



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:27 AM UTC

PDB ID : 7W1C / pdb_00007w1c
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 types of validation reports are described at

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

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

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

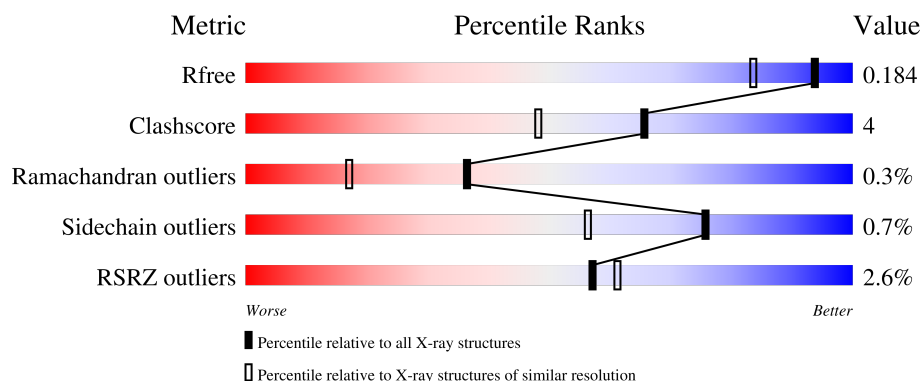
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.48 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}	180053	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	671	2% 89% 6% .
1	B	671	4% 86% 8% 6%
1	C	671	3% 88% 6% . 5%
1	D	671	2% 84% 8% 7%
1	E	671	0% 88% 8% .

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Mol	Chain	Length	Quality of chain
1	F	671	

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	A	801	-	X	-	-
2	LMR	B	703	-	X	-	-
2	LMR	D	702	-	X	-	-
2	LMR	E	707	-	X	-	-
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	D	705	-	X	-	-
4	GOL	E	703	-	X	-	-
4	GOL	F	702	-	X	-	-

2 Entry composition

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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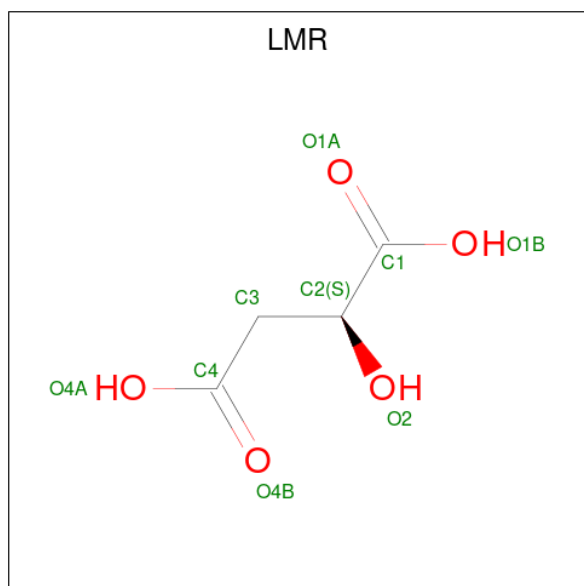
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E	-14	HIS	-	expression tag	UNP A0A068Q5Q5
E	-13	HIS	-	expression tag	UNP A0A068Q5Q5
E	-12	HIS	-	expression tag	UNP A0A068Q5Q5
E	-11	HIS	-	expression tag	UNP A0A068Q5Q5
E	-10	HIS	-	expression tag	UNP A0A068Q5Q5
E	-9	SER	-	expression tag	UNP A0A068Q5Q5
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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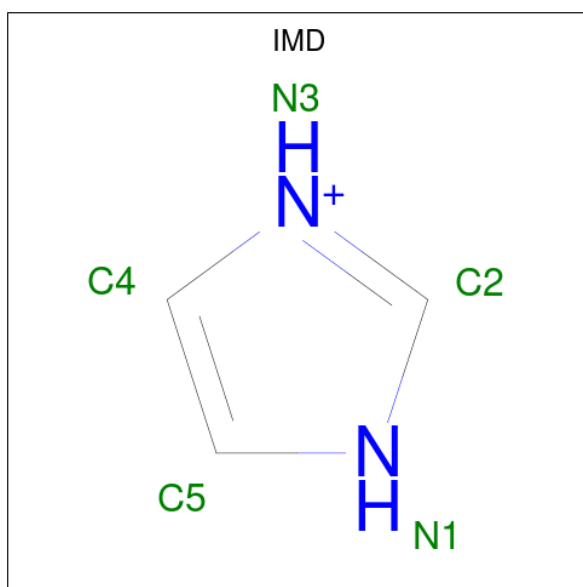
Chain	Residue	Modelled	Actual	Comment	Reference
F	392	ALA	ASP	engineered mutation	UNP A0A068Q5Q5

- Molecule 2 is (2S)-2-hydroxybutanedioic acid (CCD ID: 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 (CCD ID: IMD) (formula: $C_3H_5N_2$) (labeled as "Ligand of Interest" by depositor).



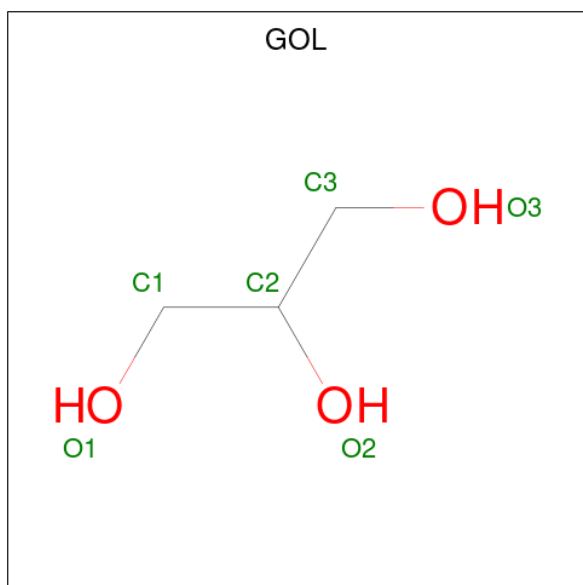
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		
3	A	1	Total	C	N	0	0
			5	3	2		
3	A	1	Total	C	N	0	0
			5	3	2		
3	B	1	Total	C	N	0	0
			5	3	2		
3	B	1	Total	C	N	0	0
			5	3	2		
3	B	1	Total	C	N	0	0
			5	3	2		
3	B	1	Total	C	N	0	0
			5	3	2		
3	C	1	Total	C	N	0	0
			5	3	2		
3	C	1	Total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

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

- Molecule 4 is GLYCEROL (CCD ID: 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	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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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

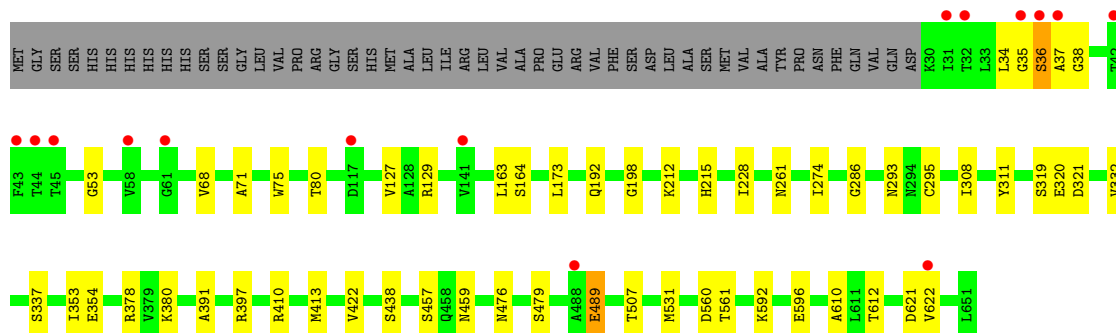
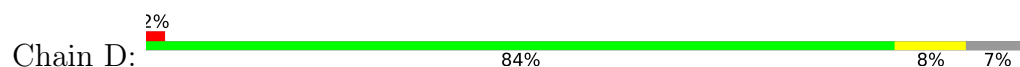
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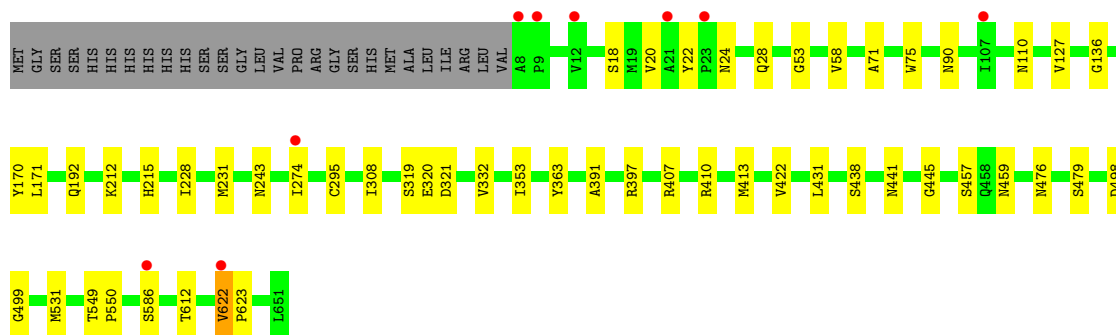
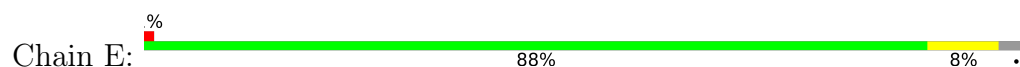
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	722	Total 722	O 722	0	0
5	E	728	Total 728	O 728	0	0
5	F	713	Total 713	O 713	0	0



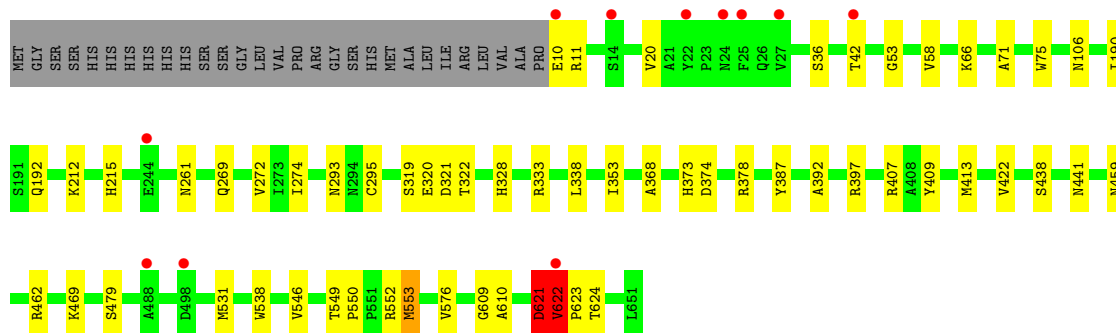
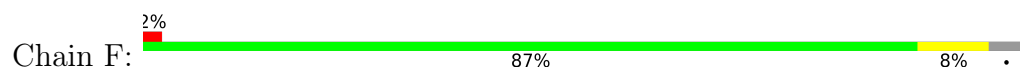
• Molecule 1: K1 LYASE



• Molecule 1: K1 LYASE



• Molecule 1: K1 LYASE



4 Data and refinement statistics

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 30.00 – 1.48	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.00-1.48) 96.8 (30.00-1.48)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.137 , 0.184 0.137 , 0.184	Depositor DCC
R_{free} test set	32922 reflections (4.86%)	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)	0.37 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.10	2/4976 (0.0%)	0.94	2/6774 (0.0%)
1	B	1.12	5/4896 (0.1%)	1.00	6/6666 (0.1%)
1	C	1.11	6/4959 (0.1%)	0.99	7/6752 (0.1%)
1	D	1.12	5/4796 (0.1%)	0.95	3/6529 (0.0%)
1	E	1.12	2/4981 (0.0%)	0.94	1/6782 (0.0%)
1	F	1.17	8/4982 (0.2%)	0.99	8/6782 (0.1%)
All	All	1.12	28/29590 (0.1%)	0.97	27/40285 (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 (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	413	MET	CA-C	6.82	1.55	1.52
1	B	38	GLY	CA-C	6.81	1.61	1.51
1	B	56	PHE	CA-C	6.32	1.60	1.52
1	C	42	THR	N-CA	6.29	1.53	1.45
1	F	609	GLY	C-O	-6.14	1.16	1.23
1	F	462	ARG	CD-NE	-6.01	1.37	1.46
1	D	198	GLY	N-CA	5.87	1.51	1.45
1	F	106	ASN	CG-ND2	-5.76	1.21	1.33
1	B	507	THR	CA-C	5.76	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	322	THR	CA-CB	5.67	1.62	1.53
1	F	576	VAL	C-O	-5.41	1.18	1.24
1	F	36	SER	C-O	5.41	1.30	1.24
1	B	50	VAL	CA-C	5.39	1.59	1.52
1	E	531	MET	SD-CE	-5.38	1.66	1.79
1	A	54	THR	CA-C	5.37	1.59	1.52
1	A	54	THR	CB-CG2	-5.36	1.34	1.52
1	B	507	THR	CA-CB	5.36	1.61	1.52
1	D	622	VAL	CA-C	5.28	1.57	1.52
1	C	117	ASP	N-CA	5.22	1.52	1.46
1	F	462	ARG	CZ-NH2	-5.19	1.26	1.33
1	F	462	ARG	NE-CZ	5.19	1.38	1.33
1	C	117	ASP	C-O	5.15	1.30	1.24
1	F	322	THR	CB-OG1	-5.14	1.35	1.43
1	D	507	THR	CB-OG1	5.13	1.51	1.43
1	C	198	GLY	N-CA	5.09	1.50	1.45
1	E	136	GLY	C-O	-5.09	1.19	1.24
1	D	173	LEU	CA-C	-5.08	1.46	1.52
1	D	228	ILE	N-CA	-5.04	1.42	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	17	ALA	N-CA-C	-14.35	91.37	112.04
1	F	553	MET	CG-SD-CE	-10.83	77.08	100.90
1	E	531	MET	CG-SD-CE	-10.21	78.44	100.90
1	C	553	MET	CG-SD-CE	-9.46	80.09	100.90
1	B	553	MET	CG-SD-CE	-7.81	83.72	100.90
1	F	531	MET	CG-SD-CE	-6.91	85.69	100.90
1	D	531	MET	CG-SD-CE	-6.80	85.94	100.90
1	F	622	VAL	CA-C-N	-6.67	111.51	119.84
1	F	622	VAL	C-N-CA	-6.67	111.51	119.84
1	F	621	ASP	O-C-N	6.35	130.62	122.81
1	B	58	VAL	CA-C-N	-6.24	113.33	119.76
1	B	58	VAL	C-N-CA	-6.24	113.33	119.76
1	C	58	VAL	CB-CA-C	6.00	116.38	109.89
1	C	531	MET	CG-SD-CE	-5.96	87.78	100.90
1	F	621	ASP	CA-C-N	5.94	133.12	122.13
1	F	621	ASP	C-N-CA	5.94	133.12	122.13
1	A	54	THR	OG1-CB-CG2	5.92	121.14	109.30
1	B	531	MET	CG-SD-CE	-5.83	88.07	100.90
1	C	15	ASP	N-CA-C	5.82	123.20	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	THR	N-CA-CB	-5.81	102.87	110.59
1	B	37	ALA	CA-C-N	5.50	132.19	121.41
1	B	37	ALA	C-N-CA	5.50	132.19	121.41
1	C	16	LEU	N-CA-C	5.50	122.52	110.80
1	D	596	GLU	CB-CG-CD	5.19	121.42	112.60
1	D	489	GLU	N-CA-C	5.09	118.75	112.54
1	F	190	ILE	N-CA-C	5.07	116.54	109.80
1	C	117	ASP	N-CA-C	5.02	117.48	111.71

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	30	0
1	B	4793	0	4650	38	0
1	C	4852	0	4711	33	0
1	D	4696	0	4562	37	0
1	E	4876	0	4728	37	0
1	F	4878	0	4725	48	0
2	A	9	0	4	0	0
2	B	9	0	4	1	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	5	1
5	C	586	0	0	5	0
5	D	722	0	0	4	0
5	E	728	0	0	6	0
5	F	713	0	0	6	1
All	All	33294	0	28388	218	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 (218) 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
1:B:538:TRP:CH2	1:B:553:MET:HE1	2.20	0.77
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
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:F:413:MET:HE3	5:F:1377:HOH:O	1.91	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:705:IMD:H5	5:F:1091:HOH:O	1.97	0.65
1:F:538:TRP:CH2	1:F:553:MET:HE1	2.31	0.64
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
1:C:538:TRP:CH2	1:C:553:MET:HE1	2.32	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:D:391:ALA:HA	1:D:413:MET:HE2	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:B:310:TRP:HE1	4:B:707:GOL:C3	2.19	0.55
3:F:703:IMD:H2	5:F:1040:HOH:O	2.06	0.55
1:D:413:MET:HE3	5:D:1373:HOH:O	2.05	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:B:413:MET:HE3	5:B:1309:HOH:O	2.07	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
1:C:391:ALA:HA	1:C:413:MET:HE2	1.90	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:413:MET:HE3	5:E:1391:HOH:O	2.11	0.50
1:A:612:THR:HB	1:C:610:ALA:HA	1.93	0.50
1:C:413:MET:HE3	5:C:1382:HOH:O	2.12	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:B:35:GLY:C	1:B:37:ALA:H	2.16	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
1:B:552:ARG:C	1:B:553:MET:HG2	2.36	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:163:LEU:C	1:D:163:LEU:HD12	2.38	0.49
1:A:494[B]:SER:OG	5:A:901:HOH:O	2.13	0.48
1:D:35:GLY:CA	1:D:36:SER:HB3	2.43	0.48
1:F:552:ARG:C	1:F:553:MET:HG2	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:560:ASP:OD1	1:A:561:THR:HG23	2.15	0.46
1:F:212:LYS:NZ	1:F:321:ASP:OD2	2.33	0.46
1:B:413:MET:HE2	5:B:937:HOH:O	2.14	0.46
1:D:36:SER:C	1:D:38:GLY:H	2.23	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:D:71:ALA:HA	1:D:75:TRP:CZ3	2.50	0.46
1:B:35:GLY:C	1:B:37:ALA:N	2.71	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:58:VAL:O	1:B:59:PRO:C	2.53	0.45
1:F:413:MET:HE2	5:F:948:HOH:O	2.15	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
1:B:19:MET:HE1	1:B:33:LEU:HB2	1.99	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:A:441:ASN:C	1:A:441:ASN:HD22	2.28	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:E:212:LYS:NZ	1:E:321:ASP:OD2	2.51	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: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:441:ASN:HD22	1:F:441:ASN:C	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:19:MET:HE2	1:B:31:ILE:HG22	2.01	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: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:E:391:ALA:HA	1:E:413:MET:HE2	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:B:163:LEU:HD12	1:B:163:LEU:C	2.45	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: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: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:441:ASN:C	1:E:441:ASN:HD22	2.29	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	642/671 (96%)	618 (96%)	23 (4%)	1 (0%)	43	22
1	B	632/671 (94%)	605 (96%)	25 (4%)	2 (0%)	36	17
1	C	640/671 (95%)	612 (96%)	26 (4%)	2 (0%)	36	17
1	D	620/671 (92%)	594 (96%)	23 (4%)	3 (0%)	24	8
1	E	643/671 (96%)	617 (96%)	24 (4%)	2 (0%)	36	17
1	F	643/671 (96%)	619 (96%)	22 (3%)	2 (0%)	36	17
All	All	3820/4026 (95%)	3665 (96%)	143 (4%)	12 (0%)	36	17

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

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%)	520 (100%)	2 (0%)	84	70
1	B	513/544 (94%)	507 (99%)	6 (1%)	63	36
1	C	520/544 (96%)	516 (99%)	4 (1%)	73	52
1	D	502/544 (92%)	497 (99%)	5 (1%)	68	43
1	E	522/544 (96%)	518 (99%)	4 (1%)	73	52
1	F	523/544 (96%)	520 (99%)	3 (1%)	78	60
All	All	3102/3264 (95%)	3078 (99%)	24 (1%)	76	52

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	54	THR
1	B	26	GLN
1	B	31	ILE
1	B	120	ARG
1	B	546	VAL
1	B	553	MET
1	B	622	VAL
1	C	78	ASN
1	C	244	GLU
1	C	274[A]	ILE
1	C	274[B]	ILE
1	D	34	LEU
1	D	68	VAL
1	D	164	SER
1	D	489	GLU
1	D	592	LYS
1	E	18	SER
1	E	28	GLN
1	E	127	VAL
1	E	622	VAL
1	F	10	GLU
1	F	11	ARG
1	F	546	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	192	GLN
1	A	215	HIS
1	A	234	ASN
1	A	261	ASN
1	A	307	ASN
1	A	328	HIS
1	A	441	ASN
1	B	26	GLN
1	B	110	ASN
1	B	133	ASN
1	B	307	ASN
1	B	328	HIS
1	B	458	GLN
1	B	459	ASN
1	C	293	ASN
1	C	307	ASN
1	C	328	HIS
1	C	441	ASN
1	D	110	ASN
1	D	192	GLN
1	D	234	ASN
1	D	293	ASN
1	D	441	ASN
1	D	577	ASN
1	E	28	GLN
1	E	192	GLN
1	E	215	HIS
1	E	293	ASN
1	E	307	ASN
1	E	367	GLN
1	E	441	ASN
1	E	476	ASN
1	F	110	ASN
1	F	130	GLN
1	F	133	ASN
1	F	192	GLN
1	F	215	HIS
1	F	234	ASN
1	F	293	ASN
1	F	307	ASN
1	F	328	HIS
1	F	373	HIS

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Mol	Chain	Res	Type
1	F	441	ASN
1	F	458	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
3	IMD	C	805	-	5,5,5	0.69	0	5,5,5	0.32	0
3	IMD	E	705	-	5,5,5	0.68	0	5,5,5	0.47	0
4	GOL	B	701	-	5,5,5	0.25	0	5,5,5	0.70	0
3	IMD	C	804	-	5,5,5	0.51	0	5,5,5	0.91	0
2	LMR	C	809	-	8,8,8	2.46	1 (12%)	10,10,10	2.55	4 (40%)
2	LMR	A	801	-	8,8,8	1.74	1 (12%)	10,10,10	2.70	3 (30%)
4	GOL	B	707	-	5,5,5	1.31	0	5,5,5	1.51	1 (20%)
2	LMR	B	703	-	8,8,8	2.32	5 (62%)	10,10,10	1.92	4 (40%)
4	GOL	F	701	-	5,5,5	0.77	0	5,5,5	0.81	0
3	IMD	A	805	-	5,5,5	0.49	0	5,5,5	0.58	0
3	IMD	F	705	-	5,5,5	0.70	0	5,5,5	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	707	-	5,5,5	0.43	0	5,5,5	0.50	0
3	IMD	B	705	-	5,5,5	0.45	0	5,5,5	1.07	0
4	GOL	C	801	-	5,5,5	1.01	0	5,5,5	0.77	0
4	GOL	C	807	-	5,5,5	0.41	0	5,5,5	1.13	0
3	IMD	B	708	-	5,5,5	0.83	0	5,5,5	0.72	0
4	GOL	E	706	-	5,5,5	0.98	0	5,5,5	0.75	0
3	IMD	F	709	-	5,5,5	0.81	0	5,5,5	0.46	0
3	IMD	A	802	-	5,5,5	0.47	0	5,5,5	0.43	0
2	LMR	F	708	-	8,8,8	1.32	0	10,10,10	1.77	4 (40%)
3	IMD	C	806	-	5,5,5	0.36	0	5,5,5	0.93	0
4	GOL	B	702	-	5,5,5	1.22	0	5,5,5	1.07	0
4	GOL	F	706	-	5,5,5	1.88	2 (40%)	5,5,5	1.29	0
3	IMD	C	810	-	5,5,5	0.46	0	5,5,5	0.26	0
4	GOL	C	803	-	5,5,5	0.56	0	5,5,5	0.90	0
2	LMR	F	707	-	8,8,8	1.23	0	10,10,10	2.33	5 (50%)
4	GOL	D	705	-	5,5,5	2.88	4 (80%)	5,5,5	1.38	2 (40%)
4	GOL	A	806	-	5,5,5	0.23	0	5,5,5	0.85	0
4	GOL	E	703	-	5,5,5	2.17	2 (40%)	5,5,5	1.87	2 (40%)
4	GOL	F	702	-	5,5,5	1.45	1 (20%)	5,5,5	1.80	2 (40%)
4	GOL	D	704	-	5,5,5	0.71	0	5,5,5	1.81	2 (40%)
4	GOL	E	701	-	5,5,5	0.55	0	5,5,5	0.22	0
3	IMD	D	706	-	5,5,5	0.50	0	5,5,5	0.60	0
3	IMD	B	704	-	5,5,5	0.62	0	5,5,5	0.51	0
2	LMR	D	702	-	8,8,8	2.22	3 (37%)	10,10,10	1.10	1 (10%)
3	IMD	A	804	-	5,5,5	0.58	0	5,5,5	0.35	0
3	IMD	E	702	-	5,5,5	0.48	0	5,5,5	0.48	0
3	IMD	F	704	-	5,5,5	0.59	0	5,5,5	0.51	0
3	IMD	D	703	-	5,5,5	0.67	0	5,5,5	0.52	0
4	GOL	C	802	-	5,5,5	2.15	2 (40%)	5,5,5	1.43	1 (20%)
3	IMD	E	704	-	5,5,5	0.85	0	5,5,5	0.91	0
3	IMD	F	703	-	5,5,5	0.44	0	5,5,5	0.30	0
4	GOL	A	803	-	5,5,5	1.11	0	5,5,5	1.92	3 (60%)
2	LMR	E	707	-	8,8,8	2.09	3 (37%)	10,10,10	1.48	1 (10%)
3	IMD	E	708	-	5,5,5	0.63	0	5,5,5	0.72	0
3	IMD	D	701	-	5,5,5	0.51	0	5,5,5	0.28	0
3	IMD	B	706	-	5,5,5	0.93	0	5,5,5	0.51	0
3	IMD	C	808	-	5,5,5	0.59	0	5,5,5	0.43	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
3	IMD	C	805	-	-	-	0/1/1/1
4	GOL	B	701	-	-	0/4/4/4	-
3	IMD	E	705	-	-	-	0/1/1/1
3	IMD	C	804	-	-	-	0/1/1/1
2	LMR	C	809	-	-	5/8/8/8	-
2	LMR	A	801	-	-	7/8/8/8	-
4	GOL	B	707	-	-	2/4/4/4	-
2	LMR	B	703	-	-	4/8/8/8	-
4	GOL	F	701	-	-	2/4/4/4	-
3	IMD	A	805	-	-	-	0/1/1/1
3	IMD	F	705	-	-	-	0/1/1/1
4	GOL	D	707	-	-	0/4/4/4	-
3	IMD	B	705	-	-	-	0/1/1/1
4	GOL	C	801	-	-	2/4/4/4	-
4	GOL	C	807	-	-	0/4/4/4	-
3	IMD	B	708	-	-	-	0/1/1/1
4	GOL	E	706	-	-	0/4/4/4	-
3	IMD	F	709	-	-	-	0/1/1/1
3	IMD	A	802	-	-	-	0/1/1/1
2	LMR	F	708	-	-	2/8/8/8	-
3	IMD	C	806	-	-	-	0/1/1/1
4	GOL	B	702	-	-	2/4/4/4	-
4	GOL	F	706	-	-	2/4/4/4	-
3	IMD	C	810	-	-	-	0/1/1/1
4	GOL	C	803	-	-	0/4/4/4	-
2	LMR	F	707	-	-	4/8/8/8	-
4	GOL	D	705	-	-	0/4/4/4	-
4	GOL	A	806	-	-	2/4/4/4	-
4	GOL	E	703	-	-	2/4/4/4	-
4	GOL	F	702	-	-	4/4/4/4	-
4	GOL	D	704	-	-	4/4/4/4	-
4	GOL	E	701	-	-	2/4/4/4	-
3	IMD	D	706	-	-	-	0/1/1/1
3	IMD	B	704	-	-	-	0/1/1/1
2	LMR	D	702	-	-	7/8/8/8	-
3	IMD	A	804	-	-	-	0/1/1/1
3	IMD	E	702	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IMD	F	704	-	-	-	0/1/1/1
4	GOL	C	802	-	-	2/4/4/4	-
3	IMD	D	703	-	-	-	0/1/1/1
3	IMD	E	704	-	-	-	0/1/1/1
3	IMD	F	703	-	-	-	0/1/1/1
4	GOL	A	803	-	-	4/4/4/4	-
2	LMR	E	707	-	-	7/8/8/8	-
3	IMD	E	708	-	-	-	0/1/1/1
3	IMD	D	701	-	-	-	0/1/1/1
3	IMD	B	706	-	-	-	0/1/1/1
3	IMD	C	808	-	-	-	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	809	LMR	C2-C1	6.00	1.60	1.52
2	D	702	LMR	C2-C1	4.65	1.58	1.52
2	E	707	LMR	C2-C1	4.34	1.58	1.52
2	A	801	LMR	C2-C1	4.27	1.58	1.52
4	C	802	GOL	O2-C2	3.87	1.54	1.43
4	E	703	GOL	O2-C2	3.83	1.54	1.43
4	F	706	GOL	C1-C2	3.59	1.65	1.51
2	B	703	LMR	C3-C2	3.36	1.59	1.52
4	D	705	GOL	O1-C1	3.32	1.56	1.42
4	D	705	GOL	C1-C2	3.31	1.64	1.51
4	D	705	GOL	O3-C3	3.17	1.55	1.42
4	D	705	GOL	O2-C2	2.93	1.51	1.43
2	B	703	LMR	O1A-C1	2.86	1.30	1.22
2	B	703	LMR	O1B-C1	-2.81	1.21	1.30
2	B	703	LMR	C3-C4	2.68	1.58	1.51
2	D	702	LMR	O1B-C1	-2.60	1.22	1.30
4	E	703	GOL	C1-C2	2.54	1.61	1.51
2	E	707	LMR	C3-C2	-2.45	1.47	1.52
4	F	702	GOL	O2-C2	2.38	1.50	1.43
2	B	703	LMR	O2-C2	-2.34	1.37	1.42
2	D	702	LMR	C3-C4	2.15	1.56	1.51
4	C	802	GOL	C1-C2	2.13	1.59	1.51
2	E	707	LMR	O1A-C1	2.09	1.28	1.22
4	F	706	GOL	C3-C2	-2.06	1.43	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	LMR	O1A-C1-C2	-5.48	111.65	122.60
2	C	809	LMR	O1B-C1-C2	5.38	124.12	112.74
2	A	801	LMR	O1B-C1-C2	5.08	123.47	112.74
2	C	809	LMR	O1A-C1-C2	-4.46	113.69	122.60
2	F	707	LMR	C3-C2-C1	3.77	119.79	110.53
2	F	707	LMR	O1A-C1-C2	-3.67	115.26	122.60
2	B	703	LMR	C2-C3-C4	-3.47	103.01	112.08
2	F	707	LMR	O4B-C4-C3	-3.25	112.87	122.84
4	B	707	GOL	C3-C2-C1	-3.11	100.38	111.80
2	E	707	LMR	O4B-C4-C3	-3.08	113.37	122.84
4	E	703	GOL	O3-C3-C2	3.00	123.90	110.38
4	A	803	GOL	O3-C3-C2	-2.98	96.96	110.38
4	F	702	GOL	O2-C2-C1	2.89	121.16	109.18
2	F	708	LMR	O1A-C1-C2	-2.81	116.99	122.60
4	D	704	GOL	O3-C3-C2	-2.76	97.96	110.38
2	A	801	LMR	O4B-C4-C3	-2.71	114.53	122.84
4	C	802	GOL	O2-C2-C1	2.55	119.73	109.18
2	B	703	LMR	O2-C2-C3	2.54	116.08	109.96
2	F	708	LMR	O2-C2-C1	-2.48	104.05	110.36
2	B	703	LMR	O4A-C4-C3	2.38	121.38	114.00
4	D	704	GOL	C3-C2-C1	2.31	120.26	111.80
4	F	702	GOL	O1-C1-C2	2.30	120.72	110.38
2	F	708	LMR	O2-C2-C3	2.29	115.48	109.96
2	F	707	LMR	O4A-C4-O4B	2.27	129.18	123.33
2	C	809	LMR	O2-C2-C1	-2.26	104.63	110.36
2	C	809	LMR	O2-C2-C3	2.21	115.27	109.96
2	B	703	LMR	C3-C2-C1	-2.20	105.12	110.53
4	D	705	GOL	O3-C3-C2	2.18	120.18	110.38
2	F	708	LMR	O1B-C1-C2	2.18	117.35	112.74
4	A	803	GOL	C3-C2-C1	2.14	119.66	111.80
4	A	803	GOL	O2-C2-C1	2.10	117.88	109.18
2	F	707	LMR	O1B-C1-O1A	2.07	128.78	124.08
2	D	702	LMR	O4B-C4-C3	-2.05	116.54	122.84
4	D	705	GOL	O1-C1-C2	2.05	119.61	110.38
4	E	703	GOL	C3-C2-C1	-2.03	104.35	111.80

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	LMR	O1A-C1-C2-O2
2	A	801	LMR	O1A-C1-C2-C3
2	A	801	LMR	O1B-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	801	LMR	O1B-C1-C2-C3
2	B	703	LMR	O1A-C1-C2-O2
2	C	809	LMR	O1A-C1-C2-O2
2	C	809	LMR	O1A-C1-C2-C3
2	C	809	LMR	O1B-C1-C2-C3
2	F	707	LMR	O1A-C1-C2-O2
2	F	707	LMR	O1B-C1-C2-O2
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
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	B	703	LMR	O1B-C1-C2-O2
2	C	809	LMR	O1B-C1-C2-O2
2	D	702	LMR	O1A-C1-C2-O2
2	E	707	LMR	O1A-C1-C2-O2
2	D	702	LMR	O1A-C1-C2-C3
2	B	703	LMR	O2-C2-C3-C4
2	C	809	LMR	O2-C2-C3-C4
2	E	707	LMR	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	E	707	LMR	C2-C3-C4-O4A
2	D	702	LMR	O1B-C1-C2-O2
2	E	707	LMR	O1B-C1-C2-O2
2	D	702	LMR	C2-C3-C4-O4A
4	D	704	GOL	O1-C1-C2-O2
2	B	703	LMR	O1A-C1-C2-C3
2	E	707	LMR	O1A-C1-C2-C3
2	F	707	LMR	O1A-C1-C2-C3
2	F	707	LMR	O1B-C1-C2-C3
2	A	801	LMR	O2-C2-C3-C4
2	D	702	LMR	C2-C3-C4-O4B
2	E	707	LMR	C2-C3-C4-O4B
2	A	801	LMR	C2-C3-C4-O4A
2	A	801	LMR	C2-C3-C4-O4B
2	F	708	LMR	O1A-C1-C2-O2
4	A	803	GOL	O1-C1-C2-O2
4	B	707	GOL	O1-C1-C2-O2
2	D	702	LMR	O1B-C1-C2-C3
2	E	707	LMR	O1B-C1-C2-C3
2	D	702	LMR	O2-C2-C3-C4
2	F	708	LMR	O1B-C1-C2-O2

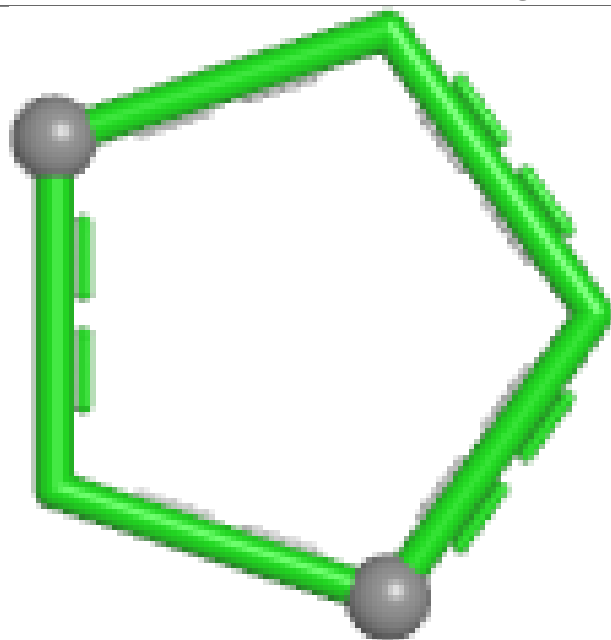
There are no ring outliers.

15 monomers are involved in 41 short contacts:

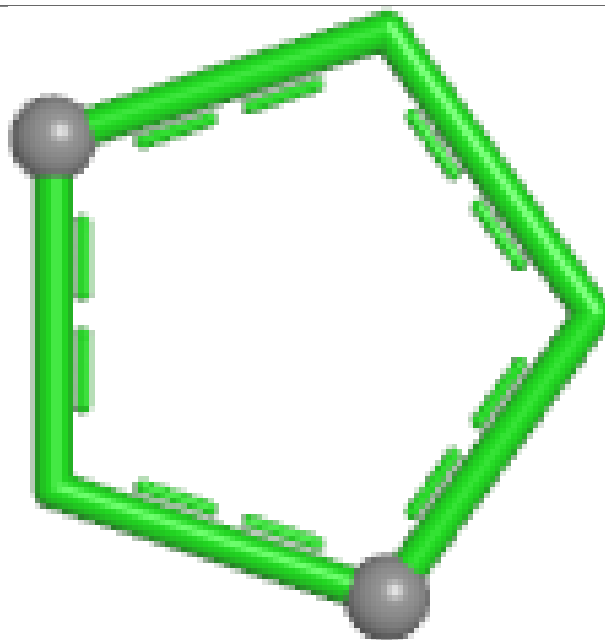
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	805	IMD	1	0
3	C	804	IMD	1	0
4	B	707	GOL	5	0
2	B	703	LMR	1	0
3	F	705	IMD	1	0
3	B	708	IMD	3	0
3	F	709	IMD	5	0
2	F	708	LMR	7	0
2	F	707	LMR	7	0
4	D	705	GOL	2	0
3	B	704	IMD	1	0
4	C	802	GOL	1	0
3	E	704	IMD	10	0
3	F	703	IMD	1	0
3	B	706	IMD	1	0

