Full wwPDB X-ray Structure Validation Report ⓘ

Feb 24, 2025 – 03:12 pm GMT

PDB ID	:	8Q83
Title	:	Photorhabdus laumondii lectin PLL5 in complex with alpha-methyl-fucoside
Authors	:	Melicher, F.; Houser, J.; Paulenova, E.; Wimmerova, M.
Deposited on	:	2023-08-17
Resolution	:	1.70 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:

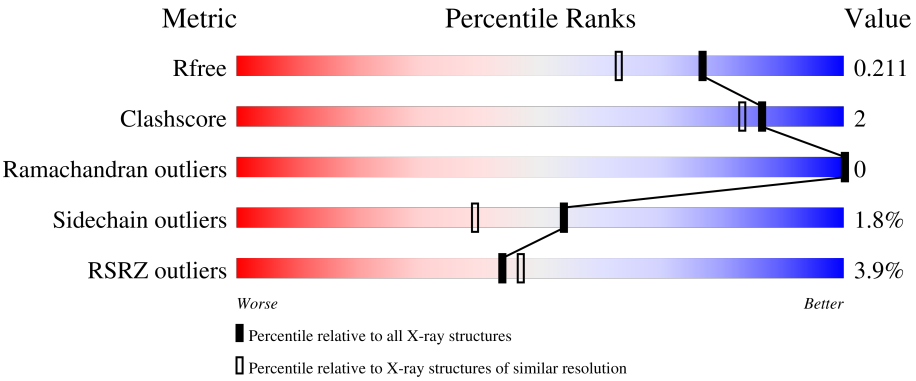
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.70 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}	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	371	3% 87% 7% 6%
1	B	371	2% 87% 6% 7%
1	C	371	4% 84% 6% 9%
1	D	371	5% 89% 8%

2 Entry composition (i)

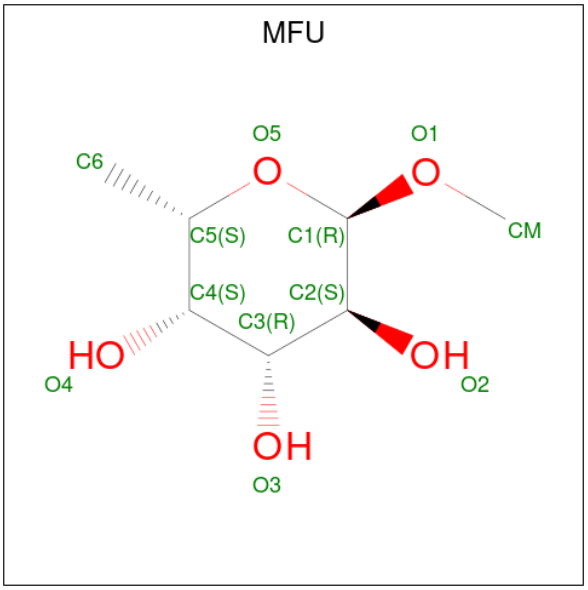
There are 3 unique types of molecules in this entry. The entry contains 11423 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Photorhabdus luminescens subsp. laumondii TTO1 complete genome segment 3/17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	348	Total 2685	C 1699	N 480	O 506	0	1	0
1	B	344	Total 2655	C 1681	N 475	O 499	0	2	0
1	C	338	Total 2609	C 1652	N 469	O 488	0	1	0
1	D	342	Total 2630	C 1665	N 473	O 492	0	0	0

- Molecule 2 is methyl alpha-L-fucopyranoside (three-letter code: MFU) (formula: $C_7H_{14}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 12	C 7	O 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 7 5	0	0
2	A	1	Total C O 12 7 5	0	0
2	A	1	Total C O 12 7 5	0	0
2	B	1	Total C O 12 7 5	0	0
2	B	1	Total C O 12 7 5	0	0
2	B	1	Total C O 12 7 5	0	0
2	B	1	Total C O 12 7 5	0	0
2	C	1	Total C O 12 7 5	0	0
2	C	1	Total C O 12 7 5	0	0
2	C	1	Total C O 12 7 5	0	0
2	C	1	Total C O 12 7 5	0	0
2	D	1	Total C O 12 7 5	0	0
2	D	1	Total C O 12 7 5	0	0
2	D	1	Total C O 12 7 5	0	0
2	D	1	Total C O 12 7 5	0	0

- Molecule 3 is water.

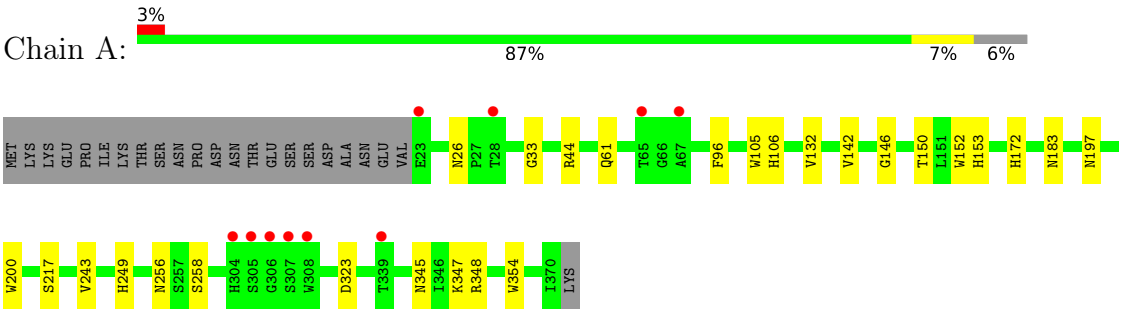
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	192	Total O 192 192	0	0
3	B	188	Total O 189 189	0	1
3	C	146	Total O 146 146	0	0
3	D	124	Total O 125 125	0	1

3 Residue-property plots (i)

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

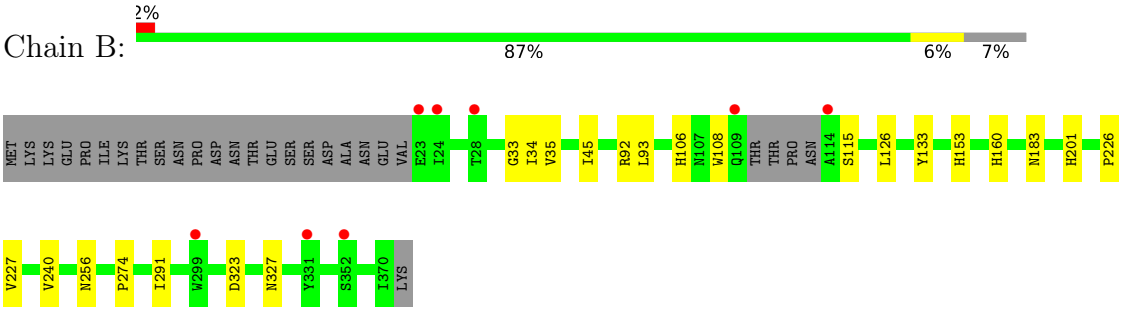
• Molecule 1: Photorhabdus luminescens subsp. laumondii TTO1 complete genome segment 3/17

Chain A:



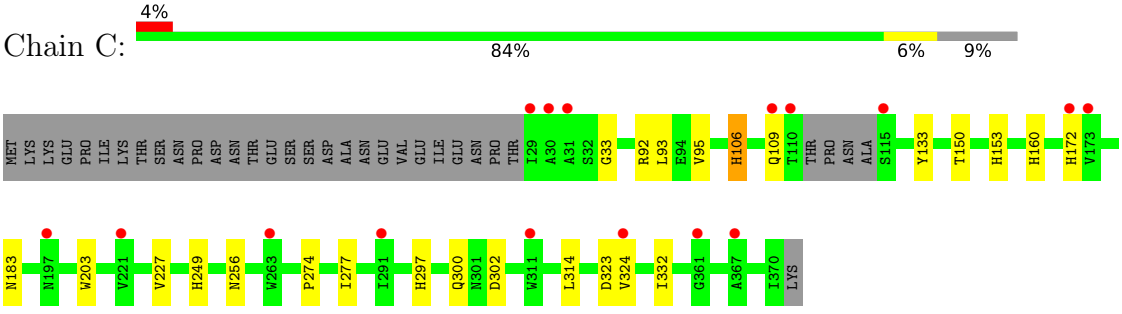
• Molecule 1: Photorhabdus luminescens subsp. laumondii TTO1 complete genome segment 3/17

Chain B:



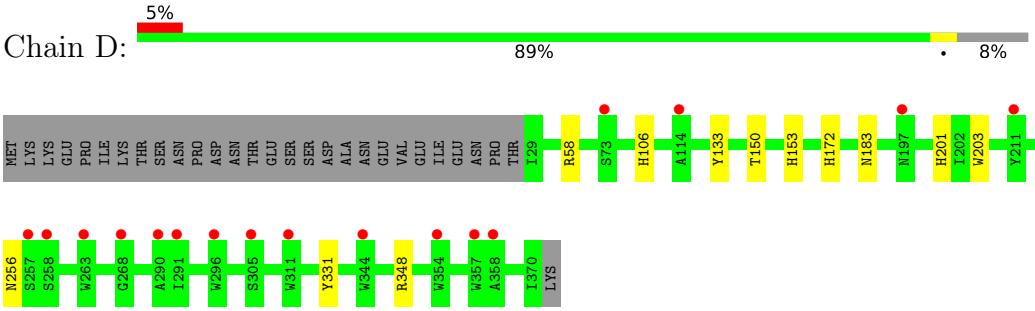
• Molecule 1: Photorhabdus luminescens subsp. laumondii TTO1 complete genome segment 3/17

Chain C:



• Molecule 1: Photorhabdus luminescens subsp. laumondii TTO1 complete genome segment 3/17

Chain D:


5%
89%
8%
MET LYS LYS GLU PRO ILE LYS THR SER ASN PRO ASP ASN THR GLU SER SER ASP ALA ASN GLU VAL GLU ILE GLU ASN PRO THR I29 R58 S73 H106 A114 Y133 T150 H153 H172 N183 N197 H201 I202 W203 Y211 H216 V243
N256 S257 S258 W263 G268 A290 I291 W296 S305 W311 Y331 W344 R348 W354 W357 A358 I370 LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.71Å 102.94Å 97.48Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	45.52 – 1.70 45.52 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.52-1.70) 99.2 (45.52-1.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.182 , 0.200 0.195 , 0.211	Depositor DCC
R_{free} test set	11774 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 23.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.057 for h,-k,-l 0.005 for l,-k,h	Xtriage
Reported twinning fraction	0.679 for H, K, L 0.321 for -h,-k,l	Depositor
Outliers	0 of 201995 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11423	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MFU

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	0.65	0/2778	0.73	0/3819
1	B	0.65	0/2749	0.74	0/3775
1	C	0.65	0/2696	0.74	0/3702
1	D	0.65	0/2719	0.74	0/3737
All	All	0.65	0/10942	0.74	0/15033

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	2685	0	2499	14	0
1	B	2655	0	2471	10	0
1	C	2609	0	2424	14	0
1	D	2630	0	2446	4	0
2	A	48	0	56	2	0
2	B	48	0	56	0	0
2	C	48	0	56	1	0
2	D	48	0	56	1	0
3	A	192	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	189	0	0	0	0
3	C	146	0	0	0	0
3	D	125	0	0	0	0
All	All	11423	0	10064	42	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 2.

All (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ARG:NH1	1:C:160:HIS:O	2.29	0.61
1:B:33:GLY:HA3	1:B:323:ASP:OD1	2.00	0.61
1:B:92:ARG:NH2	1:B:160:HIS:O	2.34	0.60
1:A:26:ASN:HA	1:A:197:ASN:HD21	1.73	0.54
1:B:45:ILE:HD11	1:B:327:ASN:HB3	1.92	0.51
1:D:203:TRP:CZ2	2:D:404:MFU:H5	2.45	0.51
1:A:183:ASN:HB3	1:A:256:ASN:ND2	2.25	0.51
1:D:331:TYR:HB3	1:D:348:ARG:HB2	1.94	0.49
1:C:150:THR:HG22	1:C:172:HIS:O	2.13	0.49
1:A:150:THR:HG22	1:A:172:HIS:O	2.13	0.49
1:B:92:ARG:HD2	1:B:108:TRP:CD1	2.49	0.47
1:A:105:TRP:CE2	2:A:403:MFU:H4	2.49	0.47
1:C:183:ASN:HB3	1:C:256:ASN:ND2	2.29	0.47
1:D:150:THR:HG22	1:D:172:HIS:O	2.15	0.47
1:C:183:ASN:HB3	1:C:256:ASN:HD22	1.80	0.46
1:B:183:ASN:HB3	1:B:256:ASN:HD22	1.80	0.46
1:A:132:VAL:HG22	1:A:142:VAL:HG22	1.98	0.45
1:C:33:GLY:HA3	1:C:323:ASP:OD1	2.18	0.44
1:C:324:VAL:HG13	1:C:332:ILE:HG23	1.99	0.44
1:A:183:ASN:HB3	1:A:256:ASN:HD22	1.83	0.43
1:C:203:TRP:CZ2	2:C:402:MFU:H5	2.54	0.43
1:C:277:ILE:HG21	1:C:324:VAL:HG11	1.99	0.43
1:A:348:ARG:HD3	1:A:354:TRP:CE2	2.53	0.43
1:A:44:ARG:HD2	1:A:61:GLN:O	2.19	0.42
1:B:227:VAL:HG11	1:B:274:PRO:O	2.19	0.42
1:C:300:GLN:HB3	1:C:302:ASP:O	2.19	0.42
1:A:258:SER:HA	2:A:404:MFU:H63	2.01	0.42
1:B:126:LEU:HD12	1:B:126:LEU:N	2.34	0.42
1:A:96:PHE:CD1	1:A:132:VAL:HG21	2.54	0.42
1:A:345:ASN:HD21	1:A:347:LYS:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLY:HA3	1:A:152:TRP:CE2	2.55	0.41
1:A:200:TRP:CZ2	1:A:217:SER:HB2	2.55	0.41
1:C:227:VAL:HG21	1:C:274:PRO:O	2.21	0.41
1:C:93:LEU:HB2	1:C:109:GLN:OE1	2.21	0.41
1:C:297:HIS:CE1	1:C:314:LEU:HD21	2.56	0.41
1:B:34:ILE:HG23	1:B:35:VAL:HG13	2.01	0.41
1:D:183:ASN:HB3	1:D:256:ASN:ND2	2.36	0.41
1:C:92:ARG:HD3	1:C:109:GLN:O	2.20	0.41
1:B:183:ASN:HB3	1:B:256:ASN:ND2	2.36	0.40
1:C:95:VAL:O	1:C:106:HIS:HA	2.22	0.40
1:A:33:GLY:HA3	1:A:323:ASP:OD1	2.22	0.40
1:B:226:PRO:HA	1:B:240:VAL:HG12	2.03	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	347/371 (94%)	338 (97%)	9 (3%)	0	100	100
1	B	342/371 (92%)	336 (98%)	6 (2%)	0	100	100
1	C	335/371 (90%)	327 (98%)	8 (2%)	0	100	100
1	D	340/371 (92%)	331 (97%)	9 (3%)	0	100	100
All	All	1364/1484 (92%)	1332 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	277/298 (93%)	273 (99%)	4 (1%)	62	49
1	B	274/298 (92%)	267 (97%)	7 (3%)	41	24
1	C	268/298 (90%)	264 (98%)	4 (2%)	60	47
1	D	270/298 (91%)	265 (98%)	5 (2%)	52	37
All	All	1089/1192 (91%)	1069 (98%)	20 (2%)	54	39

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	153	HIS
1	A	243	VAL
1	A	249	HIS
1	B	93	LEU
1	B	106	HIS
1	B	115	SER
1	B	133	TYR
1	B	153	HIS
1	B	201	HIS
1	B	291	ILE
1	C	106	HIS
1	C	133	TYR
1	C	153	HIS
1	C	249	HIS
1	D	58	ARG
1	D	106	HIS
1	D	133	TYR
1	D	153	HIS
1	D	201	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	197	ASN
1	A	256	ASN

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Mol	Chain	Res	Type
1	A	301	ASN
1	A	304	HIS
1	A	341	ASN
1	A	345	ASN
1	B	26	ASN
1	B	39	ASN
1	B	109	GLN
1	B	197	ASN
1	B	256	ASN
1	B	282	ASN
1	B	341	ASN
1	C	39	ASN
1	C	197	ASN
1	C	256	ASN
1	C	301	ASN
1	C	345	ASN
1	D	64	HIS
1	D	256	ASN
1	D	301	ASN
1	D	304	HIS
1	D	345	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)

16 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	MFU	A	402	-	12,12,12	0.76	0	17,17,17	0.86	1 (5%)
2	MFU	A	403	-	12,12,12	0.76	1 (8%)	17,17,17	0.75	0
2	MFU	C	403	-	12,12,12	0.65	0	17,17,17	0.73	0
2	MFU	D	401	-	12,12,12	0.72	1 (8%)	17,17,17	1.00	1 (5%)
2	MFU	C	402	-	12,12,12	0.76	0	17,17,17	0.96	0
2	MFU	D	404	-	12,12,12	0.79	0	17,17,17	1.02	1 (5%)
2	MFU	A	401	-	12,12,12	0.70	0	17,17,17	0.83	1 (5%)
2	MFU	A	404	-	12,12,12	0.72	0	17,17,17	1.18	1 (5%)
2	MFU	B	402	-	12,12,12	0.94	1 (8%)	17,17,17	1.17	2 (11%)
2	MFU	B	403	-	12,12,12	0.62	0	17,17,17	0.88	0
2	MFU	B	404	-	12,12,12	0.67	0	17,17,17	0.68	0
2	MFU	D	402	-	12,12,12	0.78	1 (8%)	17,17,17	1.09	1 (5%)
2	MFU	B	401	-	12,12,12	0.63	0	17,17,17	0.75	0
2	MFU	C	401	-	12,12,12	0.78	1 (8%)	17,17,17	1.11	0
2	MFU	D	403	-	12,12,12	0.62	0	17,17,17	0.45	0
2	MFU	C	404	-	12,12,12	0.67	0	17,17,17	0.82	1 (5%)

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	MFU	A	402	-	-	0/2/22/22	0/1/1/1
2	MFU	A	403	-	-	0/2/22/22	0/1/1/1
2	MFU	C	403	-	-	0/2/22/22	0/1/1/1
2	MFU	D	401	-	-	0/2/22/22	0/1/1/1
2	MFU	C	402	-	-	0/2/22/22	0/1/1/1
2	MFU	D	404	-	-	0/2/22/22	0/1/1/1
2	MFU	A	401	-	-	0/2/22/22	0/1/1/1
2	MFU	A	404	-	-	0/2/22/22	0/1/1/1
2	MFU	B	402	-	-	0/2/22/22	0/1/1/1
2	MFU	B	403	-	-	0/2/22/22	0/1/1/1
2	MFU	B	404	-	-	0/2/22/22	0/1/1/1
2	MFU	D	402	-	-	0/2/22/22	0/1/1/1
2	MFU	B	401	-	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MFU	C	401	-	-	0/2/22/22	0/1/1/1
2	MFU	D	403	-	-	0/2/22/22	0/1/1/1
2	MFU	C	404	-	-	0/2/22/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	MFU	O1-C1	2.41	1.44	1.40
2	C	401	MFU	O1-C1	2.23	1.44	1.40
2	D	402	MFU	O1-C1	2.15	1.43	1.40
2	D	401	MFU	O1-C1	2.06	1.43	1.40
2	A	403	MFU	O1-C1	2.05	1.43	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	MFU	O1-C1-C2	3.22	111.92	108.15
2	B	402	MFU	CM-O1-C1	-3.03	108.60	113.27
2	D	402	MFU	O1-C1-C2	2.68	111.29	108.15
2	A	401	MFU	O1-C1-C2	2.57	111.16	108.15
2	A	404	MFU	O1-C1-C2	2.55	111.14	108.15
2	D	404	MFU	O5-C5-C6	2.34	111.76	106.70
2	B	402	MFU	O5-C5-C6	2.34	111.76	106.70
2	C	404	MFU	O1-C1-C2	2.24	110.77	108.15
2	A	402	MFU	O1-C1-C2	2.05	110.55	108.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

