



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 03:11 AM UTC

PDB ID : 9X6I / pdb_00009x6i
Title : Crystal structure of L-threonate 3-dehydrogenase from *Paracoccus litorisediminis* (ligand-free form)
Authors : Watanabe, S.; Sato, H.
Deposited on : 2025-10-15
Resolution : 1.90 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

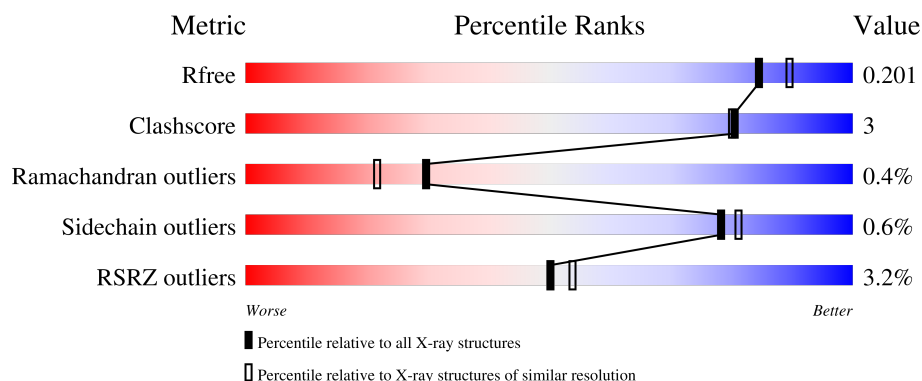
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	255	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
1	B	255	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>7%</div> </div> </div>
1	C	255	<div> <div></div> <div> <div></div> <div>86%</div> <div>6%</div> <div>7%</div> </div> </div>
1	D	255	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
1	E	255	<div> <div>0%</div> <div> <div></div> <div>88%</div> <div>•</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	255	<div><div>%</div><div><div></div><div>87%</div><div>5%7%</div></div></div>
1	G	255	<div><div></div><div>91%</div><div>•5%</div></div>
1	H	255	<div><div>%</div><div><div></div><div>87%</div><div>5%7%</div></div></div>
1	I	255	<div><div>%</div><div><div></div><div>88%</div><div>•8%</div></div></div>
1	J	255	<div><div>3%</div><div><div></div><div>89%</div><div>•8%</div></div></div>
1	K	255	<div><div>5%</div><div><div></div><div>88%</div><div>5%7%</div></div></div>
1	L	255	<div><div>15%</div><div><div></div><div>88%</div><div>•8%</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22752 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 SDR family NAD(P)-dependent oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	1	0
			1765	1102	317	336	10			
1	B	237	Total	C	N	O	S	0	1	0
			1735	1083	308	334	10			
1	C	237	Total	C	N	O	S	0	0	0
			1740	1085	311	334	10			
1	D	243	Total	C	N	O	S	0	0	0
			1774	1106	317	341	10			
1	E	236	Total	C	N	O	S	0	0	0
			1724	1075	306	333	10			
1	F	236	Total	C	N	O	S	0	0	0
			1733	1082	310	331	10			
1	G	243	Total	C	N	O	S	0	1	0
			1780	1110	317	341	12			
1	H	237	Total	C	N	O	S	0	1	0
			1736	1082	307	337	10			
1	I	235	Total	C	N	O	S	0	0	0
			1705	1067	301	327	10			
1	J	234	Total	C	N	O	S	0	0	0
			1684	1051	302	321	10			
1	K	237	Total	C	N	O	S	0	0	0
			1699	1064	299	326	10			
1	L	235	Total	C	N	O	S	0	0	0
			1655	1035	295	315	10			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP A0A844HLS7
A	-9	ARG	-	expression tag	UNP A0A844HLS7
A	-8	GLY	-	expression tag	UNP A0A844HLS7
A	-7	SER	-	expression tag	UNP A0A844HLS7
A	-6	HIS	-	expression tag	UNP A0A844HLS7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP A0A844HLS7
A	-4	HIS	-	expression tag	UNP A0A844HLS7
A	-3	HIS	-	expression tag	UNP A0A844HLS7
A	-2	HIS	-	expression tag	UNP A0A844HLS7
A	-1	HIS	-	expression tag	UNP A0A844HLS7
A	0	GLY	-	expression tag	UNP A0A844HLS7
A	1	SER	-	expression tag	UNP A0A844HLS7
B	-10	MET	-	initiating methionine	UNP A0A844HLS7
B	-9	ARG	-	expression tag	UNP A0A844HLS7
B	-8	GLY	-	expression tag	UNP A0A844HLS7
B	-7	SER	-	expression tag	UNP A0A844HLS7
B	-6	HIS	-	expression tag	UNP A0A844HLS7
B	-5	HIS	-	expression tag	UNP A0A844HLS7
B	-4	HIS	-	expression tag	UNP A0A844HLS7
B	-3	HIS	-	expression tag	UNP A0A844HLS7
B	-2	HIS	-	expression tag	UNP A0A844HLS7
B	-1	HIS	-	expression tag	UNP A0A844HLS7
B	0	GLY	-	expression tag	UNP A0A844HLS7
B	1	SER	-	expression tag	UNP A0A844HLS7
C	-10	MET	-	initiating methionine	UNP A0A844HLS7
C	-9	ARG	-	expression tag	UNP A0A844HLS7
C	-8	GLY	-	expression tag	UNP A0A844HLS7
C	-7	SER	-	expression tag	UNP A0A844HLS7
C	-6	HIS	-	expression tag	UNP A0A844HLS7
C	-5	HIS	-	expression tag	UNP A0A844HLS7
C	-4	HIS	-	expression tag	UNP A0A844HLS7
C	-3	HIS	-	expression tag	UNP A0A844HLS7
C	-2	HIS	-	expression tag	UNP A0A844HLS7
C	-1	HIS	-	expression tag	UNP A0A844HLS7
C	0	GLY	-	expression tag	UNP A0A844HLS7
C	1	SER	-	expression tag	UNP A0A844HLS7
D	-10	MET	-	initiating methionine	UNP A0A844HLS7
D	-9	ARG	-	expression tag	UNP A0A844HLS7
D	-8	GLY	-	expression tag	UNP A0A844HLS7
D	-7	SER	-	expression tag	UNP A0A844HLS7
D	-6	HIS	-	expression tag	UNP A0A844HLS7
D	-5	HIS	-	expression tag	UNP A0A844HLS7
D	-4	HIS	-	expression tag	UNP A0A844HLS7
D	-3	HIS	-	expression tag	UNP A0A844HLS7
D	-2	HIS	-	expression tag	UNP A0A844HLS7
D	-1	HIS	-	expression tag	UNP A0A844HLS7
D	0	GLY	-	expression tag	UNP A0A844HLS7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	SER	-	expression tag	UNP A0A844HLS7
E	-10	MET	-	initiating methionine	UNP A0A844HLS7
E	-9	ARG	-	expression tag	UNP A0A844HLS7
E	-8	GLY	-	expression tag	UNP A0A844HLS7
E	-7	SER	-	expression tag	UNP A0A844HLS7
E	-6	HIS	-	expression tag	UNP A0A844HLS7
E	-5	HIS	-	expression tag	UNP A0A844HLS7
E	-4	HIS	-	expression tag	UNP A0A844HLS7
E	-3	HIS	-	expression tag	UNP A0A844HLS7
E	-2	HIS	-	expression tag	UNP A0A844HLS7
E	-1	HIS	-	expression tag	UNP A0A844HLS7
E	0	GLY	-	expression tag	UNP A0A844HLS7
E	1	SER	-	expression tag	UNP A0A844HLS7
F	-10	MET	-	initiating methionine	UNP A0A844HLS7
F	-9	ARG	-	expression tag	UNP A0A844HLS7
F	-8	GLY	-	expression tag	UNP A0A844HLS7
F	-7	SER	-	expression tag	UNP A0A844HLS7
F	-6	HIS	-	expression tag	UNP A0A844HLS7
F	-5	HIS	-	expression tag	UNP A0A844HLS7
F	-4	HIS	-	expression tag	UNP A0A844HLS7
F	-3	HIS	-	expression tag	UNP A0A844HLS7
F	-2	HIS	-	expression tag	UNP A0A844HLS7
F	-1	HIS	-	expression tag	UNP A0A844HLS7
F	0	GLY	-	expression tag	UNP A0A844HLS7
F	1	SER	-	expression tag	UNP A0A844HLS7
G	-10	MET	-	initiating methionine	UNP A0A844HLS7
G	-9	ARG	-	expression tag	UNP A0A844HLS7
G	-8	GLY	-	expression tag	UNP A0A844HLS7
G	-7	SER	-	expression tag	UNP A0A844HLS7
G	-6	HIS	-	expression tag	UNP A0A844HLS7
G	-5	HIS	-	expression tag	UNP A0A844HLS7
G	-4	HIS	-	expression tag	UNP A0A844HLS7
G	-3	HIS	-	expression tag	UNP A0A844HLS7
G	-2	HIS	-	expression tag	UNP A0A844HLS7
G	-1	HIS	-	expression tag	UNP A0A844HLS7
G	0	GLY	-	expression tag	UNP A0A844HLS7
G	1	SER	-	expression tag	UNP A0A844HLS7
H	-10	MET	-	initiating methionine	UNP A0A844HLS7
H	-9	ARG	-	expression tag	UNP A0A844HLS7
H	-8	GLY	-	expression tag	UNP A0A844HLS7
H	-7	SER	-	expression tag	UNP A0A844HLS7
H	-6	HIS	-	expression tag	UNP A0A844HLS7

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	HIS	-	expression tag	UNP A0A844HLS7
H	-4	HIS	-	expression tag	UNP A0A844HLS7
H	-3	HIS	-	expression tag	UNP A0A844HLS7
H	-2	HIS	-	expression tag	UNP A0A844HLS7
H	-1	HIS	-	expression tag	UNP A0A844HLS7
H	0	GLY	-	expression tag	UNP A0A844HLS7
H	1	SER	-	expression tag	UNP A0A844HLS7
I	-10	MET	-	initiating methionine	UNP A0A844HLS7
I	-9	ARG	-	expression tag	UNP A0A844HLS7
I	-8	GLY	-	expression tag	UNP A0A844HLS7
I	-7	SER	-	expression tag	UNP A0A844HLS7
I	-6	HIS	-	expression tag	UNP A0A844HLS7
I	-5	HIS	-	expression tag	UNP A0A844HLS7
I	-4	HIS	-	expression tag	UNP A0A844HLS7
I	-3	HIS	-	expression tag	UNP A0A844HLS7
I	-2	HIS	-	expression tag	UNP A0A844HLS7
I	-1	HIS	-	expression tag	UNP A0A844HLS7
I	0	GLY	-	expression tag	UNP A0A844HLS7
I	1	SER	-	expression tag	UNP A0A844HLS7
J	-10	MET	-	initiating methionine	UNP A0A844HLS7
J	-9	ARG	-	expression tag	UNP A0A844HLS7
J	-8	GLY	-	expression tag	UNP A0A844HLS7
J	-7	SER	-	expression tag	UNP A0A844HLS7
J	-6	HIS	-	expression tag	UNP A0A844HLS7
J	-5	HIS	-	expression tag	UNP A0A844HLS7
J	-4	HIS	-	expression tag	UNP A0A844HLS7
J	-3	HIS	-	expression tag	UNP A0A844HLS7
J	-2	HIS	-	expression tag	UNP A0A844HLS7
J	-1	HIS	-	expression tag	UNP A0A844HLS7
J	0	GLY	-	expression tag	UNP A0A844HLS7
J	1	SER	-	expression tag	UNP A0A844HLS7
K	-10	MET	-	initiating methionine	UNP A0A844HLS7
K	-9	ARG	-	expression tag	UNP A0A844HLS7
K	-8	GLY	-	expression tag	UNP A0A844HLS7
K	-7	SER	-	expression tag	UNP A0A844HLS7
K	-6	HIS	-	expression tag	UNP A0A844HLS7
K	-5	HIS	-	expression tag	UNP A0A844HLS7
K	-4	HIS	-	expression tag	UNP A0A844HLS7
K	-3	HIS	-	expression tag	UNP A0A844HLS7
K	-2	HIS	-	expression tag	UNP A0A844HLS7
K	-1	HIS	-	expression tag	UNP A0A844HLS7
K	0	GLY	-	expression tag	UNP A0A844HLS7

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1	SER	-	expression tag	UNP A0A844HLS7
L	-10	MET	-	initiating methionine	UNP A0A844HLS7
L	-9	ARG	-	expression tag	UNP A0A844HLS7
L	-8	GLY	-	expression tag	UNP A0A844HLS7
L	-7	SER	-	expression tag	UNP A0A844HLS7
L	-6	HIS	-	expression tag	UNP A0A844HLS7
L	-5	HIS	-	expression tag	UNP A0A844HLS7
L	-4	HIS	-	expression tag	UNP A0A844HLS7
L	-3	HIS	-	expression tag	UNP A0A844HLS7
L	-2	HIS	-	expression tag	UNP A0A844HLS7
L	-1	HIS	-	expression tag	UNP A0A844HLS7
L	0	GLY	-	expression tag	UNP A0A844HLS7
L	1	SER	-	expression tag	UNP A0A844HLS7

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



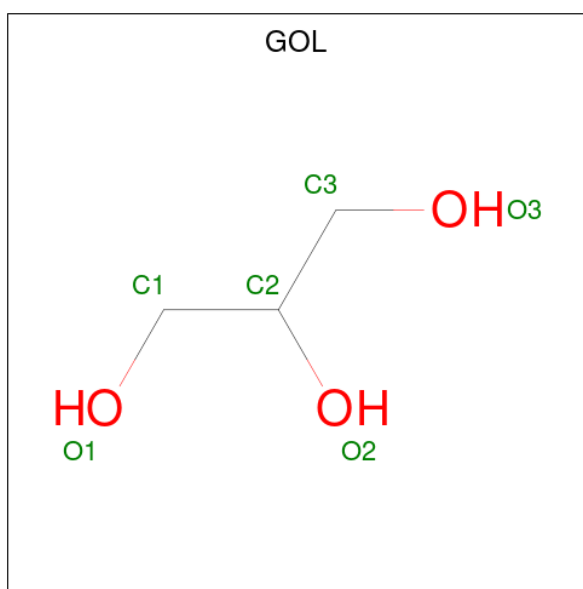
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	H	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	162	Total	O	0	0
			162	162		
5	B	187	Total	O	0	0
			187	187		
5	C	183	Total	O	0	0
			183	183		
5	D	175	Total	O	0	0
			175	175		
5	E	164	Total	O	0	0
			164	164		
5	F	151	Total	O	0	0
			151	151		
5	G	163	Total	O	0	0
			163	163		
5	H	187	Total	O	0	0
			187	187		

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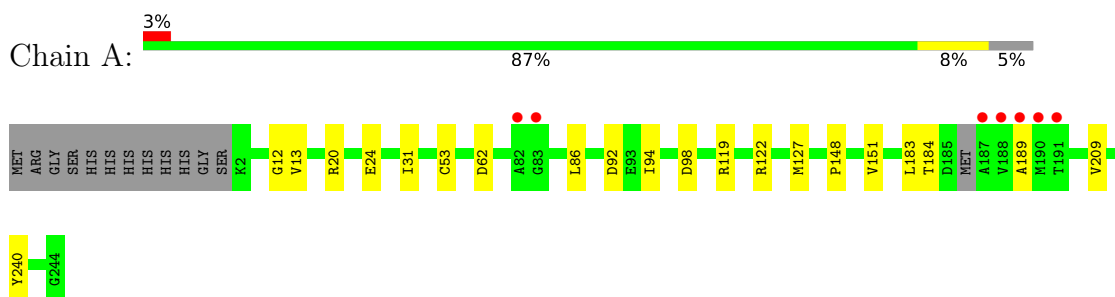
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	153	Total 153	O 153	0	0
5	J	111	Total 111	O 111	0	0
5	K	110	Total 110	O 110	0	0
5	L	80	Total 80	O 80	0	0

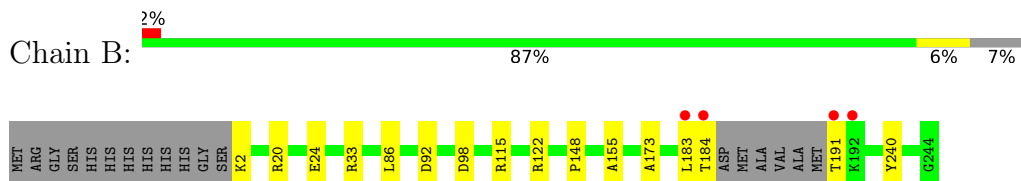
3 Residue-property plots [i](#)

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

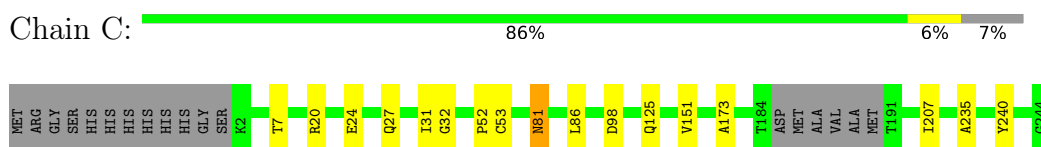
- Molecule 1: SDR family NAD(P)-dependent oxidoreductase



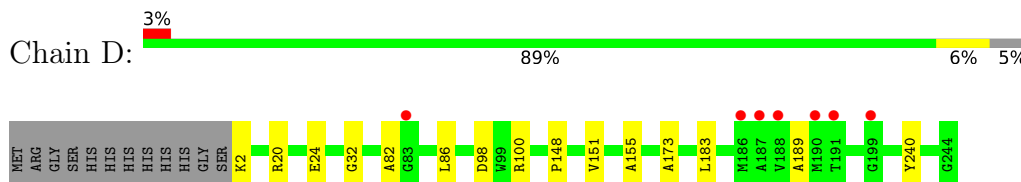
- Molecule 1: SDR family NAD(P)-dependent oxidoreductase



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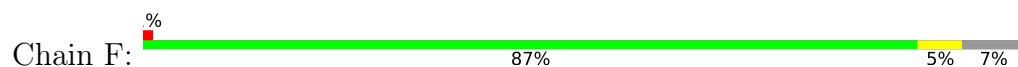


- Molecule 1: SDR family NAD(P)-dependent oxidoreductase





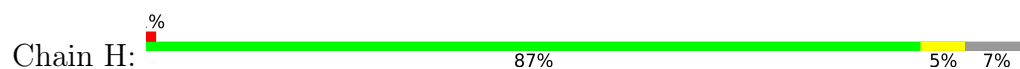
- Molecule 1: SDR family NAD(P)-dependent oxidoreductase



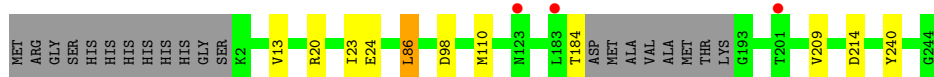
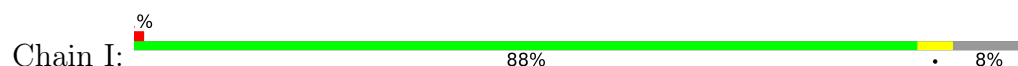
- Molecule 1: SDR family NAD(P)-dependent oxidoreductase



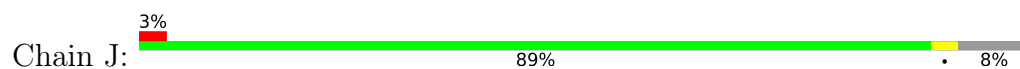
- Molecule 1: SDR family NAD(P)-dependent oxidoreductase



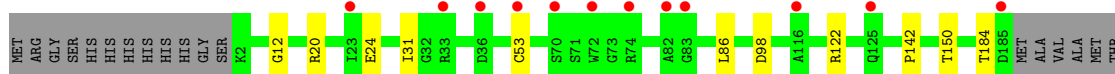
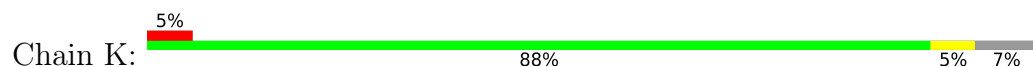
- Molecule 1: SDR family NAD(P)-dependent oxidoreductase



- Molecule 1: SDR family NAD(P)-dependent oxidoreductase

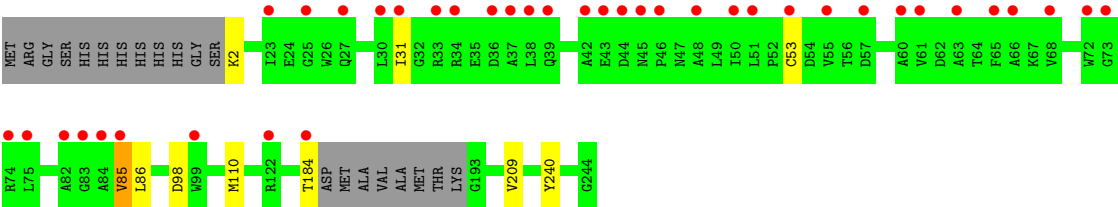
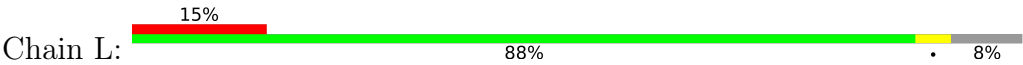


- Molecule 1: SDR family NAD(P)-dependent oxidoreductase





● Molecule 1: SDR family NAD(P)-dependent oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.76Å 73.45Å 141.29Å 83.15° 80.76° 83.81°	Depositor
Resolution (Å)	47.74 – 1.90 47.74 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.74-1.90) 97.9 (47.74-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.169 , 0.199 0.170 , 0.201	Depositor DCC
R_{free} test set	10441 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22752	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PEG, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/1795	0.58	0/2450
1	B	0.41	0/1765	0.56	0/2410
1	C	0.42	0/1770	0.59	0/2416
1	D	0.39	0/1805	0.57	0/2465
1	E	0.35	0/1754	0.53	0/2395
1	F	0.36	0/1763	0.55	0/2405
1	G	0.35	0/1811	0.54	0/2473
1	H	0.38	0/1766	0.55	0/2413
1	I	0.35	0/1735	0.52	0/2371
1	J	0.31	0/1714	0.49	0/2343
1	K	0.32	0/1729	0.50	0/2365
1	L	0.28	0/1685	0.47	0/2308
All	All	0.36	0/21092	0.54	0/28814

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1765	0	1725	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1735	0	1688	11	0
1	C	1740	0	1704	11	0
1	D	1774	0	1732	14	0
1	E	1724	0	1675	7	0
1	F	1733	0	1702	9	0
1	G	1780	0	1742	7	0
1	H	1736	0	1684	8	0
1	I	1705	0	1659	7	0
1	J	1684	0	1619	4	0
1	K	1699	0	1635	6	0
1	L	1655	0	1566	7	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
3	A	24	0	32	2	0
3	B	18	0	24	2	0
3	C	12	0	16	1	0
3	D	12	0	16	1	0
3	E	12	0	16	0	0
3	F	12	0	16	0	0
3	G	6	0	8	2	0
3	I	6	0	8	0	0
3	J	6	0	8	1	0
4	A	7	0	10	2	0
4	B	7	0	10	2	0
4	D	7	0	10	2	0
4	H	7	0	10	1	0
5	A	162	0	0	2	0
5	B	187	0	0	4	0
5	C	183	0	0	2	0
5	D	175	0	0	3	0
5	E	164	0	0	2	0
5	F	151	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	163	0	0	0	0
5	H	187	0	0	2	0
5	I	153	0	0	1	0
5	J	111	0	0	0	0
5	K	110	0	0	1	0
5	L	80	0	0	3	0
All	All	22752	0	20315	105	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (105) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:THR:O	1:C:81:ASN:ND2	1.89	1.05
1:C:20:ARG:NH1	1:C:24:GLU:OE2	2.12	0.83
1:G:20:ARG:NH1	1:G:24:GLU:OE2	2.15	0.80
1:H:20:ARG:NH1	1:H:24:GLU:OE2	2.13	0.77
1:A:12:GLY:H	4:A:306:PEG:H42	1.49	0.77
1:B:2:LYS:N	5:B:401:HOH:O	2.20	0.73
1:D:20:ARG:NH1	1:D:24:GLU:OE2	2.21	0.70
1:F:20:ARG:NH1	1:F:24:GLU:OE2	2.21	0.70
1:D:100:ARG:NH2	5:D:404:HOH:O	2.26	0.67
1:D:2:LYS:N	5:D:403:HOH:O	2.26	0.67
1:A:62:ASP:OD1	5:A:401:HOH:O	2.11	0.67
1:E:3:ASN:HB3	5:E:2405:HOH:O	1.96	0.66
1:B:20:ARG:NH1	1:B:24:GLU:OE2	2.30	0.63
1:L:86:LEU:HD11	1:L:98:ASP:HB3	1.80	0.62
1:J:86:LEU:HD11	1:J:98:ASP:HB3	1.82	0.61
1:B:191:THR:N	5:B:402:HOH:O	2.32	0.61
1:F:86:LEU:HD11	1:F:98:ASP:HB3	1.83	0.61
1:I:20:ARG:NH1	1:I:24:GLU:OE2	2.30	0.61
1:K:20:ARG:NH1	1:K:24:GLU:OE2	2.28	0.60
1:A:20:ARG:NH1	1:A:24:GLU:OE2	2.28	0.59
1:A:13:VAL:HA	1:A:209:VAL:CG2	2.33	0.59
1:C:86:LEU:HD11	1:C:98:ASP:HB3	1.87	0.57
1:D:173:ALA:HB2	3:D:302:GOL:H31	1.88	0.56
1:E:86:LEU:HD11	1:E:98:ASP:HB3	1.88	0.55
1:D:100:ARG:HG2	1:D:100:ARG:HH11	1.72	0.55
1:A:184:THR:HG22	1:A:209:VAL:HG11	1.89	0.54
1:A:94:ILE:HA	3:A:304:GOL:H32	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:214:ASP:HB3	5:I:532:HOH:O	2.08	0.53
1:A:92:ASP:OD2	1:B:122:ARG:HD3	2.09	0.53
1:K:86:LEU:HD11	1:K:98:ASP:HB3	1.90	0.53
1:A:98:ASP:OD2	3:A:304:GOL:O3	2.24	0.52
1:C:7:THR:HA	1:C:31:ILE:HB	1.92	0.52
1:D:32:GLY:CA	4:D:304:PEG:H31	2.40	0.52
1:G:186:MET:HE3	1:G:190:MET:HE3	1.91	0.52
1:G:86:LEU:HD22	1:G:87:PRO:HD2	1.90	0.52
1:F:2:LYS:N	5:F:402:HOH:O	2.43	0.51
1:F:20:ARG:O	1:F:23:ILE:HG22	2.10	0.51
1:H:86:LEU:HD12	1:H:148:PRO:HG2	1.93	0.51
1:I:13:VAL:HA	1:I:209:VAL:CG2	2.40	0.51
1:J:173:ALA:HB2	3:J:302:GOL:H12	1.92	0.51
1:B:173:ALA:HB2	3:B:303:GOL:H12	1.94	0.50
1:C:20:ARG:HD3	5:C:479:HOH:O	2.11	0.50
1:A:122:ARG:HD3	1:B:92:ASP:OD2	2.11	0.49
1:A:13:VAL:HG22	1:A:209:VAL:HG23	1.94	0.49
1:A:92:ASP:HA	1:B:115:ARG:HG3	1.94	0.49
1:B:86:LEU:HD11	1:B:98:ASP:HB3	1.95	0.49
1:J:82:ALA:HB1	1:J:105:VAL:HG12	1.95	0.49
1:F:183:LEU:HD22	1:F:206:VAL:HG11	1.94	0.49
1:D:32:GLY:HA3	4:D:304:PEG:H31	1.96	0.48
1:F:82:ALA:HB2	5:F:449:HOH:O	2.13	0.48
1:H:36:ASP:OD1	1:H:37:ALA:N	2.47	0.48
1:C:151:VAL:HG13	1:G:155:ALA:HB1	1.95	0.48
1:I:86:LEU:HD11	1:I:98:ASP:HB3	1.94	0.48
1:J:20:ARG:NH1	1:J:24:GLU:OE2	2.45	0.48
1:I:13:VAL:HG22	1:I:209:VAL:HG23	1.96	0.48
1:K:31:ILE:HG23	1:K:53:CYS:HB3	1.96	0.48
1:C:31:ILE:HG23	1:C:53:CYS:HB3	1.96	0.48
1:D:86:LEU:HD12	1:D:148:PRO:HG2	1.97	0.47
1:H:183:LEU:HD22	1:H:206:VAL:HG21	1.96	0.47
1:A:183:LEU:HD12	1:A:189:ALA:HB2	1.96	0.47
1:A:31:ILE:HG23	1:A:53:CYS:HB3	1.98	0.46
4:B:304:PEG:H22	5:B:478:HOH:O	2.15	0.46
1:A:86:LEU:HD11	1:A:98:ASP:HB3	1.98	0.46
1:H:104:ASP:OD1	5:H:401:HOH:O	2.20	0.46
1:L:85:VAL:HG22	5:L:444:HOH:O	2.15	0.46
1:A:12:GLY:N	4:A:306:PEG:H42	2.26	0.46
1:G:173:ALA:HB2	3:G:302:GOL:H11	1.98	0.46
1:B:33:ARG:H	4:B:304:PEG:H41	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:VAL:HA	1:F:209:VAL:CG2	2.46	0.45
1:C:173:ALA:HB2	3:C:302:GOL:H12	1.97	0.45
1:E:115:ARG:HG3	1:F:92:ASP:HA	1.98	0.45
1:D:86:LEU:HD11	1:D:98:ASP:HB3	1.99	0.45
1:A:86:LEU:HD12	1:A:148:PRO:HG2	1.98	0.45
1:L:31:ILE:HG23	1:L:53:CYS:HB3	1.99	0.45
1:C:207:ILE:HG23	1:C:235:ALA:HA	1.99	0.44
1:K:12:GLY:HA2	1:K:184:THR:CG2	2.47	0.44
1:L:184:THR:HG21	5:L:469:HOH:O	2.16	0.44
1:G:36:ASP:OD1	1:G:36:ASP:N	2.49	0.44
1:F:142:PRO:HB3	1:F:150:THR:HG21	1.99	0.44
1:E:82:ALA:HB2	5:E:2510:HOH:O	2.18	0.44
1:C:27:GLN:OE1	5:C:401:HOH:O	2.21	0.44
1:D:82:ALA:HB3	5:D:497:HOH:O	2.18	0.43
1:D:183:LEU:HD12	1:D:189:ALA:HB2	2.00	0.43
1:K:122:ARG:NH2	5:K:403:HOH:O	2.43	0.43
1:H:86:LEU:HD21	1:H:98:ASP:HB3	2.01	0.43
1:L:2:LYS:N	5:L:408:HOH:O	2.51	0.43
1:I:20:ARG:O	1:I:23:ILE:HG22	2.19	0.43
1:G:171:ASN:O	3:G:302:GOL:H31	2.18	0.42
1:B:86:LEU:HD12	1:B:148:PRO:HG2	2.00	0.42
1:A:127:MET:HE2	1:A:127:MET:HB3	1.88	0.42
1:A:151:VAL:HG13	1:B:155:ALA:HB1	2.01	0.42
4:H:302:PEG:H41	5:H:403:HOH:O	2.20	0.42
1:E:82:ALA:HB1	1:E:105:VAL:HG12	2.03	0.41
1:D:151:VAL:HG13	1:H:155:ALA:HB1	2.02	0.41
1:D:155:ALA:HB1	1:H:151:VAL:HG13	2.02	0.41
1:C:32:GLY:O	1:C:52:PRO:HA	2.21	0.41
1:E:110:MET:HE3	1:E:110:MET:HB3	1.85	0.41
1:L:184:THR:HA	1:L:209:VAL:HG22	2.03	0.41
1:D:100:ARG:HG2	1:D:100:ARG:NH1	2.35	0.41
1:E:142:PRO:HB3	1:E:150:THR:HG21	2.03	0.41
1:I:110:MET:HE3	1:I:110:MET:HB3	1.87	0.40
3:B:305:GOL:H11	5:B:439:HOH:O	2.22	0.40
1:L:110:MET:HE3	1:L:110:MET:HB3	2.02	0.40
1:A:119:ARG:NH2	5:A:409:HOH:O	2.55	0.40
1:K:142:PRO:HB3	1:K:150:THR:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/255 (94%)	234 (98%)	4 (2%)	1 (0%)	30	22
1	B	234/255 (92%)	231 (99%)	2 (1%)	1 (0%)	30	22
1	C	233/255 (91%)	229 (98%)	3 (1%)	1 (0%)	30	22
1	D	241/255 (94%)	238 (99%)	2 (1%)	1 (0%)	30	22
1	E	232/255 (91%)	228 (98%)	3 (1%)	1 (0%)	30	22
1	F	232/255 (91%)	230 (99%)	1 (0%)	1 (0%)	30	22
1	G	242/255 (95%)	239 (99%)	2 (1%)	1 (0%)	30	22
1	H	234/255 (92%)	231 (99%)	2 (1%)	1 (0%)	30	22
1	I	231/255 (91%)	227 (98%)	3 (1%)	1 (0%)	30	22
1	J	230/255 (90%)	226 (98%)	3 (1%)	1 (0%)	30	22
1	K	233/255 (91%)	231 (99%)	1 (0%)	1 (0%)	30	22
1	L	231/255 (91%)	226 (98%)	4 (2%)	1 (0%)	30	22
All	All	2812/3060 (92%)	2770 (98%)	30 (1%)	12 (0%)	30	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	TYR
1	B	240	TYR
1	C	240	TYR
1	D	240	TYR
1	E	240	TYR
1	F	240	TYR
1	G	240	TYR
1	H	240	TYR
1	I	240	TYR
1	J	240	TYR
1	K	240	TYR
1	L	240	TYR

