



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 02:24 AM UTC

PDB ID : 9HDE / pdb_00009hde
Title : Crystal structure of methionine gamma-lyase (K209Q variant) from *Brevibacterium aurantiacum* in complex with PLP and alpha-ketobutyrate
Authors : Kopecny, D.; Ferchaud, N.; Briozzo, P.
Deposited on : 2024-11-12
Resolution : 2.52 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 types of validation reports are described at

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

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

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

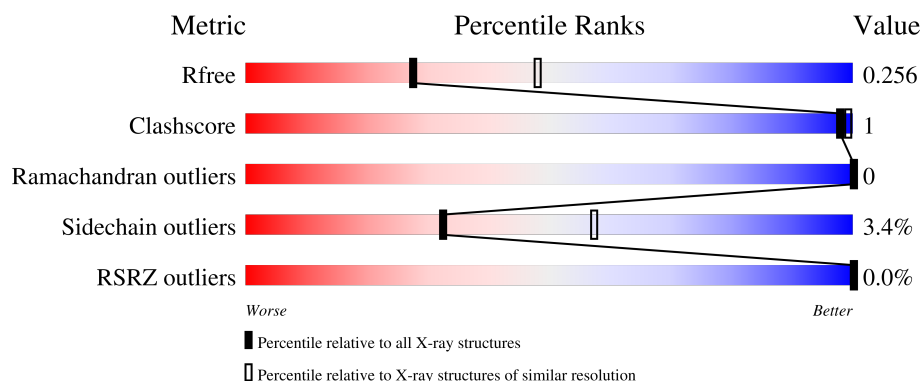
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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.
















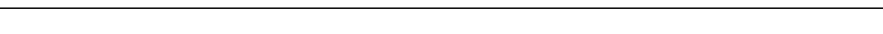





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	413	<div> <div>90%</div> <div>6%</div> </div>
1	B	413	<div> <div>88%</div> <div>5%</div> <div>6%</div> </div>
1	C	413	<div> <div>90%</div> <div>6%</div> </div>
1	D	413	<div> <div>91%</div> <div>6%</div> </div>
1	E	413	<div> <div>90%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	413	 90% • 6%
1	G	413	 90% • 6%
1	H	413	 90% • 6%
1	I	413	 90% • 6%
1	J	413	 90% • 6%
1	K	413	 89% 5% 6%
1	L	413	 91% • 6%
1	M	413	 89% 5% 6%
1	N	413	 89% 5% 6%
1	O	413	 89% 5% 6%
1	P	413	 89% • 6%
1	Q	413	 89% 5% 6%
1	R	413	 90% • 6%
1	S	413	 90% • 6%
1	T	413	 90% • 7%
1	U	413	 90% • 6%
1	V	413	 87% 6% 7%
1	W	413	 89% • 7%
1	X	413	 88% 5% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 135917 atoms, of which 67360 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 Cystathionine gamma-synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	387	Total	C	H	N	O	S	0	0	0
			5600	1759	2790	500	538	13			
1	B	387	Total	C	H	N	O	S	0	0	0
			5600	1759	2790	500	538	13			
1	C	387	Total	C	H	N	O	S	0	0	0
			5600	1759	2790	500	538	13			
1	D	387	Total	C	H	N	O	S	0	0	0
			5600	1759	2790	500	538	13			
1	E	388	Total	C	H	N	O	S	0	0	0
			5614	1763	2797	501	540	13			
1	F	387	Total	C	H	N	O	S	0	0	0
			5603	1760	2792	500	538	13			
1	G	387	Total	C	H	N	O	S	0	0	0
			5600	1759	2790	500	538	13			
1	H	387	Total	C	H	N	O	S	0	0	0
			5600	1759	2790	500	538	13			
1	I	387	Total	C	H	N	O	S	0	0	0
			5603	1760	2792	500	538	13			
1	J	387	Total	C	H	N	O	S	0	0	0
			5600	1759	2790	500	538	13			
1	K	387	Total	C	H	N	O	S	0	0	0
			5600	1759	2790	500	538	13			
1	L	388	Total	C	H	N	O	S	0	0	0
			5614	1763	2797	501	540	13			
1	M	388	Total	C	H	N	O	S	0	0	0
			5614	1763	2797	501	540	13			
1	N	388	Total	C	H	N	O	S	0	0	0
			5614	1763	2797	501	540	13			
1	O	388	Total	C	H	N	O	S	0	0	0
			5614	1763	2797	501	540	13			
1	P	388	Total	C	H	N	O	S	0	0	0
			5614	1763	2797	501	540	13			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	388	Total	C	H	N	O	S	0	0	0
			5614	1763	2797	501	540	13			
1	R	387	Total	C	H	N	O	S	0	0	0
			5600	1759	2790	500	538	13			
1	S	388	Total	C	H	N	O	S	0	0	0
			5614	1763	2797	501	540	13			
1	T	386	Total	C	H	N	O	S	0	0	0
			5589	1756	2785	499	536	13			
1	U	387	Total	C	H	N	O	S	0	0	0
			5600	1759	2790	500	538	13			
1	V	385	Total	C	H	N	O	S	0	0	0
			5578	1753	2780	498	534	13			
1	W	386	Total	C	H	N	O	S	0	0	0
			5589	1756	2785	499	536	13			
1	X	387	Total	C	H	N	O	S	0	0	0
			5603	1760	2792	500	538	13			

There are 504 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
A	-18	GLY	-	expression tag	UNP A0A2H1K3G9
A	-17	SER	-	expression tag	UNP A0A2H1K3G9
A	-16	SER	-	expression tag	UNP A0A2H1K3G9
A	-15	HIS	-	expression tag	UNP A0A2H1K3G9
A	-14	HIS	-	expression tag	UNP A0A2H1K3G9
A	-13	HIS	-	expression tag	UNP A0A2H1K3G9
A	-12	HIS	-	expression tag	UNP A0A2H1K3G9
A	-11	HIS	-	expression tag	UNP A0A2H1K3G9
A	-10	HIS	-	expression tag	UNP A0A2H1K3G9
A	-9	SER	-	expression tag	UNP A0A2H1K3G9
A	-8	SER	-	expression tag	UNP A0A2H1K3G9
A	-7	GLY	-	expression tag	UNP A0A2H1K3G9
A	-6	LEU	-	expression tag	UNP A0A2H1K3G9
A	-5	VAL	-	expression tag	UNP A0A2H1K3G9
A	-4	PRO	-	expression tag	UNP A0A2H1K3G9
A	-3	ARG	-	expression tag	UNP A0A2H1K3G9
A	-2	GLY	-	expression tag	UNP A0A2H1K3G9
A	-1	SER	-	expression tag	UNP A0A2H1K3G9
A	0	HIS	-	expression tag	UNP A0A2H1K3G9
A	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
B	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
B	-18	GLY	-	expression tag	UNP A0A2H1K3G9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP A0A2H1K3G9
B	-16	SER	-	expression tag	UNP A0A2H1K3G9
B	-15	HIS	-	expression tag	UNP A0A2H1K3G9
B	-14	HIS	-	expression tag	UNP A0A2H1K3G9
B	-13	HIS	-	expression tag	UNP A0A2H1K3G9
B	-12	HIS	-	expression tag	UNP A0A2H1K3G9
B	-11	HIS	-	expression tag	UNP A0A2H1K3G9
B	-10	HIS	-	expression tag	UNP A0A2H1K3G9
B	-9	SER	-	expression tag	UNP A0A2H1K3G9
B	-8	SER	-	expression tag	UNP A0A2H1K3G9
B	-7	GLY	-	expression tag	UNP A0A2H1K3G9
B	-6	LEU	-	expression tag	UNP A0A2H1K3G9
B	-5	VAL	-	expression tag	UNP A0A2H1K3G9
B	-4	PRO	-	expression tag	UNP A0A2H1K3G9
B	-3	ARG	-	expression tag	UNP A0A2H1K3G9
B	-2	GLY	-	expression tag	UNP A0A2H1K3G9
B	-1	SER	-	expression tag	UNP A0A2H1K3G9
B	0	HIS	-	expression tag	UNP A0A2H1K3G9
B	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
C	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
C	-18	GLY	-	expression tag	UNP A0A2H1K3G9
C	-17	SER	-	expression tag	UNP A0A2H1K3G9
C	-16	SER	-	expression tag	UNP A0A2H1K3G9
C	-15	HIS	-	expression tag	UNP A0A2H1K3G9
C	-14	HIS	-	expression tag	UNP A0A2H1K3G9
C	-13	HIS	-	expression tag	UNP A0A2H1K3G9
C	-12	HIS	-	expression tag	UNP A0A2H1K3G9
C	-11	HIS	-	expression tag	UNP A0A2H1K3G9
C	-10	HIS	-	expression tag	UNP A0A2H1K3G9
C	-9	SER	-	expression tag	UNP A0A2H1K3G9
C	-8	SER	-	expression tag	UNP A0A2H1K3G9
C	-7	GLY	-	expression tag	UNP A0A2H1K3G9
C	-6	LEU	-	expression tag	UNP A0A2H1K3G9
C	-5	VAL	-	expression tag	UNP A0A2H1K3G9
C	-4	PRO	-	expression tag	UNP A0A2H1K3G9
C	-3	ARG	-	expression tag	UNP A0A2H1K3G9
C	-2	GLY	-	expression tag	UNP A0A2H1K3G9
C	-1	SER	-	expression tag	UNP A0A2H1K3G9
C	0	HIS	-	expression tag	UNP A0A2H1K3G9
C	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
D	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
D	-18	GLY	-	expression tag	UNP A0A2H1K3G9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	expression tag	UNP A0A2H1K3G9
D	-16	SER	-	expression tag	UNP A0A2H1K3G9
D	-15	HIS	-	expression tag	UNP A0A2H1K3G9
D	-14	HIS	-	expression tag	UNP A0A2H1K3G9
D	-13	HIS	-	expression tag	UNP A0A2H1K3G9
D	-12	HIS	-	expression tag	UNP A0A2H1K3G9
D	-11	HIS	-	expression tag	UNP A0A2H1K3G9
D	-10	HIS	-	expression tag	UNP A0A2H1K3G9
D	-9	SER	-	expression tag	UNP A0A2H1K3G9
D	-8	SER	-	expression tag	UNP A0A2H1K3G9
D	-7	GLY	-	expression tag	UNP A0A2H1K3G9
D	-6	LEU	-	expression tag	UNP A0A2H1K3G9
D	-5	VAL	-	expression tag	UNP A0A2H1K3G9
D	-4	PRO	-	expression tag	UNP A0A2H1K3G9
D	-3	ARG	-	expression tag	UNP A0A2H1K3G9
D	-2	GLY	-	expression tag	UNP A0A2H1K3G9
D	-1	SER	-	expression tag	UNP A0A2H1K3G9
D	0	HIS	-	expression tag	UNP A0A2H1K3G9
D	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
E	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
E	-18	GLY	-	expression tag	UNP A0A2H1K3G9
E	-17	SER	-	expression tag	UNP A0A2H1K3G9
E	-16	SER	-	expression tag	UNP A0A2H1K3G9
E	-15	HIS	-	expression tag	UNP A0A2H1K3G9
E	-14	HIS	-	expression tag	UNP A0A2H1K3G9
E	-13	HIS	-	expression tag	UNP A0A2H1K3G9
E	-12	HIS	-	expression tag	UNP A0A2H1K3G9
E	-11	HIS	-	expression tag	UNP A0A2H1K3G9
E	-10	HIS	-	expression tag	UNP A0A2H1K3G9
E	-9	SER	-	expression tag	UNP A0A2H1K3G9
E	-8	SER	-	expression tag	UNP A0A2H1K3G9
E	-7	GLY	-	expression tag	UNP A0A2H1K3G9
E	-6	LEU	-	expression tag	UNP A0A2H1K3G9
E	-5	VAL	-	expression tag	UNP A0A2H1K3G9
E	-4	PRO	-	expression tag	UNP A0A2H1K3G9
E	-3	ARG	-	expression tag	UNP A0A2H1K3G9
E	-2	GLY	-	expression tag	UNP A0A2H1K3G9
E	-1	SER	-	expression tag	UNP A0A2H1K3G9
E	0	HIS	-	expression tag	UNP A0A2H1K3G9
E	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
F	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
F	-18	GLY	-	expression tag	UNP A0A2H1K3G9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-17	SER	-	expression tag	UNP A0A2H1K3G9
F	-16	SER	-	expression tag	UNP A0A2H1K3G9
F	-15	HIS	-	expression tag	UNP A0A2H1K3G9
F	-14	HIS	-	expression tag	UNP A0A2H1K3G9
F	-13	HIS	-	expression tag	UNP A0A2H1K3G9
F	-12	HIS	-	expression tag	UNP A0A2H1K3G9
F	-11	HIS	-	expression tag	UNP A0A2H1K3G9
F	-10	HIS	-	expression tag	UNP A0A2H1K3G9
F	-9	SER	-	expression tag	UNP A0A2H1K3G9
F	-8	SER	-	expression tag	UNP A0A2H1K3G9
F	-7	GLY	-	expression tag	UNP A0A2H1K3G9
F	-6	LEU	-	expression tag	UNP A0A2H1K3G9
F	-5	VAL	-	expression tag	UNP A0A2H1K3G9
F	-4	PRO	-	expression tag	UNP A0A2H1K3G9
F	-3	ARG	-	expression tag	UNP A0A2H1K3G9
F	-2	GLY	-	expression tag	UNP A0A2H1K3G9
F	-1	SER	-	expression tag	UNP A0A2H1K3G9
F	0	HIS	-	expression tag	UNP A0A2H1K3G9
F	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
G	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
G	-18	GLY	-	expression tag	UNP A0A2H1K3G9
G	-17	SER	-	expression tag	UNP A0A2H1K3G9
G	-16	SER	-	expression tag	UNP A0A2H1K3G9
G	-15	HIS	-	expression tag	UNP A0A2H1K3G9
G	-14	HIS	-	expression tag	UNP A0A2H1K3G9
G	-13	HIS	-	expression tag	UNP A0A2H1K3G9
G	-12	HIS	-	expression tag	UNP A0A2H1K3G9
G	-11	HIS	-	expression tag	UNP A0A2H1K3G9
G	-10	HIS	-	expression tag	UNP A0A2H1K3G9
G	-9	SER	-	expression tag	UNP A0A2H1K3G9
G	-8	SER	-	expression tag	UNP A0A2H1K3G9
G	-7	GLY	-	expression tag	UNP A0A2H1K3G9
G	-6	LEU	-	expression tag	UNP A0A2H1K3G9
G	-5	VAL	-	expression tag	UNP A0A2H1K3G9
G	-4	PRO	-	expression tag	UNP A0A2H1K3G9
G	-3	ARG	-	expression tag	UNP A0A2H1K3G9
G	-2	GLY	-	expression tag	UNP A0A2H1K3G9
G	-1	SER	-	expression tag	UNP A0A2H1K3G9
G	0	HIS	-	expression tag	UNP A0A2H1K3G9
G	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
H	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
H	-18	GLY	-	expression tag	UNP A0A2H1K3G9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-17	SER	-	expression tag	UNP A0A2H1K3G9
H	-16	SER	-	expression tag	UNP A0A2H1K3G9
H	-15	HIS	-	expression tag	UNP A0A2H1K3G9
H	-14	HIS	-	expression tag	UNP A0A2H1K3G9
H	-13	HIS	-	expression tag	UNP A0A2H1K3G9
H	-12	HIS	-	expression tag	UNP A0A2H1K3G9
H	-11	HIS	-	expression tag	UNP A0A2H1K3G9
H	-10	HIS	-	expression tag	UNP A0A2H1K3G9
H	-9	SER	-	expression tag	UNP A0A2H1K3G9
H	-8	SER	-	expression tag	UNP A0A2H1K3G9
H	-7	GLY	-	expression tag	UNP A0A2H1K3G9
H	-6	LEU	-	expression tag	UNP A0A2H1K3G9
H	-5	VAL	-	expression tag	UNP A0A2H1K3G9
H	-4	PRO	-	expression tag	UNP A0A2H1K3G9
H	-3	ARG	-	expression tag	UNP A0A2H1K3G9
H	-2	GLY	-	expression tag	UNP A0A2H1K3G9
H	-1	SER	-	expression tag	UNP A0A2H1K3G9
H	0	HIS	-	expression tag	UNP A0A2H1K3G9
H	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
I	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
I	-18	GLY	-	expression tag	UNP A0A2H1K3G9
I	-17	SER	-	expression tag	UNP A0A2H1K3G9
I	-16	SER	-	expression tag	UNP A0A2H1K3G9
I	-15	HIS	-	expression tag	UNP A0A2H1K3G9
I	-14	HIS	-	expression tag	UNP A0A2H1K3G9
I	-13	HIS	-	expression tag	UNP A0A2H1K3G9
I	-12	HIS	-	expression tag	UNP A0A2H1K3G9
I	-11	HIS	-	expression tag	UNP A0A2H1K3G9
I	-10	HIS	-	expression tag	UNP A0A2H1K3G9
I	-9	SER	-	expression tag	UNP A0A2H1K3G9
I	-8	SER	-	expression tag	UNP A0A2H1K3G9
I	-7	GLY	-	expression tag	UNP A0A2H1K3G9
I	-6	LEU	-	expression tag	UNP A0A2H1K3G9
I	-5	VAL	-	expression tag	UNP A0A2H1K3G9
I	-4	PRO	-	expression tag	UNP A0A2H1K3G9
I	-3	ARG	-	expression tag	UNP A0A2H1K3G9
I	-2	GLY	-	expression tag	UNP A0A2H1K3G9
I	-1	SER	-	expression tag	UNP A0A2H1K3G9
I	0	HIS	-	expression tag	UNP A0A2H1K3G9
I	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
J	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
J	-18	GLY	-	expression tag	UNP A0A2H1K3G9

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-17	SER	-	expression tag	UNP A0A2H1K3G9
J	-16	SER	-	expression tag	UNP A0A2H1K3G9
J	-15	HIS	-	expression tag	UNP A0A2H1K3G9
J	-14	HIS	-	expression tag	UNP A0A2H1K3G9
J	-13	HIS	-	expression tag	UNP A0A2H1K3G9
J	-12	HIS	-	expression tag	UNP A0A2H1K3G9
J	-11	HIS	-	expression tag	UNP A0A2H1K3G9
J	-10	HIS	-	expression tag	UNP A0A2H1K3G9
J	-9	SER	-	expression tag	UNP A0A2H1K3G9
J	-8	SER	-	expression tag	UNP A0A2H1K3G9
J	-7	GLY	-	expression tag	UNP A0A2H1K3G9
J	-6	LEU	-	expression tag	UNP A0A2H1K3G9
J	-5	VAL	-	expression tag	UNP A0A2H1K3G9
J	-4	PRO	-	expression tag	UNP A0A2H1K3G9
J	-3	ARG	-	expression tag	UNP A0A2H1K3G9
J	-2	GLY	-	expression tag	UNP A0A2H1K3G9
J	-1	SER	-	expression tag	UNP A0A2H1K3G9
J	0	HIS	-	expression tag	UNP A0A2H1K3G9
J	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
K	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
K	-18	GLY	-	expression tag	UNP A0A2H1K3G9
K	-17	SER	-	expression tag	UNP A0A2H1K3G9
K	-16	SER	-	expression tag	UNP A0A2H1K3G9
K	-15	HIS	-	expression tag	UNP A0A2H1K3G9
K	-14	HIS	-	expression tag	UNP A0A2H1K3G9
K	-13	HIS	-	expression tag	UNP A0A2H1K3G9
K	-12	HIS	-	expression tag	UNP A0A2H1K3G9
K	-11	HIS	-	expression tag	UNP A0A2H1K3G9
K	-10	HIS	-	expression tag	UNP A0A2H1K3G9
K	-9	SER	-	expression tag	UNP A0A2H1K3G9
K	-8	SER	-	expression tag	UNP A0A2H1K3G9
K	-7	GLY	-	expression tag	UNP A0A2H1K3G9
K	-6	LEU	-	expression tag	UNP A0A2H1K3G9
K	-5	VAL	-	expression tag	UNP A0A2H1K3G9
K	-4	PRO	-	expression tag	UNP A0A2H1K3G9
K	-3	ARG	-	expression tag	UNP A0A2H1K3G9
K	-2	GLY	-	expression tag	UNP A0A2H1K3G9
K	-1	SER	-	expression tag	UNP A0A2H1K3G9
K	0	HIS	-	expression tag	UNP A0A2H1K3G9
K	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
L	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
L	-18	GLY	-	expression tag	UNP A0A2H1K3G9

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-17	SER	-	expression tag	UNP A0A2H1K3G9
L	-16	SER	-	expression tag	UNP A0A2H1K3G9
L	-15	HIS	-	expression tag	UNP A0A2H1K3G9
L	-14	HIS	-	expression tag	UNP A0A2H1K3G9
L	-13	HIS	-	expression tag	UNP A0A2H1K3G9
L	-12	HIS	-	expression tag	UNP A0A2H1K3G9
L	-11	HIS	-	expression tag	UNP A0A2H1K3G9
L	-10	HIS	-	expression tag	UNP A0A2H1K3G9
L	-9	SER	-	expression tag	UNP A0A2H1K3G9
L	-8	SER	-	expression tag	UNP A0A2H1K3G9
L	-7	GLY	-	expression tag	UNP A0A2H1K3G9
L	-6	LEU	-	expression tag	UNP A0A2H1K3G9
L	-5	VAL	-	expression tag	UNP A0A2H1K3G9
L	-4	PRO	-	expression tag	UNP A0A2H1K3G9
L	-3	ARG	-	expression tag	UNP A0A2H1K3G9
L	-2	GLY	-	expression tag	UNP A0A2H1K3G9
L	-1	SER	-	expression tag	UNP A0A2H1K3G9
L	0	HIS	-	expression tag	UNP A0A2H1K3G9
L	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
M	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
M	-18	GLY	-	expression tag	UNP A0A2H1K3G9
M	-17	SER	-	expression tag	UNP A0A2H1K3G9
M	-16	SER	-	expression tag	UNP A0A2H1K3G9
M	-15	HIS	-	expression tag	UNP A0A2H1K3G9
M	-14	HIS	-	expression tag	UNP A0A2H1K3G9
M	-13	HIS	-	expression tag	UNP A0A2H1K3G9
M	-12	HIS	-	expression tag	UNP A0A2H1K3G9
M	-11	HIS	-	expression tag	UNP A0A2H1K3G9
M	-10	HIS	-	expression tag	UNP A0A2H1K3G9
M	-9	SER	-	expression tag	UNP A0A2H1K3G9
M	-8	SER	-	expression tag	UNP A0A2H1K3G9
M	-7	GLY	-	expression tag	UNP A0A2H1K3G9
M	-6	LEU	-	expression tag	UNP A0A2H1K3G9
M	-5	VAL	-	expression tag	UNP A0A2H1K3G9
M	-4	PRO	-	expression tag	UNP A0A2H1K3G9
M	-3	ARG	-	expression tag	UNP A0A2H1K3G9
M	-2	GLY	-	expression tag	UNP A0A2H1K3G9
M	-1	SER	-	expression tag	UNP A0A2H1K3G9
M	0	HIS	-	expression tag	UNP A0A2H1K3G9
M	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
N	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
N	-18	GLY	-	expression tag	UNP A0A2H1K3G9

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-17	SER	-	expression tag	UNP A0A2H1K3G9
N	-16	SER	-	expression tag	UNP A0A2H1K3G9
N	-15	HIS	-	expression tag	UNP A0A2H1K3G9
N	-14	HIS	-	expression tag	UNP A0A2H1K3G9
N	-13	HIS	-	expression tag	UNP A0A2H1K3G9
N	-12	HIS	-	expression tag	UNP A0A2H1K3G9
N	-11	HIS	-	expression tag	UNP A0A2H1K3G9
N	-10	HIS	-	expression tag	UNP A0A2H1K3G9
N	-9	SER	-	expression tag	UNP A0A2H1K3G9
N	-8	SER	-	expression tag	UNP A0A2H1K3G9
N	-7	GLY	-	expression tag	UNP A0A2H1K3G9
N	-6	LEU	-	expression tag	UNP A0A2H1K3G9
N	-5	VAL	-	expression tag	UNP A0A2H1K3G9
N	-4	PRO	-	expression tag	UNP A0A2H1K3G9
N	-3	ARG	-	expression tag	UNP A0A2H1K3G9
N	-2	GLY	-	expression tag	UNP A0A2H1K3G9
N	-1	SER	-	expression tag	UNP A0A2H1K3G9
N	0	HIS	-	expression tag	UNP A0A2H1K3G9
N	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
O	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
O	-18	GLY	-	expression tag	UNP A0A2H1K3G9
O	-17	SER	-	expression tag	UNP A0A2H1K3G9
O	-16	SER	-	expression tag	UNP A0A2H1K3G9
O	-15	HIS	-	expression tag	UNP A0A2H1K3G9
O	-14	HIS	-	expression tag	UNP A0A2H1K3G9
O	-13	HIS	-	expression tag	UNP A0A2H1K3G9
O	-12	HIS	-	expression tag	UNP A0A2H1K3G9
O	-11	HIS	-	expression tag	UNP A0A2H1K3G9
O	-10	HIS	-	expression tag	UNP A0A2H1K3G9
O	-9	SER	-	expression tag	UNP A0A2H1K3G9
O	-8	SER	-	expression tag	UNP A0A2H1K3G9
O	-7	GLY	-	expression tag	UNP A0A2H1K3G9
O	-6	LEU	-	expression tag	UNP A0A2H1K3G9
O	-5	VAL	-	expression tag	UNP A0A2H1K3G9
O	-4	PRO	-	expression tag	UNP A0A2H1K3G9
O	-3	ARG	-	expression tag	UNP A0A2H1K3G9
O	-2	GLY	-	expression tag	UNP A0A2H1K3G9
O	-1	SER	-	expression tag	UNP A0A2H1K3G9
O	0	HIS	-	expression tag	UNP A0A2H1K3G9
O	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
P	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
P	-18	GLY	-	expression tag	UNP A0A2H1K3G9

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-17	SER	-	expression tag	UNP A0A2H1K3G9
P	-16	SER	-	expression tag	UNP A0A2H1K3G9
P	-15	HIS	-	expression tag	UNP A0A2H1K3G9
P	-14	HIS	-	expression tag	UNP A0A2H1K3G9
P	-13	HIS	-	expression tag	UNP A0A2H1K3G9
P	-12	HIS	-	expression tag	UNP A0A2H1K3G9
P	-11	HIS	-	expression tag	UNP A0A2H1K3G9
P	-10	HIS	-	expression tag	UNP A0A2H1K3G9
P	-9	SER	-	expression tag	UNP A0A2H1K3G9
P	-8	SER	-	expression tag	UNP A0A2H1K3G9
P	-7	GLY	-	expression tag	UNP A0A2H1K3G9
P	-6	LEU	-	expression tag	UNP A0A2H1K3G9
P	-5	VAL	-	expression tag	UNP A0A2H1K3G9
P	-4	PRO	-	expression tag	UNP A0A2H1K3G9
P	-3	ARG	-	expression tag	UNP A0A2H1K3G9
P	-2	GLY	-	expression tag	UNP A0A2H1K3G9
P	-1	SER	-	expression tag	UNP A0A2H1K3G9
P	0	HIS	-	expression tag	UNP A0A2H1K3G9
P	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
Q	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
Q	-18	GLY	-	expression tag	UNP A0A2H1K3G9
Q	-17	SER	-	expression tag	UNP A0A2H1K3G9
Q	-16	SER	-	expression tag	UNP A0A2H1K3G9
Q	-15	HIS	-	expression tag	UNP A0A2H1K3G9
Q	-14	HIS	-	expression tag	UNP A0A2H1K3G9
Q	-13	HIS	-	expression tag	UNP A0A2H1K3G9
Q	-12	HIS	-	expression tag	UNP A0A2H1K3G9
Q	-11	HIS	-	expression tag	UNP A0A2H1K3G9
Q	-10	HIS	-	expression tag	UNP A0A2H1K3G9
Q	-9	SER	-	expression tag	UNP A0A2H1K3G9
Q	-8	SER	-	expression tag	UNP A0A2H1K3G9
Q	-7	GLY	-	expression tag	UNP A0A2H1K3G9
Q	-6	LEU	-	expression tag	UNP A0A2H1K3G9
Q	-5	VAL	-	expression tag	UNP A0A2H1K3G9
Q	-4	PRO	-	expression tag	UNP A0A2H1K3G9
Q	-3	ARG	-	expression tag	UNP A0A2H1K3G9
Q	-2	GLY	-	expression tag	UNP A0A2H1K3G9
Q	-1	SER	-	expression tag	UNP A0A2H1K3G9
Q	0	HIS	-	expression tag	UNP A0A2H1K3G9
Q	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
R	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
R	-18	GLY	-	expression tag	UNP A0A2H1K3G9

