



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 06:26 PM BST

PDB ID : 6QXL
Title : Crystal Structure of Pyruvate Kinase II (PykA) from *Pseudomonas aeruginosa* in complex with sodium malonate, magnesium and glucose-6-phosphate
Authors : Abdelhamid, Y.; Brear, P.; Welch, M.
Deposited on : 2019-03-07
Resolution : 2.43 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

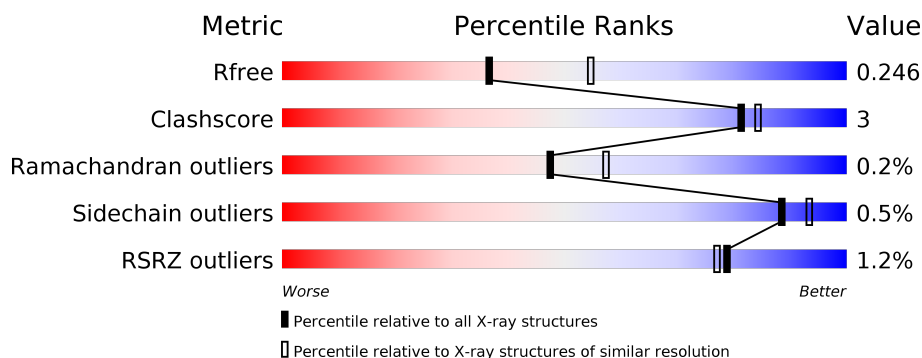
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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 on 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	483	 91% 8% .
1	B	483	 94% 5% .
1	C	483	 93% 6% .
1	D	483	 94% 5% .
1	E	483	 92% 7% .
1	F	483	 92% 8% .

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Mol	Chain	Length	Quality of chain
1	G	483	<div><div></div><div>%</div><div>93%</div><div>6%</div><div>.</div></div>
1	H	483	<div><div></div><div>2%</div><div>92%</div><div>7%</div><div></div></div>
1	I	483	<div><div></div><div>%</div><div>91%</div><div>8%</div><div>.</div></div>
1	J	483	<div><div></div><div>%</div><div>78%</div><div>.</div><div>.</div><div>16%</div><div></div></div>
1	K	483	<div><div></div><div>%</div><div>93%</div><div>6%</div><div>.</div></div>
1	L	483	<div><div></div><div>6%</div><div>89%</div><div>9%</div><div>.</div></div>

2 Entry composition

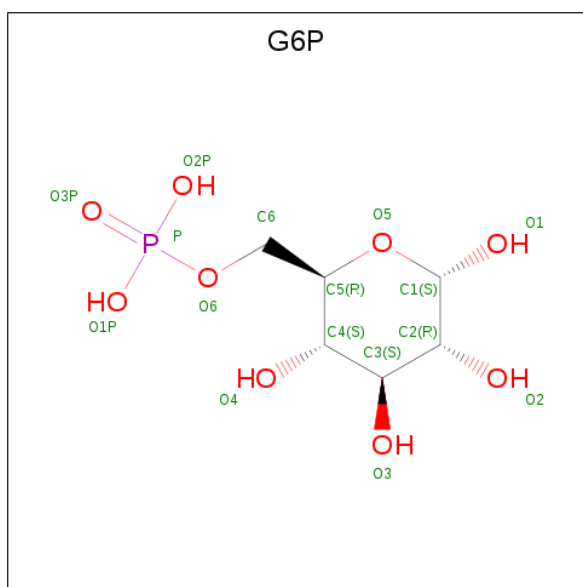
There are 6 unique types of molecules in this entry. The entry contains 45923 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3662	2286	661	695	20			
1	B	483	Total	C	N	O	S	0	0	0
			3662	2286	661	695	20			
1	C	483	Total	C	N	O	S	0	0	0
			3662	2286	661	695	20			
1	D	483	Total	C	N	O	S	0	0	0
			3662	2286	661	695	20			
1	E	483	Total	C	N	O	S	0	2	0
			3680	2296	664	700	20			
1	F	483	Total	C	N	O	S	0	0	0
			3662	2286	661	695	20			
1	G	483	Total	C	N	O	S	0	0	0
			3662	2286	661	695	20			
1	H	483	Total	C	N	O	S	0	0	0
			3662	2286	661	695	20			
1	I	483	Total	C	N	O	S	0	0	0
			3662	2286	661	695	20			
1	J	404	Total	C	N	O	S	0	0	0
			3057	1910	555	575	17			
1	K	482	Total	C	N	O	S	0	0	0
			3654	2282	660	692	20			
1	L	483	Total	C	N	O	S	0	0	0
			3662	2286	661	695	20			

- Molecule 2 is 6-O-phosphono-alpha-D-glucopyranose (three-letter code: G6P) (formula: C₆H₁₃O₉P) (labeled as "Ligand of Interest" by author).

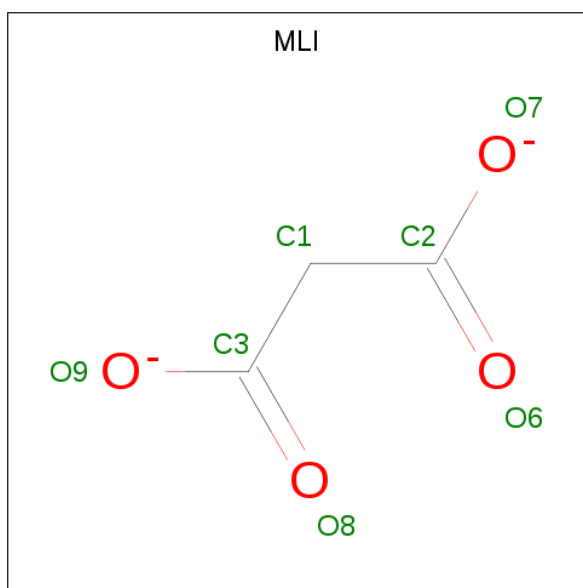


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		
2	C	1	Total	C	O	P	0	0
			16	6	9	1		
2	D	1	Total	C	O	P	0	0
			16	6	9	1		
2	E	1	Total	C	O	P	0	0
			16	6	9	1		
2	F	1	Total	C	O	P	0	0
			16	6	9	1		
2	G	1	Total	C	O	P	0	0
			16	6	9	1		
2	H	1	Total	C	O	P	0	0
			16	6	9	1		
2	I	1	Total	C	O	P	0	0
			16	6	9	1		
2	J	1	Total	C	O	P	0	0
			16	6	9	1		
2	K	1	Total	C	O	P	0	0
			16	6	9	1		
2	L	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

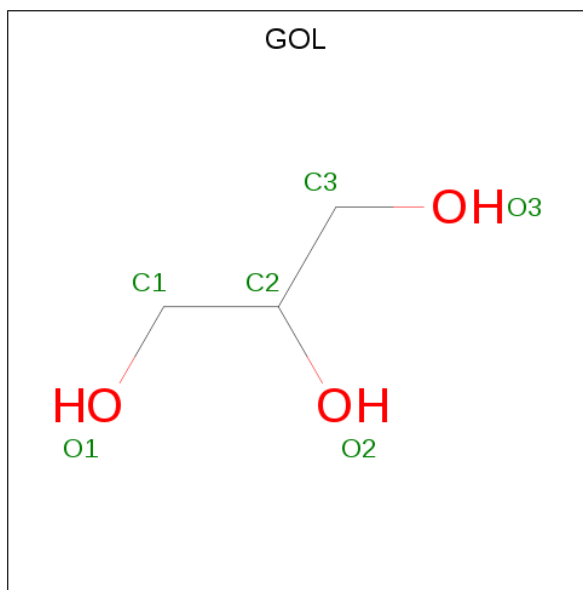
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total 1 Mg 1	0	0
3	J	1	Total 1 Mg 1	0	0
3	D	1	Total 1 Mg 1	0	0
3	K	1	Total 1 Mg 1	0	0
3	E	1	Total 1 Mg 1	0	0
3	H	1	Total 1 Mg 1	0	0
3	B	1	Total 1 Mg 1	0	0
3	I	1	Total 1 Mg 1	0	0
3	C	1	Total 1 Mg 1	0	0
3	A	1	Total 1 Mg 1	0	0
3	L	1	Total 1 Mg 1	0	0
3	F	1	Total 1 Mg 1	0	0

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	3	4		
4	B	1	Total	C	O	0	0
			7	3	4		
4	C	1	Total	C	O	0	0
			7	3	4		
4	D	1	Total	C	O	0	0
			7	3	4		
4	E	1	Total	C	O	0	0
			7	3	4		
4	F	1	Total	C	O	0	0
			7	3	4		
4	G	1	Total	C	O	0	0
			7	3	4		
4	H	1	Total	C	O	0	0
			7	3	4		
4	I	1	Total	C	O	0	0
			7	3	4		
4	J	1	Total	C	O	0	0
			7	3	4		
4	K	1	Total	C	O	0	0
			7	3	4		
4	L	1	Total	C	O	0	0
			7	3	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0

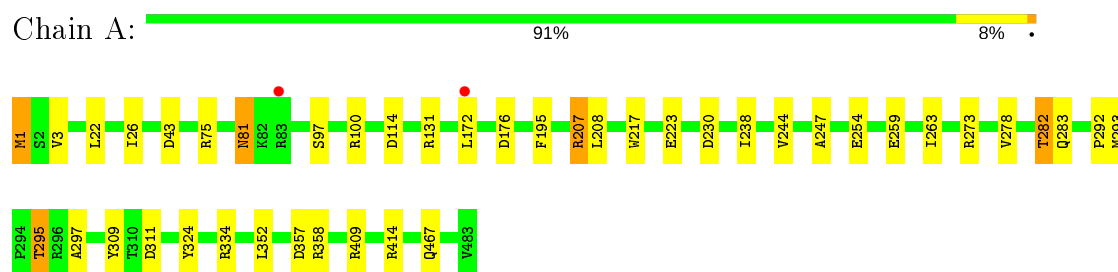
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	238	Total O 238 238	0	0
6	B	301	Total O 301 301	0	0
6	C	245	Total O 245 245	0	0
6	D	272	Total O 272 272	0	0
6	E	270	Total O 270 270	0	0
6	F	164	Total O 164 164	0	0
6	G	154	Total O 154 154	0	0
6	H	150	Total O 150 150	0	0
6	I	114	Total O 114 114	0	0
6	J	128	Total O 128 128	0	0
6	K	150	Total O 150 150	0	0
6	L	82	Total O 82 82	0	0

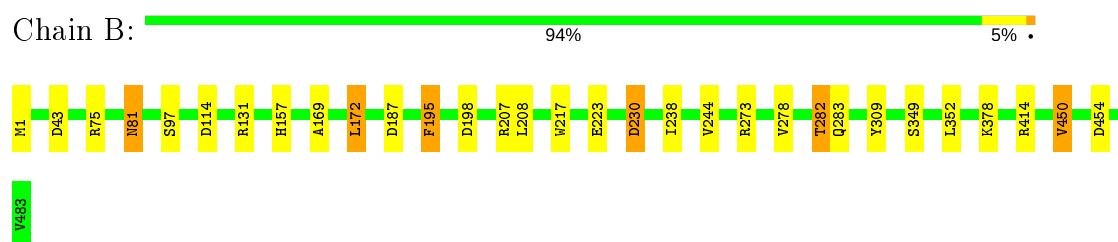
3 Residue-property plots

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

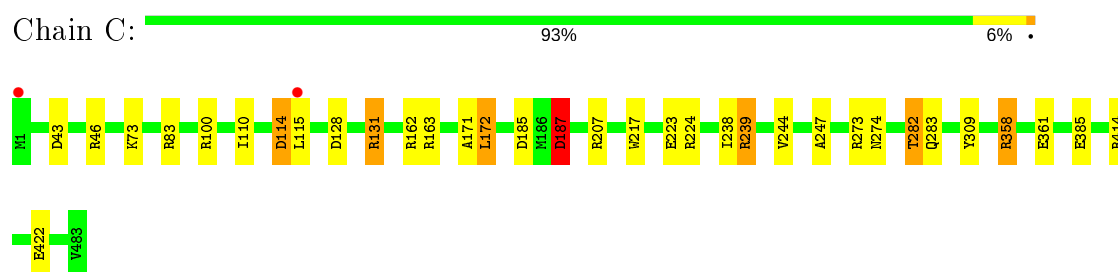
- Molecule 1: Pyruvate kinase



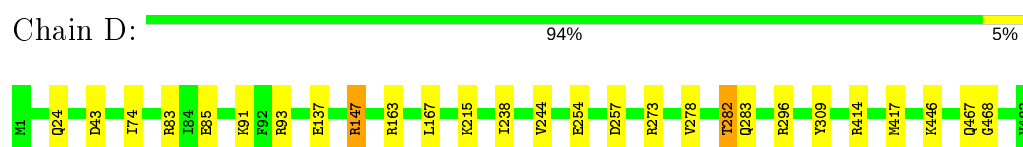
- Molecule 1: Pyruvate kinase



- Molecule 1: Pyruvate kinase



- Molecule 1: Pyruvate kinase



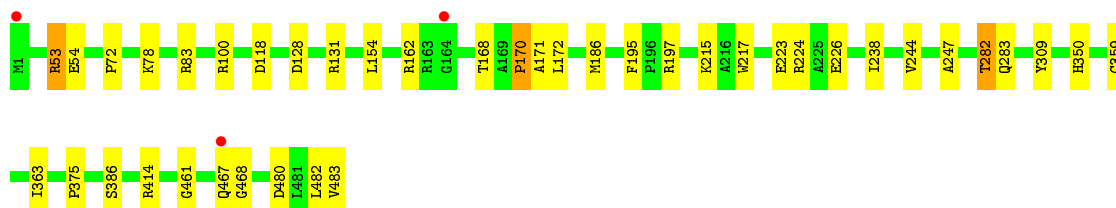
- Molecule 1: Pyruvate kinase

Chain E:  92% 7% .



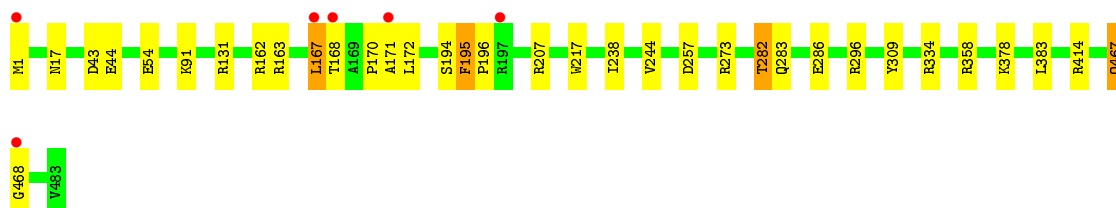
• Molecule 1: Pyruvate kinase

Chain F:  92% 8% .



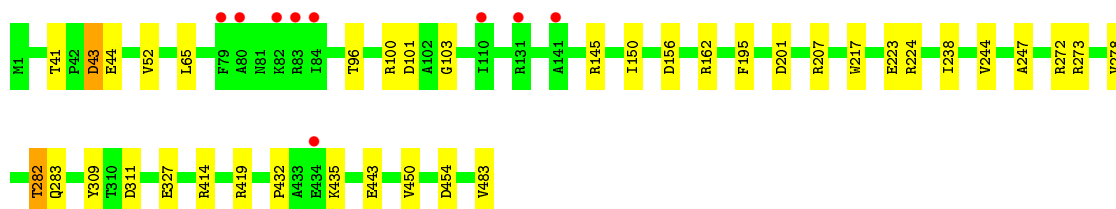
• Molecule 1: Pyruvate kinase

Chain G:  93% 6% .




• Molecule 1: Pyruvate kinase

Chain H:  92% 7% 2% .



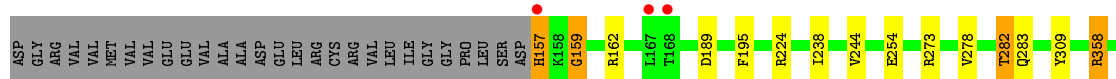
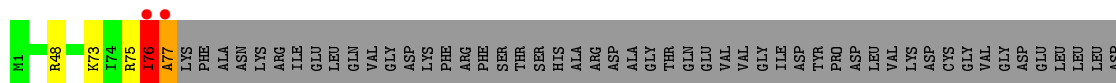
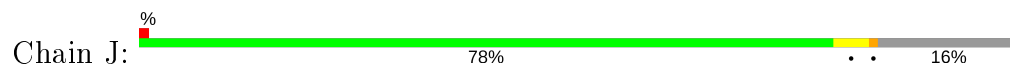
• Molecule 1: Pyruvate kinase

Chain I:  91% 8% .





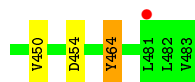
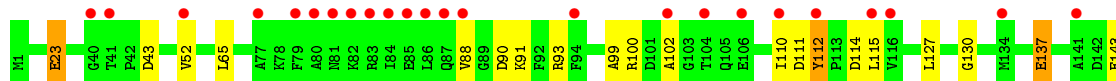
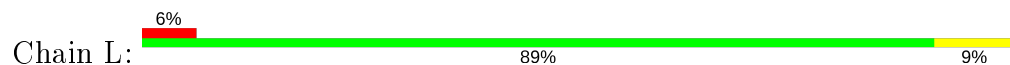
- Molecule 1: Pyruvate kinase



- Molecule 1: Pyruvate kinase



- Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.48Å 182.48Å 405.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	158.03 – 2.43 158.03 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.9 (158.03-2.43) 98.7 (158.03-2.43)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.43Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.227 , 0.251 0.221 , 0.246	Depositor DCC
R_{free} test set	14353 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.809	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	45923	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.47% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, MLI, G6P

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	0.69	3/3716 (0.1%)	0.86	19/5025 (0.4%)
1	B	0.73	1/3716 (0.0%)	0.91	15/5025 (0.3%)
1	C	0.68	1/3716 (0.0%)	0.93	19/5025 (0.4%)
1	D	0.66	0/3716	0.85	9/5025 (0.2%)
1	E	0.70	0/3734	0.90	16/5049 (0.3%)
1	F	0.72	3/3716 (0.1%)	0.95	15/5025 (0.3%)
1	G	0.67	1/3716 (0.0%)	0.90	16/5025 (0.3%)
1	H	0.72	1/3716 (0.0%)	0.92	13/5025 (0.3%)
1	I	0.71	1/3716 (0.0%)	0.96	21/5025 (0.4%)
1	J	0.75	3/3103 (0.1%)	0.99	15/4196 (0.4%)
1	K	0.69	0/3707	0.92	14/5011 (0.3%)
1	L	0.77	3/3716 (0.1%)	1.11	34/5025 (0.7%)
All	All	0.71	17/43988 (0.0%)	0.94	206/59481 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	1
1	D	0	1
1	E	0	1
1	G	0	2
1	H	0	1
1	J	0	2
1	K	0	1
1	L	0	2
All	All	0	16

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	157	HIS	N-CA	-11.85	1.22	1.46
1	J	254	GLU	CD-OE1	-8.73	1.16	1.25
1	L	464	TYR	CG-CD2	-7.38	1.29	1.39
1	A	254	GLU	CG-CD	-6.30	1.42	1.51
1	F	72	PRO	C-O	-6.21	1.10	1.23

The worst 5 of 206 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	272	ARG	NE-CZ-NH2	22.93	131.77	120.30
1	J	76	ILE	O-C-N	-18.61	92.93	122.70
1	F	53	ARG	NE-CZ-NH2	18.36	129.48	120.30
1	J	254	GLU	OE1-CD-OE2	-15.19	105.07	123.30
1	L	198	ASP	CB-CG-OD1	14.69	131.52	118.30

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	ASP	Mainchain
1	A	81	ASN	Mainchain
1	B	114	ASP	Mainchain
1	B	230	ASP	Sidechain
1	B	81	ASN	Mainchain

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	3662	0	3726	26	0
1	B	3662	0	3726	15	0
1	C	3662	0	3726	19	0
1	D	3662	0	3726	13	0
1	E	3680	0	3738	21	0
1	F	3662	0	3726	28	0
1	G	3662	0	3726	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3662	0	3726	19	0
1	I	3662	0	3726	24	0
1	J	3057	0	3123	21	0
1	K	3654	0	3721	14	0
1	L	3662	0	3726	20	0
2	A	16	0	11	1	0
2	B	16	0	11	0	0
2	C	16	0	11	0	0
2	D	16	0	11	0	0
2	E	16	0	11	0	0
2	F	16	0	11	2	0
2	G	16	0	11	0	0
2	H	16	0	11	0	0
2	I	16	0	11	0	0
2	J	16	0	11	0	0
2	K	16	0	11	0	0
2	L	16	0	11	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	7	0	2	0	0
4	B	7	0	2	0	0
4	C	7	0	2	0	0
4	D	7	0	2	0	0
4	E	7	0	2	1	0
4	F	7	0	2	0	0
4	G	7	0	2	0	0
4	H	7	0	2	0	0
4	I	7	0	2	0	0
4	J	7	0	2	0	0
4	K	7	0	2	1	0
4	L	7	0	2	0	0
5	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	6	0	8	0	0
5	E	6	0	8	0	0
6	A	238	0	0	10	0
6	B	301	0	0	7	0
6	C	245	0	0	7	0
6	D	272	0	0	7	0
6	E	270	0	0	8	0
6	F	164	0	0	3	0
6	G	154	0	0	4	0
6	H	150	0	0	3	0
6	I	114	0	0	3	0
6	J	128	0	0	8	0
6	K	150	0	0	1	0
6	L	82	0	0	2	0
All	All	45923	0	44296	225	0

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

The worst 5 of 225 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:A:263:ILE:HD11	6:A:791:HOH:O	1.01	1.18
1:C:187:ASP:OD2	6:C:601:HOH:O	1.79	0.98
1:B:378:LYS:HE3	6:B:785:HOH:O	1.65	0.96
1:E:207:ARG:HD2	6:E:771:HOH:O	1.65	0.95
1:J:73:LYS:HG3	6:J:643:HOH:O	1.67	0.93

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	481/483 (100%)	469 (98%)	11 (2%)	1 (0%)	47	57
1	B	481/483 (100%)	469 (98%)	11 (2%)	1 (0%)	47	57
1	C	481/483 (100%)	467 (97%)	13 (3%)	1 (0%)	47	57
1	D	481/483 (100%)	465 (97%)	15 (3%)	1 (0%)	47	57
1	E	483/483 (100%)	468 (97%)	14 (3%)	1 (0%)	47	57
1	F	481/483 (100%)	464 (96%)	15 (3%)	2 (0%)	34	41
1	G	481/483 (100%)	466 (97%)	14 (3%)	1 (0%)	47	57
1	H	481/483 (100%)	467 (97%)	13 (3%)	1 (0%)	47	57
1	I	481/483 (100%)	465 (97%)	15 (3%)	1 (0%)	47	57
1	J	400/483 (83%)	389 (97%)	10 (2%)	1 (0%)	41	49
1	K	478/483 (99%)	461 (96%)	16 (3%)	1 (0%)	47	57
1	L	481/483 (100%)	468 (97%)	12 (2%)	1 (0%)	47	57
All	All	5690/5796 (98%)	5518 (97%)	159 (3%)	13 (0%)	47	57

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	THR
1	B	282	THR
1	C	282	THR
1	D	282	THR
1	E	282	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/386 (100%)	385 (100%)	1 (0%)	92	95
1	B	386/386 (100%)	385 (100%)	1 (0%)	92	95
1	C	386/386 (100%)	384 (100%)	2 (0%)	88	93
1	D	386/386 (100%)	384 (100%)	2 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	388/386 (100%)	386 (100%)	2 (0%)	88	93
1	F	386/386 (100%)	384 (100%)	2 (0%)	88	93
1	G	386/386 (100%)	384 (100%)	2 (0%)	88	93
1	H	386/386 (100%)	385 (100%)	1 (0%)	92	95
1	I	386/386 (100%)	383 (99%)	3 (1%)	81	88
1	J	320/386 (83%)	319 (100%)	1 (0%)	92	95
1	K	385/386 (100%)	382 (99%)	3 (1%)	81	88
1	L	386/386 (100%)	385 (100%)	1 (0%)	92	95
All	All	4567/4632 (99%)	4546 (100%)	21 (0%)	88	93

