



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:17 PM UTC

PDB ID : 6QXL / pdb_00006qxl
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

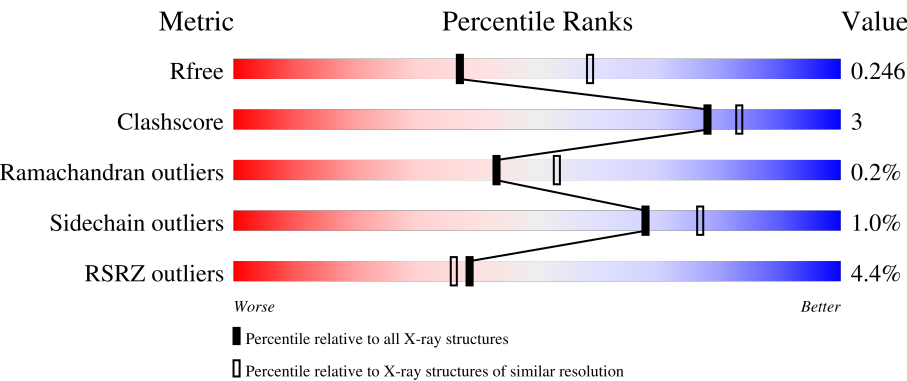
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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}	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	483	2% 92% 7% .
1	B	483	2% 93% 6% .
1	C	483	2% 93% 6% .
1	D	483	% 94% 5% .
1	E	483	% 92% 7% .

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Mol	Chain	Length	Quality of chain
1	F	483	
1	G	483	
1	H	483	
1	I	483	
1	J	483	
1	K	483	
1	L	483	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MLI	D	504	-	X	-	-

2 Entry composition

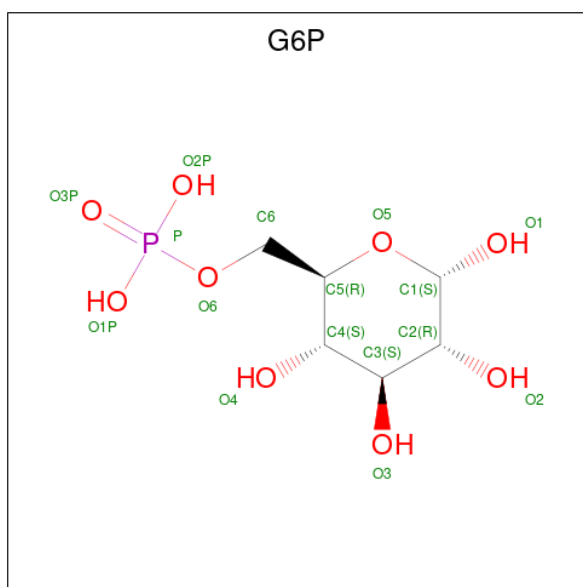
There are 6 unique types of molecules in this entry. The entry contains 45923 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: G6P) (formula: C₆H₁₃O₉P) (labeled as "Ligand of Interest" by depositor).

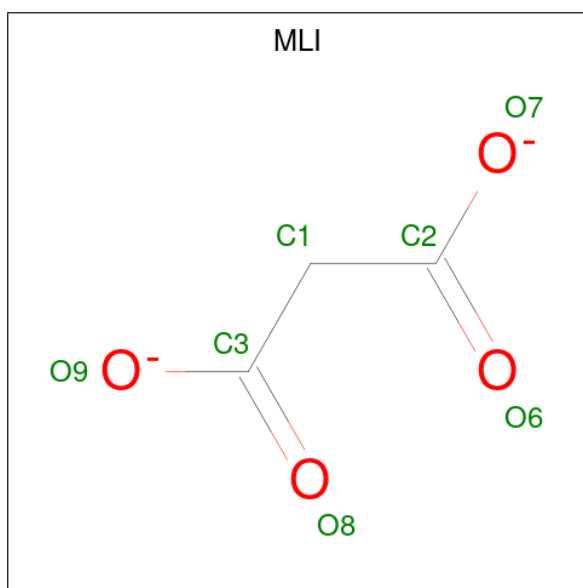


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		
2	C	1	Total	C	O	P	0	0
			16	6	9	1		
2	D	1	Total	C	O	P	0	0
			16	6	9	1		
2	E	1	Total	C	O	P	0	0
			16	6	9	1		
2	F	1	Total	C	O	P	0	0
			16	6	9	1		
2	G	1	Total	C	O	P	0	0
			16	6	9	1		
2	H	1	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 (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

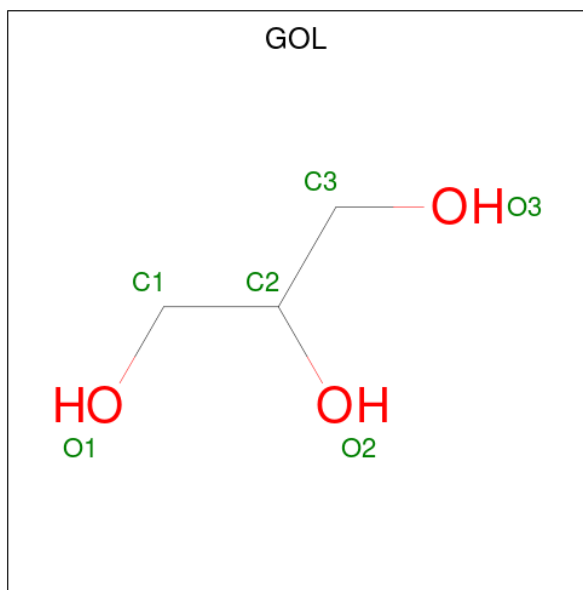
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total 1 Mg 1	0	0
3	B	1	Total 1 Mg 1	0	0
3	C	1	Total 1 Mg 1	0	0
3	D	1	Total 1 Mg 1	0	0
3	E	1	Total 1 Mg 1	0	0
3	F	1	Total 1 Mg 1	0	0
3	G	1	Total 1 Mg 1	0	0
3	H	1	Total 1 Mg 1	0	0
3	I	1	Total 1 Mg 1	0	0
3	J	1	Total 1 Mg 1	0	0
3	K	1	Total 1 Mg 1	0	0
3	L	1	Total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

- Molecule 4 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is GLYCEROL (CCD ID: 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

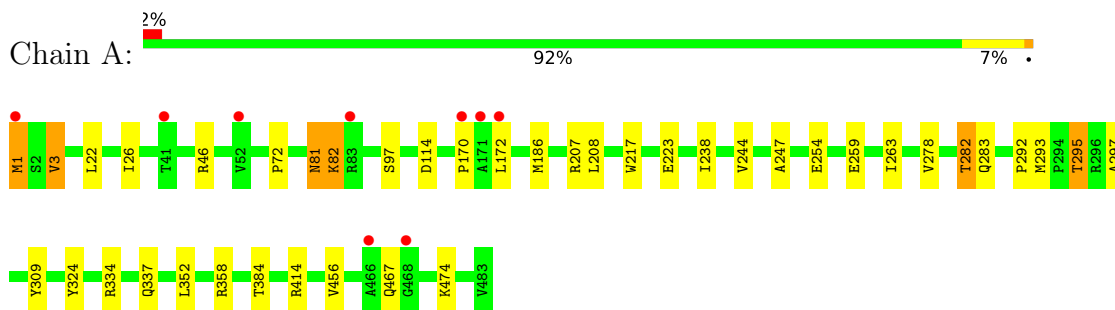
- Molecule 6 is water.

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

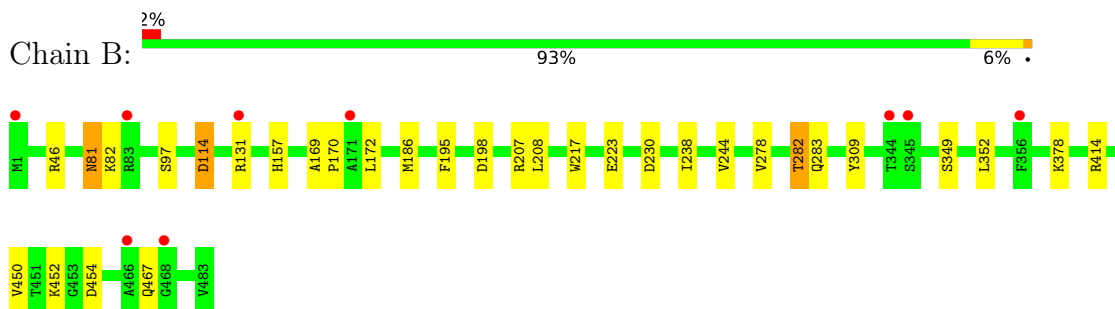
3 Residue-property plots

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.

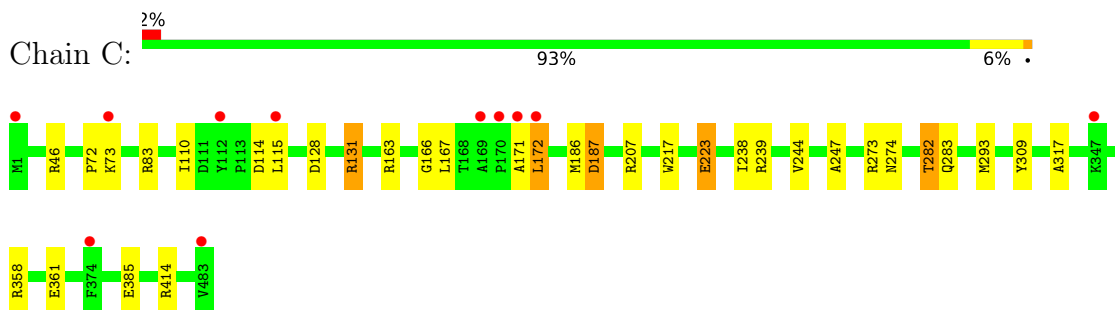
• Molecule 1: Pyruvate kinase



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• Molecule 1: Pyruvate kinase

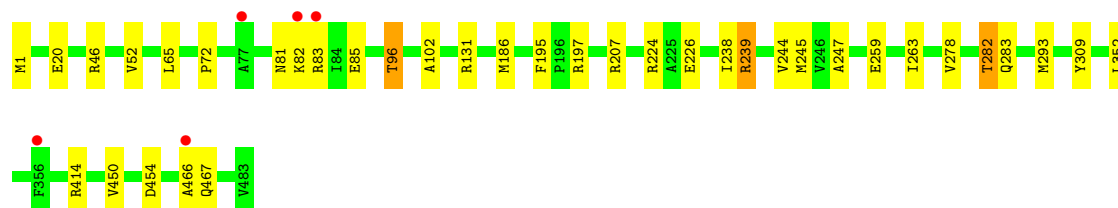
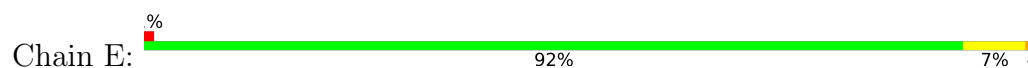


• Molecule 1: Pyruvate kinase

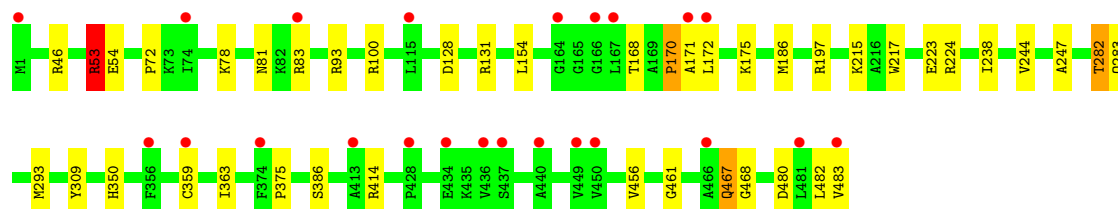
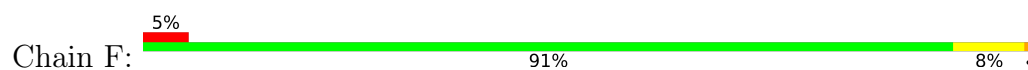




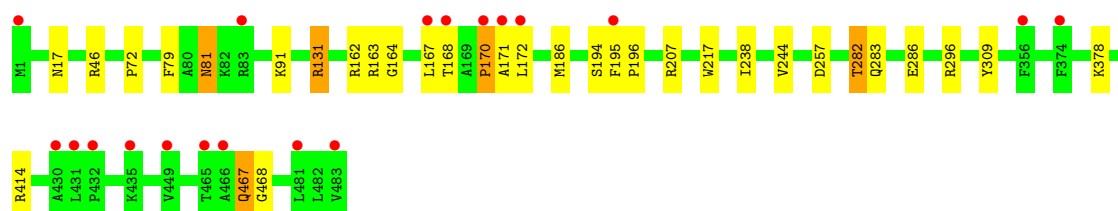
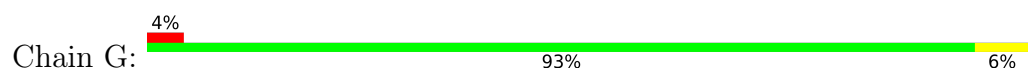
• Molecule 1: Pyruvate kinase



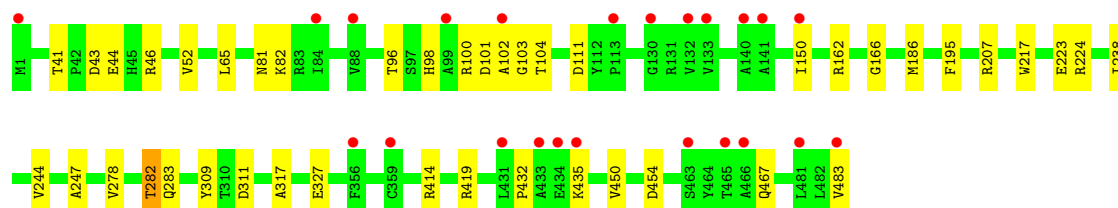
• Molecule 1: Pyruvate kinase



• Molecule 1: Pyruvate kinase

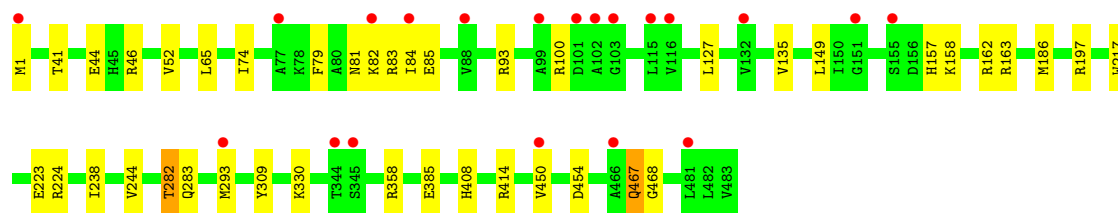


• Molecule 1: Pyruvate kinase

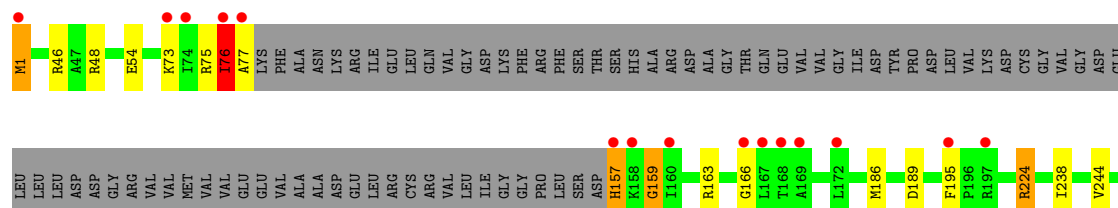
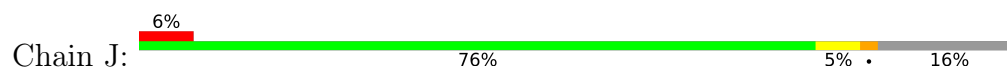


• Molecule 1: Pyruvate kinase

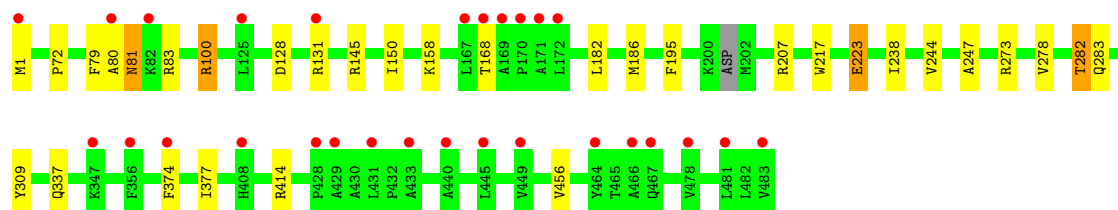
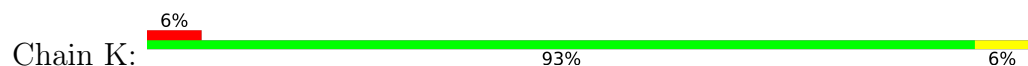




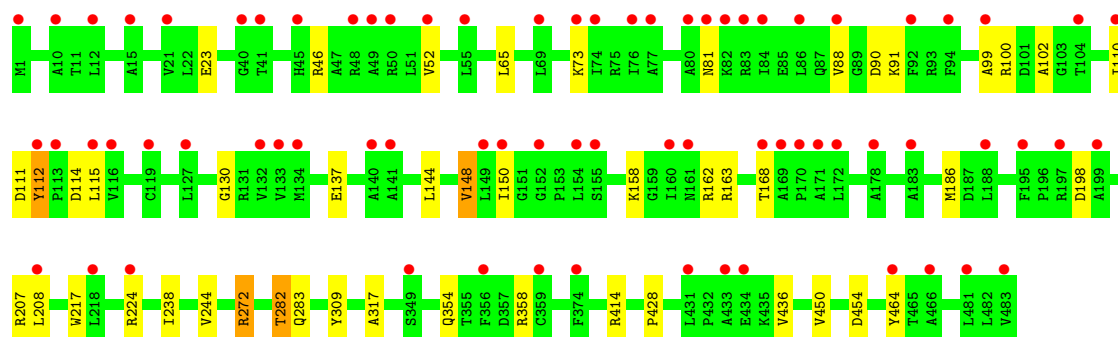
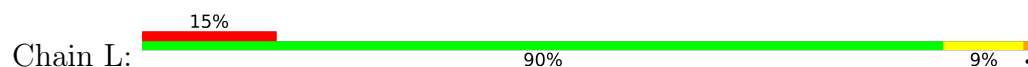
● Molecule 1: Pyruvate kinase



● 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) 98.9 (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	14500 reflections (4.95%)	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)	0.32 , 39.0	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: MG, GOL, G6P, MLI

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	0.87	3/3716 (0.1%)	0.86	7/5025 (0.1%)
1	B	0.91	1/3716 (0.0%)	0.87	4/5025 (0.1%)
1	C	0.86	4/3716 (0.1%)	0.88	4/5025 (0.1%)
1	D	0.82	1/3716 (0.0%)	0.84	4/5025 (0.1%)
1	E	0.86	2/3734 (0.1%)	0.87	8/5049 (0.2%)
1	F	0.90	3/3716 (0.1%)	0.92	12/5025 (0.2%)
1	G	0.86	4/3716 (0.1%)	0.94	11/5025 (0.2%)
1	H	0.90	5/3716 (0.1%)	0.92	9/5025 (0.2%)
1	I	0.90	4/3716 (0.1%)	0.94	12/5025 (0.2%)
1	J	0.90	5/3103 (0.2%)	1.03	13/4196 (0.3%)
1	K	0.85	1/3707 (0.0%)	0.89	6/5011 (0.1%)
1	L	0.91	5/3716 (0.1%)	1.02	13/5025 (0.3%)
All	All	0.88	38/43988 (0.1%)	0.91	103/59481 (0.2%)

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

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	72	PRO	C-O	-13.03	1.10	1.23
1	J	157	HIS	N-CA	-12.42	1.22	1.46
1	H	102	ALA	C-O	-8.47	1.14	1.24
1	F	171	ALA	C-O	-8.08	1.13	1.24
1	A	295	THR	CA-CB	8.05	1.66	1.53
1	J	76	ILE	C-O	-7.91	1.14	1.24
1	J	358	ARG	CA-C	-7.44	1.43	1.52
1	G	170	PRO	CA-C	7.34	1.62	1.52
1	L	111	ASP	C-O	-6.99	1.14	1.23
1	I	408	HIS	ND1-CE1	6.97	1.39	1.32
1	G	72	PRO	C-O	-6.51	1.15	1.24
1	L	272	ARG	CZ-NH2	-6.50	1.25	1.33
1	I	82	LYS	C-O	-6.38	1.16	1.24
1	E	72	PRO	C-O	-5.95	1.19	1.24
1	L	163	ARG	C-O	-5.94	1.16	1.24
1	H	101	ASP	CA-CB	-5.93	1.43	1.53
1	J	76	ILE	C-N	5.92	1.41	1.33
1	J	357	ASP	C-N	-5.85	1.25	1.33
1	E	245	MET	C-O	-5.67	1.17	1.24
1	K	72	PRO	C-O	-5.62	1.16	1.24
1	B	170	PRO	C-O	-5.53	1.17	1.23
1	L	354	GLN	CD-OE1	5.53	1.34	1.23
1	I	162	ARG	CZ-NH2	-5.49	1.26	1.33
1	A	72	PRO	CA-CB	-5.45	1.49	1.53
1	C	166	GLY	C-O	-5.41	1.16	1.24
1	C	167	LEU	C-O	-5.33	1.17	1.23
1	G	164	GLY	CA-C	5.26	1.58	1.52
1	H	166	GLY	C-O	-5.16	1.17	1.24
1	G	172	LEU	CA-C	-5.11	1.46	1.52
1	L	168	THR	C-O	-5.11	1.17	1.23
1	F	467	GLN	CD-OE1	5.09	1.33	1.23
1	H	98	HIS	C-O	5.09	1.30	1.23
1	C	72	PRO	CA-C	5.07	1.57	1.53
1	I	1	MET	N-CA	5.07	1.55	1.46
1	H	111	ASP	C-N	-5.06	1.29	1.33
1	A	170	PRO	C-O	-5.04	1.18	1.23
1	D	73	LYS	C-O	-5.04	1.18	1.24
1	C	223	GLU	C-O	-5.04	1.17	1.24

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	76	ILE	O-C-N	-23.71	92.93	122.57
1	G	171	ALA	N-CA-C	20.74	138.30	111.75
1	L	112	TYR	CA-C-N	-15.93	104.26	120.03
1	L	112	TYR	C-N-CA	-15.93	104.26	120.03
1	L	272	ARG	NE-CZ-NH2	13.96	131.77	119.20
1	I	81	ASN	N-CA-C	-13.16	89.39	110.32
1	F	53	ARG	NE-CZ-NH2	11.42	129.48	119.20
1	J	159	GLY	CA-C-O	-11.27	111.27	121.64
1	J	76	ILE	CA-C-N	10.54	140.67	121.70
1	J	76	ILE	C-N-CA	10.54	140.67	121.70
1	I	408	HIS	CB-CG-CD2	-9.94	118.28	131.20
1	B	82	LYS	N-CA-C	9.54	124.31	112.87
1	B	81	ASN	N-CA-C	-9.47	93.08	108.52
1	A	82	LYS	N-CA-C	9.15	124.23	112.34
1	I	408	HIS	CB-CG-ND1	9.08	136.32	122.70
1	A	81	ASN	N-CA-C	-9.07	94.46	109.07
1	F	54	GLU	CA-CB-CG	8.95	132.00	114.10
1	I	93	ARG	NE-CZ-NH2	8.71	127.04	119.20
1	L	272	ARG	NE-CZ-NH1	-8.53	112.97	121.50
1	G	172	LEU	N-CA-C	-8.28	95.14	108.55
1	E	414	ARG	NE-CZ-NH2	8.25	126.63	119.20
1	F	53	ARG	CB-CG-CD	8.07	129.86	111.30
1	I	81	ASN	CB-CA-C	8.02	123.22	109.51
1	J	157	HIS	N-CA-C	7.98	133.35	111.00
1	E	81	ASN	N-CA-C	-7.61	96.83	109.24
1	J	254	GLU	OE1-CD-OE2	-7.43	105.07	122.90
1	D	93	ARG	NE-CZ-NH2	7.21	125.69	119.20
1	G	17	ASN	CB-CG-ND2	-7.21	105.59	116.40
1	K	145	ARG	NE-CZ-NH1	-7.17	114.33	121.50
1	L	272	ARG	CD-NE-CZ	7.05	134.28	124.40
1	I	358	ARG	NE-CZ-NH2	6.97	125.47	119.20
1	G	172	LEU	CA-C-O	-6.96	112.22	120.43
1	C	273	ARG	NE-CZ-NH1	-6.93	114.56	121.50
1	H	102	ALA	CA-C-N	6.87	130.18	122.15
1	H	102	ALA	C-N-CA	6.87	130.18	122.15
1	I	93	ARG	NE-CZ-NH1	-6.86	114.64	121.50
1	F	170	PRO	N-CA-C	6.78	126.45	112.47
1	H	82	LYS	N-CA-C	6.76	118.65	111.28
1	J	414	ARG	CG-CD-NE	6.71	126.77	112.00
1	H	96	THR	OG1-CB-CG2	-6.64	96.03	109.30
1	E	414	ARG	CG-CD-NE	-6.58	97.52	112.00
1	J	76	ILE	N-CA-C	-6.57	95.69	109.34
1	H	162	ARG	CB-CG-CD	6.56	126.38	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	172	LEU	N-CA-CB	-6.55	98.75	109.56
1	L	158	LYS	CD-CE-NZ	-6.53	91.02	111.90
1	I	163	ARG	NE-CZ-NH2	6.50	125.05	119.20
1	K	273	ARG	NE-CZ-NH1	-6.45	115.05	121.50
1	G	172	LEU	N-CA-CB	6.37	122.26	110.99
1	G	81	ASN	N-CA-C	-6.34	102.35	110.53
1	E	72	PRO	O-C-N	-6.31	118.25	122.73
1	L	224	ARG	NH1-CZ-NH2	6.30	127.50	119.30
1	D	93	ARG	NE-CZ-NH1	-6.29	115.20	121.50
1	F	81	ASN	N-CA-C	-6.27	99.49	109.59
1	C	131	ARG	CB-CG-CD	6.24	125.65	111.30
1	D	414	ARG	CG-CD-NE	-6.16	98.45	112.00
1	L	207	ARG	CA-CB-CG	6.15	126.41	114.10
1	G	17	ASN	CB-CG-OD1	6.13	133.06	120.80
1	H	81	ASN	N-CA-C	-5.99	102.46	110.55
1	K	100	ARG	O-C-N	-5.95	114.25	122.46
1	E	82	LYS	N-CA-C	5.92	119.33	111.75
1	C	317	ALA	N-CA-C	-5.91	105.16	112.90
1	H	100	ARG	CB-CG-CD	5.89	124.85	111.30
1	A	295	THR	N-CA-CB	-5.88	101.50	110.45
1	A	254	GLU	CA-CB-CG	-5.85	102.39	114.10
1	L	317	ALA	N-CA-C	-5.84	105.25	112.90
1	G	171	ALA	CB-CA-C	-5.83	99.15	110.46
1	E	414	ARG	NE-CZ-NH1	-5.79	115.71	121.50
1	K	207	ARG	CA-CB-CG	5.79	125.68	114.10
1	H	317	ALA	N-CA-C	-5.75	105.37	112.90
1	K	81	ASN	N-CA-C	-5.73	102.00	110.48
1	C	172	LEU	CB-CG-CD2	5.71	127.83	110.70
1	L	198	ASP	CB-CG-OD1	5.70	131.52	118.40
1	E	239	ARG	NE-CZ-NH2	5.68	124.32	119.20
1	D	147	ARG	NH1-CZ-NH2	-5.66	111.94	119.30
1	I	157	HIS	N-CA-C	5.66	119.48	112.47
1	G	131	ARG	CB-CG-CD	5.61	124.21	111.30
1	J	414	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	I	100	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	I	81	ASN	CA-C-O	-5.51	114.75	121.36
1	L	100	ARG	NE-CZ-NH2	5.46	124.11	119.20
1	F	100	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	E	96	THR	OG1-CB-CG2	5.35	120.01	109.30
1	A	358	ARG	CD-NE-CZ	5.34	131.88	124.40
1	G	378	LYS	CD-CE-NZ	5.26	128.74	111.90
1	J	166	GLY	O-C-N	-5.26	116.94	122.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	175	LYS	CB-CG-CD	5.26	123.39	111.30
1	A	293	MET	CG-SD-CE	5.20	112.34	100.90
1	L	224	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	B	114	ASP	N-CA-C	5.18	119.09	112.87
1	F	53	ARG	CD-NE-CZ	5.18	131.66	124.40
1	K	80	ALA	N-CA-C	-5.16	105.55	111.07
1	F	172	LEU	N-CA-C	5.14	117.55	110.35
1	J	54	GLU	CA-CB-CG	5.14	124.38	114.10
1	G	131	ARG	CA-CB-CG	-5.11	103.87	114.10
1	B	198	ASP	CB-CG-OD1	5.08	130.07	118.40
1	H	104	THR	OG1-CB-CG2	-5.04	99.23	109.30
1	J	273	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	A	1	MET	CB-CG-SD	5.03	127.79	112.70
1	I	162	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	L	81	ASN	N-CA-C	-5.01	104.06	110.53
1	J	163	ARG	CB-CG-CD	5.01	122.83	111.30
1	F	171	ALA	CA-C-N	5.00	128.76	121.31
1	F	171	ALA	C-N-CA	5.00	128.76	121.31

There are no chirality outliers.