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-17	SER	-	expression tag	UNP A0A2H1K3G9
R	-16	SER	-	expression tag	UNP A0A2H1K3G9
R	-15	HIS	-	expression tag	UNP A0A2H1K3G9
R	-14	HIS	-	expression tag	UNP A0A2H1K3G9
R	-13	HIS	-	expression tag	UNP A0A2H1K3G9
R	-12	HIS	-	expression tag	UNP A0A2H1K3G9
R	-11	HIS	-	expression tag	UNP A0A2H1K3G9
R	-10	HIS	-	expression tag	UNP A0A2H1K3G9
R	-9	SER	-	expression tag	UNP A0A2H1K3G9
R	-8	SER	-	expression tag	UNP A0A2H1K3G9
R	-7	GLY	-	expression tag	UNP A0A2H1K3G9
R	-6	LEU	-	expression tag	UNP A0A2H1K3G9
R	-5	VAL	-	expression tag	UNP A0A2H1K3G9
R	-4	PRO	-	expression tag	UNP A0A2H1K3G9
R	-3	ARG	-	expression tag	UNP A0A2H1K3G9
R	-2	GLY	-	expression tag	UNP A0A2H1K3G9
R	-1	SER	-	expression tag	UNP A0A2H1K3G9
R	0	HIS	-	expression tag	UNP A0A2H1K3G9
R	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
S	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
S	-18	GLY	-	expression tag	UNP A0A2H1K3G9
S	-17	SER	-	expression tag	UNP A0A2H1K3G9
S	-16	SER	-	expression tag	UNP A0A2H1K3G9
S	-15	HIS	-	expression tag	UNP A0A2H1K3G9
S	-14	HIS	-	expression tag	UNP A0A2H1K3G9
S	-13	HIS	-	expression tag	UNP A0A2H1K3G9
S	-12	HIS	-	expression tag	UNP A0A2H1K3G9
S	-11	HIS	-	expression tag	UNP A0A2H1K3G9
S	-10	HIS	-	expression tag	UNP A0A2H1K3G9
S	-9	SER	-	expression tag	UNP A0A2H1K3G9
S	-8	SER	-	expression tag	UNP A0A2H1K3G9
S	-7	GLY	-	expression tag	UNP A0A2H1K3G9
S	-6	LEU	-	expression tag	UNP A0A2H1K3G9
S	-5	VAL	-	expression tag	UNP A0A2H1K3G9
S	-4	PRO	-	expression tag	UNP A0A2H1K3G9
S	-3	ARG	-	expression tag	UNP A0A2H1K3G9
S	-2	GLY	-	expression tag	UNP A0A2H1K3G9
S	-1	SER	-	expression tag	UNP A0A2H1K3G9
S	0	HIS	-	expression tag	UNP A0A2H1K3G9
S	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
T	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
T	-18	GLY	-	expression tag	UNP A0A2H1K3G9

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-17	SER	-	expression tag	UNP A0A2H1K3G9
T	-16	SER	-	expression tag	UNP A0A2H1K3G9
T	-15	HIS	-	expression tag	UNP A0A2H1K3G9
T	-14	HIS	-	expression tag	UNP A0A2H1K3G9
T	-13	HIS	-	expression tag	UNP A0A2H1K3G9
T	-12	HIS	-	expression tag	UNP A0A2H1K3G9
T	-11	HIS	-	expression tag	UNP A0A2H1K3G9
T	-10	HIS	-	expression tag	UNP A0A2H1K3G9
T	-9	SER	-	expression tag	UNP A0A2H1K3G9
T	-8	SER	-	expression tag	UNP A0A2H1K3G9
T	-7	GLY	-	expression tag	UNP A0A2H1K3G9
T	-6	LEU	-	expression tag	UNP A0A2H1K3G9
T	-5	VAL	-	expression tag	UNP A0A2H1K3G9
T	-4	PRO	-	expression tag	UNP A0A2H1K3G9
T	-3	ARG	-	expression tag	UNP A0A2H1K3G9
T	-2	GLY	-	expression tag	UNP A0A2H1K3G9
T	-1	SER	-	expression tag	UNP A0A2H1K3G9
T	0	HIS	-	expression tag	UNP A0A2H1K3G9
T	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
U	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
U	-18	GLY	-	expression tag	UNP A0A2H1K3G9
U	-17	SER	-	expression tag	UNP A0A2H1K3G9
U	-16	SER	-	expression tag	UNP A0A2H1K3G9
U	-15	HIS	-	expression tag	UNP A0A2H1K3G9
U	-14	HIS	-	expression tag	UNP A0A2H1K3G9
U	-13	HIS	-	expression tag	UNP A0A2H1K3G9
U	-12	HIS	-	expression tag	UNP A0A2H1K3G9
U	-11	HIS	-	expression tag	UNP A0A2H1K3G9
U	-10	HIS	-	expression tag	UNP A0A2H1K3G9
U	-9	SER	-	expression tag	UNP A0A2H1K3G9
U	-8	SER	-	expression tag	UNP A0A2H1K3G9
U	-7	GLY	-	expression tag	UNP A0A2H1K3G9
U	-6	LEU	-	expression tag	UNP A0A2H1K3G9
U	-5	VAL	-	expression tag	UNP A0A2H1K3G9
U	-4	PRO	-	expression tag	UNP A0A2H1K3G9
U	-3	ARG	-	expression tag	UNP A0A2H1K3G9
U	-2	GLY	-	expression tag	UNP A0A2H1K3G9
U	-1	SER	-	expression tag	UNP A0A2H1K3G9
U	0	HIS	-	expression tag	UNP A0A2H1K3G9
U	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
V	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
V	-18	GLY	-	expression tag	UNP A0A2H1K3G9

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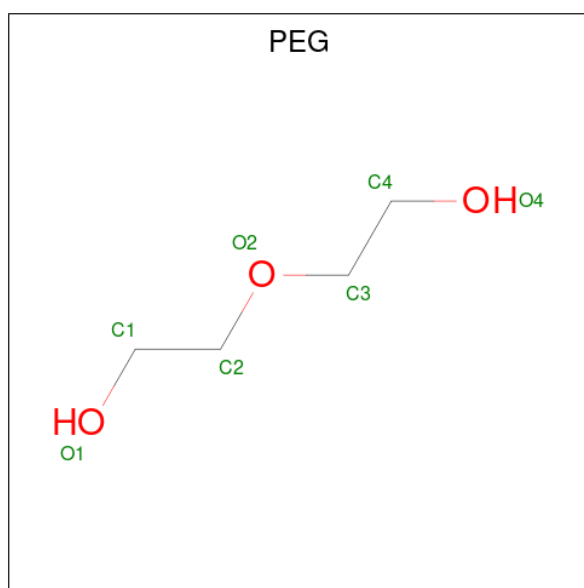
Chain	Residue	Modelled	Actual	Comment	Reference
V	-17	SER	-	expression tag	UNP A0A2H1K3G9
V	-16	SER	-	expression tag	UNP A0A2H1K3G9
V	-15	HIS	-	expression tag	UNP A0A2H1K3G9
V	-14	HIS	-	expression tag	UNP A0A2H1K3G9
V	-13	HIS	-	expression tag	UNP A0A2H1K3G9
V	-12	HIS	-	expression tag	UNP A0A2H1K3G9
V	-11	HIS	-	expression tag	UNP A0A2H1K3G9
V	-10	HIS	-	expression tag	UNP A0A2H1K3G9
V	-9	SER	-	expression tag	UNP A0A2H1K3G9
V	-8	SER	-	expression tag	UNP A0A2H1K3G9
V	-7	GLY	-	expression tag	UNP A0A2H1K3G9
V	-6	LEU	-	expression tag	UNP A0A2H1K3G9
V	-5	VAL	-	expression tag	UNP A0A2H1K3G9
V	-4	PRO	-	expression tag	UNP A0A2H1K3G9
V	-3	ARG	-	expression tag	UNP A0A2H1K3G9
V	-2	GLY	-	expression tag	UNP A0A2H1K3G9
V	-1	SER	-	expression tag	UNP A0A2H1K3G9
V	0	HIS	-	expression tag	UNP A0A2H1K3G9
V	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
W	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
W	-18	GLY	-	expression tag	UNP A0A2H1K3G9
W	-17	SER	-	expression tag	UNP A0A2H1K3G9
W	-16	SER	-	expression tag	UNP A0A2H1K3G9
W	-15	HIS	-	expression tag	UNP A0A2H1K3G9
W	-14	HIS	-	expression tag	UNP A0A2H1K3G9
W	-13	HIS	-	expression tag	UNP A0A2H1K3G9
W	-12	HIS	-	expression tag	UNP A0A2H1K3G9
W	-11	HIS	-	expression tag	UNP A0A2H1K3G9
W	-10	HIS	-	expression tag	UNP A0A2H1K3G9
W	-9	SER	-	expression tag	UNP A0A2H1K3G9
W	-8	SER	-	expression tag	UNP A0A2H1K3G9
W	-7	GLY	-	expression tag	UNP A0A2H1K3G9
W	-6	LEU	-	expression tag	UNP A0A2H1K3G9
W	-5	VAL	-	expression tag	UNP A0A2H1K3G9
W	-4	PRO	-	expression tag	UNP A0A2H1K3G9
W	-3	ARG	-	expression tag	UNP A0A2H1K3G9
W	-2	GLY	-	expression tag	UNP A0A2H1K3G9
W	-1	SER	-	expression tag	UNP A0A2H1K3G9
W	0	HIS	-	expression tag	UNP A0A2H1K3G9
W	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9
X	-19	MET	-	initiating methionine	UNP A0A2H1K3G9
X	-18	GLY	-	expression tag	UNP A0A2H1K3G9

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-17	SER	-	expression tag	UNP A0A2H1K3G9
X	-16	SER	-	expression tag	UNP A0A2H1K3G9
X	-15	HIS	-	expression tag	UNP A0A2H1K3G9
X	-14	HIS	-	expression tag	UNP A0A2H1K3G9
X	-13	HIS	-	expression tag	UNP A0A2H1K3G9
X	-12	HIS	-	expression tag	UNP A0A2H1K3G9
X	-11	HIS	-	expression tag	UNP A0A2H1K3G9
X	-10	HIS	-	expression tag	UNP A0A2H1K3G9
X	-9	SER	-	expression tag	UNP A0A2H1K3G9
X	-8	SER	-	expression tag	UNP A0A2H1K3G9
X	-7	GLY	-	expression tag	UNP A0A2H1K3G9
X	-6	LEU	-	expression tag	UNP A0A2H1K3G9
X	-5	VAL	-	expression tag	UNP A0A2H1K3G9
X	-4	PRO	-	expression tag	UNP A0A2H1K3G9
X	-3	ARG	-	expression tag	UNP A0A2H1K3G9
X	-2	GLY	-	expression tag	UNP A0A2H1K3G9
X	-1	SER	-	expression tag	UNP A0A2H1K3G9
X	0	HIS	-	expression tag	UNP A0A2H1K3G9
X	209	GLN	LYS	engineered mutation	UNP A0A2H1K3G9

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



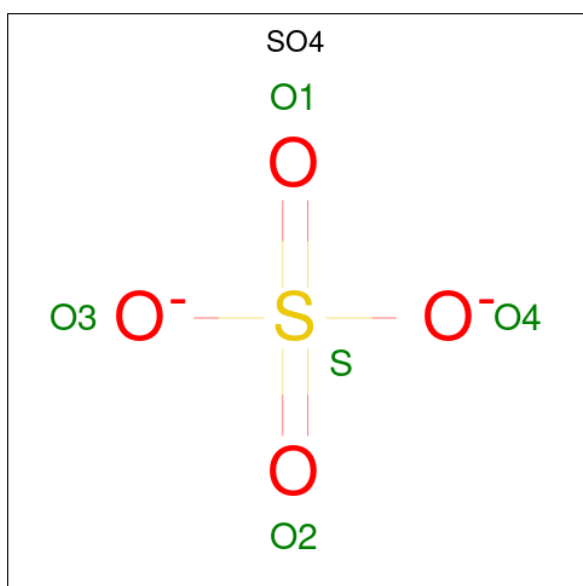
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			17	4	10	3		
2	A	1	Total	C	H	O	0	0
			17	4	10	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			17	4	10	3		
2	B	1	Total	C	H	O	0	0
			17	4	10	3		
2	H	1	Total	C	H	O	0	0
			17	4	10	3		
2	N	1	Total	C	H	O	0	0
			17	4	10	3		
2	X	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



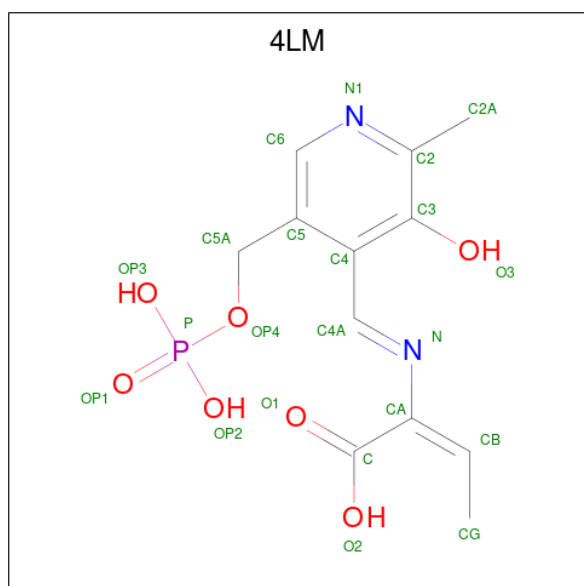
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			5	4 1		
3	A	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	C	1	Total	O S	0	0
			5	4 1		
3	D	1	Total	O S	0	0
			5	4 1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	N	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		
3	P	1	Total	O	S	0	0
			5	4	1		
3	V	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is (2E)-2-{[(1E)-{3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl}methylidene]amino}but-2-enoic acid (CCD ID: 4LM) (formula: C₁₂H₁₅N₂O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	
			34	12	12	2	7	1	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	C	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	D	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	E	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	F	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	G	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	H	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	I	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	J	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	K	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	L	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	M	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	N	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	O	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	P	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	Q	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	R	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	S	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	T	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	U	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0
4	V	1	Total 34	C 12	H 12	N 2	O 7	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	W	1	Total	C	H	N	O	P	
			34	12	12	2	7	1	0
4	X	1	Total	C	H	N	O	P	
			34	12	12	2	7	1	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	47	Total	O		
			47	47	0	0
5	B	51	Total	O		
			51	51	0	0
5	C	27	Total	O		
			27	27	0	0
5	D	26	Total	O		
			26	26	0	0
5	E	16	Total	O		
			16	16	0	0
5	F	14	Total	O		
			14	14	0	0
5	G	32	Total	O		
			32	32	0	0
5	H	34	Total	O		
			34	34	0	0
5	I	6	Total	O		
			6	6	0	0
5	J	5	Total	O		
			5	5	0	0
5	K	9	Total	O		
			9	9	0	0
5	L	8	Total	O		
			8	8	0	0
5	M	41	Total	O		
			41	41	0	0
5	N	23	Total	O		
			23	23	0	0
5	O	27	Total	O		
			27	27	0	0
5	P	22	Total	O		
			22	22	0	0
5	Q	13	Total	O		
			13	13	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	R	4	Total 4	O 4	0	0
5	S	7	Total 7	O 7	0	0
5	T	5	Total 5	O 5	0	0
5	U	5	Total 5	O 5	0	0
5	V	3	Total 3	O 3	0	0
5	W	3	Total 3	O 3	0	0
5	X	2	Total 2	O 2	0	0

3 Residue-property plots [i](#)


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

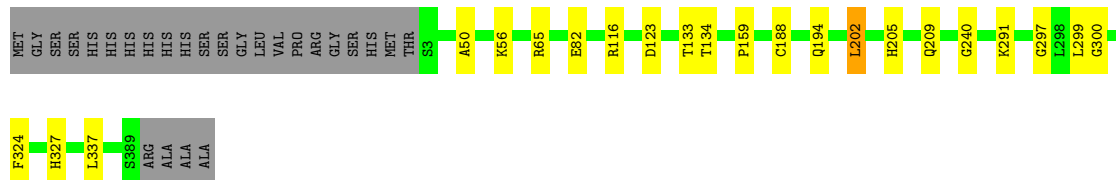
- Molecule 1: Cystathionine gamma-synthase

Chain A:  90% 6%




- Molecule 1: Cystathionine gamma-synthase

Chain B:  88% 5% 6%



- Molecule 1: Cystathionine gamma-synthase

Chain C:  90% 6%




- Molecule 1: Cystathionine gamma-synthase

Chain D:  91% 6%




- Molecule 1: Cystathionine gamma-synthase

Chain E:  90% 6%



ALA
ALA


• Molecule 1: Cystathionine gamma-synthase

Chain F:  90% 6%

MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	SER	HIS	MET	T2	G52	F90	A96	T158	Q194	L202	Q209	R233	G240	L290	Q293	L299	M312	R322	S323	F324	L337	A368	SER	ARG	ALA	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----


ALA

• Molecule 1: Cystathionine gamma-synthase

Chain G:  90% 6%

MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	SER	HIS	MET	THR	S3	Q64	R116	D123	T158	P159	C188	Q194	L202	Q209	G240	L290	Q293	L299	M312	F324	L337	S369	ARG	ALA	ALA	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----

• Molecule 1: Cystathionine gamma-synthase

Chain H:  90% 6%


MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	SER	HIS	MET	THR	S3	L81	R116	Q194	L202	G240	R253	R275	A278	L290	K291	G292	Q293	L299	M312	F324	L337	D376	S369	ARG	ALA	ALA	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----

• Molecule 1: Cystathionine gamma-synthase

Chain I:  90% 6%

MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	SER	HIS	MET	THR	T2	Q64	T112	R116	T158	Q194	L202	G240	G292	Q293	L299	M312	E313	F324	L337	A368	SER	ARG	ALA	ALA	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----


• Molecule 1: Cystathionine gamma-synthase

Chain J:  90% 6%

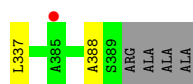
MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	SER	HIS	MET	THR	S3	W48	H53	I112	R116	D123	T158	Q194	L202	H205	G240	L290	L299	M312	F324	L337	H346	L365	S389	ARG
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----

ALA
ALA
ALA

• Molecule 1: Cystathionine gamma-synthase

Chain K:  89% 5% 6%

MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	SER	HIS	MET	THR	S3	W48	H53	R65	I112	R116	Y119	D123	T158	Q194	L202	G240	A278	L290	Q293	L299	M312	F324	H327
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------



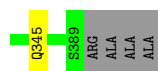
- Molecule 1: Cystathionine gamma-synthase

Chain L: 91% 6%



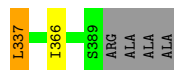
- Molecule 1: Cystathionine gamma-synthase

Chain M: 89% 5% 6%



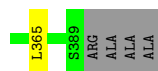
- Molecule 1: Cystathionine gamma-synthase

Chain N: 89% 5% 6%



- Molecule 1: Cystathionine gamma-synthase

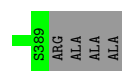
Chain O: 89% 5% 6%




- Molecule 1: Cystathionine gamma-synthase

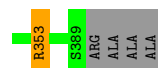
Chain P: 89% 5% 6%





- Molecule 1: Cystathionine gamma-synthase

Chain Q:  89% 5% 6%




- Molecule 1: Cystathionine gamma-synthase

Chain R:  90% 6%




- Molecule 1: Cystathionine gamma-synthase

Chain S:  90% 6%




- Molecule 1: Cystathionine gamma-synthase

Chain T:  90% 7%




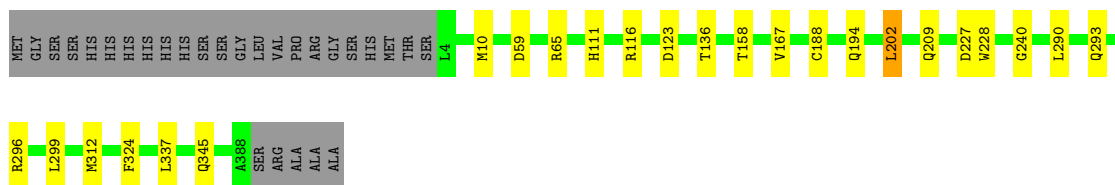
- Molecule 1: Cystathionine gamma-synthase

Chain U:  90% 6%




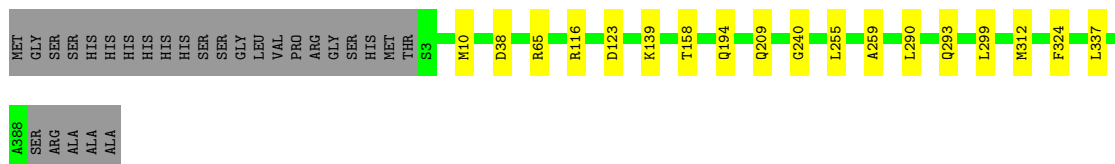
- Molecule 1: Cystathionine gamma-synthase

Chain V:  87% 6% 7%




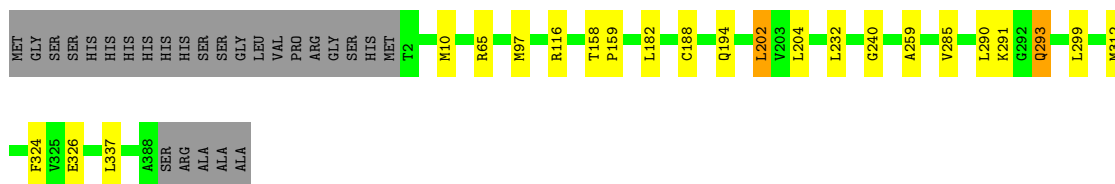
- Molecule 1: Cystathionine gamma-synthase

Chain W:  89% 0% 7%



- Molecule 1: Cystathionine gamma-synthase

Chain X:  88% 5% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	133.33Å 155.89Å 232.08Å 90.00° 90.24° 90.00°	Depositor
Resolution (Å)	232.08 – 2.52 232.08 – 2.52	Depositor EDS
% Data completeness (in resolution range)	67.2 (232.08-2.52) 66.5 (232.08-2.52)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.52Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.258 , 0.265 0.247 , 0.256	Depositor DCC
R_{free} test set	10624 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 20.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	135917	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4606e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 4LM, PEG

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	0.71	0/2865	1.02	2/3914 (0.1%)
1	B	0.74	0/2865	1.04	2/3914 (0.1%)
1	C	0.72	0/2865	1.01	2/3914 (0.1%)
1	D	0.71	0/2865	1.02	1/3914 (0.0%)
1	E	0.72	0/2872	1.01	2/3924 (0.1%)
1	F	0.71	0/2866	1.01	2/3916 (0.1%)
1	G	0.72	0/2865	1.03	2/3914 (0.1%)
1	H	0.72	0/2865	1.03	3/3914 (0.1%)
1	I	0.73	0/2866	1.03	3/3916 (0.1%)
1	J	0.72	0/2865	1.01	2/3914 (0.1%)
1	K	0.71	0/2865	1.01	2/3914 (0.1%)
1	L	0.71	0/2872	1.01	2/3924 (0.1%)
1	M	0.72	0/2872	1.02	3/3924 (0.1%)
1	N	0.72	0/2872	1.01	2/3924 (0.1%)
1	O	0.72	0/2872	1.01	2/3924 (0.1%)
1	P	0.72	0/2872	1.02	3/3924 (0.1%)
1	Q	0.71	0/2872	1.01	1/3924 (0.0%)
1	R	0.71	0/2865	1.00	2/3914 (0.1%)
1	S	0.72	0/2872	1.02	1/3924 (0.0%)
1	T	0.72	0/2859	1.01	2/3906 (0.1%)
1	U	0.74	0/2865	1.02	2/3914 (0.1%)
1	V	0.74	0/2853	1.02	2/3898 (0.1%)
1	W	0.72	0/2859	1.01	2/3906 (0.1%)
1	X	0.74	0/2866	1.02	3/3916 (0.1%)
All	All	0.72	0/68795	1.02	50/93990 (0.1%)

There are no bond length outliers.