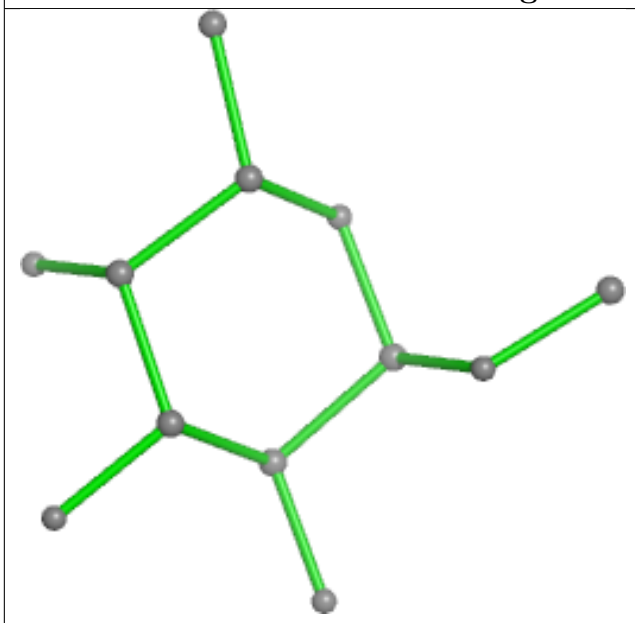
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	MFU	1	0
2	C	402	MFU	1	0
2	D	404	MFU	1	0
2	A	404	MFU	1	0

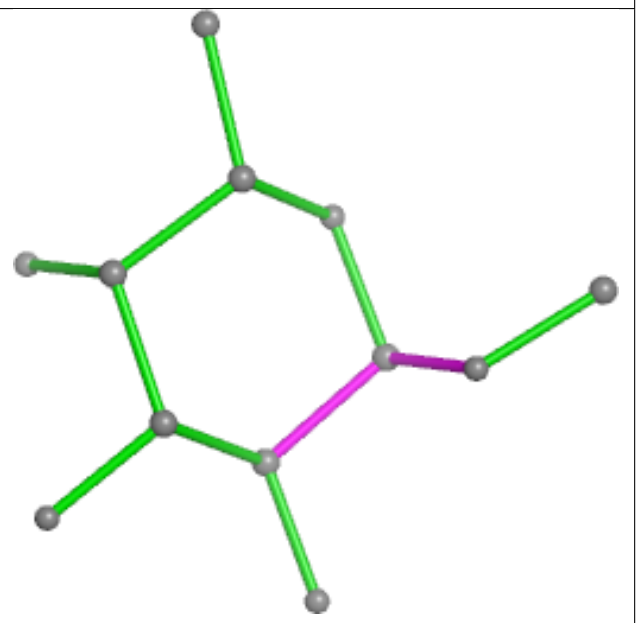
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

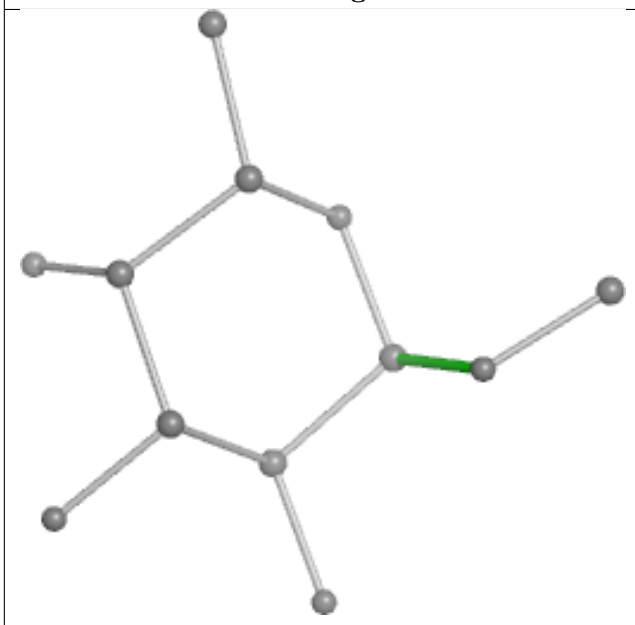
Ligand MFU A 402



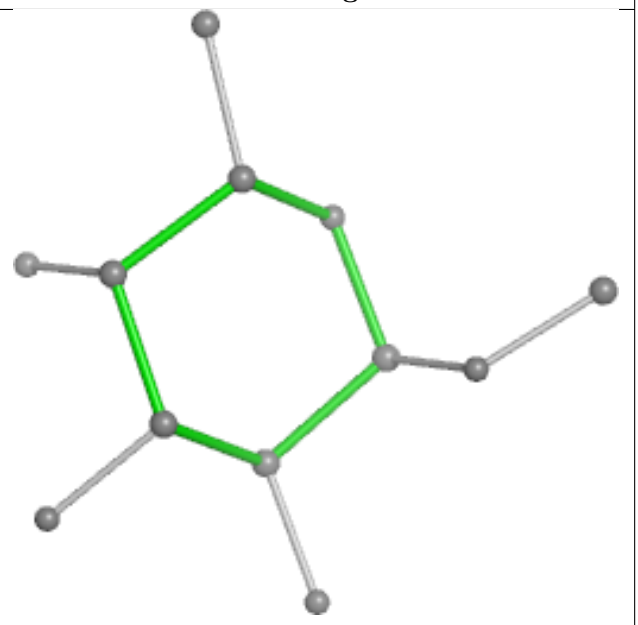
Bond lengths



Bond angles

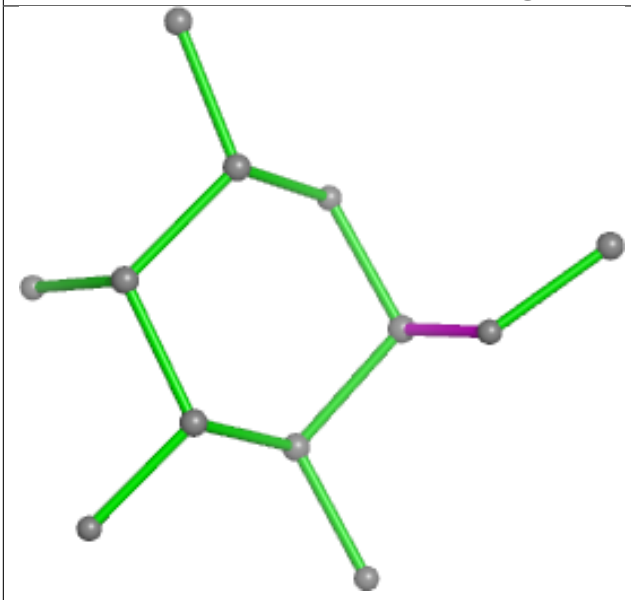


Torsions



Rings

Ligand MFU A 403



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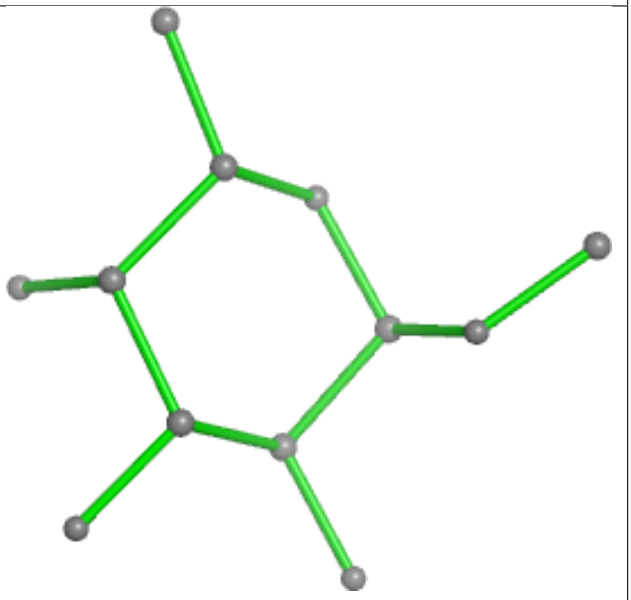
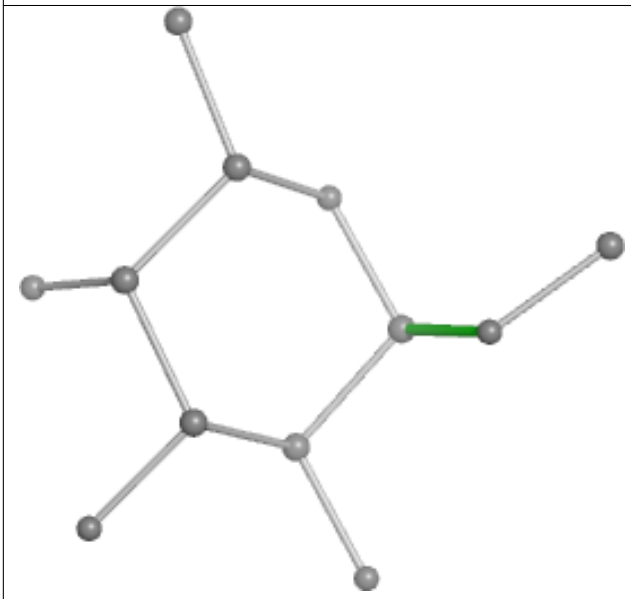


Bond angles



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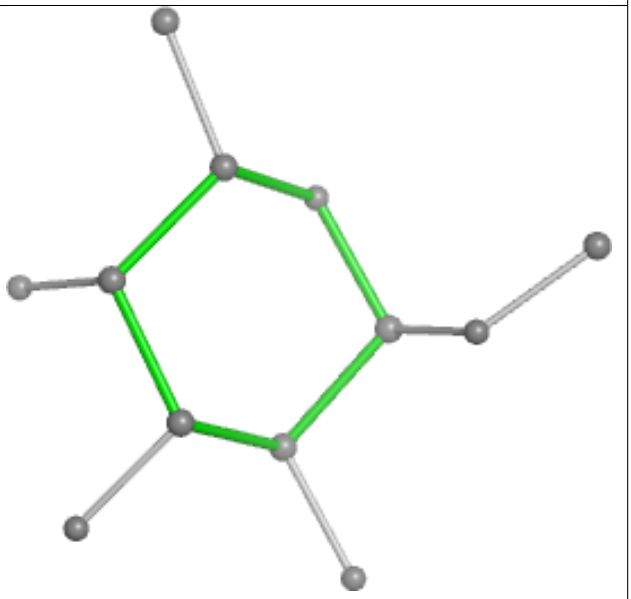
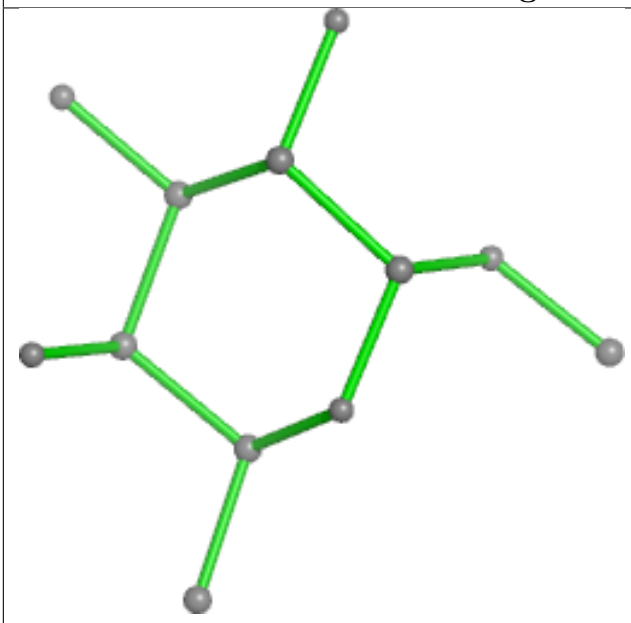


Rings

Ligand MFU C 403



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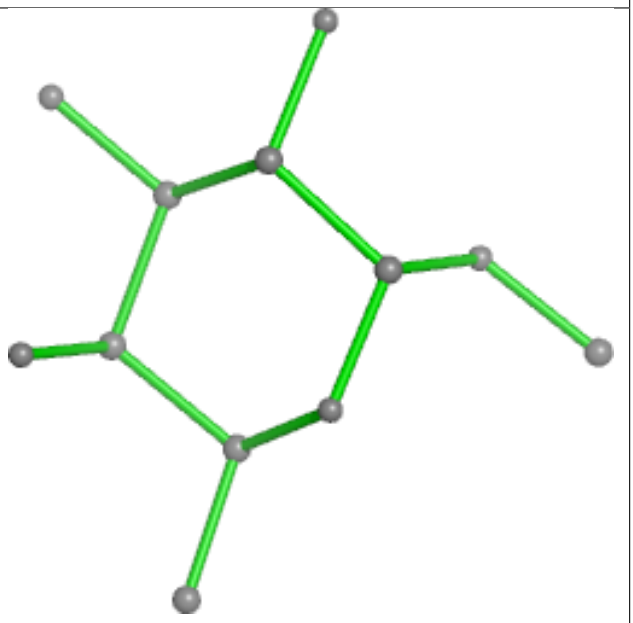
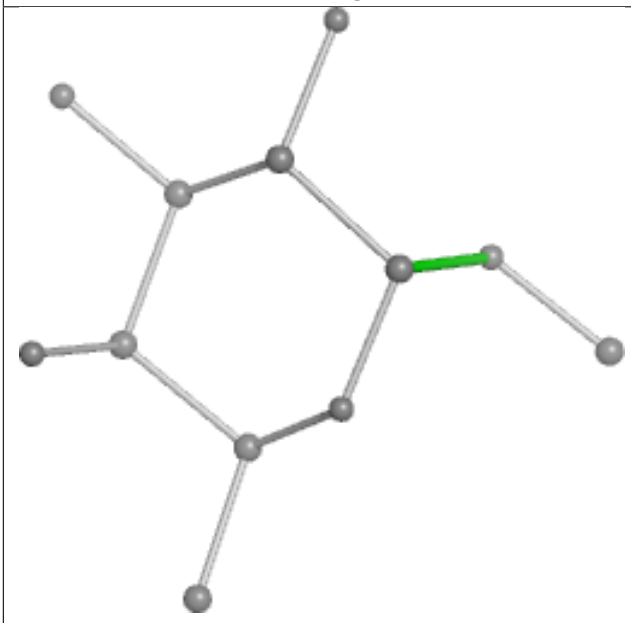


Bond angles



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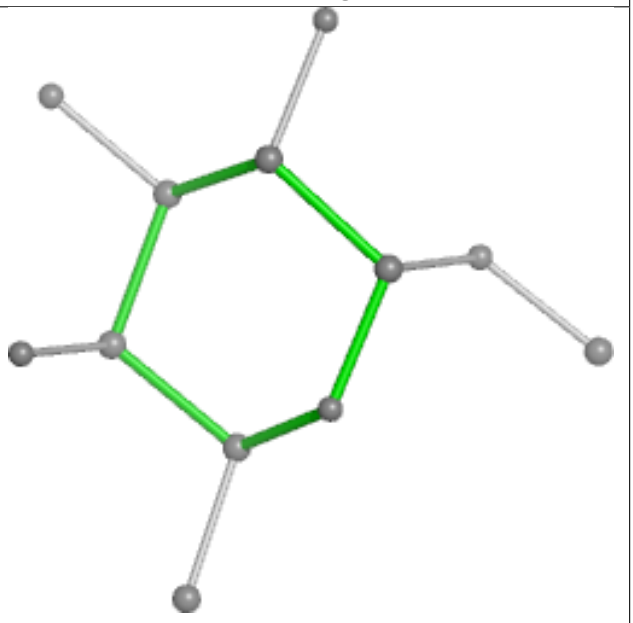
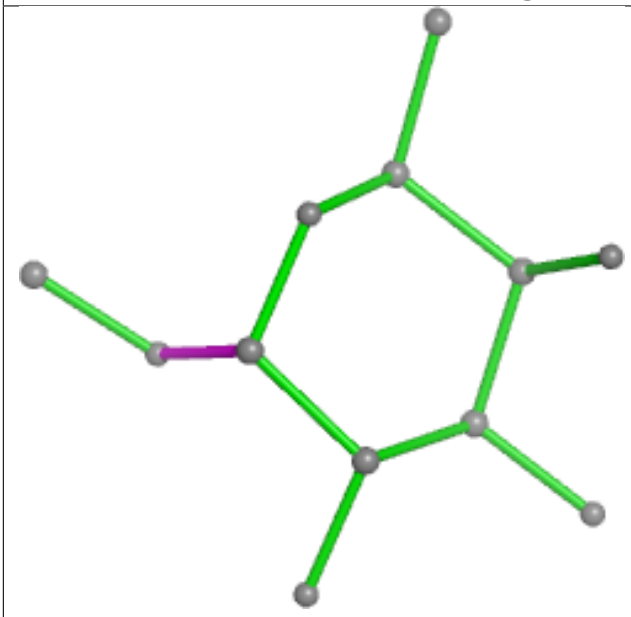


Rings

Ligand MFU D 401



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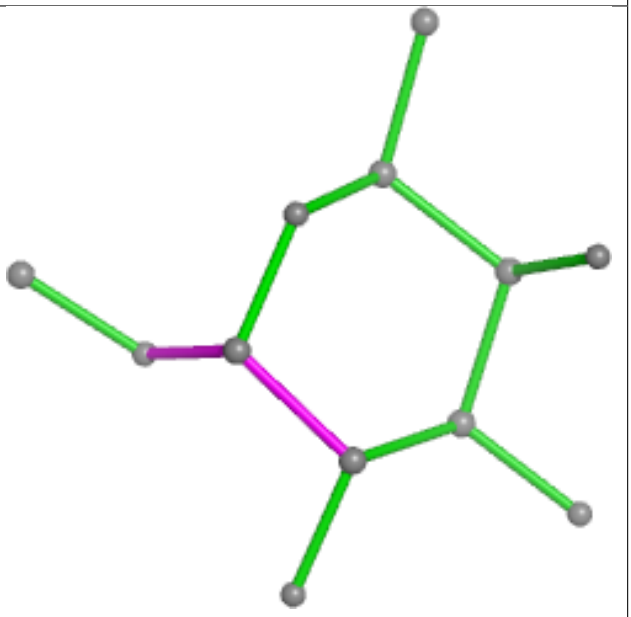

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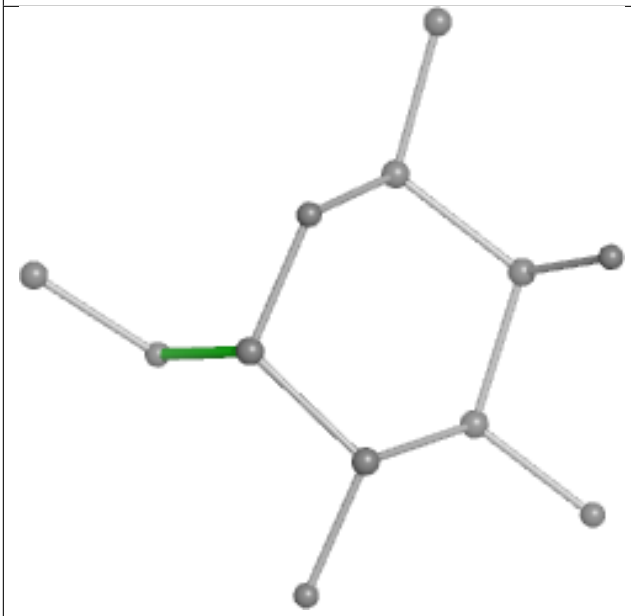

