



Full wwPDB EM Validation Report ⓘ

Jul 13, 2026 – 02:01 PM EDT

PDB ID : 9PIN / pdb_00009pin
EMDB ID : EMD-71673
Title : Inner Curvature of Thick Flagellar Filament from T.denticola
Authors : Troman, L.A.; Paul, B.; Ghosal, D.
Deposited on : 2025-07-10
Resolution : 2.90 Å(reported)
Based on initial model : .

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

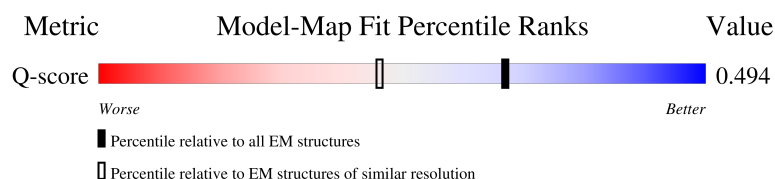
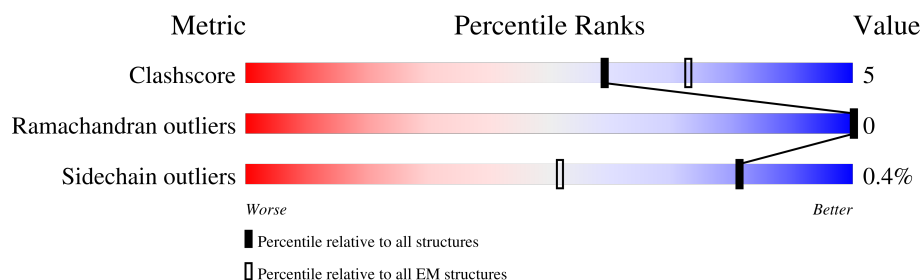
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A0	246	26% 83% 7% 10%
1	A4	246	16% 83% 7% 10%
1	A6	246	22% 84% 6% 10%
1	BI	246	8% 74% 6% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	BJ	246	
1	BM	246	
2	A3	349	
2	A5	349	
2	A9	349	
2	BQ	349	
2	BR	349	
2	BS	349	
3	A7	236	
3	A8	236	
3	BA	236	
3	BK	236	
3	BL	236	
3	BN	236	
4	E	139	
4	F	139	
4	G	139	
5	P2	234	
5	P3	234	
5	P4	234	
6	C0	286	
6	DA	286	
6	DB	286	
6	DC	286	
6	DD	286	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	DE	286	
6	DF	286	
6	DG	286	
6	DH	286	
6	DI	286	
6	DJ	286	
6	DK	286	
6	DL	286	
6	DM	286	
6	DN	286	
6	DO	286	
6	DP	286	
6	DQ	286	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 84288 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Flagellar filament outer layer protein FlaA, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A0	221	Total	C	N	O	S	0	0
			1768	1129	294	337	8		
1	A4	221	Total	C	N	O	S	0	0
			1768	1129	294	337	8		
1	A6	221	Total	C	N	O	S	0	0
			1768	1129	294	337	8		
1	BI	198	Total	C	N	O	S	0	0
			1608	1032	268	300	8		
1	BJ	198	Total	C	N	O	S	0	0
			1608	1032	268	300	8		
1	BM	198	Total	C	N	O	S	0	0
			1608	1032	268	300	8		

- Molecule 2 is a protein called Flagellar filament outer layer protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A3	324	Total	C	N	O	S	0	0
			2580	1638	439	495	8		
2	A5	324	Total	C	N	O	S	0	0
			2580	1638	439	495	8		
2	A9	324	Total	C	N	O	S	0	0
			2580	1638	439	495	8		
2	BQ	318	Total	C	N	O	S	0	0
			2487	1583	427	469	8		
2	BR	318	Total	C	N	O	S	0	0
			2487	1583	427	469	8		
2	BS	318	Total	C	N	O	S	0	0
			2487	1583	427	469	8		

- Molecule 3 is a protein called Flagellar filament outer layer protein FlaA, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A7	198	Total	C	N	O	S	0	0
			1628	1061	269	292	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A8	198	Total	C	N	O	S	0	0
			1628	1061	269	292	6		
3	BA	198	Total	C	N	O	S	0	0
			1628	1061	269	292	6		
3	BK	200	Total	C	N	O	S	0	0
			1653	1075	273	298	7		
3	BL	200	Total	C	N	O	S	0	0
			1653	1075	273	298	7		
3	BN	200	Total	C	N	O	S	0	0
			1653	1075	273	298	7		

- Molecule 4 is a protein called FlaL2.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	110	Total	C	N	O	0	0
			909	595	154	160		
4	F	110	Total	C	N	O	0	0
			909	595	154	160		
4	G	110	Total	C	N	O	0	0
			909	595	154	160		

- Molecule 5 is a protein called HEAT repeat domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P2	190	Total	C	N	O	S	0	0
			1473	922	260	282	9		
5	P3	190	Total	C	N	O	S	0	0
			1473	922	260	282	9		
5	P4	190	Total	C	N	O	S	0	0
			1473	922	260	282	9		

- Molecule 6 is a protein called Flagellin.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C0	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		
6	DA	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		
6	DB	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		
6	DC	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
6	DD	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		
6	DE	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		
6	DF	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		
6	DG	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		
6	DH	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		
6	DI	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		
6	DJ	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		
6	DK	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		
6	DL	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		
6	DM	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		
6	DN	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		
6	DO	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		
6	DP	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		
6	DQ	286	Total	C	N	O	S	0	0
			2206	1349	407	436	14		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

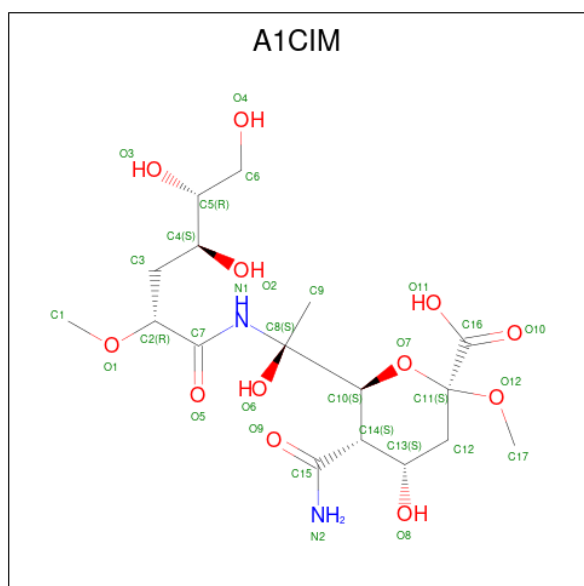
Mol	Chain	Residues	Atoms		AltConf
7	A0	1	Total	Ca	0
			1	1	
7	A4	1	Total	Ca	0
			1	1	
7	A6	1	Total	Ca	0
			1	1	
7	A7	1	Total	Ca	0
			1	1	
7	A8	1	Total	Ca	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
7	BA	1	Total	Ca	0
			1	1	
7	BI	1	Total	Ca	0
			1	1	
7	BJ	1	Total	Ca	0
			1	1	
7	BK	1	Total	Ca	0
			1	1	
7	BL	1	Total	Ca	0
			1	1	
7	BM	1	Total	Ca	0
			1	1	
7	BN	1	Total	Ca	0
			1	1	

- Molecule 8 is (2S,4S,5S,6S)-5-carbamoyl-4-hydroxy-6-[(1S)-1-hydroxy-1-[(2R,4S,5R)-4,5,6-trihydroxy-2-methoxyhexanamido]ethyl]-2-methoxyoxane-2-carboxylic acid (CCD ID: A1CIM) (formula: C₁₇H₃₀N₂O₁₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
8	C0	1	Total	C	N	O	0
			29	16	2	11	
8	C0	1	Total	C	N	O	0
			19	10	2	7	
8	C0	1	Total	C	N	O	0
			29	16	2	11	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
8	C0	1	Total	C	N	O	0
			29	16	2	11	
8	C0	1	Total	C	N	O	0
			19	10	2	7	
8	DA	1	Total	C	N	O	0
			29	16	2	11	
8	DA	1	Total	C	N	O	0
			19	10	2	7	
8	DA	1	Total	C	N	O	0
			29	16	2	11	
8	DA	1	Total	C	N	O	0
			29	16	2	11	
8	DA	1	Total	C	N	O	0
			19	10	2	7	
8	DB	1	Total	C	N	O	0
			29	16	2	11	
8	DB	1	Total	C	N	O	0
			19	10	2	7	
8	DB	1	Total	C	N	O	0
			29	16	2	11	
8	DB	1	Total	C	N	O	0
			29	16	2	11	
8	DB	1	Total	C	N	O	0
			19	10	2	7	
8	DC	1	Total	C	N	O	0
			29	16	2	11	
8	DC	1	Total	C	N	O	0
			19	10	2	7	
8	DC	1	Total	C	N	O	0
			29	16	2	11	
8	DC	1	Total	C	N	O	0
			29	16	2	11	
8	DC	1	Total	C	N	O	0
			19	10	2	7	
8	DD	1	Total	C	N	O	0
			29	16	2	11	
8	DD	1	Total	C	N	O	0
			19	10	2	7	
8	DD	1	Total	C	N	O	0
			29	16	2	11	
8	DD	1	Total	C	N	O	0
			29	16	2	11	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
8	DD	1	Total	C	N	O	0
			19	10	2	7	
8	DE	1	Total	C	N	O	0
			29	16	2	11	
8	DE	1	Total	C	N	O	0
			19	10	2	7	
8	DE	1	Total	C	N	O	0
			29	16	2	11	
8	DE	1	Total	C	N	O	0
			29	16	2	11	
8	DE	1	Total	C	N	O	0
			19	10	2	7	
8	DF	1	Total	C	N	O	0
			29	16	2	11	
8	DF	1	Total	C	N	O	0
			19	10	2	7	
8	DF	1	Total	C	N	O	0
			29	16	2	11	
8	DF	1	Total	C	N	O	0
			29	16	2	11	
8	DF	1	Total	C	N	O	0
			19	10	2	7	
8	DG	1	Total	C	N	O	0
			29	16	2	11	
8	DG	1	Total	C	N	O	0
			19	10	2	7	
8	DG	1	Total	C	N	O	0
			29	16	2	11	
8	DG	1	Total	C	N	O	0
			29	16	2	11	
8	DG	1	Total	C	N	O	0
			19	10	2	7	
8	DH	1	Total	C	N	O	0
			29	16	2	11	
8	DH	1	Total	C	N	O	0
			19	10	2	7	
8	DH	1	Total	C	N	O	0
			29	16	2	11	
8	DH	1	Total	C	N	O	0
			29	16	2	11	
8	DH	1	Total	C	N	O	0
			19	10	2	7	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
8	DI	1	Total	C	N	O	0
			29	16	2	11	
8	DI	1	Total	C	N	O	0
			19	10	2	7	
8	DI	1	Total	C	N	O	0
			29	16	2	11	
8	DI	1	Total	C	N	O	0
			29	16	2	11	
8	DI	1	Total	C	N	O	0
			19	10	2	7	
8	DJ	1	Total	C	N	O	0
			29	16	2	11	
8	DJ	1	Total	C	N	O	0
			19	10	2	7	
8	DJ	1	Total	C	N	O	0
			29	16	2	11	
8	DJ	1	Total	C	N	O	0
			29	16	2	11	
8	DJ	1	Total	C	N	O	0
			19	10	2	7	
8	DK	1	Total	C	N	O	0
			29	16	2	11	
8	DK	1	Total	C	N	O	0
			19	10	2	7	
8	DK	1	Total	C	N	O	0
			29	16	2	11	
8	DK	1	Total	C	N	O	0
			29	16	2	11	
8	DK	1	Total	C	N	O	0
			19	10	2	7	
8	DL	1	Total	C	N	O	0
			29	16	2	11	
8	DL	1	Total	C	N	O	0
			19	10	2	7	
8	DL	1	Total	C	N	O	0
			29	16	2	11	
8	DL	1	Total	C	N	O	0
			29	16	2	11	
8	DL	1	Total	C	N	O	0
			19	10	2	7	
8	DM	1	Total	C	N	O	0
			29	16	2	11	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
8	DM	1	Total	C	N	O	0
			19	10	2	7	
8	DM	1	Total	C	N	O	0
			29	16	2	11	
8	DM	1	Total	C	N	O	0
			29	16	2	11	
8	DM	1	Total	C	N	O	0
			19	10	2	7	
8	DN	1	Total	C	N	O	0
			29	16	2	11	
8	DN	1	Total	C	N	O	0
			19	10	2	7	
8	DN	1	Total	C	N	O	0
			29	16	2	11	
8	DN	1	Total	C	N	O	0
			19	10	2	7	
8	DO	1	Total	C	N	O	0
			29	16	2	11	
8	DO	1	Total	C	N	O	0
			19	10	2	7	
8	DO	1	Total	C	N	O	0
			29	16	2	11	
8	DO	1	Total	C	N	O	0
			29	16	2	11	
8	DO	1	Total	C	N	O	0
			19	10	2	7	
8	DP	1	Total	C	N	O	0
			29	16	2	11	
8	DP	1	Total	C	N	O	0
			19	10	2	7	
8	DP	1	Total	C	N	O	0
			29	16	2	11	
8	DP	1	Total	C	N	O	0
			29	16	2	11	
8	DP	1	Total	C	N	O	0
			19	10	2	7	
8	DQ	1	Total	C	N	O	0
			29	16	2	11	
8	DQ	1	Total	C	N	O	0
			19	10	2	7	

Continued on next page...

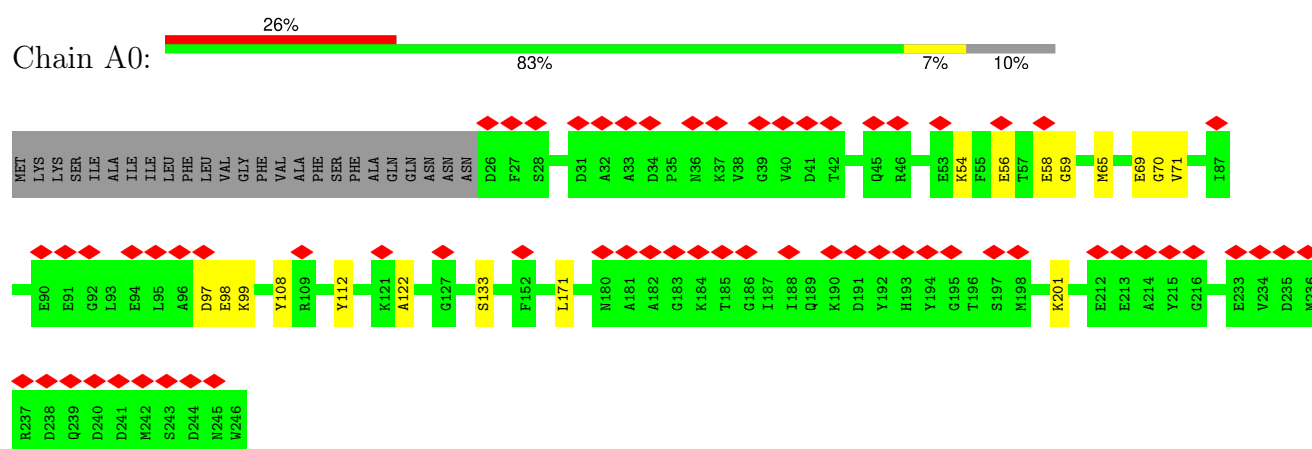
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
8	DQ	1	Total	C	N	O	0
			29	16	2	11	
8	DQ	1	Total	C	N	O	0
			29	16	2	11	
8	DQ	1	Total	C	N	O	0
			19	10	2	7	

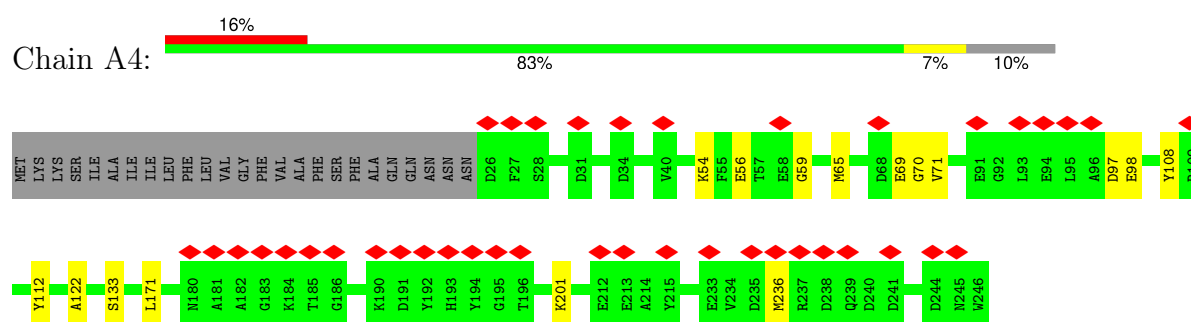
3 Residue-property plots

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 and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

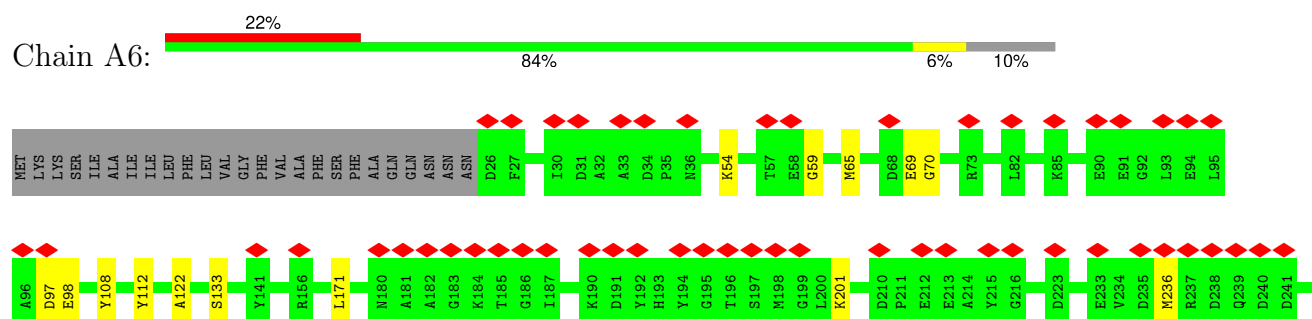
- Molecule 1: Flagellar filament outer layer protein FlaA, putative



- Molecule 1: Flagellar filament outer layer protein FlaA, putative

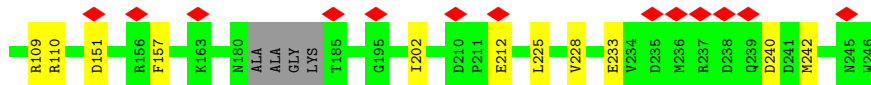
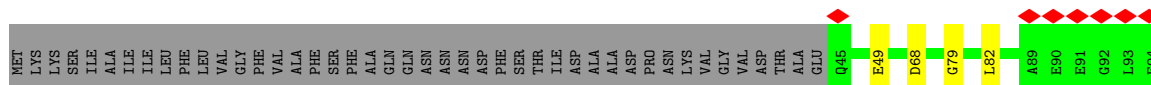
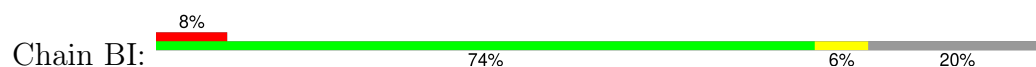


- Molecule 1: Flagellar filament outer layer protein FlaA, putative

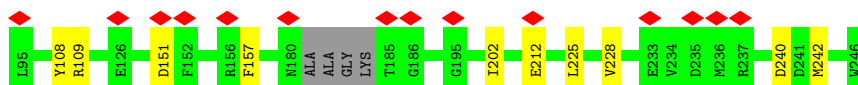
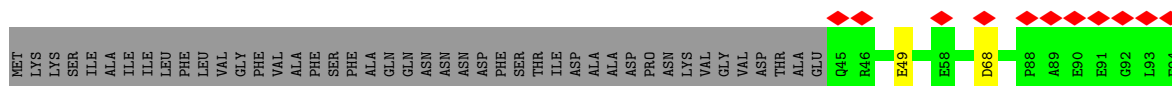
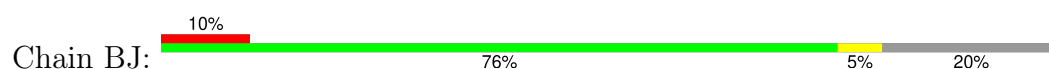




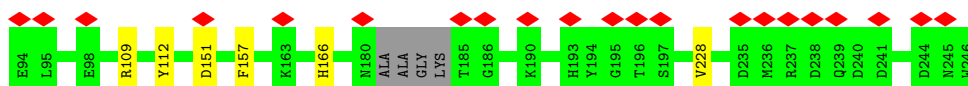
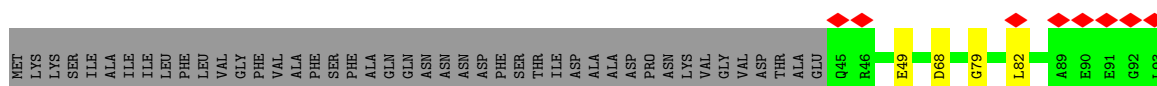
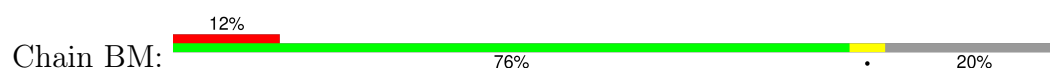
- Molecule 1: Flagellar filament outer layer protein FlaA, putative



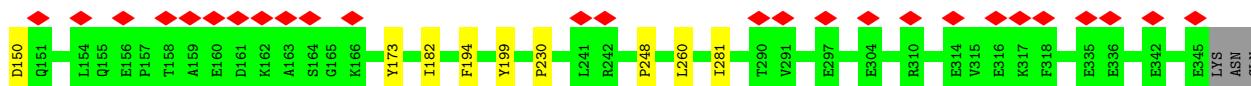
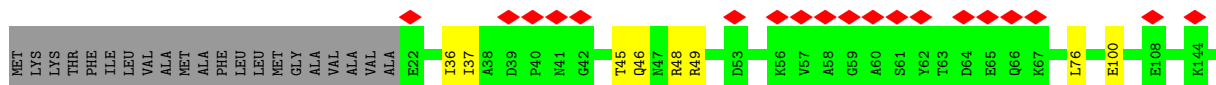
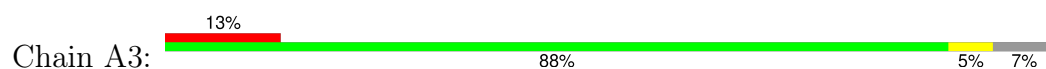
- Molecule 1: Flagellar filament outer layer protein FlaA, putative



- Molecule 1: Flagellar filament outer layer protein FlaA, putative

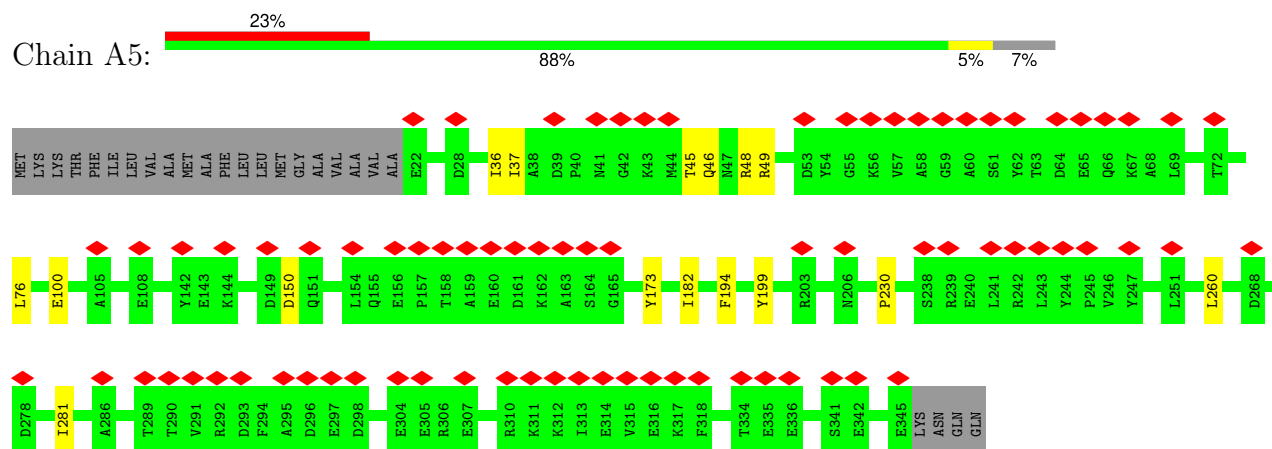


- Molecule 2: Flagellar filament outer layer protein



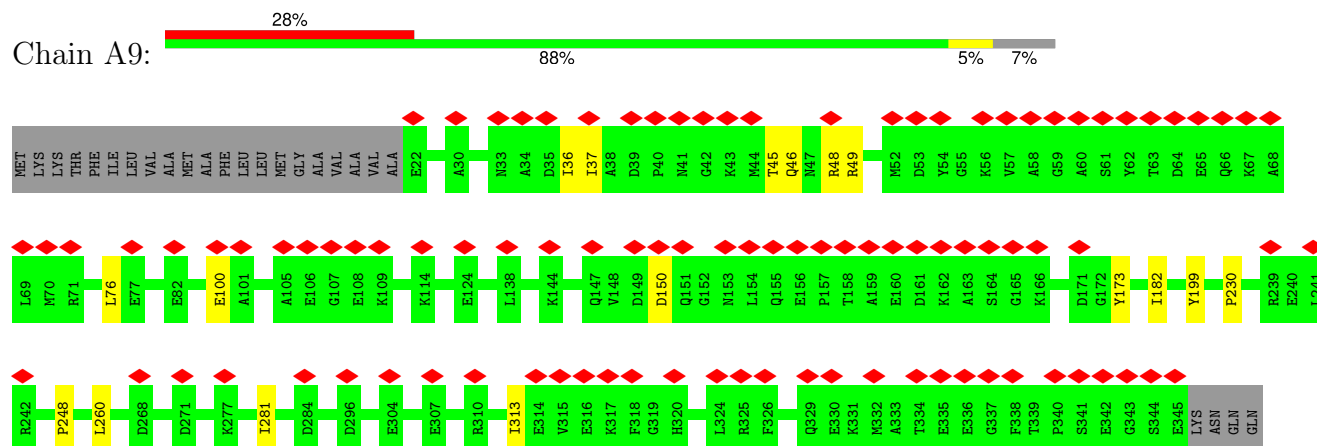
- Molecule 2: Flagellar filament outer layer protein

Chain A5:



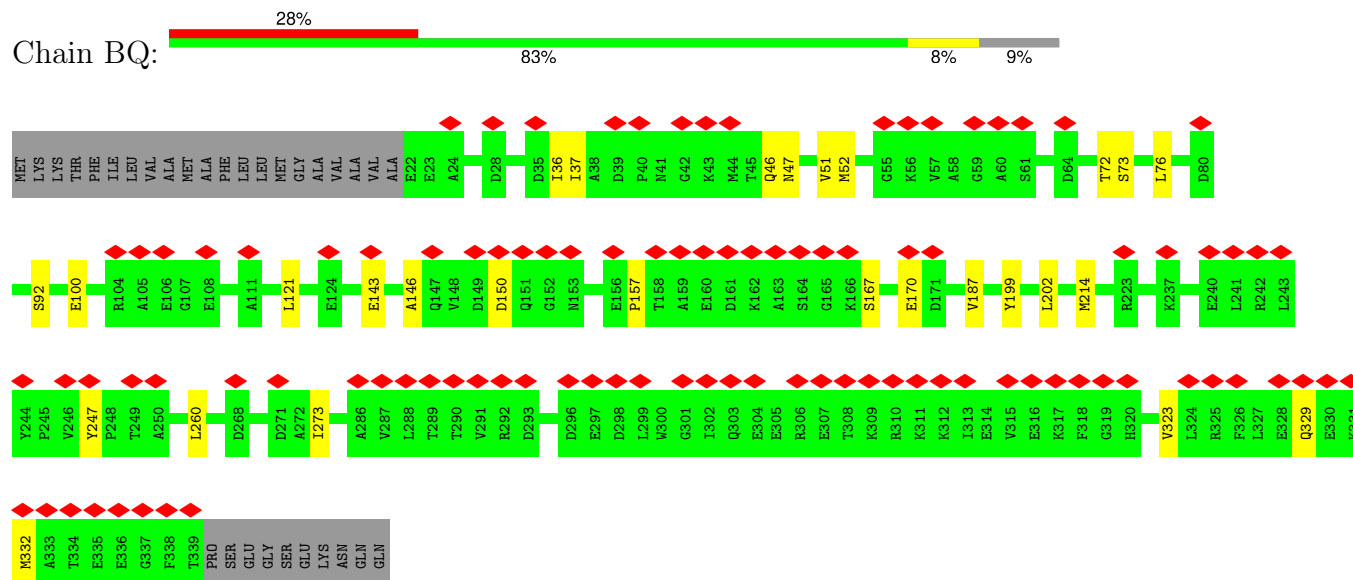
- Molecule 2: Flagellar filament outer layer protein

Chain A9:



- Molecule 2: Flagellar filament outer layer protein

Chain BQ:



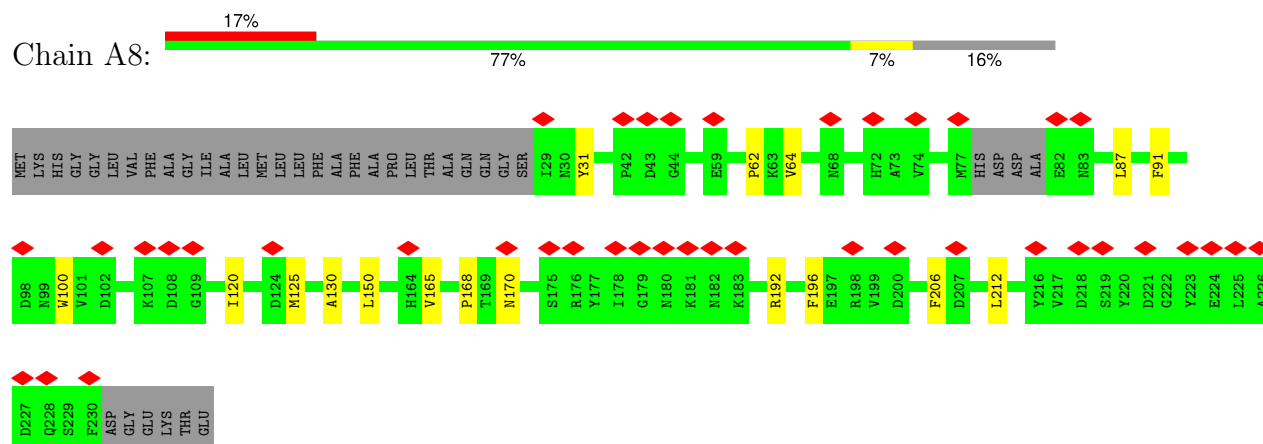
- Molecule 2: Flagellar filament outer layer protein

A295	A296	A297	D298	L299	W300	G301	L302	Q303	E304	E305	R306	E307	T308	K309	R310	K311	K312	I313	E314	V315	E316	K317	F318	G319	H320	T321	Q322	V323	L324	R325	F326	L327	E328	Q329	E330	K331	M332	A333	T334	E335	E336	F337	F338	T339	PRO	SER	GLU	GLY	SER	GLU	LYS	ASN	GLN	GLN
W222	R223	S231	Y232	I233	A234	N235	V236	K237	S238	R239	E240	L241	R242	L243	Y244	P245	V246	Y247	P248	T249	A250	L251	P252	E257	L260	D264	A265	A266	H267	D268	G269	G270	D271	A272	I273	A274	K277	D278	V279	K280	I281	V282	V283	D284	K285	A286	V287	L288	T289	T290	R291	R292	D293	T294
M153	L154	Q155	P157	T158	A159	D161	K162	A163	S164	G165	K166	S167	R168	F169	D170	G172	V173	R177	M178	T179	G180	V181	I182	K183	S184	V187	N188	T189	V190	G191	M192	N193	F194	Y199	V200	L201	L202	R203	D204	Q205	N206	W207	K210	R211	W214	L217	L218	F219	D220	G221				
D64	E65	R71	T72	S73	L76	E77	Q78	W79	D80	V81	E82	S85	Q88	S92	E100	A101	E102	V103	R104	A105	E106	G107	E108	K109	F110	A111	G112	Q113	K114	L115	M116	G117	L121	E124	W125	A131	A141	Y142	E143	K144	M145	A146	Q147	V148	D149	D150	Q151	G152						
THR	PHE	ILE	LEU	VAL	MET	ALA	PHE	LEU	MET	GLY	ALA	VAL	VAL	ALA	E22	E23	A24	I25	I26	I27	D28	F29	A30	L31	L32	N33	A34	D35	I36	I37	A38	D39	P40	N41	G42	K43	M44	T45	Q46	N47	R48	V51	D52	Y54	G55	K56	V57	A58	G59	A60	S61			
MET	LYS	THR	PHE	ILE	LEU	VAL	MET	ALA	PHE	LEU	MET	GLY	ALA	VAL	VAL	ALA	E22	E23	A24	I25	I26	I27	D28	F29	A30	L31	L32	N33	A34	D35	I36	I37	A38	D39	P40	N41	G42	K43	M44	T45	Q46	N47	R48	V51	D52	Y54	G55	K56	V57	A58	G59	A60	S61	

[illegible]

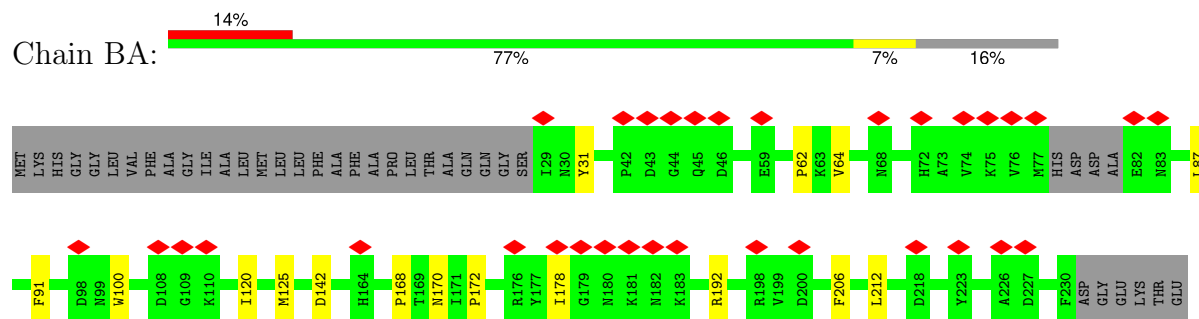
- Molecule 3: Flagellar filament outer layer protein FlaA, putative

Chain A8:



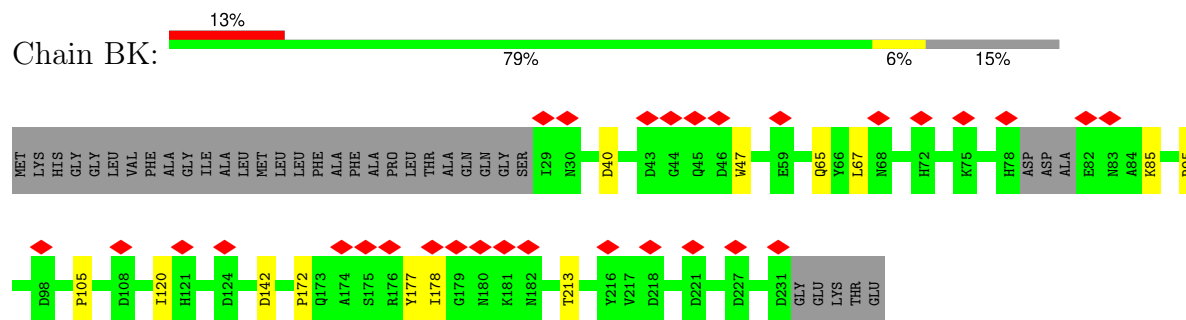
- Molecule 3: Flagellar filament outer layer protein FlaA, putative

Chain BA:



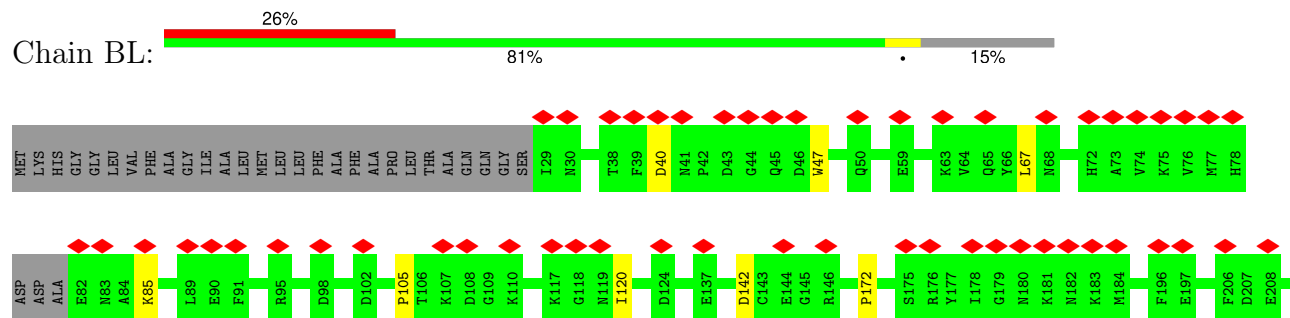
- Molecule 3: Flagellar filament outer layer protein FlaA, putative

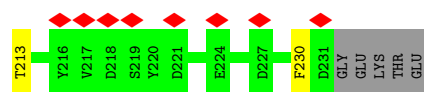
Chain BK:



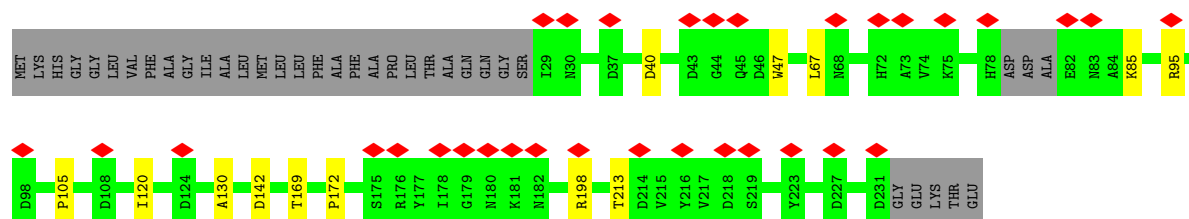
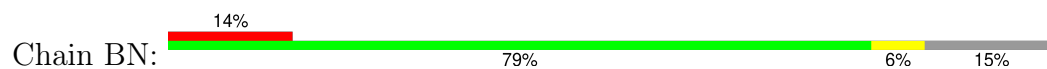
- Molecule 3: Flagellar filament outer layer protein FlaA, putative

Chain BL:

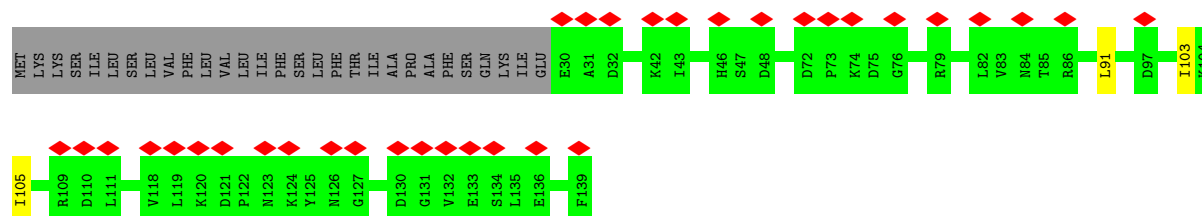




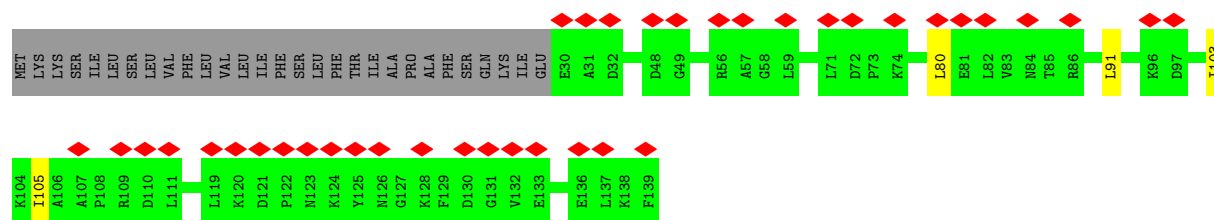
- Molecule 3: Flagellar filament outer layer protein FlaA, putative