The worst 5 of 50 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	116	ARG	CD-NE-CZ	7.98	135.57	124.40
1	I	116	ARG	CD-NE-CZ	7.92	135.48	124.40
1	H	116	ARG	CD-NE-CZ	7.49	134.89	124.40
1	M	116	ARG	CD-NE-CZ	7.44	134.81	124.40
1	X	324	PHE	CA-CB-CG	6.78	120.58	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2810	2790	2790	4	0
1	B	2810	2790	2790	10	0
1	C	2810	2790	2790	3	0
1	D	2810	2790	2790	2	0
1	E	2817	2797	2797	4	0
1	F	2811	2792	2792	3	0
1	G	2810	2790	2790	2	0
1	H	2810	2790	2790	5	0
1	I	2811	2792	2792	1	0
1	J	2810	2790	2790	3	0
1	K	2810	2790	2790	5	1
1	L	2817	2797	2797	2	0
1	M	2817	2797	2797	6	0
1	N	2817	2797	2797	6	0
1	O	2817	2797	2797	4	1
1	P	2817	2797	2797	5	0
1	Q	2817	2797	2797	11	0
1	R	2810	2790	2790	6	0
1	S	2817	2797	2797	3	0
1	T	2804	2785	2785	4	0
1	U	2810	2790	2790	3	0
1	V	2798	2780	2780	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	2804	2785	2785	5	0
1	X	2811	2792	2792	7	0
2	A	14	20	20	0	0
2	B	14	20	20	2	0
2	H	7	10	10	0	0
2	N	7	10	10	0	0
2	X	7	10	10	1	0
3	A	10	0	0	0	0
3	B	10	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
3	H	5	0	0	0	0
3	J	5	0	0	0	0
3	L	5	0	0	0	0
3	M	5	0	0	0	0
3	N	5	0	0	0	0
3	O	5	0	0	0	0
3	P	5	0	0	0	0
3	V	5	0	0	0	0
4	A	22	12	12	1	0
4	B	22	12	12	1	0
4	C	22	12	12	0	0
4	D	22	12	12	0	0
4	E	22	12	12	0	0
4	F	22	12	12	1	0
4	G	22	12	12	0	0
4	H	22	12	12	0	0
4	I	22	12	12	0	0
4	J	22	12	12	1	0
4	K	22	12	12	0	0
4	L	22	12	12	1	0
4	M	22	12	12	0	0
4	N	22	12	12	2	0
4	O	22	12	12	0	0
4	P	22	12	12	1	0
4	Q	22	12	12	1	0
4	R	22	12	12	1	0
4	S	22	12	12	1	0
4	T	22	12	12	0	0
4	U	22	12	12	1	0
4	V	22	12	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	W	22	12	12	1	0
4	X	22	12	12	1	0
5	A	47	0	0	0	0
5	B	51	0	0	0	0
5	C	27	0	0	0	0
5	D	26	0	0	0	0
5	E	16	0	0	0	0
5	F	14	0	0	0	0
5	G	32	0	0	0	0
5	H	34	0	0	0	0
5	I	6	0	0	0	0
5	J	5	0	0	0	0
5	K	9	0	0	0	0
5	L	8	0	0	0	0
5	M	41	0	0	0	0
5	N	23	0	0	0	0
5	O	27	0	0	0	0
5	P	22	0	0	0	0
5	Q	13	0	0	0	0
5	R	4	0	0	0	0
5	S	7	0	0	0	0
5	T	5	0	0	0	0
5	U	5	0	0	0	0
5	V	3	0	0	0	0
5	W	3	0	0	0	0
5	X	2	0	0	0	0
All	All	68557	67360	67360	96	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 96 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)
4:W:401:4LM:OP3	1:X:65:ARG:NH1	2.21	0.74
4:A:405:4LM:OP1	1:B:65:ARG:NH1	2.32	0.63
4:B:401:4LM:H4A	4:B:401:4LM:OP1	2.00	0.61
1:K:119:TYR:OH	1:L:65:ARG:NH1	2.32	0.60
1:X:159:PRO:HD3	1:X:188:CYS:SG	2.41	0.60

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:278:ALA:O	1:O:280:PRO:CB[1_545]	2.12	0.08

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	385/413 (93%)	373 (97%)	12 (3%)	0	100	100
1	B	385/413 (93%)	372 (97%)	13 (3%)	0	100	100
1	C	385/413 (93%)	375 (97%)	10 (3%)	0	100	100
1	D	385/413 (93%)	373 (97%)	12 (3%)	0	100	100
1	E	386/413 (94%)	374 (97%)	12 (3%)	0	100	100
1	F	385/413 (93%)	373 (97%)	12 (3%)	0	100	100
1	G	385/413 (93%)	373 (97%)	12 (3%)	0	100	100
1	H	385/413 (93%)	373 (97%)	12 (3%)	0	100	100
1	I	385/413 (93%)	374 (97%)	11 (3%)	0	100	100
1	J	385/413 (93%)	374 (97%)	11 (3%)	0	100	100
1	K	385/413 (93%)	371 (96%)	14 (4%)	0	100	100
1	L	386/413 (94%)	373 (97%)	13 (3%)	0	100	100
1	M	386/413 (94%)	374 (97%)	12 (3%)	0	100	100
1	N	386/413 (94%)	374 (97%)	12 (3%)	0	100	100
1	O	386/413 (94%)	374 (97%)	12 (3%)	0	100	100
1	P	386/413 (94%)	373 (97%)	13 (3%)	0	100	100
1	Q	386/413 (94%)	374 (97%)	12 (3%)	0	100	100
1	R	385/413 (93%)	373 (97%)	12 (3%)	0	100	100
1	S	386/413 (94%)	372 (96%)	14 (4%)	0	100	100
1	T	384/413 (93%)	372 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	385/413 (93%)	372 (97%)	13 (3%)	0	100	100
1	V	383/413 (93%)	371 (97%)	12 (3%)	0	100	100
1	W	384/413 (93%)	372 (97%)	12 (3%)	0	100	100
1	X	385/413 (93%)	373 (97%)	12 (3%)	0	100	100
All	All	9244/9912 (93%)	8952 (97%)	292 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	286/306 (94%)	280 (98%)	6 (2%)	47	72
1	B	286/306 (94%)	278 (97%)	8 (3%)	38	64
1	C	286/306 (94%)	279 (98%)	7 (2%)	43	69
1	D	286/306 (94%)	278 (97%)	8 (3%)	38	64
1	E	287/306 (94%)	277 (96%)	10 (4%)	32	56
1	F	286/306 (94%)	276 (96%)	10 (4%)	32	56
1	G	286/306 (94%)	276 (96%)	10 (4%)	32	56
1	H	286/306 (94%)	278 (97%)	8 (3%)	38	64
1	I	286/306 (94%)	276 (96%)	10 (4%)	32	56
1	J	286/306 (94%)	277 (97%)	9 (3%)	35	60
1	K	286/306 (94%)	277 (97%)	9 (3%)	35	60
1	L	287/306 (94%)	281 (98%)	6 (2%)	47	72
1	M	287/306 (94%)	277 (96%)	10 (4%)	32	56
1	N	287/306 (94%)	277 (96%)	10 (4%)	32	56
1	O	287/306 (94%)	277 (96%)	10 (4%)	32	56
1	P	287/306 (94%)	276 (96%)	11 (4%)	29	53
1	Q	287/306 (94%)	276 (96%)	11 (4%)	29	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	286/306 (94%)	275 (96%)	11 (4%)	29	53
1	S	287/306 (94%)	274 (96%)	13 (4%)	24	46
1	T	285/306 (93%)	276 (97%)	9 (3%)	34	60
1	U	286/306 (94%)	275 (96%)	11 (4%)	29	53
1	V	284/306 (93%)	268 (94%)	16 (6%)	19	37
1	W	285/306 (93%)	276 (97%)	9 (3%)	34	60
1	X	286/306 (94%)	275 (96%)	11 (4%)	29	53
All	All	6868/7344 (94%)	6635 (97%)	233 (3%)	32	57

5 of 233 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	290	LEU
1	W	337	LEU
1	Q	194	GLN
1	W	299	LEU
1	V	158	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	148	GLN
1	T	53	HIS
1	P	53	HIS
1	Q	53	HIS
1	V	53	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

46 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PEG	H	402	-	6,6,6	0.23	0	5,5,5	0.26	0
3	SO4	A	403	-	4,4,4	0.29	0	6,6,6	0.19	0
2	PEG	A	401	-	6,6,6	0.12	0	5,5,5	0.12	0
3	SO4	A	404	-	4,4,4	0.29	0	6,6,6	0.12	0
4	4LM	X	402	-	21,22,22	1.08	1 (4%)	26,31,31	0.84	0
4	4LM	Q	401	-	21,22,22	1.24	1 (4%)	26,31,31	0.99	2 (7%)
2	PEG	A	402	-	6,6,6	0.22	0	5,5,5	0.21	0
3	SO4	N	402	-	4,4,4	0.30	0	6,6,6	0.35	0
4	4LM	C	402	-	21,22,22	1.11	1 (4%)	26,31,31	1.10	3 (11%)
4	4LM	D	401	-	21,22,22	1.19	1 (4%)	26,31,31	0.87	1 (3%)
4	4LM	B	401	-	21,22,22	1.24	1 (4%)	26,31,31	0.95	1 (3%)
4	4LM	L	401	-	21,22,22	1.34	1 (4%)	26,31,31	1.07	2 (7%)
4	4LM	M	401	-	21,22,22	1.17	1 (4%)	26,31,31	1.03	2 (7%)
4	4LM	T	401	-	21,22,22	1.19	1 (4%)	26,31,31	1.06	3 (11%)
3	SO4	B	404	-	4,4,4	0.29	0	6,6,6	0.16	0
4	4LM	O	402	-	21,22,22	0.95	1 (4%)	26,31,31	1.09	3 (11%)
3	SO4	B	403	-	4,4,4	0.29	0	6,6,6	0.18	0
3	SO4	M	402	-	4,4,4	0.30	0	6,6,6	0.13	0
4	4LM	F	401	-	21,22,22	1.21	1 (4%)	26,31,31	1.09	3 (11%)
4	4LM	P	401	-	21,22,22	1.31	1 (4%)	26,31,31	1.14	2 (7%)
3	SO4	O	401	-	4,4,4	0.29	0	6,6,6	0.27	0
4	4LM	K	401	-	21,22,22	1.26	1 (4%)	26,31,31	0.90	1 (3%)
4	4LM	E	401	-	21,22,22	1.47	1 (4%)	26,31,31	1.19	4 (15%)
4	4LM	R	401	-	21,22,22	1.33	1 (4%)	26,31,31	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	F	402	-	4,4,4	0.28	0	6,6,6	0.40	0
3	SO4	L	402	-	4,4,4	0.29	0	6,6,6	0.11	0
2	PEG	X	401	-	6,6,6	0.17	0	5,5,5	0.50	0
4	4LM	U	401	-	21,22,22	1.15	1 (4%)	26,31,31	0.96	1 (3%)
4	4LM	N	401	-	21,22,22	1.17	1 (4%)	26,31,31	1.01	2 (7%)
3	SO4	C	401	-	4,4,4	0.29	0	6,6,6	0.30	0
4	4LM	J	401	-	21,22,22	1.29	1 (4%)	26,31,31	0.85	0
4	4LM	A	405	-	21,22,22	1.05	1 (4%)	26,31,31	0.76	0
4	4LM	H	401	-	21,22,22	1.20	1 (4%)	26,31,31	1.09	3 (11%)
4	4LM	W	401	-	21,22,22	1.07	1 (4%)	26,31,31	1.05	3 (11%)
2	PEG	N	403	-	6,6,6	0.27	0	5,5,5	0.36	0
3	SO4	J	402	-	4,4,4	0.29	0	6,6,6	0.12	0
2	PEG	B	402	-	6,6,6	0.21	0	5,5,5	0.20	0
4	4LM	V	401	-	21,22,22	1.09	1 (4%)	26,31,31	0.99	1 (3%)
2	PEG	B	405	-	6,6,6	0.33	0	5,5,5	0.33	0
4	4LM	G	401	-	21,22,22	1.02	1 (4%)	26,31,31	1.07	3 (11%)
3	SO4	D	402	-	4,4,4	0.29	0	6,6,6	0.22	0
3	SO4	P	402	-	4,4,4	0.30	0	6,6,6	0.22	0
3	SO4	V	402	-	4,4,4	0.28	0	6,6,6	0.23	0
4	4LM	I	401	-	21,22,22	0.95	1 (4%)	26,31,31	1.10	3 (11%)
4	4LM	S	401	-	21,22,22	1.31	1 (4%)	26,31,31	0.93	2 (7%)
3	SO4	H	403	-	4,4,4	0.29	0	6,6,6	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	H	402	-	-	2/4/4/4	-
2	PEG	A	401	-	-	2/4/4/4	-
4	4LM	X	402	-	-	3/15/17/17	0/1/1/1
4	4LM	Q	401	-	-	3/15/17/17	0/1/1/1
2	PEG	A	402	-	-	2/4/4/4	-
4	4LM	C	402	-	-	5/15/17/17	0/1/1/1
4	4LM	D	401	-	-	2/15/17/17	0/1/1/1
4	4LM	L	401	-	-	2/15/17/17	0/1/1/1
4	4LM	B	401	-	-	5/15/17/17	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	4LM	M	401	-	-	2/15/17/17	0/1/1/1
4	4LM	T	401	-	-	2/15/17/17	0/1/1/1
4	4LM	O	402	-	-	6/15/17/17	0/1/1/1
4	4LM	F	401	-	-	2/15/17/17	0/1/1/1
4	4LM	P	401	-	-	2/15/17/17	0/1/1/1
4	4LM	K	401	-	-	4/15/17/17	0/1/1/1
4	4LM	E	401	-	-	2/15/17/17	0/1/1/1
4	4LM	R	401	-	-	6/15/17/17	0/1/1/1
4	4LM	U	401	-	-	4/15/17/17	0/1/1/1
2	PEG	X	401	-	-	3/4/4/4	-
4	4LM	N	401	-	-	2/15/17/17	0/1/1/1
4	4LM	J	401	-	-	4/15/17/17	0/1/1/1
4	4LM	A	405	-	-	7/15/17/17	0/1/1/1
4	4LM	H	401	-	-	2/15/17/17	0/1/1/1
2	PEG	N	403	-	-	3/4/4/4	-
2	PEG	B	402	-	-	1/4/4/4	-
4	4LM	V	401	-	-	4/15/17/17	0/1/1/1
2	PEG	B	405	-	-	2/4/4/4	-
4	4LM	G	401	-	-	2/15/17/17	0/1/1/1
4	4LM	I	401	-	-	2/15/17/17	0/1/1/1
4	4LM	S	401	-	-	2/15/17/17	0/1/1/1
4	4LM	W	401	-	-	2/15/17/17	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	401	4LM	CA-N	-5.97	1.34	1.41
4	R	401	4LM	CA-N	-5.27	1.35	1.41
4	L	401	4LM	CA-N	-5.16	1.35	1.41
4	P	401	4LM	CA-N	-5.09	1.35	1.41
4	S	401	4LM	CA-N	-5.08	1.35	1.41

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	401	4LM	O1-C-CA	-3.01	117.26	122.02
4	Q	401	4LM	O1-C-CA	-2.99	117.29	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	402	4LM	O1-C-CA	-2.97	117.33	122.02
4	V	401	4LM	C4A-N-CA	2.91	129.95	122.63
4	P	401	4LM	O1-C-CA	-2.88	117.46	122.02

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	405	4LM	C-CA-CB-CG
4	A	405	4LM	N-CA-CB-CG
4	B	401	4LM	C-CA-CB-CG
4	B	401	4LM	N-CA-CB-CG
4	C	402	4LM	C-CA-CB-CG

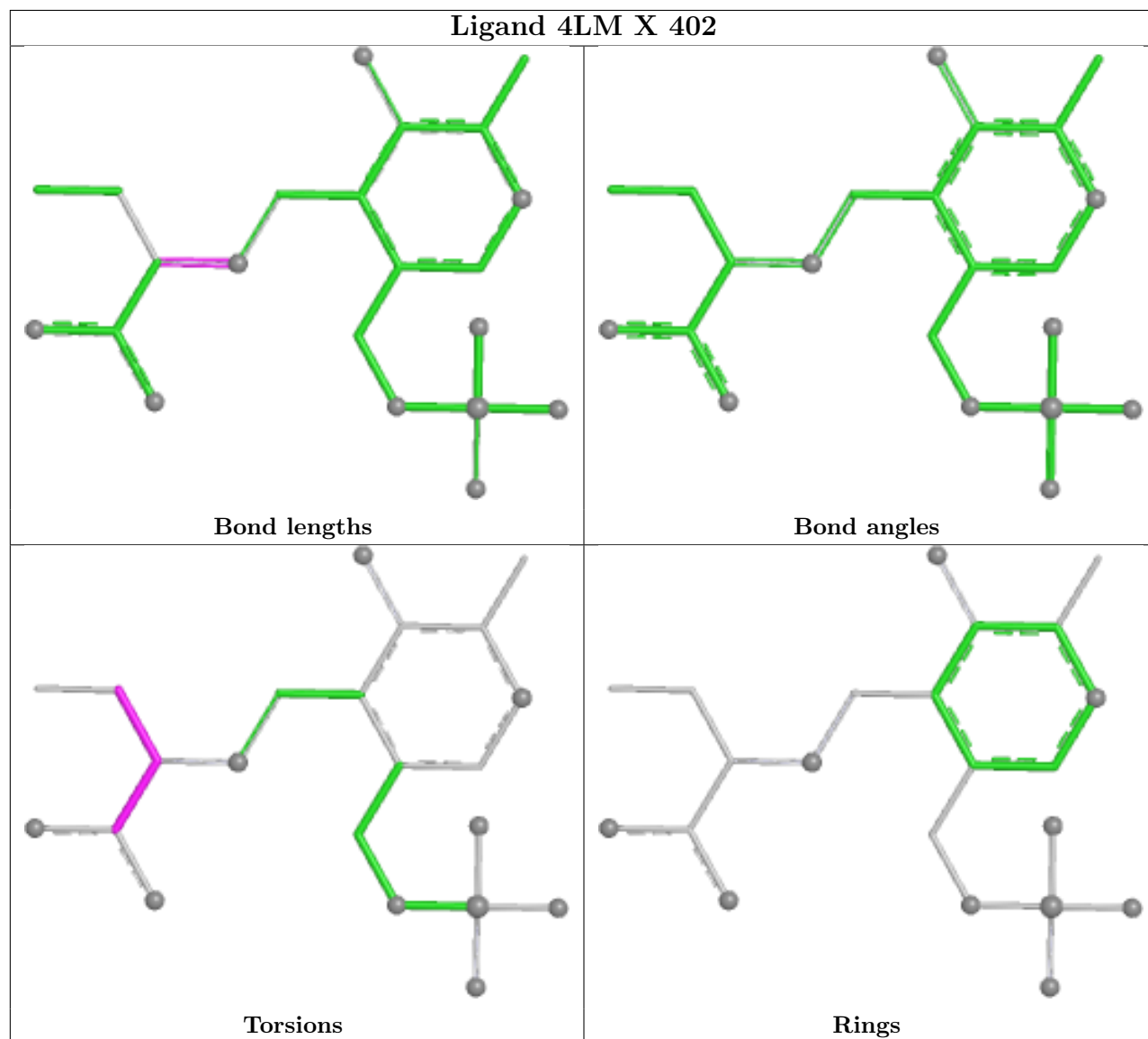
There are no ring outliers.

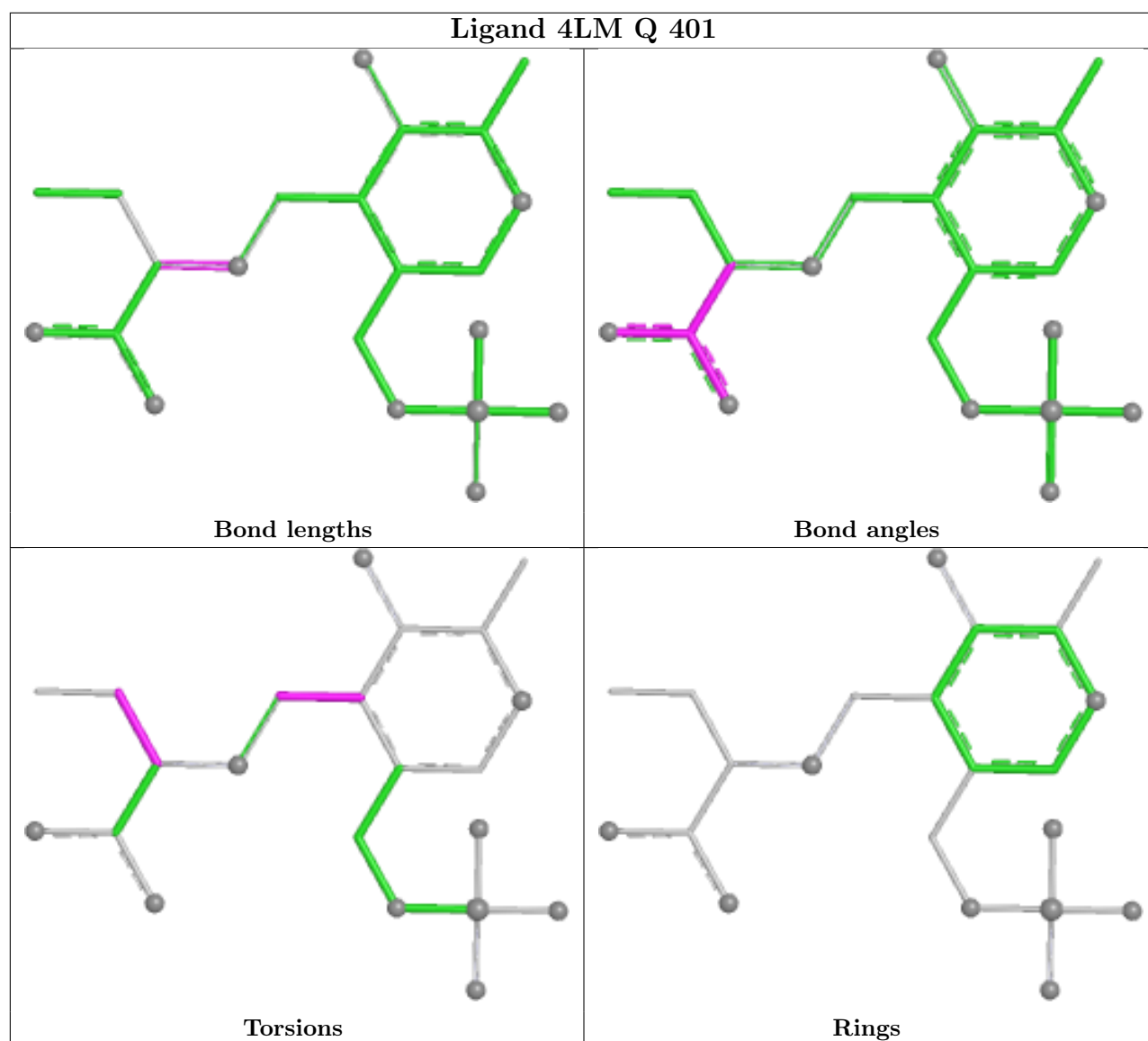
18 monomers are involved in 19 short contacts:

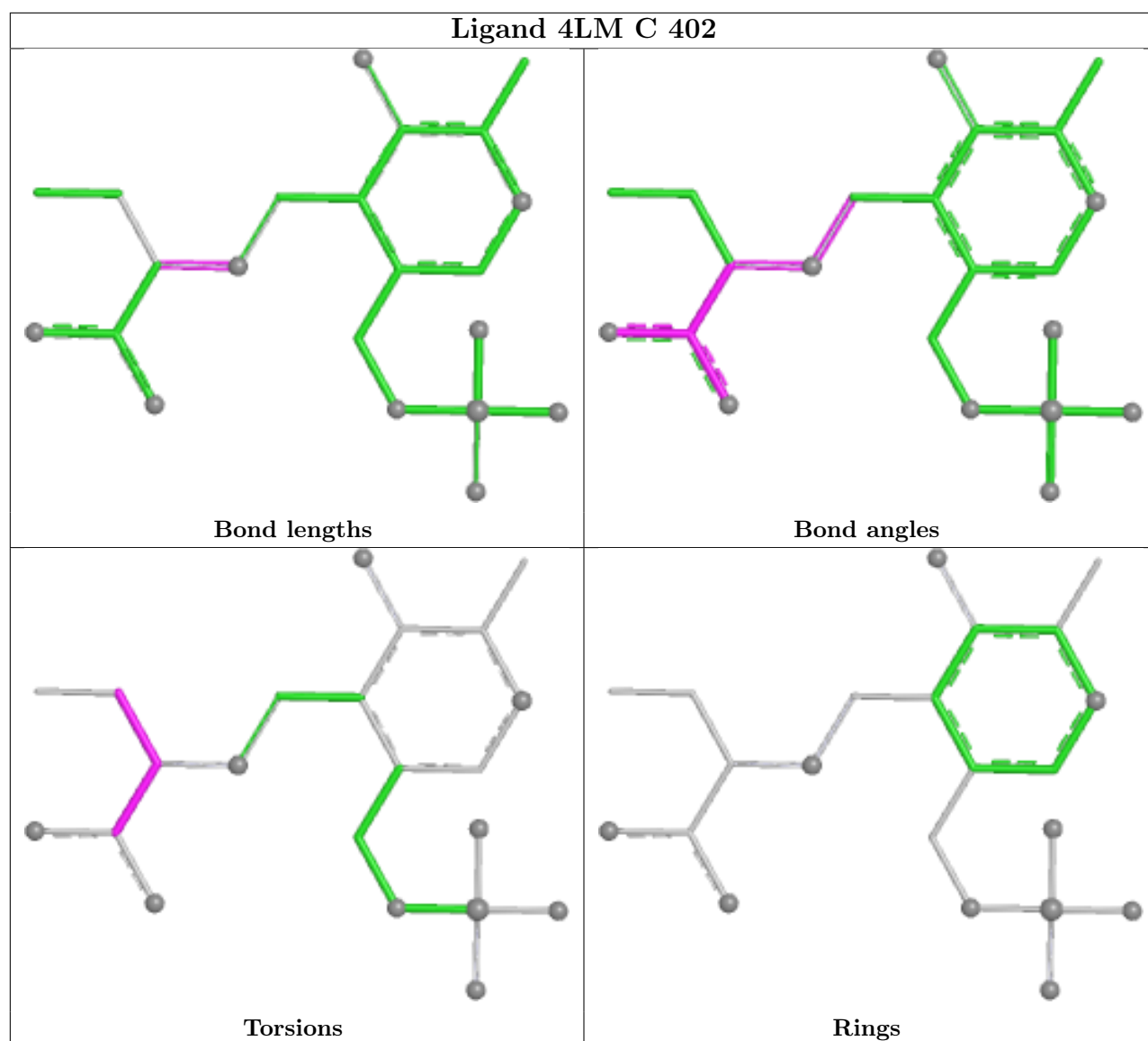
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	402	4LM	1	0
4	Q	401	4LM	1	0
4	B	401	4LM	1	0
4	L	401	4LM	1	0
3	B	403	SO4	1	0
4	F	401	4LM	1	0
4	P	401	4LM	1	0
4	R	401	4LM	1	0
2	X	401	PEG	1	0
4	U	401	4LM	1	0
4	N	401	4LM	2	0
4	J	401	4LM	1	0
4	A	405	4LM	1	0
4	W	401	4LM	1	0
2	B	402	PEG	1	0
4	V	401	4LM	1	0
2	B	405	PEG	1	0
4	S	401	4LM	1	0

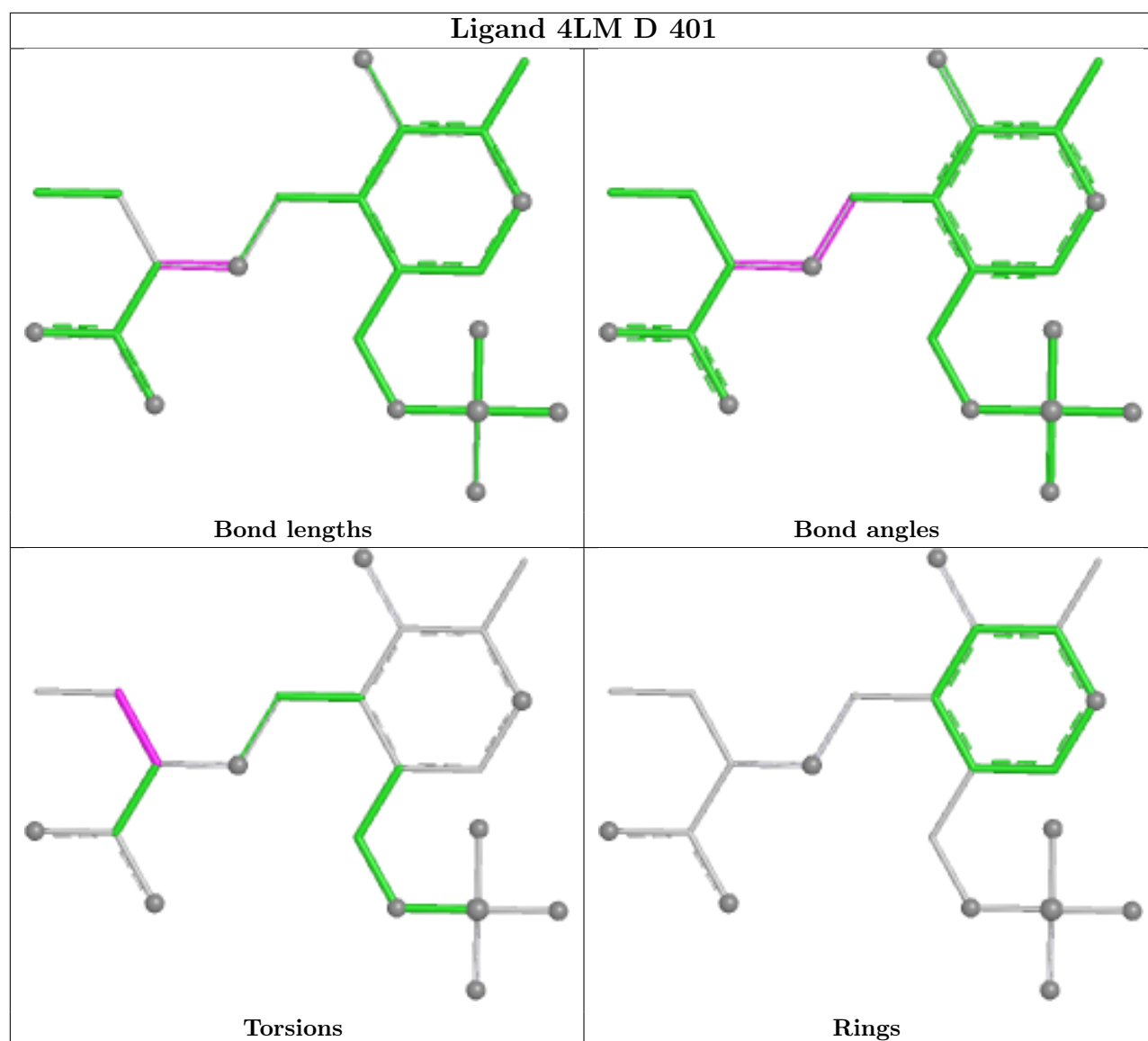
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

