



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2025 – 12:35 pm GMT

PDB ID : 8S88
Title : Crystal structure of human L-lactate Dehydrogenase B protein in complex with NADH, oxamate and fluoxetine
Authors : Van Gysel, M.; Wouters, J.
Deposited on : 2024-03-06
Resolution : 2.07 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

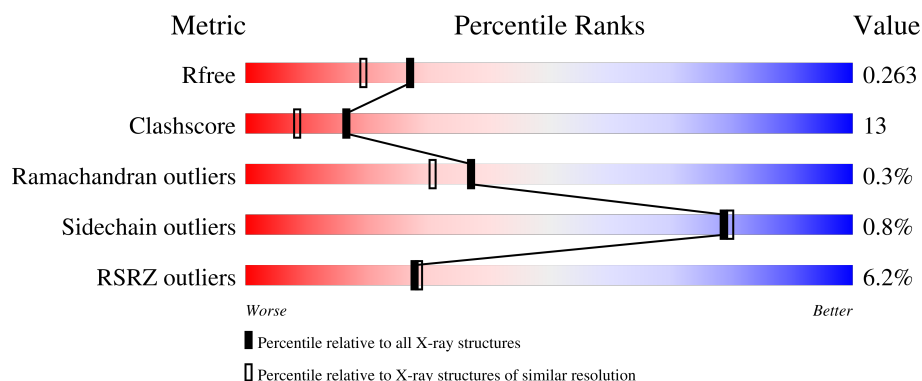
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 Å.

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



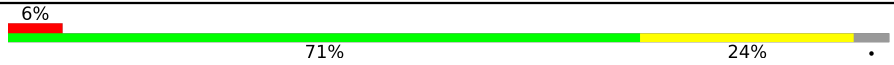

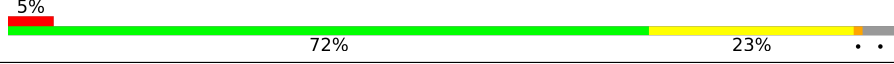
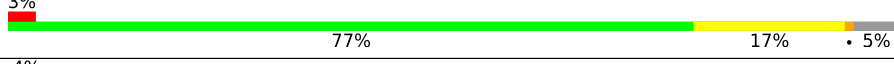

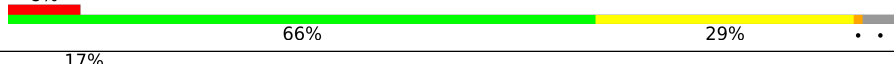
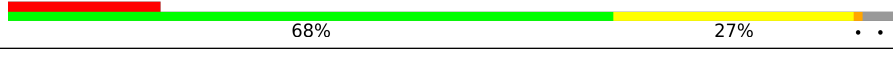
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3436 (2.08-2.04)
Clashscore	180529	3661 (2.08-2.04)
Ramachandran outliers	177936	3649 (2.08-2.04)
Sidechain outliers	177891	3649 (2.08-2.04)
RSRZ outliers	164620	3436 (2.08-2.04)

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	349	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>5%</div> </div> </div>
1	B	349	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>• 5%</div> </div> </div>
1	C	349	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>•</div> </div> </div>
1	D	349	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>5%</div> </div> </div>
1	E	349	<div> <div>7%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	349	
1	G	349	
1	H	349	
1	I	349	
1	J	349	
1	K	349	
1	L	349	

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
2	SFX	B	401	-	-	X	-
2	SFX	F	401	-	-	X	-
3	OXM	A	402	-	-	X	-
3	OXM	F	402	-	-	X	-
3	OXM	L	401	-	-	X	-
7	GOL	K	405	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 33474 atoms, of which 356 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 L-lactate dehydrogenase B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	4	0	0
			2560	1628	431	487	14			
1	B	333	Total	C	N	O	S	0	0	0
			2560	1628	431	487	14			
1	C	334	Total	C	N	O	S	3	1	0
			2580	1639	436	491	14			
1	D	332	Total	C	N	O	S	4	0	0
			2552	1622	430	486	14			
1	E	332	Total	C	N	O	S	0	0	0
			2555	1625	430	486	14			
1	F	334	Total	C	N	O	S	0	0	0
			2569	1633	432	490	14			
1	G	333	Total	C	N	O	S	0	0	0
			2560	1628	431	487	14			
1	H	334	Total	C	N	O	S	1	1	0
			2578	1639	434	491	14			
1	I	333	Total	C	N	O	S	0	0	0
			2560	1628	431	487	14			
1	J	332	Total	C	N	O	S	3	0	0
			2552	1622	430	486	14			
1	K	334	Total	C	N	O	S	0	0	0
			2569	1633	432	490	14			
1	L	334	Total	C	N	O	S	14	0	0
			2569	1633	432	490	14			

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	GLU	-	expression tag	UNP P07195
A	335	ASN	-	expression tag	UNP P07195
A	336	LEU	-	expression tag	UNP P07195
A	337	TYR	-	expression tag	UNP P07195
A	338	PHE	-	expression tag	UNP P07195

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Chain	Residue	Modelled	Actual	Comment	Reference
A	339	GLN	-	expression tag	UNP P07195
A	340	GLY	-	expression tag	UNP P07195
A	341	LEU	-	expression tag	UNP P07195
A	342	GLU	-	expression tag	UNP P07195
A	343	HIS	-	expression tag	UNP P07195
A	344	HIS	-	expression tag	UNP P07195
A	345	HIS	-	expression tag	UNP P07195
A	346	HIS	-	expression tag	UNP P07195
A	347	HIS	-	expression tag	UNP P07195
A	348	HIS	-	expression tag	UNP P07195
B	334	GLU	-	expression tag	UNP P07195
B	335	ASN	-	expression tag	UNP P07195
B	336	LEU	-	expression tag	UNP P07195
B	337	TYR	-	expression tag	UNP P07195
B	338	PHE	-	expression tag	UNP P07195
B	339	GLN	-	expression tag	UNP P07195
B	340	GLY	-	expression tag	UNP P07195
B	341	LEU	-	expression tag	UNP P07195
B	342	GLU	-	expression tag	UNP P07195
B	343	HIS	-	expression tag	UNP P07195
B	344	HIS	-	expression tag	UNP P07195
B	345	HIS	-	expression tag	UNP P07195
B	346	HIS	-	expression tag	UNP P07195
B	347	HIS	-	expression tag	UNP P07195
B	348	HIS	-	expression tag	UNP P07195
C	334	GLU	-	expression tag	UNP P07195
C	335	ASN	-	expression tag	UNP P07195
C	336	LEU	-	expression tag	UNP P07195
C	337	TYR	-	expression tag	UNP P07195
C	338	PHE	-	expression tag	UNP P07195
C	339	GLN	-	expression tag	UNP P07195
C	340	GLY	-	expression tag	UNP P07195
C	341	LEU	-	expression tag	UNP P07195
C	342	GLU	-	expression tag	UNP P07195
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C	345	HIS	-	expression tag	UNP P07195
C	346	HIS	-	expression tag	UNP P07195
C	347	HIS	-	expression tag	UNP P07195
C	348	HIS	-	expression tag	UNP P07195
D	334	GLU	-	expression tag	UNP P07195
D	335	ASN	-	expression tag	UNP P07195

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Chain	Residue	Modelled	Actual	Comment	Reference
D	336	LEU	-	expression tag	UNP P07195
D	337	TYR	-	expression tag	UNP P07195
D	338	PHE	-	expression tag	UNP P07195
D	339	GLN	-	expression tag	UNP P07195
D	340	GLY	-	expression tag	UNP P07195
D	341	LEU	-	expression tag	UNP P07195
D	342	GLU	-	expression tag	UNP P07195
D	343	HIS	-	expression tag	UNP P07195
D	344	HIS	-	expression tag	UNP P07195
D	345	HIS	-	expression tag	UNP P07195
D	346	HIS	-	expression tag	UNP P07195
D	347	HIS	-	expression tag	UNP P07195
D	348	HIS	-	expression tag	UNP P07195
E	334	GLU	-	expression tag	UNP P07195
E	335	ASN	-	expression tag	UNP P07195
E	336	LEU	-	expression tag	UNP P07195
E	337	TYR	-	expression tag	UNP P07195
E	338	PHE	-	expression tag	UNP P07195
E	339	GLN	-	expression tag	UNP P07195
E	340	GLY	-	expression tag	UNP P07195
E	341	LEU	-	expression tag	UNP P07195
E	342	GLU	-	expression tag	UNP P07195
E	343	HIS	-	expression tag	UNP P07195
E	344	HIS	-	expression tag	UNP P07195
E	345	HIS	-	expression tag	UNP P07195
E	346	HIS	-	expression tag	UNP P07195
E	347	HIS	-	expression tag	UNP P07195
E	348	HIS	-	expression tag	UNP P07195
F	334	GLU	-	expression tag	UNP P07195
F	335	ASN	-	expression tag	UNP P07195
F	336	LEU	-	expression tag	UNP P07195
F	337	TYR	-	expression tag	UNP P07195
F	338	PHE	-	expression tag	UNP P07195
F	339	GLN	-	expression tag	UNP P07195
F	340	GLY	-	expression tag	UNP P07195
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F	342	GLU	-	expression tag	UNP P07195
F	343	HIS	-	expression tag	UNP P07195
F	344	HIS	-	expression tag	UNP P07195
F	345	HIS	-	expression tag	UNP P07195
F	346	HIS	-	expression tag	UNP P07195
F	347	HIS	-	expression tag	UNP P07195

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Chain	Residue	Modelled	Actual	Comment	Reference
F	348	HIS	-	expression tag	UNP P07195
G	334	GLU	-	expression tag	UNP P07195
G	335	ASN	-	expression tag	UNP P07195
G	336	LEU	-	expression tag	UNP P07195
G	337	TYR	-	expression tag	UNP P07195
G	338	PHE	-	expression tag	UNP P07195
G	339	GLN	-	expression tag	UNP P07195
G	340	GLY	-	expression tag	UNP P07195
G	341	LEU	-	expression tag	UNP P07195
G	342	GLU	-	expression tag	UNP P07195
G	343	HIS	-	expression tag	UNP P07195
G	344	HIS	-	expression tag	UNP P07195
G	345	HIS	-	expression tag	UNP P07195
G	346	HIS	-	expression tag	UNP P07195
G	347	HIS	-	expression tag	UNP P07195
G	348	HIS	-	expression tag	UNP P07195
H	334	GLU	-	expression tag	UNP P07195
H	335	ASN	-	expression tag	UNP P07195
H	336	LEU	-	expression tag	UNP P07195
H	337	TYR	-	expression tag	UNP P07195
H	338	PHE	-	expression tag	UNP P07195
H	339	GLN	-	expression tag	UNP P07195
H	340	GLY	-	expression tag	UNP P07195
H	341	LEU	-	expression tag	UNP P07195
H	342	GLU	-	expression tag	UNP P07195
H	343	HIS	-	expression tag	UNP P07195
H	344	HIS	-	expression tag	UNP P07195
H	345	HIS	-	expression tag	UNP P07195
H	346	HIS	-	expression tag	UNP P07195
H	347	HIS	-	expression tag	UNP P07195
H	348	HIS	-	expression tag	UNP P07195
I	334	GLU	-	expression tag	UNP P07195
I	335	ASN	-	expression tag	UNP P07195
I	336	LEU	-	expression tag	UNP P07195
I	337	TYR	-	expression tag	UNP P07195
I	338	PHE	-	expression tag	UNP P07195
I	339	GLN	-	expression tag	UNP P07195
I	340	GLY	-	expression tag	UNP P07195
I	341	LEU	-	expression tag	UNP P07195
I	342	GLU	-	expression tag	UNP P07195
I	343	HIS	-	expression tag	UNP P07195
I	344	HIS	-	expression tag	UNP P07195

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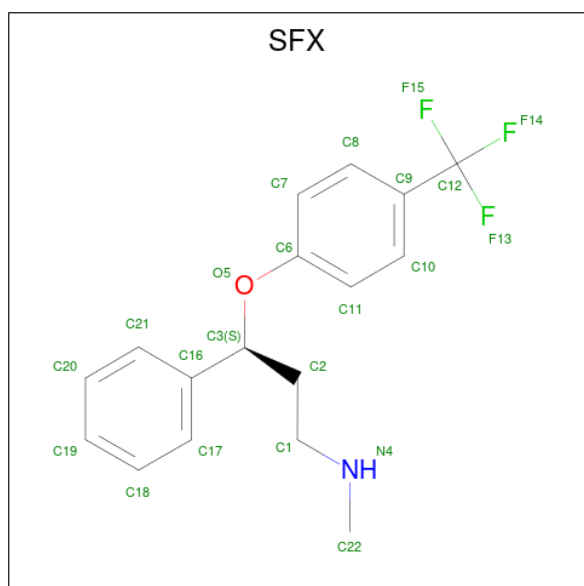
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I	347	HIS	-	expression tag	UNP P07195
I	348	HIS	-	expression tag	UNP P07195
J	334	GLU	-	expression tag	UNP P07195
J	335	ASN	-	expression tag	UNP P07195
J	336	LEU	-	expression tag	UNP P07195
J	337	TYR	-	expression tag	UNP P07195
J	338	PHE	-	expression tag	UNP P07195
J	339	GLN	-	expression tag	UNP P07195
J	340	GLY	-	expression tag	UNP P07195
J	341	LEU	-	expression tag	UNP P07195
J	342	GLU	-	expression tag	UNP P07195
J	343	HIS	-	expression tag	UNP P07195
J	344	HIS	-	expression tag	UNP P07195
J	345	HIS	-	expression tag	UNP P07195
J	346	HIS	-	expression tag	UNP P07195
J	347	HIS	-	expression tag	UNP P07195
J	348	HIS	-	expression tag	UNP P07195
K	334	GLU	-	expression tag	UNP P07195
K	335	ASN	-	expression tag	UNP P07195
K	336	LEU	-	expression tag	UNP P07195
K	337	TYR	-	expression tag	UNP P07195
K	338	PHE	-	expression tag	UNP P07195
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K	343	HIS	-	expression tag	UNP P07195
K	344	HIS	-	expression tag	UNP P07195
K	345	HIS	-	expression tag	UNP P07195
K	346	HIS	-	expression tag	UNP P07195
K	347	HIS	-	expression tag	UNP P07195
K	348	HIS	-	expression tag	UNP P07195
L	334	GLU	-	expression tag	UNP P07195
L	335	ASN	-	expression tag	UNP P07195
L	336	LEU	-	expression tag	UNP P07195
L	337	TYR	-	expression tag	UNP P07195
L	338	PHE	-	expression tag	UNP P07195
L	339	GLN	-	expression tag	UNP P07195
L	340	GLY	-	expression tag	UNP P07195
L	341	LEU	-	expression tag	UNP P07195

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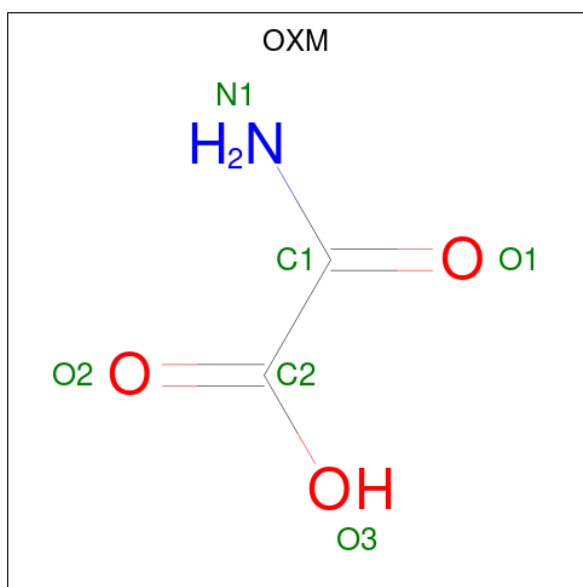
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L	343	HIS	-	expression tag	UNP P07195
L	344	HIS	-	expression tag	UNP P07195
L	345	HIS	-	expression tag	UNP P07195
L	346	HIS	-	expression tag	UNP P07195
L	347	HIS	-	expression tag	UNP P07195
L	348	HIS	-	expression tag	UNP P07195

- Molecule 2 is (3S)-N-methyl-3-phenyl-3-[4-(trifluoromethyl)phenoxy]propan-1-amine (three-letter code: SFX) (formula: C₁₇H₁₈F₃NO) (labeled as "Ligand of Interest" by depositor).



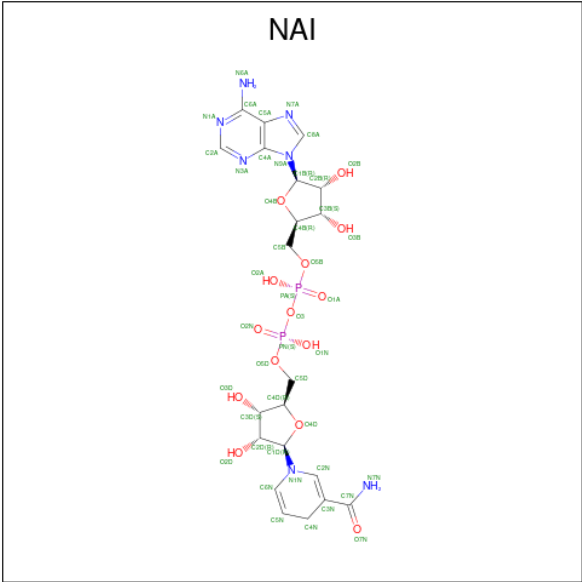
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			22	17	3	1	1		
2	B	1	Total	C	F	N	O	0	0
			22	17	3	1	1		
2	C	1	Total	C	F	N	O	0	0
			22	17	3	1	1		
2	F	1	Total	C	F	N	O	0	0
			22	17	3	1	1		
2	I	1	Total	C	F	N	O	0	0
			22	17	3	1	1		

- Molecule 3 is OXAMIC ACID (three-letter code: OXM) (formula: C₂H₃NO₃) (labeled as "Ligand of Interest" by depositor).



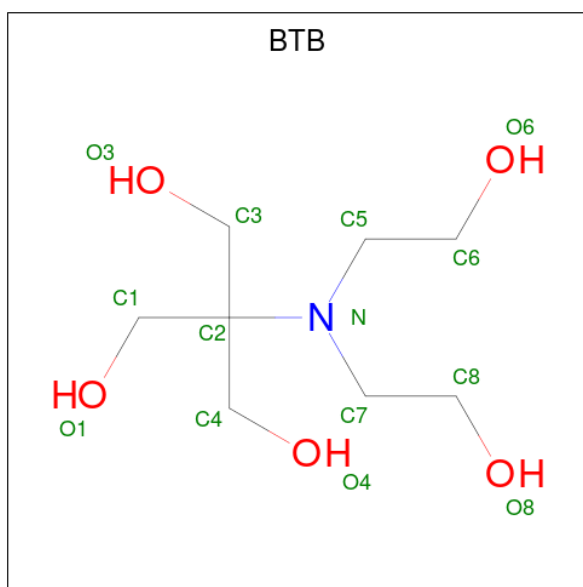
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			8	2	2	1	3		
3	B	1	Total	C	H	N	O	0	0
			8	2	2	1	3		
3	C	1	Total	C	H	N	O	0	0
			8	2	2	1	3		
3	D	1	Total	C	H	N	O	0	0
			8	2	2	1	3		
3	E	1	Total	C	H	N	O	0	0
			8	2	2	1	3		
3	F	1	Total	C	H	N	O	0	0
			8	2	2	1	3		
3	G	1	Total	C	H	N	O	0	0
			8	2	2	1	3		
3	H	1	Total	C	H	N	O	0	0
			8	2	2	1	3		
3	I	1	Total	C	H	N	O	0	0
			8	2	2	1	3		
3	J	1	Total	C	H	N	O	0	0
			8	2	2	1	3		
3	K	1	Total	C	H	N	O	0	0
			8	2	2	1	3		
3	L	1	Total	C	H	N	O	0	0
			8	2	2	1	3		

- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



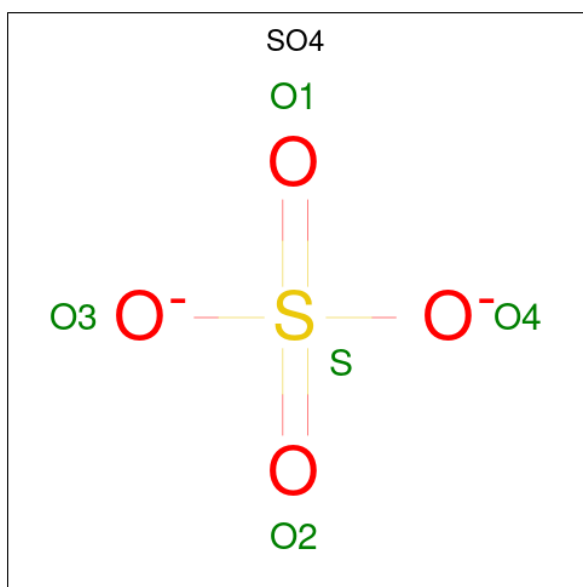
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
4	B	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
4	C	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
4	D	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
4	E	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
4	F	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
4	G	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
4	H	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
4	I	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
4	J	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
4	K	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		
4	L	1	Total	C	H	N	O	P	0	0
			71	21	27	7	14	2		

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



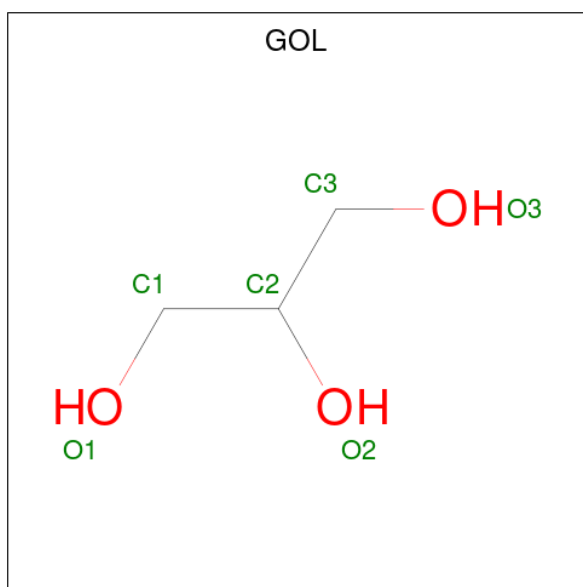
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



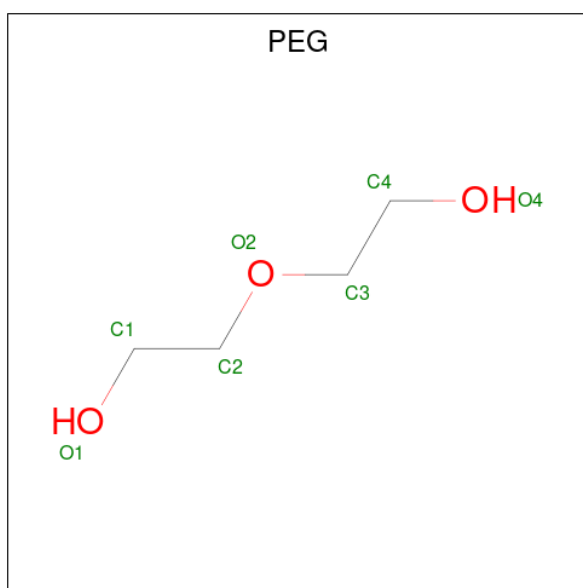
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		
7	G	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		
7	H	1	Total	C	O	0	0
			6	3	3		
7	I	1	Total	C	O	0	0
			6	3	3		
7	J	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	K	1	Total	C	O		0	0
			6	3	3			
7	K	1	Total	C	O		0	0
			6	3	3			
7	L	1	Total	C	O		0	0
			6	3	3			
7	L	1	Total	C	O		0	0
			6	3	3			
7	L	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	O		0	0
			7	4	3			
8	D	1	Total	C	O		0	0
			7	4	3			
8	D	1	Total	C	O		0	0
			7	4	3			
8	E	1	Total	C	O		0	0
			7	4	3			
8	H	1	Total	C	O		0	0
			7	4	3			
8	J	1	Total	C	O		0	0
			7	4	3			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	J	1	Total	C	O	0	0
			7	4	3		

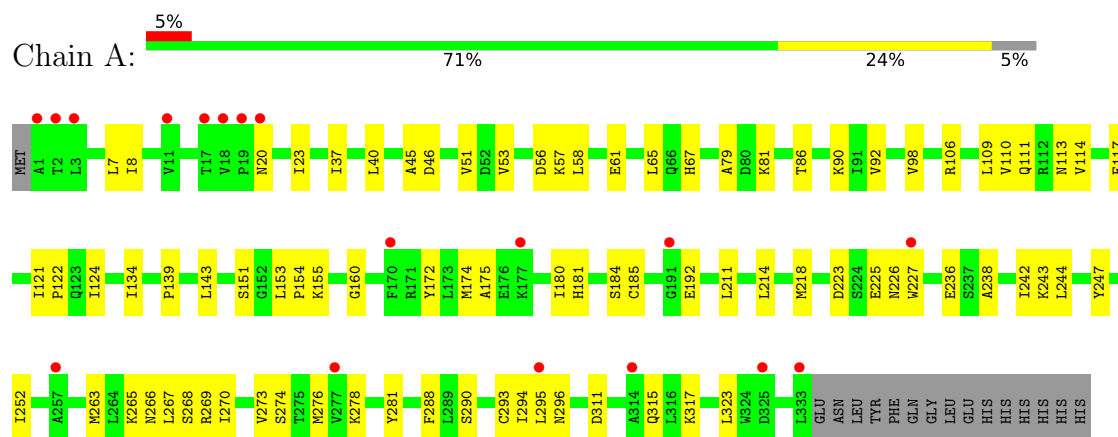
- Molecule 9 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	122	Total	O		0	0
			122	122			
9	B	133	Total	O		0	0
			133	133			
9	C	134	Total	O		0	0
			134	134			
9	D	121	Total	O		0	0
			121	121			
9	E	119	Total	O		0	0
			119	119			
9	F	98	Total	O		0	0
			98	98			
9	G	119	Total	O		0	0
			119	119			
9	H	101	Total	O		0	0
			101	101			
9	I	141	Total	O		0	0
			141	141			
9	J	99	Total	O		0	0
			99	99			
9	K	96	Total	O		0	0
			96	96			
9	L	54	Total	O		0	0
			54	54			

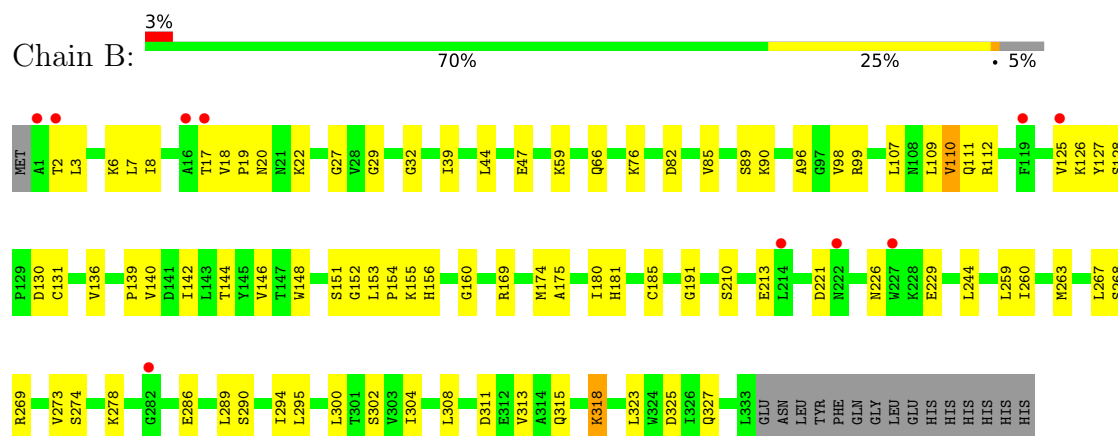
3 Residue-property plots [i](#)

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.