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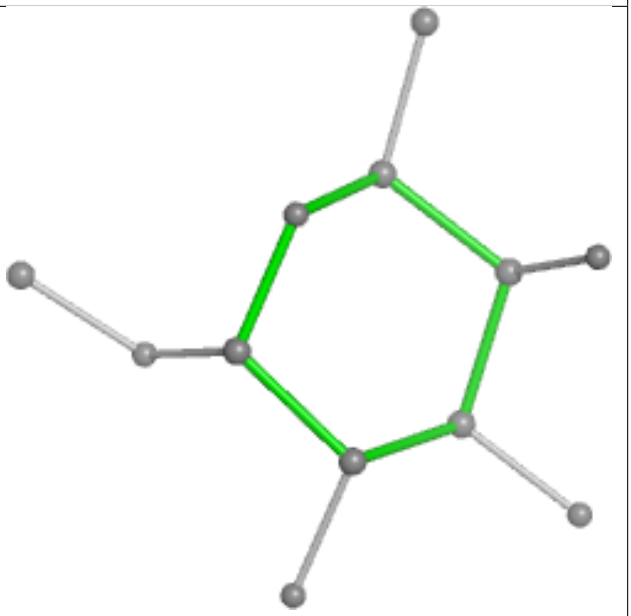
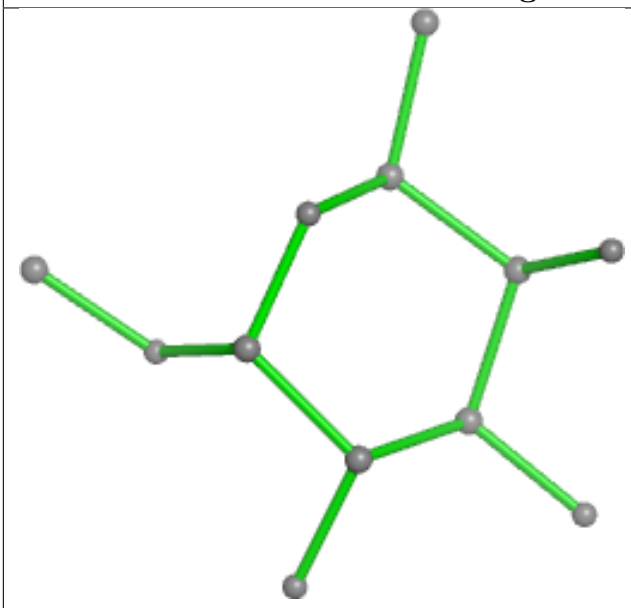


Rings

Ligand MFU C 402



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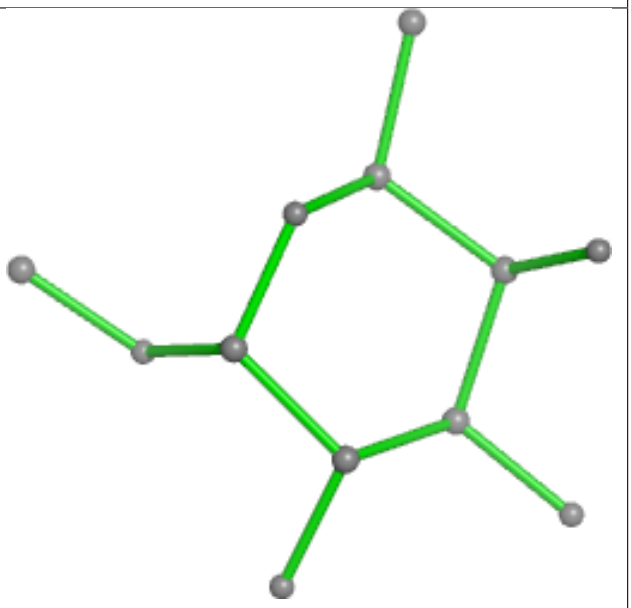

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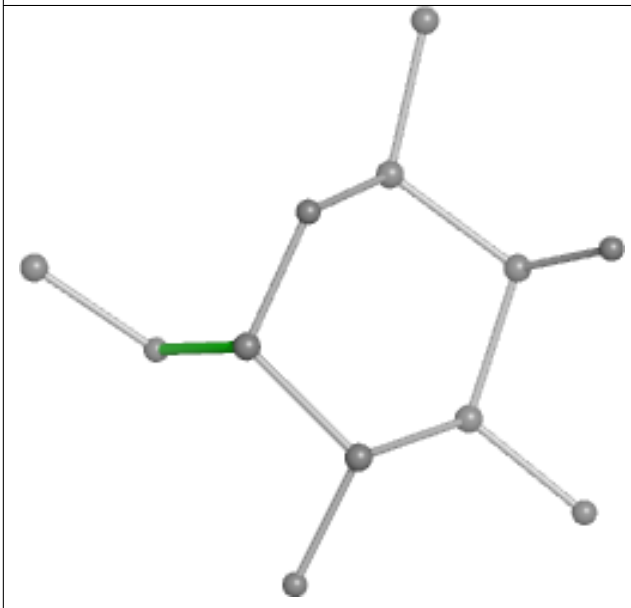

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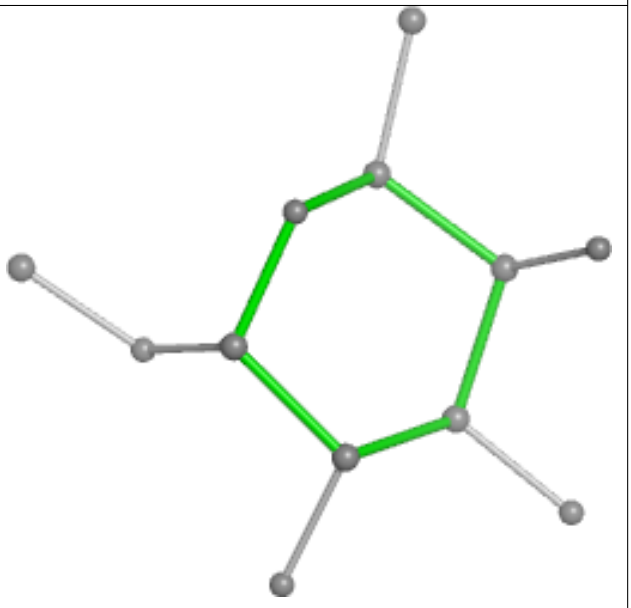
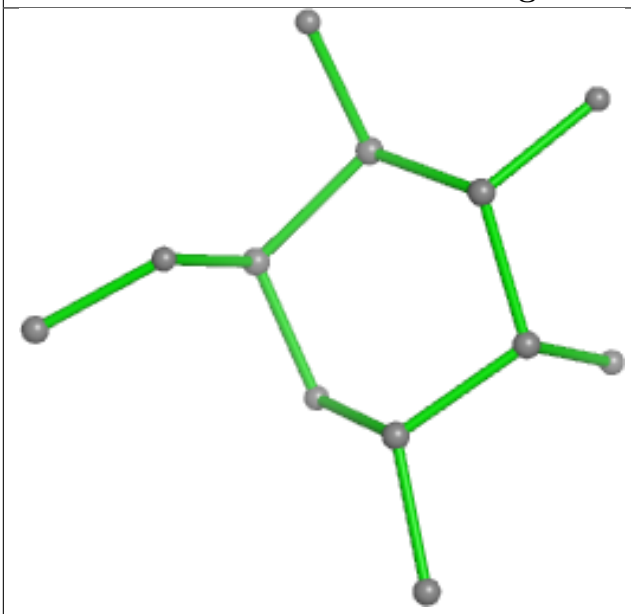


Rings

Ligand MFU D 404



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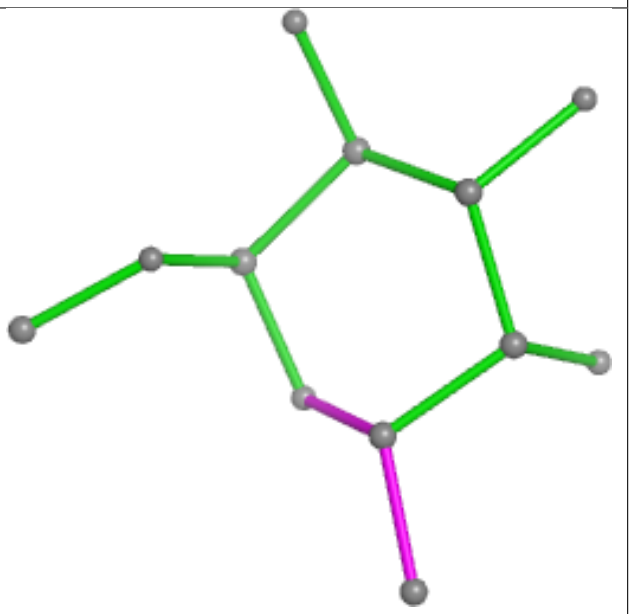

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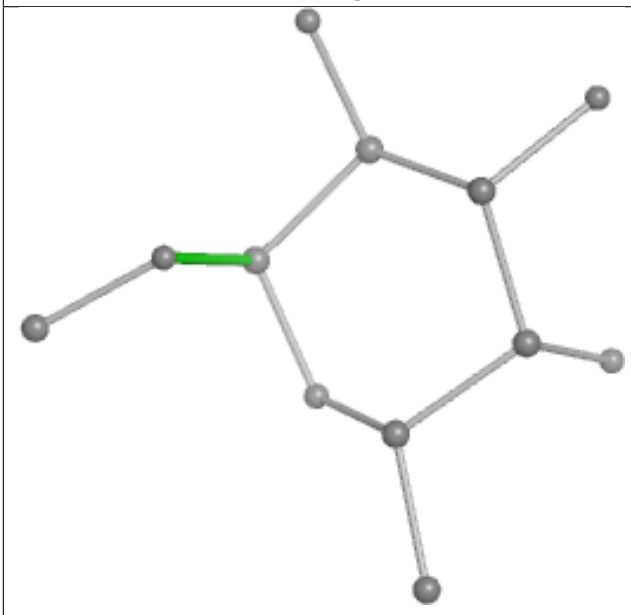

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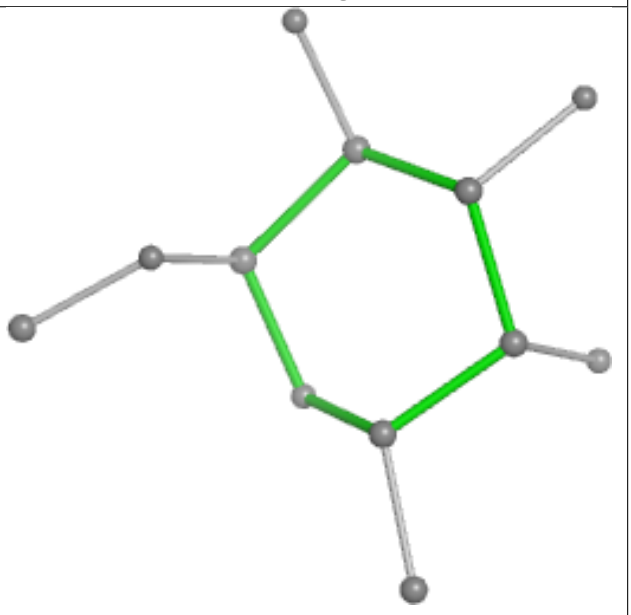
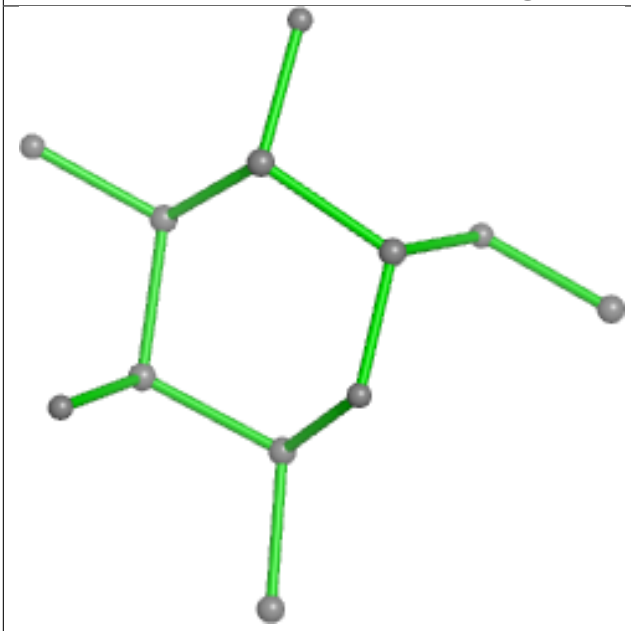


Rings

Ligand MFU A 401



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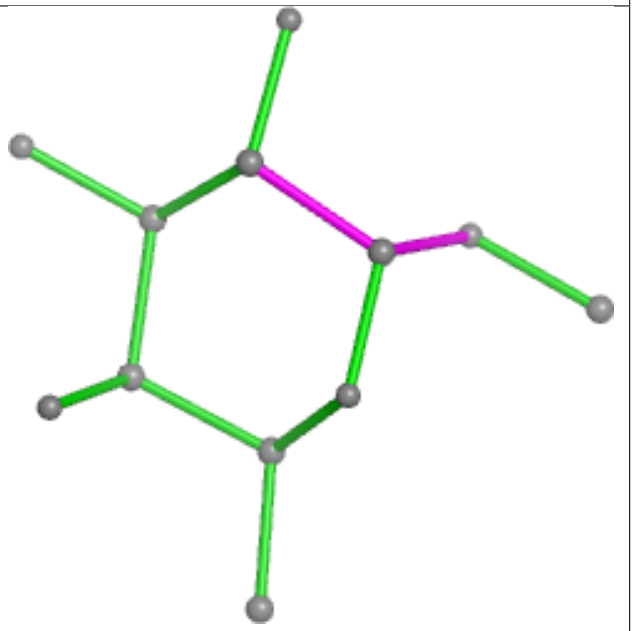

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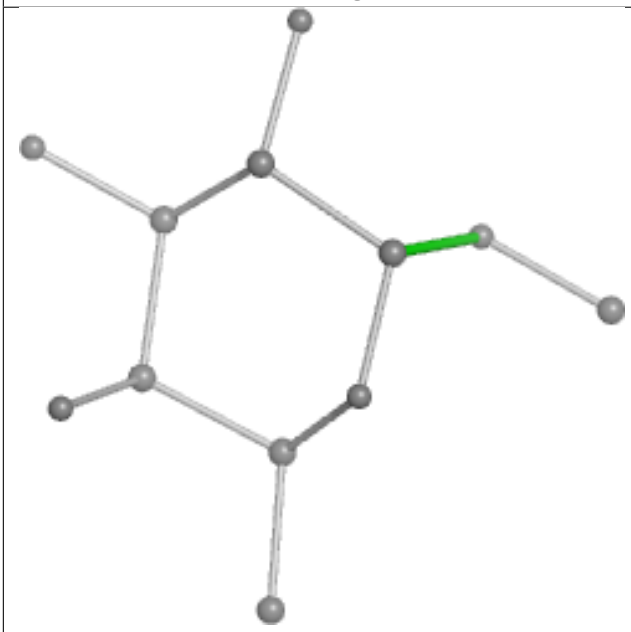

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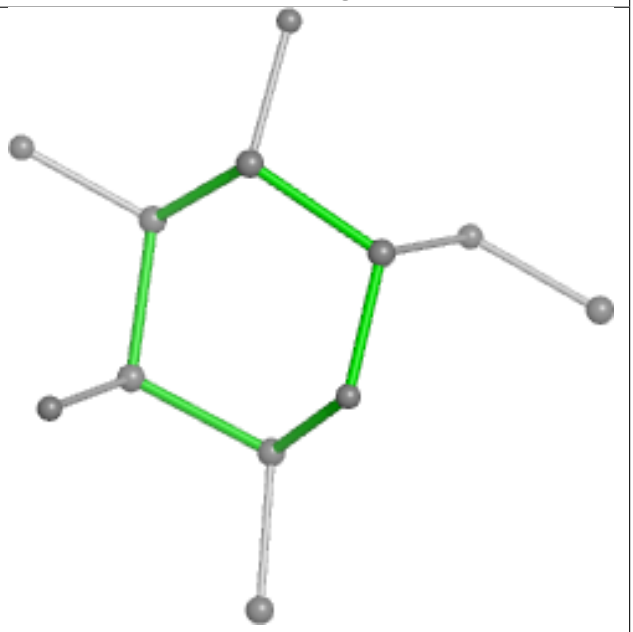
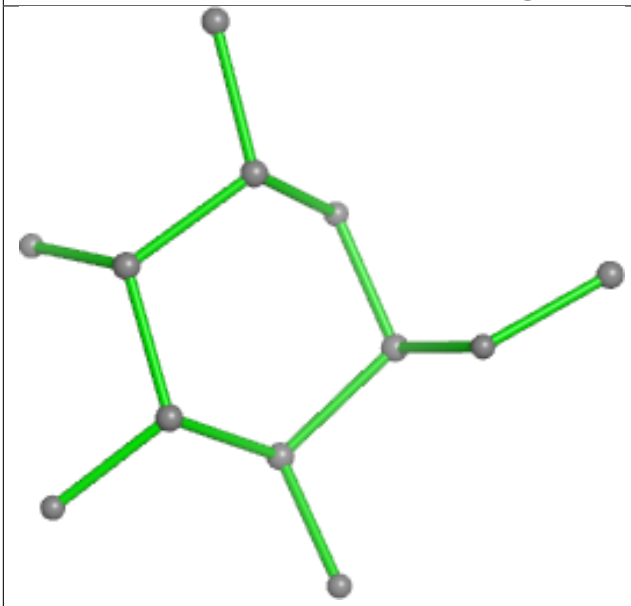


Rings

Ligand MFU A 404



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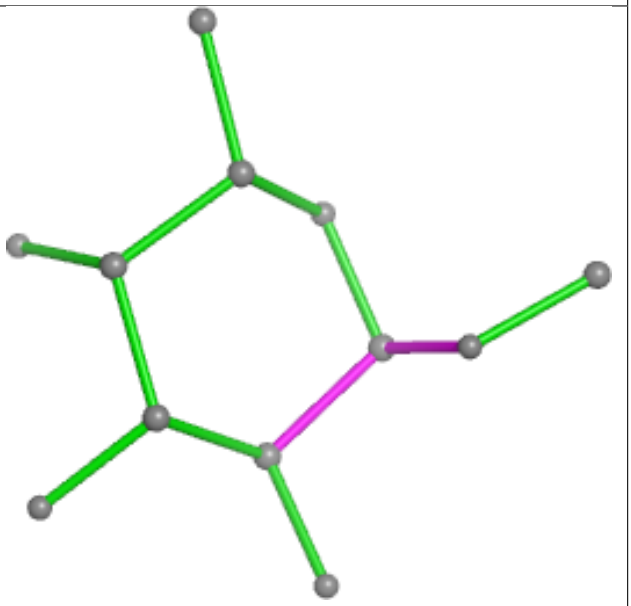

