



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:29 PM UTC

PDB ID : 6Y6A / pdb_00006y6a
Title : Structure of Finch Polyomavirus VP1 in complex with 2-O-Methyl-5-N-acetyl- α -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 types of validation reports are described at

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

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

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

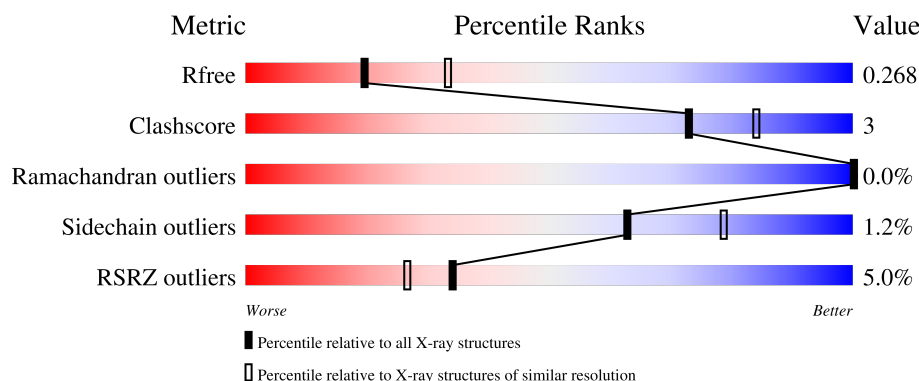
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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.



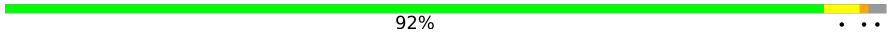
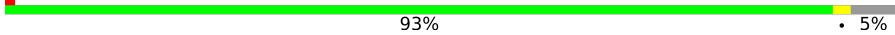
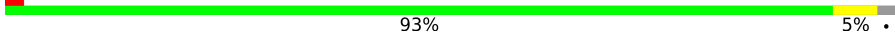
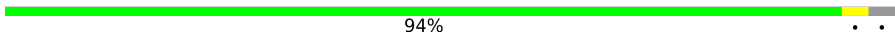
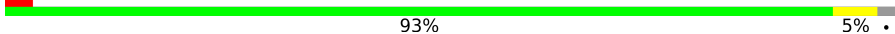
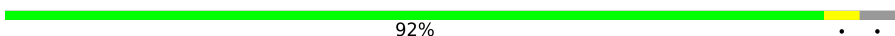
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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

Mol	Chain	Length	Quality of chain
1	A	274	% 90% 7% . .
1	B	274	% 89% 5% 5%
1	C	274	92% 5% . .
1	D	274	% 90% 5% 5%
1	E	274	% 92% . .

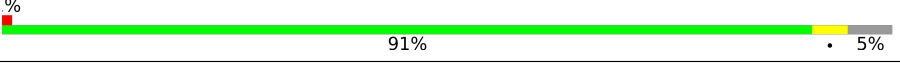
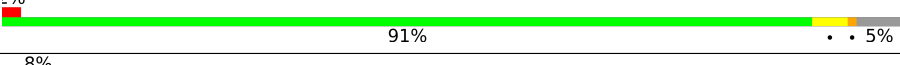
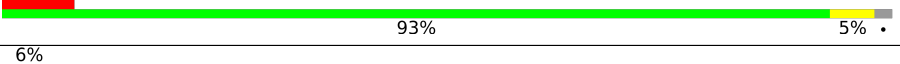
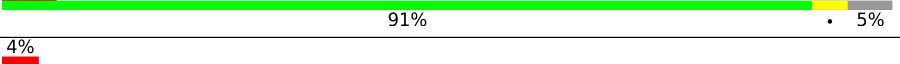
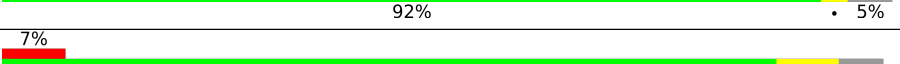
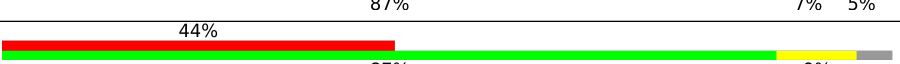
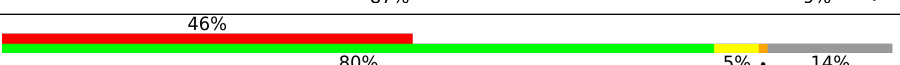
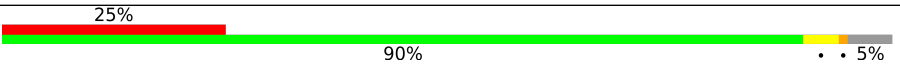
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Mol	Chain	Length	Quality of chain
1	F	274	 92% . .
1	G	274	 90% 5% 5%
1	H	274	 93% . 5%
1	I	274	 93% 5% .
1	J	274	 94% . .
1	K	274	 91% 7% .
1	L	274	 89% 6% .
1	M	274	 93% 5% .
1	N	274	 91% 5% . .
1	O	274	 91% 5% .
1	P	274	 92% 6% .
1	Q	274	 89% 8% .
1	R	274	 92% . .
1	S	274	 91% . 5%
1	T	274	 91% 5% .
1	U	274	 92% . 5%
1	V	274	 91% 5% .
1	W	274	 87% 8% .
1	X	274	 92% . 5%
1	Y	274	 90% 5% 5%
1	Z	274	 91% . 5%
1	a	274	 92% . 5%
1	b	274	 91% . 5%
1	c	274	 88% 5% 7%
1	d	274	 90% 5% 5%

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Mol	Chain	Length	Quality of chain
1	e	274	 91% 5%
1	f	274	 91% 5%
1	g	274	 93% 5%
1	h	274	 91% 5%
1	i	274	 92% 5%
1	j	274	 87% 7% 5%
1	k	274	 87% 9%
1	l	274	 80% 5% 14%
1	m	274	 90% 5%
1	n	274	 90% 8%

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

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

There are 240 discrepancies between the modelled and reference sequences:

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

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

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

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

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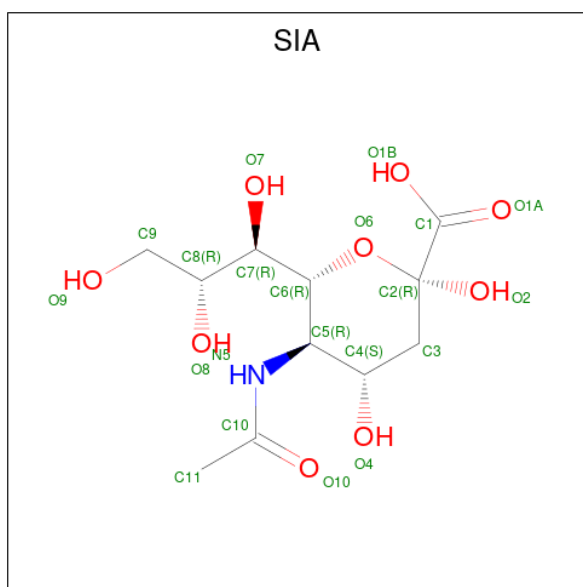
Chain	Residue	Modelled	Actual	Comment	Reference
a	20	HIS	-	expression tag	UNP R4UMH0
a	21	MET	-	expression tag	UNP R4UMH0
a	78	SER	CYS	conflict	UNP R4UMH0
a	92	SER	CYS	conflict	UNP R4UMH0
b	18	GLY	-	expression tag	UNP R4UMH0
b	19	SER	-	expression tag	UNP R4UMH0
b	20	HIS	-	expression tag	UNP R4UMH0
b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

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

- Molecule 2 is N-acetyl-alpha-neuraminic acid (CCD ID: SIA) (formula: C₁₁H₁₉NO₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 21	C 11	N 1	O 9	0	0
2	B	1	Total 21	C 11	N 1	O 9	0	0
2	C	1	Total 21	C 11	N 1	O 9	0	0
2	E	1	Total 21	C 11	N 1	O 9	0	0
2	F	1	Total 21	C 11	N 1	O 9	0	0
2	G	1	Total 21	C 11	N 1	O 9	0	0
2	I	1	Total 21	C 11	N 1	O 9	0	0
2	J	1	Total 21	C 11	N 1	O 9	0	0
2	K	1	Total 21	C 11	N 1	O 9	0	0
2	L	1	Total 21	C 11	N 1	O 9	0	0
2	M	1	Total 21	C 11	N 1	O 9	0	0
2	N	1	Total 21	C 11	N 1	O 9	0	0
2	O	1	Total 21	C 11	N 1	O 9	0	0
2	Q	1	Total 21	C 11	N 1	O 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 (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	3	Total	Cl	0	0
			3	3		
3	D	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	2	Total 2	Cl 2	0	0
3	G	2	Total 2	Cl 2	0	0
3	H	2	Total 2	Cl 2	0	0
3	I	1	Total 1	Cl 1	0	0
3	J	2	Total 2	Cl 2	0	0
3	L	1	Total 1	Cl 1	0	0
3	M	2	Total 2	Cl 2	0	0
3	N	2	Total 2	Cl 2	0	0
3	O	1	Total 1	Cl 1	0	0
3	P	2	Total 2	Cl 2	0	0
3	Q	2	Total 2	Cl 2	0	0
3	R	1	Total 1	Cl 1	0	0
3	S	2	Total 2	Cl 2	0	0
3	T	1	Total 1	Cl 1	0	0
3	U	2	Total 2	Cl 2	0	0
3	V	1	Total 1	Cl 1	0	0
3	W	2	Total 2	Cl 2	0	0
3	X	2	Total 2	Cl 2	0	0
3	Y	2	Total 2	Cl 2	0	0
3	Z	2	Total 2	Cl 2	0	0
3	c	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	d	2	Total 2	Cl 2	0	0
3	e	2	Total 2	Cl 2	0	0
3	f	2	Total 2	Cl 2	0	0
3	g	1	Total 1	Cl 1	0	0
3	h	1	Total 1	Cl 1	0	0
3	j	2	Total 2	Cl 2	0	0
3	n	2	Total 2	Cl 2	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is water.

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

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

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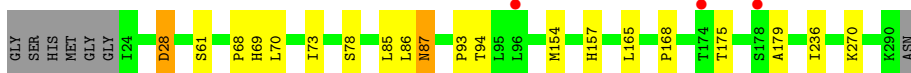
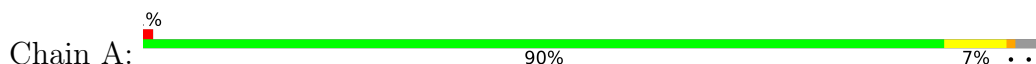
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	e	50	Total 50	O 50	0	0
5	f	33	Total 33	O 33	0	0
5	g	34	Total 34	O 34	0	0
5	h	32	Total 32	O 32	0	0
5	i	39	Total 39	O 39	0	0
5	j	25	Total 25	O 25	0	0
5	k	15	Total 15	O 15	0	0
5	l	15	Total 15	O 15	0	0
5	m	11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

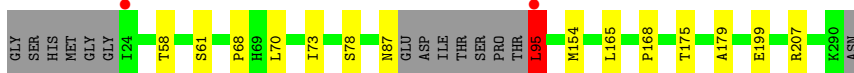
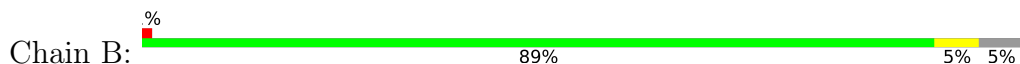
3 Residue-property plots [i](#)

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

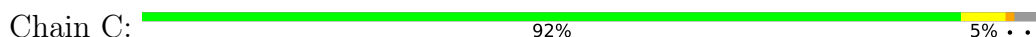
- Molecule 1: Capsid protein VP1



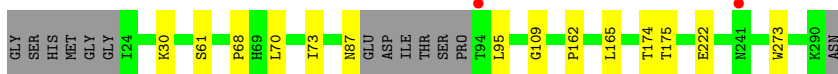
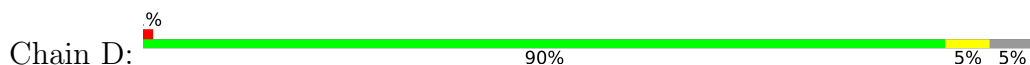
- Molecule 1: Capsid protein VP1



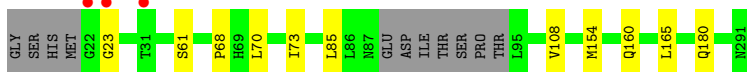
- Molecule 1: Capsid protein VP1



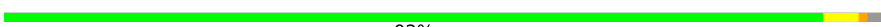
- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1



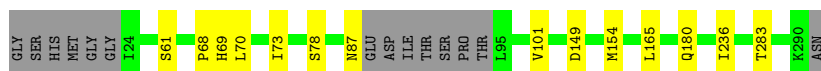
- Molecule 1: Capsid protein VP1

Chain F:  92% . . .



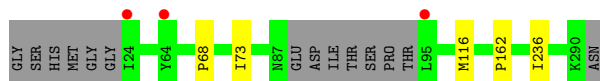
- Molecule 1: Capsid protein VP1

Chain G:  90% 5% 5%



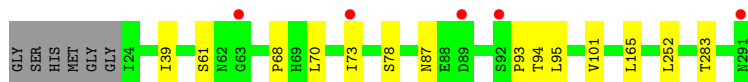
- Molecule 1: Capsid protein VP1

Chain H:  93% . 5%



- Molecule 1: Capsid protein VP1

Chain I:  93% 5% .



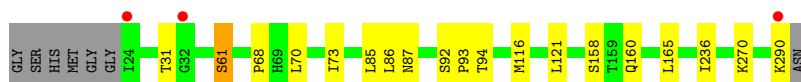
- Molecule 1: Capsid protein VP1

Chain J:  94% . .



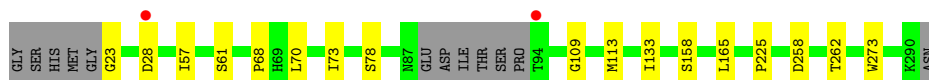
- Molecule 1: Capsid protein VP1

Chain K:  91% 7% .

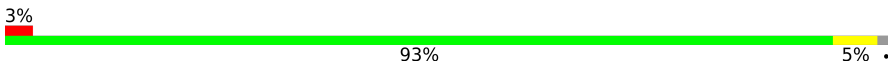


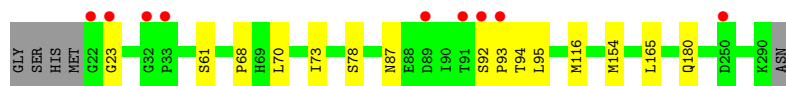
- Molecule 1: Capsid protein VP1

Chain L:  89% 6% .

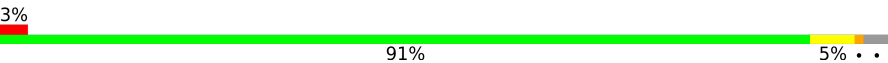


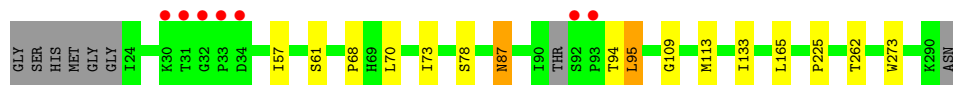
● Molecule 1: Capsid protein VP1

Chain M:  3% 93% 5%

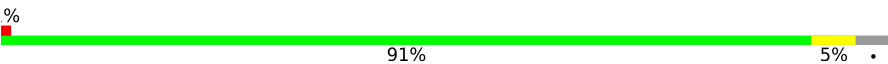


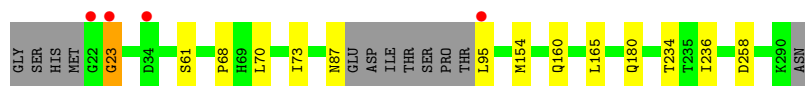
● Molecule 1: Capsid protein VP1

Chain N:  3% 91% 5%

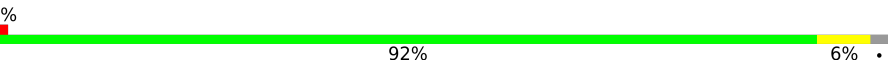


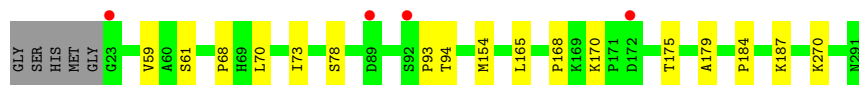
● Molecule 1: Capsid protein VP1

Chain O:  % 91% 5%



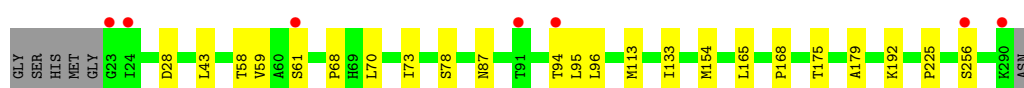
● Molecule 1: Capsid protein VP1

Chain P:  % 92% 6%

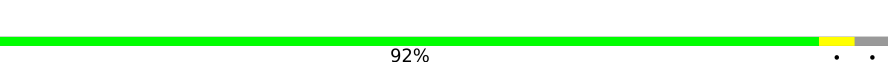


● Molecule 1: Capsid protein VP1

Chain Q:  3% 89% 8%

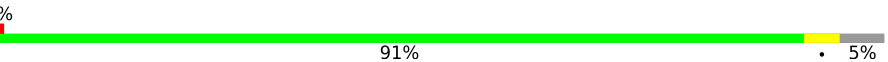


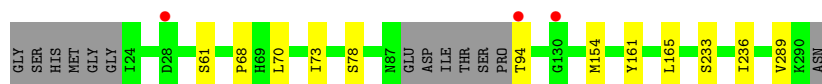
● Molecule 1: Capsid protein VP1

Chain R:  92%

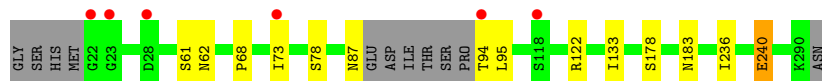
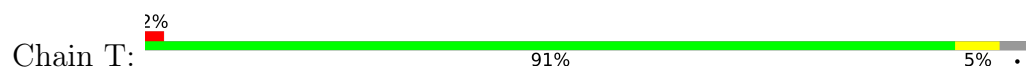


● Molecule 1: Capsid protein VP1

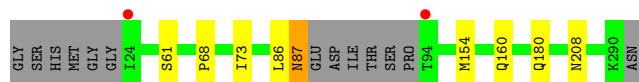
Chain S:  % 91% 5%



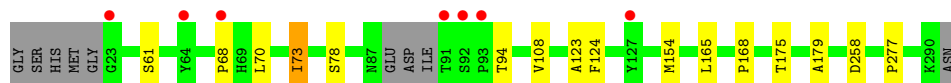
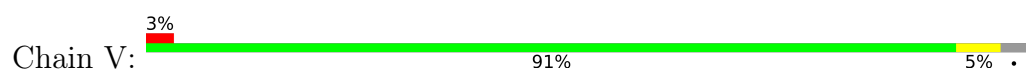
- Molecule 1: Capsid protein VP1



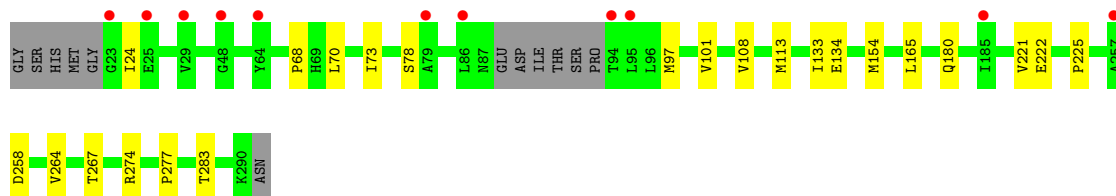
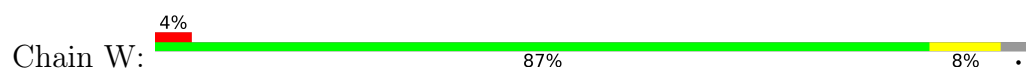
- Molecule 1: Capsid protein VP1



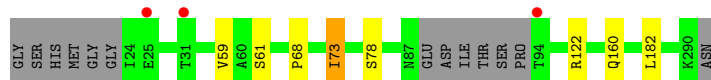
- Molecule 1: Capsid protein VP1



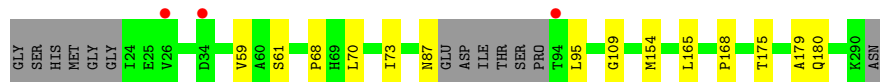
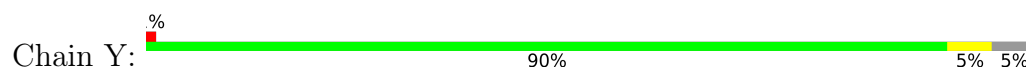
- Molecule 1: Capsid protein VP1



- Molecule 1: Capsid protein VP1

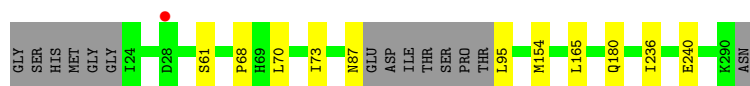


- Molecule 1: Capsid protein VP1



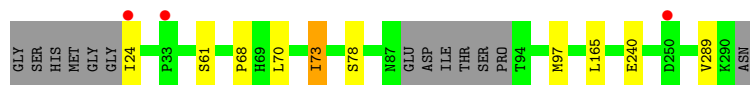
- Molecule 1: Capsid protein VP1

Chain Z:  91% 5%



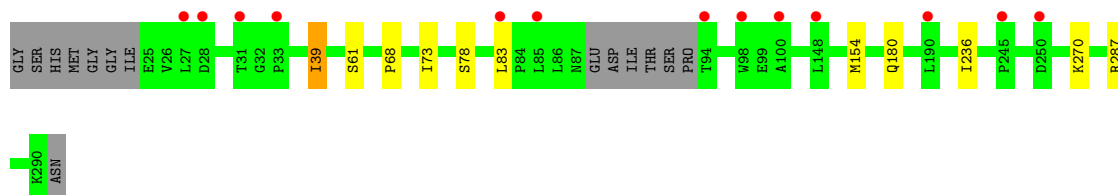
- Molecule 1: Capsid protein VP1

Chain a:  92% 5%



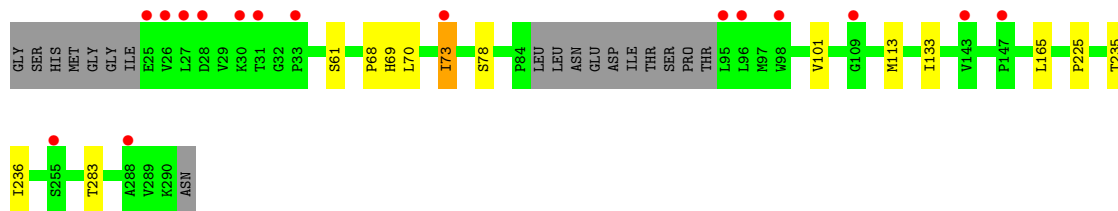
- Molecule 1: Capsid protein VP1

Chain b:  91% 5% 5%



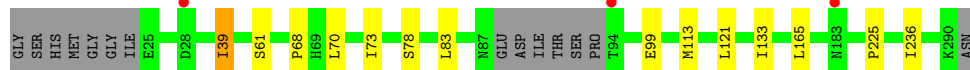
- Molecule 1: Capsid protein VP1

Chain c:  88% 5% 7%



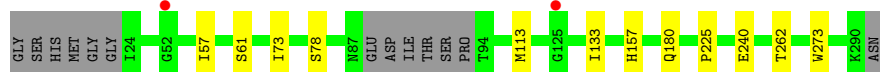
- Molecule 1: Capsid protein VP1

Chain d:  90% 5% 5%



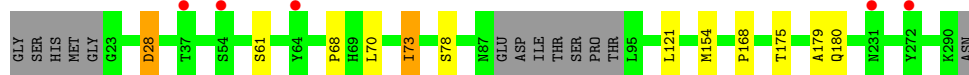
- Molecule 1: Capsid protein VP1

Chain e:  91% 5%

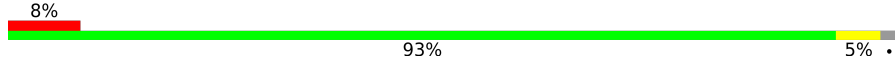


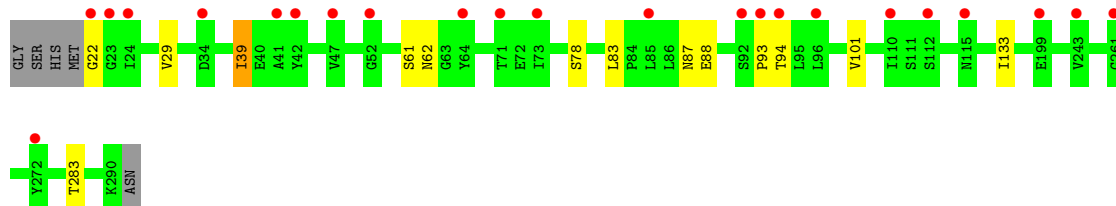
● Molecule 1: Capsid protein VP1

Chain f:  91% 2% 5%

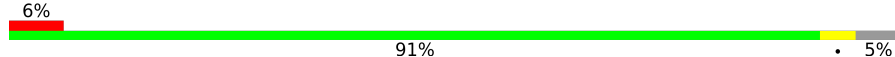


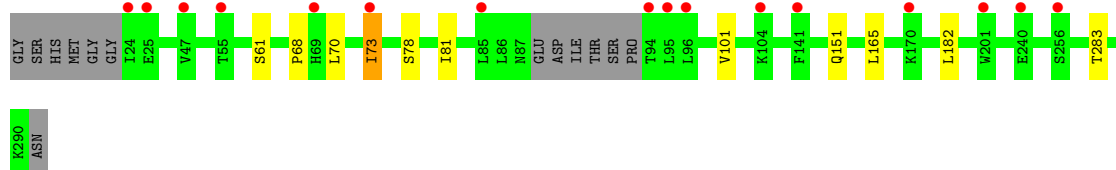
● Molecule 1: Capsid protein VP1

Chain g:  93% 8% 5%

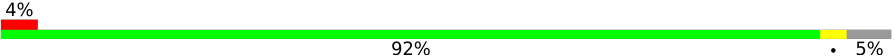


● Molecule 1: Capsid protein VP1

Chain h:  91% 6% 5%



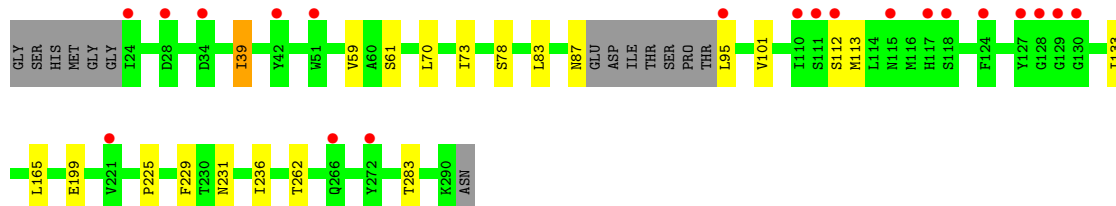
● Molecule 1: Capsid protein VP1

Chain i:  92% 4% 5%



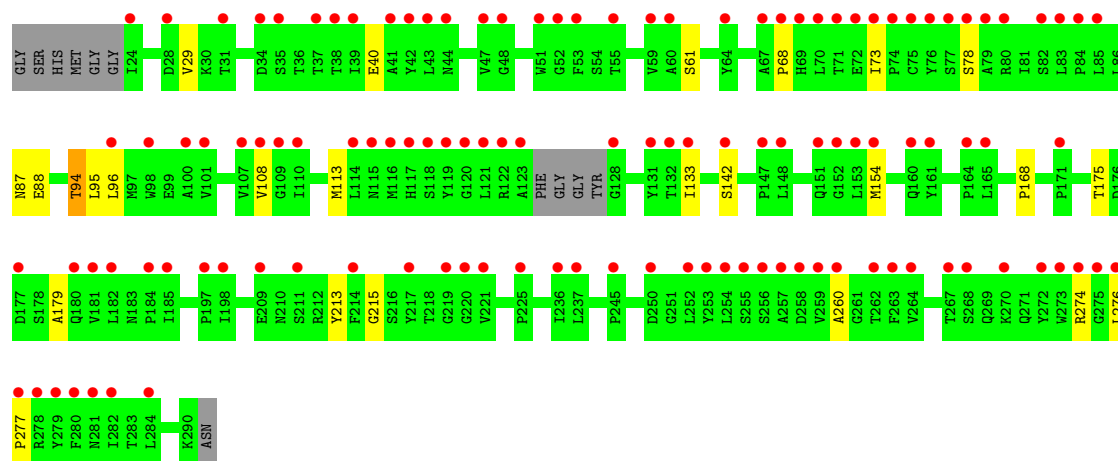
● Molecule 1: Capsid protein VP1

Chain j:  87% 7% 5%

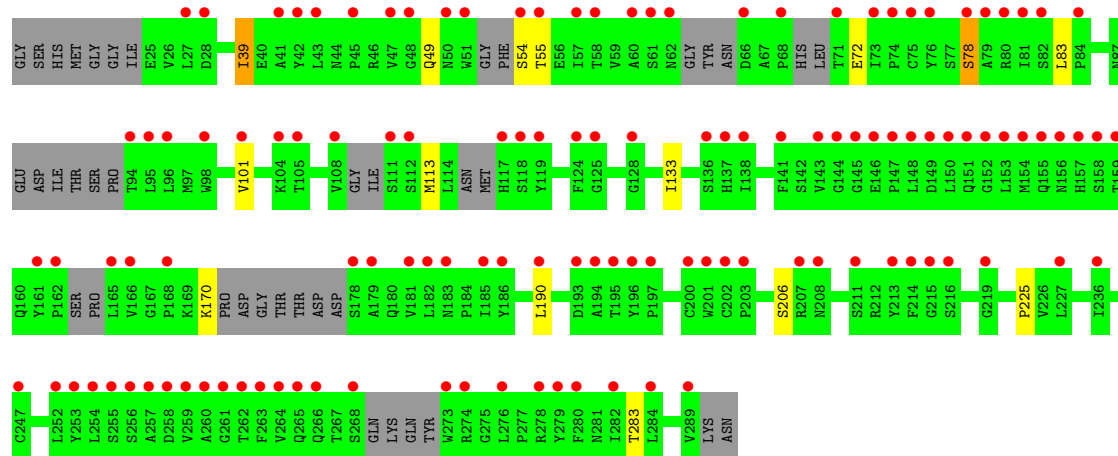
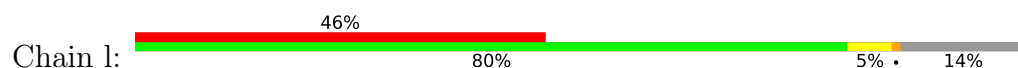


● Molecule 1: Capsid protein VP1

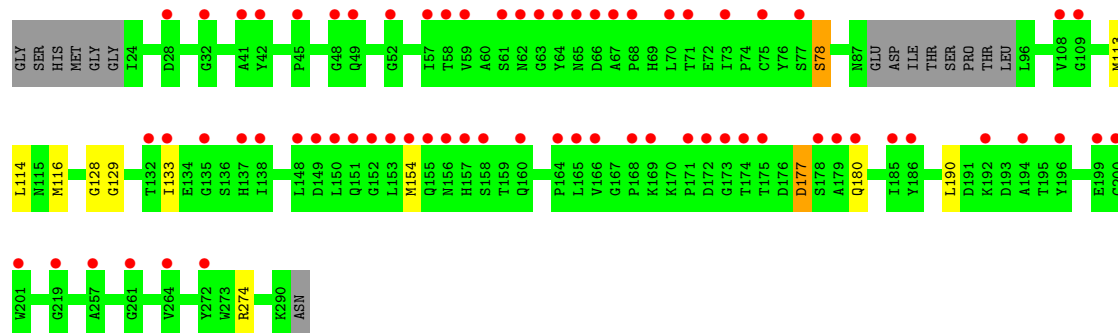
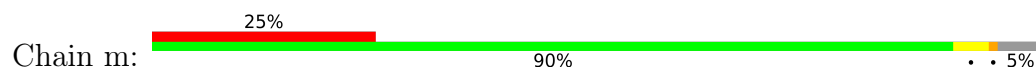
Chain k:  87% 44% 9%



• Molecule 1: Capsid protein VP1

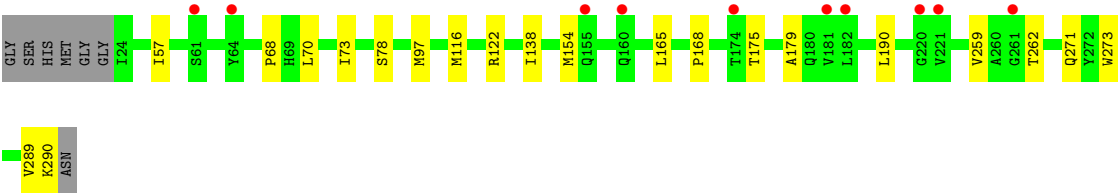


• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	86.50Å 172.06Å 245.62Å 107.09° 97.93° 93.93°	Depositor
Resolution (Å)	49.94 – 2.65 49.94 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.7 (49.94-2.65) 98.0 (49.94-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.65Å)	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)	0.29 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, SIA

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	1.04	2/2077 (0.1%)	1.27	7/2842 (0.2%)
1	B	0.98	0/2011	1.20	1/2749 (0.0%)
1	C	1.03	2/2081 (0.1%)	1.24	6/2846 (0.2%)
1	D	0.97	0/2032	1.21	0/2775
1	E	0.98	0/2029	1.22	3/2772 (0.1%)
1	F	1.01	3/2079 (0.1%)	1.25	2/2843 (0.1%)
1	G	0.97	0/2012	1.20	0/2751
1	H	0.98	0/2014	1.19	0/2753
1	I	1.01	1/2076 (0.0%)	1.24	2/2840 (0.1%)
1	J	1.00	2/2080 (0.1%)	1.21	0/2845
1	K	1.03	2/2075 (0.1%)	1.25	4/2839 (0.1%)
1	L	0.97	0/2027	1.21	3/2770 (0.1%)
1	M	1.04	1/2077 (0.0%)	1.25	3/2840 (0.1%)
1	N	1.00	1/2053 (0.0%)	1.22	1/2806 (0.0%)
1	O	0.98	0/2026	1.23	3/2767 (0.1%)
1	P	1.02	1/2078 (0.0%)	1.23	2/2843 (0.1%)
1	Q	1.03	3/2071 (0.1%)	1.23	1/2833 (0.0%)
1	R	0.98	0/2038	1.22	0/2784
1	S	0.97	0/2022	1.20	0/2763
1	T	0.97	0/2038	1.21	0/2783
1	U	1.00	1/2025 (0.0%)	1.22	1/2767 (0.0%)
1	V	1.01	2/2043 (0.1%)	1.21	0/2793
1	W	0.99	1/2016 (0.0%)	1.21	0/2756
1	X	0.98	0/2019	1.19	0/2760
1	Y	0.97	0/2022	1.20	0/2763
1	Z	0.97	0/2022	1.20	0/2761
1	a	0.98	0/2032	1.20	0/2774
1	b	1.01	1/1986 (0.1%)	1.25	2/2717 (0.1%)
1	c	0.98	0/1952	1.21	0/2667
1	d	0.98	0/2003	1.22	1/2738 (0.0%)
1	e	0.97	0/2023	1.20	0/2766
1	f	0.98	0/2013	1.21	1/2752 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	g	1.05	1/2036 (0.0%)	1.24	3/2788 (0.1%)
1	h	0.98	0/2009	1.20	0/2746
1	i	0.98	0/2000	1.20	0/2734
1	j	0.98	0/1982	1.21	1/2712 (0.0%)
1	k	1.08	2/1863 (0.1%)	1.28	3/2558 (0.1%)
1	l	1.04	0/1599	1.24	2/2188 (0.1%)
1	m	1.02	0/1882	1.25	1/2584 (0.0%)
1	n	1.00	0/2045	1.22	0/2800
All	All	1.00	26/80568 (0.0%)	1.22	53/110168 (0.0%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	94	THR	C-O	11.48	1.37	1.23
1	k	94	THR	C-O	9.32	1.35	1.23
1	C	94	THR	C-O	9.29	1.34	1.23
1	Q	94	THR	C-O	9.08	1.33	1.23
1	P	94	THR	C-O	-9.02	1.13	1.24
1	A	86	LEU	C-O	8.89	1.34	1.24
1	I	94	THR	C-O	-8.83	1.14	1.24
1	b	287	ARG	CD-NE	-8.53	1.34	1.46
1	V	94	THR	C-O	-8.01	1.15	1.24
1	M	94	THR	C-O	-7.80	1.14	1.24
1	U	86	LEU	C-O	7.55	1.34	1.23
1	J	94	THR	C-O	7.31	1.32	1.23
1	F	94	THR	C-O	7.27	1.32	1.23
1	F	86	LEU	C-O	7.05	1.33	1.23
1	K	86	LEU	C-O	6.94	1.31	1.24
1	Q	87	ASN	C-O	6.87	1.36	1.23
1	A	85	LEU	C-O	-6.17	1.16	1.23
1	C	85	LEU	C-O	5.98	1.30	1.23
1	Q	95	LEU	N-CA	5.89	1.53	1.45
1	J	87	ASN	C-O	5.49	1.33	1.23
1	N	94	THR	C-O	-5.28	1.18	1.24
1	F	95	LEU	N-CA	5.20	1.52	1.45
1	K	85	LEU	C-O	-5.08	1.17	1.23
1	k	95	LEU	N-CA	5.08	1.52	1.46
1	W	258	ASP	CG-OD2	5.06	1.34	1.25
1	V	258	ASP	CG-OD2	5.00	1.34	1.25

