



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2020 – 02:31 PM BST

PDB ID : 6Y6A
Title : Structure of Finch Polyomavirus VP1 in complex with 2-O-Methyl-5-N-acetyl-
l-alpha-D-neuraminic acid
Authors : Stroh, L.J.; Rustmeier, N.H.; Stehle, T.
Deposited on : 2020-02-26
Resolution : 2.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

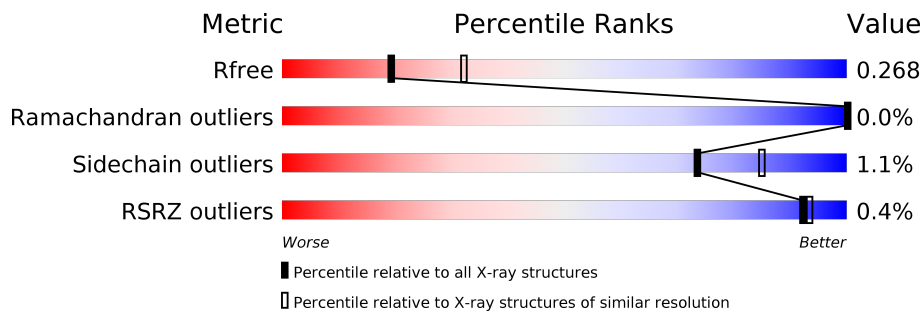
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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

Mol	Chain	Length	Quality of chain
1	A	274	96% . .
1	B	274	93% . 5%
1	C	274	96% . .
1	D	274	95% . 5%
1	E	274	96% .
1	F	274	96% . .
1	G	274	94% . 5%

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Mol	Chain	Length	Quality of chain
1	H	274	94% . 5%
1	I	274	97% ..
1	J	274	96% ..
1	K	274	96% ..
1	L	274	95% ..
1	M	274	97% ..
1	N	274	96% ..
1	O	274	95% ..
1	P	274	97% ..
1	Q	274	96% ..
1	R	274	95% ..
1	S	274	94% . 5%
1	T	274	95% ..
1	U	274	94% . 5%
1	V	274	% 96% ..
1	W	274	% 95% ..
1	X	274	95% . 5%
1	Y	274	95% . 5%
1	Z	274	94% . 5%
1	a	274	% 95% . 5%
1	b	274	93% . 5%
1	c	274	% 92% . 7%
1	d	274	93% . 5%
1	e	274	% 94% . 5%
1	f	274	94% . 5%

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Mol	Chain	Length	Quality of chain
1	g	274	<p>% 97% • •</p>
1	h	274	<p>95% • 5%</p>
1	i	274	<p>95% 5%</p>
1	j	274	<p>94% • 5%</p>
1	k	274	<p>3% 95% • •</p>
1	l	274	<p>4% 85% • 14%</p>
1	m	274	<p>2% 94% 5%</p>
1	n	274	<p>97% •</p>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 81587 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	267	Total 2024	C 1284	N 336	O 396	S 8	0	0	0
1	B	260	Total 1960	C 1245	N 327	O 380	S 8	0	0	0
1	C	267	Total 2028	C 1286	N 335	O 399	S 8	0	0	0
1	D	261	Total 1981	C 1257	N 331	O 385	S 8	0	0	0
1	E	263	Total 1978	C 1254	N 331	O 385	S 8	0	0	0
1	F	268	Total 2026	C 1287	N 336	O 395	S 8	0	0	0
1	G	260	Total 1961	C 1244	N 327	O 382	S 8	0	0	0
1	H	260	Total 1963	C 1247	N 328	O 380	S 8	0	0	0
1	I	268	Total 2023	C 1284	N 336	O 395	S 8	0	0	0
1	J	267	Total 2027	C 1285	N 335	O 399	S 8	0	0	0
1	K	267	Total 2022	C 1284	N 336	O 394	S 8	0	0	0
1	L	262	Total 1976	C 1253	N 329	O 386	S 8	0	0	0
1	M	269	Total 2024	C 1284	N 338	O 394	S 8	0	0	0
1	N	266	Total 2002	C 1268	N 334	O 392	S 8	0	0	0
1	O	262	Total 1975	C 1252	N 331	O 384	S 8	0	0	0
1	P	269	Total 2025	C 1284	N 338	O 395	S 8	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	268	Total 2018	C 1281	N 335	O 394	S 8	0	0	0
1	R	263	Total 1987	C 1259	N 332	O 388	S 8	0	0	0
1	S	261	Total 1971	C 1251	N 328	O 384	S 8	0	0	0
1	T	263	Total 1987	C 1261	N 330	O 388	S 8	0	0	0
1	U	261	Total 1974	C 1254	N 329	O 383	S 8	0	0	0
1	V	265	Total 1991	C 1262	N 334	O 387	S 8	0	0	0
1	W	262	Total 1965	C 1243	N 330	O 384	S 8	0	0	0
1	X	261	Total 1968	C 1245	N 329	O 386	S 8	0	0	0
1	Y	261	Total 1971	C 1253	N 330	O 380	S 8	0	0	0
1	Z	260	Total 1971	C 1249	N 330	O 384	S 8	0	0	0
1	a	261	Total 1981	C 1254	N 331	O 388	S 8	0	0	0
1	b	260	Total 1935	C 1229	N 325	O 373	S 8	0	0	0
1	c	256	Total 1903	C 1198	N 322	O 375	S 8	0	0	0
1	d	260	Total 1952	C 1236	N 326	O 382	S 8	0	0	0
1	e	261	Total 1972	C 1251	N 328	O 385	S 8	0	0	0
1	f	261	Total 1962	C 1241	N 328	O 385	S 8	0	0	0
1	g	269	Total 1984	C 1253	N 335	O 388	S 8	0	0	0
1	h	261	Total 1959	C 1243	N 326	O 382	S 8	0	0	0
1	i	260	Total 1949	C 1239	N 326	O 376	S 8	0	0	0
1	j	260	Total 1932	C 1224	N 324	O 376	S 8	0	0	0
1	k	263	Total 1822	C 1137	N 315	O 362	S 8	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	l	235	Total	C	N	O	S	0	0	0
			1571	992	275	298	6			
1	m	259	Total	C	N	O	S	0	0	0
			1834	1162	312	353	7			
1	n	267	Total	C	N	O	S	0	0	0
			1992	1262	333	389	8			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP R4UMH0
A	19	SER	-	expression tag	UNP R4UMH0
A	20	HIS	-	expression tag	UNP R4UMH0
A	21	MET	-	expression tag	UNP R4UMH0
A	78	SER	CYS	conflict	UNP R4UMH0
A	92	SER	CYS	conflict	UNP R4UMH0
B	18	GLY	-	expression tag	UNP R4UMH0
B	19	SER	-	expression tag	UNP R4UMH0
B	20	HIS	-	expression tag	UNP R4UMH0
B	21	MET	-	expression tag	UNP R4UMH0
B	78	SER	CYS	conflict	UNP R4UMH0
B	92	SER	CYS	conflict	UNP R4UMH0
C	18	GLY	-	expression tag	UNP R4UMH0
C	19	SER	-	expression tag	UNP R4UMH0
C	20	HIS	-	expression tag	UNP R4UMH0
C	21	MET	-	expression tag	UNP R4UMH0
C	78	SER	CYS	conflict	UNP R4UMH0
C	92	SER	CYS	conflict	UNP R4UMH0
D	18	GLY	-	expression tag	UNP R4UMH0
D	19	SER	-	expression tag	UNP R4UMH0
D	20	HIS	-	expression tag	UNP R4UMH0
D	21	MET	-	expression tag	UNP R4UMH0
D	78	SER	CYS	conflict	UNP R4UMH0
D	92	SER	CYS	conflict	UNP R4UMH0
E	18	GLY	-	expression tag	UNP R4UMH0
E	19	SER	-	expression tag	UNP R4UMH0
E	20	HIS	-	expression tag	UNP R4UMH0
E	21	MET	-	expression tag	UNP R4UMH0
E	78	SER	CYS	conflict	UNP R4UMH0
E	92	SER	CYS	conflict	UNP R4UMH0
F	18	GLY	-	expression tag	UNP R4UMH0
F	19	SER	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	20	HIS	-	expression tag	UNP R4UMH0
F	21	MET	-	expression tag	UNP R4UMH0
F	78	SER	CYS	conflict	UNP R4UMH0
F	92	SER	CYS	conflict	UNP R4UMH0
G	18	GLY	-	expression tag	UNP R4UMH0
G	19	SER	-	expression tag	UNP R4UMH0
G	20	HIS	-	expression tag	UNP R4UMH0
G	21	MET	-	expression tag	UNP R4UMH0
G	78	SER	CYS	conflict	UNP R4UMH0
G	92	SER	CYS	conflict	UNP R4UMH0
H	18	GLY	-	expression tag	UNP R4UMH0
H	19	SER	-	expression tag	UNP R4UMH0
H	20	HIS	-	expression tag	UNP R4UMH0
H	21	MET	-	expression tag	UNP R4UMH0
H	78	SER	CYS	conflict	UNP R4UMH0
H	92	SER	CYS	conflict	UNP R4UMH0
I	18	GLY	-	expression tag	UNP R4UMH0
I	19	SER	-	expression tag	UNP R4UMH0
I	20	HIS	-	expression tag	UNP R4UMH0
I	21	MET	-	expression tag	UNP R4UMH0
I	78	SER	CYS	conflict	UNP R4UMH0
I	92	SER	CYS	conflict	UNP R4UMH0
J	18	GLY	-	expression tag	UNP R4UMH0
J	19	SER	-	expression tag	UNP R4UMH0
J	20	HIS	-	expression tag	UNP R4UMH0
J	21	MET	-	expression tag	UNP R4UMH0
J	78	SER	CYS	conflict	UNP R4UMH0
J	92	SER	CYS	conflict	UNP R4UMH0
K	18	GLY	-	expression tag	UNP R4UMH0
K	19	SER	-	expression tag	UNP R4UMH0
K	20	HIS	-	expression tag	UNP R4UMH0
K	21	MET	-	expression tag	UNP R4UMH0
K	78	SER	CYS	conflict	UNP R4UMH0
K	92	SER	CYS	conflict	UNP R4UMH0
L	18	GLY	-	expression tag	UNP R4UMH0
L	19	SER	-	expression tag	UNP R4UMH0
L	20	HIS	-	expression tag	UNP R4UMH0
L	21	MET	-	expression tag	UNP R4UMH0
L	78	SER	CYS	conflict	UNP R4UMH0
L	92	SER	CYS	conflict	UNP R4UMH0
M	18	GLY	-	expression tag	UNP R4UMH0
M	19	SER	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
M	20	HIS	-	expression tag	UNP R4UMH0
M	21	MET	-	expression tag	UNP R4UMH0
M	78	SER	CYS	conflict	UNP R4UMH0
M	92	SER	CYS	conflict	UNP R4UMH0
N	18	GLY	-	expression tag	UNP R4UMH0
N	19	SER	-	expression tag	UNP R4UMH0
N	20	HIS	-	expression tag	UNP R4UMH0
N	21	MET	-	expression tag	UNP R4UMH0
N	78	SER	CYS	conflict	UNP R4UMH0
N	92	SER	CYS	conflict	UNP R4UMH0
O	18	GLY	-	expression tag	UNP R4UMH0
O	19	SER	-	expression tag	UNP R4UMH0
O	20	HIS	-	expression tag	UNP R4UMH0
O	21	MET	-	expression tag	UNP R4UMH0
O	78	SER	CYS	conflict	UNP R4UMH0
O	92	SER	CYS	conflict	UNP R4UMH0
P	18	GLY	-	expression tag	UNP R4UMH0
P	19	SER	-	expression tag	UNP R4UMH0
P	20	HIS	-	expression tag	UNP R4UMH0
P	21	MET	-	expression tag	UNP R4UMH0
P	78	SER	CYS	conflict	UNP R4UMH0
P	92	SER	CYS	conflict	UNP R4UMH0
Q	18	GLY	-	expression tag	UNP R4UMH0
Q	19	SER	-	expression tag	UNP R4UMH0
Q	20	HIS	-	expression tag	UNP R4UMH0
Q	21	MET	-	expression tag	UNP R4UMH0
Q	78	SER	CYS	conflict	UNP R4UMH0
Q	92	SER	CYS	conflict	UNP R4UMH0
R	18	GLY	-	expression tag	UNP R4UMH0
R	19	SER	-	expression tag	UNP R4UMH0
R	20	HIS	-	expression tag	UNP R4UMH0
R	21	MET	-	expression tag	UNP R4UMH0
R	78	SER	CYS	conflict	UNP R4UMH0
R	92	SER	CYS	conflict	UNP R4UMH0
S	18	GLY	-	expression tag	UNP R4UMH0
S	19	SER	-	expression tag	UNP R4UMH0
S	20	HIS	-	expression tag	UNP R4UMH0
S	21	MET	-	expression tag	UNP R4UMH0
S	78	SER	CYS	conflict	UNP R4UMH0
S	92	SER	CYS	conflict	UNP R4UMH0
T	18	GLY	-	expression tag	UNP R4UMH0
T	19	SER	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
T	20	HIS	-	expression tag	UNP R4UMH0
T	21	MET	-	expression tag	UNP R4UMH0
T	78	SER	CYS	conflict	UNP R4UMH0
T	92	SER	CYS	conflict	UNP R4UMH0
U	18	GLY	-	expression tag	UNP R4UMH0
U	19	SER	-	expression tag	UNP R4UMH0
U	20	HIS	-	expression tag	UNP R4UMH0
U	21	MET	-	expression tag	UNP R4UMH0
U	78	SER	CYS	conflict	UNP R4UMH0
U	92	SER	CYS	conflict	UNP R4UMH0
V	18	GLY	-	expression tag	UNP R4UMH0
V	19	SER	-	expression tag	UNP R4UMH0
V	20	HIS	-	expression tag	UNP R4UMH0
V	21	MET	-	expression tag	UNP R4UMH0
V	78	SER	CYS	conflict	UNP R4UMH0
V	92	SER	CYS	conflict	UNP R4UMH0
W	18	GLY	-	expression tag	UNP R4UMH0
W	19	SER	-	expression tag	UNP R4UMH0
W	20	HIS	-	expression tag	UNP R4UMH0
W	21	MET	-	expression tag	UNP R4UMH0
W	78	SER	CYS	conflict	UNP R4UMH0
W	92	SER	CYS	conflict	UNP R4UMH0
X	18	GLY	-	expression tag	UNP R4UMH0
X	19	SER	-	expression tag	UNP R4UMH0
X	20	HIS	-	expression tag	UNP R4UMH0
X	21	MET	-	expression tag	UNP R4UMH0
X	78	SER	CYS	conflict	UNP R4UMH0
X	92	SER	CYS	conflict	UNP R4UMH0
Y	18	GLY	-	expression tag	UNP R4UMH0
Y	19	SER	-	expression tag	UNP R4UMH0
Y	20	HIS	-	expression tag	UNP R4UMH0
Y	21	MET	-	expression tag	UNP R4UMH0
Y	78	SER	CYS	conflict	UNP R4UMH0
Y	92	SER	CYS	conflict	UNP R4UMH0
Z	18	GLY	-	expression tag	UNP R4UMH0
Z	19	SER	-	expression tag	UNP R4UMH0
Z	20	HIS	-	expression tag	UNP R4UMH0
Z	21	MET	-	expression tag	UNP R4UMH0
Z	78	SER	CYS	conflict	UNP R4UMH0
Z	92	SER	CYS	conflict	UNP R4UMH0
a	18	GLY	-	expression tag	UNP R4UMH0
a	19	SER	-	expression tag	UNP R4UMH0

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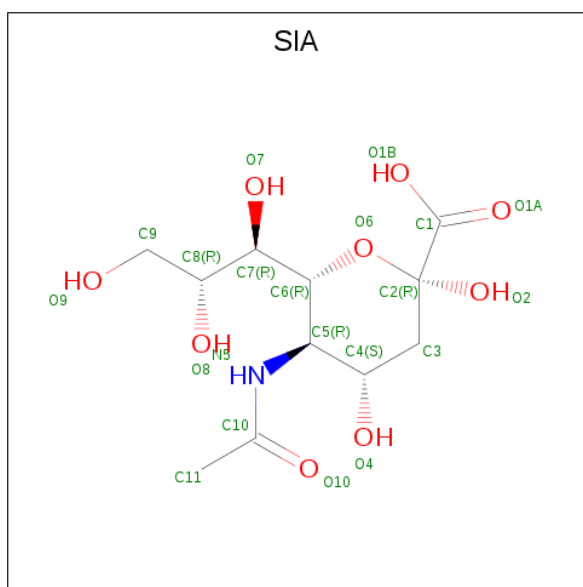
Chain	Residue	Modelled	Actual	Comment	Reference
a	20	HIS	-	expression tag	UNP R4UMH0
a	21	MET	-	expression tag	UNP R4UMH0
a	78	SER	CYS	conflict	UNP R4UMH0
a	92	SER	CYS	conflict	UNP R4UMH0
b	18	GLY	-	expression tag	UNP R4UMH0
b	19	SER	-	expression tag	UNP R4UMH0
b	20	HIS	-	expression tag	UNP R4UMH0
b	21	MET	-	expression tag	UNP R4UMH0
b	78	SER	CYS	conflict	UNP R4UMH0
b	92	SER	CYS	conflict	UNP R4UMH0
c	18	GLY	-	expression tag	UNP R4UMH0
c	19	SER	-	expression tag	UNP R4UMH0
c	20	HIS	-	expression tag	UNP R4UMH0
c	21	MET	-	expression tag	UNP R4UMH0
c	78	SER	CYS	conflict	UNP R4UMH0
c	92	SER	CYS	conflict	UNP R4UMH0
d	18	GLY	-	expression tag	UNP R4UMH0
d	19	SER	-	expression tag	UNP R4UMH0
d	20	HIS	-	expression tag	UNP R4UMH0
d	21	MET	-	expression tag	UNP R4UMH0
d	78	SER	CYS	conflict	UNP R4UMH0
d	92	SER	CYS	conflict	UNP R4UMH0
e	18	GLY	-	expression tag	UNP R4UMH0
e	19	SER	-	expression tag	UNP R4UMH0
e	20	HIS	-	expression tag	UNP R4UMH0
e	21	MET	-	expression tag	UNP R4UMH0
e	78	SER	CYS	conflict	UNP R4UMH0
e	92	SER	CYS	conflict	UNP R4UMH0
f	18	GLY	-	expression tag	UNP R4UMH0
f	19	SER	-	expression tag	UNP R4UMH0
f	20	HIS	-	expression tag	UNP R4UMH0
f	21	MET	-	expression tag	UNP R4UMH0
f	78	SER	CYS	conflict	UNP R4UMH0
f	92	SER	CYS	conflict	UNP R4UMH0
g	18	GLY	-	expression tag	UNP R4UMH0
g	19	SER	-	expression tag	UNP R4UMH0
g	20	HIS	-	expression tag	UNP R4UMH0
g	21	MET	-	expression tag	UNP R4UMH0
g	78	SER	CYS	conflict	UNP R4UMH0
g	92	SER	CYS	conflict	UNP R4UMH0
h	18	GLY	-	expression tag	UNP R4UMH0
h	19	SER	-	expression tag	UNP R4UMH0

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Chain	Residue	Modelled	Actual	Comment	Reference
h	20	HIS	-	expression tag	UNP R4UMH0
h	21	MET	-	expression tag	UNP R4UMH0
h	78	SER	CYS	conflict	UNP R4UMH0
h	92	SER	CYS	conflict	UNP R4UMH0
i	18	GLY	-	expression tag	UNP R4UMH0
i	19	SER	-	expression tag	UNP R4UMH0
i	20	HIS	-	expression tag	UNP R4UMH0
i	21	MET	-	expression tag	UNP R4UMH0
i	78	SER	CYS	conflict	UNP R4UMH0
i	92	SER	CYS	conflict	UNP R4UMH0
j	18	GLY	-	expression tag	UNP R4UMH0
j	19	SER	-	expression tag	UNP R4UMH0
j	20	HIS	-	expression tag	UNP R4UMH0
j	21	MET	-	expression tag	UNP R4UMH0
j	78	SER	CYS	conflict	UNP R4UMH0
j	92	SER	CYS	conflict	UNP R4UMH0
k	18	GLY	-	expression tag	UNP R4UMH0
k	19	SER	-	expression tag	UNP R4UMH0
k	20	HIS	-	expression tag	UNP R4UMH0
k	21	MET	-	expression tag	UNP R4UMH0
k	78	SER	CYS	conflict	UNP R4UMH0
k	92	SER	CYS	conflict	UNP R4UMH0
l	18	GLY	-	expression tag	UNP R4UMH0
l	19	SER	-	expression tag	UNP R4UMH0
l	20	HIS	-	expression tag	UNP R4UMH0
l	21	MET	-	expression tag	UNP R4UMH0
l	78	SER	CYS	conflict	UNP R4UMH0
l	92	SER	CYS	conflict	UNP R4UMH0
m	18	GLY	-	expression tag	UNP R4UMH0
m	19	SER	-	expression tag	UNP R4UMH0
m	20	HIS	-	expression tag	UNP R4UMH0
m	21	MET	-	expression tag	UNP R4UMH0
m	78	SER	CYS	conflict	UNP R4UMH0
m	92	SER	CYS	conflict	UNP R4UMH0
n	18	GLY	-	expression tag	UNP R4UMH0
n	19	SER	-	expression tag	UNP R4UMH0
n	20	HIS	-	expression tag	UNP R4UMH0
n	21	MET	-	expression tag	UNP R4UMH0
n	78	SER	CYS	conflict	UNP R4UMH0
n	92	SER	CYS	conflict	UNP R4UMH0

- Molecule 2 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: C₁₁H₁₉N₁O₉) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			21	11	1	9		
2	B	1	Total	C	N	O	0	0
			21	11	1	9		
2	C	1	Total	C	N	O	0	0
			21	11	1	9		
2	E	1	Total	C	N	O	0	0
			21	11	1	9		
2	F	1	Total	C	N	O	0	0
			21	11	1	9		
2	G	1	Total	C	N	O	0	0
			21	11	1	9		
2	I	1	Total	C	N	O	0	0
			21	11	1	9		
2	J	1	Total	C	N	O	0	0
			21	11	1	9		
2	K	1	Total	C	N	O	0	0
			21	11	1	9		
2	L	1	Total	C	N	O	0	0
			21	11	1	9		
2	M	1	Total	C	N	O	0	0
			21	11	1	9		
2	N	1	Total	C	N	O	0	0
			21	11	1	9		
2	O	1	Total	C	N	O	0	0
			21	11	1	9		
2	Q	1	Total	C	N	O	0	0
			21	11	1	9		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	R	1	Total	C	N	O	0	0
			21	11	1	9		
2	S	1	Total	C	N	O	0	0
			21	11	1	9		
2	T	1	Total	C	N	O	0	0
			21	11	1	9		
2	V	1	Total	C	N	O	0	0
			21	11	1	9		
2	X	1	Total	C	N	O	0	0
			21	11	1	9		
2	Y	1	Total	C	N	O	0	0
			21	11	1	9		
2	Z	1	Total	C	N	O	0	0
			21	11	1	9		
2	a	1	Total	C	N	O	0	0
			21	11	1	9		
2	b	1	Total	C	N	O	0	0
			21	11	1	9		
2	c	1	Total	C	N	O	0	0
			21	11	1	9		
2	d	1	Total	C	N	O	0	0
			21	11	1	9		
2	e	1	Total	C	N	O	0	0
			21	11	1	9		
2	f	1	Total	C	N	O	0	0
			21	11	1	9		
2	j	1	Total	C	N	O	0	0
			21	11	1	9		
2	n	1	Total	C	N	O	0	0
			21	11	1	9		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	2	Total	Cl	0	0
			2	2		
3	g	1	Total	Cl	0	0
			1	1		
3	h	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	c	1	Total Cl 1 1	0	0
3	W	2	Total Cl 2 2	0	0
3	N	2	Total Cl 2 2	0	0
3	X	2	Total Cl 2 2	0	0
3	S	2	Total Cl 2 2	0	0
3	f	2	Total Cl 2 2	0	0
3	J	2	Total Cl 2 2	0	0
3	V	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0
3	n	2	Total Cl 2 2	0	0
3	R	1	Total Cl 1 1	0	0
3	M	2	Total Cl 2 2	0	0
3	j	2	Total Cl 2 2	0	0
3	D	1	Total Cl 1 1	0	0
3	e	2	Total Cl 2 2	0	0
3	I	1	Total Cl 1 1	0	0
3	Z	2	Total Cl 2 2	0	0
3	U	2	Total Cl 2 2	0	0
3	L	1	Total Cl 1 1	0	0
3	G	2	Total Cl 2 2	0	0
3	Q	2	Total Cl 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	d	2	Total Cl 2 2	0	0
3	H	2	Total Cl 2 2	0	0
3	C	3	Total Cl 3 3	0	0
3	T	1	Total Cl 1 1	0	0
3	O	1	Total Cl 1 1	0	0
3	Y	2	Total Cl 2 2	0	0
3	F	2	Total Cl 2 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Mg 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	97	Total O 98 98	0	1
5	B	82	Total O 82 82	0	0
5	C	107	Total O 107 107	0	0
5	D	89	Total O 89 89	0	0
5	E	84	Total O 84 84	0	0
5	F	107	Total O 107 107	0	0
5	G	56	Total O 56 56	0	0
5	H	59	Total O 59 59	0	0
5	I	62	Total O 62 62	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	91	Total O 91 91	0	0
5	K	72	Total O 72 72	0	0
5	L	76	Total O 76 76	0	0
5	M	83	Total O 83 83	0	0
5	N	98	Total O 98 98	0	0
5	O	82	Total O 83 83	0	1
5	P	65	Total O 65 65	0	0
5	Q	79	Total O 79 79	0	0
5	R	81	Total O 81 81	0	0
5	S	55	Total O 55 55	0	0
5	T	67	Total O 68 68	0	1
5	U	83	Total O 83 83	0	0
5	V	43	Total O 43 43	0	0
5	W	41	Total O 41 41	0	0
5	X	40	Total O 40 40	0	0
5	Y	67	Total O 67 67	0	0
5	Z	63	Total O 63 63	0	0
5	a	47	Total O 47 47	0	0
5	b	30	Total O 30 30	0	0
5	c	34	Total O 34 34	0	0
5	d	46	Total O 46 46	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	e	50	Total 50	O 50	0	0
5	f	33	Total 33	O 33	0	0
5	g	34	Total 34	O 34	0	0
5	h	32	Total 32	O 32	0	0
5	i	39	Total 39	O 39	0	0
5	j	25	Total 25	O 25	0	0
5	k	15	Total 15	O 15	0	0
5	l	15	Total 15	O 15	0	0
5	m	11	Total 11	O 11	0	0
5	n	35	Total 35	O 35	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: Capsid protein VP1

Chain A:  96%



- Molecule 1: Capsid protein VP1

Chain B:  93% 5%



- Molecule 1: Capsid protein VP1

Chain C:  96%



- Molecule 1: Capsid protein VP1

Chain D:  95% 5%



- Molecule 1: Capsid protein VP1

Chain E:  96%



- Molecule 1: Capsid protein VP1

Chain F:  96%



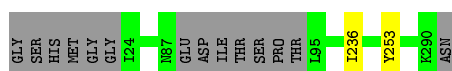
- Molecule 1: Capsid protein VP1

Chain G: 94% 5%



- Molecule 1: Capsid protein VP1

Chain H: 94% 5%



- Molecule 1: Capsid protein VP1

Chain I: 97% ..



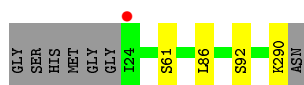
- Molecule 1: Capsid protein VP1

Chain J: 96% ..



- Molecule 1: Capsid protein VP1

Chain K: 96% ..



- Molecule 1: Capsid protein VP1

Chain L: 95% ..



- Molecule 1: Capsid protein VP1

Chain M: 97% ..