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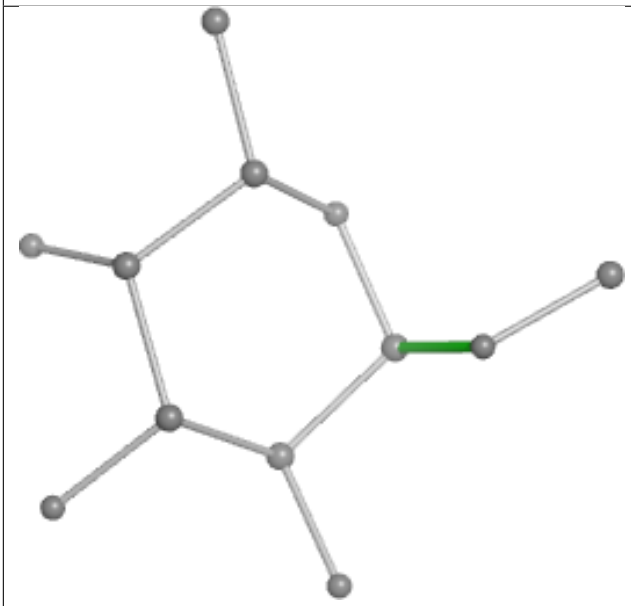

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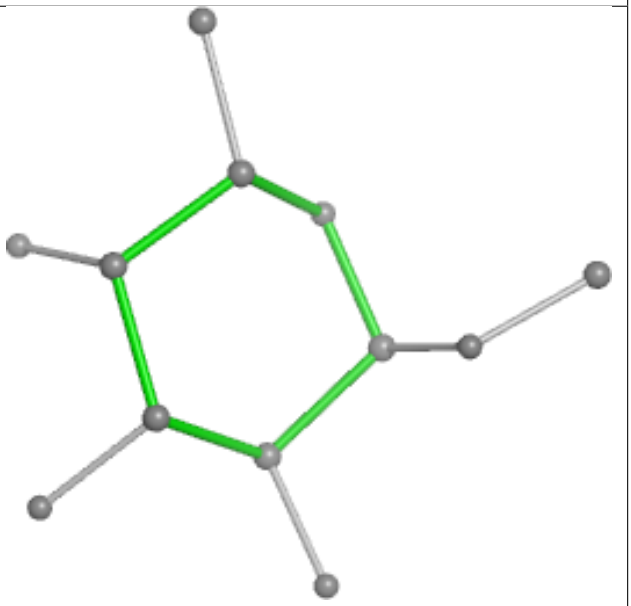
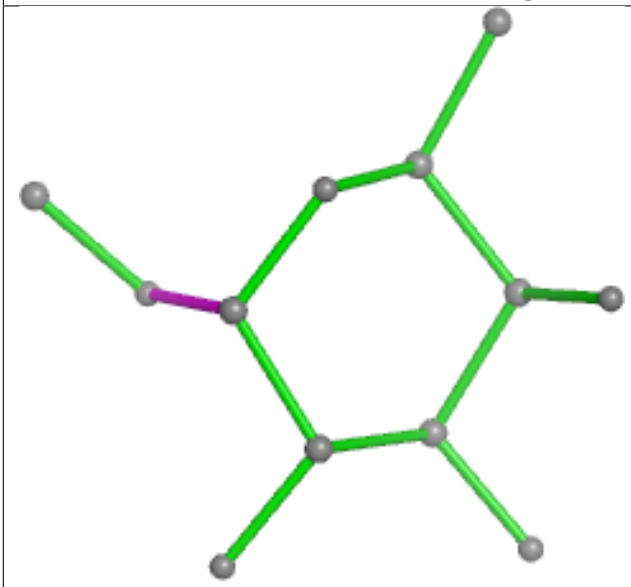


Rings

Ligand MFU B 402



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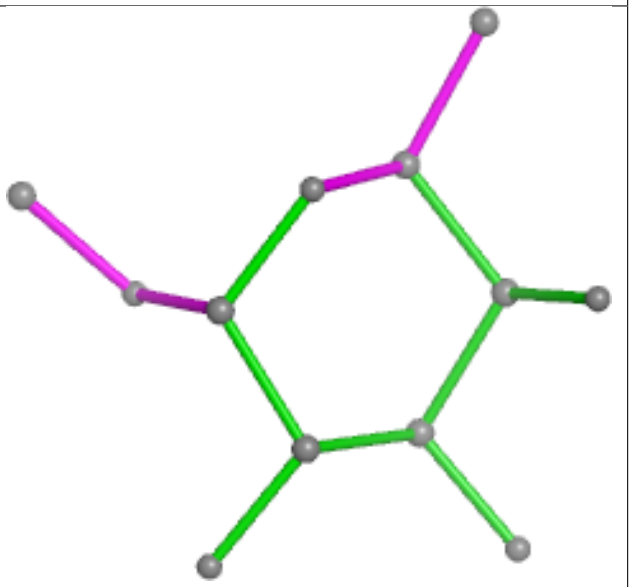
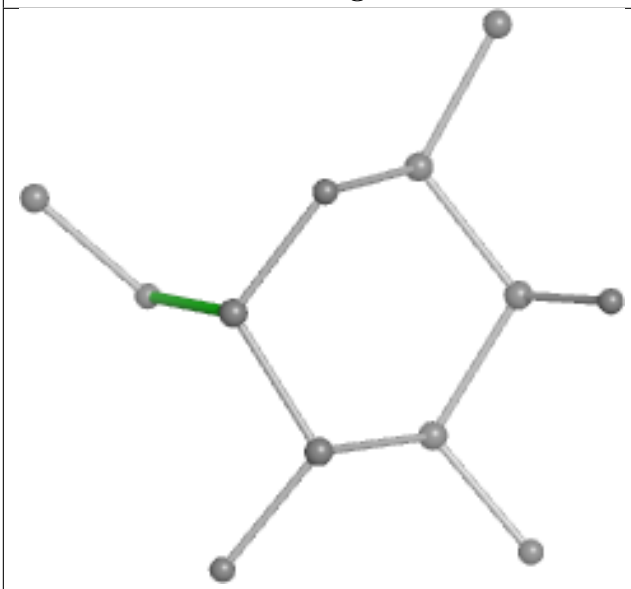


Bond angles



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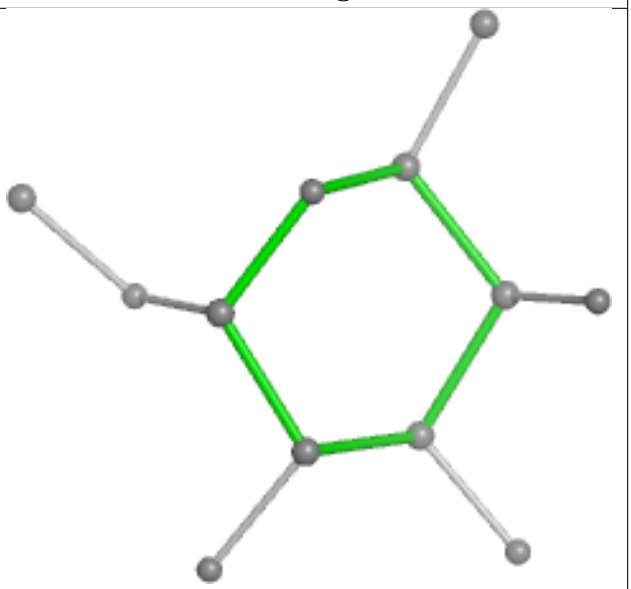
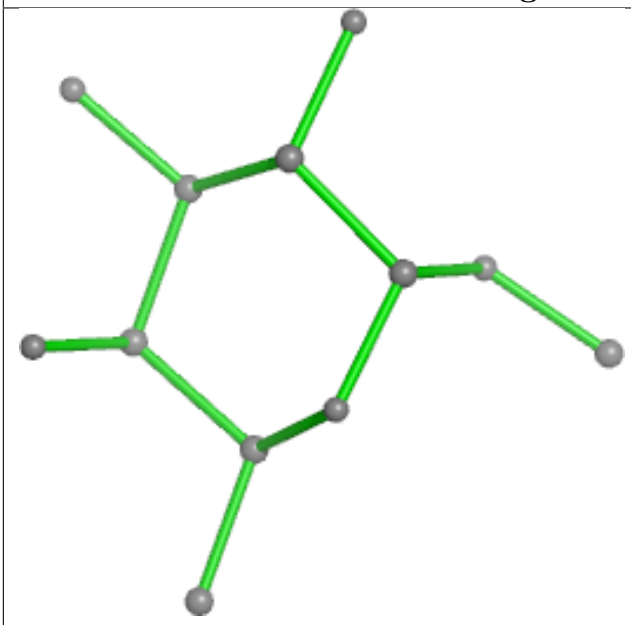


Rings

Ligand MFU B 403



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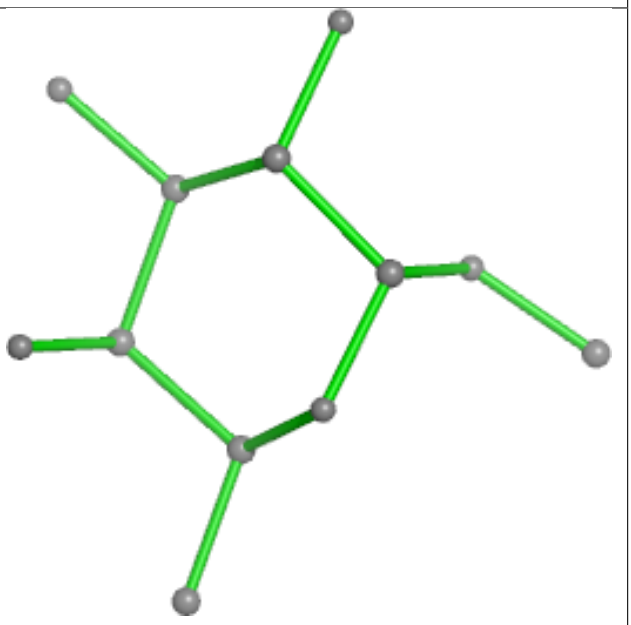

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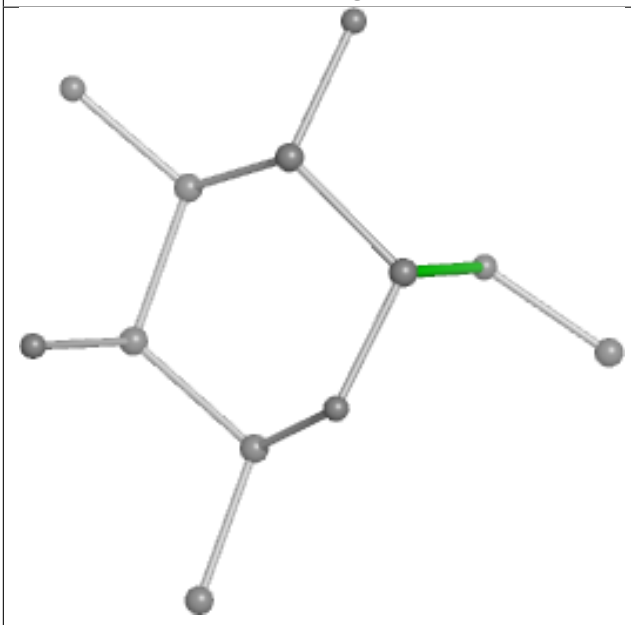

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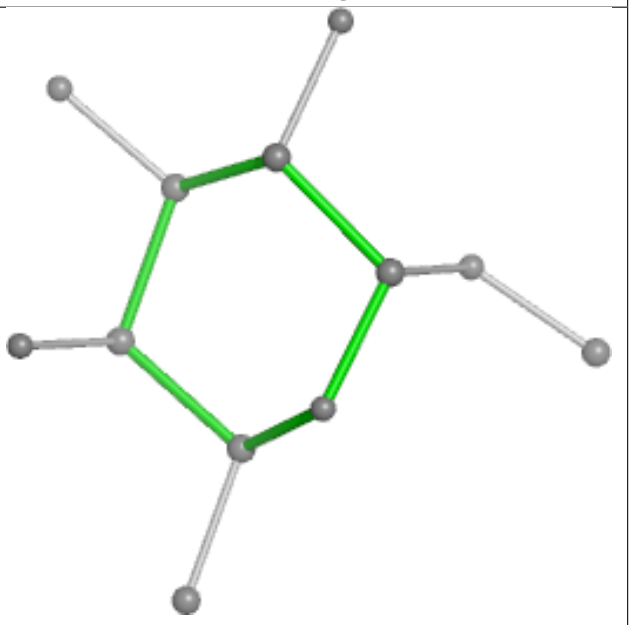
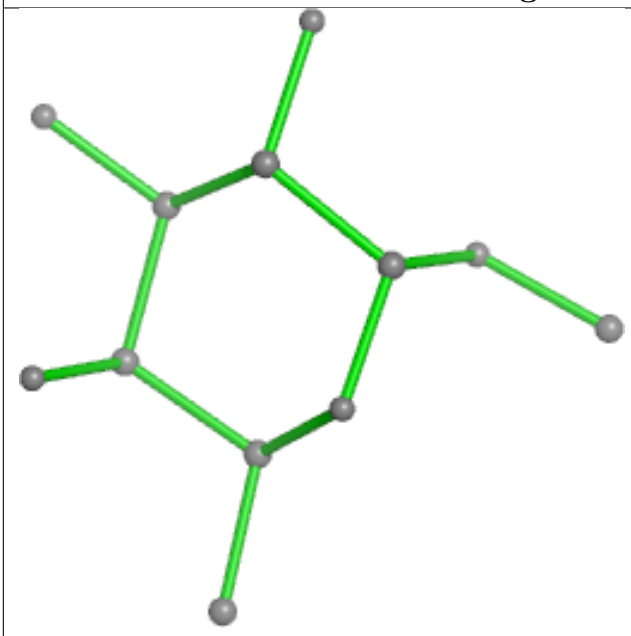


Rings

Ligand MFU B 404



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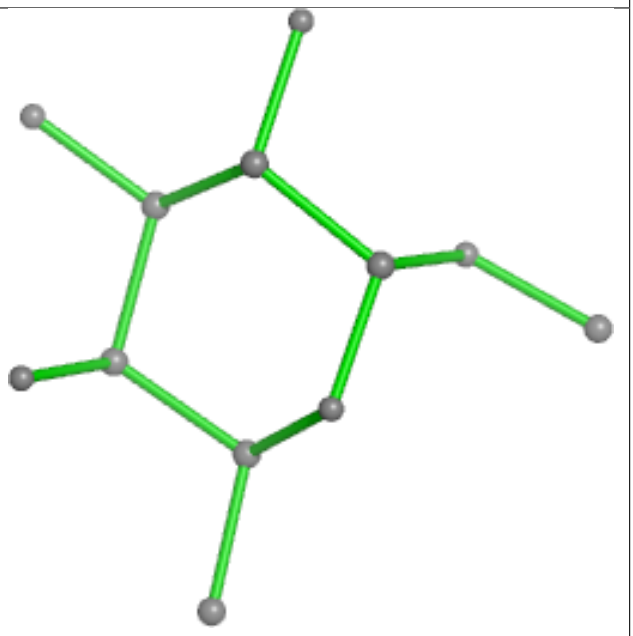

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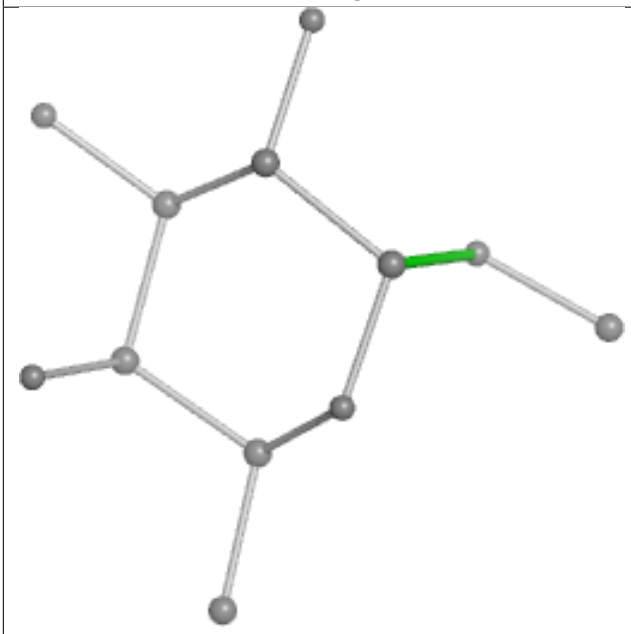

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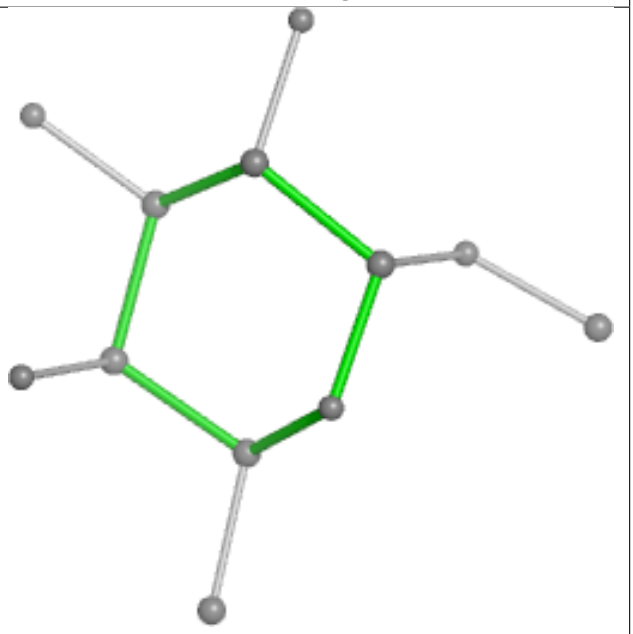
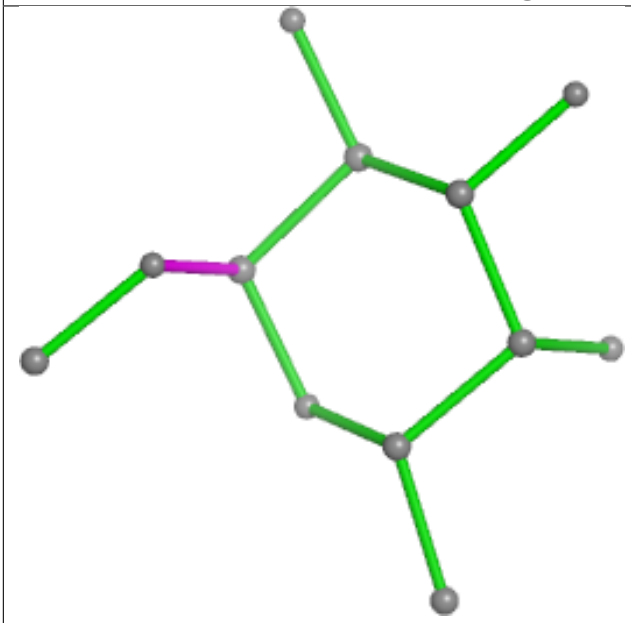