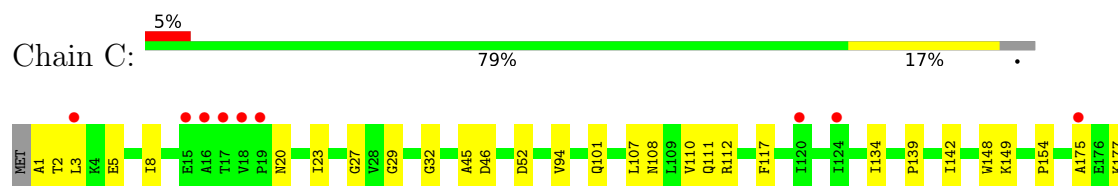
- Molecule 1: L-lactate dehydrogenase B chain

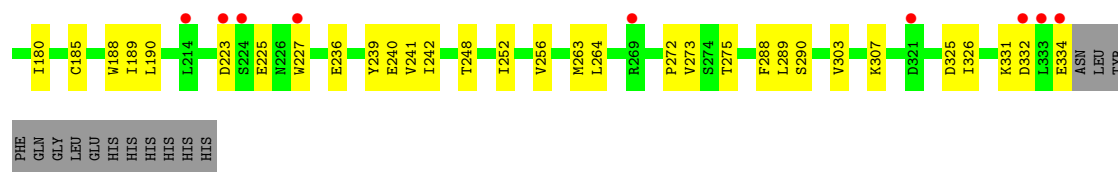


- Molecule 1: L-lactate dehydrogenase B chain

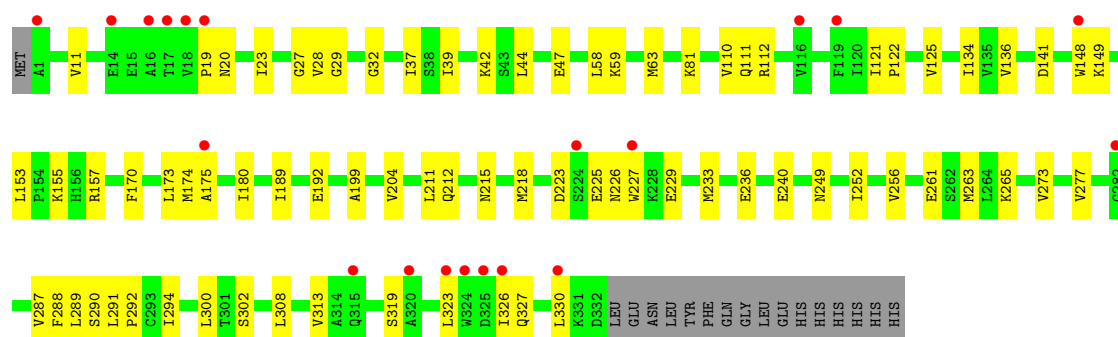
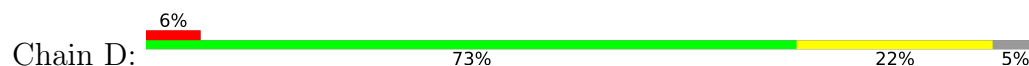


- Molecule 1: L-lactate dehydrogenase B chain

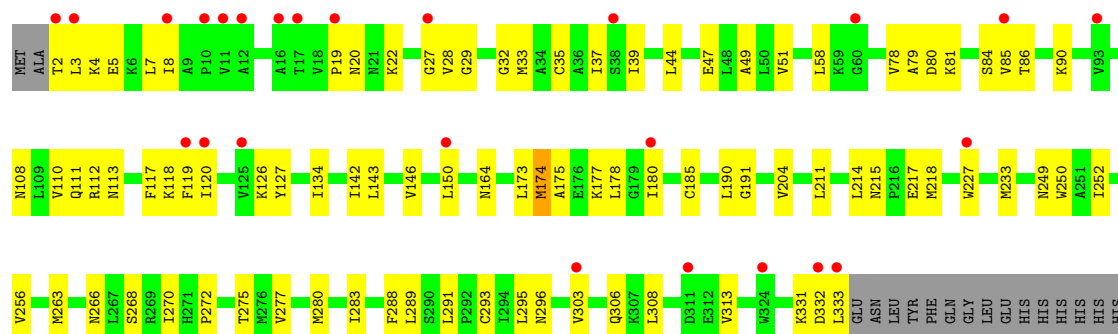




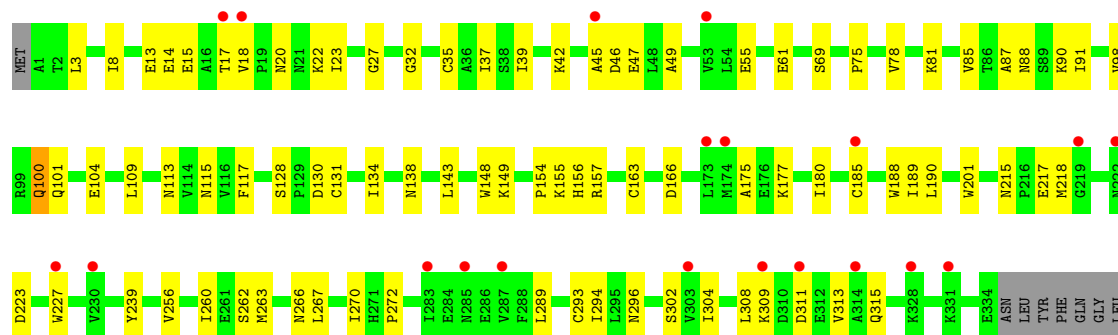
• Molecule 1: L-lactate dehydrogenase B chain



• Molecule 1: L-lactate dehydrogenase B chain




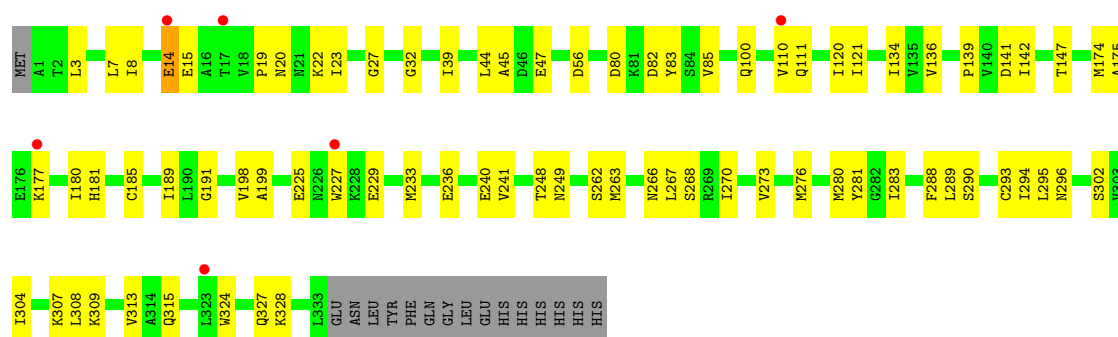
• Molecule 1: L-lactate dehydrogenase B chain



GLU
HIS
HIS
HIS
HIS
HIS
HIS

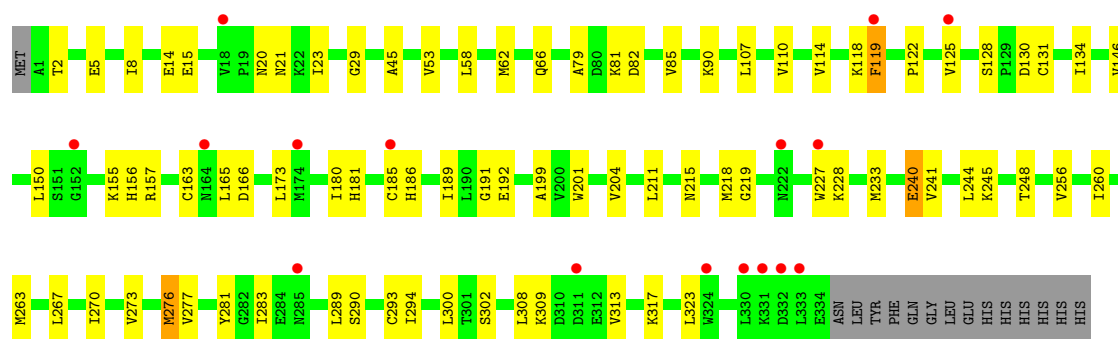
• Molecule 1: L-lactate dehydrogenase B chain

Chain G: 



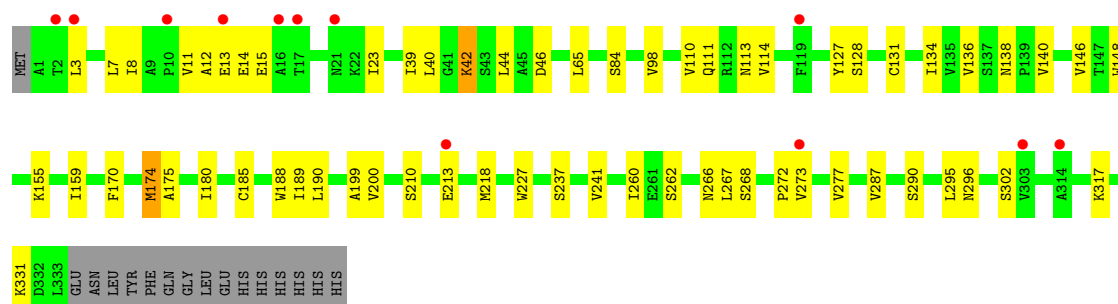
• Molecule 1: L-lactate dehydrogenase B chain

Chain H: 



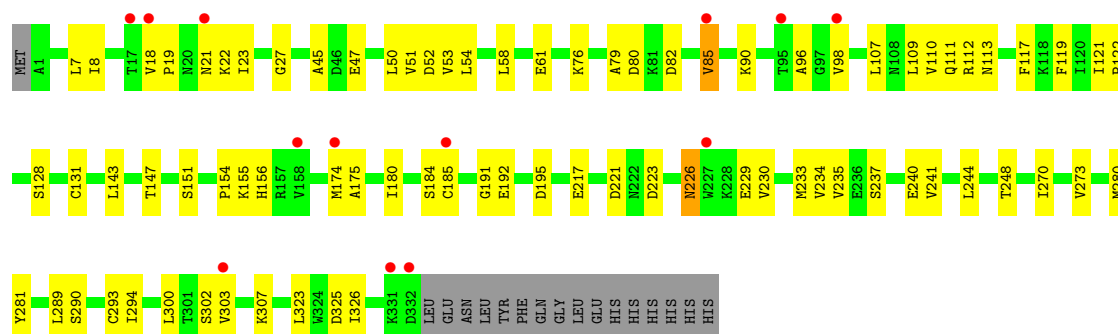
• Molecule 1: L-lactate dehydrogenase B chain

Chain I: 

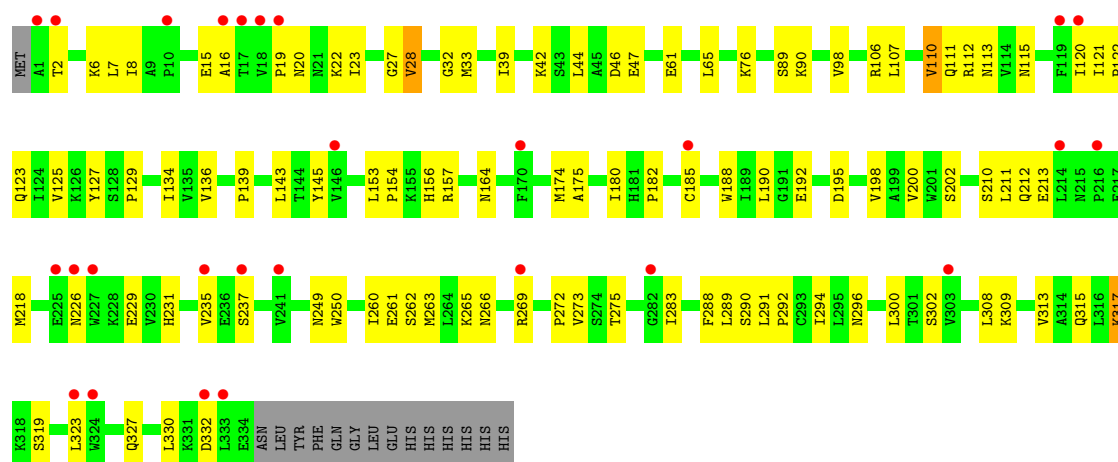


• Molecule 1: L-lactate dehydrogenase B chain

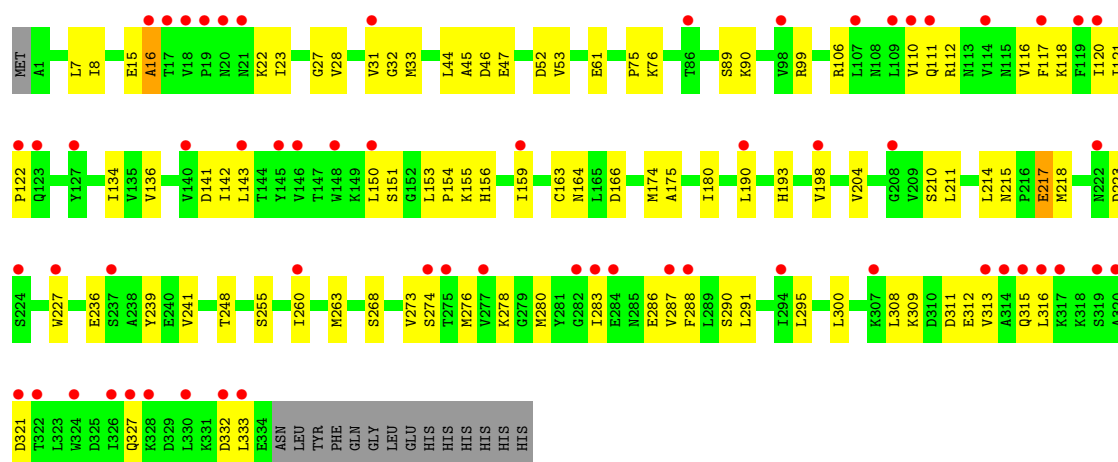
Chain J: 



• Molecule 1: L-lactate dehydrogenase B chain



• Molecule 1: L-lactate dehydrogenase B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.53Å 413.96Å 85.30Å 90.00° 109.57° 90.00°	Depositor
Resolution (Å)	48.67 – 2.07 48.67 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.67-2.07) 99.3 (48.67-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.213 , 0.264 0.212 , 0.263	Depositor DCC
R_{free} test set	14069 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.756	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33474	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SFX, GOL, SO4, PEG, BTB, NAI, OXM

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	0.42	0/2601	0.60	0/3526
1	B	0.42	0/2601	0.58	0/3526
1	C	0.47	0/2621	0.61	0/3552
1	D	0.43	0/2593	0.58	0/3515
1	E	0.41	0/2596	0.60	1/3519 (0.0%)
1	F	0.44	0/2610	0.60	0/3538
1	G	0.41	0/2601	0.58	0/3526
1	H	0.39	0/2619	0.58	1/3549 (0.0%)
1	I	0.45	0/2601	0.59	0/3526
1	J	0.38	0/2593	0.56	0/3515
1	K	0.38	0/2610	0.59	0/3538
1	L	0.37	0/2610	0.54	0/3538
All	All	0.42	0/31256	0.58	2/42368 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	276	MET	CA-CB-CG	-6.49	102.27	113.30
1	E	174	MET	CA-CB-CG	5.84	123.23	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2560	0	2633	74	0
1	B	2560	0	2633	81	0
1	C	2580	0	2651	50	0
1	D	2552	0	2622	60	0
1	E	2555	0	2625	70	0
1	F	2569	0	2639	69	0
1	G	2560	0	2633	67	0
1	H	2578	0	2651	70	0
1	I	2560	0	2633	48	0
1	J	2552	0	2622	53	0
1	K	2569	0	2639	91	0
1	L	2569	0	2639	89	0
2	A	22	0	18	8	0
2	B	22	0	18	12	0
2	C	22	0	18	4	0
2	F	22	0	18	11	0
2	I	22	0	18	7	0
3	A	6	2	2	2	0
3	B	6	2	2	1	0
3	C	6	2	2	0	0
3	D	6	2	2	1	0
3	E	6	2	2	0	0
3	F	6	2	2	4	0
3	G	6	2	2	0	0
3	H	6	2	2	0	0
3	I	6	2	2	1	0
3	J	6	2	2	1	0
3	K	6	2	2	1	0
3	L	6	2	2	4	0
4	A	44	27	27	5	0
4	B	44	27	27	6	0
4	C	44	27	27	3	0
4	D	44	27	27	3	0
4	E	44	27	27	1	0
4	F	44	27	27	2	0
4	G	44	27	27	1	0
4	H	44	27	27	3	0
4	I	44	27	27	2	0
4	J	44	27	27	2	0
4	K	44	27	27	2	0
4	L	44	27	27	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	14	0	19	2	0
5	C	14	0	19	4	0
5	F	14	0	19	5	0
5	G	14	0	19	2	0
5	K	14	0	19	1	0
5	L	14	0	19	4	0
6	A	5	0	0	0	0
6	B	10	0	0	0	0
6	C	10	0	0	0	0
6	D	10	0	0	0	0
6	G	5	0	0	0	0
6	J	10	0	0	0	0
6	L	10	0	0	0	0
7	B	12	0	16	1	0
7	C	6	0	8	0	0
7	D	6	0	8	0	0
7	F	12	0	16	1	0
7	G	12	0	16	0	0
7	H	24	0	32	1	0
7	I	6	0	8	1	0
7	J	6	0	8	0	0
7	K	12	0	16	7	0
7	L	18	8	24	3	0
8	B	7	0	10	0	0
8	D	14	0	20	0	0
8	E	7	0	10	1	0
8	H	7	0	10	1	0
8	J	14	0	20	3	0
9	A	122	0	0	5	0
9	B	133	0	0	4	0
9	C	134	0	0	7	0
9	D	121	0	0	2	0
9	E	119	0	0	1	0
9	F	98	0	0	2	0
9	G	119	0	0	2	0
9	H	101	0	0	4	0
9	I	141	0	0	2	0
9	J	99	0	0	4	0
9	K	96	0	0	4	0
9	L	54	0	0	1	0
All	All	33118	356	32394	817	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 13.

The worst 5 of 817 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:H:204:VAL:HG12	1:H:211:LEU:HD12	1.41	1.03
1:F:23:ILE:HD12	1:F:45:ALA:HB2	1.40	0.98
1:J:217:GLU:HG3	1:J:223:ASP:HA	1.49	0.94
1:F:311:ASP:OD1	1:F:315:GLN:NE2	2.04	0.91
1:C:149:LYS:HD2	1:C:334:GLU:HG2	1.53	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/349 (95%)	318 (96%)	13 (4%)	0	100	100
1	B	331/349 (95%)	320 (97%)	10 (3%)	1 (0%)	37	31
1	C	333/349 (95%)	315 (95%)	18 (5%)	0	100	100
1	D	330/349 (95%)	320 (97%)	9 (3%)	1 (0%)	37	31
1	E	330/349 (95%)	318 (96%)	11 (3%)	1 (0%)	37	31
1	F	332/349 (95%)	317 (96%)	14 (4%)	1 (0%)	37	31
1	G	331/349 (95%)	317 (96%)	13 (4%)	1 (0%)	37	31
1	H	333/349 (95%)	320 (96%)	13 (4%)	0	100	100
1	I	331/349 (95%)	317 (96%)	14 (4%)	0	100	100
1	J	330/349 (95%)	315 (96%)	14 (4%)	1 (0%)	37	31
1	K	332/349 (95%)	318 (96%)	10 (3%)	4 (1%)	11	4
1	L	332/349 (95%)	314 (95%)	17 (5%)	1 (0%)	37	31
All	All	3976/4188 (95%)	3809 (96%)	156 (4%)	11 (0%)	37	31

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	226	ASN
1	F	69	SER
1	K	332	ASP
1	E	249	ASN
1	G	249	ASN

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	289/304 (95%)	287 (99%)	2 (1%)	81	82
1	B	289/304 (95%)	286 (99%)	3 (1%)	73	73
1	C	291/304 (96%)	289 (99%)	2 (1%)	81	82
1	D	288/304 (95%)	287 (100%)	1 (0%)	91	92
1	E	289/304 (95%)	287 (99%)	2 (1%)	81	82
1	F	290/304 (95%)	288 (99%)	2 (1%)	81	82
1	G	289/304 (95%)	288 (100%)	1 (0%)	91	92
1	H	291/304 (96%)	288 (99%)	3 (1%)	73	73
1	I	289/304 (95%)	285 (99%)	4 (1%)	62	62
1	J	288/304 (95%)	284 (99%)	4 (1%)	62	62
1	K	290/304 (95%)	288 (99%)	2 (1%)	81	82
1	L	290/304 (95%)	287 (99%)	3 (1%)	73	73
All	All	3473/3648 (95%)	3444 (99%)	29 (1%)	79	80

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	119	PHE
1	L	255	SER
1	I	42	LYS
1	K	237	SER

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Mol	Chain	Res	Type
1	I	3	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	111	GLN
1	L	156	HIS
1	E	306	GLN
1	F	100	GLN
1	F	108	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

73 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	SFX	C	401	-	23,23,23	1.11	2 (8%)	30,31,31	1.00	1 (3%)
2	SFX	B	401	-	23,23,23	1.18	1 (4%)	30,31,31	1.35	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OXM	G	401	-	5,5,5	2.75	3 (60%)	4,6,6	1.51	1 (25%)
4	NAI	D	402	-	42,48,48	2.02	9 (21%)	47,73,73	2.46	15 (31%)
7	GOL	L	405	-	5,5,5	0.52	0	5,5,5	0.41	0
7	GOL	F	406	-	5,5,5	0.56	0	5,5,5	0.24	0
4	NAI	L	402	-	42,48,48	2.21	10 (23%)	47,73,73	2.88	18 (38%)
4	NAI	C	403	-	42,48,48	1.96	9 (21%)	47,73,73	2.23	15 (31%)
3	OXM	C	402	-	5,5,5	3.10	3 (60%)	4,6,6	1.42	1 (25%)
5	BTB	L	403	-	13,13,13	0.79	0	7,16,16	0.79	0
6	SO4	J	404	-	4,4,4	0.31	0	6,6,6	0.22	0
7	GOL	H	406	-	5,5,5	0.53	0	5,5,5	0.29	0
7	GOL	L	406	-	5,5,5	0.24	0	5,5,5	2.36	2 (40%)
7	GOL	B	404	-	5,5,5	0.57	0	5,5,5	0.55	0
7	GOL	H	405	-	5,5,5	0.52	0	5,5,5	0.22	0
5	BTB	G	403	-	13,13,13	1.06	2 (15%)	7,16,16	1.14	0
7	GOL	D	403	-	5,5,5	0.52	0	5,5,5	0.27	0
7	GOL	F	405	-	5,5,5	0.57	0	5,5,5	0.45	0
4	NAI	I	403	-	42,48,48	2.07	9 (21%)	47,73,73	1.93	11 (23%)
3	OXM	I	402	-	5,5,5	2.66	2 (40%)	4,6,6	1.14	0
4	NAI	H	402	-	42,48,48	2.17	12 (28%)	47,73,73	2.35	20 (42%)
6	SO4	C	407	-	4,4,4	0.16	0	6,6,6	0.39	0
7	GOL	C	405	-	5,5,5	0.54	0	5,5,5	0.33	0
3	OXM	H	401	-	5,5,5	2.63	3 (60%)	4,6,6	1.06	0
7	GOL	H	404	-	5,5,5	0.47	0	5,5,5	0.55	0
4	NAI	J	402	-	42,48,48	2.14	12 (28%)	47,73,73	2.02	17 (36%)
8	PEG	H	407	-	6,6,6	0.13	0	5,5,5	0.10	0
6	SO4	C	406	-	4,4,4	0.13	0	6,6,6	0.46	0
6	SO4	B	406	-	4,4,4	0.14	0	6,6,6	0.46	0
3	OXM	L	401	-	5,5,5	2.80	3 (60%)	4,6,6	1.22	0
8	PEG	B	408	-	6,6,6	0.22	0	5,5,5	0.10	0
8	PEG	J	407	-	6,6,6	0.16	0	5,5,5	0.12	0
4	NAI	F	403	-	42,48,48	2.05	11 (26%)	47,73,73	2.11	15 (31%)
8	PEG	D	407	-	6,6,6	0.19	0	5,5,5	0.04	0
3	OXM	A	402	-	5,5,5	2.81	2 (40%)	4,6,6	1.13	0
8	PEG	D	406	-	6,6,6	0.16	0	5,5,5	0.11	0
7	GOL	H	403	-	5,5,5	0.54	0	5,5,5	0.27	0
6	SO4	L	408	-	4,4,4	0.20	0	6,6,6	0.32	0
2	SFX	A	401	-	23,23,23	1.11	2 (8%)	30,31,31	1.02	2 (6%)
6	SO4	L	407	-	4,4,4	0.15	0	6,6,6	0.29	0
7	GOL	G	405	-	5,5,5	0.57	0	5,5,5	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BTB	K	403	-	13,13,13	0.81	0	7,16,16	1.08	1 (14%)
7	GOL	B	405	-	5,5,5	0.39	0	5,5,5	0.63	0
6	SO4	A	405	-	4,4,4	0.18	0	6,6,6	0.23	0
4	NAI	G	402	-	42,48,48	2.05	10 (23%)	47,73,73	2.17	20 (42%)
3	OXM	K	401	-	5,5,5	2.78	3 (60%)	4,6,6	1.93	1 (25%)
5	BTB	F	404	-	13,13,13	0.72	0	7,16,16	0.69	0
4	NAI	K	402	-	42,48,48	2.02	8 (19%)	47,73,73	2.08	15 (31%)
7	GOL	K	404	-	5,5,5	0.55	0	5,5,5	0.21	0
7	GOL	G	404	-	5,5,5	0.55	0	5,5,5	0.21	0
4	NAI	B	403	-	42,48,48	2.07	9 (21%)	47,73,73	2.15	13 (27%)
7	GOL	I	404	-	5,5,5	0.60	0	5,5,5	0.55	0
7	GOL	L	404	-	5,5,5	0.49	0	5,5,5	0.33	0
2	SFX	I	401	-	23,23,23	1.02	1 (4%)	30,31,31	1.67	4 (13%)
6	SO4	G	406	-	4,4,4	0.20	0	6,6,6	0.37	0
5	BTB	A	404	-	13,13,13	0.88	1 (7%)	7,16,16	1.14	0
3	OXM	D	401	-	5,5,5	2.67	3 (60%)	4,6,6	1.28	1 (25%)
8	PEG	E	403	-	6,6,6	0.12	0	5,5,5	0.12	0
3	OXM	F	402	-	5,5,5	2.55	2 (40%)	4,6,6	1.53	1 (25%)
3	OXM	B	402	-	5,5,5	2.61	2 (40%)	4,6,6	1.47	1 (25%)
5	BTB	C	404	-	13,13,13	0.98	1 (7%)	7,16,16	1.36	1 (14%)
3	OXM	J	401	-	5,5,5	2.55	2 (40%)	4,6,6	1.83	2 (50%)
6	SO4	D	405	-	4,4,4	0.22	0	6,6,6	0.38	0
2	SFX	F	401	-	23,23,23	1.21	1 (4%)	30,31,31	2.15	4 (13%)
4	NAI	A	403	-	42,48,48	2.10	7 (16%)	47,73,73	2.21	19 (40%)
6	SO4	J	405	-	4,4,4	0.21	0	6,6,6	0.28	0
3	OXM	E	401	-	5,5,5	2.85	3 (60%)	4,6,6	1.18	0
7	GOL	J	403	-	5,5,5	0.63	0	5,5,5	0.43	0
6	SO4	B	407	-	4,4,4	0.12	0	6,6,6	0.32	0
8	PEG	J	406	-	6,6,6	0.20	0	5,5,5	0.06	0
4	NAI	E	402	-	42,48,48	1.90	8 (19%)	47,73,73	2.68	19 (40%)
6	SO4	D	404	-	4,4,4	0.24	0	6,6,6	0.10	0
7	GOL	K	405	-	5,5,5	0.48	0	5,5,5	0.40	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	SFX	C	401	-	-	9/18/18/18	0/2/2/2
2	SFX	B	401	-	-	8/18/18/18	0/2/2/2
3	OXM	G	401	-	-	0/3/4/4	-
4	NAI	D	402	-	-	5/25/72/72	0/5/5/5
7	GOL	L	405	-	-	0/4/4/4	-
7	GOL	F	406	-	-	2/4/4/4	-
4	NAI	L	402	-	-	13/25/72/72	0/5/5/5
4	NAI	C	403	-	-	3/25/72/72	0/5/5/5
3	OXM	C	402	-	-	0/3/4/4	-
5	BTB	L	403	-	-	8/21/21/21	-
7	GOL	H	406	-	-	0/4/4/4	-
7	GOL	L	406	-	-	0/4/4/4	-
8	PEG	B	408	-	-	2/4/4/4	-
7	GOL	B	404	-	-	2/4/4/4	-
7	GOL	H	405	-	-	2/4/4/4	-
5	BTB	G	403	-	-	9/21/21/21	-
7	GOL	D	403	-	-	0/4/4/4	-
7	GOL	F	405	-	-	2/4/4/4	-
4	NAI	I	403	-	-	5/25/72/72	0/5/5/5
3	OXM	I	402	-	-	3/3/4/4	-
4	NAI	H	402	-	-	4/25/72/72	0/5/5/5
7	GOL	C	405	-	-	4/4/4/4	-
7	GOL	H	404	-	-	4/4/4/4	-
3	OXM	H	401	-	-	0/3/4/4	-
4	NAI	J	402	-	-	4/25/72/72	0/5/5/5
8	PEG	H	407	-	-	3/4/4/4	-
3	OXM	L	401	-	-	0/3/4/4	-
8	PEG	J	407	-	-	2/4/4/4	-
4	NAI	F	403	-	-	3/25/72/72	0/5/5/5
8	PEG	D	407	-	-	3/4/4/4	-
3	OXM	A	402	-	-	0/3/4/4	-
8	PEG	D	406	-	-	1/4/4/4	-
7	GOL	H	403	-	-	4/4/4/4	-
2	SFX	A	401	-	-	9/18/18/18	0/2/2/2
7	GOL	G	405	-	-	3/4/4/4	-
5	BTB	K	403	-	-	7/21/21/21	-
7	GOL	B	405	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAI	G	402	-	-	7/25/72/72	0/5/5/5
3	OXM	K	401	-	-	0/3/4/4	-
5	BTB	F	404	-	-	8/21/21/21	-
4	NAI	K	402	-	-	6/25/72/72	0/5/5/5
7	GOL	K	404	-	-	2/4/4/4	-
7	GOL	G	404	-	-	4/4/4/4	-
4	NAI	B	403	-	-	7/25/72/72	0/5/5/5
7	GOL	I	404	-	-	2/4/4/4	-
7	GOL	L	404	-	-	4/4/4/4	-
2	SFX	I	401	-	-	5/18/18/18	0/2/2/2
5	BTB	A	404	-	-	7/21/21/21	-
3	OXM	D	401	-	-	0/3/4/4	-
8	PEG	E	403	-	-	0/4/4/4	-
3	OXM	F	402	-	-	0/3/4/4	-
3	OXM	B	402	-	-	1/3/4/4	-
5	BTB	C	404	-	-	9/21/21/21	-
3	OXM	J	401	-	-	0/3/4/4	-
2	SFX	F	401	-	-	11/18/18/18	0/2/2/2
4	NAI	A	403	-	-	6/25/72/72	0/5/5/5
3	OXM	E	401	-	-	0/3/4/4	-
7	GOL	J	403	-	-	4/4/4/4	-
8	PEG	J	406	-	-	3/4/4/4	-
4	NAI	E	402	-	-	7/25/72/72	0/5/5/5
7	GOL	K	405	-	-	2/4/4/4	-

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	NAI	C2A-N3A	7.46	1.44	1.32
4	B	403	NAI	C2A-N3A	7.36	1.44	1.32
4	K	402	NAI	C2A-N3A	7.36	1.44	1.32
4	H	402	NAI	PA-O1A	7.34	1.76	1.50
4	J	402	NAI	PA-O1A	7.30	1.76	1.50

The worst 5 of 223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	SFX	C6-O5-C3	-9.78	112.10	118.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	402	NAI	PN-O3-PA	-9.78	99.27	132.83
4	E	402	NAI	PN-O3-PA	-8.91	102.25	132.83
4	L	402	NAI	O3B-C3B-C4B	8.19	134.73	111.05
4	A	403	NAI	PN-O3-PA	-7.47	107.18	132.83

There are no chirality outliers.