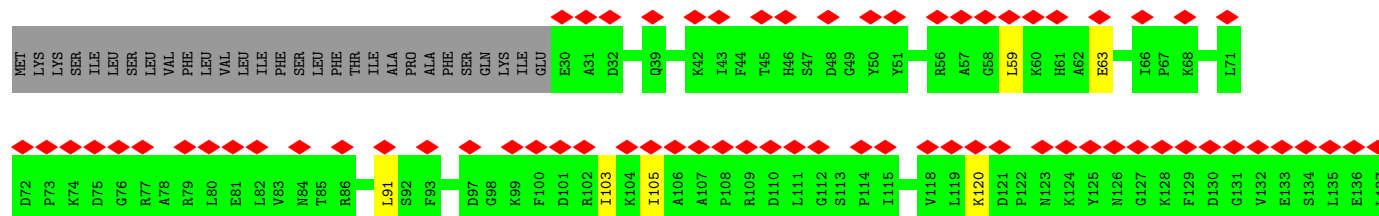
- Molecule 4: FlaL2

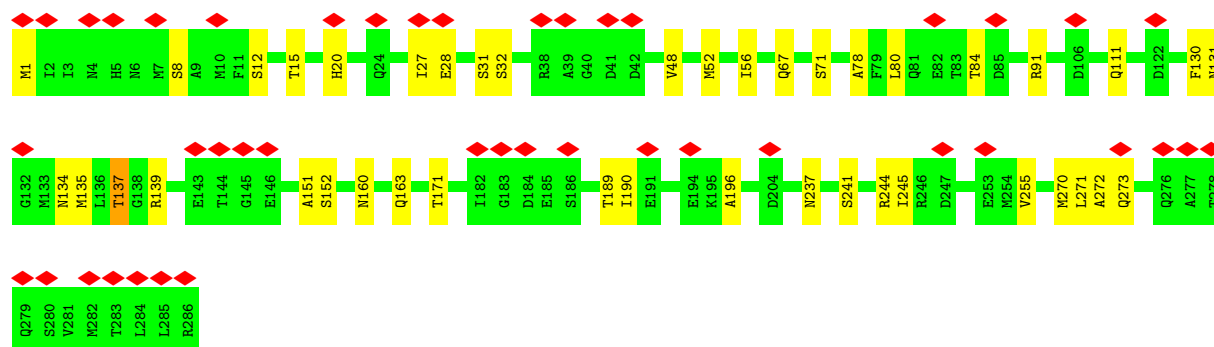


- Molecule 4: FlaL2

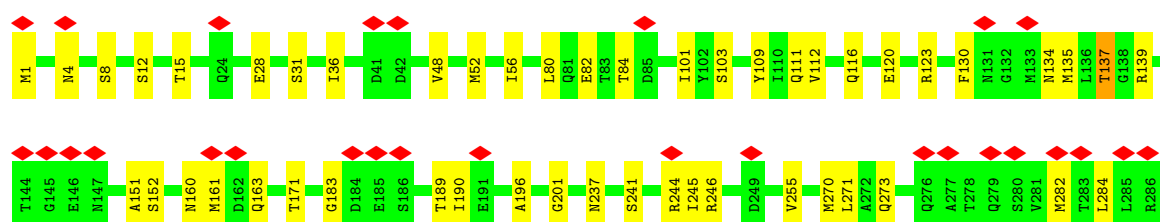
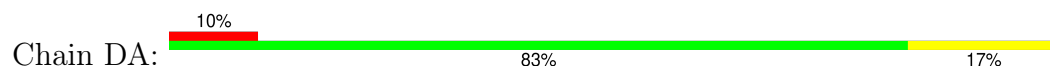


- Molecule 4: FlaL2

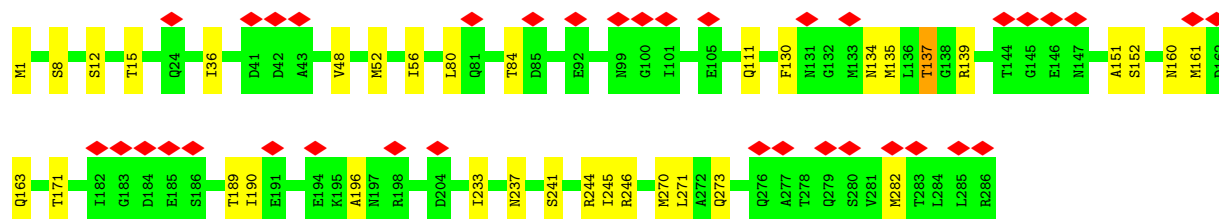
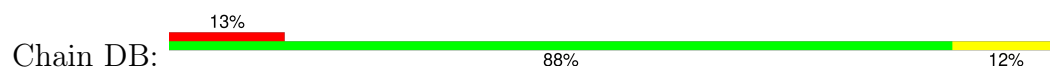




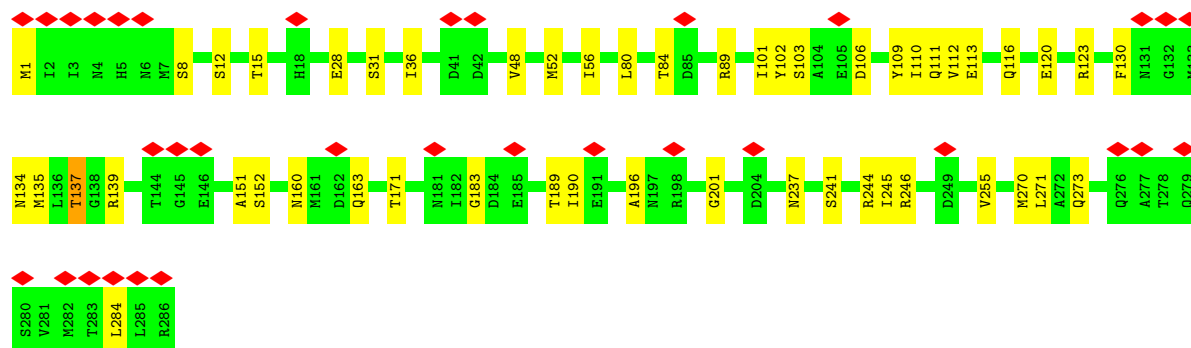
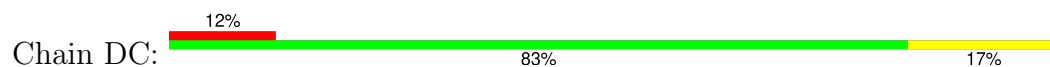
• Molecule 6: Flagellin



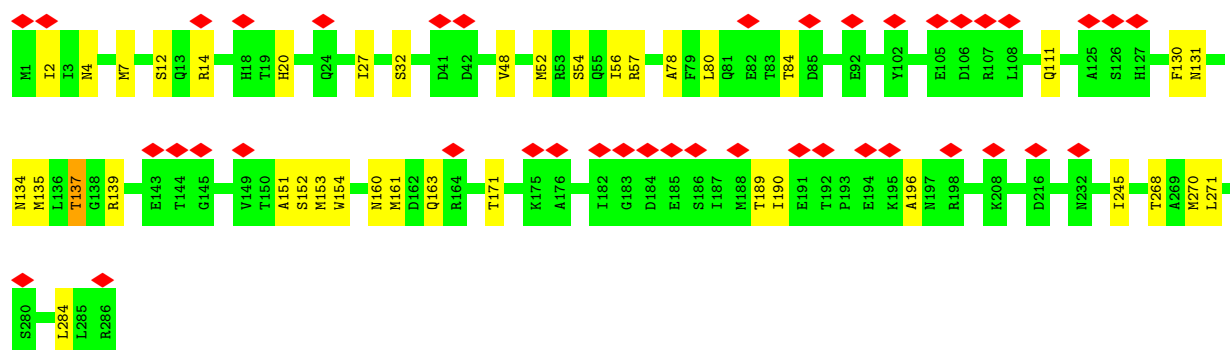
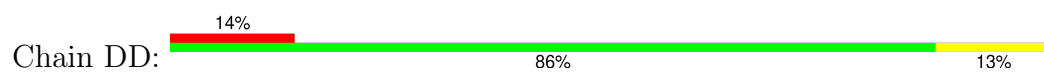
• Molecule 6: Flagellin



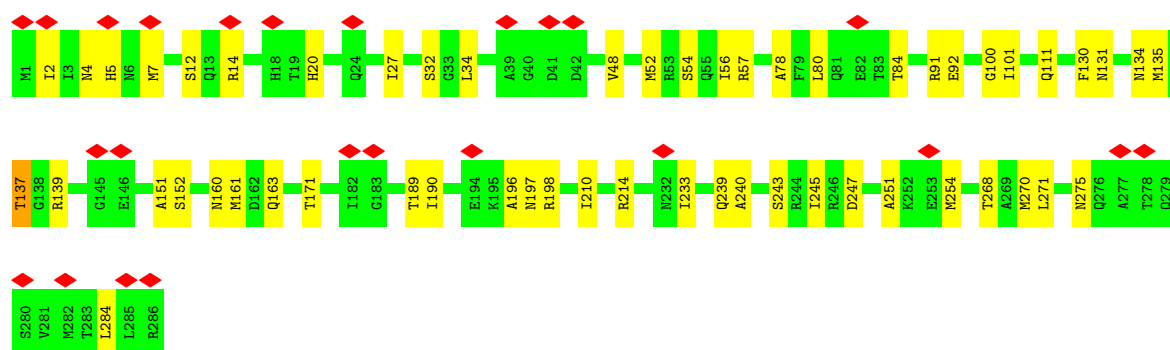
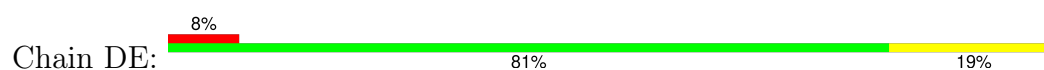
• Molecule 6: Flagellin



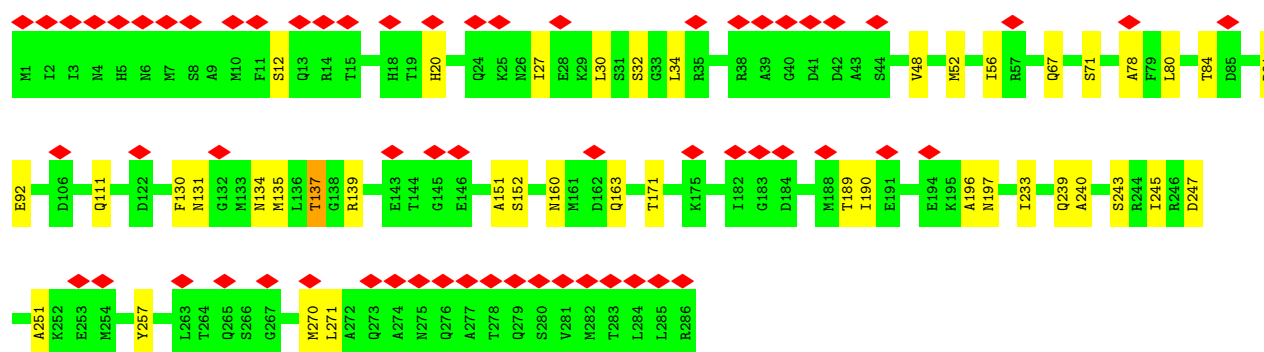
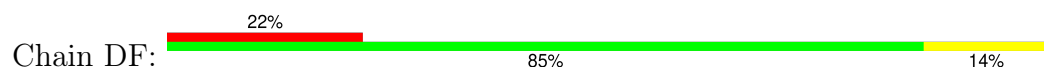
• Molecule 6: Flagellin



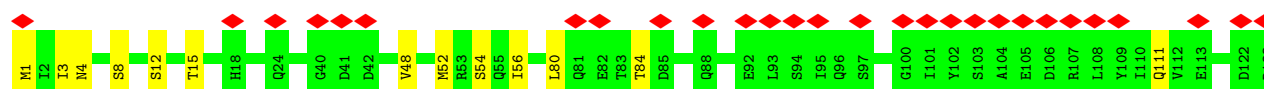
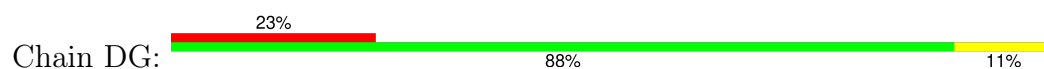
• Molecule 6: Flagellin

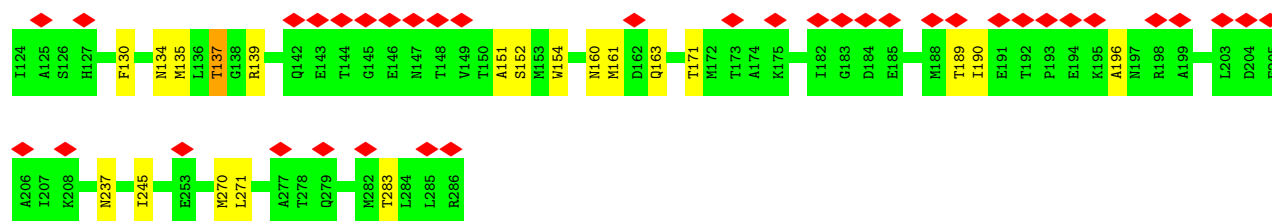


• Molecule 6: Flagellin

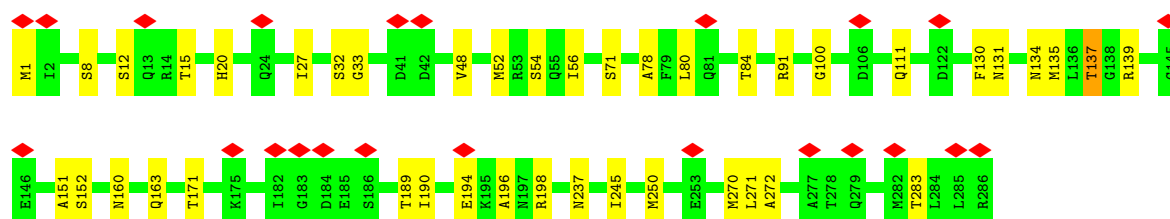
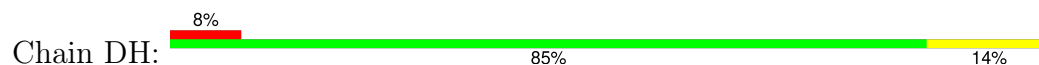


• Molecule 6: Flagellin

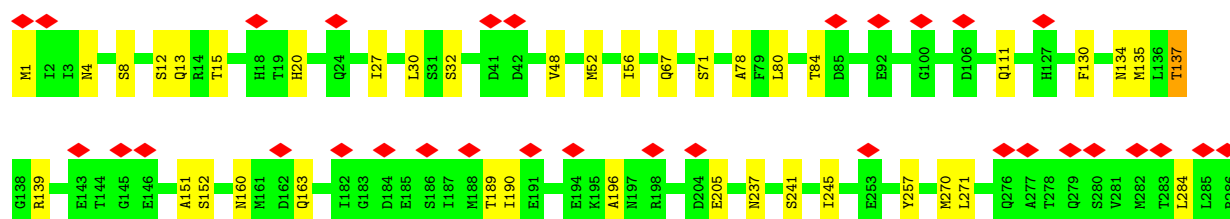
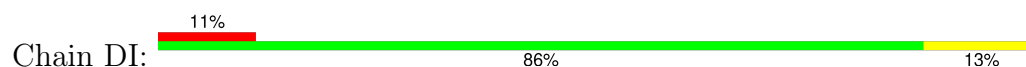




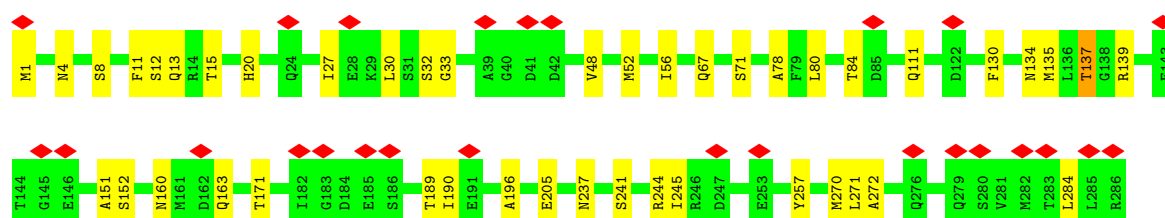
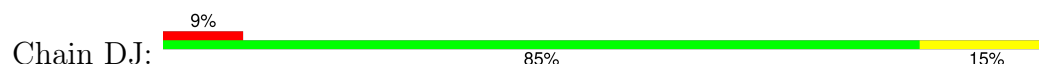
• Molecule 6: Flagellin



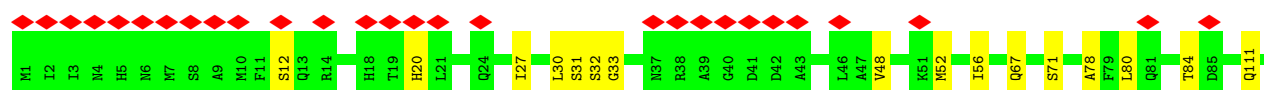
• Molecule 6: Flagellin

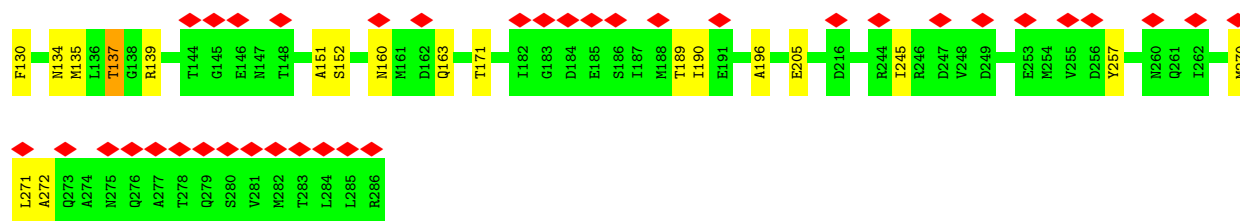


• Molecule 6: Flagellin

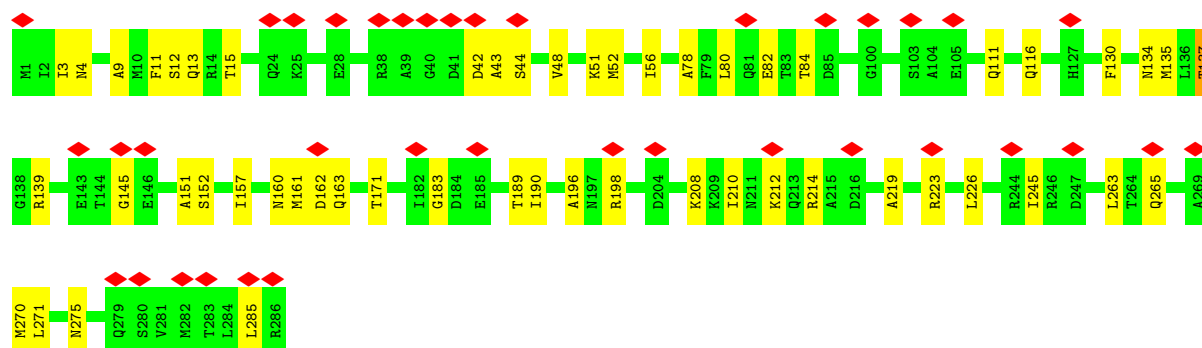
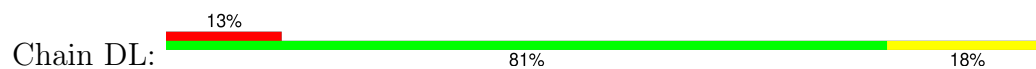


• Molecule 6: Flagellin

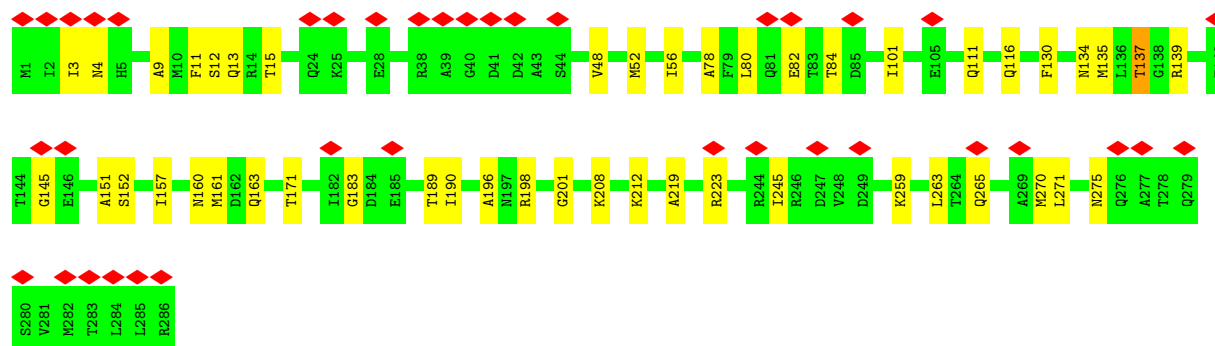
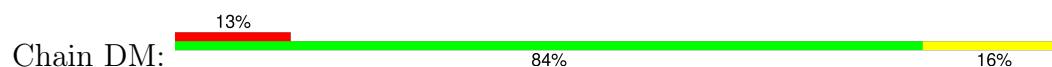




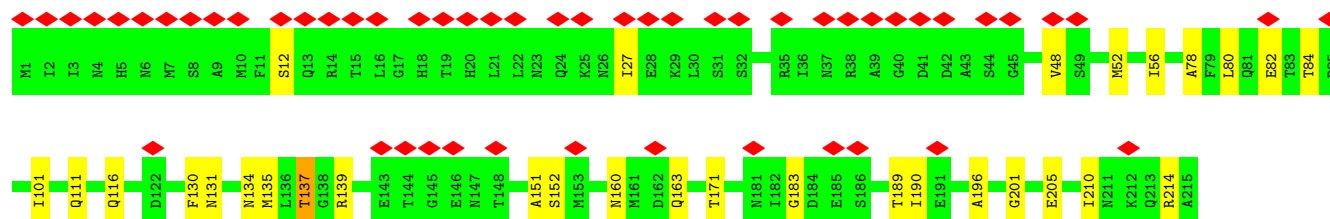
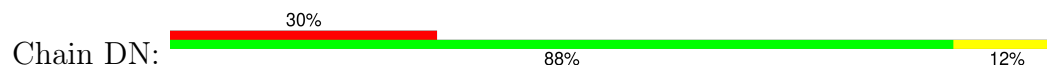
• Molecule 6: Flagellin

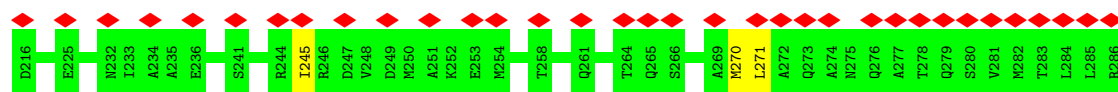


• Molecule 6: Flagellin

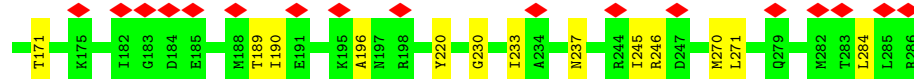
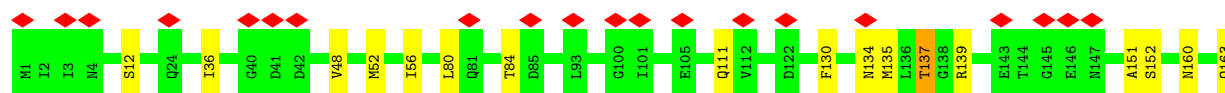
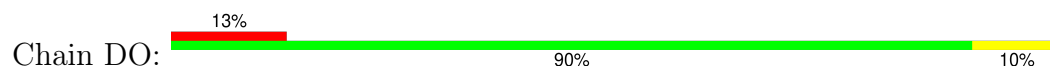


• Molecule 6: Flagellin

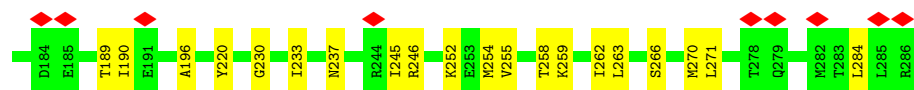
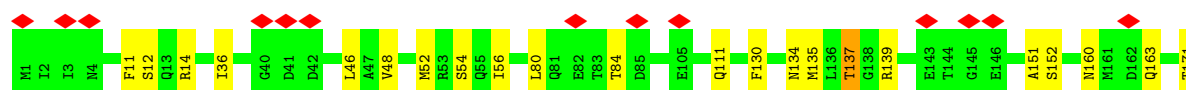
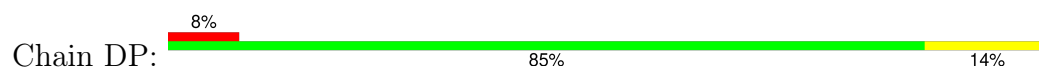




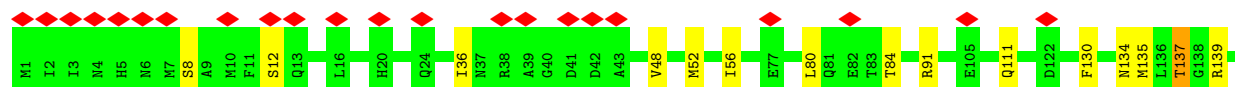
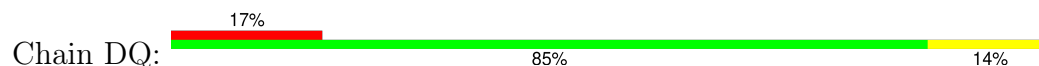
• Molecule 6: Flagellin



• Molecule 6: Flagellin



• Molecule 6: Flagellin



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	
Number of segments used	56413	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57.7	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.024	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size ($\text{\AA}$)	373.184, 373.184, 373.184	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.833, 0.833, 0.833	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, A1CIM

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	A0	0.14	0/1812	0.33	2/2452 (0.1%)
1	A4	0.14	0/1812	0.33	2/2452 (0.1%)
1	A6	0.14	0/1812	0.33	2/2452 (0.1%)
1	BI	0.07	0/1649	0.22	0/2228
1	BJ	0.07	0/1649	0.22	0/2228
1	BM	0.07	0/1649	0.22	0/2228
2	A3	0.07	0/2633	0.21	0/3561
2	A5	0.07	0/2633	0.21	0/3561
2	A9	0.07	0/2633	0.21	0/3561
2	BQ	0.07	0/2538	0.23	0/3439
2	BR	0.07	0/2538	0.23	0/3439
2	BS	0.07	0/2538	0.23	0/3439
3	A7	0.07	0/1679	0.24	0/2277
3	A8	0.07	0/1679	0.24	0/2277
3	BA	0.07	0/1679	0.24	0/2277
3	BK	0.08	0/1705	0.25	0/2311
3	BL	0.08	0/1705	0.25	0/2311
3	BN	0.08	0/1705	0.25	0/2311
4	E	0.05	0/934	0.20	0/1261
4	F	0.05	0/934	0.20	0/1261
4	G	0.05	0/934	0.20	0/1261
5	P2	0.07	0/1487	0.20	0/2006
5	P3	0.07	0/1487	0.20	0/2006
5	P4	0.07	0/1487	0.20	0/2006
6	C0	0.08	0/2224	0.25	0/2992
6	DA	0.08	0/2224	0.25	0/2992
6	DB	0.08	0/2224	0.25	0/2992
6	DC	0.08	0/2224	0.25	0/2992
6	DD	0.08	0/2224	0.25	0/2992
6	DE	0.08	0/2224	0.25	0/2992
6	DF	0.08	0/2224	0.25	0/2992
6	DG	0.08	0/2224	0.25	0/2992

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	DH	0.08	0/2224	0.25	0/2992
6	DI	0.08	0/2224	0.25	0/2992
6	DJ	0.08	0/2224	0.25	0/2992
6	DK	0.08	0/2224	0.25	0/2992
6	DL	0.08	0/2224	0.25	0/2992
6	DM	0.08	0/2224	0.25	0/2992
6	DN	0.08	0/2224	0.25	0/2992
6	DO	0.08	0/2224	0.25	0/2992
6	DP	0.08	0/2224	0.25	0/2992
6	DQ	0.08	0/2224	0.25	0/2992
All	All	0.08	0/83343	0.24	6/112461 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A0	98	GLU	CA-C-N	-5.07	113.92	122.29
1	A0	98	GLU	C-N-CA	-5.07	113.92	122.29
1	A4	98	GLU	CA-C-N	-5.07	113.92	122.29
1	A4	98	GLU	C-N-CA	-5.07	113.92	122.29
1	A6	98	GLU	CA-C-N	-5.07	113.92	122.29
1	A6	98	GLU	C-N-CA	-5.07	113.92	122.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	A0	1768	0	1710	13	0
1	A4	1768	0	1710	14	0
1	A6	1768	0	1710	10	0
1	BI	1608	0	1560	13	0
1	BJ	1608	0	1560	12	0
1	BM	1608	0	1560	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A3	2580	0	2534	12	0
2	A5	2580	0	2534	11	0
2	A9	2580	0	2534	12	0
2	BQ	2487	0	2413	17	0
2	BR	2487	0	2413	22	0
2	BS	2487	0	2413	18	0
3	A7	1628	0	1551	12	0
3	A8	1628	0	1551	12	0
3	BA	1628	0	1551	10	0
3	BK	1653	0	1573	9	0
3	BL	1653	0	1573	6	0
3	BN	1653	0	1573	9	0
4	E	909	0	913	2	0
4	F	909	0	913	3	0
4	G	909	0	913	5	0
5	P2	1473	0	1516	9	0
5	P3	1473	0	1516	7	0
5	P4	1473	0	1516	7	0
6	C0	2206	0	2213	40	0
6	DA	2206	0	2213	61	0
6	DB	2206	0	2213	31	0
6	DC	2206	0	2213	63	0
6	DD	2206	0	2213	45	0
6	DE	2206	0	2213	61	0
6	DF	2206	0	2213	41	0
6	DG	2206	0	2213	32	0
6	DH	2206	0	2213	42	0
6	DI	2206	0	2213	40	0
6	DJ	2206	0	2213	44	0
6	DK	2206	0	2213	27	0
6	DL	2206	0	2213	80	0
6	DM	2206	0	2213	59	0
6	DN	2206	0	2213	30	0
6	DO	2206	0	2213	23	0
6	DP	2206	0	2213	44	0
6	DQ	2206	0	2213	42	0
7	A0	1	0	0	0	0
7	A4	1	0	0	1	0
7	A6	1	0	0	0	0
7	A7	1	0	0	0	0
7	A8	1	0	0	0	0
7	BA	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	BI	1	0	0	0	0
7	BJ	1	0	0	0	0
7	BK	1	0	0	0	0
7	BL	1	0	0	0	0
7	BM	1	0	0	0	0
7	BN	1	0	0	0	0
8	C0	125	0	0	3	0
8	DA	125	0	0	1	0
8	DB	125	0	0	2	0
8	DC	125	0	0	1	0
8	DD	125	0	0	2	0
8	DE	125	0	0	0	0
8	DF	125	0	0	0	0
8	DG	125	0	0	1	0
8	DH	125	0	0	4	0
8	DI	125	0	0	0	0
8	DJ	125	0	0	0	0
8	DK	125	0	0	1	0
8	DL	125	0	0	0	0
8	DM	125	0	0	0	0
8	DN	125	0	0	0	0
8	DO	125	0	0	0	0
8	DP	125	0	0	0	0
8	DQ	125	0	0	0	0
All	All	84288	0	81144	757	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 5.