Rings

Ligand MFU D 402



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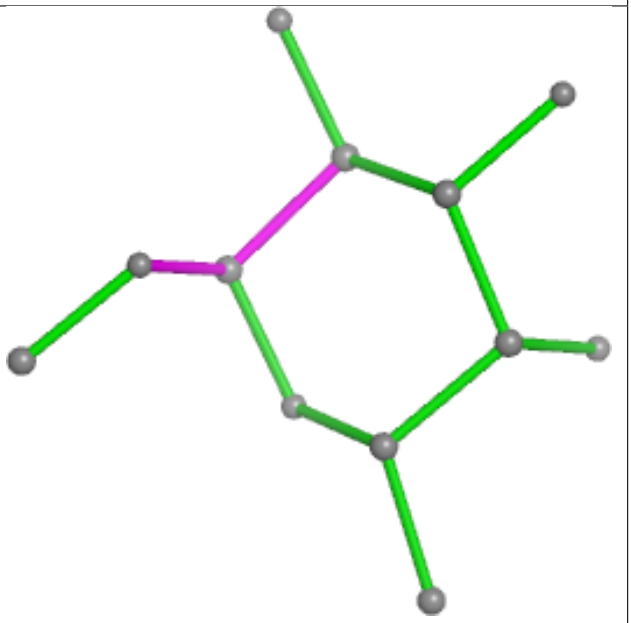
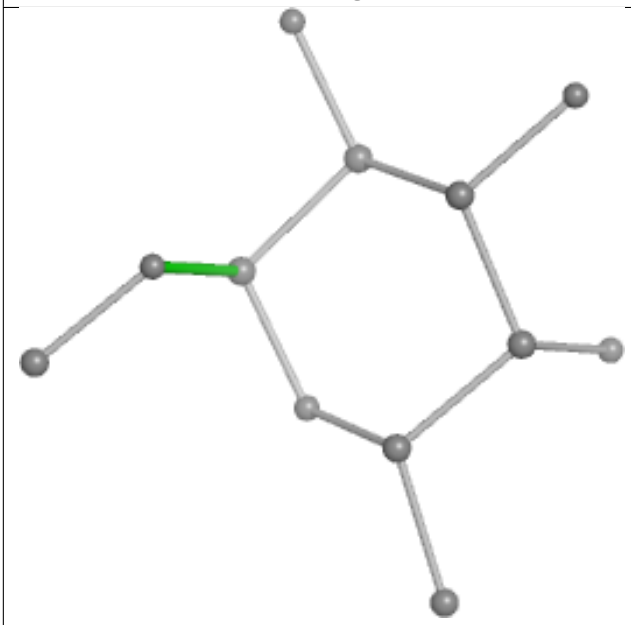
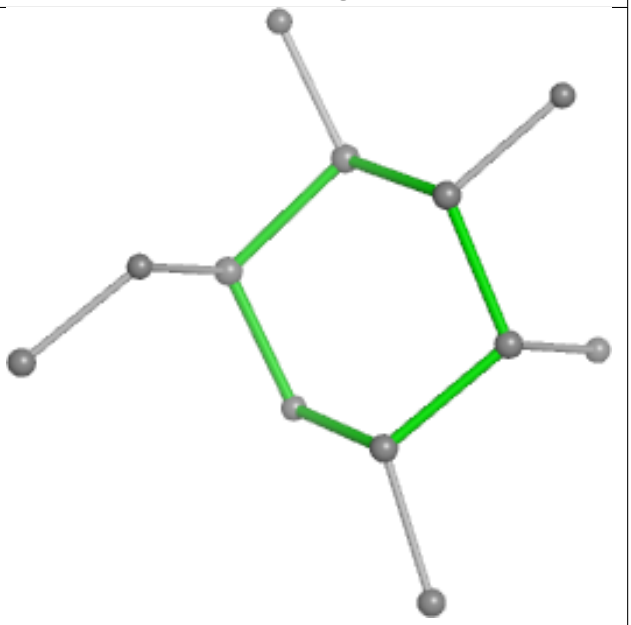