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

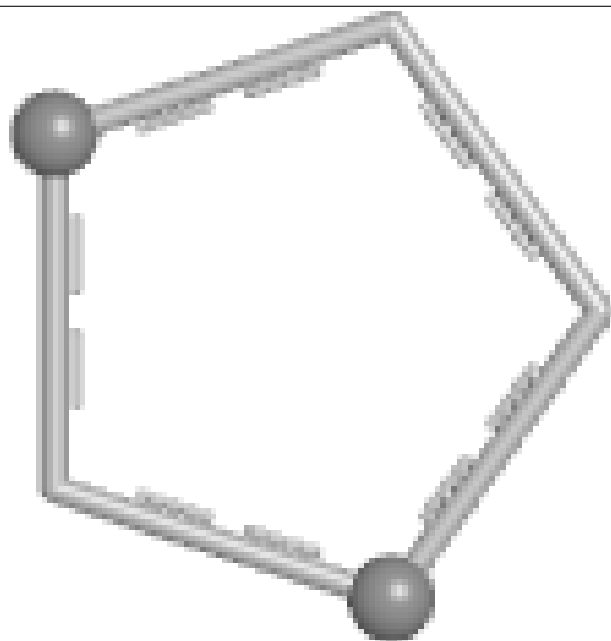
Ligand IMD C 805



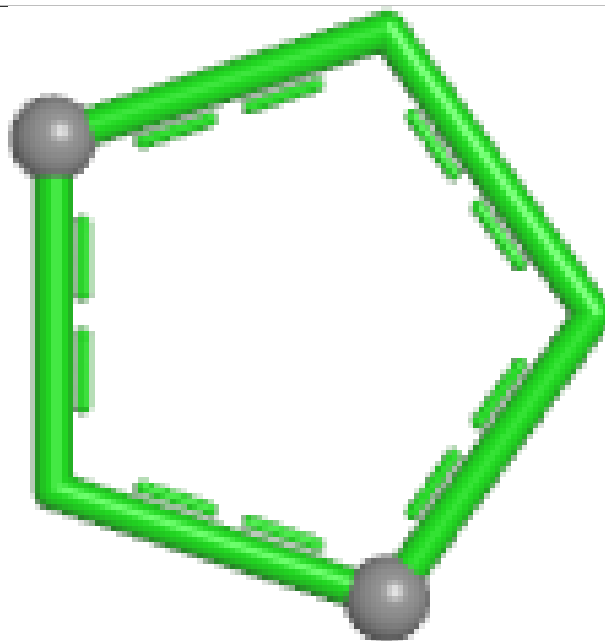
Bond lengths



Bond angles

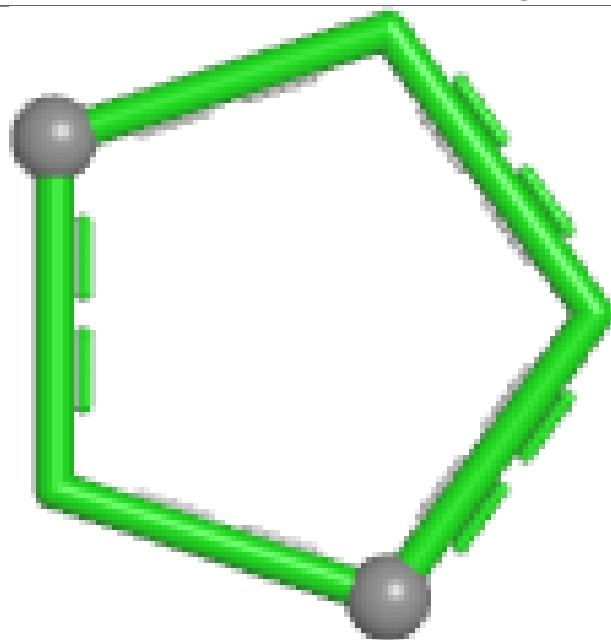


Torsions

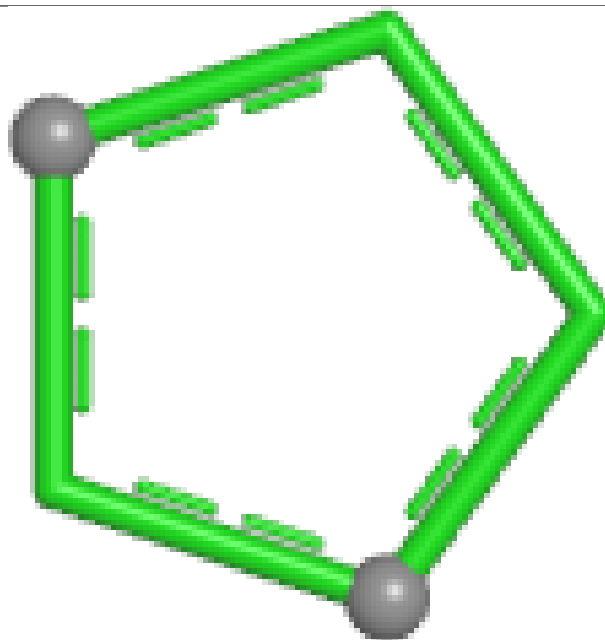


Rings

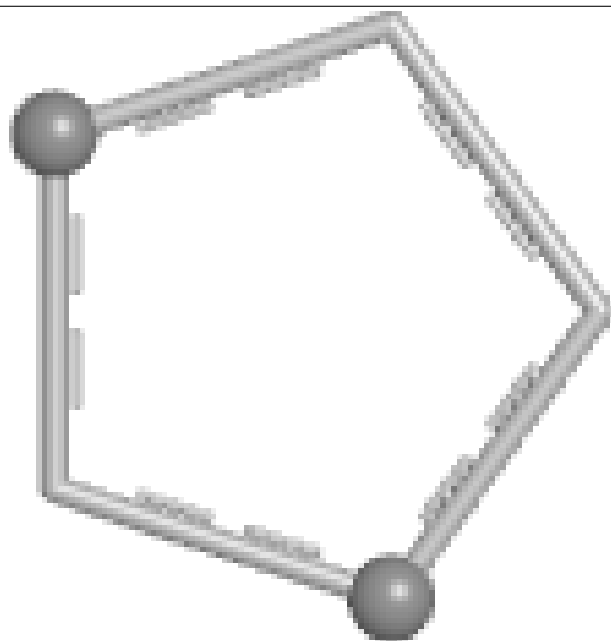
Ligand IMD E 705



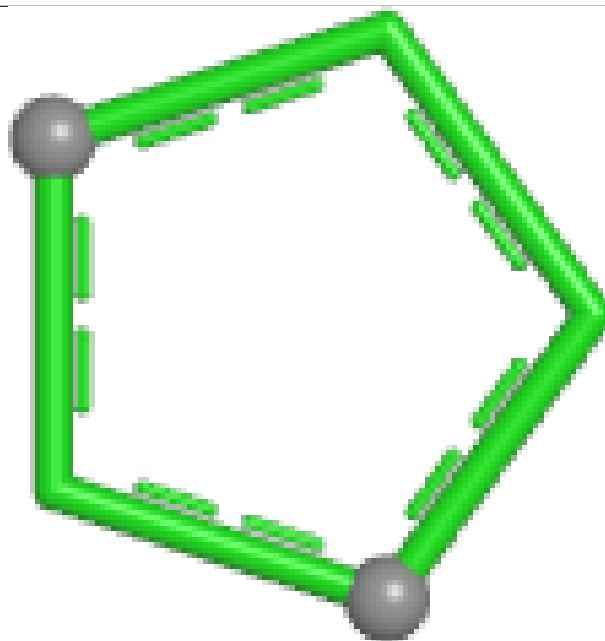
Bond lengths



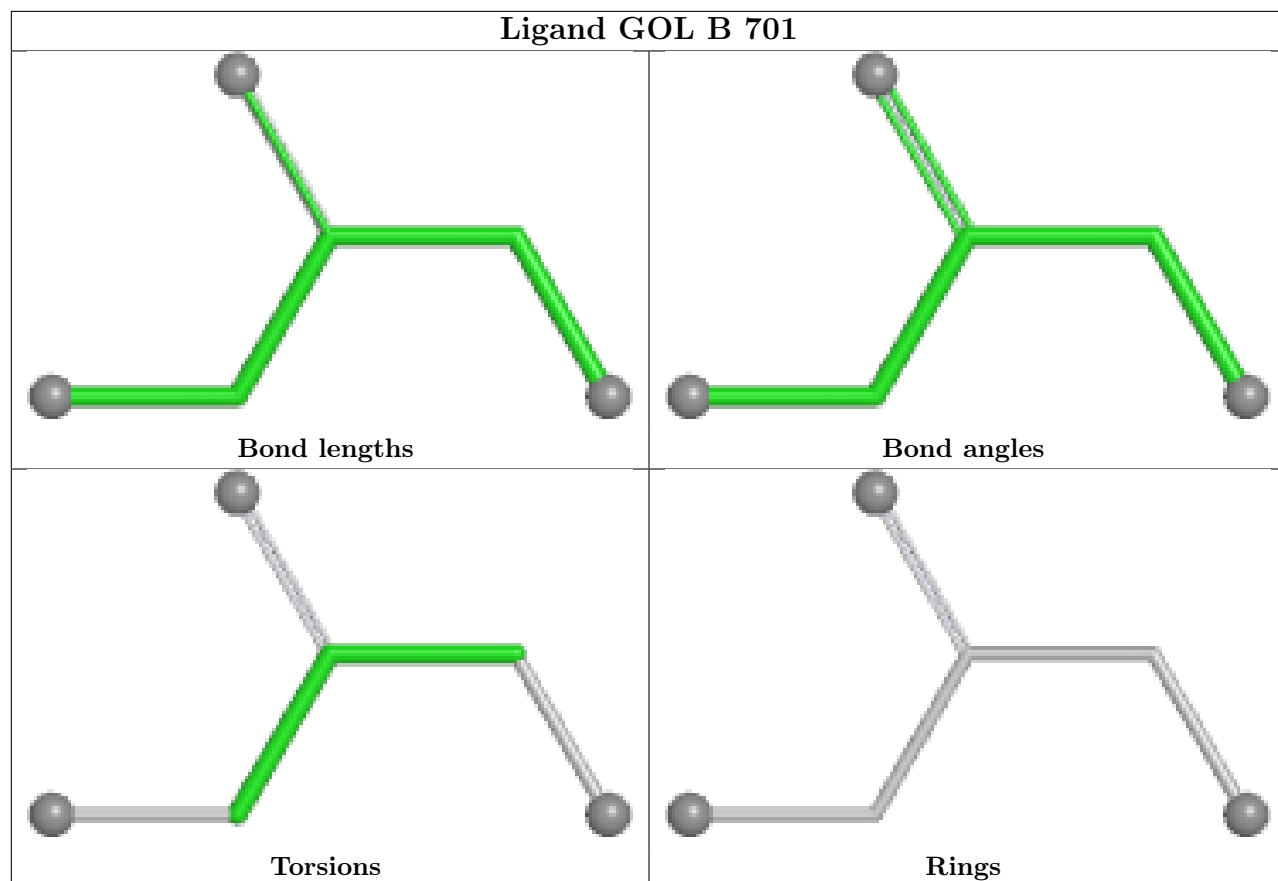
Bond angles

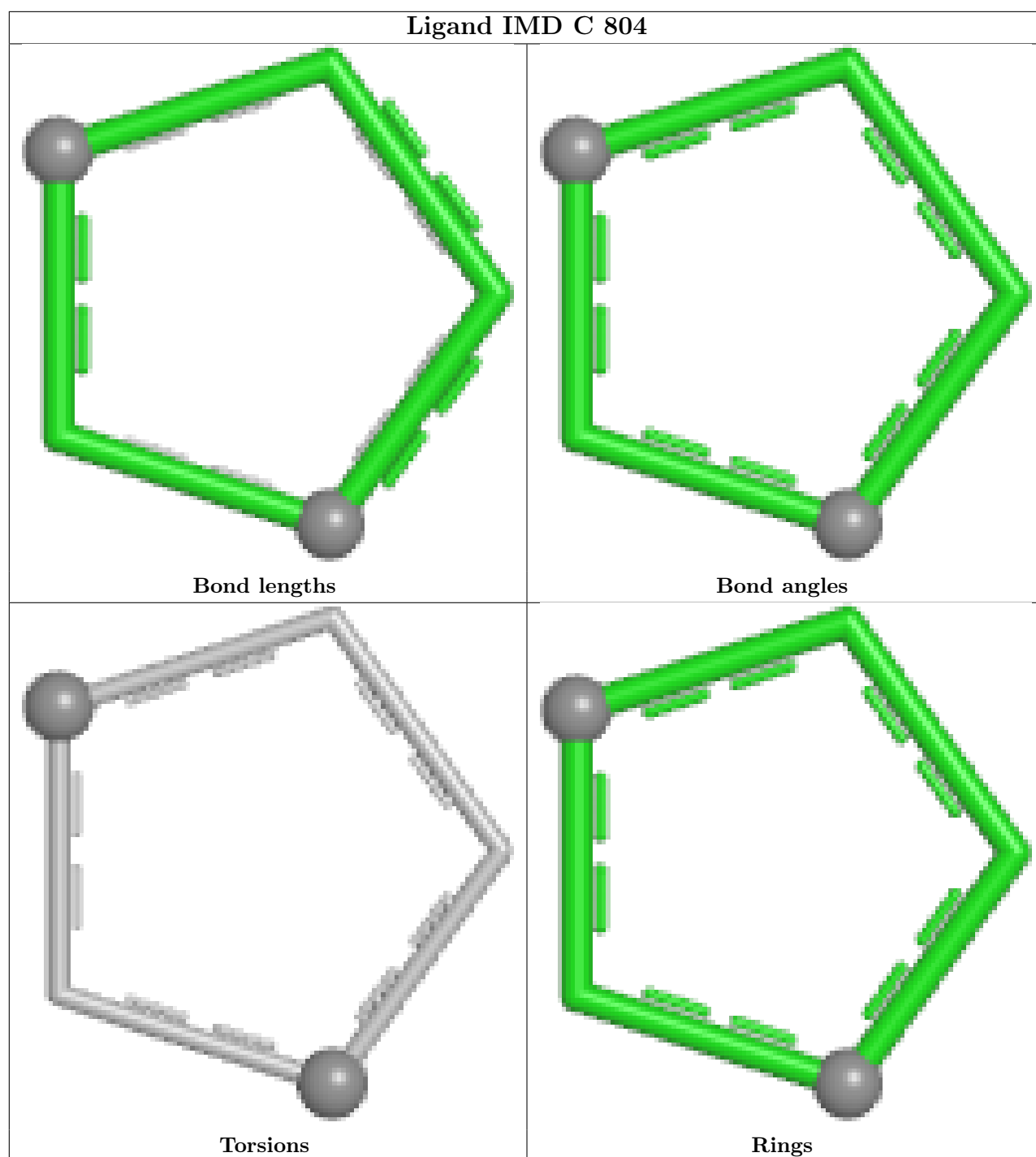


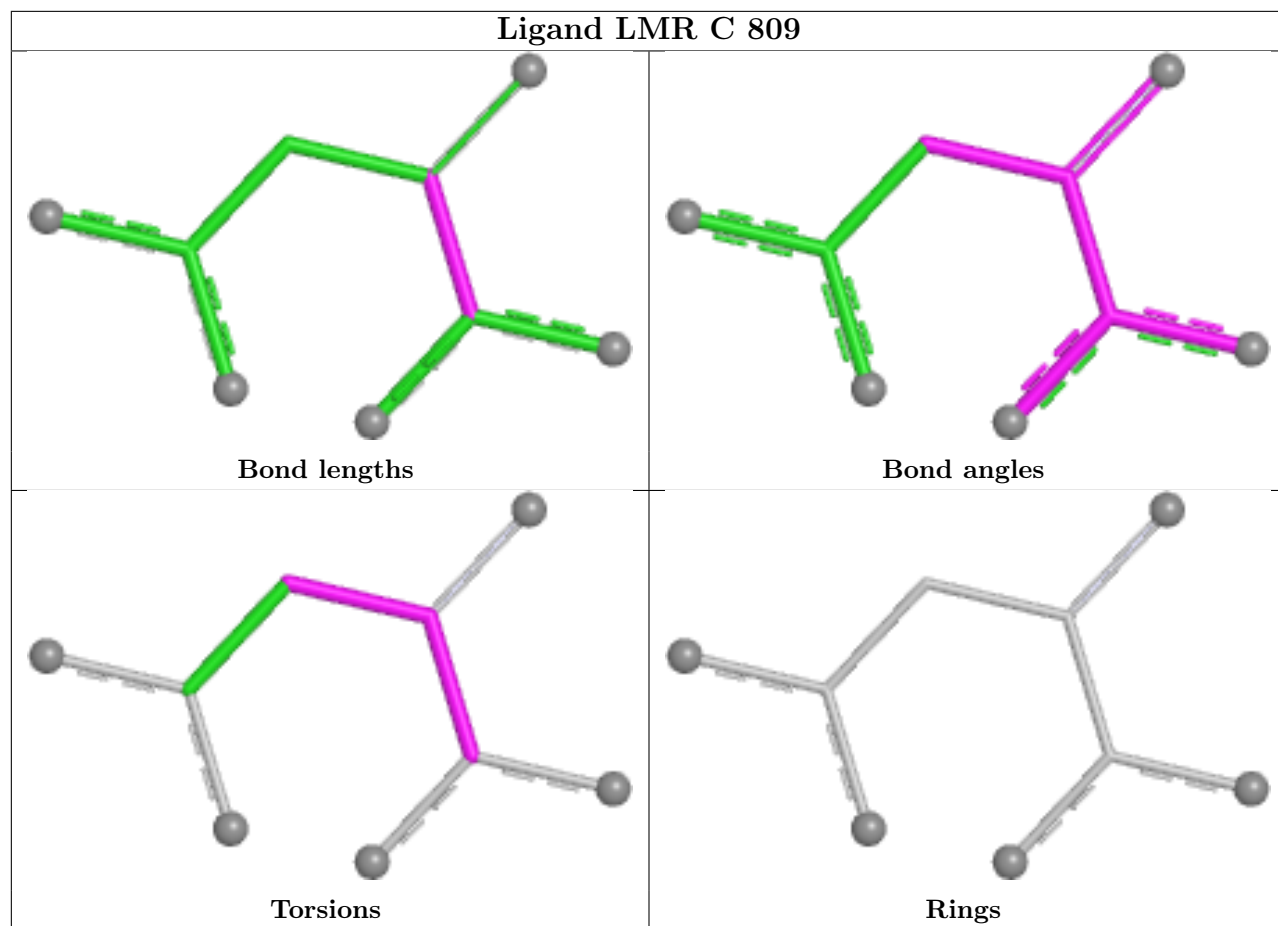
Torsions

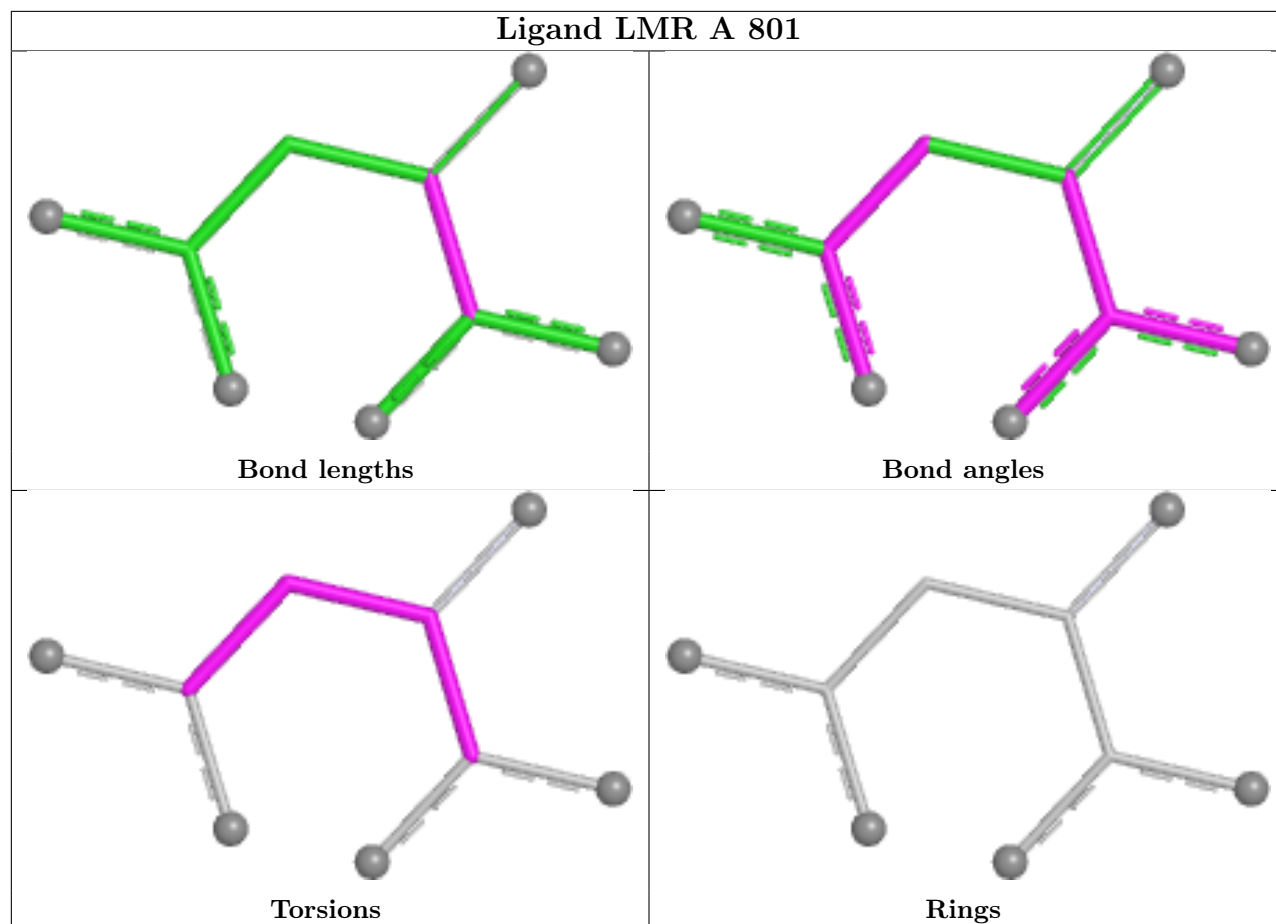


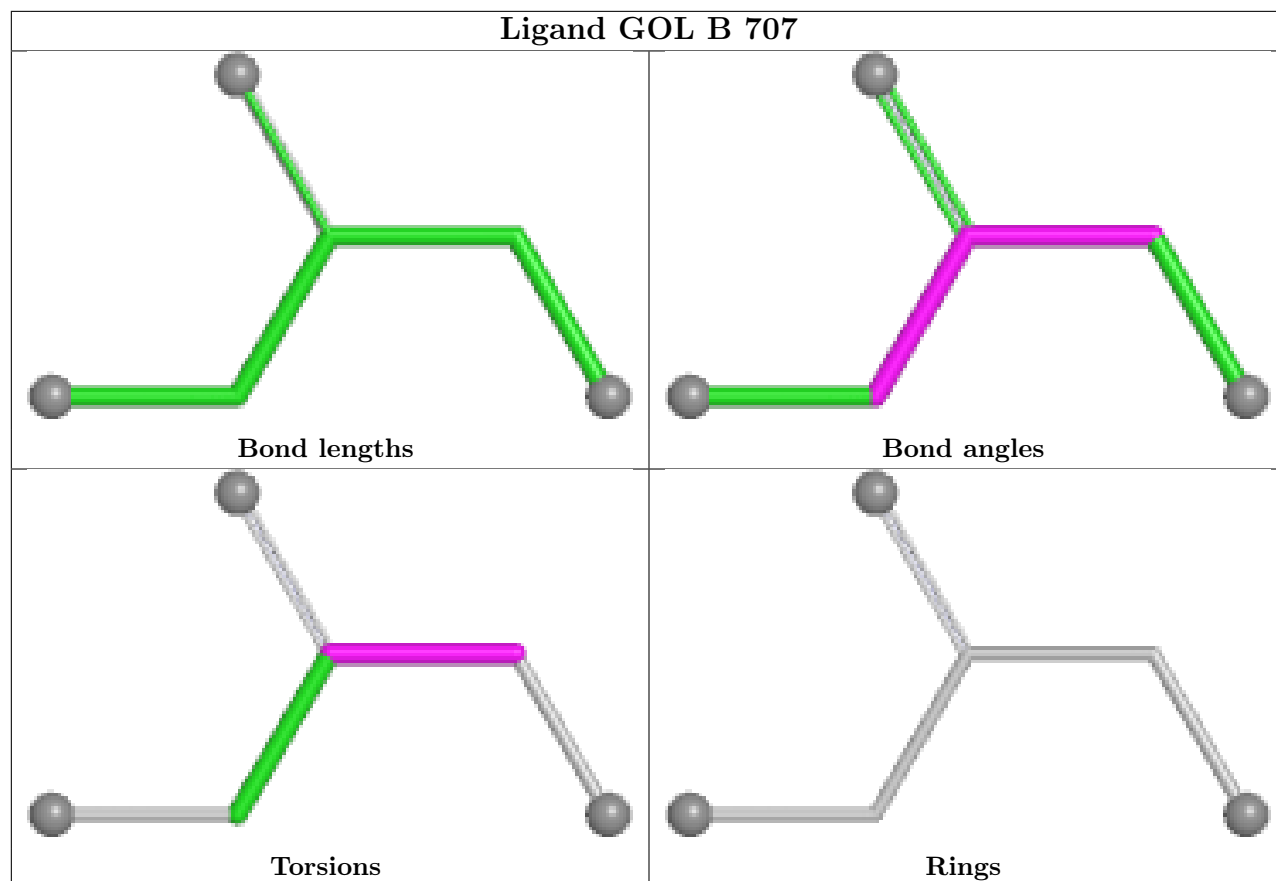
Rings

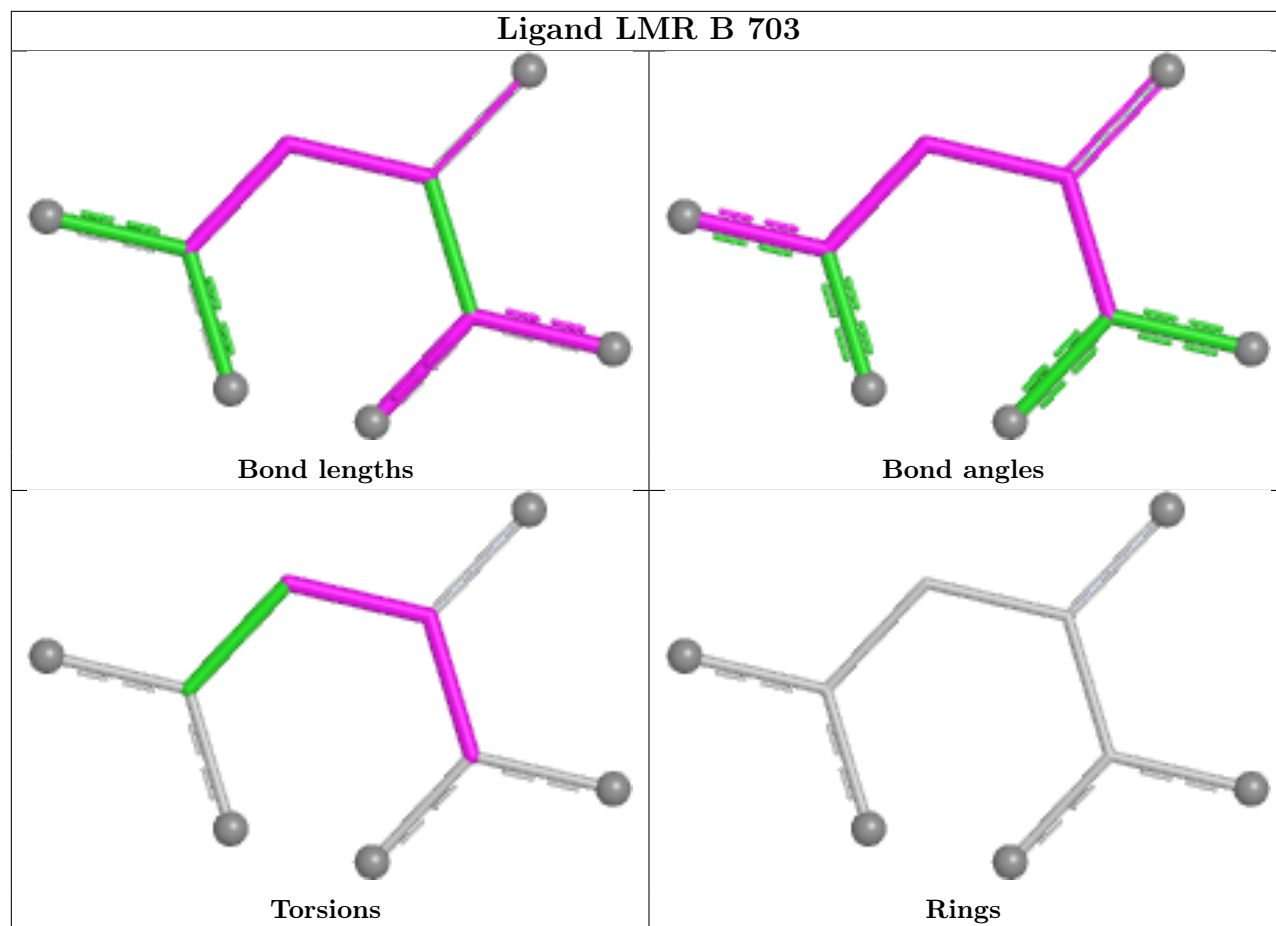


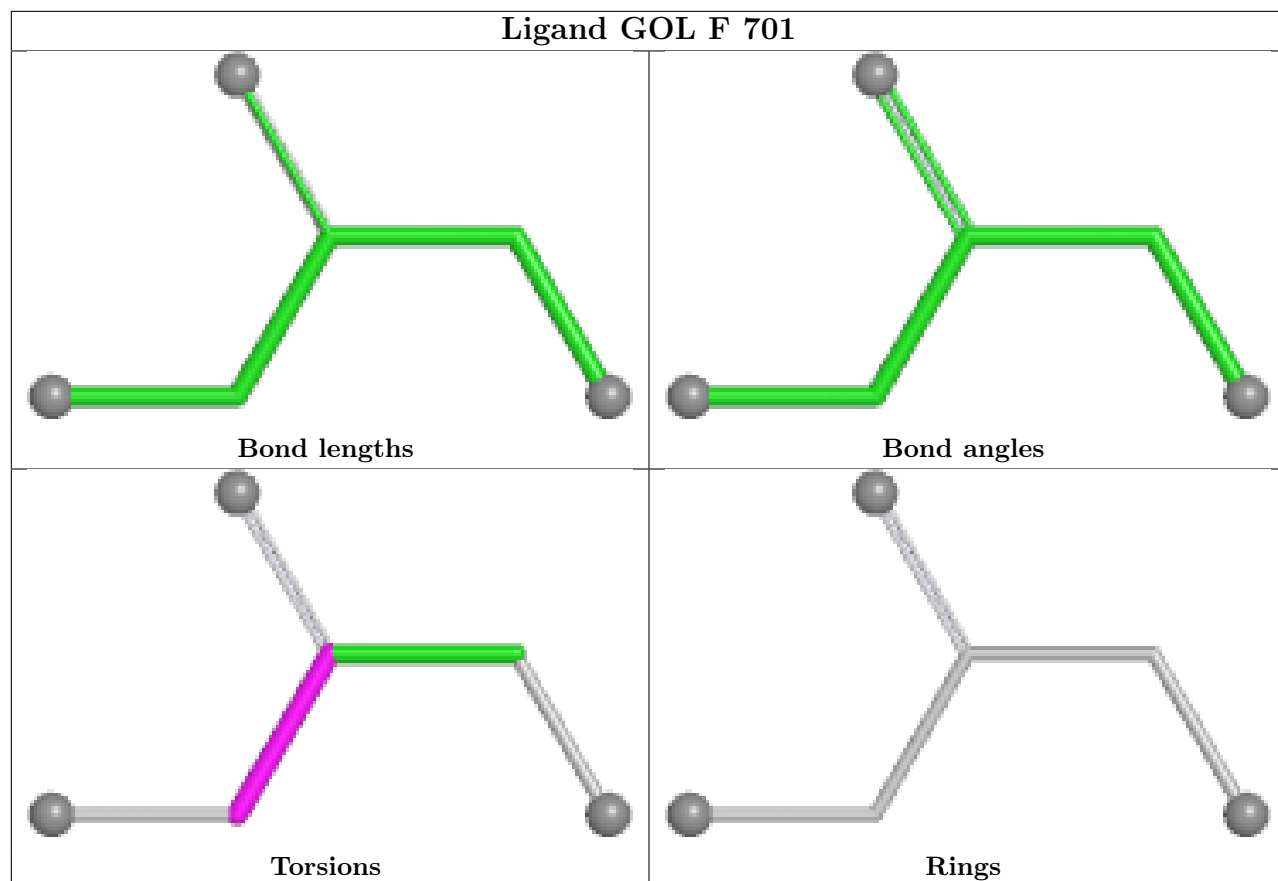




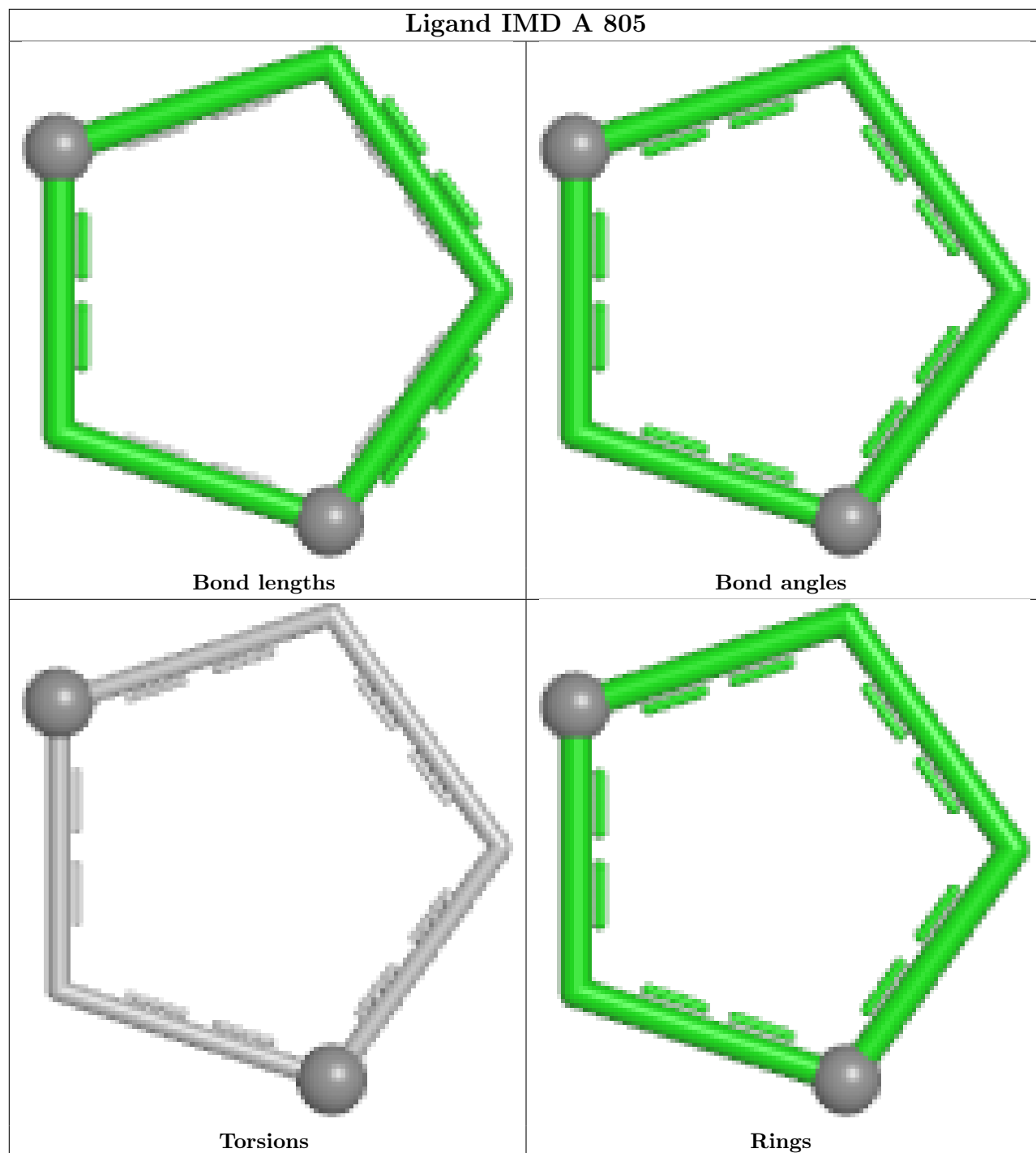




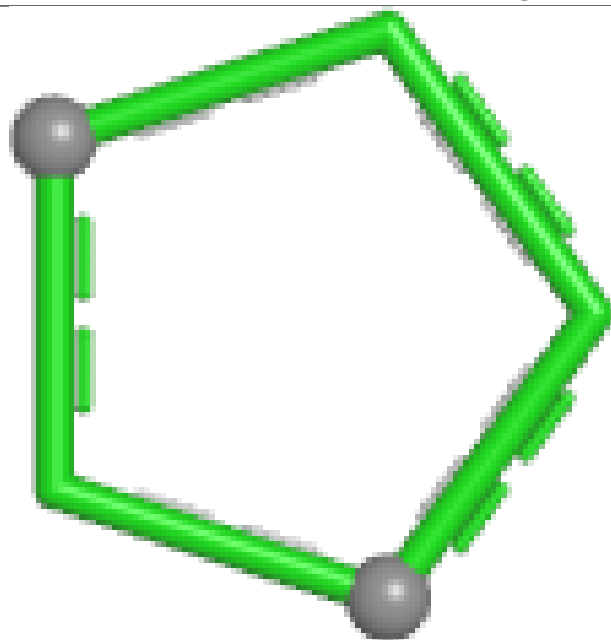




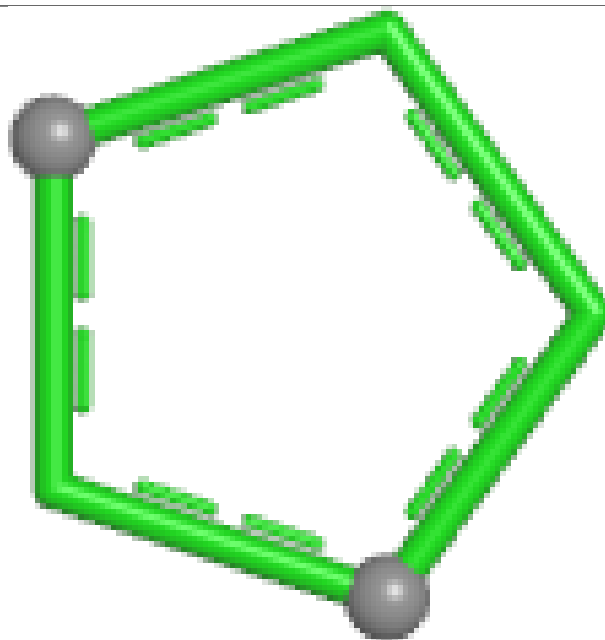
Ligand IMD A 805



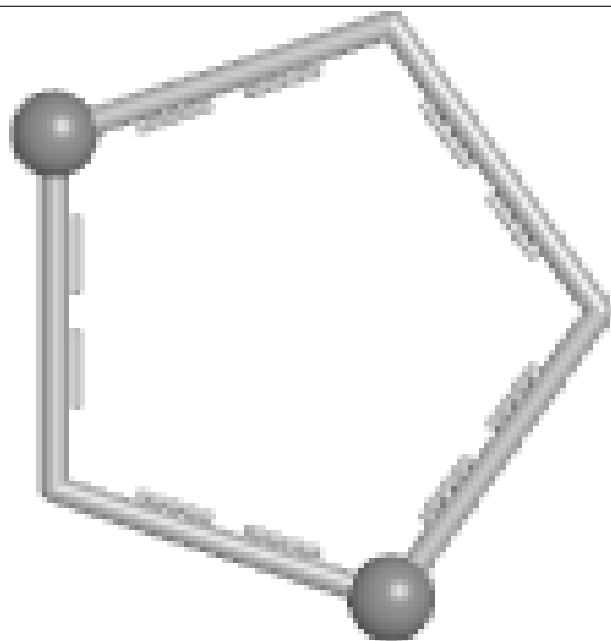
Ligand IMD F 705



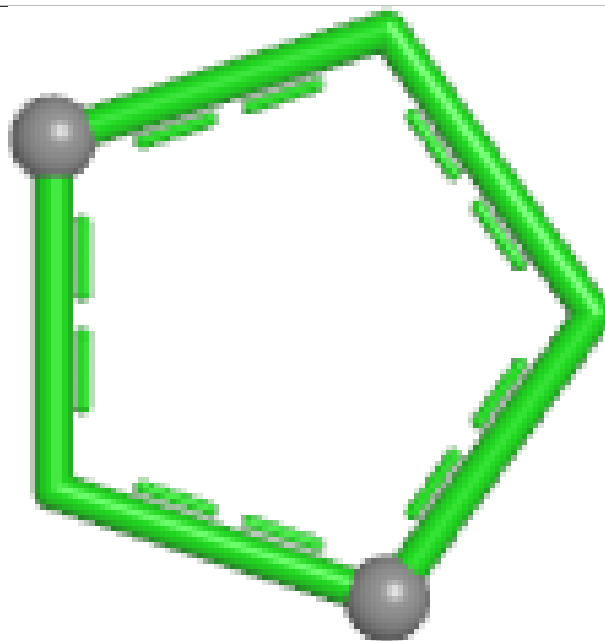
Bond lengths



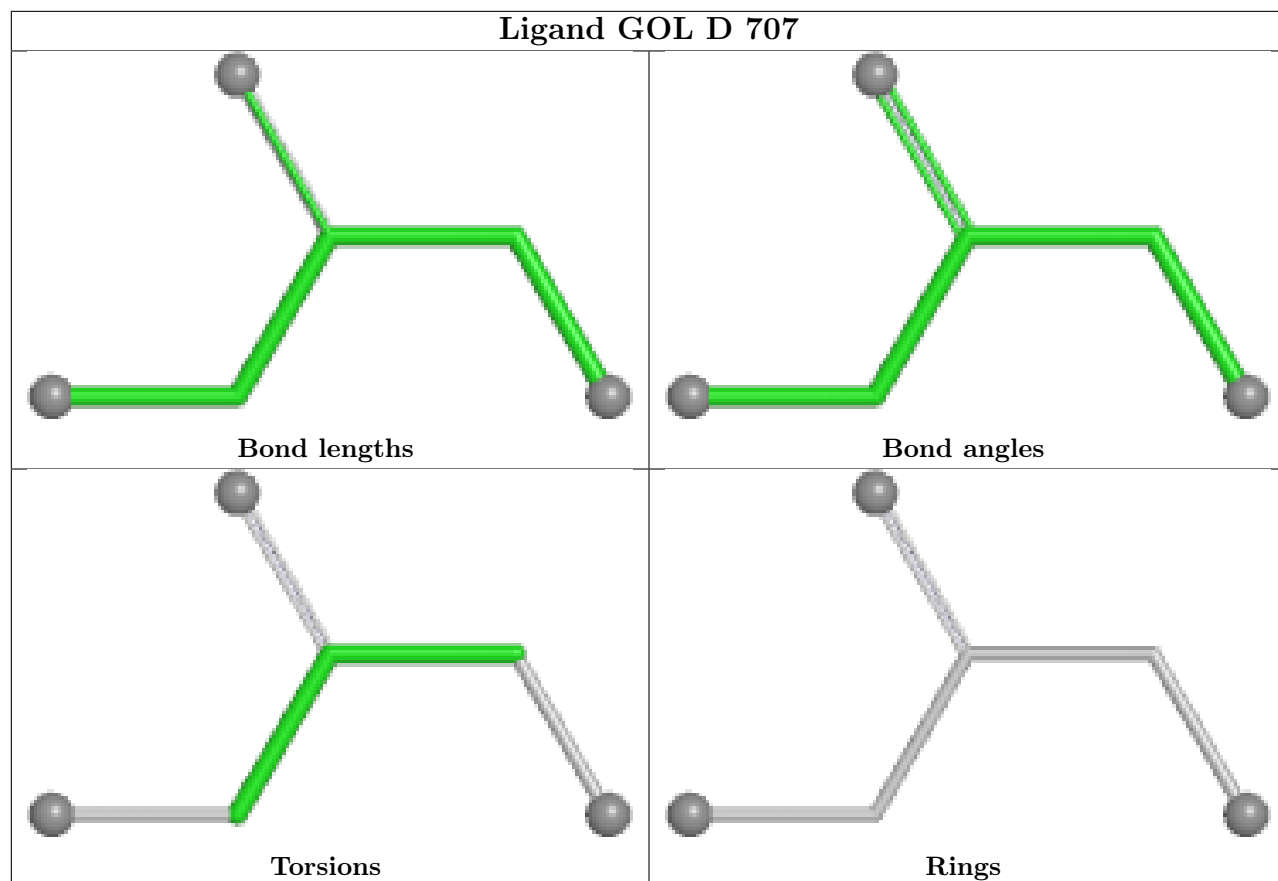
Bond angles



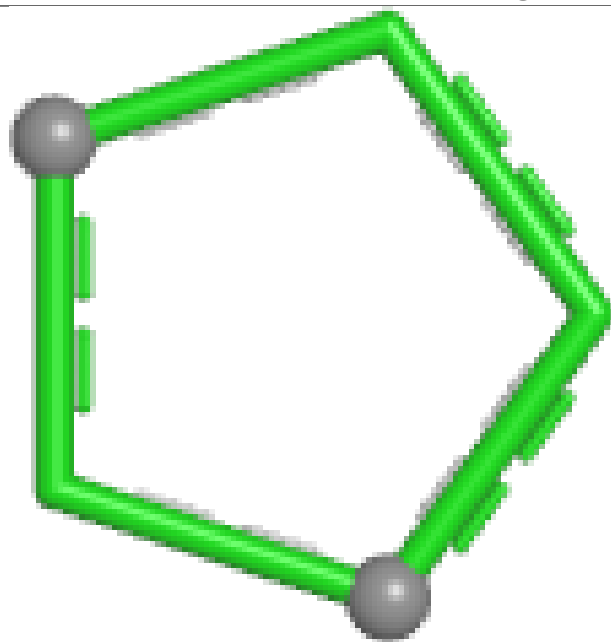
