Full wwPDB X-ray Structure Validation 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-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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

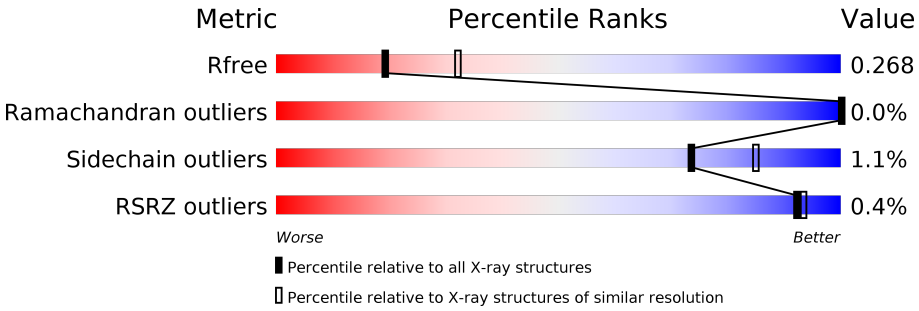
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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 <=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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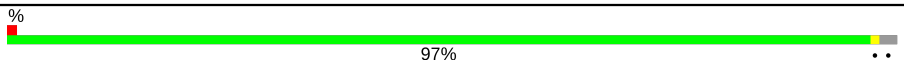
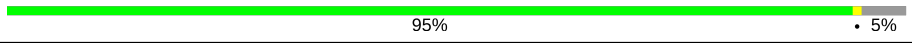
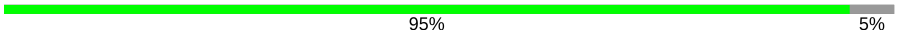
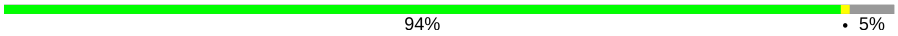
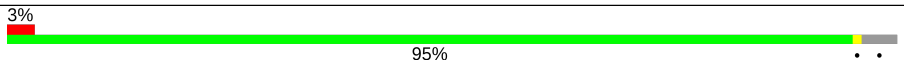
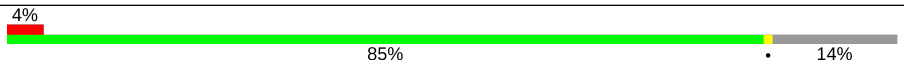
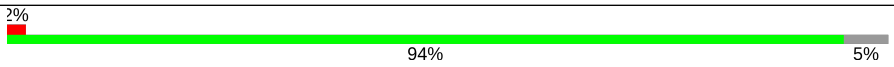
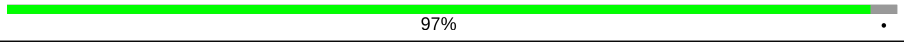
Mol	Chain	Length	Quality of chain
1	g	274	
1	h	274	
1	i	274	
1	j	274	
1	k	274	
1	l	274	
1	m	274	
1	n	274	

2 Entry composition

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

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

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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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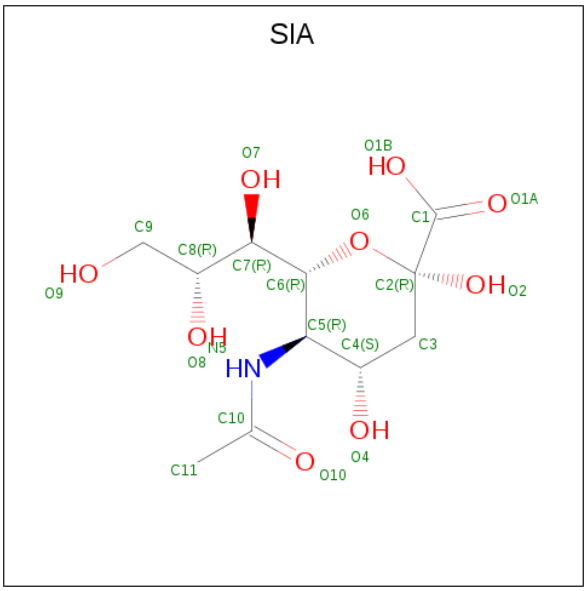
Chain	Residue	Modelled	Actual	Comment	Reference
h	20	HIS	-	expression tag	UNP R4UMH0
h	21	MET	-	expression tag	UNP R4UMH0
h	78	SER	CYS	conflict	UNP R4UMH0
h	92	SER	CYS	conflict	UNP R4UMH0
i	18	GLY	-	expression tag	UNP R4UMH0
i	19	SER	-	expression tag	UNP R4UMH0
i	20	HIS	-	expression tag	UNP R4UMH0
i	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: $C_{11}H_{19}NO_9$) (labeled as "Ligand of Interest" by author).



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

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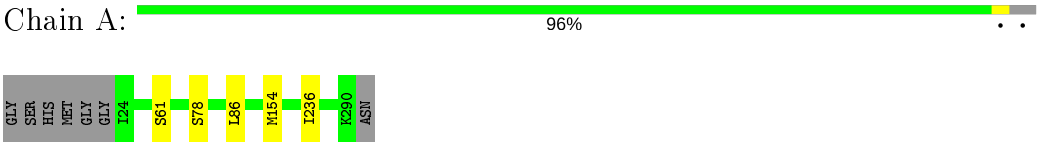
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	e	50	Total O 50 50	0	0
5	f	33	Total O 33 33	0	0
5	g	34	Total O 34 34	0	0
5	h	32	Total O 32 32	0	0
5	i	39	Total O 39 39	0	0
5	j	25	Total O 25 25	0	0
5	k	15	Total O 15 15	0	0
5	l	15	Total O 15 15	0	0
5	m	11	Total O 11 11	0	0
5	n	35	Total O 35 35	0	0

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.

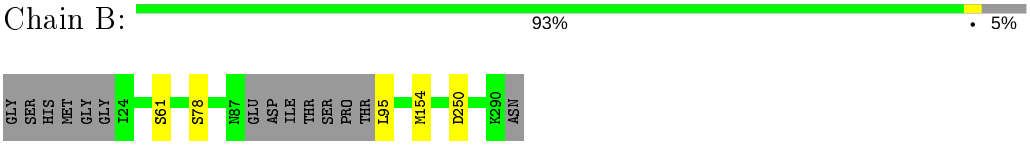
- Molecule 1: Capsid protein VP1

Chain A:



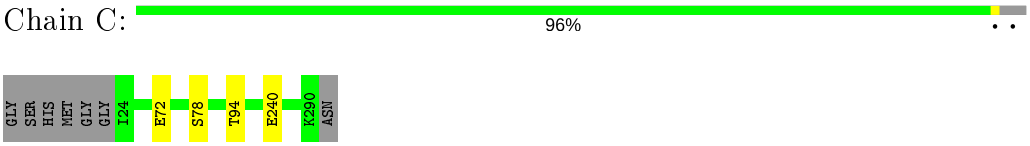
- Molecule 1: Capsid protein VP1

Chain B:



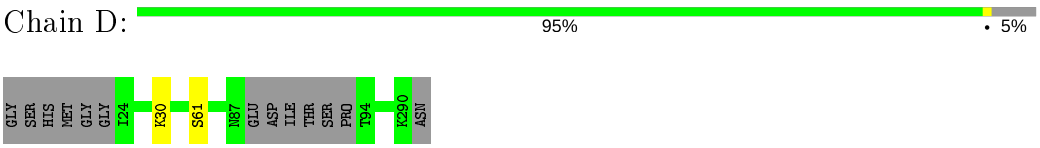
- Molecule 1: Capsid protein VP1

Chain C:



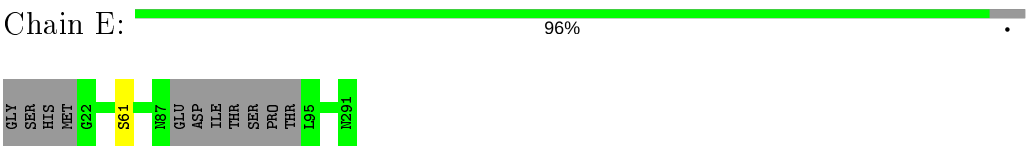
- Molecule 1: Capsid protein VP1

Chain D:



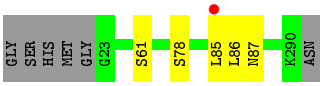
- Molecule 1: Capsid protein VP1

Chain E:



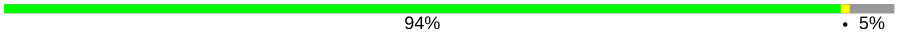
- Molecule 1: Capsid protein VP1

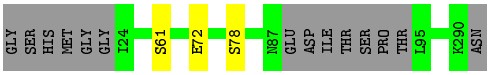
Chain F:



• Molecule 1: Capsid protein VP1

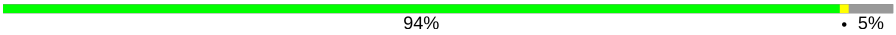
Chain G:





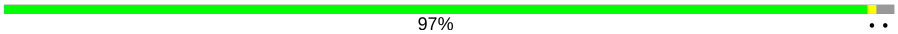
• Molecule 1: Capsid protein VP1

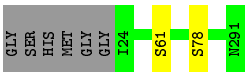
Chain H:



• Molecule 1: Capsid protein VP1

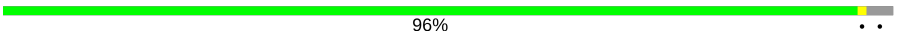
Chain I:

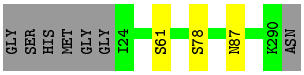




• Molecule 1: Capsid protein VP1

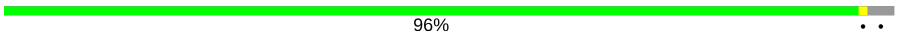
Chain J:

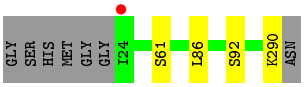




• Molecule 1: Capsid protein VP1

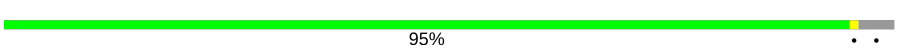
Chain K:

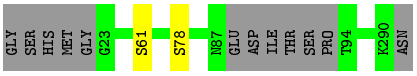




• Molecule 1: Capsid protein VP1

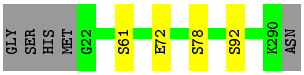
Chain L:





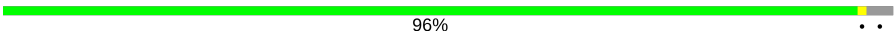
• Molecule 1: Capsid protein VP1

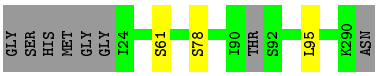
Chain M:



• Molecule 1: Capsid protein VP1

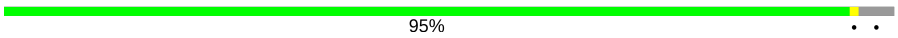
Chain N:





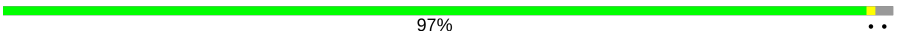
• Molecule 1: Capsid protein VP1

Chain O:



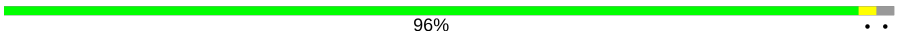
• Molecule 1: Capsid protein VP1

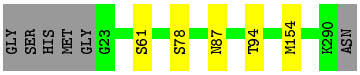
Chain P:



• Molecule 1: Capsid protein VP1

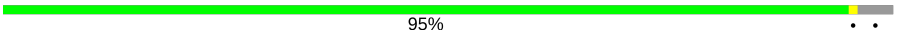
Chain Q:

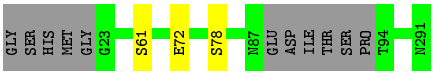




• Molecule 1: Capsid protein VP1

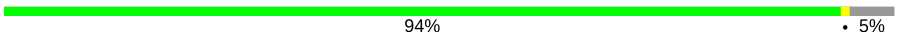
Chain R:

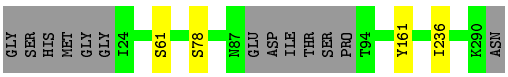




• Molecule 1: Capsid protein VP1

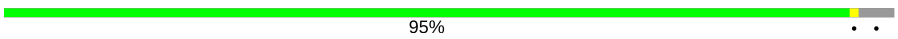
Chain S:





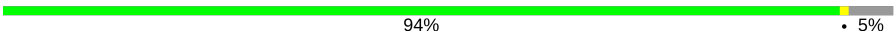
• Molecule 1: Capsid protein VP1

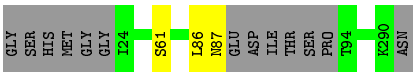
Chain T:



• Molecule 1: Capsid protein VP1

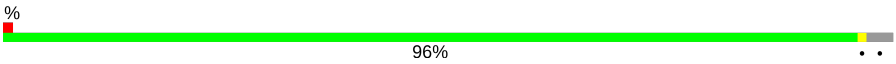
Chain U:

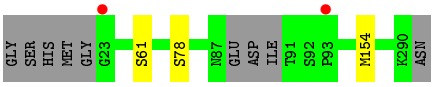




• Molecule 1: Capsid protein VP1

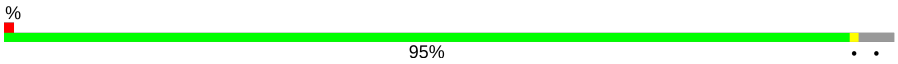
Chain V:

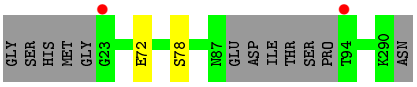




• Molecule 1: Capsid protein VP1

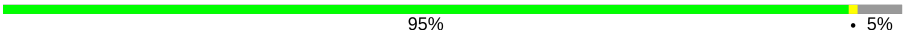
Chain W:

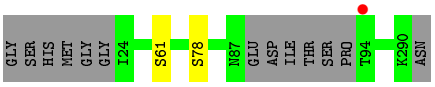




• Molecule 1: Capsid protein VP1

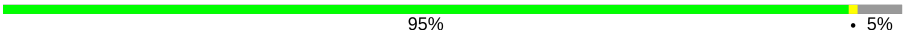
Chain X:

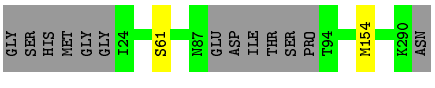




• Molecule 1: Capsid protein VP1

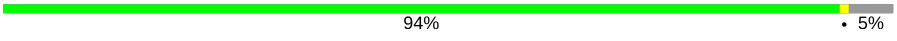
Chain Y:

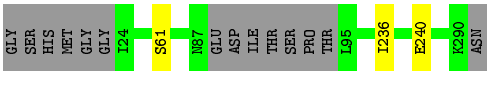




• Molecule 1: Capsid protein VP1

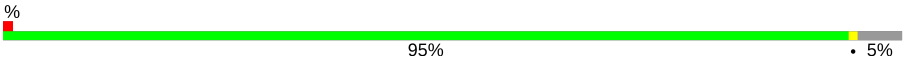
Chain Z:





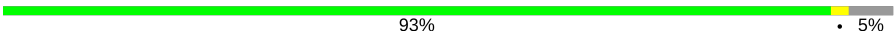
• Molecule 1: Capsid protein VP1

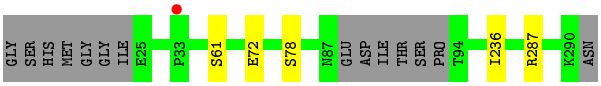
Chain a:



• Molecule 1: Capsid protein VP1

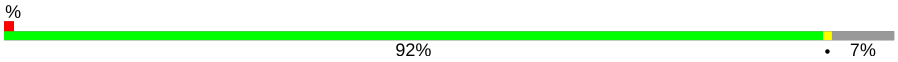
Chain b:

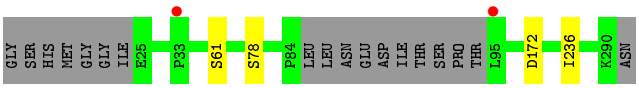




• Molecule 1: Capsid protein VP1

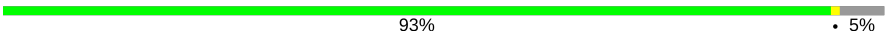
Chain c:

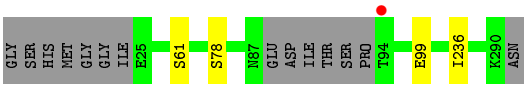




• Molecule 1: Capsid protein VP1

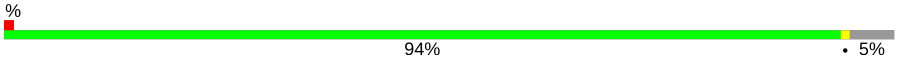
Chain d:

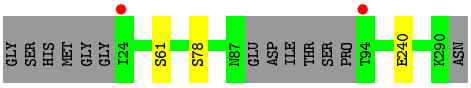




• Molecule 1: Capsid protein VP1

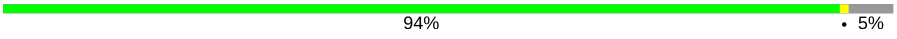
Chain e:

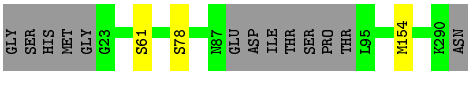




• Molecule 1: Capsid protein VP1

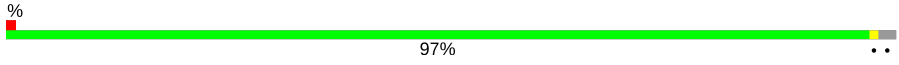
Chain f:

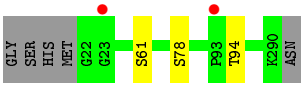




• Molecule 1: Capsid protein VP1

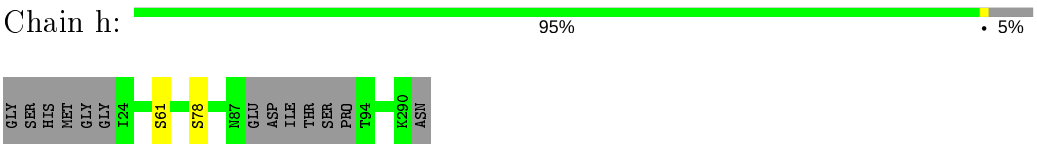
Chain g:





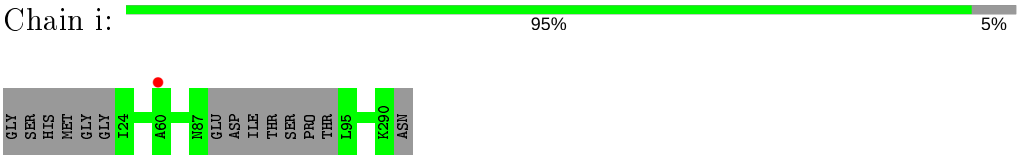
• Molecule 1: Capsid protein VP1

Chain h:



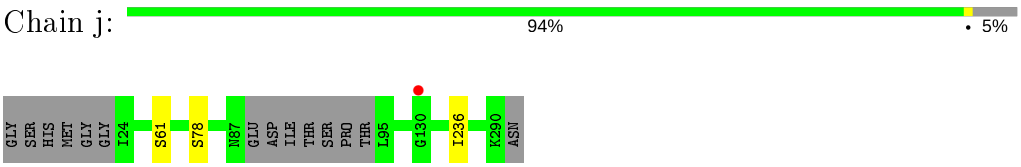
• Molecule 1: Capsid protein VP1

Chain i:



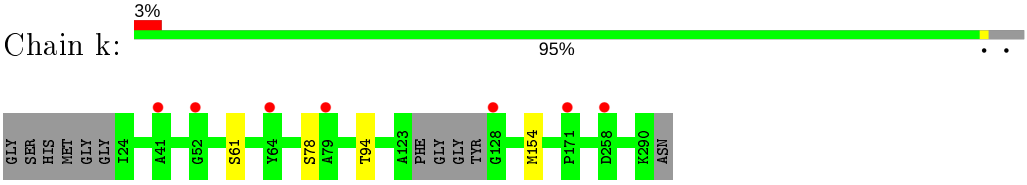
• Molecule 1: Capsid protein VP1

Chain j:



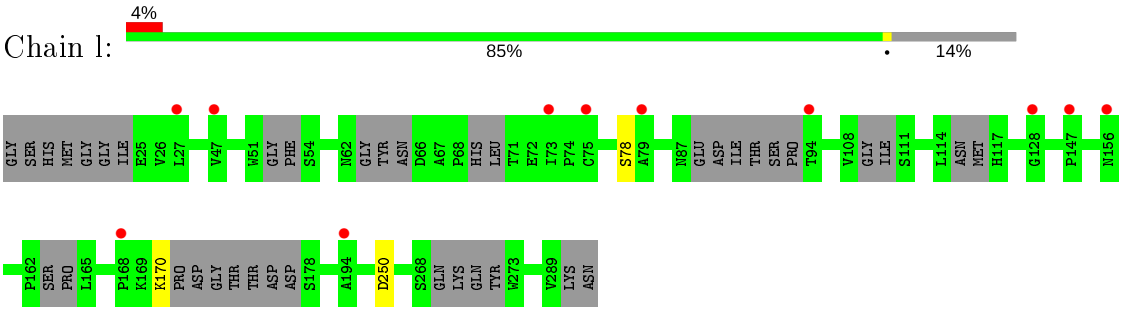
• Molecule 1: Capsid protein VP1

Chain k:



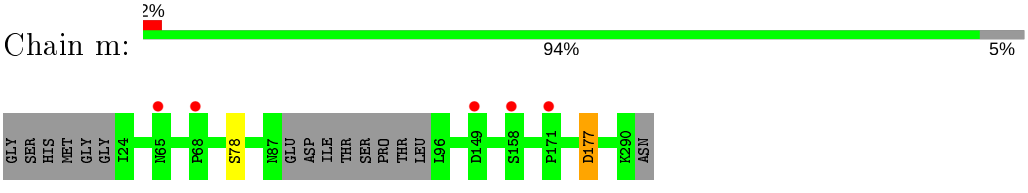
• Molecule 1: Capsid protein VP1

Chain l:



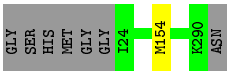
• Molecule 1: Capsid protein VP1

Chain m:



• Molecule 1: Capsid protein VP1

Chain n:


GLY
SER
HIS
MET
GLY
GLY
I24
M154
K290
ASN

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.35 (at 2.65Å)	Xtriage
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	Xtriage
Anisotropy	0.841	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 36.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,h+k+l	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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%)

All (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
1	C	94	THR	C-O	6.04	1.34	1.23
1	U	86	LEU	C-O	6.00	1.34	1.23
1	R	72	GLU	CD-OE1	-5.92	1.19	1.25
1	W	72	GLU	CD-OE1	-5.89	1.19	1.25
1	M	72	GLU	CD-OE1	-5.86	1.19	1.25
1	A	86	LEU	C-O	5.62	1.34	1.23
1	G	72	GLU	CD-OE1	-5.62	1.19	1.25
1	Q	94	THR	C-O	5.59	1.33	1.23
1	J	87	ASN	C-O	5.53	1.33	1.23
1	C	72	GLU	CD-OE1	-5.48	1.19	1.25
1	b	72	GLU	CD-OE2	-5.23	1.19	1.25
1	F	86	LEU	C-O	5.11	1.33	1.23
1	W	72	GLU	CD-OE2	-5.01	1.20	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	F	87	ASN	CB-CA-C	6.28	122.96	110.40
1	H	253	TYR	CB-CG-CD2	-5.93	117.44	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	86	LEU	N-CA-C	-5.64	95.77	111.00
1	m	177	ASP	CA-CB-CG	5.62	125.78	113.40
1	B	95	LEU	CB-CA-C	5.54	120.73	110.20
1	S	161	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	l	170	LYS	CB-CA-C	5.31	121.01	110.40
1	c	172	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	S	161	TYR	CB-CG-CD2	5.06	124.04	121.00
1	K	86	LEU	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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
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

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	SER
1	A	78	SER
1	A	154	MET
1	A	236	ILE
1	B	61	SER
1	B	78	SER
1	B	154	MET

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Mol	Chain	Res	Type
1	B	250	ASP
1	C	78	SER
1	C	240	GLU
1	D	30	LYS
1	D	61	SER
1	E	61	SER
1	F	61	SER
1	F	78	SER
1	F	85	LEU
1	G	61	SER
1	G	78	SER
1	H	236	ILE
1	I	61	SER
1	I	78	SER
1	J	61	SER
1	J	78	SER
1	K	61	SER
1	K	92	SER
1	L	61	SER
1	L	78	SER
1	M	61	SER
1	M	78	SER
1	N	61	SER
1	N	78	SER
1	N	95	LEU
1	O	61	SER
1	O	236	ILE
1	P	61	SER
1	P	78	SER
1	P	154	MET
1	Q	61	SER
1	Q	78	SER
1	Q	154	MET
1	R	61	SER
1	R	78	SER
1	S	61	SER
1	S	78	SER
1	S	236	ILE
1	T	61	SER
1	T	78	SER
1	T	236	ILE
1	T	240	GLU

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Mol	Chain	Res	Type
1	U	61	SER
1	U	87	ASN
1	V	61	SER
1	V	78	SER
1	V	154	MET
1	W	78	SER
1	X	61	SER
1	X	78	SER
1	Y	61	SER
1	Y	154	MET
1	Z	61	SER
1	Z	236	ILE
1	Z	240	GLU
1	a	61	SER
1	a	78	SER
1	b	61	SER
1	b	78	SER
1	b	236	ILE
1	c	61	SER
1	c	78	SER
1	c	236	ILE
1	d	61	SER
1	d	78	SER
1	d	236	ILE
1	e	61	SER
1	e	78	SER
1	e	240	GLU
1	f	61	SER
1	f	78	SER
1	f	154	MET
1	g	61	SER
1	g	78	SER
1	h	61	SER
1	h	78	SER
1	j	61	SER
1	j	78	SER
1	j	236	ILE
1	k	61	SER
1	k	78	SER
1	k	154	MET
1	l	78	SER
1	l	250	ASP

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Mol	Chain	Res	Type
1	m	78	SER
1	m	177	ASP
1	n	154	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	B	269	GLN
1	C	269	GLN
1	G	265	GLN
1	H	269	GLN
1	I	65	ASN
1	K	160	GLN
1	K	265	GLN
1	K	269	GLN
1	M	49	GLN
1	M	65	ASN
1	M	269	GLN
1	Q	265	GLN
1	S	265	GLN
1	X	65	ASN
1	Z	65	ASN
1	Z	265	GLN
1	b	269	GLN
1	e	180	GLN
1	e	265	GLN
1	f	65	ASN
1	g	269	GLN
1	m	69	HIS
1	n	65	ASN
1	n	269	GLN
1	n	271	GLN

5.3.3 RNA

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 (i)

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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%)
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (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
2	a	401	SIA	O2-C2	3.51	1.44	1.39
2	Q	401	SIA	C3-C2	3.37	1.55	1.51
2	T	401	SIA	O2-C2	3.35	1.44	1.39
2	X	401	SIA	O2-C2	3.34	1.44	1.39
2	e	401	SIA	O2-C2	3.33	1.44	1.39
2	J	401	SIA	O2-C2	3.31	1.44	1.39
2	O	401	SIA	O2-C2	3.26	1.44	1.39
2	Z	401	SIA	O2-C2	3.26	1.44	1.39
2	N	401	SIA	O2-C2	3.17	1.44	1.39
2	C	401	SIA	O2-C2	3.07	1.44	1.39
2	L	401	SIA	O2-C2	3.05	1.43	1.39
2	f	401	SIA	O2-C2	3.04	1.43	1.39
2	A	401	SIA	C7-C6	3.03	1.56	1.53
2	c	401	SIA	O2-C2	2.99	1.43	1.39
2	S	401	SIA	O2-C2	2.98	1.43	1.39
2	R	401	SIA	C7-C6	2.87	1.56	1.53
2	J	401	SIA	C3-C2	2.83	1.55	1.51
2	K	401	SIA	O2-C2	2.80	1.43	1.39
2	R	401	SIA	O2-C2	2.77	1.43	1.39
2	O	401	SIA	C3-C2	2.76	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	401	SIA	O2-C2	2.73	1.43	1.39
2	A	401	SIA	O2-C2	2.72	1.43	1.39
2	d	401	SIA	O2-C2	2.71	1.43	1.39
2	J	401	SIA	O6-C2	2.69	1.45	1.43
2	B	401	SIA	O2-C2	2.58	1.43	1.39
2	M	401	SIA	O2-C2	2.55	1.43	1.39
2	Z	401	SIA	C3-C2	2.55	1.54	1.51
2	a	401	SIA	C7-C6	2.50	1.56	1.53
2	a	401	SIA	O6-C2	2.49	1.45	1.43
2	F	401	SIA	O2-C2	2.47	1.43	1.39
2	V	401	SIA	C4-C5	2.45	1.55	1.53
2	B	401	SIA	C7-C6	2.43	1.56	1.53
2	b	401	SIA	O2-C2	2.41	1.43	1.39
2	j	401	SIA	C3-C2	2.39	1.54	1.51
2	T	401	SIA	C3-C2	2.39	1.54	1.51
2	I	401	SIA	O2-C2	2.38	1.43	1.39
2	V	401	SIA	C3-C2	2.32	1.54	1.51
2	e	401	SIA	C7-C6	2.31	1.55	1.53
2	X	401	SIA	C3-C2	2.31	1.54	1.51
2	Z	401	SIA	C7-C6	2.29	1.55	1.53
2	a	401	SIA	C3-C2	2.27	1.54	1.51
2	f	401	SIA	C3-C2	2.22	1.54	1.51
2	n	401	SIA	O2-C2	2.22	1.42	1.39
2	j	401	SIA	C4-C5	2.13	1.55	1.53
2	N	401	SIA	C4-C5	-2.11	1.51	1.53
2	I	401	SIA	C3-C2	2.11	1.54	1.51
2	Y	401	SIA	C3-C2	2.10	1.54	1.51
2	b	401	SIA	C3-C2	2.04	1.54	1.51
2	V	401	SIA	O6-C2	2.03	1.45	1.43
2	f	401	SIA	O6-C2	2.03	1.45	1.43
2	R	401	SIA	O6-C2	2.02	1.45	1.43

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
2	a	401	SIA	O6-C6-C5	-3.82	106.05	109.78
2	n	401	SIA	O6-C6-C5	3.59	113.28	109.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	e	401	SIA	O2-C2-C3	-3.52	104.44	109.35
2	K	401	SIA	O2-C2-C3	-3.48	104.49	109.35
2	I	401	SIA	C3-C4-C5	3.34	115.12	109.98
2	a	401	SIA	C3-C4-C5	3.22	114.94	109.98
2	a	401	SIA	O6-C6-C7	3.22	112.26	107.29
2	Q	401	SIA	O2-C2-O6	-3.21	102.51	109.85
2	R	401	SIA	O2-C2-C3	-3.21	104.87	109.35
2	Q	401	SIA	C3-C4-C5	3.16	114.84	109.98
2	c	401	SIA	C3-C4-C5	3.11	114.77	109.98
2	I	401	SIA	O2-C2-O6	-3.09	102.78	109.85
2	N	401	SIA	O2-C2-O6	-2.81	103.42	109.85
2	A	401	SIA	O7-C7-C6	2.81	115.56	109.50
2	A	401	SIA	O6-C6-C7	2.80	111.61	107.29
2	B	401	SIA	O2-C2-O6	-2.79	103.47	109.85
2	G	401	SIA	O6-C6-C5	-2.77	107.08	109.78
2	G	401	SIA	C4-C5-C6	2.72	115.99	109.10
2	X	401	SIA	C9-C8-C7	2.69	118.24	112.41
2	F	401	SIA	C4-C5-N5	-2.68	105.07	110.38
2	O	401	SIA	O2-C2-O6	-2.61	103.89	109.85
2	V	401	SIA	C6-C5-N5	-2.59	106.62	110.91
2	F	401	SIA	O2-C2-C3	-2.47	105.90	109.35
2	f	401	SIA	C3-C4-C5	2.47	113.77	109.98
2	M	401	SIA	O8-C8-C7	2.43	115.00	109.10
2	d	401	SIA	O2-C2-O6	-2.41	104.34	109.85
2	O	401	SIA	O6-C6-C7	2.41	111.00	107.29
2	Z	401	SIA	O6-C6-C7	2.40	110.99	107.29
2	O	401	SIA	C4-C5-C6	2.33	114.99	109.10
2	I	401	SIA	C8-C7-C6	-2.33	108.62	113.03
2	F	401	SIA	C3-C4-C5	2.30	113.51	109.98
2	G	401	SIA	C11-C10-N5	2.29	119.97	116.10
2	R	401	SIA	O6-C6-C7	2.26	110.78	107.29
2	R	401	SIA	C4-C5-N5	-2.24	105.94	110.38
2	F	401	SIA	O9-C9-C8	-2.23	106.22	111.07
2	c	401	SIA	O6-C6-C5	-2.23	107.60	109.78
2	T	401	SIA	O2-C2-O6	-2.22	104.77	109.85
2	G	401	SIA	C3-C4-C5	2.22	113.40	109.98
2	O	401	SIA	O4-C4-C5	-2.22	104.66	109.77
2	I	401	SIA	O7-C7-C6	2.22	114.29	109.50
2	Z	401	SIA	O7-C7-C6	2.22	114.28	109.50
2	j	401	SIA	O4-C4-C5	2.21	114.85	109.77
2	a	401	SIA	O2-C2-C3	-2.19	106.30	109.35
2	V	401	SIA	C9-C8-C7	2.18	117.14	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	SIA	C6-C5-N5	-2.18	107.30	110.91
2	b	401	SIA	O6-C6-C5	2.17	111.90	109.78
2	e	401	SIA	O2-C2-O6	-2.14	104.95	109.85
2	Y	401	SIA	O2-C2-C3	-2.11	106.41	109.35
2	B	401	SIA	O4-C4-C3	-2.10	105.01	109.91
2	e	401	SIA	O9-C9-C8	2.07	115.58	111.07
2	T	401	SIA	C3-C4-C5	2.06	113.15	109.98
2	Q	401	SIA	C6-C5-N5	-2.05	107.51	110.91
2	F	401	SIA	C8-C7-C6	-2.05	109.15	113.03
2	X	401	SIA	O8-C8-C9	-2.05	104.35	109.14
2	E	401	SIA	O4-C4-C3	-2.04	105.16	109.91
2	J	401	SIA	O6-C6-C7	2.02	110.41	107.29
2	e	401	SIA	C11-C10-N5	-2.00	112.71	116.10

There are no chirality outliers.

