



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2026 – 09:47 PM UTC

PDB ID : 8JBO / pdb_00008jbo
Title : Crystal structure of TxGH116 from Thermoanaerobacterium xylanolyticum
with isofagomine
Authors : Pengthaisong, S.; Ketudat Cairns, J.R.
Deposited on : 2023-05-09
Resolution : 2.00 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

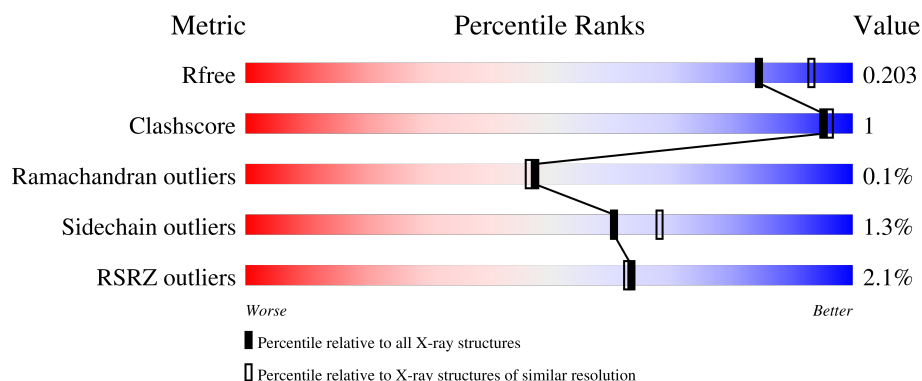
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	798	2% 93%
1	B	798	2% 93%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13604 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.

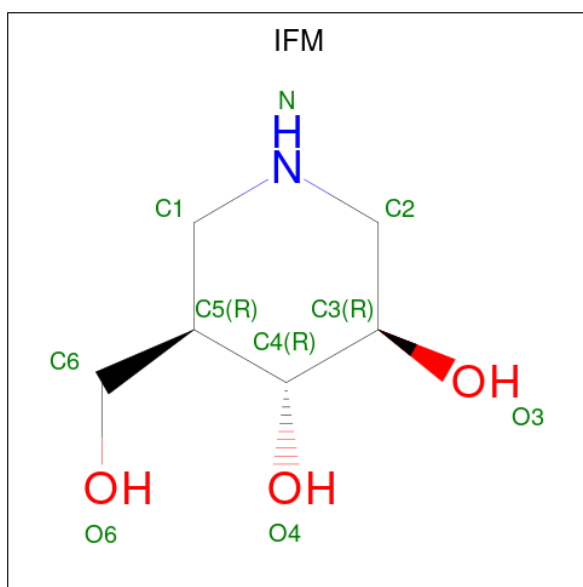
- Molecule 1 is a protein called Glucosylceramidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	769	Total	C	N	O	S	0	2	0
			6238	4028	1004	1179	27			
1	B	769	Total	C	N	O	S	0	3	0
			6248	4034	1007	1180	27			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP F6BL85
A	18	ALA	-	expression tag	UNP F6BL85
A	807	LEU	-	expression tag	UNP F6BL85
A	808	GLU	-	expression tag	UNP F6BL85
A	809	HIS	-	expression tag	UNP F6BL85
A	810	HIS	-	expression tag	UNP F6BL85
A	811	HIS	-	expression tag	UNP F6BL85
A	812	HIS	-	expression tag	UNP F6BL85
A	813	HIS	-	expression tag	UNP F6BL85
A	814	HIS	-	expression tag	UNP F6BL85
B	17	MET	-	initiating methionine	UNP F6BL85
B	18	ALA	-	expression tag	UNP F6BL85
B	807	LEU	-	expression tag	UNP F6BL85
B	808	GLU	-	expression tag	UNP F6BL85
B	809	HIS	-	expression tag	UNP F6BL85
B	810	HIS	-	expression tag	UNP F6BL85
B	811	HIS	-	expression tag	UNP F6BL85
B	812	HIS	-	expression tag	UNP F6BL85
B	813	HIS	-	expression tag	UNP F6BL85
B	814	HIS	-	expression tag	UNP F6BL85

- Molecule 2 is 5-HYDROXYMETHYL-3,4-DIHYDROXYPIPERIDINE (CCD ID: IFM) (formula: C₆H₁₃NO₃) (labeled as "Ligand of Interest" by depositor).

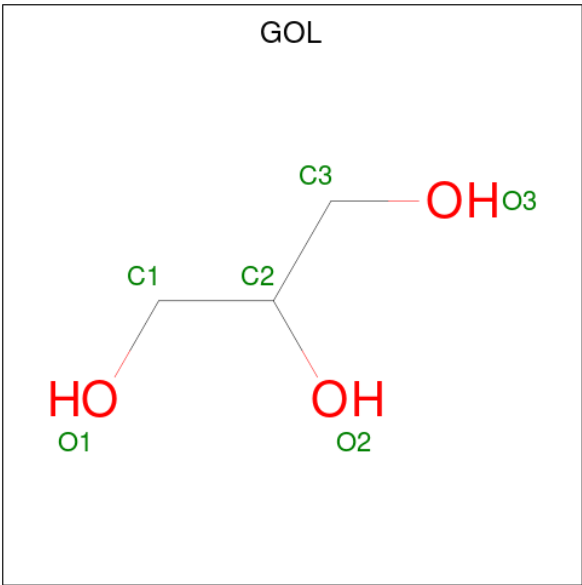


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	1	3		
2	B	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



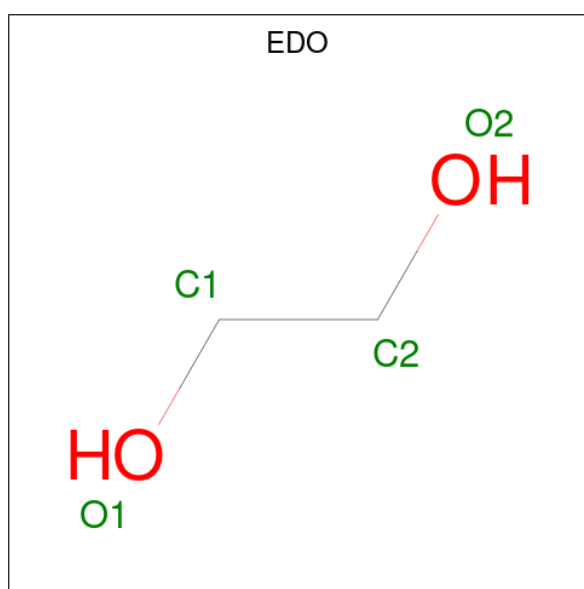
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	508	Total	O	0	0
			508	508		

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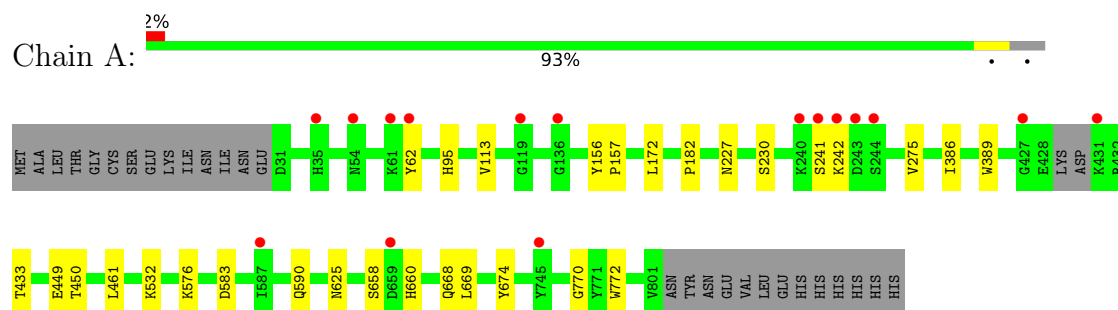
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	459	Total	O	0	0
			459	459		

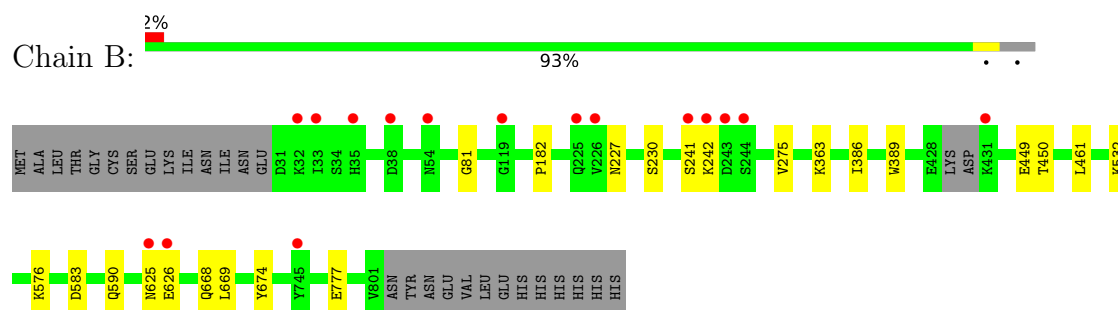
3 Residue-property plots

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

• Molecule 1: Glucosylceramidase



• Molecule 1: Glucosylceramidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.79Å 164.40Å 179.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.00 50.01 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.01-2.00) 98.7 (50.01-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.27 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.155 , 0.193 0.168 , 0.203	Depositor DCC
R_{free} test set	5466 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.3	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	13604	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0588e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, EDO, IFM, CA

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	0.80	0/6418	0.84	0/8698
1	B	0.80	0/6429	0.84	0/8713
All	All	0.80	0/12847	0.84	0/17411

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

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	6238	0	5973	15	0
1	B	6248	0	5979	8	0
2	A	10	0	13	0	0
2	B	10	0	13	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	60	0	80	6	0
4	B	60	0	80	3	0
5	A	4	0	6	3	0
5	B	4	0	6	2	0
6	A	508	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	459	0	0	3	0
All	All	13604	0	12150	29	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 1.

All (29) 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)
5:A:913:EDO:H22	6:A:1123:HOH:O	1.94	0.65
1:A:660:HIS:HB2	4:A:912:GOL:H32	1.79	0.65
1:B:363:LYS:H	4:B:906:GOL:H31	1.64	0.62
5:B:912:EDO:H11	6:B:1233:HOH:O	2.00	0.61
1:B:81:GLY:HA2	5:B:912:EDO:O1	2.02	0.59
1:B:449:GLU:O	1:B:450:THR:C	2.50	0.55
1:A:95:HIS:O	5:A:913:EDO:H21	2.09	0.53
4:A:908:GOL:C3	6:A:1034:HOH:O	2.56	0.53
1:A:449:GLU:O	1:A:450:THR:C	2.55	0.49
1:B:386:ILE:HA	1:B:389[A]:TRP:CD1	2.47	0.49
4:B:905:GOL:H12	6:B:1001:HOH:O	2.12	0.49
1:A:62:TYR:H	4:A:906:GOL:HO2	1.61	0.48
4:A:908:GOL:H31	6:A:1034:HOH:O	2.12	0.48
1:A:95:HIS:HB3	5:A:913:EDO:H21	1.96	0.48
1:A:668:GLN:HG3	1:A:669:LEU:HG	1.96	0.47
1:A:532:LYS:HE2	1:A:583:ASP:O	2.15	0.46
1:A:386:ILE:HA	1:A:389[A]:TRP:CD1	2.51	0.45
1:B:668:GLN:HG3	1:B:669:LEU:HG	1.97	0.45
1:A:156:TYR:CD1	1:A:157:PRO:HA	2.53	0.44
1:B:532:LYS:HE2	1:B:583:ASP:O	2.19	0.43
1:A:660:HIS:CB	4:A:912:GOL:H32	2.48	0.43
1:B:227:ASN:HB3	1:B:230:SER:HB2	2.01	0.42
1:A:113:VAL:HG21	1:A:172:LEU:HD11	2.01	0.41
1:B:182:PRO:HD2	1:B:389[A]:TRP:CD1	2.54	0.41
1:A:227:ASN:HB3	1:A:230:SER:HB2	2.01	0.41
1:A:182:PRO:HD2	1:A:389[A]:TRP:CD1	2.56	0.40
4:B:905:GOL:C1	6:B:1001:HOH:O	2.68	0.40
1:A:658:SER:HB3	4:A:912:GOL:H31	2.03	0.40
1:A:770:GLY:HA2	1:A:772:TRP:CZ3	2.56	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	767/798 (96%)	737 (96%)	29 (4%)	1 (0%)	48	46
1	B	768/798 (96%)	739 (96%)	28 (4%)	1 (0%)	48	46
All	All	1535/1596 (96%)	1476 (96%)	57 (4%)	2 (0%)	48	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	LYS
1	B	242	LYS

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	656/685 (96%)	648 (99%)	8 (1%)	63	70
1	B	657/685 (96%)	648 (99%)	9 (1%)	59	66
All	All	1313/1370 (96%)	1296 (99%)	17 (1%)	61	68

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	SER
1	A	275	VAL
1	A	433	THR
1	A	461	LEU

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Mol	Chain	Res	Type
1	A	576	LYS
1	A	590	GLN
1	A	625	ASN
1	A	674	TYR
1	B	241	SER
1	B	275	VAL
1	B	461	LEU
1	B	576	LYS
1	B	590	GLN
1	B	625	ASN
1	B	626	GLU
1	B	674	TYR
1	B	777	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	256	ASN
1	A	323	ASN
1	A	660	HIS
1	B	101	ASN
1	B	323	ASN

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](#)

Of 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	GOL	A	910	-	5,5,5	0.50	0	5,5,5	0.51	0
4	GOL	B	909	-	5,5,5	0.41	0	5,5,5	0.53	0
4	GOL	B	904	-	5,5,5	0.45	0	5,5,5	0.46	0
2	IFM	B	901	-	10,10,10	0.98	0	9,13,13	2.44	2 (22%)
4	GOL	B	910	-	5,5,5	0.39	0	5,5,5	0.50	0
4	GOL	B	911	-	5,5,5	0.50	0	5,5,5	0.63	0
4	GOL	B	902	-	5,5,5	0.38	0	5,5,5	0.57	0
4	GOL	B	907	-	5,5,5	0.36	0	5,5,5	0.45	0
2	IFM	A	901	-	10,10,10	0.93	0	9,13,13	1.96	1 (11%)
4	GOL	A	904	-	5,5,5	0.45	0	5,5,5	0.92	0
4	GOL	A	905	-	5,5,5	0.73	0	5,5,5	0.63	0
4	GOL	A	911	-	5,5,5	0.18	0	5,5,5	0.21	0
4	GOL	B	906	-	5,5,5	0.27	0	5,5,5	0.53	0
4	GOL	A	903	-	5,5,5	0.46	0	5,5,5	1.24	1 (20%)
4	GOL	A	906	-	5,5,5	0.50	0	5,5,5	1.43	1 (20%)
4	GOL	A	908	-	5,5,5	0.60	0	5,5,5	1.64	1 (20%)
5	EDO	B	912	-	3,3,3	0.42	0	2,2,2	0.38	0
4	GOL	A	909	-	5,5,5	0.35	0	5,5,5	0.76	0
5	EDO	A	913	-	3,3,3	0.30	0	2,2,2	0.38	0
4	GOL	B	903	-	5,5,5	0.30	0	5,5,5	0.57	0
4	GOL	B	905	-	5,5,5	0.48	0	5,5,5	1.08	0
4	GOL	A	907	-	5,5,5	0.32	0	5,5,5	0.26	0
4	GOL	B	908	-	5,5,5	0.34	0	5,5,5	0.51	0
4	GOL	A	912	-	5,5,5	0.75	0	5,5,5	1.95	2 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	910	-	-	2/4/4/4	-
4	GOL	B	909	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	904	-	-	3/4/4/4	-
2	IFM	B	901	-	-	0/2/16/16	0/1/1/1
4	GOL	B	910	-	-	0/4/4/4	-
4	GOL	B	911	-	-	0/4/4/4	-
4	GOL	B	902	-	-	0/4/4/4	-
4	GOL	B	907	-	-	0/4/4/4	-
2	IFM	A	901	-	-	0/2/16/16	0/1/1/1
4	GOL	A	904	-	-	2/4/4/4	-
4	GOL	A	905	-	-	2/4/4/4	-
4	GOL	A	911	-	-	0/4/4/4	-
4	GOL	B	906	-	-	2/4/4/4	-
4	GOL	A	903	-	-	2/4/4/4	-
4	GOL	A	906	-	-	0/4/4/4	-
4	GOL	A	908	-	-	2/4/4/4	-
5	EDO	B	912	-	-	1/1/1/1	-
4	GOL	A	909	-	-	3/4/4/4	-
5	EDO	A	913	-	-	0/1/1/1	-
4	GOL	B	903	-	-	2/4/4/4	-
4	GOL	B	905	-	-	2/4/4/4	-
4	GOL	A	907	-	-	3/4/4/4	-
4	GOL	B	908	-	-	2/4/4/4	-
4	GOL	A	912	-	-	0/4/4/4	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	IFM	C1-N-C2	6.40	119.21	111.78
2	A	901	IFM	C1-N-C2	5.53	118.19	111.78
4	A	912	GOL	O2-C2-C1	2.99	121.57	109.18
4	A	912	GOL	C3-C2-C1	-2.79	101.57	111.80
4	A	906	GOL	C3-C2-C1	2.45	120.78	111.80
2	B	901	IFM	C2-C3-C4	2.41	113.19	110.25
4	A	908	GOL	O2-C2-C3	-2.19	100.13	109.18
4	A	903	GOL	O2-C2-C1	2.03	117.59	109.18

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	903	GOL	C1-C2-C3-O3
4	A	903	GOL	O2-C2-C3-O3
4	A	904	GOL	C1-C2-C3-O3
4	A	907	GOL	C1-C2-C3-O3
4	A	910	GOL	C1-C2-C3-O3
4	B	905	GOL	C1-C2-C3-O3
4	B	906	GOL	C1-C2-C3-O3
4	B	906	GOL	O2-C2-C3-O3
4	B	908	GOL	C1-C2-C3-O3
4	B	908	GOL	O2-C2-C3-O3
4	A	905	GOL	O1-C1-C2-C3
4	A	908	GOL	O1-C1-C2-C3
4	A	909	GOL	C1-C2-C3-O3
4	B	903	GOL	O1-C1-C2-C3
4	B	904	GOL	O1-C1-C2-C3
4	A	904	GOL	O2-C2-C3-O3
4	A	907	GOL	O2-C2-C3-O3
4	A	910	GOL	O2-C2-C3-O3
4	B	903	GOL	O1-C1-C2-O2
4	B	905	GOL	O2-C2-C3-O3
4	A	908	GOL	O1-C1-C2-O2
4	A	909	GOL	O2-C2-C3-O3
5	B	912	EDO	O1-C1-C2-O2
4	A	905	GOL	O1-C1-C2-O2
4	B	904	GOL	O2-C2-C3-O3
4	A	909	GOL	O1-C1-C2-O2
4	B	904	GOL	O1-C1-C2-O2
4	A	907	GOL	O1-C1-C2-O2

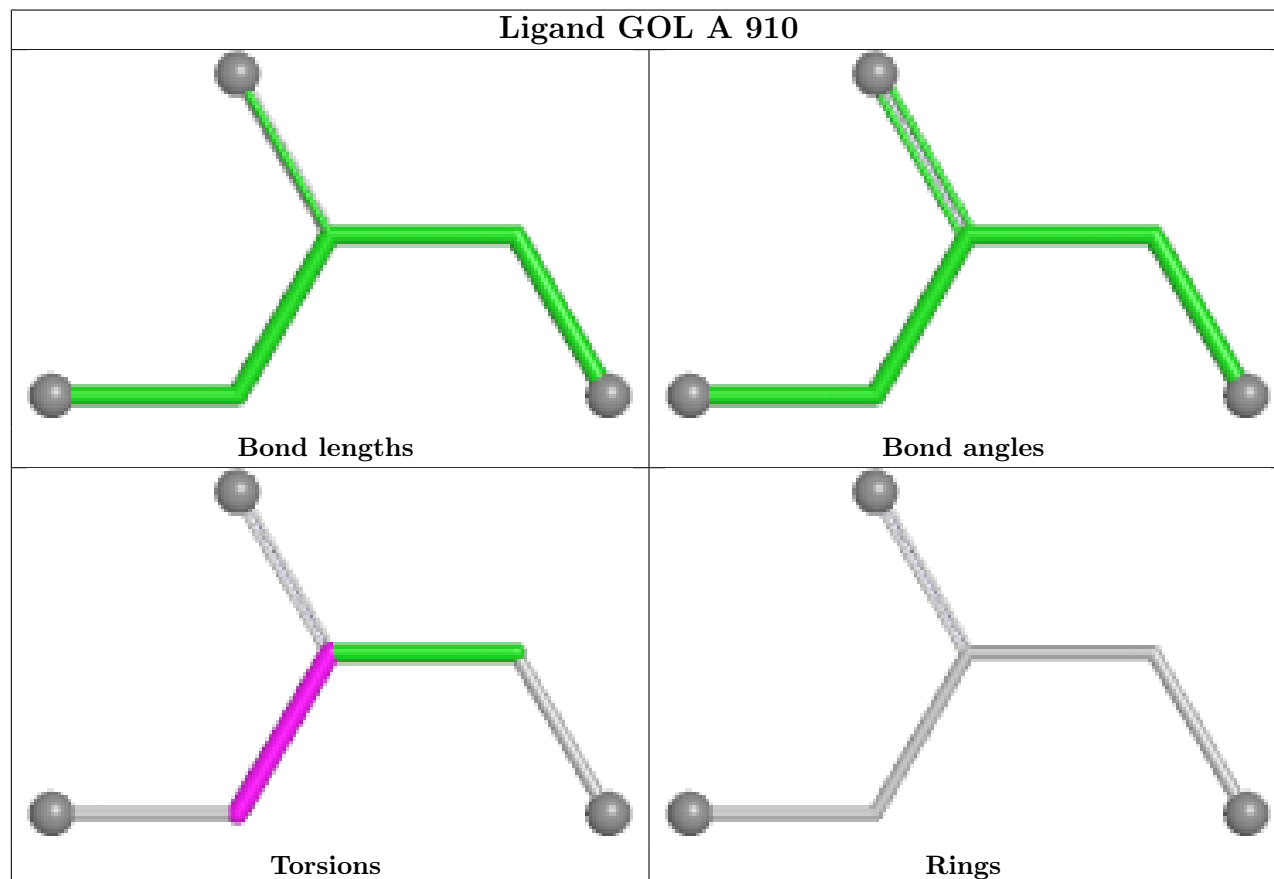
There are no ring outliers.