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	309	TYR
1	G	467	GLN
1	K	83	ARG
1	F	78	LYS
1	K	168	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	157	HIS
1	L	350	HIS
1	J	283	GLN
1	F	467	GLN
1	K	467	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 12 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MLI	J	503	3	0,6,6	0.00	-	0,7,7	0.00	-
2	G6P	B	501	-	16,16,16	1.09	1 (6%)	24,24,24	2.20	9 (37%)
4	MLI	I	503	3	0,6,6	0.00	-	0,7,7	0.00	-
4	MLI	B	504	3	0,6,6	0.00	-	0,7,7	0.00	-
4	MLI	G	503	3	0,6,6	0.00	-	0,7,7	0.00	-
2	G6P	I	501	-	16,16,16	0.84	1 (6%)	24,24,24	1.76	7 (29%)
2	G6P	J	501	-	16,16,16	0.92	0	24,24,24	1.46	4 (16%)
2	G6P	H	501	-	16,16,16	0.65	0	24,24,24	1.51	5 (20%)
2	G6P	A	501	-	16,16,16	0.83	0	24,24,24	2.59	12 (50%)
2	G6P	E	501	-	16,16,16	1.02	1 (6%)	24,24,24	1.95	8 (33%)
2	G6P	F	501	-	16,16,16	0.52	0	24,24,24	1.67	6 (25%)
5	GOL	D	503	-	5,5,5	0.49	0	5,5,5	0.86	0
2	G6P	D	501	-	16,16,16	1.06	2 (12%)	24,24,24	2.03	6 (25%)
5	GOL	E	503	-	5,5,5	0.31	0	5,5,5	0.66	0
4	MLI	E	504	3	0,6,6	0.00	-	0,7,7	0.00	-
4	MLI	L	503	3	0,6,6	0.00	-	0,7,7	0.00	-
2	G6P	K	501	-	16,16,16	0.89	1 (6%)	24,24,24	1.69	5 (20%)
4	MLI	F	503	3	0,6,6	0.00	-	0,7,7	0.00	-
2	G6P	L	501	-	16,16,16	0.74	0	24,24,24	1.83	10 (41%)
2	G6P	C	501	-	16,16,16	0.73	0	24,24,24	1.75	9 (37%)
4	MLI	C	503	3	0,6,6	0.00	-	0,7,7	0.00	-
4	MLI	D	504	3	0,6,6	0.00	-	0,7,7	0.00	-
2	G6P	G	501	-	16,16,16	0.78	0	24,24,24	1.58	5 (20%)
5	GOL	B	503	-	5,5,5	0.45	0	5,5,5	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MLI	K	503	3	0,6,6	0.00	-	0,7,7	0.00	-
4	MLI	A	503	3	0,6,6	0.00	-	0,7,7	0.00	-
4	MLI	H	503	3	0,6,6	0.00	-	0,7,7	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MLI	J	503	3	-	0/0/4/4	-
2	G6P	B	501	-	-	4/6/26/26	0/1/1/1
4	MLI	I	503	3	-	0/0/4/4	-
4	MLI	B	504	3	-	0/0/4/4	-
4	MLI	G	503	3	-	0/0/4/4	-
2	G6P	I	501	-	-	5/6/26/26	0/1/1/1
2	G6P	J	501	-	-	5/6/26/26	0/1/1/1
2	G6P	H	501	-	-	2/6/26/26	0/1/1/1
2	G6P	A	501	-	-	5/6/26/26	0/1/1/1
2	G6P	E	501	-	-	1/6/26/26	0/1/1/1
2	G6P	F	501	-	-	5/6/26/26	0/1/1/1
5	GOL	D	503	-	-	3/4/4/4	-
2	G6P	D	501	-	-	3/6/26/26	0/1/1/1
5	GOL	E	503	-	-	2/4/4/4	-
4	MLI	E	504	3	-	0/0/4/4	-
4	MLI	L	503	3	-	0/0/4/4	-
2	G6P	K	501	-	-	1/6/26/26	0/1/1/1
4	MLI	F	503	3	-	0/0/4/4	-
2	G6P	L	501	-	-	2/6/26/26	0/1/1/1
2	G6P	C	501	-	-	3/6/26/26	0/1/1/1
4	MLI	C	503	3	-	0/0/4/4	-
4	MLI	D	504	3	-	0/0/4/4	-
2	G6P	G	501	-	-	2/6/26/26	0/1/1/1
5	GOL	B	503	-	-	2/4/4/4	-
4	MLI	K	503	3	-	0/0/4/4	-
4	MLI	A	503	3	-	0/0/4/4	-
4	MLI	H	503	3	-	0/0/4/4	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	G6P	O1-C1	2.59	1.47	1.39
2	D	501	G6P	O1-C1	2.38	1.47	1.39
2	B	501	G6P	C1-C2	-2.32	1.46	1.52
2	D	501	G6P	O4-C4	2.13	1.48	1.43
2	I	501	G6P	O1-C1	2.07	1.46	1.39

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	G6P	O2P-P-O6	-6.97	88.18	106.73
2	D	501	G6P	O5-C1-C2	-6.14	99.33	110.28
2	B	501	G6P	O5-C1-C2	-5.67	100.17	110.28
2	E	501	G6P	C1-O5-C5	5.06	123.21	113.66
2	F	501	G6P	C4-C3-C2	-5.00	102.09	110.82

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	G6P	C6-O6-P-O1P
2	B	501	G6P	C6-O6-P-O2P
2	B	501	G6P	C6-O6-P-O3P
2	J	501	G6P	C4-C5-C6-O6
2	J	501	G6P	O5-C5-C6-O6

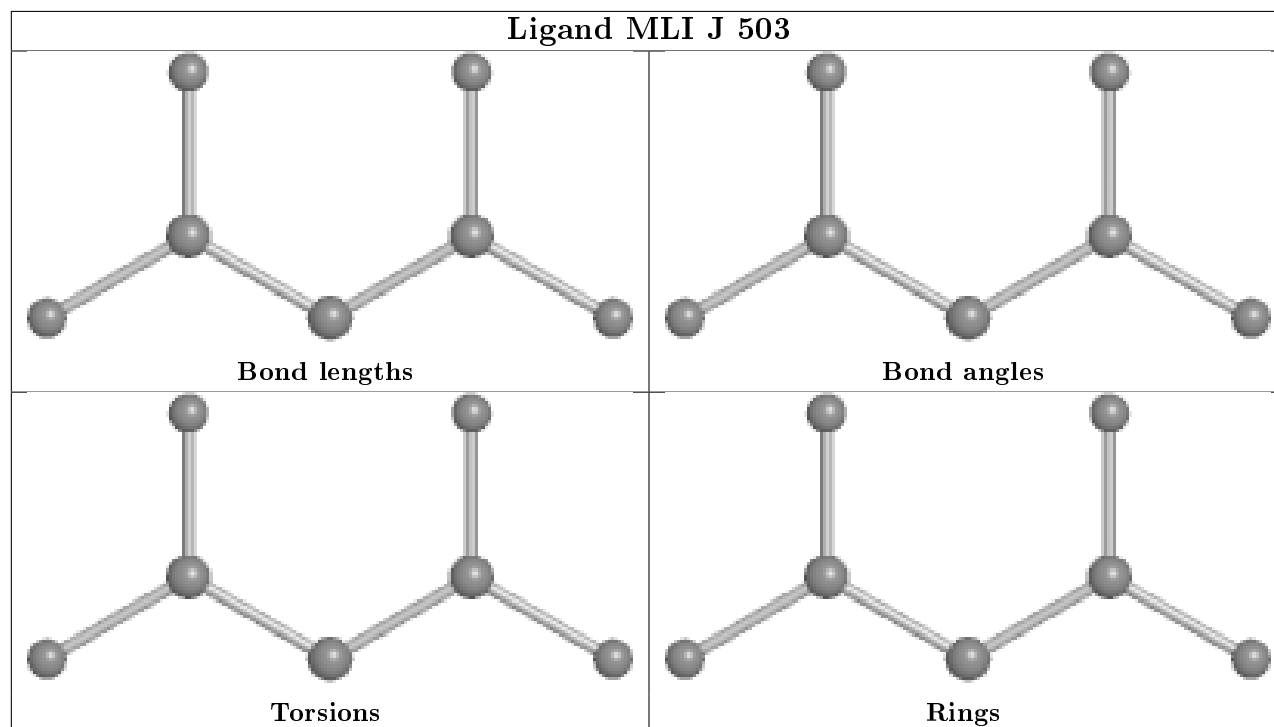
There are no ring outliers.

4 monomers are involved in 5 short contacts:

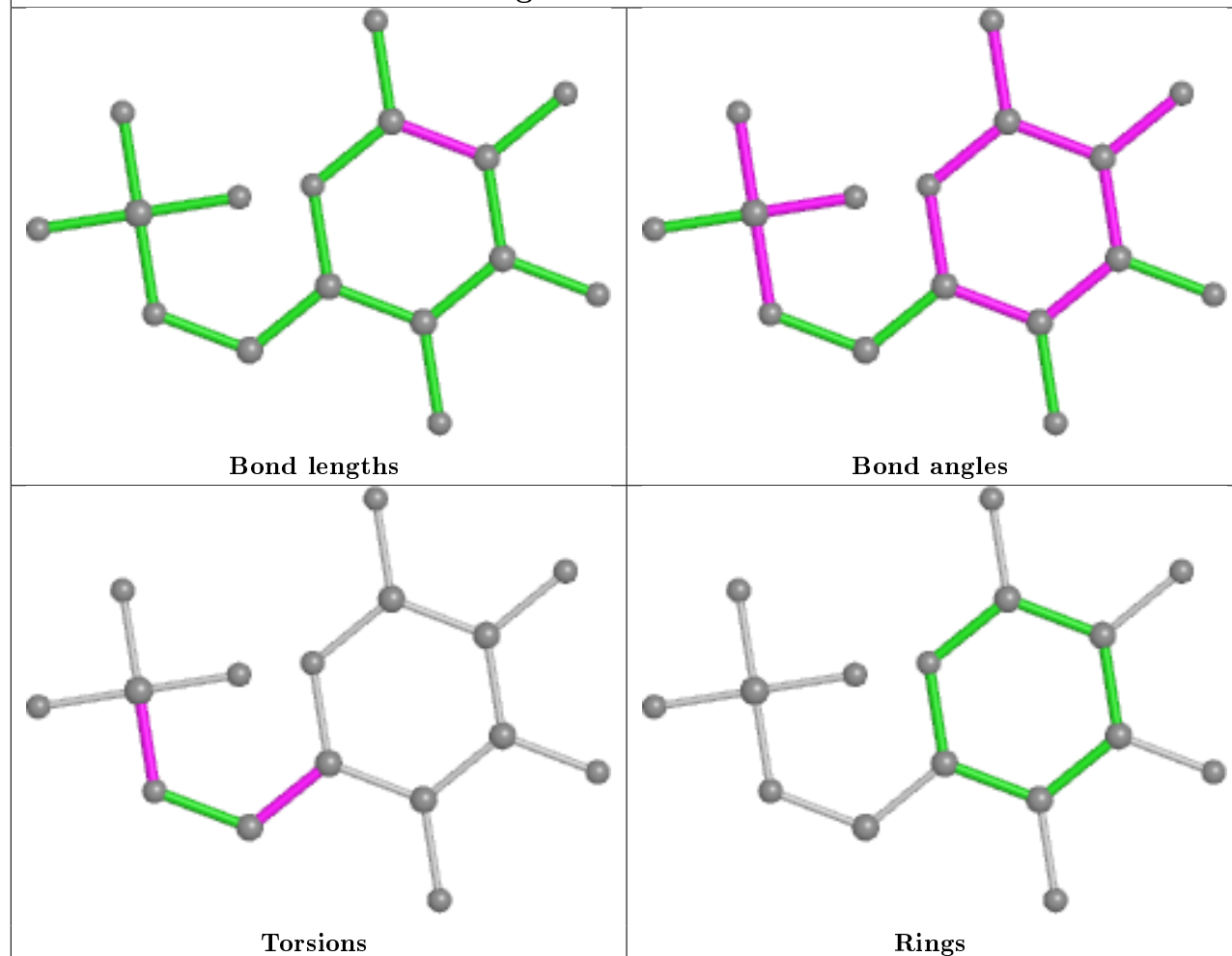
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	G6P	1	0
2	F	501	G6P	2	0
4	E	504	MLI	1	0
4	K	503	MLI	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

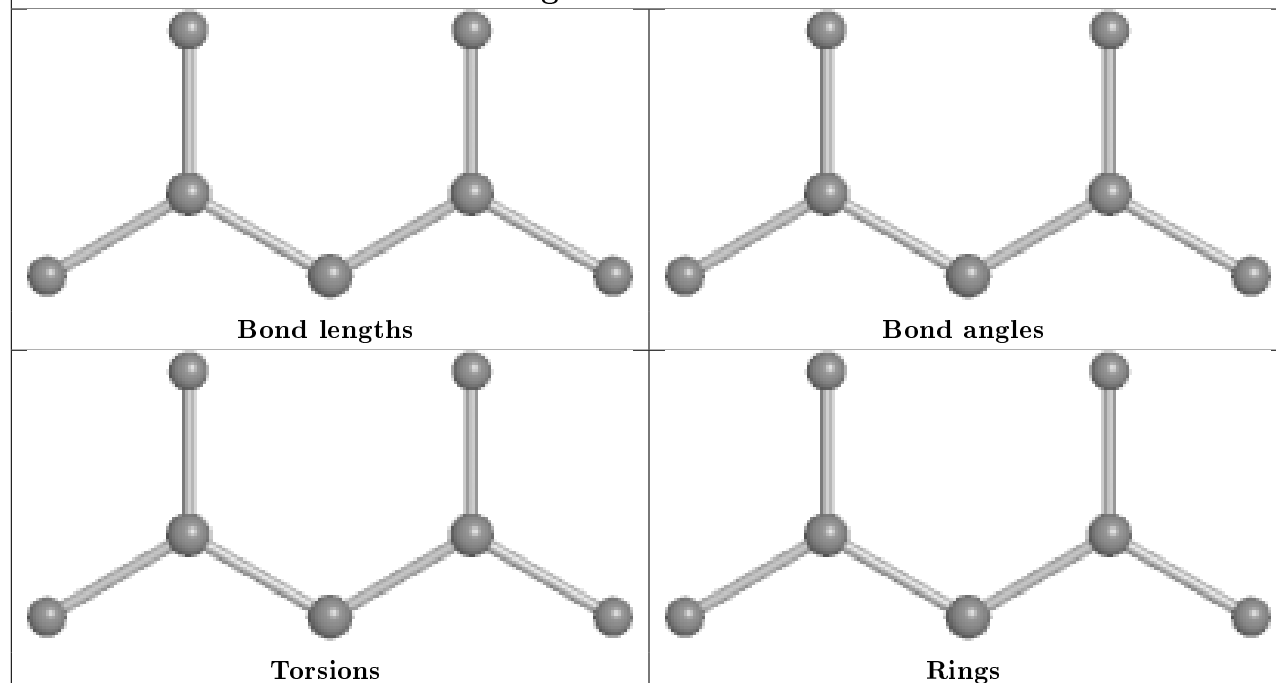
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

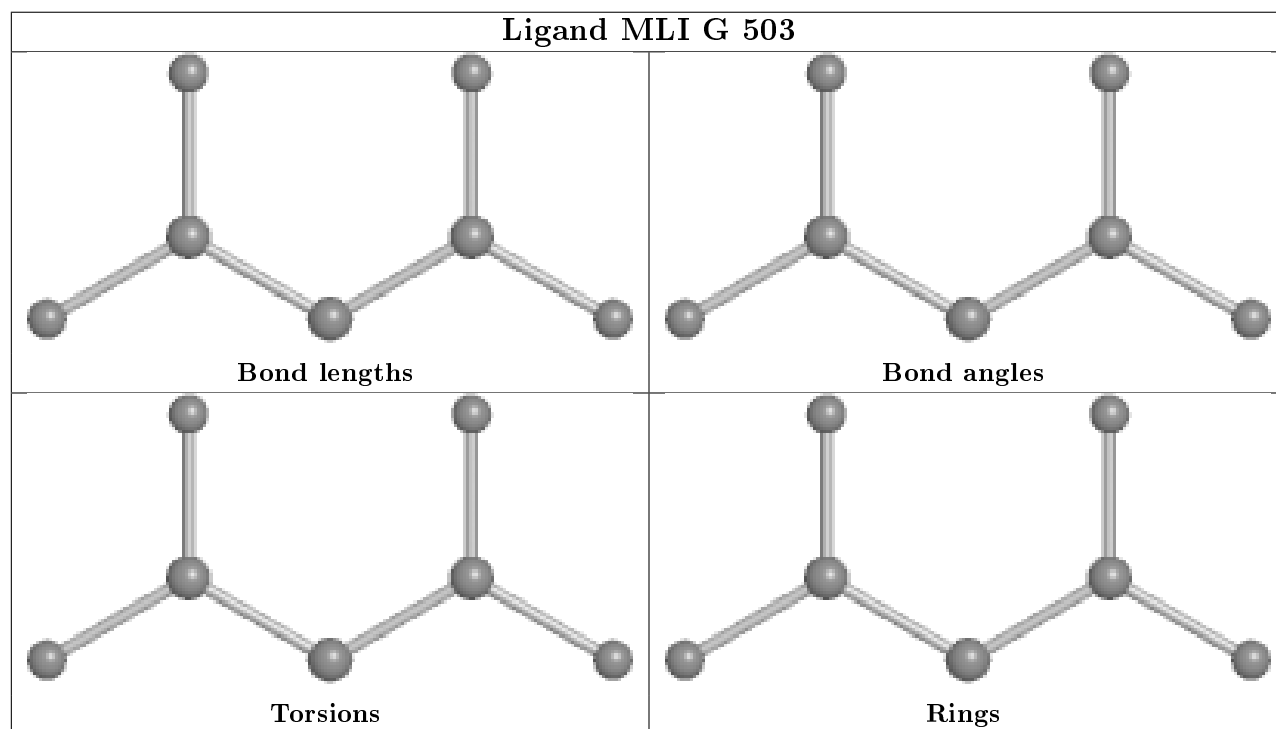
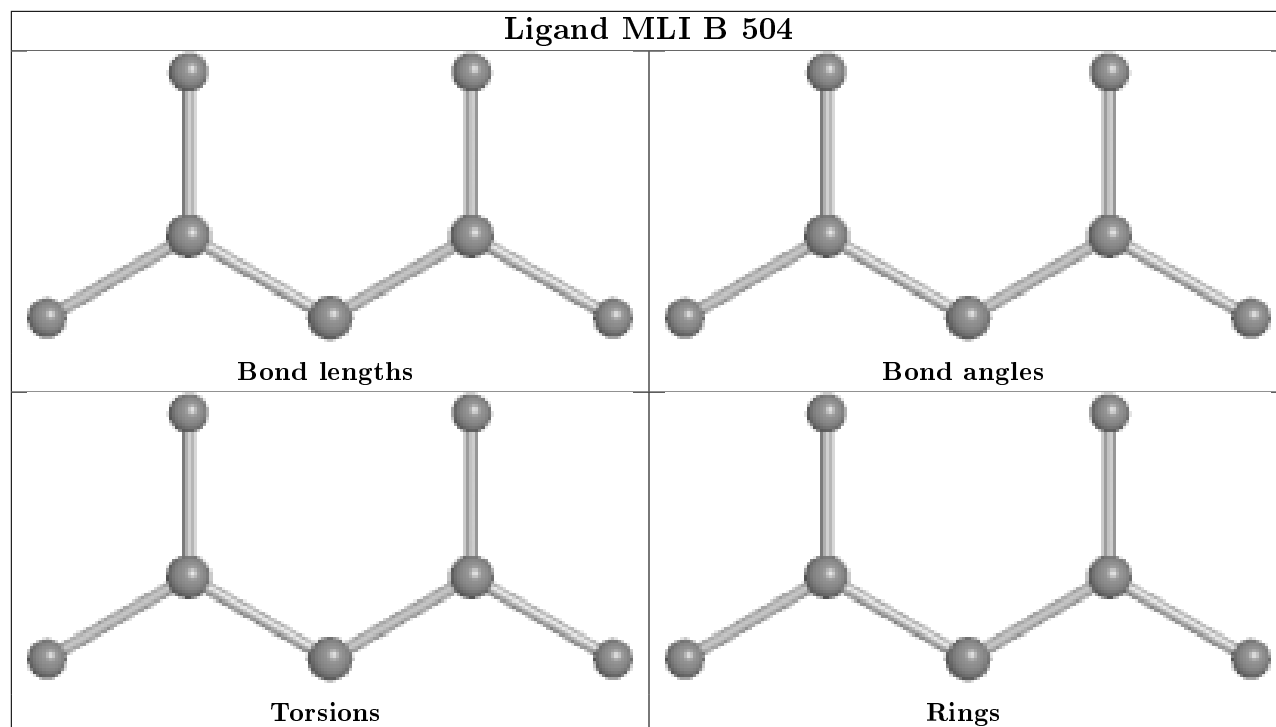