Bond angles

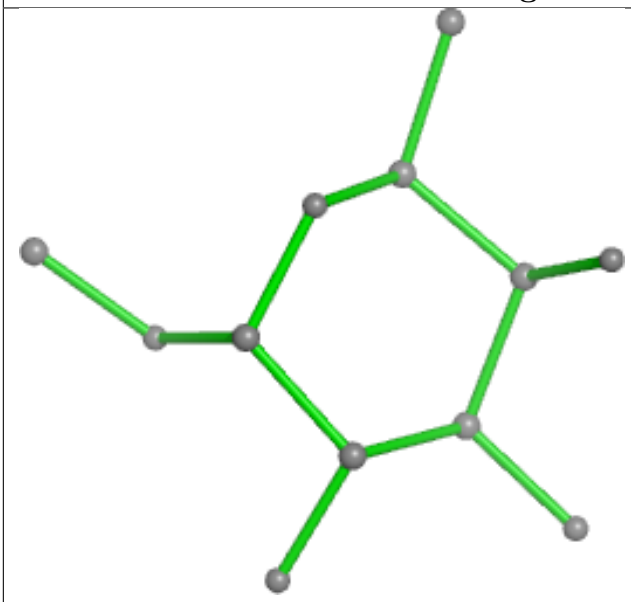


Torsions

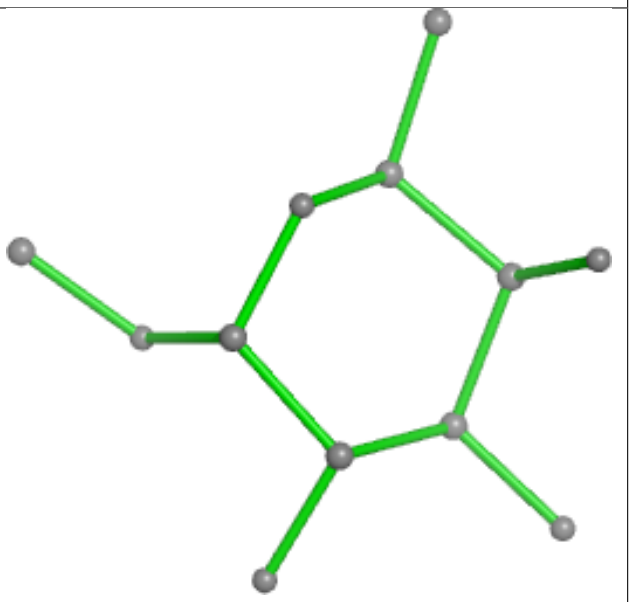


Rings

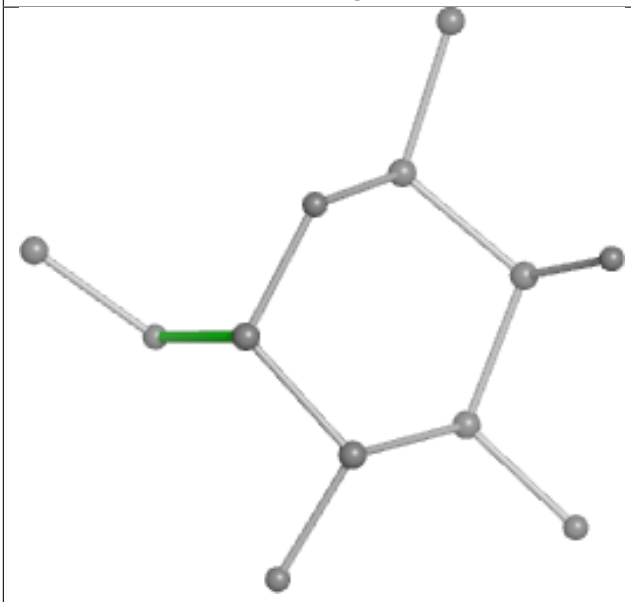
Ligand MFU B 401



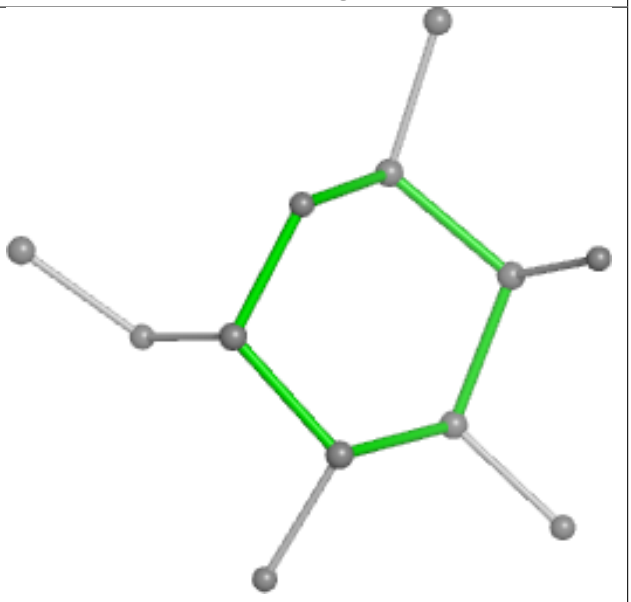
Bond lengths



Bond angles

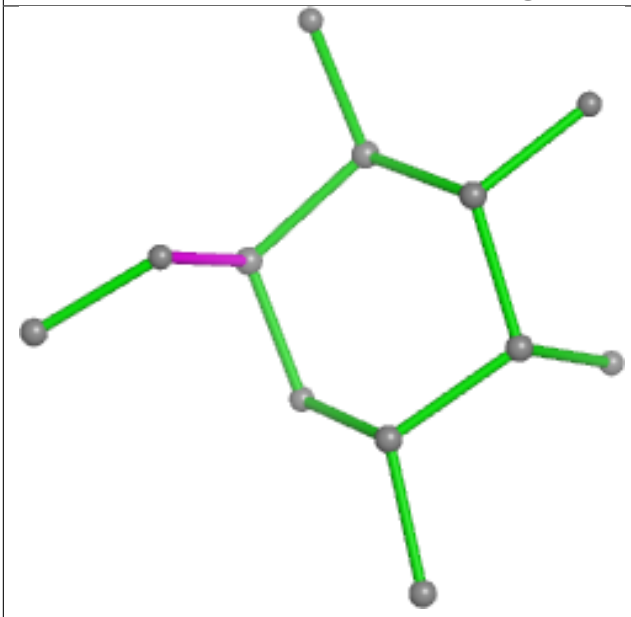


Torsions

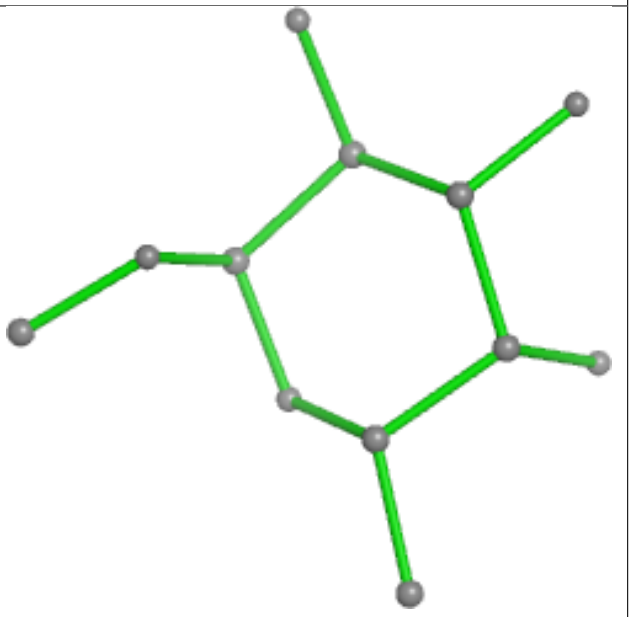


Rings

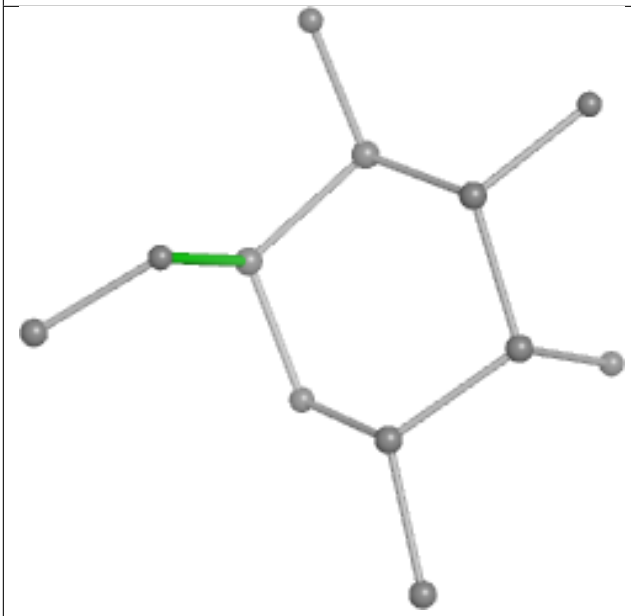
Ligand MFU C 401



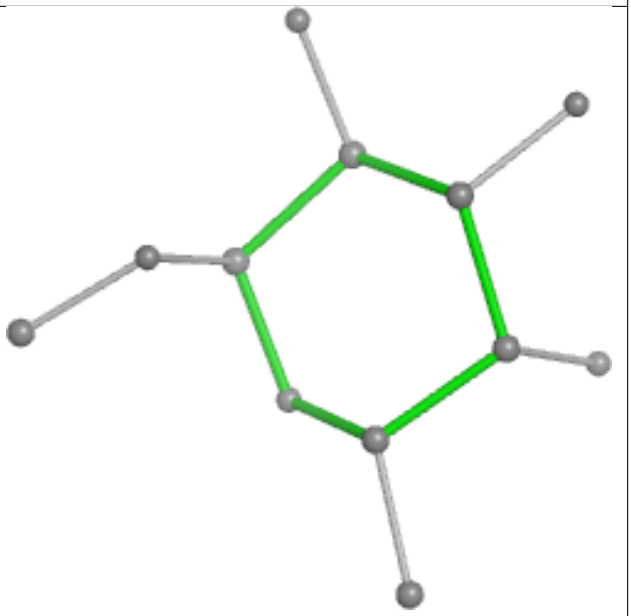
Bond lengths



Bond angles

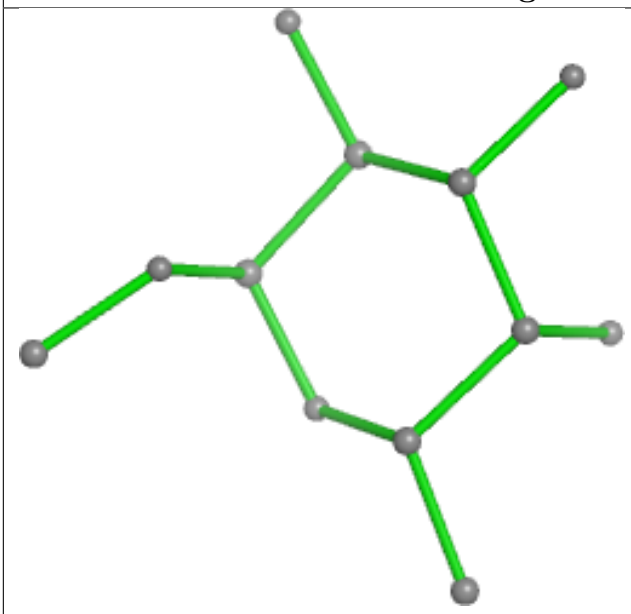


Torsions

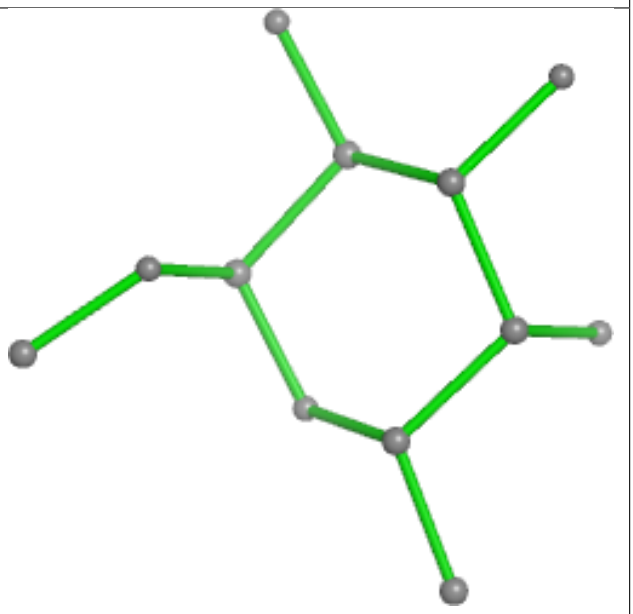


Rings

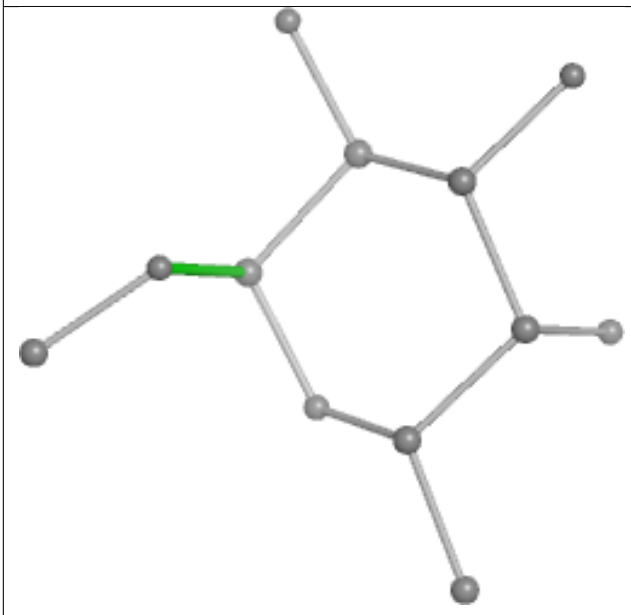
Ligand MFU D 403



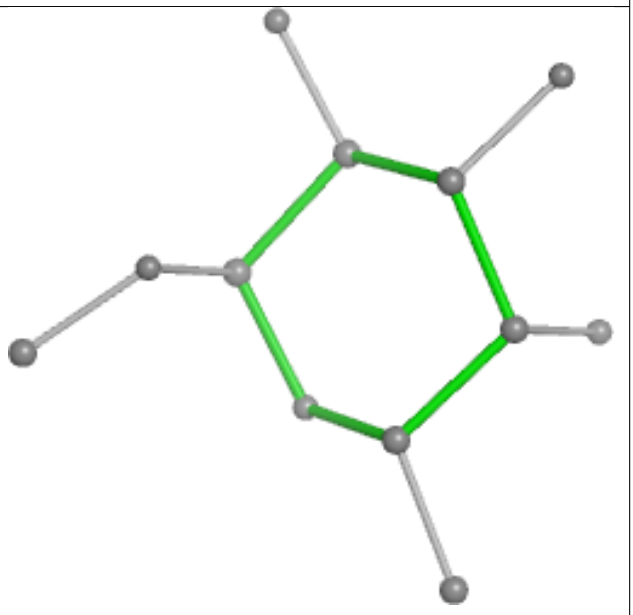
Bond lengths



Bond angles

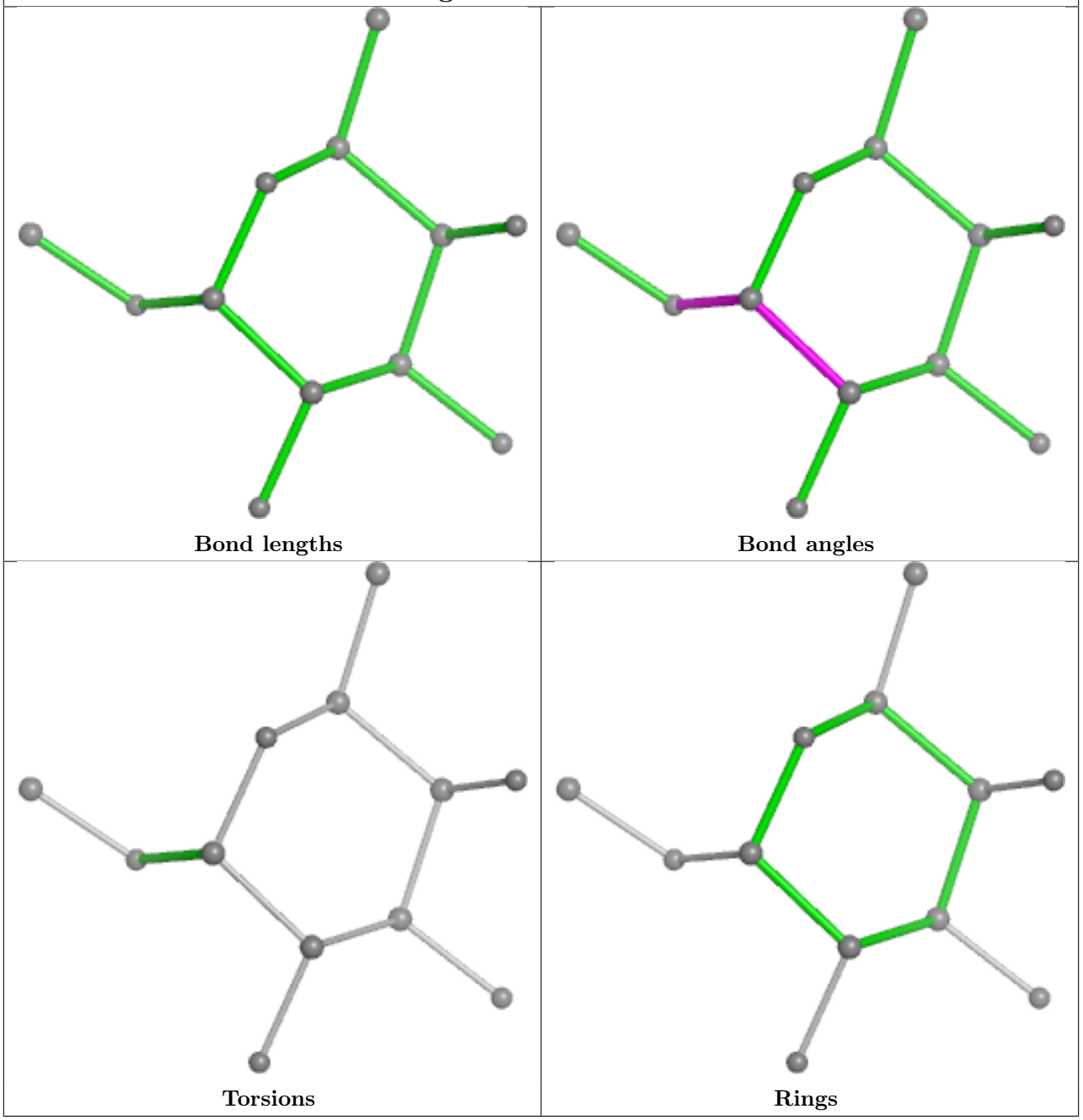


Torsions



Rings

Ligand MFU C 404



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	348/371 (93%)	0.29	10 (2%) 54 57	13, 18, 27, 40	1 (0%)
1	B	344/371 (92%)	0.28	8 (2%) 61 64	12, 19, 25, 36	2 (0%)
1	C	338/371 (91%)	0.52	16 (4%) 37 40	9, 21, 29, 35	1 (0%)
1	D	342/371 (92%)	0.68	19 (5%) 31 33	14, 22, 30, 35	0
All	All	1372/1484 (92%)	0.45	53 (3%) 44 47	9, 20, 28, 40	4 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	SER	4.1
1	B	24	ILE	3.8
1	B	28	THR	3.8
1	B	299	TRP	3.8
1	D	114	ALA	3.8
1	D	305	SER	3.7
1	A	307	SER	3.3
1	A	67	ALA	3.2
1	B	114	ALA	3.1
1	A	306	GLY	3.1
1	B	109	GLN	3.0
1	A	304	HIS	3.0
1	D	291	ILE	2.9
1	C	115	SER	2.9
1	C	263	TRP	2.8
1	C	110	THR	2.8
1	A	23	GLU	2.8
1	C	109	GLN	2.8
1	D	243	VAL	2.7
1	D	257	SER	2.7
1	A	308	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	357	TRP	2.6
1	A	65	THR	2.6
1	D	216	HIS	2.6
1	D	311	TRP	2.5
1	C	221	VAL	2.5
1	B	23	GLU	2.5
1	D	73	SER	2.4
1	C	29	ILE	2.4
1	C	30	ALA	2.4
1	C	291	ILE	2.4
1	C	197	ASN	2.4
1	D	354	TRP	2.4
1	C	172	HIS	2.4
1	C	324	VAL	2.3
1	B	352	SER	2.3
1	A	28	THR	2.2
1	D	258	SER	2.2
1	D	211	TYR	2.2
1	D	197	ASN	2.2
1	D	268	GLY	2.2
1	D	263	TRP	2.2
1	B	331	TYR	2.2
1	C	367	ALA	2.1
1	D	344	TRP	2.1
1	C	311	TRP	2.1
1	D	296	TRP	2.1
1	C	361	GLY	2.1
1	C	173	VAL	2.1
1	C	31	ALA	2.1
1	D	358	ALA	2.1
1	A	339	THR	2.0
1	D	290	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

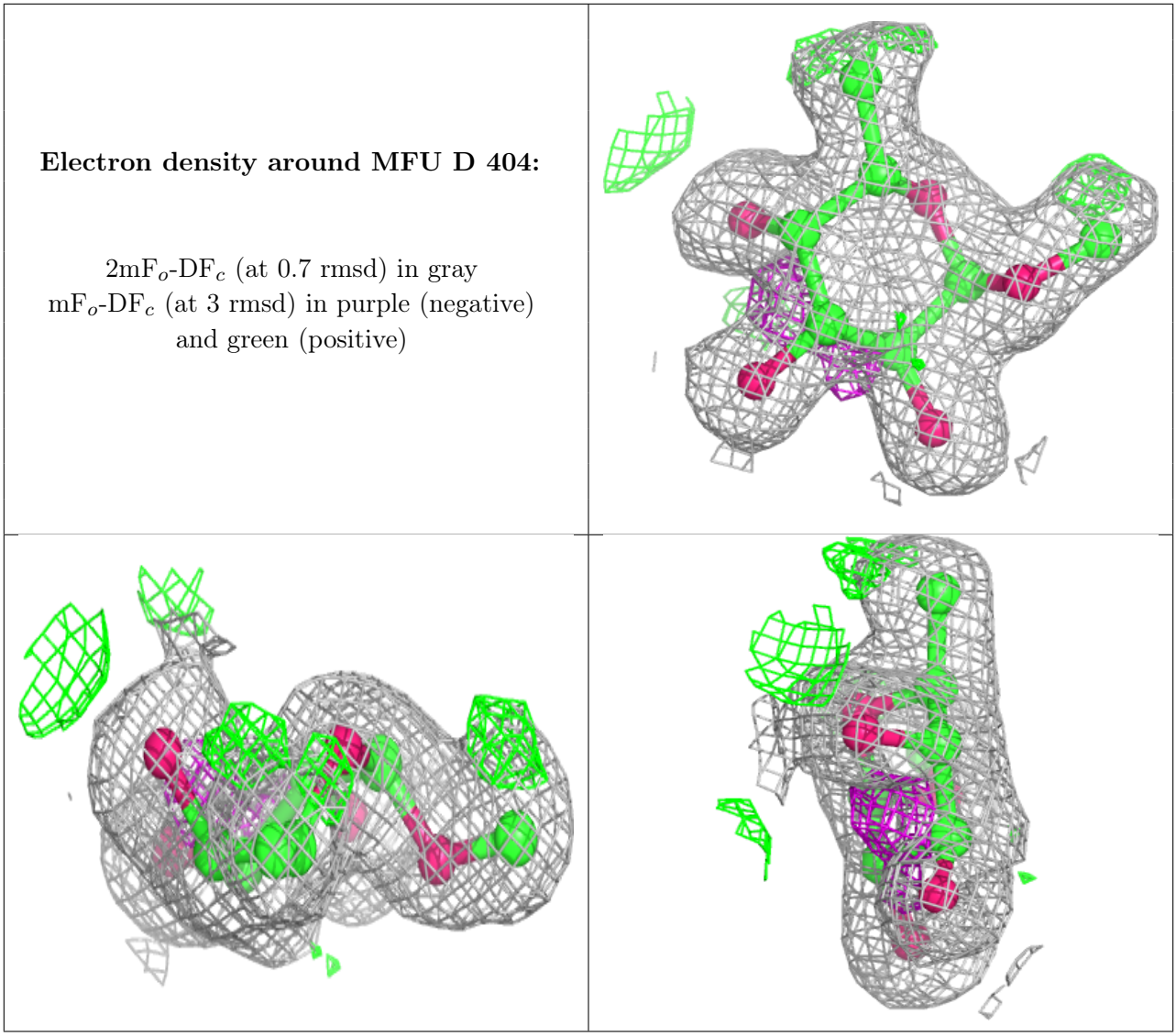
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MFU	D	404	12/12	0.83	0.14	23,25,26,26	0
2	MFU	D	403	12/12	0.84	0.13	30,33,34,35	0
2	MFU	B	404	12/12	0.88	0.12	25,27,28,29	0
2	MFU	C	403	12/12	0.91	0.11	30,31,33,34	0
2	MFU	C	402	12/12	0.92	0.10	20,22,22,23	0
2	MFU	A	404	12/12	0.92	0.10	19,22,23,23	0
2	MFU	B	401	12/12	0.93	0.09	20,21,22,22	0
2	MFU	C	404	12/12	0.94	0.08	20,21,24,24	0
2	MFU	D	402	12/12	0.94	0.08	19,20,22,22	0
2	MFU	B	403	12/12	0.94	0.08	18,20,21,22	0
2	MFU	A	402	12/12	0.94	0.08	24,25,26,26	0
2	MFU	A	403	12/12	0.95	0.07	19,20,22,22	0
2	MFU	C	401	12/12	0.95	0.07	18,18,19,19	0
2	MFU	D	401	12/12	0.96	0.07	17,18,19,20	0
2	MFU	A	401	12/12	0.96	0.06	15,16,17,18	0
2	MFU	B	402	12/12	0.97	0.05	14,15,16,16	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.

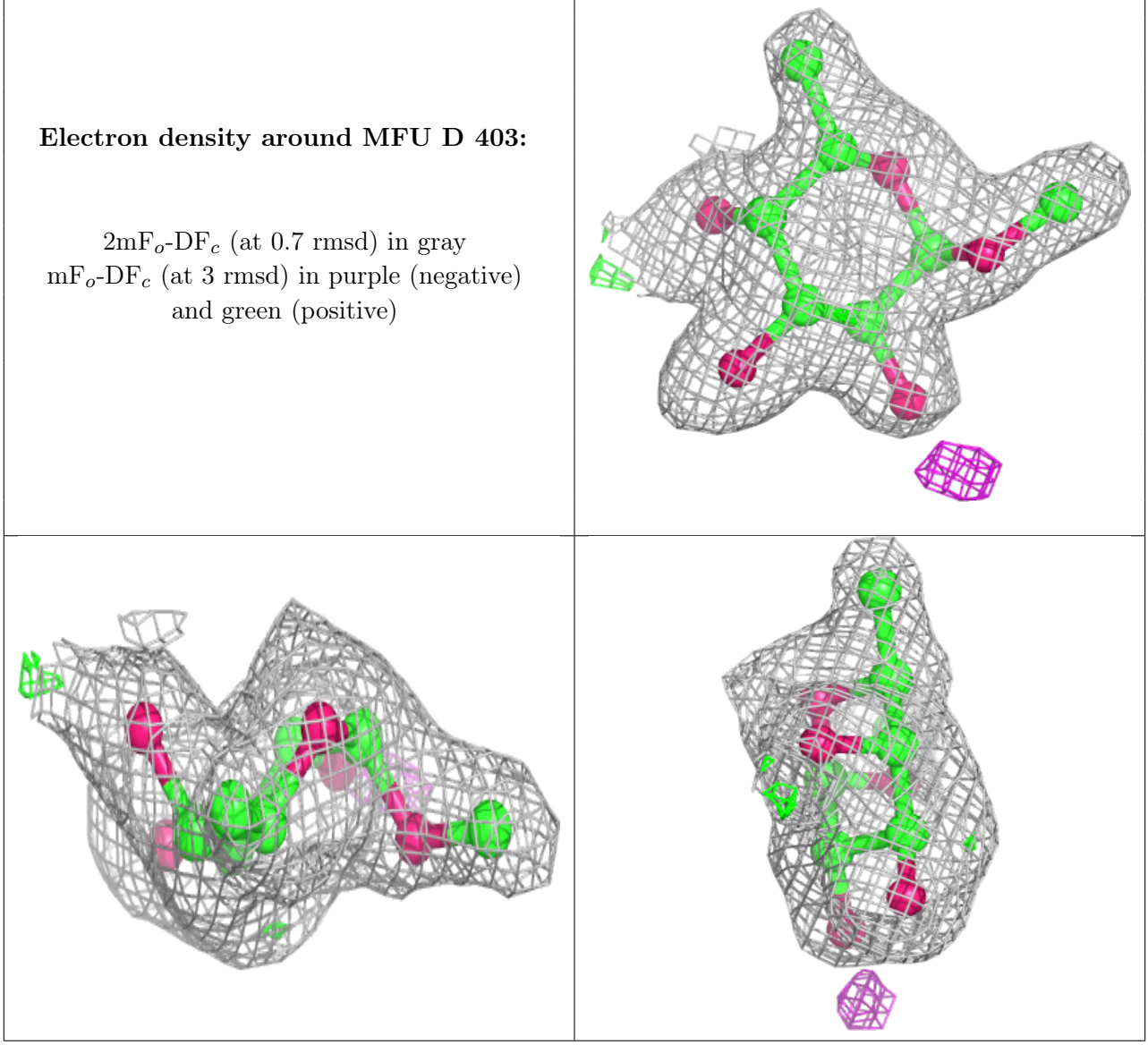
Electron density around MFU D 404:

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



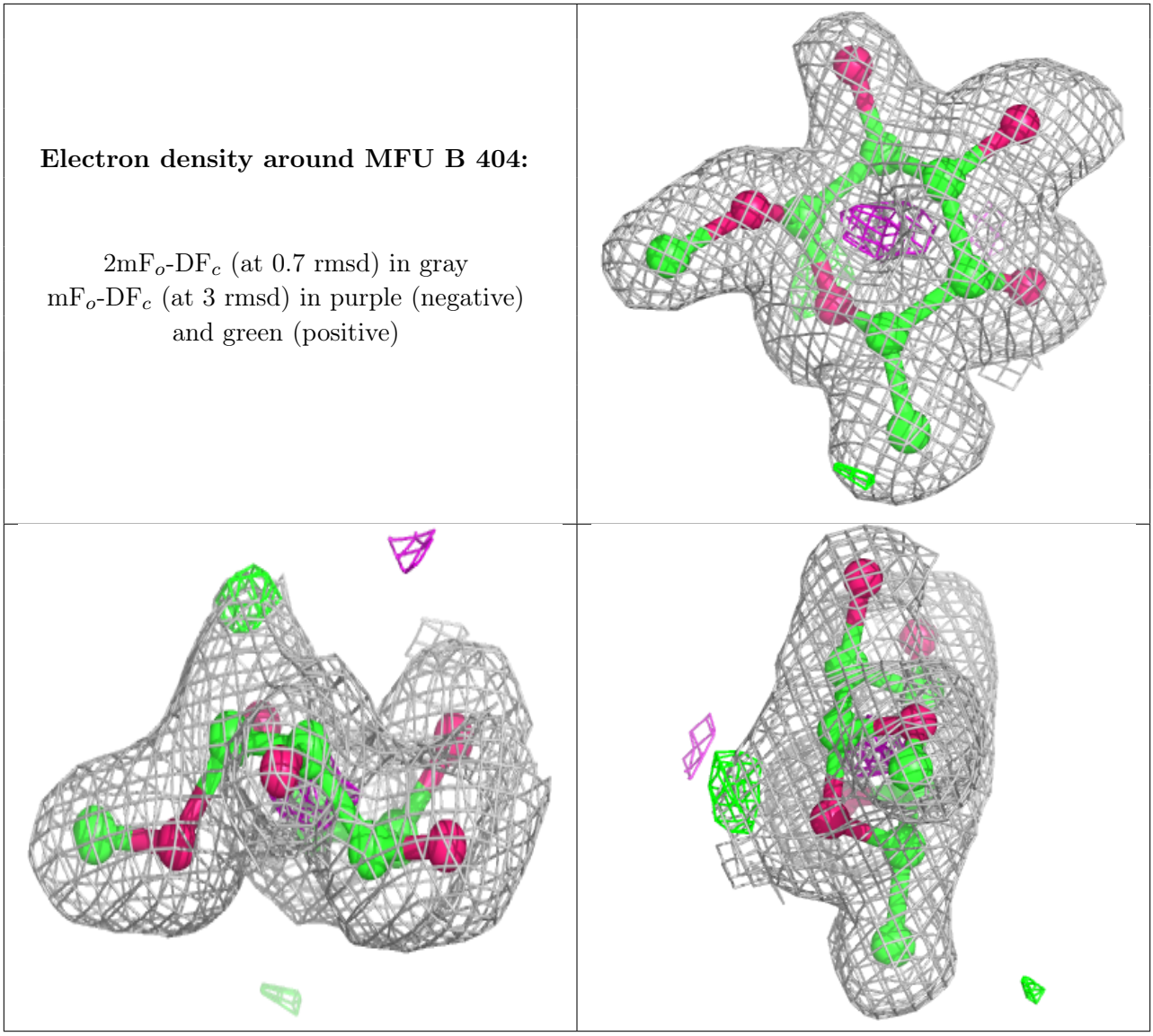
Electron density around MFU D 403:

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



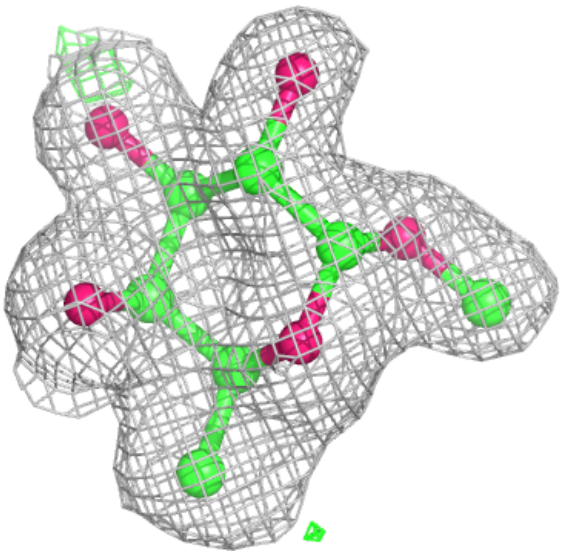
Electron density around MFU B 404:

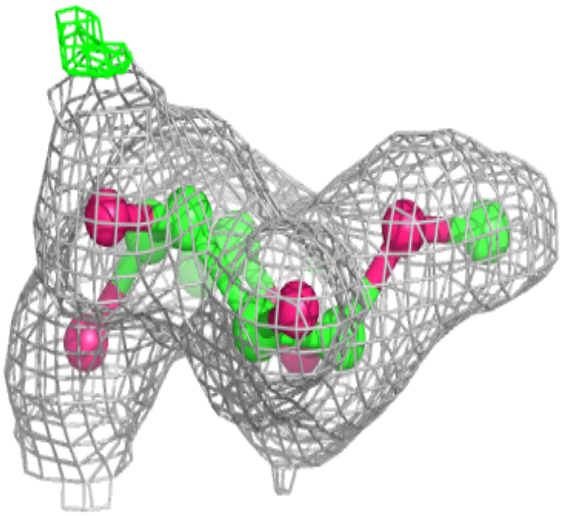
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