Torsions



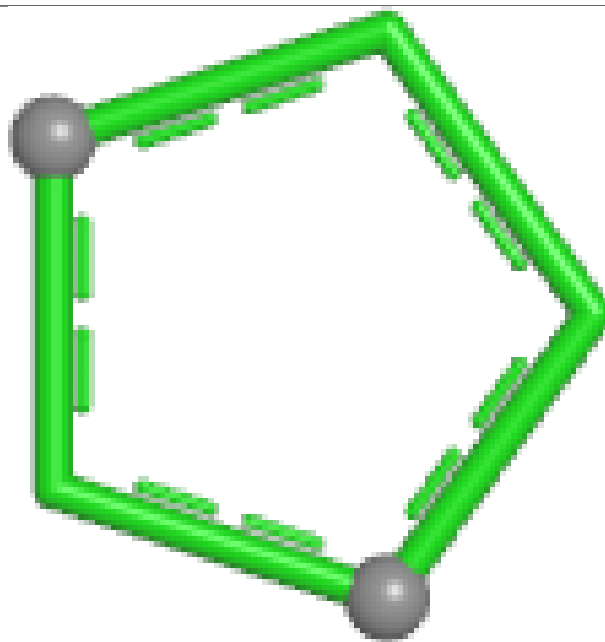
Rings



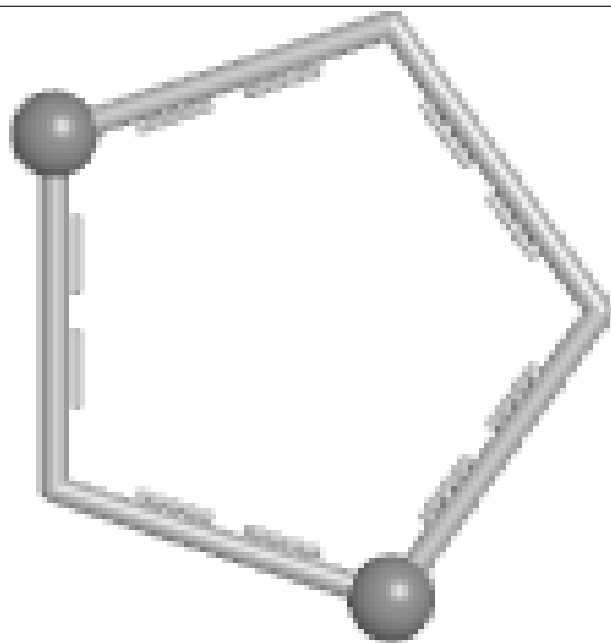
Ligand IMD B 705



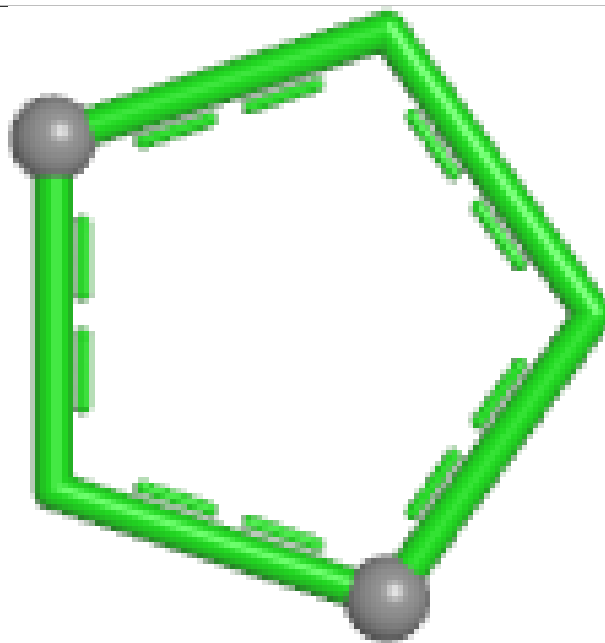
Bond lengths



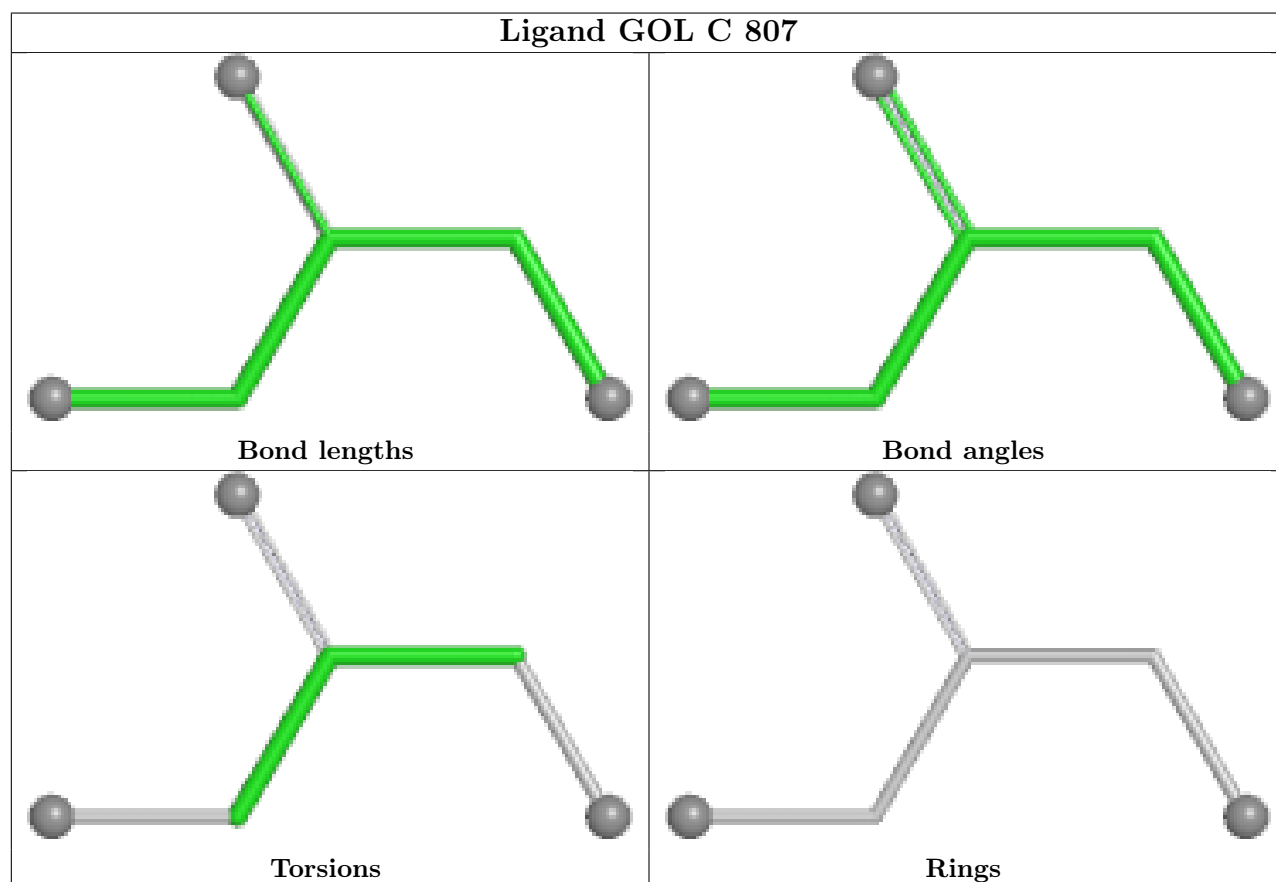
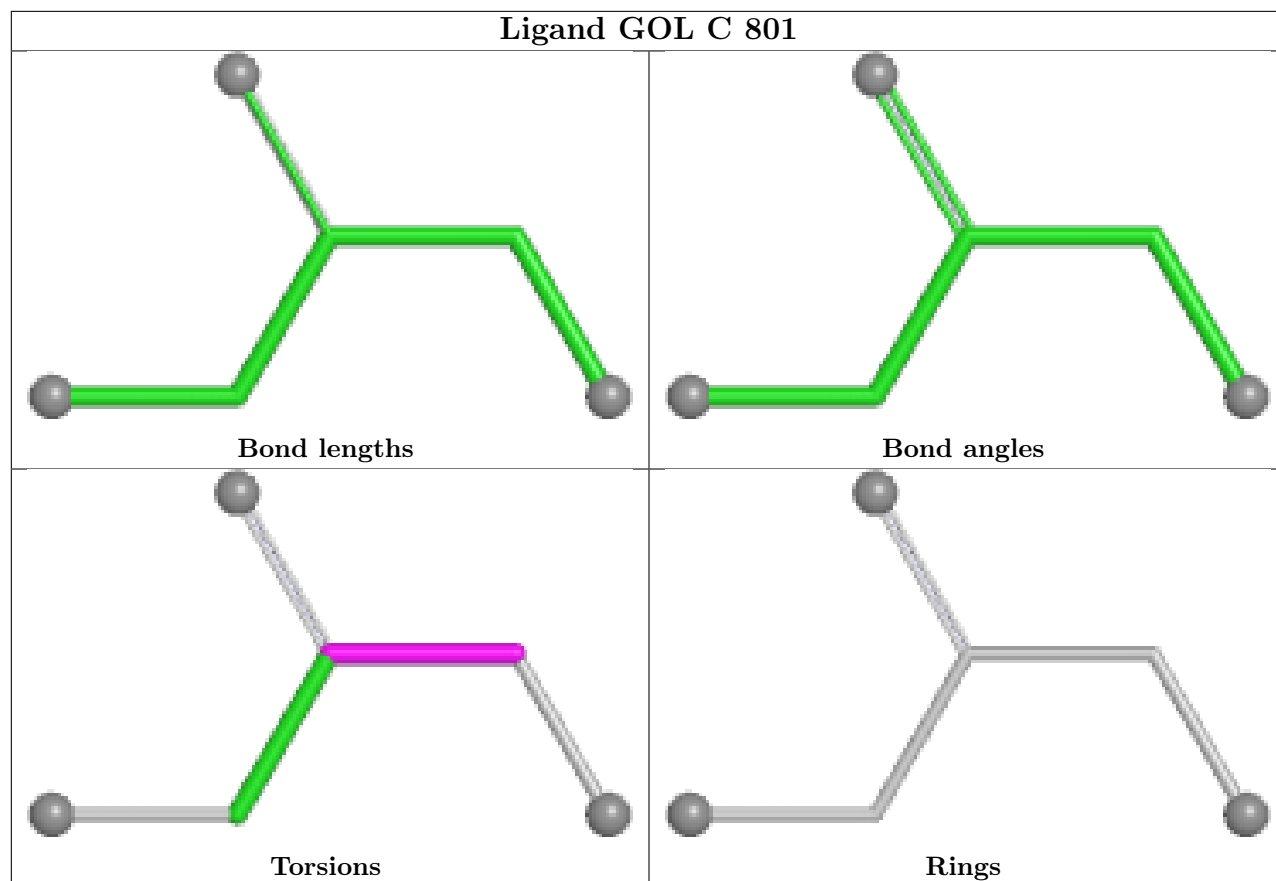
Bond angles



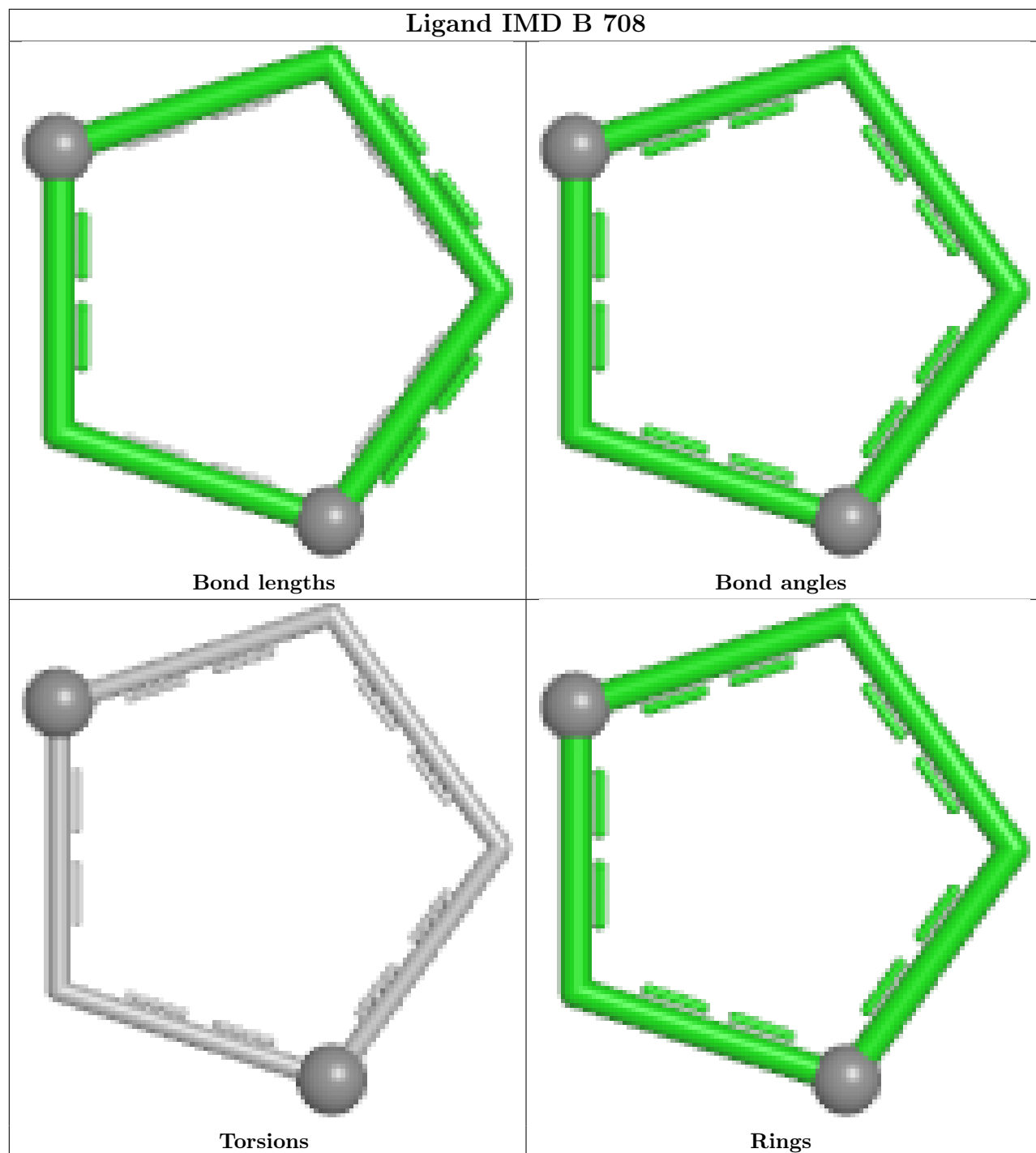
Torsions

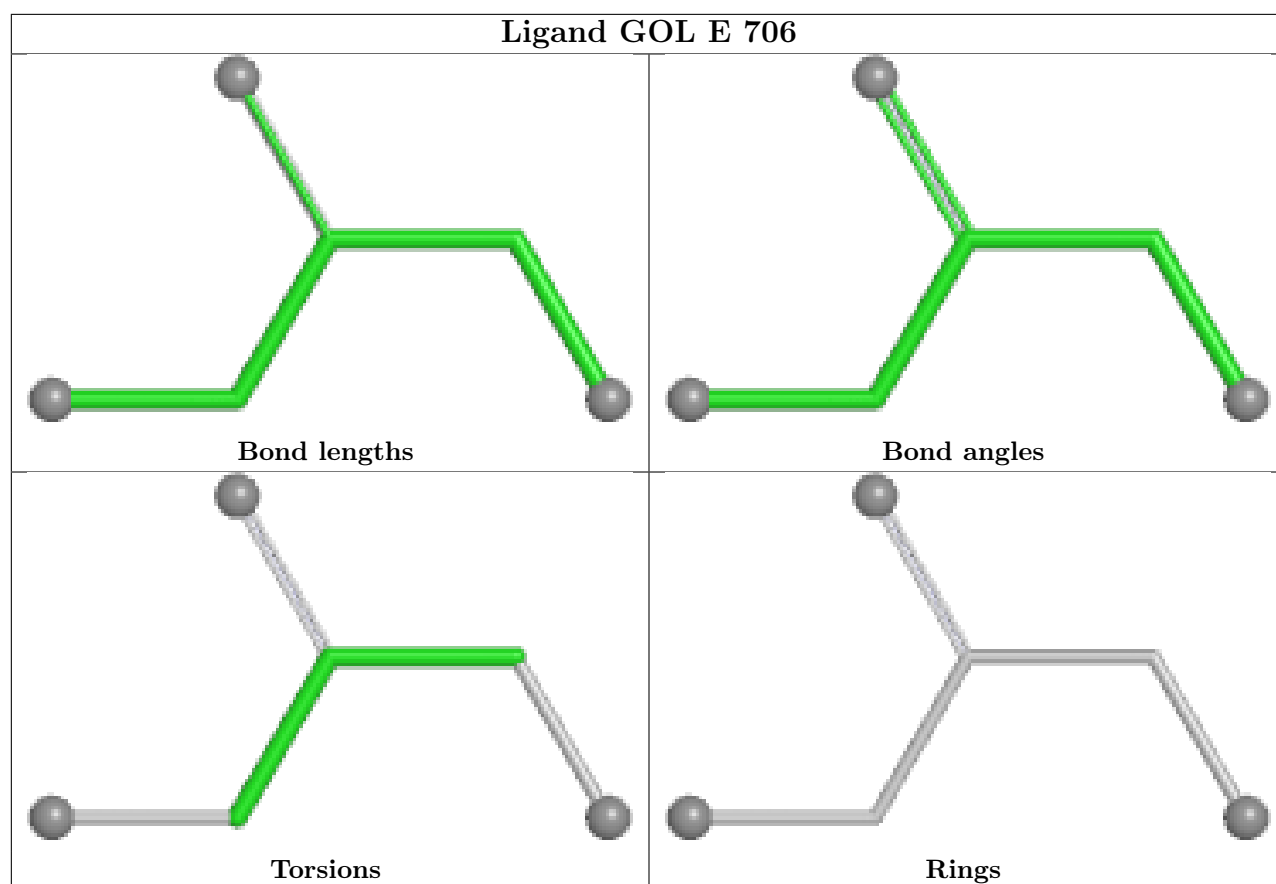


Rings

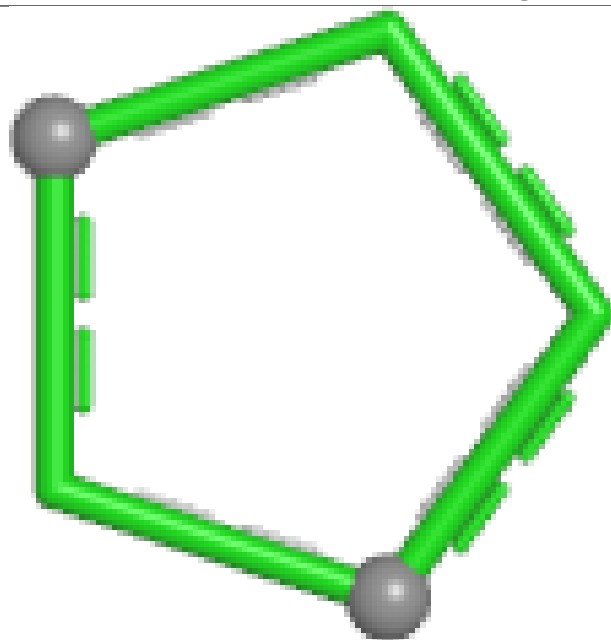


Ligand IMD B 708

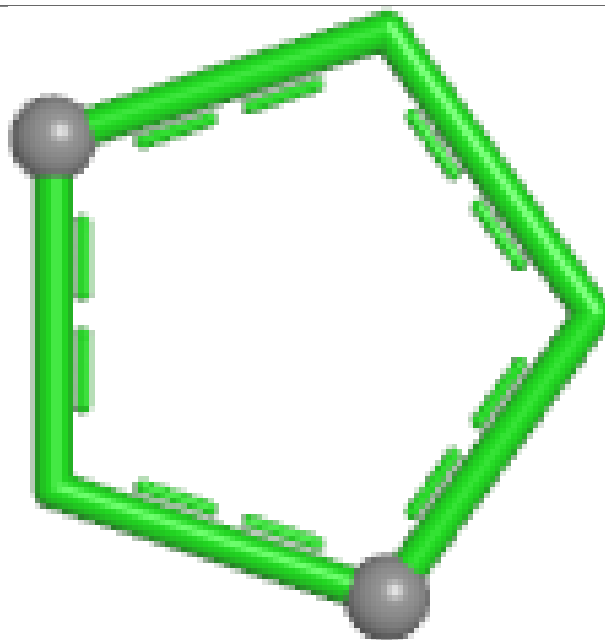




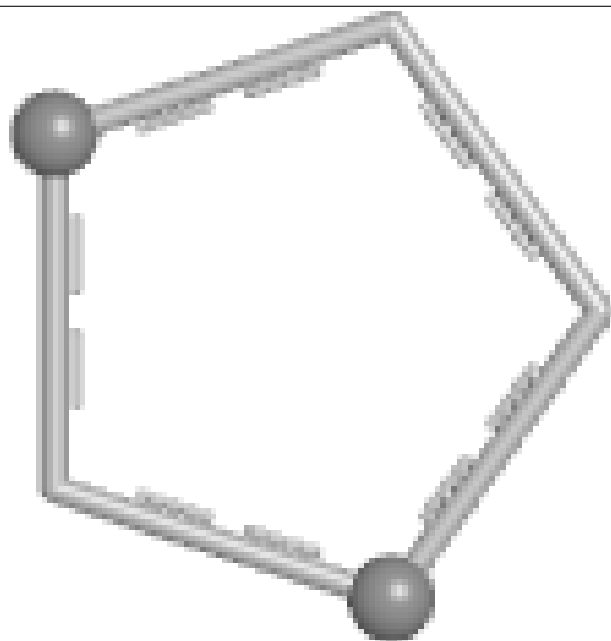
Ligand IMD F 709



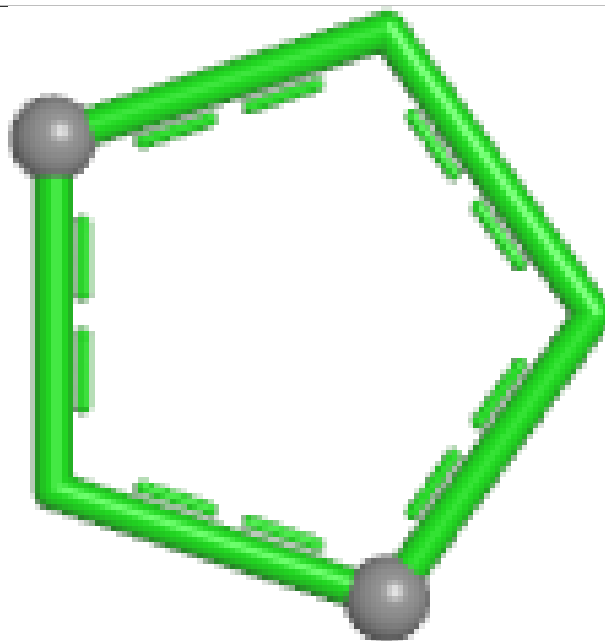
Bond lengths



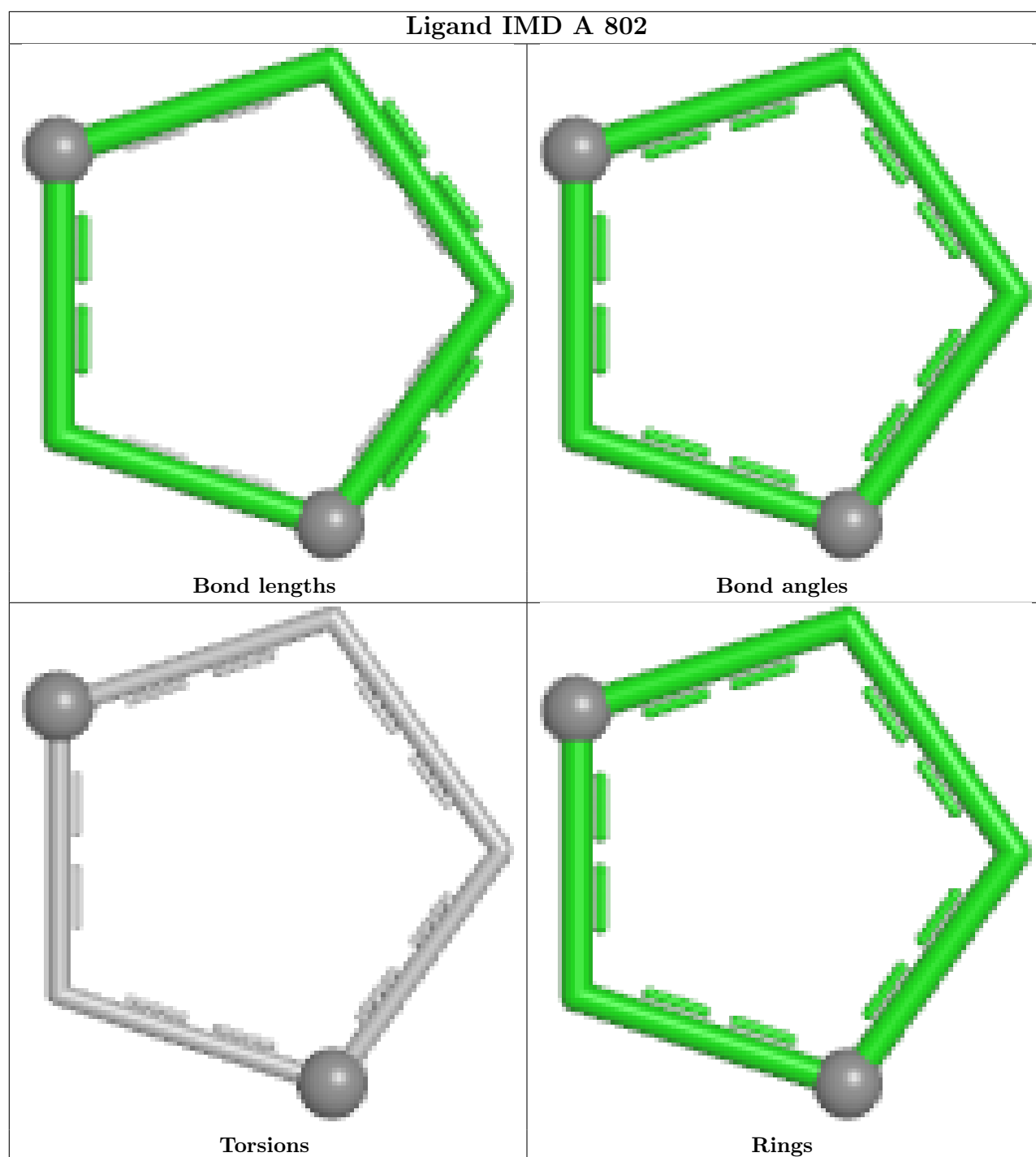
Bond angles

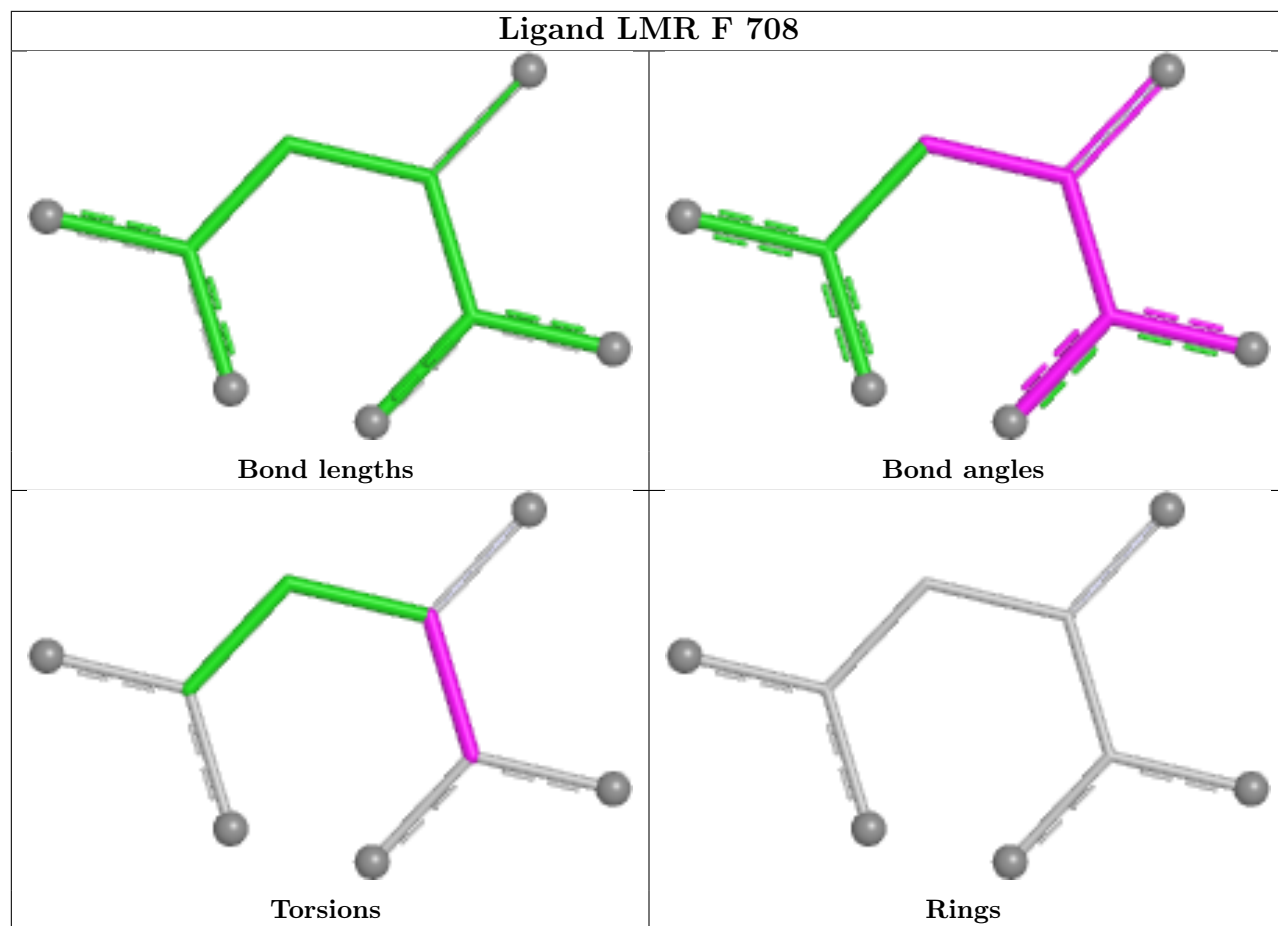


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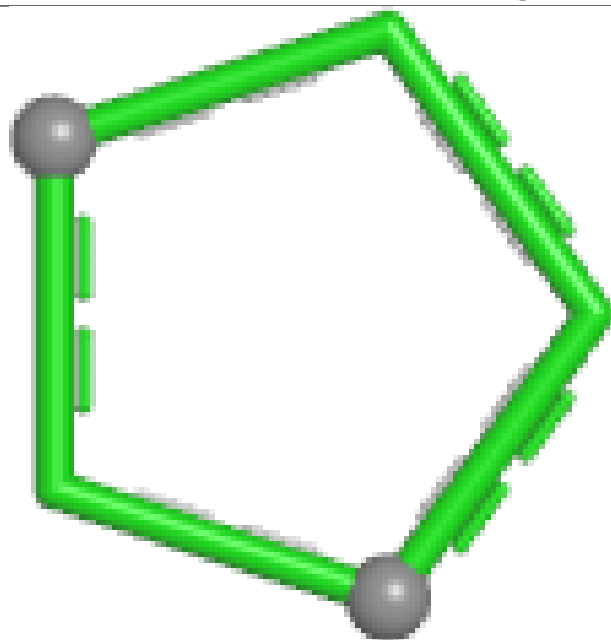


Rings

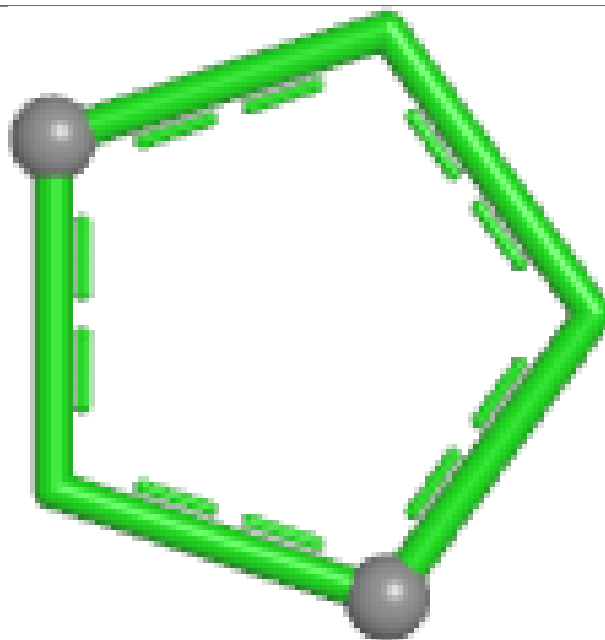




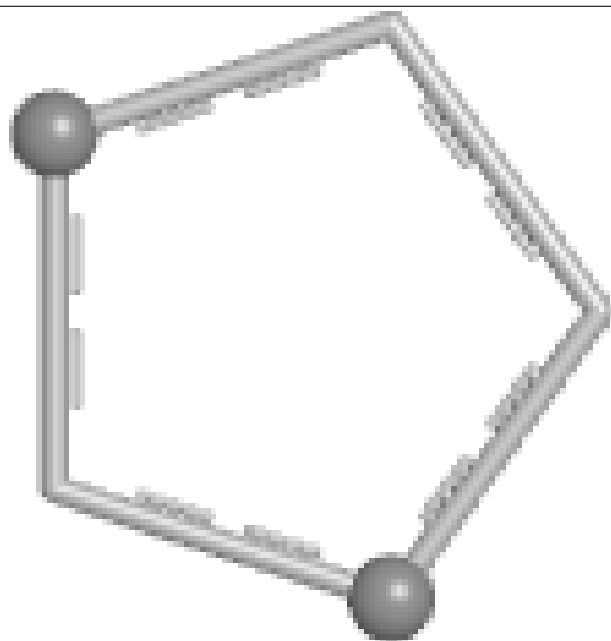
Ligand IMD C 806



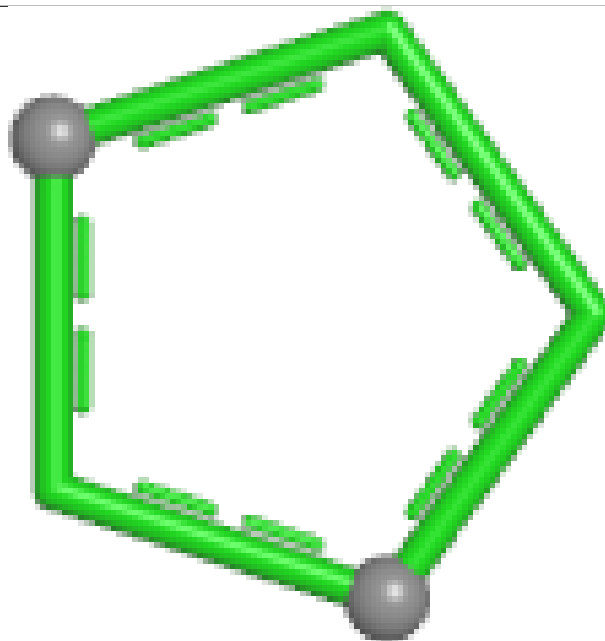
Bond lengths



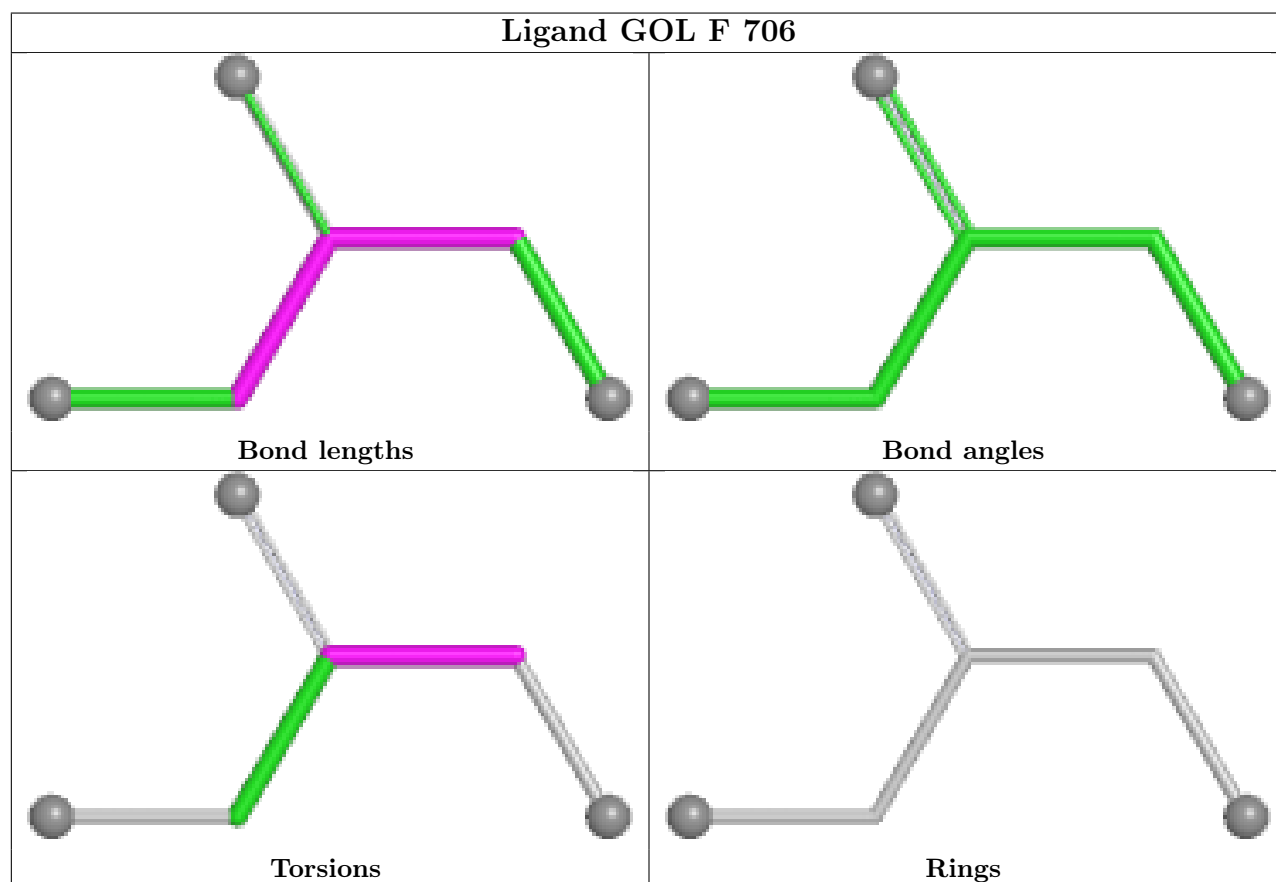
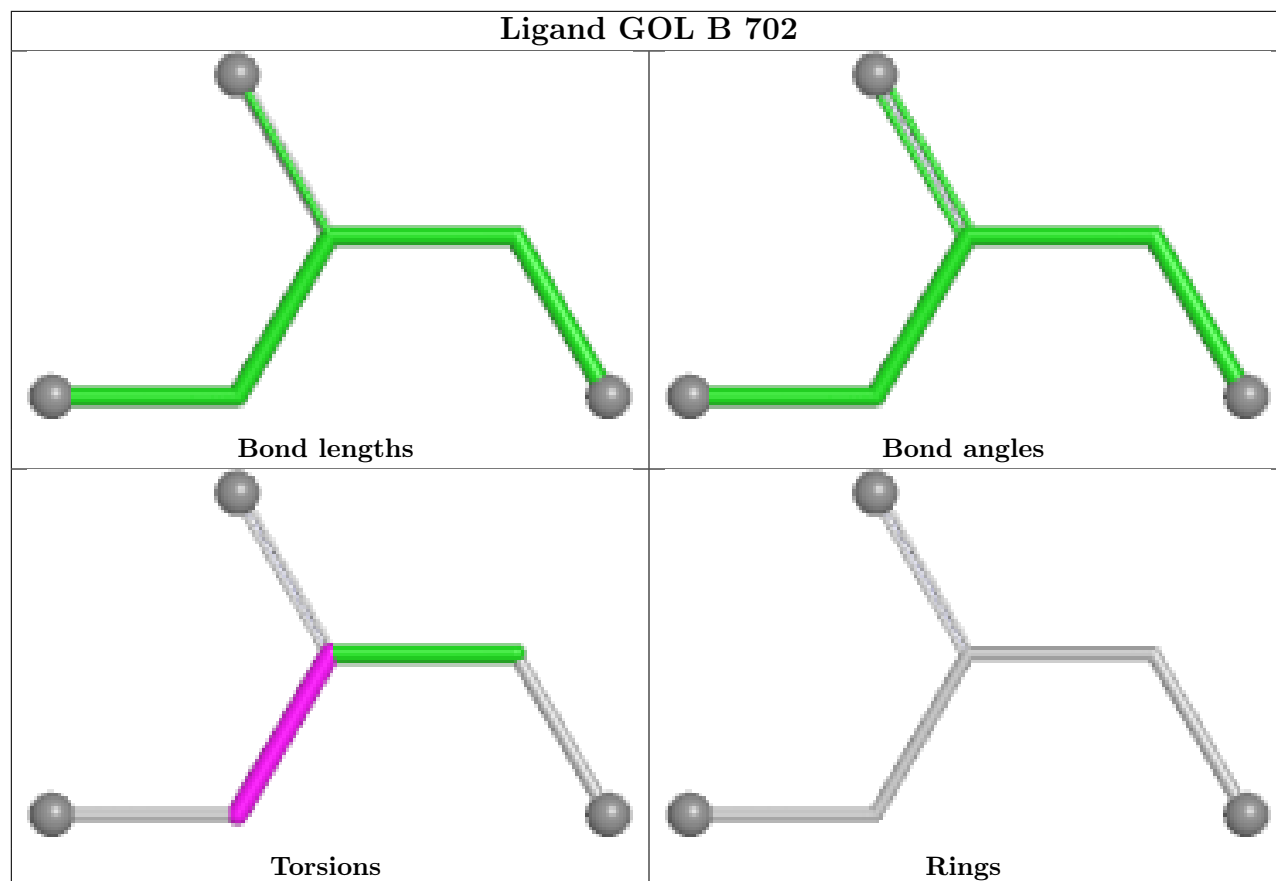
Bond angles