Ligand G6P B 501

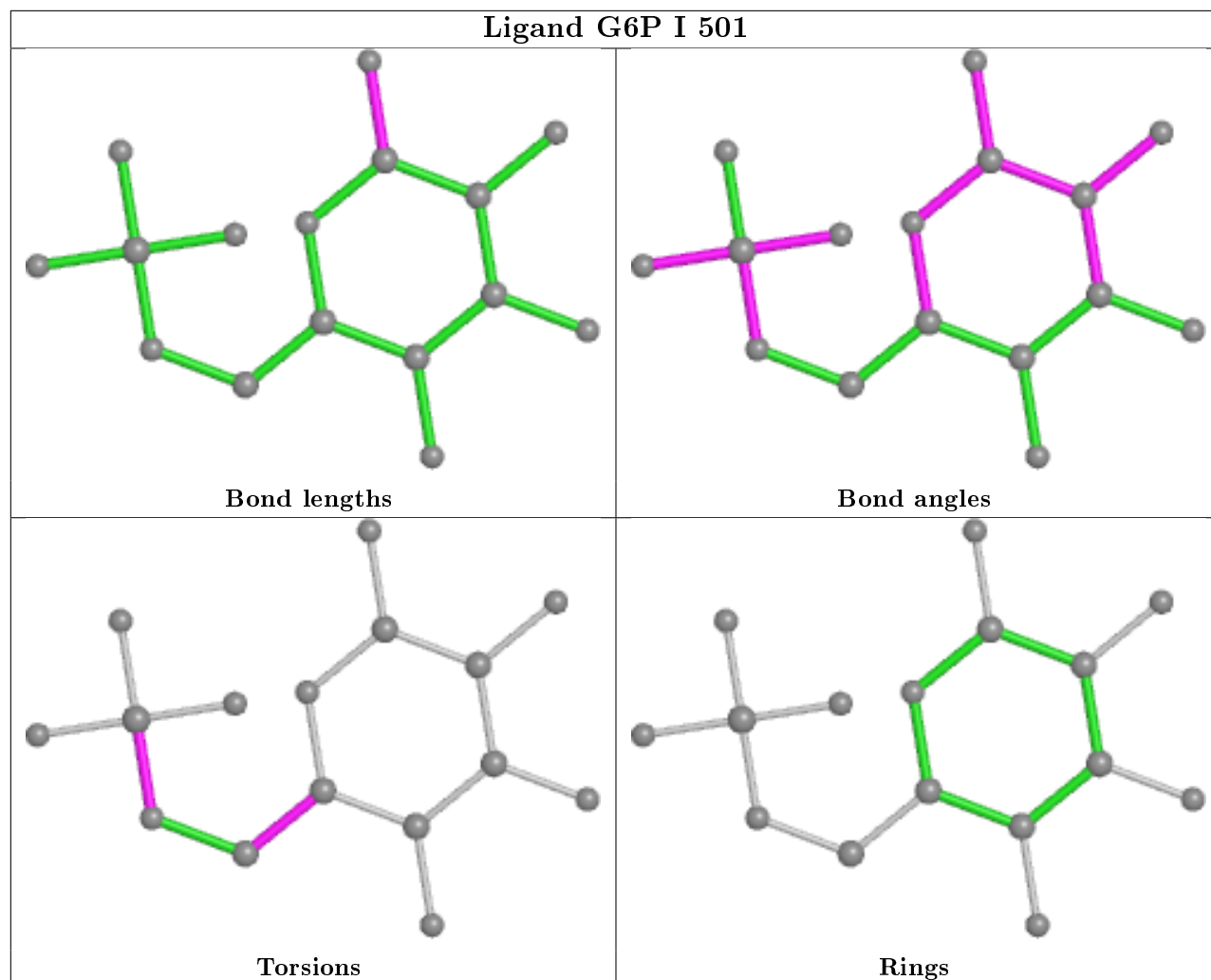


Ligand MLI I 503

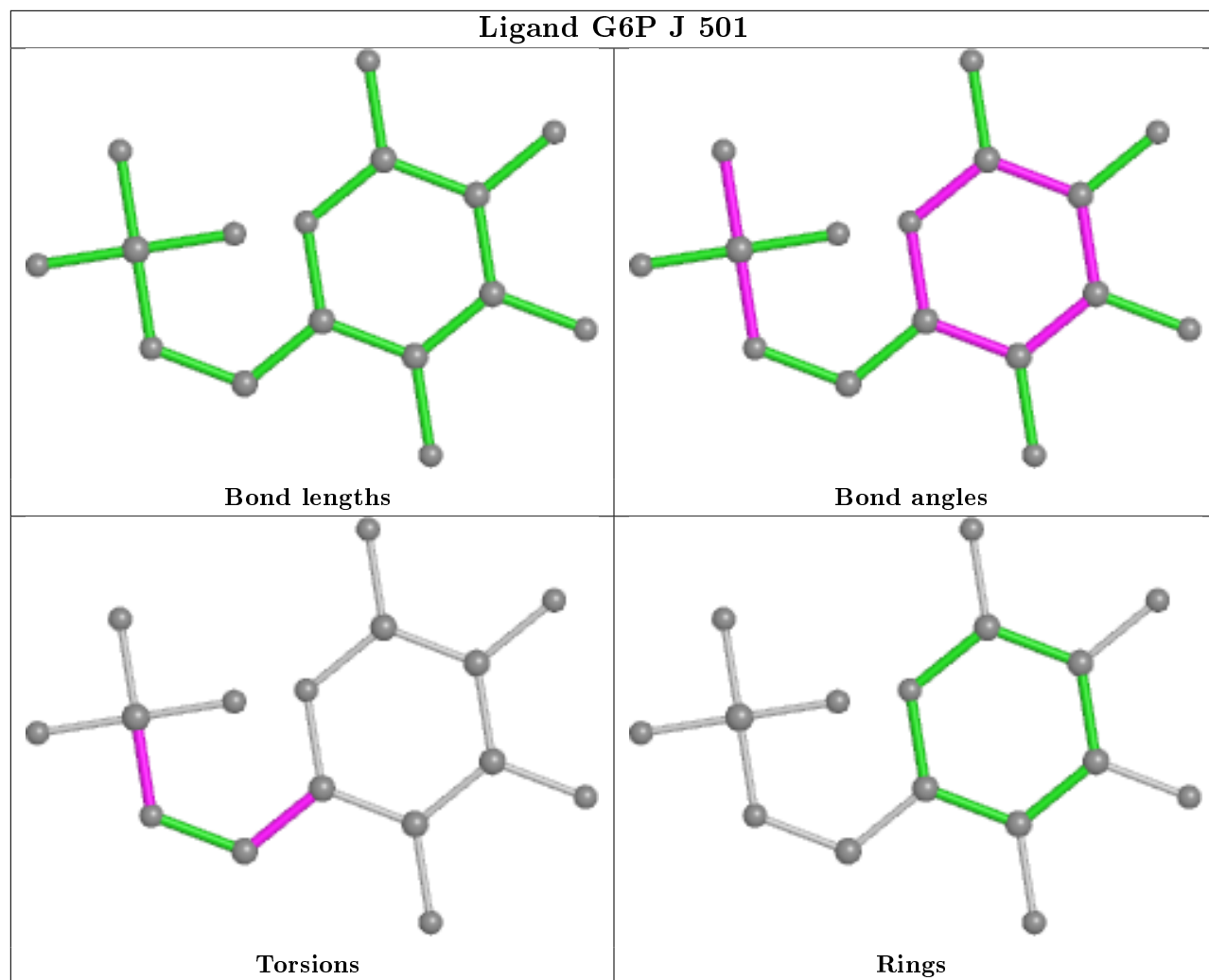




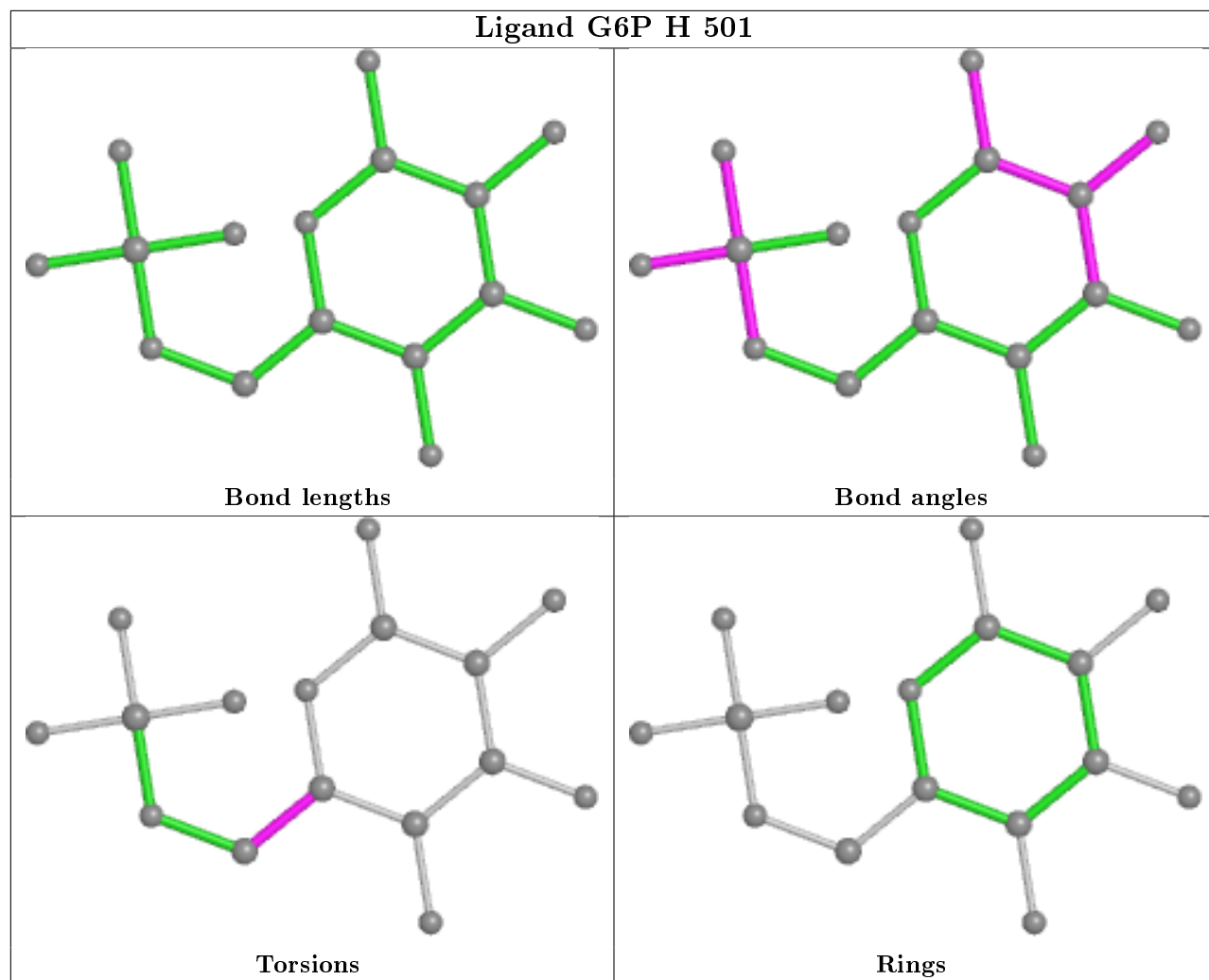
Ligand G6P I 501



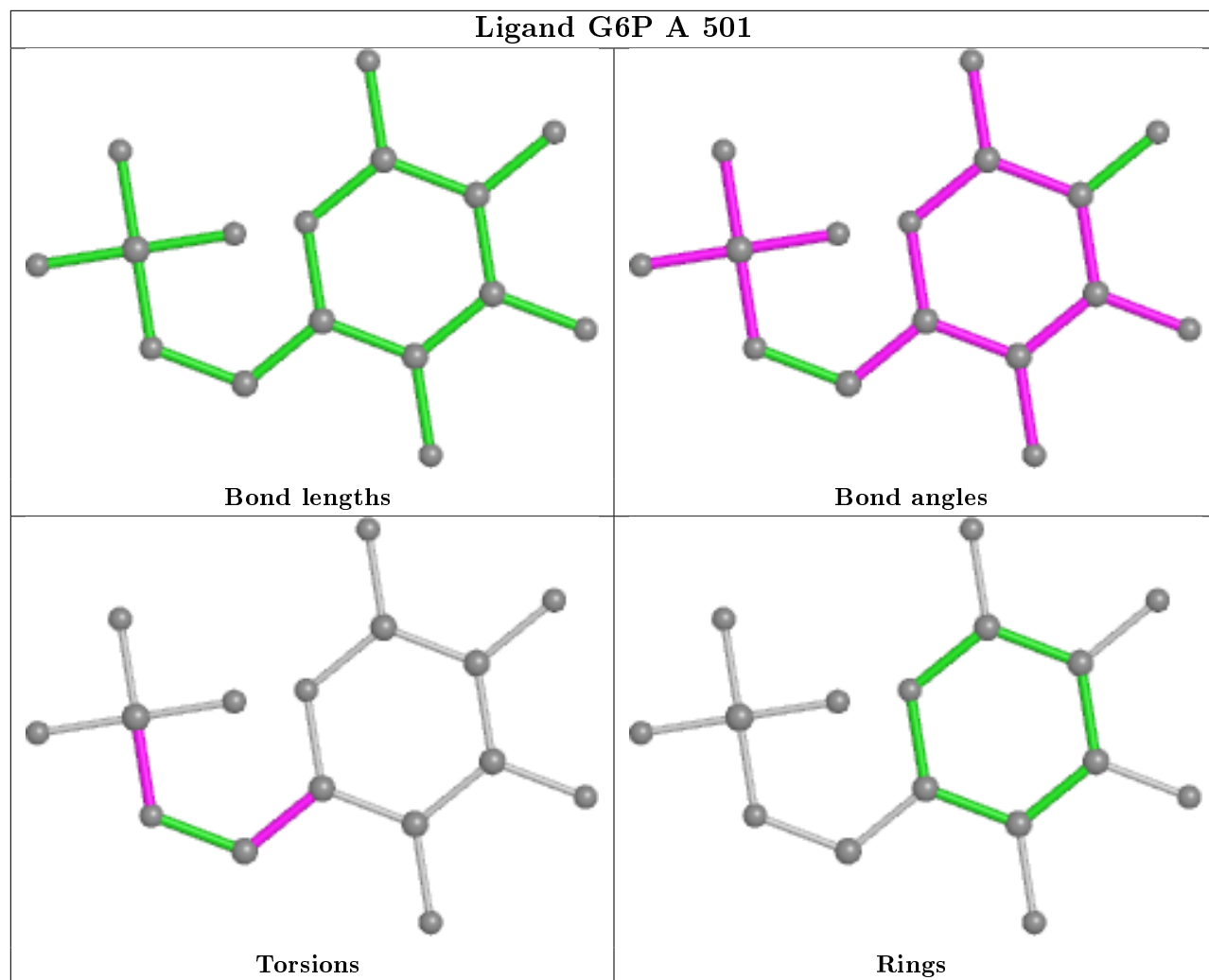
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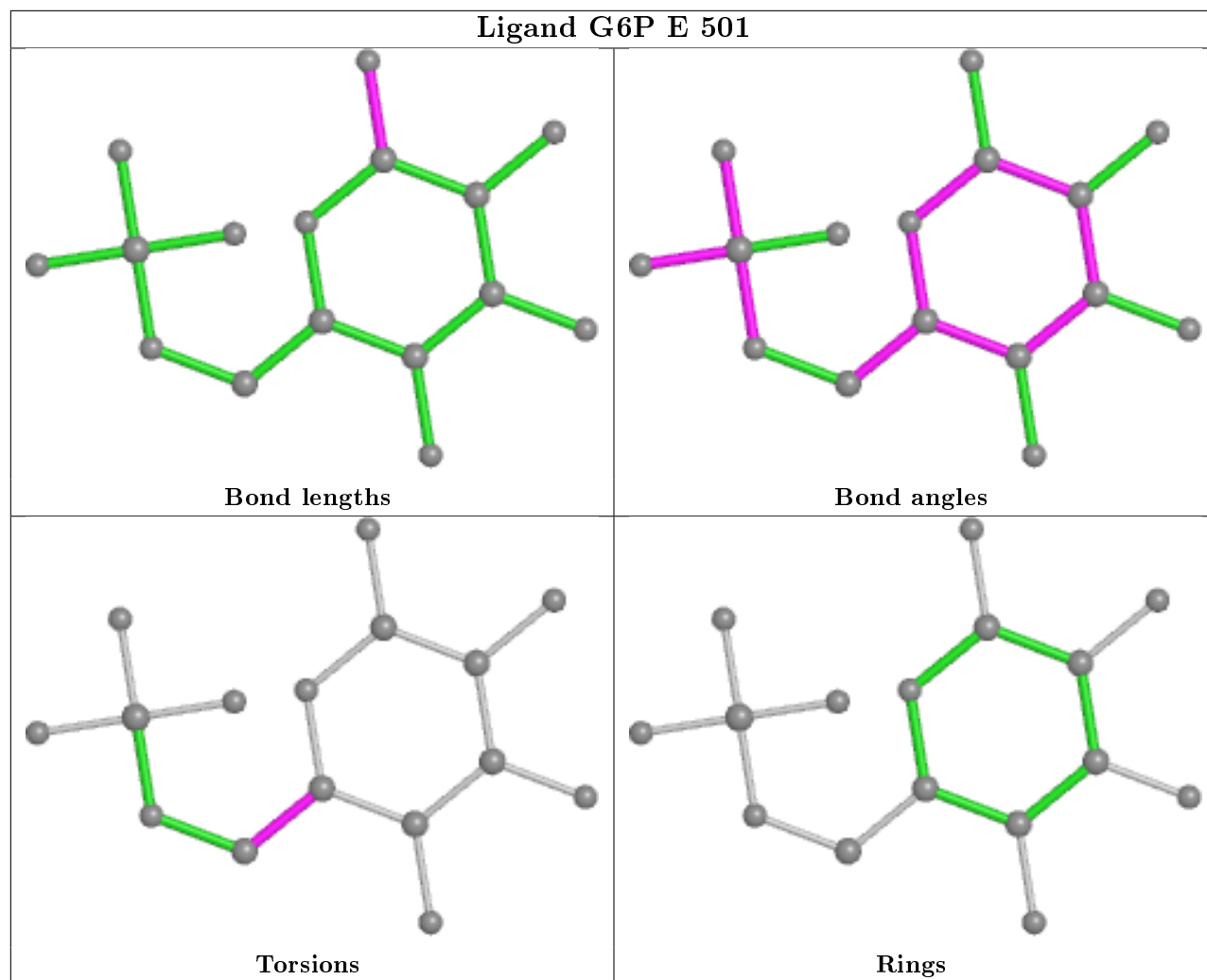
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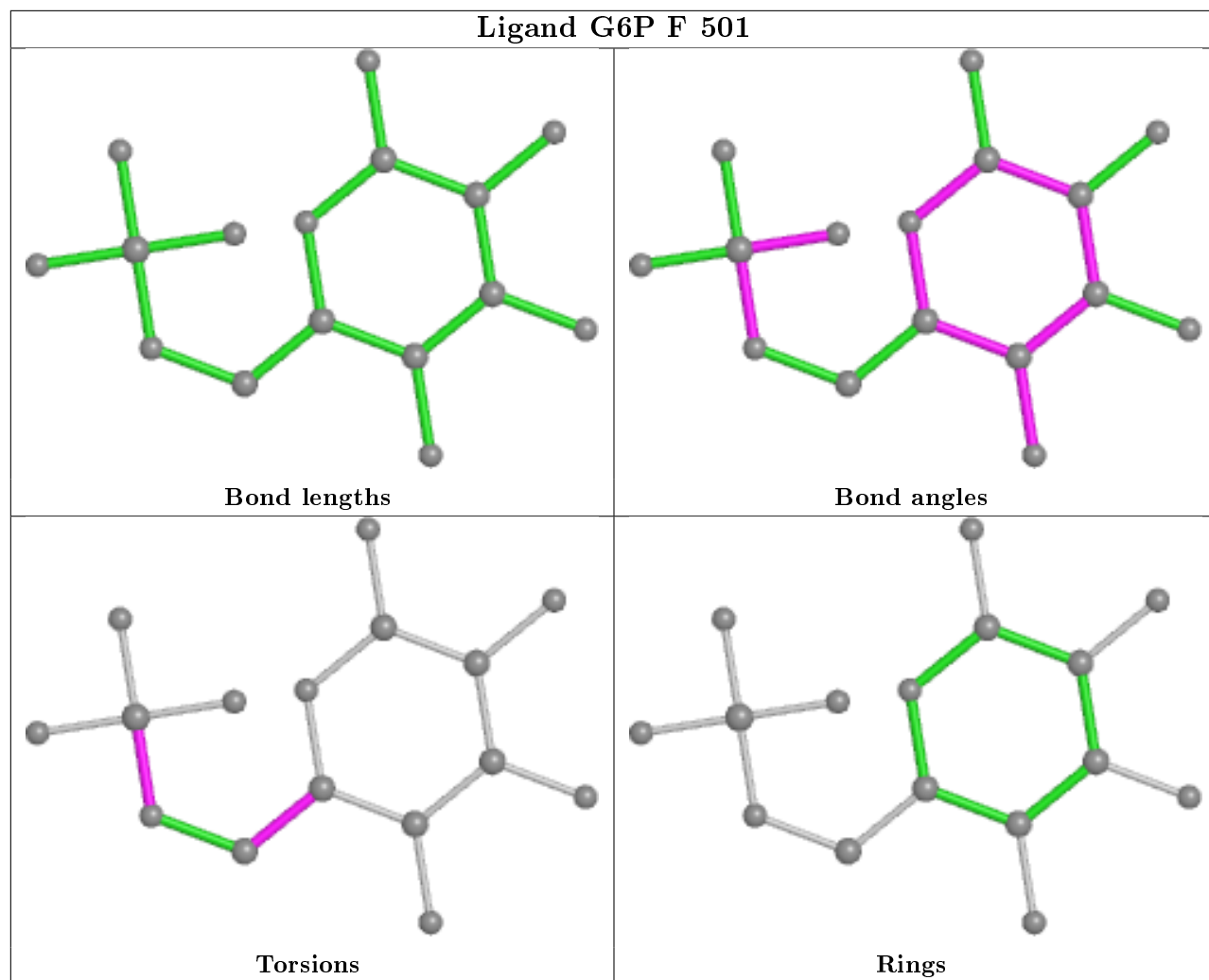
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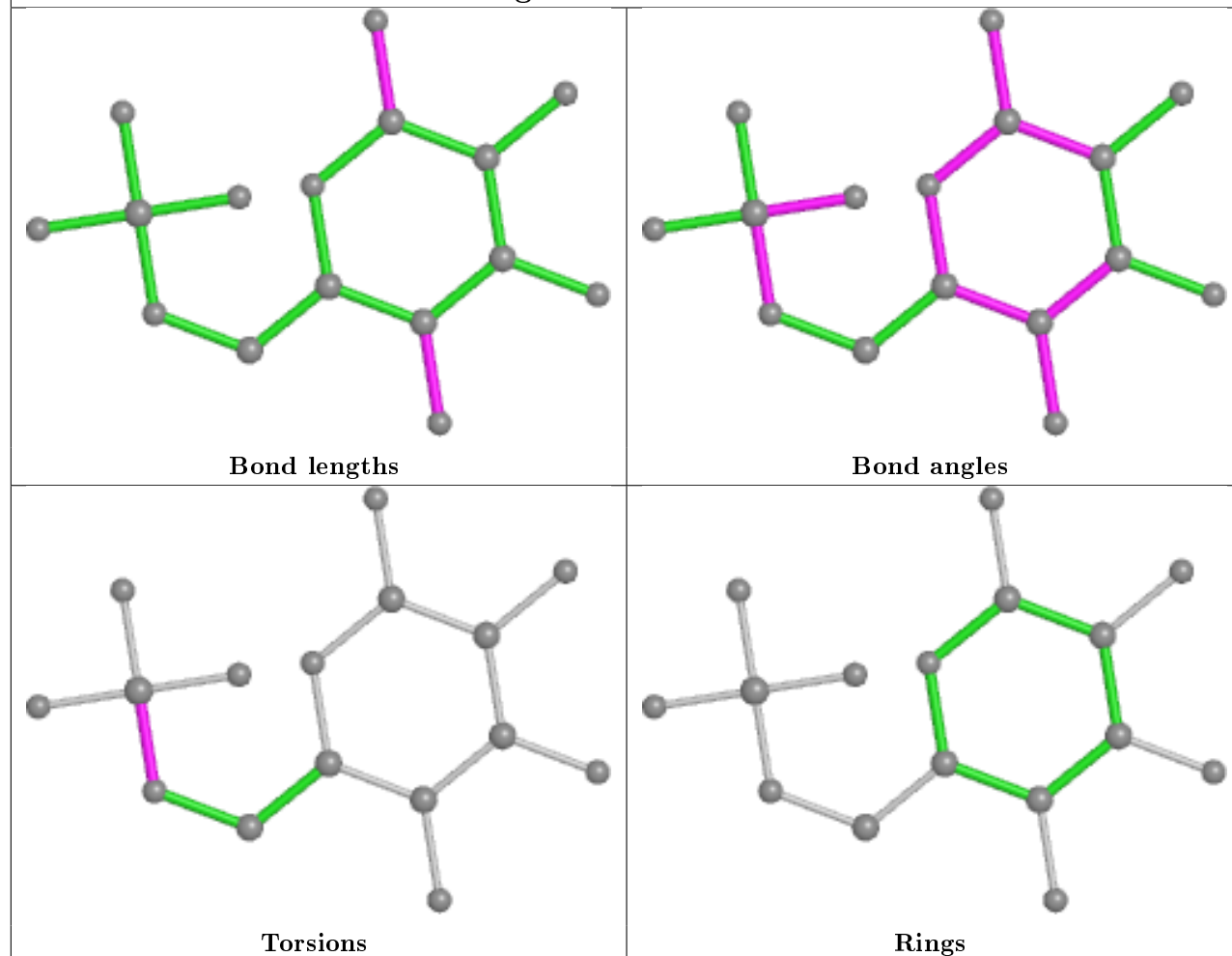
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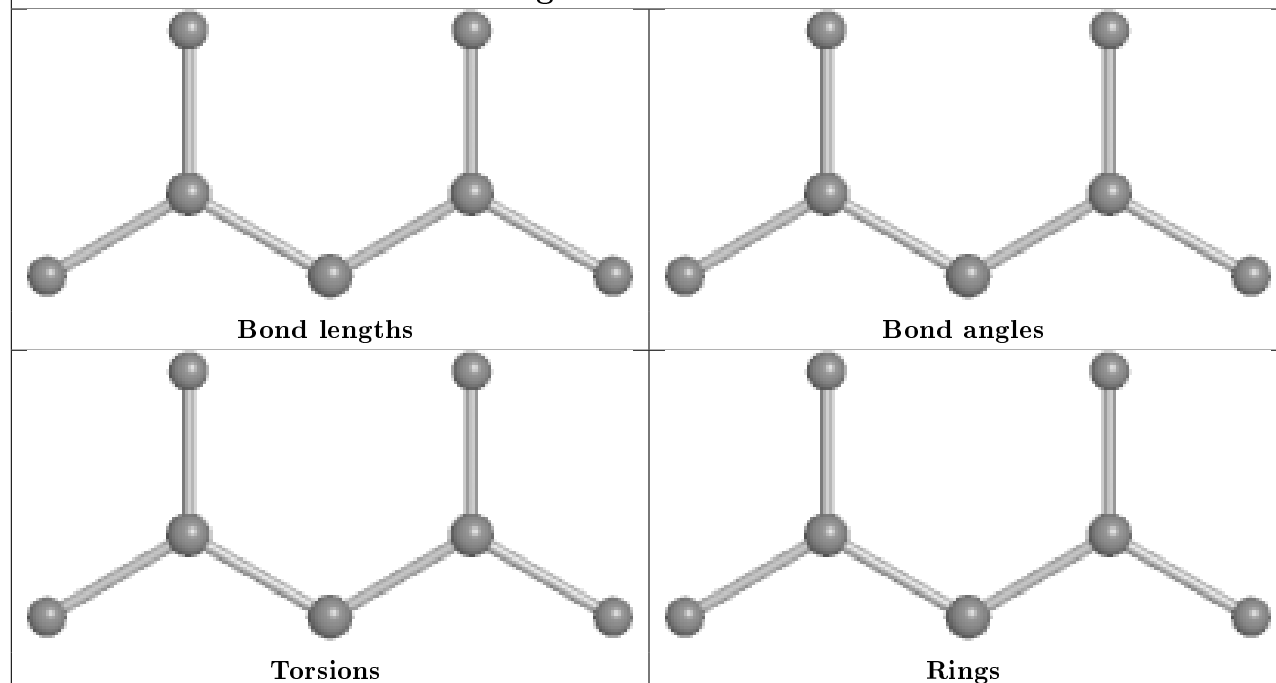
Ligand G6P F 501