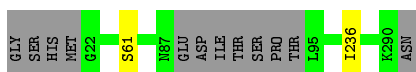
- Molecule 1: Capsid protein VP1

Chain N: 96%



- Molecule 1: Capsid protein VP1

Chain O: 95%



- Molecule 1: Capsid protein VP1

Chain P: 97%



- Molecule 1: Capsid protein VP1

Chain Q: 96%



- Molecule 1: Capsid protein VP1

Chain R: 95%



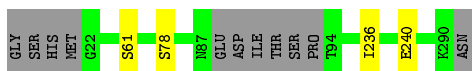
- Molecule 1: Capsid protein VP1

Chain S: 94%

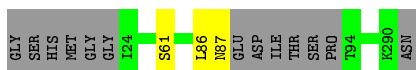


- Molecule 1: Capsid protein VP1

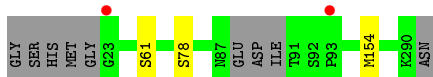
Chain T: 95%



● Molecule 1: Capsid protein VP1



● Molecule 1: Capsid protein VP1



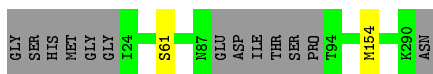
● Molecule 1: Capsid protein VP1



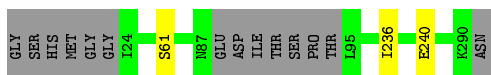
● Molecule 1: Capsid protein VP1



● Molecule 1: Capsid protein VP1

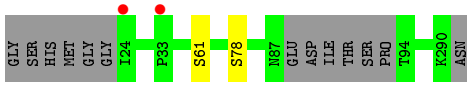


● Molecule 1: Capsid protein VP1



● Molecule 1: Capsid protein VP1

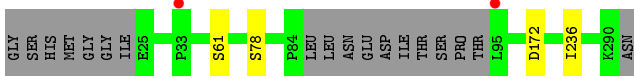
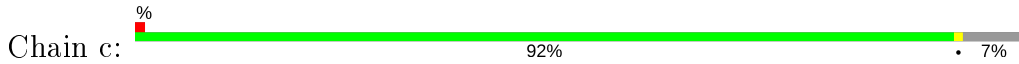




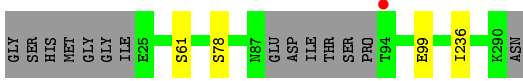
● Molecule 1: Capsid protein VP1



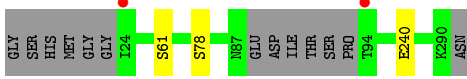
● Molecule 1: Capsid protein VP1



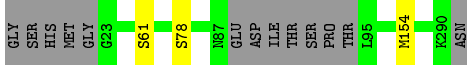
● Molecule 1: Capsid protein VP1



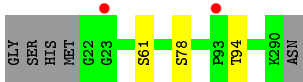
● Molecule 1: Capsid protein VP1



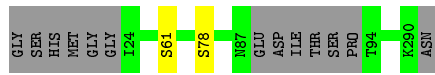
● Molecule 1: Capsid protein VP1



● Molecule 1: Capsid protein VP1



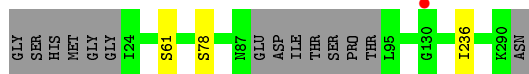
● Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1



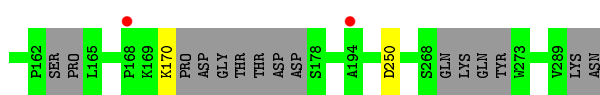
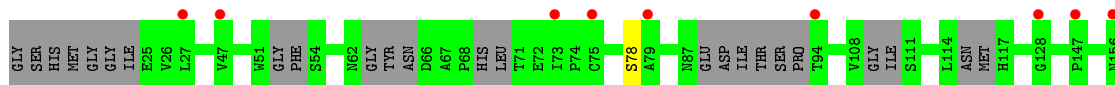
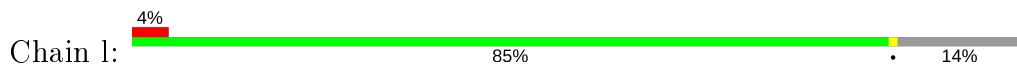
• Molecule 1: Capsid protein VP1



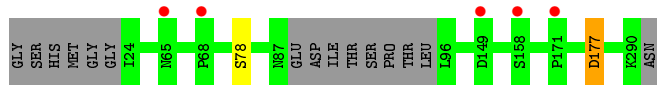
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1



GLY	GLY
SER	SER
HIS	HIS
MET	MET
GLY	GLY
GLY	GLY
I24	I24
M154	M154
K290	K290
ASN	ASN

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	86.50Å 172.06Å 245.62Å 107.09° 97.93° 93.93°	Depositor
Resolution (Å)	49.94 – 2.65 49.94 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.7 (49.94-2.65) 98.0 (49.94-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.65Å)	Xtrriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.245 , 0.267 0.246 , 0.268	Depositor DCC
R_{free} test set	3778 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtrriage
Anisotropy	0.841	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,h+k+l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	81587	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: SIA, MG, CL

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	0.68	1/2077 (0.0%)	0.82	1/2842 (0.0%)
1	B	0.64	0/2011	0.77	1/2749 (0.0%)
1	C	0.69	2/2081 (0.1%)	0.79	0/2846
1	D	0.64	0/2032	0.75	0/2775
1	E	0.64	0/2029	0.76	0/2772
1	F	0.67	1/2079 (0.0%)	0.79	1/2843 (0.0%)
1	G	0.65	1/2012 (0.0%)	0.75	0/2751
1	H	0.65	0/2014	0.77	2/2753 (0.1%)
1	I	0.66	0/2076	0.78	0/2840
1	J	0.65	1/2080 (0.0%)	0.75	0/2845
1	K	0.67	0/2075	0.80	2/2839 (0.1%)
1	L	0.63	0/2027	0.75	0/2770
1	M	0.70	1/2077 (0.0%)	0.79	0/2840
1	N	0.66	0/2053	0.77	0/2806
1	O	0.64	0/2026	0.76	0/2767
1	P	0.67	0/2078	0.77	0/2843
1	Q	0.68	2/2071 (0.1%)	0.77	0/2833
1	R	0.66	1/2038 (0.0%)	0.76	0/2784
1	S	0.63	0/2022	0.76	2/2763 (0.1%)
1	T	0.64	0/2038	0.75	0/2783
1	U	0.66	1/2025 (0.0%)	0.77	0/2767
1	V	0.66	0/2043	0.76	0/2793
1	W	0.68	2/2016 (0.1%)	0.76	0/2756
1	X	0.64	0/2019	0.75	0/2760
1	Y	0.63	0/2022	0.75	0/2763
1	Z	0.63	0/2022	0.74	0/2761
1	a	0.63	0/2032	0.74	0/2774
1	b	0.69	3/1986 (0.2%)	0.81	2/2717 (0.1%)
1	c	0.64	0/1952	0.77	1/2667 (0.0%)
1	d	0.64	0/2003	0.78	1/2738 (0.0%)
1	e	0.64	0/2023	0.74	0/2766
1	f	0.64	0/2013	0.75	0/2752

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	g	0.68	1/2036 (0.0%)	0.78	0/2788
1	h	0.64	0/2009	0.75	0/2746
1	i	0.64	0/2000	0.76	0/2734
1	j	0.64	0/1982	0.76	0/2712
1	k	0.71	1/1863 (0.1%)	0.81	0/2558
1	l	0.70	0/1599	0.79	1/2188 (0.0%)
1	m	0.66	0/1882	0.77	1/2584 (0.0%)
1	n	0.65	0/2045	0.77	0/2800
All	All	0.66	18/80568 (0.0%)	0.77	15/110168 (0.0%)

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	94	THR	C-O	7.24	1.37	1.23
1	b	287	ARG	CD-NE	-7.14	1.34	1.46
1	Q	87	ASN	C-O	6.88	1.36	1.23
1	k	94	THR	C-O	6.24	1.35	1.23
1	b	72	GLU	CD-OE1	-6.12	1.19	1.25

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	287	ARG	CB-CG-CD	-11.60	81.43	111.60
1	d	99	GLU	CG-CD-OE2	-8.32	101.66	118.30
1	K	290	LYS	CB-CA-C	-8.10	94.20	110.40
1	b	287	ARG	CG-CD-NE	7.42	127.37	111.80
1	H	253	TYR	CB-CG-CD1	6.79	125.07	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	265/274 (97%)	257 (97%)	8 (3%)	0	100	100
1	B	256/274 (93%)	248 (97%)	8 (3%)	0	100	100
1	C	265/274 (97%)	256 (97%)	9 (3%)	0	100	100
1	D	257/274 (94%)	249 (97%)	8 (3%)	0	100	100
1	E	259/274 (94%)	251 (97%)	8 (3%)	0	100	100
1	F	266/274 (97%)	257 (97%)	9 (3%)	0	100	100
1	G	256/274 (93%)	248 (97%)	8 (3%)	0	100	100
1	H	256/274 (93%)	248 (97%)	8 (3%)	0	100	100
1	I	266/274 (97%)	258 (97%)	8 (3%)	0	100	100
1	J	265/274 (97%)	256 (97%)	9 (3%)	0	100	100
1	K	265/274 (97%)	257 (97%)	8 (3%)	0	100	100
1	L	258/274 (94%)	250 (97%)	8 (3%)	0	100	100
1	M	267/274 (97%)	257 (96%)	9 (3%)	1 (0%)	34	48
1	N	262/274 (96%)	253 (97%)	9 (3%)	0	100	100
1	O	258/274 (94%)	250 (97%)	8 (3%)	0	100	100
1	P	267/274 (97%)	259 (97%)	8 (3%)	0	100	100
1	Q	266/274 (97%)	257 (97%)	9 (3%)	0	100	100
1	R	259/274 (94%)	252 (97%)	7 (3%)	0	100	100
1	S	257/274 (94%)	249 (97%)	8 (3%)	0	100	100
1	T	259/274 (94%)	251 (97%)	8 (3%)	0	100	100
1	U	257/274 (94%)	249 (97%)	8 (3%)	0	100	100
1	V	261/274 (95%)	253 (97%)	8 (3%)	0	100	100
1	W	258/274 (94%)	250 (97%)	8 (3%)	0	100	100
1	X	257/274 (94%)	249 (97%)	8 (3%)	0	100	100
1	Y	257/274 (94%)	249 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	256/274 (93%)	248 (97%)	8 (3%)	0	100	100
1	a	257/274 (94%)	249 (97%)	8 (3%)	0	100	100
1	b	256/274 (93%)	248 (97%)	8 (3%)	0	100	100
1	c	252/274 (92%)	244 (97%)	8 (3%)	0	100	100
1	d	256/274 (93%)	248 (97%)	8 (3%)	0	100	100
1	e	257/274 (94%)	249 (97%)	8 (3%)	0	100	100
1	f	257/274 (94%)	249 (97%)	8 (3%)	0	100	100
1	g	267/274 (97%)	259 (97%)	8 (3%)	0	100	100
1	h	257/274 (94%)	248 (96%)	9 (4%)	0	100	100
1	i	256/274 (93%)	248 (97%)	8 (3%)	0	100	100
1	j	256/274 (93%)	248 (97%)	8 (3%)	0	100	100
1	k	259/274 (94%)	250 (96%)	9 (4%)	0	100	100
1	l	215/274 (78%)	207 (96%)	8 (4%)	0	100	100
1	m	255/274 (93%)	247 (97%)	8 (3%)	0	100	100
1	n	265/274 (97%)	257 (97%)	8 (3%)	0	100	100
All	All	10340/10960 (94%)	10012 (97%)	327 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	92	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/233 (94%)	214 (98%)	4 (2%)	59	75
1	B	206/233 (88%)	202 (98%)	4 (2%)	57	74
1	C	220/233 (94%)	218 (99%)	2 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	213/233 (91%)	211 (99%)	2 (1%)	78	87
1	E	208/233 (89%)	207 (100%)	1 (0%)	88	94
1	F	217/233 (93%)	214 (99%)	3 (1%)	67	81
1	G	208/233 (89%)	206 (99%)	2 (1%)	76	86
1	H	207/233 (89%)	206 (100%)	1 (0%)	88	94
1	I	216/233 (93%)	214 (99%)	2 (1%)	78	87
1	J	220/233 (94%)	218 (99%)	2 (1%)	78	87
1	K	217/233 (93%)	215 (99%)	2 (1%)	78	87
1	L	209/233 (90%)	207 (99%)	2 (1%)	76	86
1	M	215/233 (92%)	213 (99%)	2 (1%)	78	87
1	N	212/233 (91%)	209 (99%)	3 (1%)	67	81
1	O	210/233 (90%)	208 (99%)	2 (1%)	76	86
1	P	215/233 (92%)	212 (99%)	3 (1%)	67	81
1	Q	213/233 (91%)	210 (99%)	3 (1%)	67	81
1	R	213/233 (91%)	211 (99%)	2 (1%)	78	87
1	S	209/233 (90%)	206 (99%)	3 (1%)	67	81
1	T	211/233 (91%)	207 (98%)	4 (2%)	57	74
1	U	210/233 (90%)	208 (99%)	2 (1%)	76	86
1	V	210/233 (90%)	207 (99%)	3 (1%)	67	81
1	W	206/233 (88%)	205 (100%)	1 (0%)	88	94
1	X	210/233 (90%)	208 (99%)	2 (1%)	76	86
1	Y	209/233 (90%)	207 (99%)	2 (1%)	76	86
1	Z	211/233 (91%)	208 (99%)	3 (1%)	67	81
1	a	213/233 (91%)	211 (99%)	2 (1%)	78	87
1	b	196/233 (84%)	193 (98%)	3 (2%)	65	80
1	c	196/233 (84%)	193 (98%)	3 (2%)	65	80
1	d	205/233 (88%)	202 (98%)	3 (2%)	65	80
1	e	210/233 (90%)	207 (99%)	3 (1%)	67	81
1	f	207/233 (89%)	204 (99%)	3 (1%)	67	81
1	g	201/233 (86%)	199 (99%)	2 (1%)	76	86
1	h	205/233 (88%)	203 (99%)	2 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	i	202/233 (87%)	202 (100%)	0	100	100
1	j	201/233 (86%)	198 (98%)	3 (2%)	65	80
1	k	168/233 (72%)	165 (98%)	3 (2%)	59	75
1	l	129/233 (55%)	127 (98%)	2 (2%)	62	78
1	m	174/233 (75%)	172 (99%)	2 (1%)	73	85
1	n	206/233 (88%)	205 (100%)	1 (0%)	88	94
All	All	8226/9320 (88%)	8132 (99%)	94 (1%)	73	85

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	61	SER
1	V	78	SER
1	k	61	SER
1	S	78	SER
1	T	236	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	269	GLN
1	X	65	ASN
1	n	269	GLN
1	Q	265	GLN
1	S	265	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 83 ligands modelled in this entry, 54 are monoatomic - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	M	401	-	18,21,21	0.99	1 (5%)	21,31,31	1.03	1 (4%)
2	SIA	V	401	-	18,21,21	1.49	4 (22%)	21,31,31	1.64	3 (14%)
2	SIA	e	401	-	18,21,21	1.20	2 (11%)	21,31,31	1.33	4 (19%)
2	SIA	a	401	-	18,21,21	1.40	4 (22%)	21,31,31	1.63	4 (19%)
2	SIA	N	401	-	18,21,21	1.15	2 (11%)	21,31,31	1.15	1 (4%)
2	SIA	d	401	-	18,21,21	1.02	1 (5%)	21,31,31	0.96	1 (4%)
2	SIA	K	401	-	18,21,21	1.09	1 (5%)	21,31,31	1.15	1 (4%)
2	SIA	Z	401	-	18,21,21	1.30	3 (16%)	21,31,31	1.64	3 (14%)
2	SIA	C	401	-	18,21,21	0.93	1 (5%)	21,31,31	0.95	0
2	SIA	L	401	-	18,21,21	0.93	1 (5%)	21,31,31	0.81	0
2	SIA	n	401	-	18,21,21	0.85	1 (5%)	21,31,31	1.13	1 (4%)
2	SIA	F	401	-	18,21,21	0.90	1 (5%)	21,31,31	1.40	5 (23%)
2	SIA	Q	401	-	18,21,21	1.36	2 (11%)	21,31,31	1.38	3 (14%)
2	SIA	G	401	-	18,21,21	1.21	1 (5%)	21,31,31	1.44	4 (19%)
2	SIA	T	401	-	18,21,21	1.12	2 (11%)	21,31,31	1.10	2 (9%)
2	SIA	I	401	-	18,21,21	0.90	2 (11%)	21,31,31	1.46	4 (19%)
2	SIA	c	401	-	18,21,21	1.11	1 (5%)	21,31,31	1.11	2 (9%)
2	SIA	J	401	-	18,21,21	1.29	3 (16%)	21,31,31	1.03	1 (4%)
2	SIA	Y	401	-	18,21,21	1.04	2 (11%)	21,31,31	1.04	1 (4%)
2	SIA	f	401	-	18,21,21	1.12	3 (16%)	21,31,31	1.03	1 (4%)
2	SIA	B	401	-	18,21,21	1.13	2 (11%)	21,31,31	1.16	2 (9%)
2	SIA	O	401	-	18,21,21	1.21	2 (11%)	21,31,31	1.85	6 (28%)
2	SIA	X	401	-	18,21,21	1.17	2 (11%)	21,31,31	1.10	2 (9%)
2	SIA	E	401	-	18,21,21	0.95	1 (5%)	21,31,31	1.11	1 (4%)
2	SIA	R	401	-	18,21,21	1.23	3 (16%)	21,31,31	1.34	3 (14%)
2	SIA	A	401	-	18,21,21	1.26	2 (11%)	21,31,31	1.37	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	j	401	-	18,21,21	1.31	3 (16%)	21,31,31	1.23	1 (4%)
2	SIA	S	401	-	18,21,21	1.04	1 (5%)	21,31,31	1.38	1 (4%)
2	SIA	b	401	-	18,21,21	0.97	2 (11%)	21,31,31	1.07	1 (4%)

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	SIA	M	401	-	-	4/14/38/38	0/1/1/1
2	SIA	V	401	-	-	2/14/38/38	0/1/1/1
2	SIA	e	401	-	-	6/14/38/38	0/1/1/1
2	SIA	a	401	-	-	4/14/38/38	0/1/1/1
2	SIA	N	401	-	-	4/14/38/38	0/1/1/1
2	SIA	d	401	-	-	2/14/38/38	0/1/1/1
2	SIA	K	401	-	-	4/14/38/38	0/1/1/1
2	SIA	Z	401	-	-	4/14/38/38	0/1/1/1
2	SIA	C	401	-	-	4/14/38/38	0/1/1/1
2	SIA	L	401	-	-	0/14/38/38	0/1/1/1
2	SIA	n	401	-	-	7/14/38/38	0/1/1/1
2	SIA	F	401	-	-	4/14/38/38	0/1/1/1
2	SIA	Q	401	-	-	1/14/38/38	0/1/1/1
2	SIA	G	401	-	-	4/14/38/38	0/1/1/1
2	SIA	T	401	-	-	2/14/38/38	0/1/1/1
2	SIA	I	401	-	-	4/14/38/38	0/1/1/1
2	SIA	c	401	-	-	2/14/38/38	0/1/1/1
2	SIA	J	401	-	-	6/14/38/38	0/1/1/1
2	SIA	Y	401	-	-	6/14/38/38	0/1/1/1
2	SIA	f	401	-	-	2/14/38/38	0/1/1/1
2	SIA	B	401	-	-	6/14/38/38	0/1/1/1
2	SIA	O	401	-	-	3/14/38/38	0/1/1/1
2	SIA	X	401	-	-	6/14/38/38	0/1/1/1
2	SIA	E	401	-	-	2/14/38/38	0/1/1/1
2	SIA	R	401	-	-	4/14/38/38	0/1/1/1
2	SIA	A	401	-	-	2/14/38/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	j	401	-	-	6/14/38/38	0/1/1/1
2	SIA	S	401	-	-	6/14/38/38	0/1/1/1
2	SIA	b	401	-	-	6/14/38/38	0/1/1/1

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	401	SIA	O2-C2	3.77	1.45	1.39
2	G	401	SIA	O2-C2	3.75	1.44	1.39
2	V	401	SIA	O2-C2	3.64	1.44	1.39
2	j	401	SIA	O2-C2	3.60	1.44	1.39
2	E	401	SIA	O2-C2	3.54	1.44	1.39

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	401	SIA	C3-C4-C5	5.24	118.04	109.98
2	O	401	SIA	C3-C4-C5	4.61	117.06	109.98
2	V	401	SIA	C3-C4-C5	4.47	116.86	109.98
2	S	401	SIA	C3-C4-C5	4.18	116.40	109.98
2	O	401	SIA	O6-C6-C5	-3.86	106.02	109.78

There are no chirality outliers.

5 of 113 torsion outliers are listed below:

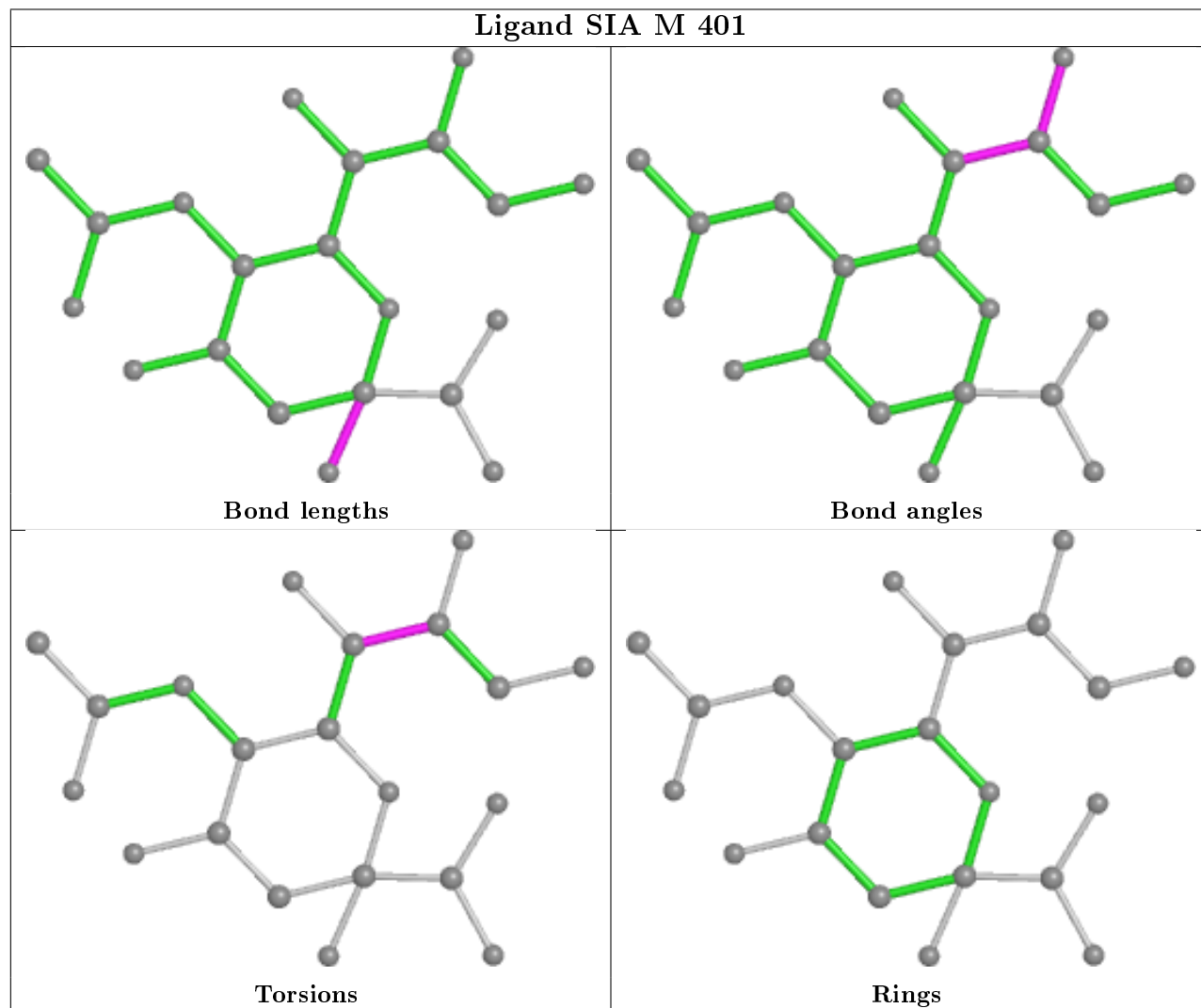
Mol	Chain	Res	Type	Atoms
2	M	401	SIA	C6-C7-C8-C9
2	M	401	SIA	C6-C7-C8-O8
2	M	401	SIA	O7-C7-C8-C9
2	M	401	SIA	O7-C7-C8-O8
2	V	401	SIA	O8-C8-C9-O9

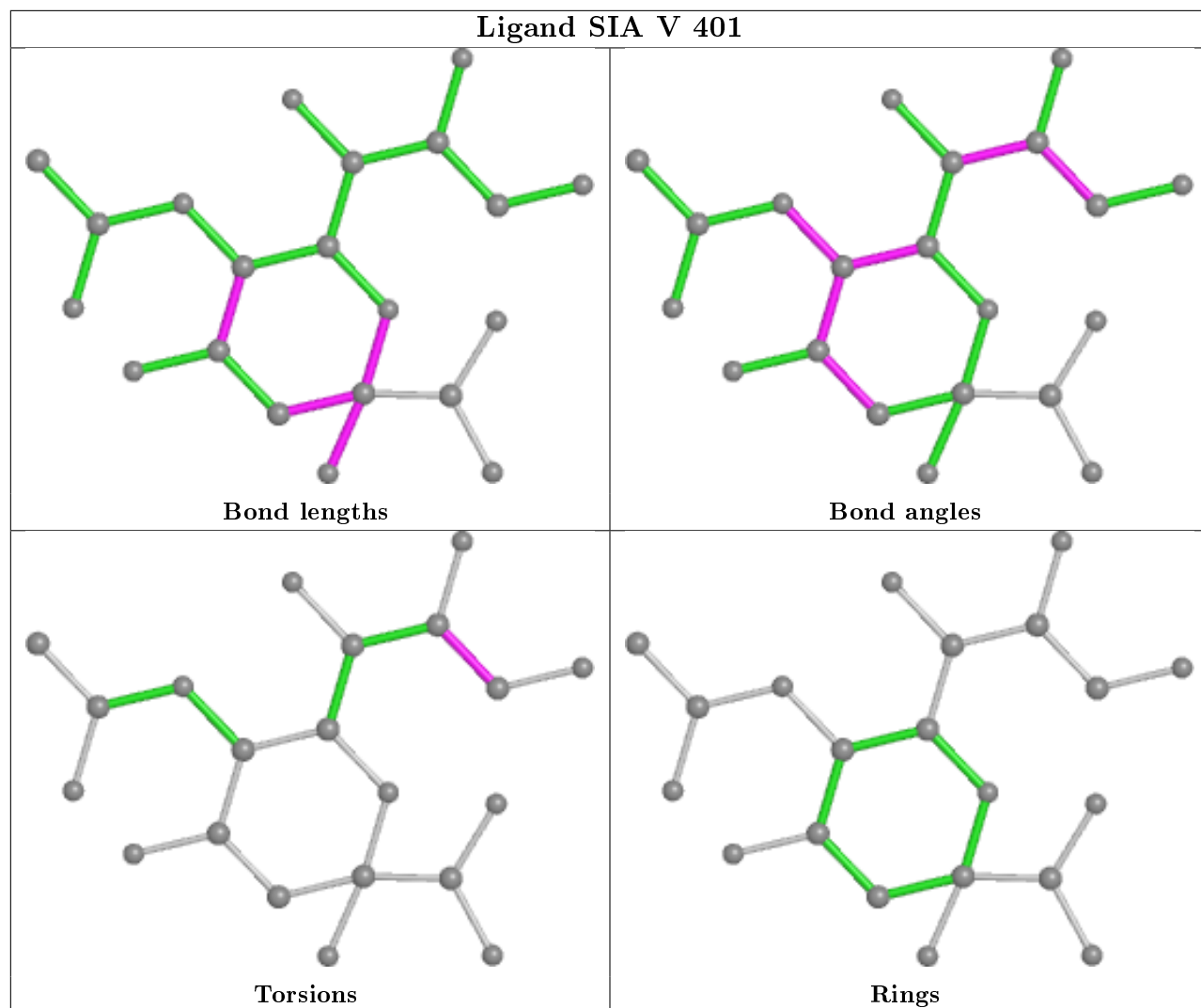
There are no ring outliers.

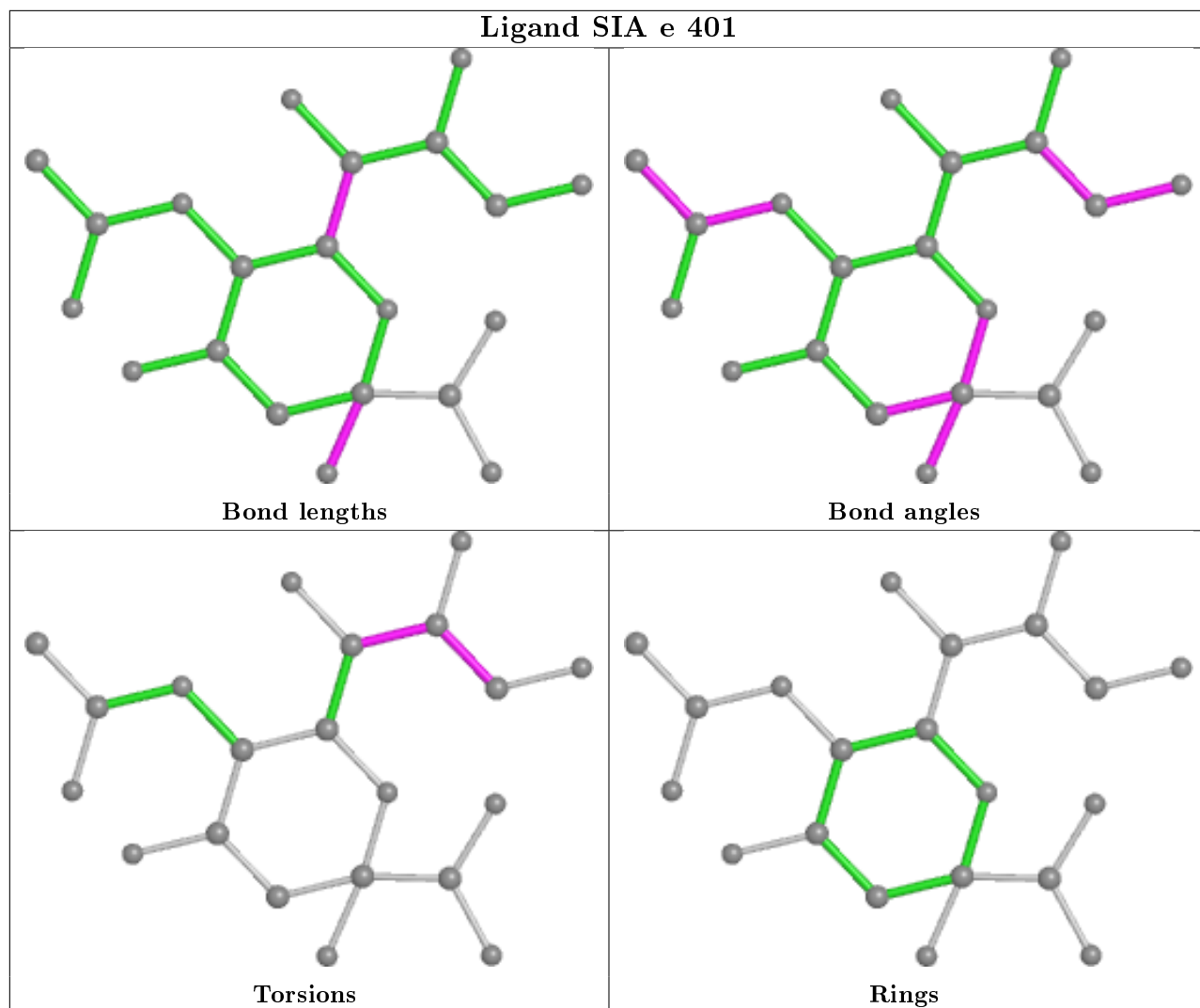
No monomer is involved in short contacts.