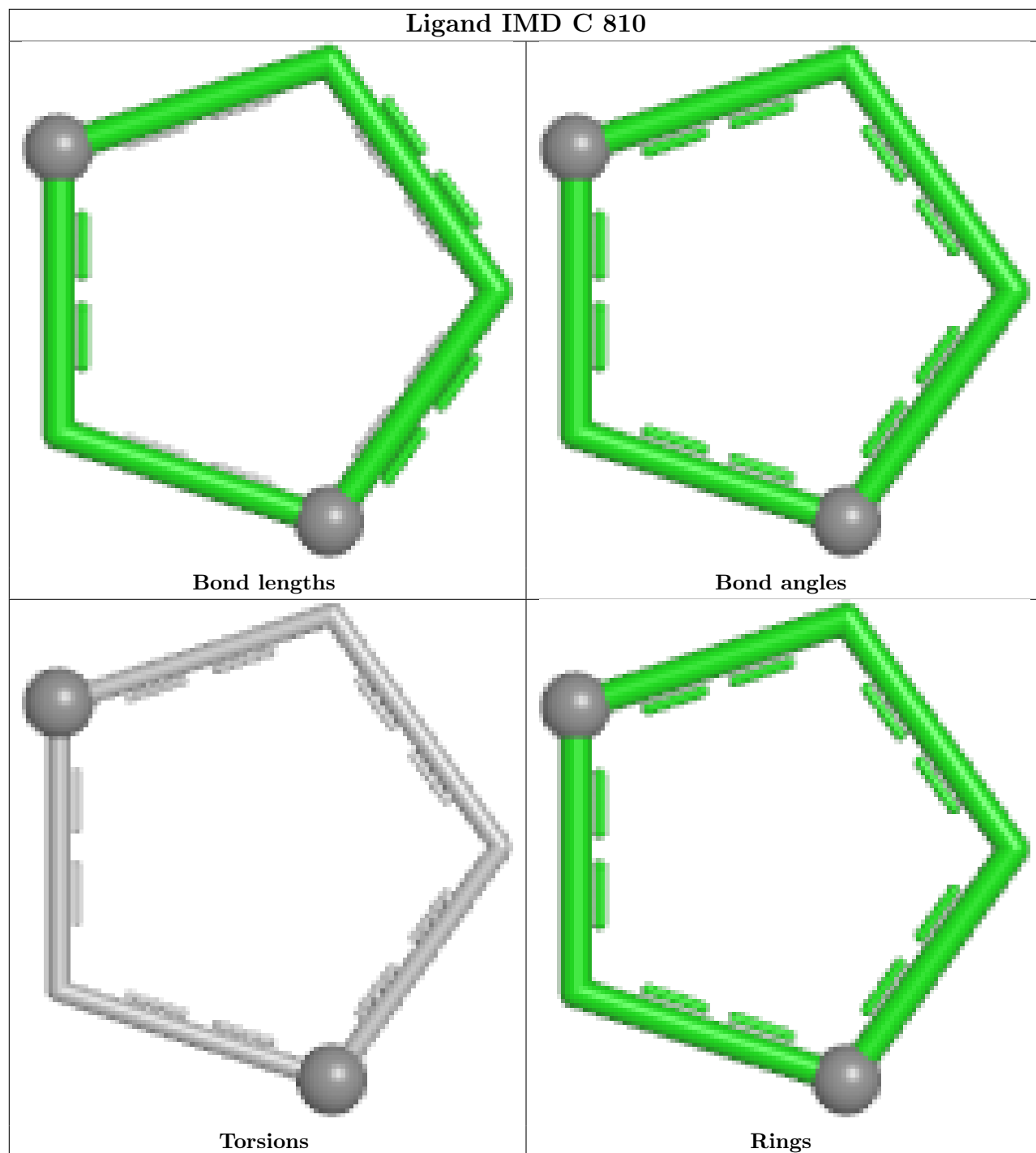
Torsions

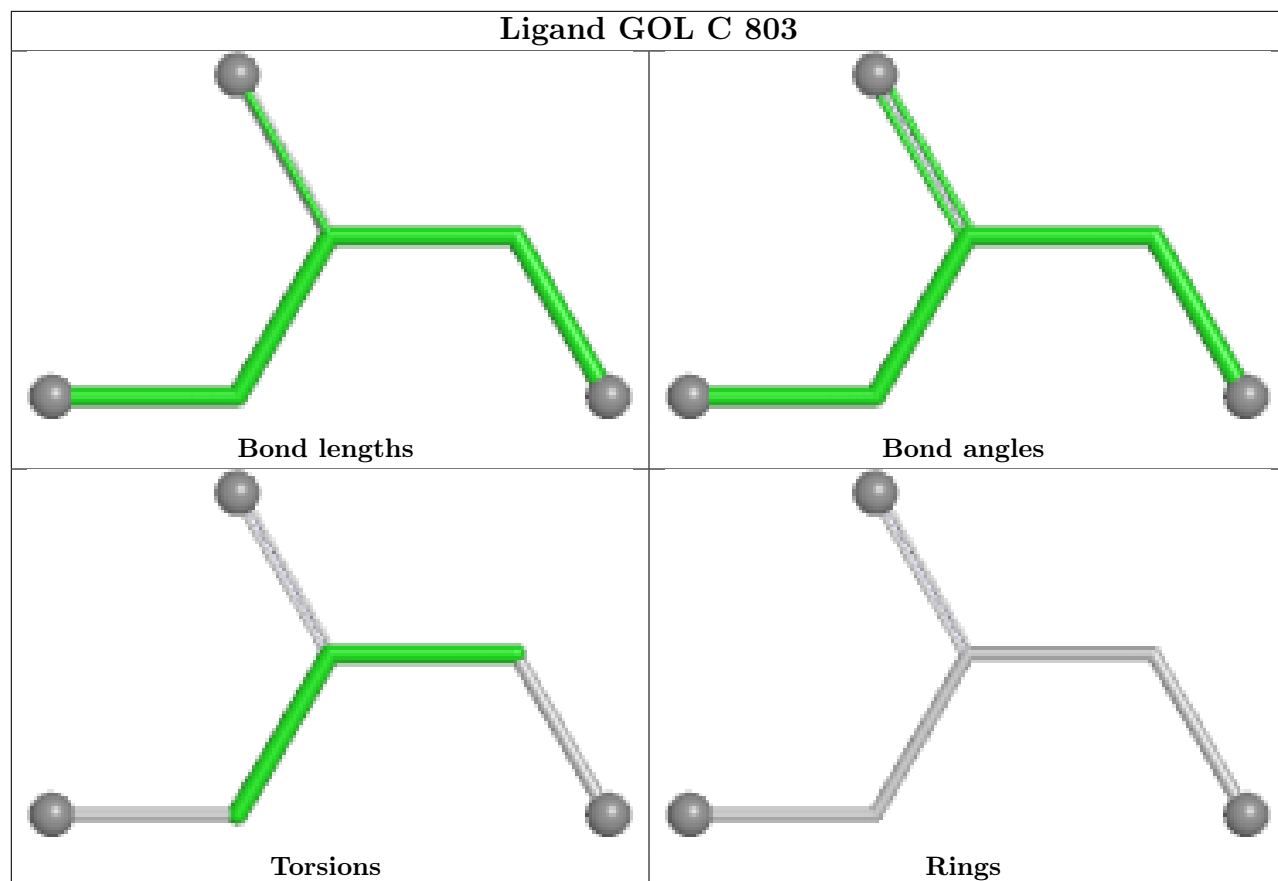


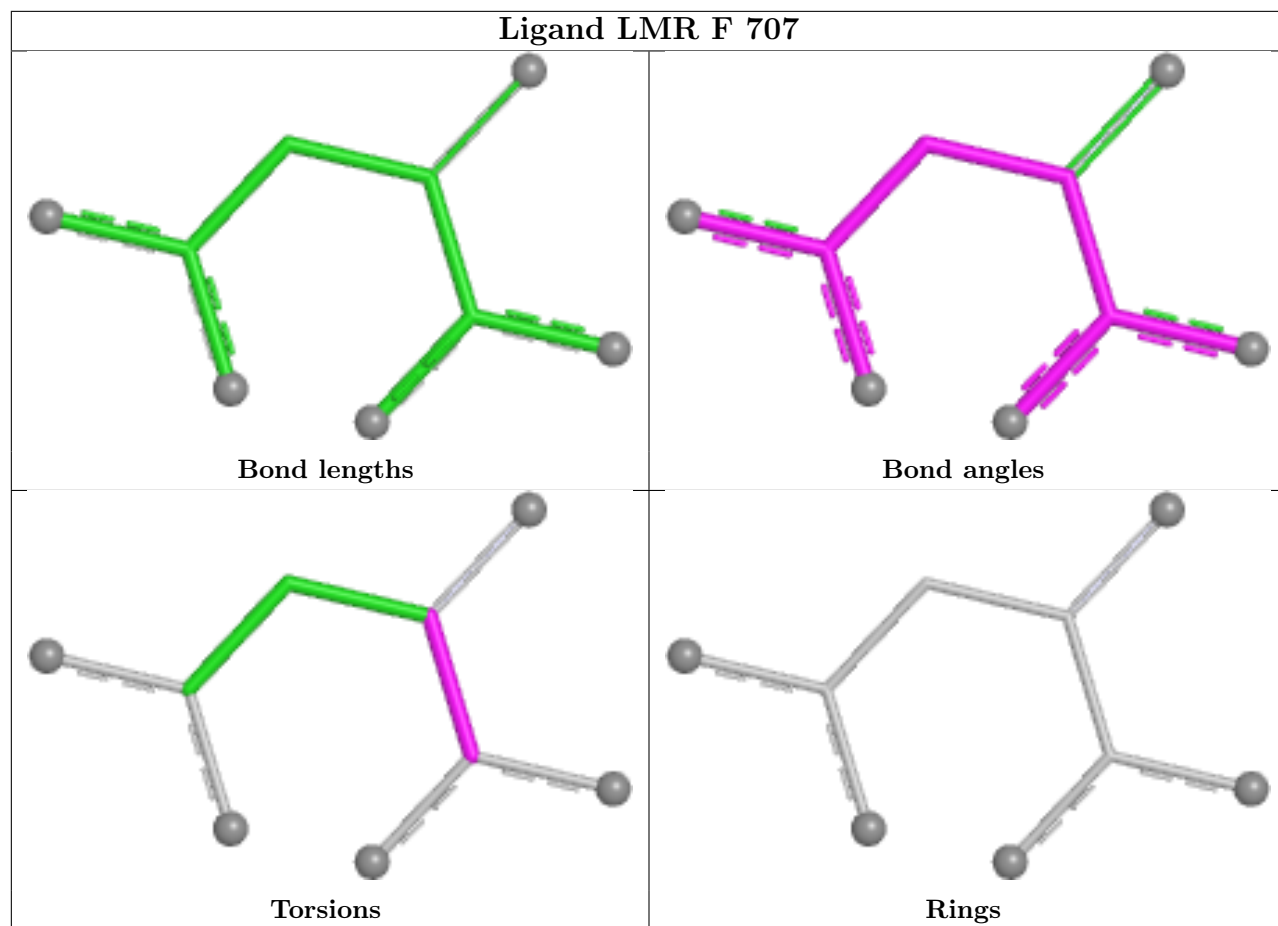
Rings

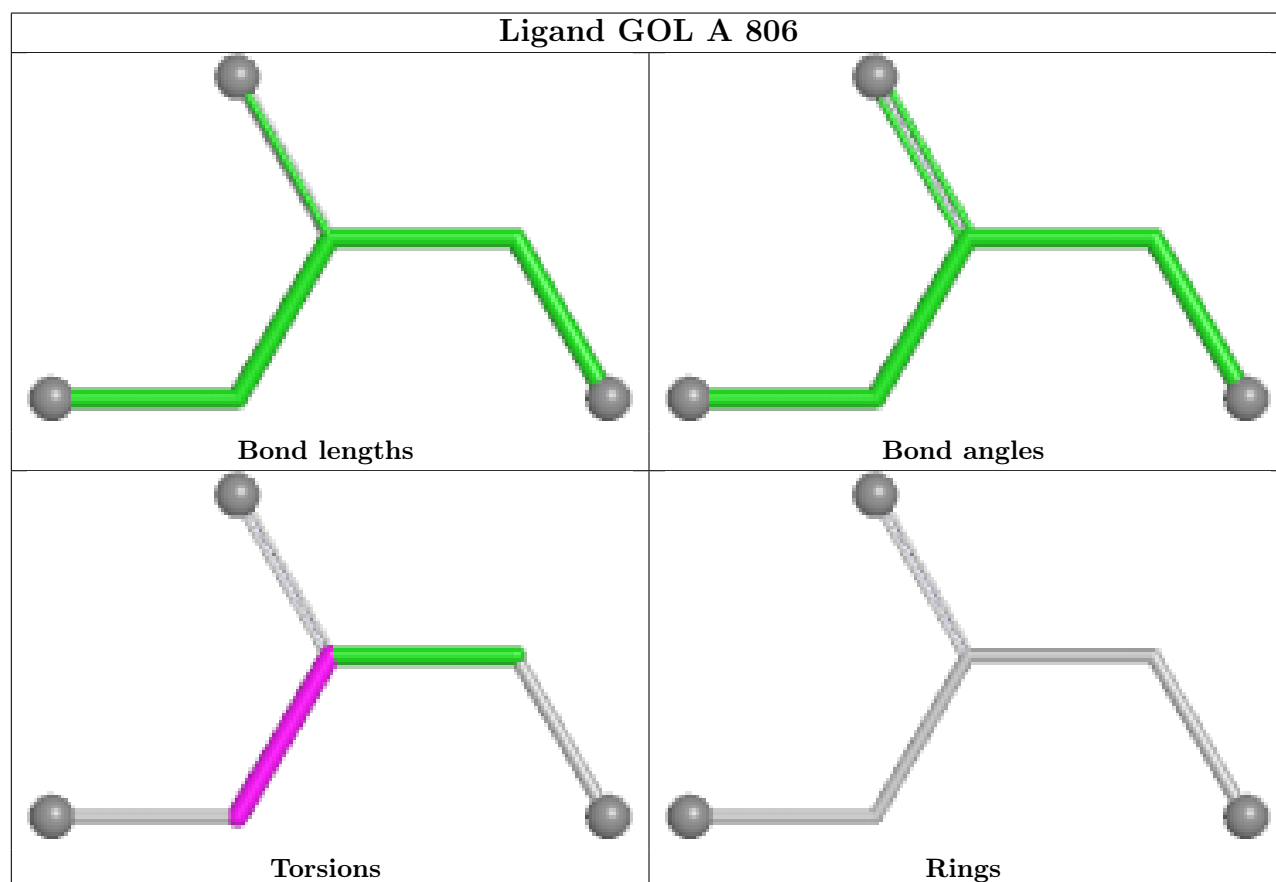
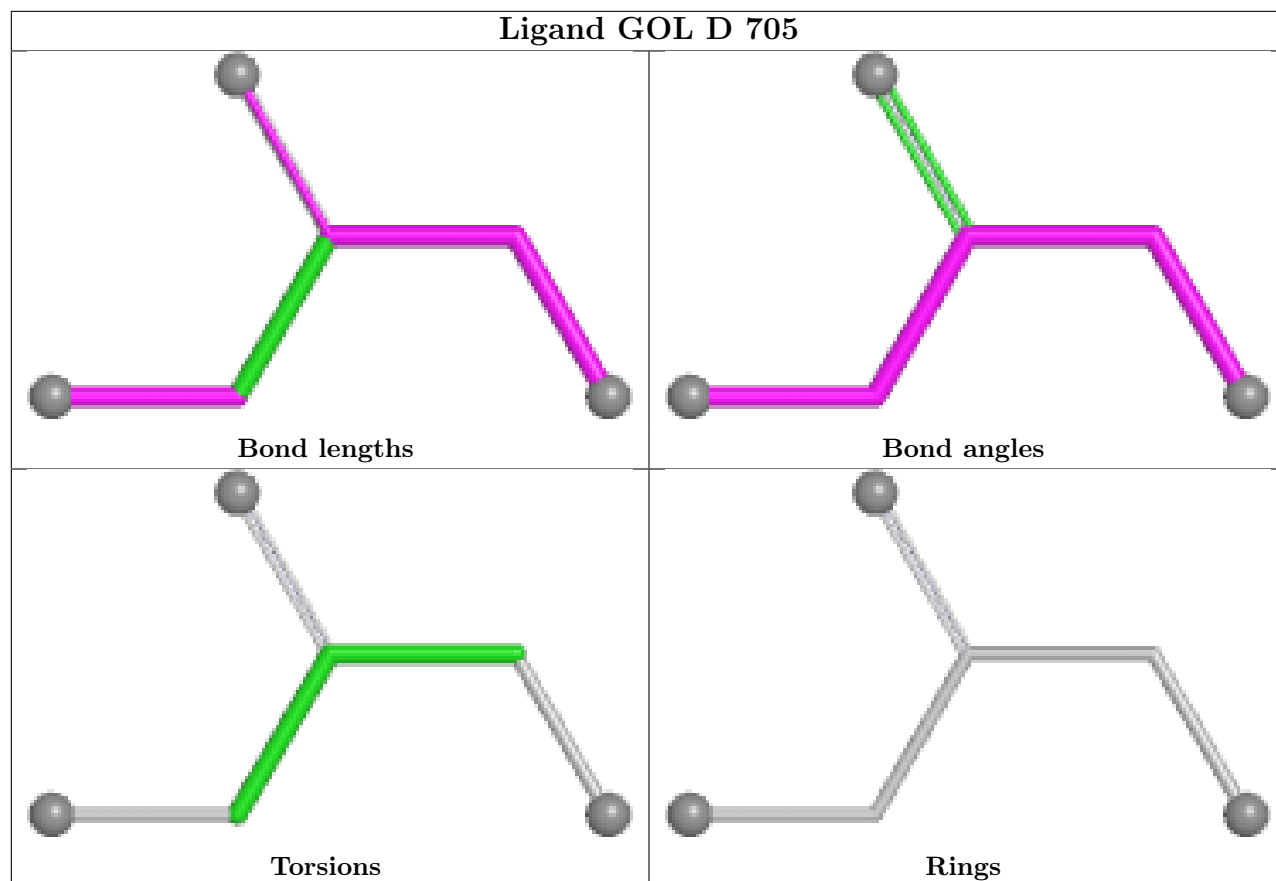


Ligand IMD C 810

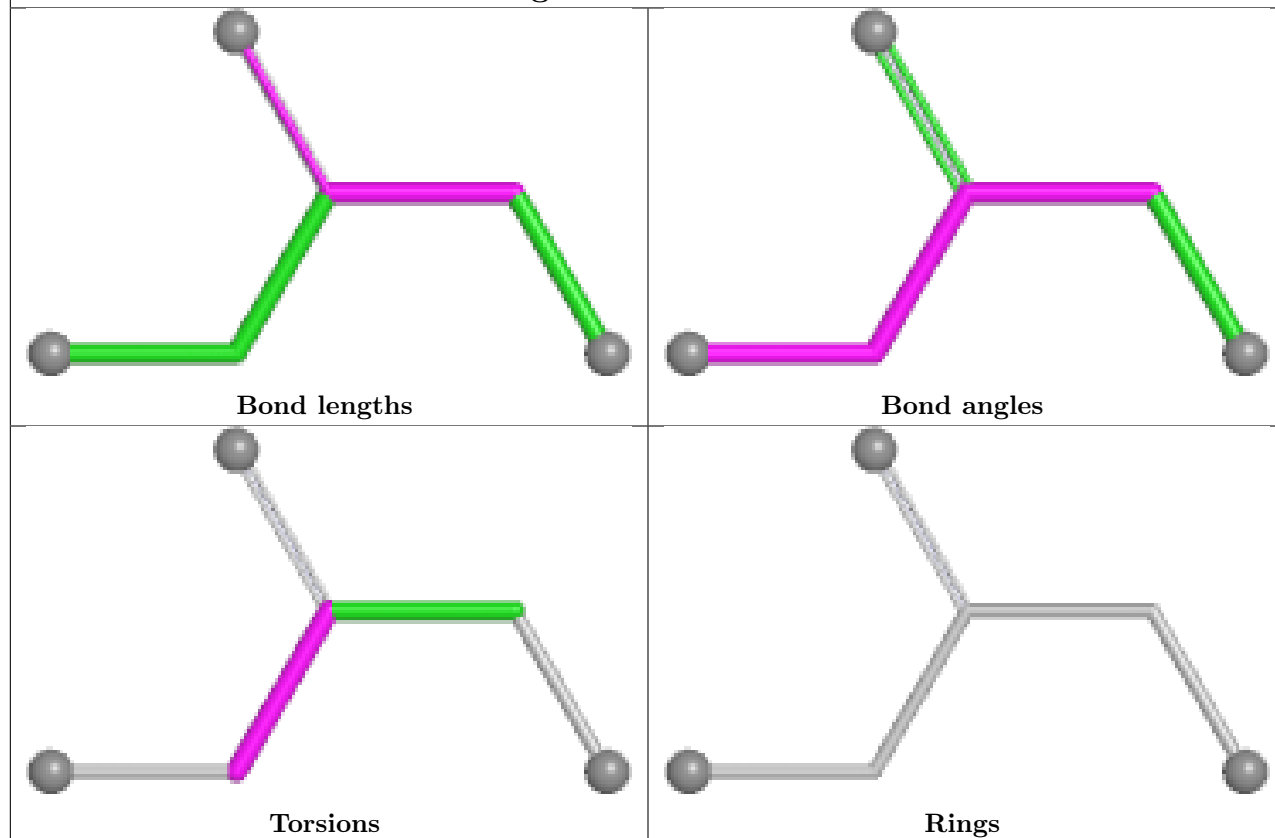




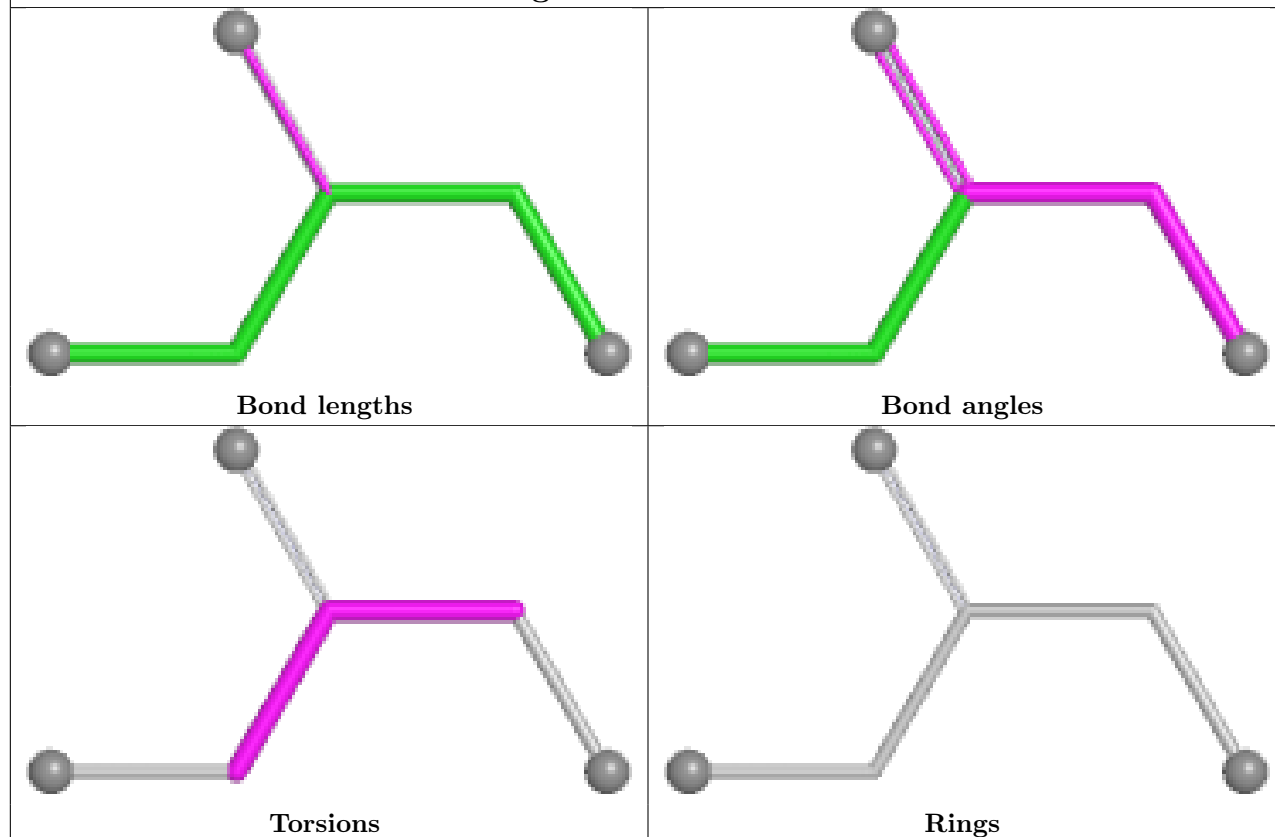


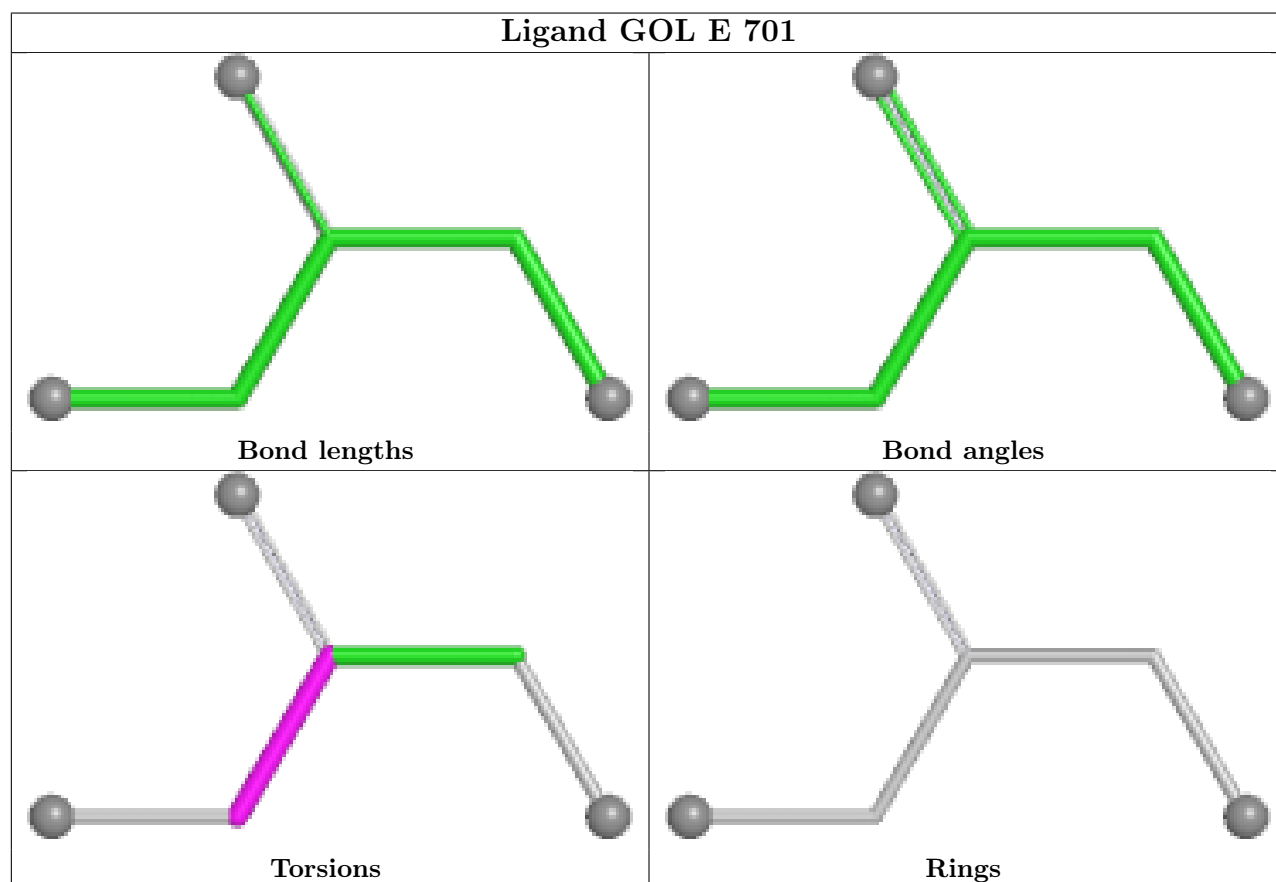
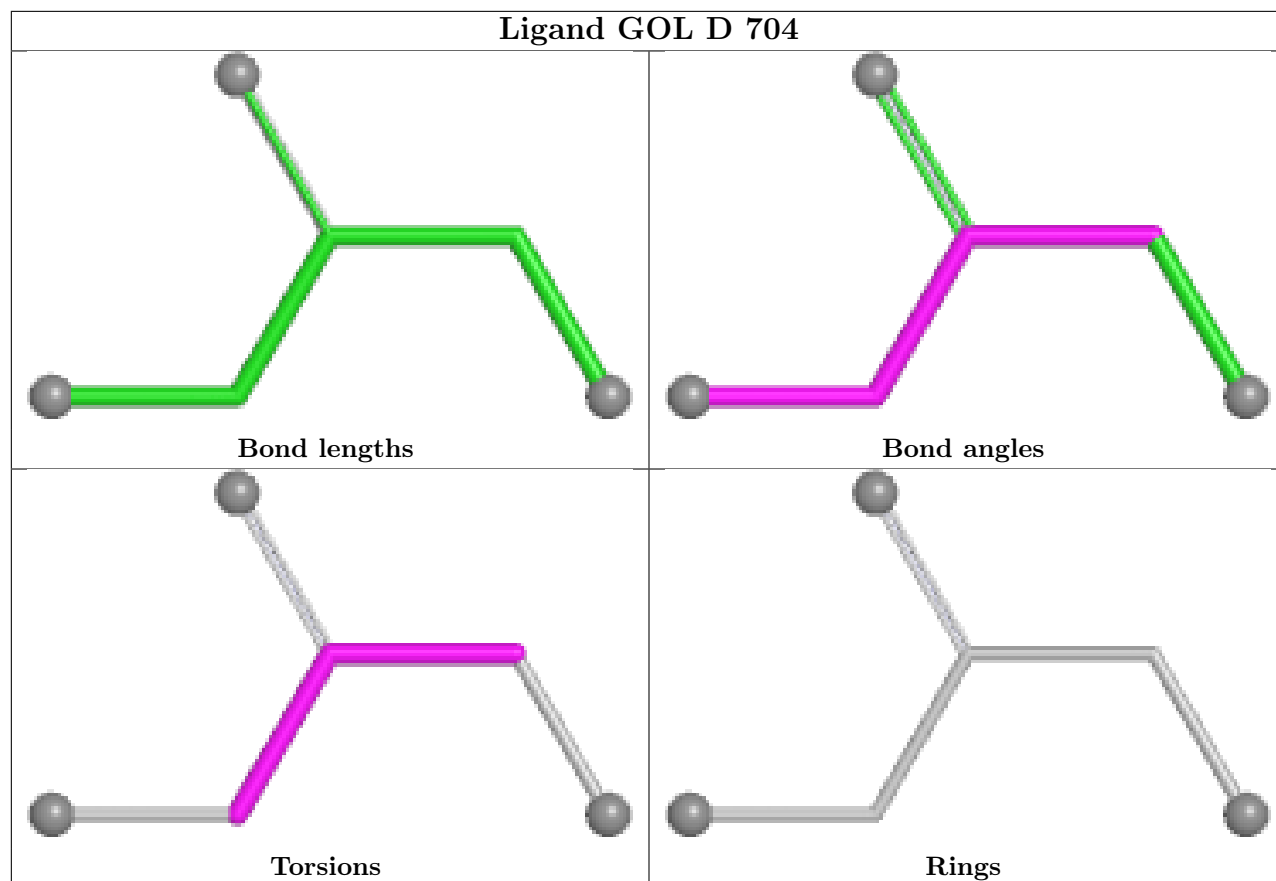


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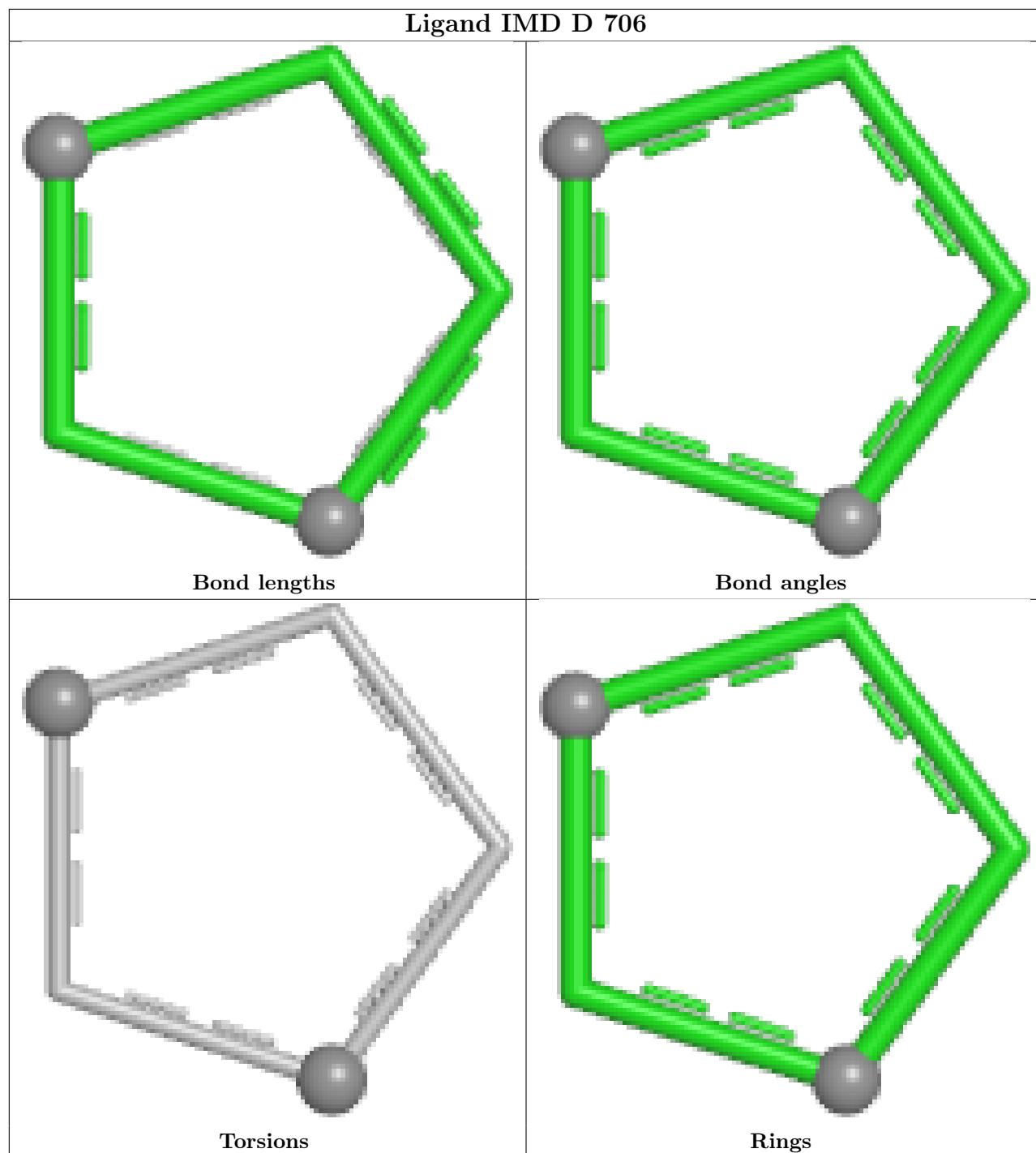


Ligand GOL F 702

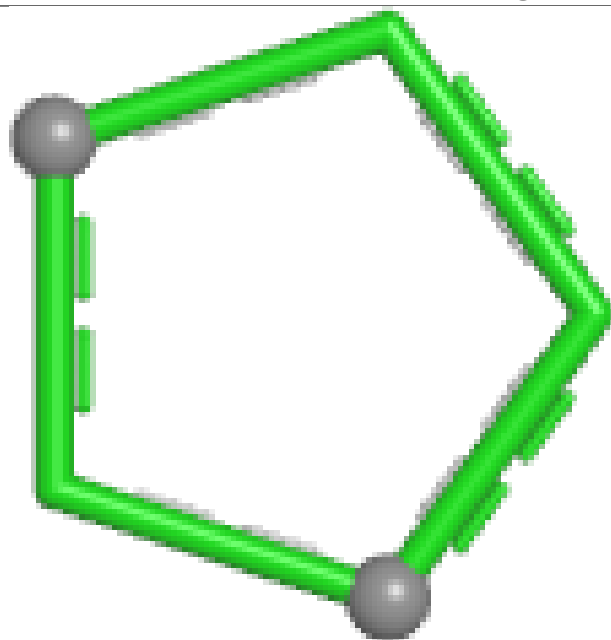




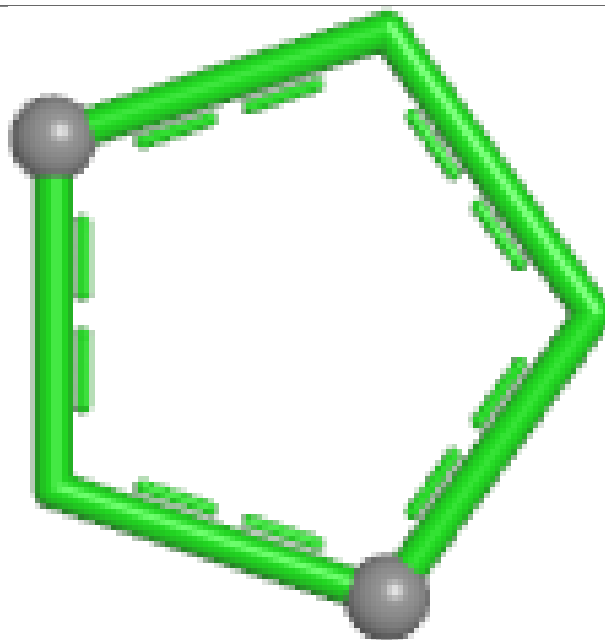
Ligand IMD D 706



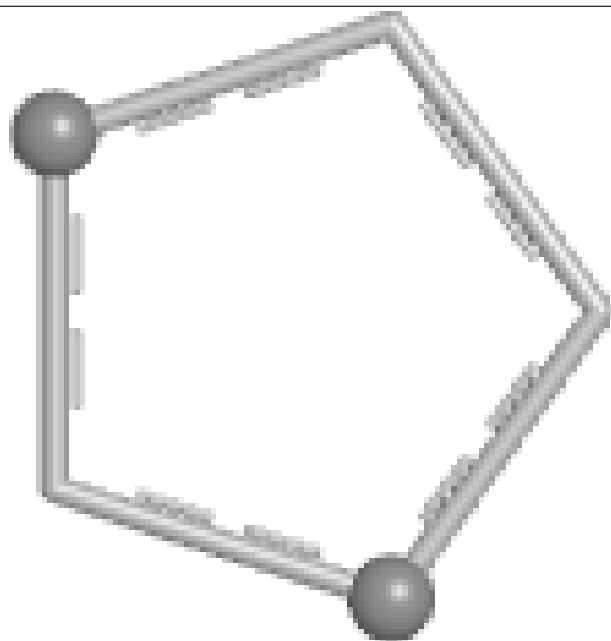
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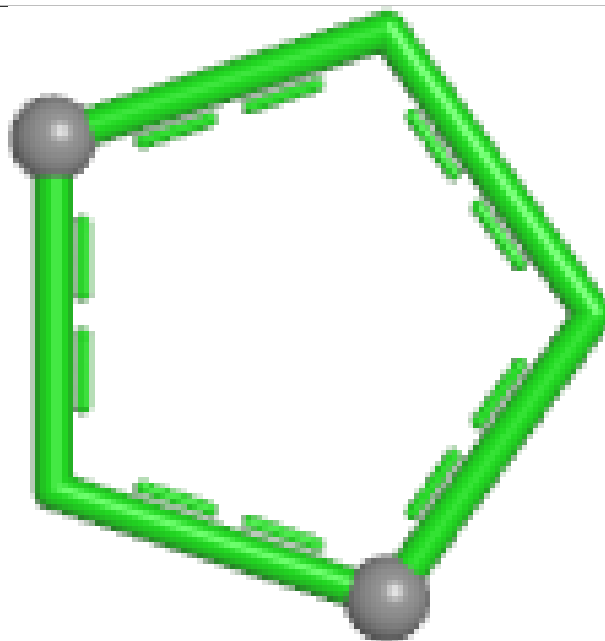
Bond lengths