All (757) 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:A4:71:VAL:HG21	8:DH:301:A1CIM:O3	1.27	1.26
1:A4:71:VAL:CG2	8:DH:301:A1CIM:O3	1.85	1.23
1:A0:71:VAL:HG21	8:C0:301:A1CIM:O3	1.47	1.15
1:A0:71:VAL:CG2	8:C0:301:A1CIM:O3	2.04	1.05
6:DC:109:TYR:HE2	6:DL:51:LYS:HZ2	1.06	0.99
6:DL:3:ILE:HG22	6:DP:263:LEU:HD22	1.52	0.89
6:DC:106:ASP:OD1	6:DL:51:LYS:HE3	1.74	0.87
6:DN:78:ALA:HB2	6:DQ:237:ASN:HD22	1.39	0.87
3:A8:196:PHE:HE1	6:DA:183:GLY:HA2	1.40	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DD:27:ILE:HG21	6:DG:8:SER:HB3	1.59	0.83
6:DN:78:ALA:HB2	6:DQ:237:ASN:ND2	1.97	0.80
6:DC:110:ILE:HG12	6:DL:44:SER:HB2	1.64	0.80
1:A0:56:GLU:OE2	1:A0:99:LYS:N	2.15	0.79
6:DH:27:ILE:HG21	6:DI:8:SER:HB3	1.65	0.79
6:DL:4:ASN:O	6:DP:259:LYS:HD2	1.83	0.78
6:DM:78:ALA:HB2	6:DP:237:ASN:HD22	1.49	0.77
6:DE:2:ILE:HG21	6:DF:243:SER:OG	1.85	0.76
6:DA:120:GLU:OE1	6:DL:223:ARG:HG3	1.85	0.76
6:DD:20:HIS:HE1	6:DG:1:MET:HE3	1.51	0.76
3:A8:170:ASN:HB3	8:DB:302:A1CIM:C7	2.17	0.75
6:DL:4:ASN:OD1	6:DP:263:LEU:HD11	1.86	0.74
2:BR:36:ILE:HD11	2:BR:150:ASP:HA	1.70	0.74
6:DA:255:VAL:HG21	6:DI:13:GLN:HE21	1.52	0.74
1:A6:108:TYR:CE1	8:DG:301:A1CIM:N2	2.55	0.74
2:BQ:36:ILE:HD11	2:BQ:150:ASP:HA	1.70	0.74
6:DM:3:ILE:HG22	6:DQ:263:LEU:HD22	1.69	0.74
6:DD:78:ALA:HB2	6:DG:237:ASN:HD22	1.53	0.73
1:BI:68:ASP:OD2	6:DC:103:SER:HB3	1.89	0.73
6:DC:255:VAL:HG21	6:DJ:13:GLN:HE21	1.53	0.73
6:DM:4:ASN:OD1	6:DQ:263:LEU:HD11	1.89	0.73
2:BS:36:ILE:HD11	2:BS:150:ASP:HA	1.70	0.73
6:DB:8:SER:HB3	6:DI:27:ILE:HG21	1.70	0.72
6:DA:31:SER:HB3	6:DL:15:THR:HG21	1.72	0.72
1:A0:54:LYS:HE2	1:A0:97:ASP:HB2	1.72	0.71
1:A4:54:LYS:HE2	1:A4:97:ASP:HB2	1.72	0.70
6:DA:28:GLU:HG2	6:DL:11:PHE:CZ	2.26	0.70
1:A0:59:GLY:HA3	2:BS:323:VAL:HG11	1.73	0.70
6:DD:2:ILE:HG21	6:DE:243:SER:OG	1.92	0.70
6:DE:27:ILE:HG21	6:DH:8:SER:HB3	1.73	0.70
6:DM:78:ALA:HB2	6:DP:237:ASN:ND2	2.06	0.70
1:A6:54:LYS:HE2	1:A6:97:ASP:HB2	1.72	0.69
1:BI:79:GLY:HA3	1:BJ:242:MET:HE1	1.74	0.69
6:DC:109:TYR:CE2	6:DL:51:LYS:NZ	2.57	0.69
6:DC:110:ILE:HG12	6:DL:44:SER:CB	2.22	0.69
6:DB:237:ASN:HD22	6:DI:78:ALA:HB2	1.58	0.69
6:DE:54:SER:HB3	6:DF:91:ARG:NH1	2.08	0.69
6:DA:123:ARG:HD2	6:DL:223:ARG:HE	1.57	0.68
2:A3:36:ILE:HD13	2:A3:48:ARG:HE	1.58	0.68
2:A9:36:ILE:HD13	2:A9:48:ARG:HE	1.58	0.68
6:DE:4:ASN:HB2	6:DF:247:ASP:OD2	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A5:36:ILE:HD13	2:A5:48:ARG:HE	1.58	0.68
6:DC:120:GLU:OE1	6:DM:223:ARG:HG3	1.94	0.67
1:A6:70:GLY:HA2	1:A6:108:TYR:CE1	2.30	0.67
1:A0:70:GLY:HA2	1:A0:108:TYR:CE1	2.30	0.67
6:DB:48:VAL:HG12	6:DB:52:MET:HE2	1.76	0.67
3:A7:170:ASN:HB3	8:DA:302:A1CIM:C7	2.25	0.67
3:A7:196:PHE:HE1	6:DC:183:GLY:HA2	1.60	0.67
6:DE:20:HIS:HE1	6:DH:1:MET:HE3	1.58	0.67
1:A4:70:GLY:HA2	1:A4:108:TYR:CE1	2.30	0.67
6:DL:48:VAL:HG12	6:DL:52:MET:HE2	1.76	0.67
1:BI:68:ASP:HB3	1:BI:109:ARG:HH12	1.60	0.67
1:BJ:68:ASP:HB3	1:BJ:109:ARG:HH12	1.60	0.67
6:DO:48:VAL:HG12	6:DO:52:MET:HE2	1.76	0.66
1:BM:68:ASP:HB3	1:BM:109:ARG:HH12	1.60	0.66
6:DD:48:VAL:HG12	6:DD:52:MET:HE2	1.76	0.66
6:DP:48:VAL:HG12	6:DP:52:MET:HE2	1.76	0.66
6:DA:48:VAL:HG12	6:DA:52:MET:HE2	1.76	0.66
2:A9:230:PRO:HG3	6:DN:183:GLY:HA3	1.77	0.66
6:DC:48:VAL:HG12	6:DC:52:MET:HE2	1.76	0.66
6:DE:48:VAL:HG12	6:DE:52:MET:HE2	1.76	0.66
6:C0:48:VAL:HG12	6:C0:52:MET:HE2	1.76	0.66
6:DH:48:VAL:HG12	6:DH:52:MET:HE2	1.76	0.66
6:DM:48:VAL:HG12	6:DM:52:MET:HE2	1.76	0.66
6:DA:123:ARG:HG3	6:DL:223:ARG:HH21	1.61	0.65
6:DF:48:VAL:HG12	6:DF:52:MET:HE2	1.76	0.65
6:DG:48:VAL:HG12	6:DG:52:MET:HE2	1.76	0.65
6:DI:48:VAL:HG12	6:DI:52:MET:HE2	1.76	0.65
6:DE:78:ALA:HB2	6:DH:237:ASN:HD22	1.61	0.65
6:DK:48:VAL:HG12	6:DK:52:MET:HE2	1.76	0.65
6:DQ:48:VAL:HG12	6:DQ:52:MET:HE2	1.76	0.65
6:DJ:48:VAL:HG12	6:DJ:52:MET:HE2	1.76	0.65
6:DA:8:SER:HB3	6:DJ:27:ILE:HG21	1.77	0.65
6:DN:48:VAL:HG12	6:DN:52:MET:HE2	1.76	0.65
1:A4:97:ASP:OD1	7:A4:301:CA:CA	1.74	0.65
6:C0:27:ILE:HG21	6:DJ:8:SER:HB3	1.79	0.65
6:DC:270:MET:SD	6:DK:30:LEU:HD13	2.37	0.65
6:DD:161:MET:HG3	6:DE:197:ASN:ND2	2.11	0.65
6:DC:31:SER:HB3	6:DM:15:THR:HG21	1.79	0.65
6:DC:28:GLU:HG2	6:DM:11:PHE:CZ	2.31	0.65
6:DE:7:MET:SD	6:DF:240:ALA:HB2	2.37	0.65
6:DD:4:ASN:ND2	6:DE:34:LEU:HD23	2.12	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DA:123:ARG:CG	6:DL:223:ARG:HH21	2.09	0.64
6:DL:4:ASN:HA	6:DP:263:LEU:HD21	1.79	0.64
1:A4:59:GLY:HA3	2:BQ:323:VAL:HG11	1.80	0.64
1:A4:71:VAL:HG22	8:DH:301:A1CIM:O3	1.91	0.63
6:DL:9:ALA:HB1	6:DP:255:VAL:HG22	1.81	0.63
6:DD:78:ALA:HB2	6:DG:237:ASN:ND2	2.13	0.63
6:DE:14:ARG:NE	6:DF:233:ILE:HG12	2.12	0.63
6:DN:82:GLU:CD	6:DQ:230:GLY:HA3	2.23	0.63
6:DM:78:ALA:HB1	6:DP:233:ILE:HG22	1.80	0.63
6:DL:78:ALA:HB2	6:DO:237:ASN:HD22	1.64	0.63
6:DE:131:ASN:HD21	6:DH:48:VAL:HG13	1.64	0.63
6:DE:161:MET:HG3	6:DF:197:ASN:ND2	2.14	0.62
1:BJ:68:ASP:OD2	6:DA:103:SER:HB3	2.00	0.62
6:C0:15:THR:HG21	6:DF:32:SER:HA	1.81	0.62
6:DE:4:ASN:HD21	6:DF:34:LEU:HD23	1.64	0.62
6:DD:131:ASN:HD21	6:DG:48:VAL:HG13	1.64	0.62
6:DM:13:GLN:HE21	6:DQ:255:VAL:CG2	2.12	0.62
6:DL:3:ILE:HG22	6:DP:263:LEU:CD2	2.26	0.62
6:DA:237:ASN:HD22	6:DJ:78:ALA:HB2	1.65	0.61
6:DM:82:GLU:CD	6:DP:230:GLY:HA3	2.25	0.61
6:DM:13:GLN:HE21	6:DQ:255:VAL:HG21	1.66	0.61
6:C0:20:HIS:CE1	6:DJ:1:MET:HB3	2.35	0.61
6:DA:109:TYR:OH	6:DL:208:LYS:HG2	2.01	0.61
6:DD:4:ASN:HD21	6:DE:34:LEU:HD23	1.64	0.61
6:C0:8:SER:HB3	6:DF:27:ILE:HG21	1.82	0.61
6:DC:15:THR:HG21	6:DK:32:SER:HA	1.83	0.61
6:DH:78:ALA:HB2	6:DI:237:ASN:HD22	1.66	0.61
6:DC:106:ASP:OD1	6:DL:51:LYS:CE	2.48	0.61
1:BM:49:GLU:HG2	1:BM:228:VAL:HG22	1.83	0.60
6:DM:4:ASN:O	6:DQ:259:LYS:HD2	2.00	0.60
1:A0:58:GLU:HB2	4:G:59:LEU:HD11	1.83	0.60
1:BI:49:GLU:HG2	1:BI:228:VAL:HG22	1.83	0.60
6:DA:101:ILE:HB	6:DB:130:PHE:CE2	2.36	0.60
6:DC:89:ARG:NH2	6:DL:42:ASP:OD1	2.28	0.60
6:DC:8:SER:HB3	6:DK:27:ILE:HG21	1.83	0.60
1:BI:242:MET:HE1	1:BM:79:GLY:HA3	1.83	0.60
6:DM:4:ASN:HA	6:DQ:263:LEU:HD21	1.83	0.60
6:DE:284:LEU:HD13	6:DF:251:ALA:HA	1.84	0.59
6:C0:32:SER:HA	6:DJ:15:THR:HG21	1.83	0.59
6:DC:241:SER:OG	6:DK:71:SER:HB3	2.02	0.59
6:DH:20:HIS:CE1	6:DI:1:MET:HB3	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BJ:49:GLU:HG2	1:BJ:228:VAL:HG22	1.83	0.59
6:DL:13:GLN:NE2	6:DP:252:LYS:HA	2.17	0.59
6:DC:123:ARG:HD2	6:DM:223:ARG:HE	1.68	0.59
6:C0:71:SER:HB3	6:DJ:241:SER:OG	2.03	0.59
6:DE:4:ASN:ND2	6:DF:34:LEU:HD23	2.16	0.59
6:DL:78:ALA:HB1	6:DO:233:ILE:HG22	1.84	0.58
6:DJ:4:ASN:ND2	6:DK:33:GLY:O	2.36	0.58
2:BQ:273:ILE:HG13	2:BS:247:TYR:HD2	1.68	0.58
6:DE:32:SER:HA	6:DH:15:THR:HG21	1.84	0.57
6:DC:244:ARG:HD2	6:DK:67:GLN:OE1	2.04	0.57
2:BS:36:ILE:HG23	2:BS:37:ILE:HG13	1.86	0.57
6:DA:15:THR:HG21	6:DJ:32:SER:HA	1.86	0.57
6:DD:14:ARG:NE	6:DE:233:ILE:HG12	2.19	0.57
6:DE:4:ASN:HB2	6:DF:247:ASP:CG	2.29	0.57
2:A9:36:ILE:HD11	2:A9:150:ASP:HA	1.86	0.57
2:BQ:36:ILE:HG23	2:BQ:37:ILE:HG13	1.86	0.57
6:DD:4:ASN:HB2	6:DE:247:ASP:OD2	2.05	0.57
6:DI:4:ASN:ND2	6:DJ:33:GLY:O	2.38	0.57
2:A5:36:ILE:HD11	2:A5:150:ASP:HA	1.86	0.57
2:A3:36:ILE:HD11	2:A3:150:ASP:HA	1.86	0.57
6:DC:123:ARG:CG	6:DM:223:ARG:HH21	2.16	0.56
6:DA:270:MET:SD	6:DJ:30:LEU:HD13	2.45	0.56
6:C0:237:ASN:HD22	6:DF:78:ALA:HB2	1.70	0.56
6:DC:109:TYR:OH	6:DM:208:LYS:HG2	2.06	0.56
3:A7:178:ILE:HD11	3:A8:130:ALA:HA	1.88	0.56
2:A9:313:ILE:HD13	6:DQ:146:GLU:HB2	1.87	0.56
6:DA:112:VAL:HG21	6:DL:212:LYS:HD2	1.87	0.56
2:A9:76:LEU:HD12	2:A9:100:GLU:HG2	1.88	0.56
6:DN:78:ALA:HB1	6:DQ:233:ILE:HG22	1.86	0.56
2:BR:36:ILE:HG23	2:BR:37:ILE:HG13	1.86	0.56
6:DH:20:HIS:HE1	6:DI:1:MET:HE3	1.70	0.56
6:DK:111:GLN:HE22	6:DK:189:THR:HA	1.71	0.56
2:BQ:76:LEU:HD12	2:BQ:100:GLU:HG2	1.87	0.56
2:BR:76:LEU:HD12	2:BR:100:GLU:HG2	1.87	0.56
6:C0:111:GLN:HE22	6:C0:189:THR:HA	1.71	0.56
6:DE:161:MET:HG3	6:DF:197:ASN:HD21	1.69	0.56
6:DH:111:GLN:HE22	6:DH:189:THR:HA	1.71	0.56
6:DC:111:GLN:HE22	6:DC:189:THR:HA	1.71	0.56
6:DG:111:GLN:HE22	6:DG:189:THR:HA	1.71	0.56
6:DI:111:GLN:HE22	6:DI:189:THR:HA	1.71	0.56
6:DJ:111:GLN:HE22	6:DJ:189:THR:HA	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DA:111:GLN:HE22	6:DA:189:THR:HA	1.71	0.55
6:DB:282:MET:HE1	6:DL:265:GLN:OE1	2.07	0.55
6:DC:237:ASN:HD22	6:DK:78:ALA:HB2	1.71	0.55
2:A3:76:LEU:HD12	2:A3:100:GLU:HG2	1.88	0.55
6:C0:1:MET:HE3	6:DF:20:HIS:HE1	1.71	0.55
6:C0:48:VAL:HG13	6:DF:131:ASN:HD21	1.71	0.55
6:DF:111:GLN:HE22	6:DF:189:THR:HA	1.71	0.55
1:A6:59:GLY:HA3	2:BR:323:VAL:HG11	1.88	0.55
1:BJ:212:GLU:HG2	6:DL:198:ARG:NH1	2.20	0.55
6:DE:111:GLN:HE22	6:DE:189:THR:HA	1.71	0.55
6:DM:111:GLN:HE22	6:DM:189:THR:HA	1.71	0.55
6:DN:111:GLN:HE22	6:DN:189:THR:HA	1.71	0.55
2:BS:76:LEU:HD12	2:BS:100:GLU:HG2	1.87	0.55
6:DB:15:THR:HG21	6:DI:32:SER:HA	1.87	0.55
6:DD:20:HIS:CE1	6:DG:1:MET:HE3	2.38	0.55
6:DD:111:GLN:HE22	6:DD:189:THR:HA	1.71	0.55
6:C0:1:MET:HB3	6:DF:20:HIS:CE1	2.42	0.55
6:DB:237:ASN:ND2	6:DI:78:ALA:HB2	2.21	0.55
6:DO:111:GLN:HE22	6:DO:189:THR:HA	1.71	0.55
2:A3:230:PRO:HG3	6:DM:183:GLY:HA3	1.89	0.55
6:DC:123:ARG:HG3	6:DM:223:ARG:HH21	1.71	0.55
6:DP:111:GLN:HE22	6:DP:189:THR:HA	1.71	0.55
6:DQ:111:GLN:HE22	6:DQ:189:THR:HA	1.71	0.55
1:BI:151:ASP:HB2	1:BI:157:PHE:HE1	1.72	0.55
1:BJ:151:ASP:HB2	1:BJ:157:PHE:HE1	1.72	0.55
1:BM:151:ASP:HB2	1:BM:157:PHE:HE1	1.72	0.55
6:DA:130:PHE:CE2	6:DC:101:ILE:HB	2.42	0.55
6:DB:111:GLN:HE22	6:DB:189:THR:HA	1.71	0.55
6:DL:111:GLN:HE22	6:DL:189:THR:HA	1.71	0.55
6:DD:57:ARG:NE	6:DE:92:GLU:OE2	2.40	0.55
6:DE:78:ALA:HB2	6:DH:237:ASN:ND2	2.22	0.55
5:P3:108:ARG:HG2	5:P3:139:VAL:HG11	1.88	0.55
6:DL:13:GLN:HE21	6:DP:255:VAL:CG2	2.19	0.55
5:P2:108:ARG:HG2	5:P2:139:VAL:HG11	1.88	0.54
6:DE:4:ASN:HD22	6:DF:247:ASP:CG	2.15	0.54
5:P4:108:ARG:HG2	5:P4:139:VAL:HG11	1.88	0.54
6:DC:273:GLN:HB3	6:DK:257:TYR:OH	2.07	0.54
2:A5:76:LEU:HD12	2:A5:100:GLU:HG2	1.88	0.54
6:DE:20:HIS:CE1	6:DH:1:MET:HB3	2.43	0.54
2:A3:194:PHE:HZ	2:A9:248:PRO:HG3	1.71	0.54
2:A5:182:ILE:HD12	2:A5:281:ILE:HD11	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DD:284:LEU:HD13	6:DE:251:ALA:HA	1.90	0.54
2:BQ:247:TYR:HD2	2:BR:273:ILE:HG13	1.73	0.54
4:F:91:LEU:HG	4:F:103:ILE:HD11	1.89	0.54
4:G:91:LEU:HG	4:G:103:ILE:HD11	1.89	0.54
6:DA:116:GLN:HB3	6:DL:219:ALA:HB1	1.90	0.54
6:DL:3:ILE:HG23	6:DP:262:ILE:HG22	1.89	0.53
2:BS:336:GLU:HG2	4:G:120:LYS:HB2	1.90	0.53
4:E:91:LEU:HG	4:E:103:ILE:HD11	1.89	0.53
6:DA:101:ILE:HB	6:DB:130:PHE:HE2	1.72	0.53
6:DL:130:PHE:HE2	6:DM:101:ILE:HB	1.72	0.53
6:DA:282:MET:HE1	6:DM:265:GLN:OE1	2.09	0.53
6:DC:89:ARG:NH2	6:DL:42:ASP:HA	2.22	0.53
3:BN:169:THR:HG21	8:DK:301:A1CIM:O5	2.09	0.53
6:DD:20:HIS:CE1	6:DG:1:MET:HB3	2.43	0.53
6:DE:57:ARG:NE	6:DF:92:GLU:OE2	2.42	0.53
6:DD:54:SER:HB3	6:DE:91:ARG:NH1	2.24	0.53
6:DC:102:TYR:HE1	6:DL:48:VAL:HG21	1.74	0.53
6:DL:78:ALA:HB2	6:DO:237:ASN:ND2	2.23	0.53
2:A3:182:ILE:HD12	2:A3:281:ILE:HD11	1.90	0.53
6:DC:109:TYR:CD2	6:DL:51:LYS:NZ	2.75	0.53
2:A9:182:ILE:HD12	2:A9:281:ILE:HD11	1.90	0.53
6:DA:255:VAL:CG2	6:DI:13:GLN:HE21	2.19	0.52
3:A7:130:ALA:HA	3:BA:178:ILE:HD11	1.91	0.52
6:DC:113:GLU:OE1	6:DL:43:ALA:HB3	2.09	0.52
1:A0:112:TYR:CD1	6:DK:205:GLU:HG3	2.44	0.52
3:BA:170:ASN:HB3	8:DC:302:A1CIM:C7	2.38	0.52
6:DB:270:MET:SD	6:DI:30:LEU:HD13	2.48	0.52
3:A8:125:MET:HE2	3:A8:206:PHE:HB3	1.92	0.52
1:BJ:157:PHE:HD2	6:DL:145:GLY:HA3	1.74	0.52
6:C0:272:ALA:HB2	6:DJ:284:LEU:HD23	1.92	0.52
1:A4:112:TYR:CD1	6:DJ:205:GLU:HG3	2.45	0.52
6:DC:112:VAL:HG21	6:DM:212:LYS:HD2	1.90	0.52
6:DC:255:VAL:CG2	6:DJ:13:GLN:HE21	2.20	0.52
6:DD:7:MET:SD	6:DE:240:ALA:HB2	2.50	0.52
6:DH:131:ASN:HD21	6:DI:48:VAL:HG13	1.74	0.52
2:A3:248:PRO:HG3	2:A5:194:PHE:HZ	1.75	0.52
3:A7:125:MET:HE2	3:A7:206:PHE:HB3	1.92	0.51
6:DD:4:ASN:HB2	6:DE:247:ASP:CG	2.35	0.51
6:DA:201:GLY:HA3	6:DB:161:MET:HE3	1.92	0.51
6:DA:31:SER:O	6:DL:263:LEU:HD12	2.10	0.51
6:DE:2:ILE:HG21	6:DF:243:SER:HG	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DL:130:PHE:CE2	6:DM:101:ILE:HB	2.45	0.51
6:DM:275:ASN:HB3	6:DQ:258:THR:HG21	1.92	0.51
6:C0:78:ALA:HB2	6:DJ:237:ASN:HD22	1.76	0.51
6:DA:116:GLN:CB	6:DL:219:ALA:HB1	2.41	0.51
1:BJ:212:GLU:HG2	6:DL:198:ARG:HH12	1.76	0.51
6:DA:241:SER:OG	6:DJ:71:SER:HB3	2.10	0.51
6:DD:161:MET:HG3	6:DE:197:ASN:HD21	1.74	0.51
1:BI:82:LEU:HD13	1:BJ:240:ASP:HB3	1.91	0.51
6:DL:13:GLN:HE21	6:DP:255:VAL:HG21	1.76	0.51
6:DB:1:MET:HE3	6:DI:20:HIS:HE1	1.76	0.51
3:BA:125:MET:HE2	3:BA:206:PHE:HB3	1.92	0.50
2:BR:187:VAL:HG23	2:BR:214:MET:HE2	1.93	0.50
6:DA:161:MET:HE3	6:DC:201:GLY:HA3	1.92	0.50
6:DD:32:SER:HA	6:DG:15:THR:HG21	1.92	0.50
6:DH:32:SER:HA	6:DI:15:THR:HG21	1.91	0.50
6:DL:9:ALA:HB1	6:DP:255:VAL:CG2	2.40	0.50
6:DL:82:GLU:CD	6:DO:230:GLY:HA3	2.37	0.50
6:DD:131:ASN:HD21	6:DG:48:VAL:CG1	2.24	0.50
6:C0:28:GLU:HA	6:DJ:11:PHE:CE1	2.46	0.50
1:A6:236:MET:HB2	3:BK:95:ARG:NH2	2.26	0.50
2:BQ:187:VAL:HG23	2:BQ:214:MET:HE2	1.93	0.50
6:DD:161:MET:HE2	6:DE:198:ARG:HA	1.94	0.50
6:DM:82:GLU:OE1	6:DP:230:GLY:HA3	2.12	0.50
6:C0:241:SER:OG	6:DF:71:SER:HB3	2.12	0.50
2:BS:52:MET:HE1	2:BS:143:GLU:HG3	1.94	0.50
6:DB:111:GLN:HE22	6:DB:190:ILE:H	1.60	0.50
6:DD:2:ILE:HG21	6:DE:243:SER:HG	1.77	0.50
6:DO:12:SER:HB2	6:DO:271:LEU:HD13	1.94	0.50
6:DD:111:GLN:HE22	6:DD:190:ILE:H	1.60	0.49
6:DG:111:GLN:HE22	6:DG:190:ILE:H	1.60	0.49
6:DI:111:GLN:HE22	6:DI:190:ILE:H	1.60	0.49
6:DM:111:GLN:HE22	6:DM:190:ILE:H	1.60	0.49
2:BQ:52:MET:HE1	2:BQ:143:GLU:HG3	1.94	0.49
2:BS:187:VAL:HG23	2:BS:214:MET:HE2	1.94	0.49
6:DC:111:GLN:HE22	6:DC:190:ILE:H	1.60	0.49
6:DE:111:GLN:HE22	6:DE:190:ILE:H	1.60	0.49
6:DH:111:GLN:HE22	6:DH:190:ILE:H	1.60	0.49
6:DQ:111:GLN:HE22	6:DQ:190:ILE:H	1.60	0.49
6:C0:27:ILE:HG13	6:DJ:8:SER:HB3	1.95	0.49
6:DJ:111:GLN:HE22	6:DJ:190:ILE:H	1.60	0.49
6:DK:111:GLN:HE22	6:DK:190:ILE:H	1.61	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DP:111:GLN:HE22	6:DP:190:ILE:H	1.60	0.49
6:DF:12:SER:HB2	6:DF:271:LEU:HD13	1.94	0.49
6:DN:111:GLN:HE22	6:DN:190:ILE:H	1.61	0.49
6:DP:12:SER:HB2	6:DP:271:LEU:HD13	1.94	0.49
6:DA:111:GLN:HE22	6:DA:190:ILE:H	1.60	0.49
6:C0:111:GLN:HE22	6:C0:190:ILE:H	1.60	0.49
6:DN:131:ASN:OD1	6:DQ:48:VAL:HG13	2.12	0.49
2:BR:52:MET:HE1	2:BR:143:GLU:HG3	1.94	0.49
5:P3:128:MET:HE1	5:P3:158:VAL:HG22	1.94	0.49
6:DL:111:GLN:HE22	6:DL:190:ILE:H	1.60	0.49
6:DL:4:ASN:O	6:DP:259:LYS:CD	2.57	0.49
6:DM:9:ALA:HB1	6:DQ:255:VAL:HG22	1.95	0.49
6:DA:12:SER:HB2	6:DA:271:LEU:HD13	1.94	0.49
6:DB:12:SER:HB2	6:DB:271:LEU:HD13	1.94	0.49
6:DC:255:VAL:HG21	6:DJ:13:GLN:NE2	2.26	0.49
6:DF:111:GLN:HE22	6:DF:190:ILE:H	1.60	0.49
3:BA:168:PRO:HB2	3:BA:170:ASN:ND2	2.28	0.49
6:DO:111:GLN:HE22	6:DO:190:ILE:H	1.61	0.49
1:A4:108:TYR:CE1	8:DH:301:A1CIM:N2	2.81	0.48
6:DA:244:ARG:HD2	6:DJ:67:GLN:OE1	2.13	0.48
6:DE:12:SER:HB2	6:DE:271:LEU:HD13	1.94	0.48
6:DG:12:SER:HB2	6:DG:271:LEU:HD13	1.94	0.48
6:DK:12:SER:HB2	6:DK:271:LEU:HD13	1.94	0.48
6:DA:123:ARG:HE	6:DL:157:ILE:HD11	1.78	0.48
6:DD:12:SER:HB2	6:DD:271:LEU:HD13	1.94	0.48
6:DA:112:VAL:HG22	6:DL:212:LYS:HE2	1.95	0.48
6:DH:12:SER:HB2	6:DH:271:LEU:HD13	1.94	0.48
6:DN:12:SER:HB2	6:DN:271:LEU:HD13	1.94	0.48
6:DQ:12:SER:HB2	6:DQ:271:LEU:HD13	1.94	0.48
5:P4:128:MET:HE1	5:P4:158:VAL:HG22	1.94	0.48
6:C0:31:SER:O	6:DJ:15:THR:HG21	2.14	0.48
6:DN:116:GLN:OE1	6:DQ:223:ARG:NH1	2.44	0.48
3:A7:168:PRO:HB2	3:A7:170:ASN:ND2	2.28	0.48
2:BS:37:ILE:HD12	2:BS:46:GLN:HG3	1.96	0.48
5:P2:128:MET:HE1	5:P2:158:VAL:HG22	1.94	0.48
6:DA:130:PHE:HE2	6:DC:101:ILE:HB	1.77	0.48
6:DC:12:SER:HB2	6:DC:271:LEU:HD13	1.94	0.48
6:DI:12:SER:HB2	6:DI:271:LEU:HD13	1.94	0.48
6:DJ:12:SER:HB2	6:DJ:271:LEU:HD13	1.94	0.48
1:A4:236:MET:HB2	3:BN:95:ARG:NH2	2.29	0.48
6:DM:12:SER:HB2	6:DM:271:LEU:HD13	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DM:130:PHE:HE2	6:DN:101:ILE:HB	1.77	0.48
2:BQ:37:ILE:HD12	2:BQ:46:GLN:HG3	1.96	0.48
6:C0:131:ASN:HD21	6:DJ:48:VAL:HG13	1.77	0.48
3:A8:168:PRO:HB2	3:A8:170:ASN:ND2	2.28	0.48
6:DA:270:MET:HE2	6:DA:270:MET:HA	1.96	0.48
6:DG:270:MET:HA	6:DG:270:MET:HE2	1.96	0.48
6:DL:12:SER:HB2	6:DL:271:LEU:HD13	1.94	0.48
6:DN:78:ALA:CB	6:DQ:237:ASN:HD22	2.19	0.48
2:BR:267:HIS:CE1	8:DD:301:A1CIM:O2	2.67	0.47
2:BS:72:THR:HG22	2:BS:73:SER:H	1.78	0.47
6:C0:12:SER:HB2	6:C0:271:LEU:HD13	1.94	0.47
6:DB:270:MET:HE2	6:DB:270:MET:HA	1.96	0.47
6:DD:131:ASN:ND2	6:DG:48:VAL:HG13	2.29	0.47
6:DH:270:MET:HA	6:DH:270:MET:HE2	1.96	0.47
6:DQ:270:MET:HE2	6:DQ:270:MET:HA	1.96	0.47
6:DP:270:MET:HA	6:DP:270:MET:HE2	1.96	0.47
2:BR:37:ILE:HD12	2:BR:46:GLN:HG3	1.96	0.47
6:DE:160:ASN:HD22	6:DE:163:GLN:HE22	1.63	0.47
6:DN:160:ASN:HD22	6:DN:163:GLN:HE22	1.63	0.47
6:C0:20:HIS:HE1	6:DJ:1:MET:HE3	1.78	0.47
6:DC:160:ASN:HD22	6:DC:163:GLN:HE22	1.63	0.47
6:DC:270:MET:HA	6:DC:270:MET:HE2	1.96	0.47
6:DD:160:ASN:HD22	6:DD:163:GLN:HE22	1.63	0.47
6:DH:160:ASN:HD22	6:DH:163:GLN:HE22	1.63	0.47
6:DJ:160:ASN:HD22	6:DJ:163:GLN:HE22	1.63	0.47
6:DK:160:ASN:HD22	6:DK:163:GLN:HE22	1.63	0.47
6:DA:273:GLN:HB3	6:DJ:257:TYR:OH	2.14	0.47
6:DE:268:THR:HG22	6:DH:283:THR:OG1	2.14	0.47
6:DO:270:MET:HE2	6:DO:270:MET:HA	1.96	0.47
2:BQ:72:THR:HG22	2:BQ:73:SER:H	1.78	0.47
6:C0:160:ASN:HD22	6:C0:163:GLN:HE22	1.63	0.47
6:DG:160:ASN:HD22	6:DG:163:GLN:HE22	1.63	0.47
6:DL:270:MET:HA	6:DL:270:MET:HE2	1.96	0.47
1:A6:65:MET:HE2	1:A6:69:GLU:HB3	1.96	0.47
1:BM:112:TYR:CD1	6:DN:205:GLU:HG3	2.49	0.47
2:BR:72:THR:HG22	2:BR:73:SER:H	1.78	0.47
6:C0:270:MET:HE2	6:C0:270:MET:HA	1.96	0.47
6:DA:160:ASN:HD22	6:DA:163:GLN:HE22	1.62	0.47
6:DA:237:ASN:ND2	6:DJ:78:ALA:HB2	2.30	0.47
6:DB:160:ASN:HD22	6:DB:163:GLN:HE22	1.62	0.47
6:DE:131:ASN:HD21	6:DH:48:VAL:CG1	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DF:160:ASN:HD22	6:DF:163:GLN:HE22	1.63	0.47
6:DF:270:MET:HE2	6:DF:270:MET:HA	1.96	0.47
6:DJ:270:MET:HE2	6:DJ:270:MET:HA	1.96	0.47
6:DK:270:MET:HA	6:DK:270:MET:HE2	1.96	0.47
6:DM:3:ILE:HG22	6:DQ:263:LEU:CD2	2.41	0.47
6:DM:160:ASN:HD22	6:DM:163:GLN:HE22	1.62	0.47
6:DQ:160:ASN:HD22	6:DQ:163:GLN:HE22	1.62	0.47
6:DL:3:ILE:HG23	6:DP:262:ILE:CG2	2.45	0.47
6:DI:160:ASN:HD22	6:DI:163:GLN:HE22	1.63	0.47
6:DN:270:MET:HE2	6:DN:270:MET:HA	1.96	0.47
6:DC:31:SER:O	6:DM:263:LEU:HD12	2.15	0.47
6:DE:270:MET:HE2	6:DE:270:MET:HA	1.96	0.47
6:DM:116:GLN:NE2	6:DP:220:TYR:HE1	2.13	0.46
6:DM:130:PHE:CE2	6:DN:101:ILE:HB	2.50	0.46
6:DP:160:ASN:HD22	6:DP:163:GLN:HE22	1.63	0.46
3:A8:196:PHE:CE1	6:DA:183:GLY:HA2	2.33	0.46
6:DA:82:GLU:OE2	6:DL:226:LEU:HB3	2.16	0.46
6:DL:82:GLU:OE1	6:DO:230:GLY:HA3	2.15	0.46
6:DL:160:ASN:HD22	6:DL:163:GLN:HE22	1.63	0.46
1:A4:65:MET:HE2	1:A4:69:GLU:HB3	1.96	0.46
6:C0:91:ARG:NH1	6:DH:54:SER:HB3	2.30	0.46
6:DI:270:MET:HE2	6:DI:270:MET:HA	1.96	0.46
6:C0:255:VAL:HG22	6:DE:275:ASN:OD1	2.15	0.46
6:DO:160:ASN:HD22	6:DO:163:GLN:HE22	1.63	0.46
6:DO:284:LEU:HD13	6:DP:254:MET:HG3	1.97	0.46
1:A0:65:MET:HE2	1:A0:69:GLU:HB3	1.96	0.46
6:DC:284:LEU:HD23	6:DK:272:ALA:HB2	1.98	0.46
6:DD:270:MET:HA	6:DD:270:MET:HE2	1.96	0.46
6:DA:80:LEU:O	6:DA:84:THR:HG23	2.16	0.46
6:DA:130:PHE:HB2	6:DA:135:MET:HE1	1.98	0.46
6:DC:123:ARG:HD2	6:DM:223:ARG:HH21	1.80	0.46
6:DG:130:PHE:HB2	6:DG:135:MET:HE1	1.98	0.46
6:DM:3:ILE:HG23	6:DQ:262:ILE:HG22	1.97	0.46
6:DM:270:MET:HE2	6:DM:270:MET:HA	1.96	0.46
6:DP:130:PHE:HB2	6:DP:135:MET:HE1	1.98	0.46
6:DQ:80:LEU:O	6:DQ:84:THR:HG23	2.16	0.46
6:C0:67:GLN:OE1	6:DJ:244:ARG:HD2	2.16	0.46
6:C0:130:PHE:HB2	6:C0:135:MET:HE1	1.98	0.46
6:DB:130:PHE:HB2	6:DB:135:MET:HE1	1.98	0.46
6:DE:130:PHE:HB2	6:DE:135:MET:HE1	1.98	0.46
6:DF:130:PHE:HB2	6:DF:135:MET:HE1	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DI:130:PHE:HB2	6:DI:135:MET:HE1	1.98	0.46
6:DK:130:PHE:HB2	6:DK:135:MET:HE1	1.98	0.46
6:DL:80:LEU:O	6:DL:84:THR:HG23	2.16	0.46
6:DL:130:PHE:HB2	6:DL:135:MET:HE1	1.98	0.46
6:DM:80:LEU:O	6:DM:84:THR:HG23	2.16	0.46
6:DO:130:PHE:HB2	6:DO:135:MET:HE1	1.98	0.46
6:DO:139:ARG:HG2	6:DO:151:ALA:HB3	1.98	0.46
6:DQ:130:PHE:HB2	6:DQ:135:MET:HE1	1.98	0.46
3:BA:120:ILE:HD12	3:BA:120:ILE:H	1.81	0.46
6:DC:130:PHE:HB2	6:DC:135:MET:HE1	1.98	0.46
6:DD:153:MET:HE1	6:DE:101:ILE:HG22	1.98	0.46
6:DI:80:LEU:O	6:DI:84:THR:HG23	2.16	0.46
6:DM:130:PHE:HB2	6:DM:135:MET:HE1	1.98	0.46
6:DP:80:LEU:O	6:DP:84:THR:HG23	2.16	0.46
3:BK:65:GLN:NE2	3:BL:230:PHE:HA	2.31	0.46
6:DB:80:LEU:O	6:DB:84:THR:HG23	2.16	0.46
6:DD:130:PHE:HB2	6:DD:135:MET:HE1	1.98	0.46
6:DH:130:PHE:HB2	6:DH:135:MET:HE1	1.98	0.46
6:DP:139:ARG:HG2	6:DP:151:ALA:HB3	1.98	0.46
1:BI:110:ARG:HB3	6:DL:162:ASP:OD2	2.15	0.46
1:BM:166:HIS:HA	5:P2:210:PHE:CG	2.51	0.46
6:DC:80:LEU:O	6:DC:84:THR:HG23	2.16	0.46
6:DG:80:LEU:O	6:DG:84:THR:HG23	2.16	0.46
6:DH:78:ALA:HB2	6:DI:237:ASN:ND2	2.29	0.46
6:DL:139:ARG:HG2	6:DL:151:ALA:HB3	1.98	0.46
6:DL:275:ASN:HB3	6:DP:258:THR:HG21	1.97	0.46
3:A7:120:ILE:HD12	3:A7:120:ILE:H	1.81	0.45
3:BA:31:TYR:HB3	3:BA:212:LEU:HD11	1.99	0.45
2:BQ:92:SER:HA	2:BQ:121:LEU:HD23	1.98	0.45
2:BR:92:SER:HA	2:BR:121:LEU:HD23	1.98	0.45
6:DB:241:SER:OG	6:DI:71:SER:HB3	2.16	0.45
6:DC:112:VAL:HG22	6:DM:212:LYS:HE2	1.97	0.45
6:DN:130:PHE:HB2	6:DN:135:MET:HE1	1.98	0.45
2:BS:92:SER:HA	2:BS:121:LEU:HD23	1.98	0.45
6:DB:1:MET:HB3	6:DI:20:HIS:CE1	2.52	0.45
6:DB:139:ARG:HG2	6:DB:151:ALA:HB3	1.98	0.45
6:DJ:130:PHE:HB2	6:DJ:135:MET:HE1	1.98	0.45
6:DM:139:ARG:HG2	6:DM:151:ALA:HB3	1.98	0.45
2:A5:199:TYR:HB2	2:A5:260:LEU:HB3	1.99	0.45
3:A7:31:TYR:HB3	3:A7:212:LEU:HD11	1.99	0.45
6:DA:139:ARG:HG2	6:DA:151:ALA:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DD:268:THR:HG22	6:DG:283:THR:OG1	2.16	0.45
6:DF:139:ARG:HG2	6:DF:151:ALA:HB3	1.98	0.45
6:DH:80:LEU:O	6:DH:84:THR:HG23	2.16	0.45
6:DL:161:MET:HE3	6:DM:201:GLY:HA3	1.98	0.45
6:DO:80:LEU:O	6:DO:84:THR:HG23	2.16	0.45
6:DQ:139:ARG:HG2	6:DQ:151:ALA:HB3	1.98	0.45
6:DE:139:ARG:HG2	6:DE:151:ALA:HB3	1.98	0.45
6:DJ:80:LEU:O	6:DJ:84:THR:HG23	2.16	0.45
6:DN:80:LEU:O	6:DN:84:THR:HG23	2.16	0.45
6:DA:123:ARG:HD2	6:DL:223:ARG:HH21	1.82	0.45
6:DC:139:ARG:HG2	6:DC:151:ALA:HB3	1.98	0.45
6:DD:80:LEU:O	6:DD:84:THR:HG23	2.16	0.45
6:DF:80:LEU:O	6:DF:84:THR:HG23	2.16	0.45
6:DH:71:SER:HB3	6:DI:241:SER:OG	2.16	0.45
3:A8:120:ILE:H	3:A8:120:ILE:HD12	1.80	0.45
6:C0:139:ARG:HG2	6:C0:151:ALA:HB3	1.98	0.45
6:DG:154:TRP:O	6:DH:100:GLY:N	2.48	0.45
6:DH:27:ILE:HG13	6:DI:8:SER:HB3	1.99	0.45
6:DI:139:ARG:HG2	6:DI:151:ALA:HB3	1.98	0.45
1:A0:71:VAL:HG22	8:C0:301:A1CIM:O3	2.04	0.45
1:A6:133:SER:HB3	1:A6:171:LEU:HD11	1.98	0.45
3:BL:67:LEU:O	3:BL:85:LYS:HA	2.16	0.45
6:C0:273:GLN:HB3	6:DF:257:TYR:OH	2.17	0.45
6:DJ:139:ARG:HG2	6:DJ:151:ALA:HB3	1.98	0.45
2:A9:49:ARG:HG2	2:A9:173:TYR:CZ	2.52	0.45
1:BJ:157:PHE:CD2	6:DL:145:GLY:HA3	2.51	0.45
6:DC:116:GLN:CB	6:DM:219:ALA:HB1	2.47	0.45
6:DD:139:ARG:HG2	6:DD:151:ALA:HB3	1.98	0.45
6:DH:139:ARG:HG2	6:DH:151:ALA:HB3	1.98	0.45
6:DK:139:ARG:HG2	6:DK:151:ALA:HB3	1.98	0.45
6:DN:139:ARG:HG2	6:DN:151:ALA:HB3	1.98	0.45
2:A5:36:ILE:HG22	2:A5:46:GLN:O	2.17	0.45
3:A8:31:TYR:HB3	3:A8:212:LEU:HD11	1.99	0.45
2:A9:36:ILE:HG22	2:A9:46:GLN:O	2.17	0.45
3:BN:67:LEU:O	3:BN:85:LYS:HA	2.16	0.45
6:DG:4:ASN:ND2	6:DH:33:GLY:O	2.50	0.45
2:A3:36:ILE:HG22	2:A3:46:GLN:O	2.17	0.45
2:A3:49:ARG:HG2	2:A3:173:TYR:CZ	2.52	0.45
2:A3:199:TYR:HB2	2:A3:260:LEU:HB3	1.99	0.45
3:BL:40:ASP:HA	3:BL:85:LYS:HB2	1.99	0.45
6:DA:123:ARG:HE	6:DL:157:ILE:CD1	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DD:134:ASN:HD22	6:DD:137:THR:HG21	1.82	0.45
6:DG:139:ARG:HG2	6:DG:151:ALA:HB3	1.98	0.45
6:DK:80:LEU:O	6:DK:84:THR:HG23	2.16	0.45
3:BK:67:LEU:O	3:BK:85:LYS:HA	2.16	0.44
6:DC:116:GLN:HB3	6:DM:219:ALA:HB1	1.99	0.44
6:DE:5:HIS:CE1	6:DF:239:GLN:NE2	2.86	0.44
1:A4:133:SER:HB3	1:A4:171:LEU:HD11	1.98	0.44
2:A5:49:ARG:HG2	2:A5:173:TYR:CZ	2.52	0.44
2:A9:199:TYR:HB2	2:A9:260:LEU:HB3	1.99	0.44
6:C0:80:LEU:O	6:C0:84:THR:HG23	2.16	0.44
6:DA:1:MET:HE3	6:DJ:20:HIS:HE1	1.83	0.44
6:DE:134:ASN:HD22	6:DE:137:THR:HG21	1.82	0.44
6:DL:116:GLN:NE2	6:DO:220:TYR:HE1	2.15	0.44
6:DM:13:GLN:NE2	6:DQ:252:LYS:HA	2.32	0.44
6:DM:134:ASN:HD22	6:DM:137:THR:HG21	1.82	0.44
6:DN:134:ASN:HD22	6:DN:137:THR:HG21	1.82	0.44
1:A6:112:TYR:CD1	6:DI:205:GLU:HG3	2.52	0.44
3:A8:64:VAL:HG13	3:A8:87:LEU:HD11	2.00	0.44
6:C0:134:ASN:HD22	6:C0:137:THR:HG21	1.82	0.44
6:DA:134:ASN:HD22	6:DA:137:THR:HG21	1.82	0.44
6:DE:80:LEU:O	6:DE:84:THR:HG23	2.16	0.44
6:DL:285:LEU:HD21	6:DP:266:SER:HA	1.98	0.44
6:DP:14:ARG:HG3	6:DQ:232:ASN:HB3	1.99	0.44
3:A7:64:VAL:HG13	3:A7:87:LEU:HD11	2.00	0.44
1:BJ:108:TYR:CE1	8:DB:301:A1CIM:N2	2.85	0.44
6:C0:237:ASN:ND2	6:DF:78:ALA:HB2	2.33	0.44
6:DC:123:ARG:HE	6:DM:157:ILE:HD11	1.82	0.44
6:DB:134:ASN:HD22	6:DB:137:THR:HG21	1.82	0.44
6:DD:154:TRP:O	6:DE:100:GLY:HA3	2.18	0.44
2:BR:125:TRP:CH2	6:DG:161:MET:HE1	2.52	0.44
5:P4:138:VAL:HA	5:P4:141:MET:HE3	2.00	0.44
6:DH:134:ASN:HD22	6:DH:137:THR:HG21	1.82	0.44
6:DK:134:ASN:HD22	6:DK:137:THR:HG21	1.82	0.44
1:A0:133:SER:HB3	1:A0:171:LEU:HD11	1.98	0.44
3:BA:64:VAL:HG13	3:BA:87:LEU:HD11	2.00	0.44
6:DQ:134:ASN:HD22	6:DQ:137:THR:HG21	1.82	0.44
6:DC:134:ASN:HD22	6:DC:137:THR:HG21	1.83	0.44
6:DP:284:LEU:HD13	6:DQ:254:MET:HG3	1.99	0.44
2:A9:36:ILE:HG23	2:A9:37:ILE:HG12	2.00	0.44
3:BN:40:ASP:HA	3:BN:85:LYS:HB2	1.99	0.44
5:P2:138:VAL:HA	5:P2:141:MET:HE3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DL:134:ASN:HD22	6:DL:137:THR:HG21	1.82	0.44
5:P4:109:ARG:HD3	5:P4:138:VAL:HG12	2.00	0.43
6:DG:3:ILE:HG13	6:DH:250:MET:HG3	2.00	0.43
3:BK:40:ASP:HA	3:BK:85:LYS:HB2	1.99	0.43
6:DF:134:ASN:HD22	6:DF:137:THR:HG21	1.82	0.43
5:P3:138:VAL:HA	5:P3:141:MET:HE3	2.00	0.43
6:DG:134:ASN:HD22	6:DG:137:THR:HG21	1.82	0.43
6:DO:134:ASN:HD22	6:DO:137:THR:HG21	1.82	0.43
2:A3:36:ILE:HG23	2:A3:37:ILE:HG12	2.00	0.43
6:DA:1:MET:HB3	6:DJ:20:HIS:CE1	2.54	0.43
6:DD:284:LEU:O	6:DE:254:MET:HE2	2.19	0.43
6:DI:134:ASN:HD22	6:DI:137:THR:HG21	1.83	0.43
6:DN:27:ILE:HG21	6:DQ:8:SER:HB3	2.00	0.43
6:DP:134:ASN:HD22	6:DP:137:THR:HG21	1.82	0.43
3:A8:62:PRO:HB3	3:A8:91:PHE:HB3	2.01	0.43
2:BS:199:TYR:HB2	2:BS:260:LEU:HB3	2.01	0.43
5:P2:109:ARG:HD3	5:P2:138:VAL:HG12	2.00	0.43
6:DP:46:LEU:HD11	6:DQ:214:ARG:NH1	2.33	0.43
6:DA:112:VAL:HG21	6:DL:212:LYS:CD	2.48	0.43
6:DJ:134:ASN:HD22	6:DJ:137:THR:HG21	1.82	0.43
2:BR:167:SER:HB3	2:BR:170:GLU:HB2	2.01	0.43
2:BS:36:ILE:HG22	2:BS:46:GLN:O	2.19	0.43
6:C0:270:MET:SD	6:DF:30:LEU:HD13	2.59	0.43
6:DB:244:ARG:HD2	6:DI:67:GLN:OE1	2.19	0.43
6:DP:54:SER:HB3	6:DQ:91:ARG:NH1	2.34	0.43
2:BQ:167:SER:HB3	2:BQ:170:GLU:HB2	2.01	0.43
2:BQ:199:TYR:HB2	2:BQ:260:LEU:HB3	2.01	0.43
2:BR:125:TRP:CZ2	6:DG:161:MET:HE1	2.53	0.43
3:A7:62:PRO:HB3	3:A7:91:PHE:HB3	2.01	0.42
1:BI:157:PHE:HD2	6:DM:145:GLY:HA3	1.84	0.42
3:BK:142:ASP:HB3	3:BK:172:PRO:HG2	2.01	0.42
5:P4:58:LYS:HB3	5:P4:107:VAL:HG21	2.01	0.42
6:DC:112:VAL:CG2	6:DM:212:LYS:HE2	2.48	0.42
2:A5:36:ILE:HG23	2:A5:37:ILE:HG12	2.00	0.42
3:BK:177:TYR:CE2	3:BN:198:ARG:HD3	2.55	0.42
3:BL:142:ASP:HB3	3:BL:172:PRO:HG2	2.01	0.42
2:BQ:36:ILE:HG22	2:BQ:46:GLN:O	2.19	0.42
5:P2:58:LYS:HB3	5:P2:107:VAL:HG21	2.01	0.42
6:DC:15:THR:HG21	6:DK:31:SER:O	2.19	0.42
6:DM:161:MET:HE3	6:DN:201:GLY:HA3	2.00	0.42
2:BR:267:HIS:HE1	8:DD:301:A1CIM:O2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BN:142:ASP:HB3	3:BN:172:PRO:HG2	2.01	0.42
2:BS:167:SER:HB3	2:BS:170:GLU:HB2	2.01	0.42
5:P3:109:ARG:HD3	5:P3:138:VAL:HG12	2.00	0.42
5:P3:58:LYS:HB3	5:P3:107:VAL:HG21	2.01	0.42
6:DA:123:ARG:CD	6:DL:223:ARG:HH21	2.32	0.42
6:DB:233:ILE:HG22	6:DI:78:ALA:HB1	2.00	0.42
2:BR:199:TYR:HB2	2:BR:260:LEU:HB3	2.01	0.42
6:DD:7:MET:HE1	6:DE:239:GLN:HG3	2.02	0.42
6:DG:54:SER:HB3	6:DH:91:ARG:NH1	2.34	0.42
6:DK:52:MET:O	6:DK:56:ILE:HG13	2.20	0.42
6:C0:111:GLN:NE2	6:C0:190:ILE:H	2.17	0.42
6:DB:52:MET:O	6:DB:56:ILE:HG13	2.20	0.42
6:DB:273:GLN:HB3	6:DI:257:TYR:OH	2.20	0.42
6:DN:52:MET:O	6:DN:56:ILE:HG13	2.20	0.42
6:DO:111:GLN:NE2	6:DO:190:ILE:H	2.17	0.42
1:A0:122:ALA:HB1	1:A0:201:LYS:HB3	2.02	0.42
3:BL:120:ILE:HG12	3:BL:213:THR:HB	2.02	0.42
2:BQ:47:ASN:O	2:BQ:51:VAL:HG23	2.20	0.42
2:BS:47:ASN:O	2:BS:51:VAL:HG23	2.20	0.42
6:DD:111:GLN:NE2	6:DD:190:ILE:H	2.17	0.42
6:DG:111:GLN:NE2	6:DG:190:ILE:H	2.17	0.42
6:DH:111:GLN:NE2	6:DH:190:ILE:H	2.17	0.42
1:A4:56:GLU:OE2	1:A4:97:ASP:OD1	2.38	0.42
3:BA:62:PRO:HB3	3:BA:91:PHE:HB3	2.01	0.42
1:BI:212:GLU:HG2	6:DM:198:ARG:NH1	2.35	0.42
2:BR:47:ASN:O	2:BR:51:VAL:HG23	2.19	0.42
6:DO:52:MET:O	6:DO:56:ILE:HG13	2.20	0.42
1:A4:122:ALA:HB1	1:A4:201:LYS:HB3	2.02	0.42
3:BN:120:ILE:HG12	3:BN:213:THR:HB	2.02	0.42
2:BR:36:ILE:HG22	2:BR:46:GLN:O	2.19	0.42
2:BR:85:SER:HB2	6:DH:194:GLU:HG2	2.01	0.42
5:P3:75:THR:HG23	5:P3:78:LEU:H	1.85	0.42
6:C0:52:MET:O	6:C0:56:ILE:HG13	2.20	0.42
6:C0:244:ARG:HD2	6:DF:67:GLN:OE1	2.20	0.42
6:DA:82:GLU:HG3	6:DL:226:LEU:HB3	2.01	0.42
6:DJ:111:GLN:NE2	6:DJ:190:ILE:H	2.17	0.42
6:DL:52:MET:O	6:DL:56:ILE:HG13	2.20	0.42
3:BK:120:ILE:HG12	3:BK:213:THR:HB	2.02	0.41
4:F:91:LEU:HD12	4:F:105:ILE:HA	2.02	0.41
6:DA:190:ILE:HG22	6:DA:196:ALA:HA	2.02	0.41
6:DA:284:LEU:HD23	6:DJ:272:ALA:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DD:190:ILE:HG22	6:DD:196:ALA:HA	2.03	0.41
6:DI:111:GLN:NE2	6:DI:190:ILE:H	2.17	0.41
6:DI:190:ILE:HG22	6:DI:196:ALA:HA	2.02	0.41
6:DJ:52:MET:O	6:DJ:56:ILE:HG13	2.20	0.41
6:DM:190:ILE:HG22	6:DM:196:ALA:HA	2.02	0.41
6:DP:190:ILE:HG22	6:DP:196:ALA:HA	2.02	0.41
6:DQ:190:ILE:HG22	6:DQ:196:ALA:HA	2.02	0.41
1:A6:245:ASN:HD22	4:F:80:LEU:HD23	1.85	0.41
6:DB:111:GLN:NE2	6:DB:190:ILE:H	2.17	0.41
6:DC:190:ILE:HG22	6:DC:196:ALA:HA	2.03	0.41
6:DE:190:ILE:HG22	6:DE:196:ALA:HA	2.03	0.41
6:DF:52:MET:O	6:DF:56:ILE:HG13	2.20	0.41
6:DH:190:ILE:HG22	6:DH:196:ALA:HA	2.03	0.41
6:DJ:190:ILE:HG22	6:DJ:196:ALA:HA	2.03	0.41
6:DK:111:GLN:NE2	6:DK:190:ILE:H	2.17	0.41
6:DP:52:MET:O	6:DP:56:ILE:HG13	2.20	0.41
1:A0:56:GLU:OE2	1:A0:97:ASP:OD1	2.38	0.41
1:A6:122:ALA:HB1	1:A6:201:LYS:HB3	2.02	0.41
1:BI:240:ASP:HB3	1:BM:82:LEU:HD13	2.03	0.41
6:DC:52:MET:O	6:DC:56:ILE:HG13	2.20	0.41
6:DG:190:ILE:HG22	6:DG:196:ALA:HA	2.02	0.41
6:DQ:52:MET:O	6:DQ:56:ILE:HG13	2.20	0.41
2:BR:146:ALA:HA	2:BR:157:PRO:HB3	2.03	0.41
4:E:91:LEU:HD12	4:E:105:ILE:HA	2.02	0.41
4:G:91:LEU:HD12	4:G:105:ILE:HA	2.02	0.41
6:C0:190:ILE:HG22	6:C0:196:ALA:HA	2.03	0.41
6:DC:109:TYR:HE2	6:DL:51:LYS:NZ	1.93	0.41
6:DD:161:MET:CG	6:DE:197:ASN:HD21	2.33	0.41
6:DE:52:MET:O	6:DE:56:ILE:HG13	2.20	0.41
6:DM:52:MET:O	6:DM:56:ILE:HG13	2.20	0.41
6:DO:52:MET:HE1	6:DO:245:ILE:HD12	2.03	0.41
2:BR:329:GLN:HA	2:BR:332:MET:HE2	2.02	0.41
6:C0:52:MET:HE1	6:C0:245:ILE:HD12	2.02	0.41
6:DC:1:MET:HB3	6:DK:20:HIS:CE1	2.55	0.41
6:DE:111:GLN:NE2	6:DE:190:ILE:H	2.17	0.41
6:DF:52:MET:HE1	6:DF:245:ILE:HD12	2.03	0.41
6:DG:137:THR:O	6:DG:171:THR:HG23	2.21	0.41
6:DH:52:MET:O	6:DH:56:ILE:HG13	2.20	0.41
6:DH:272:ALA:HB2	6:DI:284:LEU:HD23	2.02	0.41
6:DL:52:MET:HE1	6:DL:245:ILE:HD12	2.03	0.41
6:DL:111:GLN:NE2	6:DL:190:ILE:H	2.17	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DL:190:ILE:HG22	6:DL:196:ALA:HA	2.03	0.41
6:DM:52:MET:HE1	6:DM:245:ILE:HD12	2.02	0.41
6:DN:82:GLU:OE1	6:DQ:230:GLY:HA3	2.20	0.41
6:DN:190:ILE:HG22	6:DN:196:ALA:HA	2.03	0.41
3:A8:100:TRP:HB3	3:A8:192:ARG:HD3	2.03	0.41
6:DE:52:MET:HE1	6:DE:245:ILE:HD12	2.02	0.41
6:DF:111:GLN:NE2	6:DF:190:ILE:H	2.17	0.41
6:DF:190:ILE:HG22	6:DF:196:ALA:HA	2.03	0.41
6:DK:190:ILE:HG22	6:DK:196:ALA:HA	2.03	0.41
6:DP:52:MET:HE1	6:DP:245:ILE:HD12	2.03	0.41
6:DQ:111:GLN:NE2	6:DQ:190:ILE:H	2.17	0.41
1:BI:233:GLU:HG3	5:P2:213:ILE:HD11	2.01	0.41
5:P4:75:THR:HG23	5:P4:78:LEU:H	1.85	0.41
6:DA:52:MET:HE1	6:DA:245:ILE:HD12	2.02	0.41
6:DA:52:MET:O	6:DA:56:ILE:HG13	2.20	0.41
6:DA:137:THR:O	6:DA:171:THR:HG23	2.21	0.41
6:DB:52:MET:HE1	6:DB:245:ILE:HD12	2.03	0.41
6:DC:52:MET:HE1	6:DC:245:ILE:HD12	2.02	0.41
6:DK:52:MET:HE1	6:DK:245:ILE:HD12	2.03	0.41
6:DP:111:GLN:NE2	6:DP:190:ILE:H	2.17	0.41
2:BS:329:GLN:HA	2:BS:332:MET:HE2	2.02	0.41
5:P2:75:THR:HG23	5:P2:78:LEU:H	1.85	0.41
6:DA:4:ASN:O	6:DM:259:LYS:HD3	2.21	0.41
6:DA:255:VAL:HG21	6:DI:13:GLN:NE2	2.27	0.41
6:DD:52:MET:O	6:DD:56:ILE:HG13	2.20	0.41
6:DH:137:THR:O	6:DH:171:THR:HG23	2.21	0.41
6:DI:52:MET:O	6:DI:56:ILE:HG13	2.20	0.41
6:DJ:52:MET:HE1	6:DJ:245:ILE:HD12	2.02	0.41
6:DO:137:THR:O	6:DO:171:THR:HG23	2.21	0.41
6:DO:190:ILE:HG22	6:DO:196:ALA:HA	2.02	0.41
6:DQ:52:MET:HE1	6:DQ:245:ILE:HD12	2.02	0.41
6:DQ:137:THR:O	6:DQ:171:THR:HG23	2.21	0.41
3:A7:100:TRP:HB3	3:A7:192:ARG:HD3	2.03	0.41
3:BK:47:TRP:CE3	3:BK:105:PRO:HB3	2.56	0.41
3:BL:47:TRP:CE3	3:BL:105:PRO:HB3	2.56	0.41
1:BM:112:TYR:CG	6:DN:205:GLU:HG3	2.56	0.41
2:BQ:146:ALA:HA	2:BQ:157:PRO:HB3	2.03	0.41
6:DB:190:ILE:HG22	6:DB:196:ALA:HA	2.03	0.41
6:DC:112:VAL:HG21	6:DM:212:LYS:CD	2.51	0.41
6:DC:137:THR:O	6:DC:171:THR:HG23	2.21	0.41
6:DG:52:MET:O	6:DG:56:ILE:HG13	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DH:52:MET:HE1	6:DH:245:ILE:HD12	2.03	0.41
6:DK:137:THR:O	6:DK:171:THR:HG23	2.21	0.41
6:DL:3:ILE:CG2	6:DP:262:ILE:HG22	2.50	0.41
6:DL:137:THR:O	6:DL:171:THR:HG23	2.21	0.41
6:DN:52:MET:HE1	6:DN:245:ILE:HD12	2.03	0.41
6:DP:137:THR:O	6:DP:171:THR:HG23	2.21	0.41
1:BJ:202:ILE:HD13	1:BJ:225:LEU:HD21	2.03	0.41
5:P2:138:VAL:O	5:P2:141:MET:HG2	2.21	0.41
5:P3:138:VAL:O	5:P3:141:MET:HG2	2.21	0.41
5:P4:138:VAL:O	5:P4:141:MET:HG2	2.21	0.41
6:DF:137:THR:O	6:DF:171:THR:HG23	2.21	0.41
6:DI:52:MET:HE1	6:DI:245:ILE:HD12	2.03	0.41
3:BK:178:ILE:HG22	3:BN:130:ALA:O	2.21	0.40
2:BQ:329:GLN:HA	2:BQ:332:MET:HE2	2.02	0.40
6:DB:137:THR:O	6:DB:171:THR:HG23	2.21	0.40
6:DD:52:MET:HE1	6:DD:245:ILE:HD12	2.03	0.40
6:DE:131:ASN:ND2	6:DH:48:VAL:HG13	2.31	0.40
6:DE:137:THR:O	6:DE:171:THR:HG23	2.21	0.40
6:DO:36:ILE:HB	6:DO:246:ARG:HD2	2.04	0.40
6:DP:36:ILE:HB	6:DP:246:ARG:HD2	2.04	0.40
2:A3:45:THR:HG23	2:A3:46:GLN:HG2	2.01	0.40
2:A5:230:PRO:HG3	6:DL:183:GLY:HA3	2.03	0.40
3:BA:100:TRP:HB3	3:BA:192:ARG:HD3	2.03	0.40
3:BN:47:TRP:CE3	3:BN:105:PRO:HB3	2.56	0.40
6:C0:137:THR:O	6:C0:171:THR:HG23	2.21	0.40
6:DC:111:GLN:NE2	6:DC:190:ILE:H	2.17	0.40
6:DN:137:THR:O	6:DN:171:THR:HG23	2.21	0.40
1:BI:202:ILE:HD13	1:BI:225:LEU:HD21	2.03	0.40
2:BR:88:GLN:H	6:DH:198:ARG:HH12	1.69	0.40
2:BS:146:ALA:HA	2:BS:157:PRO:HB3	2.03	0.40
6:DA:112:VAL:CG2	6:DL:212:LYS:HE2	2.51	0.40
6:DD:137:THR:O	6:DD:171:THR:HG23	2.21	0.40
6:DN:210:ILE:O	6:DN:214:ARG:HG3	2.21	0.40
6:DP:11:PHE:HD2	6:DQ:236:GLU:OE2	2.04	0.40
3:A7:150:LEU:HB3	3:A7:165:VAL:HG21	2.04	0.40
3:A8:150:LEU:HB3	3:A8:165:VAL:HG21	2.04	0.40
2:A9:45:THR:HG23	2:A9:46:GLN:HG2	2.01	0.40
3:BA:142:ASP:HB3	3:BA:172:PRO:HG2	2.03	0.40
6:DA:36:ILE:HB	6:DA:246:ARG:HD2	2.03	0.40
6:DJ:137:THR:O	6:DJ:171:THR:HG23	2.21	0.40
6:DL:210:ILE:O	6:DL:214:ARG:HG3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:DM:137:THR:O	6:DM:171:THR:HG23	2.21	0.40
6:DQ:36:ILE:HB	6:DQ:246:ARG:HD2	2.04	0.40
2:A5:45:THR:HG23	2:A5:46:GLN:HG2	2.02	0.40
2:BS:338:PHE:HB2	4:G:63:GLU:OE2	2.21	0.40
6:DA:111:GLN:NE2	6:DA:190:ILE:H	2.18	0.40
6:DB:36:ILE:HB	6:DB:246:ARG:HD2	2.04	0.40
6:DC:36:ILE:HB	6:DC:246:ARG:HD2	2.04	0.40
6:DC:123:ARG:HE	6:DM:157:ILE:CD1	2.34	0.40
6:DE:210:ILE:O	6:DE:214:ARG:HG3	2.21	0.40
6:DG:52:MET:HE1	6:DG:245:ILE:HD12	2.03	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 PDB entries followed by that with respect to all EM entries.

