



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 14, 2024 – 04:44 PM EST

PDB ID : 1J0B  
Title : Crystal Structure Analysis of the ACC deaminase homologue complexed with inhibitor  
Authors : Fujino, A.; Ose, T.; Honma, M.; Yao, M.; Tanaka, I.  
Deposited on : 2002-11-12  
Resolution : 2.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40



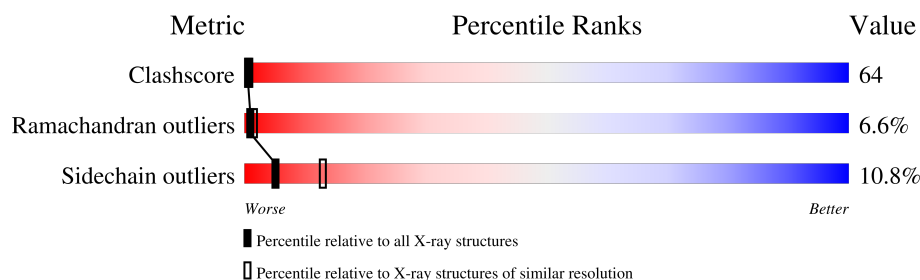
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)

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  $\geq 3$ , 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  $\leq 5\%$ .


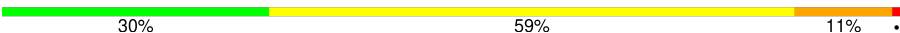



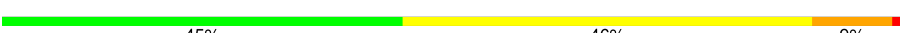




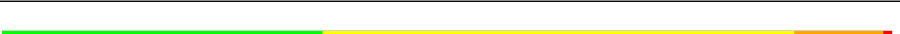


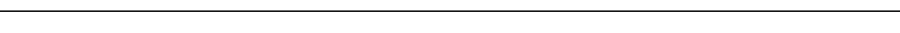
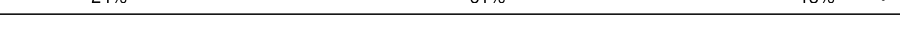
Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	325	42% 50% 7% .
1	B	325	32% 58% 8% .
1	C	325	37% 54% 8% .
1	D	325	41% 51% 7% .
1	E	325	38% 51% 9% .
1	F	325	31% 57% 11% .
1	G	325	16% 70% 13% .
1	H	325	29% 60% 10%

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Mol	Chain	Length	Quality of chain
1	I	325	
1	J	325	
1	K	325	
1	L	325	
1	M	325	
1	N	325	
1	O	325	
1	P	325	
1	Q	325	
1	R	325	
1	S	325	
1	T	325	
1	U	325	
1	V	325	
1	W	325	
1	X	325	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	5PA	B	1021	-	-	X	-
2	5PA	D	1041	-	-	X	-
2	5PA	E	1051	-	-	X	-
2	5PA	F	1061	-	-	X	-
2	5PA	H	1081	-	-	X	-
2	5PA	I	1091	-	-	X	-
2	5PA	J	1101	-	-	X	-
2	5PA	K	1111	-	-	X	-
2	5PA	M	1131	-	-	X	-
2	5PA	P	1161	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	5PA	Q	1171	-	-	X	-
2	5PA	R	1181	-	-	X	-
2	5PA	S	1191	-	-	X	-
2	5PA	V	1221	-	-	X	-
2	5PA	W	1231	-	-	X	-



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 60948 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 1-aminocyclopropane-1-carboxylate deaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	B	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	C	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	D	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	E	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	F	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	G	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	H	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	I	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	J	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	K	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	L	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	M	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	N	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	O	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	P	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			

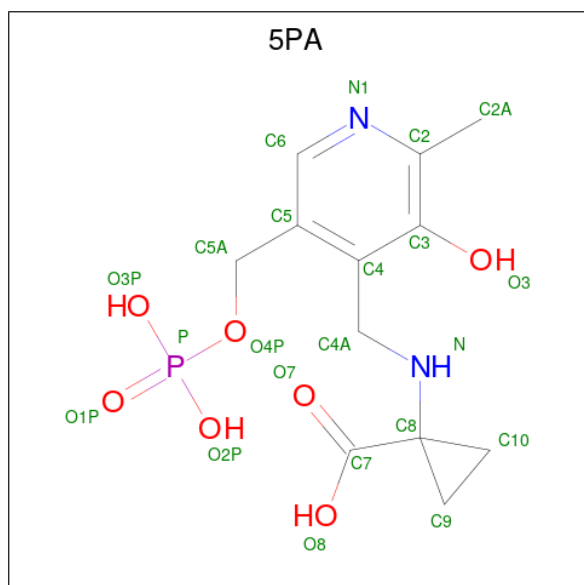
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	R	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	S	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	T	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	U	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	V	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	W	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	X	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			

- Molecule 2 is N-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-Y-LMETHYL]-1-AMINO-CYCLOPROPANECARBOXYLIC ACID (three-letter code: 5PA) (formula: C<sub>12</sub>H<sub>17</sub>N<sub>2</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	12	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			22	12	2	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	D	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	E	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	F	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	G	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	H	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	I	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	J	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	K	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	L	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	M	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	N	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	O	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	P	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	Q	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	R	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	S	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	T	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	U	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	V	1	Total 22	C 12	N 2	O 7	P 1	0	0
2	W	1	Total 22	C 12	N 2	O 7	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	X	1	Total	C	N	O	P	0	0
			22	12	2	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	34	Total	O	0	0
			34	34		
3	C	26	Total	O	0	0
			26	26		
3	D	38	Total	O	0	0
			38	38		
3	E	35	Total	O	0	0
			35	35		
3	F	40	Total	O	0	0
			40	40		
3	G	34	Total	O	0	0
			34	34		
3	H	38	Total	O	0	0
			38	38		
3	I	29	Total	O	0	0
			29	29		
3	J	30	Total	O	0	0
			30	30		
3	K	33	Total	O	0	0
			33	33		
3	L	29	Total	O	0	0
			29	29		
3	M	29	Total	O	0	0
			29	29		
3	N	38	Total	O	0	0
			38	38		
3	O	28	Total	O	0	0
			28	28		
3	P	20	Total	O	0	0
			20	20		
3	Q	25	Total	O	0	0
			25	25		
3	R	21	Total	O	0	0
			21	21		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	42	Total 42	O 42	0	0
3	T	40	Total 40	O 40	0	0
3	U	48	Total 48	O 48	0	0
3	V	40	Total 40	O 40	0	0
3	W	34	Total 34	O 34	0	0
3	X	26	Total 26	O 26	0	0

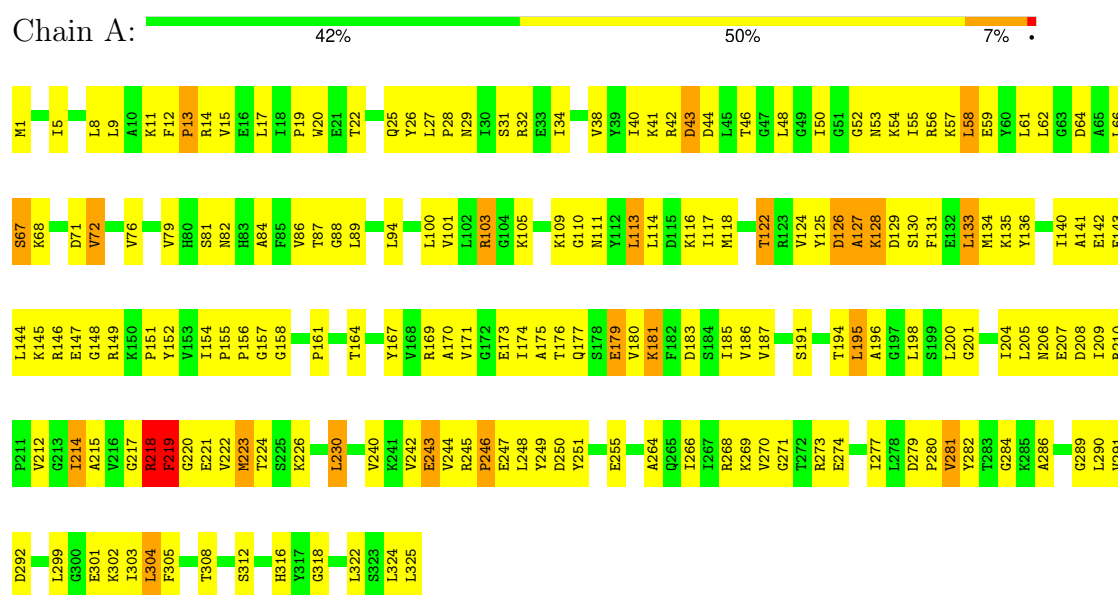


### 3 Residue-property plots

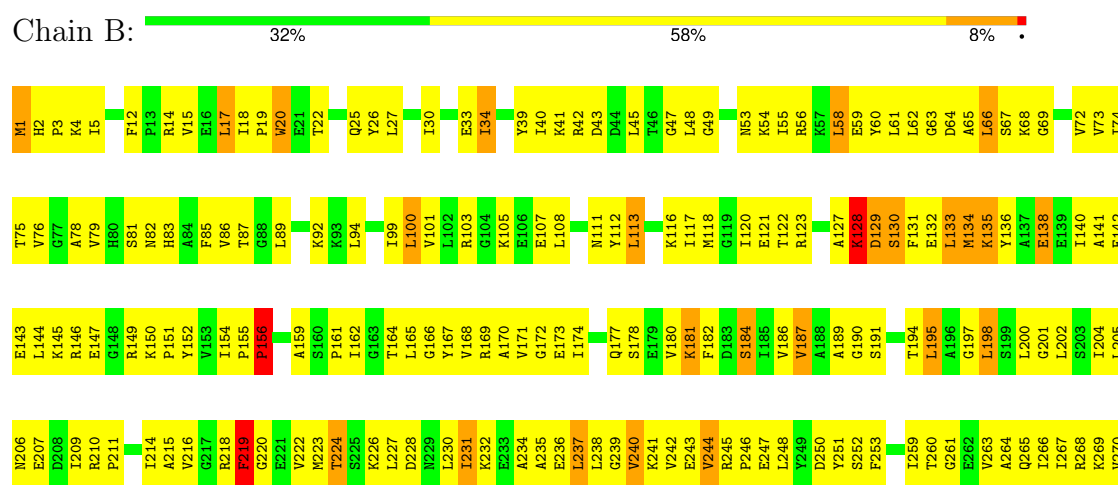
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase





- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

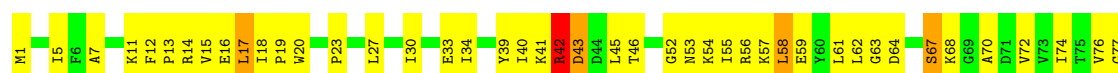
Chain C:  37% 54% 8%

- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

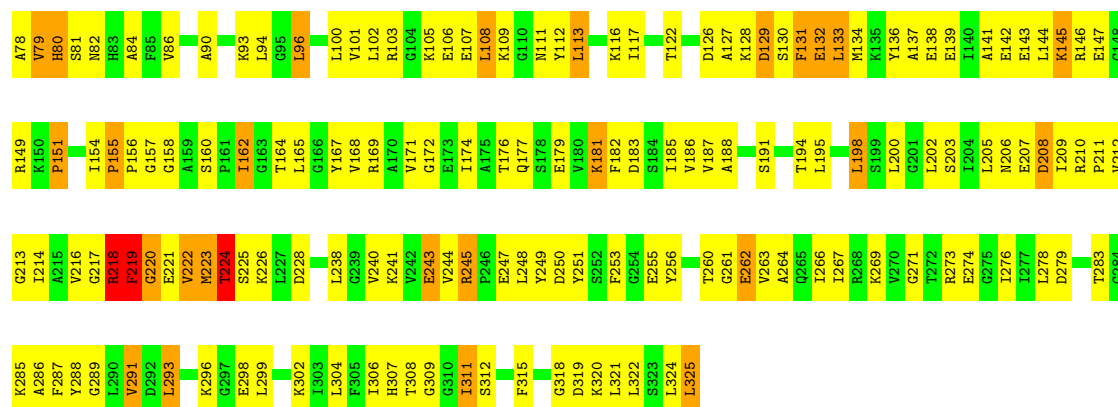
Chain D:  41% 51% 7%

- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain E:  38% 51% 9%

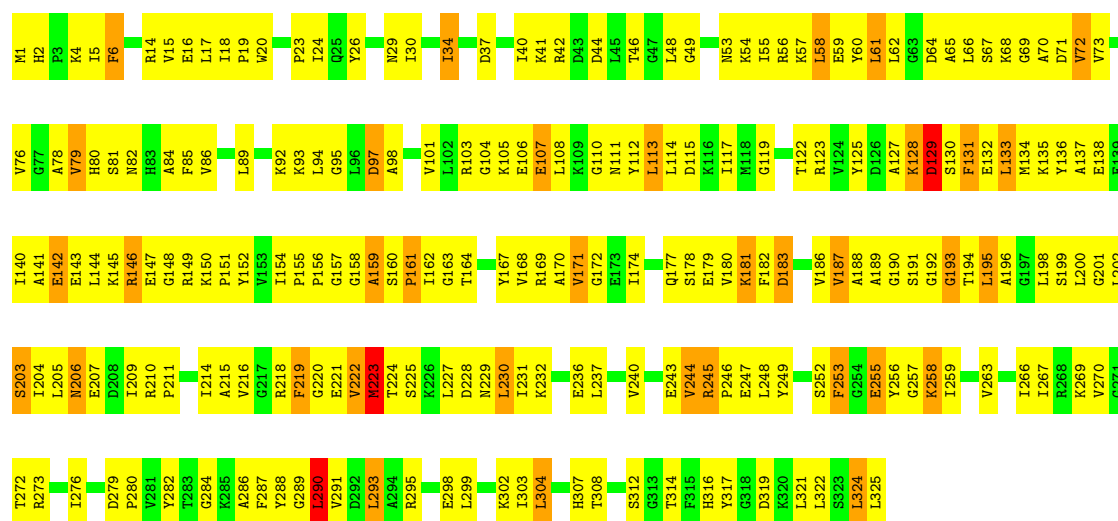






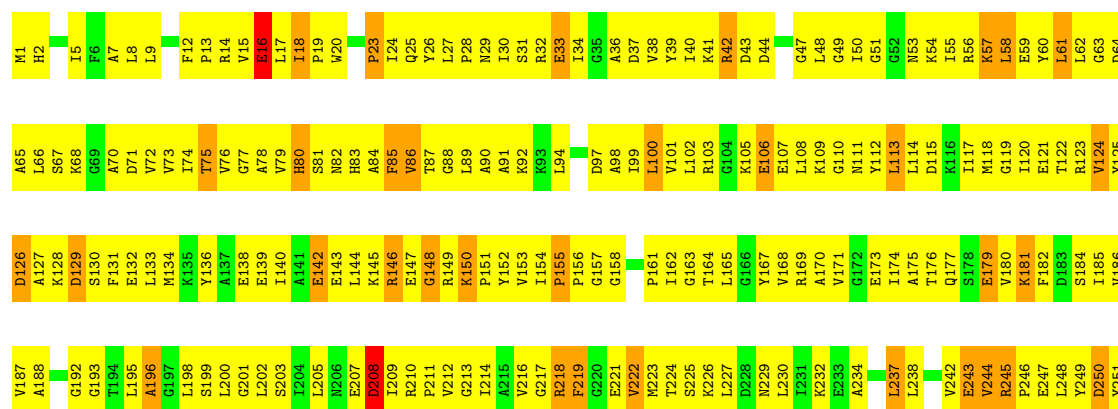
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain F: 31% 57% 11% .

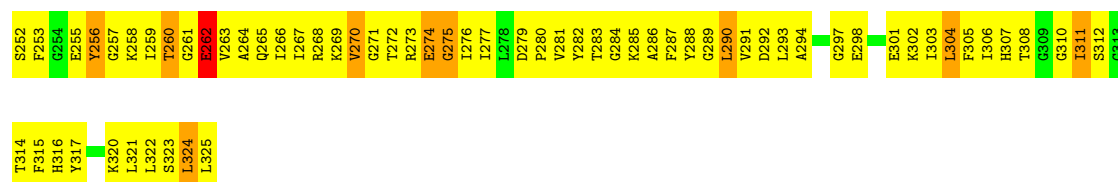


• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

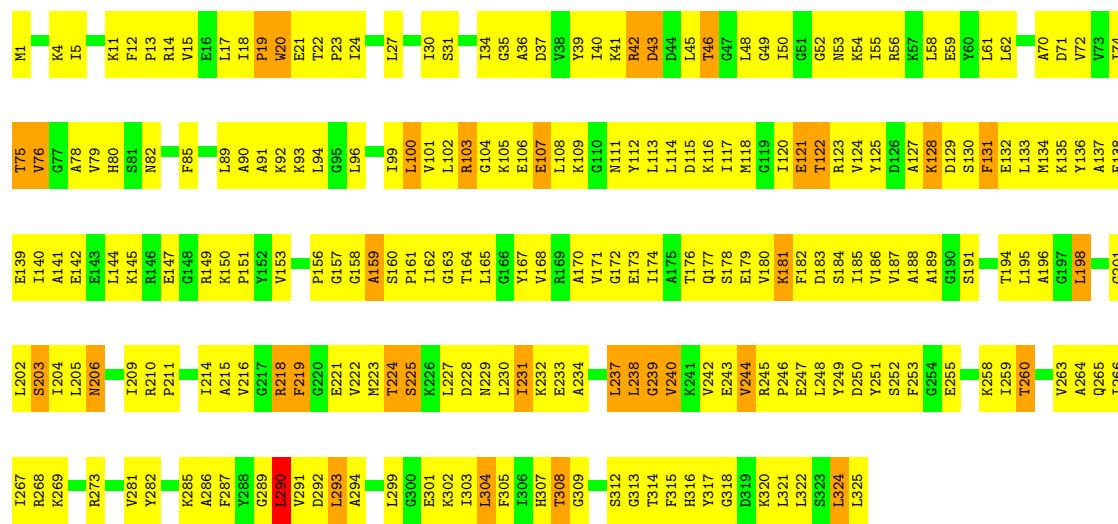
Chain G: 16% 70% 13% .