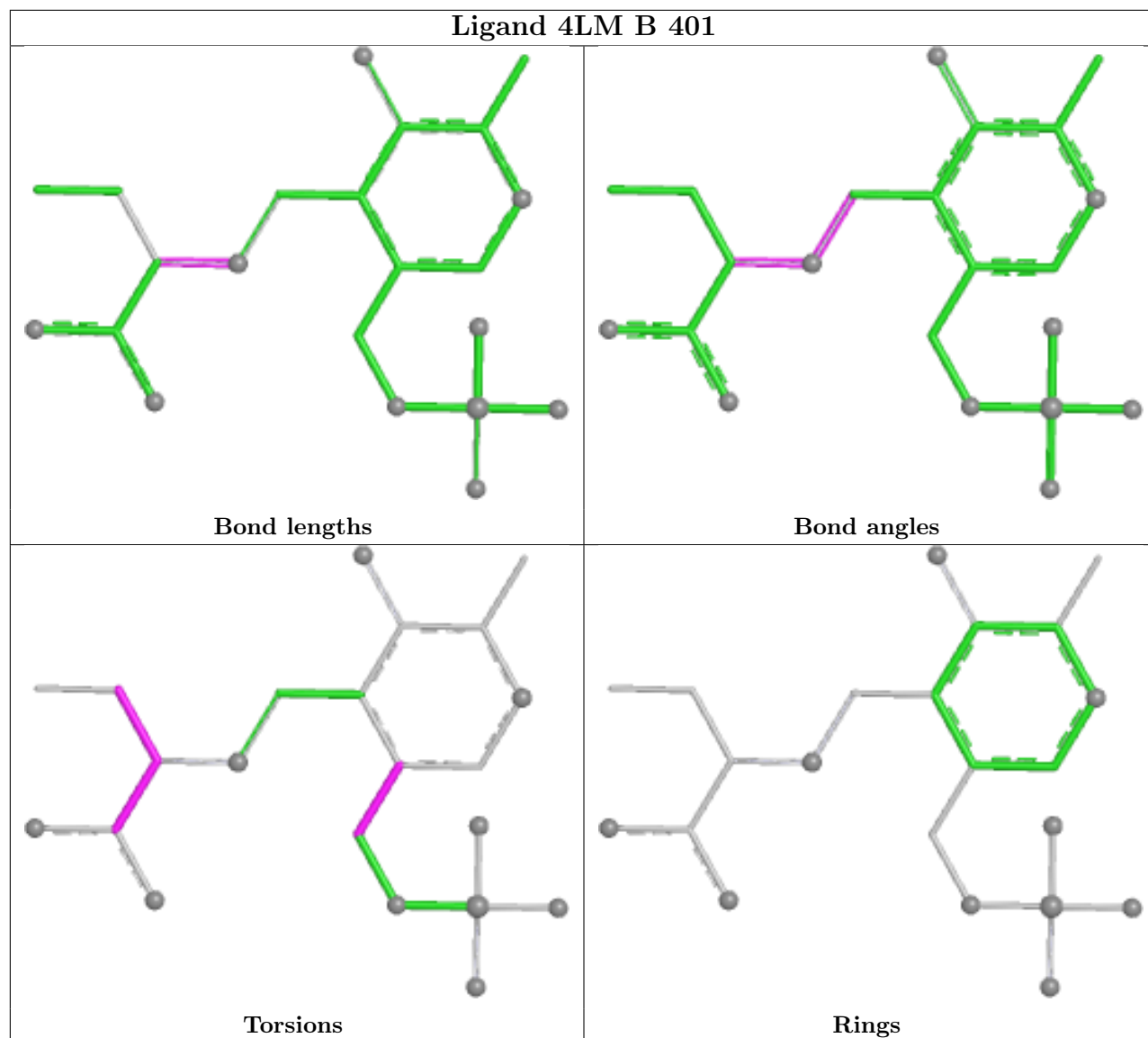
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD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

