



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 10:27 am BST

PDB ID : 8B5O
Title : Structure of haloalkane dehalogenase DmmarA from *Mycobacterium marinum* at pH 5.5
Authors : Snajdarova, K.; Marek, M.
Deposited on : 2022-09-23
Resolution : 1.60 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

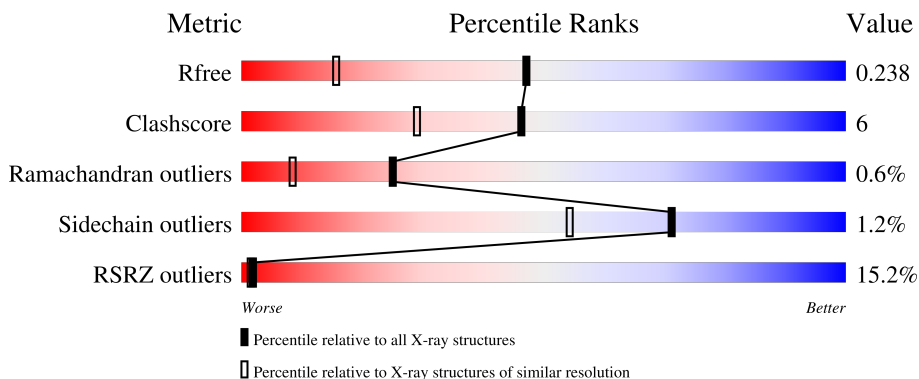
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	296	
1	B	296	
1	C	296	
1	D	296	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FMT	A	402	-	X	-	-
3	FMT	A	403	-	X	-	-
3	FMT	A	405	-	X	-	-
3	FMT	A	406	-	X	-	-
3	FMT	B	304	-	X	-	-
3	FMT	B	305	-	X	-	-
3	FMT	B	306	-	X	-	-
3	FMT	C	302	-	X	-	-
3	FMT	C	304	-	X	-	-
3	FMT	C	305	-	X	-	-
3	FMT	C	307	-	X	-	-
3	FMT	C	308	-	X	-	-
3	FMT	D	301	-	X	-	-

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 9744 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 Haloalkane dehalogenase DhaA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	283	2257	1438	393	417	9	0	3	0
1	B	282	2230	1422	386	413	9	0	1	0
1	C	284	2268	1444	397	418	9	0	3	0
1	D	277	2194	1401	377	407	9	0	1	0

There are 24 discrepancies between the modelled and reference sequences:

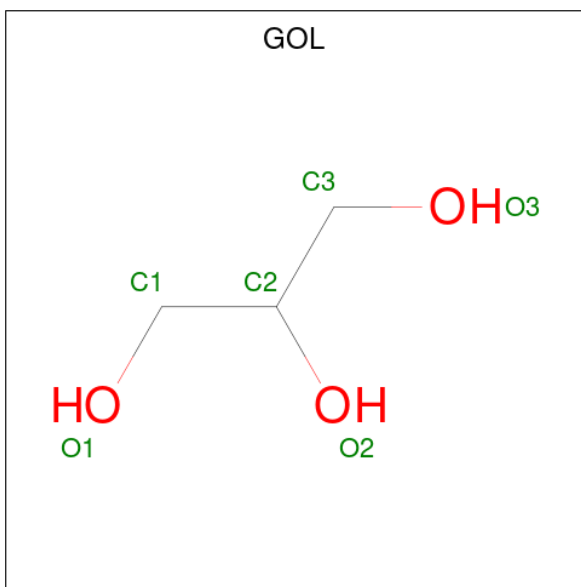
Chain	Residue	Modelled	Actual	Comment	Reference
A	291	HIS	-	expression tag	UNP B2HR89
A	292	HIS	-	expression tag	UNP B2HR89
A	293	HIS	-	expression tag	UNP B2HR89
A	294	HIS	-	expression tag	UNP B2HR89
A	295	HIS	-	expression tag	UNP B2HR89
A	296	HIS	-	expression tag	UNP B2HR89
B	291	HIS	-	expression tag	UNP B2HR89
B	292	HIS	-	expression tag	UNP B2HR89
B	293	HIS	-	expression tag	UNP B2HR89
B	294	HIS	-	expression tag	UNP B2HR89
B	295	HIS	-	expression tag	UNP B2HR89
B	296	HIS	-	expression tag	UNP B2HR89
C	291	HIS	-	expression tag	UNP B2HR89
C	292	HIS	-	expression tag	UNP B2HR89
C	293	HIS	-	expression tag	UNP B2HR89
C	294	HIS	-	expression tag	UNP B2HR89
C	295	HIS	-	expression tag	UNP B2HR89
C	296	HIS	-	expression tag	UNP B2HR89
D	291	HIS	-	expression tag	UNP B2HR89
D	292	HIS	-	expression tag	UNP B2HR89
D	293	HIS	-	expression tag	UNP B2HR89

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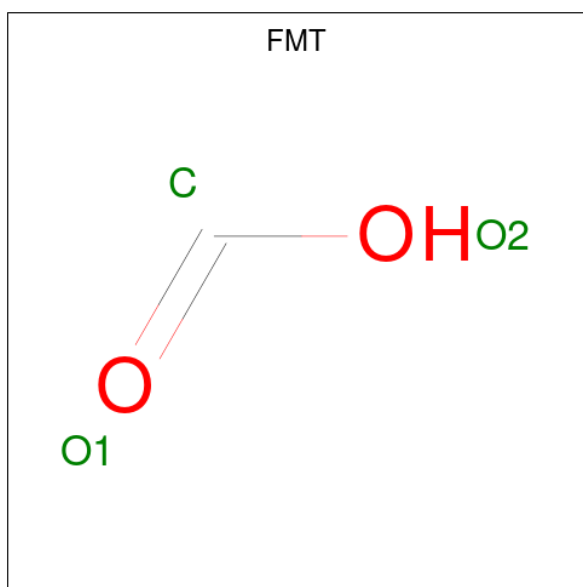
Chain	Residue	Modelled	Actual	Comment	Reference
D	294	HIS	-	expression tag	UNP B2HR89
D	295	HIS	-	expression tag	UNP B2HR89
D	296	HIS	-	expression tag	UNP B2HR89

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).



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

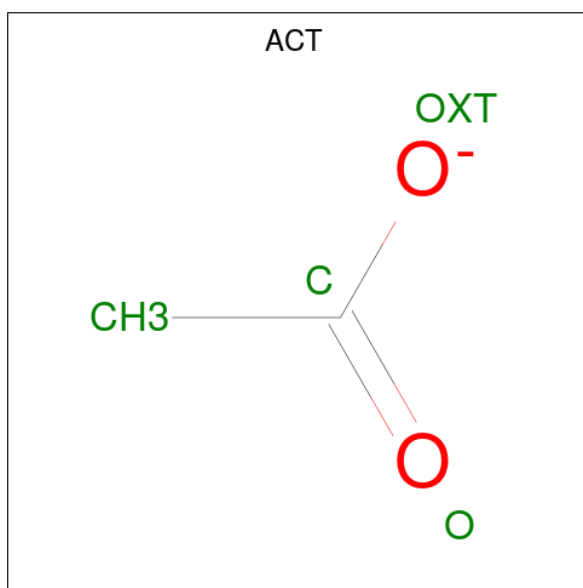
- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂) (labeled as

"Ligand of Interest" by depositor).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	229	Total	O	0	0
			229	229		
5	B	187	Total	O	0	0
			187	187		
5	C	246	Total	O	0	2
			248	248		
5	D	46	Total	O	0	0
			46	46		

G231	HIS
A232	HIS
I233	HIS
LEU	HIS
HIS	HIS
F236	HIS
G237	HIS
G238	HIS
S239	HIS
E240	HIS
L241	HIS
D242	HIS
F243	HIS
A244	HIS
R245	HIS
S246	HIS
W247	HIS
P248	HIS
R249	HIS
Q250	HIS
R251	HIS
E252	HIS
V253	HIS
K254	HIS
V255	HIS
A256	HIS
G257	HIS
R258	HIS
H259	HIS
F260	HIS
L261	HIS
Q262	HIS
E263	HIS
D264	HIS
S265	HIS
P266	HIS
D267	HIS
A268	HIS
I269	HIS
G270	HIS
A271	HIS
A272	HIS
V273	HIS
R274	HIS
A275	HIS
F276	HIS
V277	HIS
L278	HIS
D279	HIS
V280	HIS
R281	HIS
GLU	HIS
ARG	HIS
GLN	HIS
ASP	HIS
GLY	HIS
ALA	HIS
ASP	HIS
ARG	HIS
ALA	HIS

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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.70Å 60.77Å 104.78Å 90.00° 105.49° 90.00°	Depositor
Resolution (Å)	43.70 – 1.60 43.70 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (43.70-1.60) 98.8 (43.70-1.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.60Å)	Xtrriage
Refinement program	PHENIX 1.14-3260	Depositor
R, R_{free}	0.198 , 0.238 0.198 , 0.238	Depositor DCC
R_{free} test set	7081 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtrriage
Anisotropy	0.404	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9744	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, FMT, 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	0.67	0/2318	0.77	1/3158 (0.0%)
1	B	0.64	0/2291	0.75	1/3122 (0.0%)
1	C	0.73	0/2329	0.79	2/3172 (0.1%)
1	D	0.46	0/2249	0.61	0/3064
All	All	0.63	0/9187	0.73	4/12516 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	ASP	CB-CG-OD1	6.53	124.17	118.30
1	C	204	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	137	MET	CG-SD-CE	-5.21	91.87	100.20
1	C	125	ARG	NE-CZ-NH1	-5.02	117.79	120.30

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	2257	0	2208	11	0
1	B	2230	0	2180	10	0
1	C	2268	0	2221	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2194	0	2144	74	0
2	A	12	0	16	1	0
2	B	12	0	16	0	0
2	C	18	0	24	0	0
3	A	12	0	8	1	0
3	B	9	0	6	0	0
3	C	15	0	10	0	0
3	D	3	0	2	0	0
4	B	4	0	3	0	0
5	A	229	0	0	4	0
5	B	187	0	0	2	0
5	C	248	0	0	3	0
5	D	46	0	0	0	0
All	All	9744	0	8838	112	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 6.

All (112) 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:D:53:LEU:HB2	1:D:56:MET:HE3	1.23	1.16
1:D:95:ASP:O	1:D:98:SER:HB3	1.63	0.98
1:D:42:LEU:HD22	1:D:45:VAL:CG2	1.99	0.91
1:D:42:LEU:HD22	1:D:45:VAL:HG21	1.59	0.82
1:A:144[A]:GLN:NE2	5:A:503:HOH:O	2.23	0.71
1:C:119:ASP:OD2	1:C:259:HIS:ND1	2.20	0.71
1:D:20:ASP:O	1:D:47:ARG:N	2.25	0.70
1:D:53:LEU:HB2	1:D:56:MET:CE	2.14	0.70
1:D:166:ARG:NH1	1:D:263:GLU:OE1	2.24	0.69
1:D:131:THR:OG1	1:D:132:ASP:N	2.26	0.69
1:D:251:ARG:O	1:D:252:GLU:OE2	2.09	0.69
1:D:251:ARG:O	1:D:252:GLU:HG3	1.93	0.68
1:D:42:LEU:HD11	1:D:274:ARG:HA	1.75	0.68
1:D:42:LEU:HD22	1:D:45:VAL:HG22	1.75	0.68
1:D:265:SER:O	1:D:269:ILE:HG13	1.93	0.68
1:D:29:PRO:HG3	1:D:155:PHE:HB3	1.76	0.67
1:D:221:ILE:H	1:D:221:ILE:HD12	1.58	0.67
1:D:281:ARG:HG2	1:D:281:ARG:HH11	1.59	0.67
1:D:251:ARG:O	1:D:252:GLU:CG	2.44	0.66
1:B:229:GLU:OE1	1:B:254:LYS:HD3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:THR:OG1	1:D:87:GLU:N	2.30	0.64
1:C:14:ILE:HD12	1:C:32:SER:HB2	1.81	0.62
1:D:261:LEU:HD23	1:D:261:LEU:H	1.64	0.61
1:C:170:GLU:HG3	5:C:434:HOH:O	2.01	0.60
1:D:106:LEU:HD12	1:D:212:TYR:HA	1.84	0.60
1:D:202:PRO:HB2	1:D:205:VAL:HG12	1.83	0.59
1:D:198:VAL:HG12	1:D:199:GLU:HG2	1.85	0.56
1:D:197:PRO:HB3	1:D:205:VAL:HG13	1.87	0.56
1:D:21:PRO:HG2	1:D:89:VAL:HG12	1.87	0.56
1:D:229:GLU:OE2	1:D:254:LYS:NZ	2.38	0.56
1:D:160:VAL:HG12	1:D:260:PHE:CZ	2.41	0.55
1:A:261:LEU:H	1:A:261:LEU:HD23	1.72	0.54
1:B:154:VAL:HG23	1:B:158:LYS:HE2	1.88	0.54
1:A:16[A]:VAL:HG22	2:A:401:GOL:H32	1.90	0.53
1:D:118:MET:HG3	1:D:261:LEU:HD21	1.89	0.53
1:D:231:GLY:O	1:D:258:ARG:HG2	2.08	0.53
1:A:18:GLN:NE2	5:A:507:HOH:O	2.34	0.53
1:B:154:VAL:HA	1:B:158:LYS:HE2	1.90	0.53
1:D:209:VAL:HA	1:D:212:TYR:CE2	2.44	0.53
1:D:45:VAL:HG21	1:D:277:VAL:HG11	1.92	0.52
1:B:261:LEU:H	1:B:261:LEU:HD23	1.75	0.52
1:C:143:GLU:H	1:C:143:GLU:CD	2.14	0.51
1:D:112:ILE:HD11	1:D:115:ILE:HG13	1.92	0.51
1:C:169:THR:OG1	1:C:171:GLU:HG2	2.10	0.51
1:D:222:PRO:HG2	1:D:280:VAL:HG23	1.92	0.51
1:D:127:TRP:CD2	1:D:198:VAL:HG11	2.47	0.50
1:D:127:TRP:CD1	1:D:199:GLU:HG3	2.47	0.50
1:D:281:ARG:HG2	1:D:281:ARG:NH1	2.26	0.50
1:D:41:HIS:NE2	1:D:267:ASP:OD1	2.44	0.49
1:B:277:VAL:O	1:B:281:ARG:HG2	2.11	0.49
1:D:86:THR:O	1:D:87:GLU:HB2	2.13	0.49
1:D:53:LEU:CB	1:D:56:MET:HE3	2.16	0.49
1:D:160:VAL:HA	1:D:260:PHE:CE2	2.48	0.49
1:D:251:ARG:NH1	1:D:279:ASP:OD2	2.42	0.48
1:B:87:GLU:OE2	5:B:401:HOH:O	2.20	0.47
1:C:184:GLN:O	5:C:401:HOH:O	2.20	0.47
1:B:228:ALA:HB2	1:B:261:LEU:HD13	1.97	0.47
1:D:221:ILE:O	1:D:223:LYS:HE2	2.15	0.46
1:A:144[A]:GLN:CD	1:A:147:ARG:HH11	2.19	0.45
1:C:68[B]:ARG:HH12	1:C:204:ASP:CG	2.20	0.45
1:D:14:ILE:HD12	1:D:32:SER:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:TRP:HA	1:D:192:TRP:CE3	2.52	0.45
1:D:212:TYR:O	1:D:216:LEU:HD23	2.17	0.44
1:D:229:GLU:HA	1:D:229:GLU:OE1	2.18	0.44
1:D:251:ARG:HB3	1:D:252:GLU:H	1.58	0.44
1:B:14:ILE:O	1:B:49:LEU:HA	2.17	0.44
1:D:262:GLN:O	1:D:266:PRO:HB3	2.17	0.44
1:C:33:TYR:CD1	1:C:175:VAL:HG11	2.53	0.44
1:A:29:PRO:HG3	1:A:155:PHE:HB3	2.00	0.43
1:A:14:ILE:HD12	1:A:32:SER:HB2	2.01	0.43
1:D:219:SER:HB2	1:D:221:ILE:HD12	1.99	0.43
1:D:277:VAL:HA	1:D:280:VAL:HG12	2.00	0.43
1:A:26:HIS:CD2	1:A:31:SER:HA	2.54	0.43
1:A:201:GLU:OE1	5:A:501:HOH:O	2.21	0.43
1:B:132:ASP:OD1	5:B:402:HOH:O	2.21	0.43
1:D:93:VAL:HB	1:D:98:SER:HA	2.01	0.43
1:D:169:THR:HB	1:D:172:GLU:HG2	2.00	0.43
1:C:219:SER:O	1:C:248:PRO:HG2	2.18	0.43
1:D:42:LEU:HD23	1:D:42:LEU:HA	1.68	0.43
1:D:220:ASP:O	1:D:220:ASP:OD1	2.37	0.43
1:D:86:THR:OG1	1:D:111:GLN:HG2	2.18	0.42
1:D:227:VAL:O	1:D:254:LYS:HA	2.19	0.42
1:D:22:ILE:HD11	1:D:45:VAL:HG23	2.00	0.42
1:D:195:GLU:O	1:D:205:VAL:HG11	2.20	0.42
1:C:93:VAL:HB	1:C:98:SER:HA	2.02	0.42
1:D:28:ASN:HA	1:D:29:PRO:HA	1.89	0.42
1:A:14:ILE:O	1:A:49:LEU:HA	2.20	0.42
1:C:277:VAL:O	1:C:281:ARG:HG2	2.20	0.42
1:D:109:PRO:C	1:D:111:GLN:H	2.22	0.42
3:A:406:FMT:H	5:A:590:HOH:O	2.20	0.42
1:D:160:VAL:HG22	1:D:161:PRO:HD3	2.01	0.42
1:A:228:ALA:HB2	1:A:261:LEU:HD13	2.00	0.42
1:C:26:HIS:CD2	1:C:31:SER:HA	2.54	0.42
1:C:29:PRO:HG3	1:C:155:PHE:HB3	2.02	0.41
1:D:155:PHE:O	1:D:160:VAL:HG13	2.19	0.41
1:D:140:LEU:HD23	1:D:145:GLY:HA2	2.02	0.41
1:D:172:GLU:HG2	1:D:172:GLU:H	1.71	0.41
1:D:115:ILE:O	1:D:223:LYS:HA	2.21	0.41
1:C:134:GLU:HB3	1:C:135:PRO:HD3	2.03	0.41
1:C:147[B]:ARG:NH2	5:C:402:HOH:O	2.42	0.41
1:D:122:VAL:HG23	1:D:123:GLN:HG2	2.01	0.41
1:D:42:LEU:O	1:D:45:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:TYR:HE1	1:D:223:LYS:HG2	1.86	0.41
1:D:219:SER:HB2	1:D:221:ILE:CD1	2.51	0.41
1:D:2:LYS:HE3	1:D:15:ASP:HB3	2.02	0.41
1:D:127:TRP:CE2	1:D:198:VAL:HG11	2.55	0.41
1:D:56:MET:CE	1:D:192:TRP:HE1	2.34	0.40
1:B:93:VAL:HB	1:B:98:SER:HA	2.03	0.40
1:D:220:ASP:OD1	1:D:249:ASN:ND2	2.52	0.40
1:D:21:PRO:HA	1:D:47:ARG:O	2.22	0.40
1:D:137:MET:HE2	1:D:137:MET:HB3	1.59	0.40
1:C:14:ILE:O	1:C:49:LEU:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	284/296 (96%)	274 (96%)	9 (3%)	1 (0%)	34	15
1	B	281/296 (95%)	271 (96%)	10 (4%)	0	100	100
1	C	285/296 (96%)	274 (96%)	11 (4%)	0	100	100
1	D	272/296 (92%)	248 (91%)	18 (7%)	6 (2%)	6	1
All	All	1122/1184 (95%)	1067 (95%)	48 (4%)	7 (1%)	25	8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	251	ARG
1	D	252	GLU
1	D	87	GLU
1	D	249	ASN
1	D	42	LEU