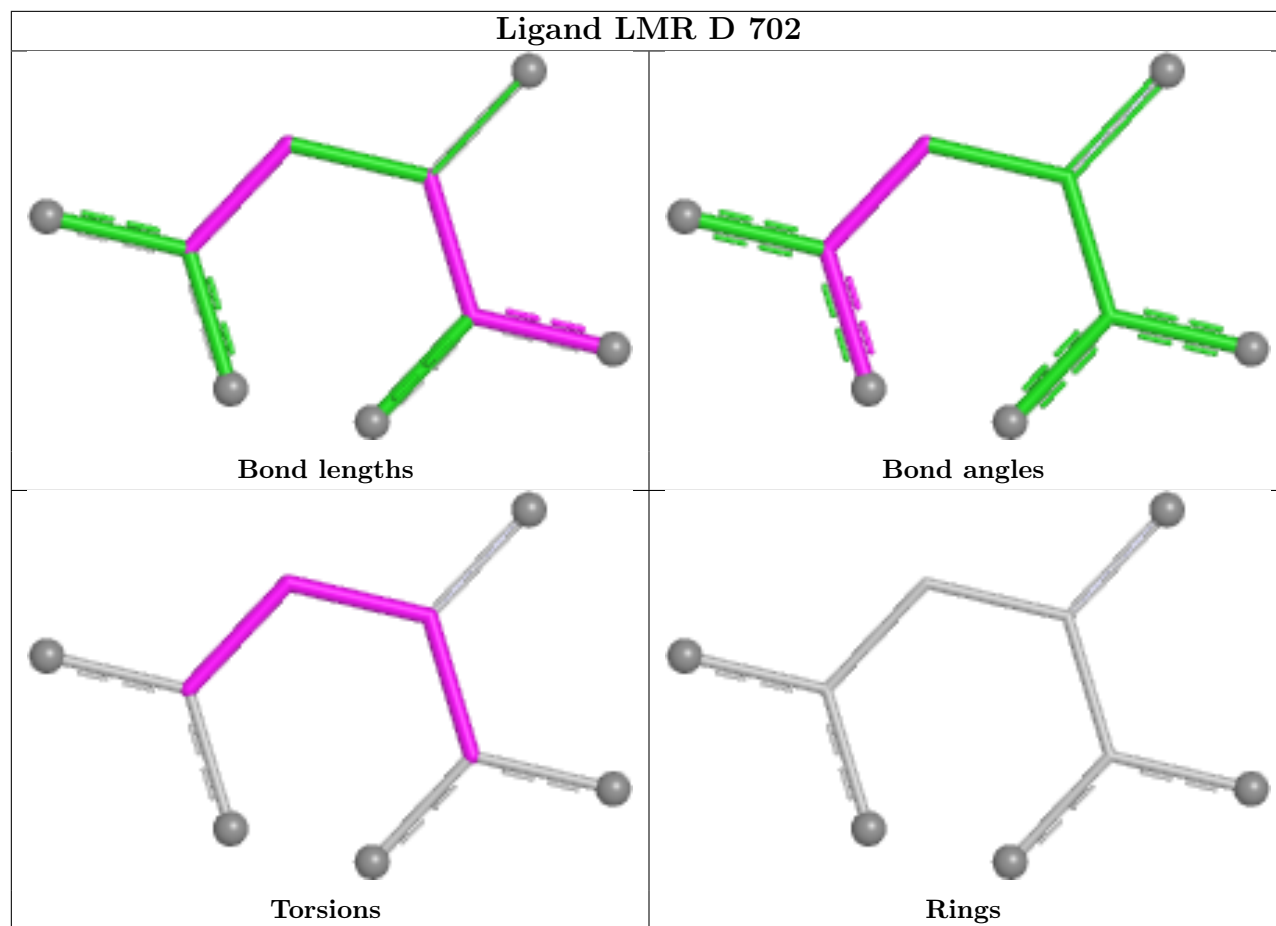
Bond angles



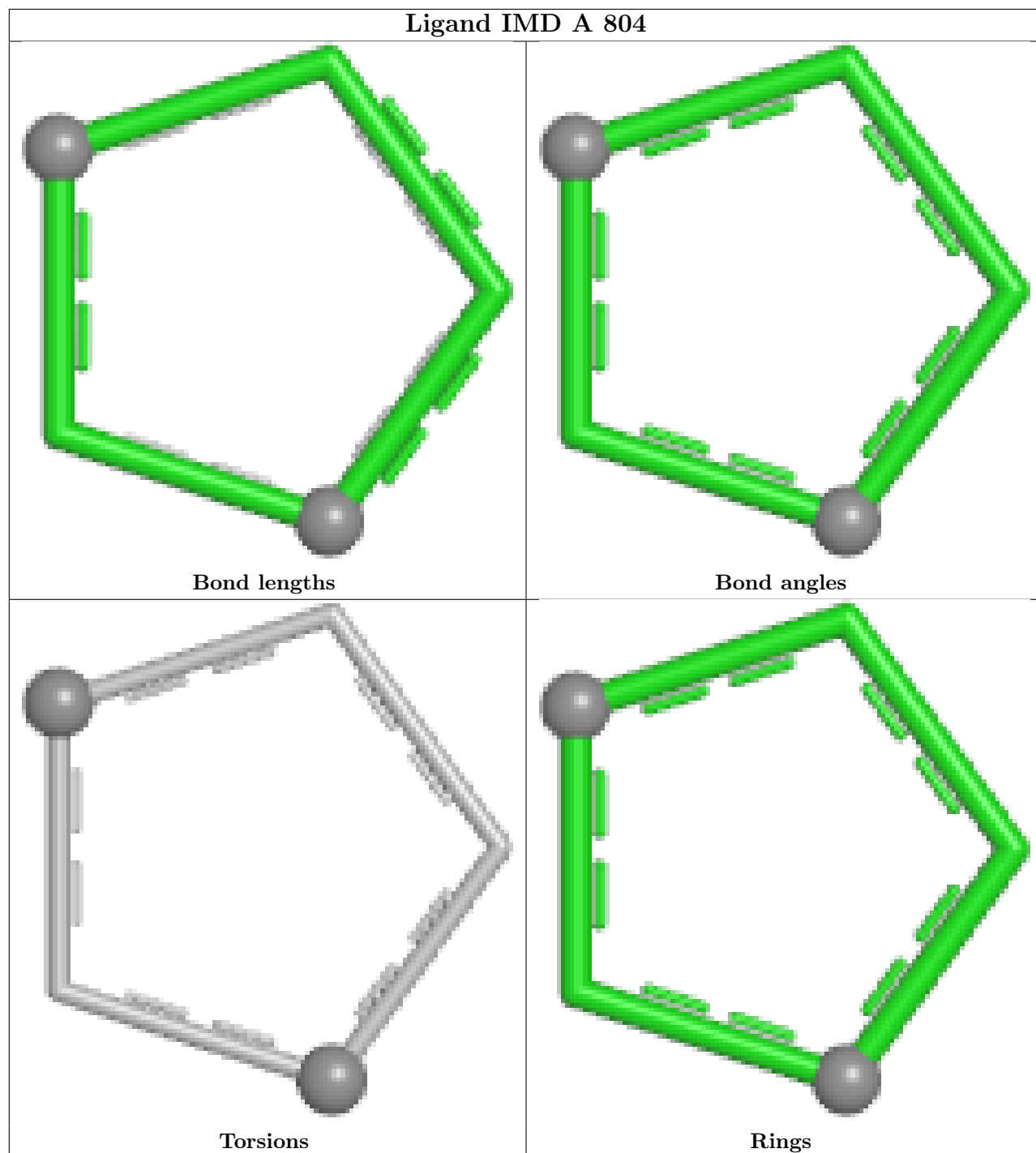
Torsions



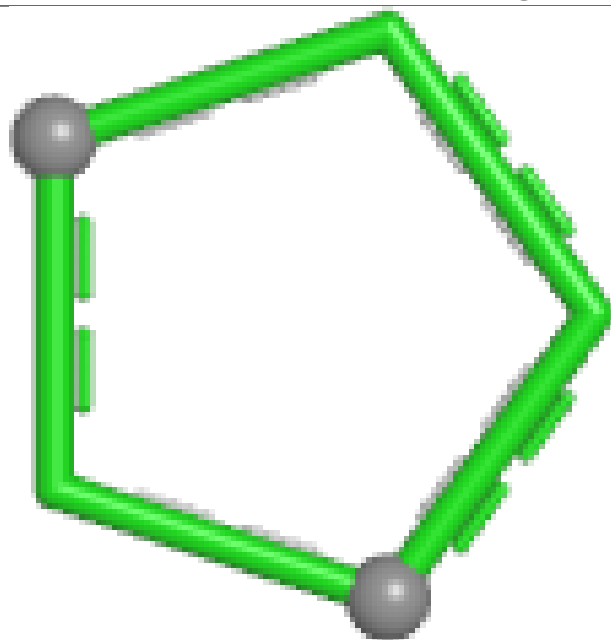
Rings



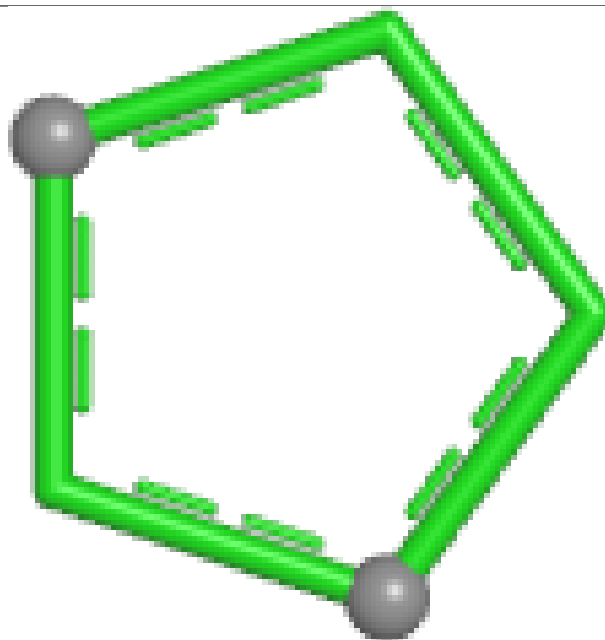
Ligand IMD A 804



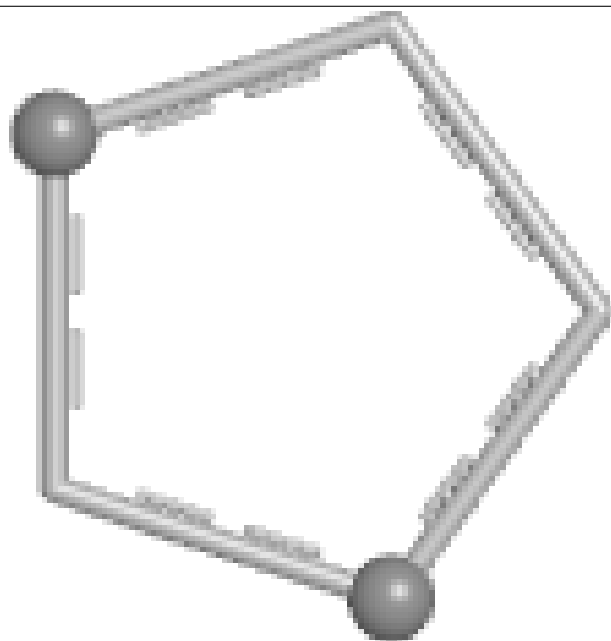
Ligand IMD E 702



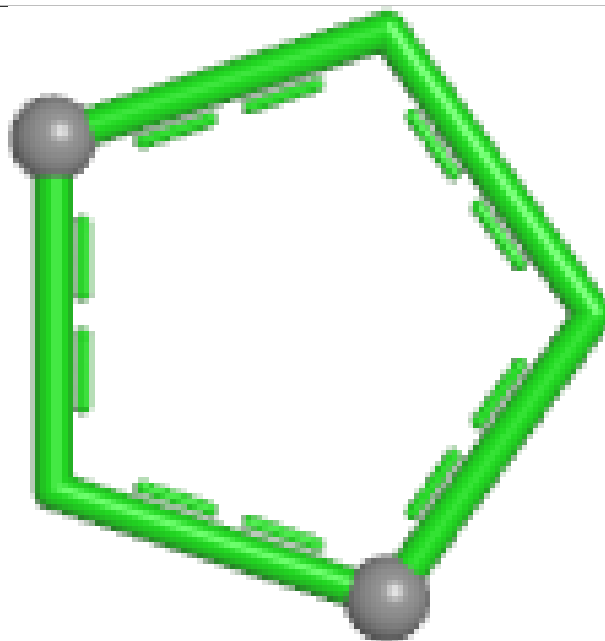
Bond lengths



Bond angles

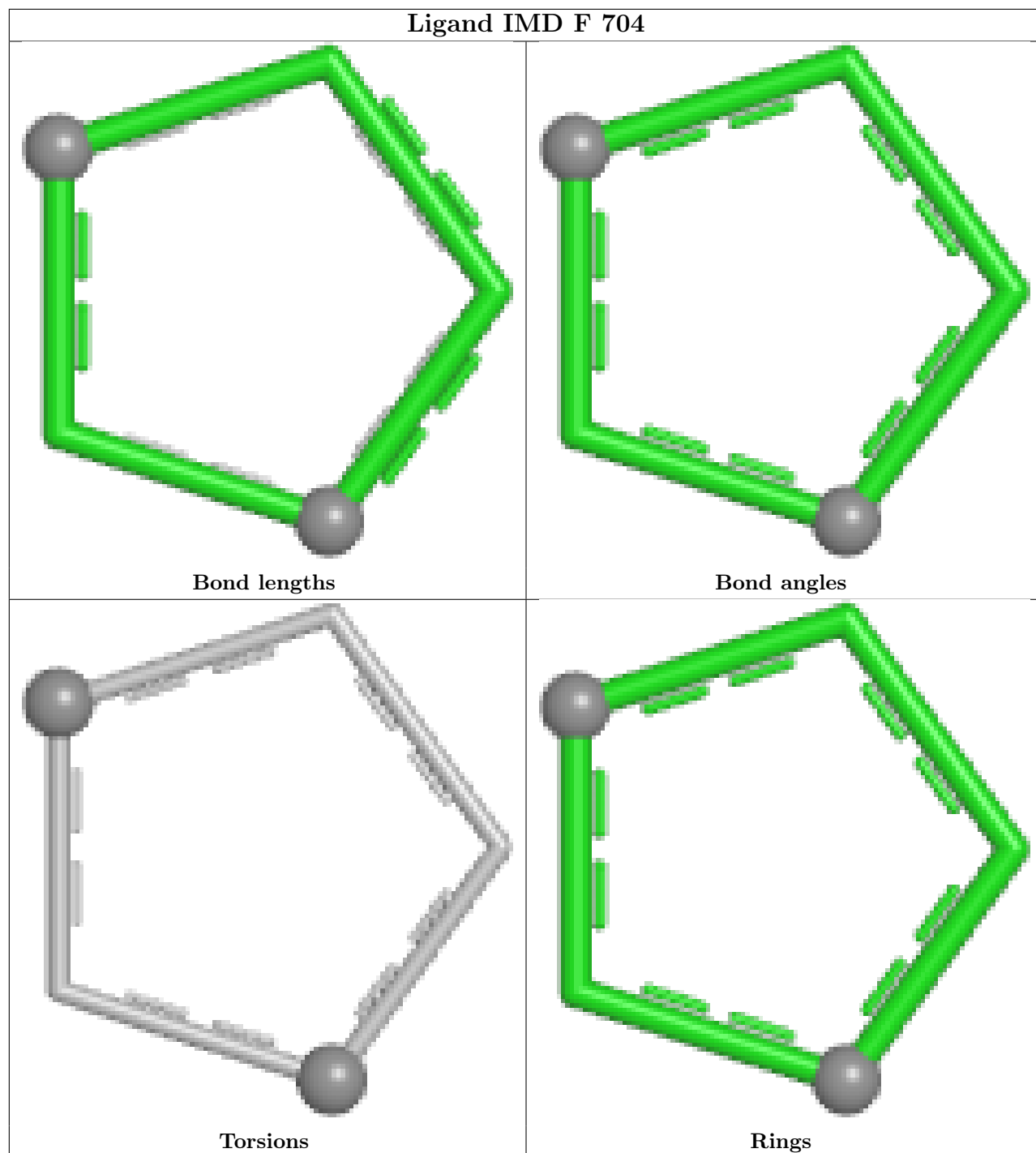


Torsions

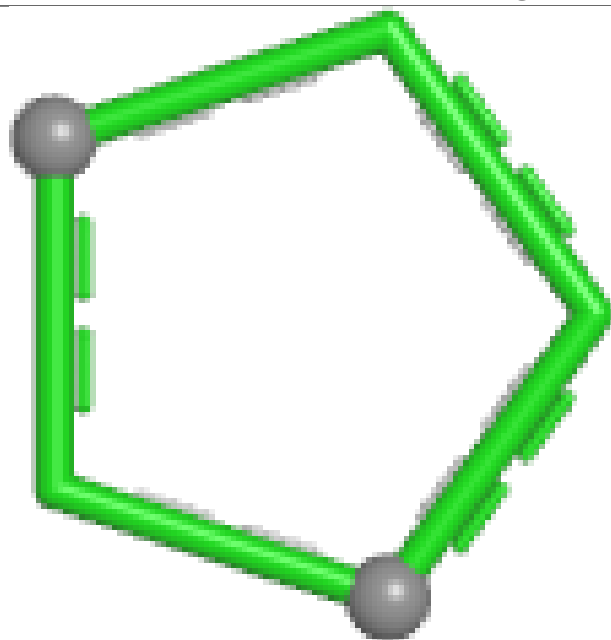


Rings

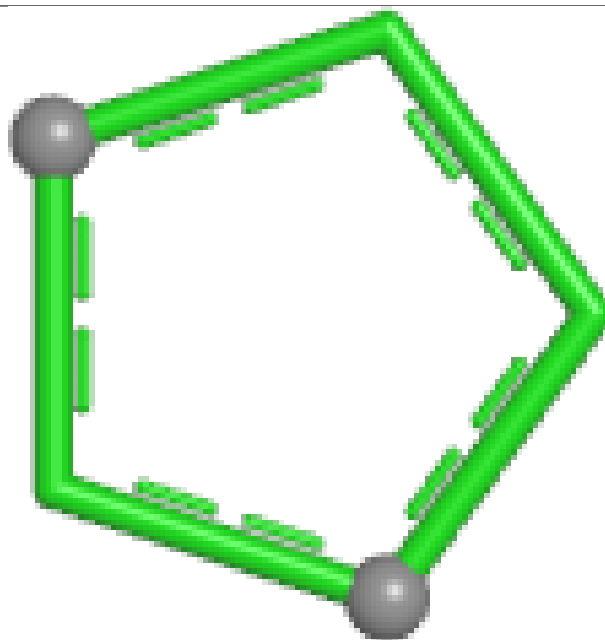
Ligand IMD F 704



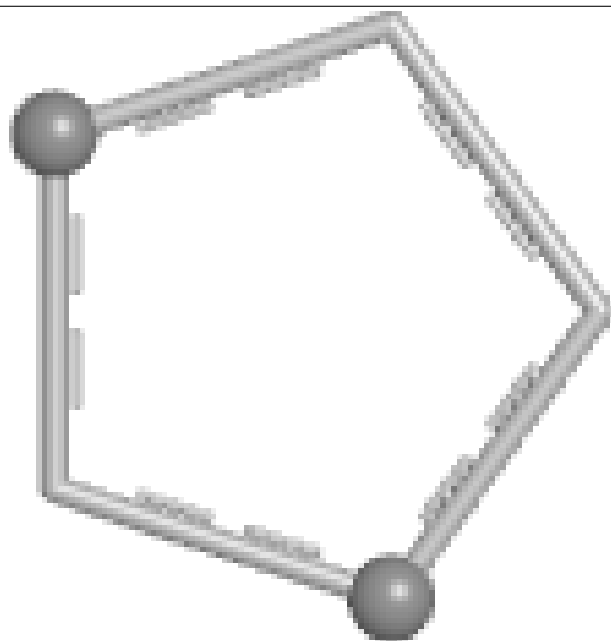
Ligand IMD D 703



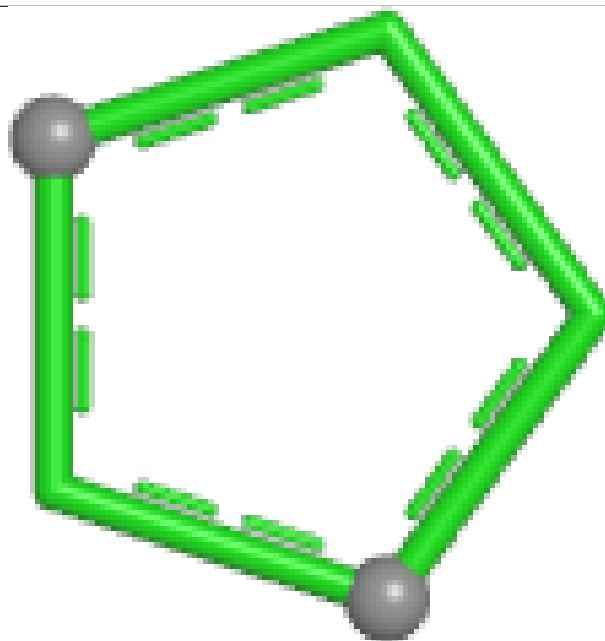
Bond lengths



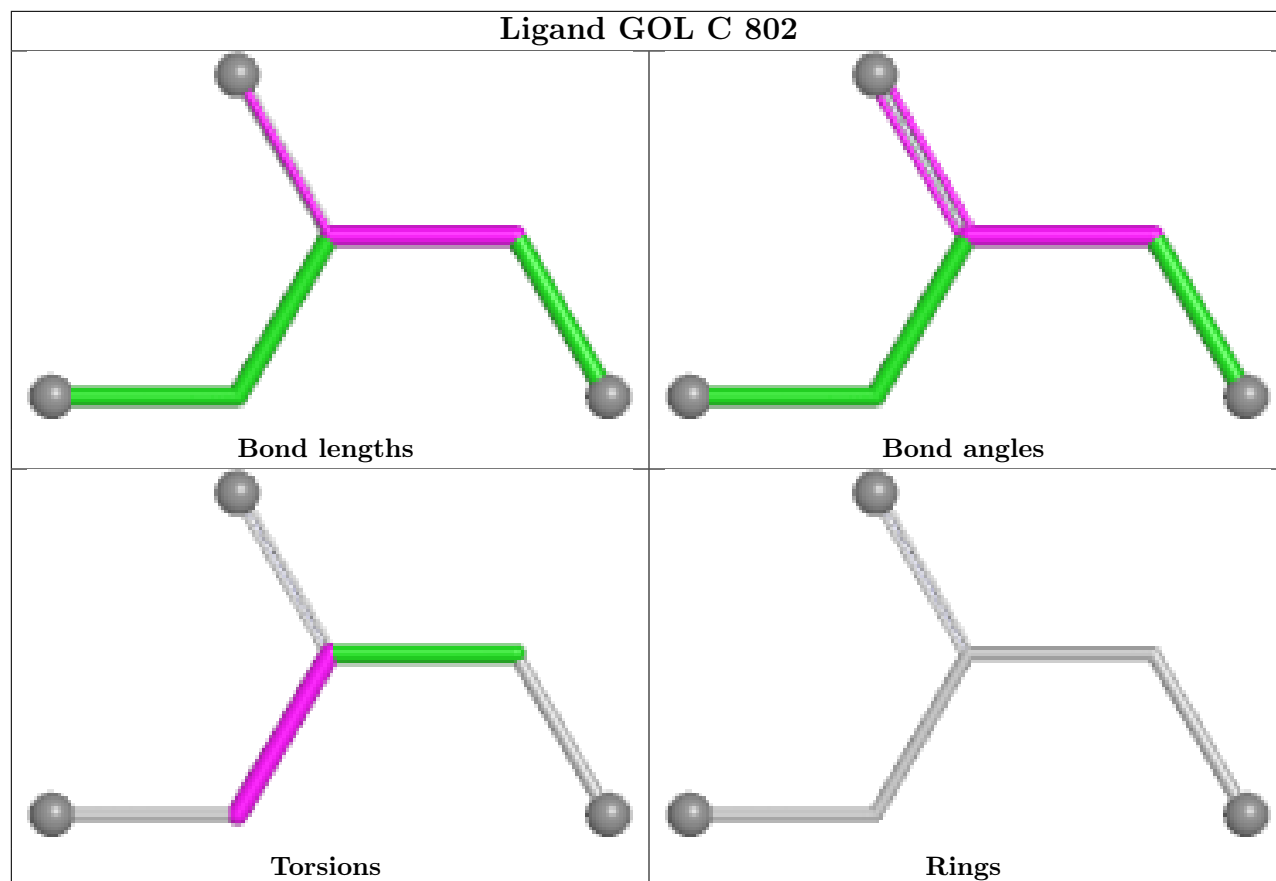
Bond angles



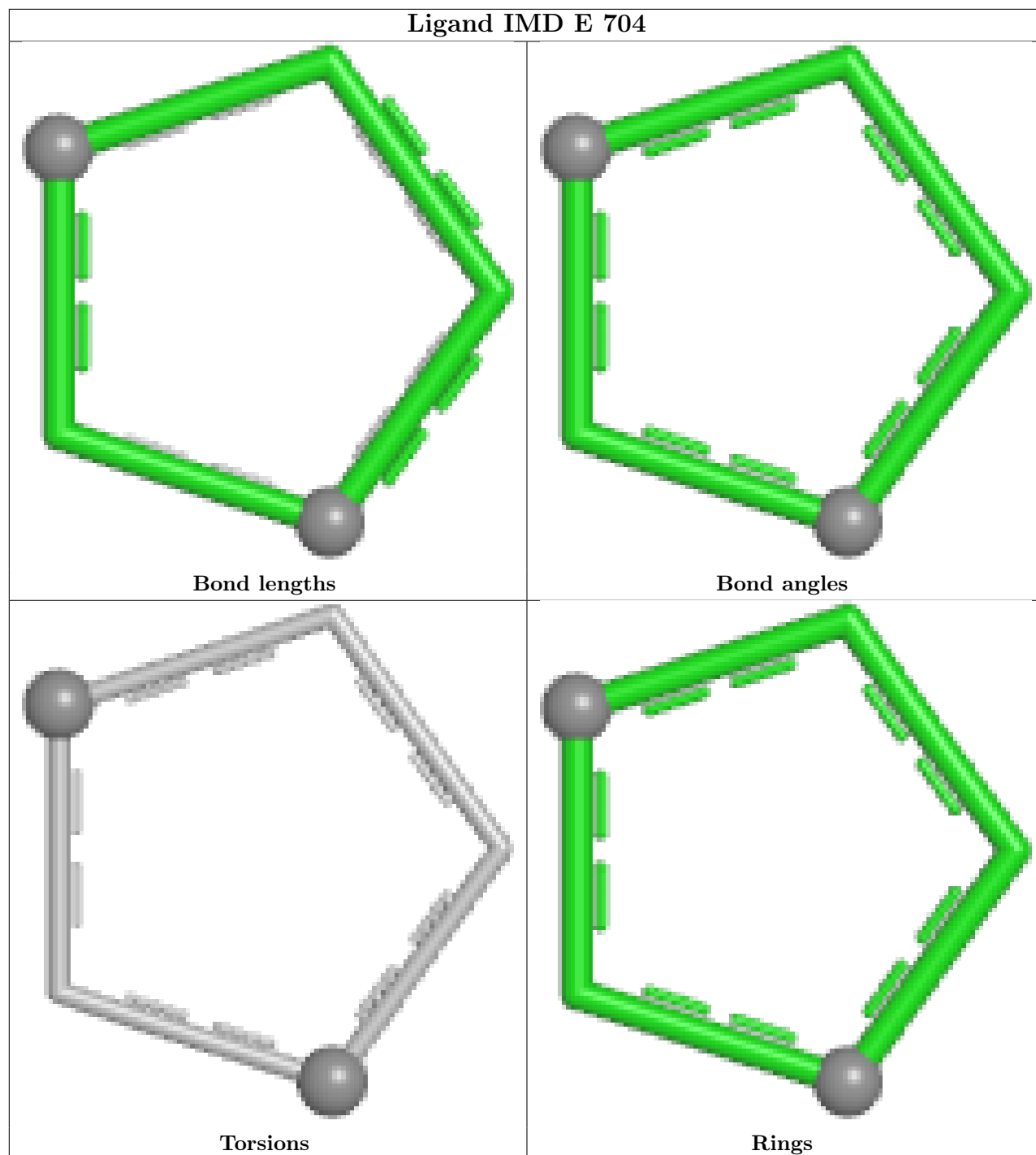
Torsions



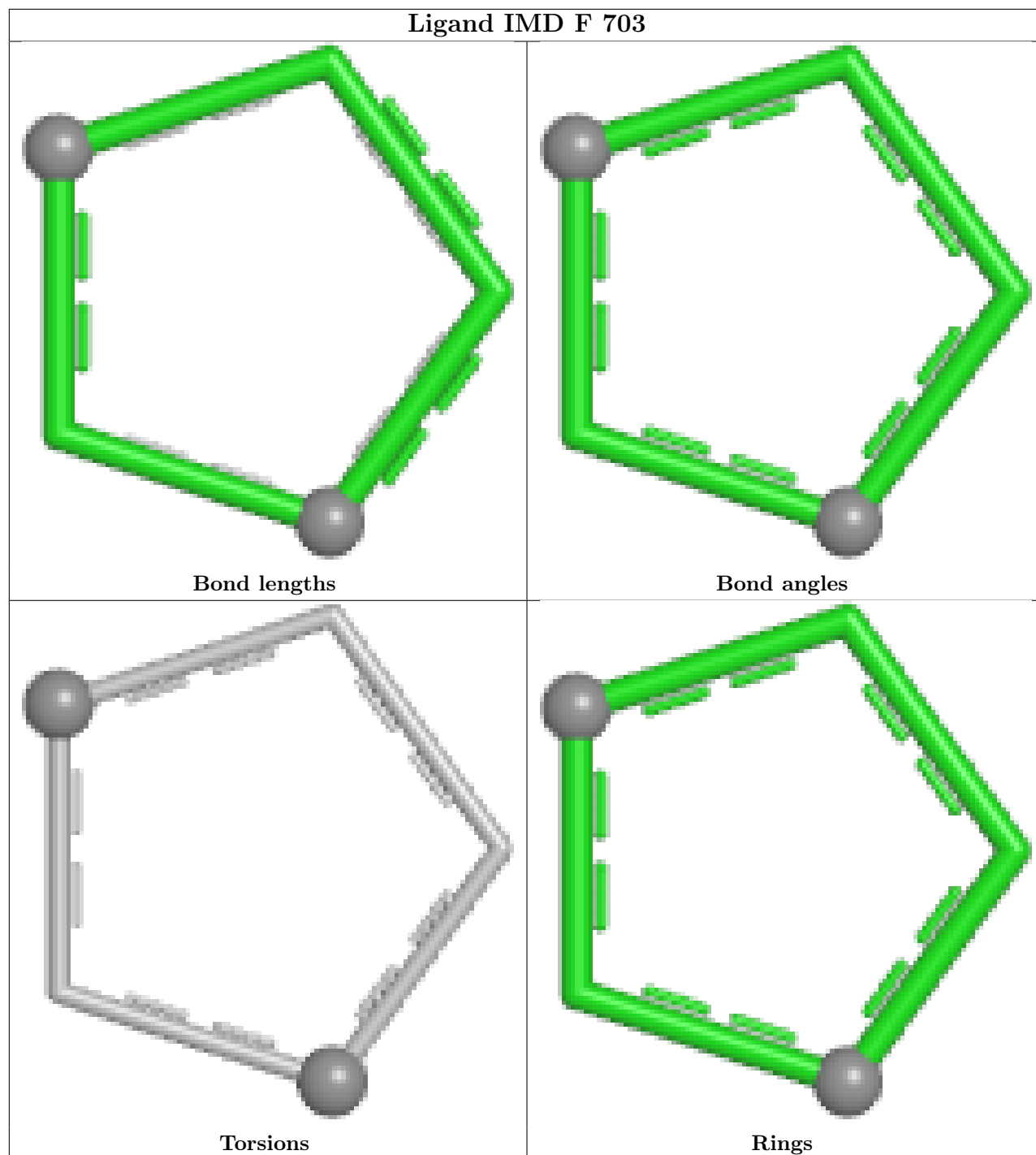
Rings

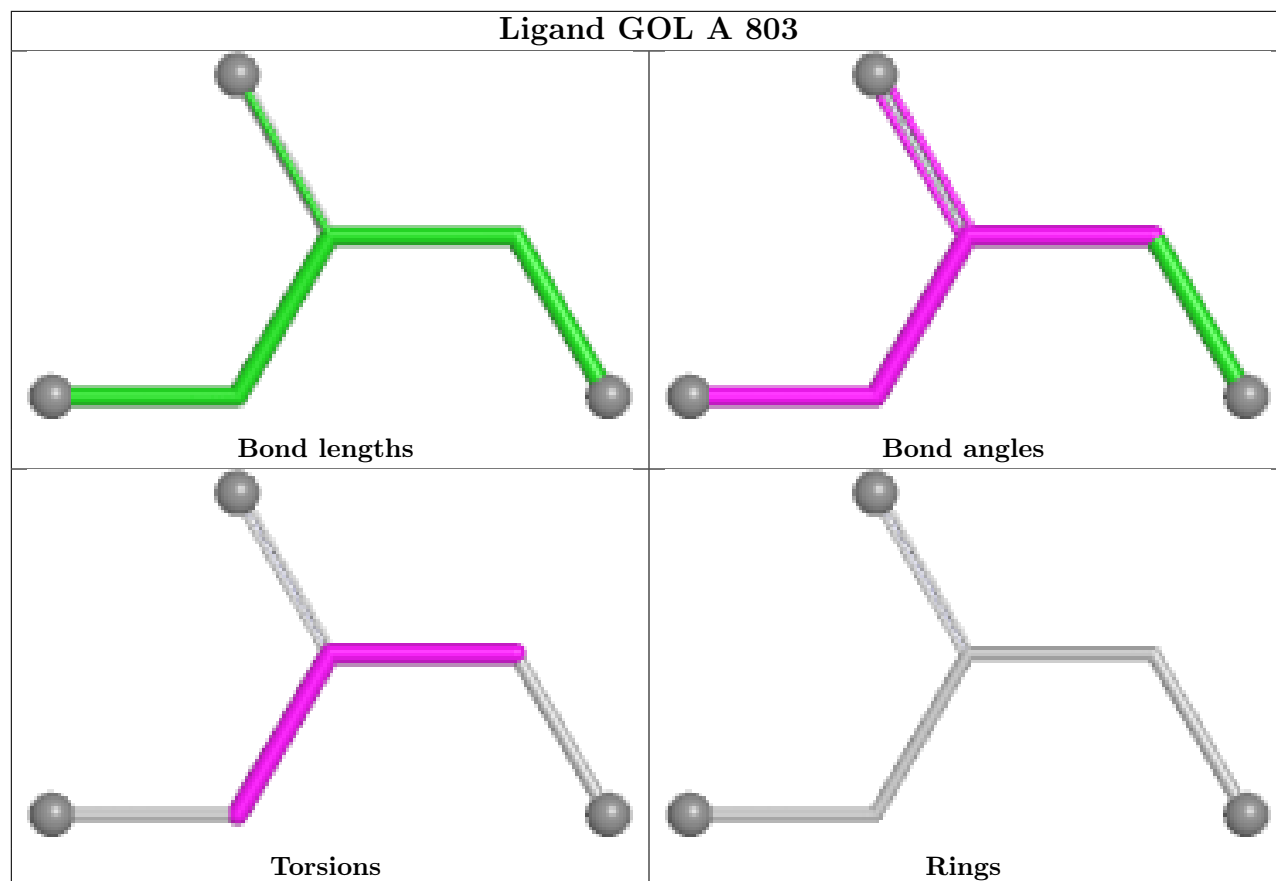


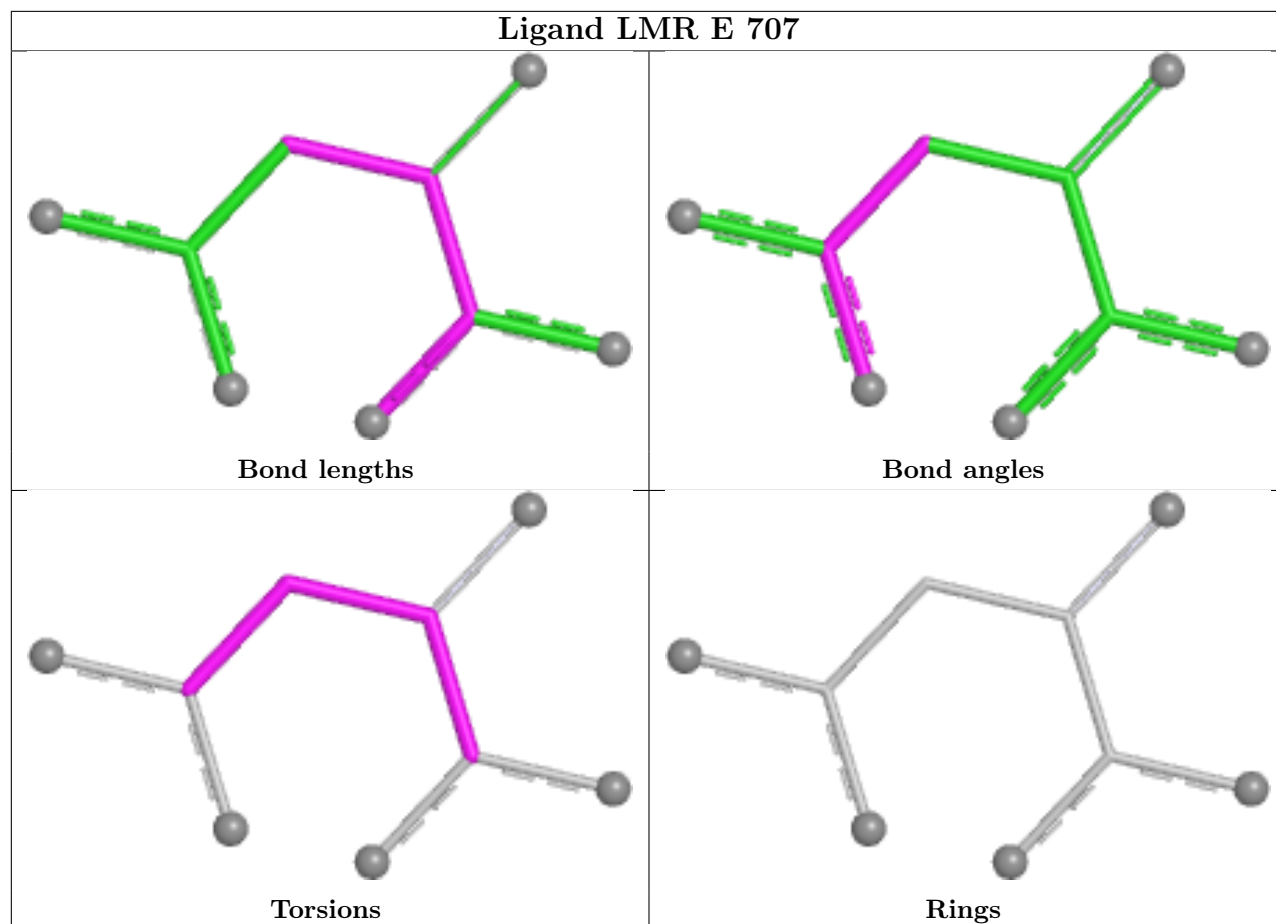
Ligand IMD E 704



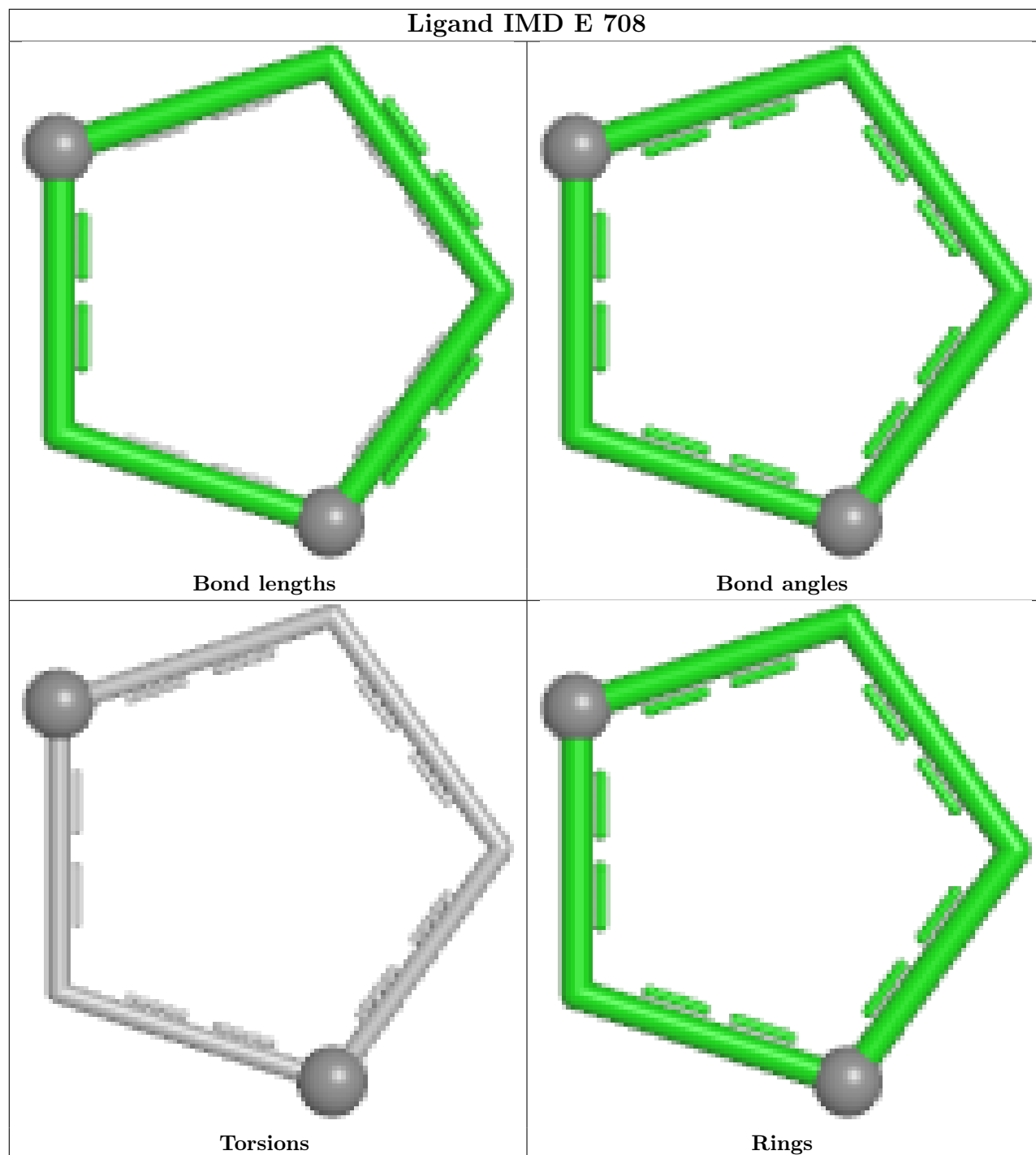
Ligand IMD F 703

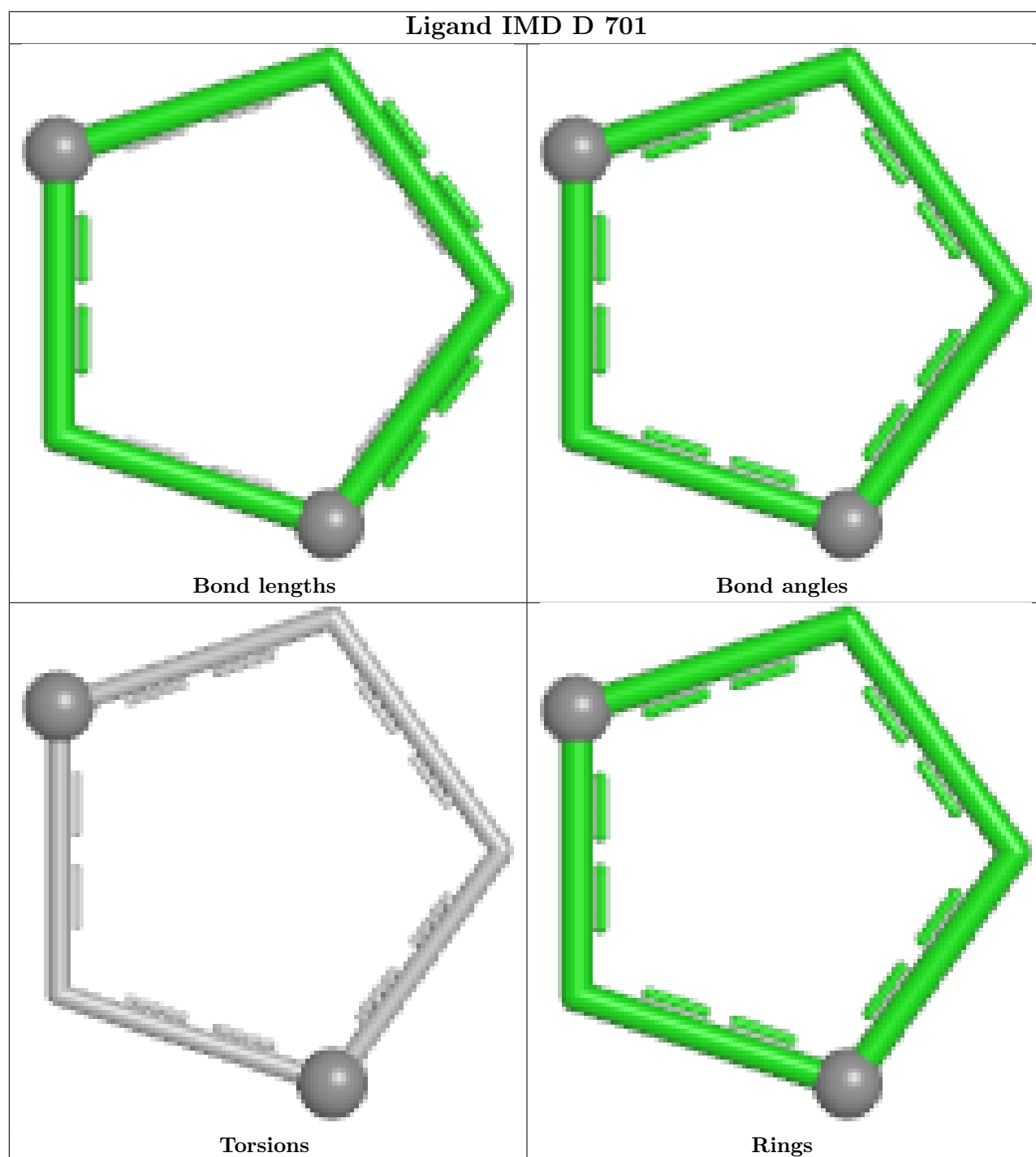




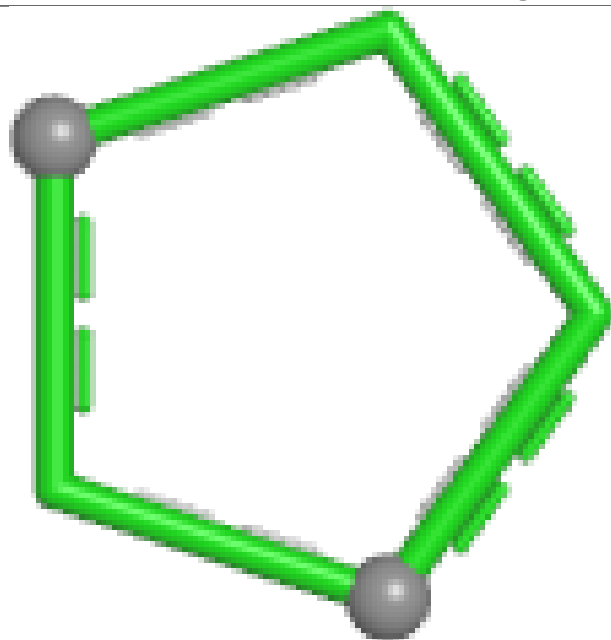


Ligand IMD E 708

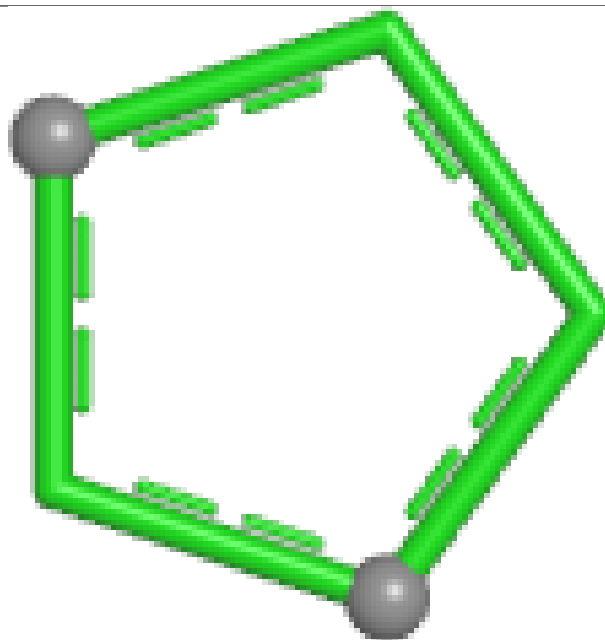




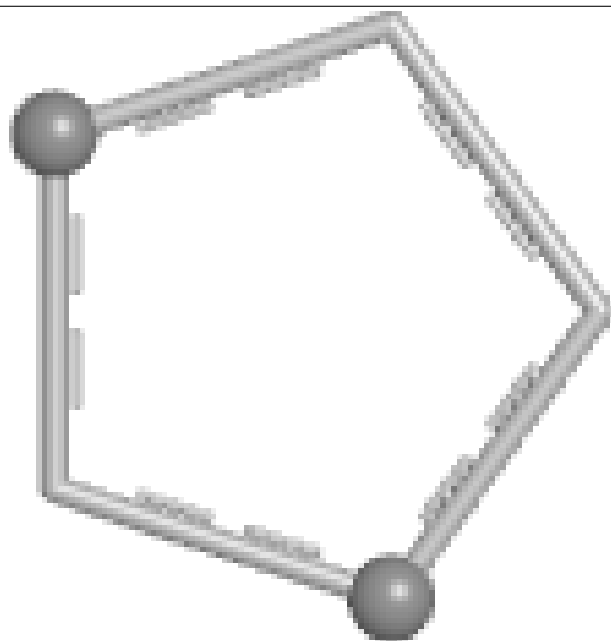
Ligand IMD B 706



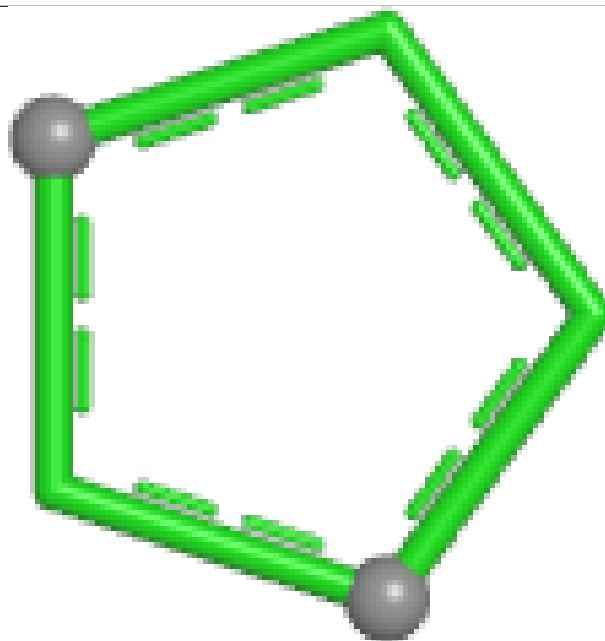
Bond lengths



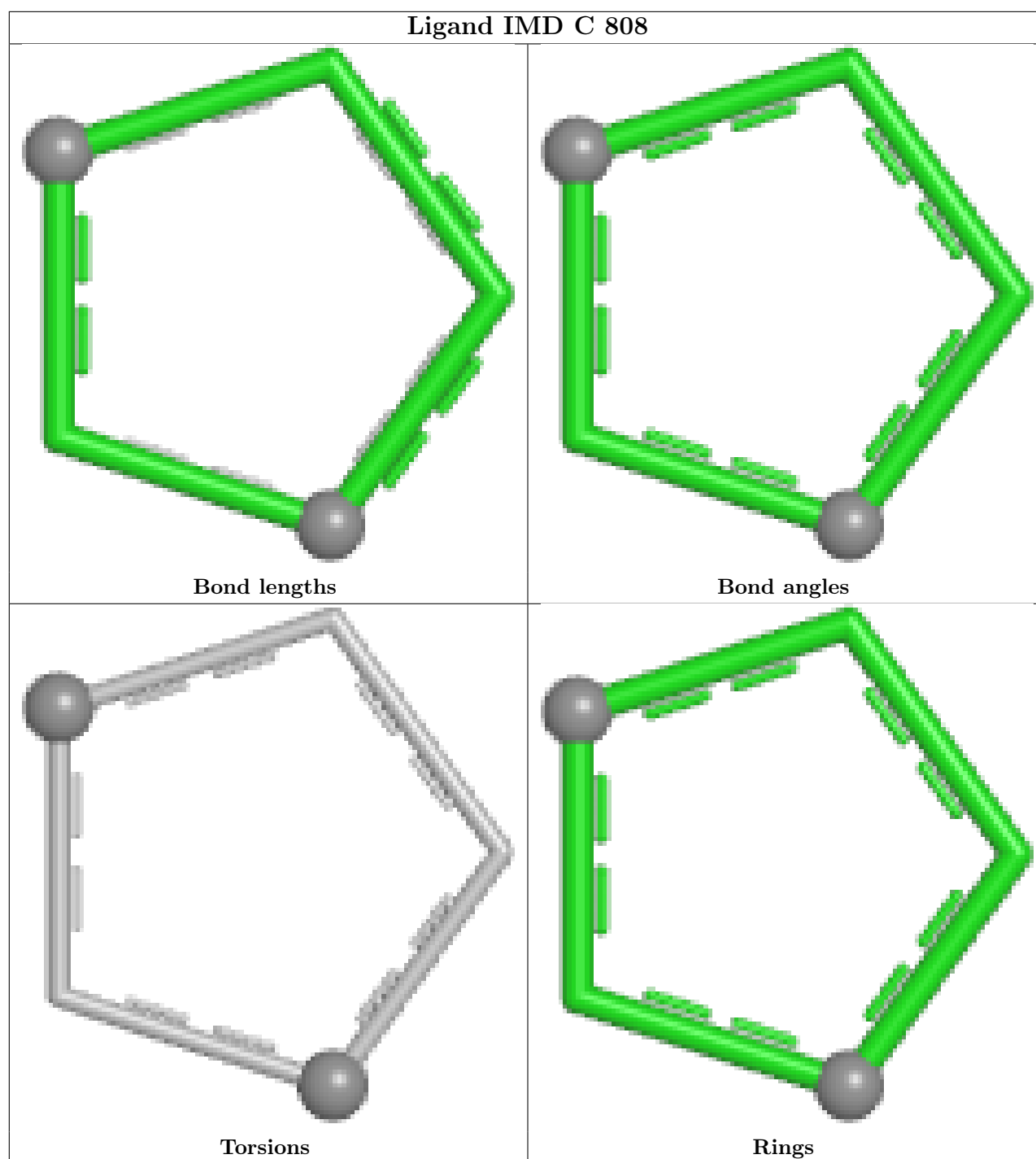
Bond angles



Torsions



Rings



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	642/671 (95%)	0.09	12 (1%) 66 70	6, 20, 34, 68	5 (0%)
1	B	634/671 (94%)	0.13	29 (4%) 37 41	8, 20, 45, 102	3 (0%)
1	C	640/671 (95%)	0.21	23 (3%) 46 50	8, 21, 49, 79	2 (0%)
1	D	622/671 (92%)	-0.08	15 (2%) 59 63	8, 16, 33, 74	2 (0%)
1	E	644/671 (95%)	-0.03	9 (1%) 73 77	5, 17, 33, 76	4 (0%)
1	F	642/671 (95%)	-0.07	11 (1%) 69 73	7, 17, 41, 80	4 (0%)
All	All	3824/4026 (94%)	0.04	99 (2%) 57 61	5, 18, 40, 102	20 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	16	LEU	8.0
1	E	274	ILE	6.8
1	F	622	VAL	6.1
1	B	37	ALA	5.5
1	C	27	VAL	5.3
1	B	622	VAL	4.8
1	B	25	PHE	4.7
1	B	140	SER	4.7
1	C	12	VAL	4.7
1	B	77	SER	4.5
1	E	622	VAL	4.4
1	C	58	VAL	4.2
1	D	36	SER	4.1
1	E	586	SER	4.1
1	C	17	ALA	4.0
1	B	59	PRO	4.0
1	F	27	VAL	3.8
1	C	45	THR	3.8
1	C	29	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	45	THR	3.7
1	B	38	GLY	3.7
1	D	58	VAL	3.7
1	A	36	SER	3.6
1	B	23	PRO	3.5
1	E	107	ILE	3.5
1	D	35	GLY	3.4
1	C	22	TYR	3.4
1	C	43	PHE	3.3
1	C	13	PHE	3.2
1	A	624	THR	3.2
1	D	61	GLY	3.1
1	B	27	VAL	3.1
1	C	25	PHE	3.1
1	E	8	ALA	3.0
1	B	36	SER	3.0
1	B	47	ALA	2.9
1	C	62	TYR	2.9
1	C	42	THR	2.9
1	C	623	PRO	2.9
1	F	22	TYR	2.8
1	A	622	VAL	2.8
1	B	20	VAL	2.8
1	B	22	TYR	2.7
1	B	31	ILE	2.7
1	A	219	TYR	2.7
1	D	37	ALA	2.7
1	F	488	ALA	2.7
1	B	34	LEU	2.7
1	A	21	ALA	2.6
1	D	488	ALA	2.6
1	A	498	ASP	2.6
1	C	622	VAL	2.6
1	E	9	PRO	2.6
1	E	23	PRO	2.6
1	B	42	THR	2.5
1	D	43	PHE	2.5
1	A	623	PRO	2.5
1	F	498	ASP	2.5
1	B	244	GLU	2.5
1	A	488	ALA	2.5
1	F	14	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	31	ILE	2.4
1	A	545	THR	2.4
1	C	63	LEU	2.4
1	B	624	THR	2.4
1	B	32	THR	2.4
1	D	32	THR	2.4
1	B	29	ASP	2.3
1	C	34	LEU	2.3
1	B	41	PHE	2.3
1	F	25	PHE	2.3
1	D	42	THR	2.3
1	B	160	ALA	2.2
1	D	117	ASP	2.2
1	C	26	GLN	2.2
1	A	578	ALA	2.2
1	B	498	ASP	2.2
1	C	498	ASP	2.2
1	A	546	VAL	2.2
1	F	24	ASN	2.1
1	B	546	VAL	2.1
1	C	141	VAL	2.1
1	E	12	VAL	2.1
1	C	28	GLN	2.1
1	F	244	GLU	2.1
1	D	141	VAL	2.1
1	D	622	VAL	2.1
1	C	488	ALA	2.1
1	B	43	PHE	2.0
1	F	42	THR	2.0
1	A	34	LEU	2.0
1	B	28	GLN	2.0
1	F	10	GLU	2.0
1	B	623	PRO	2.0
1	D	44	THR	2.0
1	B	21	ALA	2.0
1	C	617	ALA	2.0
1	E	21	ALA	2.0
1	B	629	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	IMD	C	806	5/5	0.60	0.20	41,44,49,56	0
3	IMD	E	708	5/5	0.60	0.20	47,49,53,54	0
3	IMD	F	709	5/5	0.68	0.19	25,34,40,44	0
3	IMD	B	708	5/5	0.74	0.20	26,27,45,47	0
3	IMD	B	705	5/5	0.74	0.14	35,42,44,45	0
3	IMD	A	804	5/5	0.78	0.14	37,44,45,46	0
3	IMD	C	805	5/5	0.80	0.14	28,33,40,41	0
3	IMD	A	802	5/5	0.81	0.17	44,47,66,73	0
3	IMD	F	704	5/5	0.81	0.14	37,41,45,53	0
3	IMD	D	706	5/5	0.81	0.16	39,42,45,47	0
3	IMD	E	704	5/5	0.83	0.13	21,26,44,45	0
3	IMD	F	703	5/5	0.84	0.11	33,33,39,42	0
3	IMD	F	705	5/5	0.86	0.12	23,33,43,44	0
