



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:46 PM UTC

PDB ID : 1J0B / pdb_00001j0b
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

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

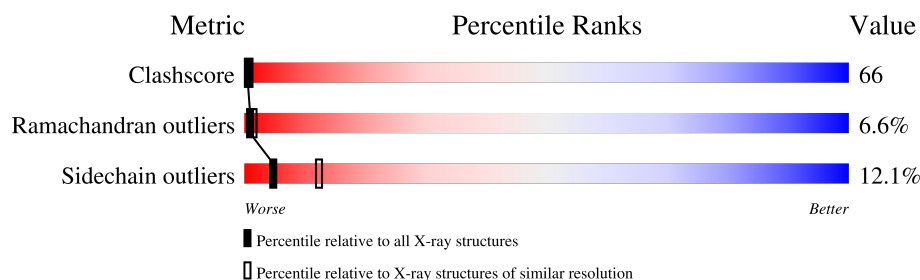
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

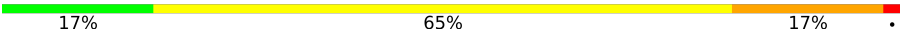
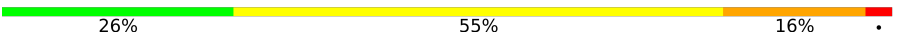
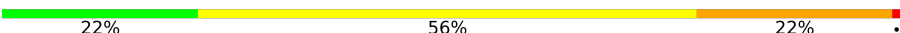
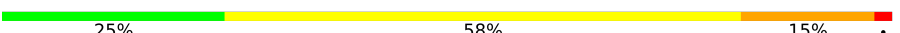
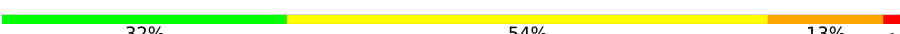
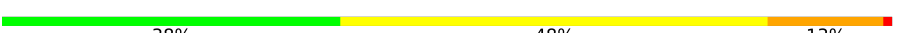
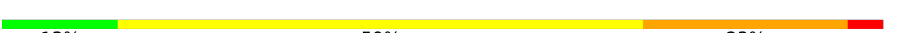
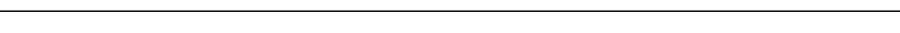
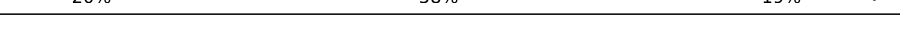
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	39% 48% 12% .
1	B	325	29% 55% 14% .
1	C	325	33% 50% 15% .
1	D	325	37% 47% 13% .
1	E	325	35% 52% 11% .
1	F	325	29% 55% 14% .
1	G	325	12% 64% 22% .
1	H	325	26% 56% 17% .

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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	C	1031	-	-	X	-
2	5PA	D	1041	-	-	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	T	1201	-	-	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.

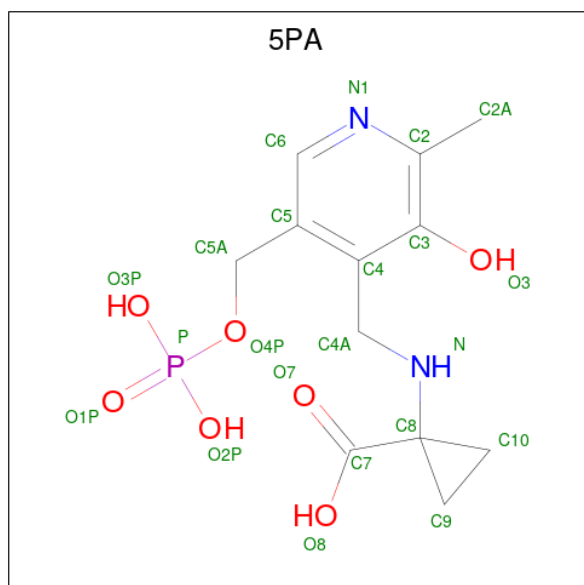
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	B	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	C	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	D	325	Total	C	N	O	S	0	0	0
			2484	1604	415	461	4			
1	E	325	Total	C	N	O	S	0	0	0
			2484	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 (CCD ID: 5PA) (formula: C₁₂H₁₇N₂O₇P).



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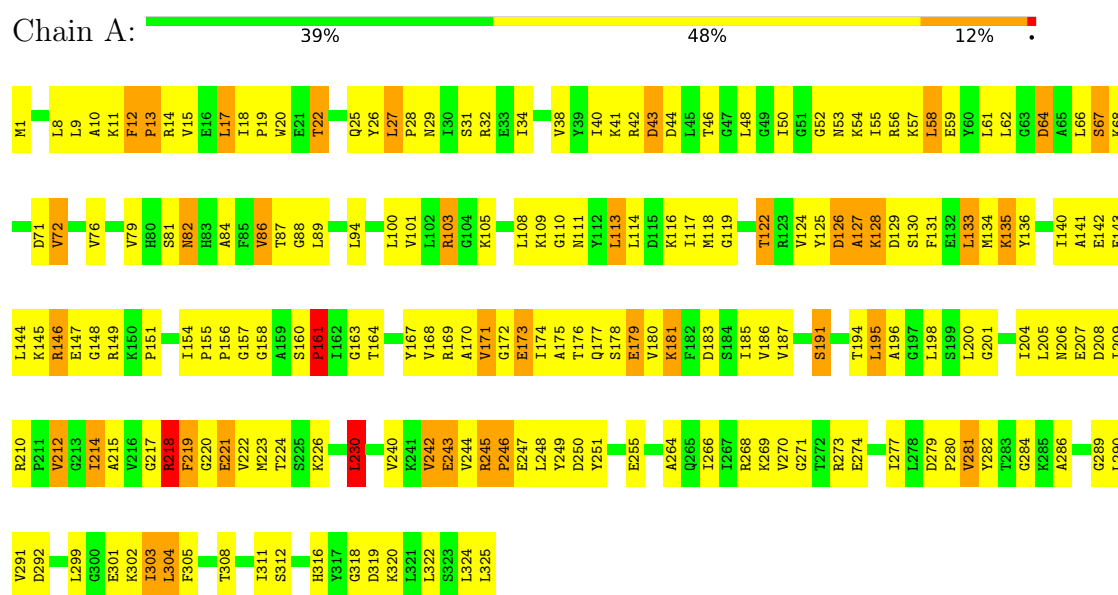
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	S	42	Total 42	O 42	0	0
3	T	40	Total 40	O 40	0	0
3	U	48	Total 48	O 48	0	0
3	V	40	Total 40	O 40	0	0
3	W	34	Total 34	O 34	0	0
3	X	26	Total 26	O 26	0	0

3 Residue-property plots

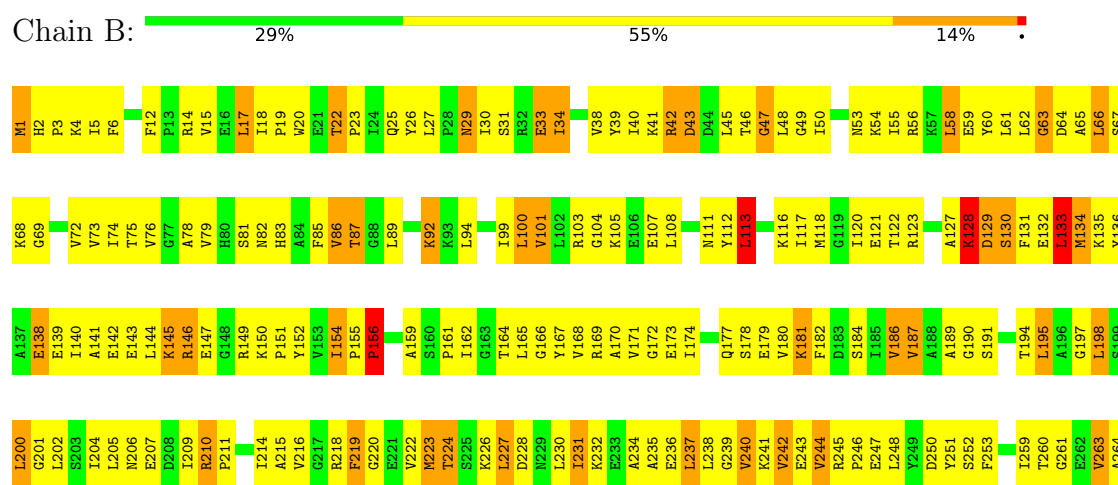
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



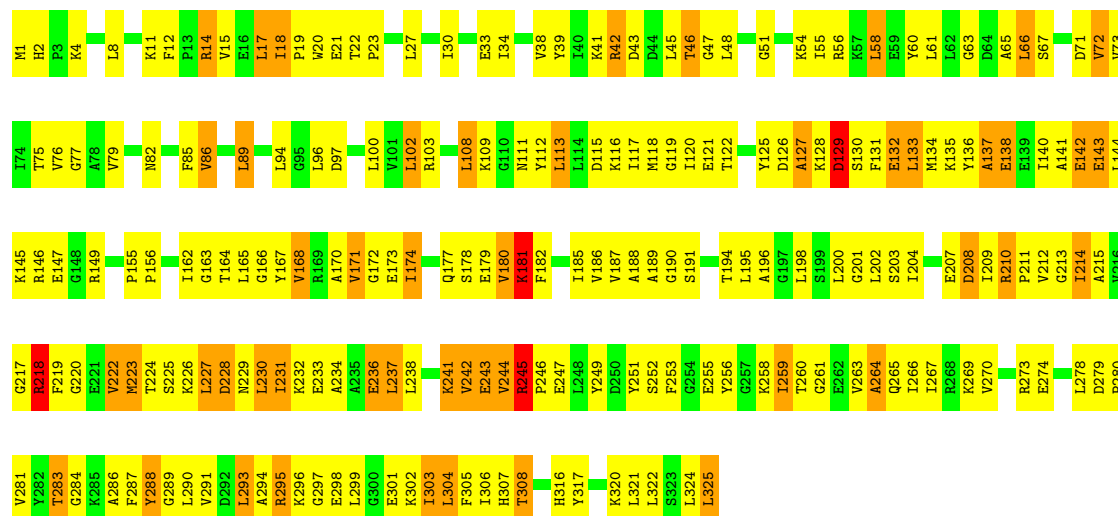
- Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase





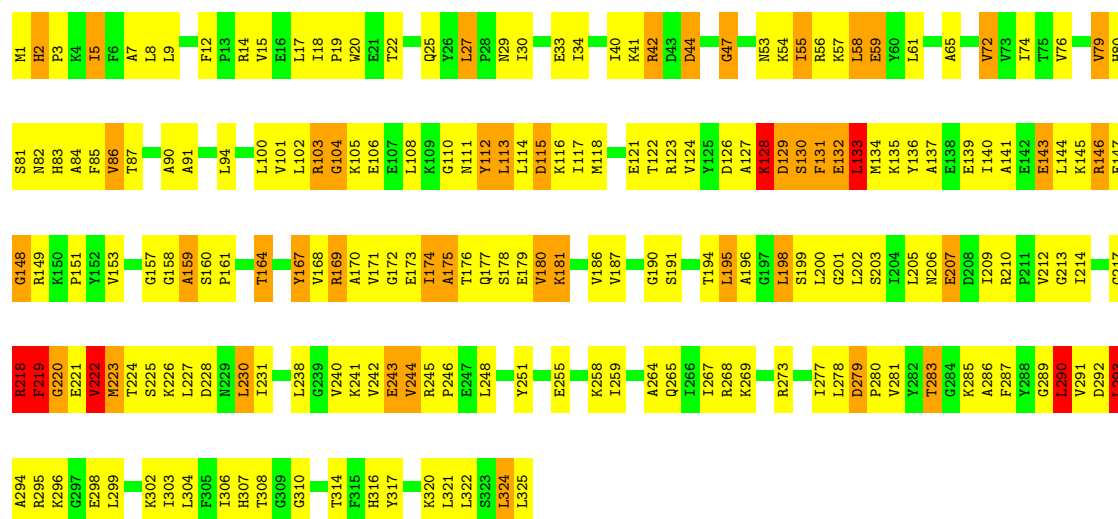
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain C: 33% 50% 15% .



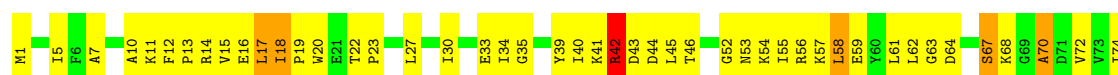
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

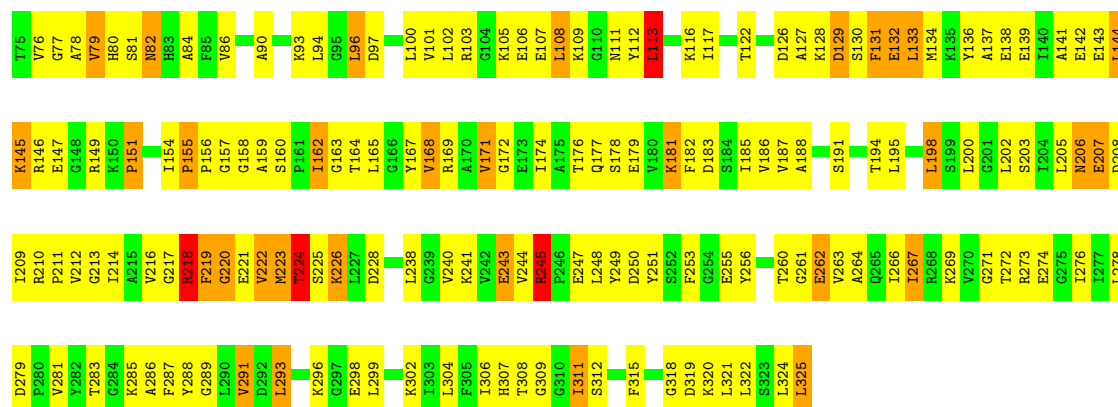
Chain D: 37% 47% 13% .



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

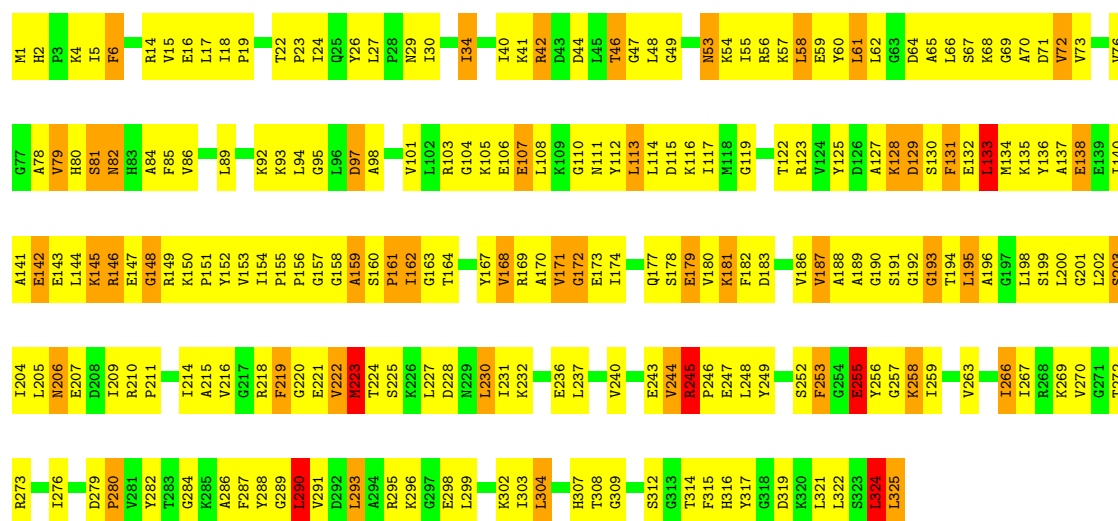
Chain E: 35% 52% 11% .





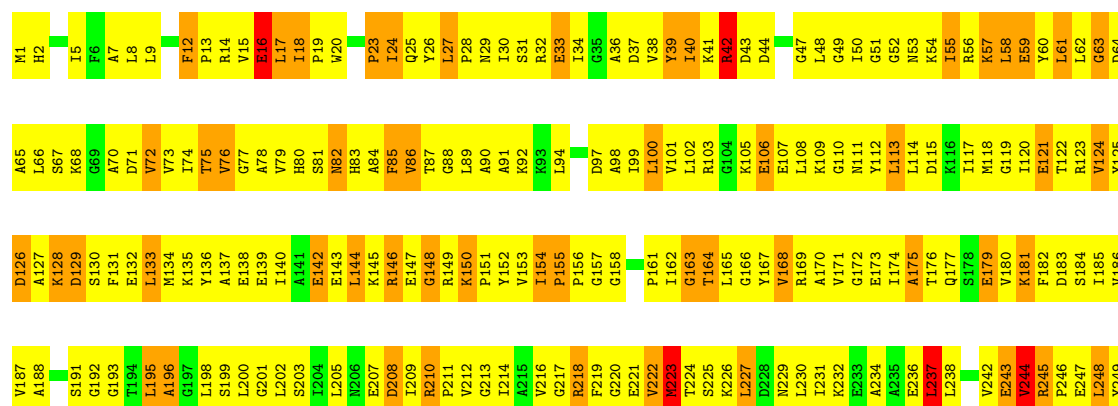
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

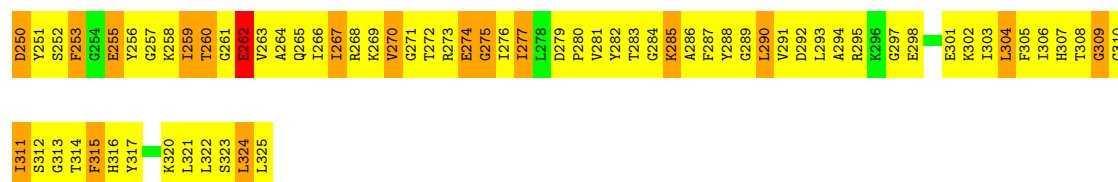
Chain F: 29% 55% 14% .



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

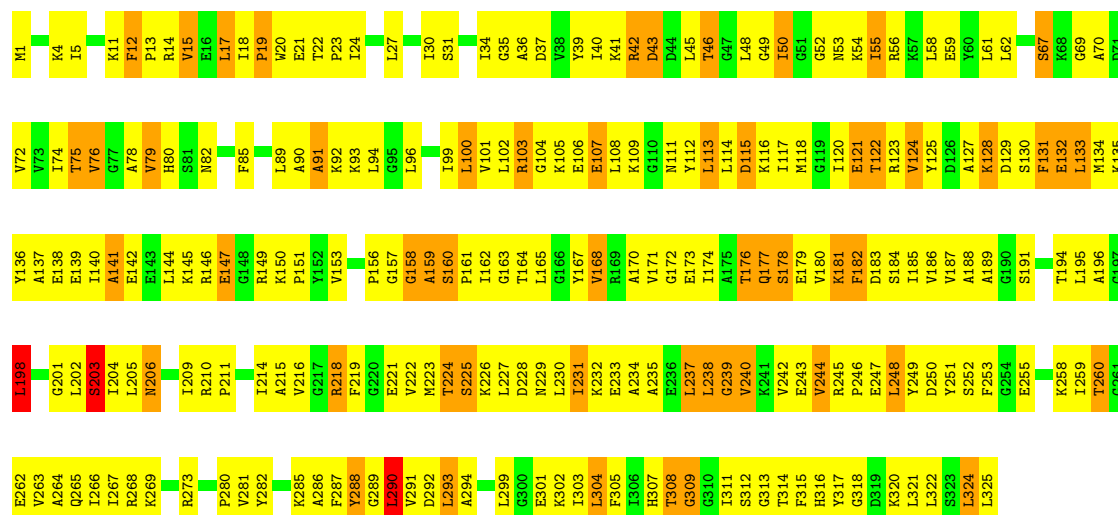
Chain G: 12% 64% 22% .