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	A0	219/246 (89%)	213 (97%)	6 (3%)	0	100	100
1	A4	219/246 (89%)	213 (97%)	6 (3%)	0	100	100
1	A6	219/246 (89%)	213 (97%)	6 (3%)	0	100	100
1	BI	194/246 (79%)	192 (99%)	2 (1%)	0	100	100
1	BJ	194/246 (79%)	192 (99%)	2 (1%)	0	100	100
1	BM	194/246 (79%)	192 (99%)	2 (1%)	0	100	100
2	A3	322/349 (92%)	316 (98%)	6 (2%)	0	100	100
2	A5	322/349 (92%)	316 (98%)	6 (2%)	0	100	100
2	A9	322/349 (92%)	315 (98%)	7 (2%)	0	100	100
2	BQ	316/349 (90%)	314 (99%)	2 (1%)	0	100	100
2	BR	316/349 (90%)	314 (99%)	2 (1%)	0	100	100
2	BS	316/349 (90%)	314 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A7	194/236 (82%)	190 (98%)	4 (2%)	0	100	100
3	A8	194/236 (82%)	190 (98%)	4 (2%)	0	100	100
3	BA	194/236 (82%)	190 (98%)	4 (2%)	0	100	100
3	BK	196/236 (83%)	190 (97%)	6 (3%)	0	100	100
3	BL	196/236 (83%)	190 (97%)	6 (3%)	0	100	100
3	BN	196/236 (83%)	190 (97%)	6 (3%)	0	100	100
4	E	108/139 (78%)	108 (100%)	0	0	100	100
4	F	108/139 (78%)	108 (100%)	0	0	100	100
4	G	108/139 (78%)	108 (100%)	0	0	100	100
5	P2	188/234 (80%)	185 (98%)	3 (2%)	0	100	100
5	P3	188/234 (80%)	185 (98%)	3 (2%)	0	100	100
5	P4	188/234 (80%)	185 (98%)	3 (2%)	0	100	100
6	C0	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
6	DA	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
6	DB	284/286 (99%)	280 (99%)	4 (1%)	0	100	100
6	DC	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
6	DD	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
6	DE	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
6	DF	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
6	DG	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
6	DH	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
6	DI	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
6	DJ	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
6	DK	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
6	DL	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
6	DM	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
6	DN	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
6	DO	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
6	DP	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
6	DQ	284/286 (99%)	281 (99%)	3 (1%)	0	100	100
All	All	10323/11253 (92%)	10180 (99%)	143 (1%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	A0	187/208 (90%)	187 (100%)	0	100	100
1	A4	187/208 (90%)	187 (100%)	0	100	100
1	A6	187/208 (90%)	187 (100%)	0	100	100
1	BI	171/208 (82%)	171 (100%)	0	100	100
1	BJ	171/208 (82%)	171 (100%)	0	100	100
1	BM	171/208 (82%)	171 (100%)	0	100	100
2	A3	271/290 (93%)	271 (100%)	0	100	100
2	A5	271/290 (93%)	271 (100%)	0	100	100
2	A9	271/290 (93%)	271 (100%)	0	100	100
2	BQ	252/290 (87%)	251 (100%)	1 (0%)	84	94
2	BR	252/290 (87%)	251 (100%)	1 (0%)	84	94
2	BS	252/290 (87%)	251 (100%)	1 (0%)	84	94
3	A7	170/199 (85%)	170 (100%)	0	100	100
3	A8	170/199 (85%)	170 (100%)	0	100	100
3	BA	170/199 (85%)	170 (100%)	0	100	100
3	BK	174/199 (87%)	174 (100%)	0	100	100
3	BL	174/199 (87%)	174 (100%)	0	100	100
3	BN	174/199 (87%)	174 (100%)	0	100	100
4	E	96/123 (78%)	96 (100%)	0	100	100
4	F	96/123 (78%)	96 (100%)	0	100	100
4	G	96/123 (78%)	96 (100%)	0	100	100
5	P2	162/204 (79%)	162 (100%)	0	100	100
5	P3	162/204 (79%)	162 (100%)	0	100	100
5	P4	162/204 (79%)	162 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	C0	236/236 (100%)	234 (99%)	2 (1%)	73	90
6	DA	236/236 (100%)	234 (99%)	2 (1%)	73	90
6	DB	236/236 (100%)	234 (99%)	2 (1%)	73	90
6	DC	236/236 (100%)	234 (99%)	2 (1%)	73	90
6	DD	236/236 (100%)	234 (99%)	2 (1%)	73	90
6	DE	236/236 (100%)	234 (99%)	2 (1%)	73	90
6	DF	236/236 (100%)	234 (99%)	2 (1%)	73	90
6	DG	236/236 (100%)	234 (99%)	2 (1%)	73	90
6	DH	236/236 (100%)	234 (99%)	2 (1%)	73	90
6	DI	236/236 (100%)	234 (99%)	2 (1%)	73	90
6	DJ	236/236 (100%)	234 (99%)	2 (1%)	73	90
6	DK	236/236 (100%)	234 (99%)	2 (1%)	73	90
6	DL	236/236 (100%)	234 (99%)	2 (1%)	73	90
6	DM	236/236 (100%)	234 (99%)	2 (1%)	73	90
6	DN	236/236 (100%)	234 (99%)	2 (1%)	73	90
6	DO	236/236 (100%)	234 (99%)	2 (1%)	73	90
6	DP	236/236 (100%)	234 (99%)	2 (1%)	73	90
6	DQ	236/236 (100%)	234 (99%)	2 (1%)	73	90
All	All	8697/9411 (92%)	8658 (100%)	39 (0%)	81	94

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	BQ	202	LEU
2	BR	202	LEU
2	BS	202	LEU
6	C0	137	THR
6	C0	152	SER
6	DA	137	THR
6	DA	152	SER
6	DB	137	THR
6	DB	152	SER
6	DC	137	THR
6	DC	152	SER
6	DD	137	THR
6	DD	152	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	DE	137	THR
6	DE	152	SER
6	DF	137	THR
6	DF	152	SER
6	DG	137	THR
6	DG	152	SER
6	DH	137	THR
6	DH	152	SER
6	DI	137	THR
6	DI	152	SER
6	DJ	137	THR
6	DJ	152	SER
6	DK	137	THR
6	DK	152	SER
6	DL	137	THR
6	DL	152	SER
6	DM	137	THR
6	DM	152	SER
6	DN	137	THR
6	DN	152	SER
6	DO	137	THR
6	DO	152	SER
6	DP	137	THR
6	DP	152	SER
6	DQ	137	THR
6	DQ	152	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (279) such sidechains are listed below:

Mol	Chain	Res	Type
1	A0	166	HIS
1	A0	217	HIS
2	A3	128	ASN
2	A3	130	ASN
2	A3	303	GLN
1	A4	166	HIS
1	A4	217	HIS
2	A5	128	ASN
2	A5	130	ASN
2	A5	303	GLN
1	A6	166	HIS
1	A6	217	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A7	32	GLN
3	A7	50	GLN
3	A7	65	GLN
3	A7	72	HIS
3	A7	99	ASN
3	A7	170	ASN
3	A8	32	GLN
3	A8	50	GLN
3	A8	65	GLN
3	A8	99	ASN
3	A8	170	ASN
2	A9	130	ASN
2	A9	188	ASN
2	A9	193	ASN
2	A9	303	GLN
3	BA	65	GLN
3	BA	72	HIS
3	BA	99	ASN
3	BA	170	ASN
1	BI	217	HIS
3	BK	65	GLN
1	BM	217	HIS
2	BQ	78	GLN
2	BQ	147	GLN
2	BQ	228	ASN
2	BQ	267	HIS
2	BQ	322	GLN
2	BQ	329	GLN
2	BR	78	GLN
2	BR	147	GLN
2	BR	228	ASN
2	BR	267	HIS
2	BR	322	GLN
2	BR	329	GLN
2	BS	66	GLN
2	BS	78	GLN
2	BS	147	GLN
2	BS	228	ASN
2	BS	322	GLN
2	BS	329	GLN
4	E	37	ASN
4	F	37	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	G	37	ASN
5	P2	166	ASN
5	P3	166	ASN
6	C0	5	HIS
6	C0	20	HIS
6	C0	55	GLN
6	C0	60	ASN
6	C0	74	GLN
6	C0	111	GLN
6	C0	142	GLN
6	C0	156	HIS
6	C0	160	ASN
6	C0	237	ASN
6	C0	261	GLN
6	C0	276	GLN
6	DA	5	HIS
6	DA	20	HIS
6	DA	55	GLN
6	DA	60	ASN
6	DA	74	GLN
6	DA	111	GLN
6	DA	142	GLN
6	DA	156	HIS
6	DA	160	ASN
6	DA	237	ASN
6	DA	261	GLN
6	DA	276	GLN
6	DB	5	HIS
6	DB	20	HIS
6	DB	55	GLN
6	DB	60	ASN
6	DB	74	GLN
6	DB	111	GLN
6	DB	142	GLN
6	DB	156	HIS
6	DB	160	ASN
6	DB	237	ASN
6	DB	261	GLN
6	DB	275	ASN
6	DB	276	GLN
6	DC	5	HIS
6	DC	20	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	DC	55	GLN
6	DC	60	ASN
6	DC	74	GLN
6	DC	111	GLN
6	DC	142	GLN
6	DC	156	HIS
6	DC	160	ASN
6	DC	237	ASN
6	DC	239	GLN
6	DC	261	GLN
6	DC	273	GLN
6	DC	276	GLN
6	DD	20	HIS
6	DD	24	GLN
6	DD	55	GLN
6	DD	60	ASN
6	DD	74	GLN
6	DD	111	GLN
6	DD	142	GLN
6	DD	156	HIS
6	DD	160	ASN
6	DD	261	GLN
6	DD	276	GLN
6	DE	20	HIS
6	DE	24	GLN
6	DE	55	GLN
6	DE	60	ASN
6	DE	74	GLN
6	DE	111	GLN
6	DE	142	GLN
6	DE	156	HIS
6	DE	160	ASN
6	DE	261	GLN
6	DE	276	GLN
6	DF	5	HIS
6	DF	20	HIS
6	DF	55	GLN
6	DF	60	ASN
6	DF	74	GLN
6	DF	111	GLN
6	DF	142	GLN
6	DF	156	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	DF	160	ASN
6	DF	239	GLN
6	DF	261	GLN
6	DF	276	GLN
6	DG	5	HIS
6	DG	20	HIS
6	DG	55	GLN
6	DG	60	ASN
6	DG	74	GLN
6	DG	111	GLN
6	DG	142	GLN
6	DG	156	HIS
6	DG	160	ASN
6	DG	237	ASN
6	DG	261	GLN
6	DG	273	GLN
6	DG	276	GLN
6	DH	5	HIS
6	DH	20	HIS
6	DH	55	GLN
6	DH	60	ASN
6	DH	74	GLN
6	DH	111	GLN
6	DH	134	ASN
6	DH	142	GLN
6	DH	156	HIS
6	DH	160	ASN
6	DH	237	ASN
6	DH	239	GLN
6	DH	261	GLN
6	DH	276	GLN
6	DI	13	GLN
6	DI	18	HIS
6	DI	20	HIS
6	DI	55	GLN
6	DI	60	ASN
6	DI	74	GLN
6	DI	111	GLN
6	DI	142	GLN
6	DI	156	HIS
6	DI	160	ASN
6	DI	237	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	DI	261	GLN
6	DI	275	ASN
6	DI	276	GLN
6	DJ	13	GLN
6	DJ	20	HIS
6	DJ	55	GLN
6	DJ	60	ASN
6	DJ	74	GLN
6	DJ	111	GLN
6	DJ	142	GLN
6	DJ	156	HIS
6	DJ	160	ASN
6	DJ	237	ASN
6	DJ	261	GLN
6	DJ	275	ASN
6	DJ	276	GLN
6	DK	5	HIS
6	DK	20	HIS
6	DK	55	GLN
6	DK	60	ASN
6	DK	74	GLN
6	DK	96	GLN
6	DK	111	GLN
6	DK	142	GLN
6	DK	156	HIS
6	DK	160	ASN
6	DK	261	GLN
6	DK	276	GLN
6	DL	5	HIS
6	DL	13	GLN
6	DL	20	HIS
6	DL	55	GLN
6	DL	60	ASN
6	DL	74	GLN
6	DL	111	GLN
6	DL	142	GLN
6	DL	156	HIS
6	DL	160	ASN
6	DL	261	GLN
6	DL	276	GLN
6	DM	5	HIS
6	DM	13	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	DM	20	HIS
6	DM	55	GLN
6	DM	60	ASN
6	DM	74	GLN
6	DM	111	GLN
6	DM	142	GLN
6	DM	156	HIS
6	DM	160	ASN
6	DM	261	GLN
6	DM	276	GLN
6	DN	5	HIS
6	DN	20	HIS
6	DN	55	GLN
6	DN	60	ASN
6	DN	74	GLN
6	DN	111	GLN
6	DN	142	GLN
6	DN	156	HIS
6	DN	160	ASN
6	DN	261	GLN
6	DN	276	GLN
6	DO	5	HIS
6	DO	20	HIS
6	DO	55	GLN
6	DO	60	ASN
6	DO	74	GLN
6	DO	111	GLN
6	DO	142	GLN
6	DO	156	HIS
6	DO	160	ASN
6	DO	237	ASN
6	DO	261	GLN
6	DO	276	GLN
6	DP	5	HIS
6	DP	20	HIS
6	DP	55	GLN
6	DP	60	ASN
6	DP	74	GLN
6	DP	111	GLN
6	DP	142	GLN
6	DP	156	HIS
6	DP	160	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	DP	237	ASN
6	DP	261	GLN
6	DP	276	GLN
6	DQ	5	HIS
6	DQ	20	HIS
6	DQ	55	GLN
6	DQ	60	ASN
6	DQ	74	GLN
6	DQ	111	GLN
6	DQ	142	GLN
6	DQ	156	HIS
6	DQ	160	ASN
6	DQ	237	ASN
6	DQ	261	GLN
6	DQ	276	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 102 ligands modelled in this entry, 12 are monoatomic - leaving 90 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
8	A1CIM	DB	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DL	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	DH	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	DC	305	6	17,19,31	4.16	6 (35%)	18,28,46	2.36	7 (38%)
8	A1CIM	DG	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)
8	A1CIM	DH	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)
8	A1CIM	C0	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	DK	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	DN	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DI	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DI	305	6	17,19,31	4.16	6 (35%)	18,28,46	2.36	7 (38%)
8	A1CIM	DK	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)
8	A1CIM	DN	305	6	17,19,31	4.16	6 (35%)	18,28,46	2.36	7 (38%)
8	A1CIM	DB	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)
8	A1CIM	DO	305	6	17,19,31	4.16	6 (35%)	18,28,46	2.36	7 (38%)
8	A1CIM	DF	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)
8	A1CIM	DN	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	DI	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	C0	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DP	305	6	17,19,31	4.16	6 (35%)	18,28,46	2.36	7 (38%)
8	A1CIM	DE	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	DO	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	DD	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	DL	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)
8	A1CIM	DE	305	6	17,19,31	4.16	6 (35%)	18,28,46	2.36	7 (38%)
8	A1CIM	DA	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DP	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)
8	A1CIM	DQ	305	6	17,19,31	4.16	6 (35%)	18,28,46	2.36	7 (38%)
8	A1CIM	C0	305	6	17,19,31	4.16	6 (35%)	18,28,46	2.36	7 (38%)
8	A1CIM	DG	305	6	17,19,31	4.16	6 (35%)	18,28,46	2.36	7 (38%)
8	A1CIM	DB	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)
8	A1CIM	DL	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DK	305	6	17,19,31	4.16	6 (35%)	18,28,46	2.36	7 (38%)
8	A1CIM	DQ	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	DL	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	A1CIM	DO	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DD	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DG	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	DP	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)
8	A1CIM	DQ	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)
8	A1CIM	DA	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)
8	A1CIM	DO	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)
8	A1CIM	DG	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)
8	A1CIM	DM	305	6	17,19,31	4.16	6 (35%)	18,28,46	2.36	7 (38%)
8	A1CIM	DB	305	6	17,19,31	4.15	6 (35%)	18,28,46	2.36	7 (38%)
8	A1CIM	DA	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)
8	A1CIM	DC	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)
8	A1CIM	DK	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DH	305	6	17,19,31	4.16	6 (35%)	18,28,46	2.36	7 (38%)
8	A1CIM	DN	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)
8	A1CIM	DM	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)
8	A1CIM	C0	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)
8	A1CIM	DF	305	6	17,19,31	4.16	6 (35%)	18,28,46	2.36	7 (38%)
8	A1CIM	DG	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DI	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)
8	A1CIM	DK	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)
8	A1CIM	DC	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)
8	A1CIM	DP	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	C0	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)
8	A1CIM	DD	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)
8	A1CIM	DD	305	6	17,19,31	4.16	6 (35%)	18,28,46	2.36	7 (38%)
8	A1CIM	DE	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)
8	A1CIM	DJ	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)
8	A1CIM	DA	305	6	17,19,31	4.16	6 (35%)	18,28,46	2.36	7 (38%)
8	A1CIM	DN	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)
8	A1CIM	DQ	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)
8	A1CIM	DF	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)
8	A1CIM	DB	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	DQ	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DM	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	A1CIM	DC	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	DJ	305	6	17,19,31	4.16	6 (35%)	18,28,46	2.36	7 (38%)
8	A1CIM	DA	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	DJ	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	DJ	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)
8	A1CIM	DI	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)
8	A1CIM	DC	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DF	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	DM	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DO	304	6	27,29,31	2.21	6 (22%)	29,42,46	1.42	5 (17%)
8	A1CIM	DH	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)
8	A1CIM	DJ	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DD	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)
8	A1CIM	DF	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DE	301	6	27,29,31	2.35	7 (25%)	29,42,46	1.89	6 (20%)
8	A1CIM	DH	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DP	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DM	302	6	17,19,31	4.09	5 (29%)	18,28,46	2.52	7 (38%)
8	A1CIM	DE	303	6	27,29,31	2.27	8 (29%)	29,42,46	2.14	6 (20%)
8	A1CIM	DL	305	6	17,19,31	4.16	6 (35%)	18,28,46	2.36	7 (38%)

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
8	A1CIM	DB	303	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DL	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DH	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DC	305	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DG	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DH	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	C0	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DK	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DN	303	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DI	303	6	-	14/31/51/58	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	A1CIM	DI	305	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DK	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DN	305	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DB	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DO	305	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DF	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DN	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DI	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	C0	303	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DP	305	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DE	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DO	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DD	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DL	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DE	305	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DA	303	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DP	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DQ	305	6	-	0/13/34/58	0/1/1/1
8	A1CIM	C0	305	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DG	305	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DB	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DL	303	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DK	305	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DQ	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DL	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DO	303	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DD	303	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DG	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DP	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DQ	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DA	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DO	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DG	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DM	305	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DB	305	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DA	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DC	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DK	303	6	-	14/31/51/58	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	A1CIM	DH	305	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DN	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DM	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	C0	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DF	305	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DG	303	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DI	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DK	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DC	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DP	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	C0	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DD	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DD	305	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DE	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DJ	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DA	305	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DN	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DQ	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DF	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DB	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DQ	303	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DM	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DC	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DJ	305	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DA	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DJ	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DJ	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DI	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DC	303	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DF	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DM	303	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DO	304	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DH	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DJ	303	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DD	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DF	303	6	-	14/31/51/58	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	A1CIM	DE	301	6	-	17/31/51/58	0/1/1/1
8	A1CIM	DH	303	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DP	303	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DM	302	6	-	0/13/34/58	0/1/1/1
8	A1CIM	DE	303	6	-	14/31/51/58	0/1/1/1
8	A1CIM	DL	305	6	-	0/13/34/58	0/1/1/1