All (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
2	e	401	SIA	O8-C8-C9-O9
2	a	401	SIA	C6-C7-C8-C9
2	a	401	SIA	C6-C7-C8-O8
2	a	401	SIA	O7-C7-C8-C9
2	a	401	SIA	O7-C7-C8-O8
2	d	401	SIA	C7-C8-C9-O9
2	d	401	SIA	O8-C8-C9-O9
2	K	401	SIA	C6-C7-C8-C9
2	K	401	SIA	C6-C7-C8-O8
2	K	401	SIA	O7-C7-C8-C9
2	K	401	SIA	O7-C7-C8-O8
2	C	401	SIA	C6-C7-C8-C9
2	C	401	SIA	C6-C7-C8-O8
2	C	401	SIA	O7-C7-C8-C9
2	C	401	SIA	O7-C7-C8-O8
2	F	401	SIA	O8-C8-C9-O9
2	T	401	SIA	C7-C8-C9-O9
2	T	401	SIA	O8-C8-C9-O9
2	J	401	SIA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	J	401	SIA	C6-C7-C8-O8
2	J	401	SIA	O7-C7-C8-C9
2	J	401	SIA	O7-C7-C8-O8
2	J	401	SIA	C7-C8-C9-O9
2	J	401	SIA	O8-C8-C9-O9
2	f	401	SIA	O8-C8-C9-O9
2	X	401	SIA	C7-C8-C9-O9
2	X	401	SIA	O8-C8-C9-O9
2	E	401	SIA	C7-C8-C9-O9
2	E	401	SIA	O8-C8-C9-O9
2	R	401	SIA	C6-C7-C8-O8
2	R	401	SIA	O7-C7-C8-C9
2	R	401	SIA	O7-C7-C8-O8
2	A	401	SIA	O8-C8-C9-O9
2	S	401	SIA	C6-C7-C8-C9
2	S	401	SIA	C6-C7-C8-O8
2	S	401	SIA	O7-C7-C8-C9
2	S	401	SIA	O7-C7-C8-O8
2	B	401	SIA	O8-C8-C9-O9
2	V	401	SIA	C7-C8-C9-O9
2	e	401	SIA	C7-C8-C9-O9
2	F	401	SIA	C7-C8-C9-O9
2	f	401	SIA	C7-C8-C9-O9
2	A	401	SIA	C7-C8-C9-O9
2	b	401	SIA	O7-C7-C8-O8
2	e	401	SIA	C6-C7-C8-O8
2	n	401	SIA	C6-C7-C8-O8
2	b	401	SIA	C6-C7-C8-O8
2	G	401	SIA	O7-C7-C8-C9
2	b	401	SIA	O7-C7-C8-C9
2	B	401	SIA	C6-C7-C8-C9
2	R	401	SIA	C6-C7-C8-C9
2	b	401	SIA	O8-C8-C9-O9
2	n	401	SIA	C7-C8-C9-O9
2	Y	401	SIA	C7-C8-C9-O9
2	F	401	SIA	C11-C10-N5-C5
2	F	401	SIA	O10-C10-N5-C5
2	G	401	SIA	O7-C7-C8-O8
2	Y	401	SIA	C6-C7-C8-O8
2	B	401	SIA	C6-C7-C8-O8
2	X	401	SIA	C6-C7-C8-O8
2	j	401	SIA	C6-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
2	b	401	SIA	C7-C8-C9-O9
2	n	401	SIA	O7-C7-C8-C9
2	X	401	SIA	O7-C7-C8-C9
2	e	401	SIA	C6-C7-C8-C9
2	n	401	SIA	C6-C7-C8-C9
2	G	401	SIA	C6-C7-C8-C9
2	I	401	SIA	C6-C7-C8-C9
2	X	401	SIA	C6-C7-C8-C9
2	j	401	SIA	C6-C7-C8-C9
2	b	401	SIA	C6-C7-C8-C9
2	Z	401	SIA	O8-C8-C9-O9
2	n	401	SIA	O8-C8-C9-O9
2	B	401	SIA	O7-C7-C8-O8
2	Z	401	SIA	C7-C8-C9-O9
2	O	401	SIA	C7-C8-C9-O9
2	I	401	SIA	C6-C7-C8-O8
2	B	401	SIA	O7-C7-C8-C9
2	Y	401	SIA	O8-C8-C9-O9
2	e	401	SIA	O7-C7-C8-O8
2	n	401	SIA	O7-C7-C8-O8
2	Y	401	SIA	O7-C7-C8-O8
2	X	401	SIA	O7-C7-C8-O8
2	I	401	SIA	O7-C7-C8-C9
2	j	401	SIA	O7-C7-C8-C9
2	j	401	SIA	O8-C8-C9-O9
2	S	401	SIA	O8-C8-C9-O9
2	O	401	SIA	O8-C8-C9-O9
2	j	401	SIA	O7-C7-C8-O8
2	G	401	SIA	C6-C7-C8-O8
2	S	401	SIA	C7-C8-C9-O9
2	N	401	SIA	O7-C7-C8-C9
2	I	401	SIA	O7-C7-C8-O8
2	N	401	SIA	O7-C7-C8-O8
2	N	401	SIA	C6-C7-C8-O8
2	B	401	SIA	C7-C8-C9-O9
2	e	401	SIA	O7-C7-C8-C9
2	N	401	SIA	C6-C7-C8-C9
2	Y	401	SIA	C6-C7-C8-C9
2	c	401	SIA	O8-C8-C9-O9
2	c	401	SIA	C7-C8-C9-O9
2	Z	401	SIA	C4-C5-N5-C10
2	Y	401	SIA	O7-C7-C8-C9

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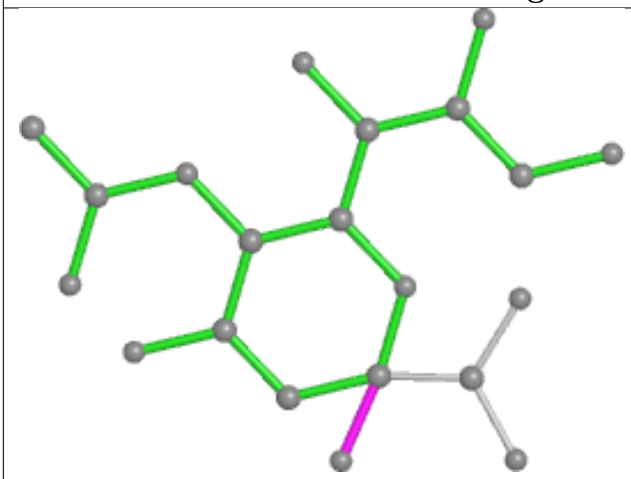
Mol	Chain	Res	Type	Atoms
2	n	401	SIA	C4-C5-N5-C10
2	O	401	SIA	C4-C5-N5-C10
2	Z	401	SIA	C6-C5-N5-C10
2	j	401	SIA	C7-C8-C9-O9
2	Q	401	SIA	C4-C5-N5-C10

There are no ring outliers.

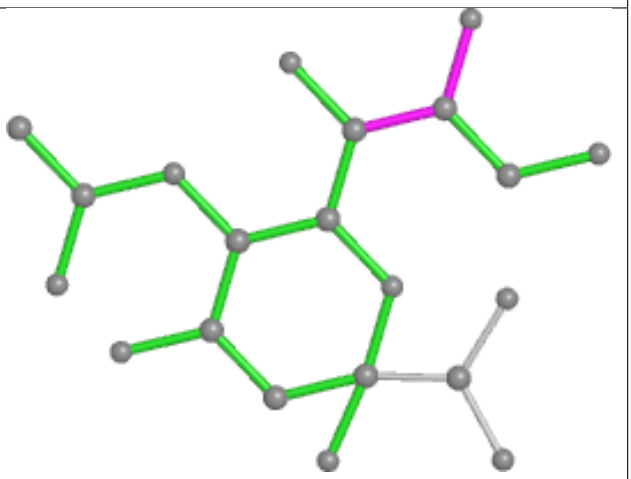
No monomer is involved in short contacts.

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 then 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.

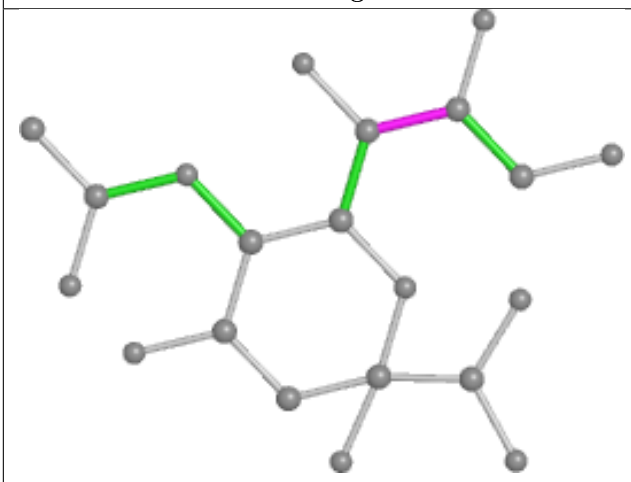
Ligand SIA M 401



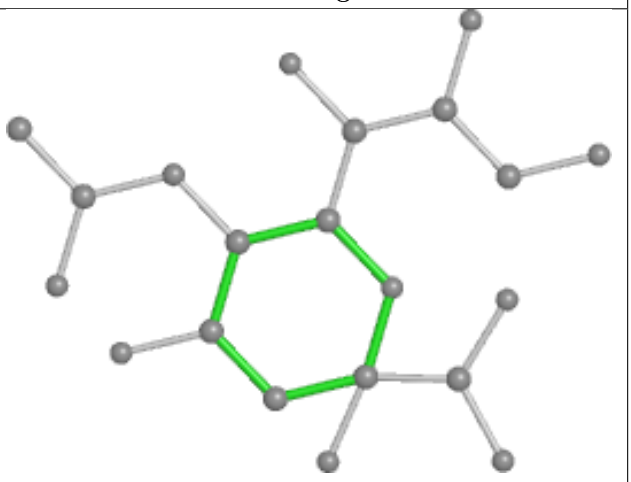
Bond lengths



Bond angles

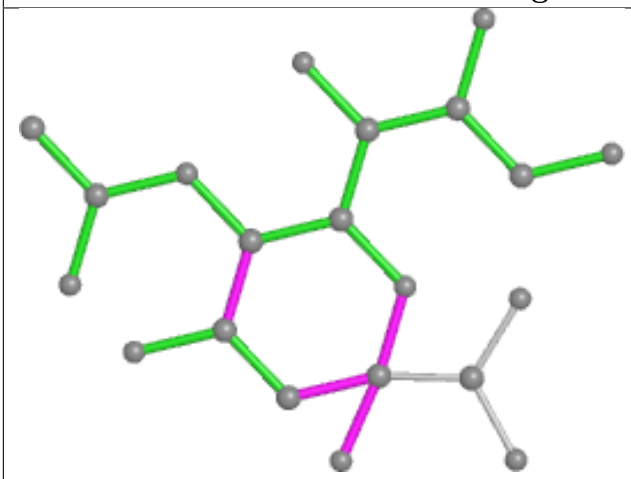


Torsions



Rings

Ligand SIA V 401



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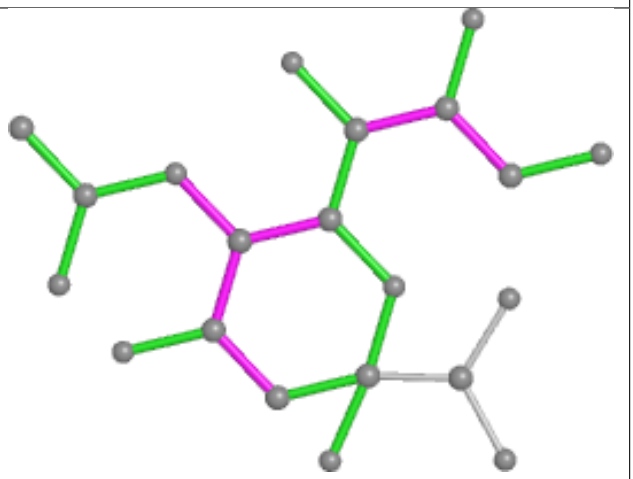

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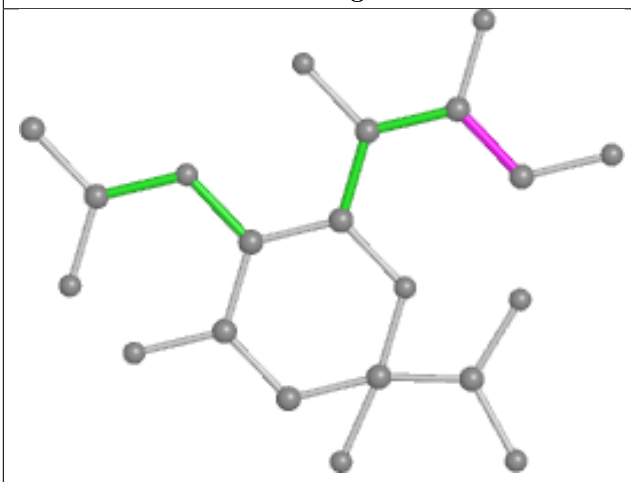

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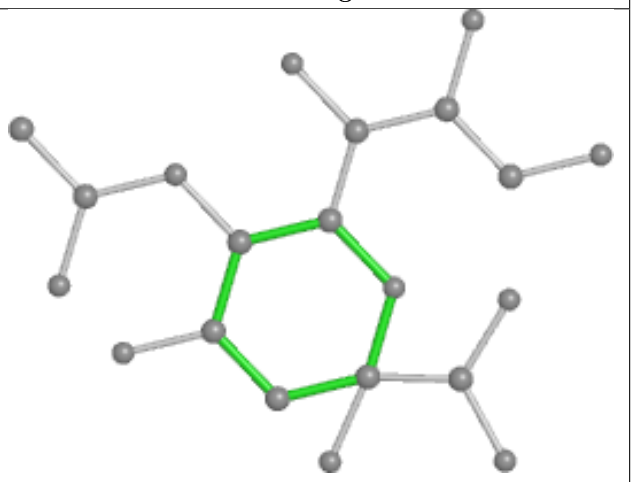
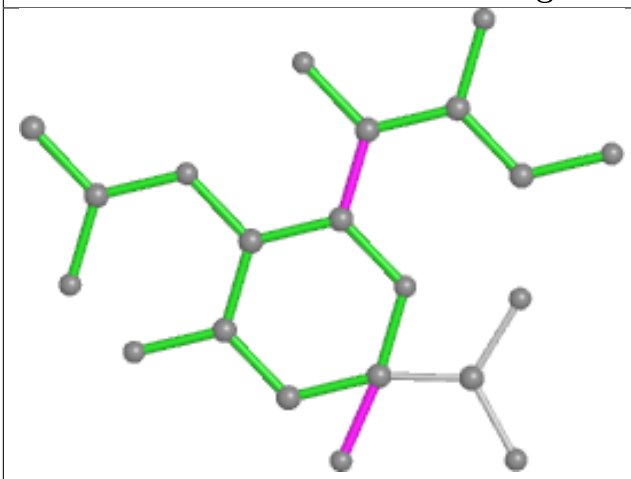


Rings

Ligand SIA e 401



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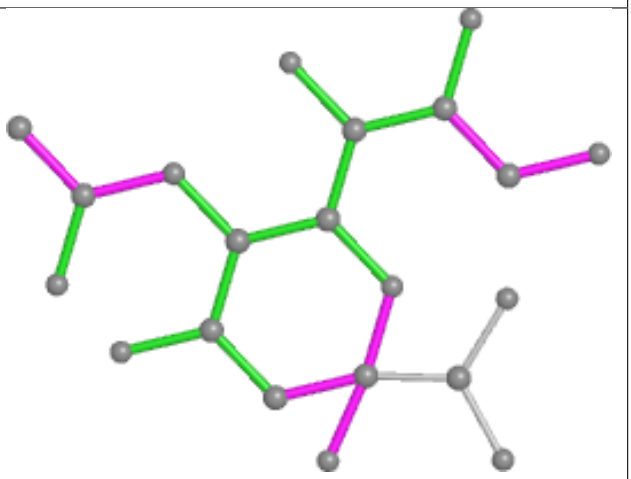

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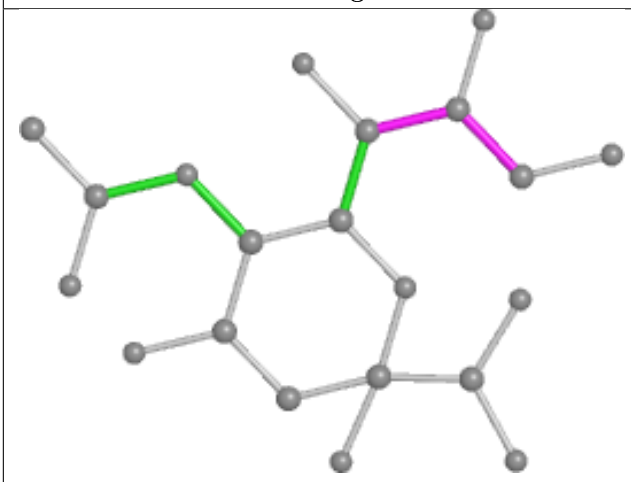

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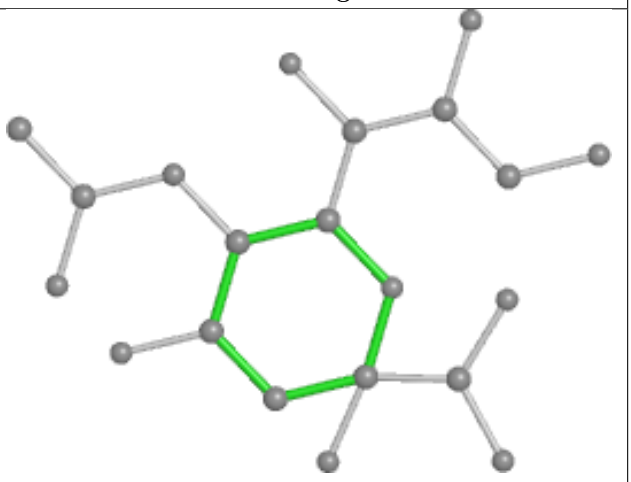
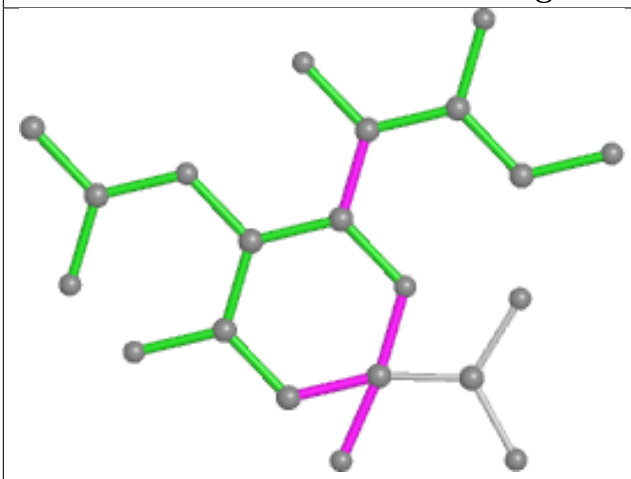


Rings

Ligand SIA a 401



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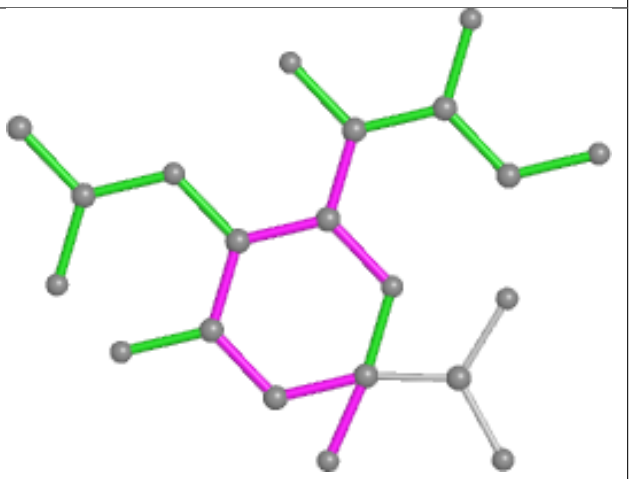

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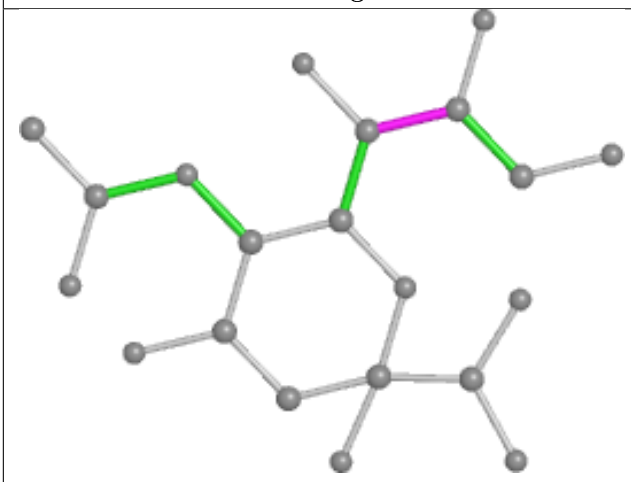

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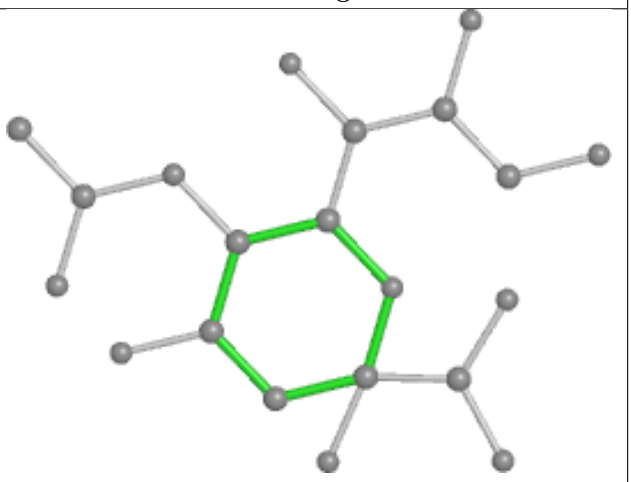
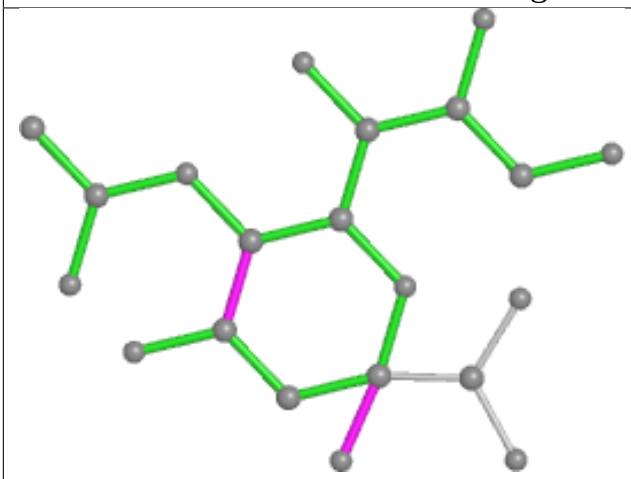


Rings

Ligand SIA N 401



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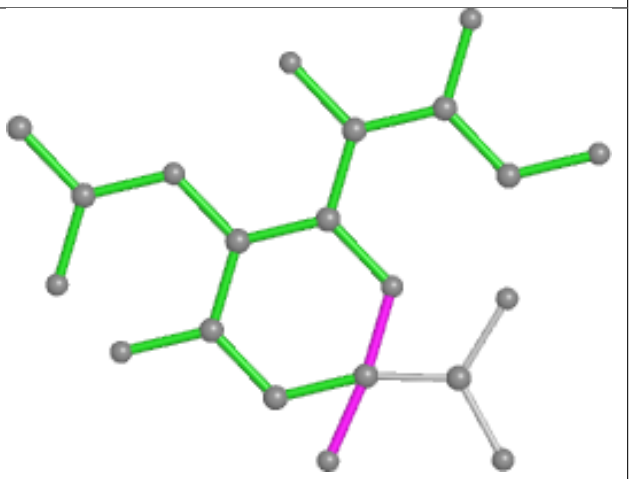

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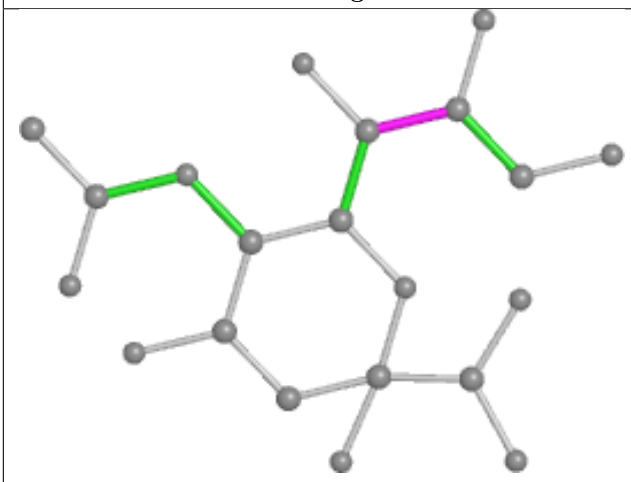

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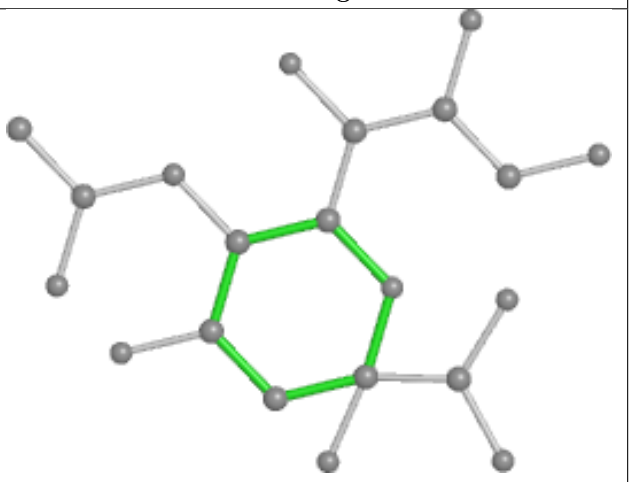
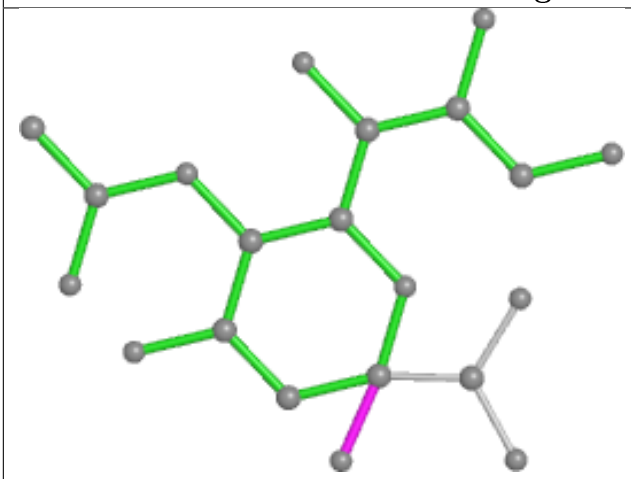