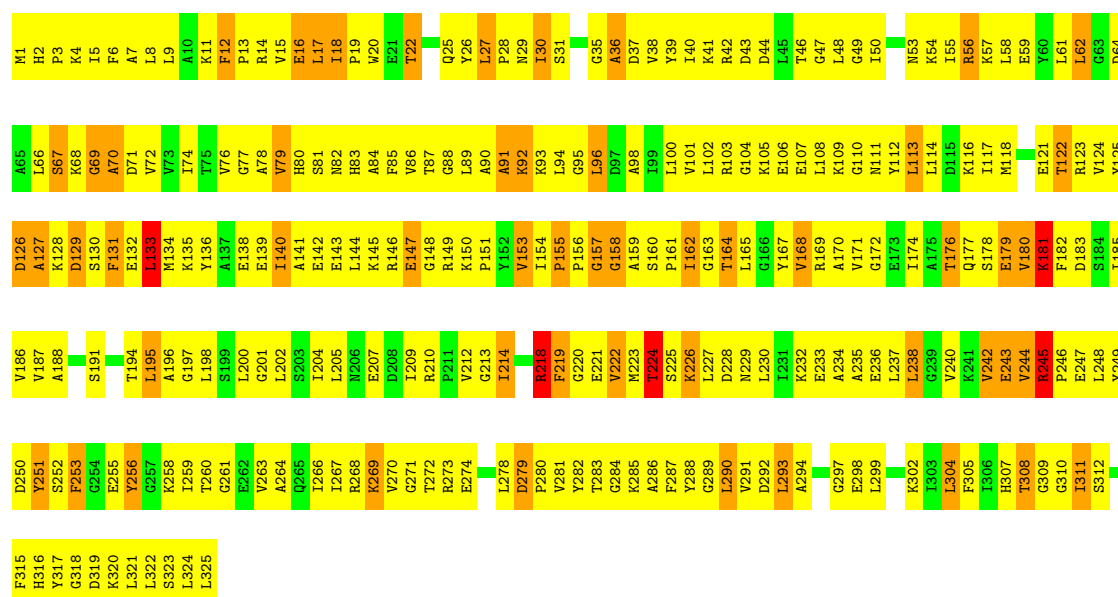
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain H: 26% 56% 17%

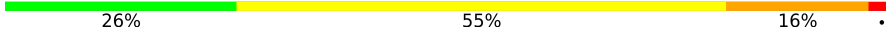


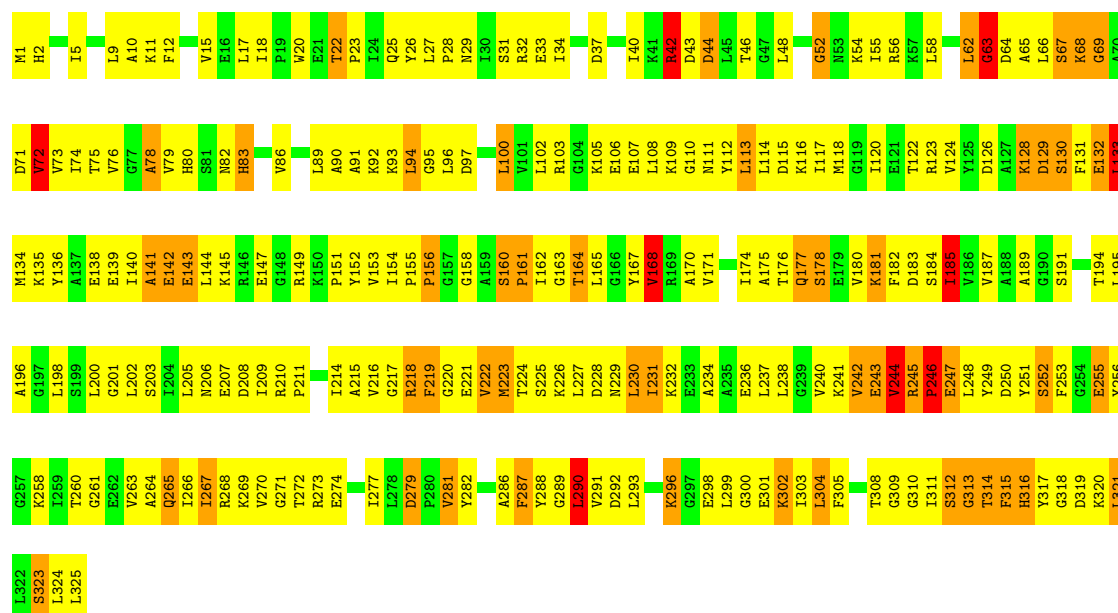
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain I: 17% 65% 17%

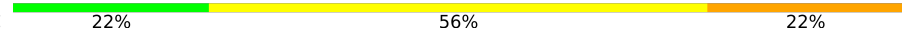


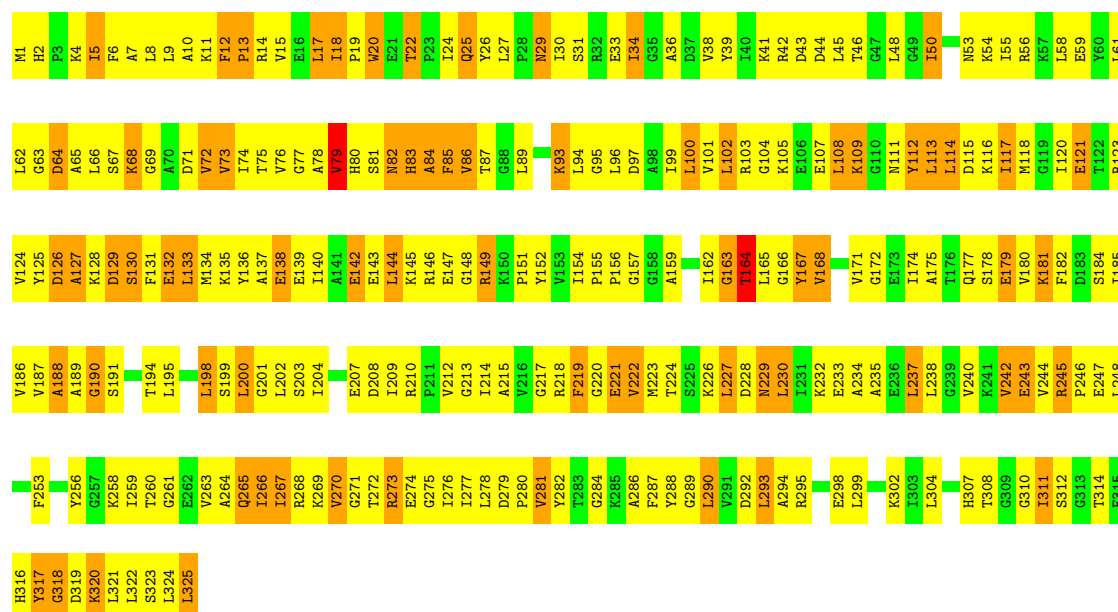
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain J:  26% 55% 16% .



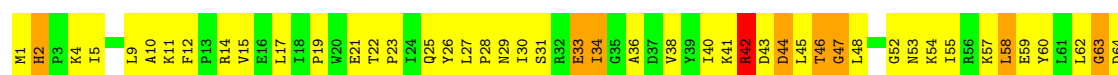
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

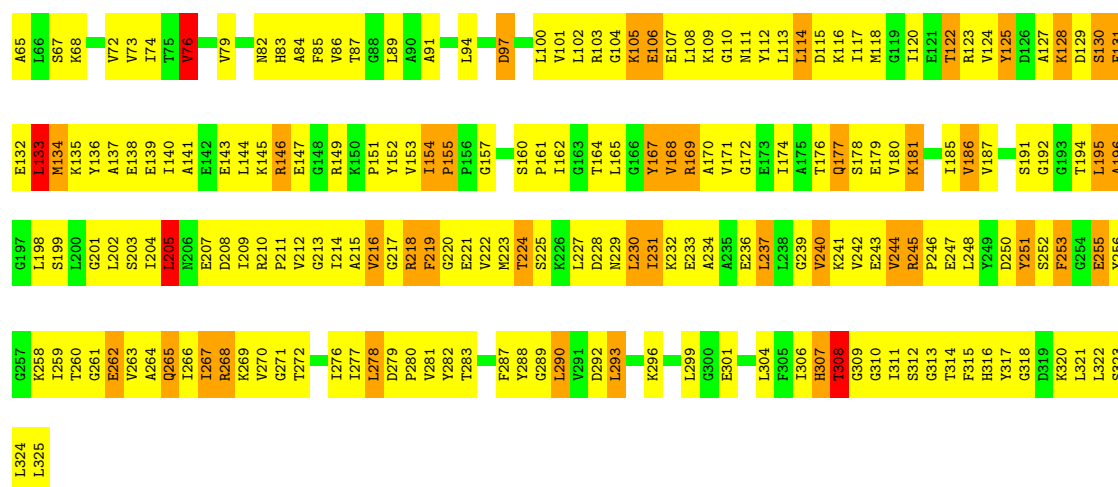
Chain K:  22% 56% 22% .



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

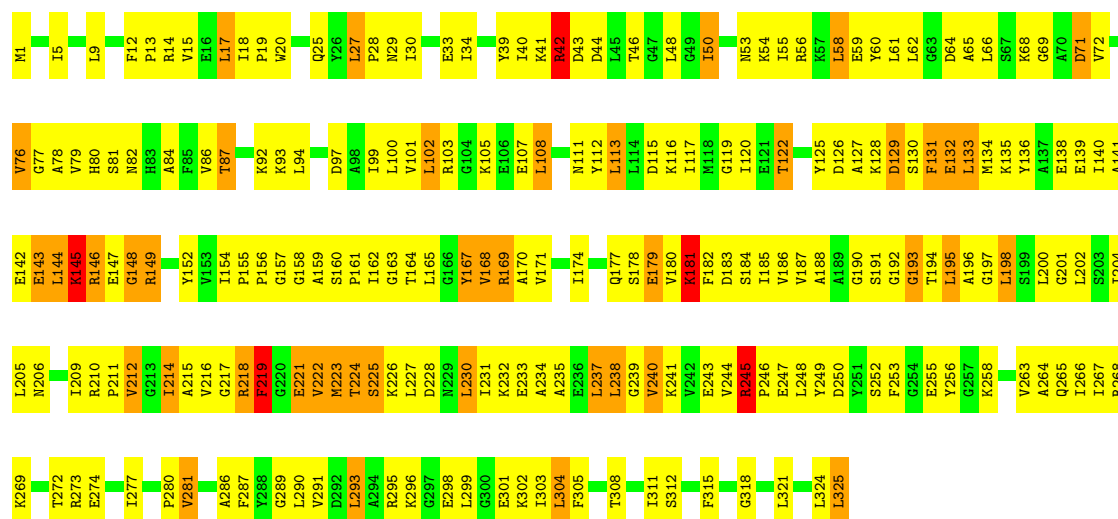
Chain L:  25% 58% 15% .





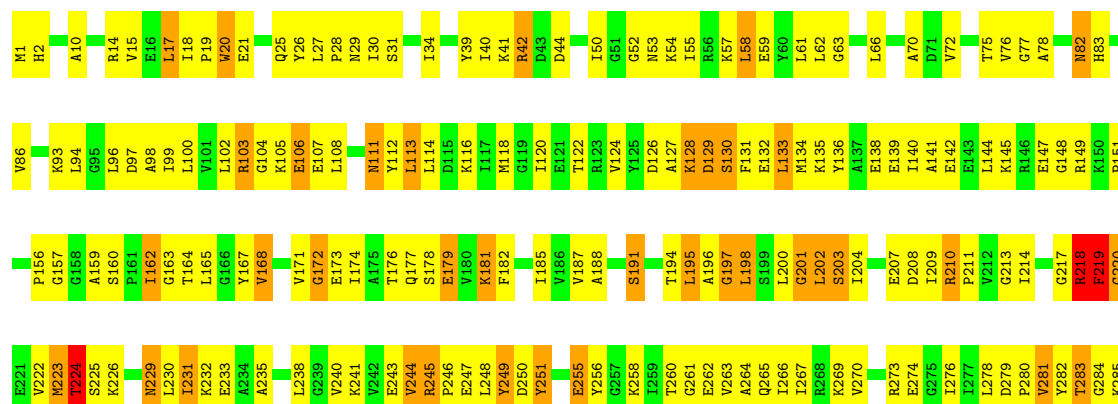
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain M: 32% 54% 13%



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

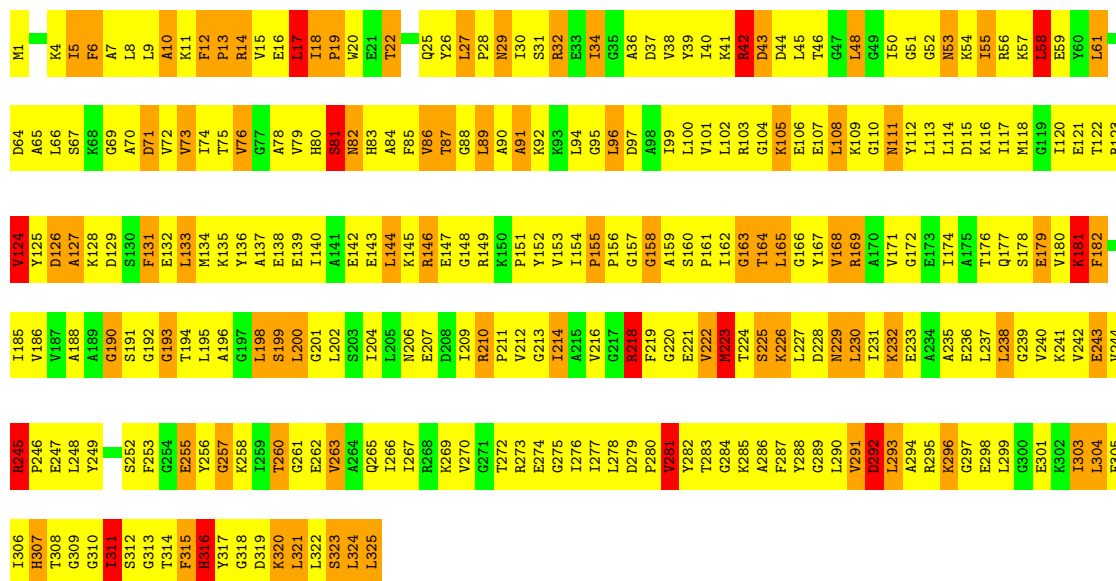
Chain N: 38% 48% 13%





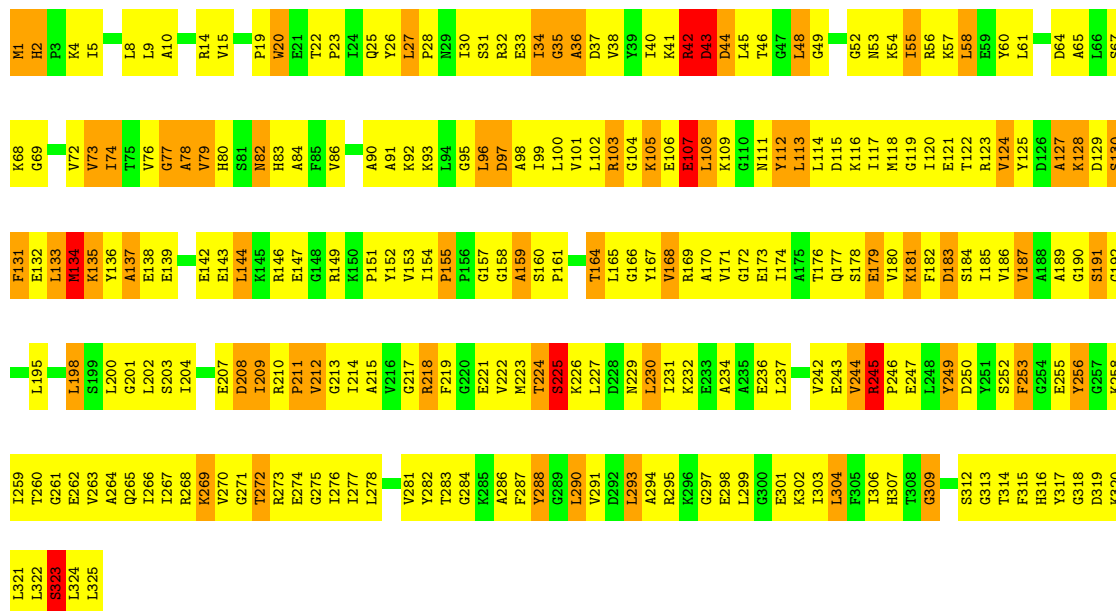
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain O: 13% 59% 23% .



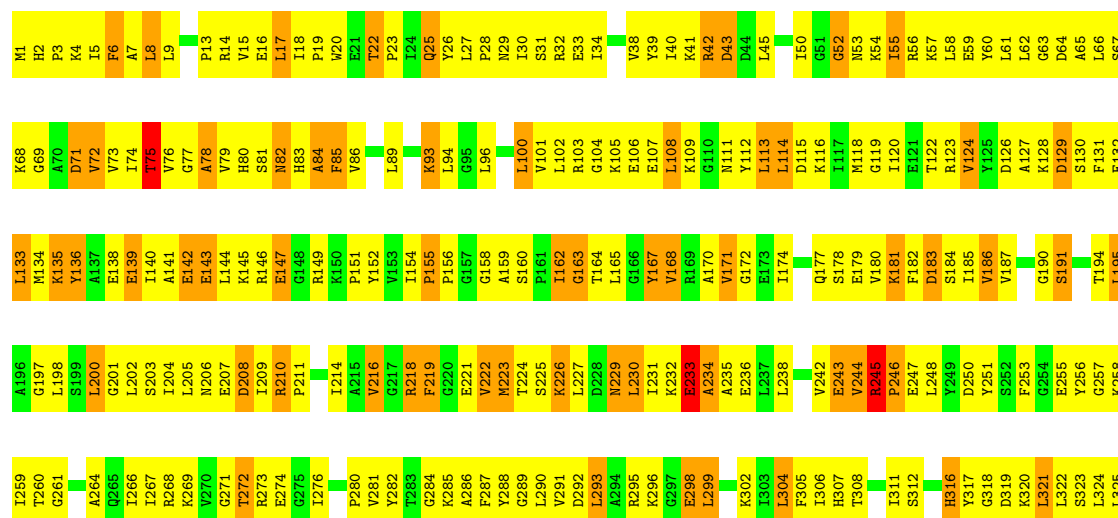
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain P: 22% 57% 19% .



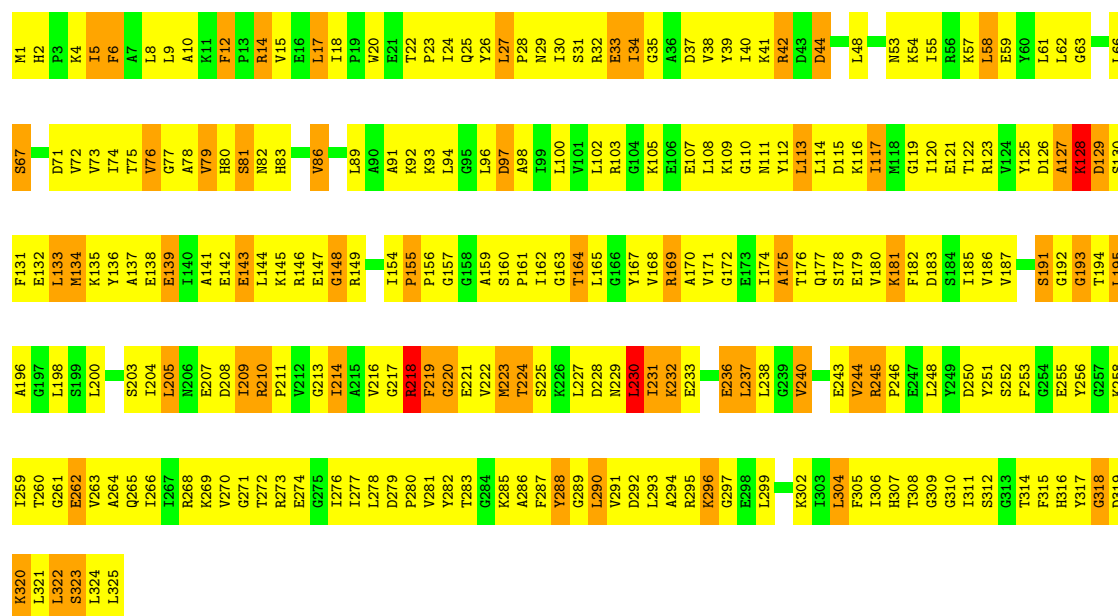
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain Q: 24% 56% 19% .