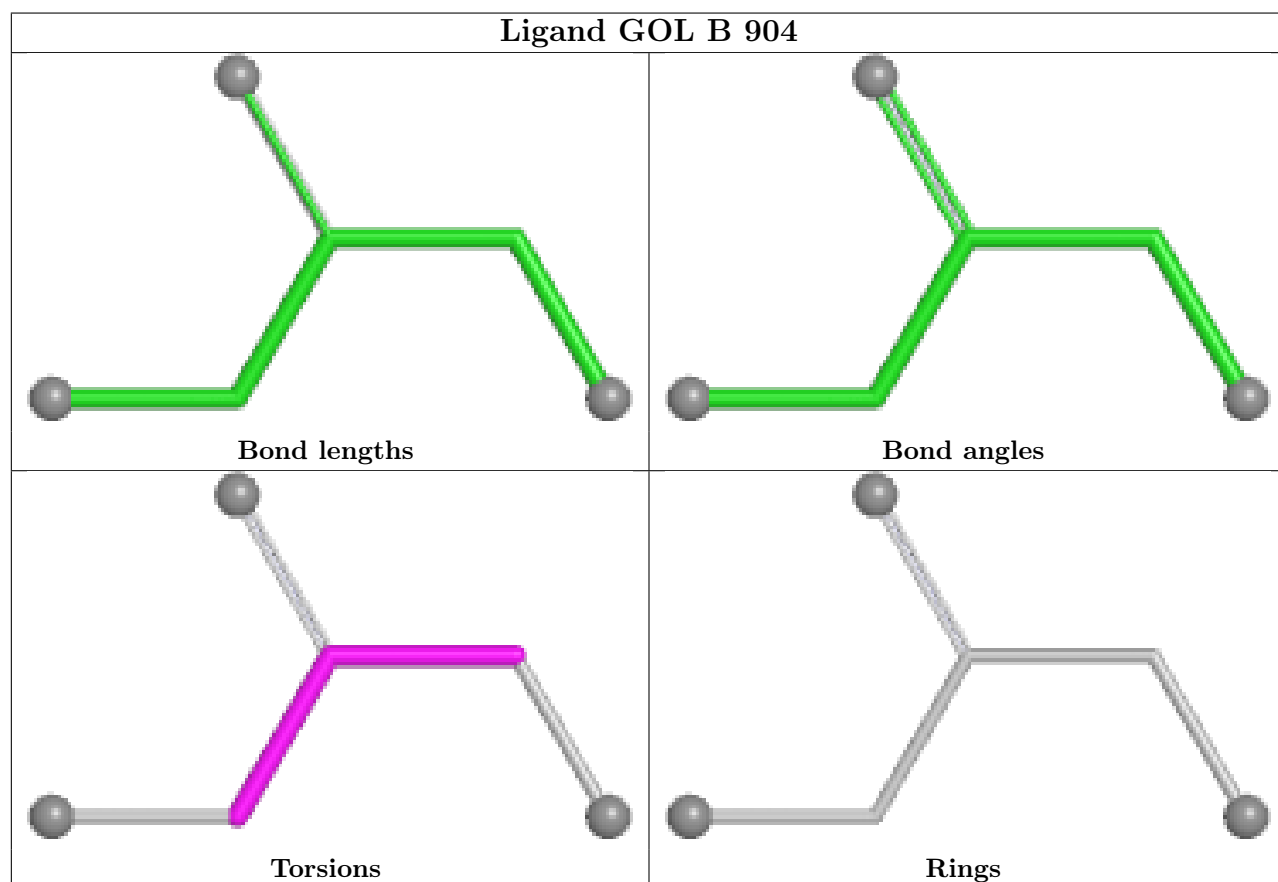
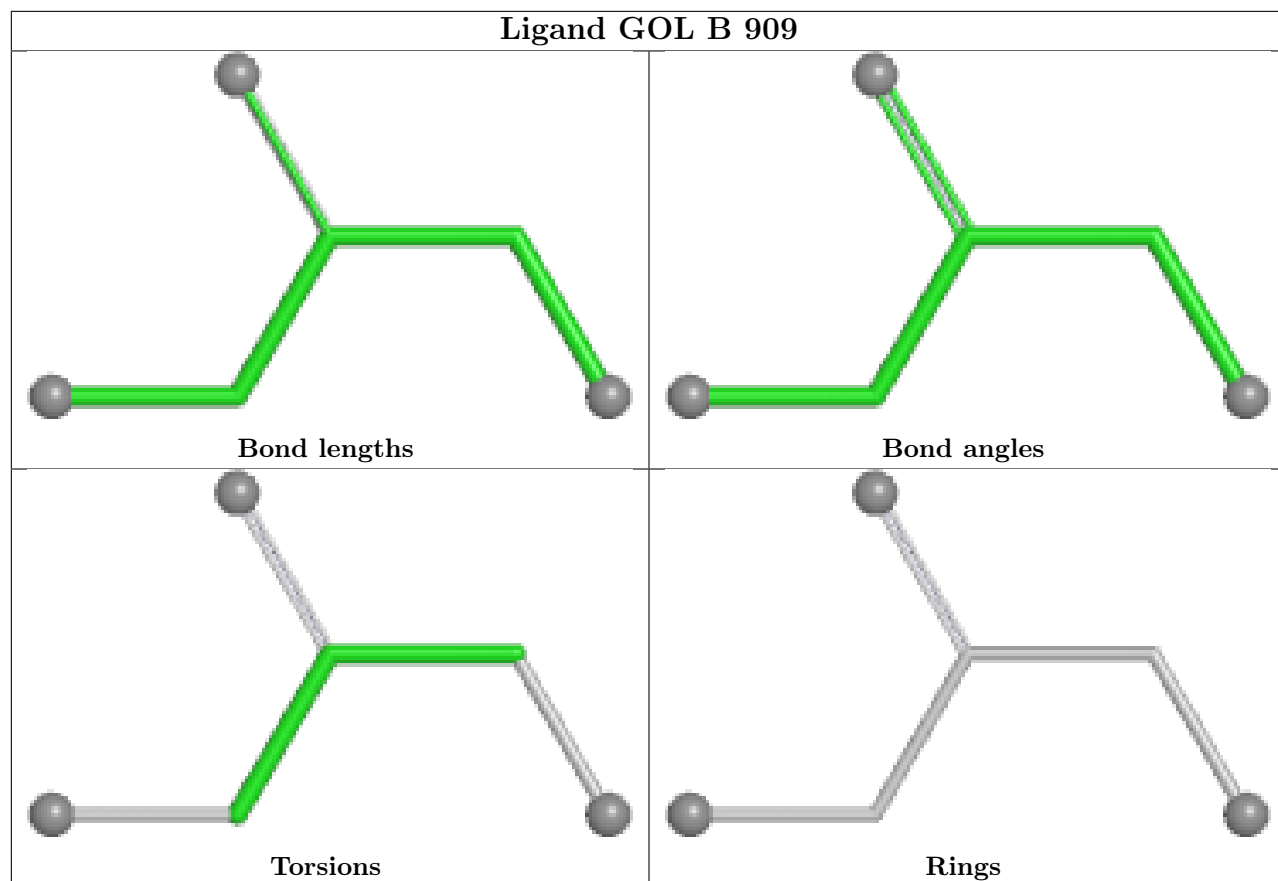
7 monomers are involved in 14 short contacts:

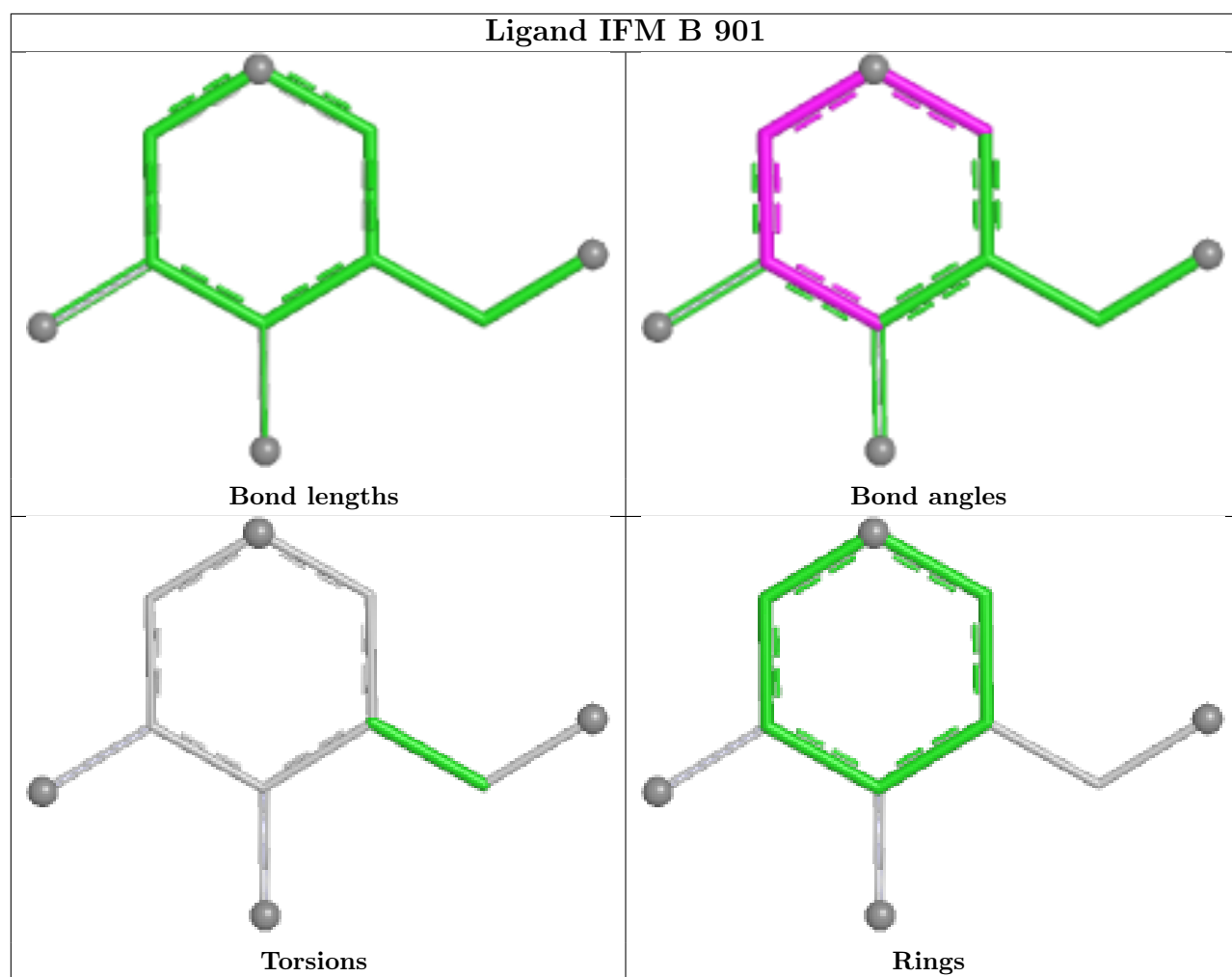
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	906	GOL	1	0
4	A	906	GOL	1	0
4	A	908	GOL	2	0
5	B	912	EDO	2	0
5	A	913	EDO	3	0
4	B	905	GOL	2	0
4	A	912	GOL	3	0

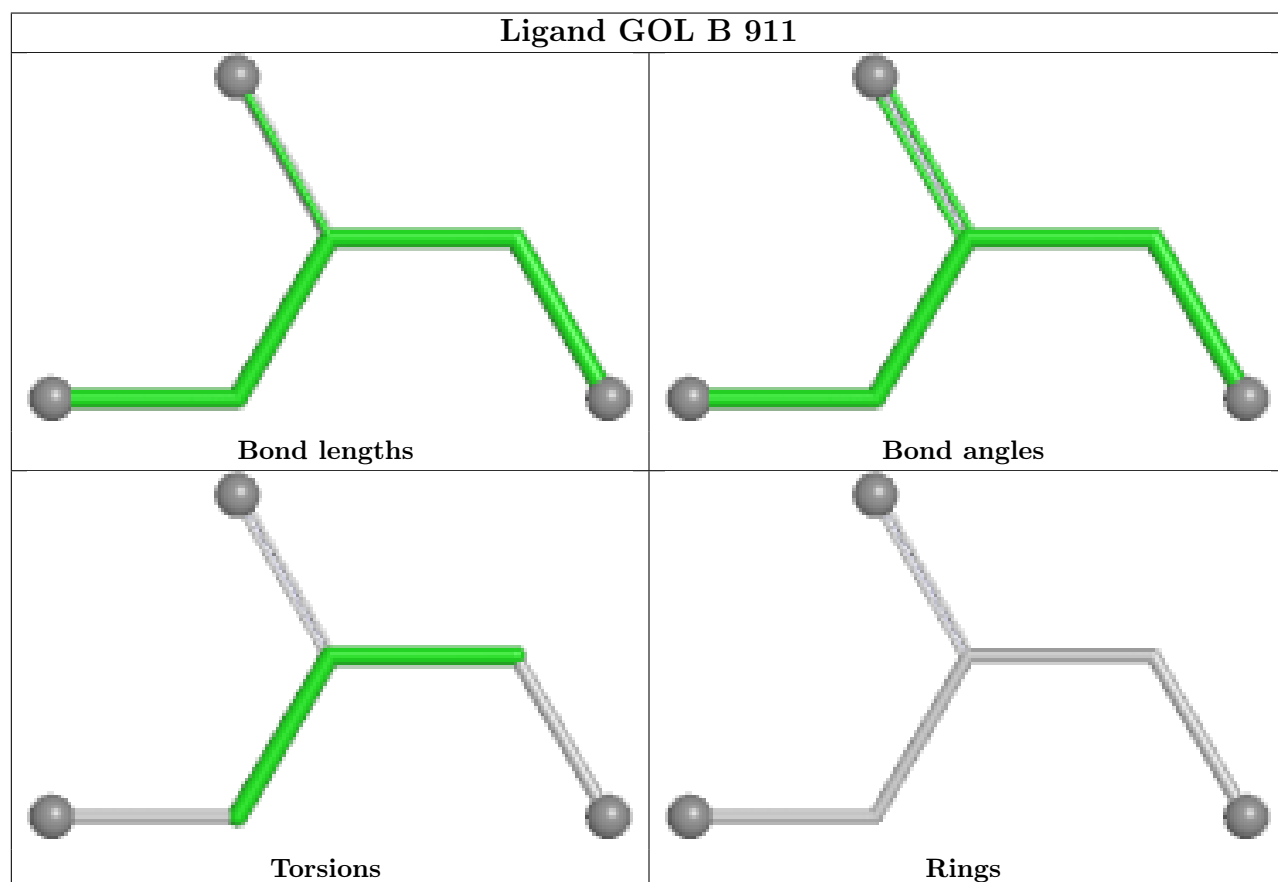
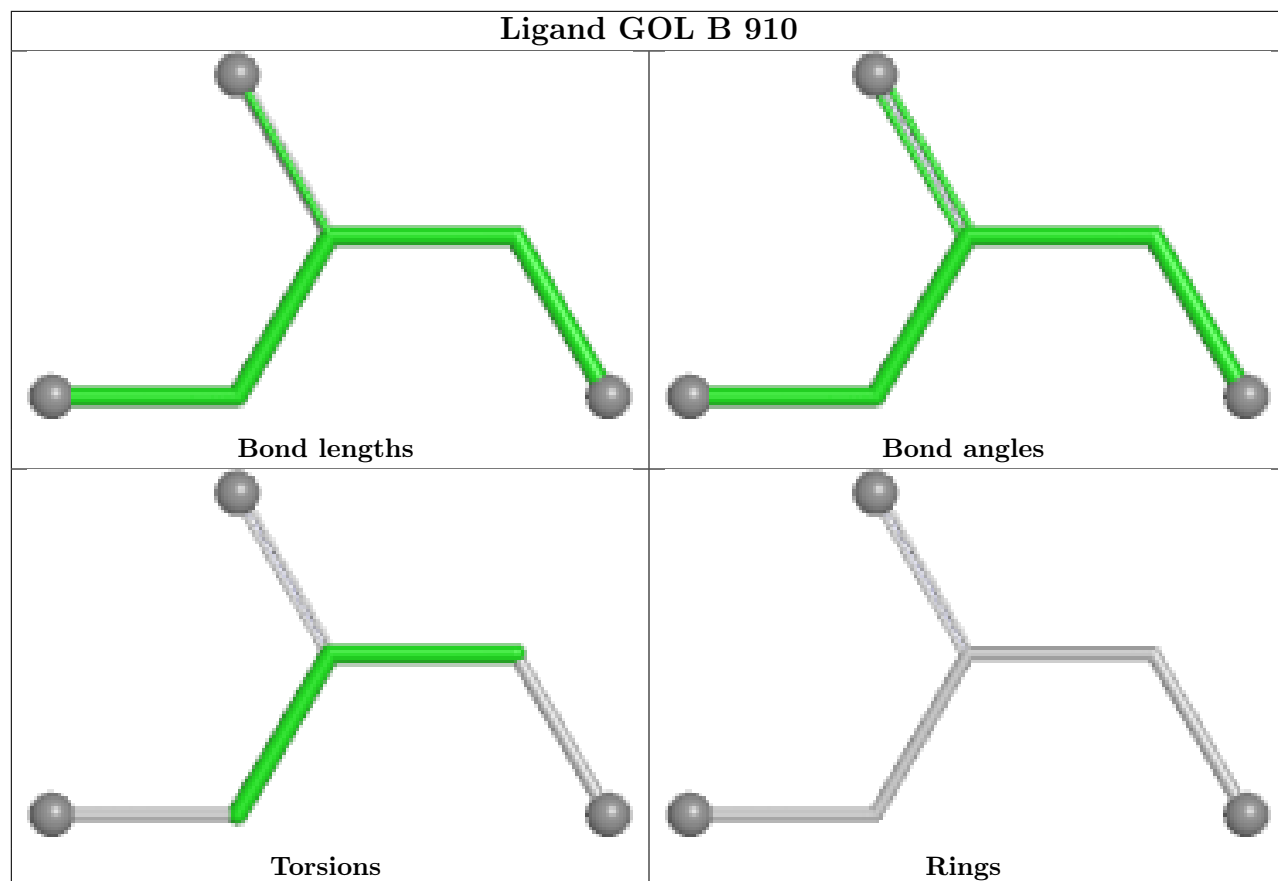
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