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Mol	Chain	Res	Type
1	D	110	GLU
1	A	119	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/244 (97%)	232 (98%)	5 (2%)	53	29
1	B	234/244 (96%)	233 (100%)	1 (0%)	91	84
1	C	238/244 (98%)	238 (100%)	0	100	100
1	D	231/244 (95%)	225 (97%)	6 (3%)	46	21
All	All	940/976 (96%)	928 (99%)	12 (1%)	71	50

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	GLN
1	A	212	TYR
1	A	251[A]	ARG
1	A	251[B]	ARG
1	A	283	ARG
1	B	212	TYR
1	D	98	SER
1	D	134	GLU
1	D	170	GLU
1	D	212	TYR
1	D	249	ASN
1	D	251	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	167	GLN
1	C	18	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	C	301	-	5,5,5	0.57	0	5,5,5	0.70	0
2	GOL	B	301	-	5,5,5	0.47	0	5,5,5	0.29	0
3	FMT	A	402	-	2,2,2	3.04	2 (100%)	1,1,1	1.51	0
3	FMT	B	306	-	2,2,2	3.04	2 (100%)	1,1,1	1.52	0
3	FMT	B	305	-	2,2,2	3.00	2 (100%)	1,1,1	1.62	0
3	FMT	A	406	-	2,2,2	2.95	2 (100%)	1,1,1	1.36	0
3	FMT	A	405	-	2,2,2	3.09	2 (100%)	1,1,1	1.75	0
4	ACT	B	303	-	3,3,3	1.04	0	3,3,3	0.65	0
2	GOL	C	303	-	5,5,5	0.50	0	5,5,5	0.57	0
3	FMT	C	305	-	2,2,2	3.00	2 (100%)	1,1,1	1.63	0
3	FMT	A	403	-	2,2,2	3.04	2 (100%)	1,1,1	1.36	0
3	FMT	D	301	-	2,2,2	3.35	2 (100%)	1,1,1	1.35	0
3	FMT	C	302	-	2,2,2	3.16	2 (100%)	1,1,1	1.25	0
2	GOL	C	306	-	5,5,5	0.45	0	5,5,5	0.27	0
2	GOL	A	401	-	5,5,5	0.29	0	5,5,5	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FMT	B	304	-	2,2,2	2.96	2 (100%)	1,1,1	1.51	0
2	GOL	B	302	-	5,5,5	0.65	0	5,5,5	0.74	0
3	FMT	C	307	-	2,2,2	3.17	2 (100%)	1,1,1	0.76	0
2	GOL	A	404	-	5,5,5	0.49	0	5,5,5	0.27	0
3	FMT	C	304	-	2,2,2	2.98	2 (100%)	1,1,1	1.68	0
3	FMT	C	308	-	2,2,2	2.97	2 (100%)	1,1,1	1.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	301	-	-	0/4/4/4	-
2	GOL	B	301	-	-	2/4/4/4	-
2	GOL	B	302	-	-	4/4/4/4	-
2	GOL	C	303	-	-	2/4/4/4	-
2	GOL	A	404	-	-	2/4/4/4	-
2	GOL	C	306	-	-	2/4/4/4	-
2	GOL	A	401	-	-	2/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	FMT	O1-C	3.98	1.43	1.22
3	C	307	FMT	O1-C	3.70	1.41	1.22
3	C	302	FMT	O1-C	3.68	1.41	1.22
3	A	402	FMT	O1-C	3.67	1.41	1.22
3	B	306	FMT	O1-C	3.57	1.41	1.22
3	A	403	FMT	O1-C	3.56	1.40	1.22
3	A	405	FMT	O1-C	3.55	1.40	1.22
3	C	305	FMT	O1-C	3.53	1.40	1.22
3	B	305	FMT	O1-C	3.52	1.40	1.22
3	C	304	FMT	O1-C	3.51	1.40	1.22
3	A	406	FMT	O1-C	3.50	1.40	1.22
3	C	308	FMT	O1-C	3.48	1.40	1.22
3	B	304	FMT	O1-C	3.44	1.40	1.22
3	D	301	FMT	O2-C	2.56	1.41	1.28
3	A	405	FMT	O2-C	2.55	1.41	1.28
3	C	302	FMT	O2-C	2.54	1.41	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	307	FMT	O2-C	2.53	1.41	1.28
3	A	403	FMT	O2-C	2.42	1.40	1.28
3	B	306	FMT	O2-C	2.38	1.40	1.28
3	B	304	FMT	O2-C	2.37	1.40	1.28
3	B	305	FMT	O2-C	2.37	1.40	1.28
3	C	305	FMT	O2-C	2.36	1.40	1.28
3	C	308	FMT	O2-C	2.36	1.40	1.28
3	C	304	FMT	O2-C	2.35	1.40	1.28
3	A	406	FMT	O2-C	2.27	1.40	1.28
3	A	402	FMT	O2-C	2.26	1.40	1.28

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	GOL	C1-C2-C3-O3
2	B	302	GOL	C1-C2-C3-O3
2	B	302	GOL	O2-C2-C3-O3
2	A	401	GOL	C1-C2-C3-O3
2	A	404	GOL	C1-C2-C3-O3
2	B	302	GOL	O1-C1-C2-C3
2	C	306	GOL	O1-C1-C2-C3
2	B	301	GOL	O2-C2-C3-O3
2	C	306	GOL	O1-C1-C2-O2
2	A	401	GOL	O2-C2-C3-O3
2	C	303	GOL	C1-C2-C3-O3
2	B	302	GOL	O1-C1-C2-O2
2	A	404	GOL	O1-C1-C2-O2
2	C	303	GOL	O2-C2-C3-O3

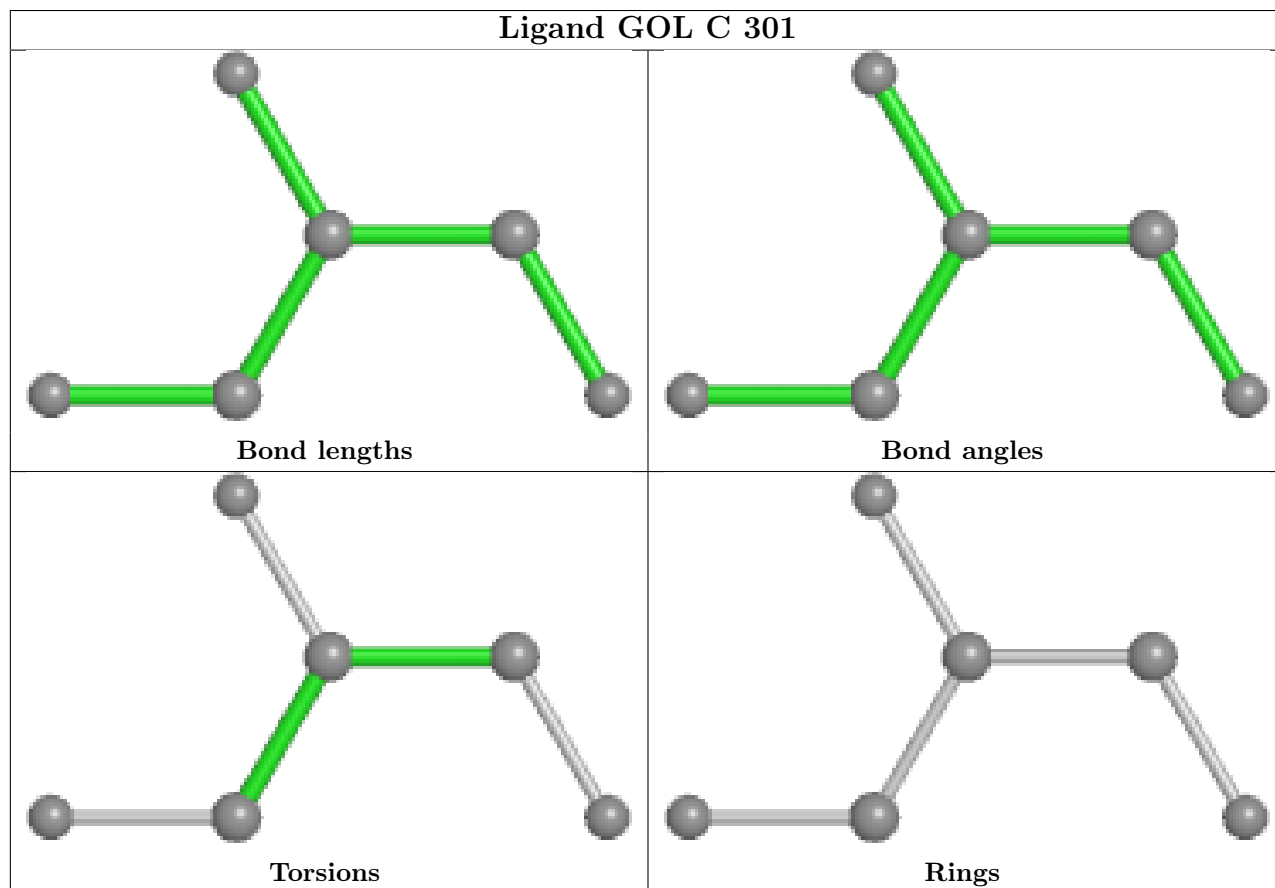
There are no ring outliers.

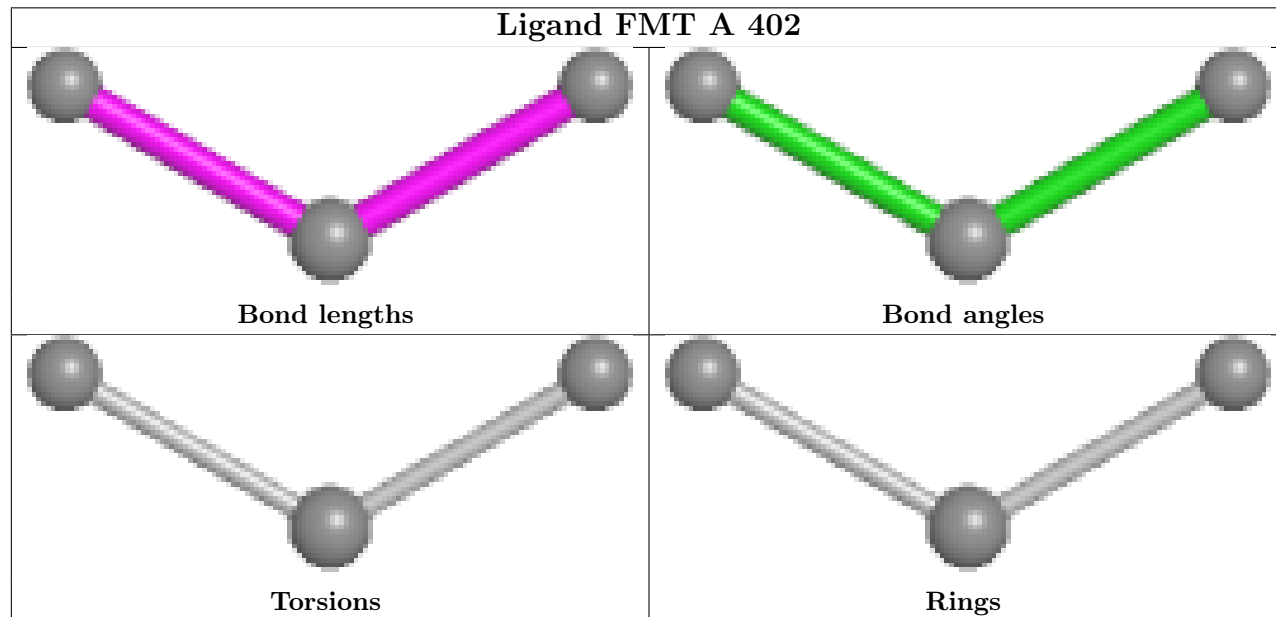
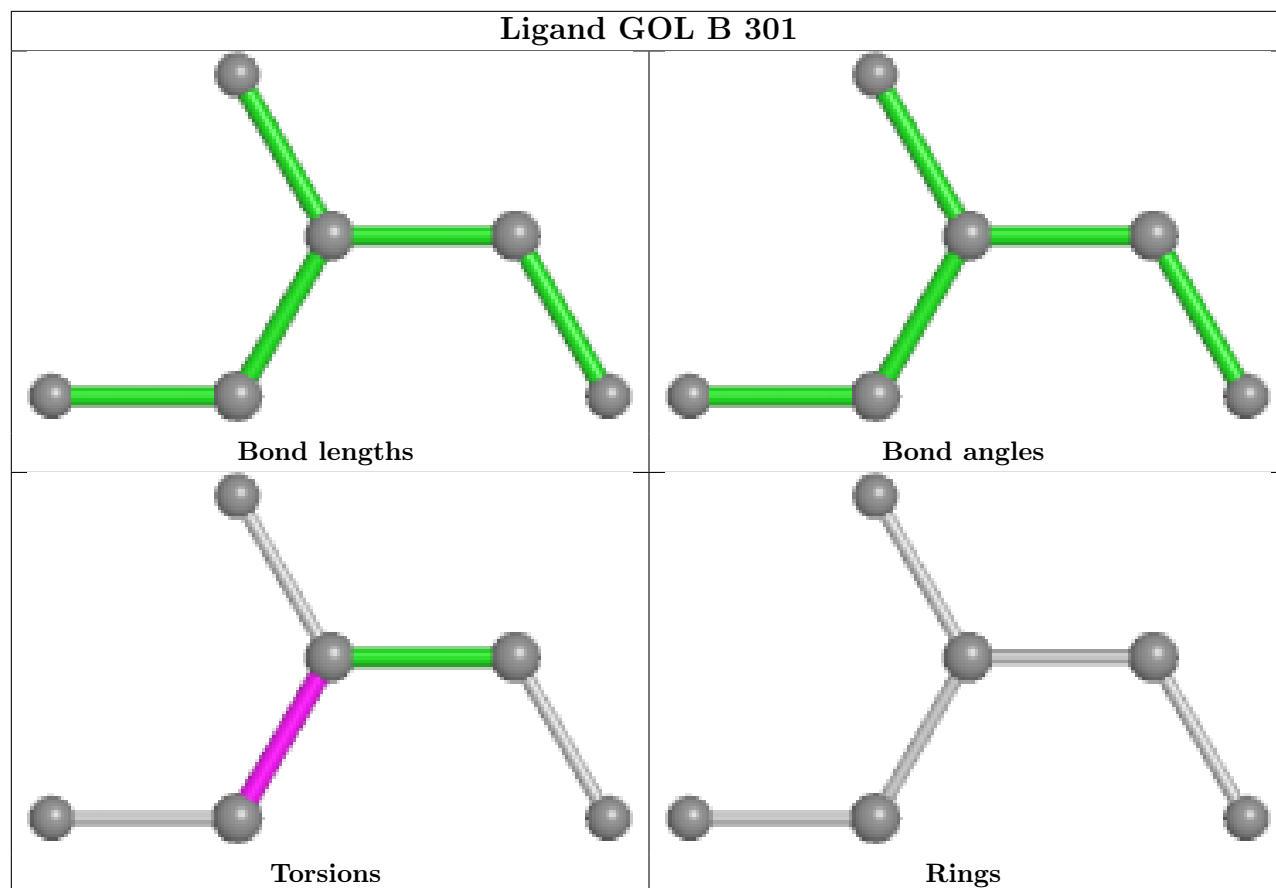
2 monomers are involved in 2 short contacts:

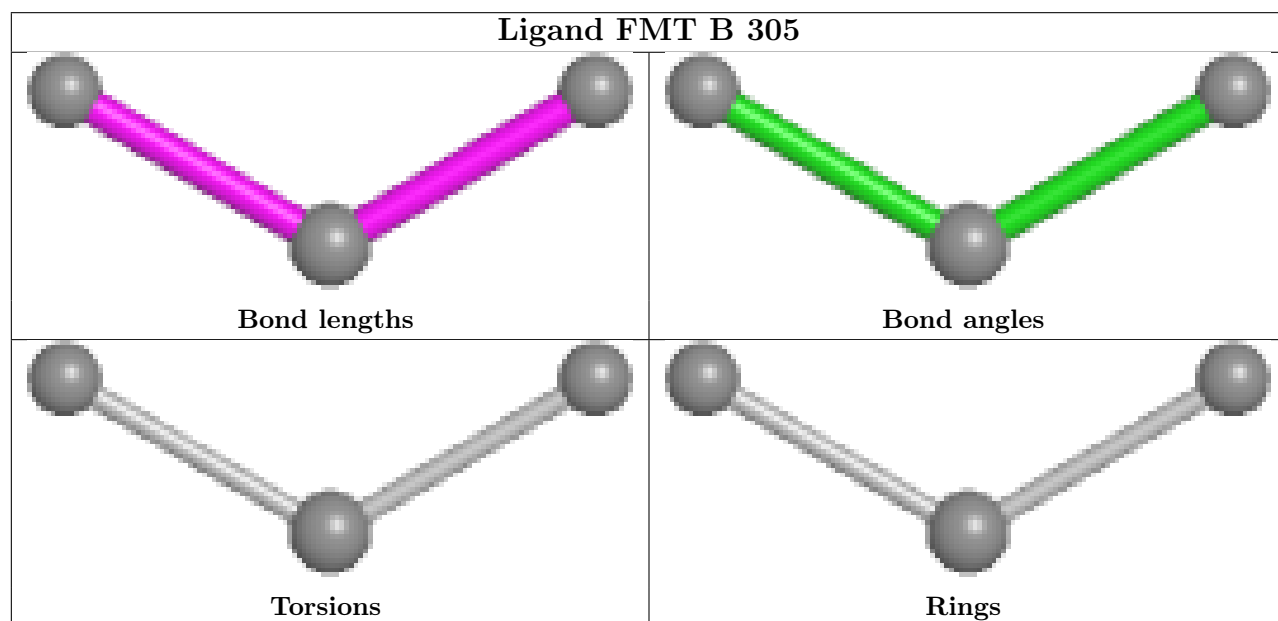
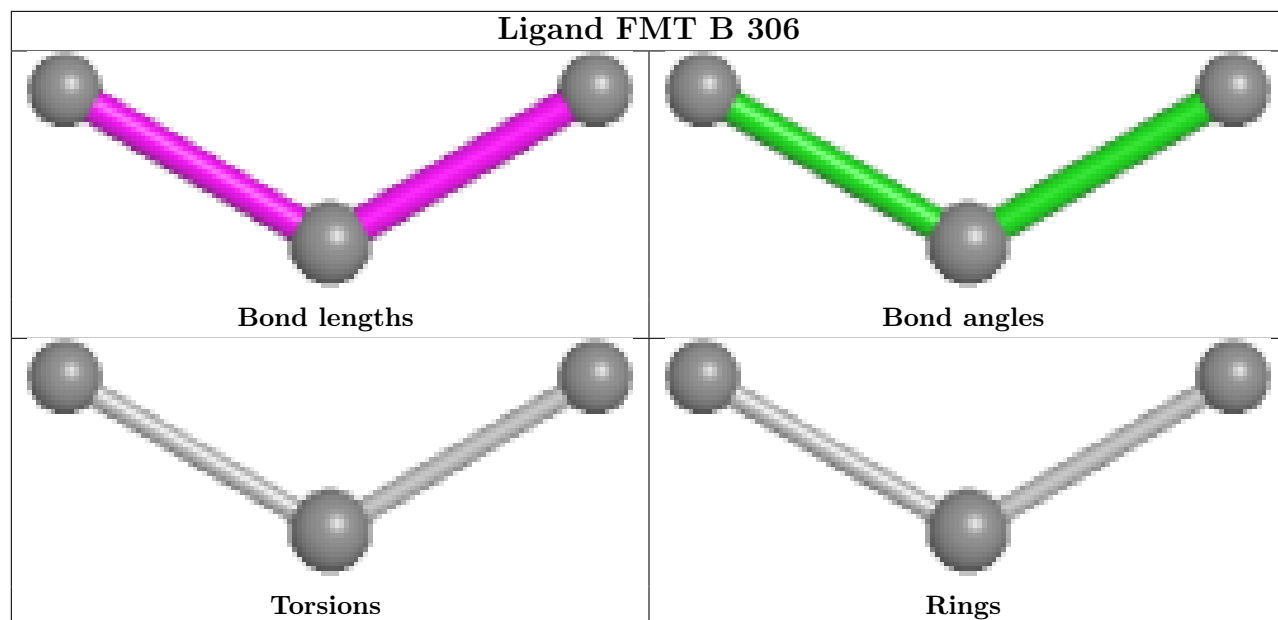
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	406	FMT	1	0
2	A	401	GOL	1	0

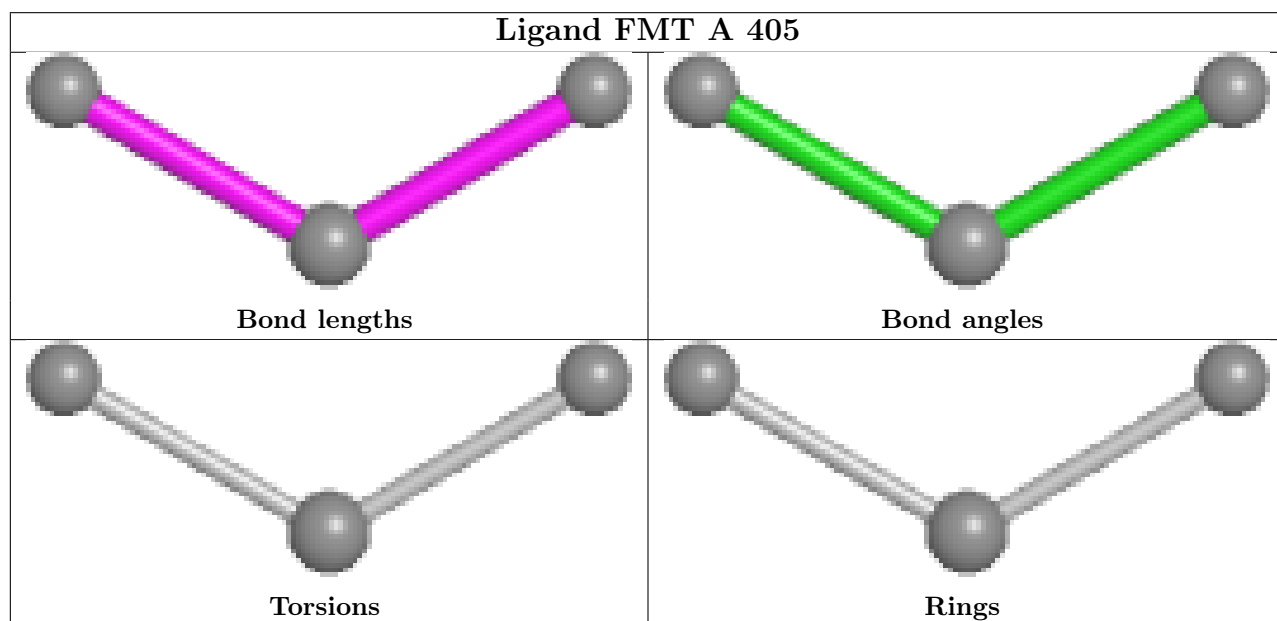
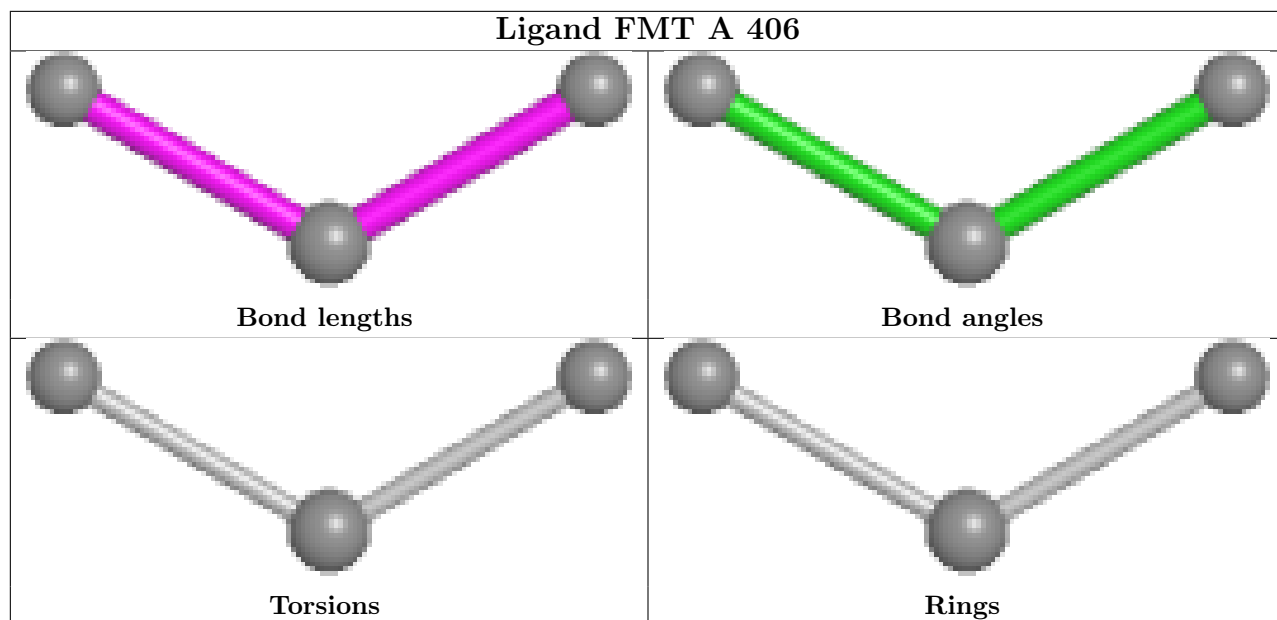
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

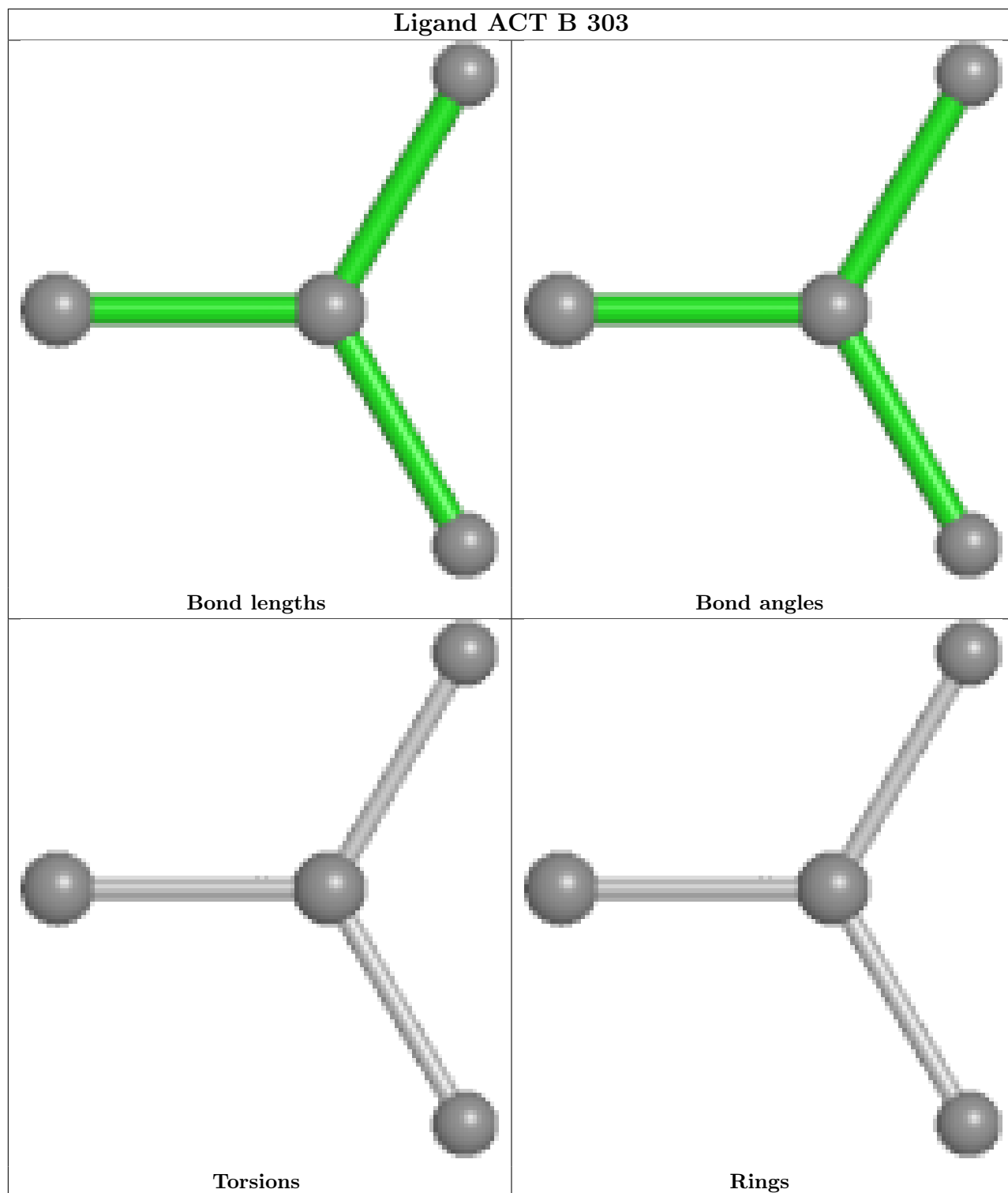
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

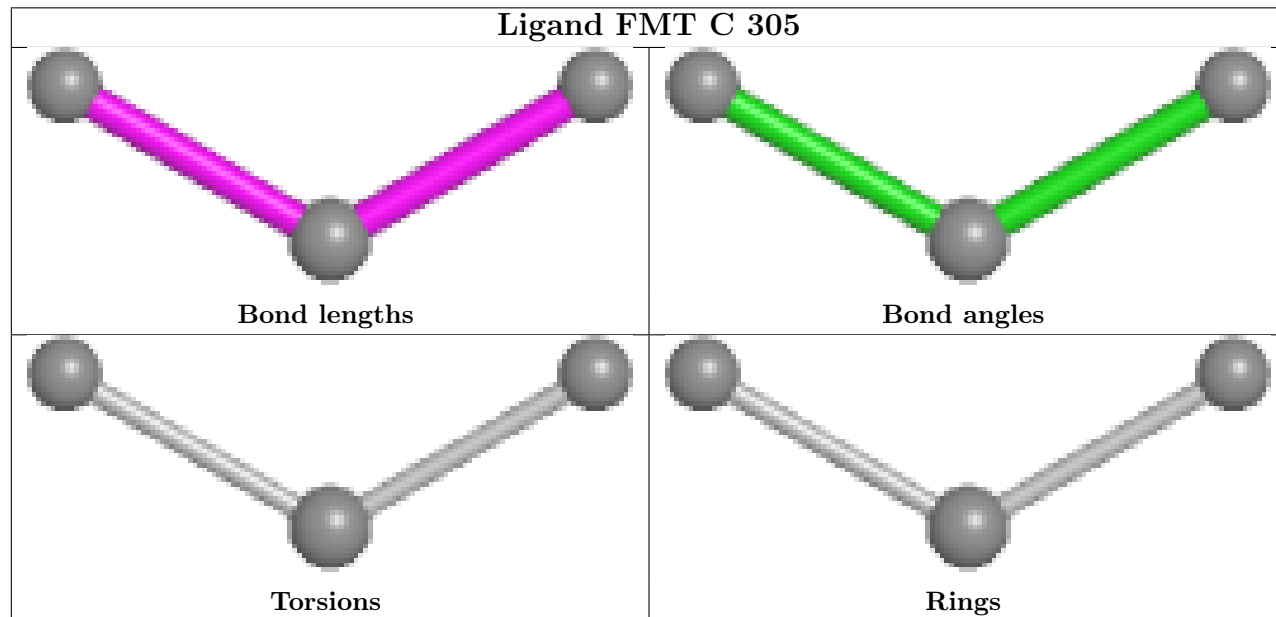
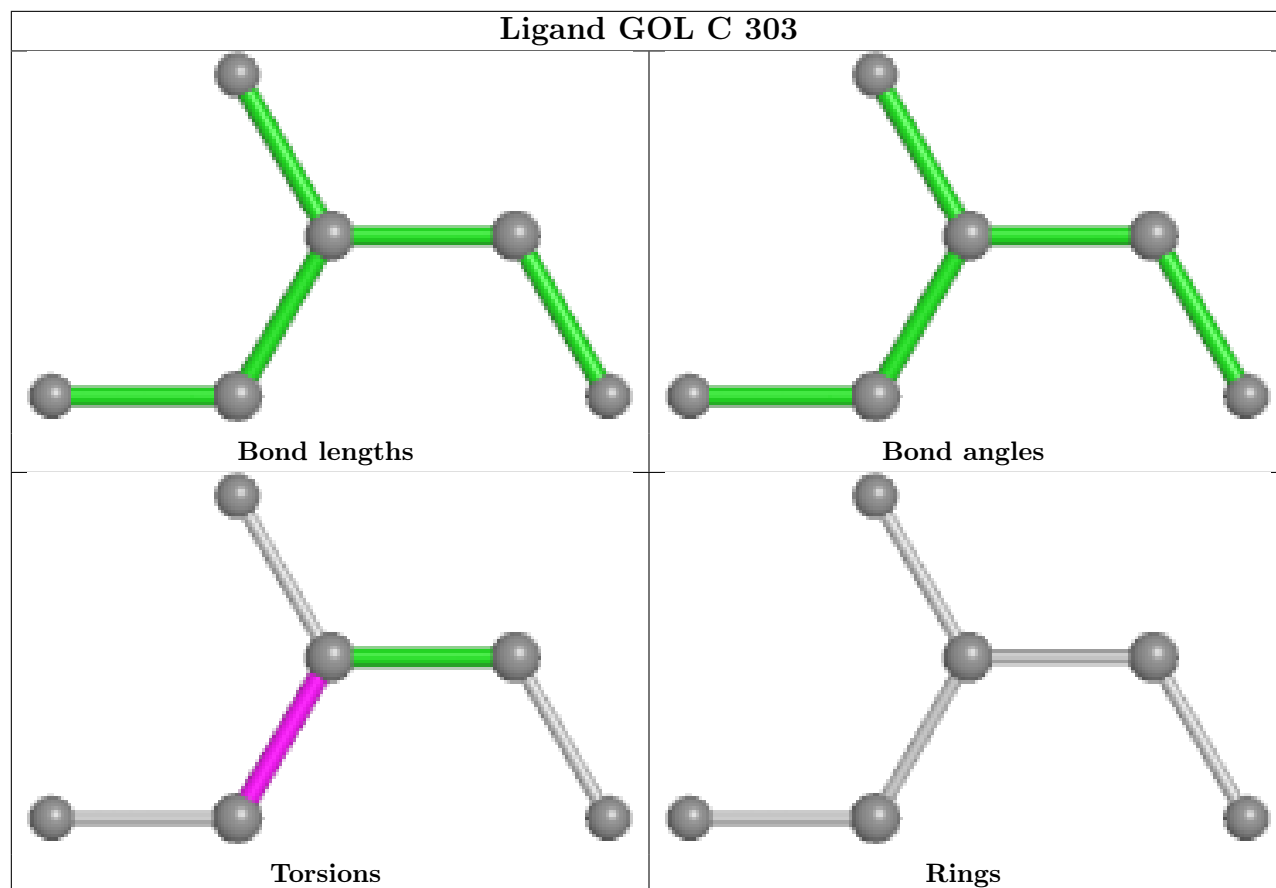