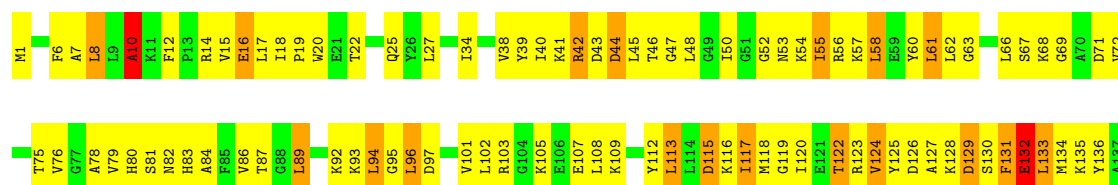
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

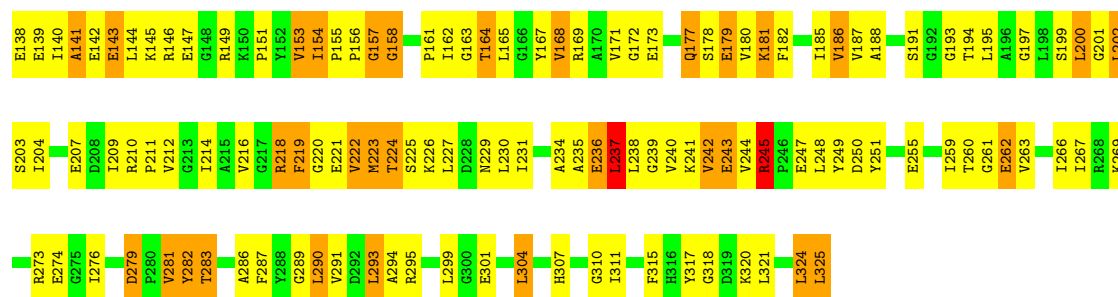
Chain R: 22% 59% 18% .



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

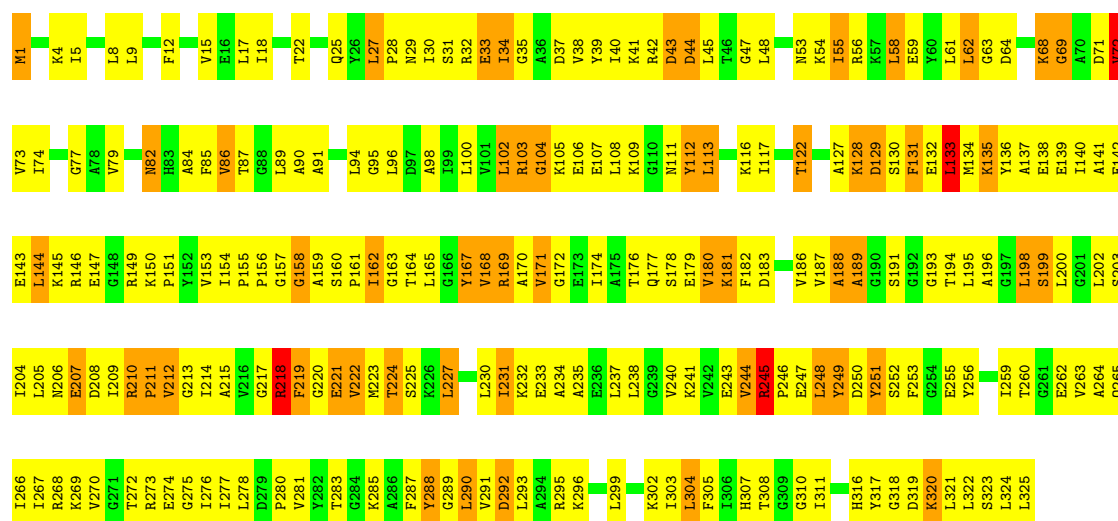
Chain S: 33% 50% 15% .





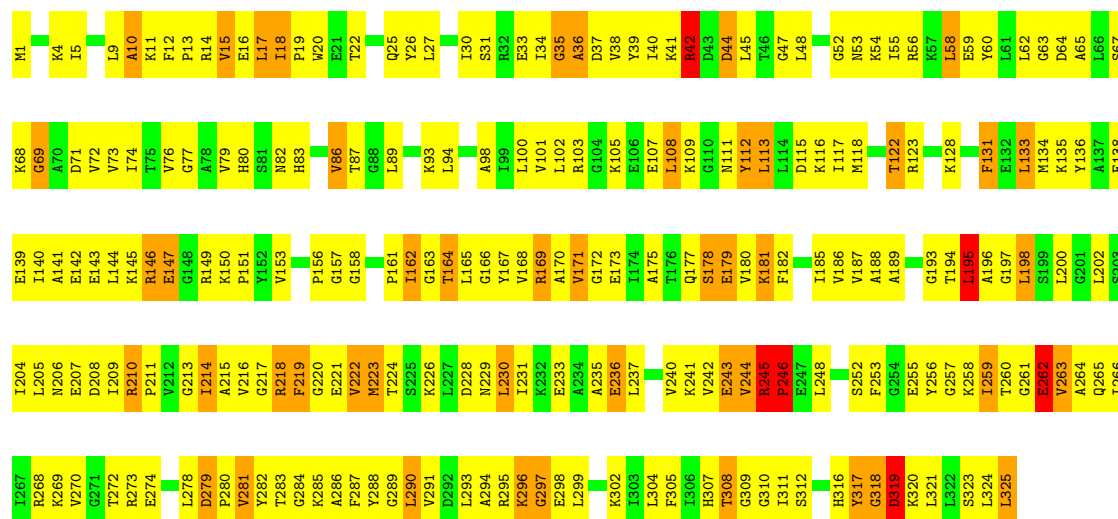
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain T: 27% 55% 17%

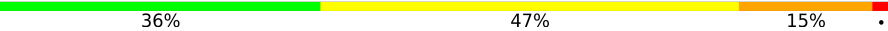


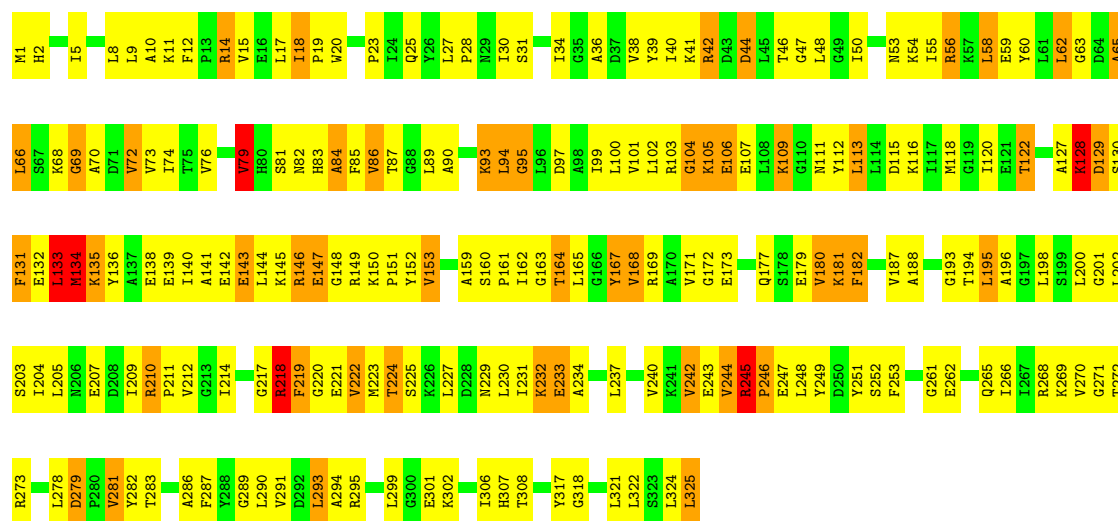
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain U: 28% 56% 14%

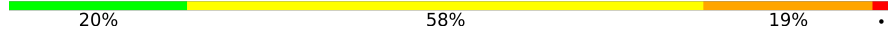


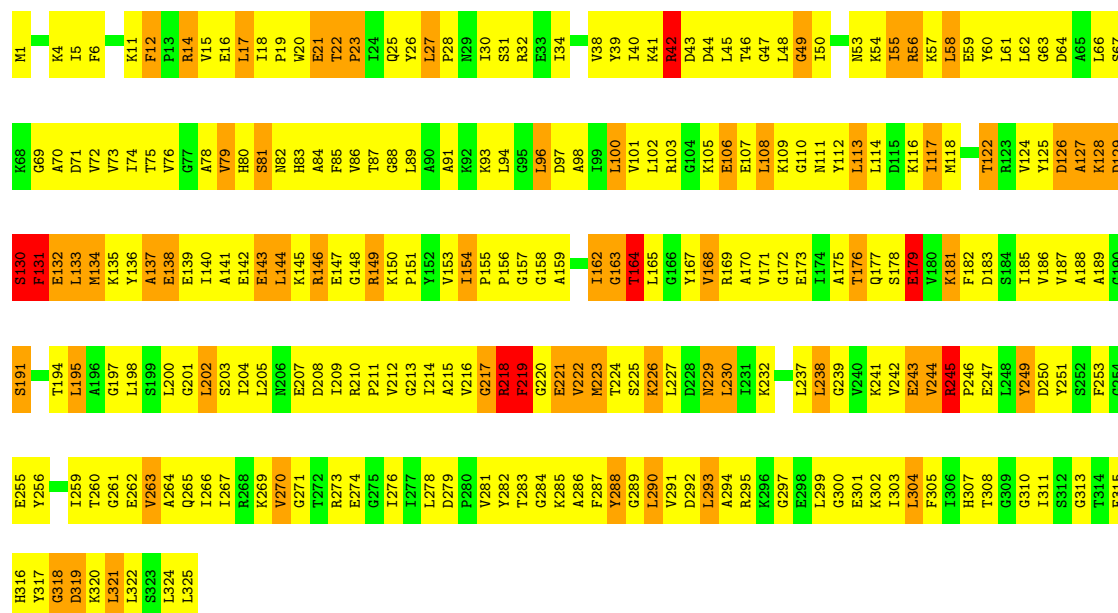
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain V: 

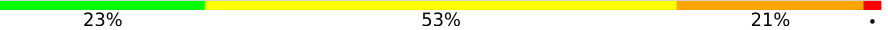


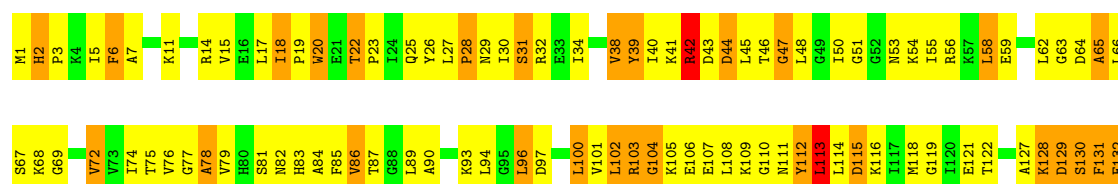
• Molecule 1: 1-aminocyclopropane-1-carboxylate deaminase

Chain W: 



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

Chain X: 



L324 L325	L259	L198	L133
	T260	S199	M134
	G261	L200	K135
	E262	G201	Y136
	V263	L202	A137
	A264	S203	E138
	Q265	L204	E139
	L266	L205	T140
	T267	N206	A141
	K268	E207	E142
L326	K269	D208	E143
	V270	L209	L144
	G271	R210	K145
	T272	P211	R146
	T273	V212	E147
	E274	G213	G148
	G275	L214	R149
	L276	A215	K150
	L277	V216	P151
	L278	G217	Y152
L327	D279	R218	V153
	P280	E219	T154
	V281	G220	I155
	Y282	E221	P155
	T283	V222	F156
	G284	M223	G158
	K285	T224	A159
	A286	S225	S160
	T287	K226	P161
	Y288	L227	T162
L328	G289	D228	G163
	L290	N229	T164
	V291	L230	L165
		I231	G166
	K296	K232	Y167
	E297	E233	V168
	G298	A234	R169
	L299	A235	A170
	G300	E236	V171
		L237	
L329	L303	L238	I174
	L304	G339	
	F305	V240	Q177
		K241	S178
	T308	V242	E179
	G309	E243	V180
	G310	V244	K181
	L311	R245	F182
	S312	P246	
	G313	E247	V186
L330	T314	L248	V187
	F315	Y249	A188
	H316	D250	A189
		Y251	G190
	K317	S252	S191
	G318	F253	
	D319	G254	T194
	K320	E255	L195
	L321		A196
	L322		G197

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, α , β , γ	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 ²)	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	0.59	0/2526	1.23	27/3407 (0.8%)
1	B	0.55	0/2526	1.19	25/3407 (0.7%)
1	C	0.54	0/2526	1.19	28/3407 (0.8%)
1	D	0.59	0/2526	1.20	32/3407 (0.9%)
1	E	0.56	0/2526	1.15	19/3407 (0.6%)
1	F	0.57	0/2526	1.15	25/3407 (0.7%)
1	G	0.58	0/2526	1.28	40/3407 (1.2%)
1	H	0.57	0/2526	1.17	23/3407 (0.7%)
1	I	0.61	0/2526	1.25	39/3407 (1.1%)
1	J	0.55	0/2526	1.20	40/3407 (1.2%)
1	K	0.58	0/2526	1.23	33/3407 (1.0%)
1	L	0.56	0/2526	1.25	33/3407 (1.0%)
1	M	0.55	0/2526	1.15	25/3407 (0.7%)
1	N	0.56	0/2526	1.20	33/3407 (1.0%)
1	O	0.59	0/2526	1.27	41/3407 (1.2%)
1	P	0.55	0/2526	1.20	32/3407 (0.9%)
1	Q	0.58	0/2526	1.18	24/3407 (0.7%)
1	R	0.57	0/2526	1.22	29/3407 (0.9%)
1	S	0.60	0/2526	1.19	26/3407 (0.8%)
1	T	0.61	1/2526 (0.0%)	1.22	34/3407 (1.0%)
1	U	0.58	0/2526	1.24	38/3407 (1.1%)
1	V	0.58	0/2526	1.22	32/3407 (0.9%)
1	W	0.55	0/2526	1.25	36/3407 (1.1%)
1	X	0.57	0/2526	1.29	45/3407 (1.3%)
All	All	0.57	1/60624 (0.0%)	1.21	759/81768 (0.9%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	1	MET	SD-CE	-5.23	1.66	1.79

The worst 5 of 759 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	226	LYS	N-CA-C	-14.44	95.54	111.14
1	E	133	LEU	N-CA-C	-13.66	96.58	113.38
1	N	133	LEU	N-CA-C	-13.19	97.22	113.18
1	O	309	GLY	N-CA-C	12.17	123.86	111.56
1	A	168	VAL	N-CA-C	-11.94	99.31	110.53

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2484	0	2583	244	0
1	B	2484	0	2583	302	0
1	C	2484	0	2583	298	1
1	D	2484	0	2583	274	0
1	E	2484	0	2583	249	0
1	F	2484	0	2583	287	1
1	G	2484	0	2583	522	0
1	H	2484	0	2583	345	0
1	I	2484	0	2583	423	0
1	J	2484	0	2583	381	0
1	K	2484	0	2583	437	0
1	L	2484	0	2583	352	0
1	M	2484	0	2583	331	0
1	N	2484	0	2583	228	0
1	O	2484	0	2583	474	0
1	P	2484	0	2583	382	0
1	Q	2484	0	2583	406	0
1	R	2484	0	2583	360	0
1	S	2484	0	2583	302	0
1	T	2484	0	2583	336	0
1	U	2484	0	2583	285	0
1	V	2484	0	2583	267	0
1	W	2484	0	2583	424	0
1	X	2484	0	2583	351	0
2	A	22	0	13	5	0
2	B	22	0	13	9	0
2	C	22	0	13	7	0
2	D	22	0	13	8	0
2	E	22	0	13	5	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	12	0
2	J	22	0	13	9	0
2	K	22	0	13	9	0
2	L	22	0	13	5	0
2	M	22	0	13	10	0
2	N	22	0	13	4	0
2	O	22	0	13	5	0
2	P	22	0	13	10	0
2	Q	22	0	13	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	22	0	13	13	0
2	S	22	0	13	9	0
2	T	22	0	13	7	0
2	U	22	0	13	6	0
2	V	22	0	13	4	0
2	W	22	0	13	10	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	13	0
3	H	38	0	0	11	0
3	I	29	0	0	8	0
3	J	30	0	0	8	0
3	K	33	0	0	9	0
3	L	29	0	0	12	0
3	M	29	0	0	8	0
3	N	38	0	0	7	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	8068	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 66.