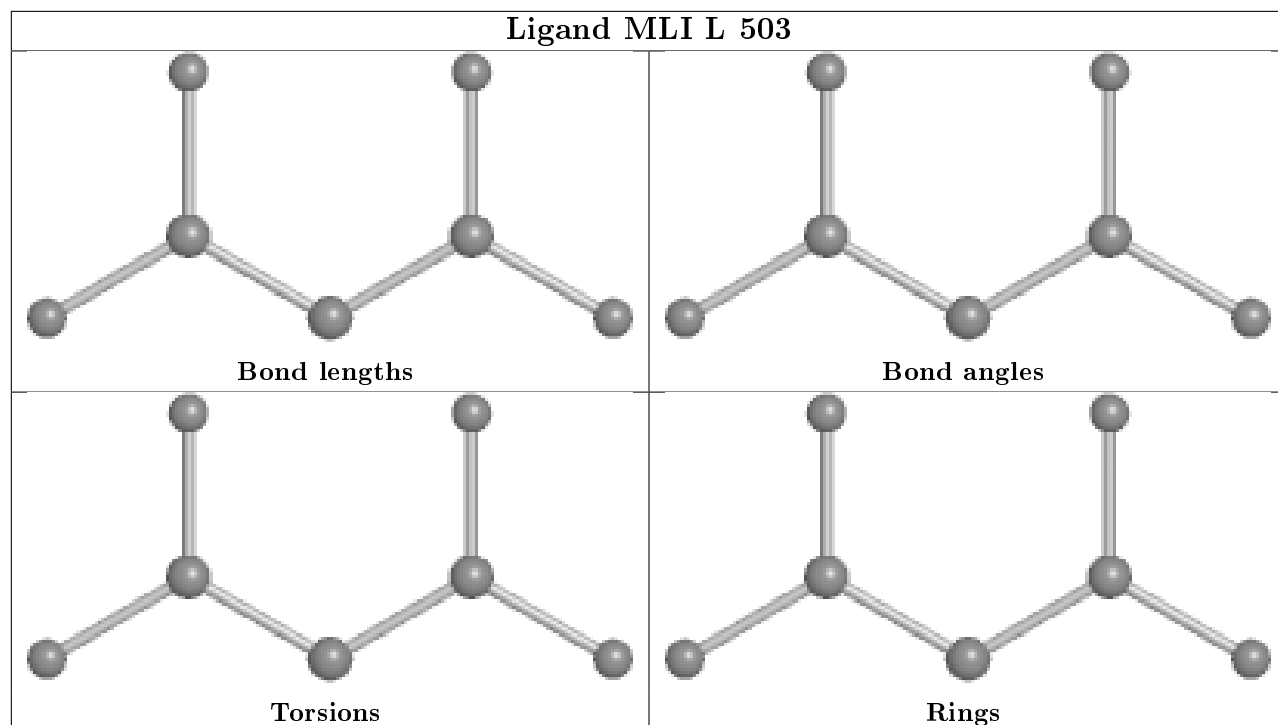
Ligand G6P D 501



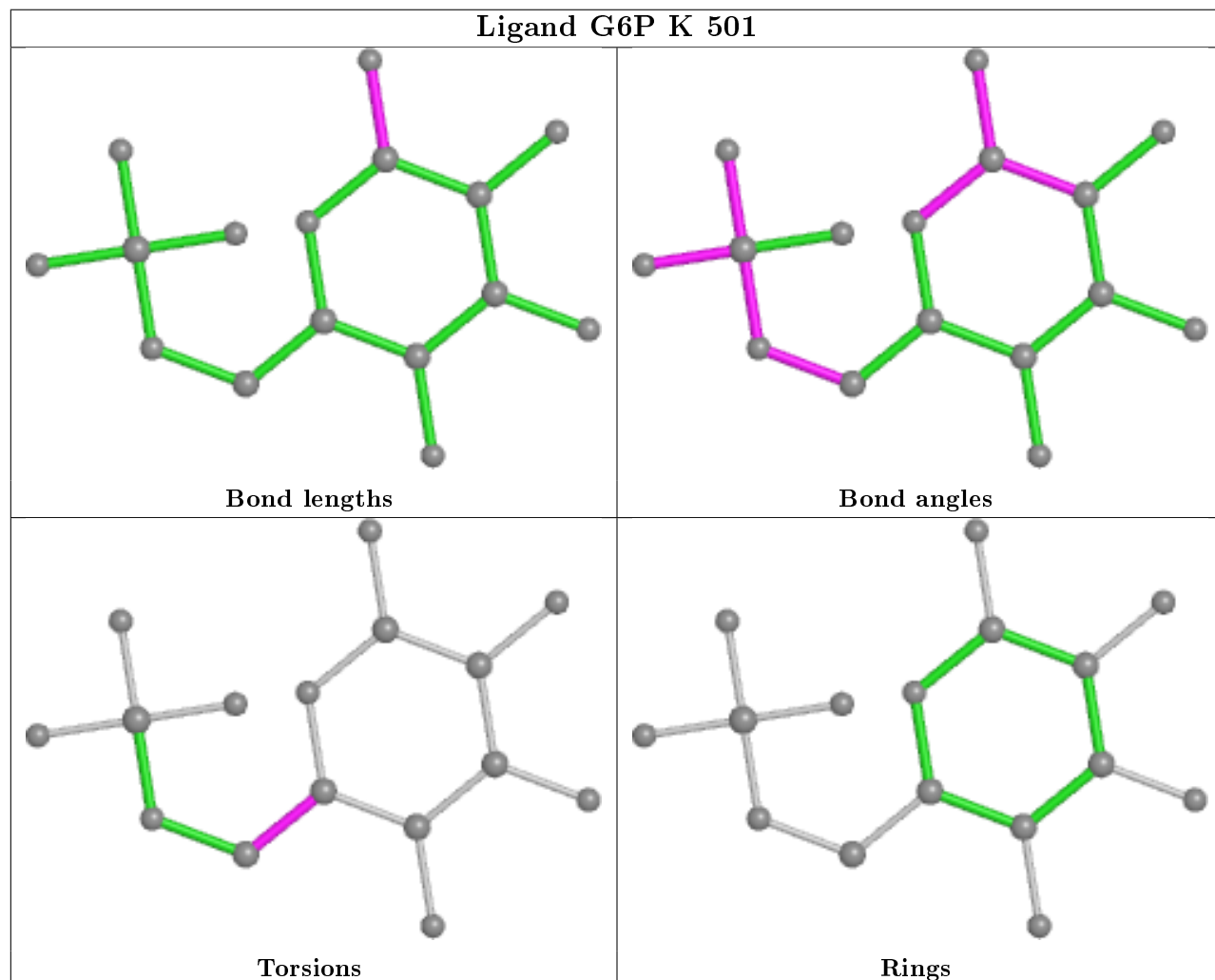
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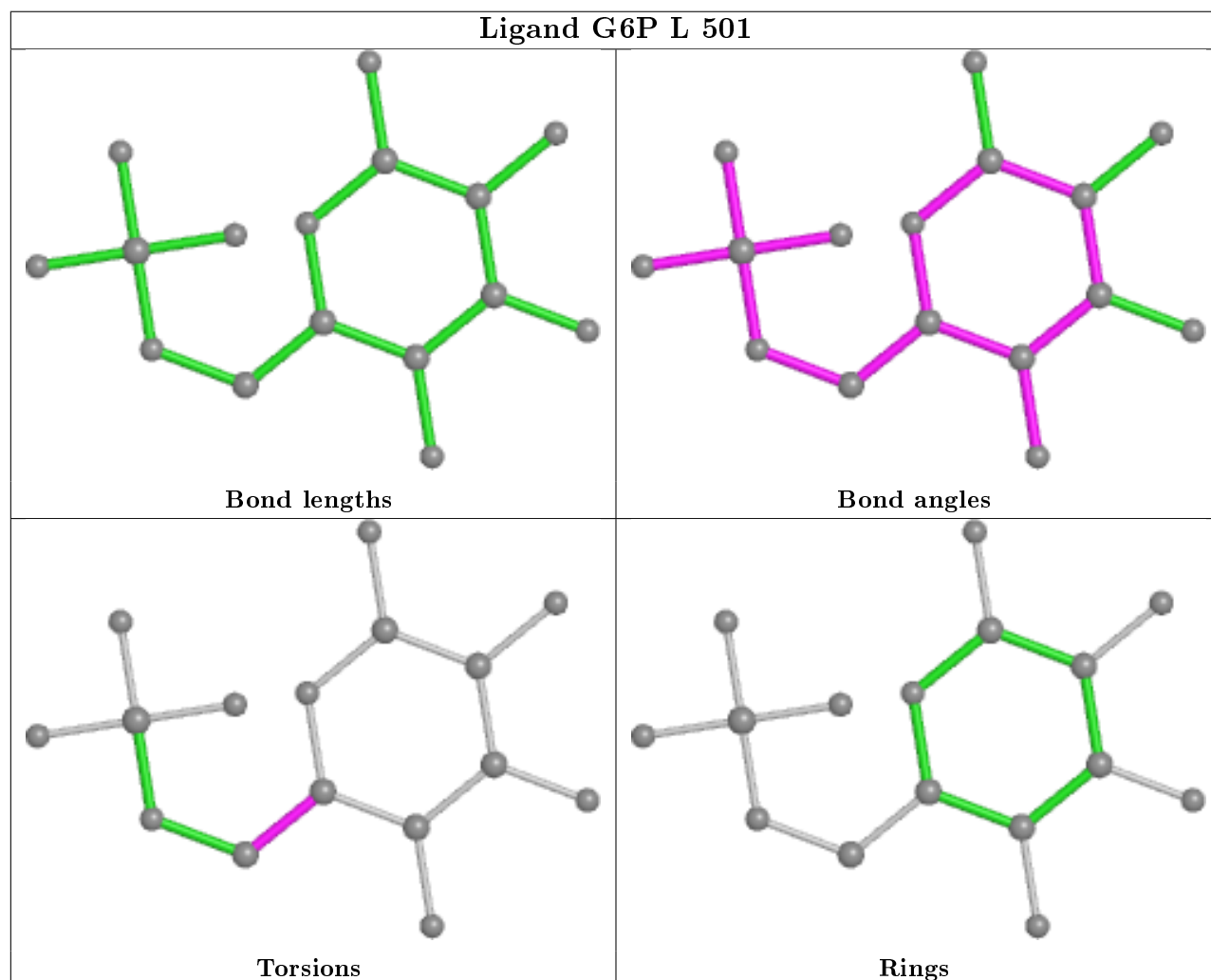
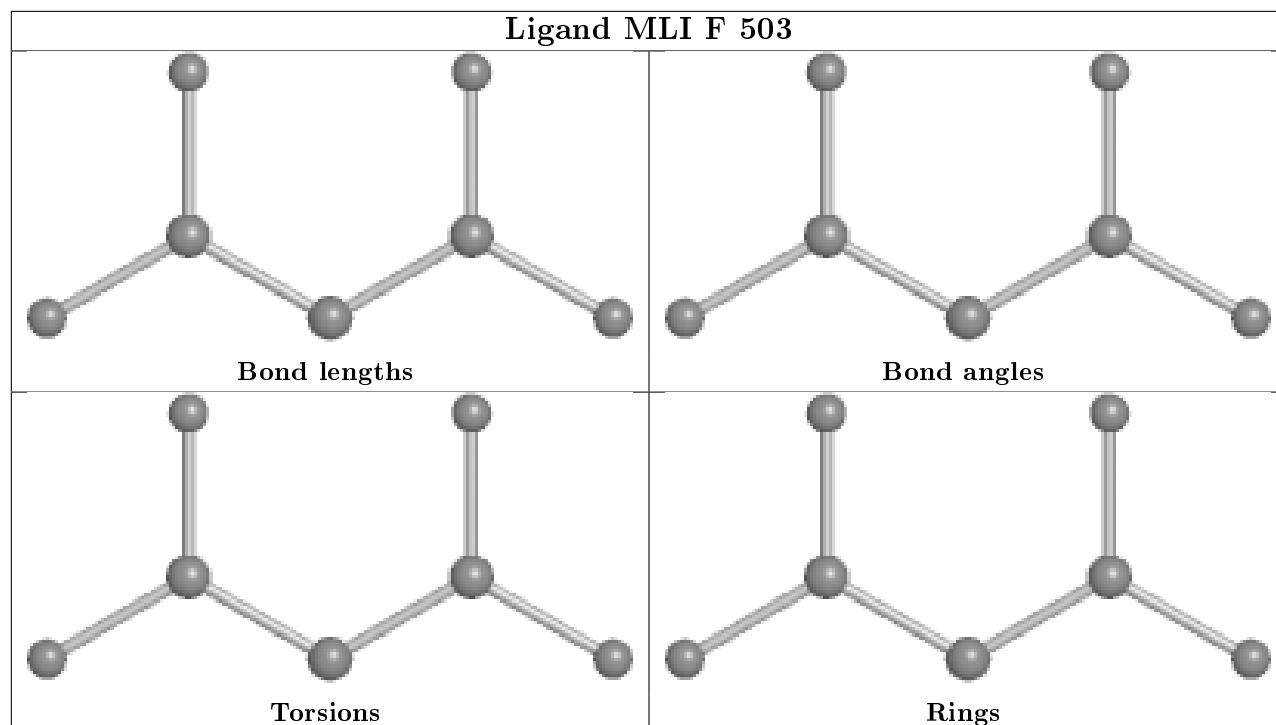


Ligand MLI L 503

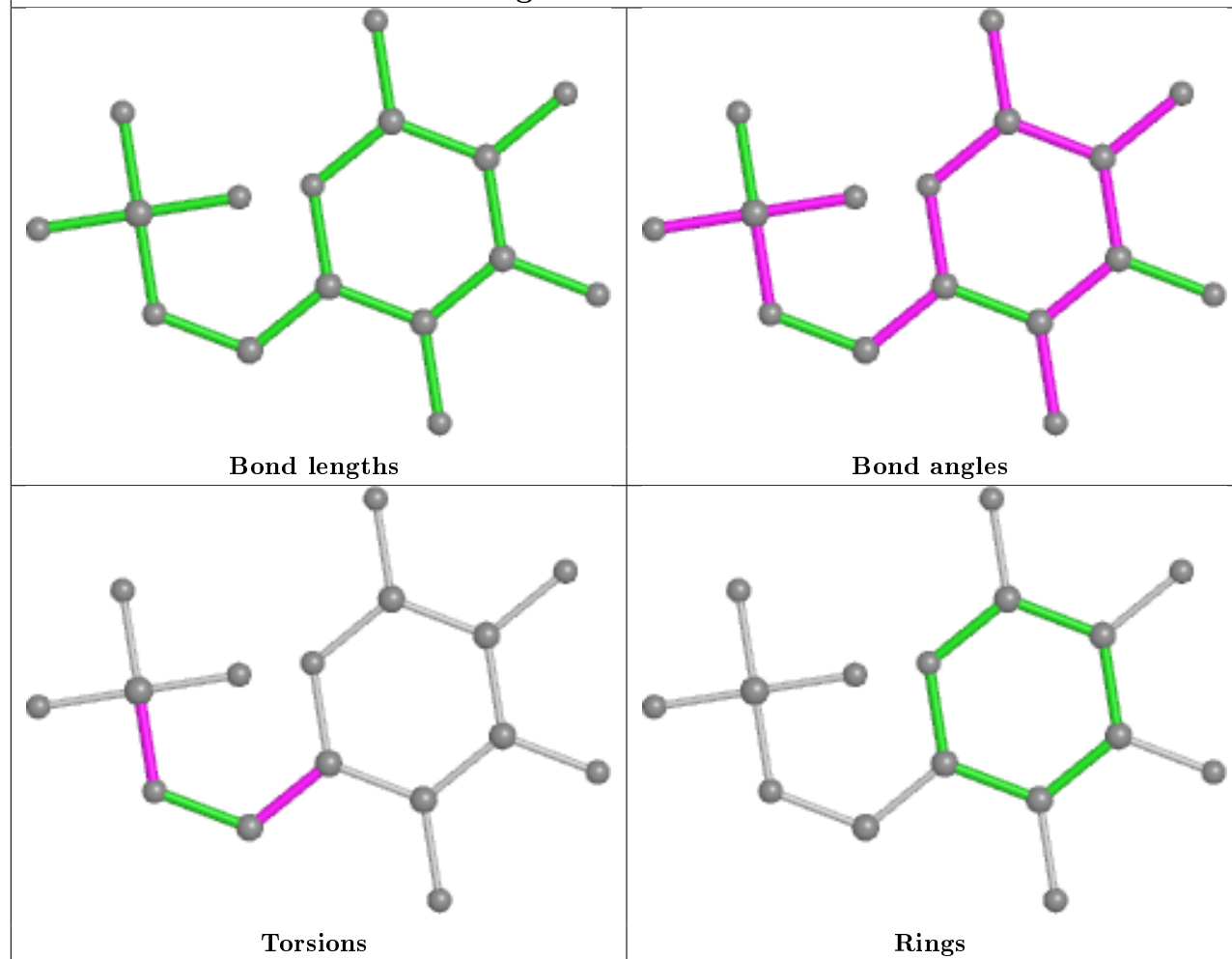


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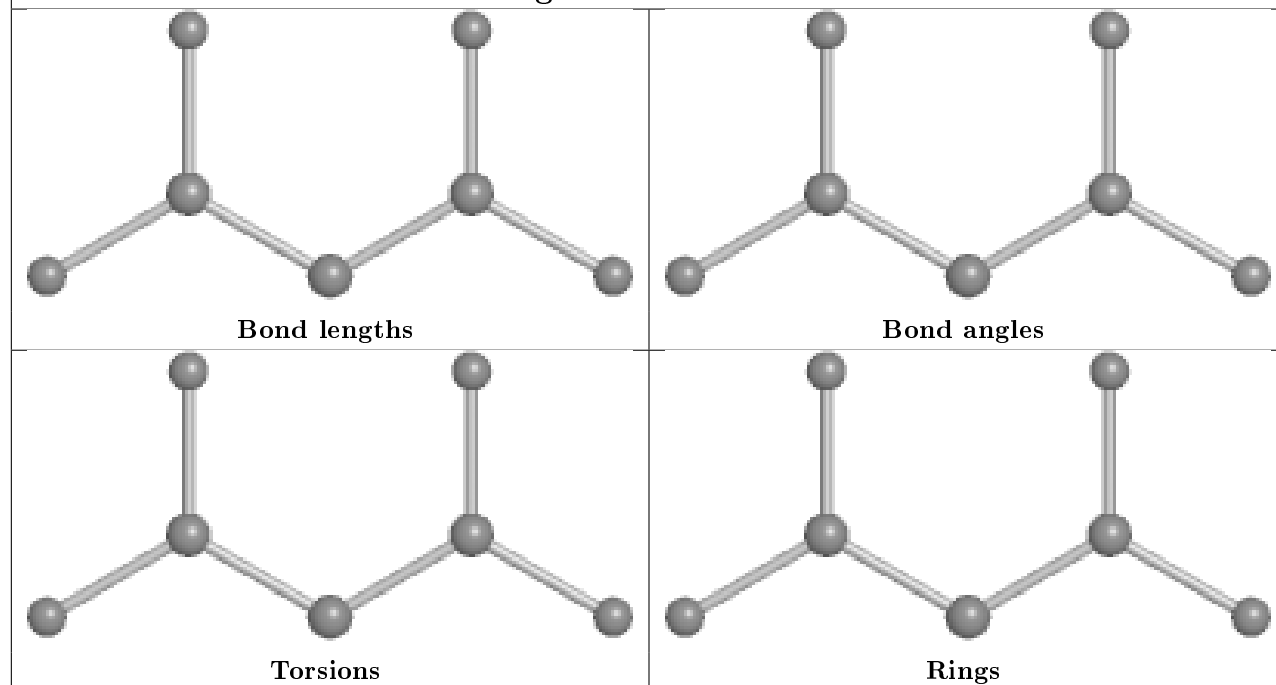


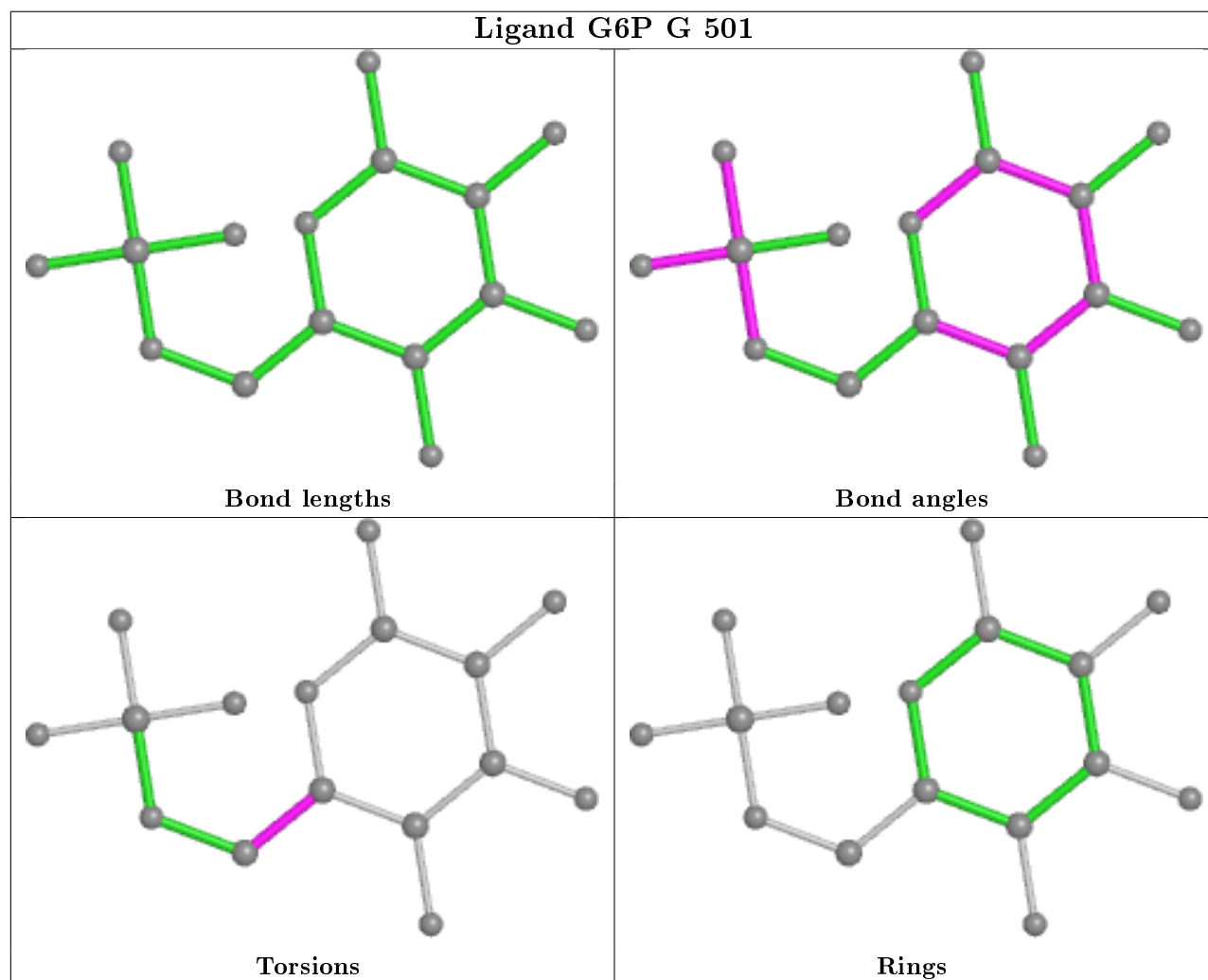
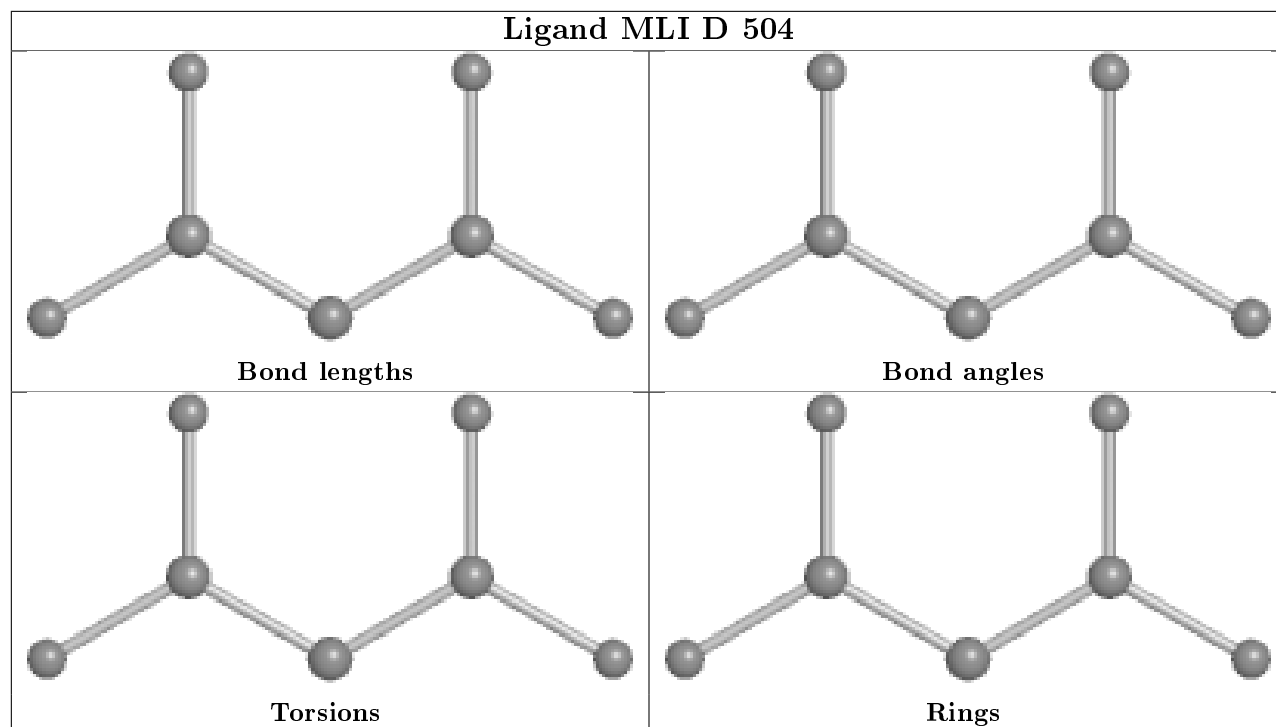