All (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
1	C	114	ASP	Mainchain
1	D	147	ARG	Sidechain
1	E	102	ALA	Mainchain
1	G	163	ARG	Mainchain
1	G	170	PRO	Peptide
1	H	103	GLY	Mainchain
1	J	159	GLY	Mainchain
1	J	76	ILE	Mainchain
1	K	100	ARG	Mainchain
1	L	23	GLU	Sidechain
1	L	358	ARG	Sidechain

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	3662	0	3726	30	0
1	B	3662	0	3726	17	0
1	C	3662	0	3726	23	0
1	D	3662	0	3726	15	0
1	E	3680	0	3738	23	0
1	F	3662	0	3726	30	0
1	G	3662	0	3726	18	0
1	H	3662	0	3726	21	0
1	I	3662	0	3726	26	0
1	J	3057	0	3123	24	0
1	K	3654	0	3721	15	0
1	L	3662	0	3726	22	0
2	A	16	0	11	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
5	D	6	0	8	0	0
5	E	6	0	8	0	0
6	A	238	0	0	11	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	249	0

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

All (249) 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:K:182:LEU:HG	1:K:186:MET:HE2	1.46	0.94
1:J:73:LYS:HG3	6:J:643:HOH:O	1.67	0.93
1:E:226:GLU:HG2	6:E:858:HOH:O	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ARG:NH1	6:A:601:HOH:O	2.05	0.89
1:E:466:ALA:HB1	6:E:747:HOH:O	1.77	0.85
1:D:163:ARG:HG3	6:D:659:HOH:O	1.82	0.79
1:D:446:LYS:NZ	6:D:601:HOH:O	1.73	0.76
1:F:359:CYS:SG	1:J:475:VAL:HG23	2.25	0.76
1:A:263:ILE:HD12	6:A:636:HOH:O	1.86	0.75
1:D:215:LYS:HE2	6:D:784:HOH:O	1.86	0.75
1:B:207:ARG:HD2	6:B:774:HOH:O	1.87	0.74
1:H:327:GLU:HG3	6:H:744:HOH:O	1.89	0.71
1:A:1:MET:HE2	6:A:754:HOH:O	1.91	0.71
1:D:296:ARG:HG2	1:J:283:GLN:HE21	1.57	0.70
1:C:73:LYS:HE2	6:C:647:HOH:O	1.92	0.69
1:B:414:ARG:NH1	6:B:601:HOH:O	2.25	0.69
1:H:207:ARG:HD3	6:H:719:HOH:O	1.91	0.68
1:A:97:SER:HB3	6:A:689:HOH:O	1.94	0.67
1:E:131:ARG:HG3	6:E:659:HOH:O	1.94	0.67
1:L:91:LYS:HE3	1:L:137:GLU:OE1	1.95	0.67
1:E:293:MET:HE3	1:H:150:ILE:HG21	1.77	0.66
1:I:41:THR:HG23	1:I:44:GLU:H	1.60	0.66
1:H:41:THR:HG23	1:H:44:GLU:H	1.61	0.66
1:F:128:ASP:O	1:F:131:ARG:HG2	1.95	0.65
1:E:1:MET:HA	6:E:623:HOH:O	1.96	0.64
1:A:3:VAL:HG13	6:A:766:HOH:O	1.96	0.64
1:E:197:ARG:NH1	6:E:602:HOH:O	2.23	0.64
1:J:48:ARG:HD2	6:J:606:HOH:O	1.96	0.64
1:H:52:VAL:CG2	1:H:65:LEU:HD21	2.29	0.63
1:I:83:ARG:O	1:I:84:ILE:HD13	1.99	0.63
1:H:41:THR:HG22	1:H:44:GLU:OE1	2.00	0.61
1:E:195:PHE:O	1:E:224:ARG:NH1	2.32	0.60
1:L:52:VAL:HG21	1:L:65:LEU:HD21	1.83	0.60
1:I:84:ILE:HG22	1:I:85:GLU:N	2.16	0.60
1:F:168:THR:HG21	1:F:224:ARG:NH2	2.16	0.59
1:I:52:VAL:CG2	1:I:65:LEU:HD21	2.33	0.59
1:E:52:VAL:CG2	1:E:65:LEU:HD21	2.33	0.59
1:F:386:SER:CB	1:F:467:GLN:HE21	2.14	0.59
1:K:79:PHE:HB2	1:K:81:ASN:O	2.03	0.58
1:L:52:VAL:CG2	1:L:65:LEU:HD21	2.32	0.58
1:C:172:LEU:N	1:C:172:LEU:HD12	2.19	0.58
1:I:293:MET:SD	1:L:130:GLY:O	2.61	0.58
1:A:295:THR:HG22	1:A:297:ALA:H	1.67	0.58
1:C:223:GLU:HG2	1:C:247:ALA:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:375:PRO:HB3	6:F:710:HOH:O	2.04	0.58
1:I:135:VAL:HG12	1:I:149:LEU:CD1	2.34	0.58
1:A:22:LEU:O	1:A:26:ILE:HG12	2.04	0.57
1:F:128:ASP:O	1:F:131:ARG:CG	2.52	0.57
1:A:334:ARG:NH1	1:G:257:ASP:OD1	2.38	0.56
1:F:467:GLN:HG2	1:F:468:GLY:N	2.20	0.56
1:I:135:VAL:HG12	1:I:149:LEU:HD11	1.86	0.56
1:F:215:LYS:HD3	6:F:729:HOH:O	2.05	0.56
1:K:247:ALA:HB1	4:K:503:MLI:H11	1.88	0.56
1:C:385:GLU:HG2	6:C:748:HOH:O	2.04	0.56
1:I:79:PHE:CD2	1:I:84:ILE:HG12	2.41	0.56
1:I:293:MET:CE	1:L:150:ILE:HG21	2.35	0.56
1:C:110:ILE:CD1	1:C:115:LEU:HD23	2.36	0.56
1:G:167:LEU:O	1:G:168:THR:HG23	2.05	0.56
1:I:197:ARG:HG2	1:I:224:ARG:CD	2.36	0.56
1:K:79:PHE:CB	1:K:81:ASN:O	2.53	0.56
1:A:474:LYS:NZ	6:A:602:HOH:O	2.17	0.56
1:B:131:ARG:HA	1:F:293:MET:HE1	1.89	0.55
1:A:1:MET:CE	6:A:754:HOH:O	2.52	0.55
1:D:24:GLN:HG2	6:D:839:HOH:O	2.07	0.54
1:F:363:ILE:HD11	1:J:475:VAL:HG22	1.88	0.54
1:E:20[B]:GLU:HG2	6:E:603:HOH:O	2.06	0.54
1:C:110:ILE:HD12	1:C:115:LEU:HD23	1.90	0.54
1:C:163:ARG:HG3	6:C:687:HOH:O	2.08	0.54
1:H:223:GLU:HG3	1:H:247:ALA:HB3	1.89	0.54
1:I:52:VAL:HG21	1:I:65:LEU:HD21	1.89	0.54
1:C:239:ARG:HD3	6:C:805:HOH:O	2.08	0.54
1:A:1:MET:HE3	1:A:337:GLN:HB3	1.89	0.53
1:B:169:ALA:CB	6:B:824:HOH:O	2.56	0.53
1:F:168:THR:HG21	1:F:224:ARG:HH22	1.72	0.53
1:F:461:GLY:N	2:F:501:G6P:H2	2.24	0.53
1:J:195:PHE:HE2	6:J:683:HOH:O	1.91	0.53
1:J:414:ARG:NH1	6:J:601:HOH:O	2.41	0.53
1:E:20[B]:GLU:CG	6:E:603:HOH:O	2.56	0.53
1:G:207:ARG:HD3	6:G:648:HOH:O	2.07	0.53
1:F:359:CYS:SG	1:J:475:VAL:CG2	2.97	0.53
1:G:194:SER:C	1:G:196:PRO:HD3	2.33	0.53
1:A:207:ARG:HG2	6:A:646:HOH:O	2.09	0.52
1:F:197:ARG:HD3	1:F:224:ARG:NH2	2.23	0.52
1:B:97:SER:HB3	6:B:739:HOH:O	2.10	0.52
1:E:197:ARG:HG2	1:E:224:ARG:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:358:ARG:HB3	6:J:666:HOH:O	2.10	0.52
1:F:482:LEU:CD1	1:F:482:LEU:N	2.73	0.52
1:G:131:ARG:NH2	1:G:286:GLU:OE2	2.41	0.52
1:L:272:ARG:HD2	6:L:603:HOH:O	2.10	0.52
1:F:461:GLY:H	2:F:501:G6P:H2	1.76	0.51
1:A:263:ILE:CD1	6:A:791:HOH:O	1.87	0.51
1:E:52:VAL:HG21	1:E:65:LEU:HD21	1.91	0.51
1:F:197:ARG:HD3	1:F:224:ARG:CZ	2.40	0.51
1:B:172:LEU:HD23	1:B:208:LEU:HD12	1.94	0.50
1:B:450:VAL:CG2	1:B:454:ASP:HB2	2.40	0.50
1:G:414:ARG:NH1	6:G:603:HOH:O	2.45	0.50
1:J:1:MET:HE3	1:J:337:GLN:CB	2.42	0.50
1:K:1:MET:HE3	1:K:337:GLN:HB3	1.93	0.50
1:I:330:LYS:HE2	6:I:689:HOH:O	2.11	0.50
1:K:128:ASP:OD2	1:K:158:LYS:HE3	2.12	0.50
1:I:450:VAL:CG2	1:I:454:ASP:HB2	2.42	0.49
1:D:190:TYR:CZ	1:D:417:MET:HE2	2.46	0.49
1:J:73:LYS:CG	6:J:643:HOH:O	2.39	0.49
1:C:46:ARG:HA	1:C:186:MET:HE3	1.94	0.49
1:C:171:ALA:C	1:C:172:LEU:HD12	2.38	0.49
1:B:46:ARG:HA	1:B:186:MET:HE3	1.95	0.49
1:D:257:ASP:HB3	6:D:796:HOH:O	2.13	0.49
1:I:84:ILE:CG2	1:I:85:GLU:N	2.75	0.49
1:I:385:GLU:HG2	6:I:681:HOH:O	2.10	0.49
1:L:450:VAL:CG2	1:L:454:ASP:HB2	2.43	0.49
1:F:197:ARG:HG2	1:F:224:ARG:HD3	1.95	0.49
1:A:46:ARG:HA	1:A:186:MET:HE3	1.95	0.49
1:F:482:LEU:N	1:F:482:LEU:HD12	2.28	0.49
1:I:46:ARG:HA	1:I:186:MET:HE3	1.95	0.48
1:F:131:ARG:HH21	1:F:131:ARG:HG3	1.79	0.48
1:D:467:GLN:HG2	1:D:468:GLY:N	2.27	0.48
1:E:46:ARG:HA	1:E:186:MET:HE3	1.94	0.48
1:G:167:LEU:O	1:G:168:THR:CG2	2.62	0.48
1:H:450:VAL:CG2	1:H:454:ASP:HB2	2.44	0.47
1:E:450:VAL:CG2	1:E:454:ASP:HB2	2.45	0.47
1:J:1:MET:HE3	1:J:337:GLN:HB3	1.95	0.47
1:D:182:LEU:HG	1:D:186:MET:HE2	1.96	0.47
1:H:217:TRP:CE2	1:H:414:ARG:HD3	2.50	0.47
1:I:414:ARG:NH1	6:I:603:HOH:O	2.46	0.47
1:J:46:ARG:HA	1:J:186:MET:HE3	1.96	0.47
1:A:238:ILE:HG12	1:A:244:VAL:HG11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:ARG:HA	1:F:186:MET:HE3	1.96	0.47
1:J:77:ALA:HA	1:J:157:HIS:CE1	2.50	0.47
1:L:238:ILE:HG12	1:L:244:VAL:HG11	1.97	0.47
1:H:46:ARG:HA	1:H:186:MET:HE3	1.96	0.47
1:H:282:THR:HG22	1:H:283:GLN:HG3	1.97	0.47
1:J:73:LYS:HG2	6:J:683:HOH:O	2.15	0.47
1:D:238:ILE:HG12	1:D:244:VAL:HG11	1.97	0.47
1:F:217:TRP:CE2	1:F:414:ARG:HD3	2.50	0.47
1:L:162:ARG:NH1	6:L:601:HOH:O	2.48	0.47
1:B:238:ILE:HG12	1:B:244:VAL:HG11	1.97	0.46
1:G:46:ARG:HA	1:G:186:MET:HE3	1.96	0.46
1:G:195:PHE:N	1:G:196:PRO:HD3	2.30	0.46
1:C:223:GLU:HG2	1:C:247:ALA:CB	2.46	0.46
1:L:282:THR:HG22	1:L:283:GLN:HG3	1.98	0.46
1:I:217:TRP:CE2	1:I:414:ARG:HD3	2.50	0.46
1:H:483:VAL:HG23	1:H:483:VAL:O	2.15	0.46
1:K:217:TRP:CE2	1:K:414:ARG:HD3	2.50	0.46
1:I:197:ARG:HG2	1:I:224:ARG:HD3	1.97	0.46
1:I:238:ILE:HG12	1:I:244:VAL:HG11	1.98	0.46
1:A:217:TRP:CE2	1:A:414:ARG:HD3	2.50	0.46
1:C:238:ILE:HG12	1:C:244:VAL:HG11	1.97	0.46
1:F:238:ILE:HG12	1:F:244:VAL:HG11	1.97	0.46
1:G:217:TRP:CE2	1:G:414:ARG:HD3	2.50	0.46
1:E:238:ILE:HG12	1:E:244:VAL:HG11	1.98	0.46
1:J:238:ILE:HG12	1:J:244:VAL:HG11	1.98	0.46
1:L:46:ARG:HA	1:L:186:MET:HE3	1.97	0.46
1:L:114:ASP:O	1:L:115:LEU:C	2.59	0.46
1:D:282:THR:HG22	1:D:283:GLN:HG3	1.98	0.45
1:A:282:THR:HG22	1:A:283:GLN:HG3	1.98	0.45
1:D:83:ARG:NH1	6:D:602:HOH:O	2.41	0.45
1:H:238:ILE:HG12	1:H:244:VAL:HG11	1.97	0.45
1:K:238:ILE:HG12	1:K:244:VAL:HG11	1.98	0.45
1:B:282:THR:HG22	1:B:283:GLN:HG3	1.98	0.45
1:E:247:ALA:HB1	4:E:504:MLI:H11	1.97	0.45
1:H:52:VAL:HG21	1:H:65:LEU:HD21	1.99	0.45
1:J:282:THR:HG22	1:J:283:GLN:HG3	1.98	0.45
1:E:293:MET:CE	1:H:150:ILE:HD13	2.47	0.45
1:D:91:LYS:HD2	6:D:720:HOH:O	2.15	0.45
1:F:223:GLU:HG2	1:F:247:ALA:HB3	1.99	0.44
1:G:238:ILE:HG12	1:G:244:VAL:HG11	1.98	0.44
1:I:282:THR:HG22	1:I:283:GLN:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLU:HG2	1:A:247:ALA:HB3	1.98	0.44
1:C:128:ASP:O	1:C:131:ARG:HD3	2.18	0.44
1:C:282:THR:HG22	1:C:283:GLN:HG3	1.98	0.44
1:D:74:ILE:CD1	1:D:167:LEU:HB3	2.47	0.44
1:F:282:THR:HG22	1:F:283:GLN:HG3	1.98	0.44
1:C:83:ARG:HD2	6:C:820:HOH:O	2.17	0.44
1:C:293:MET:HE3	1:K:150:ILE:HD13	1.99	0.44
1:I:158:LYS:HD3	1:I:158:LYS:HA	1.76	0.44
1:E:282:THR:HG22	1:E:283:GLN:HG3	2.00	0.44
1:J:422:GLU:HG2	6:J:708:HOH:O	2.17	0.44
1:A:259:GLU:O	1:A:263:ILE:CD1	2.66	0.44
1:A:384:THR:OG1	2:A:501:G6P:O2P	2.34	0.44
1:B:217:TRP:CE2	1:B:414:ARG:HD3	2.52	0.44
1:A:223:GLU:CG	1:A:247:ALA:HB3	2.48	0.43
1:K:282:THR:HG22	1:K:283:GLN:HG3	1.99	0.43
1:B:195:PHE:N	1:B:223:GLU:OE2	2.50	0.43
1:C:358:ARG:HD3	1:C:361:GLU:CD	2.43	0.43
1:H:43:ASP:HB2	6:H:642:HOH:O	2.16	0.43
1:C:217:TRP:CE2	1:C:414:ARG:HD3	2.53	0.43
1:E:259:GLU:O	1:E:263:ILE:HD13	2.18	0.43
1:J:412:GLN:NE2	1:J:425:PRO:HB3	2.33	0.43
1:B:349:SER:O	1:B:352:LEU:HD13	2.18	0.43
1:G:162:ARG:HB2	1:G:167:LEU:HD13	2.00	0.43
1:I:135:VAL:CG1	1:I:149:LEU:HD11	2.47	0.43
1:L:52:VAL:HG21	1:L:65:LEU:CD2	2.48	0.43
1:I:293:MET:HE3	1:L:150:ILE:HG21	2.00	0.43
1:C:207:ARG:HD2	6:C:660:HOH:O	2.17	0.43
1:L:88:VAL:HA	1:L:148:VAL:HG22	2.00	0.43
1:L:217:TRP:CE2	1:L:414:ARG:HD3	2.54	0.43
1:J:75:ARG:C	1:J:76:ILE:O	2.55	0.42
1:J:189:ASP:OD1	1:J:413:ALA:HB3	2.19	0.42
1:F:483:VAL:HG21	1:J:462:ASP:HB3	2.00	0.42
1:A:467:GLN:HA	2:A:501:G6P:H62	2.01	0.42
1:A:259:GLU:O	1:A:263:ILE:HD13	2.19	0.42
1:B:169:ALA:HB2	6:B:824:HOH:O	2.19	0.42
1:L:436:VAL:HG21	1:L:464:TYR:HE2	1.84	0.42
1:G:467:GLN:HG3	1:G:468:GLY:N	2.34	0.42
1:F:350:HIS:HD2	6:F:635:HOH:O	2.02	0.42
1:L:99:ALA:HB3	1:L:102:ALA:HB3	2.01	0.42
1:A:172:LEU:CD2	1:A:208:LEU:HD12	2.49	0.41
6:G:678:HOH:O	1:H:483:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:PHE:C	1:G:81:ASN:O	2.63	0.41
1:L:428:PRO:HB2	1:L:464:TYR:CD2	2.56	0.41
1:E:83:ARG:NH1	1:E:85:GLU:HG3	2.35	0.41
1:I:467:GLN:HG2	1:I:468:GLY:N	2.35	0.41
1:K:128:ASP:OD2	1:K:131:ARG:HD2	2.20	0.41
1:E:244:VAL:HG23	1:E:278:VAL:HG23	2.02	0.41
1:H:244:VAL:HG23	1:H:278:VAL:HG23	2.03	0.41
1:K:374:PHE:HB3	1:K:377:ILE:HD12	2.02	0.41
1:G:282:THR:HG22	1:G:283:GLN:HG3	2.02	0.41
1:A:283:GLN:OE1	1:G:296:ARG:HG2	2.21	0.41
1:J:244:VAL:HG23	1:J:278:VAL:HG23	2.03	0.41
1:L:110:ILE:HD12	1:L:112:TYR:HB3	2.03	0.41
1:B:157:HIS:HE1	6:B:854:HOH:O	2.04	0.41
1:B:244:VAL:HG23	1:B:278:VAL:HG23	2.03	0.41
1:F:53:ARG:NH1	1:F:186:MET:O	2.54	0.41
1:F:83:ARG:HG3	1:F:154:LEU:O	2.21	0.41
1:L:90:ASP:O	1:L:148:VAL:HG13	2.20	0.41
1:A:352:LEU:HD22	1:E:352:LEU:HD22	2.02	0.41
1:C:293:MET:HE2	1:C:293:MET:HB3	2.03	0.41
1:A:244:VAL:HG23	1:A:278:VAL:HG23	2.03	0.40
1:H:432:PRO:HG2	1:H:435:LYS:HD3	2.03	0.40
1:J:195:PHE:HB3	1:J:224:ARG:HE	1.86	0.40
1:A:334:ARG:HG2	6:A:754:HOH:O	2.21	0.40
1:C:239:ARG:NH1	1:C:274:ASN:OD1	2.54	0.40
1:C:358:ARG:HD3	1:C:361:GLU:OE2	2.22	0.40
1:G:195:PHE:N	1:G:196:PRO:CD	2.85	0.40
1:K:81:ASN:ND2	6:K:602:HOH:O	2.55	0.40
1:K:244:VAL:HG23	1:K:278:VAL:HG23	2.04	0.40
1:F:480:ASP:O	1:F:482:LEU:HD13	2.21	0.40
1:G:91:LYS:HE2	6:G:613:HOH:O	2.22	0.40
1:K:195:PHE:N	1:K:223:GLU:OE2	2.51	0.40
1:L:115:LEU:HD11	1:L:144:LEU:HD12	2.02	0.40
1:A:292:PRO:HB3	1:A:324:TYR:CE2	2.56	0.40
1:D:244:VAL:HG23	1:D:278:VAL:HG23	2.03	0.40
1:H:195:PHE:HB3	1:H:224:ARG:HE	1.86	0.40
1:H:311:ASP:HA	1:H:419:ARG:HB2	2.04	0.40
1:I:84:ILE:CG2	1:I:85:GLU:H	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	481/483 (100%)	469 (98%)	11 (2%)	1 (0%)	43	53
1	B	481/483 (100%)	469 (98%)	11 (2%)	1 (0%)	43	53
1	C	481/483 (100%)	467 (97%)	13 (3%)	1 (0%)	43	53
1	D	481/483 (100%)	465 (97%)	15 (3%)	1 (0%)	43	53
1	E	483/483 (100%)	468 (97%)	14 (3%)	1 (0%)	43	53
1	F	481/483 (100%)	464 (96%)	15 (3%)	2 (0%)	30	36
1	G	481/483 (100%)	466 (97%)	14 (3%)	1 (0%)	43	53
1	H	481/483 (100%)	467 (97%)	13 (3%)	1 (0%)	43	53
1	I	481/483 (100%)	465 (97%)	15 (3%)	1 (0%)	43	53
1	J	400/483 (83%)	389 (97%)	10 (2%)	1 (0%)	36	44
1	K	478/483 (99%)	461 (96%)	16 (3%)	1 (0%)	43	53
1	L	481/483 (100%)	468 (97%)	12 (2%)	1 (0%)	43	53
All	All	5690/5796 (98%)	5518 (97%)	159 (3%)	13 (0%)	43	53

All (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
1	F	282	THR
1	G	282	THR
1	H	282	THR
1	I	282	THR
1	K	282	THR
1	L	282	THR
1	J	282	THR

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Mol	Chain	Res	Type
1	F	170	PRO

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%)	382 (99%)	4 (1%)	68	77
1	B	386/386 (100%)	383 (99%)	3 (1%)	73	81
1	C	386/386 (100%)	384 (100%)	2 (0%)	81	87
1	D	386/386 (100%)	383 (99%)	3 (1%)	73	81
1	E	388/386 (100%)	384 (99%)	4 (1%)	68	77
1	F	386/386 (100%)	381 (99%)	5 (1%)	61	72
1	G	386/386 (100%)	384 (100%)	2 (0%)	81	87
1	H	386/386 (100%)	384 (100%)	2 (0%)	81	87
1	I	386/386 (100%)	381 (99%)	5 (1%)	61	72
1	J	320/386 (83%)	315 (98%)	5 (2%)	55	68
1	K	385/386 (100%)	380 (99%)	5 (1%)	61	72
1	L	386/386 (100%)	382 (99%)	4 (1%)	68	77
All	All	4567/4632 (99%)	4523 (99%)	44 (1%)	68	77

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	82	LYS
1	A	309	TYR
1	A	456	VAL
1	B	309	TYR
1	B	452	LYS
1	B	467	GLN
1	C	187	ASP
1	C	309	TYR

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Mol	Chain	Res	Type
1	D	1	MET
1	D	85	GLU
1	D	309	TYR
1	E	96	THR
1	E	239	ARG
1	E	309	TYR
1	E	467	GLN
1	F	53	ARG
1	F	78	LYS
1	F	93	ARG
1	F	309	TYR
1	F	456	VAL
1	G	309	TYR
1	G	467	GLN
1	H	309	TYR
1	H	467	GLN
1	I	74	ILE
1	I	127	LEU
1	I	223	GLU
1	I	309	TYR
1	I	467	GLN
1	J	1	MET
1	J	224	ARG
1	J	263	ILE
1	J	273	ARG
1	J	309	TYR
1	K	83	ARG
1	K	168	THR
1	K	223	GLU
1	K	309	TYR
1	K	456	VAL
1	L	73	LYS
1	L	148	VAL
1	L	208	LEU
1	L	309	TYR

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	24	GLN
1	A	70	GLN
1	A	81	ASN

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Mol	Chain	Res	Type
1	B	24	GLN
1	B	157	HIS
1	B	438	GLN
1	C	438	GLN
1	D	24	GLN
1	D	274	ASN
1	D	438	GLN
1	E	438	GLN
1	E	467	GLN
1	F	39	HIS
1	F	467	GLN
1	G	24	GLN
1	I	24	GLN
1	I	438	GLN
1	J	157	HIS
1	J	283	GLN
1	J	438	GLN
1	K	438	GLN
1	K	467	GLN
1	L	45	HIS
1	L	438	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
2	G6P	K	501	-	16,16,16	0.90	1 (6%)	23,24,24	1.68	5 (21%)
2	G6P	A	501	-	16,16,16	0.84	0	23,24,24	2.65	12 (52%)
4	MLI	E	504	3	6,6,6	1.00	0	7,7,7	1.56	2 (28%)
2	G6P	E	501	-	16,16,16	1.02	1 (6%)	23,24,24	1.97	8 (34%)
2	G6P	D	501	-	16,16,16	1.05	2 (12%)	23,24,24	2.08	6 (26%)
4	MLI	B	504	3	6,6,6	1.31	0	7,7,7	1.50	1 (14%)
2	G6P	B	501	-	16,16,16	1.10	1 (6%)	23,24,24	2.23	9 (39%)
4	MLI	A	503	3	6,6,6	1.39	1 (16%)	7,7,7	1.20	1 (14%)
4	MLI	K	503	3	6,6,6	1.05	0	7,7,7	1.69	2 (28%)
5	GOL	D	503	-	5,5,5	0.51	0	5,5,5	0.93	0
4	MLI	H	503	3	6,6,6	1.47	0	7,7,7	0.74	0
2	G6P	L	501	-	16,16,16	0.73	0	23,24,24	1.82	9 (39%)
5	GOL	E	503	-	5,5,5	0.33	0	5,5,5	0.69	0
4	MLI	D	504	3	6,6,6	1.15	0	7,7,7	2.58	3 (42%)
4	MLI	I	503	3	6,6,6	1.35	0	7,7,7	1.35	0
2	G6P	G	501	-	16,16,16	0.78	0	23,24,24	1.62	5 (21%)
4	MLI	C	503	3	6,6,6	1.06	0	7,7,7	2.05	3 (42%)
5	GOL	B	503	-	5,5,5	0.47	0	5,5,5	0.55	0
4	MLI	F	503	3	6,6,6	1.10	0	7,7,7	1.78	2 (28%)
4	MLI	L	503	3	6,6,6	1.20	0	7,7,7	1.69	1 (14%)
2	G6P	H	501	-	16,16,16	0.66	0	23,24,24	1.53	5 (21%)
2	G6P	J	501	-	16,16,16	0.93	0	23,24,24	1.50	4 (17%)
4	MLI	J	503	3	6,6,6	1.62	1 (16%)	7,7,7	0.94	0
2	G6P	I	501	-	16,16,16	0.85	1 (6%)	23,24,24	1.76	6 (26%)
2	G6P	F	501	-	16,16,16	0.52	0	23,24,24	1.70	6 (26%)
4	MLI	G	503	3	6,6,6	1.06	0	7,7,7	2.35	4 (57%)
2	G6P	C	501	-	16,16,16	0.74	0	23,24,24	1.77	9 (39%)

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	G6P	K	501	-	-	1/6/26/26	0/1/1/1
2	G6P	A	501	-	-	5/6/26/26	0/1/1/1
4	MLI	E	504	3	-	2/4/4/4	-
2	G6P	E	501	-	-	1/6/26/26	0/1/1/1
2	G6P	D	501	-	-	3/6/26/26	0/1/1/1
4	MLI	B	504	3	-	2/4/4/4	-
2	G6P	B	501	-	-	4/6/26/26	0/1/1/1
4	MLI	A	503	3	-	3/4/4/4	-
4	MLI	K	503	3	-	2/4/4/4	-
5	GOL	D	503	-	-	4/4/4/4	-
4	MLI	H	503	3	-	4/4/4/4	-
2	G6P	L	501	-	-	2/6/26/26	0/1/1/1
5	GOL	E	503	-	-	2/4/4/4	-
4	MLI	D	504	3	-	4/4/4/4	-
4	MLI	I	503	3	-	2/4/4/4	-
2	G6P	G	501	-	-	2/6/26/26	0/1/1/1
4	MLI	C	503	3	-	3/4/4/4	-
5	GOL	B	503	-	-	2/4/4/4	-
4	MLI	F	503	3	-	2/4/4/4	-
4	MLI	L	503	3	-	2/4/4/4	-
2	G6P	H	501	-	-	2/6/26/26	0/1/1/1
2	G6P	J	501	-	-	5/6/26/26	0/1/1/1
4	MLI	J	503	3	-	4/4/4/4	-
2	G6P	I	501	-	-	5/6/26/26	0/1/1/1
2	G6P	F	501	-	-	5/6/26/26	0/1/1/1
4	MLI	G	503	3	-	2/4/4/4	-
2	G6P	C	501	-	-	3/6/26/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	G6P	O1-C1	2.64	1.47	1.39
2	B	501	G6P	C1-C2	-2.42	1.46	1.52
2	D	501	G6P	O1-C1	2.42	1.47	1.39
4	A	503	MLI	O7-C2	-2.32	1.23	1.30
4	J	503	MLI	C1-C2	2.19	1.54	1.51
2	I	501	G6P	O1-C1	2.10	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	501	G6P	O1-C1	2.05	1.46	1.39
2	D	501	G6P	O4-C4	2.04	1.48	1.43

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	G6P	O2P-P-O6	-7.09	88.18	106.67
2	D	501	G6P	O5-C1-C2	-6.24	99.33	110.30
2	B	501	G6P	O5-C1-C2	-5.76	100.17	110.30
2	F	501	G6P	C4-C3-C2	-4.98	102.09	110.83
2	E	501	G6P	C1-O5-C5	4.94	123.21	113.65
4	D	504	MLI	O6-C2-C1	-4.34	109.73	122.11
2	A	501	G6P	O3-C3-C2	-4.05	100.83	110.38
2	B	501	G6P	O2P-P-O6	-3.68	97.08	106.67
2	E	501	G6P	C4-C3-C2	-3.56	104.57	110.83
2	B	501	G6P	C1-O5-C5	3.52	120.46	113.65
2	A	501	G6P	C1-C2-C3	-3.52	103.18	110.36
2	K	501	G6P	O5-C1-C2	-3.50	104.14	110.30
2	B	501	G6P	O1-C1-O5	3.42	120.56	110.41
2	A	501	G6P	O6-P-O3P	3.38	115.58	106.44
4	D	504	MLI	O8-C3-C1	-3.35	112.58	122.11
2	D	501	G6P	O1-C1-O5	3.31	120.23	110.41
4	G	503	MLI	O9-C3-C1	3.29	124.70	114.51
2	I	501	G6P	O5-C1-C2	-3.28	104.54	110.30
2	G	501	G6P	C1-C2-C3	-3.27	103.69	110.36
2	I	501	G6P	C1-C2-C3	-3.22	103.79	110.36
2	I	501	G6P	O1-C1-O5	3.20	119.91	110.41
4	G	503	MLI	O8-C3-C1	-3.20	113.01	122.11
2	E	501	G6P	O5-C5-C6	3.16	112.97	106.69
2	H	501	G6P	O1-C1-C2	-3.14	99.87	108.98
4	C	503	MLI	O8-C3-C1	-3.13	113.18	122.11
2	G	501	G6P	O5-C1-C2	-3.13	104.80	110.30
2	C	501	G6P	C1-C2-C3	-3.12	103.98	110.36
4	B	504	MLI	O6-C2-C1	-3.11	113.27	122.11
2	L	501	G6P	O5-C1-C2	-3.10	104.85	110.30
4	F	503	MLI	O6-C2-C1	-3.09	113.31	122.11
2	J	501	G6P	O5-C1-C2	-3.07	104.89	110.30
2	L	501	G6P	O5-C5-C6	-3.05	100.65	106.69
2	A	501	G6P	O2P-P-O3P	3.04	122.68	110.83
2	A	501	G6P	C3-C4-C5	-3.03	104.73	110.23
2	L	501	G6P	O1P-P-O6	-3.03	98.77	106.67
4	K	503	MLI	O8-C3-C1	-3.03	113.49	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	501	G6P	O6-P-O3P	-2.98	98.39	106.44
4	L	503	MLI	O8-C3-C1	-2.97	113.64	122.11
2	E	501	G6P	O5-C1-C2	-2.96	105.09	110.30
2	H	501	G6P	C1-C2-C3	-2.95	104.34	110.36
2	J	501	G6P	C4-C3-C2	-2.90	105.74	110.83
4	G	503	MLI	O6-C2-C1	-2.89	113.89	122.11
2	K	501	G6P	O2P-P-O3P	2.88	122.06	110.83
2	D	501	G6P	C1-O5-C5	2.82	119.10	113.65
2	A	501	G6P	O2P-P-O1P	2.80	118.31	107.80
2	K	501	G6P	O1-C1-O5	2.80	118.73	110.41
2	G	501	G6P	C3-C4-C5	2.79	115.28	110.23
4	C	503	MLI	O6-C2-C1	-2.78	114.20	122.11
2	B	501	G6P	O2P-P-O1P	2.77	118.19	107.80
2	G	501	G6P	O2P-P-O6	-2.74	99.52	106.67
2	E	501	G6P	C3-C4-C5	-2.74	105.26	110.23
2	C	501	G6P	O5-C1-C2	-2.74	105.48	110.30
2	L	501	G6P	O4-C4-C5	2.72	116.03	109.32
2	L	501	G6P	O2P-P-O1P	2.70	117.91	107.80
2	D	501	G6P	O4-C4-C5	2.68	115.93	109.32
4	D	504	MLI	O7-C2-C1	2.67	122.78	114.51
2	A	501	G6P	O4-C4-C5	2.65	115.84	109.32
2	E	501	G6P	O2P-P-O3P	2.64	121.13	110.83
2	K	501	G6P	O2P-P-O6	-2.64	99.79	106.67
4	C	503	MLI	O9-C3-O8	2.62	130.08	123.33
2	J	501	G6P	O2P-P-O6	-2.58	99.94	106.67
2	C	501	G6P	O1P-P-O3P	2.56	120.83	110.83
4	G	503	MLI	O7-C2-C1	2.55	122.41	114.51
2	F	501	G6P	O4-C4-C5	2.52	115.53	109.32
2	C	501	G6P	O2-C2-C3	2.44	116.13	110.38
2	C	501	G6P	O1-C1-C2	-2.44	101.89	108.98
2	C	501	G6P	O1P-P-O6	-2.44	100.30	106.67
2	B	501	G6P	C3-C4-C5	-2.43	105.83	110.23
2	A	501	G6P	C4-C3-C2	2.40	115.04	110.83
2	H	501	G6P	O2P-P-O3P	2.39	120.15	110.83
2	D	501	G6P	O1P-P-O6	-2.37	100.48	106.67
2	A	501	G6P	O1-C1-O5	2.37	117.45	110.41
4	E	504	MLI	O6-C2-C1	-2.36	115.39	122.11
2	D	501	G6P	C3-C4-C5	-2.36	105.95	110.23
4	K	503	MLI	O9-C3-C1	2.35	121.80	114.51
2	I	501	G6P	O2-C2-C3	2.34	115.89	110.38
2	I	501	G6P	C1-O5-C5	2.31	118.12	113.65
2	L	501	G6P	O5-C5-C4	2.29	113.83	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	504	MLI	O8-C3-C1	-2.28	115.61	122.11
2	A	501	G6P	O5-C5-C6	2.28	111.22	106.69
2	H	501	G6P	O2-C2-C3	2.27	115.73	110.38
4	A	503	MLI	O8-C3-C1	-2.27	115.64	122.11
2	C	501	G6P	O5-C5-C6	2.25	111.15	106.69
2	G	501	G6P	O2P-P-O3P	2.24	119.57	110.83
2	J	501	G6P	O5-C5-C4	2.24	113.73	109.70
2	C	501	G6P	C4-C3-C2	2.22	114.73	110.83
2	E	501	G6P	C1-C2-C3	-2.21	105.86	110.36
2	E	501	G6P	O6-P-O3P	-2.20	100.49	106.44
2	F	501	G6P	O5-C5-C4	2.19	113.65	109.70
2	F	501	G6P	C1-O5-C5	-2.19	109.42	113.65
4	F	503	MLI	O8-C3-C1	-2.18	115.89	122.11
2	C	501	G6P	O4-C4-C3	-2.18	105.23	110.38
2	H	501	G6P	O2P-P-O6	-2.18	100.98	106.67
2	F	501	G6P	C1-C2-C3	2.17	114.78	110.36
2	L	501	G6P	C1-O5-C5	2.15	117.81	113.65
2	A	501	G6P	O1-C1-C2	-2.14	102.77	108.98
2	B	501	G6P	C1-C2-C3	-2.14	106.00	110.36
2	L	501	G6P	C4-C3-C2	-2.08	107.17	110.83
2	F	501	G6P	O1P-P-O6	-2.07	101.27	106.67
2	B	501	G6P	O2-C2-C1	-2.06	104.49	109.25
2	K	501	G6P	O6-P-O3P	-2.05	100.89	106.44
2	B	501	G6P	O1P-P-O6	-2.05	101.33	106.67
2	L	501	G6P	O1P-P-O3P	2.00	118.64	110.83