The worst 5 of 8068 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:S:1:MET:HE1	1:S:172:GLY:HA3	1.26	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	223 (86%)	36 (14%)	3	9
1	B	259/259 (100%)	227 (88%)	32 (12%)	4	11
1	C	259/259 (100%)	231 (89%)	28 (11%)	6	16
1	D	259/259 (100%)	232 (90%)	27 (10%)	7	17
1	E	259/259 (100%)	230 (89%)	29 (11%)	6	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	259/259 (100%)	227 (88%)	32 (12%)	4	11
1	G	259/259 (100%)	224 (86%)	35 (14%)	4	9
1	H	259/259 (100%)	227 (88%)	32 (12%)	4	11
1	I	259/259 (100%)	235 (91%)	24 (9%)	8	21
1	J	259/259 (100%)	232 (90%)	27 (10%)	7	17
1	K	259/259 (100%)	231 (89%)	28 (11%)	6	16
1	L	259/259 (100%)	235 (91%)	24 (9%)	8	21
1	M	259/259 (100%)	227 (88%)	32 (12%)	4	11
1	N	259/259 (100%)	229 (88%)	30 (12%)	5	13
1	O	259/259 (100%)	221 (85%)	38 (15%)	3	8
1	P	259/259 (100%)	223 (86%)	36 (14%)	3	9
1	Q	259/259 (100%)	228 (88%)	31 (12%)	5	12
1	R	259/259 (100%)	224 (86%)	35 (14%)	4	9
1	S	259/259 (100%)	225 (87%)	34 (13%)	4	10
1	T	259/259 (100%)	230 (89%)	29 (11%)	6	15
1	U	259/259 (100%)	231 (89%)	28 (11%)	6	16
1	V	259/259 (100%)	224 (86%)	35 (14%)	4	9
1	W	259/259 (100%)	226 (87%)	33 (13%)	4	11
1	X	259/259 (100%)	223 (86%)	36 (14%)	3	9
All	All	6216/6216 (100%)	5465 (88%)	751 (12%)	5	12

5 of 751 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	73	VAL
1	S	181	LYS
1	P	181	LYS
1	P	58	LEU
1	Q	316	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 133 such sidechains are listed below:

Mol	Chain	Res	Type
1	V	82	ASN

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Mol	Chain	Res	Type
1	V	229	ASN
1	X	111	ASN
1	J	25	GLN
1	I	316	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	Q	1171	-	22,23,23	2.49	6 (27%)	33,35,35	2.10	5 (15%)
2	5PA	A	1011	-	22,23,23	2.47	5 (22%)	33,35,35	2.25	8 (24%)
2	5PA	W	1231	-	22,23,23	2.48	7 (31%)	33,35,35	2.02	5 (15%)
2	5PA	E	1051	-	22,23,23	2.48	6 (27%)	33,35,35	2.14	7 (21%)
2	5PA	G	1071	-	22,23,23	2.46	8 (36%)	33,35,35	2.24	8 (24%)
2	5PA	V	1221	-	22,23,23	2.49	5 (22%)	33,35,35	2.15	7 (21%)
2	5PA	X	1241	-	22,23,23	2.46	5 (22%)	33,35,35	2.10	9 (27%)
2	5PA	U	1211	-	22,23,23	2.46	6 (27%)	33,35,35	2.26	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5PA	S	1191	-	22,23,23	2.46	7 (31%)	33,35,35	2.30	9 (27%)
2	5PA	L	1121	-	22,23,23	2.49	7 (31%)	33,35,35	2.20	8 (24%)
2	5PA	I	1091	-	22,23,23	2.45	6 (27%)	33,35,35	2.06	5 (15%)
2	5PA	K	1111	-	22,23,23	2.44	6 (27%)	33,35,35	2.38	6 (18%)
2	5PA	M	1131	-	22,23,23	2.47	6 (27%)	33,35,35	2.16	8 (24%)
2	5PA	B	1021	-	22,23,23	2.47	6 (27%)	33,35,35	2.12	7 (21%)
2	5PA	T	1201	-	22,23,23	2.44	6 (27%)	33,35,35	2.09	6 (18%)
2	5PA	C	1031	-	22,23,23	2.45	6 (27%)	33,35,35	2.22	8 (24%)
2	5PA	D	1041	-	22,23,23	2.47	6 (27%)	33,35,35	2.08	9 (27%)
2	5PA	R	1181	-	22,23,23	2.48	5 (22%)	33,35,35	2.19	7 (21%)
2	5PA	O	1151	-	22,23,23	2.52	7 (31%)	33,35,35	1.91	6 (18%)
2	5PA	P	1161	-	22,23,23	2.47	6 (27%)	33,35,35	2.06	7 (21%)
2	5PA	H	1081	-	22,23,23	2.54	6 (27%)	33,35,35	2.06	9 (27%)
2	5PA	J	1101	-	22,23,23	2.47	7 (31%)	33,35,35	1.98	6 (18%)
2	5PA	F	1061	-	22,23,23	2.47	5 (22%)	33,35,35	2.04	6 (18%)
2	5PA	N	1141	-	22,23,23	2.45	5 (22%)	33,35,35	2.17	6 (18%)

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	Q	1171	-	-	6/15/22/22	0/2/2/2
2	5PA	A	1011	-	-	8/15/22/22	0/2/2/2
2	5PA	W	1231	-	-	7/15/22/22	0/2/2/2
2	5PA	E	1051	-	-	6/15/22/22	0/2/2/2
2	5PA	G	1071	-	-	7/15/22/22	0/2/2/2
2	5PA	V	1221	-	-	8/15/22/22	0/2/2/2
2	5PA	X	1241	-	-	7/15/22/22	0/2/2/2
2	5PA	U	1211	-	-	9/15/22/22	0/2/2/2
2	5PA	S	1191	-	-	4/15/22/22	0/2/2/2
2	5PA	L	1121	-	-	10/15/22/22	0/2/2/2
2	5PA	I	1091	-	-	9/15/22/22	0/2/2/2
2	5PA	K	1111	-	-	8/15/22/22	0/2/2/2
2	5PA	M	1131	-	-	7/15/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5PA	B	1021	-	-	6/15/22/22	0/2/2/2
2	5PA	T	1201	-	-	6/15/22/22	0/2/2/2
2	5PA	C	1031	-	-	7/15/22/22	0/2/2/2
2	5PA	D	1041	-	-	8/15/22/22	0/2/2/2
2	5PA	R	1181	-	-	8/15/22/22	0/2/2/2
2	5PA	O	1151	-	-	9/15/22/22	0/2/2/2
2	5PA	P	1161	-	-	8/15/22/22	0/2/2/2
2	5PA	H	1081	-	-	8/15/22/22	0/2/2/2
2	5PA	J	1101	-	-	12/15/22/22	0/2/2/2
2	5PA	F	1061	-	-	8/15/22/22	0/2/2/2
2	5PA	N	1141	-	-	6/15/22/22	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

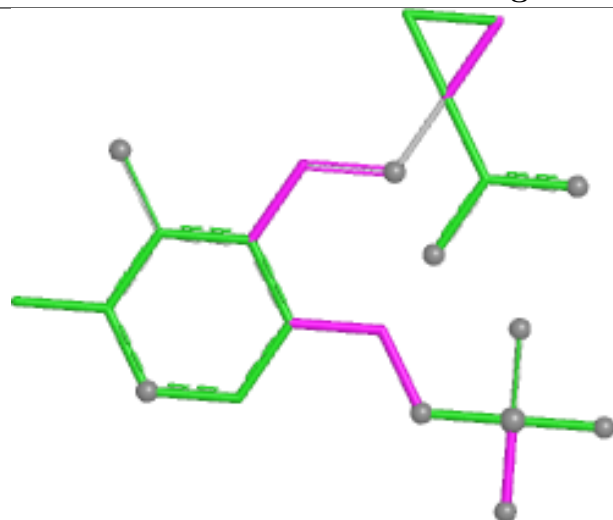
There are no ring outliers.

24 monomers are involved in 193 short contacts:

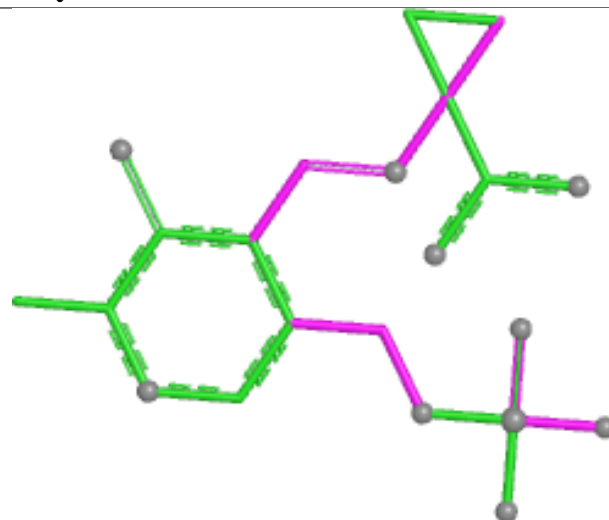
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	1171	5PA	15	0
2	A	1011	5PA	5	0
2	W	1231	5PA	10	0
2	E	1051	5PA	5	0
2	G	1071	5PA	3	0
2	V	1221	5PA	4	0
2	X	1241	5PA	6	0
2	U	1211	5PA	6	0
2	S	1191	5PA	9	0
2	L	1121	5PA	5	0
2	I	1091	5PA	12	0
2	K	1111	5PA	9	0
2	M	1131	5PA	10	0
2	B	1021	5PA	9	0
2	T	1201	5PA	7	0
2	C	1031	5PA	7	0
2	D	1041	5PA	8	0
2	R	1181	5PA	13	0
2	O	1151	5PA	5	0
2	P	1161	5PA	10	0
2	H	1081	5PA	7	0
2	J	1101	5PA	9	0
2	F	1061	5PA	15	0
2	N	1141	5PA	4	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.