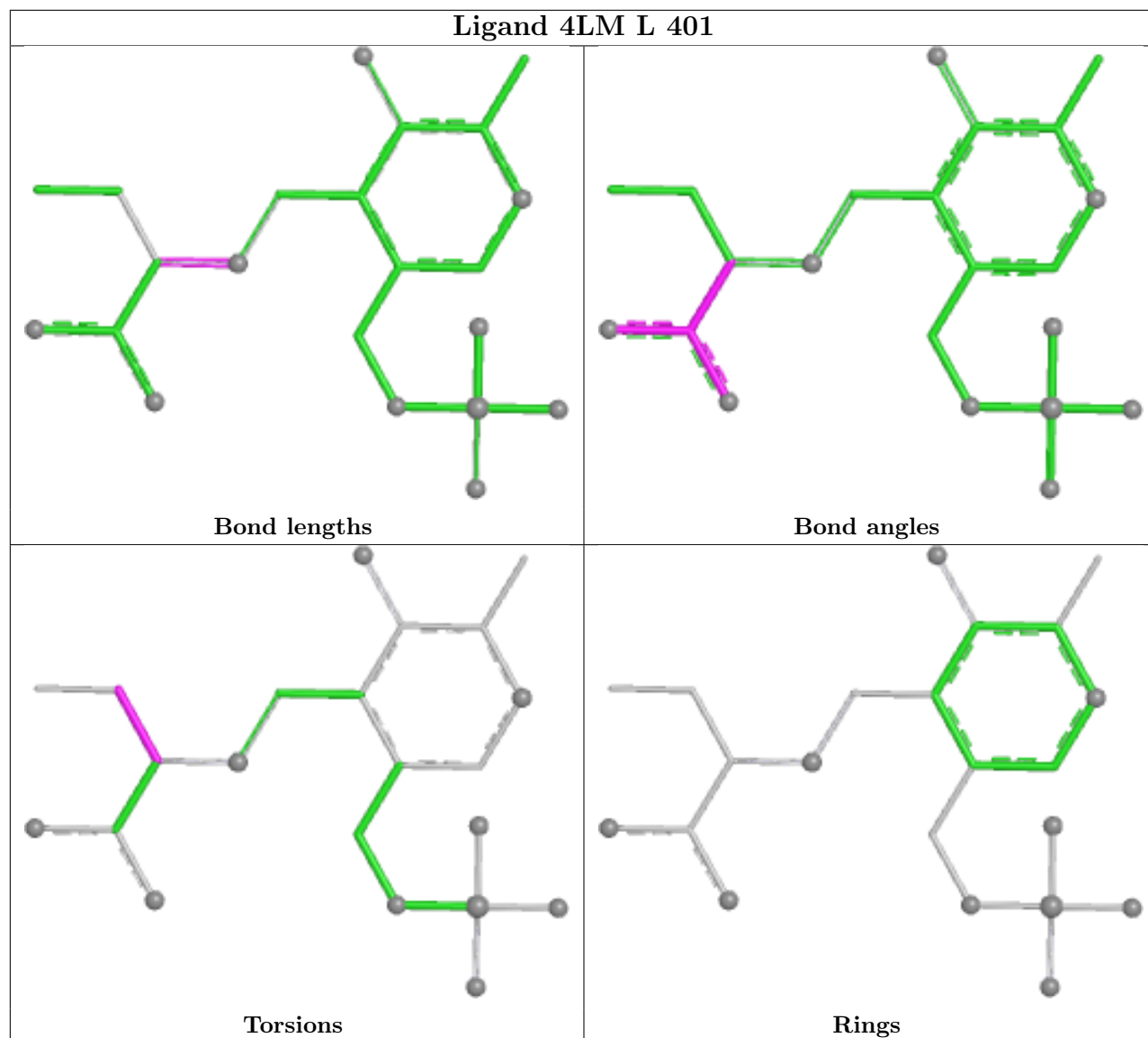


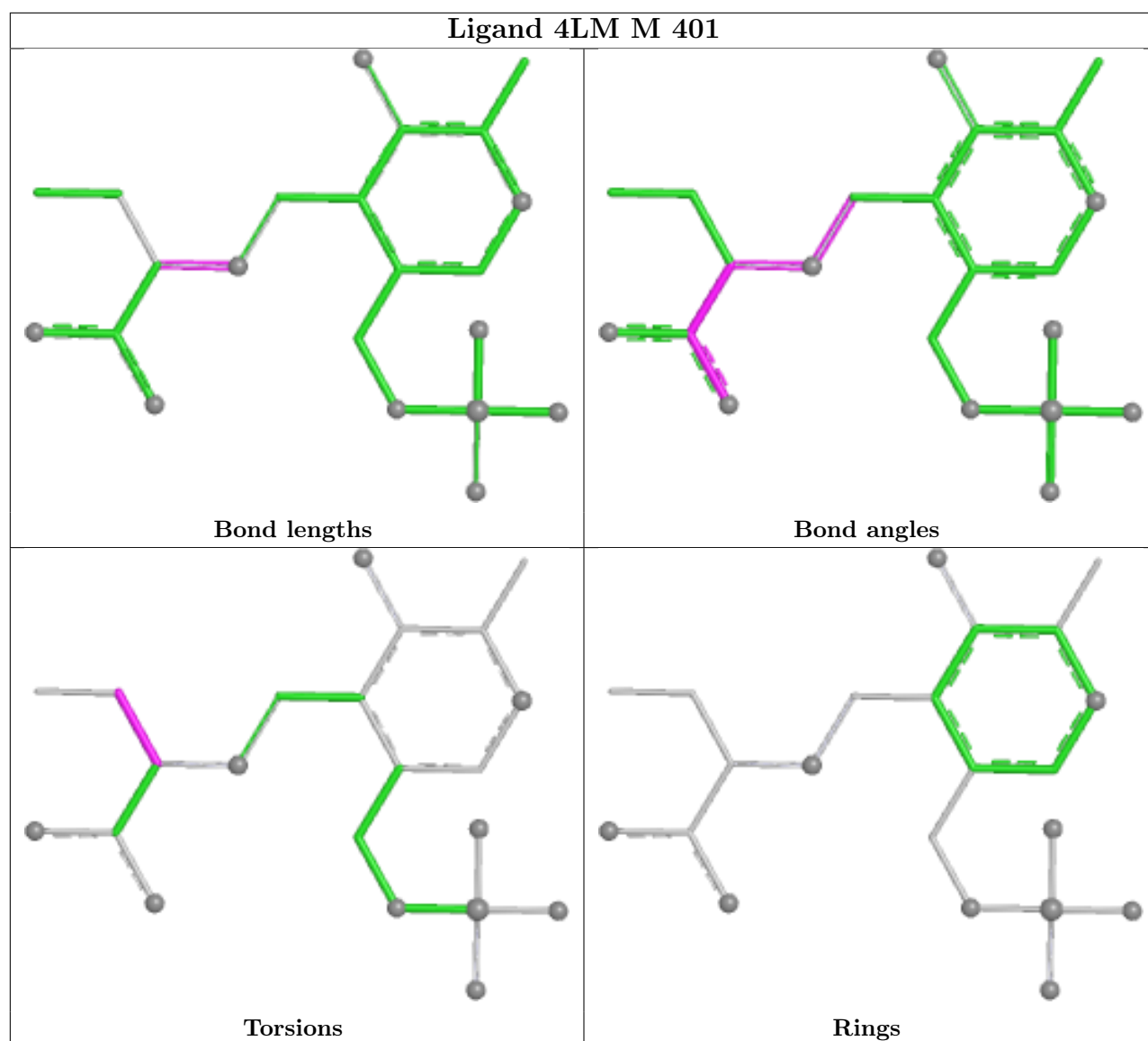


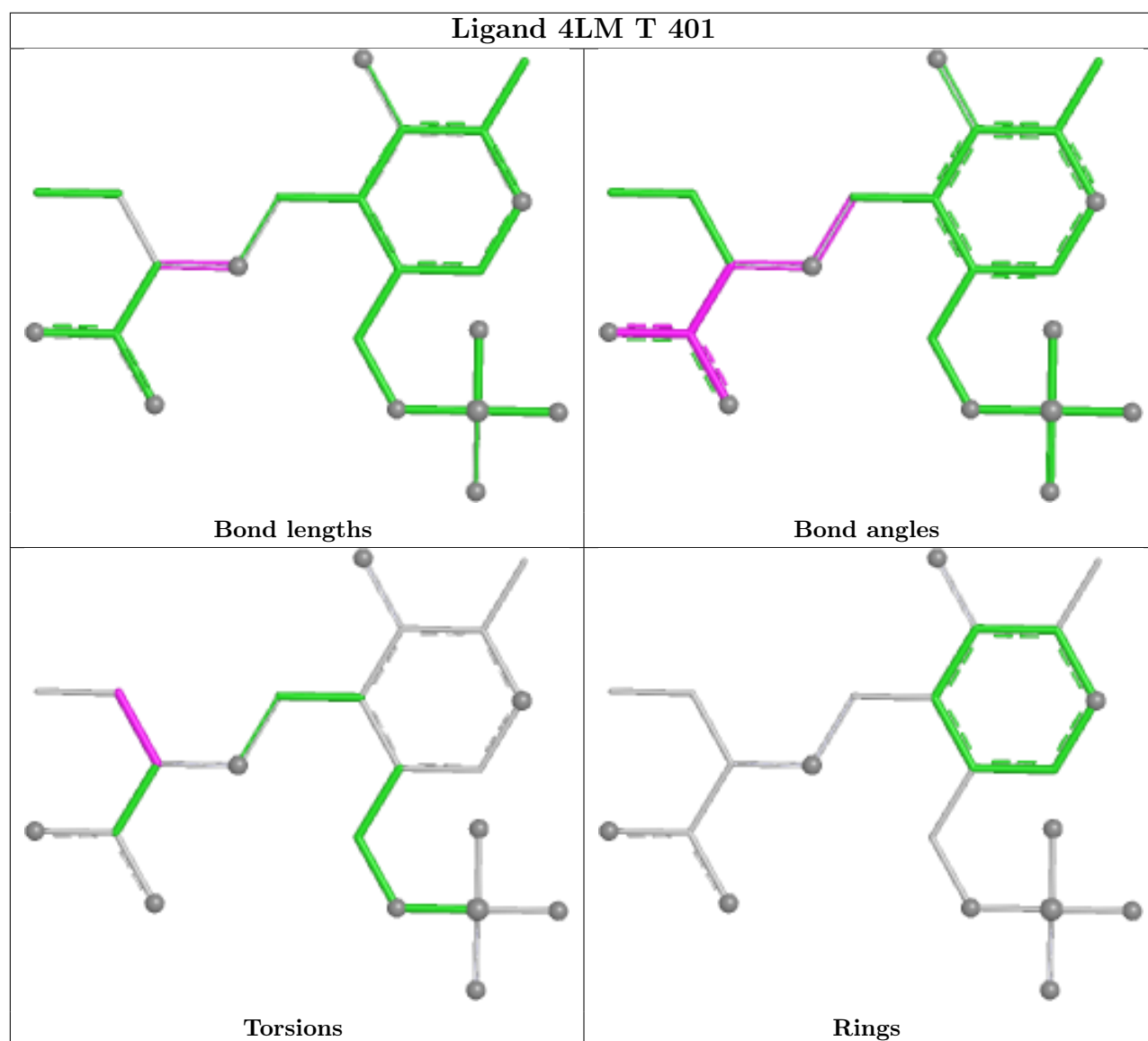


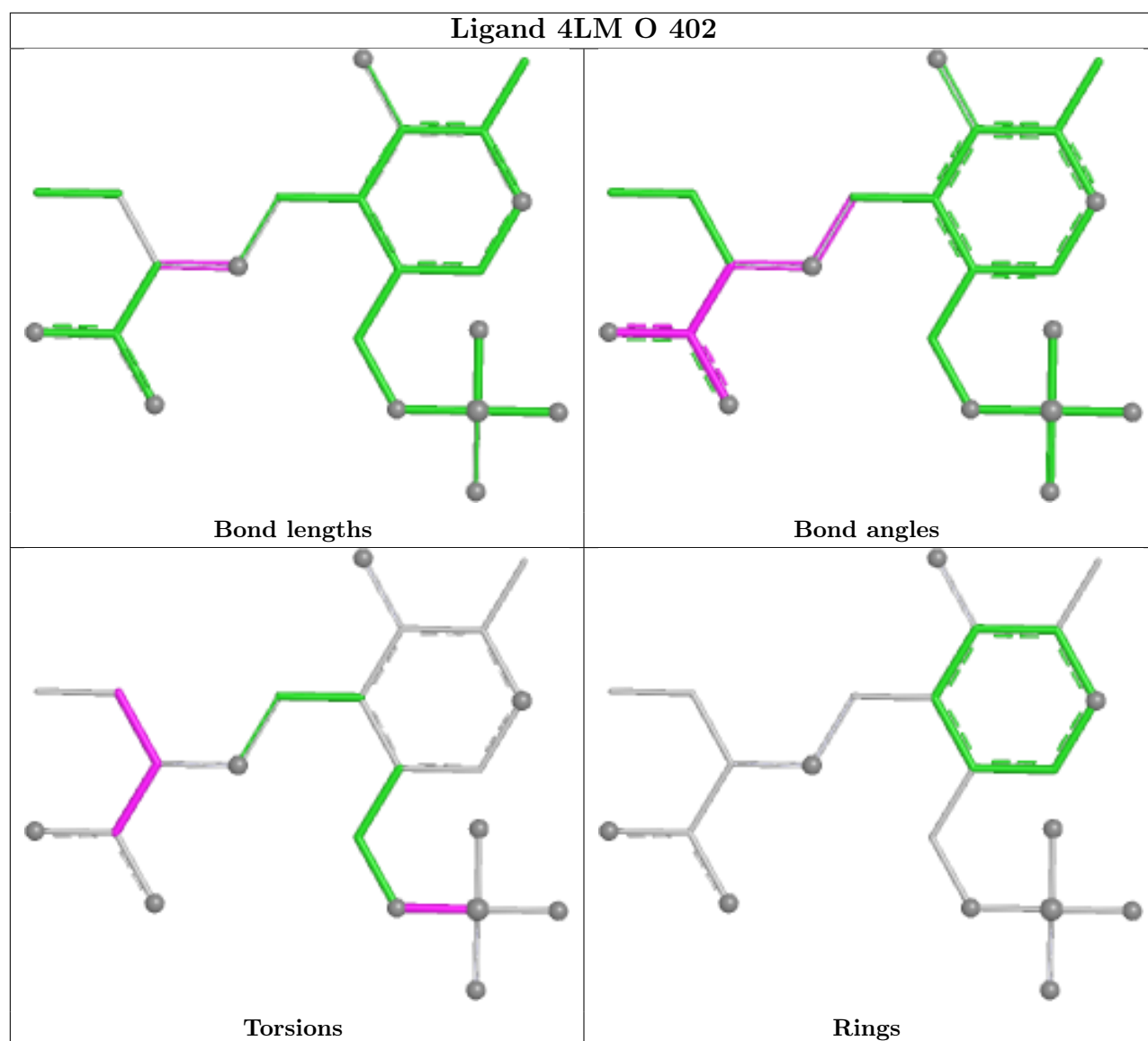


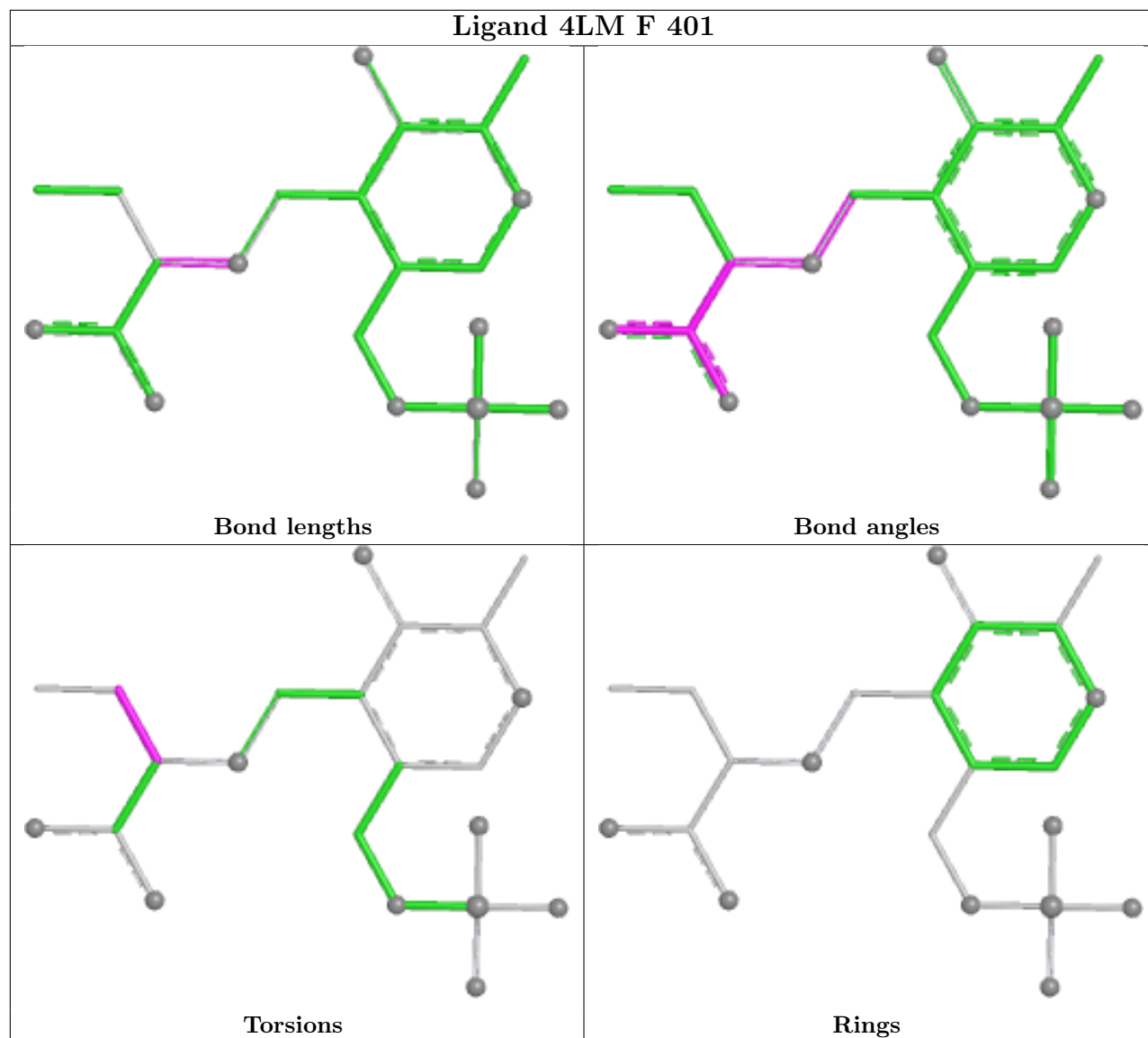


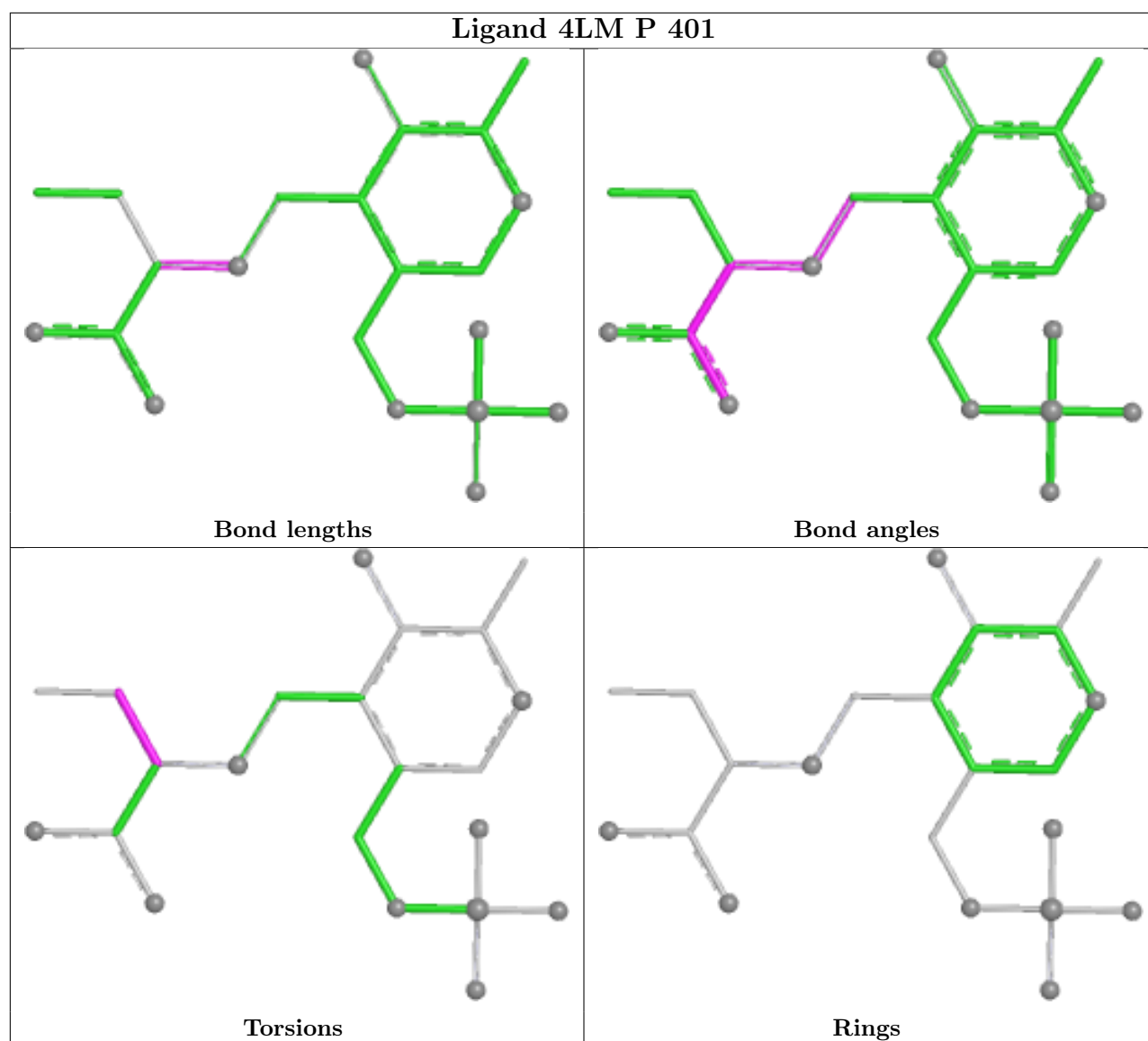


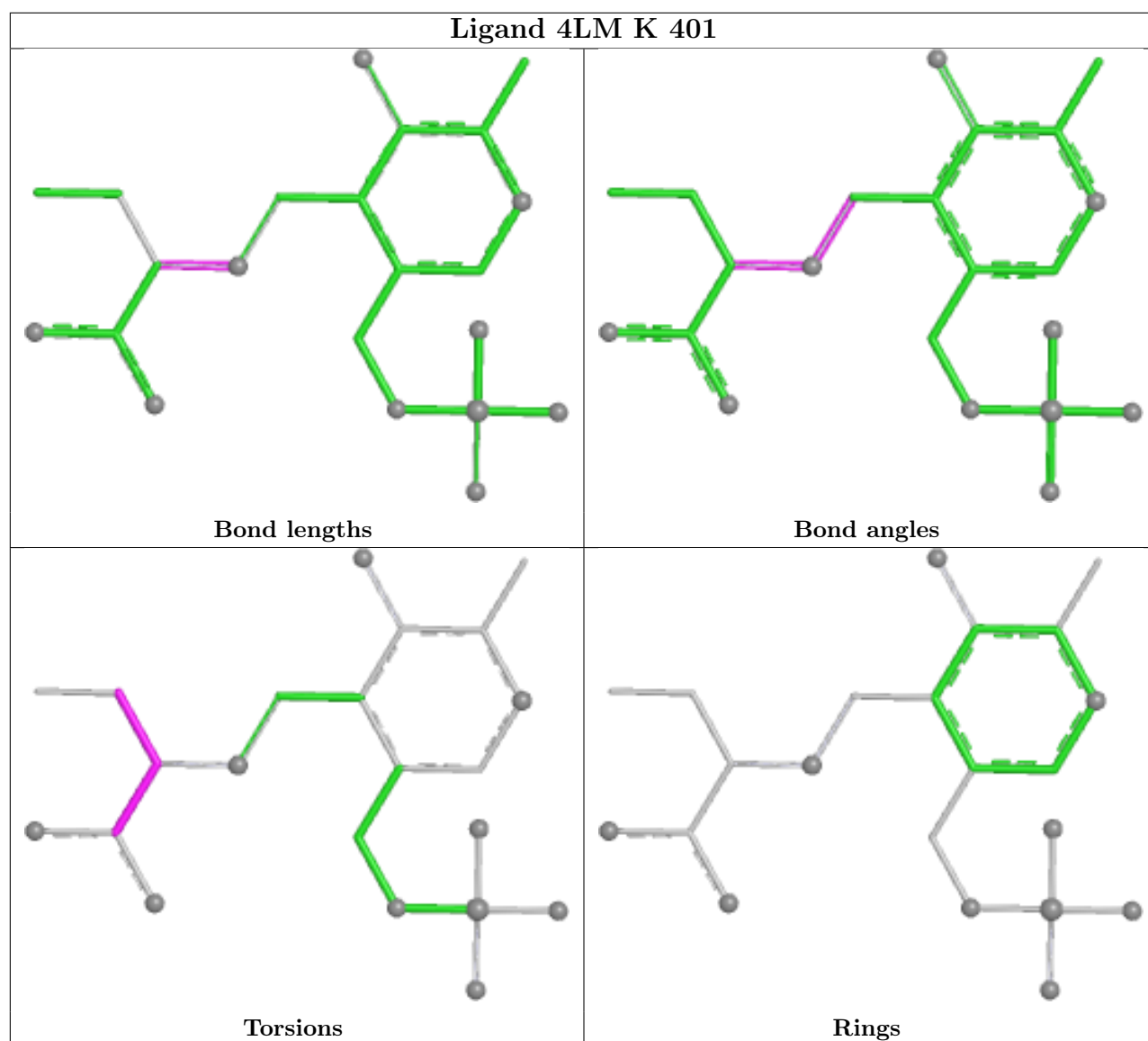


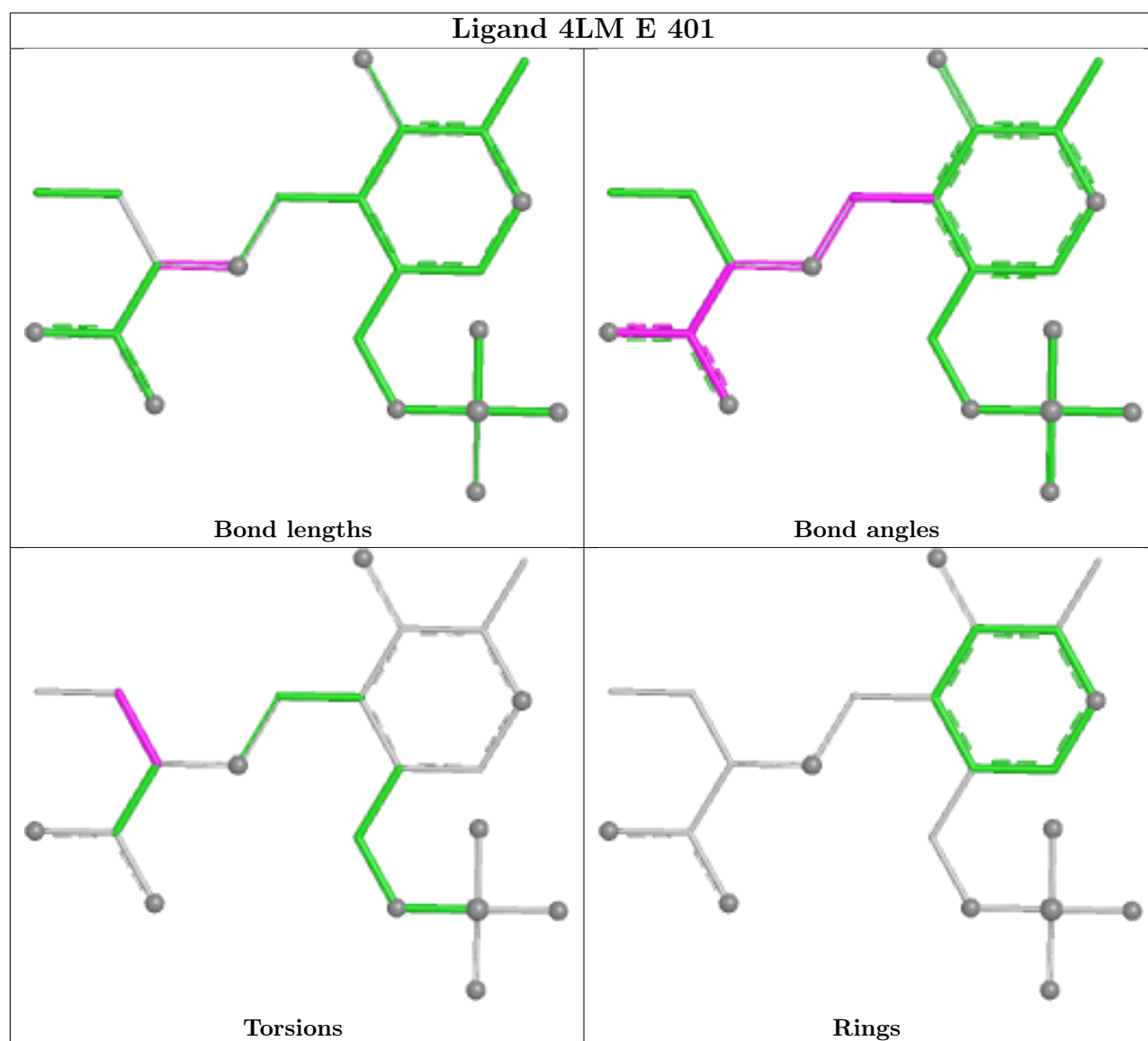


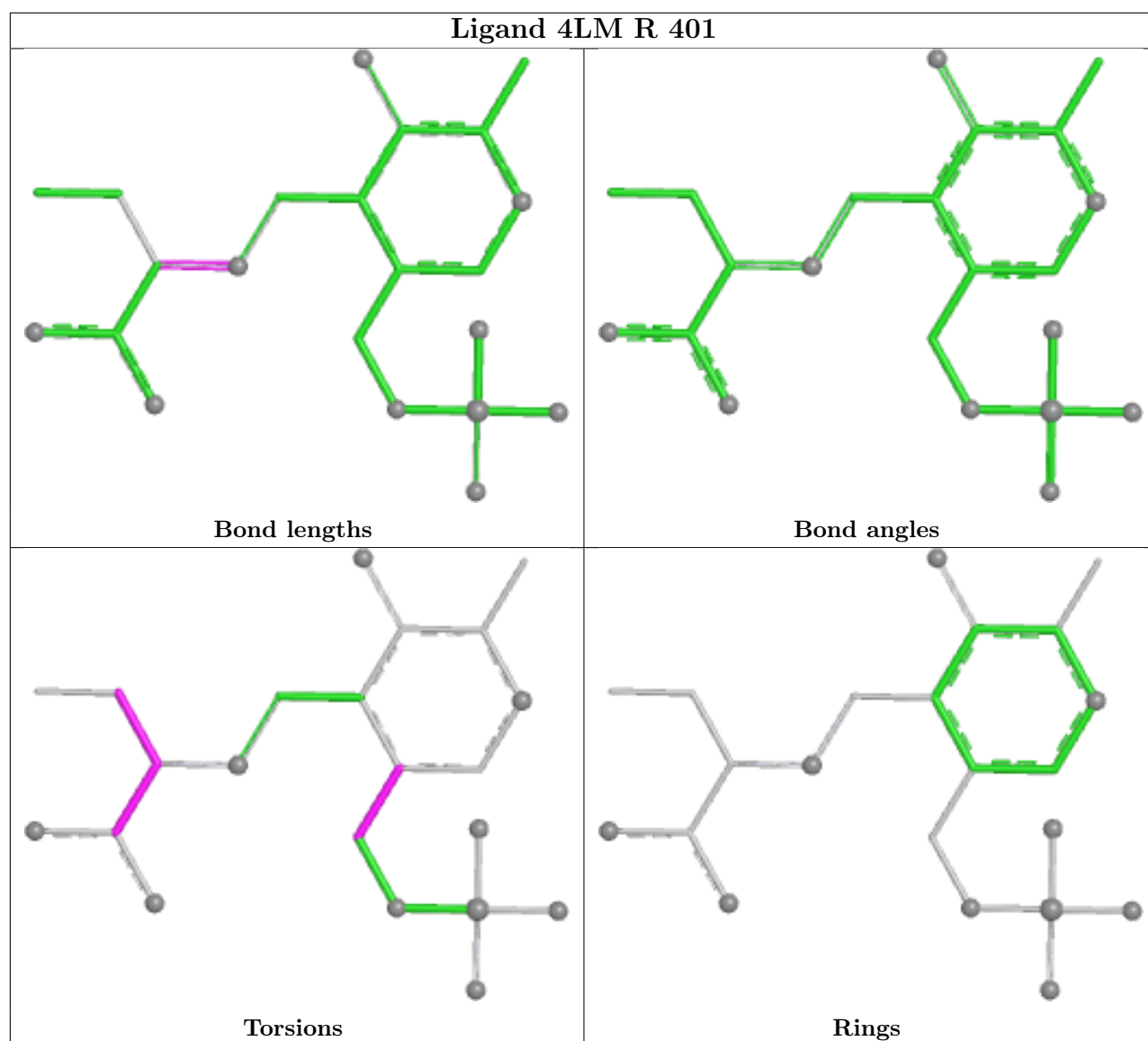


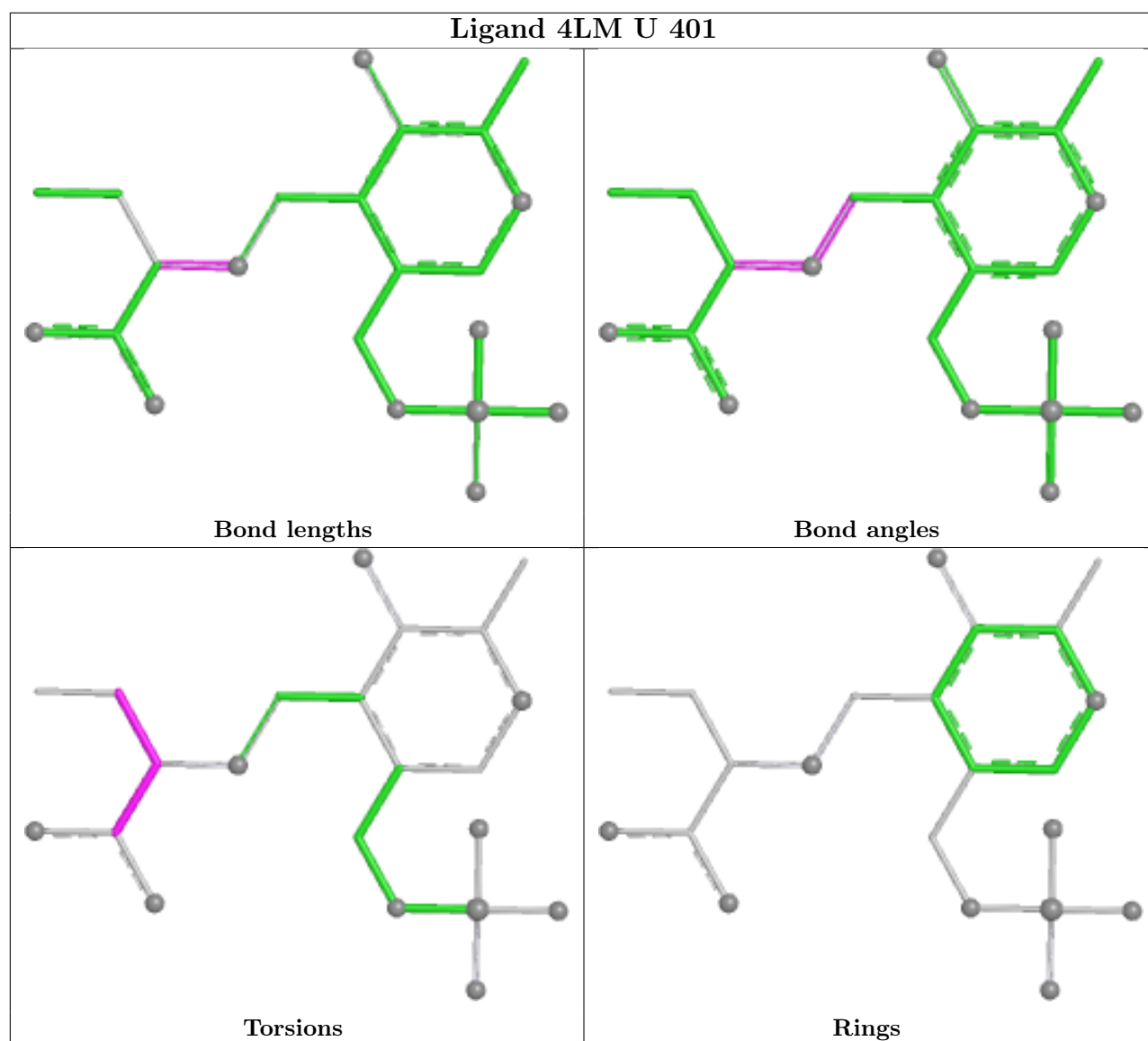


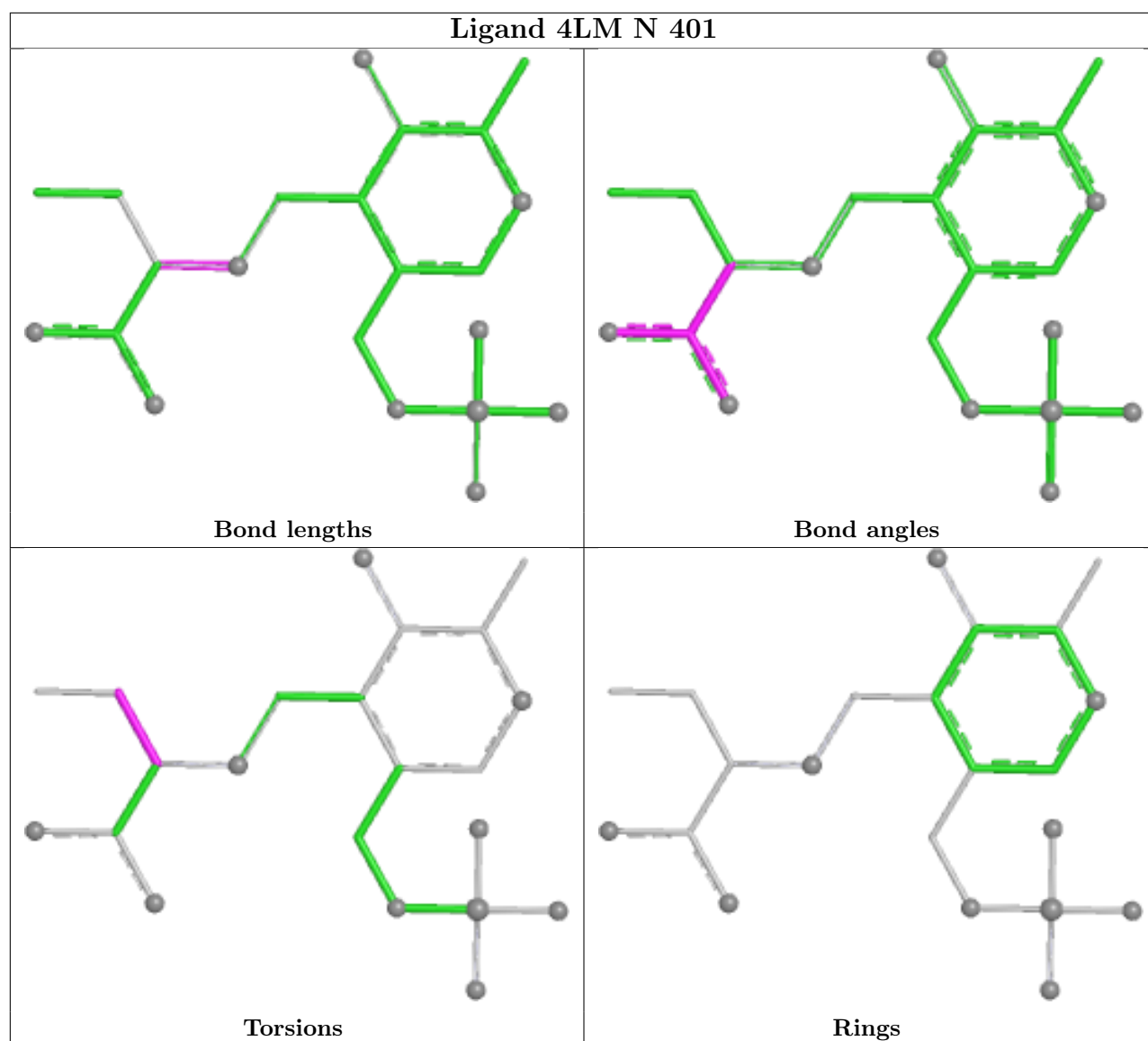


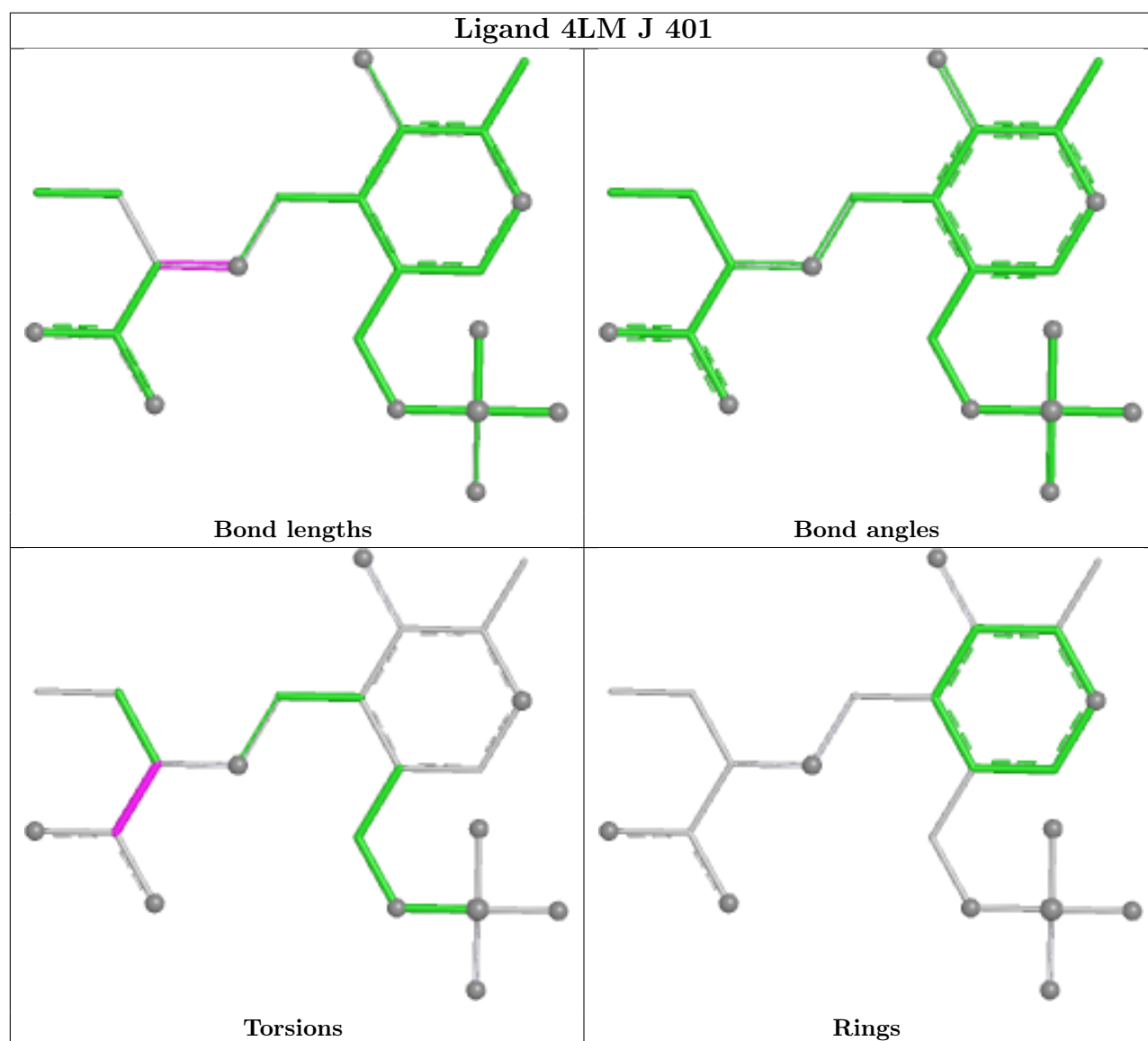


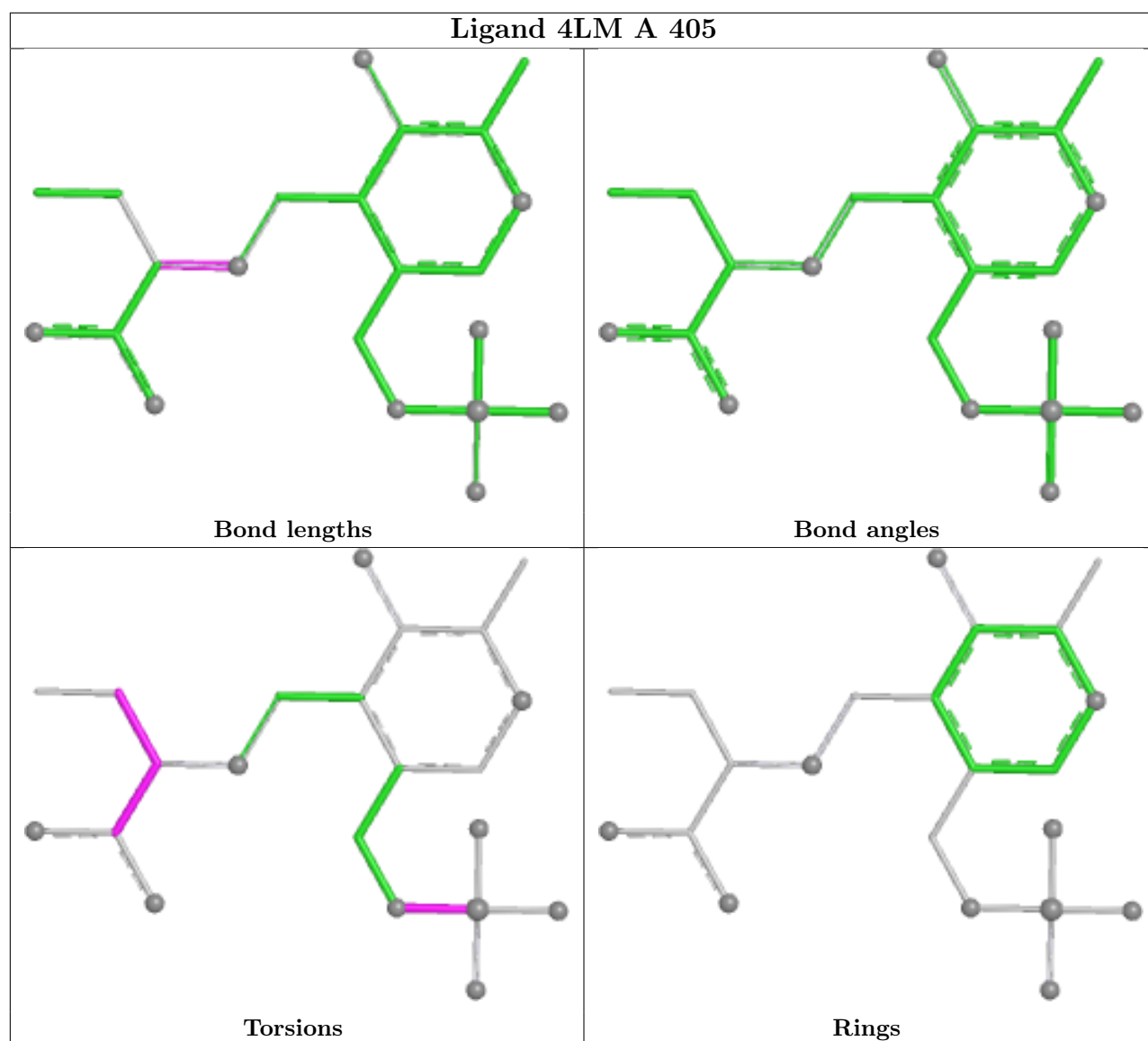


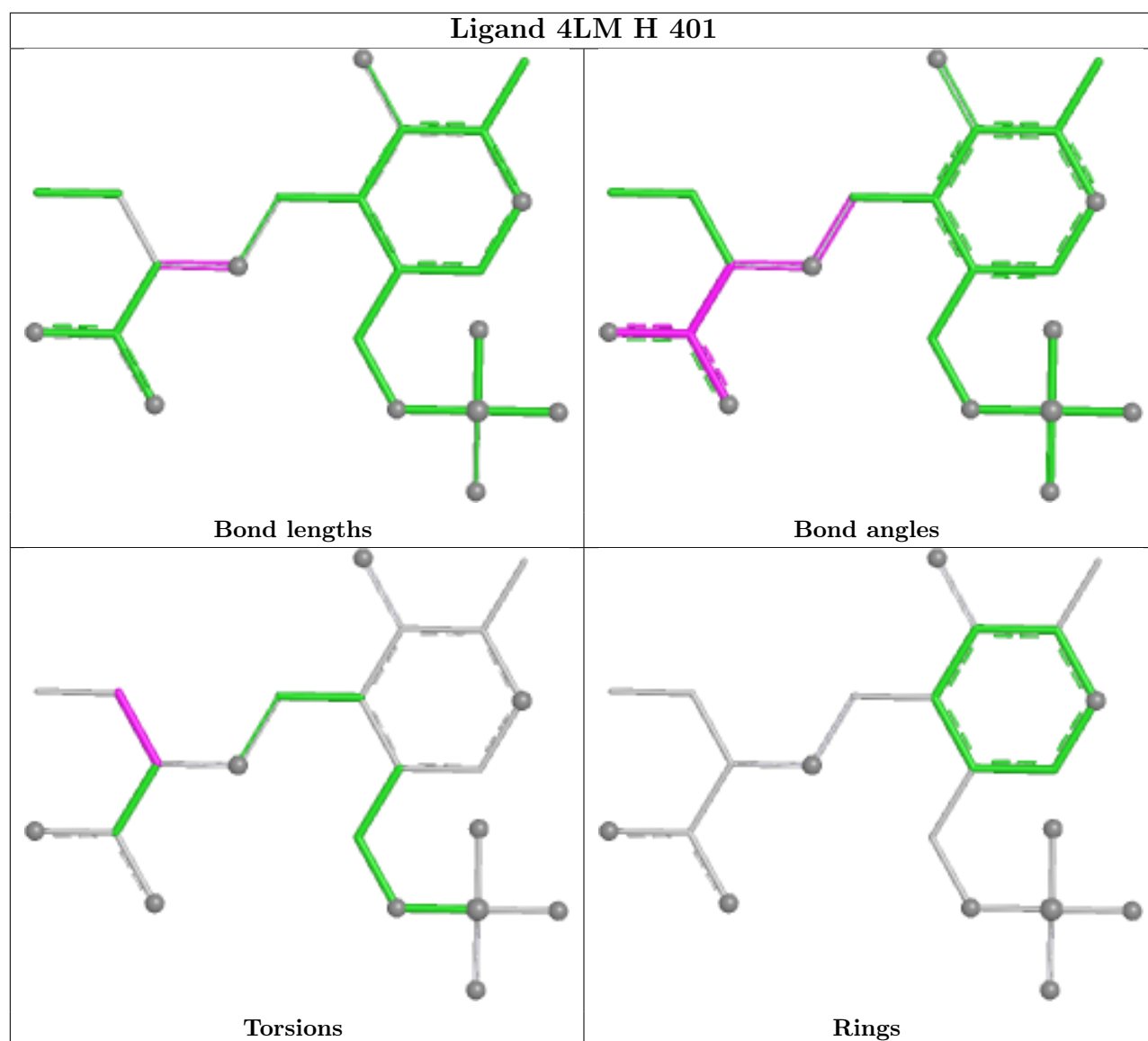


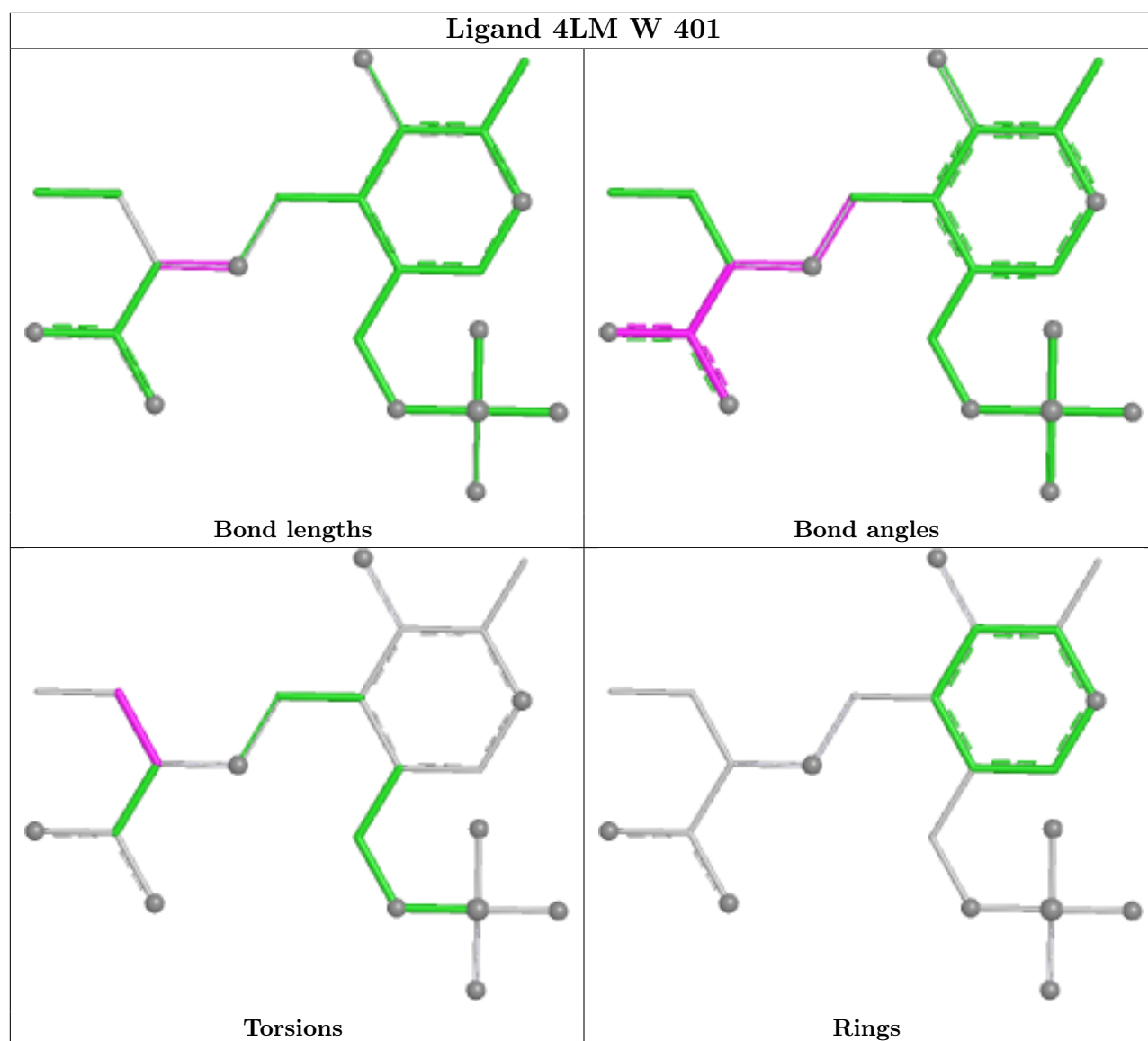


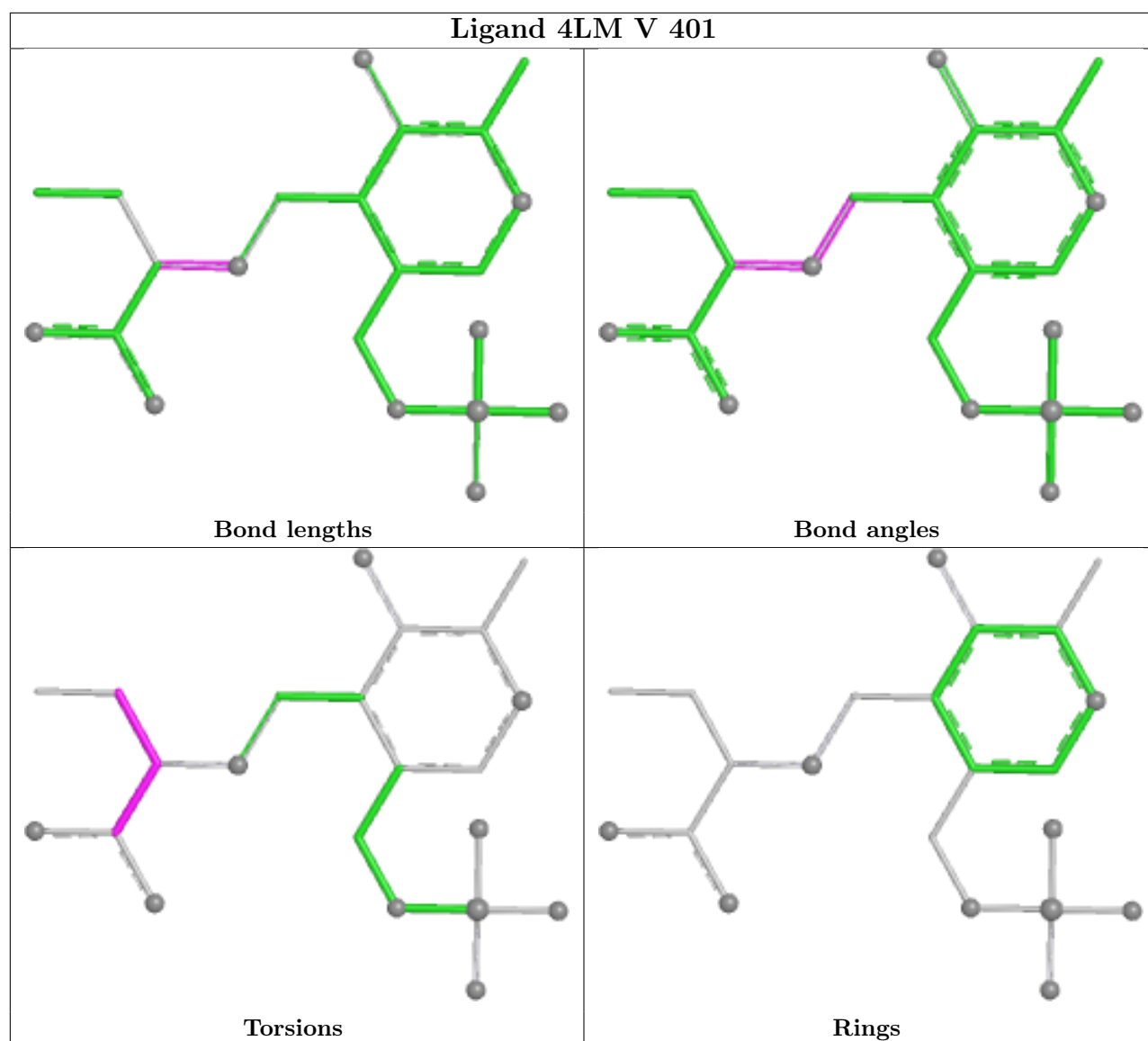


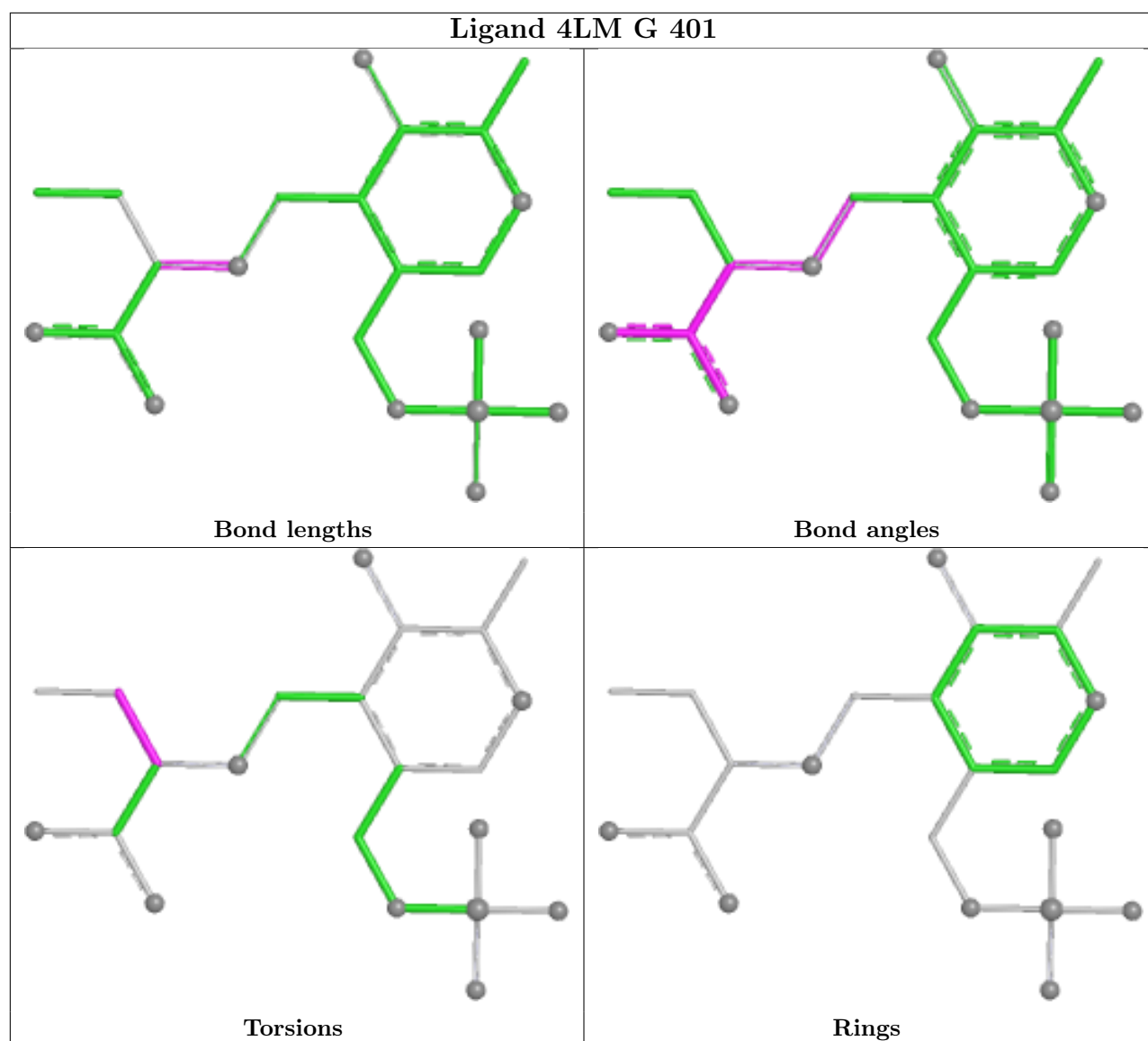


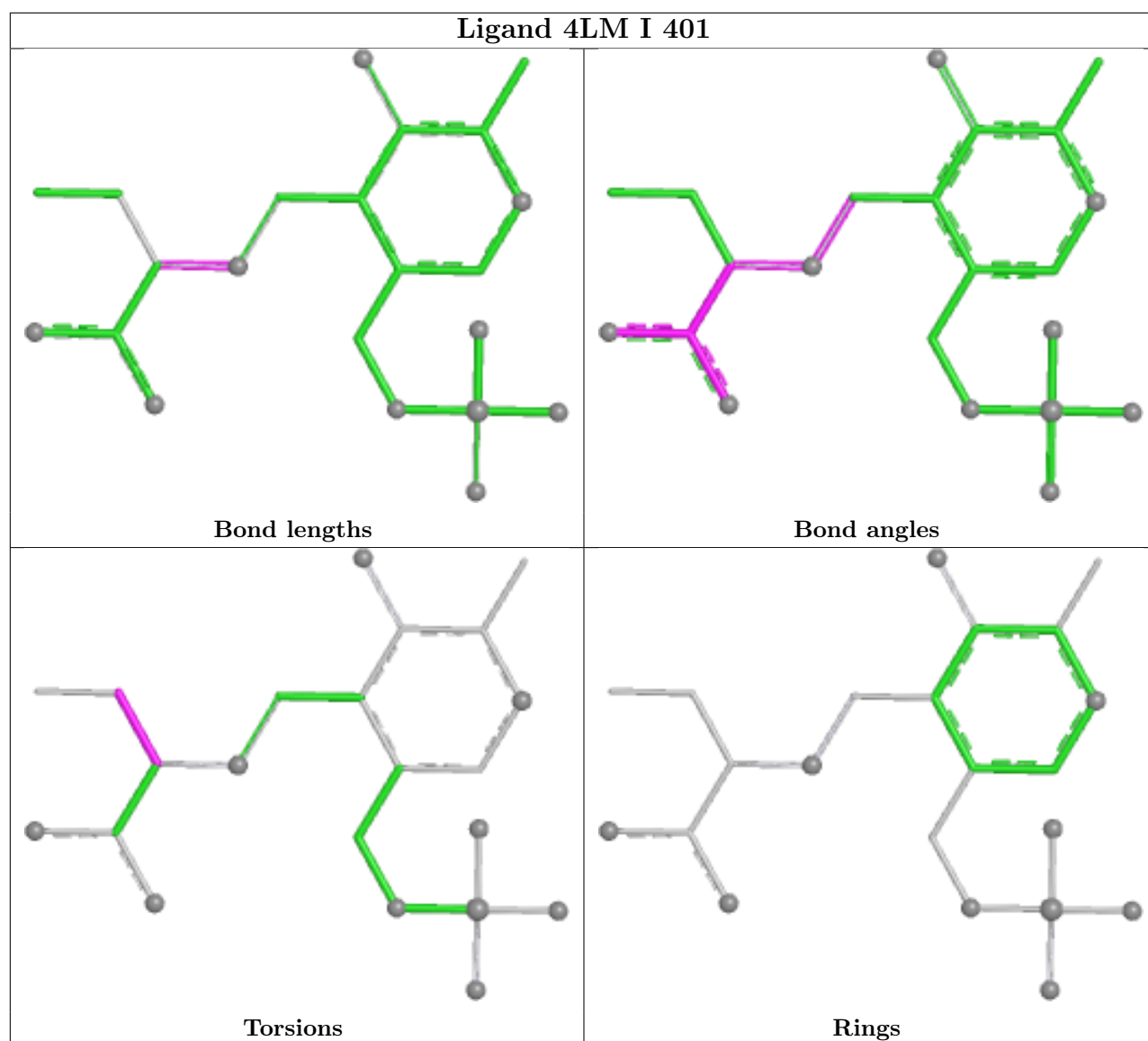


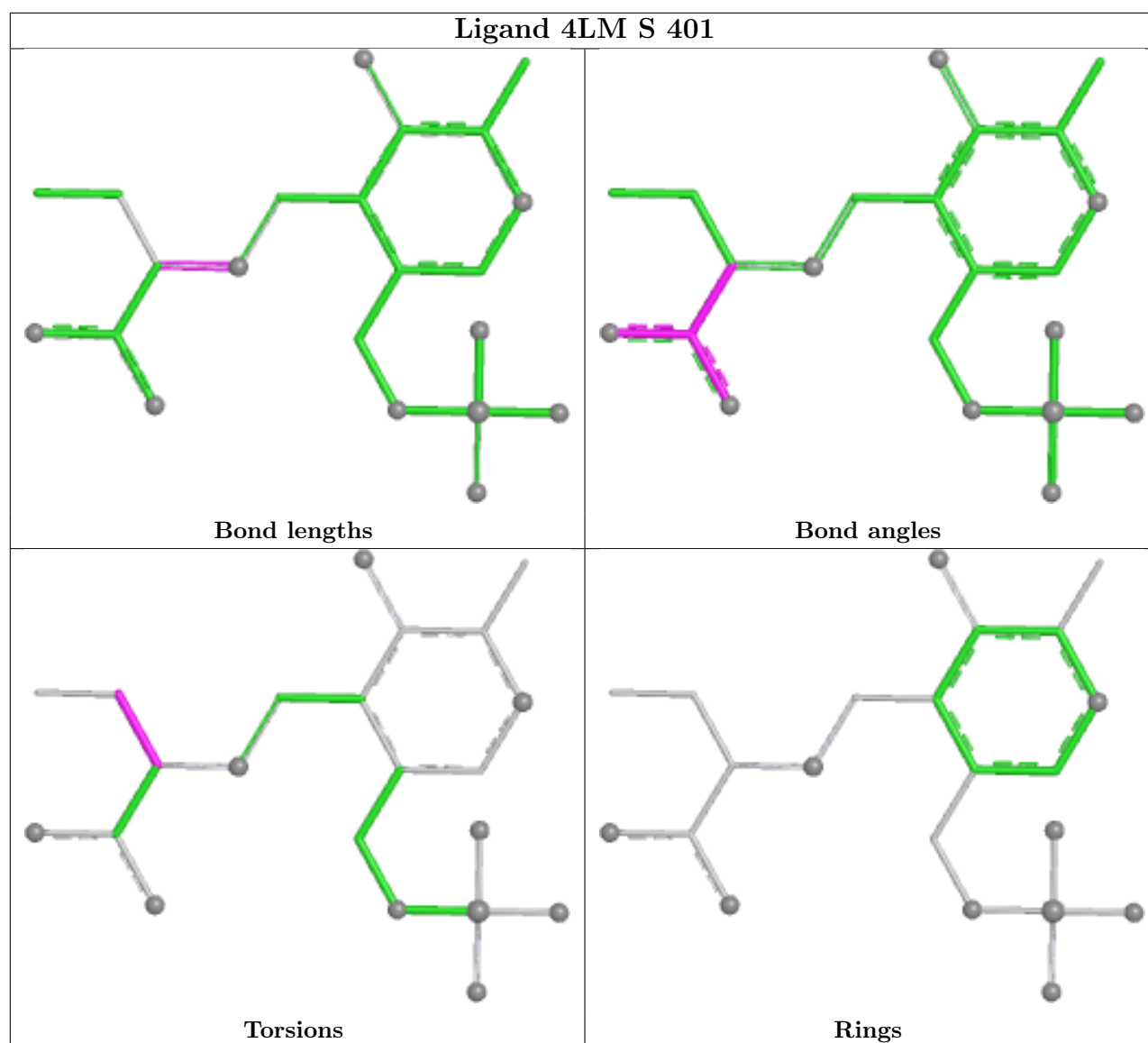












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	387/413 (93%)	-1.44	0	100	100	20, 34, 51, 61	0
1	B	387/413 (93%)	-1.45	0	100	100	17, 35, 53, 63	0
1	C	387/413 (93%)	-1.35	0	100	100	22, 44, 60, 70	0
1	D	387/413 (93%)	-1.37	0	100	100	26, 48, 69, 78	0
1	E	388/413 (93%)	-1.20	0	100	100	32, 60, 89, 99	0
1	F	387/413 (93%)	-1.10	0	100	100	27, 63, 95, 108	0
1	G	387/413 (93%)	-1.37	0	100	100	21, 42, 65, 77	0
1	H	387/413 (93%)	-1.39	0	100	100	21, 41, 59, 74	0
1	I	387/413 (93%)	-1.14	0	100	100	45, 72, 94, 106	0
1	J	387/413 (93%)	-1.00	0	100	100	51, 75, 103, 114	0
1	K	387/413 (93%)	-1.04	1 (0%)	90	88	35, 61, 112, 126	0
1	L	388/413 (93%)	-1.25	0	100	100	36, 58, 86, 98	0
1	M	388/413 (93%)	-1.43	0	100	100	16, 36, 54, 68	0
1	N	388/413 (93%)	-1.35	0	100	100	23, 47, 75, 86	0
1	O	388/413 (93%)	-1.35	0	100	100	23, 47, 80, 89	0
1	P	388/413 (93%)	-1.38	0	100	100	24, 44, 62, 76	0
1	Q	388/413 (93%)	-1.06	0	100	100	35, 64, 109, 137	0
1	R	387/413 (93%)	-0.99	0	100	100	48, 75, 101, 109	0
1	S	388/413 (93%)	-1.02	0	100	100	46, 74, 111, 120	0
1	T	386/413 (93%)	-1.11	0	100	100	47, 72, 90, 106	0
1	U	387/413 (93%)	-1.15	0	100	100	50, 67, 84, 93	0
1	V	385/413 (93%)	-1.05	0	100	100	48, 79, 110, 121	0
1	W	386/413 (93%)	-0.96	0	100	100	57, 88, 115, 127	0
1	X	387/413 (93%)	-1.09	0	100	100	51, 77, 103, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	9292/9912 (93%)	-1.21	1 (0%) 100 100	16, 58, 98, 137	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	385	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	404	5/5	0.97	0.05	103,103,103,103	0