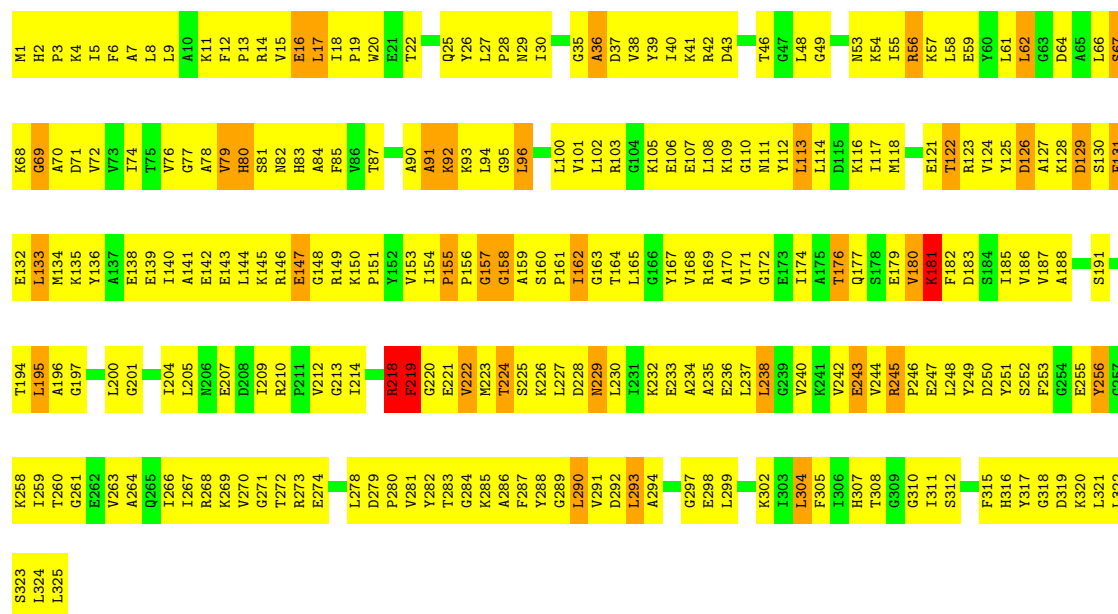




• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



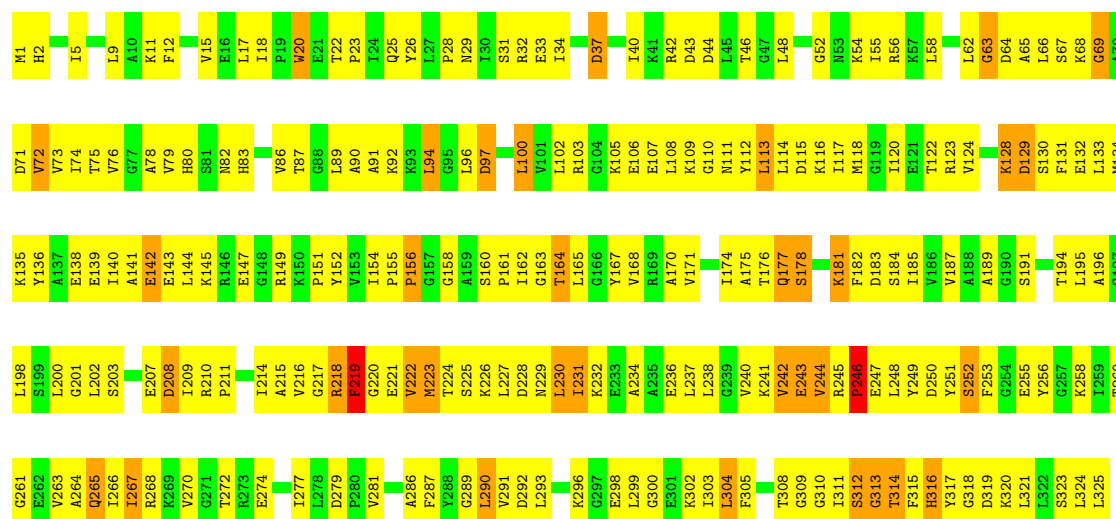
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



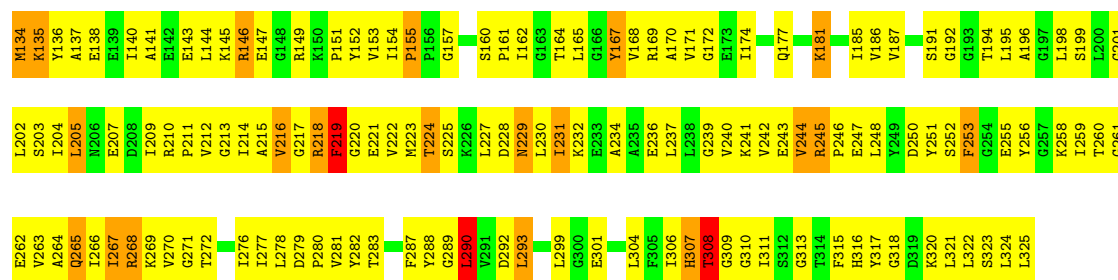
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



Chain J:  30% 59% 11%

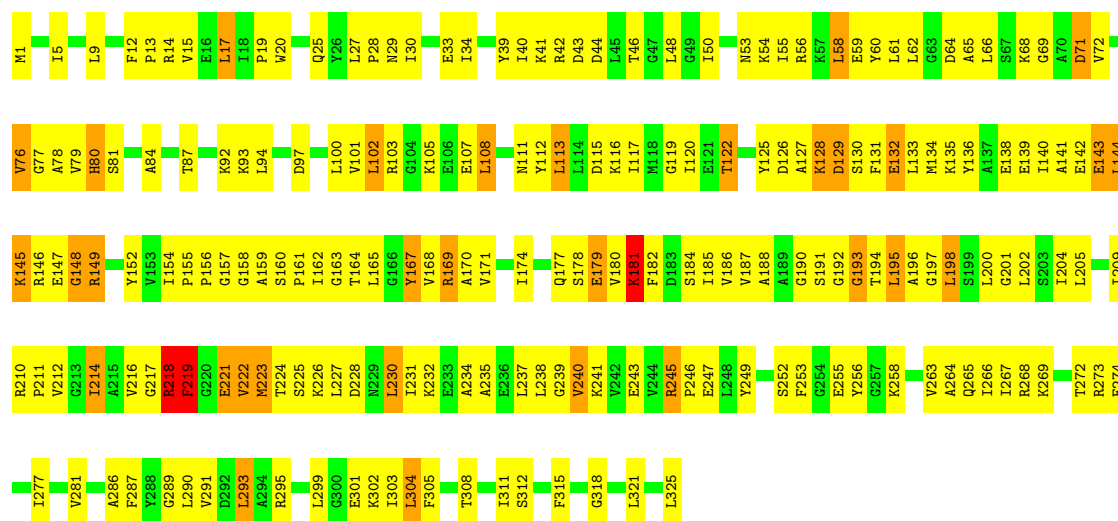






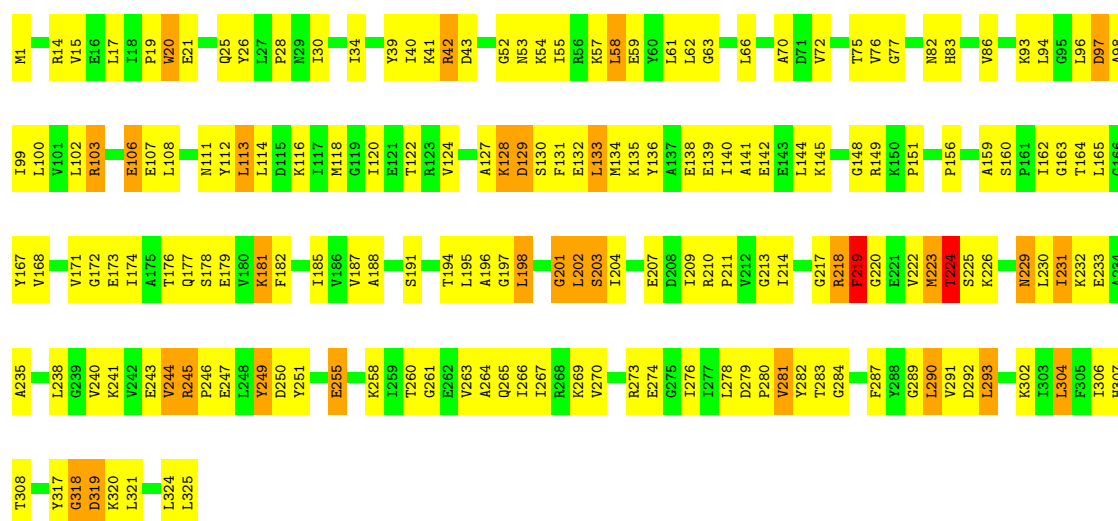
- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain M: 36% 53% 10% •



- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

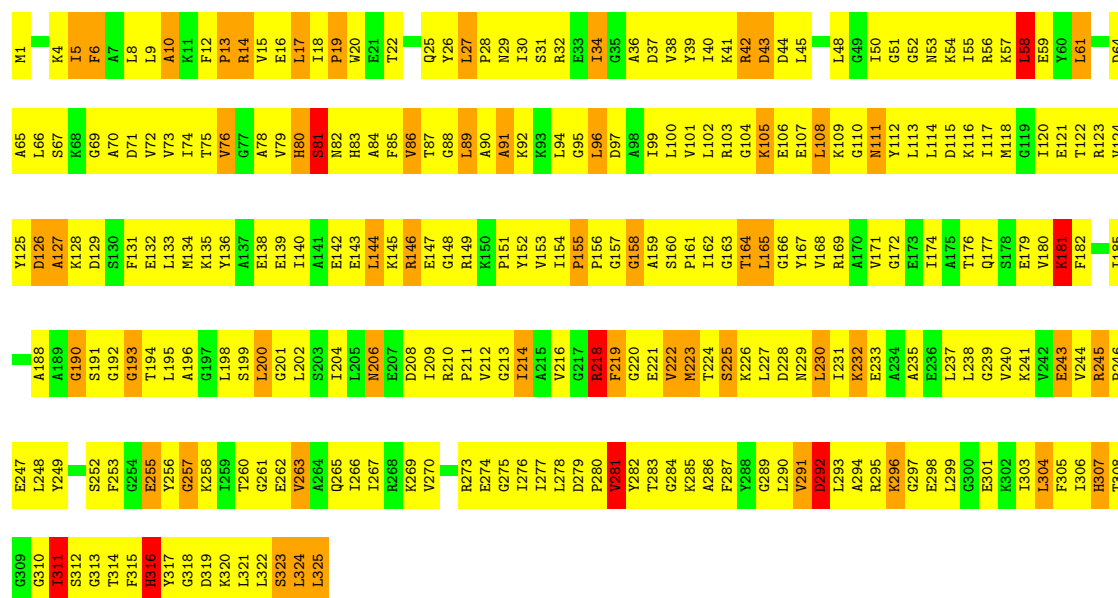
Chain N: 45% 46% 9% •



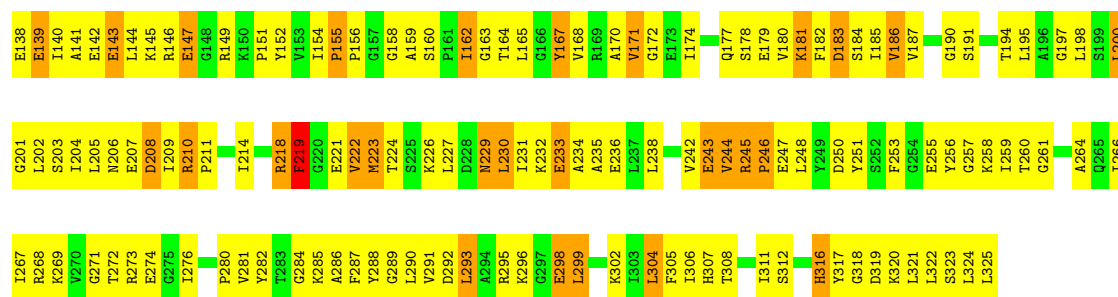
- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



Chain O:  17% 65% 16%

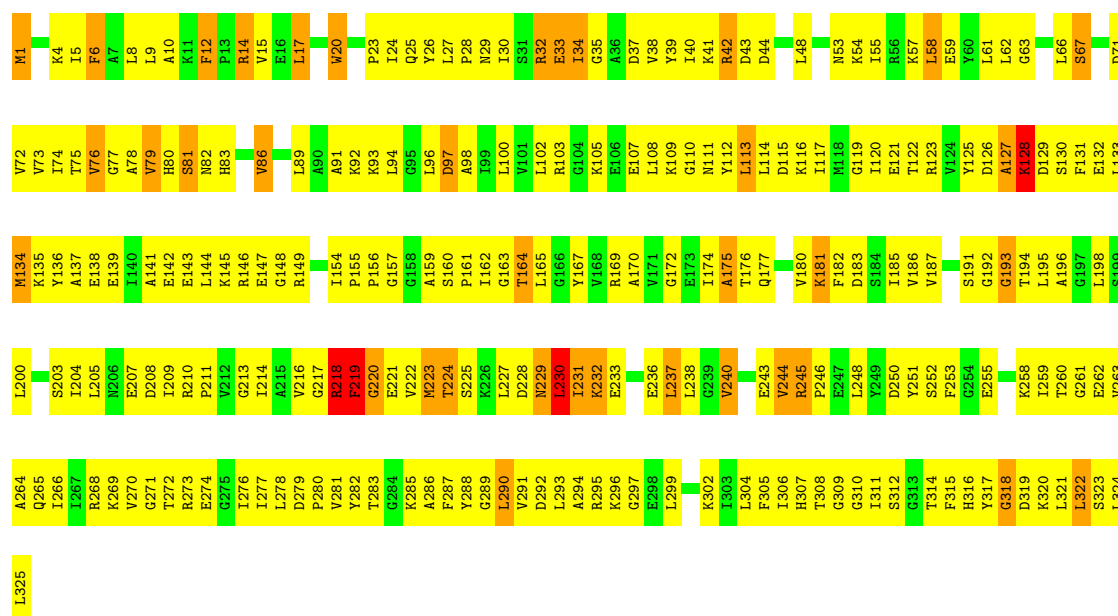






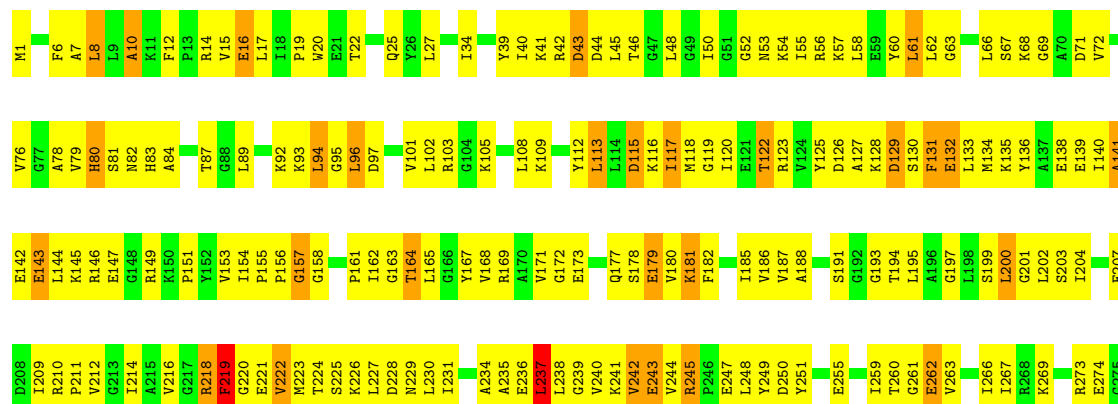
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain R: 25% 63% 11%

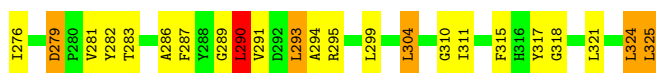


• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

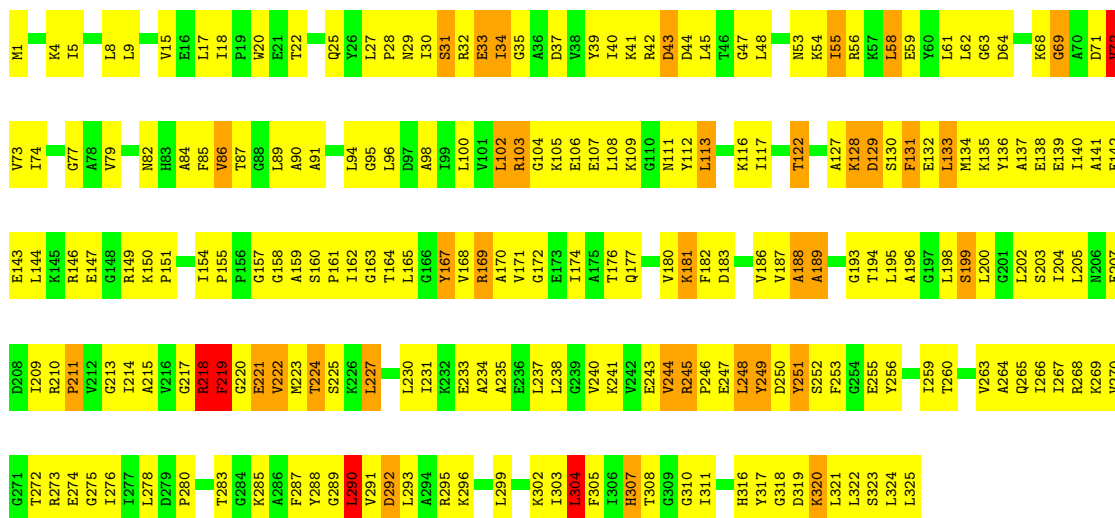
Chain S: 36% 53% 10%



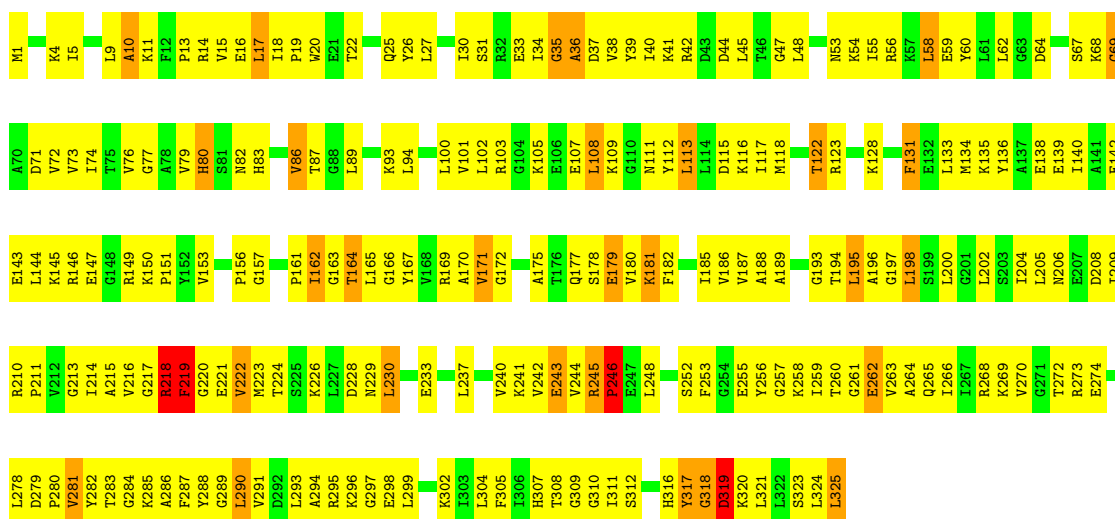




• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



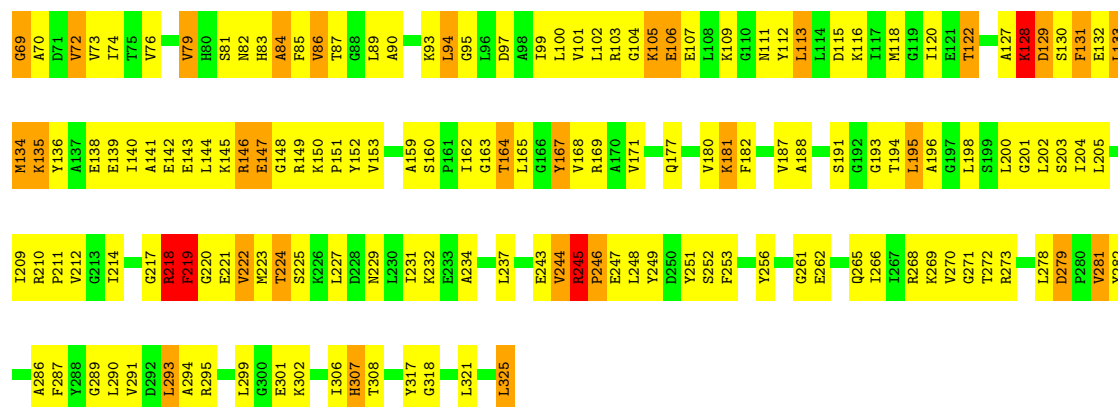
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