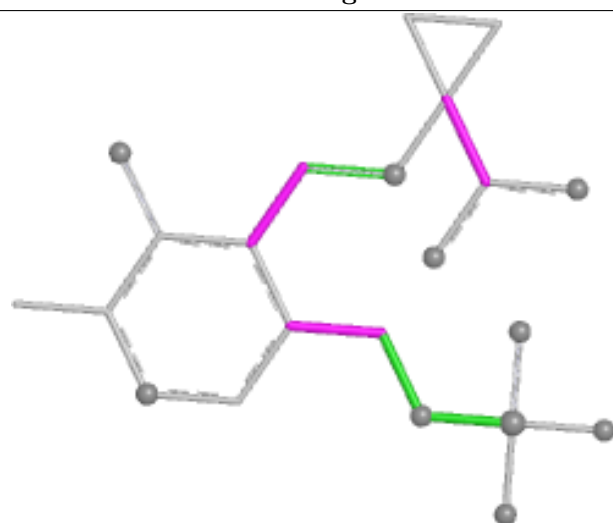
Ligand 5PA Q 1171



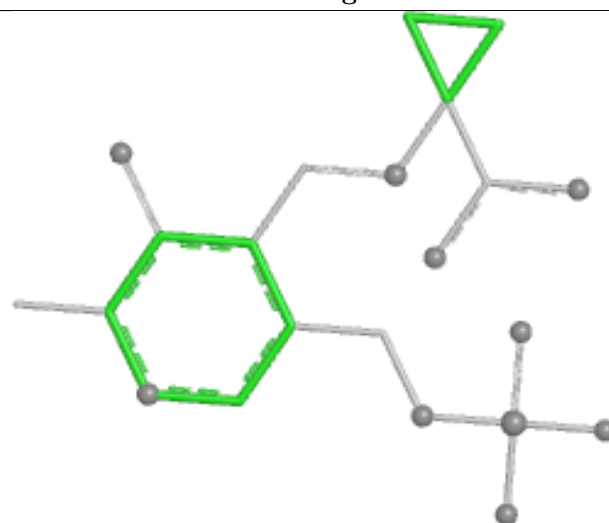
Bond lengths



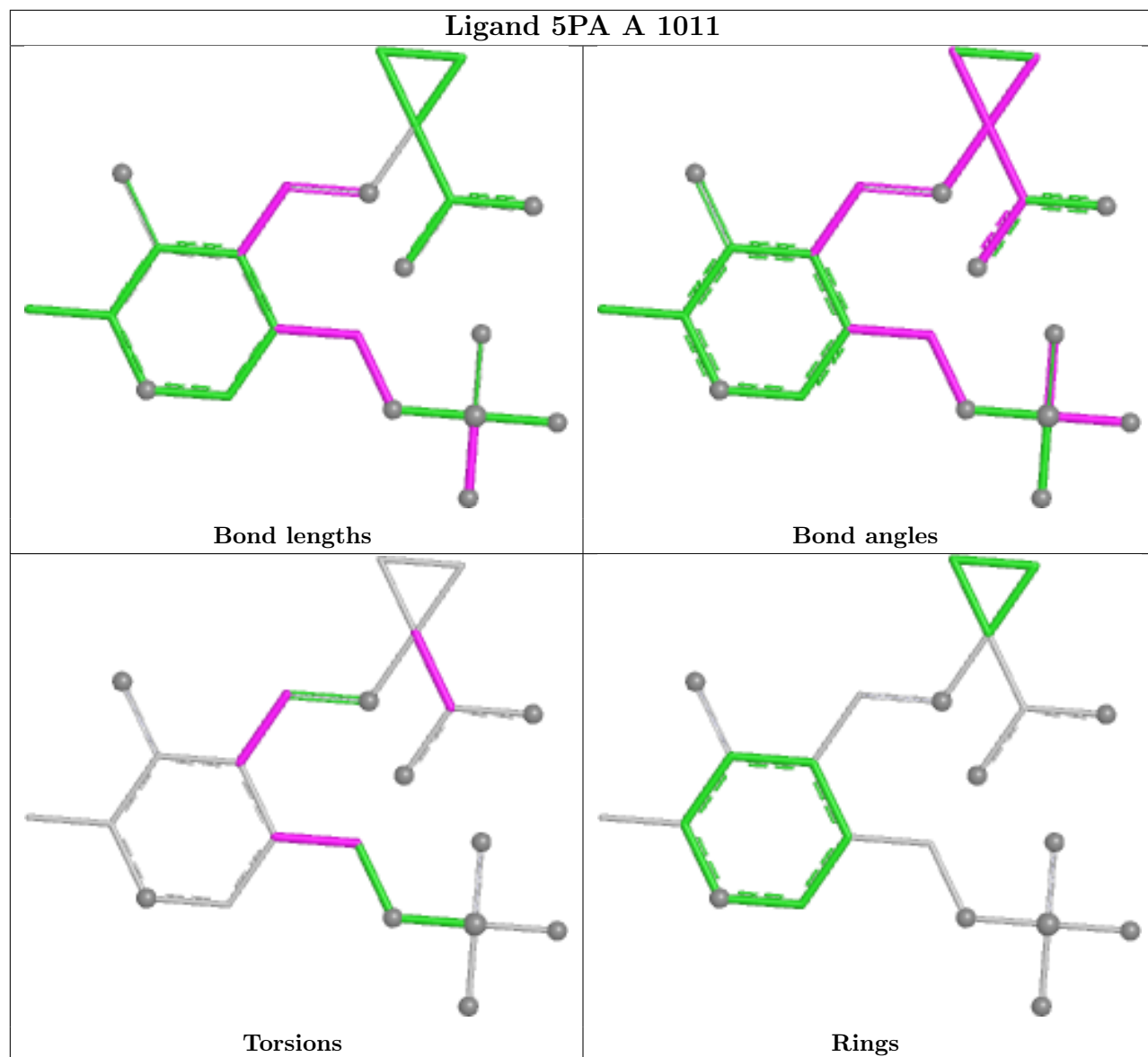
Bond angles



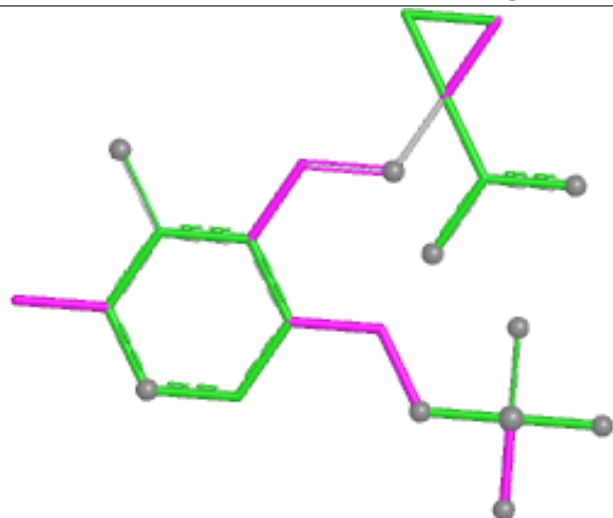
Torsions



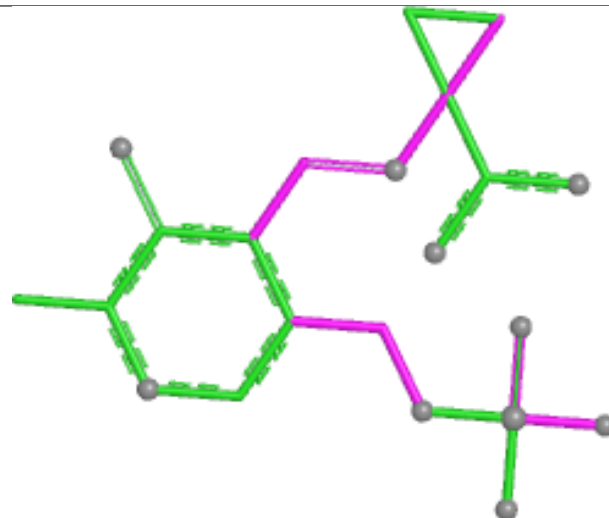
Rings



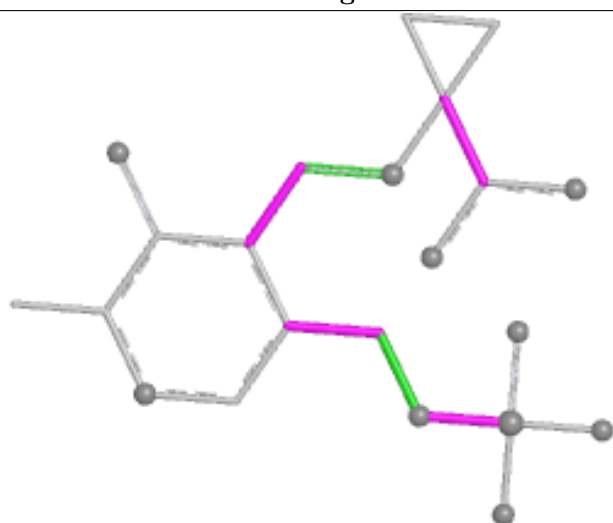
Ligand 5PA W 1231



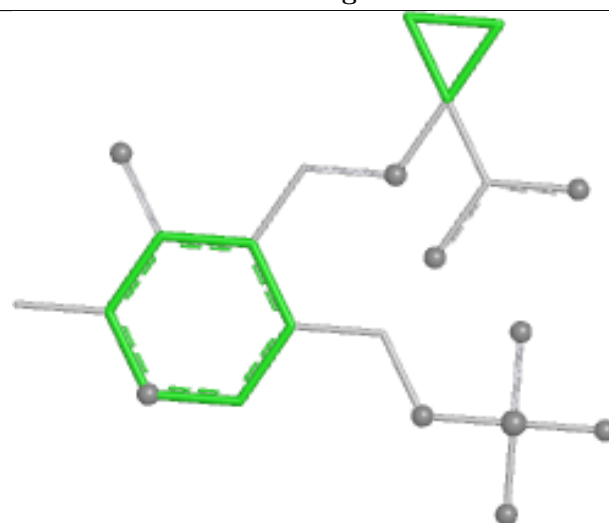
Bond lengths



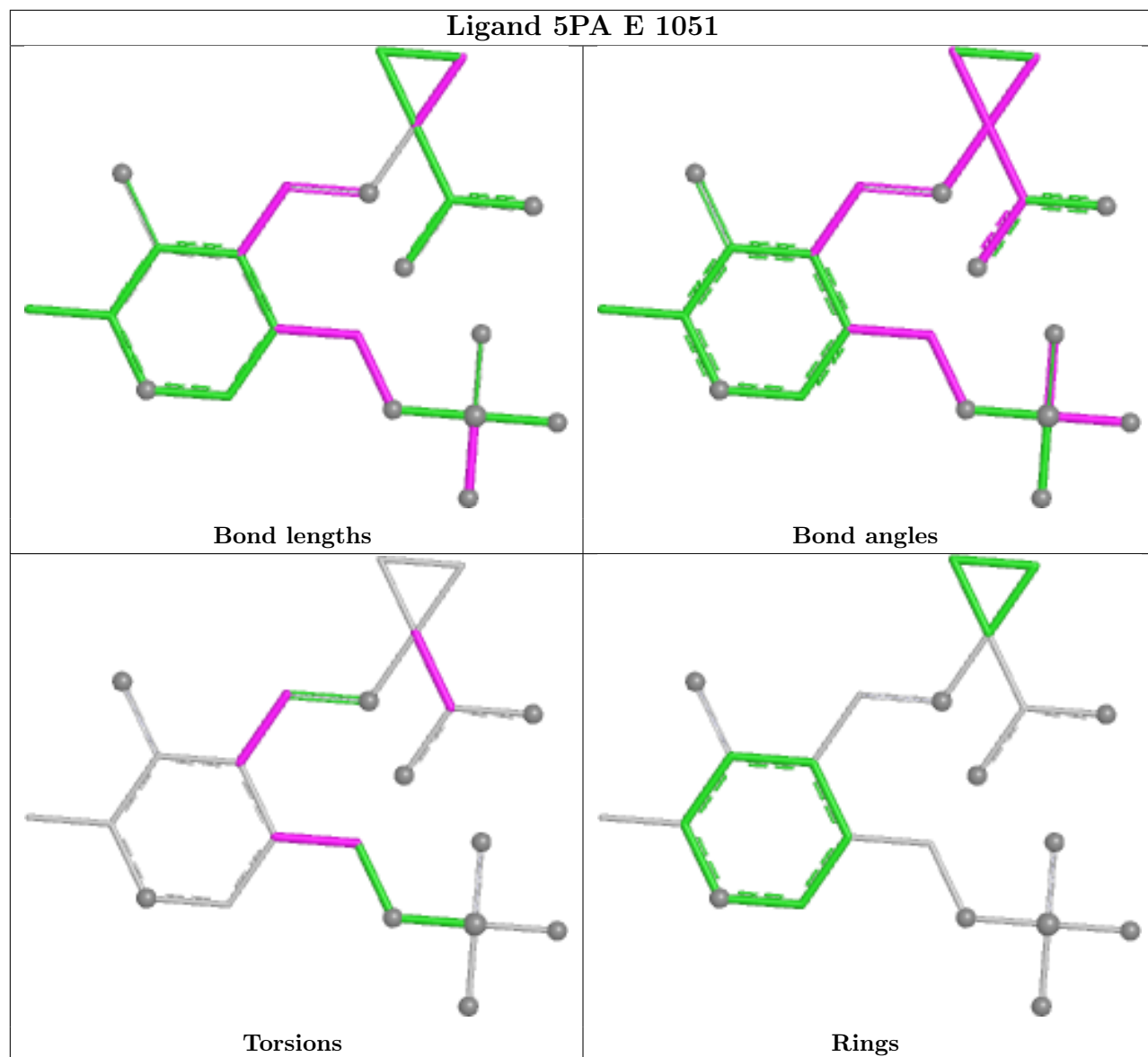
Bond angles



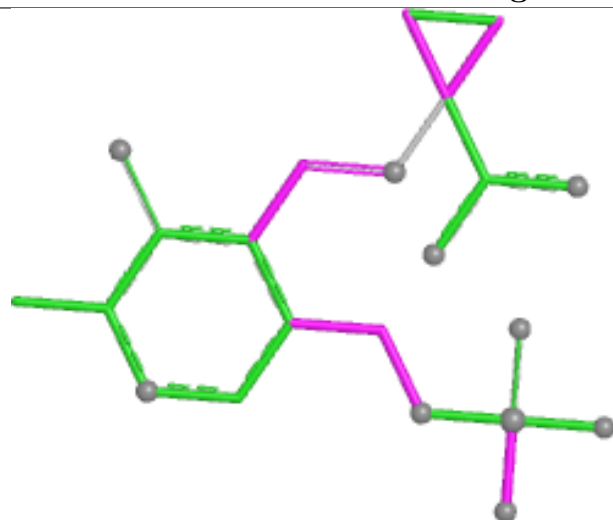
Torsions



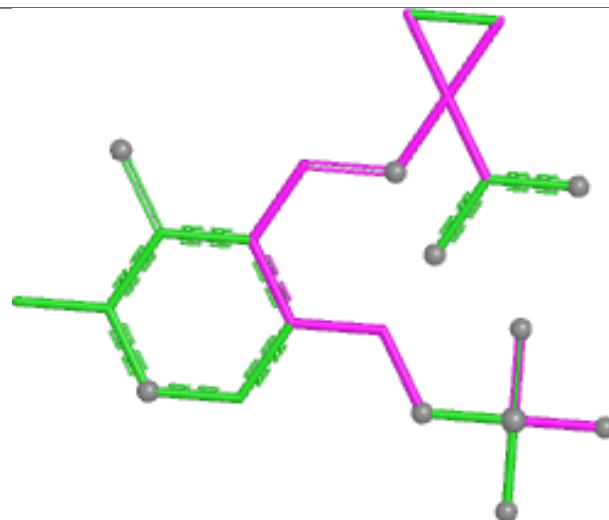
Rings



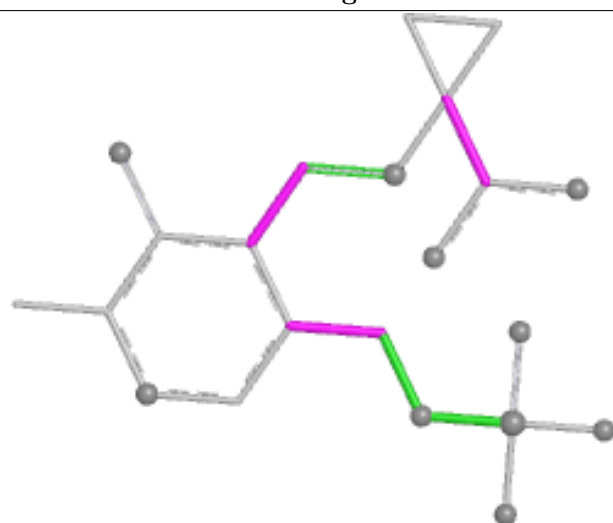
Ligand 5PA G 1071



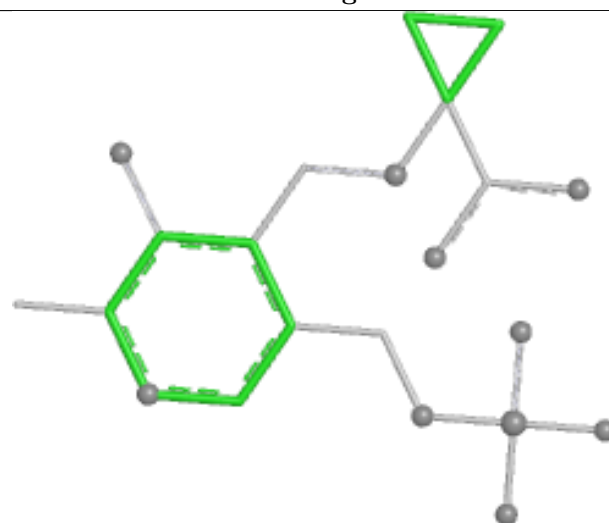