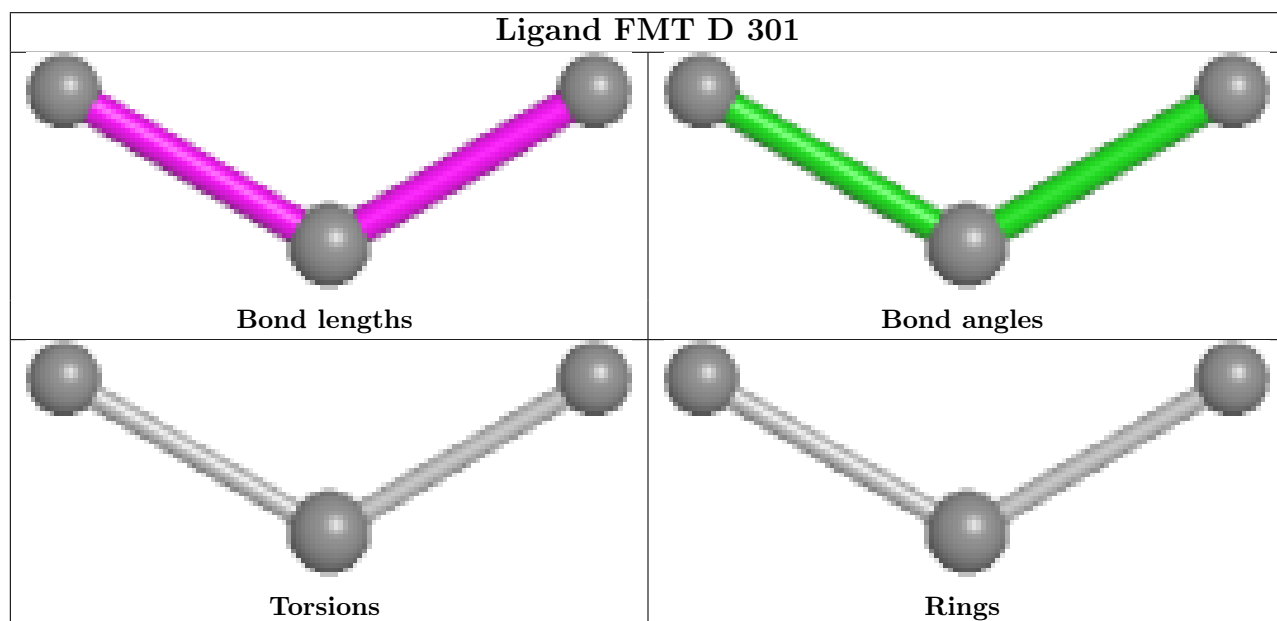
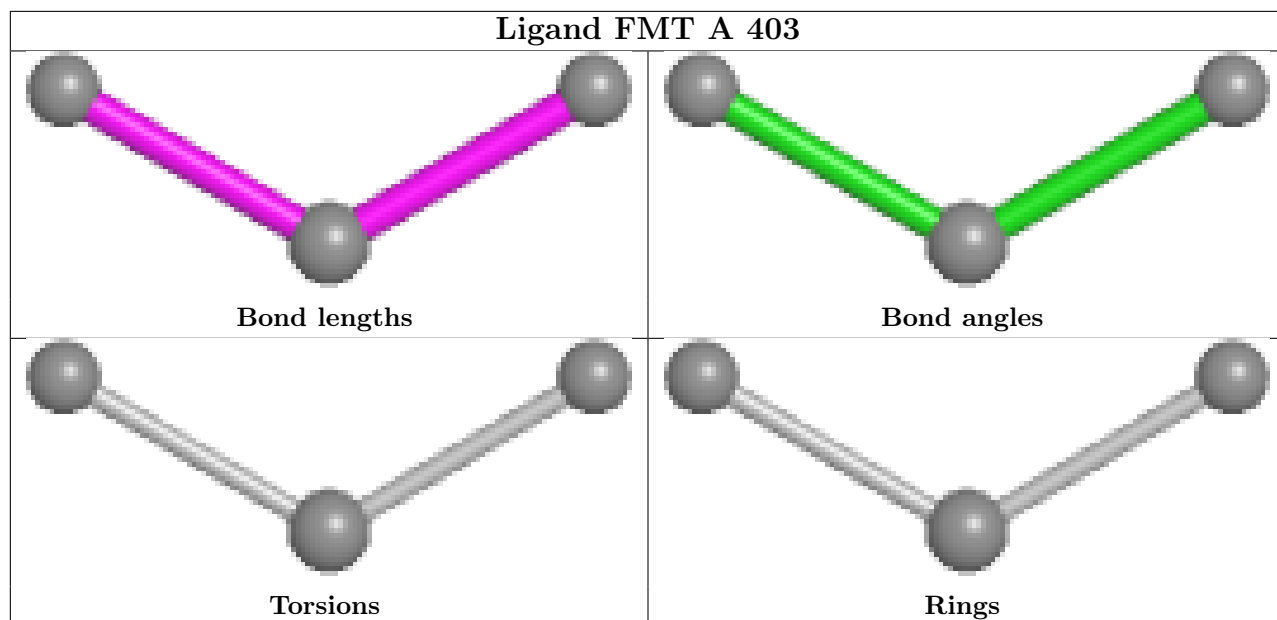


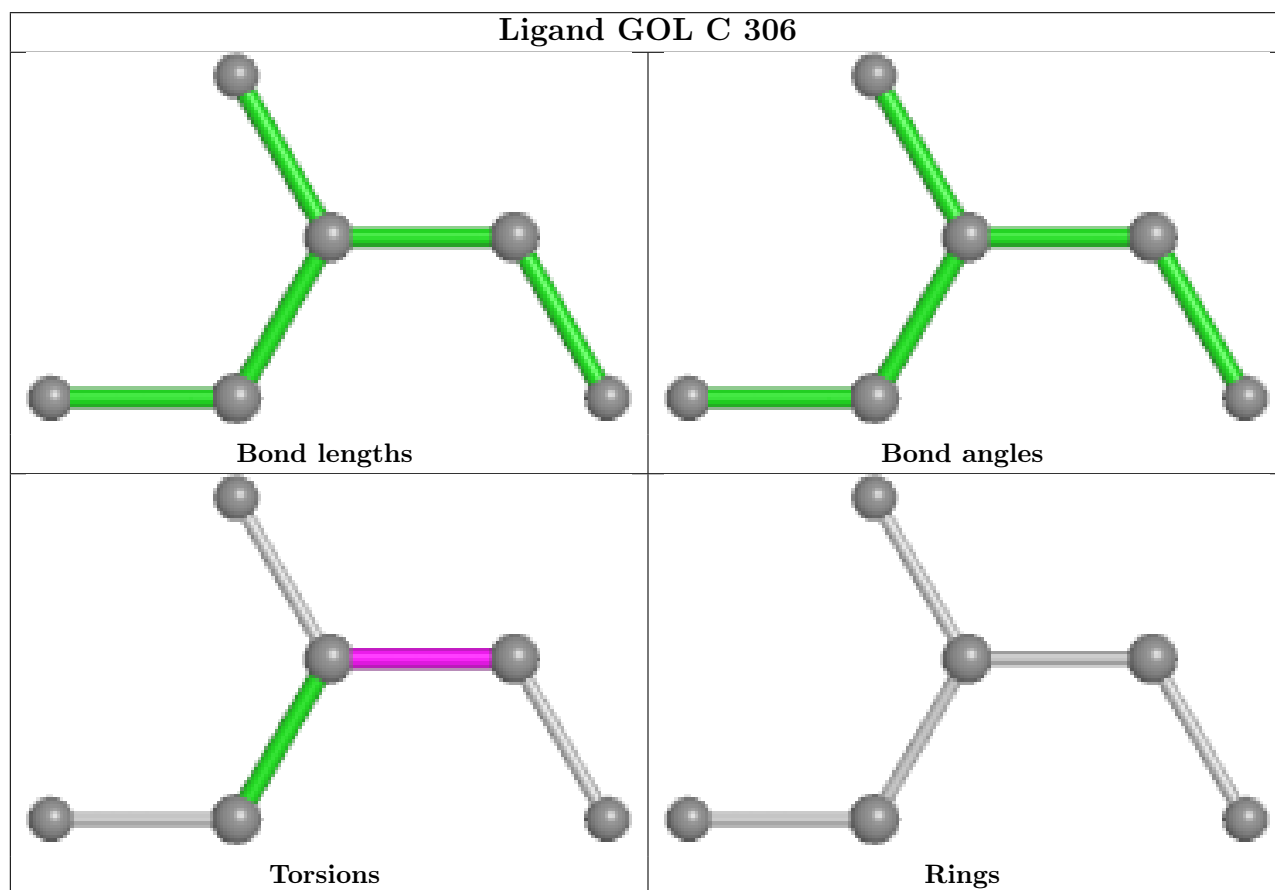
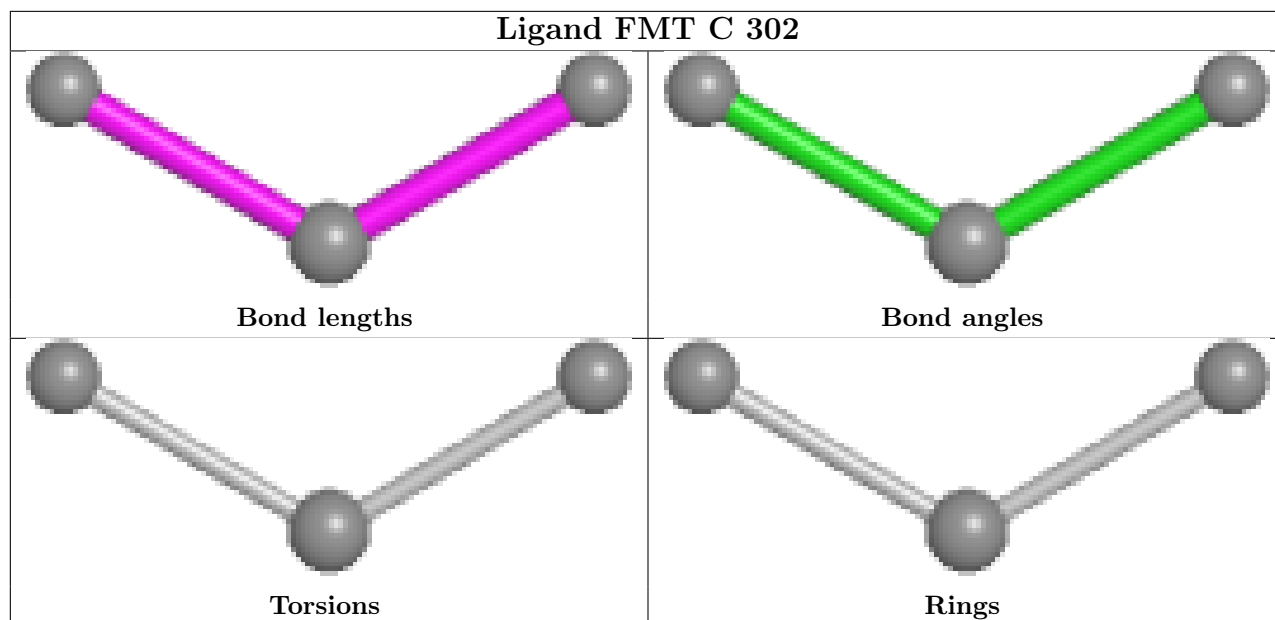


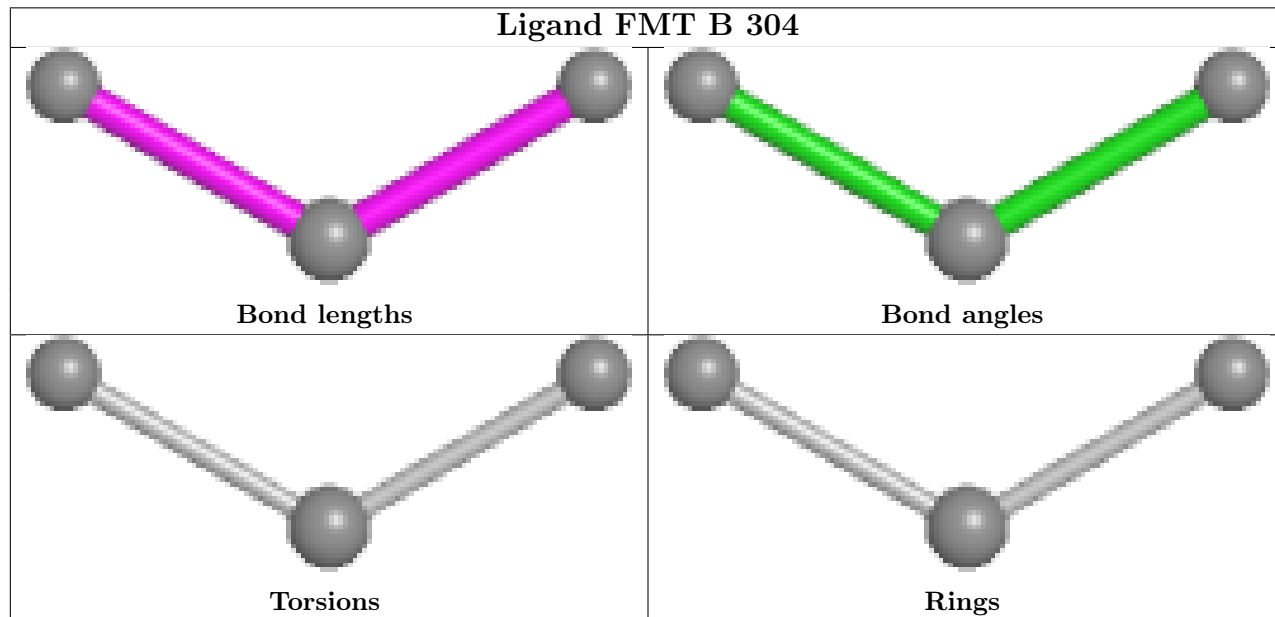
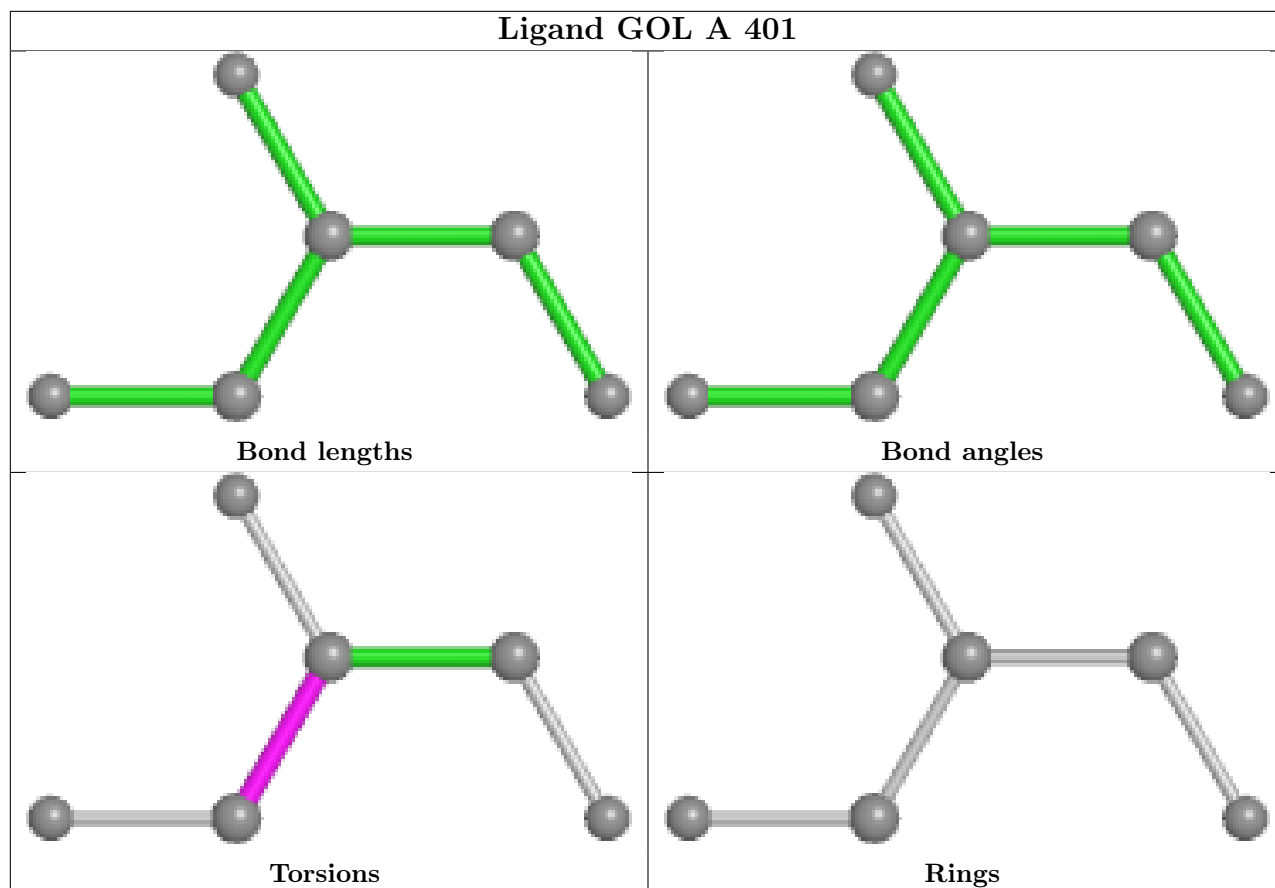