5 of 219 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	SFX	C2-C3-O5-C6
2	A	401	SFX	C16-C3-O5-C6
2	A	401	SFX	C1-C2-C3-O5
2	A	401	SFX	C1-C2-C3-C16
2	A	401	SFX	C17-C16-C3-C2

There are no ring outliers.

42 monomers are involved in 125 short contacts:

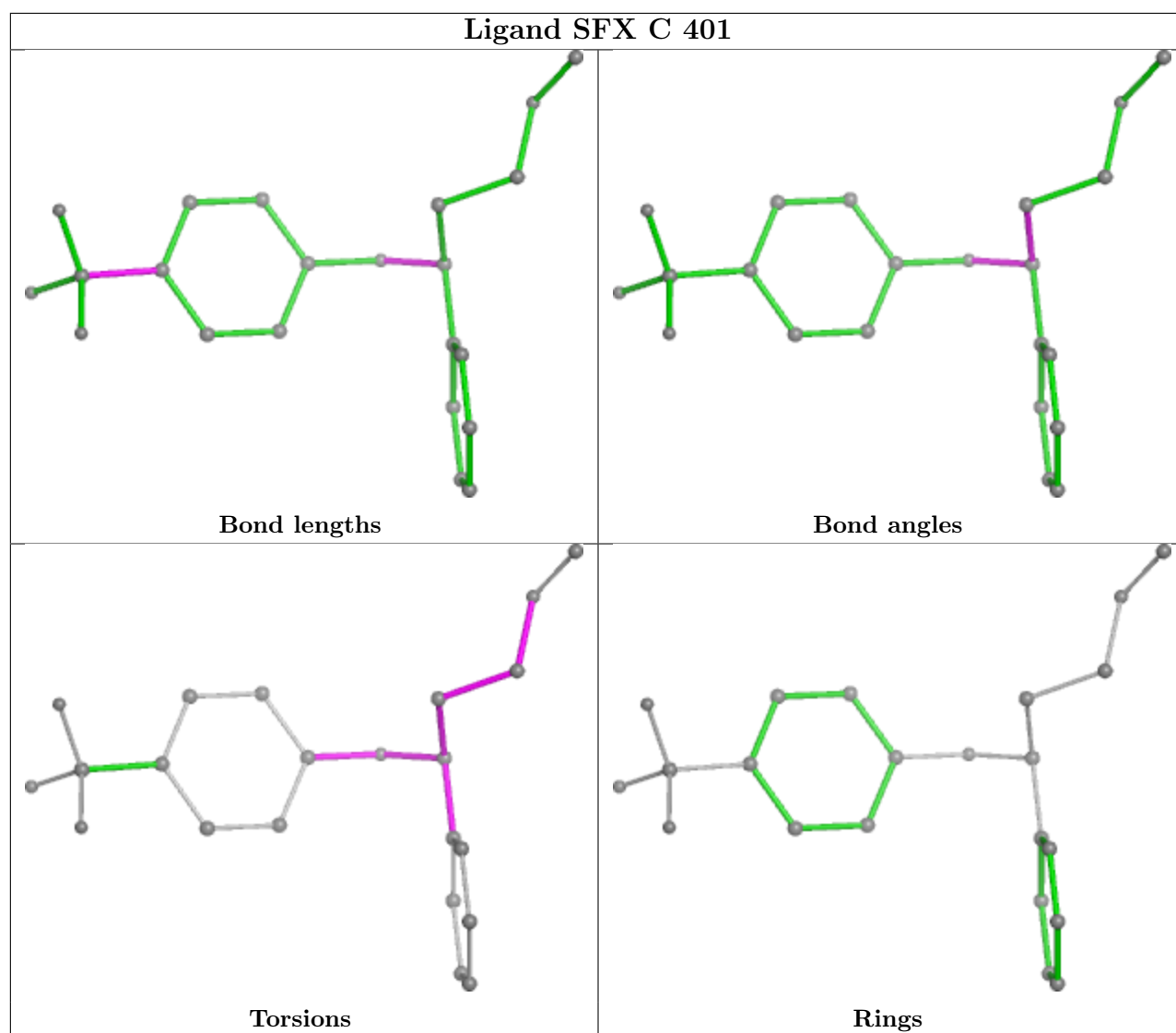
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	SFX	4	0
2	B	401	SFX	12	0
4	D	402	NAI	3	0
4	L	402	NAI	12	0
4	C	403	NAI	3	0
5	L	403	BTB	4	0
7	L	406	GOL	2	0
7	B	404	GOL	1	0
5	G	403	BTB	2	0
7	F	405	GOL	1	0
4	I	403	NAI	2	0
3	I	402	OXM	1	0
4	H	402	NAI	3	0
7	H	404	GOL	1	0
4	J	402	NAI	2	0
8	H	407	PEG	1	0
3	L	401	OXM	4	0
8	J	407	PEG	1	0
4	F	403	NAI	2	0
3	A	402	OXM	2	0
2	A	401	SFX	8	0
5	K	403	BTB	1	0

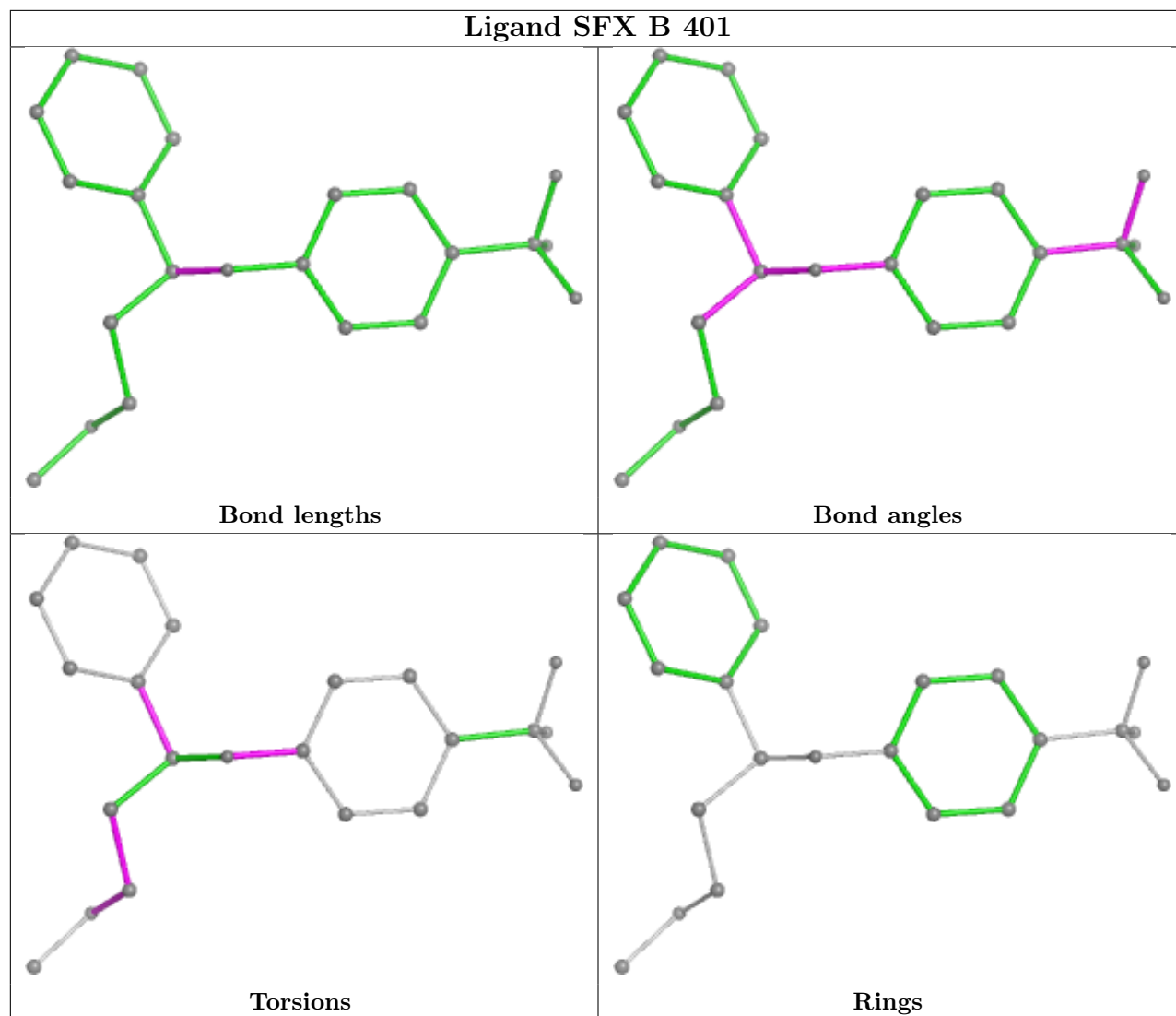
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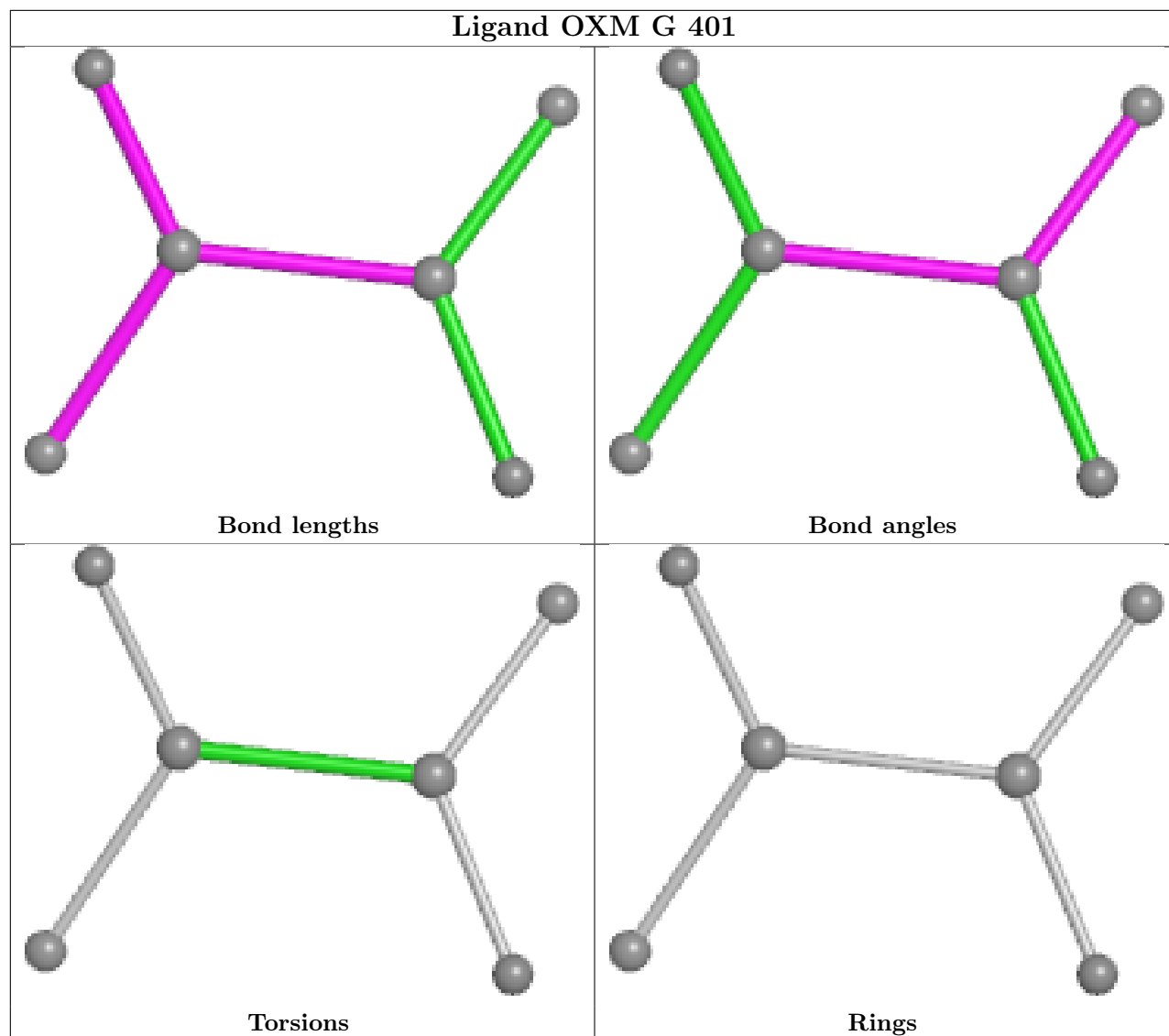
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	402	NAI	1	0
3	K	401	OXM	1	0
5	F	404	BTB	5	0
4	K	402	NAI	2	0
4	B	403	NAI	6	0
7	I	404	GOL	1	0
7	L	404	GOL	1	0
2	I	401	SFX	7	0
5	A	404	BTB	2	0
3	D	401	OXM	1	0
8	E	403	PEG	1	0
3	F	402	OXM	4	0
3	B	402	OXM	1	0
5	C	404	BTB	4	0
3	J	401	OXM	1	0
2	F	401	SFX	11	0
4	A	403	NAI	5	0
8	J	406	PEG	2	0
4	E	402	NAI	1	0
7	K	405	GOL	7	0

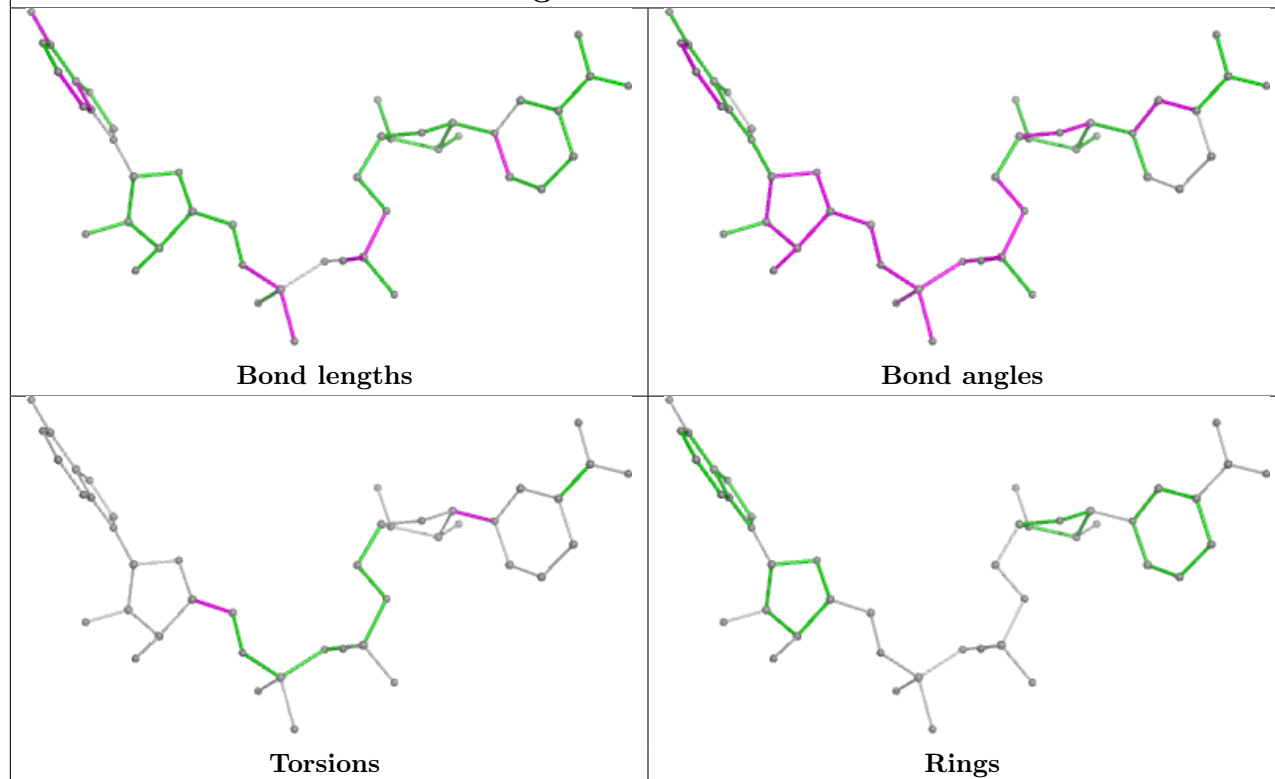
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