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	G6P	C4-C5-C6-O6
2	A	501	G6P	O5-C5-C6-O6
2	A	501	G6P	C6-O6-P-O1P
2	A	501	G6P	C6-O6-P-O2P
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	C	501	G6P	C4-C5-C6-O6
2	C	501	G6P	O5-C5-C6-O6
2	D	501	G6P	C6-O6-P-O1P
2	D	501	G6P	C6-O6-P-O3P
2	E	501	G6P	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	F	501	G6P	C4-C5-C6-O6
2	F	501	G6P	O5-C5-C6-O6
2	F	501	G6P	C6-O6-P-O1P
2	F	501	G6P	C6-O6-P-O2P
2	F	501	G6P	C6-O6-P-O3P
2	G	501	G6P	C4-C5-C6-O6
2	G	501	G6P	O5-C5-C6-O6
2	H	501	G6P	C4-C5-C6-O6
2	H	501	G6P	O5-C5-C6-O6
2	I	501	G6P	O5-C5-C6-O6
2	I	501	G6P	C6-O6-P-O1P
2	I	501	G6P	C6-O6-P-O2P
2	I	501	G6P	C6-O6-P-O3P
2	J	501	G6P	C4-C5-C6-O6
2	J	501	G6P	O5-C5-C6-O6
2	J	501	G6P	C6-O6-P-O1P
2	J	501	G6P	C6-O6-P-O3P
2	L	501	G6P	C4-C5-C6-O6
2	L	501	G6P	O5-C5-C6-O6
5	E	503	GOL	O1-C1-C2-C3
5	B	503	GOL	C1-C2-C3-O3
5	D	503	GOL	O1-C1-C2-C3
4	A	503	MLI	C2-C1-C3-O9
5	E	503	GOL	O1-C1-C2-O2
4	C	503	MLI	C2-C1-C3-O9
4	H	503	MLI	C3-C1-C2-O7
4	I	503	MLI	C2-C1-C3-O8
4	J	503	MLI	C2-C1-C3-O9
2	B	501	G6P	O5-C5-C6-O6
4	A	503	MLI	C2-C1-C3-O8
4	B	504	MLI	C2-C1-C3-O8
4	C	503	MLI	C2-C1-C3-O8
4	H	503	MLI	C3-C1-C2-O6
4	H	503	MLI	C2-C1-C3-O8
4	J	503	MLI	C2-C1-C3-O8
5	D	503	GOL	C1-C2-C3-O3
4	H	503	MLI	C2-C1-C3-O9
4	I	503	MLI	C2-C1-C3-O9
4	B	504	MLI	C2-C1-C3-O9
4	L	503	MLI	C3-C1-C2-O7
2	C	501	G6P	C6-O6-P-O3P
4	D	504	MLI	C2-C1-C3-O8

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Mol	Chain	Res	Type	Atoms
4	E	504	MLI	C3-C1-C2-O6
4	K	503	MLI	C3-C1-C2-O6
4	L	503	MLI	C3-C1-C2-O6
4	D	504	MLI	C2-C1-C3-O9
4	J	503	MLI	C3-C1-C2-O7
4	J	503	MLI	C3-C1-C2-O6
4	K	503	MLI	C3-C1-C2-O7
2	I	501	G6P	C4-C5-C6-O6
2	K	501	G6P	C4-C5-C6-O6
5	B	503	GOL	O2-C2-C3-O3
5	D	503	GOL	O1-C1-C2-O2
4	E	504	MLI	C3-C1-C2-O7
4	D	504	MLI	C3-C1-C2-O7
4	F	503	MLI	C2-C1-C3-O8
4	G	503	MLI	C3-C1-C2-O7
2	A	501	G6P	C6-O6-P-O3P
2	D	501	G6P	C6-O6-P-O2P
2	J	501	G6P	C6-O6-P-O2P
4	D	504	MLI	C3-C1-C2-O6
4	F	503	MLI	C2-C1-C3-O9
4	G	503	MLI	C3-C1-C2-O6
4	C	503	MLI	C3-C1-C2-O7
4	A	503	MLI	C3-C1-C2-O6
5	D	503	GOL	O2-C2-C3-O3

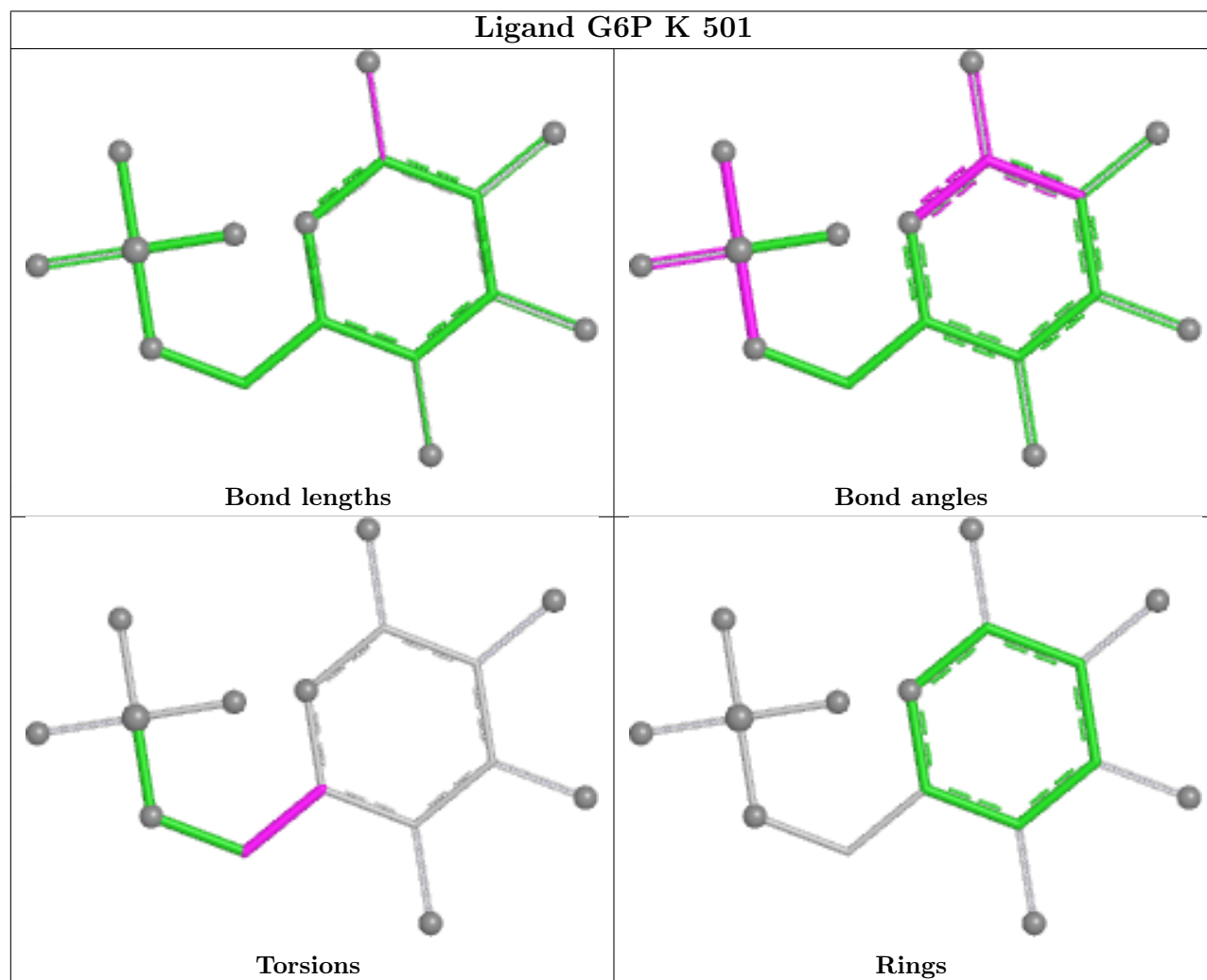
There are no ring outliers.

4 monomers are involved in 6 short contacts:

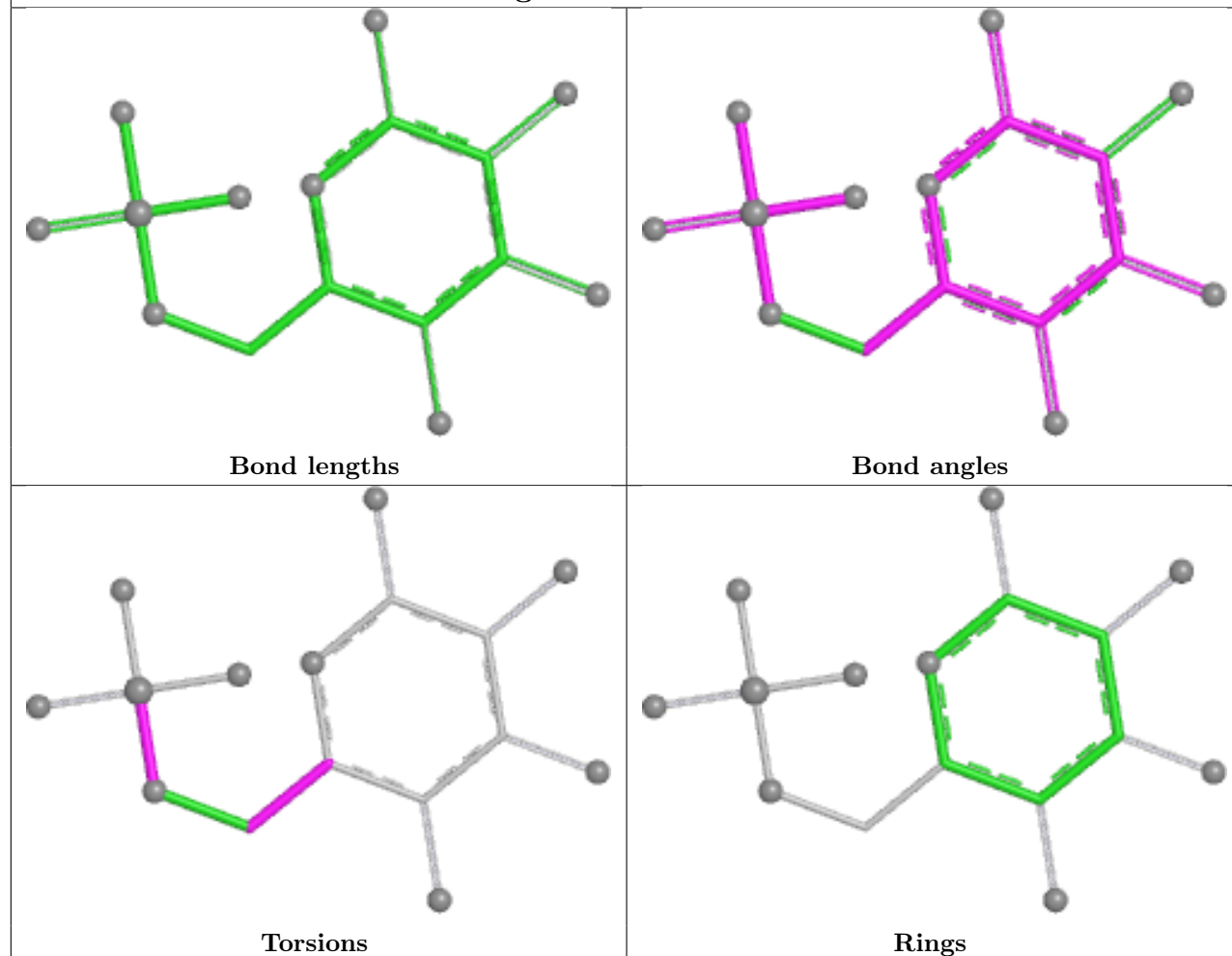
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	G6P	2	0
4	E	504	MLI	1	0
4	K	503	MLI	1	0
2	F	501	G6P	2	0

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

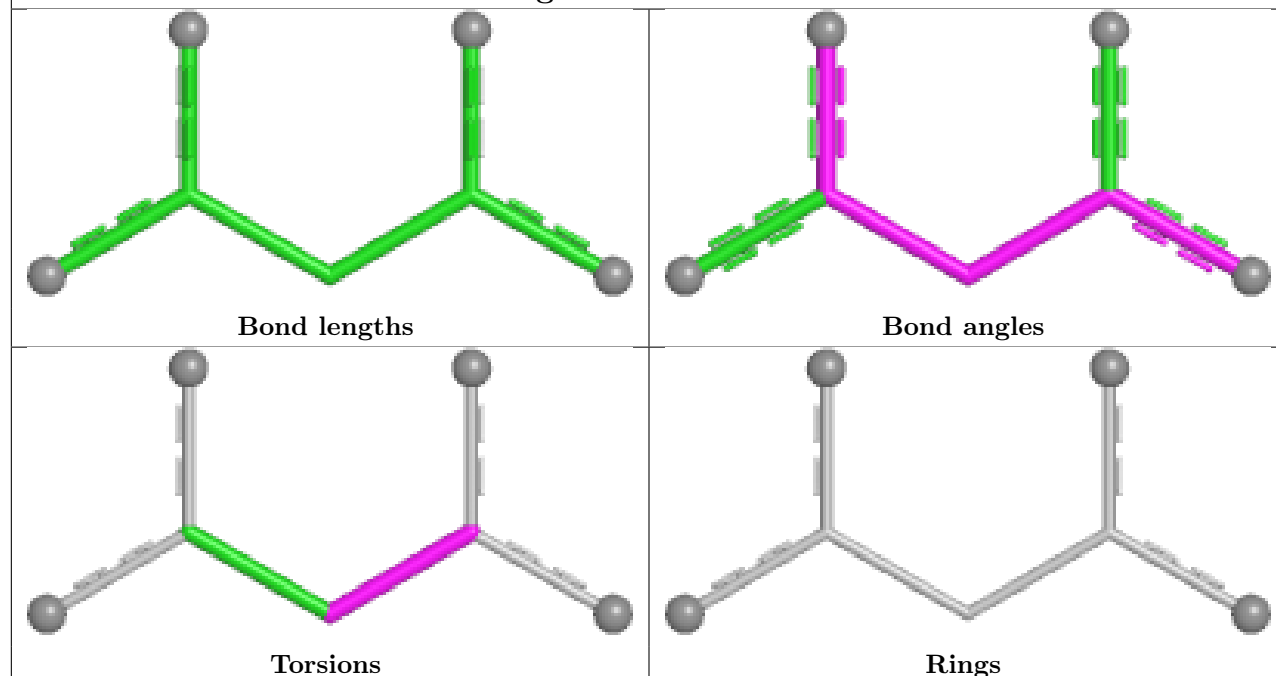
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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