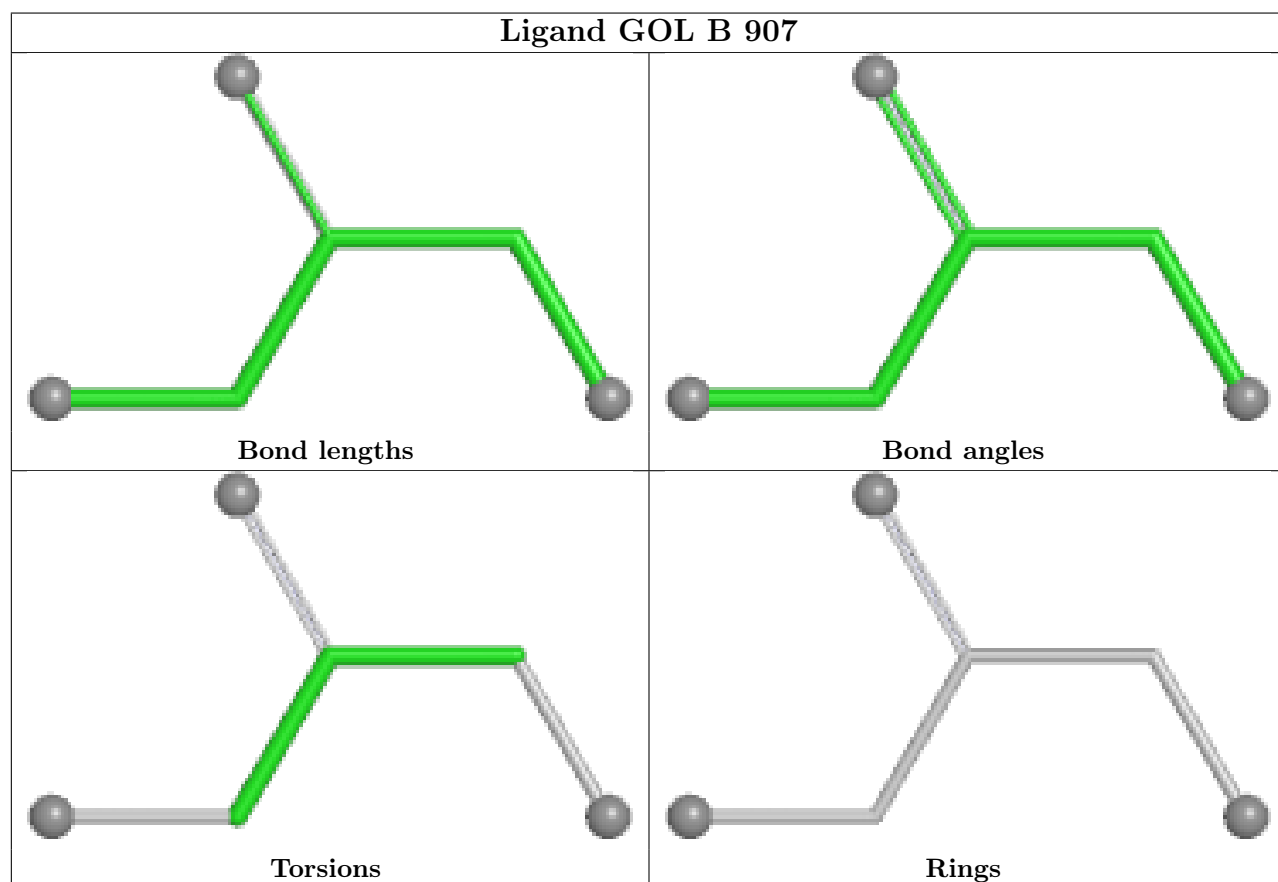
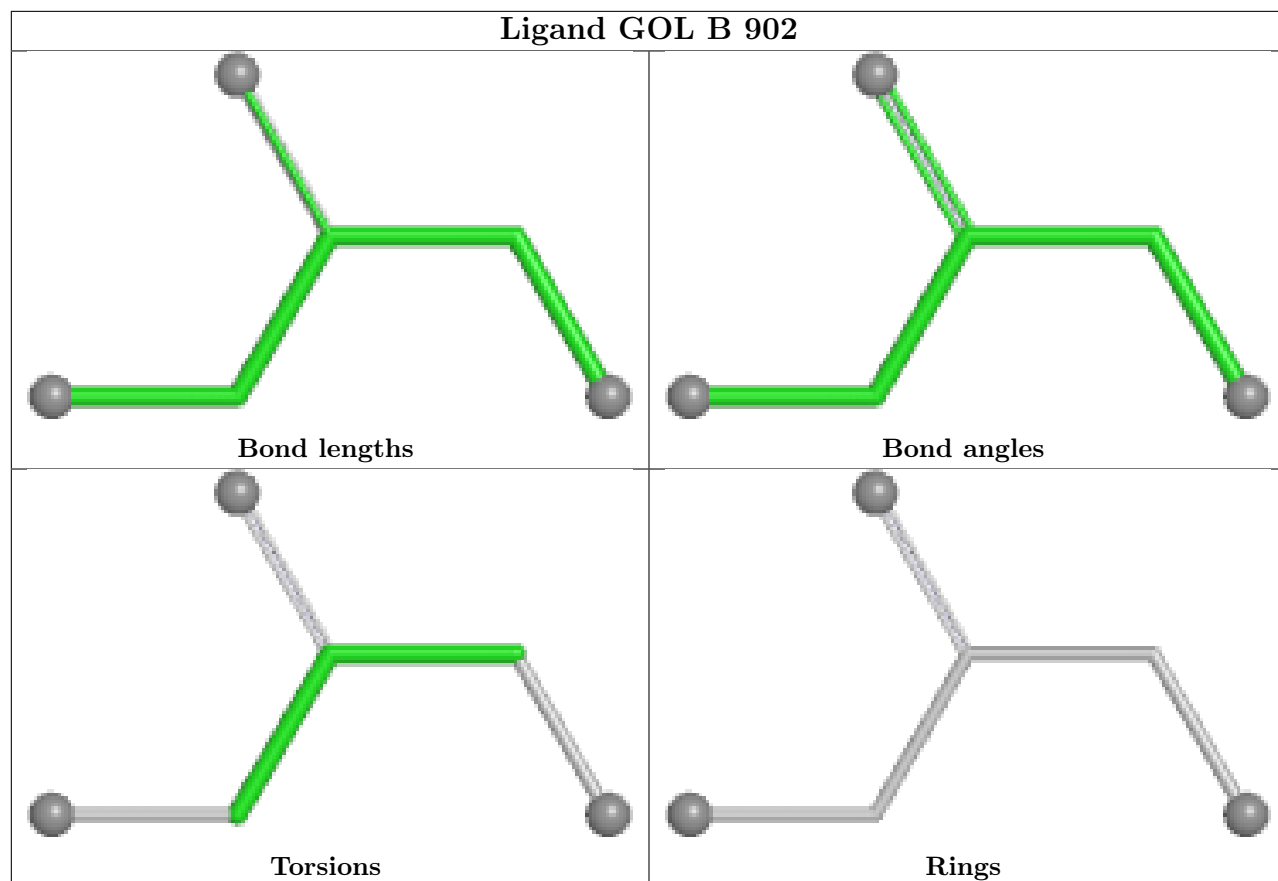
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

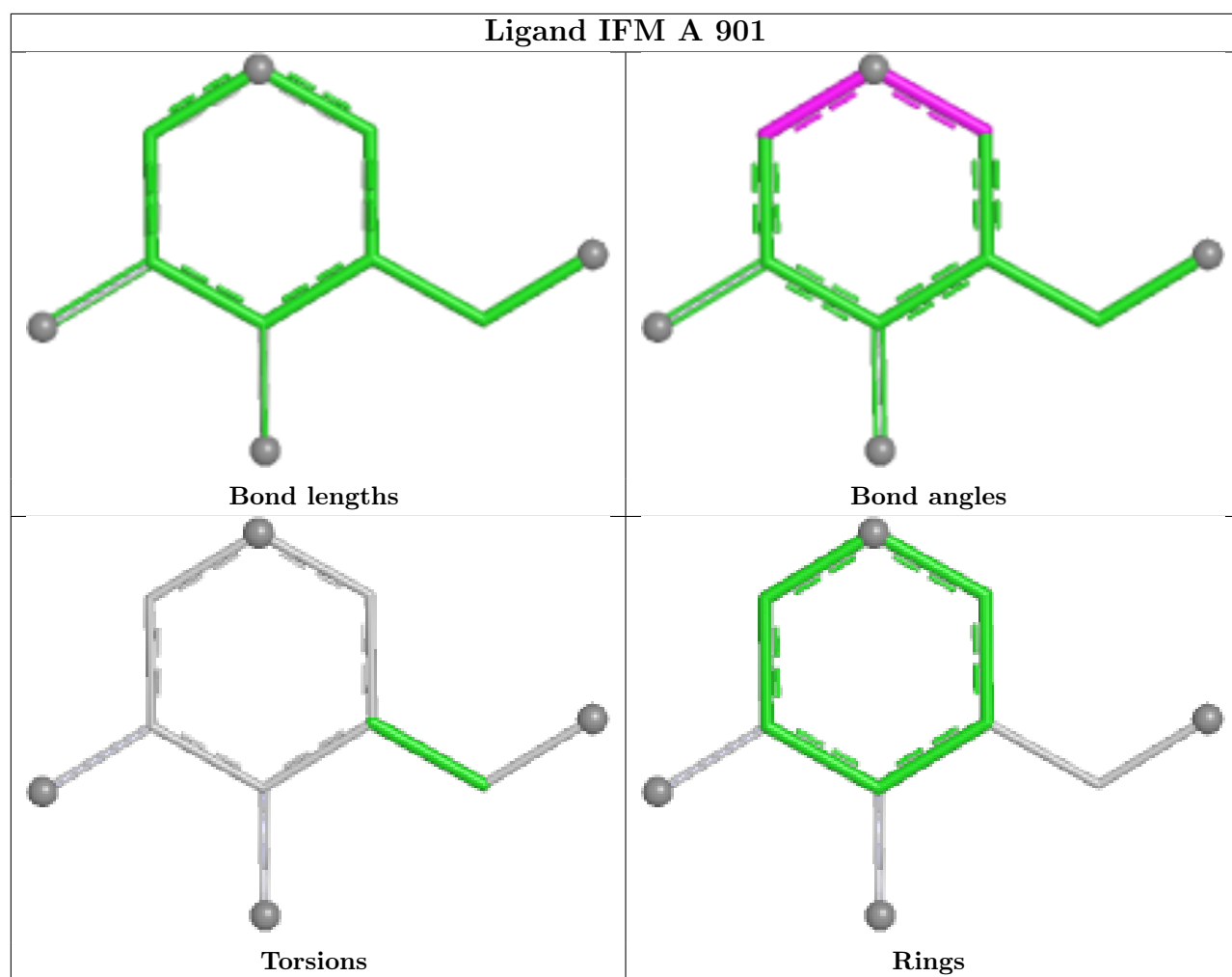


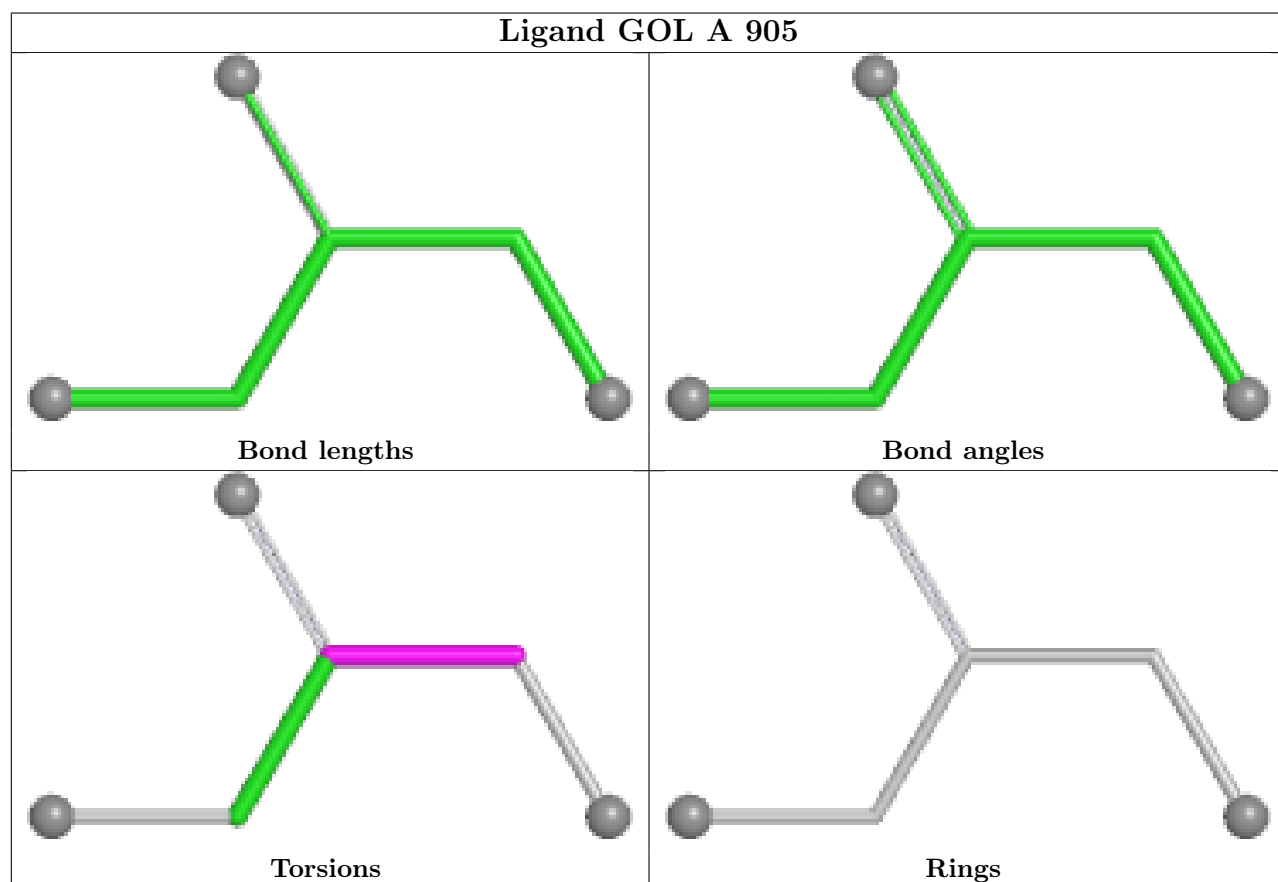
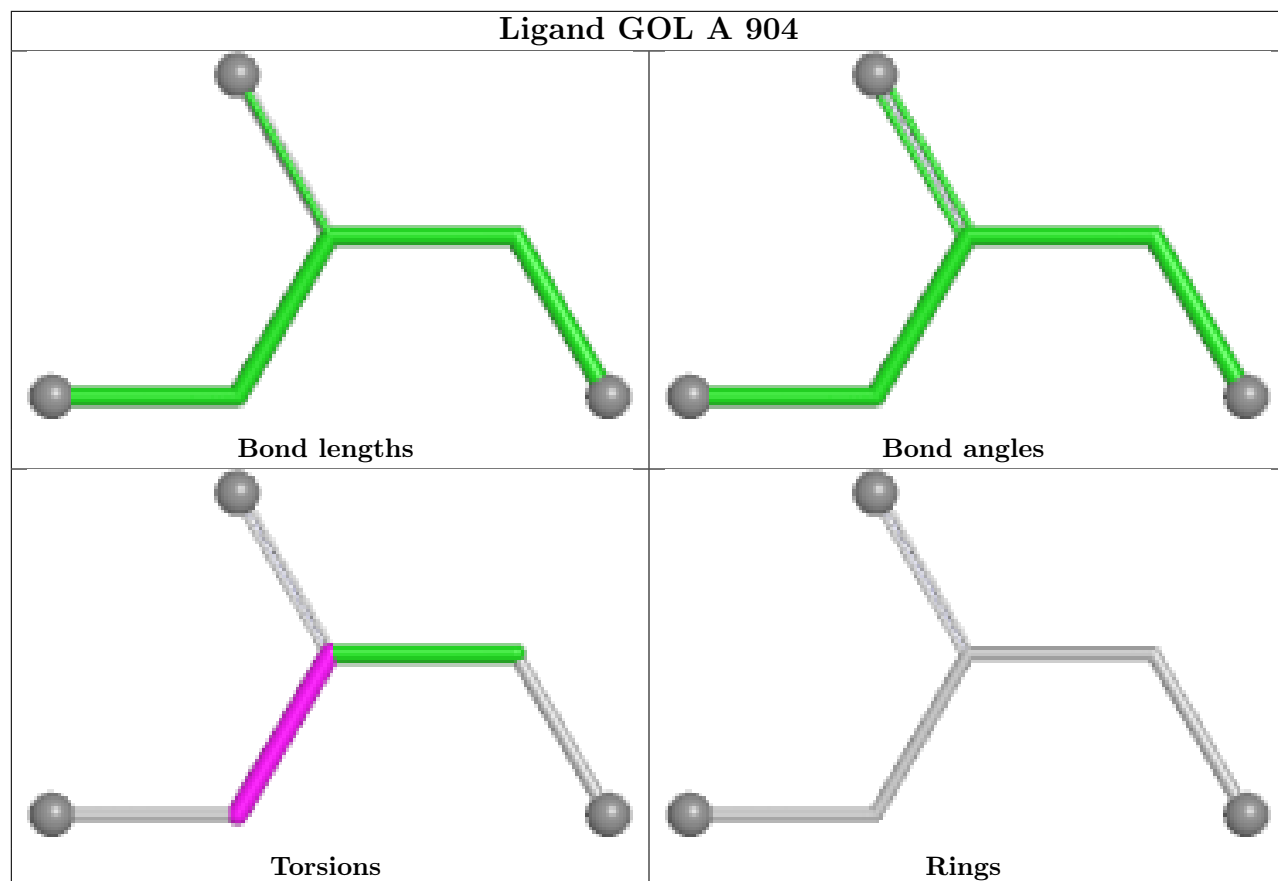