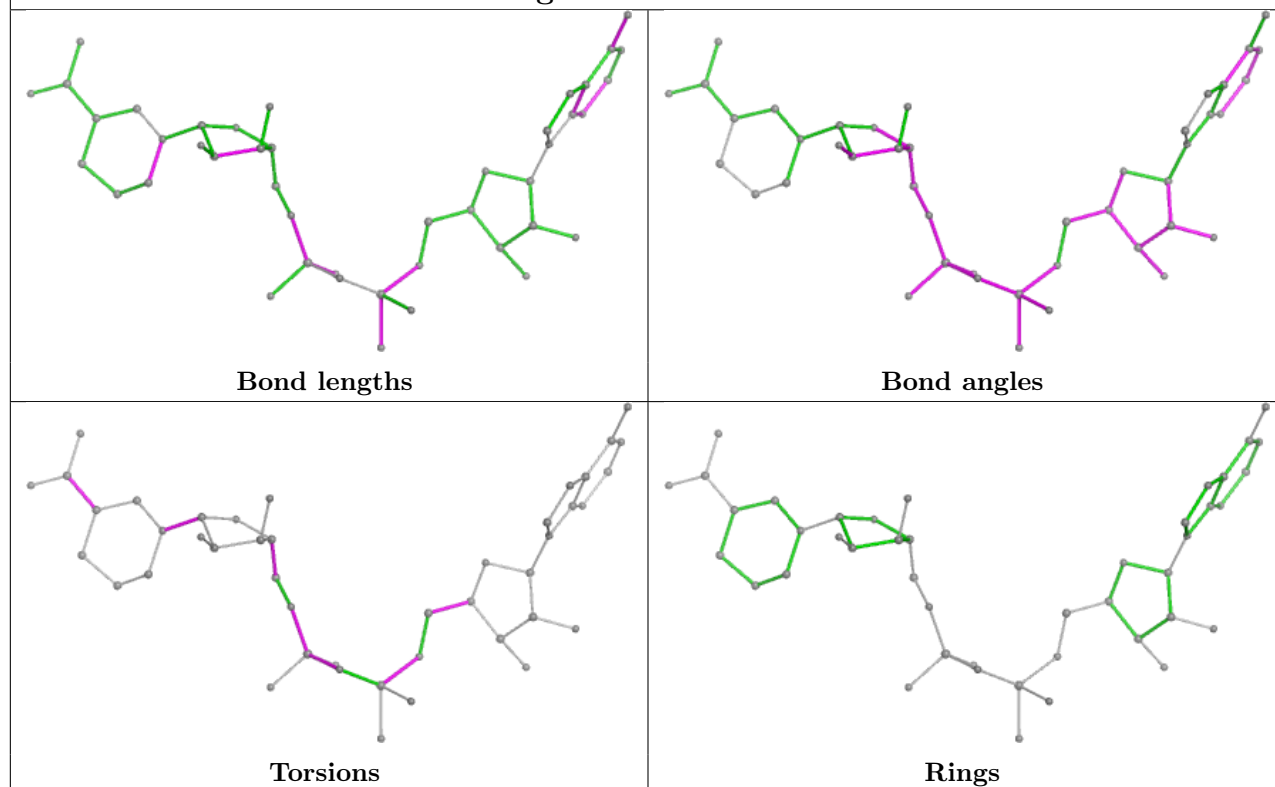


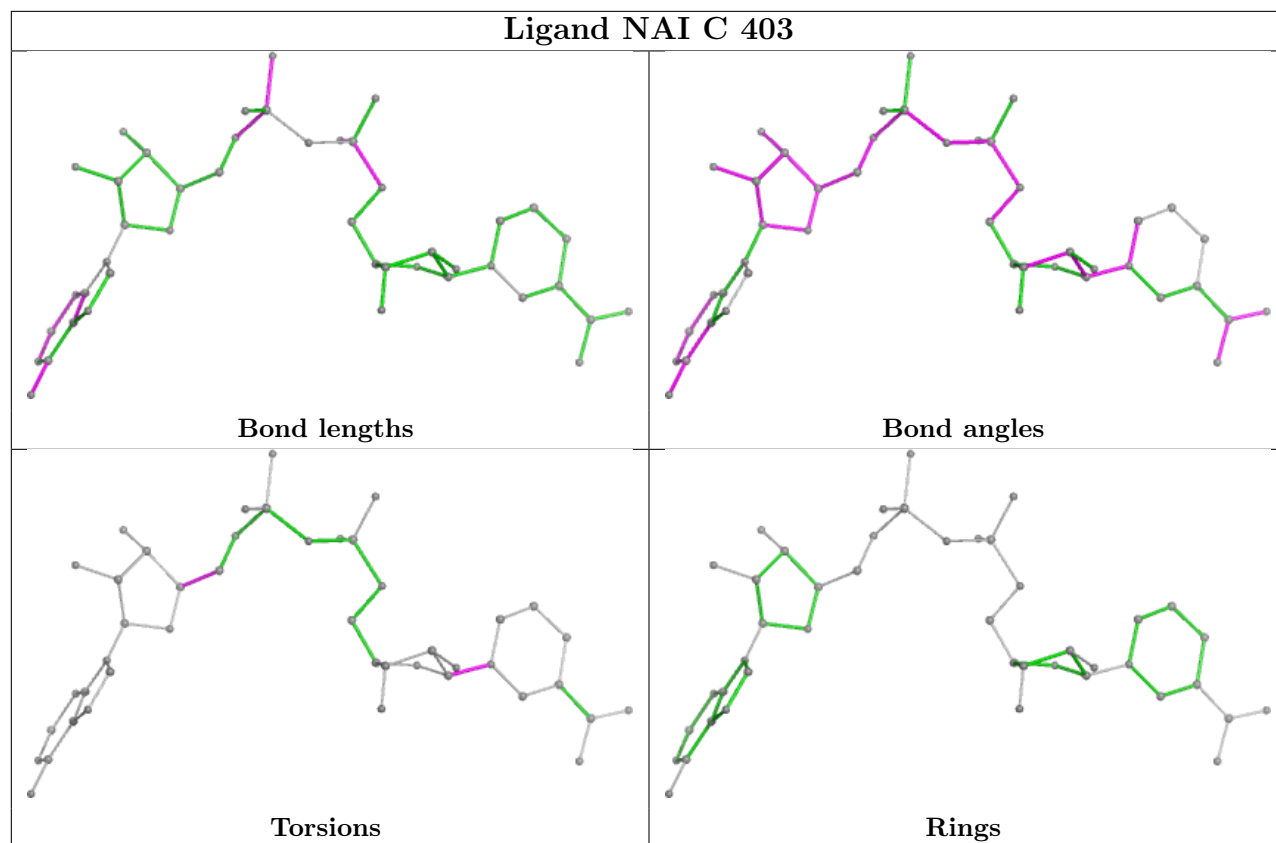


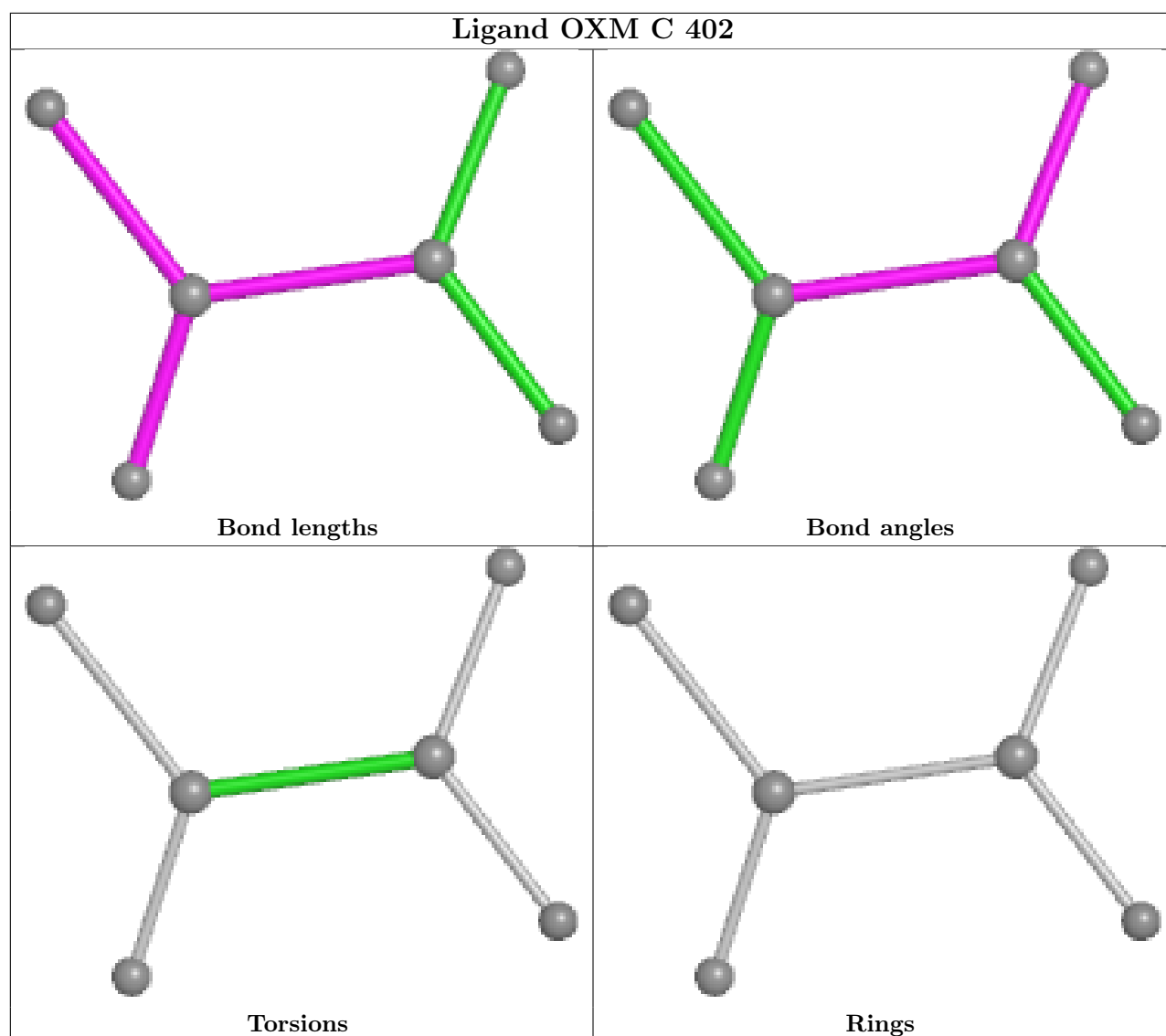
Ligand NAI D 402

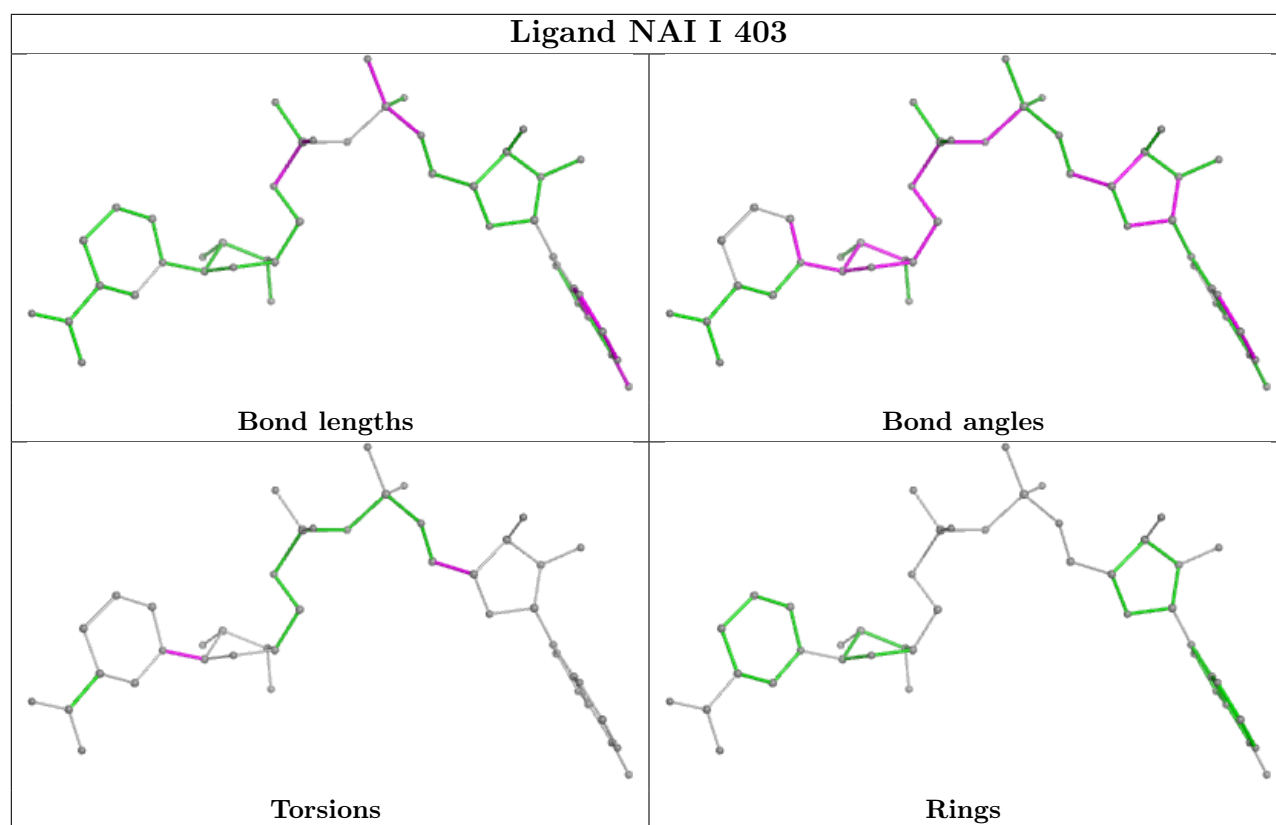


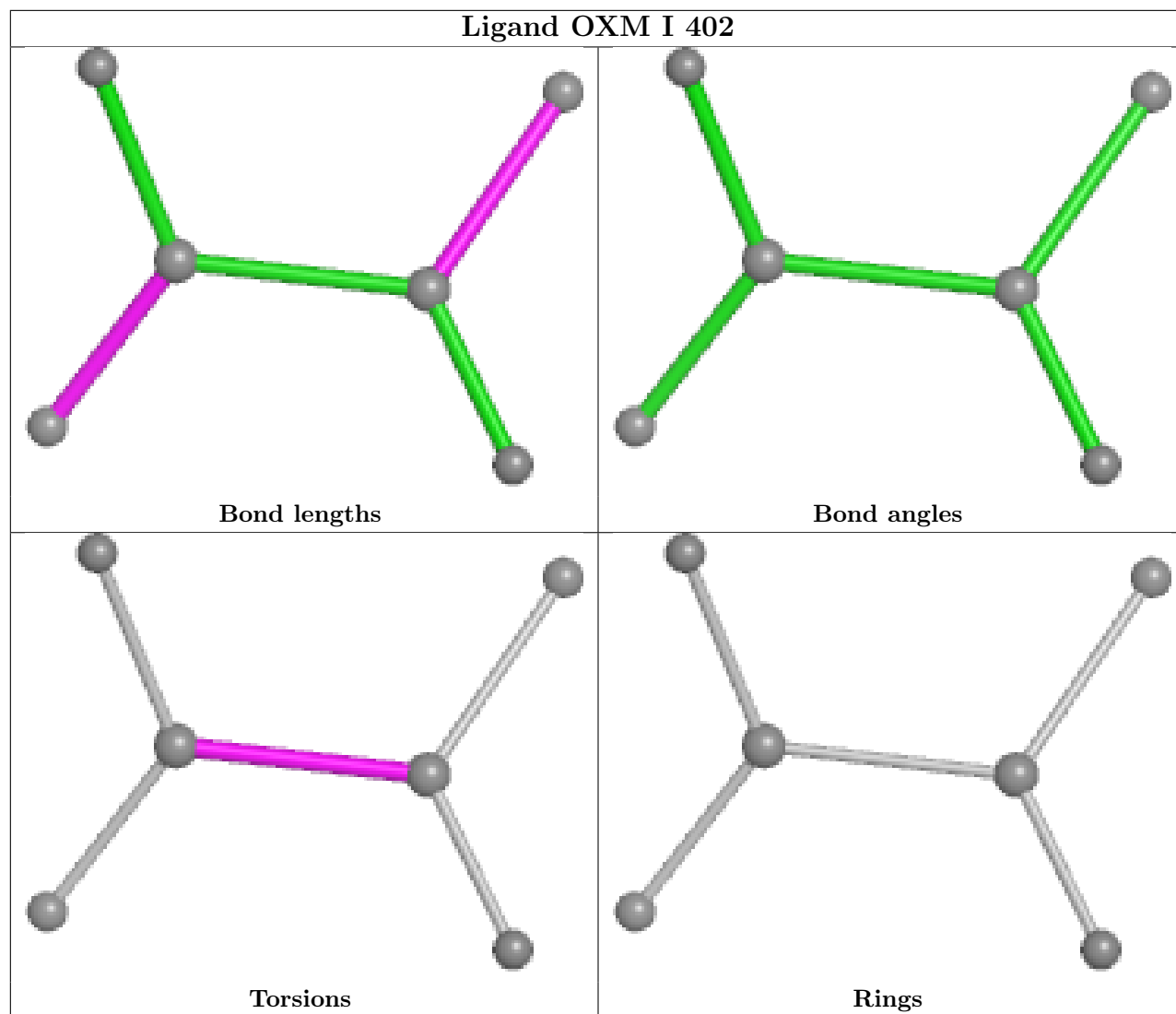
Ligand NAI L 402

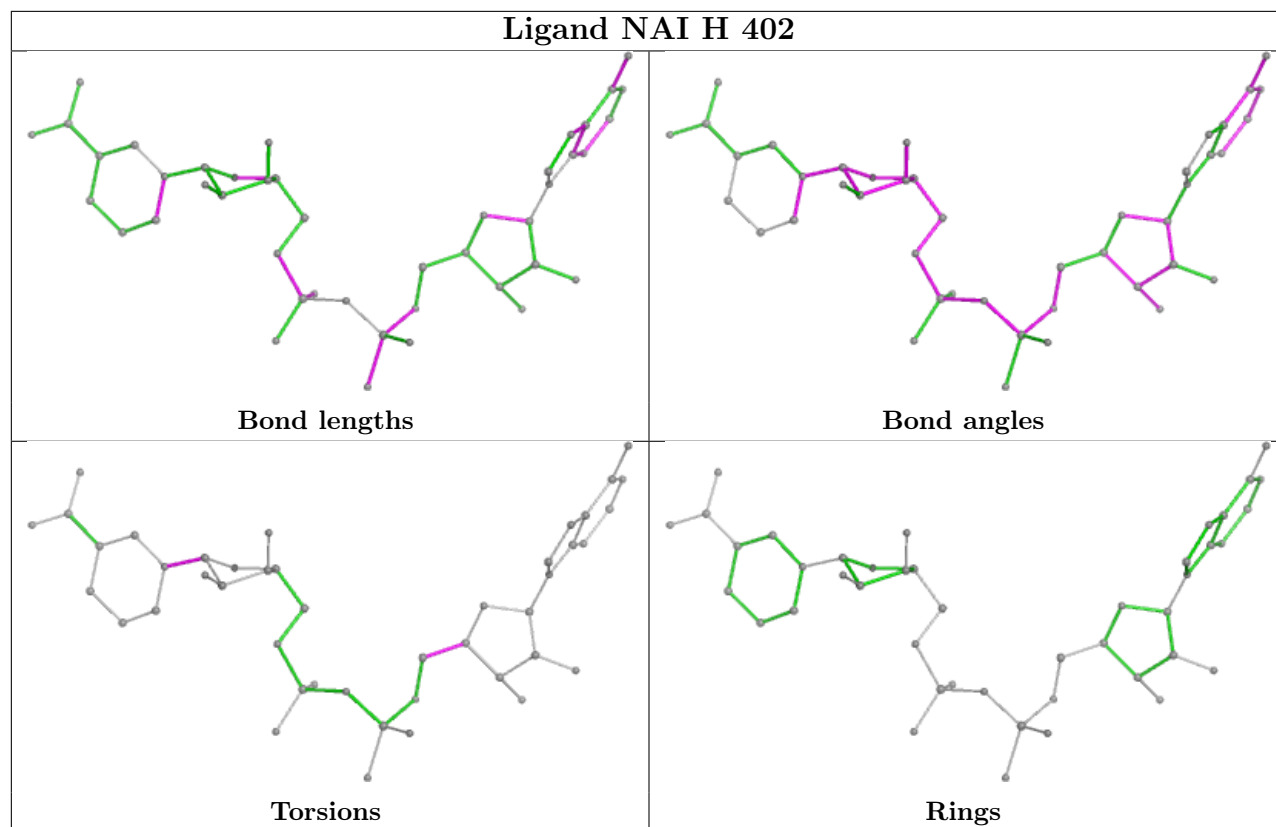


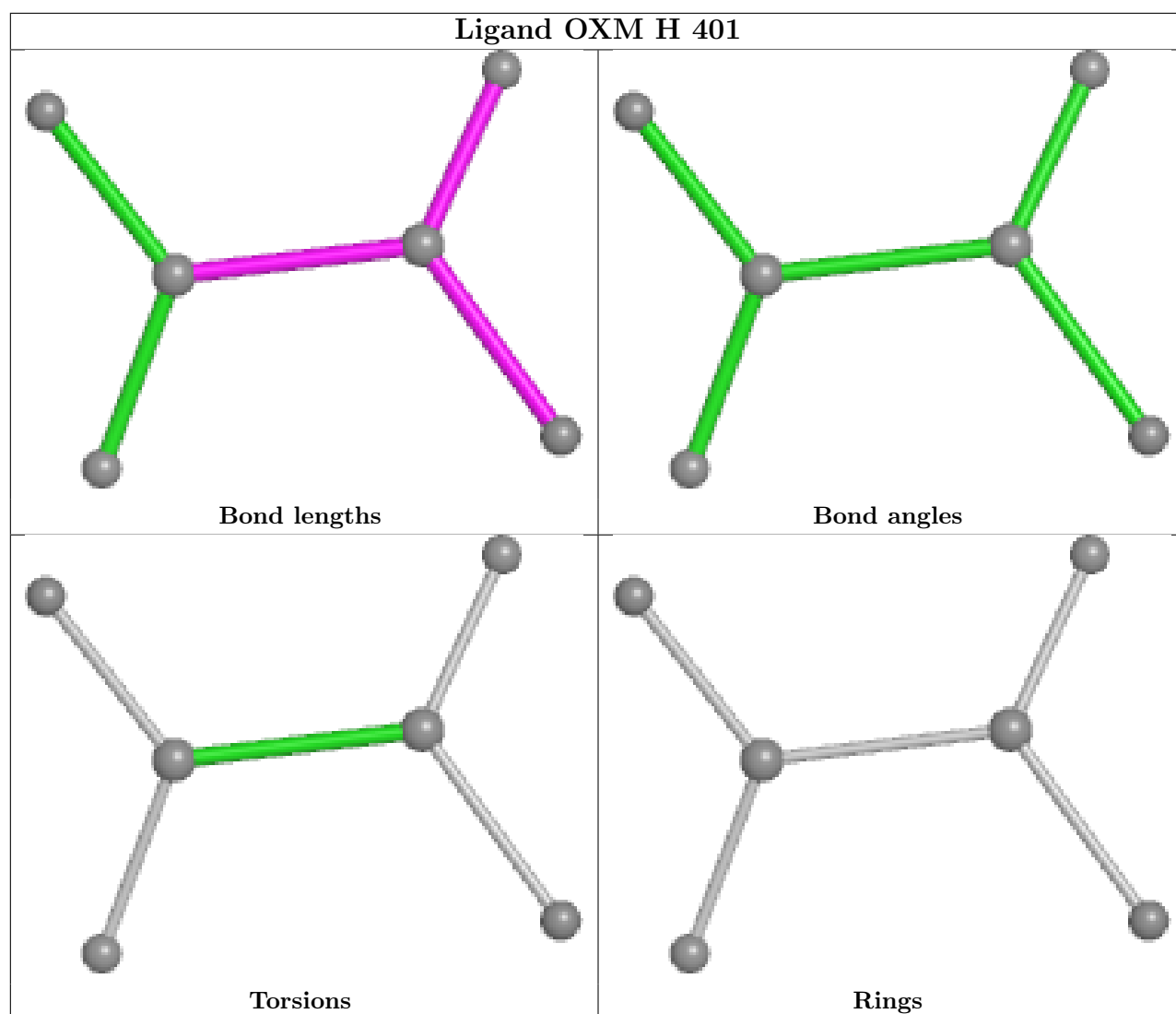


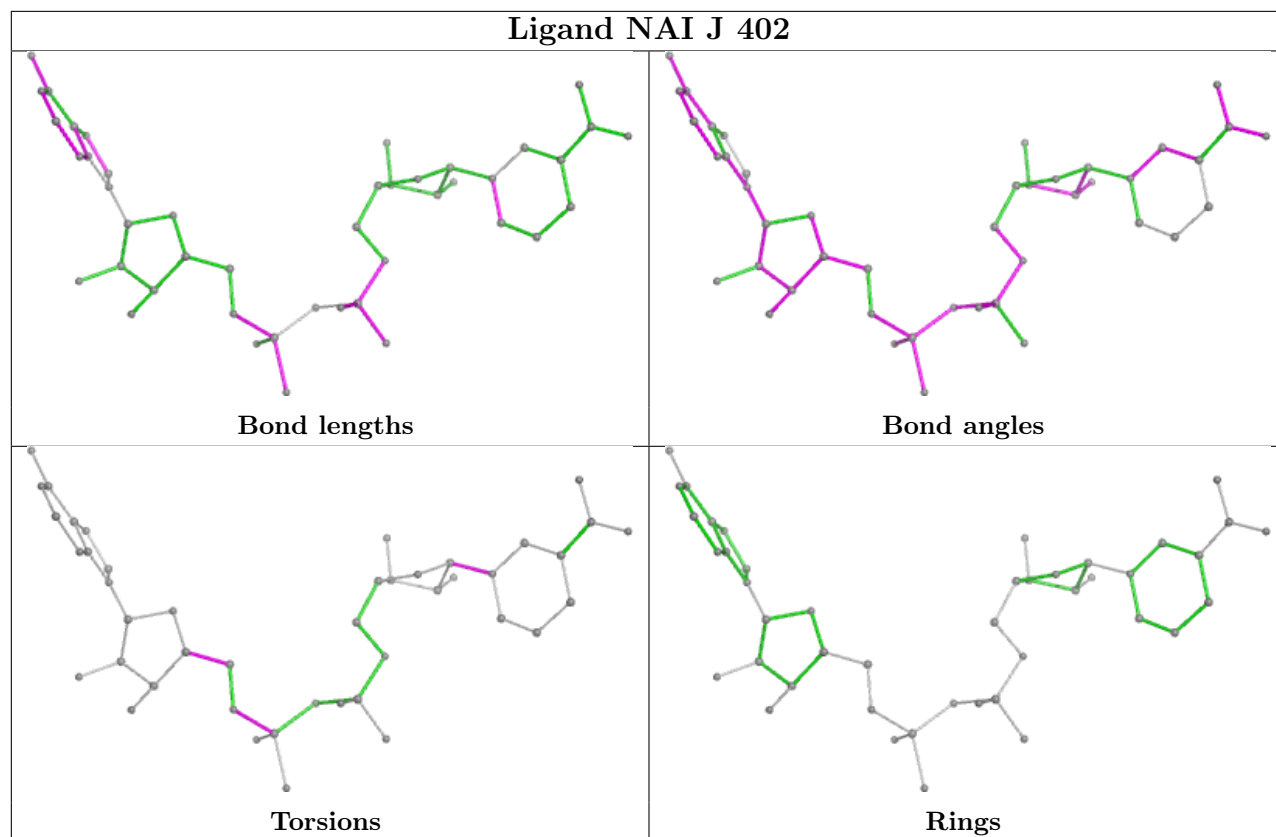


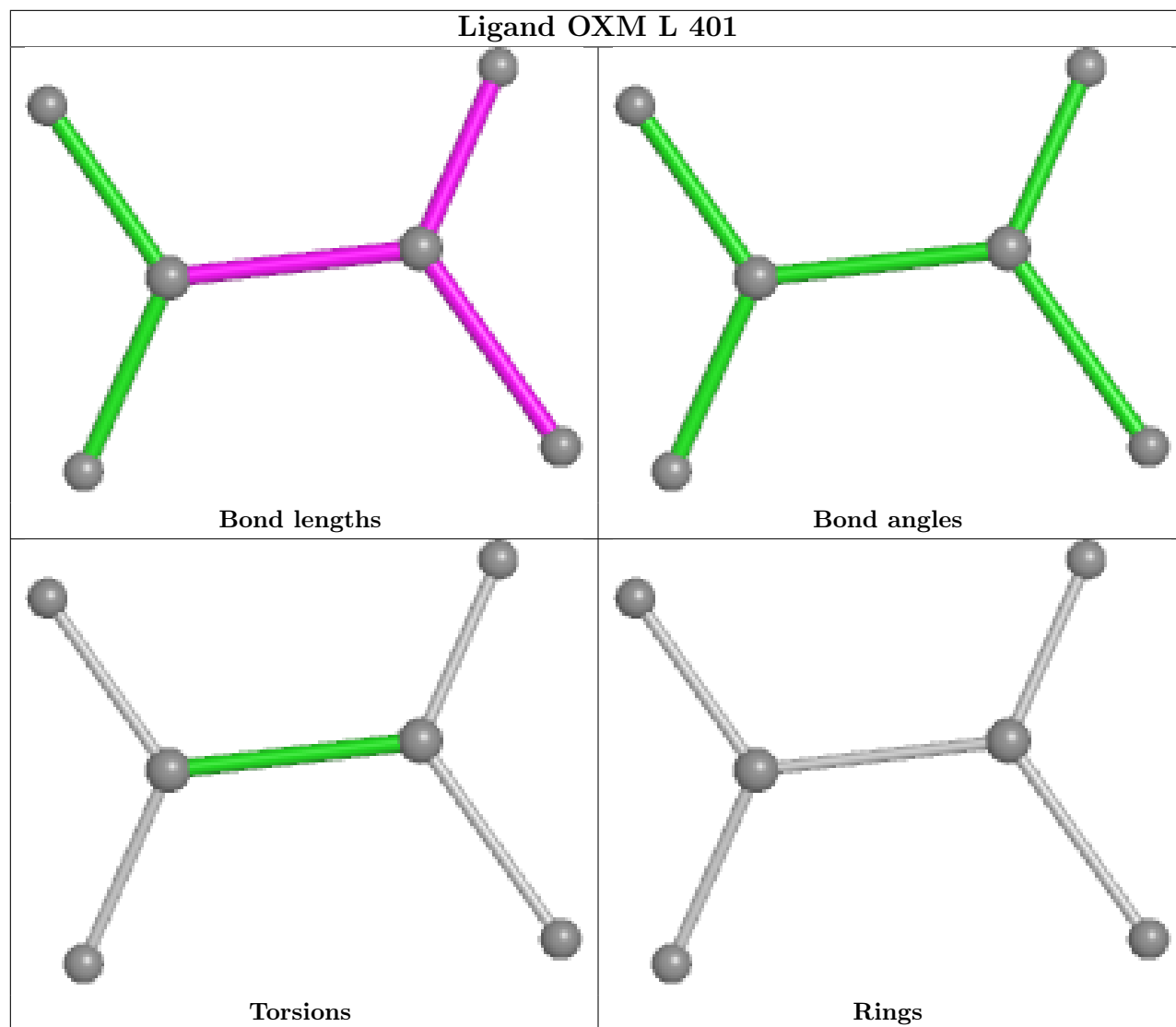


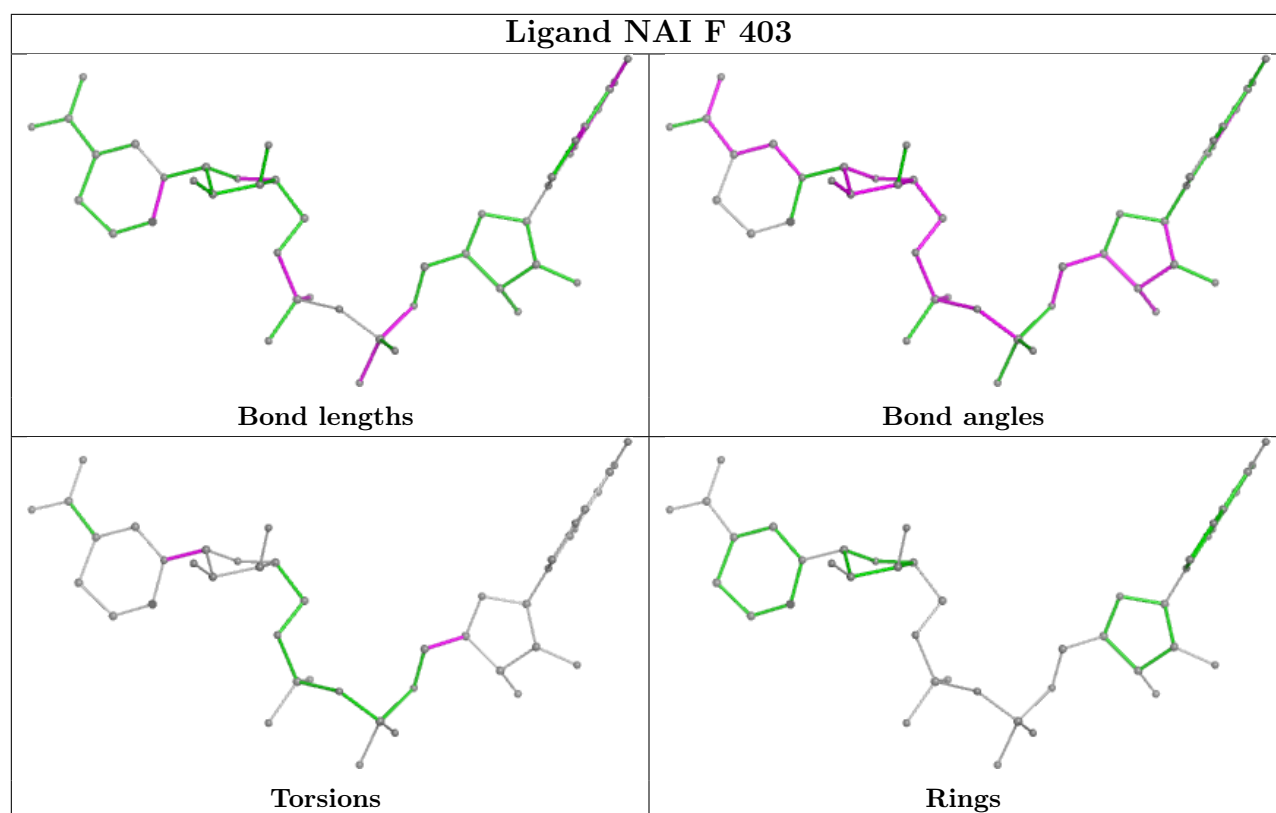


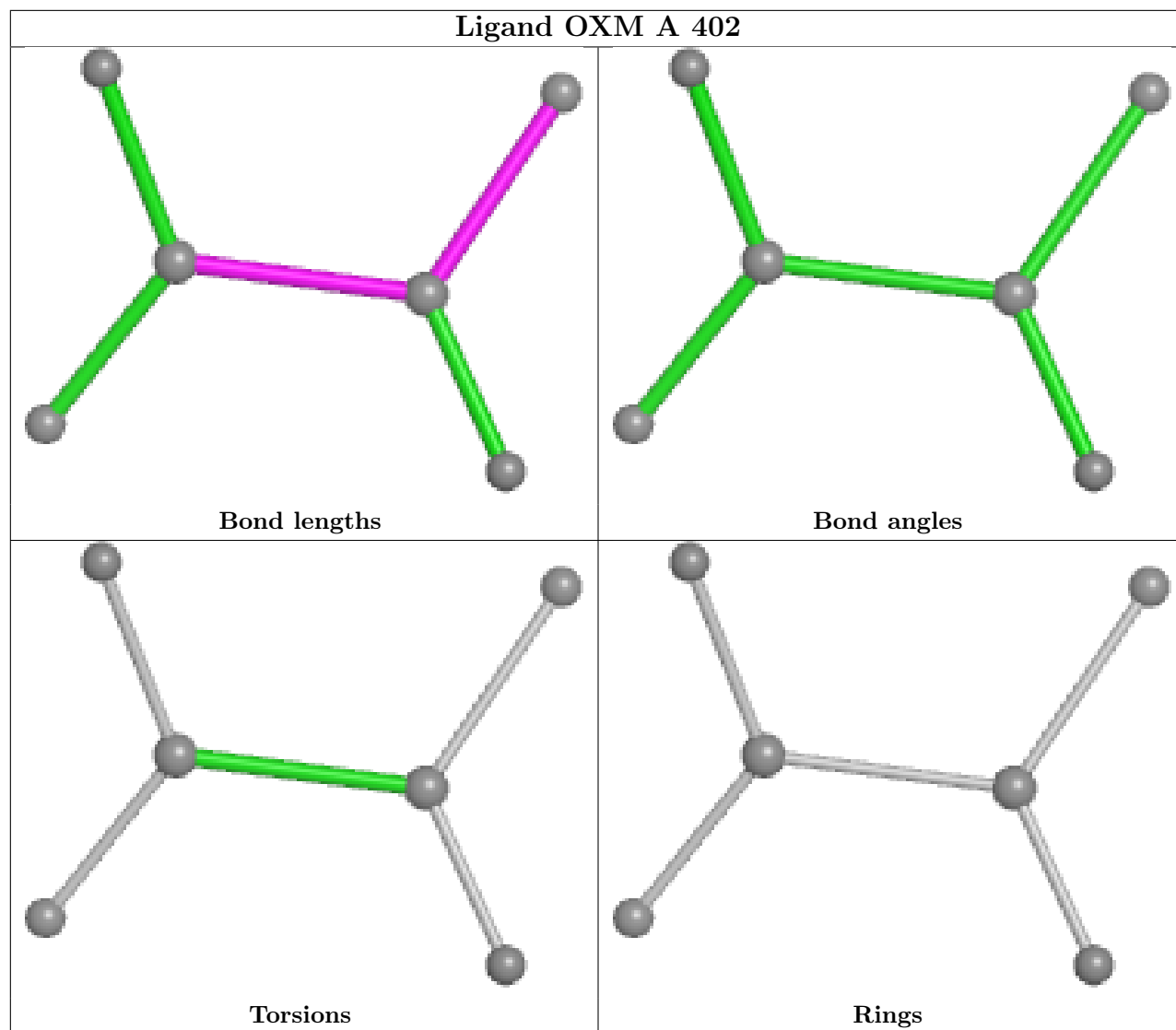


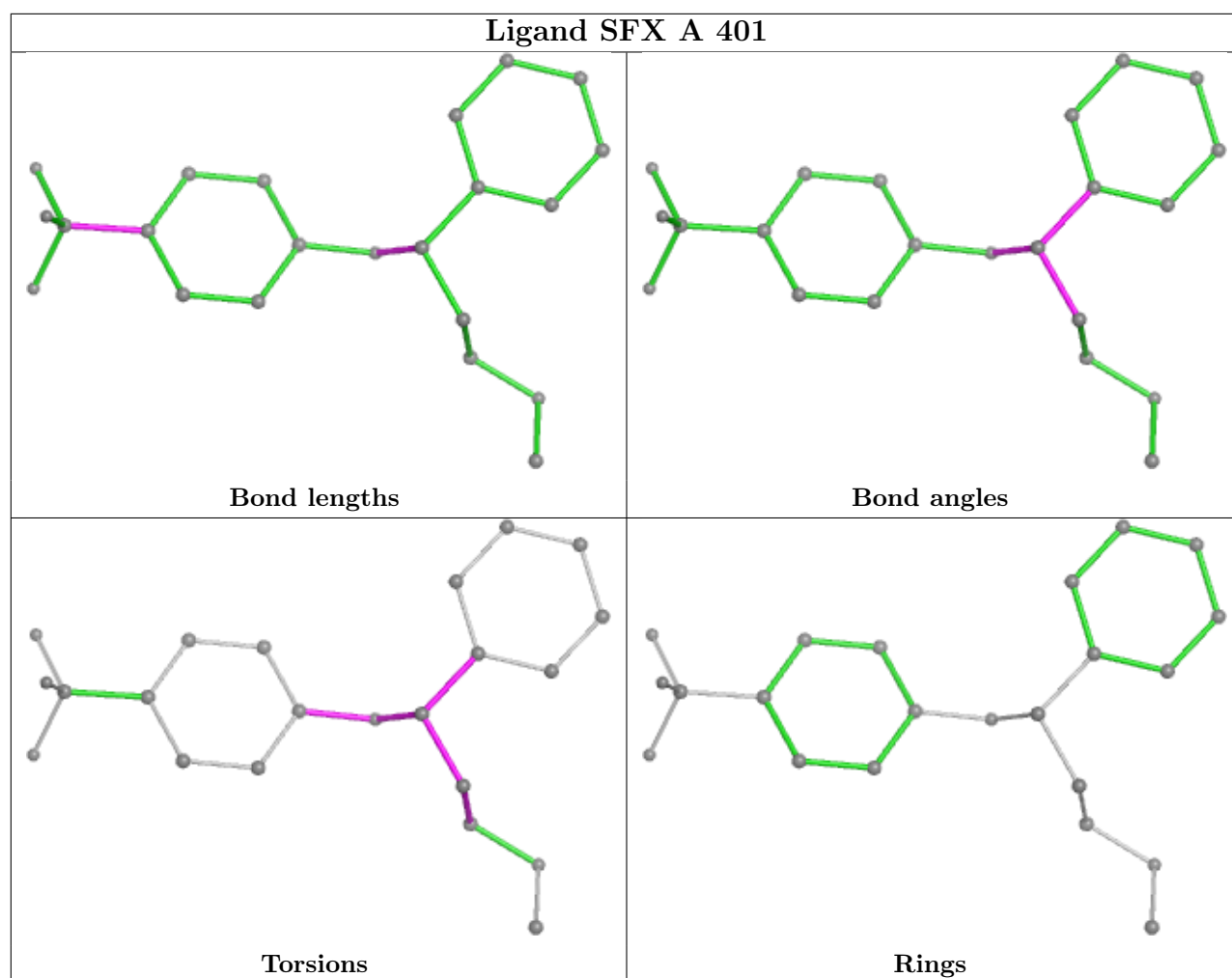


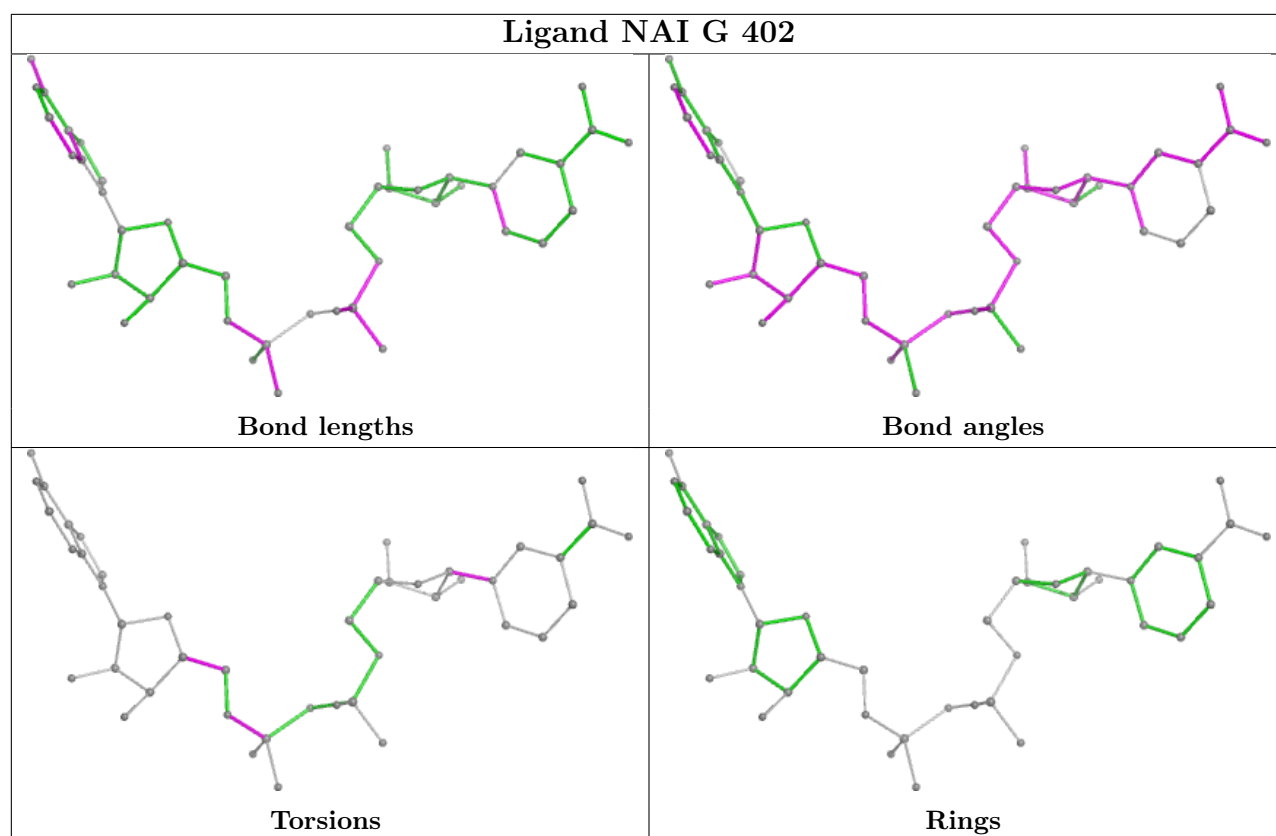


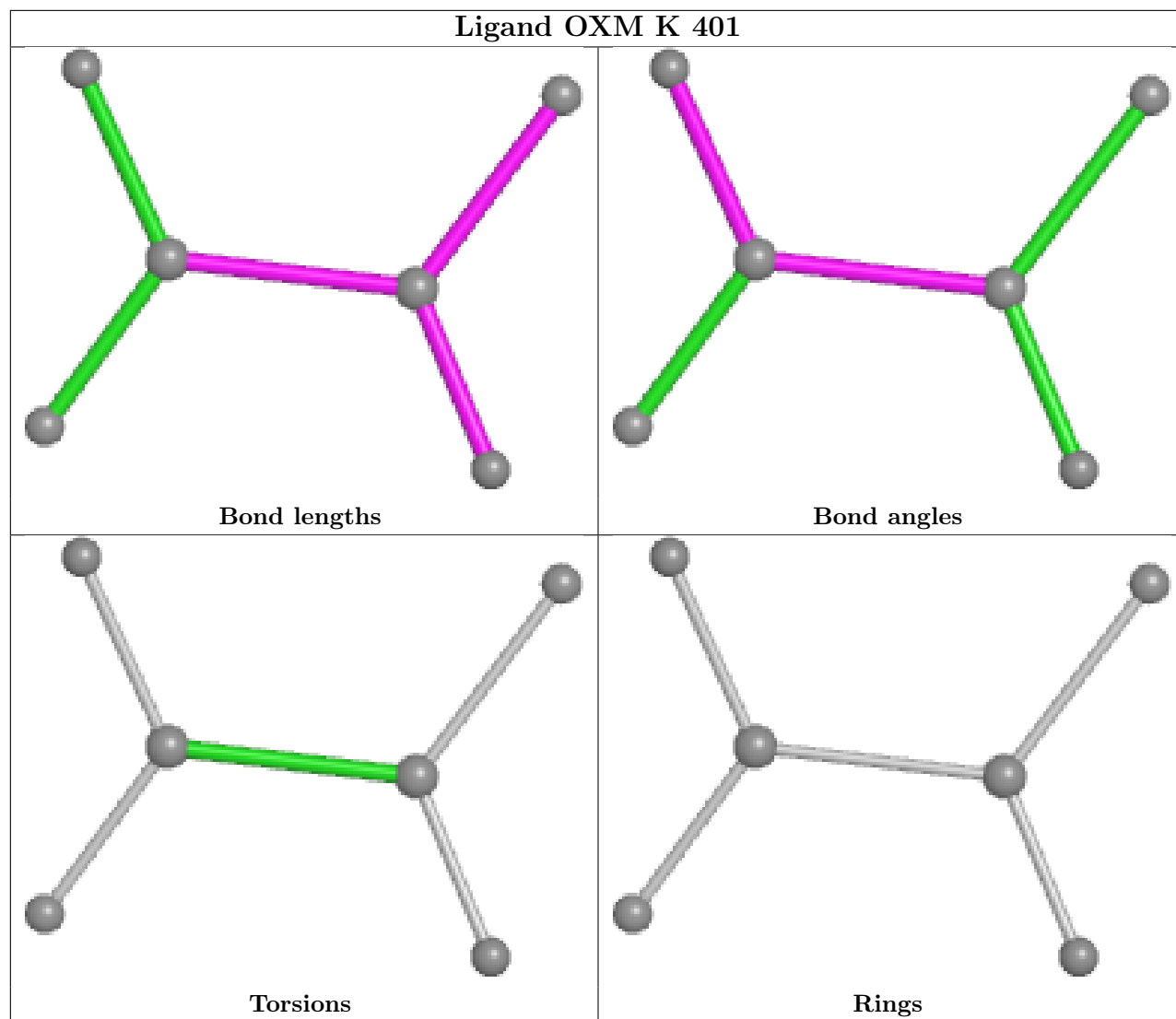




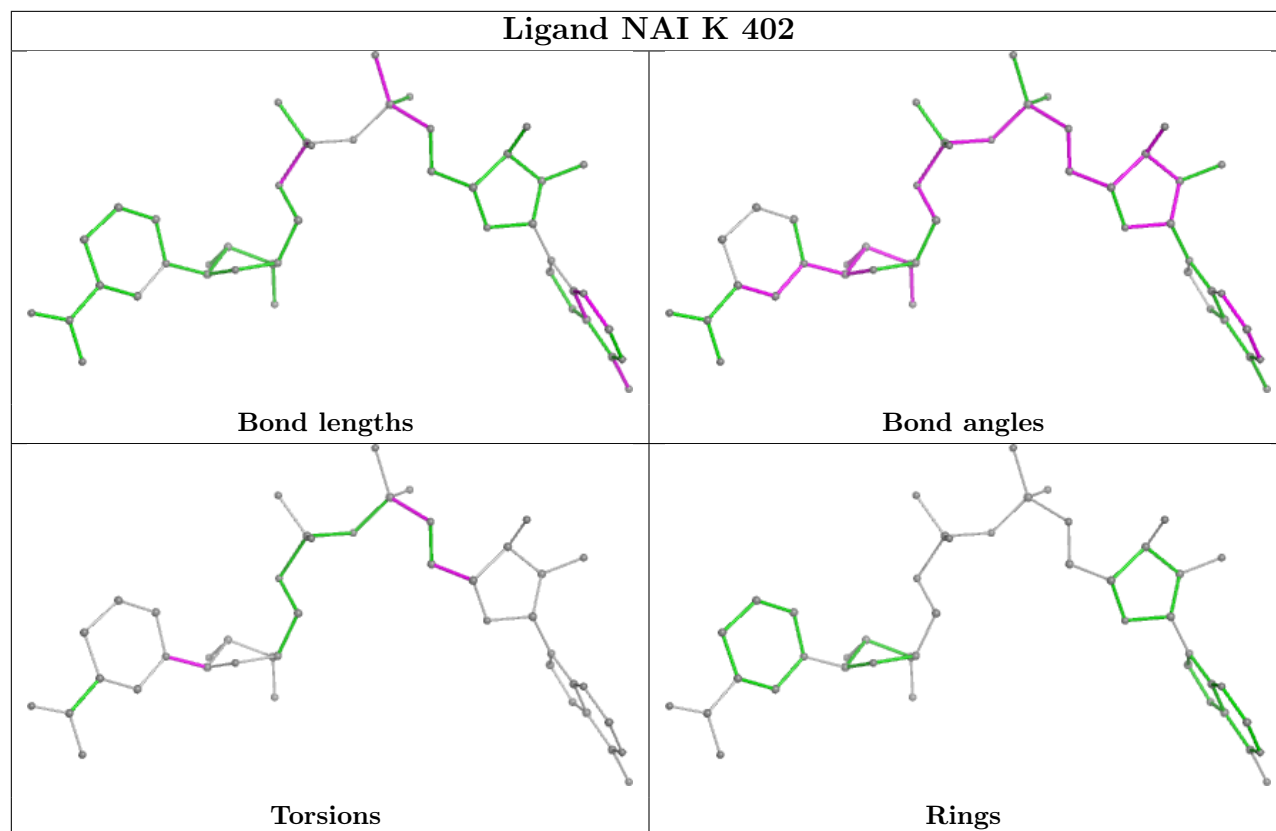




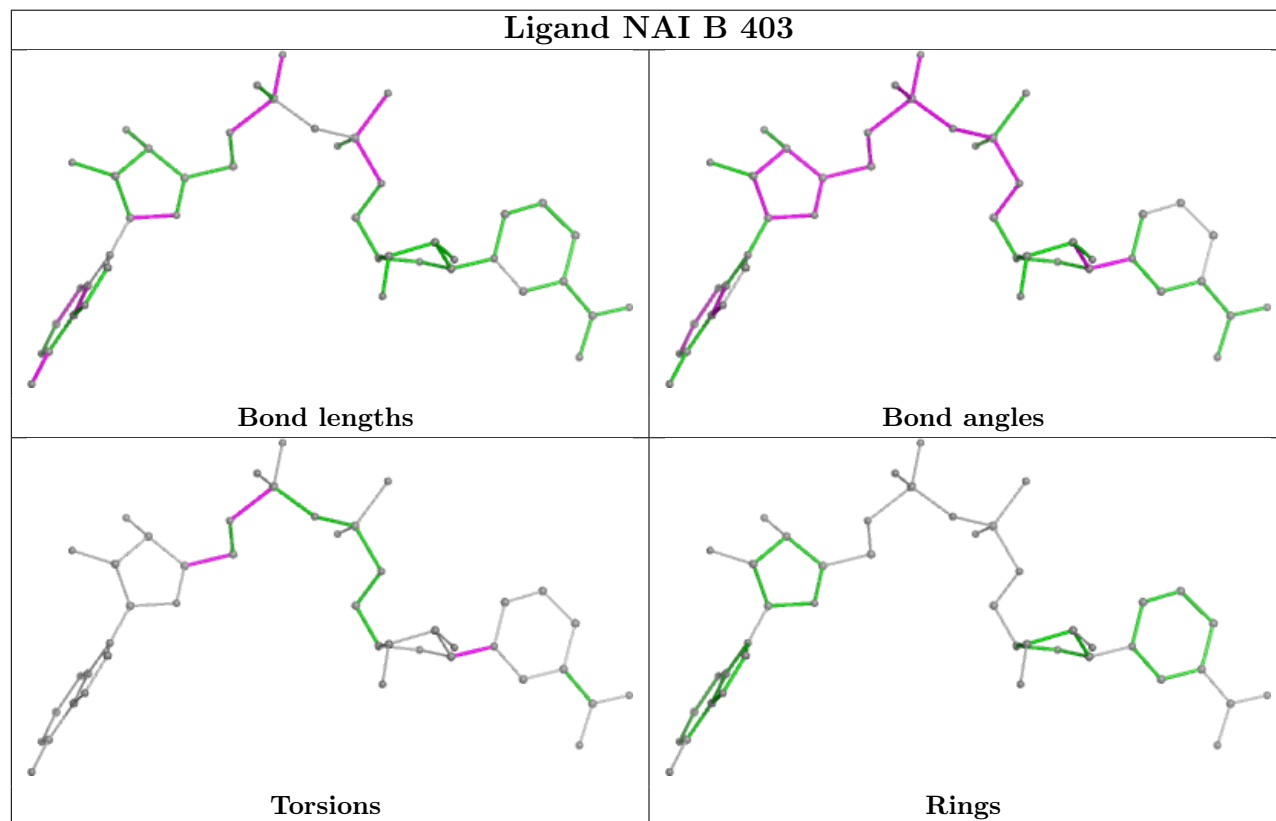


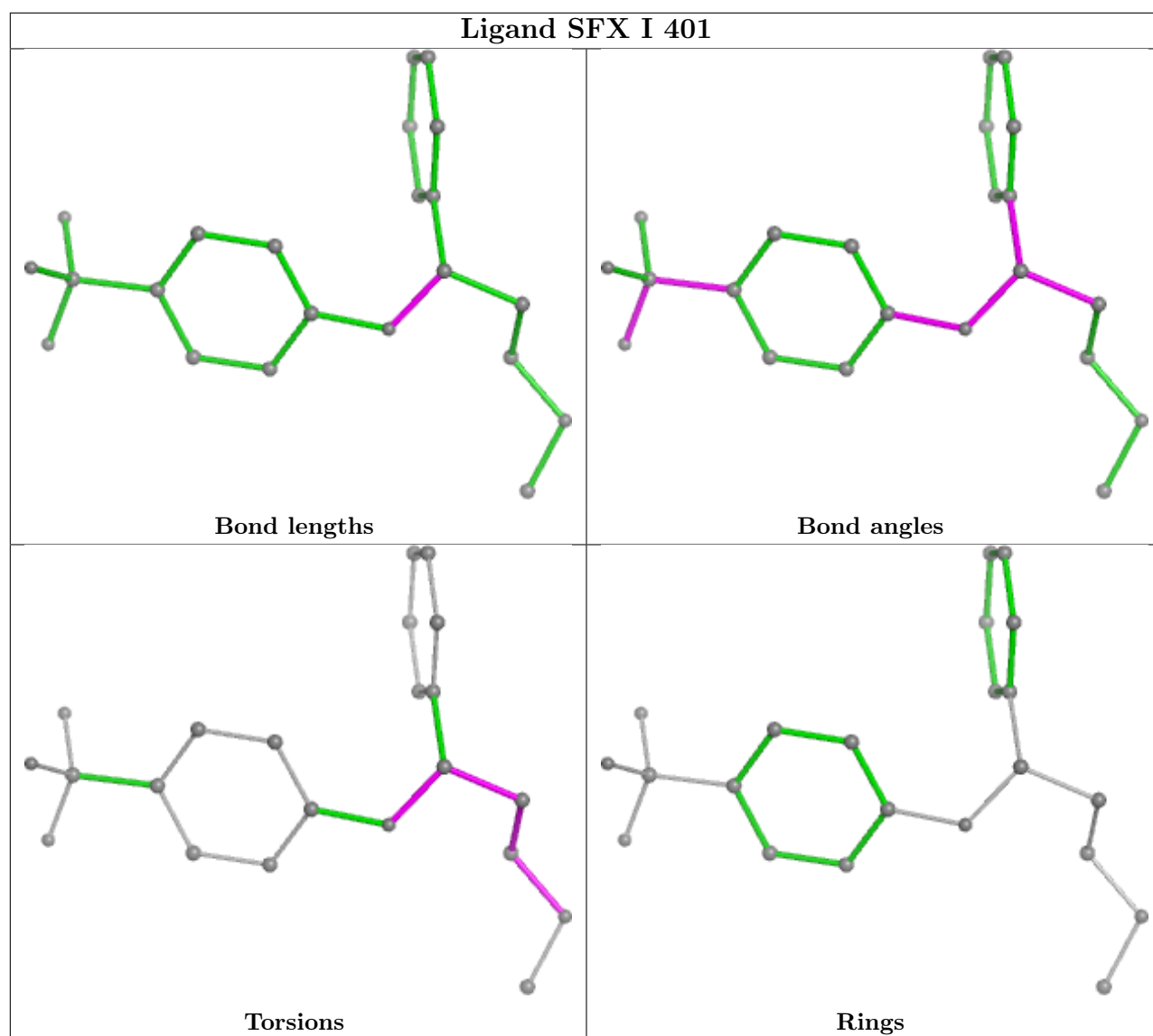


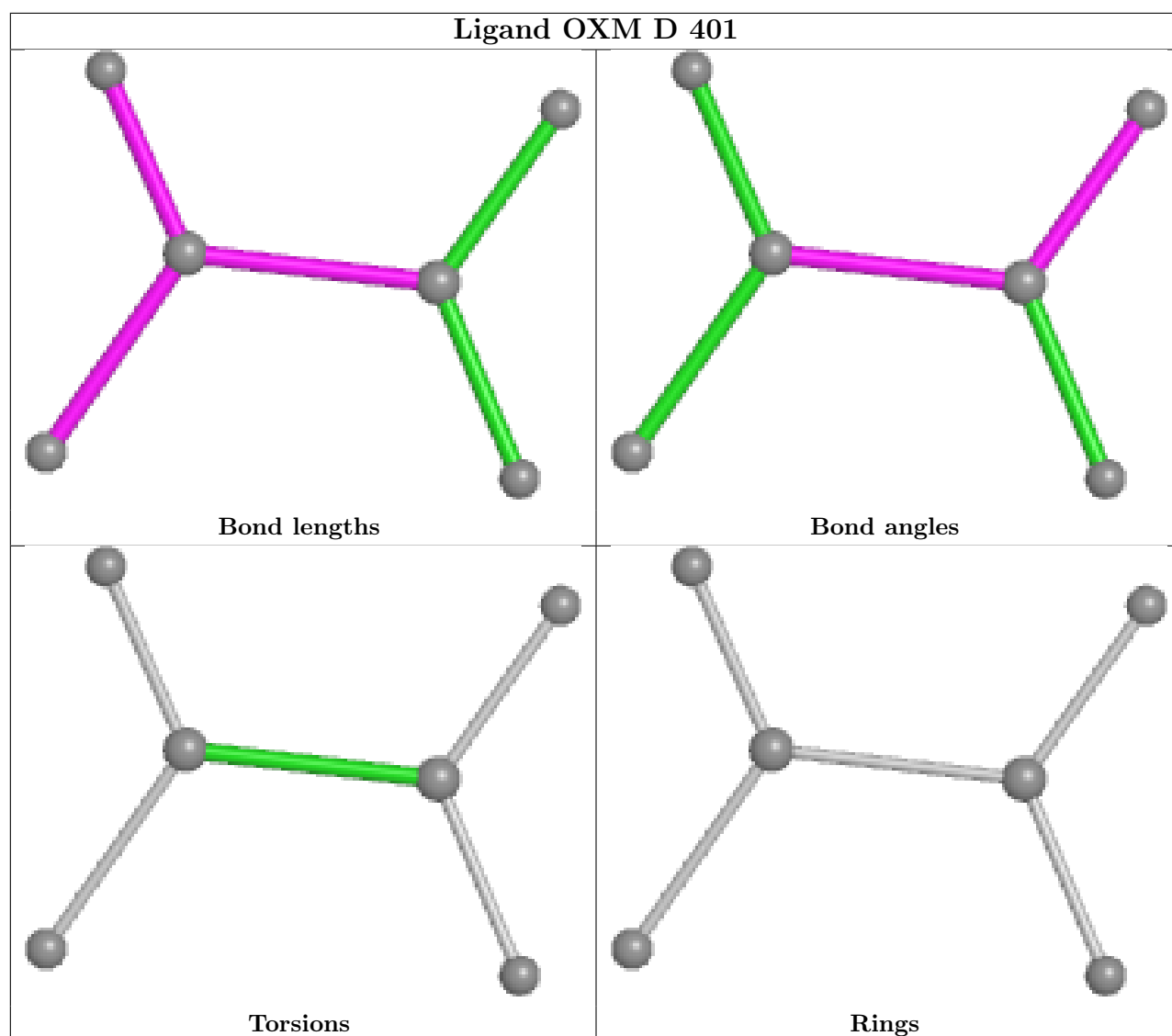
Ligand NAI K 402

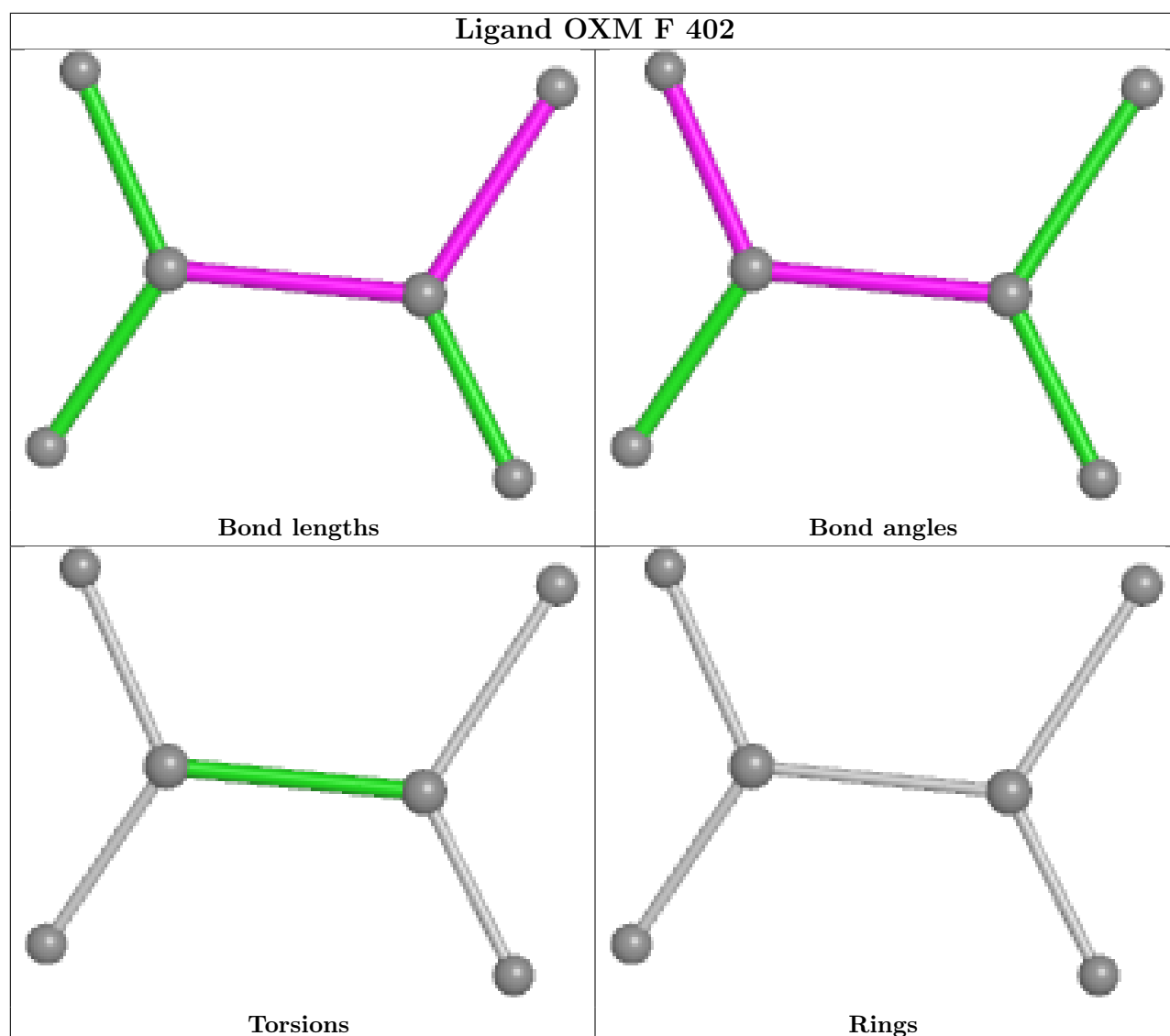


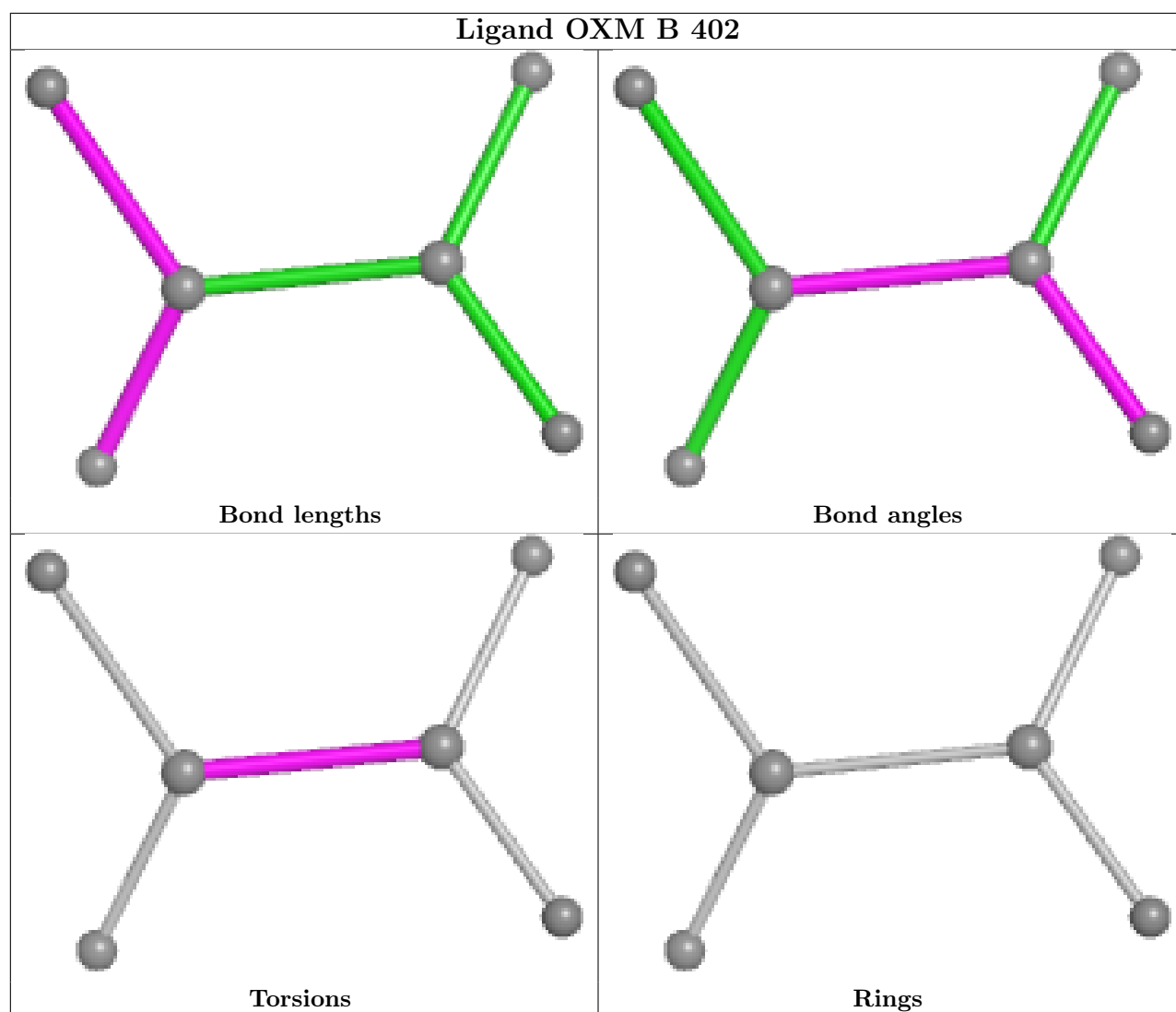
Ligand NAI B 403

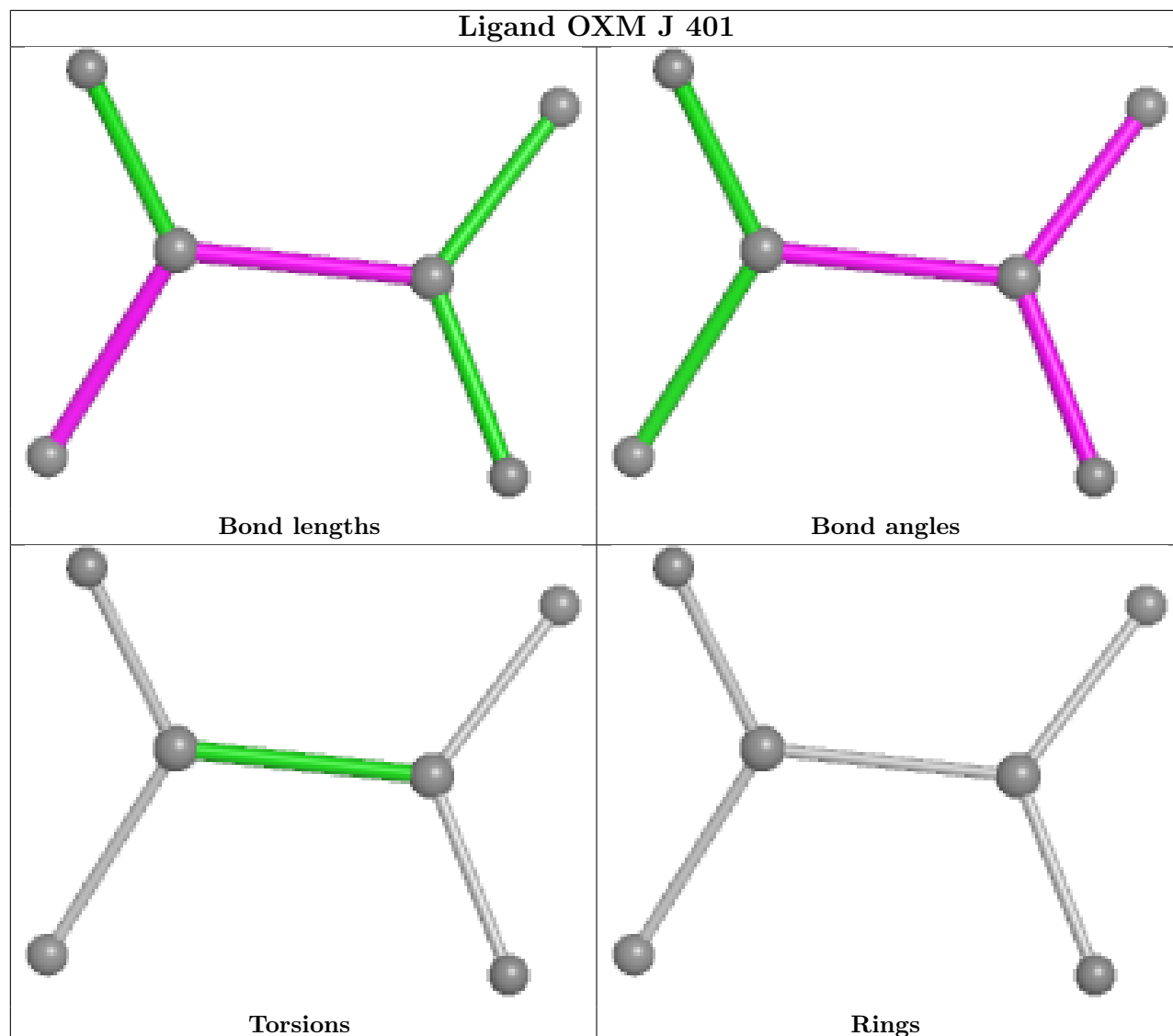




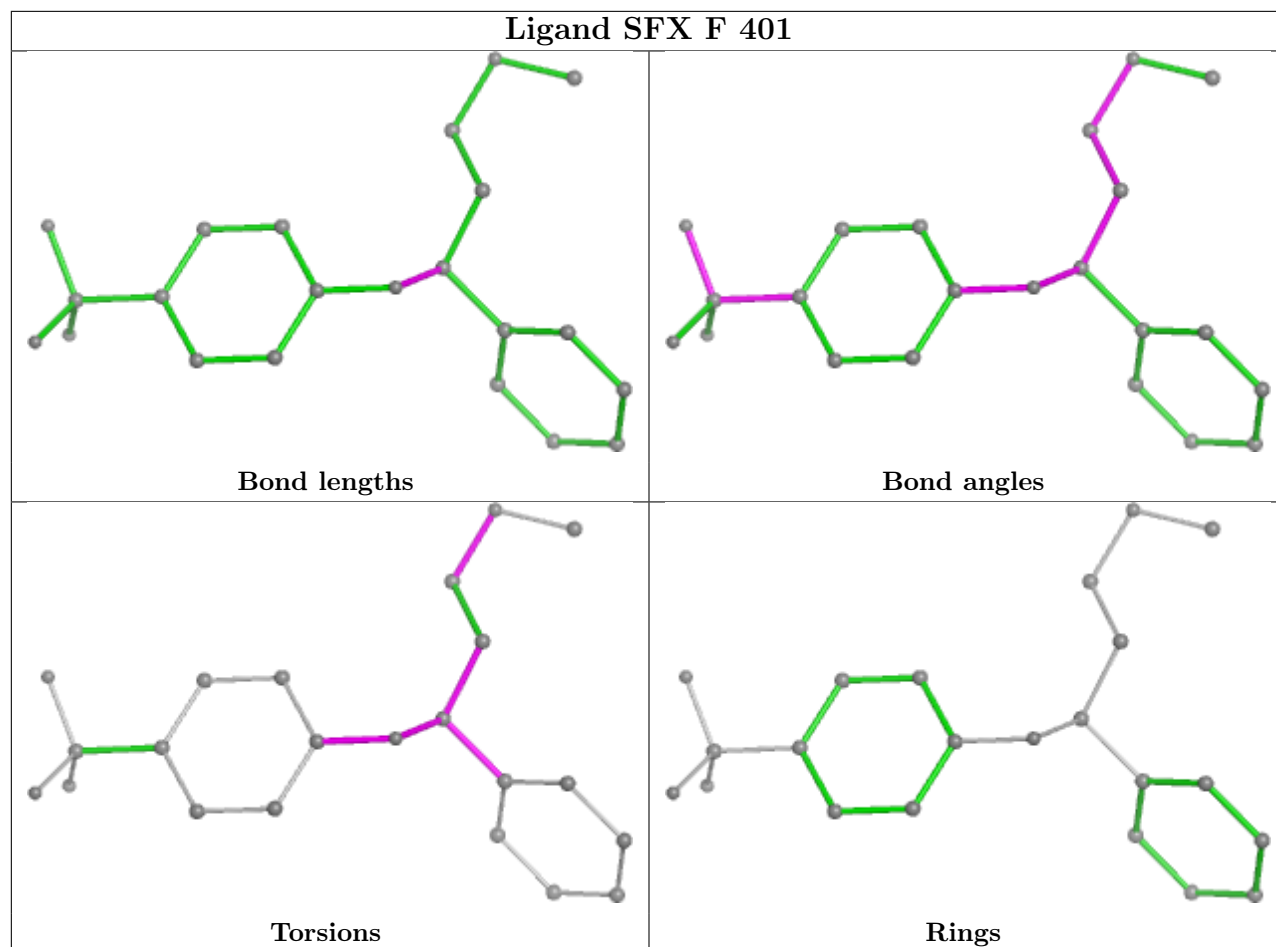




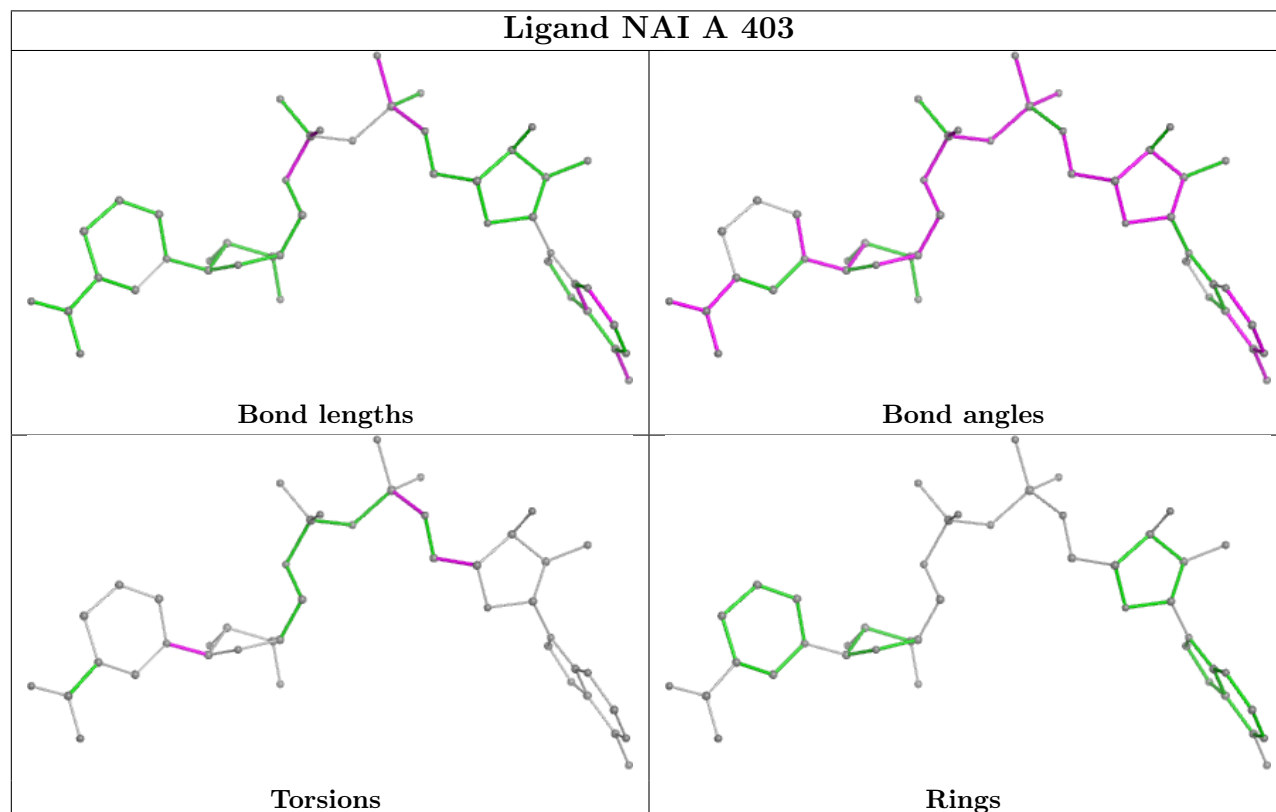


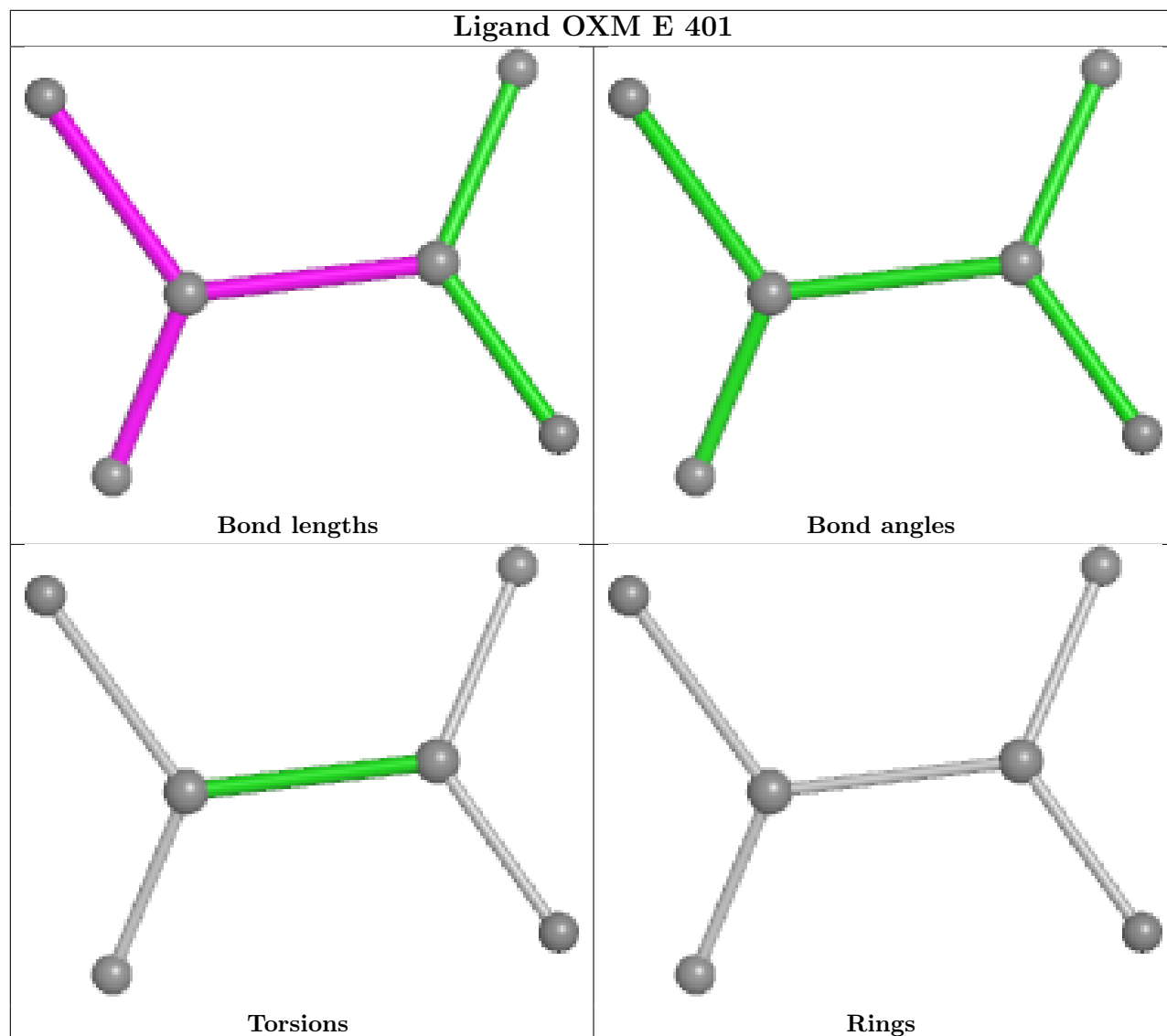


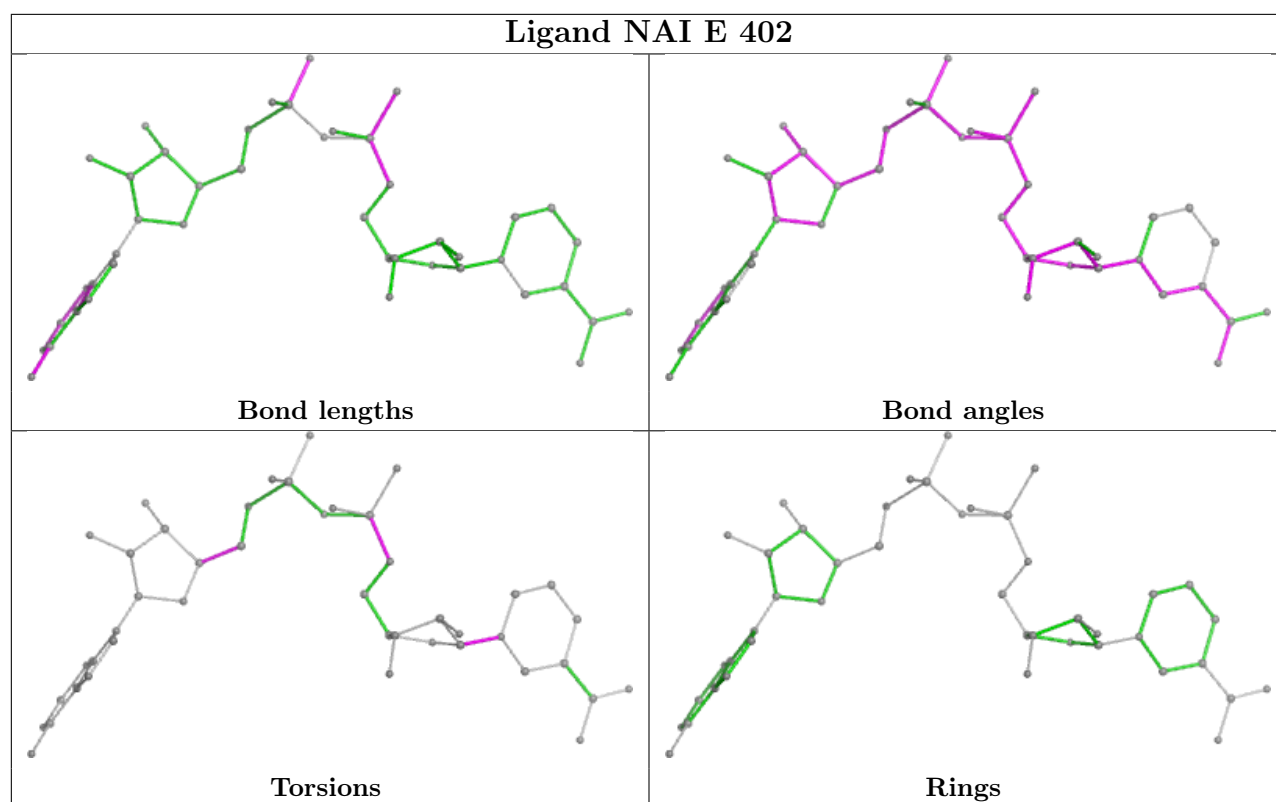
Ligand SFX F 401



Ligand NAI A 403







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	333/349 (95%)	0.90	18 (5%)	32 34	29, 40, 62, 78	1 (0%)
1	B	333/349 (95%)	0.79	10 (3%)	52 54	29, 39, 61, 83	0
1	C	334/349 (95%)	0.80	18 (5%)	32 34	17, 36, 60, 85	2 (0%)
1	D	332/349 (95%)	0.84	20 (6%)	29 30	26, 39, 57, 77	2 (0%)
1	E	332/349 (95%)	0.93	25 (7%)	22 23	29, 40, 65, 86	0
1	F	334/349 (95%)	0.89	20 (5%)	29 30	28, 38, 59, 78	0
1	G	333/349 (95%)	0.84	6 (1%)	67 69	29, 39, 58, 72	0
1	H	334/349 (95%)	0.97	16 (4%)	36 38	20, 43, 61, 80	2 (0%)
1	I	333/349 (95%)	0.78	12 (3%)	46 48	27, 37, 57, 82	0
1	J	332/349 (95%)	0.96	13 (3%)	44 45	32, 43, 59, 78	2 (0%)