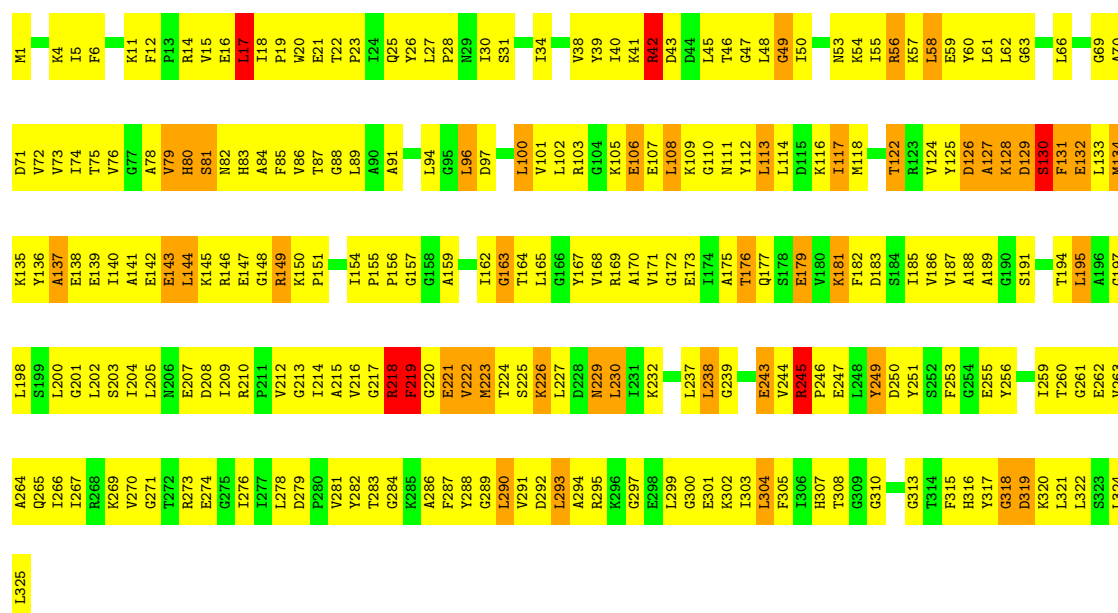
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



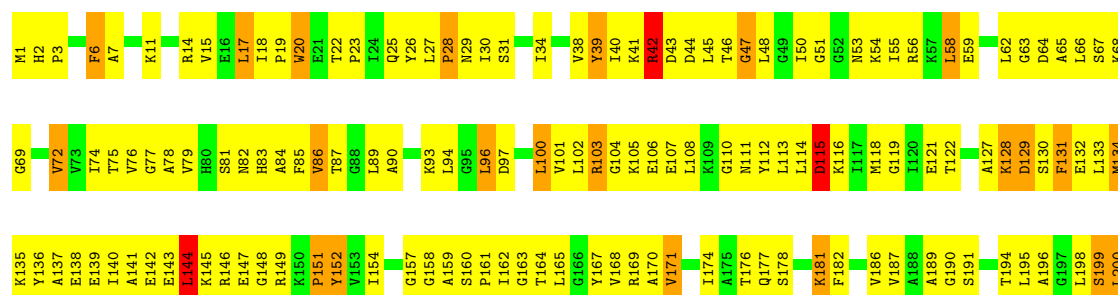




• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase



• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase





G201	L202	S203	I204	L205	N206	E207	D208	I209	R210	P211		I214		G217	R218	F219	G220	E221	V222	M223	T224	S225	K226	L227	D228	N229	L230	F231	K232	E233	A234	A235	E236	L237	L238	G239	V240	K241	V242	E243	V244	R245	P246	E247	L248	D249	N250	Y251	S252	F253	G254	E255		K258	I259	T260	G261	E262	V263
A264	Q265	I266	I267	R268	K269	Y270	G271	T272	R273	E274	G275	L276	L277	L278	D279	P280	V281	Y282	T283	G284	K285	A286	F287	Y288	G289	L290	V291		E298	L299	G300		I303	L304	F305		T308	G309	G310	I311	S312	G313	T314	F315	H316	Y317	G318	D319	K320	L321	L322	S323	L324	L325					



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.87Å 147.28Å 149.07Å 73.18° 90.11° 68.49°	Depositor
Resolution (Å)	10.00 – 2.70	Depositor
% Data completeness (in resolution range)	100.0 (10.00-2.70)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.291 , 0.342	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	60948	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5PA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.45	0/2526	0.76	1/3407 (0.0%)
1	B	0.43	0/2526	0.73	0/3407
1	C	0.42	0/2526	0.74	0/3407
1	D	0.45	0/2526	0.74	0/3407
1	E	0.43	0/2526	0.73	1/3407 (0.0%)
1	F	0.46	0/2526	0.73	1/3407 (0.0%)
1	G	0.48	0/2526	0.80	1/3407 (0.0%)
1	H	0.45	0/2526	0.73	1/3407 (0.0%)
1	I	0.49	0/2526	0.77	1/3407 (0.0%)
1	J	0.45	0/2526	0.74	0/3407
1	K	0.47	0/2526	0.76	0/3407
1	L	0.47	0/2526	0.76	2/3407 (0.1%)
1	M	0.45	0/2526	0.75	0/3407
1	N	0.44	0/2526	0.75	2/3407 (0.1%)
1	O	0.48	0/2526	0.80	0/3407
1	P	0.45	0/2526	0.75	3/3407 (0.1%)
1	Q	0.46	0/2526	0.75	0/3407
1	R	0.46	0/2526	0.76	0/3407
1	S	0.45	0/2526	0.74	1/3407 (0.0%)
1	T	0.46	0/2526	0.78	2/3407 (0.1%)
1	U	0.46	0/2526	0.76	0/3407
1	V	0.44	0/2526	0.77	3/3407 (0.1%)
1	W	0.46	0/2526	0.78	3/3407 (0.1%)
1	X	0.45	0/2526	0.77	2/3407 (0.1%)
All	All	0.45	0/60624	0.76	24/81768 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.



Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	Q	0	1
1	T	0	1
1	V	0	1
All	All	0	7

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	304	LEU	CA-CB-CG	6.44	130.11	115.30
1	W	17	LEU	CA-CB-CG	6.26	129.70	115.30
1	N	290	LEU	CA-CB-CG	6.01	129.13	115.30
1	T	290	LEU	CA-CB-CG	5.89	128.85	115.30
1	I	17	LEU	CA-CB-CG	5.83	128.72	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	167	TYR	Sidechain
1	K	167	TYR	Sidechain
1	L	167	TYR	Sidechain
1	M	167	TYR	Sidechain
1	Q	167	TYR	Sidechain

## 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	2484	0	2583	236	0
1	B	2484	0	2583	289	0
1	C	2484	0	2583	286	1
1	D	2484	0	2583	265	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2484	0	2583	245	0
1	F	2484	0	2583	278	1
1	G	2484	0	2583	501	0
1	H	2484	0	2583	328	0
1	I	2484	0	2583	413	0
1	J	2484	0	2583	363	0
1	K	2484	0	2583	430	0
1	L	2484	0	2583	341	0
1	M	2484	0	2583	325	0
1	N	2484	0	2583	219	0
1	O	2484	0	2583	457	0
1	P	2484	0	2583	362	0
1	Q	2484	0	2583	392	0
1	R	2484	0	2583	353	0
1	S	2484	0	2583	295	0
1	T	2484	0	2583	326	0
1	U	2484	0	2583	282	0
1	V	2484	0	2583	261	0
1	W	2484	0	2583	409	0
1	X	2484	0	2583	341	0
2	A	22	0	13	5	0
2	B	22	0	13	9	0
2	C	22	0	13	6	0
2	D	22	0	13	8	0
2	E	22	0	13	7	0
2	F	22	0	13	15	0
2	G	22	0	13	3	0
2	H	22	0	13	7	0
2	I	22	0	13	13	0
2	J	22	0	13	9	0
2	K	22	0	13	11	0
2	L	22	0	13	6	0
2	M	22	0	13	11	0
2	N	22	0	13	4	0
2	O	22	0	13	6	0
2	P	22	0	13	10	0
2	Q	22	0	13	15	0
2	R	22	0	13	14	0
2	S	22	0	13	9	0
2	T	22	0	13	6	0
2	U	22	0	13	6	0
2	V	22	0	13	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	22	0	13	8	0
2	X	22	0	13	6	0
3	A	47	0	0	10	0
3	B	34	0	0	7	0
3	C	26	0	0	3	0
3	D	38	0	0	9	0
3	E	35	0	0	5	0
3	F	40	0	0	6	0
3	G	34	0	0	12	0
3	H	38	0	0	11	0
3	I	29	0	0	9	0
3	J	30	0	0	8	0
3	K	33	0	0	8	0
3	L	29	0	0	12	0
3	M	29	0	0	8	0
3	N	38	0	0	6	0
3	O	28	0	0	9	0
3	P	20	0	0	11	0
3	Q	25	0	0	13	0
3	R	21	0	0	5	0
3	S	42	0	0	10	0
3	T	40	0	0	12	0
3	U	48	0	0	9	0
3	V	40	0	0	6	0
3	W	34	0	0	10	0
3	X	26	0	0	6	0
All	All	60948	0	62304	7808	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 64.

The worst 5 of 7808 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:X:128:LYS:H	1:X:128:LYS:HD3	1.06	1.19
1:C:103:ARG:HD3	1:C:133:LEU:HD22	1.21	1.15
1:G:147:GLU:CB	1:I:221:GLU:HA	1.75	1.15
1:C:214:ILE:HD13	1:C:286:ALA:HA	1.29	1.14
1:G:147:GLU:HB3	1:I:221:GLU:HA	1.18	1.14

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



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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:PHE:O	1:F:147:GLU:O[1_455]	2.12	0.08

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	323/325 (99%)	268 (83%)	42 (13%)	13 (4%)	2	5
1	B	323/325 (99%)	257 (80%)	50 (16%)	16 (5%)	1	3
1	C	323/325 (99%)	256 (79%)	51 (16%)	16 (5%)	1	3
1	D	323/325 (99%)	273 (84%)	34 (10%)	16 (5%)	1	3
1	E	323/325 (99%)	270 (84%)	36 (11%)	17 (5%)	1	3
1	F	323/325 (99%)	268 (83%)	37 (12%)	18 (6%)	1	2
1	G	323/325 (99%)	232 (72%)	63 (20%)	28 (9%)	0	0
1	H	323/325 (99%)	258 (80%)	51 (16%)	14 (4%)	2	4
1	I	323/325 (99%)	250 (77%)	50 (16%)	23 (7%)	1	1
1	J	323/325 (99%)	242 (75%)	57 (18%)	24 (7%)	1	1
1	K	323/325 (99%)	231 (72%)	61 (19%)	31 (10%)	0	0
1	L	323/325 (99%)	260 (80%)	43 (13%)	20 (6%)	1	2
1	M	323/325 (99%)	263 (81%)	45 (14%)	15 (5%)	2	4
1	N	323/325 (99%)	275 (85%)	37 (12%)	11 (3%)	3	7
1	O	323/325 (99%)	208 (64%)	69 (21%)	46 (14%)	0	0
1	P	323/325 (99%)	241 (75%)	56 (17%)	26 (8%)	1	1
1	Q	323/325 (99%)	241 (75%)	58 (18%)	24 (7%)	1	1
1	R	323/325 (99%)	259 (80%)	43 (13%)	21 (6%)	1	1
1	S	323/325 (99%)	255 (79%)	51 (16%)	17 (5%)	1	3
1	T	323/325 (99%)	259 (80%)	38 (12%)	26 (8%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	323/325 (99%)	264 (82%)	40 (12%)	19 (6%)	1	2
1	V	323/325 (99%)	266 (82%)	41 (13%)	16 (5%)	1	3
1	W	323/325 (99%)	234 (72%)	60 (19%)	29 (9%)	0	0
1	X	323/325 (99%)	235 (73%)	59 (18%)	29 (9%)	0	0
All	All	7752/7800 (99%)	6065 (78%)	1172 (15%)	515 (7%)	1	1

5 of 515 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	PHE
1	A	245	ARG
1	B	33	GLU
1	B	72	VAL
1	B	187	VAL

### 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	259/259 (100%)	230 (89%)	29 (11%)	5	12
1	B	259/259 (100%)	232 (90%)	27 (10%)	5	14
1	C	259/259 (100%)	236 (91%)	23 (9%)	8	20
1	D	259/259 (100%)	238 (92%)	21 (8%)	9	23
1	E	259/259 (100%)	231 (89%)	28 (11%)	5	13
1	F	259/259 (100%)	226 (87%)	33 (13%)	3	9
1	G	259/259 (100%)	231 (89%)	28 (11%)	5	13
1	H	259/259 (100%)	231 (89%)	28 (11%)	5	13
1	I	259/259 (100%)	236 (91%)	23 (9%)	8	20
1	J	259/259 (100%)	236 (91%)	23 (9%)	8	20
1	K	259/259 (100%)	234 (90%)	25 (10%)	6	17
1	L	259/259 (100%)	237 (92%)	22 (8%)	8	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	259/259 (100%)	232 (90%)	27 (10%)	5	14
1	N	259/259 (100%)	230 (89%)	29 (11%)	5	12
1	O	259/259 (100%)	228 (88%)	31 (12%)	4	10
1	P	259/259 (100%)	224 (86%)	35 (14%)	3	7
1	Q	259/259 (100%)	232 (90%)	27 (10%)	5	14
1	R	259/259 (100%)	223 (86%)	36 (14%)	3	7
1	S	259/259 (100%)	230 (89%)	29 (11%)	5	12
1	T	259/259 (100%)	230 (89%)	29 (11%)	5	12
1	U	259/259 (100%)	232 (90%)	27 (10%)	5	14
1	V	259/259 (100%)	228 (88%)	31 (12%)	4	10
1	W	259/259 (100%)	227 (88%)	32 (12%)	4	9
1	X	259/259 (100%)	229 (88%)	30 (12%)	4	11
All	All	6216/6216 (100%)	5543 (89%)	673 (11%)	5	13

5 of 673 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	20	TRP
1	U	246	PRO
1	R	113	LEU
1	R	17	LEU
1	S	293	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	82	ASN
1	V	229	ASN
1	O	25	GLN
1	V	206	ASN
1	X	29	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	5PA	X	1241	-	22,23,23	2.46	5 (22%)	33,35,35	2.10	9 (27%)
2	5PA	L	1121	-	22,23,23	2.49	7 (31%)	33,35,35	2.20	8 (24%)
2	5PA	T	1201	-	22,23,23	2.44	6 (27%)	33,35,35	2.09	6 (18%)
2	5PA	P	1161	-	22,23,23	2.47	6 (27%)	33,35,35	2.06	7 (21%)
2	5PA	N	1141	-	22,23,23	2.45	5 (22%)	33,35,35	2.17	6 (18%)
2	5PA	V	1221	-	22,23,23	2.49	5 (22%)	33,35,35	2.15	7 (21%)
2	5PA	S	1191	-	22,23,23	2.46	7 (31%)	33,35,35	2.30	9 (27%)
2	5PA	O	1151	-	22,23,23	2.52	7 (31%)	33,35,35	1.91	6 (18%)
2	5PA	E	1051	-	22,23,23	2.48	6 (27%)	33,35,35	2.14	7 (21%)
2	5PA	I	1091	-	22,23,23	2.45	6 (27%)	33,35,35	2.06	5 (15%)
2	5PA	Q	1171	-	22,23,23	2.49	6 (27%)	33,35,35	2.10	5 (15%)
2	5PA	H	1081	-	22,23,23	2.54	6 (27%)	33,35,35	2.06	9 (27%)
2	5PA	M	1131	-	22,23,23	2.47	6 (27%)	33,35,35	2.16	8 (24%)
2	5PA	J	1101	-	22,23,23	2.47	7 (31%)	33,35,35	1.98	6 (18%)
2	5PA	G	1071	-	22,23,23	2.46	8 (36%)	33,35,35	2.24	8 (24%)
2	5PA	R	1181	-	22,23,23	2.48	5 (22%)	33,35,35	2.19	7 (21%)
2	5PA	U	1211	-	22,23,23	2.46	6 (27%)	33,35,35	2.26	6 (18%)
2	5PA	C	1031	-	22,23,23	2.45	6 (27%)	33,35,35	2.22	8 (24%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	5PA	B	1021	-	22,23,23	2.47	6 (27%)	33,35,35	2.12	7 (21%)
2	5PA	K	1111	-	22,23,23	2.44	6 (27%)	33,35,35	2.38	6 (18%)
2	5PA	A	1011	-	22,23,23	2.47	5 (22%)	33,35,35	2.25	8 (24%)
2	5PA	D	1041	-	22,23,23	2.47	6 (27%)	33,35,35	2.08	9 (27%)
2	5PA	F	1061	-	22,23,23	2.47	5 (22%)	33,35,35	2.04	6 (18%)
2	5PA	W	1231	-	22,23,23	2.48	7 (31%)	33,35,35	2.02	5 (15%)

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	5PA	X	1241	-	-	7/15/22/22	0/2/2/2
2	5PA	L	1121	-	-	10/15/22/22	0/2/2/2
2	5PA	T	1201	-	-	6/15/22/22	0/2/2/2
2	5PA	P	1161	-	-	8/15/22/22	0/2/2/2
2	5PA	N	1141	-	-	6/15/22/22	0/2/2/2
2	5PA	V	1221	-	-	8/15/22/22	0/2/2/2
2	5PA	S	1191	-	-	4/15/22/22	0/2/2/2
2	5PA	O	1151	-	-	9/15/22/22	0/2/2/2
2	5PA	E	1051	-	-	6/15/22/22	0/2/2/2
2	5PA	I	1091	-	-	9/15/22/22	0/2/2/2
2	5PA	Q	1171	-	-	6/15/22/22	0/2/2/2
2	5PA	H	1081	-	-	8/15/22/22	0/2/2/2
2	5PA	M	1131	-	-	7/15/22/22	0/2/2/2
2	5PA	J	1101	-	-	12/15/22/22	0/2/2/2
2	5PA	G	1071	-	-	7/15/22/22	0/2/2/2
2	5PA	R	1181	-	-	8/15/22/22	0/2/2/2
2	5PA	U	1211	-	-	9/15/22/22	0/2/2/2
2	5PA	C	1031	-	-	7/15/22/22	0/2/2/2
2	5PA	B	1021	-	-	6/15/22/22	0/2/2/2
2	5PA	K	1111	-	-	8/15/22/22	0/2/2/2
2	5PA	A	1011	-	-	8/15/22/22	0/2/2/2
2	5PA	D	1041	-	-	8/15/22/22	0/2/2/2
2	5PA	F	1061	-	-	8/15/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5PA	W	1231	-	-	7/15/22/22	0/2/2/2

The worst 5 of 145 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1051	5PA	C4A-C4	-8.37	1.39	1.52
2	H	1081	5PA	C4A-C4	-8.37	1.39	1.52
2	V	1221	5PA	C4A-C4	-8.36	1.39	1.52
2	A	1011	5PA	C4A-C4	-8.33	1.39	1.52
2	M	1131	5PA	C4A-C4	-8.32	1.39	1.52

The worst 5 of 168 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1111	5PA	O4P-C5A-C5	8.12	124.57	109.36
2	C	1031	5PA	O4P-C5A-C5	6.97	122.41	109.36
2	S	1191	5PA	O4P-C5A-C5	6.88	122.25	109.36
2	U	1211	5PA	O4P-C5A-C5	6.79	122.09	109.36
2	G	1071	5PA	O4P-C5A-C5	6.53	121.59	109.36

There are no chirality outliers.