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	m	177	ASP	CA-CB-CG	13.18	125.78	112.60
1	b	287	ARG	CB-CG-CD	-12.99	81.43	111.30
1	A	28	ASP	CA-CB-CG	-9.25	103.35	112.60
1	L	28	ASP	CA-CB-CG	-9.20	103.40	112.60
1	f	28	ASP	CA-CB-CG	-8.97	103.63	112.60
1	Q	28	ASP	CA-CB-CG	-8.91	103.69	112.60
1	K	290	LYS	CB-CA-C	-8.37	94.20	110.10
1	F	86	LEU	N-CA-C	-7.94	97.67	109.81
1	O	23	GLY	CA-C-N	7.47	132.01	122.37
1	O	23	GLY	C-N-CA	7.47	132.01	122.37
1	d	99	GLU	CG-CD-OE2	-7.28	101.66	118.40
1	g	87	ASN	CB-CA-C	7.02	119.85	111.22
1	b	287	ARG	CG-CD-NE	6.99	127.37	112.00
1	U	86	LEU	CA-C-O	-6.96	110.67	120.07
1	A	86	LEU	N-CA-C	-6.88	95.77	108.02
1	k	87	ASN	CB-CA-C	6.75	119.53	111.22
1	K	86	LEU	N-CA-C	-6.70	97.49	108.41
1	C	87	ASN	CB-CA-C	6.55	119.95	111.50
1	j	112	SER	CA-CB-OG	6.55	124.19	111.10
1	E	23	GLY	CA-C-N	6.35	130.56	122.37
1	E	23	GLY	C-N-CA	6.35	130.56	122.37
1	F	87	ASN	CB-CA-C	6.30	122.96	110.42
1	K	87	ASN	CA-C-O	-6.16	113.72	120.43
1	M	23	GLY	CA-C-N	6.02	130.51	122.93
1	M	23	GLY	C-N-CA	6.02	130.51	122.93
1	A	86	LEU	N-CA-CB	5.83	119.69	110.84
1	A	87	ASN	CA-C-O	-5.76	114.15	120.43
1	l	170	LYS	CB-CA-C	5.74	121.01	110.10
1	A	86	LEU	CA-C-O	5.71	126.50	120.33
1	K	290	LYS	CA-C-O	-5.63	111.22	120.80
1	l	55	THR	CA-C-O	-5.61	115.59	121.99
1	B	95	LEU	CB-CA-C	5.59	120.73	110.10
1	C	87	ASN	CA-C-N	5.53	127.69	120.28
1	C	87	ASN	C-N-CA	5.53	127.69	120.28
1	N	87	ASN	OD1-CG-ND2	5.48	128.08	122.60
1	M	93	PRO	O-C-N	5.45	129.96	122.38
1	I	93	PRO	CA-C-O	-5.39	112.11	118.90
1	P	93	PRO	CA-C-O	-5.38	112.11	118.90
1	E	160	GLN	CB-CG-CD	-5.38	103.45	112.60
1	P	93	PRO	O-C-N	5.38	129.74	122.37
1	g	93	PRO	CA-C-N	5.36	131.22	121.89
1	g	93	PRO	C-N-CA	5.36	131.22	121.89
1	I	93	PRO	O-C-N	5.33	129.67	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	160	GLN	CB-CG-CD	-5.25	103.67	112.60
1	C	88	GLU	CA-C-O	-5.14	115.10	120.55
1	C	93	PRO	CA-C-N	5.14	131.22	122.37
1	C	93	PRO	C-N-CA	5.14	131.22	122.37
1	k	94	THR	CA-C-O	-5.10	115.14	121.06
1	L	23	GLY	CA-C-N	5.06	128.90	122.37
1	L	23	GLY	C-N-CA	5.06	128.90	122.37
1	A	85	LEU	CA-C-N	5.01	129.97	122.86
1	A	85	LEU	C-N-CA	5.01	129.97	122.86
1	k	88	GLU	CA-C-O	-5.00	115.25	120.55

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2024	0	1925	19	0
1	B	1960	0	1845	16	0
1	C	2028	0	1933	9	0
1	D	1981	0	1889	9	0
1	E	1978	0	1862	6	0
1	F	2026	0	1931	12	0
1	G	1961	0	1849	7	0
1	H	1963	0	1854	4	0
1	I	2023	0	1919	12	0
1	J	2027	0	1931	4	0
1	K	2022	0	1925	19	0
1	L	1976	0	1862	17	0
1	M	2024	0	1920	10	0
1	N	2002	0	1883	15	0
1	O	1975	0	1873	8	0
1	P	2025	0	1914	18	0
1	Q	2018	0	1902	21	0
1	R	1987	0	1886	5	0
1	S	1971	0	1862	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	1987	0	1883	8	0
1	U	1974	0	1873	5	0
1	V	1991	0	1876	20	0
1	W	1965	0	1838	29	0
1	X	1968	0	1852	5	0
1	Y	1971	0	1873	14	0
1	Z	1971	0	1871	4	0
1	a	1981	0	1880	9	0
1	b	1935	0	1789	9	0
1	c	1903	0	1751	9	0
1	d	1952	0	1825	13	0
1	e	1972	0	1862	14	0
1	f	1962	0	1836	13	0
1	g	1984	0	1821	11	0
1	h	1959	0	1835	5	0
1	i	1949	0	1828	16	0
1	j	1932	0	1800	21	0
1	k	1822	0	1579	29	0
1	l	1571	0	1322	23	0
1	m	1834	0	1627	23	0
1	n	1992	0	1848	38	0
2	A	21	0	18	1	0
2	B	21	0	18	1	0
2	C	21	0	18	0	0
2	E	21	0	18	0	0
2	F	21	0	18	2	0
2	G	21	0	18	1	0
2	I	21	0	18	0	0
2	J	21	0	18	1	0
2	K	21	0	18	0	0
2	L	21	0	18	0	0
2	M	21	0	18	0	0
2	N	21	0	18	0	0
2	O	21	0	18	0	0
2	Q	21	0	18	1	0
2	R	21	0	18	0	0
2	S	21	0	18	0	0
2	T	21	0	18	0	0
2	V	21	0	18	0	0
2	X	21	0	18	1	0
2	Y	21	0	18	0	0
2	Z	21	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	a	21	0	18	0	0
2	b	21	0	18	0	0
2	c	21	0	18	1	0
2	d	21	0	18	0	0
2	e	21	0	18	0	0
2	f	21	0	18	0	0
2	j	21	0	18	0	0
2	n	21	0	18	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	1	0	0	0	0
3	J	2	0	0	0	0
3	L	1	0	0	0	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
3	O	1	0	0	0	0
3	P	2	0	0	0	0
3	Q	2	0	0	0	0
3	R	1	0	0	0	0
3	S	2	0	0	0	0
3	T	1	0	0	0	0
3	U	2	0	0	0	0
3	V	1	0	0	0	0
3	W	2	0	0	0	0
3	X	2	0	0	0	0
3	Y	2	0	0	0	0
3	Z	2	0	0	0	0
3	c	1	0	0	0	0
3	d	2	0	0	0	0
3	e	2	0	0	0	0
3	f	2	0	0	0	0
3	g	1	0	0	0	0
3	h	1	0	0	0	0
3	j	2	0	0	0	0
3	n	2	0	0	0	0
4	C	1	0	0	0	0
5	A	98	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	82	0	0	2	0
5	C	107	0	0	1	0
5	D	89	0	0	4	0
5	E	84	0	0	2	0
5	F	107	0	0	3	0
5	G	56	0	0	2	0
5	H	59	0	0	1	0
5	I	62	0	0	1	0
5	J	91	0	0	0	0
5	K	72	0	0	5	0
5	L	76	0	0	1	0
5	M	83	0	0	1	0
5	N	98	0	0	1	0
5	O	83	0	0	4	0
5	P	65	0	0	2	0
5	Q	79	0	0	3	0
5	R	81	0	0	1	0
5	S	55	0	0	1	0
5	T	68	0	0	4	0
5	U	83	0	0	2	0
5	V	43	0	0	1	0
5	W	41	0	0	0	0
5	X	40	0	0	1	0
5	Y	67	0	0	1	0
5	Z	63	0	0	0	0
5	a	47	0	0	0	0
5	b	30	0	0	0	0
5	c	34	0	0	1	0
5	d	46	0	0	1	0
5	e	50	0	0	0	0
5	f	33	0	0	3	0
5	g	34	0	0	1	0
5	h	32	0	0	2	0
5	i	39	0	0	0	0
5	j	25	0	0	3	0
5	k	15	0	0	0	0
5	l	15	0	0	3	0
5	m	11	0	0	0	0
5	n	35	0	0	3	0
All	All	81587	0	74156	487	0

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

All (487) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:39:ILE:HD11	1:I:252:LEU:CD2	1.36	1.53
1:i:39:ILE:HD11	1:i:252:LEU:CD2	1.35	1.51
1:I:39:ILE:CD1	1:I:252:LEU:HD23	1.74	1.18
1:i:39:ILE:CD1	1:i:252:LEU:HD23	1.72	1.18
1:l:78:SER:HB2	1:l:190:LEU:HD21	1.20	1.15
1:i:39:ILE:HD11	1:i:252:LEU:HD22	1.22	1.14
1:m:78:SER:HB2	1:m:190:LEU:HD21	1.21	1.14
1:a:97:MET:CE	1:a:289:VAL:HG11	1.79	1.12
1:a:97:MET:HE2	1:a:289:VAL:HG11	1.33	1.11
1:I:39:ILE:HD11	1:I:252:LEU:HD23	1.11	1.11
1:I:39:ILE:HD11	1:I:252:LEU:HD22	1.23	1.09
1:K:31:THR:HG21	1:W:267:THR:HG21	1.35	1.09
1:i:39:ILE:CD1	1:i:252:LEU:CD2	2.27	1.09
1:I:39:ILE:CD1	1:I:252:LEU:CD2	2.29	1.08
1:i:39:ILE:HD11	1:i:252:LEU:HD23	1.09	1.08
1:P:154:MET:HE3	1:P:179:ALA:HB1	1.37	1.06
1:Y:154:MET:HE3	1:Y:179:ALA:CB	1.86	1.06
1:n:154:MET:HE3	1:n:179:ALA:CB	1.86	1.06
1:Q:154:MET:HE3	1:Q:179:ALA:HB1	1.38	1.05
1:P:154:MET:HE3	1:P:179:ALA:CB	1.86	1.05
1:V:154:MET:HE3	1:V:179:ALA:HB1	1.37	1.05
1:k:154:MET:HE3	1:k:179:ALA:CB	1.86	1.05
1:V:154:MET:HE3	1:V:179:ALA:CB	1.86	1.05
1:f:154:MET:HE3	1:f:179:ALA:CB	1.86	1.05
1:B:154:MET:HE3	1:B:179:ALA:CB	1.86	1.04
1:A:154:MET:HE3	1:A:179:ALA:CB	1.87	1.04
1:A:154:MET:HE3	1:A:179:ALA:HB1	1.39	1.03
1:Q:154:MET:HE3	1:Q:179:ALA:CB	1.86	1.03
1:B:154:MET:HE3	1:B:179:ALA:HB1	1.38	1.03
1:n:154:MET:HE3	1:n:179:ALA:HB1	1.37	1.03
1:k:154:MET:HE3	1:k:179:ALA:HB1	1.37	1.02
1:W:133:ILE:HD13	1:W:274:ARG:HG2	1.39	1.02
1:e:262:THR:HG21	1:i:116:MET:HE1	1.37	1.02
1:f:154:MET:HE3	1:f:179:ALA:HB1	1.38	1.01
1:k:133:ILE:HD13	1:k:274:ARG:HG2	1.38	1.01
1:Y:154:MET:HE3	1:Y:179:ALA:HB1	1.38	1.00
1:K:31:THR:HG21	1:W:267:THR:CG2	1.90	0.99
1:n:138:ILE:HG22	1:n:259:VAL:HG12	1.40	0.99
1:K:116:MET:HE1	1:L:262:THR:HG21	1.41	0.99
1:m:133:ILE:HD13	1:m:274:ARG:HG2	1.41	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:MET:HE3	1:D:273:TRP:CH2	1.98	0.98
1:l:39:ILE:HD11	1:l:83:LEU:HD23	1.44	0.97
1:n:97:MET:CE	1:n:289:VAL:HG11	1.95	0.97
1:V:154:MET:CE	1:V:179:ALA:HB1	1.96	0.95
1:m:116:MET:HE1	1:n:262:THR:HG21	1.46	0.95
1:Q:154:MET:CE	1:Q:179:ALA:HB1	1.97	0.95
1:n:97:MET:HE2	1:n:289:VAL:HG11	1.48	0.95
1:n:154:MET:CE	1:n:179:ALA:HB1	1.97	0.95
1:B:154:MET:CE	1:B:179:ALA:HB1	1.97	0.95
1:m:133:ILE:CD1	1:m:274:ARG:HG2	1.97	0.94
1:W:133:ILE:CD1	1:W:274:ARG:HG2	1.97	0.94
1:k:133:ILE:CD1	1:k:274:ARG:HG2	1.96	0.94
1:P:154:MET:CE	1:P:179:ALA:HB1	1.96	0.94
1:A:154:MET:CE	1:A:179:ALA:HB1	1.97	0.94
1:Y:154:MET:CE	1:Y:179:ALA:HB1	1.97	0.94
1:k:154:MET:CE	1:k:179:ALA:HB1	1.97	0.94
1:M:116:MET:HE1	1:N:262:THR:HG21	1.47	0.94
1:d:39:ILE:HD11	1:d:83:LEU:HD23	1.49	0.94
1:l:54:SER:OG	1:l:72:GLU:HA	1.68	0.94
1:j:39:ILE:HD11	1:j:83:LEU:HD23	1.49	0.93
1:g:39:ILE:HD11	1:g:83:LEU:HD23	1.50	0.93
1:f:154:MET:CE	1:f:179:ALA:HB1	1.97	0.93
1:K:116:MET:HE3	1:L:57:ILE:HD13	1.50	0.93
1:e:57:ILE:HD13	1:i:116:MET:HE3	1.47	0.93
1:b:39:ILE:HD11	1:b:83:LEU:HD23	1.48	0.92
1:M:116:MET:HE2	1:N:273:TRP:CH2	2.06	0.91
1:l:39:ILE:HA	5:l:307:HOH:O	1.70	0.90
1:m:116:MET:HE2	1:n:273:TRP:CH2	2.06	0.90
1:n:78:SER:CB	1:n:190:LEU:HD21	2.01	0.90
1:W:113:MET:HG2	1:W:133:ILE:HD12	1.53	0.90
1:l:39:ILE:HD11	1:l:83:LEU:CD2	2.02	0.90
1:m:78:SER:CB	1:m:190:LEU:HD21	2.04	0.88
1:m:113:MET:HG2	1:m:133:ILE:HD12	1.56	0.88
1:e:157:HIS:H	1:e:180:GLN:HE21	1.21	0.87
1:M:116:MET:HE3	1:N:57:ILE:HD13	1.57	0.87
1:l:190:LEU:O	1:l:190:LEU:HD23	1.76	0.86
1:l:78:SER:CB	1:l:190:LEU:HD21	2.04	0.86
1:g:39:ILE:CD1	1:g:83:LEU:HD23	2.05	0.86
1:m:190:LEU:HD23	1:m:190:LEU:O	1.75	0.85
1:M:116:MET:HE1	1:N:262:THR:CG2	2.07	0.85
1:m:116:MET:HE3	1:n:57:ILE:HD13	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:39:ILE:CD1	1:d:83:LEU:HD23	2.07	0.85
1:m:116:MET:HE1	1:n:262:THR:CG2	2.06	0.84
1:b:39:ILE:CD1	1:b:83:LEU:HD23	2.06	0.84
1:W:113:MET:HE3	1:W:133:ILE:HB	1.58	0.84
1:j:39:ILE:CD1	1:j:83:LEU:HD23	2.07	0.83
1:e:262:THR:CG2	1:i:116:MET:HE1	2.08	0.83
1:l:39:ILE:CD1	1:l:83:LEU:HD23	2.07	0.83
1:n:190:LEU:HD23	1:n:190:LEU:O	1.78	0.83
1:Q:113:MET:HE3	1:Q:133:ILE:HB	1.60	0.83
1:c:113:MET:HE3	1:c:133:ILE:HB	1.61	0.83
1:g:133:ILE:CB	5:h:421:HOH:O	2.25	0.82
1:L:113:MET:HE3	1:L:133:ILE:HB	1.60	0.82
1:N:113:MET:HE3	1:N:133:ILE:HB	1.59	0.81
1:K:116:MET:HE1	1:L:262:THR:CG2	2.10	0.81
1:l:39:ILE:CD1	1:l:83:LEU:CD2	2.58	0.81
1:j:39:ILE:HD11	1:j:83:LEU:CD2	2.10	0.81
1:e:113:MET:HE3	1:e:133:ILE:HB	1.61	0.81
1:b:39:ILE:HD11	1:b:83:LEU:CD2	2.10	0.80
1:B:87:ASN:ND2	1:B:95:LEU:N	2.29	0.80
1:d:113:MET:HE3	1:d:133:ILE:HB	1.61	0.80
1:j:113:MET:HE3	1:j:133:ILE:HB	1.60	0.80
1:d:39:ILE:HD11	1:d:83:LEU:CD2	2.12	0.80
1:k:113:MET:HG2	1:k:133:ILE:HD12	1.62	0.80
1:g:39:ILE:HD11	1:g:83:LEU:CD2	2.12	0.80
1:T:178:SER:OG	1:T:183:ASN:HB2	1.82	0.79
1:b:39:ILE:CD1	1:b:83:LEU:CD2	2.61	0.79
1:j:39:ILE:CD1	1:j:83:LEU:CD2	2.61	0.78
1:g:39:ILE:CD1	1:g:83:LEU:CD2	2.62	0.78
1:F:85:LEU:HD12	1:F:85:LEU:H	1.49	0.77
1:a:97:MET:HE2	1:a:289:VAL:CG1	2.13	0.77
1:l:101:VAL:HG22	1:l:283:THR:O	1.86	0.76
1:e:57:ILE:CD1	1:i:116:MET:HE3	2.15	0.76
1:h:101:VAL:HG22	1:h:283:THR:O	1.86	0.76
1:n:138:ILE:HG22	1:n:259:VAL:CG1	2.15	0.76
1:I:101:VAL:HG22	1:I:283:THR:O	1.86	0.76
1:W:101:VAL:HG22	1:W:283:THR:O	1.86	0.76
1:g:101:VAL:HG22	1:g:283:THR:O	1.86	0.76
1:c:101:VAL:HG22	1:c:283:THR:O	1.86	0.75
1:k:133:ILE:HD13	1:k:274:ARG:CG	2.14	0.75
1:W:24:ILE:HG21	1:W:97:MET:HE1	1.69	0.75
1:f:28:ASP:HB2	5:f:530:HOH:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:133:ILE:HD13	1:m:274:ARG:CG	2.16	0.75
1:G:101:VAL:HG22	1:G:283:THR:O	1.86	0.75
1:d:39:ILE:CD1	1:d:83:LEU:CD2	2.63	0.75
1:W:133:ILE:HD13	1:W:274:ARG:CG	2.16	0.74
1:j:101:VAL:HG22	1:j:283:THR:O	1.86	0.74
1:a:24:ILE:HG21	1:a:97:MET:HE1	1.70	0.73
1:i:39:ILE:CD1	1:i:252:LEU:HD22	2.10	0.73
1:K:116:MET:HE3	1:L:57:ILE:CD1	2.17	0.73
1:n:68:PRO:HG2	1:n:73:ILE:HD11	1.71	0.73
1:S:68:PRO:HG2	1:S:73:ILE:HD11	1.71	0.72
1:W:68:PRO:HG2	1:W:73:ILE:HD11	1.71	0.72
1:b:68:PRO:HG2	1:b:73:ILE:HD11	1.72	0.72
1:T:68:PRO:HG2	1:T:73:ILE:HD11	1.71	0.72
1:G:68:PRO:HG2	1:G:73:ILE:HD11	1.71	0.72
1:H:68:PRO:HG2	1:H:73:ILE:HD11	1.71	0.72
1:C:68:PRO:HG2	1:C:73:ILE:HD11	1.71	0.72
1:Y:68:PRO:HG2	1:Y:73:ILE:HD11	1.71	0.72
1:m:116:MET:HE2	1:n:273:TRP:CZ2	2.25	0.72
1:M:68:PRO:HG2	1:M:73:ILE:HD11	1.71	0.71
1:i:68:PRO:HG2	1:i:73:ILE:HD11	1.71	0.71
1:B:68:PRO:HG2	1:B:73:ILE:HD11	1.71	0.71
1:D:68:PRO:HG2	1:D:73:ILE:HD11	1.72	0.71
1:J:68:PRO:HG2	1:J:73:ILE:HD11	1.71	0.71
1:N:68:PRO:HG2	1:N:73:ILE:HD11	1.72	0.71
1:O:68:PRO:HG2	1:O:73:ILE:HD11	1.72	0.71
1:L:68:PRO:HG2	1:L:73:ILE:HD11	1.72	0.70
1:k:68:PRO:HG2	1:k:73:ILE:HD11	1.71	0.70
1:F:68:PRO:HG2	1:F:73:ILE:HD11	1.71	0.70
1:P:68:PRO:HG2	1:P:73:ILE:HD11	1.72	0.70
1:Q:68:PRO:HG2	1:Q:73:ILE:HD11	1.72	0.70
1:d:68:PRO:HG2	1:d:73:ILE:HD11	1.72	0.70
1:A:68:PRO:HG2	1:A:73:ILE:HD11	1.72	0.70
1:R:68:PRO:HG2	1:R:73:ILE:HD11	1.71	0.70
1:U:68:PRO:HG2	1:U:73:ILE:HD11	1.72	0.70
1:Z:68:PRO:HG2	1:Z:73:ILE:HD11	1.72	0.70
1:I:68:PRO:HG2	1:I:73:ILE:HD11	1.72	0.70
1:K:68:PRO:HG2	1:K:73:ILE:HD11	1.71	0.70
1:I:39:ILE:CD1	1:I:252:LEU:HD22	2.11	0.70
1:E:68:PRO:HG2	1:E:73:ILE:HD11	1.72	0.69
1:k:113:MET:HE2	1:k:276:LEU:HD11	1.74	0.68
1:j:262:THR:HG21	1:n:116:MET:HE1	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:108:VAL:HG22	1:V:277:PRO:O	1.94	0.67
1:i:39:ILE:HD12	1:i:252:LEU:HD23	1.73	0.67
1:l:78:SER:HB2	1:l:190:LEU:CD2	2.12	0.67
1:R:28:ASP:HB2	5:R:559:HOH:O	1.94	0.67
1:m:114:LEU:HD21	1:n:259:VAL:HG11	1.77	0.67
1:I:39:ILE:HD12	1:I:252:LEU:HD23	1.75	0.67
1:A:87:ASN:HB3	1:P:184:PRO:O	1.94	0.66
1:A:87:ASN:ND2	1:P:187:LYS:HG3	2.10	0.66
1:l:113:MET:HE1	1:l:225:PRO:HG3	1.77	0.65
1:a:97:MET:HE2	1:a:289:VAL:HG21	1.79	0.65
1:X:59:VAL:O	2:X:401:SIA:H91	1.96	0.65
1:m:78:SER:HB2	1:m:190:LEU:CD2	2.14	0.65
1:L:113:MET:HE1	1:L:225:PRO:HG3	1.79	0.65
1:R:94:THR:N	1:R:289:VAL:O	2.30	0.64
1:W:108:VAL:HG13	1:W:277:PRO:HG2	1.80	0.64
1:e:273:TRP:CH2	1:i:116:MET:HE2	2.32	0.64
1:k:142:SER:OG	1:k:213:TYR:CB	2.45	0.64
1:m:116:MET:HE3	1:n:57:ILE:CD1	2.27	0.64
1:M:116:MET:HE3	1:N:57:ILE:CD1	2.26	0.64
1:f:70:LEU:C	1:f:70:LEU:HD23	2.22	0.64
1:e:113:MET:HE1	1:e:225:PRO:HG3	1.81	0.63
1:T:94:THR:CB	5:T:528:HOH:O	2.46	0.63
5:f:521:HOH:O	1:g:62:ASN:HB3	1.99	0.63
1:L:113:MET:HE1	1:L:225:PRO:CG	2.29	0.62
1:K:116:MET:HE2	1:L:273:TRP:CH2	2.35	0.62
1:P:154:MET:HE3	1:P:179:ALA:HB3	1.80	0.62
1:c:113:MET:HE1	1:c:225:PRO:HG3	1.81	0.62
1:N:113:MET:HE1	1:N:225:PRO:HG3	1.81	0.62
1:g:39:ILE:HD12	1:g:83:LEU:CD2	2.29	0.62
1:d:113:MET:HE1	1:d:225:PRO:HG3	1.82	0.62
1:W:108:VAL:CG1	1:W:277:PRO:HG2	2.29	0.62
1:W:113:MET:HE1	1:W:225:PRO:HG3	1.82	0.61
1:l:113:MET:HE1	1:l:225:PRO:CG	2.29	0.61
1:Q:113:MET:HE1	1:Q:225:PRO:HG3	1.81	0.61
1:H:116:MET:HE1	5:I:518:HOH:O	2.01	0.61
1:B:154:MET:HE3	1:B:179:ALA:HB3	1.81	0.61
1:c:113:MET:HE1	1:c:225:PRO:CG	2.31	0.61
1:k:108:VAL:CG1	1:k:277:PRO:HG2	2.31	0.60
1:e:113:MET:HE1	1:e:225:PRO:CG	2.31	0.60
1:K:270:LYS:HE3	5:K:556:HOH:O	2.02	0.60
1:N:113:MET:HE1	1:N:225:PRO:CG	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:39:ILE:HD12	1:b:83:LEU:CD2	2.30	0.60
1:l:54:SER:HG	1:l:72:GLU:HA	1.64	0.60
1:d:39:ILE:HD12	1:d:83:LEU:CD2	2.32	0.60
1:j:113:MET:HE1	1:j:225:PRO:HG3	1.83	0.60
1:V:108:VAL:HG23	1:V:277:PRO:HG2	1.84	0.60
1:Y:154:MET:HE3	1:Y:179:ALA:HB3	1.81	0.59
1:k:108:VAL:HG13	1:k:277:PRO:HG2	1.82	0.59
1:U:87:ASN:OD1	1:U:87:ASN:N	2.35	0.59
1:M:116:MET:HE2	1:N:273:TRP:CZ2	2.38	0.59
1:d:113:MET:HE1	1:d:225:PRO:CG	2.32	0.59
1:e:157:HIS:H	1:e:180:GLN:NE2	1.97	0.59
1:B:199:GLU:HB3	5:B:550:HOH:O	2.03	0.59
1:k:113:MET:CE	1:k:276:LEU:HD11	2.31	0.59
1:n:154:MET:HE3	1:n:179:ALA:HB3	1.81	0.59
1:W:113:MET:HE1	1:W:225:PRO:CG	2.33	0.59
1:Q:113:MET:HE1	1:Q:225:PRO:CG	2.32	0.58
1:l:39:ILE:HD12	1:l:83:LEU:CD2	2.33	0.58
1:m:133:ILE:HD11	1:m:274:ARG:HG2	1.83	0.58
1:j:39:ILE:HD12	1:j:83:LEU:CD2	2.31	0.58
1:j:113:MET:HE1	1:j:225:PRO:CG	2.33	0.58
1:K:160:GLN:NE2	5:K:503:HOH:O	2.36	0.58
1:P:270:LYS:HG2	5:T:548:HOH:O	2.04	0.58
1:V:154:MET:HE3	1:V:179:ALA:HB3	1.81	0.58
1:D:109:GLY:HA2	5:D:439:HOH:O	2.04	0.58
1:W:108:VAL:HG11	1:X:182:LEU:HD22	1.84	0.58
1:A:154:MET:HE3	1:A:179:ALA:HB3	1.80	0.57
1:Q:154:MET:HE3	1:Q:179:ALA:HB3	1.81	0.57
1:f:154:MET:HE3	1:f:179:ALA:HB3	1.81	0.57
1:Q:96:LEU:HD12	5:Q:509:HOH:O	2.04	0.57
1:J:59:VAL:H	2:J:401:SIA:H91	1.70	0.57
1:P:270:LYS:HE3	5:P:441:HOH:O	2.05	0.57
1:k:142:SER:OG	1:k:213:TYR:HB3	2.05	0.57
1:B:87:ASN:HD21	1:B:95:LEU:N	2.03	0.56
1:D:162:PRO:HD3	5:D:403:HOH:O	2.04	0.56
1:Q:154:MET:HE2	1:Q:179:ALA:HB1	1.86	0.56
1:n:97:MET:HE2	1:n:289:VAL:HG21	1.87	0.56
1:K:116:MET:HE2	1:L:273:TRP:CZ2	2.41	0.56
1:g:29:VAL:O	1:g:29:VAL:HG13	2.06	0.56
1:k:94:THR:O	1:k:96:LEU:HD12	2.05	0.56
1:k:29:VAL:HG13	1:k:29:VAL:O	2.06	0.56
1:l:39:ILE:HD12	1:l:83:LEU:HD21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:154:MET:HE2	1:k:179:ALA:HB1	1.86	0.55
1:l:113:MET:HE2	5:l:301:HOH:O	2.04	0.55
1:n:78:SER:CB	1:n:190:LEU:CD2	2.82	0.55
1:j:231:ASN:HB2	5:j:506:HOH:O	2.05	0.55
1:B:154:MET:HE2	1:B:179:ALA:HB1	1.86	0.55
1:k:40:GLU:OE2	1:l:206:SER:HB2	2.07	0.55
1:C:116:MET:HE2	5:D:432:HOH:O	2.06	0.54
1:j:262:THR:HG21	1:n:116:MET:CE	2.37	0.54
1:k:133:ILE:HD11	1:k:274:ARG:HG2	1.85	0.54
1:V:154:MET:HE2	1:V:179:ALA:HB1	1.86	0.54
1:F:67:ALA:H	2:F:401:SIA:H111	1.72	0.54
1:k:154:MET:HE3	1:k:179:ALA:HB3	1.81	0.54
1:T:133:ILE:HG12	5:T:508:HOH:O	2.06	0.53
1:j:39:ILE:HD12	1:j:83:LEU:HD21	1.91	0.53
1:l:113:MET:CE	1:l:225:PRO:HG3	2.38	0.53
1:D:222:GLU:HB2	5:D:423:HOH:O	2.08	0.53
1:e:157:HIS:N	1:e:180:GLN:HE21	2.00	0.53
1:Y:154:MET:HE2	1:Y:179:ALA:HB1	1.86	0.53
1:k:113:MET:HE1	1:k:260:ALA:HB1	1.90	0.53
1:U:160:GLN:NE2	5:U:404:HOH:O	2.34	0.53
1:n:154:MET:HE2	1:n:179:ALA:HB1	1.86	0.53
1:m:190:LEU:O	1:m:190:LEU:CD2	2.54	0.53
1:M:87:ASN:HD22	1:M:95:LEU:HD22	1.73	0.52
1:j:87:ASN:HD22	1:j:95:LEU:HD22	1.74	0.52
1:Q:154:MET:HE2	1:Q:168:PRO:HG2	1.91	0.52
1:V:108:VAL:HG23	1:V:277:PRO:CG	2.39	0.52
1:W:113:MET:CG	1:W:133:ILE:HD12	2.34	0.52
1:W:133:ILE:HD11	1:W:274:ARG:HG2	1.84	0.52
1:Y:109:GLY:HA2	5:Y:529:HOH:O	2.09	0.52
1:b:39:ILE:HD12	1:b:83:LEU:HD21	1.90	0.52
1:k:154:MET:HE2	1:k:168:PRO:HG2	1.92	0.52
1:V:123:ALA:HB1	1:V:124:PHE:CD1	2.44	0.52
1:Q:192:LYS:CD	5:Q:525:HOH:O	2.58	0.52
1:P:154:MET:HE2	1:P:179:ALA:HB1	1.85	0.52
1:Y:154:MET:HE2	1:Y:168:PRO:HG2	1.92	0.52
1:F:88:GLU:HB2	5:F:552:HOH:O	2.10	0.52
1:P:154:MET:HE1	1:P:175:THR:CG2	2.40	0.52
1:V:154:MET:HE2	1:V:168:PRO:HG2	1.92	0.52
1:V:154:MET:HE1	1:V:175:THR:CG2	2.40	0.52
1:Q:154:MET:HE1	1:Q:175:THR:CG2	2.40	0.52
1:N:113:MET:CE	1:N:225:PRO:HG3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:108:VAL:HG12	1:W:277:PRO:O	2.10	0.51
1:Y:154:MET:HE1	1:Y:175:THR:CG2	2.40	0.51
1:c:113:MET:CE	1:c:225:PRO:HG3	2.40	0.51
1:T:62:ASN:ND2	5:T:502:HOH:O	2.42	0.51
1:A:154:MET:HE1	1:A:175:THR:CG2	2.41	0.51
1:n:154:MET:HE1	1:n:175:THR:CG2	2.41	0.51
1:n:190:LEU:HD22	5:n:512:HOH:O	2.09	0.51
1:A:28:ASP:OD2	1:b:270:LYS:NZ	2.40	0.51
1:A:154:MET:HE2	1:A:168:PRO:HG2	1.92	0.51
1:A:154:MET:HE2	1:A:179:ALA:HB1	1.86	0.51
1:B:154:MET:HE1	1:B:175:THR:CG2	2.41	0.51
1:k:108:VAL:HG12	1:k:277:PRO:O	2.10	0.51
1:k:154:MET:HE1	1:k:175:THR:CG2	2.40	0.51
1:Q:113:MET:CE	1:Q:225:PRO:HG3	2.41	0.51
1:e:113:MET:CE	1:e:225:PRO:HG3	2.41	0.51
1:T:87:ASN:HD22	1:T:95:LEU:HD22	1.76	0.50
1:f:154:MET:HE2	1:f:168:PRO:HG2	1.92	0.50
1:n:154:MET:HE2	1:n:168:PRO:HG2	1.92	0.50
1:B:154:MET:HE2	1:B:168:PRO:HG2	1.92	0.50
1:d:113:MET:CE	1:d:225:PRO:HG3	2.41	0.50
1:D:87:ASN:HD22	1:D:95:LEU:HD22	1.74	0.50
1:e:273:TRP:CZ2	1:i:116:MET:HE2	2.47	0.50
1:f:154:MET:HE1	1:f:175:THR:CG2	2.41	0.50
1:j:113:MET:CE	1:j:225:PRO:HG3	2.41	0.50
1:S:94:THR:N	1:S:289:VAL:O	2.45	0.50
1:c:69:HIS:NE2	2:c:401:SIA:O1A	2.44	0.50
1:K:31:THR:CG2	1:W:267:THR:HG21	2.24	0.50
1:L:113:MET:CE	1:L:225:PRO:HG3	2.41	0.50
1:P:154:MET:HE2	1:P:168:PRO:HG2	1.94	0.50
1:W:113:MET:CE	1:W:225:PRO:HG3	2.41	0.50
1:j:231:ASN:HA	5:j:503:HOH:O	2.11	0.50
1:n:97:MET:HE2	1:n:289:VAL:CG1	2.32	0.50
1:X:160:GLN:HG3	5:X:531:HOH:O	2.12	0.49
1:d:39:ILE:HD12	1:d:83:LEU:HD21	1.94	0.49
1:g:39:ILE:HD12	1:g:83:LEU:HD21	1.92	0.49
1:A:93:PRO:HG2	1:A:94:THR:HG23	1.93	0.49
1:O:87:ASN:HD22	1:O:95:LEU:HD22	1.77	0.49
1:G:69:HIS:NE2	2:G:401:SIA:O1A	2.44	0.49
1:W:108:VAL:CG1	1:W:277:PRO:CG	2.91	0.49
1:W:134:GLU:OE2	1:W:222:GLU:HG2	2.12	0.49
1:A:69:HIS:NE2	2:A:401:SIA:O1A	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:234:THR:HG23	5:O:566:HOH:O	2.12	0.49
1:f:154:MET:HE2	1:f:179:ALA:HB1	1.86	0.49
1:I:87:ASN:HD22	1:I:95:LEU:HD22	1.78	0.48
1:V:108:VAL:HG23	1:V:277:PRO:HD2	1.95	0.48
1:k:142:SER:OG	1:k:213:TYR:HB2	2.13	0.48
1:m:113:MET:CG	1:m:133:ILE:HD12	2.35	0.48
1:j:231:ASN:CB	5:j:506:HOH:O	2.60	0.48
1:k:108:VAL:CG1	1:k:277:PRO:CG	2.92	0.48
1:k:113:MET:CG	1:k:133:ILE:HD12	2.39	0.48
1:m:78:SER:CB	1:m:190:LEU:CD2	2.85	0.48
1:Q:43:LEU:HD12	1:Q:256:SER:OG	2.14	0.47
1:V:124:PHE:CE2	1:W:264:VAL:HG11	2.48	0.47
1:K:121:LEU:HD12	5:K:552:HOH:O	2.13	0.47
1:C:87:ASN:HD22	1:C:95:LEU:HD22	1.79	0.47
1:O:23:GLY:HA3	5:O:538:HOH:O	2.15	0.47
1:A:154:MET:HE1	1:A:175:THR:HG21	1.97	0.47
1:Q:154:MET:HE1	1:Q:175:THR:HG21	1.97	0.47
5:V:506:HOH:O	1:W:221:VAL:HG23	2.14	0.47
1:Z:87:ASN:HD22	1:Z:95:LEU:HD22	1.79	0.47
1:l:78:SER:CB	1:l:190:LEU:CD2	2.85	0.47
1:K:93:PRO:HG2	1:K:94:THR:HG23	1.96	0.47
1:j:229:PHE:CZ	1:k:215:GLY:HA3	2.49	0.47
1:A:154:MET:CE	1:A:179:ALA:CB	2.69	0.46
1:n:154:MET:CE	1:n:179:ALA:CB	2.69	0.46
1:V:108:VAL:CG2	1:V:277:PRO:HG2	2.45	0.46
1:k:154:MET:HE1	1:k:175:THR:HG21	1.97	0.46
1:n:190:LEU:O	1:n:190:LEU:CD2	2.56	0.46
1:Y:154:MET:HE1	1:Y:175:THR:HG21	1.97	0.46
1:N:87:ASN:ND2	1:N:95:LEU:HB3	2.31	0.46
1:l:190:LEU:O	1:l:190:LEU:CD2	2.55	0.46
1:n:154:MET:HE1	1:n:175:THR:HG21	1.97	0.46
1:Y:87:ASN:HD22	1:Y:95:LEU:HD22	1.80	0.46
1:f:154:MET:HE1	1:f:175:THR:HG21	1.97	0.46
1:A:270:LYS:HG2	5:E:544:HOH:O	2.15	0.46
1:F:85:LEU:H	1:F:85:LEU:CD1	2.24	0.46
1:P:154:MET:HE1	1:P:175:THR:HG21	1.97	0.45
1:B:154:MET:HE1	1:B:175:THR:HG21	1.97	0.45
1:K:61:SER:HB3	5:K:510:HOH:O	2.15	0.45
1:V:154:MET:HE1	1:V:175:THR:HG21	1.97	0.45
1:K:158:SER:HB2	5:O:545:HOH:O	2.16	0.45
1:d:121:LEU:HD12	5:d:513:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:VAL:HA	5:E:547:HOH:O	2.17	0.45
1:K:68:PRO:CG	1:K:73:ILE:HD11	2.46	0.45
1:a:97:MET:HE2	1:a:289:VAL:CG2	2.45	0.45
1:g:22:GLY:N	5:g:403:HOH:O	2.50	0.45
1:N:68:PRO:CG	1:N:73:ILE:HD11	2.46	0.44
1:D:174:THR:HG22	1:D:175:THR:N	2.33	0.44
1:E:85:LEU:HD12	1:E:85:LEU:H	1.82	0.44
1:S:233:SER:HA	5:S:543:HOH:O	2.16	0.44
1:B:58:THR:HB	2:B:401:SIA:H8	1.99	0.44
1:G:149:ASP:HB3	5:G:525:HOH:O	2.18	0.44
1:F:87:ASN:HD22	1:F:95:LEU:HD22	1.82	0.44
1:m:114:LEU:CD2	1:n:259:VAL:HG11	2.45	0.44
1:A:68:PRO:CG	1:A:73:ILE:HD11	2.46	0.44
1:L:258:ASP:HB2	5:L:503:HOH:O	2.17	0.44
1:H:162:PRO:HD3	5:H:402:HOH:O	2.18	0.43
1:A:157:HIS:NE2	5:A:501:HOH:O	2.23	0.43
5:K:543:HOH:O	1:L:158:SER:HB2	2.18	0.43
1:J:87:ASN:HD22	1:J:95:LEU:HD22	1.84	0.43
1:f:121:LEU:HD12	5:f:518:HOH:O	2.17	0.43
1:C:116:MET:HE3	1:D:273:TRP:CZ3	2.50	0.43
1:F:29:VAL:HG23	5:F:564:HOH:O	2.19	0.43
1:l:49:GLN:HA	5:l:309:HOH:O	2.17	0.43
1:K:116:MET:CE	1:L:57:ILE:CD1	2.93	0.43
1:N:109:GLY:HA2	5:N:512:HOH:O	2.19	0.43
1:n:290:LYS:HA	5:n:519:HOH:O	2.19	0.43
1:W:68:PRO:CG	1:W:73:ILE:HD11	2.46	0.43
1:a:24:ILE:HG21	1:a:97:MET:CE	2.45	0.42
1:l:113:MET:HE3	1:l:133:ILE:CB	2.49	0.42
1:O:68:PRO:CG	1:O:73:ILE:HD11	2.47	0.42
1:I:68:PRO:CG	1:I:73:ILE:HD11	2.46	0.42
1:L:68:PRO:CG	1:L:73:ILE:HD11	2.46	0.42
1:Q:58:THR:HB	2:Q:401:SIA:O8	2.20	0.42
1:e:57:ILE:CD1	1:i:116:MET:CE	2.95	0.42
1:n:259:VAL:HG13	1:n:259:VAL:O	2.19	0.42
1:E:68:PRO:CG	1:E:73:ILE:HD11	2.46	0.42
1:P:68:PRO:CG	1:P:73:ILE:HD11	2.46	0.42
1:Q:154:MET:CE	1:Q:179:ALA:CB	2.69	0.42
1:a:70:LEU:HD12	1:a:165:LEU:HG	2.02	0.42
1:F:86:LEU:O	1:F:87:ASN:HB2	2.20	0.42
1:j:59:VAL:HB	1:n:122:ARG:HD2	2.01	0.42
1:B:68:PRO:CG	1:B:73:ILE:HD11	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:LEU:HD12	1:E:165:LEU:HG	2.02	0.42
1:F:68:PRO:CG	1:F:73:ILE:HD11	2.46	0.42
1:S:154:MET:HE1	1:S:161:TYR:HE1	1.85	0.42
1:T:240:GLU:H	1:T:240:GLU:HG2	1.65	0.42
1:R:68:PRO:CG	1:R:73:ILE:HD11	2.46	0.41
1:d:70:LEU:HD12	1:d:165:LEU:HG	2.01	0.41
1:I:70:LEU:HD12	1:I:165:LEU:HG	2.03	0.41
1:S:70:LEU:HD12	1:S:165:LEU:HG	2.02	0.41
1:V:124:PHE:CD1	1:V:124:PHE:N	2.87	0.41
1:B:207:ARG:NE	5:B:502:HOH:O	2.33	0.41
1:D:70:LEU:HD12	1:D:165:LEU:HG	2.03	0.41
1:N:70:LEU:HD12	1:N:165:LEU:HG	2.03	0.41
1:C:70:LEU:HD12	1:C:165:LEU:HG	2.02	0.41
1:L:70:LEU:HD12	1:L:165:LEU:HG	2.02	0.41
1:P:170:LYS:HE3	5:P:432:HOH:O	2.21	0.41
1:c:235:THR:HA	5:c:504:HOH:O	2.19	0.41
1:h:70:LEU:HD12	1:h:165:LEU:HG	2.02	0.41
1:h:81:ILE:HA	5:h:414:HOH:O	2.21	0.41
1:C:88:GLU:HG3	5:C:543:HOH:O	2.21	0.41
1:M:70:LEU:HD12	1:M:165:LEU:HG	2.02	0.41
1:F:87:ASN:OD1	1:F:87:ASN:N	2.52	0.41
1:F:121:LEU:HD12	5:F:551:HOH:O	2.20	0.41
1:O:258:ASP:HB2	5:O:504:HOH:O	2.19	0.41
1:Z:70:LEU:HD12	1:Z:165:LEU:HG	2.02	0.41
1:j:70:LEU:HD12	1:j:165:LEU:HG	2.02	0.41
1:j:199:GLU:CB	5:n:522:HOH:O	2.68	0.41
1:n:70:LEU:HD12	1:n:165:LEU:HG	2.02	0.41
1:B:70:LEU:HD12	1:B:165:LEU:HG	2.03	0.41
1:P:70:LEU:HD12	1:P:165:LEU:HG	2.03	0.41
1:a:68:PRO:CG	1:a:73:ILE:HD11	2.51	0.41
1:m:129:GLY:H	1:n:271:GLN:NE2	2.18	0.41
1:A:70:LEU:HD12	1:A:165:LEU:HG	2.02	0.41
2:F:401:SIA:O9	1:J:122:ARG:NH1	2.51	0.41
1:Q:70:LEU:HD12	1:Q:165:LEU:HG	2.01	0.41
1:U:208:ASN:HA	5:U:438:HOH:O	2.21	0.41
1:V:68:PRO:CG	1:V:73:ILE:HD11	2.51	0.41
1:V:108:VAL:CG2	1:V:277:PRO:CG	2.99	0.41
1:X:122:ARG:HD2	1:Y:59:VAL:HB	2.02	0.41
1:h:151:GLN:CD	1:h:182:LEU:CD1	2.94	0.41
1:O:70:LEU:HD12	1:O:165:LEU:HG	2.03	0.41
1:P:59:VAL:HB	1:T:122:ARG:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:154:MET:CE	1:P:179:ALA:CB	2.68	0.41
1:V:70:LEU:HD12	1:V:165:LEU:HG	2.03	0.41
1:W:108:VAL:HG13	1:W:277:PRO:CG	2.49	0.41
1:X:68:PRO:CG	1:X:73:ILE:HD11	2.51	0.41
1:h:68:PRO:CG	1:h:73:ILE:HD11	2.51	0.41
1:n:138:ILE:CG2	1:n:259:VAL:HG12	2.29	0.41
1:K:70:LEU:HD12	1:K:165:LEU:HG	2.03	0.41
1:Q:113:MET:CE	1:Q:225:PRO:CG	2.99	0.41
1:R:70:LEU:HD12	1:R:165:LEU:HG	2.03	0.41
1:Y:70:LEU:HD12	1:Y:165:LEU:HG	2.02	0.41
1:V:123:ALA:CB	1:V:124:PHE:HD1	2.35	0.40
1:W:70:LEU:HD12	1:W:165:LEU:HG	2.03	0.40
1:W:154:MET:O	1:W:180:GLN:HA	2.22	0.40
1:i:70:LEU:HD12	1:i:165:LEU:HG	2.03	0.40
1:C:68:PRO:CG	1:C:73:ILE:HD11	2.46	0.40
1:F:70:LEU:HD12	1:F:165:LEU:HG	2.04	0.40
1:M:154:MET:O	1:M:180:GLN:HA	2.22	0.40
1:Q:59:VAL:O	5:Q:501:HOH:O	2.22	0.40
1:U:154:MET:O	1:U:180:GLN:HA	2.21	0.40
1:c:68:PRO:CG	1:c:73:ILE:HD11	2.51	0.40
1:E:154:MET:O	1:E:180:GLN:HA	2.22	0.40
1:G:70:LEU:HD12	1:G:165:LEU:HG	2.03	0.40
1:H:68:PRO:CG	1:H:73:ILE:HD11	2.46	0.40
1:L:109:GLY:HA2	5:M:506:HOH:O	2.20	0.40
1:O:154:MET:O	1:O:180:GLN:HA	2.22	0.40
1:b:154:MET:O	1:b:180:GLN:HA	2.22	0.40
1:f:68:PRO:CG	1:f:73:ILE:HD11	2.51	0.40
1:m:128:GLY:HA3	1:n:271:GLN:HE21	1.85	0.40
1:m:154:MET:O	1:m:180:GLN:HA	2.22	0.40
1:C:154:MET:O	1:C:180:GLN:HA	2.22	0.40
1:c:70:LEU:HD12	1:c:165:LEU:HG	2.03	0.40
1:f:154:MET:O	1:f:180:GLN:HA	2.22	0.40
1:G:87:ASN:C	5:G:503:HOH:O	2.64	0.40
1:G:154:MET:O	1:G:180:GLN:HA	2.22	0.40
1:W:24:ILE:HG21	1:W:97:MET:CE	2.45	0.40
1:Y:154:MET:O	1:Y:180:GLN:HA	2.22	0.40
1:Z:154:MET:O	1:Z:180:GLN:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	265/274 (97%)	257 (97%)	8 (3%)	0	100	100
1	B	256/274 (93%)	248 (97%)	8 (3%)	0	100	100
1	C	265/274 (97%)	256 (97%)	9 (3%)	0	100	100
1	D	257/274 (94%)	249 (97%)	8 (3%)	0	100	100
1	E	259/274 (94%)	251 (97%)	8 (3%)	0	100	100
1	F	266/274 (97%)	257 (97%)	9 (3%)	0	100	100
1	G	256/274 (93%)	248 (97%)	8 (3%)	0	100	100
1	H	256/274 (93%)	248 (97%)	8 (3%)	0	100	100
1	I	266/274 (97%)	258 (97%)	8 (3%)	0	100	100
1	J	265/274 (97%)	256 (97%)	9 (3%)	0	100	100
1	K	265/274 (97%)	257 (97%)	8 (3%)	0	100	100
1	L	258/274 (94%)	250 (97%)	8 (3%)	0	100	100
1	M	267/274 (97%)	257 (96%)	9 (3%)	1 (0%)	30	45
1	N	262/274 (96%)	253 (97%)	9 (3%)	0	100	100
1	O	258/274 (94%)	250 (97%)	8 (3%)	0	100	100
1	P	267/274 (97%)	259 (97%)	8 (3%)	0	100	100
1	Q	266/274 (97%)	257 (97%)	9 (3%)	0	100	100
1	R	259/274 (94%)	252 (97%)	7 (3%)	0	100	100
1	S	257/274 (94%)	249 (97%)	8 (3%)	0	100	100
1	T	259/274 (94%)	251 (97%)	8 (3%)	0	100	100
1	U	257/274 (94%)	249 (97%)	8 (3%)	0	100	100
1	V	261/274 (95%)	253 (97%)	8 (3%)	0	100	100
1	W	258/274 (94%)	250 (97%)	8 (3%)	0	100	100
1	X	257/274 (94%)	249 (97%)	8 (3%)	0	100	100
1	Y	257/274 (94%)	249 (97%)	8 (3%)	0	100	100