Rings

Ligand SIA d 401



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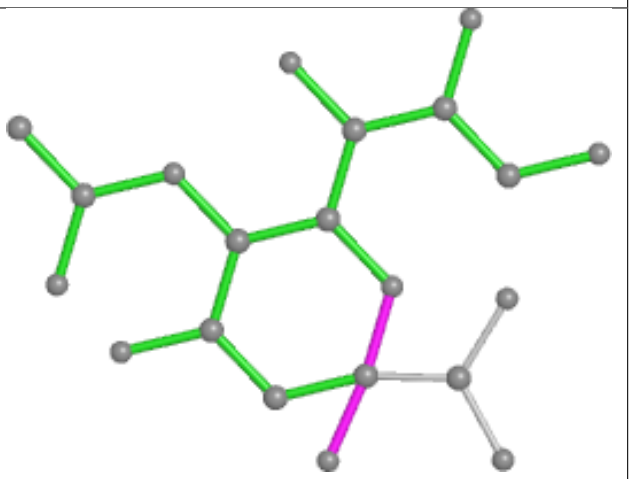

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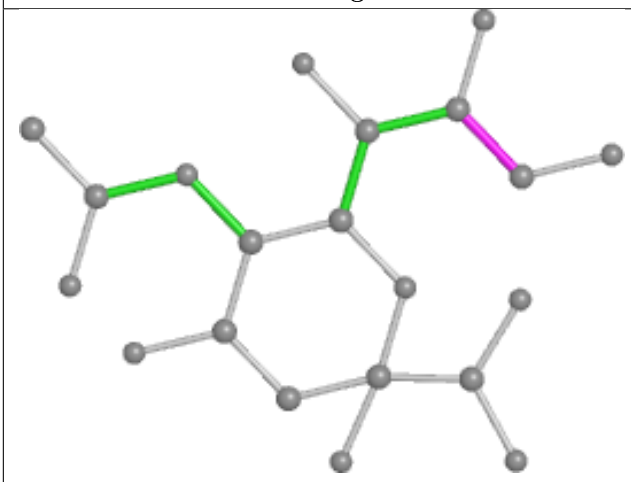

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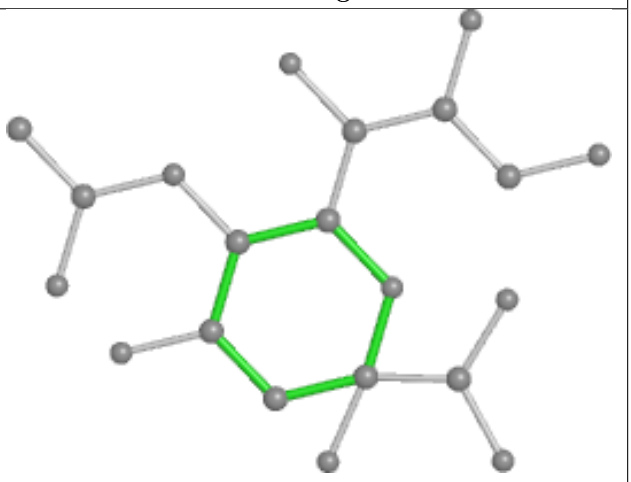
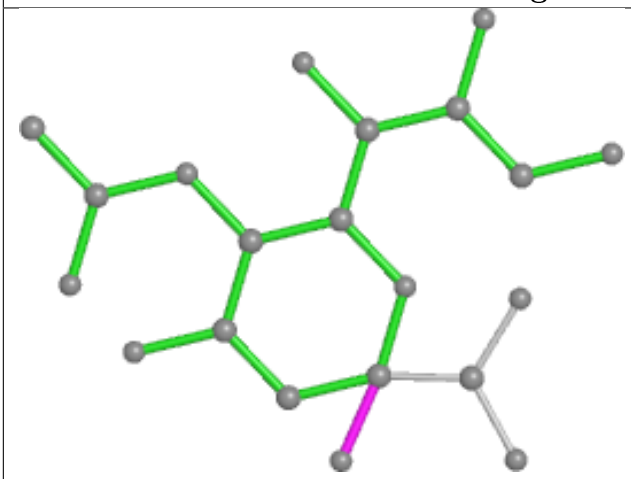


Rings

Ligand SIA K 401



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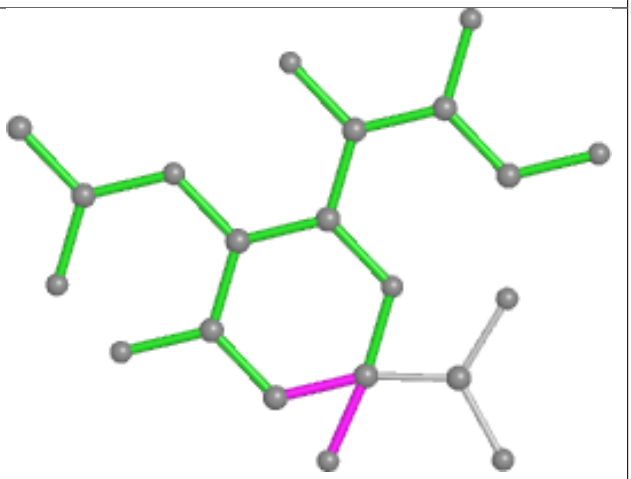

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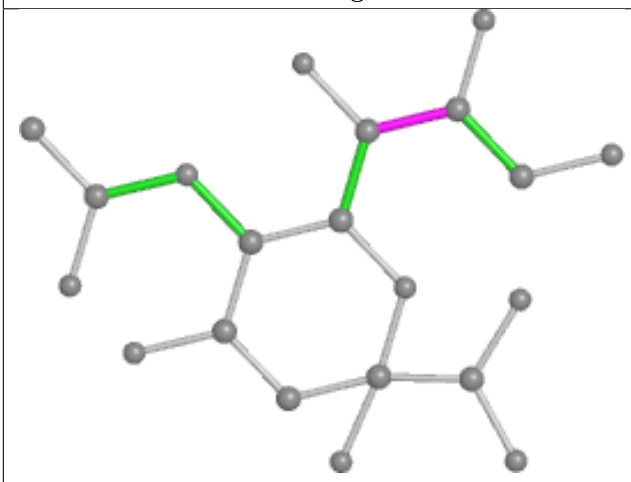
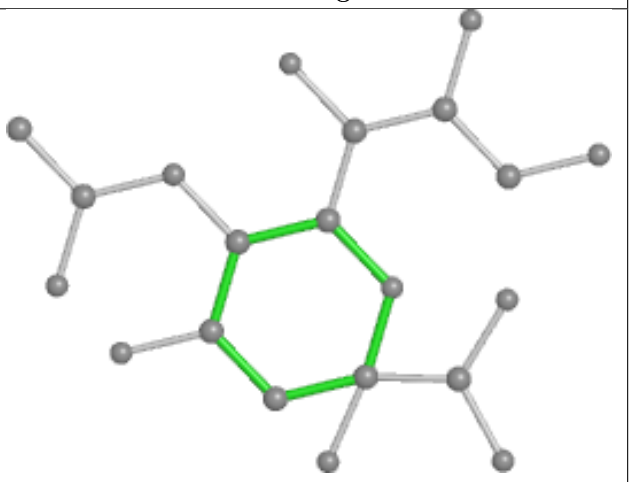


Torsions



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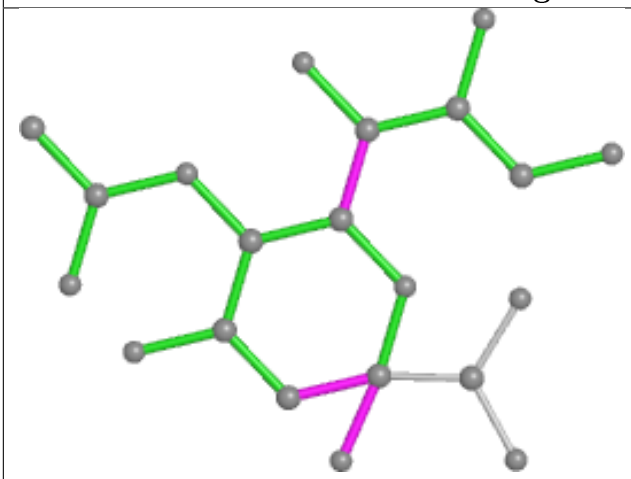

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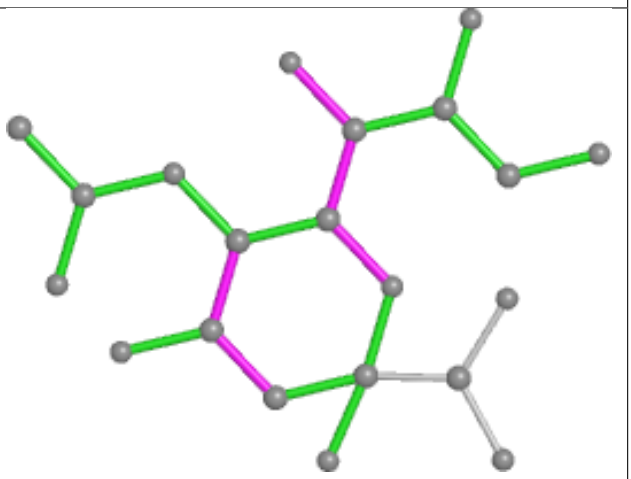

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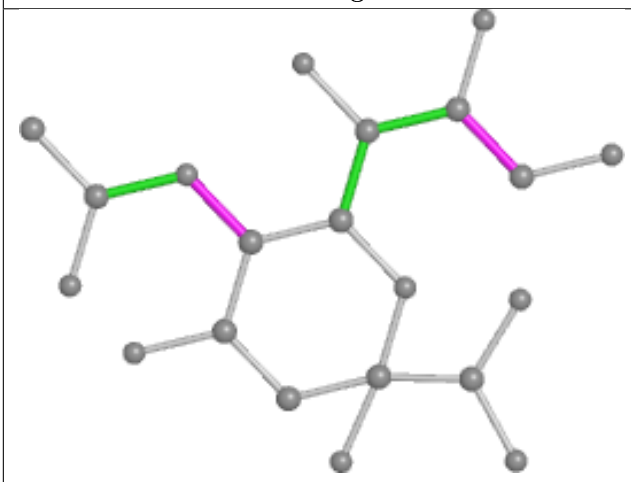

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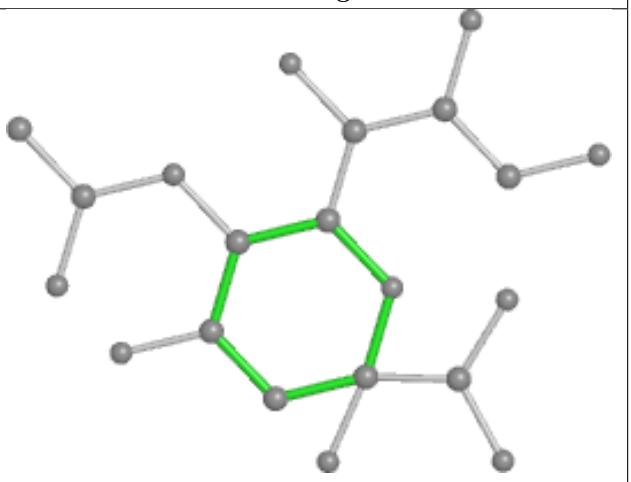

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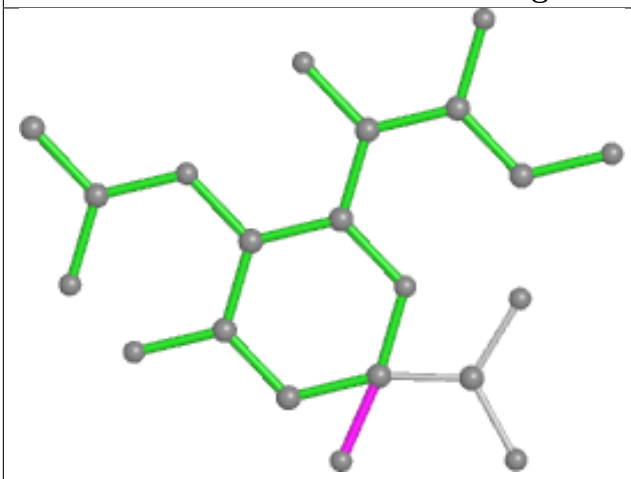

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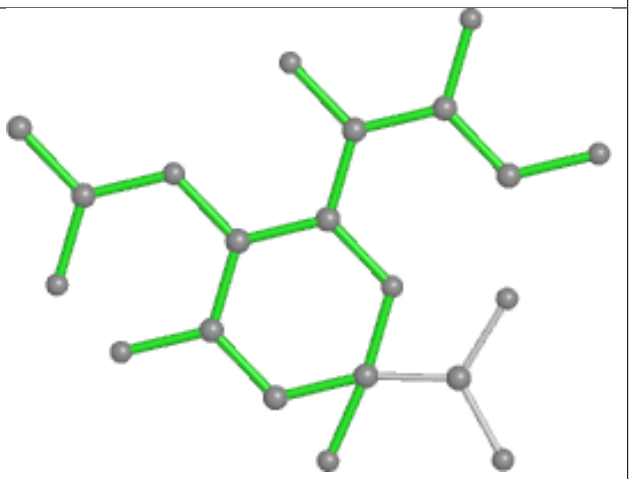

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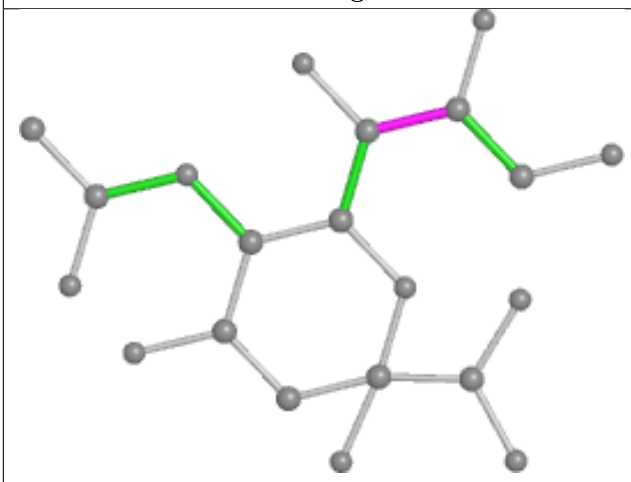

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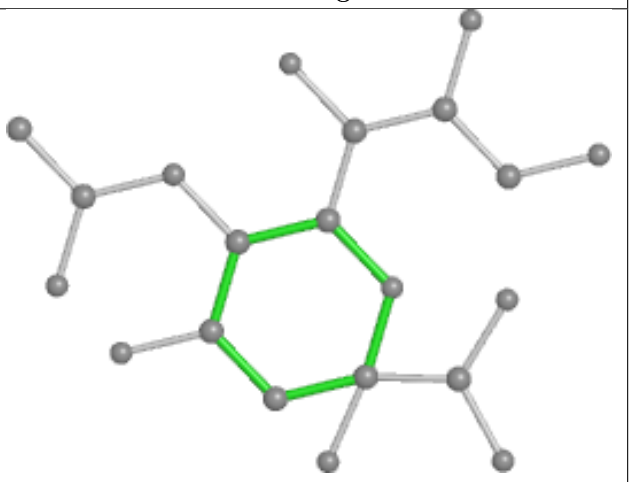

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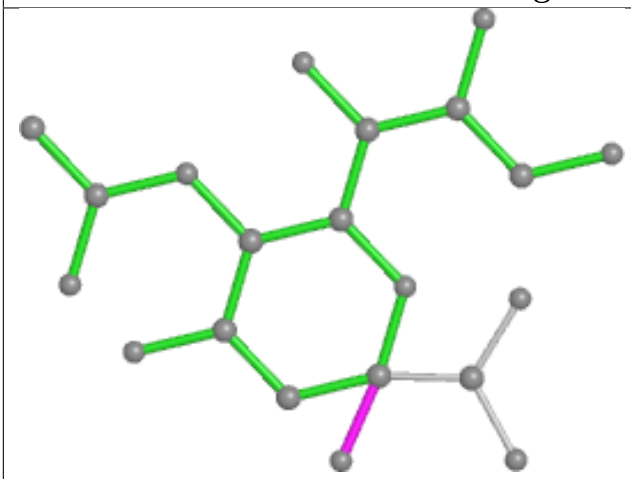

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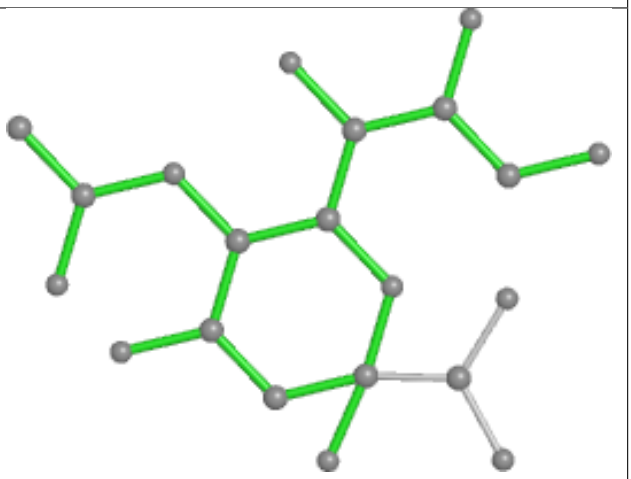

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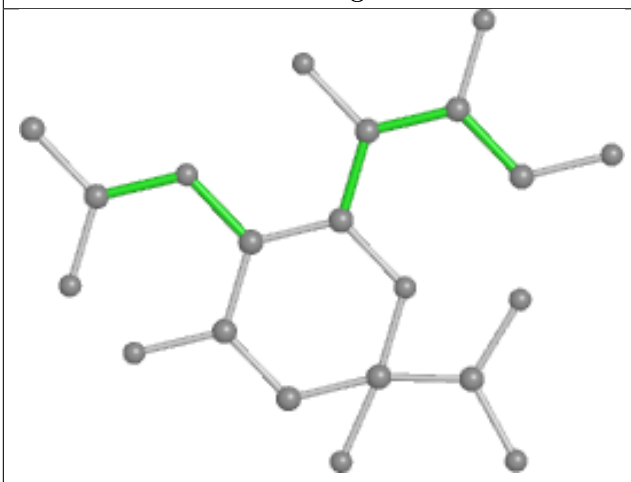

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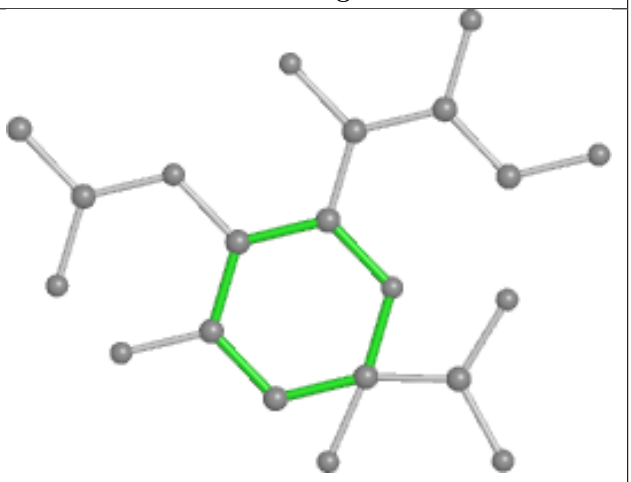

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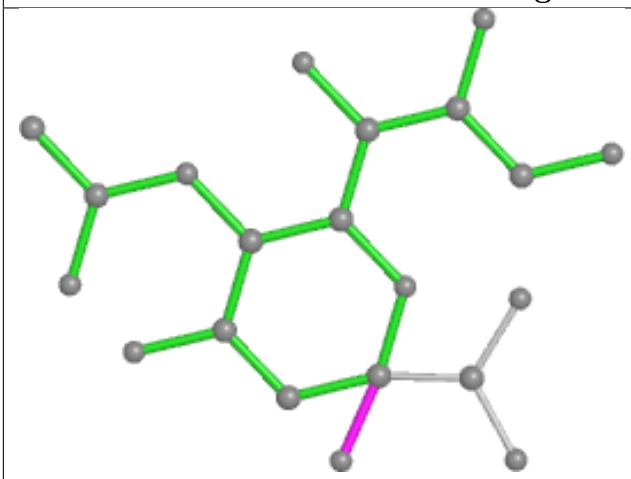

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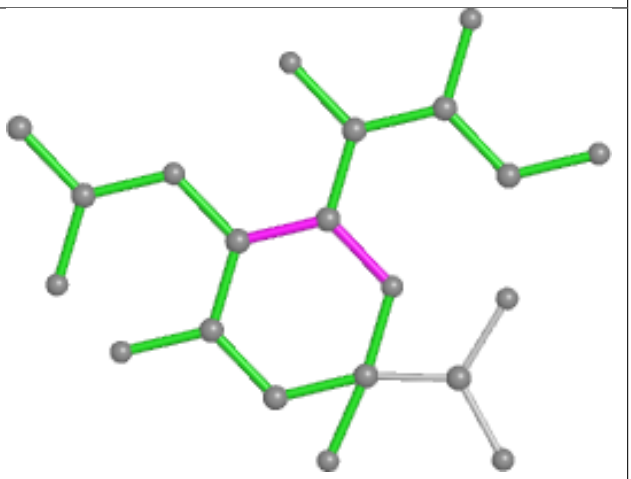

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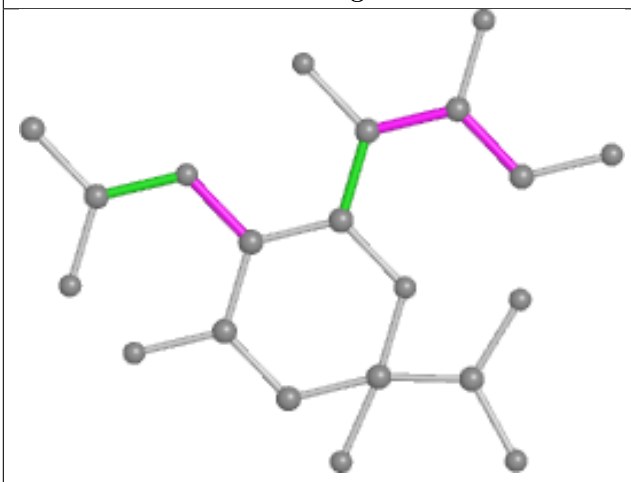

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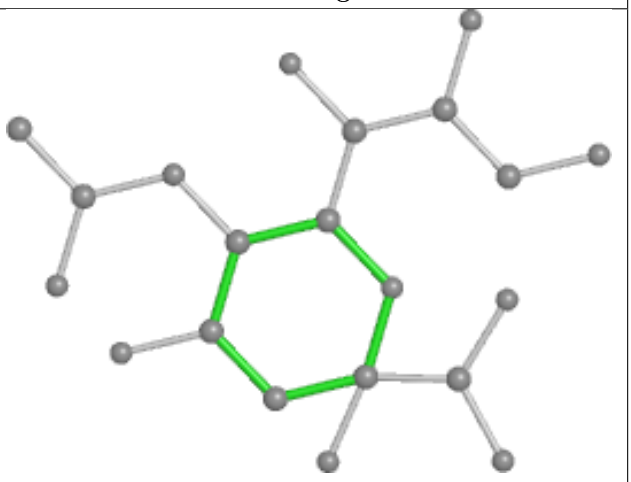

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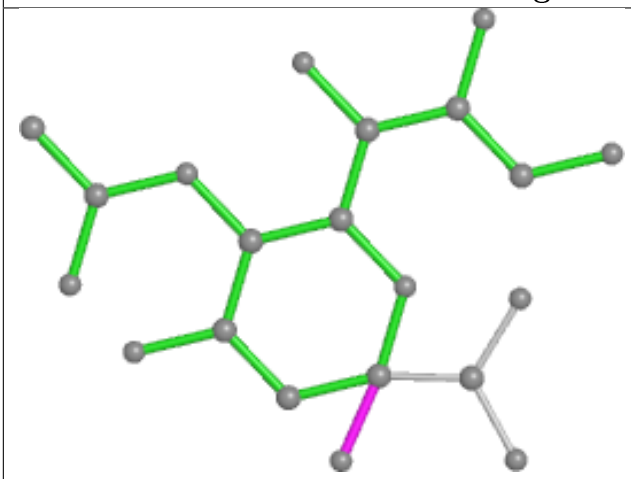

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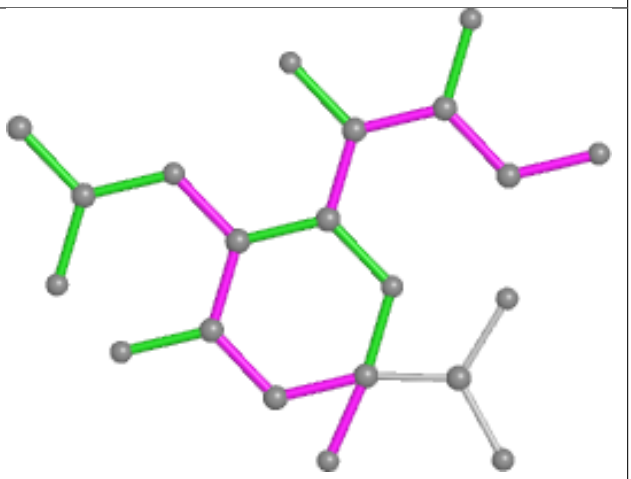

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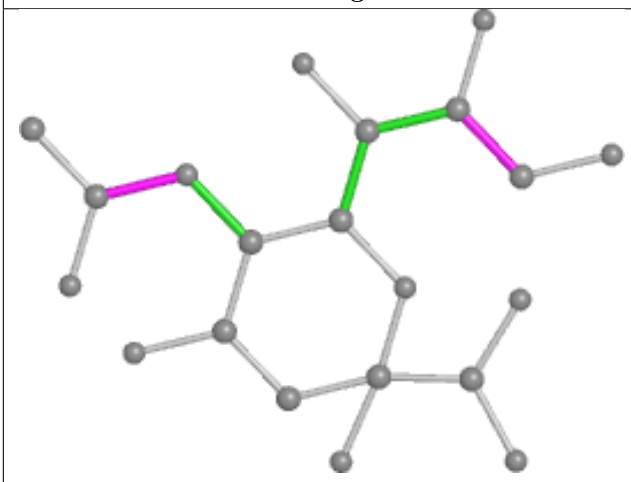

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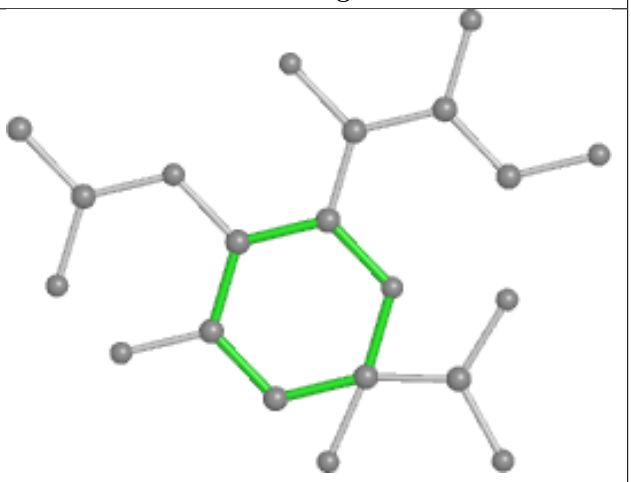

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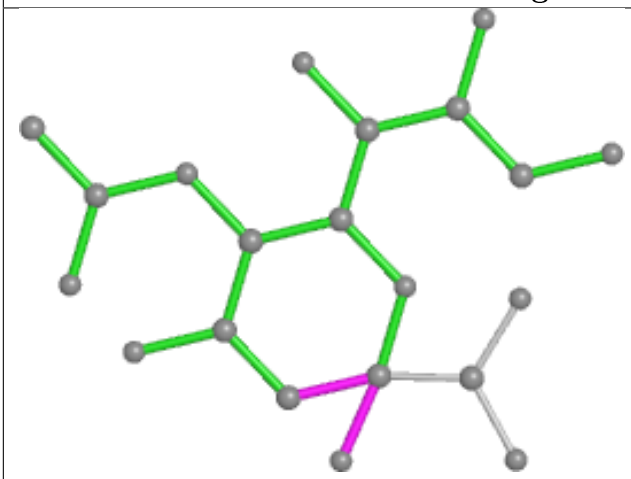

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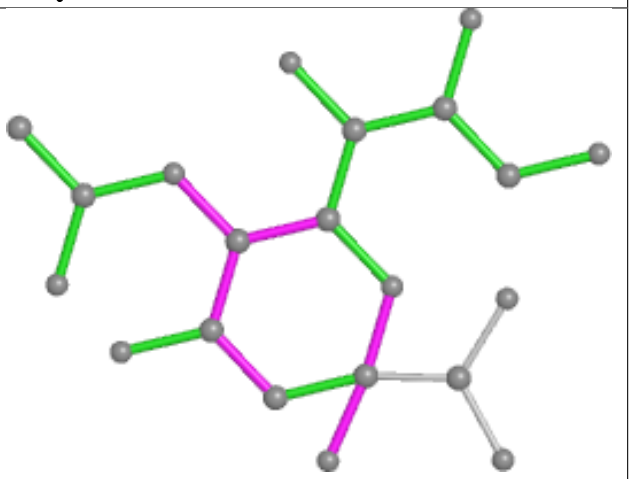

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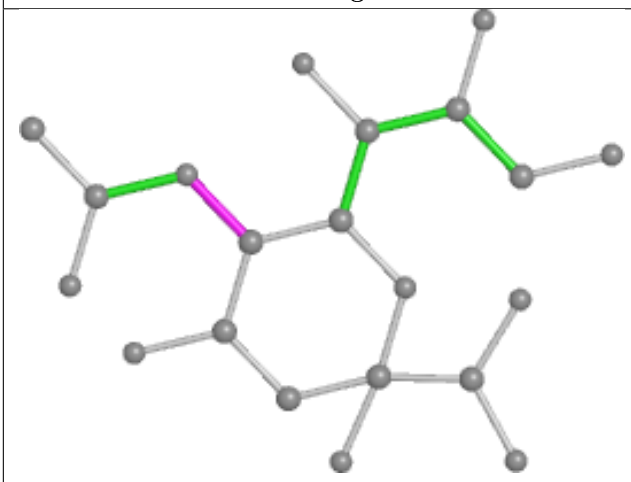