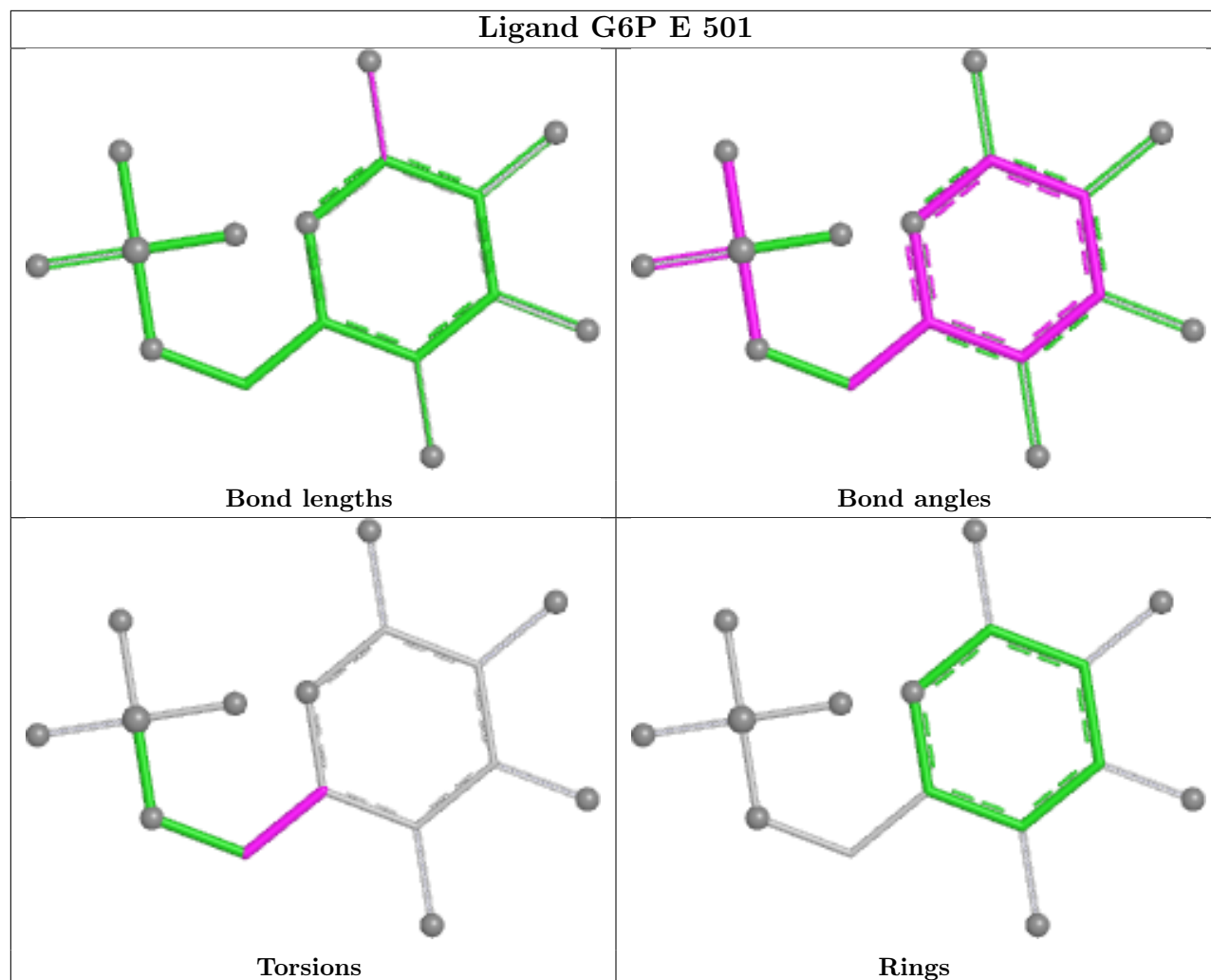
Ligand G6P A 501



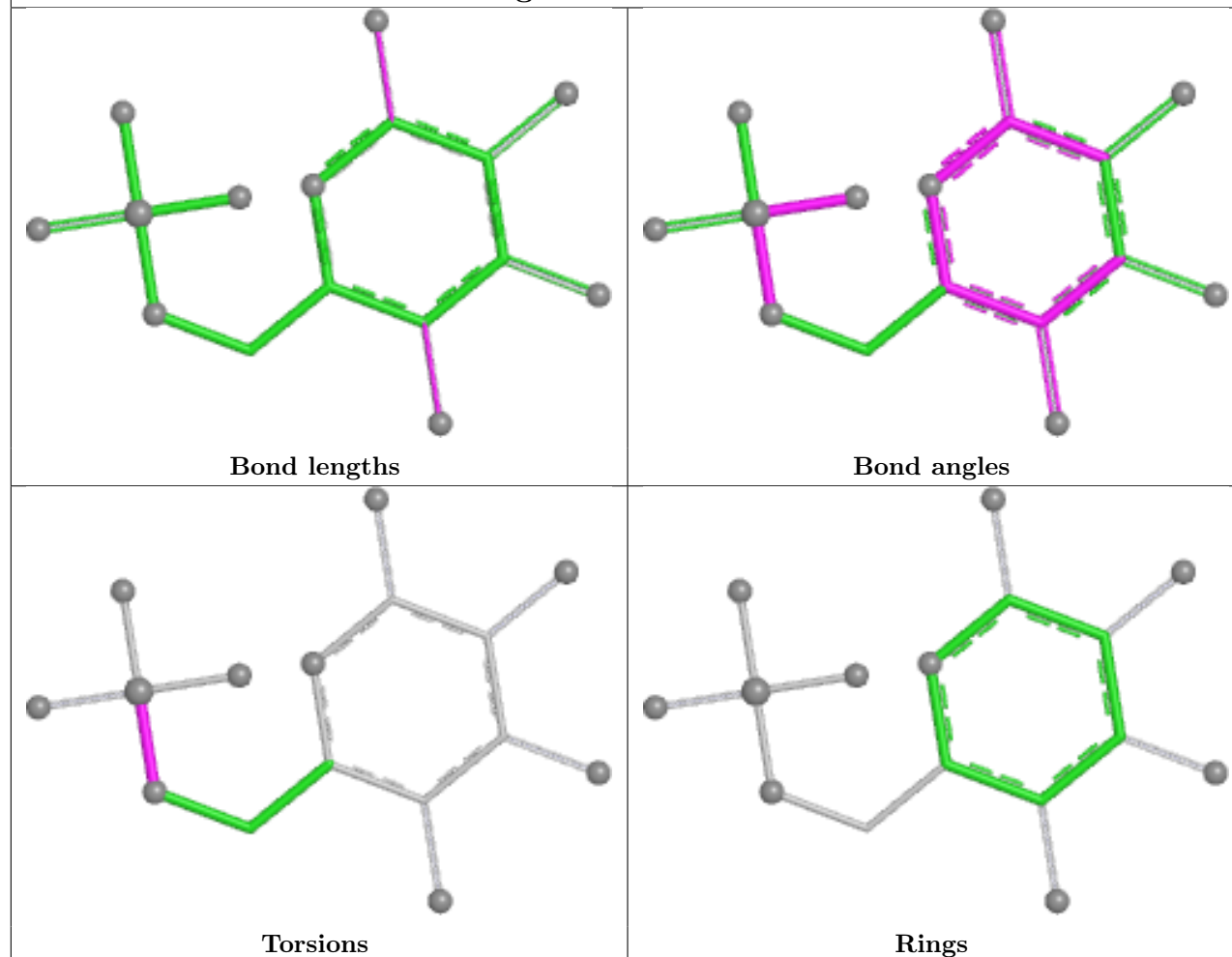
Ligand MLI E 504



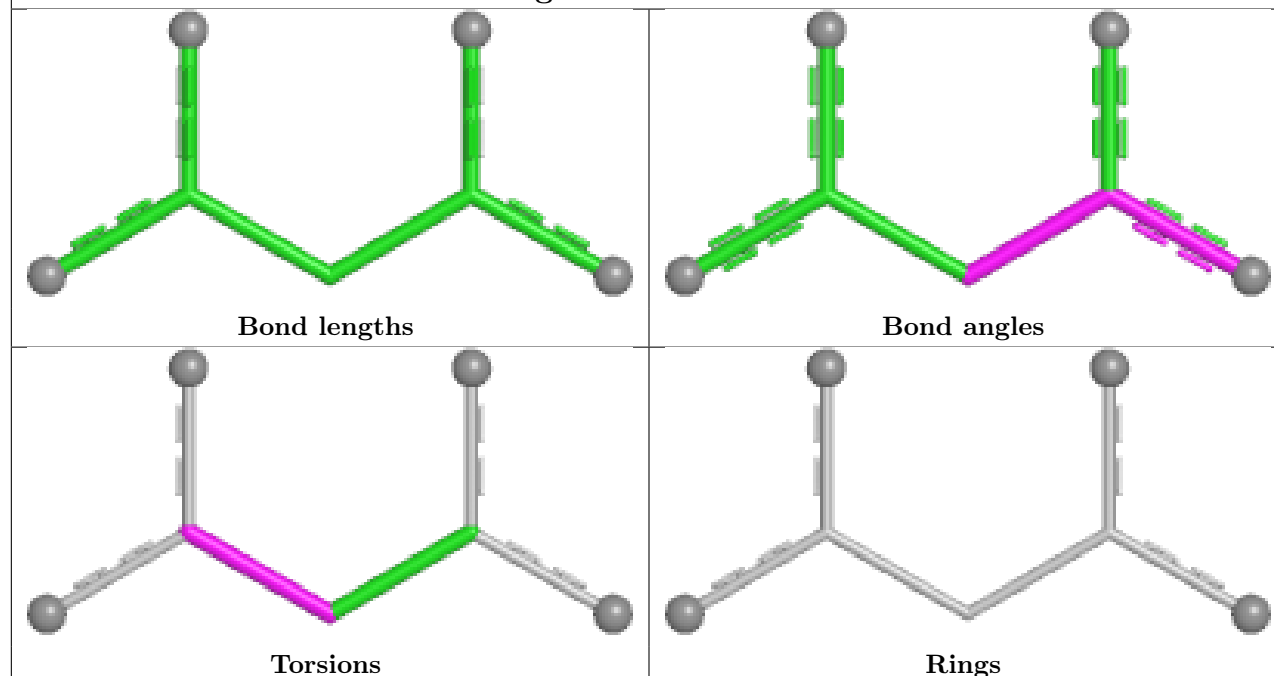
Ligand G6P E 501



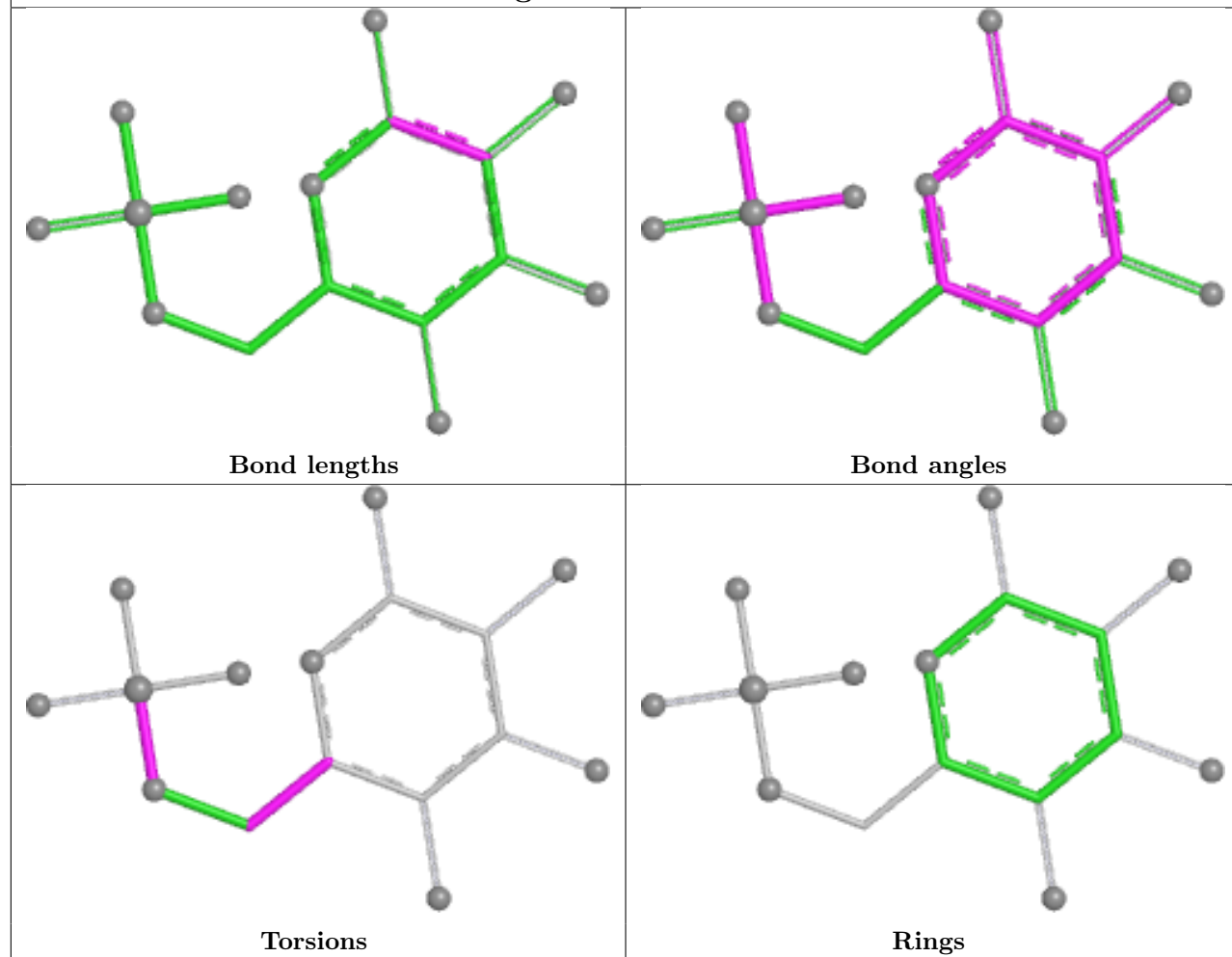
Ligand G6P D 501



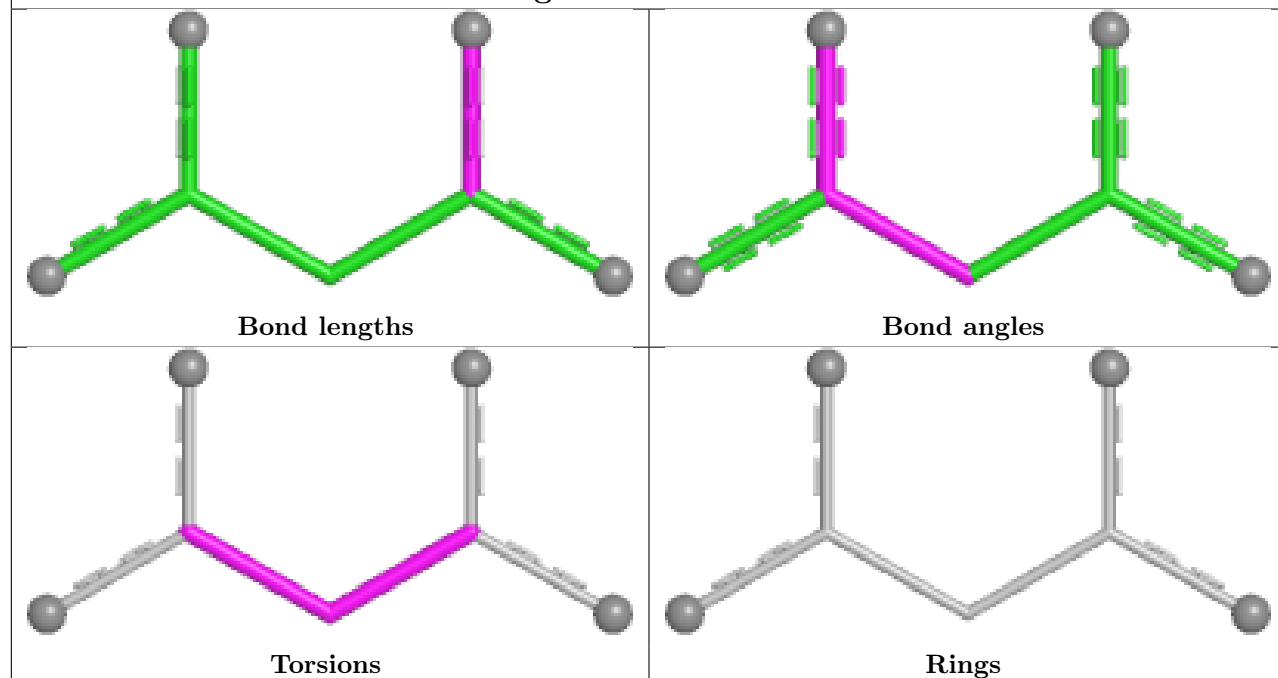
Ligand MLI B 504

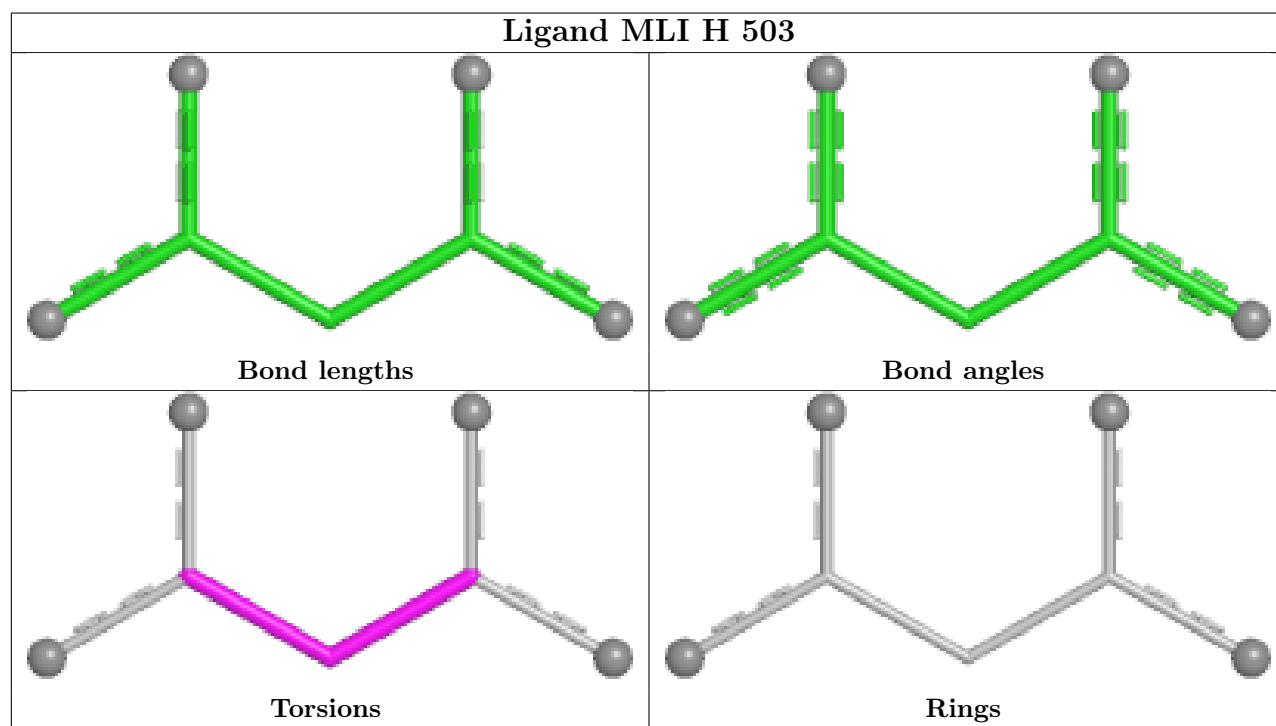
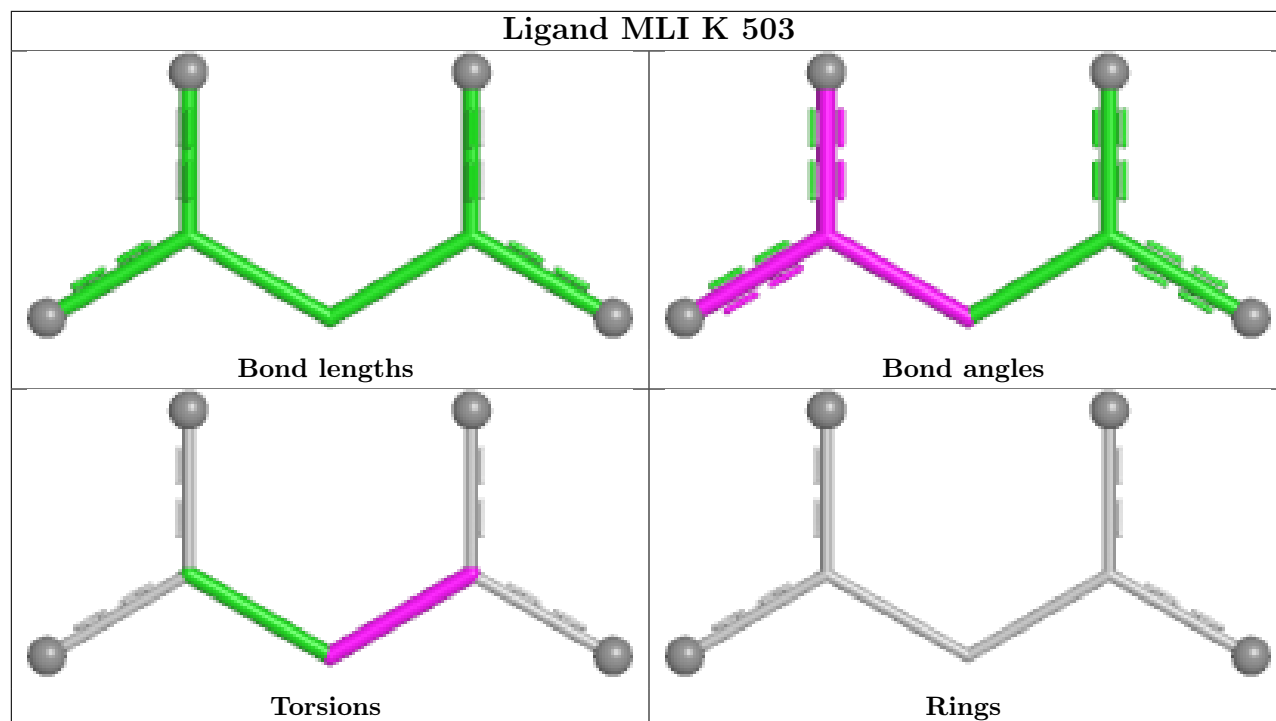


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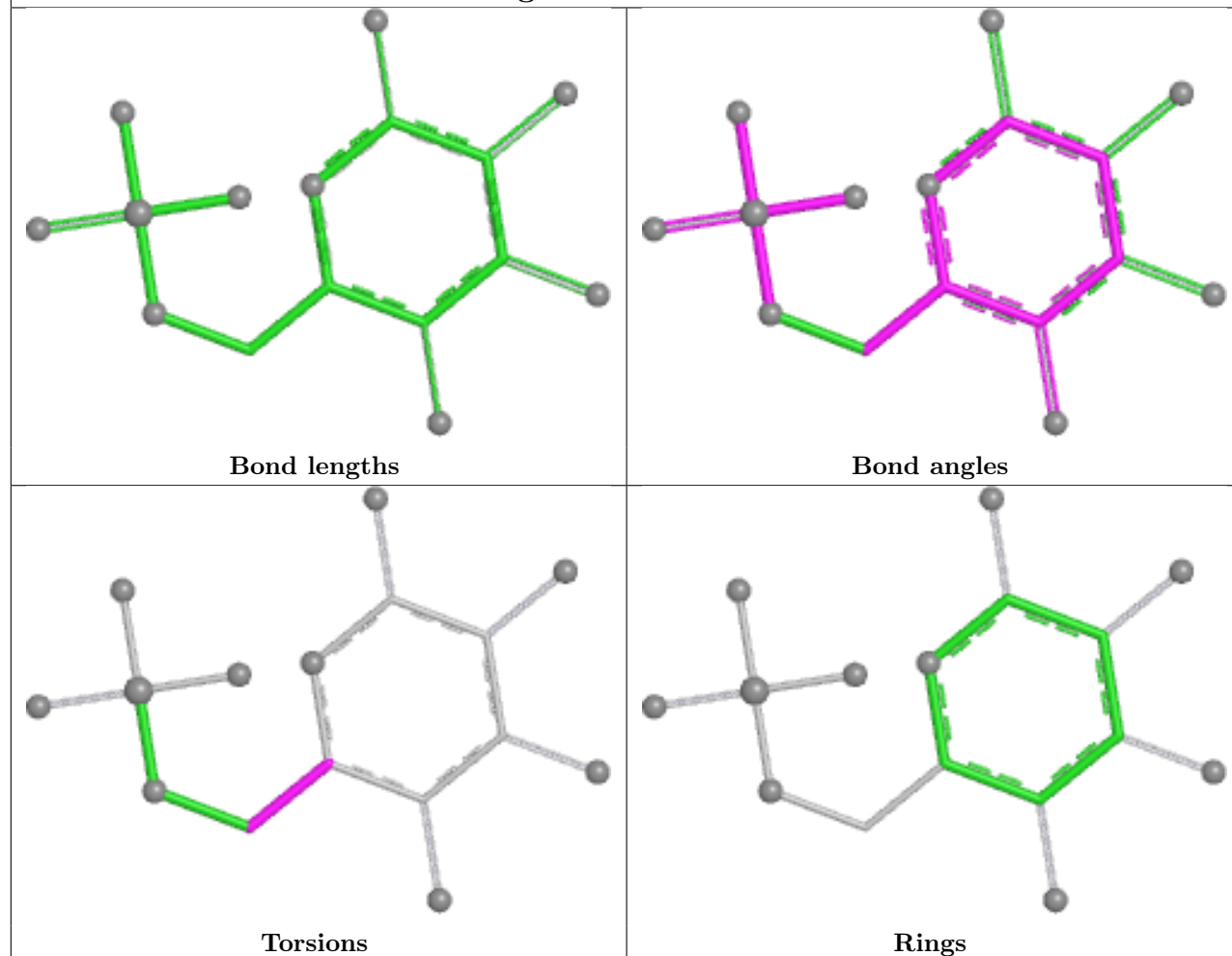


Ligand MLI A 503

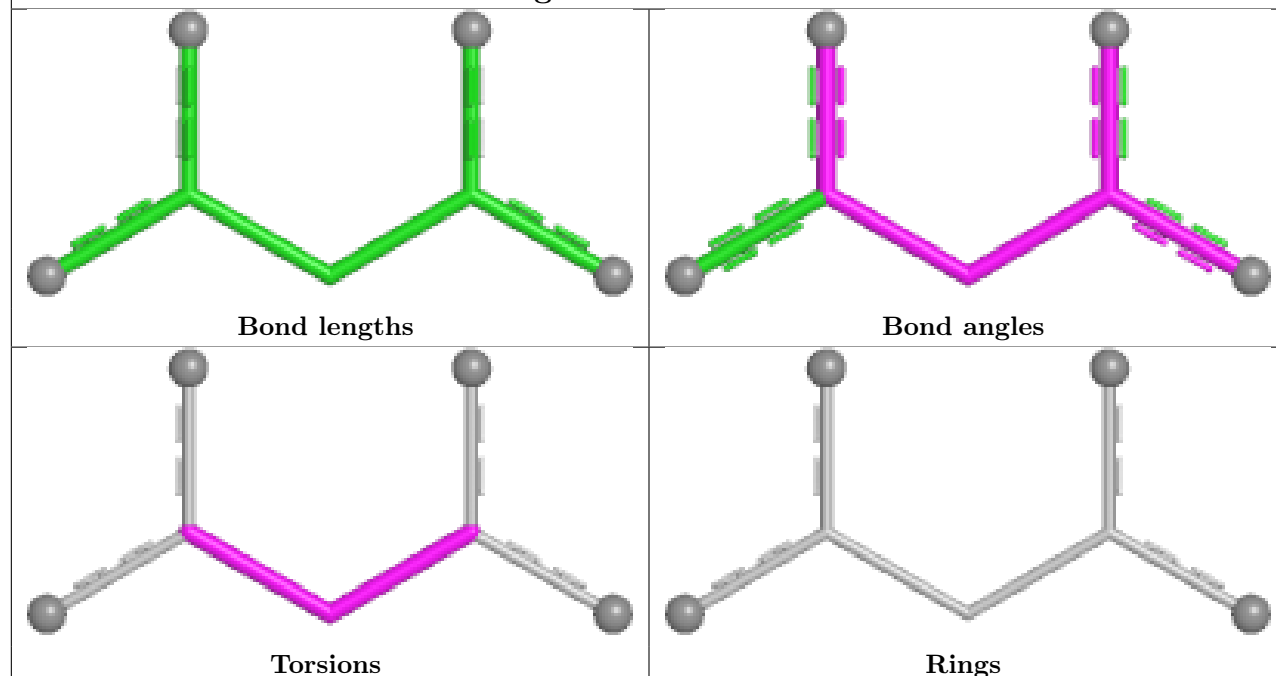




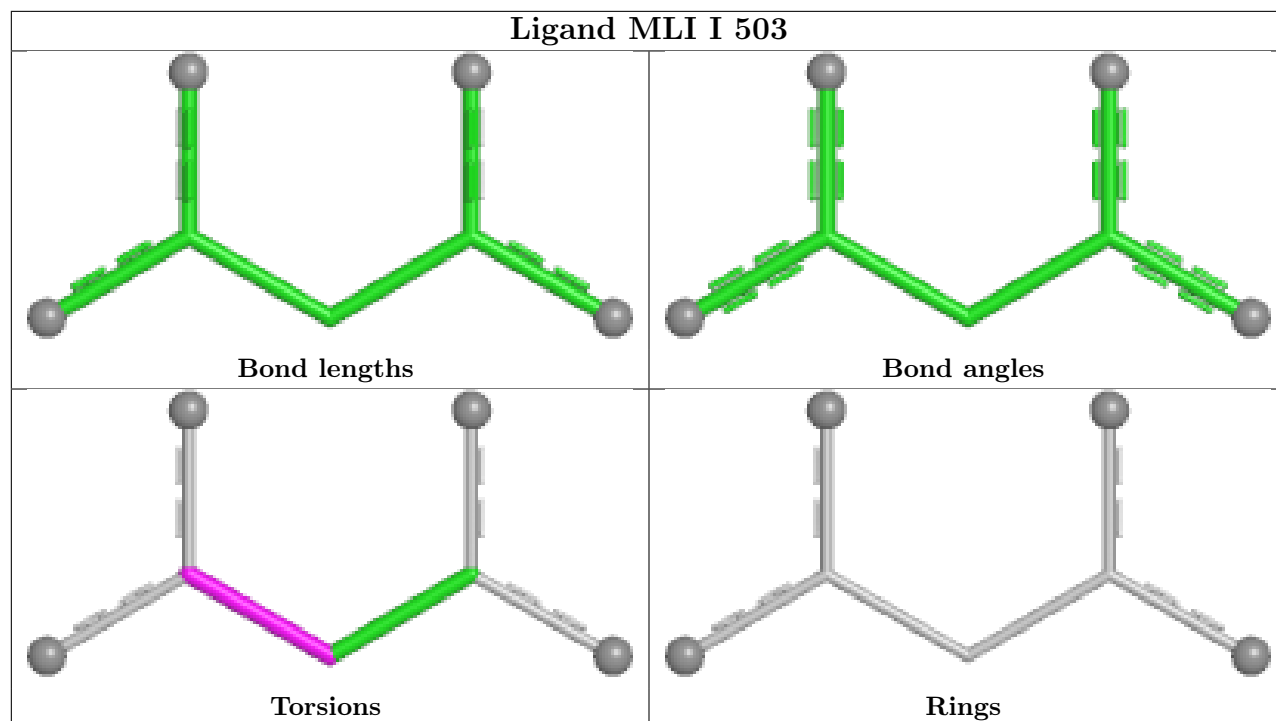
Ligand G6P L 501



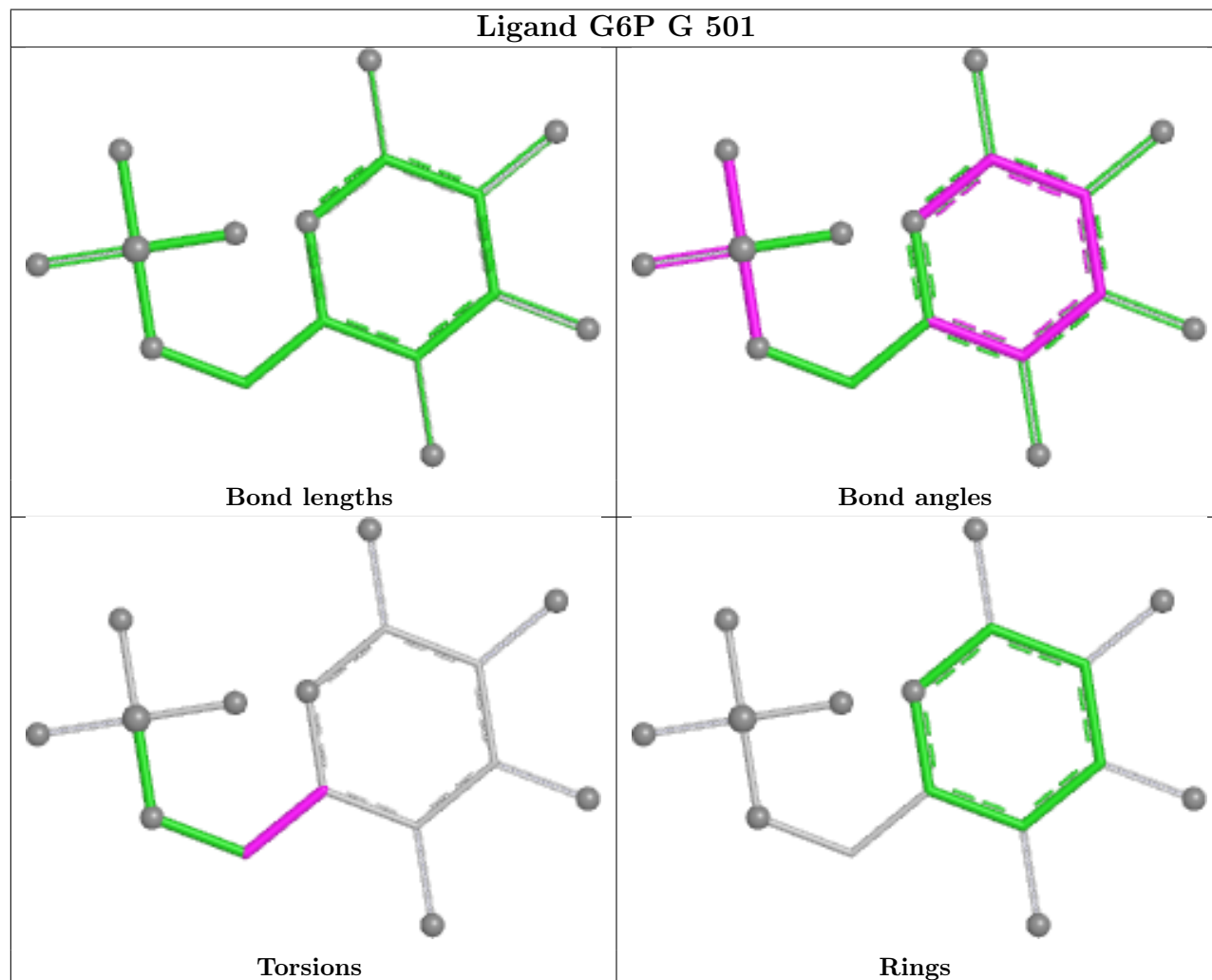
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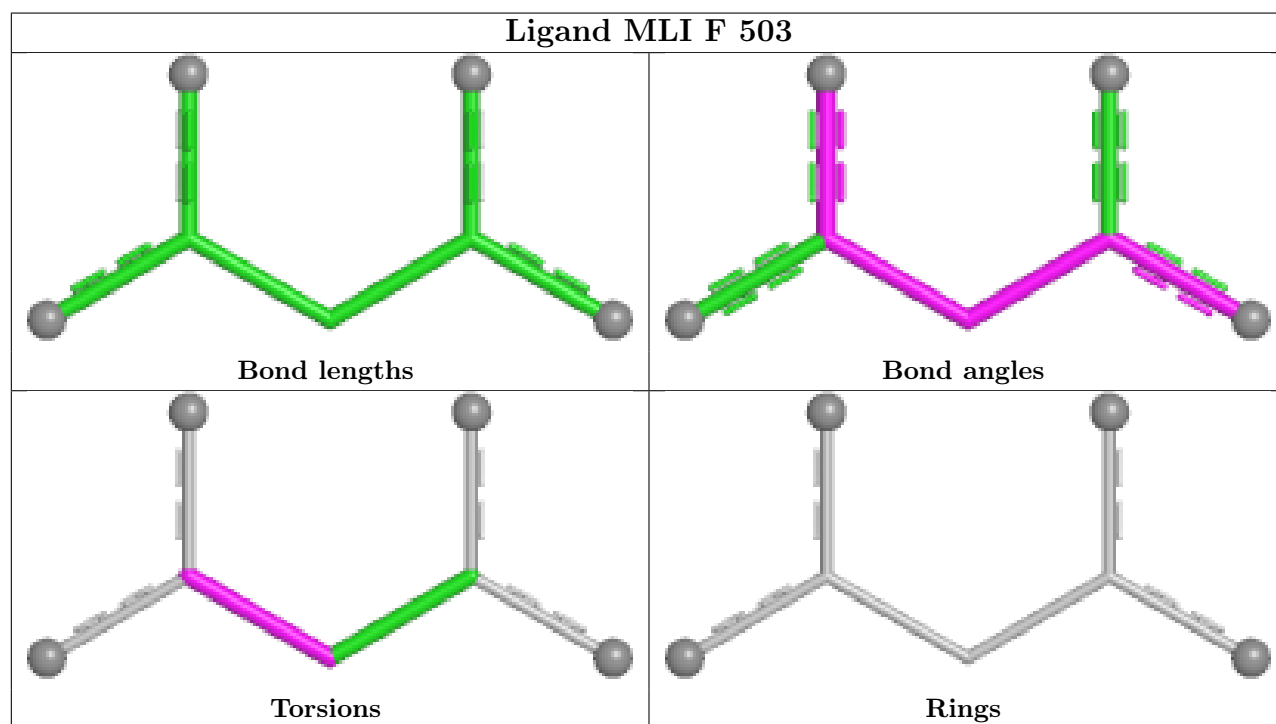
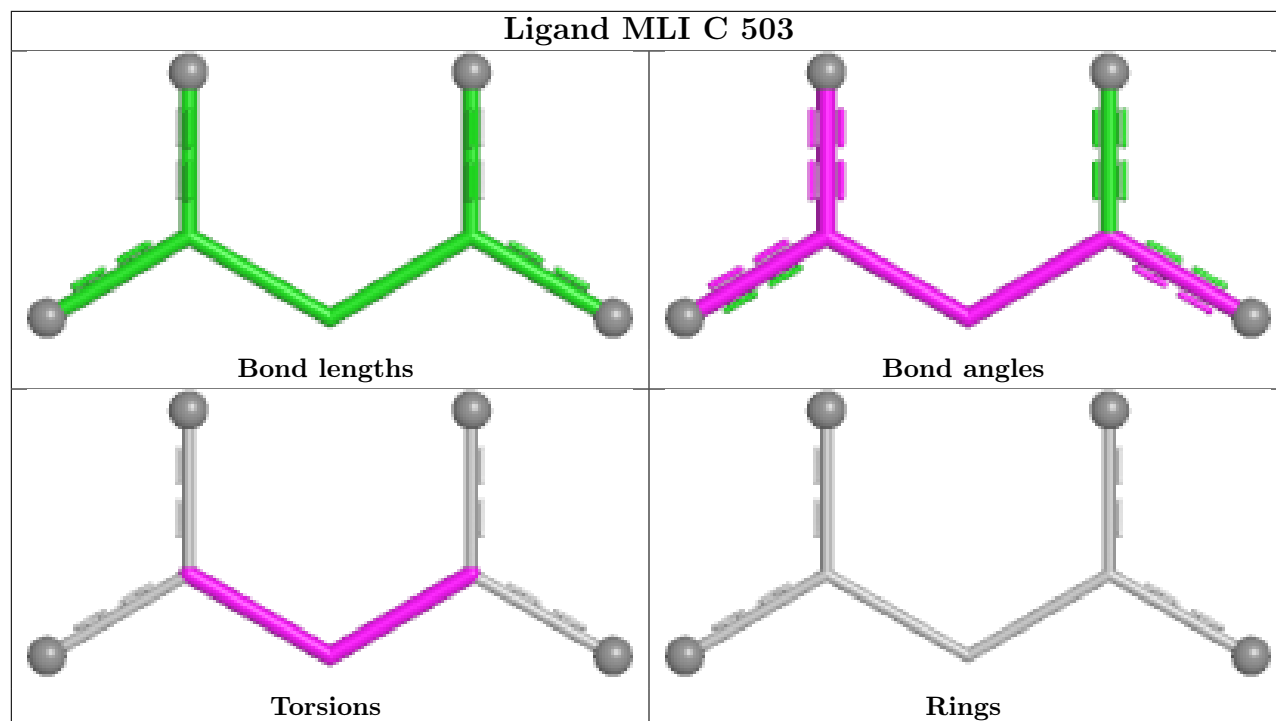