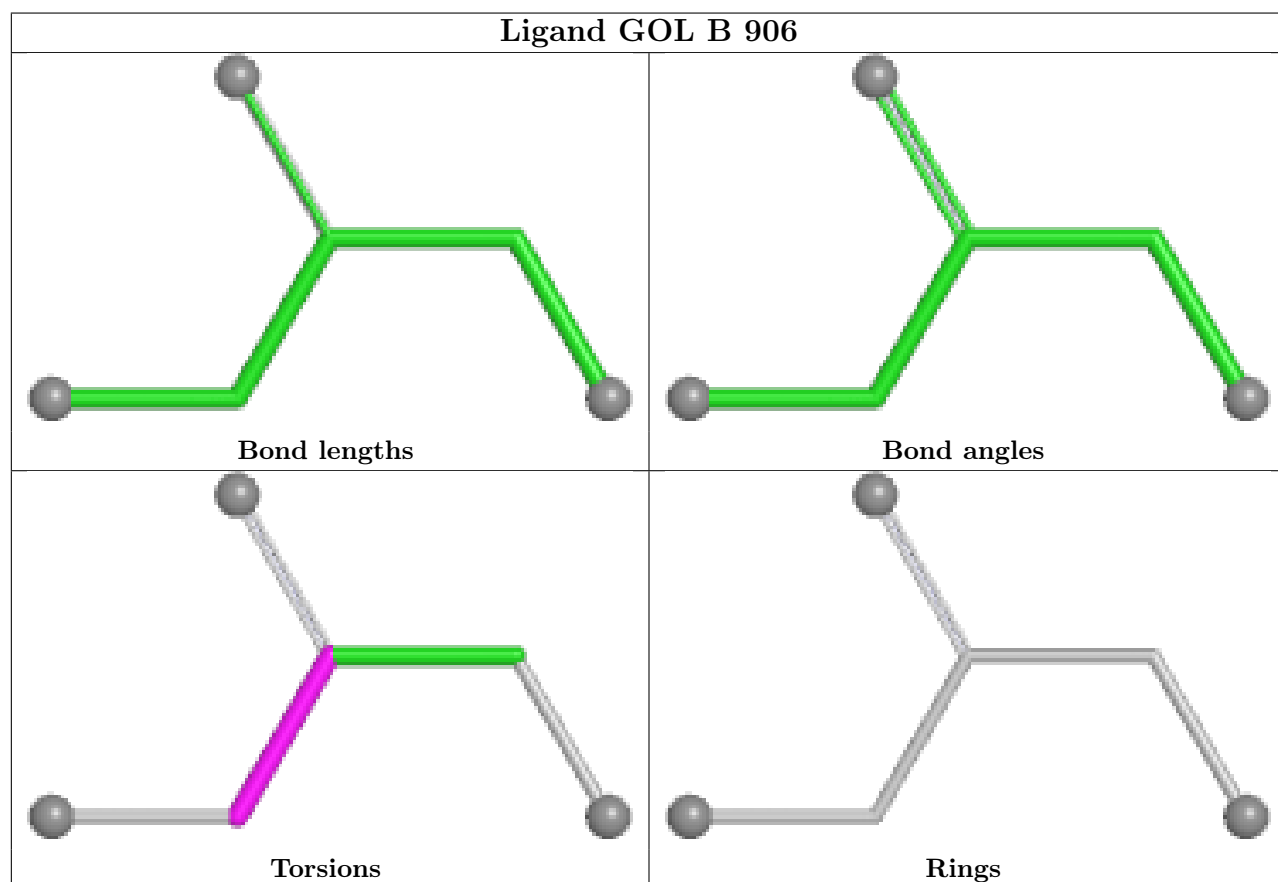
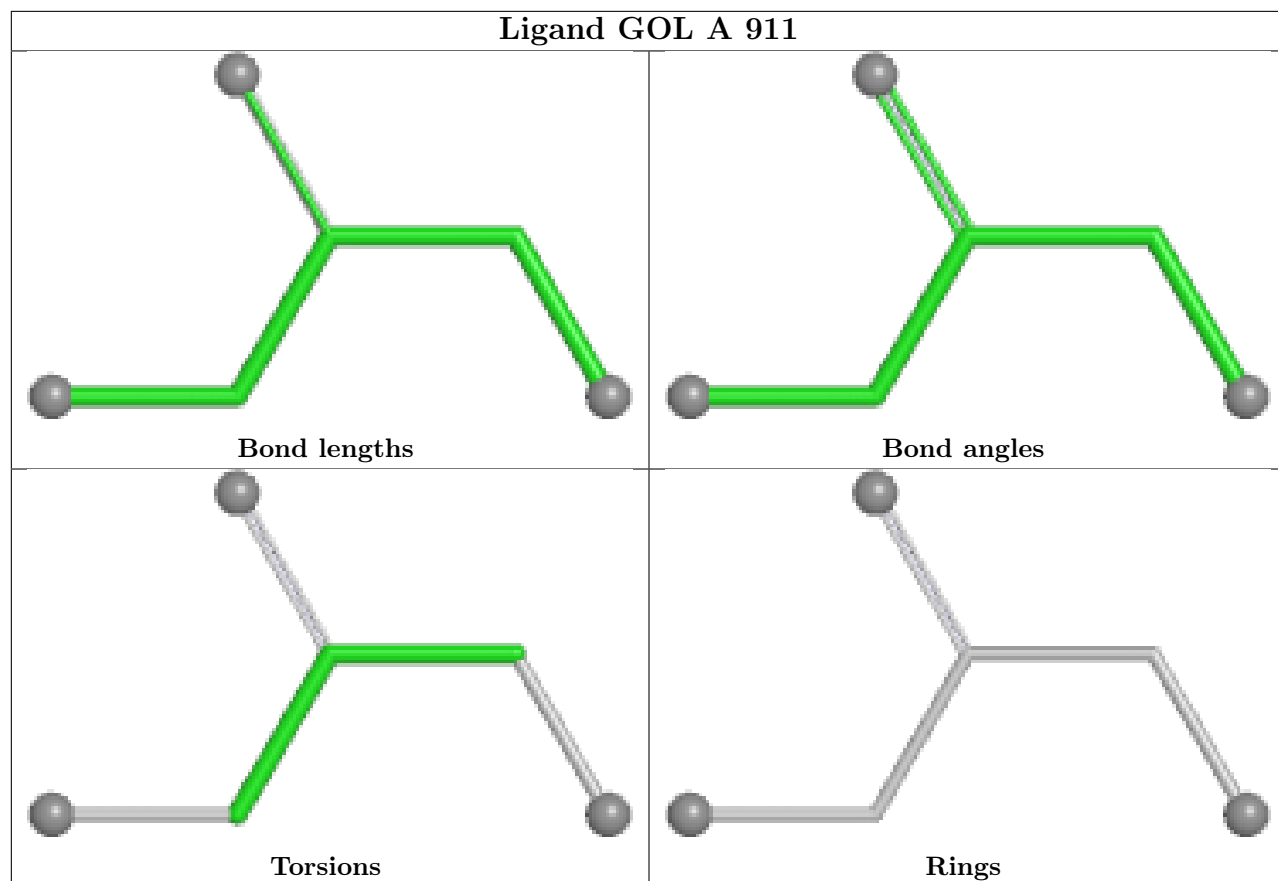


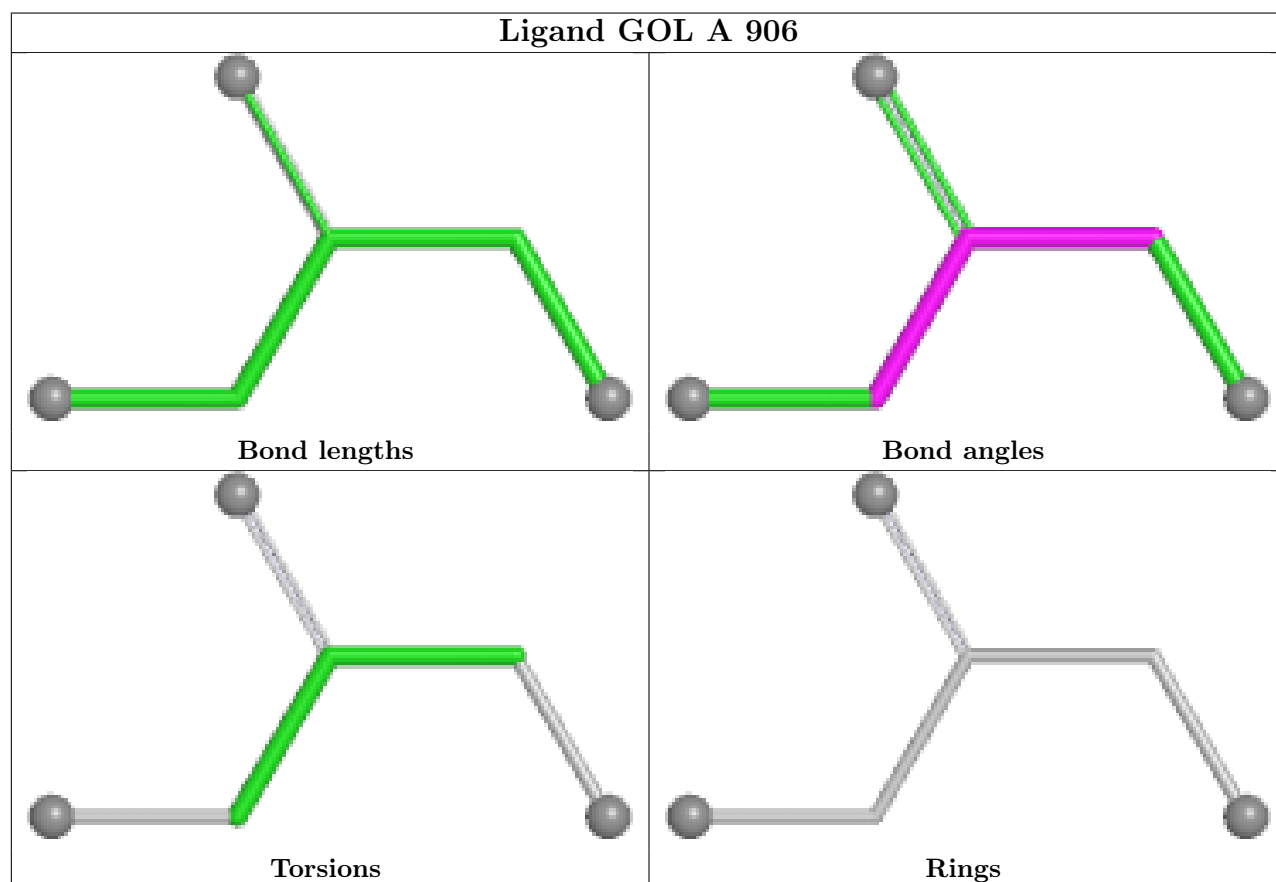
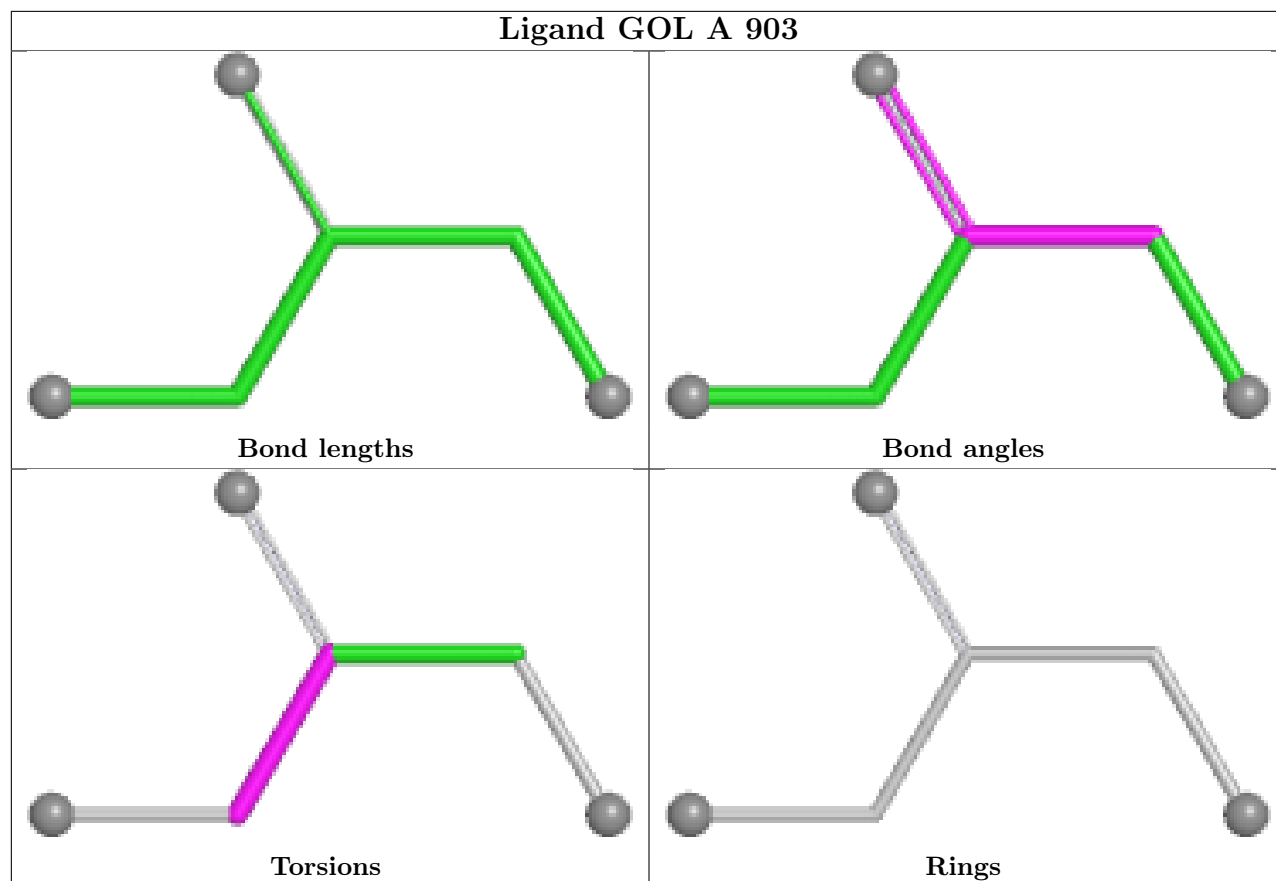


