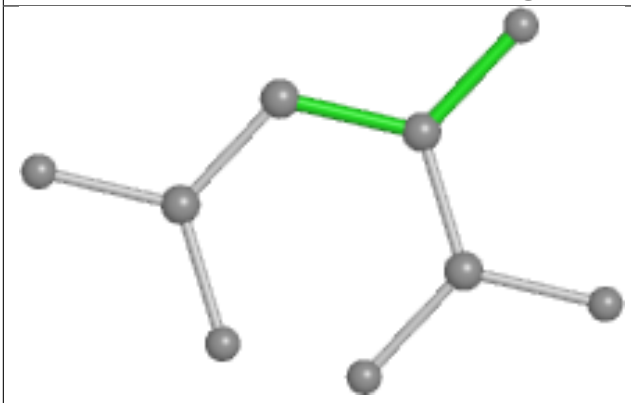


Torsions



Rings

Ligand LMR A 801



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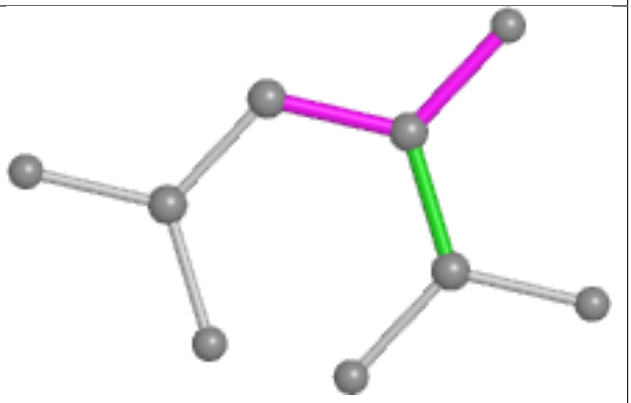
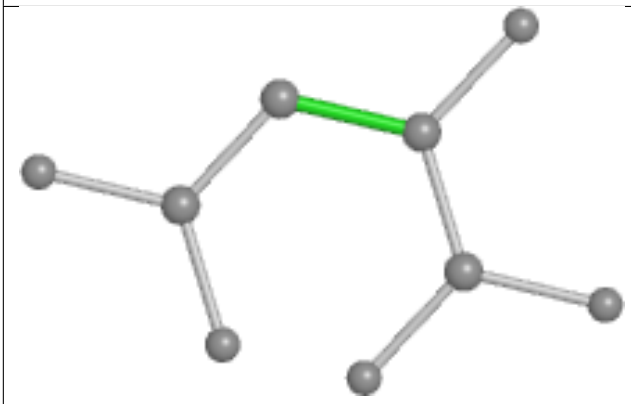
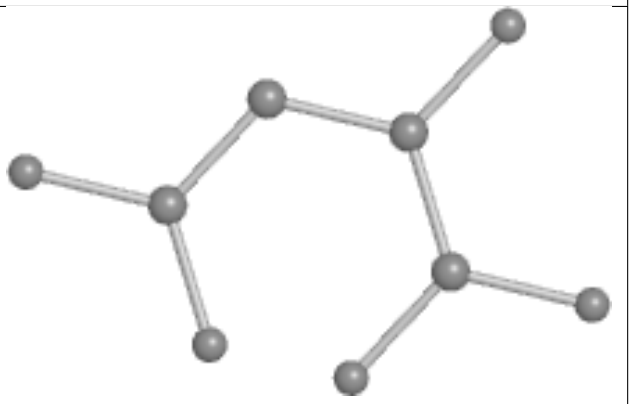


Bond angles

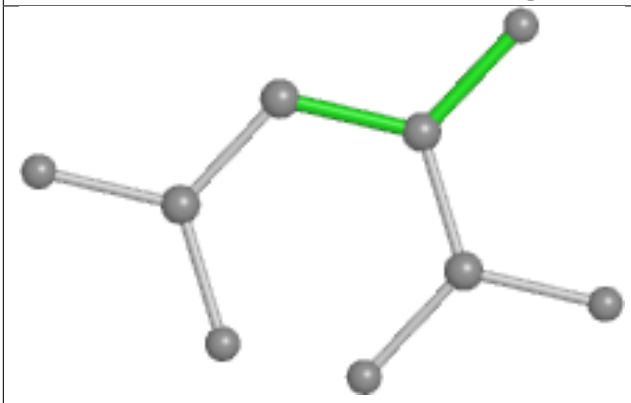


Torsions



Rings

Ligand LMR F 708



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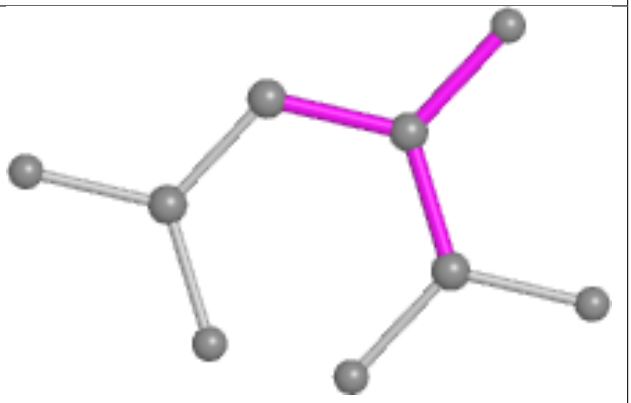
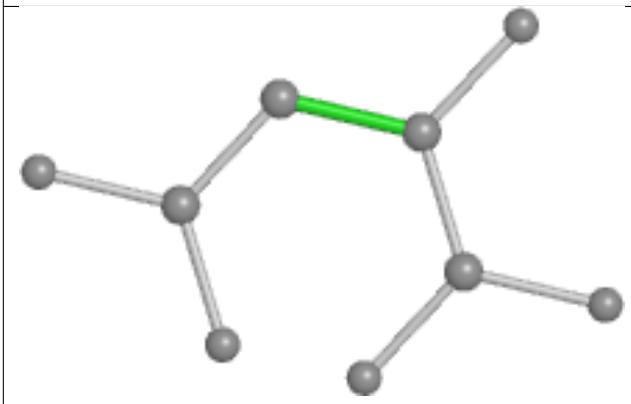


Bond angles



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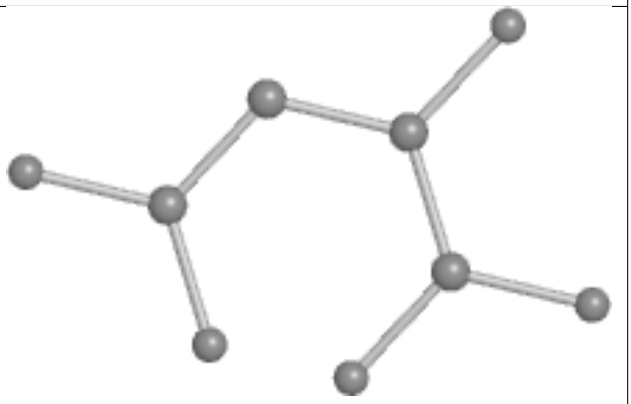
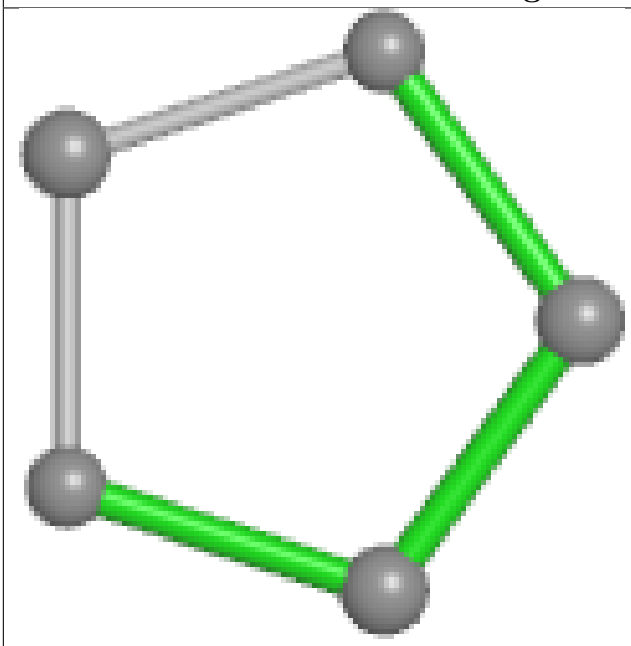


Rings

Ligand IMD A 802



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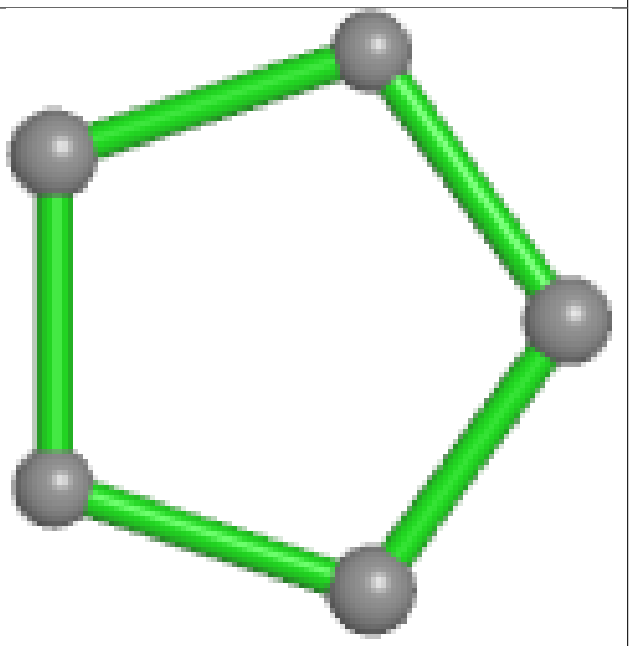
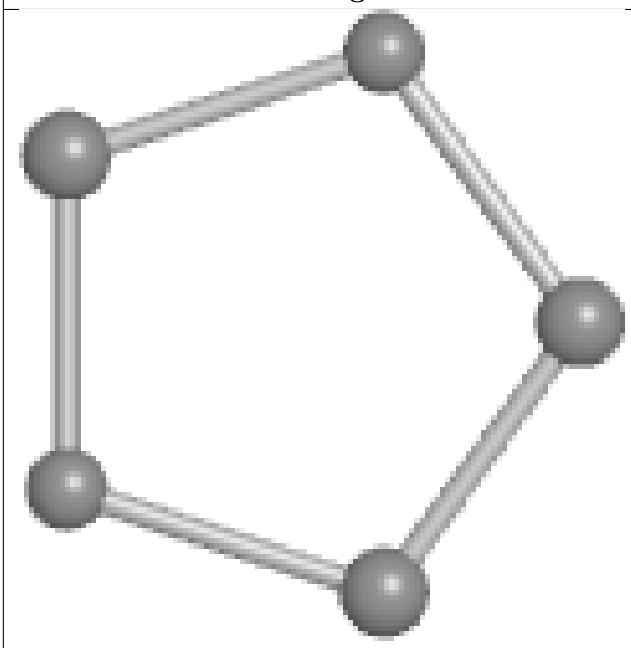


Bond angles



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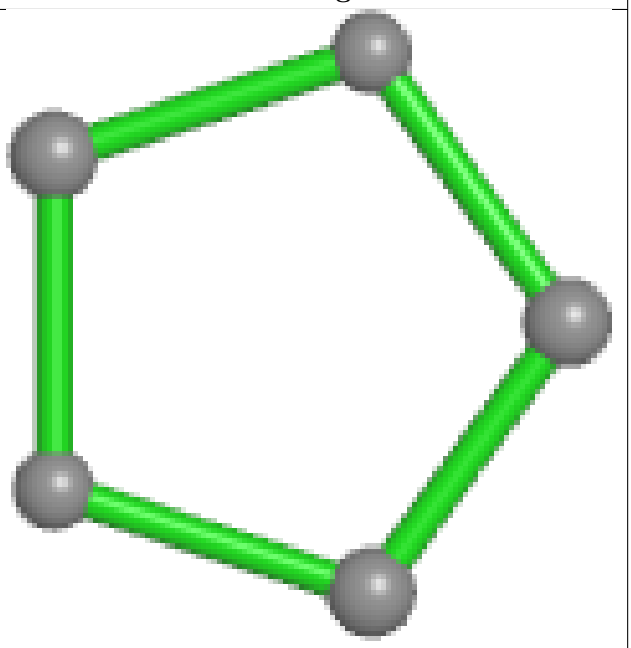
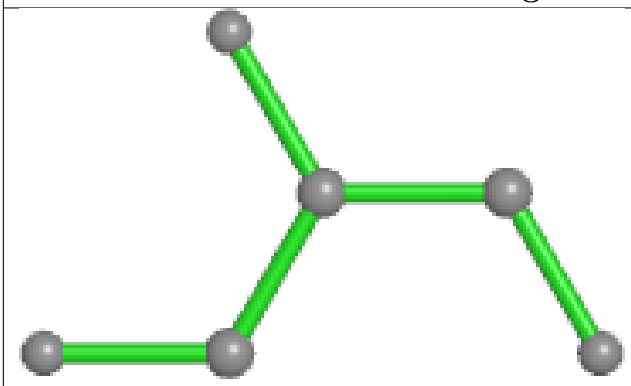


Rings

Ligand GOL D 704



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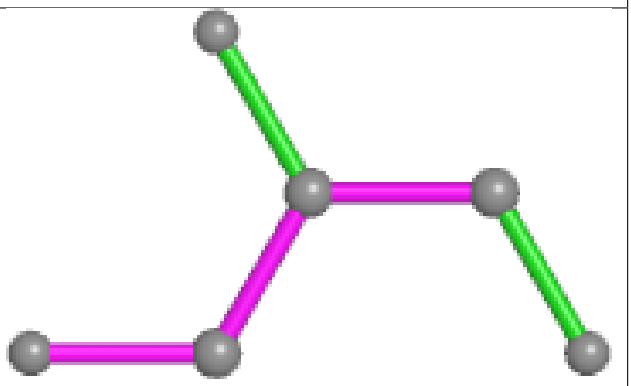
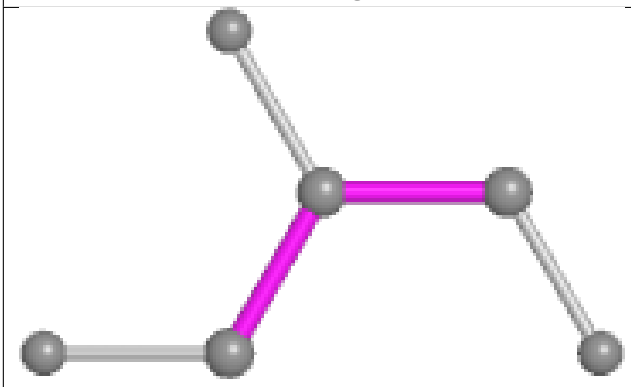
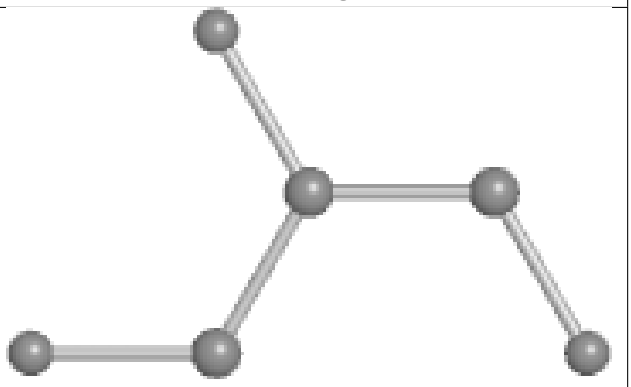