All (576) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	DD	305	A1CIM	C7-N1	14.46	1.47	1.33
8	DE	305	A1CIM	C7-N1	14.46	1.47	1.33
8	DO	305	A1CIM	C7-N1	14.46	1.47	1.33
8	DQ	305	A1CIM	C7-N1	14.46	1.47	1.33
8	DH	305	A1CIM	C7-N1	14.46	1.47	1.33
8	DA	305	A1CIM	C7-N1	14.46	1.47	1.33
8	DG	305	A1CIM	C7-N1	14.46	1.47	1.33
8	DL	305	A1CIM	C7-N1	14.46	1.47	1.33
8	DM	305	A1CIM	C7-N1	14.46	1.47	1.33
8	DN	305	A1CIM	C7-N1	14.46	1.47	1.33
8	DI	305	A1CIM	C7-N1	14.45	1.47	1.33
8	DJ	305	A1CIM	C7-N1	14.45	1.47	1.33
8	C0	305	A1CIM	C7-N1	14.45	1.47	1.33
8	DK	305	A1CIM	C7-N1	14.45	1.47	1.33
8	DP	305	A1CIM	C7-N1	14.45	1.47	1.33
8	DF	305	A1CIM	C7-N1	14.45	1.47	1.33
8	DB	305	A1CIM	C7-N1	14.45	1.47	1.33
8	DC	305	A1CIM	C7-N1	14.45	1.47	1.33
8	DD	302	A1CIM	C7-N1	14.37	1.47	1.33
8	DO	302	A1CIM	C7-N1	14.37	1.47	1.33
8	DG	302	A1CIM	C7-N1	14.37	1.47	1.33
8	DL	302	A1CIM	C7-N1	14.37	1.47	1.33
8	DB	302	A1CIM	C7-N1	14.37	1.47	1.33
8	DK	302	A1CIM	C7-N1	14.37	1.47	1.33
8	DM	302	A1CIM	C7-N1	14.37	1.47	1.33
8	DH	302	A1CIM	C7-N1	14.37	1.47	1.33
8	DE	302	A1CIM	C7-N1	14.37	1.47	1.33
8	DN	302	A1CIM	C7-N1	14.37	1.47	1.33
8	DP	302	A1CIM	C7-N1	14.37	1.47	1.33
8	C0	302	A1CIM	C7-N1	14.36	1.47	1.33
8	DC	302	A1CIM	C7-N1	14.36	1.47	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	DF	302	A1CIM	C7-N1	14.36	1.47	1.33
8	DI	302	A1CIM	C7-N1	14.36	1.47	1.33
8	DQ	302	A1CIM	C7-N1	14.36	1.47	1.33
8	DJ	302	A1CIM	C7-N1	14.36	1.47	1.33
8	DA	302	A1CIM	C7-N1	14.36	1.47	1.33
8	DJ	301	A1CIM	C7-N1	6.81	1.48	1.34
8	DQ	301	A1CIM	C7-N1	6.81	1.48	1.34
8	C0	301	A1CIM	C7-N1	6.81	1.48	1.34
8	DE	301	A1CIM	C7-N1	6.81	1.48	1.34
8	DF	301	A1CIM	C7-N1	6.81	1.48	1.34
8	DO	301	A1CIM	C7-N1	6.81	1.48	1.34
8	DB	301	A1CIM	C7-N1	6.80	1.48	1.34
8	DI	301	A1CIM	C7-N1	6.80	1.48	1.34
8	DL	301	A1CIM	C7-N1	6.80	1.48	1.34
8	DM	301	A1CIM	C7-N1	6.80	1.48	1.34
8	DA	301	A1CIM	C7-N1	6.80	1.48	1.34
8	DP	301	A1CIM	C7-N1	6.80	1.48	1.34
8	DC	301	A1CIM	C7-N1	6.80	1.48	1.34
8	DN	301	A1CIM	C7-N1	6.80	1.48	1.34
8	DK	301	A1CIM	C7-N1	6.80	1.48	1.34
8	DD	301	A1CIM	C7-N1	6.80	1.48	1.34
8	DH	301	A1CIM	C7-N1	6.80	1.48	1.34
8	DG	301	A1CIM	C7-N1	6.80	1.48	1.34
8	DM	303	A1CIM	C7-N1	6.53	1.47	1.34
8	DL	303	A1CIM	C7-N1	6.53	1.47	1.34
8	DB	303	A1CIM	C7-N1	6.52	1.47	1.34
8	C0	303	A1CIM	C7-N1	6.52	1.47	1.34
8	DA	303	A1CIM	C7-N1	6.52	1.47	1.34
8	DF	303	A1CIM	C7-N1	6.52	1.47	1.34
8	DJ	303	A1CIM	C7-N1	6.52	1.47	1.34
8	DQ	303	A1CIM	C7-N1	6.52	1.47	1.34
8	DG	303	A1CIM	C7-N1	6.52	1.47	1.34
8	DH	303	A1CIM	C7-N1	6.52	1.47	1.34
8	DK	303	A1CIM	C7-N1	6.52	1.47	1.34
8	DO	303	A1CIM	C7-N1	6.52	1.47	1.34
8	DI	303	A1CIM	C7-N1	6.52	1.47	1.34
8	DD	303	A1CIM	C7-N1	6.52	1.47	1.34
8	DE	303	A1CIM	C7-N1	6.52	1.47	1.34
8	DN	303	A1CIM	C7-N1	6.52	1.47	1.34
8	DP	303	A1CIM	C7-N1	6.52	1.47	1.34
8	DC	303	A1CIM	C7-N1	6.52	1.47	1.34
8	DP	304	A1CIM	C7-N1	6.41	1.47	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	DF	304	A1CIM	C7-N1	6.40	1.47	1.34
8	DH	304	A1CIM	C7-N1	6.40	1.47	1.34
8	DM	304	A1CIM	C7-N1	6.40	1.47	1.34
8	DJ	304	A1CIM	C7-N1	6.40	1.47	1.34
8	DG	304	A1CIM	C7-N1	6.40	1.47	1.34
8	DQ	304	A1CIM	C7-N1	6.40	1.47	1.34
8	DB	304	A1CIM	C7-N1	6.40	1.47	1.34
8	DK	304	A1CIM	C7-N1	6.40	1.47	1.34
8	DO	304	A1CIM	C7-N1	6.40	1.47	1.34
8	DE	304	A1CIM	C7-N1	6.40	1.47	1.34
8	C0	304	A1CIM	C7-N1	6.40	1.47	1.34
8	DC	304	A1CIM	C7-N1	6.40	1.47	1.34
8	DD	304	A1CIM	C7-N1	6.40	1.47	1.34
8	DL	304	A1CIM	C7-N1	6.40	1.47	1.34
8	DI	304	A1CIM	C7-N1	6.40	1.47	1.34
8	DA	304	A1CIM	C7-N1	6.40	1.47	1.34
8	DN	304	A1CIM	C7-N1	6.40	1.47	1.34
8	DA	303	A1CIM	C15-N2	5.24	1.45	1.32
8	DE	303	A1CIM	C15-N2	5.24	1.45	1.32
8	DF	303	A1CIM	C15-N2	5.24	1.45	1.32
8	DG	303	A1CIM	C15-N2	5.24	1.45	1.32
8	DO	303	A1CIM	C15-N2	5.24	1.45	1.32
8	DC	303	A1CIM	C15-N2	5.24	1.45	1.32
8	DL	303	A1CIM	C15-N2	5.24	1.45	1.32
8	C0	303	A1CIM	C15-N2	5.24	1.45	1.32
8	DH	303	A1CIM	C15-N2	5.24	1.45	1.32
8	DJ	303	A1CIM	C15-N2	5.24	1.45	1.32
8	DB	303	A1CIM	C15-N2	5.24	1.45	1.32
8	DD	303	A1CIM	C15-N2	5.24	1.45	1.32
8	DM	303	A1CIM	C15-N2	5.24	1.45	1.32
8	DN	303	A1CIM	C15-N2	5.24	1.45	1.32
8	DP	303	A1CIM	C15-N2	5.24	1.45	1.32
8	DI	303	A1CIM	C15-N2	5.24	1.45	1.32
8	DQ	303	A1CIM	C15-N2	5.24	1.45	1.32
8	DK	303	A1CIM	C15-N2	5.24	1.45	1.32
8	DF	301	A1CIM	C14-C13	-5.21	1.46	1.54
8	DG	301	A1CIM	C14-C13	-5.21	1.46	1.54
8	DC	301	A1CIM	C14-C13	-5.21	1.46	1.54
8	DM	301	A1CIM	C14-C13	-5.21	1.46	1.54
8	DA	301	A1CIM	C14-C13	-5.21	1.46	1.54
8	DB	301	A1CIM	C14-C13	-5.21	1.46	1.54
8	DI	301	A1CIM	C14-C13	-5.21	1.46	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	DL	301	A1CIM	C14-C13	-5.21	1.46	1.54
8	DP	301	A1CIM	C14-C13	-5.21	1.46	1.54
8	DE	301	A1CIM	C14-C13	-5.21	1.46	1.54
8	DK	301	A1CIM	C14-C13	-5.21	1.46	1.54
8	DO	301	A1CIM	C14-C13	-5.21	1.46	1.54
8	C0	301	A1CIM	C14-C13	-5.21	1.46	1.54
8	DH	301	A1CIM	C14-C13	-5.21	1.46	1.54
8	DJ	301	A1CIM	C14-C13	-5.21	1.46	1.54
8	DN	301	A1CIM	C14-C13	-5.21	1.46	1.54
8	DQ	301	A1CIM	C14-C13	-5.21	1.46	1.54
8	DD	301	A1CIM	C14-C13	-5.20	1.46	1.54
8	DF	304	A1CIM	C15-N2	5.20	1.45	1.32
8	DC	304	A1CIM	C15-N2	5.20	1.45	1.32
8	DJ	304	A1CIM	C15-N2	5.20	1.45	1.32
8	DN	304	A1CIM	C15-N2	5.20	1.45	1.32
8	DD	304	A1CIM	C15-N2	5.20	1.45	1.32
8	DM	304	A1CIM	C15-N2	5.20	1.45	1.32
8	DB	304	A1CIM	C15-N2	5.20	1.45	1.32
8	DI	304	A1CIM	C15-N2	5.20	1.45	1.32
8	DO	304	A1CIM	C15-N2	5.20	1.45	1.32
8	DG	304	A1CIM	C15-N2	5.20	1.45	1.32
8	DK	304	A1CIM	C15-N2	5.20	1.45	1.32
8	DQ	304	A1CIM	C15-N2	5.20	1.45	1.32
8	C0	304	A1CIM	C15-N2	5.20	1.45	1.32
8	DA	304	A1CIM	C15-N2	5.20	1.45	1.32
8	DL	304	A1CIM	C15-N2	5.20	1.45	1.32
8	DP	304	A1CIM	C15-N2	5.20	1.45	1.32
8	DH	304	A1CIM	C15-N2	5.20	1.45	1.32
8	DE	304	A1CIM	C15-N2	5.20	1.45	1.32
8	DI	305	A1CIM	C15-N2	5.16	1.45	1.32
8	DN	305	A1CIM	C15-N2	5.16	1.45	1.32
8	DL	305	A1CIM	C15-N2	5.16	1.45	1.32
8	DQ	305	A1CIM	C15-N2	5.16	1.45	1.32
8	DE	305	A1CIM	C15-N2	5.16	1.45	1.32
8	DD	305	A1CIM	C15-N2	5.16	1.45	1.32
8	DB	305	A1CIM	C15-N2	5.16	1.45	1.32
8	DK	305	A1CIM	C15-N2	5.16	1.45	1.32
8	C0	305	A1CIM	C15-N2	5.16	1.45	1.32
8	DJ	305	A1CIM	C15-N2	5.16	1.45	1.32
8	DM	305	A1CIM	C15-N2	5.16	1.45	1.32
8	DN	302	A1CIM	C15-N2	5.16	1.45	1.32
8	DO	305	A1CIM	C15-N2	5.16	1.45	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	DF	305	A1CIM	C15-N2	5.16	1.45	1.32
8	DA	305	A1CIM	C15-N2	5.16	1.45	1.32
8	DF	302	A1CIM	C15-N2	5.16	1.45	1.32
8	DK	302	A1CIM	C15-N2	5.16	1.45	1.32
8	DC	305	A1CIM	C15-N2	5.16	1.45	1.32
8	DP	302	A1CIM	C15-N2	5.16	1.45	1.32
8	DP	305	A1CIM	C15-N2	5.16	1.45	1.32
8	C0	302	A1CIM	C15-N2	5.16	1.45	1.32
8	DG	305	A1CIM	C15-N2	5.16	1.45	1.32
8	DH	302	A1CIM	C15-N2	5.16	1.45	1.32
8	DH	305	A1CIM	C15-N2	5.16	1.45	1.32
8	DQ	302	A1CIM	C15-N2	5.16	1.45	1.32
8	DG	302	A1CIM	C15-N2	5.16	1.45	1.32
8	DC	302	A1CIM	C15-N2	5.16	1.45	1.32
8	DD	302	A1CIM	C15-N2	5.16	1.45	1.32
8	DE	302	A1CIM	C15-N2	5.16	1.45	1.32
8	DJ	302	A1CIM	C15-N2	5.16	1.45	1.32
8	DL	302	A1CIM	C15-N2	5.16	1.45	1.32
8	DB	302	A1CIM	C15-N2	5.16	1.45	1.32
8	DA	302	A1CIM	C15-N2	5.16	1.45	1.32
8	DO	302	A1CIM	C15-N2	5.16	1.45	1.32
8	DI	302	A1CIM	C15-N2	5.15	1.45	1.32
8	DM	302	A1CIM	C15-N2	5.15	1.45	1.32
8	DG	301	A1CIM	C15-N2	5.06	1.44	1.32
8	DH	301	A1CIM	C15-N2	5.06	1.44	1.32
8	DP	301	A1CIM	C15-N2	5.06	1.44	1.32
8	DQ	301	A1CIM	C15-N2	5.06	1.44	1.32
8	DK	301	A1CIM	C15-N2	5.06	1.44	1.32
8	C0	301	A1CIM	C15-N2	5.06	1.44	1.32
8	DA	301	A1CIM	C15-N2	5.06	1.44	1.32
8	DB	301	A1CIM	C15-N2	5.06	1.44	1.32
8	DC	301	A1CIM	C15-N2	5.06	1.44	1.32
8	DF	301	A1CIM	C15-N2	5.06	1.44	1.32
8	DD	301	A1CIM	C15-N2	5.06	1.44	1.32
8	DL	301	A1CIM	C15-N2	5.06	1.44	1.32
8	DN	301	A1CIM	C15-N2	5.06	1.44	1.32
8	DE	301	A1CIM	C15-N2	5.06	1.44	1.32
8	DO	301	A1CIM	C15-N2	5.06	1.44	1.32
8	DJ	301	A1CIM	C15-N2	5.05	1.44	1.32
8	DM	301	A1CIM	C15-N2	5.05	1.44	1.32
8	DI	301	A1CIM	C15-N2	5.05	1.44	1.32
8	DC	305	A1CIM	C14-C13	-4.69	1.47	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C0	305	A1CIM	C14-C13	-4.69	1.47	1.54
8	DM	305	A1CIM	C14-C13	-4.69	1.47	1.54
8	DN	305	A1CIM	C14-C13	-4.68	1.47	1.54
8	DL	305	A1CIM	C14-C13	-4.68	1.47	1.54
8	DK	305	A1CIM	C14-C13	-4.68	1.47	1.54
8	DP	305	A1CIM	C14-C13	-4.68	1.47	1.54
8	DI	305	A1CIM	C14-C13	-4.68	1.47	1.54
8	DJ	305	A1CIM	C14-C13	-4.68	1.47	1.54
8	DA	305	A1CIM	C14-C13	-4.68	1.47	1.54
8	DB	305	A1CIM	C14-C13	-4.68	1.47	1.54
8	DD	305	A1CIM	C14-C13	-4.68	1.47	1.54
8	DE	305	A1CIM	C14-C13	-4.68	1.47	1.54
8	DG	305	A1CIM	C14-C13	-4.68	1.47	1.54
8	DH	305	A1CIM	C14-C13	-4.68	1.47	1.54
8	DO	305	A1CIM	C14-C13	-4.68	1.47	1.54
8	DF	305	A1CIM	C14-C13	-4.68	1.47	1.54
8	DQ	305	A1CIM	C14-C13	-4.68	1.47	1.54
8	DD	304	A1CIM	C14-C13	-4.51	1.47	1.54
8	DN	304	A1CIM	C14-C13	-4.51	1.47	1.54
8	DJ	304	A1CIM	C14-C13	-4.51	1.47	1.54
8	DK	304	A1CIM	C14-C13	-4.51	1.47	1.54
8	DP	304	A1CIM	C14-C13	-4.51	1.47	1.54
8	DM	304	A1CIM	C14-C13	-4.50	1.47	1.54
8	DI	304	A1CIM	C14-C13	-4.50	1.47	1.54
8	DE	304	A1CIM	C14-C13	-4.50	1.47	1.54
8	DF	304	A1CIM	C14-C13	-4.50	1.47	1.54
8	DC	304	A1CIM	C14-C13	-4.50	1.47	1.54
8	DQ	304	A1CIM	C14-C13	-4.50	1.47	1.54
8	DB	304	A1CIM	C14-C13	-4.50	1.47	1.54
8	DG	304	A1CIM	C14-C13	-4.50	1.47	1.54
8	DA	304	A1CIM	C14-C13	-4.50	1.47	1.54
8	DO	304	A1CIM	C14-C13	-4.50	1.47	1.54
8	C0	304	A1CIM	C14-C13	-4.50	1.47	1.54
8	DL	304	A1CIM	C14-C13	-4.50	1.47	1.54
8	DH	304	A1CIM	C14-C13	-4.50	1.47	1.54
8	DE	302	A1CIM	C14-C13	-4.49	1.47	1.54
8	DN	302	A1CIM	C14-C13	-4.49	1.47	1.54
8	DC	302	A1CIM	C14-C13	-4.49	1.47	1.54
8	DH	302	A1CIM	C14-C13	-4.49	1.47	1.54
8	DP	302	A1CIM	C14-C13	-4.49	1.47	1.54
8	DK	302	A1CIM	C14-C13	-4.49	1.47	1.54
8	DI	302	A1CIM	C14-C13	-4.48	1.47	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	DJ	302	A1CIM	C14-C13	-4.48	1.47	1.54
8	DQ	302	A1CIM	C14-C13	-4.48	1.47	1.54
8	DD	302	A1CIM	C14-C13	-4.48	1.47	1.54
8	DM	302	A1CIM	C14-C13	-4.48	1.47	1.54
8	DG	302	A1CIM	C14-C13	-4.48	1.47	1.54
8	DL	302	A1CIM	C14-C13	-4.48	1.47	1.54
8	DO	302	A1CIM	C14-C13	-4.48	1.47	1.54
8	DA	302	A1CIM	C14-C13	-4.48	1.47	1.54
8	DF	302	A1CIM	C14-C13	-4.48	1.47	1.54
8	DB	302	A1CIM	C14-C13	-4.48	1.47	1.54
8	C0	302	A1CIM	C14-C13	-4.48	1.47	1.54
8	DP	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	DJ	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	DO	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	DK	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	DN	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	DA	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	DH	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	DI	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	C0	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	DB	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	DF	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	DQ	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	DC	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	DD	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	DM	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	DE	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	DG	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	DL	303	A1CIM	C14-C13	-4.16	1.47	1.54
8	DA	301	A1CIM	C12-C13	-3.12	1.46	1.52
8	DI	301	A1CIM	C12-C13	-3.12	1.46	1.52
8	DJ	301	A1CIM	C12-C13	-3.12	1.46	1.52
8	DK	301	A1CIM	C12-C13	-3.12	1.46	1.52
8	DL	301	A1CIM	C12-C13	-3.12	1.46	1.52
8	DG	301	A1CIM	C12-C13	-3.12	1.46	1.52
8	C0	301	A1CIM	C12-C13	-3.12	1.46	1.52
8	DN	301	A1CIM	C12-C13	-3.12	1.46	1.52
8	DB	301	A1CIM	C12-C13	-3.12	1.46	1.52
8	DF	301	A1CIM	C12-C13	-3.12	1.46	1.52
8	DH	301	A1CIM	C12-C13	-3.12	1.46	1.52
8	DM	301	A1CIM	C12-C13	-3.12	1.46	1.52
8	DC	301	A1CIM	C12-C13	-3.12	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	DD	301	A1CIM	C12-C13	-3.12	1.46	1.52
8	DQ	301	A1CIM	C12-C13	-3.12	1.46	1.52
8	DE	301	A1CIM	C12-C13	-3.12	1.46	1.52
8	DO	301	A1CIM	C12-C13	-3.12	1.46	1.52
8	DP	301	A1CIM	C12-C13	-3.12	1.46	1.52
8	DB	302	A1CIM	C12-C13	-3.07	1.46	1.52
8	DC	302	A1CIM	C12-C13	-3.07	1.46	1.52
8	DF	302	A1CIM	C12-C13	-3.07	1.46	1.52
8	DO	302	A1CIM	C12-C13	-3.07	1.46	1.52
8	DA	302	A1CIM	C12-C13	-3.07	1.46	1.52
8	C0	302	A1CIM	C12-C13	-3.07	1.46	1.52
8	DI	302	A1CIM	C12-C13	-3.07	1.46	1.52
8	DJ	302	A1CIM	C12-C13	-3.07	1.46	1.52
8	DG	302	A1CIM	C12-C13	-3.07	1.46	1.52
8	DN	302	A1CIM	C12-C13	-3.07	1.46	1.52
8	DP	302	A1CIM	C12-C13	-3.07	1.46	1.52
8	DE	302	A1CIM	C12-C13	-3.07	1.46	1.52
8	DD	302	A1CIM	C12-C13	-3.07	1.46	1.52
8	DQ	302	A1CIM	C12-C13	-3.07	1.46	1.52
8	DL	302	A1CIM	C12-C13	-3.07	1.46	1.52
8	DK	302	A1CIM	C12-C13	-3.06	1.46	1.52
8	DM	302	A1CIM	C12-C13	-3.06	1.46	1.52
8	DH	302	A1CIM	C12-C13	-3.06	1.46	1.52
8	DH	303	A1CIM	C12-C13	-2.95	1.47	1.52
8	DM	303	A1CIM	C12-C13	-2.95	1.47	1.52
8	DF	303	A1CIM	C12-C13	-2.95	1.47	1.52
8	DL	303	A1CIM	C12-C13	-2.95	1.47	1.52
8	DG	303	A1CIM	C12-C13	-2.95	1.47	1.52
8	DI	303	A1CIM	C12-C13	-2.95	1.47	1.52
8	C0	303	A1CIM	C12-C13	-2.95	1.47	1.52
8	DC	303	A1CIM	C12-C13	-2.95	1.47	1.52
8	DE	303	A1CIM	C12-C13	-2.95	1.47	1.52
8	DP	303	A1CIM	C12-C13	-2.95	1.47	1.52
8	DA	303	A1CIM	C12-C13	-2.94	1.47	1.52
8	DD	303	A1CIM	C12-C13	-2.94	1.47	1.52
8	DB	303	A1CIM	C12-C13	-2.94	1.47	1.52
8	DK	303	A1CIM	C12-C13	-2.94	1.47	1.52
8	DJ	303	A1CIM	C12-C13	-2.94	1.47	1.52
8	DO	303	A1CIM	C12-C13	-2.94	1.47	1.52
8	DN	303	A1CIM	C12-C13	-2.94	1.47	1.52
8	DQ	303	A1CIM	C12-C13	-2.94	1.47	1.52
8	DL	305	A1CIM	C12-C13	-2.92	1.47	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	DM	305	A1CIM	C12-C13	-2.91	1.47	1.52
8	DQ	305	A1CIM	C12-C13	-2.91	1.47	1.52
8	DG	305	A1CIM	C12-C13	-2.91	1.47	1.52
8	DA	305	A1CIM	C12-C13	-2.91	1.47	1.52
8	DI	305	A1CIM	C12-C13	-2.91	1.47	1.52
8	DP	305	A1CIM	C12-C13	-2.91	1.47	1.52
8	C0	305	A1CIM	C12-C13	-2.91	1.47	1.52
8	DJ	305	A1CIM	C12-C13	-2.91	1.47	1.52
8	DB	305	A1CIM	C12-C13	-2.91	1.47	1.52
8	DO	305	A1CIM	C12-C13	-2.91	1.47	1.52
8	DH	305	A1CIM	C12-C13	-2.91	1.47	1.52
8	DD	305	A1CIM	C12-C13	-2.91	1.47	1.52
8	DF	305	A1CIM	C12-C13	-2.91	1.47	1.52
8	DE	305	A1CIM	C12-C13	-2.91	1.47	1.52
8	DK	305	A1CIM	C12-C13	-2.91	1.47	1.52
8	DN	305	A1CIM	C12-C13	-2.91	1.47	1.52
8	DC	305	A1CIM	C12-C13	-2.91	1.47	1.52
8	DF	304	A1CIM	C12-C13	-2.89	1.47	1.52
8	DC	304	A1CIM	C12-C13	-2.89	1.47	1.52
8	C0	304	A1CIM	C12-C13	-2.89	1.47	1.52
8	DE	304	A1CIM	C12-C13	-2.89	1.47	1.52
8	DK	304	A1CIM	C12-C13	-2.89	1.47	1.52
8	DL	304	A1CIM	C12-C13	-2.89	1.47	1.52
8	DA	304	A1CIM	C12-C13	-2.89	1.47	1.52
8	DG	304	A1CIM	C12-C13	-2.89	1.47	1.52
8	DJ	304	A1CIM	C12-C13	-2.89	1.47	1.52
8	DM	304	A1CIM	C12-C13	-2.89	1.47	1.52
8	DQ	304	A1CIM	C12-C13	-2.89	1.47	1.52
8	DB	304	A1CIM	C12-C13	-2.89	1.47	1.52
8	DH	304	A1CIM	C12-C13	-2.89	1.47	1.52
8	DI	304	A1CIM	C12-C13	-2.89	1.47	1.52
8	DN	304	A1CIM	C12-C13	-2.89	1.47	1.52
8	DO	304	A1CIM	C12-C13	-2.89	1.47	1.52
8	DP	304	A1CIM	C12-C13	-2.89	1.47	1.52
8	DD	304	A1CIM	C12-C13	-2.88	1.47	1.52
8	DE	301	A1CIM	O9-C15	-2.81	1.18	1.23
8	DJ	301	A1CIM	O9-C15	-2.81	1.18	1.23
8	DM	301	A1CIM	O9-C15	-2.81	1.18	1.23
8	DD	301	A1CIM	O9-C15	-2.81	1.18	1.23
8	DG	301	A1CIM	O9-C15	-2.81	1.18	1.23
8	C0	301	A1CIM	O9-C15	-2.80	1.18	1.23
8	DK	301	A1CIM	O9-C15	-2.80	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	DL	301	A1CIM	O9-C15	-2.80	1.18	1.23
8	DP	301	A1CIM	O9-C15	-2.80	1.18	1.23
8	DA	301	A1CIM	O9-C15	-2.80	1.18	1.23
8	DC	301	A1CIM	O9-C15	-2.80	1.18	1.23
8	DQ	301	A1CIM	O9-C15	-2.80	1.18	1.23
8	DO	301	A1CIM	O9-C15	-2.80	1.18	1.23
8	DF	301	A1CIM	O9-C15	-2.80	1.18	1.23
8	DI	301	A1CIM	O9-C15	-2.80	1.18	1.23
8	DN	301	A1CIM	O9-C15	-2.80	1.18	1.23
8	DH	301	A1CIM	O9-C15	-2.80	1.18	1.23
8	DB	301	A1CIM	O9-C15	-2.80	1.18	1.23
8	DA	303	A1CIM	O9-C15	-2.77	1.18	1.23
8	DF	303	A1CIM	O9-C15	-2.77	1.18	1.23
8	DJ	303	A1CIM	O9-C15	-2.77	1.18	1.23
8	DM	303	A1CIM	O9-C15	-2.77	1.18	1.23
8	DP	303	A1CIM	O9-C15	-2.77	1.18	1.23
8	DQ	303	A1CIM	O9-C15	-2.76	1.18	1.23
8	DG	303	A1CIM	O9-C15	-2.76	1.18	1.23
8	DC	303	A1CIM	O9-C15	-2.76	1.18	1.23
8	DC	305	A1CIM	O9-C15	-2.76	1.18	1.23
8	DH	303	A1CIM	O9-C15	-2.76	1.18	1.23
8	DO	303	A1CIM	O9-C15	-2.76	1.18	1.23
8	C0	303	A1CIM	O9-C15	-2.76	1.18	1.23
8	DJ	305	A1CIM	O9-C15	-2.76	1.18	1.23
8	DL	303	A1CIM	O9-C15	-2.76	1.18	1.23
8	DL	305	A1CIM	O9-C15	-2.76	1.18	1.23
8	DD	303	A1CIM	O9-C15	-2.76	1.18	1.23
8	DE	303	A1CIM	O9-C15	-2.76	1.18	1.23
8	DO	305	A1CIM	O9-C15	-2.76	1.18	1.23
8	DB	303	A1CIM	O9-C15	-2.76	1.18	1.23
8	DD	305	A1CIM	O9-C15	-2.76	1.18	1.23
8	DE	305	A1CIM	O9-C15	-2.76	1.18	1.23
8	DI	303	A1CIM	O9-C15	-2.76	1.18	1.23
8	DI	305	A1CIM	O9-C15	-2.76	1.18	1.23
8	DK	303	A1CIM	O9-C15	-2.76	1.18	1.23
8	DN	303	A1CIM	O9-C15	-2.76	1.18	1.23
8	DN	305	A1CIM	O9-C15	-2.76	1.18	1.23
8	C0	305	A1CIM	O9-C15	-2.76	1.18	1.23
8	DA	305	A1CIM	O9-C15	-2.76	1.18	1.23
8	DK	305	A1CIM	O9-C15	-2.76	1.18	1.23
8	DM	305	A1CIM	O9-C15	-2.76	1.18	1.23
8	DF	305	A1CIM	O9-C15	-2.76	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	DP	305	A1CIM	O9-C15	-2.76	1.18	1.23
8	DC	304	A1CIM	O9-C15	-2.76	1.18	1.23
8	DQ	305	A1CIM	O9-C15	-2.76	1.18	1.23
8	DB	305	A1CIM	O9-C15	-2.76	1.18	1.23
8	DK	304	A1CIM	O9-C15	-2.76	1.18	1.23
8	DM	304	A1CIM	O9-C15	-2.76	1.18	1.23
8	DD	304	A1CIM	O9-C15	-2.76	1.18	1.23
8	DP	304	A1CIM	O9-C15	-2.75	1.18	1.23
8	DF	304	A1CIM	O9-C15	-2.75	1.18	1.23
8	DN	304	A1CIM	O9-C15	-2.75	1.18	1.23
8	DG	305	A1CIM	O9-C15	-2.75	1.18	1.23
8	DH	305	A1CIM	O9-C15	-2.75	1.18	1.23
8	DA	304	A1CIM	O9-C15	-2.75	1.18	1.23
8	DE	304	A1CIM	O9-C15	-2.75	1.18	1.23
8	DB	304	A1CIM	O9-C15	-2.75	1.18	1.23
8	DH	304	A1CIM	O9-C15	-2.75	1.18	1.23
8	DQ	304	A1CIM	O9-C15	-2.75	1.18	1.23
8	DI	304	A1CIM	O9-C15	-2.75	1.18	1.23
8	DJ	304	A1CIM	O9-C15	-2.75	1.18	1.23
8	DL	304	A1CIM	O9-C15	-2.75	1.18	1.23
8	DO	304	A1CIM	O9-C15	-2.75	1.18	1.23
8	C0	304	A1CIM	O9-C15	-2.75	1.18	1.23
8	DG	304	A1CIM	O9-C15	-2.75	1.18	1.23
8	DJ	303	A1CIM	C14-C15	2.68	1.53	1.51
8	DQ	303	A1CIM	C14-C15	2.68	1.53	1.51
8	DF	302	A1CIM	O9-C15	-2.68	1.19	1.23
8	DL	302	A1CIM	O9-C15	-2.68	1.19	1.23
8	DQ	302	A1CIM	O9-C15	-2.68	1.19	1.23
8	DF	303	A1CIM	C14-C15	2.68	1.53	1.51
8	DM	303	A1CIM	C14-C15	2.68	1.53	1.51
8	DA	302	A1CIM	O9-C15	-2.68	1.19	1.23
8	DO	302	A1CIM	O9-C15	-2.68	1.19	1.23
8	DP	303	A1CIM	C14-C15	2.68	1.53	1.51
8	DD	302	A1CIM	O9-C15	-2.68	1.19	1.23
8	DG	302	A1CIM	O9-C15	-2.68	1.19	1.23
8	C0	302	A1CIM	O9-C15	-2.68	1.19	1.23
8	DH	302	A1CIM	O9-C15	-2.68	1.19	1.23
8	DM	302	A1CIM	O9-C15	-2.68	1.19	1.23
8	DN	302	A1CIM	O9-C15	-2.68	1.19	1.23
8	DK	302	A1CIM	O9-C15	-2.68	1.19	1.23
8	DB	303	A1CIM	C14-C15	2.68	1.53	1.51
8	DD	303	A1CIM	C14-C15	2.68	1.53	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	DB	302	A1CIM	O9-C15	-2.68	1.19	1.23
8	DC	302	A1CIM	O9-C15	-2.68	1.19	1.23
8	DP	302	A1CIM	O9-C15	-2.68	1.19	1.23
8	DE	302	A1CIM	O9-C15	-2.68	1.19	1.23
8	DJ	302	A1CIM	O9-C15	-2.68	1.19	1.23
8	DC	303	A1CIM	C14-C15	2.67	1.53	1.51
8	DG	303	A1CIM	C14-C15	2.67	1.53	1.51
8	DI	303	A1CIM	C14-C15	2.67	1.53	1.51
8	DK	303	A1CIM	C14-C15	2.67	1.53	1.51
8	DI	302	A1CIM	O9-C15	-2.67	1.19	1.23
8	DH	303	A1CIM	C14-C15	2.67	1.53	1.51
8	DN	303	A1CIM	C14-C15	2.67	1.53	1.51
8	DO	303	A1CIM	C14-C15	2.67	1.53	1.51
8	DA	303	A1CIM	C14-C15	2.67	1.53	1.51
8	C0	303	A1CIM	C14-C15	2.66	1.53	1.51
8	DE	303	A1CIM	C14-C15	2.66	1.53	1.51
8	DL	303	A1CIM	C14-C15	2.66	1.53	1.51
8	DP	305	A1CIM	O7-C10	2.59	1.48	1.43
8	DL	305	A1CIM	O7-C10	2.59	1.48	1.43
8	DM	305	A1CIM	O7-C10	2.59	1.48	1.43
8	DA	305	A1CIM	O7-C10	2.59	1.48	1.43
8	DC	305	A1CIM	O7-C10	2.59	1.48	1.43
8	DK	305	A1CIM	O7-C10	2.59	1.48	1.43
8	DO	305	A1CIM	O7-C10	2.59	1.48	1.43
8	DF	305	A1CIM	O7-C10	2.59	1.48	1.43
8	C0	305	A1CIM	O7-C10	2.59	1.48	1.43
8	DN	305	A1CIM	O7-C10	2.59	1.48	1.43
8	DE	305	A1CIM	O7-C10	2.59	1.48	1.43
8	DB	305	A1CIM	O7-C10	2.59	1.48	1.43
8	DH	305	A1CIM	O7-C10	2.59	1.48	1.43
8	DI	305	A1CIM	O7-C10	2.59	1.48	1.43
8	DQ	305	A1CIM	O7-C10	2.59	1.48	1.43
8	DJ	305	A1CIM	O7-C10	2.58	1.48	1.43
8	DD	305	A1CIM	O7-C10	2.58	1.48	1.43
8	DG	305	A1CIM	O7-C10	2.58	1.48	1.43
8	DG	301	A1CIM	O1-C2	-2.50	1.38	1.42
8	DB	301	A1CIM	O1-C2	-2.49	1.38	1.42
8	DH	301	A1CIM	O1-C2	-2.49	1.38	1.42
8	DP	301	A1CIM	O1-C2	-2.49	1.38	1.42
8	DD	301	A1CIM	O1-C2	-2.49	1.38	1.42
8	DE	301	A1CIM	O1-C2	-2.49	1.38	1.42
8	DK	301	A1CIM	O1-C2	-2.49	1.38	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	DM	301	A1CIM	O1-C2	-2.49	1.38	1.42
8	DC	301	A1CIM	O1-C2	-2.49	1.38	1.42
8	DN	301	A1CIM	O1-C2	-2.49	1.38	1.42
8	DO	301	A1CIM	O1-C2	-2.49	1.38	1.42
8	C0	301	A1CIM	O1-C2	-2.49	1.38	1.42
8	DA	301	A1CIM	O1-C2	-2.49	1.38	1.42
8	DJ	301	A1CIM	O1-C2	-2.49	1.38	1.42
8	DF	301	A1CIM	O1-C2	-2.49	1.38	1.42
8	DL	301	A1CIM	O1-C2	-2.49	1.38	1.42
8	DQ	301	A1CIM	O1-C2	-2.49	1.38	1.42
8	DI	301	A1CIM	O1-C2	-2.48	1.38	1.42
8	DQ	301	A1CIM	O5-C7	-2.41	1.18	1.23
8	DJ	301	A1CIM	O5-C7	-2.40	1.18	1.23
8	DC	301	A1CIM	O5-C7	-2.40	1.18	1.23
8	C0	301	A1CIM	O5-C7	-2.40	1.18	1.23
8	DB	301	A1CIM	O5-C7	-2.40	1.18	1.23
8	DD	301	A1CIM	O5-C7	-2.40	1.18	1.23
8	DN	301	A1CIM	O5-C7	-2.40	1.18	1.23
8	DO	301	A1CIM	O5-C7	-2.40	1.18	1.23
8	DE	301	A1CIM	O5-C7	-2.40	1.18	1.23
8	DF	301	A1CIM	O5-C7	-2.40	1.18	1.23
8	DL	301	A1CIM	O5-C7	-2.40	1.18	1.23
8	DA	301	A1CIM	O5-C7	-2.40	1.18	1.23
8	DH	301	A1CIM	O5-C7	-2.40	1.18	1.23
8	DK	301	A1CIM	O5-C7	-2.40	1.18	1.23
8	DG	301	A1CIM	O5-C7	-2.40	1.18	1.23
8	DM	301	A1CIM	O5-C7	-2.40	1.18	1.23
8	DP	301	A1CIM	O5-C7	-2.40	1.18	1.23
8	DI	301	A1CIM	O5-C7	-2.39	1.18	1.23
8	C0	303	A1CIM	O7-C10	2.35	1.48	1.43
8	DM	303	A1CIM	O7-C10	2.35	1.48	1.43
8	DA	303	A1CIM	O7-C10	2.35	1.48	1.43
8	DC	303	A1CIM	O7-C10	2.35	1.48	1.43
8	DK	303	A1CIM	O7-C10	2.35	1.48	1.43
8	DO	303	A1CIM	O7-C10	2.35	1.48	1.43
8	DL	303	A1CIM	O7-C10	2.35	1.48	1.43
8	DH	303	A1CIM	O7-C10	2.35	1.48	1.43
8	DP	303	A1CIM	O7-C10	2.35	1.48	1.43
8	DQ	303	A1CIM	O7-C10	2.35	1.48	1.43
8	DI	303	A1CIM	O7-C10	2.34	1.48	1.43
8	DJ	303	A1CIM	O7-C10	2.34	1.48	1.43
8	DN	303	A1CIM	O7-C10	2.34	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	DF	303	A1CIM	O7-C10	2.34	1.48	1.43
8	DG	303	A1CIM	O7-C10	2.34	1.48	1.43
8	DB	303	A1CIM	O7-C10	2.34	1.48	1.43
8	DE	303	A1CIM	O7-C10	2.34	1.48	1.43
8	DD	303	A1CIM	O7-C10	2.34	1.48	1.43
8	DH	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	DJ	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	DQ	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	C0	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	DI	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	DK	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	DB	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	DM	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	DP	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	DL	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	DA	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	DF	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	DD	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	DE	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	DC	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	DN	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	DO	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	DG	303	A1CIM	O5-C7	-2.32	1.18	1.23
8	DF	304	A1CIM	O5-C7	-2.27	1.19	1.23
8	DI	304	A1CIM	O5-C7	-2.27	1.19	1.23
8	DH	304	A1CIM	O5-C7	-2.27	1.19	1.23
8	DE	304	A1CIM	O5-C7	-2.27	1.19	1.23
8	DG	304	A1CIM	O5-C7	-2.27	1.19	1.23
8	DB	304	A1CIM	O5-C7	-2.27	1.19	1.23
8	DP	304	A1CIM	O5-C7	-2.27	1.19	1.23
8	C0	304	A1CIM	O5-C7	-2.27	1.19	1.23
8	DA	304	A1CIM	O5-C7	-2.27	1.19	1.23
8	DC	304	A1CIM	O5-C7	-2.27	1.19	1.23
8	DO	304	A1CIM	O5-C7	-2.27	1.19	1.23
8	DN	304	A1CIM	O5-C7	-2.27	1.19	1.23
8	DD	304	A1CIM	O5-C7	-2.27	1.19	1.23
8	DK	304	A1CIM	O5-C7	-2.27	1.19	1.23
8	DL	304	A1CIM	O5-C7	-2.27	1.19	1.23
8	DQ	304	A1CIM	O5-C7	-2.27	1.19	1.23
8	DM	304	A1CIM	O5-C7	-2.27	1.19	1.23
8	DJ	304	A1CIM	O5-C7	-2.27	1.19	1.23