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

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	92	SER

5.3.2 Protein sidechains ⓘ

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%)	215 (99%)	3 (1%)	59	76
1	B	206/233 (88%)	203 (98%)	3 (2%)	57	75
1	C	220/233 (94%)	218 (99%)	2 (1%)	70	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	213/233 (91%)	211 (99%)	2 (1%)	70	82
1	E	208/233 (89%)	207 (100%)	1 (0%)	81	91
1	F	217/233 (93%)	214 (99%)	3 (1%)	59	76
1	G	208/233 (89%)	205 (99%)	3 (1%)	59	76
1	H	207/233 (89%)	206 (100%)	1 (0%)	81	91
1	I	216/233 (93%)	214 (99%)	2 (1%)	70	82
1	J	220/233 (94%)	218 (99%)	2 (1%)	70	82
1	K	217/233 (93%)	214 (99%)	3 (1%)	59	76
1	L	209/233 (90%)	207 (99%)	2 (1%)	68	81
1	M	215/233 (92%)	213 (99%)	2 (1%)	70	82
1	N	212/233 (91%)	209 (99%)	3 (1%)	59	76
1	O	210/233 (90%)	208 (99%)	2 (1%)	68	81
1	P	215/233 (92%)	213 (99%)	2 (1%)	70	82
1	Q	213/233 (91%)	211 (99%)	2 (1%)	70	82
1	R	213/233 (91%)	210 (99%)	3 (1%)	59	76
1	S	209/233 (90%)	206 (99%)	3 (1%)	59	76
1	T	211/233 (91%)	207 (98%)	4 (2%)	50	71
1	U	210/233 (90%)	208 (99%)	2 (1%)	68	81
1	V	210/233 (90%)	207 (99%)	3 (1%)	59	76
1	W	206/233 (88%)	205 (100%)	1 (0%)	81	91
1	X	210/233 (90%)	207 (99%)	3 (1%)	59	76
1	Y	209/233 (90%)	208 (100%)	1 (0%)	81	91
1	Z	211/233 (91%)	208 (99%)	3 (1%)	59	76
1	a	213/233 (91%)	209 (98%)	4 (2%)	50	71
1	b	196/233 (84%)	192 (98%)	4 (2%)	48	69
1	c	196/233 (84%)	192 (98%)	4 (2%)	48	69
1	d	205/233 (88%)	201 (98%)	4 (2%)	48	69
1	e	210/233 (90%)	206 (98%)	4 (2%)	50	71
1	f	207/233 (89%)	204 (99%)	3 (1%)	59	76
1	g	201/233 (86%)	197 (98%)	4 (2%)	48	69
1	h	205/233 (88%)	202 (98%)	3 (2%)	57	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	i	202/233 (87%)	202 (100%)	0	100	100
1	j	201/233 (86%)	196 (98%)	5 (2%)	42	64
1	k	168/233 (72%)	166 (99%)	2 (1%)	63	79
1	l	129/233 (55%)	127 (98%)	2 (2%)	55	74
1	m	174/233 (75%)	172 (99%)	2 (1%)	65	80
1	n	206/233 (88%)	206 (100%)	0	100	100
All	All	8226/9320 (88%)	8124 (99%)	102 (1%)	63	79

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	SER
1	A	78	SER
1	A	236	ILE
1	B	61	SER
1	B	78	SER
1	B	95	LEU
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	G	236	ILE
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	K	236	ILE
1	L	61	SER
1	L	78	SER
1	M	61	SER
1	M	78	SER

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Mol	Chain	Res	Type
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	Q	61	SER
1	Q	78	SER
1	R	61	SER
1	R	78	SER
1	R	189	LYS
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
1	U	61	SER
1	U	87	ASN
1	V	61	SER
1	V	73	ILE
1	V	78	SER
1	W	78	SER
1	X	61	SER
1	X	73	ILE
1	X	78	SER
1	Y	61	SER
1	Z	61	SER
1	Z	236	ILE
1	Z	240	GLU
1	a	61	SER
1	a	73	ILE
1	a	78	SER
1	a	240	GLU
1	b	39	ILE
1	b	61	SER
1	b	78	SER
1	b	236	ILE
1	c	61	SER
1	c	73	ILE

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Mol	Chain	Res	Type
1	c	78	SER
1	c	236	ILE
1	d	39	ILE
1	d	61	SER
1	d	78	SER
1	d	236	ILE
1	e	61	SER
1	e	73	ILE
1	e	78	SER
1	e	240	GLU
1	f	61	SER
1	f	73	ILE
1	f	78	SER
1	g	39	ILE
1	g	61	SER
1	g	78	SER
1	g	88	GLU
1	h	61	SER
1	h	73	ILE
1	h	78	SER
1	j	39	ILE
1	j	61	SER
1	j	73	ILE
1	j	78	SER
1	j	236	ILE
1	k	61	SER
1	k	78	SER
1	l	39	ILE
1	l	78	SER
1	m	78	SER
1	m	177	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	155	GLN
1	B	155	GLN
1	C	269	GLN
1	D	87	ASN
1	G	155	GLN
1	H	155	GLN

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Mol	Chain	Res	Type
1	H	269	GLN
1	I	65	ASN
1	I	87	ASN
1	J	155	GLN
1	K	160	GLN
1	K	269	GLN
1	L	155	GLN
1	M	65	ASN
1	M	69	HIS
1	M	87	ASN
1	M	269	GLN
1	N	87	ASN
1	N	160	GLN
1	O	87	ASN
1	O	155	GLN
1	P	49	GLN
1	Q	69	HIS
1	Q	155	GLN
1	T	87	ASN
1	T	155	GLN
1	U	69	HIS
1	U	155	GLN
1	V	155	GLN
1	X	65	ASN
1	X	160	GLN
1	Y	87	ASN
1	Y	155	GLN
1	Y	160	GLN
1	Z	65	ASN
1	Z	69	HIS
1	Z	87	ASN
1	Z	155	GLN
1	b	155	GLN
1	b	269	GLN
1	e	62	ASN
1	e	155	GLN
1	e	180	GLN
1	e	265	GLN
1	f	65	ASN
1	f	155	GLN
1	g	269	GLN
1	i	155	GLN

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Mol	Chain	Res	Type
1	j	62	ASN
1	j	87	ASN
1	k	139	HIS
1	k	155	GLN
1	m	69	HIS
1	n	65	ASN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	M	401	-	21,21,21	1.04	1 (4%)	24,31,31	1.35	3 (12%)
2	SIA	R	401	-	21,21,21	1.20	2 (9%)	24,31,31	1.45	4 (16%)
2	SIA	f	401	-	21,21,21	1.12	1 (4%)	24,31,31	1.22	3 (12%)
2	SIA	e	401	-	21,21,21	1.17	2 (9%)	24,31,31	1.37	5 (20%)
2	SIA	a	401	-	21,21,21	1.32	4 (19%)	24,31,31	1.75	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SIA	Q	401	-	21,21,21	1.27	2 (9%)	24,31,31	1.40	4 (16%)
2	SIA	F	401	-	21,21,21	0.96	1 (4%)	24,31,31	1.43	6 (25%)
2	SIA	B	401	-	21,21,21	1.21	3 (14%)	24,31,31	1.39	3 (12%)
2	SIA	Z	401	-	21,21,21	1.23	3 (14%)	24,31,31	1.79	5 (20%)
2	SIA	T	401	-	21,21,21	1.12	2 (9%)	24,31,31	1.19	2 (8%)
2	SIA	G	401	-	21,21,21	1.19	1 (4%)	24,31,31	1.41	5 (20%)
2	SIA	Y	401	-	21,21,21	1.03	1 (4%)	24,31,31	1.10	1 (4%)
2	SIA	A	401	-	21,21,21	1.26	2 (9%)	24,31,31	1.77	5 (20%)
2	SIA	X	401	-	21,21,21	1.12	2 (9%)	24,31,31	1.21	2 (8%)
2	SIA	N	401	-	21,21,21	1.14	2 (9%)	24,31,31	1.16	2 (8%)
2	SIA	K	401	-	21,21,21	1.11	1 (4%)	24,31,31	1.21	2 (8%)
2	SIA	E	401	-	21,21,21	0.98	1 (4%)	24,31,31	1.18	3 (12%)
2	SIA	d	401	-	21,21,21	1.04	1 (4%)	24,31,31	1.18	3 (12%)
2	SIA	S	401	-	21,21,21	1.06	1 (4%)	24,31,31	1.85	4 (16%)
2	SIA	b	401	-	21,21,21	1.04	1 (4%)	24,31,31	1.29	3 (12%)
2	SIA	j	401	-	21,21,21	1.27	3 (14%)	24,31,31	1.37	3 (12%)
2	SIA	C	401	-	21,21,21	0.99	1 (4%)	24,31,31	1.08	2 (8%)
2	SIA	O	401	-	21,21,21	1.18	2 (9%)	24,31,31	1.81	6 (25%)
2	SIA	J	401	-	21,21,21	1.22	3 (14%)	24,31,31	1.15	2 (8%)
2	SIA	V	401	-	21,21,21	1.39	3 (14%)	24,31,31	1.86	5 (20%)
2	SIA	n	401	-	21,21,21	0.97	1 (4%)	24,31,31	1.22	2 (8%)
2	SIA	L	401	-	21,21,21	0.97	1 (4%)	24,31,31	0.93	0
2	SIA	c	401	-	21,21,21	1.16	2 (9%)	24,31,31	1.29	3 (12%)
2	SIA	I	401	-	21,21,21	0.92	1 (4%)	24,31,31	1.68	5 (20%)

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	-	-	8/20/38/38	0/1/1/1
2	SIA	R	401	-	-	8/20/38/38	0/1/1/1
2	SIA	f	401	-	-	3/20/38/38	0/1/1/1
2	SIA	e	401	-	-	8/20/38/38	0/1/1/1
2	SIA	a	401	-	-	5/20/38/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIA	Q	401	-	-	2/20/38/38	0/1/1/1
2	SIA	F	401	-	-	5/20/38/38	0/1/1/1
2	SIA	B	401	-	-	7/20/38/38	0/1/1/1
2	SIA	Z	401	-	-	7/20/38/38	0/1/1/1
2	SIA	T	401	-	-	3/20/38/38	0/1/1/1
2	SIA	G	401	-	-	6/20/38/38	0/1/1/1
2	SIA	Y	401	-	-	7/20/38/38	0/1/1/1
2	SIA	A	401	-	-	3/20/38/38	0/1/1/1
2	SIA	X	401	-	-	7/20/38/38	0/1/1/1
2	SIA	N	401	-	-	7/20/38/38	0/1/1/1
2	SIA	K	401	-	-	5/20/38/38	0/1/1/1
2	SIA	E	401	-	-	2/20/38/38	0/1/1/1
2	SIA	d	401	-	-	3/20/38/38	0/1/1/1
2	SIA	S	401	-	-	9/20/38/38	0/1/1/1
2	SIA	b	401	-	-	8/20/38/38	0/1/1/1
2	SIA	j	401	-	-	7/20/38/38	0/1/1/1
2	SIA	C	401	-	-	6/20/38/38	0/1/1/1
2	SIA	O	401	-	-	3/20/38/38	0/1/1/1
2	SIA	J	401	-	-	10/20/38/38	0/1/1/1
2	SIA	V	401	-	-	5/20/38/38	0/1/1/1
2	SIA	n	401	-	-	12/20/38/38	0/1/1/1
2	SIA	L	401	-	-	1/20/38/38	0/1/1/1
2	SIA	c	401	-	-	2/20/38/38	0/1/1/1
2	SIA	I	401	-	-	7/20/38/38	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	401	SIA	O2-C2	3.74	1.45	1.39
2	G	401	SIA	O2-C2	3.72	1.44	1.39
2	V	401	SIA	O2-C2	3.61	1.44	1.39
2	j	401	SIA	O2-C2	3.58	1.44	1.39
2	E	401	SIA	O2-C2	3.52	1.44	1.39
2	a	401	SIA	O2-C2	3.49	1.44	1.39
2	T	401	SIA	O2-C2	3.33	1.44	1.39
2	X	401	SIA	O2-C2	3.33	1.44	1.39
2	e	401	SIA	O2-C2	3.32	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	401	SIA	O2-C2	3.30	1.44	1.39
2	O	401	SIA	O2-C2	3.24	1.44	1.39
2	Z	401	SIA	O2-C2	3.24	1.44	1.39
2	N	401	SIA	O2-C2	3.16	1.44	1.39
2	A	401	SIA	C7-C6	3.11	1.56	1.52
2	C	401	SIA	O2-C2	3.06	1.44	1.39
2	L	401	SIA	O2-C2	3.04	1.43	1.39
2	f	401	SIA	O2-C2	3.04	1.43	1.39
2	c	401	SIA	O2-C2	2.99	1.43	1.39
2	S	401	SIA	O2-C2	2.97	1.43	1.39
2	Q	401	SIA	C3-C2	2.97	1.55	1.51
2	R	401	SIA	C7-C6	2.95	1.56	1.52
2	K	401	SIA	O2-C2	2.80	1.43	1.39
2	R	401	SIA	O2-C2	2.76	1.43	1.39
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	B	401	SIA	O2-C2	2.59	1.43	1.39
2	a	401	SIA	C7-C6	2.57	1.56	1.52
2	M	401	SIA	O2-C2	2.55	1.43	1.39
2	J	401	SIA	O6-C2	2.51	1.45	1.43
2	B	401	SIA	C7-C6	2.50	1.56	1.52
2	J	401	SIA	C3-C2	2.50	1.55	1.51
2	F	401	SIA	O2-C2	2.48	1.43	1.39
2	O	401	SIA	C3-C2	2.44	1.55	1.51
2	b	401	SIA	O2-C2	2.42	1.43	1.39
2	I	401	SIA	O2-C2	2.38	1.43	1.39
2	e	401	SIA	C7-C6	2.38	1.55	1.52
2	Z	401	SIA	C7-C6	2.36	1.55	1.52
2	V	401	SIA	C4-C5	2.33	1.55	1.53
2	a	401	SIA	O6-C2	2.31	1.45	1.43
2	Z	401	SIA	C3-C2	2.25	1.54	1.51
2	n	401	SIA	O2-C2	2.23	1.42	1.39
2	c	401	SIA	C2-C1	-2.13	1.50	1.53
2	N	401	SIA	C4-C5	-2.13	1.51	1.53
2	j	401	SIA	C3-C2	2.12	1.54	1.51
2	T	401	SIA	C3-C2	2.12	1.54	1.51
2	V	401	SIA	C3-C2	2.06	1.54	1.51
2	X	401	SIA	C3-C2	2.05	1.54	1.51
2	a	401	SIA	C3-C2	2.02	1.54	1.51
2	j	401	SIA	C4-C5	2.01	1.55	1.53
2	B	401	SIA	C2-C1	-2.01	1.50	1.53

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	401	SIA	C3-C4-C5	5.38	118.04	109.72
2	S	401	SIA	O1A-C1-C2	-5.28	115.04	123.85
2	A	401	SIA	O1A-C1-C2	-4.91	115.66	123.85
2	I	401	SIA	O1A-C1-C2	-4.77	115.89	123.85
2	O	401	SIA	C3-C4-C5	4.75	117.06	109.72
2	V	401	SIA	C3-C4-C5	4.62	116.86	109.72
2	S	401	SIA	C3-C4-C5	4.32	116.40	109.72
2	O	401	SIA	O6-C6-C5	-4.18	106.02	109.84
2	a	401	SIA	O6-C6-C5	-4.15	106.05	109.84
2	B	401	SIA	O1A-C1-C2	-4.14	116.95	123.85
2	V	401	SIA	O1A-C1-C2	-4.06	117.08	123.85
2	M	401	SIA	O1A-C1-C2	-3.94	117.28	123.85
2	n	401	SIA	O6-C6-C5	3.75	113.28	109.84
2	b	401	SIA	O1A-C1-C2	-3.68	117.70	123.85
2	a	401	SIA	O6-C6-C7	3.59	112.26	106.65
2	I	401	SIA	C3-C4-C5	3.49	115.12	109.72
2	a	401	SIA	C3-C4-C5	3.37	114.94	109.72
2	Q	401	SIA	C3-C4-C5	3.31	114.84	109.72
2	e	401	SIA	O2-C2-C3	-3.31	104.44	109.44
2	K	401	SIA	O2-C2-C3	-3.27	104.49	109.44
2	a	401	SIA	O1A-C1-C2	-3.26	118.41	123.85
2	c	401	SIA	C3-C4-C5	3.26	114.77	109.72
2	T	401	SIA	O1A-C1-C2	-3.25	118.43	123.85
2	c	401	SIA	O1A-C1-C2	-3.24	118.44	123.85
2	S	401	SIA	O2-C2-C1	-3.22	103.93	110.73
2	A	401	SIA	O6-C6-C7	3.18	111.61	106.65
2	R	401	SIA	O1A-C1-C2	-3.10	118.68	123.85
2	G	401	SIA	O6-C6-C5	-3.02	107.08	109.84
2	R	401	SIA	O2-C2-C3	-3.02	104.87	109.44
2	Z	401	SIA	O1A-C1-C2	-2.99	118.86	123.85
2	X	401	SIA	C9-C8-C7	2.98	118.24	112.17
2	f	401	SIA	O1A-C1-C2	-2.85	119.10	123.85
2	A	401	SIA	O7-C7-C6	2.83	115.56	109.44
2	d	401	SIA	C3-C2-C1	-2.80	107.64	112.84
2	O	401	SIA	O6-C6-C7	2.79	111.00	106.65
2	C	401	SIA	O1A-C1-C2	-2.78	119.21	123.85
2	Q	401	SIA	O2-C2-O6	-2.78	102.51	109.51
2	Z	401	SIA	O6-C6-C7	2.78	110.99	106.65
2	Z	401	SIA	O2-C2-C1	-2.73	104.96	110.73
2	Q	401	SIA	O1A-C1-C2	-2.73	119.30	123.85
2	F	401	SIA	C4-C5-N5	-2.73	105.07	110.44
2	j	401	SIA	O1A-C1-C2	-2.71	119.33	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	SIA	O1A-C1-C2	-2.70	119.34	123.85
2	V	401	SIA	C6-C5-N5	-2.69	106.62	110.91
2	I	401	SIA	O2-C2-O6	-2.67	102.78	109.51
2	R	401	SIA	O6-C6-C7	2.64	110.78	106.65
2	f	401	SIA	C3-C4-C5	2.62	113.77	109.72
2	d	401	SIA	O1A-C1-C2	-2.59	119.53	123.85
2	M	401	SIA	O2-C2-C1	-2.51	105.43	110.73
2	F	401	SIA	O1A-C1-C2	-2.50	119.68	123.85
2	M	401	SIA	O8-C8-C7	2.46	115.00	109.25
2	F	401	SIA	C3-C4-C5	2.45	113.51	109.72
2	c	401	SIA	O6-C6-C5	-2.45	107.60	109.84
2	V	401	SIA	C9-C8-C7	2.44	117.14	112.17
2	N	401	SIA	O2-C2-O6	-2.42	103.42	109.51
2	A	401	SIA	C3-C2-C1	-2.42	108.35	112.84
2	J	401	SIA	O6-C6-C7	2.41	110.41	106.65
2	B	401	SIA	O2-C2-O6	-2.40	103.47	109.51
2	G	401	SIA	C3-C4-C5	2.38	113.40	109.72
2	I	401	SIA	C8-C7-C6	-2.36	108.62	113.05
2	F	401	SIA	O9-C9-C8	-2.35	106.22	111.16
2	F	401	SIA	O2-C2-C3	-2.34	105.90	109.44
2	n	401	SIA	O1A-C1-C2	-2.33	119.96	123.85
2	G	401	SIA	C11-C10-N5	2.33	119.97	116.12
2	O	401	SIA	O1A-C1-C2	-2.28	120.04	123.85
2	R	401	SIA	C4-C5-N5	-2.28	105.94	110.44
2	O	401	SIA	O4-C4-C5	-2.28	104.66	109.84
2	e	401	SIA	O1A-C1-C2	-2.28	120.05	123.85
2	A	401	SIA	C6-C5-N5	-2.26	107.30	110.91
2	b	401	SIA	O6-C6-C5	2.24	111.90	109.84
2	I	401	SIA	O7-C7-C6	2.24	114.29	109.44
2	Z	401	SIA	O7-C7-C6	2.24	114.28	109.44
2	O	401	SIA	O2-C2-O6	-2.23	103.89	109.51
2	T	401	SIA	C3-C4-C5	2.22	113.15	109.72
2	j	401	SIA	O4-C4-C5	2.20	114.85	109.84
2	j	401	SIA	C3-C2-C1	-2.20	108.75	112.84
2	V	401	SIA	O2-C2-C1	-2.17	106.15	110.73
2	E	401	SIA	O1A-C1-C2	-2.15	120.27	123.85
2	B	401	SIA	O4-C4-C3	-2.13	105.01	109.97
2	Q	401	SIA	C6-C5-N5	-2.13	107.51	110.91
2	J	401	SIA	O1A-C1-C2	-2.11	120.33	123.85
2	e	401	SIA	O9-C9-C8	2.11	115.58	111.16
2	N	401	SIA	O1A-C1-C2	-2.10	120.34	123.85
2	K	401	SIA	O1A-C1-C2	-2.10	120.35	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	SIA	C3-C4-C5	2.09	112.96	109.72
2	b	401	SIA	O2-C2-C1	-2.09	106.32	110.73
2	F	401	SIA	C8-C7-C6	-2.08	109.15	113.05
2	a	401	SIA	O2-C2-C3	-2.08	106.30	109.44
2	S	401	SIA	O6-C6-C5	-2.07	107.95	109.84
2	E	401	SIA	O4-C4-C3	-2.07	105.16	109.97
2	X	401	SIA	O8-C8-C9	-2.06	104.35	109.03
2	e	401	SIA	C11-C10-N5	-2.05	112.71	116.12
2	d	401	SIA	O2-C2-O6	-2.05	104.34	109.51
2	E	401	SIA	C3-C4-C5	2.05	112.89	109.72
2	f	401	SIA	C8-C7-C6	-2.02	109.26	113.05
2	e	401	SIA	O6-C6-C7	2.01	109.80	106.65
2	Y	401	SIA	O2-C2-C3	-2.00	106.41	109.44
2	G	401	SIA	C5-N5-C10	-2.00	118.42	123.11

There are no chirality outliers.

All (166) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	SIA	O8-C8-C9-O9
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	E	401	SIA	C7-C8-C9-O9
2	E	401	SIA	O8-C8-C9-O9
2	F	401	SIA	O8-C8-C9-O9
2	G	401	SIA	O1B-C1-C2-O6
2	I	401	SIA	O1A-C1-C2-O2
2	I	401	SIA	O1B-C1-C2-O2
2	J	401	SIA	O1A-C1-C2-O2
2	J	401	SIA	O1B-C1-C2-O2
2	J	401	SIA	O1B-C1-C2-O6
2	J	401	SIA	C6-C7-C8-C9
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	K	401	SIA	C6-C7-C8-C9
2	K	401	SIA	C6-C7-C8-O8
2	K	401	SIA	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
2	K	401	SIA	O7-C7-C8-O8
2	M	401	SIA	O1A-C1-C2-O2
2	M	401	SIA	O1B-C1-C2-O2
2	M	401	SIA	O1B-C1-C2-O6
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	N	401	SIA	O1B-C1-C2-O6
2	R	401	SIA	O1A-C1-C2-O2
2	R	401	SIA	O1B-C1-C2-O2
2	R	401	SIA	O1B-C1-C2-O6
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	S	401	SIA	O1A-C1-C2-O2
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	T	401	SIA	C7-C8-C9-O9
2	T	401	SIA	O8-C8-C9-O9
2	V	401	SIA	O1A-C1-C2-O2
2	V	401	SIA	O1B-C1-C2-O2
2	V	401	SIA	O8-C8-C9-O9
2	X	401	SIA	C7-C8-C9-O9
2	X	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	b	401	SIA	O1B-C1-C2-O6
2	d	401	SIA	C7-C8-C9-O9
2	d	401	SIA	O8-C8-C9-O9
2	e	401	SIA	O8-C8-C9-O9
2	f	401	SIA	O8-C8-C9-O9
2	n	401	SIA	O1A-C1-C2-O6
2	B	401	SIA	O8-C8-C9-O9
2	A	401	SIA	C7-C8-C9-O9
2	F	401	SIA	C7-C8-C9-O9
2	V	401	SIA	C7-C8-C9-O9
2	e	401	SIA	C7-C8-C9-O9

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

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Mol	Chain	Res	Type	Atoms
2	Y	401	SIA	O8-C8-C9-O9
2	j	401	SIA	O8-C8-C9-O9
2	j	401	SIA	O7-C7-C8-O8
2	S	401	SIA	O8-C8-C9-O9
2	G	401	SIA	C6-C7-C8-O8
2	O	401	SIA	O8-C8-C9-O9
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	e	401	SIA	O7-C7-C8-C9
2	N	401	SIA	C6-C7-C8-O8
2	B	401	SIA	C7-C8-C9-O9
2	Z	401	SIA	O1A-C1-C2-C3
2	Z	401	SIA	O1B-C1-C2-C3
2	n	401	SIA	O1A-C1-C2-C3
2	n	401	SIA	O1B-C1-C2-C3
2	N	401	SIA	C6-C7-C8-C9
2	Y	401	SIA	C6-C7-C8-C9
2	A	401	SIA	O1A-C1-C2-O2
2	J	401	SIA	O1A-C1-C2-O6
2	M	401	SIA	O1A-C1-C2-O6
2	N	401	SIA	O1A-C1-C2-O6
2	R	401	SIA	O1A-C1-C2-O6
2	X	401	SIA	O1A-C1-C2-O2
2	b	401	SIA	O1A-C1-C2-O6
2	n	401	SIA	O1A-C1-C2-O2
2	c	401	SIA	C7-C8-C9-O9
2	c	401	SIA	O8-C8-C9-O9
2	Y	401	SIA	O7-C7-C8-C9
2	Z	401	SIA	C4-C5-N5-C10
2	B	401	SIA	O1B-C1-C2-O6
2	F	401	SIA	O1B-C1-C2-O2
2	G	401	SIA	O1B-C1-C2-O2
2	I	401	SIA	O1B-C1-C2-O6
2	L	401	SIA	O1B-C1-C2-O2
2	N	401	SIA	O1B-C1-C2-O2
2	Q	401	SIA	O1B-C1-C2-O2
2	S	401	SIA	O1B-C1-C2-O2
2	S	401	SIA	O1B-C1-C2-O6
2	V	401	SIA	O1B-C1-C2-O6
2	Z	401	SIA	O1B-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	d	401	SIA	O1B-C1-C2-O2
2	e	401	SIA	O1B-C1-C2-O2
2	f	401	SIA	O1B-C1-C2-O6
2	j	401	SIA	O1B-C1-C2-O2
2	n	401	SIA	O1B-C1-C2-O2
2	j	401	SIA	C7-C8-C9-O9
2	O	401	SIA	C4-C5-N5-C10
2	Z	401	SIA	C6-C5-N5-C10
2	n	401	SIA	C4-C5-N5-C10
2	C	401	SIA	O1B-C1-C2-C3
2	K	401	SIA	O1A-C1-C2-C3
2	T	401	SIA	O1B-C1-C2-C3
2	Y	401	SIA	O1A-C1-C2-C3
2	a	401	SIA	O1B-C1-C2-C3
2	e	401	SIA	O1A-C1-C2-C3
2	C	401	SIA	O8-C8-C9-O9
2	Q	401	SIA	C4-C5-N5-C10

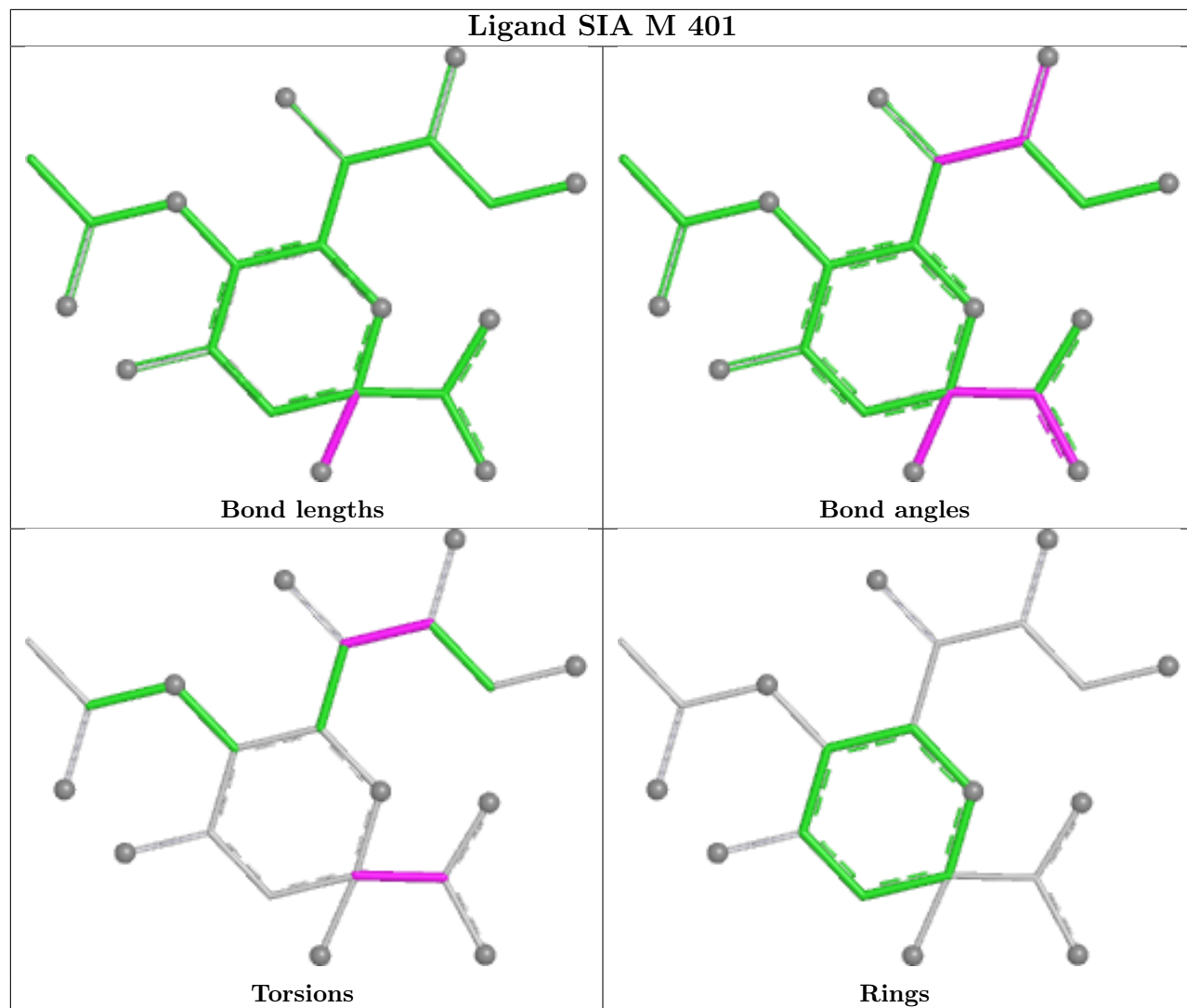
There are no ring outliers.