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	179/202 (89%)	179 (100%)	0	100	100
1	B	178/202 (88%)	176 (99%)	2 (1%)	65	67
1	C	180/202 (89%)	178 (99%)	2 (1%)	65	67
1	D	181/202 (90%)	181 (100%)	0	100	100
1	E	177/202 (88%)	176 (99%)	1 (1%)	78	81
1	F	179/202 (89%)	178 (99%)	1 (1%)	78	81
1	G	183/202 (91%)	182 (100%)	1 (0%)	81	84
1	H	179/202 (89%)	176 (98%)	3 (2%)	53	52
1	I	174/202 (86%)	172 (99%)	2 (1%)	65	67
1	J	168/202 (83%)	168 (100%)	0	100	100
1	K	170/202 (84%)	170 (100%)	0	100	100
1	L	160/202 (79%)	159 (99%)	1 (1%)	78	81
All	All	2108/2424 (87%)	2095 (99%)	13 (1%)	78	81

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	183	LEU
1	B	184	THR
1	C	81	ASN
1	C	125	GLN
1	E	184	THR
1	F	183	LEU
1	G	86	LEU
1	H	122	ARG
1	H	183	LEU
1	H	184	THR
1	I	86	LEU
1	I	184	THR
1	L	85	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	123	ASN
1	B	27	GLN
1	D	120	GLN
1	E	237	ASN
1	F	47	ASN
1	F	237	ASN
1	I	154	HIS
1	J	154	HIS
1	K	154	HIS
1	L	154	HIS
1	L	218	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

34 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	GOL	I	302	-	5,5,5	0.59	0	5,5,5	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	D	304	-	6,6,6	0.52	0	5,5,5	1.01	1 (20%)
3	GOL	C	302	-	5,5,5	0.53	0	5,5,5	0.83	0
2	SO4	D	301	-	4,4,4	0.30	0	6,6,6	0.38	0
2	SO4	I	301	-	4,4,4	0.27	0	6,6,6	0.42	0
4	PEG	A	306	-	6,6,6	0.57	0	5,5,5	0.28	0
3	GOL	E	303	-	5,5,5	0.55	0	5,5,5	0.87	0
2	SO4	L	301	-	4,4,4	0.19	0	6,6,6	0.20	0
3	GOL	E	302	-	5,5,5	0.41	0	5,5,5	0.61	0
2	SO4	B	301	-	4,4,4	0.20	0	6,6,6	0.21	0
3	GOL	F	303	-	5,5,5	0.63	0	5,5,5	0.72	0
2	SO4	J	301	-	4,4,4	0.10	0	6,6,6	0.27	0
3	GOL	G	302	-	5,5,5	0.52	0	5,5,5	0.37	0
2	SO4	H	301	-	4,4,4	0.28	0	6,6,6	0.18	0
2	SO4	G	301	-	4,4,4	0.24	0	6,6,6	0.18	0
3	GOL	A	303	-	5,5,5	0.57	0	5,5,5	0.54	0
2	SO4	F	301	-	4,4,4	0.33	0	6,6,6	0.30	0
3	GOL	B	302	-	5,5,5	0.43	0	5,5,5	0.23	0
3	GOL	A	305	-	5,5,5	0.75	0	5,5,5	0.71	0
3	GOL	B	305	-	5,5,5	0.61	0	5,5,5	0.66	0
3	GOL	B	303	-	5,5,5	0.52	0	5,5,5	0.42	0
2	SO4	C	301	-	4,4,4	0.24	0	6,6,6	0.33	0
2	SO4	A	301	-	4,4,4	0.15	0	6,6,6	0.19	0
2	SO4	K	301	-	4,4,4	0.25	0	6,6,6	0.37	0
4	PEG	B	304	-	6,6,6	0.42	0	5,5,5	0.44	0
4	PEG	H	302	-	6,6,6	0.54	0	5,5,5	0.37	0
3	GOL	D	303	-	5,5,5	0.45	0	5,5,5	0.58	0
3	GOL	C	303	-	5,5,5	0.59	0	5,5,5	0.51	0
3	GOL	D	302	-	5,5,5	0.56	0	5,5,5	0.52	0
3	GOL	A	304	-	5,5,5	0.60	0	5,5,5	0.85	0
3	GOL	A	302	-	5,5,5	0.49	0	5,5,5	0.65	0
3	GOL	J	302	-	5,5,5	0.49	0	5,5,5	0.42	0
2	SO4	E	301	-	4,4,4	0.23	0	6,6,6	0.36	0
3	GOL	F	302	-	5,5,5	0.43	0	5,5,5	0.69	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	GOL	I	302	-	-	2/4/4/4	-
4	PEG	D	304	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	302	-	-	0/4/4/4	-
4	PEG	A	306	-	-	2/4/4/4	-
3	GOL	E	303	-	-	4/4/4/4	-
3	GOL	E	302	-	-	0/4/4/4	-
3	GOL	F	303	-	-	4/4/4/4	-
3	GOL	G	302	-	-	2/4/4/4	-
3	GOL	A	303	-	-	3/4/4/4	-
3	GOL	B	302	-	-	4/4/4/4	-
3	GOL	A	305	-	-	1/4/4/4	-
3	GOL	B	305	-	-	1/4/4/4	-
3	GOL	B	303	-	-	0/4/4/4	-
4	PEG	B	304	-	-	2/4/4/4	-
4	PEG	H	302	-	-	2/4/4/4	-
3	GOL	D	303	-	-	2/4/4/4	-
3	GOL	C	303	-	-	0/4/4/4	-
3	GOL	D	302	-	-	0/4/4/4	-
3	GOL	A	304	-	-	4/4/4/4	-
3	GOL	A	302	-	-	3/4/4/4	-
3	GOL	J	302	-	-	0/4/4/4	-
3	GOL	F	302	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	304	PEG	O2-C3-C4	2.23	119.94	110.11

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	GOL	O1-C1-C2-C3
3	A	304	GOL	O1-C1-C2-C3
3	A	304	GOL	C1-C2-C3-O3
3	A	304	GOL	O2-C2-C3-O3
3	B	302	GOL	O1-C1-C2-C3
3	D	303	GOL	C1-C2-C3-O3
3	E	303	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	F	303	GOL	O1-C1-C2-O2
3	F	303	GOL	O1-C1-C2-C3
3	F	303	GOL	C1-C2-C3-O3
3	G	302	GOL	C1-C2-C3-O3
3	G	302	GOL	O2-C2-C3-O3
3	I	302	GOL	O1-C1-C2-C3
4	D	304	PEG	C1-C2-O2-C3
3	B	302	GOL	C1-C2-C3-O3
3	B	305	GOL	O1-C1-C2-C3
3	E	303	GOL	O1-C1-C2-C3
3	A	304	GOL	O1-C1-C2-O2
3	B	302	GOL	O2-C2-C3-O3
3	E	303	GOL	O2-C2-C3-O3
3	I	302	GOL	O1-C1-C2-O2
4	B	304	PEG	O2-C3-C4-O4
4	B	304	PEG	O1-C1-C2-O2
3	A	302	GOL	O2-C2-C3-O3
3	A	303	GOL	O1-C1-C2-O2
3	B	302	GOL	O1-C1-C2-O2
3	D	303	GOL	O2-C2-C3-O3
3	F	303	GOL	O2-C2-C3-O3
3	A	303	GOL	O2-C2-C3-O3
4	H	302	PEG	O1-C1-C2-O2
3	A	302	GOL	O1-C1-C2-O2
3	E	303	GOL	O1-C1-C2-O2
4	H	302	PEG	C4-C3-O2-C2
4	A	306	PEG	C4-C3-O2-C2
3	A	305	GOL	O2-C2-C3-O3
3	A	302	GOL	C1-C2-C3-O3
4	A	306	PEG	C1-C2-O2-C3

There are no ring outliers.

11 monomers are involved in 16 short contacts:

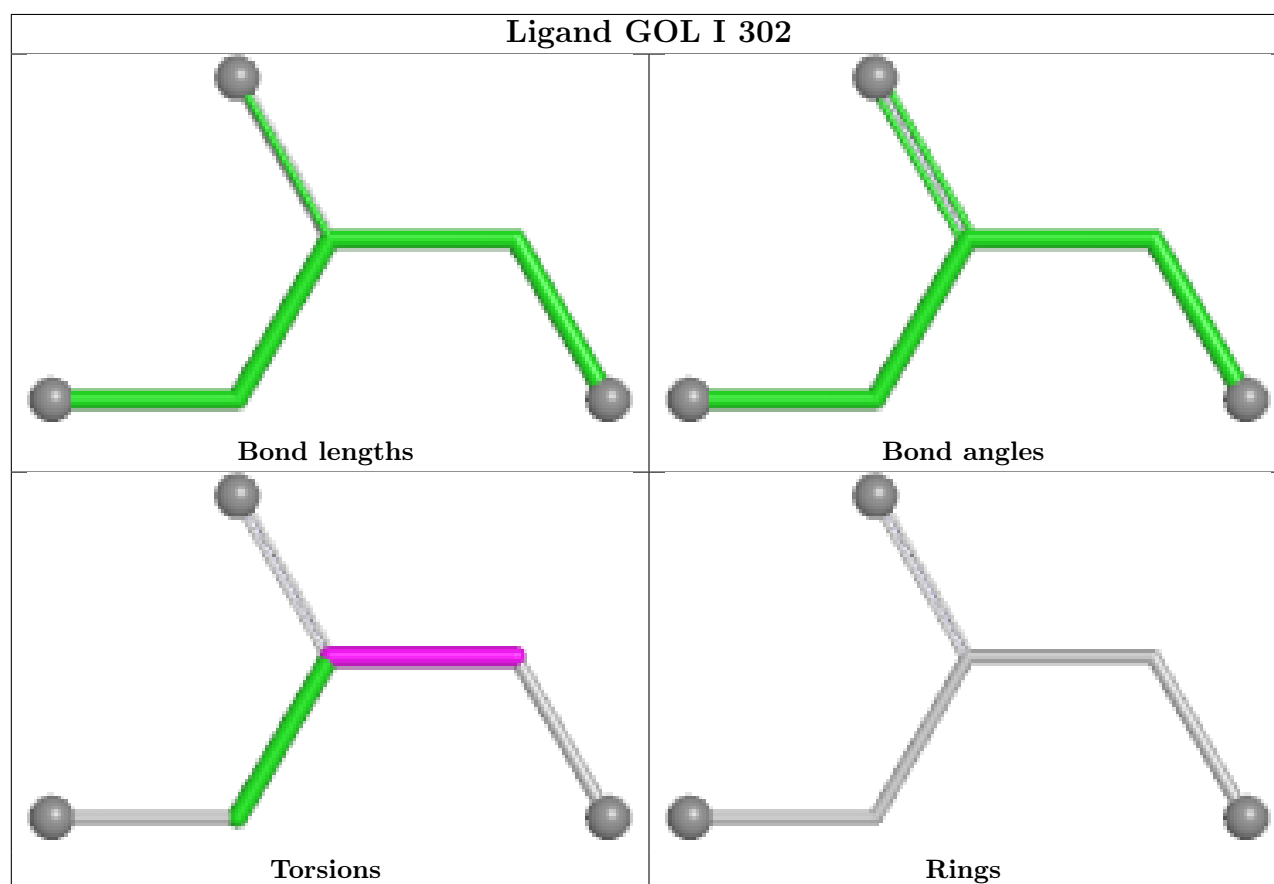
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	304	PEG	2	0
3	C	302	GOL	1	0
4	A	306	PEG	2	0
3	G	302	GOL	2	0
3	B	305	GOL	1	0
3	B	303	GOL	1	0
4	B	304	PEG	2	0

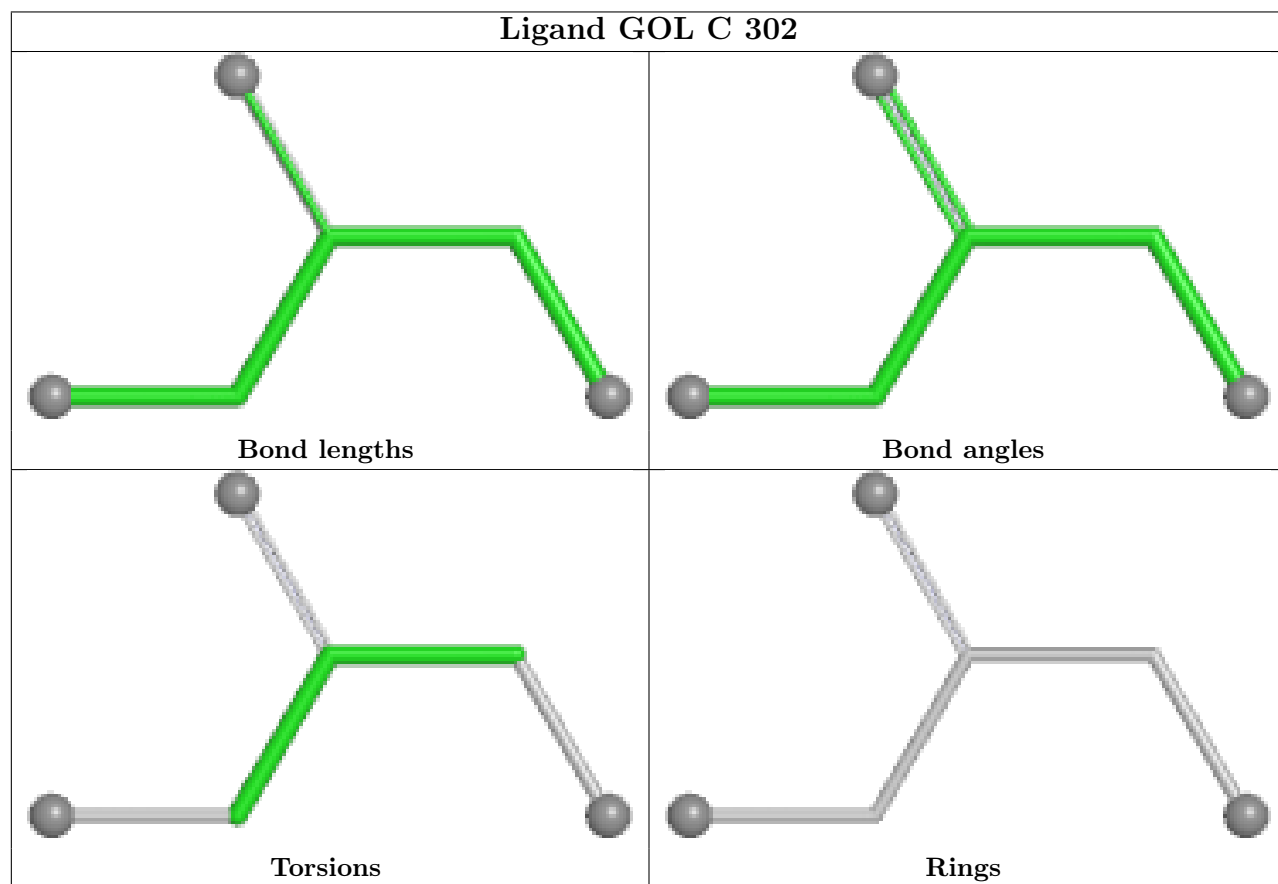
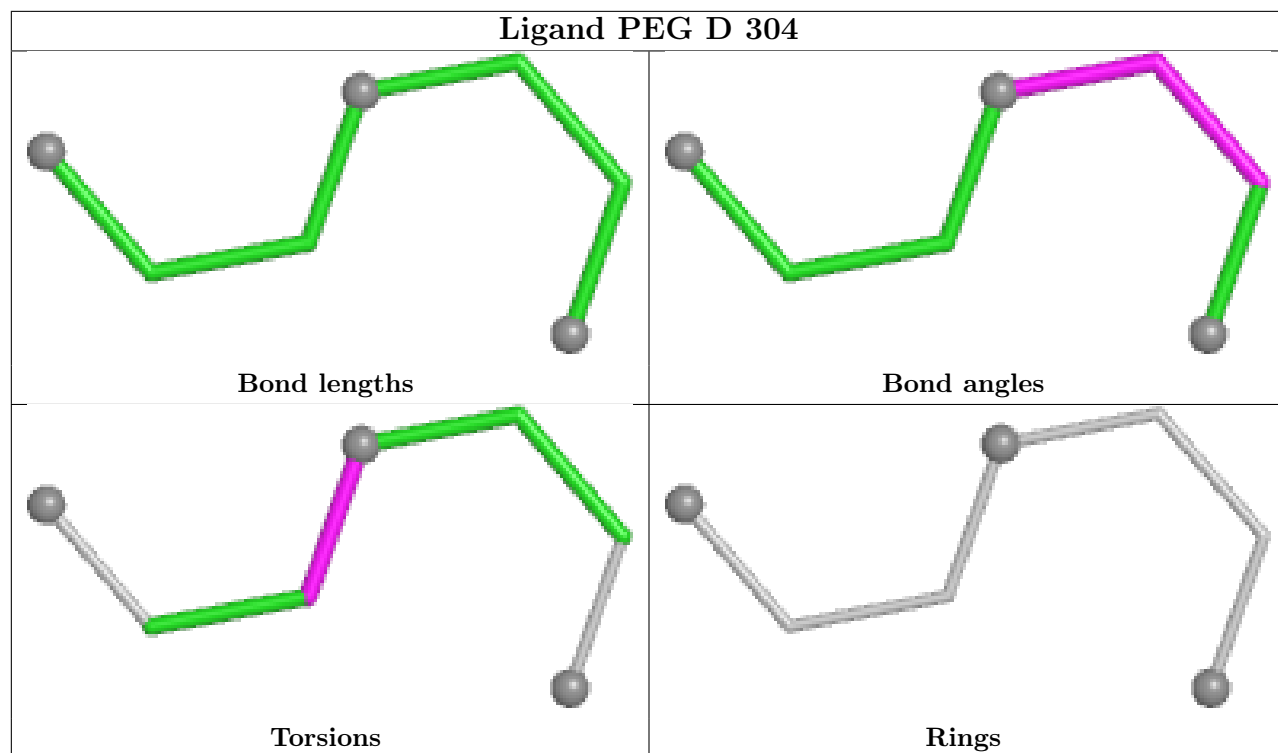
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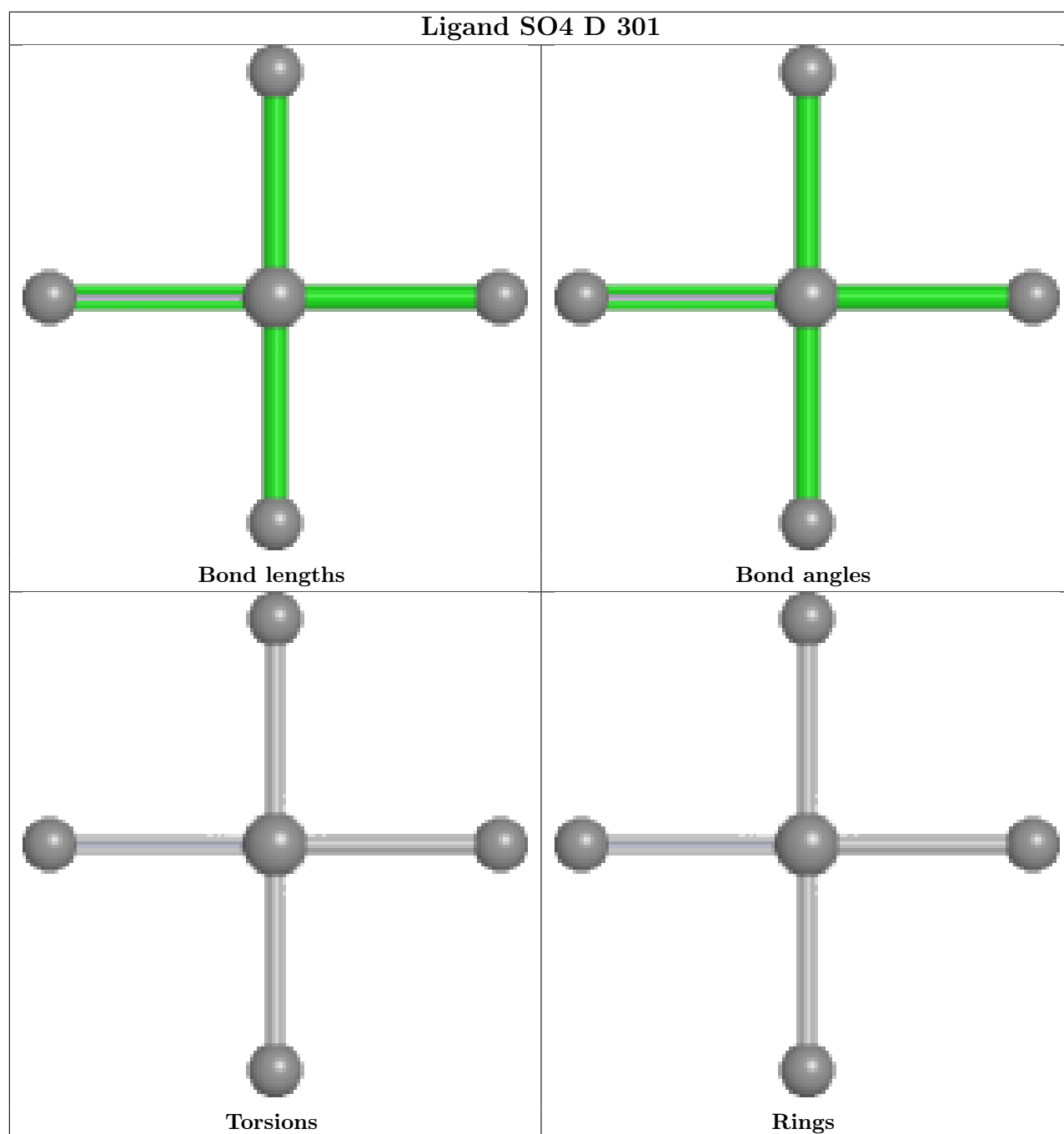
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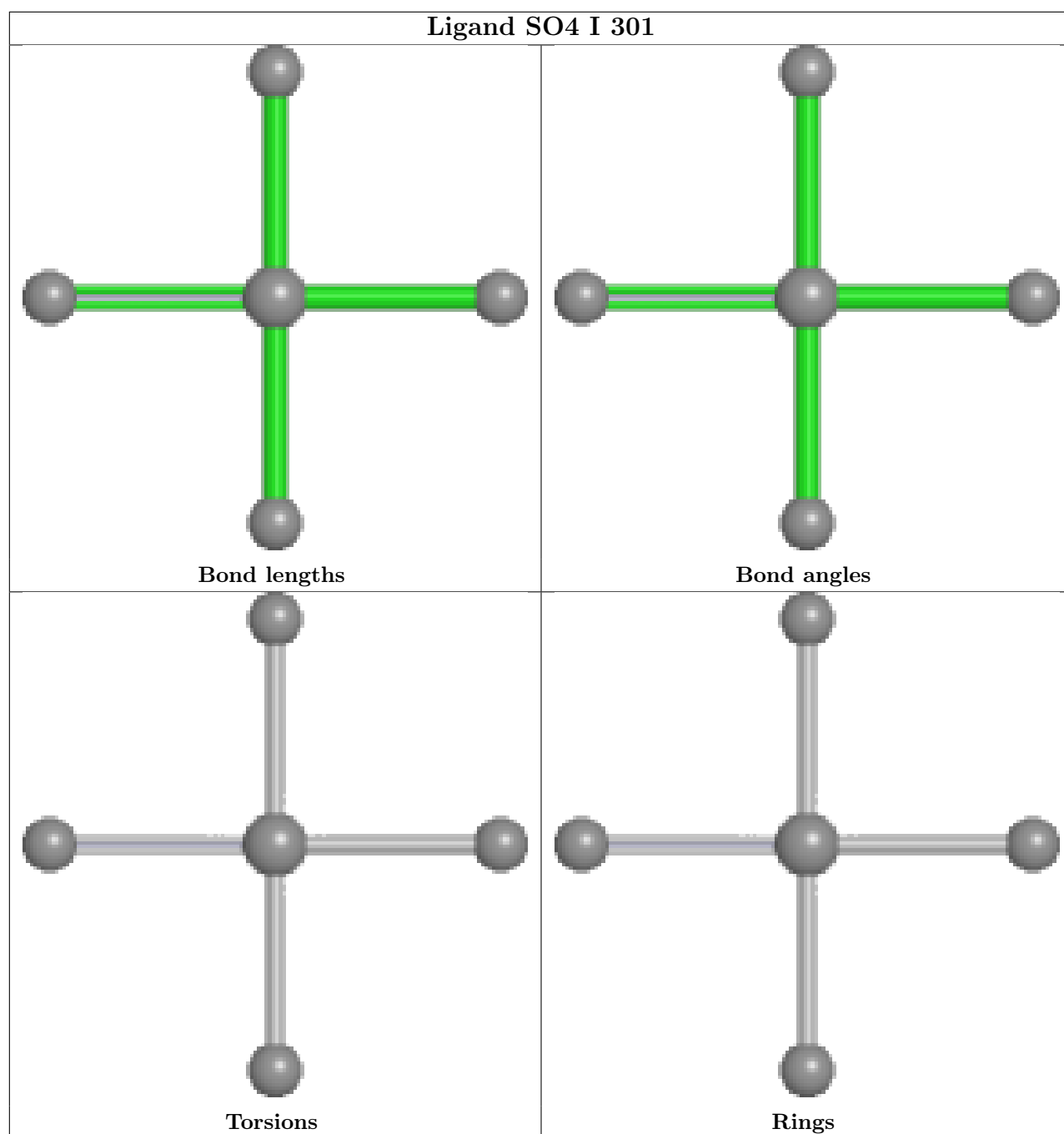
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	302	PEG	1	0
3	D	302	GOL	1	0
3	A	304	GOL	2	0
3	J	302	GOL	1	0