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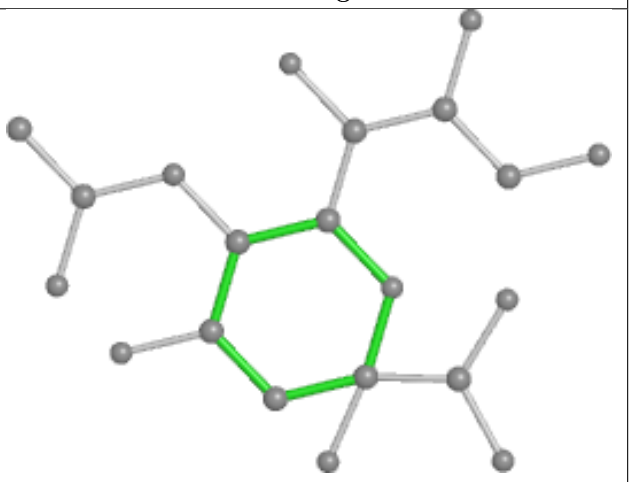

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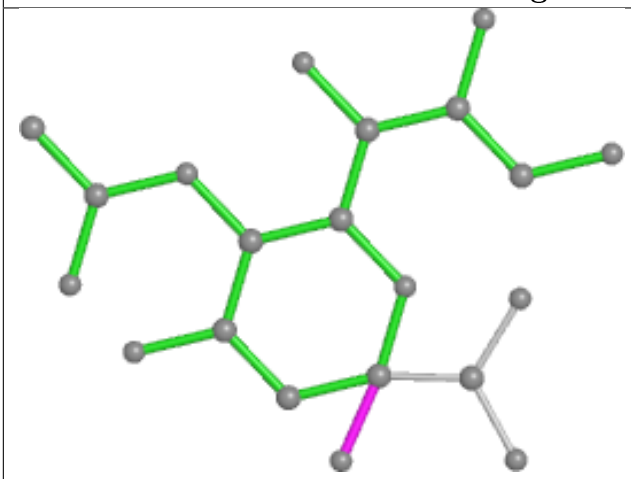

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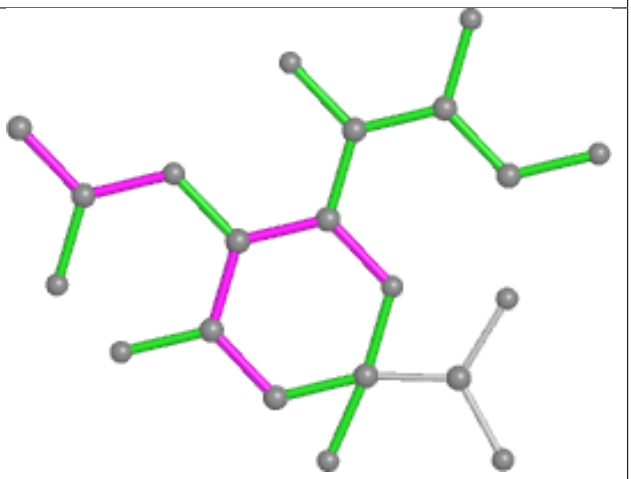

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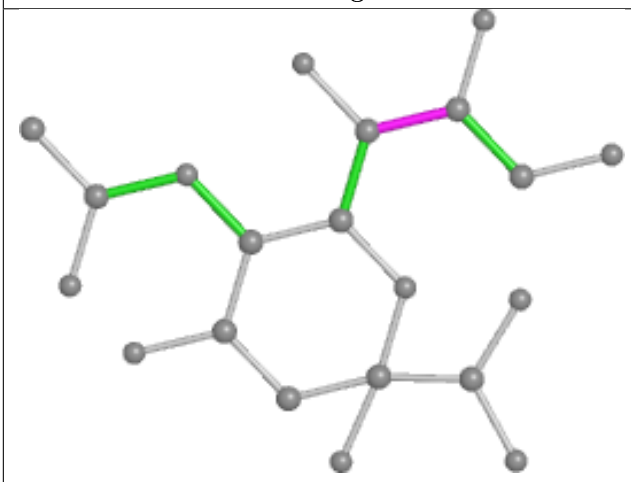

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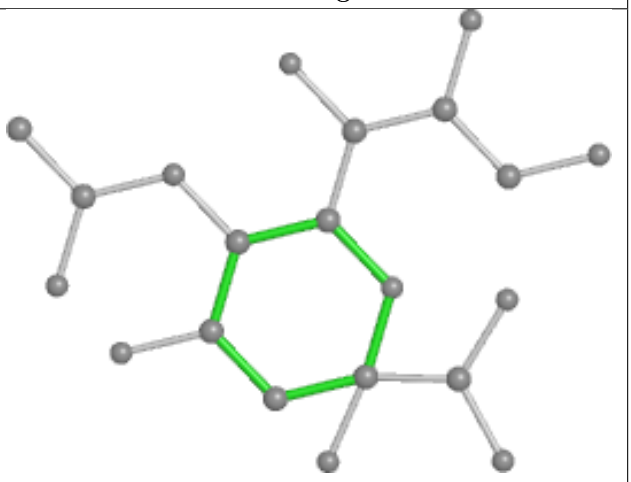

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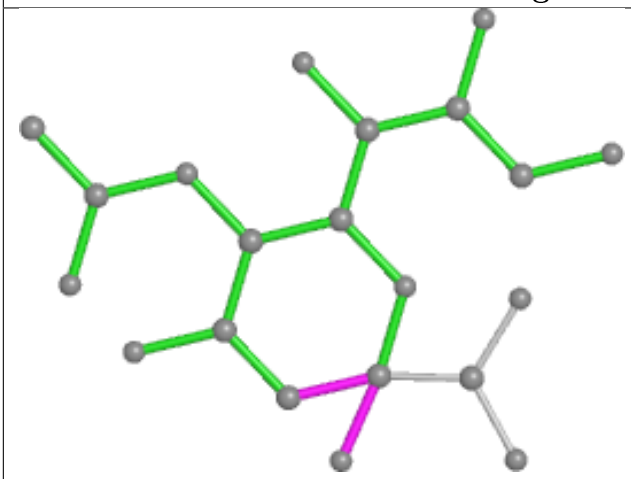

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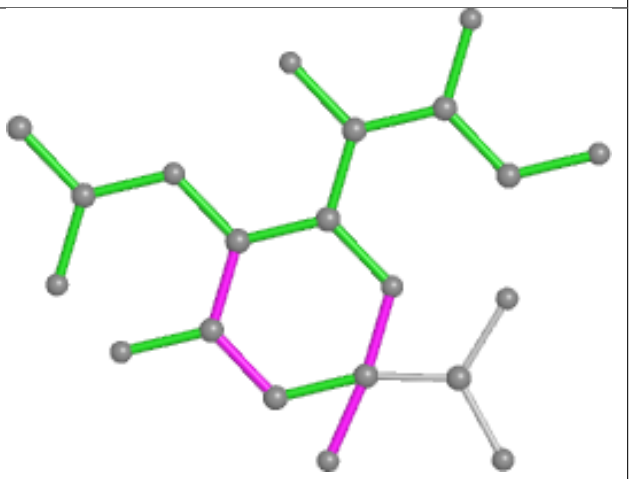

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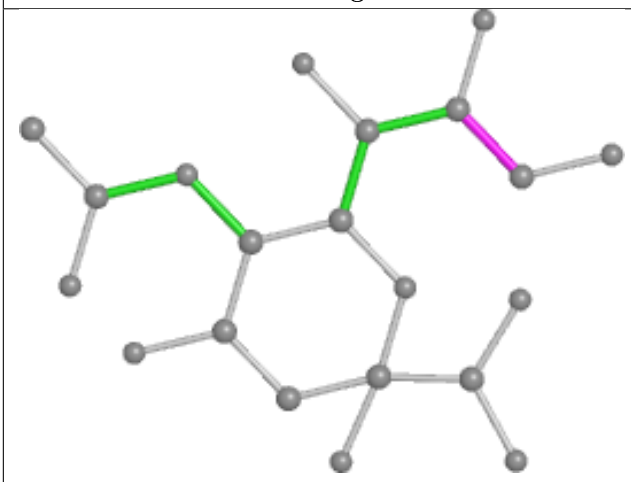

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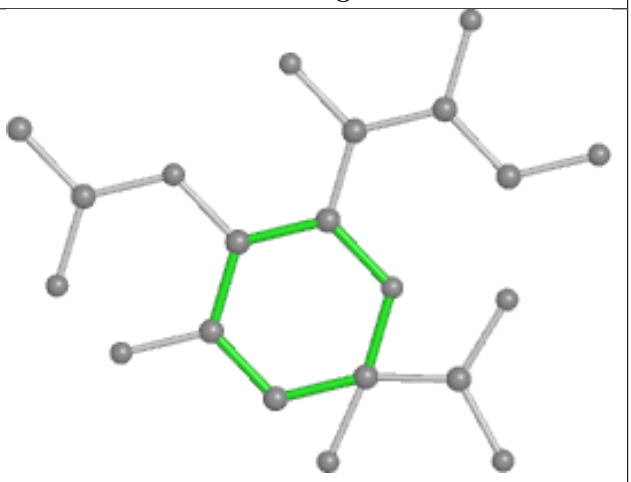

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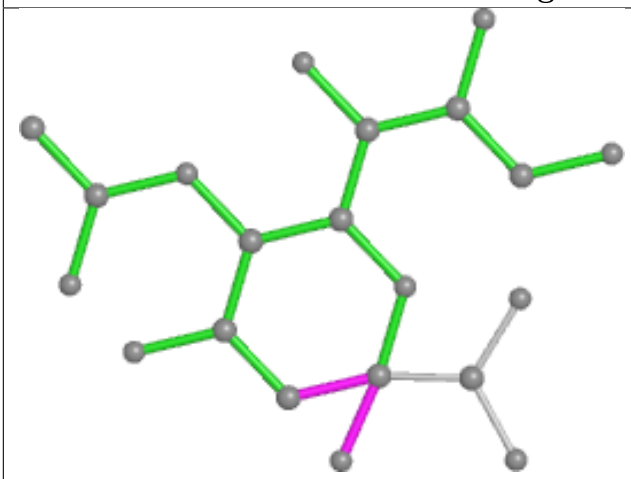

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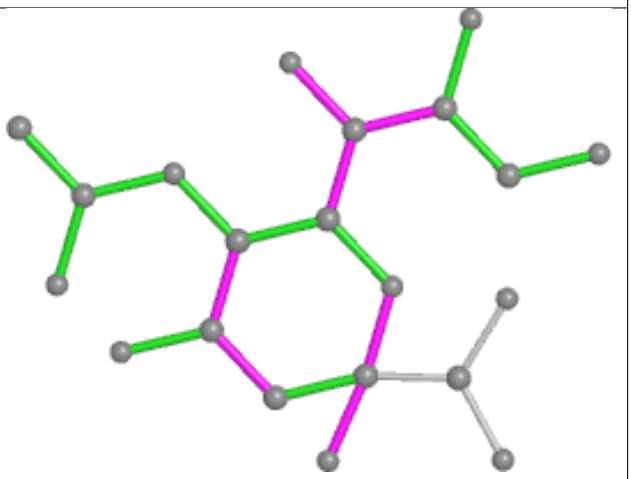

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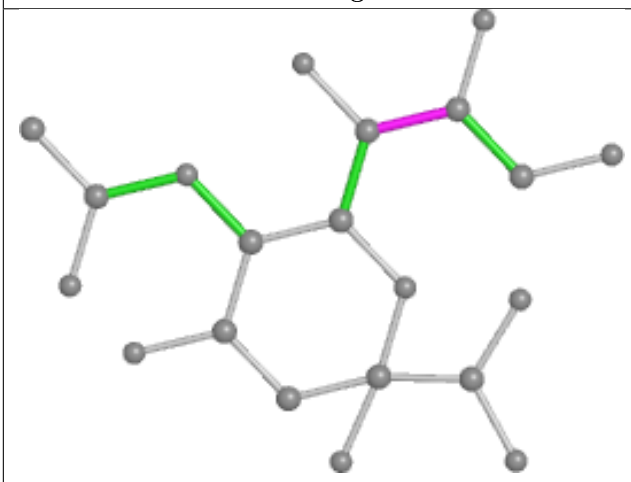

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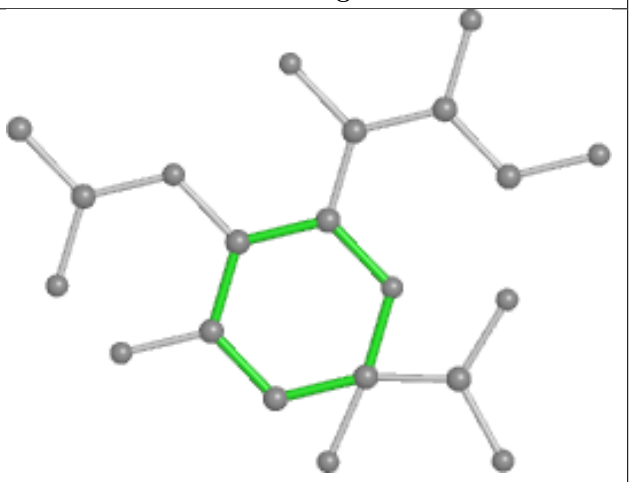

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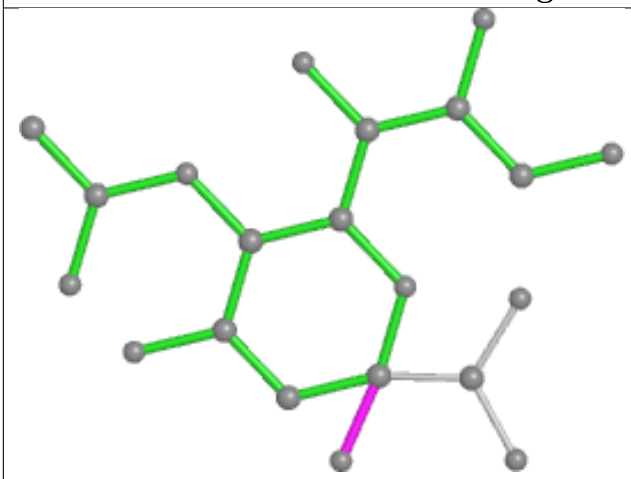

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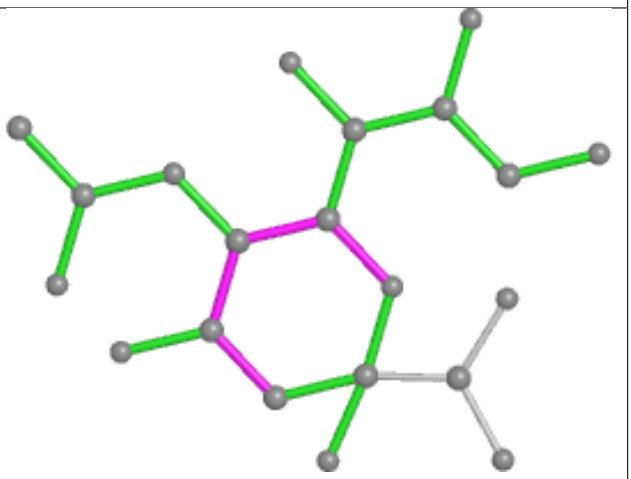

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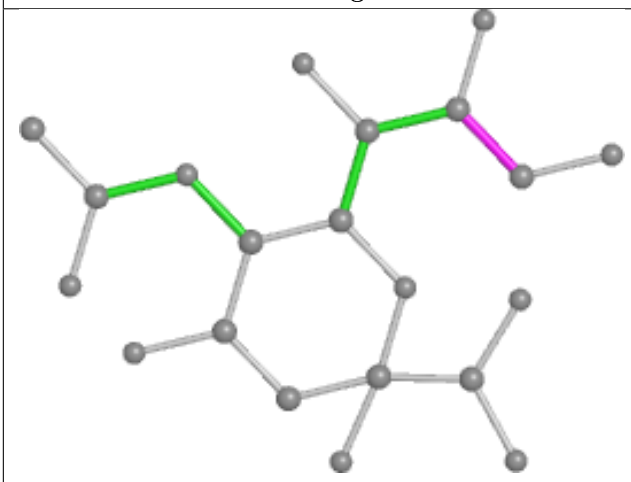

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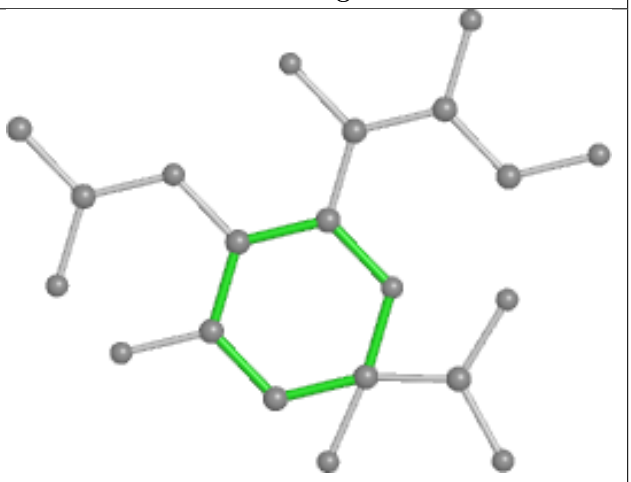

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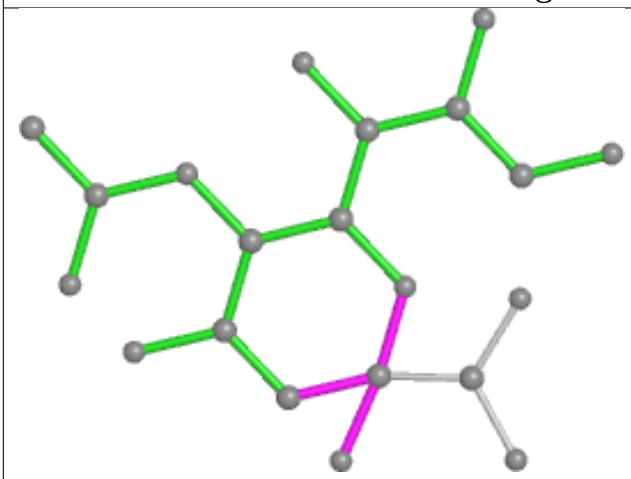

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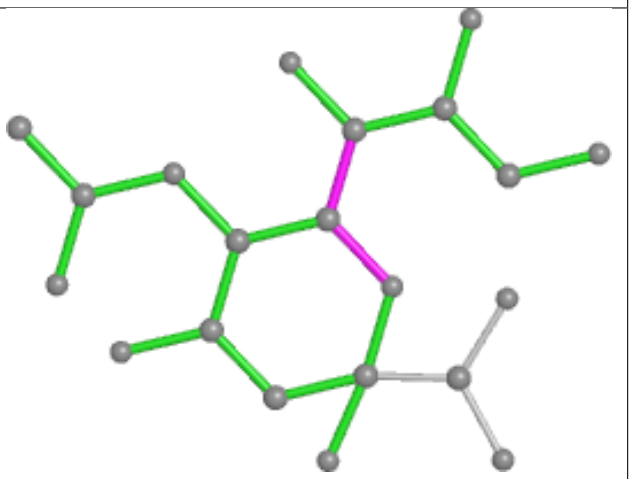

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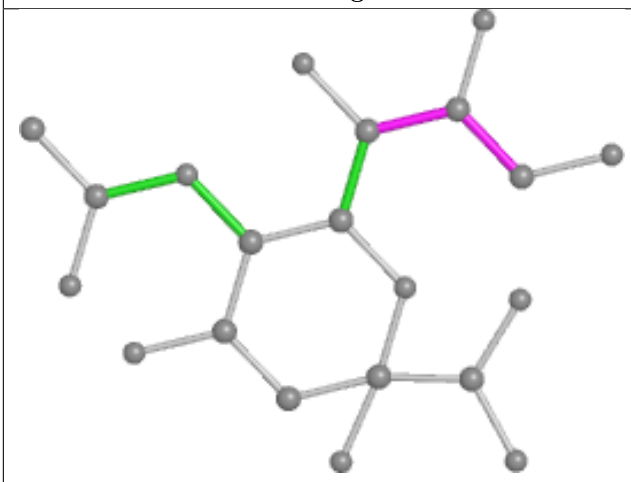

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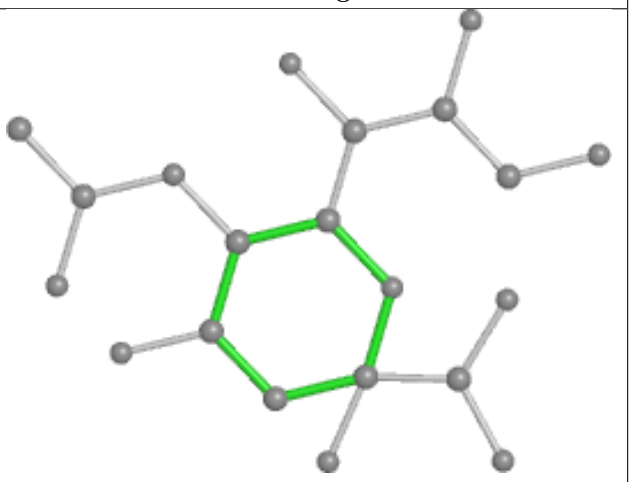

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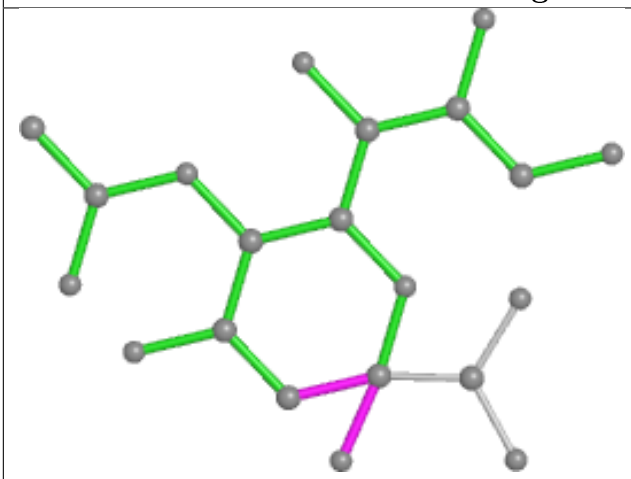

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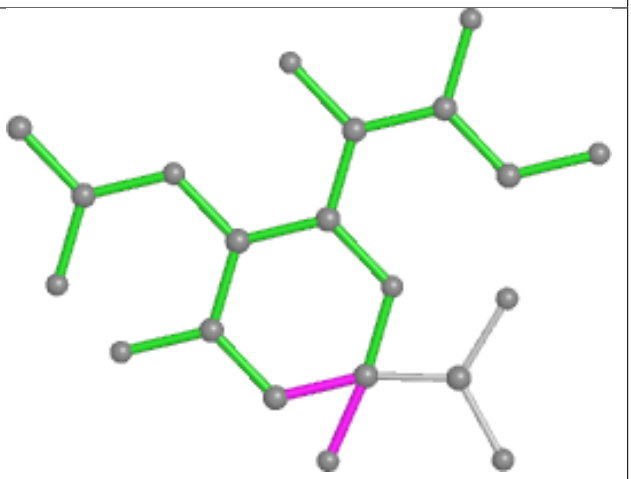

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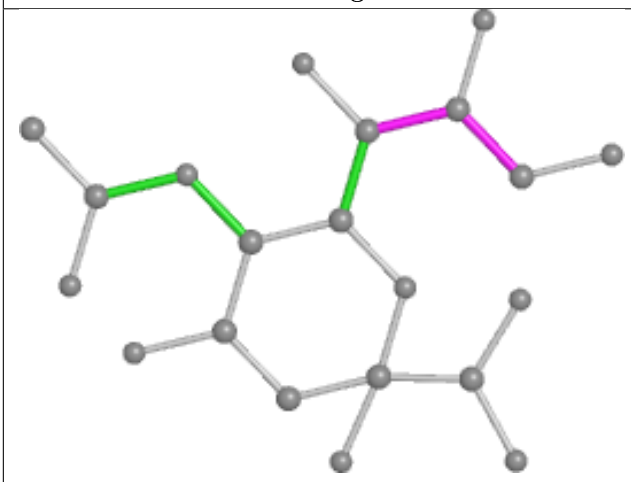

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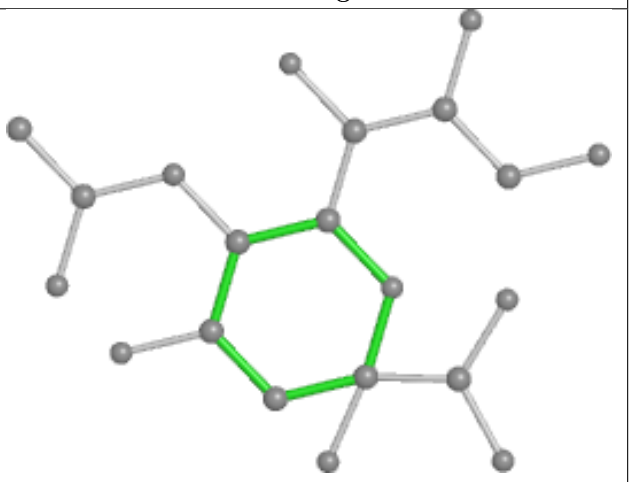

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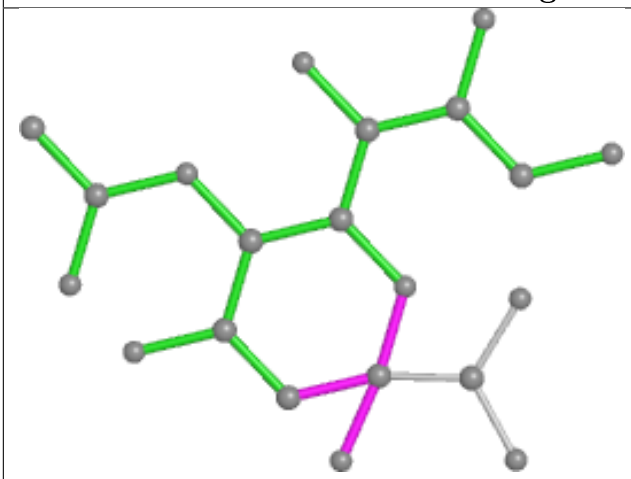

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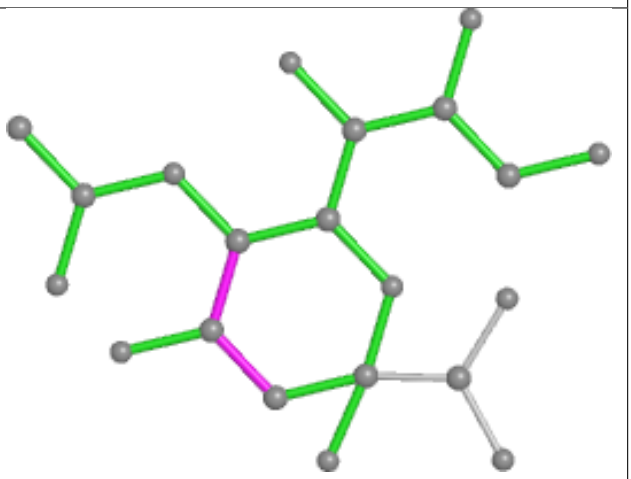

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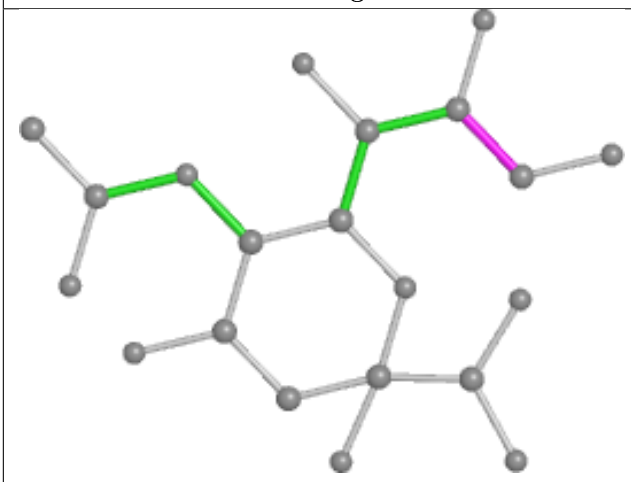

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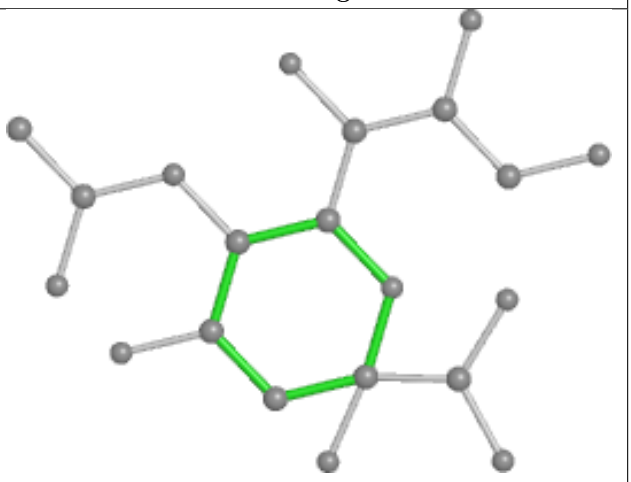

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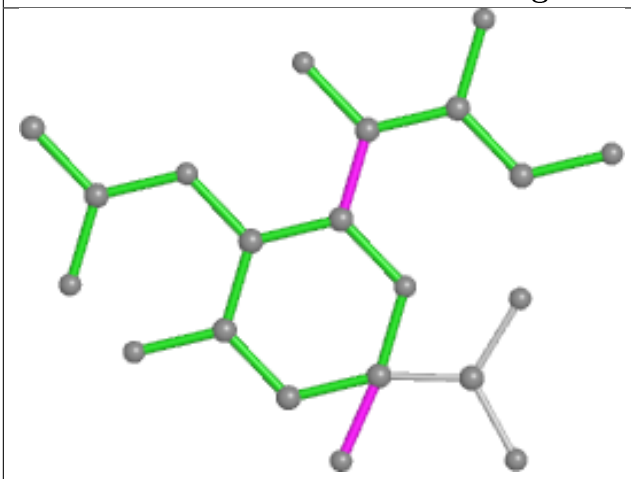

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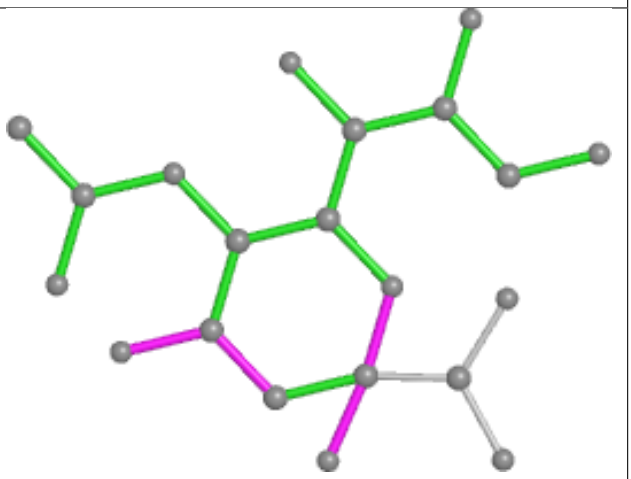