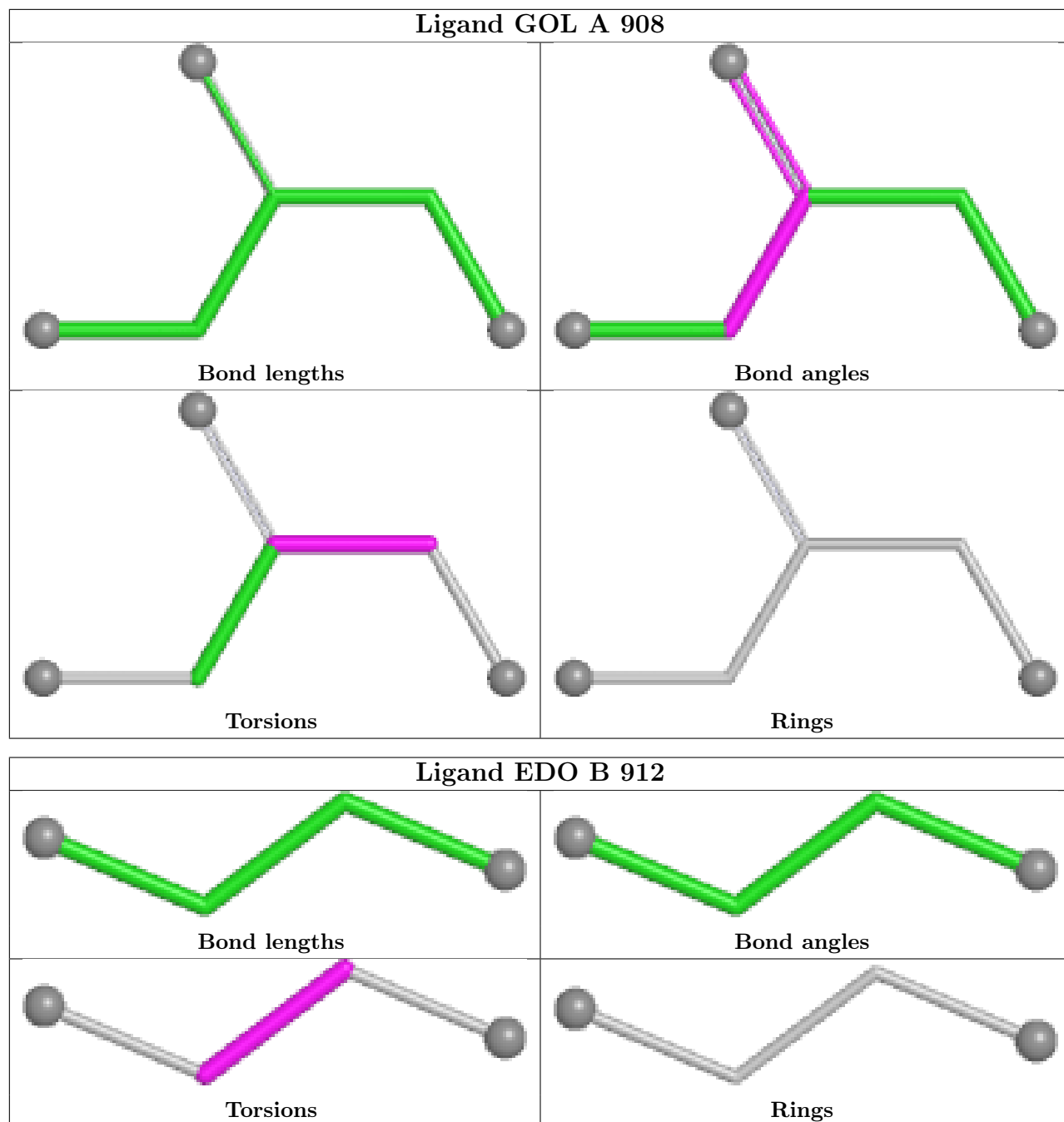


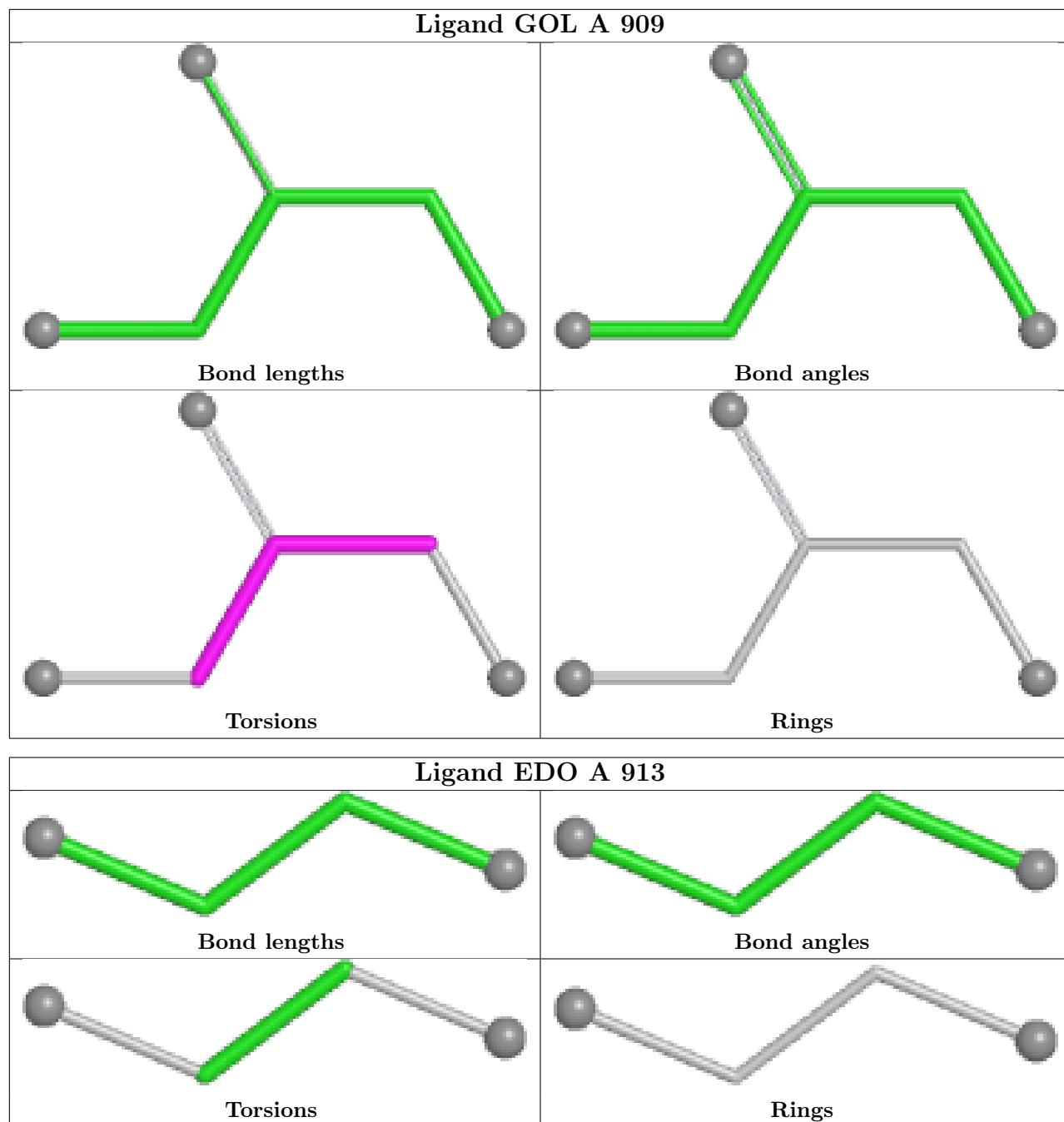


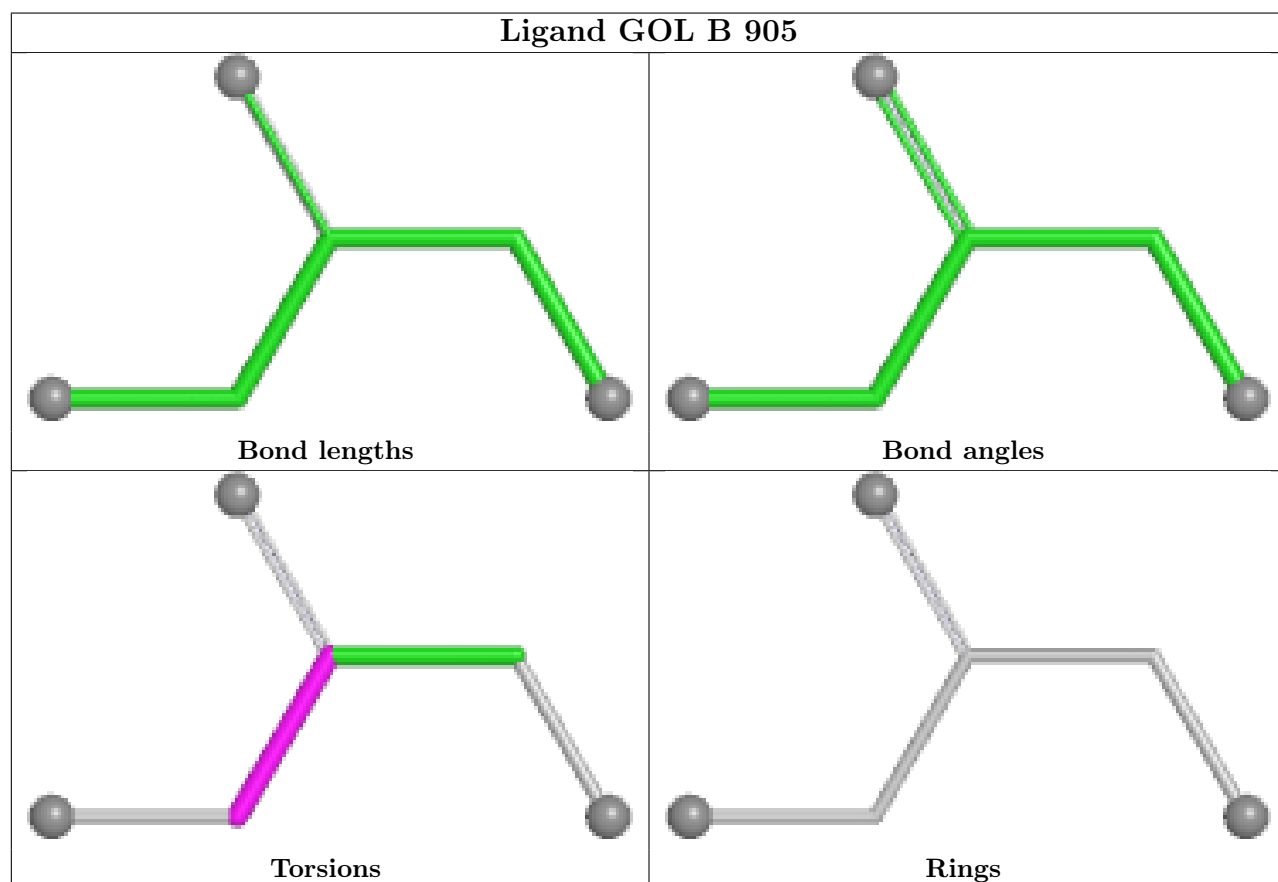
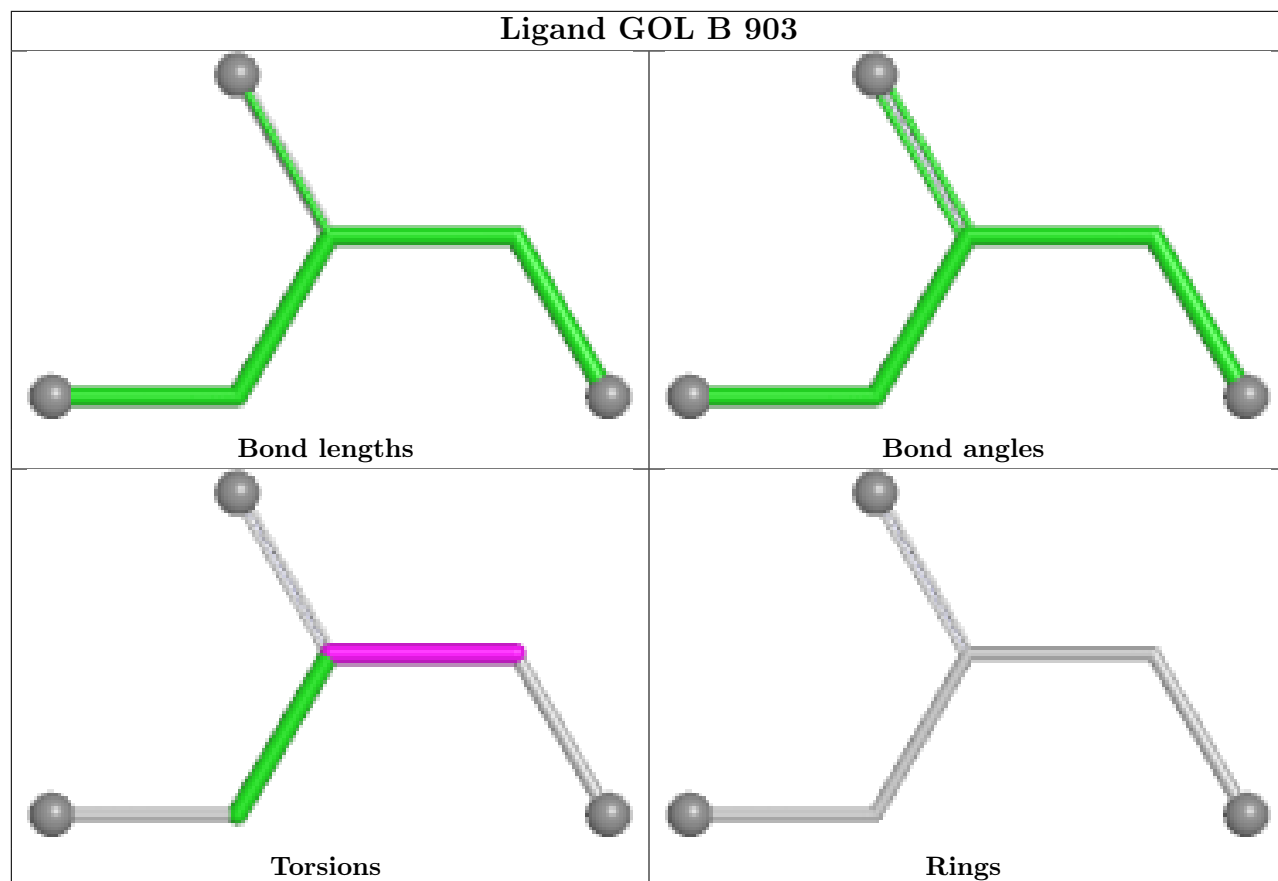


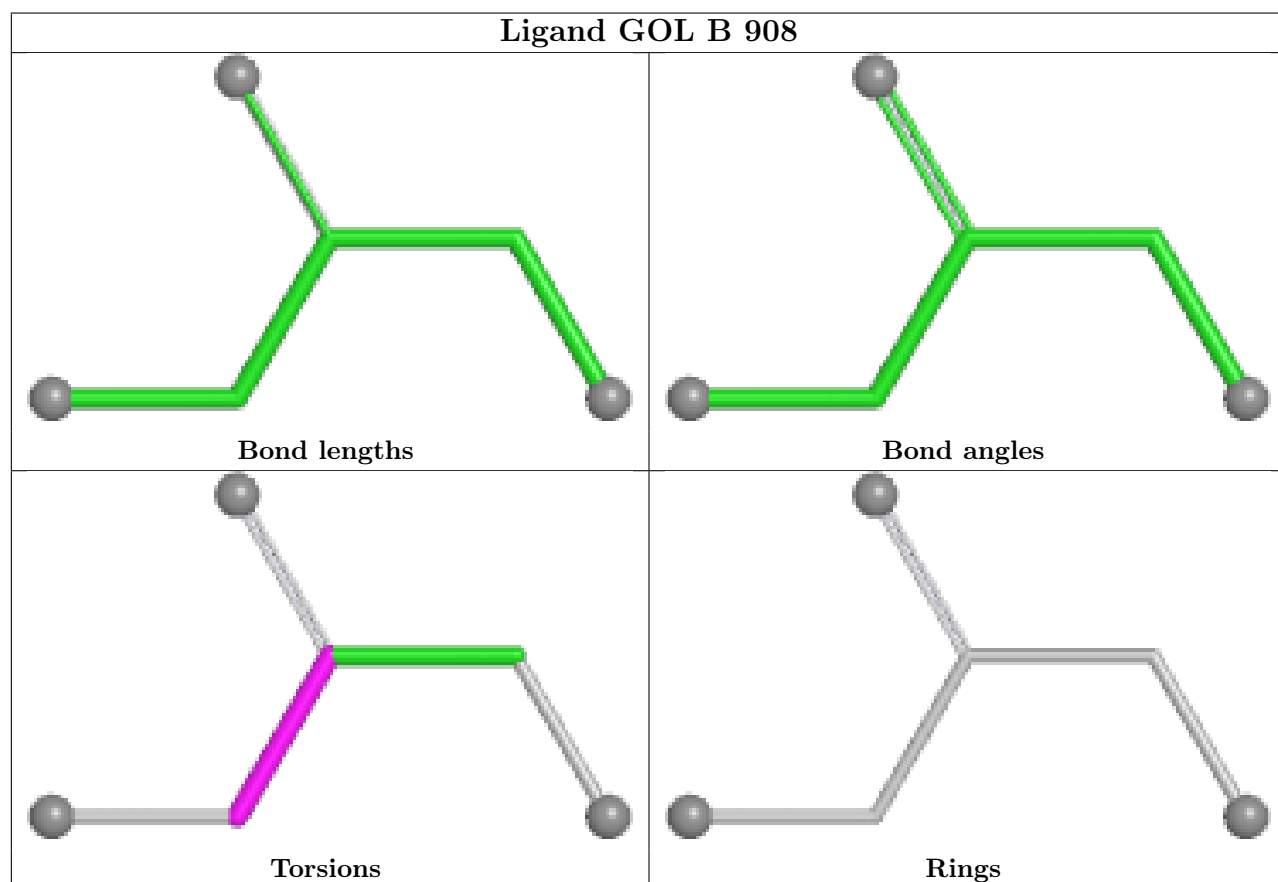
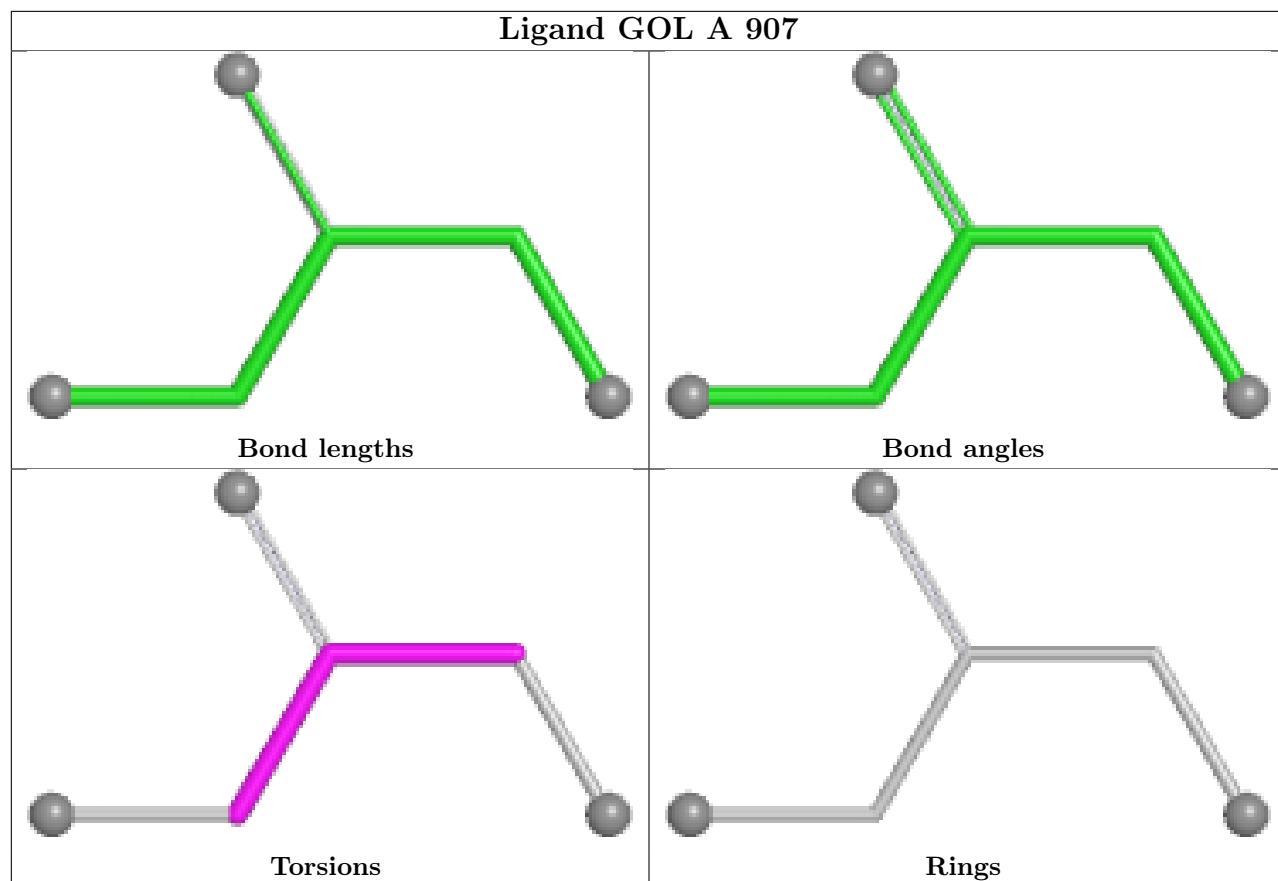


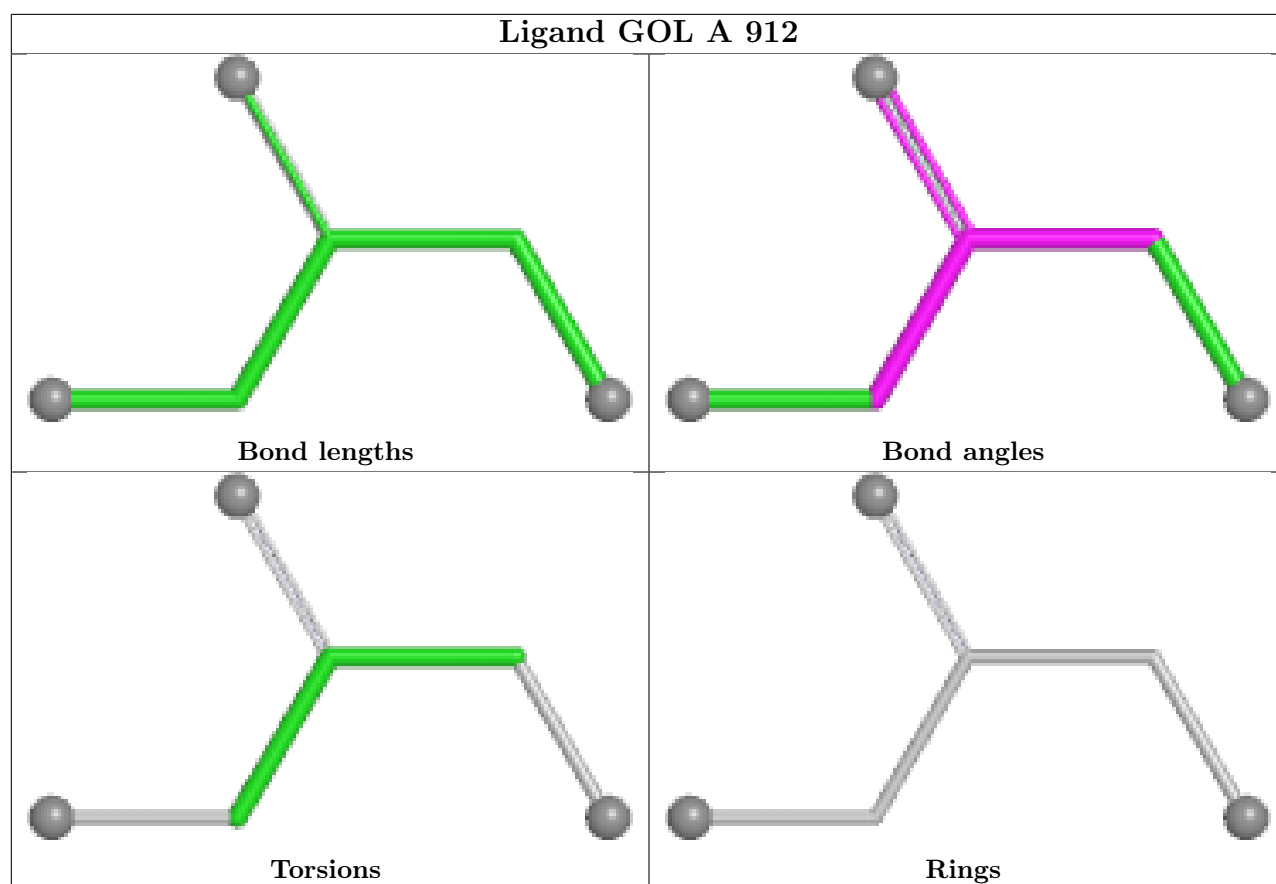












5.7 Other polymers [i](#)

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	769/798 (96%)	-0.33	16 (2%)	63 63	7, 18, 41, 80	2 (0%)
1	B	769/798 (96%)	-0.26	16 (2%)	63 63	6, 19, 43, 69	3 (0%)
All	All	1538/1596 (96%)	-0.30	32 (2%)	63 63	6, 19, 42, 80	5 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	GLN	3.9
1	A	242	LYS	3.8
1	A	243	ASP	3.6
1	B	244	SER	3.6
1	A	244	SER	3.4
1	A	54	ASN	3.2
1	B	35	HIS	3.2
1	A	62	TYR	3.1
1	A	241	SER	3.0
1	B	33	ILE	3.0
1	B	226	VAL	3.0
1	B	242	LYS	2.9
1	B	626	GLU	2.9
1	A	240	LYS	2.9
1	B	241	SER	2.9
1	A	35	HIS	2.9
1	A	745	TYR	2.7
1	B	243	ASP	2.7
1	B	745	TYR	2.7
1	A	136	GLY	2.6
1	B	625	ASN	2.5
1	B	54	ASN	2.4
1	B	119	GLY	2.3
1	A	427	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	659	ASP	2.2
1	A	431	LYS	2.2
1	A	61	LYS	2.2
1	A	119	GLY	2.1
1	B	431	LYS	2.1
1	A	587	ILE	2.0
1	B	38	ASP	2.0
1	B	32	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