8 monomers are involved in 9 short contacts:

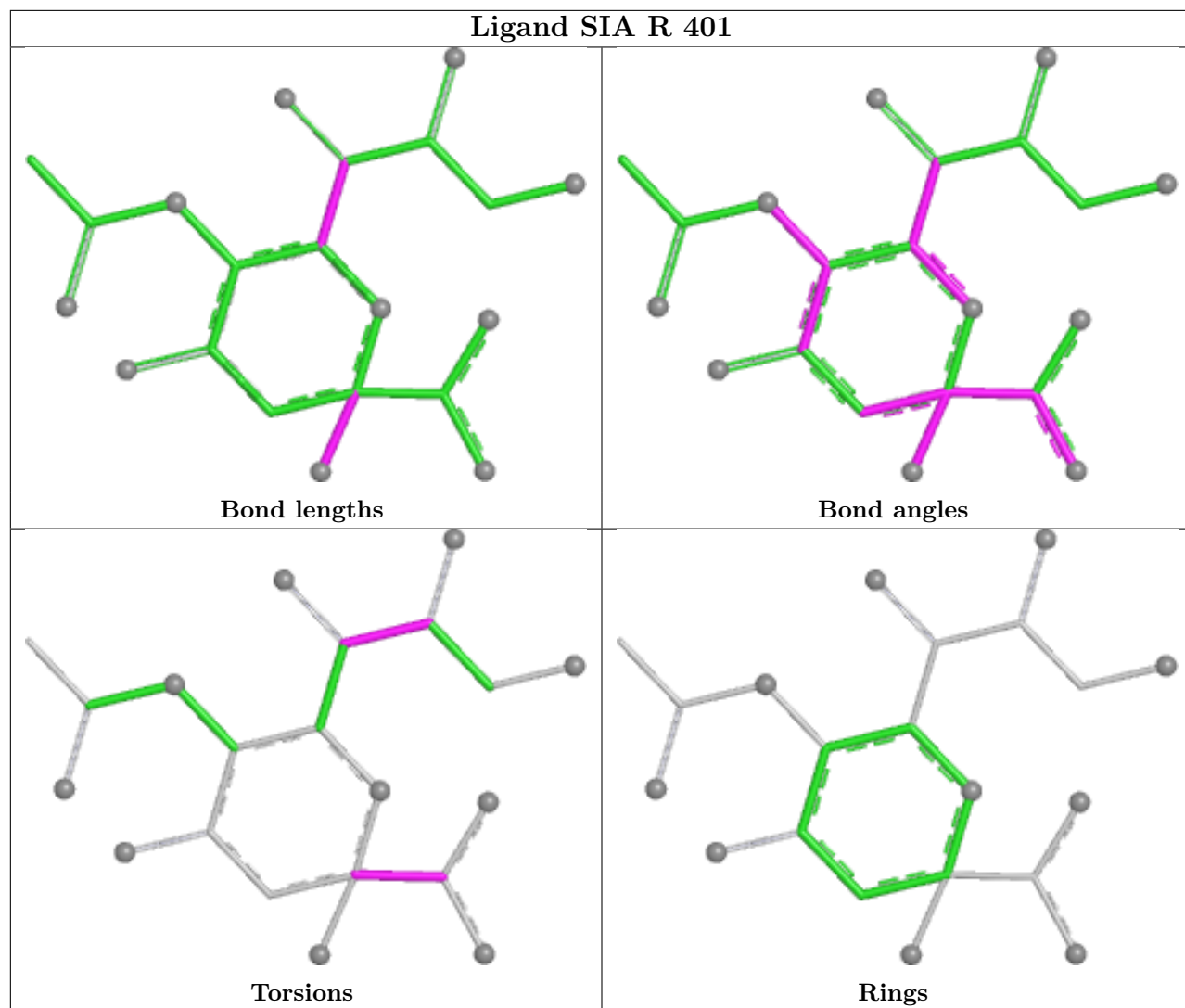
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	401	SIA	1	0
2	F	401	SIA	2	0
2	B	401	SIA	1	0
2	G	401	SIA	1	0
2	A	401	SIA	1	0
2	X	401	SIA	1	0
2	J	401	SIA	1	0
2	c	401	SIA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

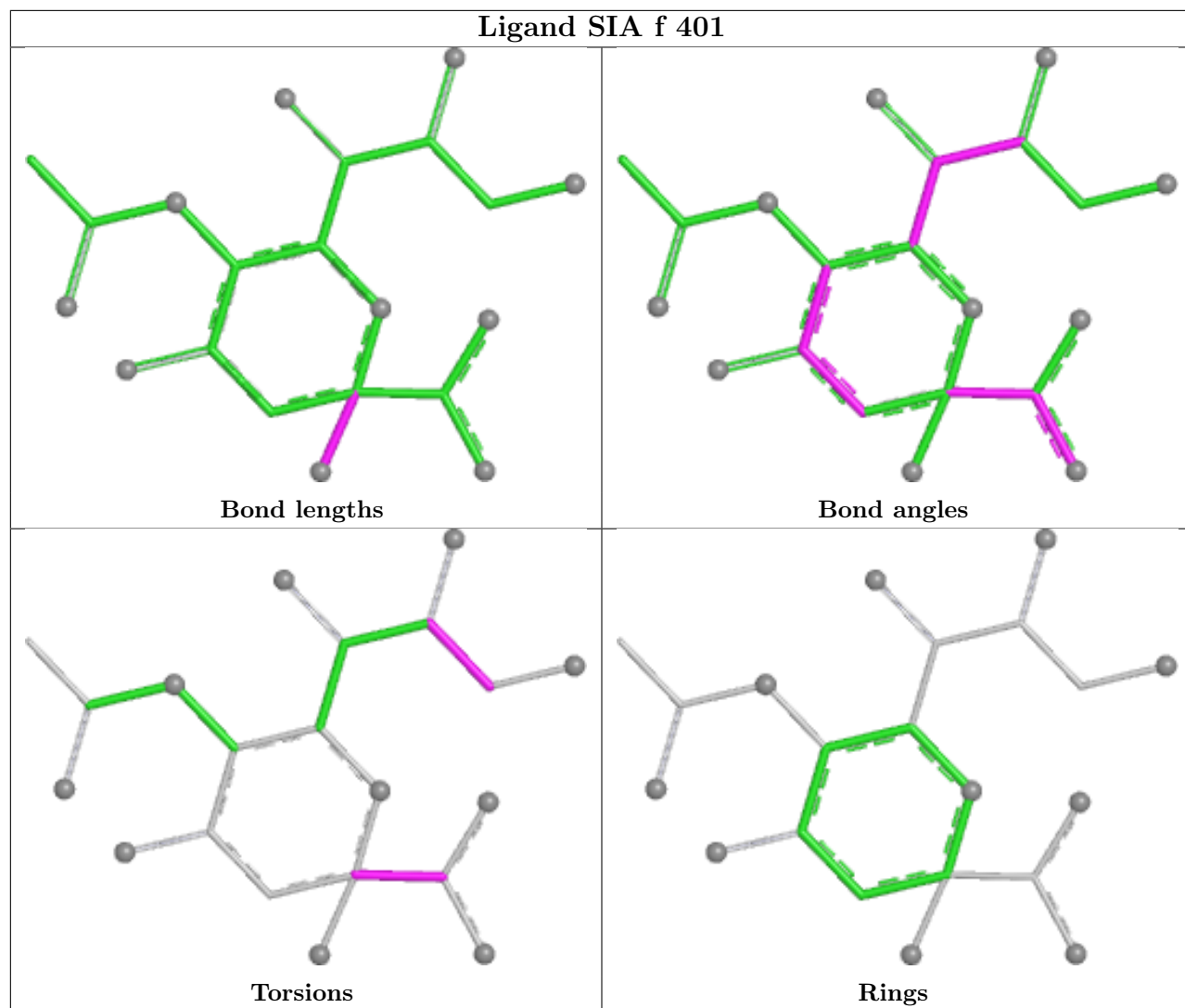
equivalents in the CSD to analyse the geometry.