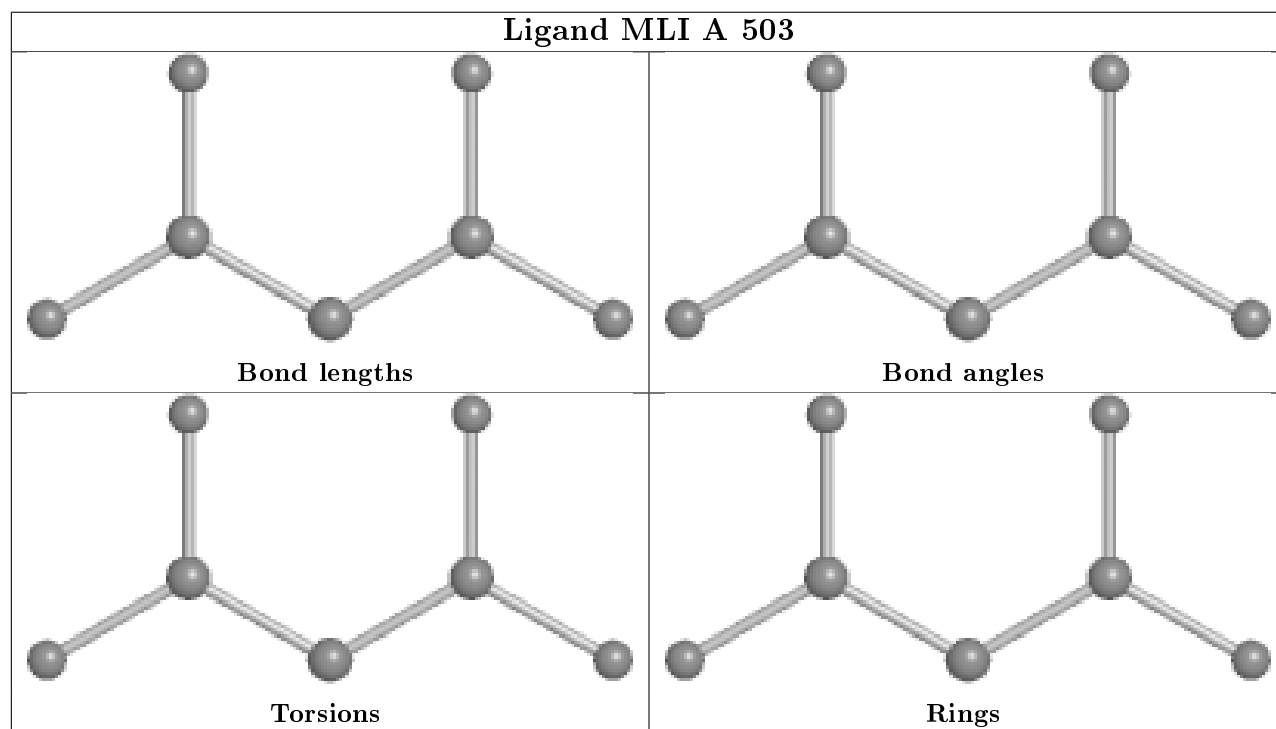
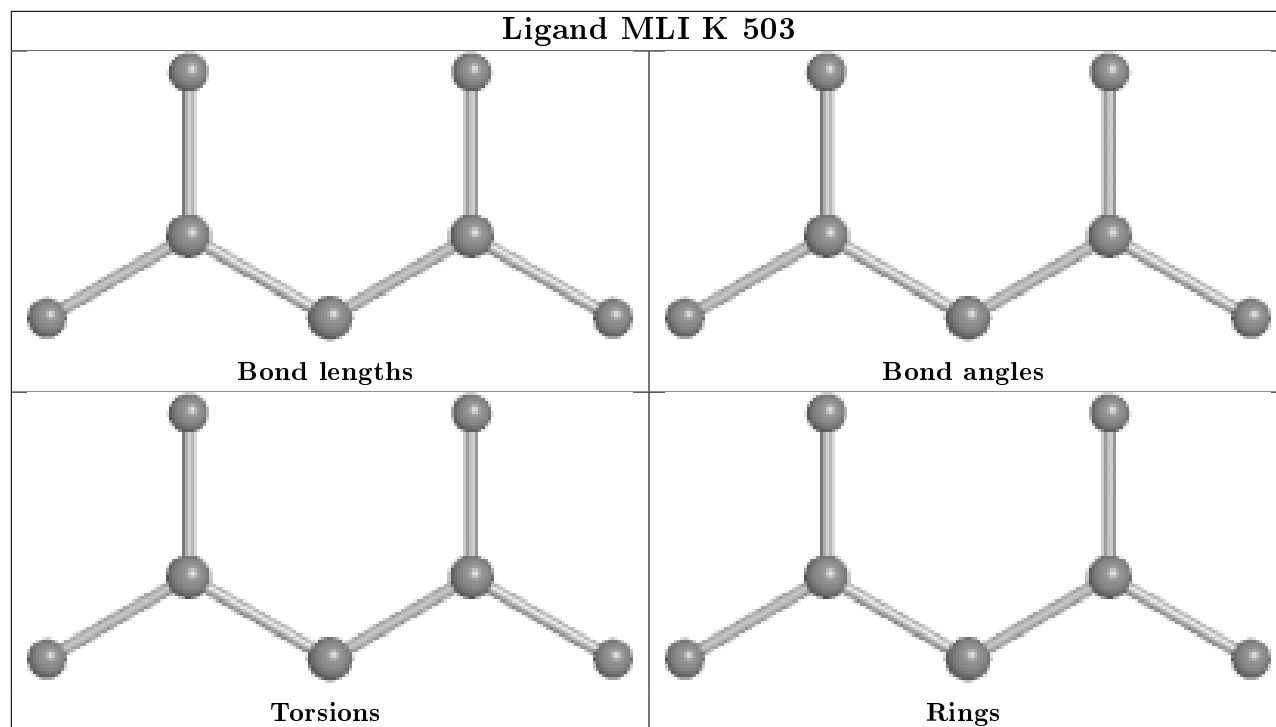
Ligand G6P C 501

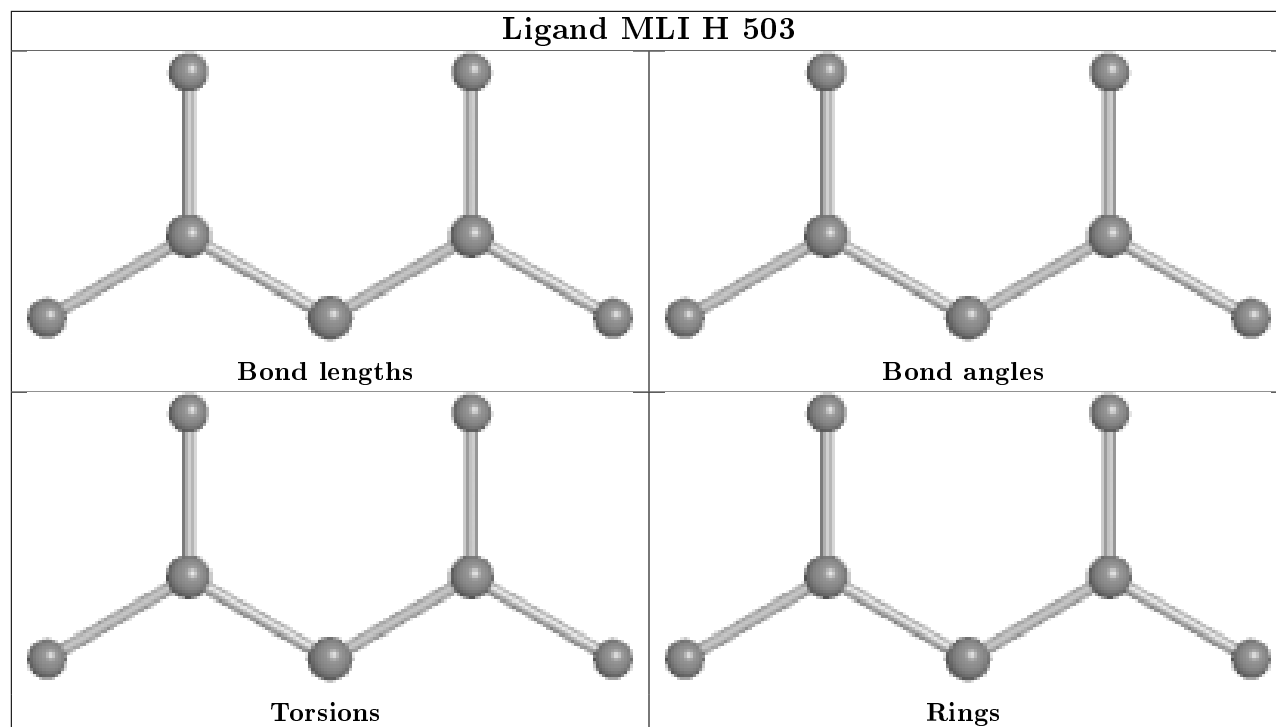


Ligand MLI C 503









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	483/483 (100%)	-0.16	2 (0%) 92 92	27, 47, 74, 105	0
1	B	483/483 (100%)	-0.20	0 100 100	22, 37, 67, 98	0
1	C	483/483 (100%)	-0.22	2 (0%) 92 92	27, 44, 72, 110	0
1	D	483/483 (100%)	-0.21	0 100 100	25, 42, 71, 102	0
1	E	483/483 (100%)	-0.20	1 (0%) 95 95	24, 39, 73, 92	0
1	F	483/483 (100%)	-0.06	3 (0%) 89 89	26, 53, 85, 111	0
1	G	483/483 (100%)	-0.10	6 (1%) 79 77	30, 56, 90, 116	0
1	H	483/483 (100%)	-0.01	9 (1%) 66 63	23, 54, 102, 138	0
1	I	483/483 (100%)	-0.04	7 (1%) 75 73	30, 62, 91, 114	0
1	J	404/483 (83%)	-0.03	5 (1%) 79 77	28, 55, 93, 214	0
1	K	482/483 (99%)	-0.06	4 (0%) 86 85	31, 58, 92, 128	0
1	L	483/483 (100%)	0.34	31 (6%) 19 16	37, 71, 118, 153	0
All	All	5716/5796 (98%)	-0.08	70 (1%) 79 77	22, 52, 92, 214	0

The worst 5 of 70 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	76	ILE	6.3
1	L	79	PHE	4.9
1	L	104	THR	4.2
1	L	77	ALA	4.2
1	L	82	LYS	4.2

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	L	502	1/1	0.68	0.09	75,75,75,75	0
3	MG	I	502	1/1	0.75	0.07	30,30,30,30	0
4	MLI	L	503	7/7	0.77	0.16	64,79,81,87	0
3	MG	B	502	1/1	0.77	0.17	44,44,44,44	0
5	GOL	D	503	6/6	0.86	0.18	45,54,60,62	0
3	MG	C	502	1/1	0.89	0.10	30,30,30,30	0
4	MLI	K	503	7/7	0.90	0.14	61,67,70,84	0
3	MG	A	502	1/1	0.90	0.05	49,49,49,49	0
5	GOL	B	503	6/6	0.91	0.16	44,52,58,58	0
4	MLI	J	503	7/7	0.91	0.16	59,61,69,75	0
4	MLI	I	503	7/7	0.91	0.14	55,62,65,83	0
3	MG	G	502	1/1	0.91	0.14	45,45,45,45	0
3	MG	J	502	1/1	0.92	0.04	55,55,55,55	0
3	MG	E	502	1/1	0.93	0.16	40,40,40,40	0
4	MLI	B	504	7/7	0.94	0.09	37,42,45,46	0
2	G6P	G	501	16/16	0.94	0.18	49,81,94,100	0
2	G6P	F	501	16/16	0.94	0.15	53,80,96,104	0
4	MLI	H	503	7/7	0.94	0.10	47,52,54,57	0
5	GOL	E	503	6/6	0.95	0.13	40,49,51,57	0
2	G6P	K	501	16/16	0.95	0.16	51,77,92,98	0
4	MLI	C	503	7/7	0.95	0.12	38,50,64,68	0
4	MLI	D	504	7/7	0.95	0.11	33,41,49,50	0
3	MG	D	502	1/1	0.95	0.17	39,39,39,39	0
2	G6P	H	501	16/16	0.95	0.16	50,69,82,92	0
3	MG	F	502	1/1	0.95	0.09	49,49,49,49	0
2	G6P	I	501	16/16	0.96	0.16	47,62,72,84	0
2	G6P	L	501	16/16	0.96	0.13	59,80,90,92	0
2	G6P	C	501	16/16	0.96	0.15	39,54,79,84	0
4	MLI	E	504	7/7	0.96	0.09	29,34,42,46	0
2	G6P	B	501	16/16	0.96	0.16	33,51,67,103	0
2	G6P	A	501	16/16	0.96	0.15	40,59,69,74	0
4	MLI	A	503	7/7	0.96	0.15	45,49,54,62	0

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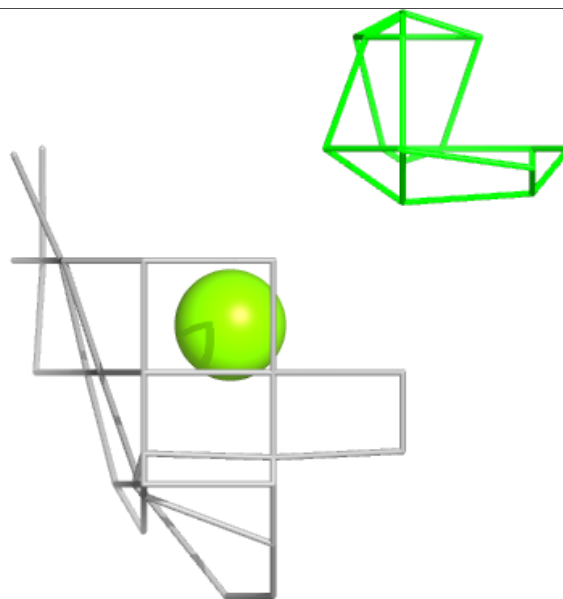
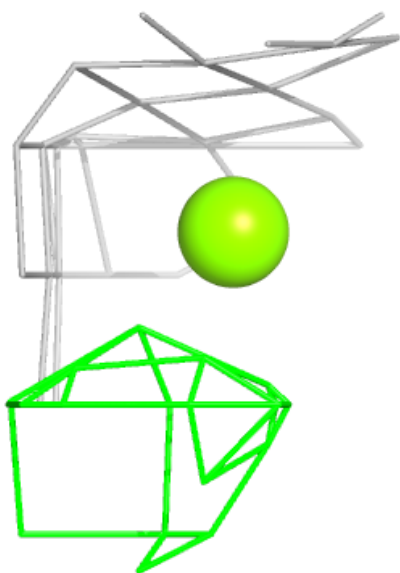
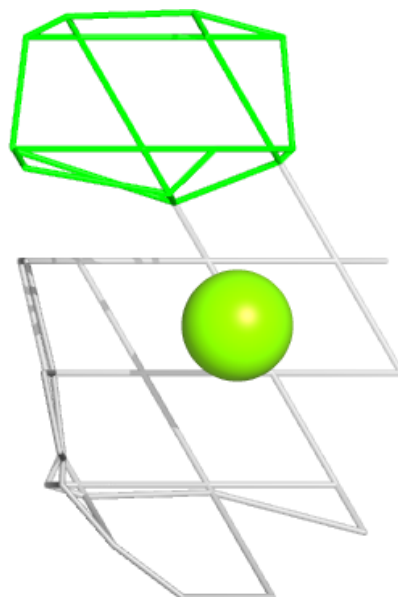
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	H	502	1/1	0.96	0.07	49,49,49,49	0
2	G6P	J	501	16/16	0.97	0.17	58,85,105,109	0
4	MLI	F	503	7/7	0.97	0.12	46,58,61,64	0
2	G6P	D	501	16/16	0.97	0.16	36,47,60,74	0
4	MLI	G	503	7/7	0.97	0.09	52,54,60,60	0
2	G6P	E	501	16/16	0.97	0.17	42,60,75,78	0
3	MG	K	502	1/1	0.98	0.12	48,48,48,48	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.

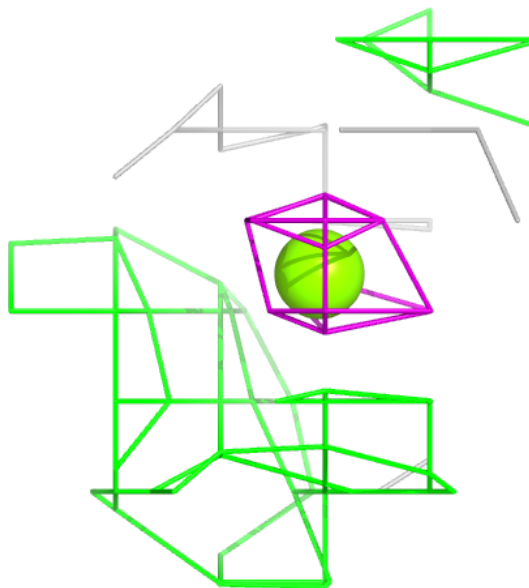
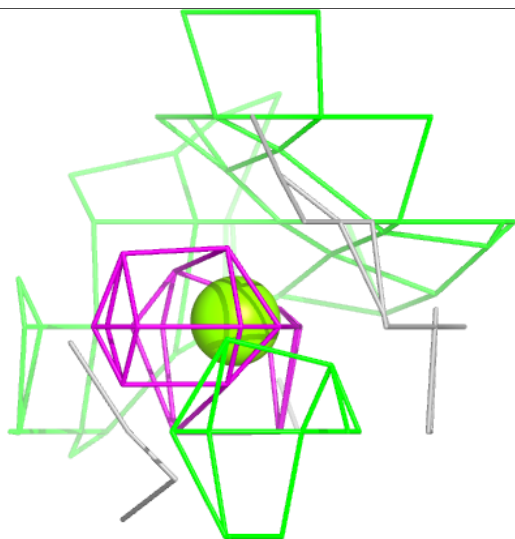
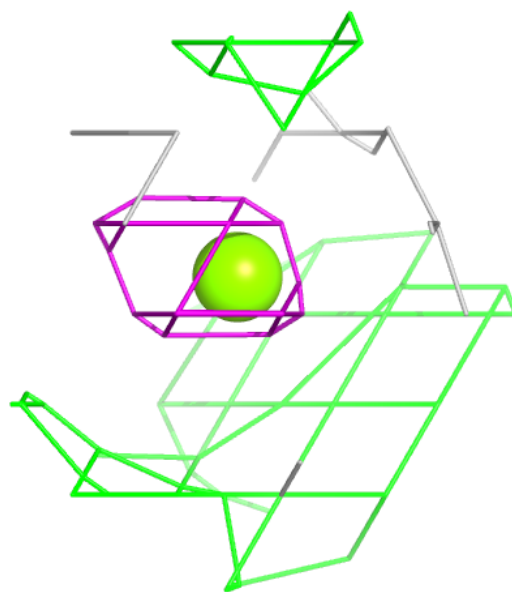
Electron density around MG L 502:

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



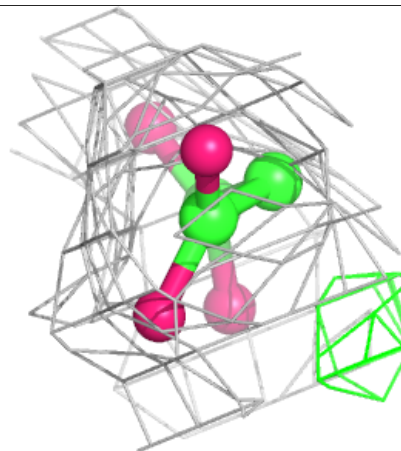
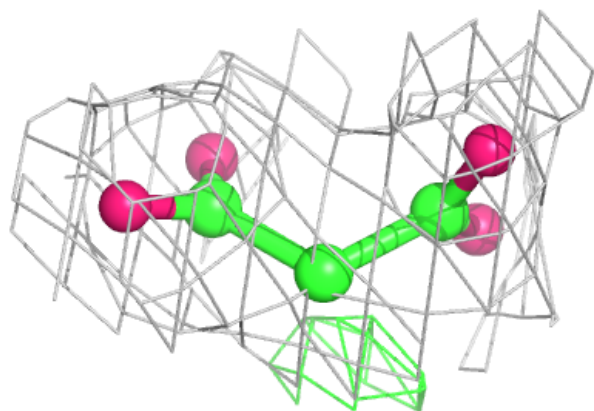
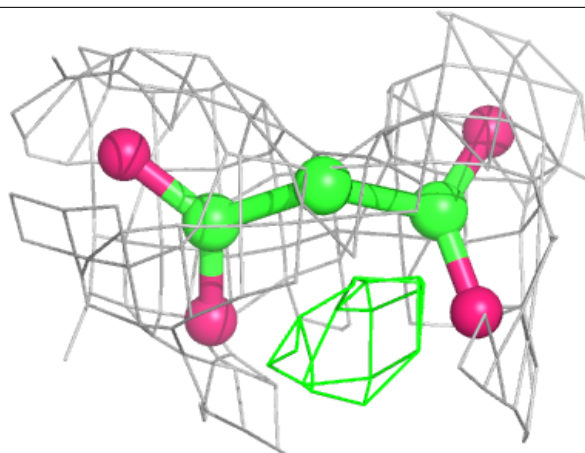
Electron density around MG I 502:

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and green (positive)