All (558) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DB	303	A1CIM	O7-C10-C14	7.71	119.30	109.95
8	DG	303	A1CIM	O7-C10-C14	7.71	119.30	109.95
8	DM	303	A1CIM	O7-C10-C14	7.71	119.30	109.95
8	C0	303	A1CIM	O7-C10-C14	7.71	119.30	109.95
8	DH	303	A1CIM	O7-C10-C14	7.71	119.30	109.95
8	DA	303	A1CIM	O7-C10-C14	7.71	119.30	109.95
8	DI	303	A1CIM	O7-C10-C14	7.71	119.30	109.95
8	DQ	303	A1CIM	O7-C10-C14	7.71	119.30	109.95
8	DJ	303	A1CIM	O7-C10-C14	7.70	119.29	109.95
8	DN	303	A1CIM	O7-C10-C14	7.70	119.29	109.95
8	DP	303	A1CIM	O7-C10-C14	7.70	119.29	109.95
8	DF	303	A1CIM	O7-C10-C14	7.70	119.29	109.95
8	DO	303	A1CIM	O7-C10-C14	7.70	119.29	109.95
8	DC	303	A1CIM	O7-C10-C14	7.70	119.29	109.95
8	DD	303	A1CIM	O7-C10-C14	7.70	119.29	109.95
8	DE	303	A1CIM	O7-C10-C14	7.70	119.29	109.95
8	DK	303	A1CIM	O7-C10-C14	7.70	119.29	109.95
8	DL	303	A1CIM	O7-C10-C14	7.70	119.29	109.95
8	DG	302	A1CIM	O7-C10-C14	7.52	119.07	109.95
8	DL	302	A1CIM	O7-C10-C14	7.52	119.07	109.95
8	DQ	302	A1CIM	O7-C10-C14	7.52	119.07	109.95
8	C0	302	A1CIM	O7-C10-C14	7.52	119.07	109.95
8	DI	302	A1CIM	O7-C10-C14	7.52	119.07	109.95
8	DA	302	A1CIM	O7-C10-C14	7.52	119.07	109.95
8	DK	302	A1CIM	O7-C10-C14	7.52	119.07	109.95
8	DP	302	A1CIM	O7-C10-C14	7.52	119.07	109.95
8	DB	302	A1CIM	O7-C10-C14	7.52	119.07	109.95
8	DM	302	A1CIM	O7-C10-C14	7.52	119.07	109.95
8	DD	302	A1CIM	O7-C10-C14	7.52	119.07	109.95
8	DF	302	A1CIM	O7-C10-C14	7.52	119.07	109.95
8	DH	302	A1CIM	O7-C10-C14	7.52	119.07	109.95
8	DJ	302	A1CIM	O7-C10-C14	7.52	119.07	109.95
8	DE	302	A1CIM	O7-C10-C14	7.52	119.06	109.95
8	DN	302	A1CIM	O7-C10-C14	7.52	119.06	109.95
8	DO	302	A1CIM	O7-C10-C14	7.52	119.06	109.95
8	DC	302	A1CIM	O7-C10-C14	7.51	119.06	109.95
8	DA	305	A1CIM	O7-C10-C14	7.00	118.44	109.95
8	DD	305	A1CIM	O7-C10-C14	7.00	118.44	109.95
8	DB	305	A1CIM	O7-C10-C14	7.00	118.44	109.95
8	DO	305	A1CIM	O7-C10-C14	7.00	118.44	109.95
8	DC	305	A1CIM	O7-C10-C14	7.00	118.44	109.95
8	DF	305	A1CIM	O7-C10-C14	7.00	118.44	109.95
8	DH	305	A1CIM	O7-C10-C14	7.00	118.44	109.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DI	305	A1CIM	O7-C10-C14	7.00	118.44	109.95
8	DK	305	A1CIM	O7-C10-C14	7.00	118.44	109.95
8	DL	305	A1CIM	O7-C10-C14	7.00	118.44	109.95
8	DM	305	A1CIM	O7-C10-C14	7.00	118.44	109.95
8	C0	305	A1CIM	O7-C10-C14	7.00	118.44	109.95
8	DE	305	A1CIM	O7-C10-C14	7.00	118.44	109.95
8	DQ	305	A1CIM	O7-C10-C14	7.00	118.44	109.95
8	DG	305	A1CIM	O7-C10-C14	7.00	118.44	109.95
8	DJ	305	A1CIM	O7-C10-C14	7.00	118.43	109.95
8	DP	305	A1CIM	O7-C10-C14	7.00	118.43	109.95
8	DN	305	A1CIM	O7-C10-C14	6.99	118.43	109.95
8	DK	303	A1CIM	C14-C15-N2	4.58	122.43	115.62
8	DD	303	A1CIM	C14-C15-N2	4.58	122.42	115.62
8	DB	303	A1CIM	C14-C15-N2	4.58	122.42	115.62
8	DC	303	A1CIM	C14-C15-N2	4.58	122.42	115.62
8	DI	303	A1CIM	C14-C15-N2	4.58	122.42	115.62
8	DM	303	A1CIM	C14-C15-N2	4.58	122.42	115.62
8	C0	303	A1CIM	C14-C15-N2	4.58	122.42	115.62
8	DG	303	A1CIM	C14-C15-N2	4.58	122.42	115.62
8	DN	303	A1CIM	C14-C15-N2	4.58	122.42	115.62
8	DQ	303	A1CIM	C14-C15-N2	4.58	122.42	115.62
8	DF	303	A1CIM	C14-C15-N2	4.57	122.42	115.62
8	DL	303	A1CIM	C14-C15-N2	4.57	122.42	115.62
8	DE	303	A1CIM	C14-C15-N2	4.57	122.42	115.62
8	DH	303	A1CIM	C14-C15-N2	4.57	122.42	115.62
8	DO	303	A1CIM	C14-C15-N2	4.57	122.42	115.62
8	DA	303	A1CIM	C14-C15-N2	4.57	122.42	115.62
8	DJ	303	A1CIM	C14-C15-N2	4.57	122.42	115.62
8	DP	303	A1CIM	C14-C15-N2	4.57	122.41	115.62
8	DI	301	A1CIM	O5-C7-N1	-4.43	113.89	123.15
8	DM	301	A1CIM	O5-C7-N1	-4.43	113.89	123.15
8	DG	301	A1CIM	O5-C7-N1	-4.43	113.89	123.15
8	DC	301	A1CIM	O5-C7-N1	-4.43	113.89	123.15
8	DE	301	A1CIM	O5-C7-N1	-4.43	113.89	123.15
8	DN	301	A1CIM	O5-C7-N1	-4.43	113.89	123.15
8	DO	301	A1CIM	O5-C7-N1	-4.43	113.89	123.15
8	DB	301	A1CIM	O5-C7-N1	-4.43	113.89	123.15
8	DJ	301	A1CIM	O5-C7-N1	-4.43	113.89	123.15
8	DP	301	A1CIM	O5-C7-N1	-4.43	113.89	123.15
8	C0	301	A1CIM	O5-C7-N1	-4.43	113.89	123.15
8	DA	301	A1CIM	O5-C7-N1	-4.43	113.89	123.15
8	DD	301	A1CIM	O5-C7-N1	-4.43	113.89	123.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DH	301	A1CIM	O5-C7-N1	-4.43	113.89	123.15
8	DK	301	A1CIM	O5-C7-N1	-4.43	113.89	123.15
8	DF	301	A1CIM	O5-C7-N1	-4.43	113.90	123.15
8	DQ	301	A1CIM	O5-C7-N1	-4.43	113.90	123.15
8	DL	301	A1CIM	O5-C7-N1	-4.43	113.90	123.15
8	DD	301	A1CIM	C14-C15-N2	4.13	121.76	115.62
8	DF	301	A1CIM	C14-C15-N2	4.13	121.76	115.62
8	DQ	301	A1CIM	C14-C15-N2	4.13	121.76	115.62
8	DB	301	A1CIM	C14-C15-N2	4.13	121.76	115.62
8	DC	301	A1CIM	C14-C15-N2	4.13	121.76	115.62
8	DI	301	A1CIM	C14-C15-N2	4.13	121.76	115.62
8	DJ	301	A1CIM	C14-C15-N2	4.13	121.76	115.62
8	DL	301	A1CIM	C14-C15-N2	4.13	121.76	115.62
8	DN	301	A1CIM	C14-C15-N2	4.13	121.76	115.62
8	DK	301	A1CIM	C14-C15-N2	4.13	121.76	115.62
8	DH	301	A1CIM	C14-C15-N2	4.13	121.75	115.62
8	DM	301	A1CIM	C14-C15-N2	4.13	121.75	115.62
8	DE	301	A1CIM	C14-C15-N2	4.13	121.75	115.62
8	DP	301	A1CIM	C14-C15-N2	4.13	121.75	115.62
8	DA	301	A1CIM	C14-C15-N2	4.13	121.75	115.62
8	DO	301	A1CIM	C14-C15-N2	4.13	121.75	115.62
8	DG	301	A1CIM	C14-C15-N2	4.13	121.75	115.62
8	C0	301	A1CIM	C14-C15-N2	4.13	121.75	115.62
8	DC	301	A1CIM	C3-C2-C7	-4.10	103.46	110.81
8	C0	301	A1CIM	C3-C2-C7	-4.10	103.47	110.81
8	DK	301	A1CIM	C3-C2-C7	-4.10	103.47	110.81
8	DB	301	A1CIM	C3-C2-C7	-4.10	103.47	110.81
8	DF	301	A1CIM	C3-C2-C7	-4.10	103.47	110.81
8	DO	301	A1CIM	C3-C2-C7	-4.10	103.47	110.81
8	DQ	301	A1CIM	C3-C2-C7	-4.10	103.47	110.81
8	DA	301	A1CIM	C3-C2-C7	-4.09	103.47	110.81
8	DD	301	A1CIM	C3-C2-C7	-4.09	103.47	110.81
8	DJ	301	A1CIM	C3-C2-C7	-4.09	103.47	110.81
8	DI	301	A1CIM	C3-C2-C7	-4.09	103.47	110.81
8	DP	301	A1CIM	C3-C2-C7	-4.09	103.47	110.81
8	DG	301	A1CIM	C3-C2-C7	-4.09	103.47	110.81
8	DL	301	A1CIM	C3-C2-C7	-4.09	103.47	110.81
8	DN	301	A1CIM	C3-C2-C7	-4.09	103.47	110.81
8	DE	301	A1CIM	C3-C2-C7	-4.09	103.47	110.81
8	DH	301	A1CIM	C3-C2-C7	-4.09	103.47	110.81
8	DM	301	A1CIM	C3-C2-C7	-4.09	103.47	110.81
8	C0	305	A1CIM	C14-C15-N2	3.29	120.50	115.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DP	305	A1CIM	C14-C15-N2	3.29	120.50	115.62
8	DG	305	A1CIM	C14-C15-N2	3.28	120.50	115.62
8	DB	305	A1CIM	C14-C15-N2	3.28	120.50	115.62
8	DH	305	A1CIM	C14-C15-N2	3.28	120.50	115.62
8	DO	305	A1CIM	C14-C15-N2	3.28	120.50	115.62
8	DA	305	A1CIM	C14-C15-N2	3.28	120.50	115.62
8	DC	305	A1CIM	C14-C15-N2	3.28	120.50	115.62
8	DK	305	A1CIM	C14-C15-N2	3.28	120.50	115.62
8	DN	305	A1CIM	C14-C15-N2	3.28	120.50	115.62
8	DJ	305	A1CIM	C14-C15-N2	3.28	120.50	115.62
8	DE	305	A1CIM	C14-C15-N2	3.28	120.50	115.62
8	DF	305	A1CIM	C14-C15-N2	3.28	120.50	115.62
8	DI	305	A1CIM	C14-C15-N2	3.28	120.50	115.62
8	DL	305	A1CIM	C14-C15-N2	3.28	120.50	115.62
8	DQ	305	A1CIM	C14-C15-N2	3.28	120.50	115.62
8	DM	305	A1CIM	C14-C15-N2	3.28	120.50	115.62
8	DD	305	A1CIM	C14-C15-N2	3.28	120.50	115.62
8	DE	302	A1CIM	C12-C13-C14	3.27	116.85	111.56
8	DP	302	A1CIM	C12-C13-C14	3.27	116.85	111.56
8	DA	302	A1CIM	C12-C13-C14	3.27	116.84	111.56
8	DC	302	A1CIM	C12-C13-C14	3.27	116.84	111.56
8	DF	302	A1CIM	C12-C13-C14	3.27	116.84	111.56
8	DN	302	A1CIM	C12-C13-C14	3.27	116.84	111.56
8	DO	302	A1CIM	C12-C13-C14	3.27	116.84	111.56
8	DB	302	A1CIM	C12-C13-C14	3.27	116.84	111.56
8	DG	302	A1CIM	C12-C13-C14	3.27	116.84	111.56
8	DI	302	A1CIM	C12-C13-C14	3.27	116.84	111.56
8	DD	302	A1CIM	C12-C13-C14	3.27	116.84	111.56
8	DK	302	A1CIM	C12-C13-C14	3.27	116.84	111.56
8	C0	302	A1CIM	C12-C13-C14	3.27	116.84	111.56
8	DQ	302	A1CIM	C12-C13-C14	3.27	116.84	111.56
8	DH	302	A1CIM	C12-C13-C14	3.27	116.84	111.56
8	DL	302	A1CIM	C12-C13-C14	3.27	116.84	111.56
8	DM	302	A1CIM	C12-C13-C14	3.27	116.84	111.56
8	DJ	302	A1CIM	C12-C13-C14	3.27	116.84	111.56
8	C0	304	A1CIM	C14-C15-N2	3.19	120.36	115.62
8	DG	304	A1CIM	C14-C15-N2	3.19	120.36	115.62
8	DI	304	A1CIM	C14-C15-N2	3.19	120.36	115.62
8	DL	304	A1CIM	C14-C15-N2	3.18	120.35	115.62
8	DQ	304	A1CIM	C14-C15-N2	3.18	120.35	115.62
8	DE	304	A1CIM	C14-C15-N2	3.18	120.35	115.62
8	DF	304	A1CIM	C14-C15-N2	3.18	120.35	115.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DJ	304	A1CIM	C14-C15-N2	3.18	120.35	115.62
8	DA	304	A1CIM	C14-C15-N2	3.18	120.35	115.62
8	DH	304	A1CIM	C14-C15-N2	3.18	120.35	115.62
8	DK	304	A1CIM	C14-C15-N2	3.18	120.35	115.62
8	DO	304	A1CIM	C14-C15-N2	3.18	120.35	115.62
8	DD	304	A1CIM	C14-C15-N2	3.18	120.35	115.62
8	DP	304	A1CIM	C14-C15-N2	3.18	120.35	115.62
8	DB	304	A1CIM	C14-C15-N2	3.18	120.35	115.62
8	DC	304	A1CIM	C14-C15-N2	3.18	120.35	115.62
8	DM	304	A1CIM	C14-C15-N2	3.18	120.35	115.62
8	DN	304	A1CIM	C14-C15-N2	3.18	120.34	115.62
8	DL	302	A1CIM	O5-C7-N1	-3.16	121.81	125.96
8	DN	302	A1CIM	O5-C7-N1	-3.16	121.81	125.96
8	DO	302	A1CIM	O5-C7-N1	-3.16	121.81	125.96
8	DG	302	A1CIM	O5-C7-N1	-3.16	121.81	125.96
8	C0	302	A1CIM	O5-C7-N1	-3.16	121.81	125.96
8	DF	302	A1CIM	O5-C7-N1	-3.16	121.81	125.96
8	DI	302	A1CIM	O5-C7-N1	-3.16	121.82	125.96
8	DJ	302	A1CIM	O5-C7-N1	-3.16	121.82	125.96
8	DK	302	A1CIM	O5-C7-N1	-3.16	121.82	125.96
8	DC	302	A1CIM	O5-C7-N1	-3.16	121.82	125.96
8	DP	302	A1CIM	O5-C7-N1	-3.16	121.82	125.96
8	DE	302	A1CIM	O5-C7-N1	-3.16	121.82	125.96
8	DH	302	A1CIM	O5-C7-N1	-3.16	121.82	125.96
8	DD	302	A1CIM	O5-C7-N1	-3.16	121.82	125.96
8	DM	302	A1CIM	O5-C7-N1	-3.16	121.82	125.96
8	DA	302	A1CIM	O5-C7-N1	-3.15	121.82	125.96
8	DB	302	A1CIM	O5-C7-N1	-3.15	121.82	125.96
8	DQ	302	A1CIM	O5-C7-N1	-3.15	121.82	125.96
8	DE	304	A1CIM	O7-C10-C14	3.09	113.70	109.95
8	DF	304	A1CIM	O7-C10-C14	3.09	113.70	109.95
8	DB	304	A1CIM	O7-C10-C14	3.09	113.70	109.95
8	DH	304	A1CIM	O7-C10-C14	3.09	113.70	109.95
8	DI	304	A1CIM	O7-C10-C14	3.09	113.70	109.95
8	DC	304	A1CIM	O7-C10-C14	3.09	113.70	109.95
8	DD	304	A1CIM	O7-C10-C14	3.09	113.70	109.95
8	DG	304	A1CIM	O7-C10-C14	3.09	113.70	109.95
8	C0	304	A1CIM	O7-C10-C14	3.09	113.70	109.95
8	DA	304	A1CIM	O7-C10-C14	3.09	113.70	109.95
8	DM	304	A1CIM	O7-C10-C14	3.09	113.70	109.95
8	DP	304	A1CIM	O7-C10-C14	3.09	113.70	109.95
8	DJ	304	A1CIM	O7-C10-C14	3.09	113.70	109.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DL	304	A1CIM	O7-C10-C14	3.09	113.70	109.95
8	DN	304	A1CIM	O7-C10-C14	3.09	113.70	109.95
8	DK	304	A1CIM	O7-C10-C14	3.09	113.70	109.95
8	DO	304	A1CIM	O7-C10-C14	3.09	113.70	109.95
8	DQ	304	A1CIM	O7-C10-C14	3.09	113.70	109.95
8	DM	303	A1CIM	O11-C16-C11	3.00	120.52	112.71
8	DK	303	A1CIM	O11-C16-C11	3.00	120.52	112.71
8	C0	303	A1CIM	O11-C16-C11	3.00	120.52	112.71
8	DE	303	A1CIM	O11-C16-C11	3.00	120.52	112.71
8	DQ	303	A1CIM	O11-C16-C11	3.00	120.52	112.71
8	DG	303	A1CIM	O11-C16-C11	3.00	120.52	112.71
8	DA	303	A1CIM	O11-C16-C11	3.00	120.52	112.71
8	DD	303	A1CIM	O11-C16-C11	3.00	120.52	112.71
8	DI	303	A1CIM	O11-C16-C11	3.00	120.52	112.71
8	DJ	303	A1CIM	O11-C16-C11	3.00	120.52	112.71
8	DP	303	A1CIM	O11-C16-C11	3.00	120.52	112.71
8	DB	303	A1CIM	O11-C16-C11	3.00	120.52	112.71
8	DF	303	A1CIM	O11-C16-C11	3.00	120.52	112.71
8	DH	303	A1CIM	O11-C16-C11	3.00	120.52	112.71
8	DL	303	A1CIM	O11-C16-C11	3.00	120.52	112.71
8	DO	303	A1CIM	O11-C16-C11	3.00	120.52	112.71
8	DC	303	A1CIM	O11-C16-C11	3.00	120.52	112.71
8	DN	303	A1CIM	O11-C16-C11	3.00	120.51	112.71
8	DH	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	DA	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	DG	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	DL	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	DP	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	C0	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	DB	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	DD	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	DK	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	DN	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	DE	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	DM	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	DQ	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	DI	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	DO	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	DC	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	DF	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	DJ	301	A1CIM	O5-C7-C2	-2.90	115.05	119.58
8	DC	302	A1CIM	C14-C15-N2	2.81	119.79	115.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DI	302	A1CIM	C14-C15-N2	2.81	119.79	115.62
8	DN	302	A1CIM	C14-C15-N2	2.81	119.79	115.62
8	DE	302	A1CIM	C14-C15-N2	2.81	119.79	115.62
8	DK	302	A1CIM	C14-C15-N2	2.81	119.79	115.62
8	DB	302	A1CIM	C14-C15-N2	2.81	119.79	115.62
8	DJ	302	A1CIM	C14-C15-N2	2.81	119.79	115.62
8	DM	302	A1CIM	C14-C15-N2	2.81	119.79	115.62
8	DP	302	A1CIM	C14-C15-N2	2.81	119.79	115.62
8	DL	302	A1CIM	C14-C15-N2	2.81	119.79	115.62
8	DD	302	A1CIM	C14-C15-N2	2.81	119.79	115.62
8	DH	302	A1CIM	C14-C15-N2	2.81	119.79	115.62
8	DF	302	A1CIM	C14-C15-N2	2.81	119.79	115.62
8	C0	302	A1CIM	C14-C15-N2	2.80	119.79	115.62
8	DA	302	A1CIM	C14-C15-N2	2.80	119.79	115.62
8	DO	302	A1CIM	C14-C15-N2	2.80	119.79	115.62
8	DG	302	A1CIM	C14-C15-N2	2.80	119.79	115.62
8	DQ	302	A1CIM	C14-C15-N2	2.80	119.78	115.62
8	DA	301	A1CIM	O11-C16-C11	2.78	119.94	112.71
8	DM	301	A1CIM	O11-C16-C11	2.78	119.94	112.71
8	DD	301	A1CIM	O11-C16-C11	2.78	119.94	112.71
8	DE	301	A1CIM	O11-C16-C11	2.78	119.94	112.71
8	DK	301	A1CIM	O11-C16-C11	2.78	119.94	112.71
8	DP	301	A1CIM	O11-C16-C11	2.78	119.94	112.71
8	DB	301	A1CIM	O11-C16-C11	2.78	119.94	112.71
8	C0	301	A1CIM	O11-C16-C11	2.78	119.93	112.71
8	DL	301	A1CIM	O11-C16-C11	2.78	119.93	112.71
8	DN	301	A1CIM	O11-C16-C11	2.78	119.93	112.71
8	DI	301	A1CIM	O11-C16-C11	2.78	119.93	112.71
8	DC	301	A1CIM	O11-C16-C11	2.78	119.93	112.71
8	DF	301	A1CIM	O11-C16-C11	2.78	119.93	112.71
8	DJ	301	A1CIM	O11-C16-C11	2.78	119.93	112.71
8	DO	301	A1CIM	O11-C16-C11	2.78	119.93	112.71
8	DH	301	A1CIM	O11-C16-C11	2.78	119.93	112.71
8	DQ	301	A1CIM	O11-C16-C11	2.78	119.93	112.71
8	DG	301	A1CIM	O11-C16-C11	2.78	119.93	112.71
8	DN	302	A1CIM	O11-C16-C11	2.63	119.56	112.71
8	DB	302	A1CIM	O11-C16-C11	2.63	119.55	112.71
8	DG	302	A1CIM	O11-C16-C11	2.63	119.55	112.71
8	DK	302	A1CIM	O11-C16-C11	2.63	119.55	112.71
8	C0	302	A1CIM	O11-C16-C11	2.63	119.55	112.71
8	DA	302	A1CIM	O11-C16-C11	2.63	119.55	112.71
8	DP	302	A1CIM	O11-C16-C11	2.63	119.55	112.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DC	302	A1CIM	O11-C16-C11	2.63	119.55	112.71
8	DJ	302	A1CIM	O11-C16-C11	2.63	119.55	112.71
8	DM	302	A1CIM	O11-C16-C11	2.63	119.55	112.71
8	DE	302	A1CIM	O11-C16-C11	2.63	119.55	112.71
8	DO	302	A1CIM	O11-C16-C11	2.63	119.55	112.71
8	DQ	302	A1CIM	O11-C16-C11	2.63	119.55	112.71
8	DL	302	A1CIM	O11-C16-C11	2.63	119.55	112.71
8	DF	302	A1CIM	O11-C16-C11	2.63	119.55	112.71
8	DH	302	A1CIM	O11-C16-C11	2.63	119.55	112.71
8	DI	302	A1CIM	O11-C16-C11	2.63	119.55	112.71
8	DD	302	A1CIM	O11-C16-C11	2.63	119.55	112.71
8	DK	304	A1CIM	C12-C13-C14	2.62	115.79	111.56
8	DE	304	A1CIM	C12-C13-C14	2.62	115.79	111.56
8	DF	304	A1CIM	C12-C13-C14	2.62	115.79	111.56
8	DM	304	A1CIM	C12-C13-C14	2.62	115.79	111.56
8	DP	304	A1CIM	C12-C13-C14	2.62	115.79	111.56
8	DB	304	A1CIM	C12-C13-C14	2.62	115.79	111.56
8	DI	304	A1CIM	C12-C13-C14	2.62	115.79	111.56
8	DN	304	A1CIM	C12-C13-C14	2.62	115.79	111.56
8	C0	304	A1CIM	C12-C13-C14	2.61	115.79	111.56
8	DJ	304	A1CIM	C12-C13-C14	2.61	115.79	111.56
8	DL	304	A1CIM	C12-C13-C14	2.61	115.79	111.56
8	DC	304	A1CIM	C12-C13-C14	2.61	115.78	111.56
8	DD	304	A1CIM	C12-C13-C14	2.61	115.78	111.56
8	DA	304	A1CIM	C12-C13-C14	2.61	115.78	111.56
8	DG	304	A1CIM	C12-C13-C14	2.61	115.78	111.56
8	DH	304	A1CIM	C12-C13-C14	2.61	115.78	111.56
8	DO	304	A1CIM	C12-C13-C14	2.61	115.78	111.56
8	DQ	304	A1CIM	C12-C13-C14	2.61	115.78	111.56
8	DH	302	A1CIM	C10-O7-C11	2.58	118.45	114.75
8	DF	302	A1CIM	C10-O7-C11	2.58	118.45	114.75
8	DO	302	A1CIM	C10-O7-C11	2.58	118.45	114.75
8	DC	302	A1CIM	C10-O7-C11	2.58	118.45	114.75
8	DD	302	A1CIM	C10-O7-C11	2.58	118.45	114.75
8	DI	302	A1CIM	C10-O7-C11	2.58	118.45	114.75
8	DN	302	A1CIM	C10-O7-C11	2.58	118.44	114.75
8	DP	302	A1CIM	C10-O7-C11	2.58	118.44	114.75
8	DQ	302	A1CIM	C10-O7-C11	2.58	118.44	114.75
8	C0	302	A1CIM	C10-O7-C11	2.58	118.44	114.75
8	DA	302	A1CIM	C10-O7-C11	2.58	118.44	114.75
8	DB	302	A1CIM	C10-O7-C11	2.58	118.44	114.75
8	DE	302	A1CIM	C10-O7-C11	2.58	118.44	114.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DK	302	A1CIM	C10-O7-C11	2.58	118.44	114.75
8	DM	302	A1CIM	C10-O7-C11	2.58	118.44	114.75
8	DJ	302	A1CIM	C10-O7-C11	2.57	118.44	114.75
8	DG	302	A1CIM	C10-O7-C11	2.57	118.44	114.75
8	DL	302	A1CIM	C10-O7-C11	2.57	118.44	114.75
8	DG	305	A1CIM	C10-O7-C11	2.55	118.41	114.75
8	DE	305	A1CIM	C10-O7-C11	2.55	118.41	114.75
8	DK	305	A1CIM	C10-O7-C11	2.55	118.41	114.75
8	DQ	305	A1CIM	C10-O7-C11	2.55	118.41	114.75
8	DA	305	A1CIM	C10-O7-C11	2.55	118.41	114.75
8	DI	305	A1CIM	C10-O7-C11	2.55	118.41	114.75
8	DJ	305	A1CIM	C10-O7-C11	2.55	118.41	114.75
8	DG	305	A1CIM	O11-C16-C11	2.55	119.34	112.71
8	DN	305	A1CIM	C10-O7-C11	2.55	118.41	114.75
8	DP	305	A1CIM	C10-O7-C11	2.55	118.41	114.75
8	DF	305	A1CIM	C10-O7-C11	2.55	118.41	114.75
8	DH	305	A1CIM	C10-O7-C11	2.55	118.41	114.75
8	DE	305	A1CIM	O11-C16-C11	2.55	119.34	112.71
8	DB	305	A1CIM	C10-O7-C11	2.55	118.41	114.75
8	DD	305	A1CIM	C10-O7-C11	2.55	118.41	114.75
8	DO	305	A1CIM	C10-O7-C11	2.55	118.41	114.75
8	DD	305	A1CIM	O11-C16-C11	2.55	119.34	112.71
8	DN	305	A1CIM	O11-C16-C11	2.55	119.34	112.71
8	DB	305	A1CIM	O11-C16-C11	2.55	119.34	112.71
8	DP	305	A1CIM	O11-C16-C11	2.55	119.34	112.71
8	C0	305	A1CIM	C10-O7-C11	2.55	118.40	114.75
8	DM	305	A1CIM	C10-O7-C11	2.55	118.40	114.75
8	DH	305	A1CIM	O11-C16-C11	2.55	119.33	112.71
8	DK	305	A1CIM	O11-C16-C11	2.55	119.33	112.71
8	C0	305	A1CIM	O11-C16-C11	2.55	119.33	112.71
8	DC	305	A1CIM	O11-C16-C11	2.55	119.33	112.71
8	DL	305	A1CIM	C10-O7-C11	2.55	118.40	114.75
8	DA	305	A1CIM	O11-C16-C11	2.55	119.33	112.71
8	DF	305	A1CIM	O11-C16-C11	2.55	119.33	112.71
8	DI	305	A1CIM	O11-C16-C11	2.55	119.33	112.71
8	DJ	305	A1CIM	O11-C16-C11	2.55	119.33	112.71
8	DL	305	A1CIM	O11-C16-C11	2.55	119.33	112.71
8	DM	305	A1CIM	O11-C16-C11	2.55	119.33	112.71
8	DQ	305	A1CIM	O11-C16-C11	2.55	119.33	112.71
8	DO	305	A1CIM	O11-C16-C11	2.55	119.33	112.71
8	DC	305	A1CIM	C10-O7-C11	2.55	118.40	114.75
8	C0	303	A1CIM	O9-C15-N2	-2.54	118.55	123.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DC	303	A1CIM	O9-C15-N2	-2.54	118.55	123.04
8	DL	303	A1CIM	O9-C15-N2	-2.54	118.55	123.04
8	DD	303	A1CIM	O9-C15-N2	-2.54	118.55	123.04
8	DI	303	A1CIM	O9-C15-N2	-2.54	118.55	123.04
8	DK	303	A1CIM	O9-C15-N2	-2.54	118.55	123.04
8	DM	303	A1CIM	O9-C15-N2	-2.54	118.55	123.04
8	DE	303	A1CIM	O9-C15-N2	-2.54	118.55	123.04
8	DH	303	A1CIM	O9-C15-N2	-2.54	118.55	123.04
8	DQ	303	A1CIM	O9-C15-N2	-2.54	118.55	123.04
8	DG	303	A1CIM	O9-C15-N2	-2.54	118.55	123.04
8	DO	303	A1CIM	O9-C15-N2	-2.54	118.55	123.04
8	DN	303	A1CIM	O9-C15-N2	-2.54	118.56	123.04
8	DJ	303	A1CIM	O9-C15-N2	-2.54	118.56	123.04
8	DA	303	A1CIM	O9-C15-N2	-2.54	118.56	123.04
8	DF	303	A1CIM	O9-C15-N2	-2.54	118.56	123.04
8	DB	303	A1CIM	O9-C15-N2	-2.54	118.56	123.04
8	DP	303	A1CIM	O9-C15-N2	-2.54	118.56	123.04
8	DF	303	A1CIM	C9-C8-C10	-2.43	108.33	111.47
8	C0	303	A1CIM	C9-C8-C10	-2.43	108.33	111.47
8	DC	303	A1CIM	C9-C8-C10	-2.43	108.33	111.47
8	DE	303	A1CIM	C9-C8-C10	-2.43	108.33	111.47
8	DG	303	A1CIM	C9-C8-C10	-2.43	108.33	111.47
8	DN	303	A1CIM	C9-C8-C10	-2.43	108.33	111.47
8	DG	303	A1CIM	O5-C7-N1	-2.43	118.08	123.15
8	DH	303	A1CIM	C9-C8-C10	-2.43	108.33	111.47
8	DQ	303	A1CIM	C9-C8-C10	-2.43	108.33	111.47
8	DD	303	A1CIM	O5-C7-N1	-2.43	118.08	123.15
8	C0	303	A1CIM	O5-C7-N1	-2.43	118.08	123.15
8	DM	303	A1CIM	O5-C7-N1	-2.43	118.08	123.15
8	DQ	303	A1CIM	O5-C7-N1	-2.43	118.08	123.15
8	DJ	303	A1CIM	C9-C8-C10	-2.43	108.34	111.47
8	DK	303	A1CIM	C9-C8-C10	-2.43	108.34	111.47
8	DL	303	A1CIM	C9-C8-C10	-2.43	108.34	111.47
8	DO	303	A1CIM	C9-C8-C10	-2.43	108.34	111.47
8	DB	303	A1CIM	O5-C7-N1	-2.43	118.08	123.15
8	DC	303	A1CIM	O5-C7-N1	-2.43	118.08	123.15
8	DK	303	A1CIM	O5-C7-N1	-2.43	118.08	123.15
8	DL	303	A1CIM	O5-C7-N1	-2.43	118.08	123.15
8	DA	303	A1CIM	C9-C8-C10	-2.43	108.34	111.47
8	DP	303	A1CIM	C9-C8-C10	-2.43	108.34	111.47
8	DA	303	A1CIM	O5-C7-N1	-2.43	118.08	123.15
8	DH	303	A1CIM	O5-C7-N1	-2.43	118.08	123.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DF	303	A1CIM	O5-C7-N1	-2.43	118.08	123.15
8	DB	303	A1CIM	C9-C8-C10	-2.43	108.34	111.47
8	DD	303	A1CIM	C9-C8-C10	-2.43	108.34	111.47
8	DI	303	A1CIM	C9-C8-C10	-2.43	108.34	111.47
8	DN	303	A1CIM	O5-C7-N1	-2.43	118.08	123.15
8	DO	303	A1CIM	O5-C7-N1	-2.43	118.08	123.15
8	DI	303	A1CIM	O5-C7-N1	-2.43	118.08	123.15
8	DE	303	A1CIM	O5-C7-N1	-2.42	118.09	123.15
8	DJ	303	A1CIM	O5-C7-N1	-2.42	118.09	123.15
8	DM	303	A1CIM	C9-C8-C10	-2.42	108.34	111.47
8	DP	303	A1CIM	O5-C7-N1	-2.42	118.09	123.15
8	DD	304	A1CIM	O11-C16-C11	2.35	118.82	112.71
8	DF	304	A1CIM	O11-C16-C11	2.35	118.81	112.71
8	DQ	304	A1CIM	O11-C16-C11	2.35	118.81	112.71
8	DB	304	A1CIM	O11-C16-C11	2.35	118.81	112.71
8	DH	304	A1CIM	O11-C16-C11	2.35	118.81	112.71
8	DN	304	A1CIM	O11-C16-C11	2.35	118.81	112.71
8	DO	304	A1CIM	O11-C16-C11	2.35	118.81	112.71
8	DA	304	A1CIM	O11-C16-C11	2.35	118.81	112.71
8	C0	304	A1CIM	O11-C16-C11	2.35	118.81	112.71
8	DC	304	A1CIM	O11-C16-C11	2.35	118.81	112.71
8	DK	304	A1CIM	O11-C16-C11	2.35	118.81	112.71
8	DL	304	A1CIM	O11-C16-C11	2.35	118.81	112.71
8	DG	304	A1CIM	O11-C16-C11	2.35	118.81	112.71
8	DI	304	A1CIM	O11-C16-C11	2.35	118.81	112.71
8	DJ	304	A1CIM	O11-C16-C11	2.35	118.81	112.71
8	DM	304	A1CIM	O11-C16-C11	2.35	118.81	112.71
8	DP	304	A1CIM	O11-C16-C11	2.35	118.81	112.71
8	DE	304	A1CIM	O11-C16-C11	2.34	118.81	112.71
8	DF	304	A1CIM	O11-C16-O10	-2.34	118.77	124.08
8	DD	304	A1CIM	O11-C16-O10	-2.34	118.77	124.08
8	DJ	304	A1CIM	O11-C16-O10	-2.34	118.77	124.08
8	DO	304	A1CIM	O11-C16-O10	-2.34	118.77	124.08
8	DB	304	A1CIM	O11-C16-O10	-2.34	118.77	124.08
8	DH	304	A1CIM	O11-C16-O10	-2.34	118.77	124.08
8	DI	304	A1CIM	O11-C16-O10	-2.34	118.77	124.08
8	DE	304	A1CIM	O11-C16-O10	-2.34	118.77	124.08
8	C0	304	A1CIM	O11-C16-O10	-2.34	118.77	124.08
8	DM	304	A1CIM	O11-C16-O10	-2.34	118.77	124.08
8	DC	304	A1CIM	O11-C16-O10	-2.34	118.78	124.08
8	DG	304	A1CIM	O11-C16-O10	-2.34	118.78	124.08
8	DN	304	A1CIM	O11-C16-O10	-2.34	118.78	124.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DP	304	A1CIM	O11-C16-O10	-2.34	118.78	124.08
8	DK	304	A1CIM	O11-C16-O10	-2.34	118.78	124.08
8	DL	304	A1CIM	O11-C16-O10	-2.34	118.78	124.08
8	DQ	304	A1CIM	O11-C16-O10	-2.34	118.78	124.08
8	DA	304	A1CIM	O11-C16-O10	-2.34	118.78	124.08
8	DA	305	A1CIM	O5-C7-N1	-2.32	122.91	125.96
8	DD	305	A1CIM	O5-C7-N1	-2.32	122.92	125.96
8	DE	305	A1CIM	O5-C7-N1	-2.32	122.92	125.96
8	DK	305	A1CIM	O5-C7-N1	-2.32	122.92	125.96
8	DH	305	A1CIM	O5-C7-N1	-2.32	122.92	125.96
8	DF	305	A1CIM	O5-C7-N1	-2.32	122.92	125.96
8	DJ	305	A1CIM	O5-C7-N1	-2.32	122.92	125.96
8	DP	305	A1CIM	O5-C7-N1	-2.32	122.92	125.96
8	DI	305	A1CIM	O5-C7-N1	-2.32	122.92	125.96
8	DN	305	A1CIM	O5-C7-N1	-2.32	122.92	125.96
8	DQ	305	A1CIM	O5-C7-N1	-2.32	122.92	125.96
8	C0	305	A1CIM	O5-C7-N1	-2.32	122.92	125.96
8	DG	305	A1CIM	O5-C7-N1	-2.32	122.92	125.96
8	DO	305	A1CIM	O5-C7-N1	-2.32	122.92	125.96
8	DC	305	A1CIM	O5-C7-N1	-2.32	122.92	125.96
8	DL	305	A1CIM	O5-C7-N1	-2.32	122.92	125.96
8	DM	305	A1CIM	O5-C7-N1	-2.32	122.92	125.96
8	DB	305	A1CIM	O5-C7-N1	-2.31	122.92	125.96
8	DB	305	A1CIM	O8-C13-C12	2.26	115.49	109.86
8	DA	305	A1CIM	O8-C13-C12	2.26	115.48	109.86
8	DE	305	A1CIM	O8-C13-C12	2.26	115.48	109.86
8	DJ	305	A1CIM	O8-C13-C12	2.26	115.48	109.86
8	DP	305	A1CIM	O8-C13-C12	2.26	115.48	109.86
8	DD	305	A1CIM	O8-C13-C12	2.26	115.48	109.86
8	DG	305	A1CIM	O8-C13-C12	2.26	115.48	109.86
8	DK	305	A1CIM	O8-C13-C12	2.26	115.48	109.86
8	DL	305	A1CIM	O8-C13-C12	2.26	115.48	109.86
8	DM	305	A1CIM	O8-C13-C12	2.26	115.48	109.86
8	DC	305	A1CIM	O8-C13-C12	2.26	115.48	109.86
8	DI	305	A1CIM	O8-C13-C12	2.26	115.48	109.86
8	DO	305	A1CIM	O8-C13-C12	2.26	115.48	109.86
8	DQ	305	A1CIM	O8-C13-C12	2.26	115.48	109.86
8	C0	305	A1CIM	O8-C13-C12	2.26	115.48	109.86
8	DF	305	A1CIM	O8-C13-C12	2.26	115.48	109.86
8	DH	305	A1CIM	O8-C13-C12	2.26	115.48	109.86
8	DN	305	A1CIM	O8-C13-C12	2.26	115.48	109.86
8	DG	305	A1CIM	O11-C16-O10	-2.24	118.99	124.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DB	305	A1CIM	O11-C16-O10	-2.24	118.99	124.08
8	DL	305	A1CIM	O11-C16-O10	-2.24	118.99	124.08
8	C0	305	A1CIM	O11-C16-O10	-2.24	119.00	124.08
8	DJ	305	A1CIM	O11-C16-O10	-2.24	119.00	124.08
8	DN	305	A1CIM	O11-C16-O10	-2.24	119.00	124.08
8	DP	305	A1CIM	O11-C16-O10	-2.24	119.00	124.08
8	DC	305	A1CIM	O11-C16-O10	-2.24	119.00	124.08
8	DE	305	A1CIM	O11-C16-O10	-2.24	119.00	124.08
8	DF	305	A1CIM	O11-C16-O10	-2.24	119.00	124.08
8	DH	305	A1CIM	O11-C16-O10	-2.24	119.00	124.08
8	DD	305	A1CIM	O11-C16-O10	-2.24	119.00	124.08
8	DA	305	A1CIM	O11-C16-O10	-2.24	119.00	124.08
8	DK	305	A1CIM	O11-C16-O10	-2.24	119.00	124.08
8	DM	305	A1CIM	O11-C16-O10	-2.24	119.00	124.08
8	DQ	305	A1CIM	O11-C16-O10	-2.24	119.00	124.08
8	DI	305	A1CIM	O11-C16-O10	-2.24	119.00	124.08
8	DO	305	A1CIM	O11-C16-O10	-2.24	119.00	124.08
8	DD	301	A1CIM	O9-C15-N2	-2.23	119.10	123.04
8	DH	301	A1CIM	O9-C15-N2	-2.23	119.10	123.04
8	DK	301	A1CIM	O9-C15-N2	-2.23	119.10	123.04
8	DC	301	A1CIM	O9-C15-N2	-2.23	119.10	123.04
8	DQ	301	A1CIM	O9-C15-N2	-2.23	119.10	123.04
8	DL	301	A1CIM	O9-C15-N2	-2.23	119.10	123.04
8	DP	301	A1CIM	O9-C15-N2	-2.23	119.10	123.04
8	DI	301	A1CIM	O9-C15-N2	-2.23	119.10	123.04
8	DB	301	A1CIM	O9-C15-N2	-2.23	119.10	123.04
8	DF	301	A1CIM	O9-C15-N2	-2.23	119.10	123.04
8	C0	301	A1CIM	O9-C15-N2	-2.23	119.11	123.04
8	DE	301	A1CIM	O9-C15-N2	-2.23	119.11	123.04
8	DG	301	A1CIM	O9-C15-N2	-2.23	119.11	123.04
8	DM	301	A1CIM	O9-C15-N2	-2.23	119.11	123.04
8	DA	301	A1CIM	O9-C15-N2	-2.23	119.11	123.04
8	DN	301	A1CIM	O9-C15-N2	-2.23	119.11	123.04
8	DJ	301	A1CIM	O9-C15-N2	-2.23	119.11	123.04
8	DO	301	A1CIM	O9-C15-N2	-2.23	119.11	123.04
8	C0	302	A1CIM	O11-C16-O10	-2.04	119.45	124.08
8	DM	302	A1CIM	O11-C16-O10	-2.04	119.45	124.08
8	DN	302	A1CIM	O11-C16-O10	-2.04	119.45	124.08
8	DA	302	A1CIM	O11-C16-O10	-2.04	119.45	124.08
8	DC	302	A1CIM	O11-C16-O10	-2.04	119.45	124.08
8	DD	302	A1CIM	O11-C16-O10	-2.04	119.45	124.08
8	DE	302	A1CIM	O11-C16-O10	-2.04	119.45	124.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	DK	302	A1CIM	O11-C16-O10	-2.04	119.45	124.08
8	DB	302	A1CIM	O11-C16-O10	-2.04	119.45	124.08
8	DG	302	A1CIM	O11-C16-O10	-2.04	119.45	124.08
8	DJ	302	A1CIM	O11-C16-O10	-2.04	119.45	124.08
8	DQ	302	A1CIM	O11-C16-O10	-2.04	119.45	124.08
8	DF	302	A1CIM	O11-C16-O10	-2.04	119.45	124.08
8	DH	302	A1CIM	O11-C16-O10	-2.04	119.45	124.08
8	DO	302	A1CIM	O11-C16-O10	-2.04	119.45	124.08
8	DL	302	A1CIM	O11-C16-O10	-2.04	119.46	124.08
8	DP	302	A1CIM	O11-C16-O10	-2.04	119.46	124.08
8	DI	302	A1CIM	O11-C16-O10	-2.04	119.46	124.08

There are no chirality outliers.