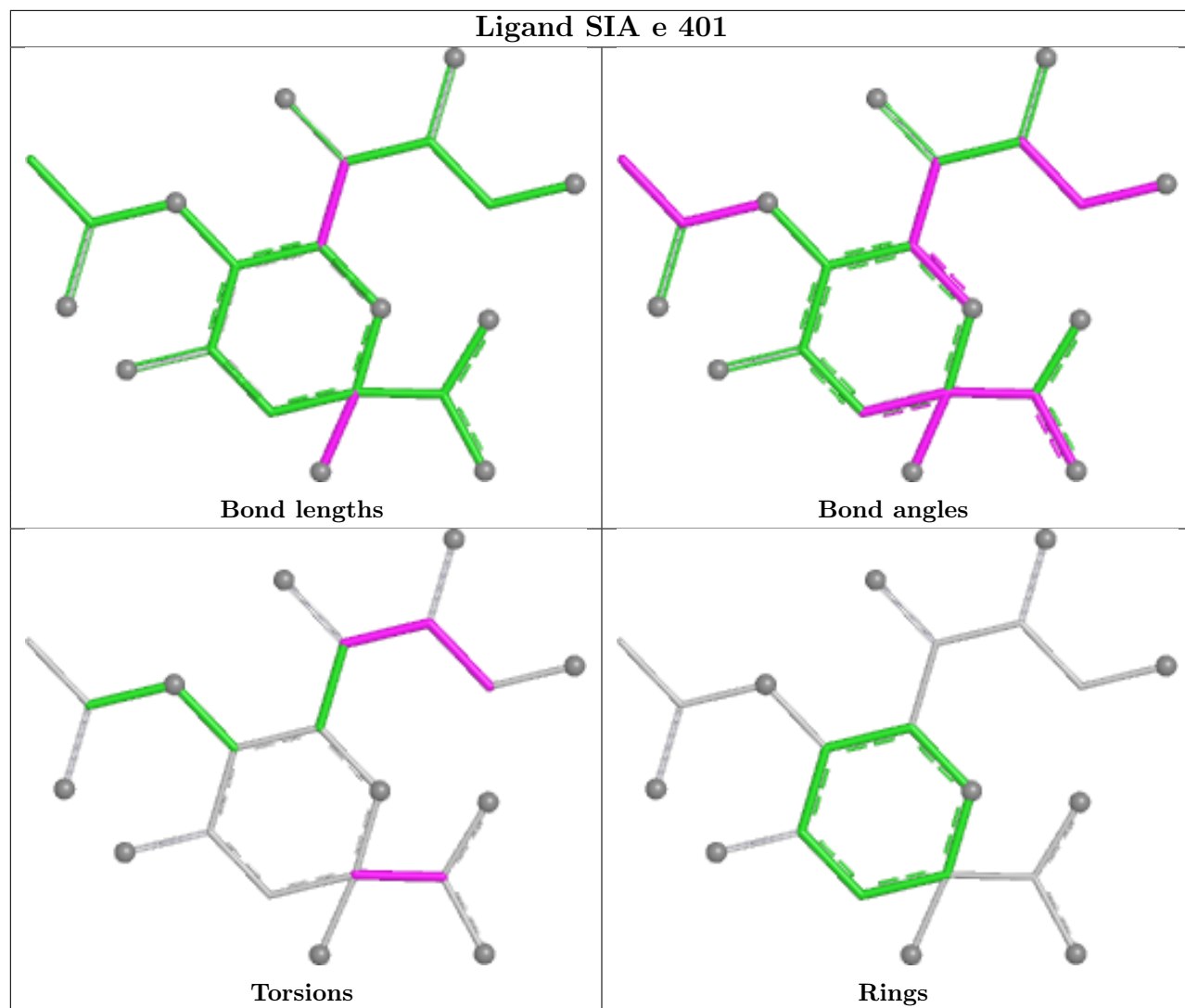
Ligand SIA R 401



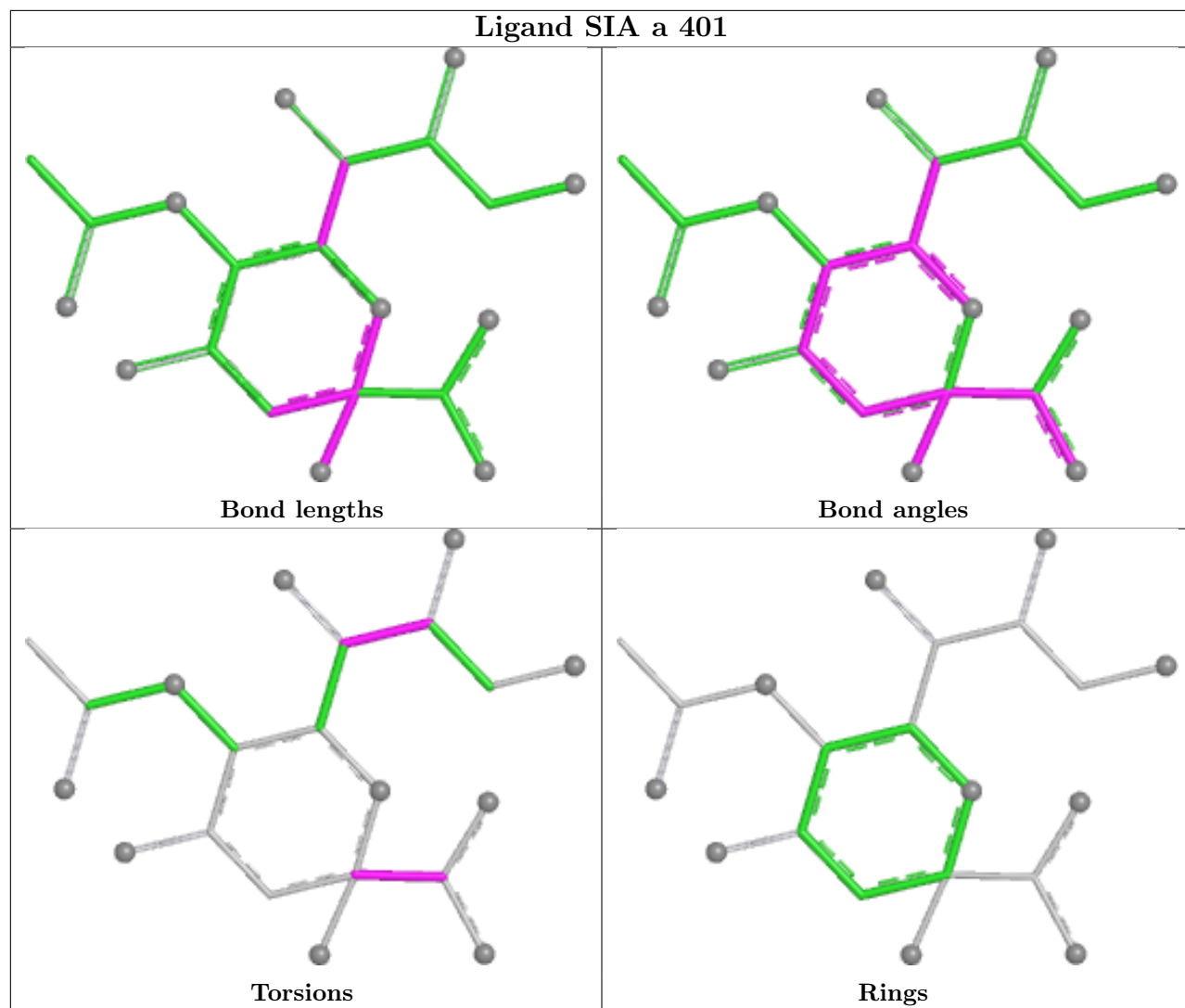
Ligand SIA f 401



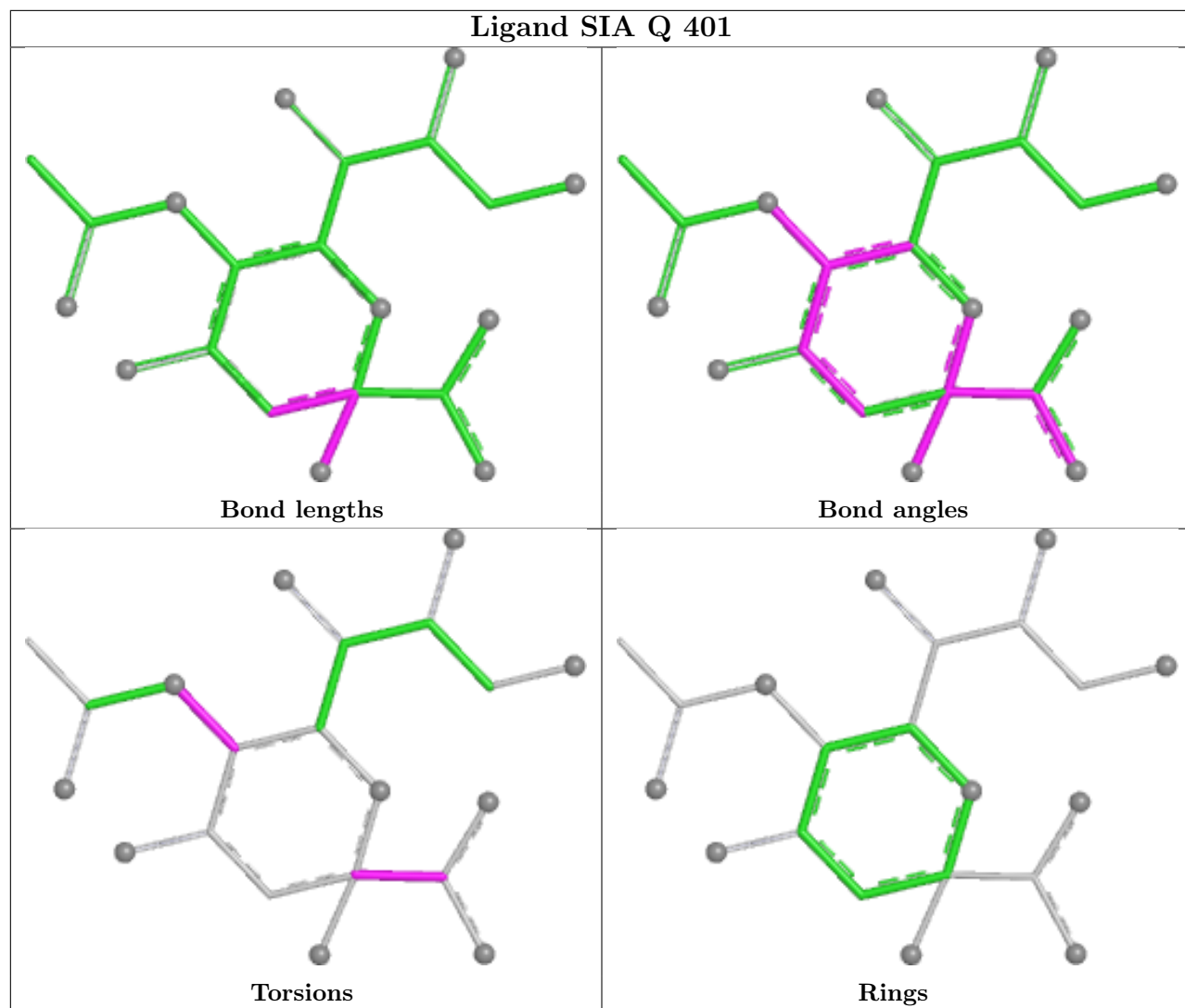
Ligand SIA e 401



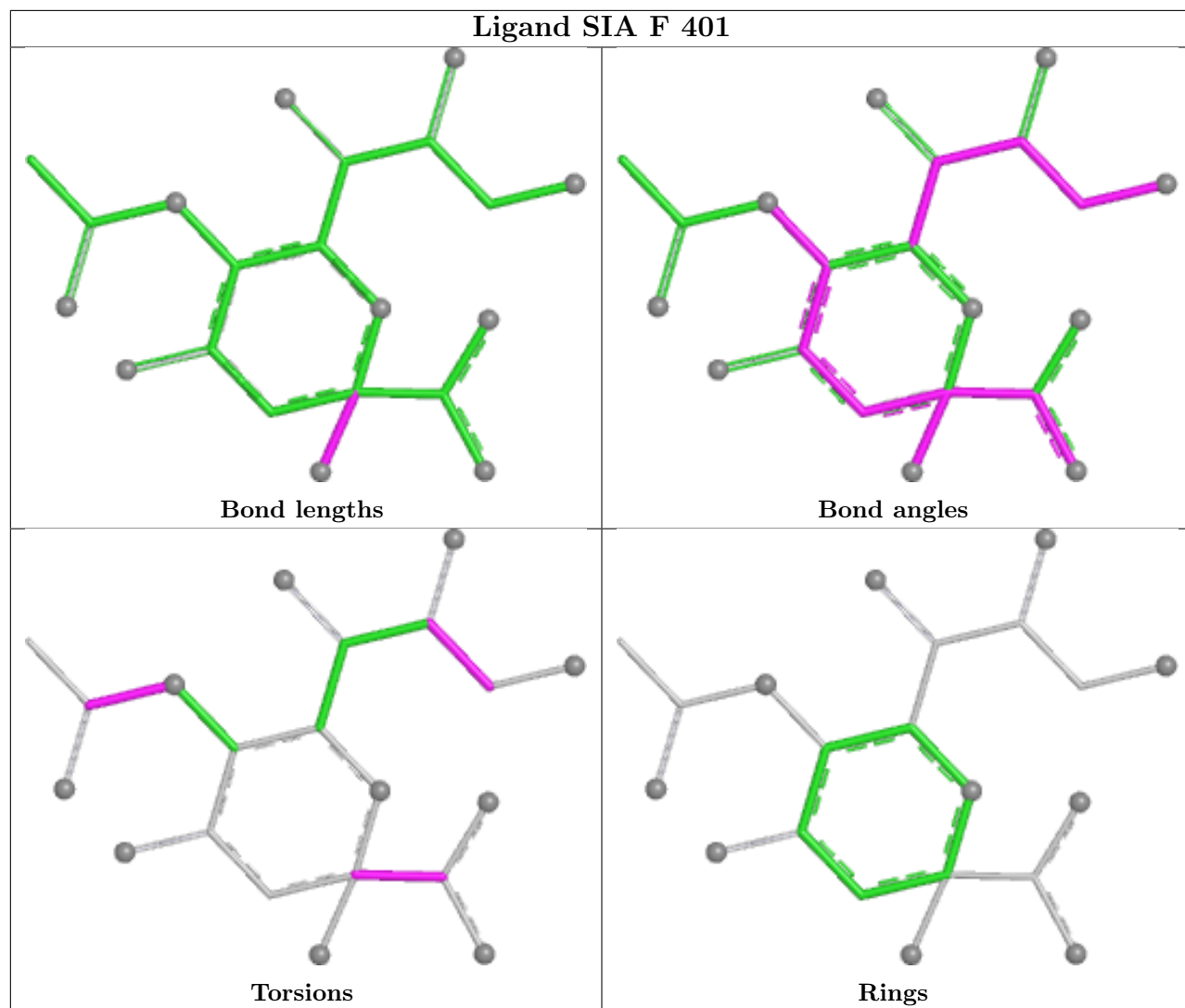
Ligand SIA a 401



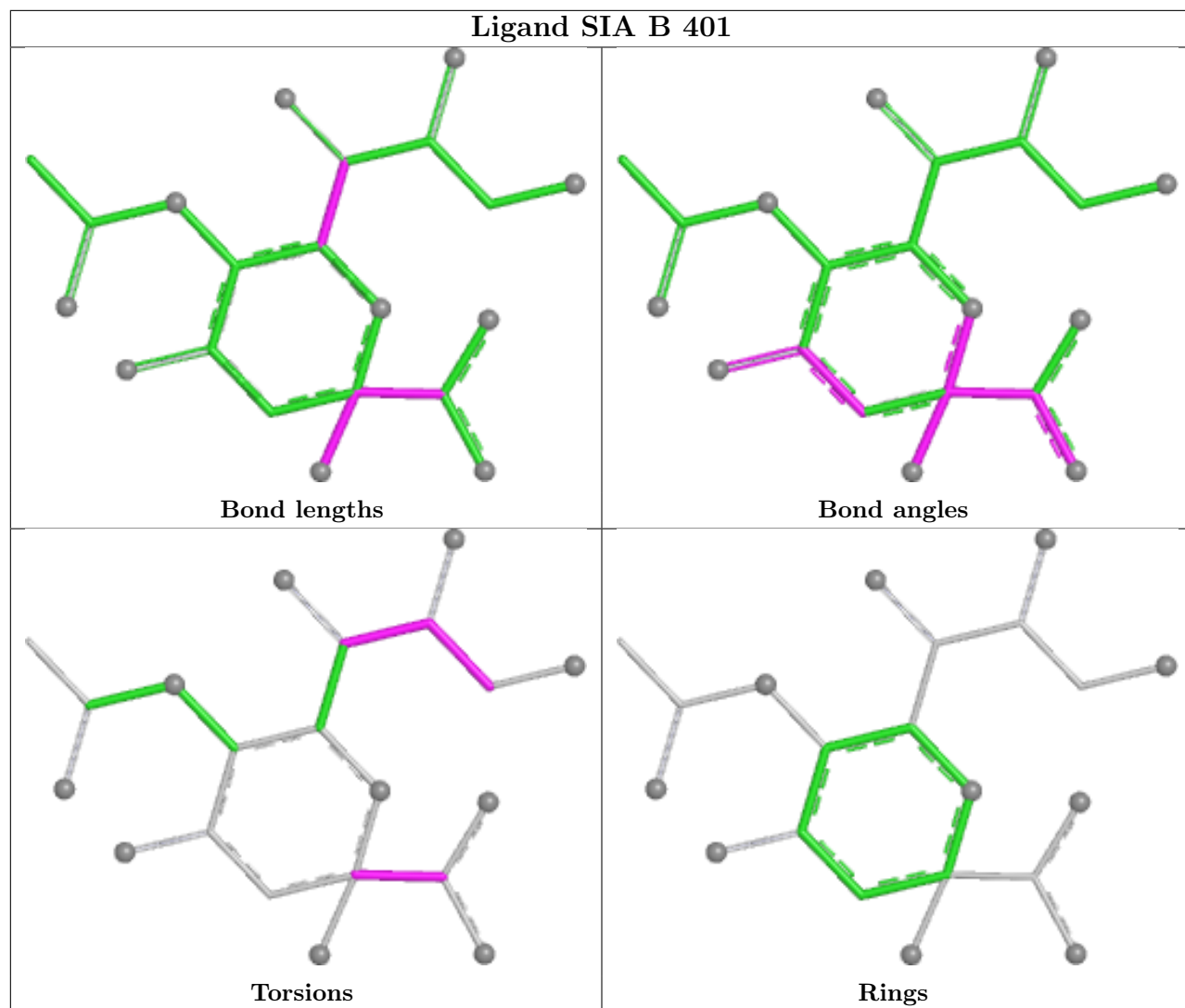
Ligand SIA Q 401



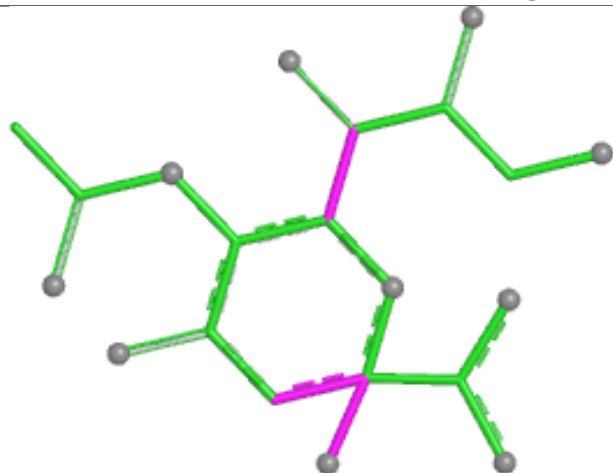
Ligand SIA F 401



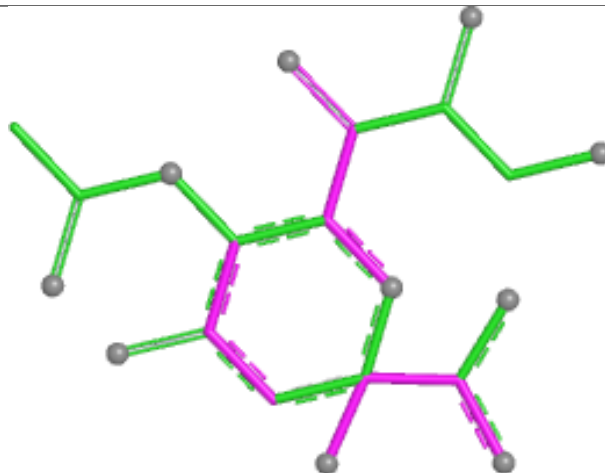
Ligand SIA B 401



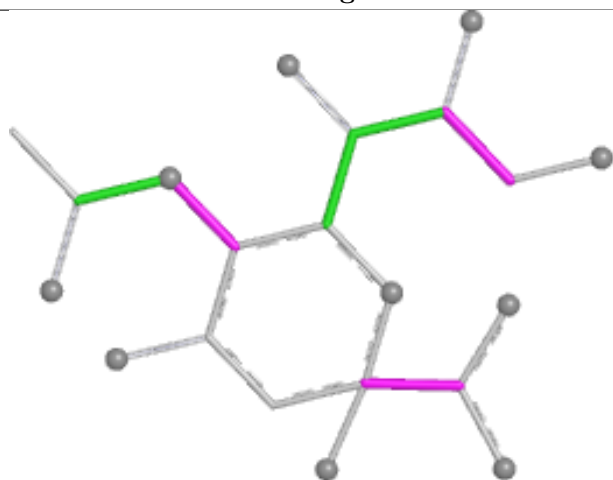
Ligand SIA Z 401



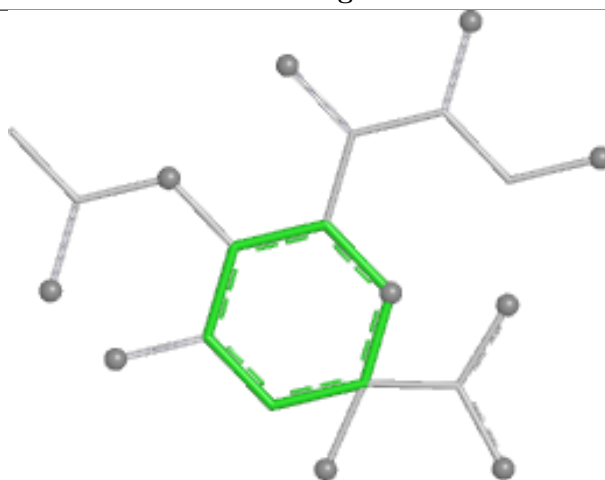
Bond lengths



Bond angles

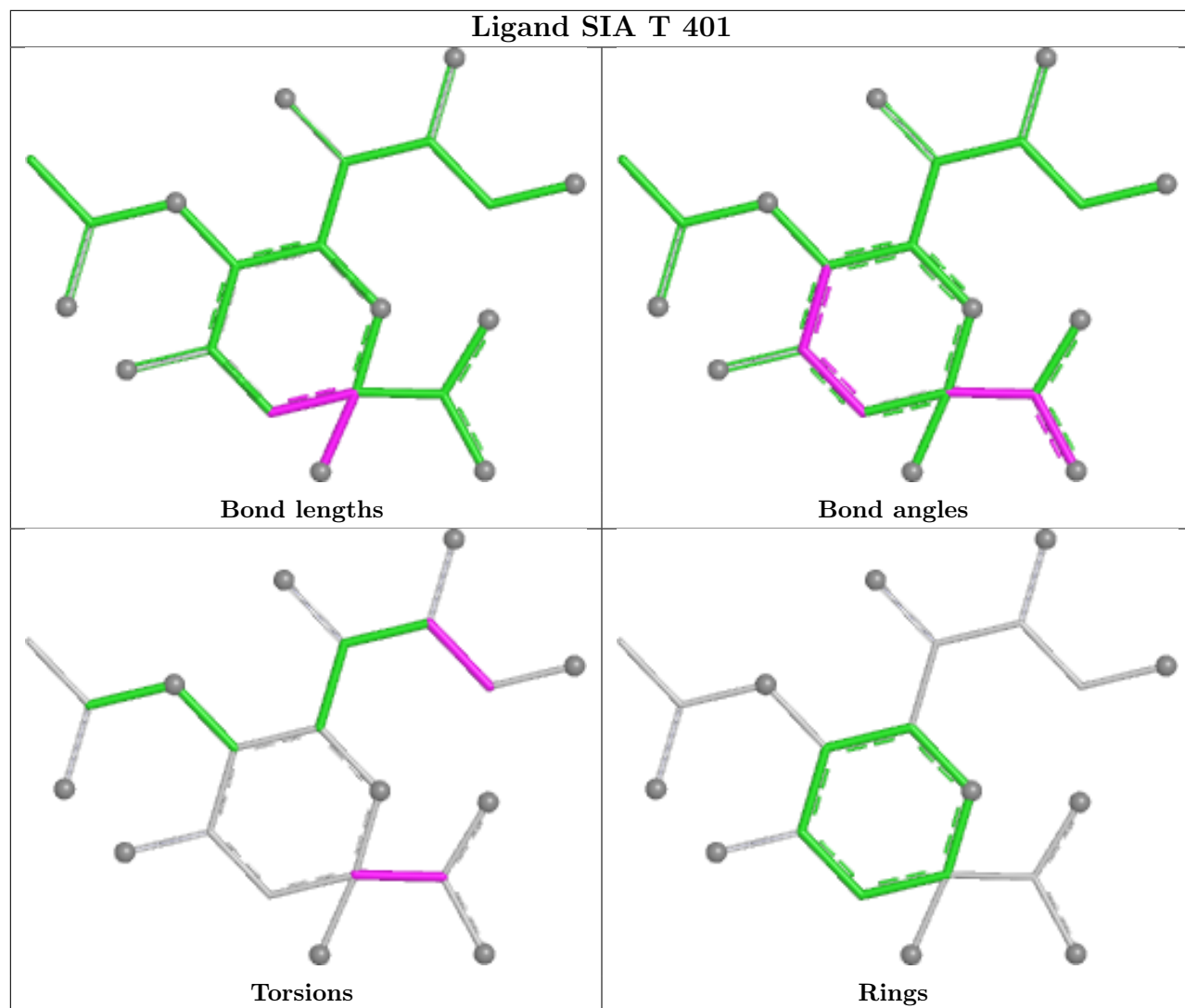


Torsions

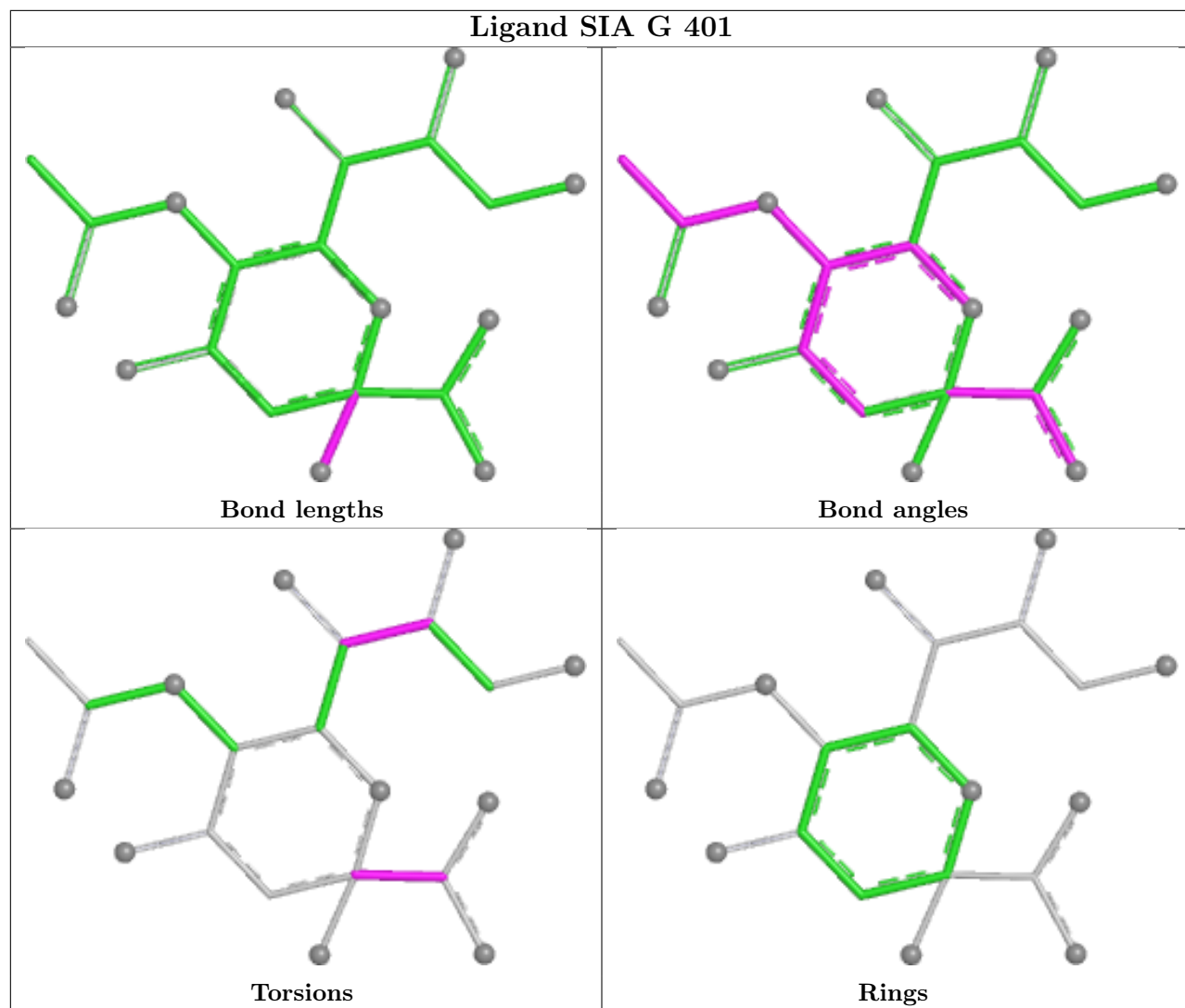


Rings

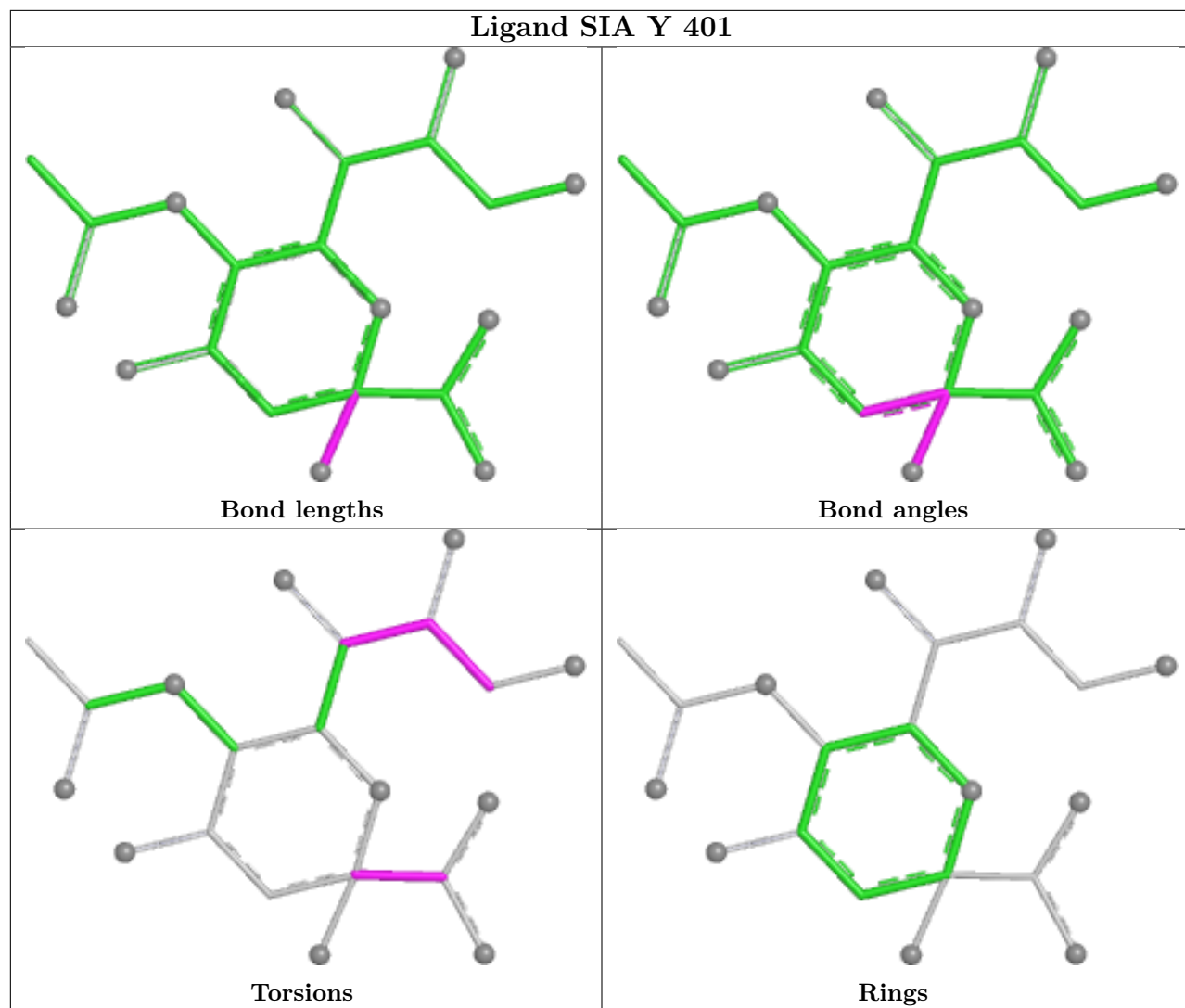
Ligand SIA T 401



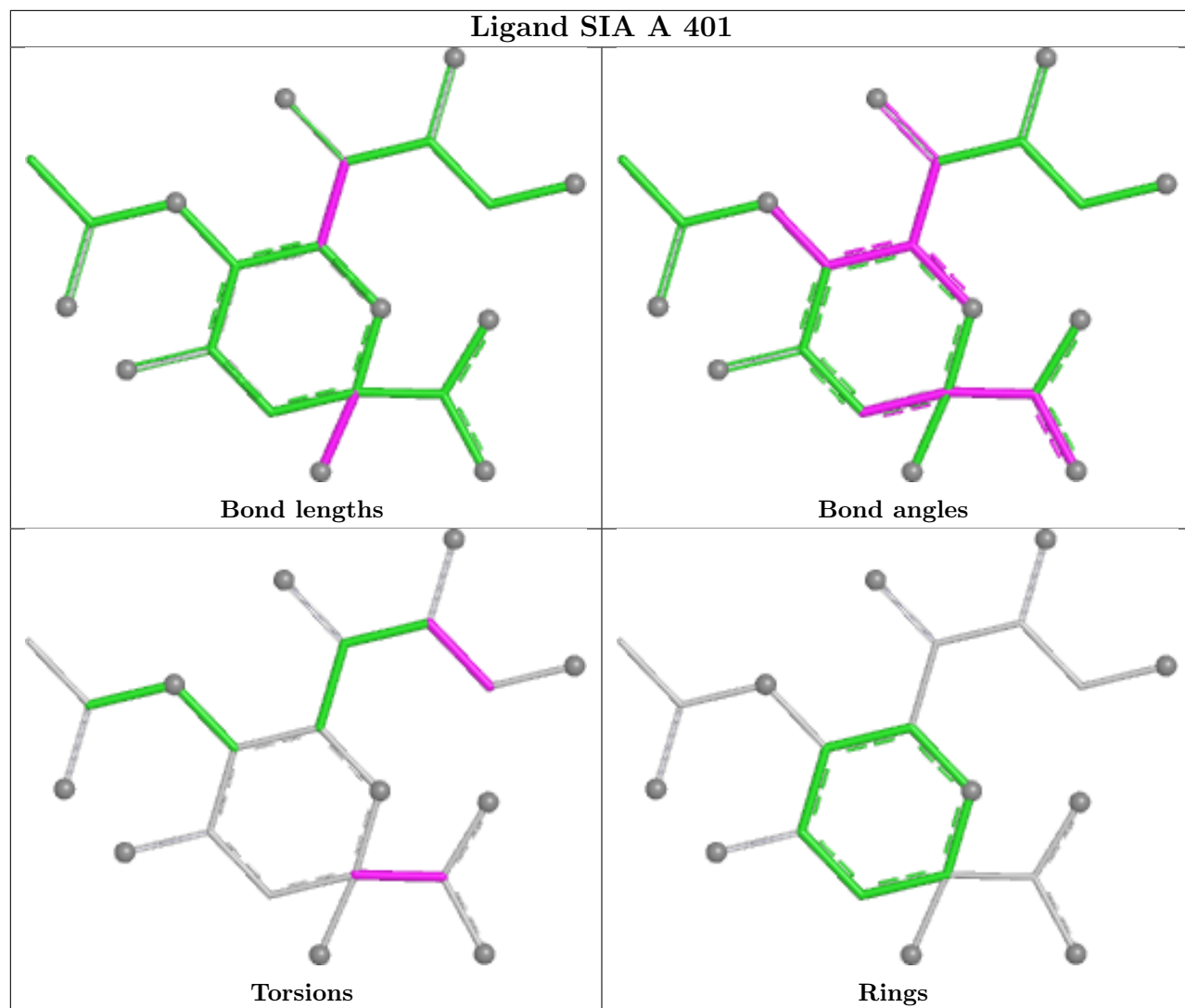
Ligand SIA G 401



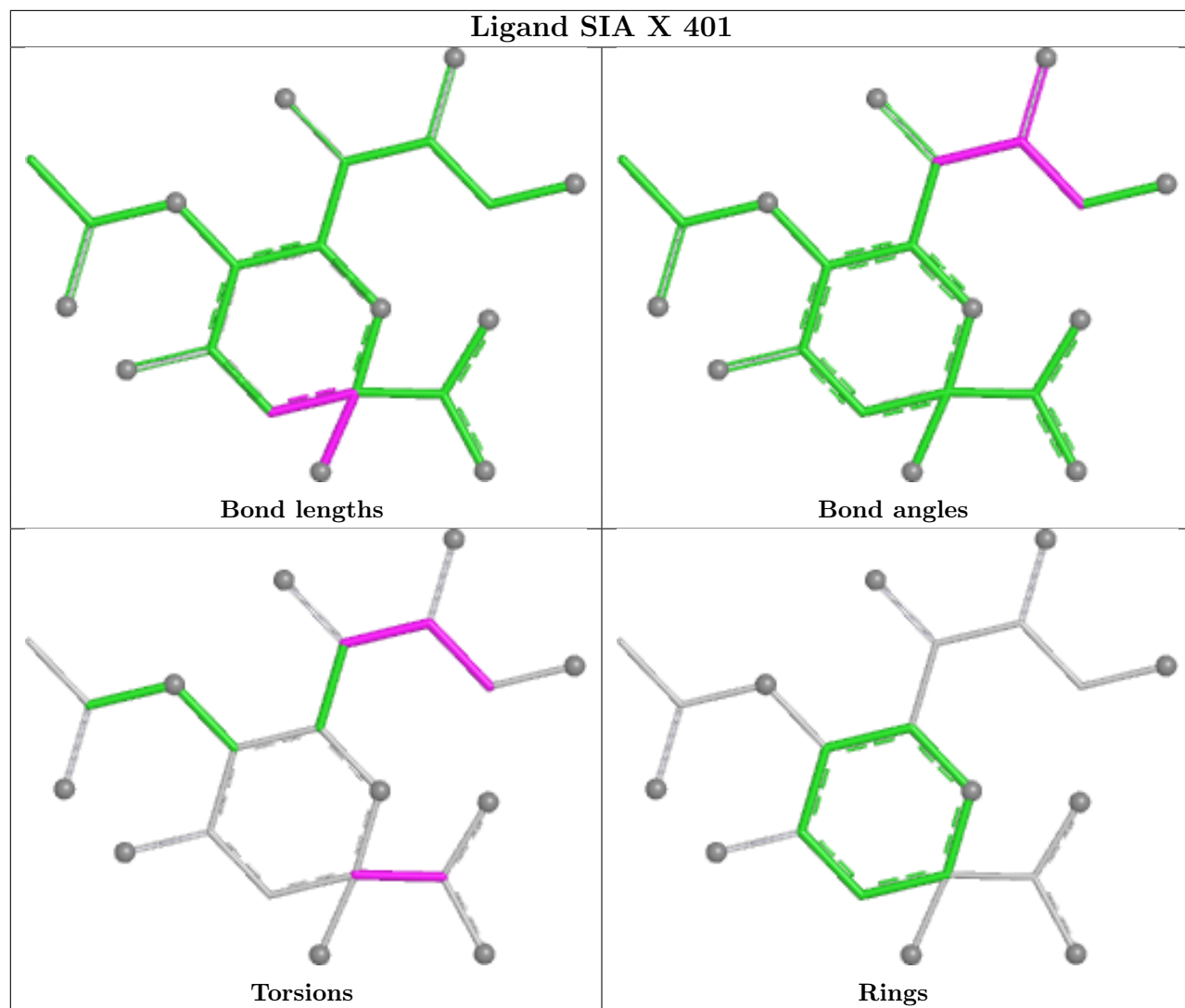
Ligand SIA Y 401



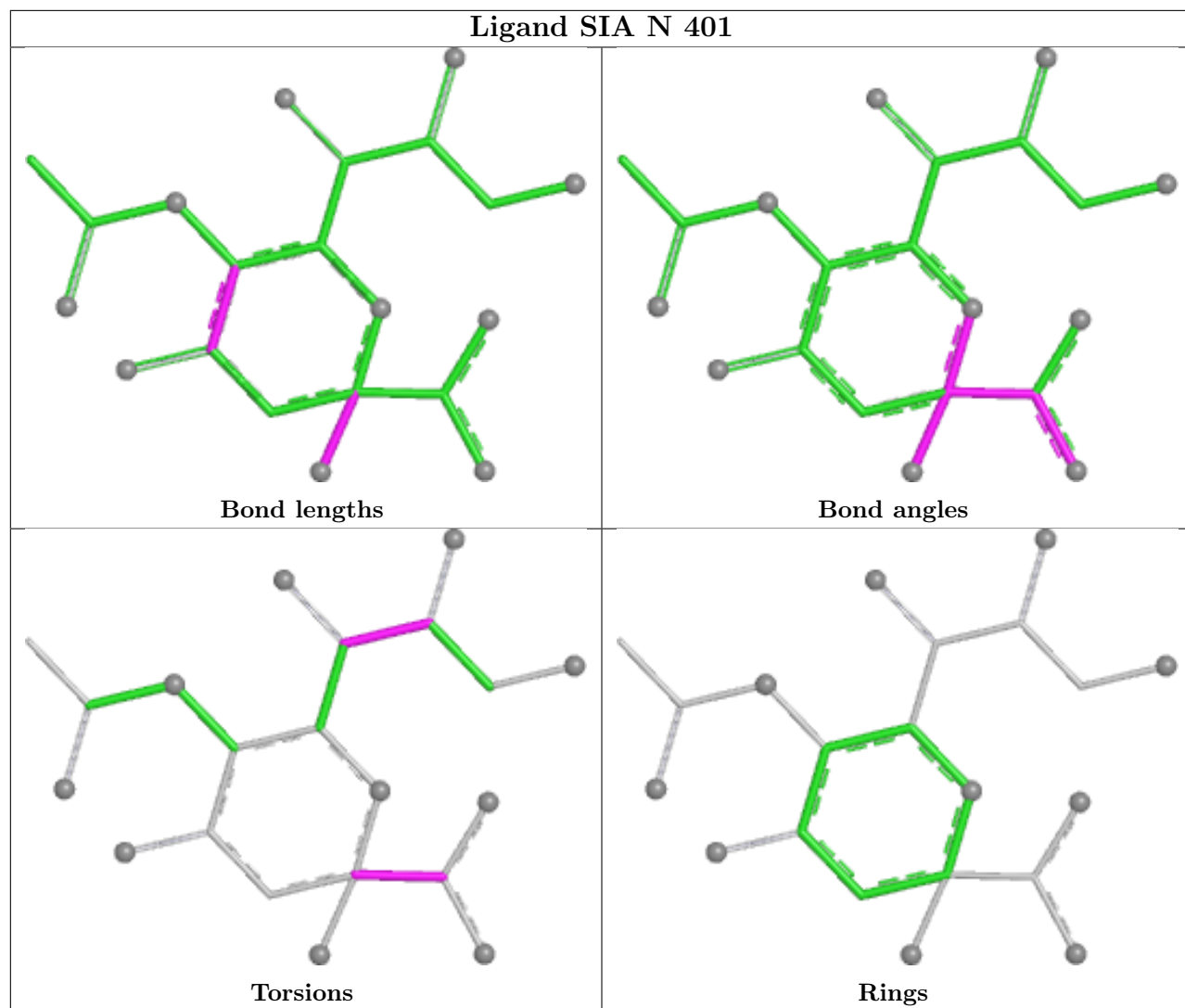
Ligand SIA A 401



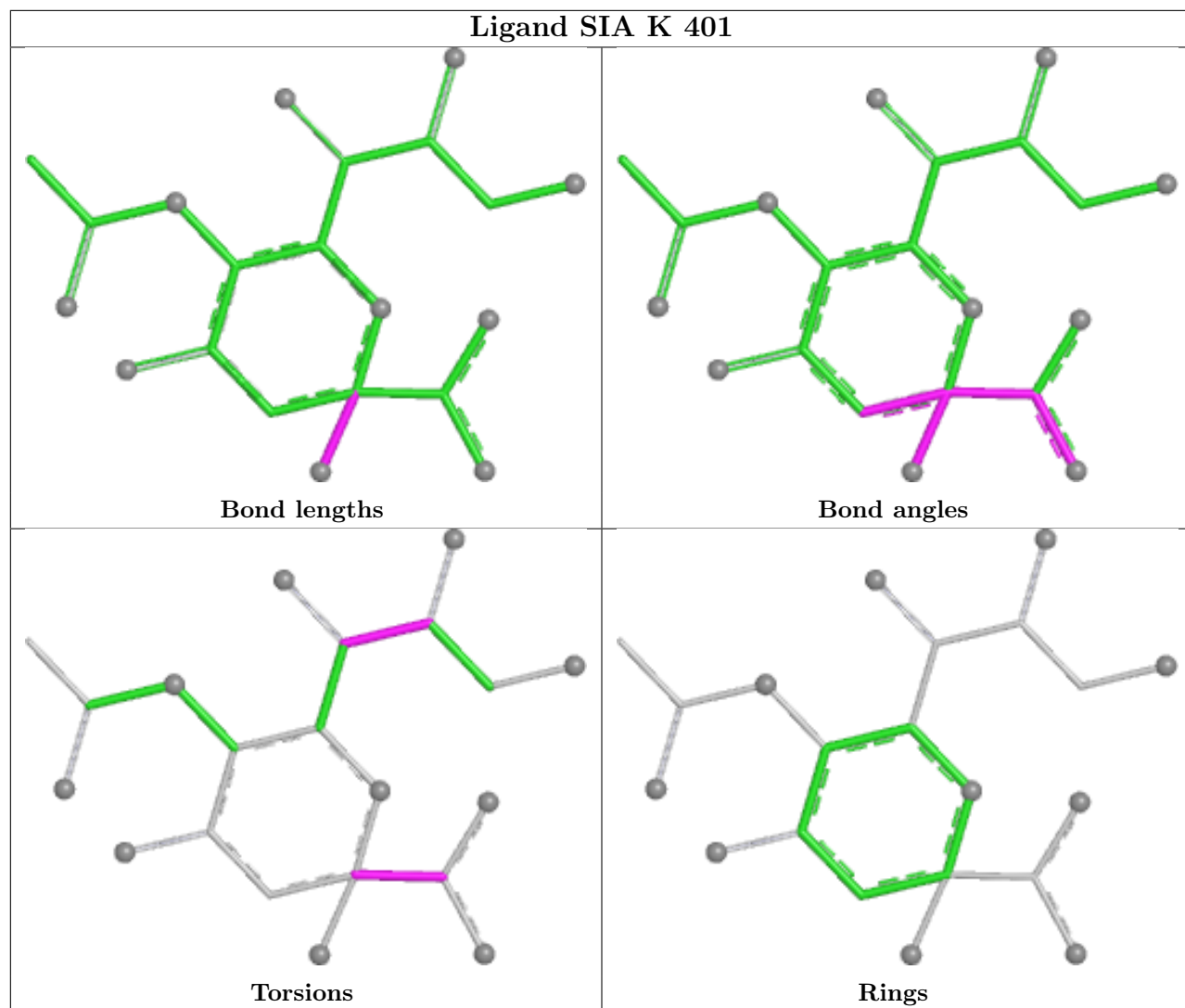
Ligand SIA X 401



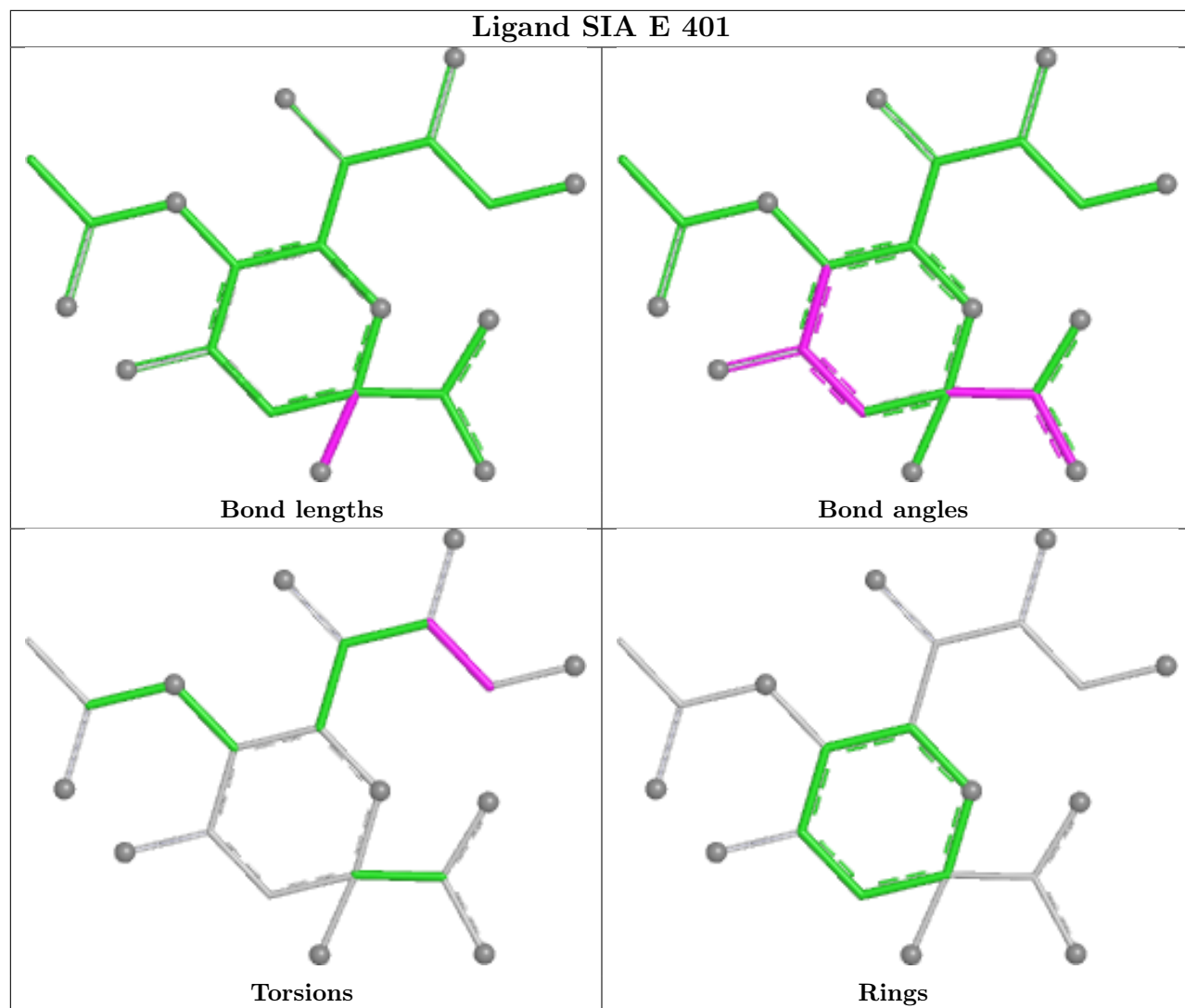
Ligand SIA N 401



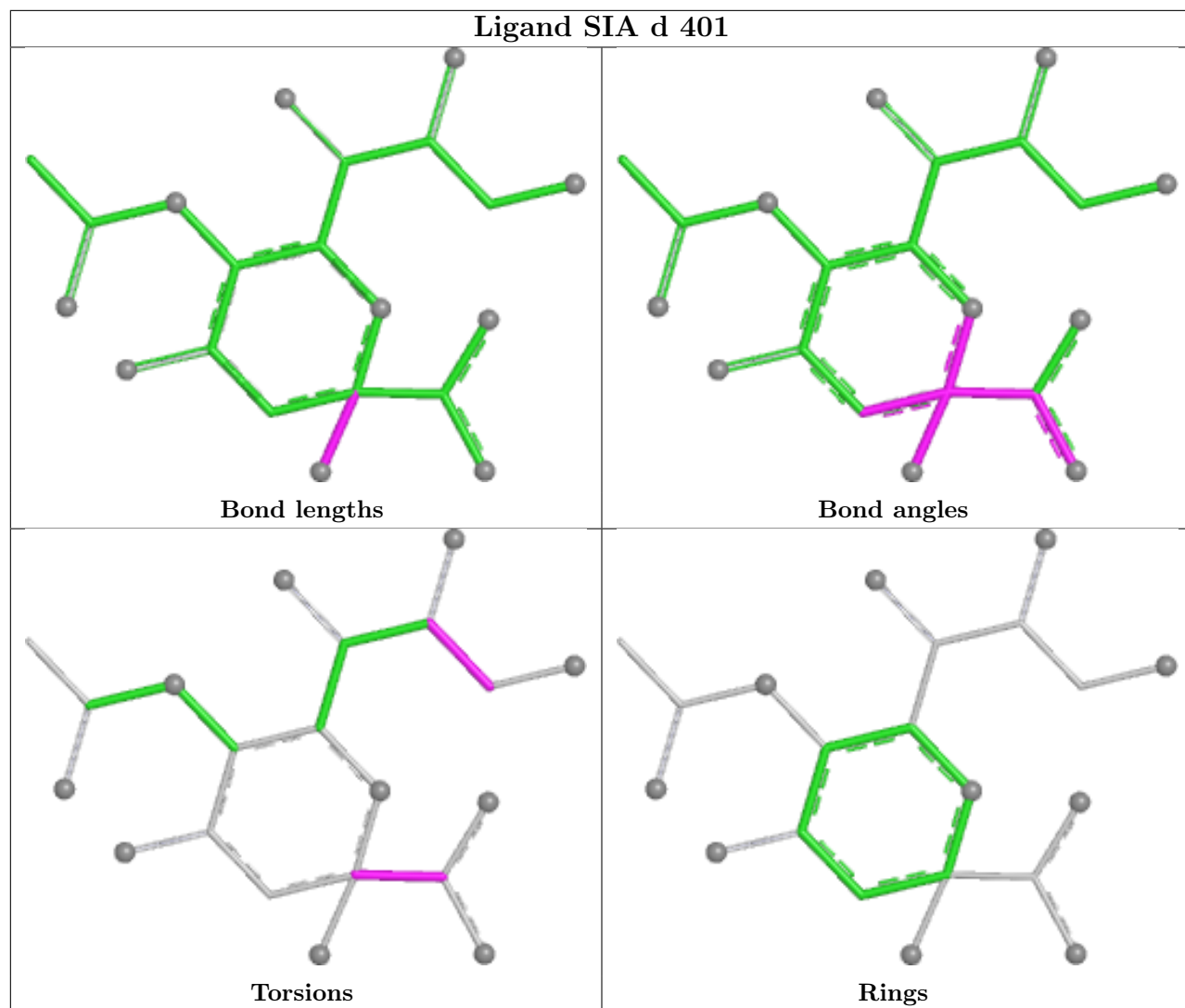
Ligand SIA K 401



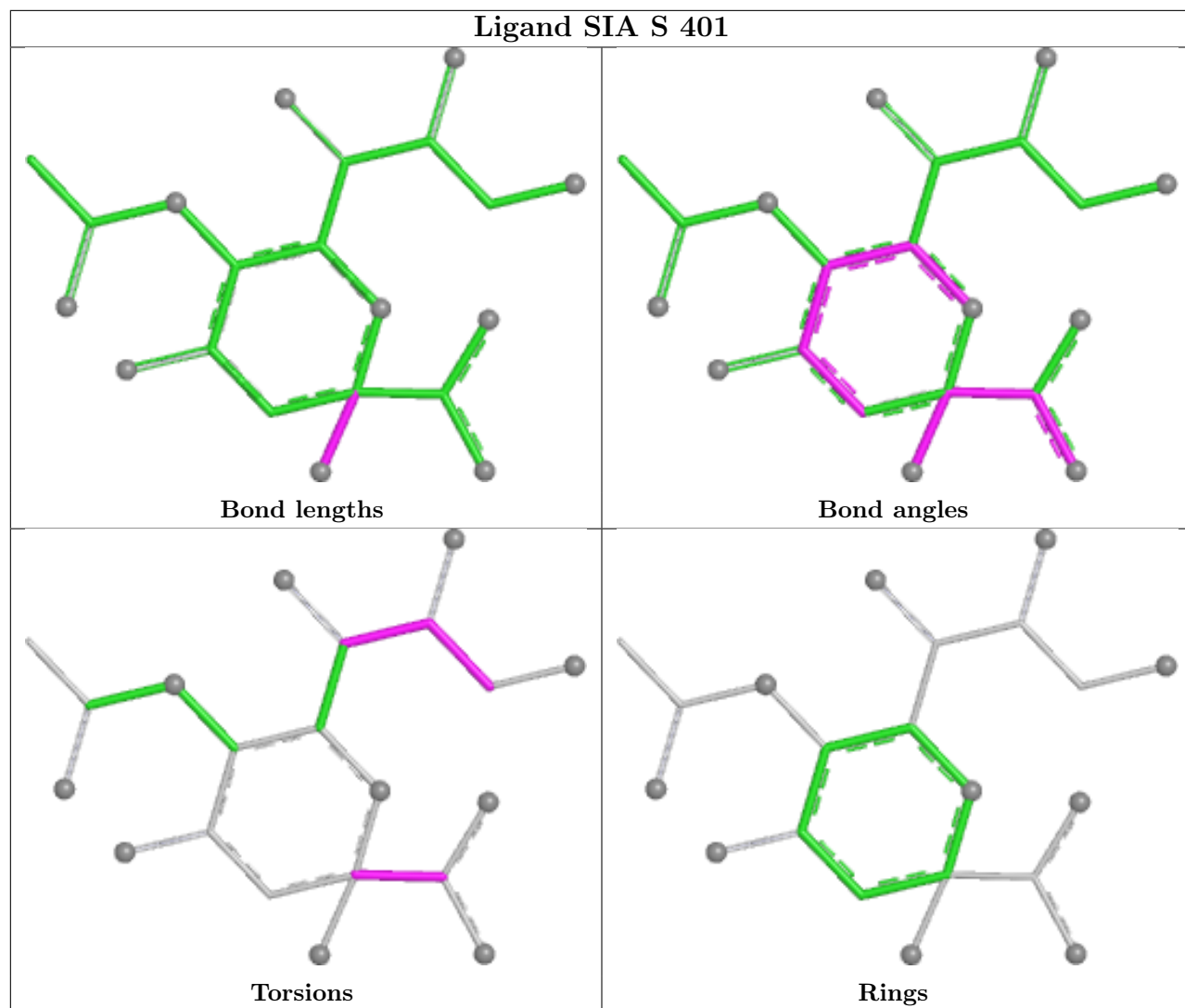
Ligand SIA E 401



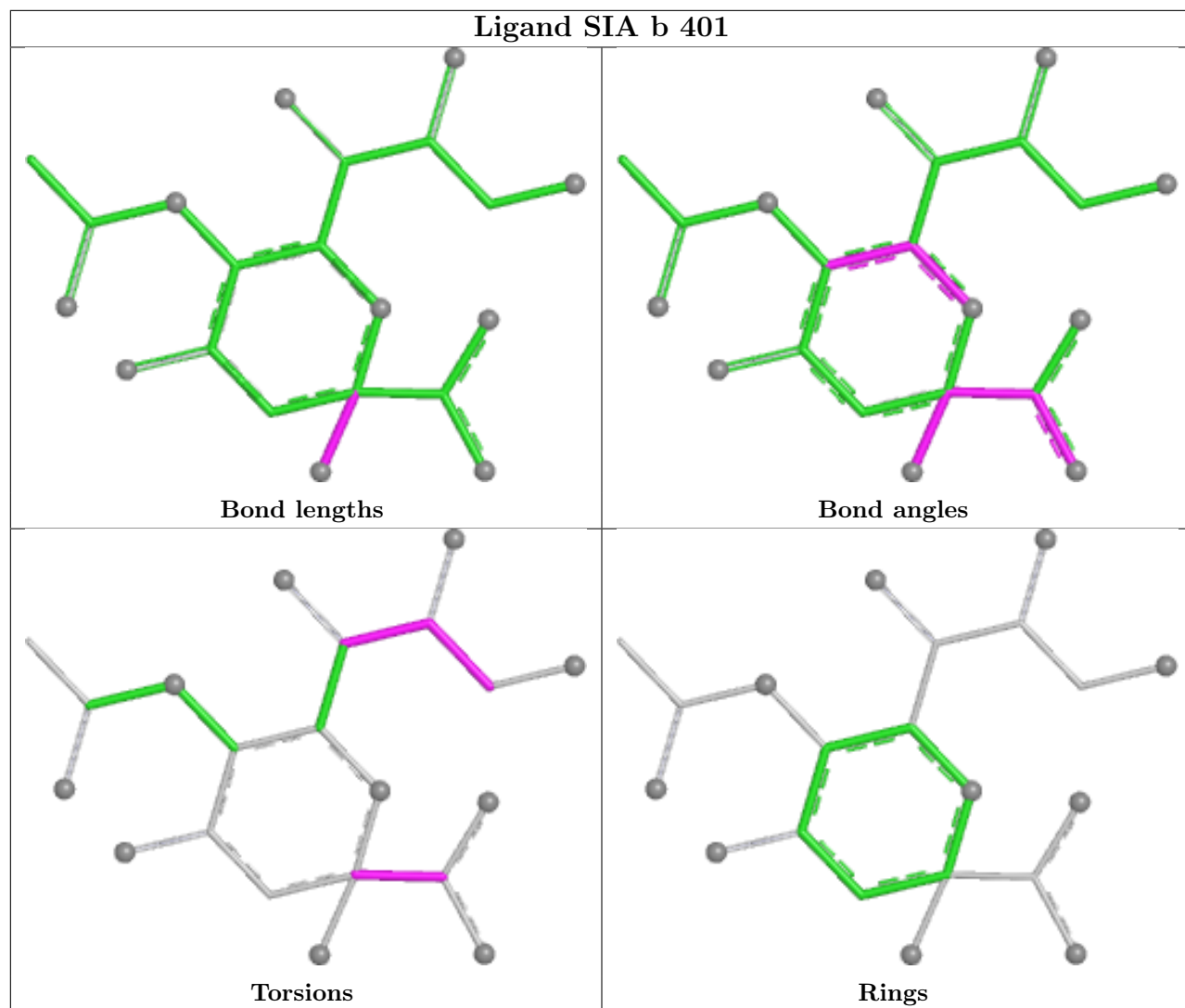
Ligand SIA d 401



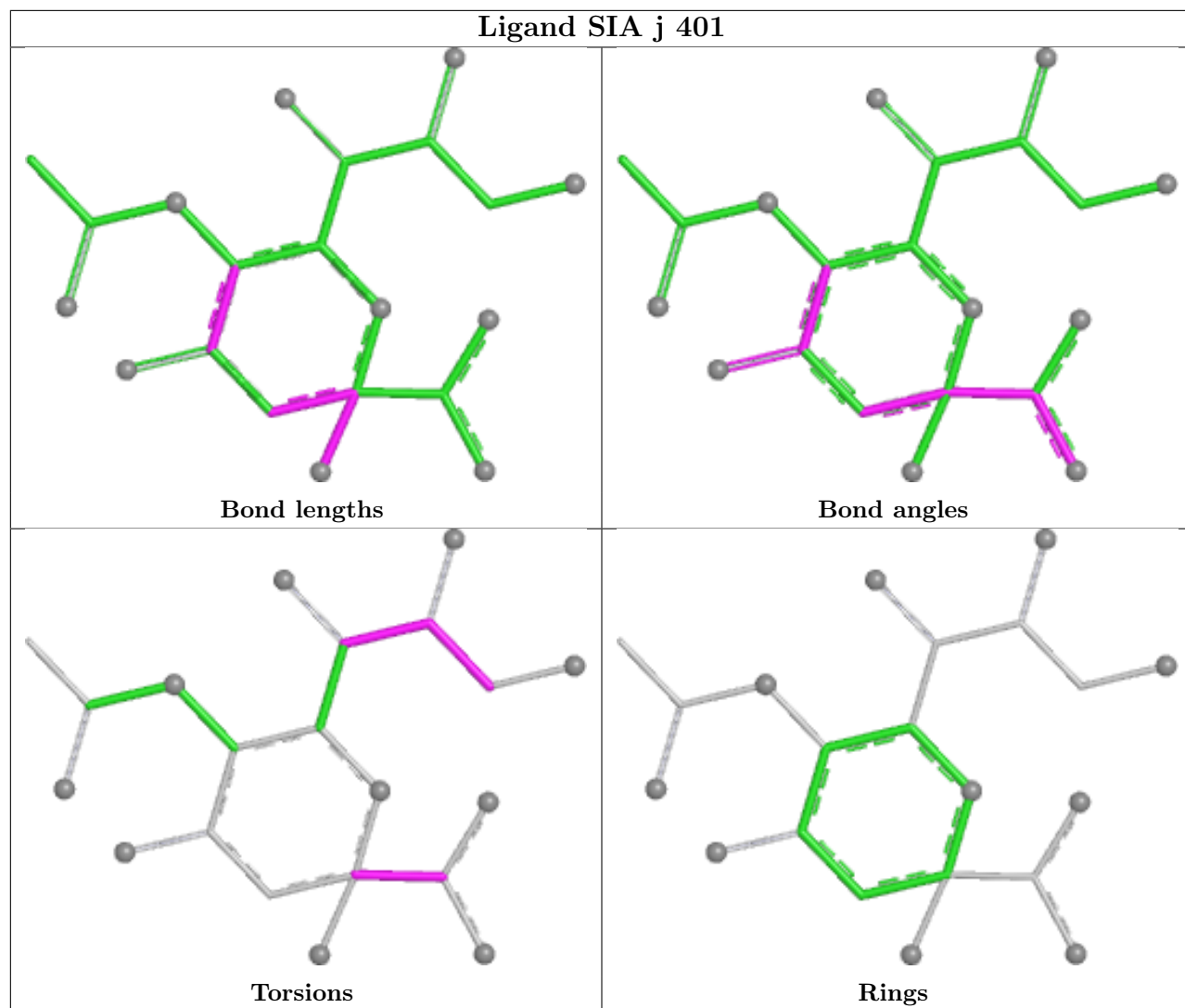
Ligand SIA S 401



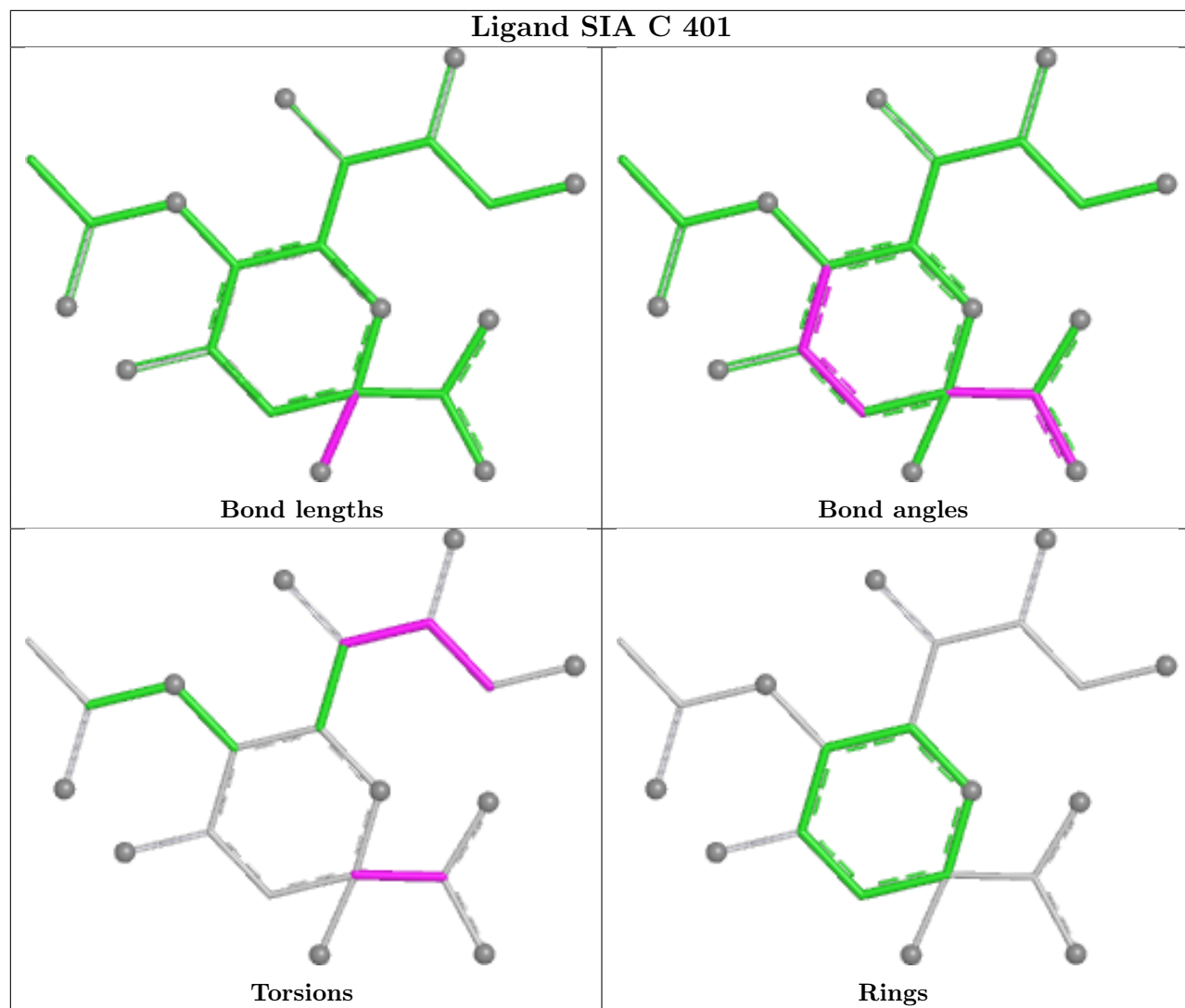
Ligand SIA b 401



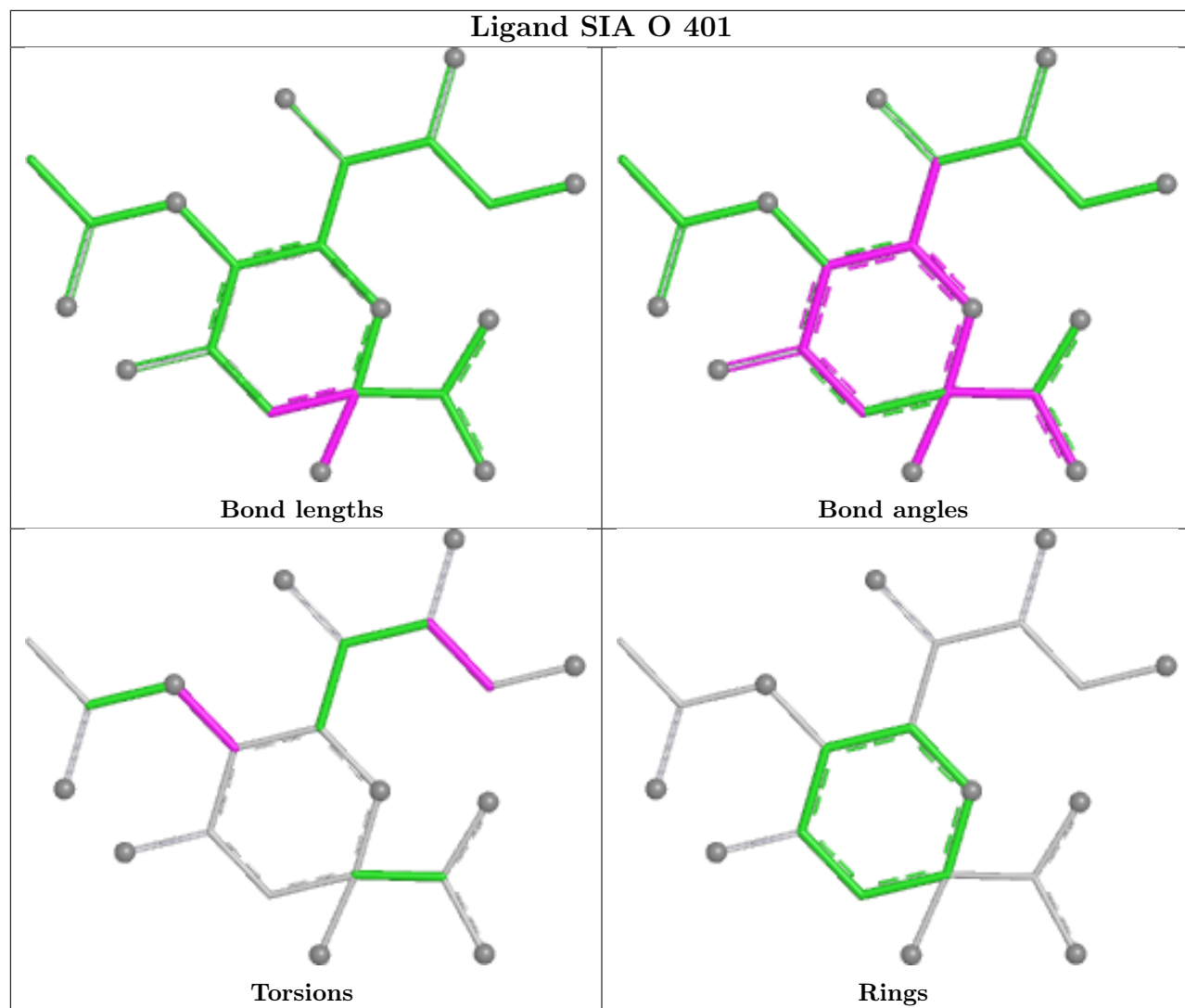
Ligand SIA j 401



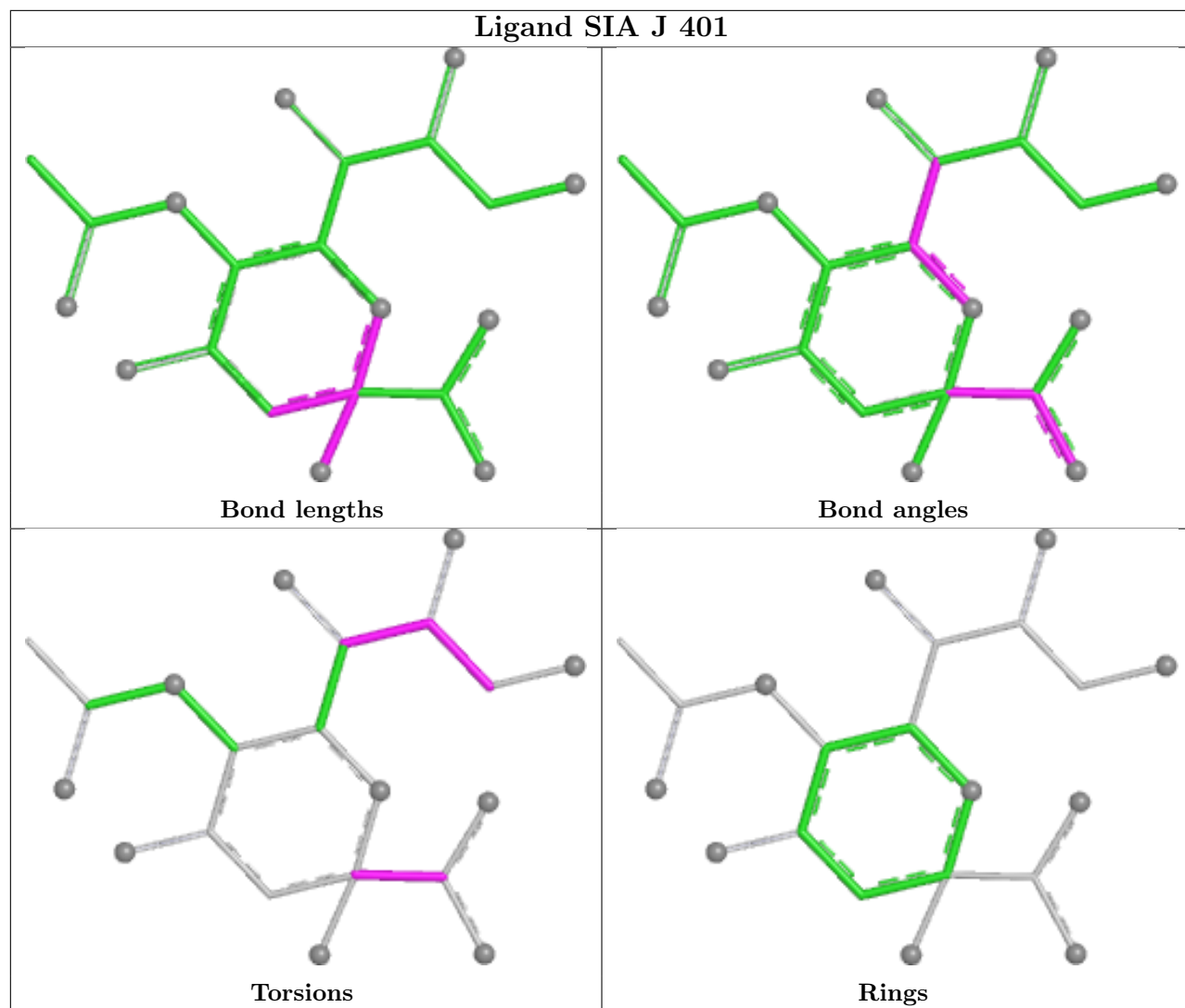
Ligand SIA C 401



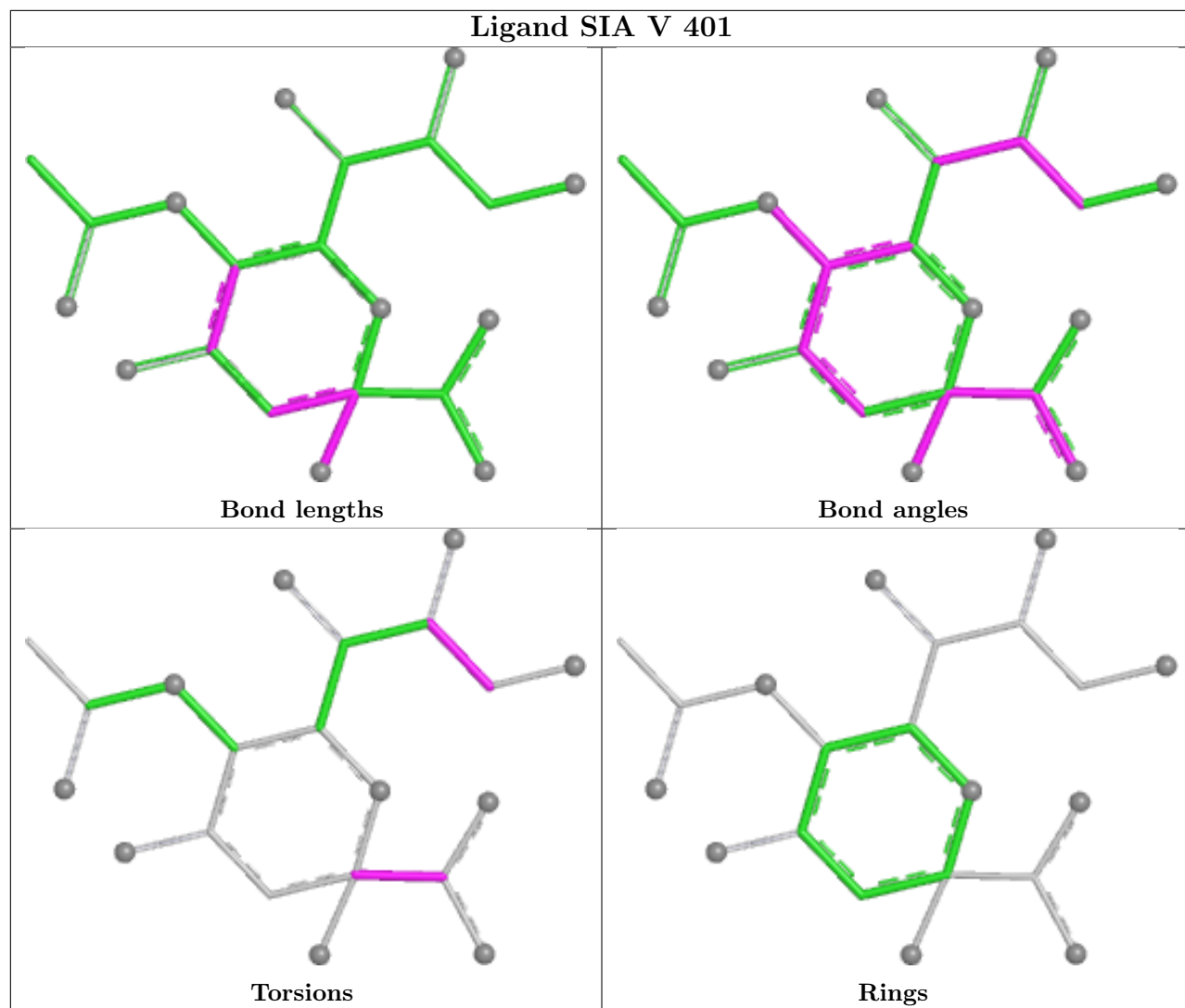
Ligand SIA O 401

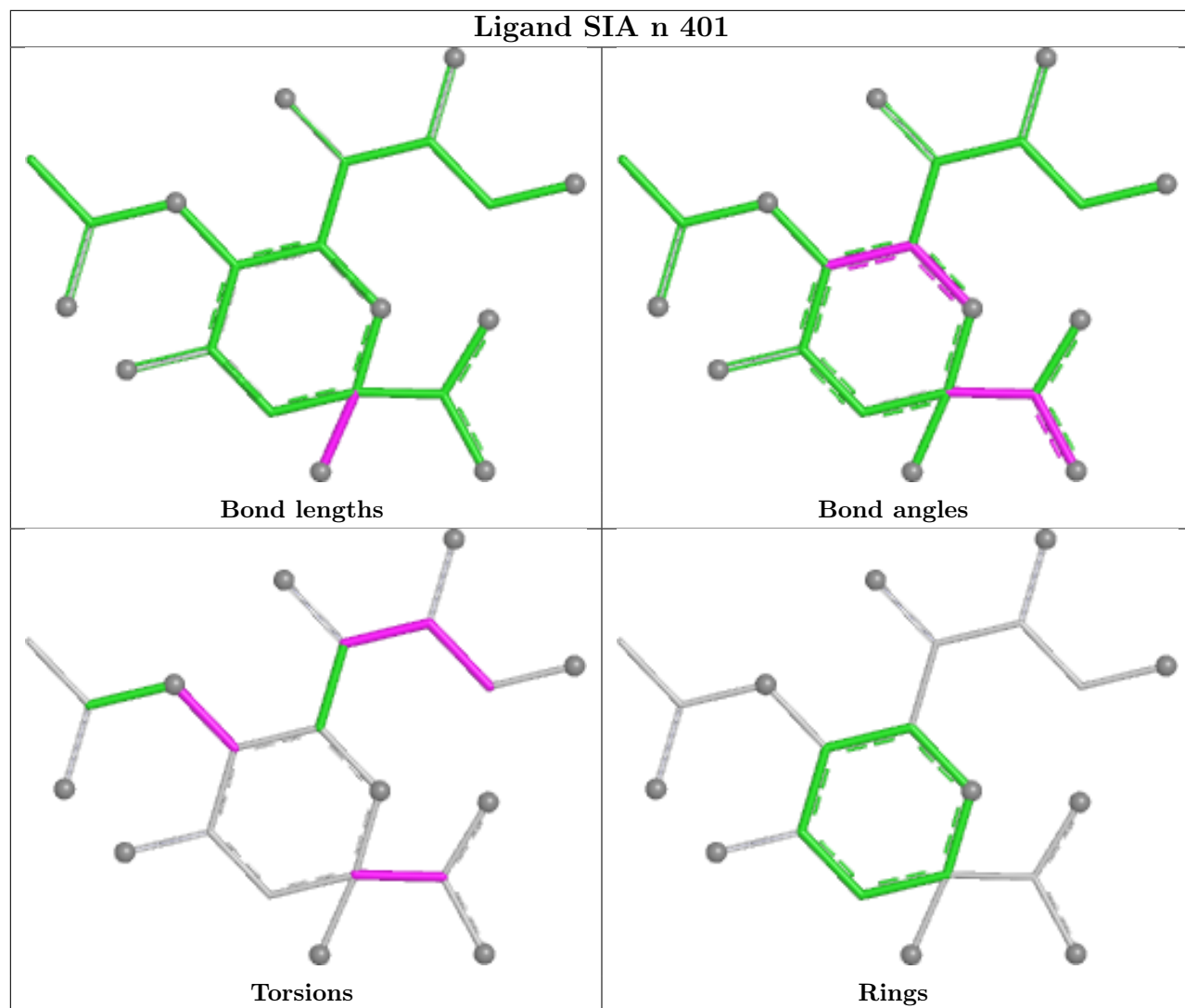


Ligand SIA J 401

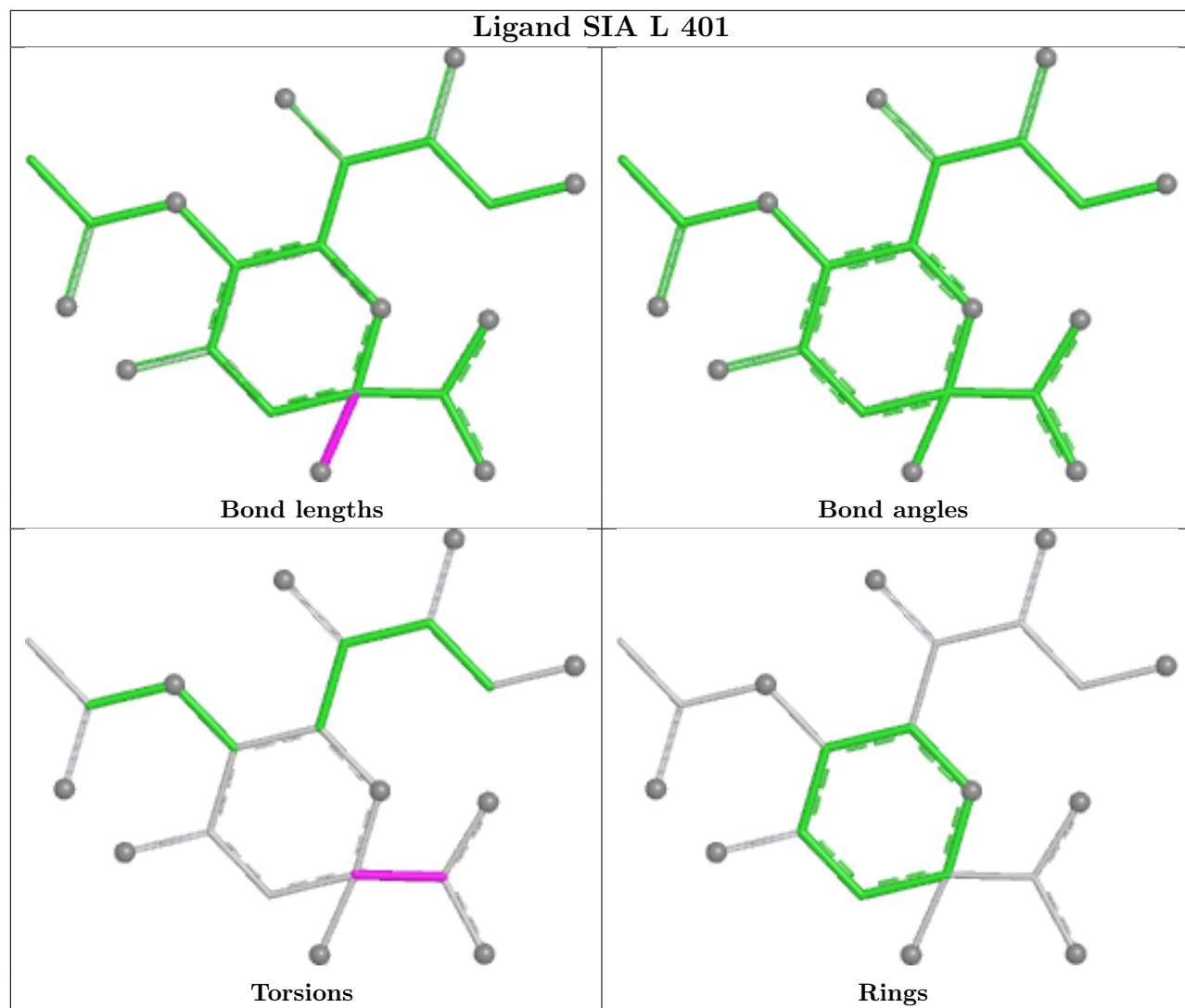


Ligand SIA V 401

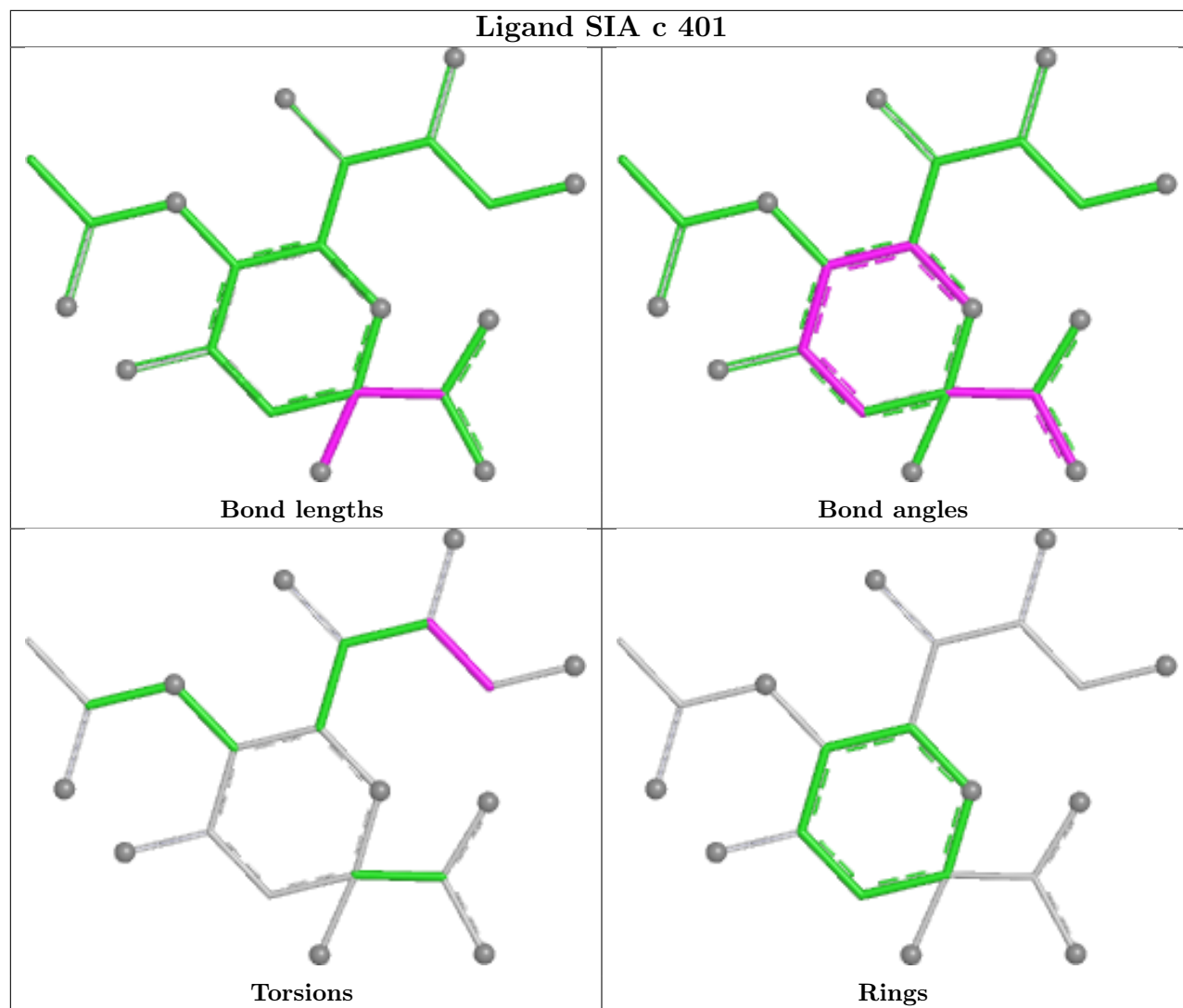


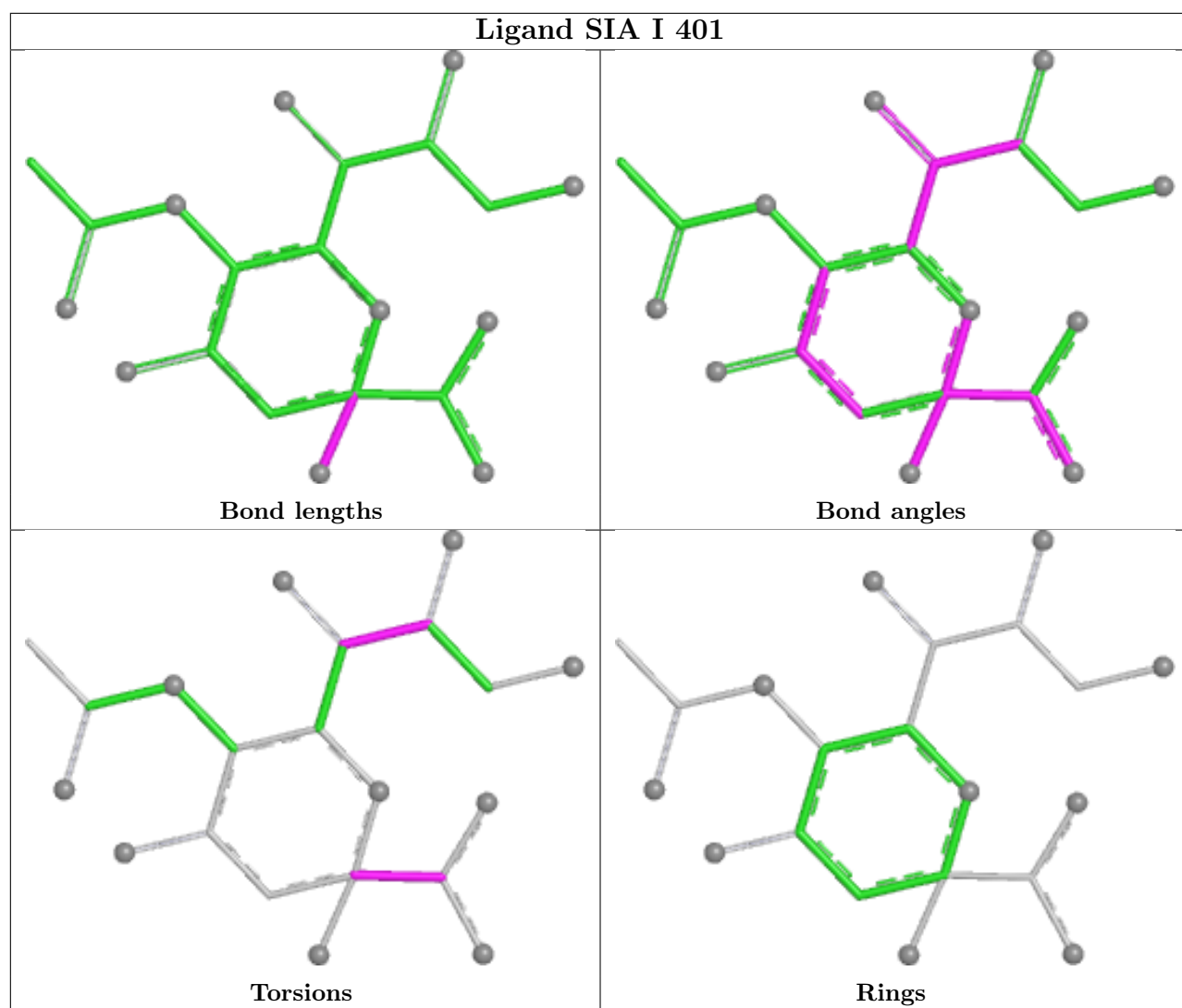


Ligand SIA L 401



Ligand SIA c 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	267/274 (97%)	0.08	3 (1%) 78 75	18, 27, 50, 55	0
1	B	260/274 (94%)	0.01	2 (0%) 82 79	16, 28, 47, 67	0
1	C	267/274 (97%)	-0.13	0 100 100	14, 24, 42, 50	0
1	D	261/274 (95%)	-0.19	2 (0%) 82 79	13, 23, 40, 73	0
1	E	263/274 (95%)	-0.03	3 (1%) 78 75	17, 27, 52, 69	0
1	F	268/274 (97%)	-0.04	1 (0%) 88 87	15, 26, 41, 55	0
1	G	260/274 (94%)	0.14	0 100 100	21, 33, 50, 66	0