5 of 182 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1011	5PA	C5-C4-C4A-N
2	A	1011	5PA	C3-C4-C4A-N
2	A	1011	5PA	C4-C5-C5A-O4P
2	A	1011	5PA	C6-C5-C5A-O4P
2	A	1011	5PA	O7-C7-C8-N

There are no ring outliers.

24 monomers are involved in 201 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	1241	5PA	6	0
2	L	1121	5PA	6	0
2	T	1201	5PA	6	0
2	P	1161	5PA	10	0
2	N	1141	5PA	4	0
2	V	1221	5PA	7	0
2	S	1191	5PA	9	0

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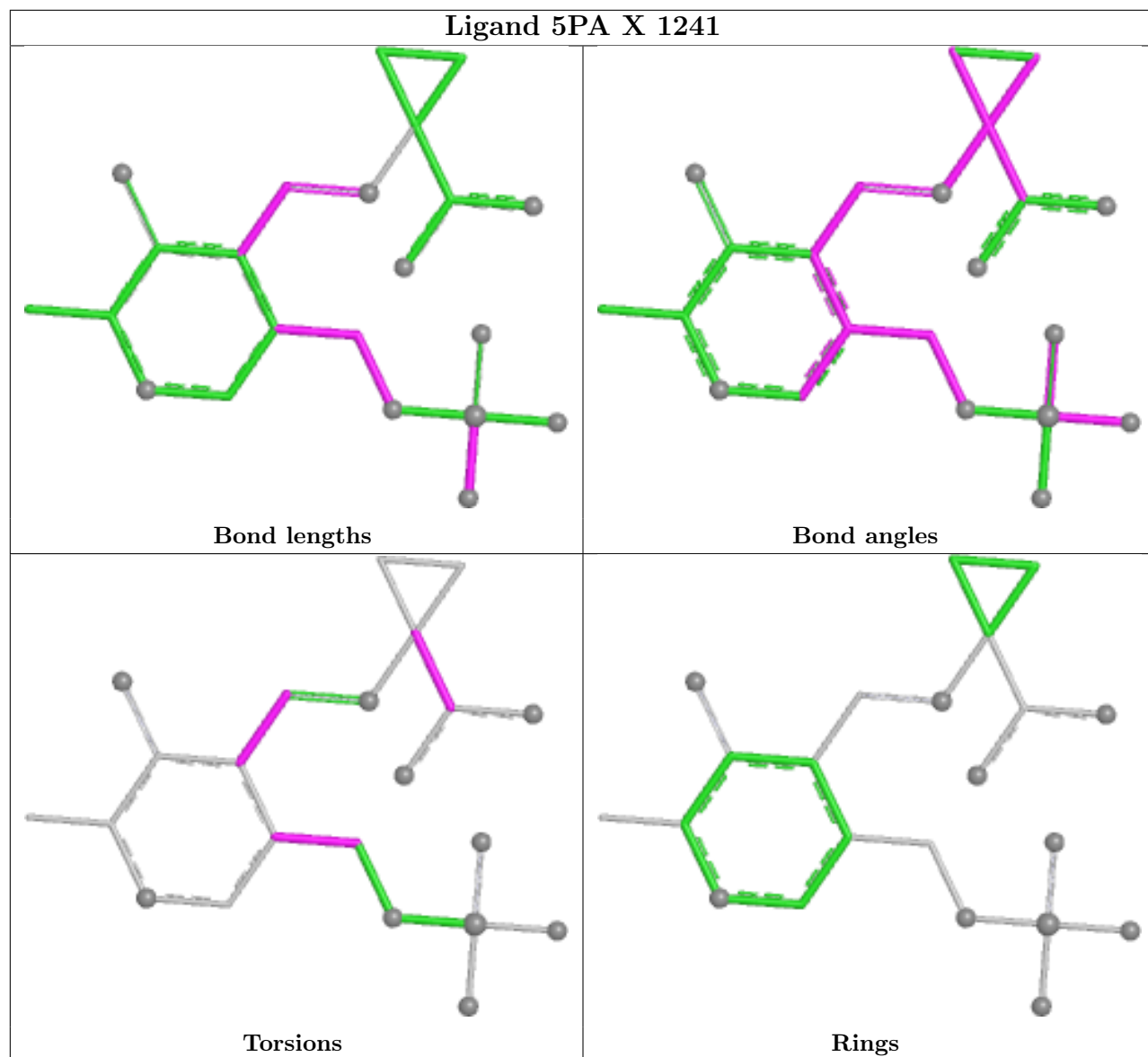


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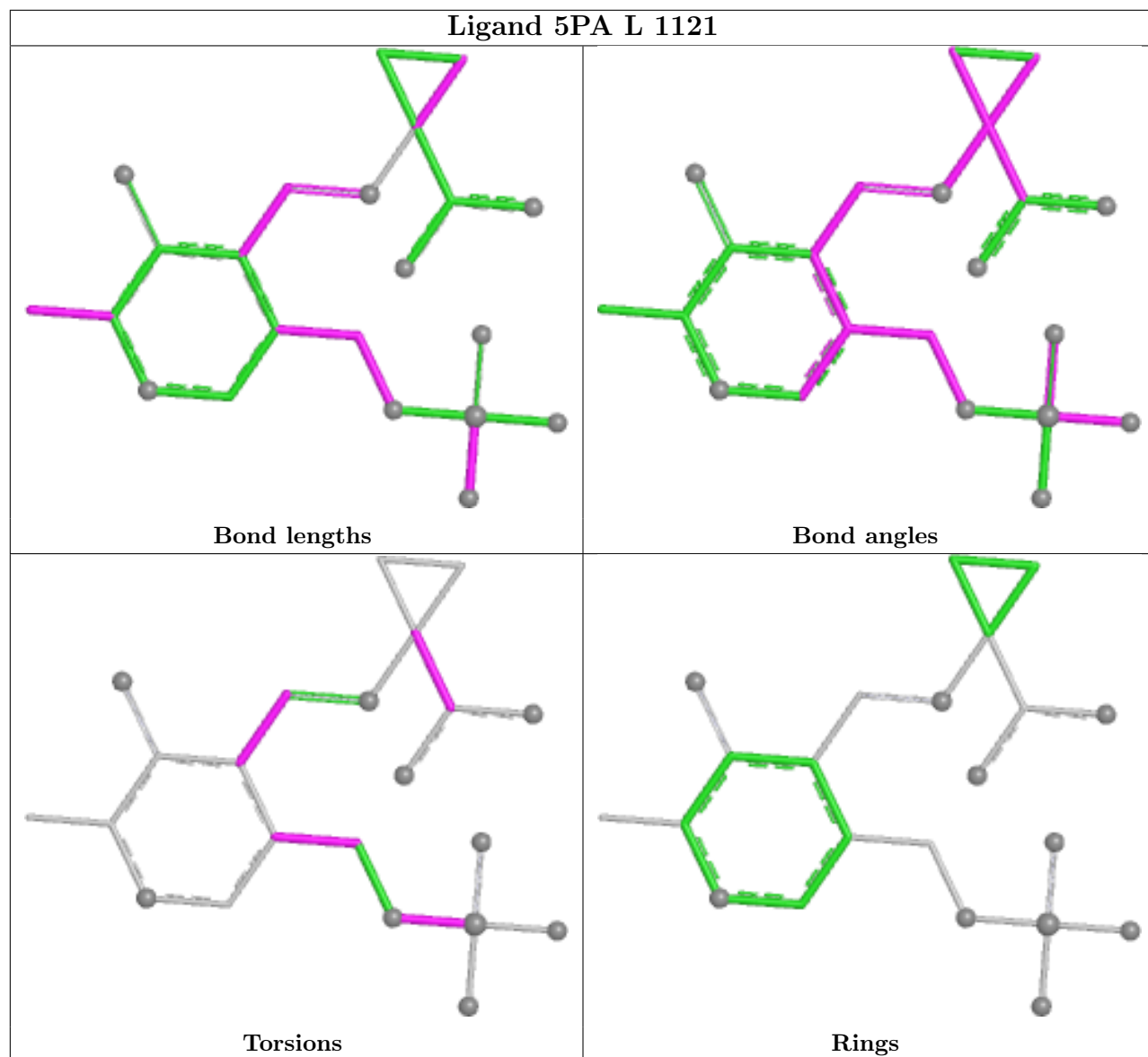
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1151	5PA	6	0
2	E	1051	5PA	7	0
2	I	1091	5PA	13	0
2	Q	1171	5PA	15	0
2	H	1081	5PA	7	0
2	M	1131	5PA	11	0
2	J	1101	5PA	9	0
2	G	1071	5PA	3	0
2	R	1181	5PA	14	0
2	U	1211	5PA	6	0
2	C	1031	5PA	6	0
2	B	1021	5PA	9	0
2	K	1111	5PA	11	0
2	A	1011	5PA	5	0
2	D	1041	5PA	8	0
2	F	1061	5PA	15	0
2	W	1231	5PA	8	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.