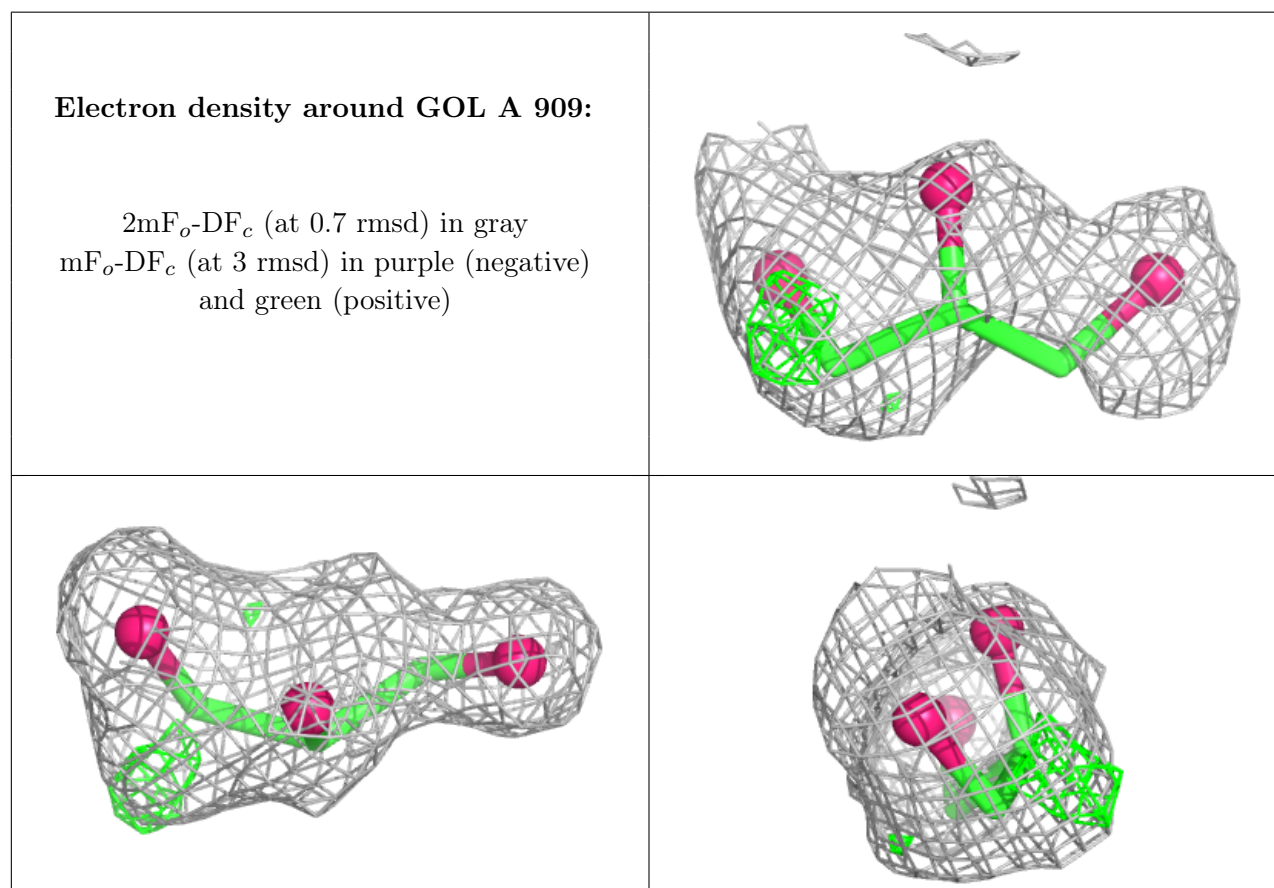
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	909	6/6	0.75	0.17	45,47,51,52	0
4	GOL	B	909	6/6	0.76	0.25	43,44,48,53	0
4	GOL	B	906	6/6	0.77	0.20	35,43,50,51	0
4	GOL	B	910	6/6	0.79	0.14	60,63,63,64	0
4	GOL	A	906	6/6	0.80	0.18	38,45,46,48	0
4	GOL	A	905	6/6	0.80	0.16	31,43,44,50	0
4	GOL	B	904	6/6	0.80	0.14	39,44,48,52	0
4	GOL	A	912	6/6	0.82	0.16	44,45,46,47	0
4	GOL	A	911	6/6	0.83	0.16	37,45,49,54	0
4	GOL	B	911	6/6	0.83	0.15	40,43,47,54	0
4	GOL	B	905	6/6	0.85	0.14	28,30,33,35	0
4	GOL	A	907	6/6	0.87	0.12	43,44,46,46	0
4	GOL	A	908	6/6	0.87	0.18	35,41,46,47	0
4	GOL	B	907	6/6	0.87	0.13	45,46,47,48	0
5	EDO	B	912	4/4	0.87	0.30	26,29,31,40	0

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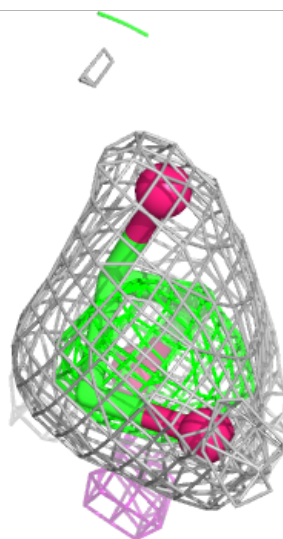
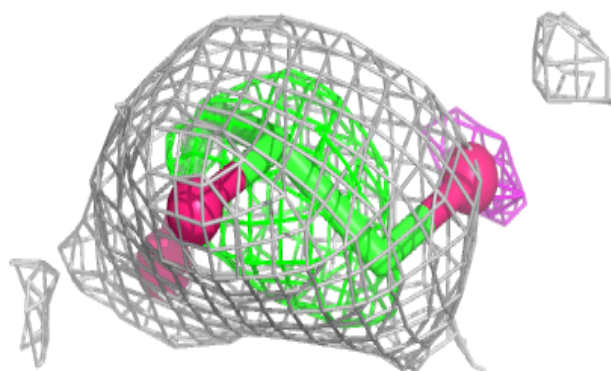
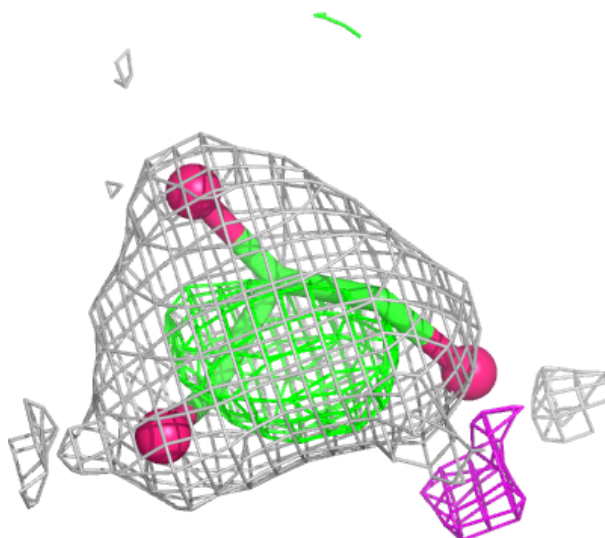
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	910	6/6	0.88	0.13	39,42,46,49	0
4	GOL	B	908	6/6	0.88	0.12	36,41,43,45	0
4	GOL	A	903	6/6	0.90	0.11	23,27,29,30	0
4	GOL	B	902	6/6	0.91	0.10	23,26,26,31	0
5	EDO	A	913	4/4	0.91	0.21	27,28,30,33	0
4	GOL	A	904	6/6	0.91	0.10	23,26,27,28	0
4	GOL	B	903	6/6	0.93	0.08	25,28,31,32	0
3	CA	B	913	1/1	0.96	0.05	32,32,32,32	0
2	IFM	B	901	10/10	0.97	0.05	12,14,15,15	0
2	IFM	A	901	10/10	0.98	0.04	12,12,13,13	0
3	CA	A	914	1/1	0.99	0.04	25,25,25,25	0
3	CA	A	902	1/1	0.99	0.02	26,26,26,26	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.



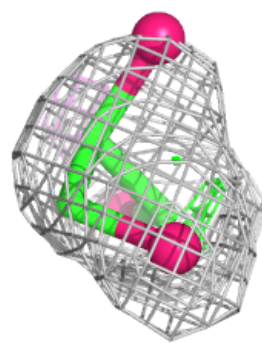
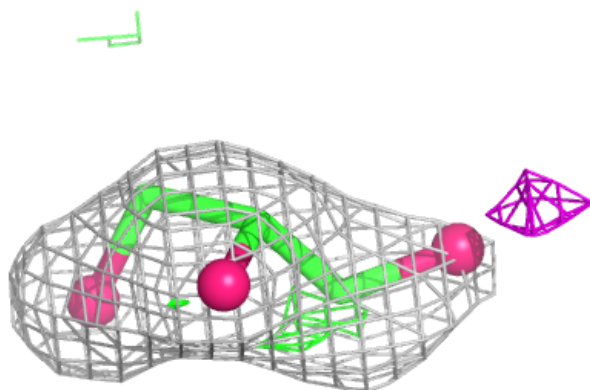
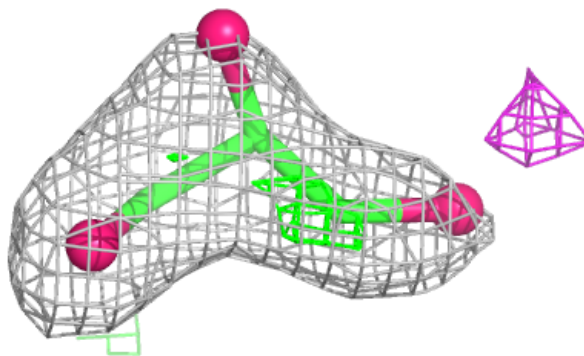
Electron density around GOL B 909:

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

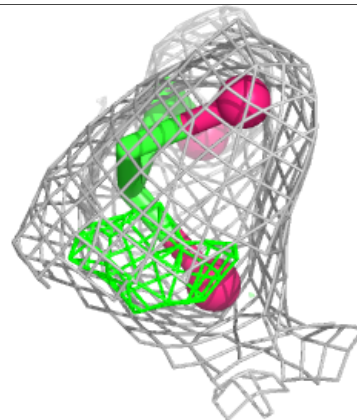
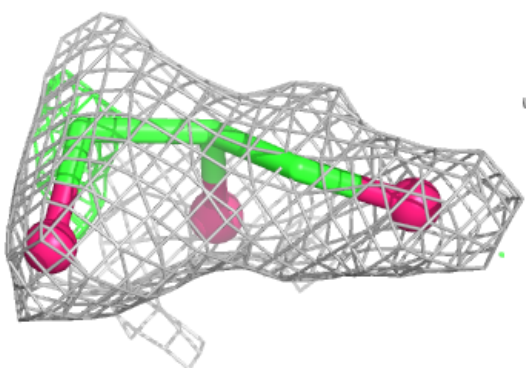
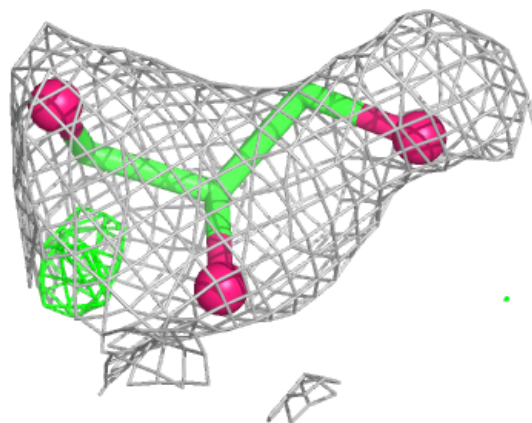


Electron density around GOL B 906:

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and green (positive)

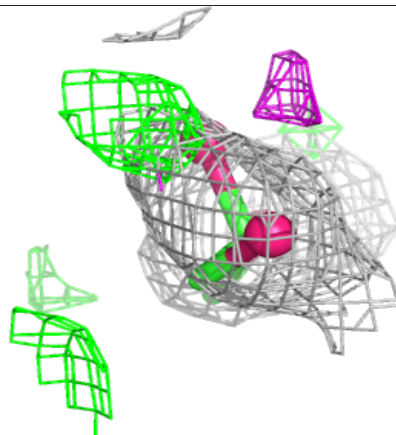
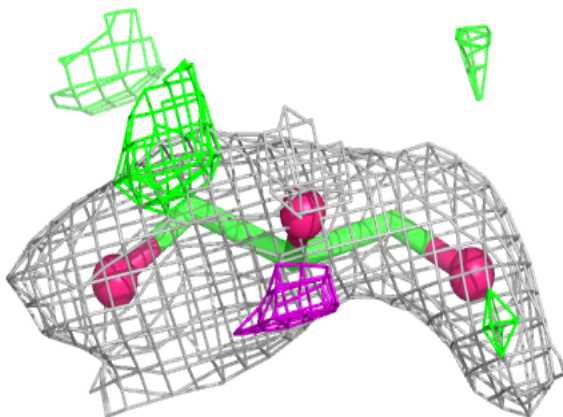
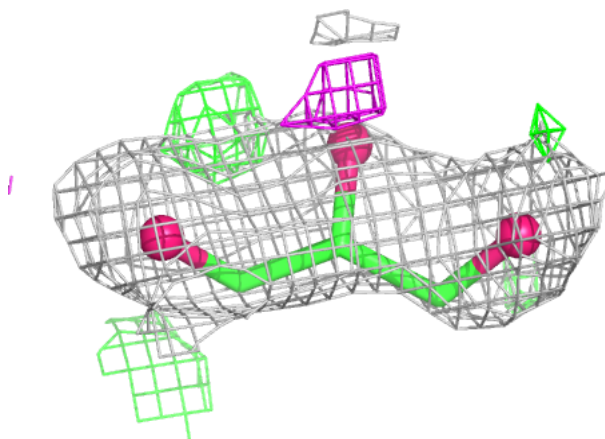
**Electron density around GOL B 910:**

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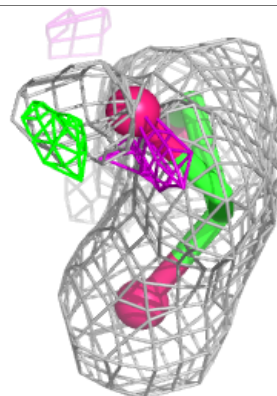
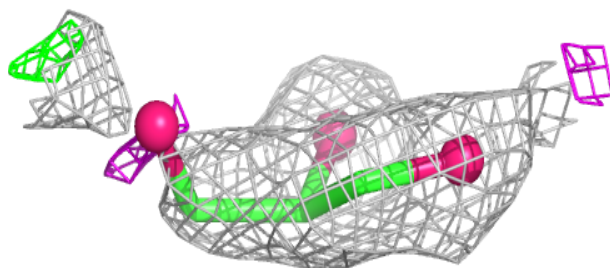
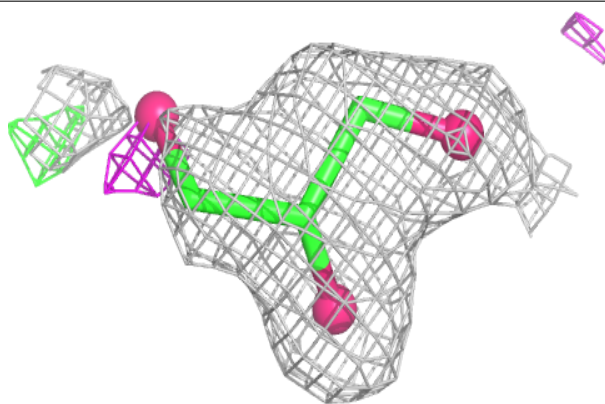


Electron density around GOL A 906:

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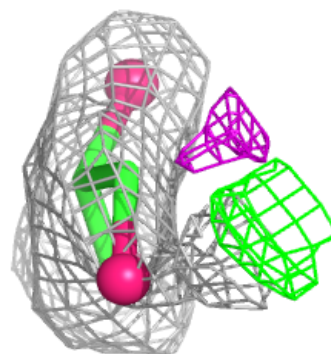
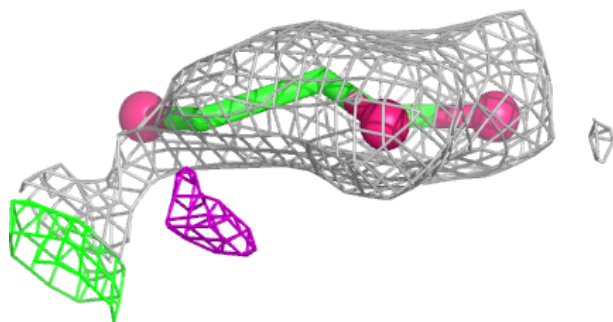
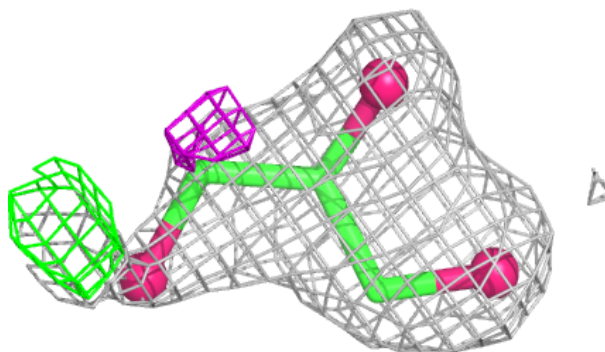
**Electron density around GOL A 905:**

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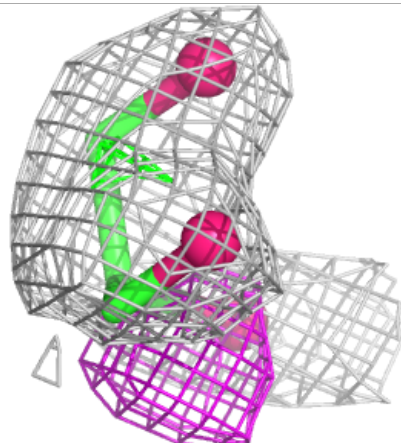
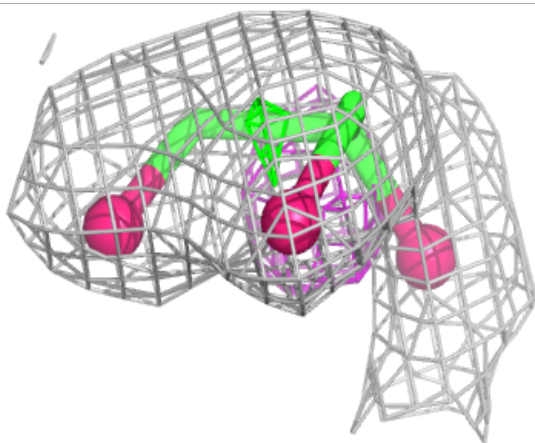
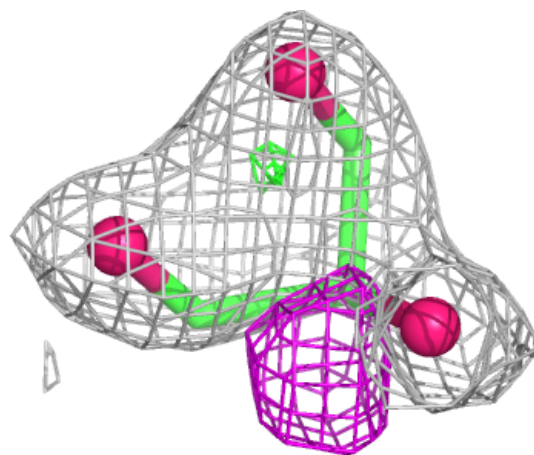
Electron density around GOL B 904:

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and green (positive)



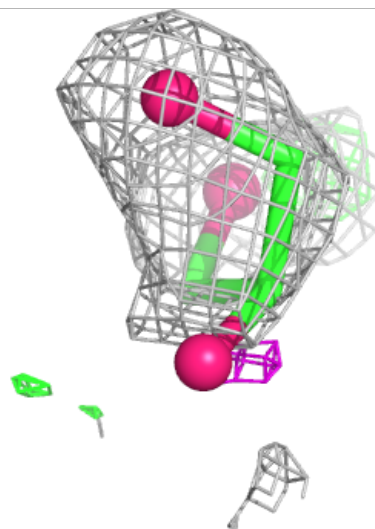
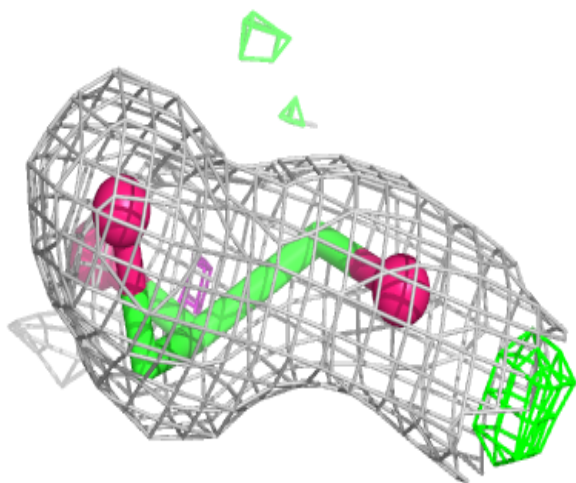
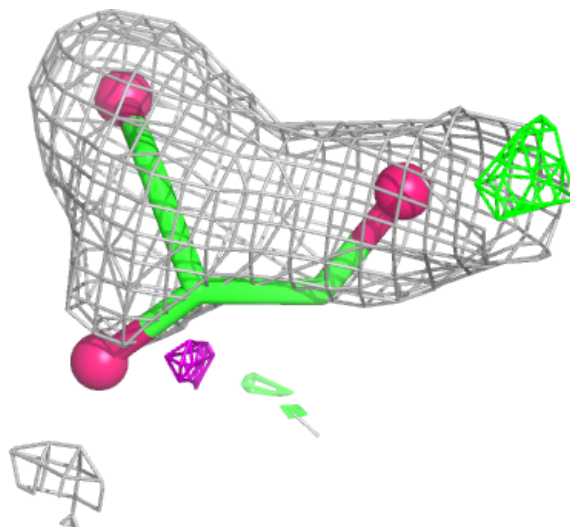
Electron density around GOL A 912:

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and green (positive)