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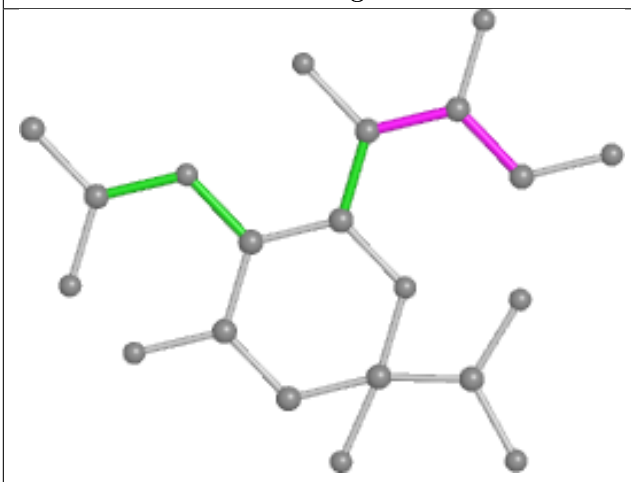

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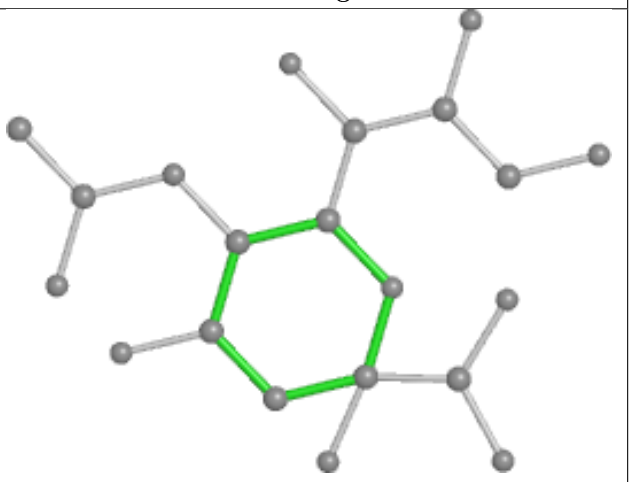
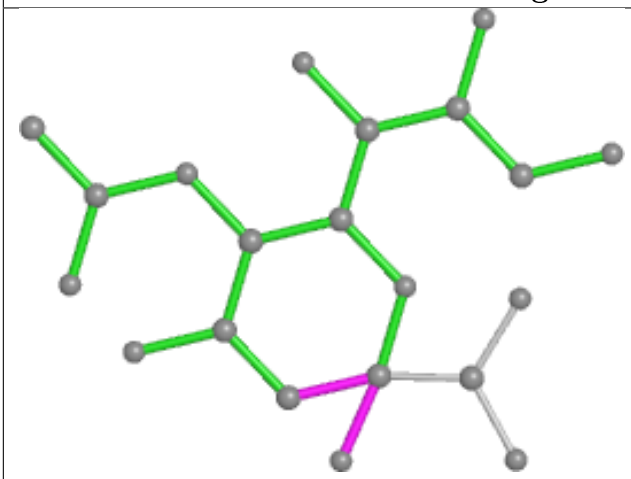
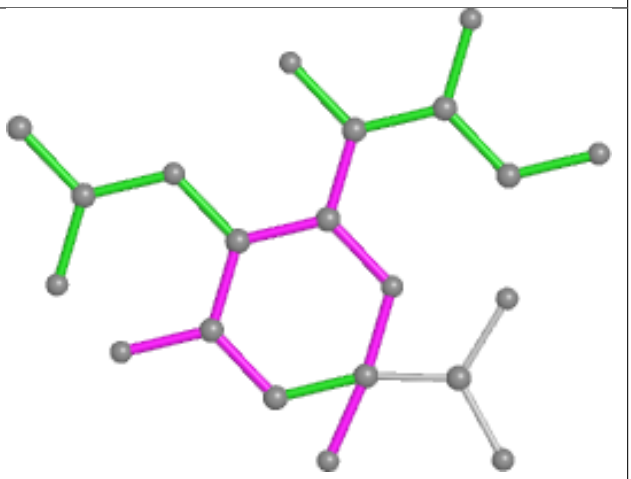


Rings

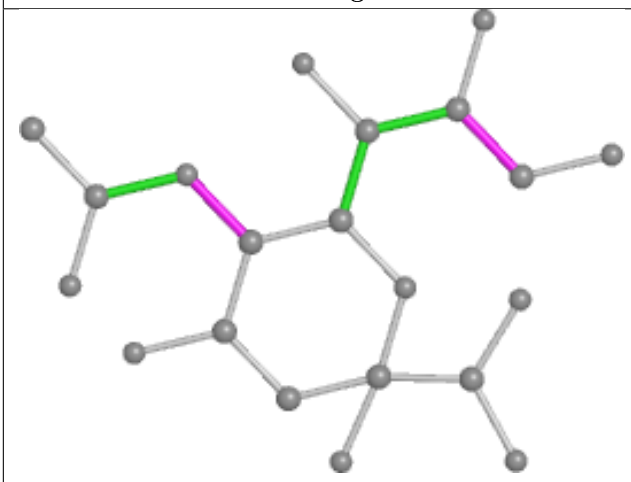
Ligand SIA O 401



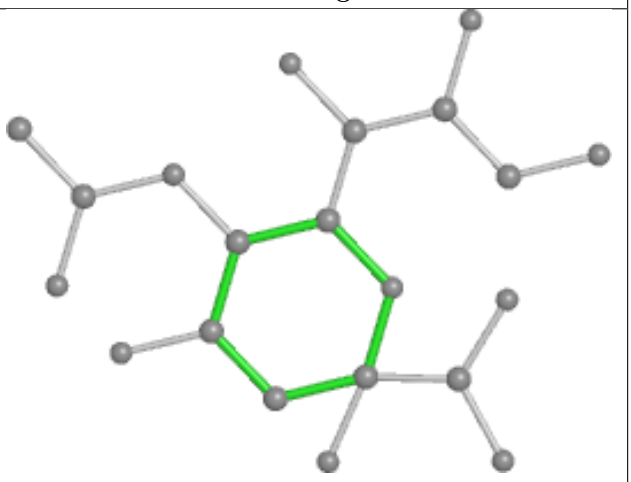
Bond lengths



Bond angles

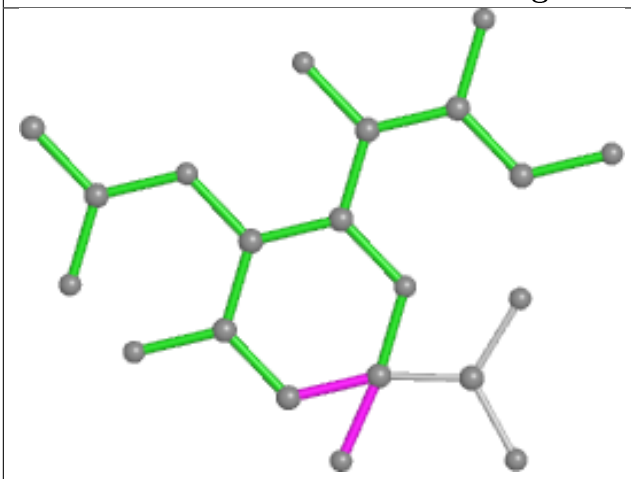


Torsions

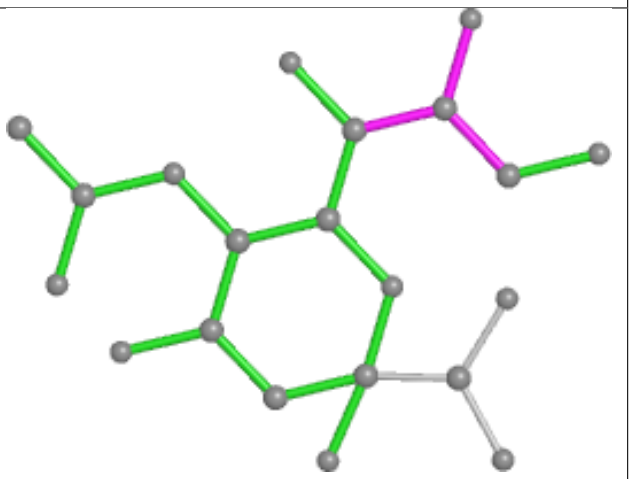


Rings

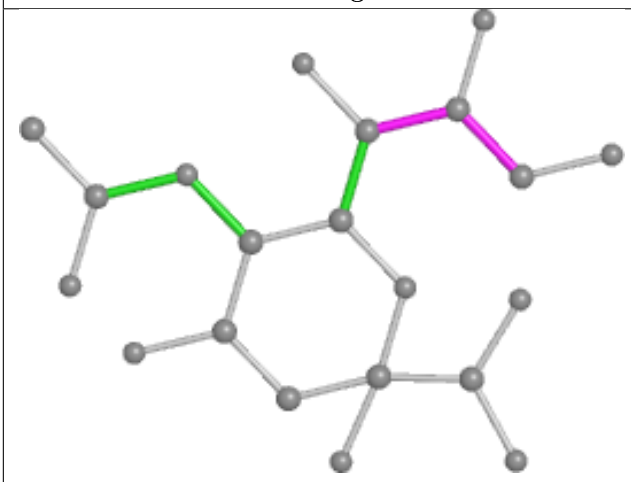
Ligand SIA X 401



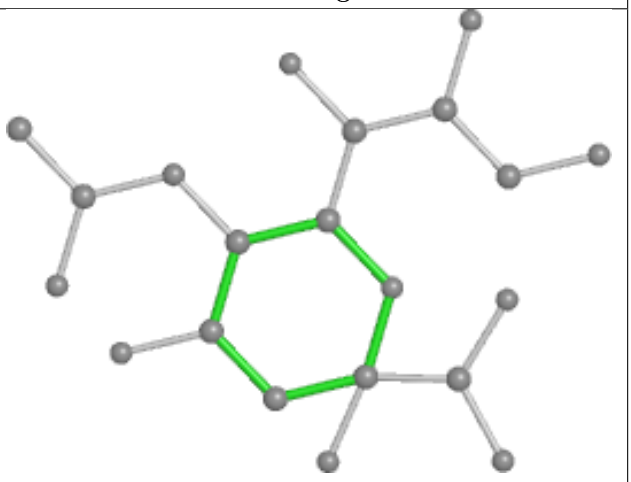
Bond lengths



Bond angles

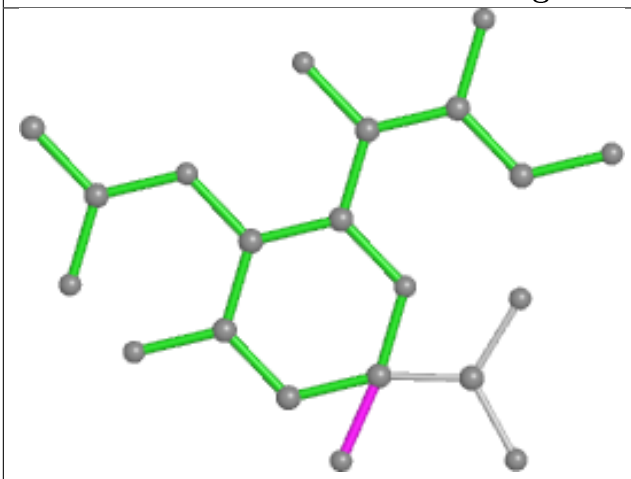


Torsions

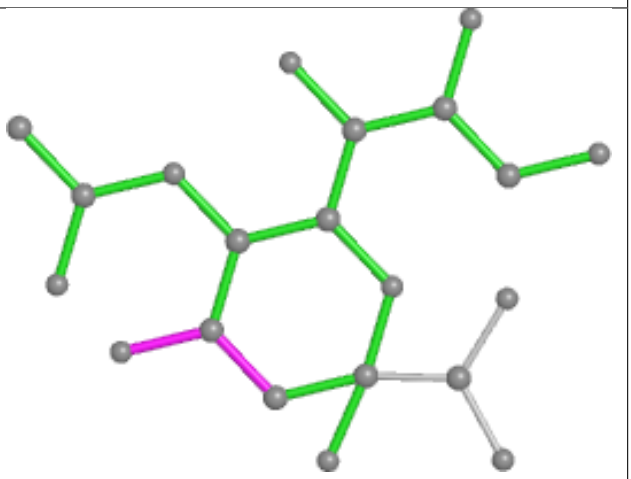


Rings

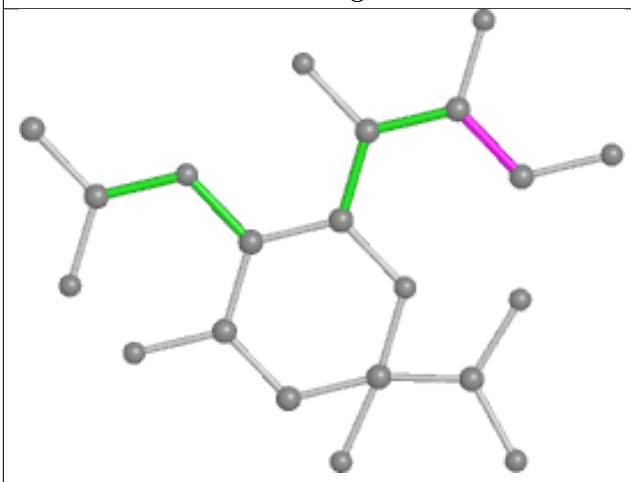
Ligand SIA E 401



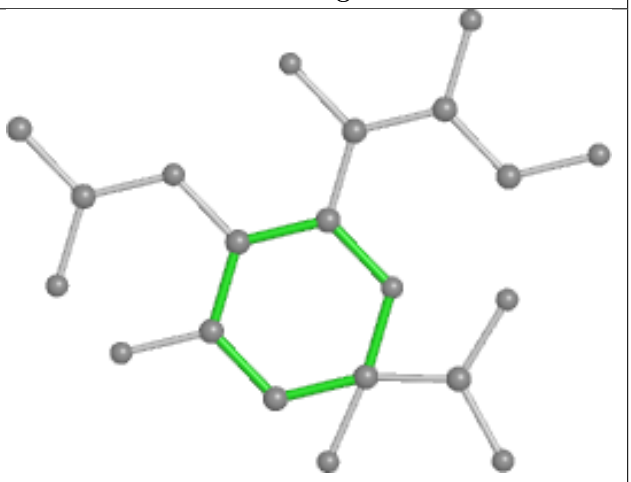
Bond lengths



Bond angles

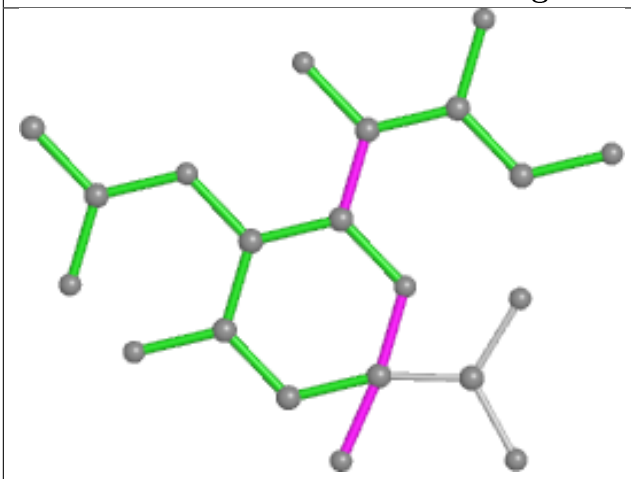


Torsions

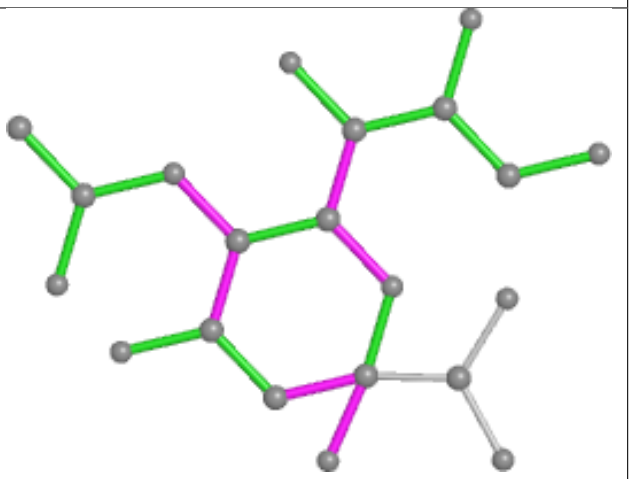


Rings

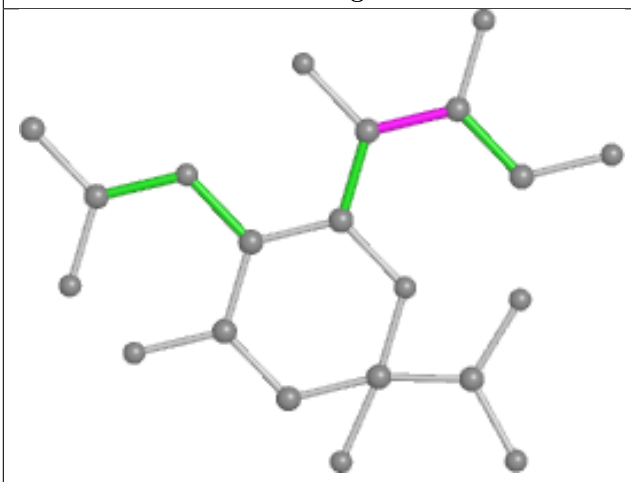
Ligand SIA R 401



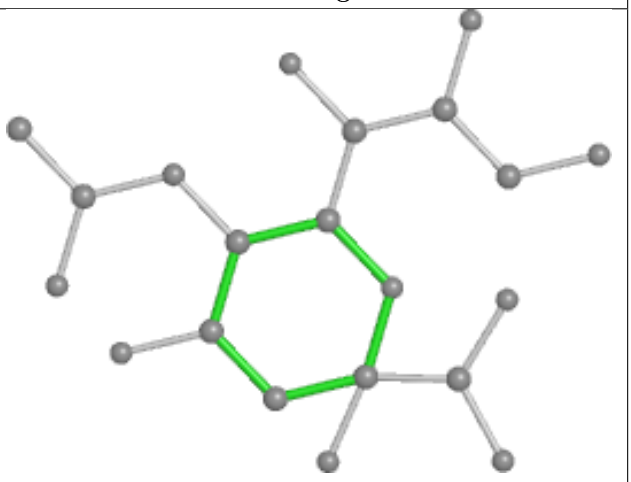
Bond lengths



Bond angles

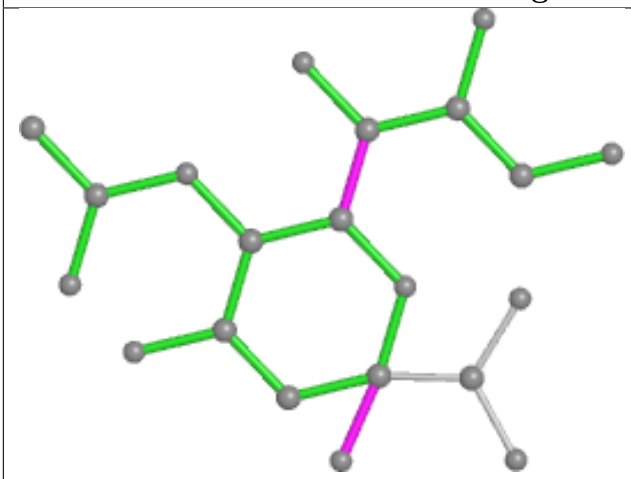


Torsions

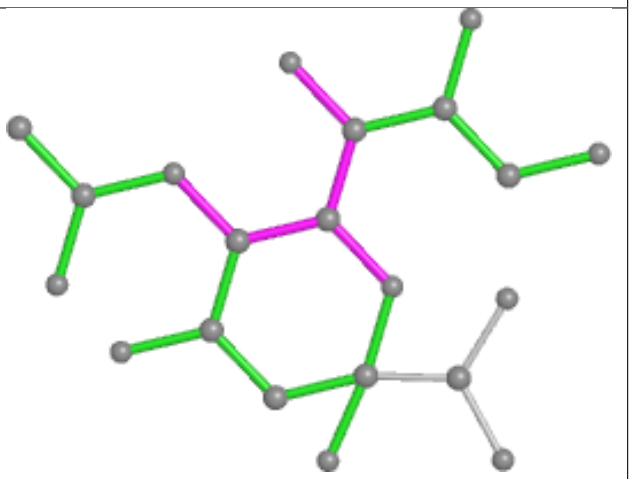


Rings

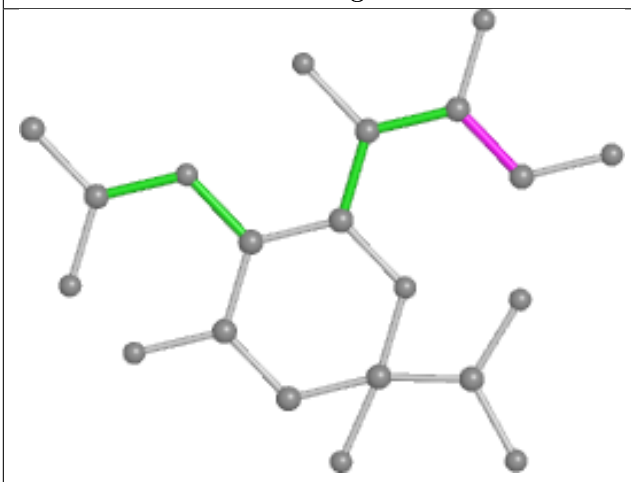
Ligand SIA A 401



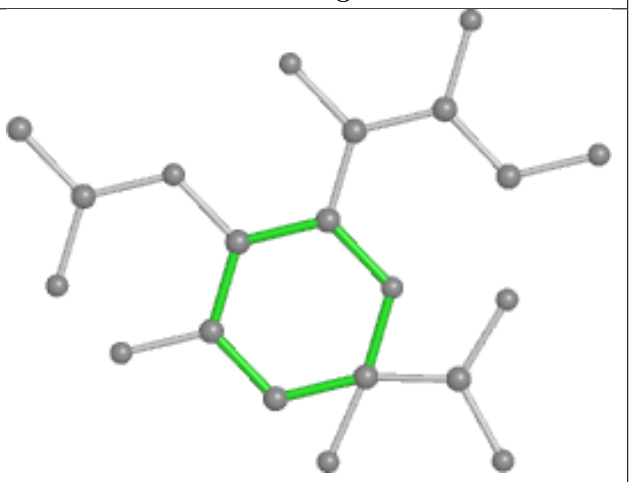
Bond lengths



Bond angles

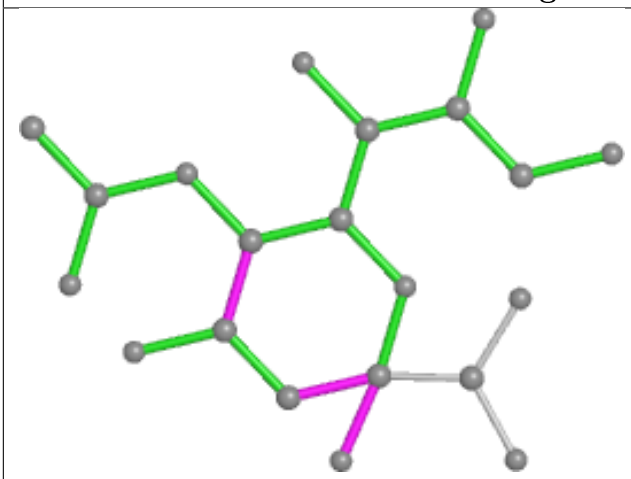


Torsions

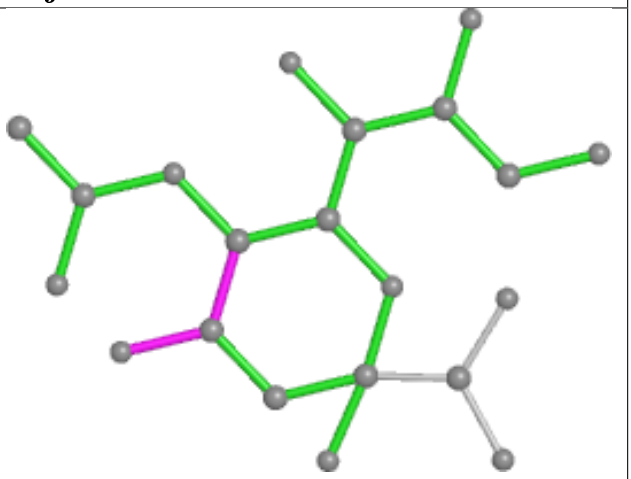


Rings

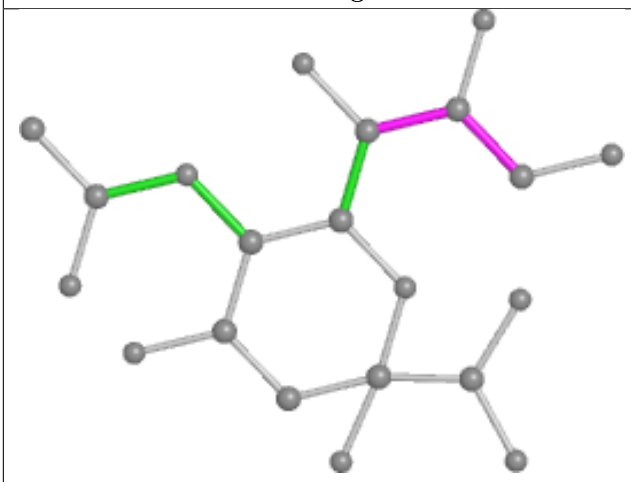
Ligand SIA j 401



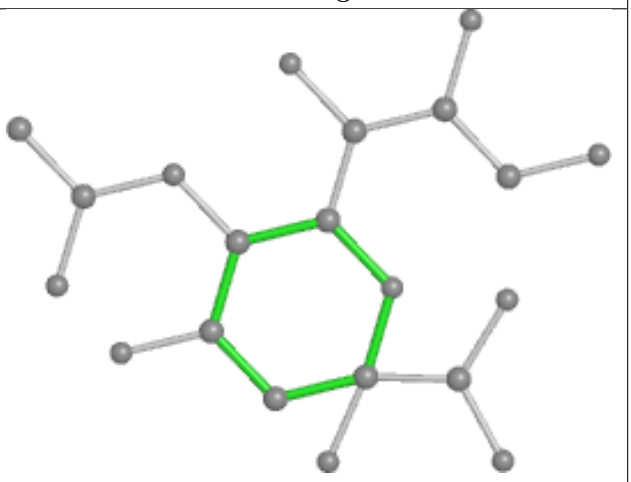
Bond lengths



Bond angles

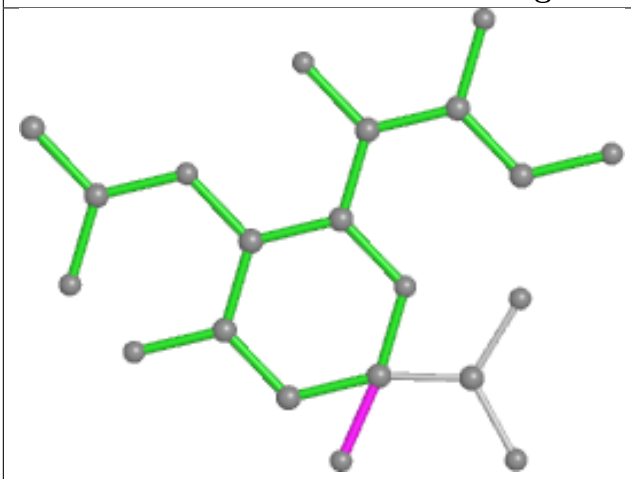


Torsions

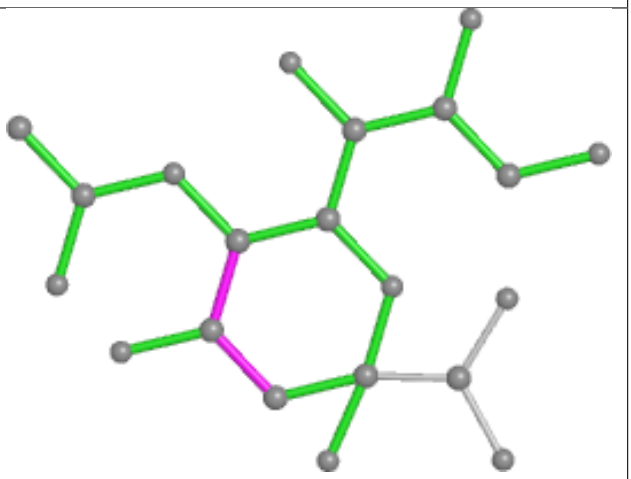


Rings

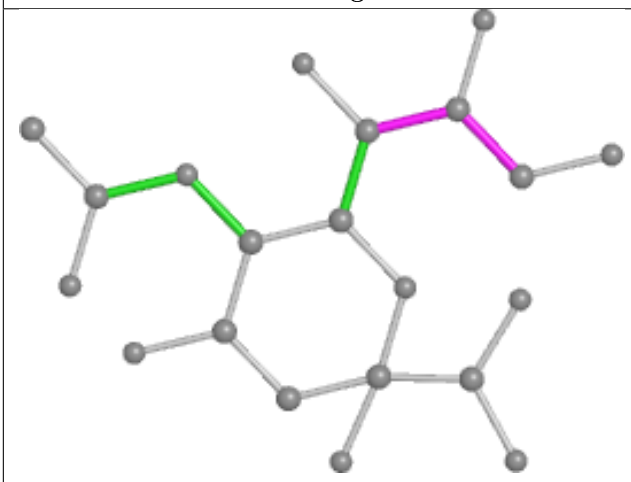
Ligand SIA S 401



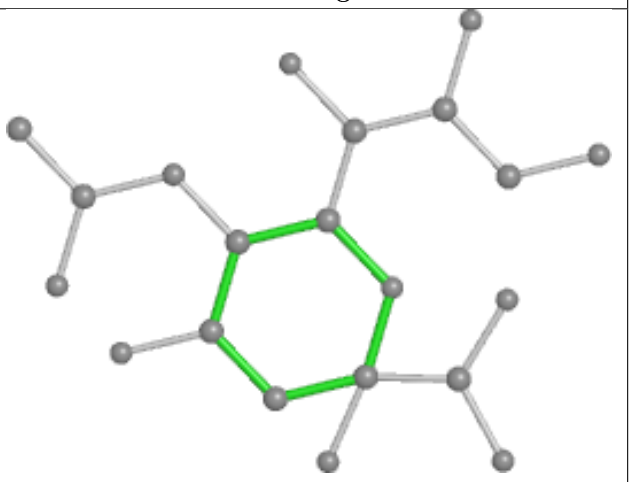
Bond lengths



Bond angles

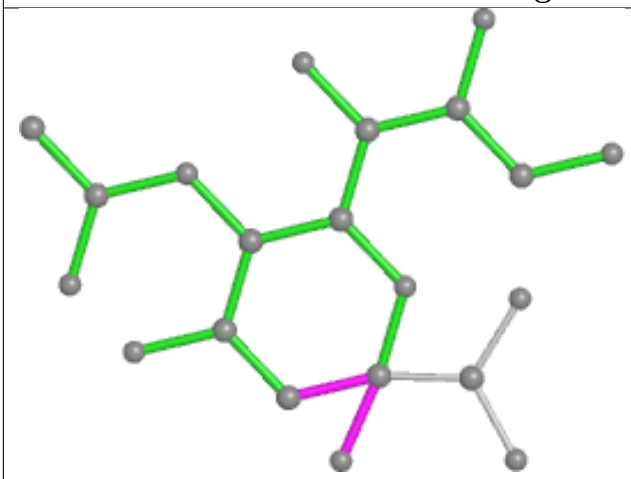


Torsions

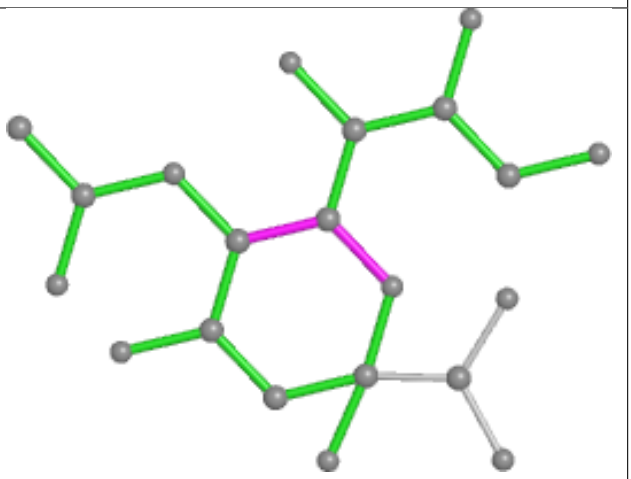


Rings

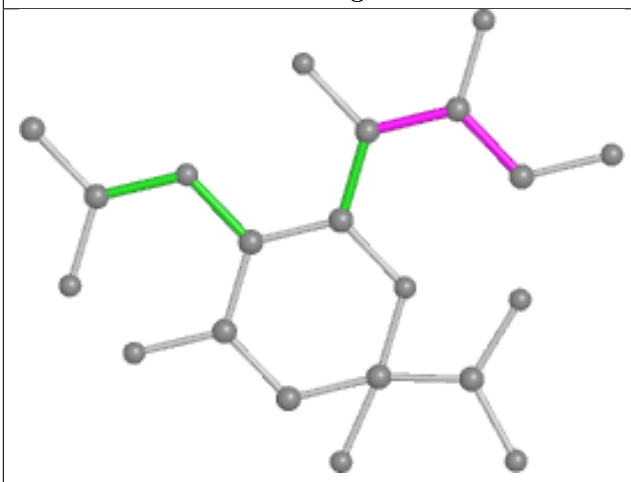
Ligand SIA b 401



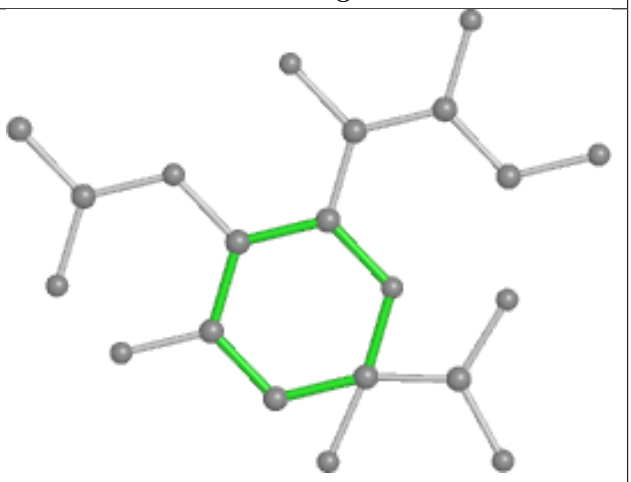
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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