Bond lengths



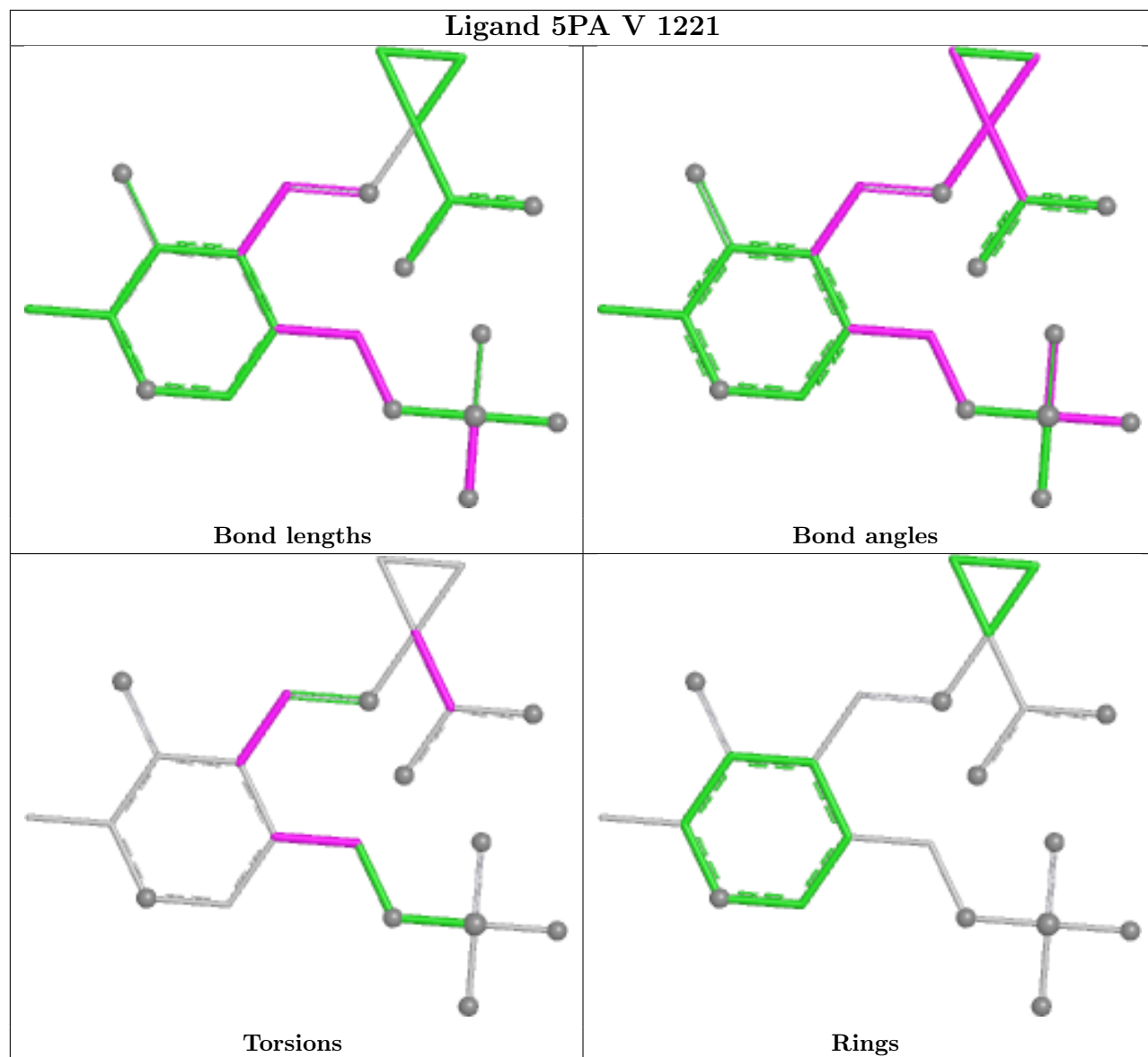
Bond angles

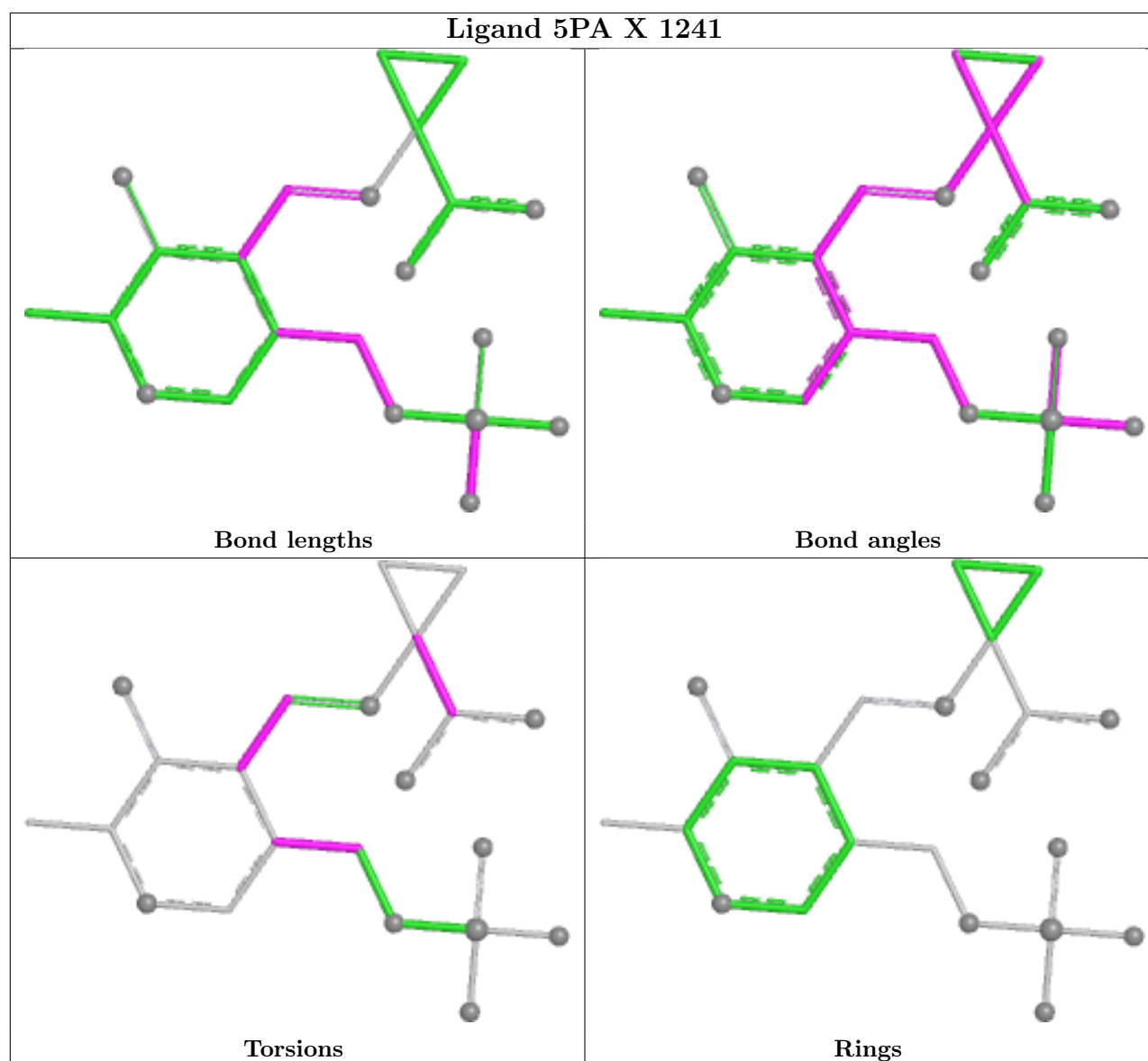


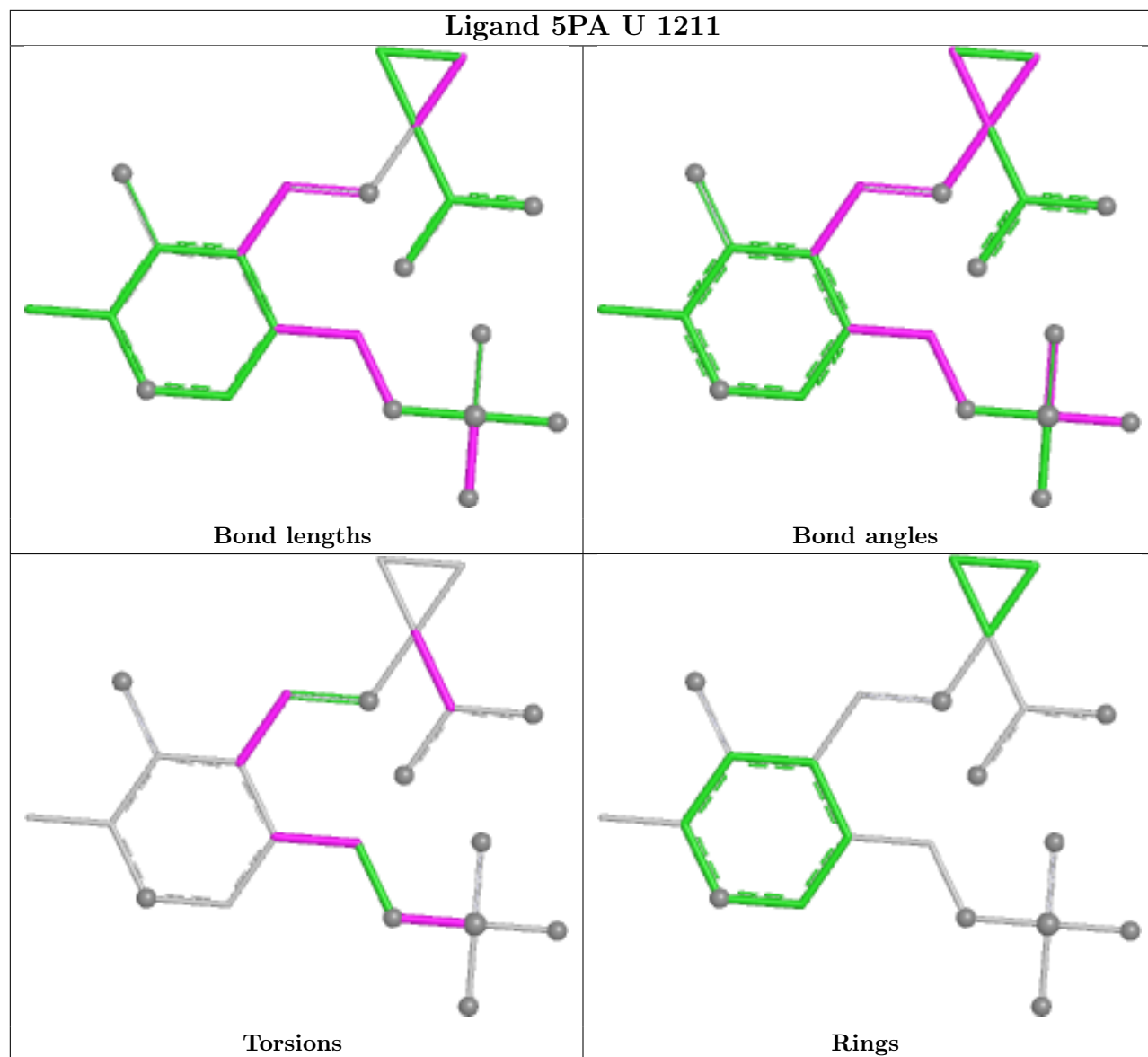
Torsions

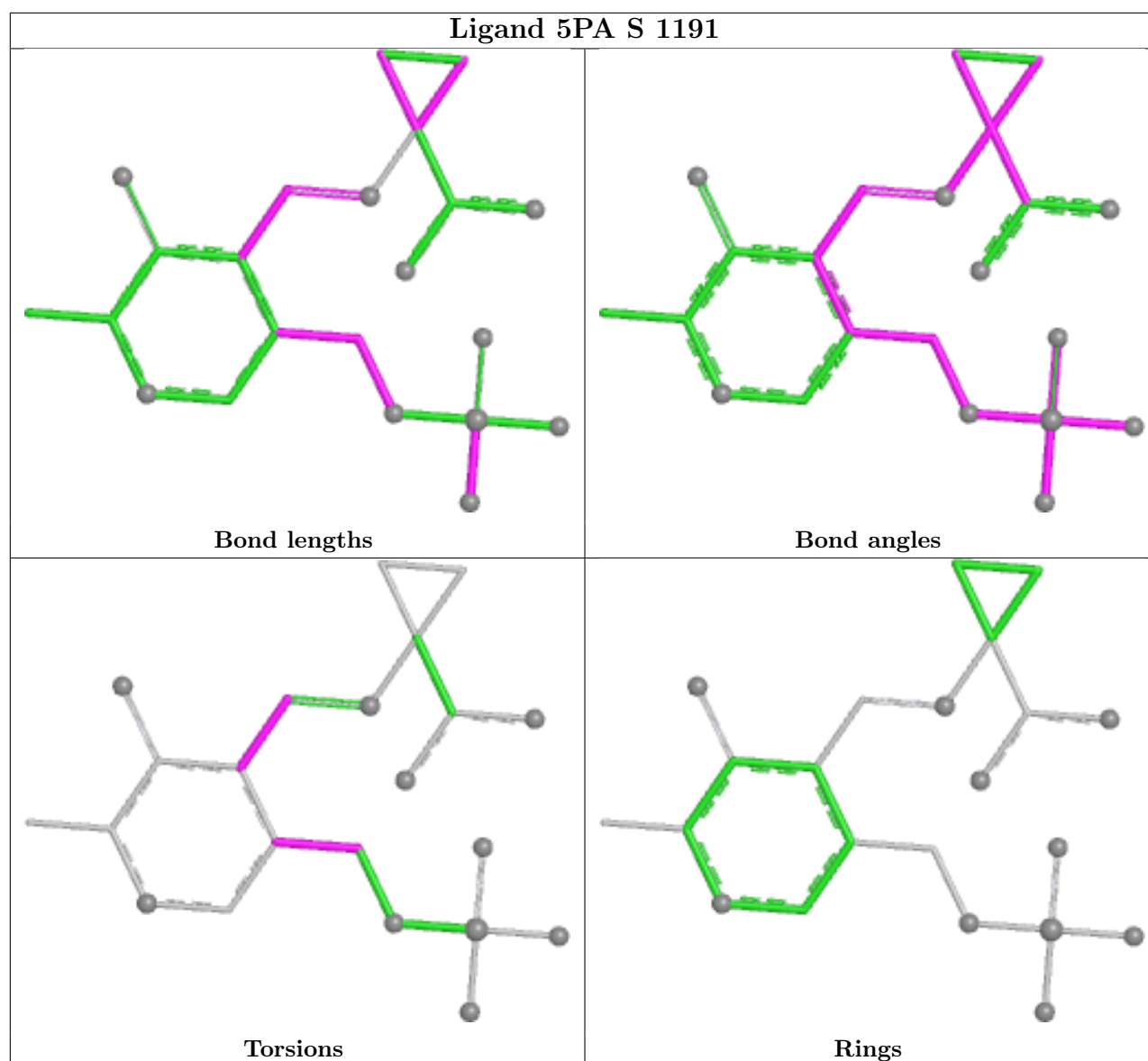


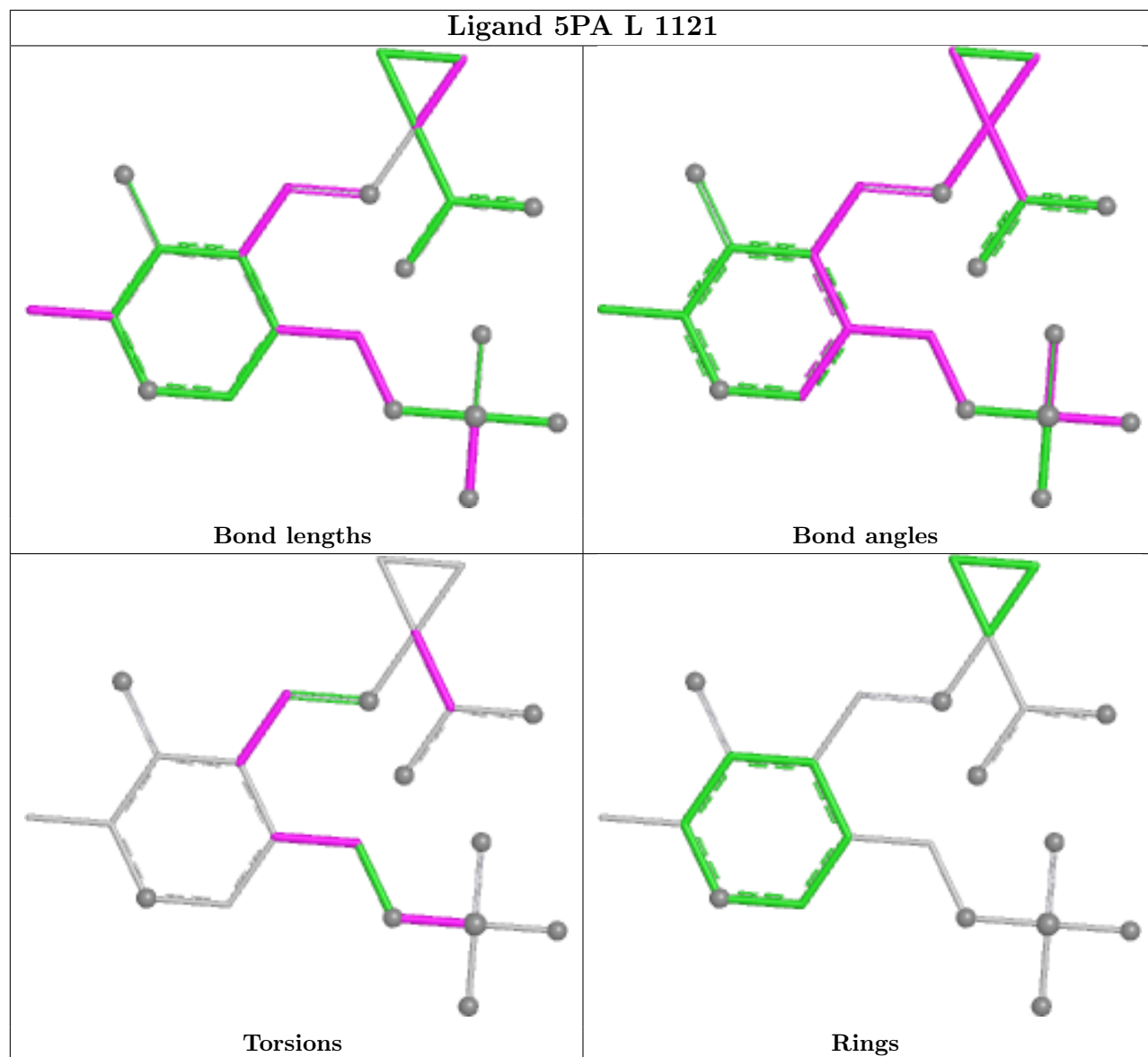
Rings



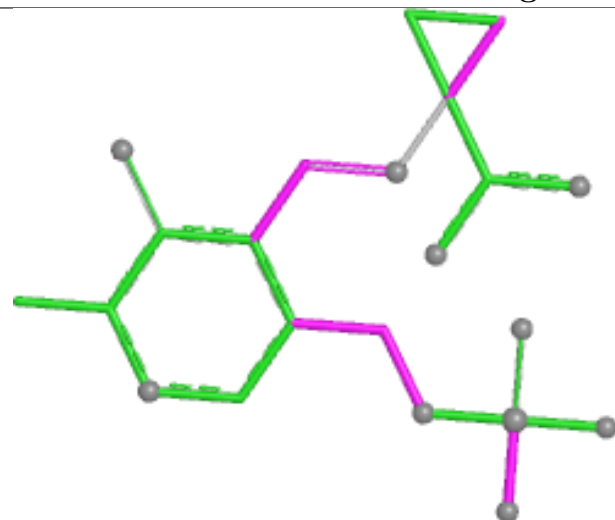




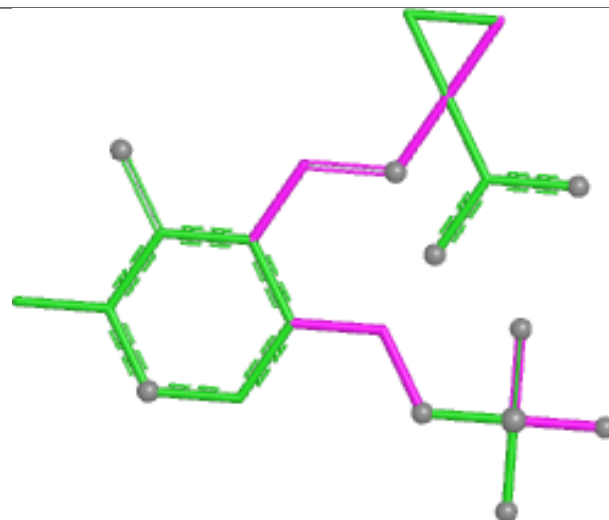




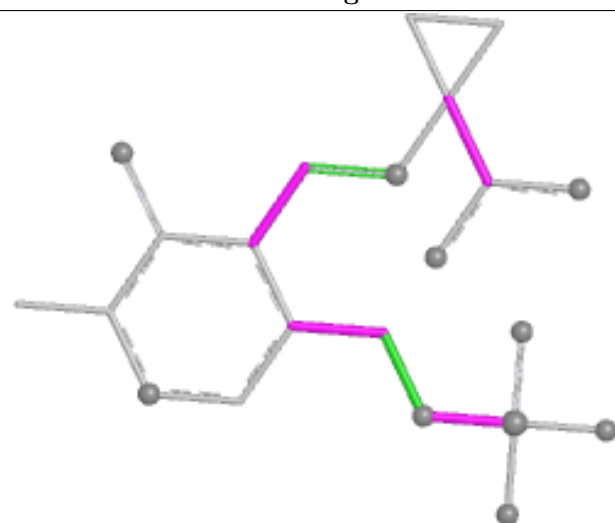
Ligand 5PA I 1091



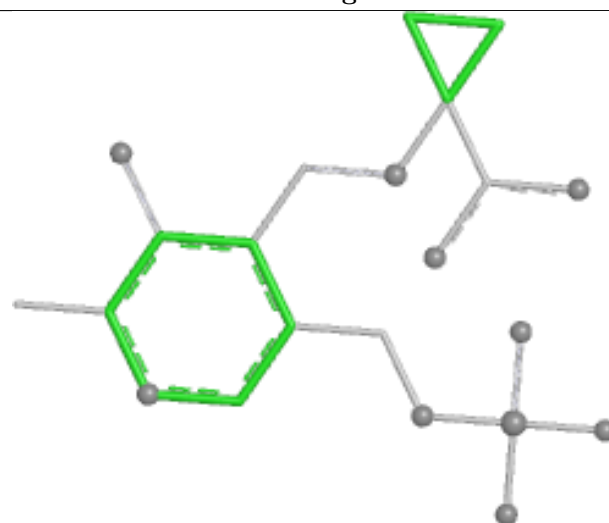
Bond lengths



Bond angles

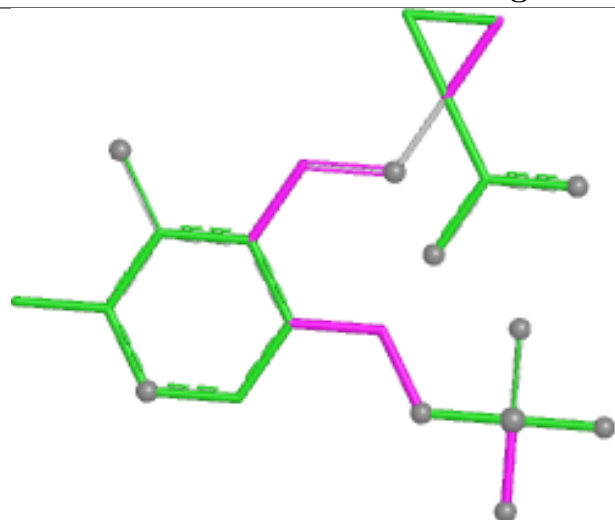


Torsions

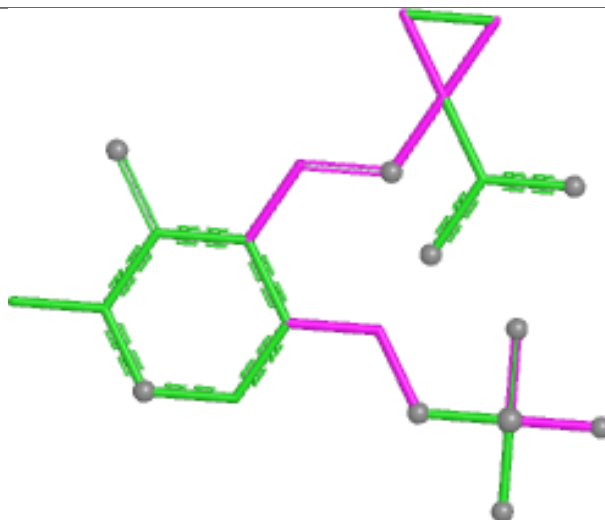


Rings

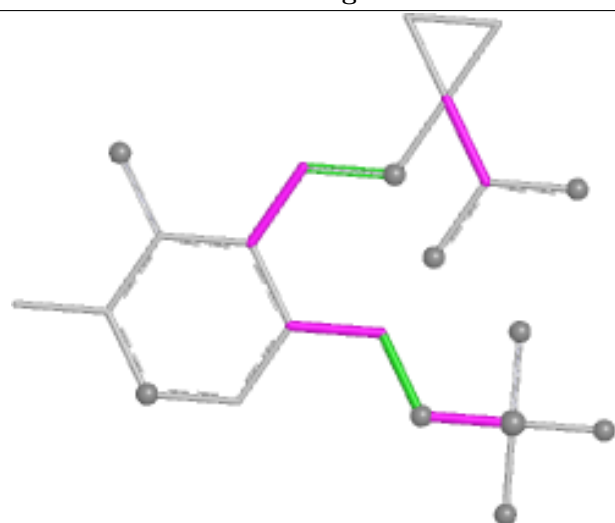