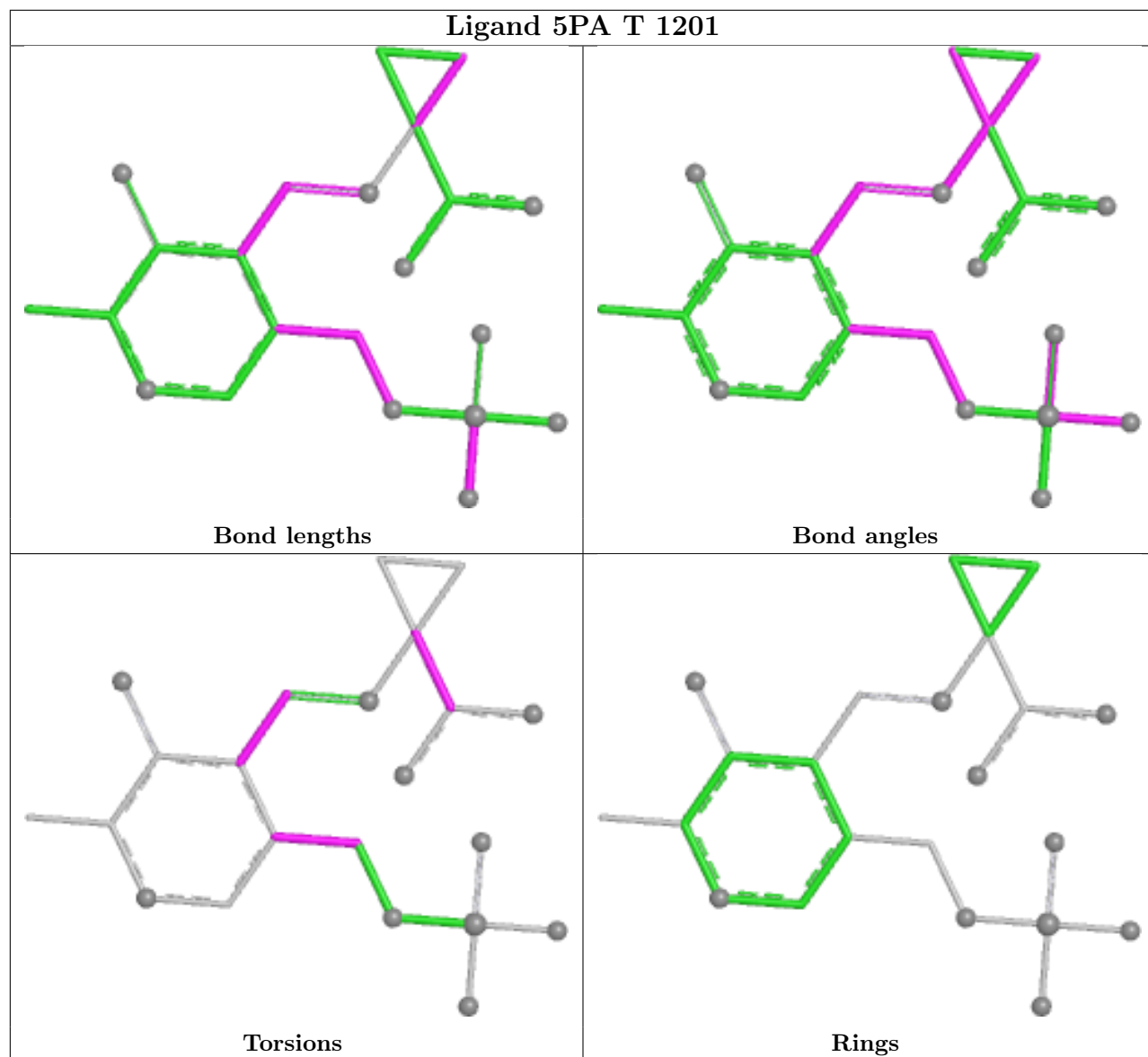




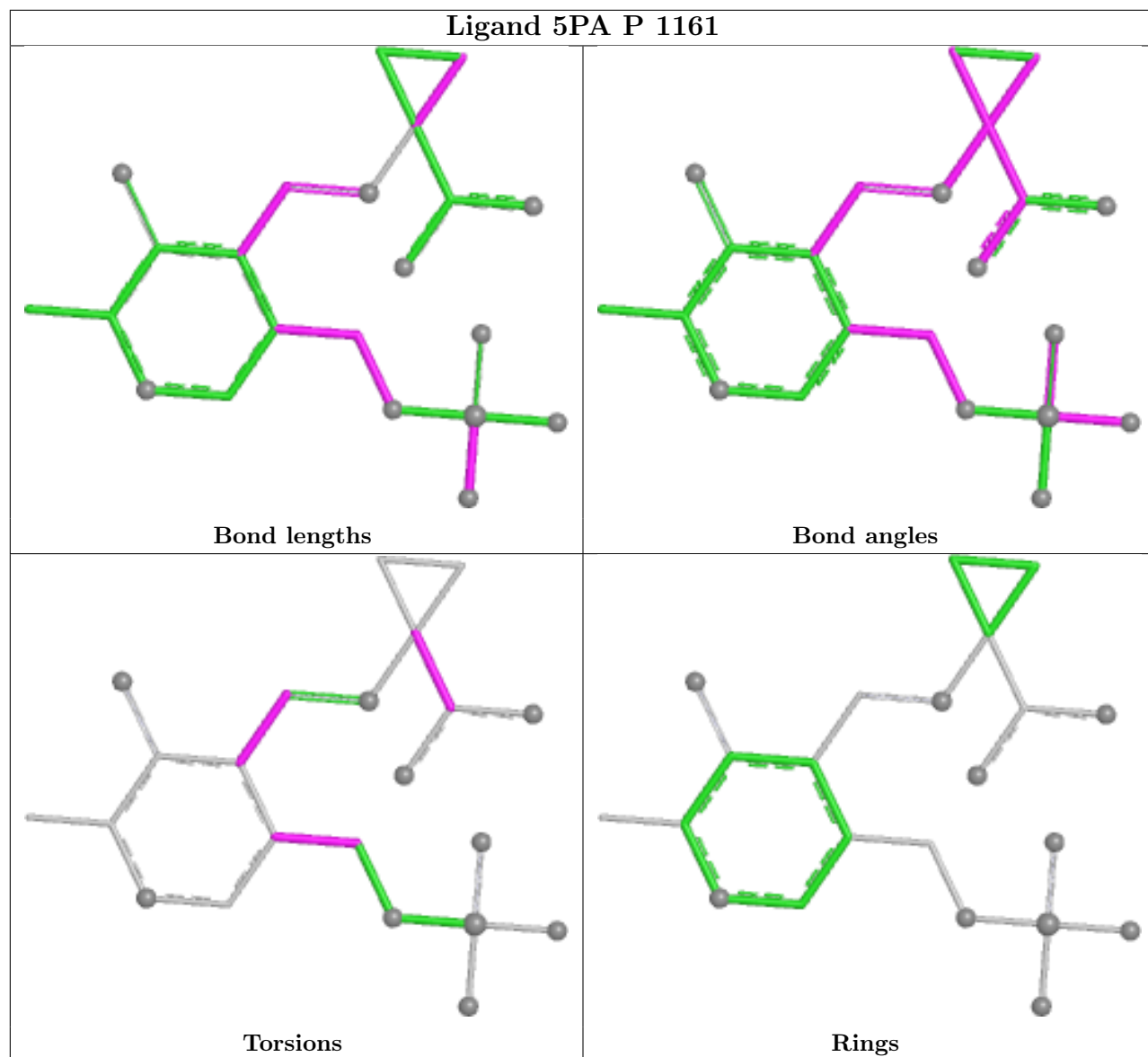




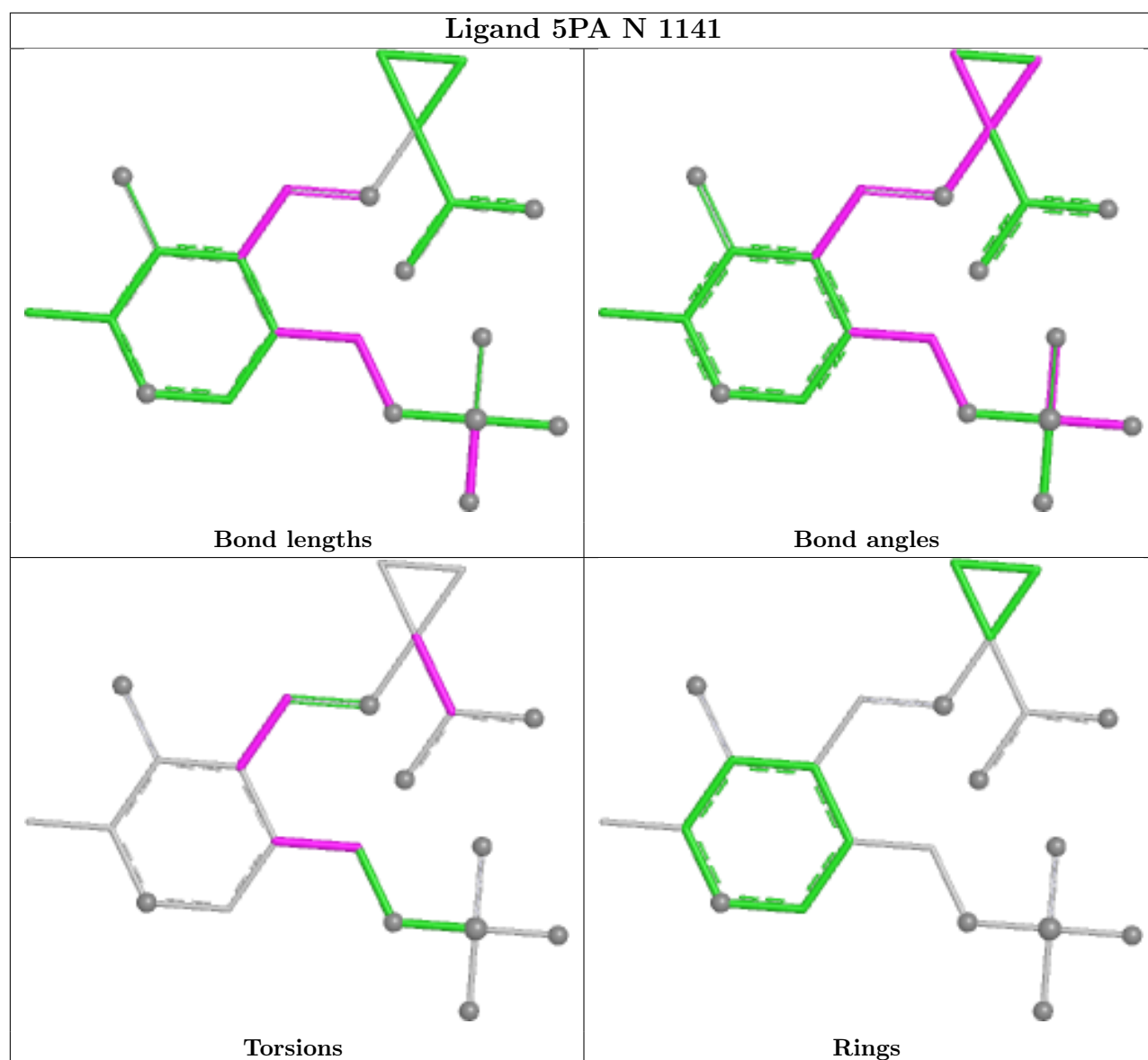




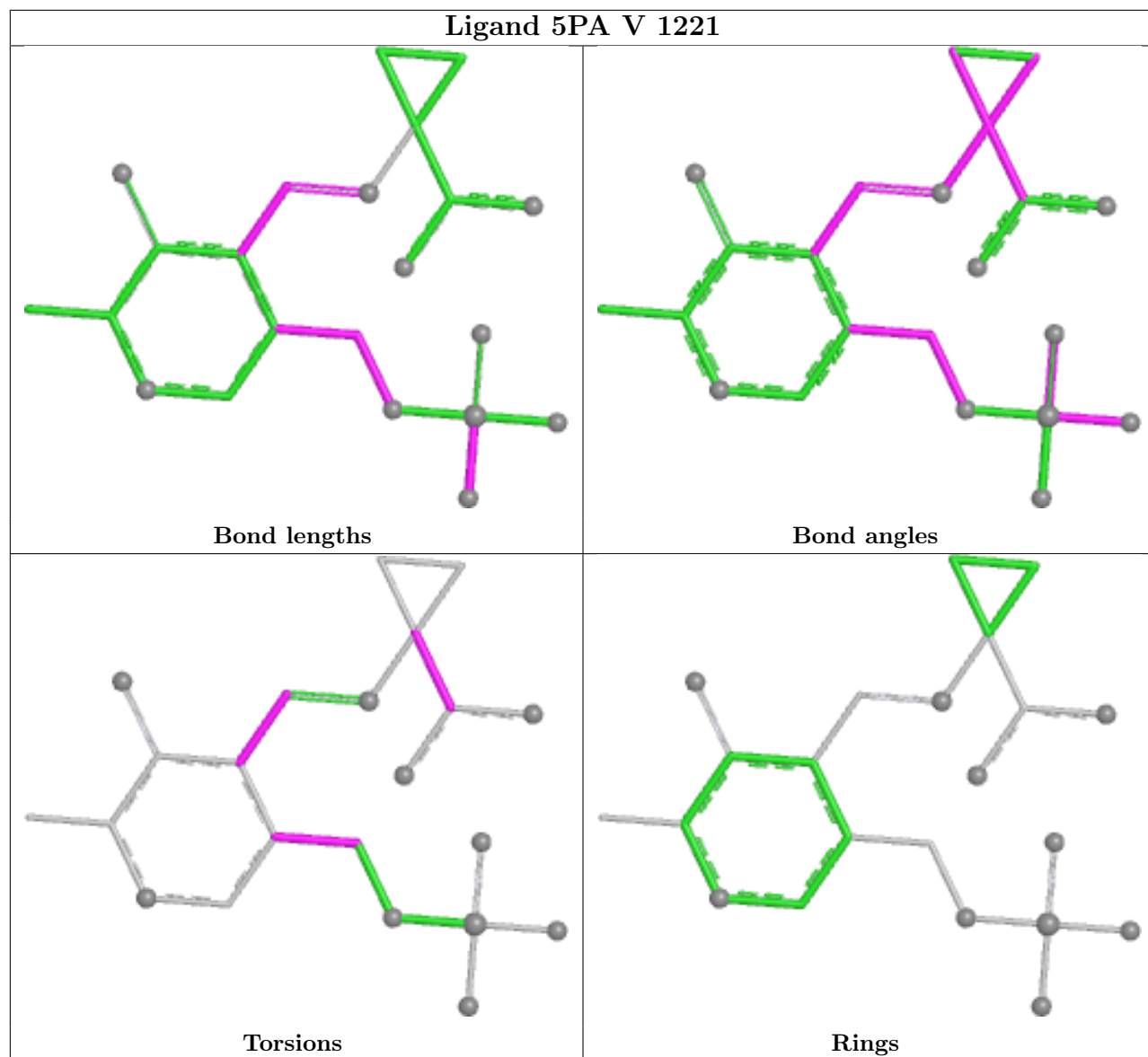




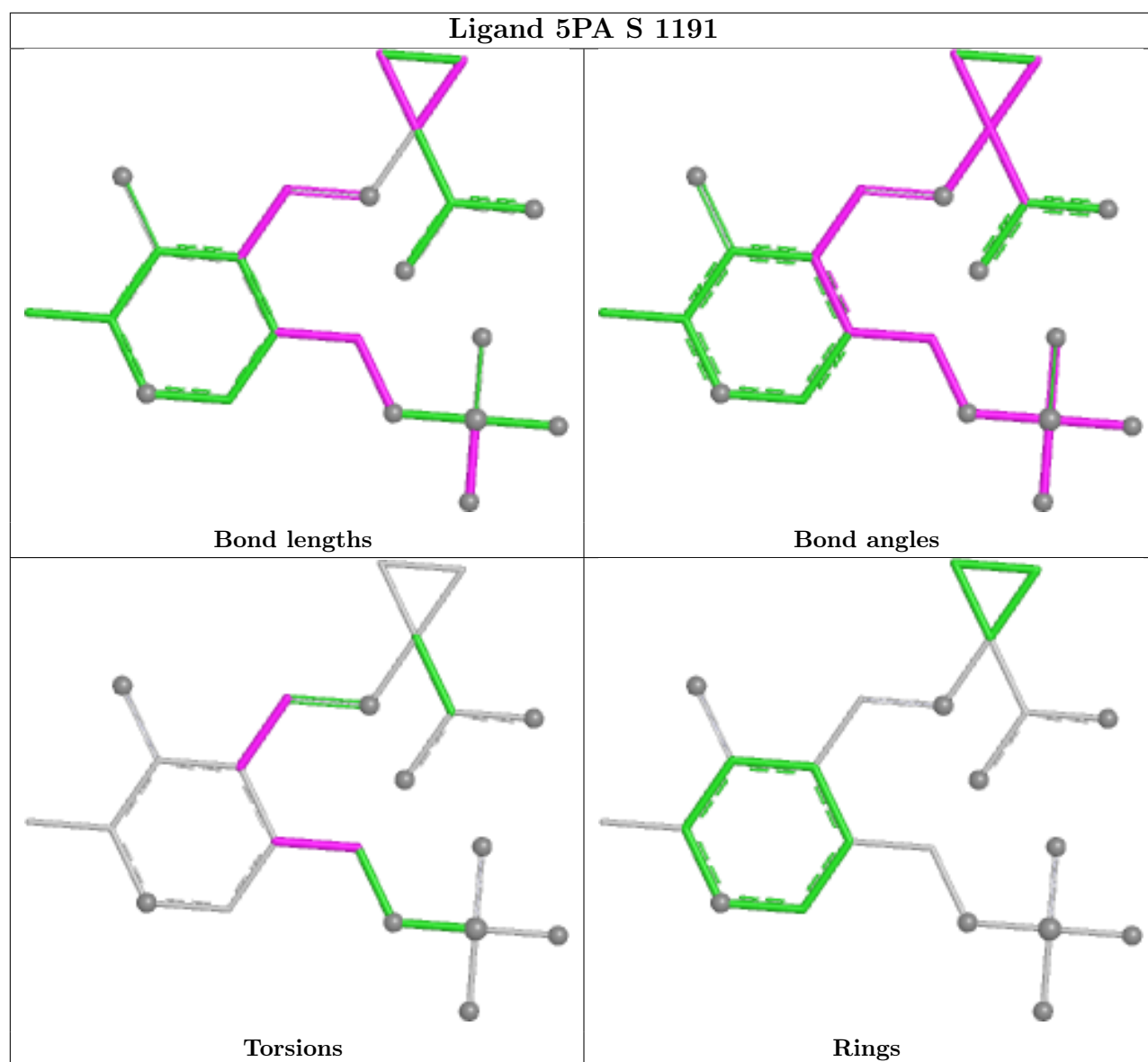




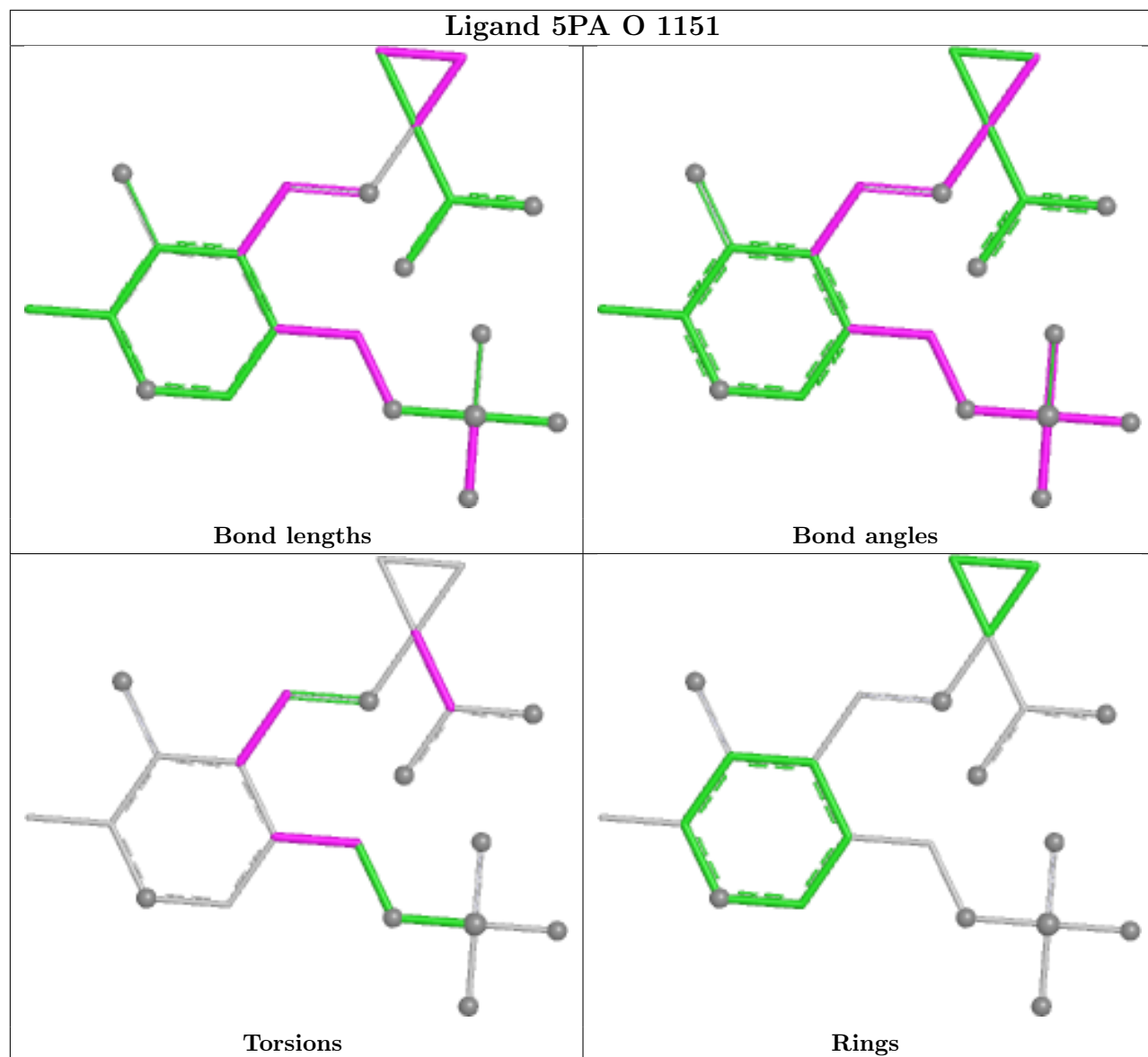






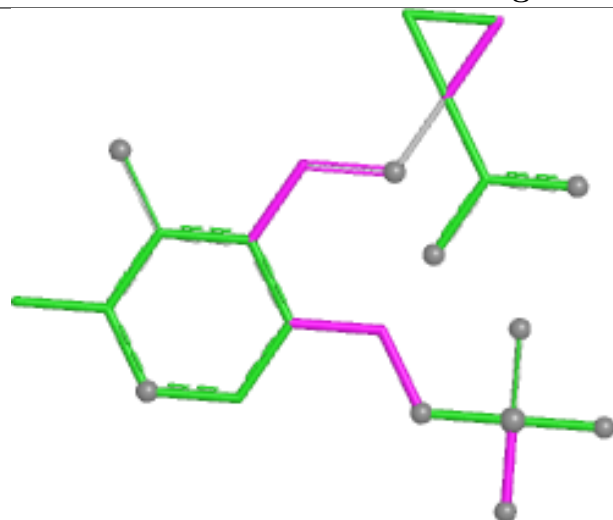




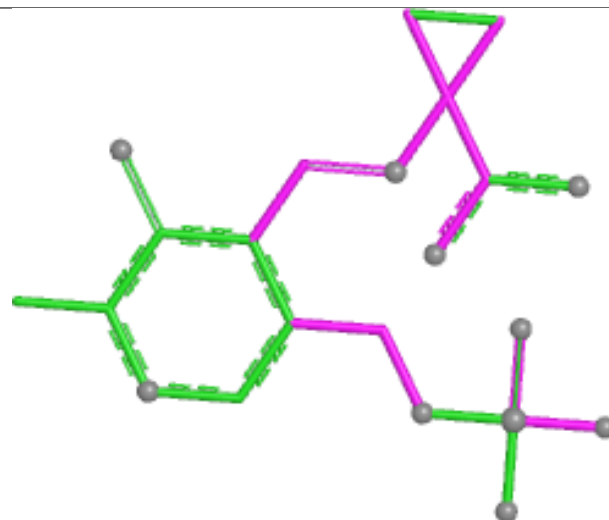




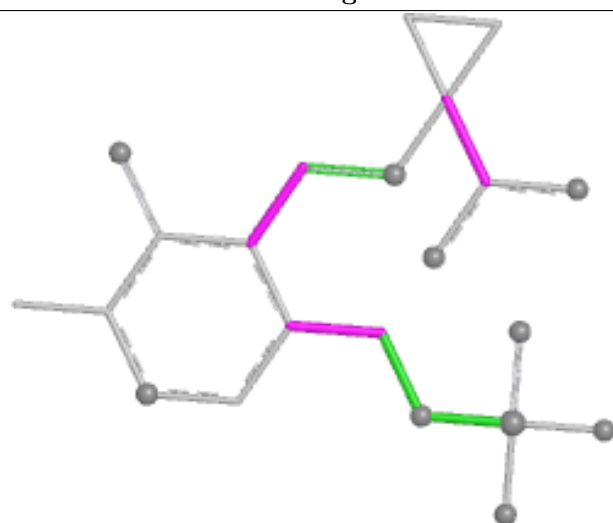
## Ligand 5PA E 1051



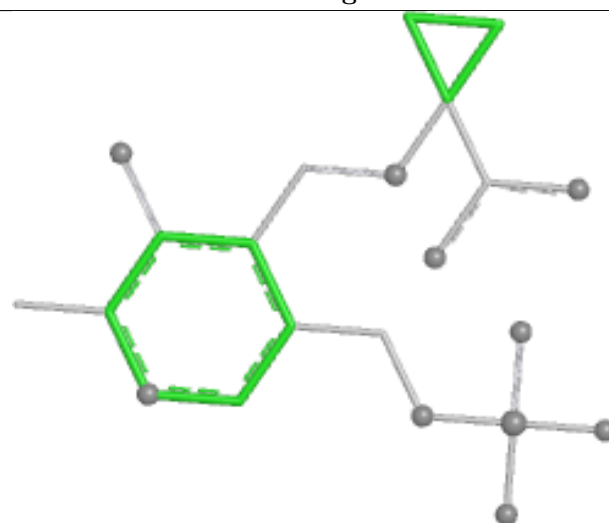
Bond lengths



Bond angles



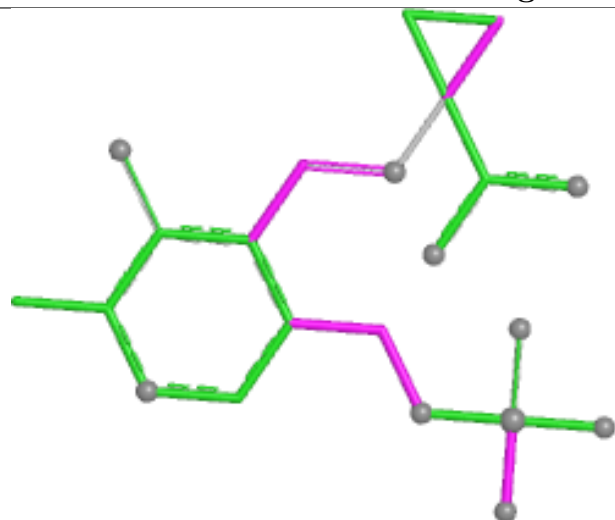
Torsions



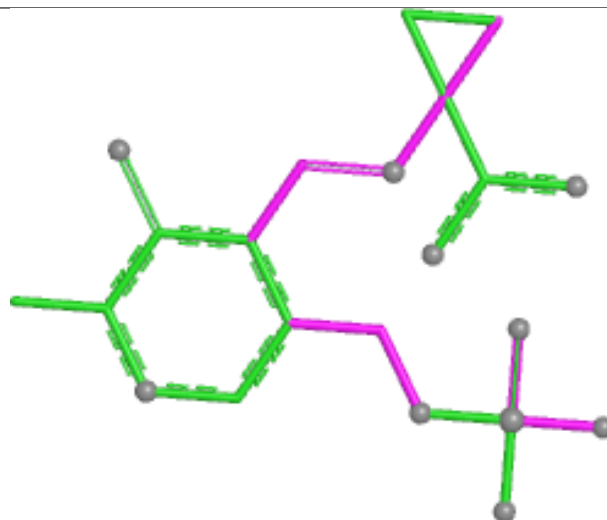
Rings



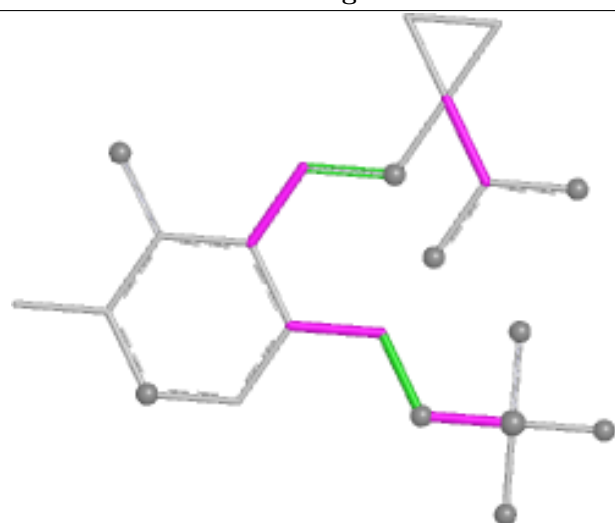