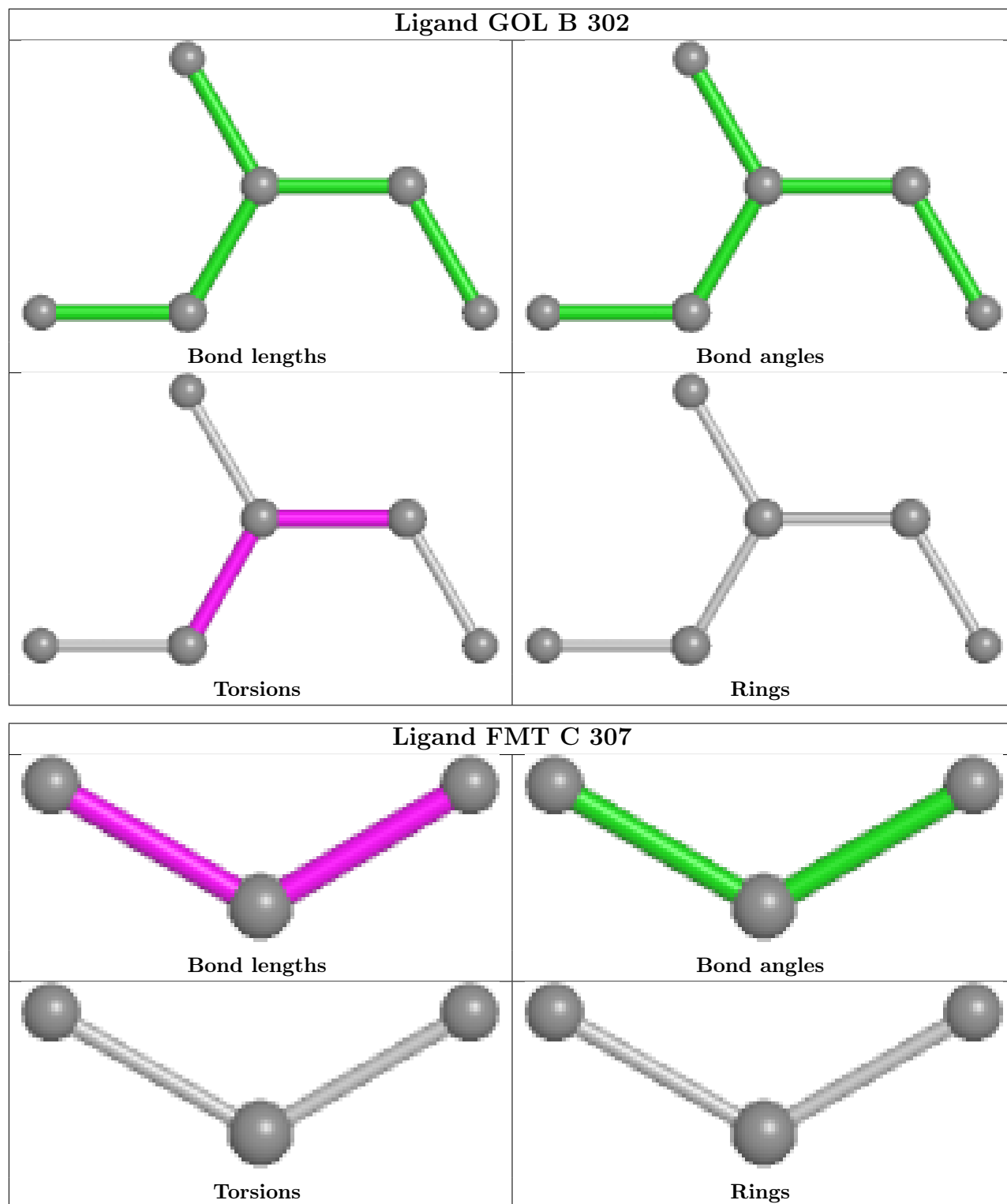


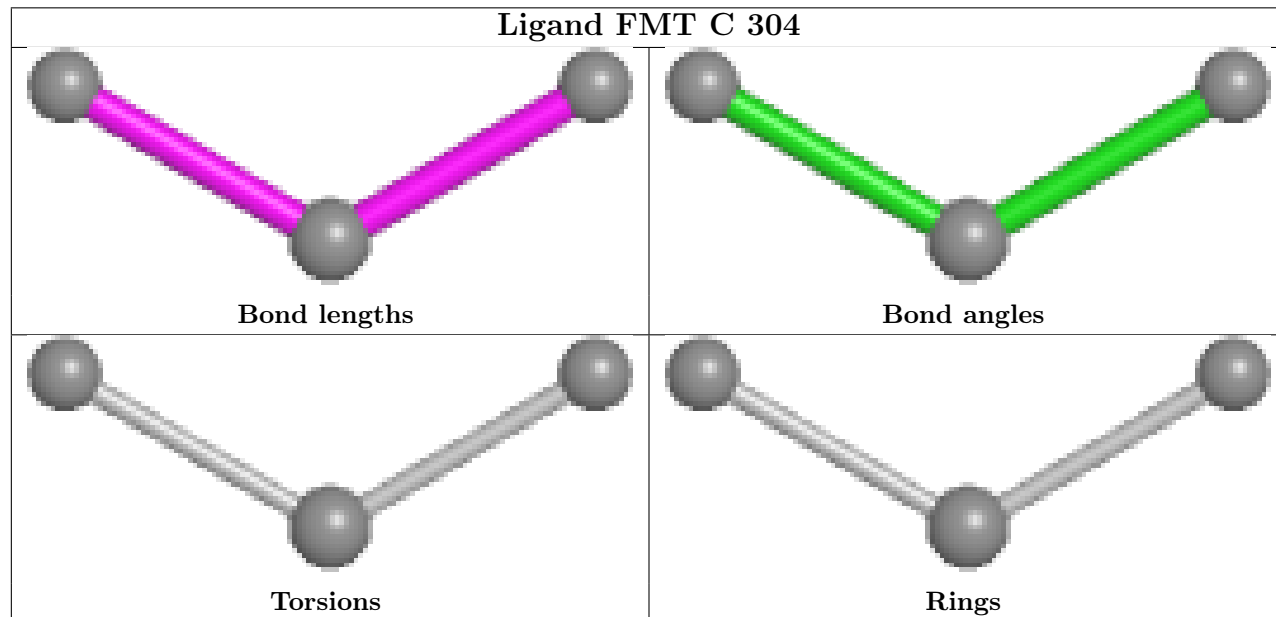
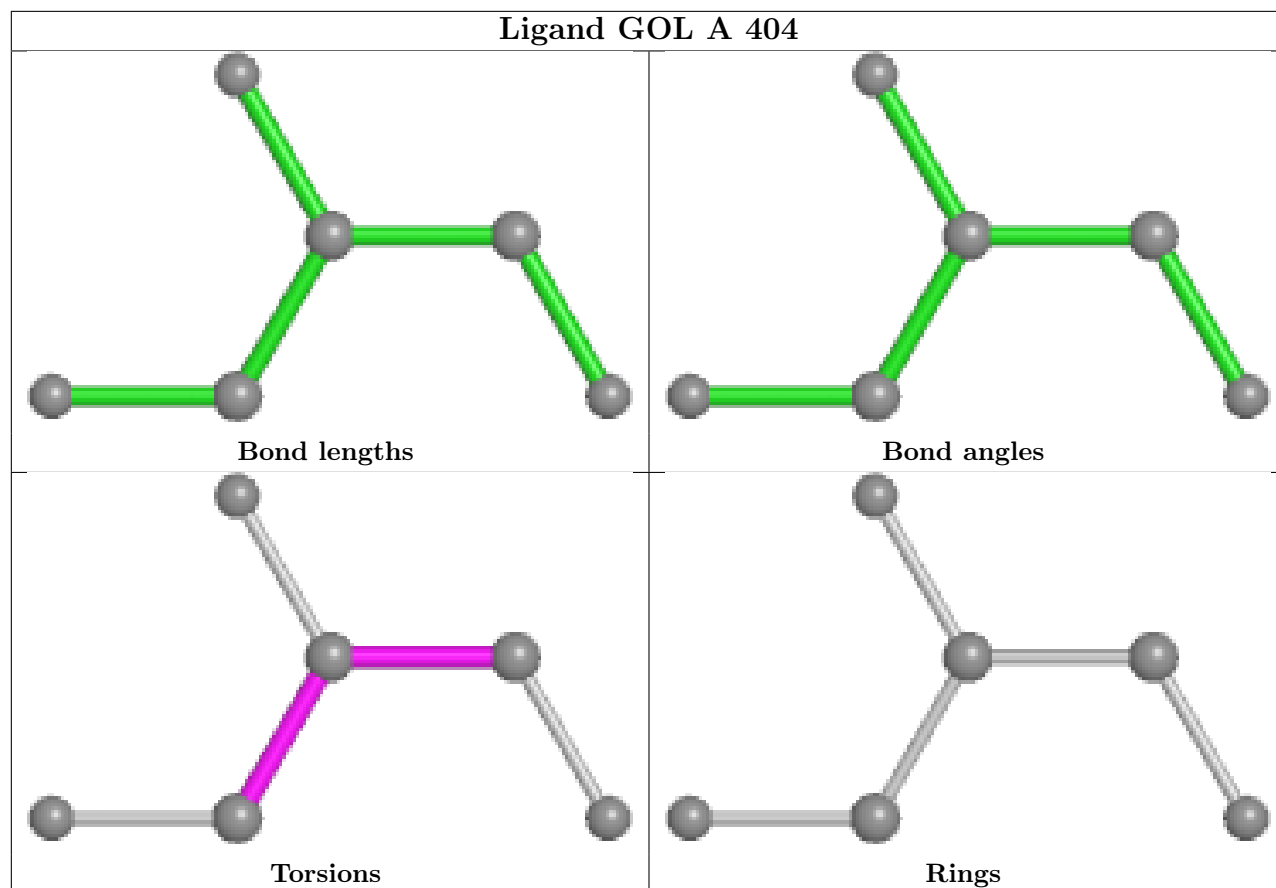


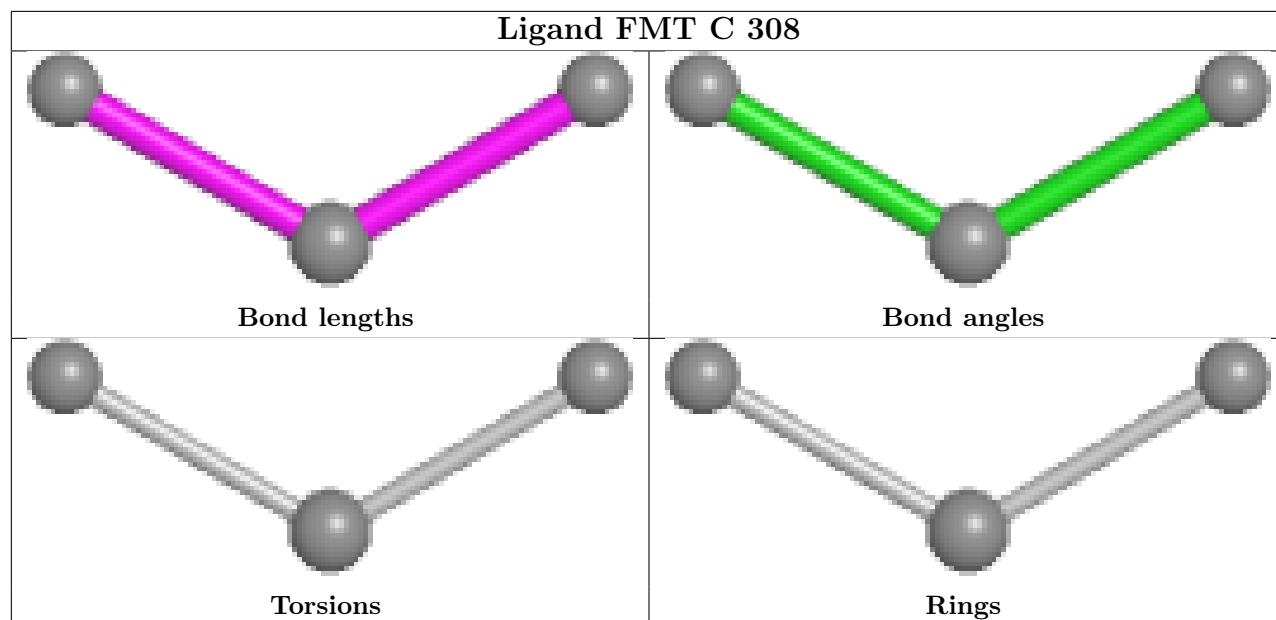












5.7 Other polymers [i](#)

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	283/296 (95%)	0.11	2 (0%) 87 87	12, 20, 32, 71	0
1	B	282/296 (95%)	0.09	4 (1%) 75 75	12, 22, 35, 55	0
1	C	284/296 (95%)	0.01	0 100 100	12, 18, 29, 47	0
1	D	277/296 (93%)	2.89	165 (59%) 0 0	20, 50, 85, 145	0
All	All	1126/1184 (95%)	0.76	171 (15%) 2 1	12, 23, 64, 145	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	244	ALA	19.9
1	D	247	TRP	11.6
1	D	277	VAL	11.0
1	D	253	VAL	9.4
1	D	216	LEU	9.3
1	D	215	PHE	8.9
1	D	217	SER	7.8
1	D	128	ALA	7.7
1	D	160	VAL	7.6
1	D	108	TYR	7.2
1	D	226	ILE	7.1
1	D	269	ILE	7.1
1	D	280	VAL	7.0
1	D	213	ALA	7.0
1	D	127	TRP	6.9
1	D	112	ILE	6.9
1	D	39	ILE	6.6
1	D	80	PHE	6.4
1	D	237	GLY	6.3
1	D	233	ILE	6.2
1	D	222	PRO	6.1

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Mol	Chain	Res	Type	RSRZ
1	D	236	GLU	5.9
1	D	218	ARG	5.8
1	D	117	TYR	5.8
1	D	42	LEU	5.8
1	D	225	LEU	5.7
1	D	45	VAL	5.7
1	D	164	VAL	5.7
1	D	243	PHE	5.7
1	D	168	LEU	5.5
1	D	103	TYR	5.5
1	D	102	PHE	5.4
1	D	49	LEU	5.4
1	D	93	VAL	5.4
1	D	116	ALA	5.3
1	D	178	THR	5.3
1	D	256	ALA	5.3
1	D	242	ASP	5.3
1	D	241	LEU	5.3
1	D	174	ALA	5.2
1	D	167	GLN	5.1
1	D	89	VAL	5.1
1	D	122	VAL	5.0
1	D	135	PRO	5.0
1	D	231	GLY	4.9
1	D	278	LEU	4.9
1	D	136	LEU	4.9
1	D	90	VAL	4.9
1	D	273	VAL	4.8
1	D	14	ILE	4.8
1	D	109	PRO	4.8
1	D	169	THR	4.7
1	D	38	VAL	4.7
1	D	21	PRO	4.7
1	D	33	TYR	4.7
1	D	24	PHE	4.6
1	D	88	ASN	4.5
1	D	266	PRO	4.5
1	D	19	GLY	4.5
1	D	257	GLY	4.5
1	D	220	ASP	4.4
1	D	48	CYS	4.4
1	D	239	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	110	GLU	4.3
1	D	173	MET	4.3
1	D	159	VAL	4.2
1	D	86	THR	4.2
1	D	105	ALA	4.2
1	D	260	PHE	4.1
1	D	230	PRO	4.1
1	D	161	PRO	4.0
1	D	258	ARG	3.9
1	D	41	HIS	3.9
1	D	270	GLY	3.9
1	D	16	VAL	3.9
1	D	126	THR	3.8
1	D	238	GLY	3.8
1	D	40	PRO	3.8
1	D	98	SER	3.8
1	D	121	LEU	3.8
1	D	224	LEU	3.8
1	D	176	TYR	3.7
1	D	232	ALA	3.7
1	D	219	SER	3.7
1	D	268	ALA	3.6
1	D	276	PHE	3.6
1	D	255	VAL	3.6
1	D	209	VAL	3.5
1	D	281	ARG	3.5
1	D	92	VAL	3.5
1	D	170	GLU	3.5
1	D	119	ASP	3.5
1	D	199	GLU	3.5
1	D	50	ALA	3.4
1	D	149	ALA	3.4
1	D	133	TYR	3.3
1	D	227	VAL	3.3
1	D	271	ALA	3.3
1	D	17	GLY	3.2
1	D	36	ARG	3.1
1	D	120	ALA	3.1
1	D	246	SER	3.1
1	D	212	TYR	3.1
1	B	279	ASP	3.0
1	D	249	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	91	LEU	3.0
1	D	131	THR	3.0
1	D	275	ALA	3.0
1	D	198	VAL	3.0
1	D	205	VAL	2.9
1	D	22	ILE	2.8
1	D	259	HIS	2.8
1	D	20	ASP	2.8
1	D	44	ASP	2.8
1	D	43	SER	2.8
1	D	272	ALA	2.8
1	D	124	PRO	2.8
1	D	34	LEU	2.8
1	D	106	LEU	2.8
1	D	156	VAL	2.7
1	D	248	PRO	2.7
1	D	79	TRP	2.7
1	D	129	GLY	2.7
1	D	175	VAL	2.6
1	D	130	PHE	2.6
1	D	134	GLU	2.6
1	D	210	GLN	2.6
1	D	201	GLU	2.6
1	D	214	ASP	2.6
1	D	99	ALA	2.5
1	D	13	TYR	2.5
1	D	261	LEU	2.5
1	D	240	GLU	2.5
1	D	208	MET	2.5
1	B	128	ALA	2.5
1	D	228	ALA	2.5
1	D	35	TRP	2.5
1	D	197	PRO	2.5
1	D	264	ASP	2.5
1	D	267	ASP	2.5
1	D	18	GLN	2.5
1	D	154	VAL	2.4
1	D	221	ILE	2.4
1	D	203	ALA	2.4
1	D	181	PRO	2.4
1	D	206	GLN	2.4
1	D	84	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	283	ARG	2.4
1	D	207	ALA	2.3
1	D	171	GLU	2.3
1	D	251	ARG	2.3
1	D	101	GLY	2.3
1	D	123	GLN	2.3
1	D	82	ALA	2.3
1	D	94	HIS	2.2
1	D	172	GLU	2.2
1	D	37	ASN	2.2
1	D	69	PHE	2.2
1	D	139	ALA	2.1
1	D	115	ILE	2.1
1	D	118	MET	2.1
1	B	280	VAL	2.1
1	B	248	PRO	2.1
1	D	76	LEU	2.1
1	D	104	ARG	2.1
1	A	82	ALA	2.1
1	D	137	MET	2.0
1	D	245	ARG	2.0
1	D	4	VAL	2.0
1	D	85	ILE	2.0
1	D	30	THR	2.0