3	SO4	N	402	5/5	0.97	0.05	88,88,88,88	0
3	SO4	V	402	5/5	0.97	0.06	100,100,100,100	0
3	SO4	J	402	5/5	0.98	0.05	106,106,106,106	0
3	SO4	A	403	5/5	0.98	0.05	88,88,88,88	0
3	SO4	B	403	5/5	0.98	0.04	124,124,124,124	0
2	PEG	A	401	7/7	0.99	0.03	29,30,30,30	0
2	PEG	B	402	7/7	0.99	0.06	53,53,54,54	0
2	PEG	B	405	7/7	0.99	0.04	22,22,22,22	0
3	SO4	B	404	5/5	0.99	0.04	86,86,86,86	0
3	SO4	C	401	5/5	0.99	0.04	78,78,78,78	0
3	SO4	D	402	5/5	0.99	0.04	99,99,99,99	0
3	SO4	F	402	5/5	0.99	0.05	87,87,87,87	0
3	SO4	H	403	5/5	0.99	0.04	90,91,91,91	0
2	PEG	H	402	7/7	0.99	0.02	39,39,39,39	0
3	SO4	L	402	5/5	0.99	0.04	86,86,86,86	0

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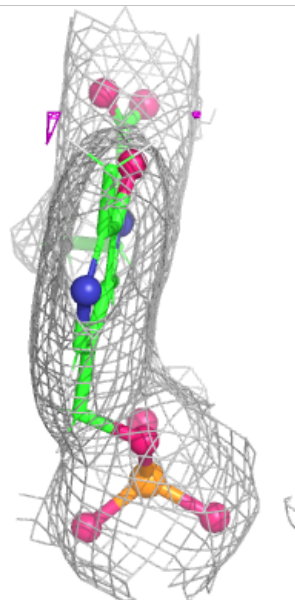
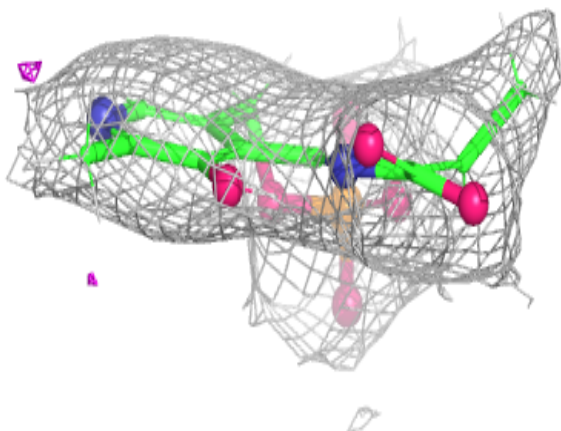
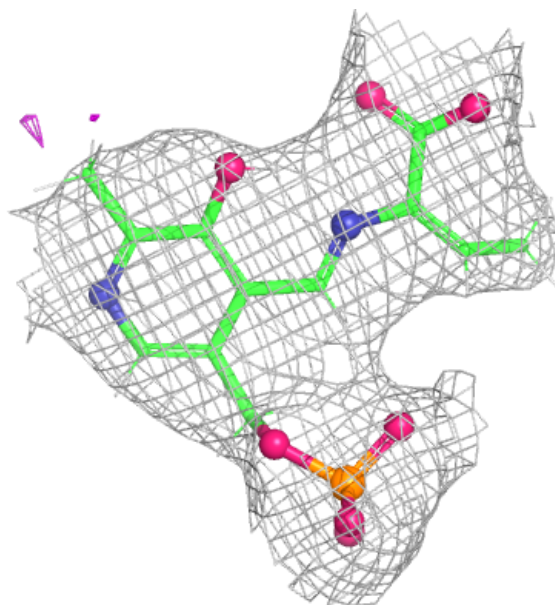
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	M	402	5/5	0.99	0.04	78,78,78,78	0
2	PEG	N	403	7/7	0.99	0.03	32,32,33,33	0
3	SO4	O	401	5/5	0.99	0.05	83,83,83,83	0
3	SO4	P	402	5/5	0.99	0.07	79,79,79,79	0
2	PEG	X	401	7/7	0.99	0.04	51,51,52,52	0
4	4LM	E	401	22/22	0.99	0.03	40,42,43,43	0
4	4LM	J	401	22/22	0.99	0.04	63,63,64,64	0
4	4LM	N	401	22/22	0.99	0.03	31,34,35,35	0
4	4LM	O	402	22/22	0.99	0.03	31,31,32,32	0
4	4LM	Q	401	22/22	0.99	0.04	57,58,59,59	0
4	4LM	R	401	22/22	0.99	0.03	51,52,52,52	0
4	4LM	S	401	22/22	0.99	0.04	70,70,71,71	0
4	4LM	T	401	22/22	0.99	0.04	54,55,55,55	0
4	4LM	U	401	22/22	0.99	0.03	52,53,54,54	0
4	4LM	W	401	22/22	0.99	0.03	74,74,75,75	0
4	4LM	A	405	22/22	1.00	0.03	26,28,29,29	0
4	4LM	K	401	22/22	1.00	0.02	41,44,47,47	0
4	4LM	L	401	22/22	1.00	0.03	46,47,50,50	0
4	4LM	M	401	22/22	1.00	0.03	19,23,25,26	0
4	4LM	B	401	22/22	1.00	0.02	18,21,21,21	0
4	4LM	C	402	22/22	1.00	0.02	33,35,35,35	0
4	4LM	P	401	22/22	1.00	0.02	24,26,27,27	0
4	4LM	D	401	22/22	1.00	0.03	29,30,30,30	0
2	PEG	A	402	7/7	1.00	0.02	32,32,34,34	0
4	4LM	F	401	22/22	1.00	0.03	52,54,55,55	0
4	4LM	G	401	22/22	1.00	0.02	29,30,30,30	0
4	4LM	H	401	22/22	1.00	0.03	21,24,26,27	0
4	4LM	V	401	22/22	1.00	0.03	68,68,68,68	0
4	4LM	I	401	22/22	1.00	0.03	63,63,63,63	0
4	4LM	X	402	22/22	1.00	0.03	71,71,72,72	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.