All (810) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C0	301	A1CIM	C3-C2-O1-C1
8	C0	301	A1CIM	C7-C2-O1-C1
8	C0	301	A1CIM	C4-C5-C6-O4
8	C0	301	A1CIM	C2-C7-N1-C8
8	C0	301	A1CIM	O5-C7-N1-C8
8	C0	301	A1CIM	C14-C10-C8-C9
8	C0	301	A1CIM	O7-C10-C8-C9
8	C0	301	A1CIM	C14-C10-C8-O6
8	C0	301	A1CIM	O7-C10-C8-O6
8	C0	303	A1CIM	C3-C4-C5-C6
8	C0	303	A1CIM	C3-C4-C5-O3
8	C0	303	A1CIM	O2-C4-C5-C6
8	C0	303	A1CIM	C2-C7-N1-C8
8	C0	303	A1CIM	O5-C7-N1-C8
8	C0	303	A1CIM	C14-C10-C8-C9
8	C0	303	A1CIM	O7-C10-C8-C9
8	C0	303	A1CIM	C14-C10-C8-O6
8	C0	303	A1CIM	O7-C10-C8-O6
8	C0	303	A1CIM	C9-C8-N1-C7
8	C0	304	A1CIM	C3-C2-C7-N1
8	C0	304	A1CIM	C3-C2-C7-O5
8	C0	304	A1CIM	O1-C2-C7-N1
8	C0	304	A1CIM	C3-C2-O1-C1
8	C0	304	A1CIM	C3-C4-C5-C6
8	C0	304	A1CIM	C3-C4-C5-O3
8	C0	304	A1CIM	O2-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	C0	304	A1CIM	O2-C4-C5-O3
8	C0	304	A1CIM	C14-C10-C8-C9
8	C0	304	A1CIM	O7-C10-C8-C9
8	C0	304	A1CIM	C14-C10-C8-O6
8	C0	304	A1CIM	O7-C10-C8-O6
8	DA	301	A1CIM	C3-C2-O1-C1
8	DA	301	A1CIM	C7-C2-O1-C1
8	DA	301	A1CIM	C4-C5-C6-O4
8	DA	301	A1CIM	C2-C7-N1-C8
8	DA	301	A1CIM	O5-C7-N1-C8
8	DA	301	A1CIM	C14-C10-C8-C9
8	DA	301	A1CIM	O7-C10-C8-C9
8	DA	301	A1CIM	C14-C10-C8-O6
8	DA	301	A1CIM	O7-C10-C8-O6
8	DA	303	A1CIM	C3-C4-C5-C6
8	DA	303	A1CIM	C3-C4-C5-O3
8	DA	303	A1CIM	O2-C4-C5-C6
8	DA	303	A1CIM	C2-C7-N1-C8
8	DA	303	A1CIM	O5-C7-N1-C8
8	DA	303	A1CIM	C14-C10-C8-C9
8	DA	303	A1CIM	O7-C10-C8-C9
8	DA	303	A1CIM	C14-C10-C8-O6
8	DA	303	A1CIM	O7-C10-C8-O6
8	DA	303	A1CIM	C9-C8-N1-C7
8	DA	304	A1CIM	C3-C2-C7-N1
8	DA	304	A1CIM	C3-C2-C7-O5
8	DA	304	A1CIM	O1-C2-C7-N1
8	DA	304	A1CIM	C3-C2-O1-C1
8	DA	304	A1CIM	C3-C4-C5-C6
8	DA	304	A1CIM	C3-C4-C5-O3
8	DA	304	A1CIM	O2-C4-C5-C6
8	DA	304	A1CIM	O2-C4-C5-O3
8	DA	304	A1CIM	C14-C10-C8-C9
8	DA	304	A1CIM	O7-C10-C8-C9
8	DA	304	A1CIM	C14-C10-C8-O6
8	DA	304	A1CIM	O7-C10-C8-O6
8	DB	301	A1CIM	C3-C2-O1-C1
8	DB	301	A1CIM	C7-C2-O1-C1
8	DB	301	A1CIM	C4-C5-C6-O4
8	DB	301	A1CIM	C2-C7-N1-C8
8	DB	301	A1CIM	O5-C7-N1-C8
8	DB	301	A1CIM	C14-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	DB	301	A1CIM	O7-C10-C8-C9
8	DB	301	A1CIM	C14-C10-C8-O6
8	DB	301	A1CIM	O7-C10-C8-O6
8	DB	303	A1CIM	C3-C4-C5-C6
8	DB	303	A1CIM	C3-C4-C5-O3
8	DB	303	A1CIM	O2-C4-C5-C6
8	DB	303	A1CIM	C2-C7-N1-C8
8	DB	303	A1CIM	O5-C7-N1-C8
8	DB	303	A1CIM	C14-C10-C8-C9
8	DB	303	A1CIM	O7-C10-C8-C9
8	DB	303	A1CIM	C14-C10-C8-O6
8	DB	303	A1CIM	O7-C10-C8-O6
8	DB	303	A1CIM	C9-C8-N1-C7
8	DB	304	A1CIM	C3-C2-C7-N1
8	DB	304	A1CIM	C3-C2-C7-O5
8	DB	304	A1CIM	O1-C2-C7-N1
8	DB	304	A1CIM	C3-C2-O1-C1
8	DB	304	A1CIM	C3-C4-C5-C6
8	DB	304	A1CIM	C3-C4-C5-O3
8	DB	304	A1CIM	O2-C4-C5-C6
8	DB	304	A1CIM	O2-C4-C5-O3
8	DB	304	A1CIM	C14-C10-C8-C9
8	DB	304	A1CIM	O7-C10-C8-C9
8	DB	304	A1CIM	C14-C10-C8-O6
8	DB	304	A1CIM	O7-C10-C8-O6
8	DC	301	A1CIM	C3-C2-O1-C1
8	DC	301	A1CIM	C7-C2-O1-C1
8	DC	301	A1CIM	C4-C5-C6-O4
8	DC	301	A1CIM	C2-C7-N1-C8
8	DC	301	A1CIM	O5-C7-N1-C8
8	DC	301	A1CIM	C14-C10-C8-C9
8	DC	301	A1CIM	O7-C10-C8-C9
8	DC	301	A1CIM	C14-C10-C8-O6
8	DC	301	A1CIM	O7-C10-C8-O6
8	DC	303	A1CIM	C3-C4-C5-C6
8	DC	303	A1CIM	C3-C4-C5-O3
8	DC	303	A1CIM	O2-C4-C5-C6
8	DC	303	A1CIM	C2-C7-N1-C8
8	DC	303	A1CIM	O5-C7-N1-C8
8	DC	303	A1CIM	C14-C10-C8-C9
8	DC	303	A1CIM	O7-C10-C8-C9
8	DC	303	A1CIM	C14-C10-C8-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	DC	303	A1CIM	O7-C10-C8-O6
8	DC	303	A1CIM	C9-C8-N1-C7
8	DC	304	A1CIM	C3-C2-C7-N1
8	DC	304	A1CIM	C3-C2-C7-O5
8	DC	304	A1CIM	O1-C2-C7-N1
8	DC	304	A1CIM	C3-C2-O1-C1
8	DC	304	A1CIM	C3-C4-C5-C6
8	DC	304	A1CIM	C3-C4-C5-O3
8	DC	304	A1CIM	O2-C4-C5-C6
8	DC	304	A1CIM	O2-C4-C5-O3
8	DC	304	A1CIM	C14-C10-C8-C9
8	DC	304	A1CIM	O7-C10-C8-C9
8	DC	304	A1CIM	C14-C10-C8-O6
8	DC	304	A1CIM	O7-C10-C8-O6
8	DD	301	A1CIM	C3-C2-O1-C1
8	DD	301	A1CIM	C7-C2-O1-C1
8	DD	301	A1CIM	C4-C5-C6-O4
8	DD	301	A1CIM	C2-C7-N1-C8
8	DD	301	A1CIM	O5-C7-N1-C8
8	DD	301	A1CIM	C14-C10-C8-C9
8	DD	301	A1CIM	O7-C10-C8-C9
8	DD	301	A1CIM	C14-C10-C8-O6
8	DD	301	A1CIM	O7-C10-C8-O6
8	DD	303	A1CIM	C3-C4-C5-C6
8	DD	303	A1CIM	C3-C4-C5-O3
8	DD	303	A1CIM	O2-C4-C5-C6
8	DD	303	A1CIM	C2-C7-N1-C8
8	DD	303	A1CIM	O5-C7-N1-C8
8	DD	303	A1CIM	C14-C10-C8-C9
8	DD	303	A1CIM	O7-C10-C8-C9
8	DD	303	A1CIM	C14-C10-C8-O6
8	DD	303	A1CIM	O7-C10-C8-O6
8	DD	303	A1CIM	C9-C8-N1-C7
8	DD	304	A1CIM	C3-C2-C7-N1
8	DD	304	A1CIM	C3-C2-C7-O5
8	DD	304	A1CIM	O1-C2-C7-N1
8	DD	304	A1CIM	C3-C2-O1-C1
8	DD	304	A1CIM	C3-C4-C5-C6
8	DD	304	A1CIM	C3-C4-C5-O3
8	DD	304	A1CIM	O2-C4-C5-C6
8	DD	304	A1CIM	O2-C4-C5-O3
8	DD	304	A1CIM	C14-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	DD	304	A1CIM	O7-C10-C8-C9
8	DD	304	A1CIM	C14-C10-C8-O6
8	DD	304	A1CIM	O7-C10-C8-O6
8	DE	301	A1CIM	C3-C2-O1-C1
8	DE	301	A1CIM	C7-C2-O1-C1
8	DE	301	A1CIM	C4-C5-C6-O4
8	DE	301	A1CIM	C2-C7-N1-C8
8	DE	301	A1CIM	O5-C7-N1-C8
8	DE	301	A1CIM	C14-C10-C8-C9
8	DE	301	A1CIM	O7-C10-C8-C9
8	DE	301	A1CIM	C14-C10-C8-O6
8	DE	301	A1CIM	O7-C10-C8-O6
8	DE	303	A1CIM	C3-C4-C5-C6
8	DE	303	A1CIM	C3-C4-C5-O3
8	DE	303	A1CIM	O2-C4-C5-C6
8	DE	303	A1CIM	C2-C7-N1-C8
8	DE	303	A1CIM	O5-C7-N1-C8
8	DE	303	A1CIM	C14-C10-C8-C9
8	DE	303	A1CIM	O7-C10-C8-C9
8	DE	303	A1CIM	C14-C10-C8-O6
8	DE	303	A1CIM	O7-C10-C8-O6
8	DE	303	A1CIM	C9-C8-N1-C7
8	DE	304	A1CIM	C3-C2-C7-N1
8	DE	304	A1CIM	C3-C2-C7-O5
8	DE	304	A1CIM	O1-C2-C7-N1
8	DE	304	A1CIM	C3-C2-O1-C1
8	DE	304	A1CIM	C3-C4-C5-C6
8	DE	304	A1CIM	C3-C4-C5-O3
8	DE	304	A1CIM	O2-C4-C5-C6
8	DE	304	A1CIM	O2-C4-C5-O3
8	DE	304	A1CIM	C14-C10-C8-C9
8	DE	304	A1CIM	O7-C10-C8-C9
8	DE	304	A1CIM	C14-C10-C8-O6
8	DE	304	A1CIM	O7-C10-C8-O6
8	DF	301	A1CIM	C3-C2-O1-C1
8	DF	301	A1CIM	C7-C2-O1-C1
8	DF	301	A1CIM	C4-C5-C6-O4
8	DF	301	A1CIM	C2-C7-N1-C8
8	DF	301	A1CIM	O5-C7-N1-C8
8	DF	301	A1CIM	C14-C10-C8-C9
8	DF	301	A1CIM	O7-C10-C8-C9
8	DF	301	A1CIM	C14-C10-C8-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	DF	301	A1CIM	O7-C10-C8-O6
8	DF	303	A1CIM	C3-C4-C5-C6
8	DF	303	A1CIM	C3-C4-C5-O3
8	DF	303	A1CIM	O2-C4-C5-C6
8	DF	303	A1CIM	C2-C7-N1-C8
8	DF	303	A1CIM	O5-C7-N1-C8
8	DF	303	A1CIM	C14-C10-C8-C9
8	DF	303	A1CIM	O7-C10-C8-C9
8	DF	303	A1CIM	C14-C10-C8-O6
8	DF	303	A1CIM	O7-C10-C8-O6
8	DF	303	A1CIM	C9-C8-N1-C7
8	DF	304	A1CIM	C3-C2-C7-N1
8	DF	304	A1CIM	C3-C2-C7-O5
8	DF	304	A1CIM	O1-C2-C7-N1
8	DF	304	A1CIM	C3-C2-O1-C1
8	DF	304	A1CIM	C3-C4-C5-C6
8	DF	304	A1CIM	C3-C4-C5-O3
8	DF	304	A1CIM	O2-C4-C5-C6
8	DF	304	A1CIM	O2-C4-C5-O3
8	DF	304	A1CIM	C14-C10-C8-C9
8	DF	304	A1CIM	O7-C10-C8-C9
8	DF	304	A1CIM	C14-C10-C8-O6
8	DF	304	A1CIM	O7-C10-C8-O6
8	DG	301	A1CIM	C3-C2-O1-C1
8	DG	301	A1CIM	C7-C2-O1-C1
8	DG	301	A1CIM	C4-C5-C6-O4
8	DG	301	A1CIM	C2-C7-N1-C8
8	DG	301	A1CIM	O5-C7-N1-C8
8	DG	301	A1CIM	C14-C10-C8-C9
8	DG	301	A1CIM	O7-C10-C8-C9
8	DG	301	A1CIM	C14-C10-C8-O6
8	DG	301	A1CIM	O7-C10-C8-O6
8	DG	303	A1CIM	C3-C4-C5-C6
8	DG	303	A1CIM	C3-C4-C5-O3
8	DG	303	A1CIM	O2-C4-C5-C6
8	DG	303	A1CIM	C2-C7-N1-C8
8	DG	303	A1CIM	O5-C7-N1-C8
8	DG	303	A1CIM	C14-C10-C8-C9
8	DG	303	A1CIM	O7-C10-C8-C9
8	DG	303	A1CIM	C14-C10-C8-O6
8	DG	303	A1CIM	O7-C10-C8-O6
8	DG	303	A1CIM	C9-C8-N1-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	DG	304	A1CIM	C3-C2-C7-N1
8	DG	304	A1CIM	C3-C2-C7-O5
8	DG	304	A1CIM	O1-C2-C7-N1
8	DG	304	A1CIM	C3-C2-O1-C1
8	DG	304	A1CIM	C3-C4-C5-C6
8	DG	304	A1CIM	C3-C4-C5-O3
8	DG	304	A1CIM	O2-C4-C5-C6
8	DG	304	A1CIM	O2-C4-C5-O3
8	DG	304	A1CIM	C14-C10-C8-C9
8	DG	304	A1CIM	O7-C10-C8-C9
8	DG	304	A1CIM	C14-C10-C8-O6
8	DG	304	A1CIM	O7-C10-C8-O6
8	DH	301	A1CIM	C3-C2-O1-C1
8	DH	301	A1CIM	C7-C2-O1-C1
8	DH	301	A1CIM	C4-C5-C6-O4
8	DH	301	A1CIM	C2-C7-N1-C8
8	DH	301	A1CIM	O5-C7-N1-C8
8	DH	301	A1CIM	C14-C10-C8-C9
8	DH	301	A1CIM	O7-C10-C8-C9
8	DH	301	A1CIM	C14-C10-C8-O6
8	DH	301	A1CIM	O7-C10-C8-O6
8	DH	303	A1CIM	C3-C4-C5-C6
8	DH	303	A1CIM	C3-C4-C5-O3
8	DH	303	A1CIM	O2-C4-C5-C6
8	DH	303	A1CIM	C2-C7-N1-C8
8	DH	303	A1CIM	O5-C7-N1-C8
8	DH	303	A1CIM	C14-C10-C8-C9
8	DH	303	A1CIM	O7-C10-C8-C9
8	DH	303	A1CIM	C14-C10-C8-O6
8	DH	303	A1CIM	O7-C10-C8-O6
8	DH	303	A1CIM	C9-C8-N1-C7
8	DH	304	A1CIM	C3-C2-C7-N1
8	DH	304	A1CIM	C3-C2-C7-O5
8	DH	304	A1CIM	O1-C2-C7-N1
8	DH	304	A1CIM	C3-C2-O1-C1
8	DH	304	A1CIM	C3-C4-C5-C6
8	DH	304	A1CIM	C3-C4-C5-O3
8	DH	304	A1CIM	O2-C4-C5-C6
8	DH	304	A1CIM	O2-C4-C5-O3
8	DH	304	A1CIM	C14-C10-C8-C9
8	DH	304	A1CIM	O7-C10-C8-C9
8	DH	304	A1CIM	C14-C10-C8-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	DH	304	A1CIM	O7-C10-C8-O6
8	DI	301	A1CIM	C3-C2-O1-C1
8	DI	301	A1CIM	C7-C2-O1-C1
8	DI	301	A1CIM	C4-C5-C6-O4
8	DI	301	A1CIM	C2-C7-N1-C8
8	DI	301	A1CIM	O5-C7-N1-C8
8	DI	301	A1CIM	C14-C10-C8-C9
8	DI	301	A1CIM	O7-C10-C8-C9
8	DI	301	A1CIM	C14-C10-C8-O6
8	DI	301	A1CIM	O7-C10-C8-O6
8	DI	303	A1CIM	C3-C4-C5-C6
8	DI	303	A1CIM	C3-C4-C5-O3
8	DI	303	A1CIM	O2-C4-C5-C6
8	DI	303	A1CIM	C2-C7-N1-C8
8	DI	303	A1CIM	O5-C7-N1-C8
8	DI	303	A1CIM	C14-C10-C8-C9
8	DI	303	A1CIM	O7-C10-C8-C9
8	DI	303	A1CIM	C14-C10-C8-O6
8	DI	303	A1CIM	O7-C10-C8-O6
8	DI	303	A1CIM	C9-C8-N1-C7
8	DI	304	A1CIM	C3-C2-C7-N1
8	DI	304	A1CIM	C3-C2-C7-O5
8	DI	304	A1CIM	O1-C2-C7-N1
8	DI	304	A1CIM	C3-C2-O1-C1
8	DI	304	A1CIM	C3-C4-C5-C6
8	DI	304	A1CIM	C3-C4-C5-O3
8	DI	304	A1CIM	O2-C4-C5-C6
8	DI	304	A1CIM	O2-C4-C5-O3
8	DI	304	A1CIM	C14-C10-C8-C9
8	DI	304	A1CIM	O7-C10-C8-C9
8	DI	304	A1CIM	C14-C10-C8-O6
8	DI	304	A1CIM	O7-C10-C8-O6
8	DJ	301	A1CIM	C3-C2-O1-C1
8	DJ	301	A1CIM	C7-C2-O1-C1
8	DJ	301	A1CIM	C4-C5-C6-O4
8	DJ	301	A1CIM	C2-C7-N1-C8
8	DJ	301	A1CIM	O5-C7-N1-C8
8	DJ	301	A1CIM	C14-C10-C8-C9
8	DJ	301	A1CIM	O7-C10-C8-C9
8	DJ	301	A1CIM	C14-C10-C8-O6
8	DJ	301	A1CIM	O7-C10-C8-O6
8	DJ	303	A1CIM	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	DJ	303	A1CIM	C3-C4-C5-O3
8	DJ	303	A1CIM	O2-C4-C5-C6
8	DJ	303	A1CIM	C2-C7-N1-C8
8	DJ	303	A1CIM	O5-C7-N1-C8
8	DJ	303	A1CIM	C14-C10-C8-C9
8	DJ	303	A1CIM	O7-C10-C8-C9
8	DJ	303	A1CIM	C14-C10-C8-O6
8	DJ	303	A1CIM	O7-C10-C8-O6
8	DJ	303	A1CIM	C9-C8-N1-C7
8	DJ	304	A1CIM	C3-C2-C7-N1
8	DJ	304	A1CIM	C3-C2-C7-O5
8	DJ	304	A1CIM	O1-C2-C7-N1
8	DJ	304	A1CIM	C3-C2-O1-C1
8	DJ	304	A1CIM	C3-C4-C5-C6
8	DJ	304	A1CIM	C3-C4-C5-O3
8	DJ	304	A1CIM	O2-C4-C5-C6
8	DJ	304	A1CIM	O2-C4-C5-O3
8	DJ	304	A1CIM	C14-C10-C8-C9
8	DJ	304	A1CIM	O7-C10-C8-C9
8	DJ	304	A1CIM	C14-C10-C8-O6
8	DJ	304	A1CIM	O7-C10-C8-O6
8	DK	301	A1CIM	C3-C2-O1-C1
8	DK	301	A1CIM	C7-C2-O1-C1
8	DK	301	A1CIM	C4-C5-C6-O4
8	DK	301	A1CIM	C2-C7-N1-C8
8	DK	301	A1CIM	O5-C7-N1-C8
8	DK	301	A1CIM	C14-C10-C8-C9
8	DK	301	A1CIM	O7-C10-C8-C9
8	DK	301	A1CIM	C14-C10-C8-O6
8	DK	301	A1CIM	O7-C10-C8-O6
8	DK	303	A1CIM	C3-C4-C5-C6
8	DK	303	A1CIM	C3-C4-C5-O3
8	DK	303	A1CIM	O2-C4-C5-C6
8	DK	303	A1CIM	C2-C7-N1-C8
8	DK	303	A1CIM	O5-C7-N1-C8
8	DK	303	A1CIM	C14-C10-C8-C9
8	DK	303	A1CIM	O7-C10-C8-C9
8	DK	303	A1CIM	C14-C10-C8-O6
8	DK	303	A1CIM	O7-C10-C8-O6
8	DK	303	A1CIM	C9-C8-N1-C7
8	DK	304	A1CIM	C3-C2-C7-N1
8	DK	304	A1CIM	C3-C2-C7-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	DK	304	A1CIM	O1-C2-C7-N1
8	DK	304	A1CIM	C3-C2-O1-C1
8	DK	304	A1CIM	C3-C4-C5-C6
8	DK	304	A1CIM	C3-C4-C5-O3
8	DK	304	A1CIM	O2-C4-C5-C6
8	DK	304	A1CIM	O2-C4-C5-O3
8	DK	304	A1CIM	C14-C10-C8-C9
8	DK	304	A1CIM	O7-C10-C8-C9
8	DK	304	A1CIM	C14-C10-C8-O6
8	DK	304	A1CIM	O7-C10-C8-O6
8	DL	301	A1CIM	C3-C2-O1-C1
8	DL	301	A1CIM	C7-C2-O1-C1
8	DL	301	A1CIM	C4-C5-C6-O4
8	DL	301	A1CIM	C2-C7-N1-C8
8	DL	301	A1CIM	O5-C7-N1-C8
8	DL	301	A1CIM	C14-C10-C8-C9
8	DL	301	A1CIM	O7-C10-C8-C9
8	DL	301	A1CIM	C14-C10-C8-O6
8	DL	301	A1CIM	O7-C10-C8-O6
8	DL	303	A1CIM	C3-C4-C5-C6
8	DL	303	A1CIM	C3-C4-C5-O3
8	DL	303	A1CIM	O2-C4-C5-C6
8	DL	303	A1CIM	C2-C7-N1-C8
8	DL	303	A1CIM	O5-C7-N1-C8
8	DL	303	A1CIM	C14-C10-C8-C9
8	DL	303	A1CIM	O7-C10-C8-C9
8	DL	303	A1CIM	C14-C10-C8-O6
8	DL	303	A1CIM	O7-C10-C8-O6
8	DL	303	A1CIM	C9-C8-N1-C7
8	DL	304	A1CIM	C3-C2-C7-N1
8	DL	304	A1CIM	C3-C2-C7-O5
8	DL	304	A1CIM	O1-C2-C7-N1
8	DL	304	A1CIM	C3-C2-O1-C1
8	DL	304	A1CIM	C3-C4-C5-C6
8	DL	304	A1CIM	C3-C4-C5-O3
8	DL	304	A1CIM	O2-C4-C5-C6
8	DL	304	A1CIM	O2-C4-C5-O3
8	DL	304	A1CIM	C14-C10-C8-C9
8	DL	304	A1CIM	O7-C10-C8-C9
8	DL	304	A1CIM	C14-C10-C8-O6
8	DL	304	A1CIM	O7-C10-C8-O6
8	DM	301	A1CIM	C3-C2-O1-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	DM	301	A1CIM	C7-C2-O1-C1
8	DM	301	A1CIM	C4-C5-C6-O4
8	DM	301	A1CIM	C2-C7-N1-C8
8	DM	301	A1CIM	O5-C7-N1-C8
8	DM	301	A1CIM	C14-C10-C8-C9
8	DM	301	A1CIM	O7-C10-C8-C9
8	DM	301	A1CIM	C14-C10-C8-O6
8	DM	301	A1CIM	O7-C10-C8-O6
8	DM	303	A1CIM	C3-C4-C5-C6
8	DM	303	A1CIM	C3-C4-C5-O3
8	DM	303	A1CIM	O2-C4-C5-C6
8	DM	303	A1CIM	C2-C7-N1-C8
8	DM	303	A1CIM	O5-C7-N1-C8
8	DM	303	A1CIM	C14-C10-C8-C9
8	DM	303	A1CIM	O7-C10-C8-C9
8	DM	303	A1CIM	C14-C10-C8-O6
8	DM	303	A1CIM	O7-C10-C8-O6
8	DM	303	A1CIM	C9-C8-N1-C7
8	DM	304	A1CIM	C3-C2-C7-N1
8	DM	304	A1CIM	C3-C2-C7-O5
8	DM	304	A1CIM	O1-C2-C7-N1
8	DM	304	A1CIM	C3-C2-O1-C1
8	DM	304	A1CIM	C3-C4-C5-C6
8	DM	304	A1CIM	C3-C4-C5-O3
8	DM	304	A1CIM	O2-C4-C5-C6
8	DM	304	A1CIM	O2-C4-C5-O3
8	DM	304	A1CIM	C14-C10-C8-C9
8	DM	304	A1CIM	O7-C10-C8-C9
8	DM	304	A1CIM	C14-C10-C8-O6
8	DM	304	A1CIM	O7-C10-C8-O6
8	DN	301	A1CIM	C3-C2-O1-C1
8	DN	301	A1CIM	C7-C2-O1-C1
8	DN	301	A1CIM	C4-C5-C6-O4
8	DN	301	A1CIM	C2-C7-N1-C8
8	DN	301	A1CIM	O5-C7-N1-C8
8	DN	301	A1CIM	C14-C10-C8-C9
8	DN	301	A1CIM	O7-C10-C8-C9
8	DN	301	A1CIM	C14-C10-C8-O6
8	DN	301	A1CIM	O7-C10-C8-O6
8	DN	303	A1CIM	C3-C4-C5-C6
8	DN	303	A1CIM	C3-C4-C5-O3
8	DN	303	A1CIM	O2-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	DN	303	A1CIM	C2-C7-N1-C8
8	DN	303	A1CIM	O5-C7-N1-C8
8	DN	303	A1CIM	C14-C10-C8-C9
8	DN	303	A1CIM	O7-C10-C8-C9
8	DN	303	A1CIM	C14-C10-C8-O6
8	DN	303	A1CIM	O7-C10-C8-O6
8	DN	303	A1CIM	C9-C8-N1-C7
8	DN	304	A1CIM	C3-C2-C7-N1
8	DN	304	A1CIM	C3-C2-C7-O5
8	DN	304	A1CIM	O1-C2-C7-N1
8	DN	304	A1CIM	C3-C2-O1-C1
8	DN	304	A1CIM	C3-C4-C5-C6
8	DN	304	A1CIM	C3-C4-C5-O3
8	DN	304	A1CIM	O2-C4-C5-C6
8	DN	304	A1CIM	O2-C4-C5-O3
8	DN	304	A1CIM	C14-C10-C8-C9
8	DN	304	A1CIM	O7-C10-C8-C9
8	DN	304	A1CIM	C14-C10-C8-O6
8	DN	304	A1CIM	O7-C10-C8-O6
8	DO	301	A1CIM	C3-C2-O1-C1
8	DO	301	A1CIM	C7-C2-O1-C1
8	DO	301	A1CIM	C4-C5-C6-O4
8	DO	301	A1CIM	C2-C7-N1-C8
8	DO	301	A1CIM	O5-C7-N1-C8
8	DO	301	A1CIM	C14-C10-C8-C9
8	DO	301	A1CIM	O7-C10-C8-C9
8	DO	301	A1CIM	C14-C10-C8-O6
8	DO	301	A1CIM	O7-C10-C8-O6
8	DO	303	A1CIM	C3-C4-C5-C6
8	DO	303	A1CIM	C3-C4-C5-O3
8	DO	303	A1CIM	O2-C4-C5-C6
8	DO	303	A1CIM	C2-C7-N1-C8
8	DO	303	A1CIM	O5-C7-N1-C8
8	DO	303	A1CIM	C14-C10-C8-C9
8	DO	303	A1CIM	O7-C10-C8-C9
8	DO	303	A1CIM	C14-C10-C8-O6
8	DO	303	A1CIM	O7-C10-C8-O6
8	DO	303	A1CIM	C9-C8-N1-C7
8	DO	304	A1CIM	C3-C2-C7-N1
8	DO	304	A1CIM	C3-C2-C7-O5
8	DO	304	A1CIM	O1-C2-C7-N1
8	DO	304	A1CIM	C3-C2-O1-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	DO	304	A1CIM	C3-C4-C5-C6
8	DO	304	A1CIM	C3-C4-C5-O3
8	DO	304	A1CIM	O2-C4-C5-C6
8	DO	304	A1CIM	O2-C4-C5-O3
8	DO	304	A1CIM	C14-C10-C8-C9
8	DO	304	A1CIM	O7-C10-C8-C9
8	DO	304	A1CIM	C14-C10-C8-O6
8	DO	304	A1CIM	O7-C10-C8-O6
8	DP	301	A1CIM	C3-C2-O1-C1
8	DP	301	A1CIM	C7-C2-O1-C1
8	DP	301	A1CIM	C4-C5-C6-O4
8	DP	301	A1CIM	C2-C7-N1-C8
8	DP	301	A1CIM	O5-C7-N1-C8
8	DP	301	A1CIM	C14-C10-C8-C9
8	DP	301	A1CIM	O7-C10-C8-C9
8	DP	301	A1CIM	C14-C10-C8-O6
8	DP	301	A1CIM	O7-C10-C8-O6
8	DP	303	A1CIM	C3-C4-C5-C6
8	DP	303	A1CIM	C3-C4-C5-O3
8	DP	303	A1CIM	O2-C4-C5-C6
8	DP	303	A1CIM	C2-C7-N1-C8
8	DP	303	A1CIM	O5-C7-N1-C8
8	DP	303	A1CIM	C14-C10-C8-C9
8	DP	303	A1CIM	O7-C10-C8-C9
8	DP	303	A1CIM	C14-C10-C8-O6
8	DP	303	A1CIM	O7-C10-C8-O6
8	DP	303	A1CIM	C9-C8-N1-C7
8	DP	304	A1CIM	C3-C2-C7-N1
8	DP	304	A1CIM	C3-C2-C7-O5
8	DP	304	A1CIM	O1-C2-C7-N1
8	DP	304	A1CIM	C3-C2-O1-C1
8	DP	304	A1CIM	C3-C4-C5-C6
8	DP	304	A1CIM	C3-C4-C5-O3
8	DP	304	A1CIM	O2-C4-C5-C6
8	DP	304	A1CIM	O2-C4-C5-O3
8	DP	304	A1CIM	C14-C10-C8-C9
8	DP	304	A1CIM	O7-C10-C8-C9
8	DP	304	A1CIM	C14-C10-C8-O6
8	DP	304	A1CIM	O7-C10-C8-O6
8	DQ	301	A1CIM	C3-C2-O1-C1
8	DQ	301	A1CIM	C7-C2-O1-C1
8	DQ	301	A1CIM	C4-C5-C6-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	DQ	301	A1CIM	C2-C7-N1-C8
8	DQ	301	A1CIM	O5-C7-N1-C8
8	DQ	301	A1CIM	C14-C10-C8-C9
8	DQ	301	A1CIM	O7-C10-C8-C9
8	DQ	301	A1CIM	C14-C10-C8-O6
8	DQ	301	A1CIM	O7-C10-C8-O6
8	DQ	303	A1CIM	C3-C4-C5-C6
8	DQ	303	A1CIM	C3-C4-C5-O3
8	DQ	303	A1CIM	O2-C4-C5-C6
8	DQ	303	A1CIM	C2-C7-N1-C8
8	DQ	303	A1CIM	O5-C7-N1-C8
8	DQ	303	A1CIM	C14-C10-C8-C9
8	DQ	303	A1CIM	O7-C10-C8-C9
8	DQ	303	A1CIM	C14-C10-C8-O6
8	DQ	303	A1CIM	O7-C10-C8-O6
8	DQ	303	A1CIM	C9-C8-N1-C7
8	DQ	304	A1CIM	C3-C2-C7-N1
8	DQ	304	A1CIM	C3-C2-C7-O5
8	DQ	304	A1CIM	O1-C2-C7-N1
8	DQ	304	A1CIM	C3-C2-O1-C1
8	DQ	304	A1CIM	C3-C4-C5-C6
8	DQ	304	A1CIM	C3-C4-C5-O3
8	DQ	304	A1CIM	O2-C4-C5-C6
8	DQ	304	A1CIM	O2-C4-C5-O3
8	DQ	304	A1CIM	C14-C10-C8-C9
8	DQ	304	A1CIM	O7-C10-C8-C9
8	DQ	304	A1CIM	C14-C10-C8-O6
8	DQ	304	A1CIM	O7-C10-C8-O6
8	C0	301	A1CIM	O3-C5-C6-O4
8	DA	301	A1CIM	O3-C5-C6-O4
8	DB	301	A1CIM	O3-C5-C6-O4
8	DC	301	A1CIM	O3-C5-C6-O4
8	DD	301	A1CIM	O3-C5-C6-O4
8	DE	301	A1CIM	O3-C5-C6-O4
8	DF	301	A1CIM	O3-C5-C6-O4
8	DG	301	A1CIM	O3-C5-C6-O4
8	DH	301	A1CIM	O3-C5-C6-O4
8	DI	301	A1CIM	O3-C5-C6-O4
8	DJ	301	A1CIM	O3-C5-C6-O4
8	DK	301	A1CIM	O3-C5-C6-O4
8	DL	301	A1CIM	O3-C5-C6-O4
8	DM	301	A1CIM	O3-C5-C6-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	DN	301	A1CIM	O3-C5-C6-O4
8	DO	301	A1CIM	O3-C5-C6-O4
8	DP	301	A1CIM	O3-C5-C6-O4
8	DQ	301	A1CIM	O3-C5-C6-O4
8	C0	304	A1CIM	O7-C11-C16-O10
8	DA	304	A1CIM	O7-C11-C16-O10
8	DB	304	A1CIM	O7-C11-C16-O10
8	DC	304	A1CIM	O7-C11-C16-O10
8	DD	304	A1CIM	O7-C11-C16-O10
8	DE	304	A1CIM	O7-C11-C16-O10
8	DF	304	A1CIM	O7-C11-C16-O10
8	DG	304	A1CIM	O7-C11-C16-O10
8	DH	304	A1CIM	O7-C11-C16-O10
8	DI	304	A1CIM	O7-C11-C16-O10
8	DJ	304	A1CIM	O7-C11-C16-O10
8	DK	304	A1CIM	O7-C11-C16-O10
8	DL	304	A1CIM	O7-C11-C16-O10
8	DM	304	A1CIM	O7-C11-C16-O10
8	DN	304	A1CIM	O7-C11-C16-O10
8	DO	304	A1CIM	O7-C11-C16-O10
8	DP	304	A1CIM	O7-C11-C16-O10
8	DQ	304	A1CIM	O7-C11-C16-O10
8	C0	301	A1CIM	C3-C2-C7-O5
8	DA	301	A1CIM	C3-C2-C7-O5
8	DB	301	A1CIM	C3-C2-C7-O5
8	DC	301	A1CIM	C3-C2-C7-O5
8	DD	301	A1CIM	C3-C2-C7-O5
8	DE	301	A1CIM	C3-C2-C7-O5
8	DF	301	A1CIM	C3-C2-C7-O5
8	DG	301	A1CIM	C3-C2-C7-O5
8	DH	301	A1CIM	C3-C2-C7-O5
8	DI	301	A1CIM	C3-C2-C7-O5
8	DJ	301	A1CIM	C3-C2-C7-O5
8	DK	301	A1CIM	C3-C2-C7-O5
8	DL	301	A1CIM	C3-C2-C7-O5
8	DM	301	A1CIM	C3-C2-C7-O5
8	DN	301	A1CIM	C3-C2-C7-O5
8	DO	301	A1CIM	C3-C2-C7-O5
8	DP	301	A1CIM	C3-C2-C7-O5
8	DQ	301	A1CIM	C3-C2-C7-O5
8	C0	301	A1CIM	C3-C2-C7-N1
8	DA	301	A1CIM	C3-C2-C7-N1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	DB	301	A1CIM	C3-C2-C7-N1
8	DC	301	A1CIM	C3-C2-C7-N1
8	DD	301	A1CIM	C3-C2-C7-N1
8	DE	301	A1CIM	C3-C2-C7-N1
8	DF	301	A1CIM	C3-C2-C7-N1
8	DG	301	A1CIM	C3-C2-C7-N1
8	DH	301	A1CIM	C3-C2-C7-N1
8	DI	301	A1CIM	C3-C2-C7-N1
8	DJ	301	A1CIM	C3-C2-C7-N1
8	DK	301	A1CIM	C3-C2-C7-N1
8	DL	301	A1CIM	C3-C2-C7-N1
8	DM	301	A1CIM	C3-C2-C7-N1
8	DN	301	A1CIM	C3-C2-C7-N1
8	DO	301	A1CIM	C3-C2-C7-N1
8	DP	301	A1CIM	C3-C2-C7-N1
8	DQ	301	A1CIM	C3-C2-C7-N1
8	C0	301	A1CIM	O1-C2-C3-C4
8	C0	301	A1CIM	O1-C2-C7-N1
8	C0	301	A1CIM	O1-C2-C7-O5
8	DA	301	A1CIM	O1-C2-C3-C4
8	DA	301	A1CIM	O1-C2-C7-N1
8	DA	301	A1CIM	O1-C2-C7-O5
8	DB	301	A1CIM	O1-C2-C3-C4
8	DB	301	A1CIM	O1-C2-C7-N1
8	DB	301	A1CIM	O1-C2-C7-O5
8	DC	301	A1CIM	O1-C2-C3-C4
8	DC	301	A1CIM	O1-C2-C7-N1
8	DC	301	A1CIM	O1-C2-C7-O5
8	DD	301	A1CIM	O1-C2-C3-C4
8	DD	301	A1CIM	O1-C2-C7-N1
8	DD	301	A1CIM	O1-C2-C7-O5
8	DE	301	A1CIM	O1-C2-C3-C4
8	DE	301	A1CIM	O1-C2-C7-N1
8	DE	301	A1CIM	O1-C2-C7-O5
8	DF	301	A1CIM	O1-C2-C3-C4
8	DF	301	A1CIM	O1-C2-C7-N1
8	DF	301	A1CIM	O1-C2-C7-O5
8	DG	301	A1CIM	O1-C2-C3-C4
8	DG	301	A1CIM	O1-C2-C7-N1
8	DG	301	A1CIM	O1-C2-C7-O5
8	DH	301	A1CIM	O1-C2-C3-C4
8	DH	301	A1CIM	O1-C2-C7-N1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	DH	301	A1CIM	O1-C2-C7-O5
8	DI	301	A1CIM	O1-C2-C3-C4
8	DI	301	A1CIM	O1-C2-C7-N1
8	DI	301	A1CIM	O1-C2-C7-O5
8	DJ	301	A1CIM	O1-C2-C3-C4
8	DJ	301	A1CIM	O1-C2-C7-N1
8	DJ	301	A1CIM	O1-C2-C7-O5
8	DK	301	A1CIM	O1-C2-C3-C4
8	DK	301	A1CIM	O1-C2-C7-N1
8	DK	301	A1CIM	O1-C2-C7-O5
8	DL	301	A1CIM	O1-C2-C3-C4
8	DL	301	A1CIM	O1-C2-C7-N1
8	DL	301	A1CIM	O1-C2-C7-O5
8	DM	301	A1CIM	O1-C2-C3-C4
8	DM	301	A1CIM	O1-C2-C7-N1
8	DM	301	A1CIM	O1-C2-C7-O5
8	DN	301	A1CIM	O1-C2-C3-C4
8	DN	301	A1CIM	O1-C2-C7-N1
8	DN	301	A1CIM	O1-C2-C7-O5
8	DO	301	A1CIM	O1-C2-C3-C4
8	DO	301	A1CIM	O1-C2-C7-N1
8	DO	301	A1CIM	O1-C2-C7-O5
8	DP	301	A1CIM	O1-C2-C3-C4
8	DP	301	A1CIM	O1-C2-C7-N1
8	DP	301	A1CIM	O1-C2-C7-O5
8	DQ	301	A1CIM	O1-C2-C3-C4
8	DQ	301	A1CIM	O1-C2-C7-N1
8	DQ	301	A1CIM	O1-C2-C7-O5
8	C0	301	A1CIM	C9-C8-N1-C7
8	DA	301	A1CIM	C9-C8-N1-C7
8	DB	301	A1CIM	C9-C8-N1-C7
8	DC	301	A1CIM	C9-C8-N1-C7
8	DD	301	A1CIM	C9-C8-N1-C7
8	DE	301	A1CIM	C9-C8-N1-C7
8	DF	301	A1CIM	C9-C8-N1-C7
8	DG	301	A1CIM	C9-C8-N1-C7
8	DH	301	A1CIM	C9-C8-N1-C7
8	DI	301	A1CIM	C9-C8-N1-C7
8	DJ	301	A1CIM	C9-C8-N1-C7
8	DK	301	A1CIM	C9-C8-N1-C7
8	DL	301	A1CIM	C9-C8-N1-C7
8	DM	301	A1CIM	C9-C8-N1-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	DN	301	A1CIM	C9-C8-N1-C7
8	DO	301	A1CIM	C9-C8-N1-C7
8	DP	301	A1CIM	C9-C8-N1-C7
8	DQ	301	A1CIM	C9-C8-N1-C7
8	C0	303	A1CIM	O2-C4-C5-O3
8	DA	303	A1CIM	O2-C4-C5-O3
8	DB	303	A1CIM	O2-C4-C5-O3
8	DC	303	A1CIM	O2-C4-C5-O3
8	DD	303	A1CIM	O2-C4-C5-O3
8	DE	303	A1CIM	O2-C4-C5-O3
8	DF	303	A1CIM	O2-C4-C5-O3
8	DG	303	A1CIM	O2-C4-C5-O3
8	DH	303	A1CIM	O2-C4-C5-O3
8	DI	303	A1CIM	O2-C4-C5-O3
8	DJ	303	A1CIM	O2-C4-C5-O3
8	DK	303	A1CIM	O2-C4-C5-O3
8	DL	303	A1CIM	O2-C4-C5-O3
8	DM	303	A1CIM	O2-C4-C5-O3
8	DN	303	A1CIM	O2-C4-C5-O3
8	DO	303	A1CIM	O2-C4-C5-O3
8	DP	303	A1CIM	O2-C4-C5-O3
8	DQ	303	A1CIM	O2-C4-C5-O3
8	C0	301	A1CIM	C7-C2-C3-C4
8	DA	301	A1CIM	C7-C2-C3-C4
8	DB	301	A1CIM	C7-C2-C3-C4
8	DC	301	A1CIM	C7-C2-C3-C4
8	DD	301	A1CIM	C7-C2-C3-C4
8	DE	301	A1CIM	C7-C2-C3-C4
8	DF	301	A1CIM	C7-C2-C3-C4
8	DG	301	A1CIM	C7-C2-C3-C4
8	DH	301	A1CIM	C7-C2-C3-C4
8	DI	301	A1CIM	C7-C2-C3-C4
8	DJ	301	A1CIM	C7-C2-C3-C4
8	DK	301	A1CIM	C7-C2-C3-C4
8	DL	301	A1CIM	C7-C2-C3-C4
8	DM	301	A1CIM	C7-C2-C3-C4
8	DN	301	A1CIM	C7-C2-C3-C4
8	DO	301	A1CIM	C7-C2-C3-C4
8	DP	301	A1CIM	C7-C2-C3-C4
8	DQ	301	A1CIM	C7-C2-C3-C4
8	C0	303	A1CIM	O1-C2-C7-N1
8	DA	303	A1CIM	O1-C2-C7-N1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	DB	303	A1CIM	O1-C2-C7-N1
8	DC	303	A1CIM	O1-C2-C7-N1
8	DD	303	A1CIM	O1-C2-C7-N1
8	DE	303	A1CIM	O1-C2-C7-N1
8	DF	303	A1CIM	O1-C2-C7-N1
8	DG	303	A1CIM	O1-C2-C7-N1
8	DH	303	A1CIM	O1-C2-C7-N1
8	DI	303	A1CIM	O1-C2-C7-N1
8	DJ	303	A1CIM	O1-C2-C7-N1
8	DK	303	A1CIM	O1-C2-C7-N1
8	DL	303	A1CIM	O1-C2-C7-N1
8	DM	303	A1CIM	O1-C2-C7-N1
8	DN	303	A1CIM	O1-C2-C7-N1
8	DO	303	A1CIM	O1-C2-C7-N1
8	DP	303	A1CIM	O1-C2-C7-N1
8	DQ	303	A1CIM	O1-C2-C7-N1
8	C0	303	A1CIM	C13-C14-C15-N2
8	C0	303	A1CIM	C13-C14-C15-O9
8	C0	304	A1CIM	C10-C14-C15-N2
8	DA	303	A1CIM	C13-C14-C15-N2
8	DA	303	A1CIM	C13-C14-C15-O9
8	DA	304	A1CIM	C10-C14-C15-N2
8	DB	303	A1CIM	C13-C14-C15-N2
8	DB	303	A1CIM	C13-C14-C15-O9
8	DB	304	A1CIM	C10-C14-C15-N2
8	DC	303	A1CIM	C13-C14-C15-N2
8	DC	303	A1CIM	C13-C14-C15-O9
8	DC	304	A1CIM	C10-C14-C15-N2
8	DD	303	A1CIM	C13-C14-C15-N2
8	DD	303	A1CIM	C13-C14-C15-O9
8	DD	304	A1CIM	C10-C14-C15-N2
8	DE	303	A1CIM	C13-C14-C15-N2
8	DE	303	A1CIM	C13-C14-C15-O9
8	DE	304	A1CIM	C10-C14-C15-N2
8	DF	303	A1CIM	C13-C14-C15-N2
8	DF	303	A1CIM	C13-C14-C15-O9
8	DF	304	A1CIM	C10-C14-C15-N2
8	DG	303	A1CIM	C13-C14-C15-N2
8	DG	303	A1CIM	C13-C14-C15-O9
8	DG	304	A1CIM	C10-C14-C15-N2
8	DH	303	A1CIM	C13-C14-C15-N2
8	DH	303	A1CIM	C13-C14-C15-O9

Continued on next page...

Continued from previous page...