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

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

6.3 Carbohydrates [i](#)

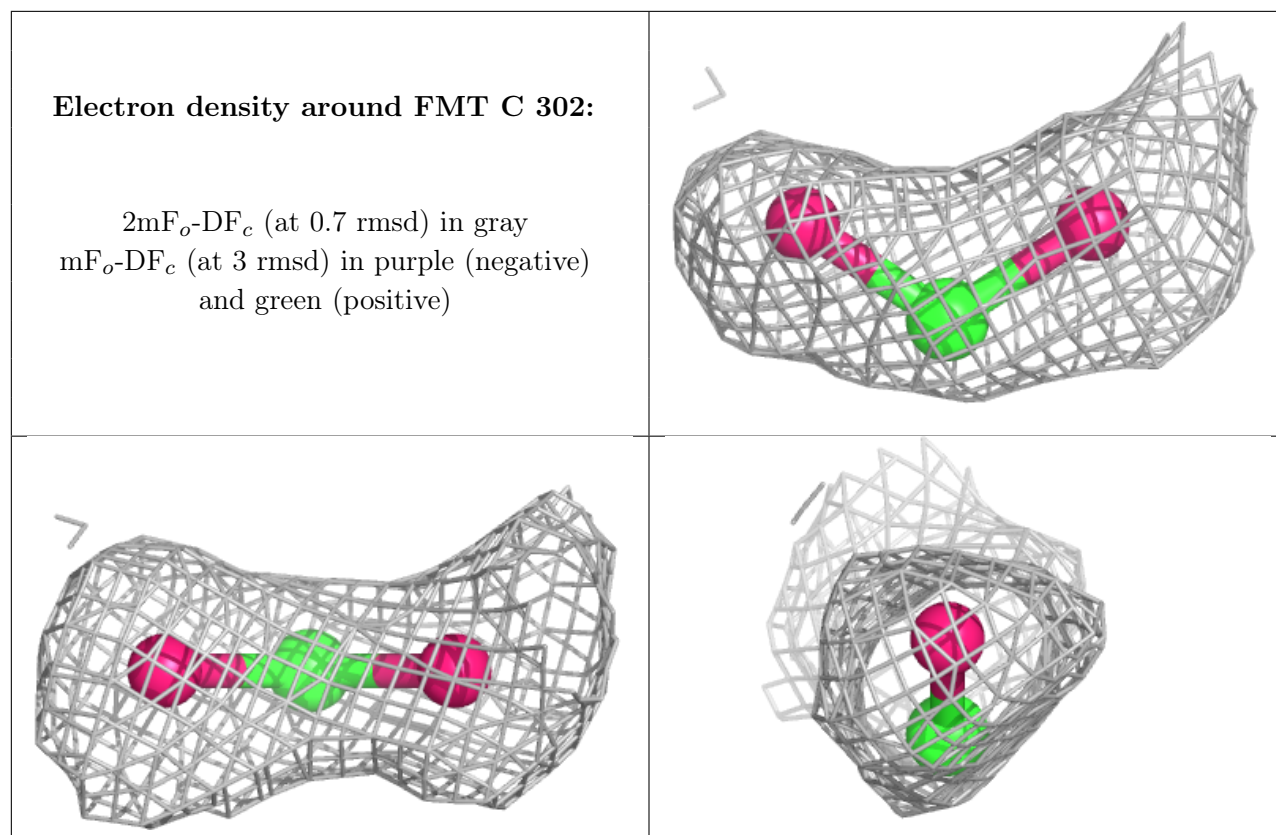
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

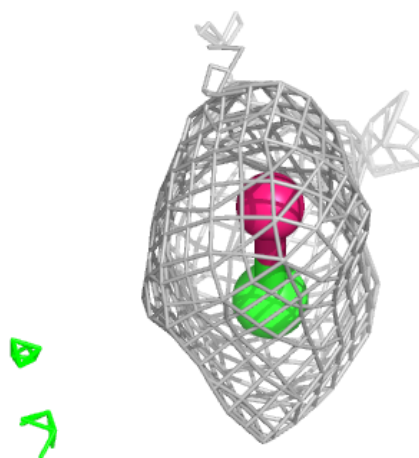
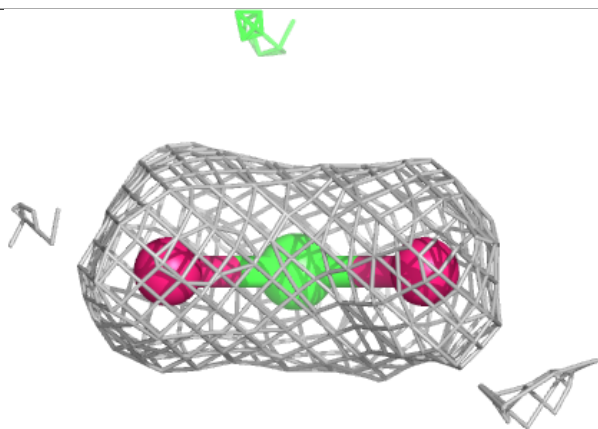
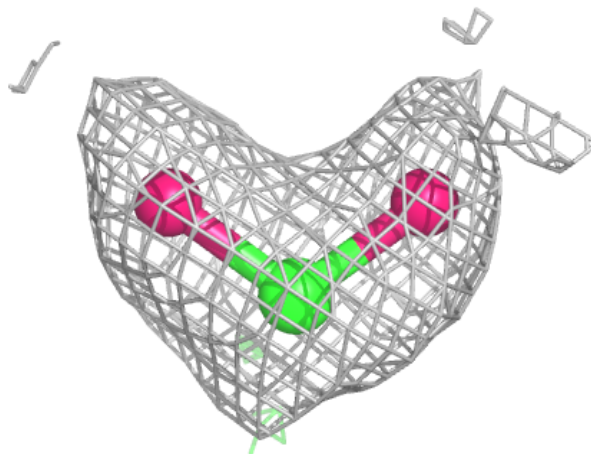
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FMT	C	302	3/3	0.71	0.13	49,49,52,52	0
3	FMT	C	304	3/3	0.76	0.14	56,56,59,61	0
2	GOL	B	301	6/6	0.78	0.14	59,61,63,68	0
2	GOL	C	303	6/6	0.81	0.15	47,51,54,56	0
2	GOL	B	302	6/6	0.82	0.17	25,46,54,55	0
3	FMT	A	405	3/3	0.83	0.13	37,37,41,42	0
3	FMT	B	306	3/3	0.84	0.15	50,50,52,54	0
3	FMT	A	406	3/3	0.85	0.21	43,43,45,47	0
2	GOL	A	401	6/6	0.86	0.10	28,30,34,35	0
3	FMT	C	305	3/3	0.87	0.10	56,56,60,63	0
2	GOL	C	301	6/6	0.88	0.14	24,33,36,37	0
3	FMT	B	304	3/3	0.88	0.12	46,46,48,53	0
3	FMT	C	308	3/3	0.88	0.18	33,33,38,40	0
3	FMT	A	403	3/3	0.89	0.10	37,37,42,43	0
3	FMT	D	301	3/3	0.89	0.08	26,26,29,33	0
4	ACT	B	303	4/4	0.89	0.10	24,31,35,39	0
2	GOL	C	306	6/6	0.91	0.10	26,43,48,50	0
3	FMT	C	307	3/3	0.92	0.12	20,20,21,22	0
3	FMT	B	305	3/3	0.94	0.08	34,34,39,43	0
3	FMT	A	402	3/3	0.95	0.08	24,24,26,27	0
2	GOL	A	404	6/6	0.96	0.08	22,32,44,53	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.



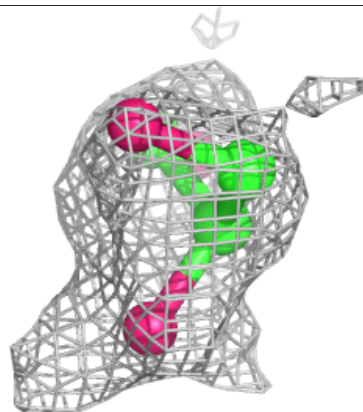
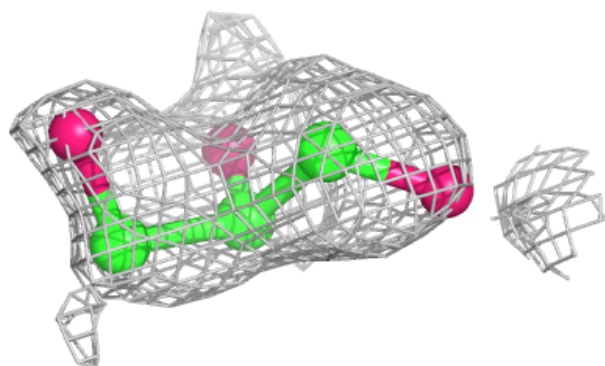
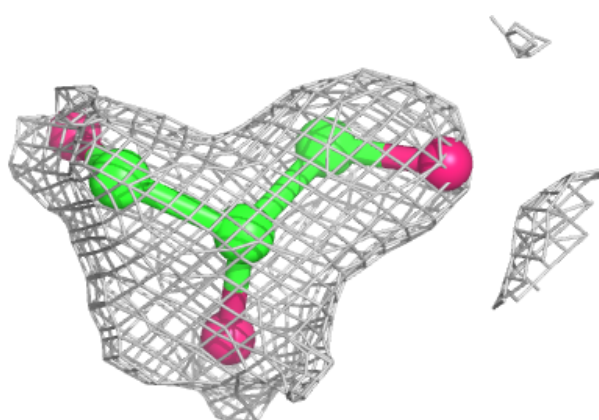
Electron density around FMT C 304:

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

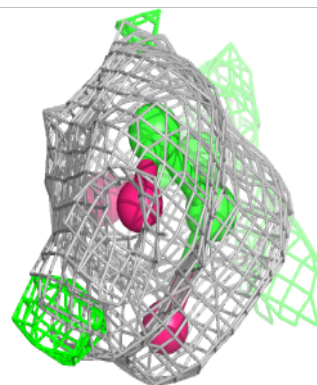
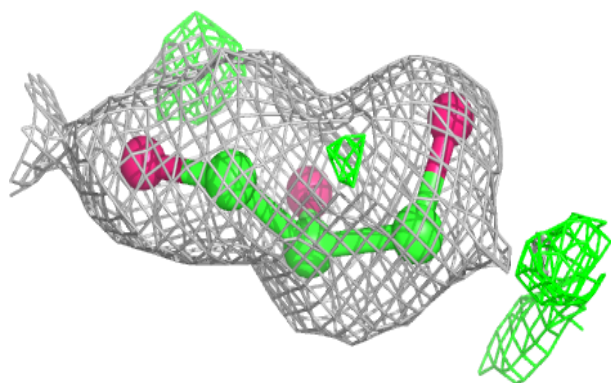
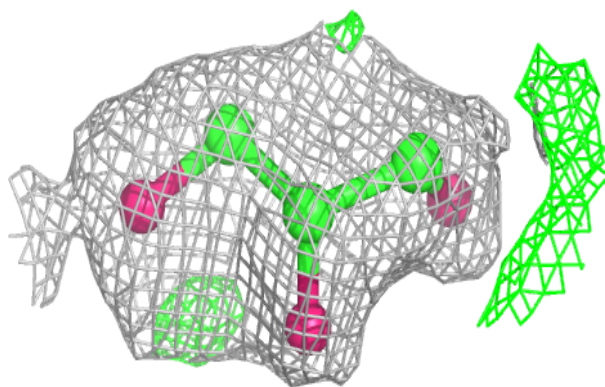


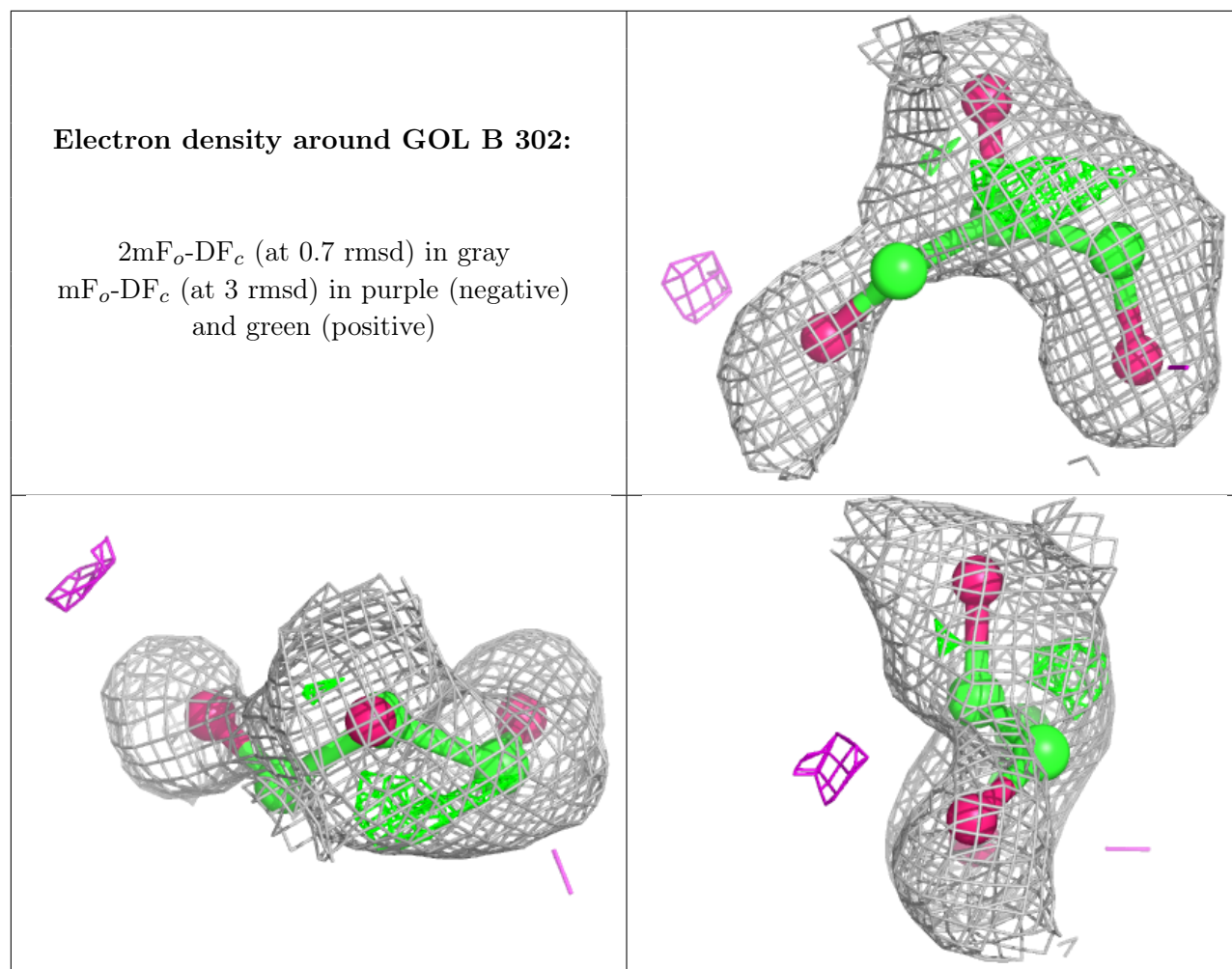
Electron density around GOL B 301:

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

**Electron density around GOL C 303:**

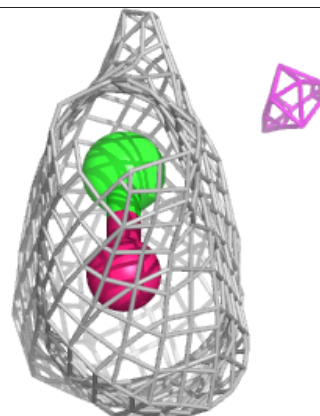
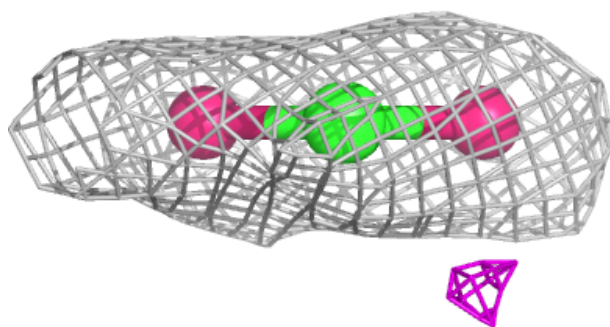
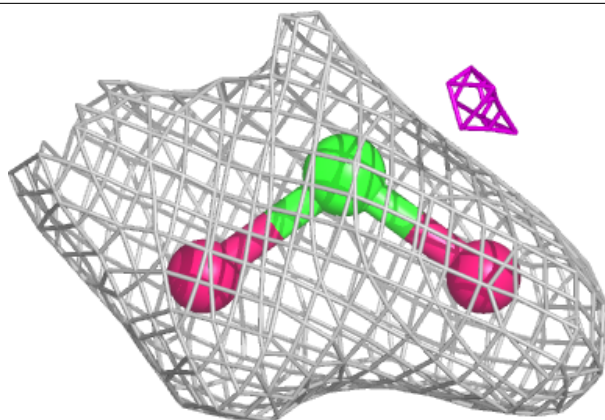
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



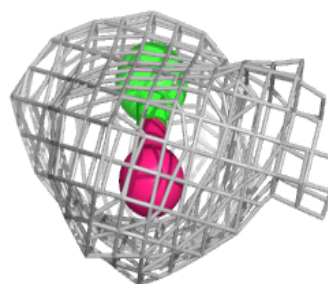
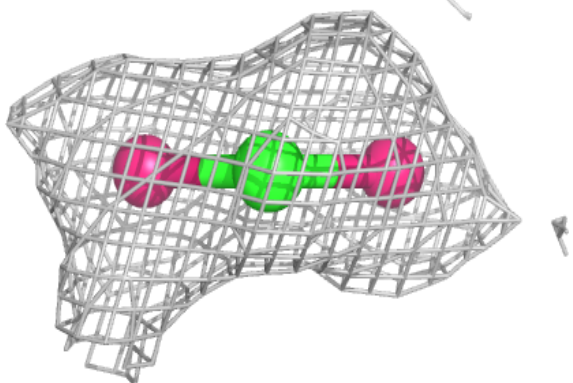
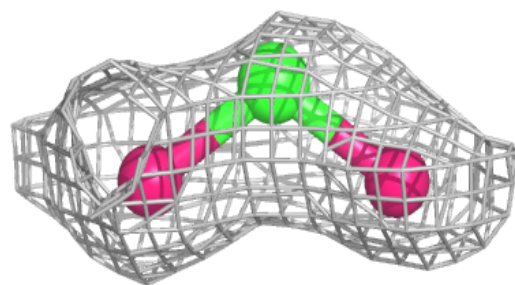