Ligand MLI I 503

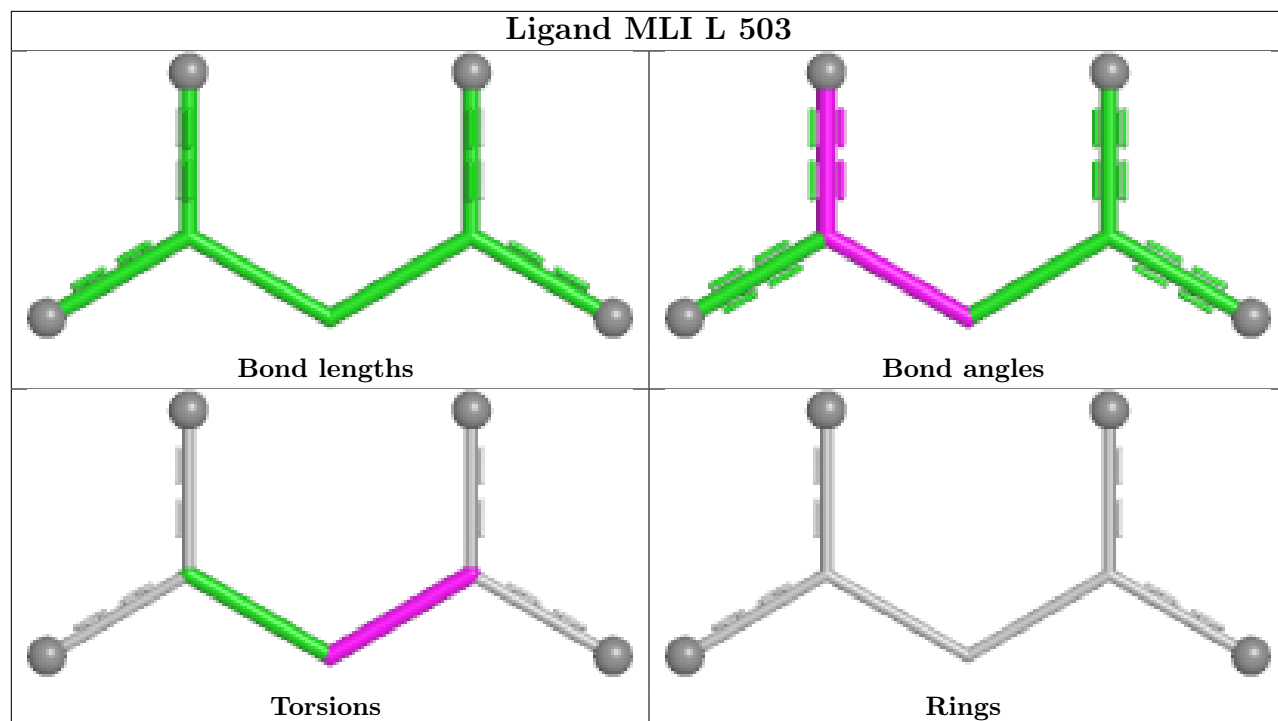


Ligand G6P G 501

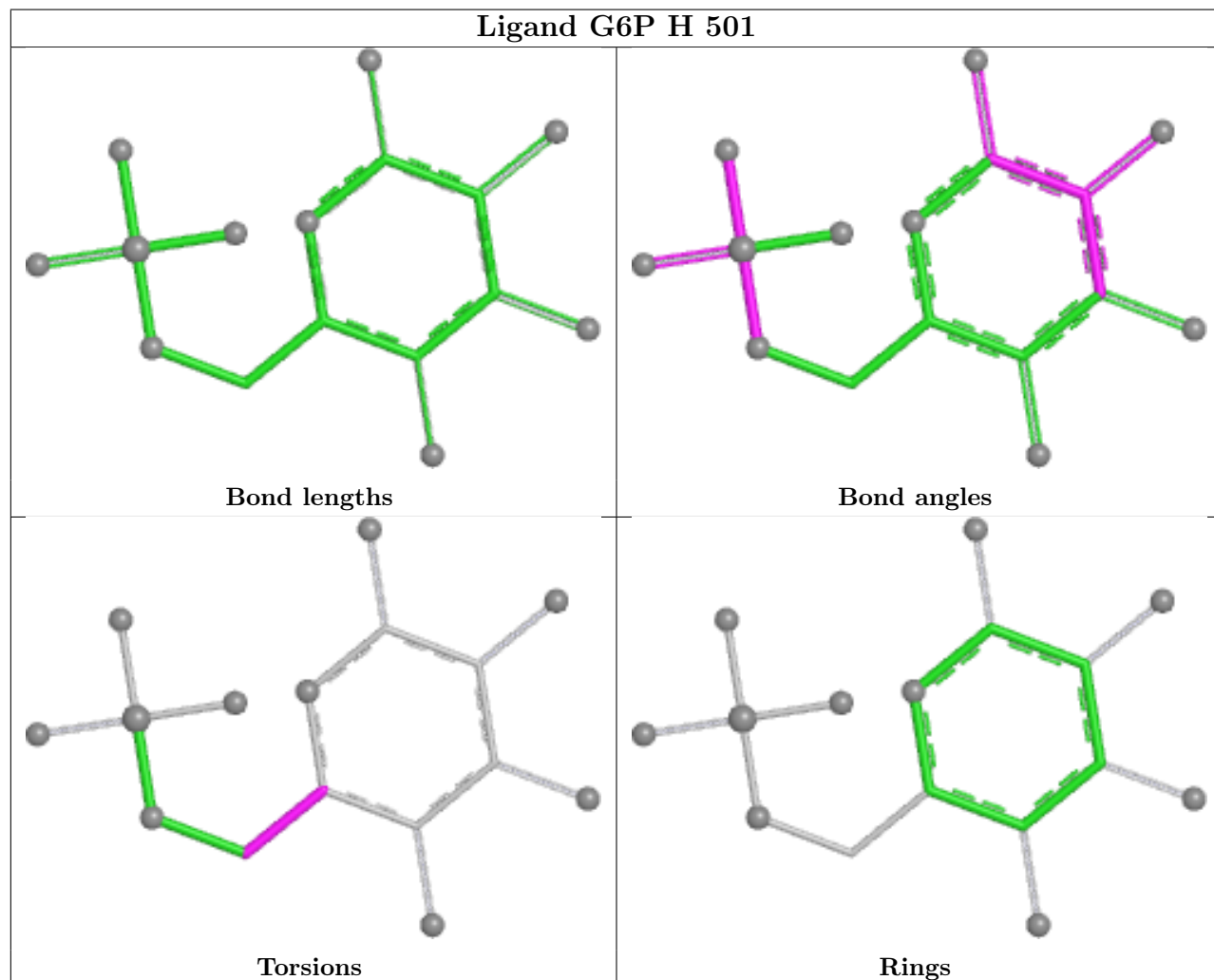




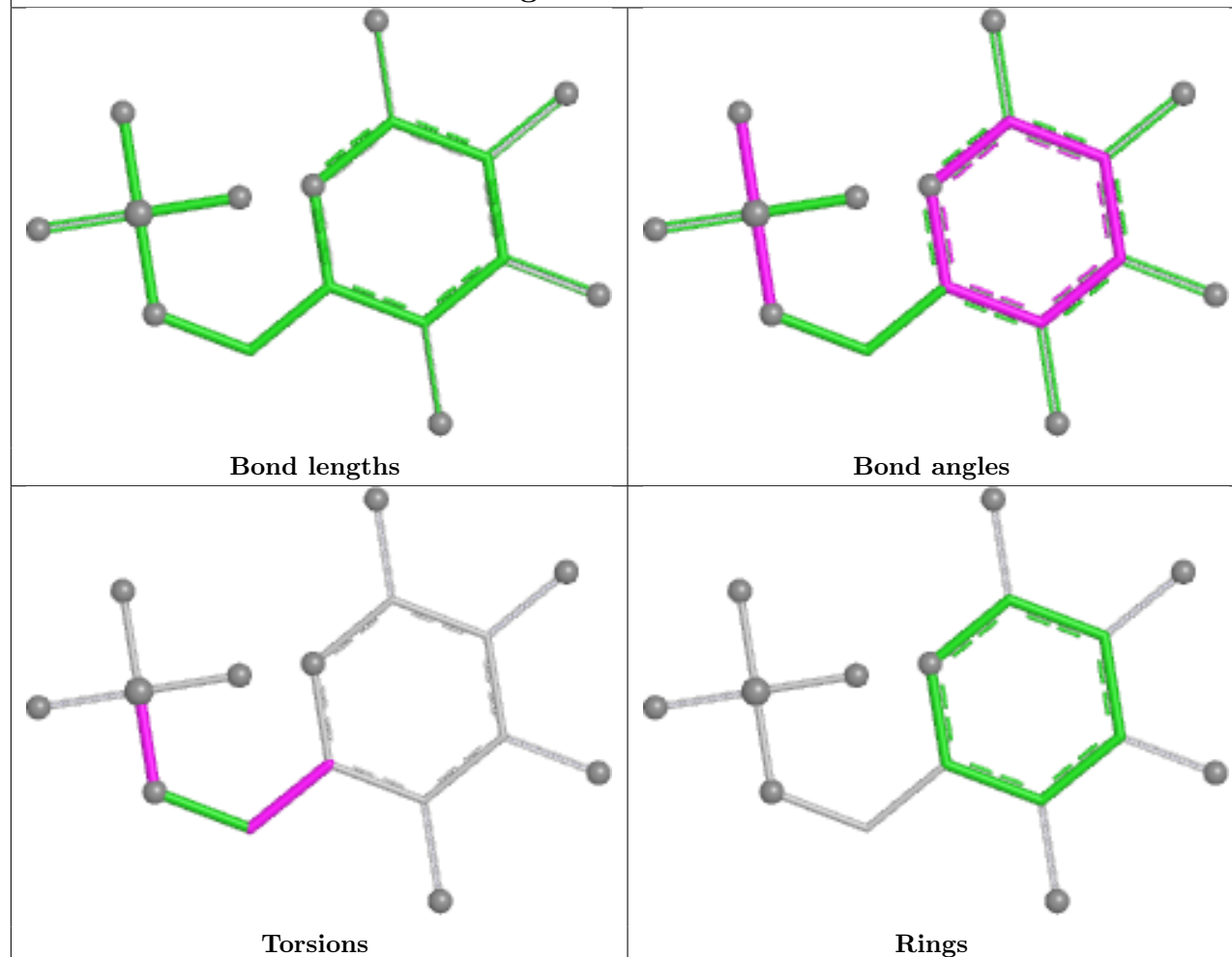
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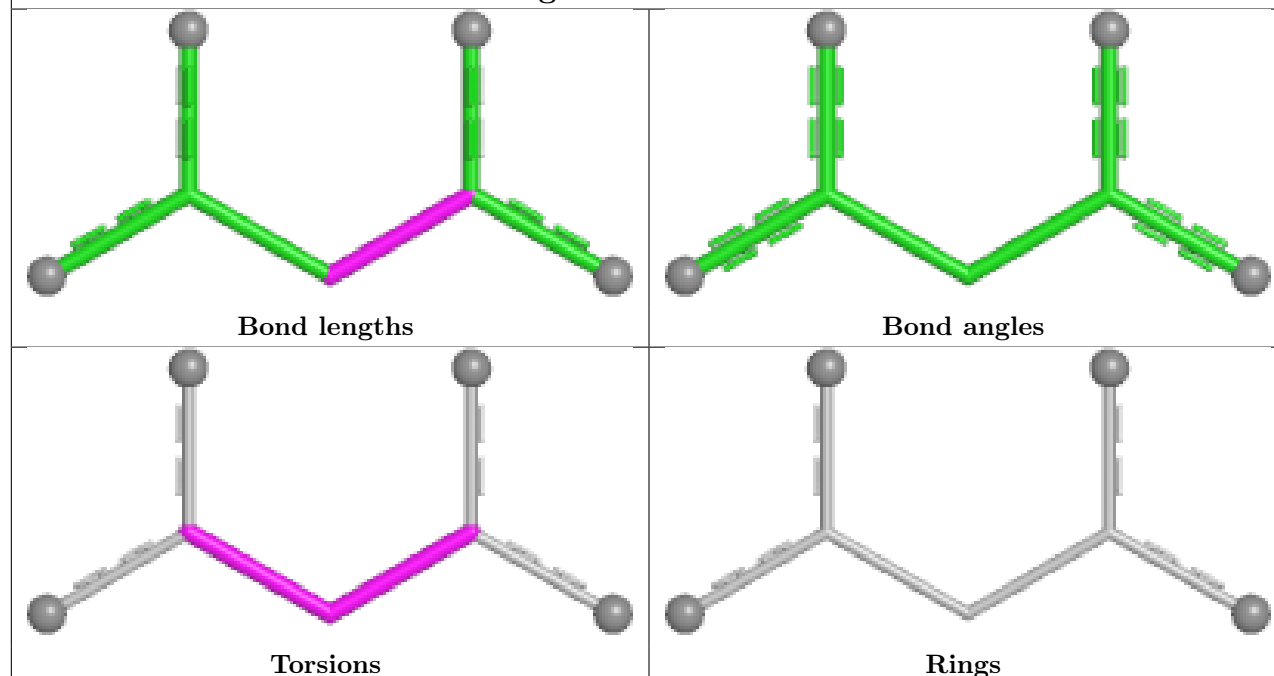
Ligand G6P H 501



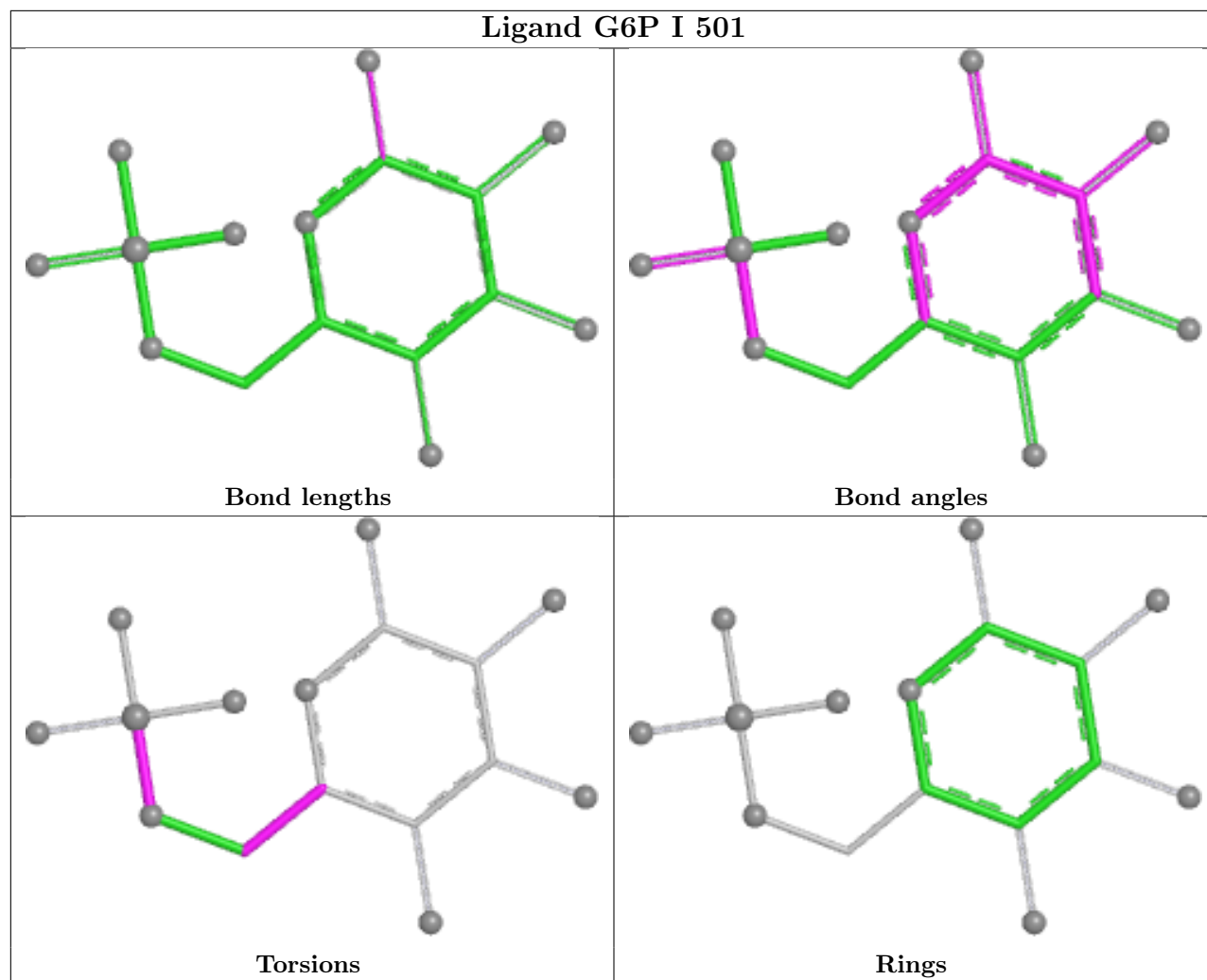
Ligand G6P J 501



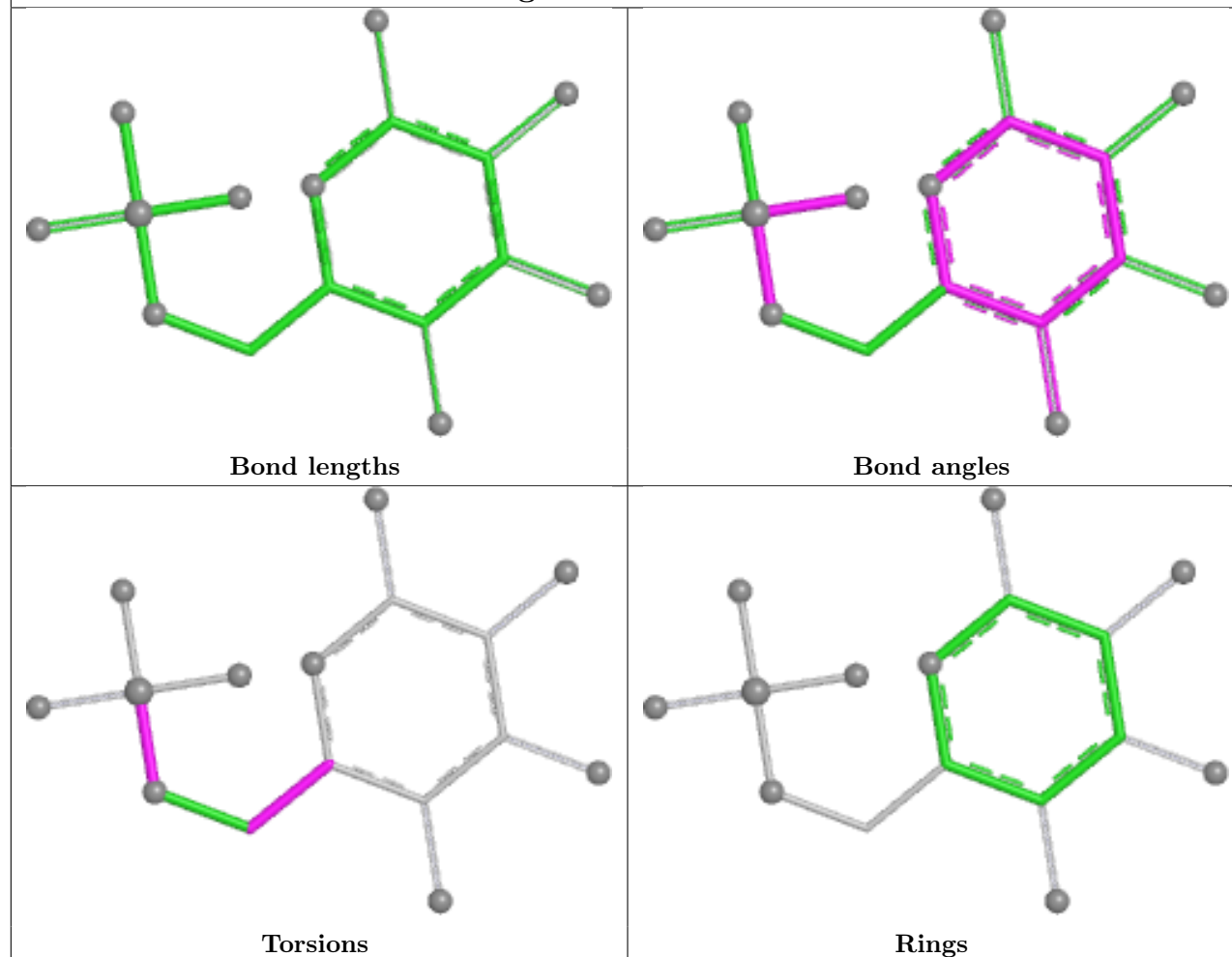
Ligand MLI J 503



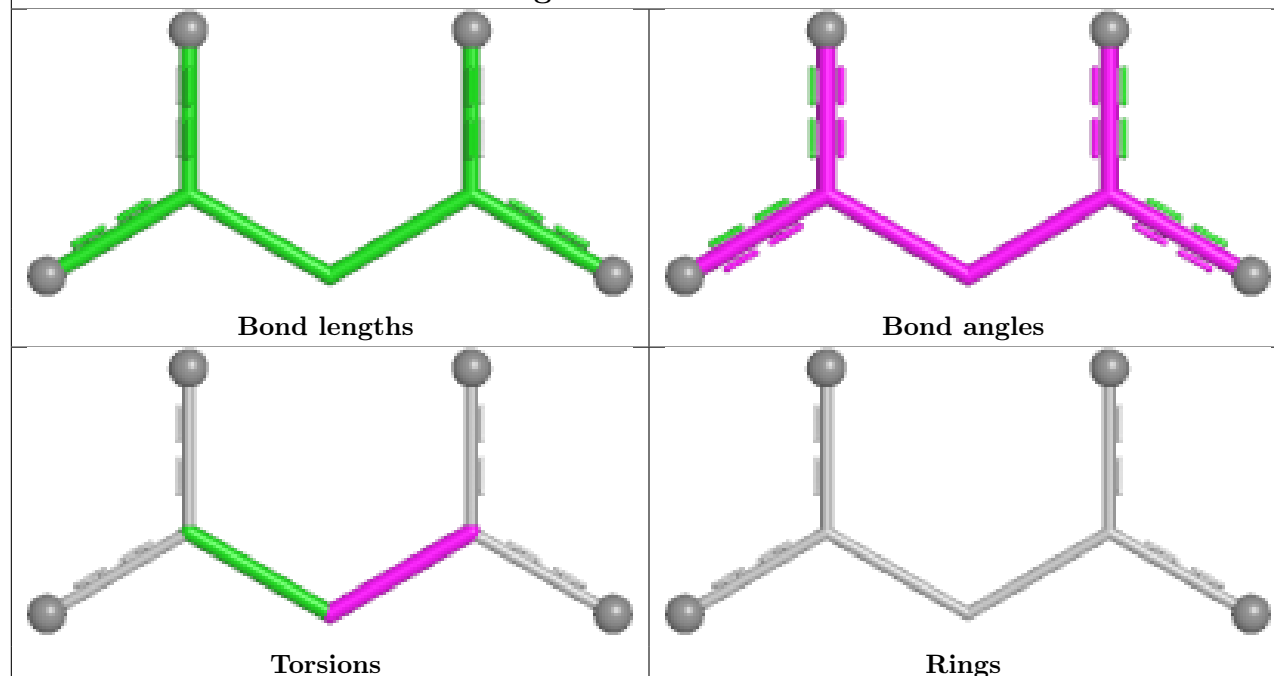
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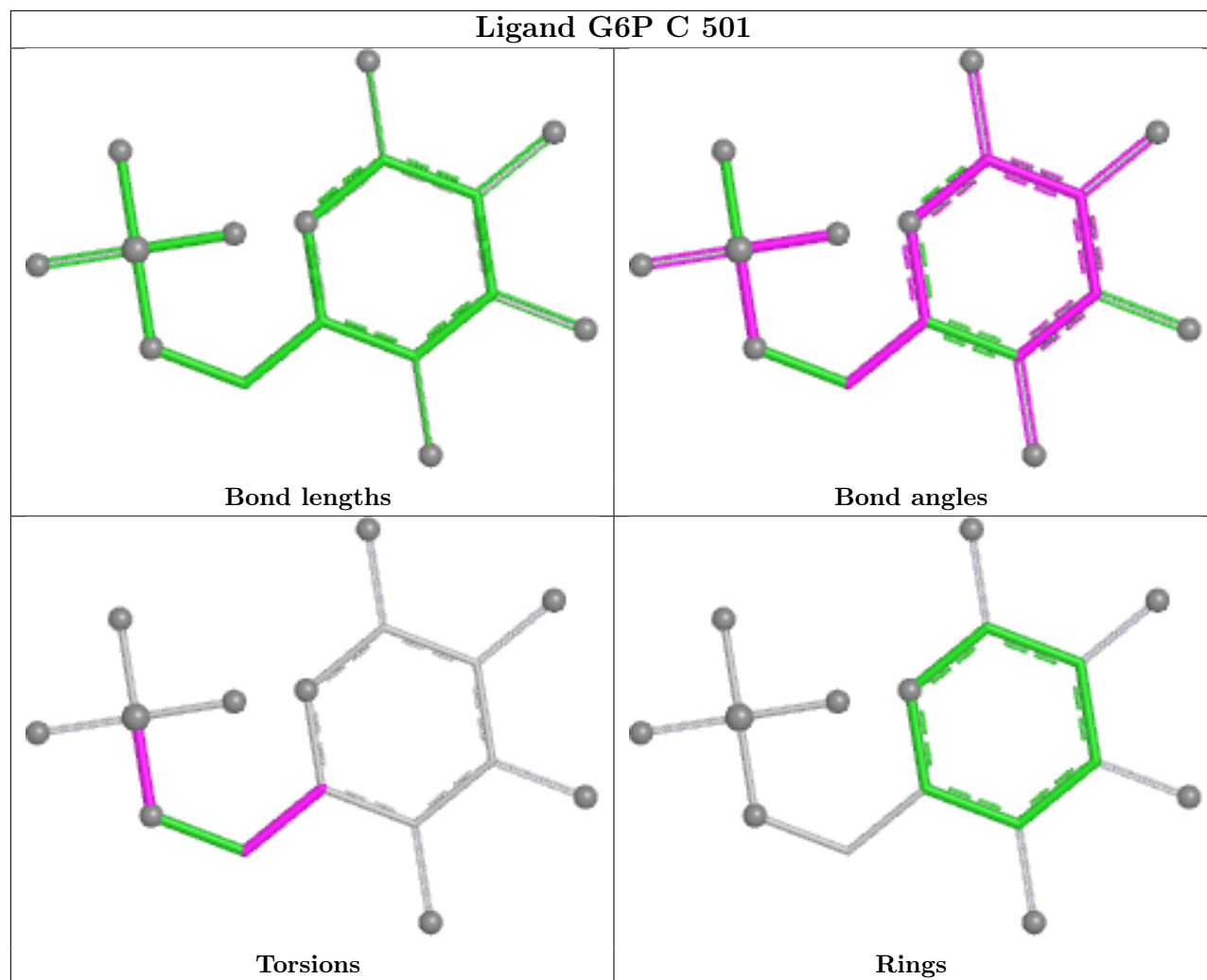


Ligand G6P F 501



Ligand MLI G 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%)	0.21	9 (1%) 66 67	27, 47, 74, 105	0
1	B	483/483 (100%)	-0.09	9 (1%) 66 67	22, 37, 67, 98	0
1	C	483/483 (100%)	0.07	11 (2%) 61 62	27, 44, 72, 110	0
1	D	483/483 (100%)	0.00	3 (0%) 85 87	25, 42, 71, 102	0
1	E	483/483 (100%)	-0.07	5 (1%) 79 81	14, 39, 73, 92	2 (0%)
1	F	483/483 (100%)	0.57	23 (4%) 35 33	26, 53, 84, 111	0
1	G	483/483 (100%)	0.48	19 (3%) 43 40	30, 56, 90, 116	0
1	H	483/483 (100%)	0.42	23 (4%) 35 33	23, 54, 102, 138	0
1	I	483/483 (100%)	0.57	20 (4%) 41 39	30, 62, 91, 114	0
1	J	404/483 (83%)	0.61	28 (6%) 23 19	28, 55, 93, 214	0
1	K	482/483 (99%)	0.50	28 (5%) 29 25	31, 58, 92, 128	0
1	L	483/483 (100%)	1.03	73 (15%) 5 4	37, 71, 118, 153	0
All	All	5716/5796 (98%)	0.36	251 (4%) 39 36	14, 52, 92, 214	2 (0%)

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	77	ALA	8.3
1	J	76	ILE	5.8
1	G	171	ALA	5.5
1	J	157	HIS	4.8
1	L	483	VAL	4.5
1	C	170	PRO	4.4
1	C	171	ALA	4.4
1	J	167	LEU	4.2
1	J	466	ALA	4.2
1	L	359	CYS	4.0
1	K	167	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	L	481	LEU	3.9
1	L	52	VAL	3.9
1	L	171	ALA	3.9
1	L	154	LEU	3.9
1	J	160	ILE	3.8
1	F	356	PHE	3.8
1	K	481	LEU	3.7
1	G	483	VAL	3.6
1	B	466	ALA	3.6
1	G	481	LEU	3.6
1	K	483	VAL	3.5
1	K	171	ALA	3.5
1	L	74	ILE	3.5
1	J	349	SER	3.5
1	H	102	ALA	3.5
1	G	1	MET	3.5
1	L	172	LEU	3.5
1	A	171	ALA	3.4
1	J	168	THR	3.4
1	J	356	PHE	3.3
1	H	1	MET	3.3
1	F	83	ARG	3.2
1	A	468	GLY	3.2
1	H	84	ILE	3.2
1	F	374	PHE	3.2
1	L	466	ALA	3.2
1	C	172	LEU	3.2
1	F	449	VAL	3.1
1	F	1	MET	3.1
1	L	15	ALA	3.1
1	B	1	MET	3.1
1	C	1	MET	3.1
1	A	172	LEU	3.1
1	I	77	ALA	3.0
1	L	433	ALA	3.0
1	L	83	ARG	3.0
1	L	349	SER	3.0
1	C	483	VAL	3.0
1	E	466	ALA	3.0
1	L	141	ALA	3.0
1	L	112	TYR	3.0
1	C	115	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	50	ARG	3.0
1	H	483	VAL	3.0
1	L	132	VAL	3.0
1	I	84	ILE	2.9
1	C	169	ALA	2.9
1	F	171	ALA	2.9
1	G	432	PRO	2.9
1	F	413	ALA	2.9
1	L	113	PRO	2.9
1	J	158	LYS	2.9
1	H	133	VAL	2.9
1	H	140	ALA	2.9
1	L	82	LYS	2.9
1	L	86	LEU	2.9
1	L	356	PHE	2.9
1	L	134	MET	2.9
1	J	359	CYS	2.9
1	L	169	ALA	2.9
1	J	461	GLY	2.9
1	I	155	SER	2.8
1	G	172	LEU	2.8
1	I	293	MET	2.8
1	L	374	PHE	2.8
1	B	345	SER	2.8
1	L	21	VAL	2.8
1	F	172	LEU	2.8
1	G	466	ALA	2.8
1	J	374	PHE	2.8
1	L	81	ASN	2.8
1	I	99	ALA	2.8
1	L	41	THR	2.8
1	L	49	ALA	2.8
1	L	149	LEU	2.8
1	I	1	MET	2.8
1	L	1	MET	2.8
1	L	152	GLY	2.7
1	F	466	ALA	2.7
1	H	466	ALA	2.7
1	F	483	VAL	2.7
1	I	82	LYS	2.7
1	K	356	PHE	2.7
1	J	431	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	99	ALA	2.7
1	H	141	ALA	2.7
1	K	169	ALA	2.7
1	K	466	ALA	2.7
1	H	130	GLY	2.7
1	H	356	PHE	2.7
1	L	94	PHE	2.7
1	L	195	PHE	2.7
1	L	88	VAL	2.7
1	L	133	VAL	2.7
1	G	465	THR	2.7
1	B	468	GLY	2.6
1	L	76	ILE	2.6
1	L	434	GLU	2.6
1	B	171	ALA	2.6
1	J	465	THR	2.6
1	G	435	LYS	2.6
1	G	170	PRO	2.6
1	H	434	GLU	2.6
1	B	83	ARG	2.6
1	L	110	ILE	2.6
1	F	481	LEU	2.6
1	L	55	LEU	2.6
1	H	88	VAL	2.6
1	L	140	ALA	2.6
1	K	374	PHE	2.6
1	J	483	VAL	2.6
1	H	113	PRO	2.5
1	G	167	LEU	2.5
1	H	465	THR	2.5
1	J	1	MET	2.5
1	F	164	GLY	2.5
1	H	150	ILE	2.5
1	K	445	LEU	2.5
1	H	435	LYS	2.5
1	J	344	THR	2.5
1	K	1	MET	2.5
1	F	167	LEU	2.5
1	G	431	LEU	2.5
1	L	116	VAL	2.5
1	E	83	ARG	2.5
1	D	1	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	428	PRO	2.5
1	J	73	LYS	2.5
1	G	168	THR	2.5
1	I	88	VAL	2.4
1	L	168	THR	2.4
1	J	74	ILE	2.4
1	L	12	LEU	2.4
1	A	83	ARG	2.4
1	I	132	VAL	2.4
1	G	430	ALA	2.4
1	L	80	ALA	2.4
1	L	45	HIS	2.4
1	L	40	GLY	2.4
1	L	160	ILE	2.4
1	L	218	LEU	2.4
1	K	449	VAL	2.4
1	L	69	LEU	2.3
1	I	466	ALA	2.3
1	L	10	ALA	2.3
1	F	166	GLY	2.3
1	L	48	ARG	2.3
1	B	344	THR	2.3
1	K	431	LEU	2.3
1	C	347	LYS	2.3
1	G	374	PHE	2.3
1	F	450	VAL	2.3
1	G	449	VAL	2.3
1	L	183	ALA	2.3
1	K	131	ARG	2.3
1	J	166	GLY	2.3
1	K	172	LEU	2.3
1	L	84	ILE	2.3
1	L	115	LEU	2.3
1	L	150	ILE	2.3
1	I	101	ASP	2.3
1	I	450	VAL	2.3
1	B	131	ARG	2.3
1	L	99	ALA	2.2
1	L	104	THR	2.2
1	E	82	LYS	2.2
1	L	127	LEU	2.2
1	G	83	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	170	PRO	2.2
1	C	112	TYR	2.2
1	L	464	TYR	2.2
1	K	347	LYS	2.2
1	I	345	SER	2.2
1	K	170	PRO	2.2
1	L	77	ALA	2.2
1	L	199	ALA	2.2
1	K	408	HIS	2.2
1	J	481	LEU	2.2
1	D	349	SER	2.2
1	J	437	SER	2.2
1	L	155	SER	2.2
1	F	434	GLU	2.2
1	G	356	PHE	2.2
1	H	132	VAL	2.2
1	C	73	LYS	2.2
1	L	73	LYS	2.2
1	L	161	ASN	2.2
1	B	356	PHE	2.2
1	G	195	PHE	2.2
1	A	1	MET	2.1
1	I	102	ALA	2.1
1	K	80	ALA	2.1
1	K	429	ALA	2.1
1	K	467	GLN	2.1
1	I	151	GLY	2.1
1	I	344	THR	2.1
1	E	356	PHE	2.1
1	K	478	VAL	2.1
1	K	433	ALA	2.1
1	A	41	THR	2.1
1	I	103	GLY	2.1
1	L	431	LEU	2.1
1	F	74	ILE	2.1
1	J	197	ARG	2.1
1	L	119	CYS	2.1
1	I	116	VAL	2.1
1	D	466	ALA	2.1
1	L	178	ALA	2.1
1	F	115	LEU	2.1
1	I	115	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	208	LEU	2.1
1	J	347	LYS	2.1
1	K	82	LYS	2.1
1	F	359	CYS	2.1
1	F	436	VAL	2.1
1	L	92	PHE	2.1
1	E	77	ALA	2.1
1	H	433	ALA	2.1
1	I	481	LEU	2.1
1	L	197	ARG	2.1
1	L	224	ARG	2.1
1	K	464	TYR	2.1
1	H	463	SER	2.1
1	A	170	PRO	2.1
1	H	359	CYS	2.1
1	K	428	PRO	2.1
1	C	374	PHE	2.0
1	J	195	PHE	2.0
1	A	466	ALA	2.0
1	K	440	ALA	2.0
1	H	431	LEU	2.0
1	L	188	LEU	2.0
1	K	168	THR	2.0
1	A	52	VAL	2.0
1	F	440	ALA	2.0
1	H	481	LEU	2.0
1	J	169	ALA	2.0
1	J	172	LEU	2.0
1	K	125	LEU	2.0
1	F	437	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	B	502	1/1	0.79	0.15	44,44,44,44	0
3	MG	L	502	1/1	0.82	0.17	75,75,75,75	0
4	MLI	L	503	7/7	0.82	0.14	64,79,81,87	0
4	MLI	J	503	7/7	0.84	0.12	59,61,69,75	0
4	MLI	I	503	7/7	0.84	0.13	55,62,65,83	0
5	GOL	D	503	6/6	0.84	0.17	45,54,60,62	0
3	MG	I	502	1/1	0.86	0.08	30,30,30,30	0
3	MG	E	502	1/1	0.87	0.12	40,40,40,40	0
3	MG	D	502	1/1	0.88	0.17	39,39,39,39	0
4	MLI	K	503	7/7	0.88	0.12	61,67,70,84	0
3	MG	C	502	1/1	0.90	0.07	30,30,30,30	0
4	MLI	F	503	7/7	0.91	0.09	46,58,61,64	0
4	MLI	C	503	7/7	0.91	0.10	38,50,64,68	0
2	G6P	F	501	16/16	0.92	0.11	53,80,96,104	0
2	G6P	L	501	16/16	0.92	0.10	59,80,90,92	0
4	MLI	H	503	7/7	0.92	0.09	47,52,54,57	0
5	GOL	B	503	6/6	0.92	0.11	44,52,58,58	0
4	MLI	A	503	7/7	0.92	0.10	45,49,54,62	0
2	G6P	G	501	16/16	0.93	0.11	49,81,94,100	0
4	MLI	B	504	7/7	0.93	0.08	37,42,45,46	0
2	G6P	K	501	16/16	0.93	0.10	51,77,92,98	0
4	MLI	D	504	7/7	0.93	0.09	33,41,49,50	0
3	MG	K	502	1/1	0.93	0.11	48,48,48,48	0
2	G6P	A	501	16/16	0.93	0.09	40,59,69,74	0
2	G6P	E	501	16/16	0.94	0.11	42,60,75,78	0
2	G6P	H	501	16/16	0.94	0.10	50,69,82,92	0
3	MG	F	502	1/1	0.94	0.07	49,49,49,49	0
2	G6P	I	501	16/16	0.94	0.09	47,62,72,84	0
3	MG	J	502	1/1	0.94	0.07	55,55,55,55	0
2	G6P	J	501	16/16	0.94	0.11	58,85,105,109	0
4	MLI	G	503	7/7	0.94	0.07	52,54,60,60	0
5	GOL	E	503	6/6	0.94	0.10	40,49,51,57	0
2	G6P	C	501	16/16	0.95	0.09	39,54,79,84	0
4	MLI	E	504	7/7	0.95	0.07	29,34,42,46	0
2	G6P	D	501	16/16	0.95	0.09	36,47,60,74	0
3	MG	H	502	1/1	0.96	0.06	49,49,49,49	0
3	MG	A	502	1/1	0.96	0.06	49,49,49,49	0

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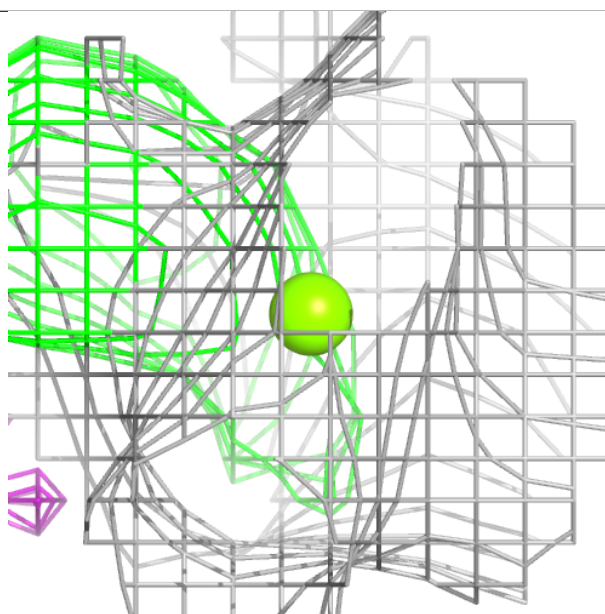
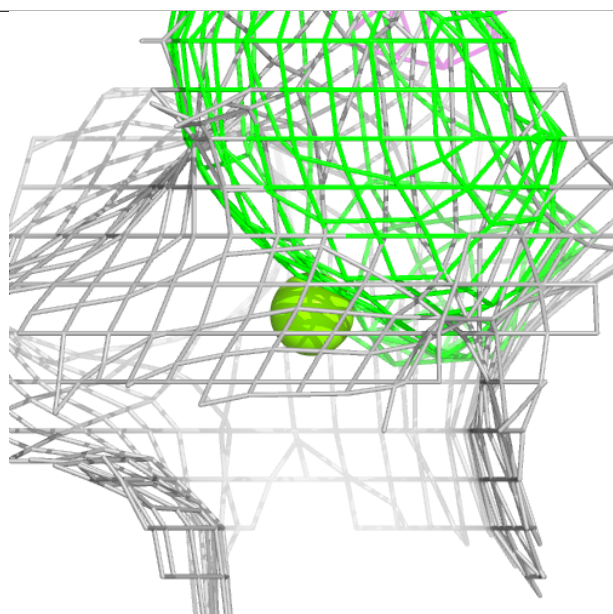
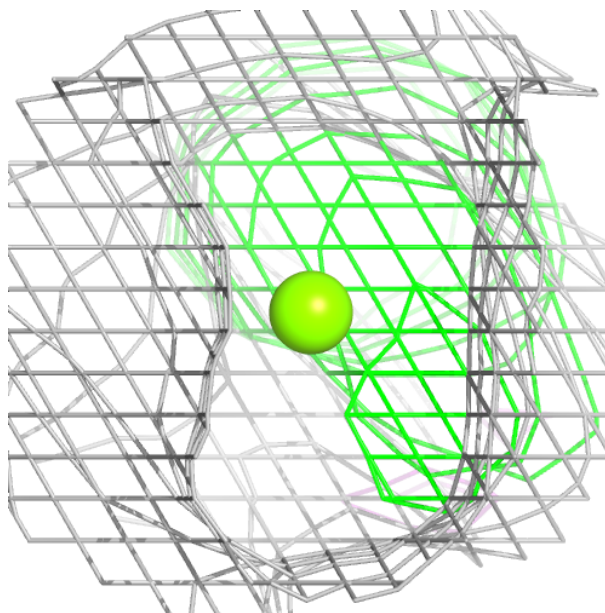
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	G6P	B	501	16/16	0.96	0.10	33,51,67,103	0
3	MG	G	502	1/1	0.96	0.11	45,45,45,45	0

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.