1	K	334/349 (95%)	1.07	27 (8%)	19 21	30, 43, 69, 83	0
1	L	334/349 (95%)	1.39	61 (18%)	4 4	35, 50, 73, 91	4 (1%)
All	All	3998/4188 (95%)	0.93	246 (6%)	28 28	17, 41, 64, 91	13 (0%)

The worst 5 of 246 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	16	ALA	5.3
1	C	16	ALA	4.8
1	D	227	TRP	4.6
1	L	227	TRP	4.4
1	J	227	TRP	4.4

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SFX	B	401	22/22	0.62	0.26	37,46,52,57	22
2	SFX	C	401	22/22	0.62	0.24	46,52,60,66	22
5	BTB	G	403	14/14	0.63	0.21	42,48,56,56	0
5	BTB	A	404	14/14	0.65	0.21	45,48,52,53	14
2	SFX	A	401	22/22	0.65	0.24	46,50,53,54	22
2	SFX	I	401	22/22	0.66	0.25	43,52,60,65	22
5	BTB	K	403	14/14	0.67	0.18	43,53,58,61	14
5	BTB	F	404	14/14	0.70	0.17	51,54,62,62	0
5	BTB	L	403	14/14	0.71	0.15	57,62,65,68	0
7	GOL	G	404	6/6	0.71	0.17	61,64,66,68	0
8	PEG	J	407	7/7	0.71	0.16	47,55,64,67	0
2	SFX	F	401	22/22	0.72	0.20	42,51,61,67	22
5	BTB	C	404	14/14	0.73	0.17	37,44,47,48	14
7	GOL	F	406	6/6	0.74	0.15	49,52,55,58	0
8	PEG	D	406	7/7	0.75	0.17	57,61,64,67	0
8	PEG	H	407	7/7	0.77	0.15	50,54,59,61	0
7	GOL	L	404	6/6	0.78	0.16	57,58,60,65	0
7	GOL	H	403	6/6	0.78	0.14	57,64,66,69	0
7	GOL	H	404	6/6	0.79	0.14	55,58,59,64	0
7	GOL	K	405	6/6	0.79	0.13	43,47,49,54	0
8	PEG	J	406	7/7	0.79	0.15	51,55,60,60	0
7	GOL	G	405	6/6	0.79	0.13	51,51,52,53	0
8	PEG	B	408	7/7	0.80	0.15	41,49,56,59	0
7	GOL	K	404	6/6	0.80	0.12	51,57,60,63	0
7	GOL	D	403	6/6	0.80	0.14	47,55,56,57	0
7	GOL	B	405	6/6	0.80	0.18	36,41,44,44	0
7	GOL	L	405	6/6	0.80	0.15	57,61,64,64	0
7	GOL	L	406	6/6	0.81	0.17	37,45,52,52	0
7	GOL	H	406	6/6	0.81	0.13	43,53,56,57	0
8	PEG	D	407	7/7	0.82	0.14	52,54,57,65	0
7	GOL	B	404	6/6	0.82	0.13	39,46,49,58	0
7	GOL	J	403	6/6	0.82	0.15	48,50,52,54	0

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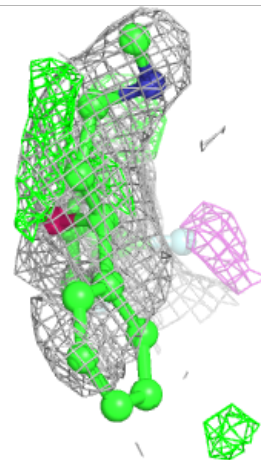
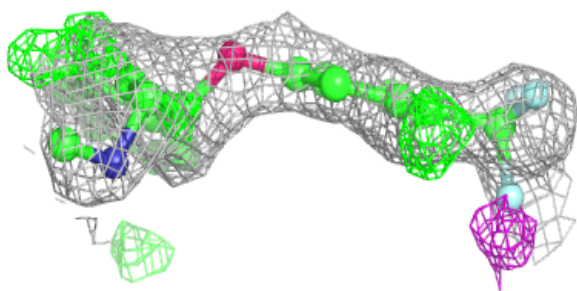