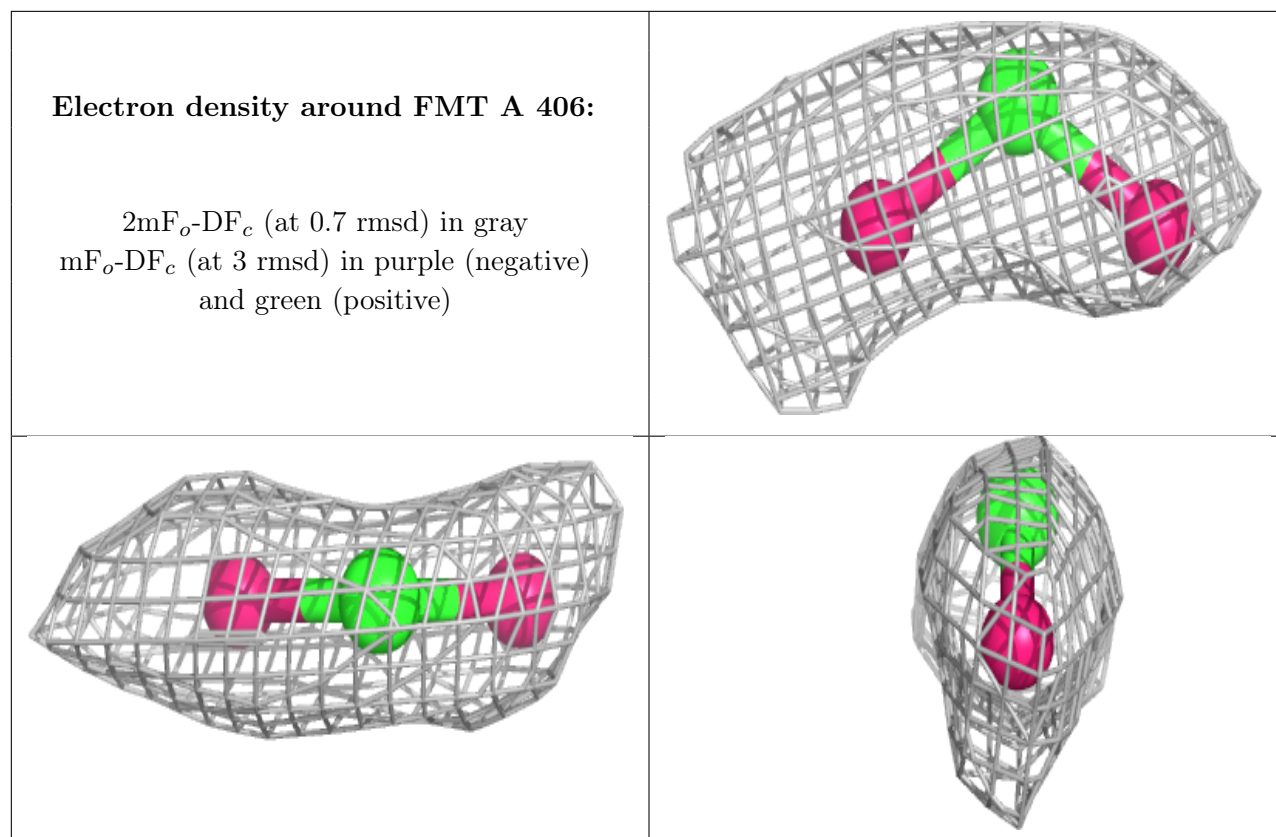
Electron density around FMT A 405:

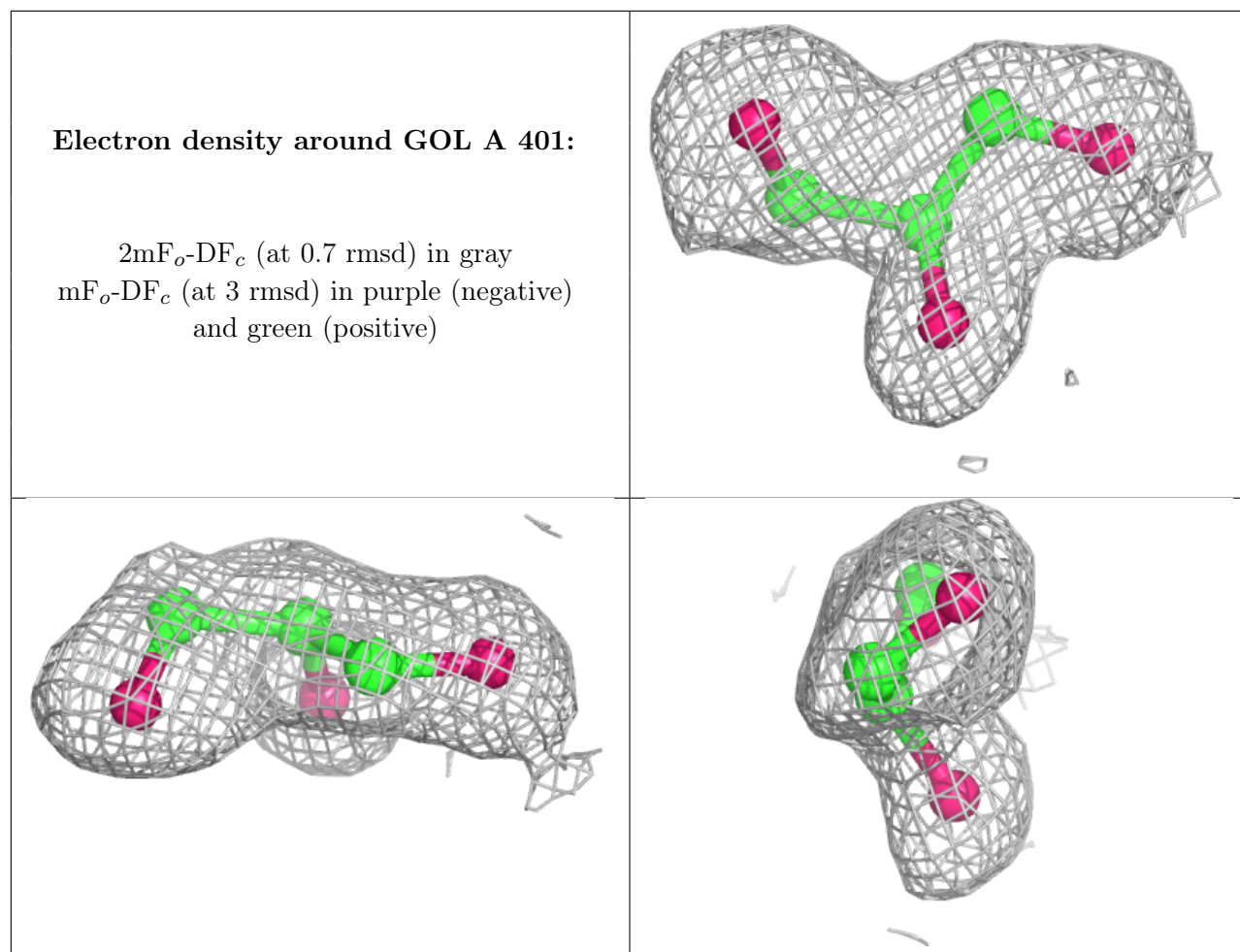
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FMT B 306:**

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

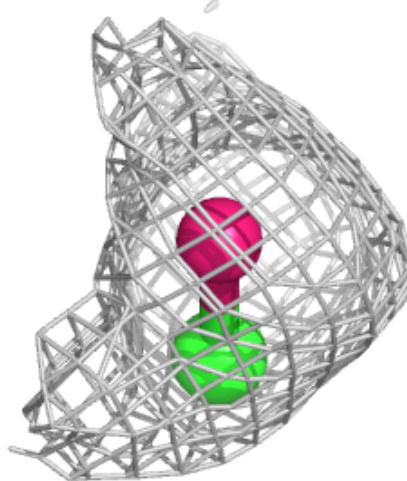
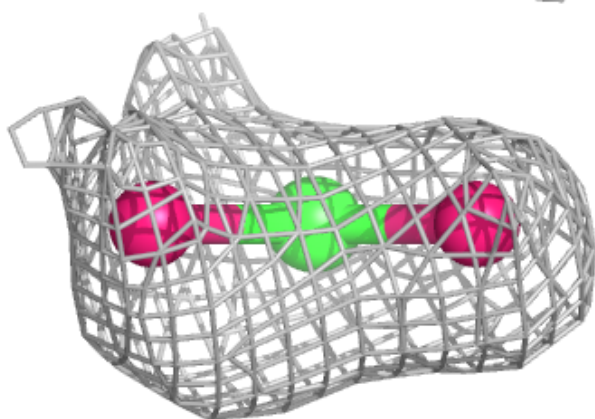
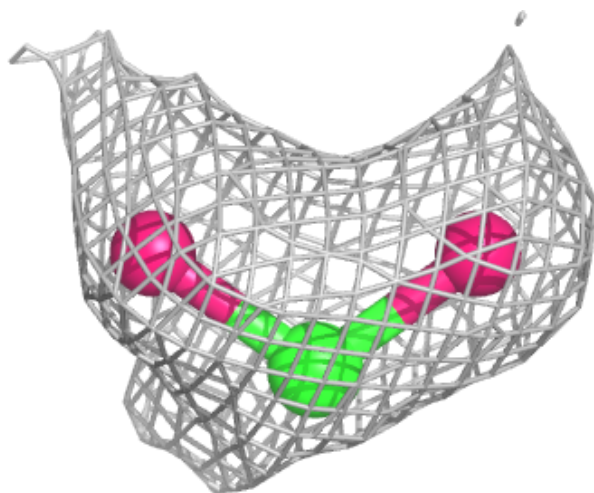


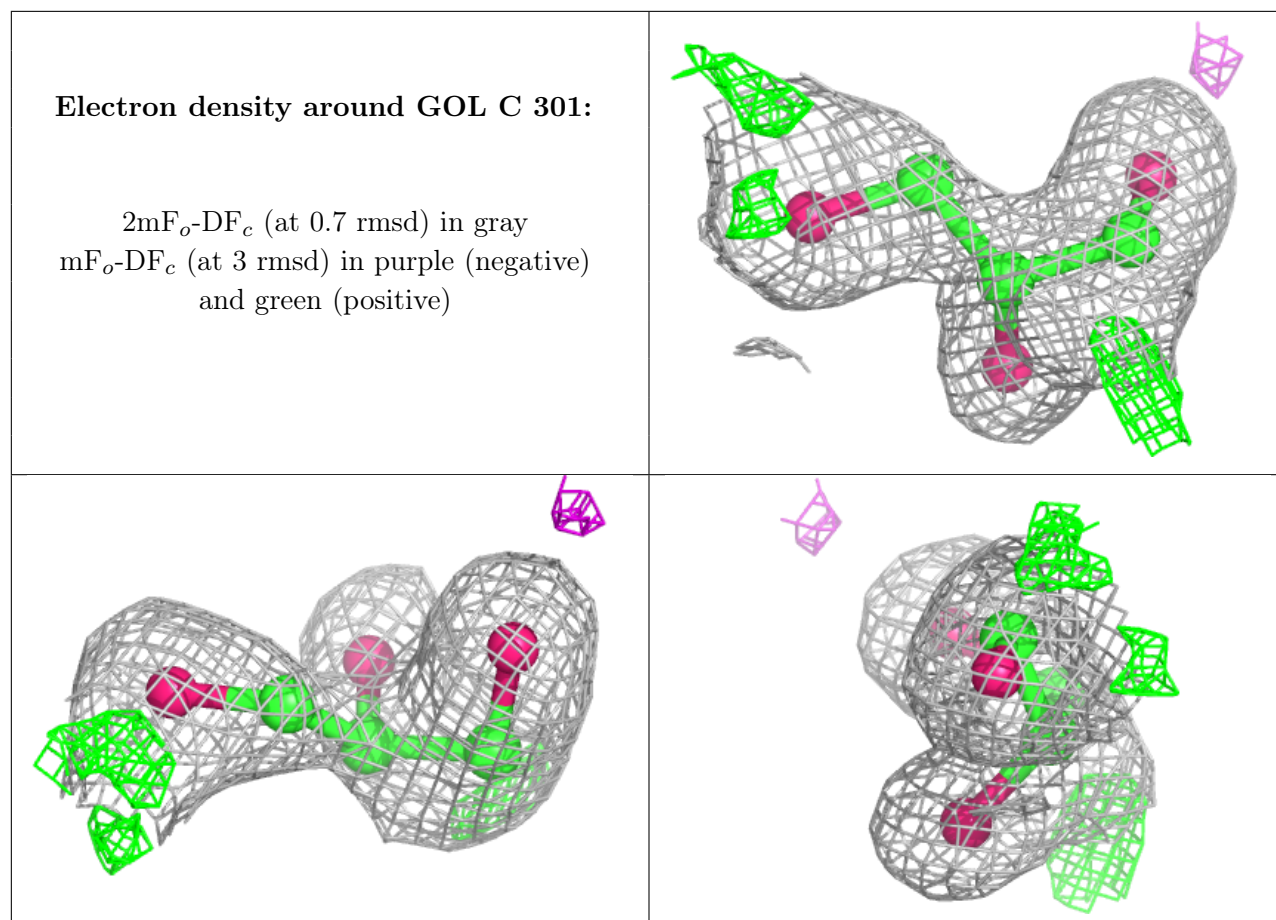




Electron density around FMT C 305:

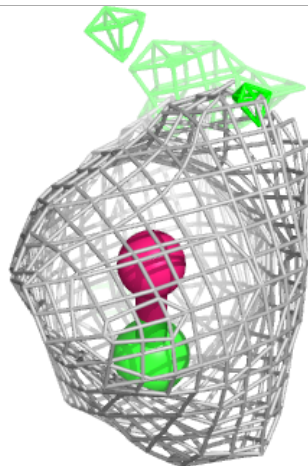
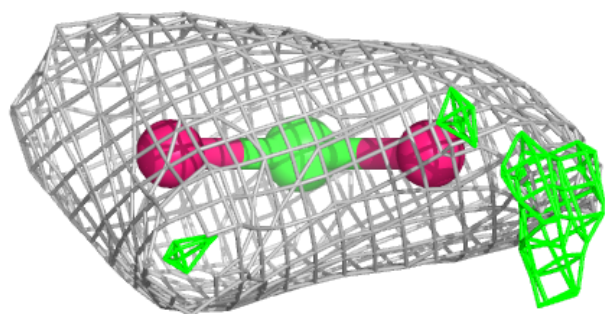
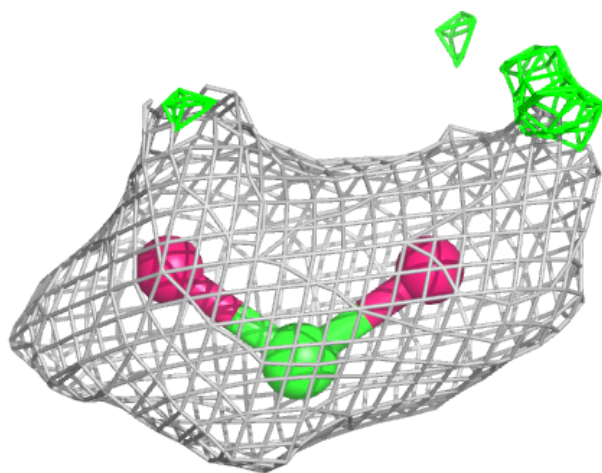
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





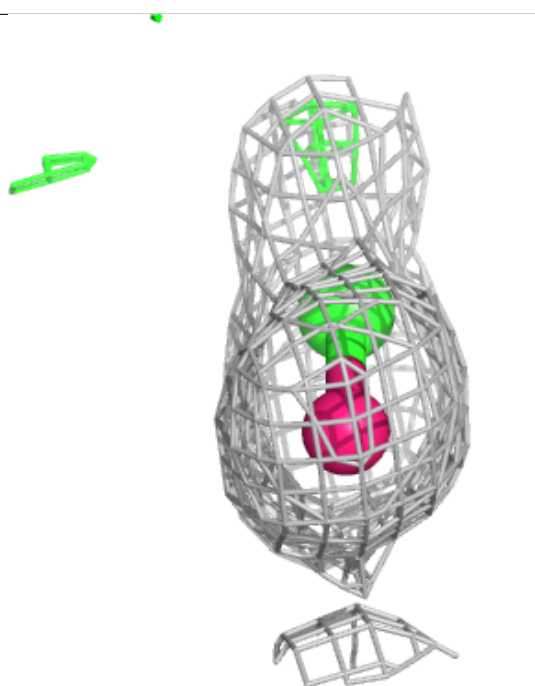
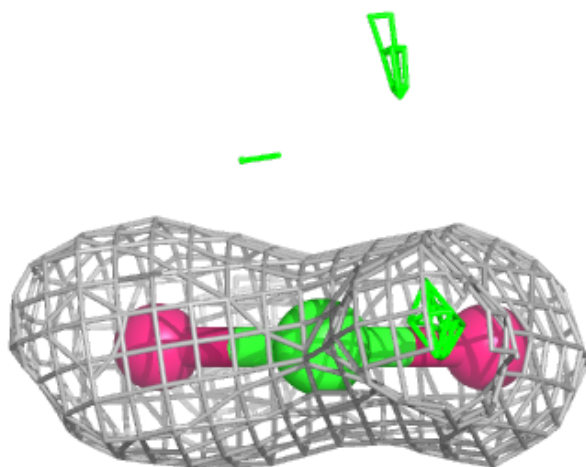
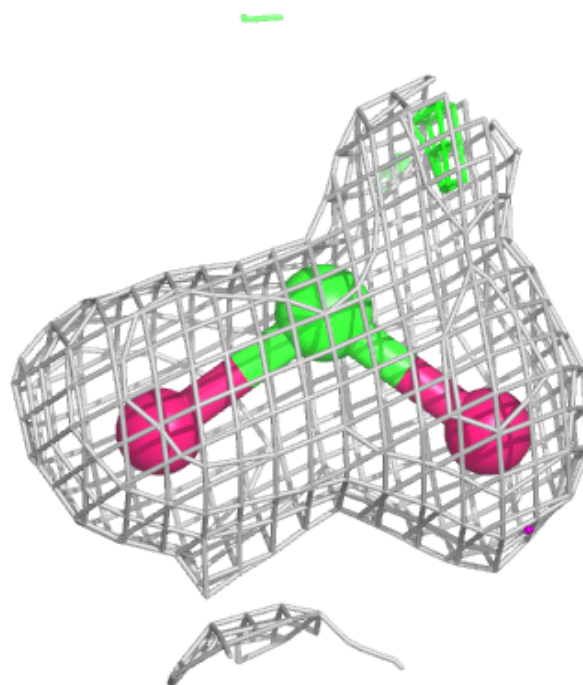
Electron density around FMT B 304:

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



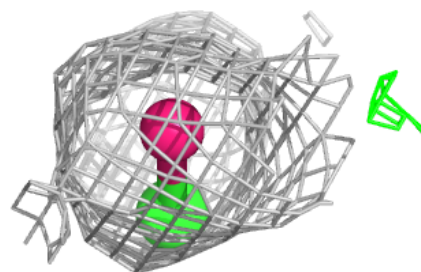
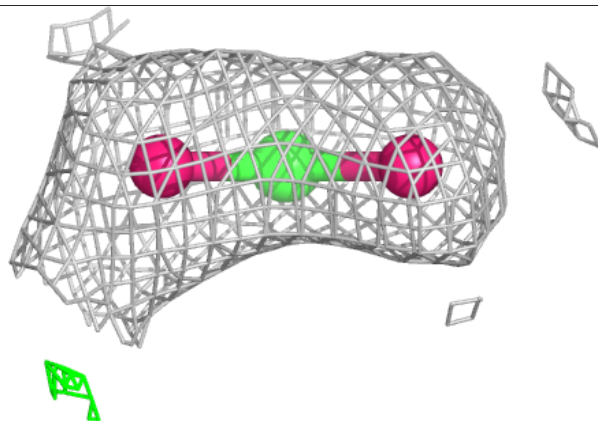
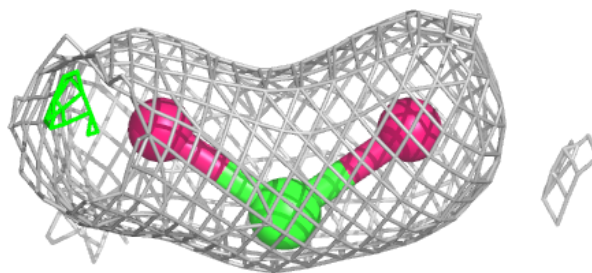
Electron density around FMT C 308:

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

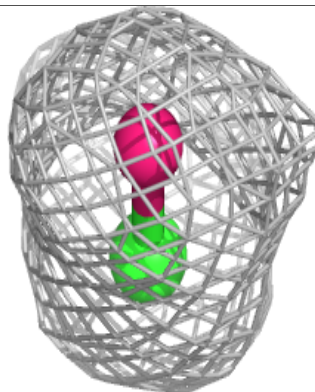
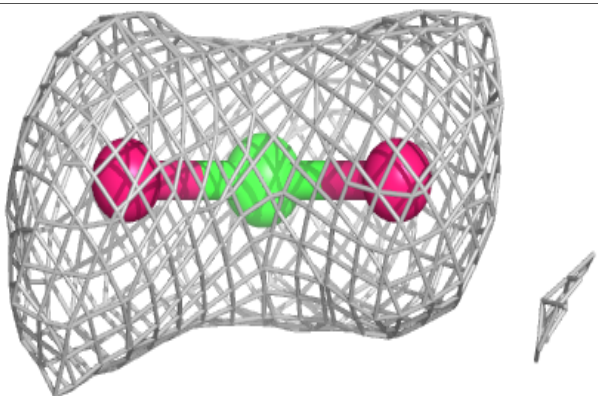
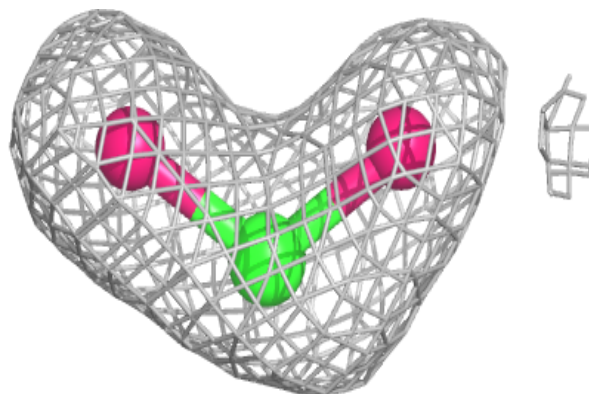


Electron density around FMT A 403:

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

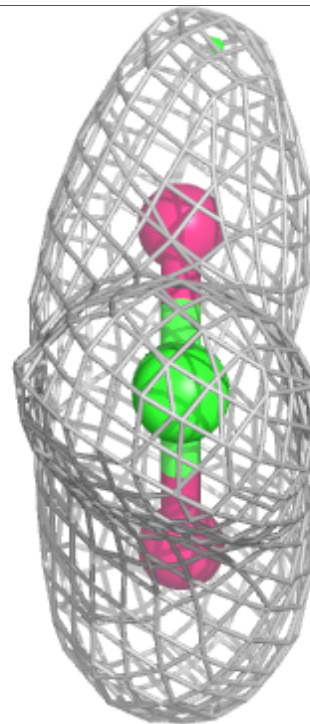
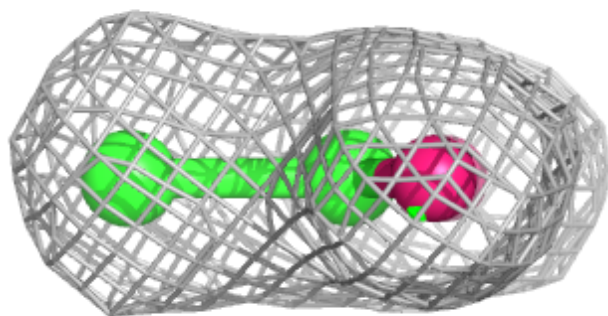
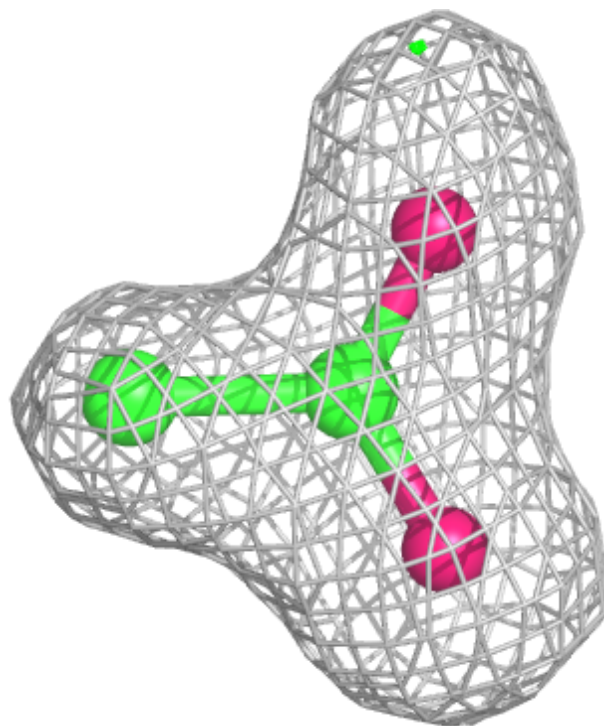
**Electron density around FMT D 301:**

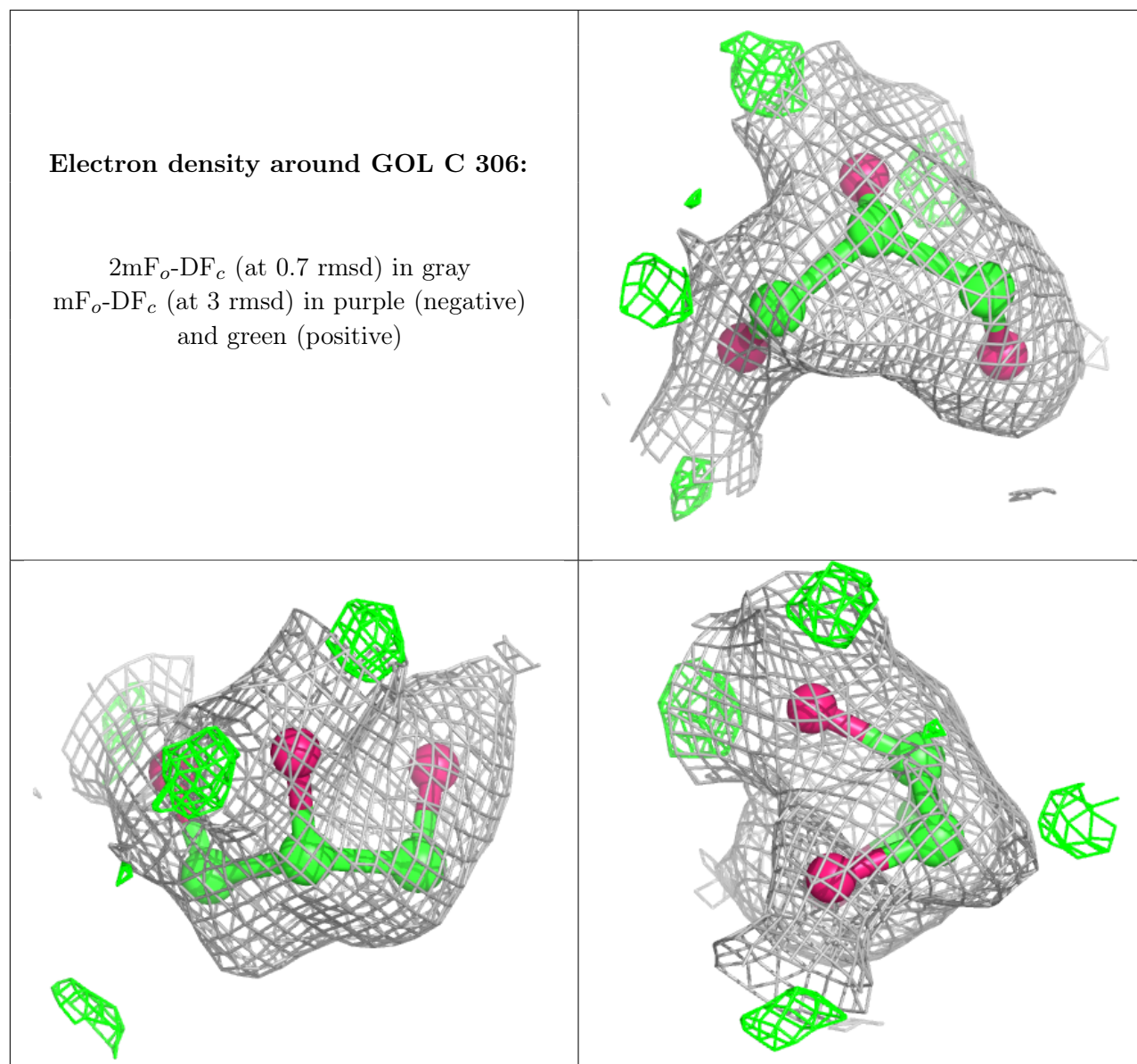
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ACT B 303:

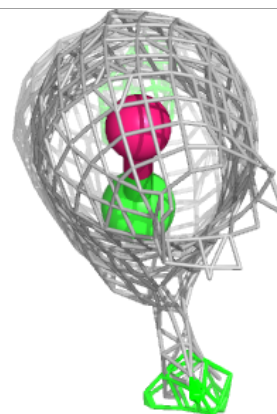
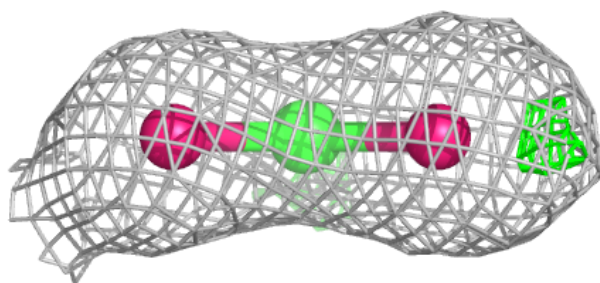
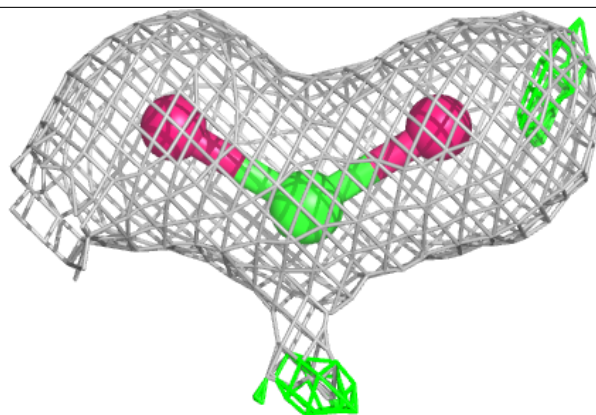
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



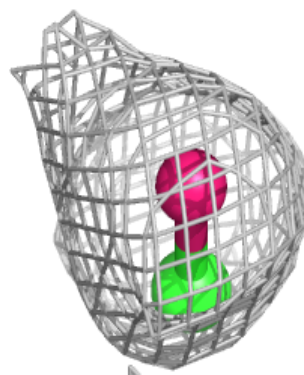
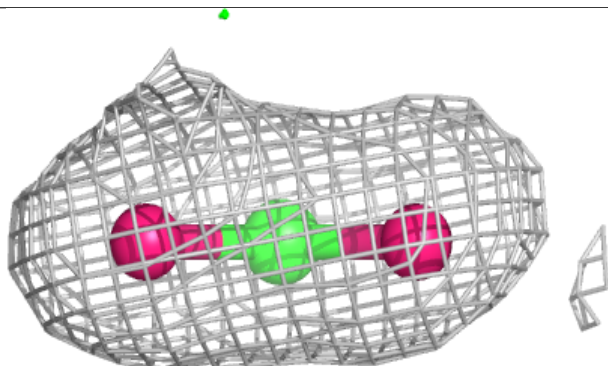
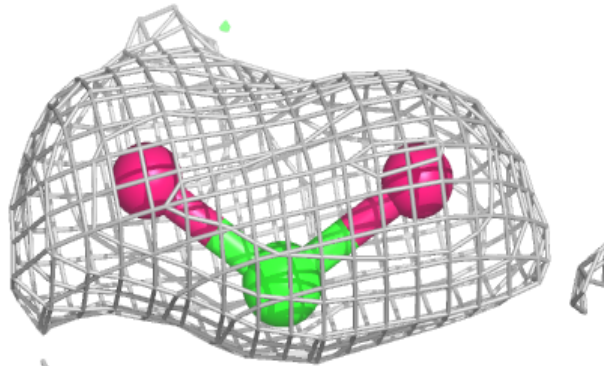


Electron density around FMT C 307:

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

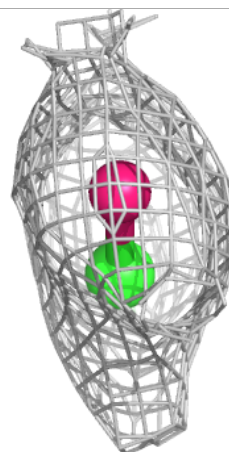
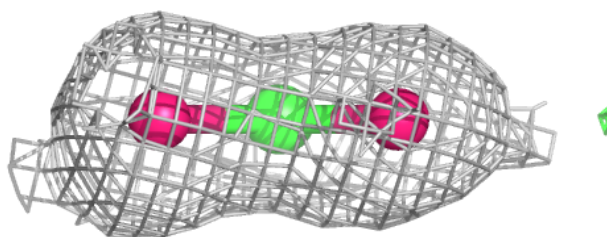
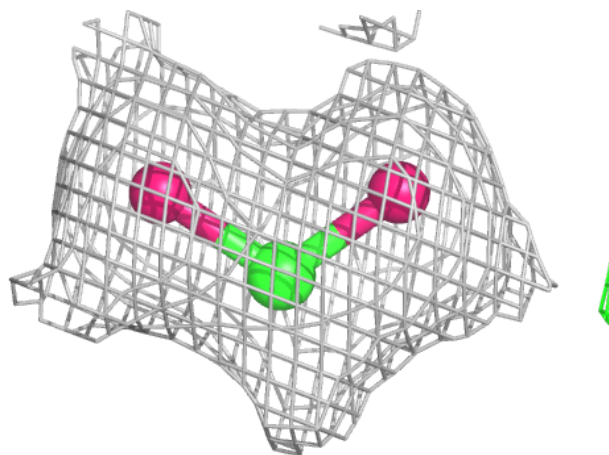
**Electron density around FMT B 305:**

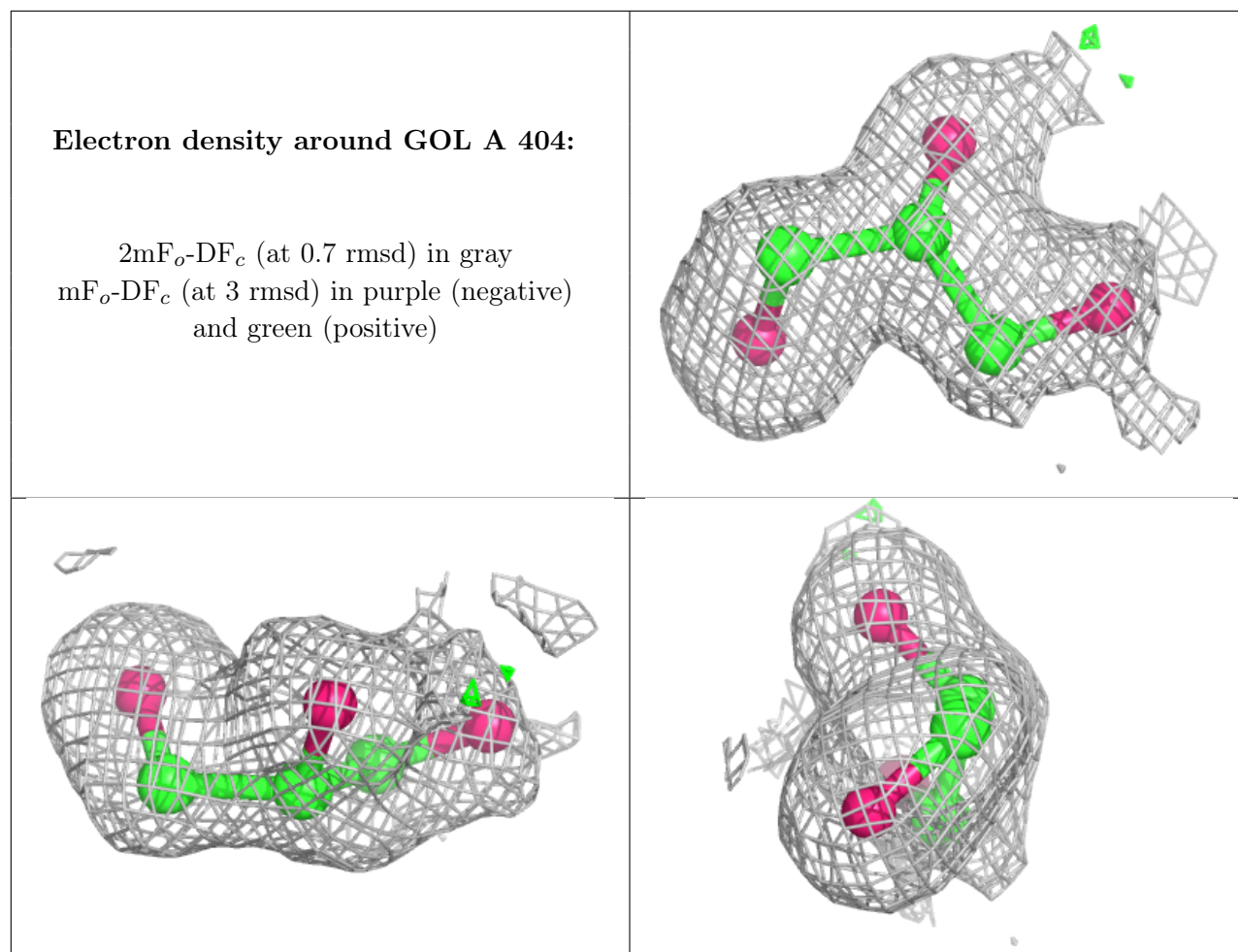
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FMT A 402:

$2mF_o-DF_c$ (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.