Ligand 5PA K 1111



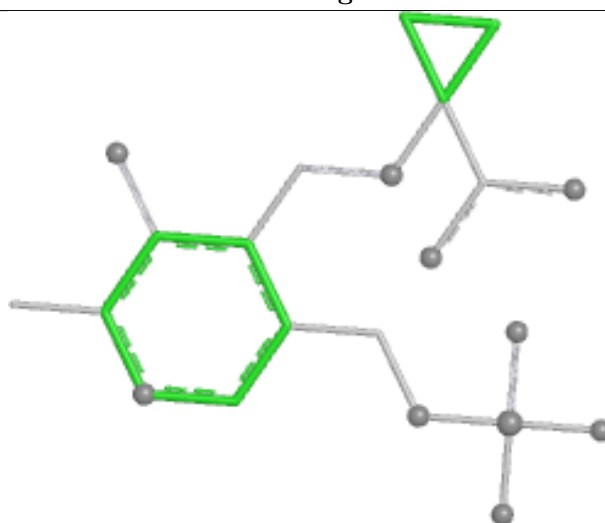
Bond lengths



Bond angles

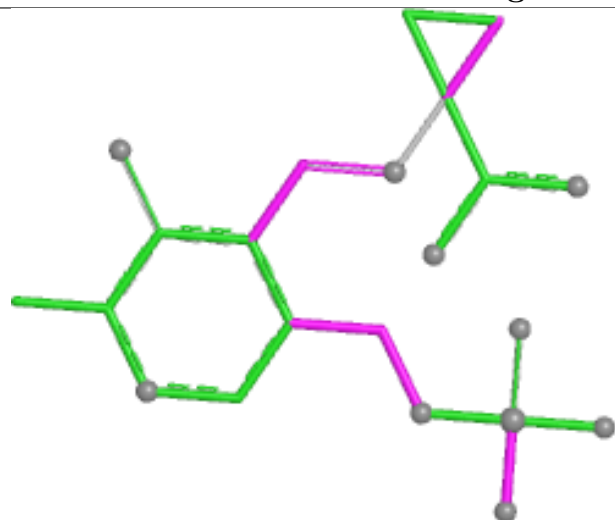


Torsions

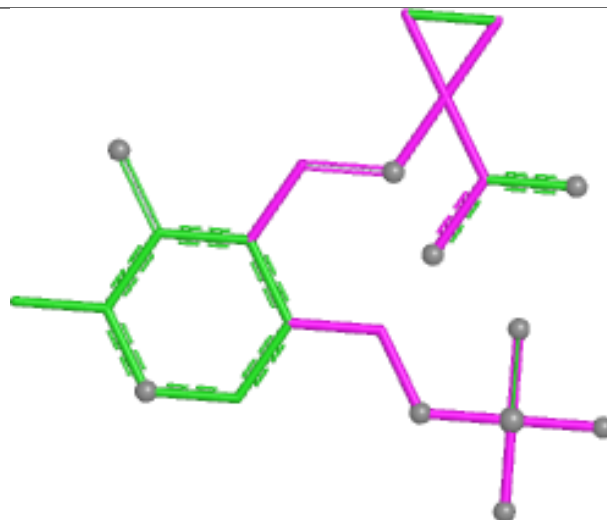


Rings

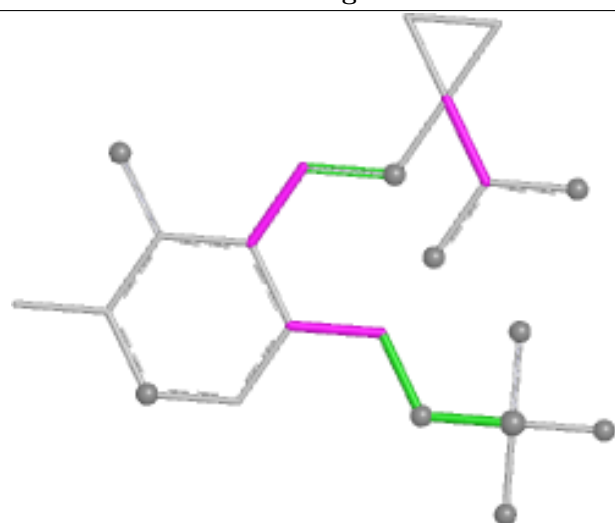
Ligand 5PA M 1131



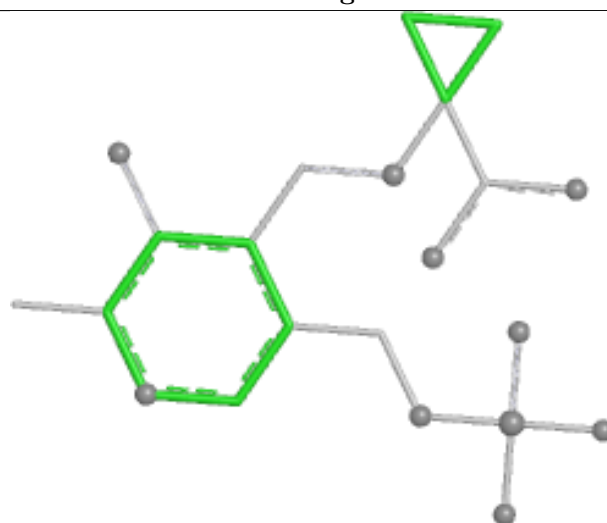
Bond lengths



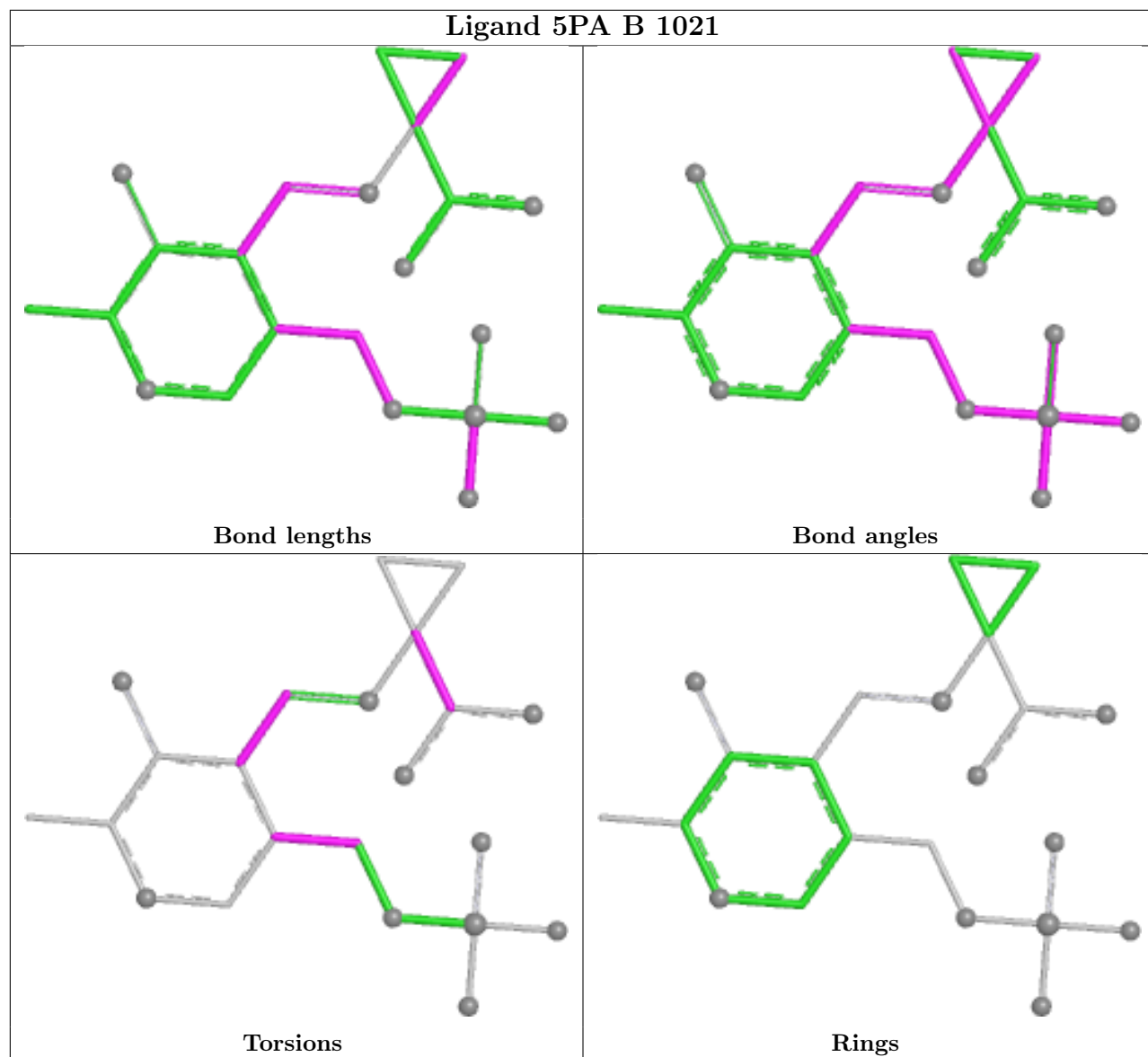
Bond angles

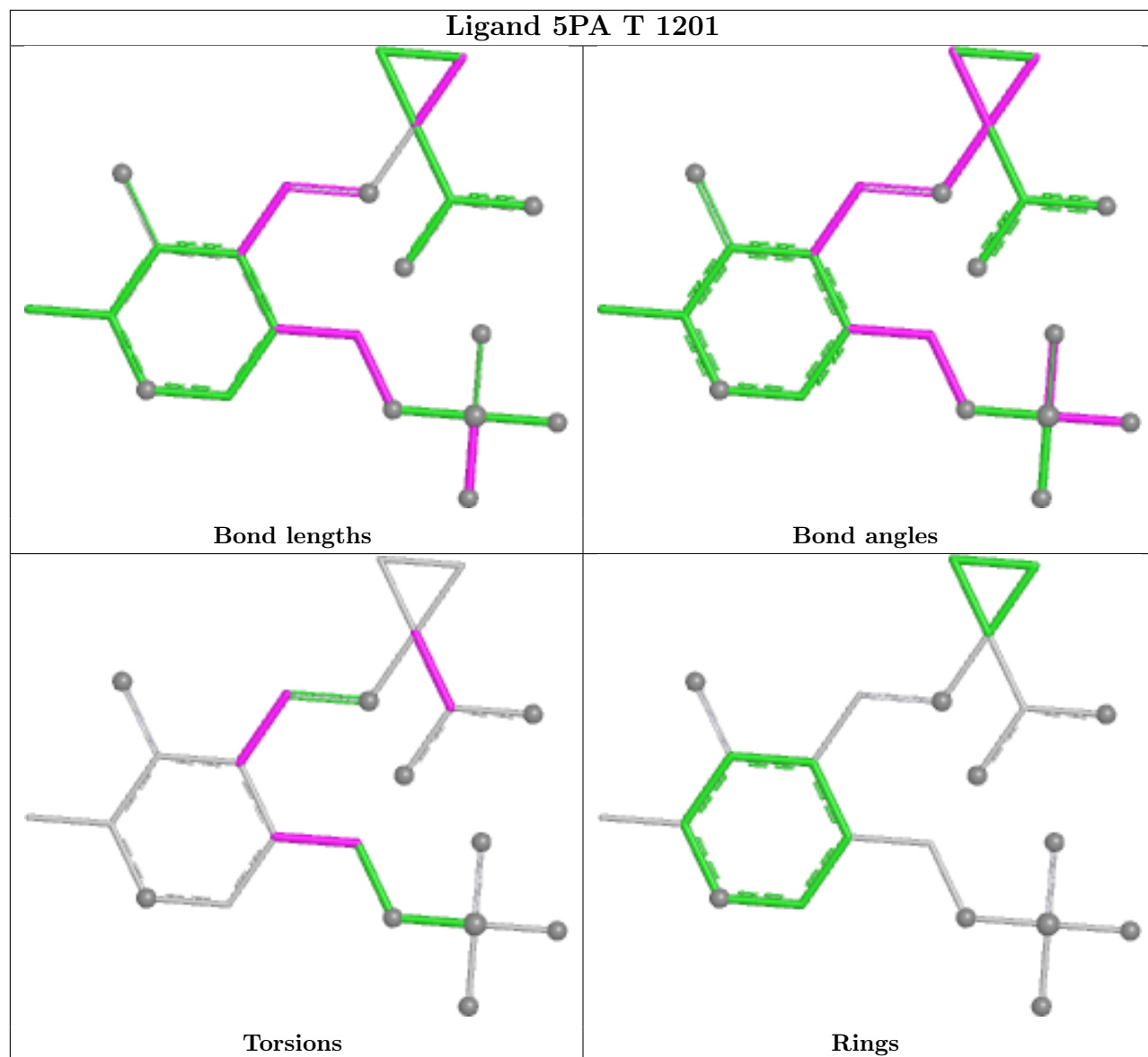


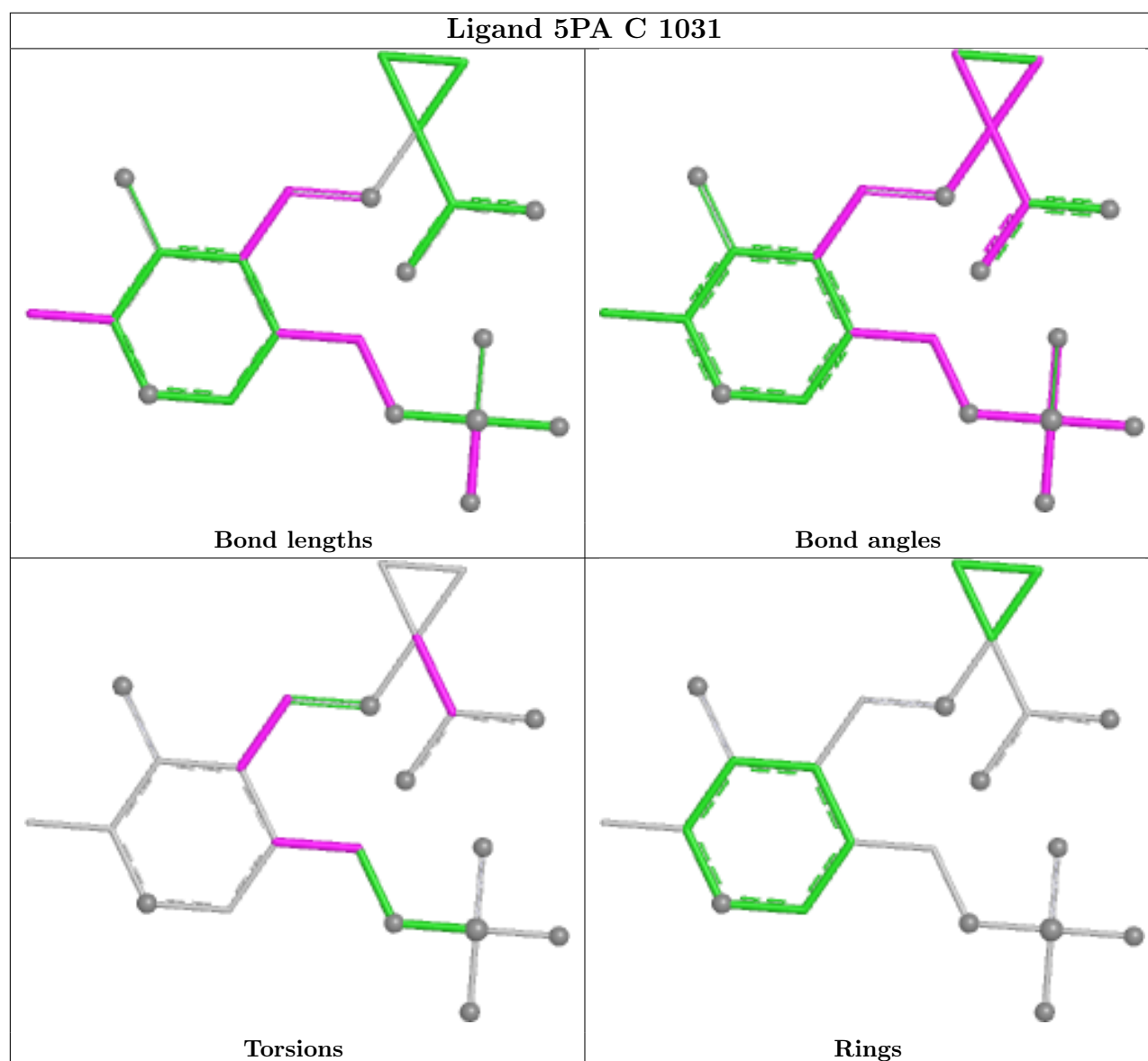
Torsions

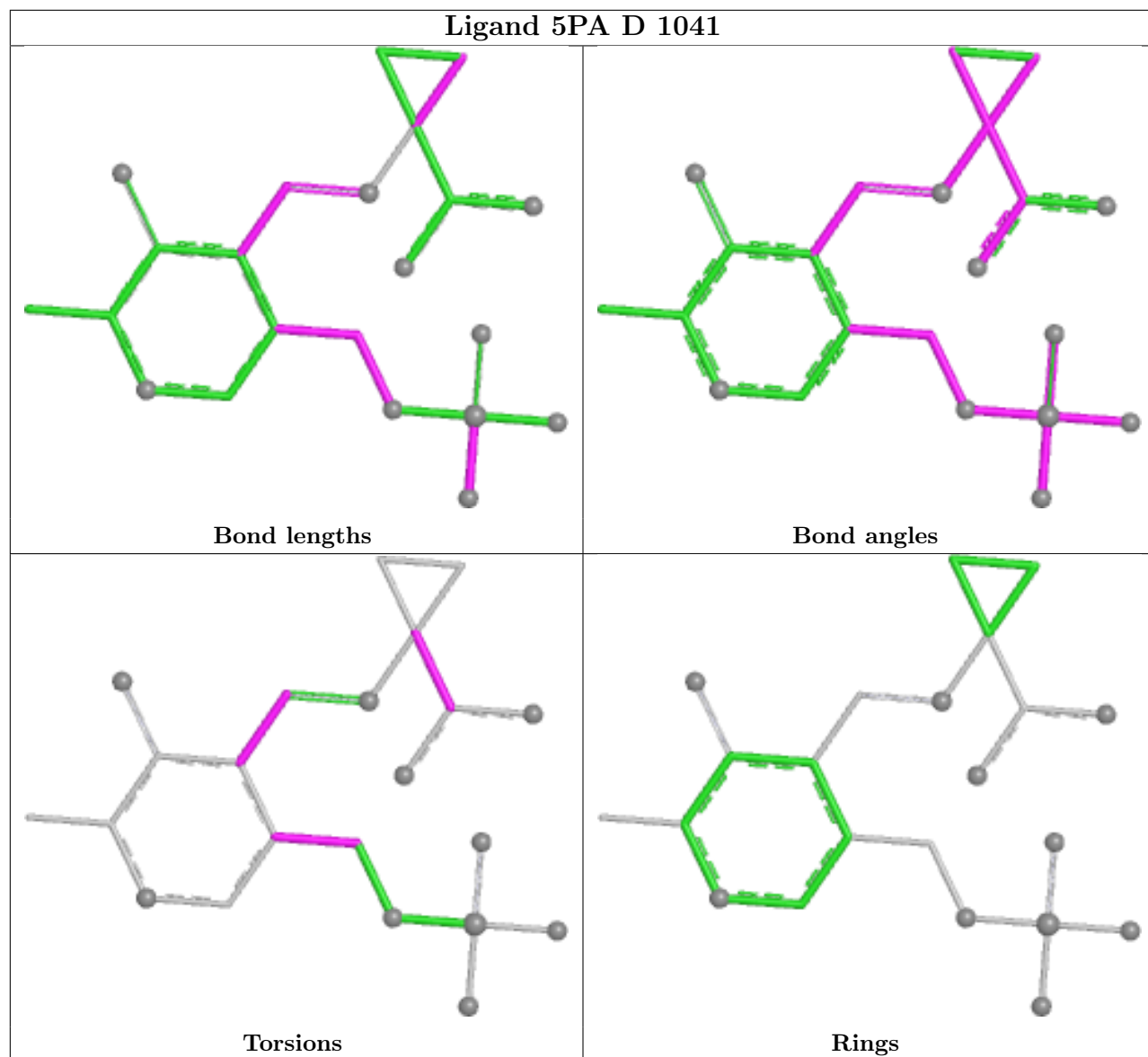


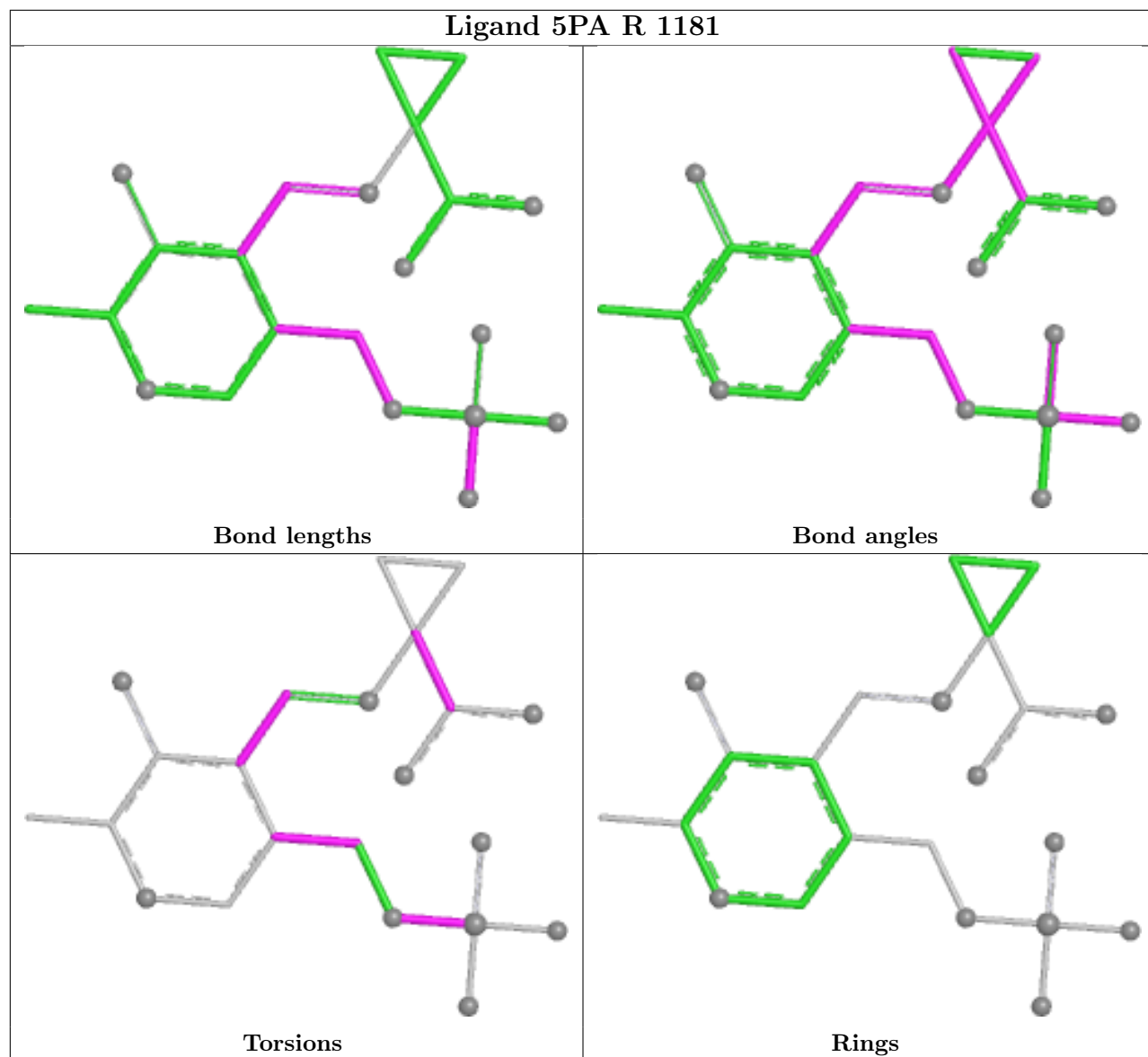
Rings

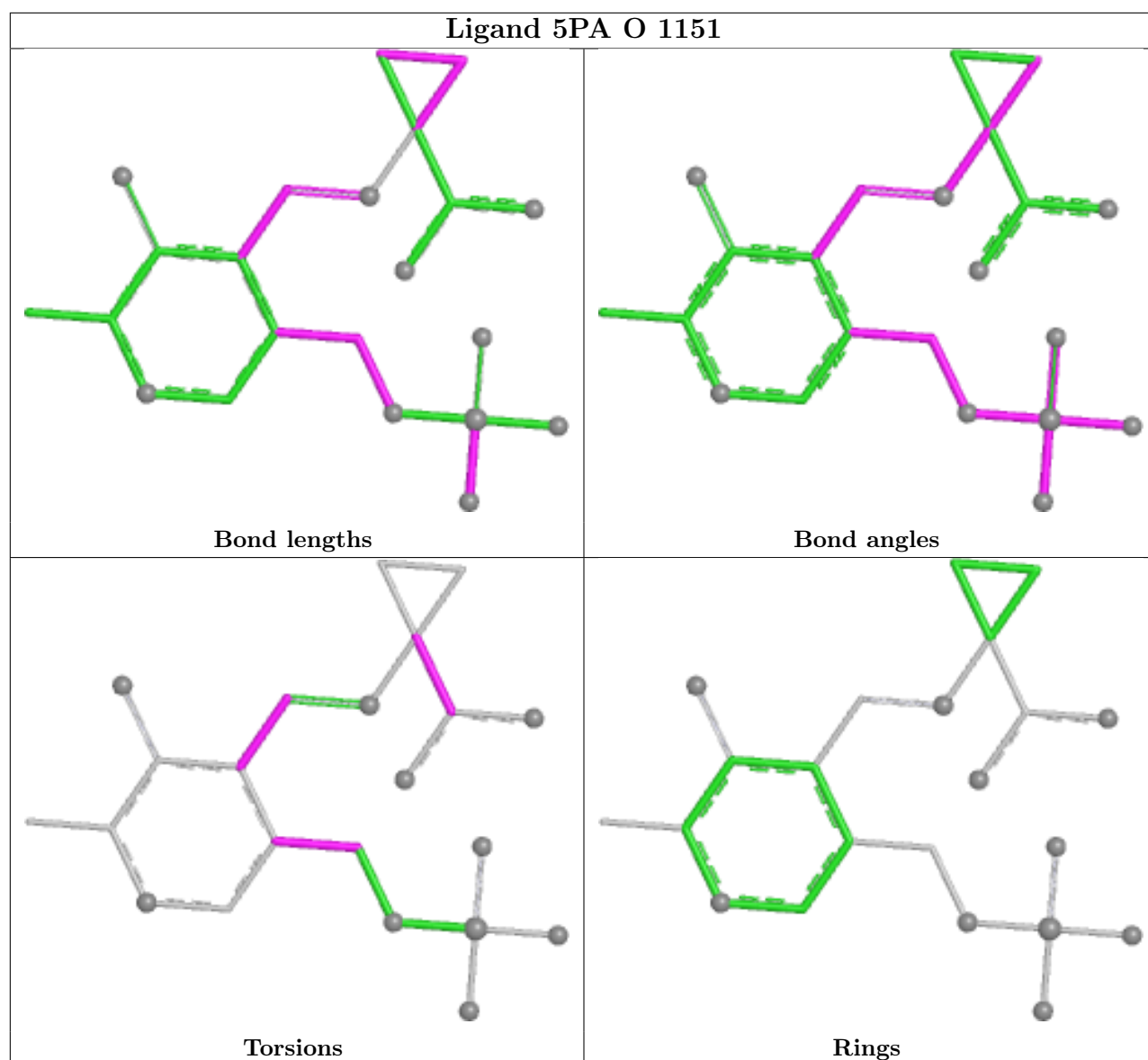




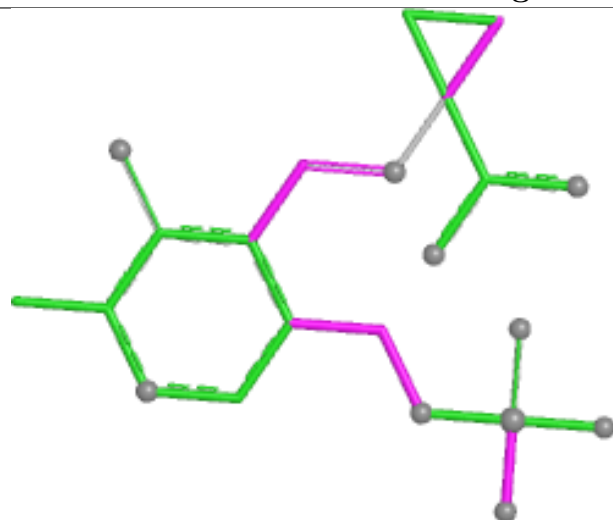