All (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
1	W	23	GLY	3.2
1	a	24	ILE	3.2
1	g	93	PRO	3.1
1	e	24	ILE	3.0
1	m	65	ASN	2.9
1	K	24	ILE	2.8
1	l	128	GLY	2.8
1	m	171	PRO	2.8
1	c	33	PRO	2.6
1	l	94	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	V	23	GLY	2.5
1	g	23	GLY	2.5
1	l	75	CYS	2.5
1	W	94	THR	2.5
1	i	60	ALA	2.4
1	l	79	ALA	2.4
1	b	33	PRO	2.4
1	a	33	PRO	2.4
1	l	47	VAL	2.4
1	k	171	PRO	2.3
1	e	94	THR	2.3
1	j	130	GLY	2.3
1	m	158	SER	2.3
1	l	168	PRO	2.3
1	l	194	ALA	2.2
1	k	52	GLY	2.2
1	l	156	ASN	2.2
1	V	93	PRO	2.2
1	X	94	THR	2.1
1	c	95	LEU	2.1
1	k	79	ALA	2.1
1	l	147	PRO	2.1
1	d	94	THR	2.1
1	m	149	ASP	2.1
1	l	73	ILE	2.0
1	F	85	LEU	2.0
1	m	68	PRO	2.0

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, 95^{th} 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
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

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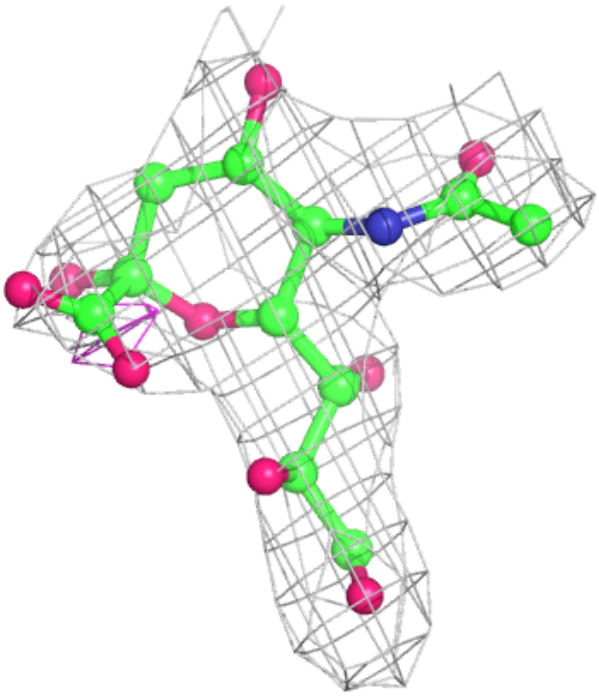
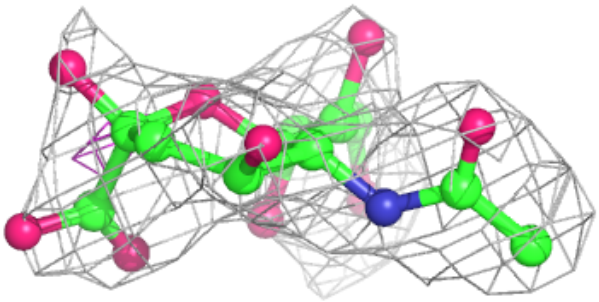
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CL	d	402	1/1	0.89	0.11	45,45,45,45	0
3	CL	M	402	1/1	0.90	0.12	41,41,41,41	0
3	CL	Y	403	1/1	0.90	0.08	47,47,47,47	0
2	SIA	B	401	21/21	0.90	0.24	46,49,60,69	0
3	CL	S	403	1/1	0.90	0.14	44,44,44,44	0
3	CL	X	403	1/1	0.90	0.14	50,50,50,50	0
2	SIA	N	401	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
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

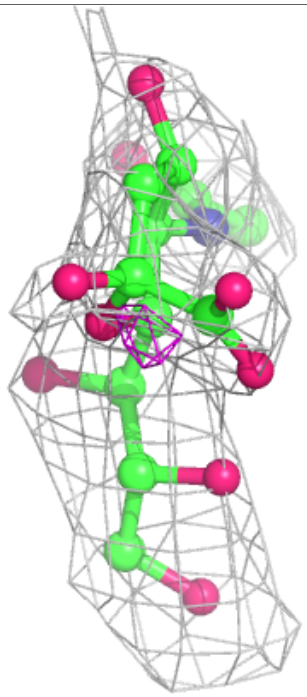
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

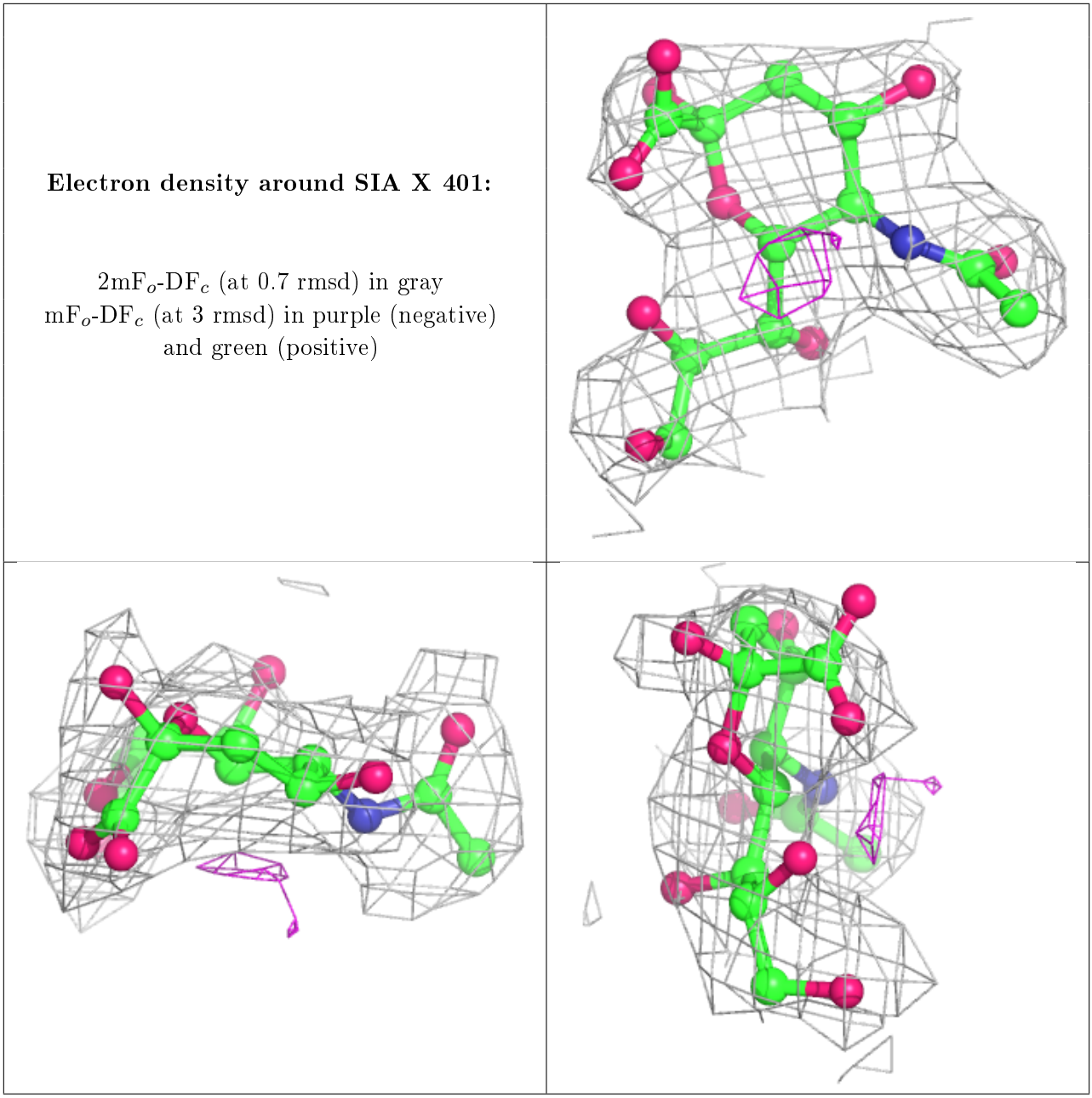






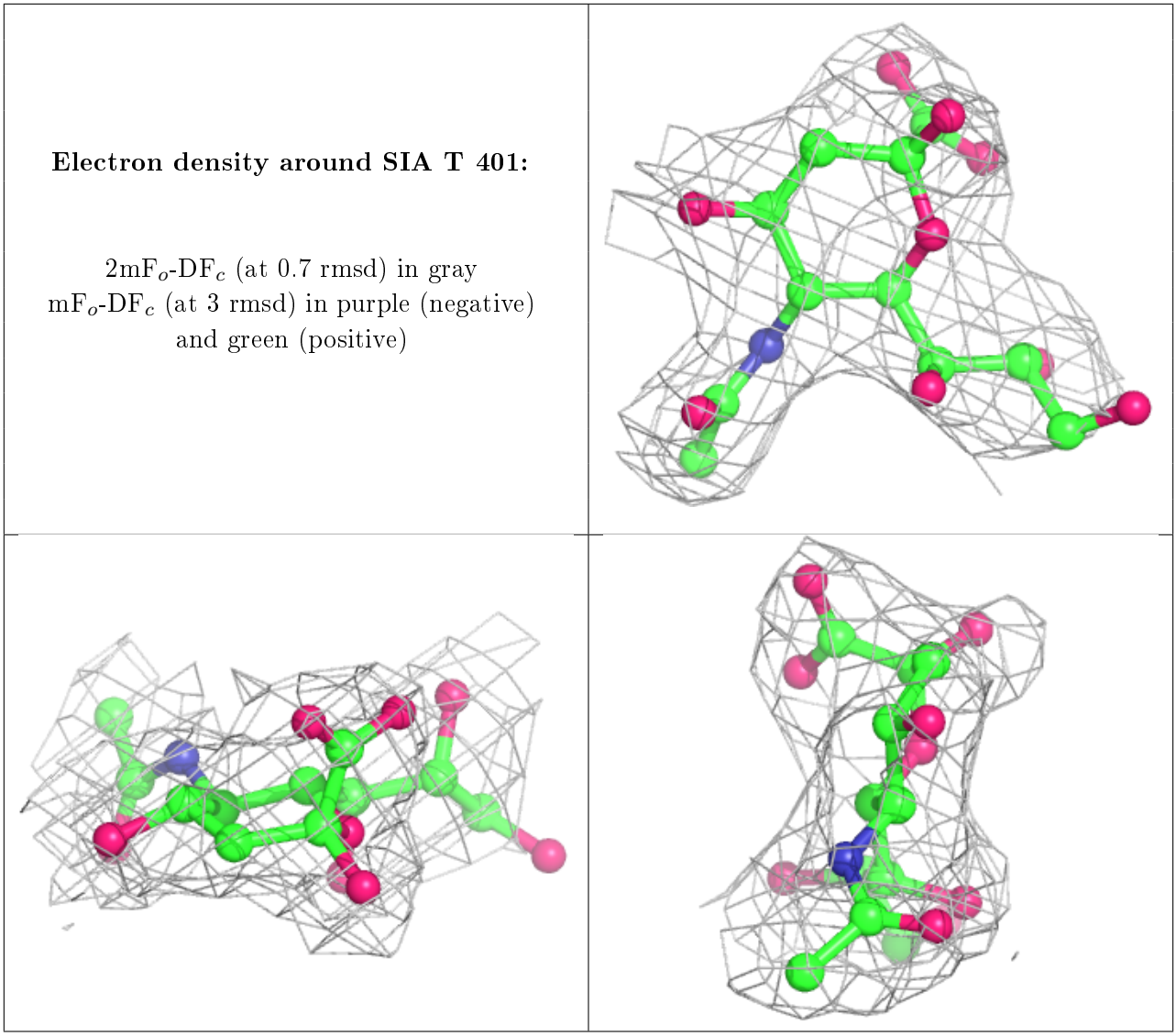
Electron density around SIA X 401:

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



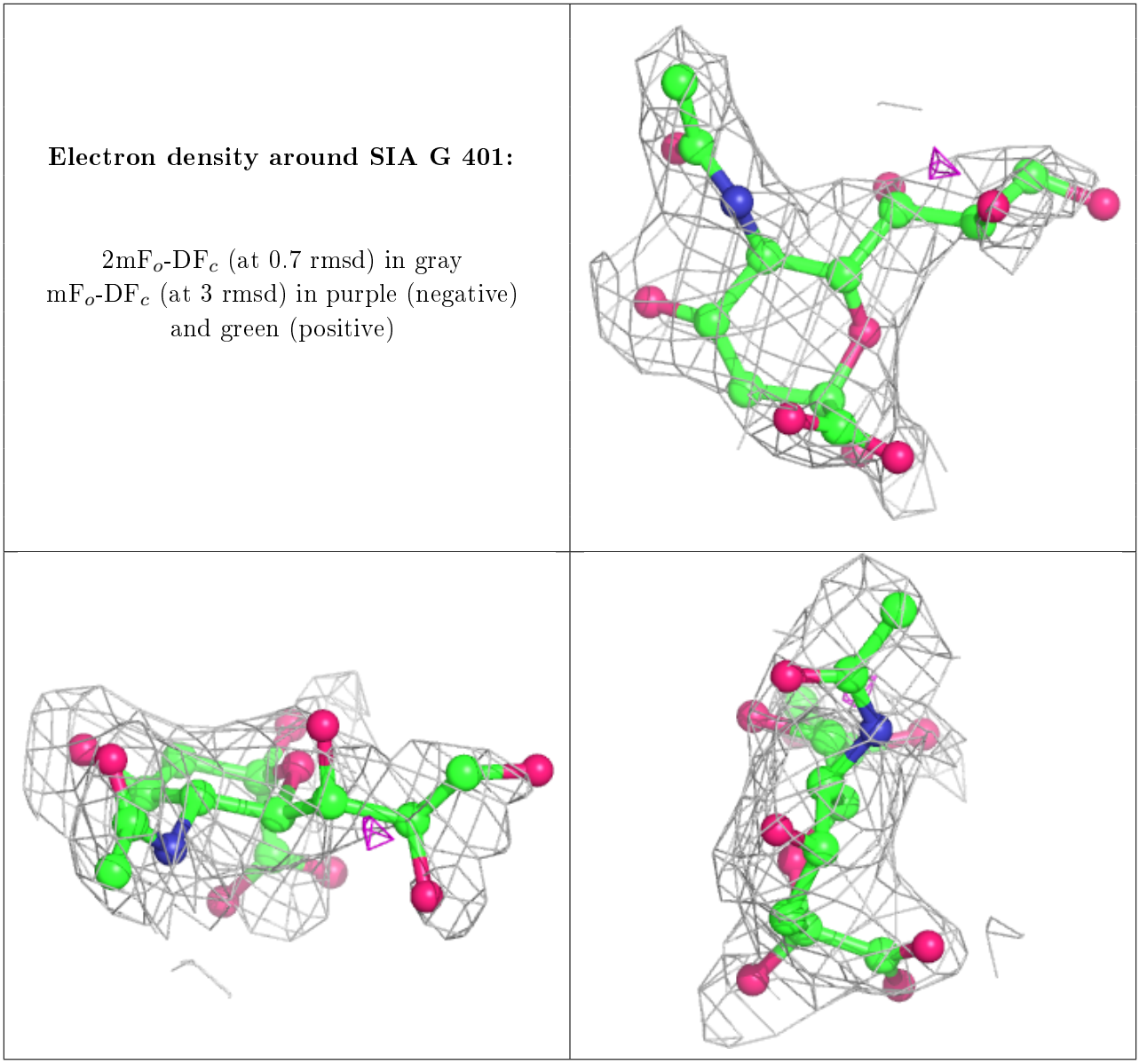
Electron density around SIA T 401:

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



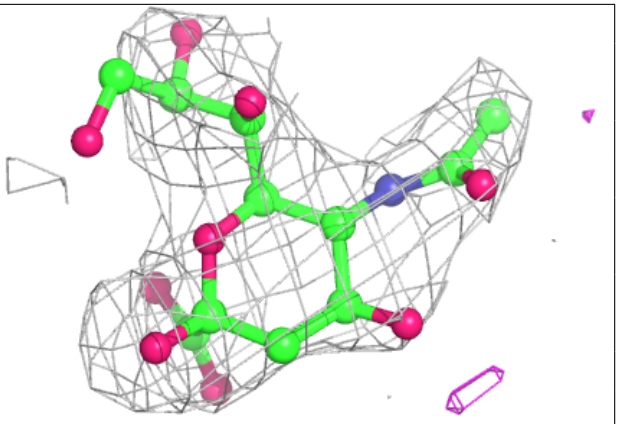
Electron density around SIA G 401:

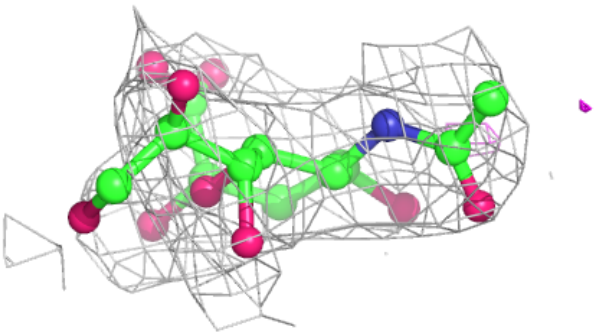
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

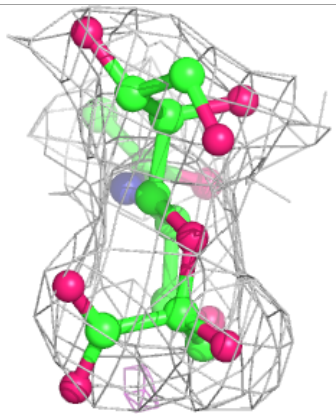


Electron density around SIA C 401:

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

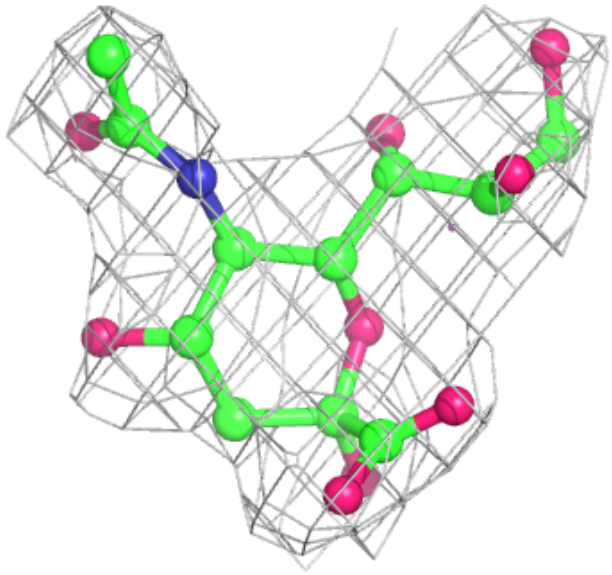


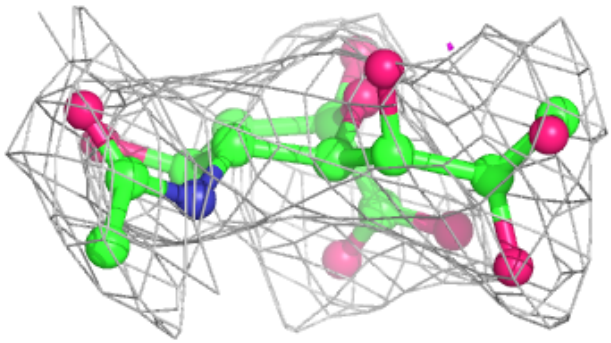


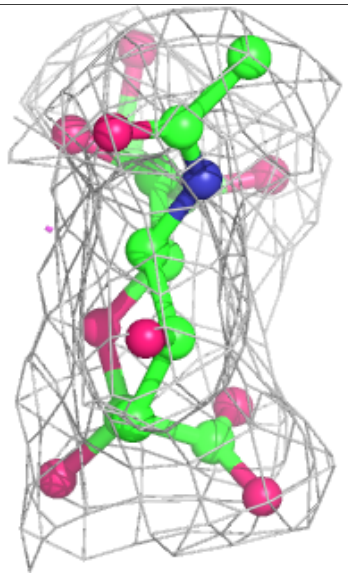


Electron density around SIA a 401:

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

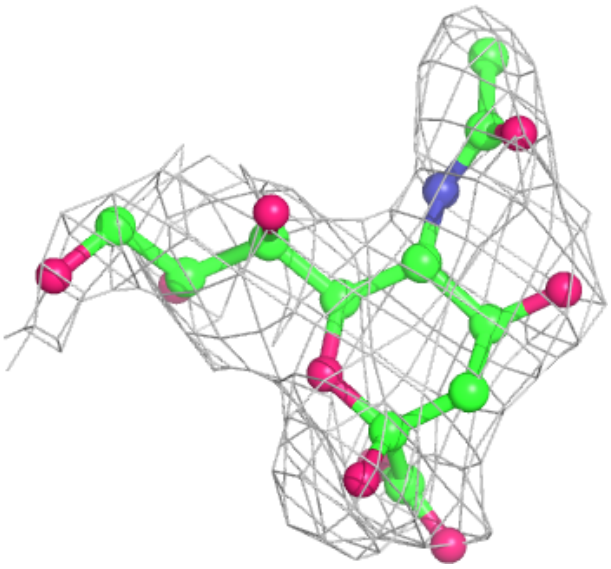


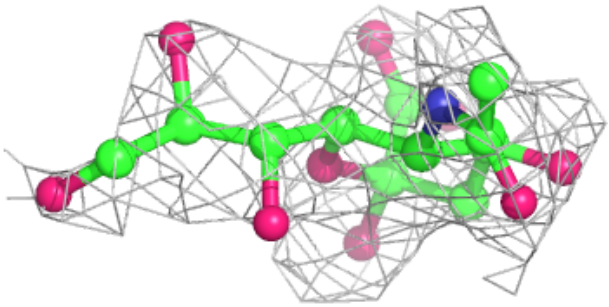


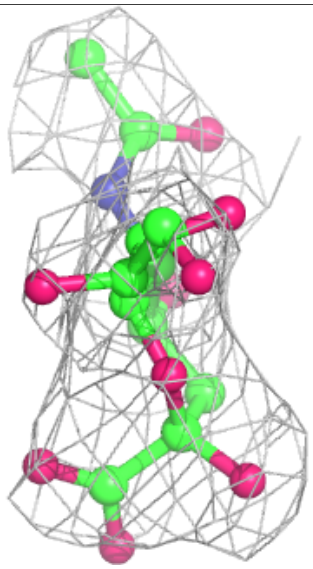


Electron density around SIA d 401:

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

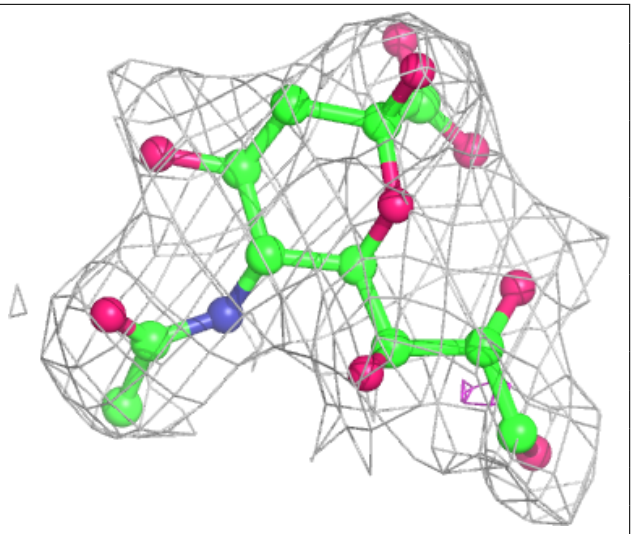


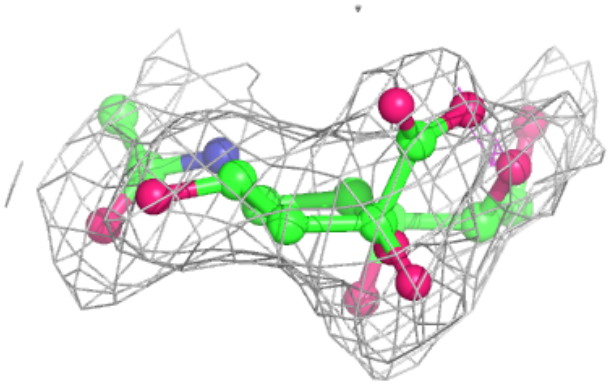


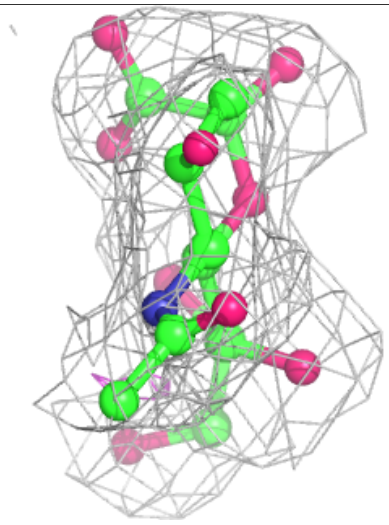


Electron density around SIA Y 401:

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

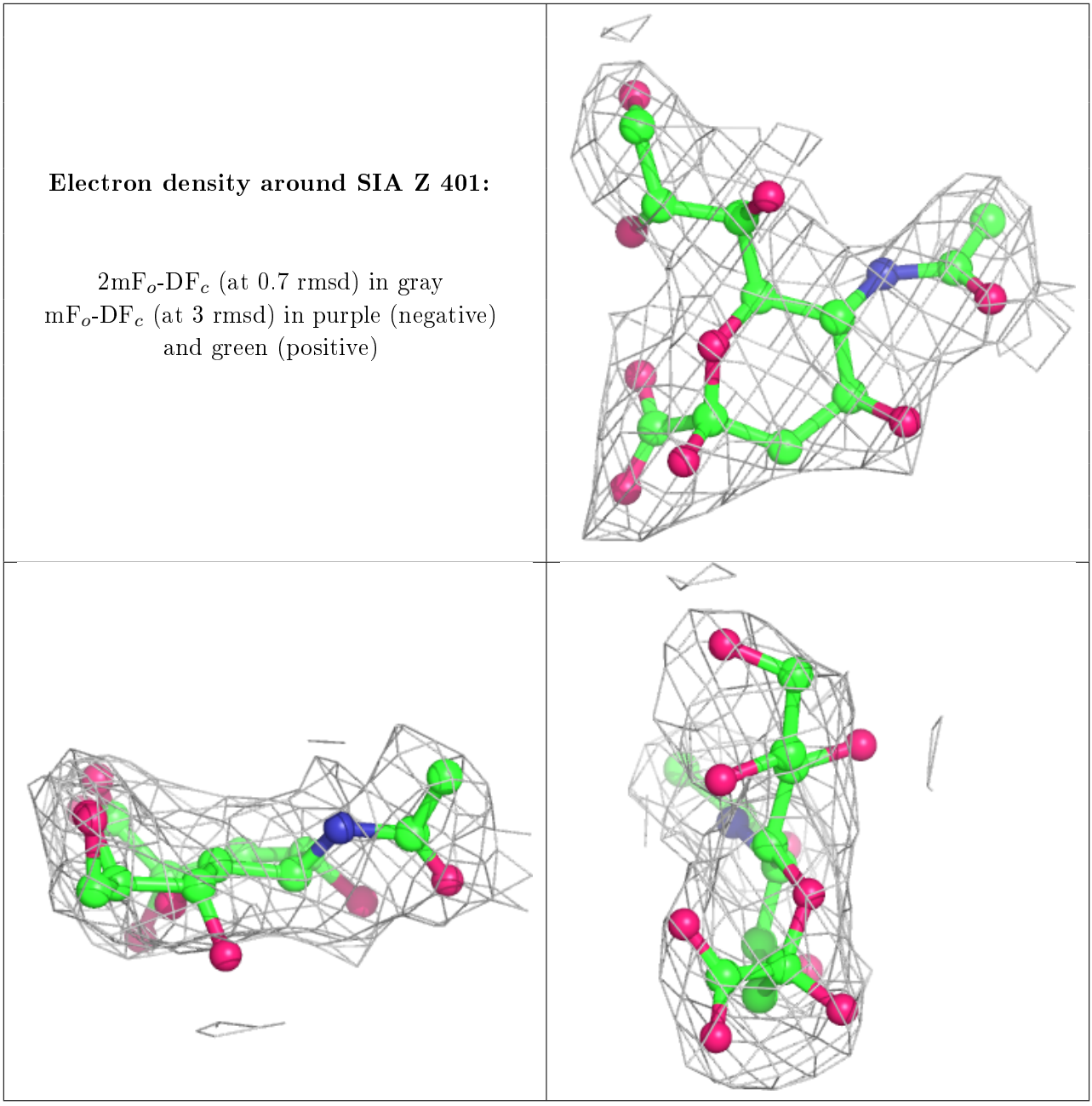






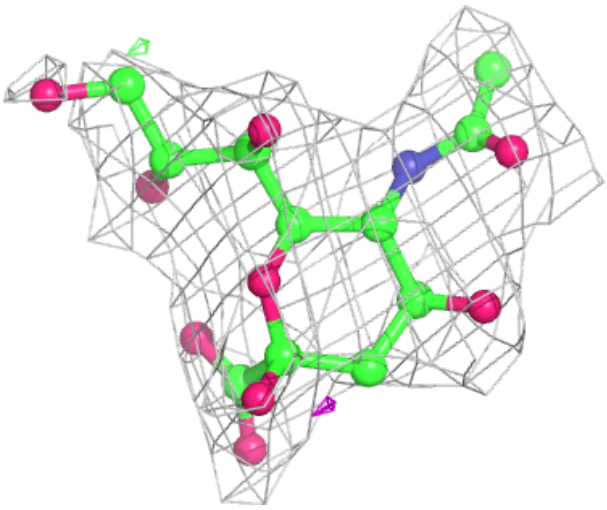
Electron density around SIA Z 401:

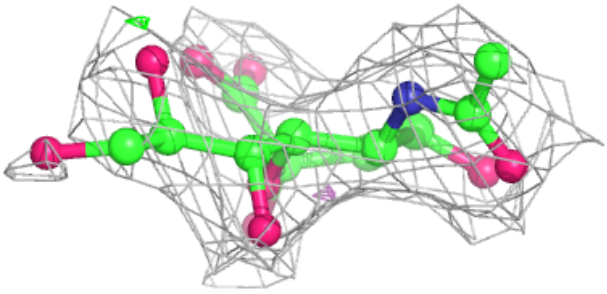
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

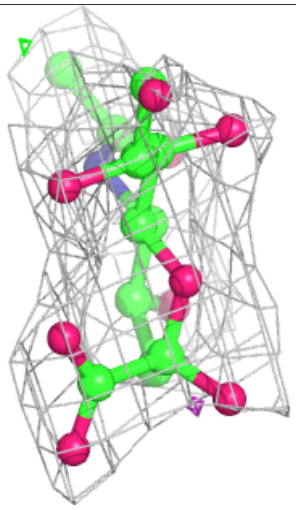


Electron density around SIA Q 401:

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

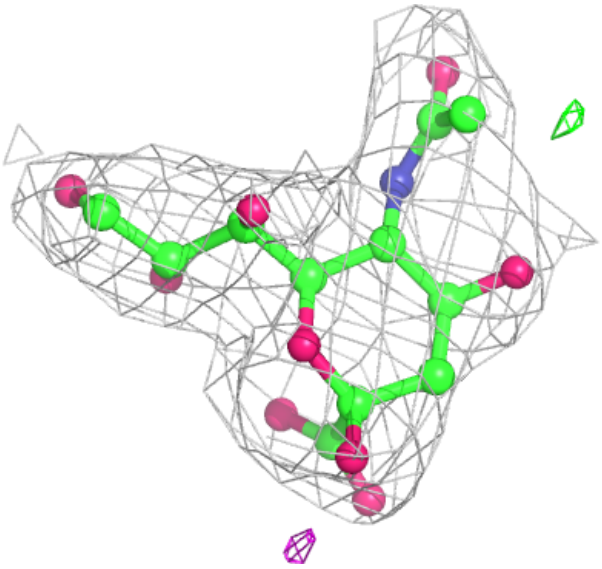


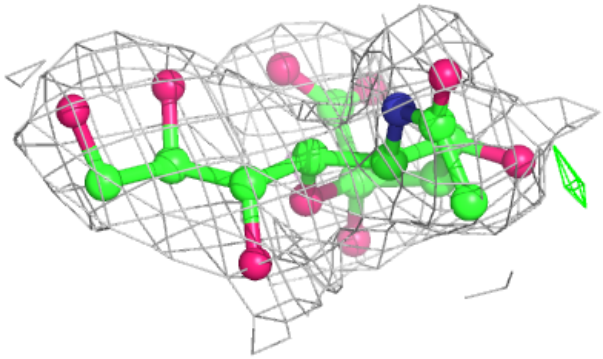


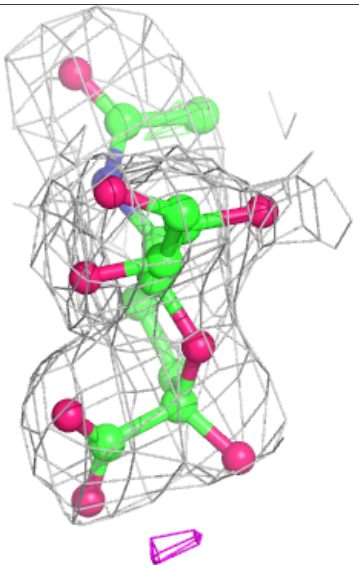


Electron density around SIA F 401:

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

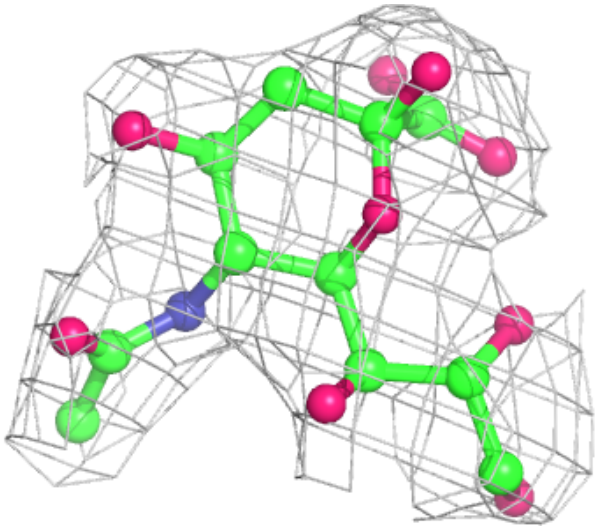


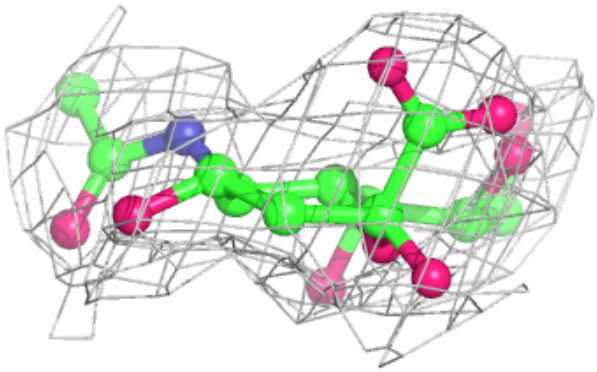


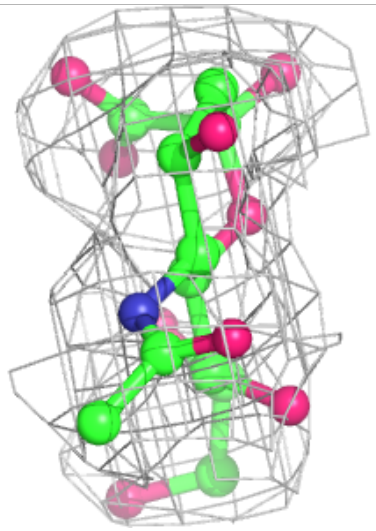


Electron density around SIA c 401:

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

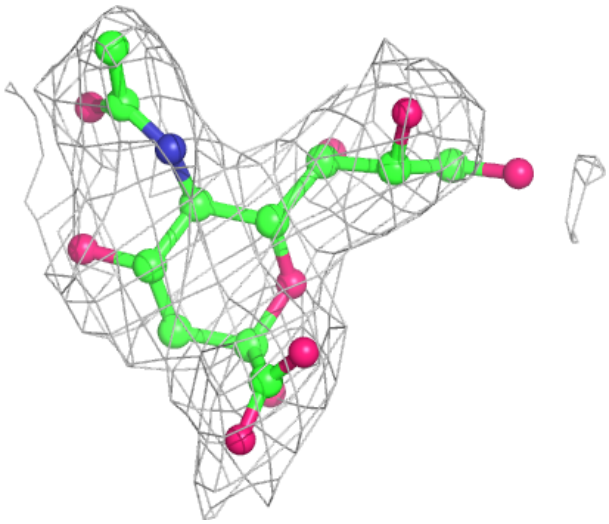


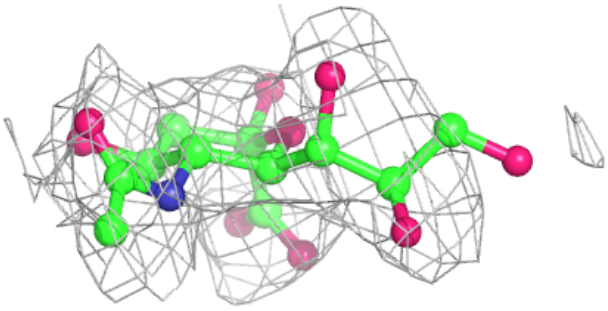


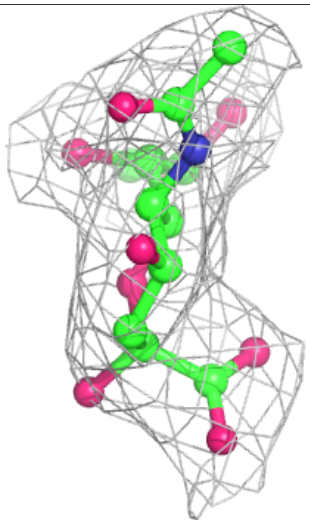


Electron density around SIA R 401:

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

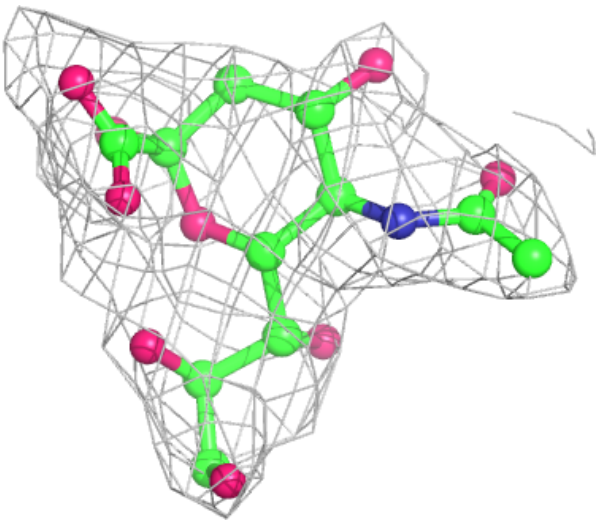


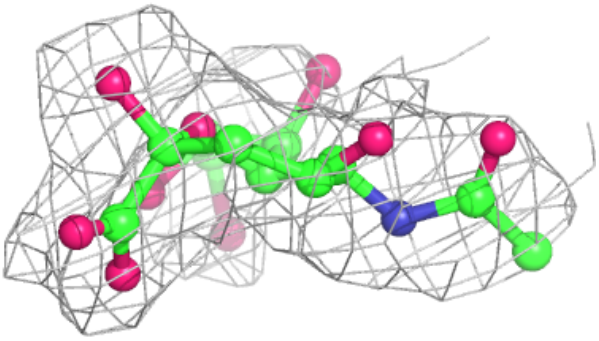


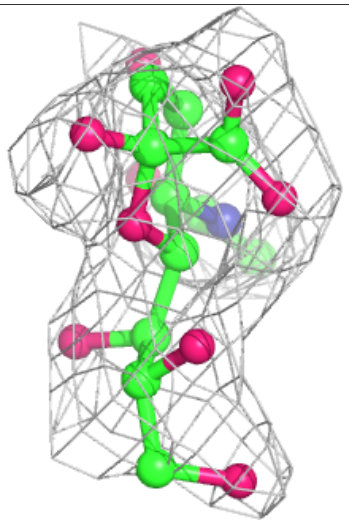


Electron density around SIA I 401:

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

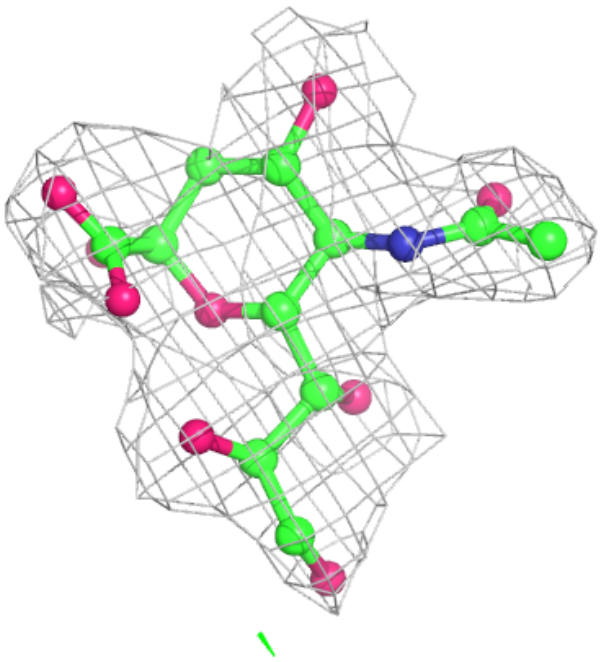


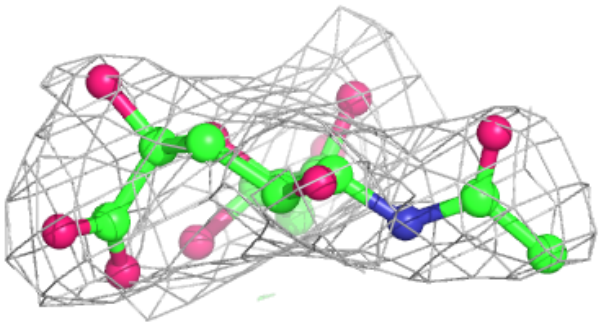


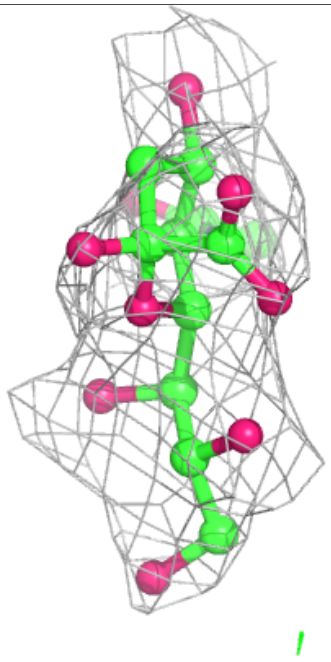


Electron density around SIA j 401:

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

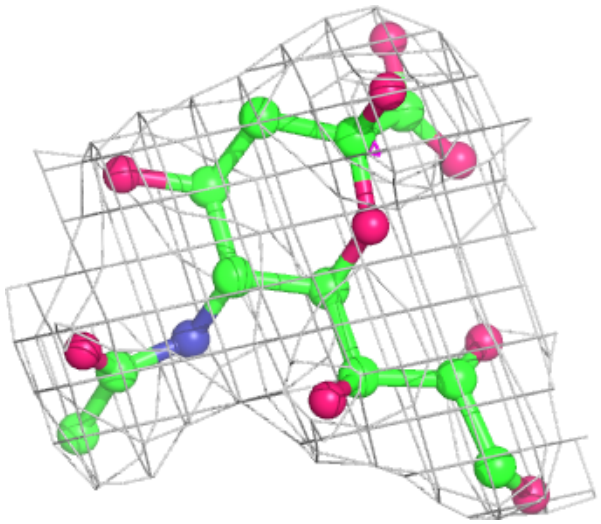


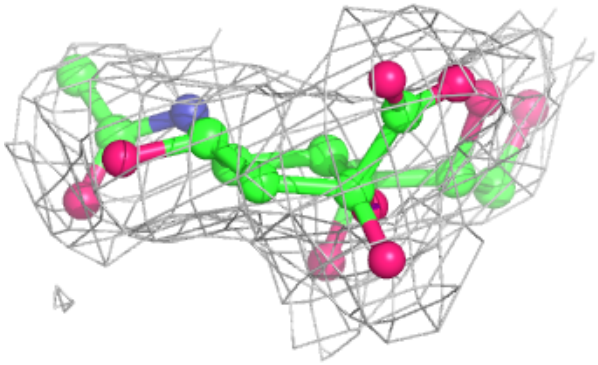


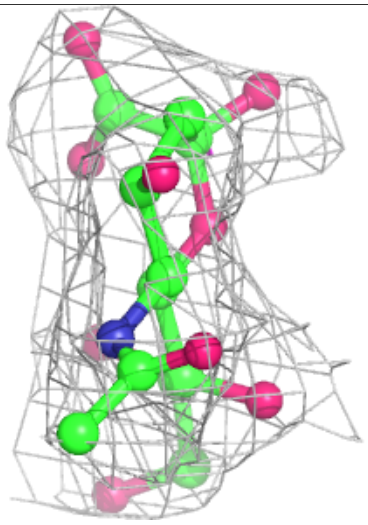


Electron density around SIA f 401:

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

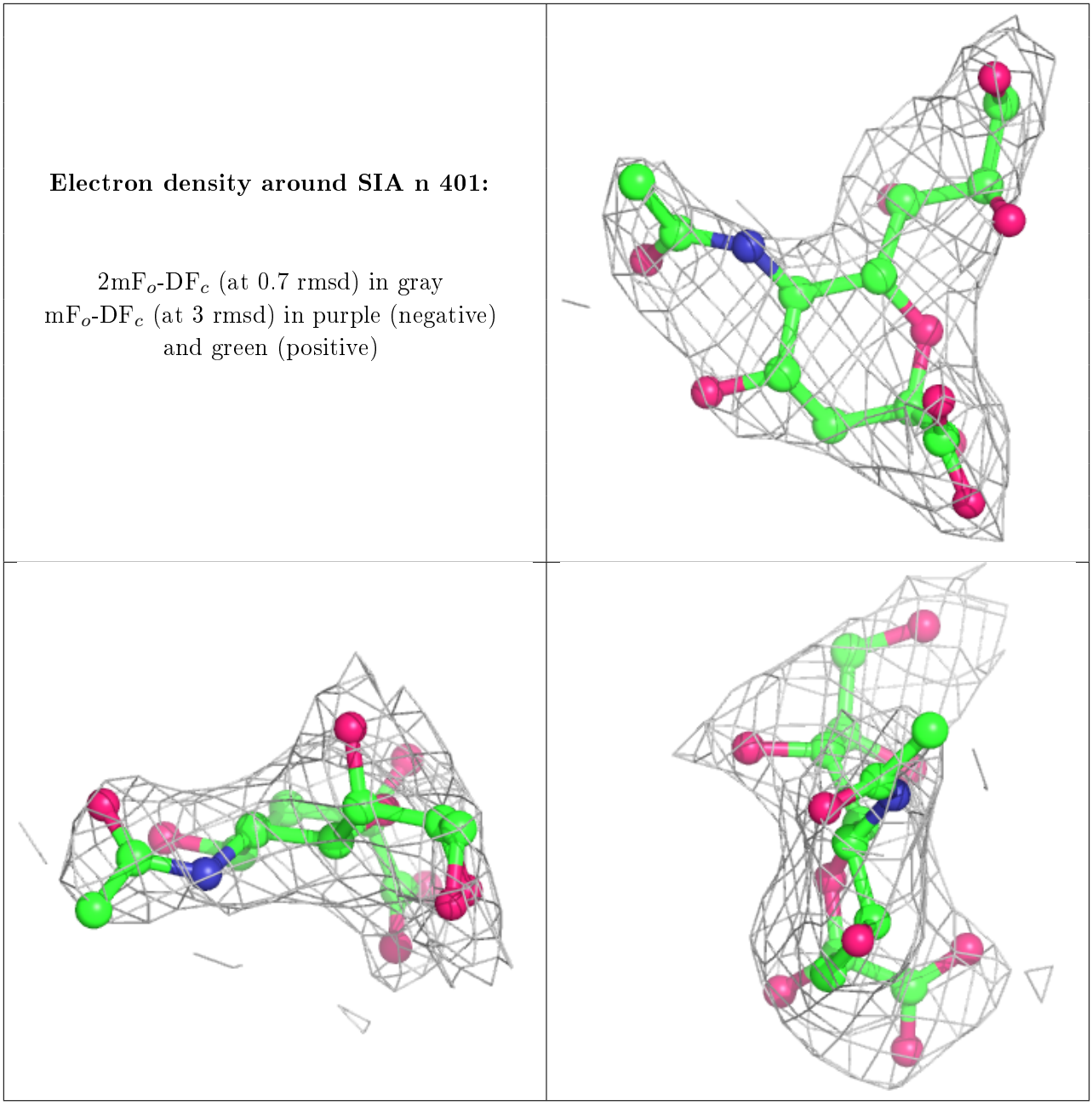






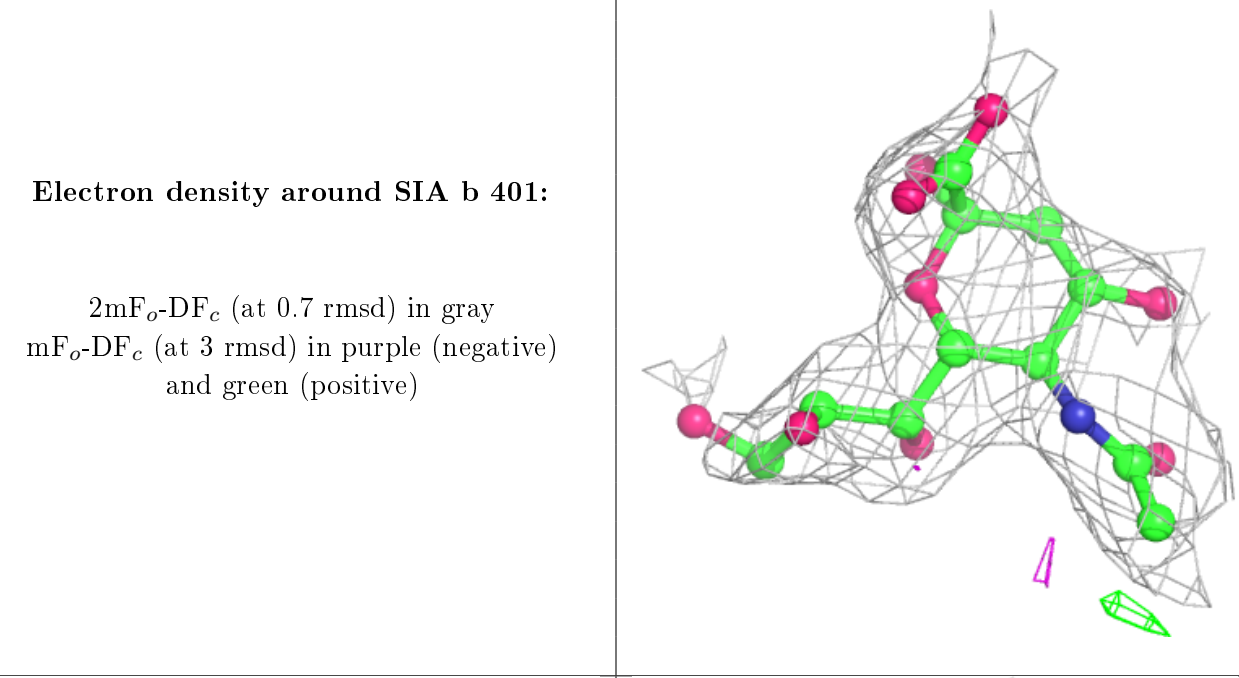
Electron density around SIA n 401:

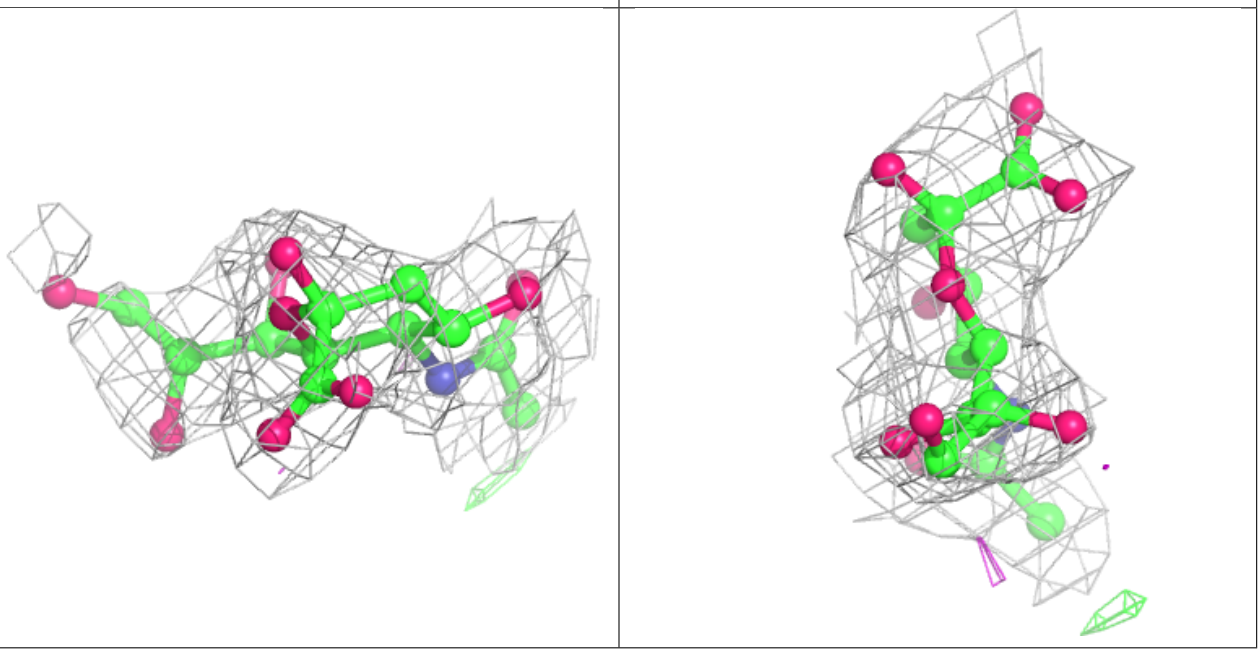
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SIA b 401:

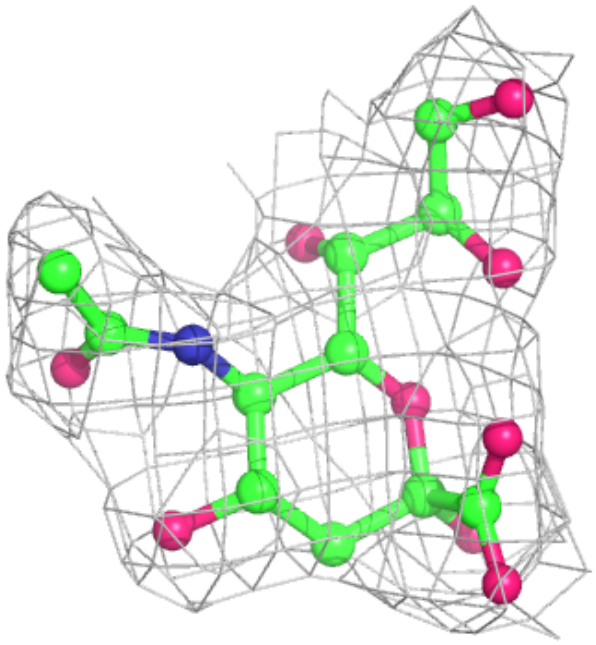
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

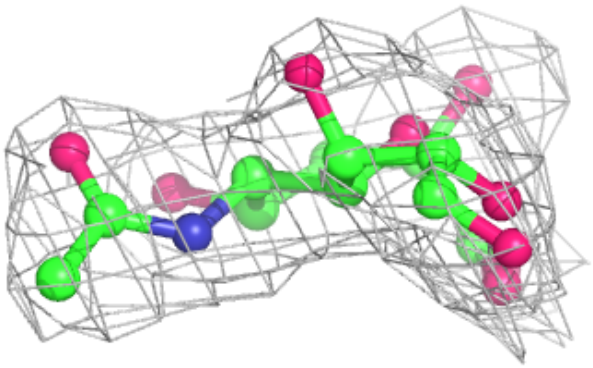


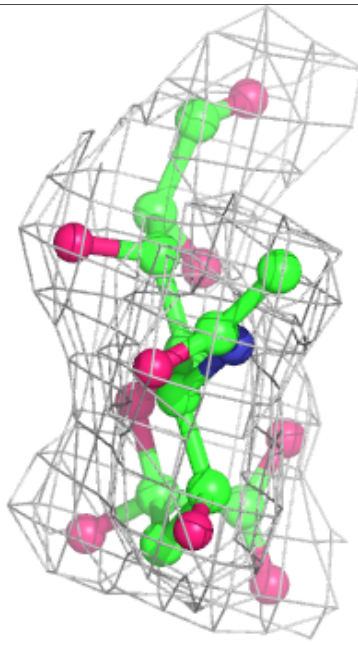


Electron density around SIA J 401:

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

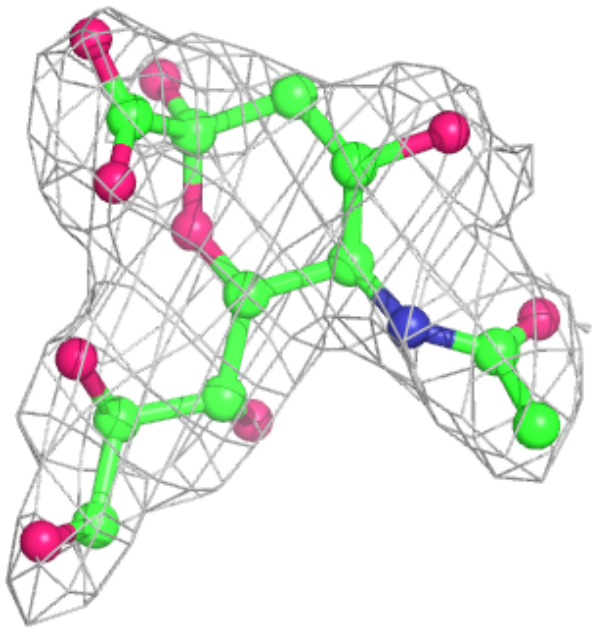


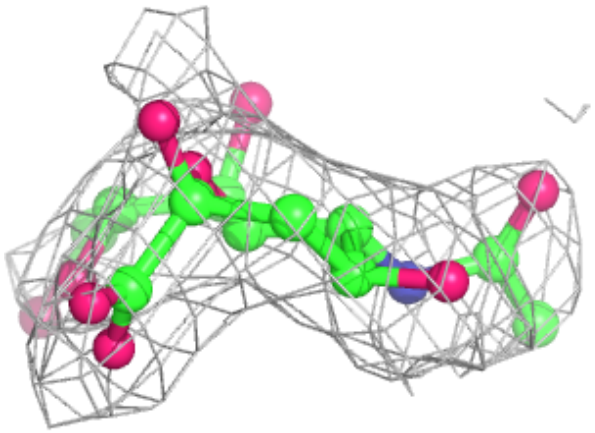


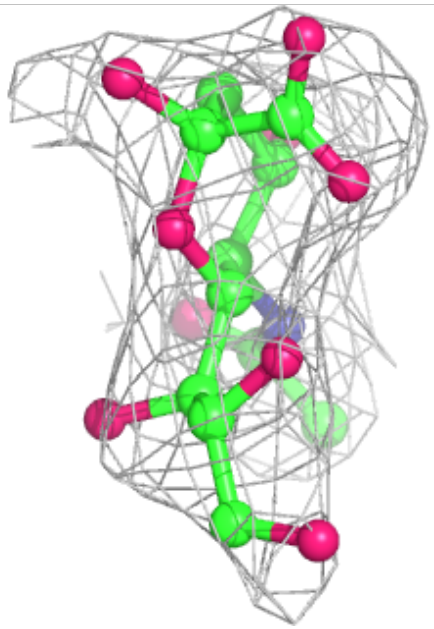


Electron density around SIA e 401:

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

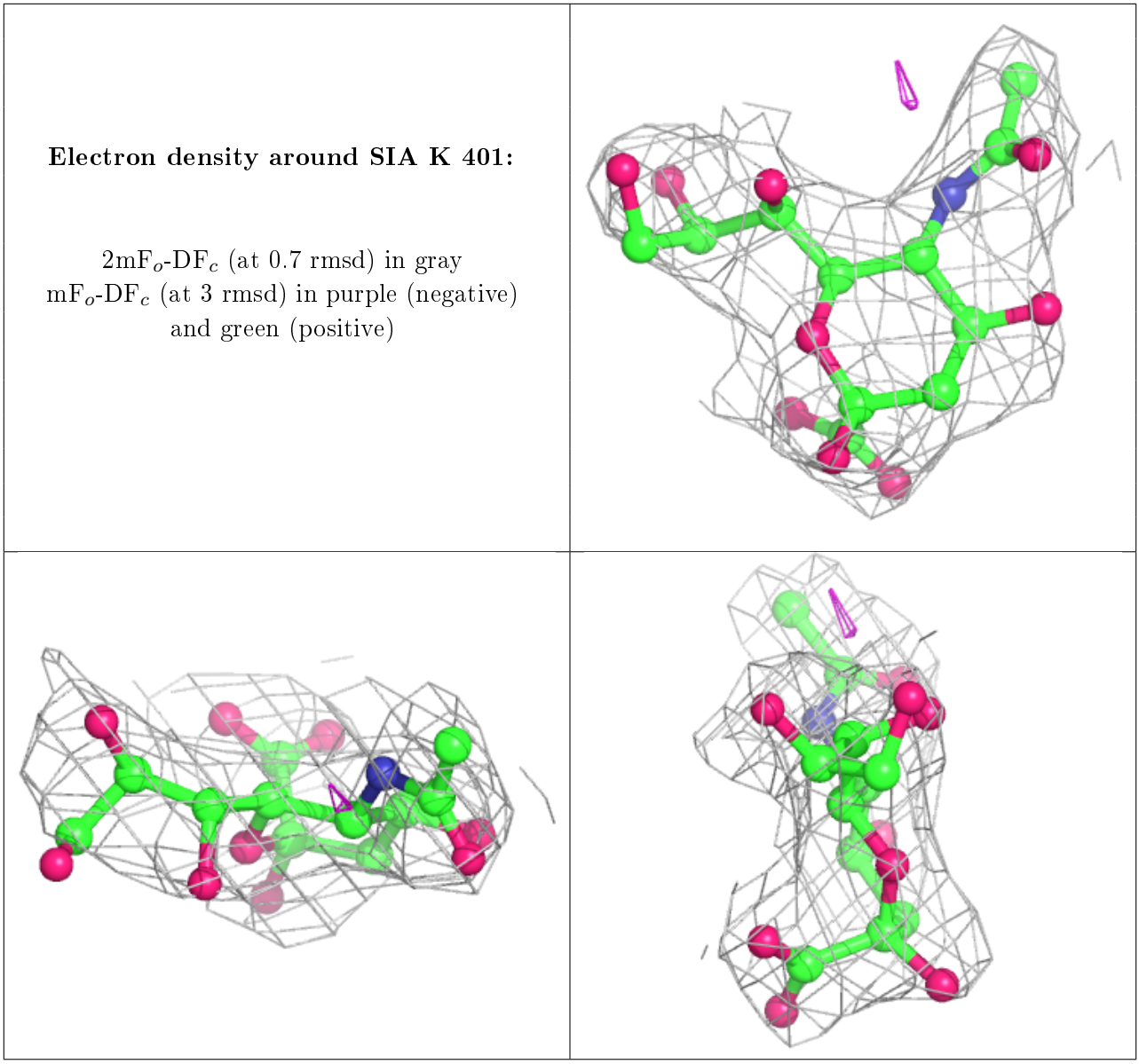






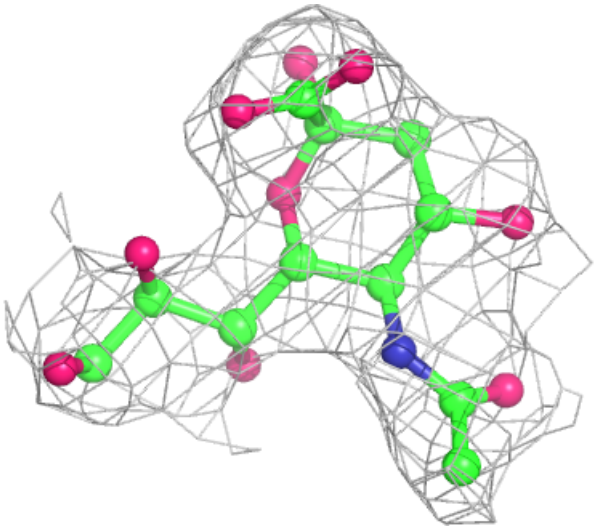
Electron density around SIA K 401:

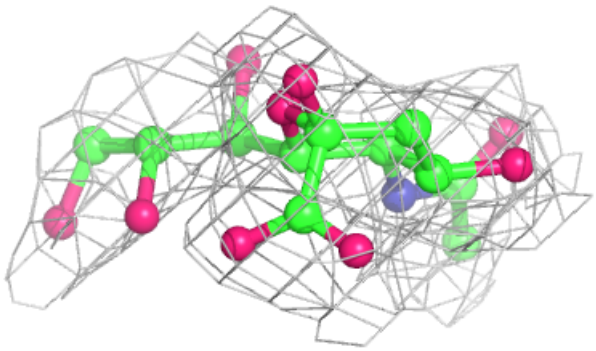
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

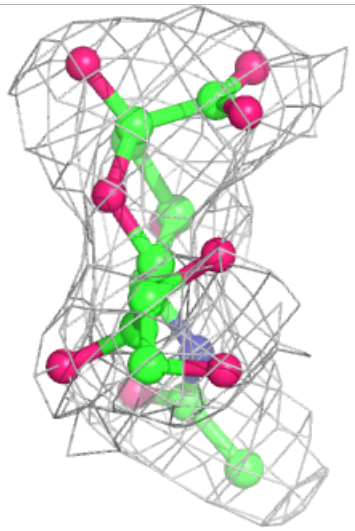


Electron density around SIA A 401:

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

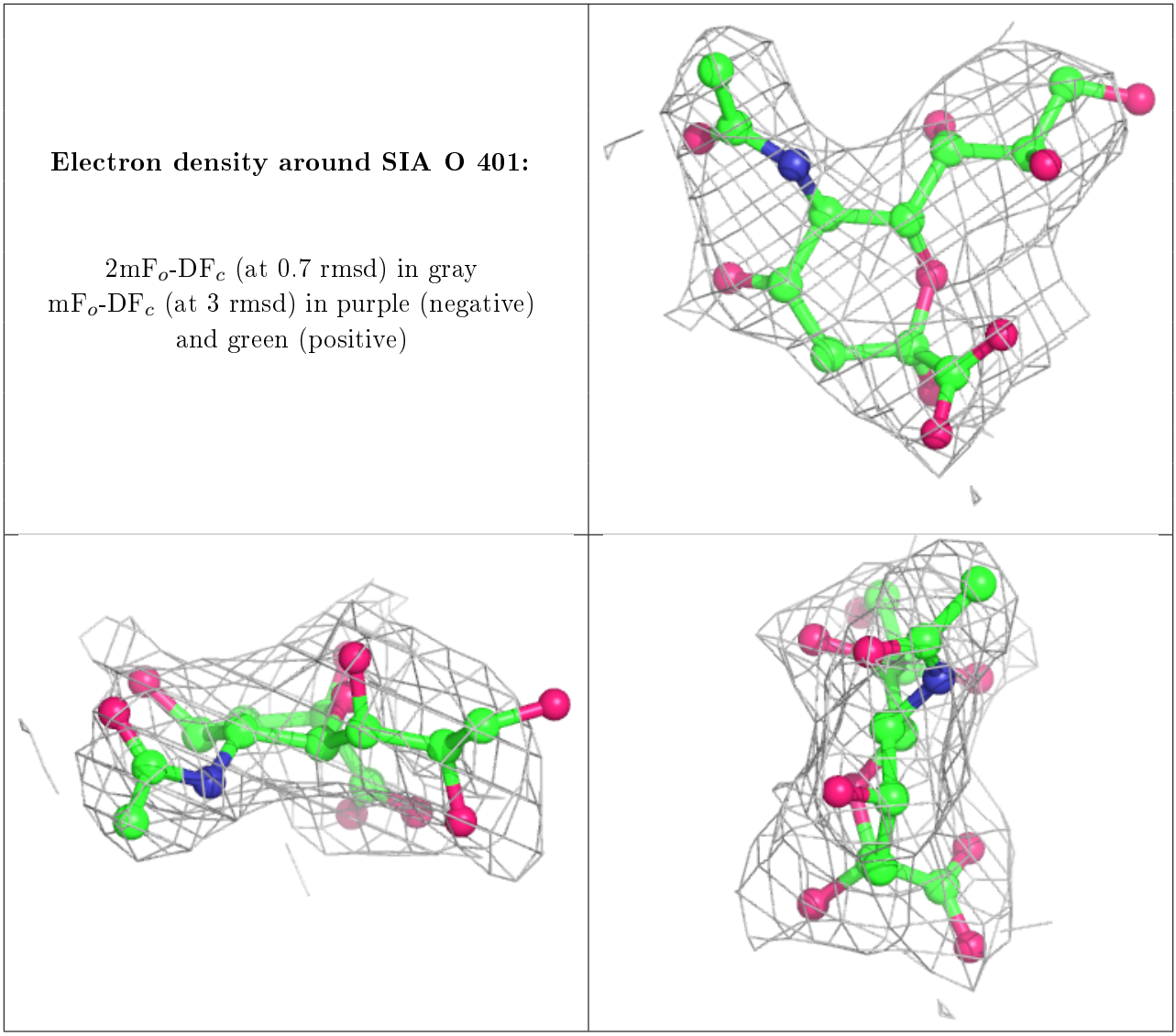






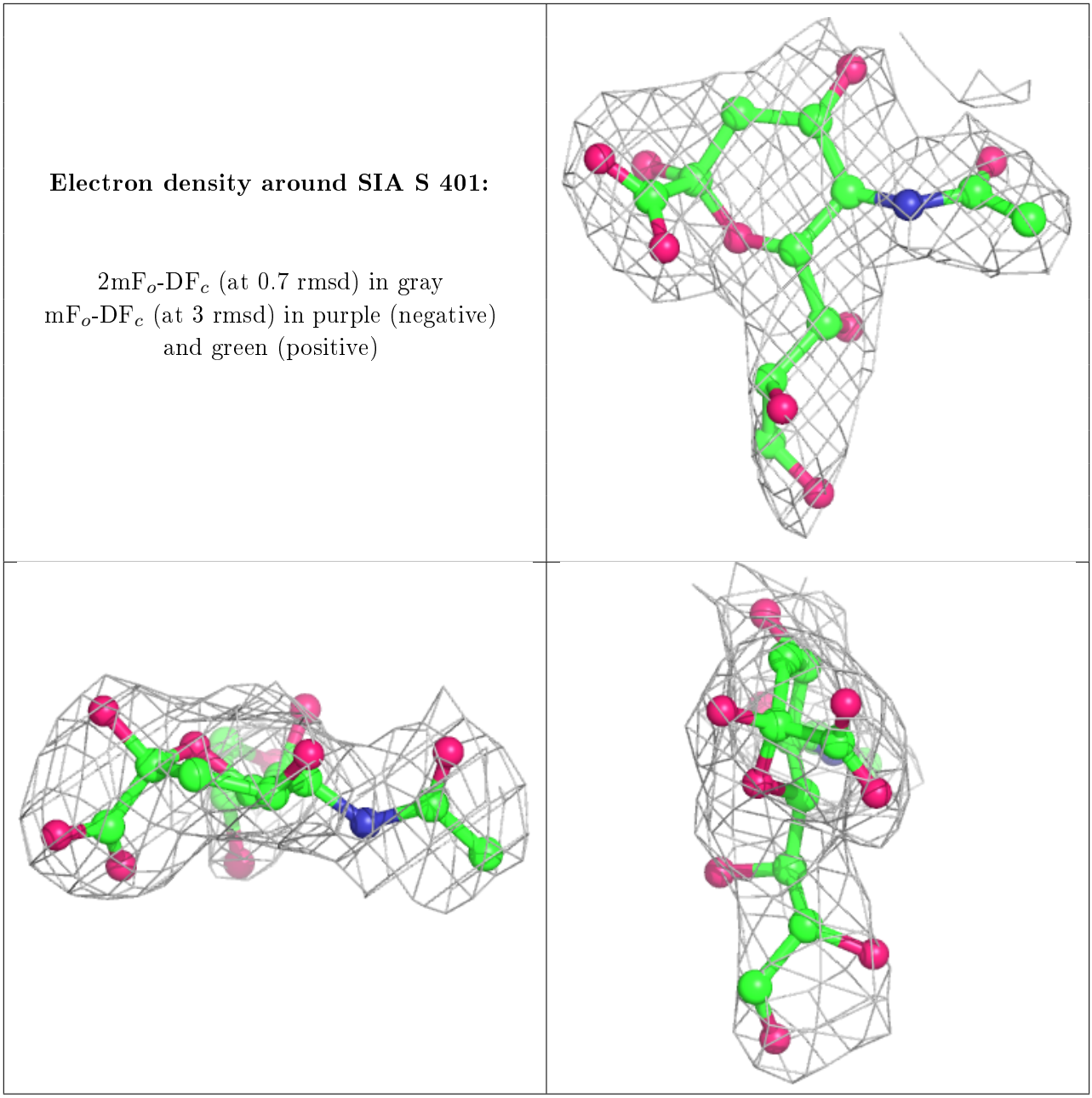
Electron density around SIA O 401:

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



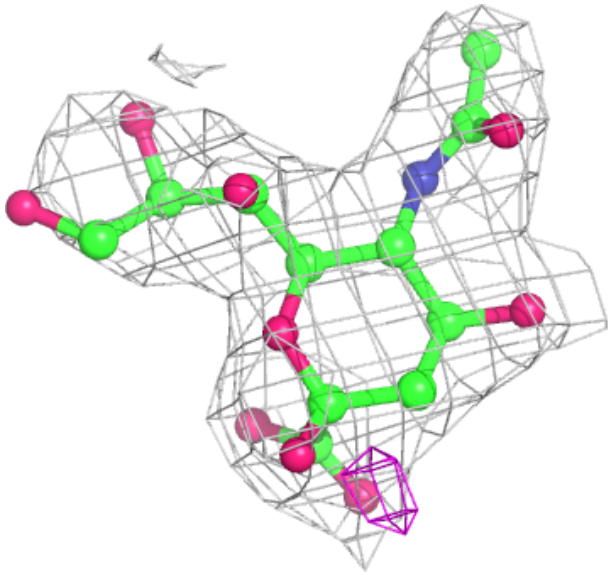
Electron density around SIA S 401:

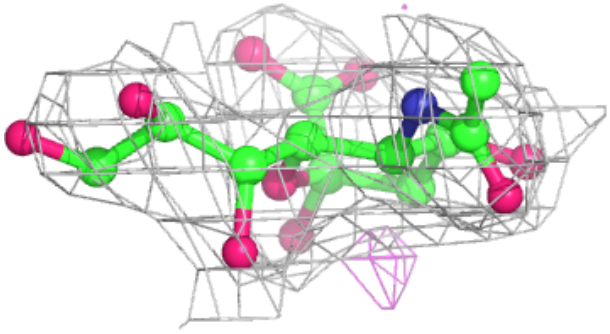
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

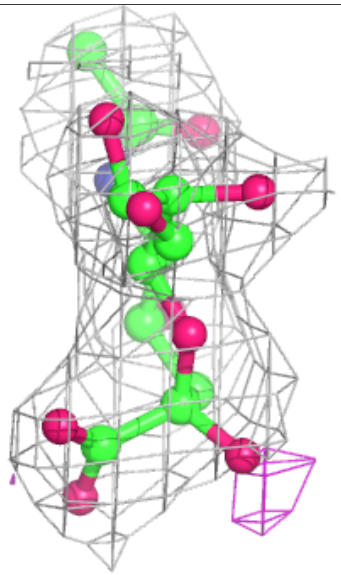


Electron density around SIA B 401:

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

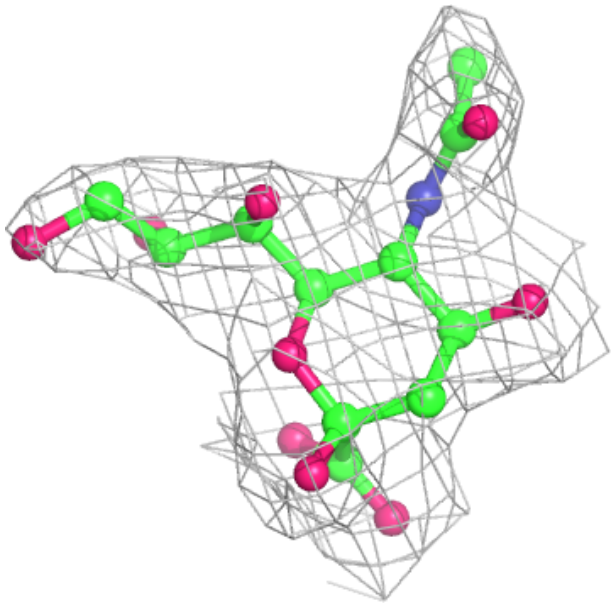


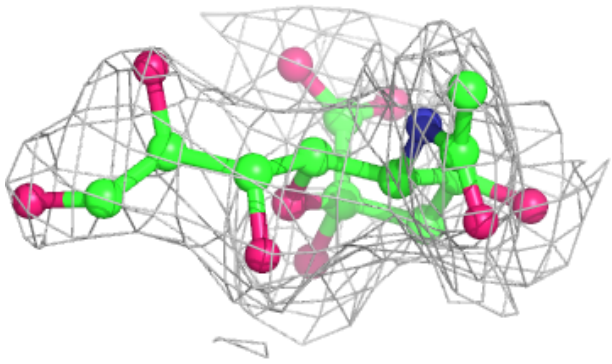


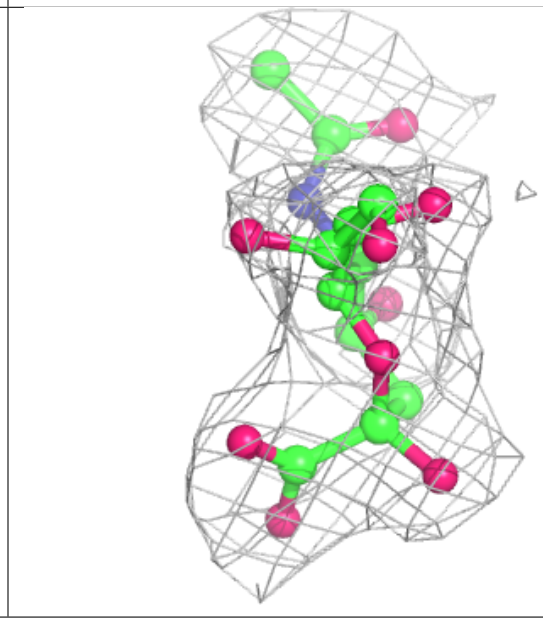


Electron density around SIA N 401:

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

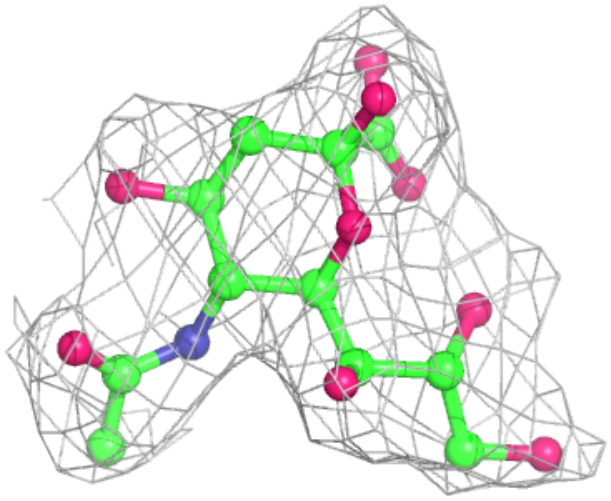


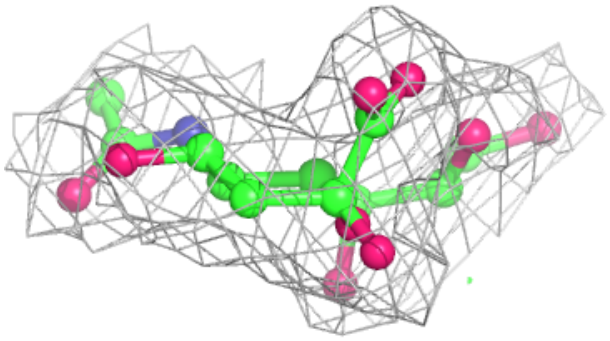


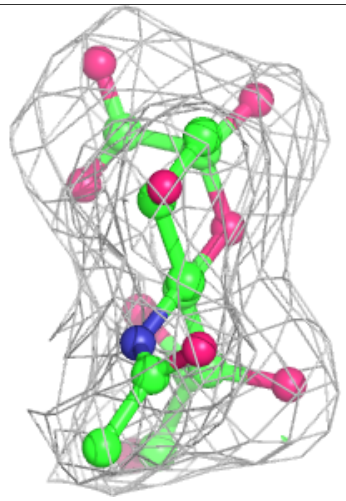


Electron density around SIA M 401:

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

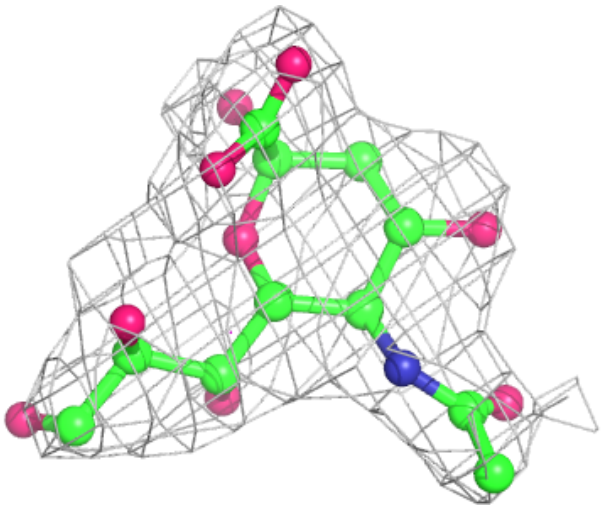


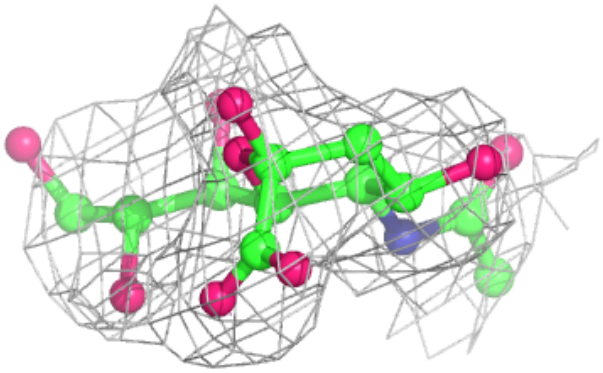


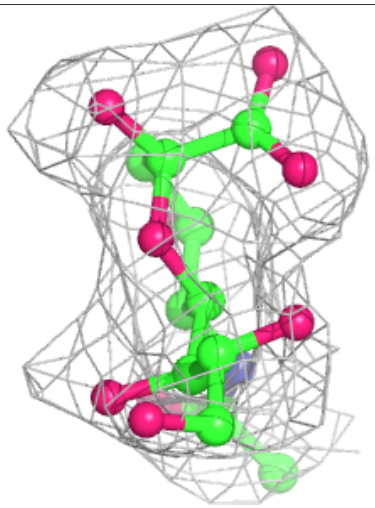


Electron density around SIA E 401:

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

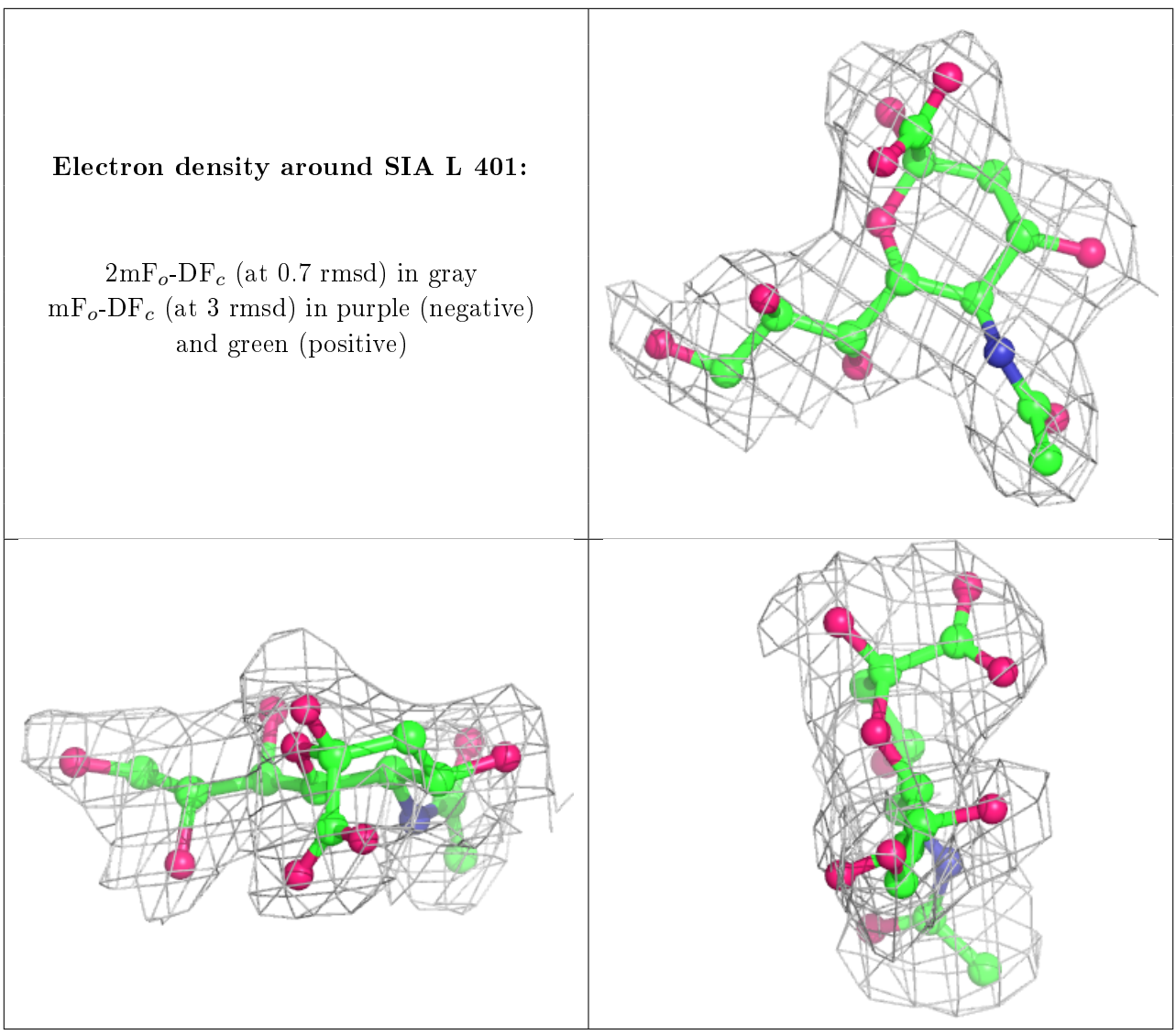






Electron density around SIA L 401:

$2mF_o$-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.