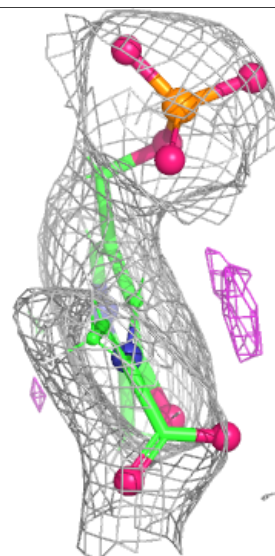
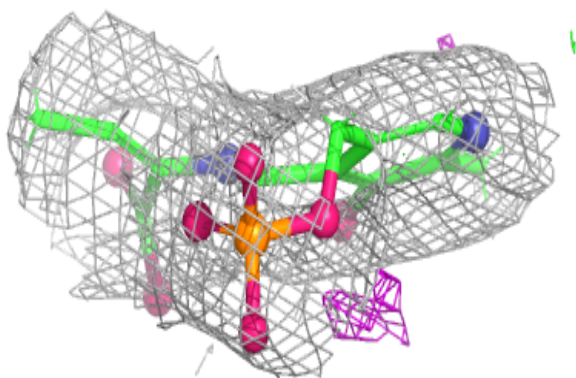
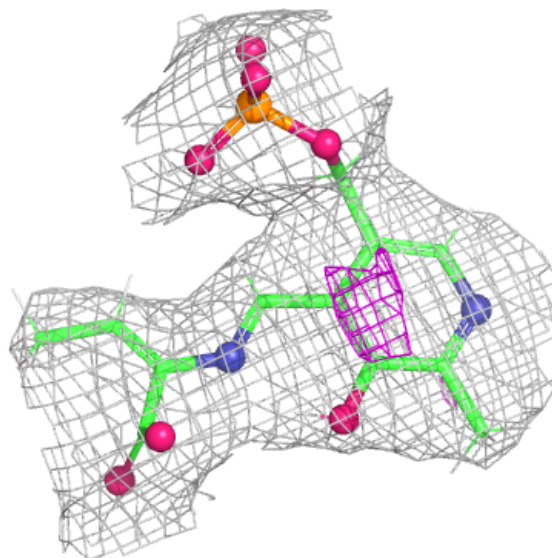
Electron density around 4LM E 401:

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



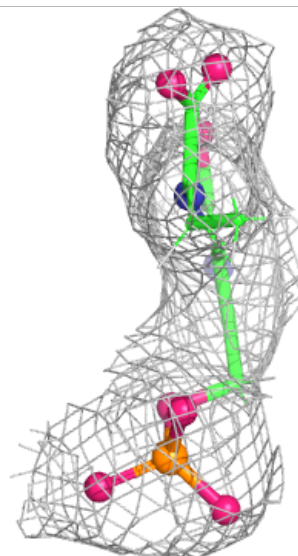
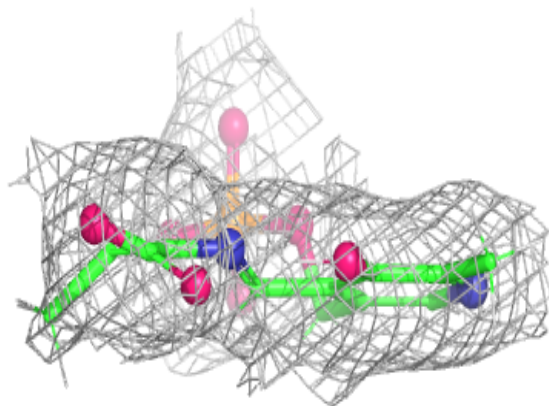
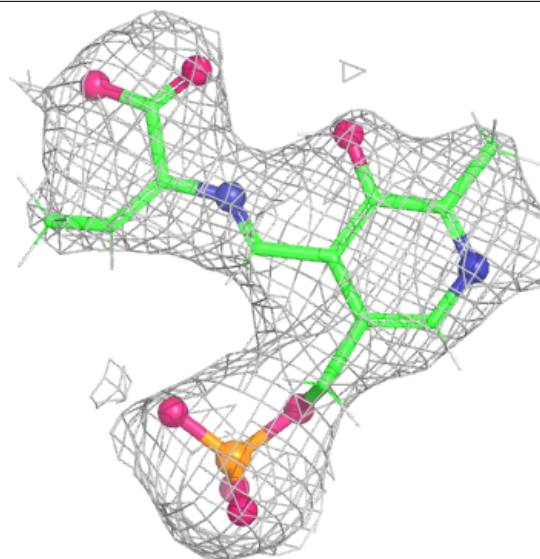
Electron density around 4LM J 401:

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



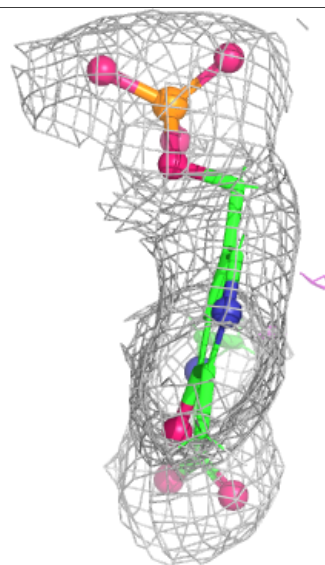
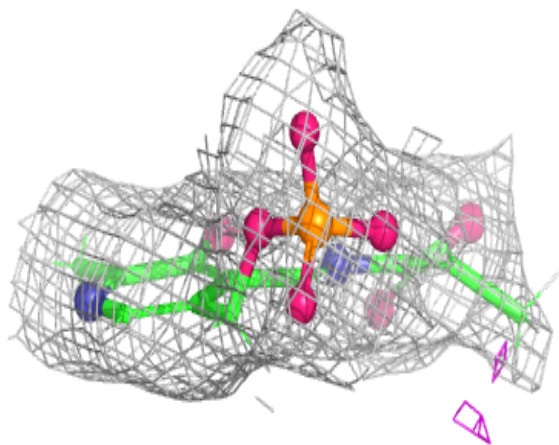
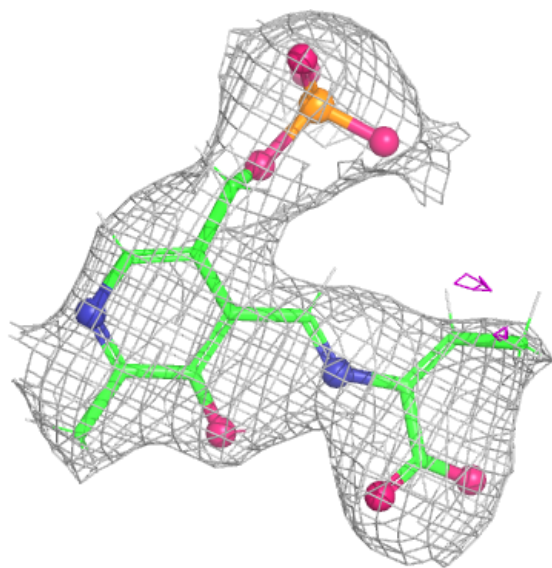
Electron density around 4LM N 401:

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



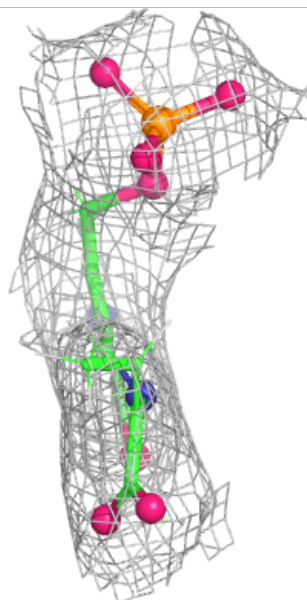
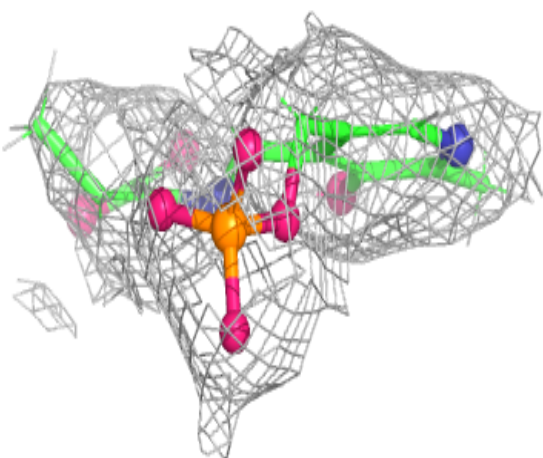
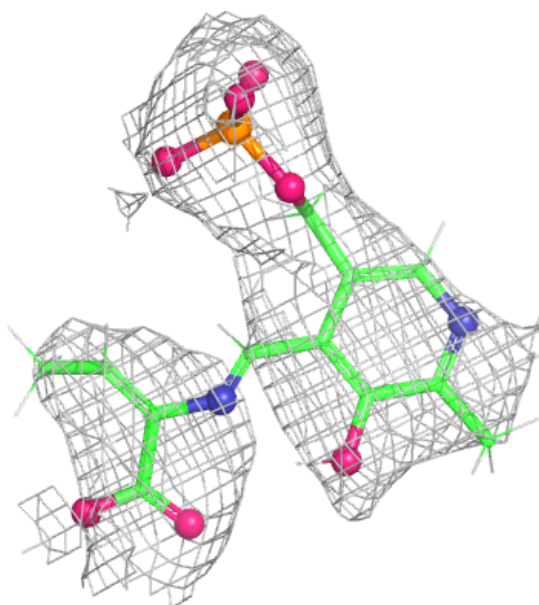
Electron density around 4LM O 402:

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and green (positive)



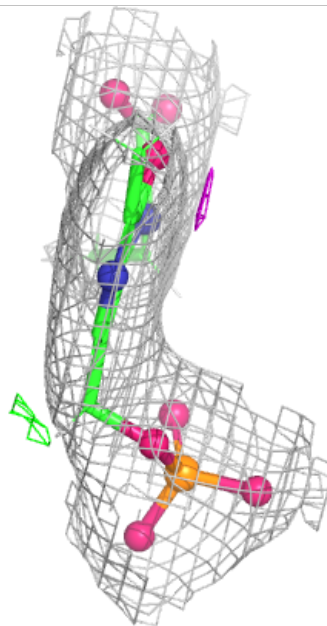
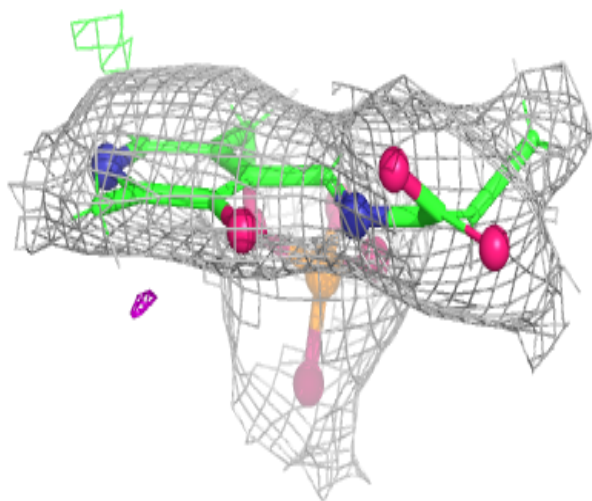
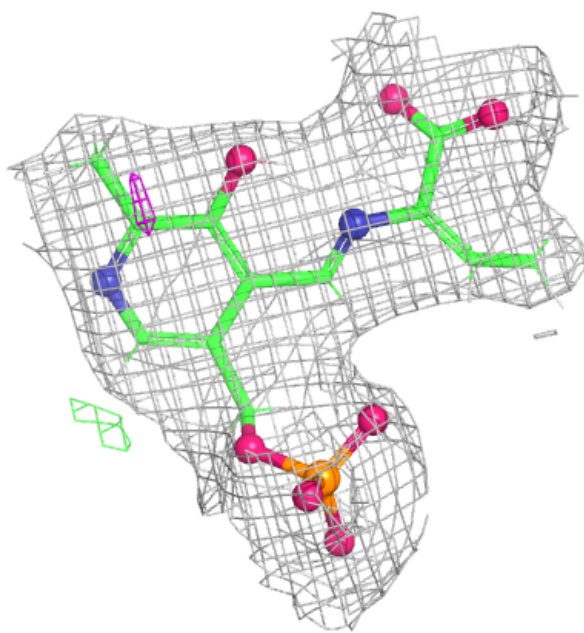
Electron density around 4LM Q 401:

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



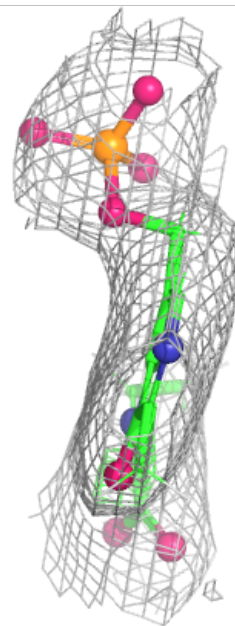
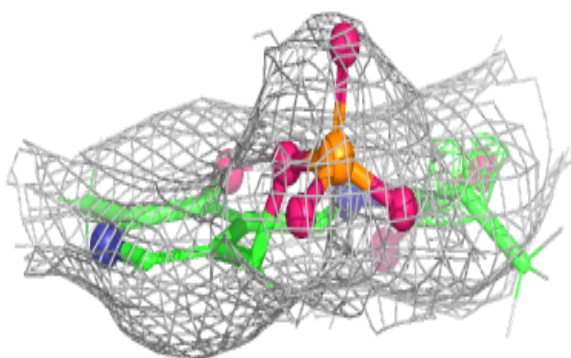
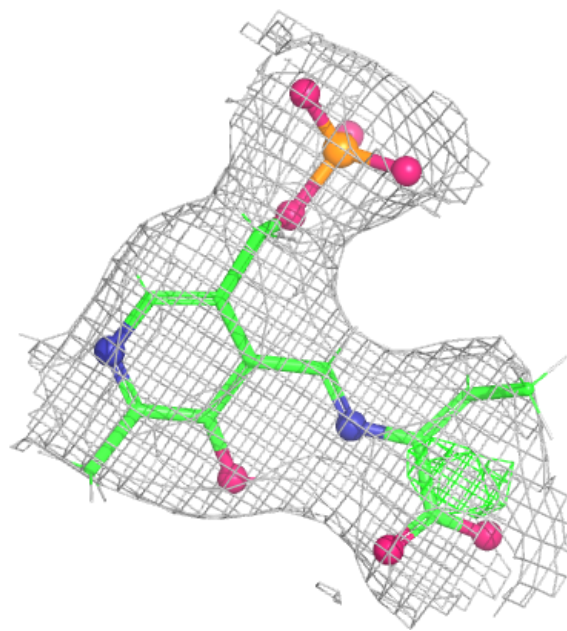
Electron density around 4LM R 401:

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and green (positive)



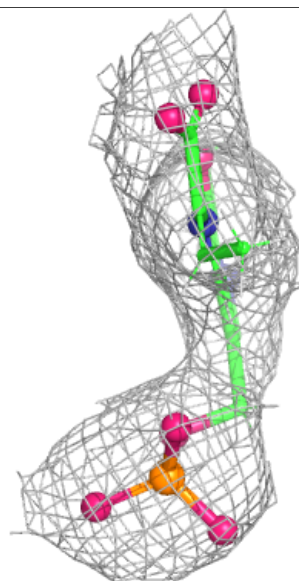
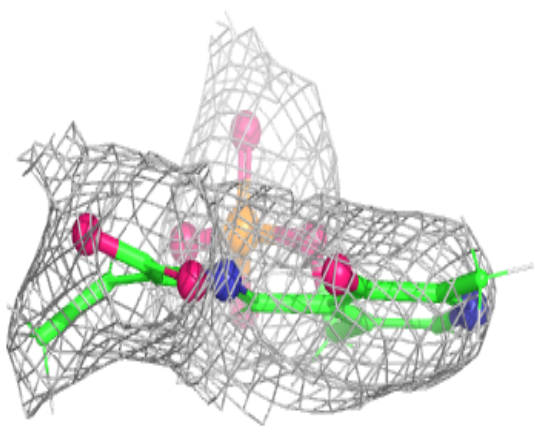
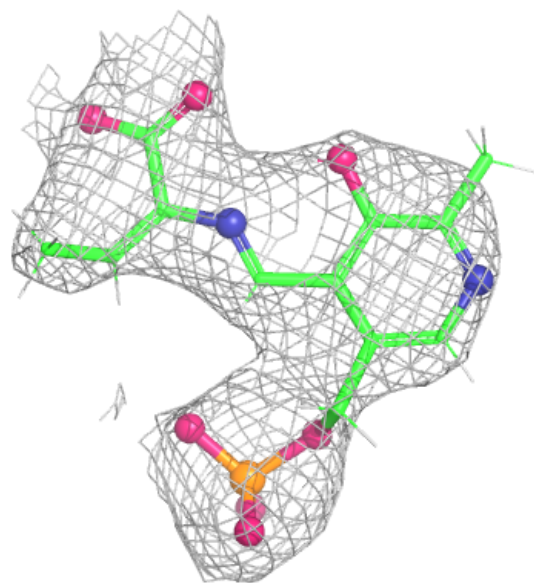
Electron density around 4LM S 401:

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



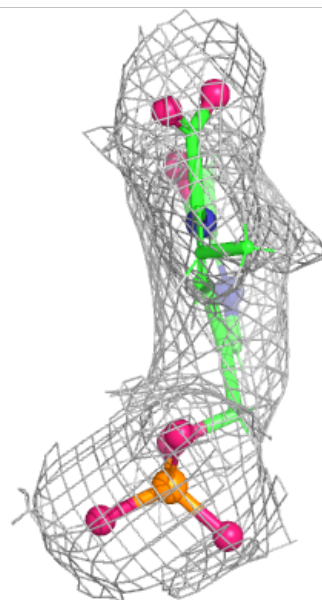
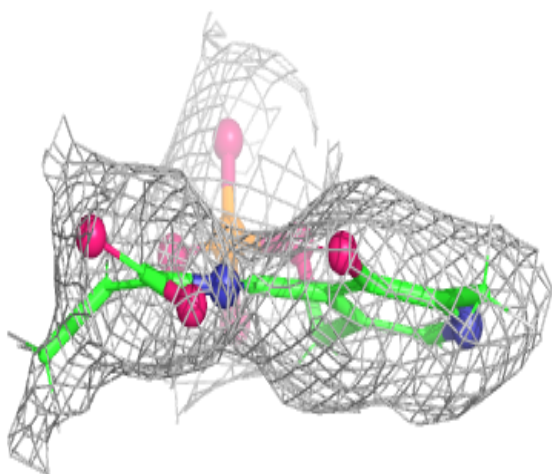
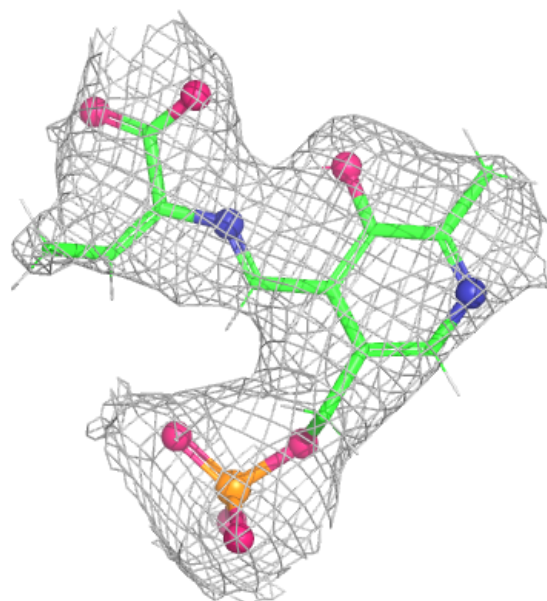
Electron density around 4LM T 401:

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and green (positive)



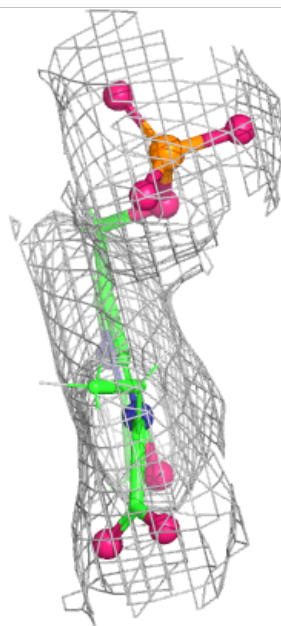
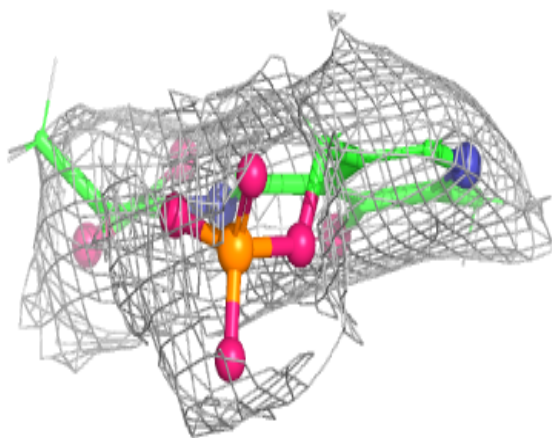
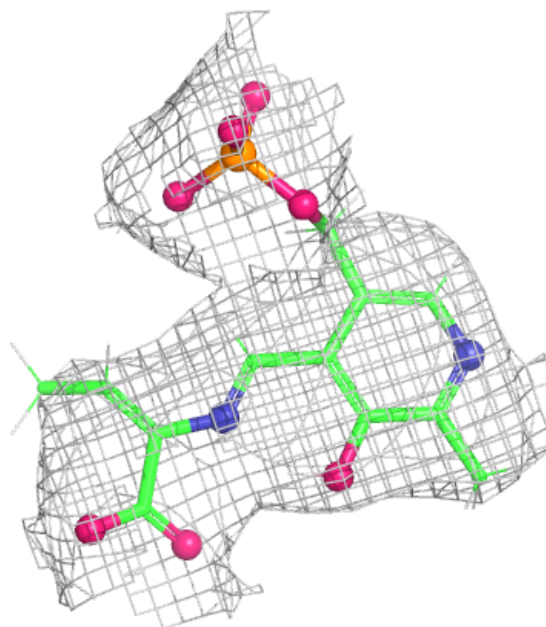
Electron density around 4LM U 401:

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and green (positive)



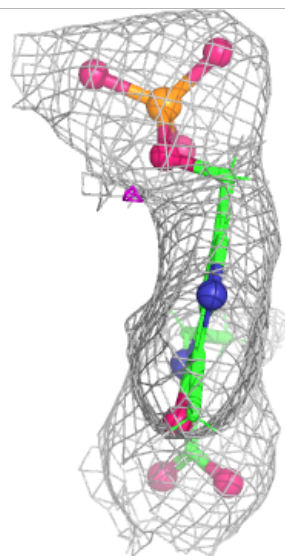
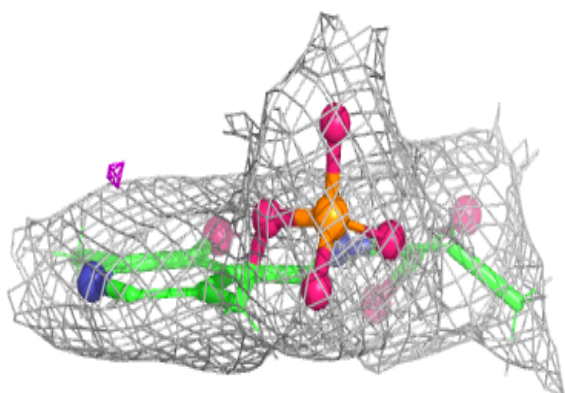
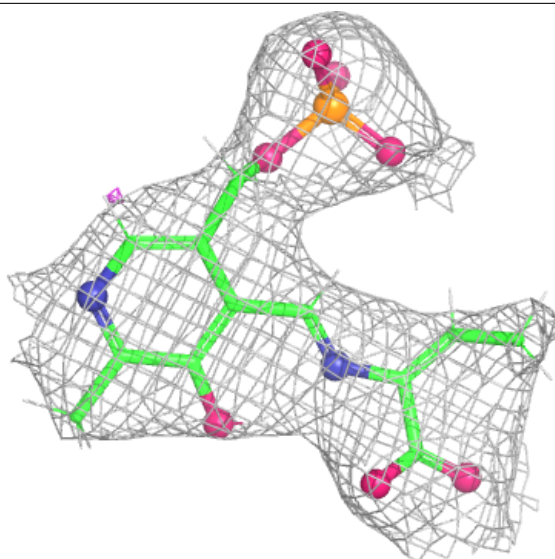
Electron density around 4LM W 401:

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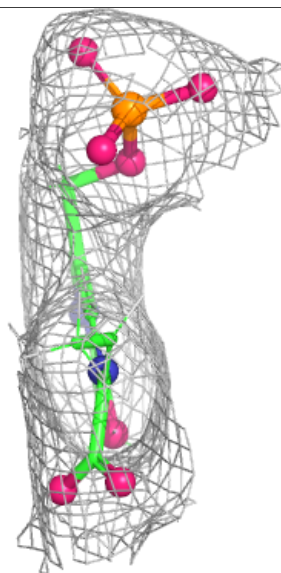
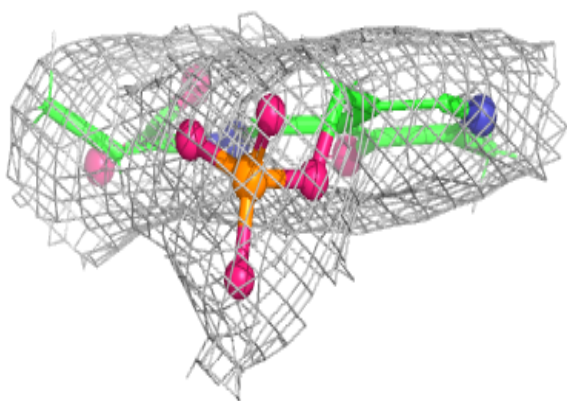
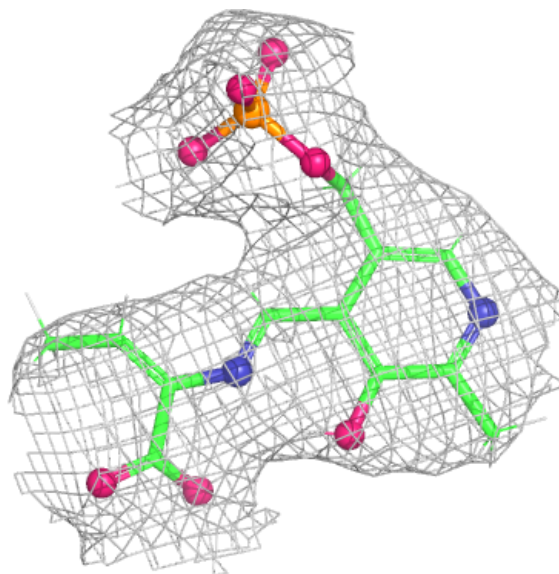
Electron density around 4LM A 405:

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



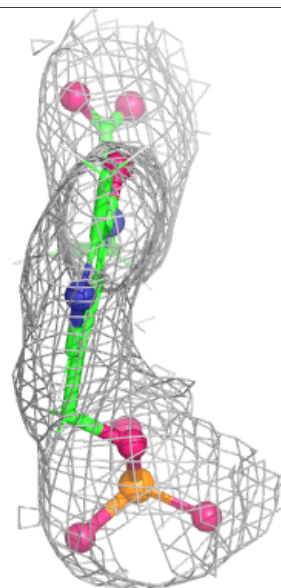
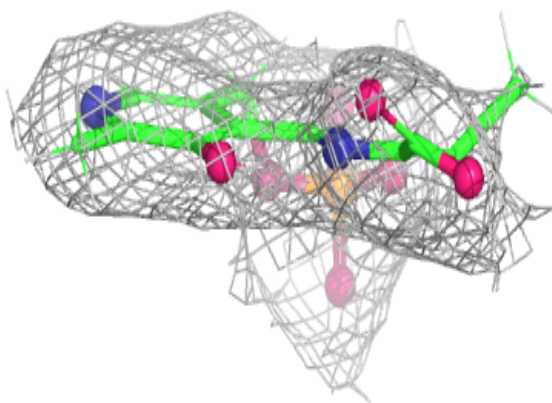
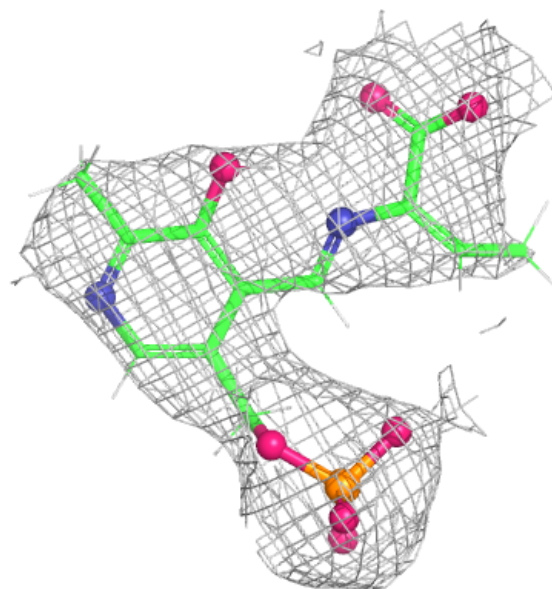
Electron density around 4LM K 401:

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



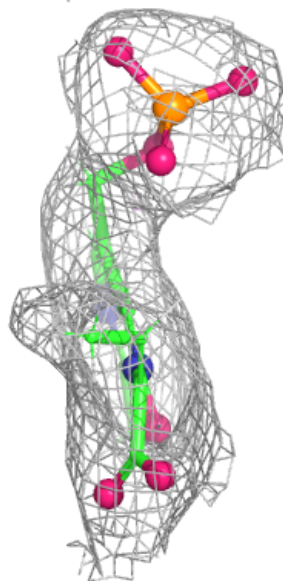
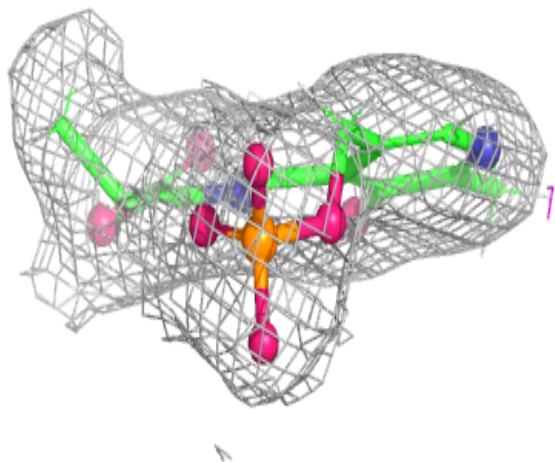
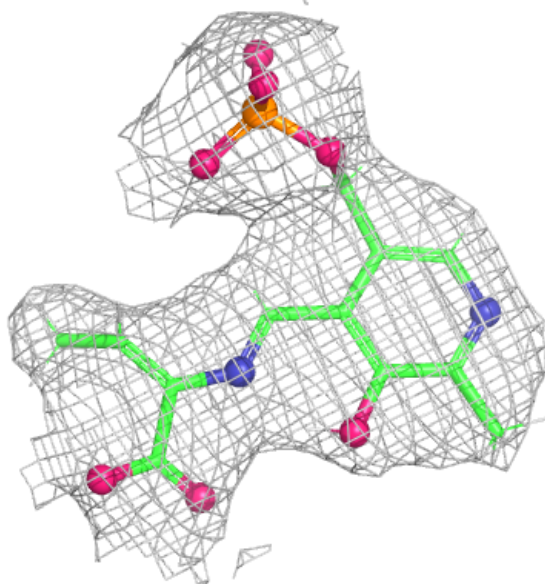
Electron density around 4LM L 401:

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



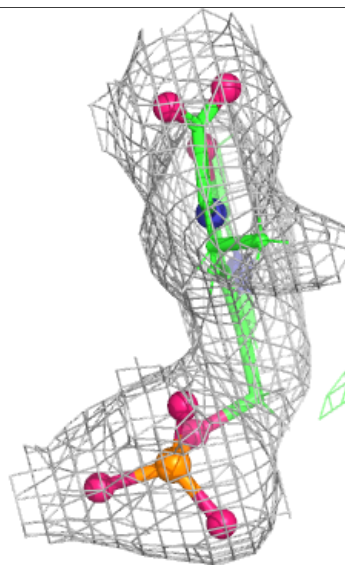
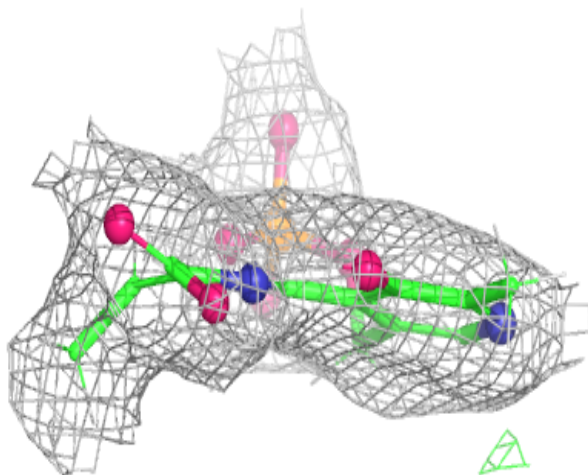
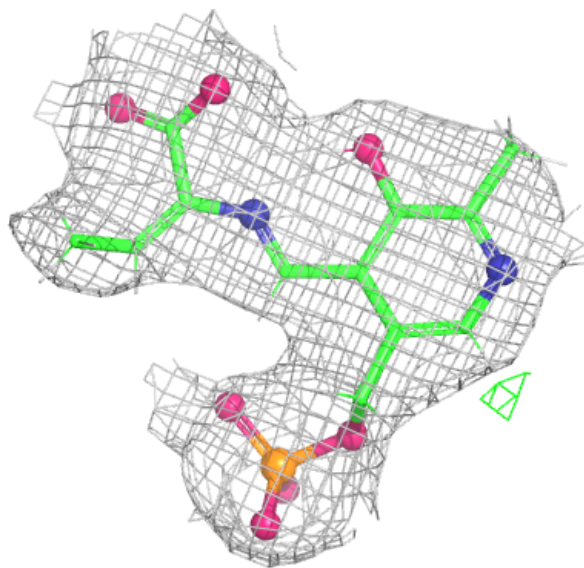
Electron density around 4LM M 401:

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



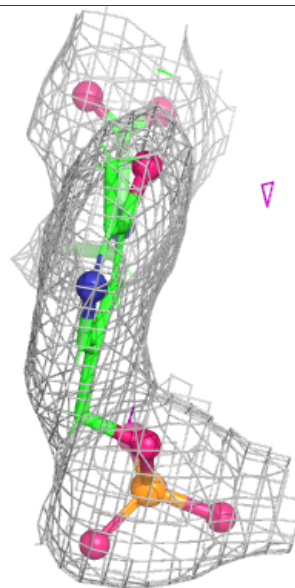
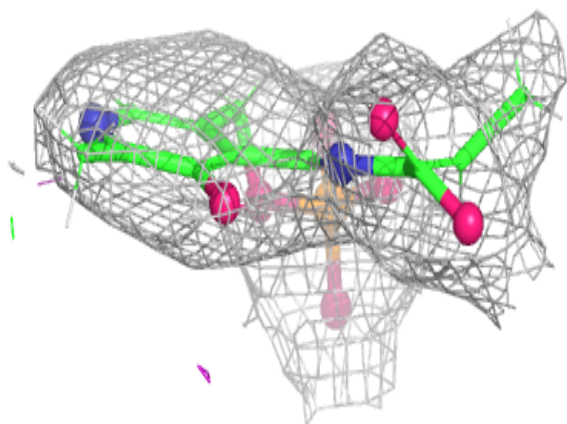
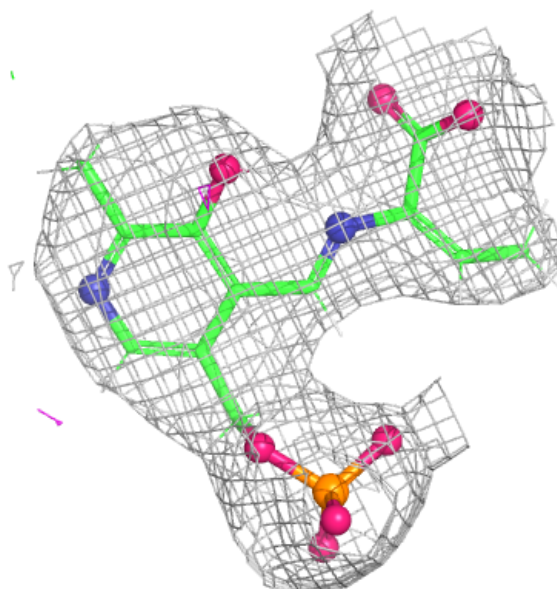
Electron density around 4LM B 401:

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



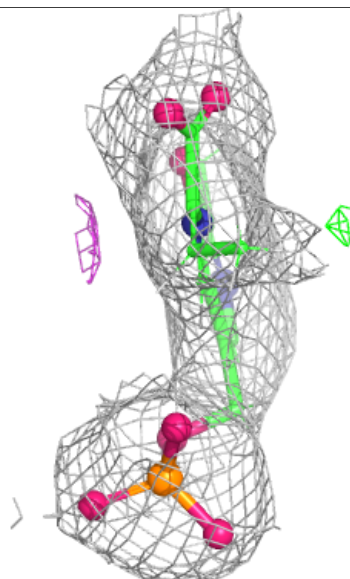
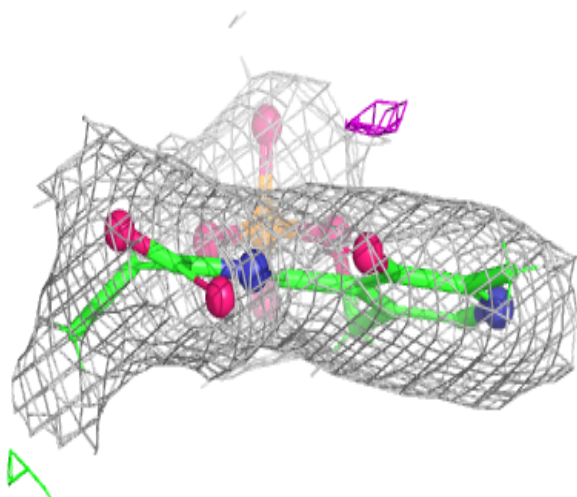
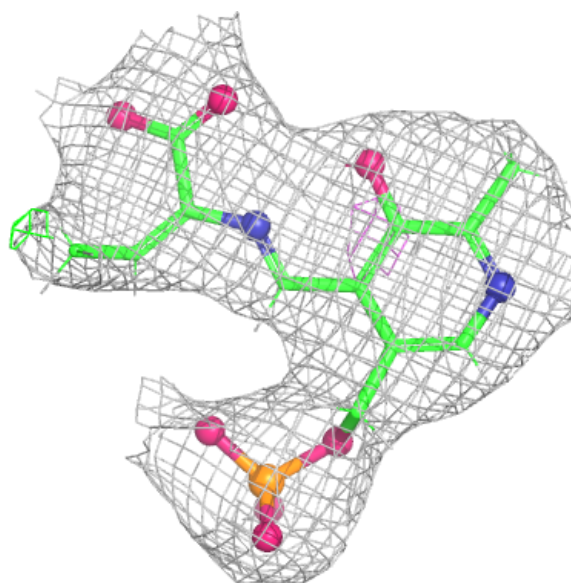
Electron density around 4LM C 402:

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



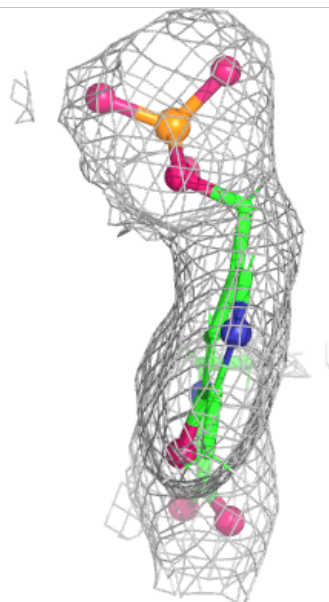
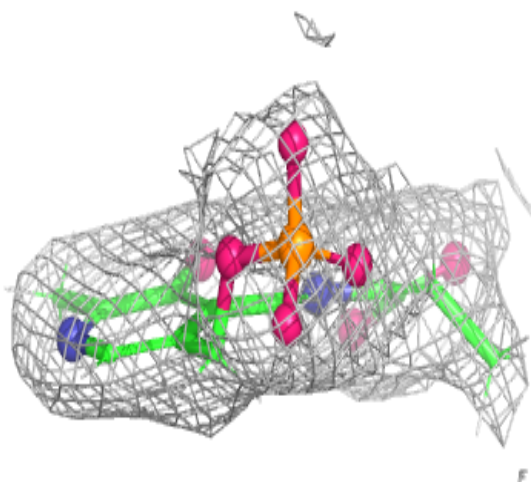
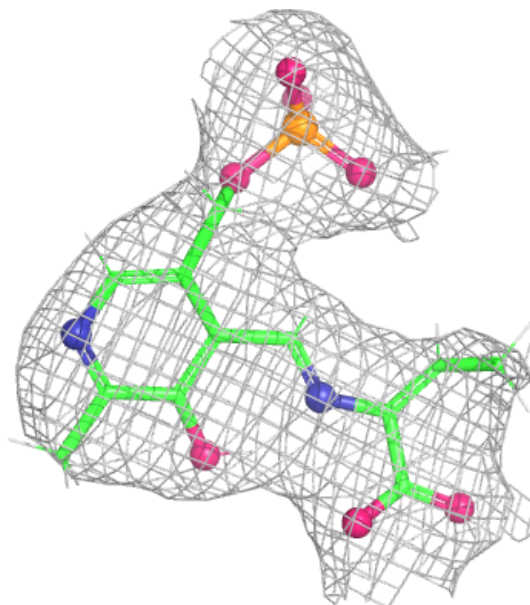
Electron density around 4LM P 401:

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



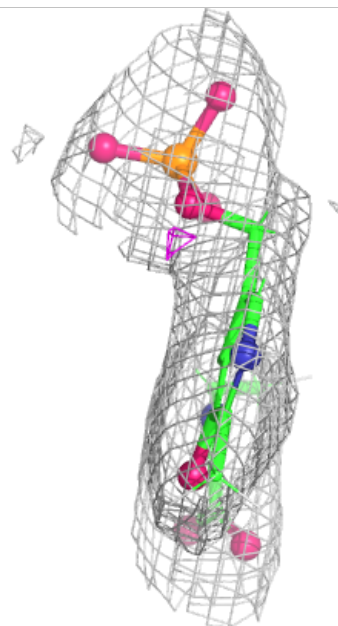
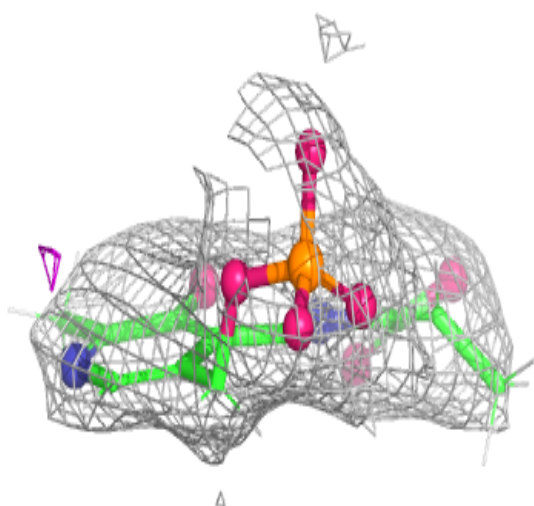
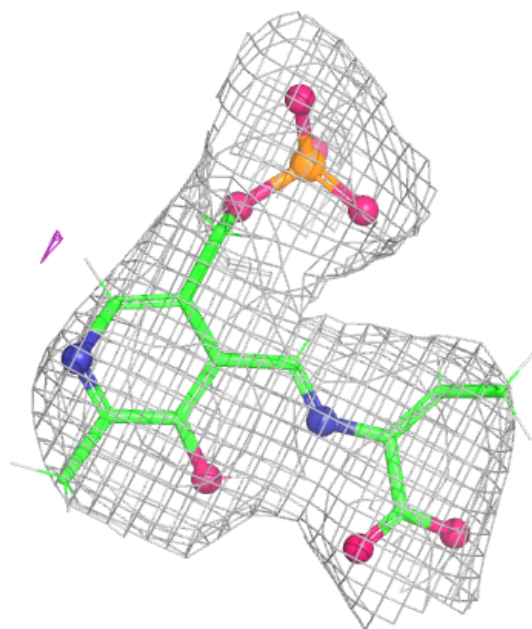
Electron density around 4LM D 401:

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



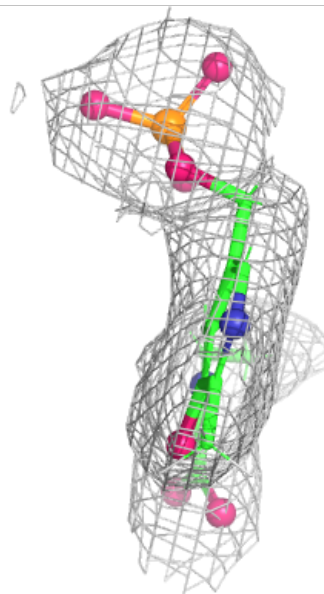
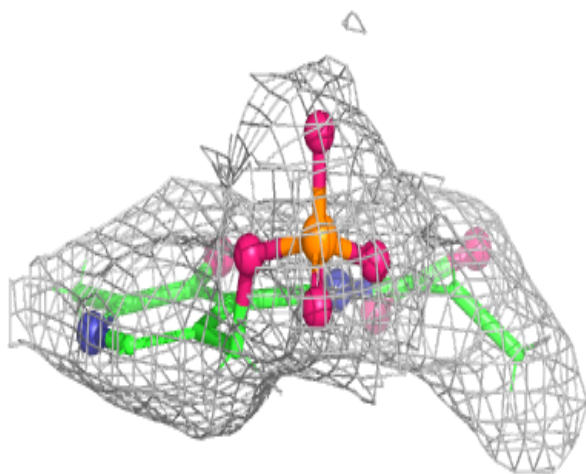
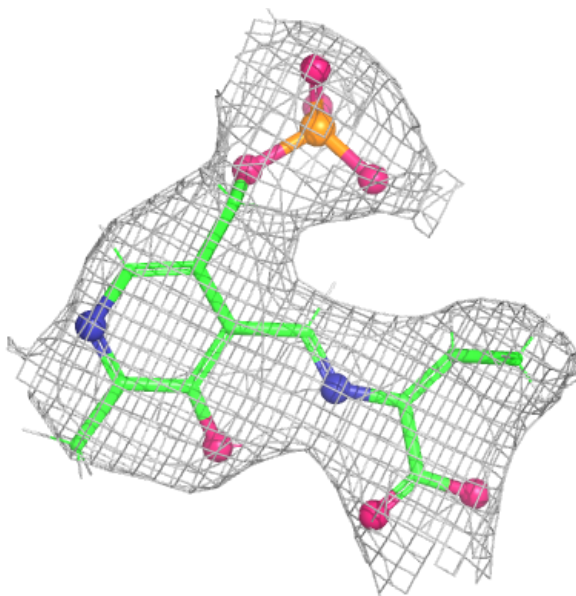
Electron density around 4LM F 401:

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



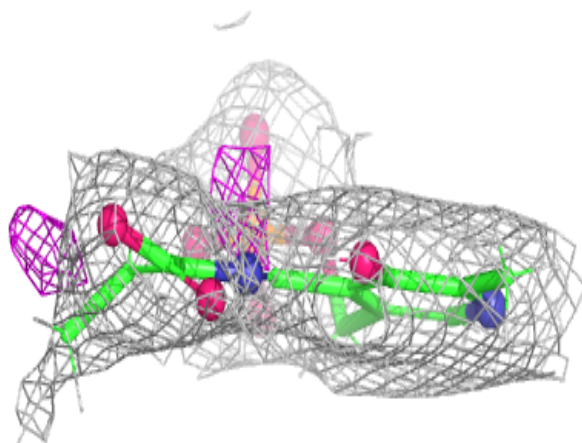
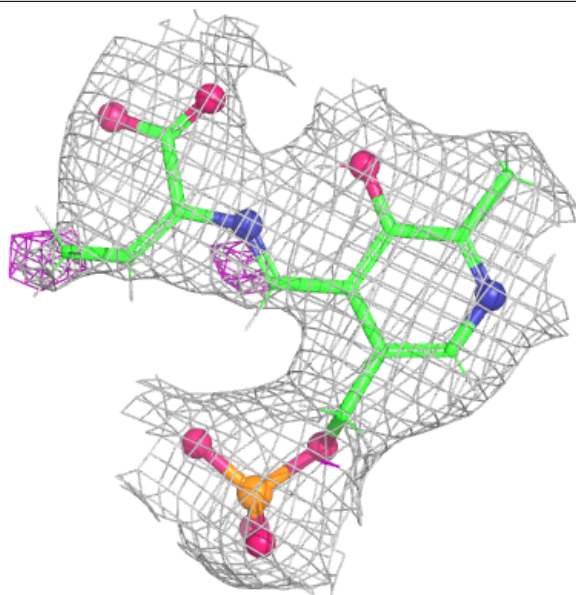
Electron density around 4LM G 401:

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



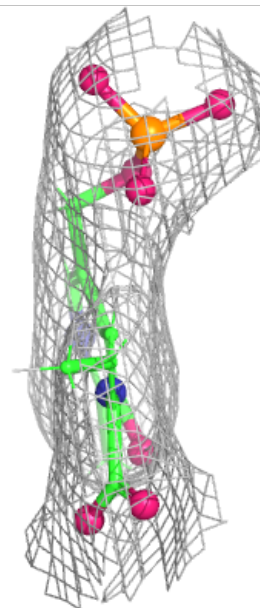
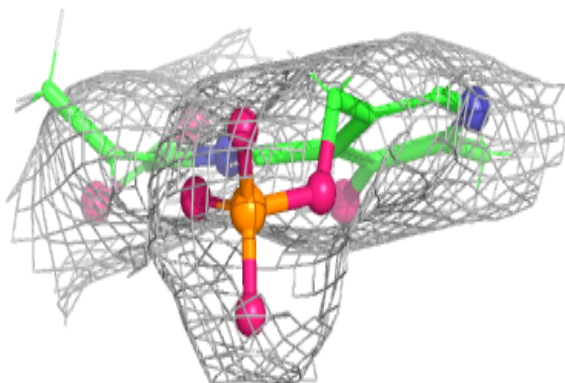
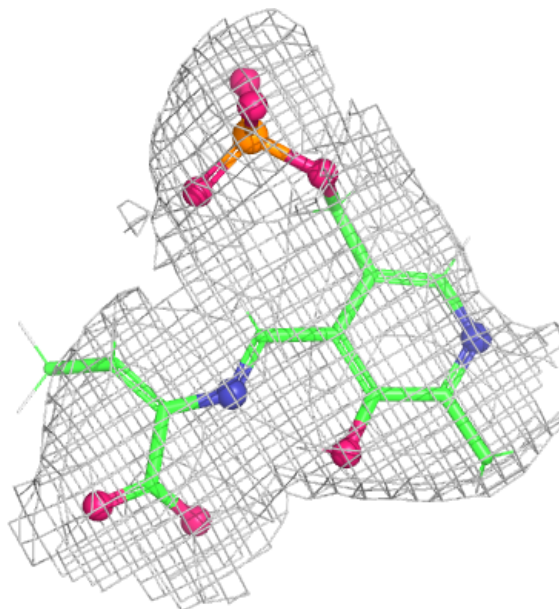
Electron density around 4LM H 401:

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



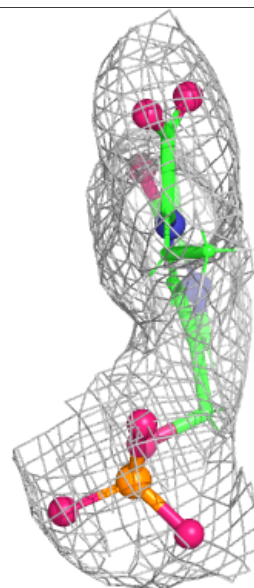
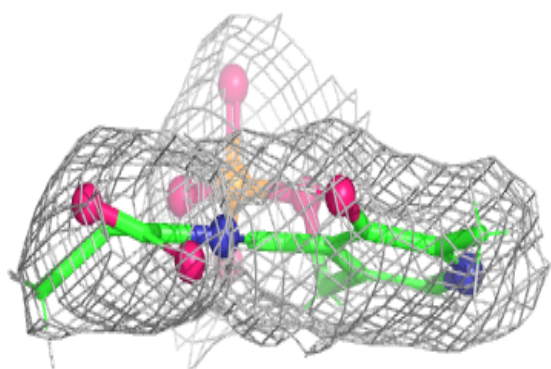
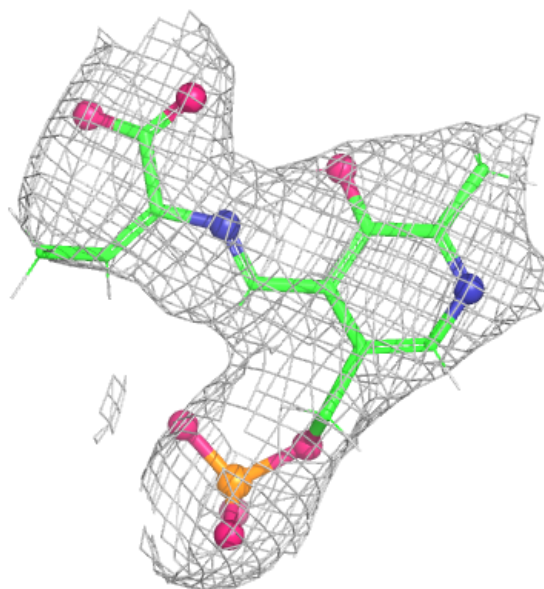
Electron density around 4LM V 401:

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



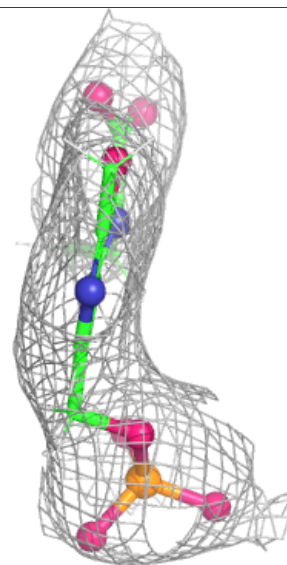
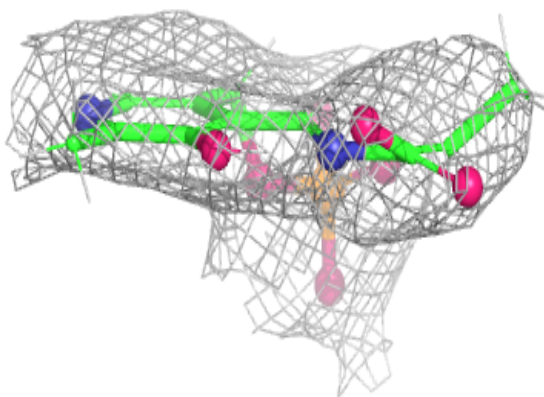
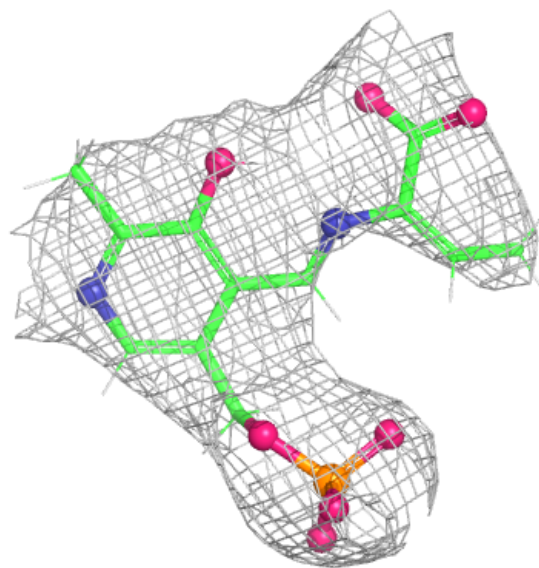
Electron density around 4LM I 401:

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



Electron density around 4LM X 402:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.