## Ligand 5PA I 1091



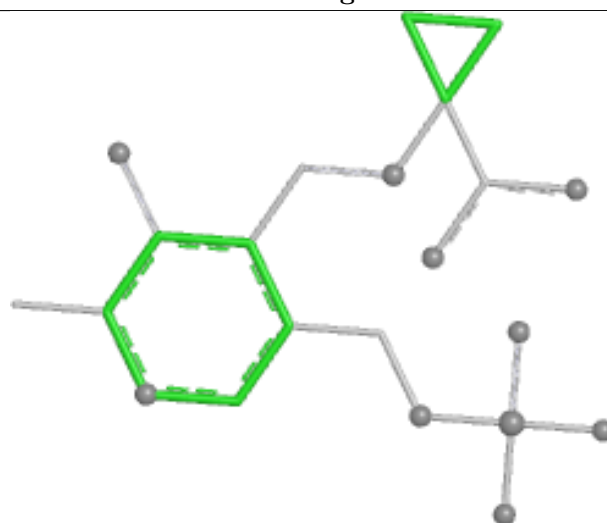
Bond lengths



Bond angles

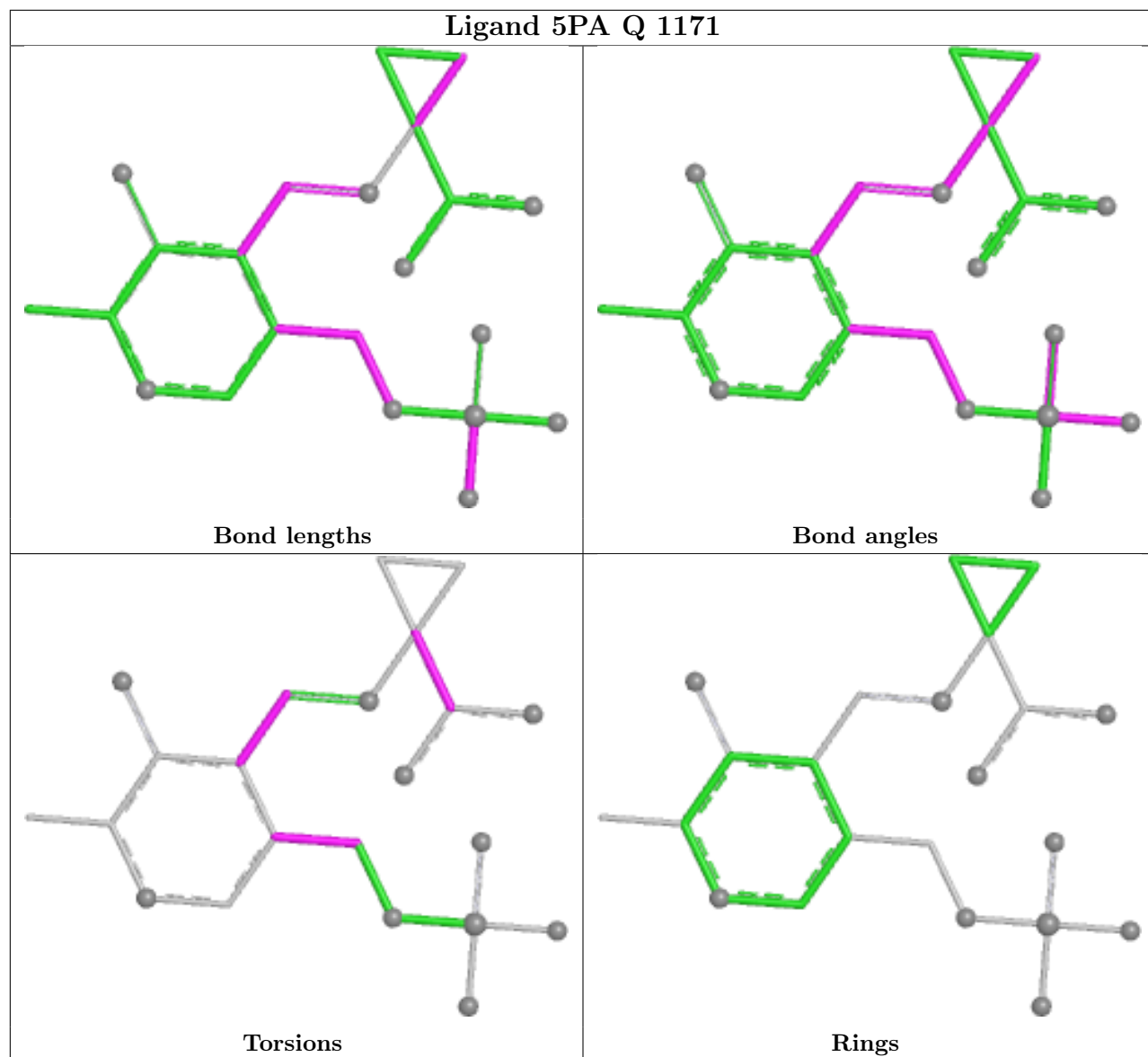


Torsions

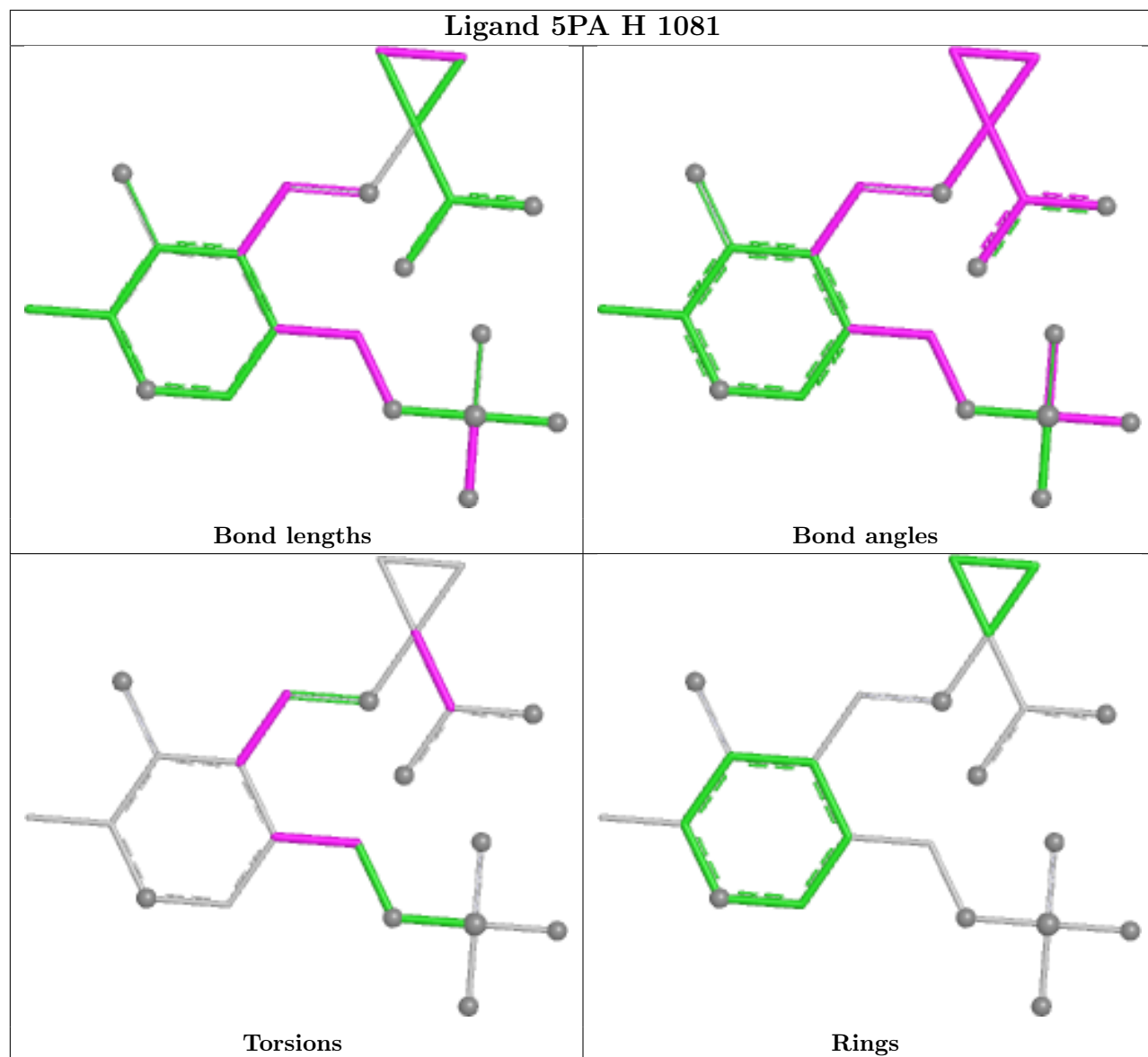


Rings



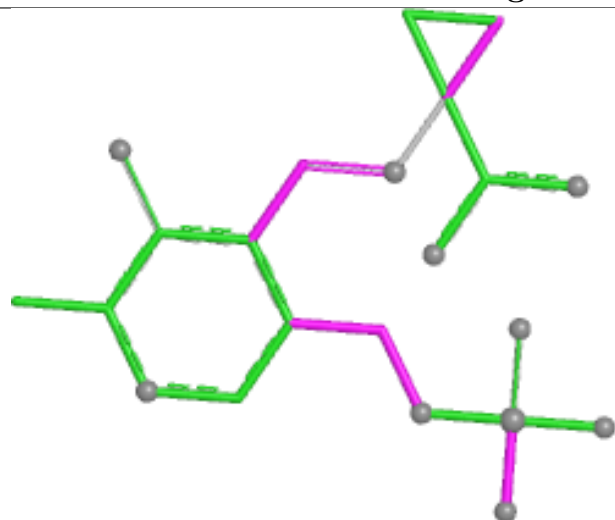




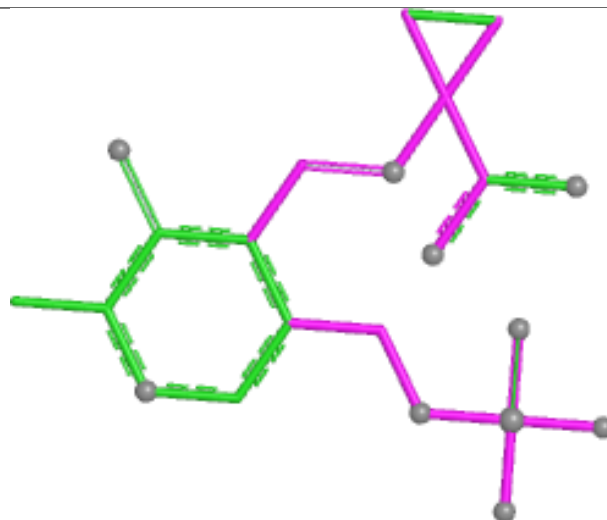




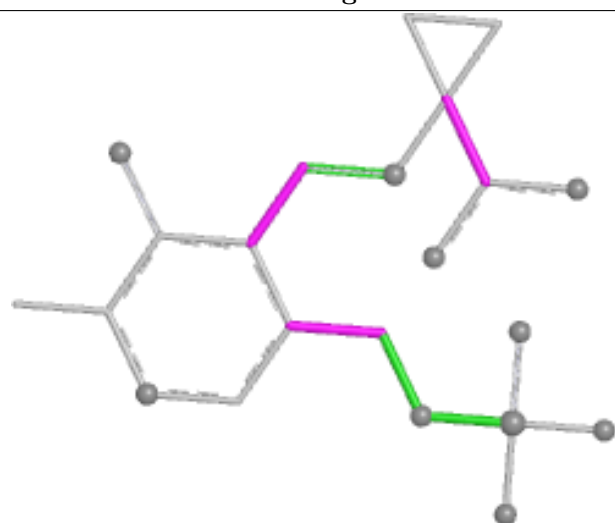
## Ligand 5PA M 1131



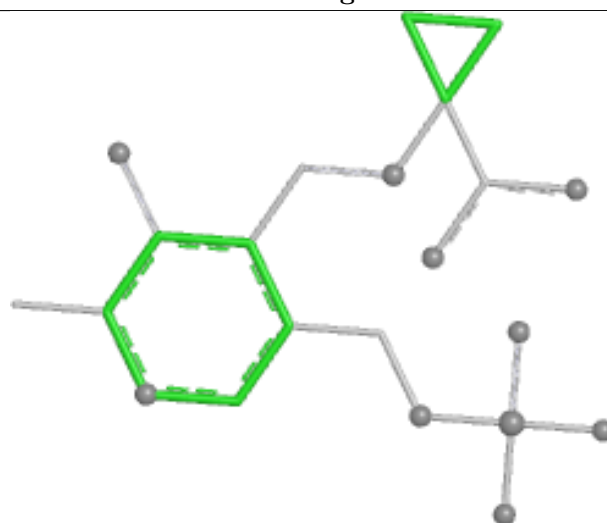
Bond lengths



Bond angles



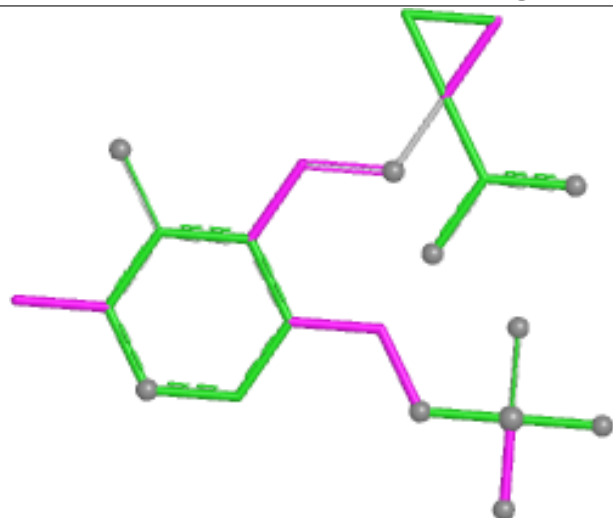
Torsions



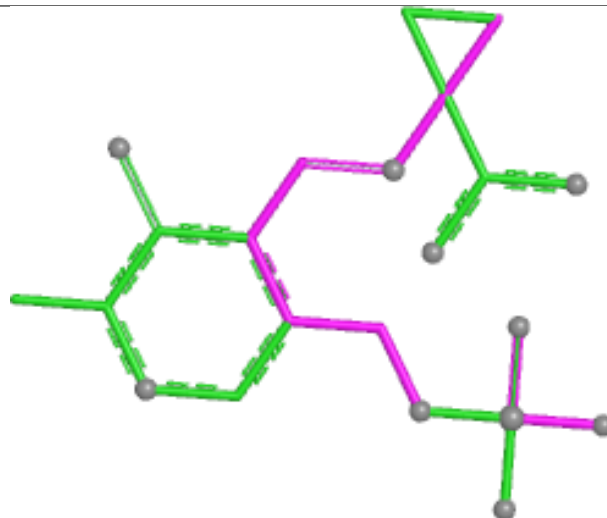
Rings



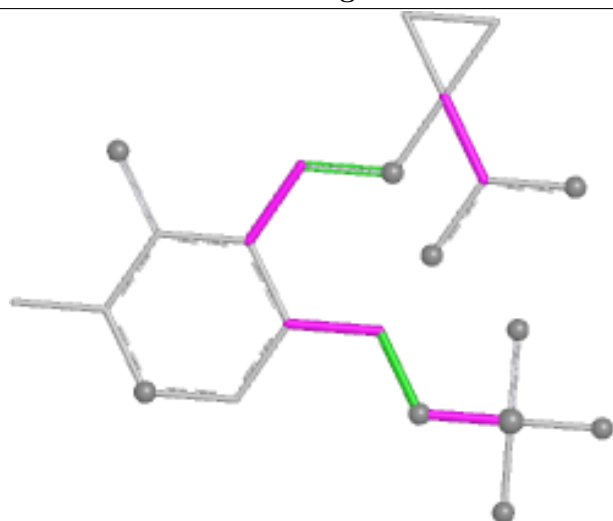
## Ligand 5PA J 1101



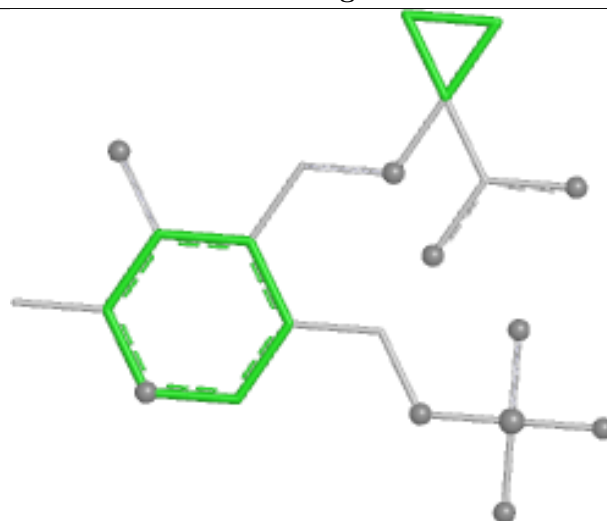