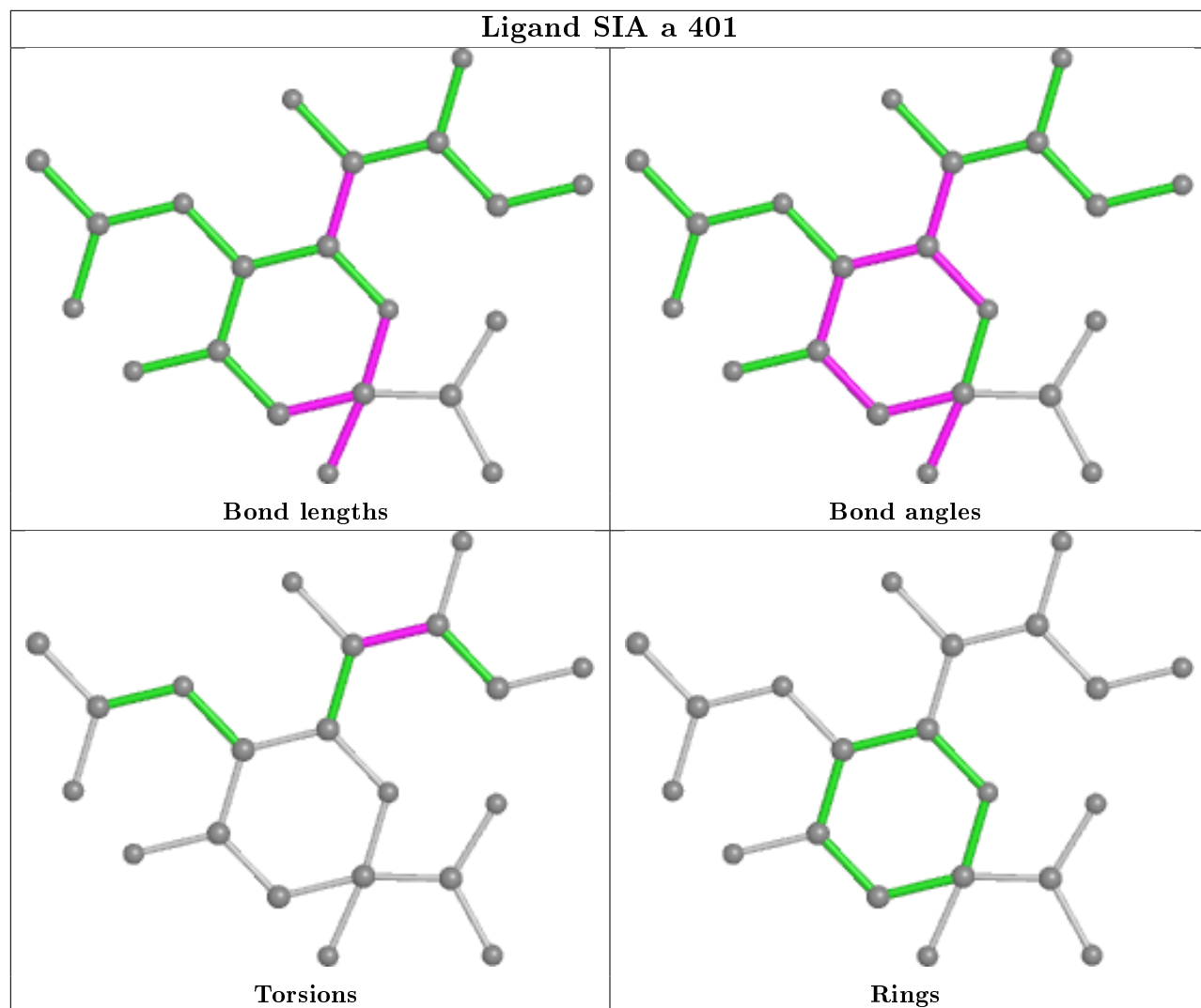
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

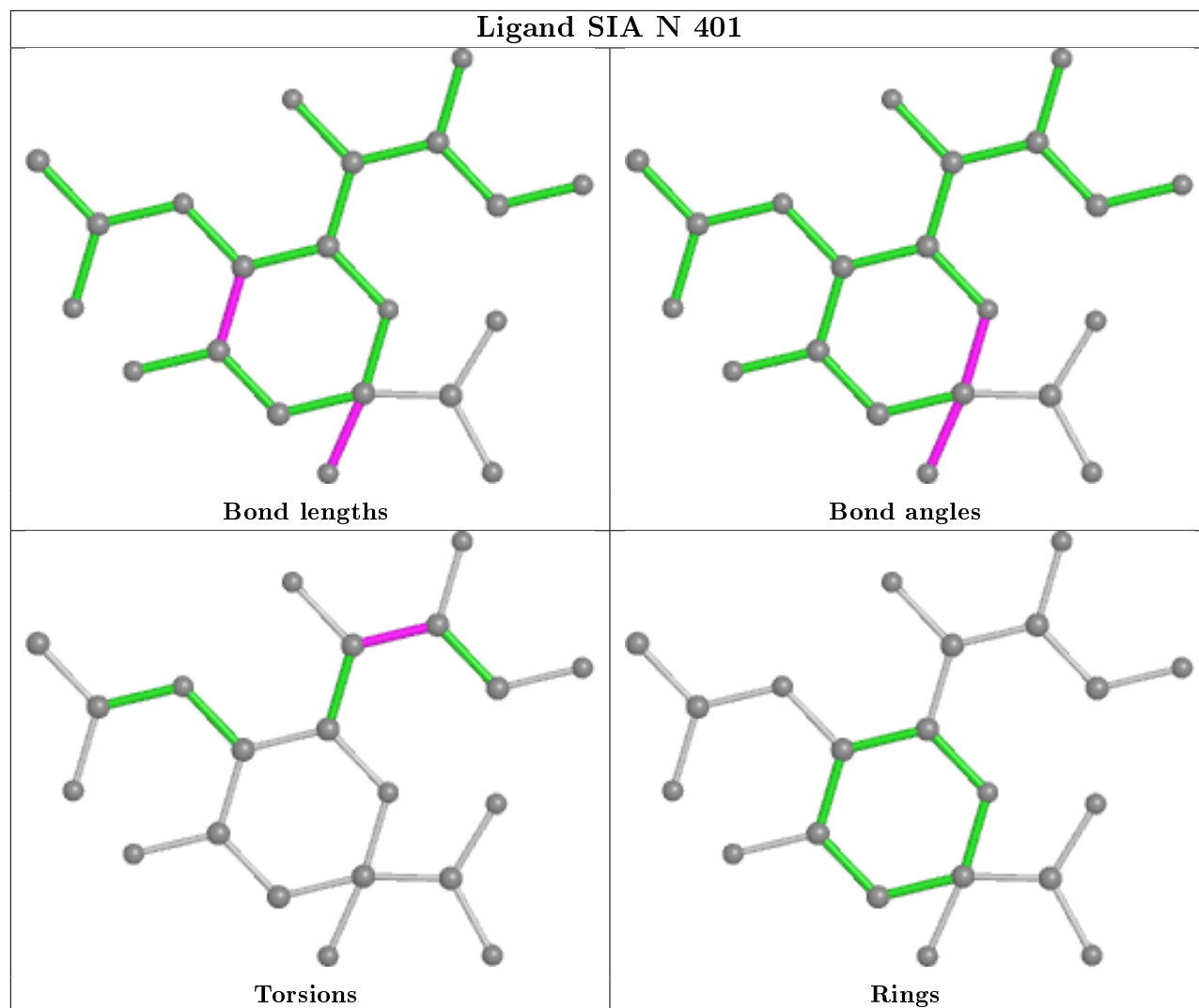
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