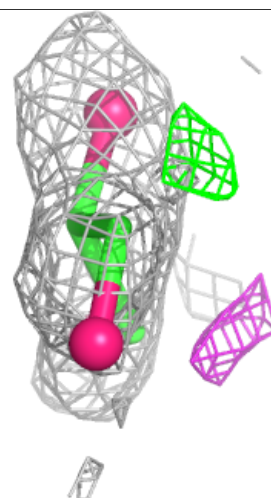
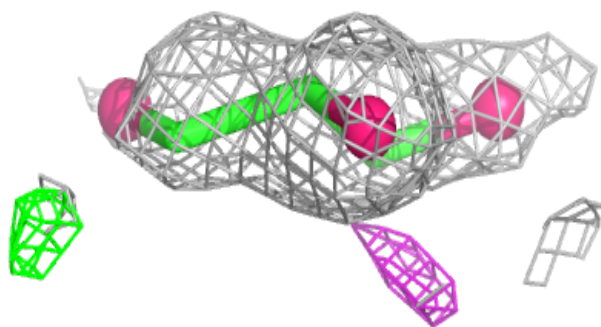
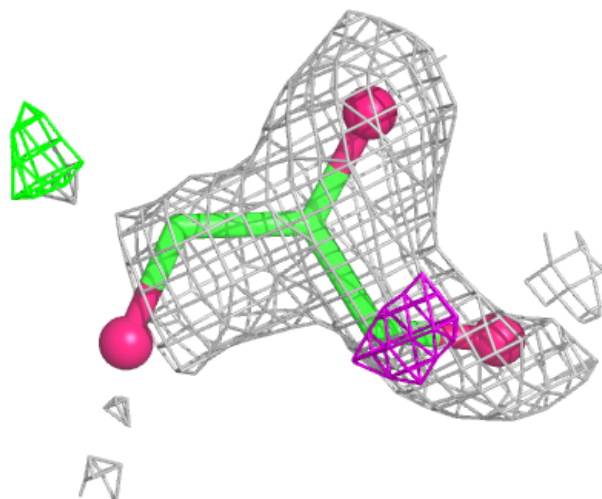
Electron density around GOL A 911:

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



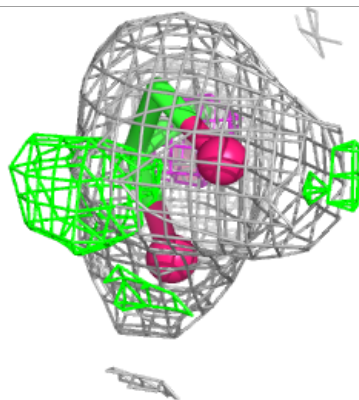
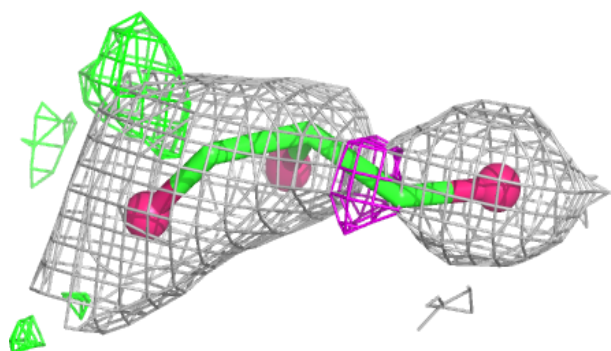
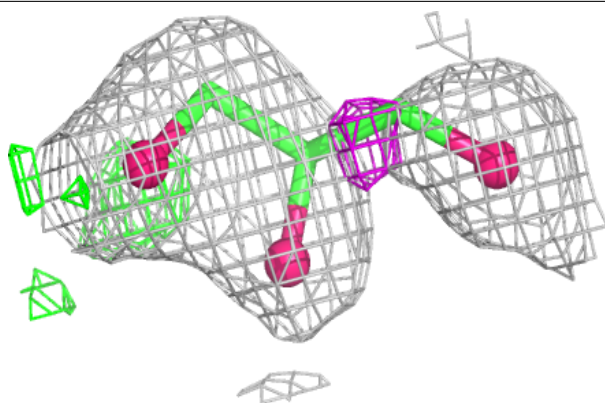
Electron density around GOL B 911:

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

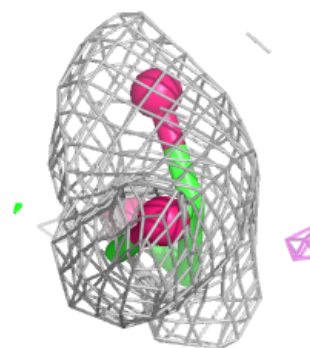
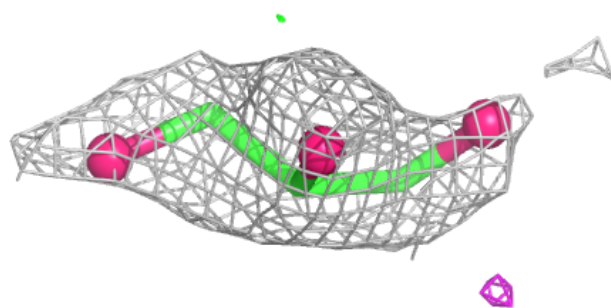
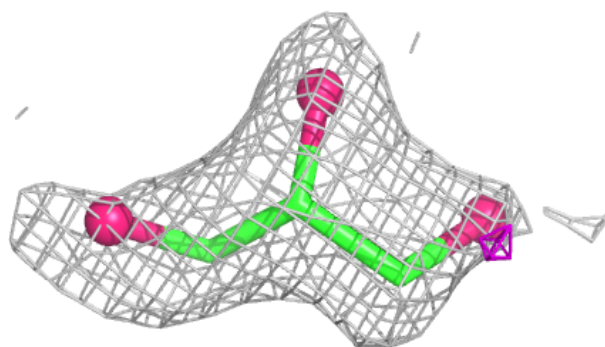


Electron density around GOL B 905:

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

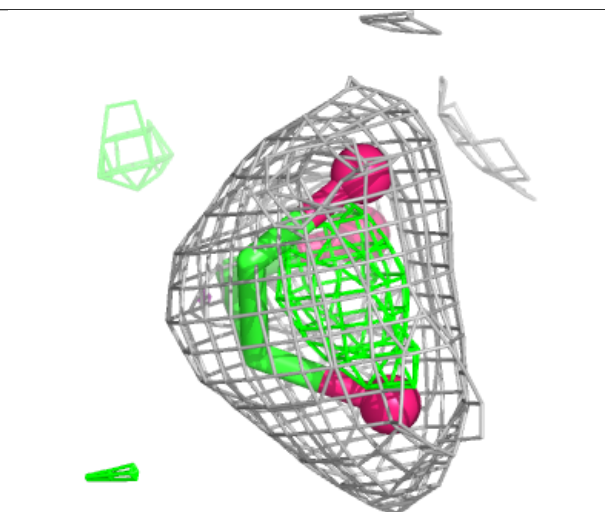
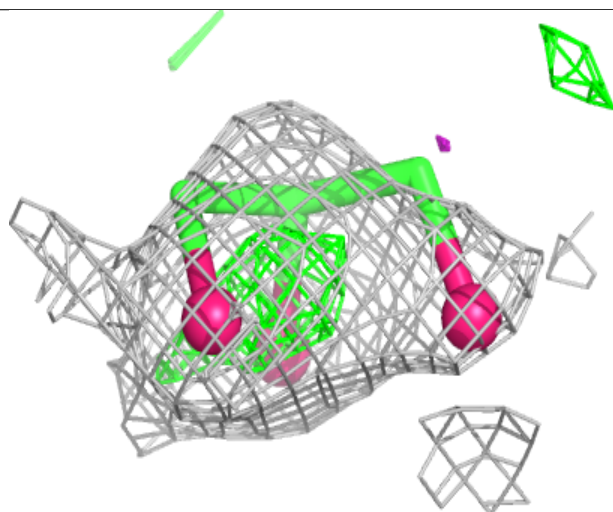
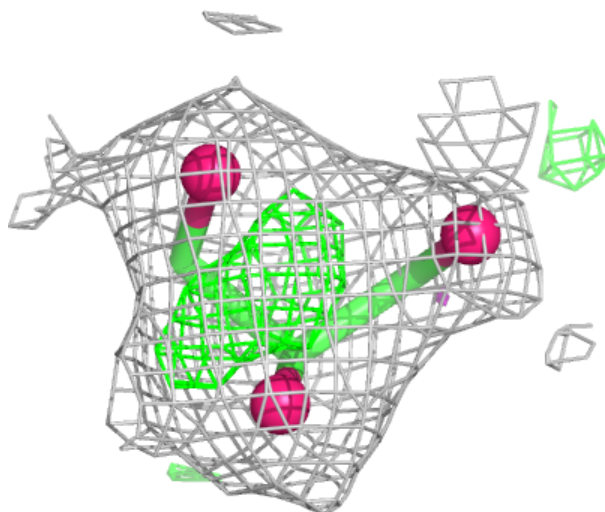
**Electron density around GOL A 907:**

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



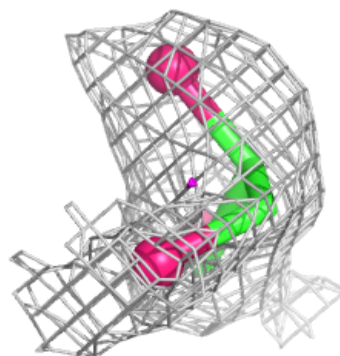
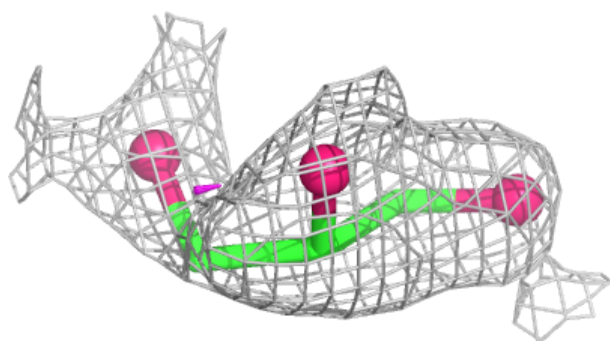
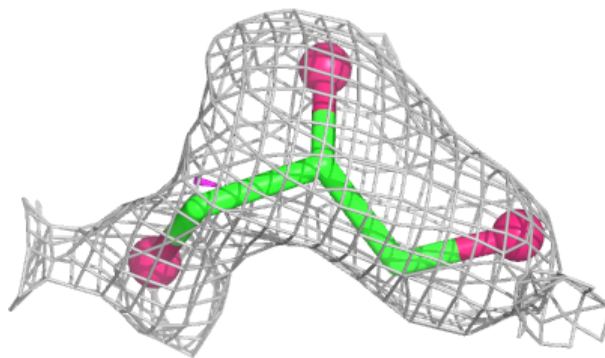
Electron density around GOL A 908:

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

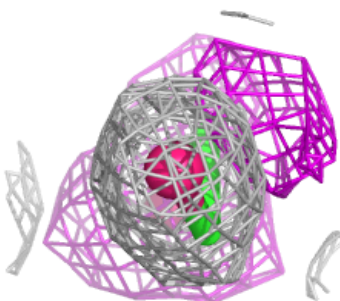
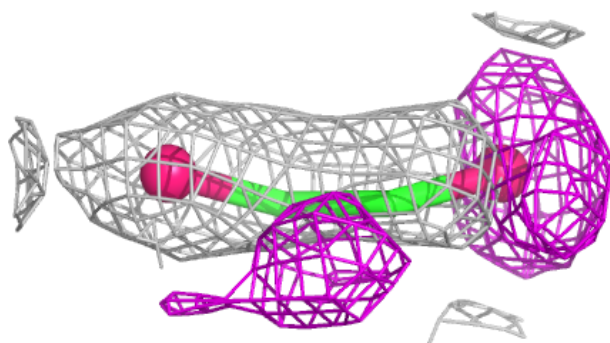
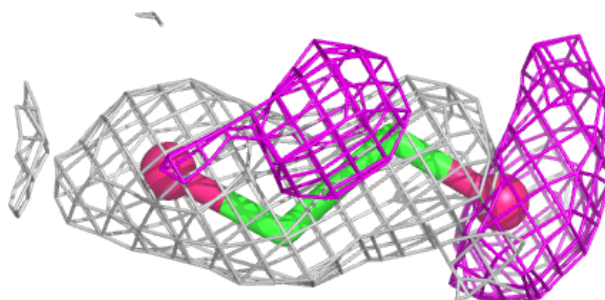


Electron density around GOL B 907:

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

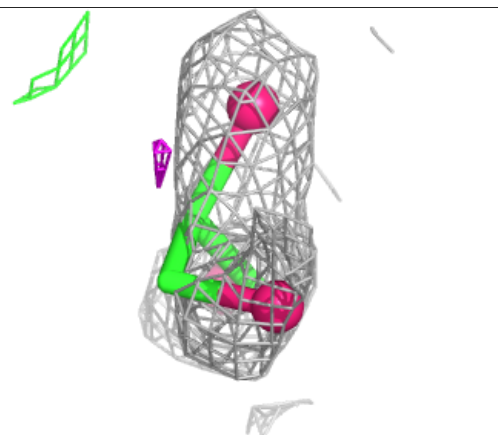
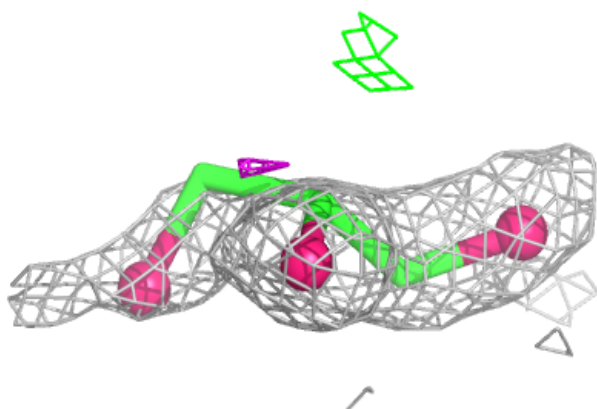
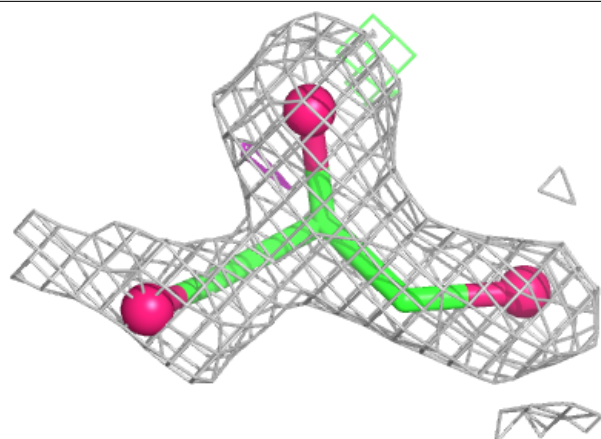
**Electron density around EDO B 912:**

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

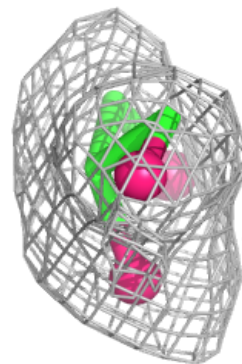
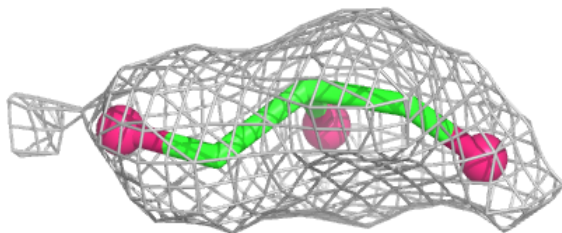
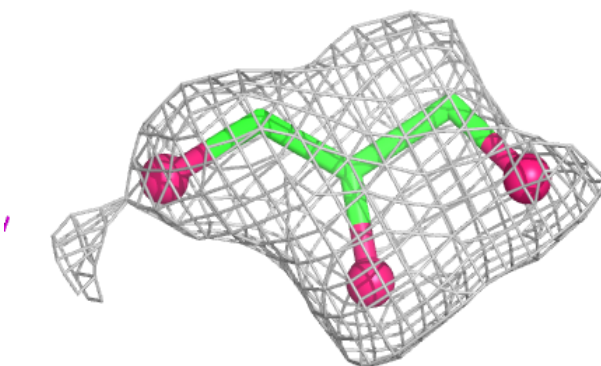


Electron density around GOL A 910:

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

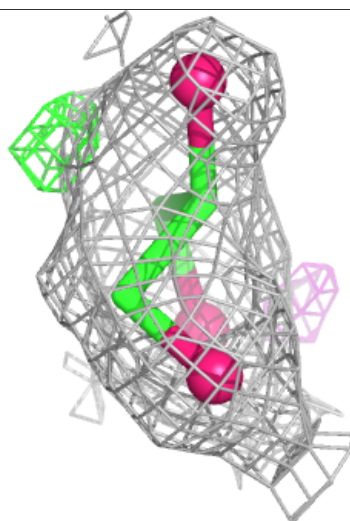
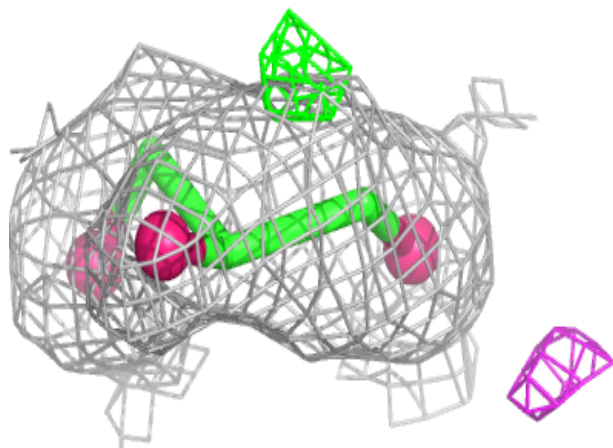
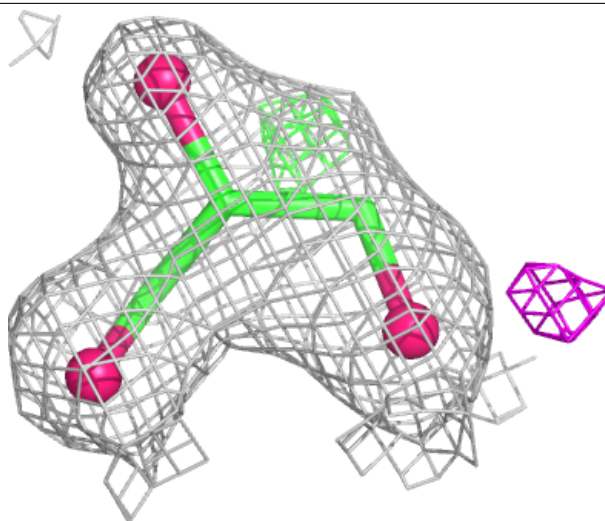
**Electron density around GOL B 908:**

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



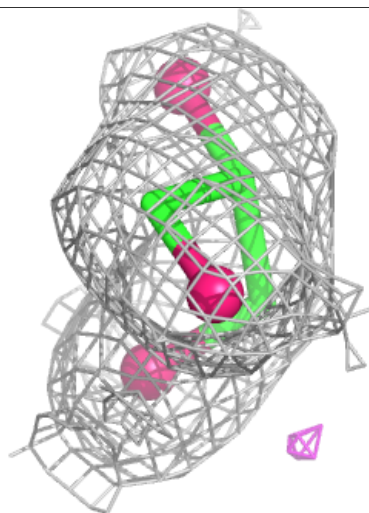
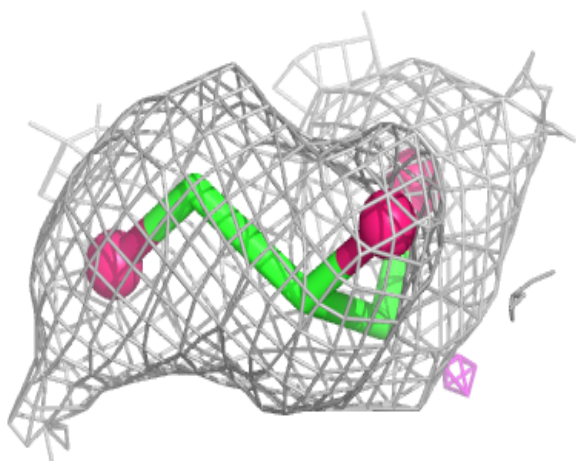
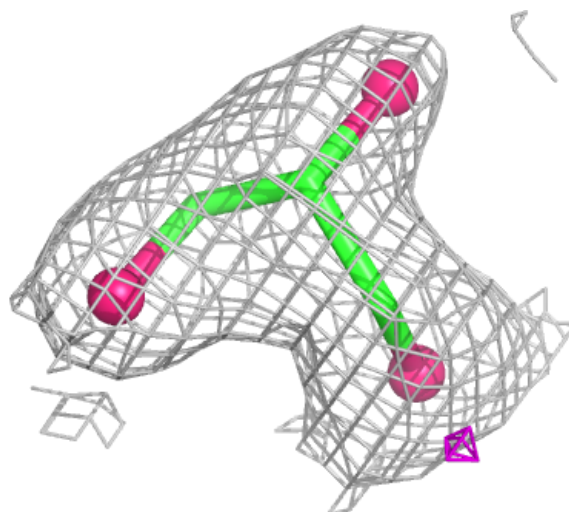
Electron density around GOL A 903:

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



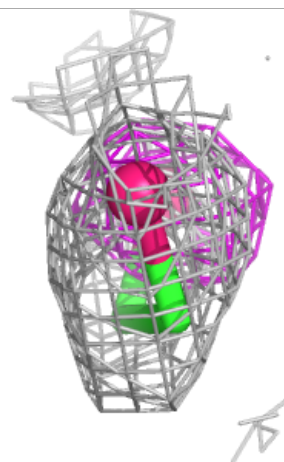
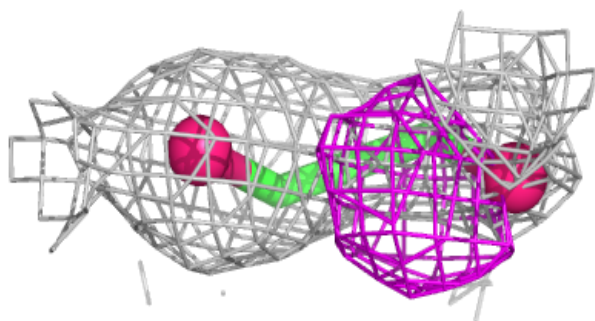
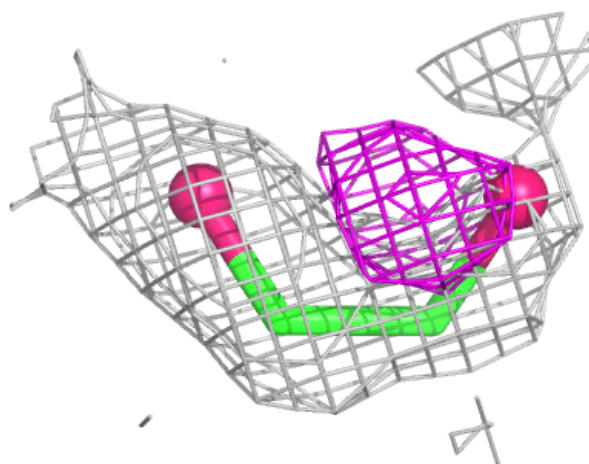
Electron density around GOL B 902:

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



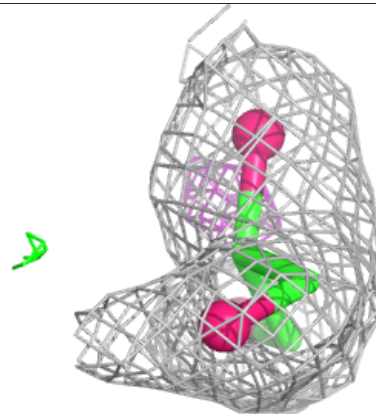
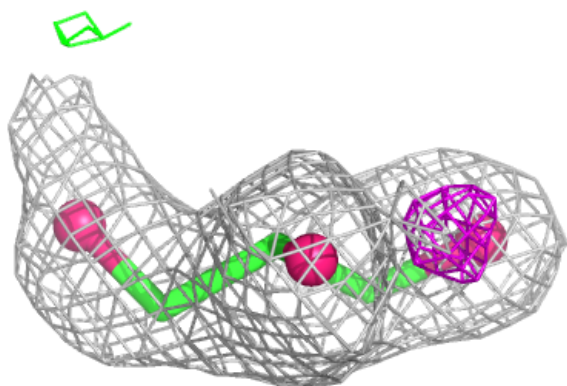
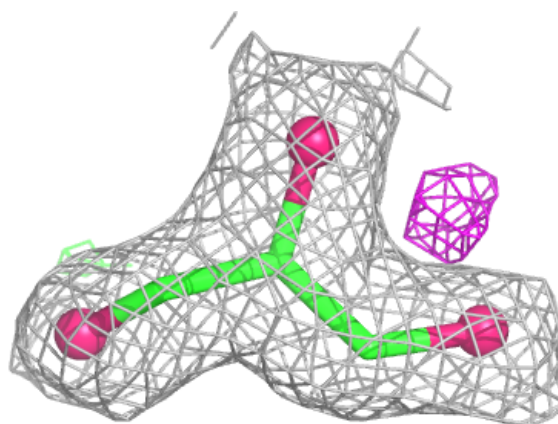
Electron density around EDO A 913:

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



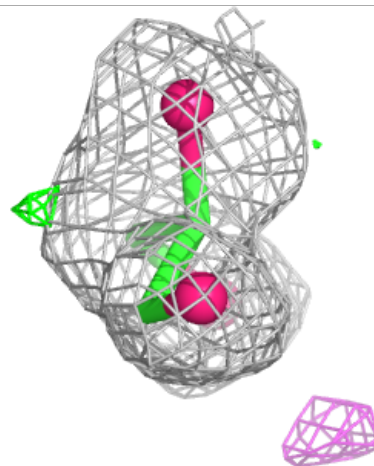
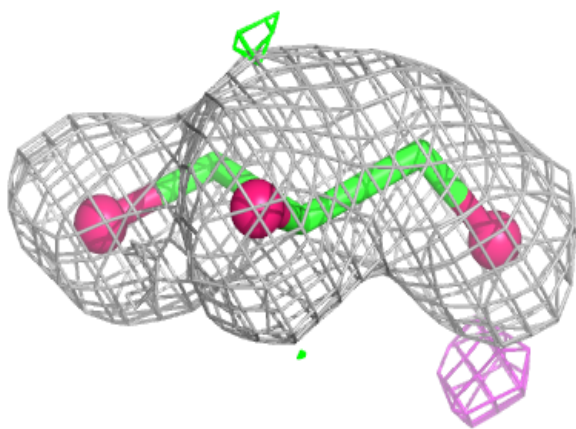
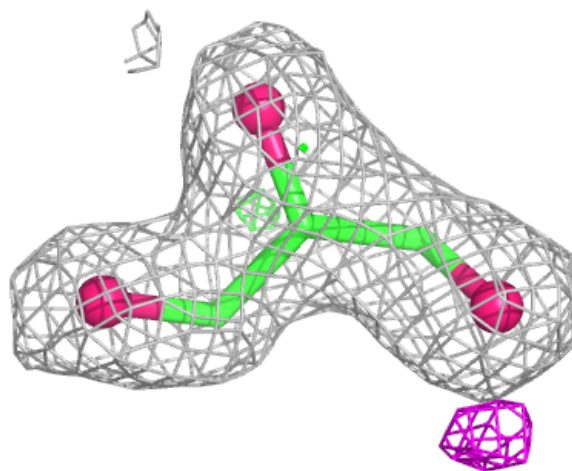
Electron density around GOL A 904:

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



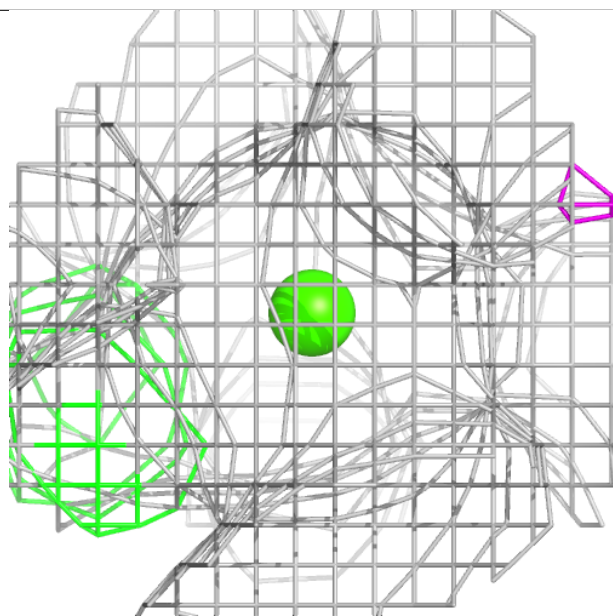
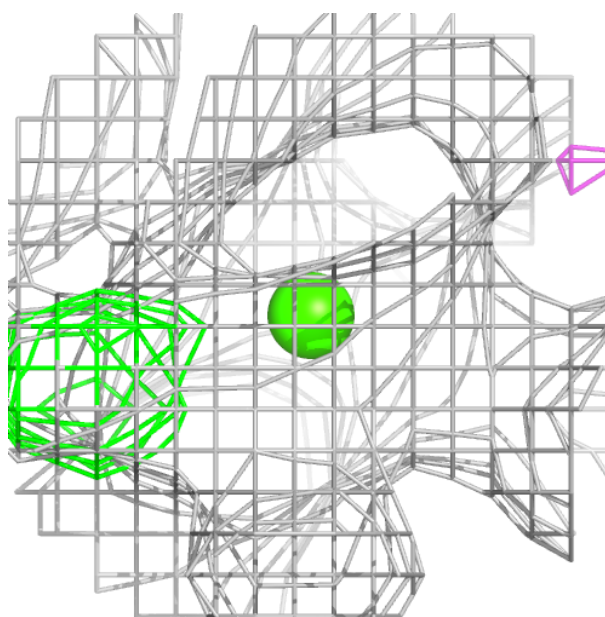
Electron density around GOL B 903:

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



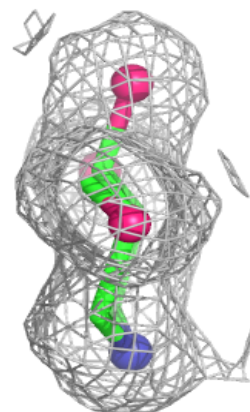
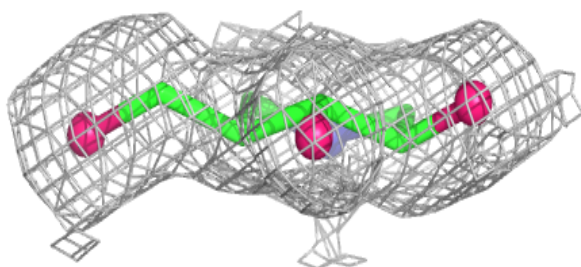
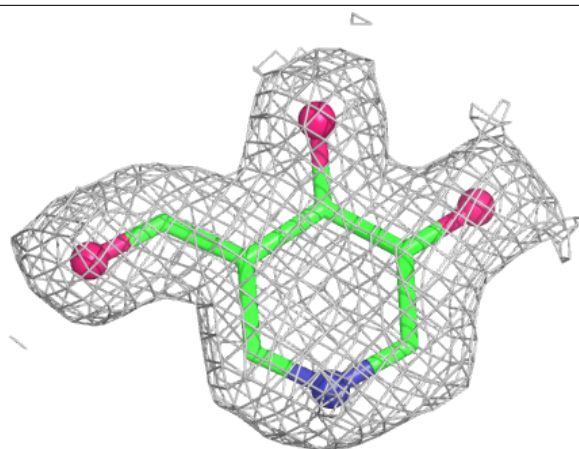
Electron density around CA B 913:

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



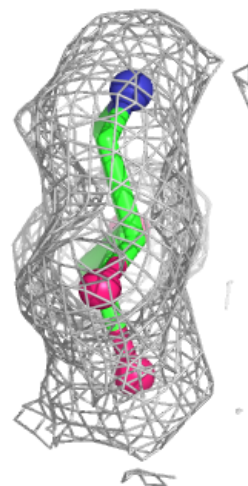
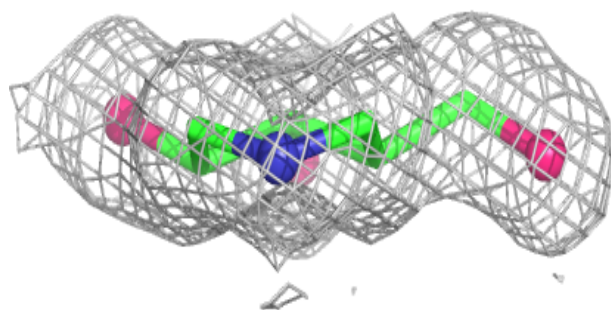
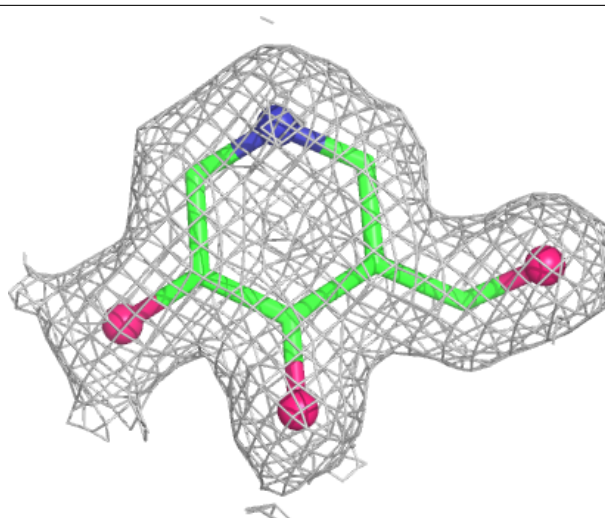
Electron density around IFM B 901:

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



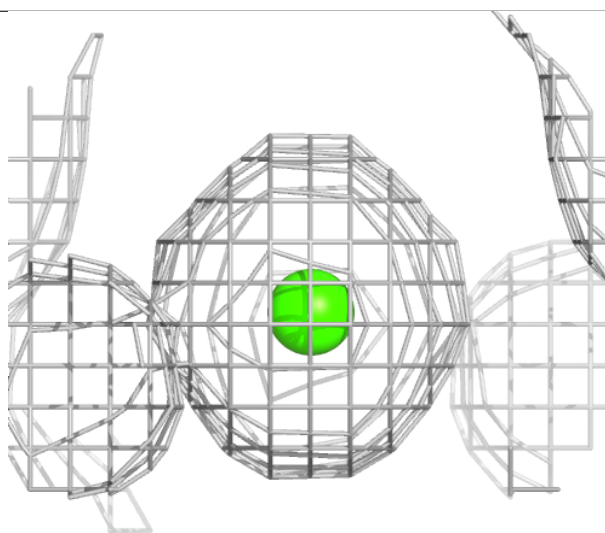
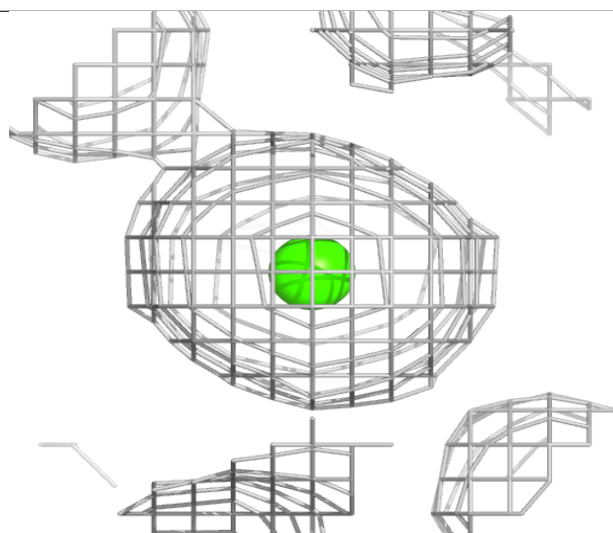
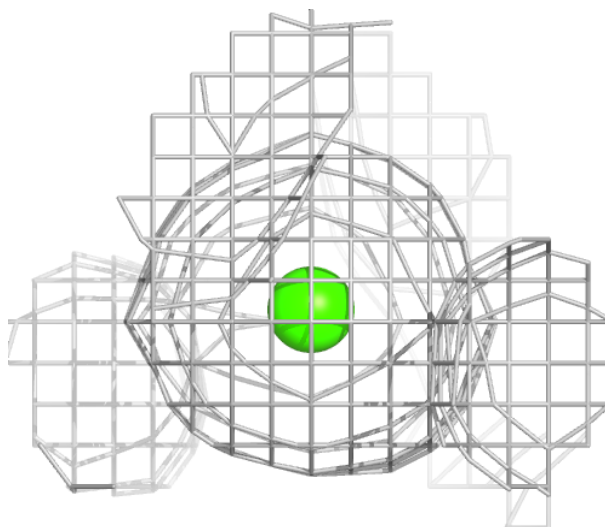
Electron density around IFM A 901:

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



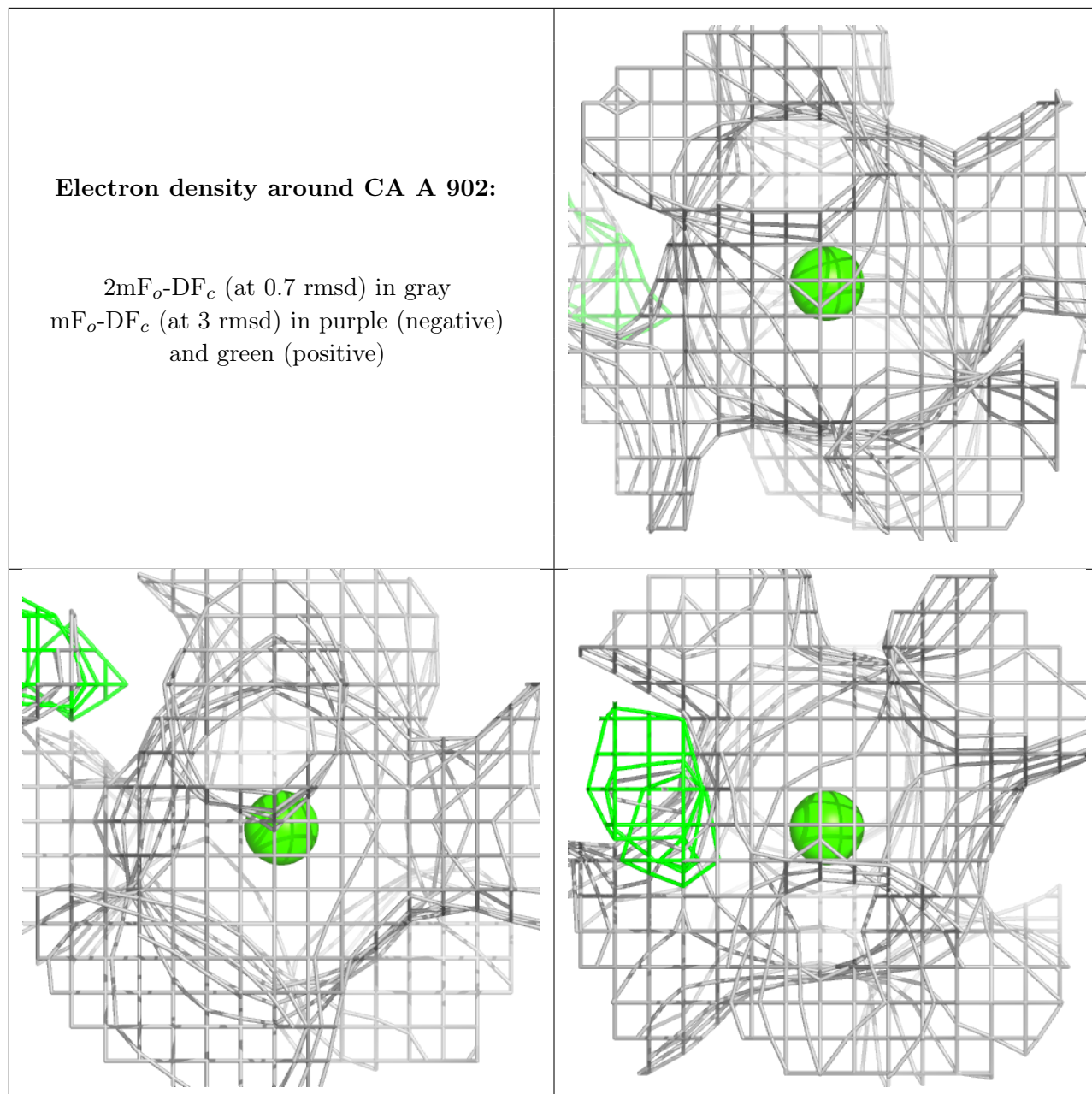
Electron density around CA A 914:

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



Electron density around CA A 902:

$2mF_o-DF_c$ (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.