Bond angles

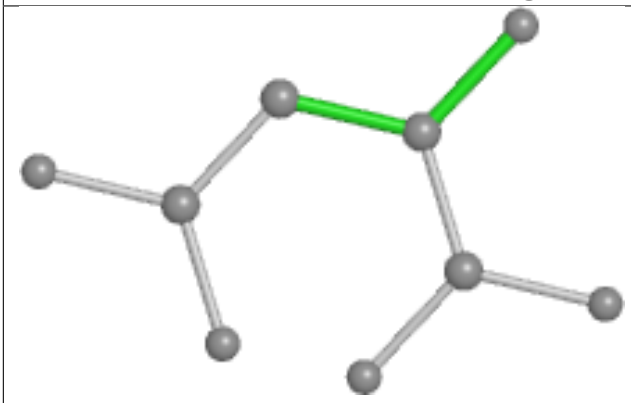


Torsions

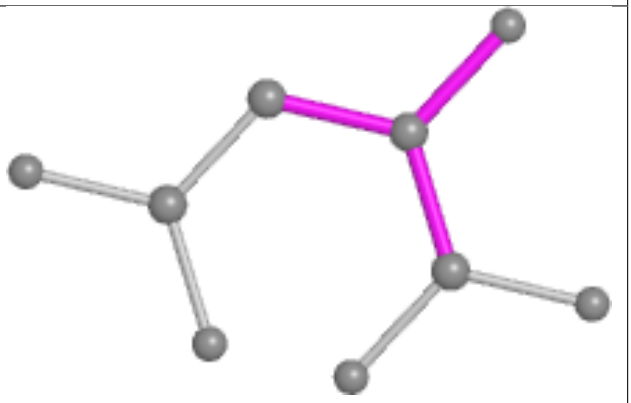


Rings

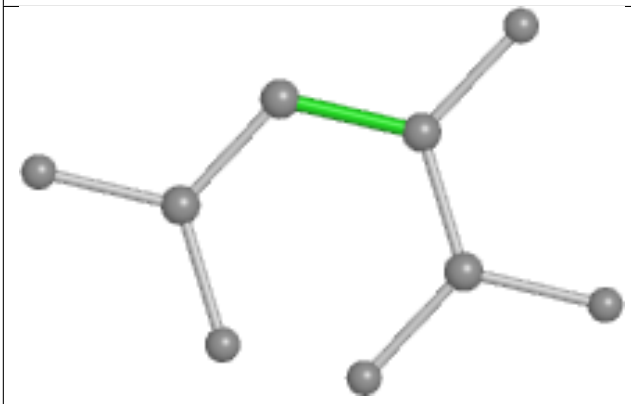
Ligand LMR C 809



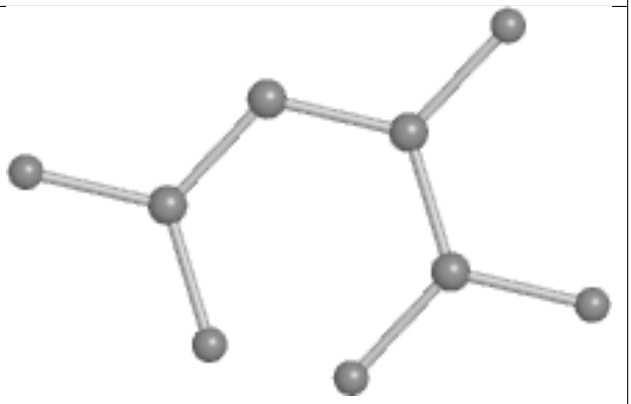
Bond lengths



Bond angles

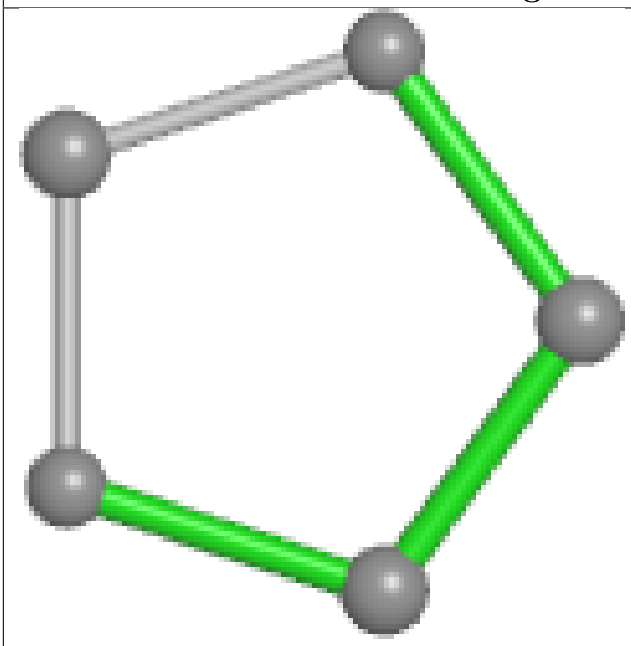


Torsions

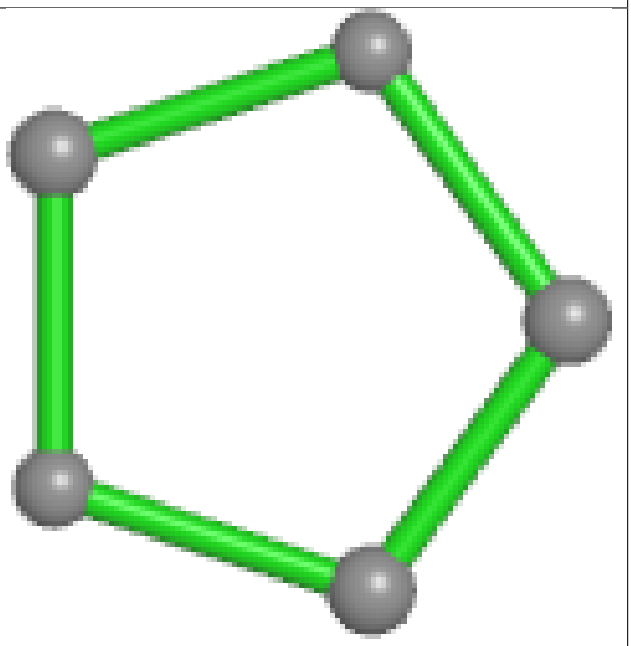


Rings

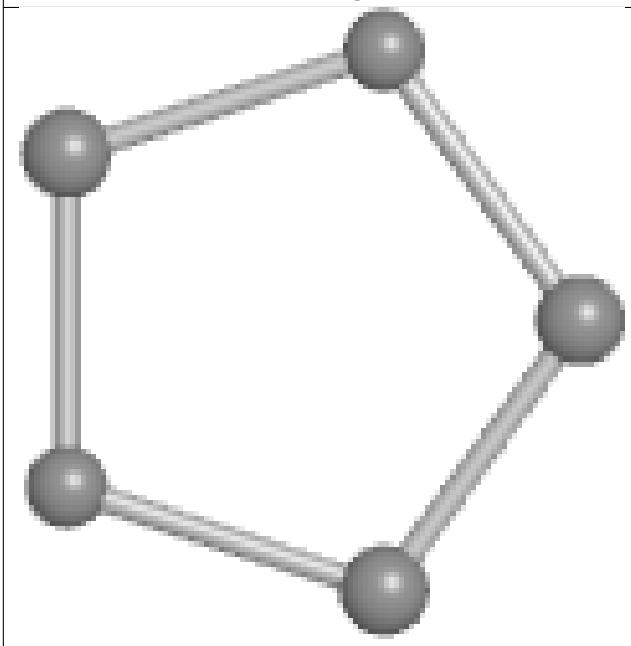
Ligand IMD D 703



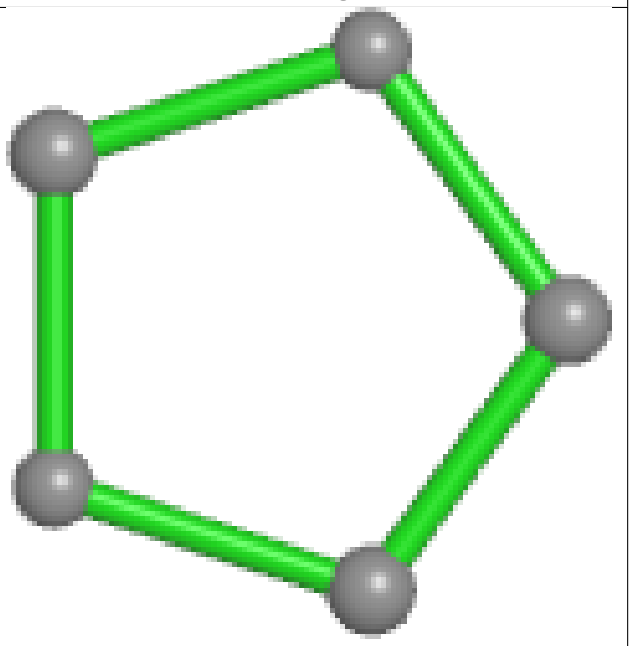
Bond lengths



Bond angles

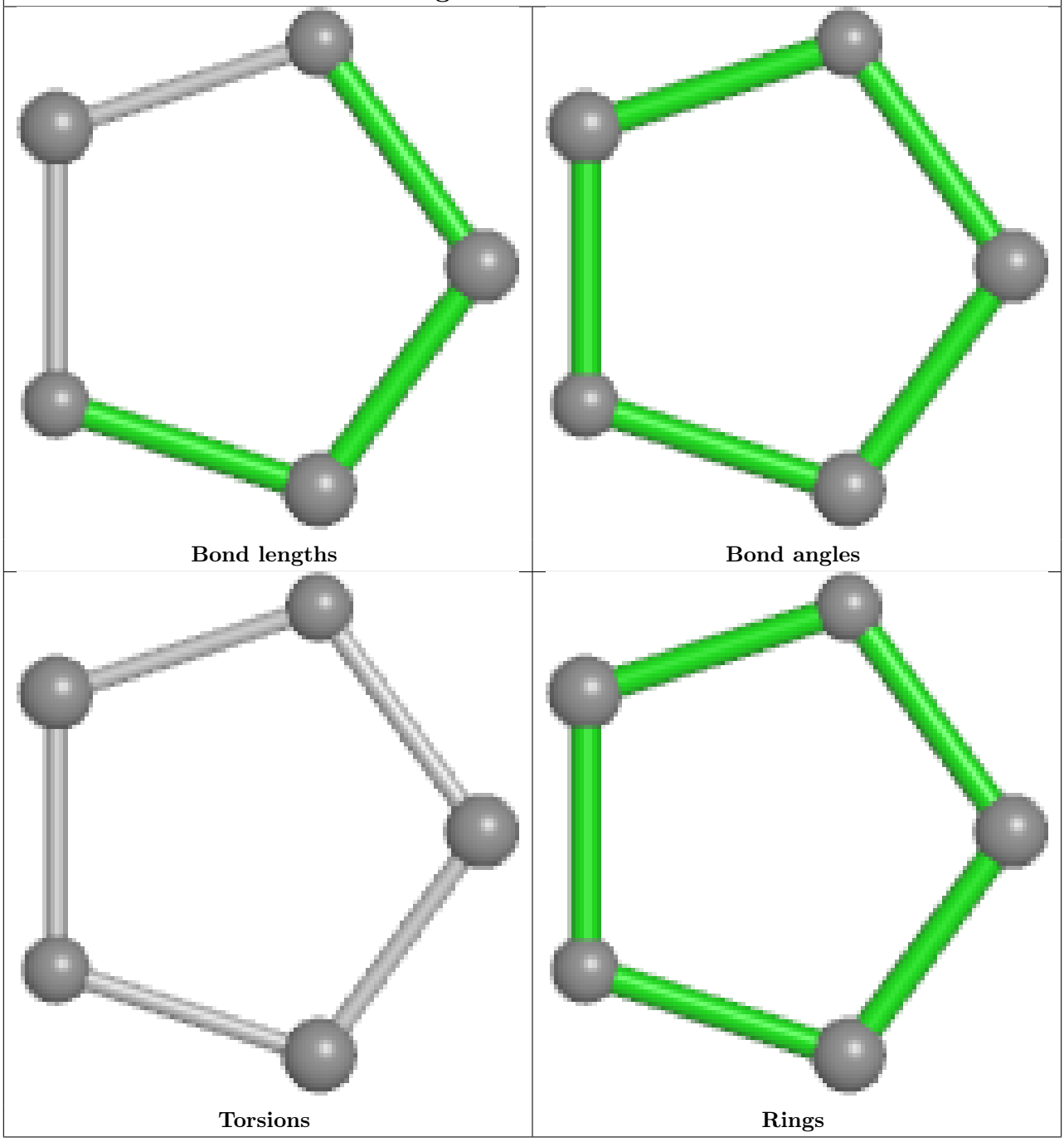


Torsions



Rings

Ligand IMD C 808



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	642/671 (95%)	-0.10	17 (2%)	56	60	11, 20, 34, 68	3 (0%)
1	B	634/671 (94%)	-0.02	40 (6%)	20	21	12, 20, 45, 102	3 (0%)
1	C	640/671 (95%)	0.12	44 (6%)	16	18	13, 21, 49, 79	0
1	D	622/671 (92%)	-0.20	19 (3%)	49	53	11, 16, 33, 74	2 (0%)
1	E	644/671 (95%)	-0.18	16 (2%)	57	61	9, 17, 33, 76	3 (0%)
1	F	642/671 (95%)	-0.19	26 (4%)	38	42	11, 17, 41, 80	1 (0%)
All	All	3824/4026 (94%)	-0.10	162 (4%)	36	39	9, 18, 40, 102	12 (0%)

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	622	VAL	10.7
1	E	274	ILE	9.5
1	B	23	PRO	9.0
1	B	22	TYR	8.5
1	B	36	SER	8.4
1	C	622	VAL	7.5
1	C	623	PRO	7.4
1	C	25	PHE	7.2
1	B	28	GLN	7.1
1	B	25	PHE	7.0
1	B	47	ALA	7.0
1	D	36	SER	6.9
1	B	20	VAL	6.6
1	D	43	PHE	6.5
1	D	58	VAL	6.5
1	F	622	VAL	6.4
1	C	22	TYR	6.3
1	A	624	THR	6.3
1	B	37	ALA	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	21	ALA	6.1
1	C	21	ALA	6.1
1	E	8	ALA	5.7
1	F	22	TYR	5.6
1	C	24	ASN	5.6
1	C	23	PRO	5.5
1	C	624	THR	5.4
1	B	24	ASN	5.3
1	B	624	THR	5.2
1	C	13	PHE	5.2
1	B	45	THR	5.1
1	C	43	PHE	5.1
1	B	59	PRO	5.0
1	A	587	VAL	5.0
1	F	24	ASN	5.0
1	E	9	PRO	4.9
1	C	59	PRO	4.9
1	A	622	VAL	4.7
1	D	61	GLY	4.6
1	F	14	SER	4.6
1	E	622	VAL	4.5
1	D	45	THR	4.4
1	A	36	SER	4.4
1	A	623	PRO	4.4
1	D	59	PRO	4.4
1	F	21	ALA	4.3
1	B	27	VAL	4.3
1	B	58	VAL	4.3
1	F	203	GLY	4.2
1	F	23	PRO	4.1
1	B	60	GLY	4.1
1	B	29	ASP	4.1
1	F	27	VAL	4.0
1	F	28	GLN	3.9
1	F	25	PHE	3.8
1	C	61	GLY	3.8
1	D	35	GLY	3.8
1	C	58	VAL	3.8
1	E	203	GLY	3.8
1	B	48	SER	3.7
1	C	36	SER	3.7
1	B	623	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	62	TYR	3.7
1	B	570	VAL	3.7
1	D	60	GLY	3.6
1	B	620	GLN	3.6
1	C	15	ASP	3.6
1	C	62	TYR	3.6
1	F	46	THR	3.6
1	C	27	VAL	3.6
1	C	546	VAL	3.6
1	B	43	PHE	3.5
1	E	107	ILE	3.5
1	D	44	THR	3.4
1	C	29	ASP	3.4
1	F	47	ALA	3.4
1	E	204	GLY	3.3
1	C	26	GLN	3.3
1	D	42	THR	3.3
1	C	20	VAL	3.3
1	B	26	GLN	3.3
1	E	623	PRO	3.3
1	E	624	THR	3.3
1	C	621	ASP	3.2
1	F	624	THR	3.2
1	D	31	ILE	3.2
1	C	16	LEU	3.1
1	A	488	ALA	3.1
1	B	34	LEU	3.1
1	F	59	PRO	3.1
1	C	202	SER	3.1
1	F	488	ALA	3.0
1	B	621	ASP	3.0
1	A	17	ALA	3.0
1	B	625	PRO	3.0
1	C	574	ALA	3.0
1	C	625	PRO	2.9
1	D	34	LEU	2.9
1	B	140	SER	2.9
1	B	46	THR	2.9
1	C	545	THR	2.9
1	B	639	ALA	2.9
1	F	11	ARG	2.9
1	C	31	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	49	VAL	2.9
1	F	17	ALA	2.8
1	B	18	SER	2.8
1	C	12	VAL	2.8
1	C	488	ALA	2.8
1	B	57	ALA	2.7
1	E	586	SER	2.7
1	C	203	GLY	2.7
1	C	45	THR	2.7
1	A	345	ASP	2.7
1	A	626	ASN	2.6
1	A	620	GLN	2.6
1	C	19	MET	2.5
1	F	45	THR	2.5
1	B	31	ILE	2.5
1	F	10	GLU	2.5
1	B	202	SER	2.5
1	C	344	ALA	2.4
1	C	18	SER	2.4
1	B	629	LEU	2.4
1	F	13	PHE	2.4
1	B	203	GLY	2.4
1	C	14	SER	2.4
1	F	60	GLY	2.4
1	A	525	SER	2.4
1	C	345	ASP	2.3
1	E	140	SER	2.3
1	D	33	LEU	2.3
1	D	46	THR	2.3
1	F	623	PRO	2.3
1	D	489	GLU	2.3
1	A	586	SER	2.3
1	F	18	SER	2.3
1	B	546	VAL	2.3
1	C	60	GLY	2.3
1	C	606	SER	2.2
1	E	202	SER	2.2
1	D	63	LEU	2.2
1	C	17	ALA	2.2
1	B	61	GLY	2.2
1	C	34	LEU	2.2
1	E	10	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	15	ASP	2.2
1	A	21	ALA	2.2
1	A	140	SER	2.2
1	D	488	ALA	2.1
1	A	261	ASN	2.1
1	E	21	ALA	2.1
1	E	346	GLY	2.1
1	C	127	VAL	2.1
1	F	20	VAL	2.1
1	A	126	ALA	2.1
1	D	57	ALA	2.1
1	E	345	ASP	2.1
1	A	332	VAL	2.1
1	F	36	SER	2.1
1	C	47	ALA	2.1
1	D	127	VAL	2.0
1	C	258	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
3	IMD	C	806	5/5	0.75	0.28	41,44,49,56	0
3	IMD	E	708	5/5	0.77	0.36	47,49,53,54	0
3	IMD	A	804	5/5	0.79	0.29	37,44,45,46	0
3	IMD	D	706	5/5	0.81	0.23	39,42,45,47	0
3	IMD	F	709	5/5	0.82	0.23	25,34,40,44	0
3	IMD	B	708	5/5	0.84	0.22	26,27,45,47	0

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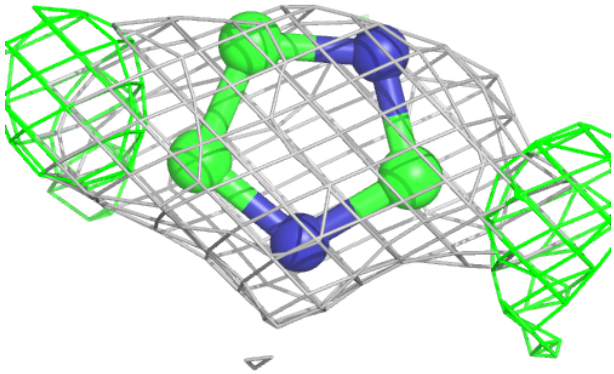
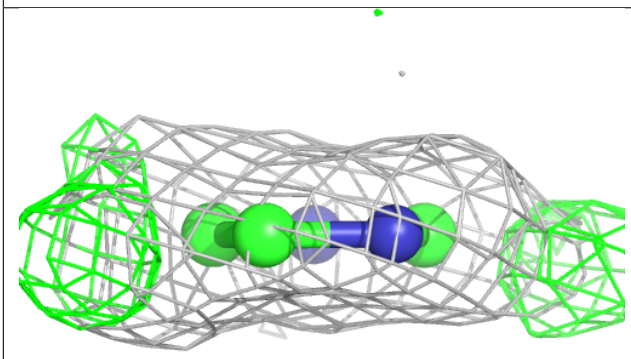
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	IMD	A	802	5/5	0.86	0.27	44,47,66,73	0
4	GOL	F	701	6/6	0.87	0.15	19,28,30,31	0
3	IMD	B	705	5/5	0.88	0.22	35,42,44,45	0
4	GOL	E	703	6/6	0.88	0.14	20,27,40,44	0
3	IMD	C	810	5/5	0.88	0.22	28,31,40,43	0
4	GOL	D	705	6/6	0.89	0.18	26,32,34,37	0
4	GOL	C	802	6/6	0.90	0.15	24,36,50,57	0
3	IMD	E	704	5/5	0.90	0.22	21,26,44,45	0
4	GOL	F	702	6/6	0.90	0.13	25,29,40,45	0
4	GOL	A	803	6/6	0.91	0.09	25,29,33,35	0
3	IMD	F	705	5/5	0.91	0.14	23,33,43,44	0
3	IMD	B	706	5/5	0.91	0.17	26,31,40,48	0
4	GOL	C	807	6/6	0.92	0.10	28,36,40,47	0
3	IMD	C	805	5/5	0.92	0.23	28,33,40,41	0
2	LMR	F	708	9/9	0.92	0.16	22,26,29,30	0
3	IMD	F	703	5/5	0.92	0.20	33,33,39,42	0
3	IMD	F	704	5/5	0.92	0.18	37,41,45,53	0
2	LMR	D	702	9/9	0.93	0.12	23,30,43,44	0
3	IMD	B	704	5/5	0.93	0.14	35,41,45,47	0
4	GOL	B	707	6/6	0.93	0.16	23,29,35,50	0
4	GOL	F	706	6/6	0.93	0.11	21,27,30,35	0
3	IMD	D	701	5/5	0.94	0.12	23,28,37,43	0
3	IMD	D	703	5/5	0.94	0.17	31,34,35,38	0
4	GOL	D	704	6/6	0.94	0.09	19,20,24,30	0
2	LMR	E	707	9/9	0.94	0.15	20,30,41,46	0
3	IMD	A	805	5/5	0.94	0.17	23,29,43,47	0
3	IMD	E	705	5/5	0.94	0.15	22,29,45,45	0
4	GOL	A	806	6/6	0.94	0.09	23,35,39,49	0
3	IMD	C	804	5/5	0.94	0.20	31,36,38,40	0
2	LMR	B	703	9/9	0.95	0.14	19,25,48,56	0
4	GOL	E	701	6/6	0.95	0.11	22,30,34,42	0
4	GOL	C	801	6/6	0.95	0.08	24,29,37,46	0
3	IMD	C	808	5/5	0.95	0.25	47,50,54,56	0
2	LMR	C	809	9/9	0.95	0.16	26,30,45,51	0
4	GOL	B	701	6/6	0.95	0.13	25,28,31,41	0
4	GOL	B	702	6/6	0.96	0.08	24,28,31,36	0
2	LMR	A	801	9/9	0.96	0.11	25,31,45,50	0
4	GOL	D	707	6/6	0.97	0.06	18,26,28,45	0
4	GOL	C	803	6/6	0.97	0.09	21,23,24,26	0
3	IMD	E	702	5/5	0.97	0.28	26,30,33,36	0
2	LMR	F	707	9/9	0.98	0.14	19,26,36,54	0
4	GOL	E	706	6/6	0.99	0.05	17,18,21,22	0

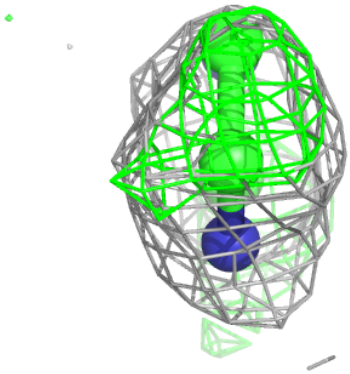
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IMD C 806:

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

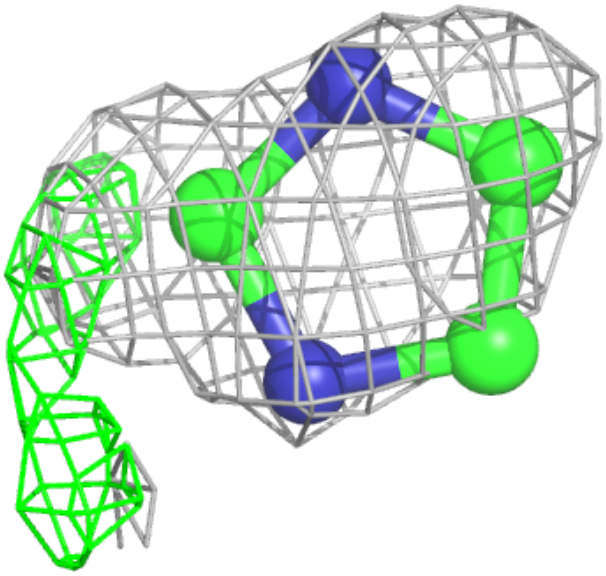


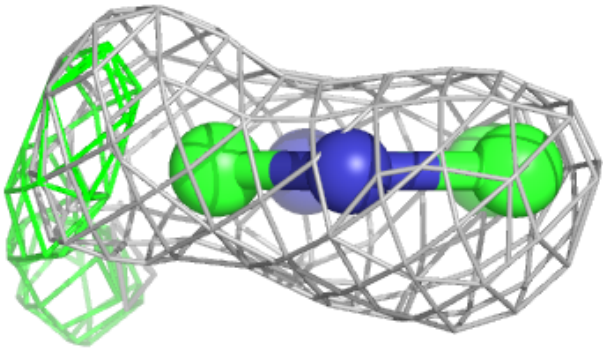


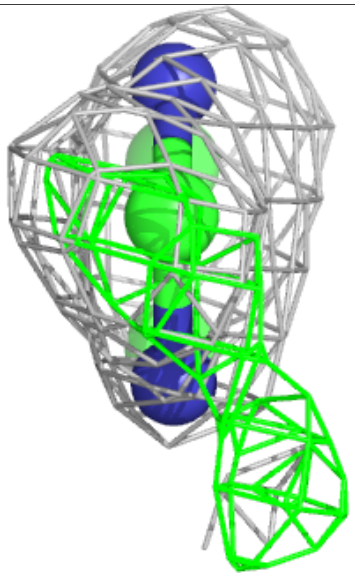


Electron density around IMD E 708:

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

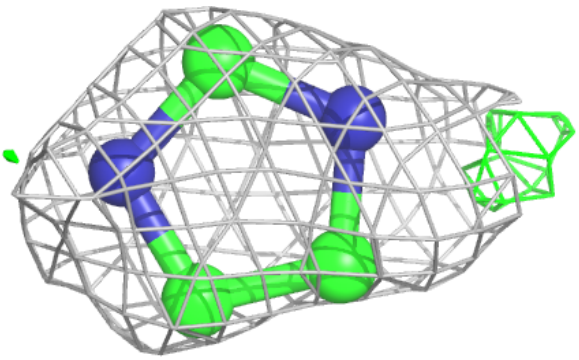


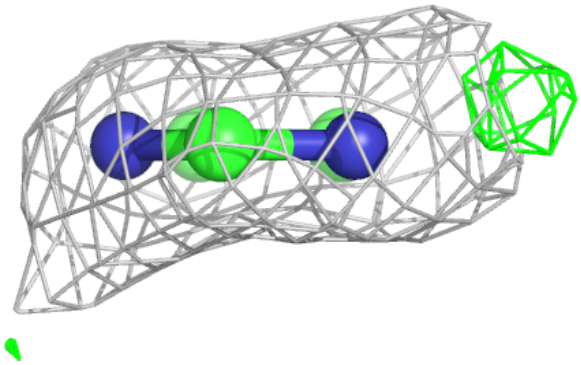


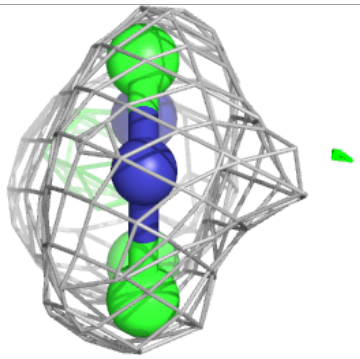


Electron density around IMD A 804:

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

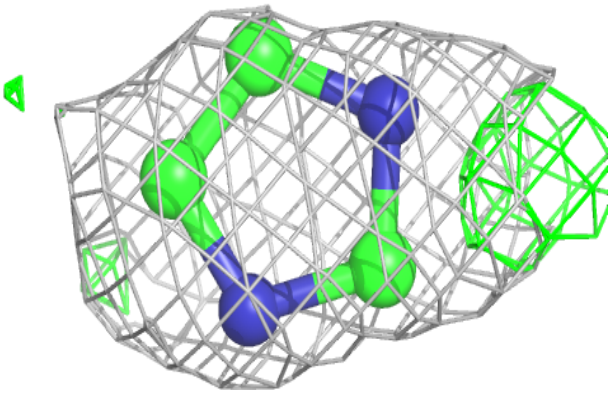


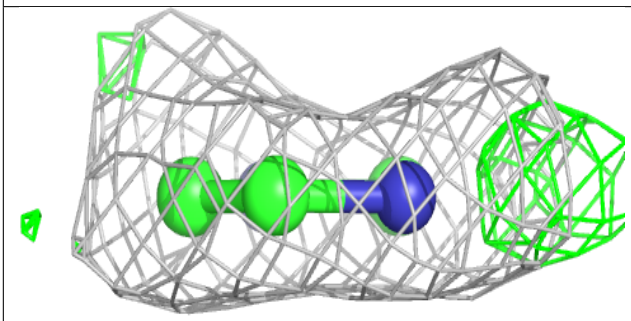


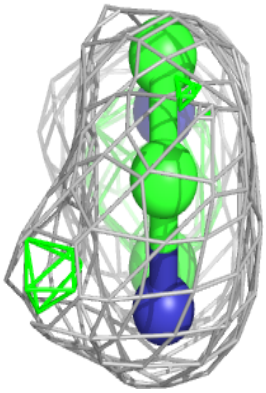


Electron density around IMD D 706:

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

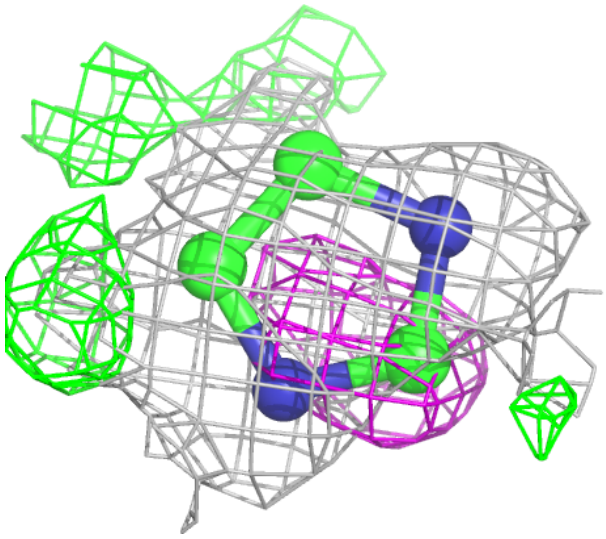


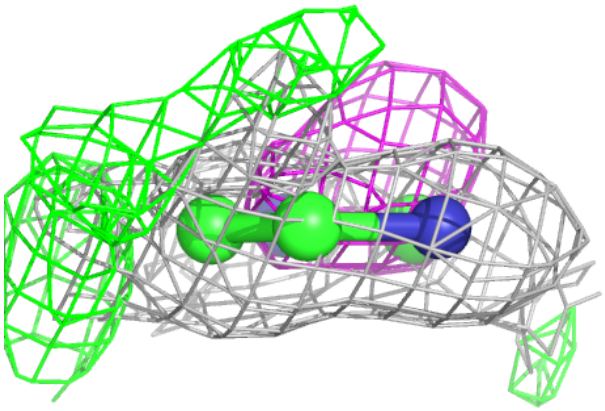


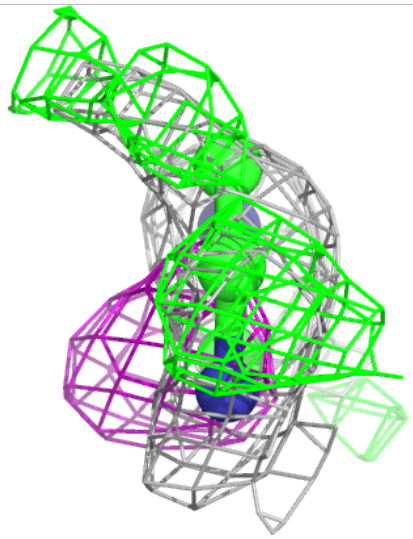


Electron density around IMD F 709:

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

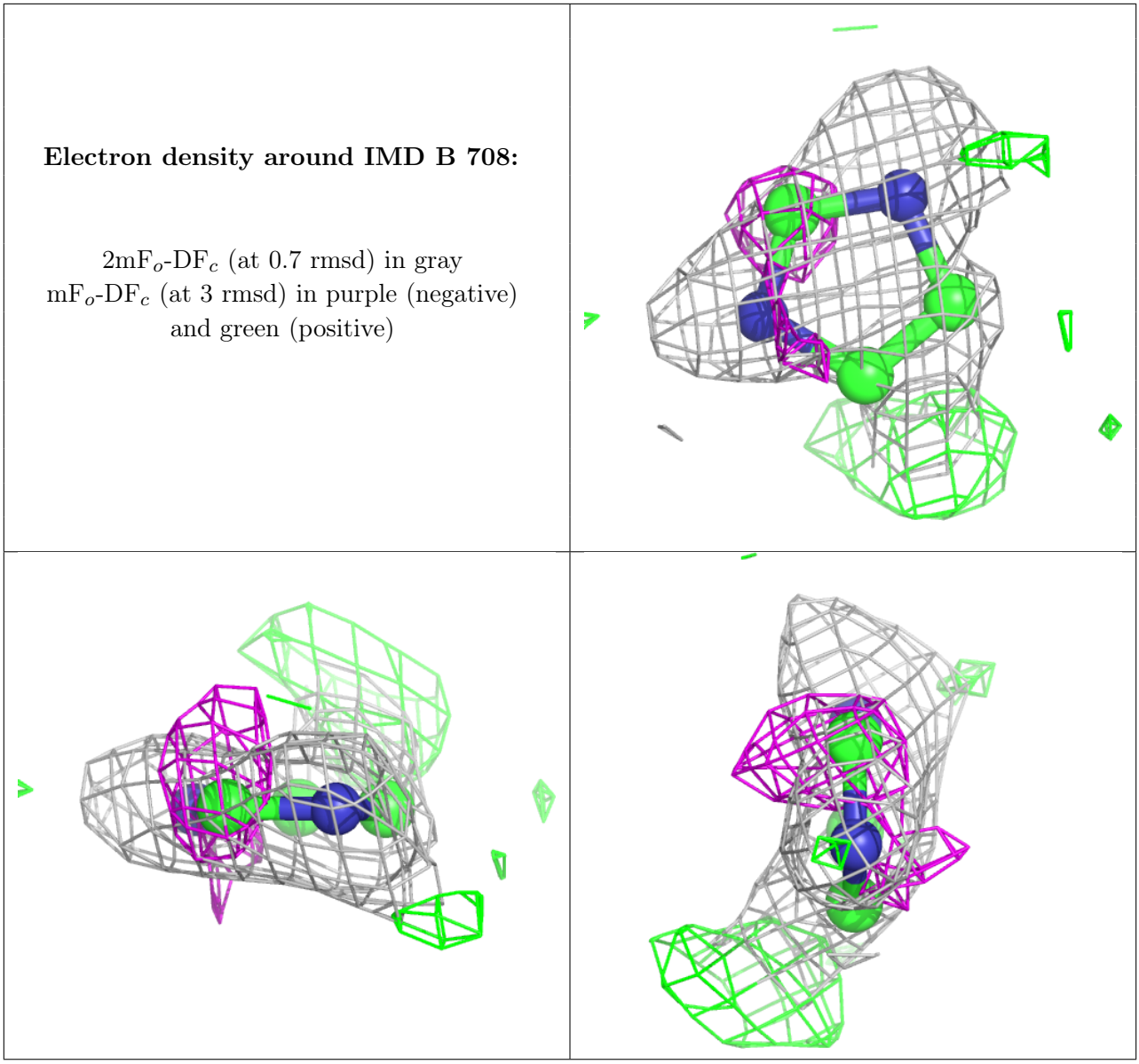






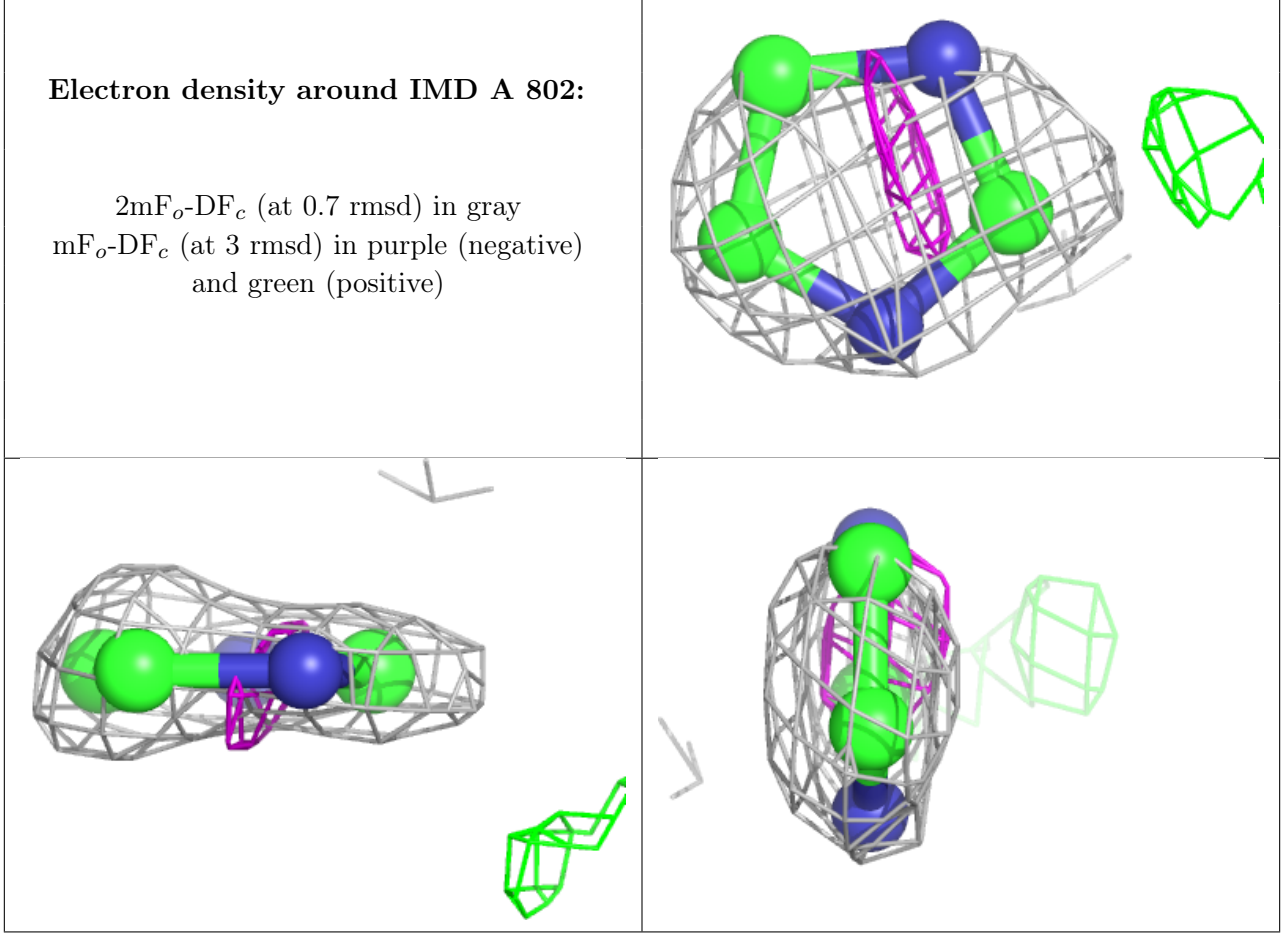
Electron density around IMD B 708:

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



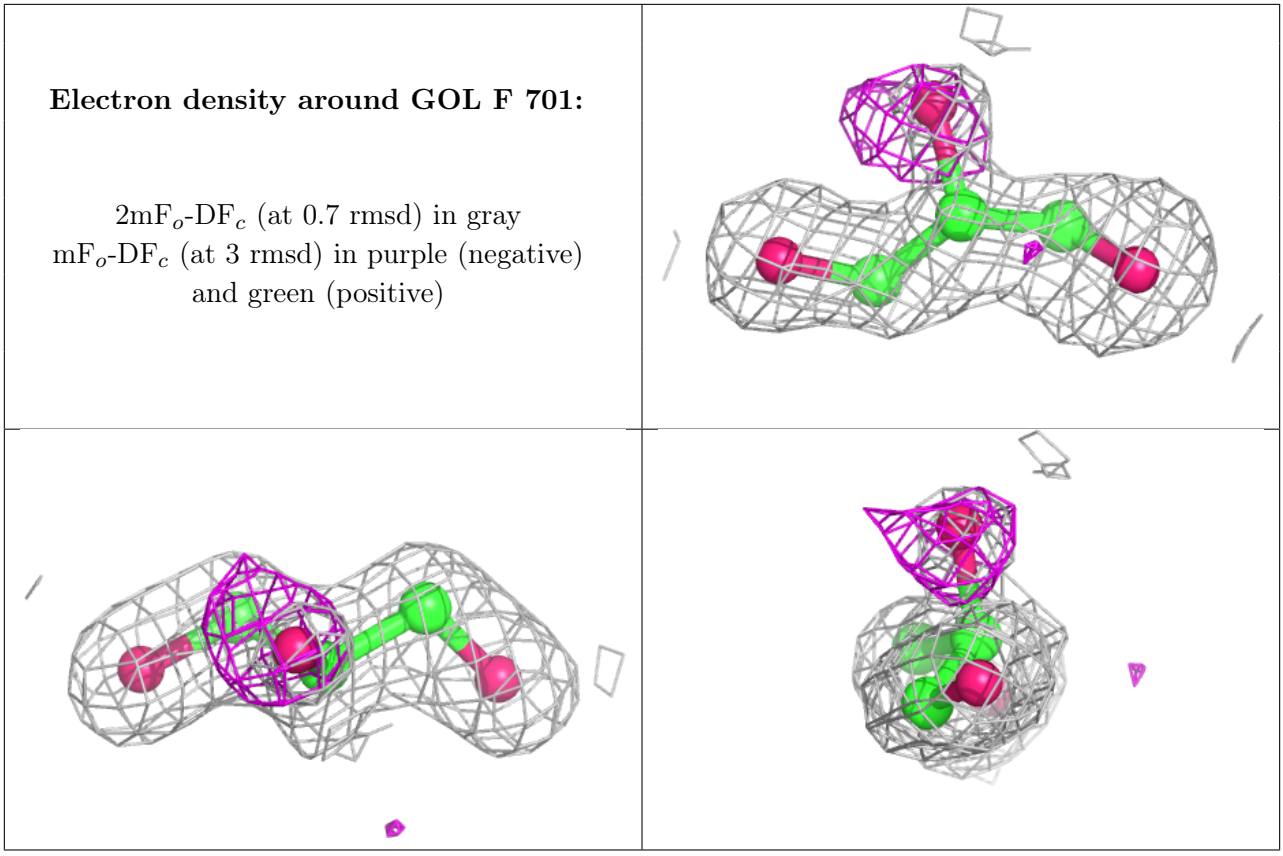
Electron density around IMD A 802:

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



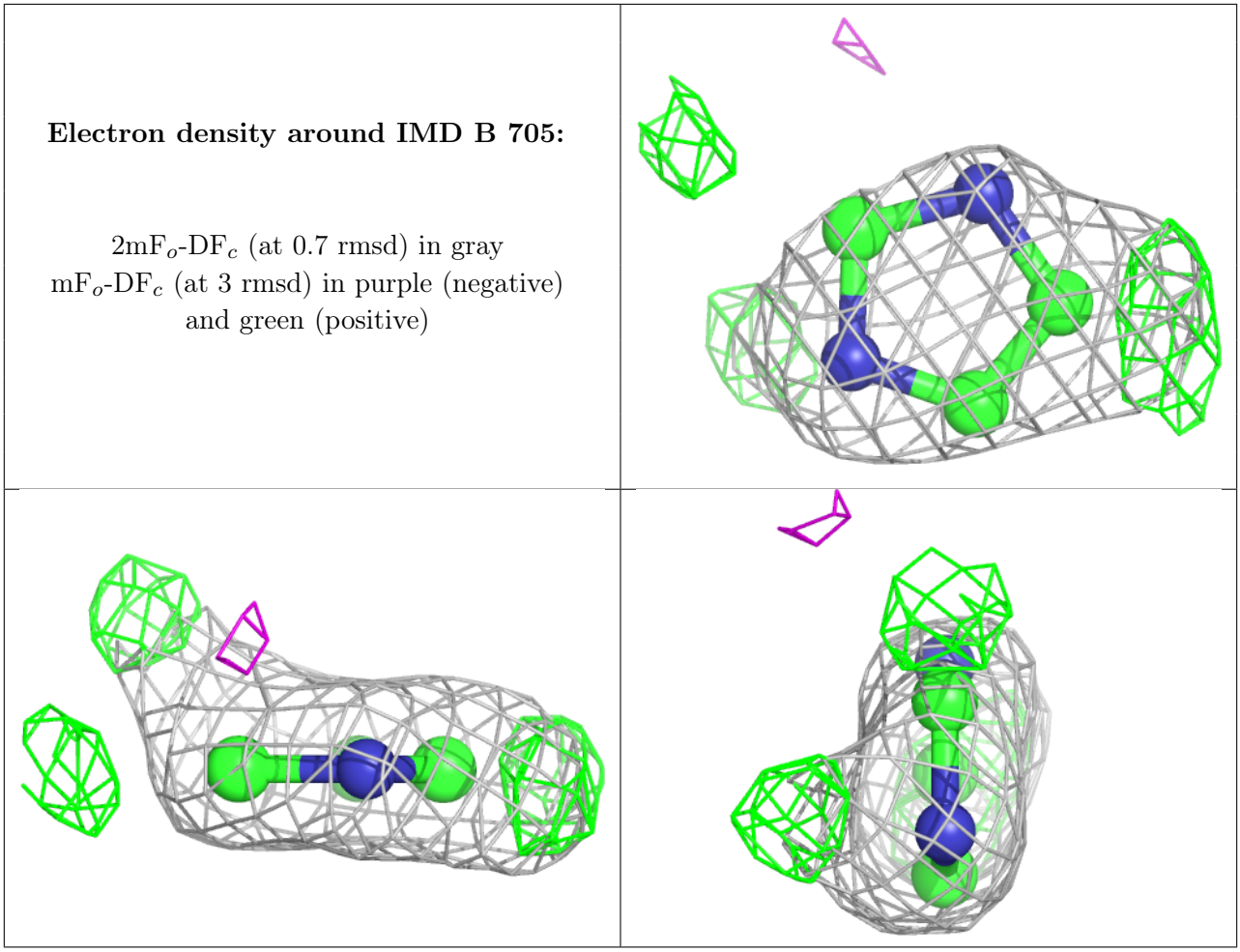
Electron density around GOL F 701:

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



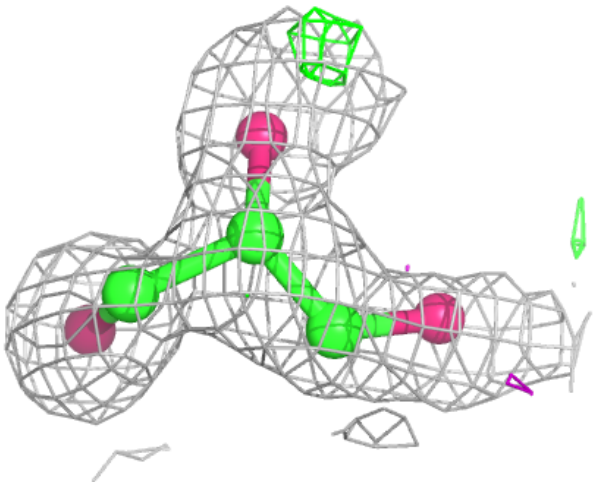
Electron density around IMD B 705:

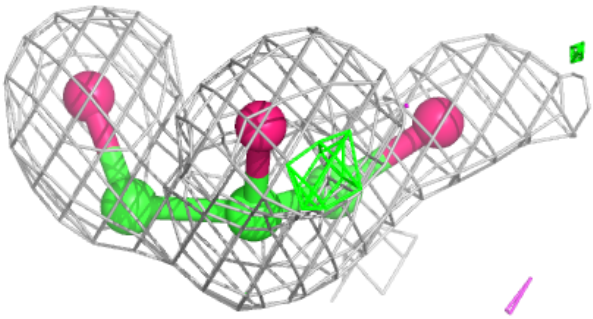
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

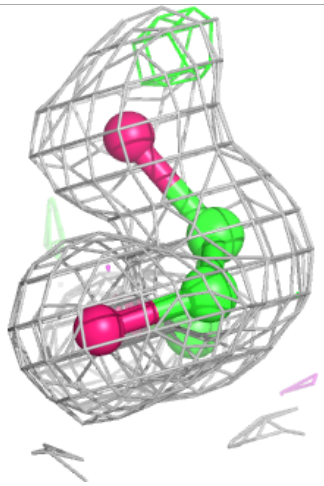


Electron density around GOL E 703:

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

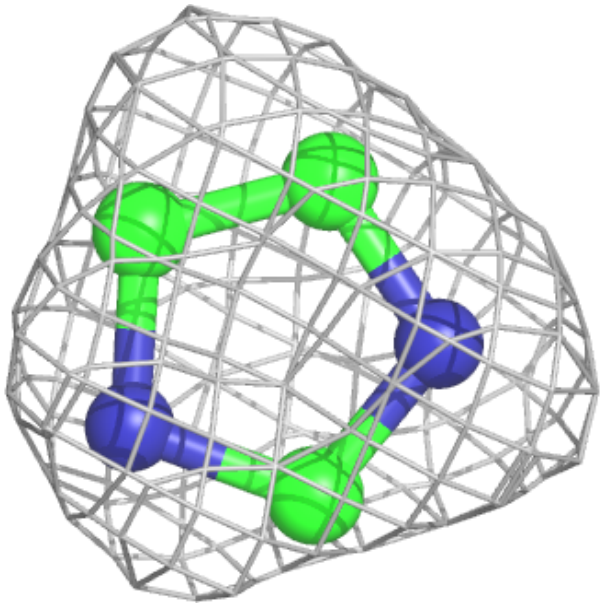


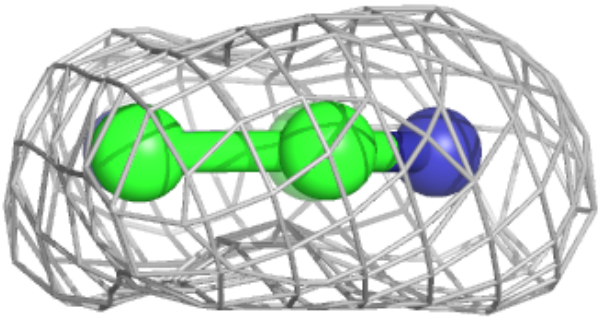


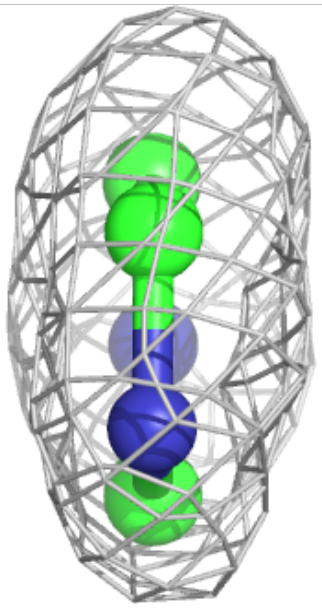


Electron density around IMD C 810:

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

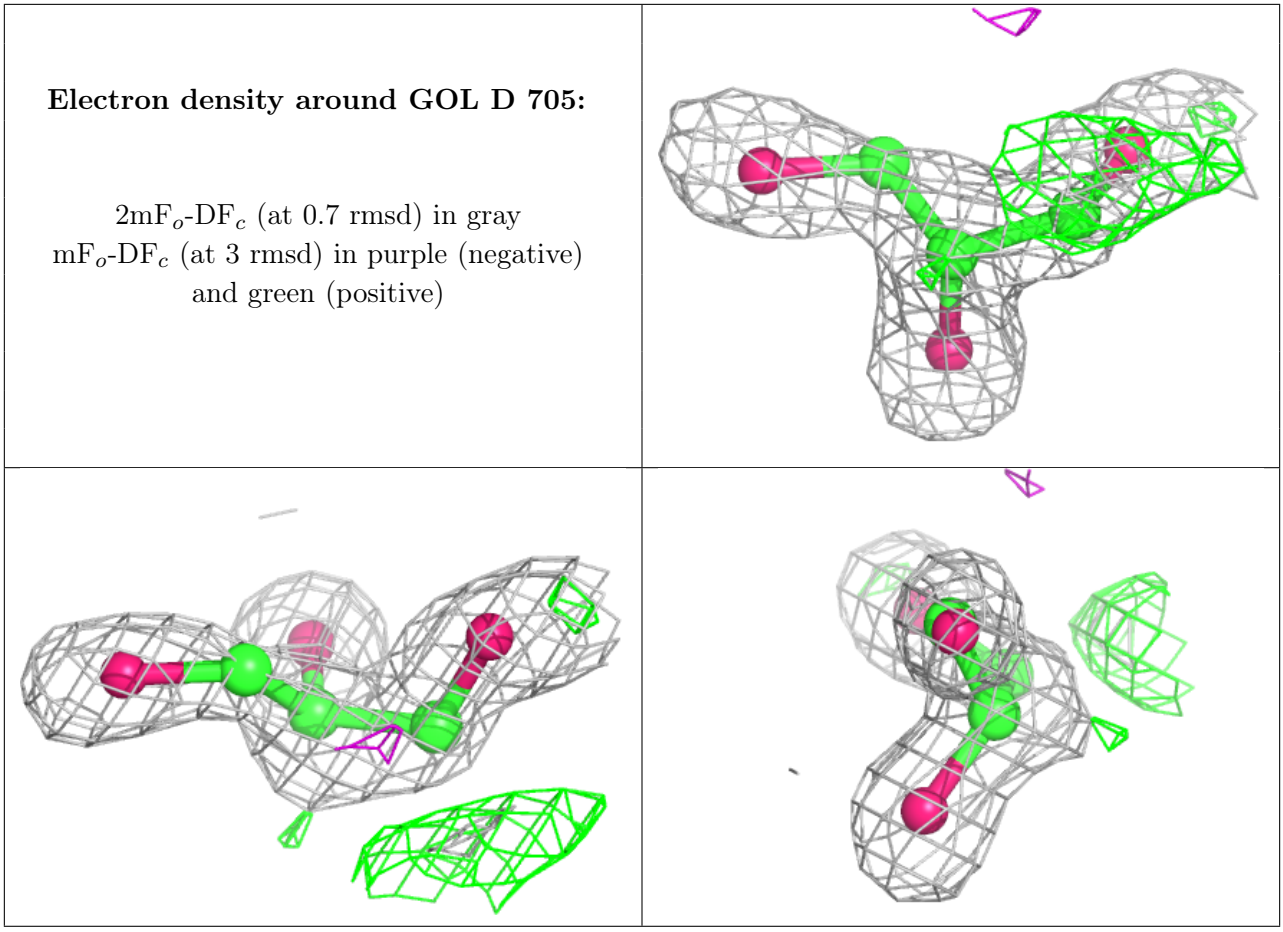






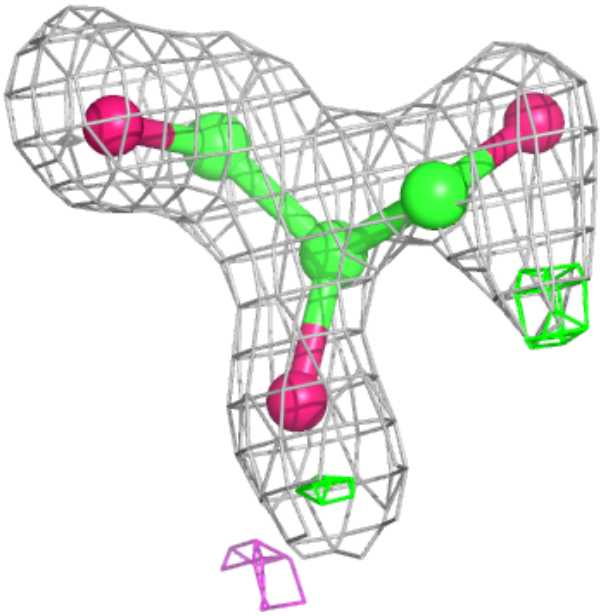
Electron density around GOL D 705:

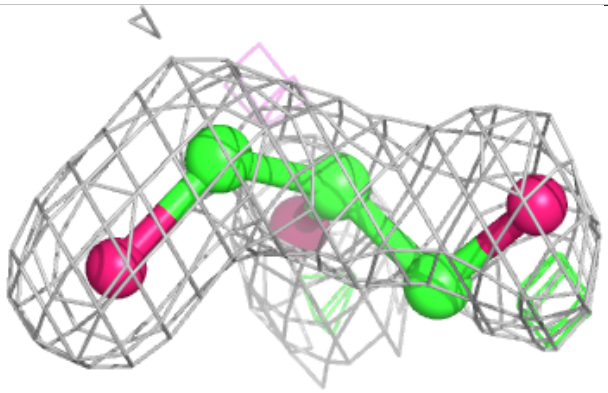
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

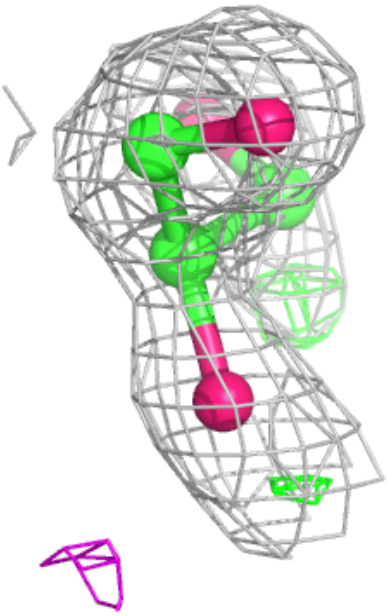


Electron density around GOL C 802:

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

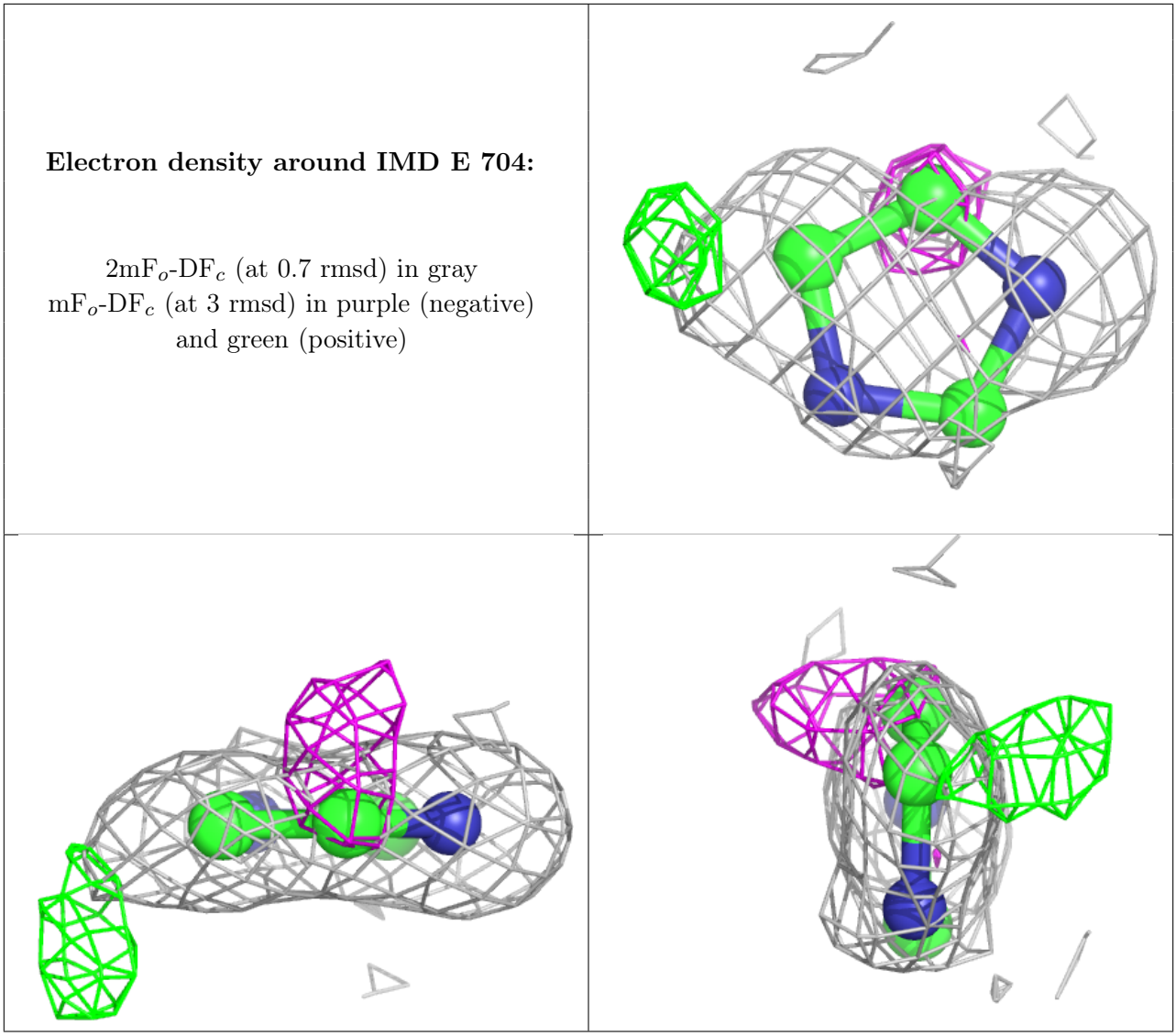






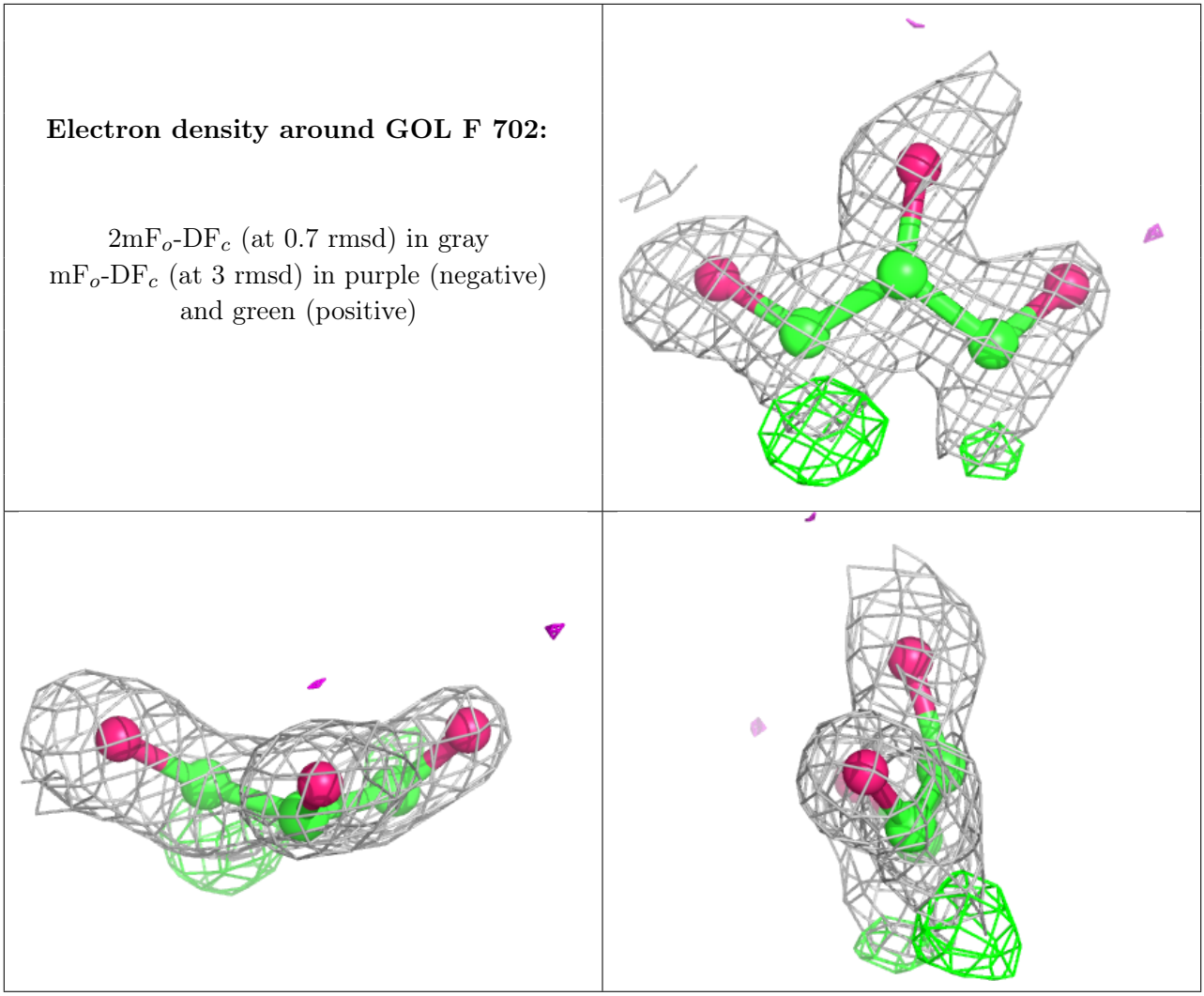
Electron density around IMD E 704:

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



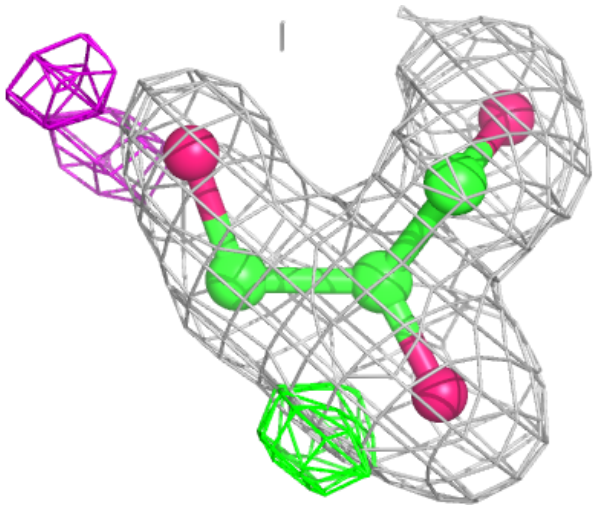
Electron density around GOL F 702:

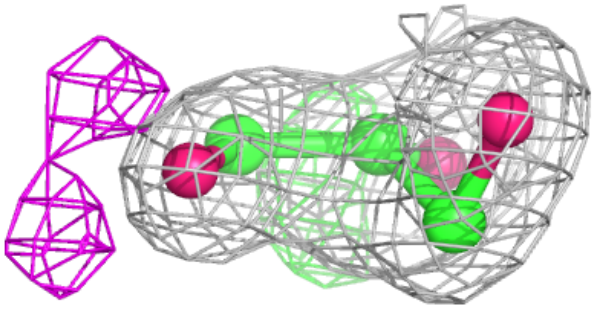
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

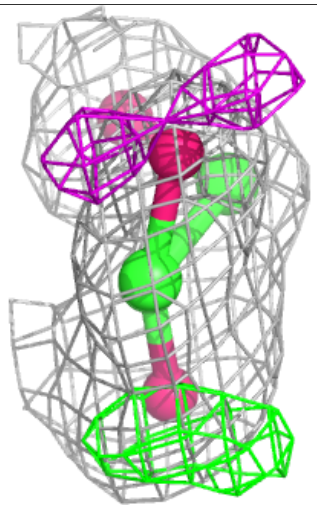


Electron density around GOL A 803:

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

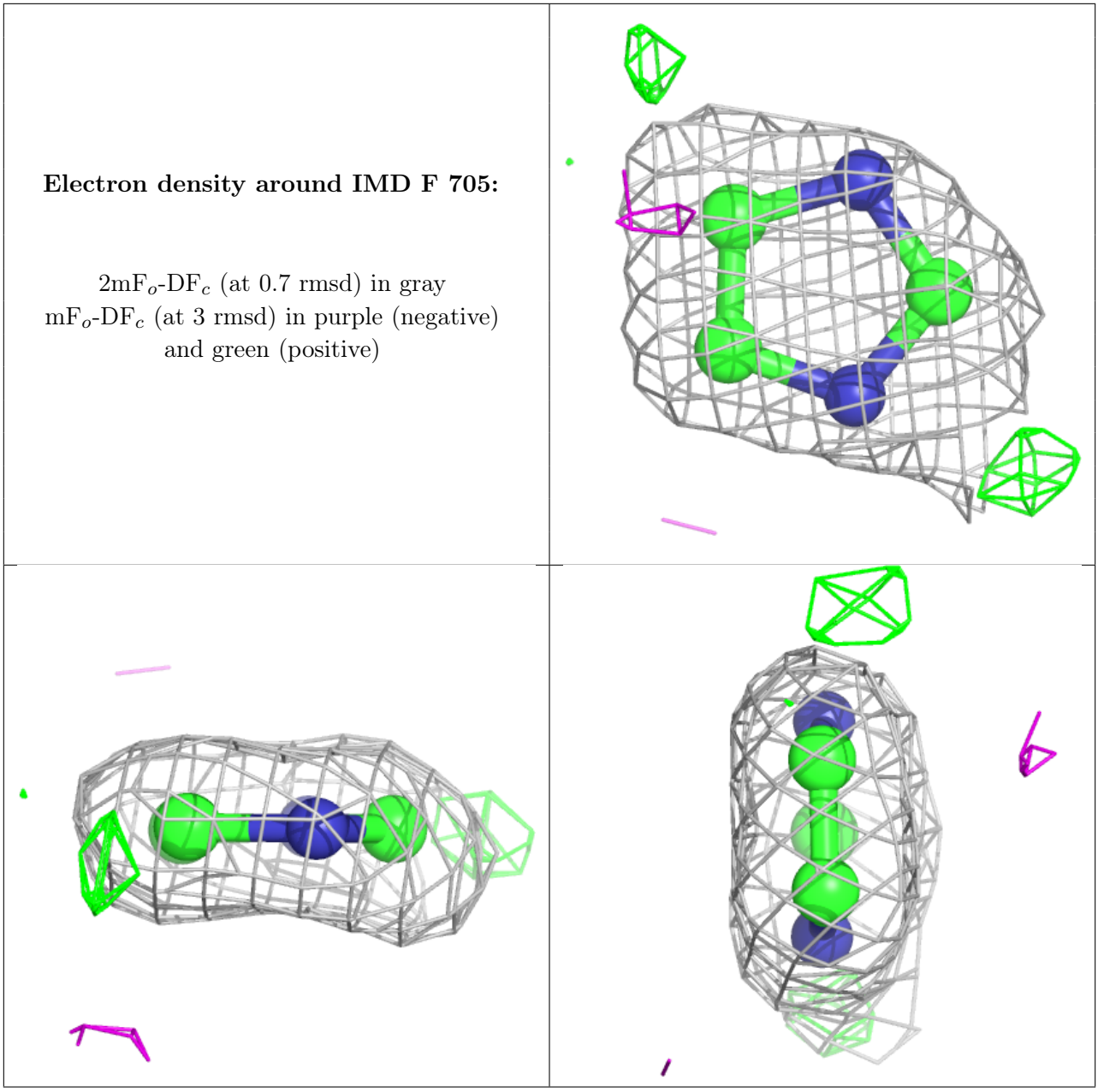






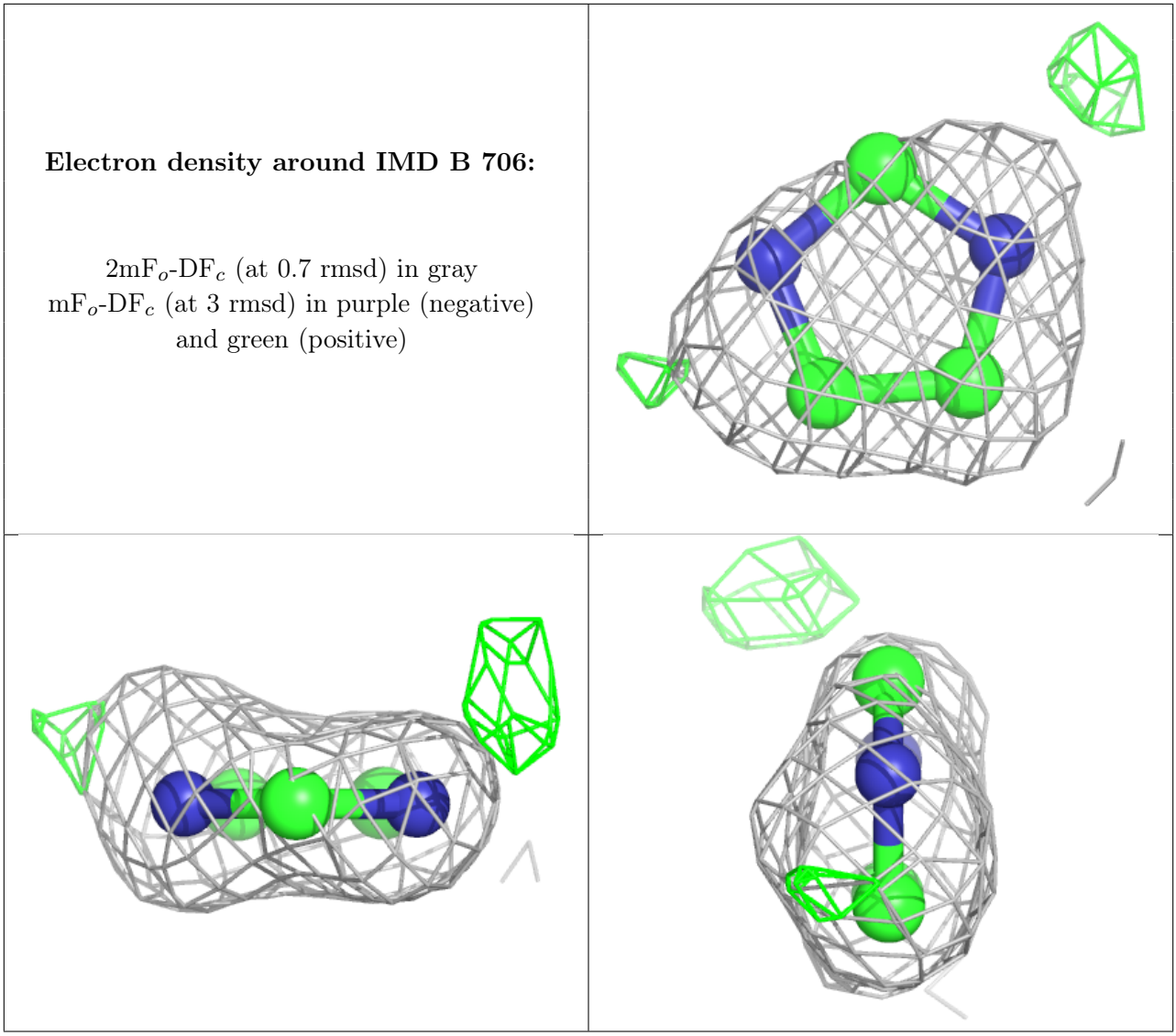
Electron density around IMD F 705:

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



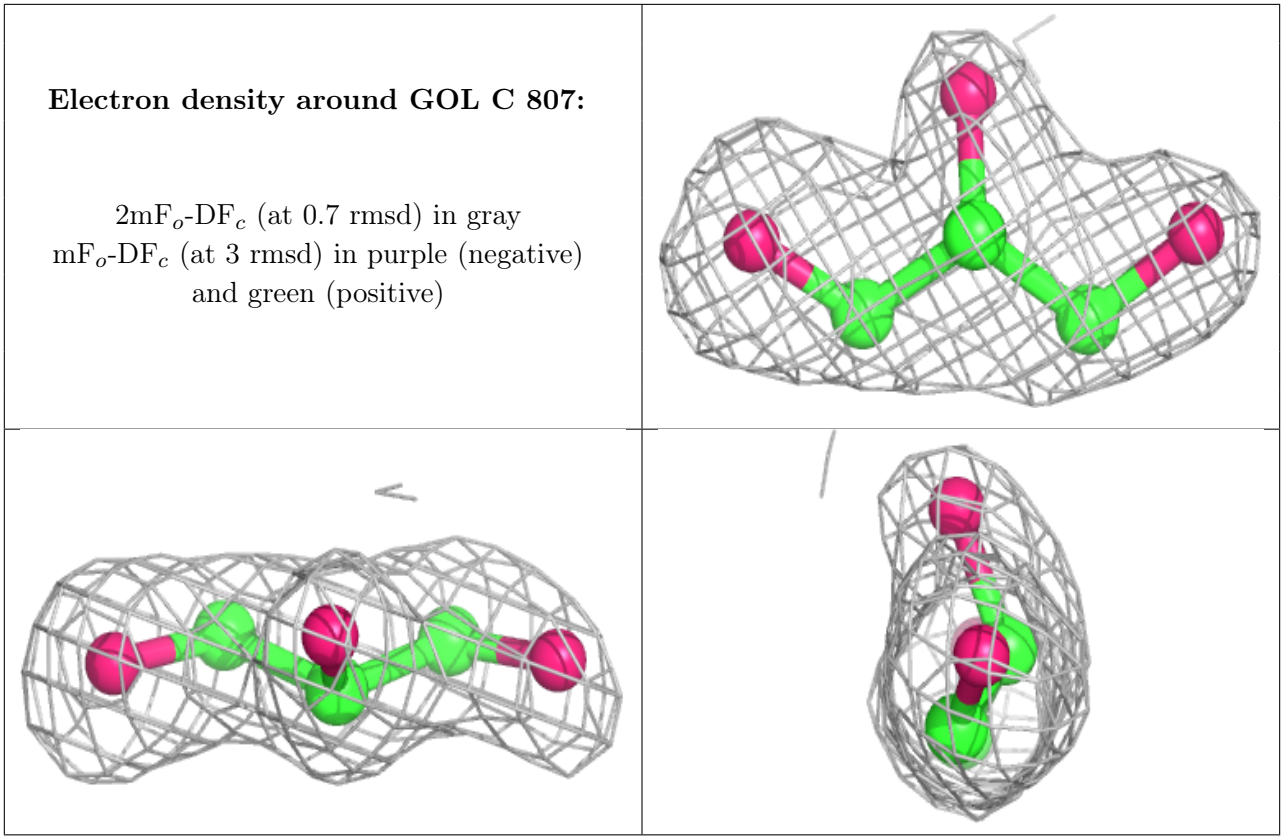
Electron density around IMD B 706:

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



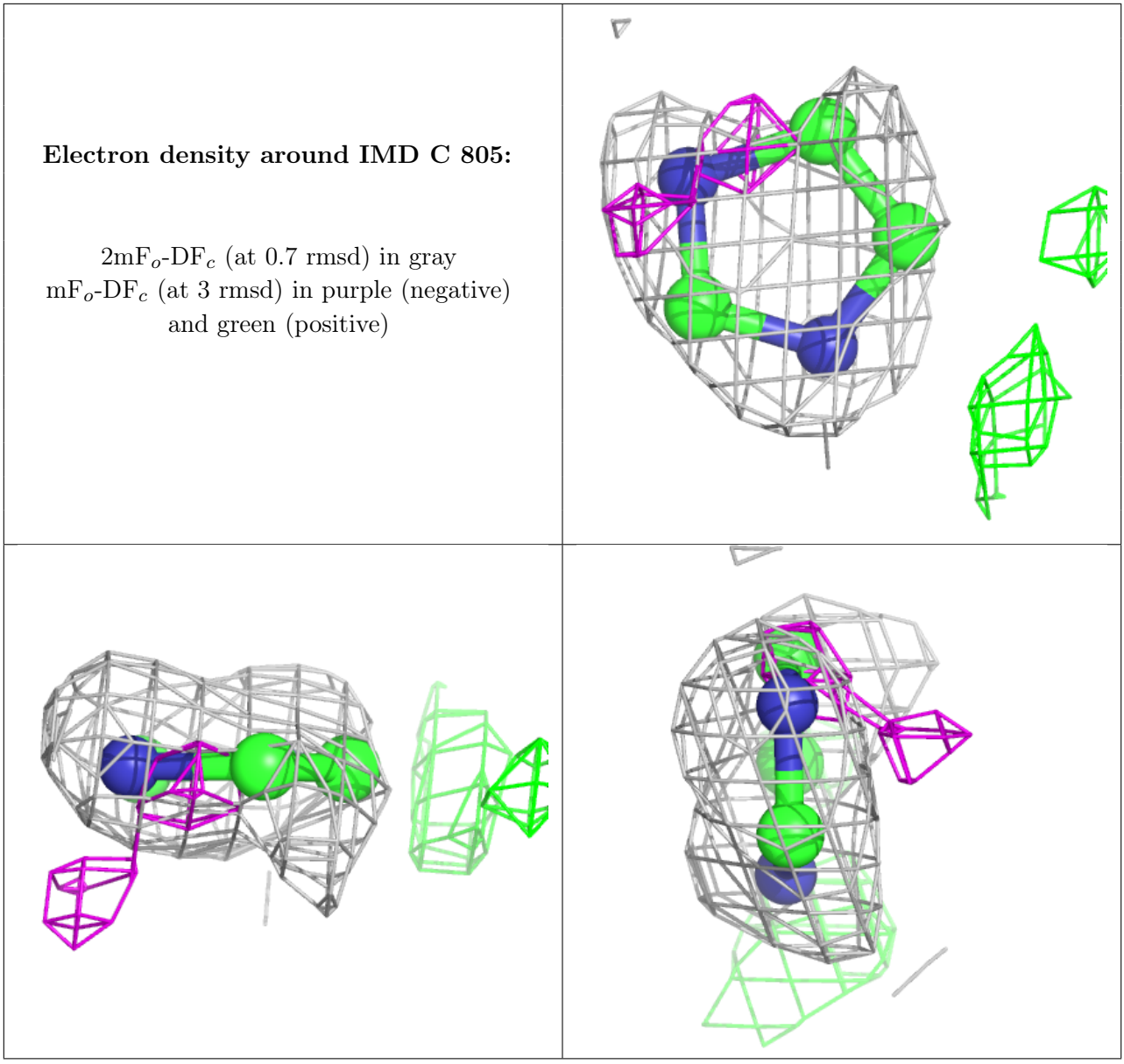
Electron density around GOL C 807:

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



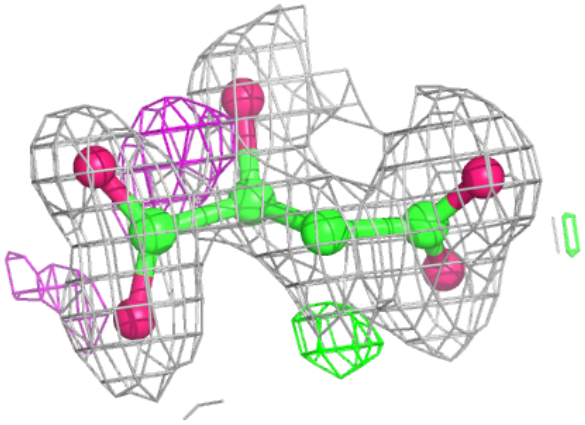
Electron density around IMD C 805:

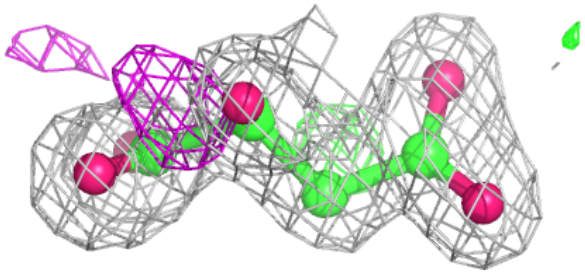
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

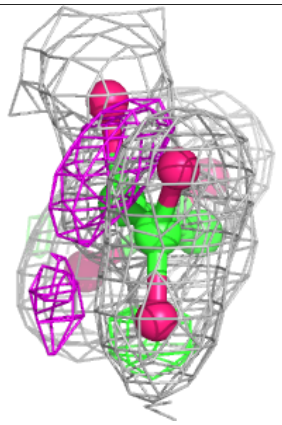


Electron density around LMR F 708:

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

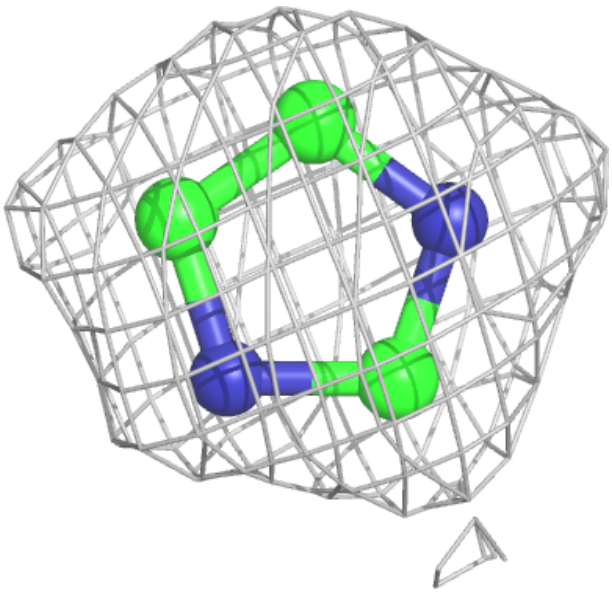


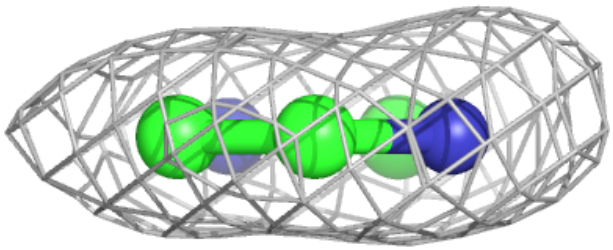


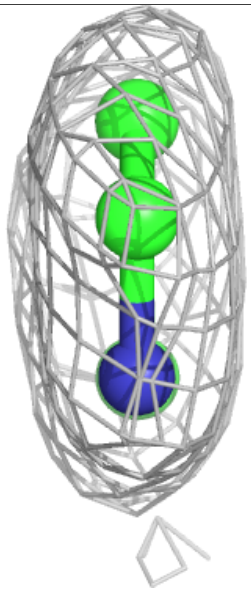


Electron density around IMD F 703:

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

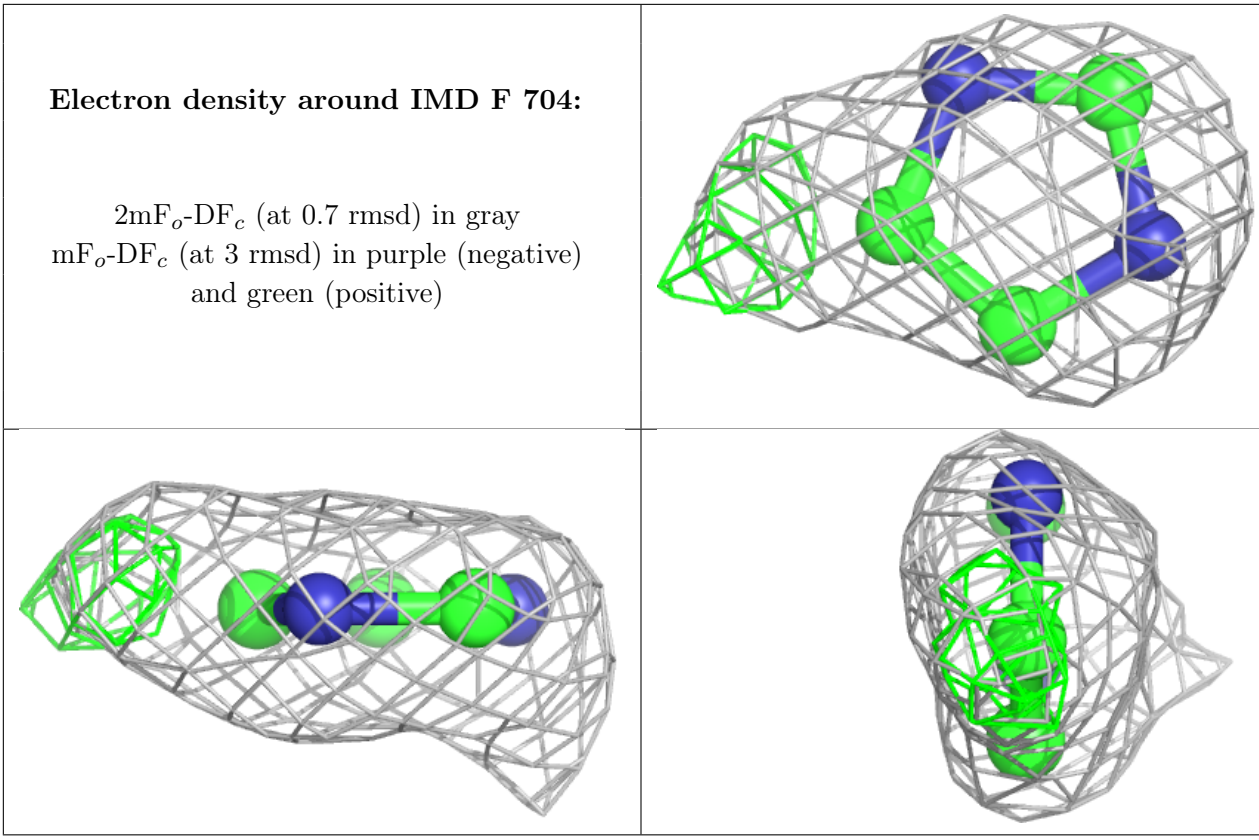






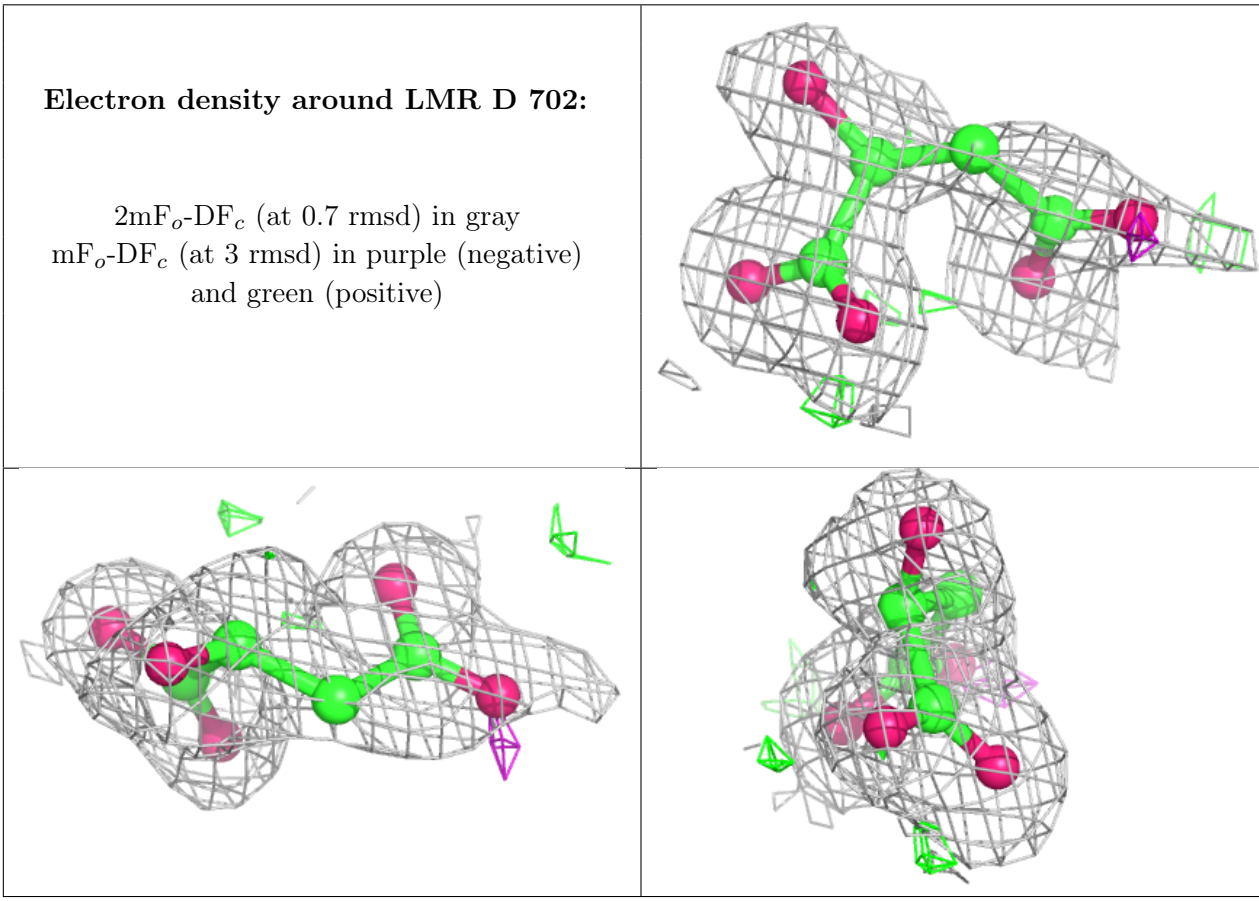
Electron density around IMD F 704:

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



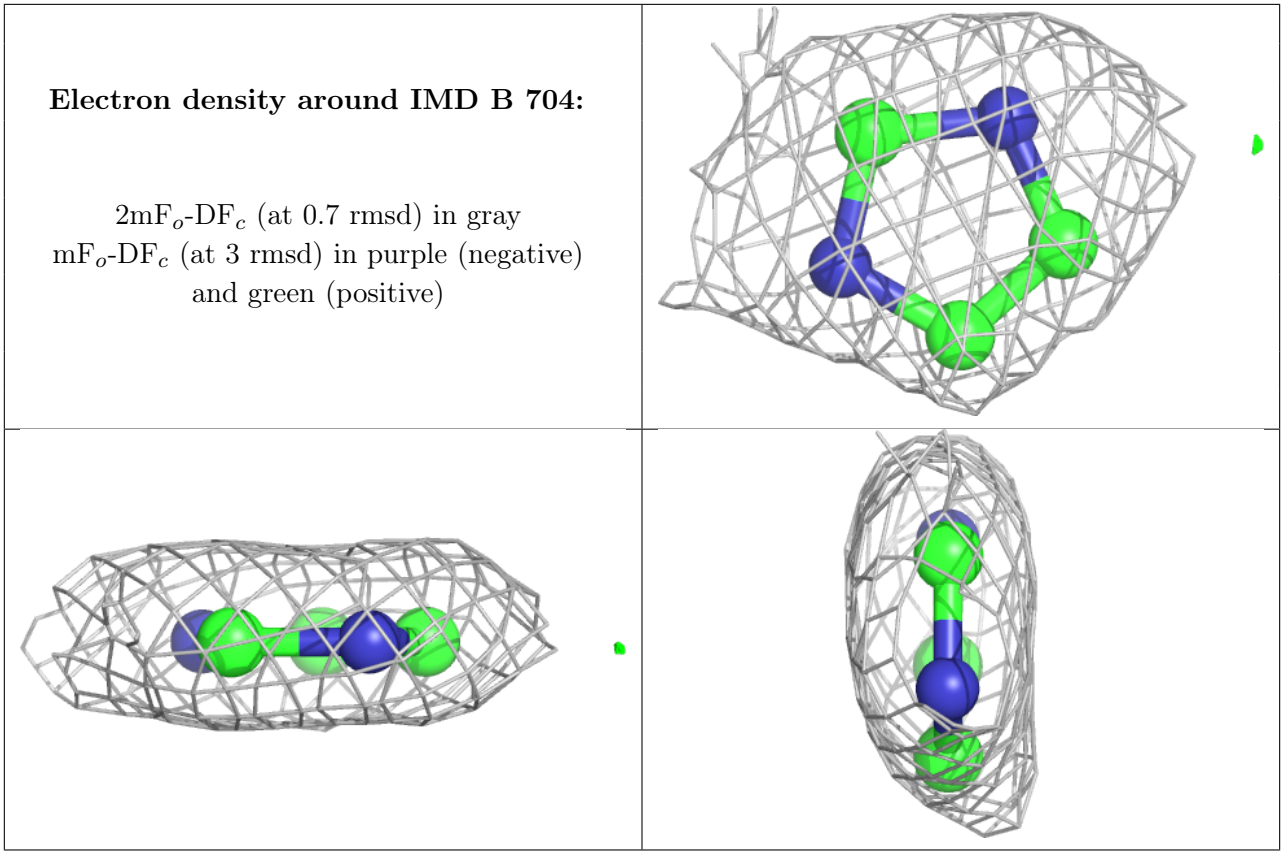
Electron density around LMR D 702:

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



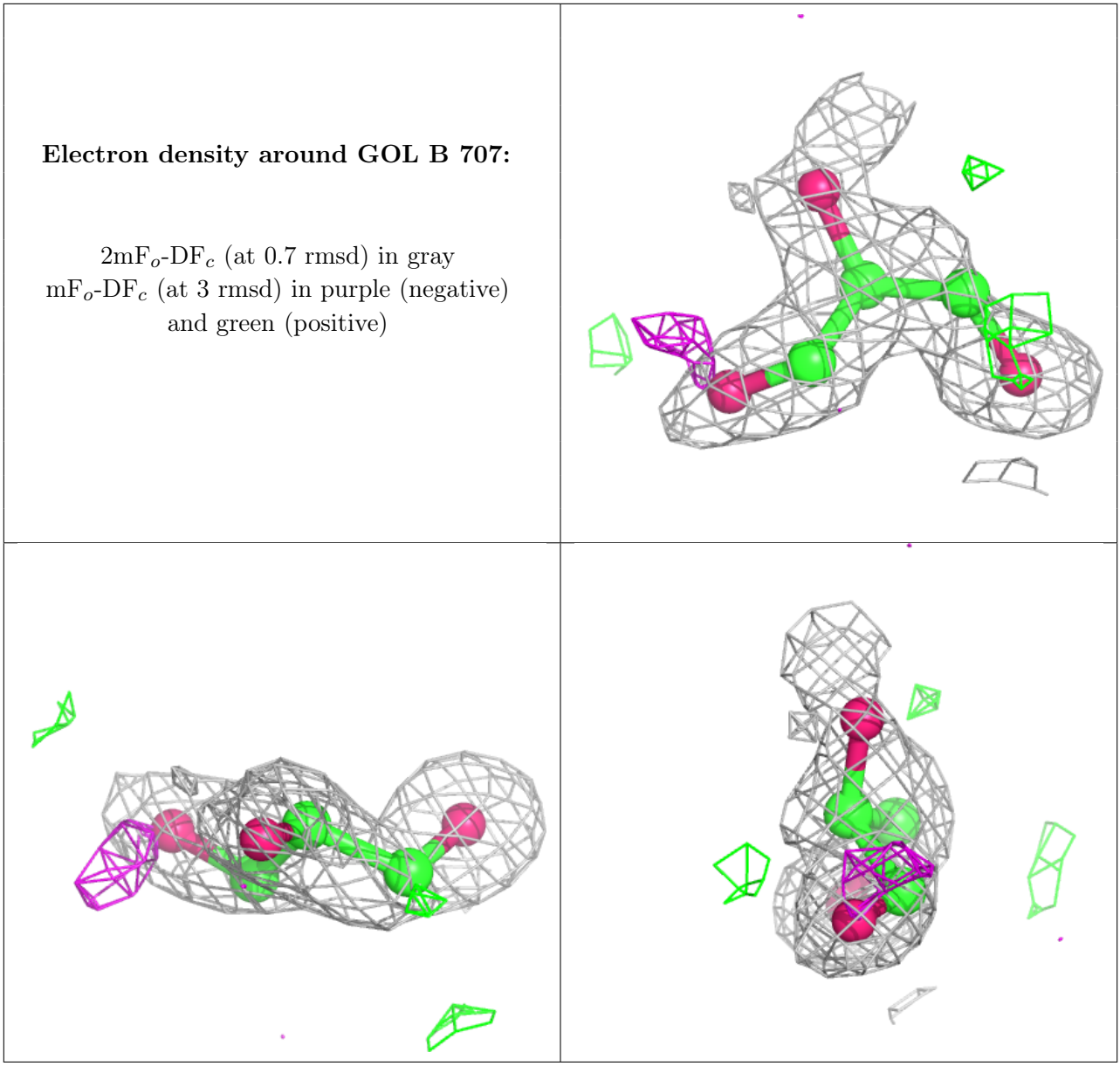
Electron density around IMD B 704:

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



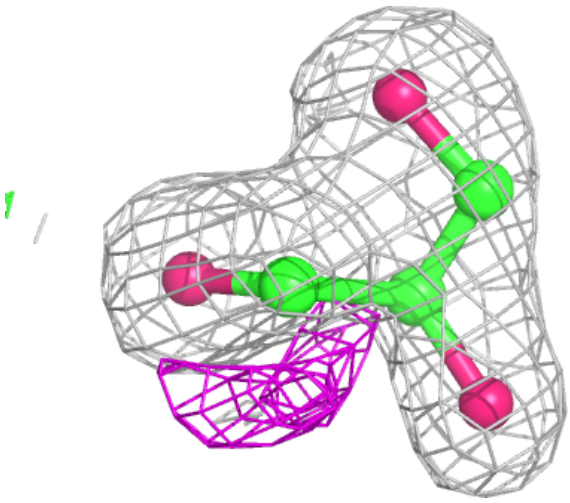
Electron density around GOL B 707:

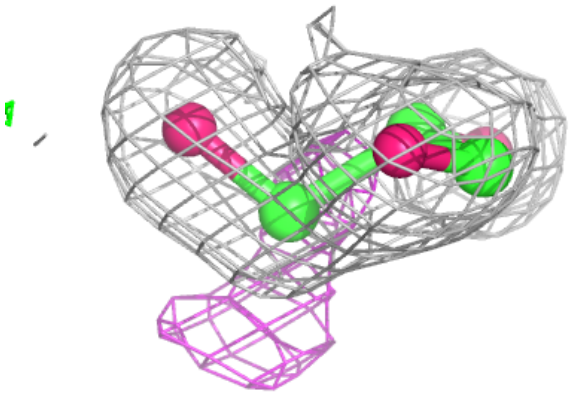
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

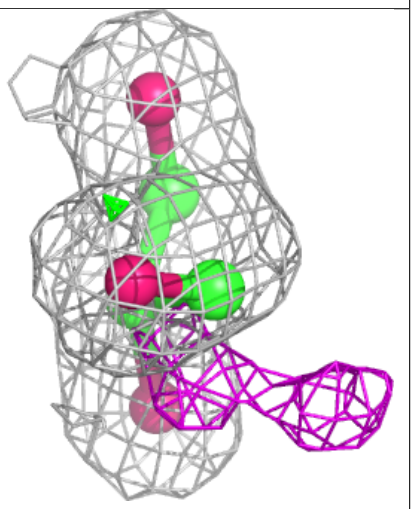


Electron density around GOL F 706:

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

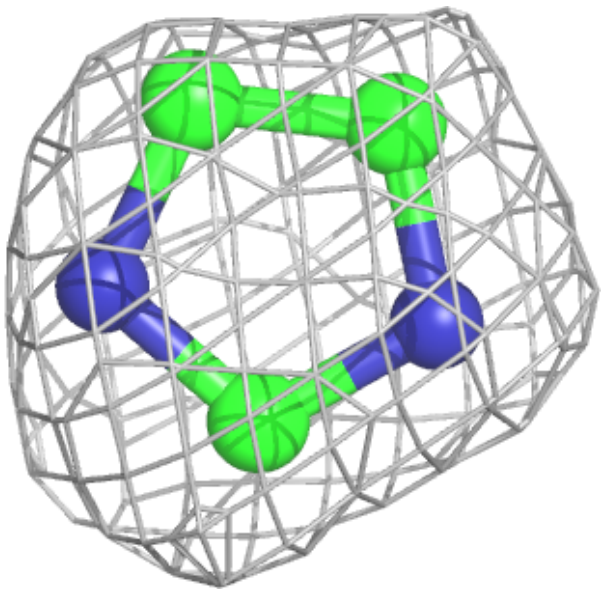


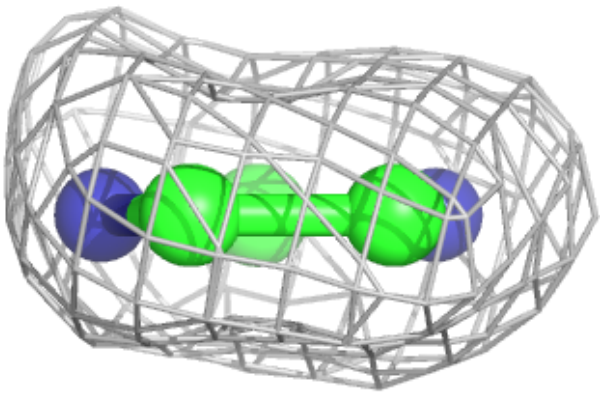


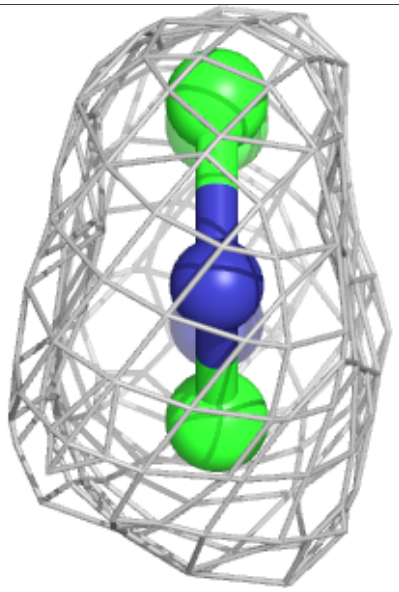


Electron density around IMD D 701:

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

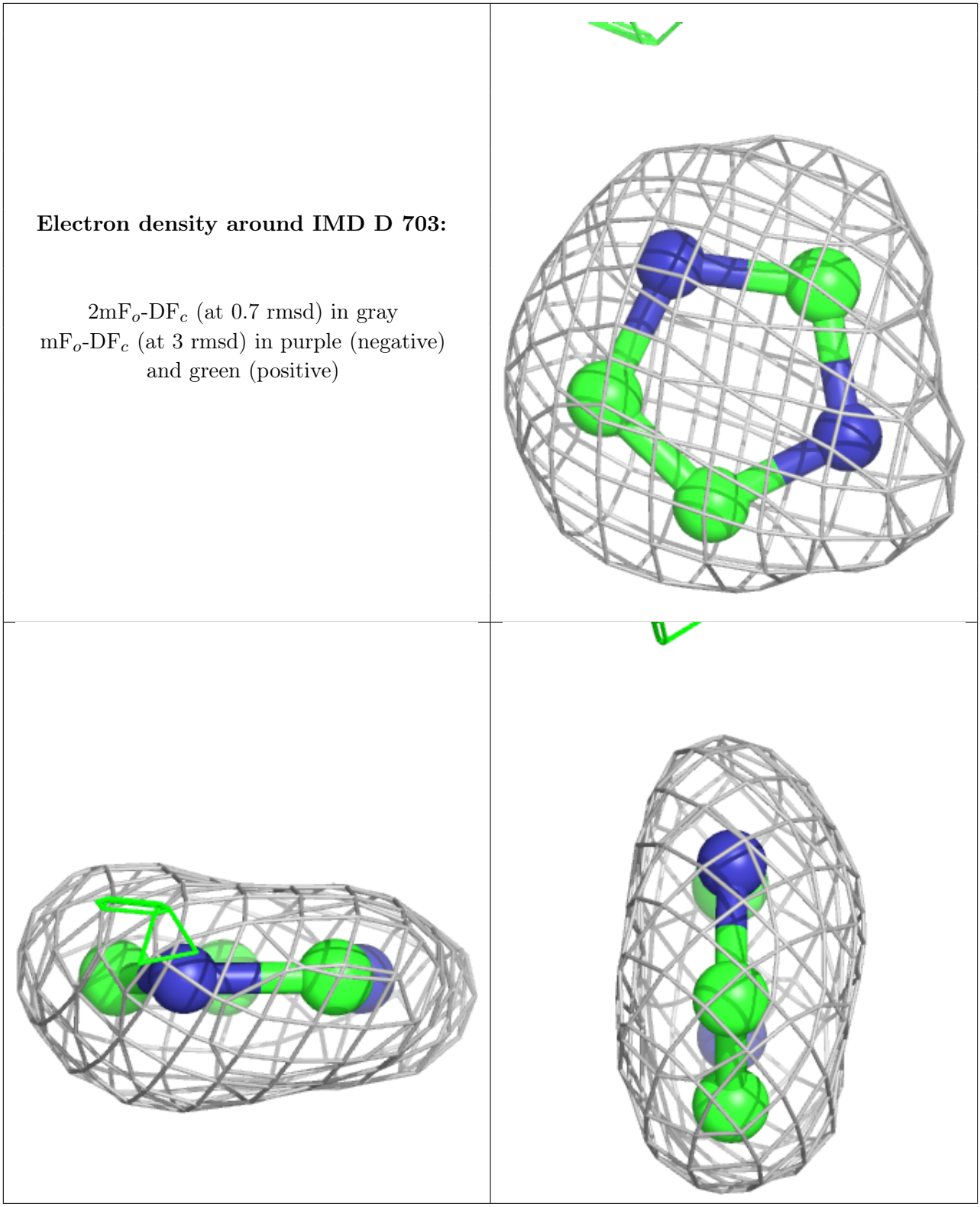






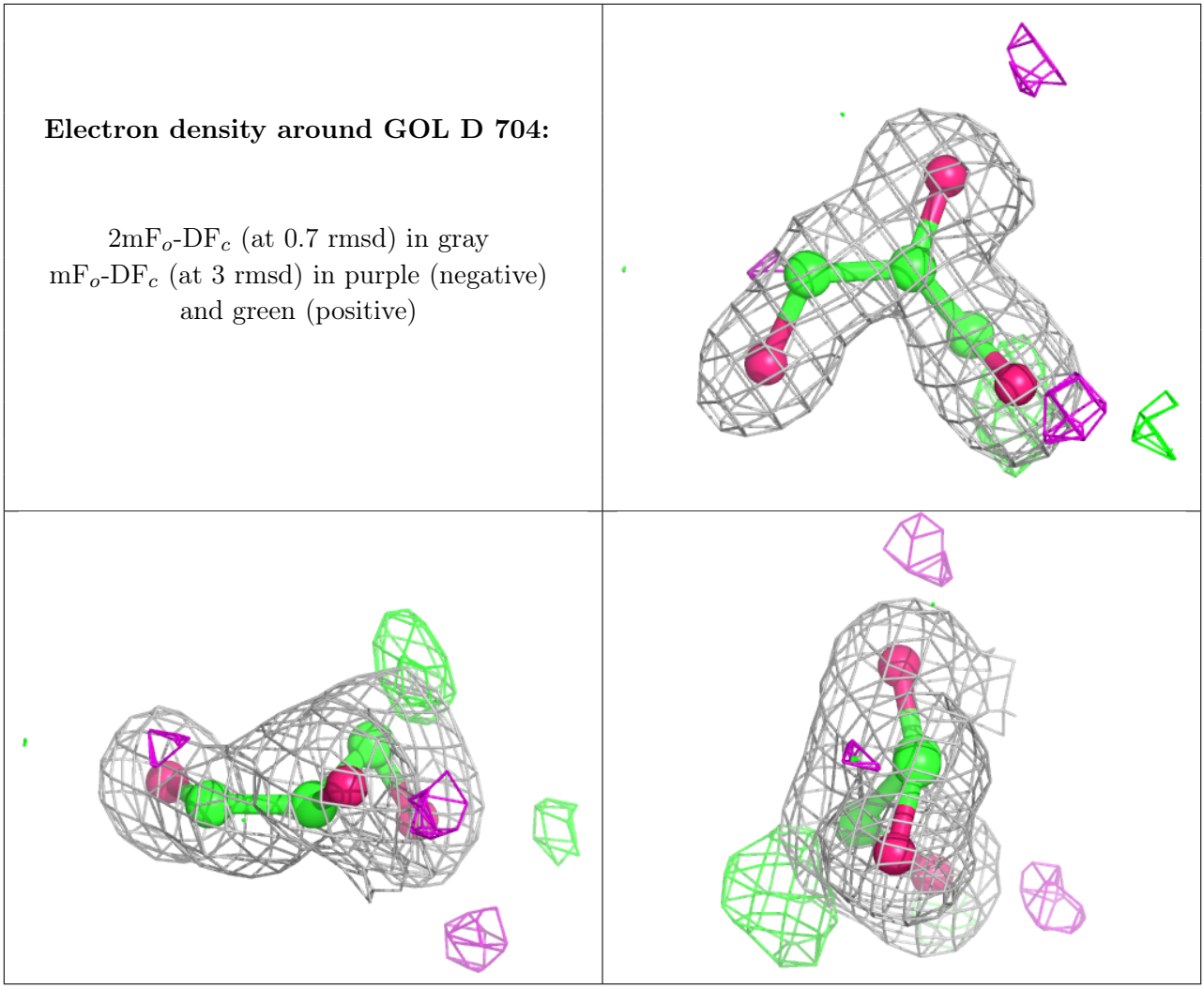
Electron density around IMD D 703:

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



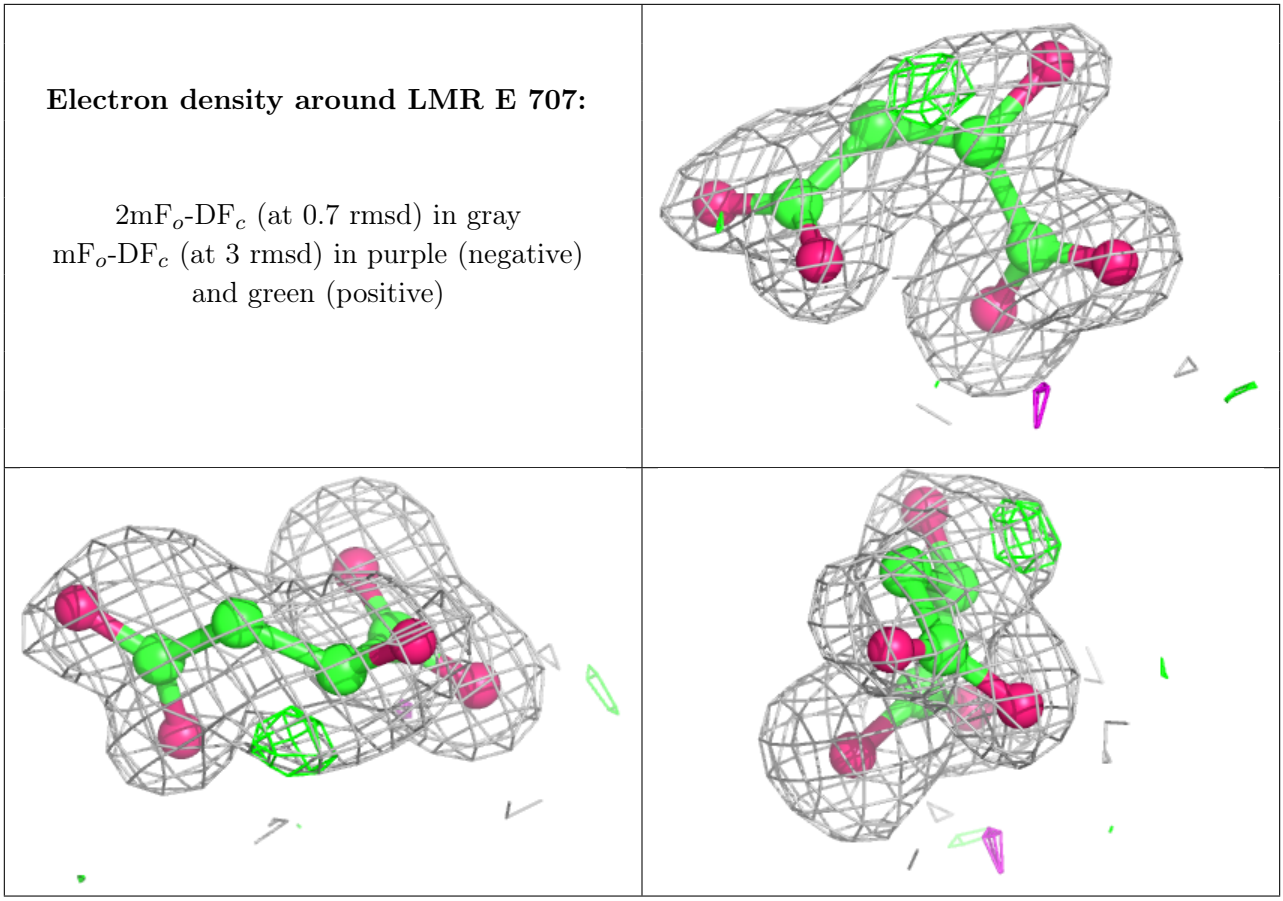
Electron density around GOL D 704:

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



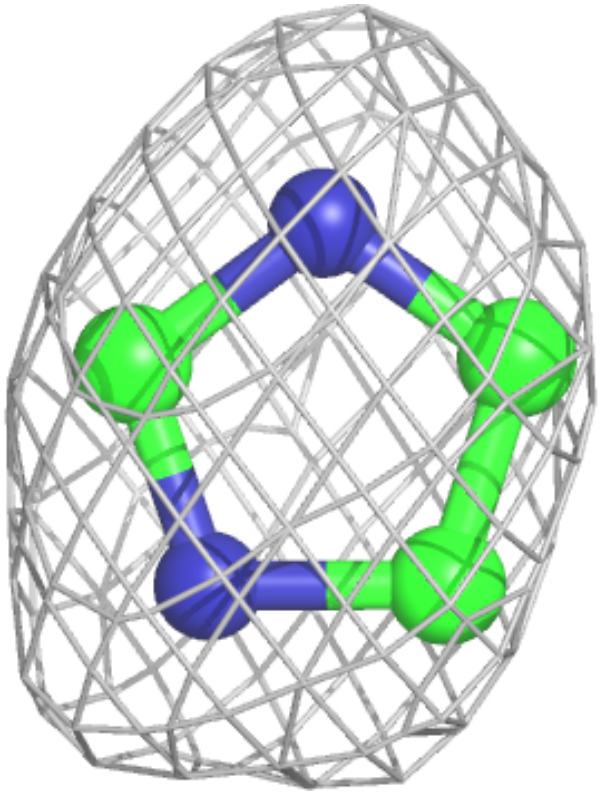
Electron density around LMR E 707:

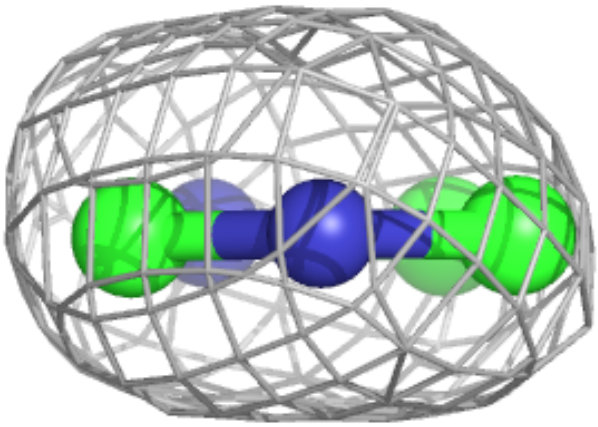
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

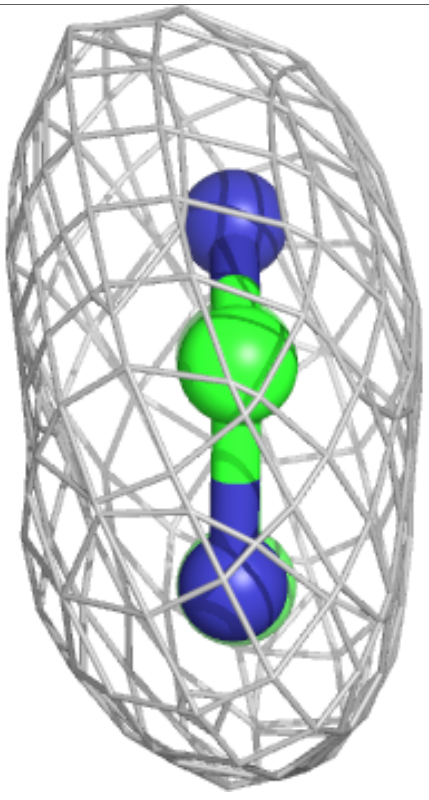


Electron density around IMD A 805:

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

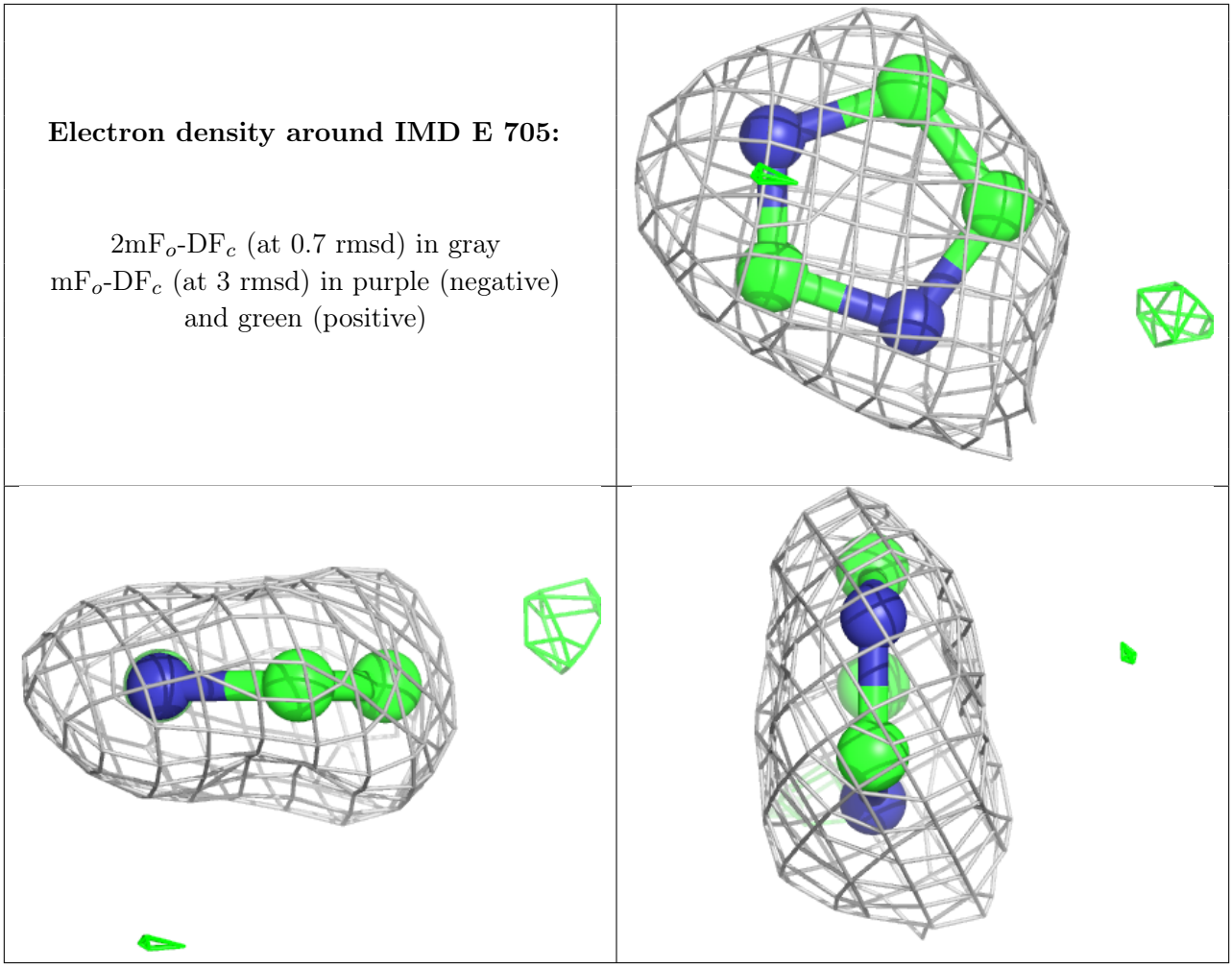






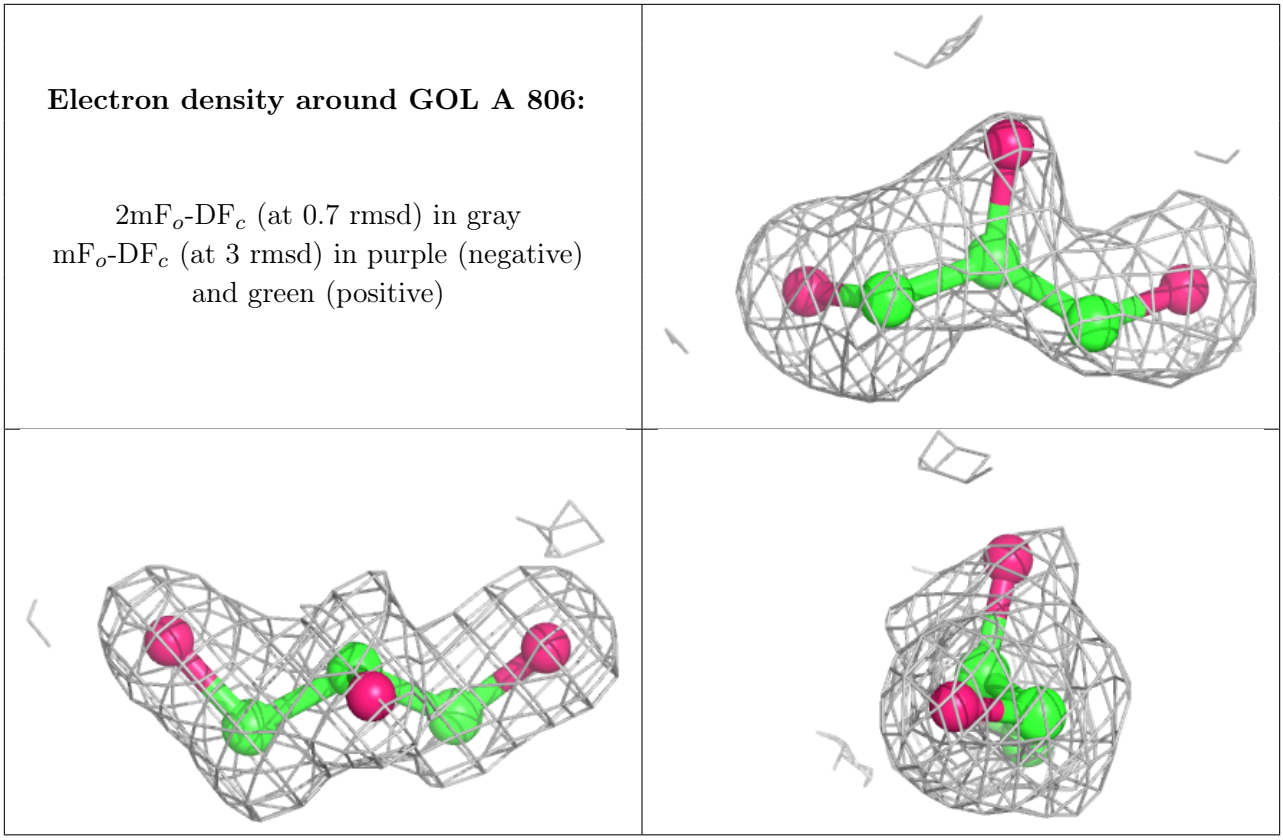
Electron density around IMD E 705:

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



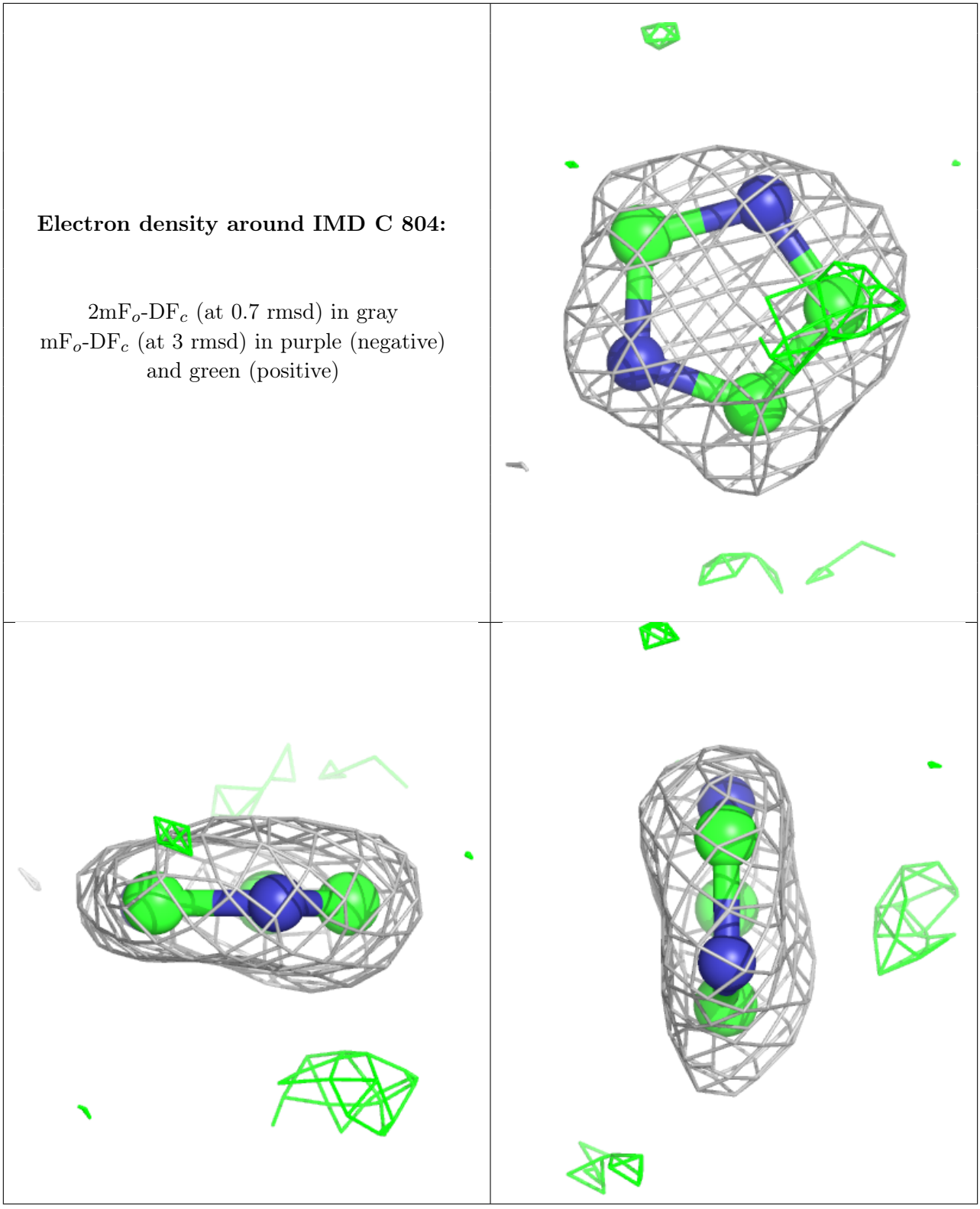
Electron density around GOL A 806:

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



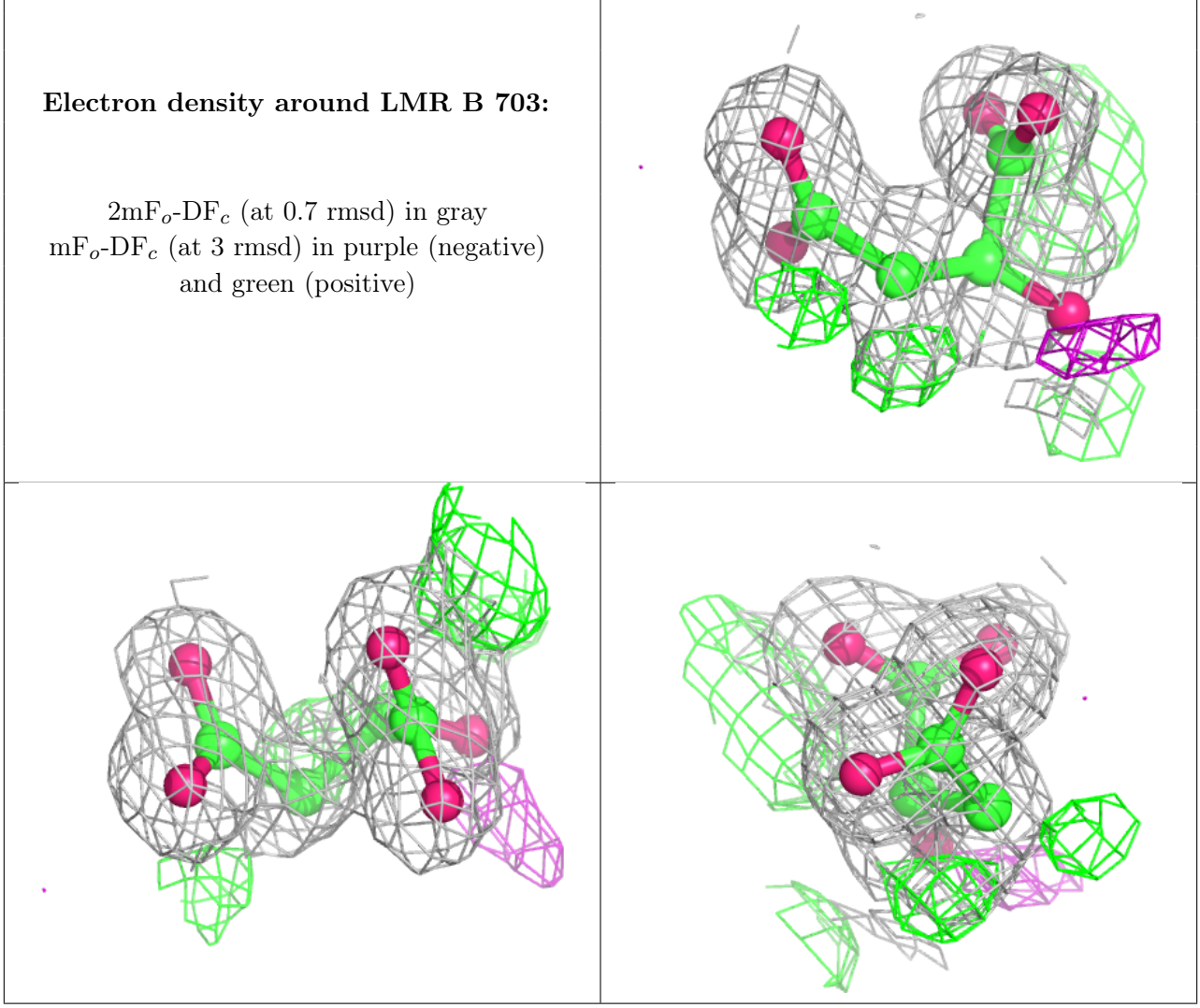
Electron density around IMD C 804:

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



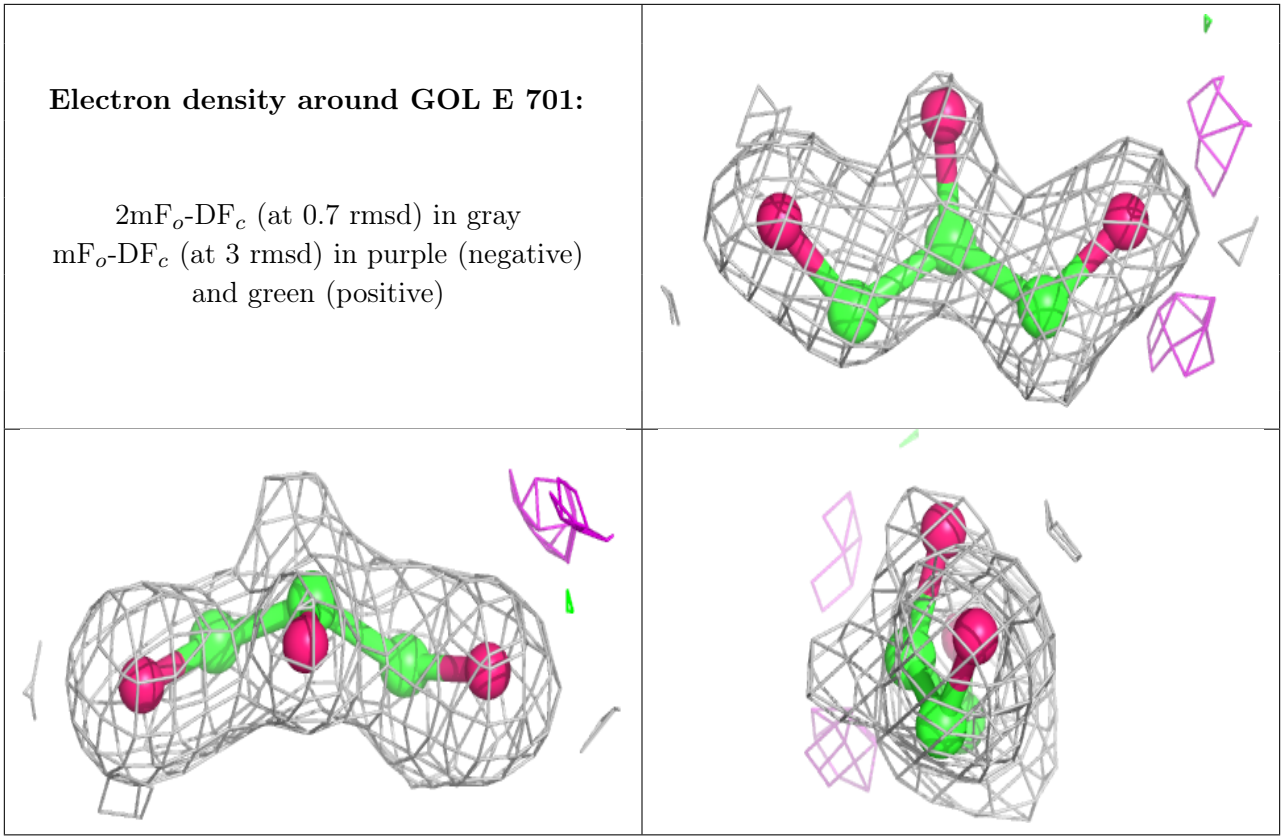
Electron density around LMR B 703:

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



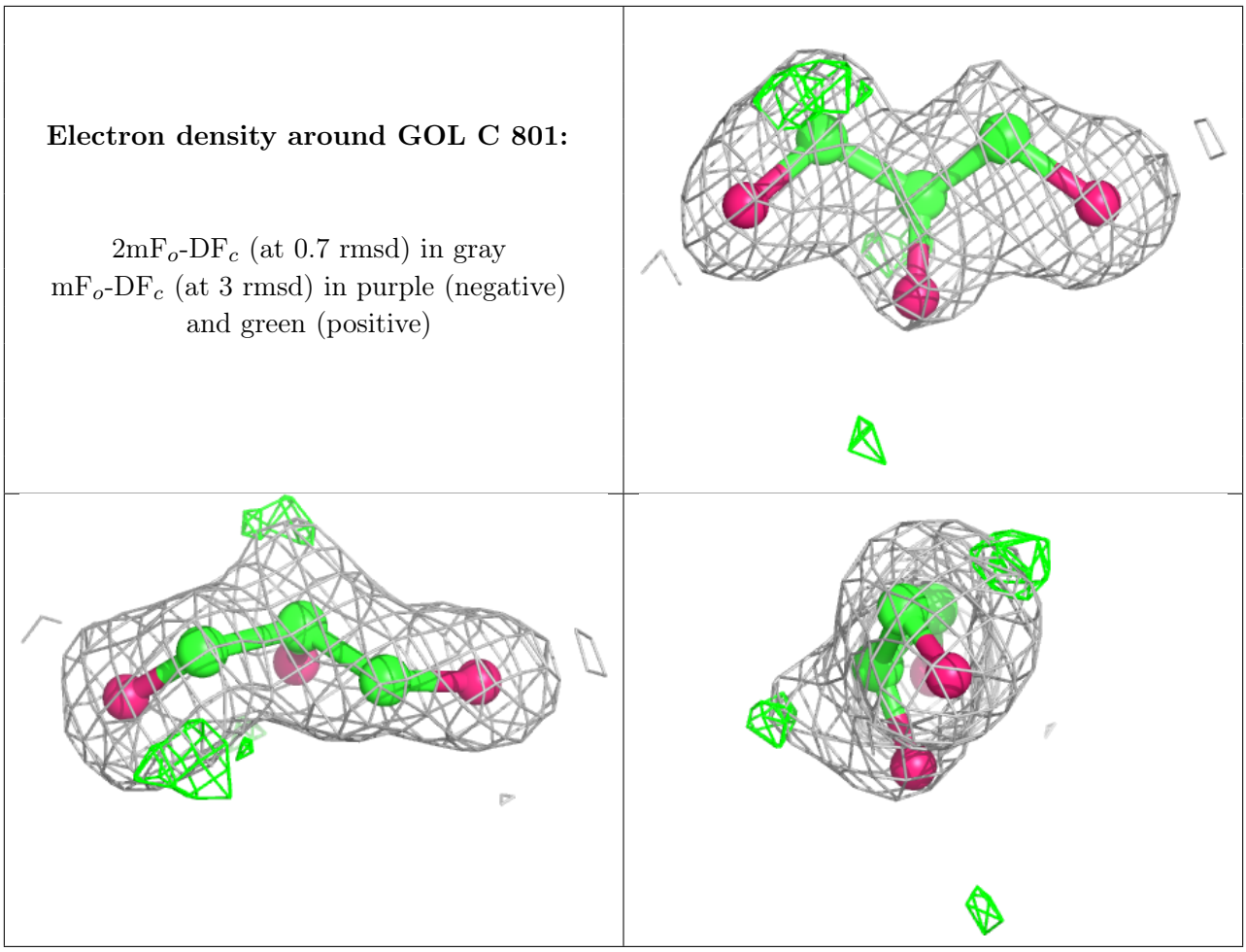
Electron density around GOL E 701:

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



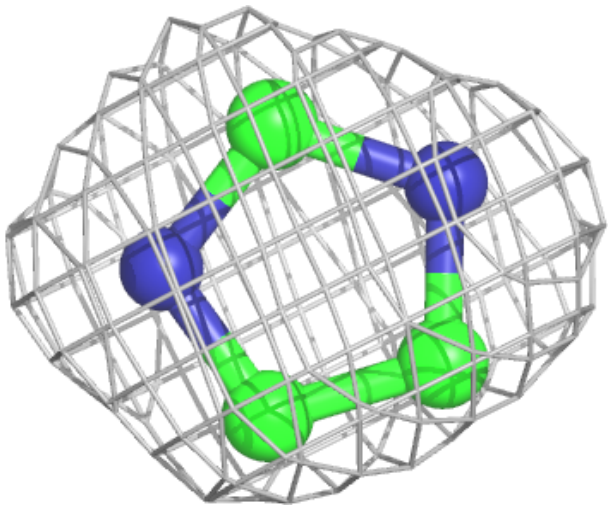
Electron density around GOL C 801:

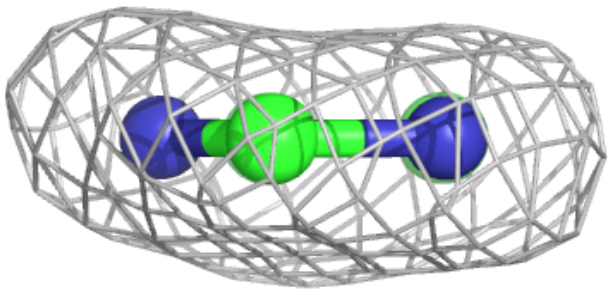
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

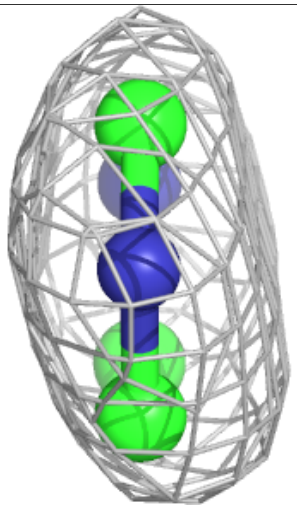


Electron density around IMD C 808:

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

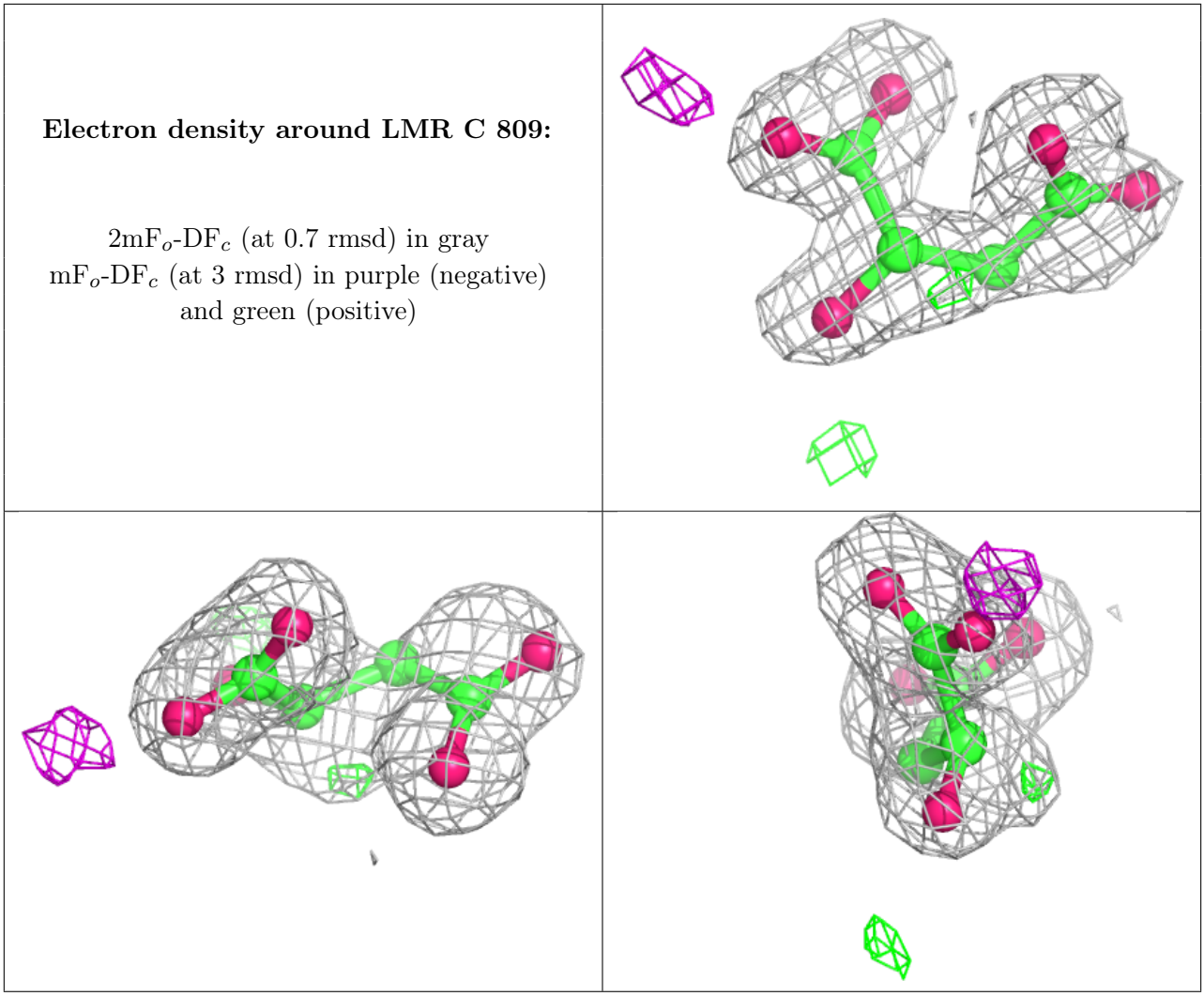






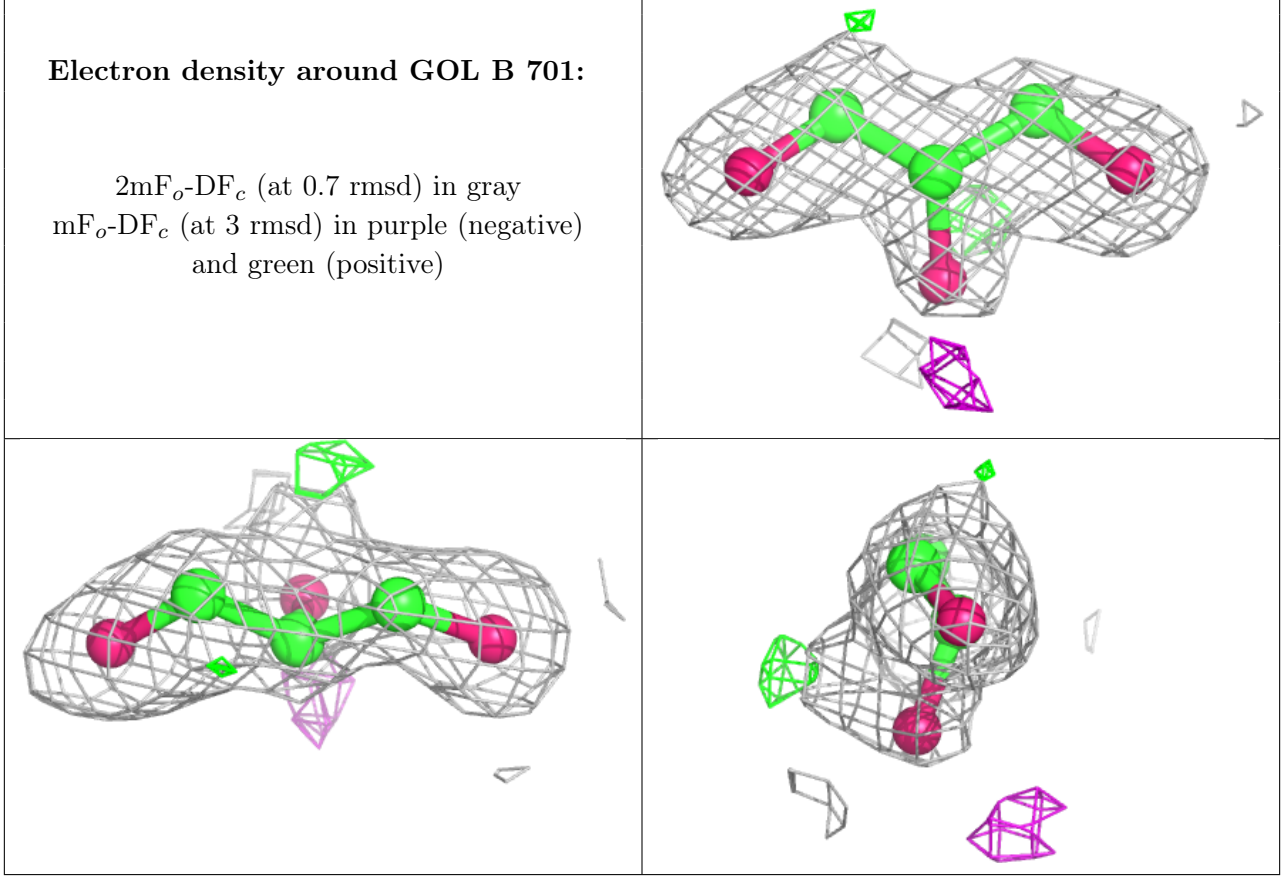
Electron density around LMR C 809:

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



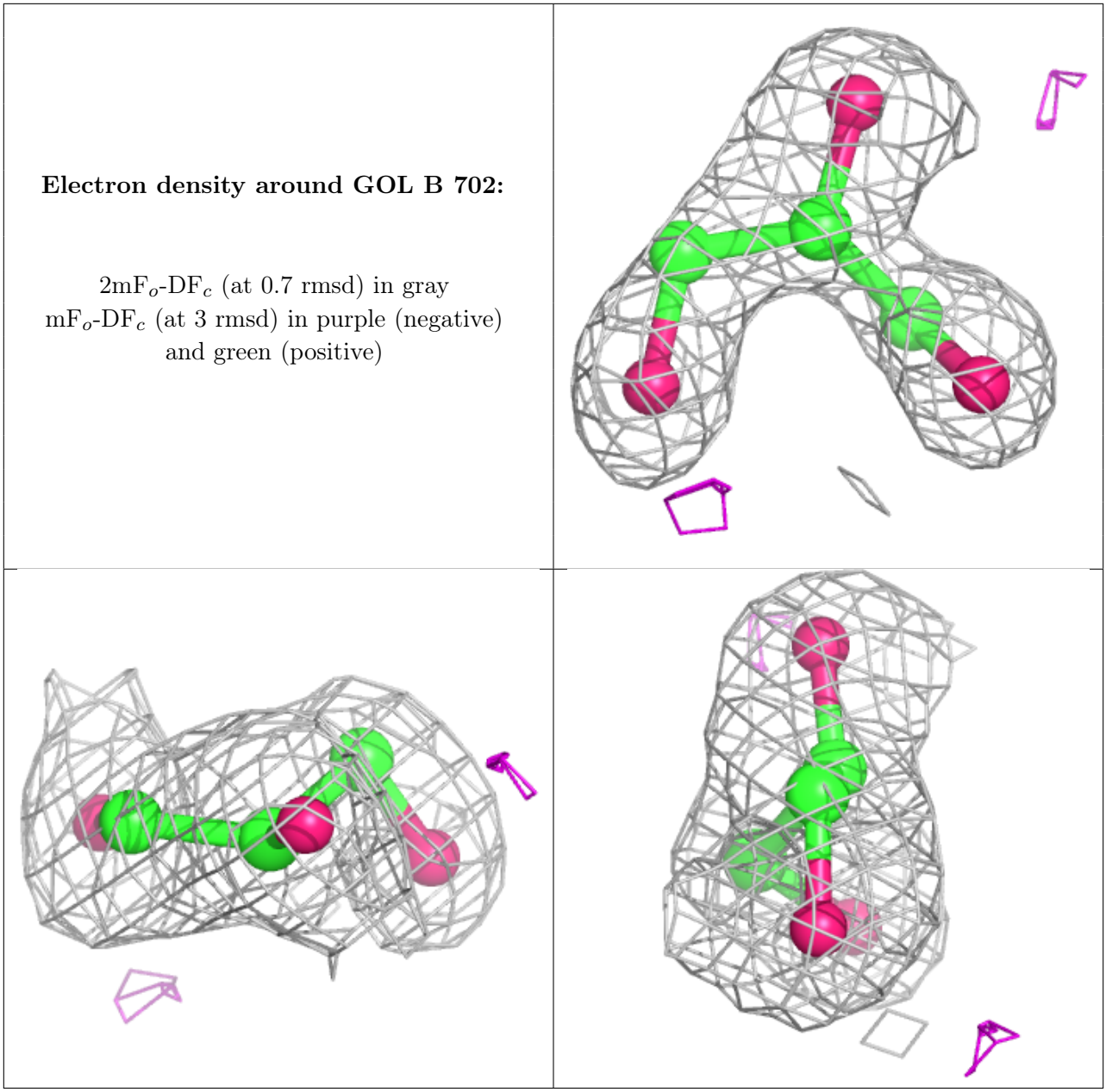
Electron density around GOL B 701:

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



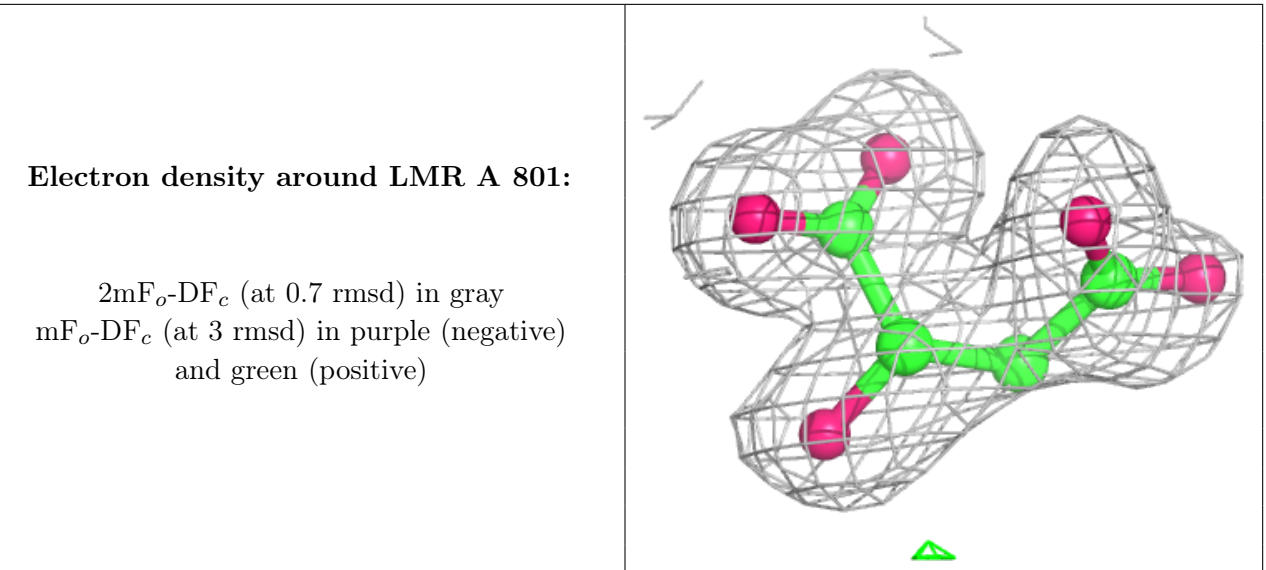
Electron density around GOL B 702:

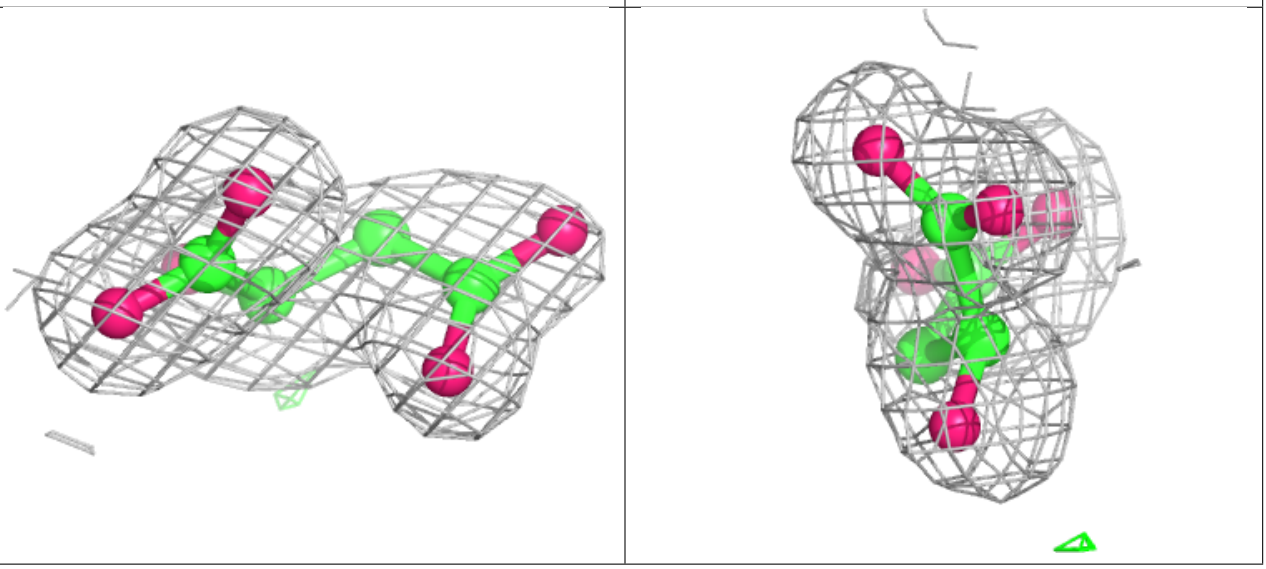
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMR A 801:

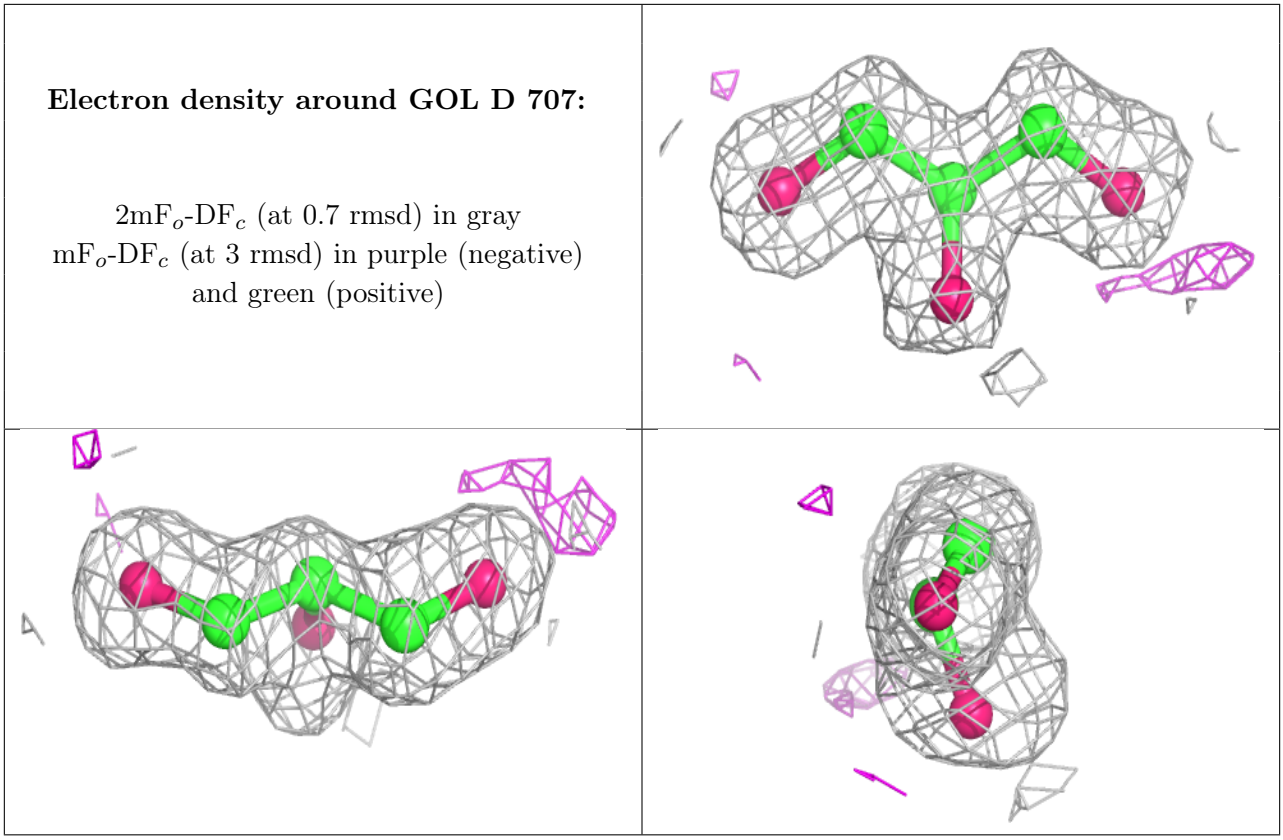
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





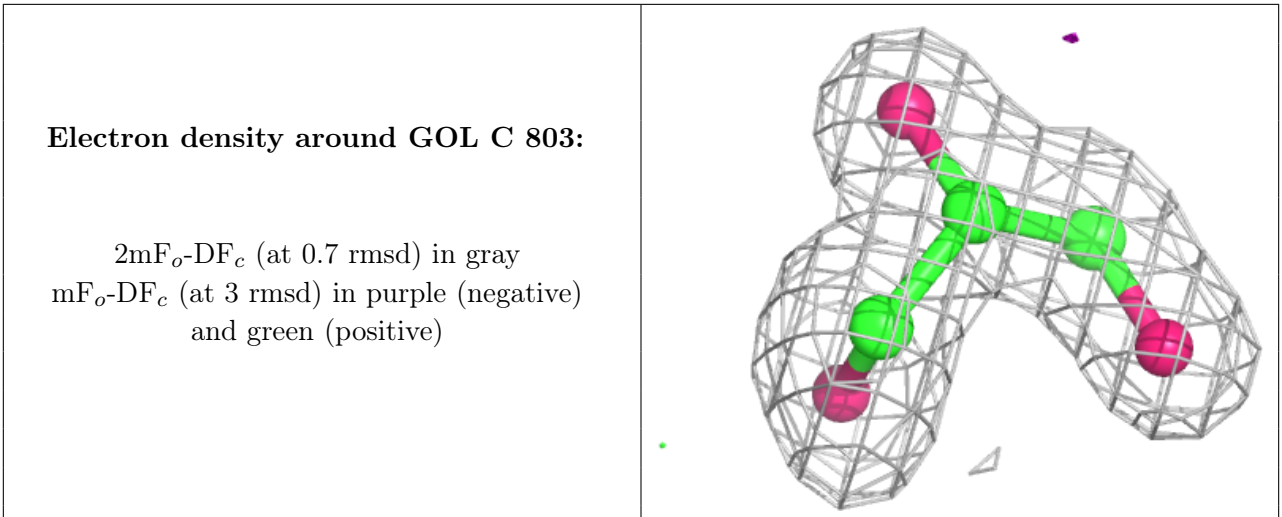
Electron density around GOL D 707:

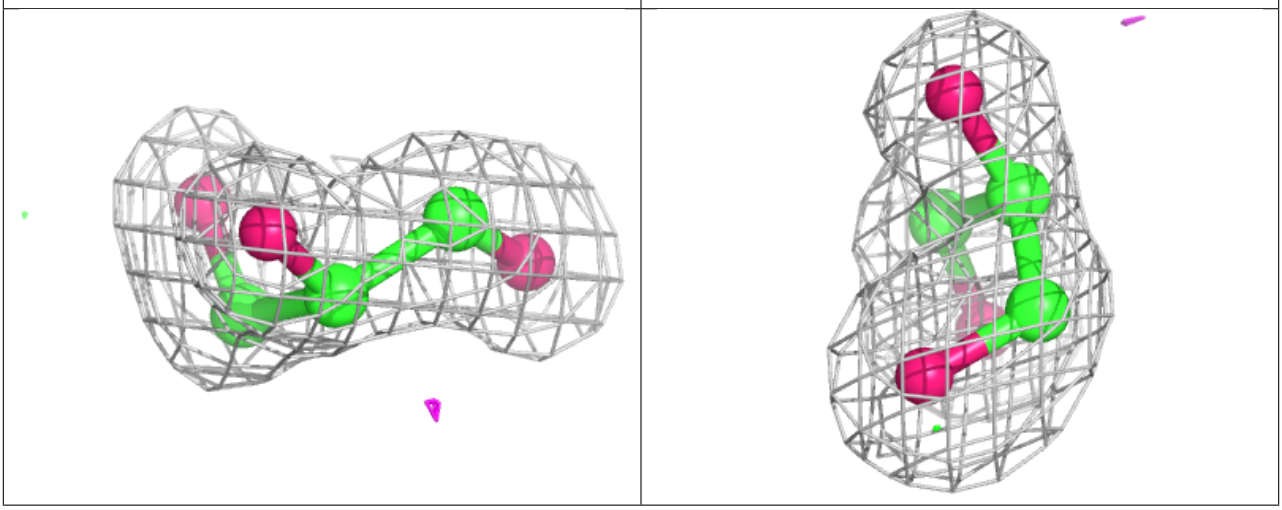
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around GOL C 803:

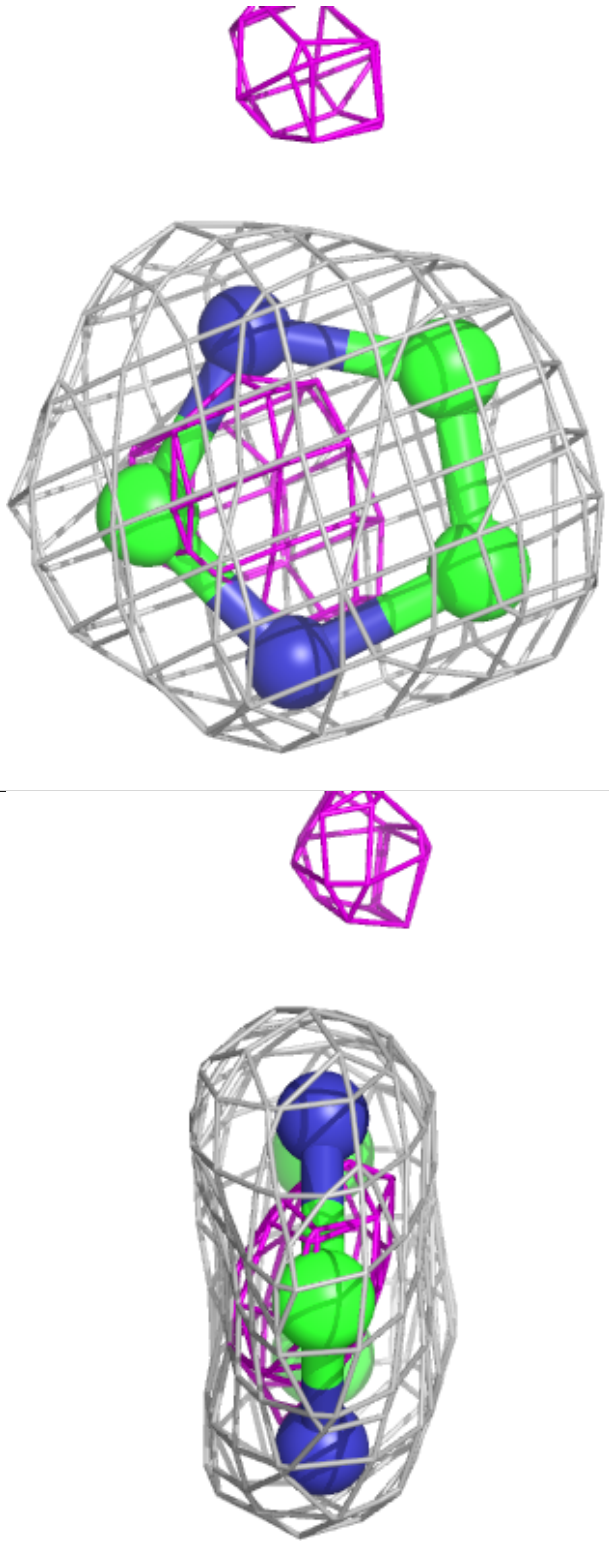
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





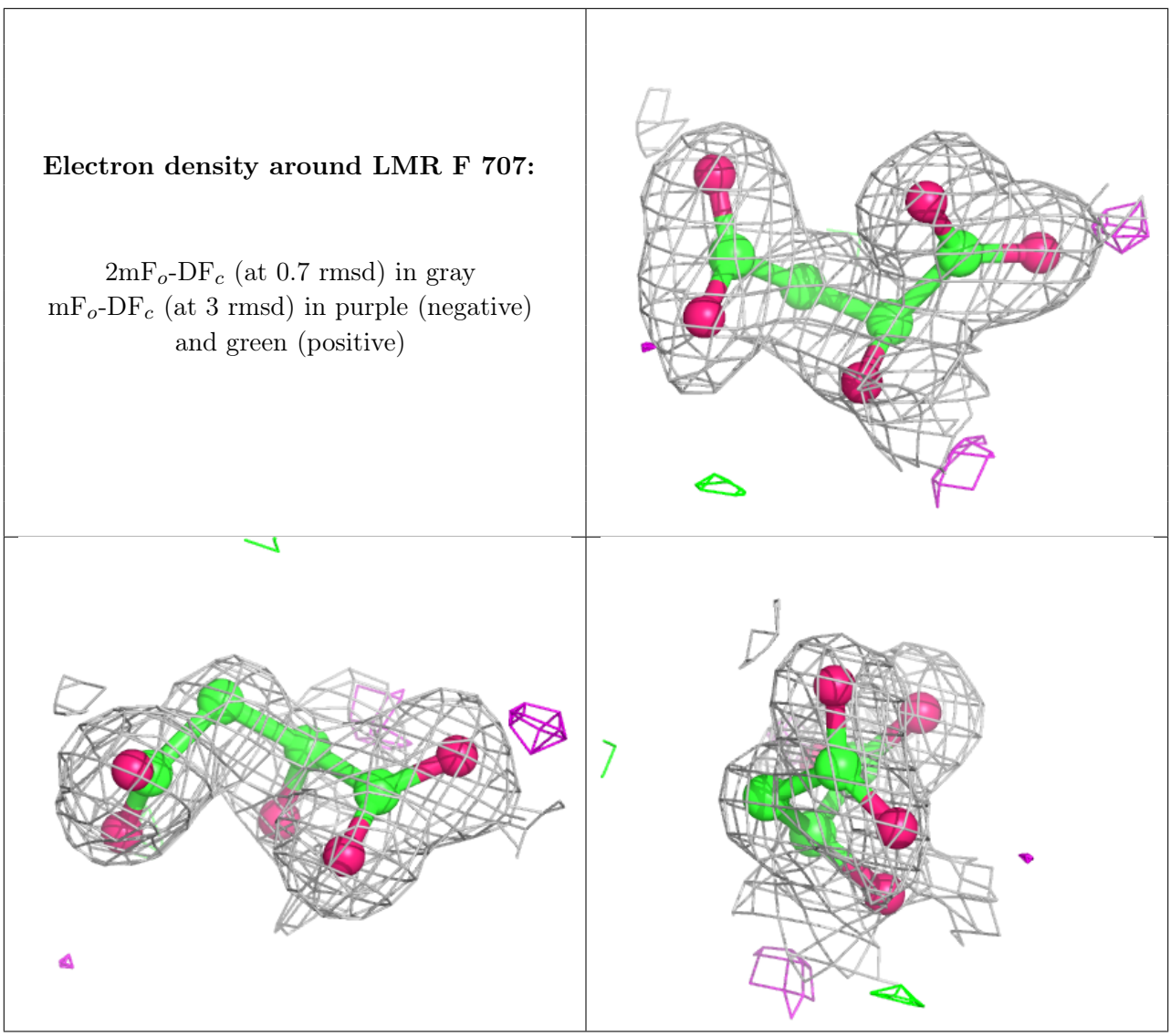
Electron density around IMD E 702:

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



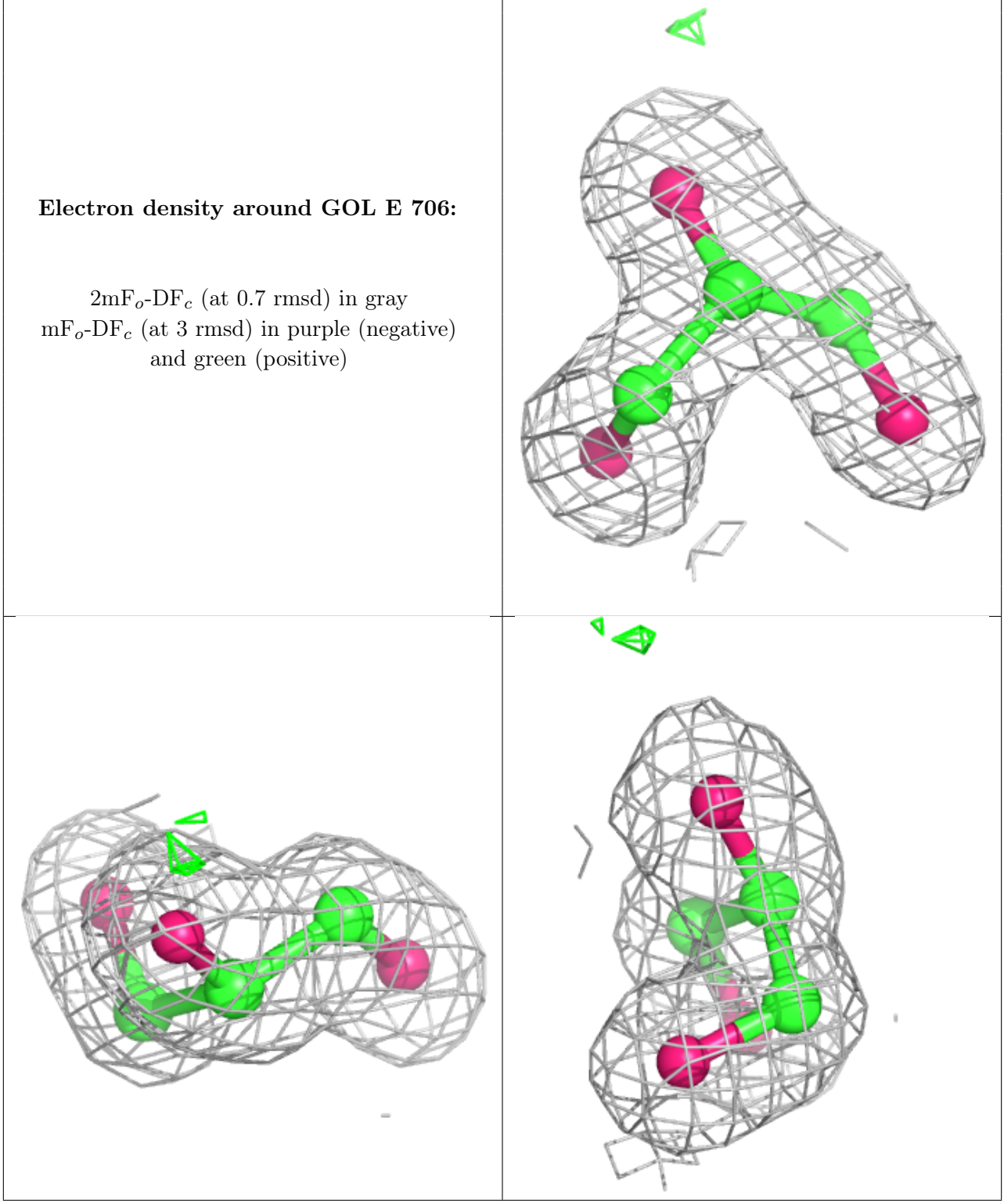
Electron density around LMR F 707:

$2mF_o$-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 706:

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



6.5 Other polymers (i)

There are no such residues in this entry.