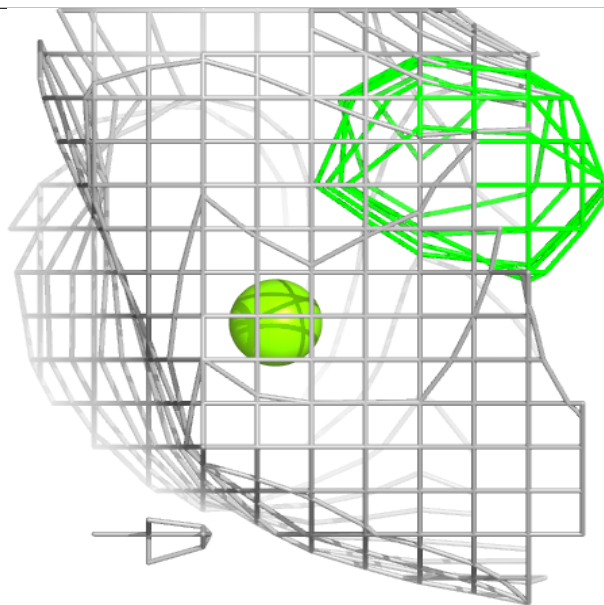
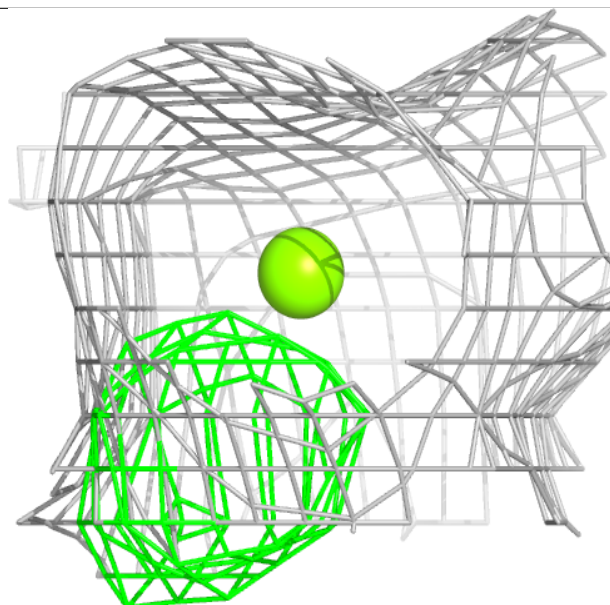
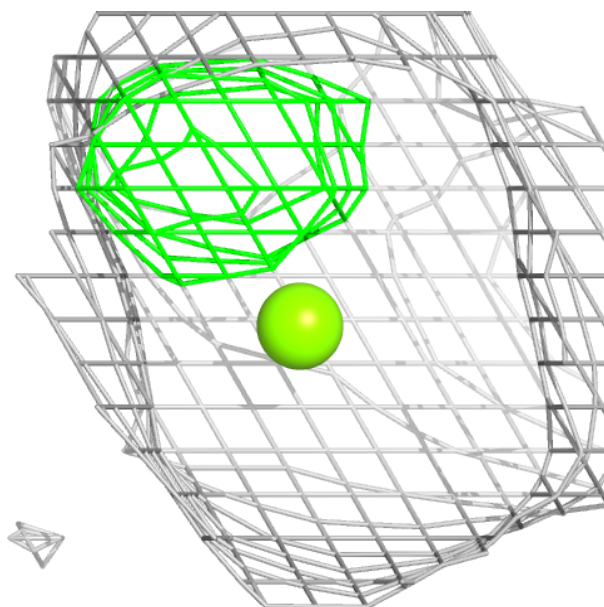
Electron density around MG B 502:

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



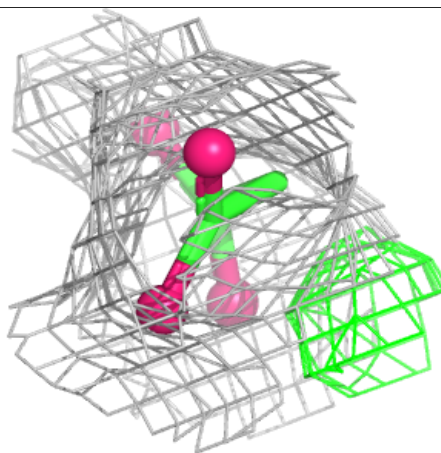
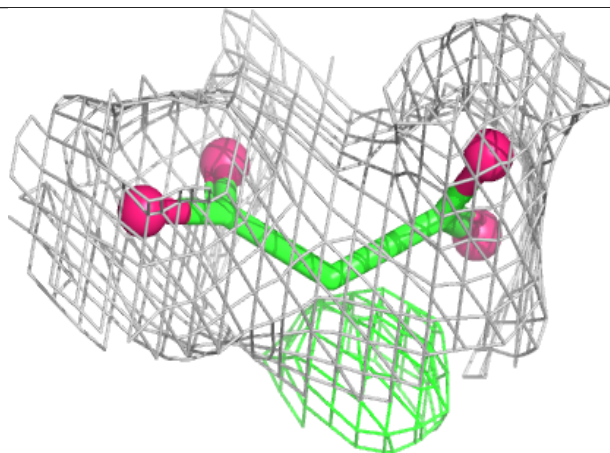
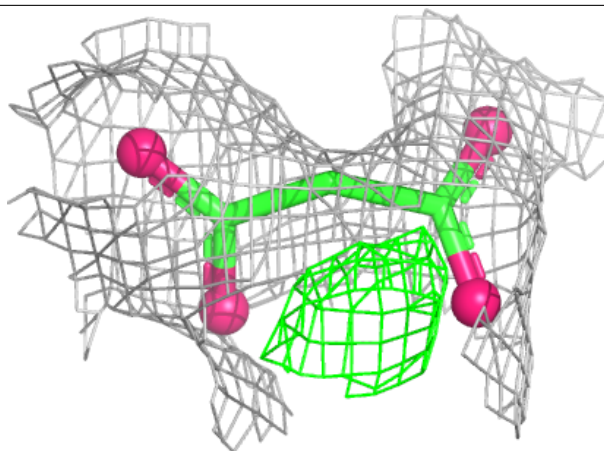
Electron density around MG L 502:

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



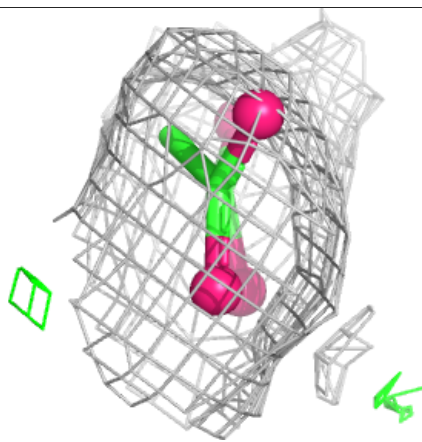
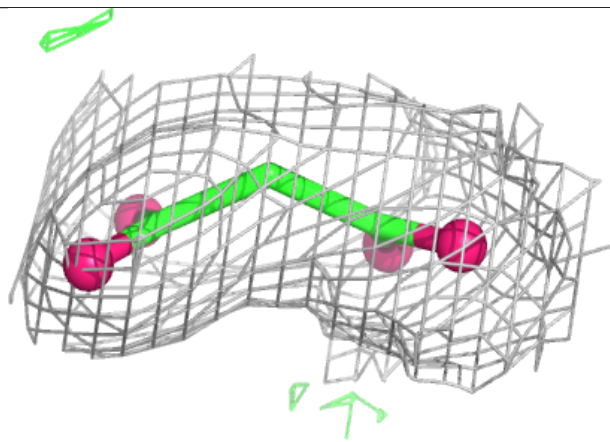
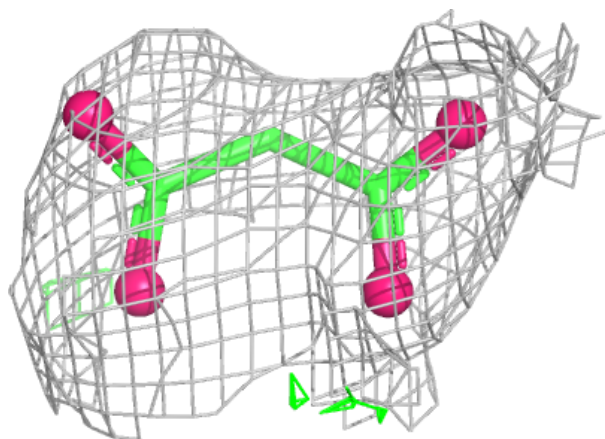
Electron density around MLI L 503:

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



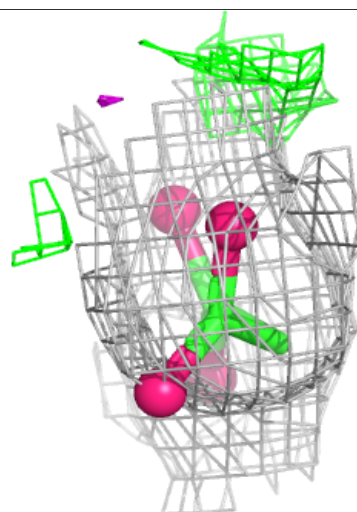
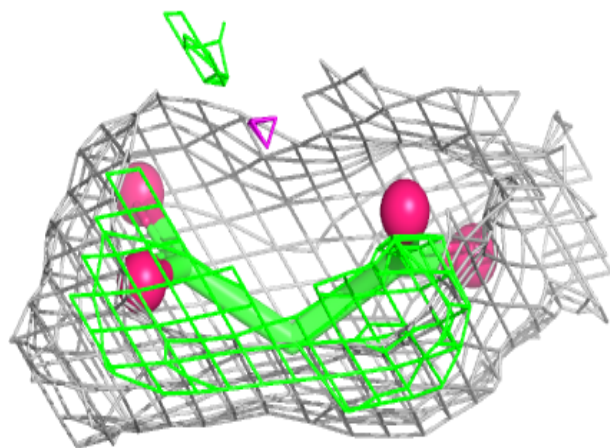
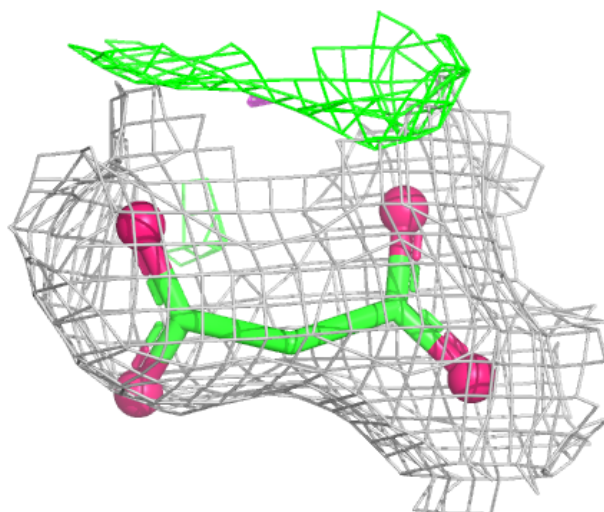
Electron density around MLI J 503:

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and green (positive)



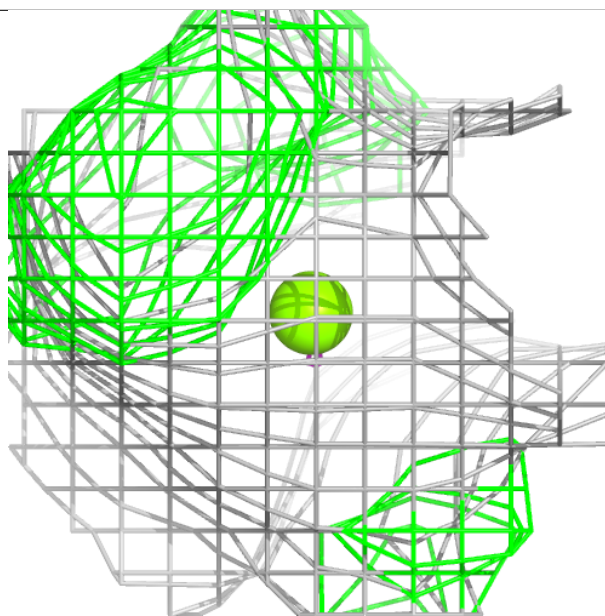
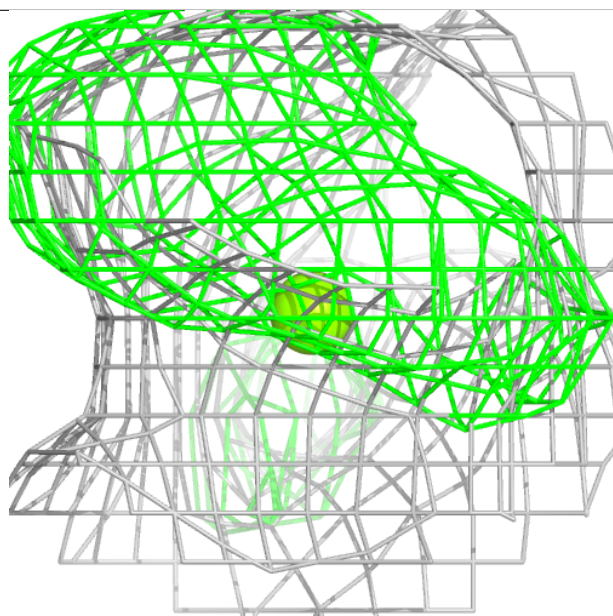
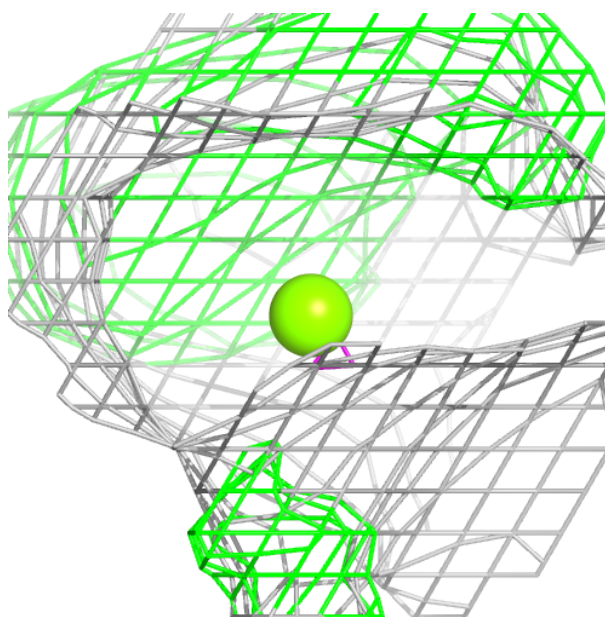
Electron density around MLI I 503:

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and green (positive)



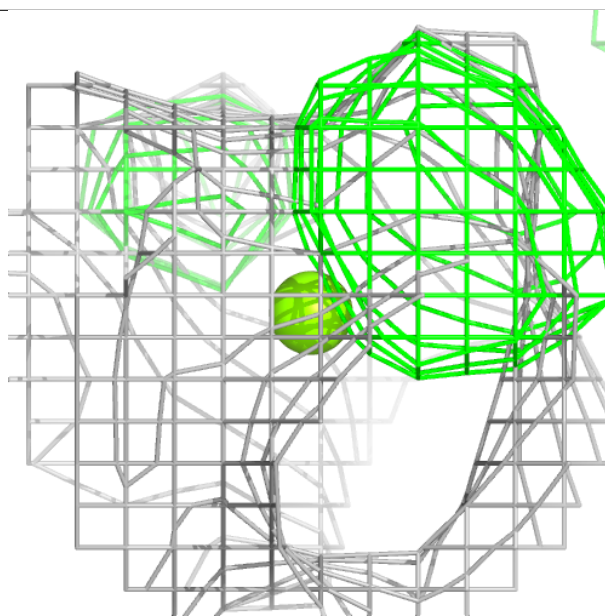
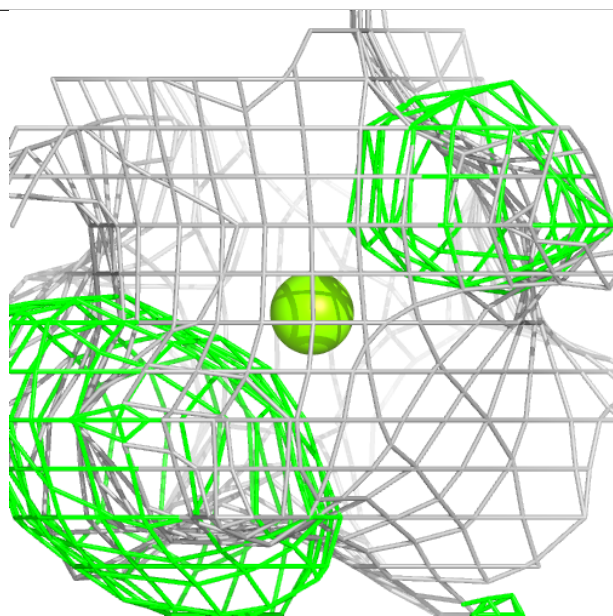
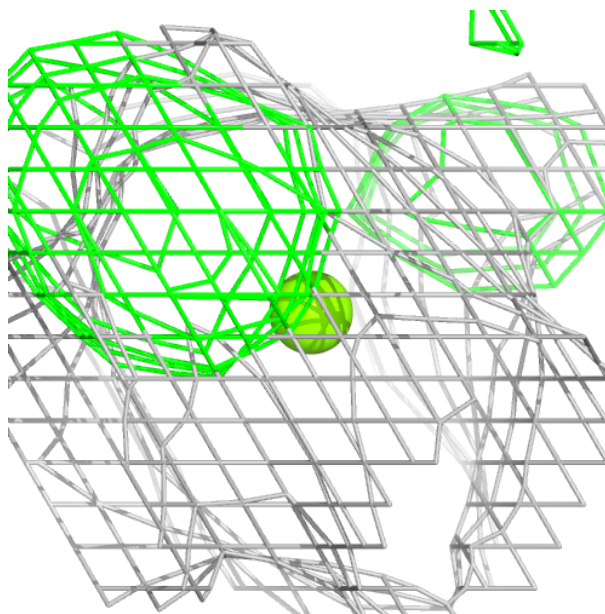
Electron density around MG I 502:

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



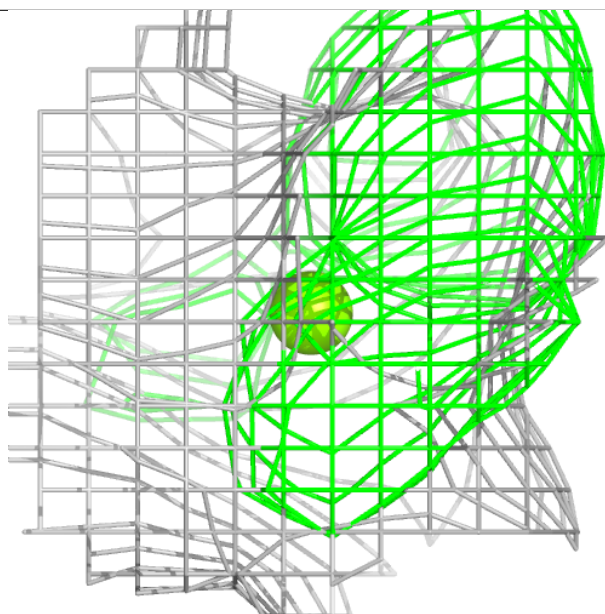
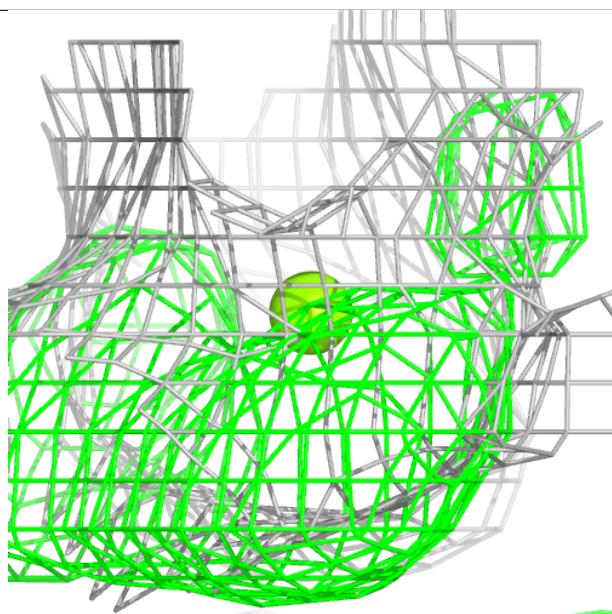
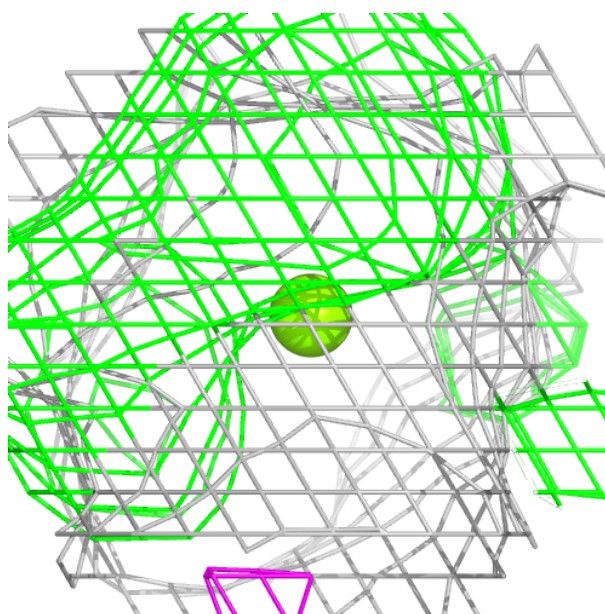
Electron density around MG E 502:

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



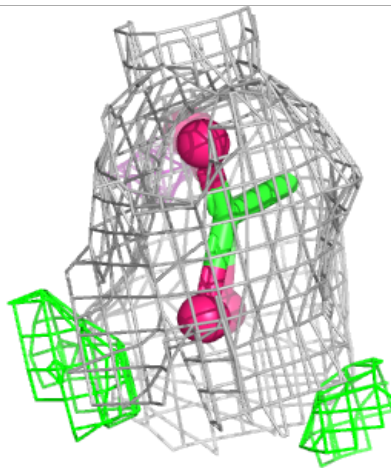
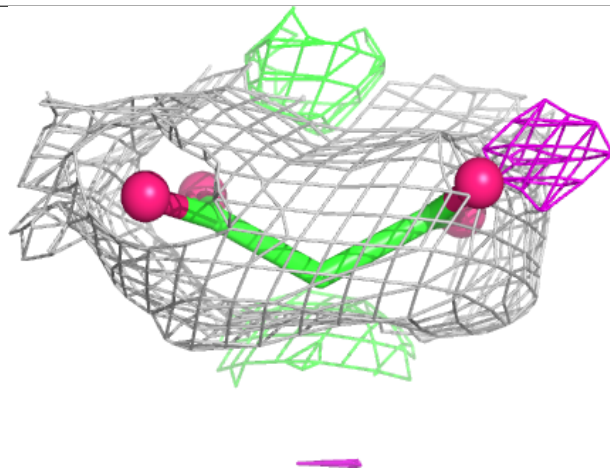
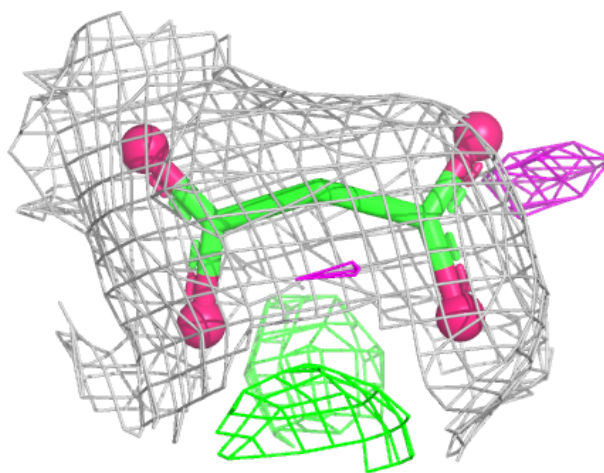
Electron density around MG D 502:

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



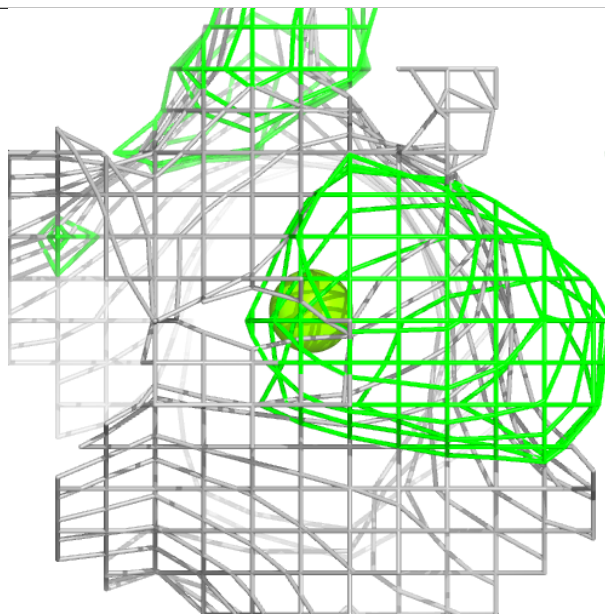
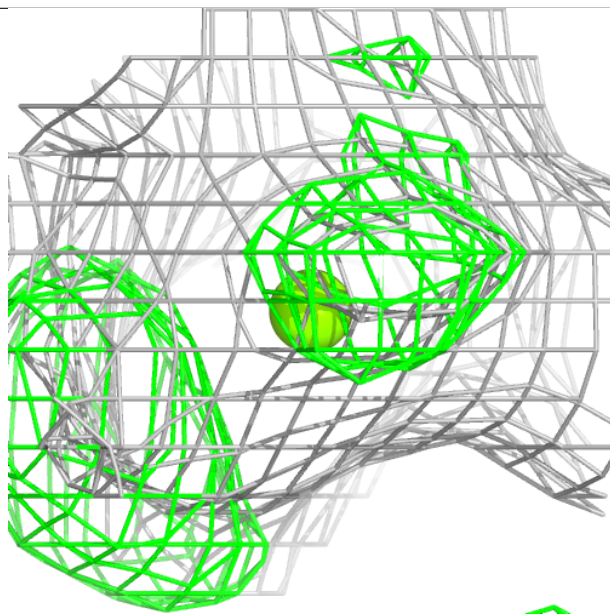
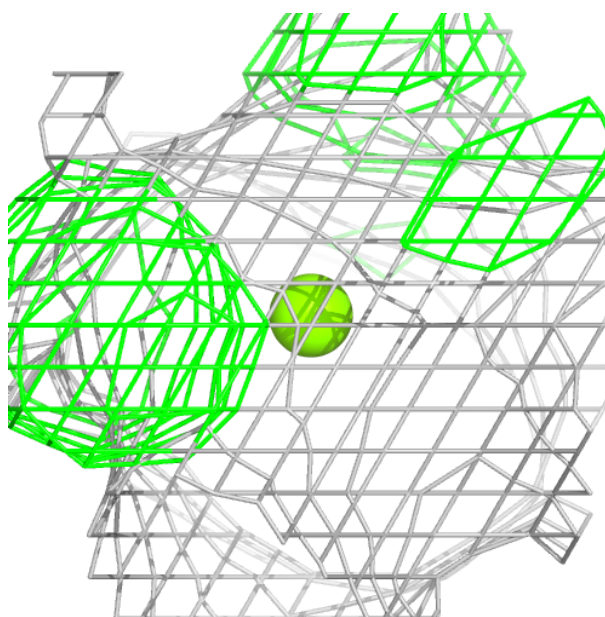
Electron density around MLI K 503:

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



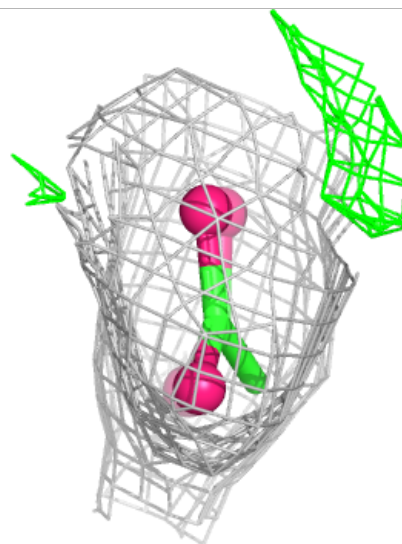
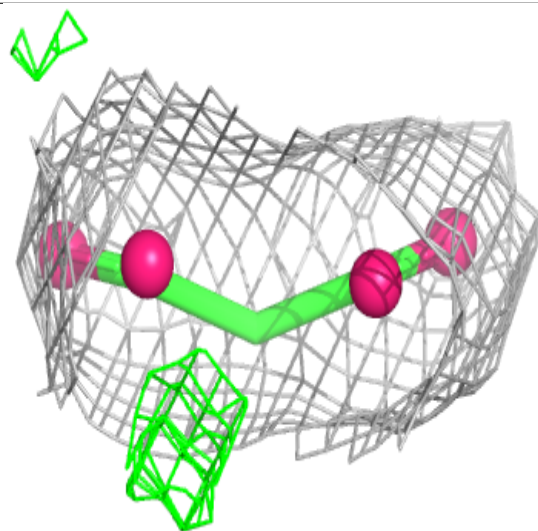
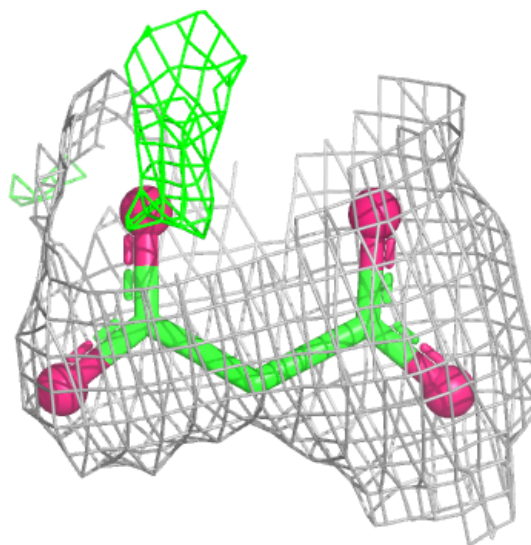
Electron density around MG C 502:

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



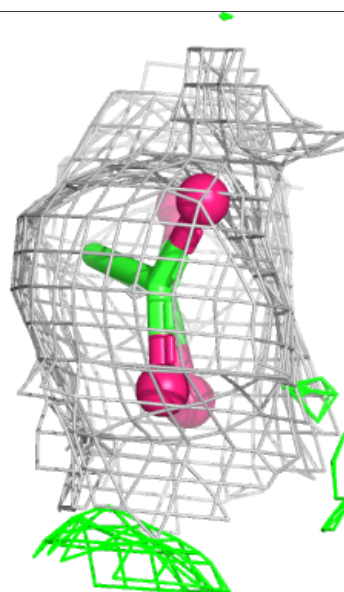
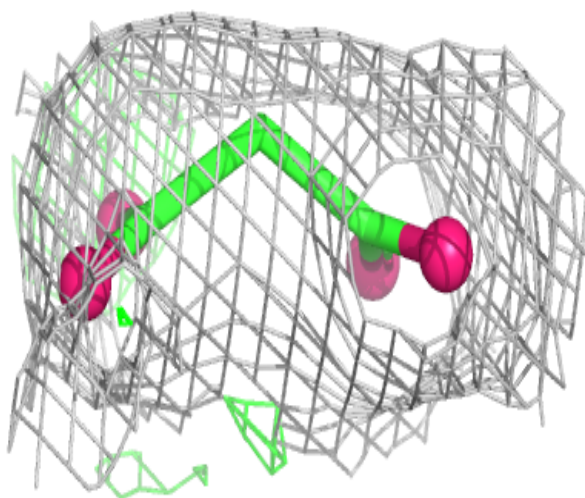
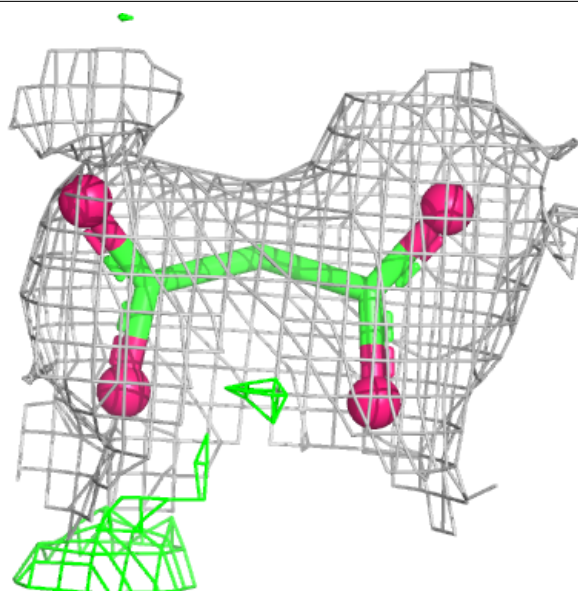
Electron density around MLI F 503:

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



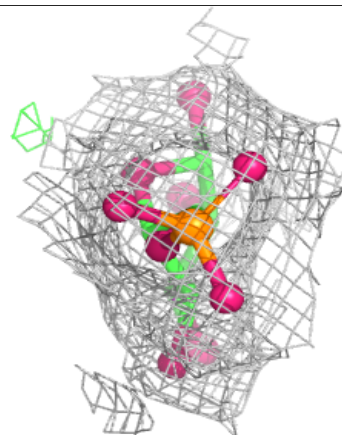
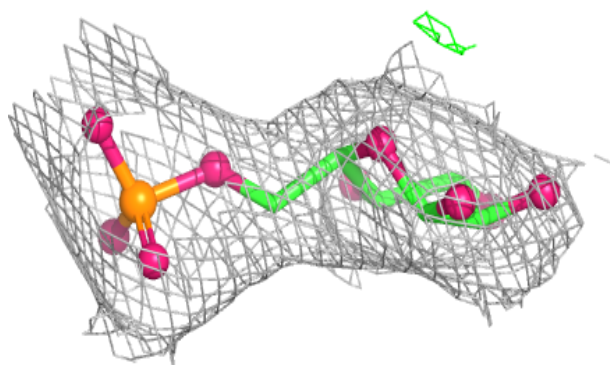
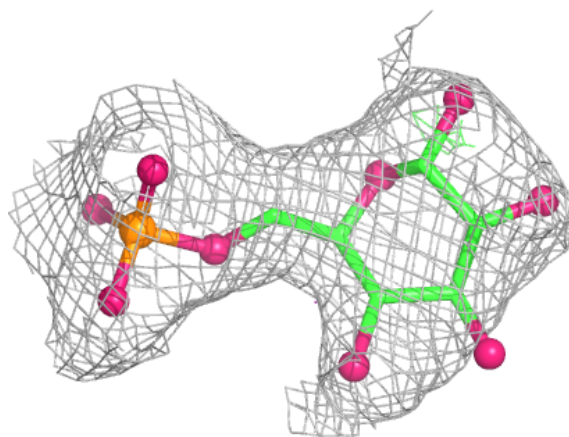
Electron density around MLI C 503:

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

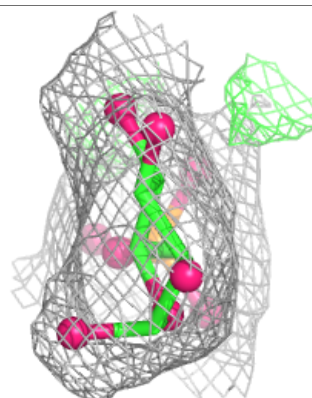
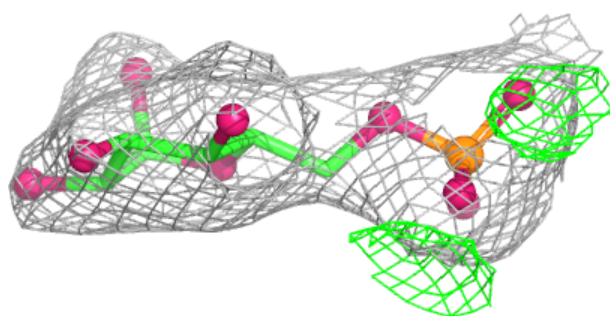
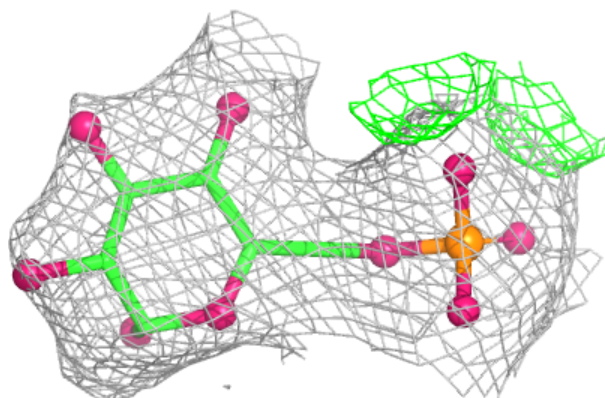


Electron density around G6P F 501:

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

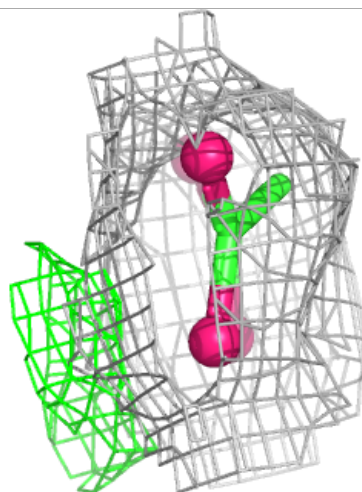
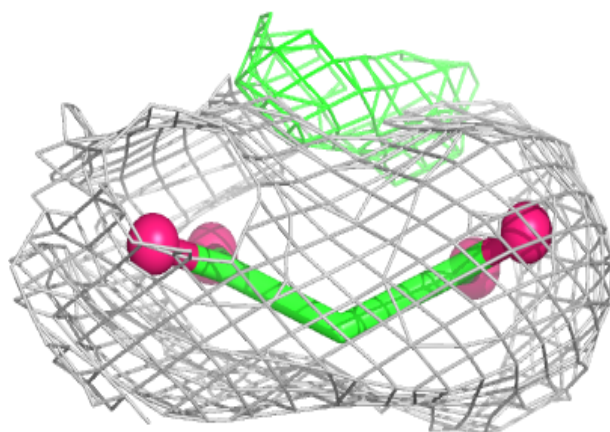
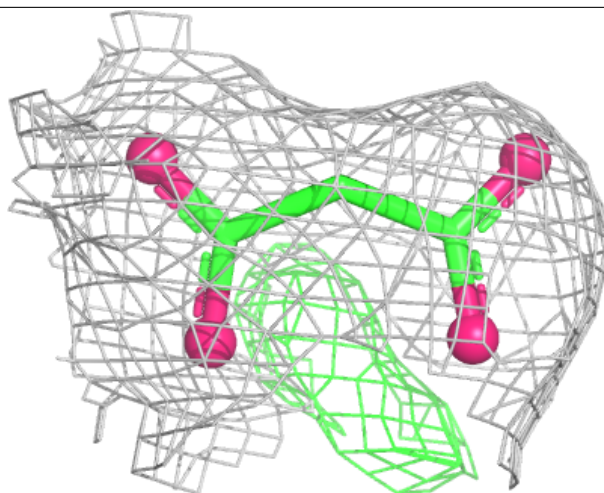
**Electron density around G6P L 501:**

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



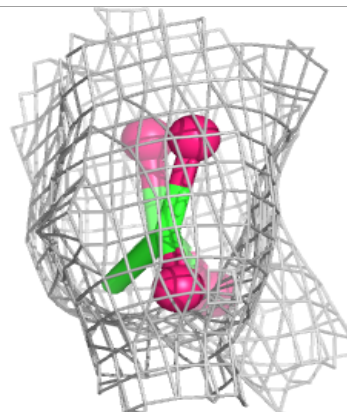
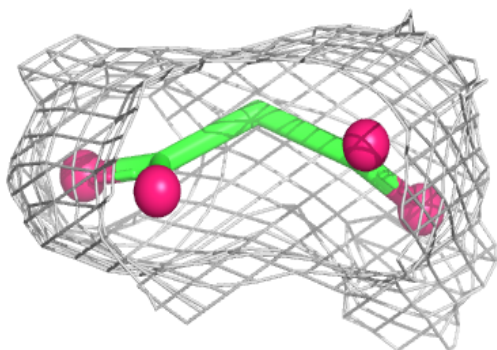
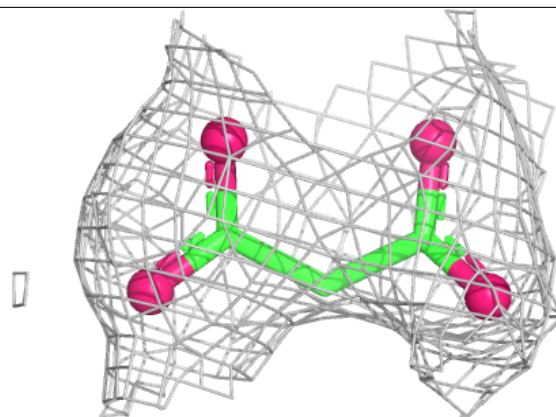
Electron density around MLI H 503:

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

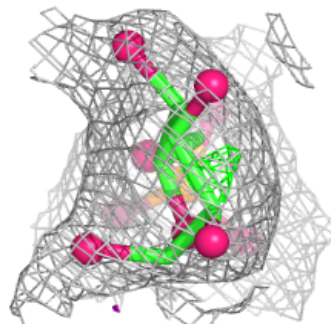
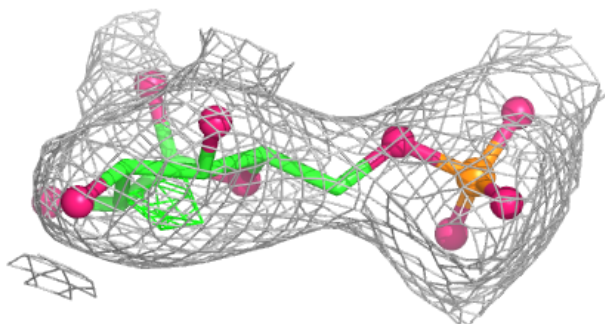
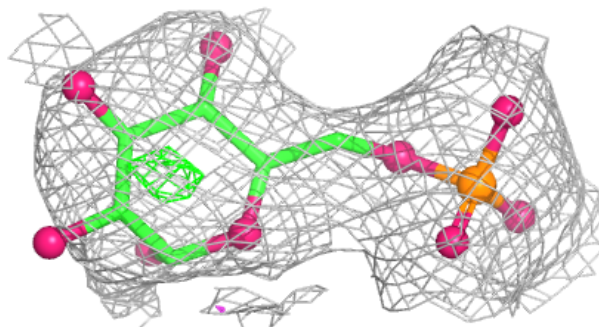


Electron density around MLI A 503:

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

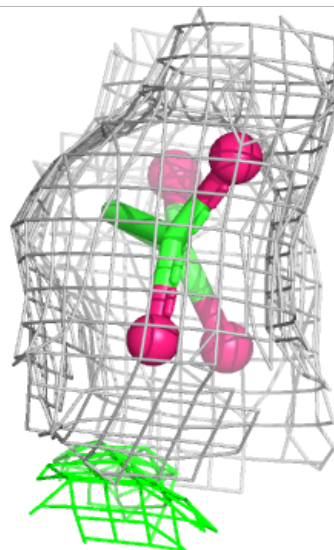
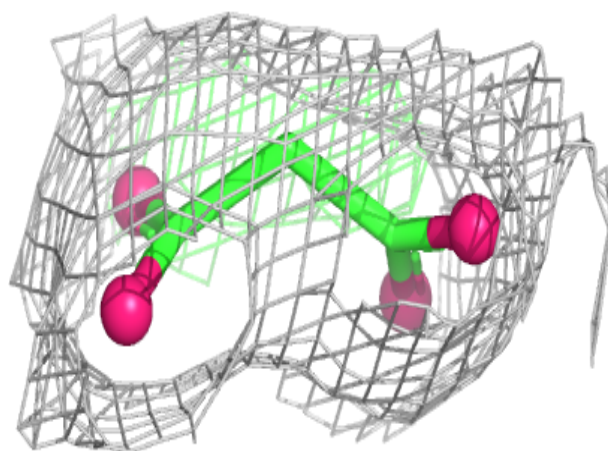
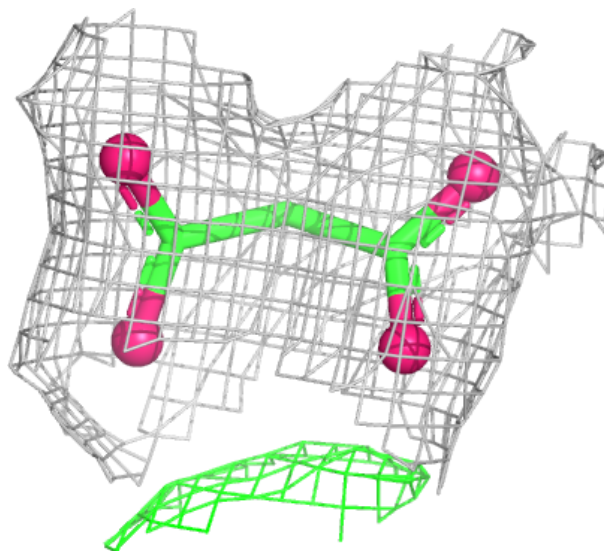
**Electron density around G6P G 501:**

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



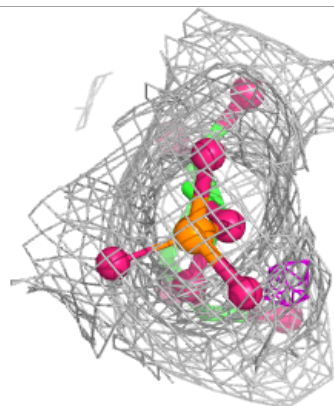
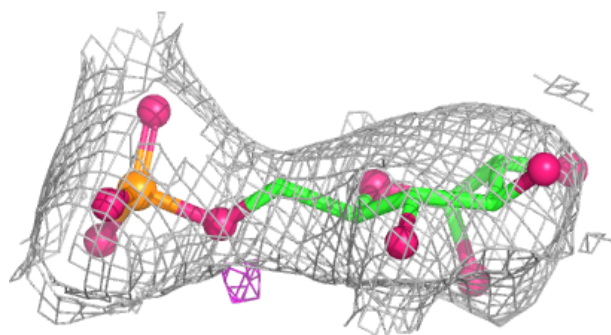
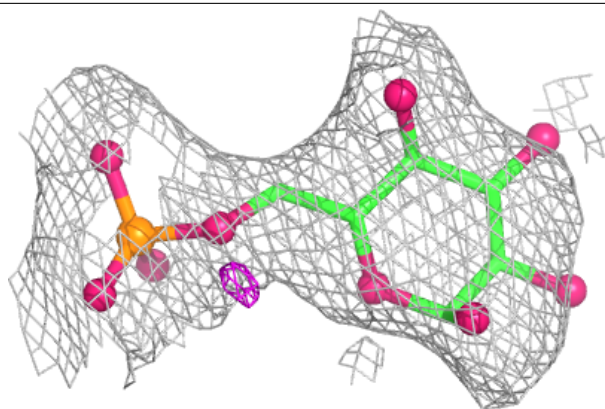
Electron density around MLI B 504:

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



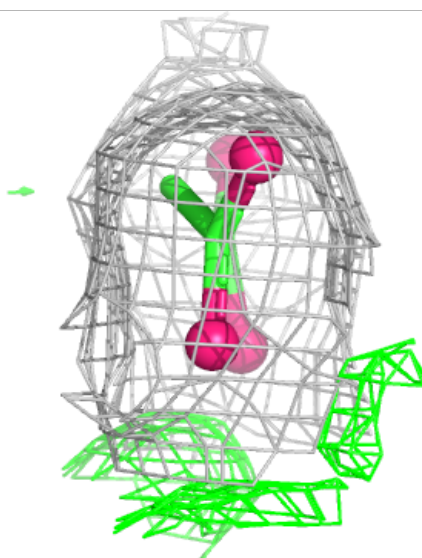
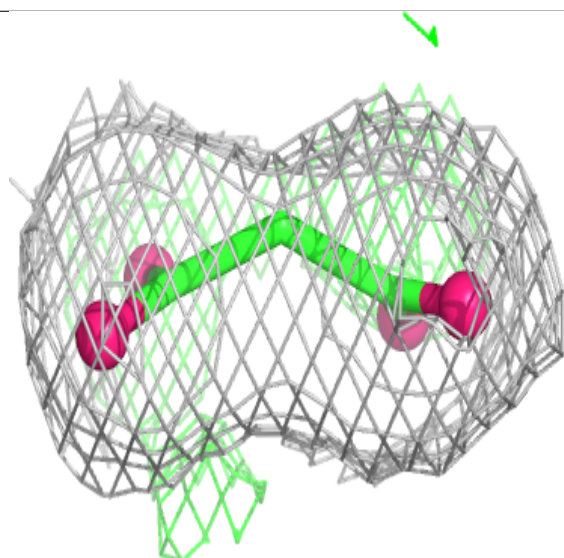
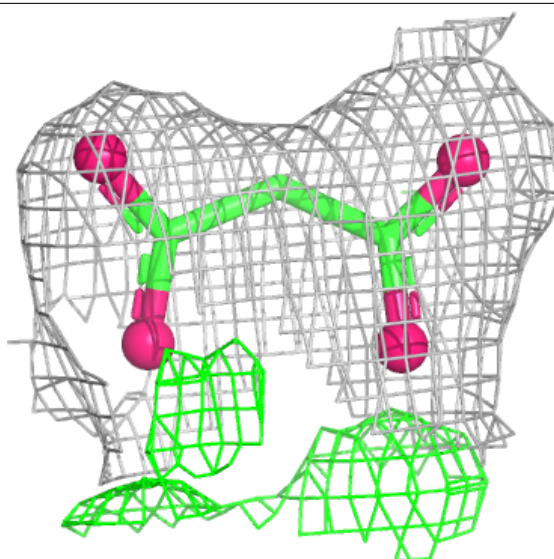
Electron density around G6P K 501:

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



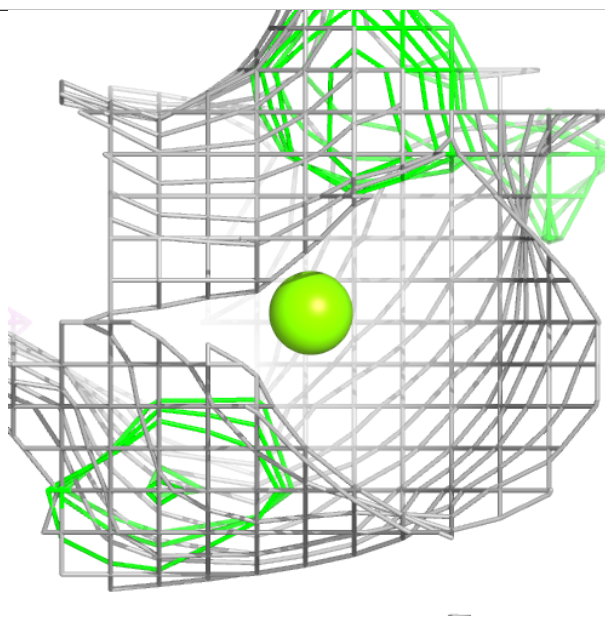
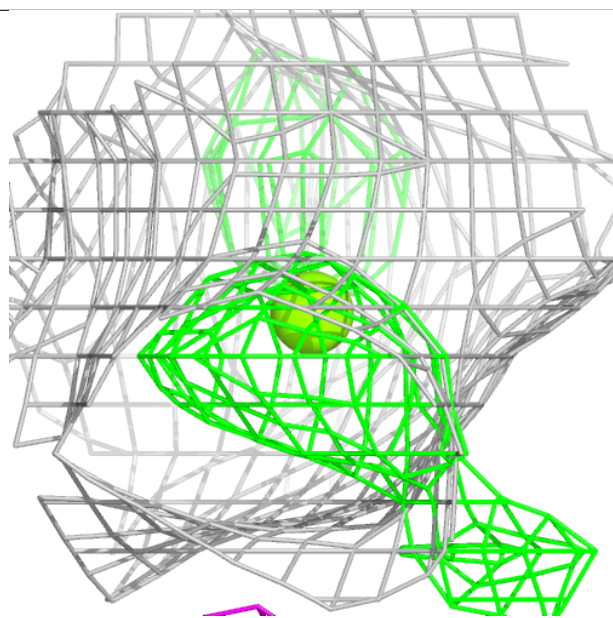
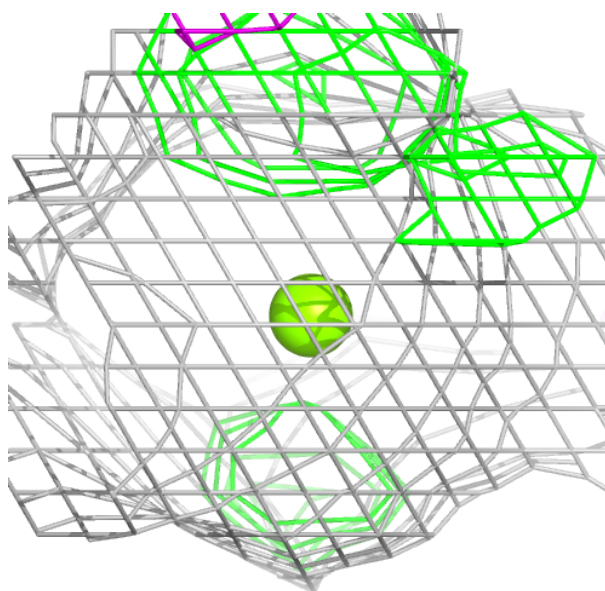
Electron density around MLI D 504:

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



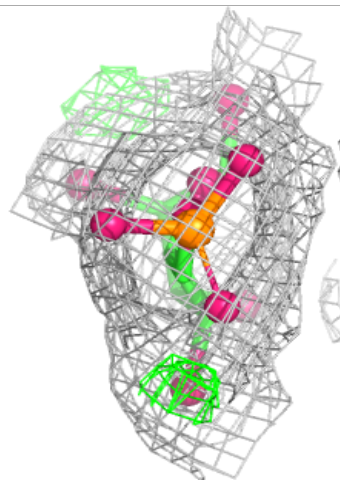
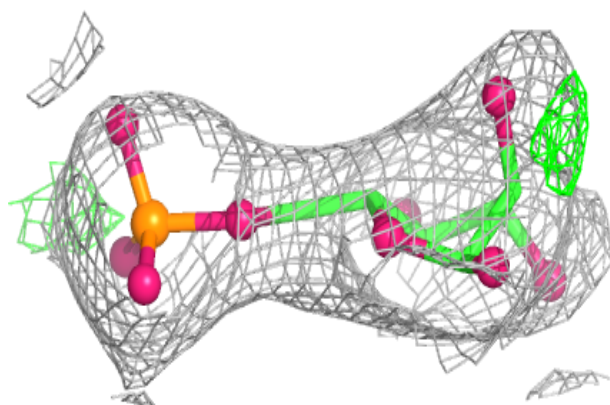
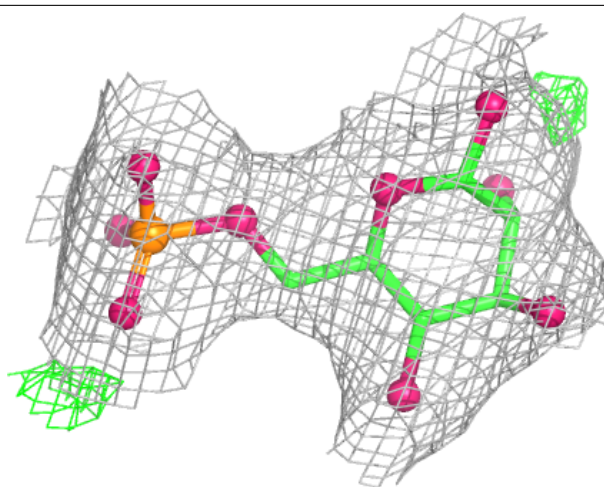
Electron density around MG K 502:

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



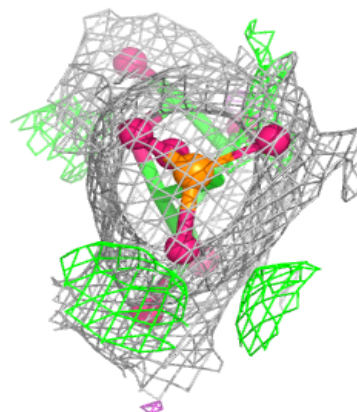
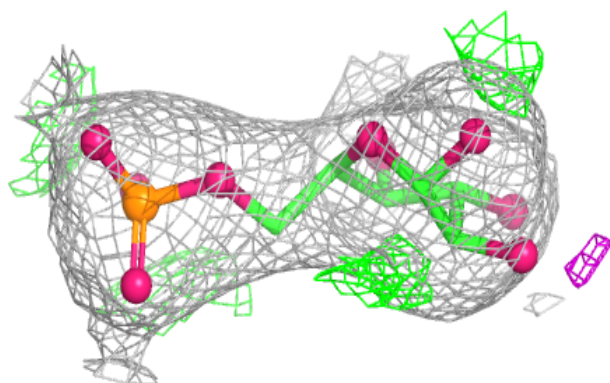
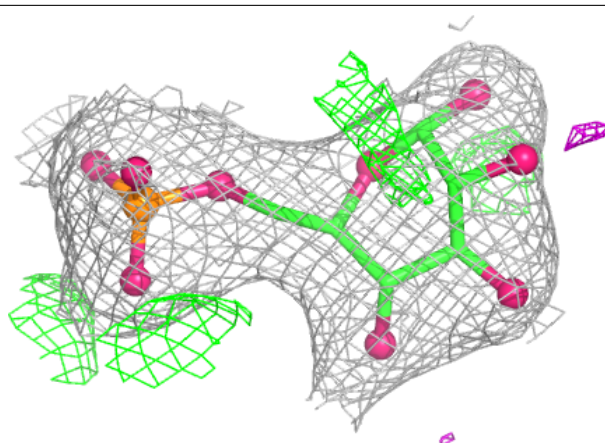
Electron density around G6P A 501:

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



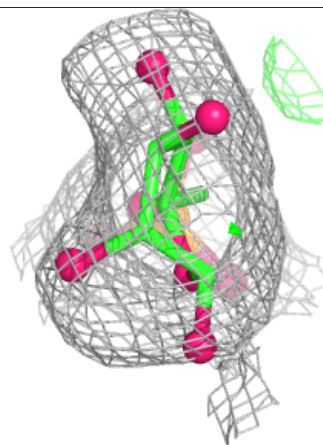
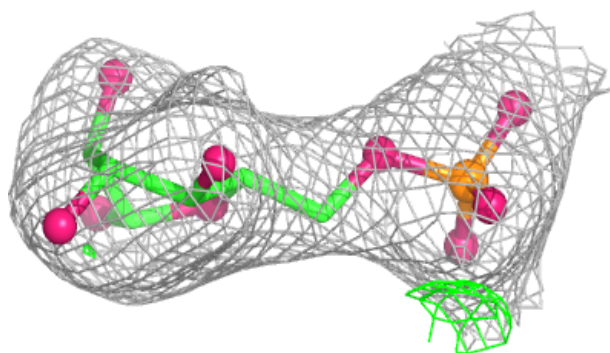
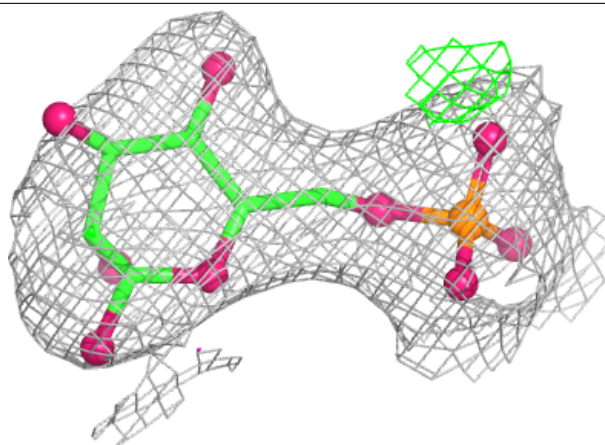
Electron density around G6P E 501:

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



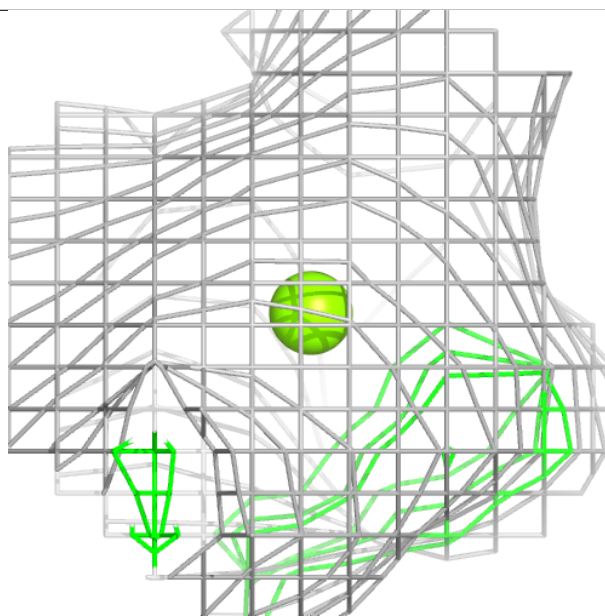
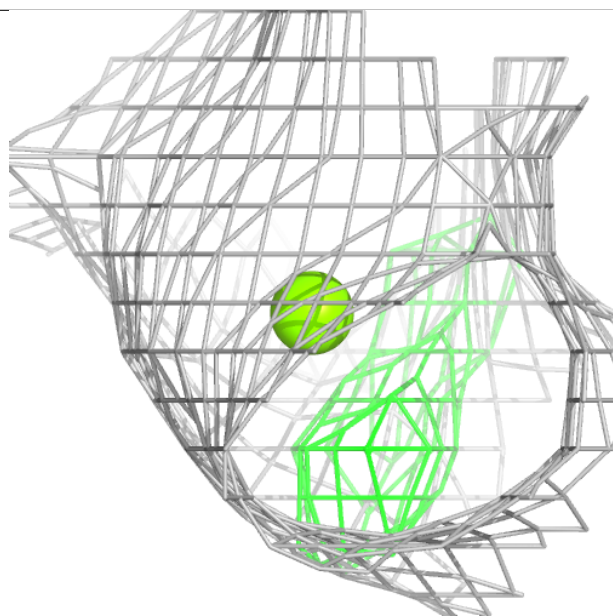
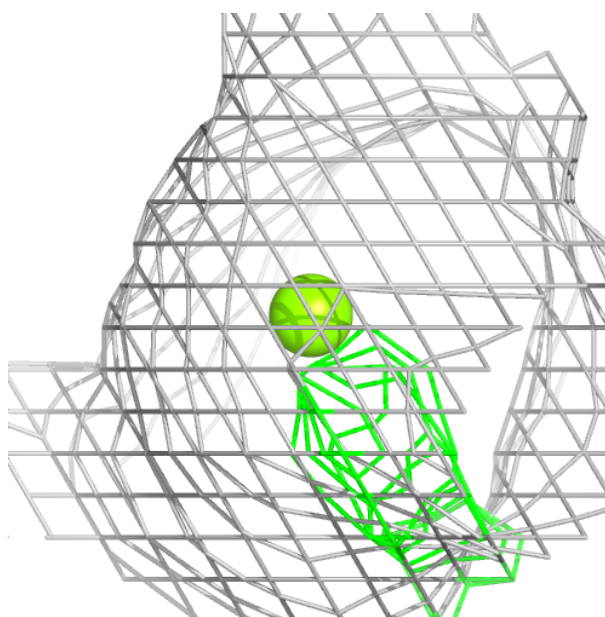
Electron density around G6P H 501:

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



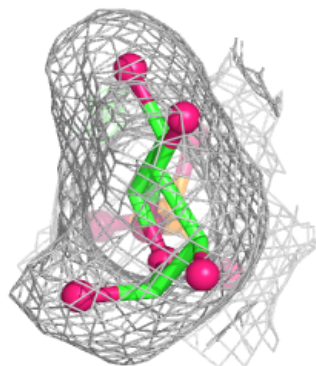
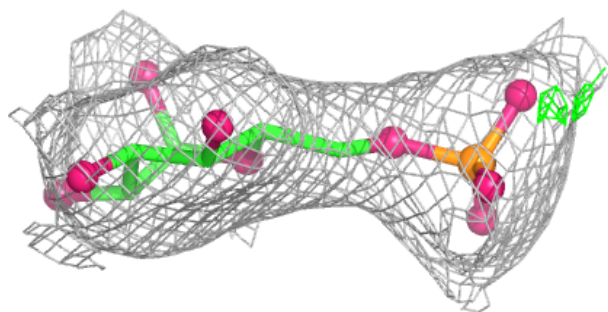
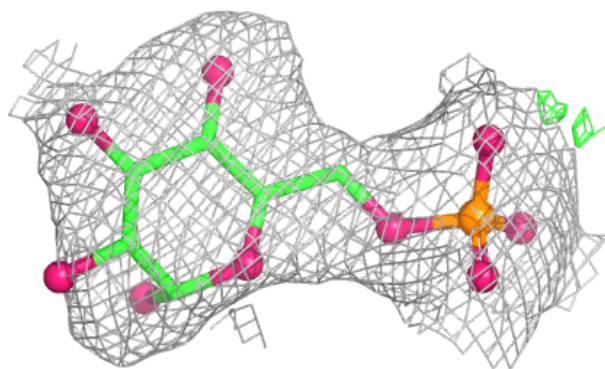
Electron density around MG F 502:

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



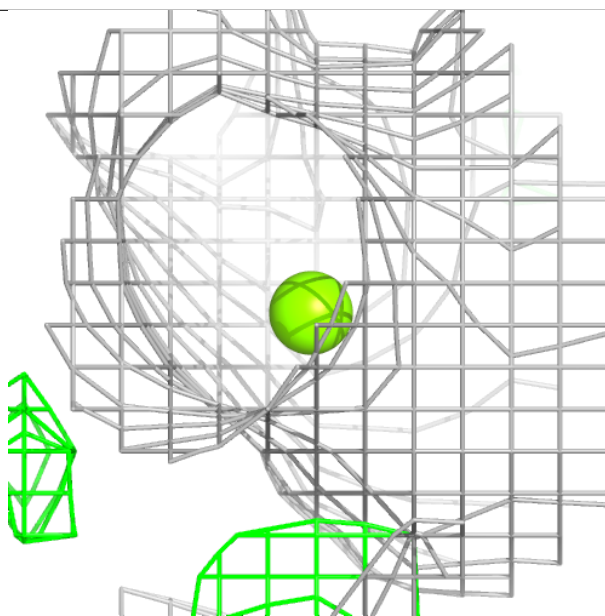
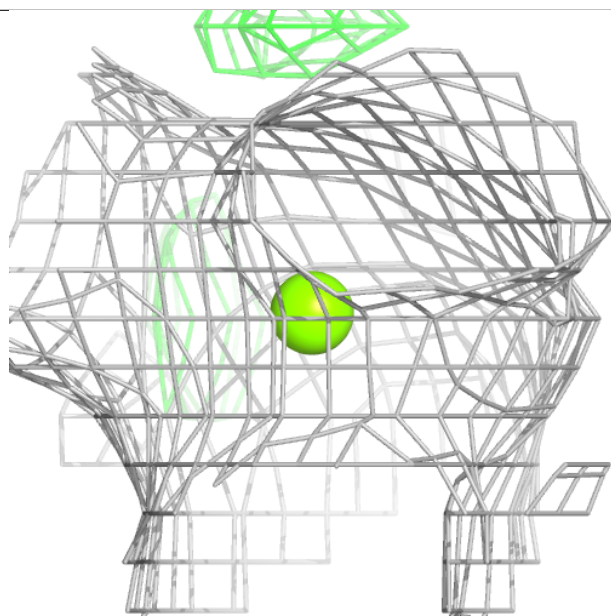
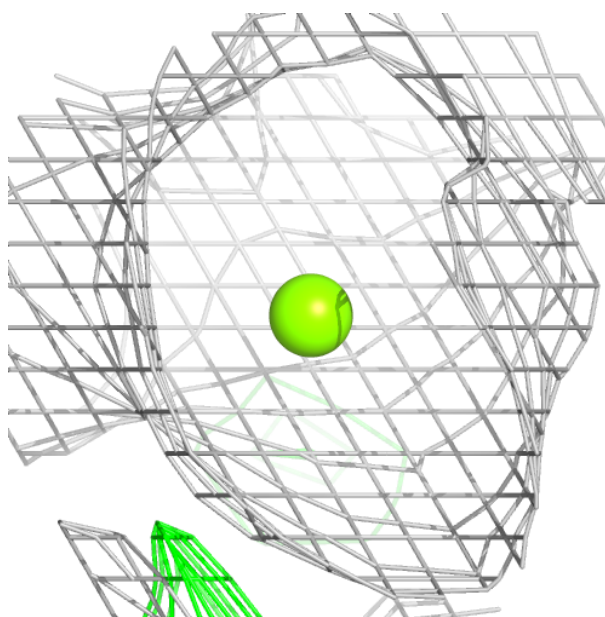
Electron density around G6P I 501:

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



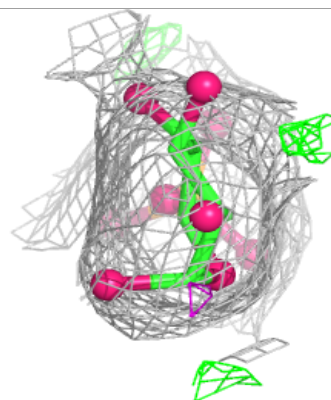
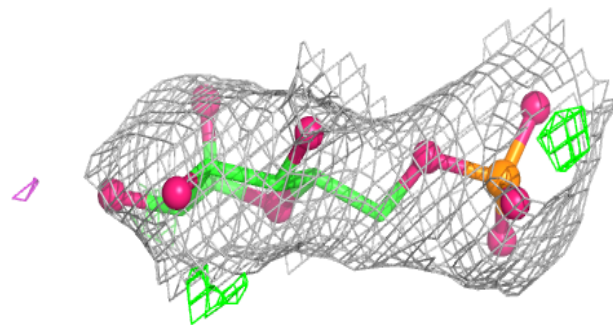
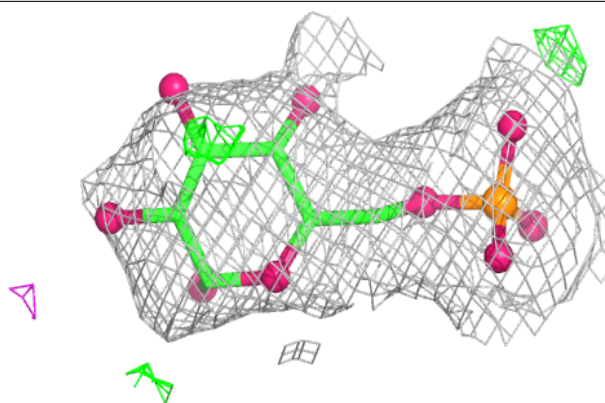
Electron density around MG J 502:

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



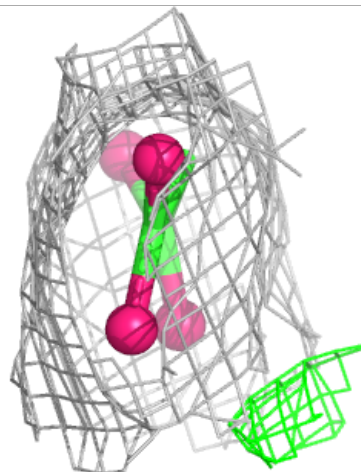
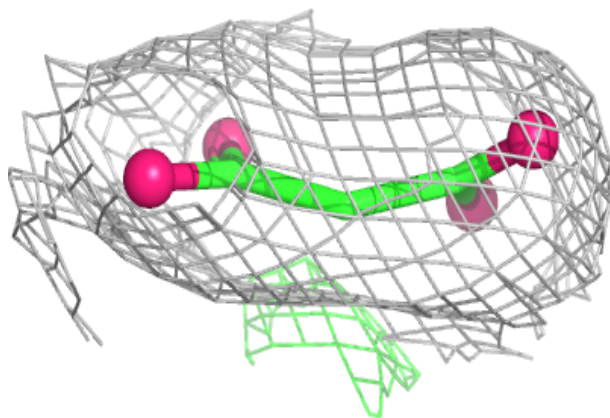
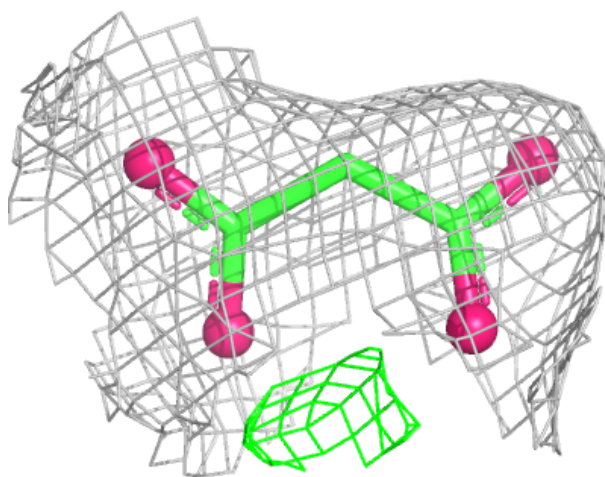
Electron density around G6P J 501:

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



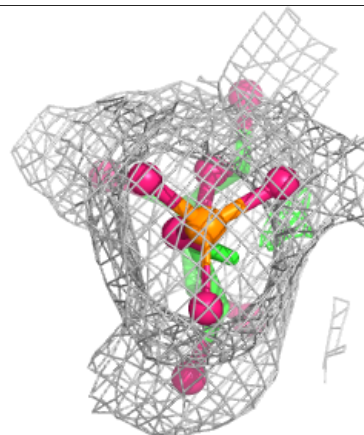
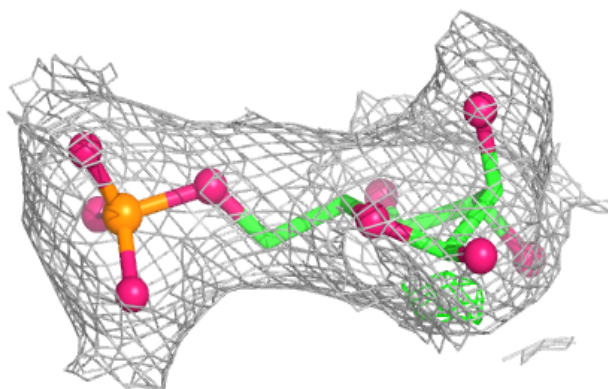
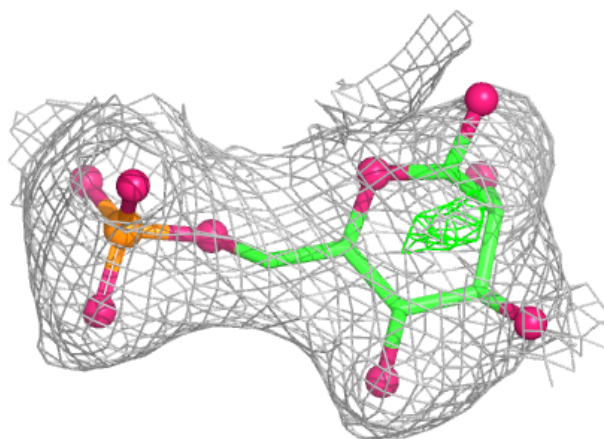
Electron density around MLI G 503:

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



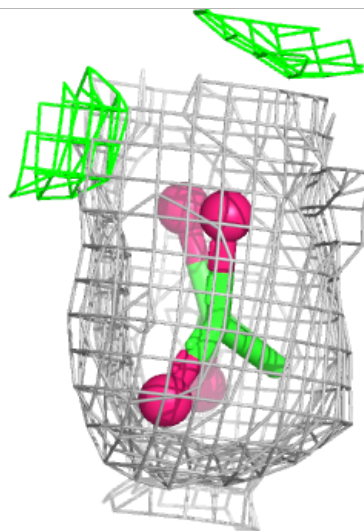
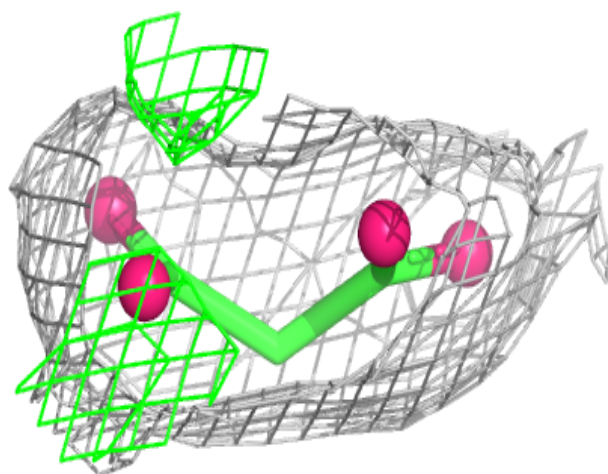
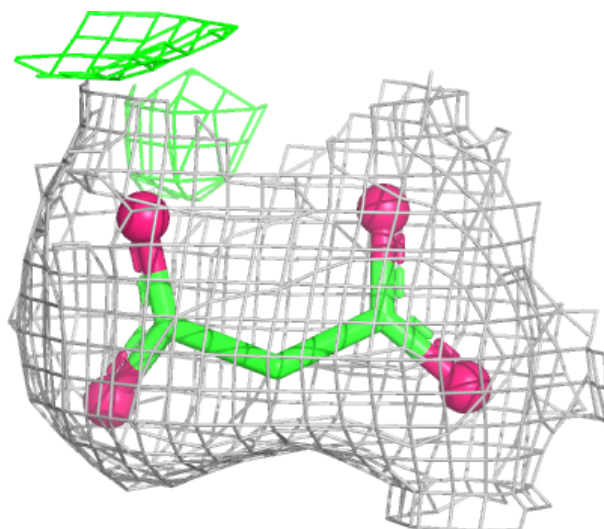
Electron density around G6P C 501:

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



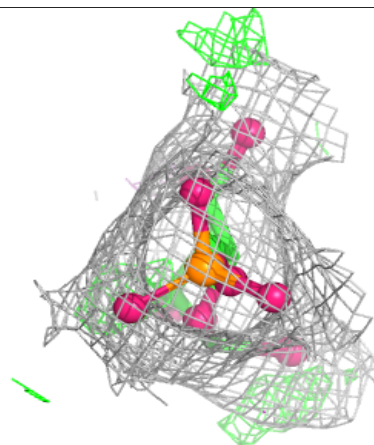
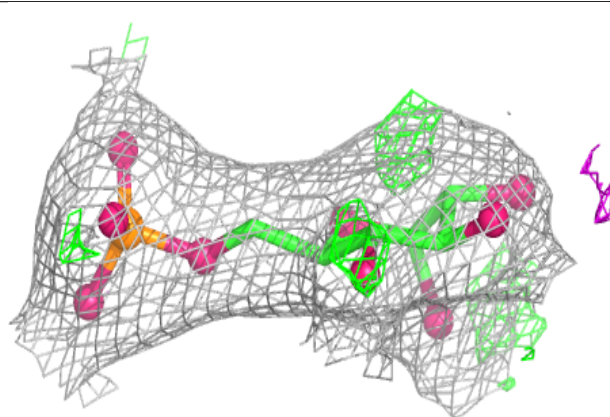
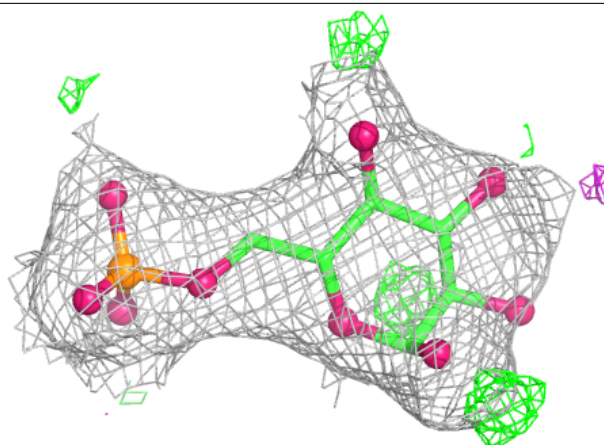
Electron density around MLI E 504:

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



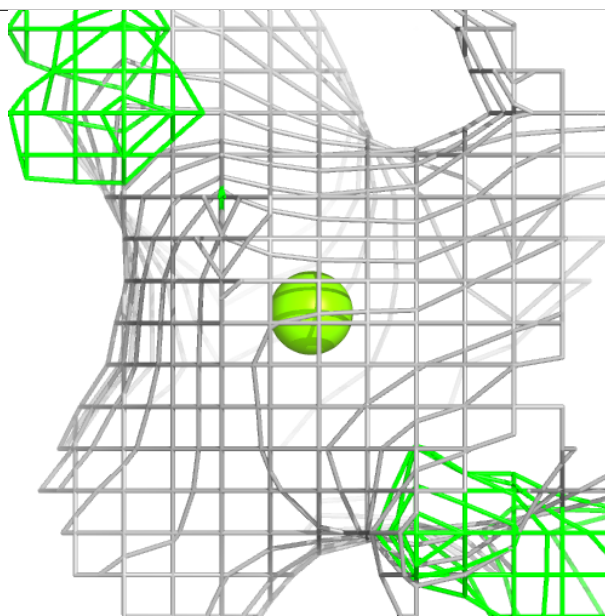
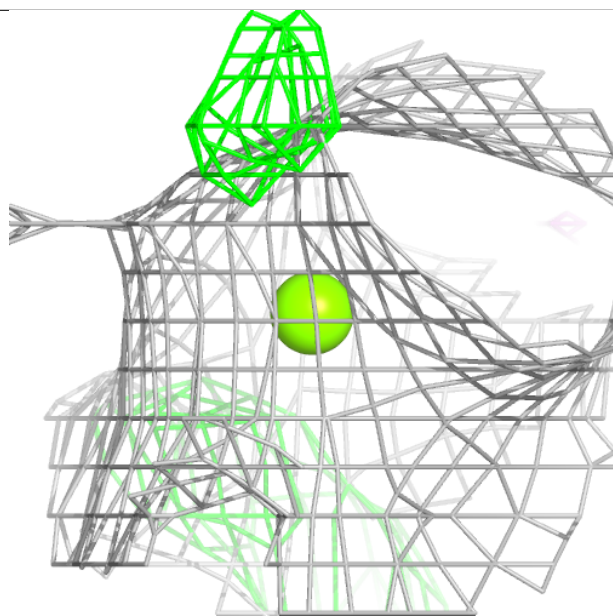
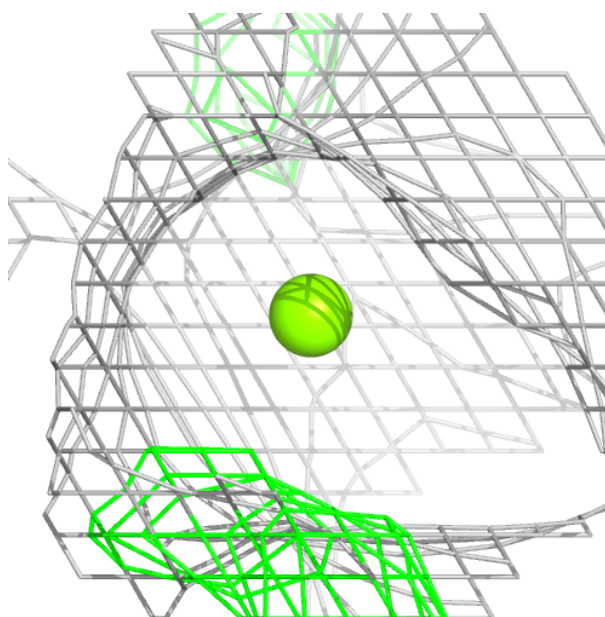
Electron density around G6P D 501:

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



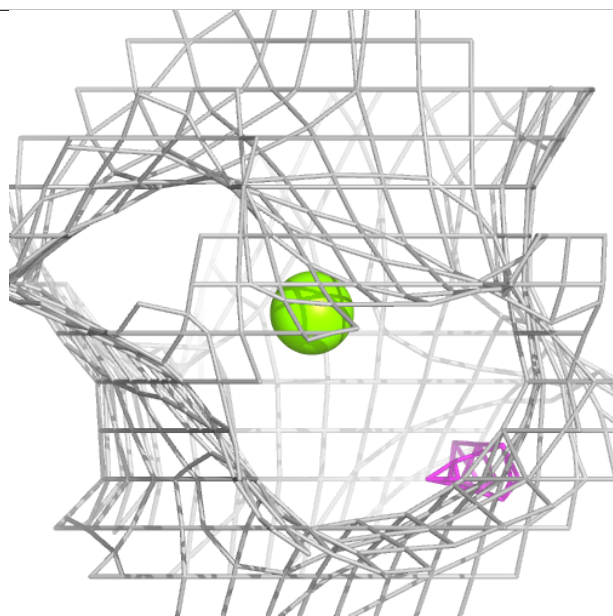
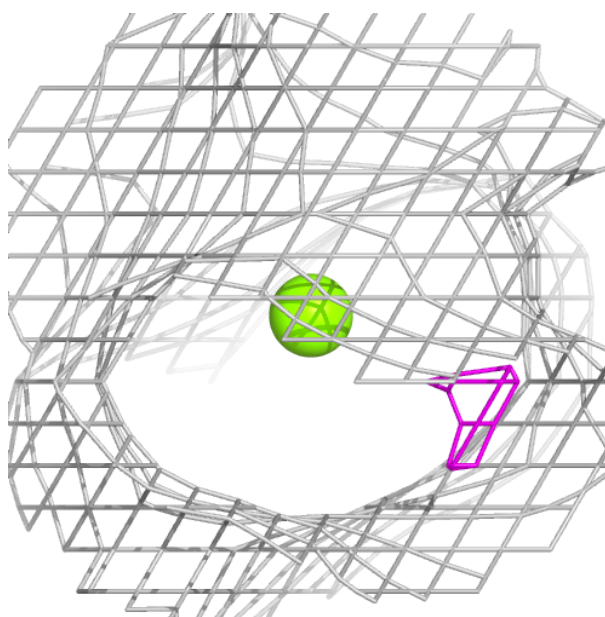
Electron density around MG H 502:

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



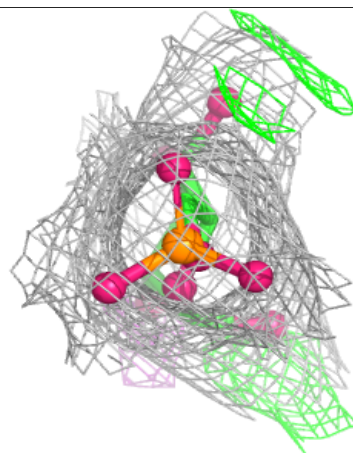
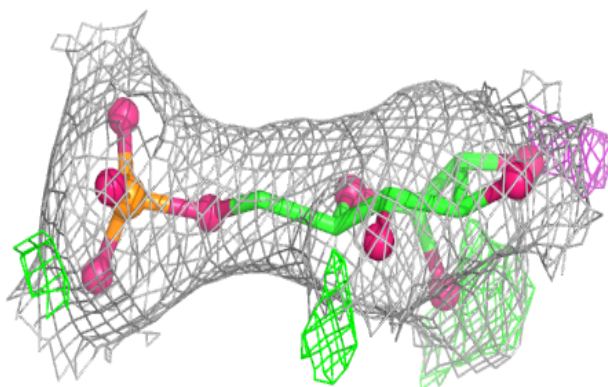
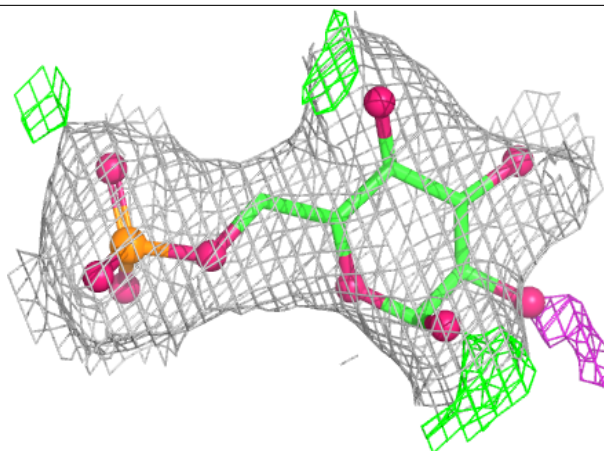
Electron density around MG A 502:

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



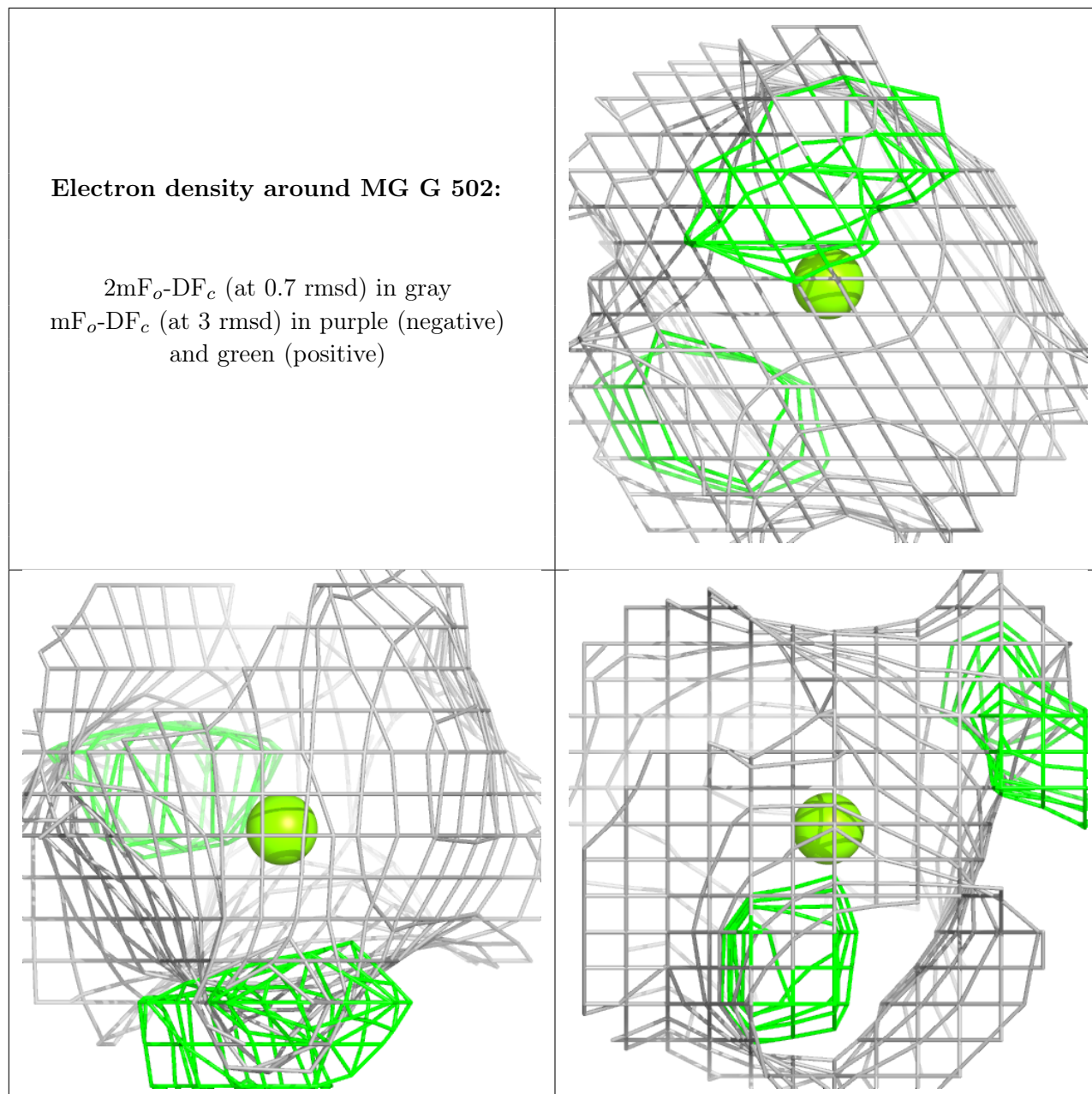
Electron density around G6P B 501:

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



Electron density around MG G 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.