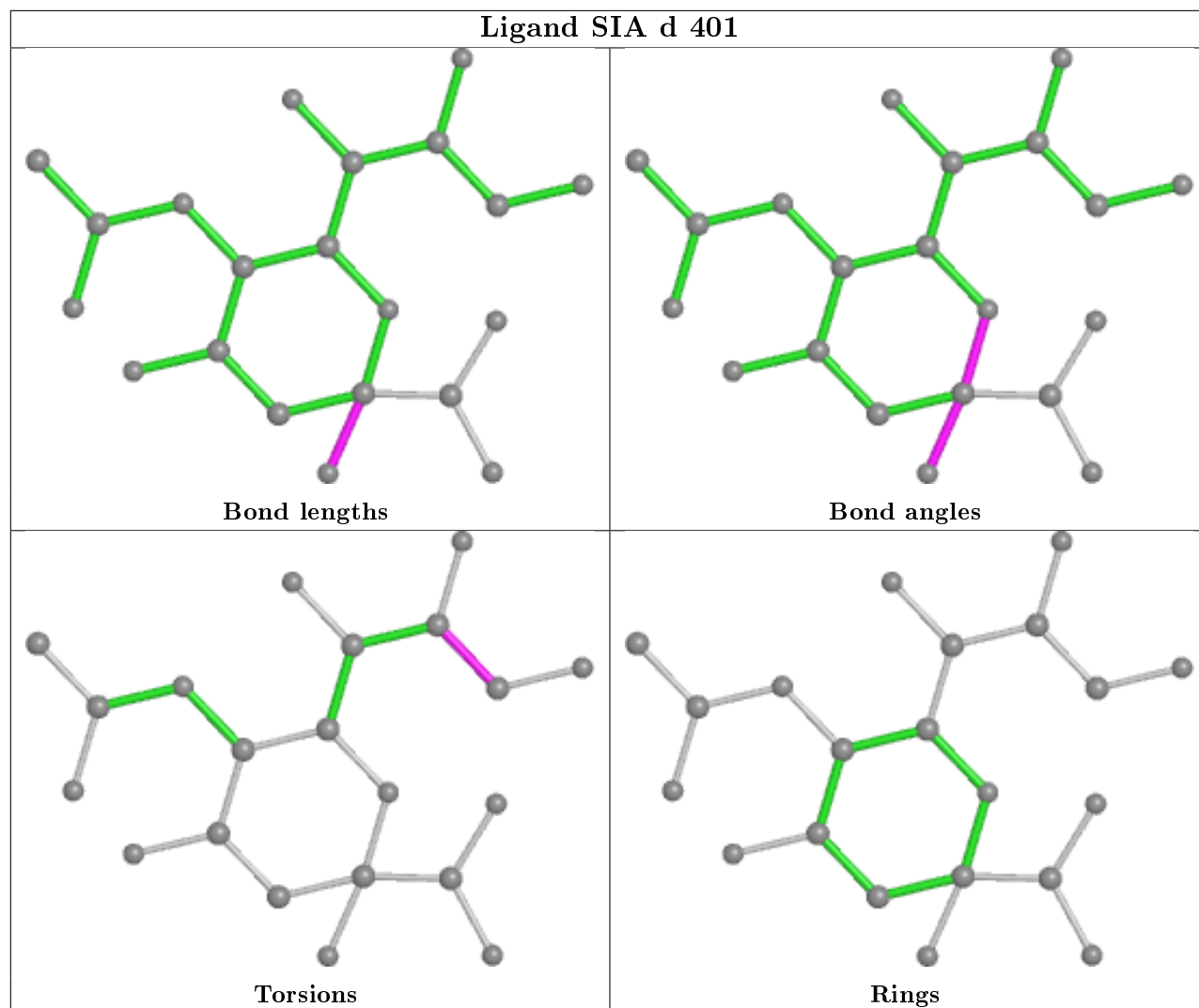


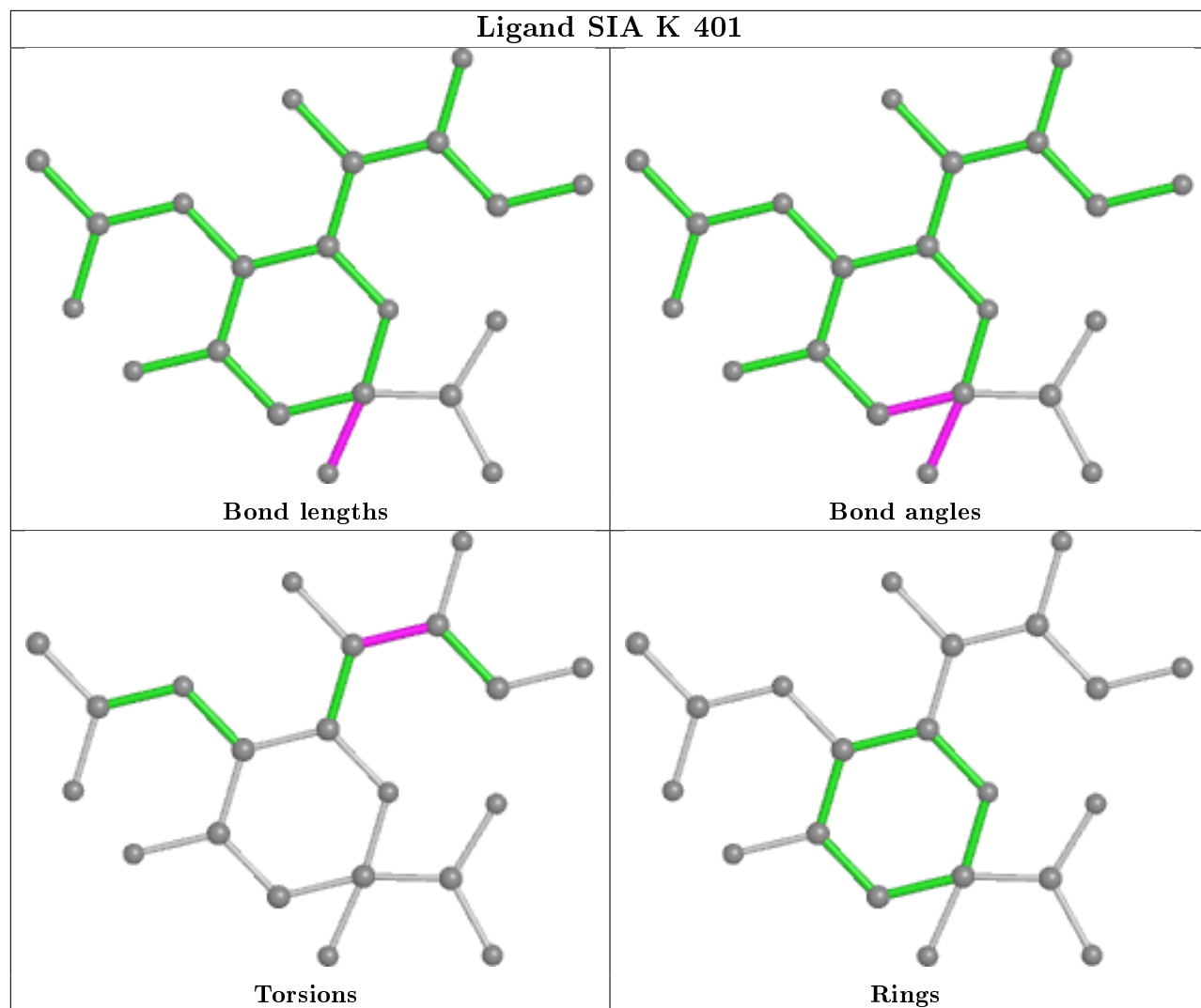


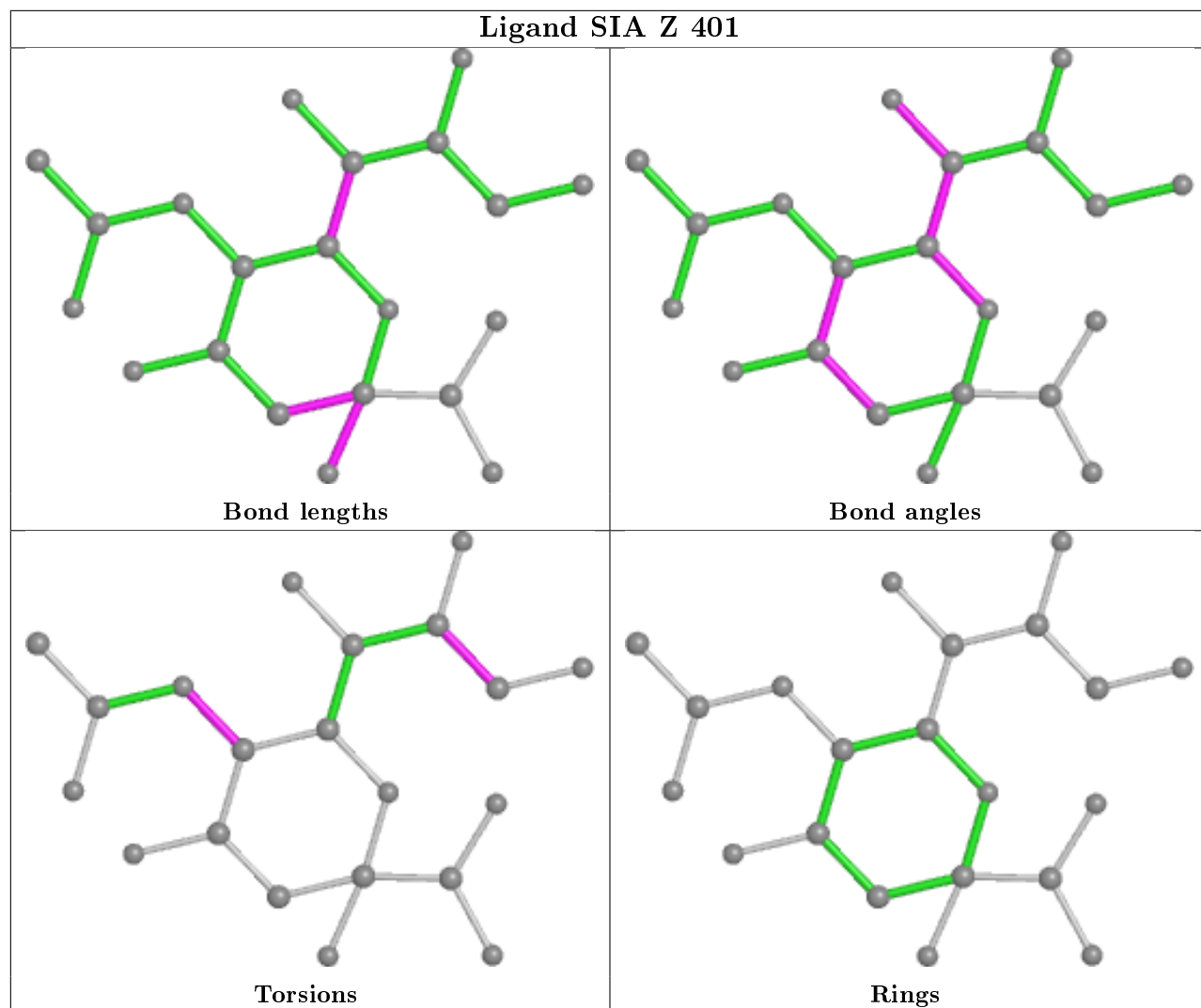


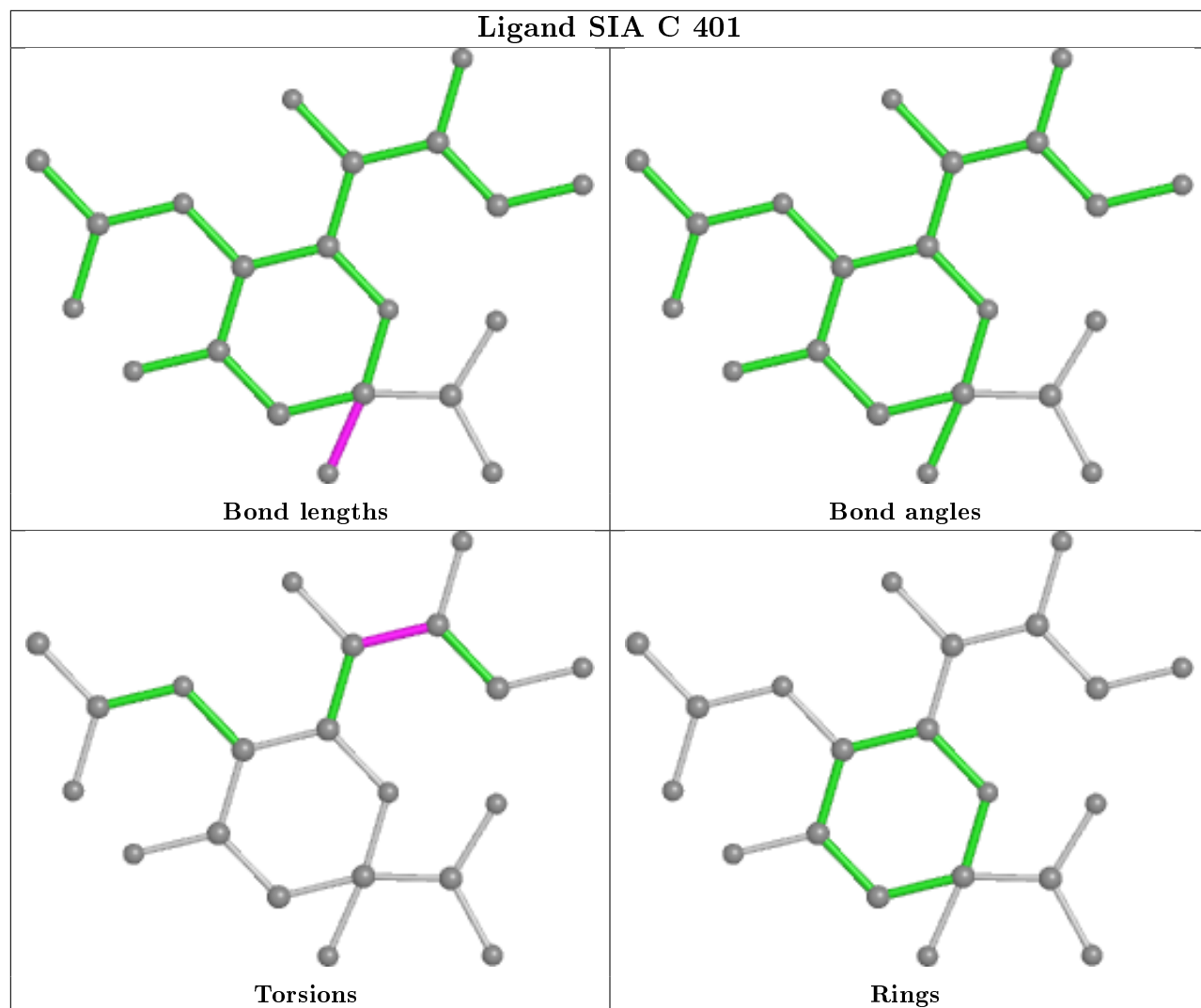


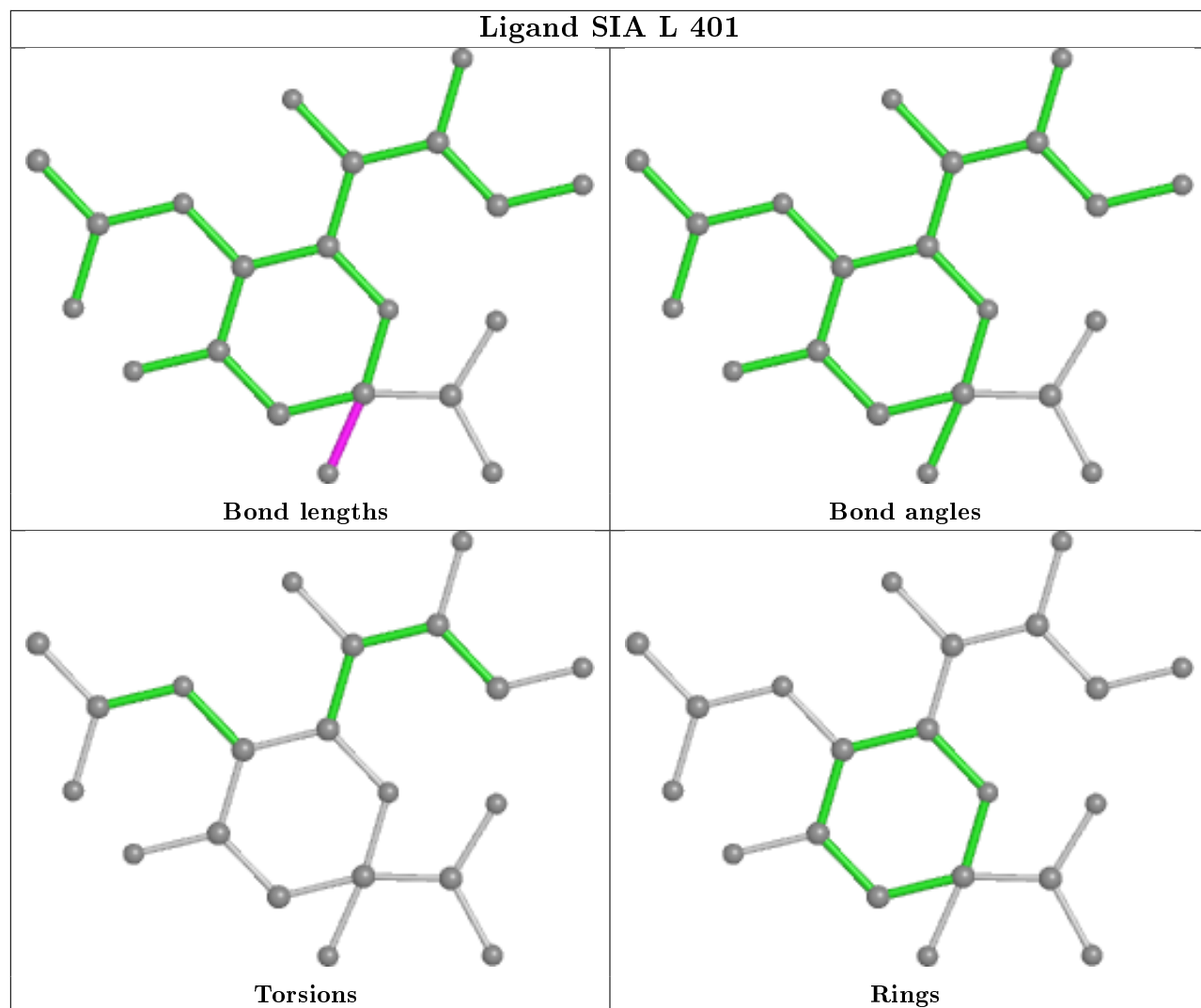


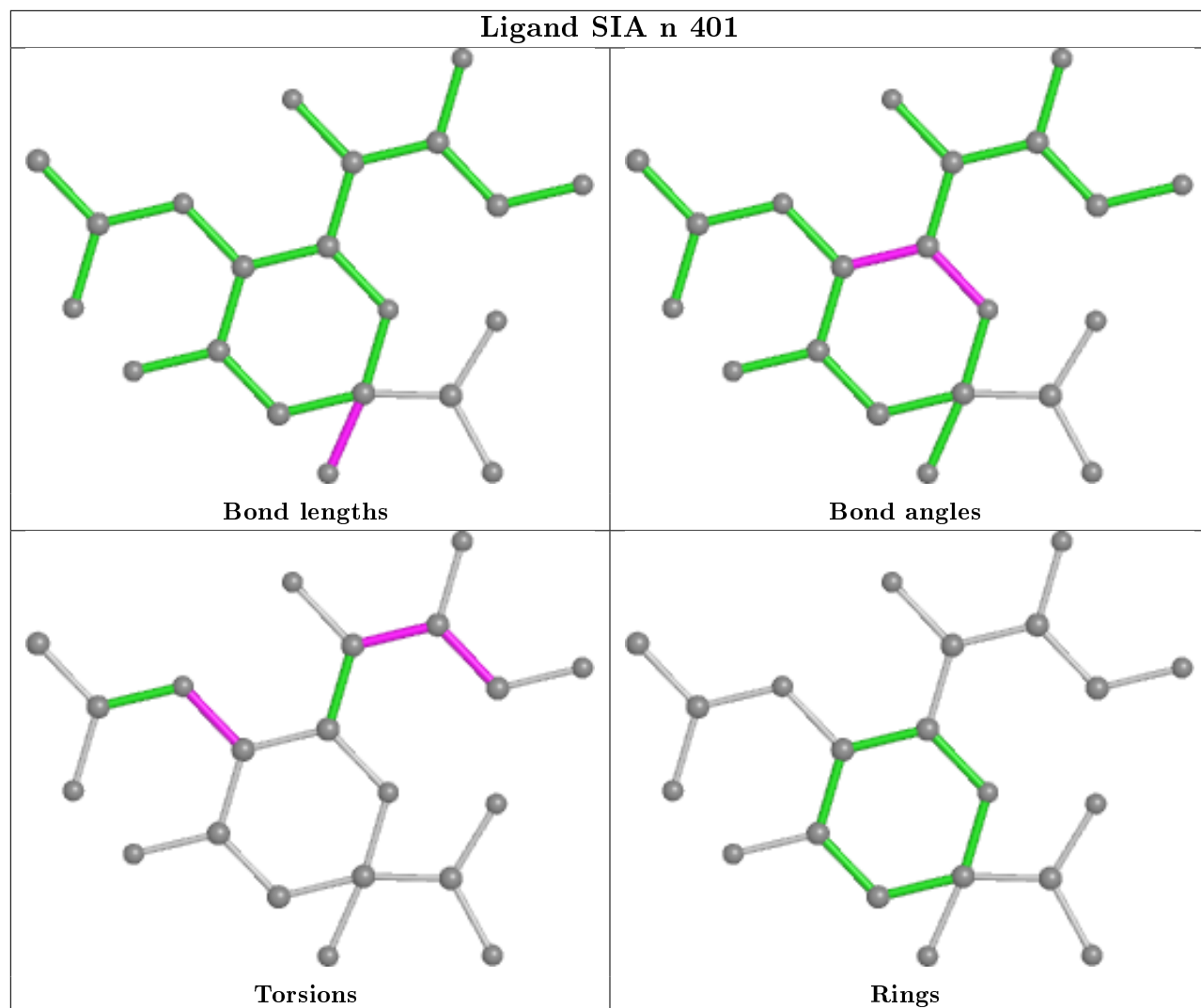


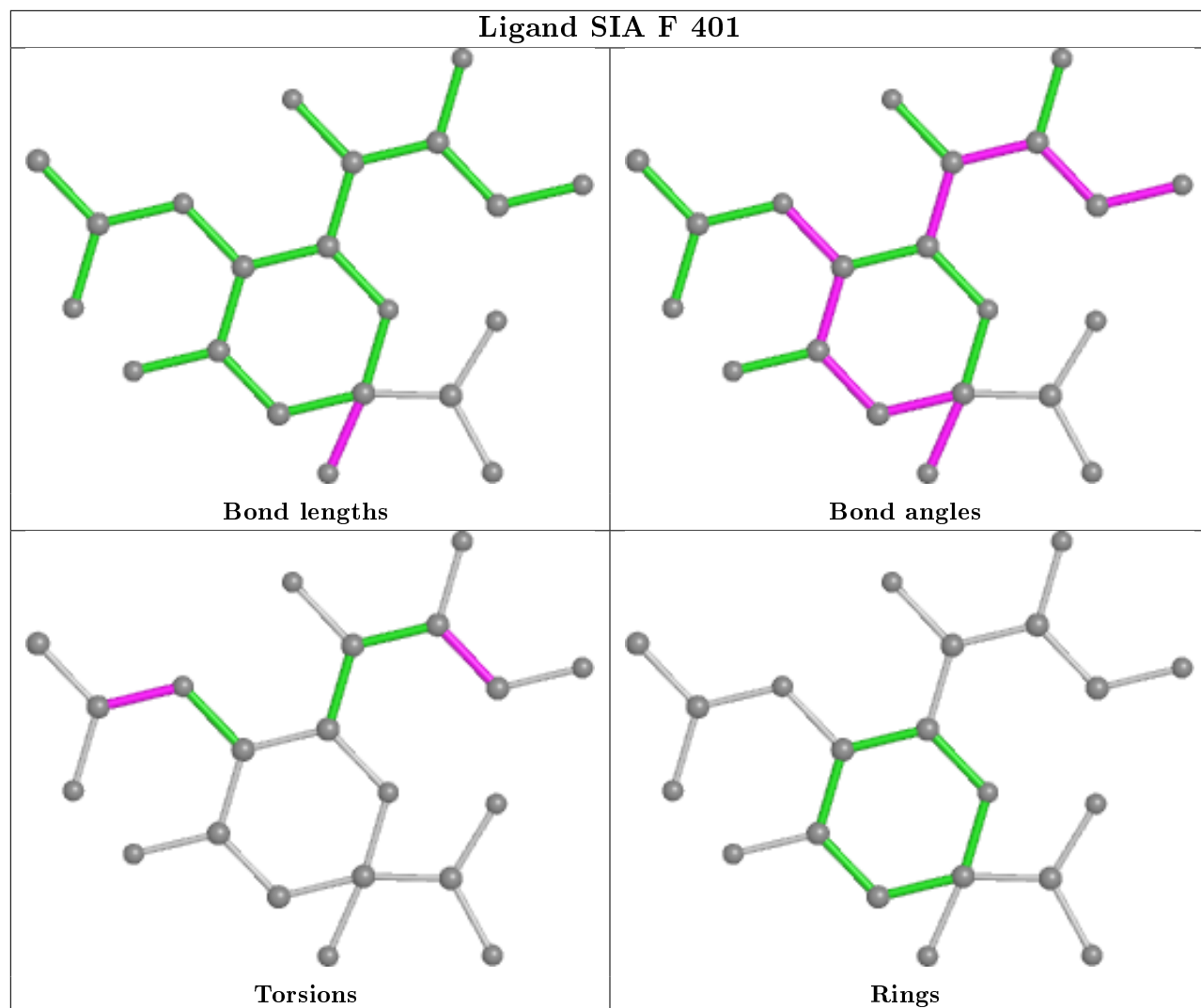


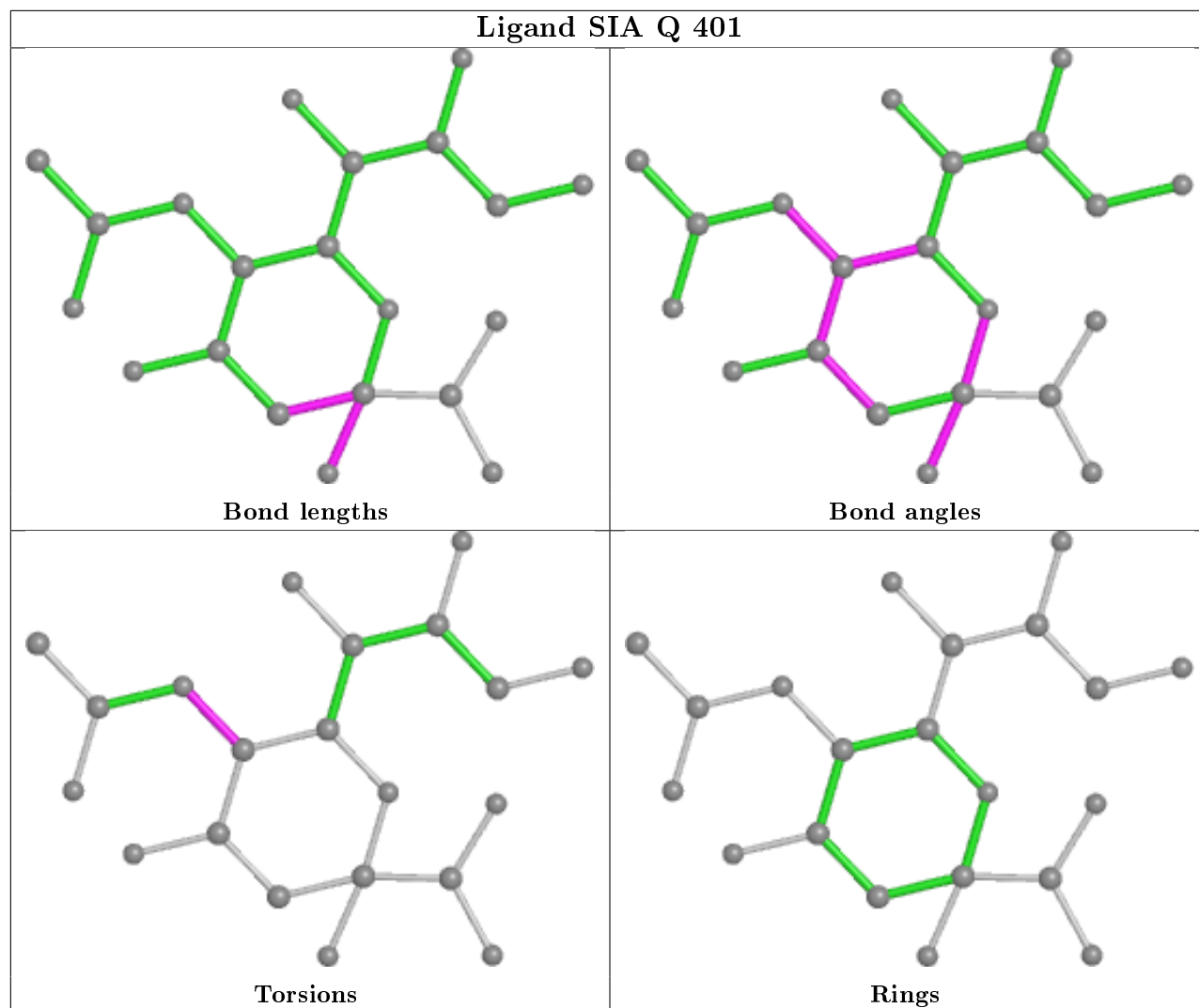


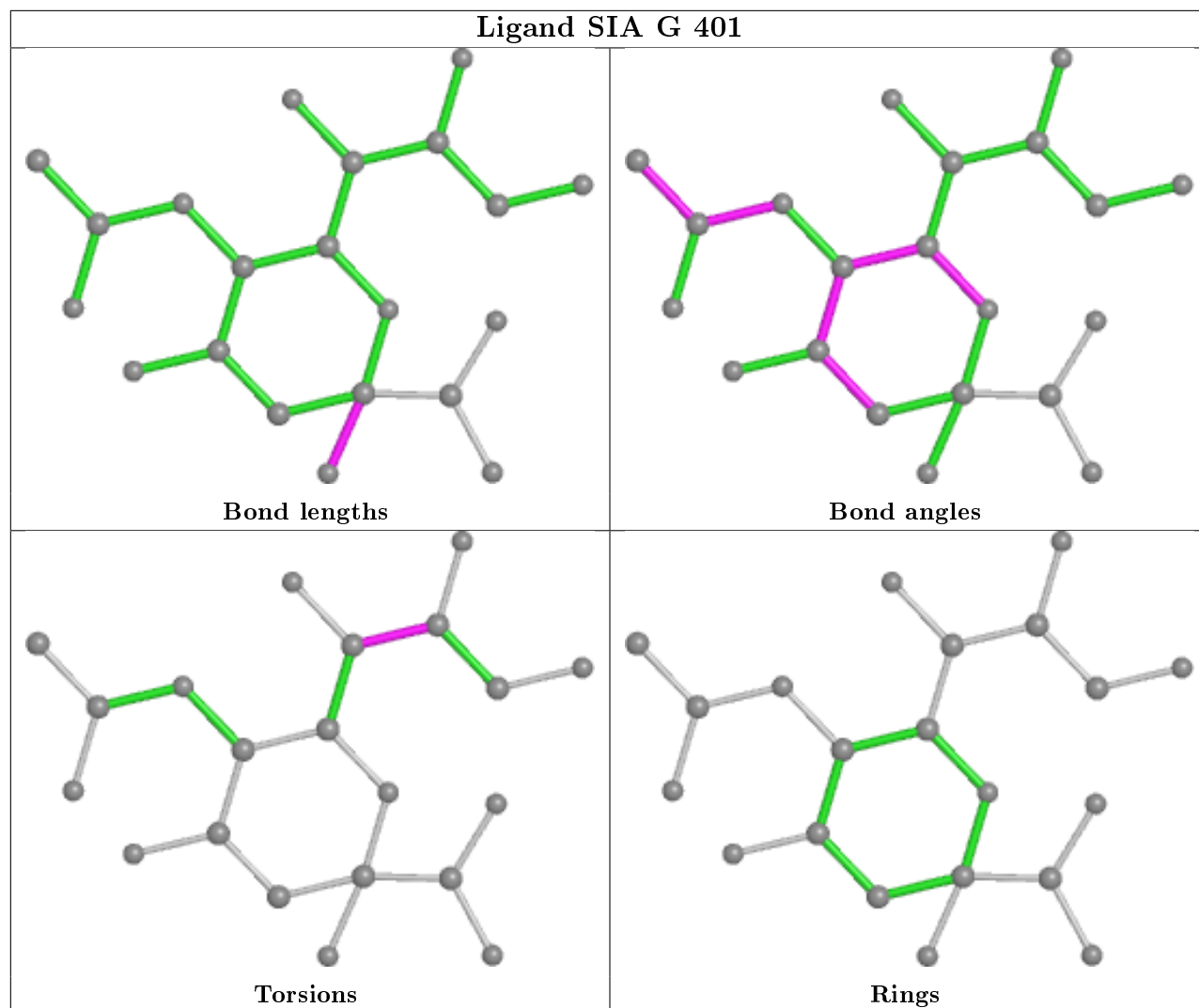


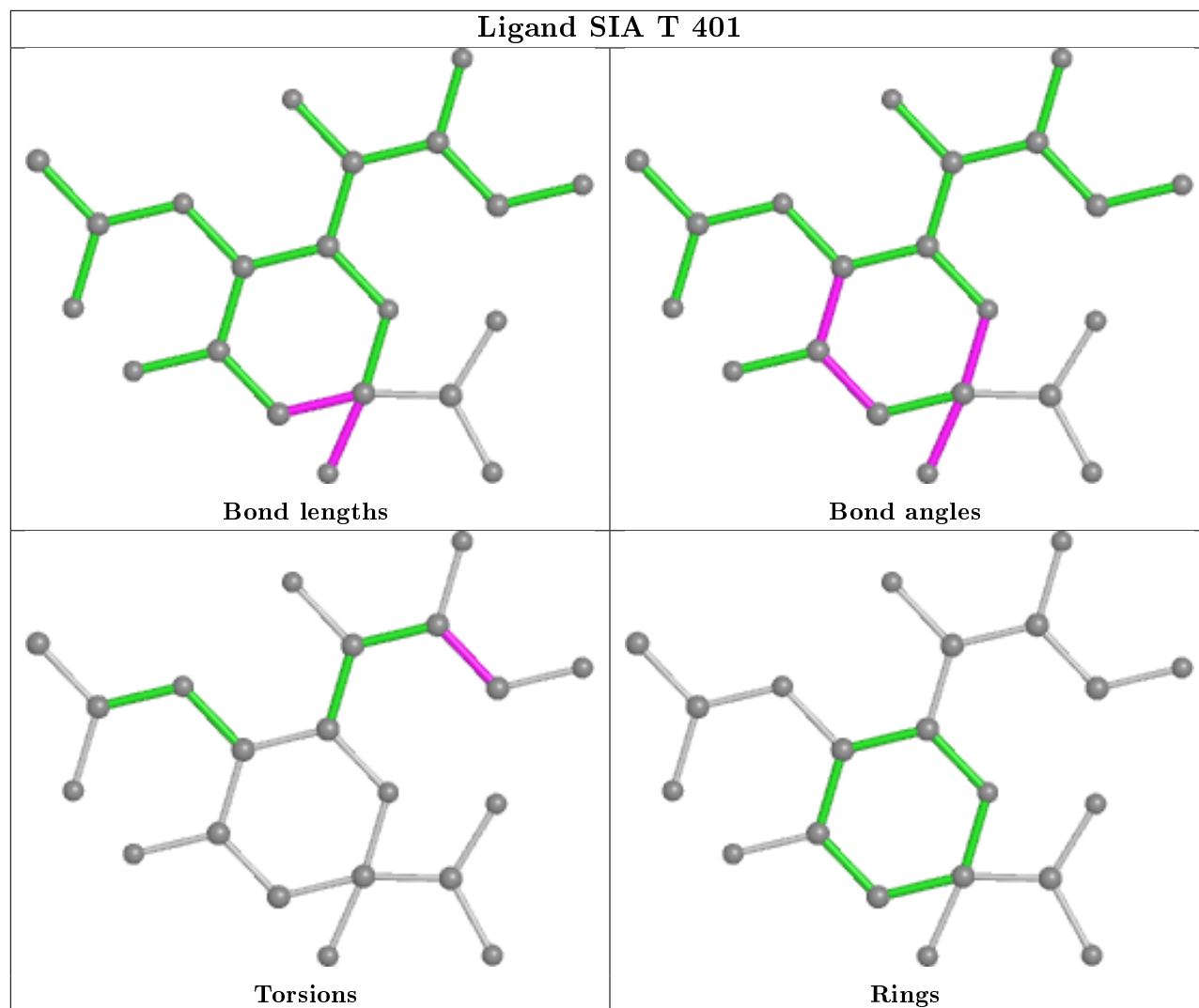


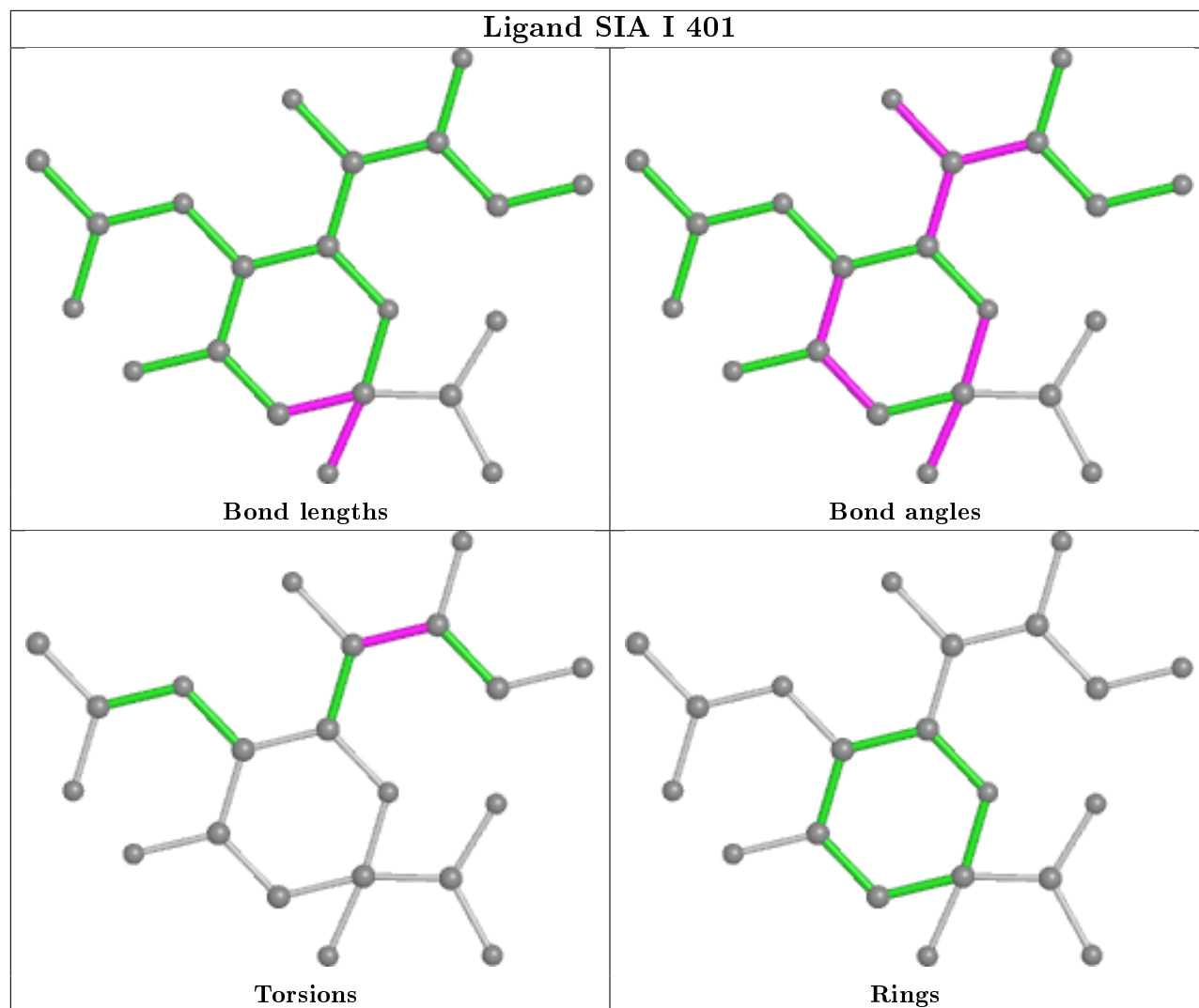


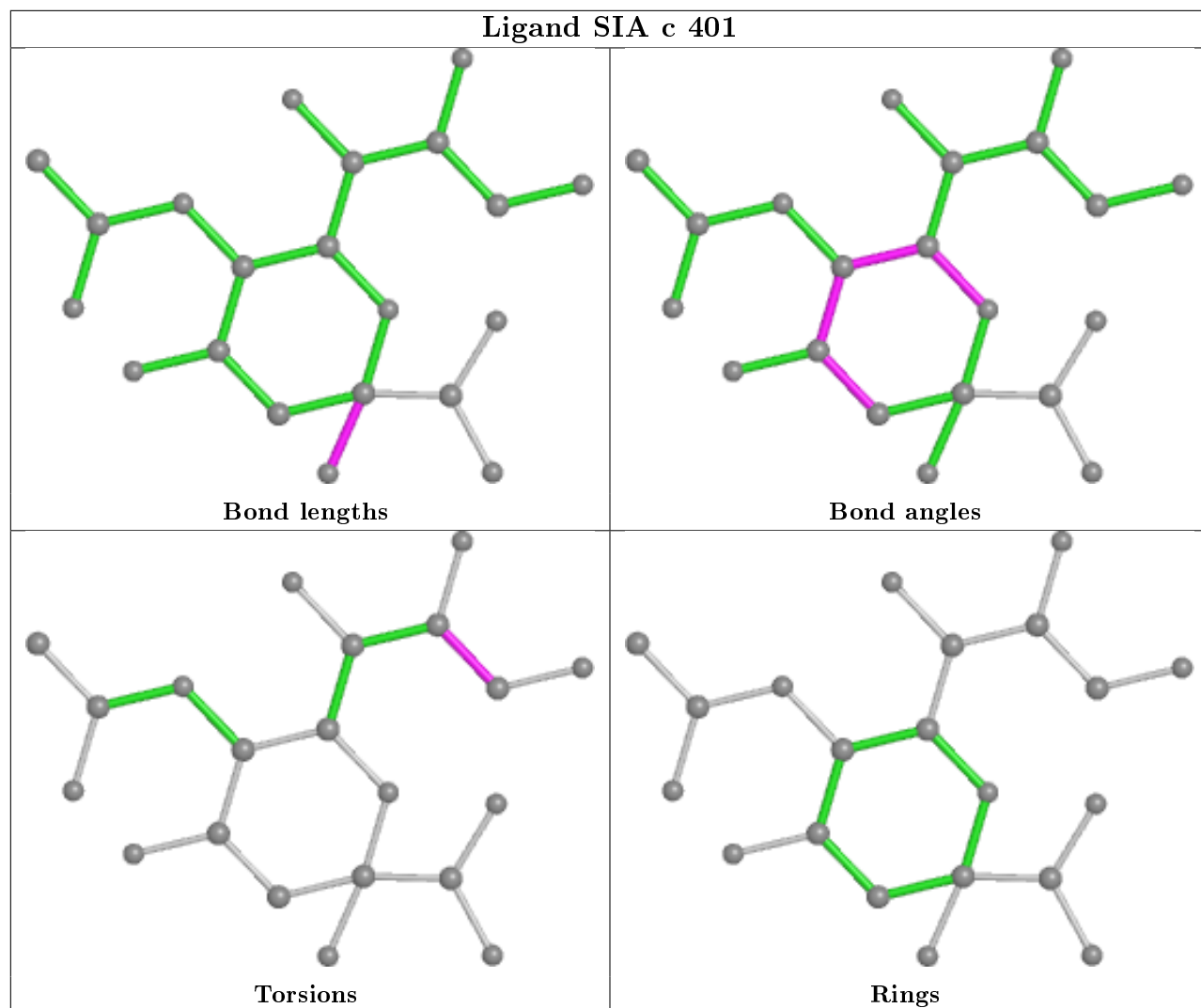


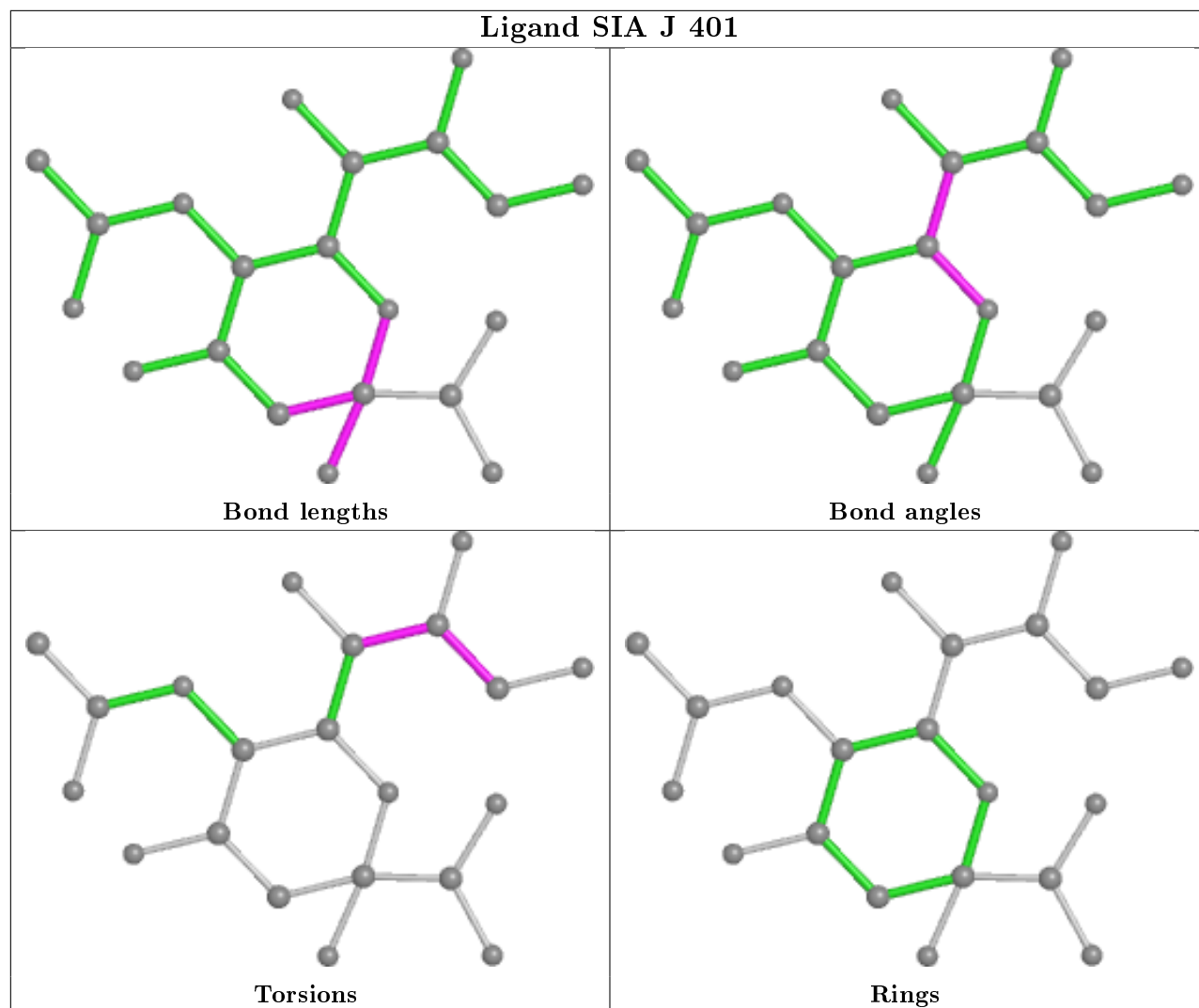


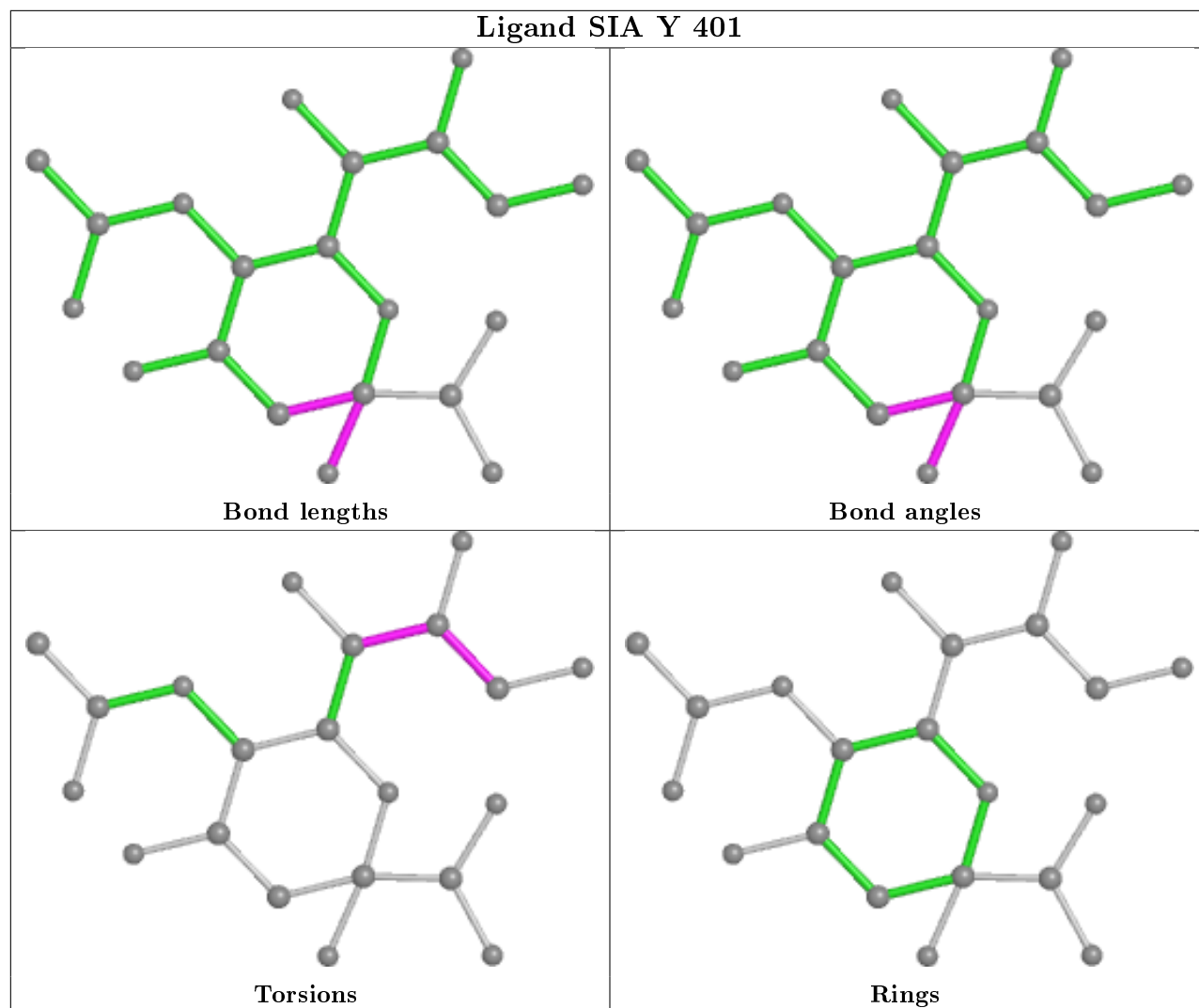


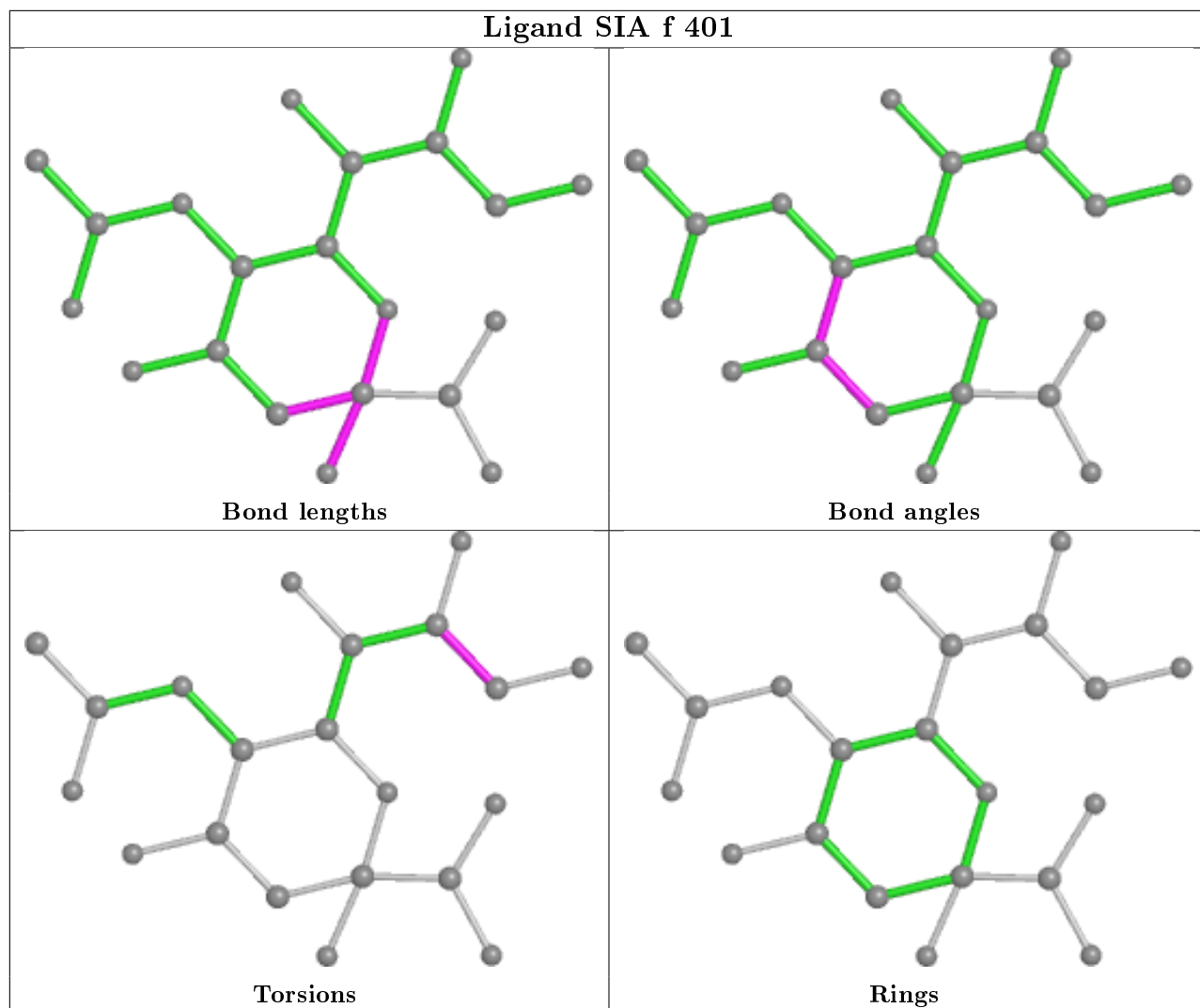


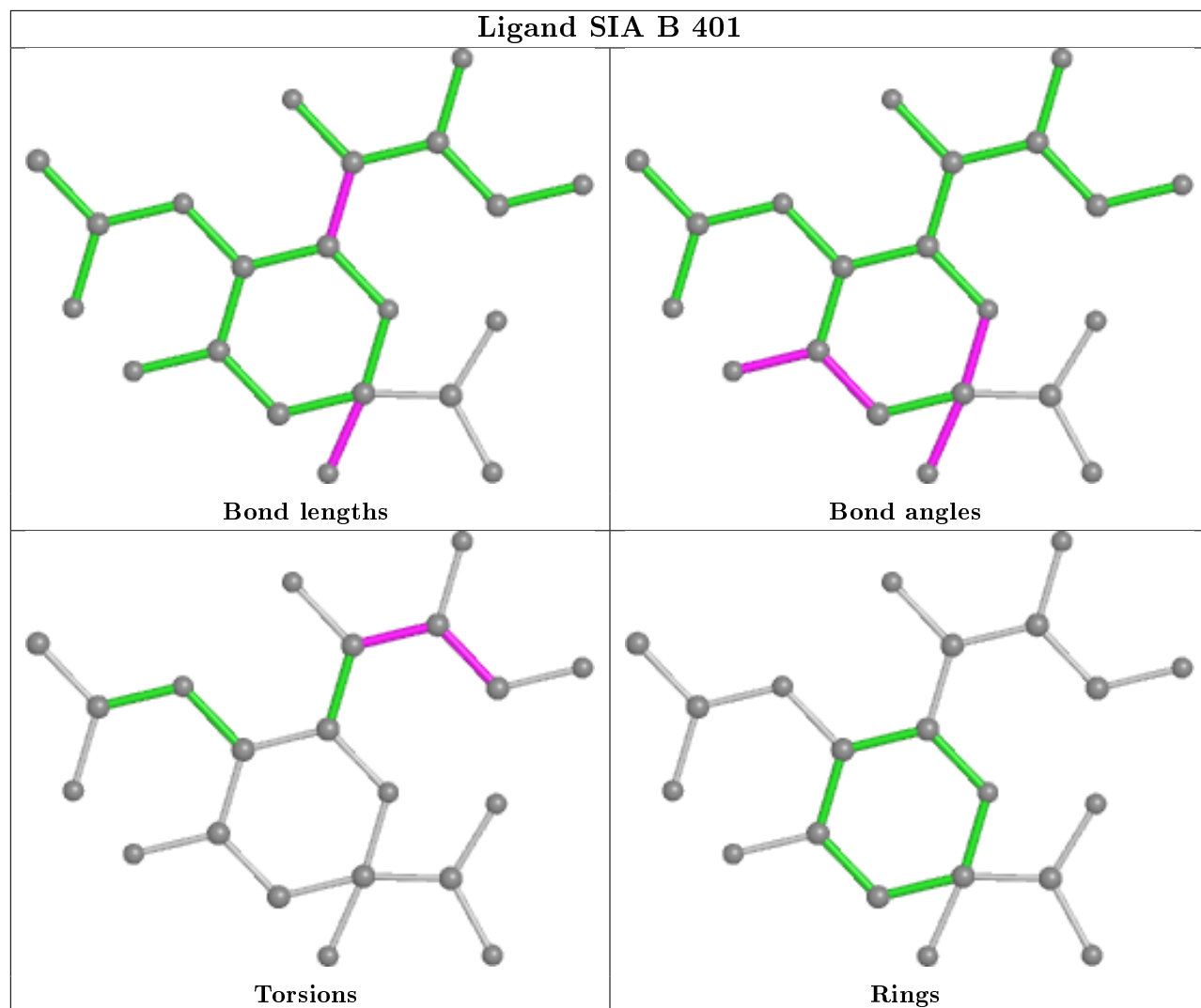


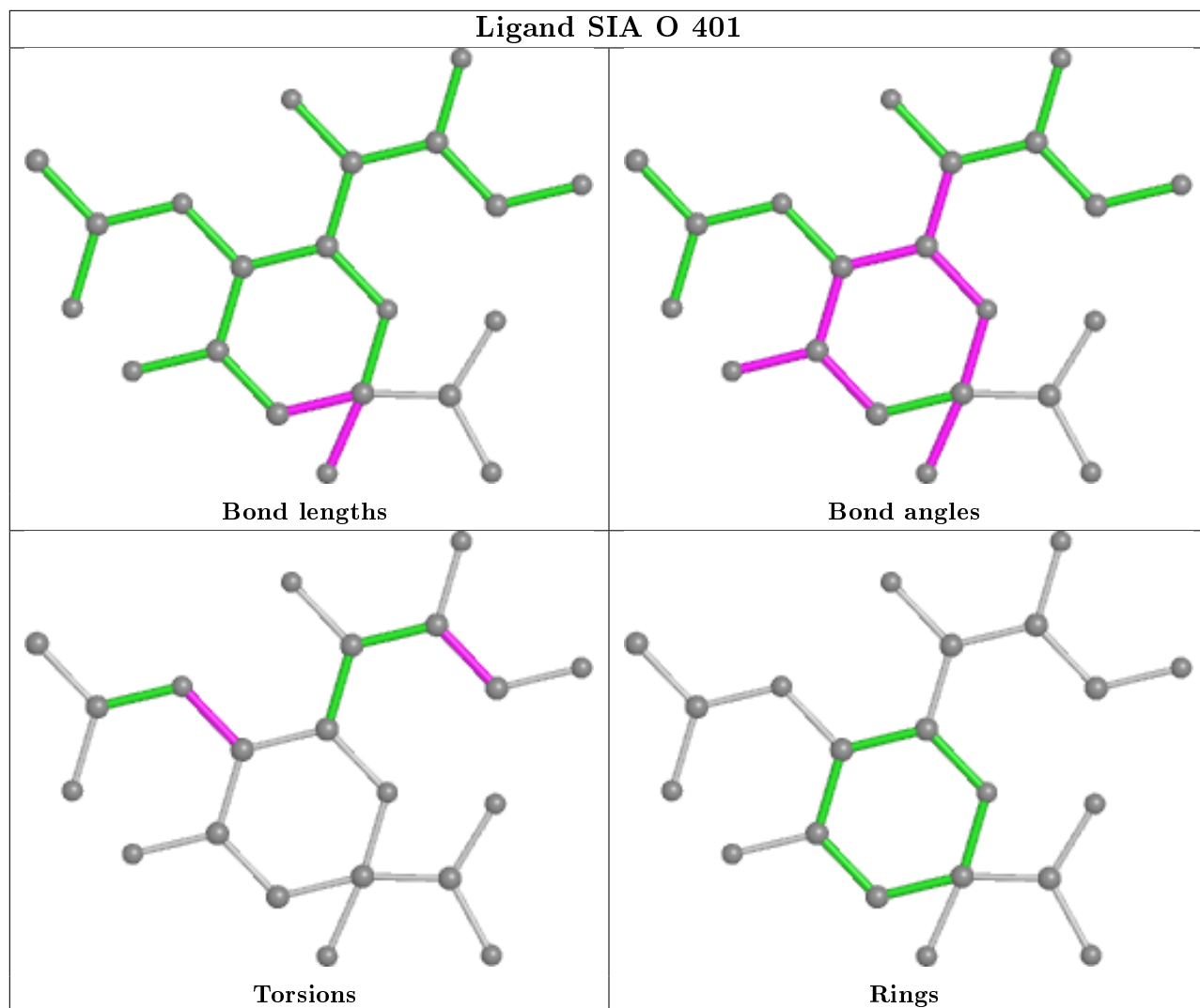


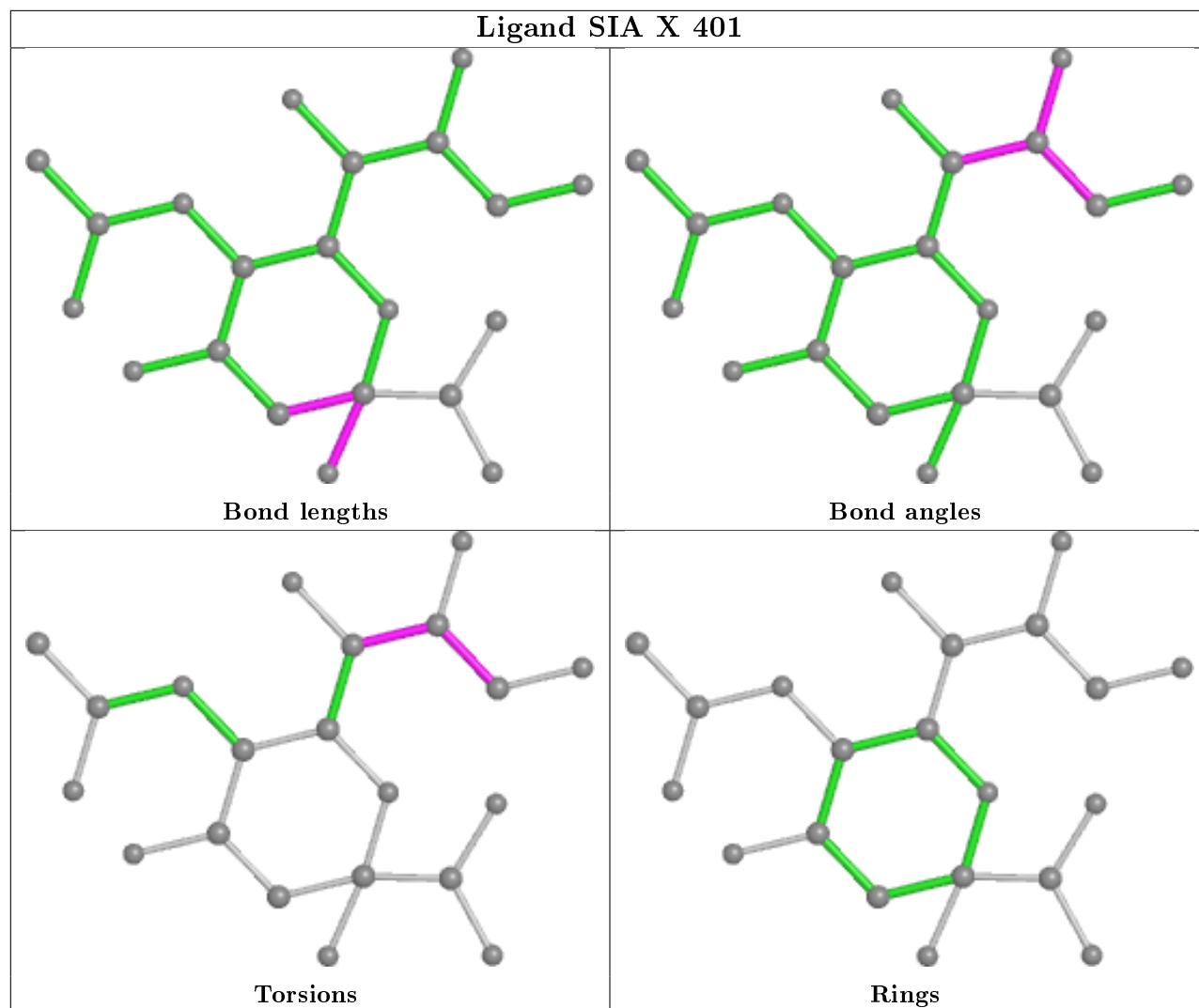


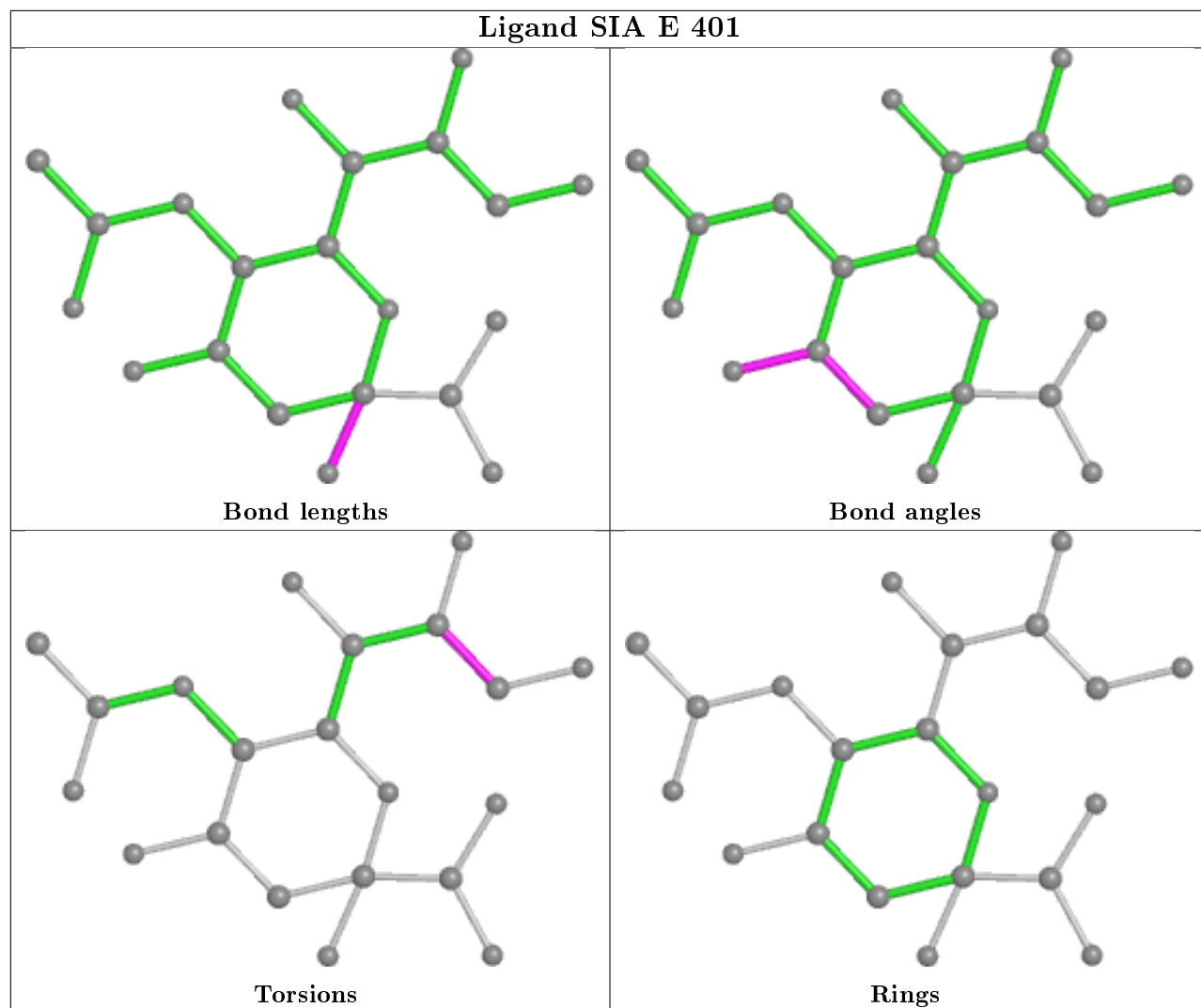


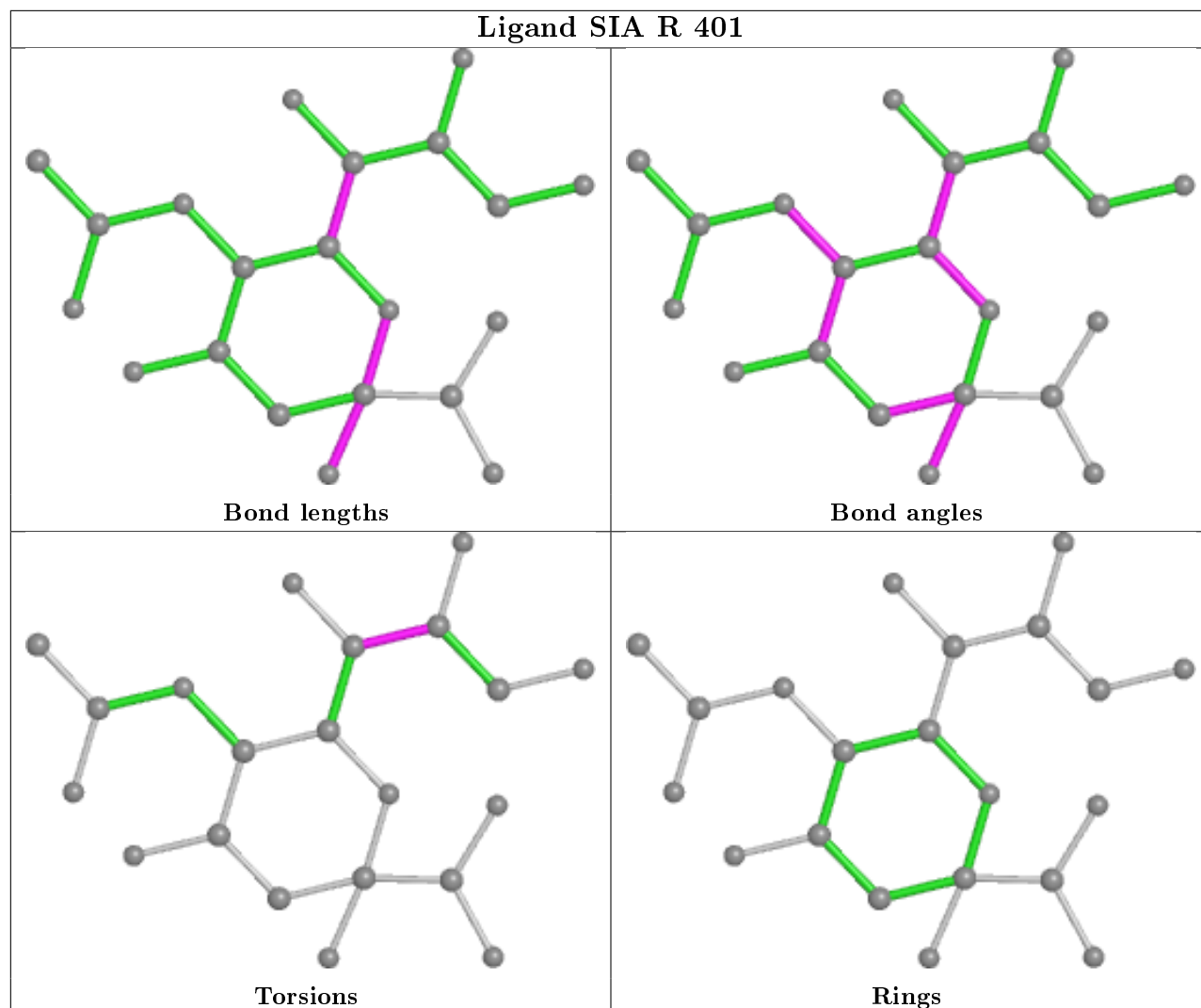


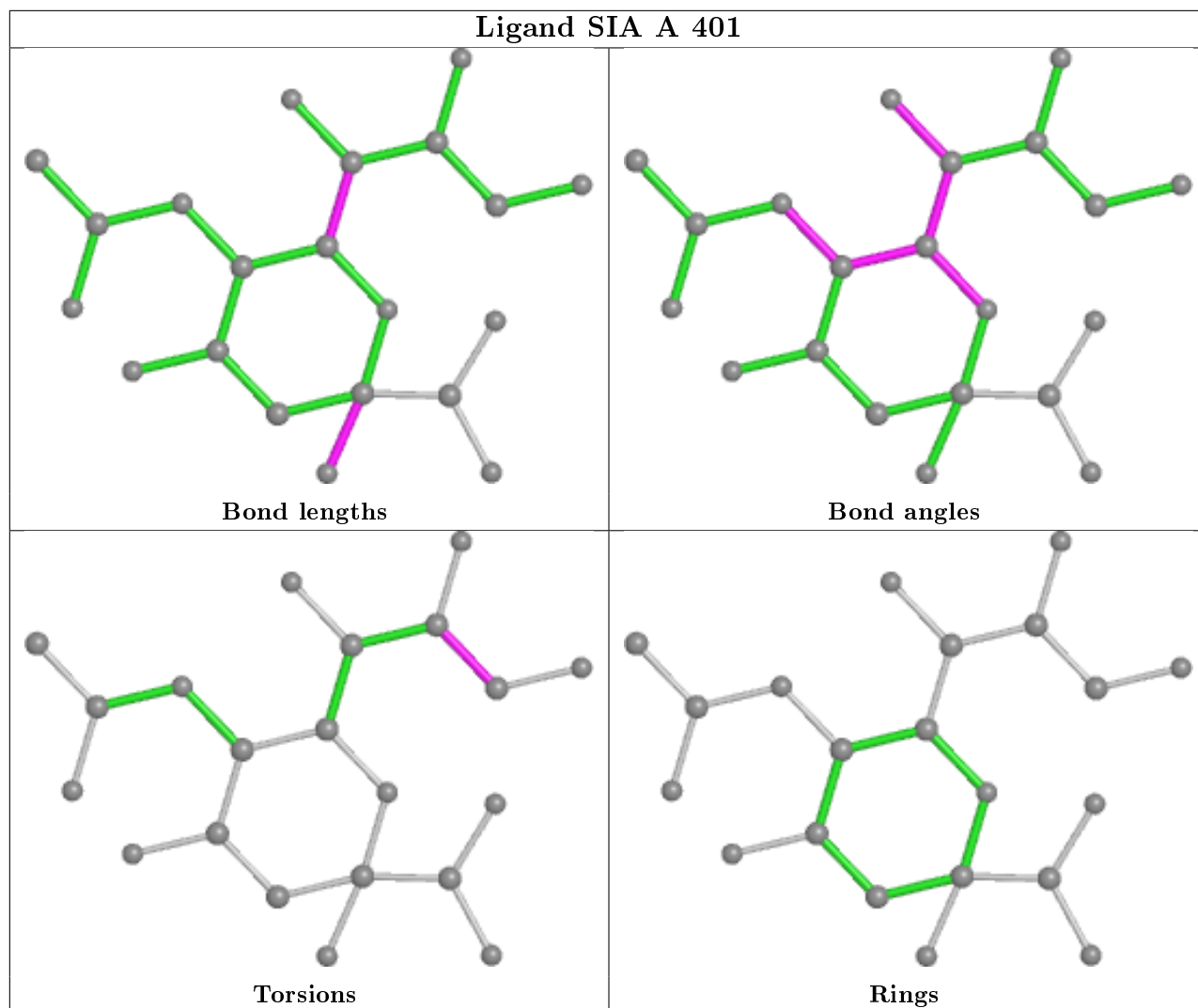


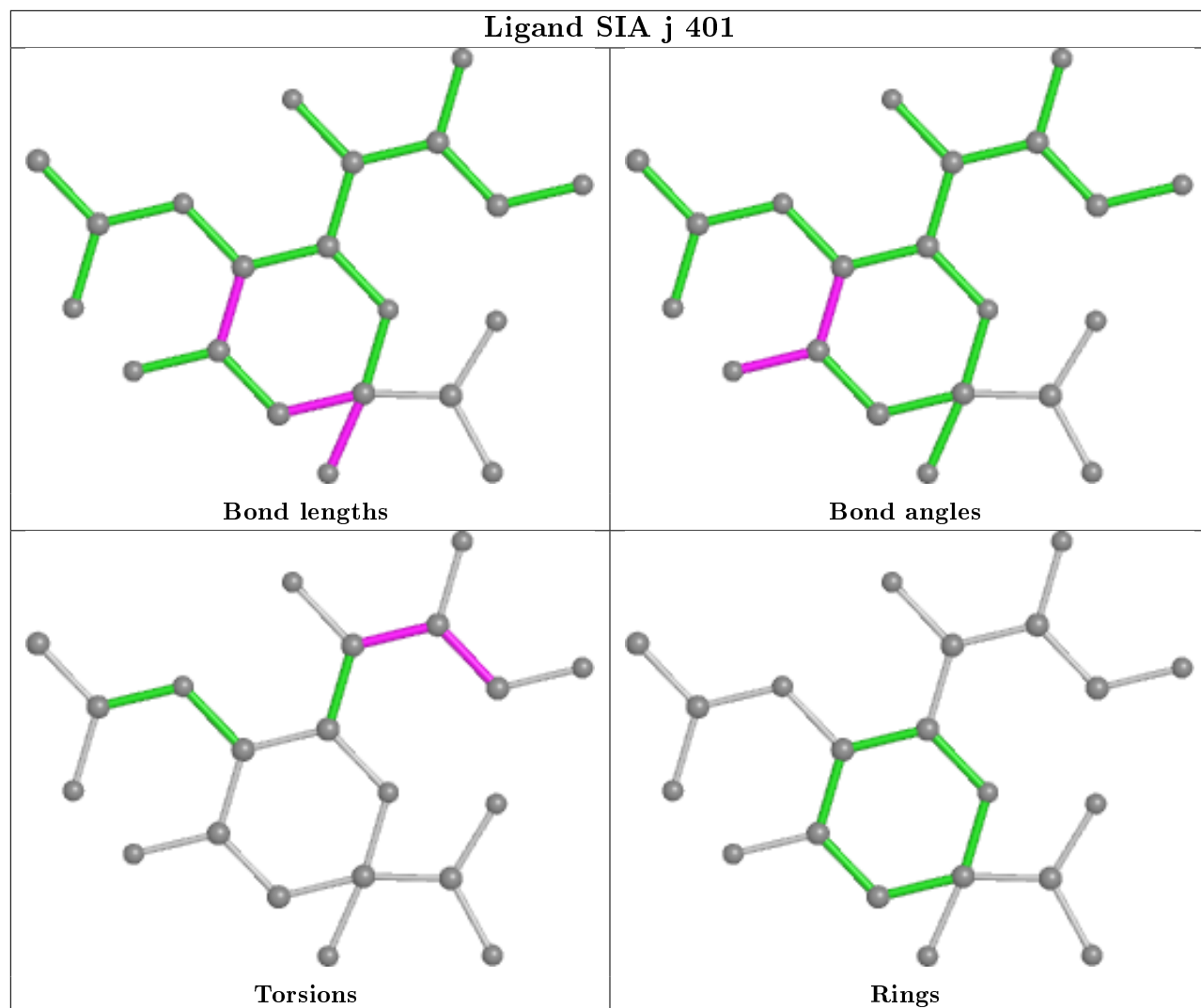


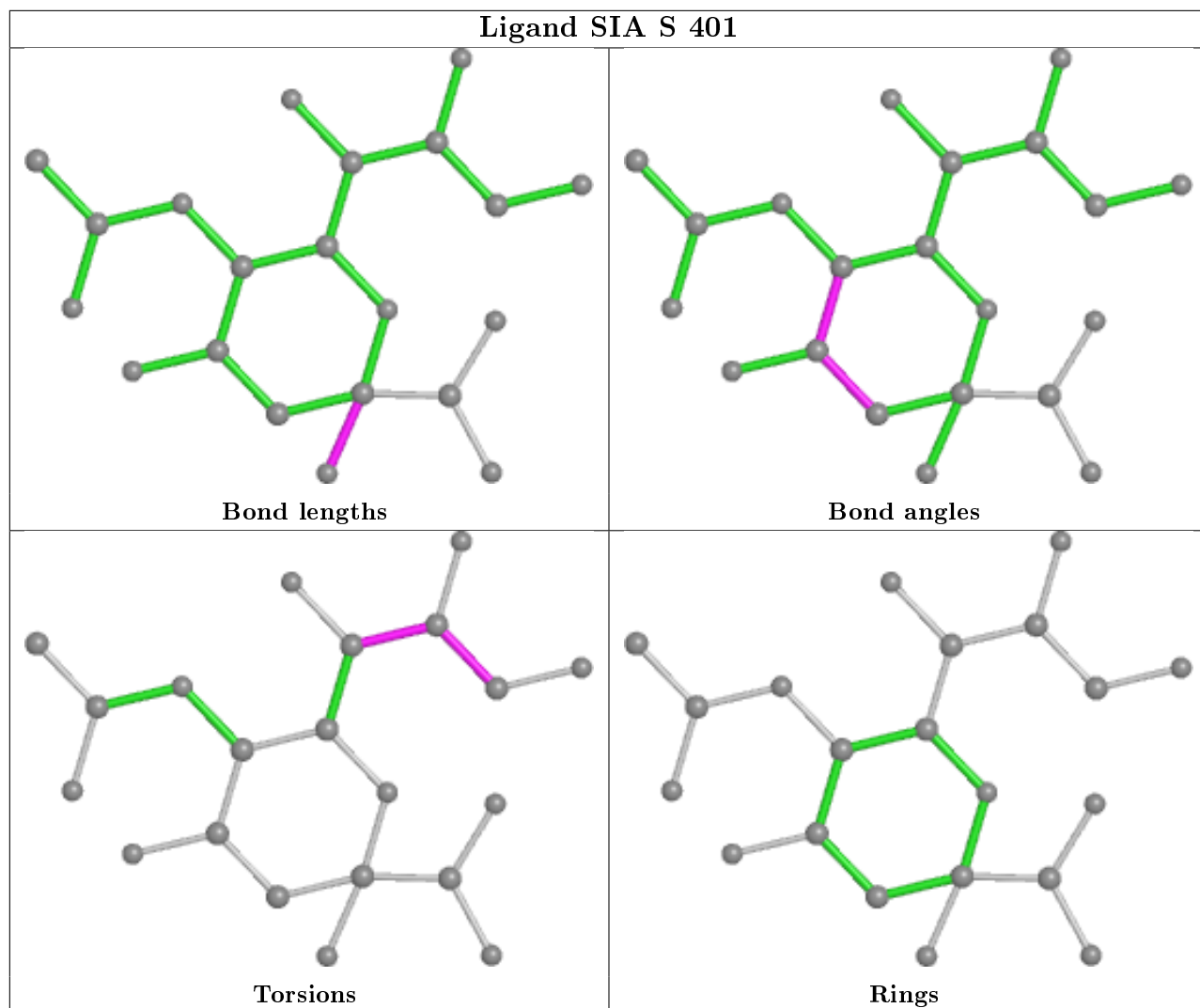


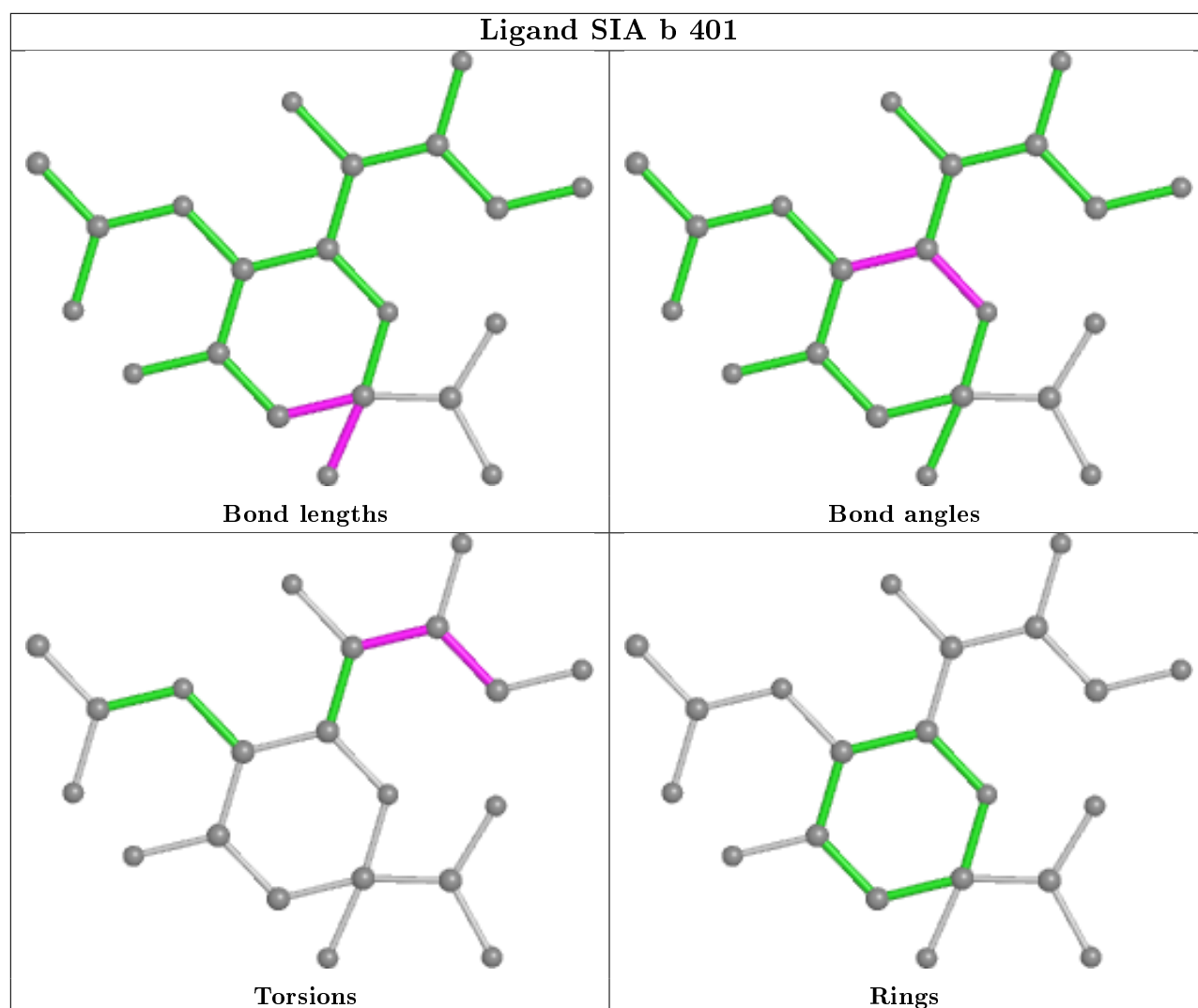












5.7 Other polymers [i](#)

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 [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	267/274 (97%)	-0.32	0 100 100	18, 27, 50, 55	0
1	B	260/274 (94%)	-0.38	0 100 100	16, 28, 47, 67	0
1	C	267/274 (97%)	-0.48	0 100 100	14, 24, 42, 50	0
1	D	261/274 (95%)	-0.50	0 100 100	13, 23, 40, 73	0
1	E	263/274 (95%)	-0.38	0 100 100	17, 27, 52, 69	0
1	F	268/274 (97%)	-0.43	1 (0%) 92 93	15, 26, 41, 55	0
1	G	260/274 (94%)	-0.39	0 100 100	21, 33, 51, 66	0
1	H	260/274 (94%)	-0.32	0 100 100	22, 35, 51, 69	0
1	I	268/274 (97%)	-0.35	0 100 100	16, 30, 46, 58	0
1	J	267/274 (97%)	-0.37	0 100 100	16, 28, 43, 57	0
1	K	267/274 (97%)	-0.32	1 (0%) 92 93	19, 29, 47, 70	0
1	L	262/274 (95%)	-0.35	0 100 100	18, 30, 52, 66	0
1	M	269/274 (98%)	-0.36	0 100 100	17, 28, 56, 92	0
1	N	266/274 (97%)	-0.39	0 100 100	18, 27, 53, 86	0
1	O	262/274 (95%)	-0.39	0 100 100	19, 29, 51, 78	0
1	P	269/274 (98%)	-0.36	0 100 100	20, 32, 47, 67	0
1	Q	268/274 (97%)	-0.37	0 100 100	20, 31, 45, 66	0
1	R	263/274 (95%)	-0.39	0 100 100	20, 30, 46, 78	0
1	S	261/274 (95%)	-0.32	0 100 100	20, 33, 50, 81	0
1	T	263/274 (95%)	-0.31	0 100 100	22, 35, 51, 79	0
1	U	261/274 (95%)	-0.36	0 100 100	19, 29, 45, 76	0
1	V	265/274 (96%)	-0.19	2 (0%) 86 85	26, 40, 60, 85	0
1	W	262/274 (95%)	-0.09	2 (0%) 86 85	25, 41, 61, 90	0
1	X	261/274 (95%)	-0.17	1 (0%) 92 93	22, 39, 57, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	261/274 (95%)	-0.38	0 100 100	19, 31, 53, 70	0
1	Z	260/274 (94%)	-0.33	0 100 100	23, 32, 46, 61	0
1	a	261/274 (95%)	-0.27	2 (0%) 86 85	25, 38, 55, 86	0
1	b	260/274 (94%)	-0.04	1 (0%) 92 93	28, 43, 64, 102	0