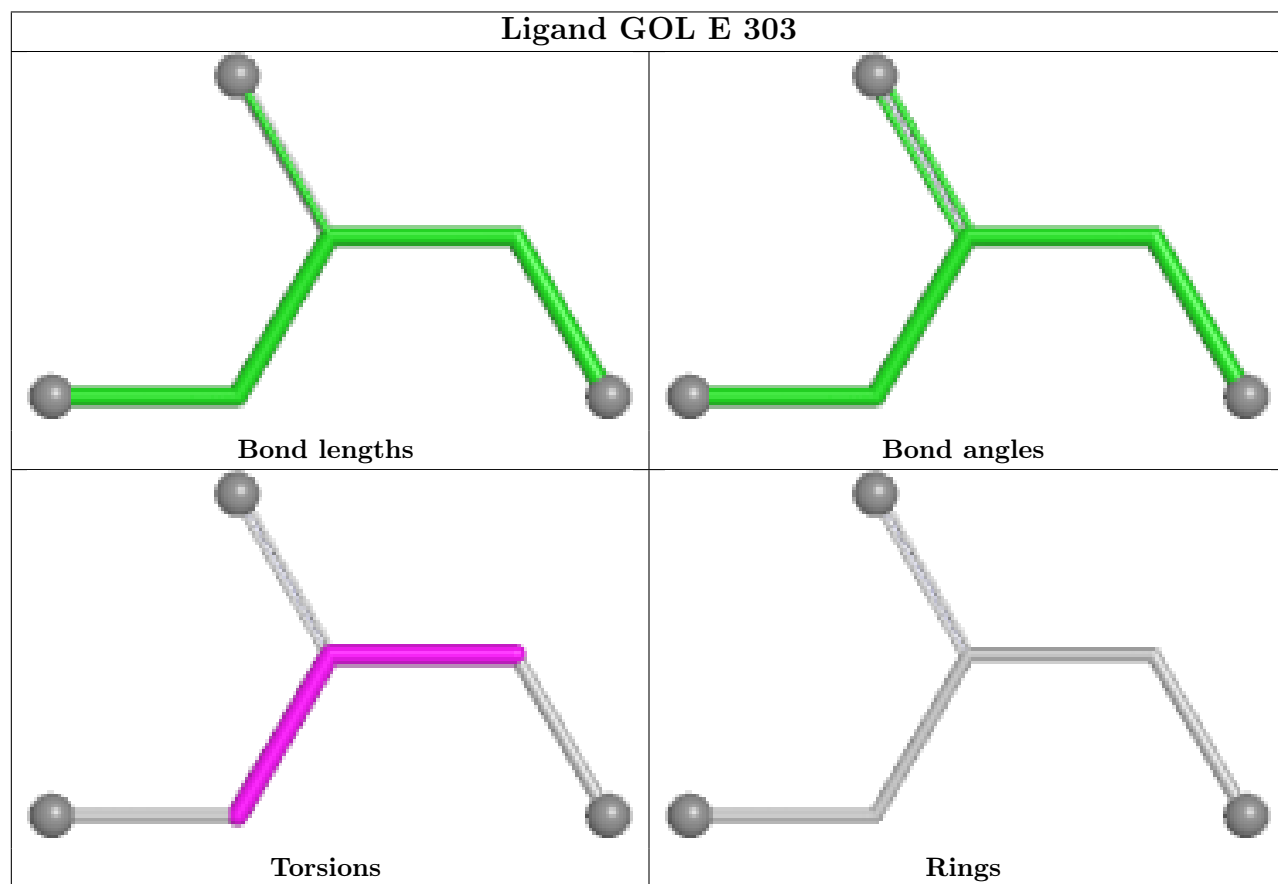
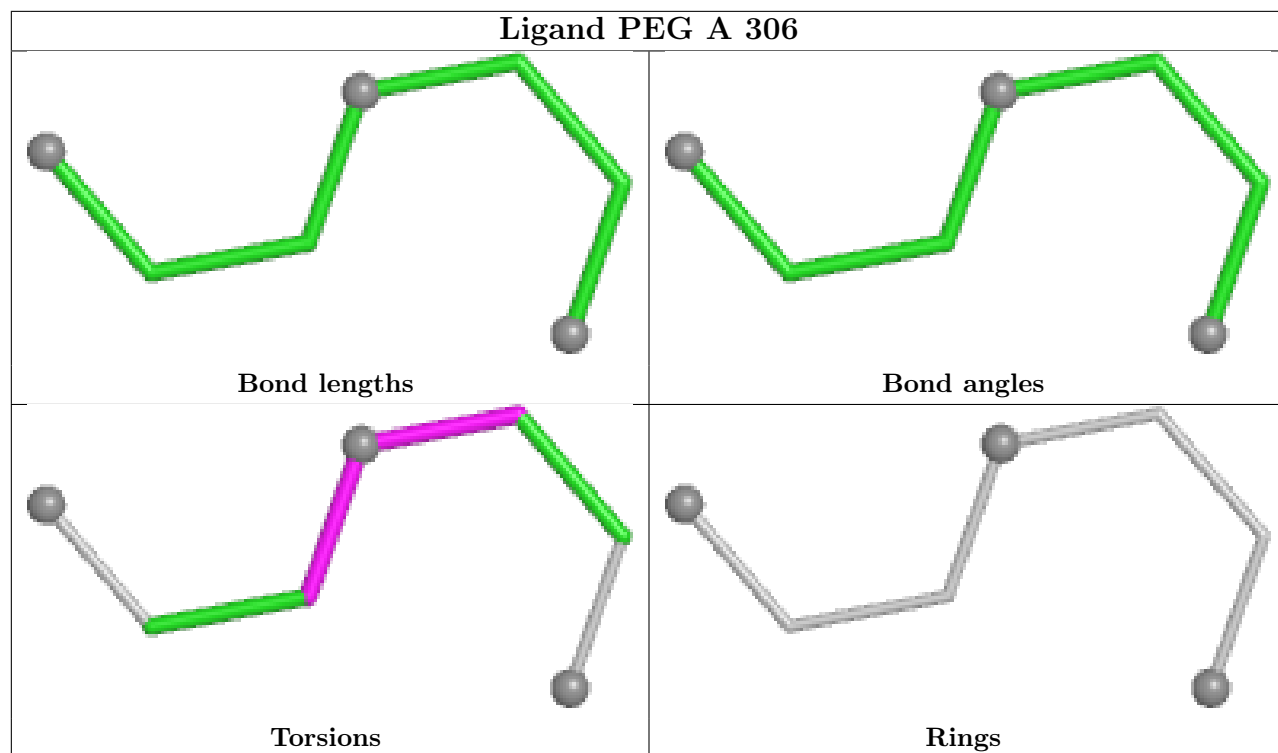
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