1	H	260/274 (94%)	0.35	3 (1%) 76 72	22, 35, 51, 69	0
1	I	268/274 (97%)	0.24	5 (1%) 66 61	16, 30, 46, 58	0
1	J	267/274 (97%)	-0.03	1 (0%) 88 87	16, 28, 43, 57	0
1	K	267/274 (97%)	0.12	3 (1%) 78 75	19, 29, 47, 70	0
1	L	262/274 (95%)	0.08	2 (0%) 82 79	18, 30, 52, 66	0
1	M	269/274 (98%)	0.12	9 (3%) 49 40	17, 28, 56, 92	0
1	N	266/274 (97%)	0.08	7 (2%) 57 51	18, 27, 53, 86	0
1	O	262/274 (95%)	0.04	4 (1%) 72 67	19, 29, 51, 78	0
1	P	269/274 (98%)	0.21	4 (1%) 72 67	20, 32, 47, 67	0
1	Q	268/274 (97%)	0.07	7 (2%) 57 51	20, 31, 45, 66	0
1	R	263/274 (95%)	0.06	1 (0%) 88 87	20, 30, 46, 78	0
1	S	261/274 (95%)	0.19	3 (1%) 78 75	20, 33, 50, 81	0
1	T	263/274 (95%)	0.33	6 (2%) 61 54	22, 35, 51, 79	0
1	U	261/274 (95%)	0.04	2 (0%) 82 79	19, 29, 45, 76	0
1	V	265/274 (96%)	0.46	7 (2%) 57 51	26, 40, 60, 85	0
1	W	262/274 (95%)	0.76	11 (4%) 40 32	25, 41, 61, 90	0
1	X	261/274 (95%)	0.60	3 (1%) 78 75	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%)	0.13	3 (1%) 78 75	19, 31, 53, 70	0
1	Z	260/274 (94%)	0.15	1 (0%) 88 87	23, 32, 46, 61	0
1	a	261/274 (95%)	0.26	3 (1%) 78 75	25, 38, 55, 86	0
1	b	260/274 (94%)	0.74	13 (5%) 34 26	28, 43, 64, 102	0
1	c	256/274 (93%)	0.77	16 (6%) 26 19	29, 45, 64, 87	0
1	d	260/274 (94%)	0.41	3 (1%) 76 72	23, 41, 64, 82	0
1	e	261/274 (95%)	0.38	2 (0%) 82 79	23, 39, 52, 77	0
1	f	261/274 (95%)	0.54	5 (1%) 66 61	29, 42, 56, 64	0
1	g	269/274 (98%)	0.95	23 (8%) 16 12	29, 46, 63, 88	0
1	h	261/274 (95%)	0.83	16 (6%) 27 20	30, 47, 60, 76	0
1	i	260/274 (94%)	0.68	11 (4%) 40 32	29, 44, 60, 91	0
1	j	260/274 (94%)	0.80	20 (7%) 19 14	29, 47, 64, 79	0
1	k	263/274 (95%)	2.06	120 (45%) 0 0	35, 61, 80, 99	0
1	l	235/274 (85%)	2.20	125 (53%) 0 0	40, 65, 85, 93	0
1	m	259/274 (94%)	1.48	69 (26%) 1 1	33, 58, 85, 100	0
1	n	267/274 (97%)	0.59	10 (3%) 45 37	28, 42, 60, 75	0
All	All	10494/10960 (95%)	0.41	529 (5%) 34 26	13, 36, 63, 102	0

All (529) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	l	51	TRP	7.1
1	l	47	VAL	6.5
1	k	258	ASP	6.0
1	k	119	TYR	5.9
1	M	22	GLY	5.5
1	k	41	ALA	5.3
1	k	52	GLY	5.3
1	l	73	ILE	5.1
1	l	149	ASP	5.1
1	k	278	ARG	5.0
1	l	128	GLY	5.0
1	l	50	ASN	4.8
1	k	64	TYR	4.8
1	m	155	GLN	4.7
1	l	154	MET	4.7