1	c	256/274 (93%)	-0.09	2 (0%) 86 85	29, 45, 64, 87	0
1	d	260/274 (94%)	-0.22	1 (0%) 92 93	23, 41, 64, 82	0
1	e	261/274 (95%)	-0.26	2 (0%) 86 85	23, 39, 52, 77	0
1	f	261/274 (95%)	-0.16	0 100 100	29, 42, 56, 64	0
1	g	269/274 (98%)	-0.06	2 (0%) 87 87	29, 46, 63, 88	0
1	h	261/274 (95%)	-0.13	0 100 100	30, 47, 60, 76	0
1	i	260/274 (94%)	-0.18	1 (0%) 92 93	29, 44, 60, 91	0
1	j	260/274 (94%)	-0.12	1 (0%) 92 93	29, 47, 64, 79	0
1	k	263/274 (95%)	0.44	7 (2%) 54 50	35, 61, 80, 99	0
1	l	235/274 (85%)	0.55	11 (4%) 31 28	40, 65, 85, 93	0
1	m	259/274 (94%)	0.26	5 (1%) 66 63	33, 58, 85, 100	0
1	n	267/274 (97%)	-0.24	0 100 100	28, 42, 60, 75	0
All	All	10494/10960 (95%)	-0.24	42 (0%) 92 93	13, 36, 63, 102	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	k	41	ALA	4.1
1	l	27	LEU	3.8
1	k	128	GLY	3.8
1	k	258	ASP	3.6
1	k	64	TYR	3.6

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	SIA	V	401	21/21	0.78	0.25	48,63,75,76	0
3	CL	S	402	1/1	0.78	0.12	53,53,53,53	0
2	SIA	X	401	21/21	0.79	0.28	54,62,68,74	0
3	CL	W	302	1/1	0.79	0.13	53,53,53,53	0
3	CL	j	403	1/1	0.82	0.11	58,58,58,58	0
2	SIA	T	401	21/21	0.82	0.24	49,60,65,68	0
2	SIA	G	401	21/21	0.83	0.30	60,76,84,89	0
2	SIA	C	401	21/21	0.83	0.31	57,68,73,86	0
2	SIA	a	401	21/21	0.83	0.21	53,62,67,69	0
3	CL	H	301	1/1	0.83	0.10	45,45,45,45	0
2	SIA	d	401	21/21	0.84	0.31	64,74,79,81	0
3	CL	H	302	1/1	0.84	0.07	48,48,48,48	0
2	SIA	Y	401	21/21	0.84	0.24	48,56,64,71	0
2	SIA	Z	401	21/21	0.84	0.20	50,65,70,72	0
3	CL	L	402	1/1	0.84	0.19	48,48,48,48	0
2	SIA	Q	401	21/21	0.84	0.25	47,55,60,63	0
3	CL	C	404	1/1	0.85	0.13	47,47,47,47	0
3	CL	G	402	1/1	0.85	0.12	58,58,58,58	0
3	CL	F	402	1/1	0.85	0.08	47,47,47,47	0
2	SIA	F	401	21/21	0.85	0.21	54,62,68,69	0
2	SIA	c	401	21/21	0.86	0.24	59,67,71,72	0
3	CL	N	402	1/1	0.86	0.10	54,54,54,54	0
2	SIA	R	401	21/21	0.86	0.22	48,60,68,77	0
2	SIA	I	401	21/21	0.86	0.26	51,60,62,63	0
2	SIA	j	401	21/21	0.86	0.21	49,60,64,65	0
2	SIA	f	401	21/21	0.86	0.22	52,61,63,66	0
2	SIA	n	401	21/21	0.87	0.28	67,73,82,82	0
3	CL	P	302	1/1	0.87	0.11	41,41,41,41	0
3	CL	d	403	1/1	0.87	0.12	43,43,43,43	0
3	CL	h	301	1/1	0.87	0.08	44,44,44,44	0
2	SIA	b	401	21/21	0.87	0.24	47,60,63,66	0
3	CL	G	403	1/1	0.88	0.10	43,43,43,43	0
3	CL	R	402	1/1	0.88	0.10	50,50,50,50	0
2	SIA	J	401	21/21	0.88	0.17	43,51,55,57	0
2	SIA	e	401	21/21	0.88	0.24	51,62,63,65	0
2	SIA	K	401	21/21	0.88	0.24	49,57,64,78	0
2	SIA	A	401	21/21	0.88	0.19	42,50,59,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	U	302	1/1	0.89	0.07	47,47,47,47	0
2	SIA	O	401	21/21	0.89	0.22	45,50,54,58	0
2	SIA	S	401	21/21	0.89	0.25	55,59,68,68	0
3	CL	F	403	1/1	0.89	0.11	45,45,45,45	0
3	CL	d	402	1/1	0.89	0.11	45,45,45,45	0
3	CL	M	402	1/1	0.90	0.12	41,41,41,41	0