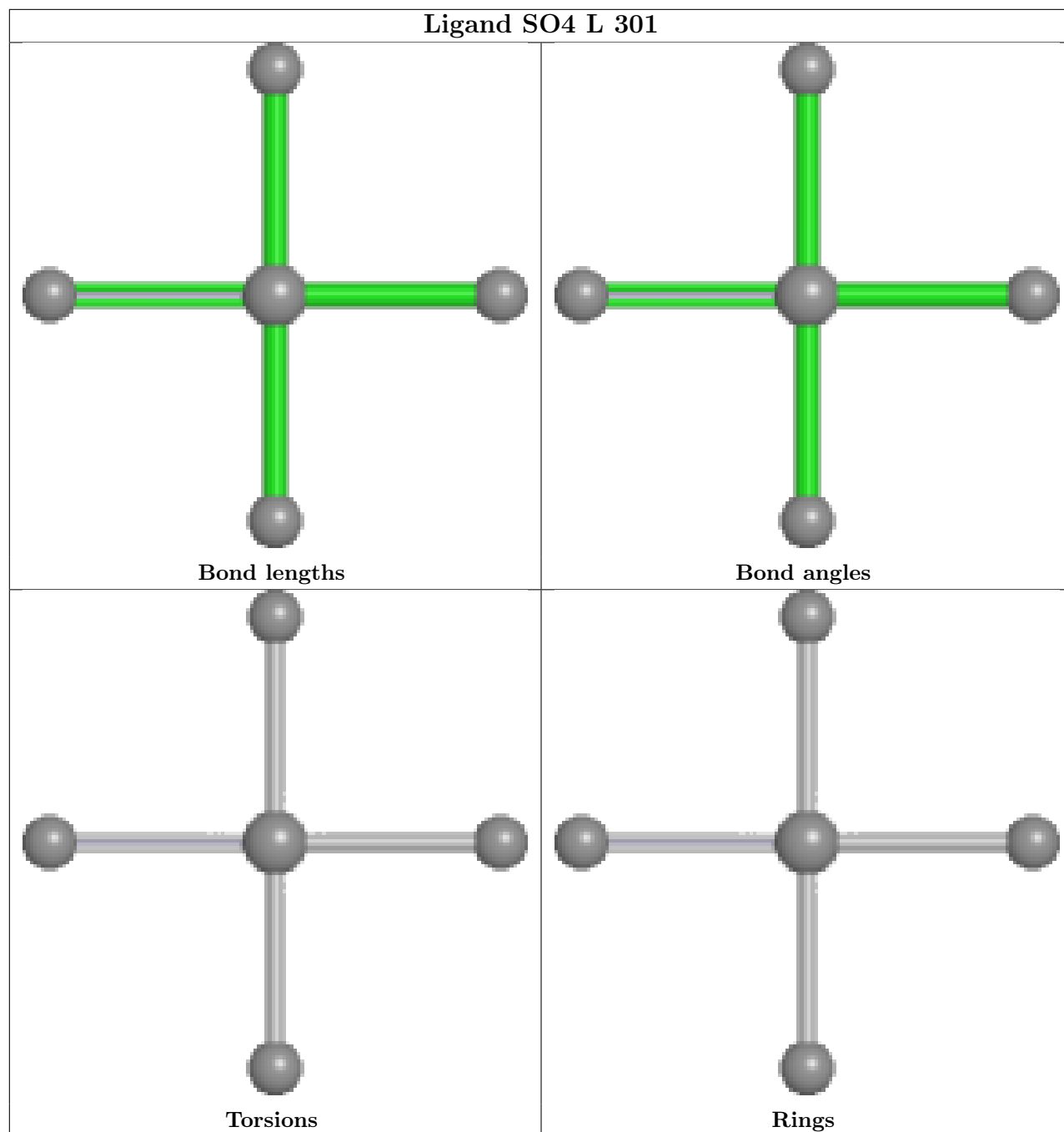


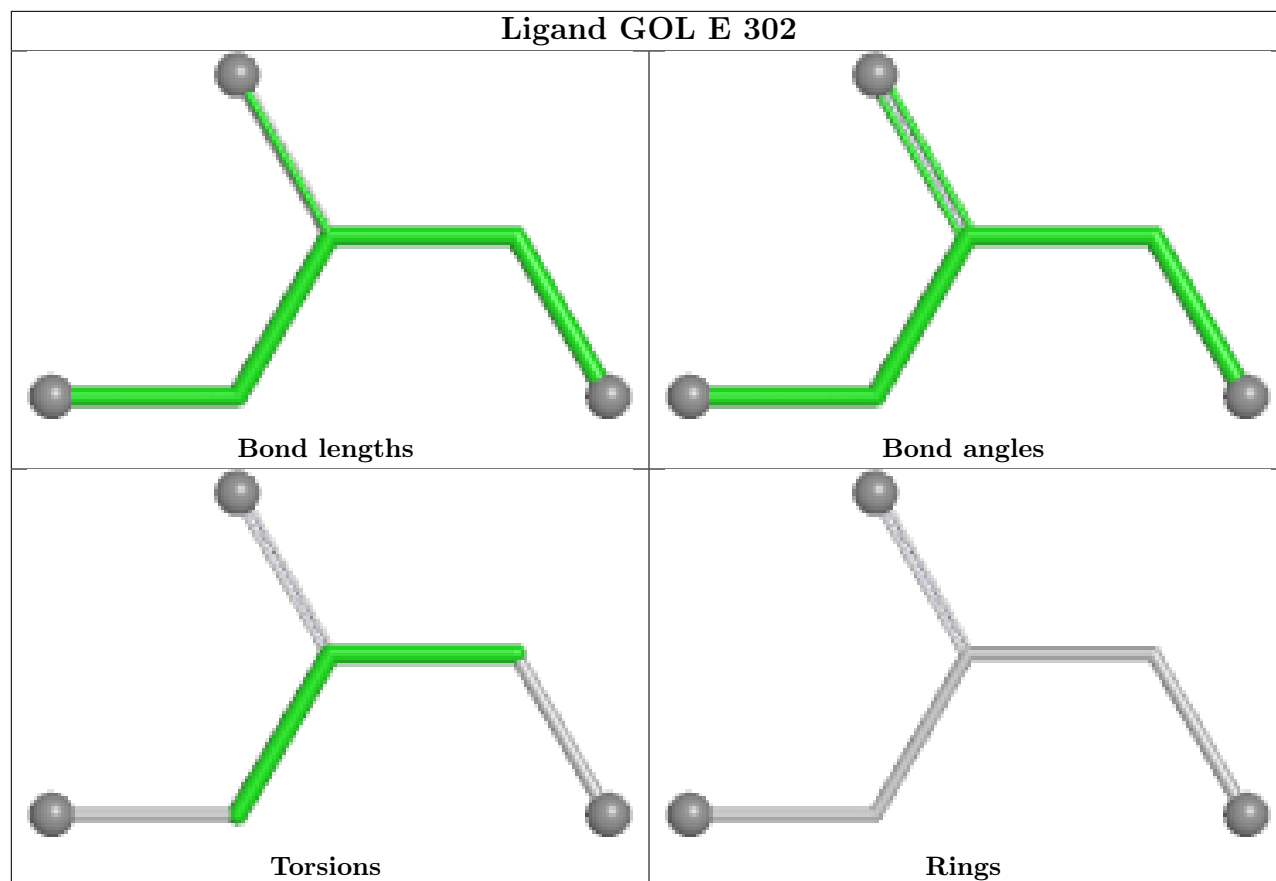


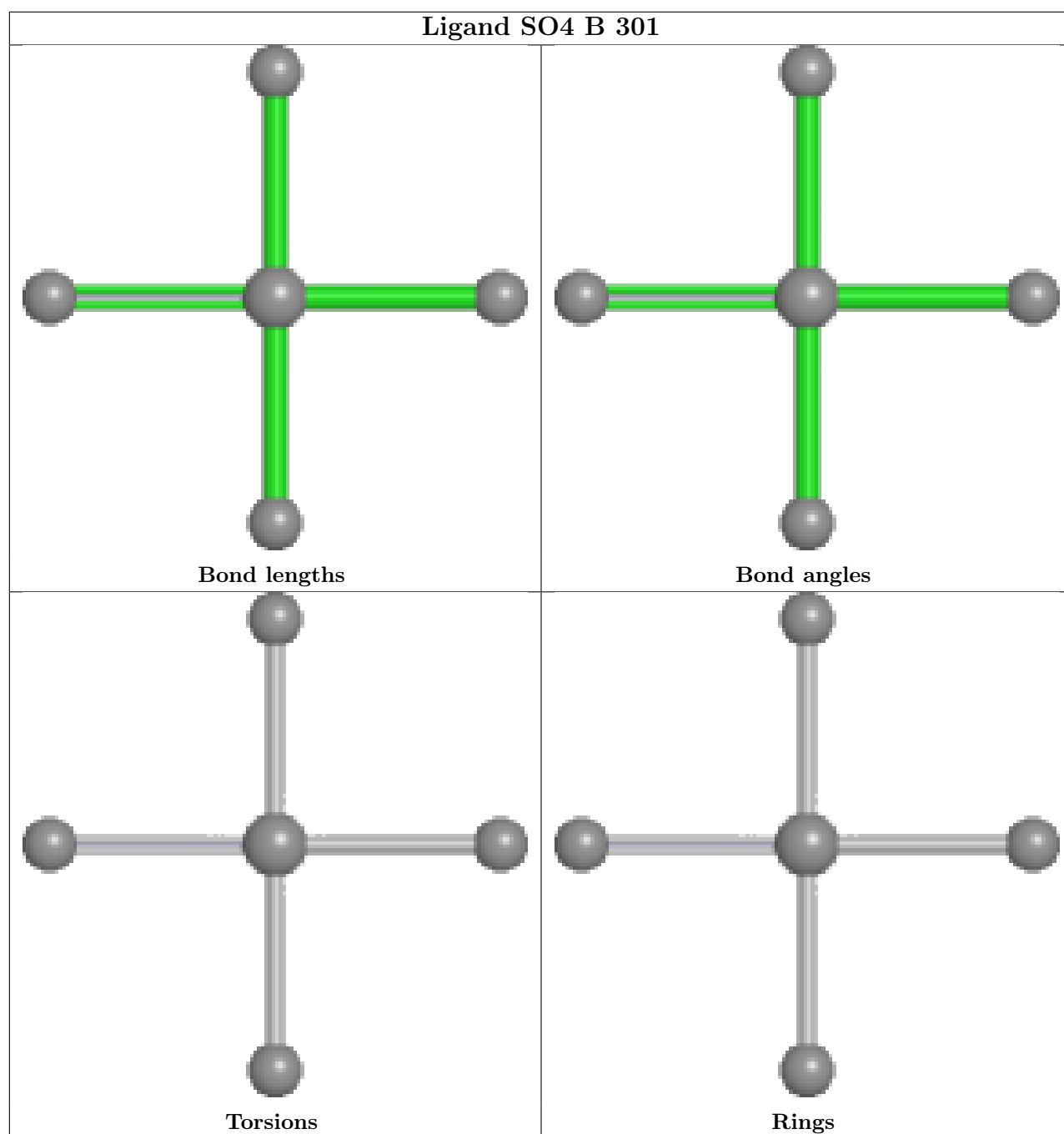


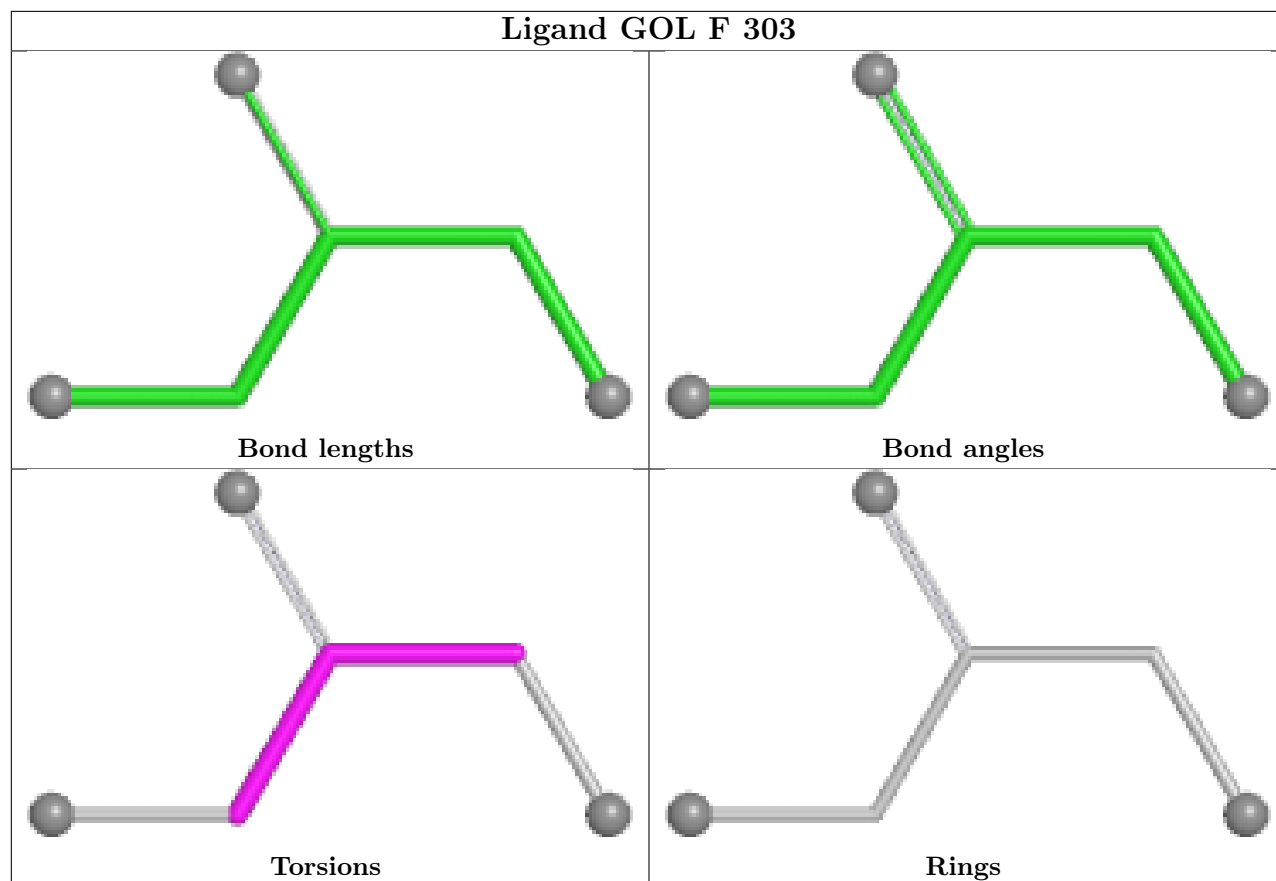


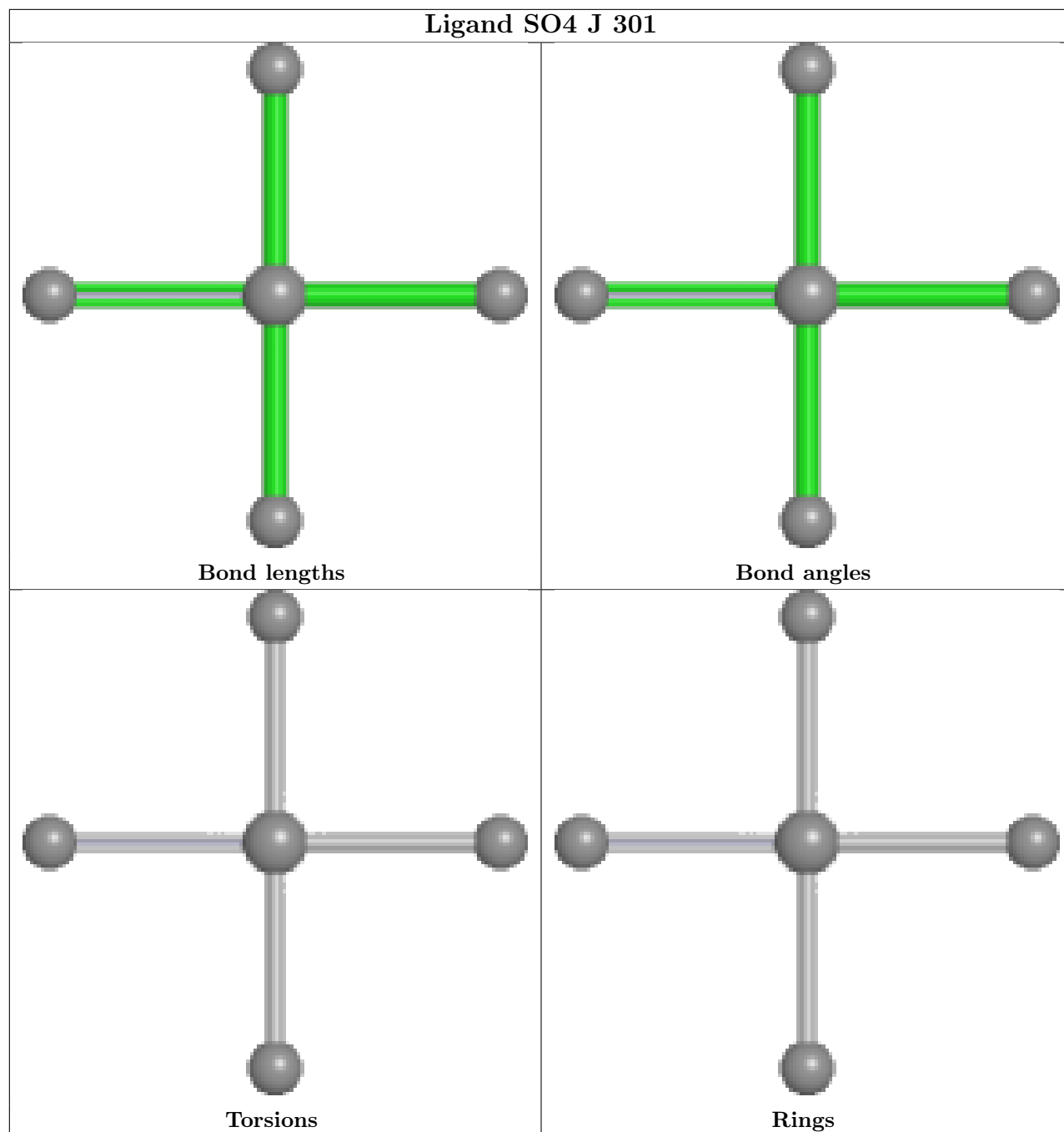


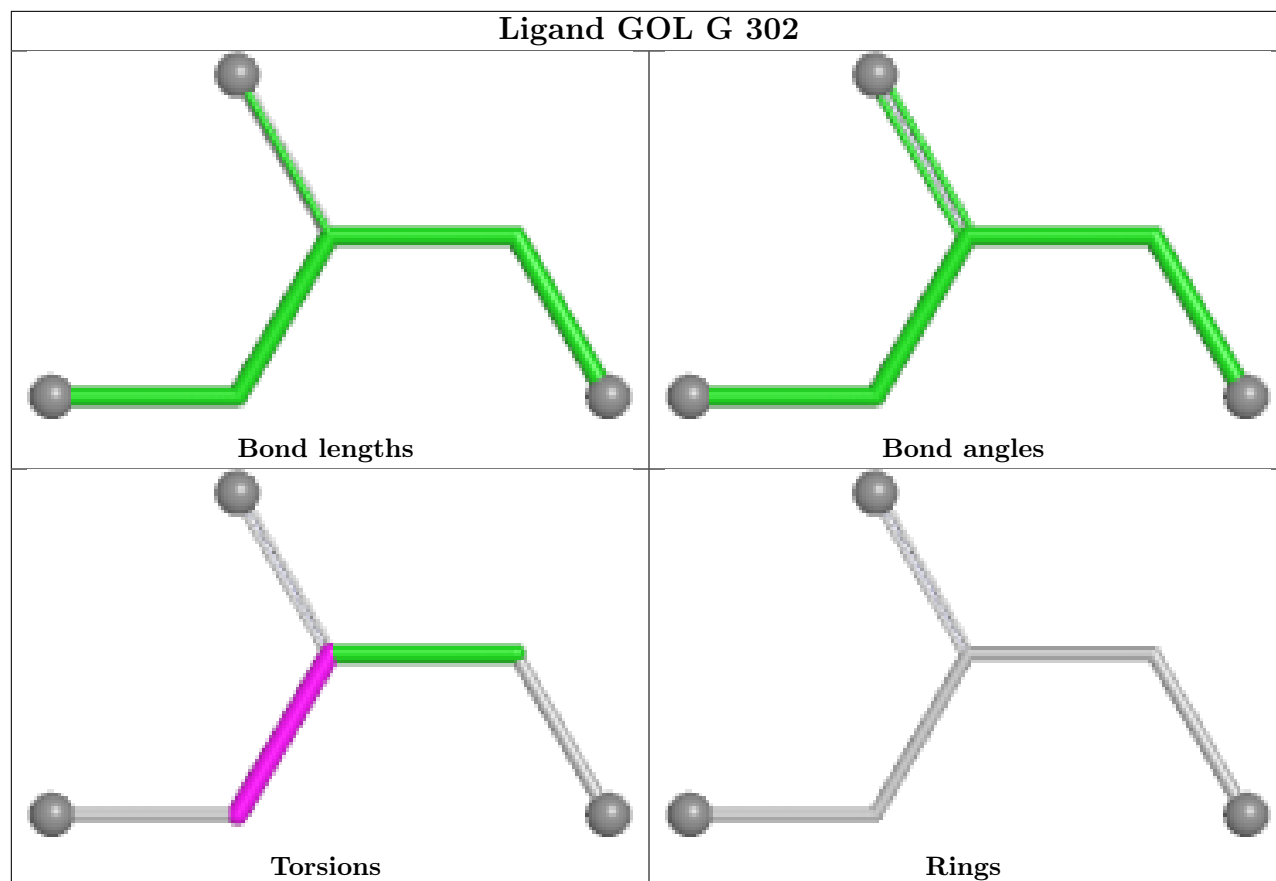


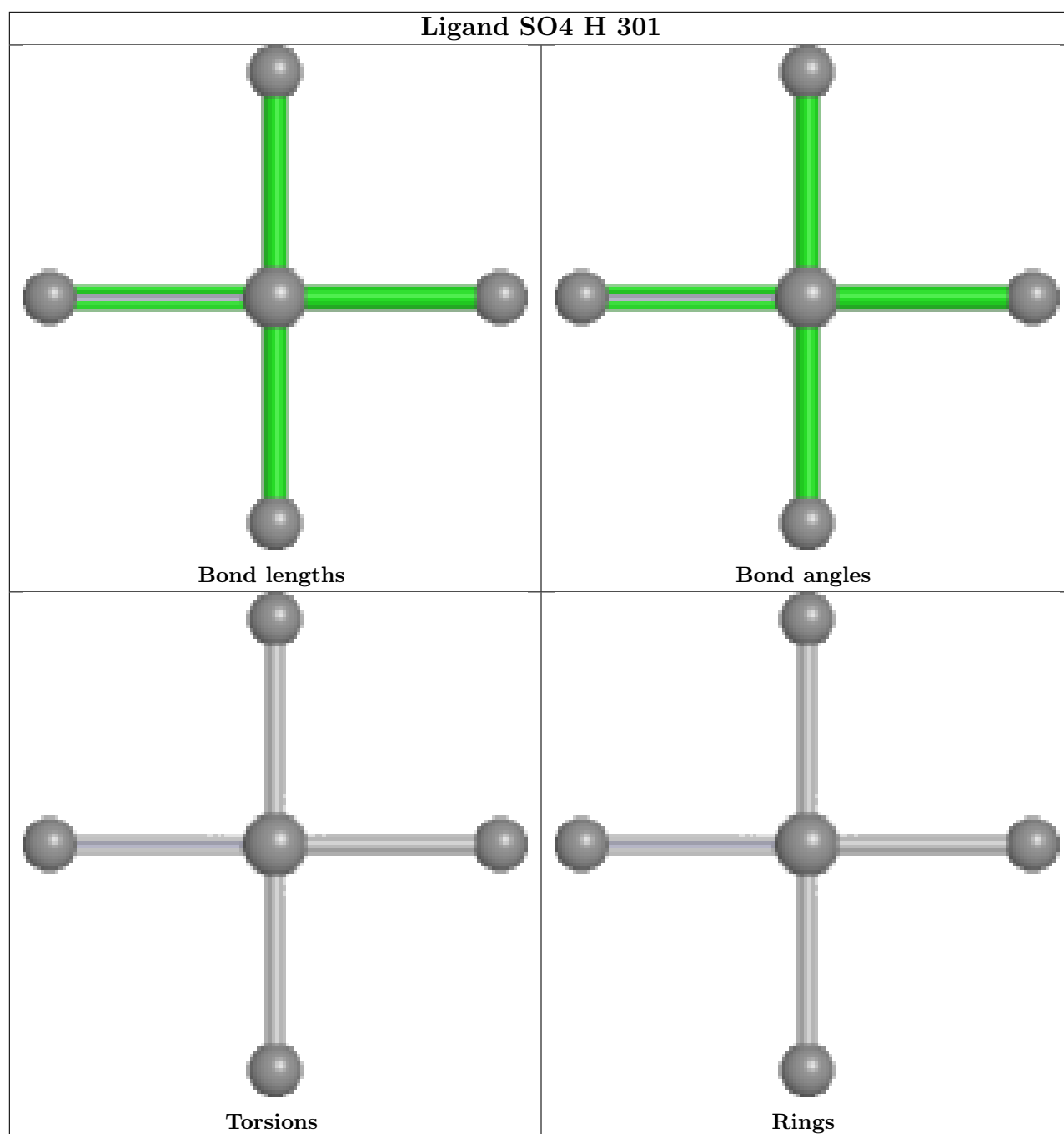


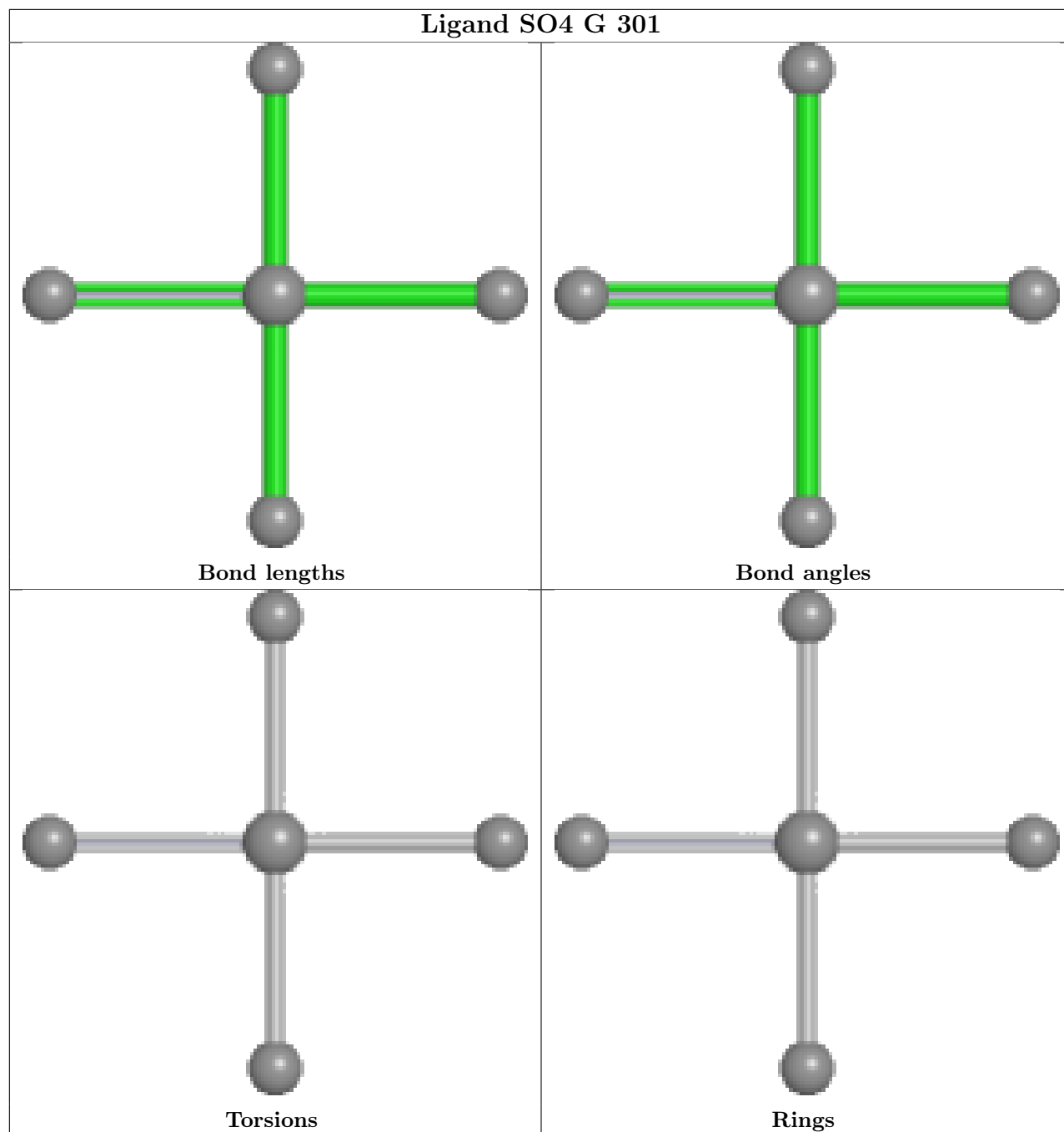


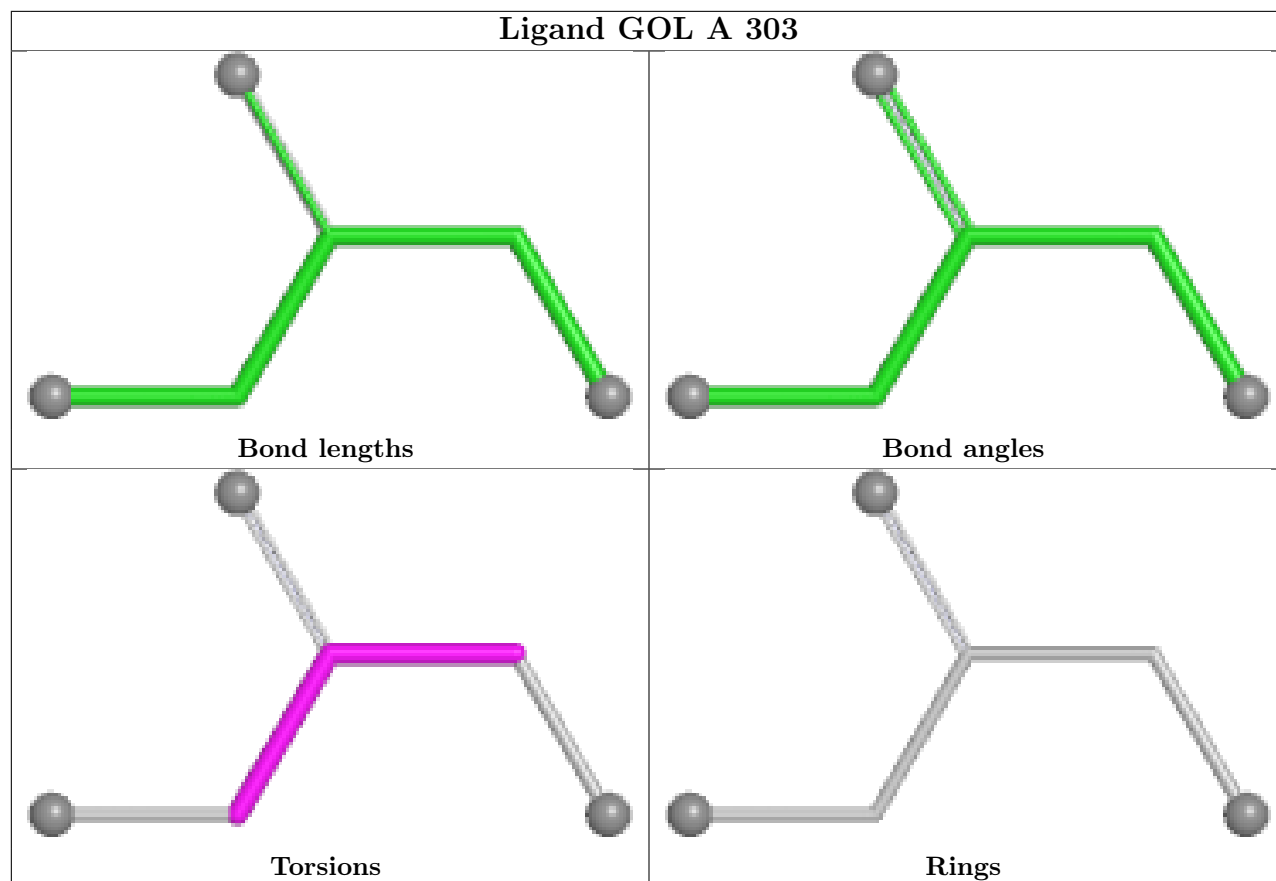


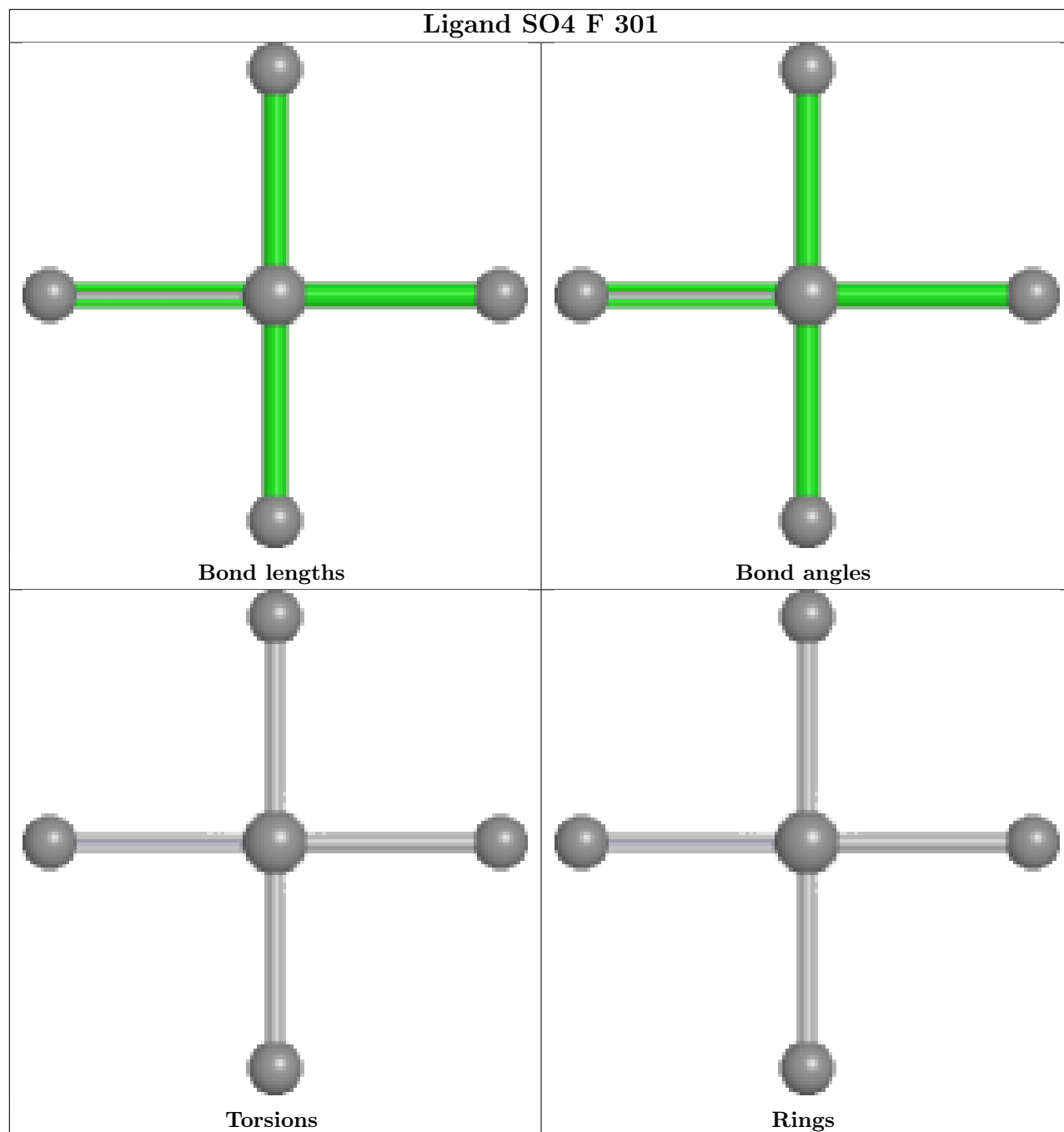


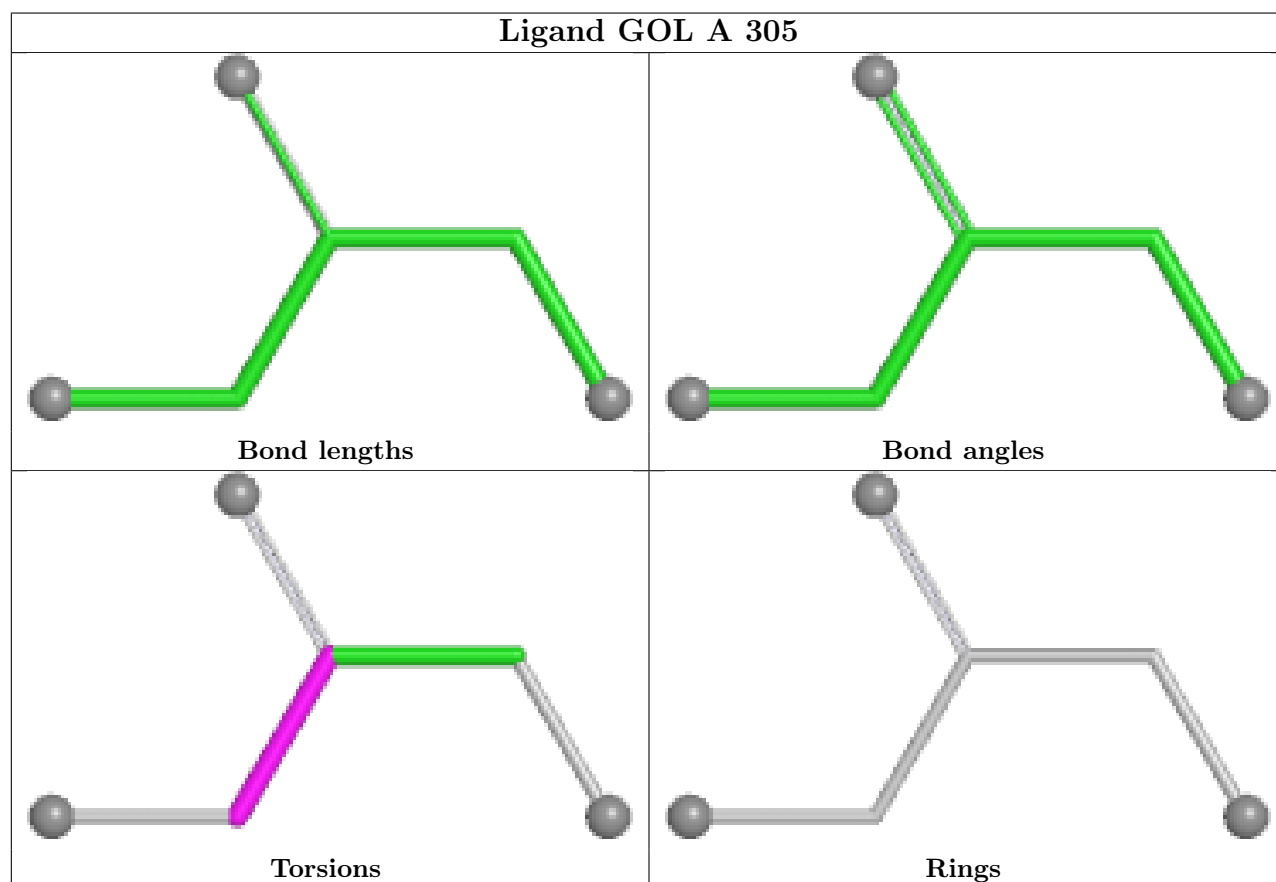
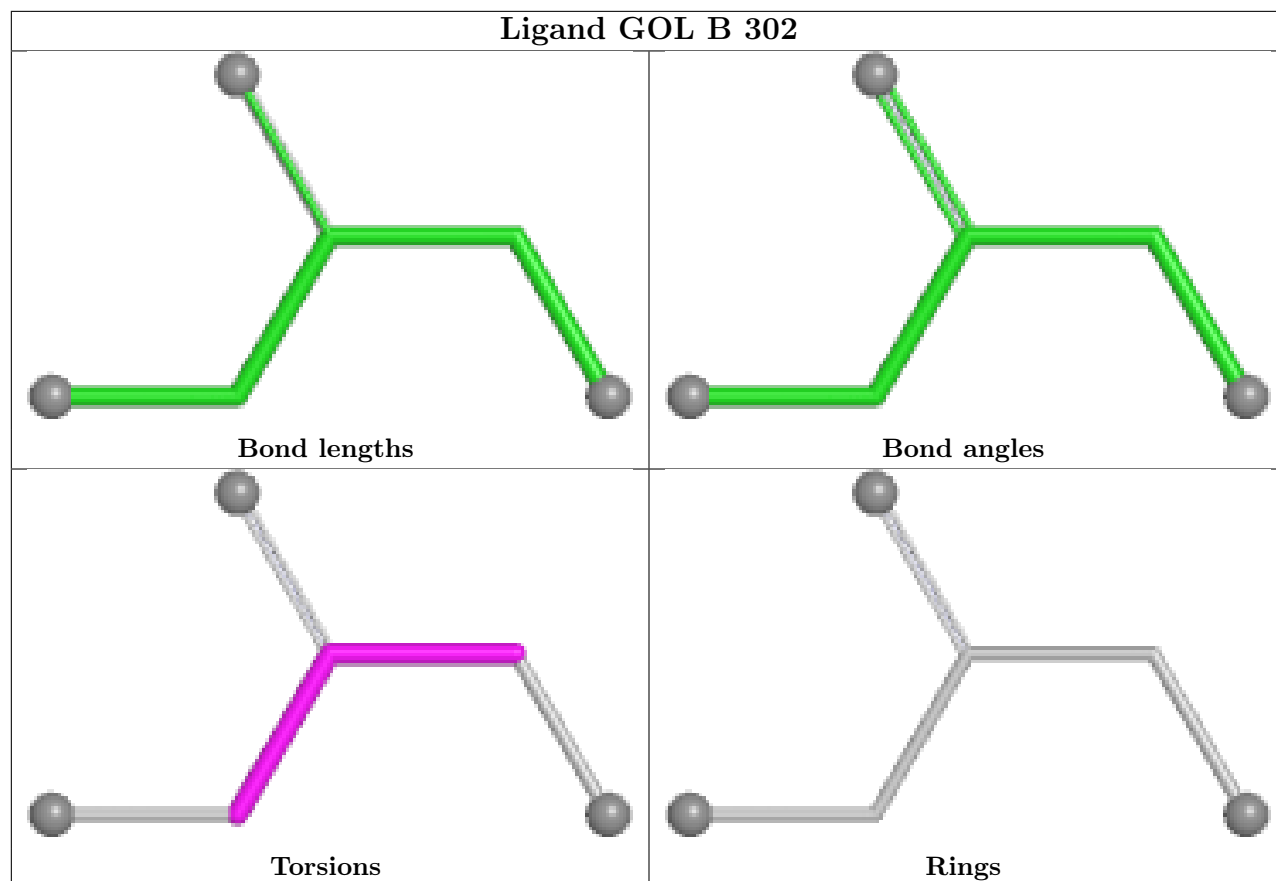


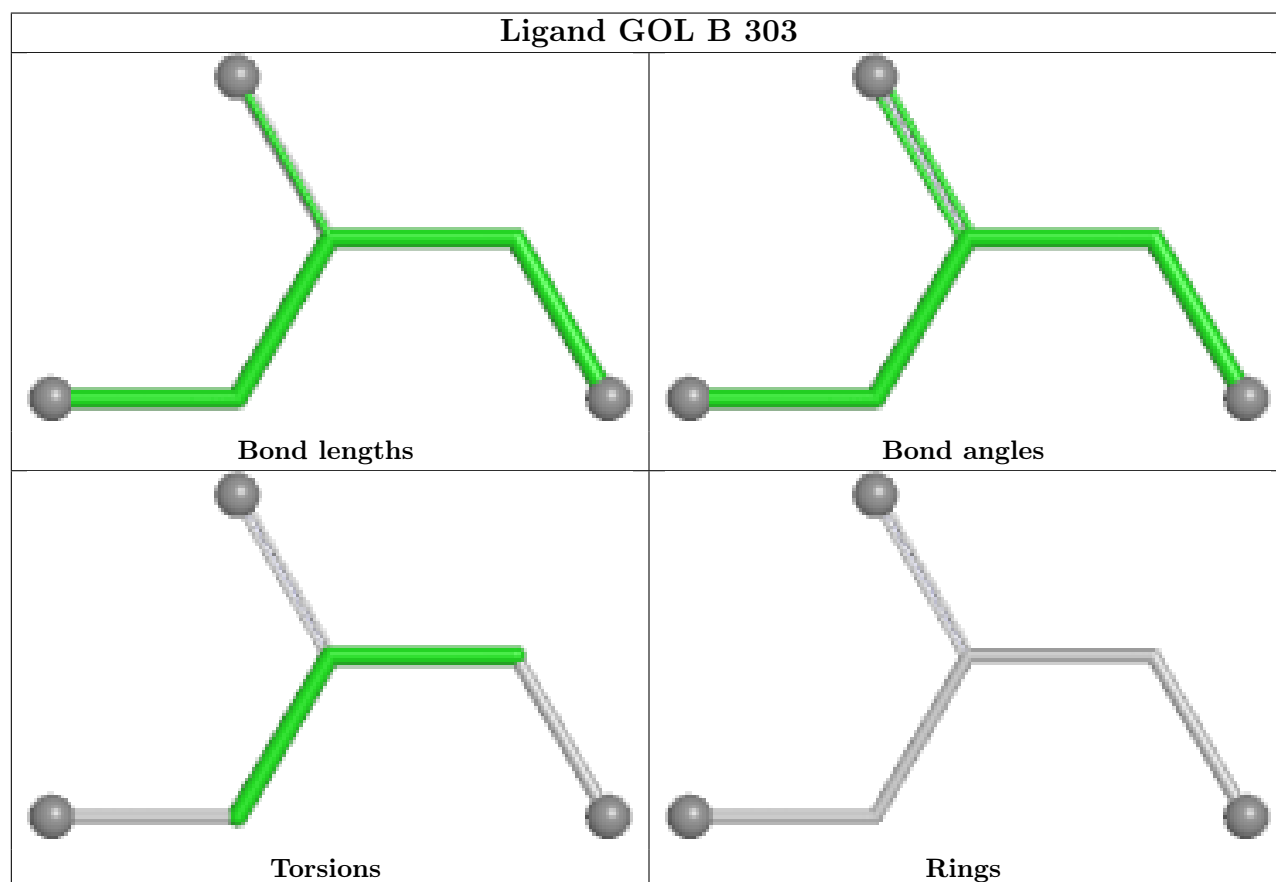
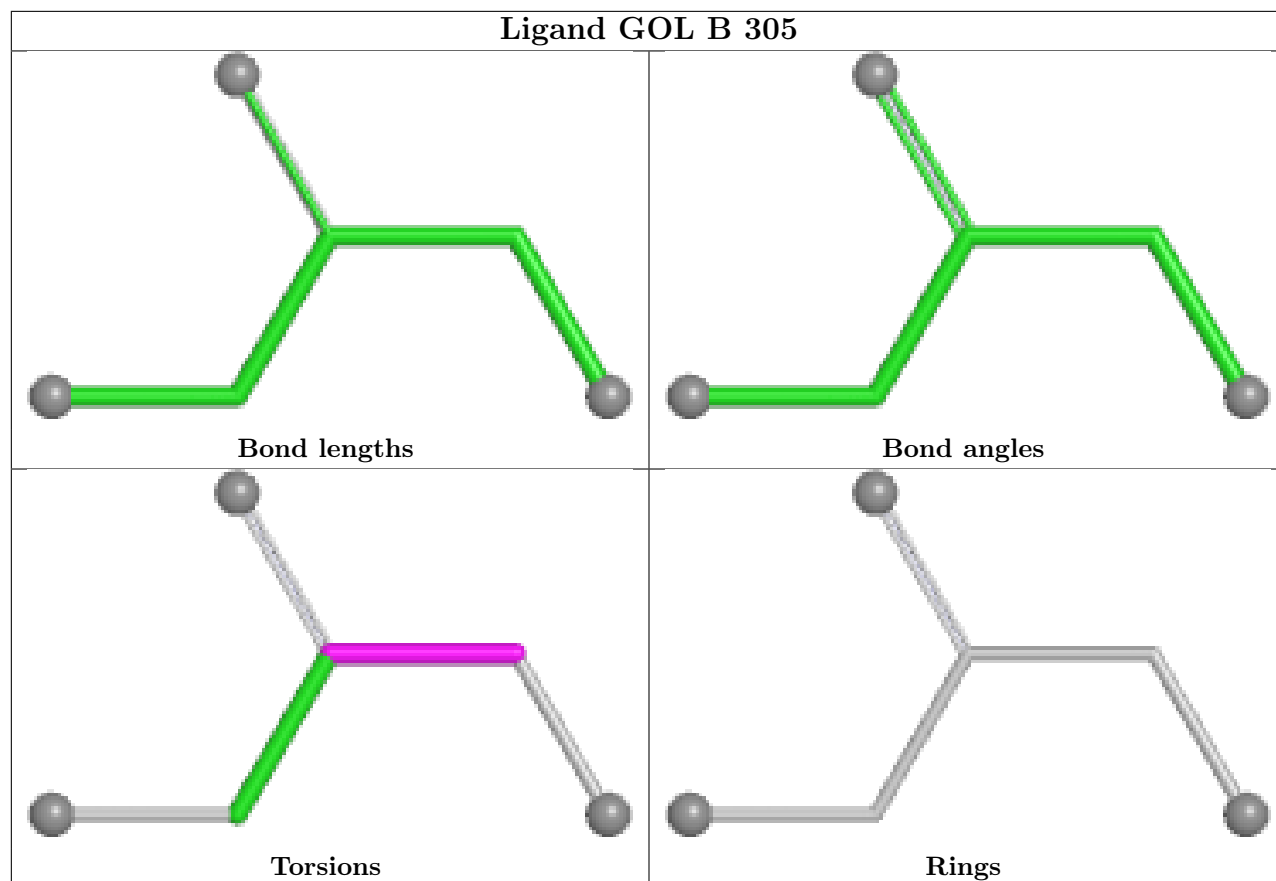