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Mol	Chain	Res	Type	RSRZ
1	l	79	ALA	4.6
1	m	174	THR	4.6
1	N	32	GLY	4.6
1	f	37	THR	4.6
1	V	91	THR	4.6
1	k	118	SER	4.5
1	l	256	SER	4.5
1	l	62	ASN	4.5
1	m	65	ASN	4.4
1	g	112	SER	4.4
1	l	74	PRO	4.4
1	k	115	ASN	4.3
1	l	156	ASN	4.3
1	l	118	SER	4.3
1	k	123	ALA	4.2
1	k	70	LEU	4.2
1	k	177	ASP	4.2
1	m	68	PRO	4.2
1	B	95	LEU	4.2
1	m	172	ASP	4.2
1	k	280	PHE	4.2
1	k	264	VAL	4.2
1	l	168	PRO	4.2
1	l	255	SER	4.2
1	k	254	LEU	4.2
1	m	168	PRO	4.1
1	k	53	PHE	4.1
1	k	148	LEU	4.1
1	k	71	THR	4.1
1	l	161	TYR	4.0
1	l	111	SER	4.0
1	k	68	PRO	4.0
1	j	130	GLY	4.0
1	k	42	TYR	3.9
1	l	183	ASN	3.8
1	l	55	THR	3.8
1	l	75	CYS	3.8
1	k	277	PRO	3.8
1	S	94	THR	3.8
1	k	256	SER	3.8
1	k	128	GLY	3.8
1	i	29	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	k	38	THR	3.8
1	k	73	ILE	3.8
1	g	93	PRO	3.8
1	N	34	ASP	3.7
1	l	157	HIS	3.7
1	l	119	TYR	3.7
1	l	186	TYR	3.7
1	l	66	ASP	3.7
1	k	279	TYR	3.7
1	l	196	TYR	3.7
1	l	194	ALA	3.7
1	m	194	ALA	3.7
1	k	116	MET	3.7
1	c	27	LEU	3.6
1	k	182	LEU	3.6
1	W	94	THR	3.6
1	N	92	SER	3.6
1	l	43	LEU	3.6
1	N	31	THR	3.6
1	k	77	SER	3.6
1	l	45	PRO	3.6
1	k	34	ASP	3.6
1	m	66	ASP	3.6
1	k	117	HIS	3.6
1	m	171	PRO	3.6
1	l	117	HIS	3.5
1	l	268	SER	3.5
1	m	152	GLY	3.5
1	m	49	GLN	3.5
1	k	257	ALA	3.5
1	k	253	TYR	3.4
1	k	272	TYR	3.4
1	l	71	THR	3.4
1	k	85	LEU	3.4
1	l	27	LEU	3.4
1	l	279	TYR	3.4
1	T	94	THR	3.4
1	g	34	ASP	3.4
1	k	79	ALA	3.4
1	c	95	LEU	3.4
1	l	276	LEU	3.4
1	j	221	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	g	42	TYR	3.4
1	l	42	TYR	3.4
1	L	94	THR	3.4
1	M	33	PRO	3.4
1	m	151	GLN	3.4
1	T	22	GLY	3.4
1	d	94	THR	3.3
1	k	28	ASP	3.3
1	k	221	VAL	3.3
1	l	201	TRP	3.3
1	l	178	SER	3.3
1	l	48	GLY	3.3
1	k	114	LEU	3.3
1	l	147	PRO	3.3
1	m	175	THR	3.3
1	m	178	SER	3.3
1	l	155	GLN	3.3
1	l	68	PRO	3.2
1	n	174	THR	3.2
1	k	82	SER	3.2
1	m	173	GLY	3.2
1	j	110	ILE	3.2
1	k	83	LEU	3.2
1	k	268	SER	3.2
1	l	261	GLY	3.2
1	m	41	ALA	3.2
1	m	186	TYR	3.2
1	l	208	ASN	3.2
1	m	62	ASN	3.2
1	k	75	CYS	3.2
1	k	270	LYS	3.2
1	m	154	MET	3.2
1	h	24	ILE	3.2
1	k	197	PRO	3.2
1	D	94	THR	3.2
1	E	22	GLY	3.2
1	m	272	TYR	3.2
1	n	221	VAL	3.2
1	k	121	LEU	3.1
1	M	93	PRO	3.1
1	m	160	GLN	3.1
1	X	94	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	l	81	ILE	3.1
1	l	101	VAL	3.1
1	O	22	GLY	3.1
1	k	273	TRP	3.1
1	k	24	ILE	3.1
1	m	73	ILE	3.1
1	l	136	SER	3.1
1	c	33	PRO	3.1
1	g	22	GLY	3.1
1	m	28	ASP	3.1
1	k	164	PRO	3.1
1	l	265	GLN	3.1
1	l	266	GLN	3.1
1	k	35	SER	3.1
1	k	161	TYR	3.0
1	l	258	ASP	3.0
1	R	94	THR	3.0
1	k	31	THR	3.0
1	m	71	THR	3.0
1	k	98	TRP	3.0
1	l	95	LEU	3.0
1	l	252	LEU	3.0
1	m	169	LYS	3.0
1	j	129	GLY	3.0
1	k	48	GLY	3.0
1	l	262	THR	3.0
1	n	220	GLY	3.0
1	F	85	LEU	3.0
1	l	200	CYS	3.0
1	l	216	SER	3.0
1	O	34	ASP	3.0
1	S	28	ASP	3.0
1	k	219	GLY	3.0
1	l	193	ASP	3.0
1	e	125	GLY	3.0
1	l	94	THR	3.0
1	l	195	THR	3.0
1	k	181	VAL	3.0
1	l	141	PHE	3.0
1	N	33	PRO	2.9
1	V	127	TYR	2.9
1	c	31	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	l	124	PHE	2.9
1	k	69	HIS	2.9
1	l	54	SER	2.9
1	b	250	ASP	2.9
1	k	153	LEU	2.9
1	k	263	PHE	2.9
1	l	182	LEU	2.9
1	f	54	SER	2.9
1	Y	34	ASP	2.9
1	g	73	ILE	2.9
1	j	24	ILE	2.9
1	m	67	ALA	2.9
1	l	148	LEU	2.9
1	b	28	ASP	2.9
1	l	213	TYR	2.9
1	l	257	ALA	2.9
1	a	33	PRO	2.8
1	k	245	PRO	2.8
1	l	273	TRP	2.8
1	k	133	ILE	2.8
1	K	32	GLY	2.8
1	k	262	THR	2.8
1	l	137	HIS	2.8
1	k	147	PRO	2.8
1	l	57	ILE	2.8
1	m	150	LEU	2.8
1	Q	94	THR	2.8
1	l	166	VAL	2.8
1	l	146	GLU	2.8
1	l	197	PRO	2.8
1	h	256	SER	2.8
1	k	142	SER	2.8
1	g	23	GLY	2.8
1	l	153	LEU	2.8
1	m	153	LEU	2.8
1	W	79	ALA	2.8
1	l	105	THR	2.8
1	l	214	PHE	2.8
1	l	264	VAL	2.8
1	b	33	PRO	2.8
1	k	160	GLN	2.8
1	Q	24	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	c	73	ILE	2.8
1	k	281	ASN	2.8
1	e	52	GLY	2.8
1	g	41	ALA	2.8
1	l	179	ALA	2.8
1	k	217	TYR	2.8
1	K	290	LYS	2.7
1	j	111	SER	2.7
1	k	211	SER	2.7
1	l	82	SER	2.7
1	l	165	LEU	2.7
1	m	70	LEU	2.7
1	k	131	TYR	2.7
1	m	148	LEU	2.7
1	l	61	SER	2.7
1	k	209	GLU	2.7
1	l	162	PRO	2.7
1	l	190	LEU	2.7
1	A	178	SER	2.7
1	k	51	TRP	2.7
1	M	250	ASP	2.7
1	j	28	ASP	2.7
1	k	275	GLY	2.7
1	l	112	SER	2.7
1	m	77	SER	2.7
1	m	158	SER	2.7
1	k	101	VAL	2.7
1	m	58	THR	2.7
1	m	179	ALA	2.7
1	l	76	TYR	2.6
1	S	130	GLY	2.6
1	l	98	TRP	2.6
1	l	158	SER	2.6
1	m	59	VAL	2.6
1	i	172	ASP	2.6
1	U	24	ILE	2.6
1	k	43	LEU	2.6
1	m	137	HIS	2.6
1	m	157	HIS	2.6
1	M	32	GLY	2.6
1	Q	23	GLY	2.6
1	W	48	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	291	ASN	2.6
1	M	92	SER	2.6
1	k	108	VAL	2.6
1	l	263	PHE	2.6
1	m	201	TRP	2.6
1	M	89	ASP	2.6
1	m	149	ASP	2.6
1	l	150	LEU	2.6
1	k	220	GLY	2.6
1	k	225	PRO	2.6
1	l	203	PRO	2.6
1	T	118	SER	2.6
1	g	110	ILE	2.6
1	k	39	ILE	2.6
1	m	185	ILE	2.6
1	l	227	LEU	2.6
1	j	127	TYR	2.6
1	g	199	GLU	2.6
1	k	72	GLU	2.6
1	W	257	ALA	2.6
1	k	59	VAL	2.6
1	l	260	ALA	2.6
1	m	45	PRO	2.6
1	g	94	THR	2.5
1	j	112	SER	2.5
1	l	159	THR	2.5
1	m	57	ILE	2.5
1	m	133	ILE	2.5
1	N	30	LYS	2.5
1	k	274	ARG	2.5
1	j	118	SER	2.5
1	K	24	ILE	2.5
1	k	165	LEU	2.5
1	j	42	TYR	2.5
1	m	135	GLY	2.5
1	k	74	PRO	2.5
1	k	37	THR	2.5
1	l	58	THR	2.5
1	l	202	CYS	2.5
1	m	75	CYS	2.5
1	a	24	ILE	2.5
1	A	96	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	l	28	ASP	2.5
1	c	25	GLU	2.5
1	j	128	GLY	2.5
1	l	181	VAL	2.5
1	k	260	ALA	2.5
1	c	30	LYS	2.5
1	m	192	LYS	2.5
1	c	96	LEU	2.5
1	g	92	SER	2.5
1	m	61	SER	2.5
1	I	89	ASP	2.5
1	L	28	ASP	2.5
1	m	64	TYR	2.5
1	h	47	VAL	2.5
1	l	60	ALA	2.5
1	U	94	THR	2.4
1	h	73	ILE	2.4
1	k	198	ILE	2.4
1	l	185	ILE	2.4
1	V	92	SER	2.4
1	M	23	GLY	2.4
1	k	171	PRO	2.4
1	m	52	GLY	2.4
1	k	259	VAL	2.4
1	Q	91	THR	2.4
1	g	96	LEU	2.4
1	j	115	ASN	2.4
1	c	28	ASP	2.4
1	N	93	PRO	2.4
1	k	120	GLY	2.4
1	c	143	VAL	2.4
1	k	76	TYR	2.4
1	i	60	ALA	2.4
1	l	274	ARG	2.4
1	l	278	ARG	2.4
1	b	148	LEU	2.4
1	k	282	ILE	2.4
1	l	236	ILE	2.4
1	m	165	LEU	2.4
1	l	78	SER	2.4
1	k	151	GLN	2.4
1	k	47	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	l	143	VAL	2.4
1	i	64	TYR	2.4
1	k	237	LEU	2.4
1	k	276	LEU	2.4
1	l	96	LEU	2.4
1	X	31	THR	2.4
1	k	267	THR	2.4
1	j	117	HIS	2.4
1	b	98	TRP	2.4
1	h	201	TRP	2.4
1	k	84	PRO	2.4
1	m	108	VAL	2.4
1	i	67	ALA	2.4
1	k	60	ALA	2.4
1	m	196	TYR	2.3
1	M	91	THR	2.3
1	k	55	THR	2.3
1	W	25	GLU	2.3
1	P	172	ASP	2.3
1	a	250	ASP	2.3
1	i	28	ASP	2.3
1	V	93	PRO	2.3
1	l	84	PRO	2.3
1	V	23	GLY	2.3
1	c	109	GLY	2.3
1	l	215	GLY	2.3
1	b	27	LEU	2.3
1	P	23	GLY	2.3
1	l	151	GLN	2.3
1	c	288	ALA	2.3
1	h	85	LEU	2.3
1	k	284	LEU	2.3
1	W	64	TYR	2.3
1	m	42	TYR	2.3
1	c	255	SER	2.3
1	l	211	SER	2.3
1	T	23	GLY	2.3
1	l	145	GLY	2.3
1	m	261	GLY	2.3
1	b	85	LEU	2.3
1	m	200	CYS	2.3
1	k	214	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	b	100	ALA	2.3
1	E	31	THR	2.3
1	J	94	THR	2.3
1	m	132	THR	2.3
1	m	199	GLU	2.3
1	Q	256	SER	2.3
1	m	180	GLN	2.3
1	g	52	GLY	2.3
1	h	95	LEU	2.3
1	k	100	ALA	2.2
1	l	247	CYS	2.2
1	m	138	ILE	2.2
1	g	64	TYR	2.2
1	D	241	ASN	2.2
1	k	44	ASN	2.2
1	d	28	ASP	2.2
1	k	255	SER	2.2
1	m	219	GLY	2.2
1	c	98	TRP	2.2
1	c	26	VAL	2.2
1	k	107	VAL	2.2
1	l	254	LEU	2.2
1	H	24	ILE	2.2
1	h	104	LYS	2.2
1	k	110	ILE	2.2
1	k	132	THR	2.2
1	i	50	ASN	2.2
1	k	184	PRO	2.2
1	T	28	ASP	2.2
1	k	109	GLY	2.2
1	O	95	LEU	2.2
1	W	95	LEU	2.2
1	g	85	LEU	2.2
1	W	29	VAL	2.2
1	T	73	ILE	2.2
1	j	124	PHE	2.2
1	k	185	ILE	2.2
1	l	280	PHE	2.2
1	b	94	THR	2.2
1	h	240	GLU	2.2
1	k	80	ARG	2.2
1	m	156	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	n	64	TYR	2.2
1	b	245	PRO	2.2
1	H	95	LEU	2.2
1	O	23	GLY	2.2
1	W	23	GLY	2.2
1	W	86	LEU	2.2
1	b	190	LEU	2.2
1	g	24	ILE	2.2
1	h	69	HIS	2.2
1	k	236	ILE	2.2
1	h	25	GLU	2.2
1	l	80	ARG	2.2
1	i	65	ASN	2.2
1	l	219	GLY	2.2
1	m	63	GLY	2.2
1	g	47	VAL	2.2
1	l	138	ILE	2.2
1	A	174	THR	2.1
1	c	147	PRO	2.1
1	l	104	LYS	2.1
1	j	95	LEU	2.1
1	k	152	GLY	2.1
1	B	24	ILE	2.1
1	i	163	SER	2.1
1	n	61	SER	2.1
1	X	25	GLU	2.1
1	g	71	THR	2.1
1	h	94	THR	2.1
1	g	115	ASN	2.1
1	i	156	ASN	2.1
1	j	266	GLN	2.1
1	k	154	MET	2.1
1	j	272	TYR	2.1
1	m	48	GLY	2.1
1	n	261	GLY	2.1
1	I	73	ILE	2.1
1	Y	26	VAL	2.1
1	j	34	ASP	2.1
1	k	250	ASP	2.1
1	l	289	VAL	2.1
1	I	92	SER	2.1
1	k	67	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	l	41	ALA	2.1
1	Y	94	THR	2.1
1	b	31	THR	2.1
1	Q	290	LYS	2.1
1	V	68	PRO	2.1
1	m	164	PRO	2.1
1	h	96	LEU	2.1
1	k	96	LEU	2.1
1	V	64	TYR	2.1
1	l	144	GLY	2.1
1	W	185	ILE	2.1
1	g	243	VAL	2.1
1	m	166	VAL	2.1
1	m	264	VAL	2.1
1	Z	28	ASP	2.1
1	h	141	PHE	2.1
1	Q	61	SER	2.1
1	k	122	ARG	2.1
1	m	257	ALA	2.1
1	j	51	TRP	2.1
1	n	160	GLN	2.1
1	n	182	LEU	2.1
1	E	23	GLY	2.1
1	g	261	GLY	2.1
1	l	152	GLY	2.1
1	H	64	TYR	2.1
1	f	64	TYR	2.1
1	l	253	TYR	2.1
1	h	55	THR	2.0
1	k	252	LEU	2.0
1	d	183	ASN	2.0
1	I	63	GLY	2.0
1	m	109	GLY	2.0
1	f	272	TYR	2.0
1	g	272	TYR	2.0
1	l	108	VAL	2.0
1	n	181	VAL	2.0
1	l	207	ARG	2.0
1	P	89	ASP	2.0
1	h	170	LYS	2.0
1	P	92	SER	2.0
1	k	78	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	i	51	TRP	2.0
1	b	83	LEU	2.0
1	k	180	GLN	2.0
1	l	284	LEU	2.0
1	n	155	GLN	2.0
1	f	231	ASN	2.0
1	l	125	GLY	2.0
1	l	282	ILE	2.0
1	m	32	GLY	2.0
1	l	259	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SIA	T	401	21/21	0.78	0.14	49,60,65,68	0
2	SIA	V	401	21/21	0.80	0.12	48,63,75,76	0
2	SIA	X	401	21/21	0.80	0.13	54,62,68,74	0
2	SIA	G	401	21/21	0.81	0.15	60,76,84,89	0
2	SIA	a	401	21/21	0.81	0.14	53,62,67,69	0
2	SIA	b	401	21/21	0.81	0.12	47,60,63,66	0
2	SIA	F	401	21/21	0.82	0.14	54,62,68,69	0
2	SIA	f	401	21/21	0.82	0.13	52,61,63,66	0
3	CL	C	404	1/1	0.82	0.10	47,47,47,47	0
2	SIA	d	401	21/21	0.83	0.15	64,74,79,81	0
2	SIA	Q	401	21/21	0.83	0.13	47,55,60,63	0
2	SIA	I	401	21/21	0.83	0.12	51,60,62,63	0
2	SIA	C	401	21/21	0.84	0.14	57,68,73,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SIA	Y	401	21/21	0.84	0.13	48,56,64,71	0
2	SIA	j	401	21/21	0.84	0.11	49,60,64,65	0
2	SIA	n	401	21/21	0.84	0.12	67,73,82,82	0
2	SIA	c	401	21/21	0.84	0.13	59,67,71,72	0
2	SIA	O	401	21/21	0.85	0.12	45,50,54,58	0
2	SIA	A	401	21/21	0.85	0.11	42,50,59,64	0
2	SIA	R	401	21/21	0.85	0.13	48,60,68,77	0
2	SIA	J	401	21/21	0.85	0.11	43,51,55,57	0
2	SIA	K	401	21/21	0.85	0.12	49,57,64,78	0
2	SIA	S	401	21/21	0.86	0.12	55,59,68,68	0
3	CL	G	403	1/1	0.86	0.11	43,43,43,43	0
3	CL	W	302	1/1	0.86	0.10	53,53,53,53	0
2	SIA	M	401	21/21	0.87	0.11	38,43,46,46	0
2	SIA	Z	401	21/21	0.87	0.11	50,65,70,72	0
2	SIA	B	401	21/21	0.88	0.11	46,49,60,69	0
3	CL	N	402	1/1	0.88	0.09	54,54,54,54	0
2	SIA	e	401	21/21	0.88	0.11	51,62,63,65	0
3	CL	d	402	1/1	0.88	0.07	45,45,45,45	0
2	SIA	L	401	21/21	0.89	0.09	37,42,44,46	0
3	CL	H	302	1/1	0.89	0.11	48,48,48,48	0
2	SIA	E	401	21/21	0.89	0.11	42,50,62,64	0
2	SIA	N	401	21/21	0.89	0.11	38,46,52,54	0
3	CL	F	403	1/1	0.89	0.10	45,45,45,45	0
3	CL	j	402	1/1	0.89	0.08	51,51,51,51	0
3	CL	j	403	1/1	0.89	0.07	58,58,58,58	0
3	CL	n	403	1/1	0.89	0.09	48,48,48,48	0
3	CL	R	402	1/1	0.90	0.07	50,50,50,50	0
3	CL	B	402	1/1	0.90	0.09	52,52,52,52	0
3	CL	A	402	1/1	0.90	0.07	45,45,45,45	0
3	CL	Z	402	1/1	0.91	0.07	49,49,49,49	0
3	CL	L	402	1/1	0.91	0.08	48,48,48,48	0
3	CL	g	301	1/1	0.91	0.09	52,52,52,52	0
3	CL	S	402	1/1	0.91	0.07	53,53,53,53	0
3	CL	W	301	1/1	0.91	0.05	37,37,37,37	0
3	CL	F	402	1/1	0.91	0.10	47,47,47,47	0
3	CL	T	402	1/1	0.92	0.07	46,46,46,46	0
3	CL	X	402	1/1	0.92	0.07	44,44,44,44	0
3	CL	h	301	1/1	0.92	0.07	44,44,44,44	0
3	CL	Y	403	1/1	0.92	0.09	47,47,47,47	0
3	CL	P	302	1/1	0.92	0.07	41,41,41,41	0
3	CL	c	402	1/1	0.92	0.06	43,43,43,43	0
3	CL	U	302	1/1	0.93	0.07	47,47,47,47	0

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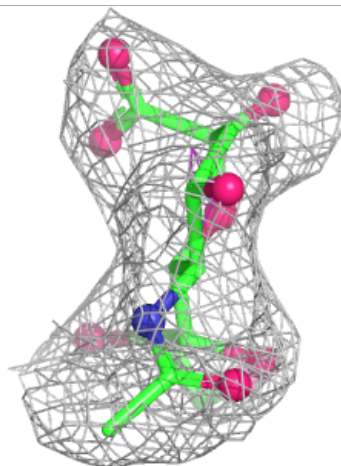
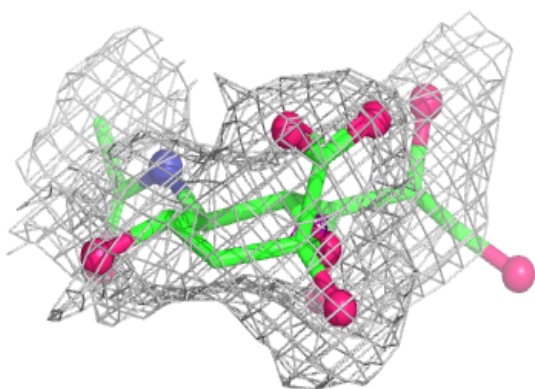
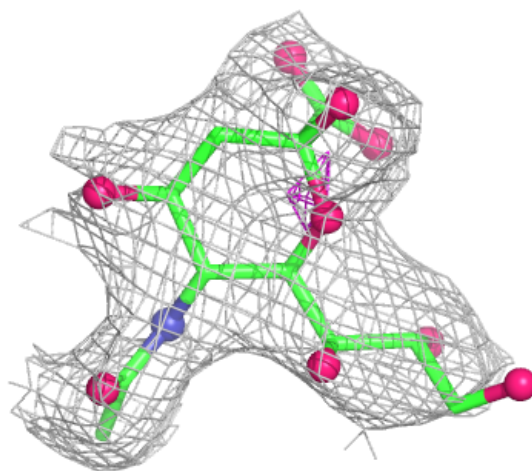
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	O	402	1/1	0.93	0.07	47,47,47,47	0
3	CL	G	402	1/1	0.93	0.06	58,58,58,58	0
3	CL	C	403	1/1	0.93	0.07	41,41,41,41	0
3	CL	Y	402	1/1	0.93	0.06	39,39,39,39	0
3	CL	H	301	1/1	0.93	0.07	45,45,45,45	0
3	CL	N	403	1/1	0.93	0.08	43,43,43,43	0
3	CL	C	402	1/1	0.94	0.07	46,46,46,46	0
3	CL	M	402	1/1	0.94	0.05	41,41,41,41	0
3	CL	e	403	1/1	0.94	0.07	51,51,51,51	0
3	CL	S	403	1/1	0.94	0.08	44,44,44,44	0
3	CL	X	403	1/1	0.94	0.06	50,50,50,50	0
3	CL	D	301	1/1	0.94	0.06	36,36,36,36	0
3	CL	Q	403	1/1	0.94	0.06	49,49,49,49	0
3	CL	V	402	1/1	0.94	0.06	43,43,43,43	0
3	CL	e	402	1/1	0.95	0.07	43,43,43,43	0
3	CL	J	403	1/1	0.95	0.06	42,42,42,42	0
3	CL	f	403	1/1	0.95	0.06	47,47,47,47	0
3	CL	d	403	1/1	0.95	0.06	43,43,43,43	0
3	CL	Q	402	1/1	0.96	0.07	46,46,46,46	0
3	CL	f	402	1/1	0.96	0.05	40,40,40,40	0
3	CL	Z	403	1/1	0.96	0.06	45,45,45,45	0
3	CL	J	402	1/1	0.96	0.05	39,39,39,39	0
4	MG	C	405	1/1	0.96	0.07	12,12,12,12	0
3	CL	M	403	1/1	0.97	0.07	38,38,38,38	0
3	CL	I	402	1/1	0.97	0.05	40,40,40,40	0
3	CL	U	301	1/1	0.98	0.04	27,27,27,27	0
3	CL	n	402	1/1	0.98	0.04	39,39,39,39	0
3	CL	P	301	1/1	0.99	0.06	41,41,41,41	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.

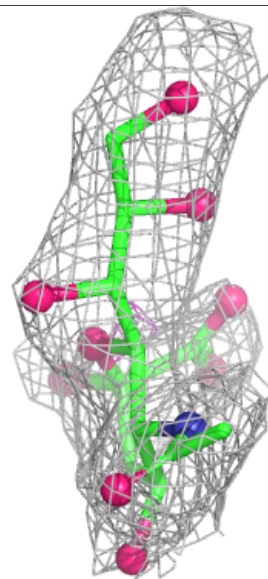
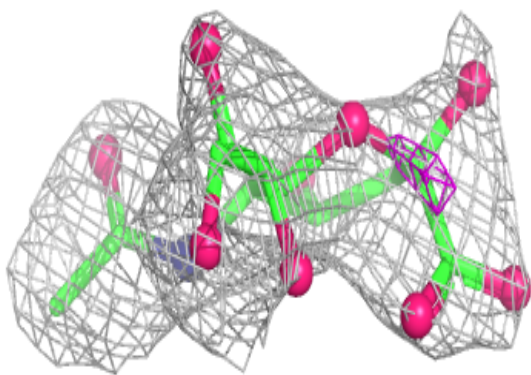
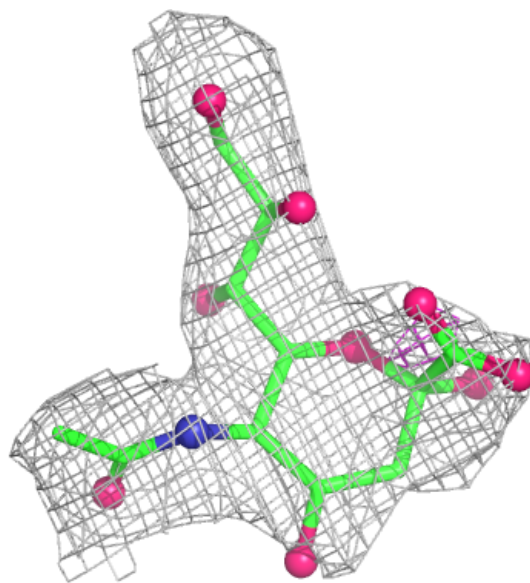
Electron density around SIA T 401:

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



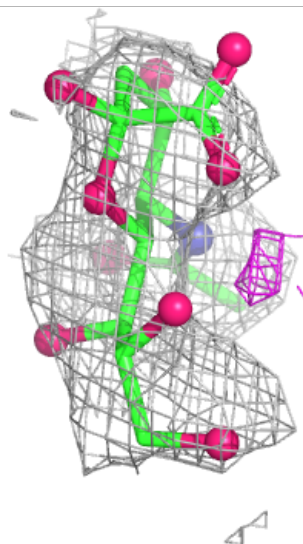
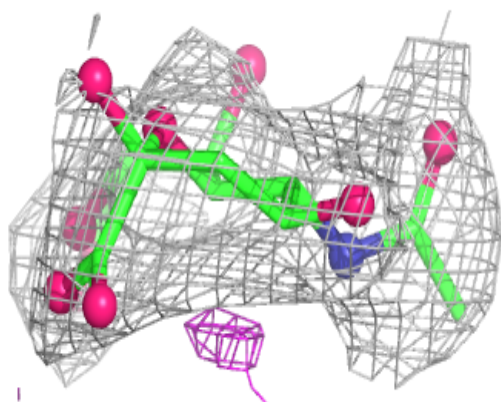
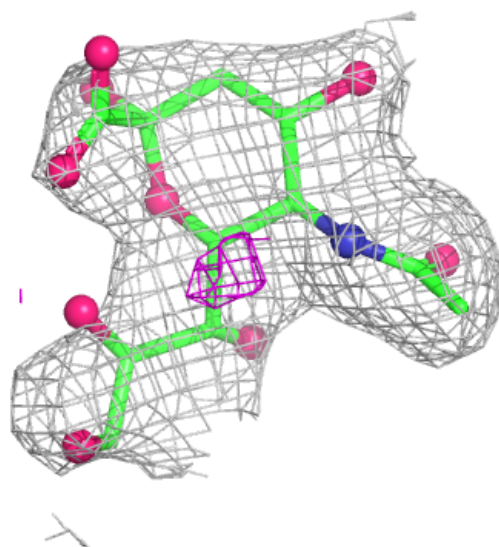
Electron density around SIA V 401:

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



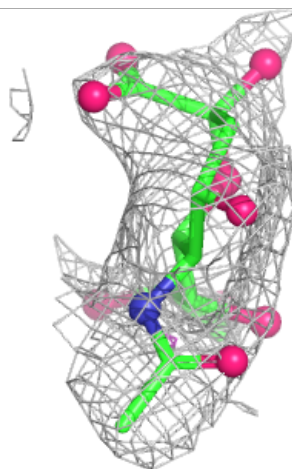
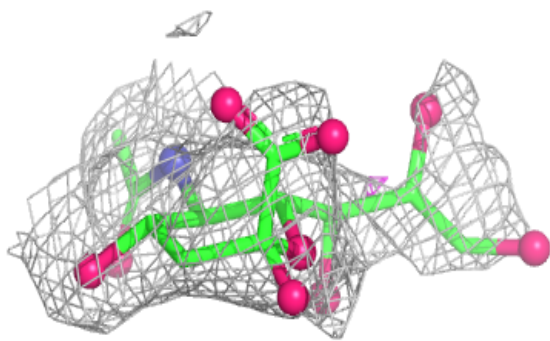
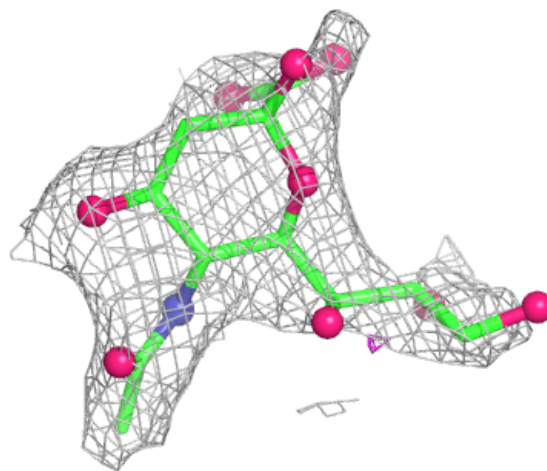
Electron density around SIA X 401:

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



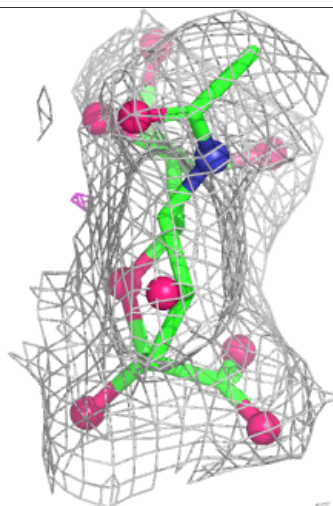
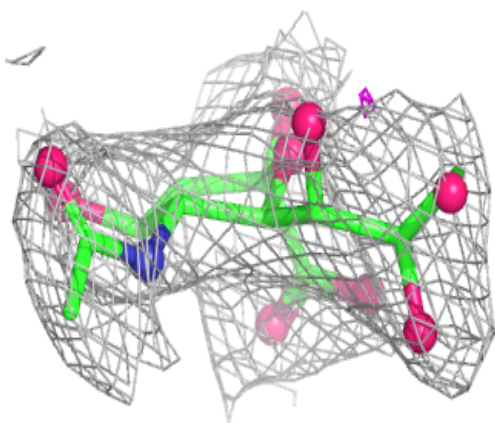
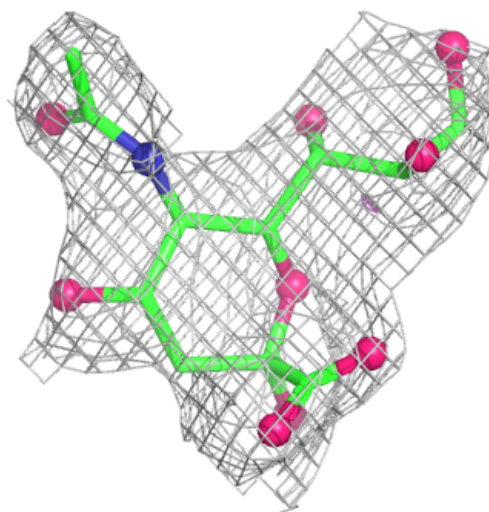
Electron density around SIA G 401:

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



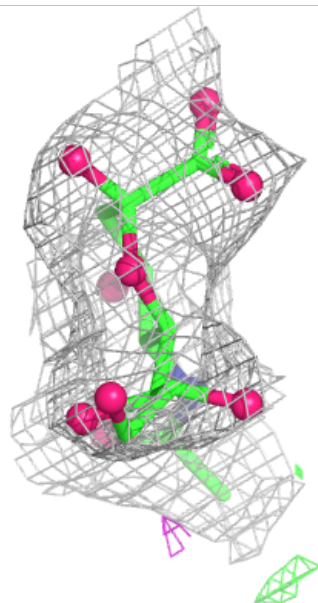
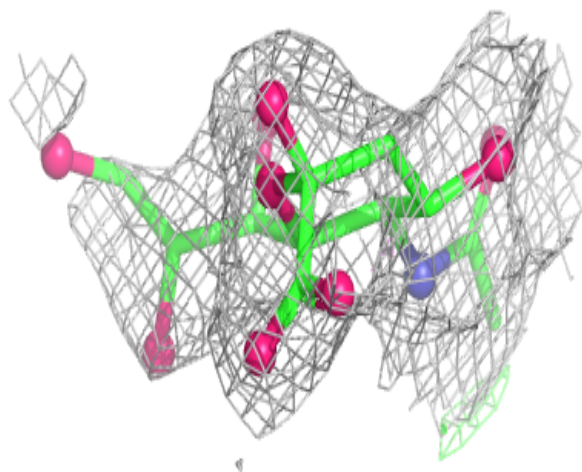
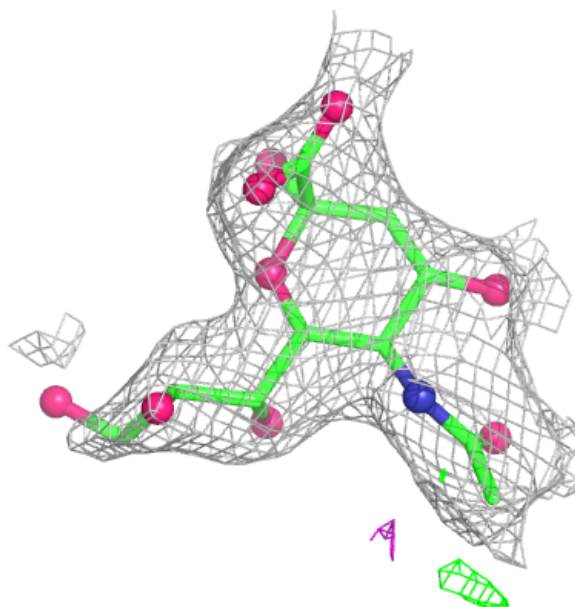
Electron density around SIA a 401:

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



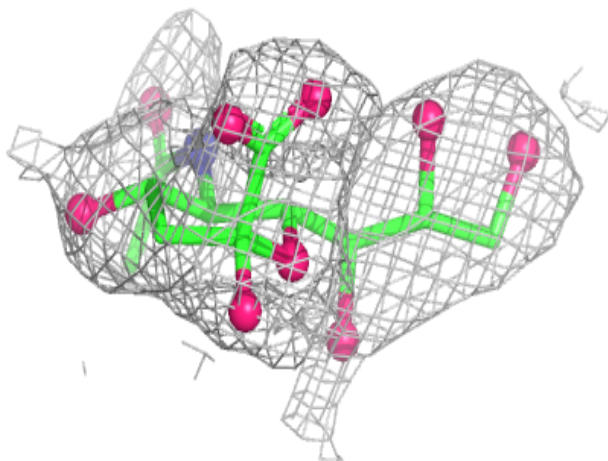
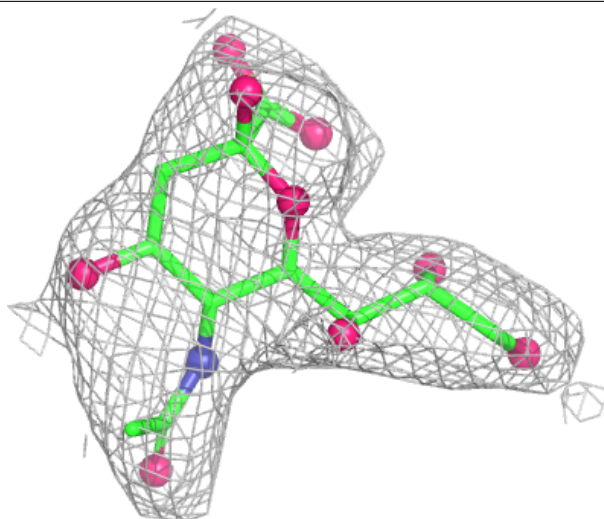
Electron density around SIA b 401:

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



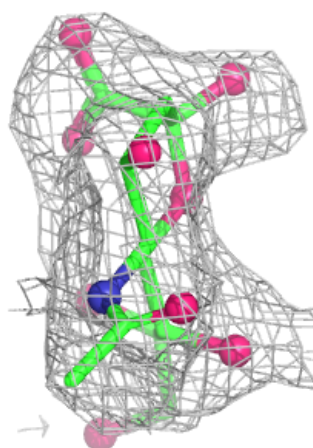
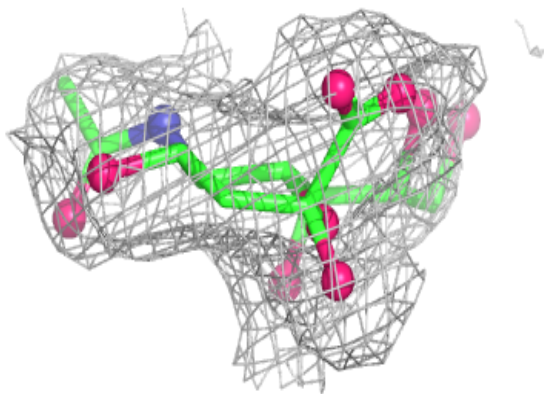
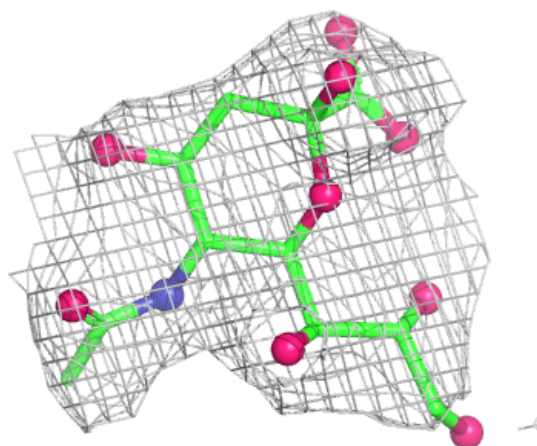
Electron density around SIA F 401:

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



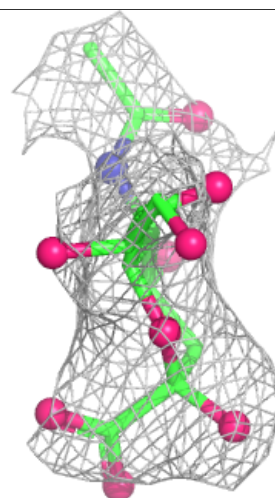
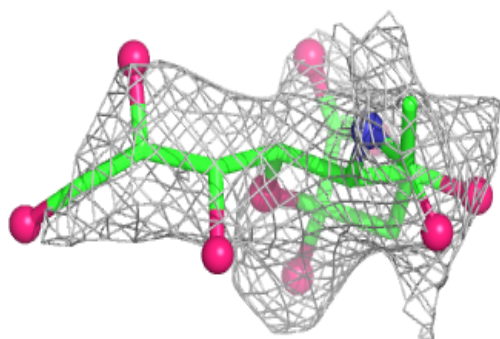
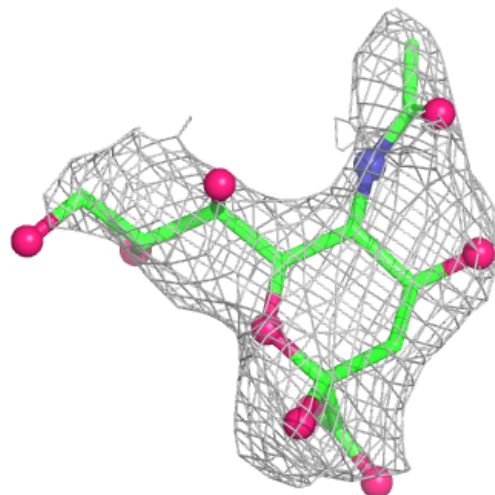
Electron density around SIA f 401:

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



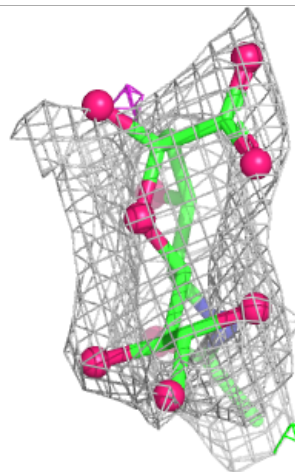
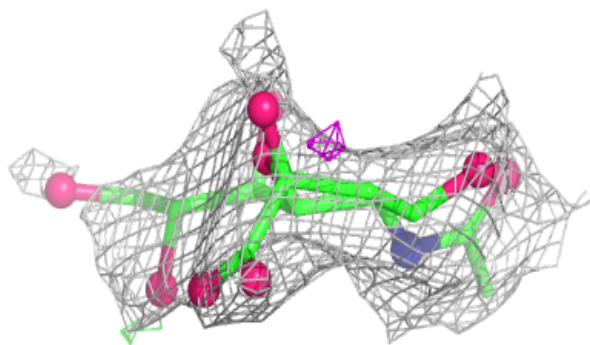
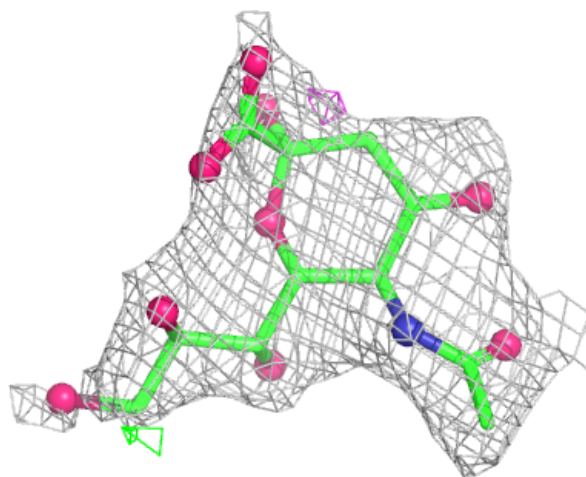
Electron density around SIA d 401:

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



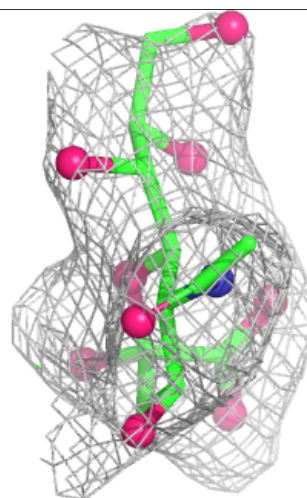
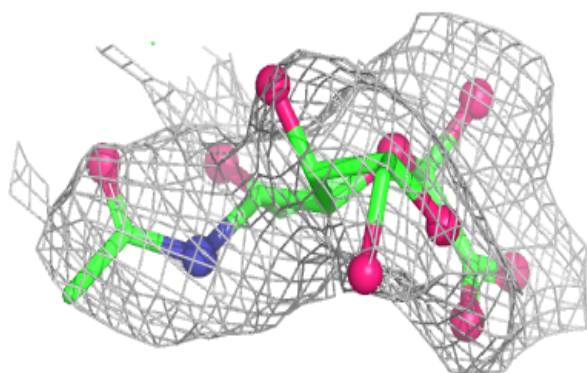
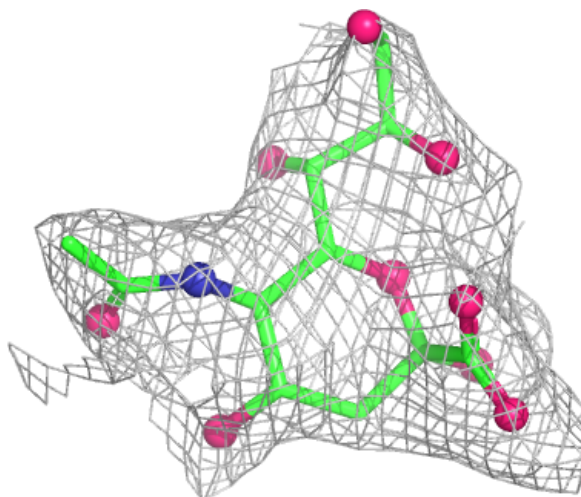
Electron density around SIA Q 401:

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



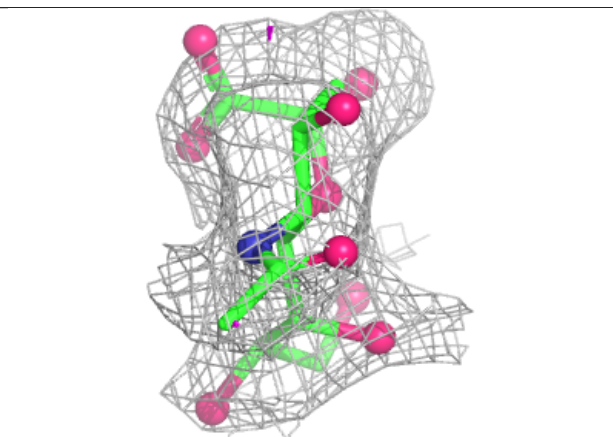
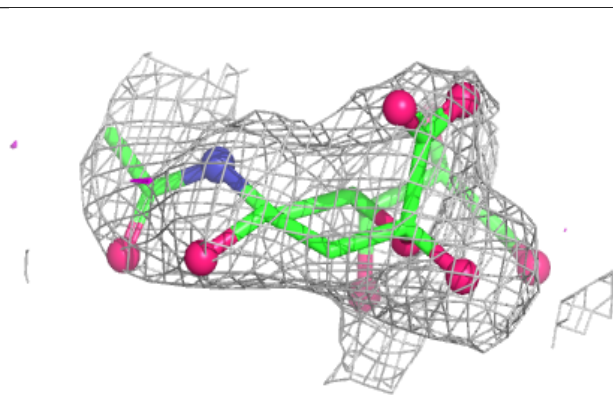
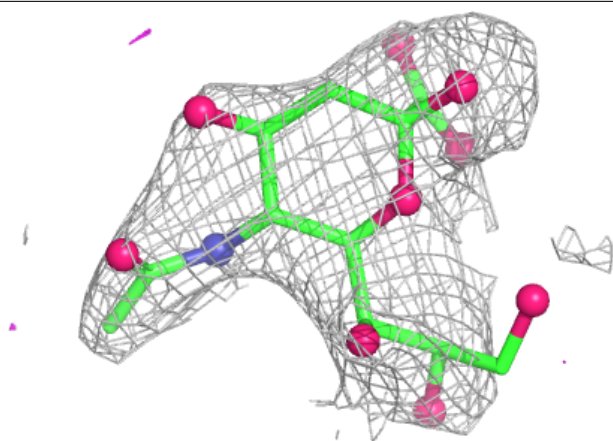
Electron density around SIA I 401:

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



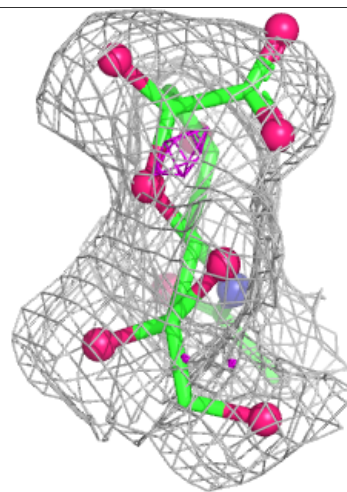
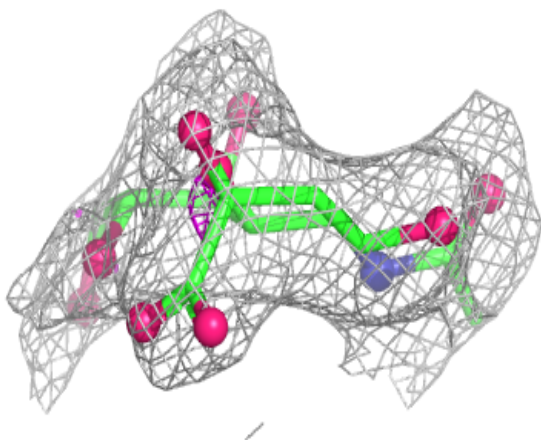
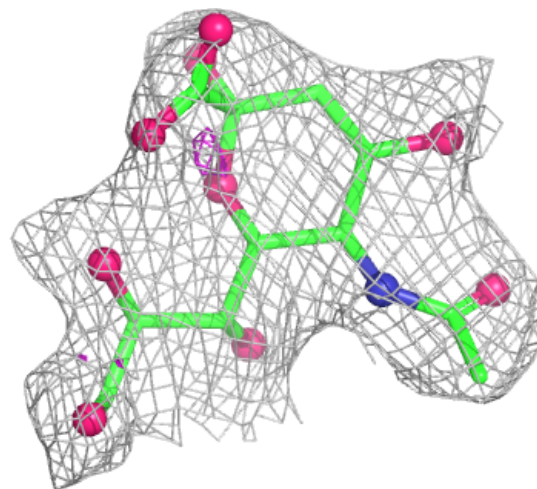
Electron density around SIA C 401:

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



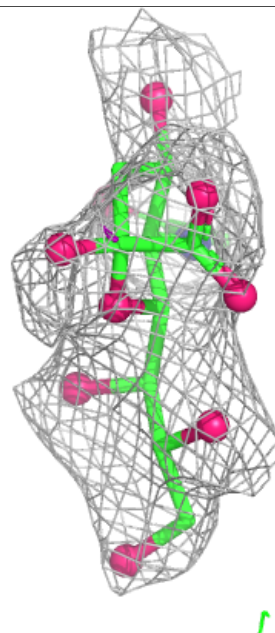
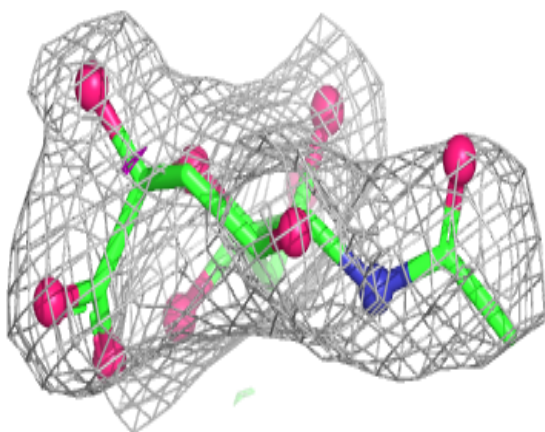
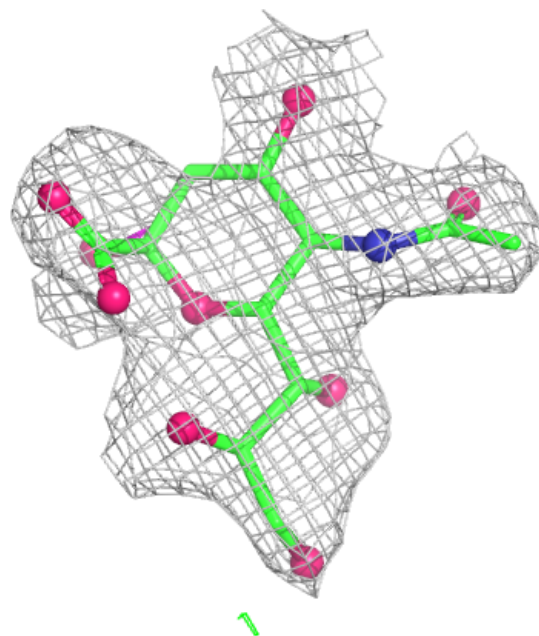
Electron density around SIA Y 401:

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



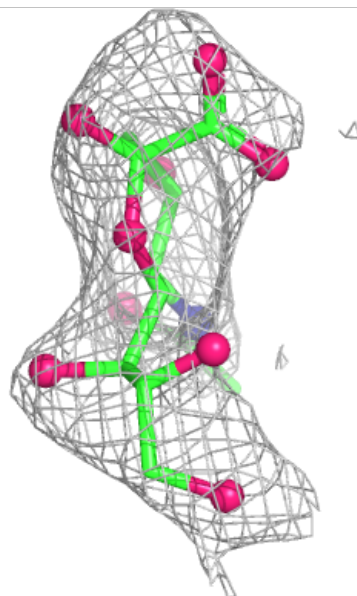
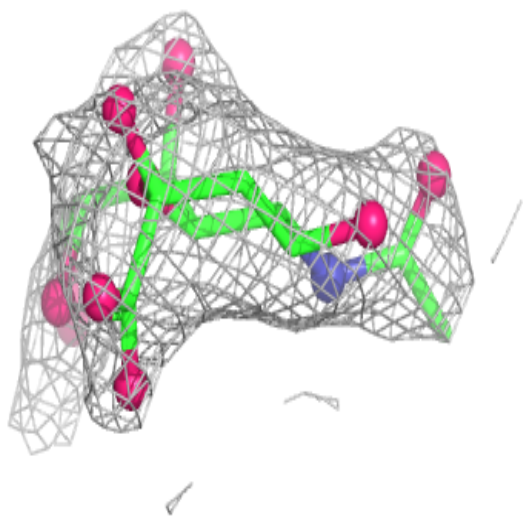
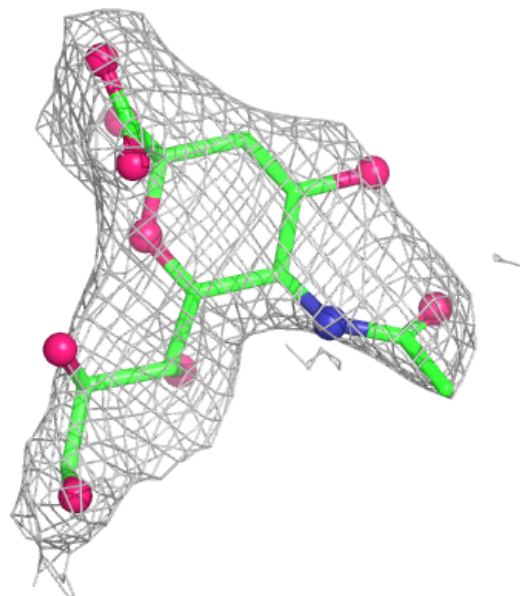
Electron density around SIA j 401:

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



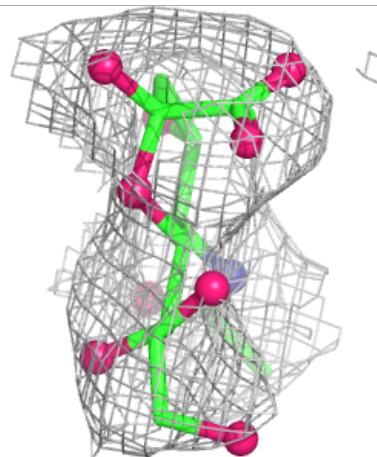
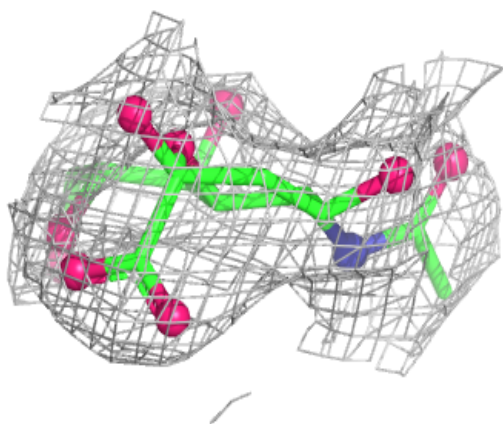
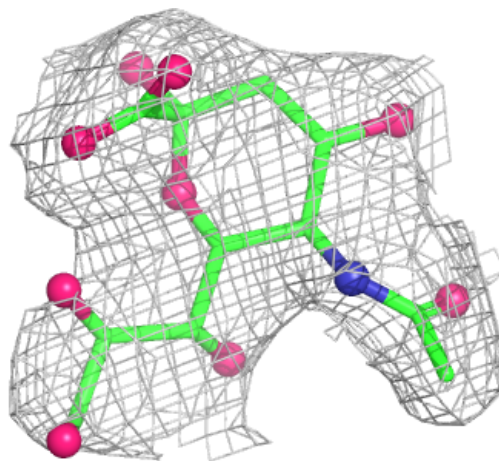
Electron density around SIA n 401:

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



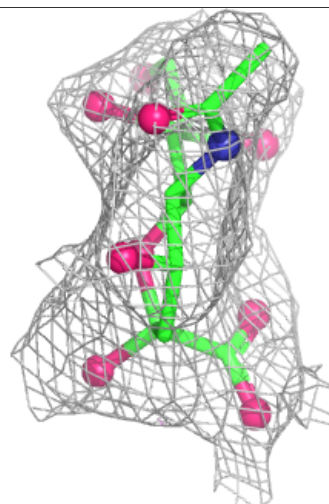
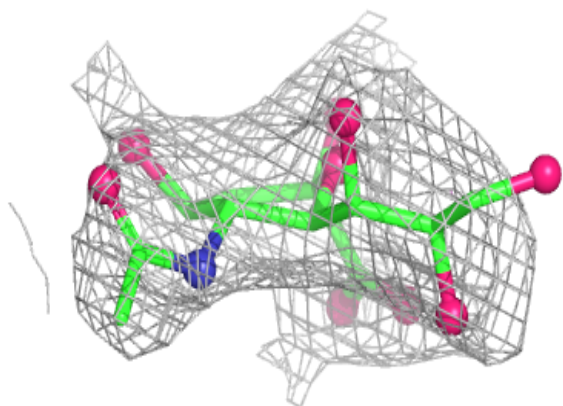
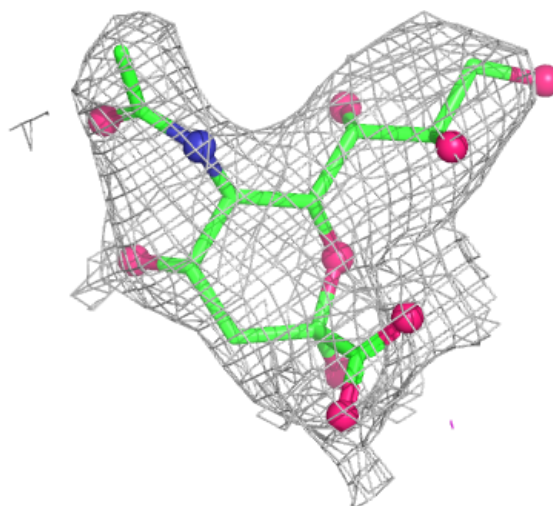
Electron density around SIA c 401:

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



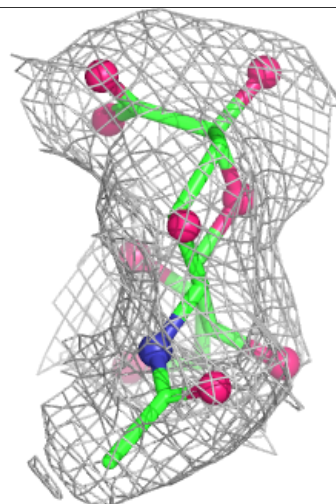
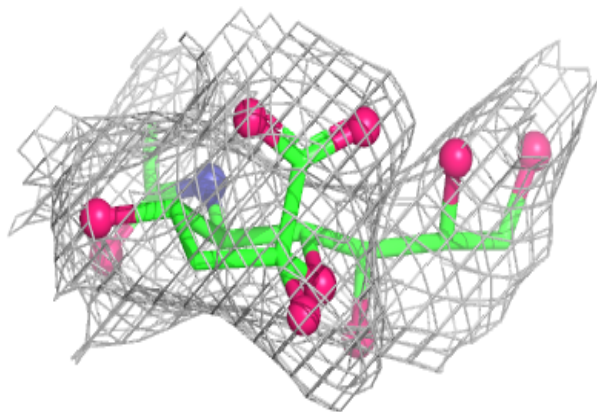
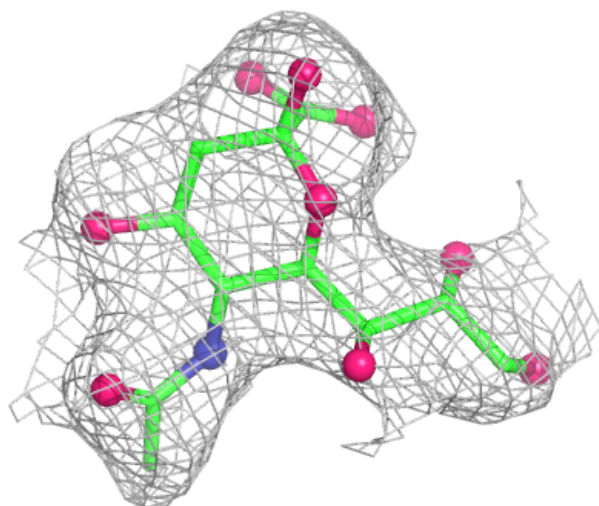
Electron density around SIA O 401:

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



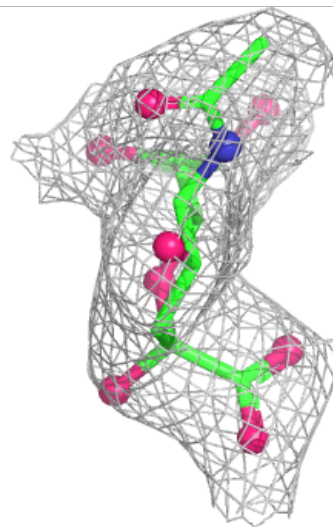
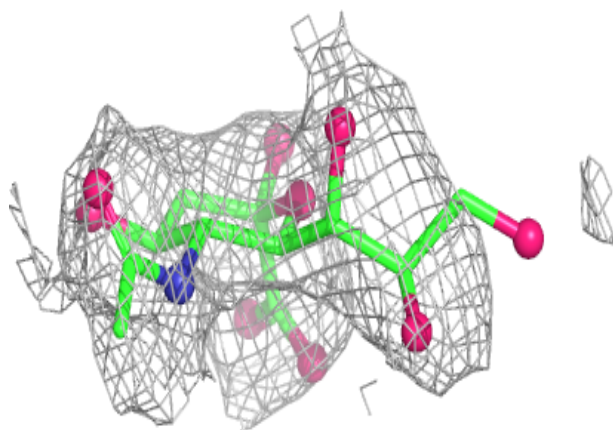
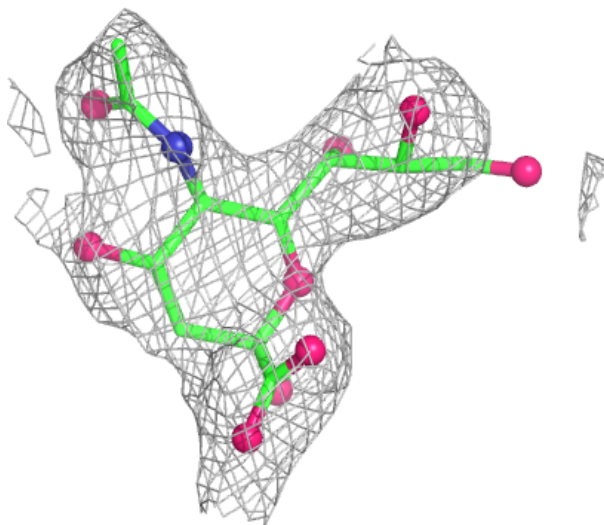
Electron density around SIA A 401:

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



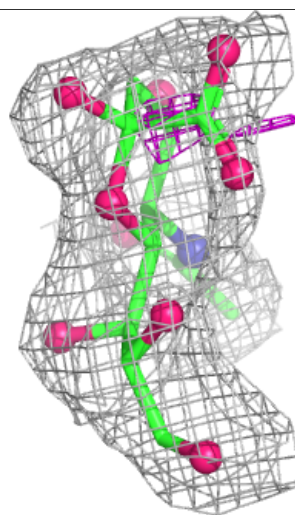
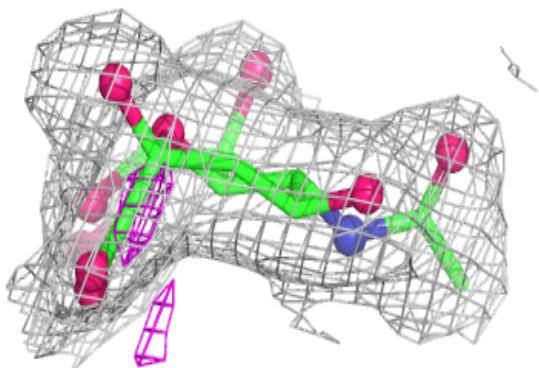
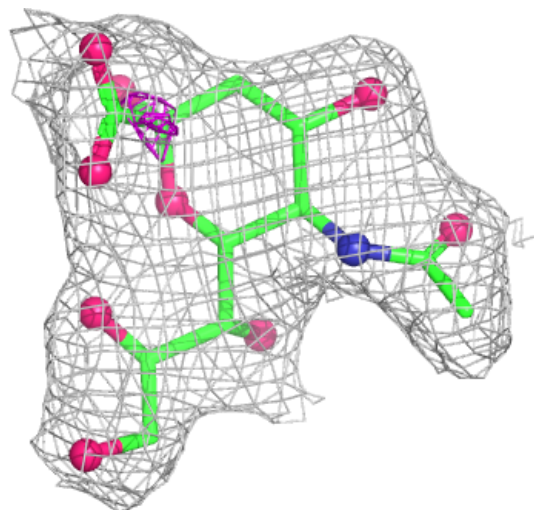
Electron density around SIA R 401:

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



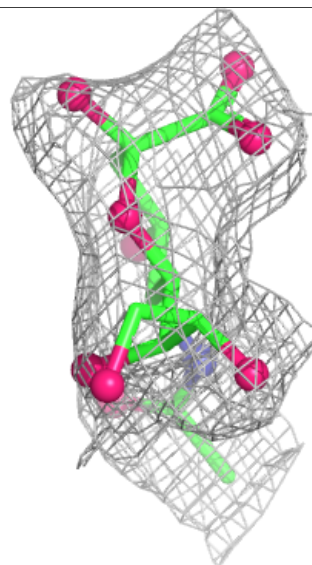
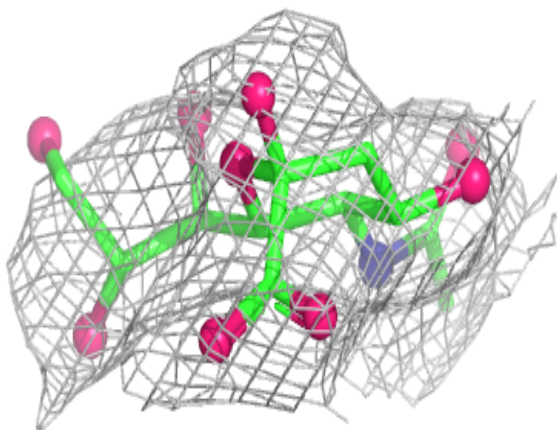
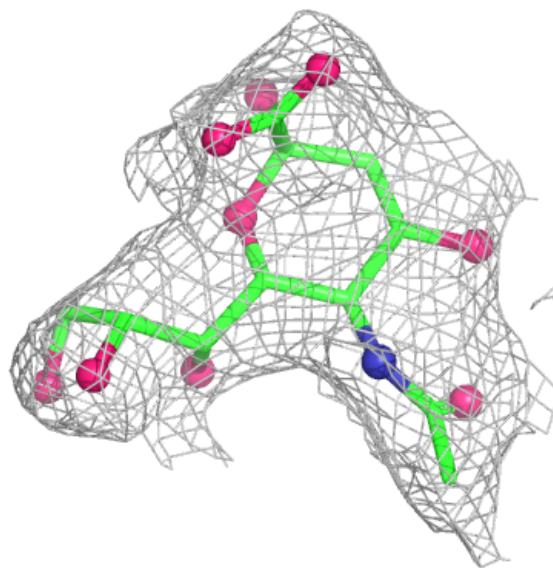
Electron density around SIA J 401:

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



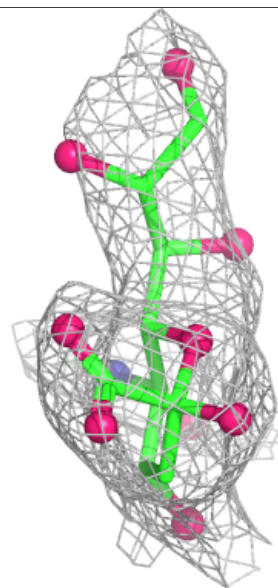
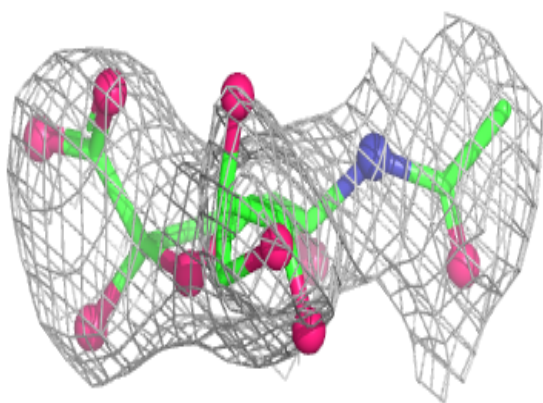
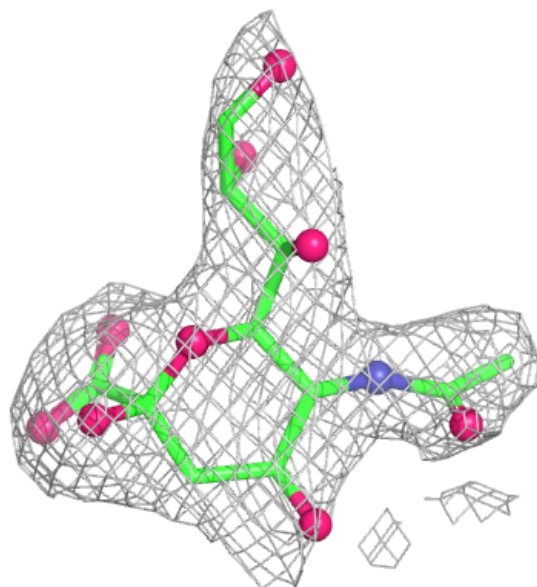
Electron density around SIA K 401:

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



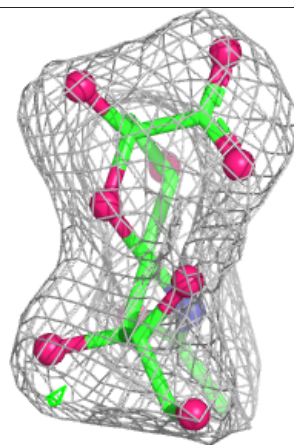
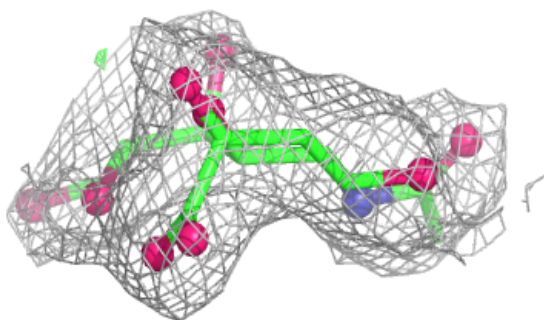
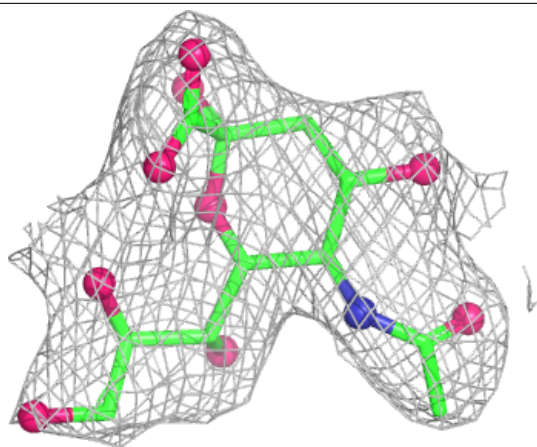
Electron density around SIA S 401:

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



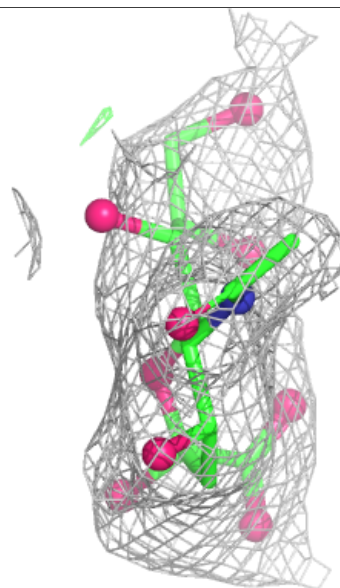
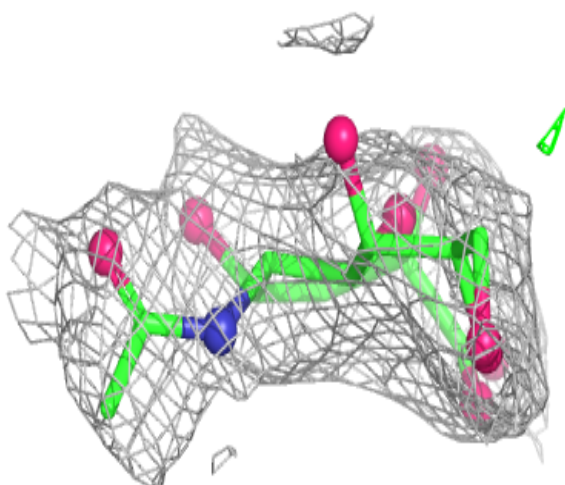
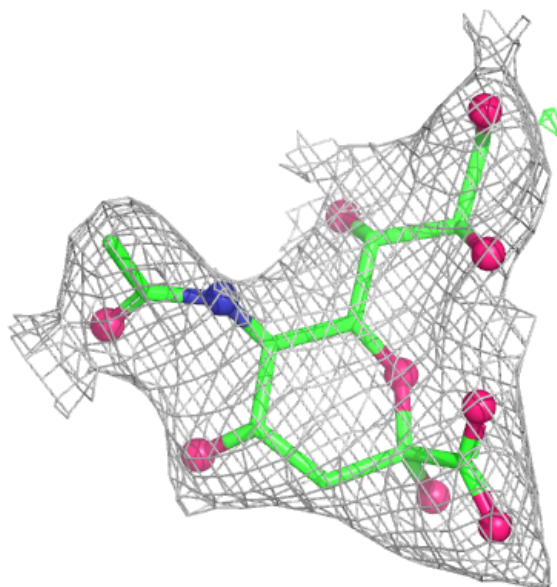
Electron density around SIA M 401:

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



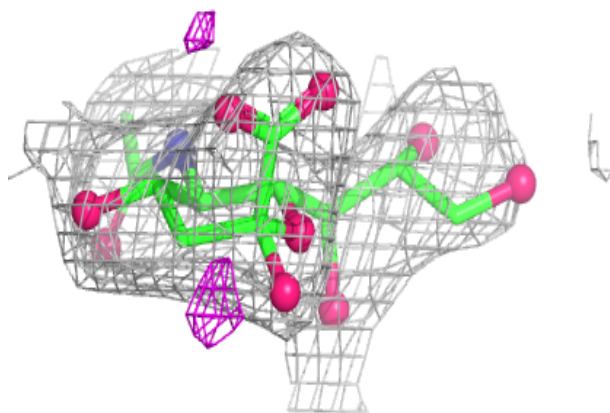
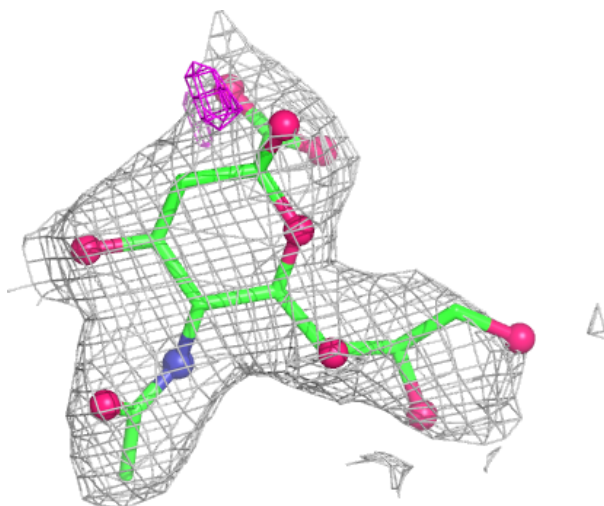
Electron density around SIA Z 401:

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



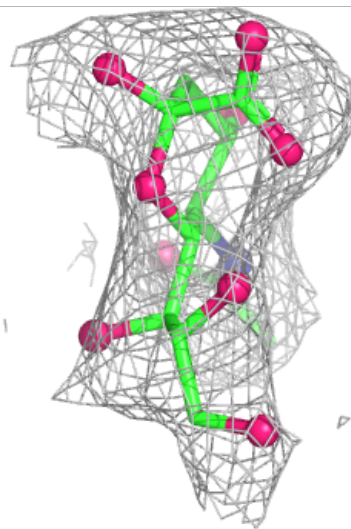
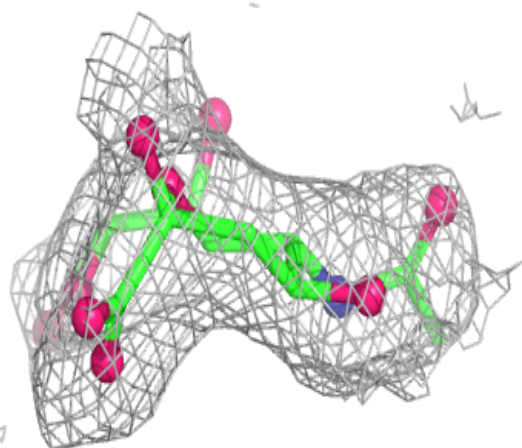
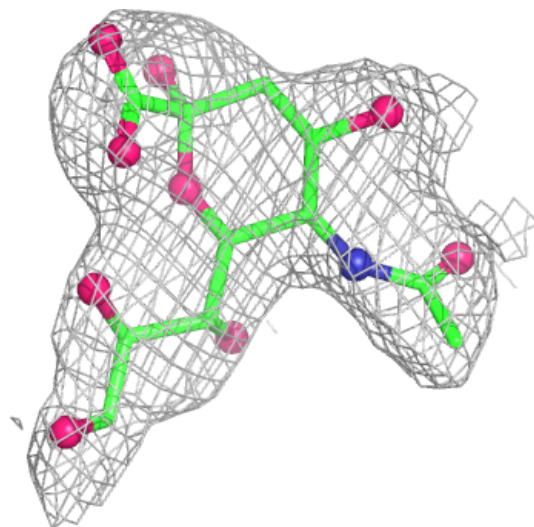
Electron density around SIA B 401:

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



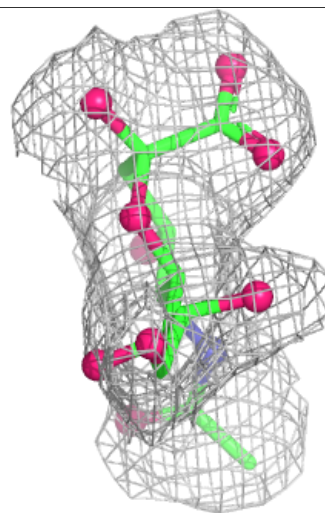
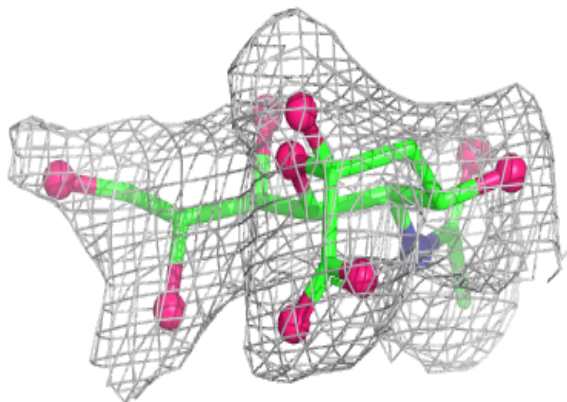
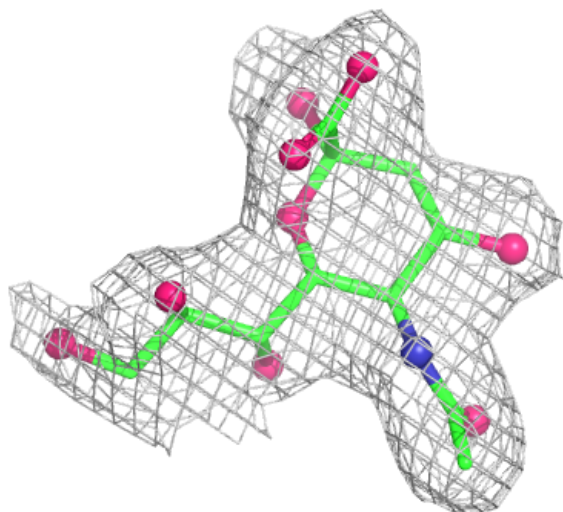
Electron density around SIA e 401:

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



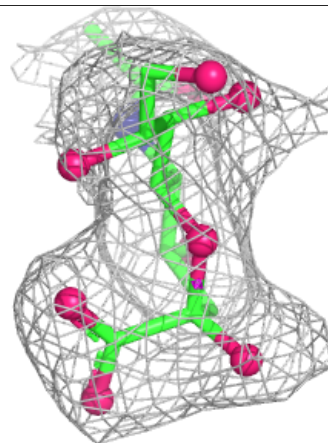
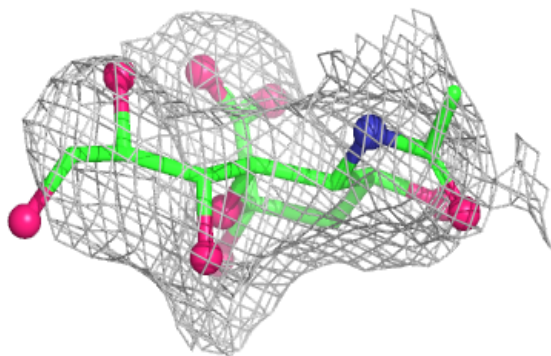
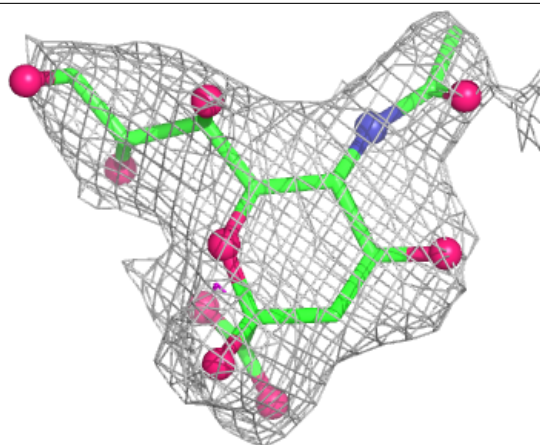
Electron density around SIA L 401:

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



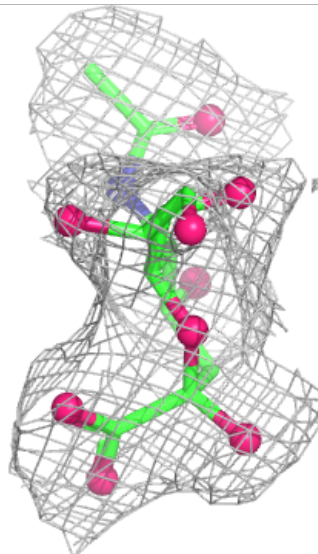
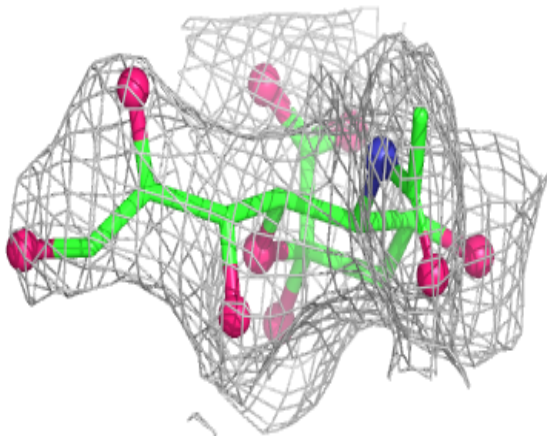
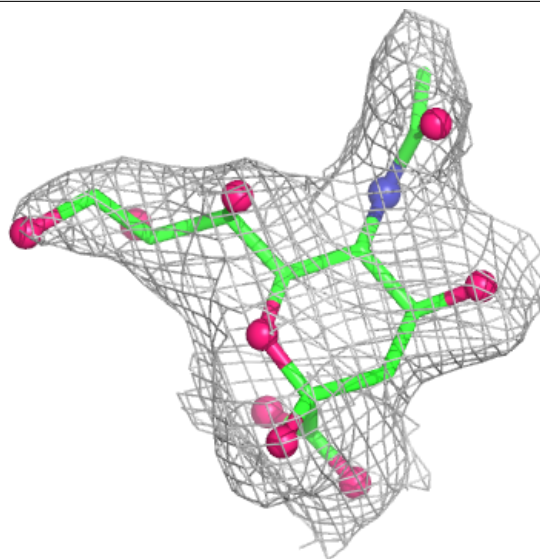
Electron density around SIA E 401:

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



Electron density around SIA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.