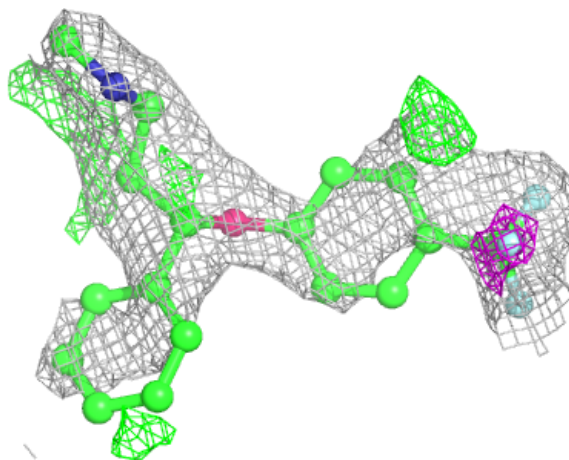
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GOL	H	405	6/6	0.82	0.13	50,55,60,62	0
7	GOL	F	405	6/6	0.83	0.15	44,48,48,48	0
7	GOL	C	405	6/6	0.83	0.14	45,46,47,61	0
7	GOL	I	404	6/6	0.83	0.15	40,42,45,47	0
3	OXM	C	402	6/6	0.84	0.15	31,35,42,42	0
8	PEG	E	403	7/7	0.85	0.13	43,48,52,60	0
3	OXM	K	401	6/6	0.85	0.13	39,40,48,48	0
3	OXM	L	401	6/6	0.86	0.14	43,45,53,53	0
3	OXM	E	401	6/6	0.87	0.11	32,35,40,40	0
3	OXM	I	402	6/6	0.87	0.11	29,31,36,36	0
3	OXM	A	402	6/6	0.87	0.13	33,37,42,42	0
3	OXM	F	402	6/6	0.88	0.12	30,36,37,43	0
3	OXM	G	401	6/6	0.89	0.10	32,36,41,41	0
3	OXM	J	401	6/6	0.89	0.10	34,36,42,42	0
3	OXM	B	402	6/6	0.90	0.11	35,37,44,44	0
4	NAI	H	402	44/44	0.91	0.10	27,35,44,50	0
4	NAI	J	402	44/44	0.91	0.10	30,36,46,52	0
4	NAI	K	402	44/44	0.91	0.10	28,36,45,48	0
4	NAI	L	402	44/44	0.91	0.10	31,39,51,55	0
3	OXM	D	401	6/6	0.91	0.11	36,38,43,43	0
4	NAI	D	402	44/44	0.91	0.10	27,35,44,48	0
4	NAI	C	403	44/44	0.92	0.09	24,31,39,44	0
6	SO4	B	406	5/5	0.92	0.10	34,38,42,43	0
3	OXM	H	401	6/6	0.92	0.09	32,40,48,48	0
4	NAI	E	402	44/44	0.92	0.10	22,34,42,46	0
4	NAI	A	403	44/44	0.93	0.09	28,35,44,47	0
4	NAI	F	403	44/44	0.93	0.09	25,32,40,42	0
4	NAI	G	402	44/44	0.93	0.09	27,34,42,50	0
4	NAI	B	403	44/44	0.93	0.09	25,33,42,46	0
6	SO4	L	408	5/5	0.94	0.09	37,40,42,45	0
4	NAI	I	403	44/44	0.94	0.09	24,31,43,45	0
6	SO4	D	405	5/5	0.94	0.09	27,32,36,39	0
6	SO4	L	407	5/5	0.95	0.08	38,38,45,47	0
6	SO4	D	404	5/5	0.95	0.07	33,37,38,39	0
6	SO4	C	406	5/5	0.95	0.09	31,32,36,39	0
6	SO4	J	404	5/5	0.95	0.07	32,34,39,42	0
6	SO4	B	407	5/5	0.96	0.07	29,37,40,42	0
6	SO4	A	405	5/5	0.96	0.07	35,36,41,45	0
6	SO4	C	407	5/5	0.96	0.07	30,35,36,37	0
6	SO4	J	405	5/5	0.96	0.07	37,39,41,42	0
6	SO4	G	406	5/5	0.97	0.06	32,35,41,42	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.