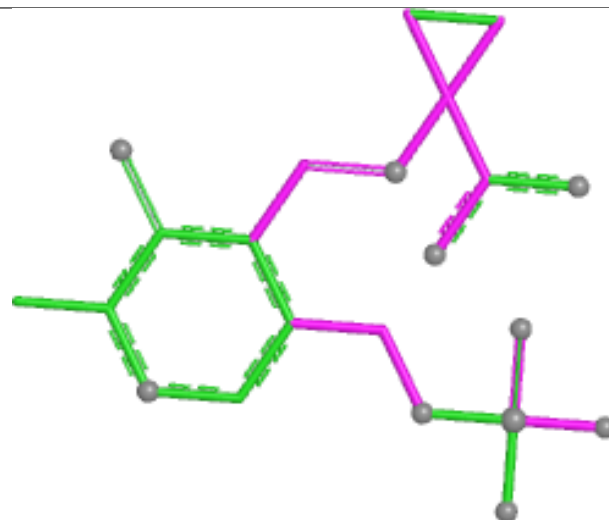




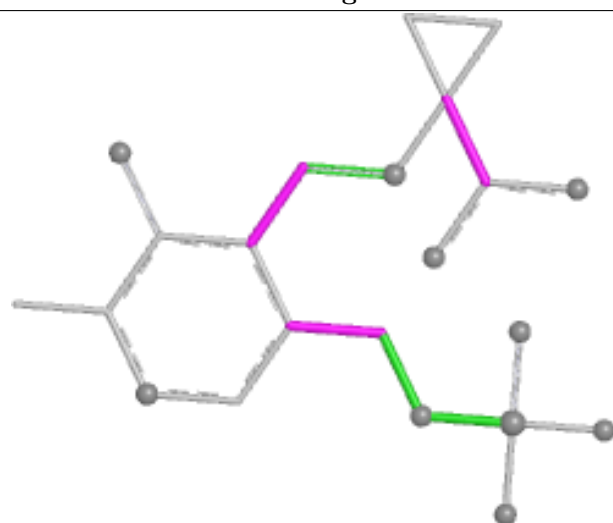
Ligand 5PA P 1161



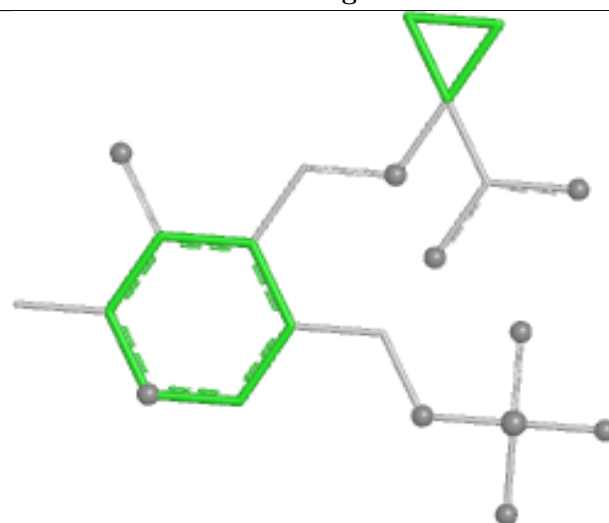
Bond lengths



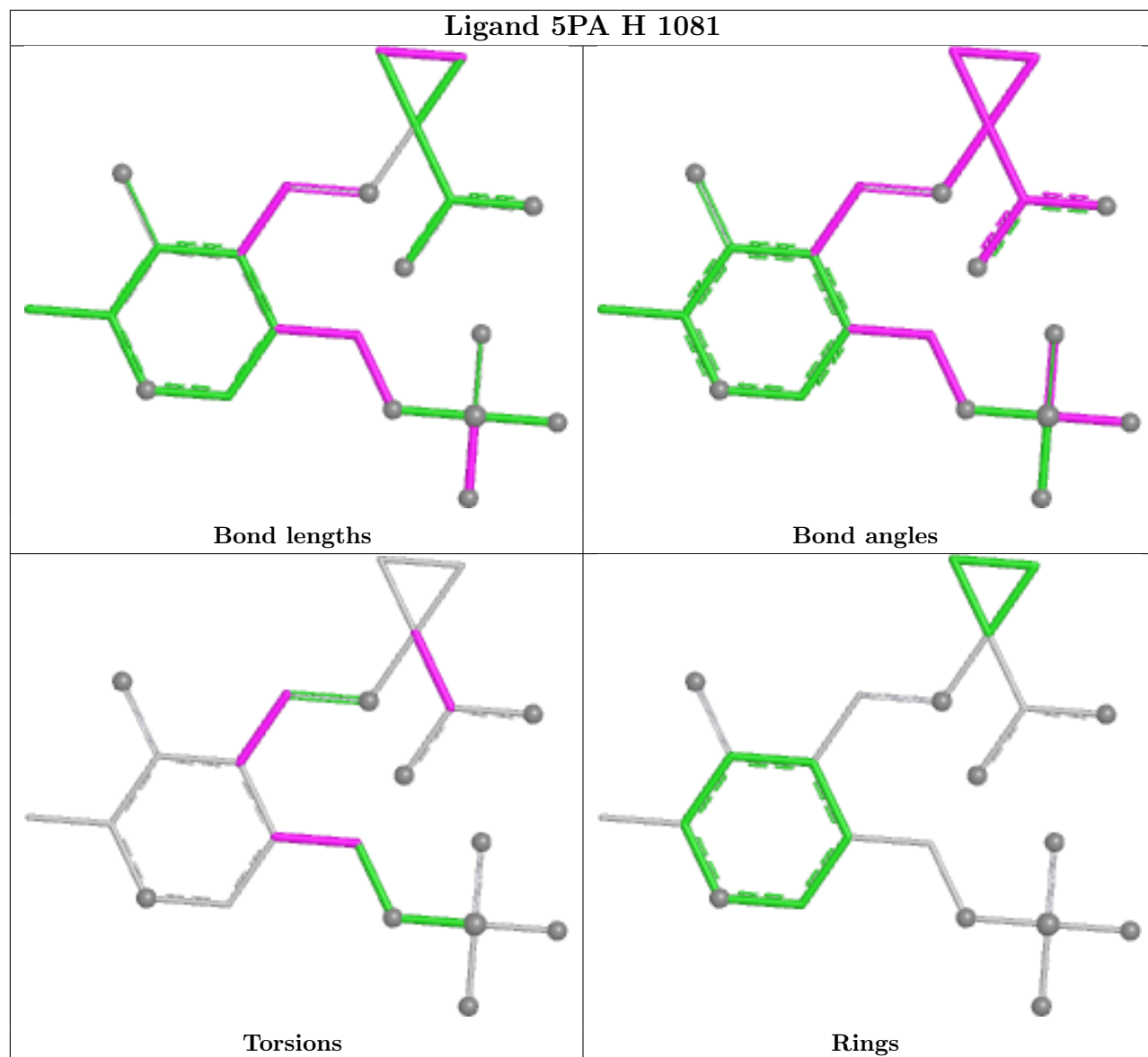
Bond angles



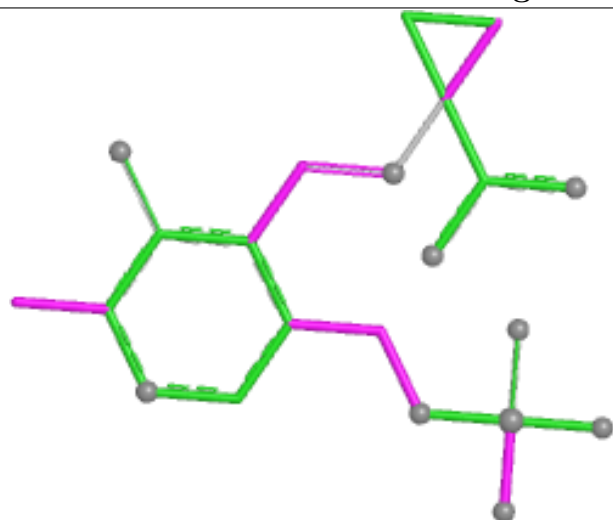
Torsions



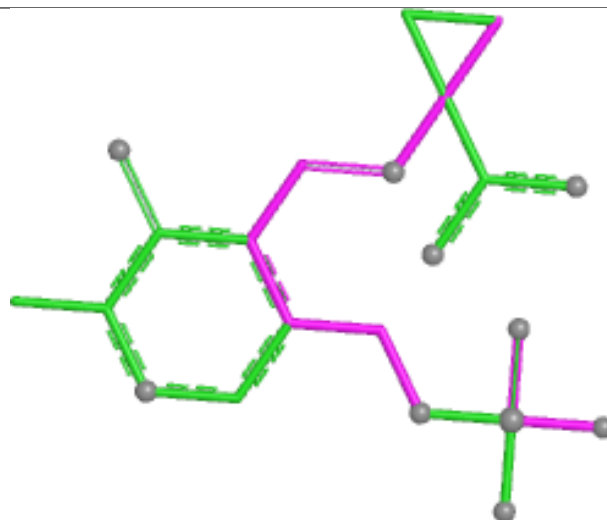
Rings



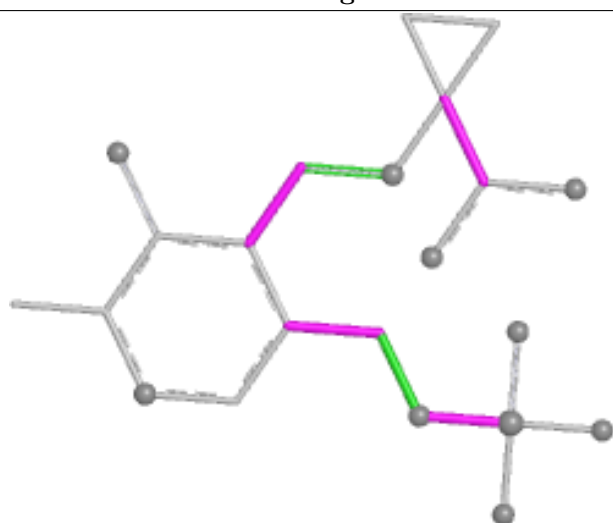
Ligand 5PA J 1101



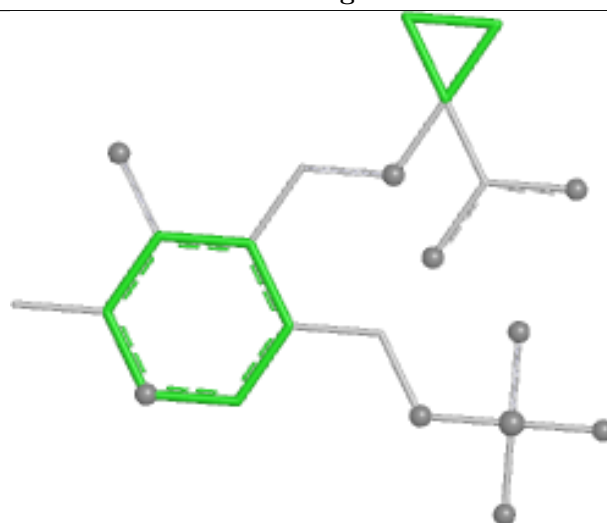
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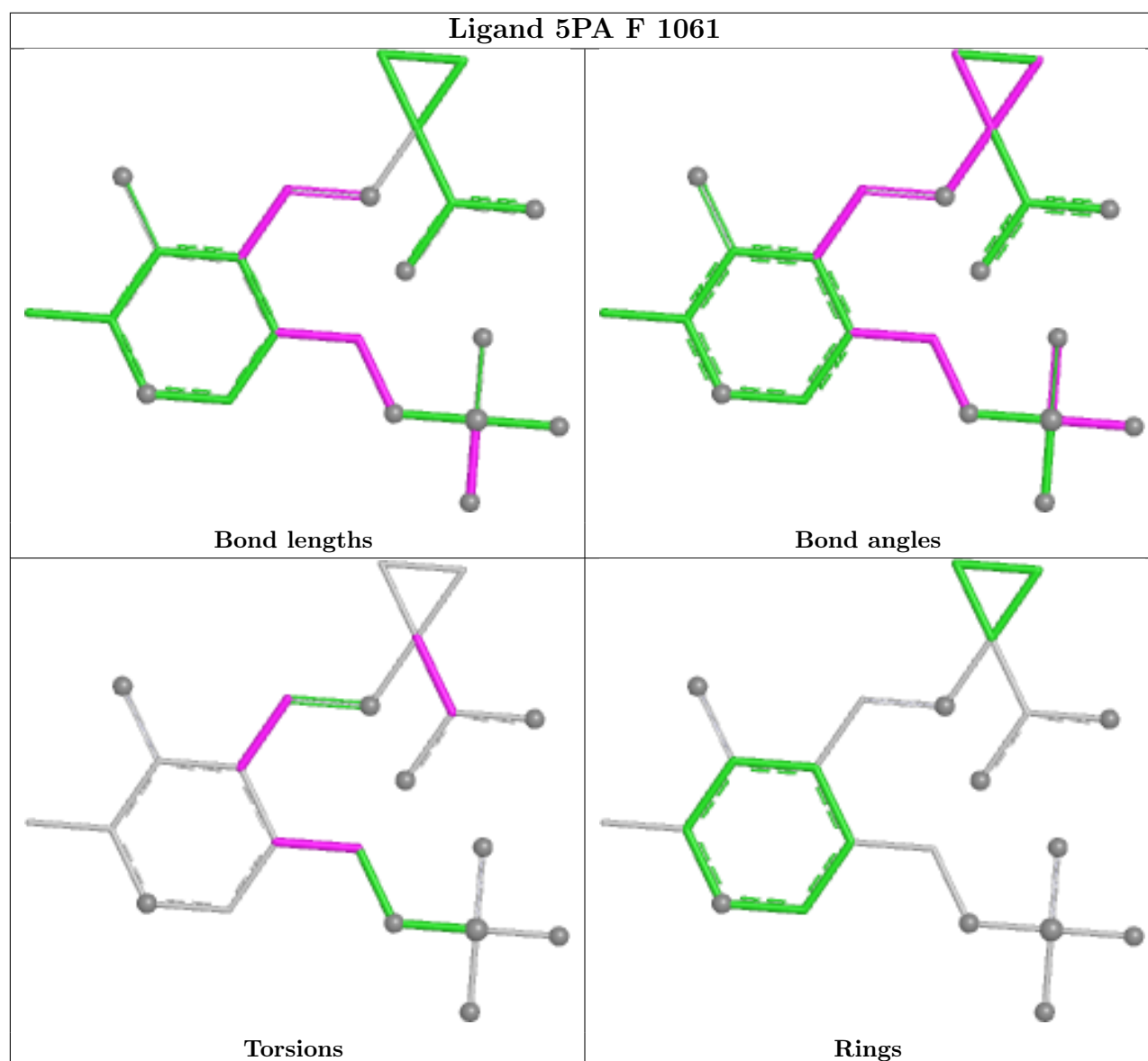
Bond angles

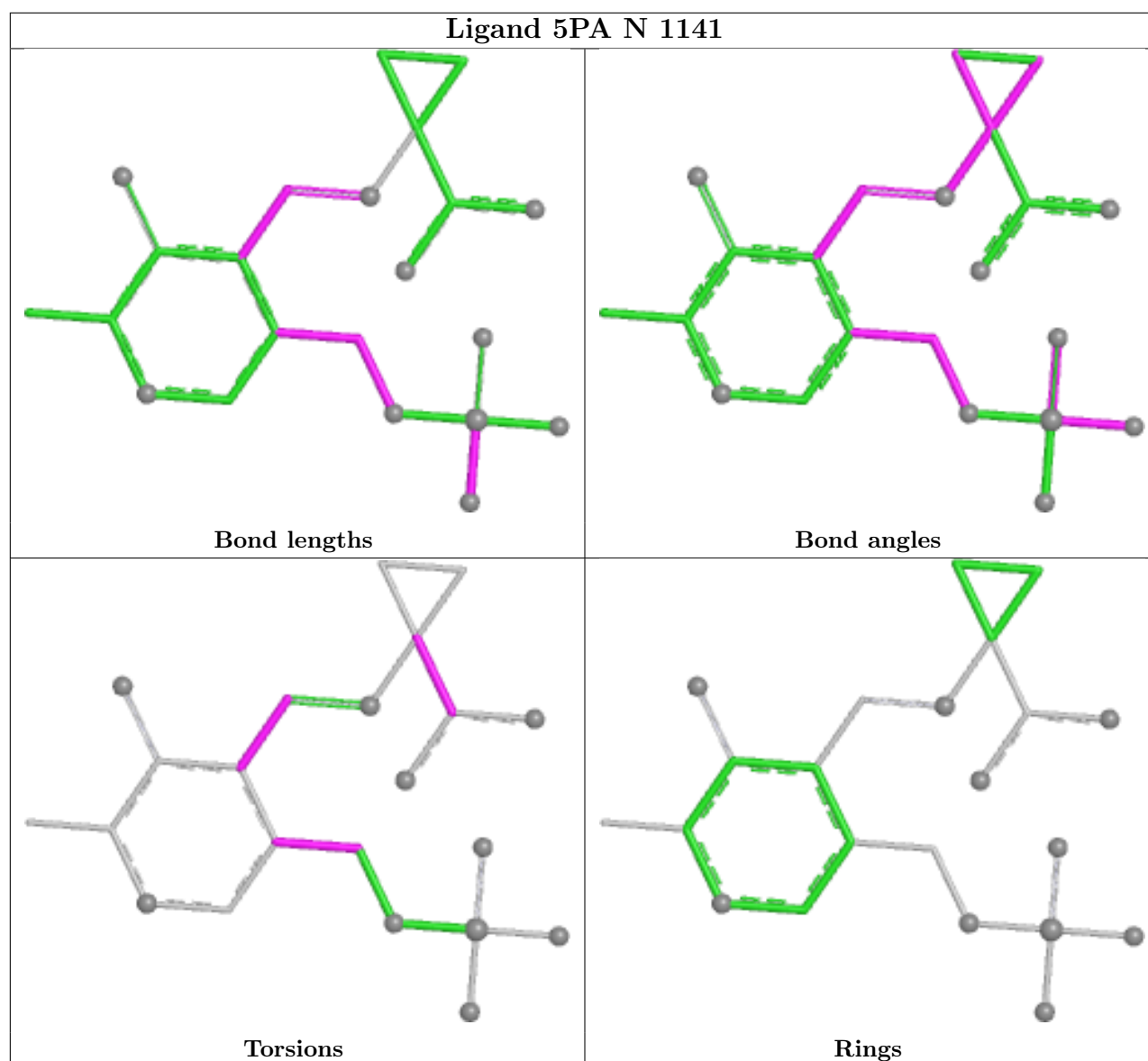


Torsions



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.