Bond lengths



Bond angles



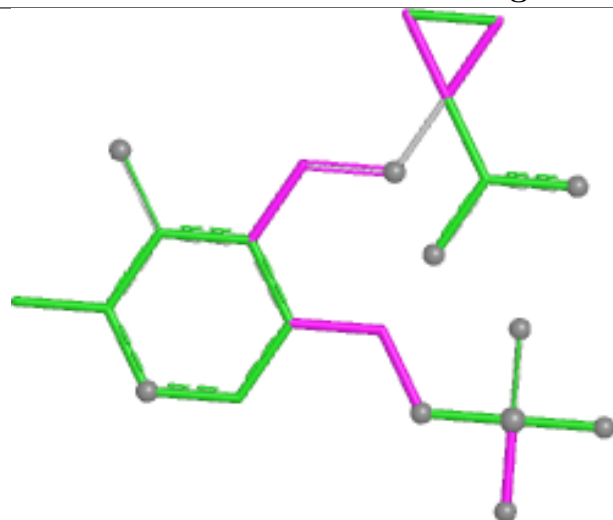
Torsions



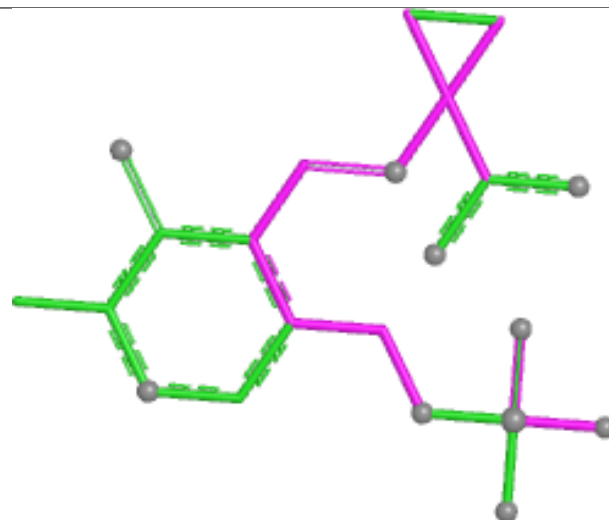
Rings



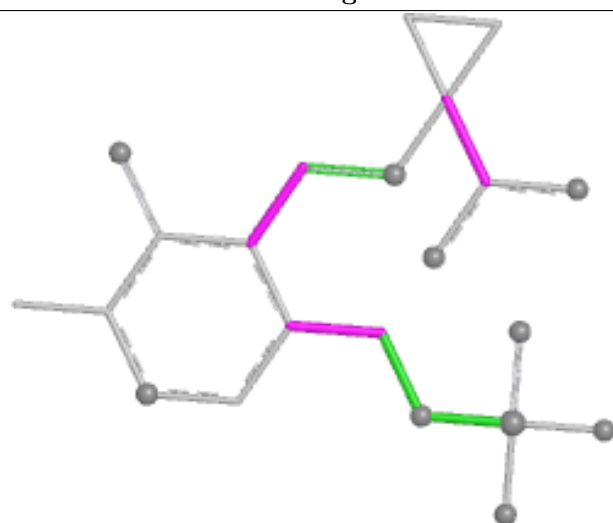
## Ligand 5PA G 1071



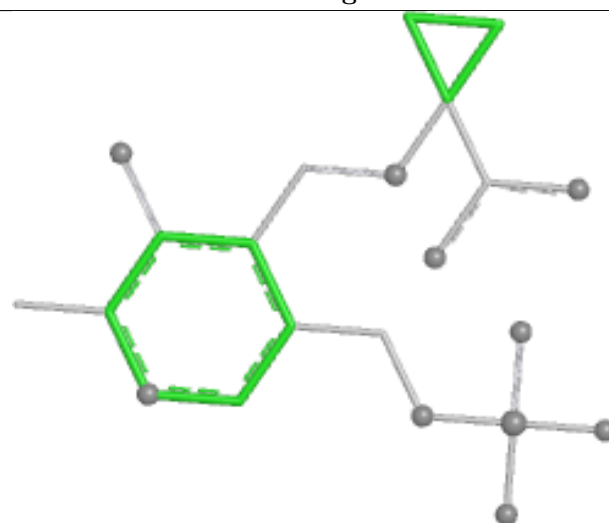
Bond lengths



Bond angles

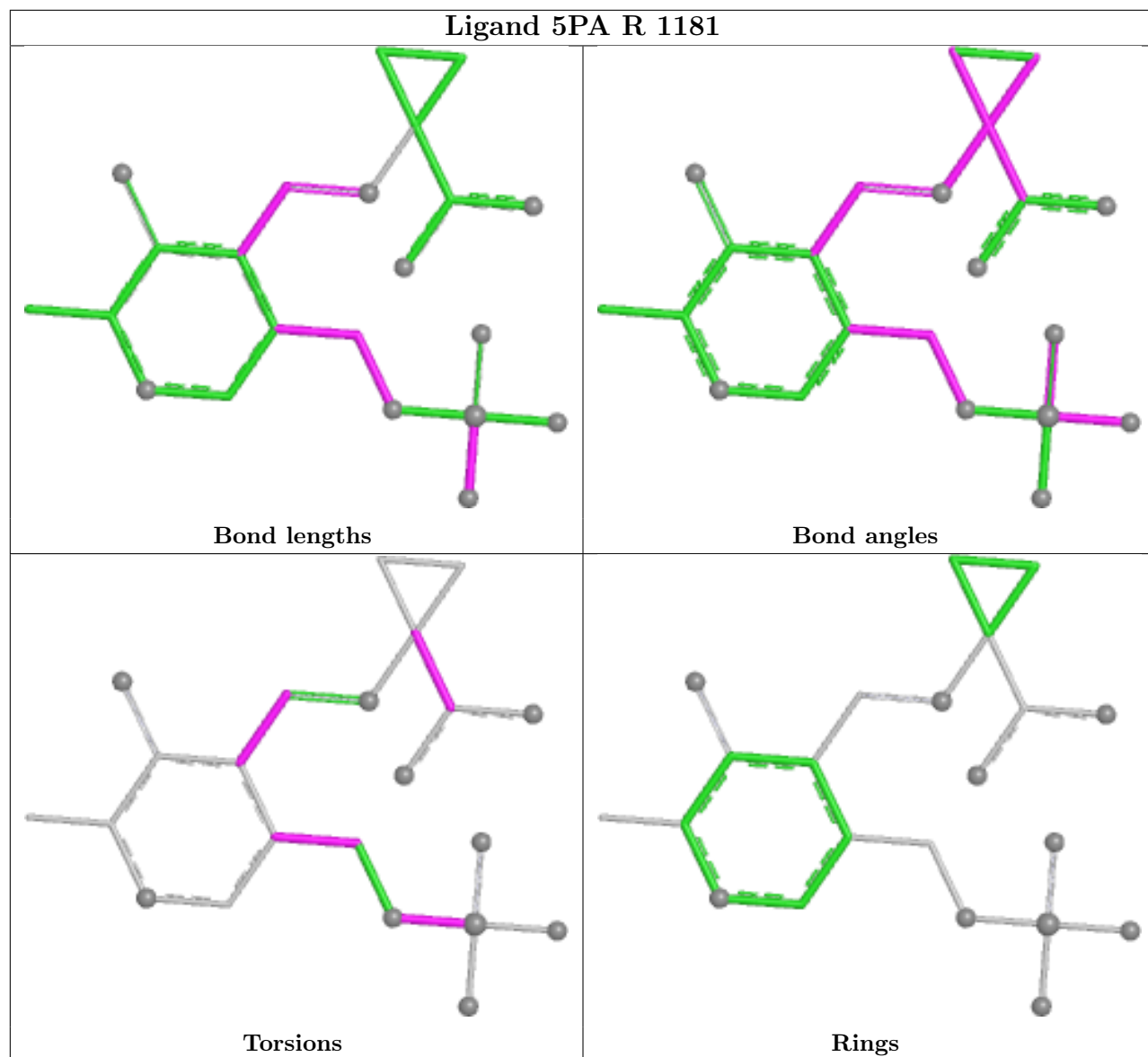


Torsions

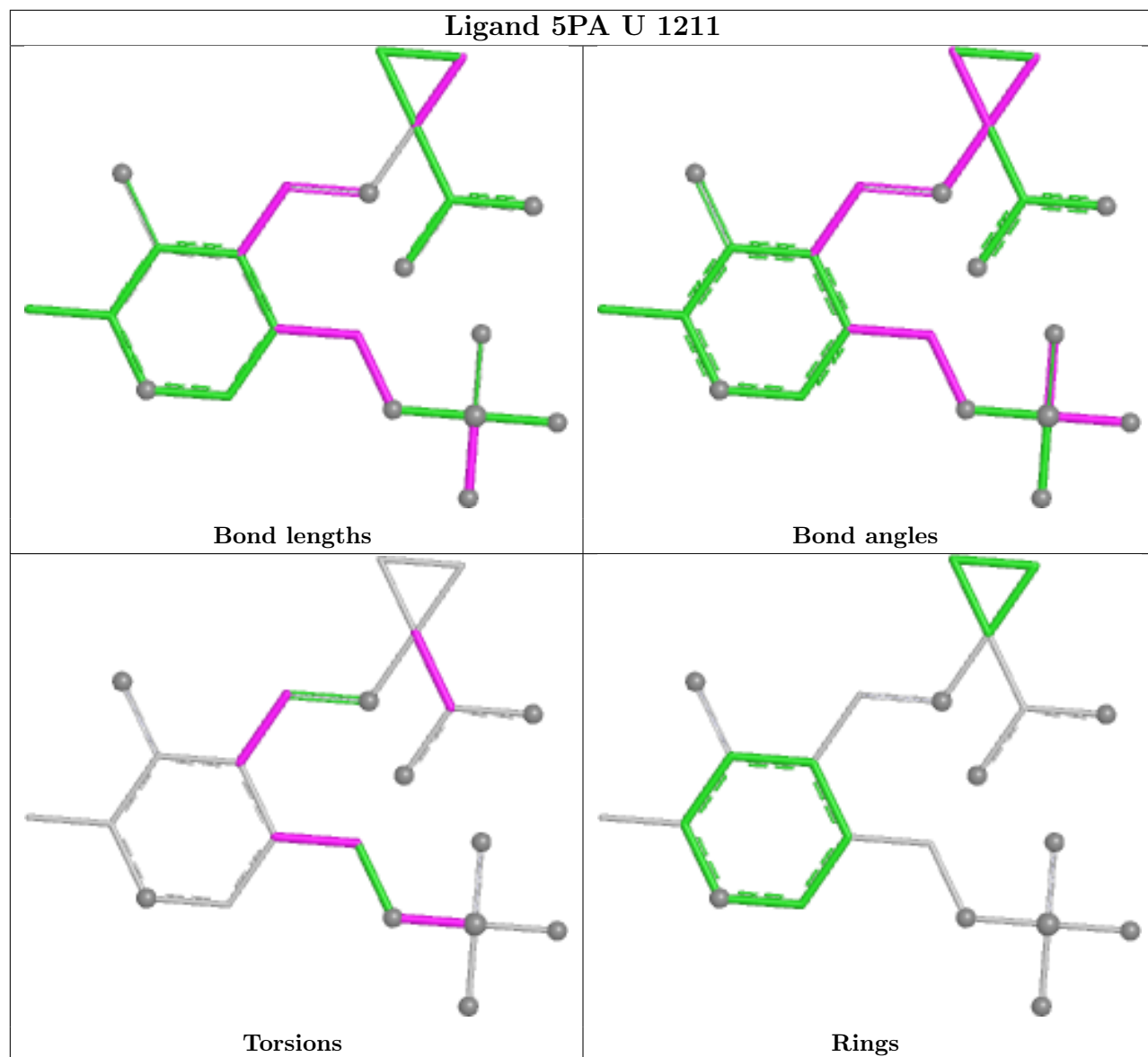


Rings

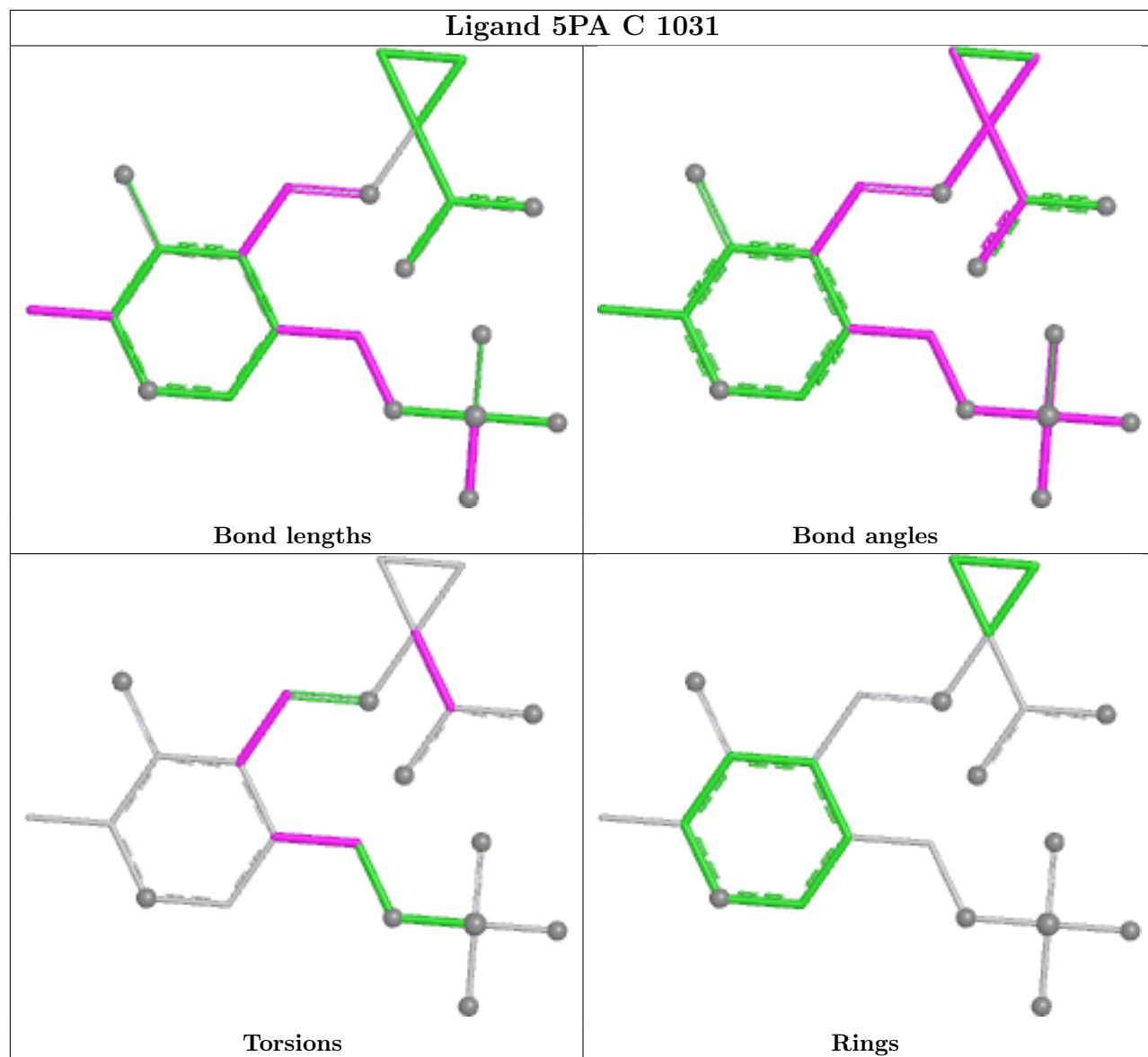






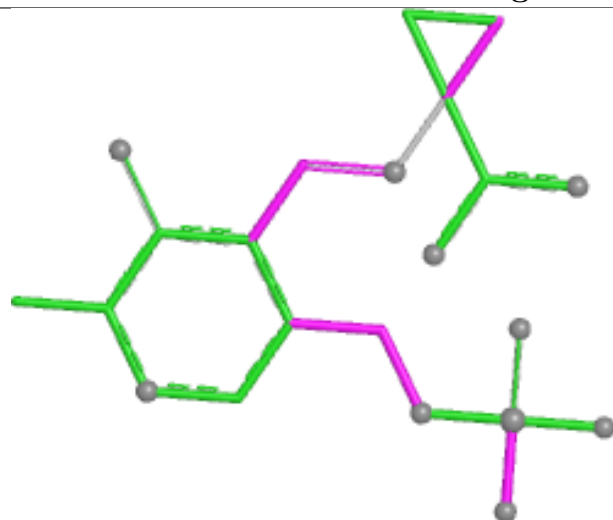




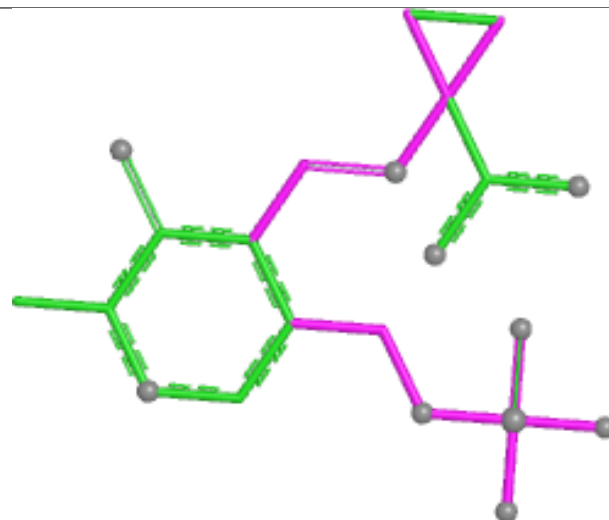




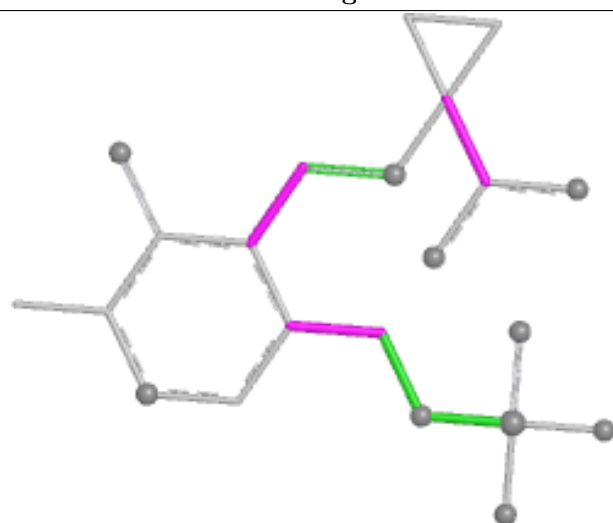
## Ligand 5PA B 1021



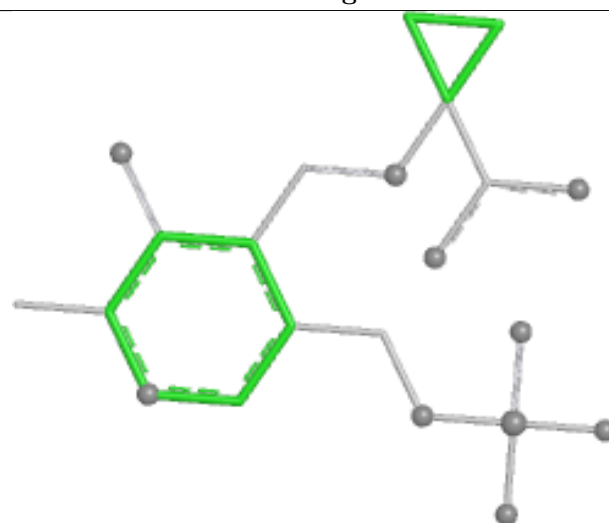