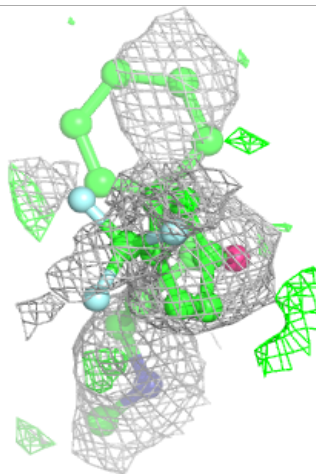
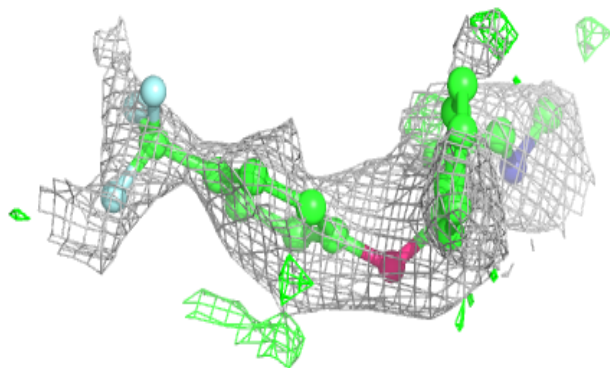
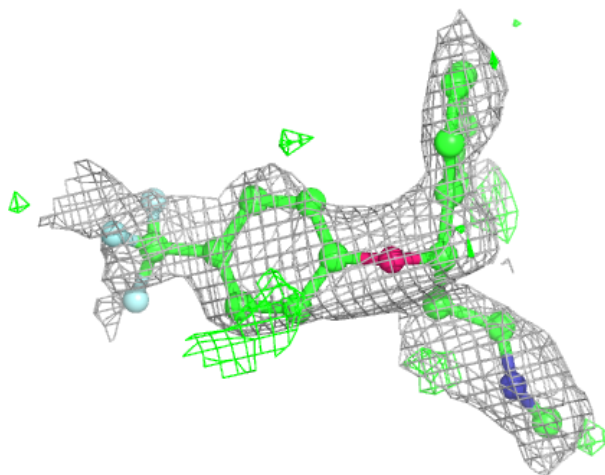
Electron density around SFX B 401:

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and green (positive)



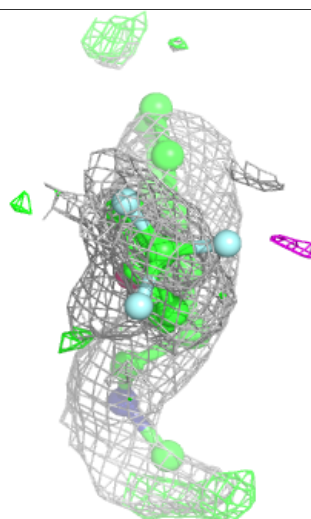
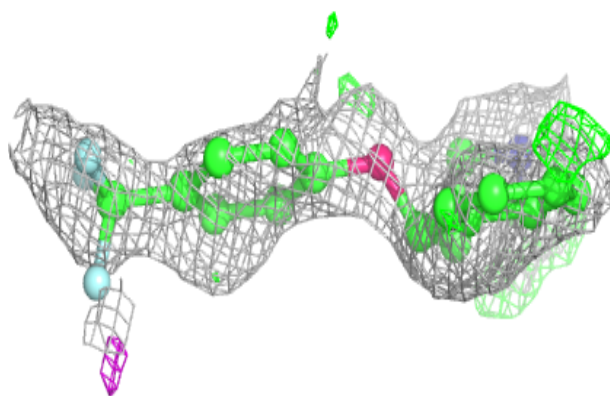
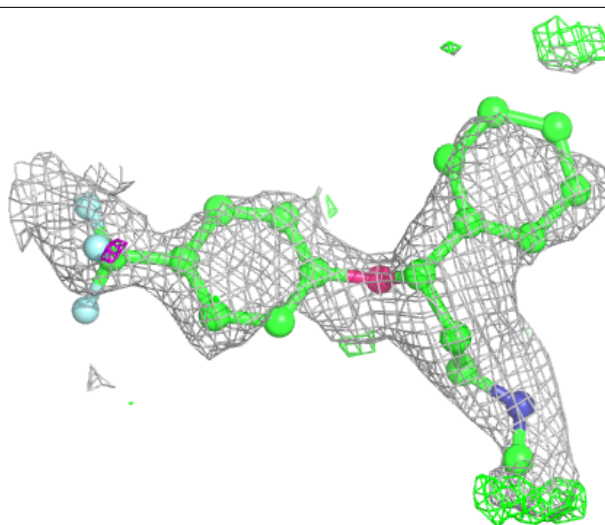
Electron density around SFX C 401:

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and green (positive)



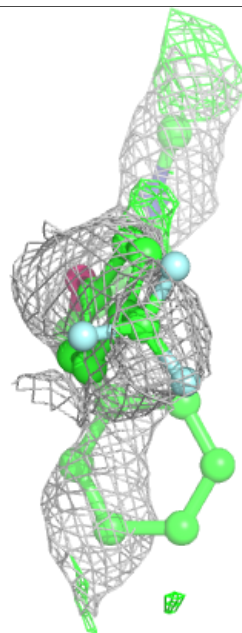
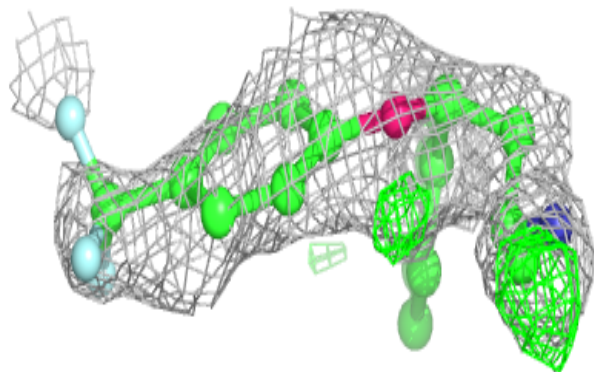
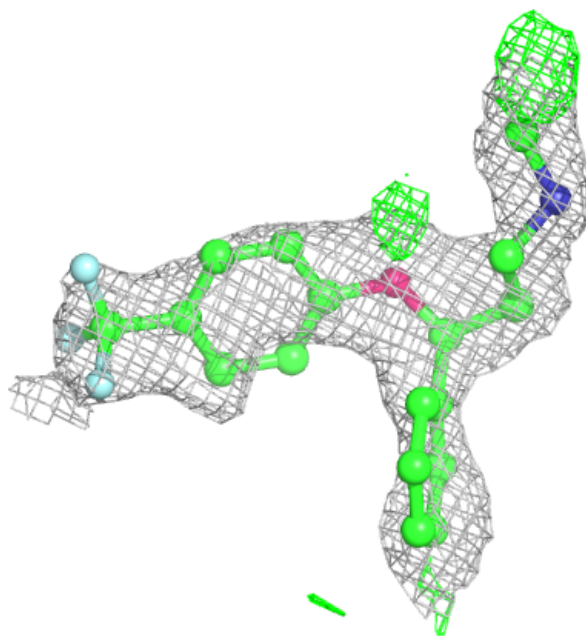
Electron density around SFX A 401:

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and green (positive)



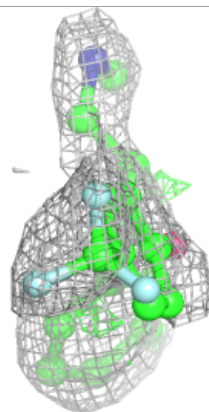
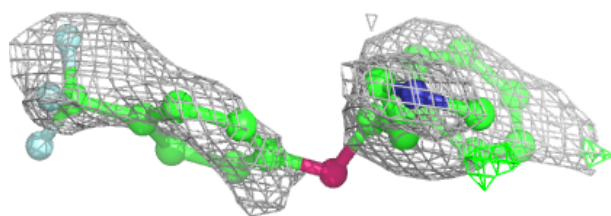
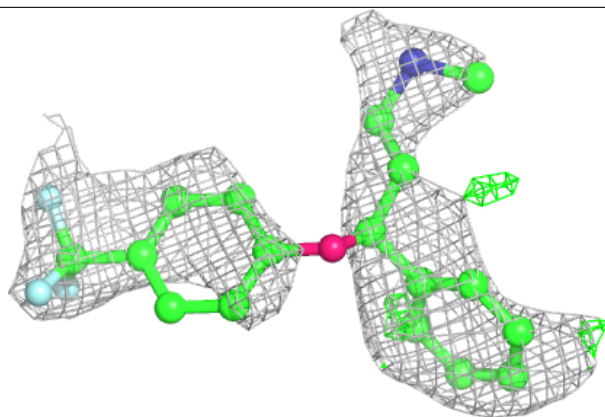
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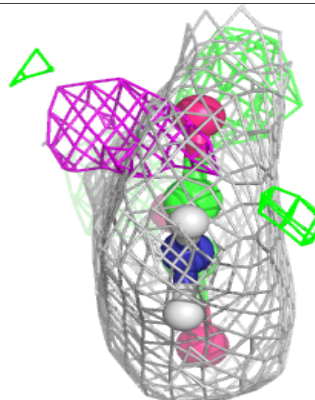
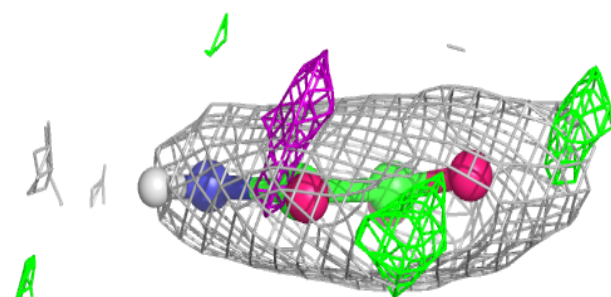
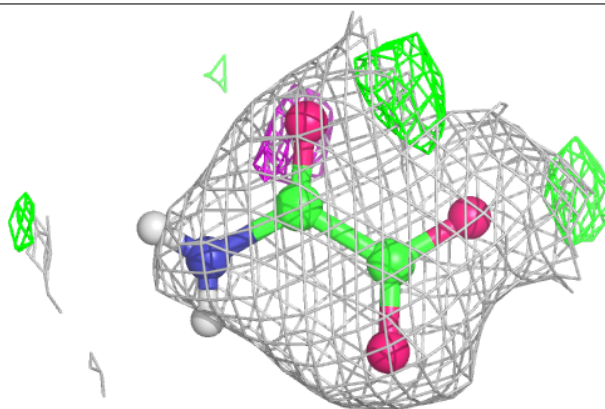


Electron density around SFX F 401:

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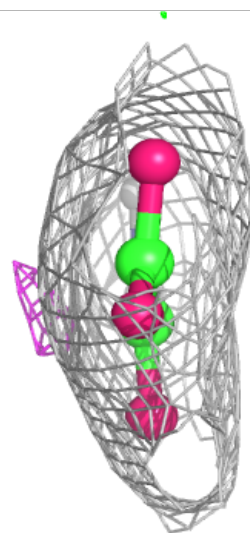
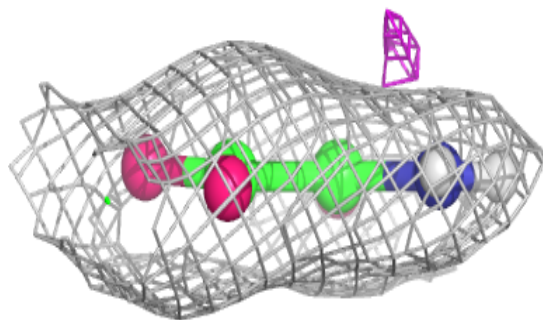
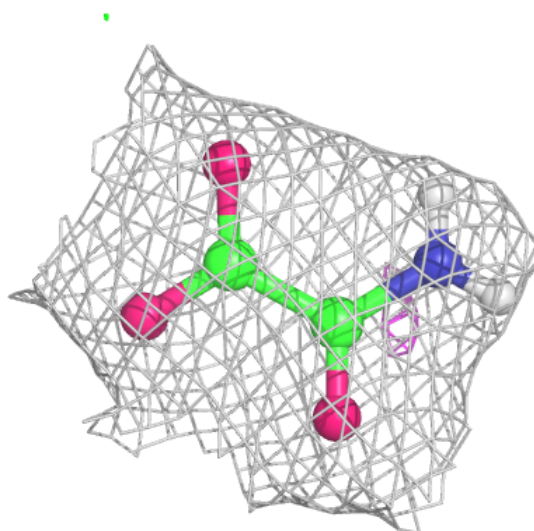
**Electron density around OXM C 402:**

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and green (positive)



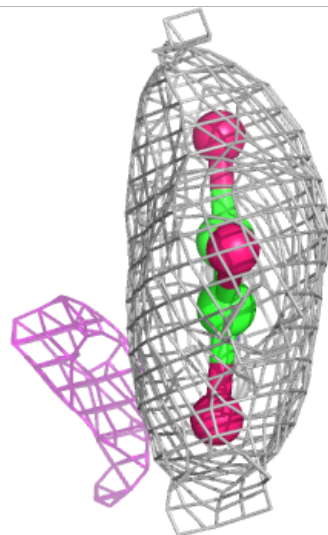
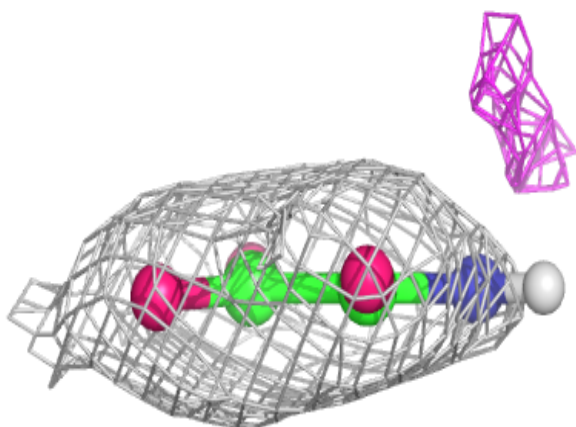
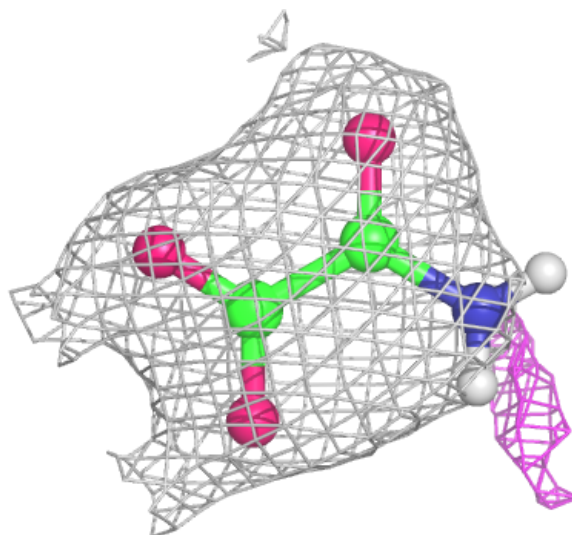
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and green (positive)



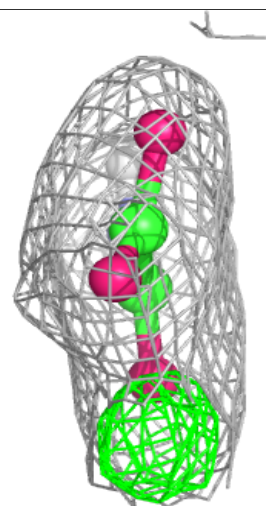
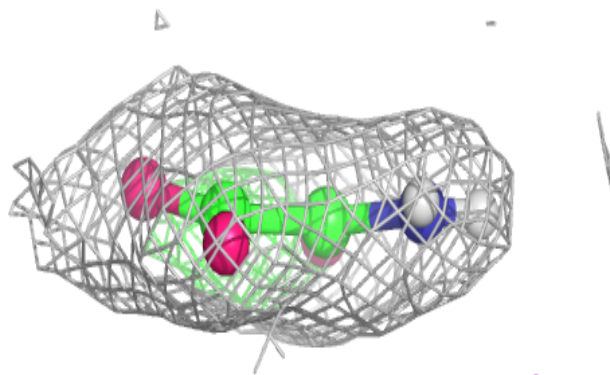
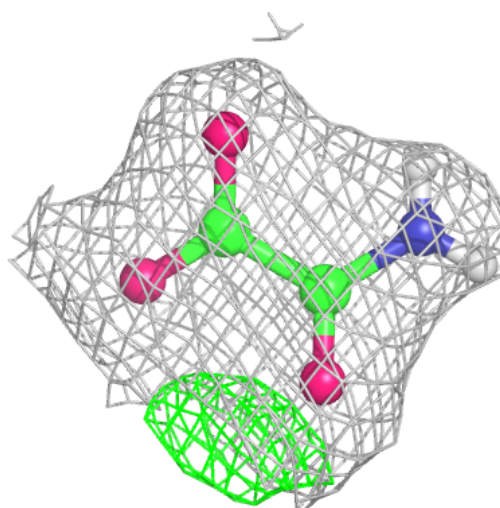
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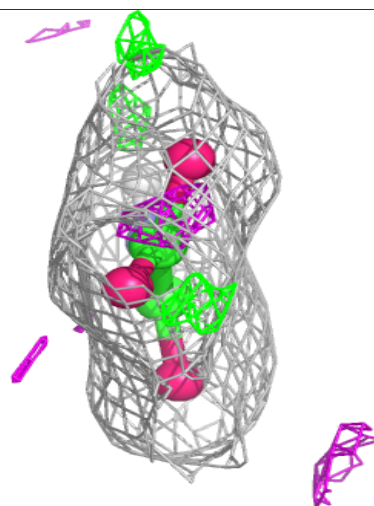
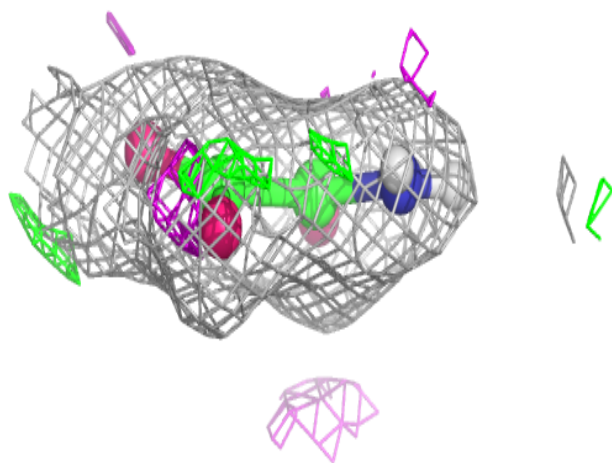
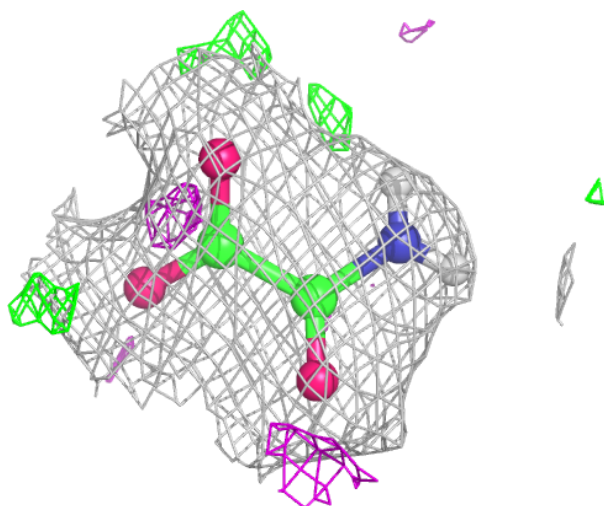
Electron density around OXM E 401:

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and green (positive)



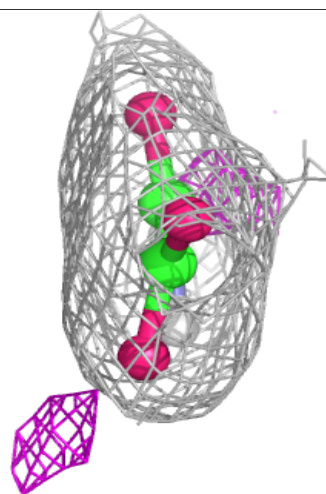
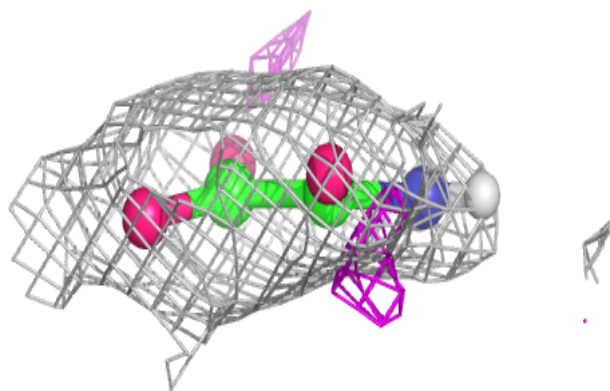
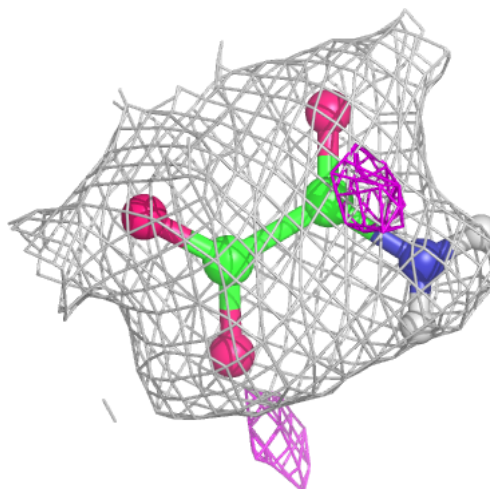
Electron density around OXM I 402:

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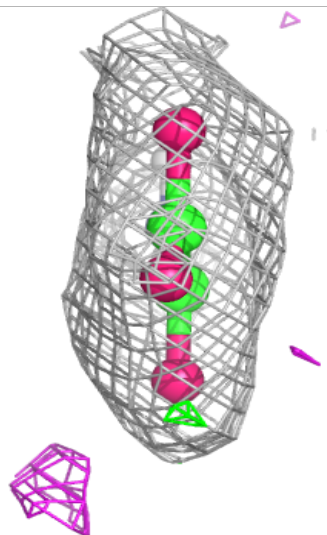
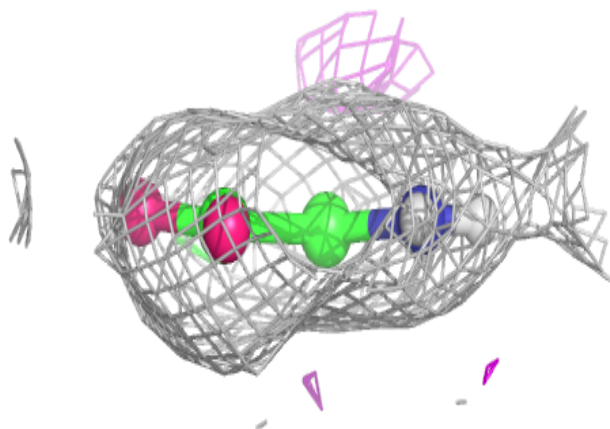
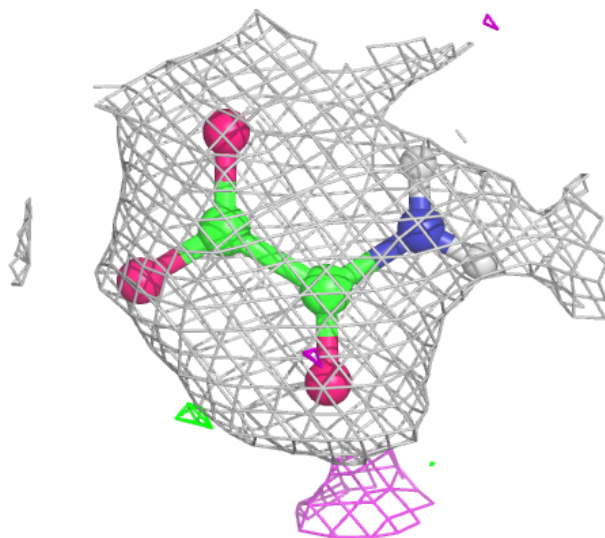
Electron density around OXM A 402:

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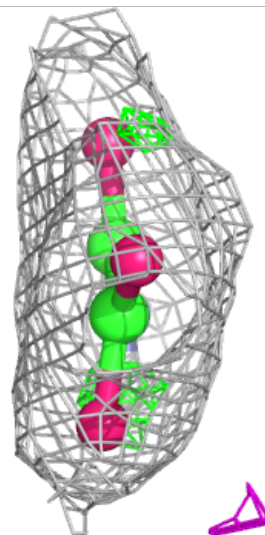
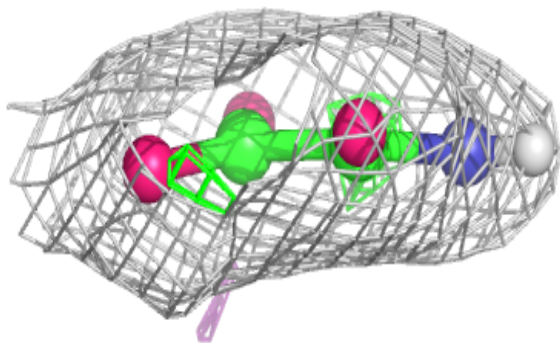
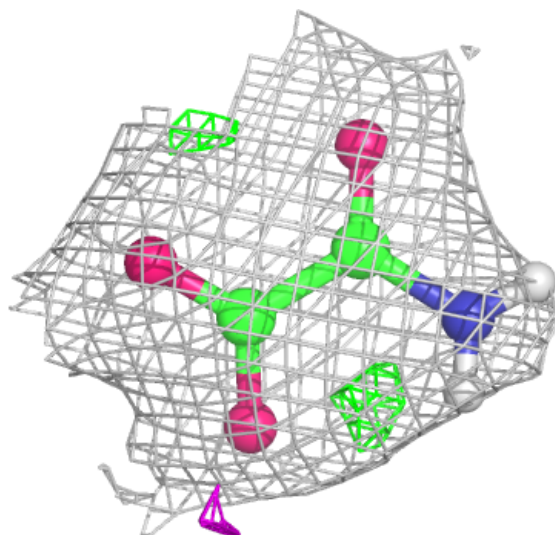
Electron density around OXM F 402:

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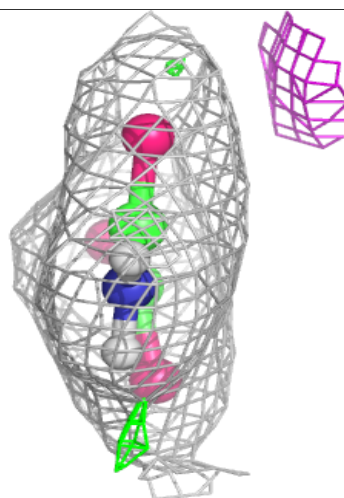
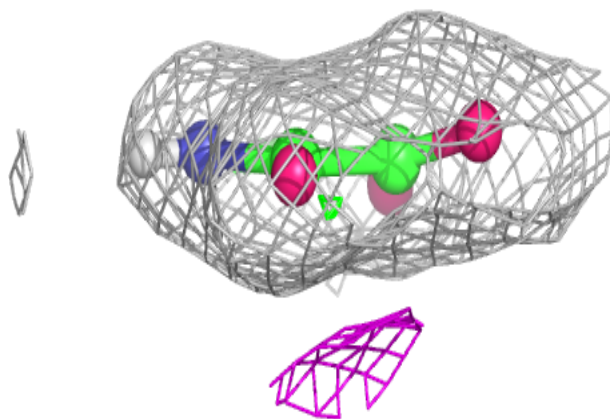
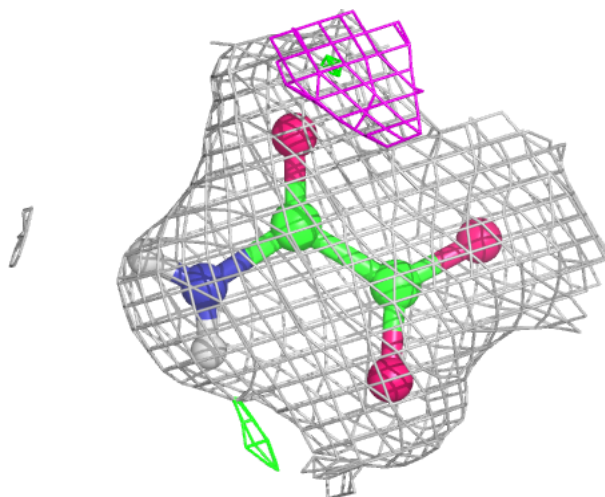
Electron density around OXM G 401:

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and green (positive)



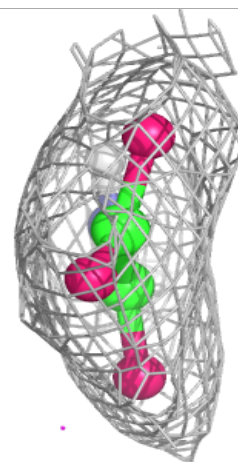
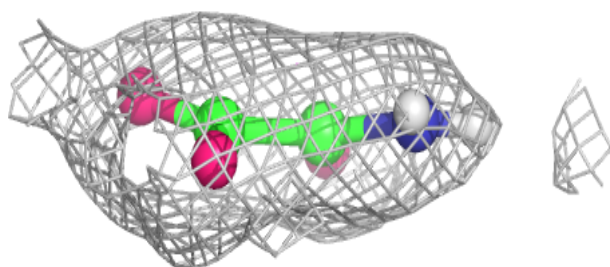
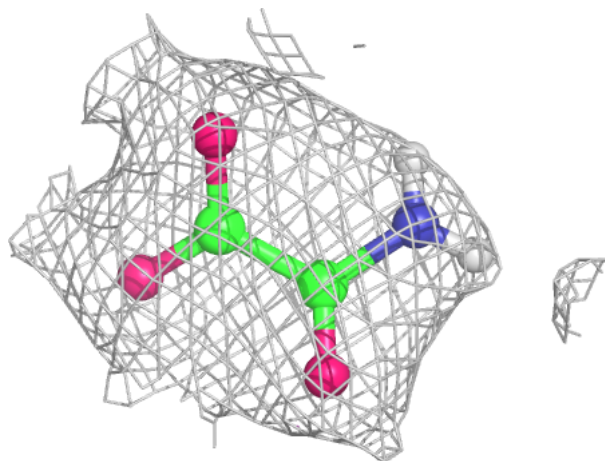
Electron density around OXM J 401:

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and green (positive)



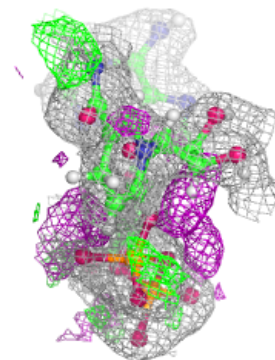
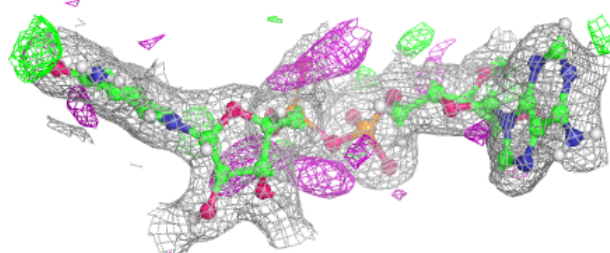
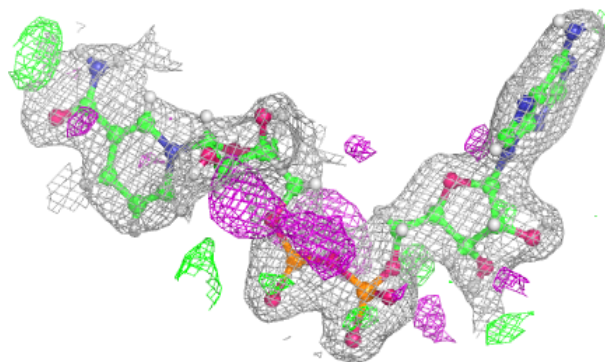
Electron density around OXM B 402:

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

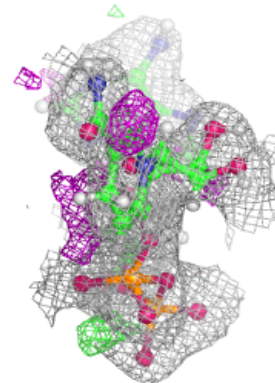
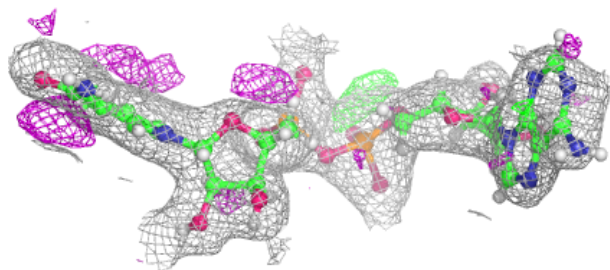
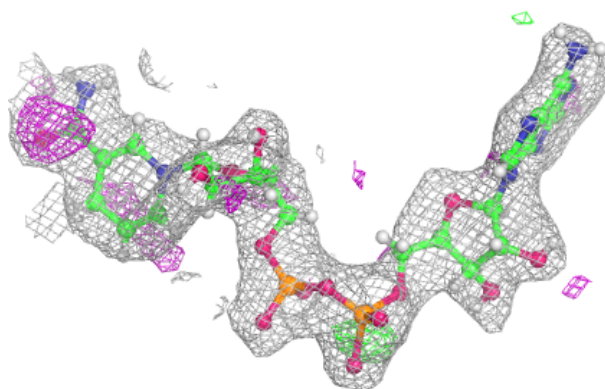


Electron density around NAI H 402:

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

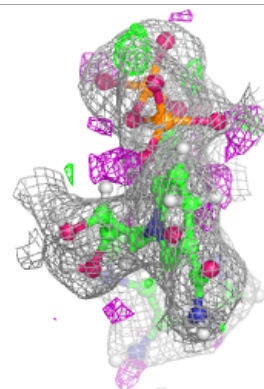
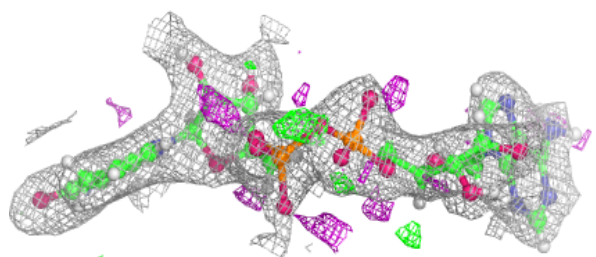
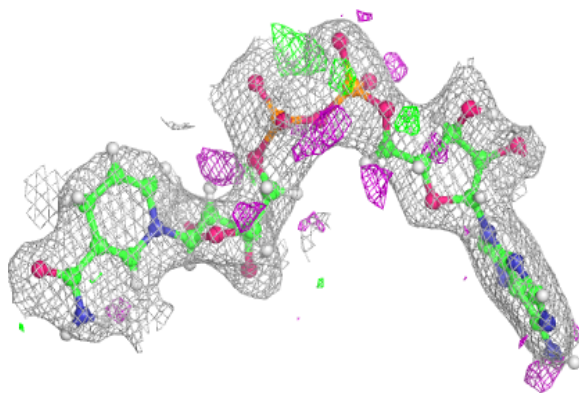
**Electron density around NAI J 402:**

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

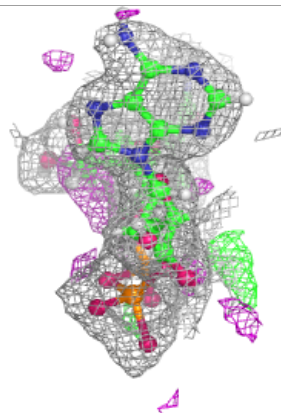
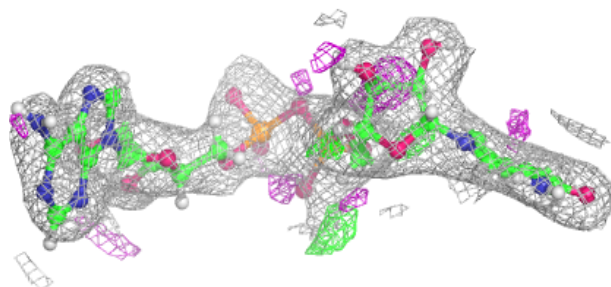
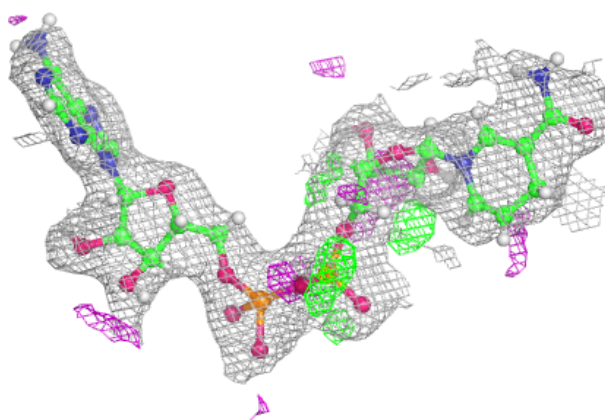


Electron density around NAI K 402:

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

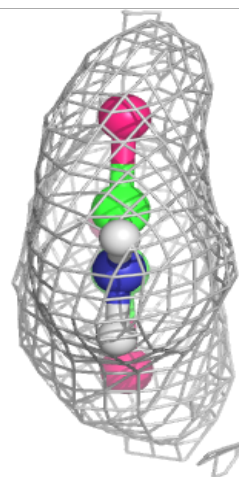
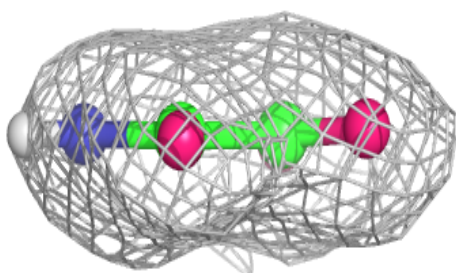
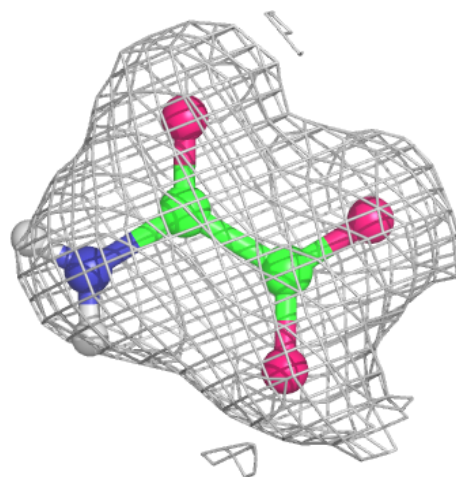
**Electron density around NAI L 402:**

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



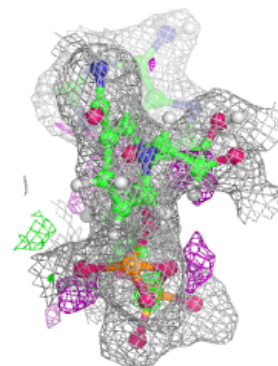
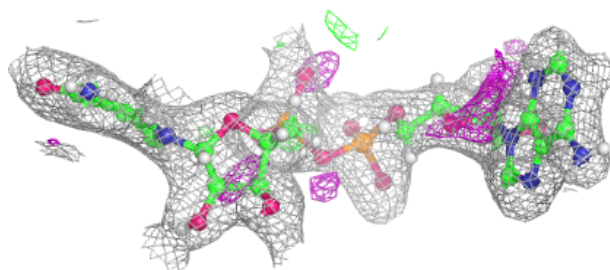
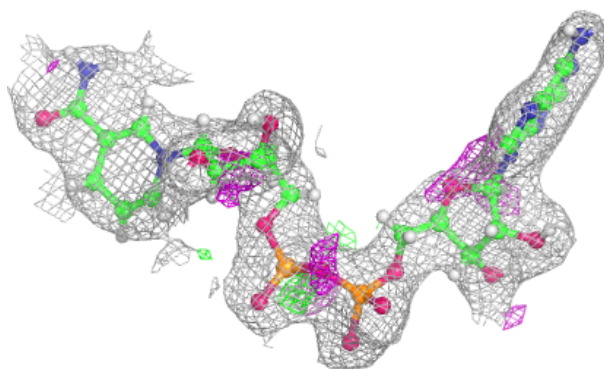
Electron density around OXM D 401:

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

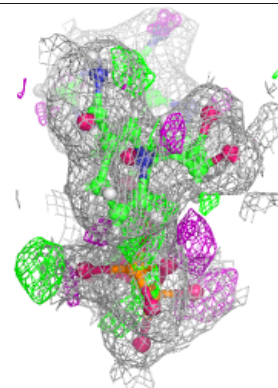
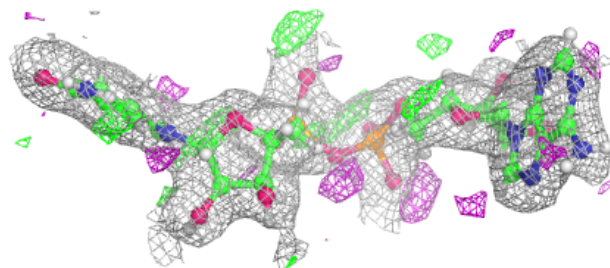
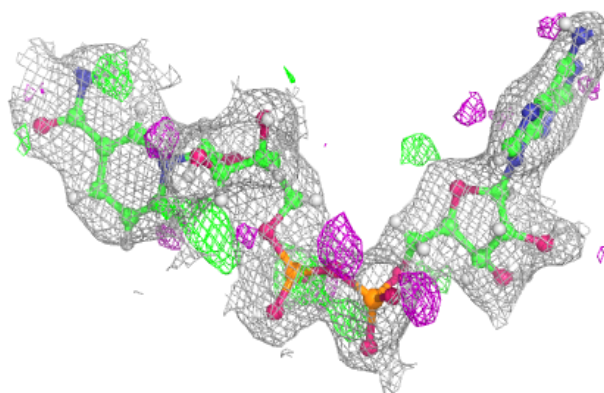


Electron density around NAI D 402:

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

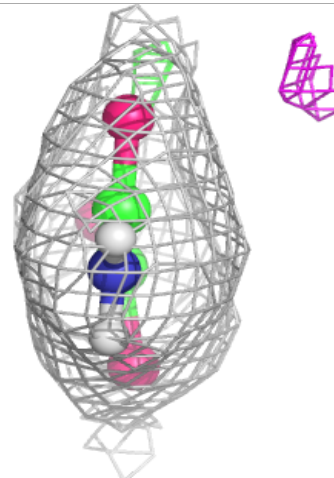
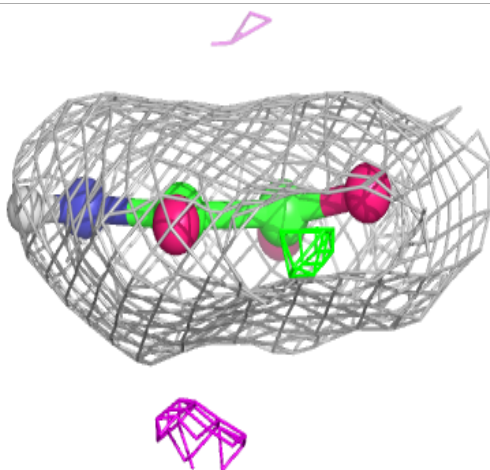
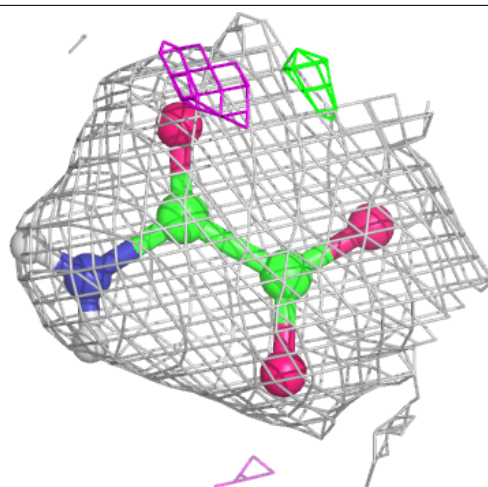
**Electron density around NAI C 403:**

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



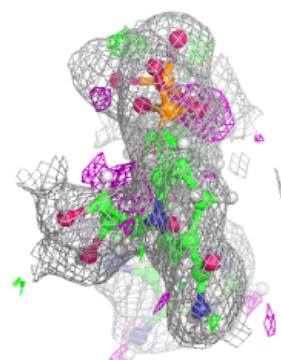
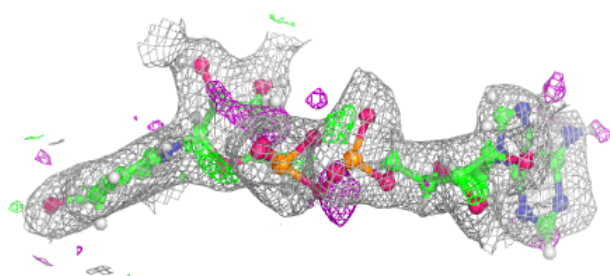
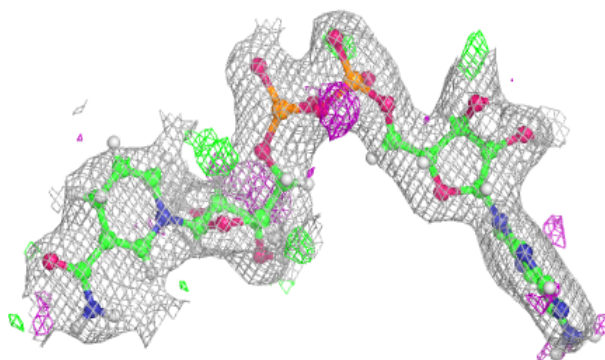
Electron density around OXM H 401:

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

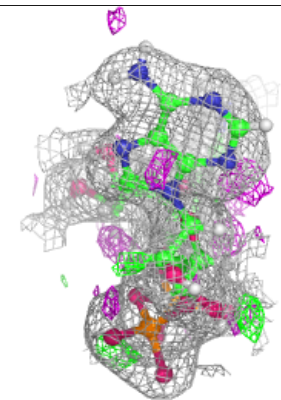
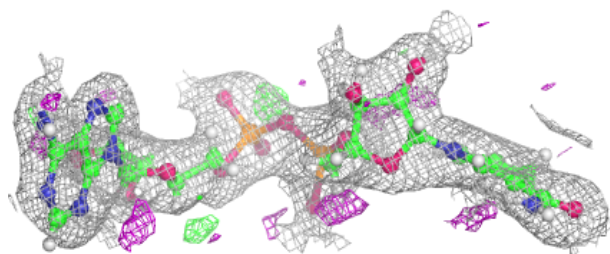
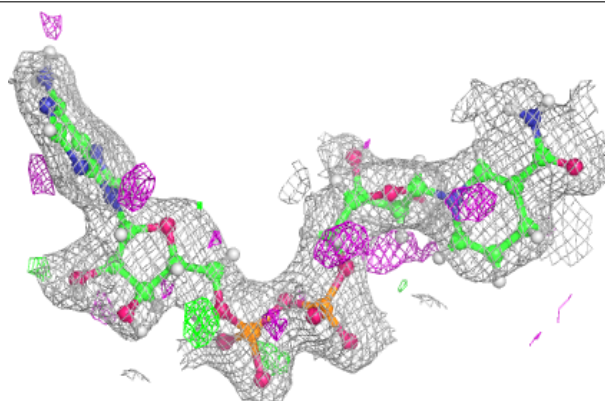


Electron density around NAI E 402:

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

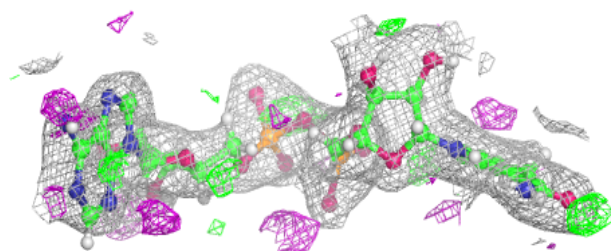
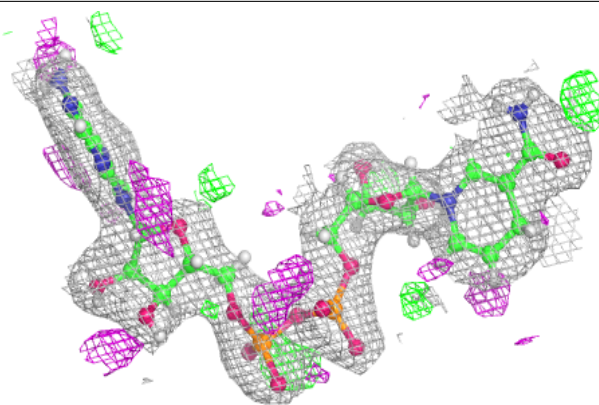
**Electron density around NAI A 403:**

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

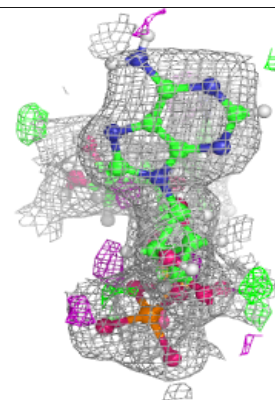
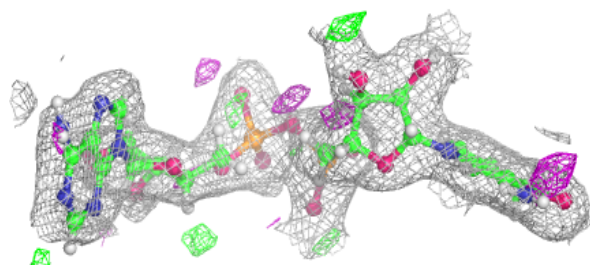
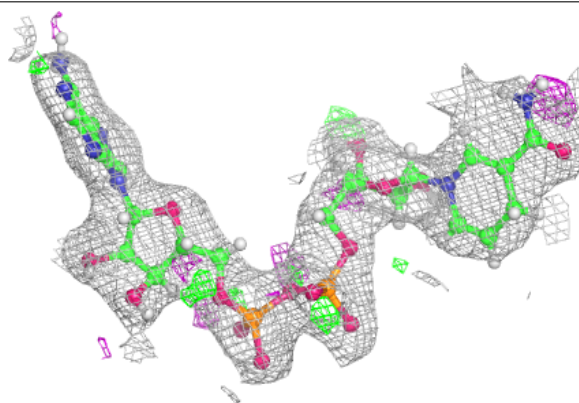


Electron density around NAI F 403:

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

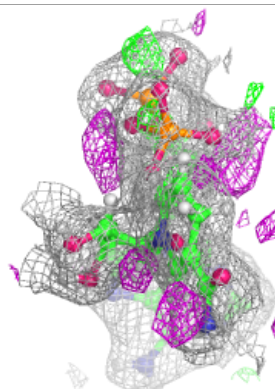
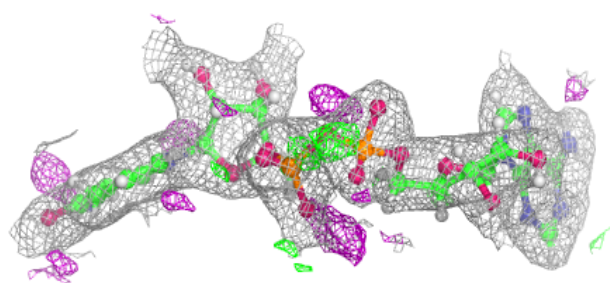
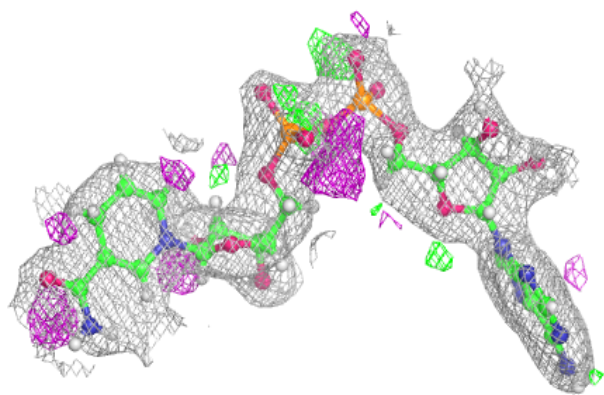
**Electron density around NAI G 402:**

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

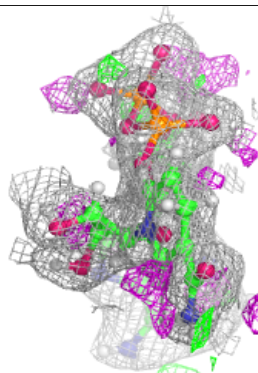
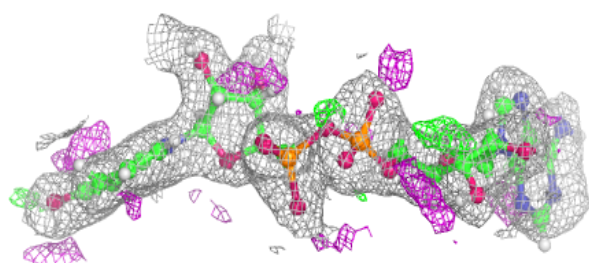
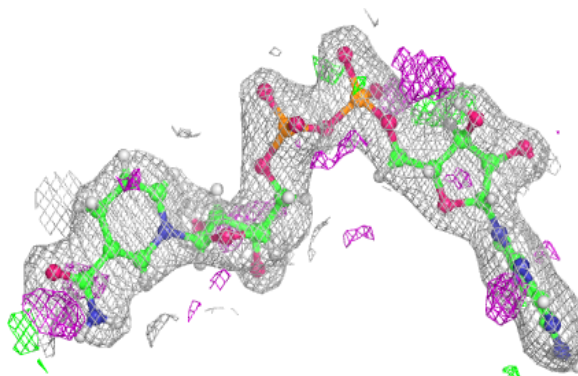


Electron density around NAI B 403:

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

**Electron density around NAI I 403:**

$2mF_o-DF_c$ (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.