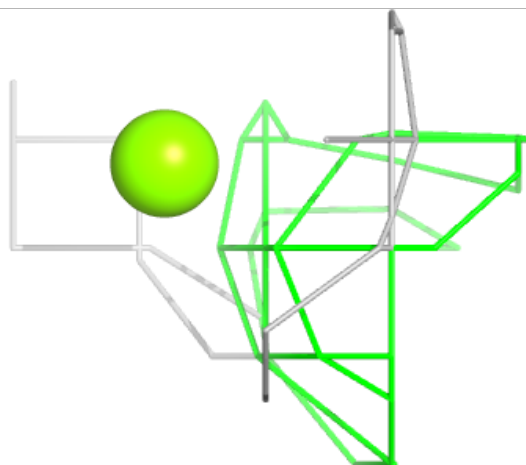
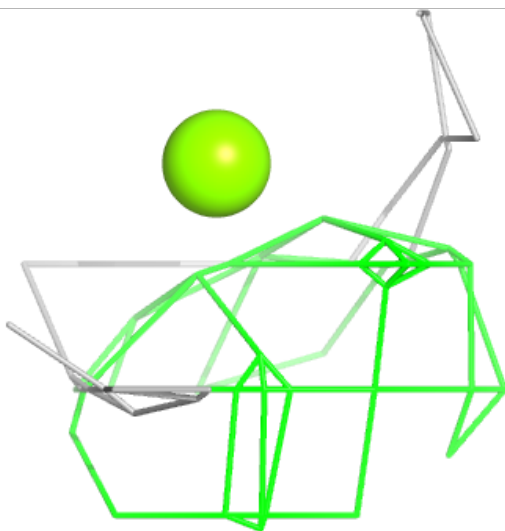
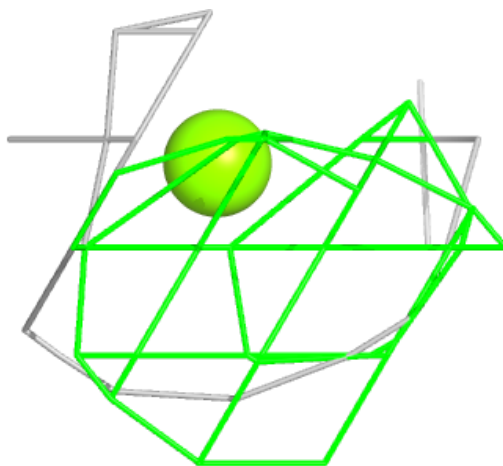
Electron density around MLI L 503:

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and green (positive)



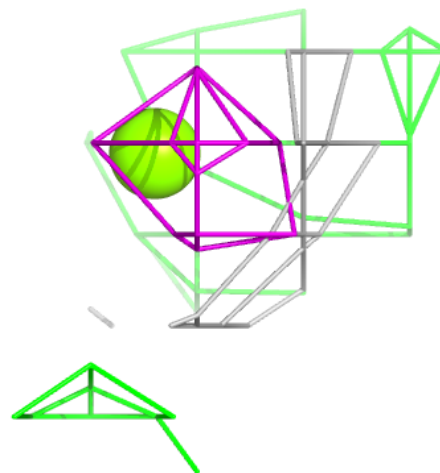
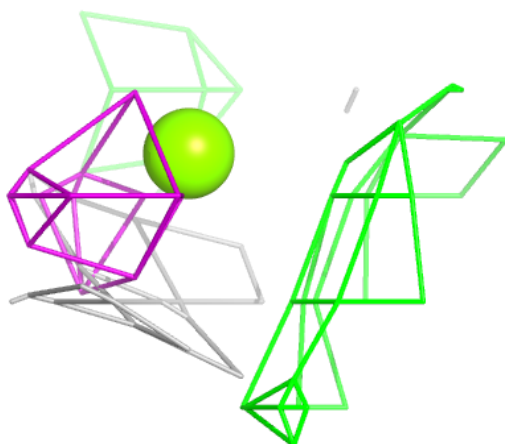
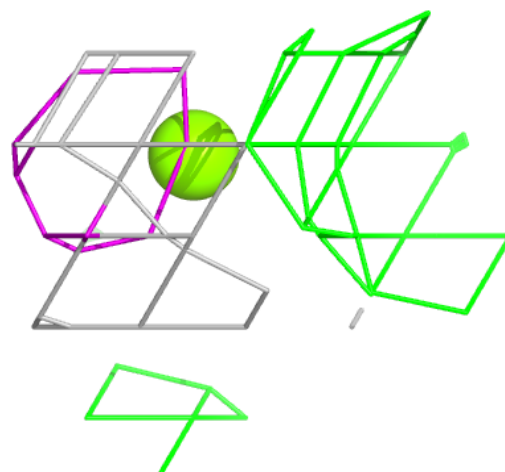
Electron density around MG B 502:

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and green (positive)



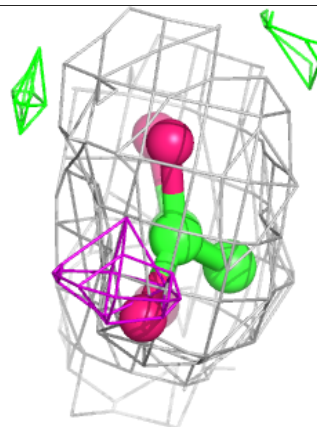
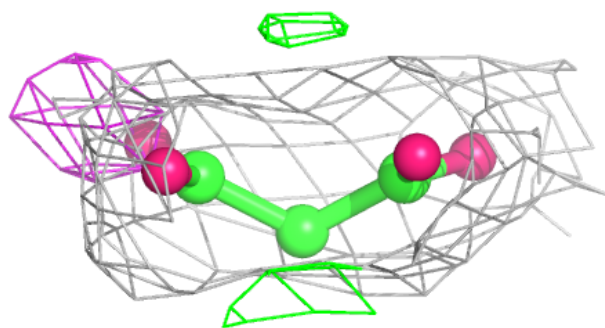
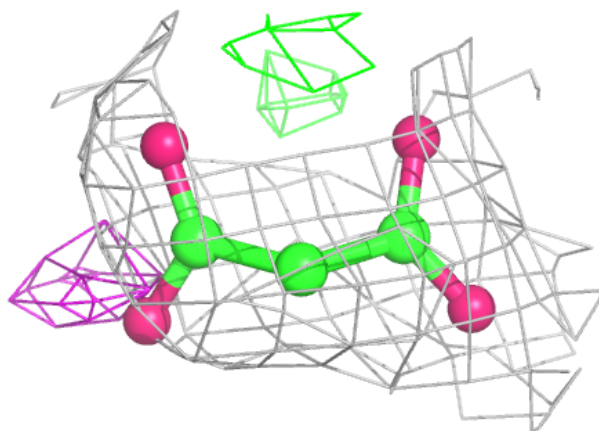
Electron density around MG C 502:

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and green (positive)



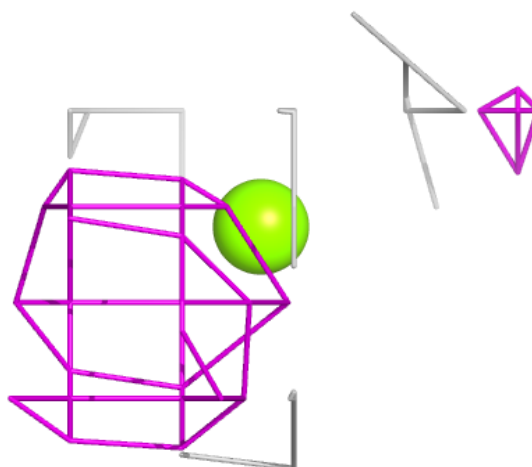
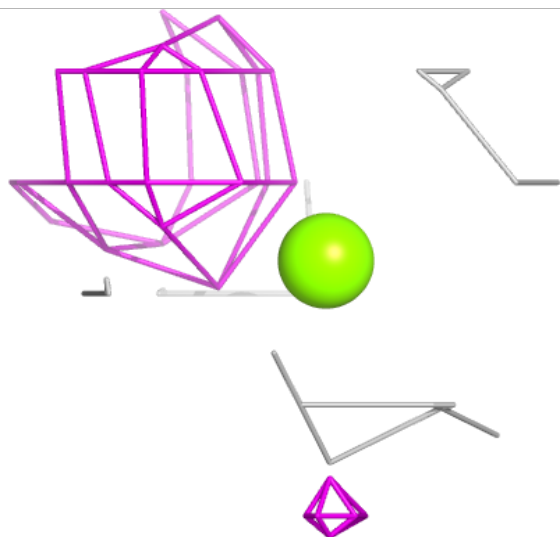
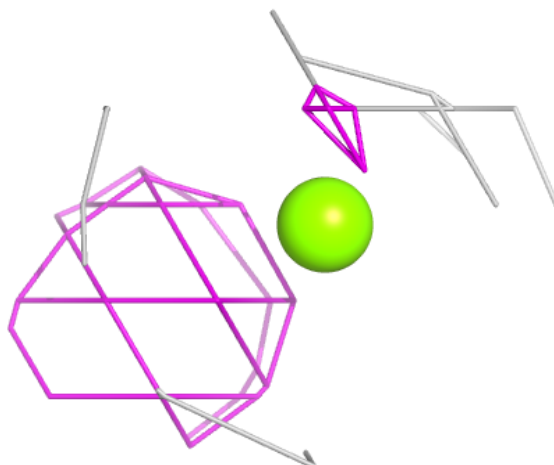
Electron density around MLI K 503:

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



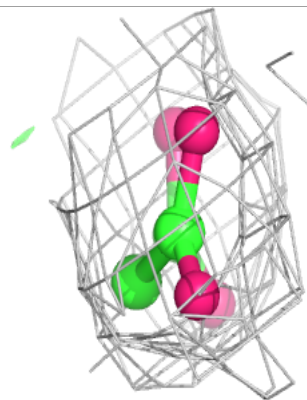
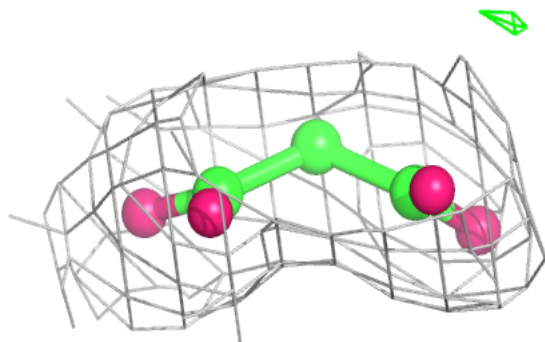
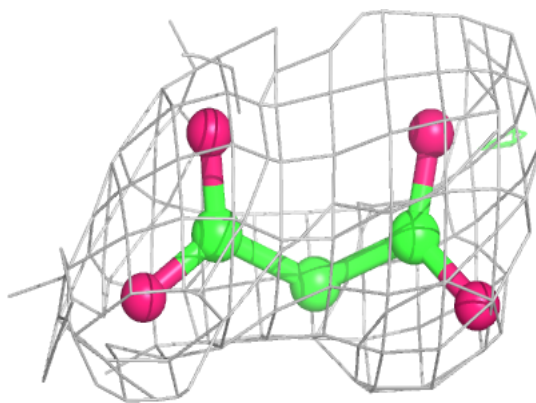
Electron density around MG A 502:

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and green (positive)



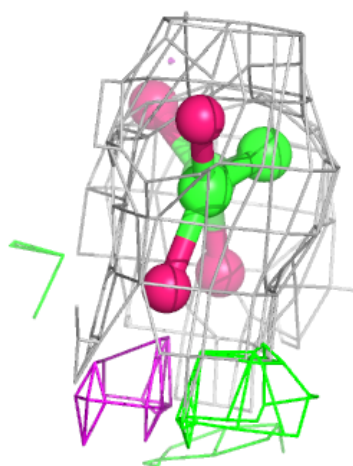
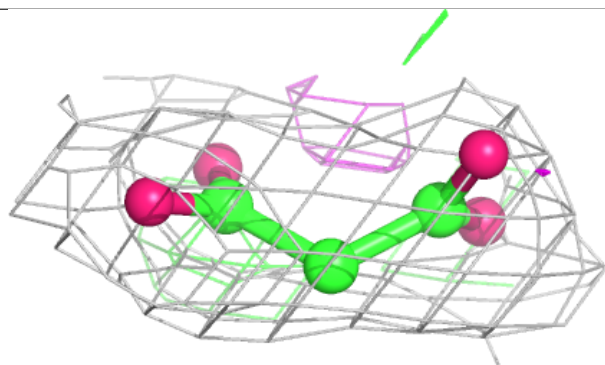
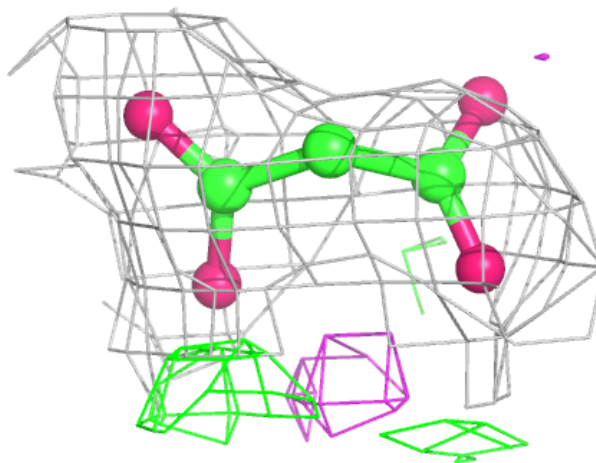
Electron density around MLI J 503:

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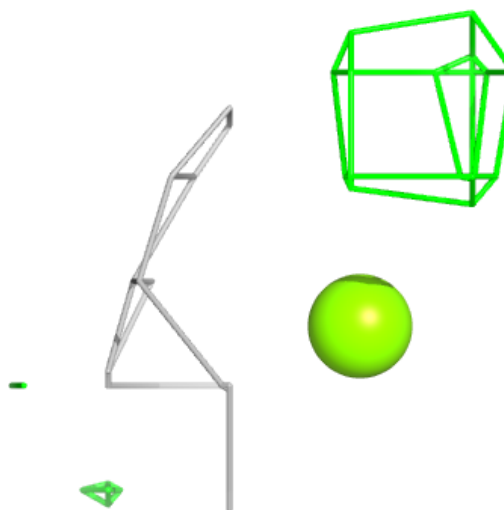
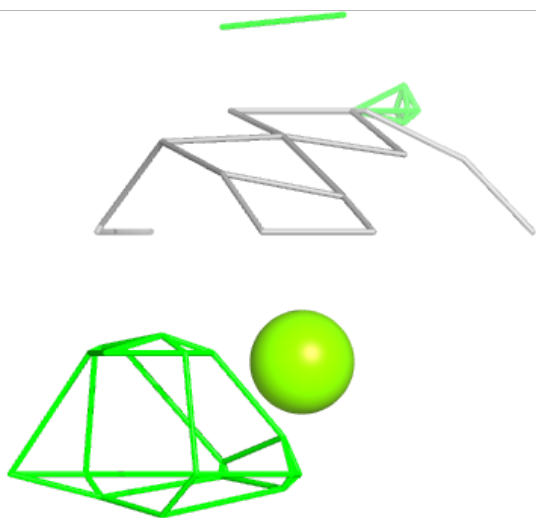
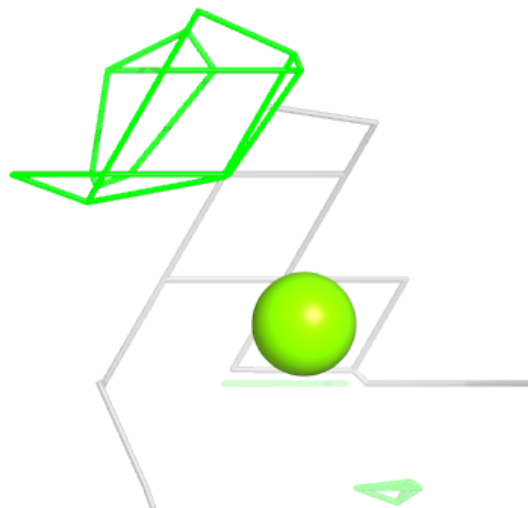
Electron density around MLI I 503:

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and green (positive)



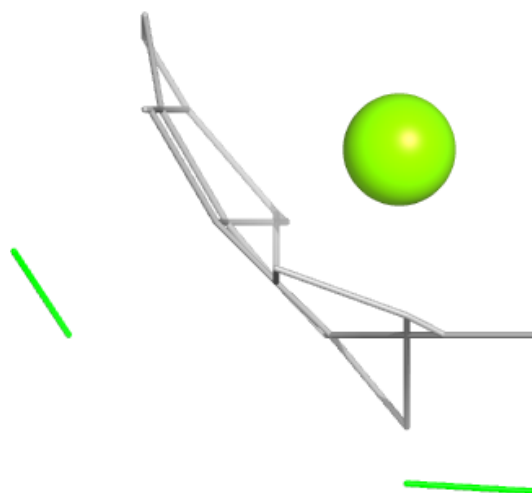
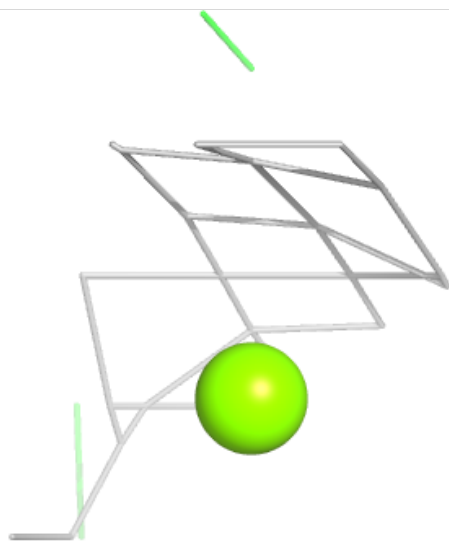
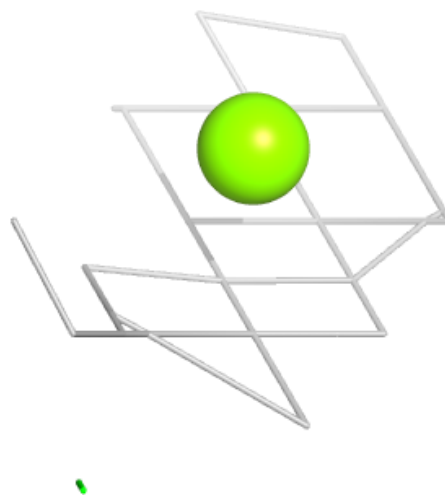
Electron density around MG G 502:

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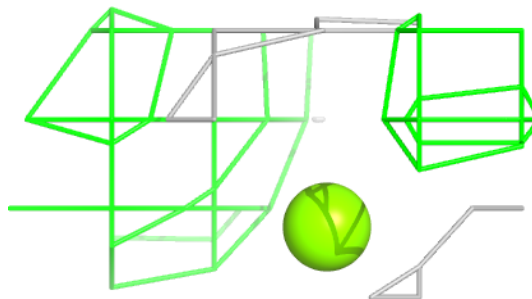
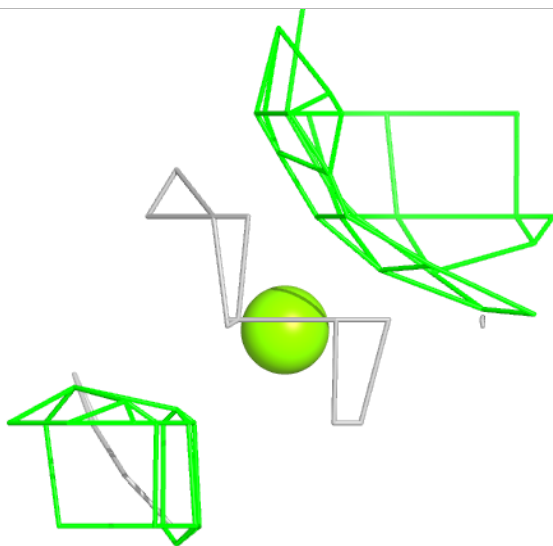
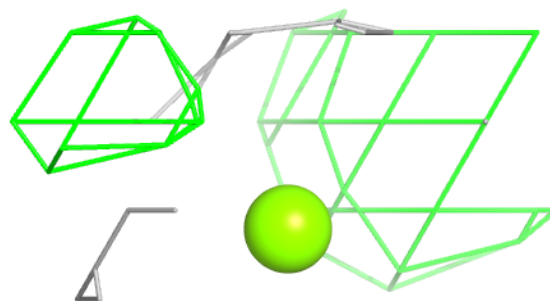
Electron density around MG J 502:

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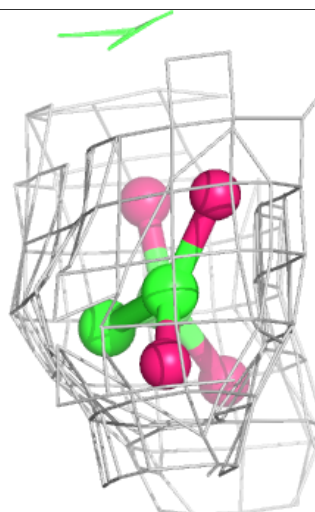
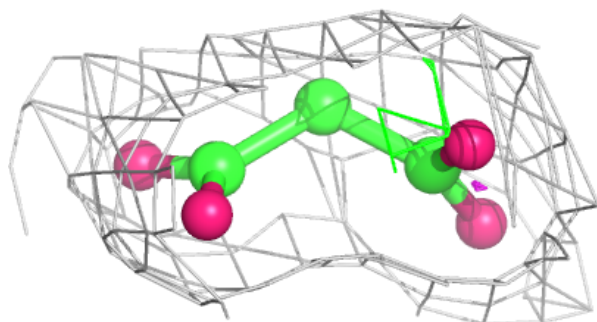
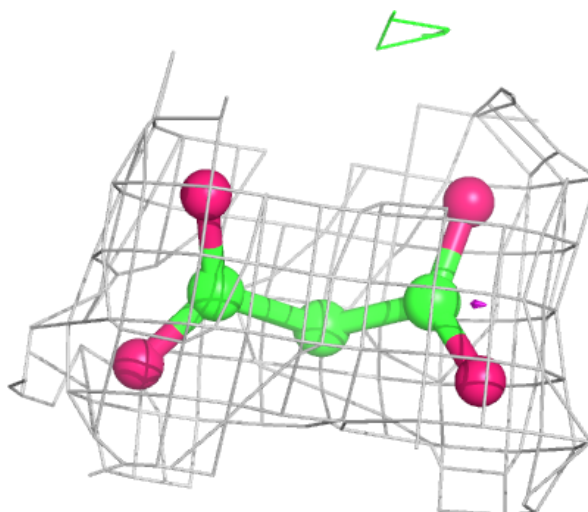
Electron density around MG E 502:

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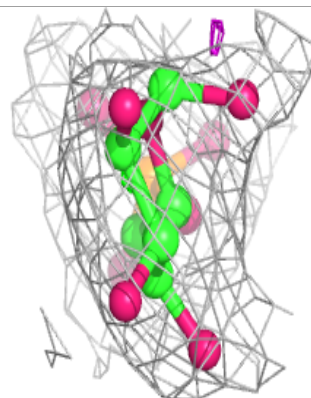
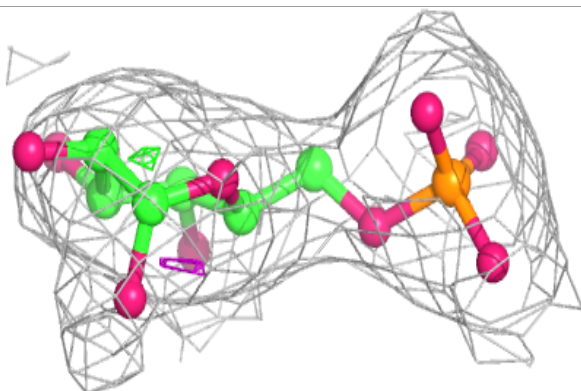
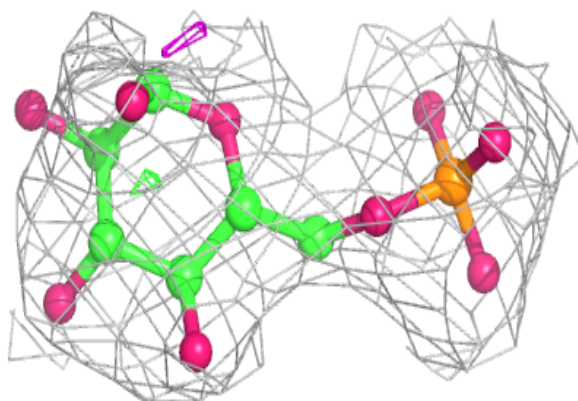
Electron density around MLI B 504:

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and green (positive)