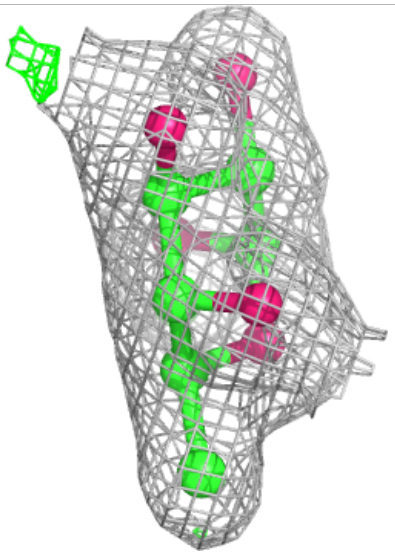


Electron density around MFU C 403:

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

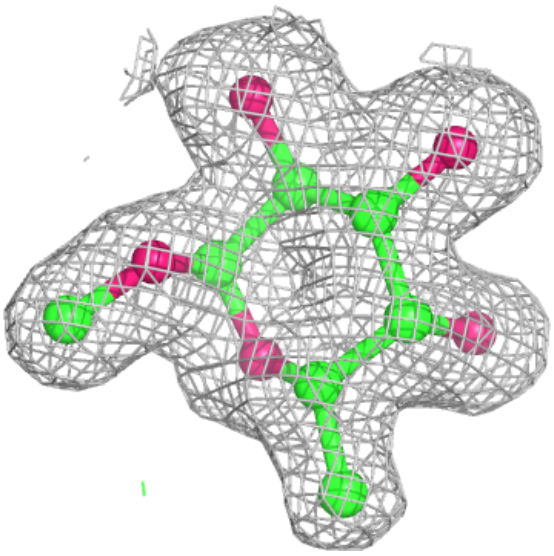


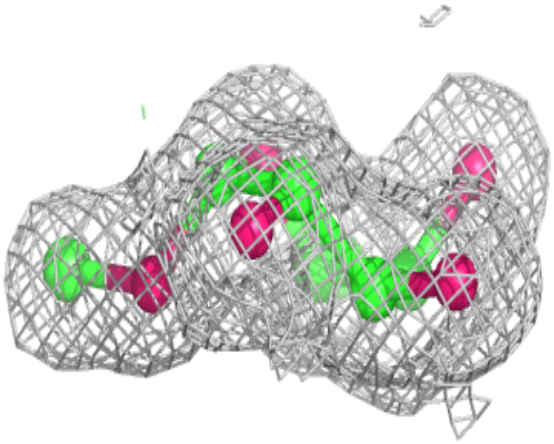


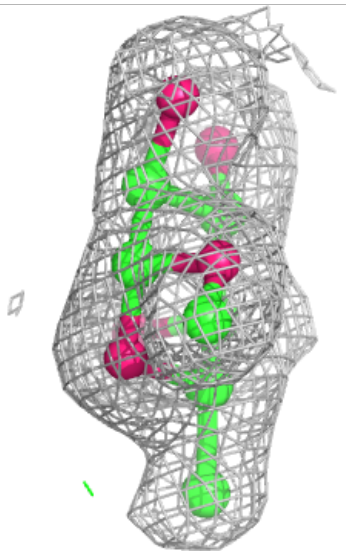


Electron density around MFU C 402:

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

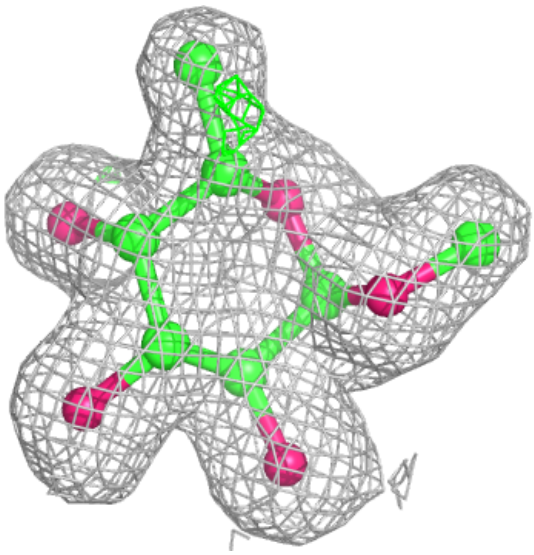


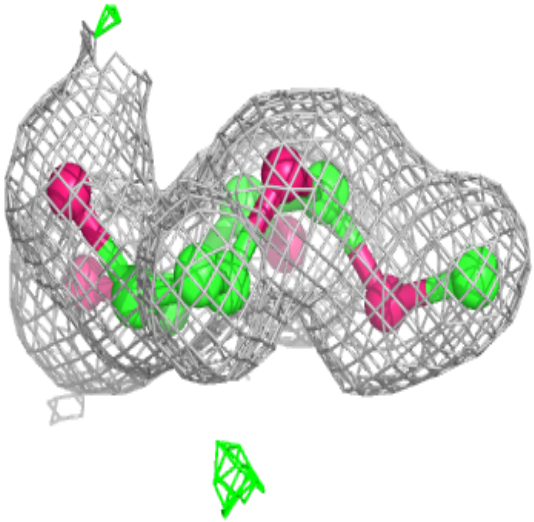


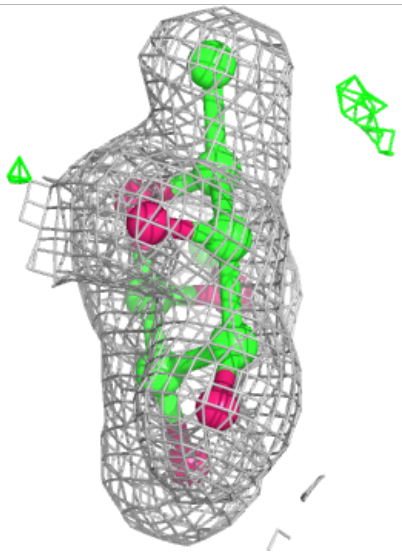


Electron density around MFU A 404:

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

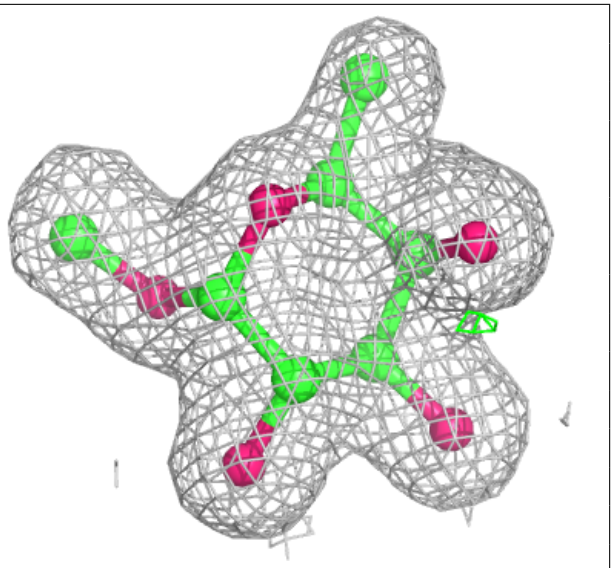


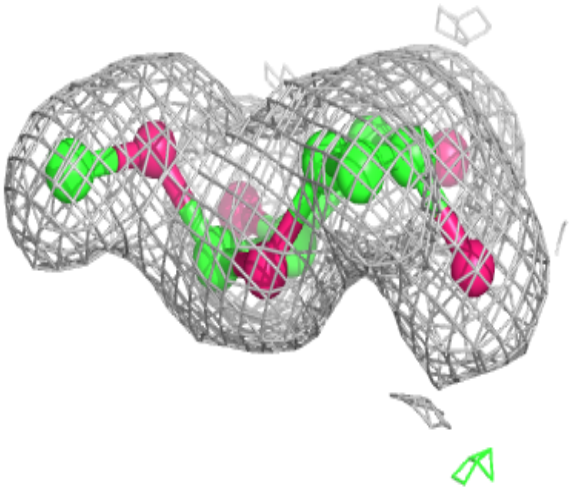


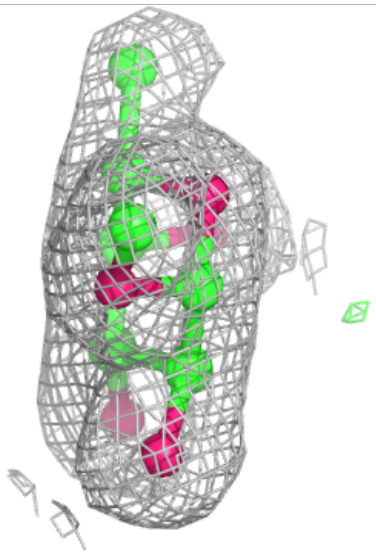


Electron density around MFU B 401:

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

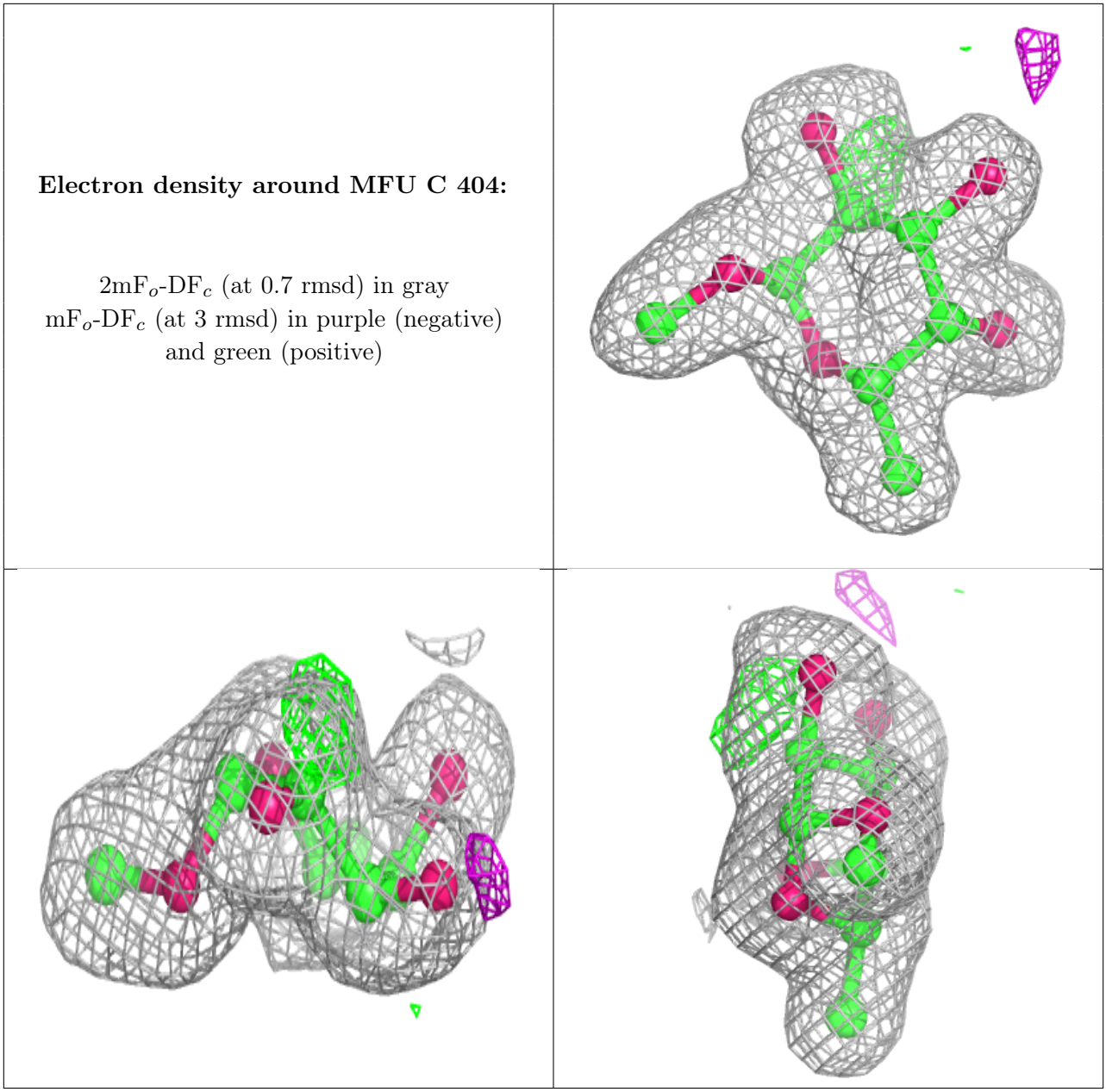






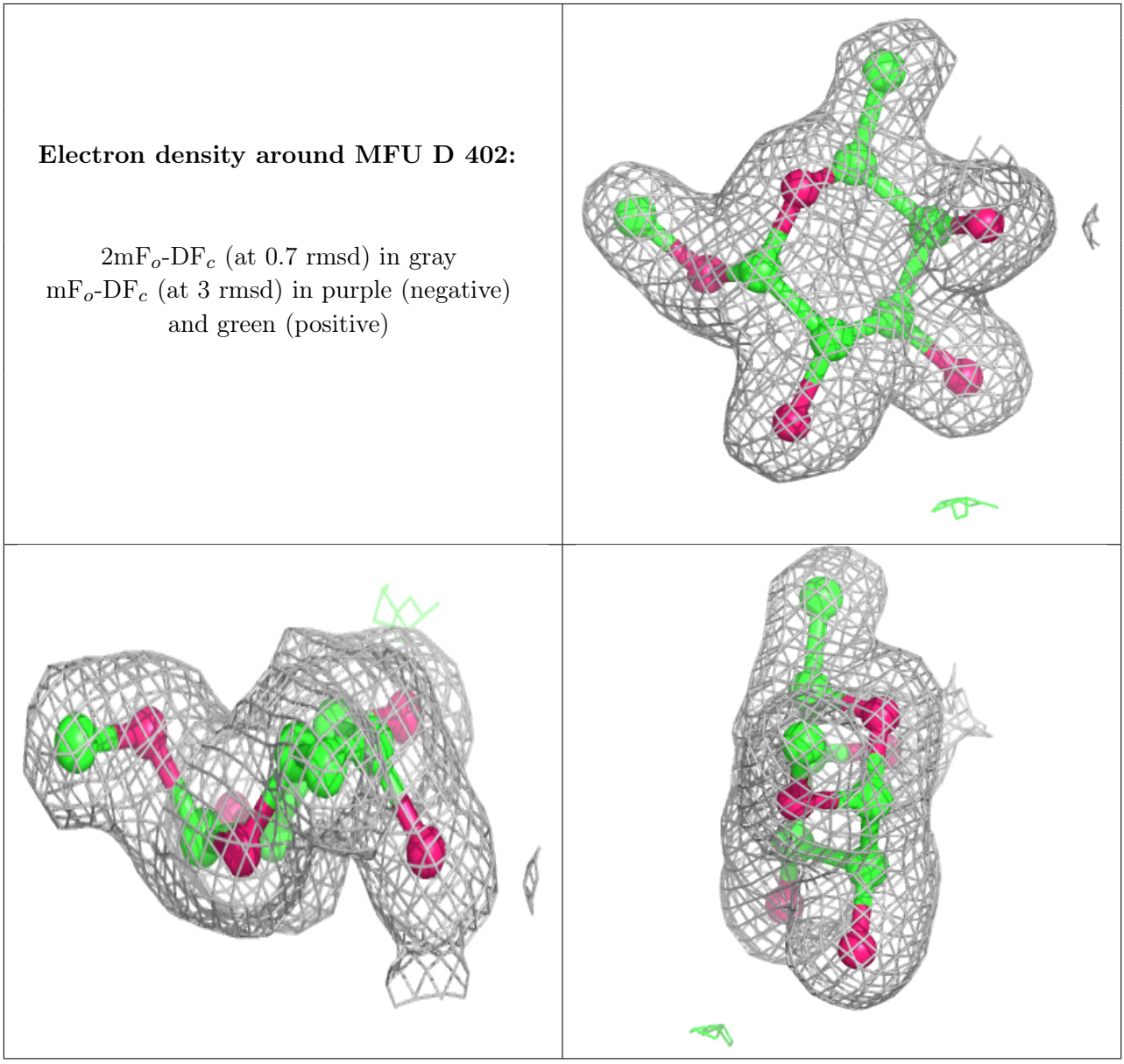
Electron density around MFU C 404:

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



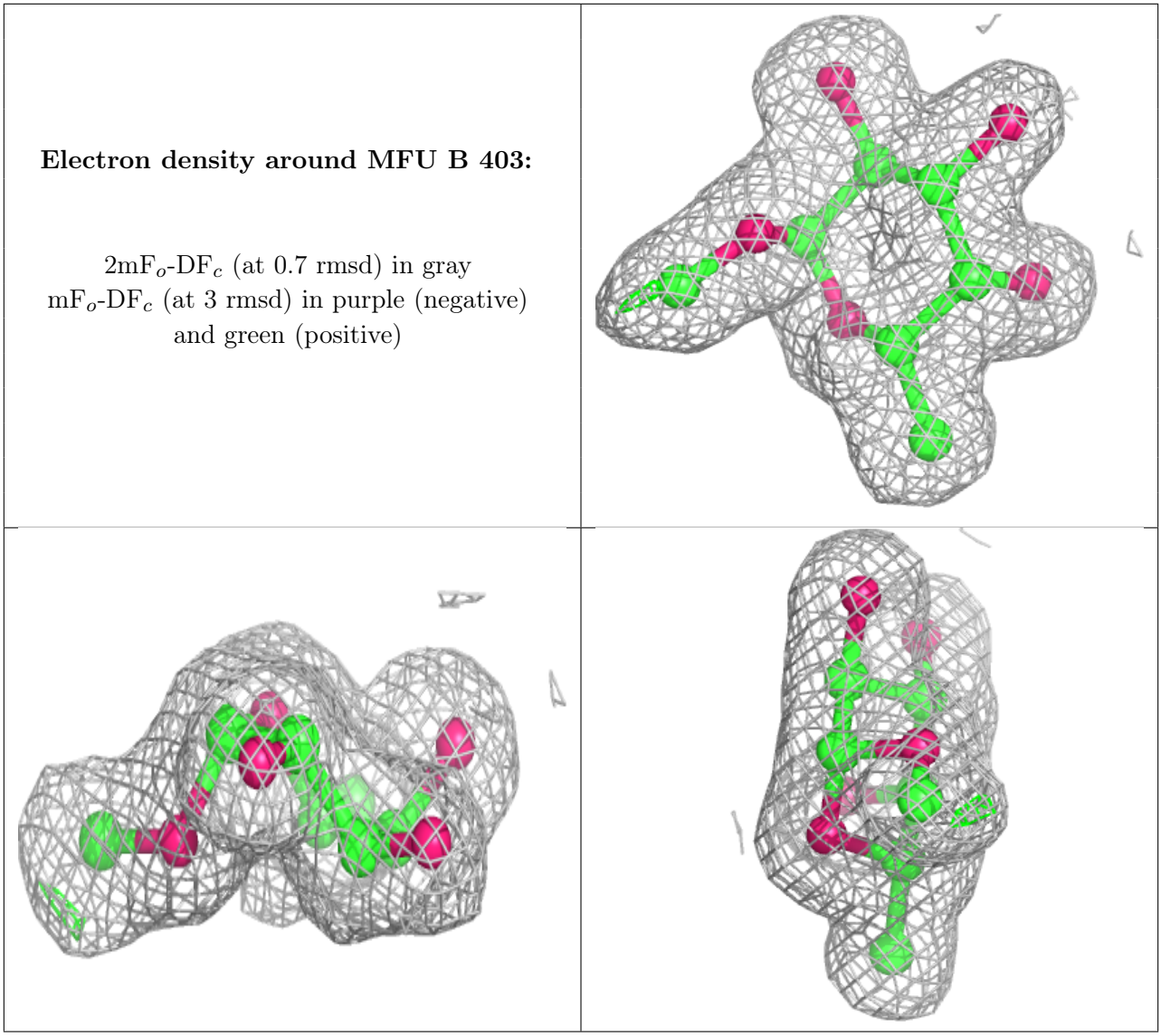
Electron density around MFU D 402:

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



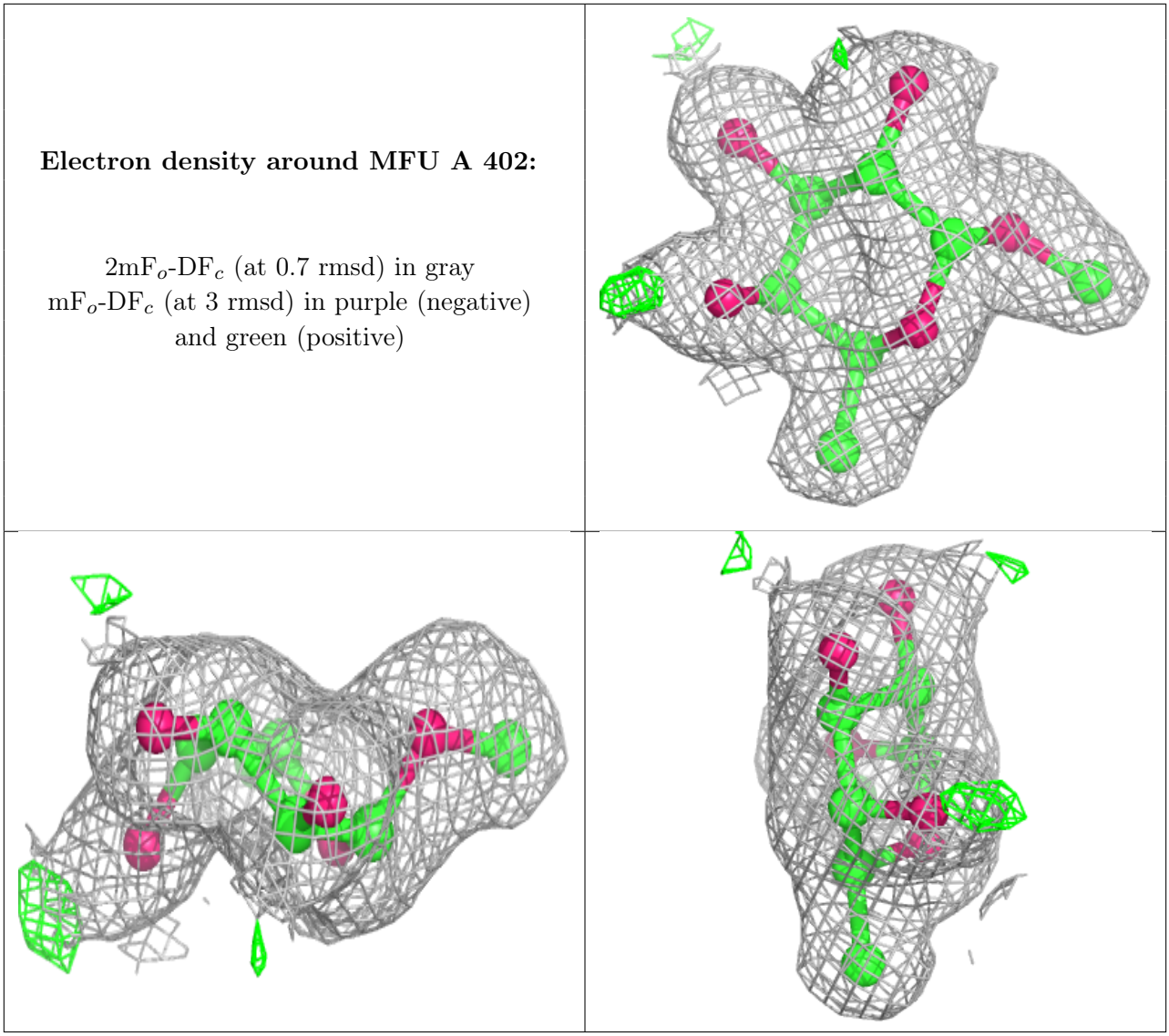
Electron density around MFU B 403:

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



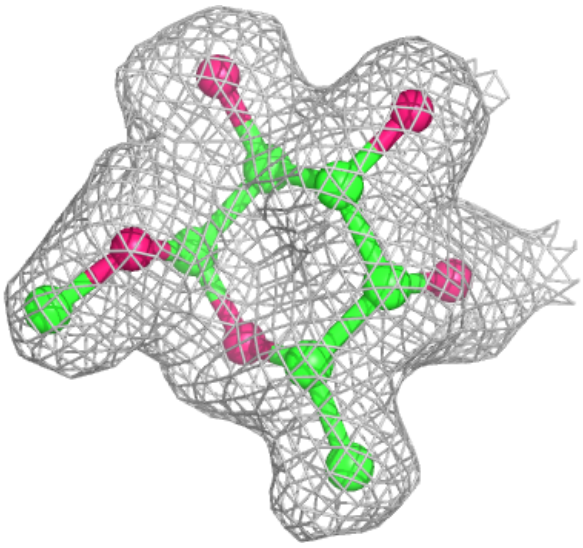
Electron density around MFU A 402:

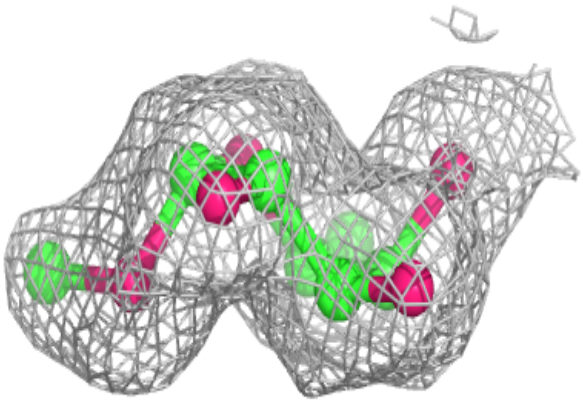
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

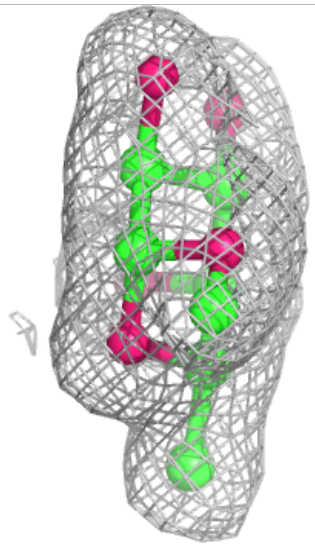


Electron density around MFU A 403:

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

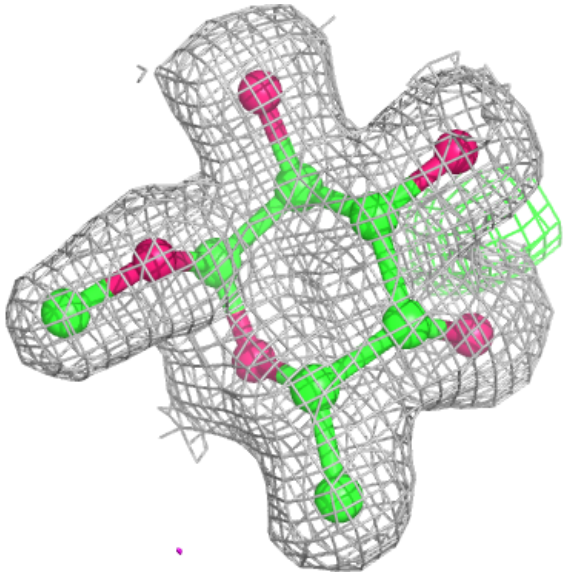


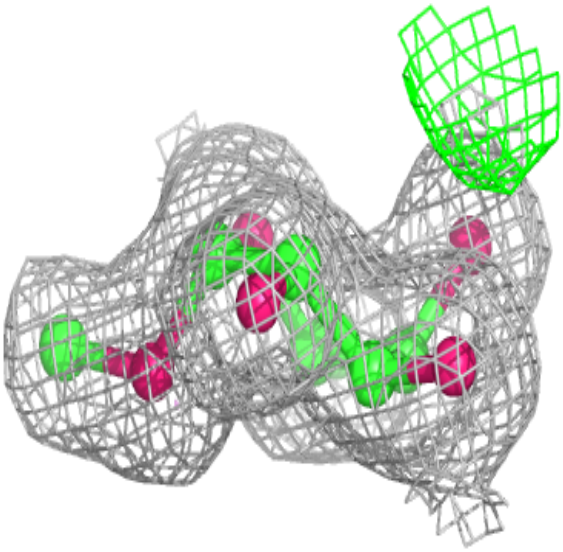


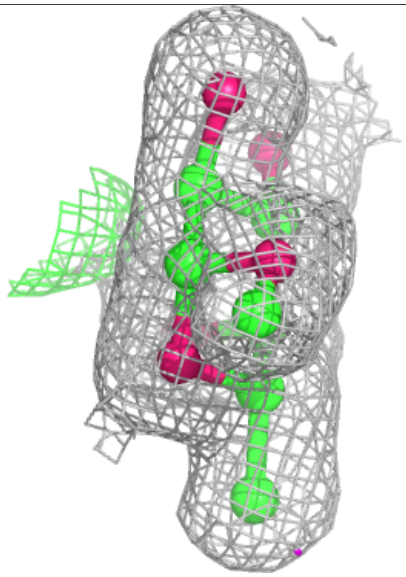


Electron density around MFU C 401:

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

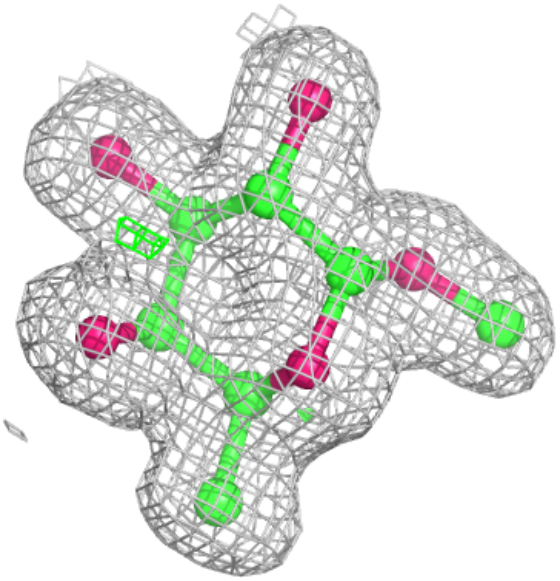


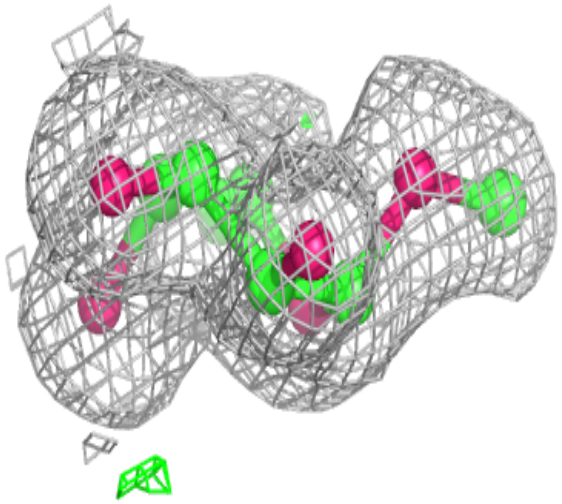


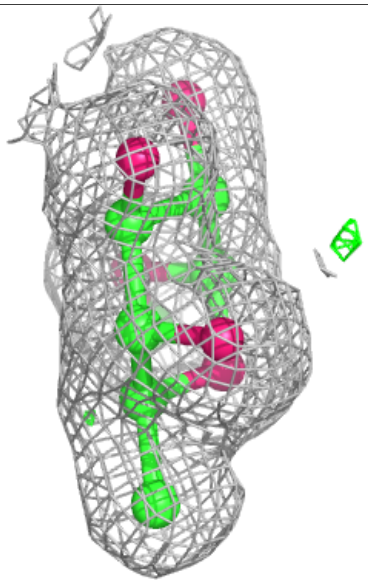


Electron density around MFU D 401:

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

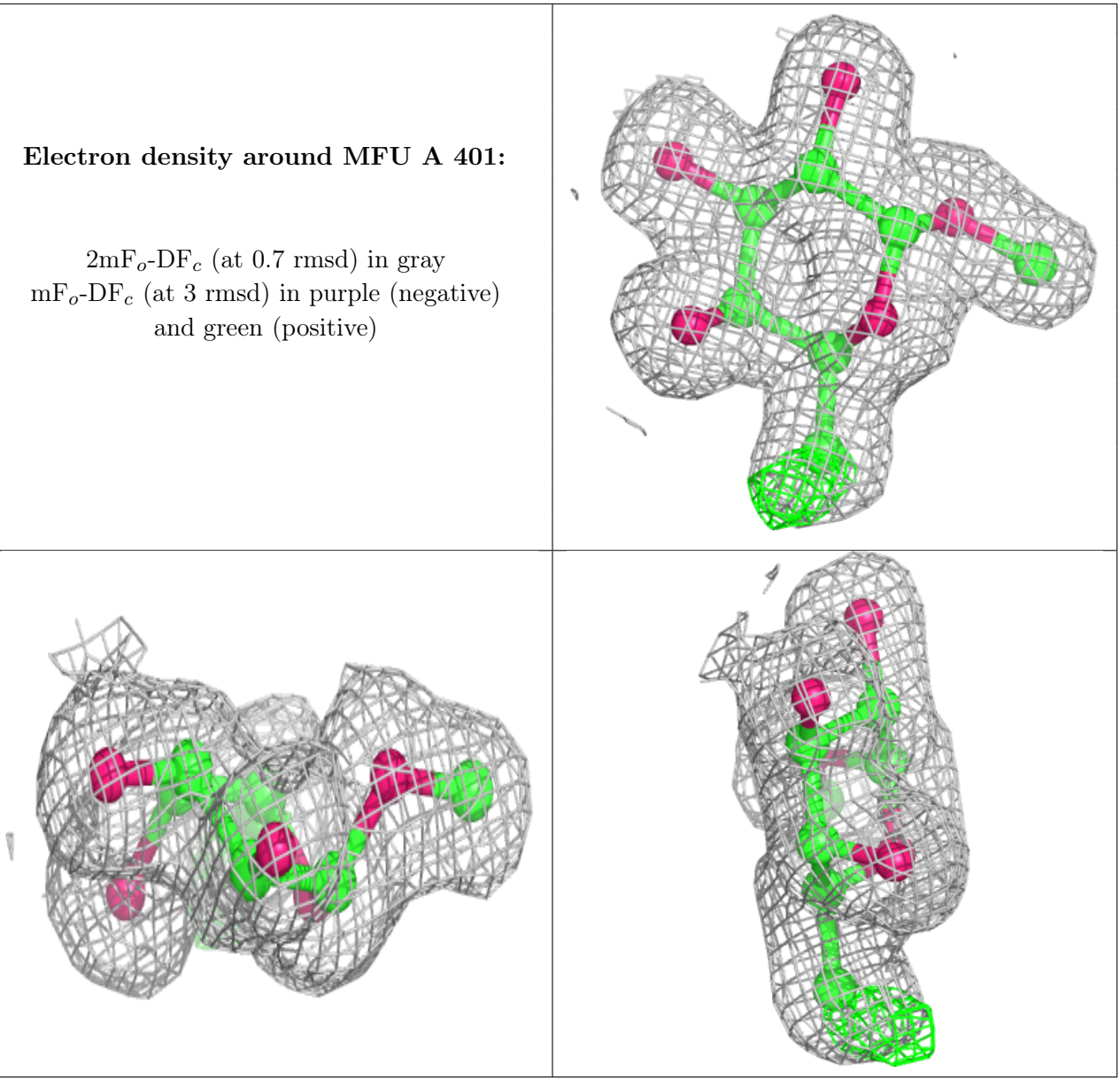






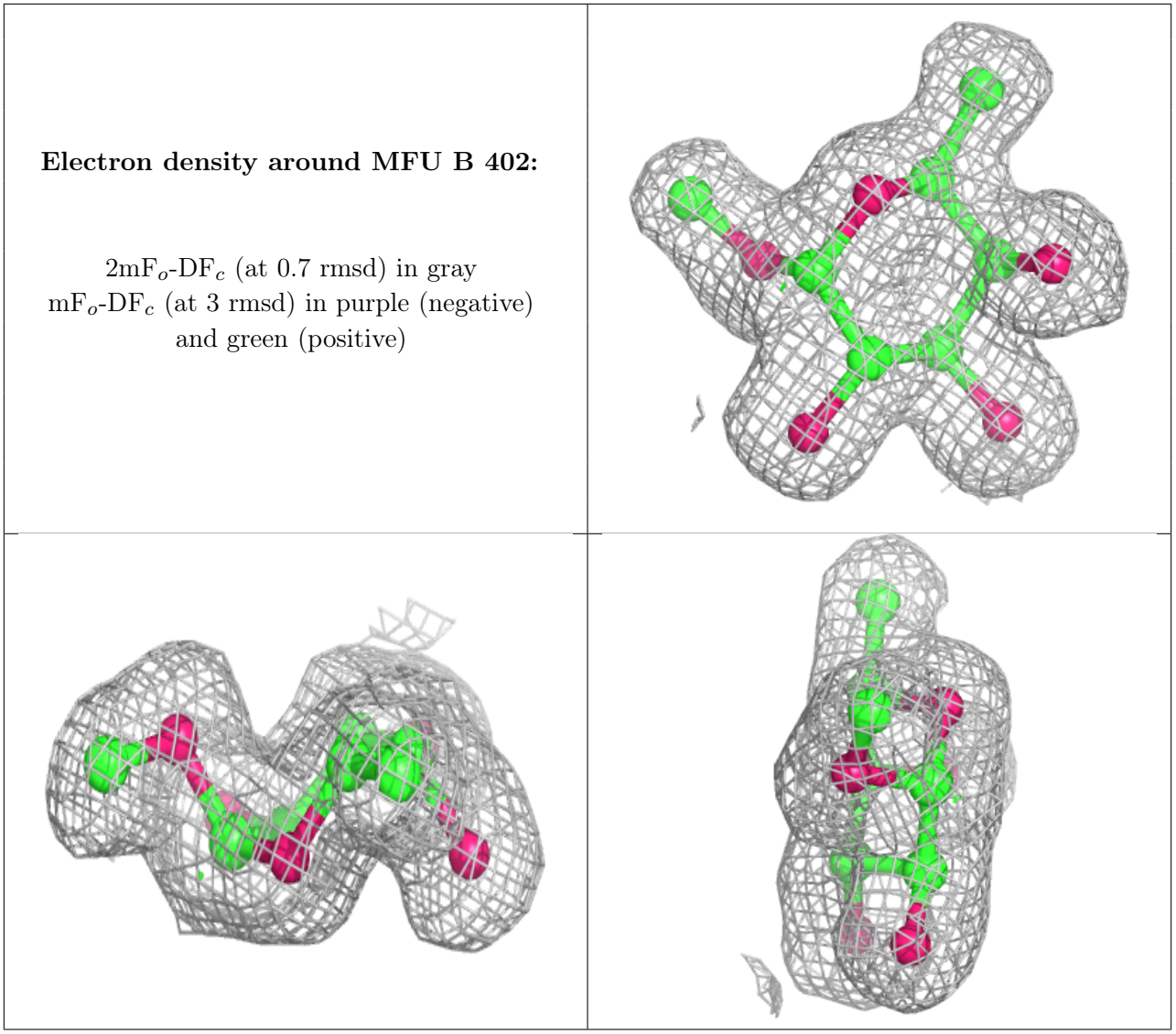
Electron density around MFU A 401:

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



Electron density around MFU B 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

There are no such residues in this entry.