Bond lengths



Bond angles



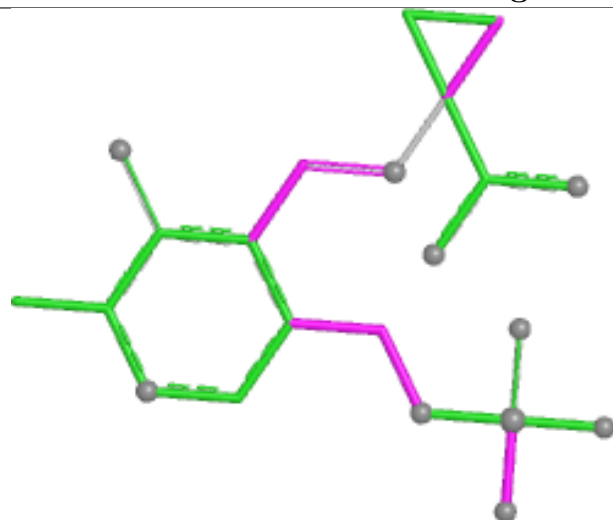
Torsions



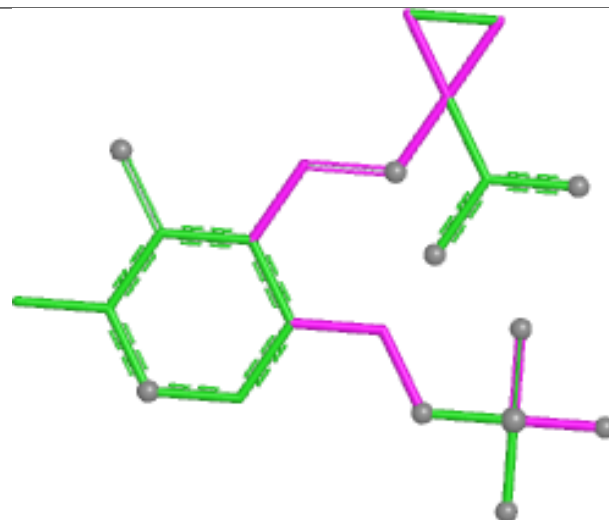
Rings



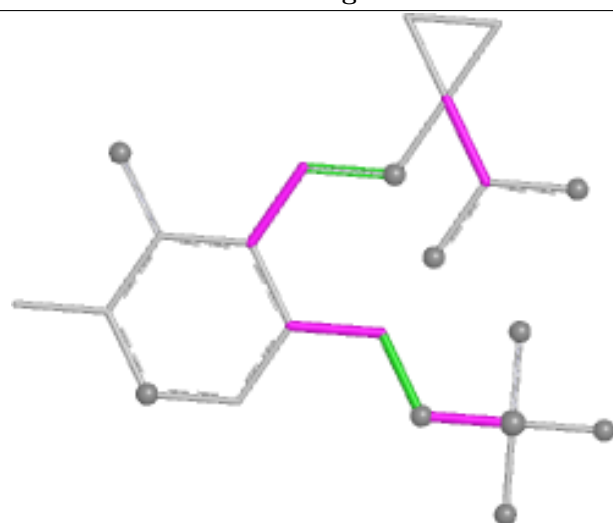
## Ligand 5PA K 1111



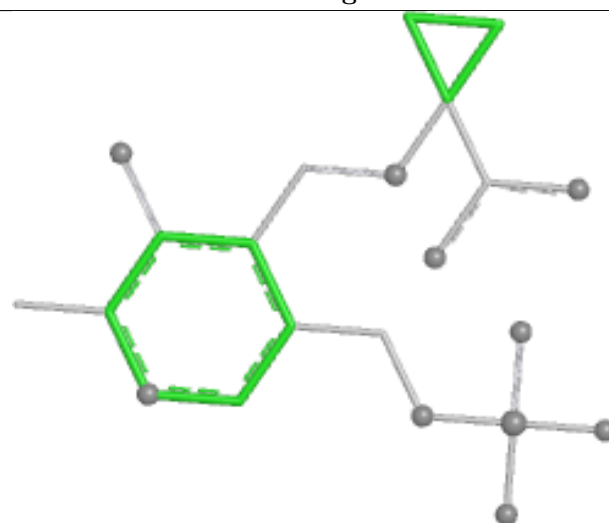
Bond lengths



Bond angles

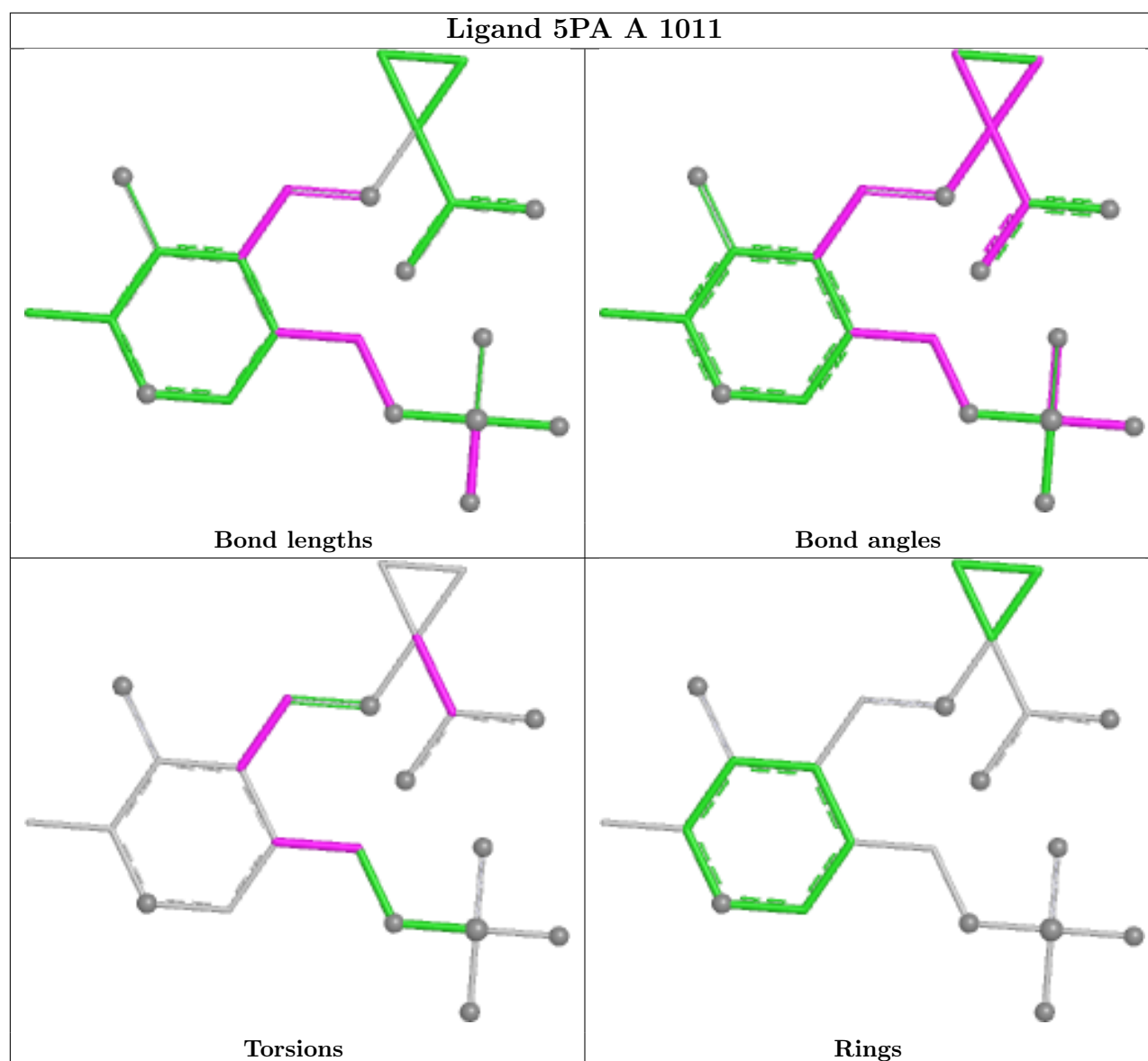


Torsions

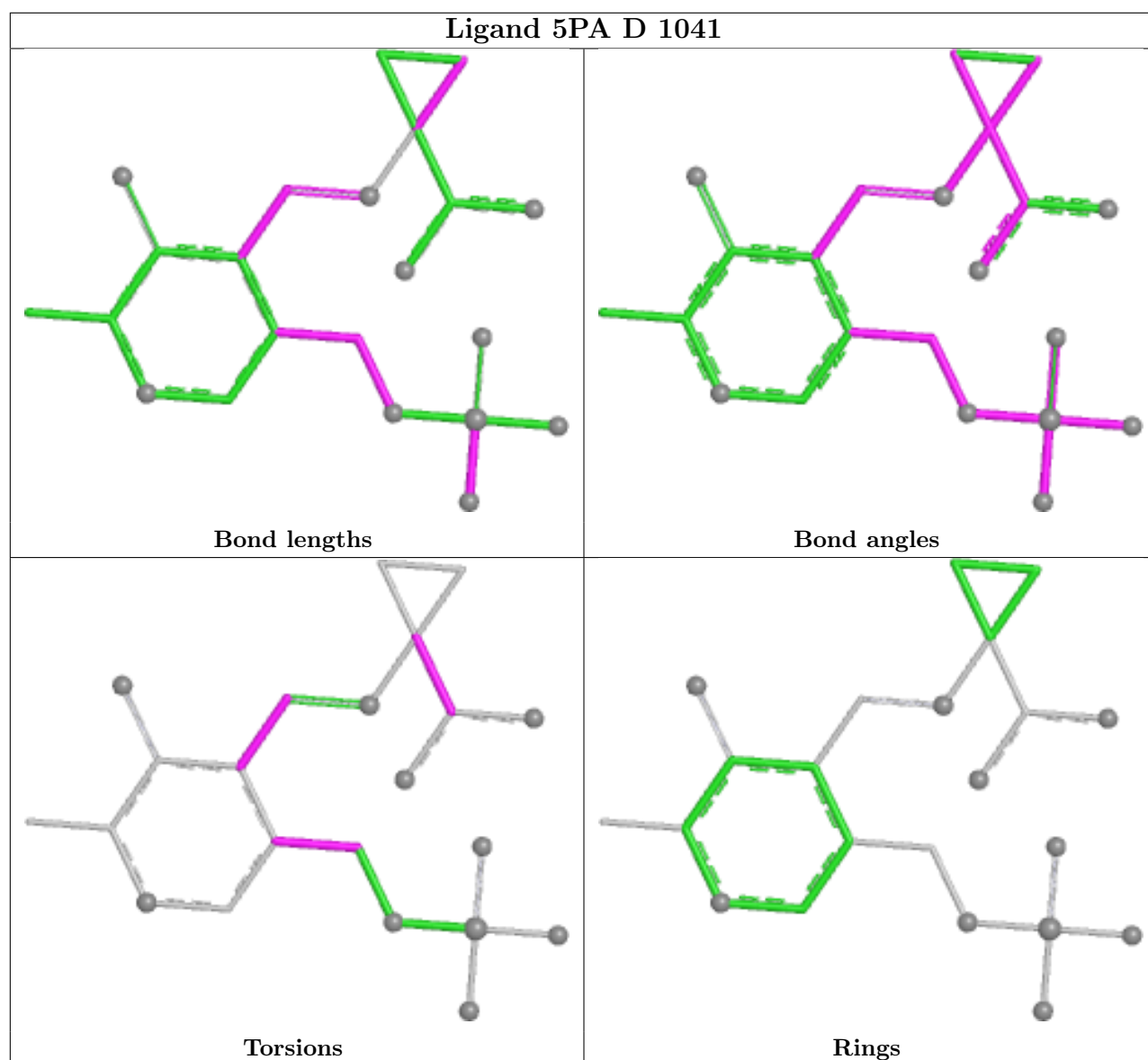


Rings

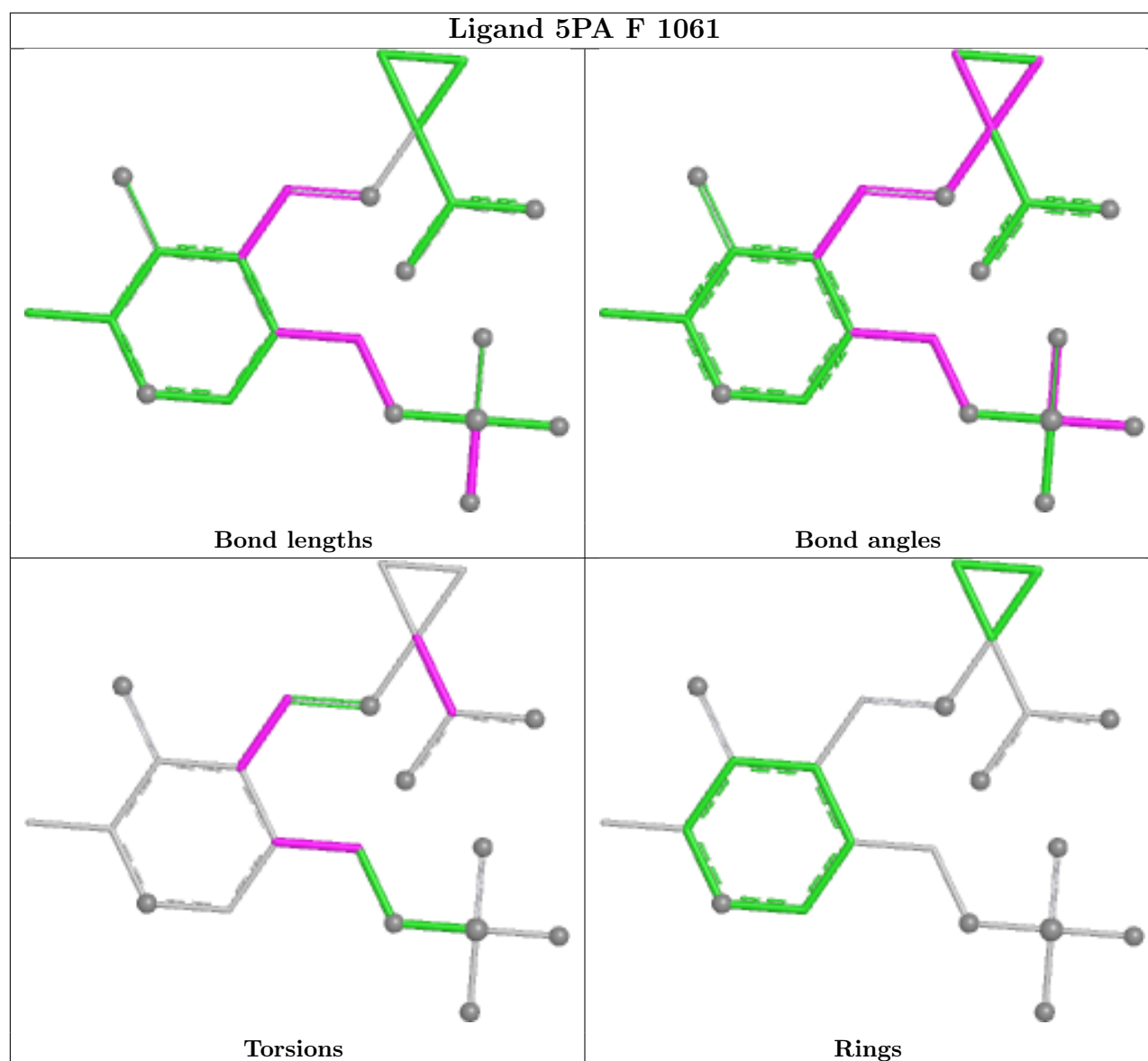




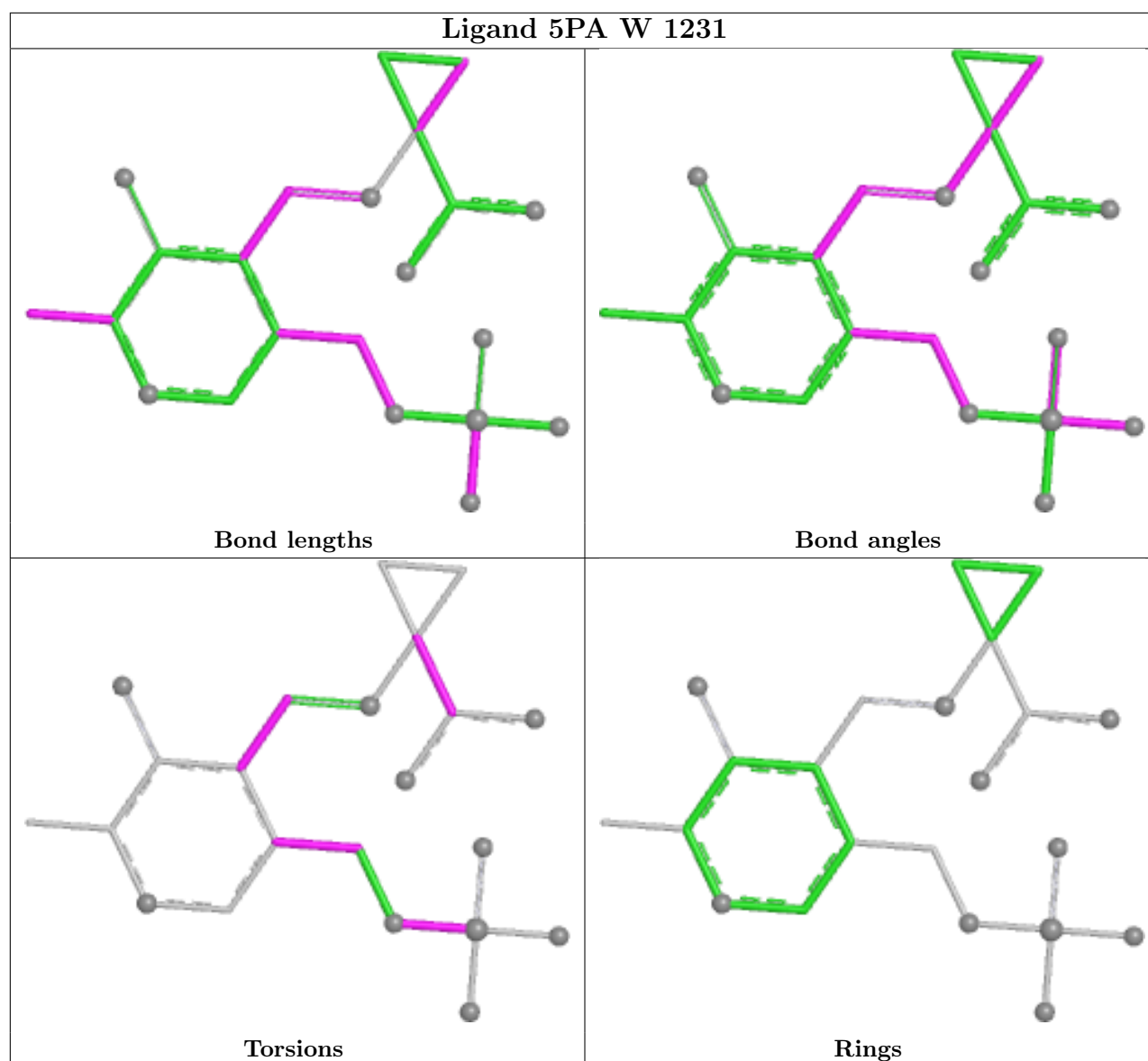












## 5.7 Other polymers [i](#)

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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.