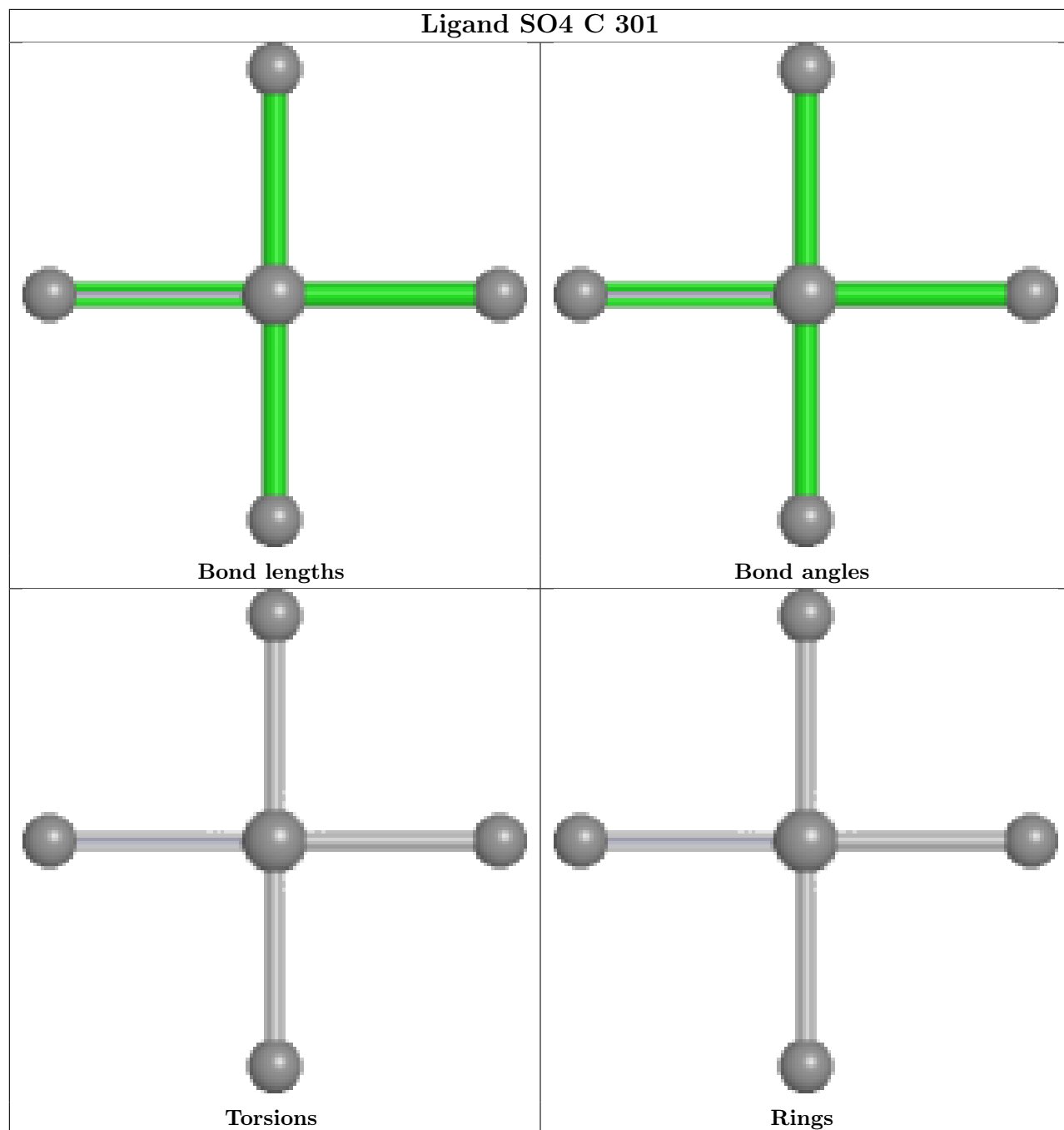


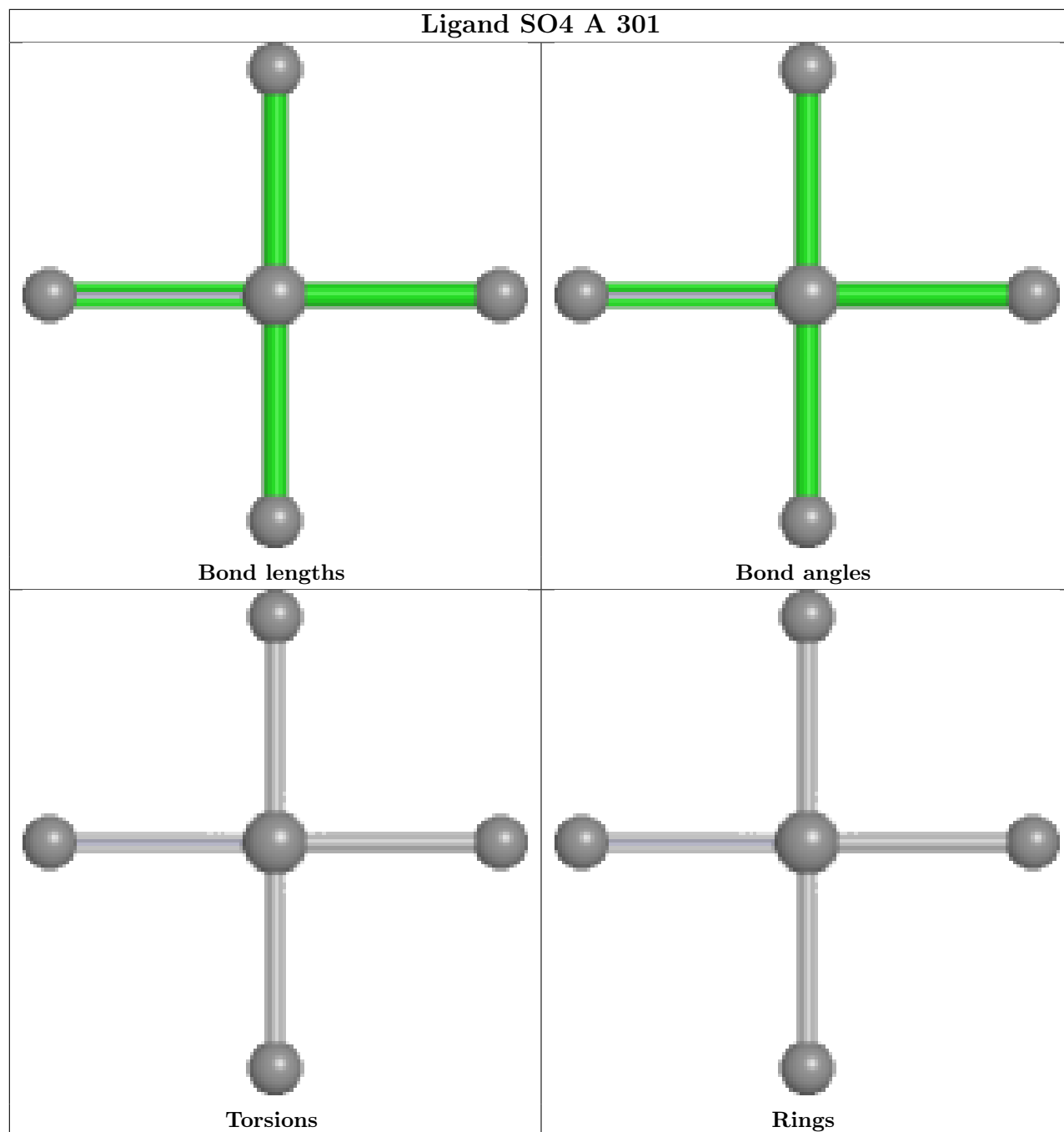


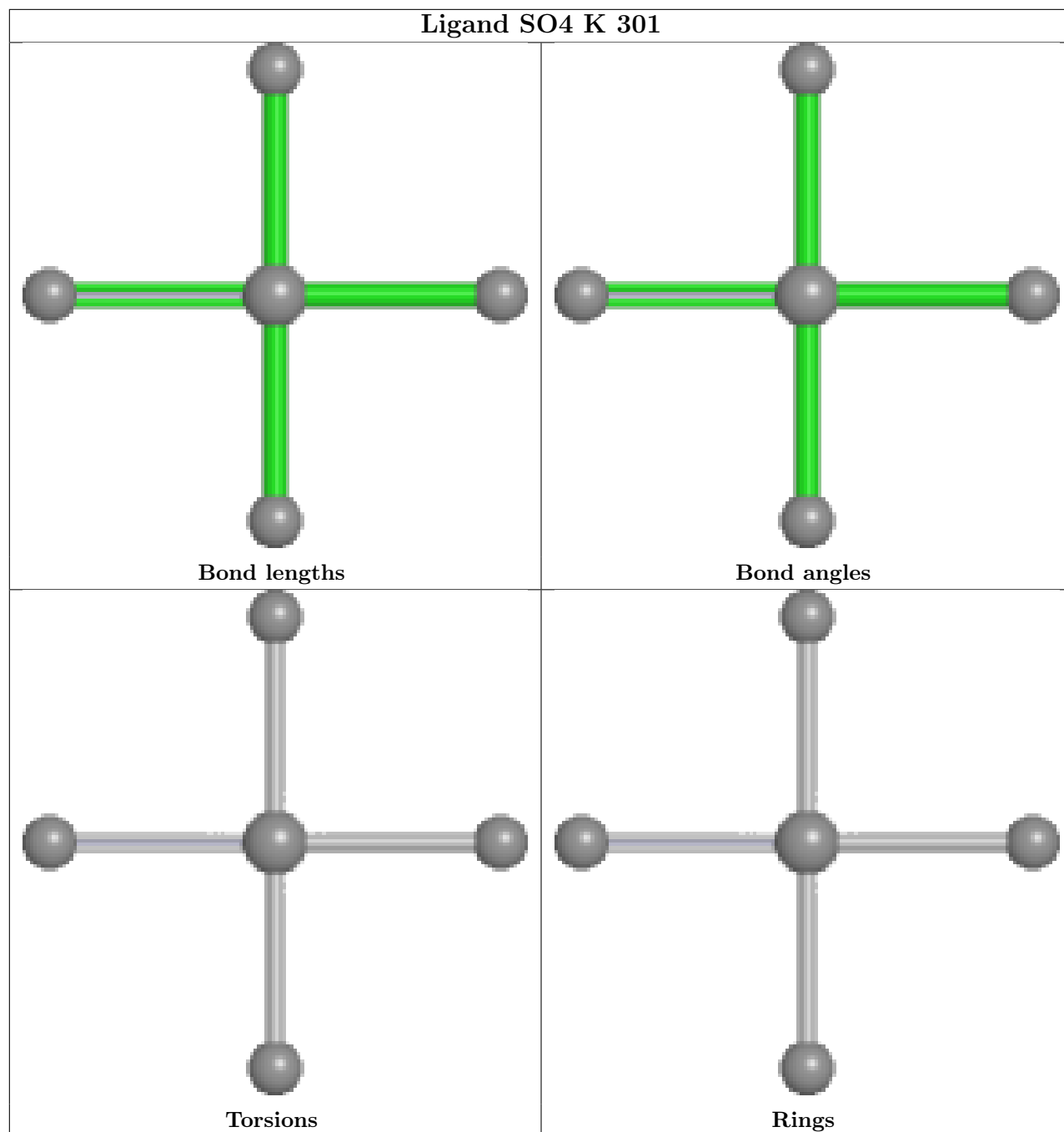


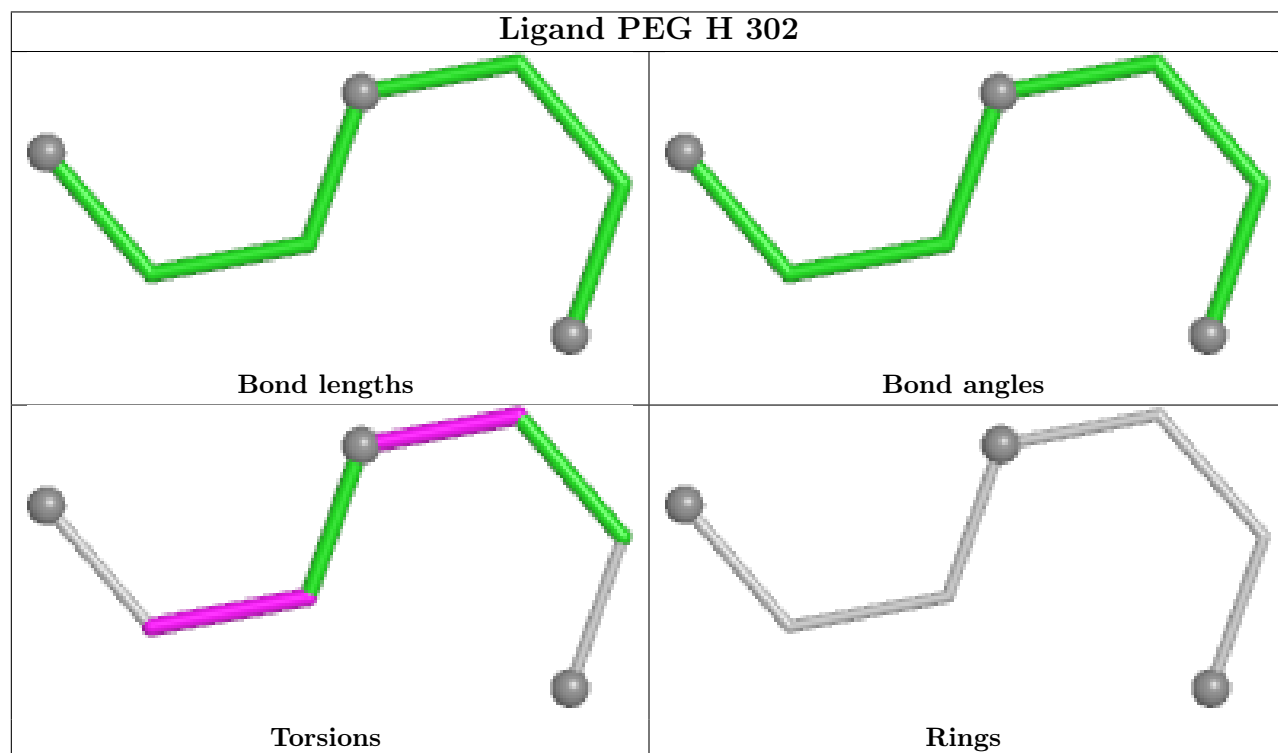
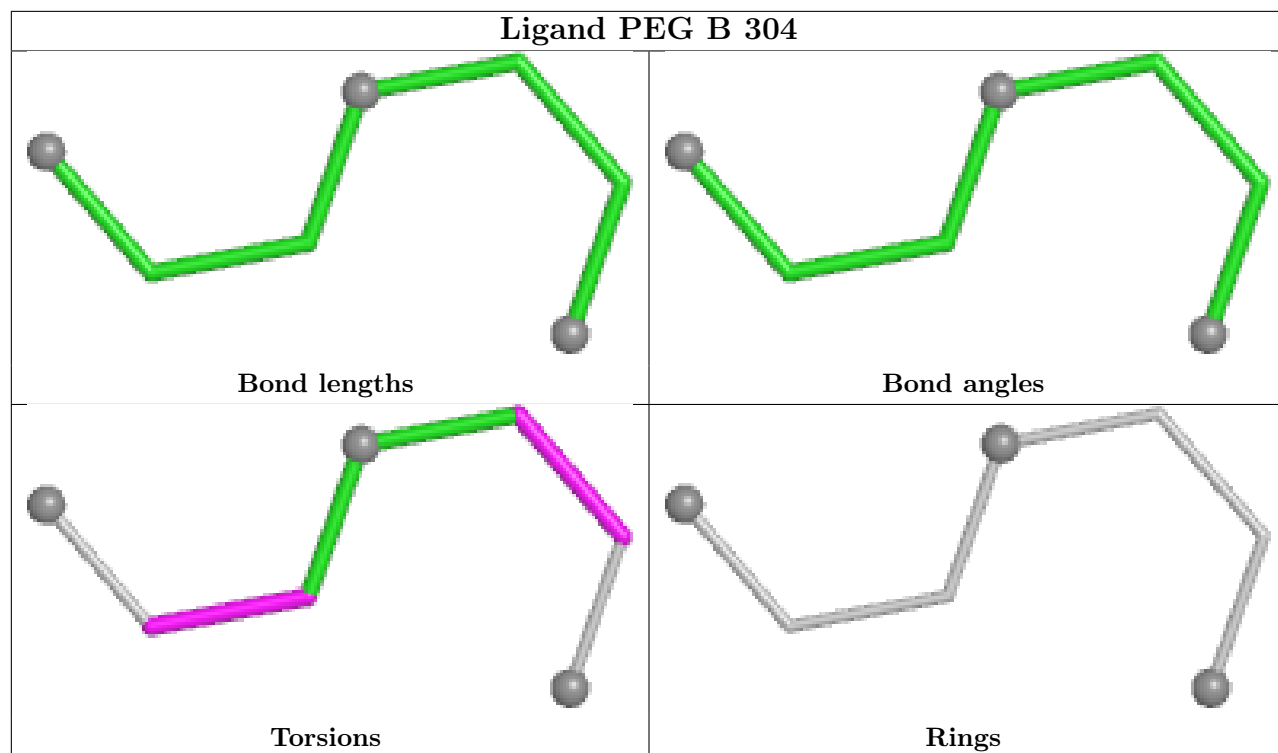


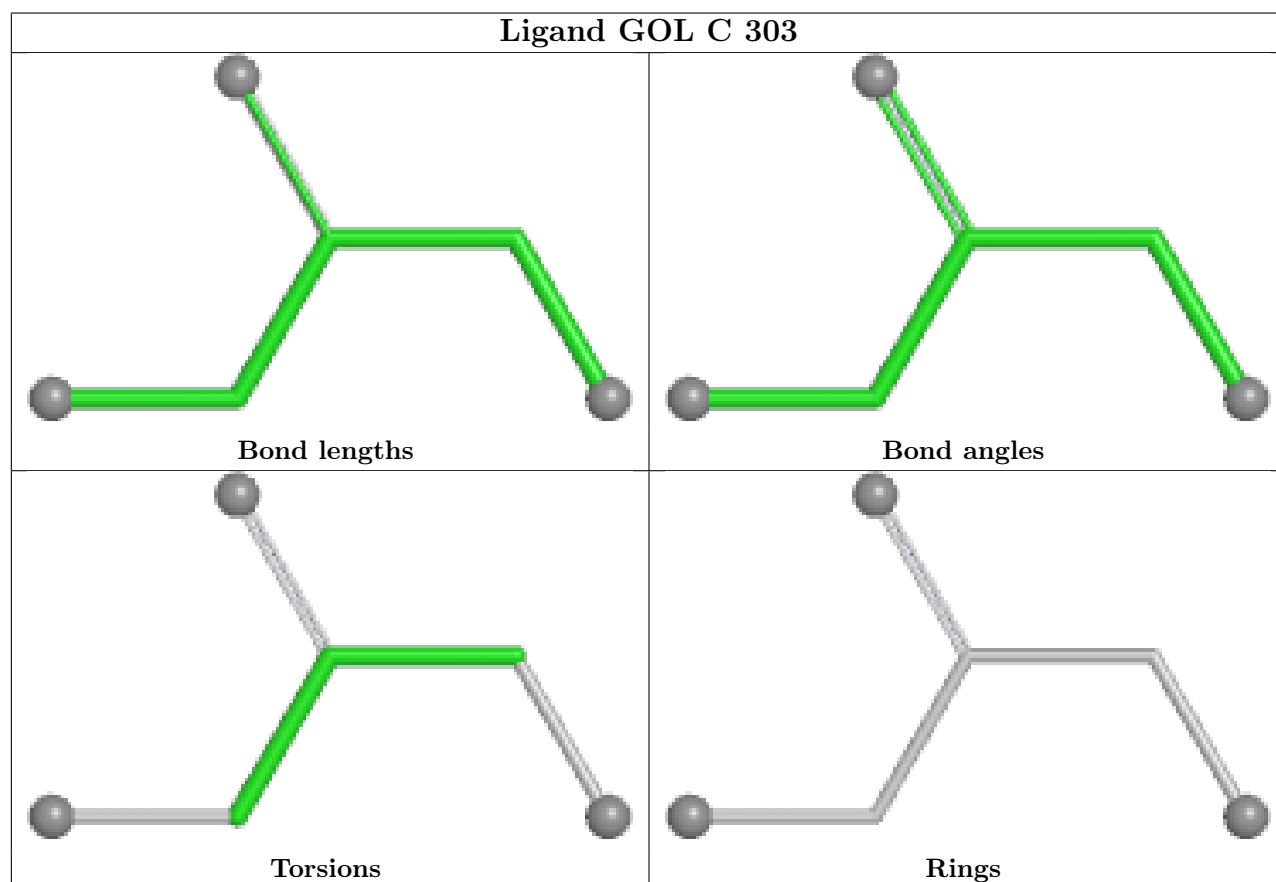
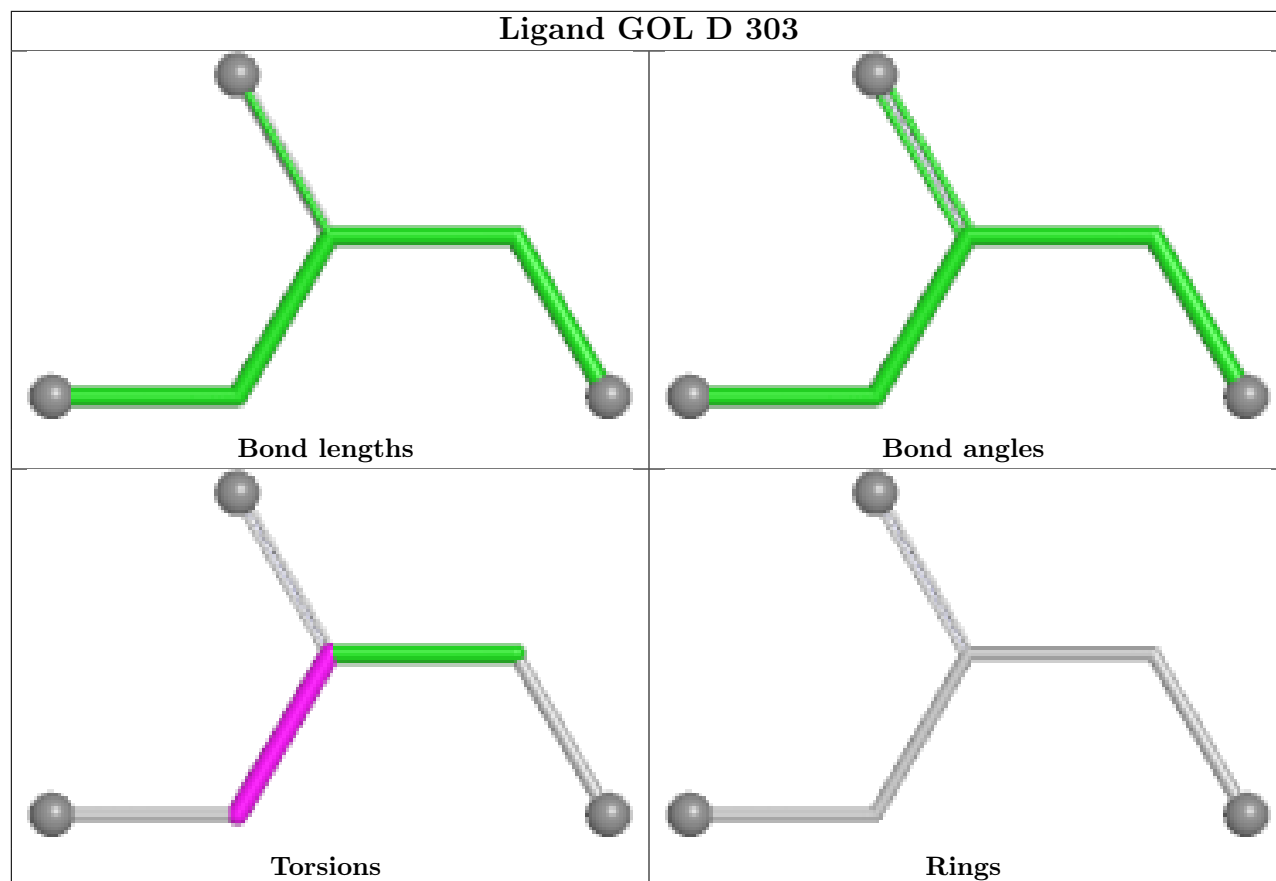


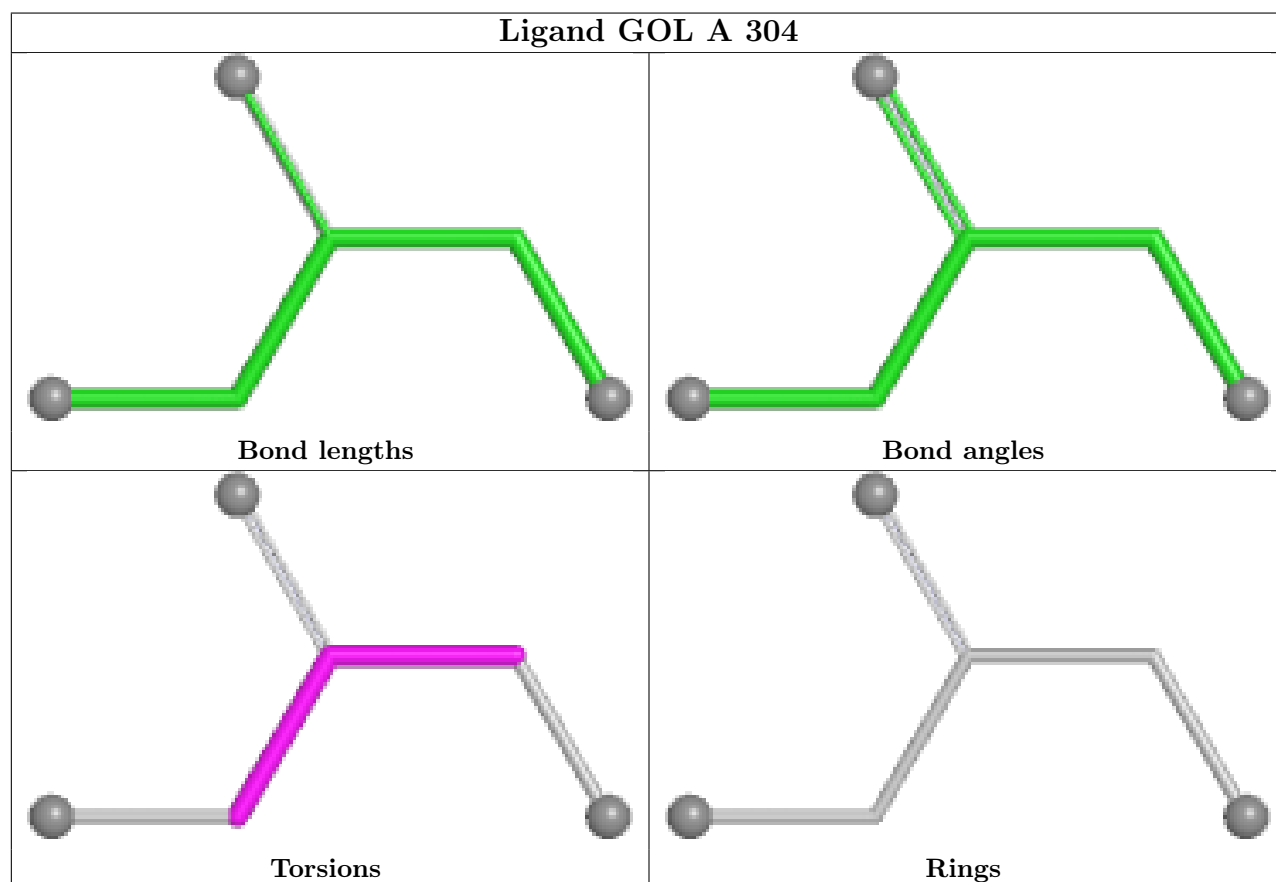
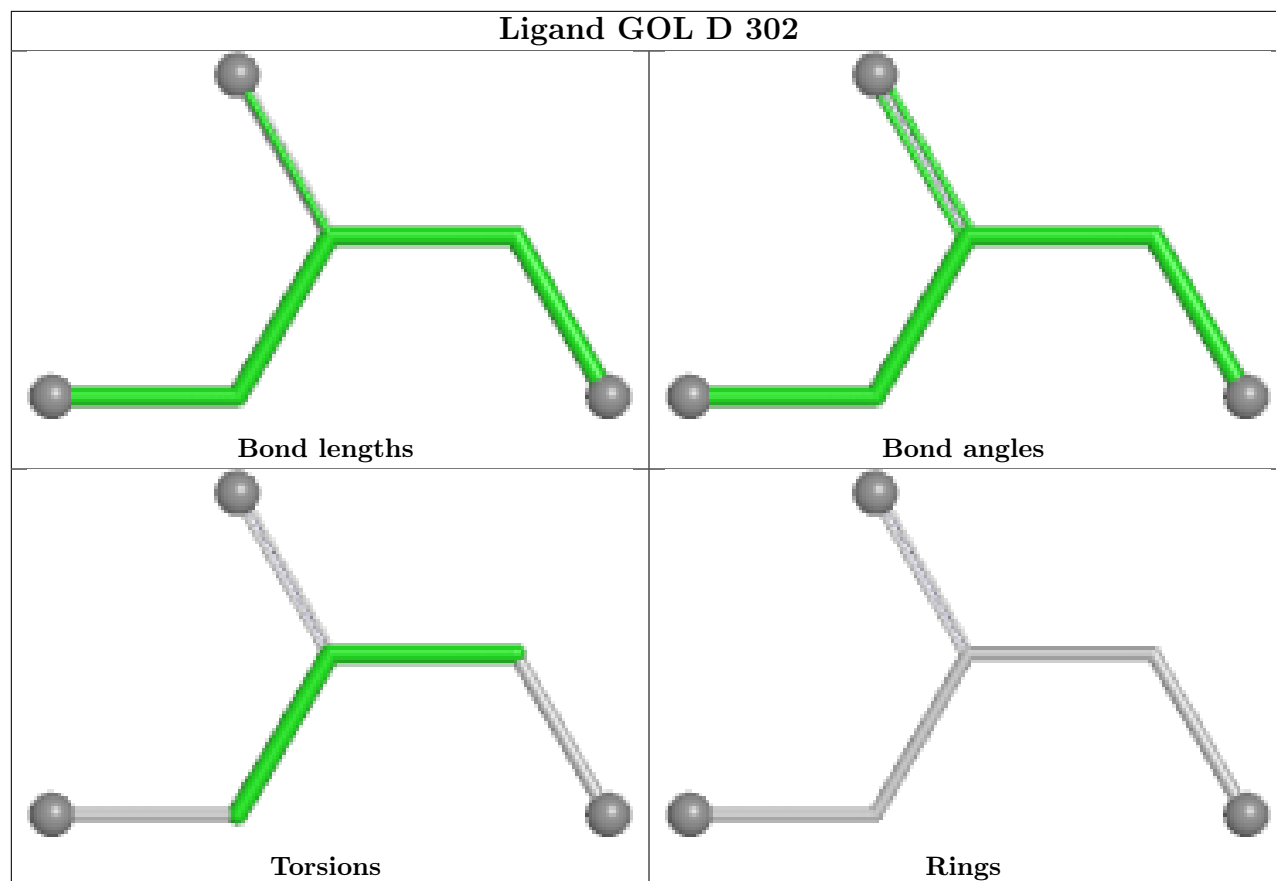


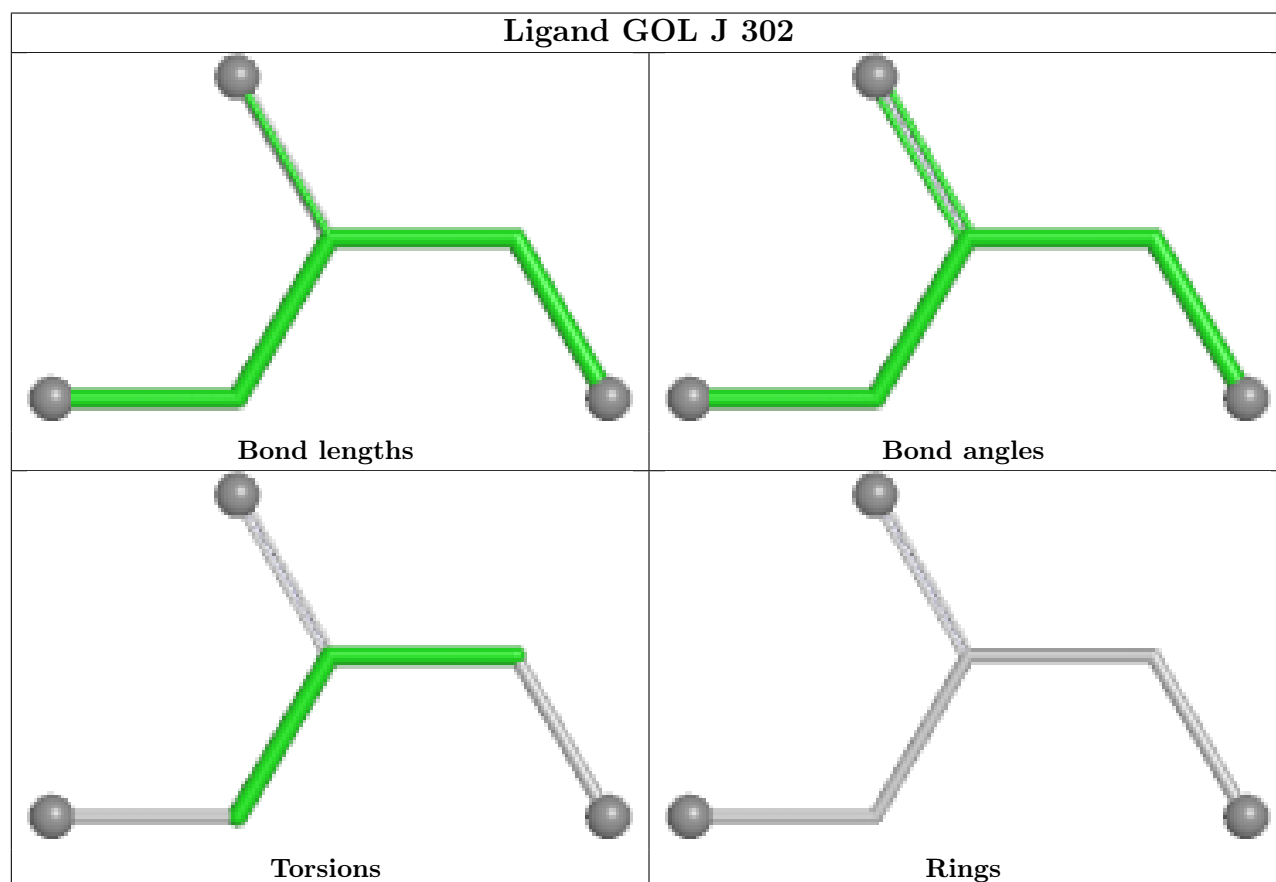
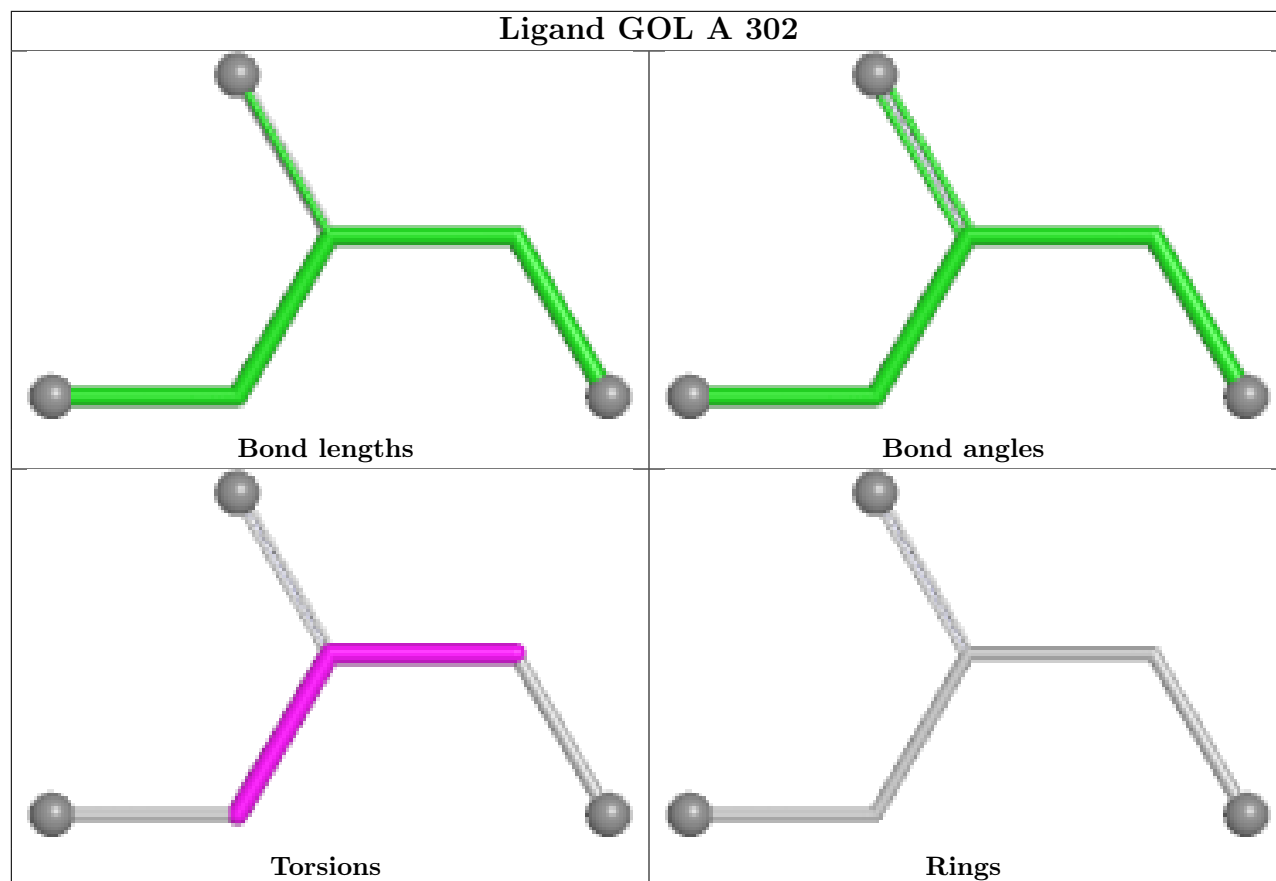