3	IMD	C	804	5/5	0.86	0.11	31,36,38,40	0
3	IMD	B	704	5/5	0.87	0.12	35,41,45,47	0
4	GOL	C	802	6/6	0.87	0.14	24,36,50,57	0
4	GOL	B	707	6/6	0.88	0.11	23,29,35,50	0
3	IMD	B	706	5/5	0.88	0.12	26,31,40,48	0
4	GOL	D	705	6/6	0.88	0.14	26,32,34,37	0
4	GOL	F	701	6/6	0.88	0.12	19,28,30,31	0
4	GOL	E	703	6/6	0.89	0.11	20,27,40,44	0
4	GOL	F	702	6/6	0.89	0.12	25,29,40,45	0
3	IMD	C	808	5/5	0.90	0.12	47,50,54,56	0
4	GOL	A	806	6/6	0.90	0.09	23,35,39,49	0
3	IMD	C	810	5/5	0.90	0.10	28,31,40,43	0
3	IMD	D	703	5/5	0.90	0.10	31,34,35,38	0
4	GOL	A	803	6/6	0.91	0.11	25,29,33,35	0
2	LMR	E	707	9/9	0.91	0.11	20,30,41,46	0
2	LMR	F	708	9/9	0.91	0.09	22,26,29,30	0
2	LMR	B	703	9/9	0.91	0.11	19,25,48,56	0
3	IMD	E	702	5/5	0.92	0.09	26,30,33,36	0
3	IMD	A	805	5/5	0.92	0.10	23,29,43,47	0

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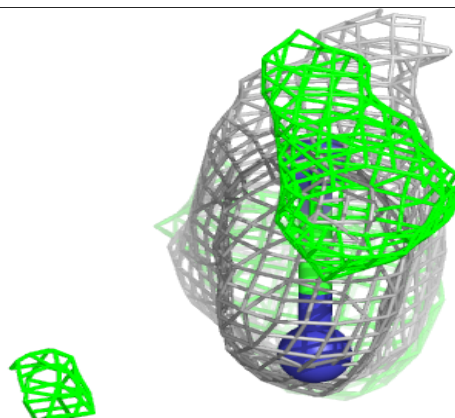
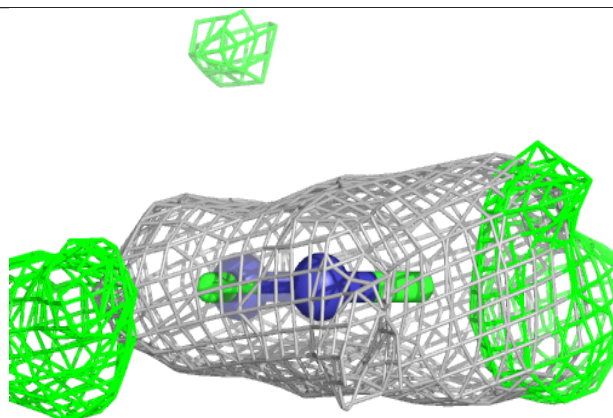
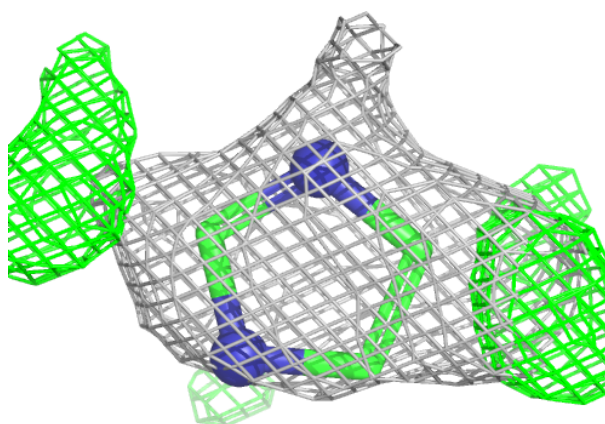
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	E	701	6/6	0.92	0.10	22,30,34,42	0
4	GOL	F	706	6/6	0.92	0.12	21,27,30,35	0
3	IMD	E	705	5/5	0.93	0.12	22,29,45,45	0
4	GOL	C	807	6/6	0.93	0.09	28,36,40,47	0
2	LMR	D	702	9/9	0.93	0.09	23,30,43,44	0
3	IMD	D	701	5/5	0.93	0.09	23,28,37,43	0
4	GOL	B	701	6/6	0.94	0.09	25,28,31,41	0
4	GOL	D	704	6/6	0.94	0.09	19,20,24,30	0
2	LMR	A	801	9/9	0.94	0.08	25,31,45,50	0
2	LMR	C	809	9/9	0.94	0.08	26,30,45,51	0
4	GOL	D	707	6/6	0.95	0.09	18,26,28,45	0
4	GOL	C	803	6/6	0.95	0.08	21,23,24,26	0
4	GOL	C	801	6/6	0.95	0.07	24,29,37,46	0
4	GOL	B	702	6/6	0.96	0.08	24,28,31,36	0
2	LMR	F	707	9/9	0.97	0.06	19,26,36,54	0
4	GOL	E	706	6/6	0.98	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.

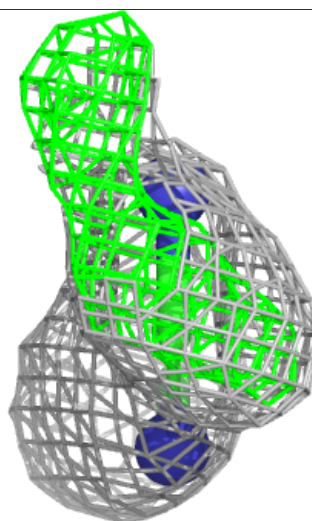
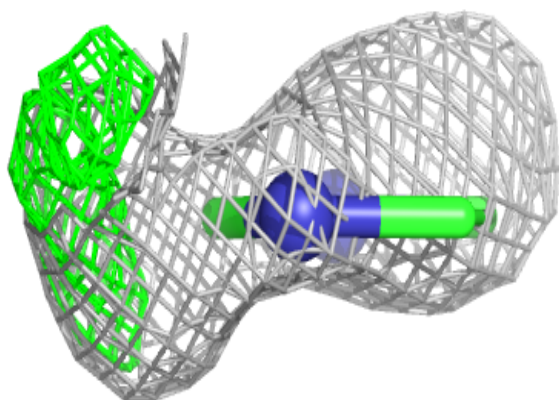
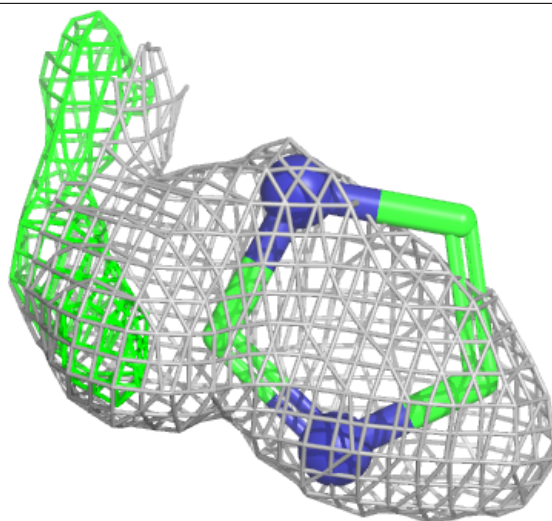
Electron density around IMD C 806:

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



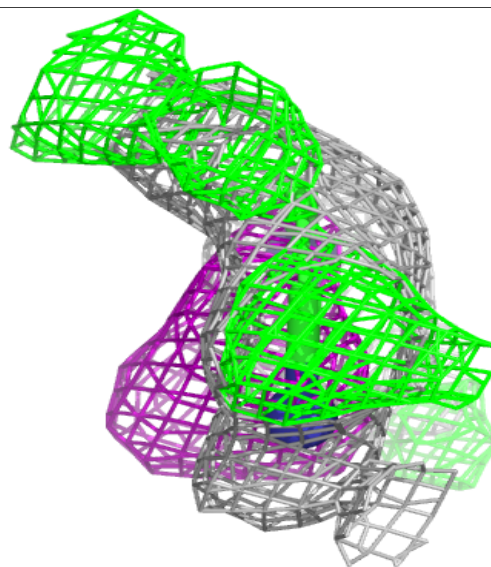
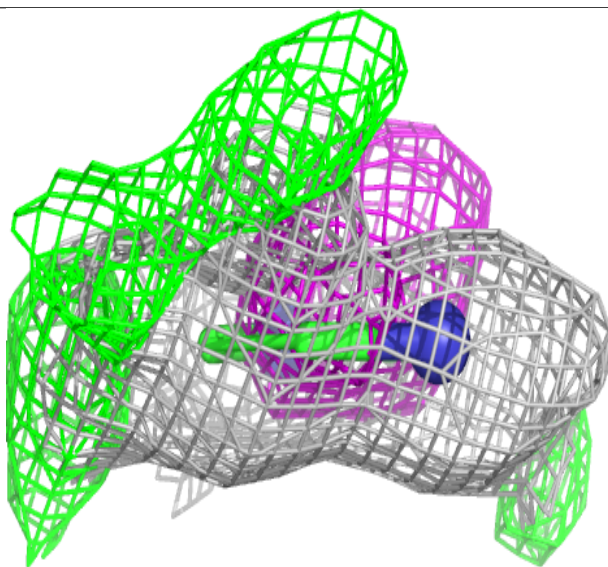
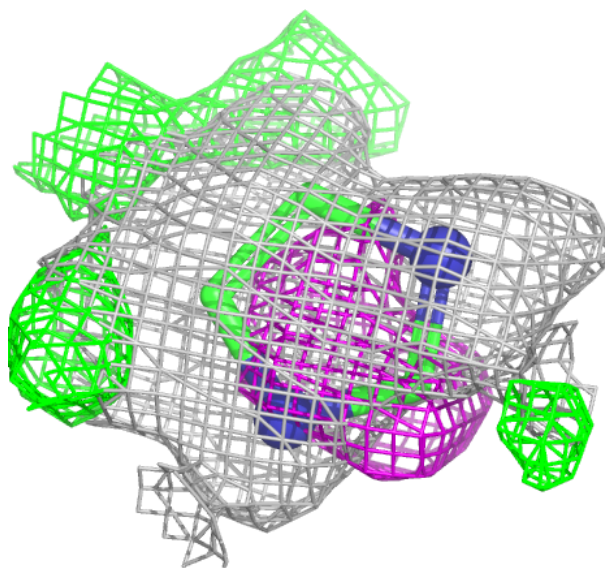
Electron density around IMD E 708:

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



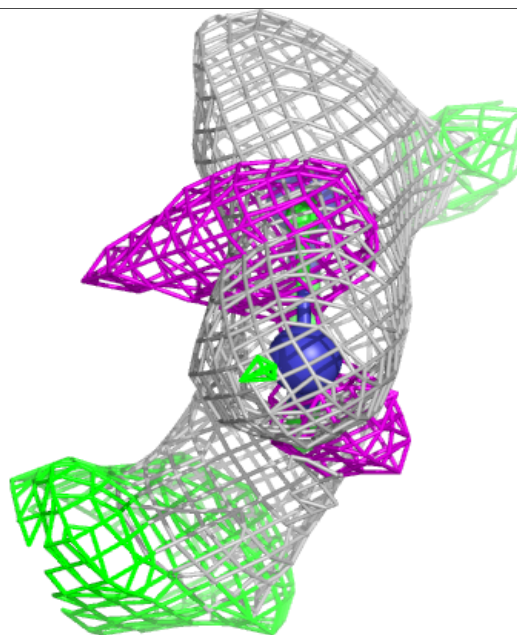
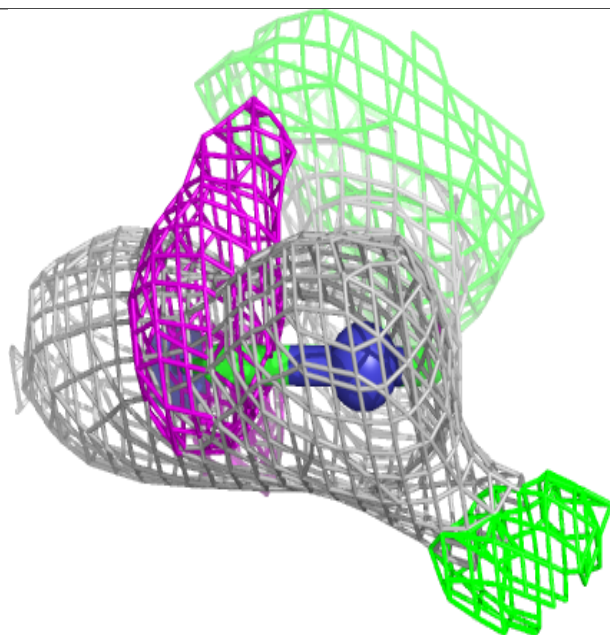
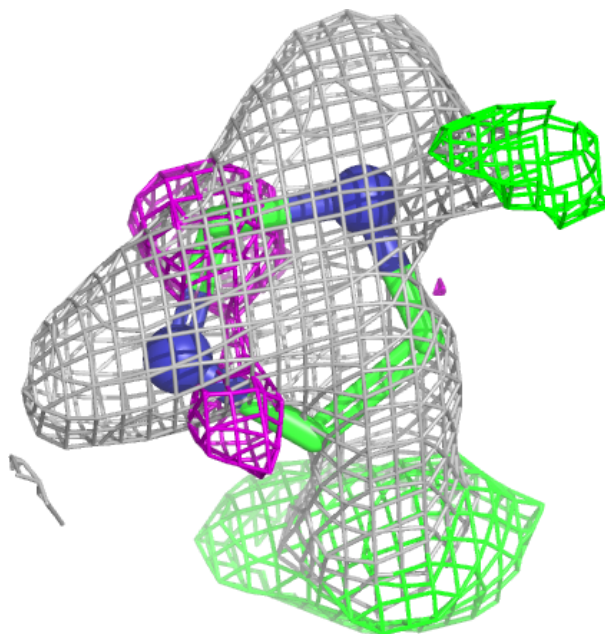
Electron density around IMD F 709:

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



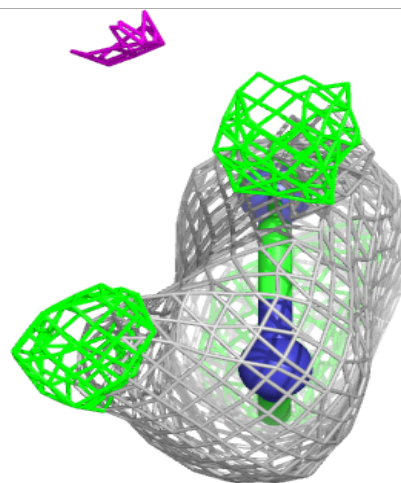
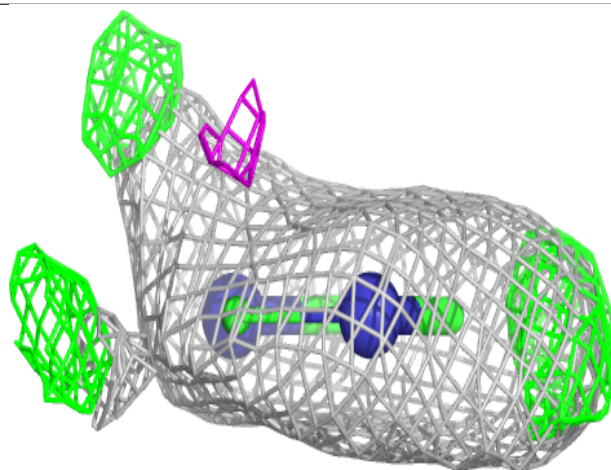
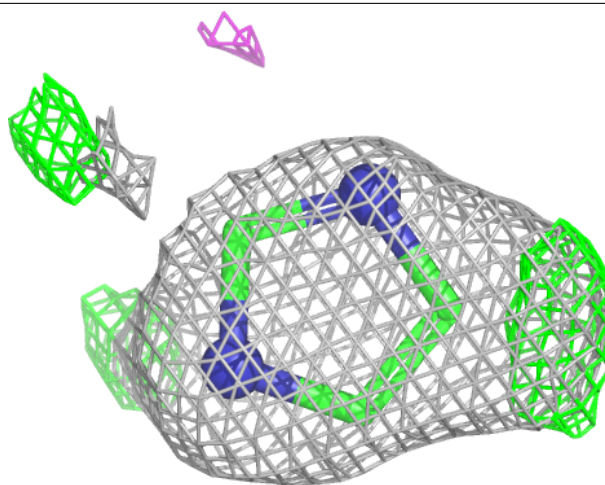
Electron density around IMD B 708:

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



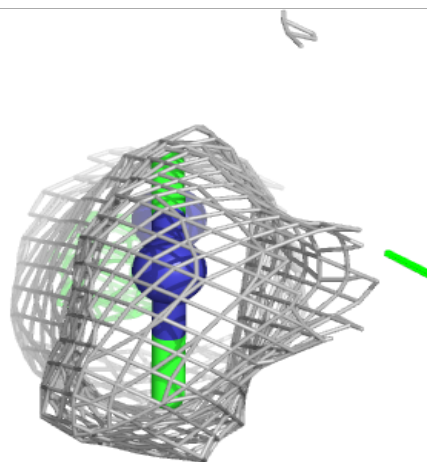
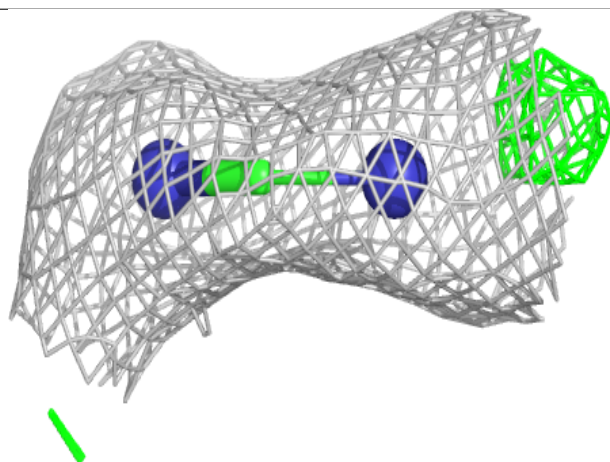
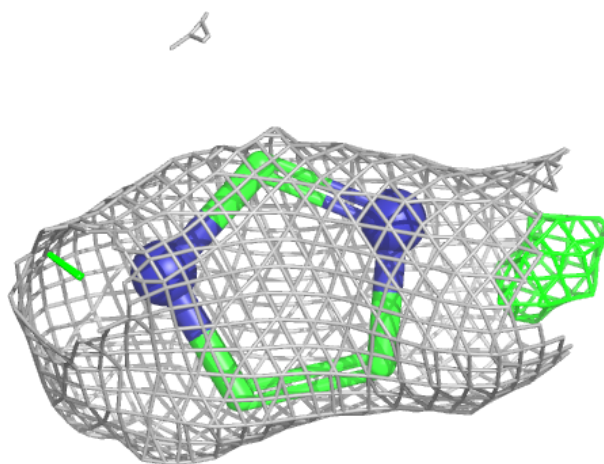
Electron density around IMD B 705:

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



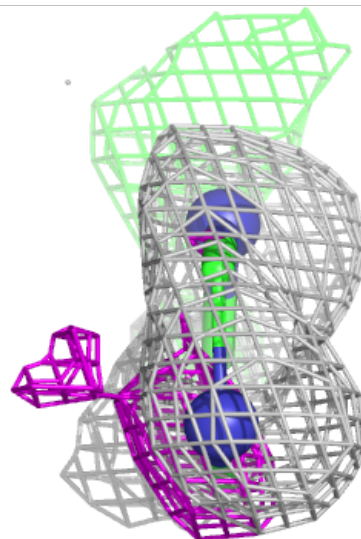
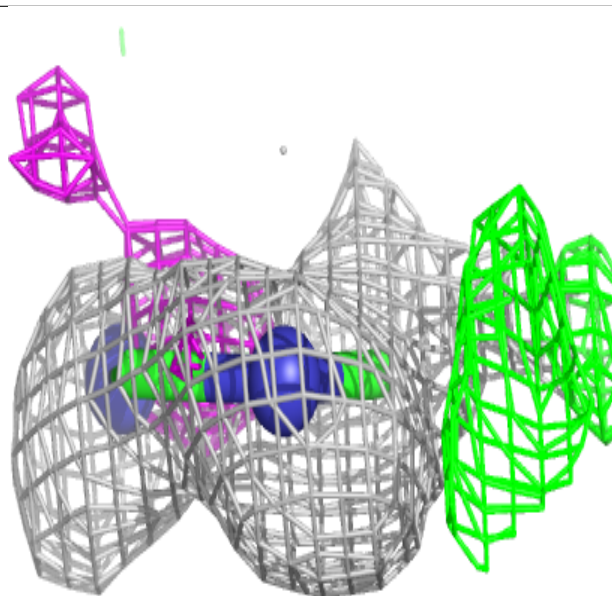
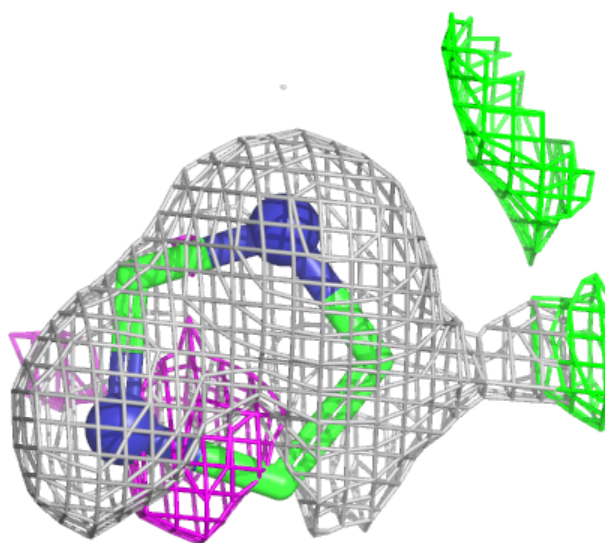
Electron density around IMD A 804:

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



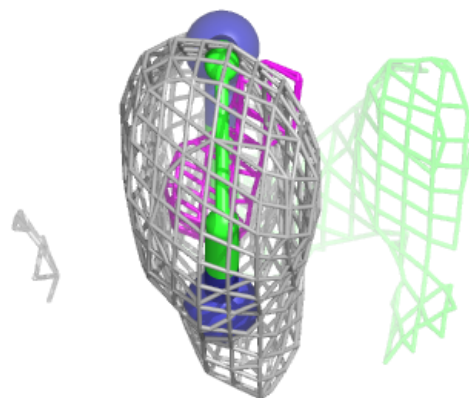
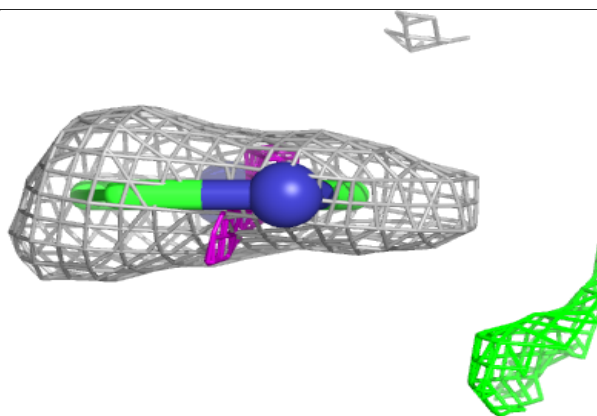
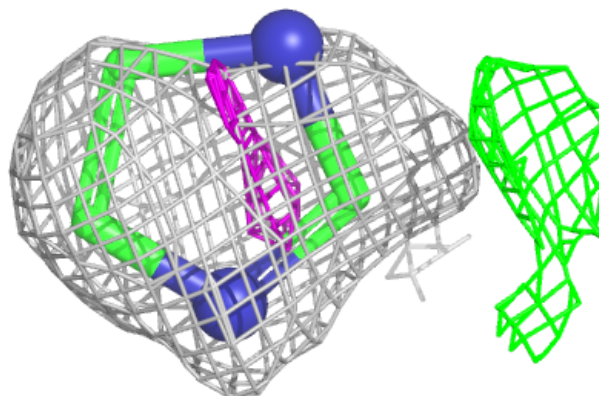
Electron density around IMD C 805:

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



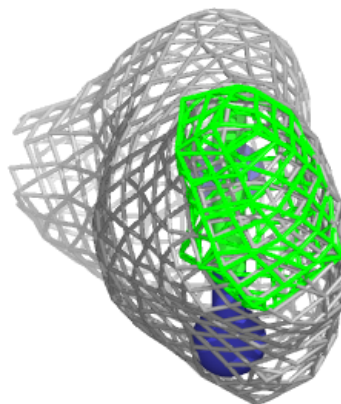
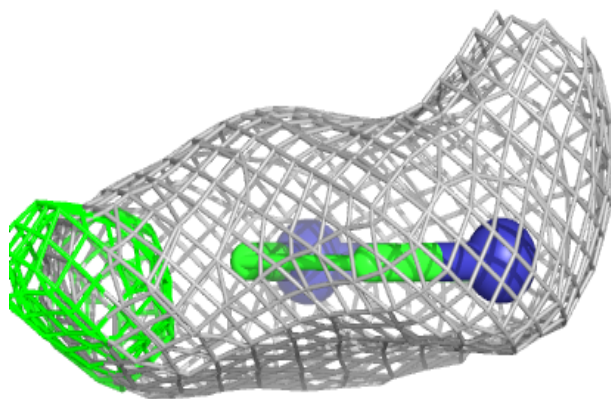
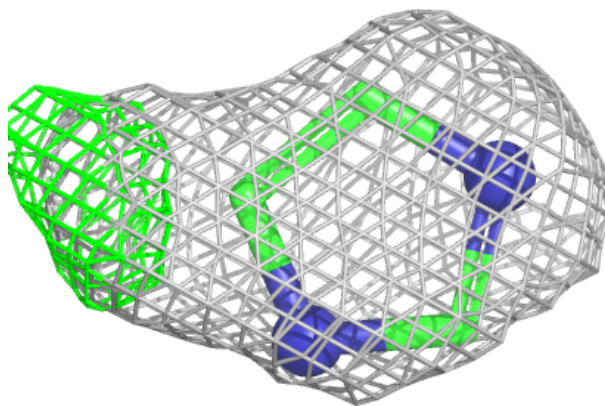
Electron density around IMD A 802:

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



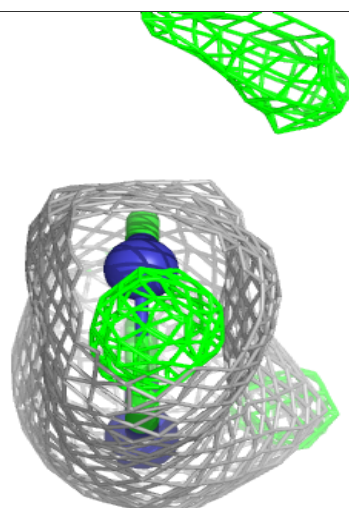
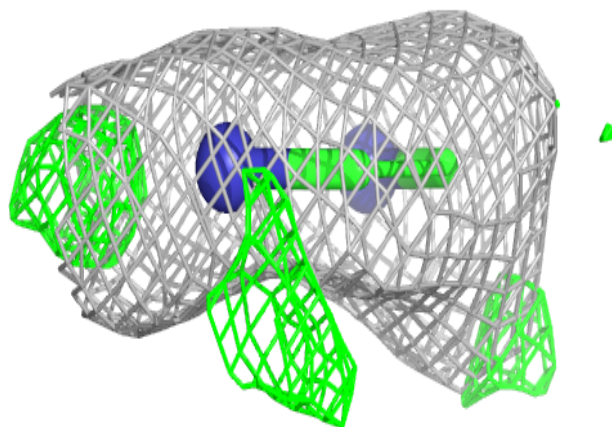
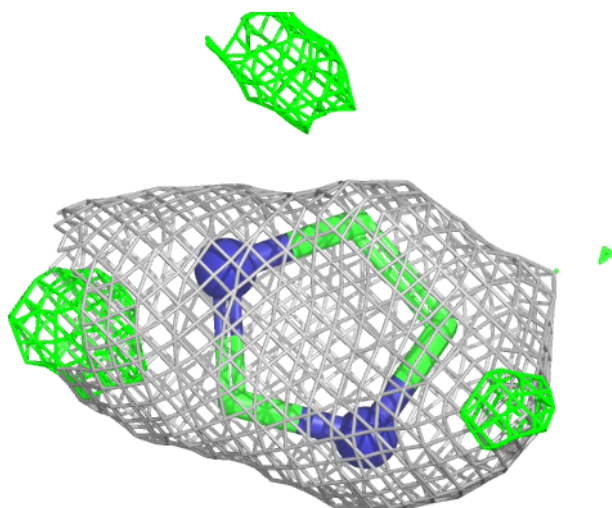
Electron density around IMD F 704:

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



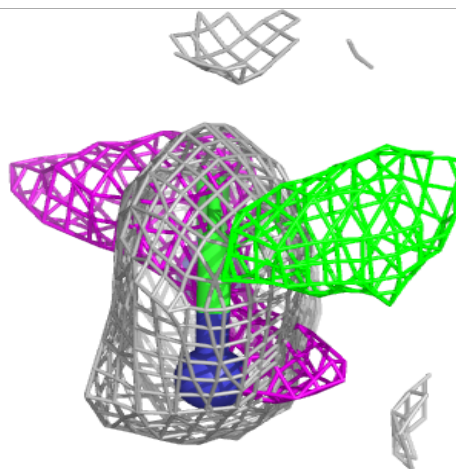
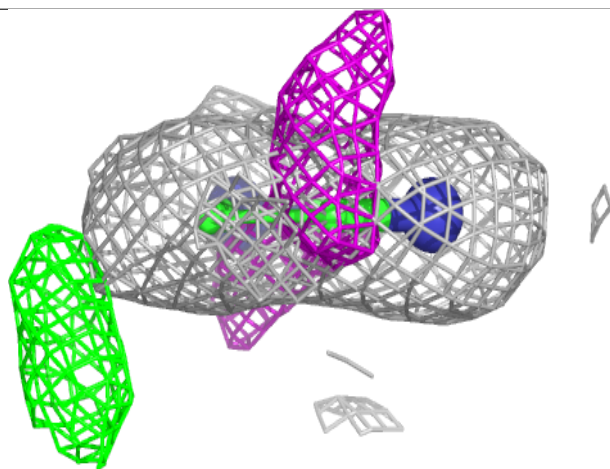
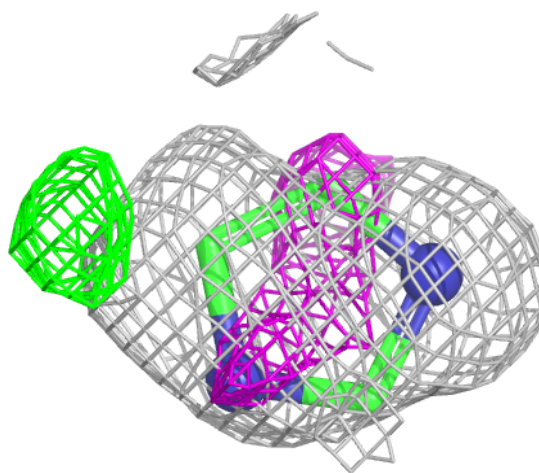
Electron density around IMD D 706:

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



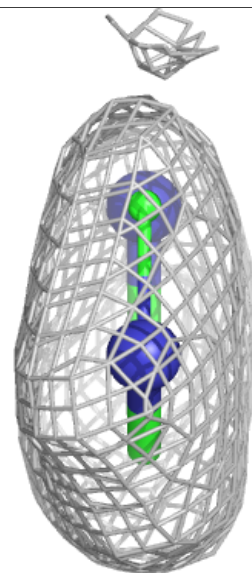
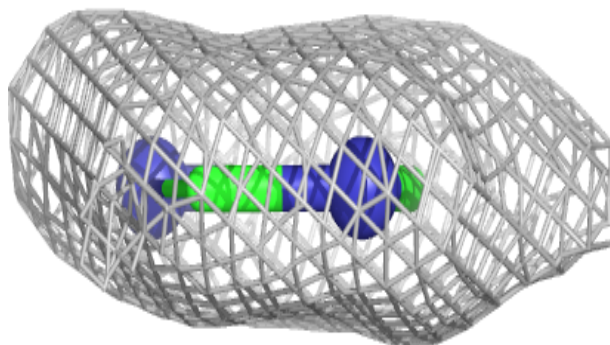
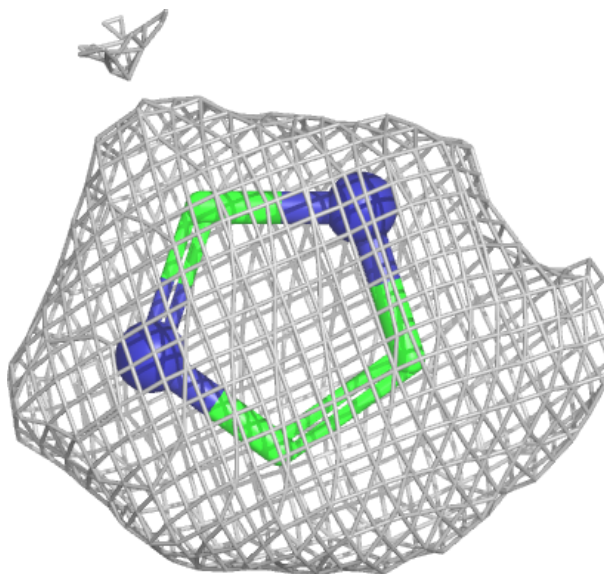
Electron density around IMD E 704:

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



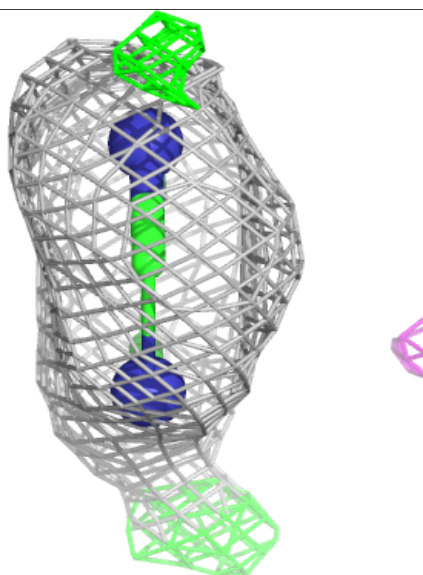
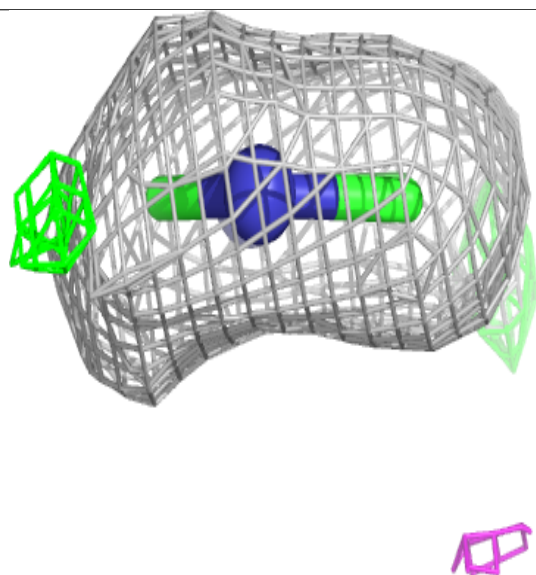
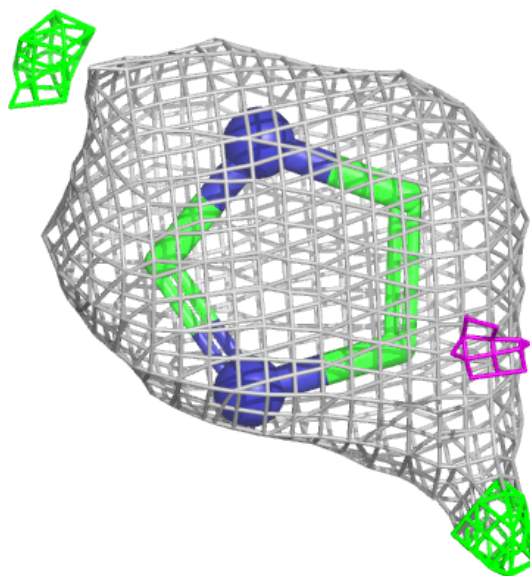
Electron density around IMD F 703:

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



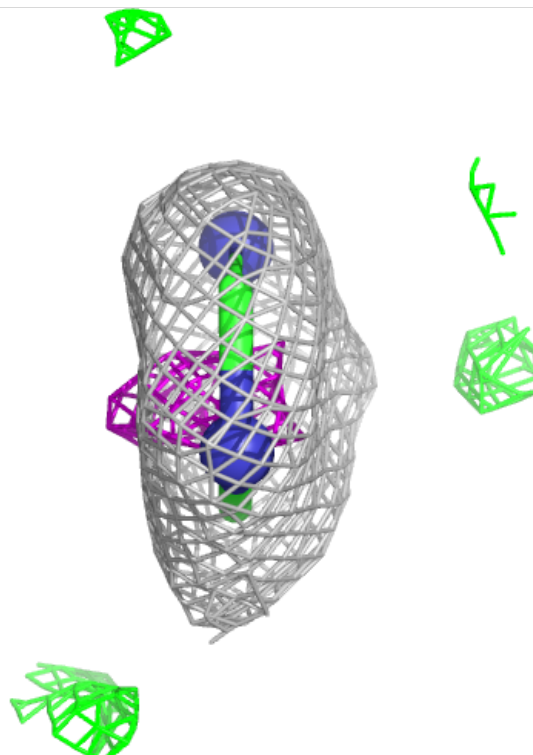
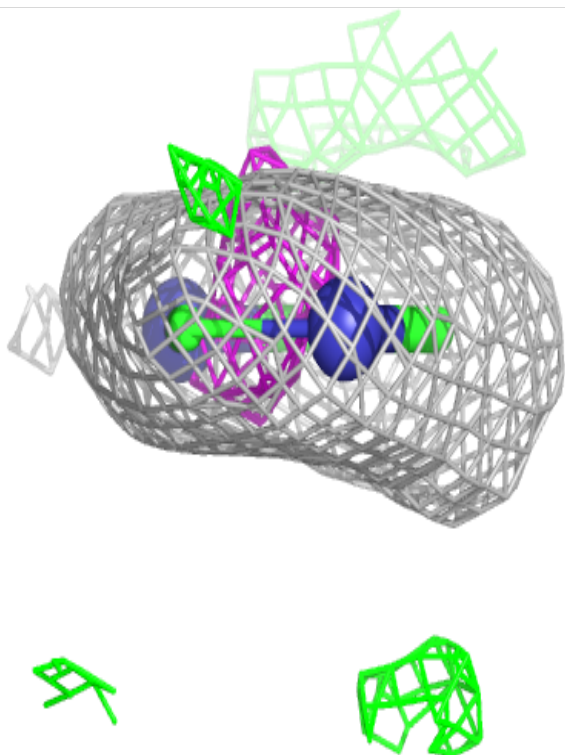
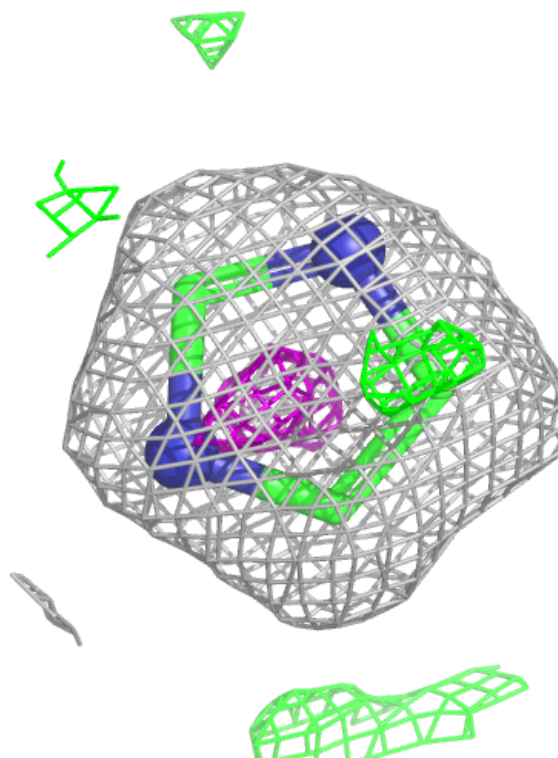
Electron density around IMD F 705:

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



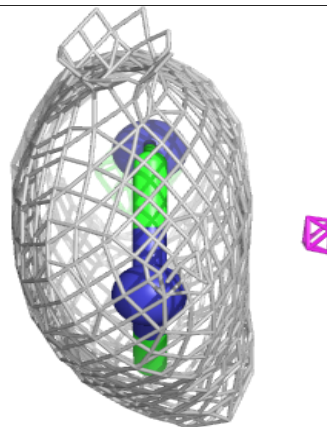
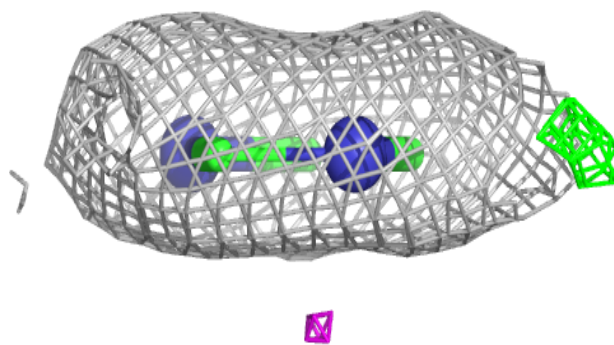
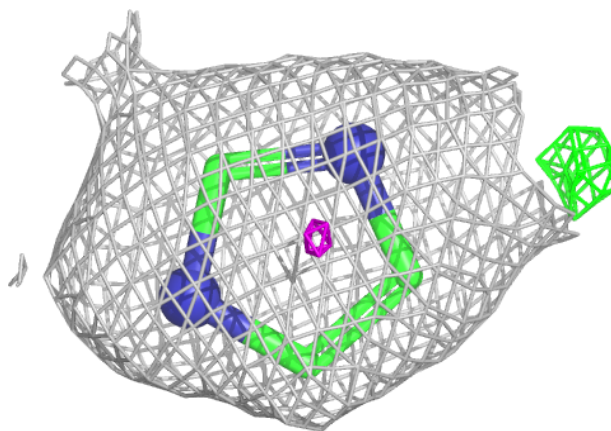
Electron density around IMD C 804:

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



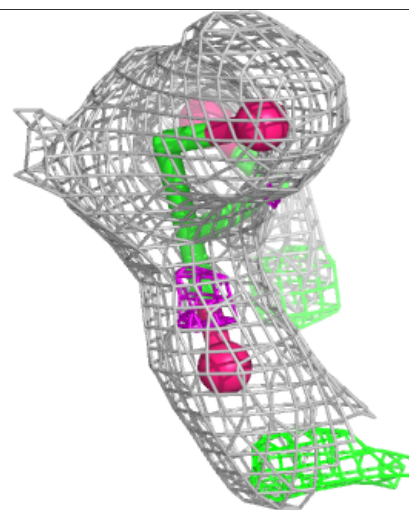
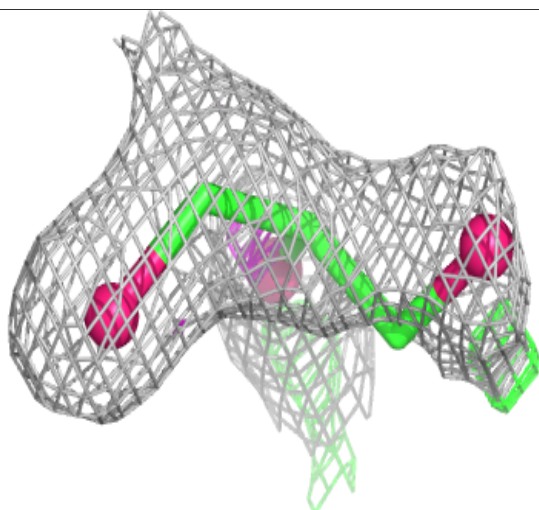
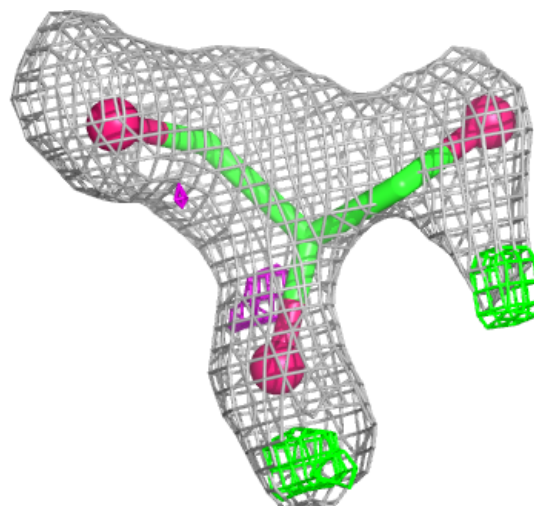
Electron density around IMD B 704:

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



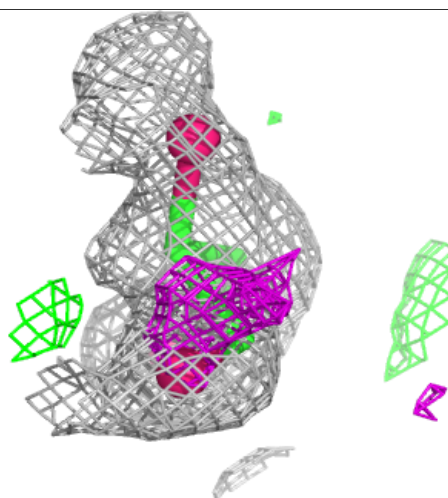
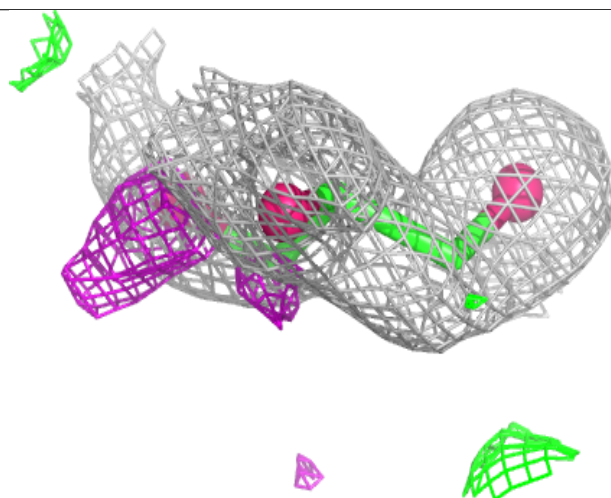
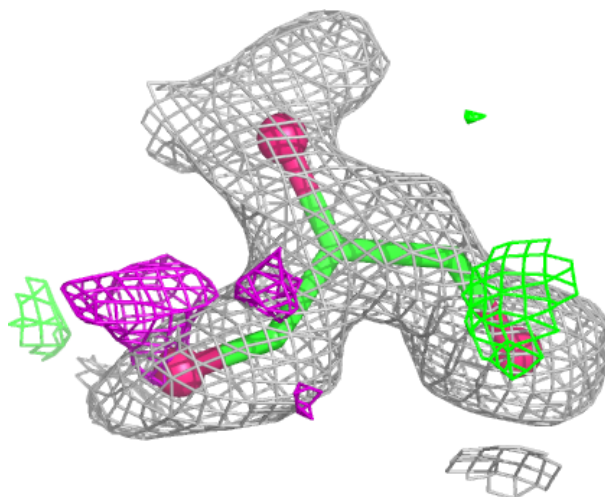
Electron density around GOL C 802:

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



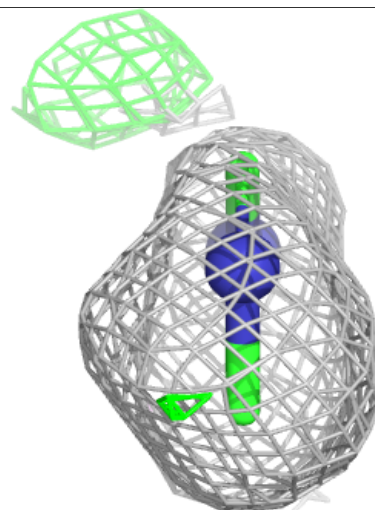
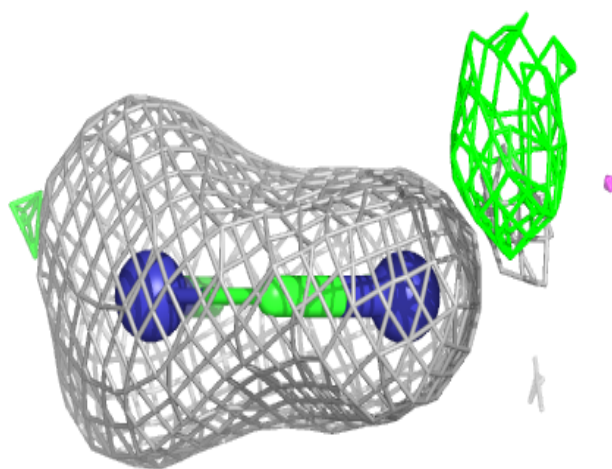
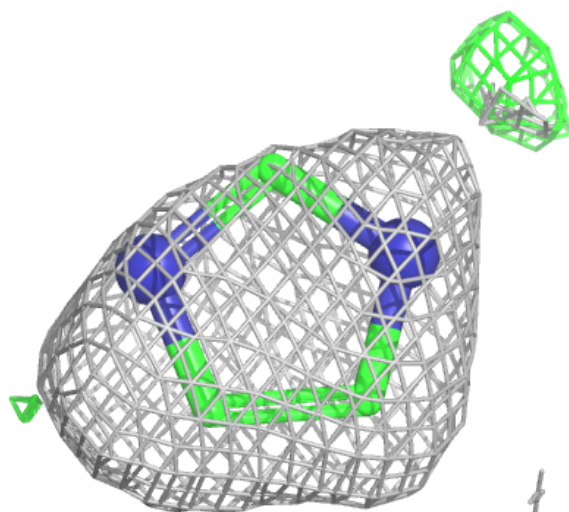
Electron density around GOL B 707:

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



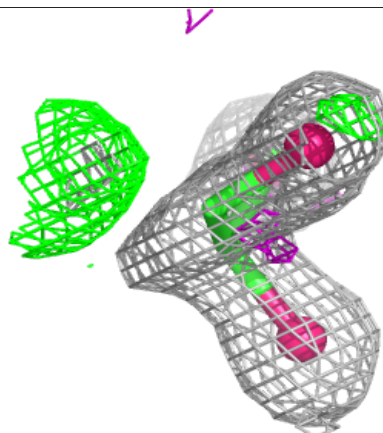
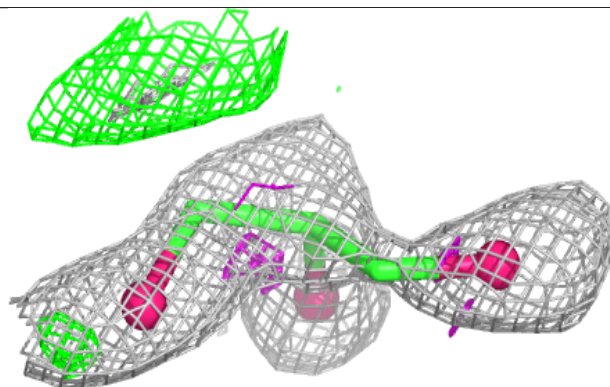
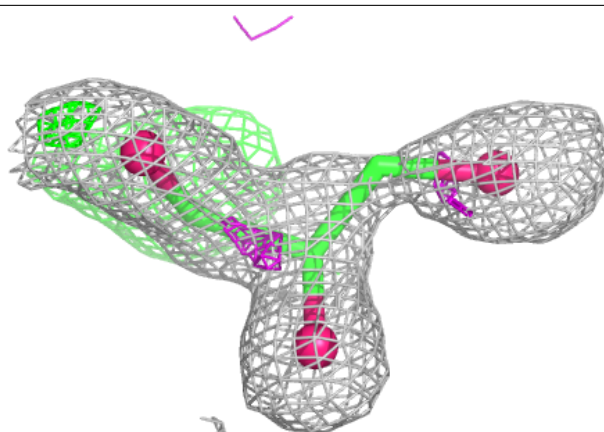
Electron density around IMD B 706:

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

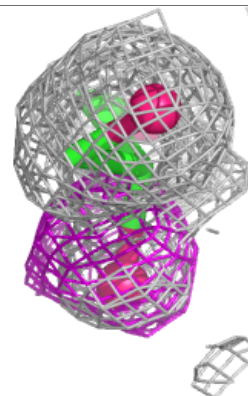
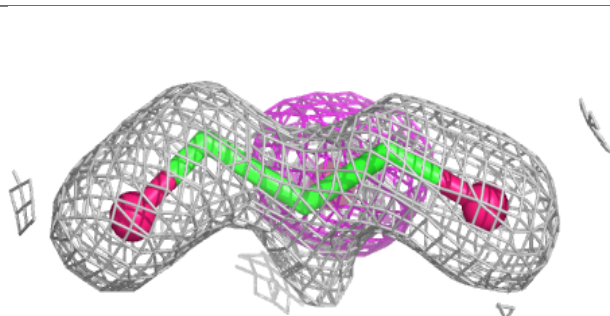
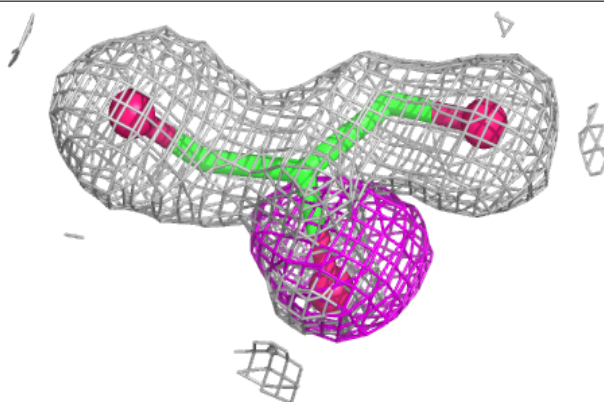


Electron density around GOL D 705:

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

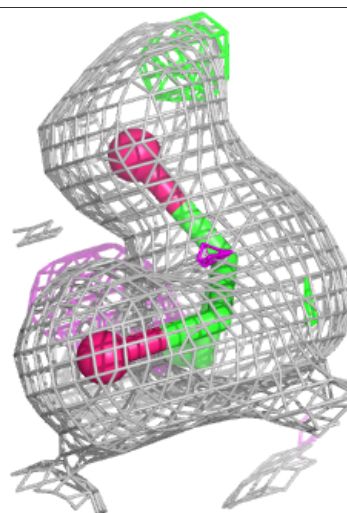
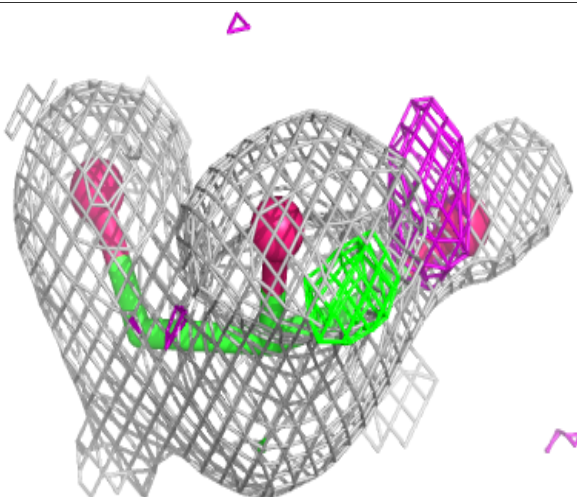
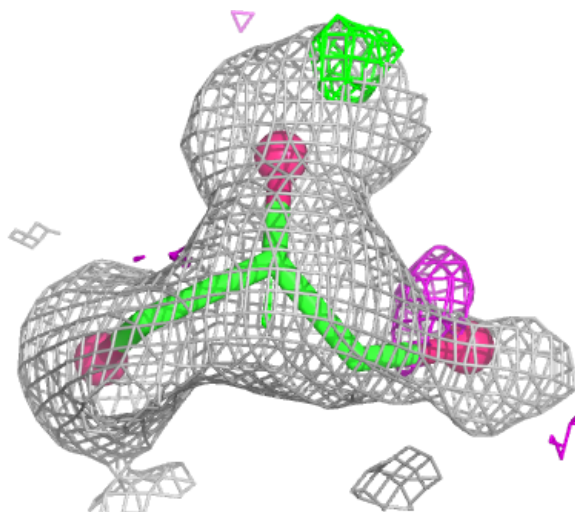
**Electron density around GOL F 701:**

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



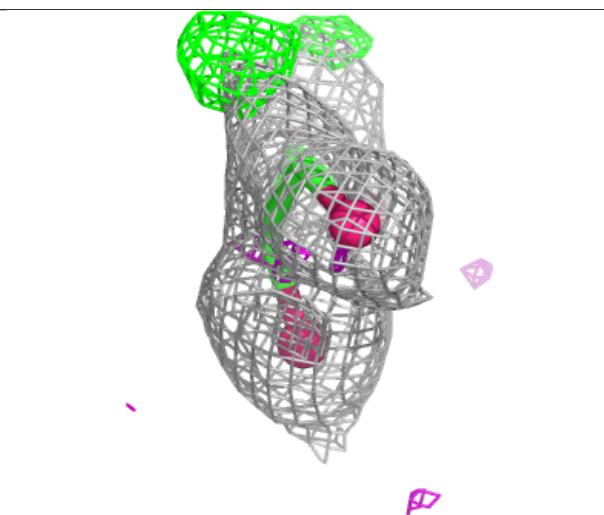
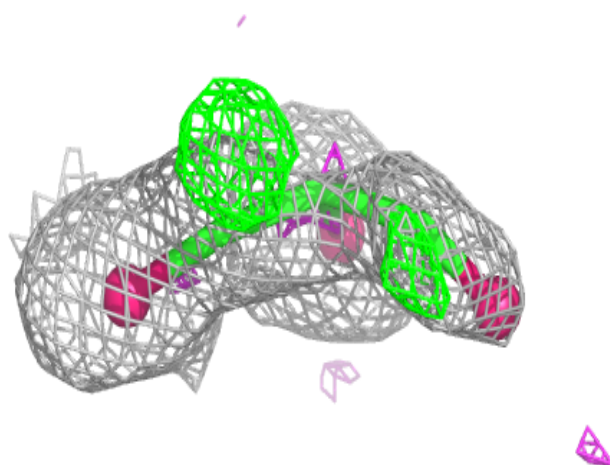
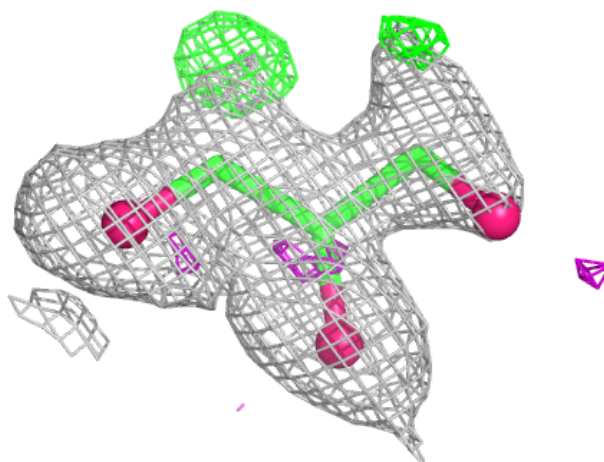
Electron density around GOL E 703:

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



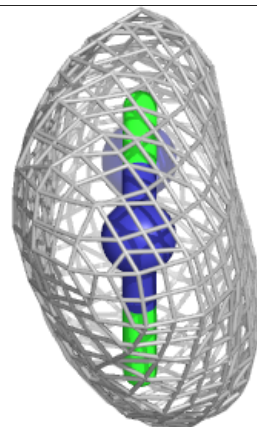
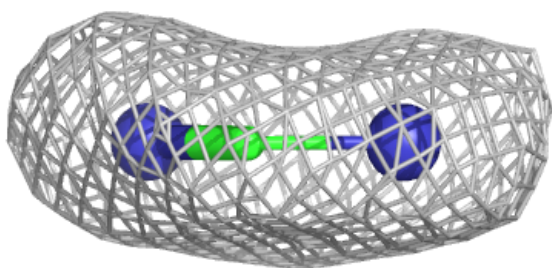
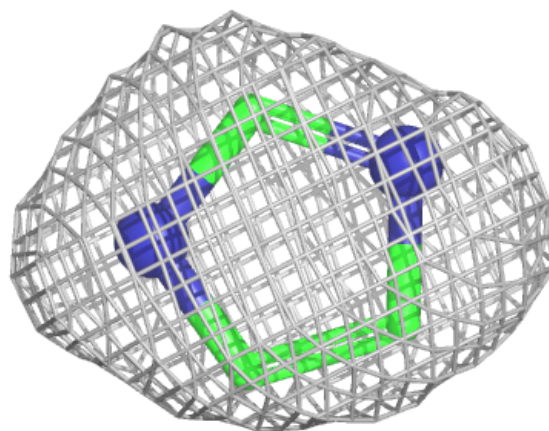
Electron density around GOL F 702:

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

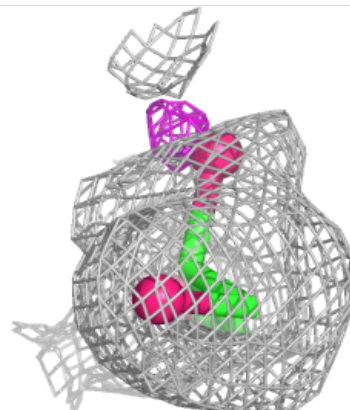
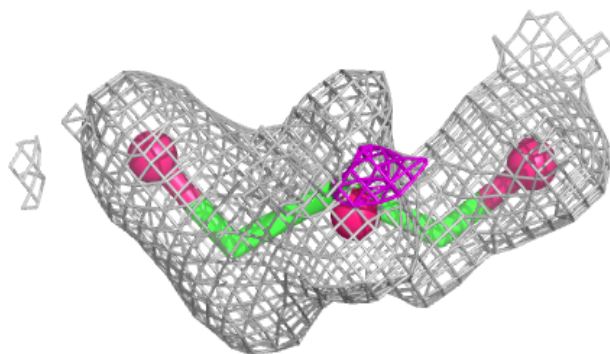
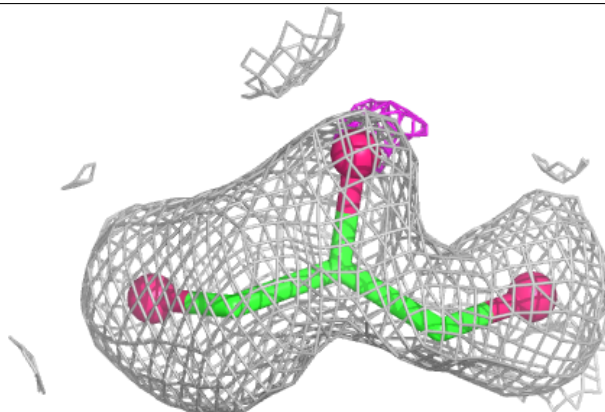


Electron density around IMD C 808:

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

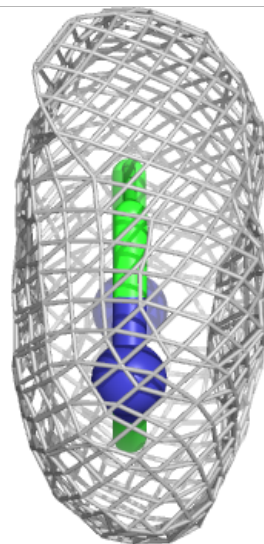
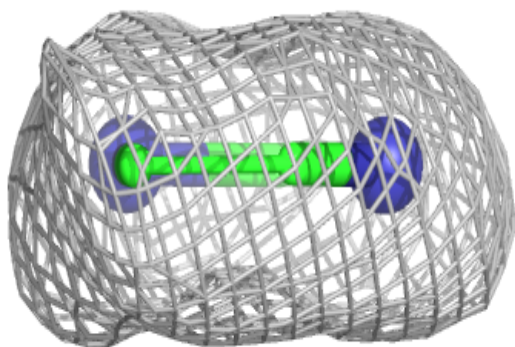
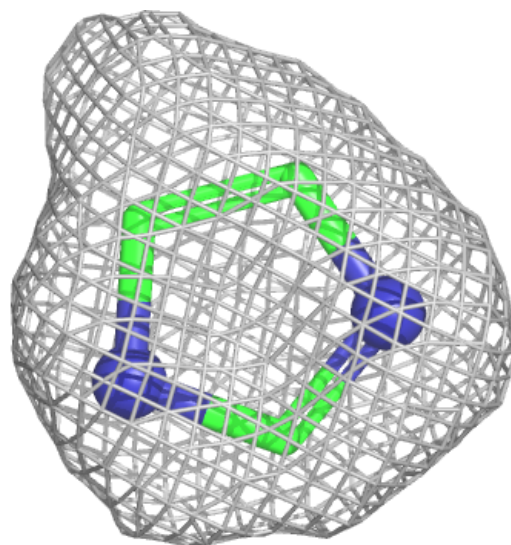
**Electron density around GOL A 806:**

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



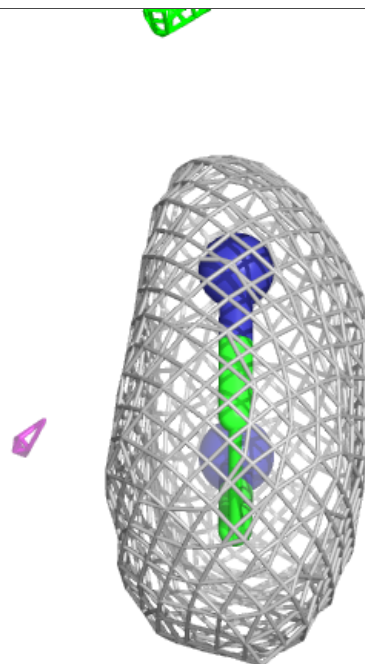
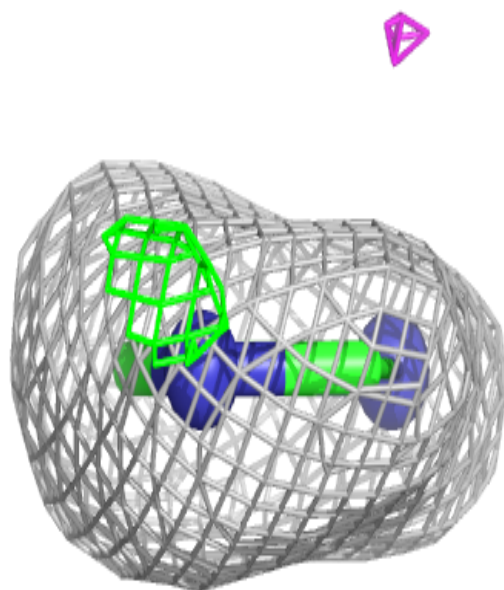
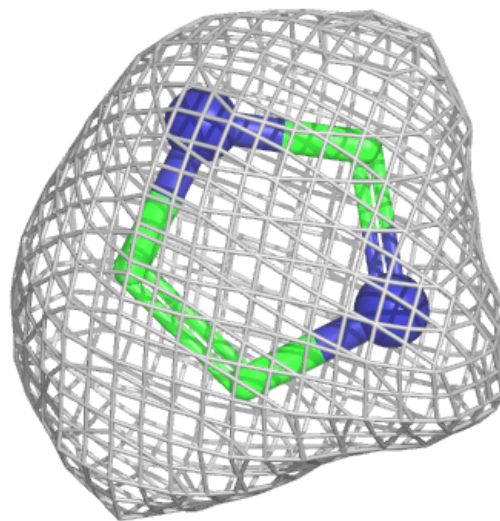
Electron density around IMD C 810:

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



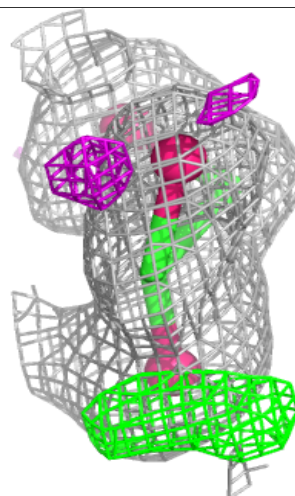
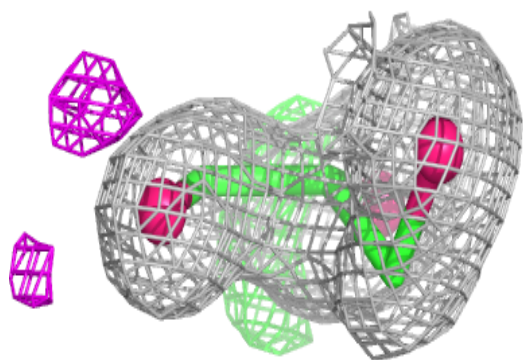
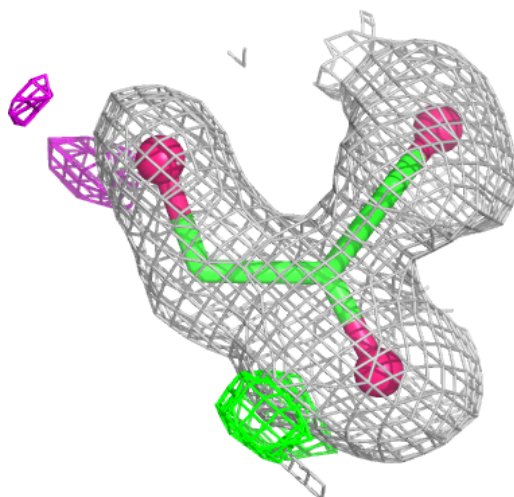
Electron density around IMD D 703:

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



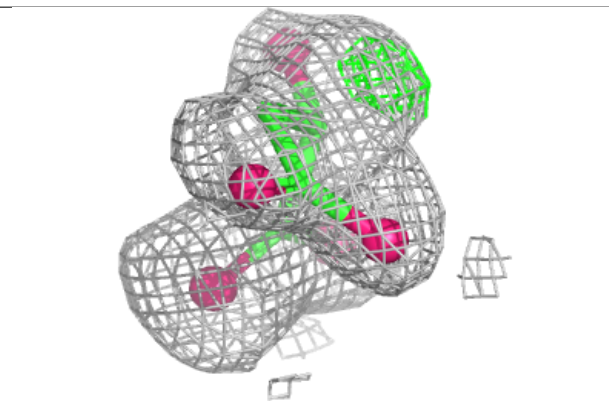
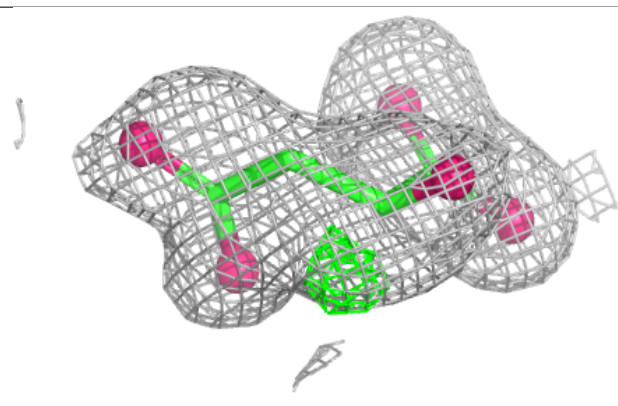
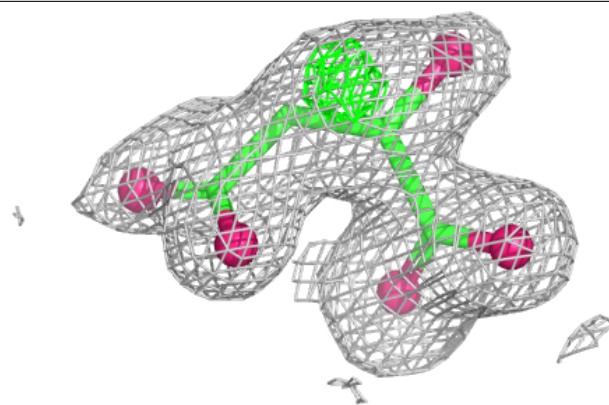
Electron density around GOL A 803:

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



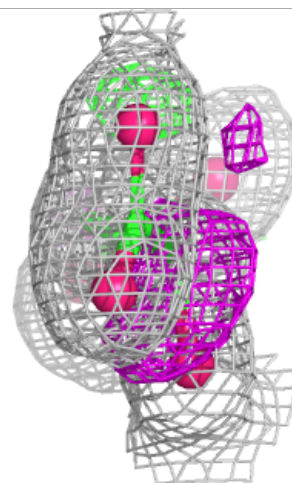
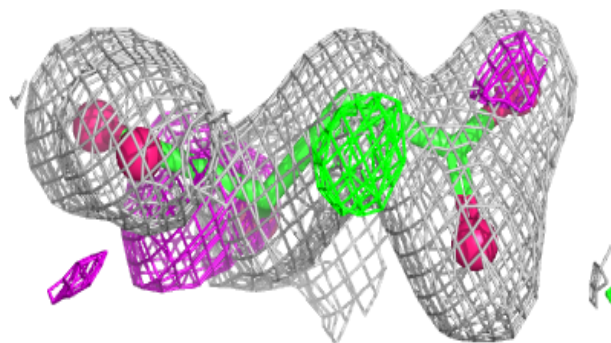
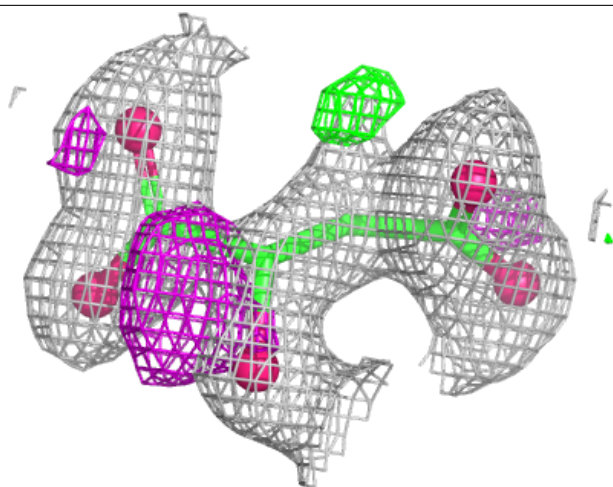
Electron density around LMR E 707:

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



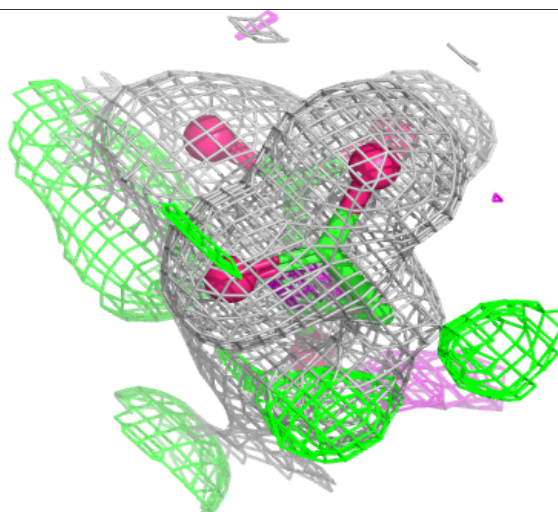
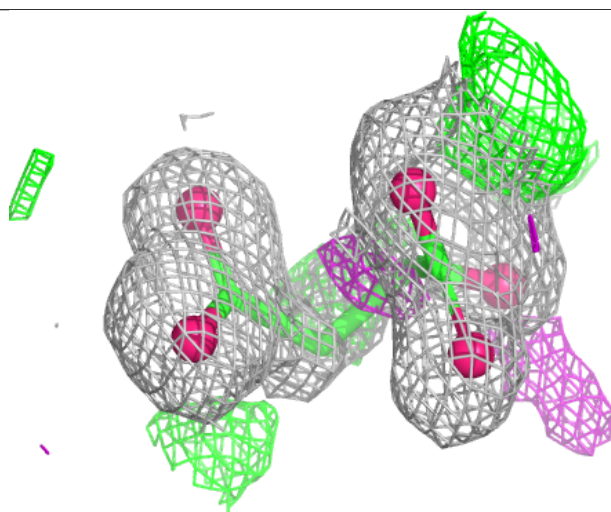
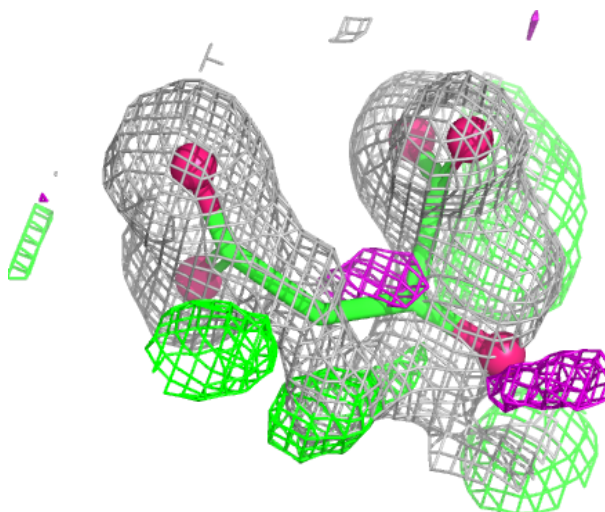
Electron density around LMR F 708:

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



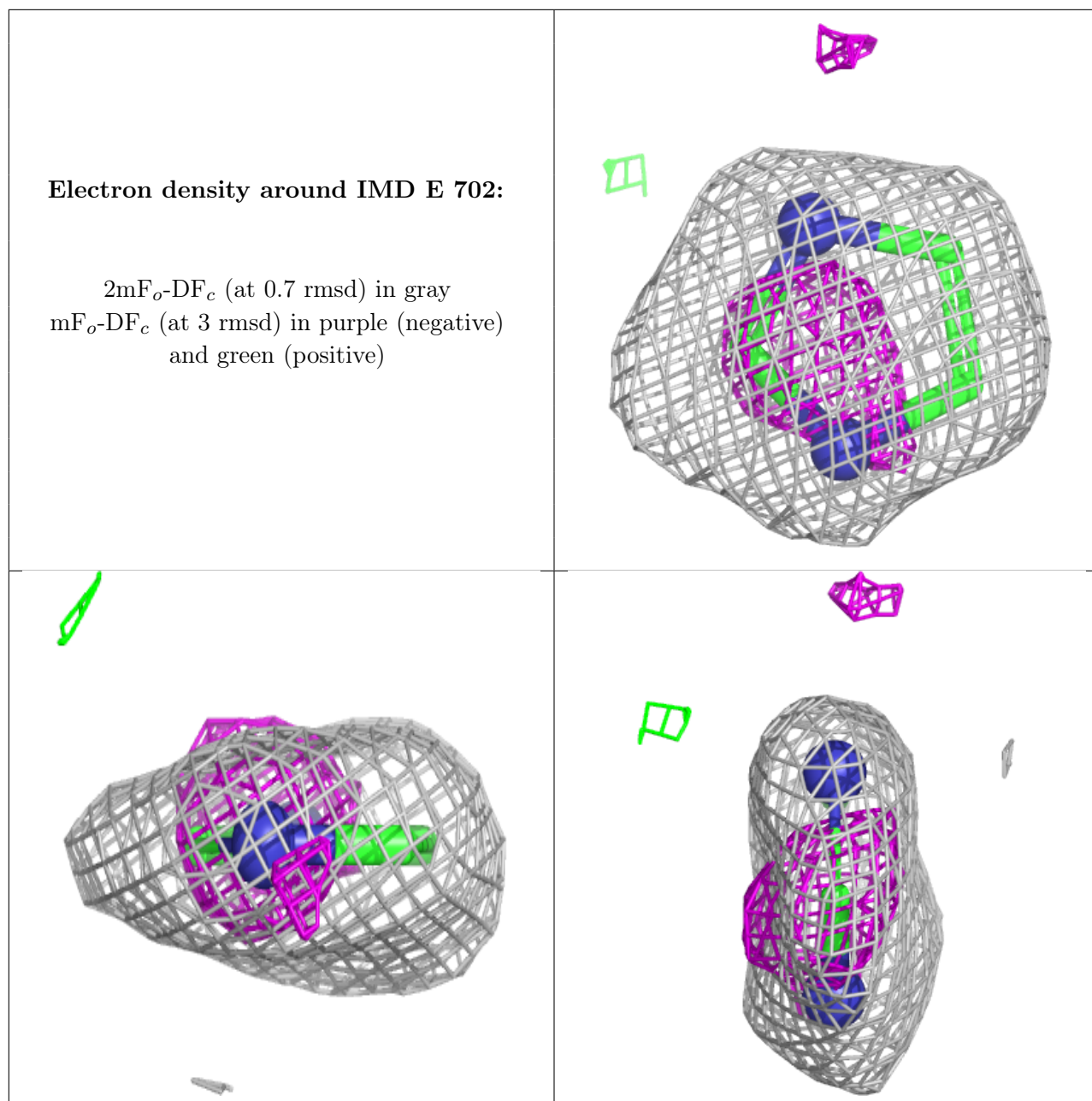
Electron density around LMR B 703:

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



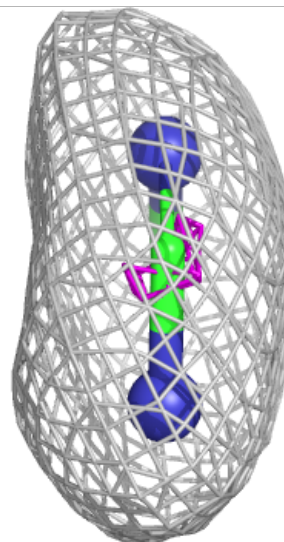
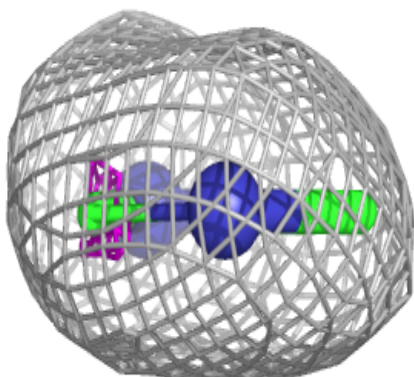
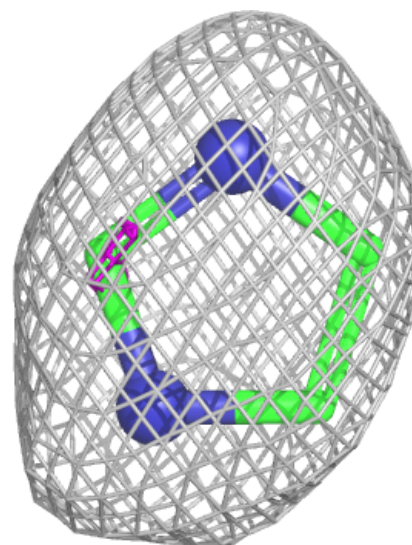
Electron density around IMD E 702:

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



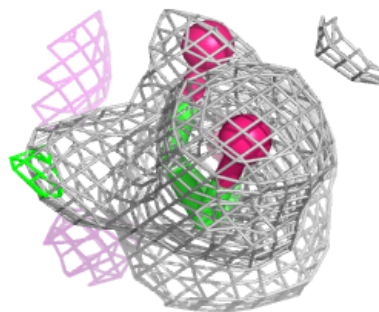
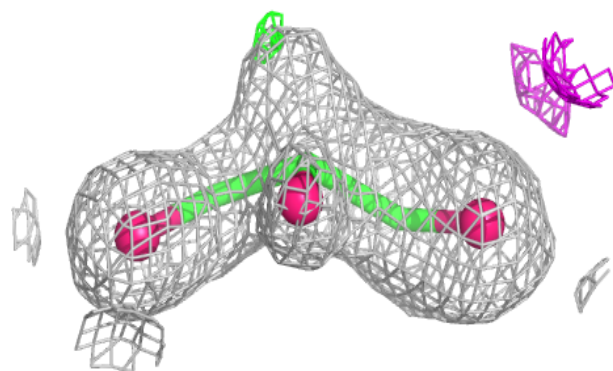
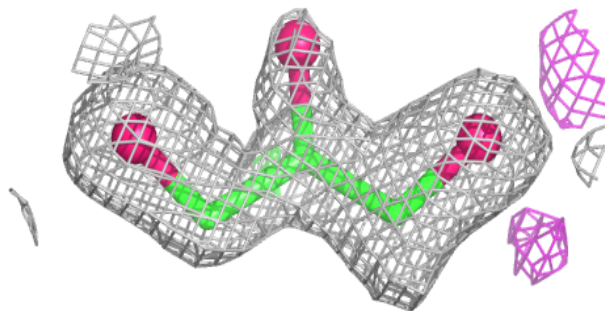
Electron density around IMD A 805:

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



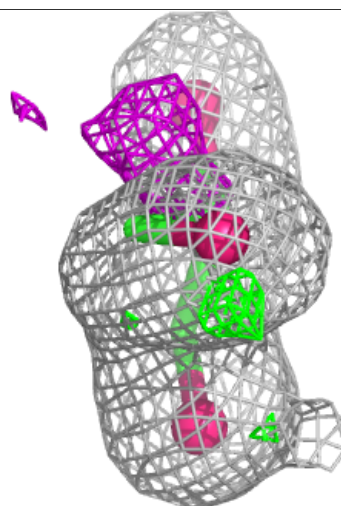
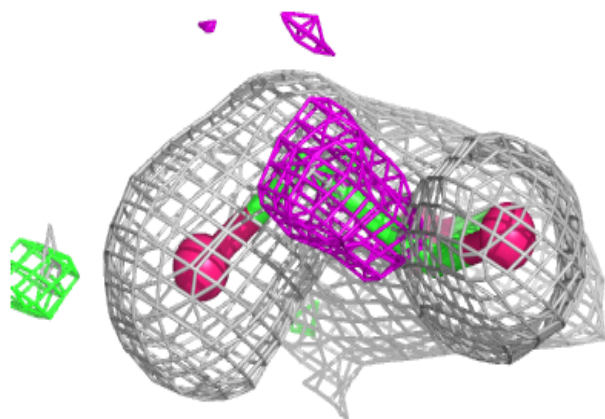
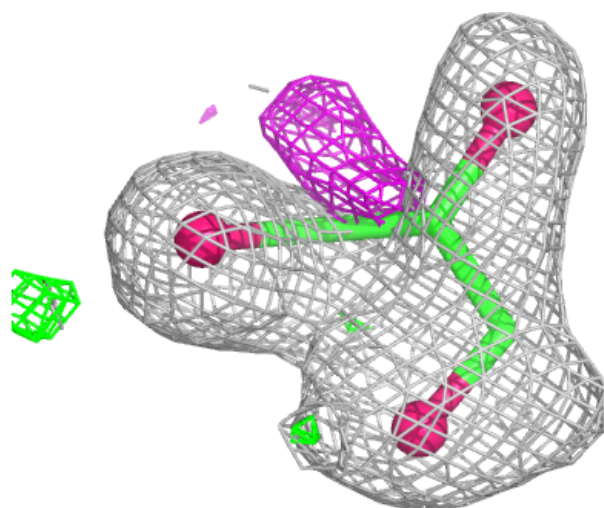
Electron density around GOL E 701:

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



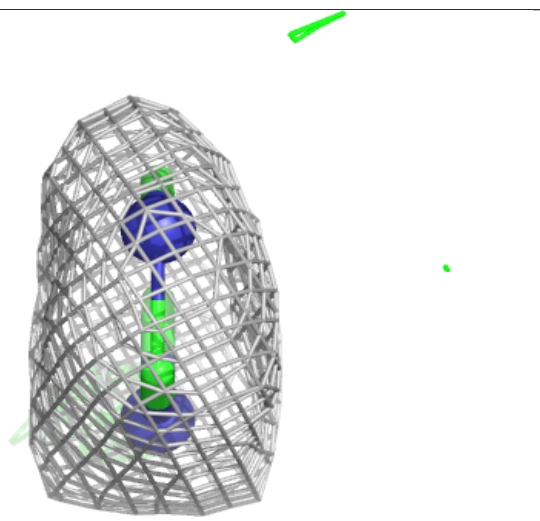
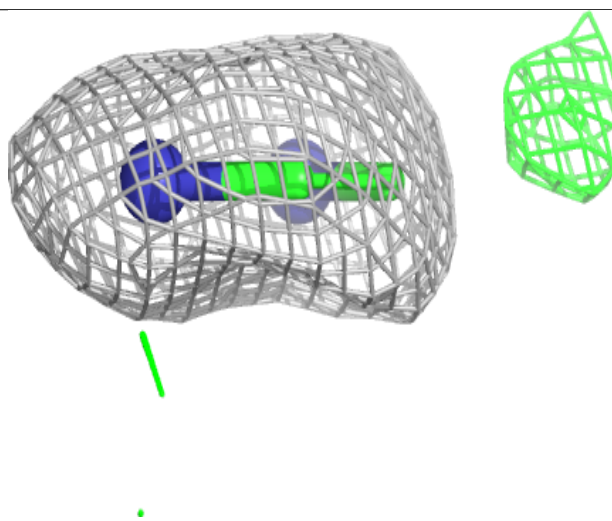
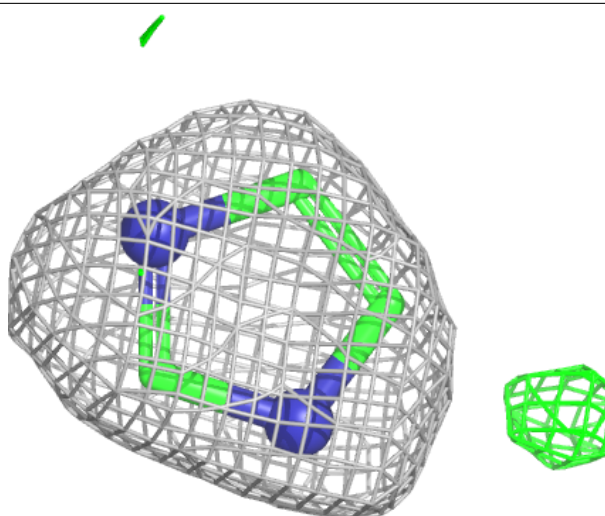
Electron density around GOL F 706:

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



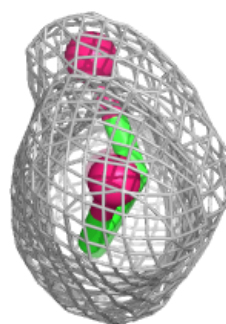
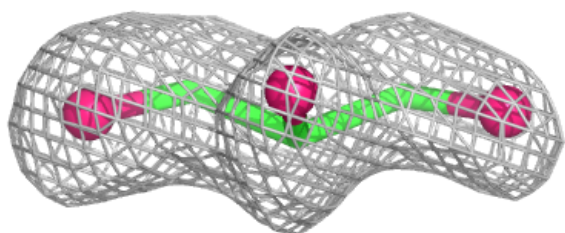
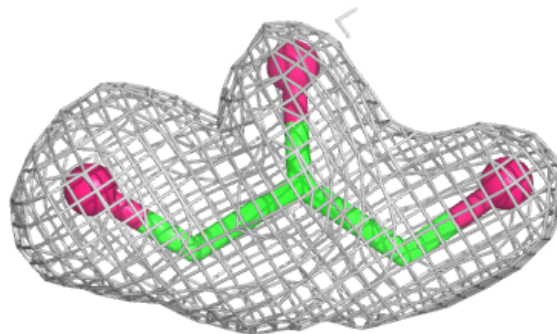
Electron density around IMD E 705:

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

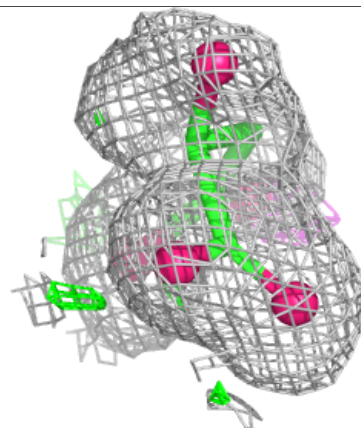
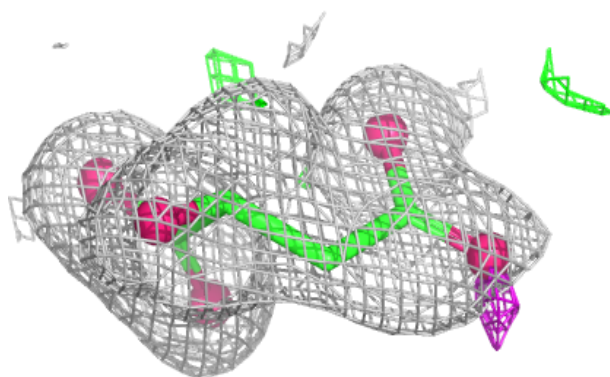
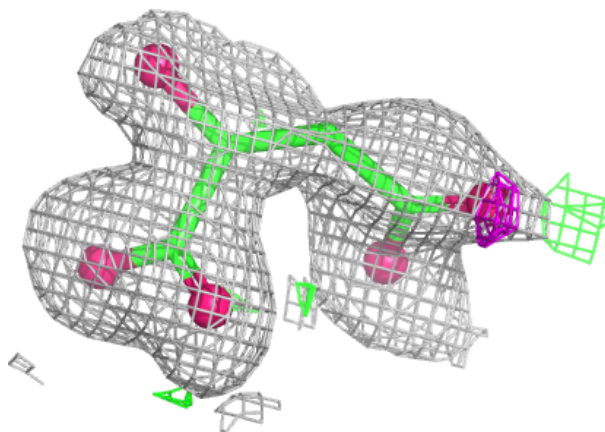


Electron density around GOL C 807:

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

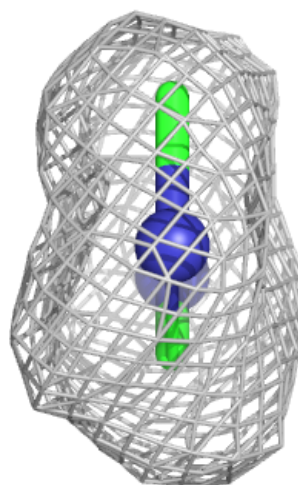
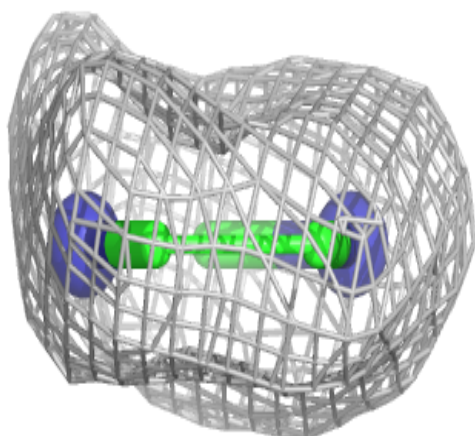
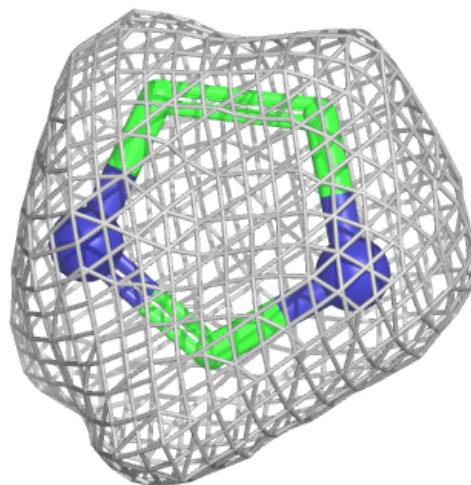
**Electron density around LMR D 702:**

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



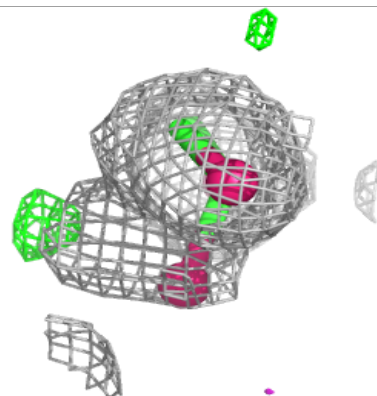
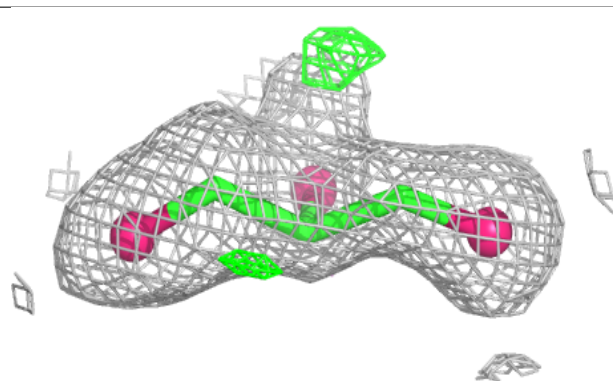
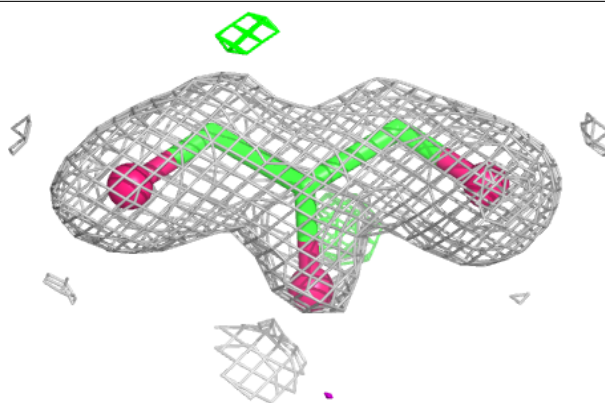
Electron density around IMD D 701:

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



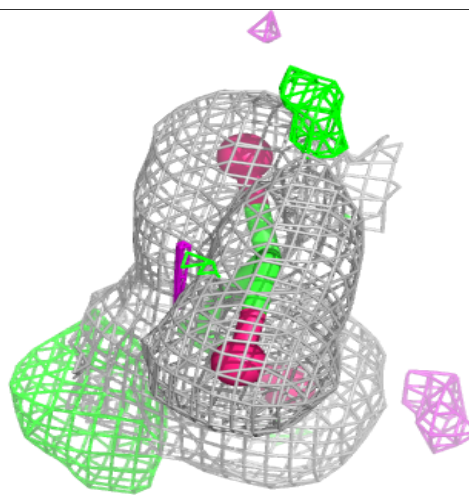
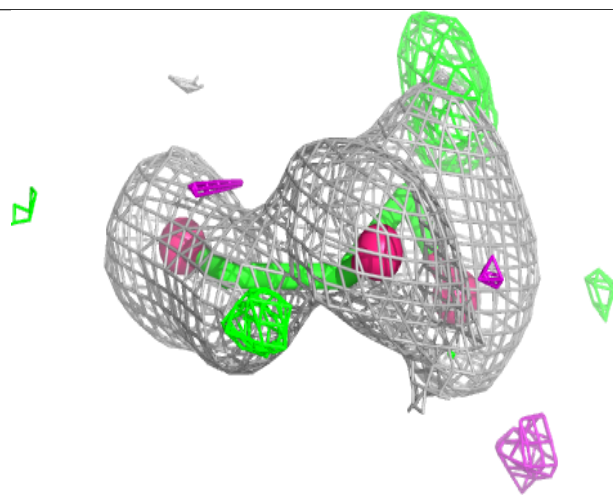
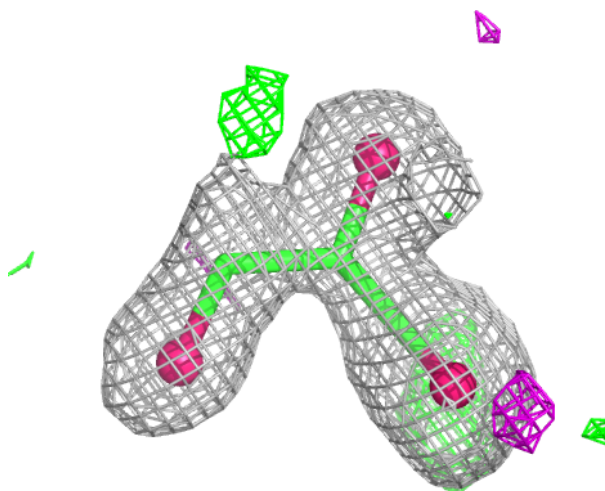
Electron density around GOL B 701:

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



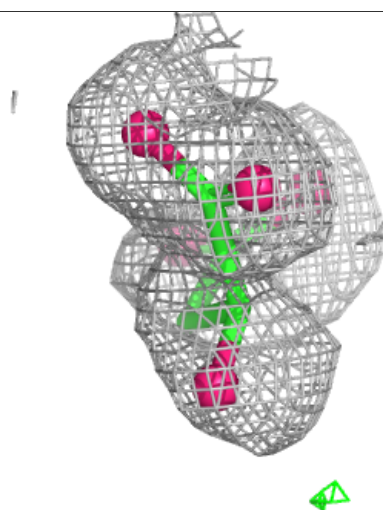
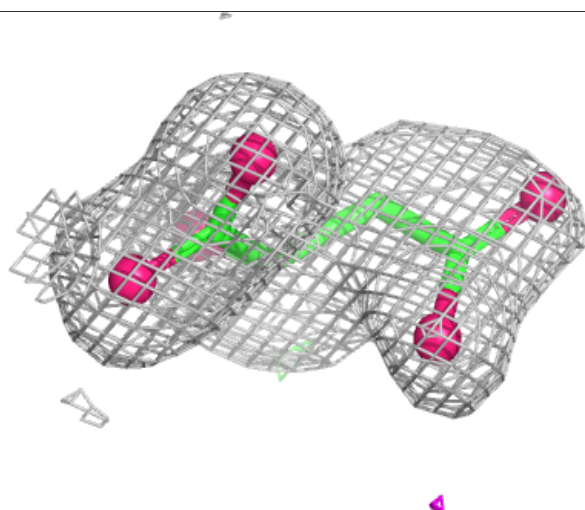
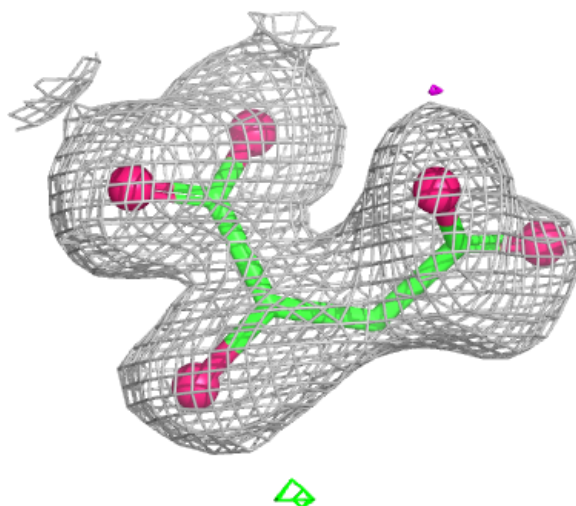
Electron density around GOL D 704:

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



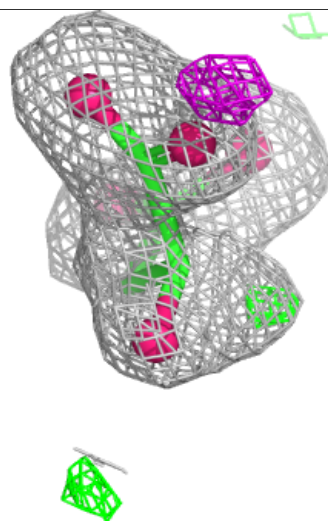
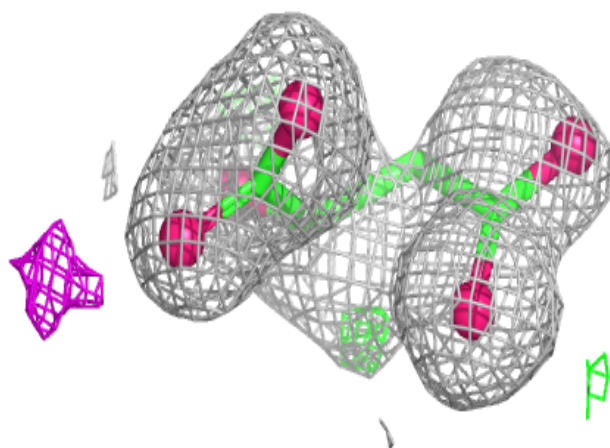
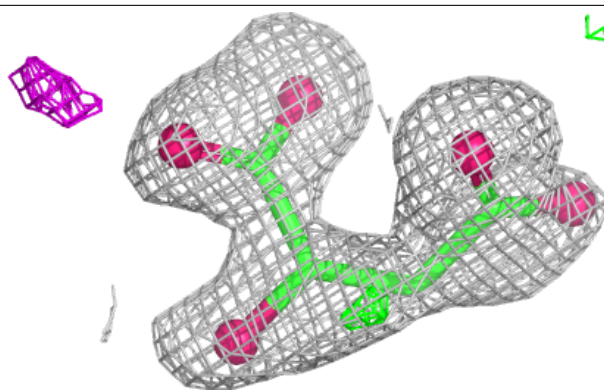
Electron density around LMR A 801:

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



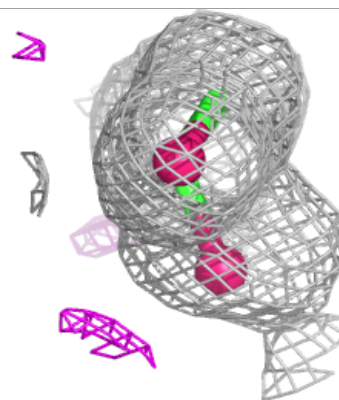
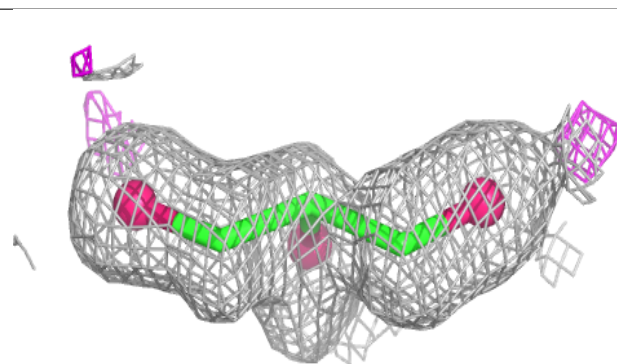
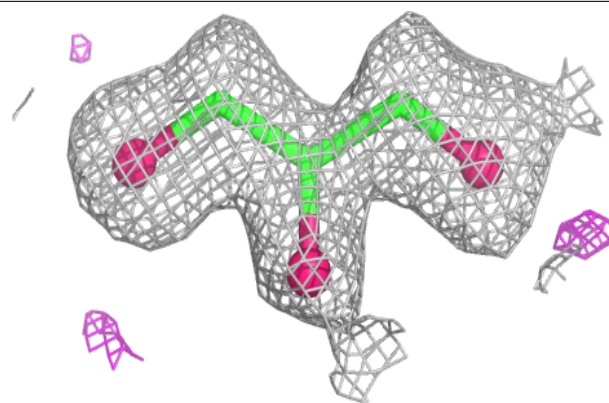
Electron density around LMR C 809:

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



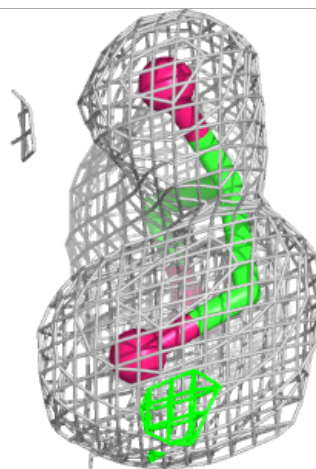
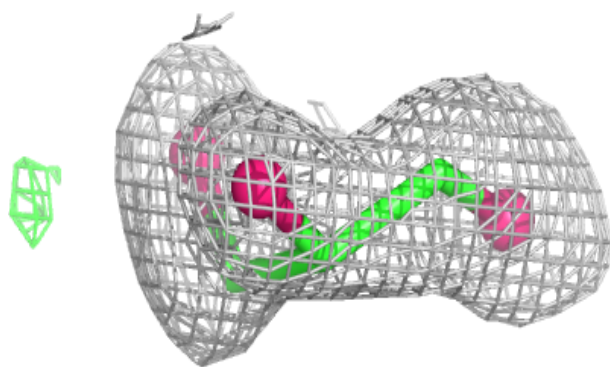
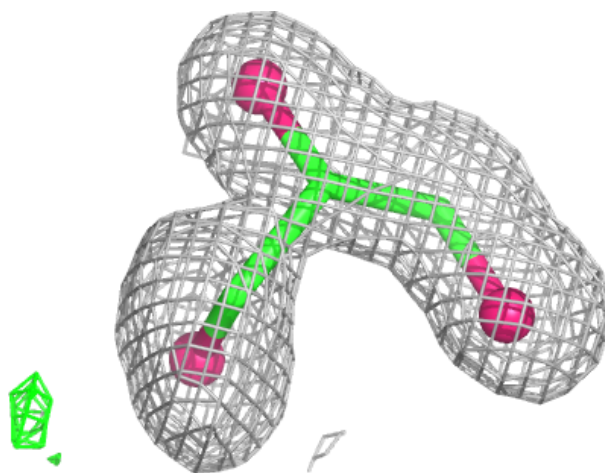
Electron density around GOL D 707:

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



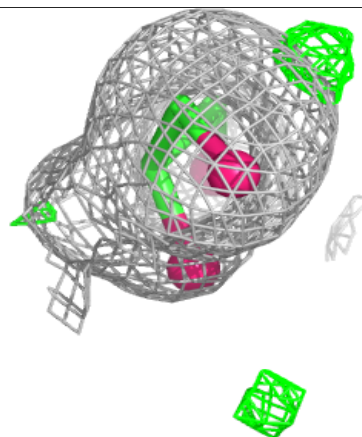
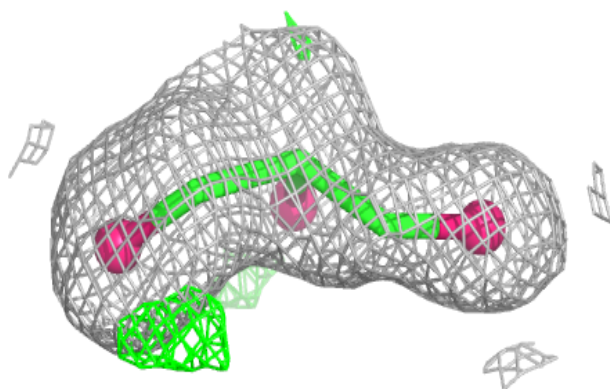
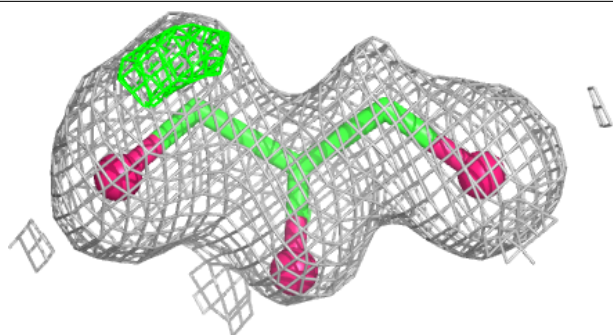
Electron density around GOL C 803:

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



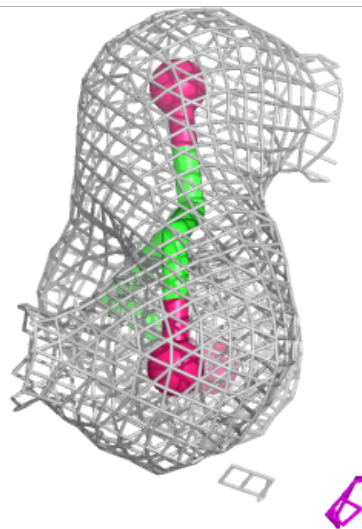
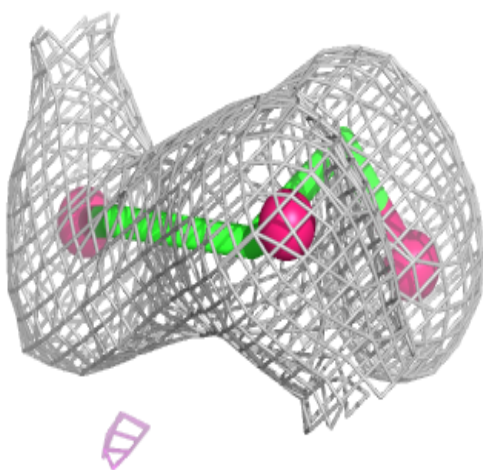
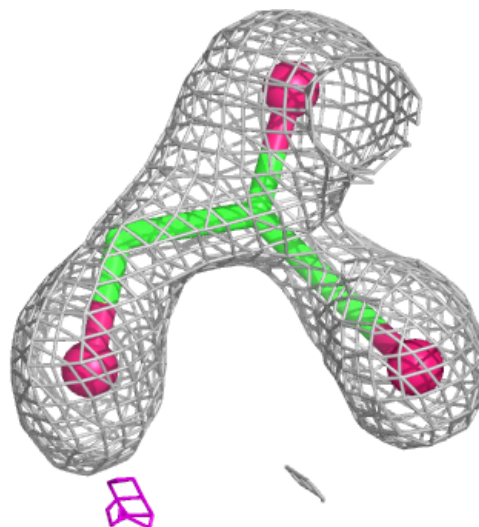
Electron density around GOL C 801:

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



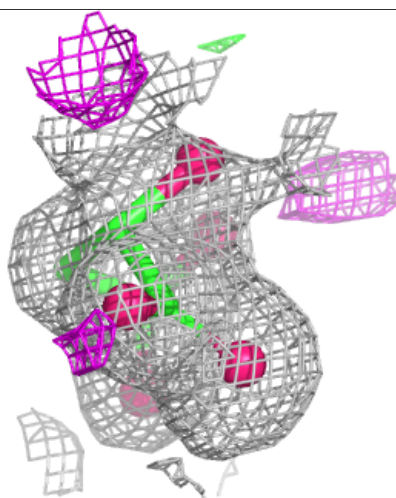
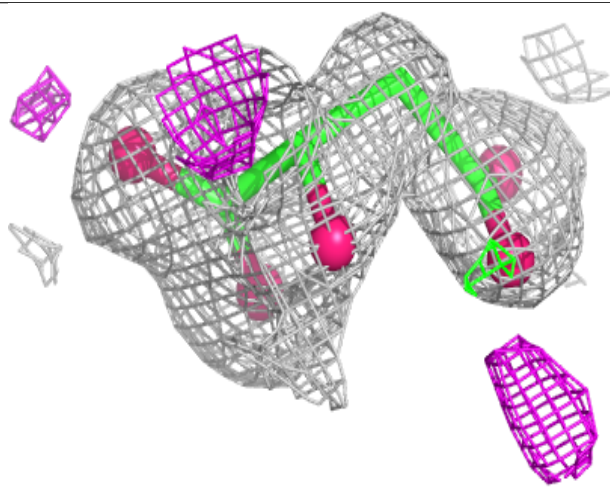
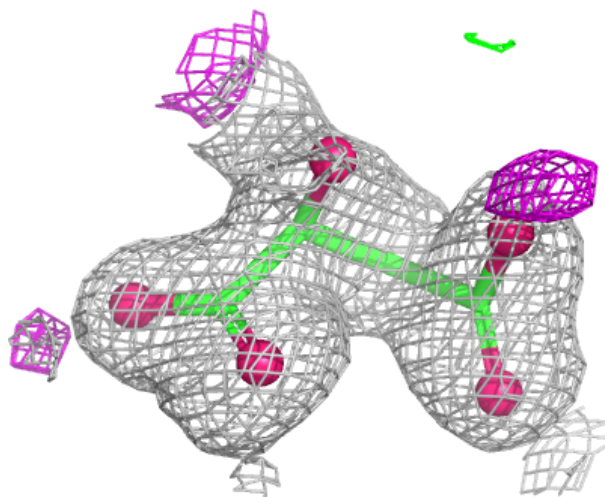
Electron density around GOL B 702:

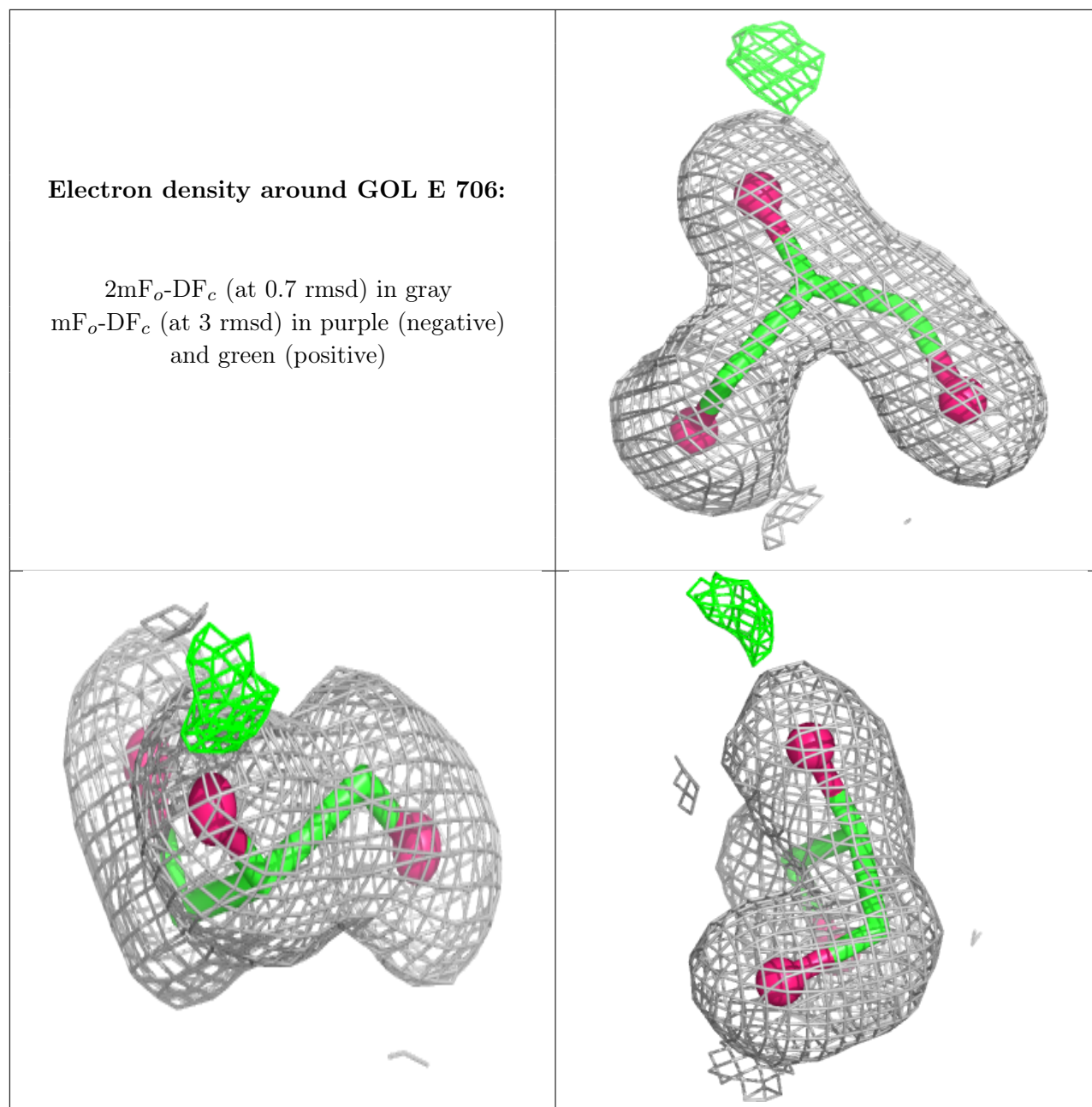
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMR 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.