3	CL	Y	403	1/1	0.90	0.08	47,47,47,47	0
2	SIA	B	401	21/21	0.90	0.24	46,49,60,69	0
3	CL	S	403	1/1	0.90	0.14	44,44,44,44	0
3	CL	X	403	1/1	0.90	0.14	50,50,50,50	0
2	SIA	N	401	21/21	0.90	0.16	38,46,52,54	0
2	SIA	M	401	21/21	0.90	0.19	38,43,46,46	0
2	SIA	E	401	21/21	0.90	0.20	42,50,62,64	0
3	CL	B	402	1/1	0.90	0.07	52,52,52,52	0
3	CL	O	402	1/1	0.91	0.12	47,47,47,47	0
3	CL	n	403	1/1	0.91	0.12	48,48,48,48	0
2	SIA	L	401	21/21	0.91	0.16	37,42,44,46	0
3	CL	Q	403	1/1	0.91	0.07	49,49,49,49	0
3	CL	f	403	1/1	0.91	0.07	47,47,47,47	0
3	CL	g	301	1/1	0.92	0.11	52,52,52,52	0
3	CL	A	402	1/1	0.92	0.09	45,45,45,45	0
3	CL	X	402	1/1	0.92	0.06	44,44,44,44	0
3	CL	N	403	1/1	0.93	0.14	43,43,43,43	0
3	CL	W	301	1/1	0.94	0.13	37,37,37,37	0
3	CL	V	402	1/1	0.94	0.06	43,43,43,43	0
3	CL	Z	403	1/1	0.94	0.06	45,45,45,45	0
3	CL	Y	402	1/1	0.94	0.14	39,39,39,39	0
3	CL	c	402	1/1	0.95	0.12	43,43,43,43	0
3	CL	T	402	1/1	0.95	0.08	46,46,46,46	0
3	CL	J	403	1/1	0.96	0.17	42,42,42,42	0
3	CL	D	301	1/1	0.96	0.08	36,36,36,36	0
3	CL	f	402	1/1	0.96	0.08	40,40,40,40	0
3	CL	I	402	1/1	0.96	0.05	40,40,40,40	0
3	CL	M	403	1/1	0.96	0.11	38,38,38,38	0
4	MG	C	405	1/1	0.96	0.17	12,12,12,12	0
3	CL	C	403	1/1	0.96	0.12	41,41,41,41	0
3	CL	J	402	1/1	0.96	0.06	39,39,39,39	0
3	CL	Z	402	1/1	0.96	0.09	49,49,49,49	0
3	CL	j	402	1/1	0.97	0.11	51,51,51,51	0
3	CL	Q	402	1/1	0.97	0.20	46,46,46,46	0
3	CL	P	301	1/1	0.97	0.16	41,41,41,41	0
3	CL	C	402	1/1	0.98	0.15	46,46,46,46	0

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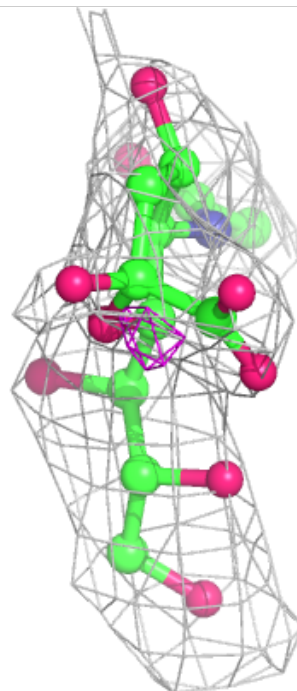
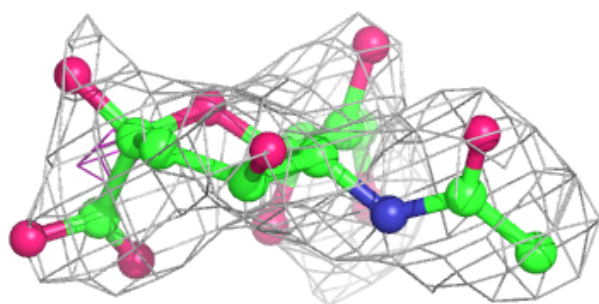
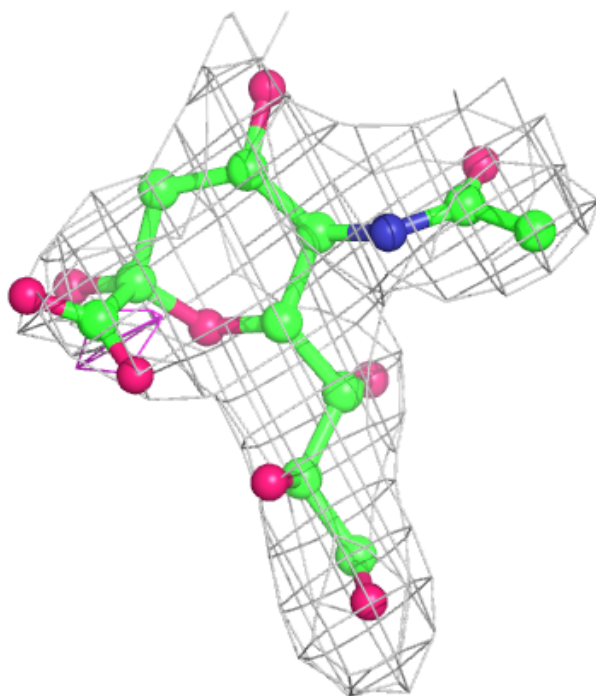
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CL	e	402	1/1	0.98	0.14	43,43,43,43	0
3	CL	U	301	1/1	0.98	0.13	27,27,27,27	0
3	CL	n	402	1/1	0.98	0.04	39,39,39,39	0
3	CL	e	403	1/1	0.98	0.06	51,51,51,51	0

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.

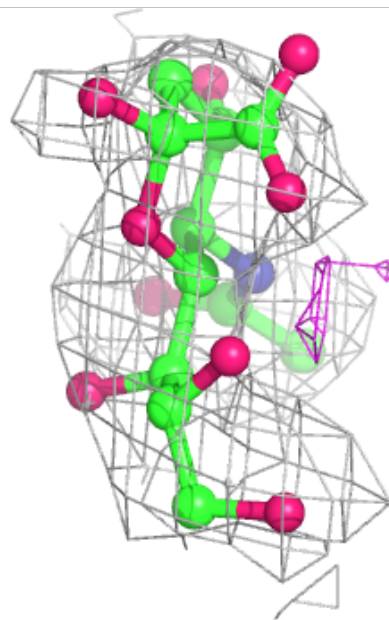
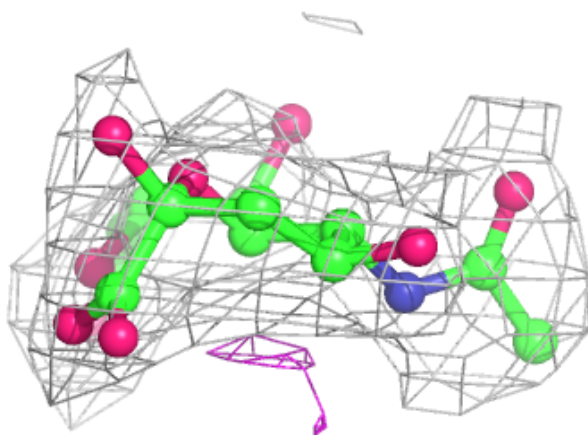
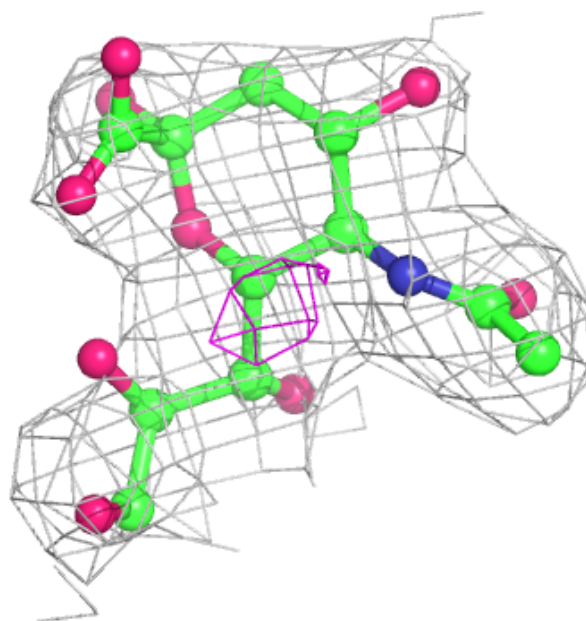
Electron density around SIA V 401:

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



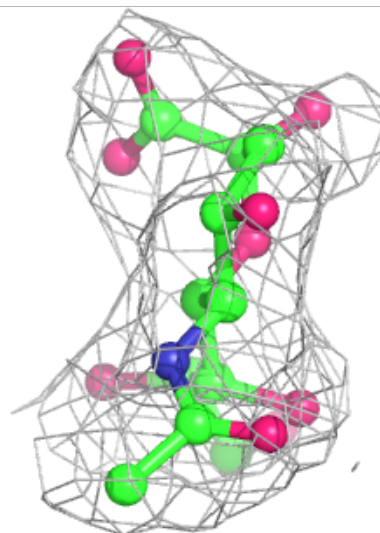
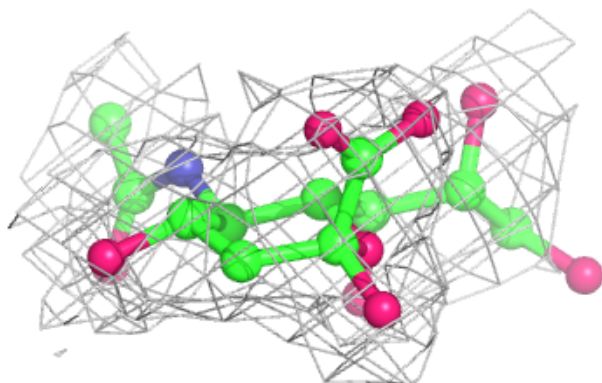
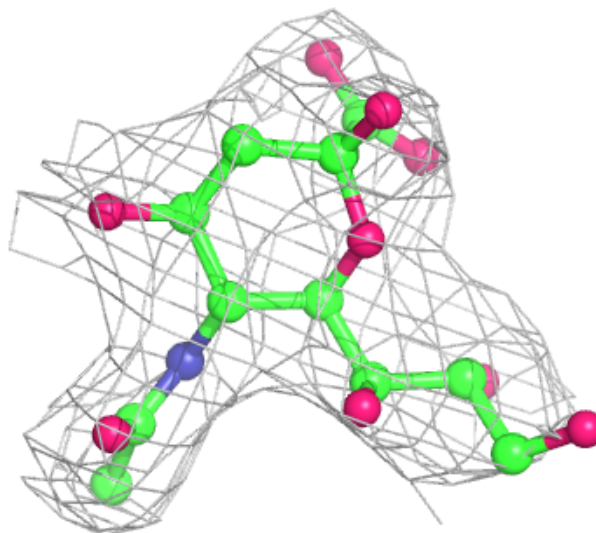
Electron density around SIA X 401:

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



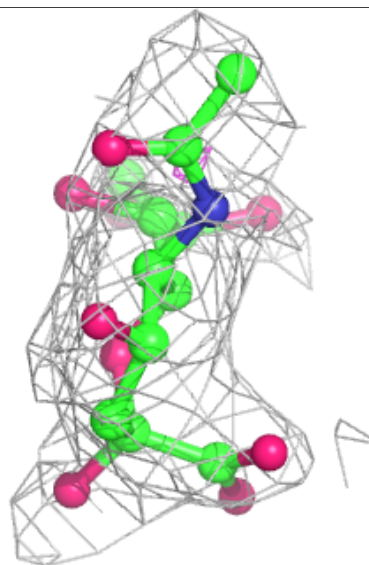
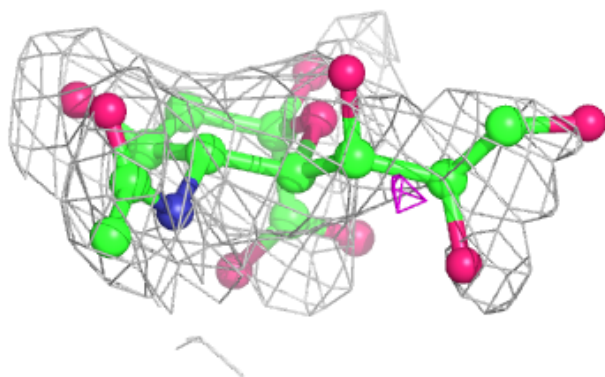
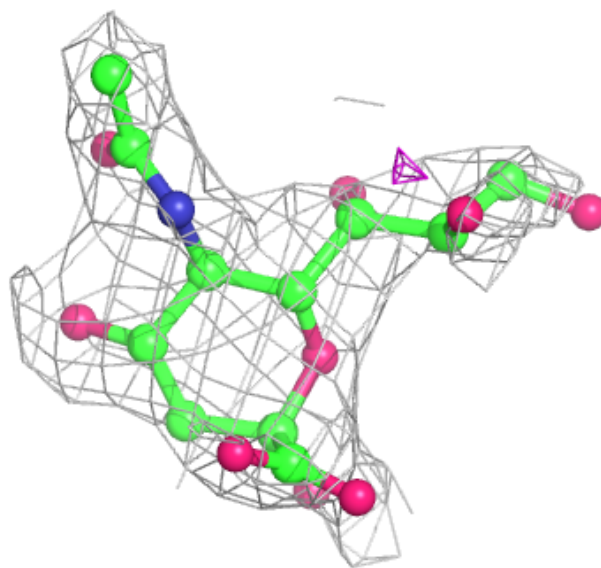
Electron density around SIA T 401:

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and green (positive)



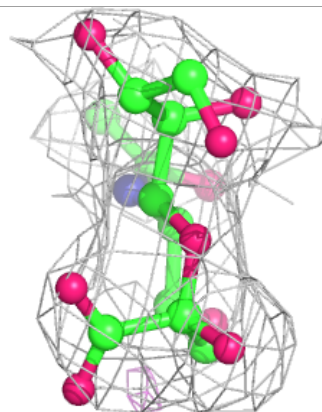
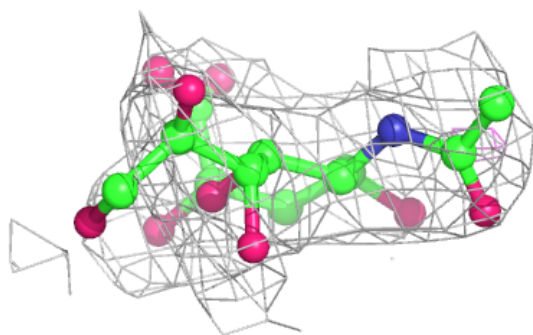
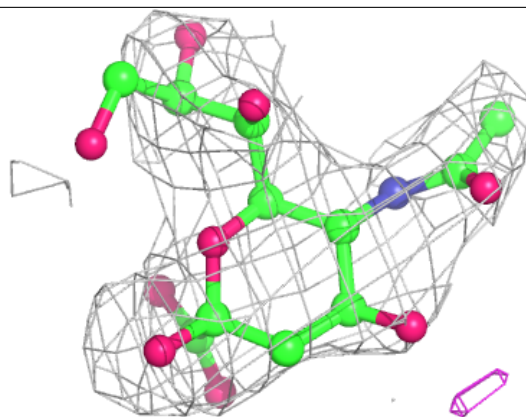
Electron density around SIA G 401:

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



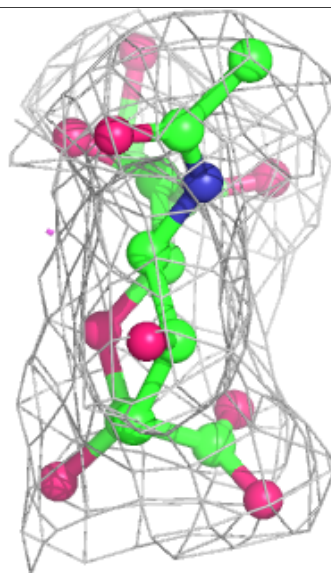
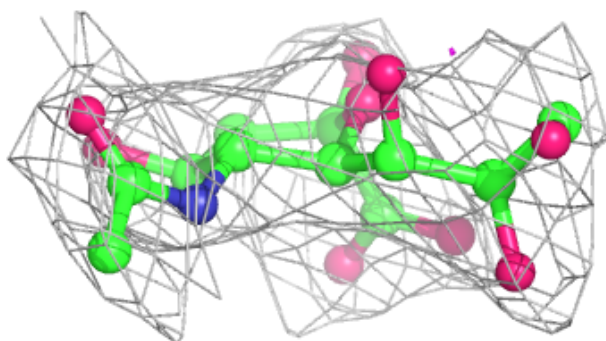
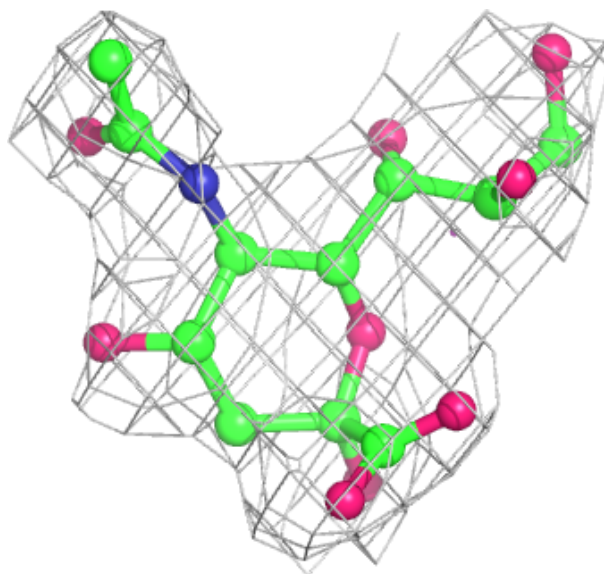
Electron density around SIA C 401:

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



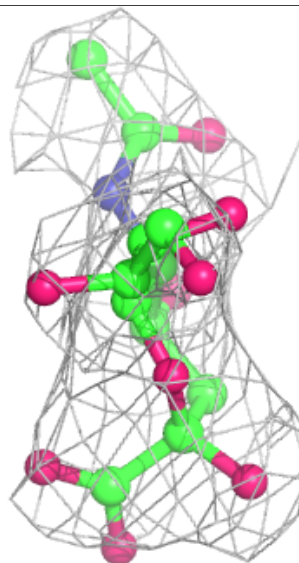
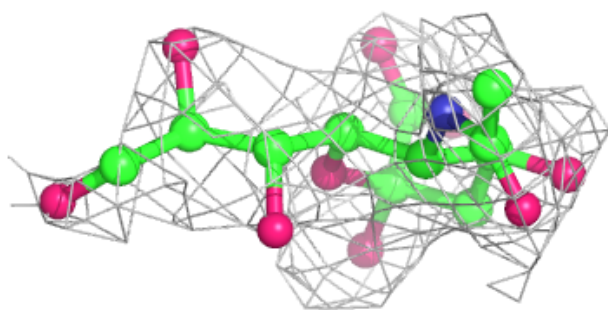
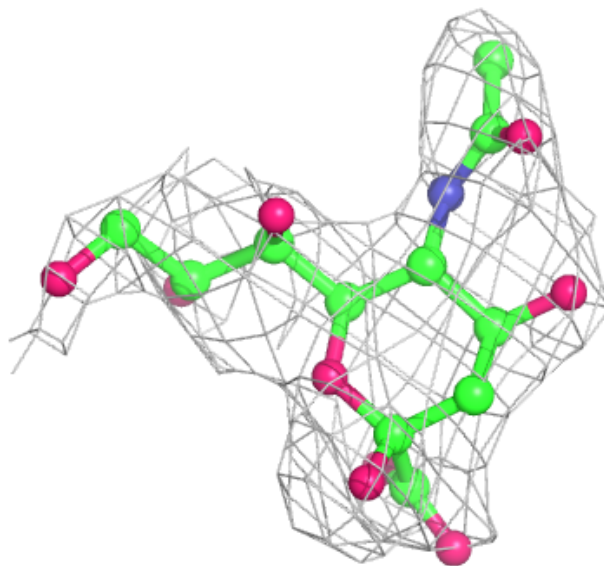
Electron density around SIA a 401:

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



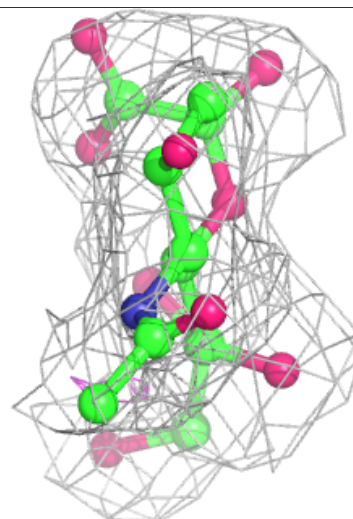
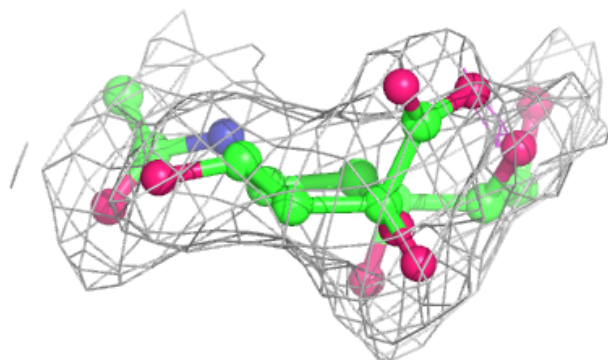
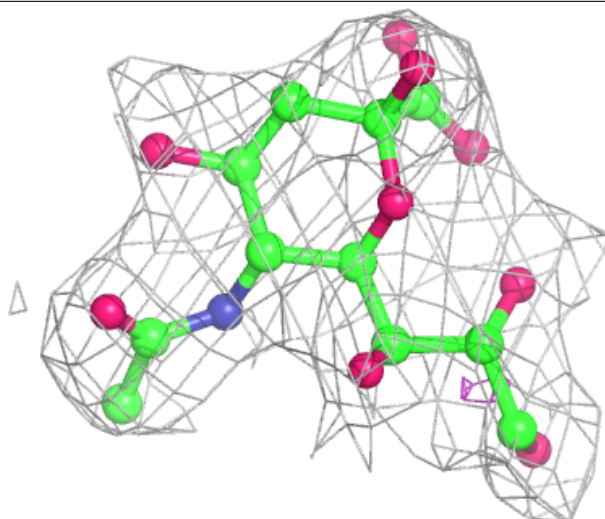
Electron density around SIA d 401:

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



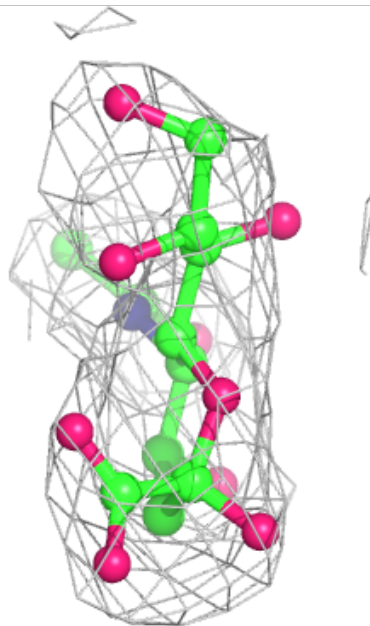
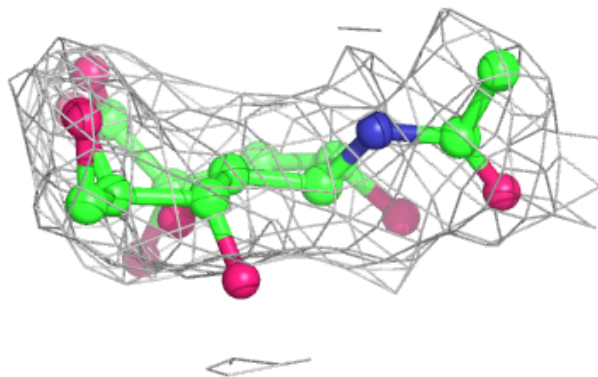
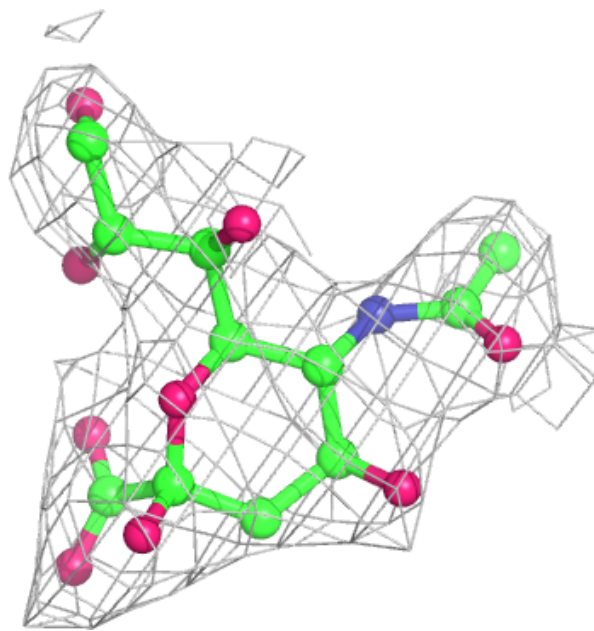
Electron density around SIA Y 401:

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and green (positive)



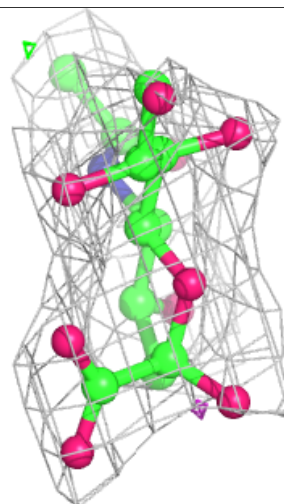
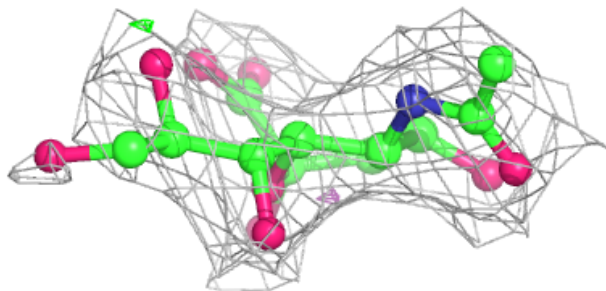
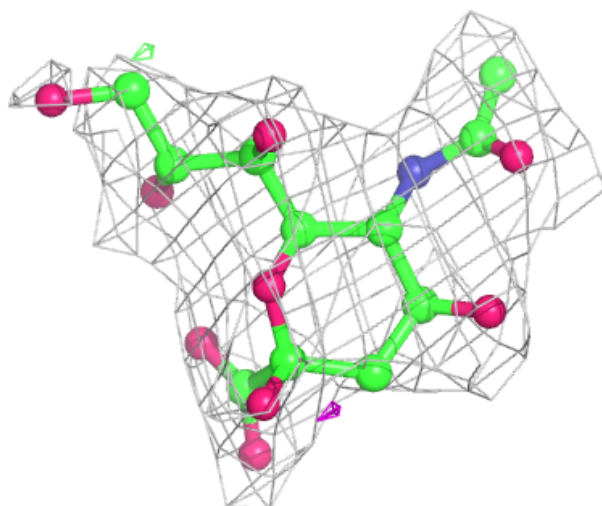
Electron density around SIA Z 401:

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and green (positive)



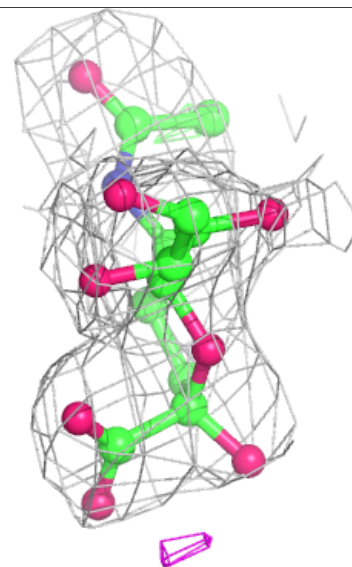
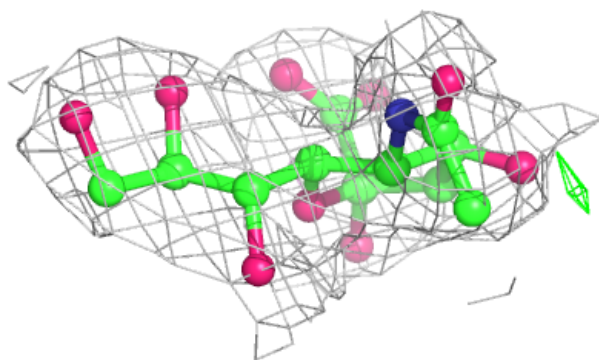
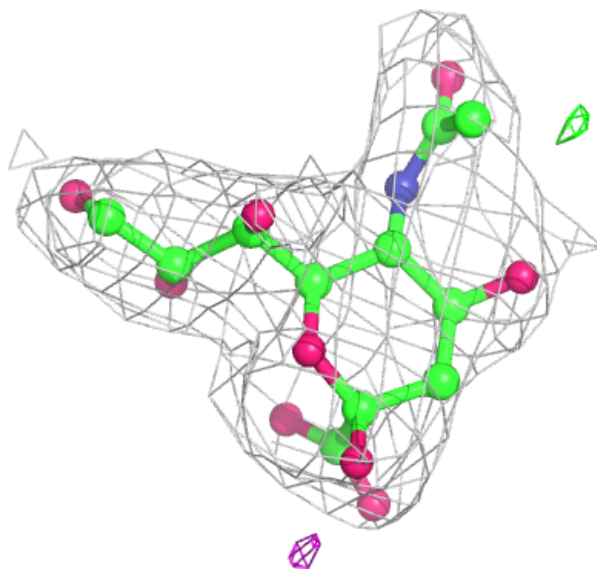
Electron density around SIA Q 401:

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and green (positive)



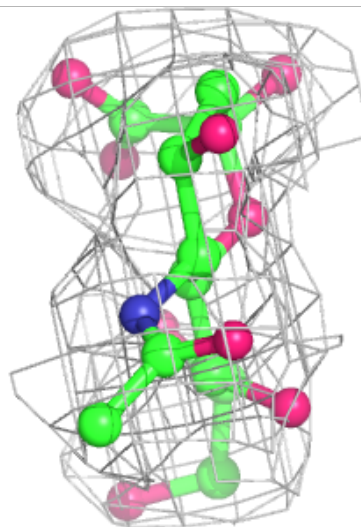
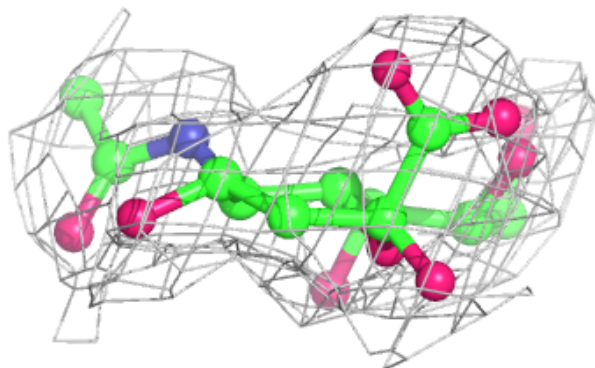
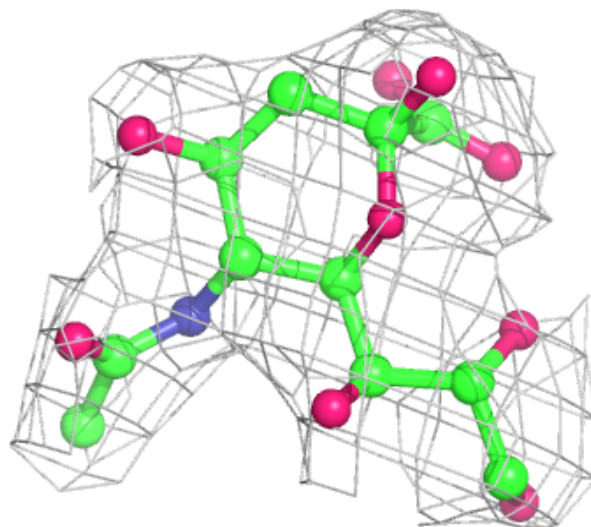
Electron density around SIA F 401:

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



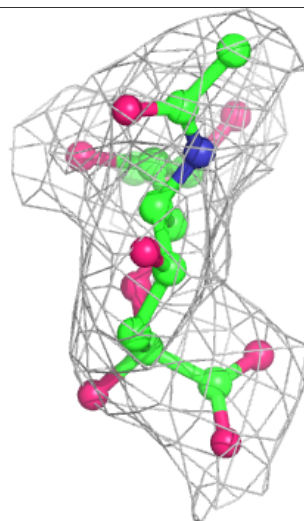
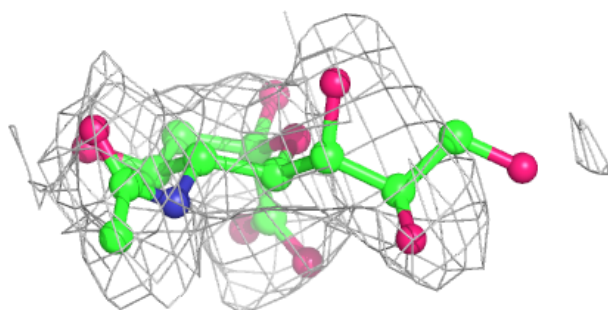
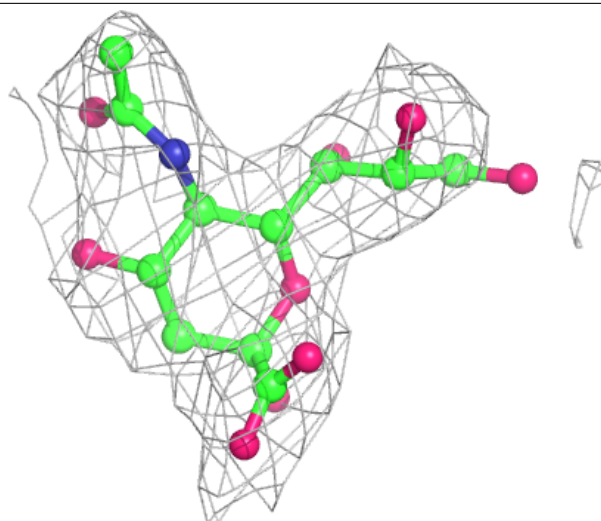
Electron density around SIA c 401:

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



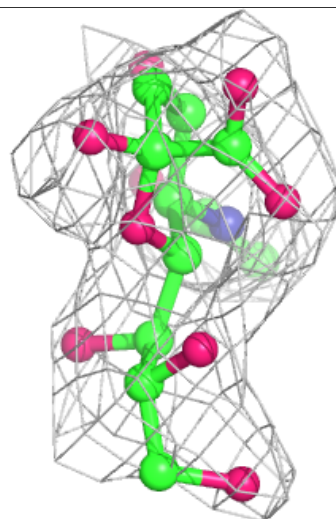
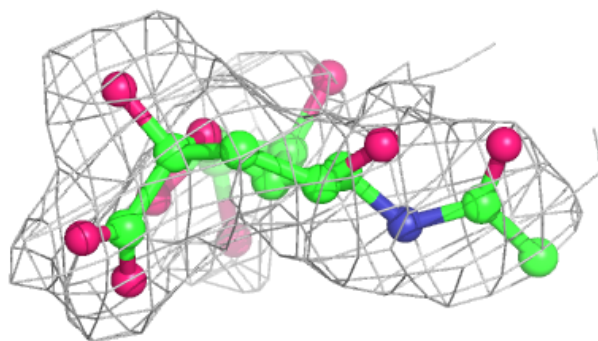
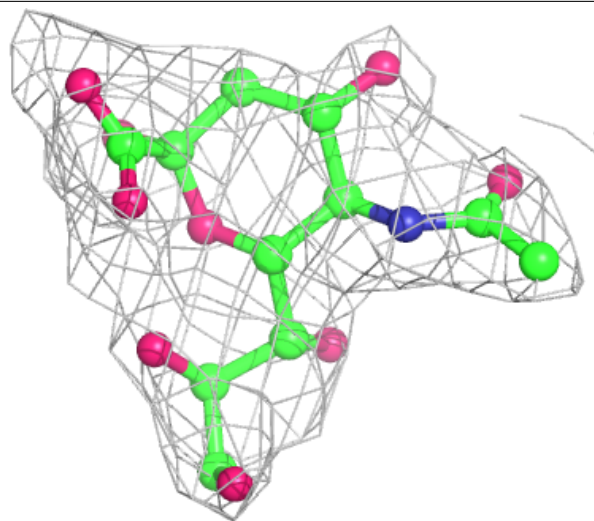
Electron density around SIA R 401:

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



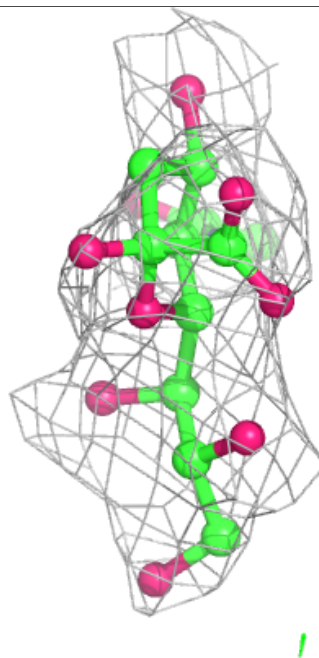
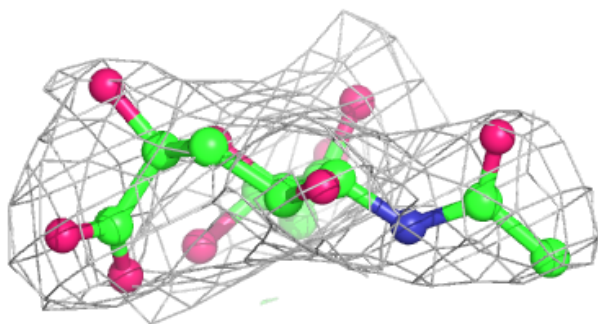
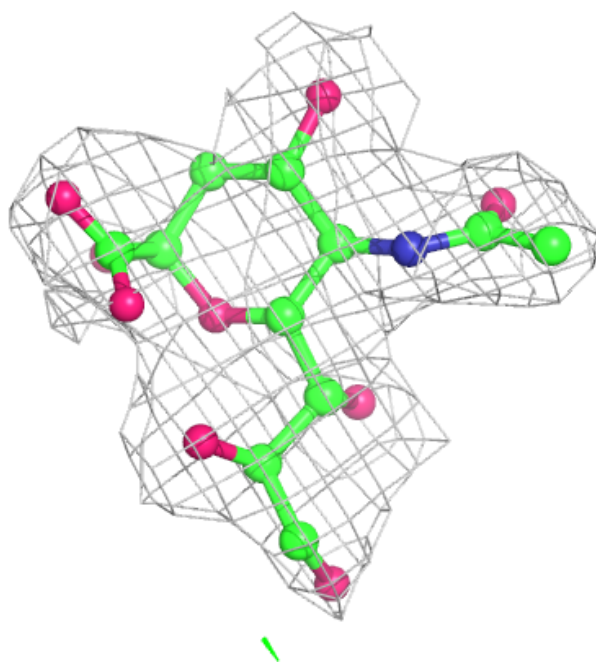
Electron density around SIA I 401:

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



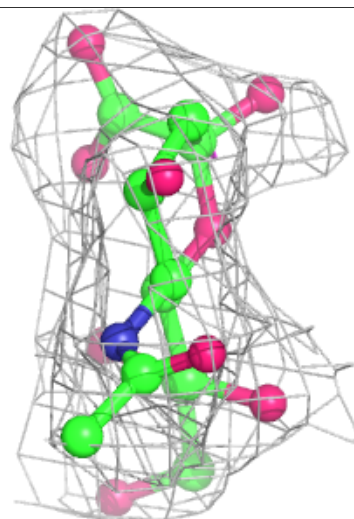
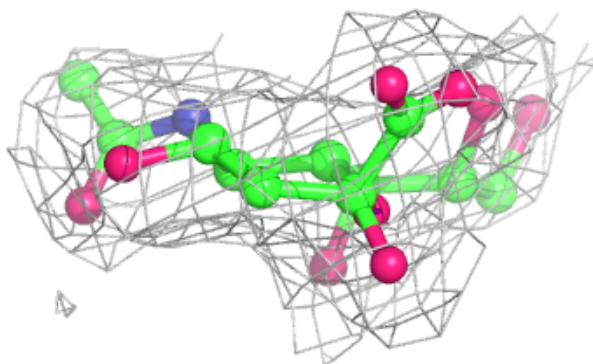
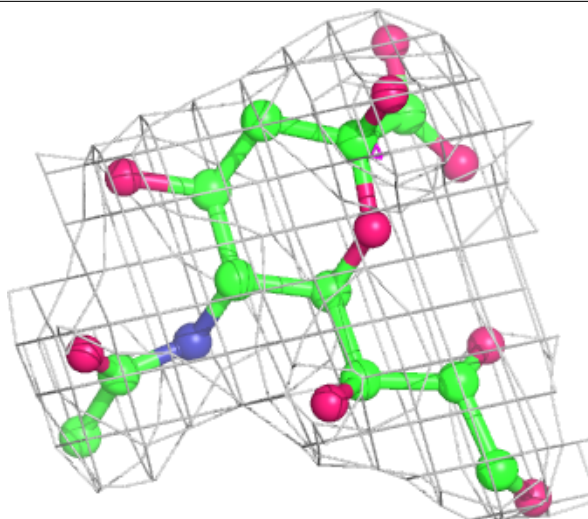
Electron density around SIA j 401:

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



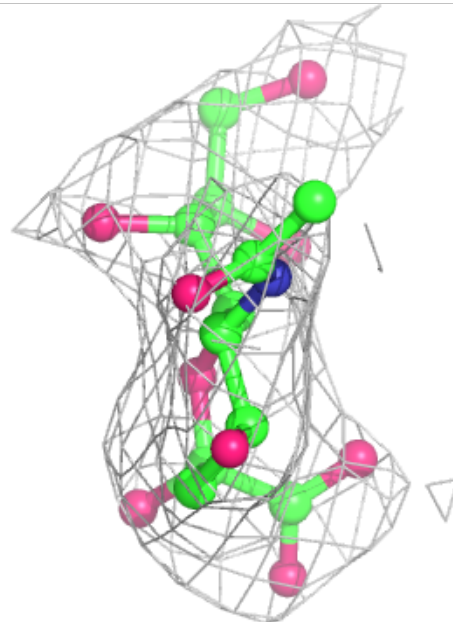
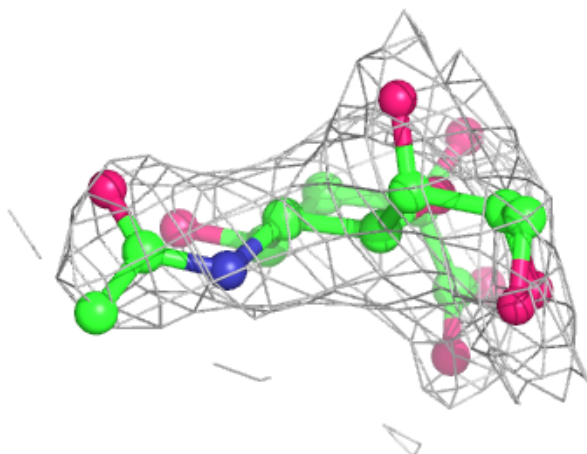
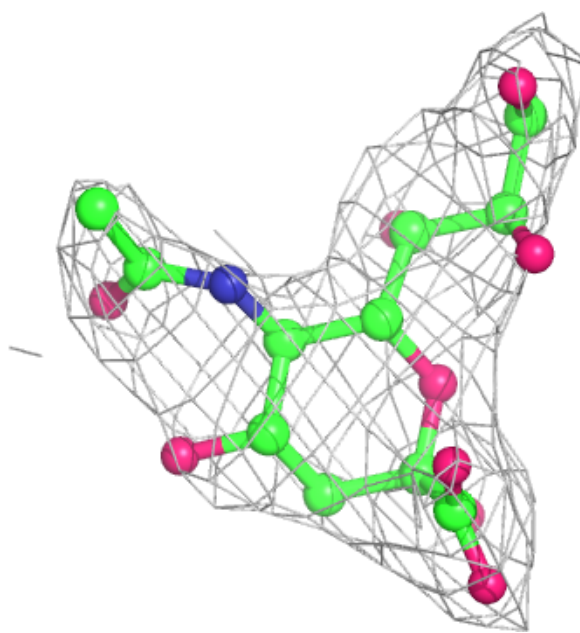
Electron density around SIA f 401:

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



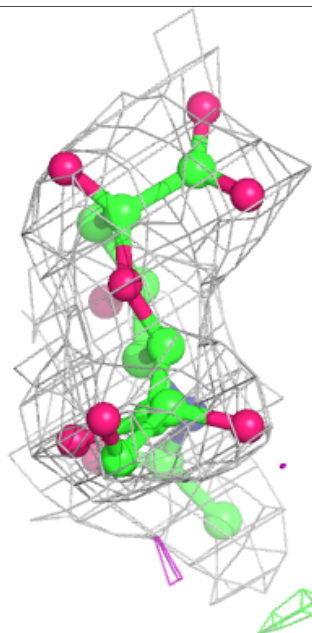
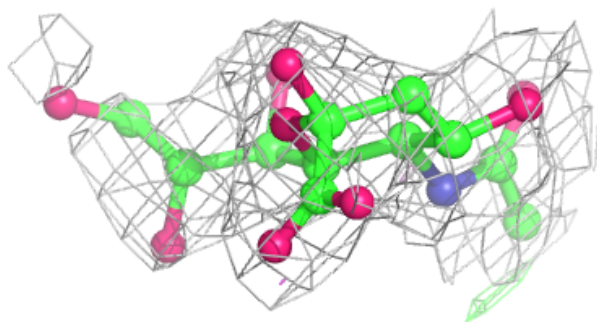
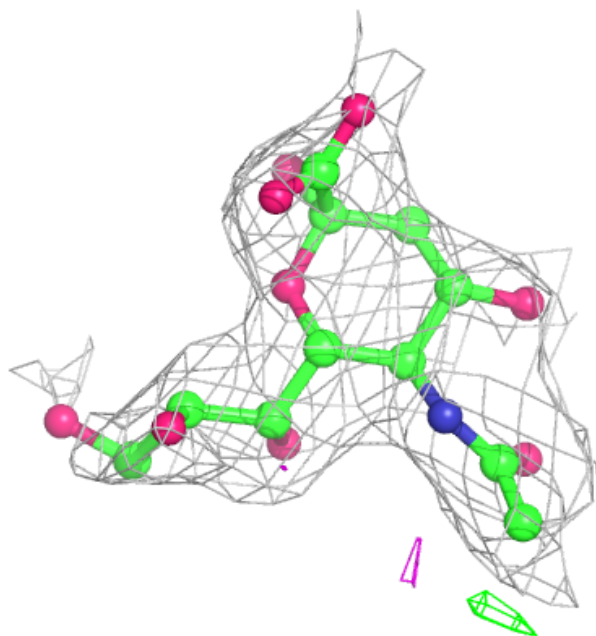
Electron density around SIA n 401:

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



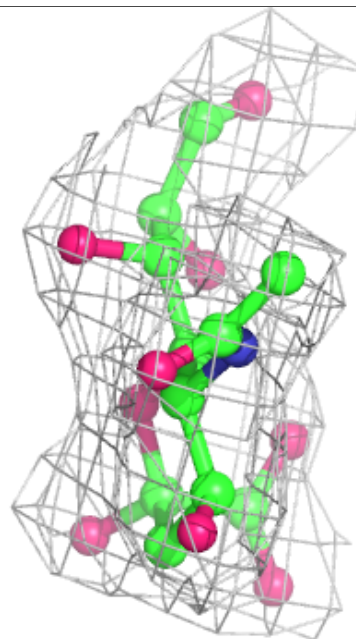
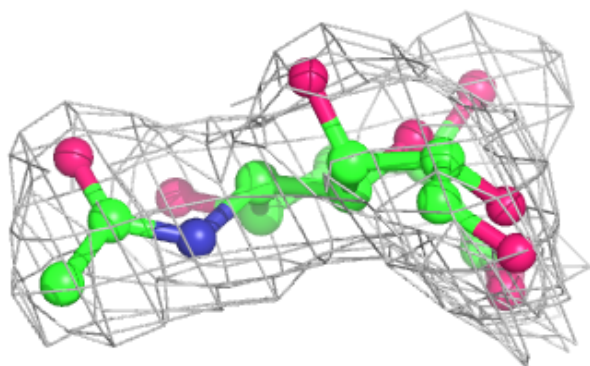
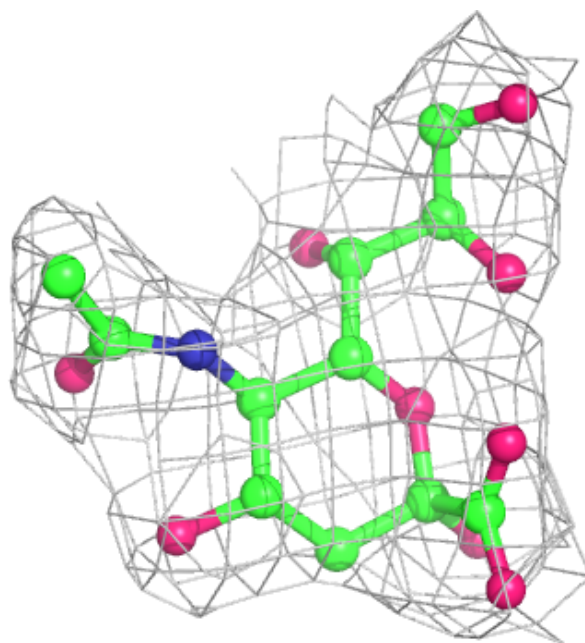
Electron density around SIA b 401:

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



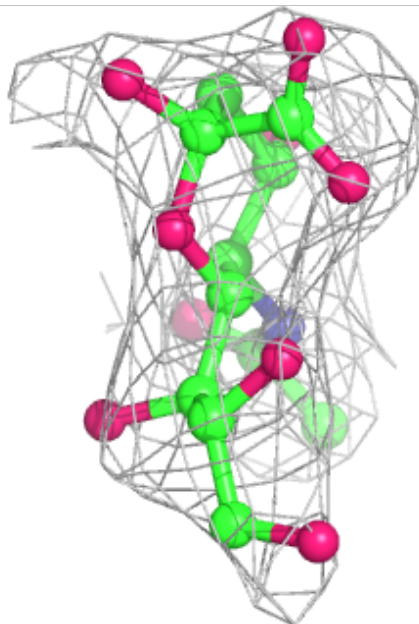
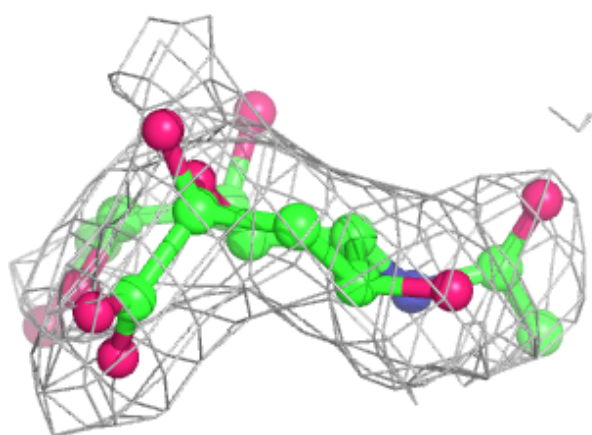
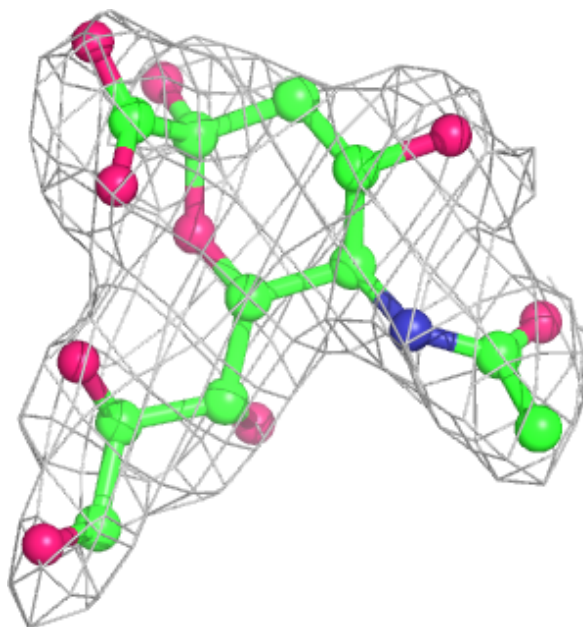
Electron density around SIA J 401:

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



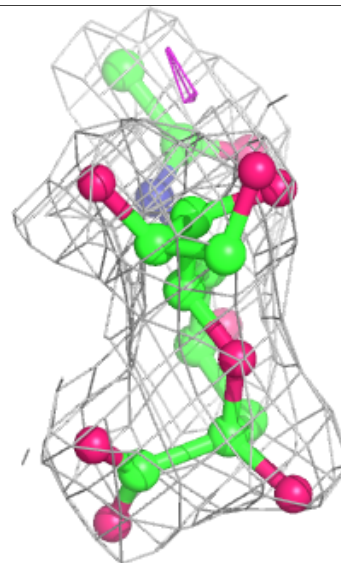
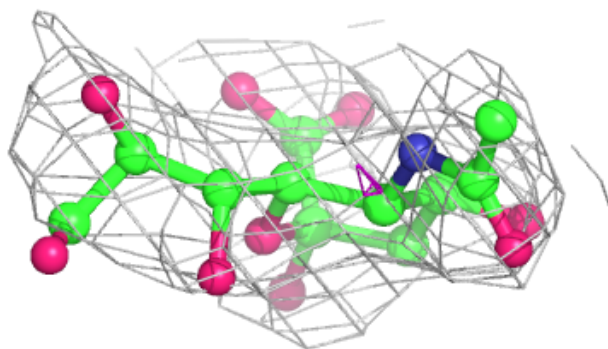
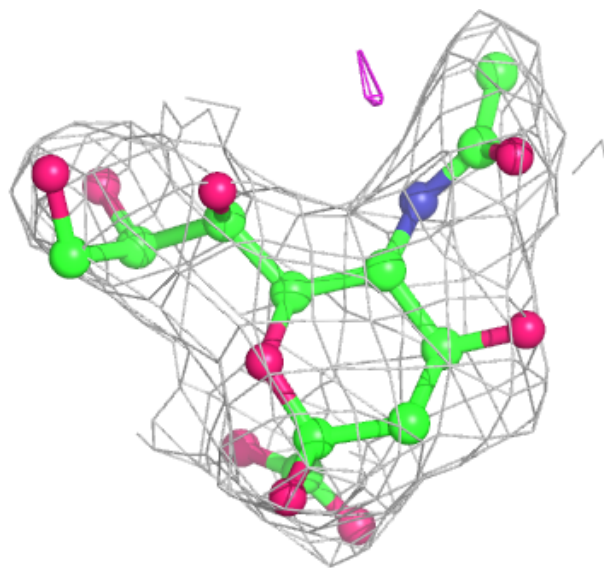
Electron density around SIA e 401:

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



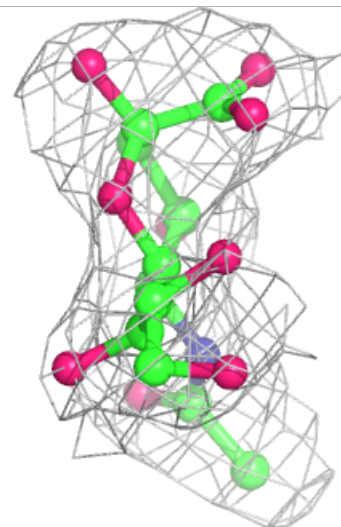
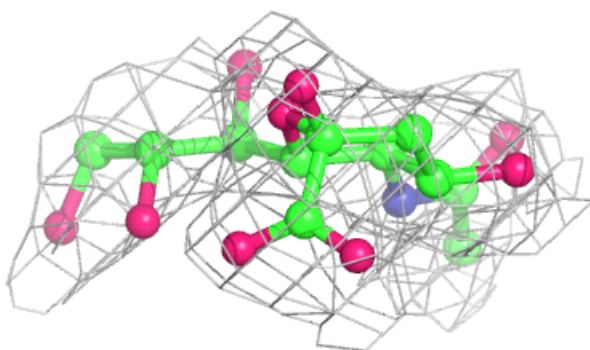
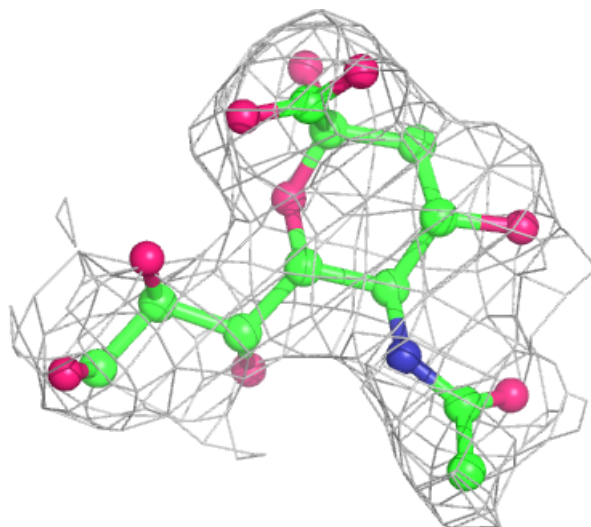
Electron density around SIA K 401:

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



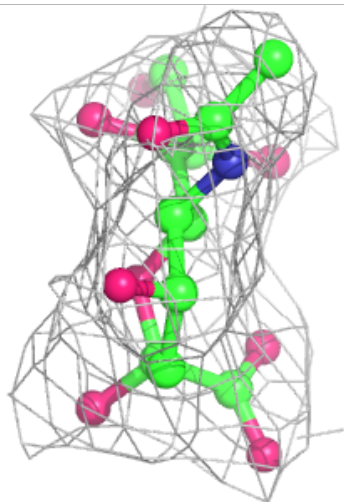
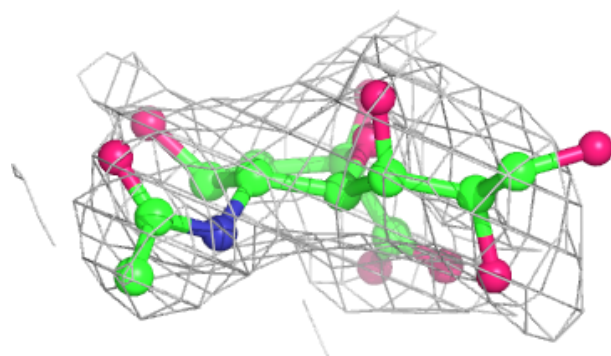
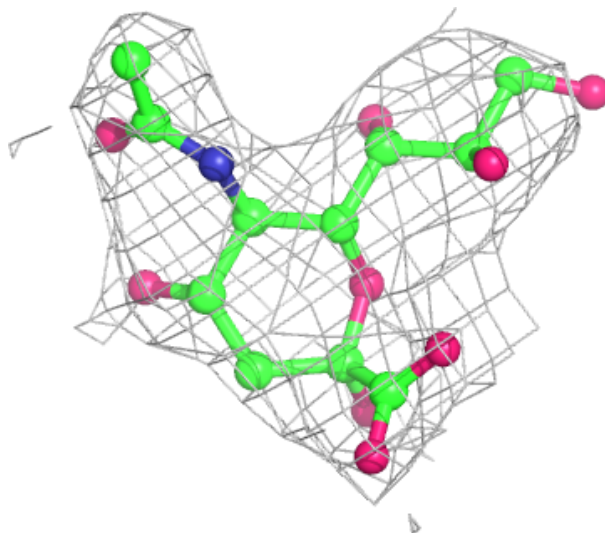
Electron density around SIA A 401:

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



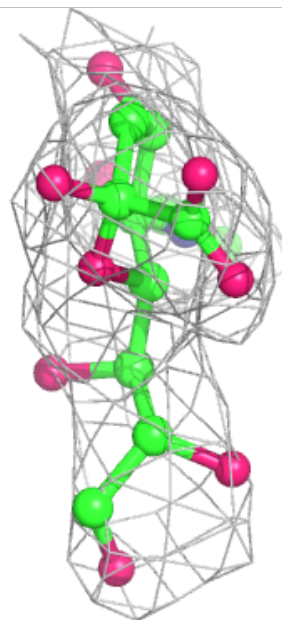
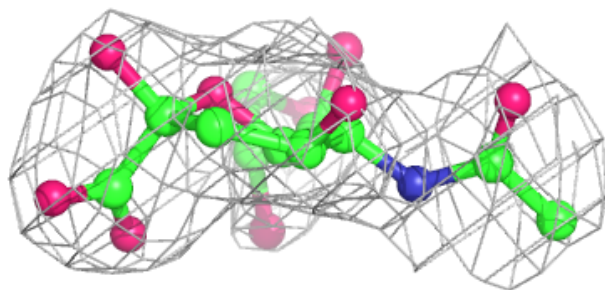
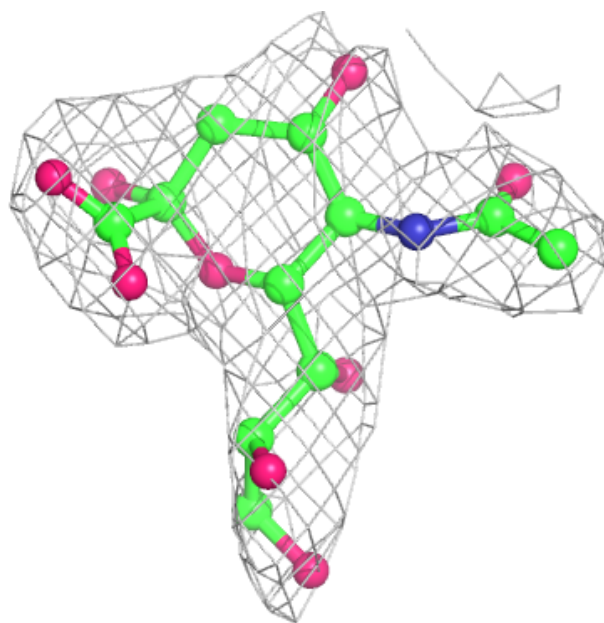
Electron density around SIA O 401:

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



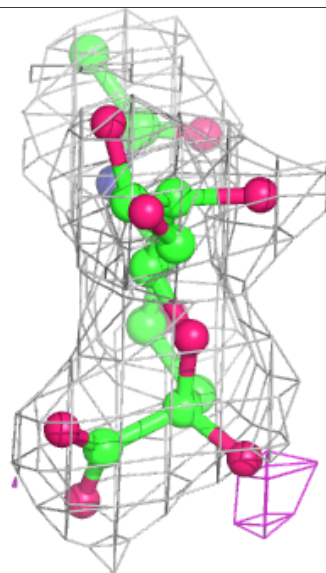
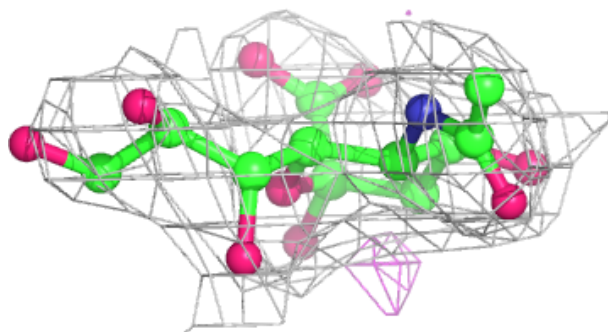
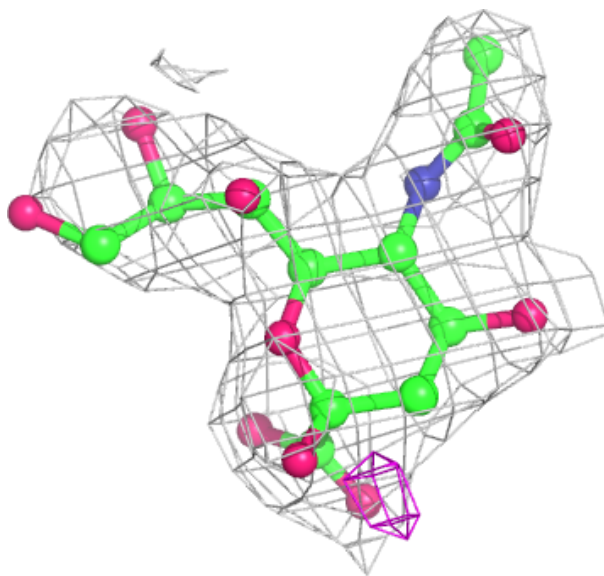
Electron density around SIA S 401:

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



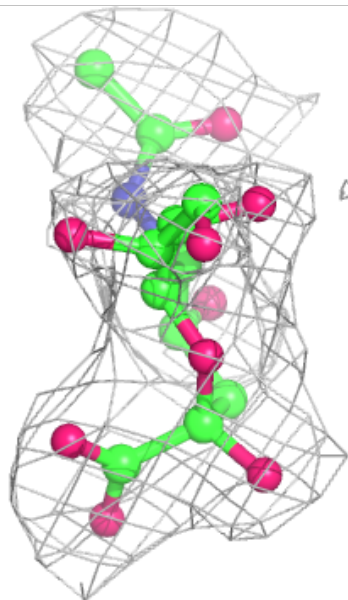
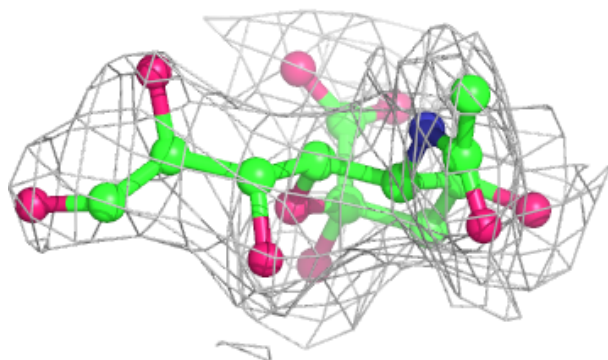
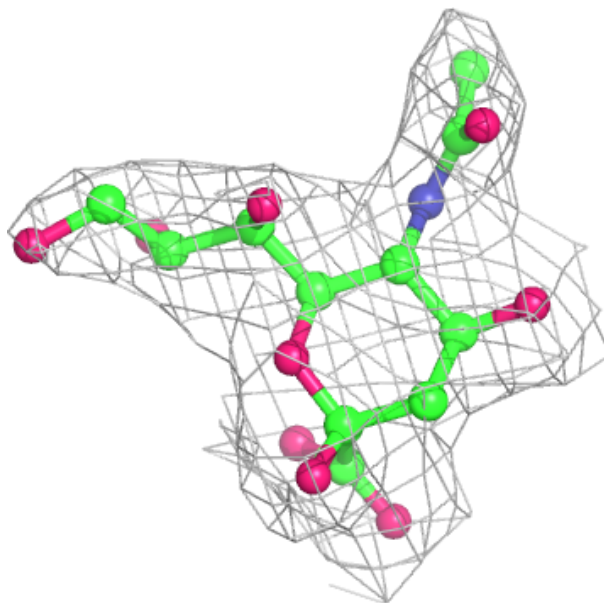
Electron density around SIA B 401:

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



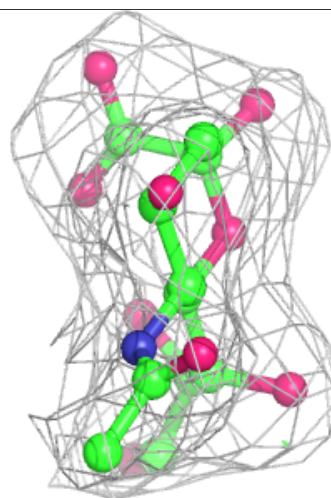
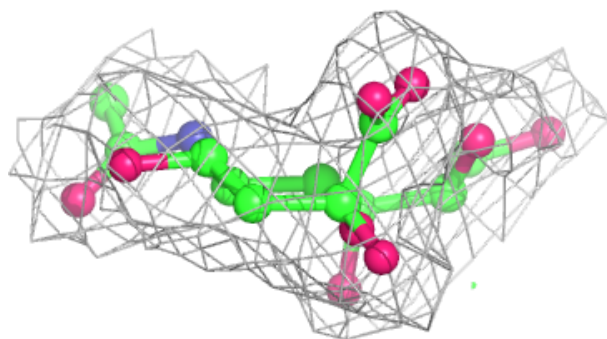
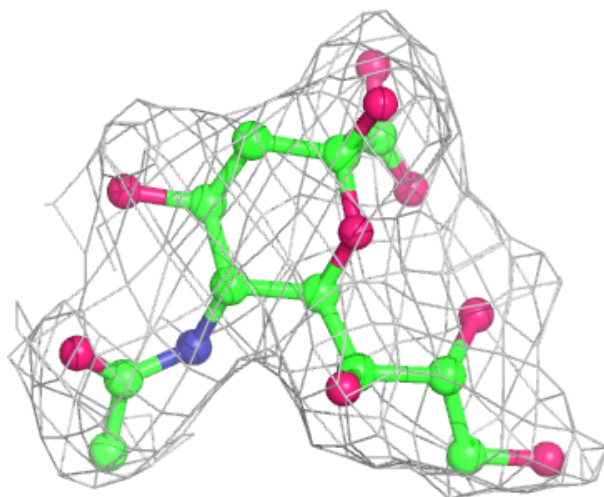
Electron density around SIA N 401:

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



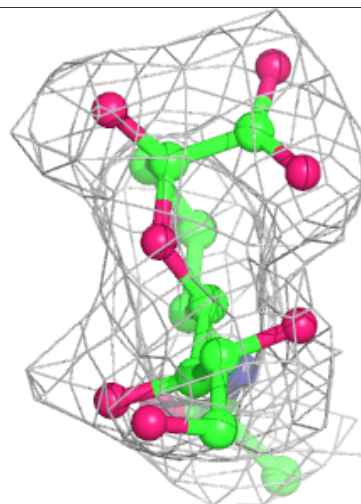
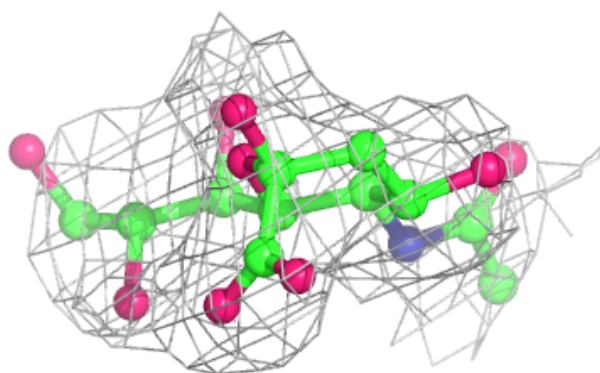
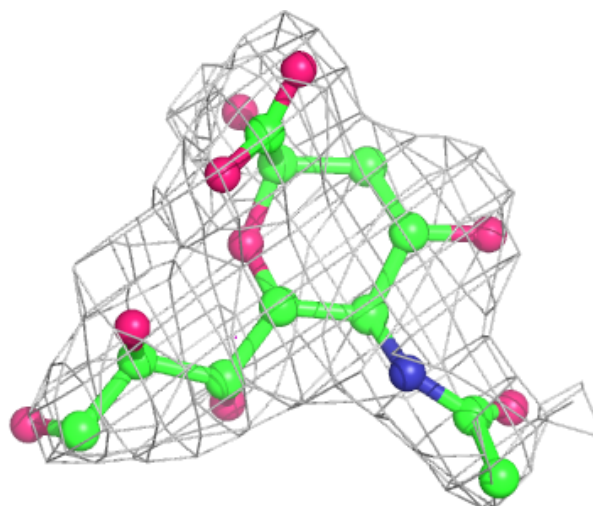
Electron density around SIA M 401:

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



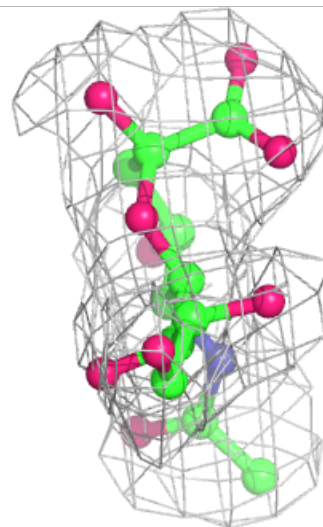
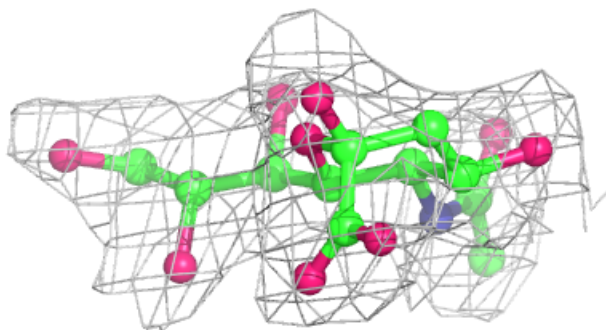
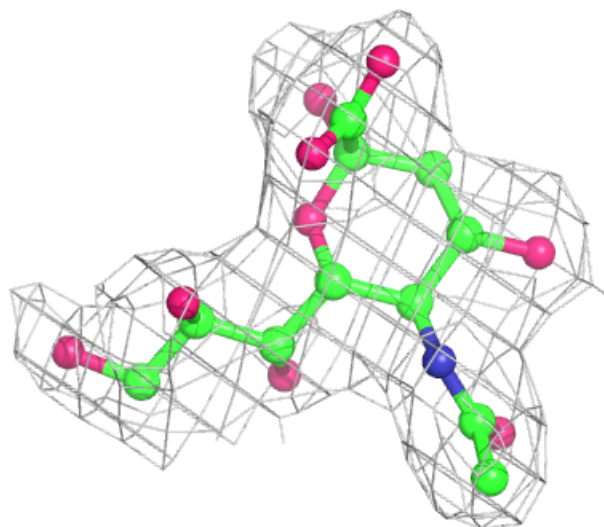
Electron density around SIA E 401:

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



Electron density around SIA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.