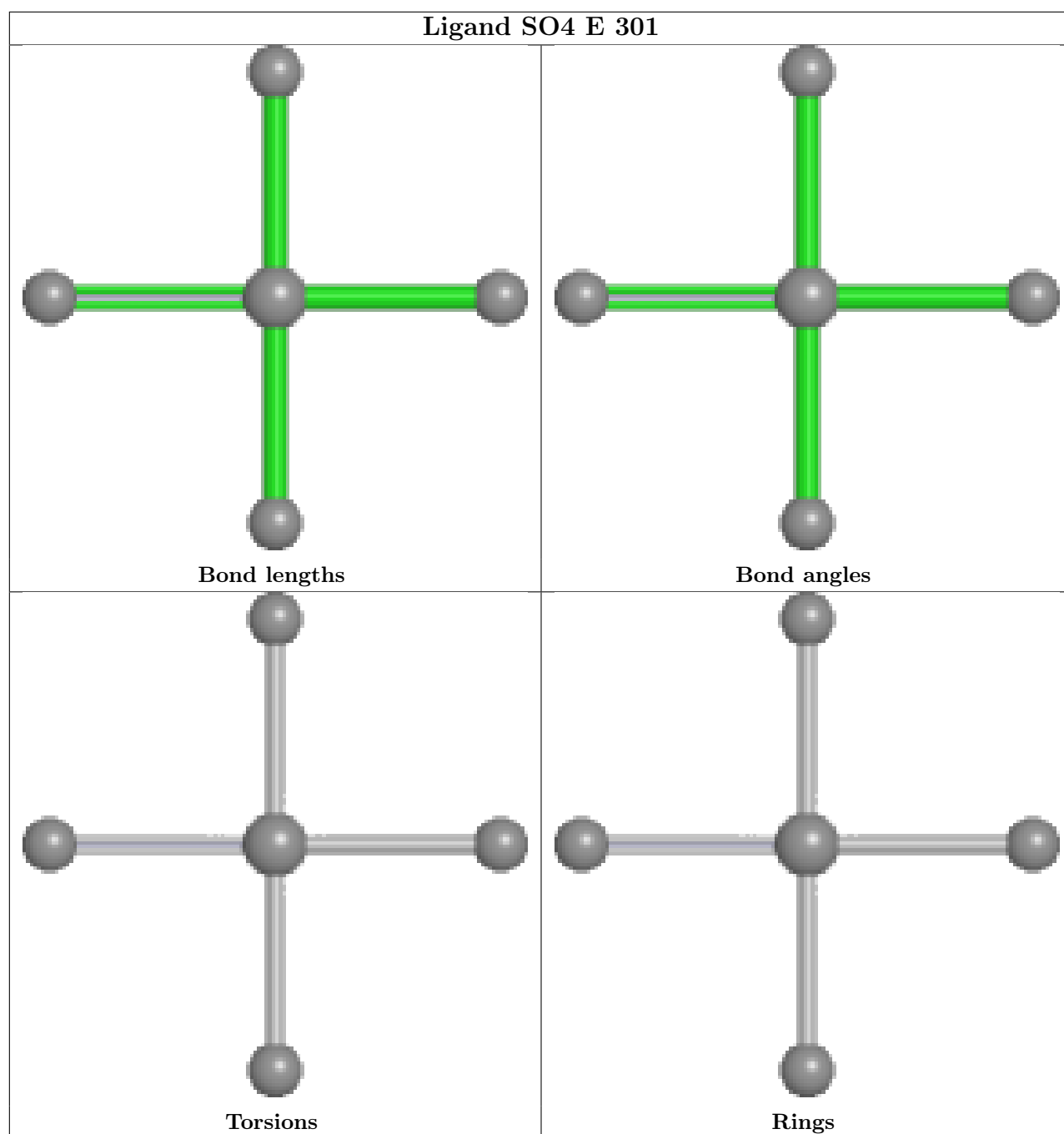


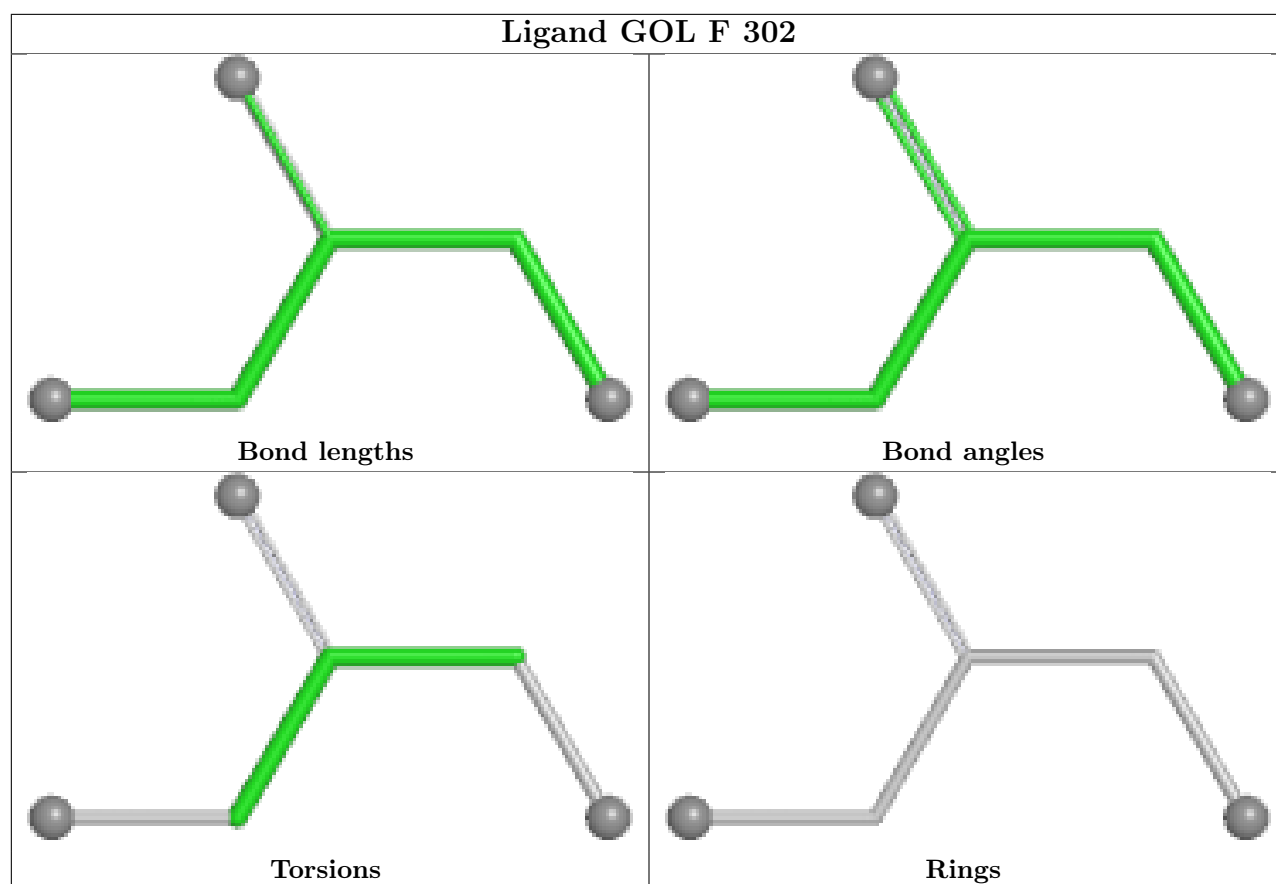












5.7 Other polymers [i](#)

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	242/255 (94%)	-0.40	7 (2%)	53	57	9, 22, 38, 57	1 (0%)
1	B	237/255 (92%)	-0.41	4 (1%)	69	72	9, 22, 36, 46	1 (0%)
1	C	237/255 (92%)	-0.48	0	100	100	13, 23, 34, 47	0
1	D	243/255 (95%)	-0.28	7 (2%)	53	57	14, 25, 41, 55	0
1	E	236/255 (92%)	-0.26	3 (1%)	75	78	17, 28, 41, 61	0
1	F	236/255 (92%)	-0.22	3 (1%)	75	78	16, 28, 41, 56	0
1	G	243/255 (95%)	-0.21	1 (0%)	88	90	9, 28, 45, 56	1 (0%)
1	H	237/255 (92%)	-0.32	3 (1%)	75	78	14, 25, 40, 55	1 (0%)
1	I	235/255 (92%)	-0.10	3 (1%)	75	78	17, 32, 46, 56	0
1	J	234/255 (91%)	0.20	8 (3%)	48	51	19, 36, 53, 65	0
1	K	237/255 (92%)	0.62	13 (5%)	30	32	23, 41, 54, 62	0
1	L	235/255 (92%)	0.83	39 (16%)	4	4	21, 44, 67, 77	0
All	All	2852/3060 (93%)	-0.09	91 (3%)	50	54	9, 28, 52, 77	4 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	83	GLY	5.5
1	J	82	ALA	4.3
1	L	82	ALA	4.0
1	L	50	ILE	4.0
1	L	48	ALA	3.8
1	J	193	GLY	3.8
1	J	199	GLY	3.6
1	J	195	PRO	3.5
1	L	85	VAL	3.4
1	L	33	ARG	3.3
1	D	83	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	184	THR	3.3
1	L	74	ARG	3.3
1	K	185	ASP	3.2
1	H	184	THR	3.0
1	L	66	ALA	3.0
1	J	44	ASP	3.0
1	B	183	LEU	3.0
1	L	72	TRP	2.9
1	L	63	ALA	2.9
1	A	190	MET	2.9
1	A	82	ALA	2.9
1	L	30	LEU	2.8
1	J	194	VAL	2.8
1	J	201	THR	2.7
1	L	44	ASP	2.7
1	L	46	PRO	2.7
1	L	34	ARG	2.7
1	I	183	LEU	2.7
1	L	55	VAL	2.7
1	L	83	GLY	2.6
1	K	72	TRP	2.6
1	L	65	PHE	2.6
1	L	43	GLU	2.6
1	H	183	LEU	2.6
1	L	23	ILE	2.6
1	B	192	LYS	2.6
1	L	25	GLY	2.6
1	L	61	VAL	2.6
1	K	83	GLY	2.5
1	F	82	ALA	2.5
1	L	184	THR	2.5
1	K	125	GLN	2.5
1	L	57	ASP	2.5
1	L	45	ASN	2.5
1	J	203	ILE	2.5
1	L	31	ILE	2.5
1	L	39	GLN	2.5
1	A	187	ALA	2.5
1	G	187	ALA	2.5
1	L	60	ALA	2.4
1	E	185	ASP	2.4
1	A	188	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	42	ALA	2.4
1	K	74	ARG	2.4
1	L	36	ASP	2.3
1	K	33	ARG	2.3
1	D	191	THR	2.3
1	L	37	ALA	2.3
1	L	27	GLN	2.3
1	L	75	LEU	2.3
1	K	82	ALA	2.3
1	E	70	SER	2.3
1	D	188	VAL	2.3
1	A	191	THR	2.3
1	D	187	ALA	2.3
1	K	116	ALA	2.3
1	L	68	VAL	2.3
1	D	186	MET	2.3
1	F	184	THR	2.3
1	L	51	LEU	2.3
1	L	99	TRP	2.2
1	I	123	ASN	2.2
1	L	53	CYS	2.2
1	F	83	GLY	2.2
1	K	70	SER	2.2
1	L	84	ALA	2.2
1	D	199	GLY	2.2
1	K	36	ASP	2.2
1	B	191	THR	2.2
1	K	192	LYS	2.2
1	L	122	ARG	2.2
1	H	191	THR	2.1
1	D	190	MET	2.1
1	L	38	LEU	2.1
1	A	189	ALA	2.1
1	I	201	THR	2.1
1	L	73	GLY	2.1
1	K	53	CYS	2.1
1	K	23	ILE	2.0
1	E	3	ASN	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.

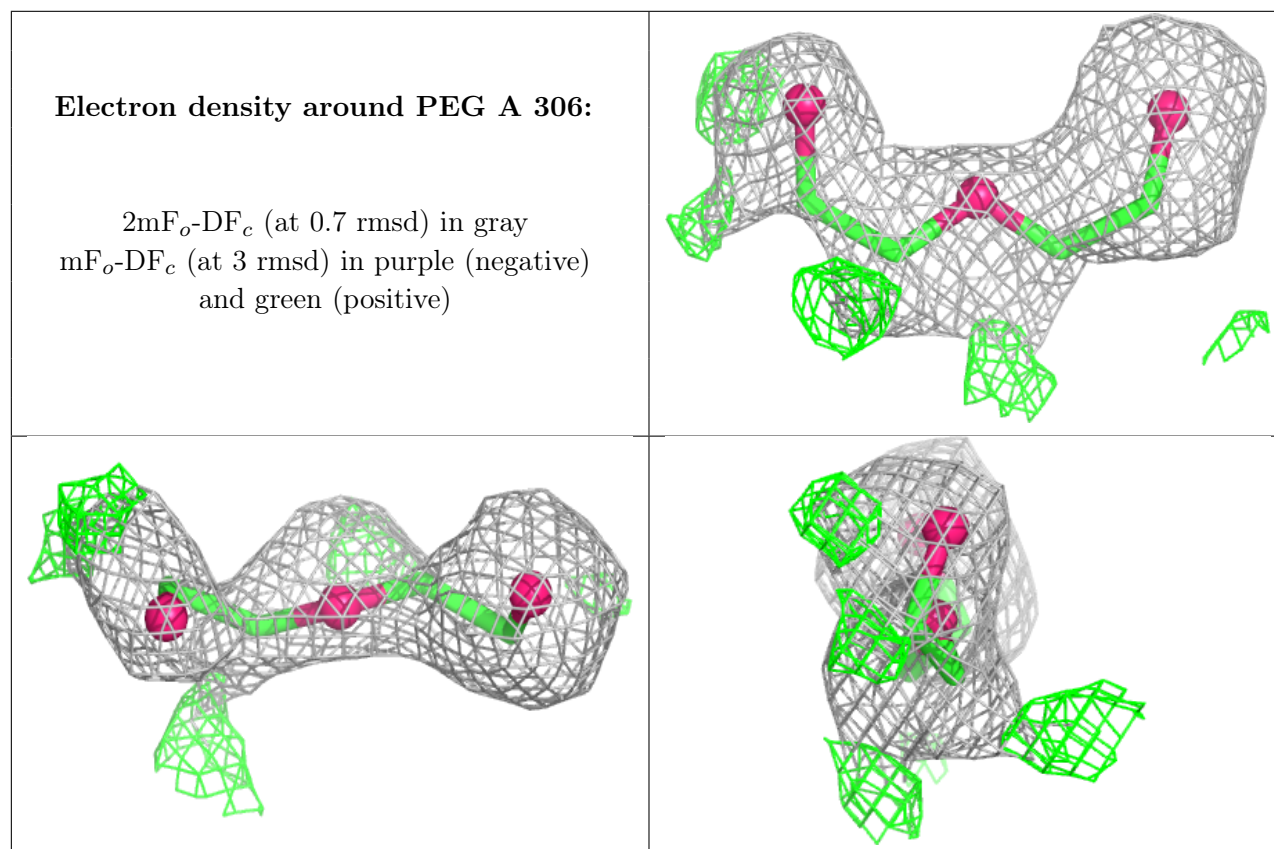
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PEG	A	306	7/7	0.75	0.17	39,46,49,56	0
4	PEG	B	304	7/7	0.76	0.16	30,32,43,44	0
4	PEG	D	304	7/7	0.79	0.14	33,37,49,54	0
3	GOL	B	302	6/6	0.82	0.12	36,40,42,44	0
3	GOL	C	303	6/6	0.82	0.13	38,39,42,43	0
3	GOL	E	303	6/6	0.82	0.14	42,45,47,50	0
3	GOL	D	303	6/6	0.87	0.10	38,51,53,59	0
4	PEG	H	302	7/7	0.87	0.13	31,39,40,40	0
3	GOL	F	303	6/6	0.88	0.13	33,34,40,41	0
3	GOL	B	305	6/6	0.90	0.13	32,35,38,39	0
3	GOL	I	302	6/6	0.90	0.12	23,30,33,38	0
3	GOL	A	304	6/6	0.90	0.12	23,37,39,43	0
3	GOL	F	302	6/6	0.92	0.11	31,35,39,42	0
3	GOL	G	302	6/6	0.93	0.09	39,41,43,47	0
3	GOL	A	305	6/6	0.93	0.10	22,25,28,31	0
3	GOL	A	302	6/6	0.93	0.11	26,34,41,41	0
3	GOL	B	303	6/6	0.94	0.08	25,27,29,32	0
3	GOL	E	302	6/6	0.95	0.08	25,27,30,36	0
3	GOL	A	303	6/6	0.96	0.09	28,29,33,34	0
3	GOL	D	302	6/6	0.96	0.07	28,34,34,38	0
3	GOL	C	302	6/6	0.96	0.06	21,25,30,33	0
3	GOL	J	302	6/6	0.96	0.06	24,27,29,32	0
2	SO4	K	301	5/5	0.97	0.07	34,37,39,39	0
2	SO4	C	301	5/5	0.98	0.06	23,23,24,26	0
2	SO4	L	301	5/5	0.98	0.04	32,35,39,40	0
2	SO4	E	301	5/5	0.98	0.05	27,29,31,33	0
2	SO4	A	301	5/5	0.99	0.04	25,25,26,28	0
2	SO4	D	301	5/5	0.99	0.05	22,23,23,25	0
2	SO4	B	301	5/5	0.99	0.04	20,21,23,25	0
2	SO4	F	301	5/5	0.99	0.04	21,22,24,29	0
2	SO4	G	301	5/5	0.99	0.04	18,22,23,24	0
2	SO4	H	301	5/5	0.99	0.03	21,22,24,26	0

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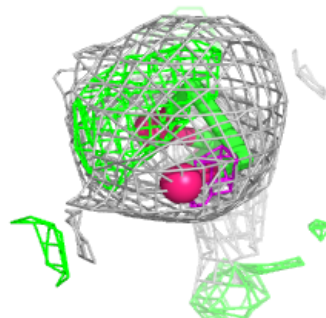
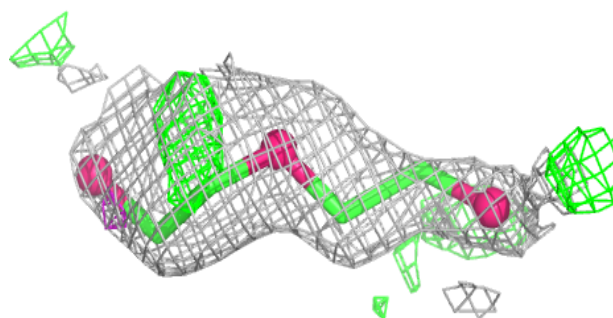
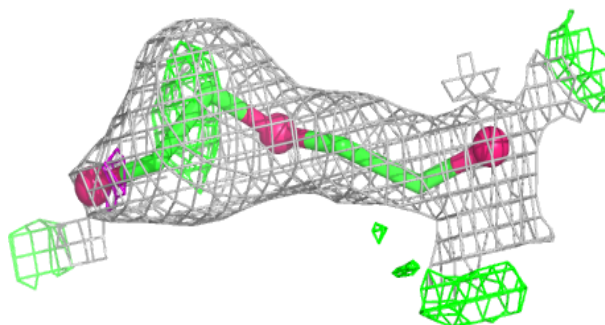
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	I	301	5/5	0.99	0.04	25,28,29,34	0
2	SO4	J	301	5/5	0.99	0.04	31,33,36,39	0

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.

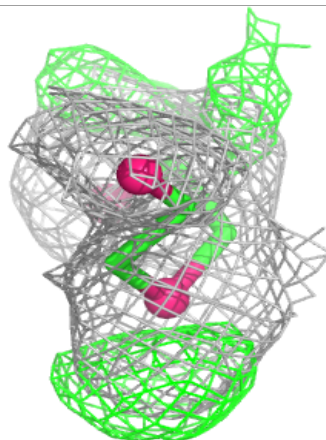
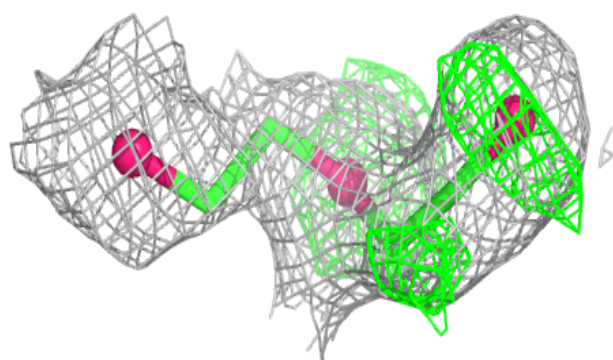
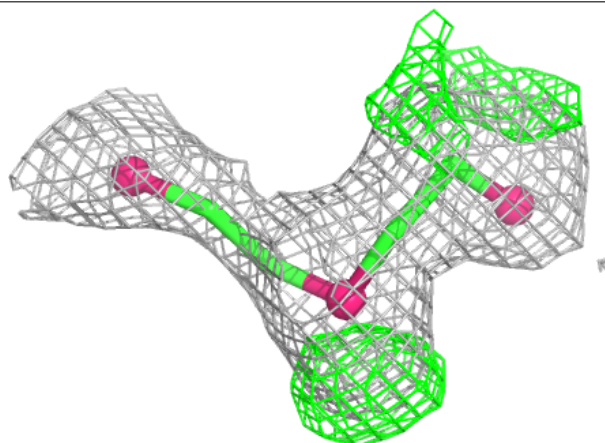


Electron density around PEG B 304:

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

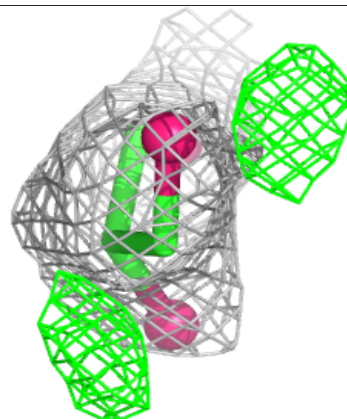
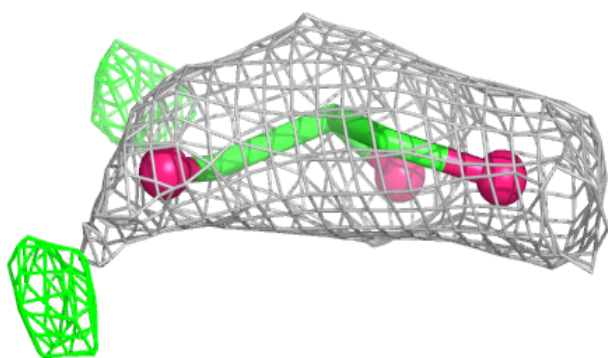
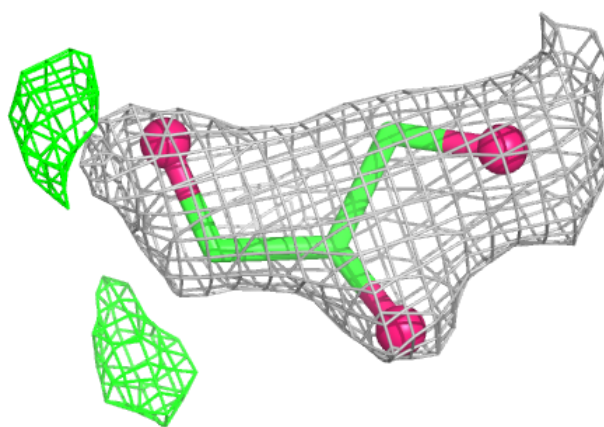
**Electron density around PEG D 304:**

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



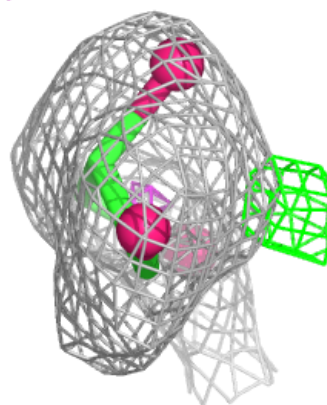
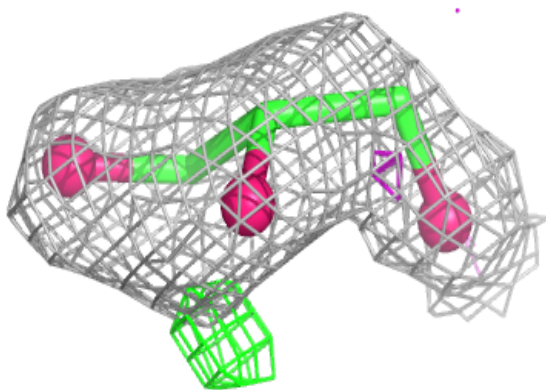
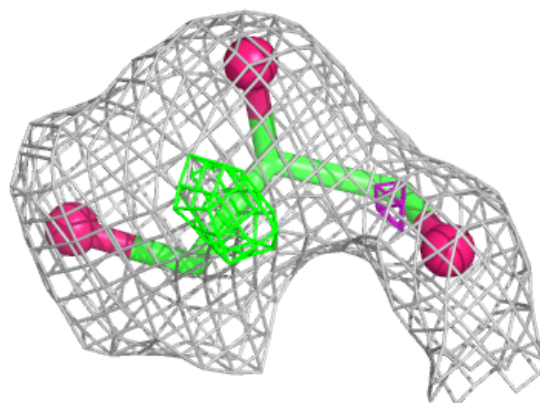
Electron density around GOL B 302:

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



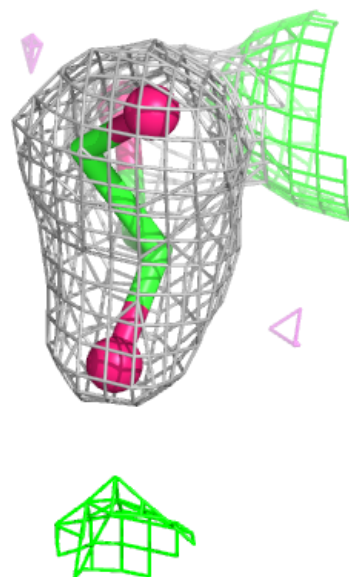
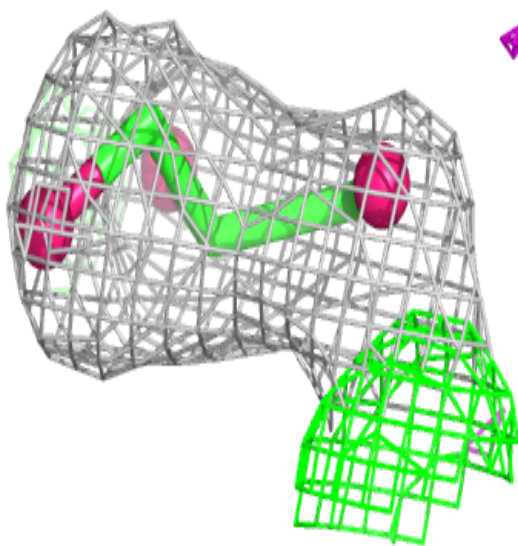
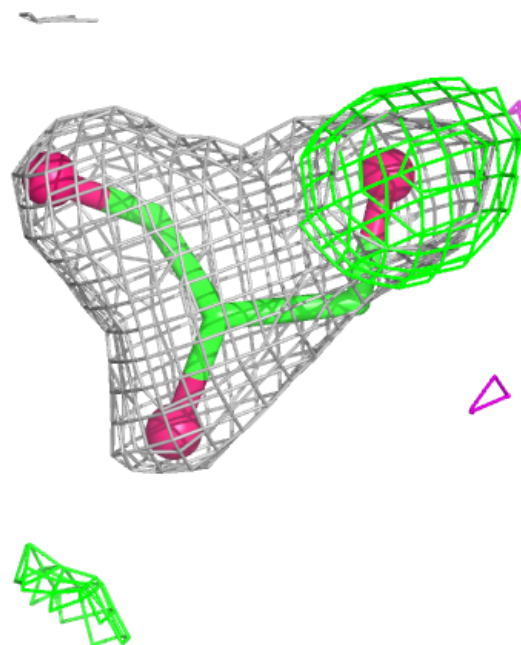
Electron density around GOL C 303:

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



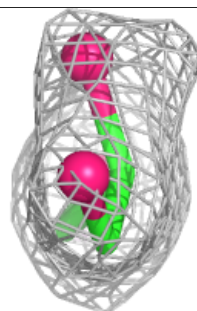
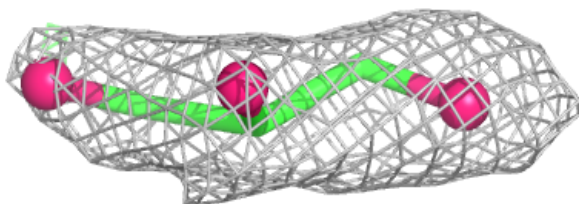
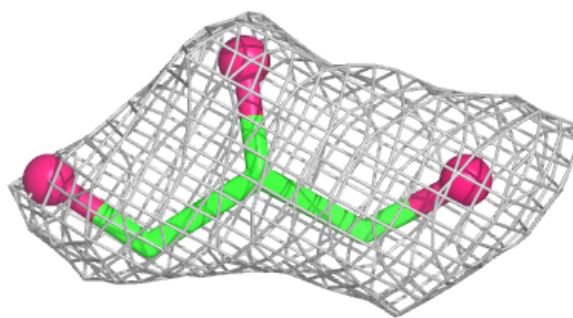
Electron density around GOL E 303:

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and green (positive)

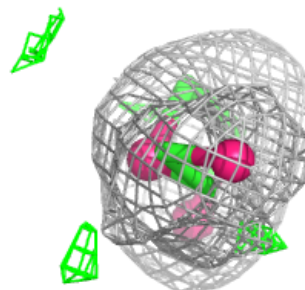
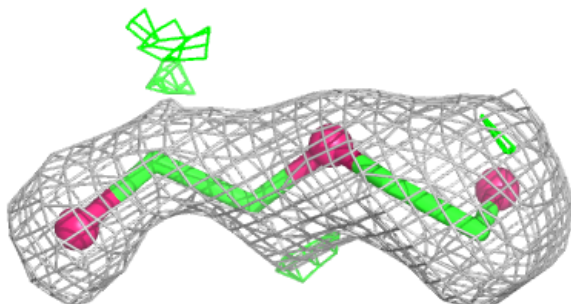
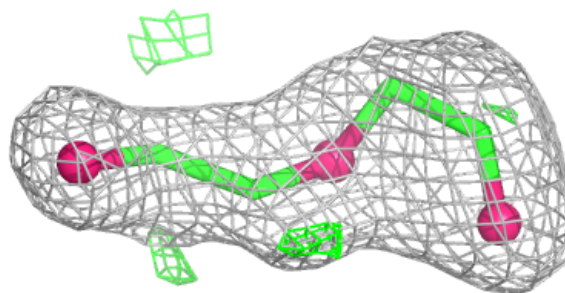


Electron density around GOL D 303:

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

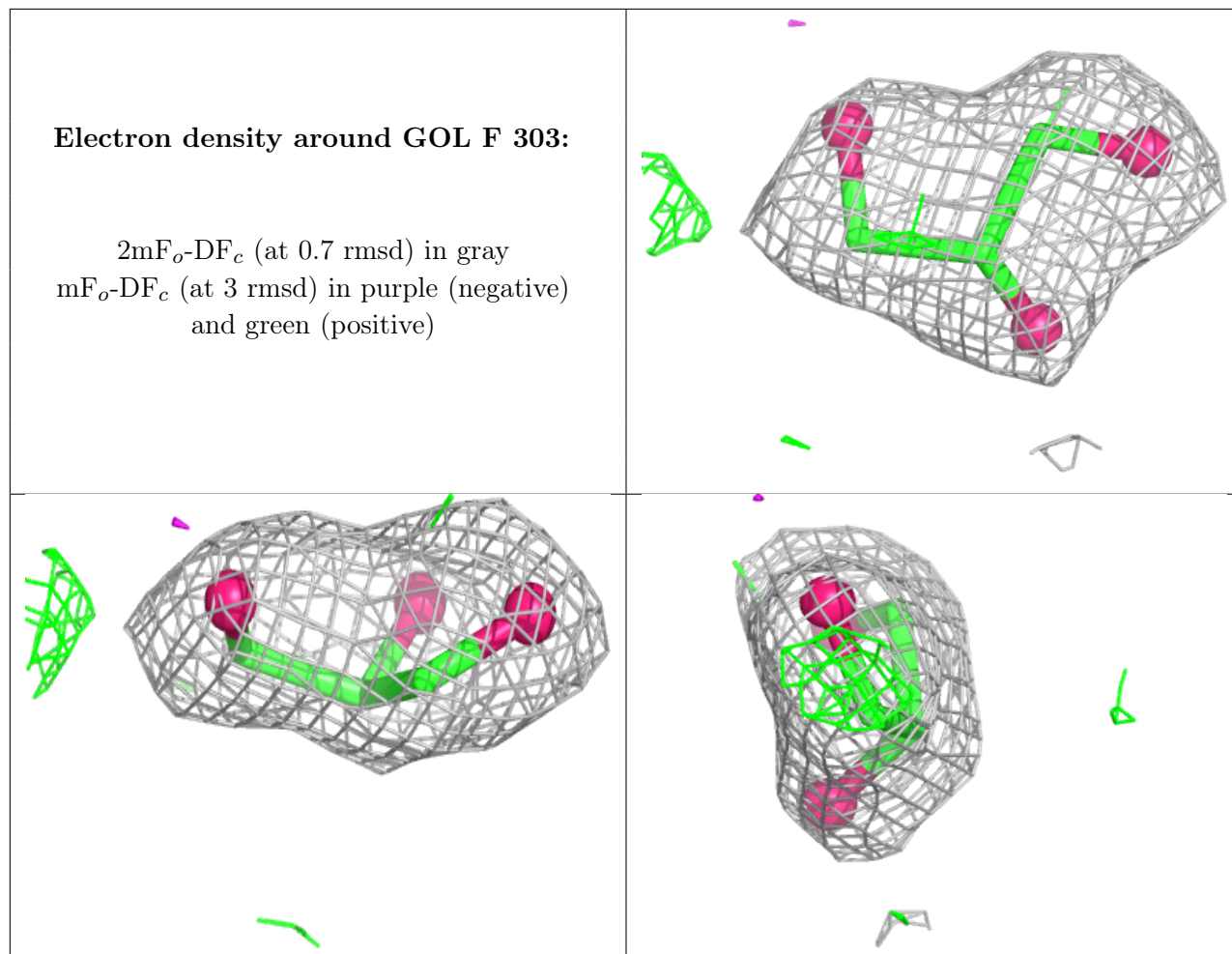
**Electron density around PEG H 302:**

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and green (positive)



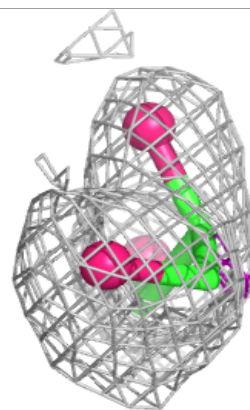
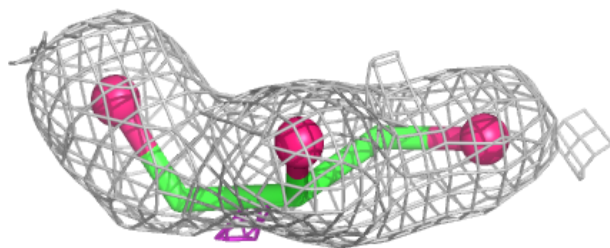
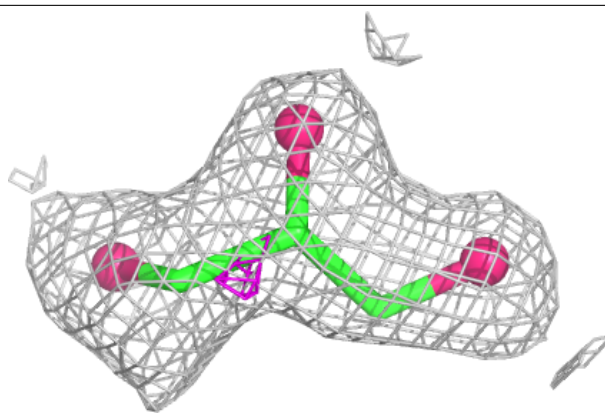
Electron density around GOL F 303:

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



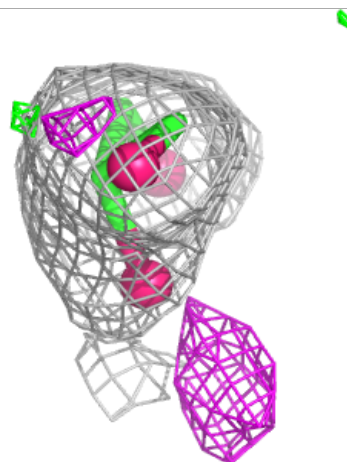
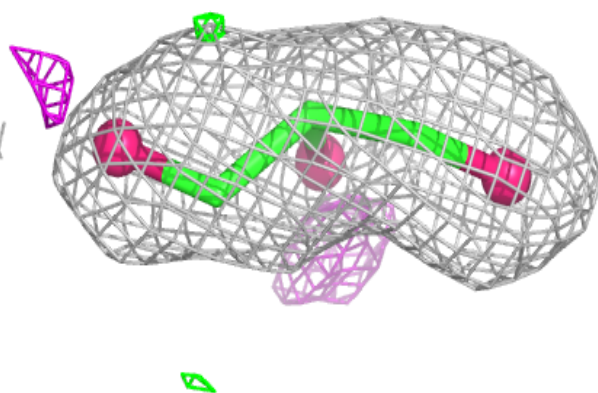
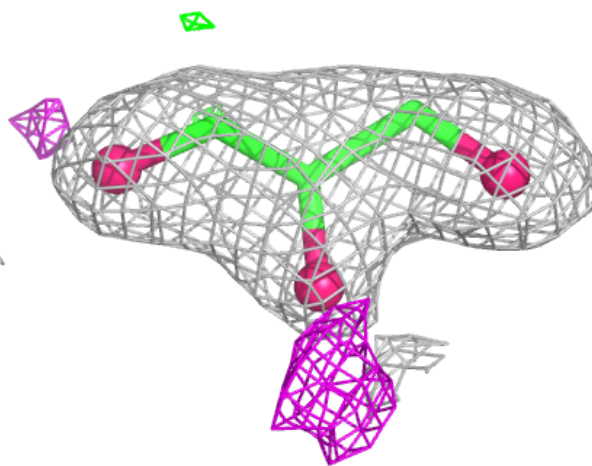
Electron density around GOL B 305:

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and green (positive)



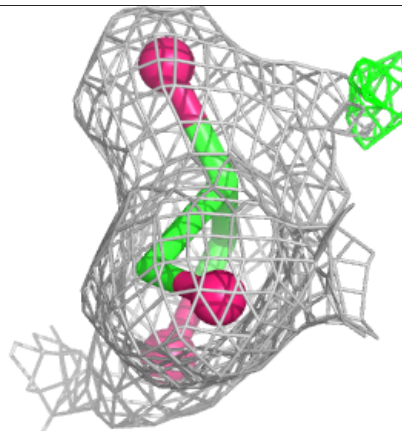
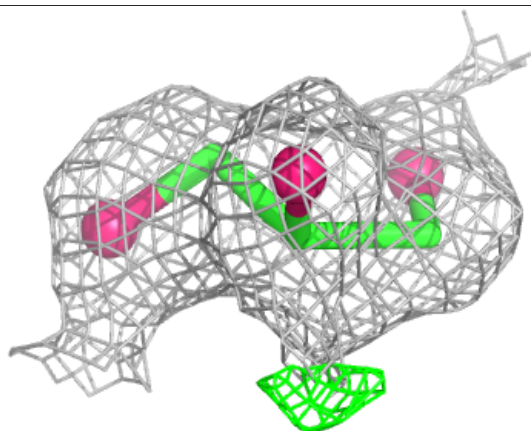
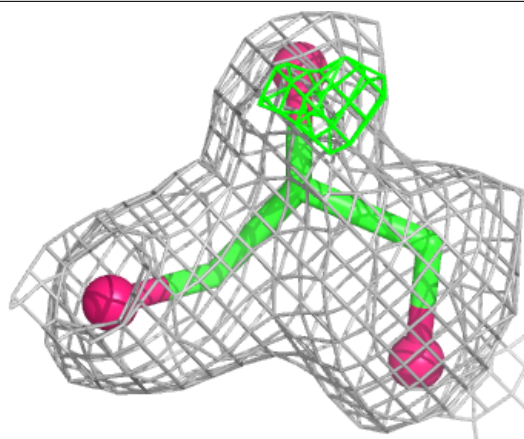
Electron density around GOL I 302:

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

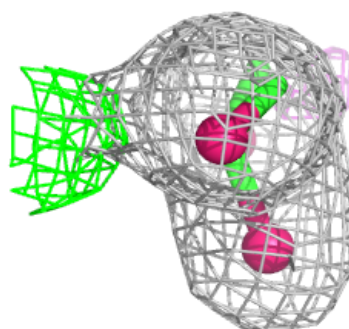
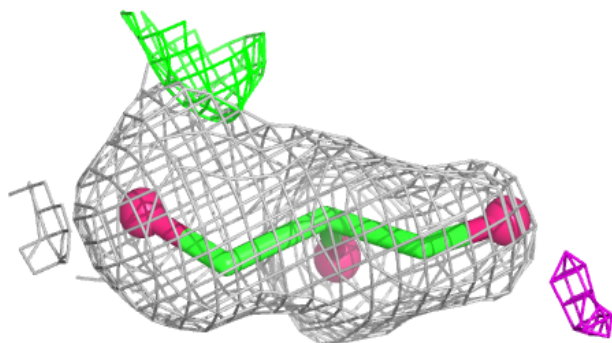
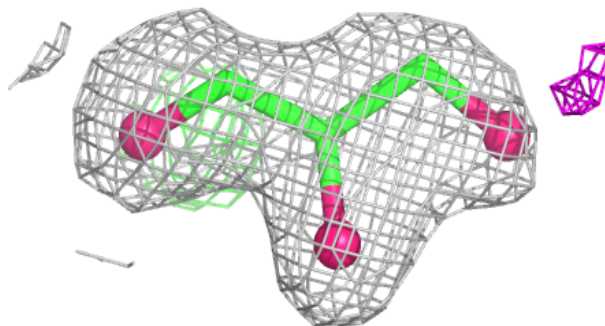


Electron density around GOL A 304:

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

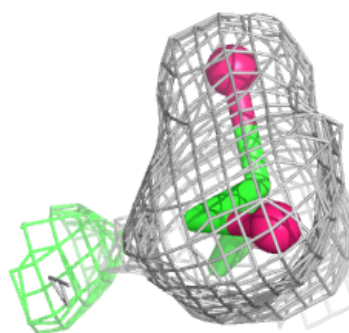
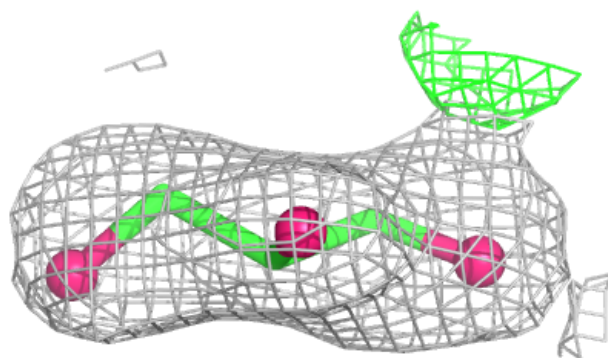
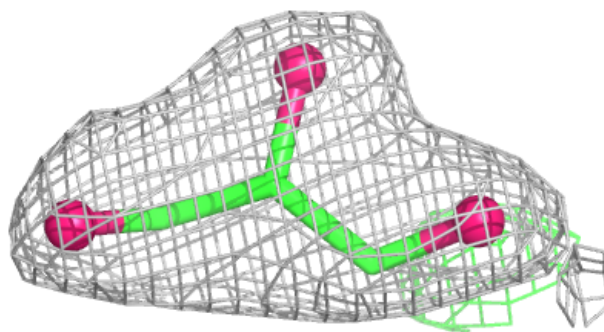
**Electron density around GOL F 302:**

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



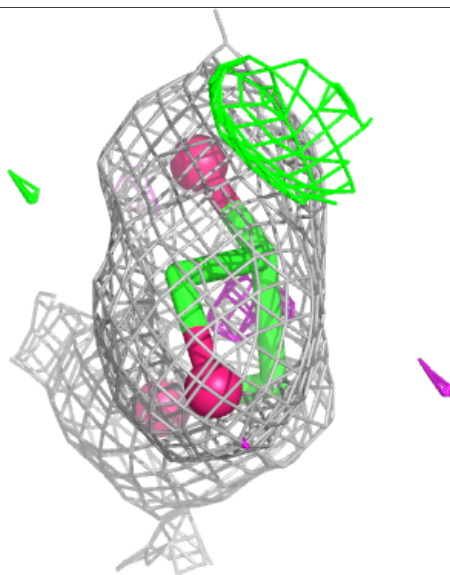
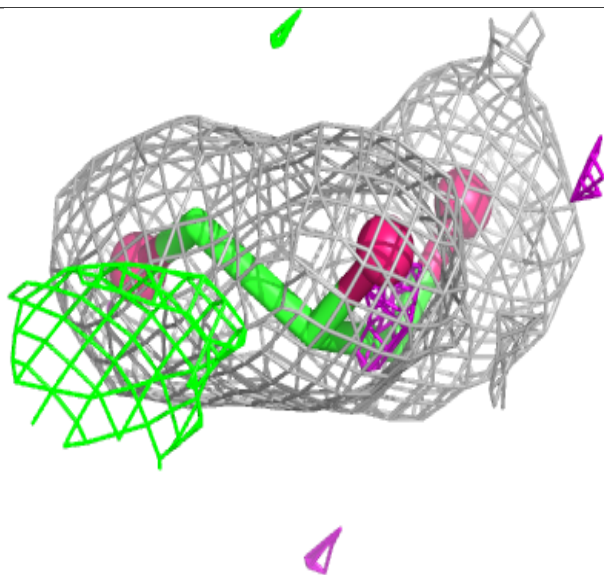
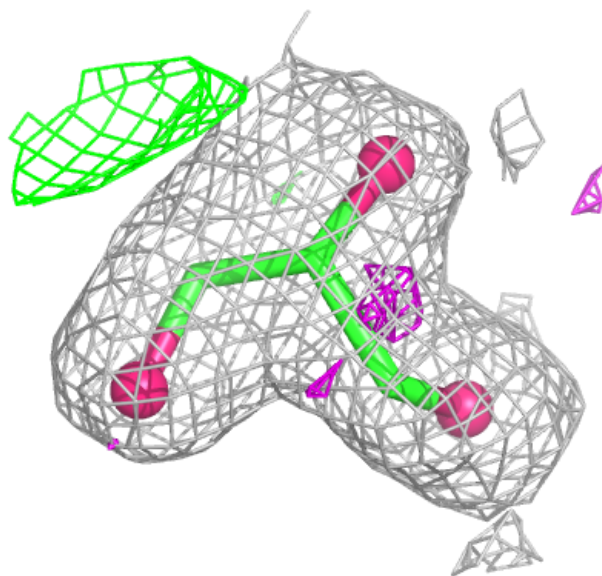
Electron density around GOL G 302:

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and green (positive)



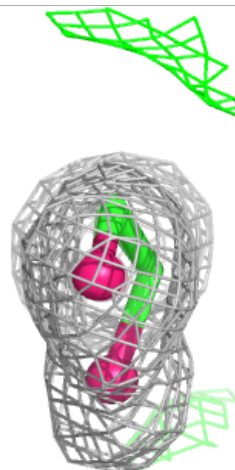
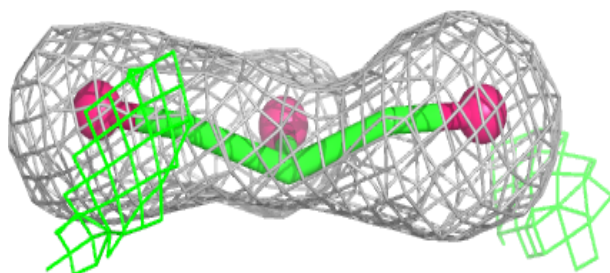
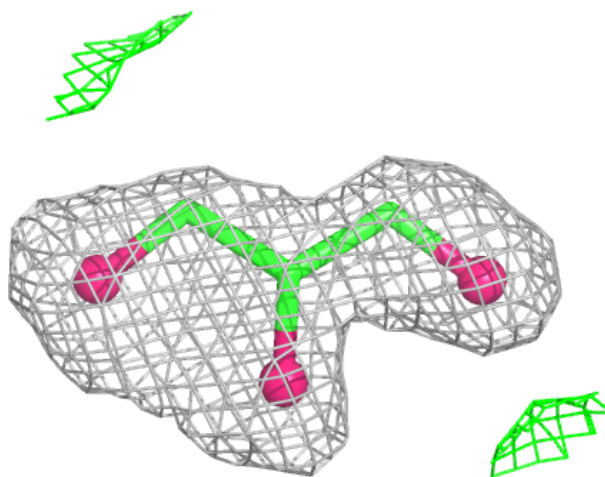
Electron density around GOL A 305:

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



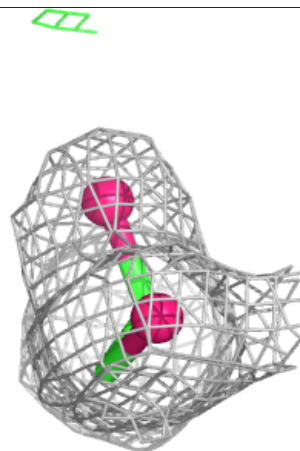
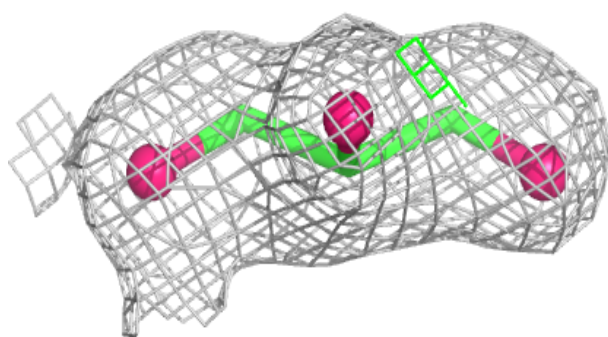
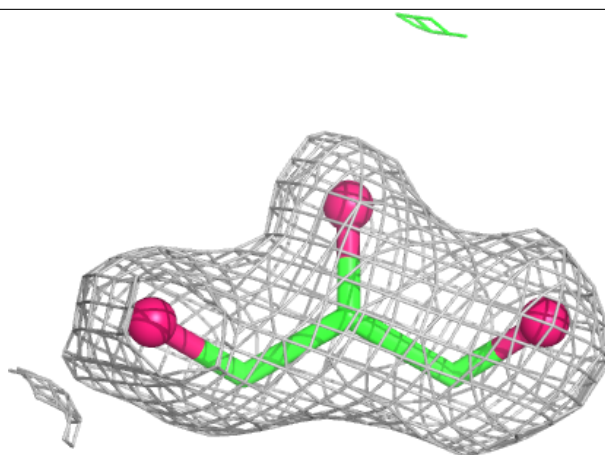
Electron density around GOL A 302:

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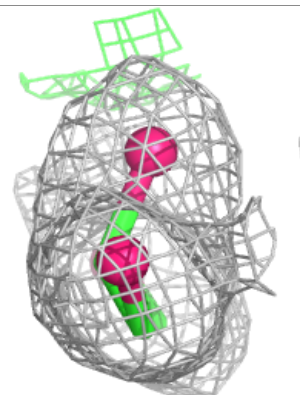
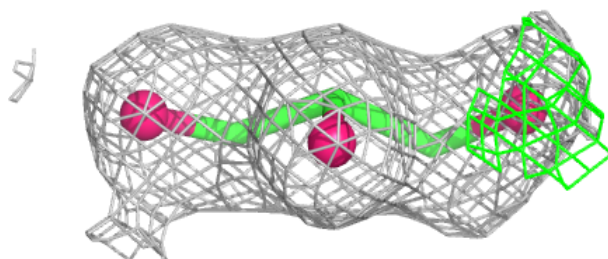
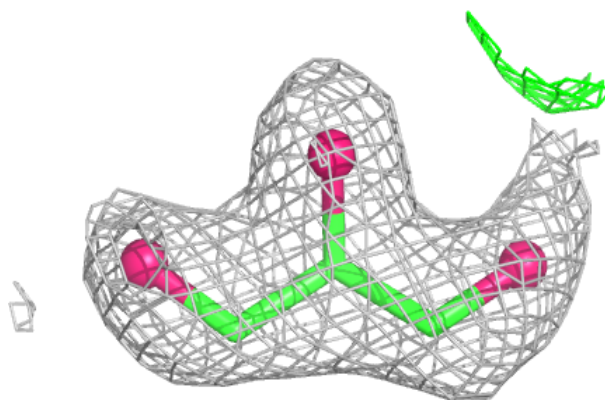


Electron density around GOL B 303:

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and green (positive)

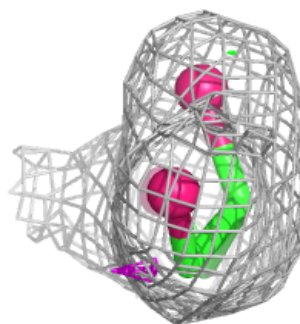
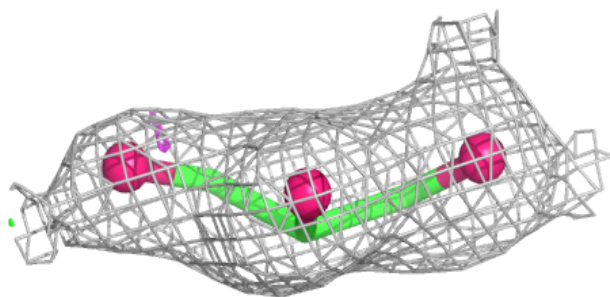
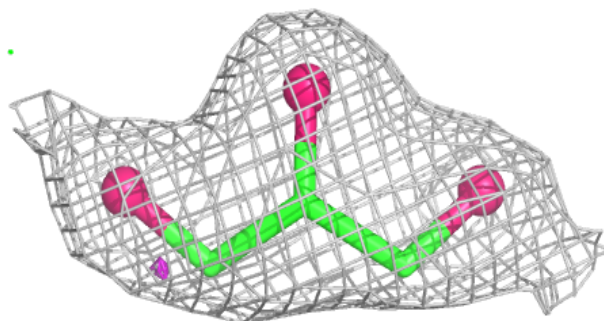
**Electron density around GOL E 302:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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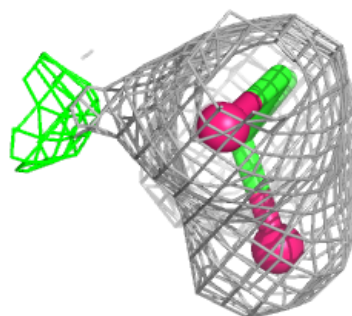
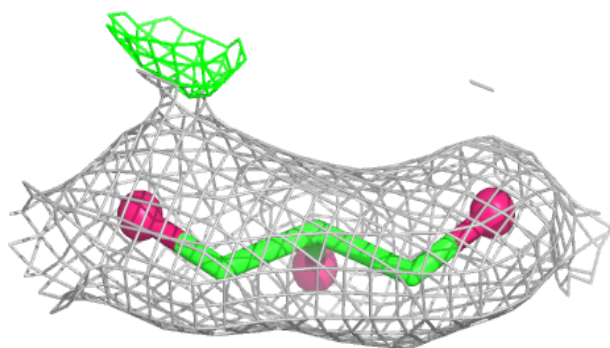
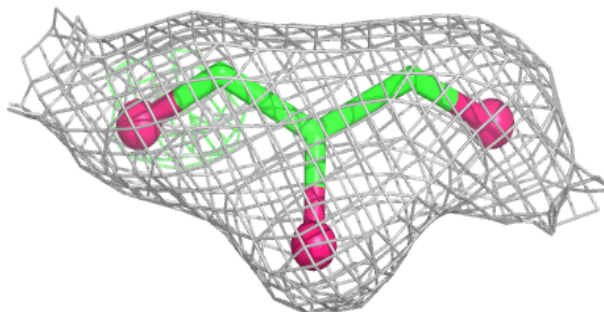


Electron density around GOL A 303:

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

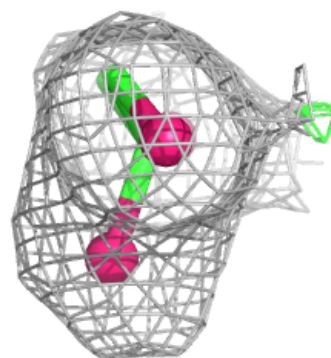
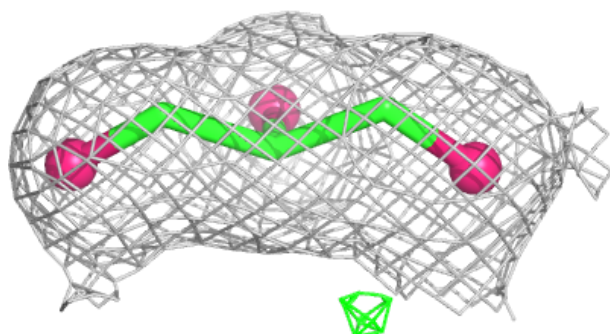
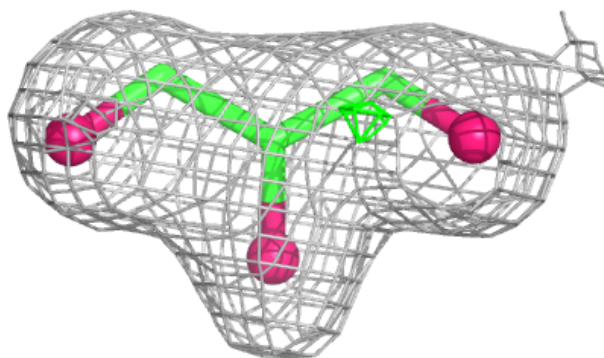
**Electron density around GOL D 302:**

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and green (positive)

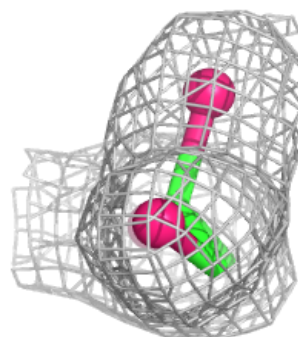
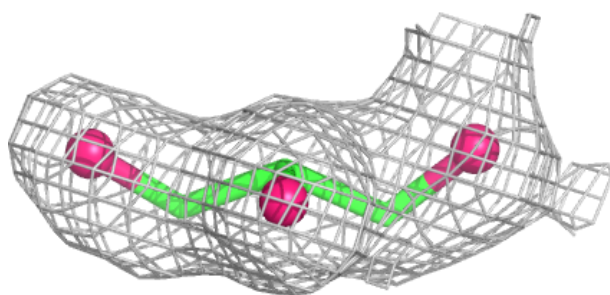
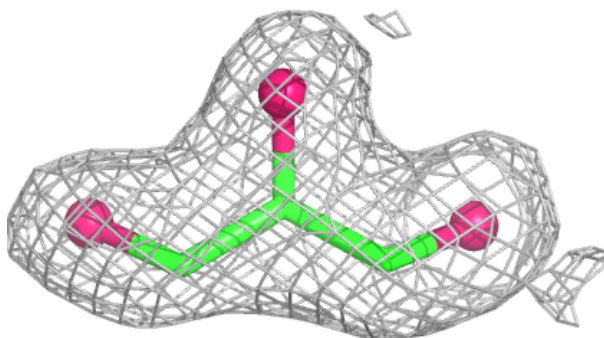


Electron density around GOL C 302:

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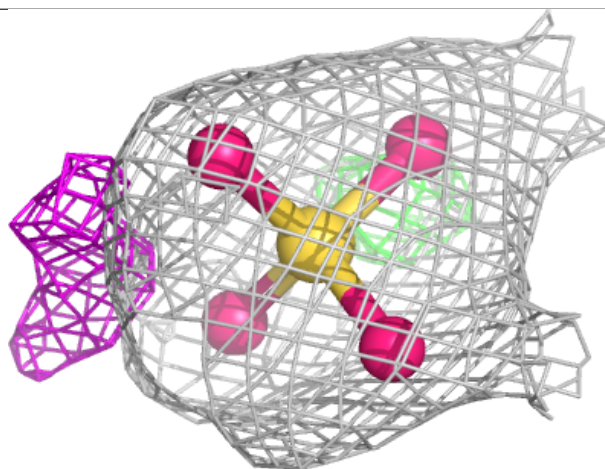
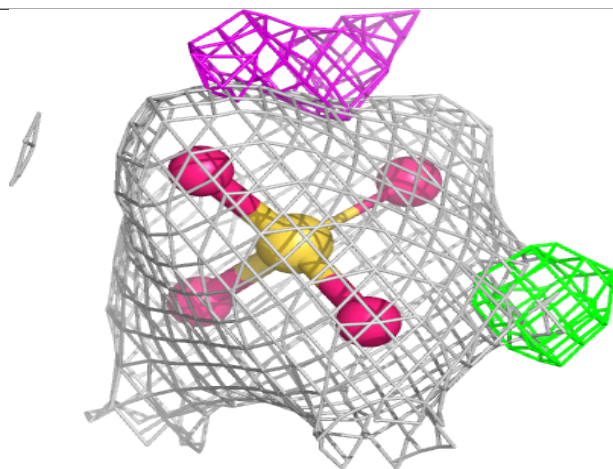
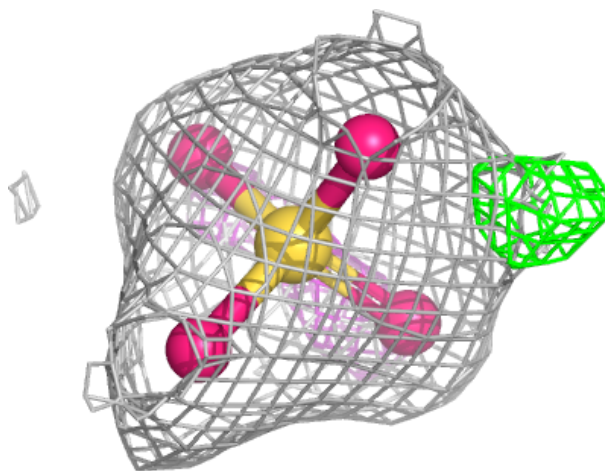
**Electron density around GOL J 302:**