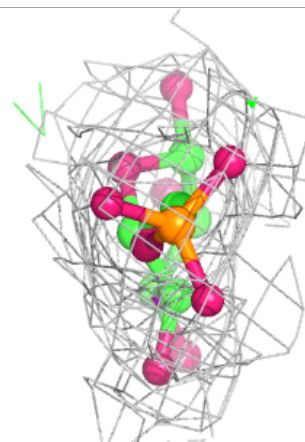
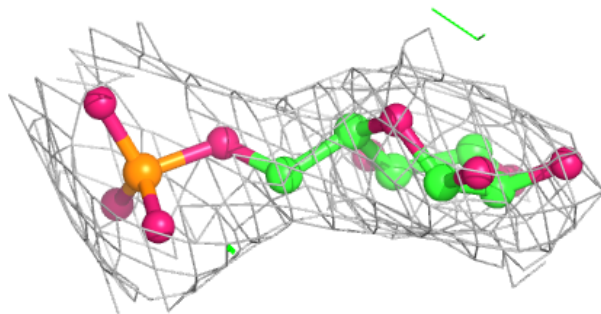
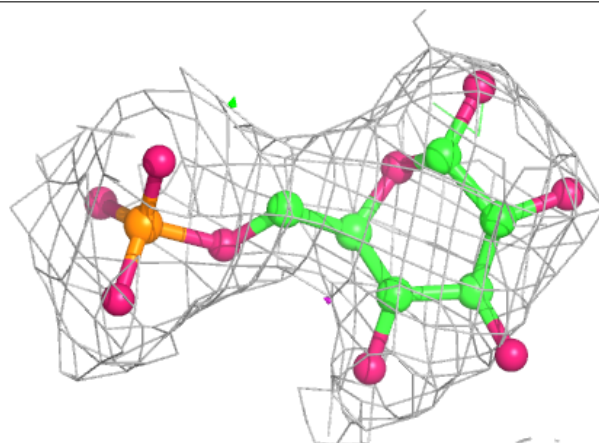


Electron density around G6P G 501:

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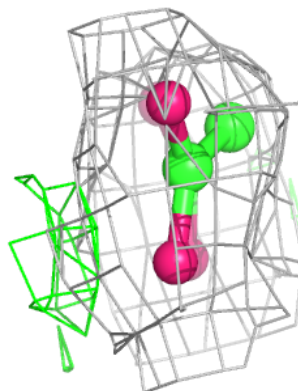
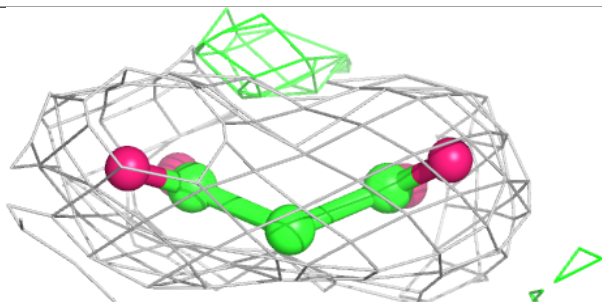
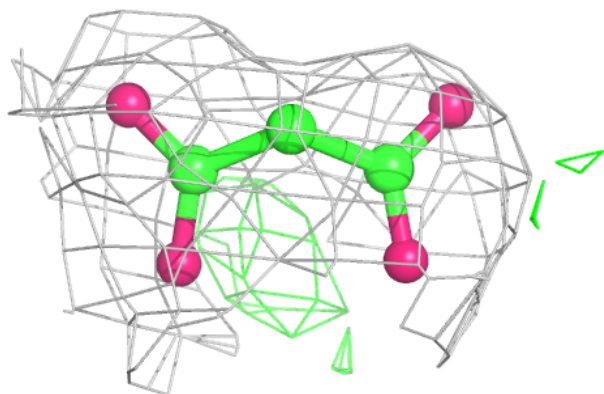
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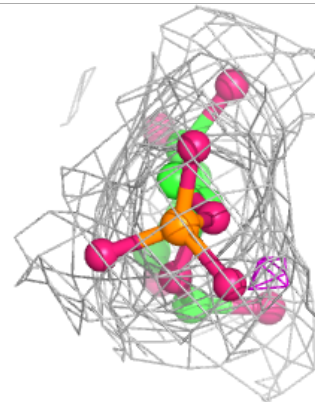
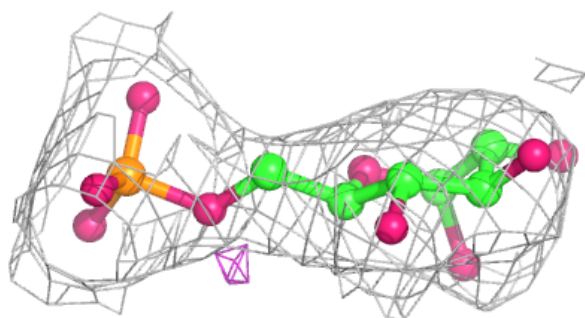
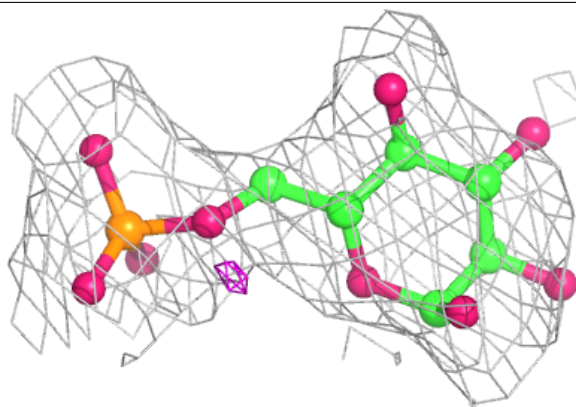


Electron density around MLI H 503:

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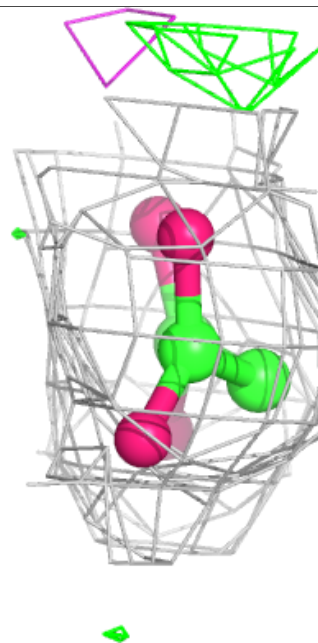
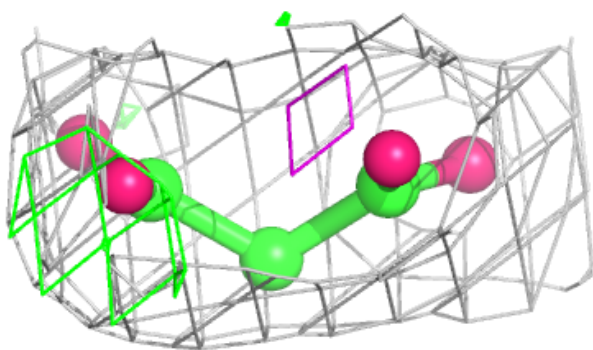
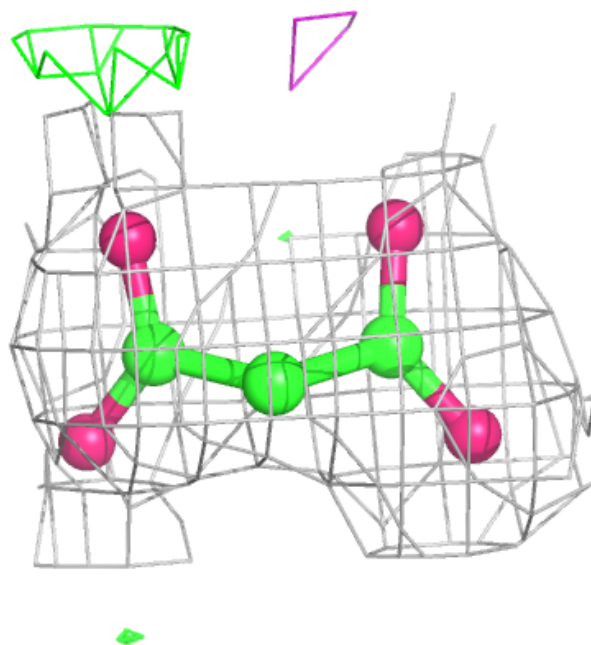
**Electron density around G6P K 501:**

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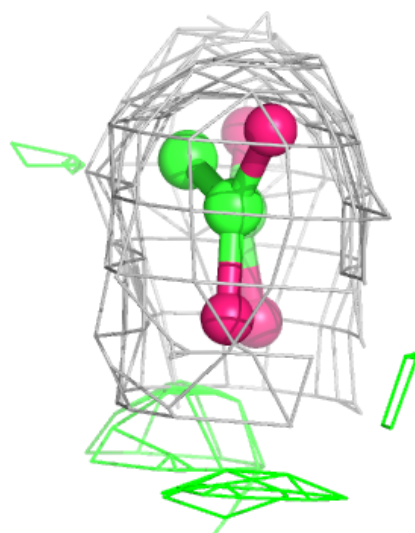
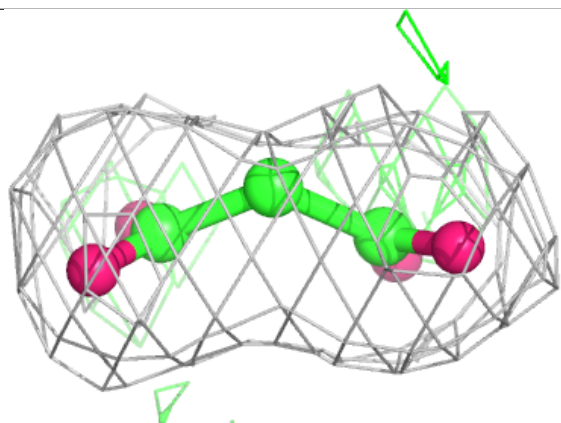
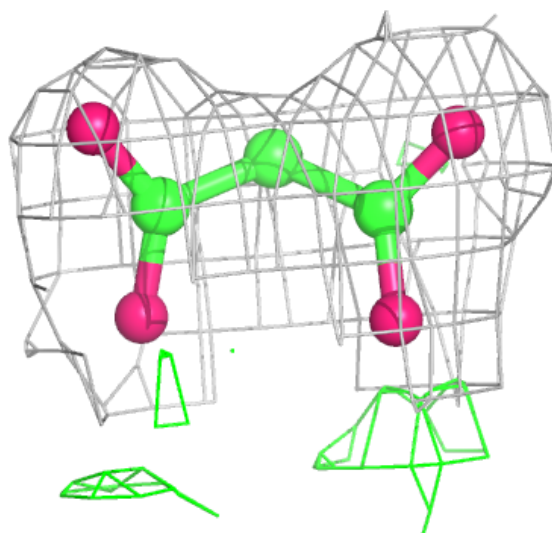
Electron density around MLI C 503:

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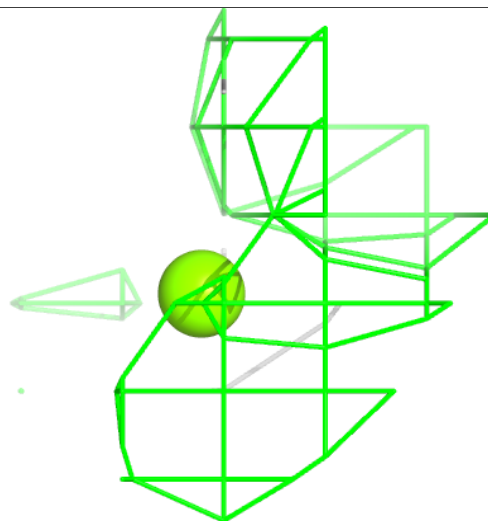
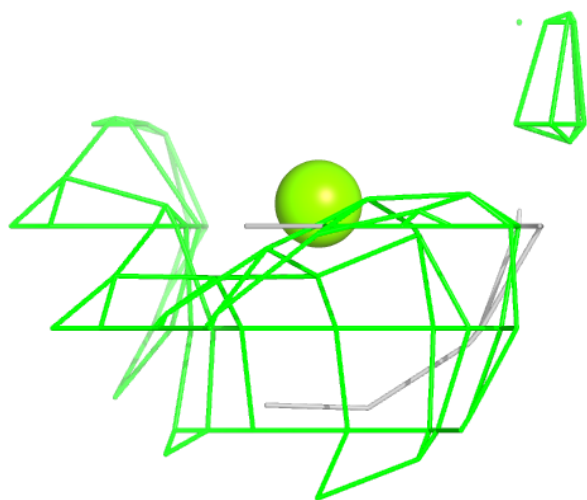
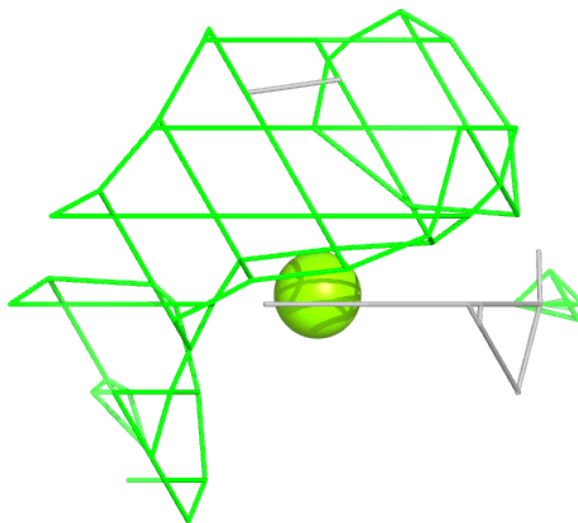
Electron density around MLI D 504:

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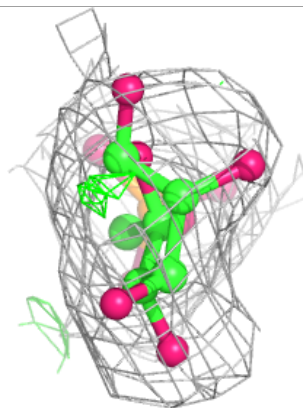
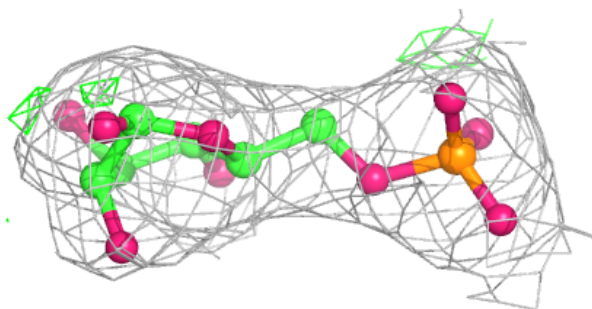
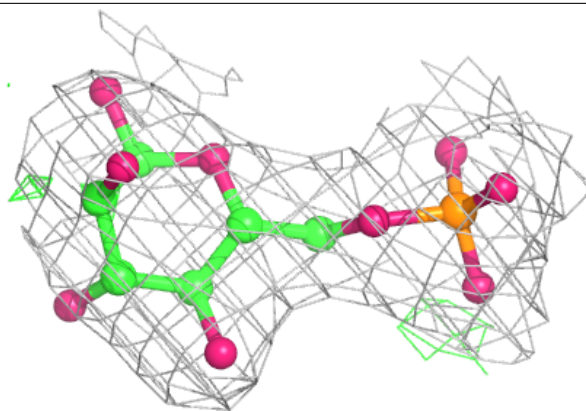
Electron density around MG D 502:

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and green (positive)



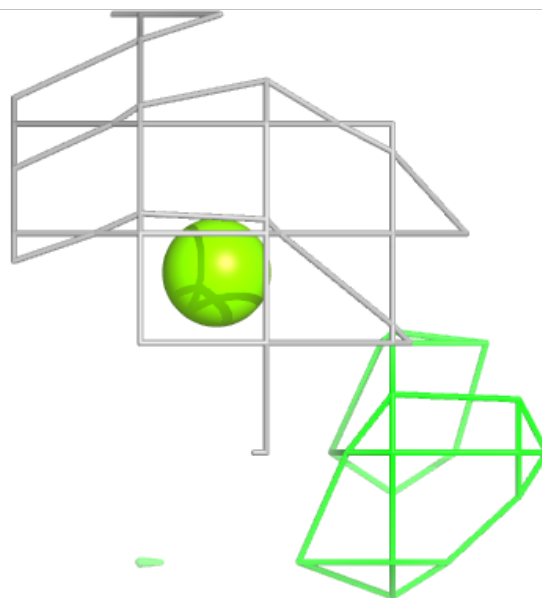
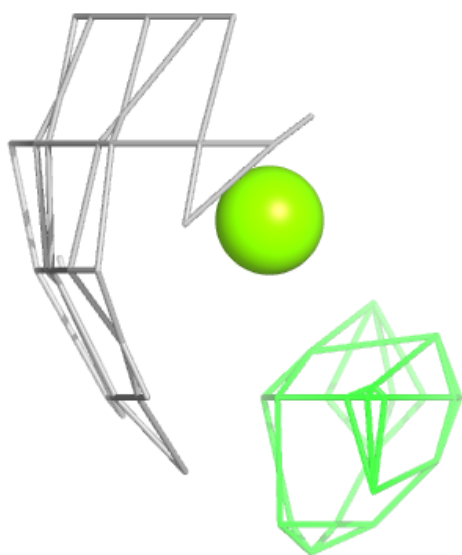
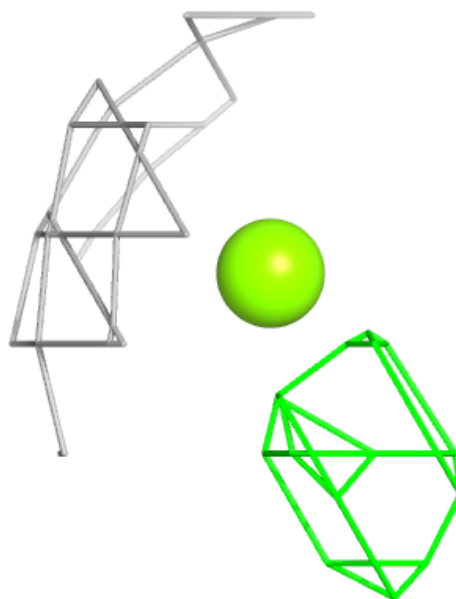
Electron density around G6P H 501:

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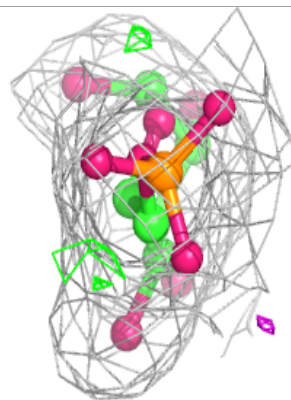
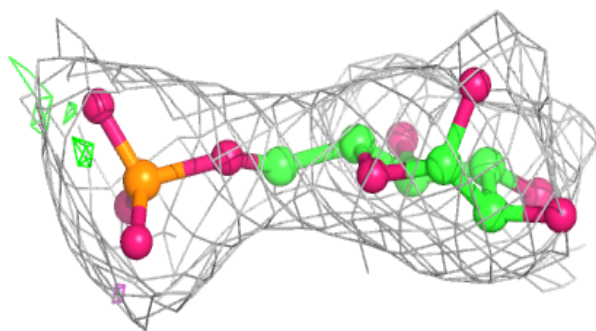
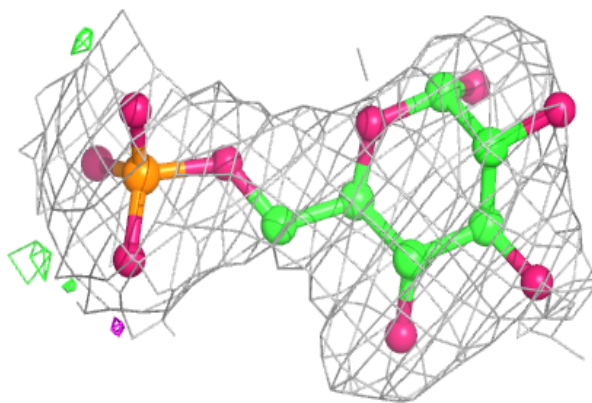
Electron density around MG F 502:

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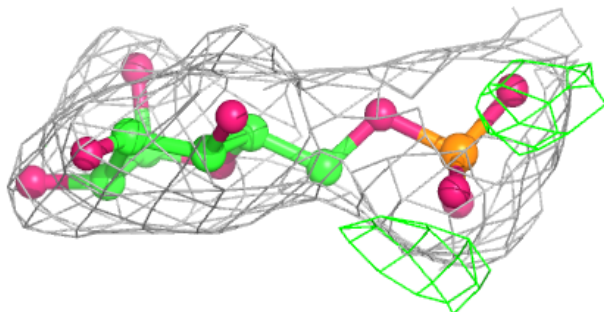
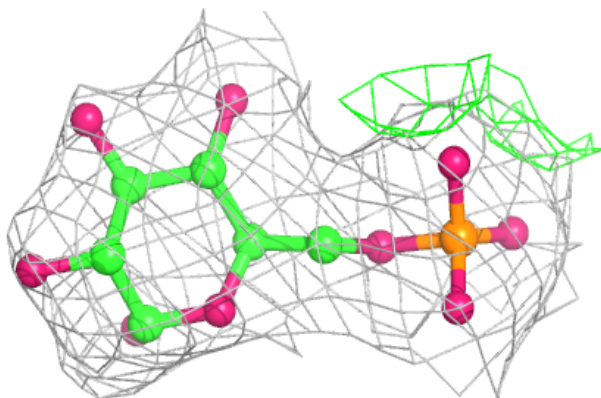


Electron density around G6P I 501:

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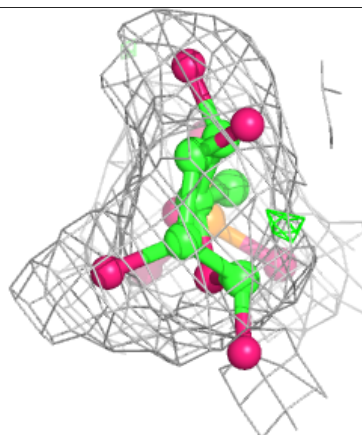
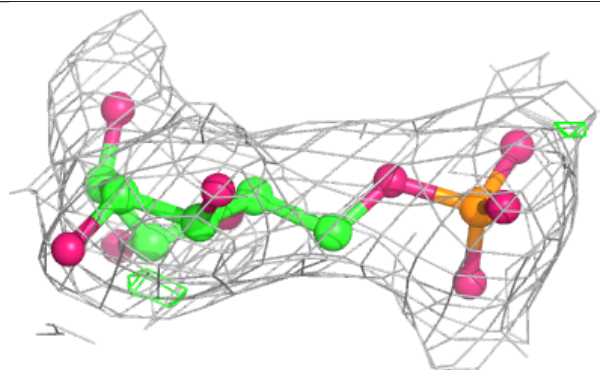
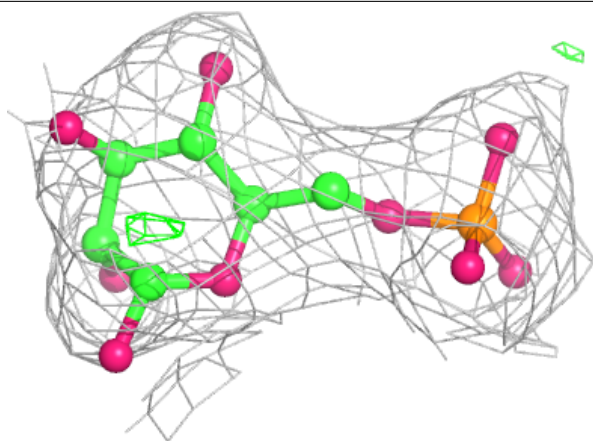
**Electron density around G6P L 501:**

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



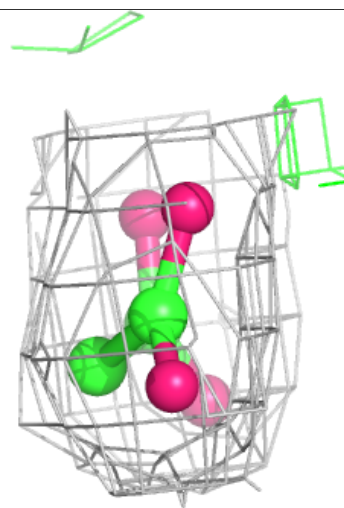
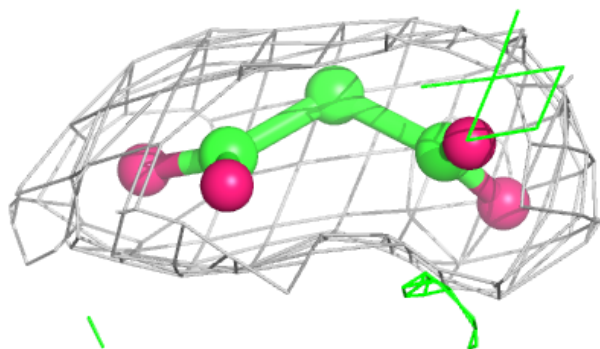
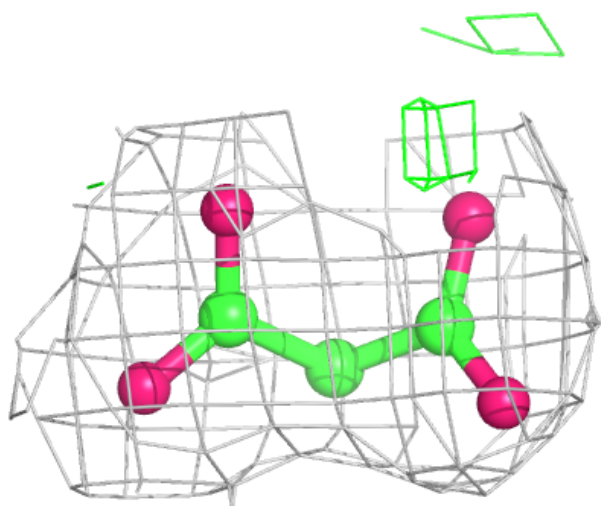
Electron density around G6P C 501:

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



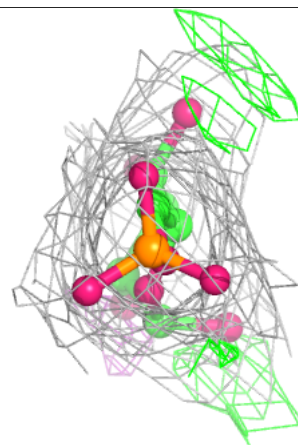
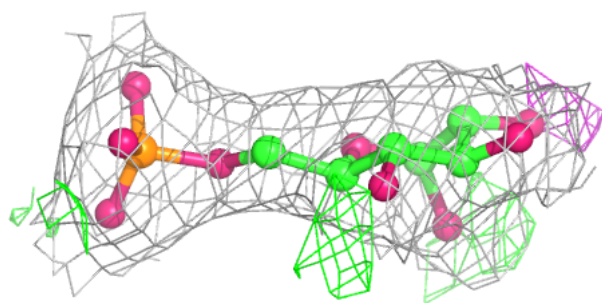
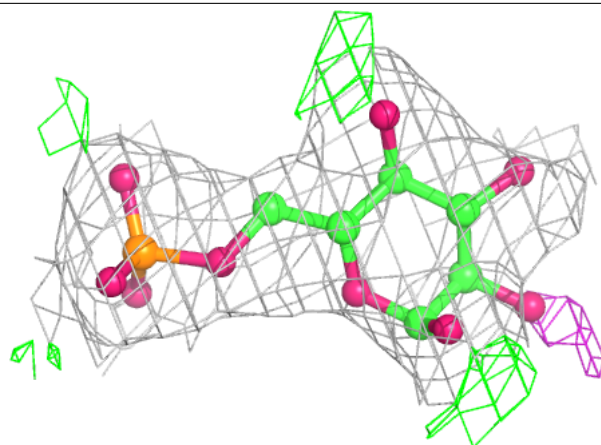
Electron density around MLI E 504:

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



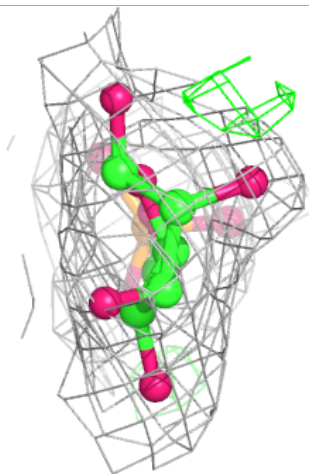
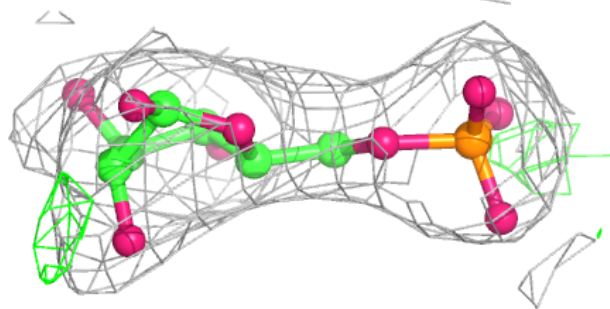
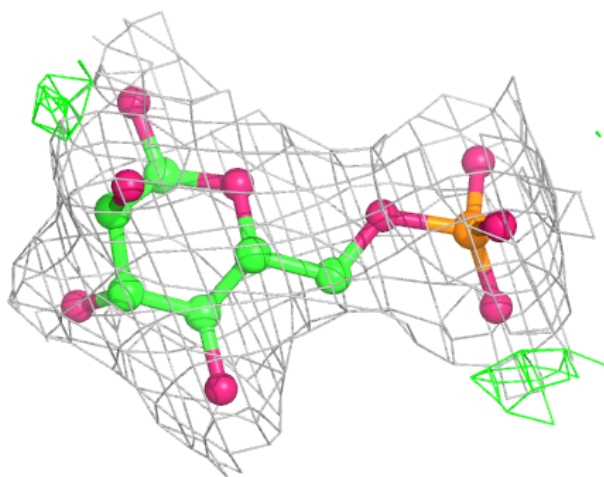
Electron density around G6P B 501:

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



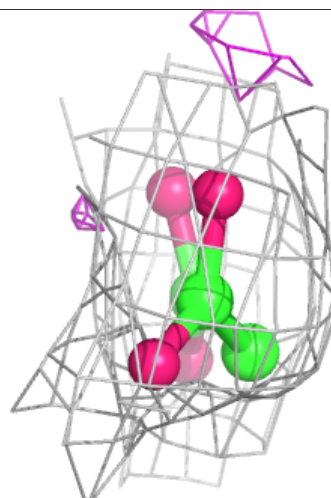
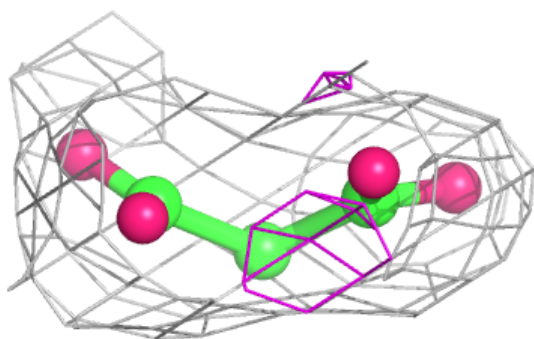
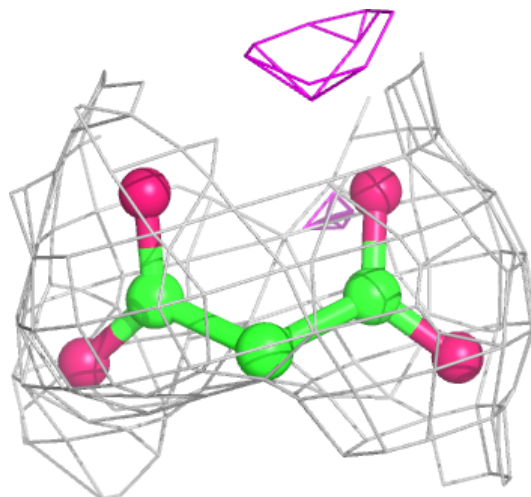
Electron density around G6P A 501:

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



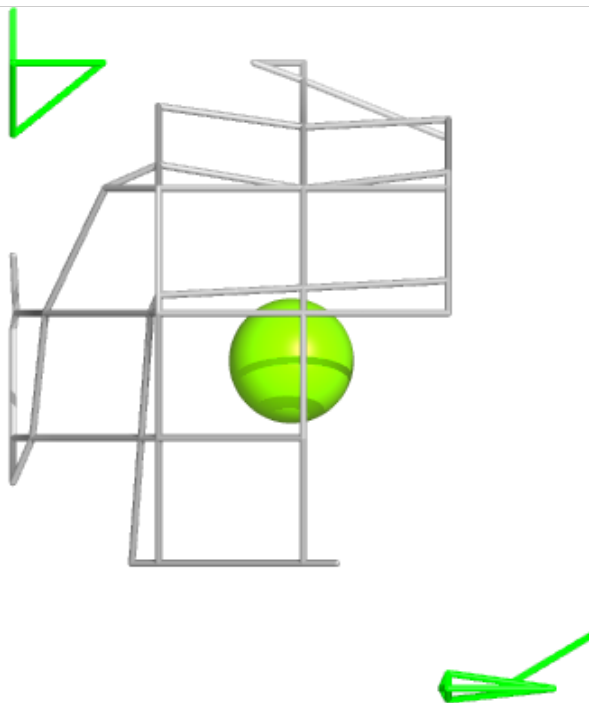
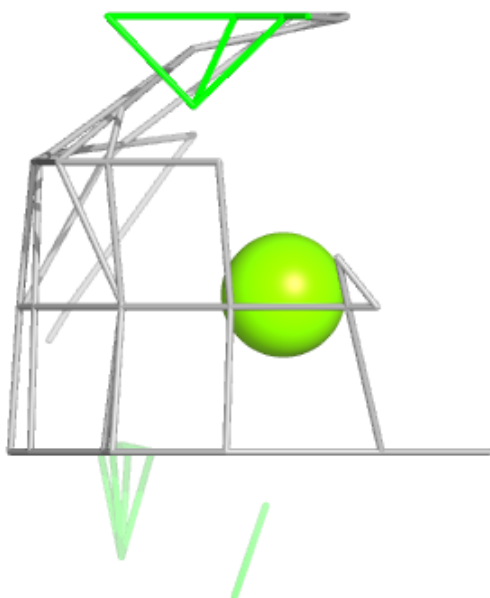
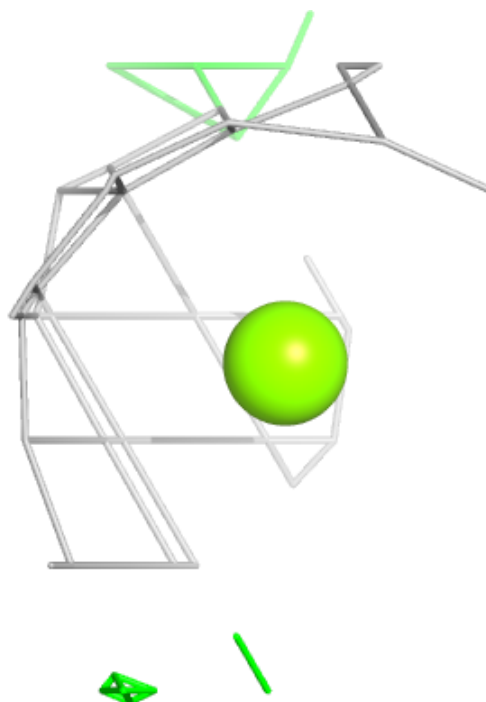
Electron density around MLI A 503:

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



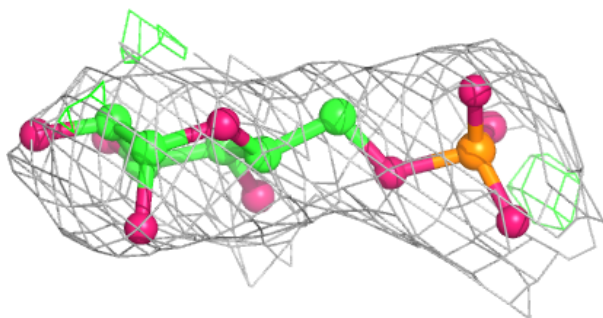
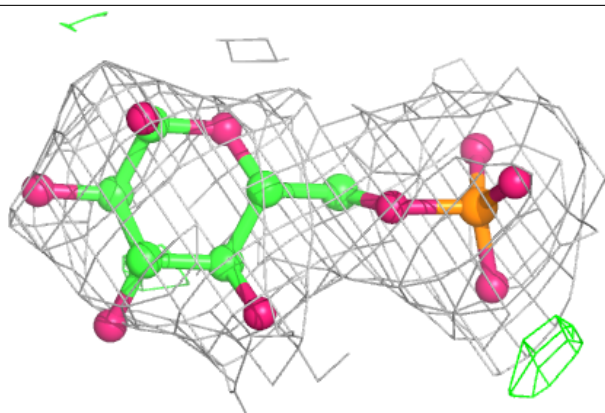
Electron density around MG H 502:

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



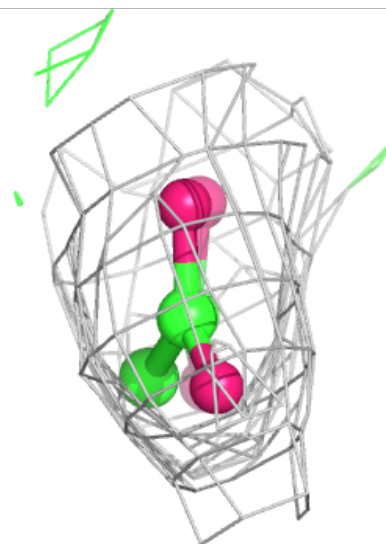
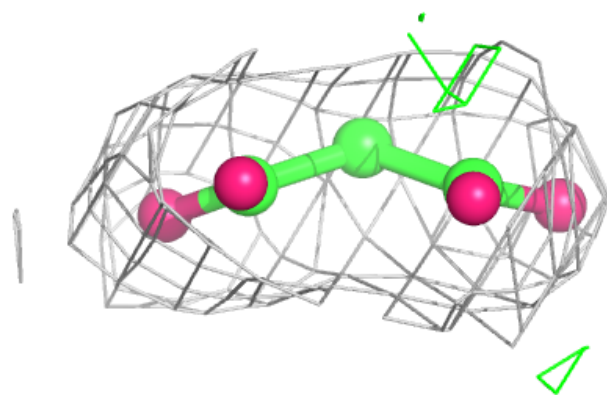
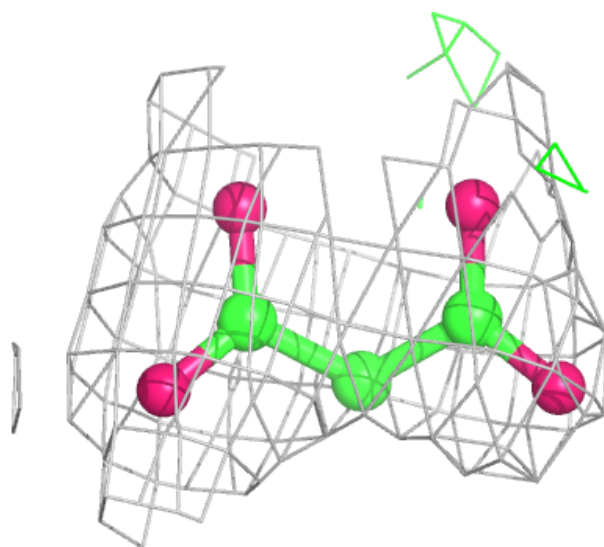
Electron density around G6P J 501:

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



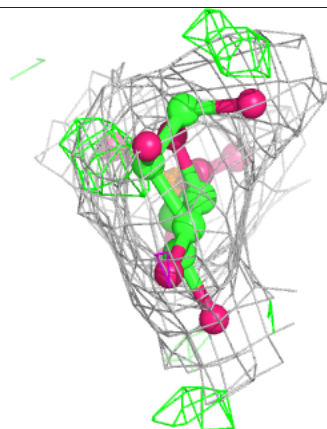
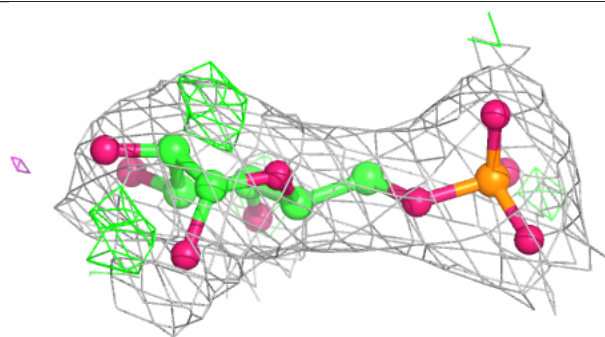
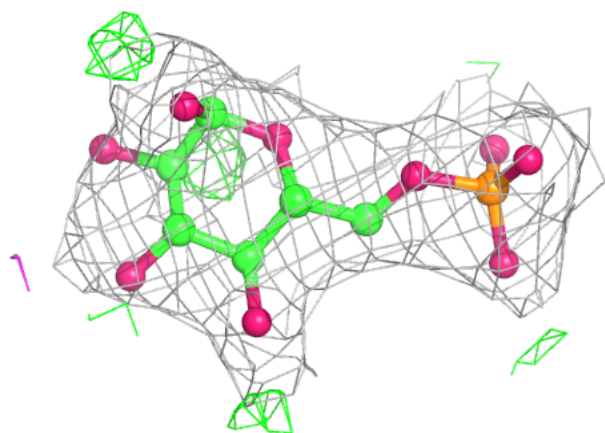
Electron density around MLI F 503:

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



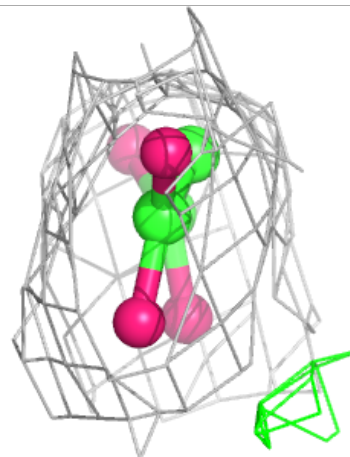
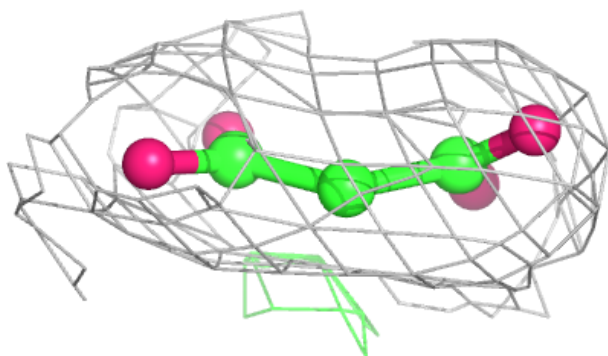
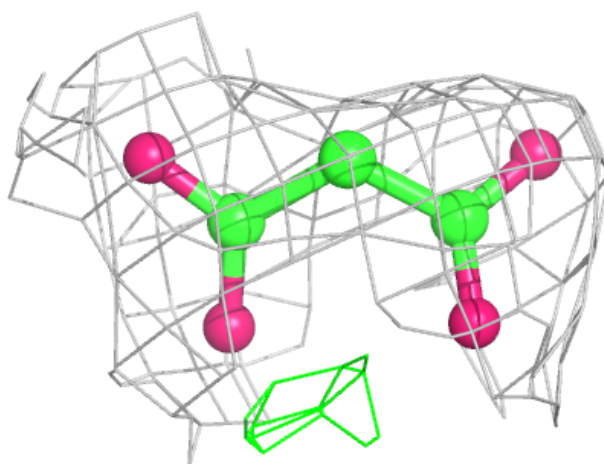
Electron density around G6P D 501:

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



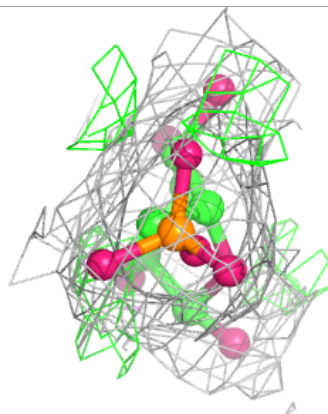
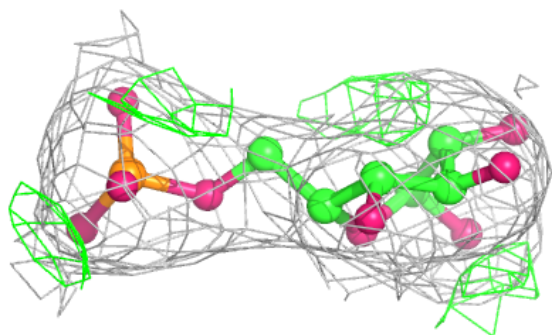
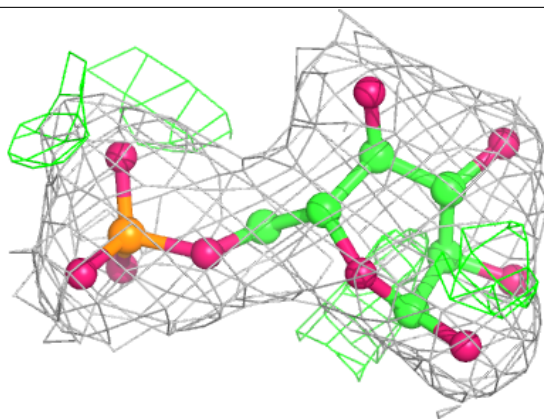
Electron density around MLI G 503:

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



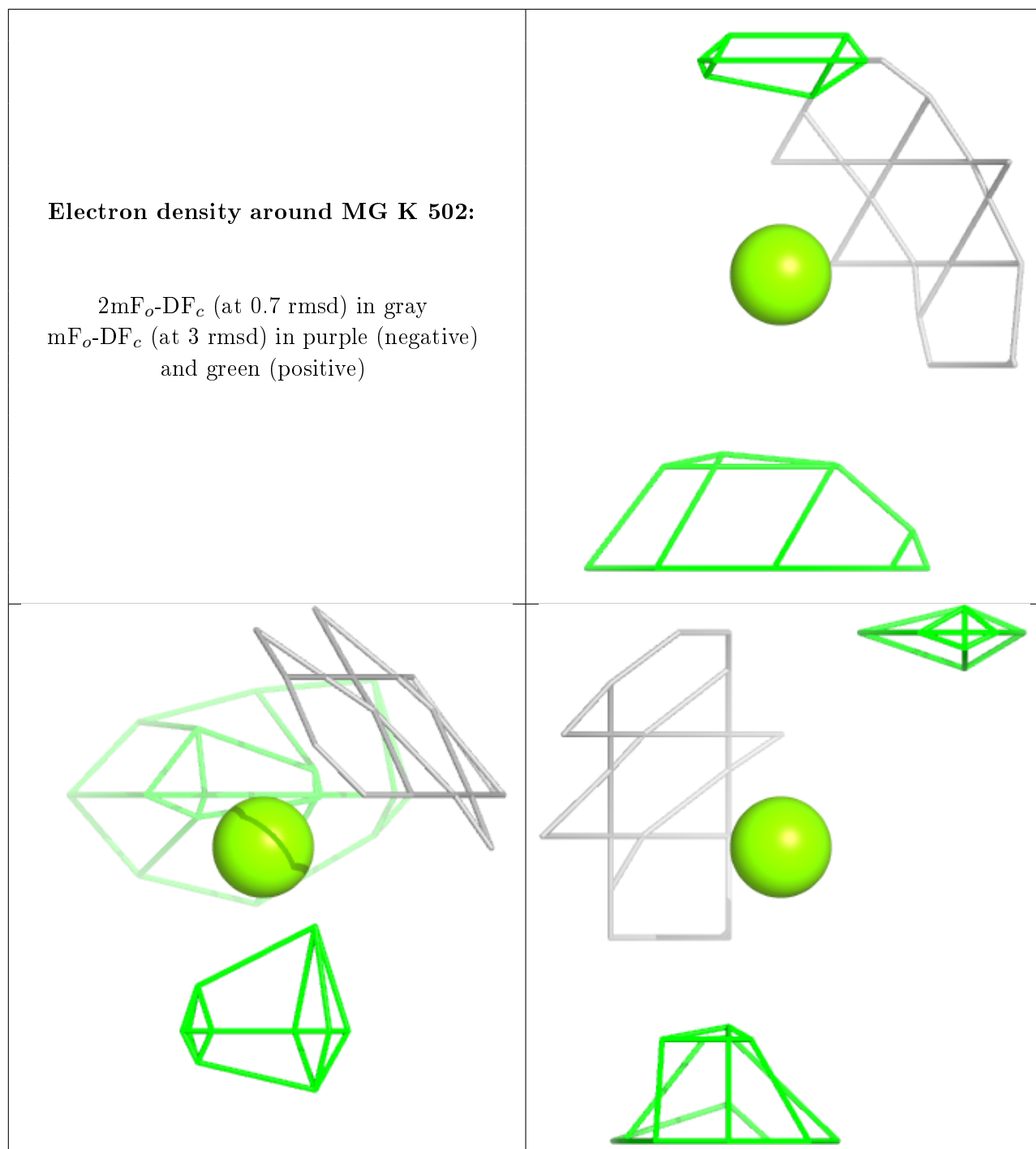
Electron density around G6P E 501:

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



Electron density around MG K 502:

$2mF_o-DF_c$ (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.