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



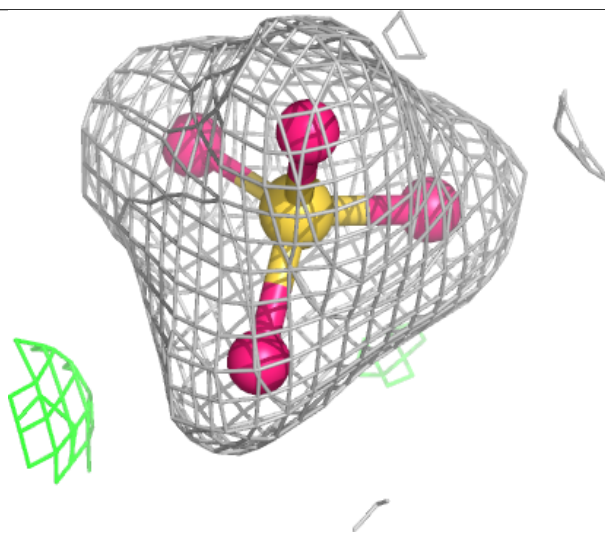
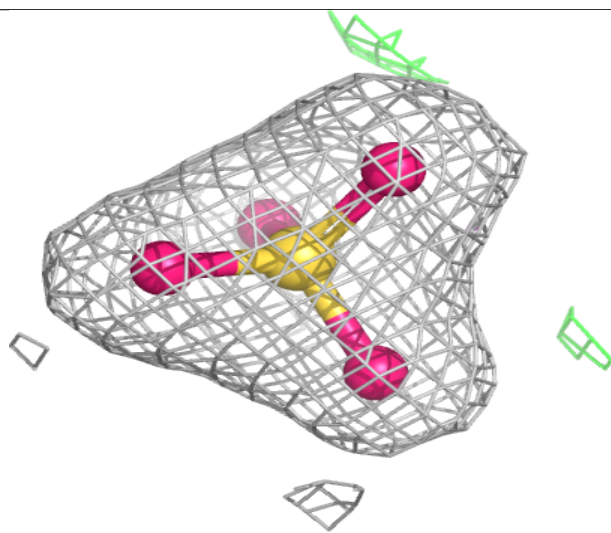
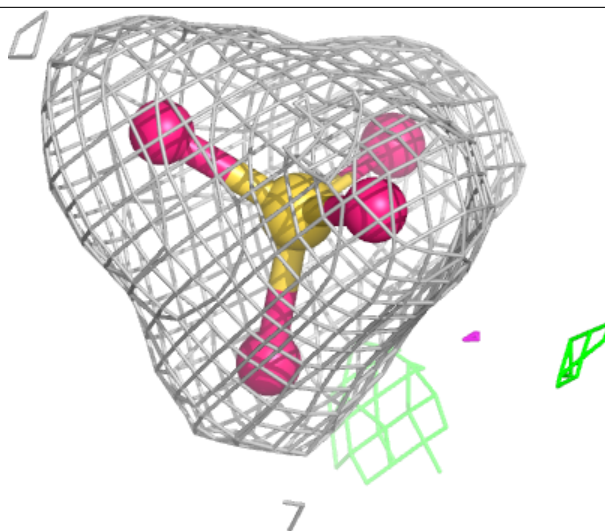
Electron density around SO4 K 301:

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



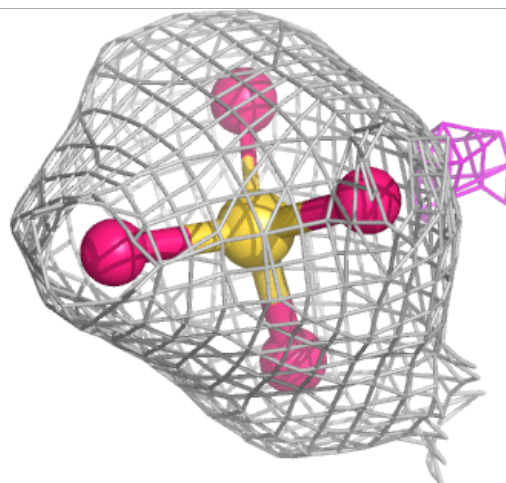
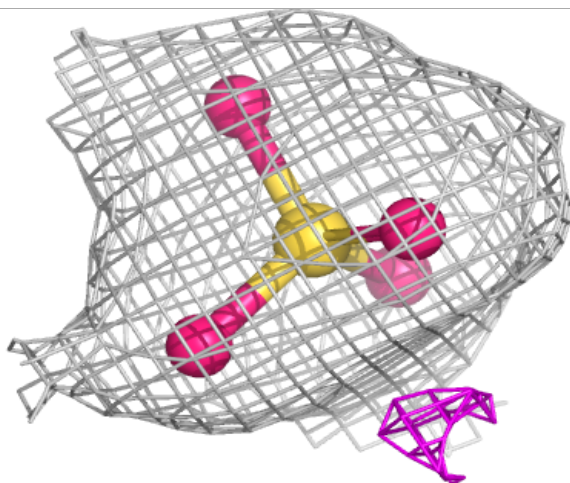
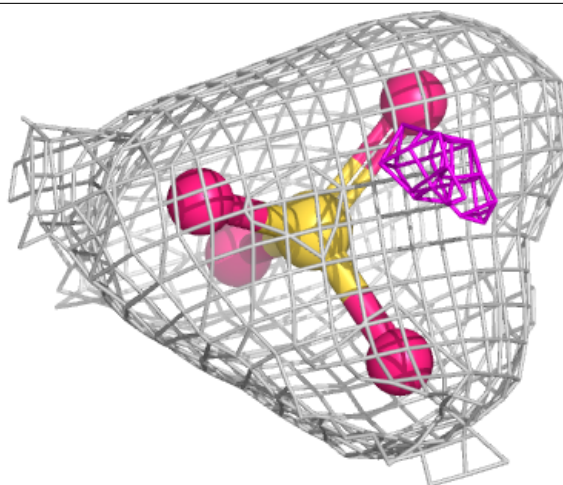
Electron density around SO4 C 301:

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



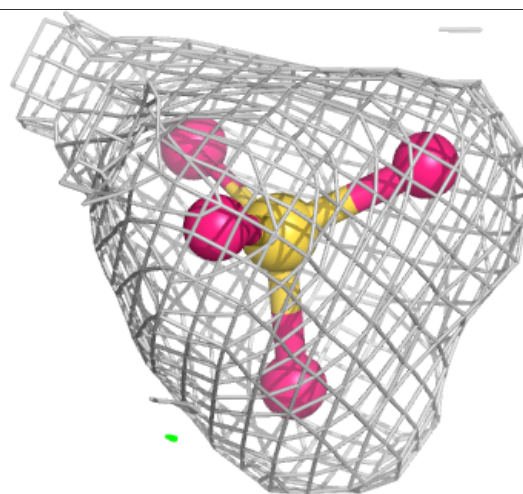
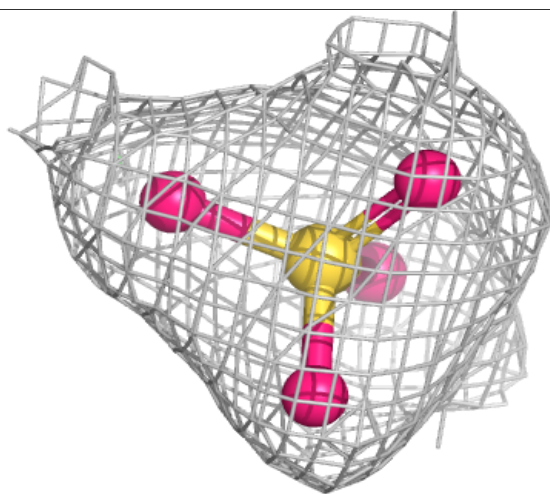
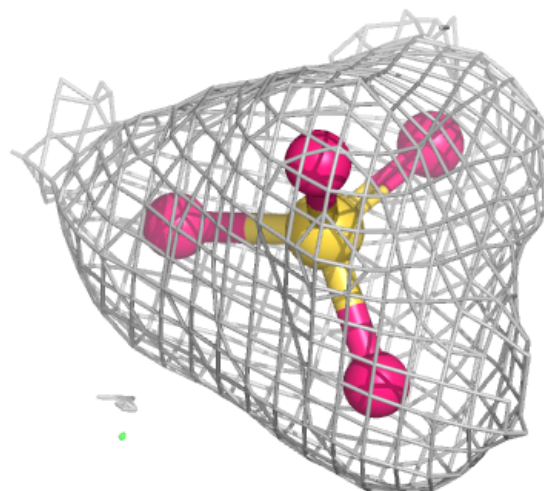
Electron density around SO4 L 301:

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



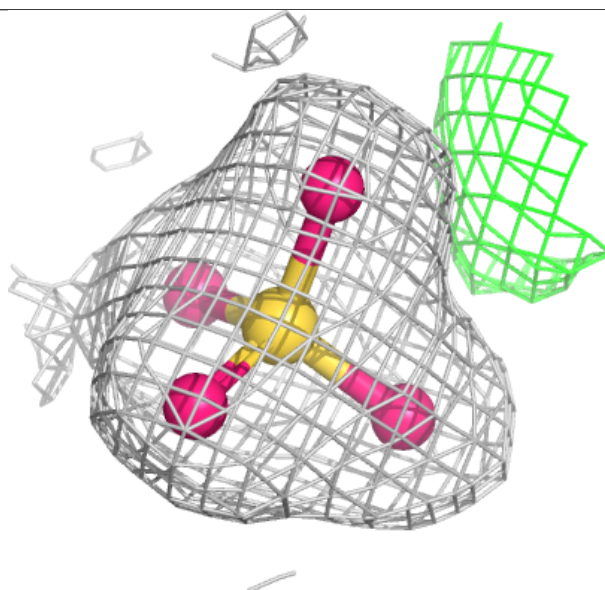
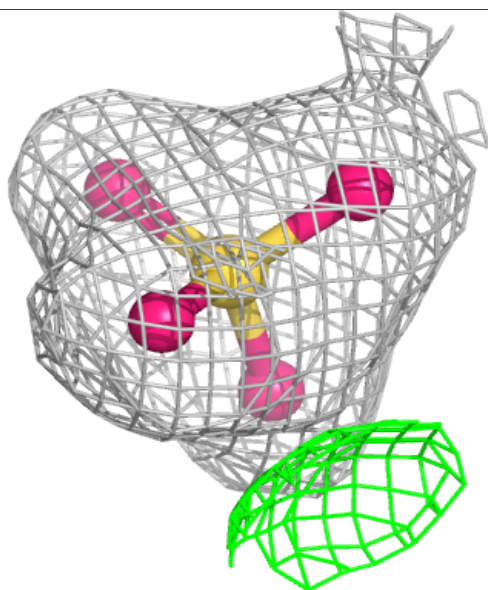
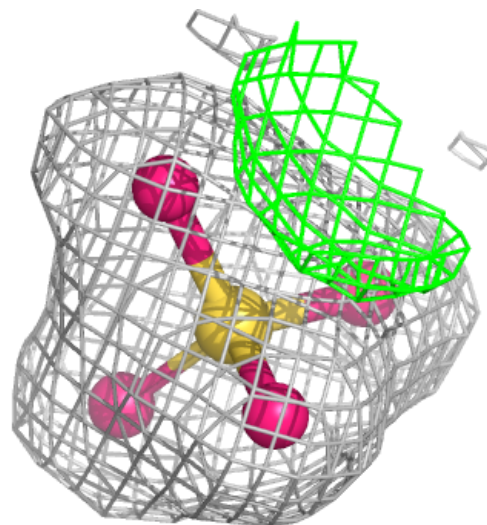
Electron density around SO4 E 301:

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



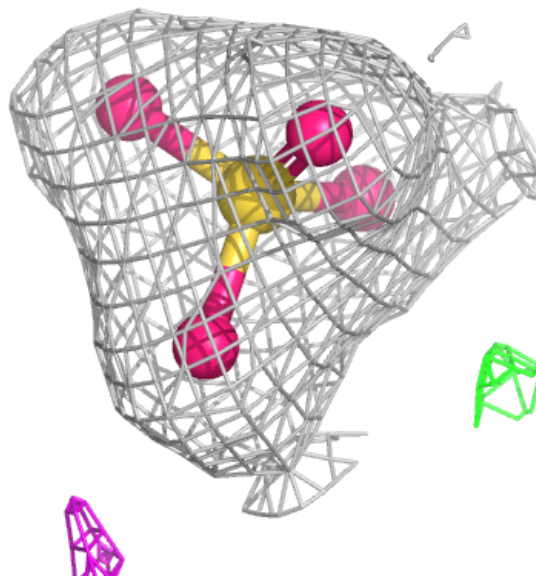
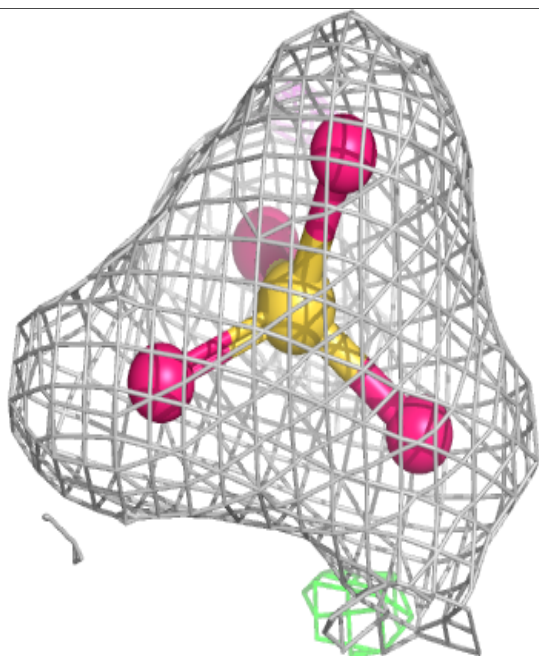
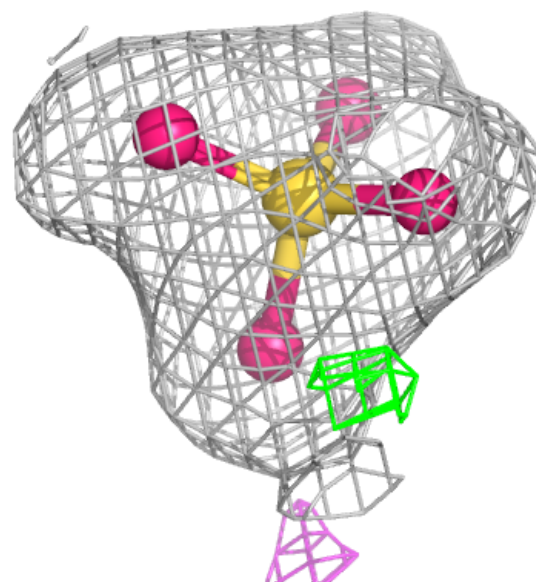
Electron density around SO4 A 301:

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



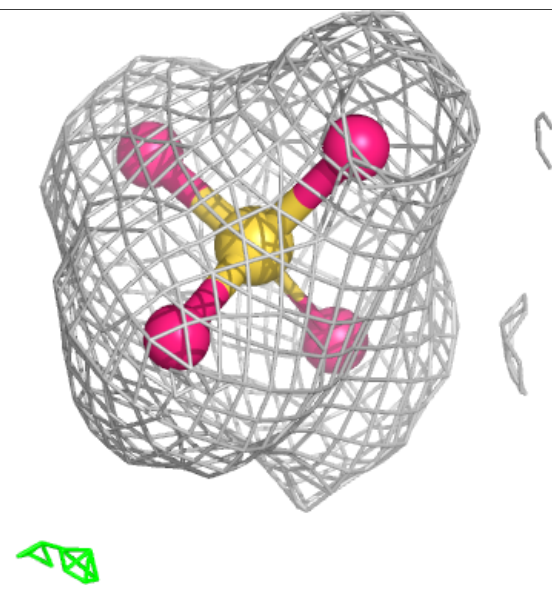
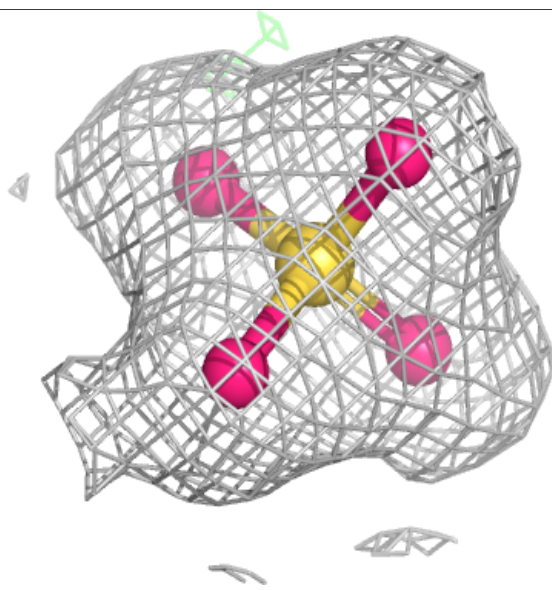
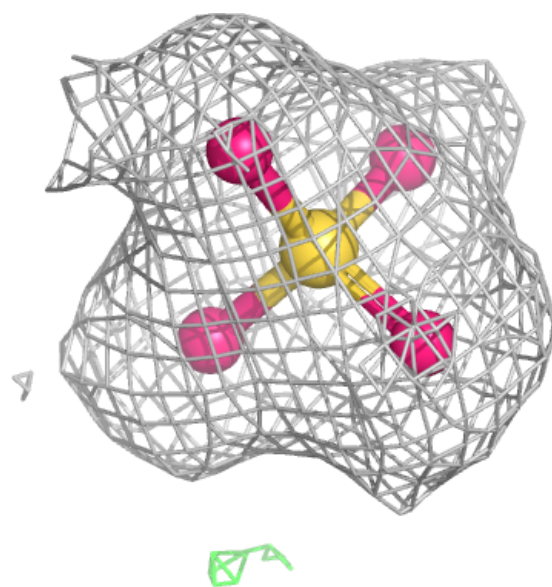
Electron density around SO4 D 301:

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



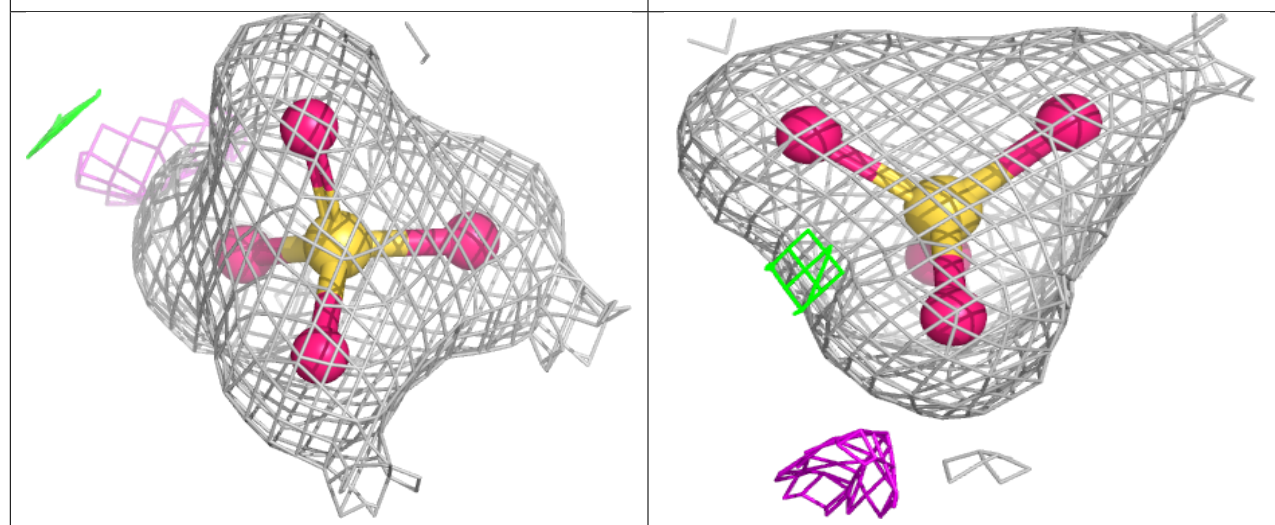
Electron density around SO4 B 301:

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



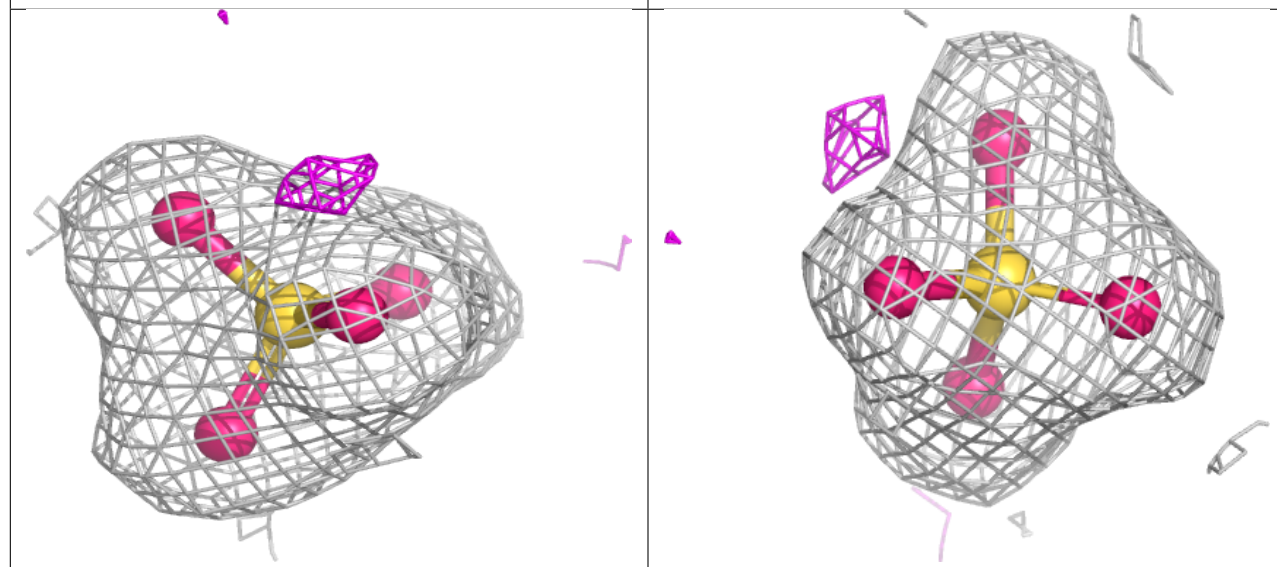
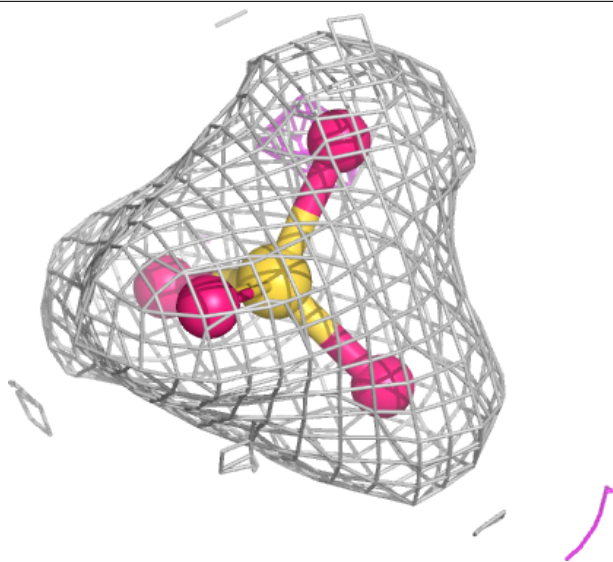
Electron density around SO4 F 301:

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



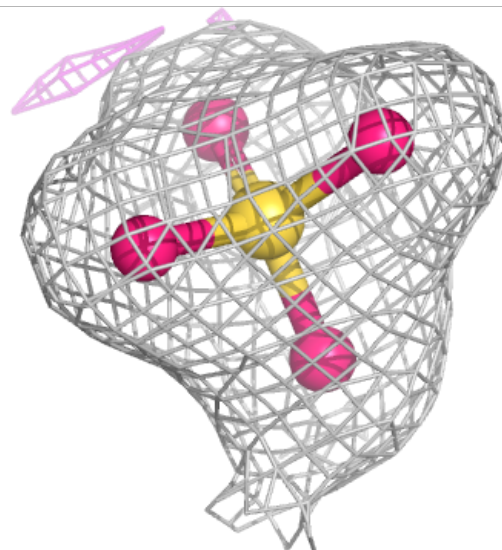
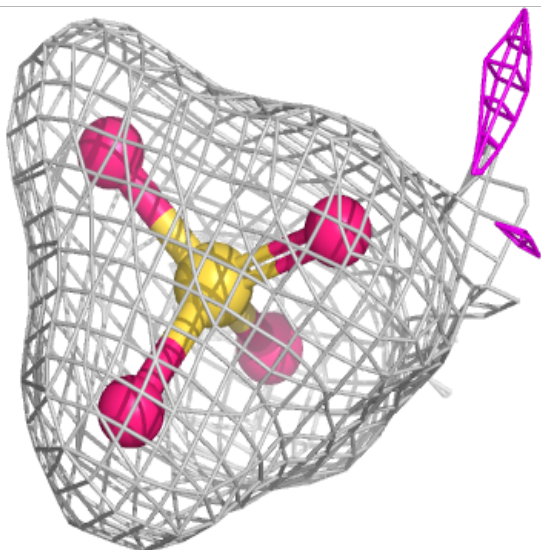
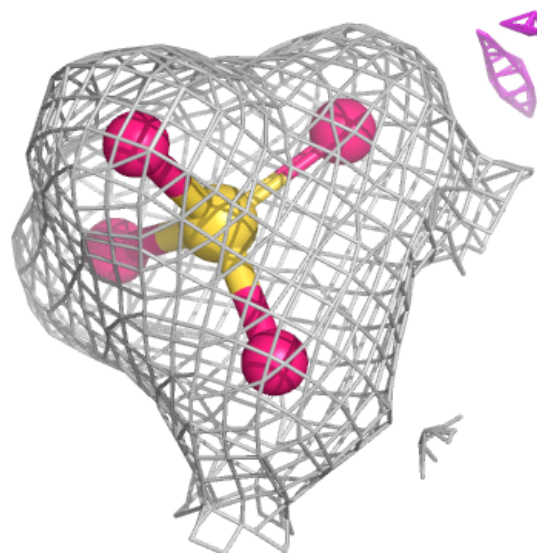
Electron density around SO4 G 301:

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



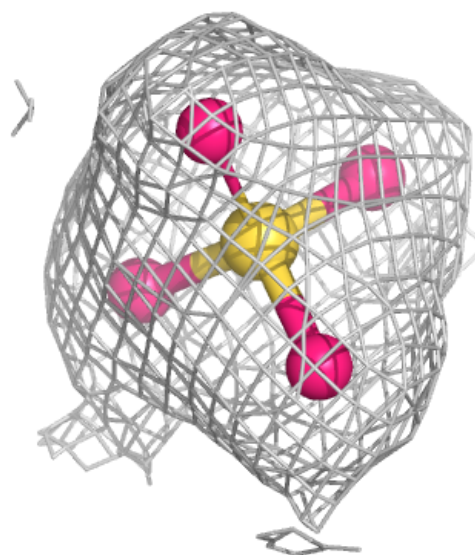
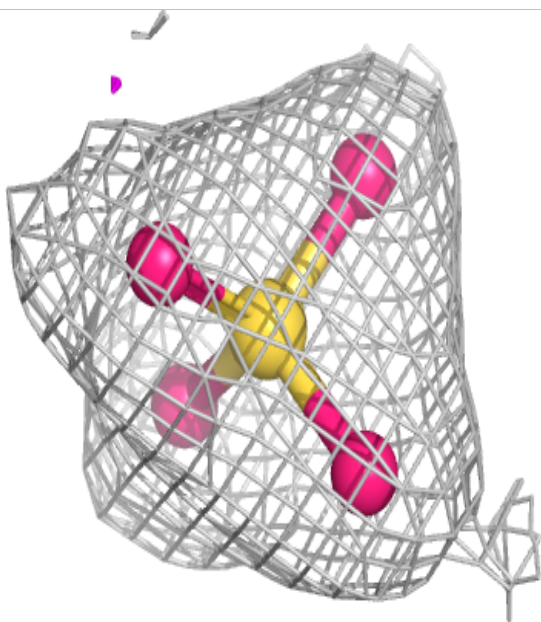
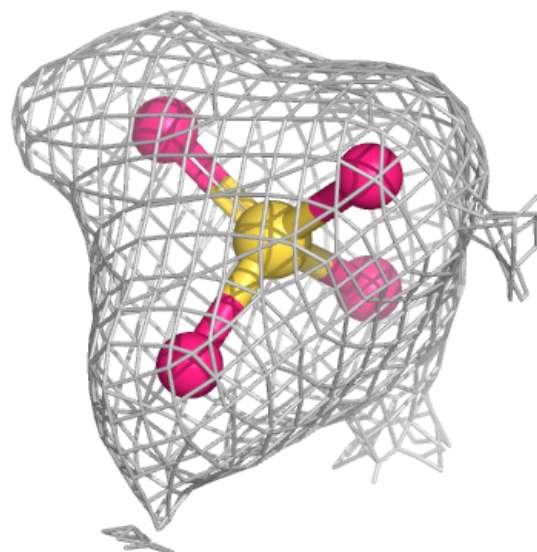
Electron density around SO4 H 301:

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



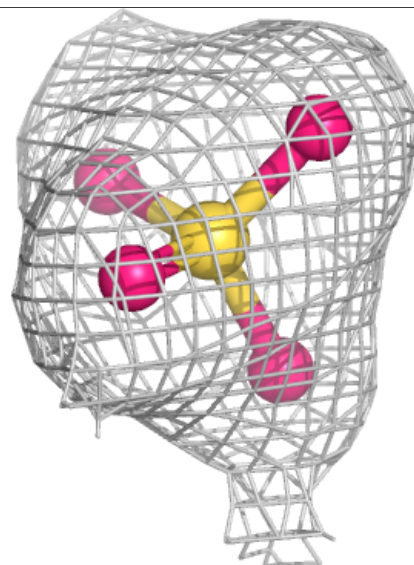
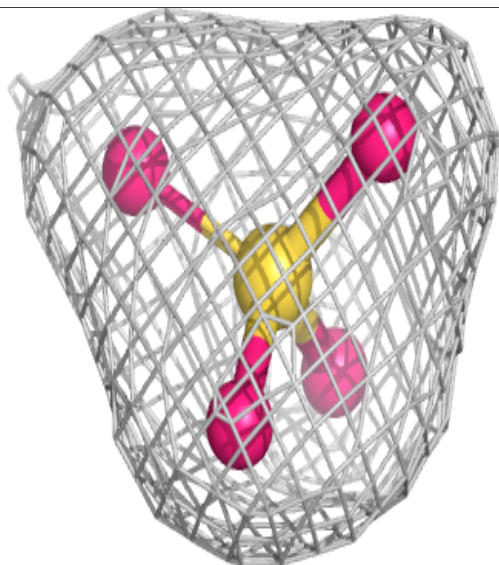
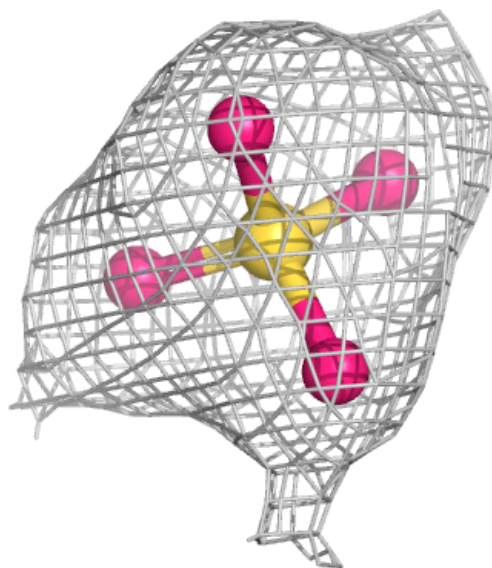
Electron density around SO4 I 301:

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



Electron density around SO4 J 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.