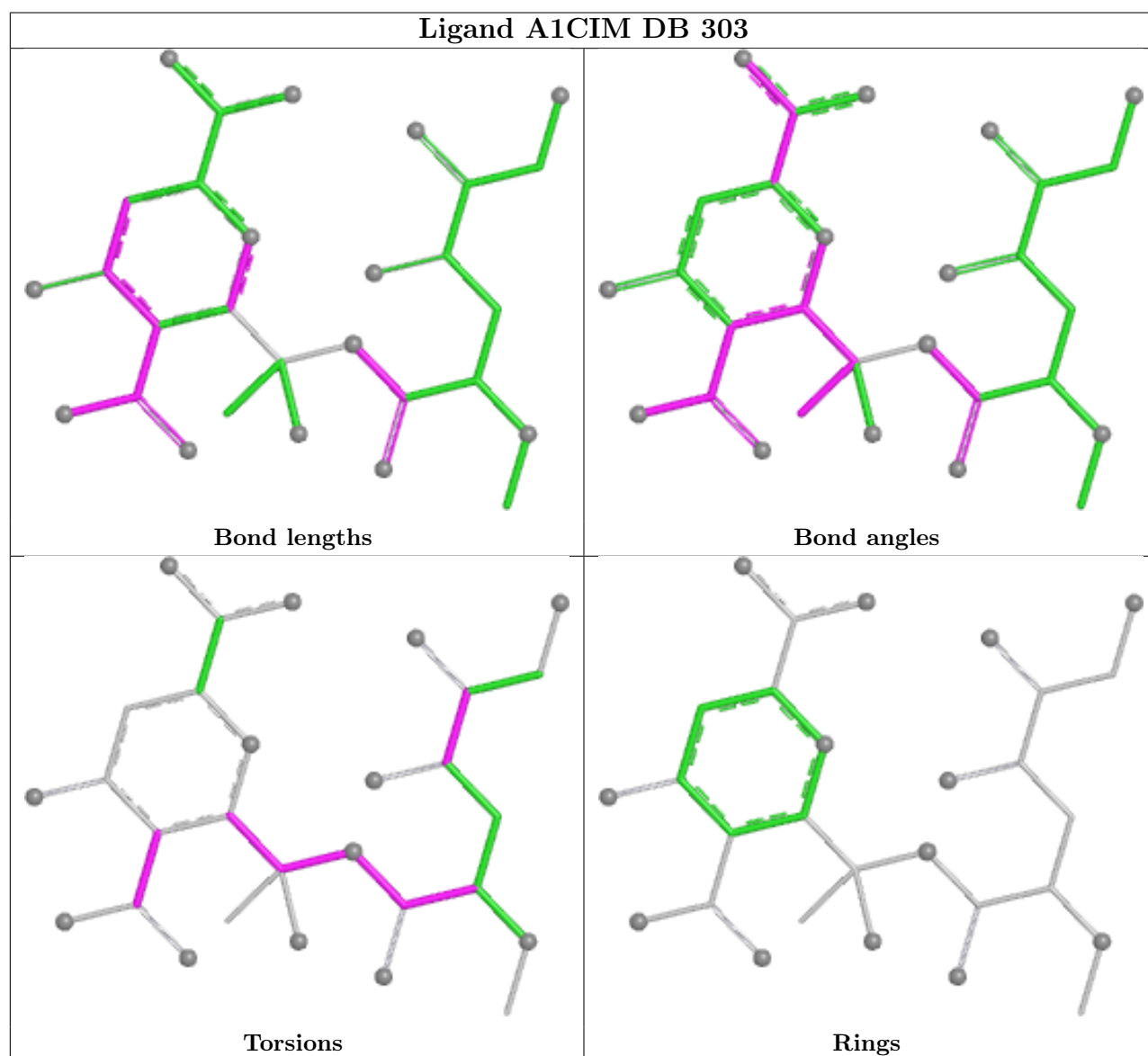
Mol	Chain	Res	Type	Atoms
8	DH	304	A1CIM	C10-C14-C15-N2
8	DI	303	A1CIM	C13-C14-C15-N2
8	DI	303	A1CIM	C13-C14-C15-O9
8	DI	304	A1CIM	C10-C14-C15-N2
8	DJ	303	A1CIM	C13-C14-C15-N2
8	DJ	303	A1CIM	C13-C14-C15-O9
8	DJ	304	A1CIM	C10-C14-C15-N2
8	DK	303	A1CIM	C13-C14-C15-N2
8	DK	303	A1CIM	C13-C14-C15-O9
8	DK	304	A1CIM	C10-C14-C15-N2
8	DL	303	A1CIM	C13-C14-C15-N2
8	DL	303	A1CIM	C13-C14-C15-O9
8	DL	304	A1CIM	C10-C14-C15-N2
8	DM	303	A1CIM	C13-C14-C15-N2
8	DM	303	A1CIM	C13-C14-C15-O9
8	DM	304	A1CIM	C10-C14-C15-N2
8	DN	303	A1CIM	C13-C14-C15-N2
8	DN	303	A1CIM	C13-C14-C15-O9
8	DN	304	A1CIM	C10-C14-C15-N2
8	DO	303	A1CIM	C13-C14-C15-N2
8	DO	303	A1CIM	C13-C14-C15-O9
8	DO	304	A1CIM	C10-C14-C15-N2
8	DP	303	A1CIM	C13-C14-C15-N2
8	DP	303	A1CIM	C13-C14-C15-O9
8	DP	304	A1CIM	C10-C14-C15-N2
8	DQ	303	A1CIM	C13-C14-C15-N2
8	DQ	303	A1CIM	C13-C14-C15-O9
8	DQ	304	A1CIM	C10-C14-C15-N2

There are no ring outliers.

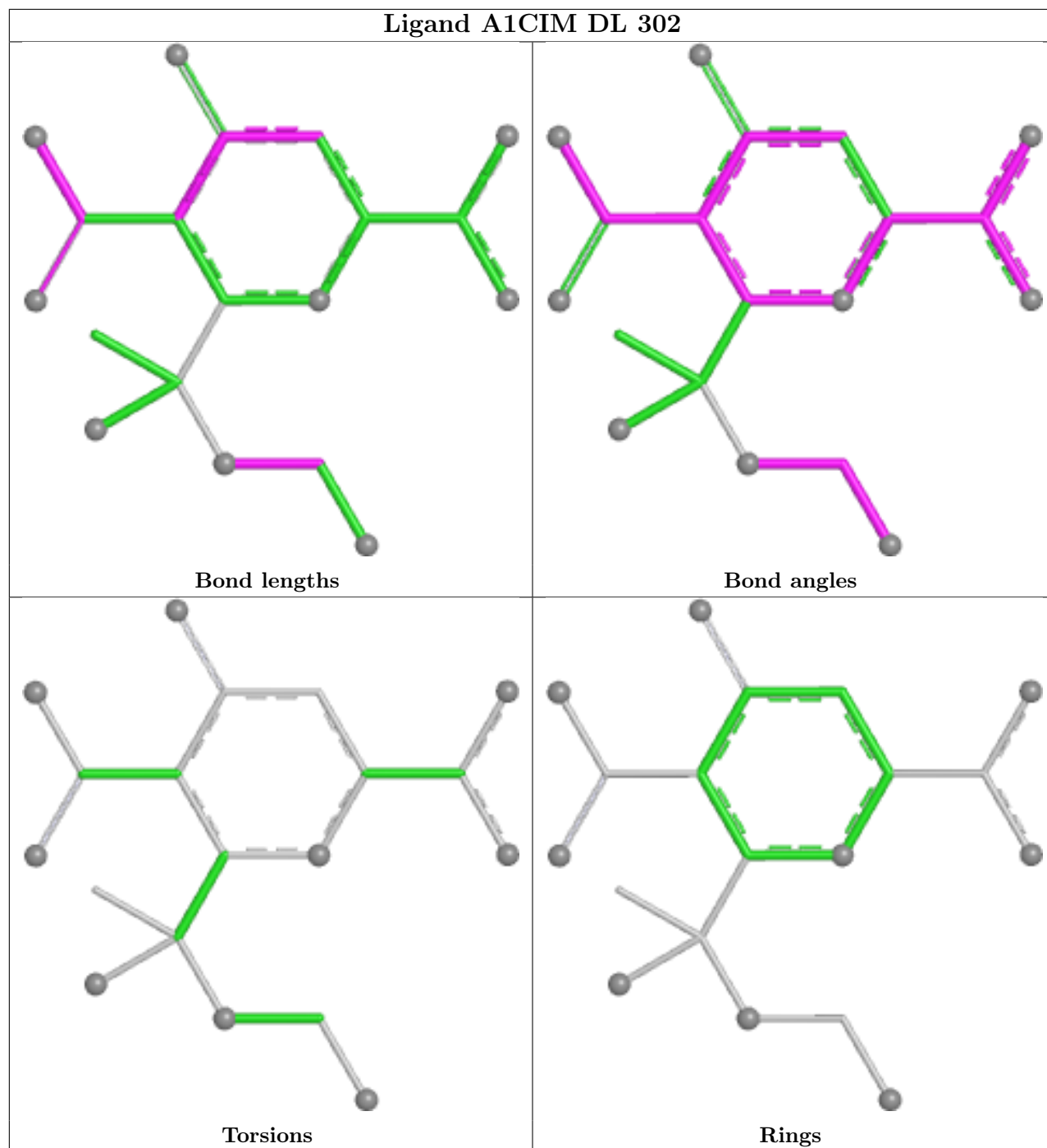
9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	DG	301	A1CIM	1	0
8	DB	301	A1CIM	1	0
8	C0	301	A1CIM	3	0
8	DK	301	A1CIM	1	0
8	DB	302	A1CIM	1	0
8	DC	302	A1CIM	1	0
8	DA	302	A1CIM	1	0
8	DH	301	A1CIM	4	0
8	DD	301	A1CIM	2	0

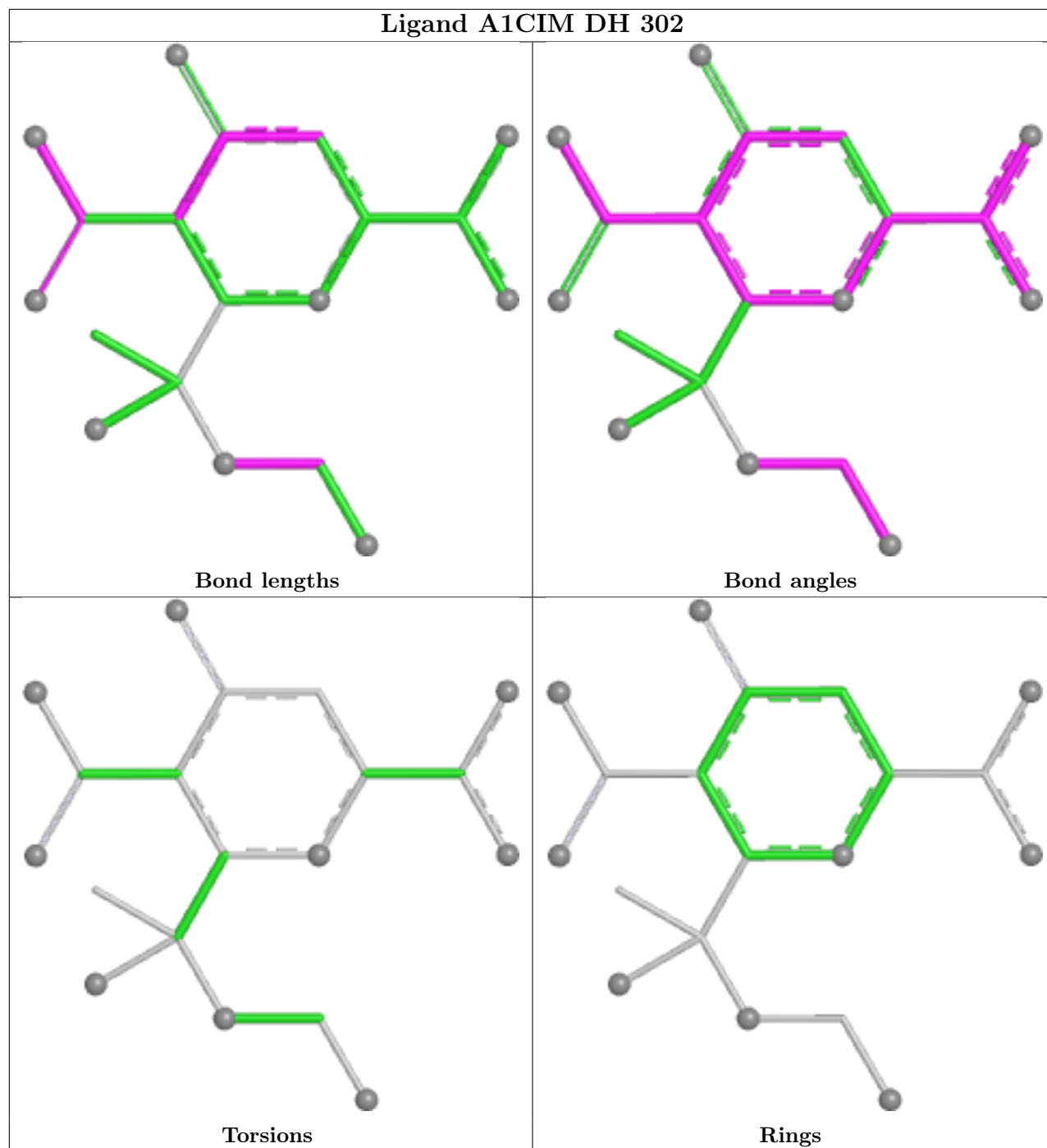
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



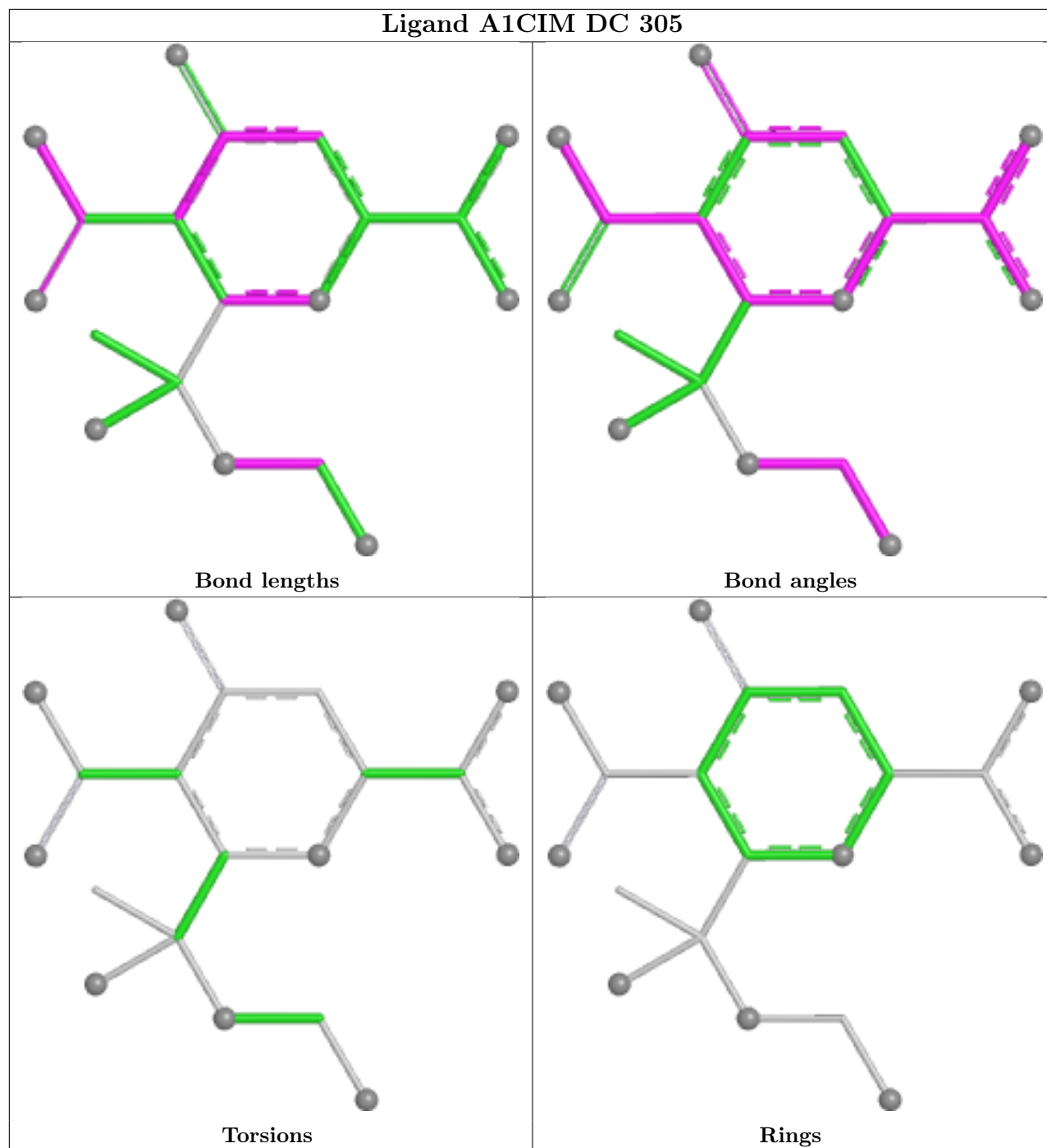
Ligand A1CIM DL 302



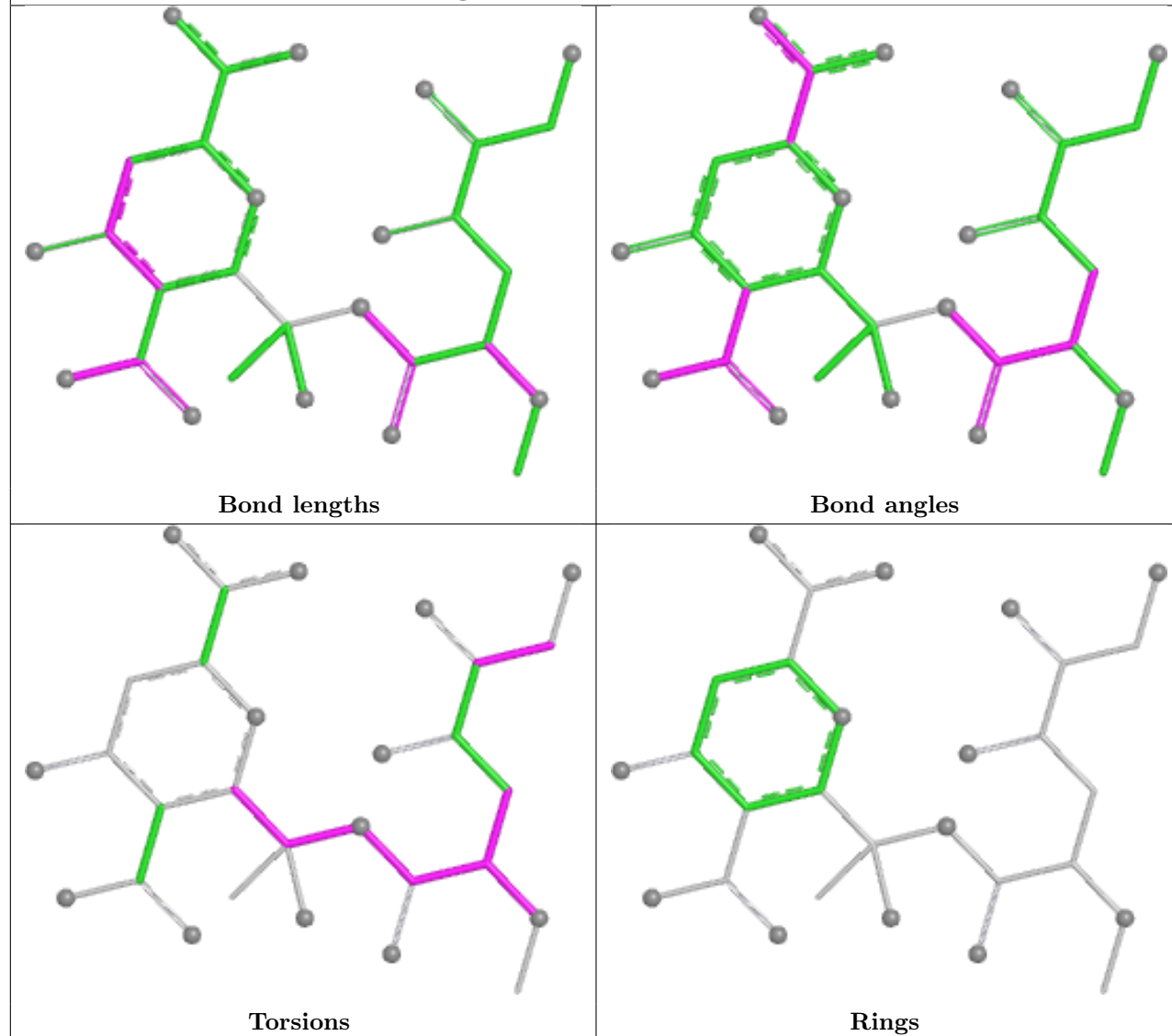
Ligand A1CIM DH 302



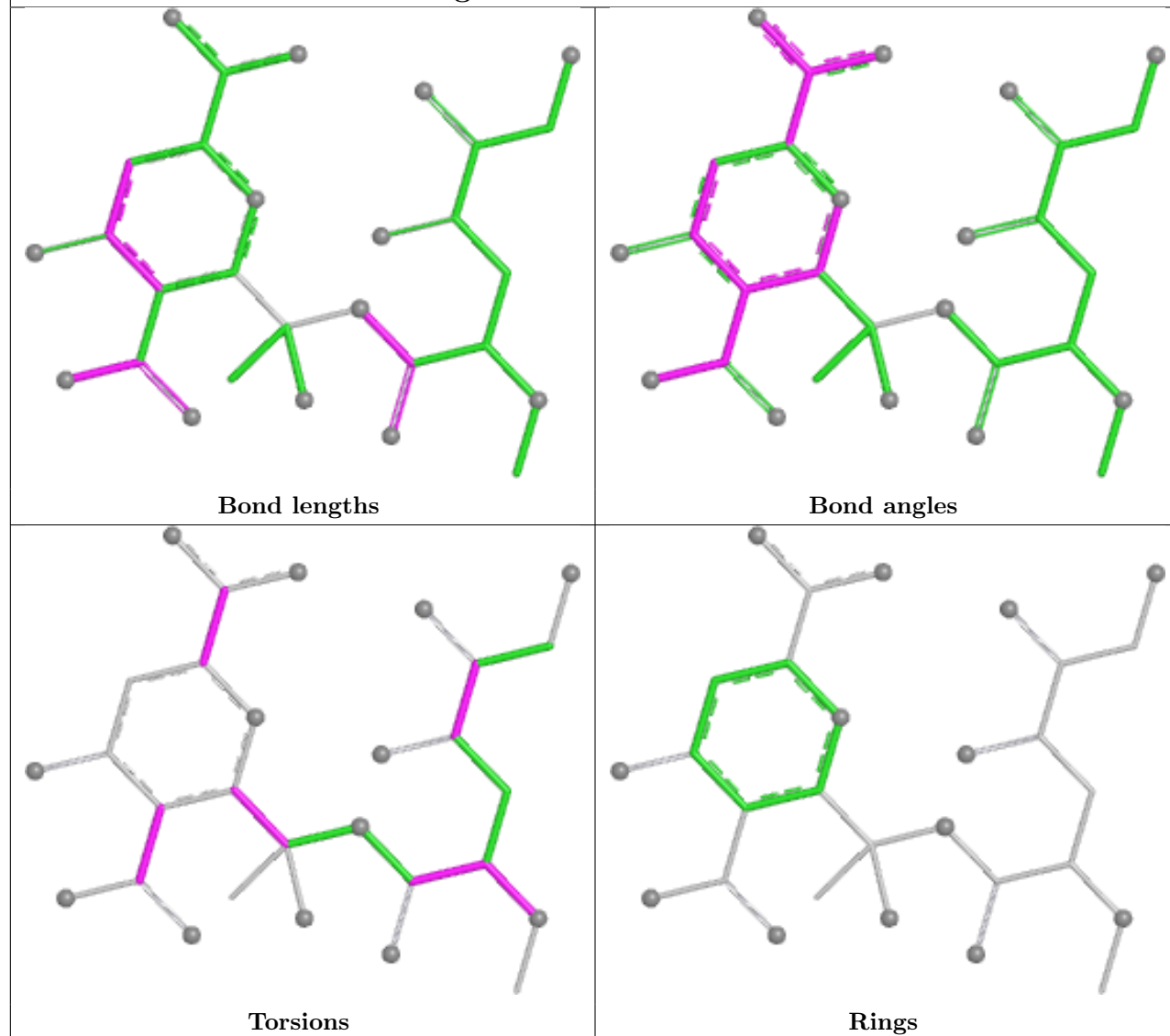
Ligand A1CIM DC 305



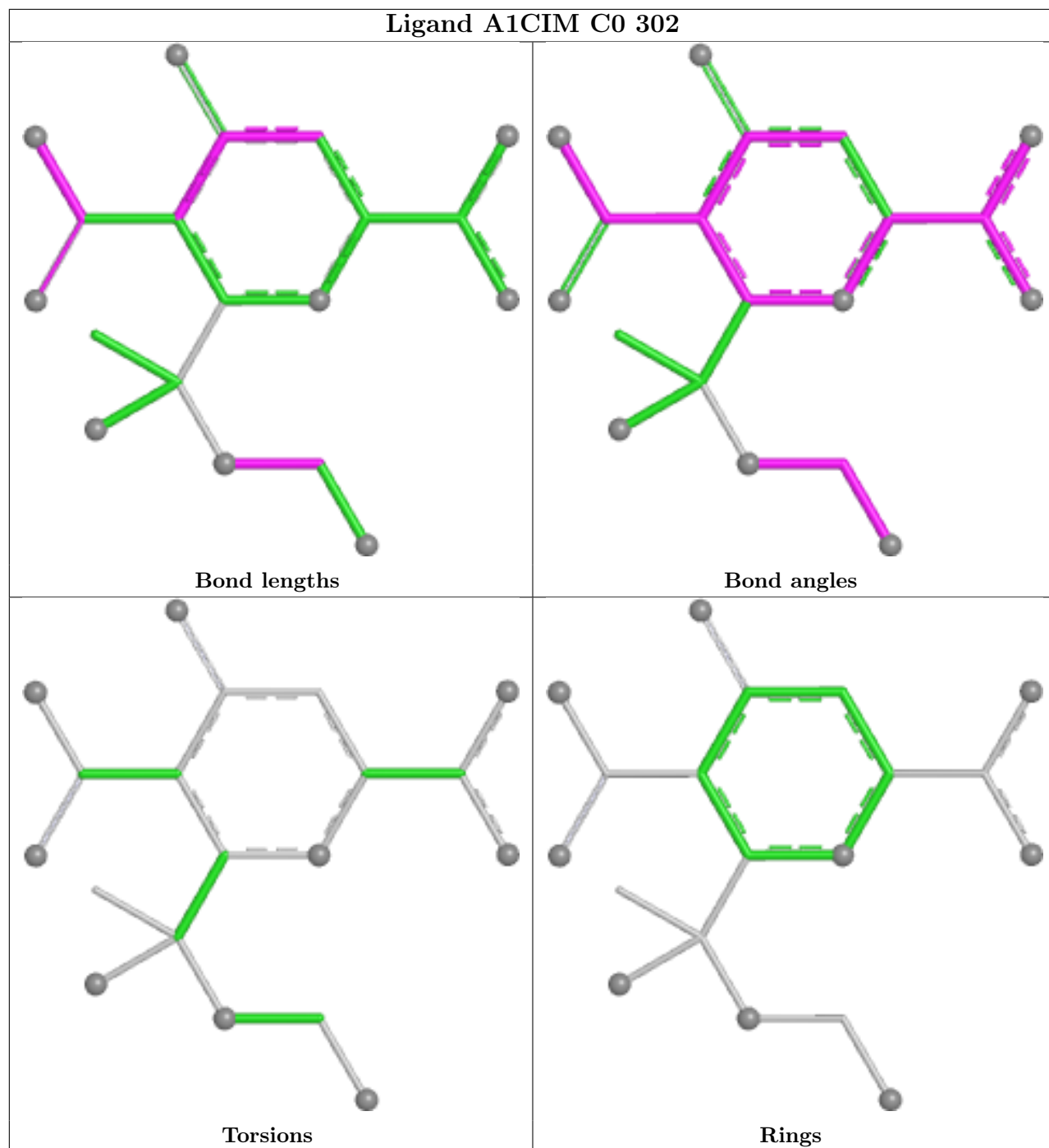
Ligand A1CIM DG 301



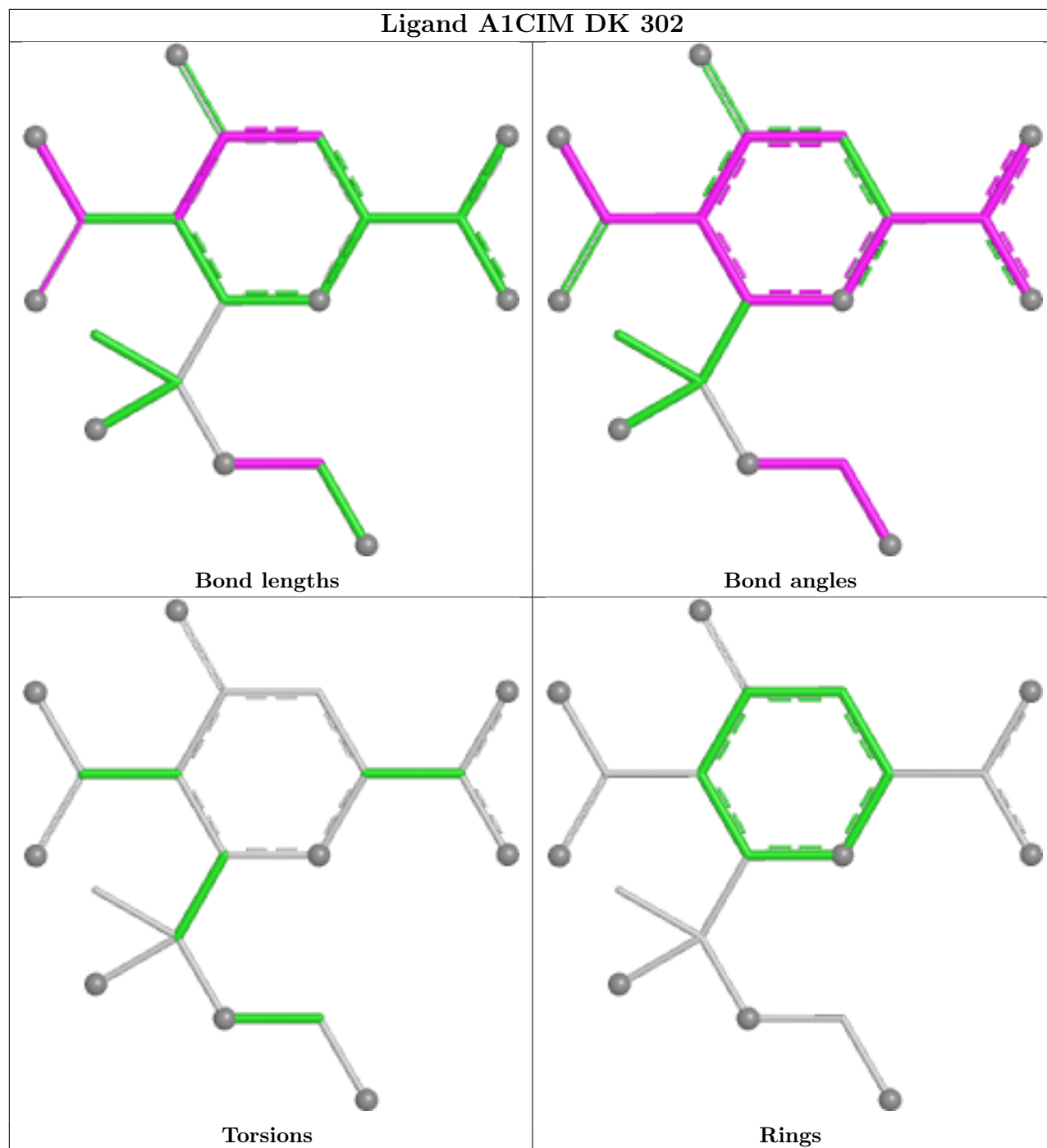
Ligand A1CIM DH 304



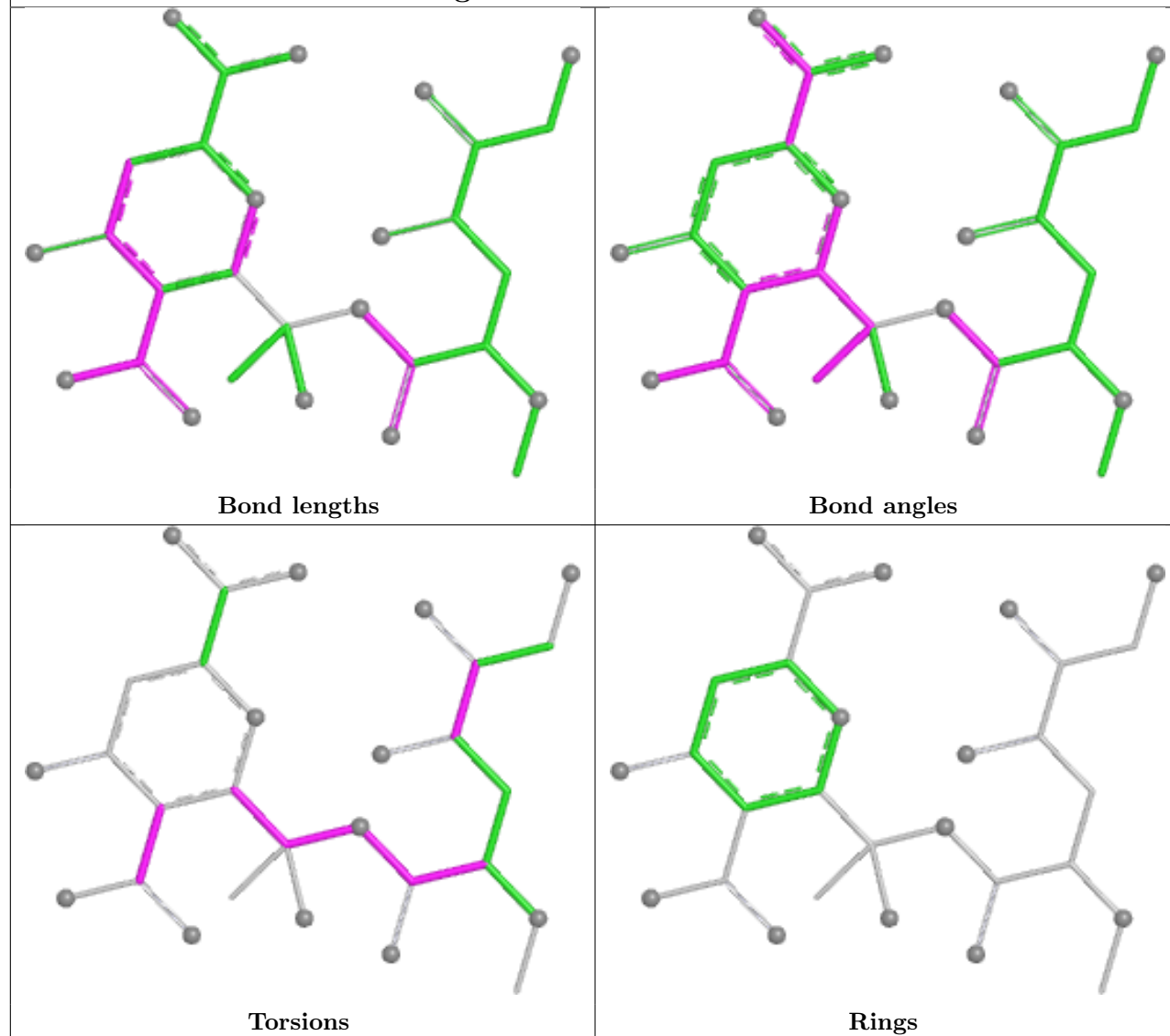
Ligand A1CIM C0 302



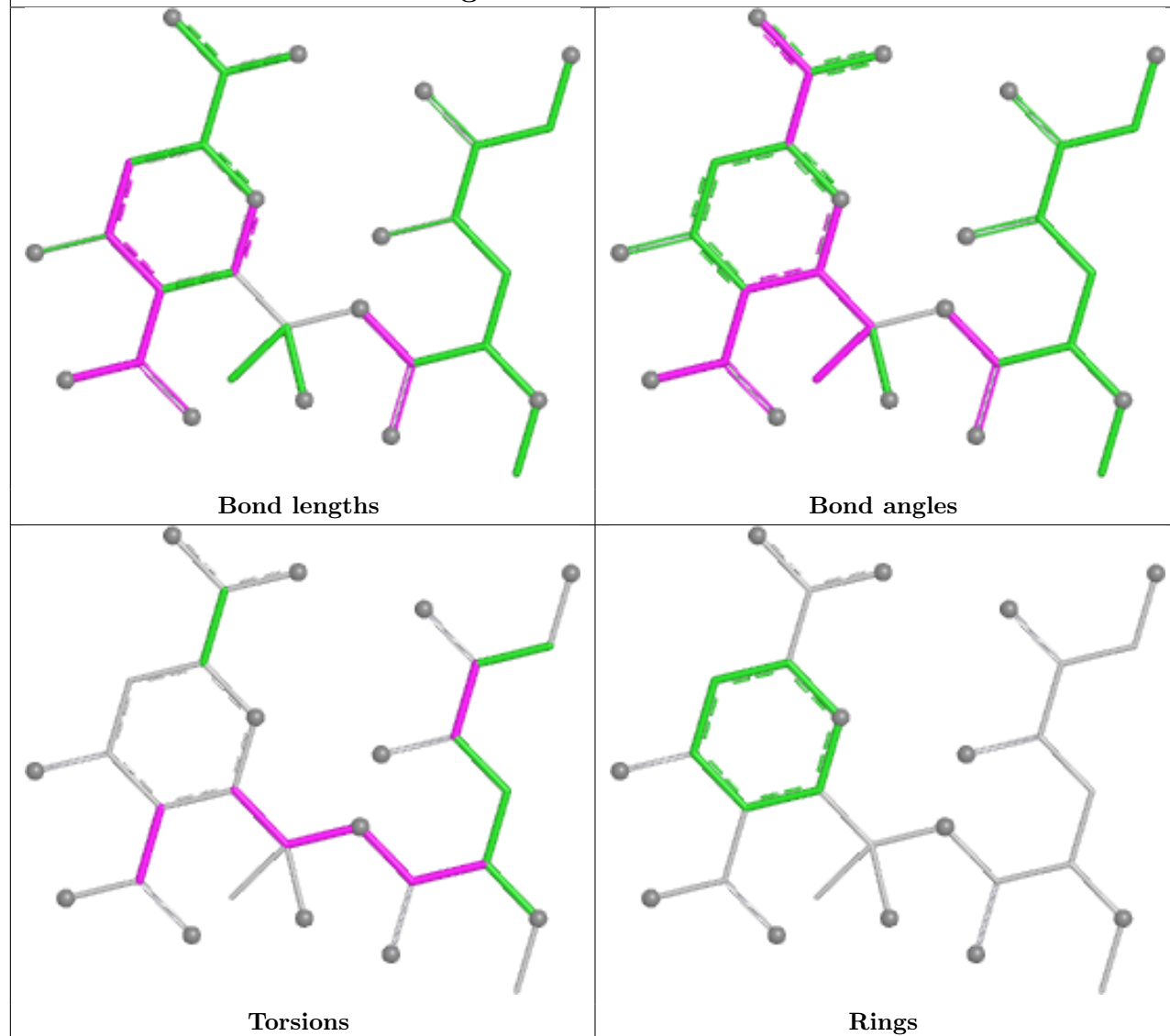
Ligand A1CIM DK 302



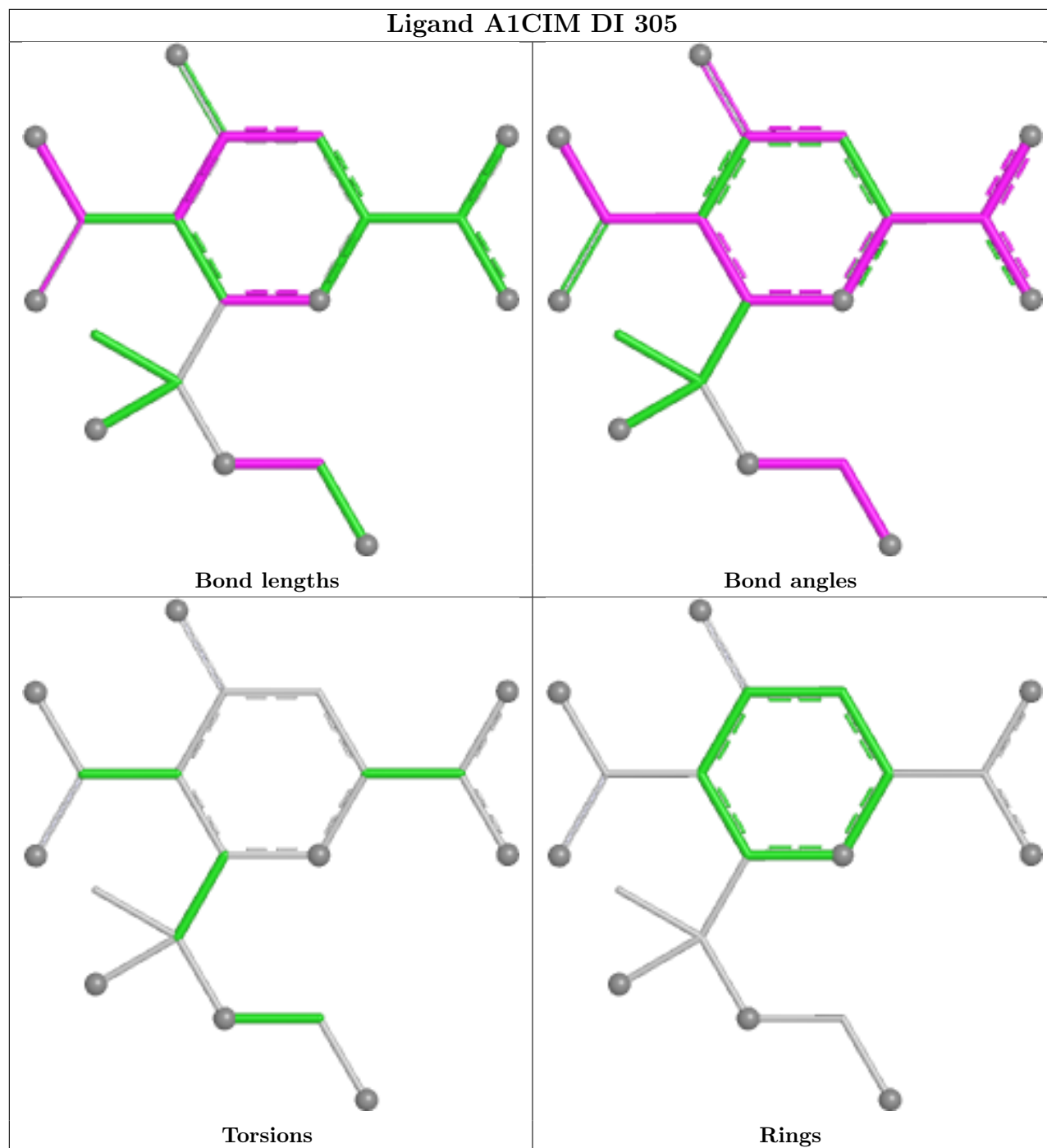
Ligand A1CIM DN 303



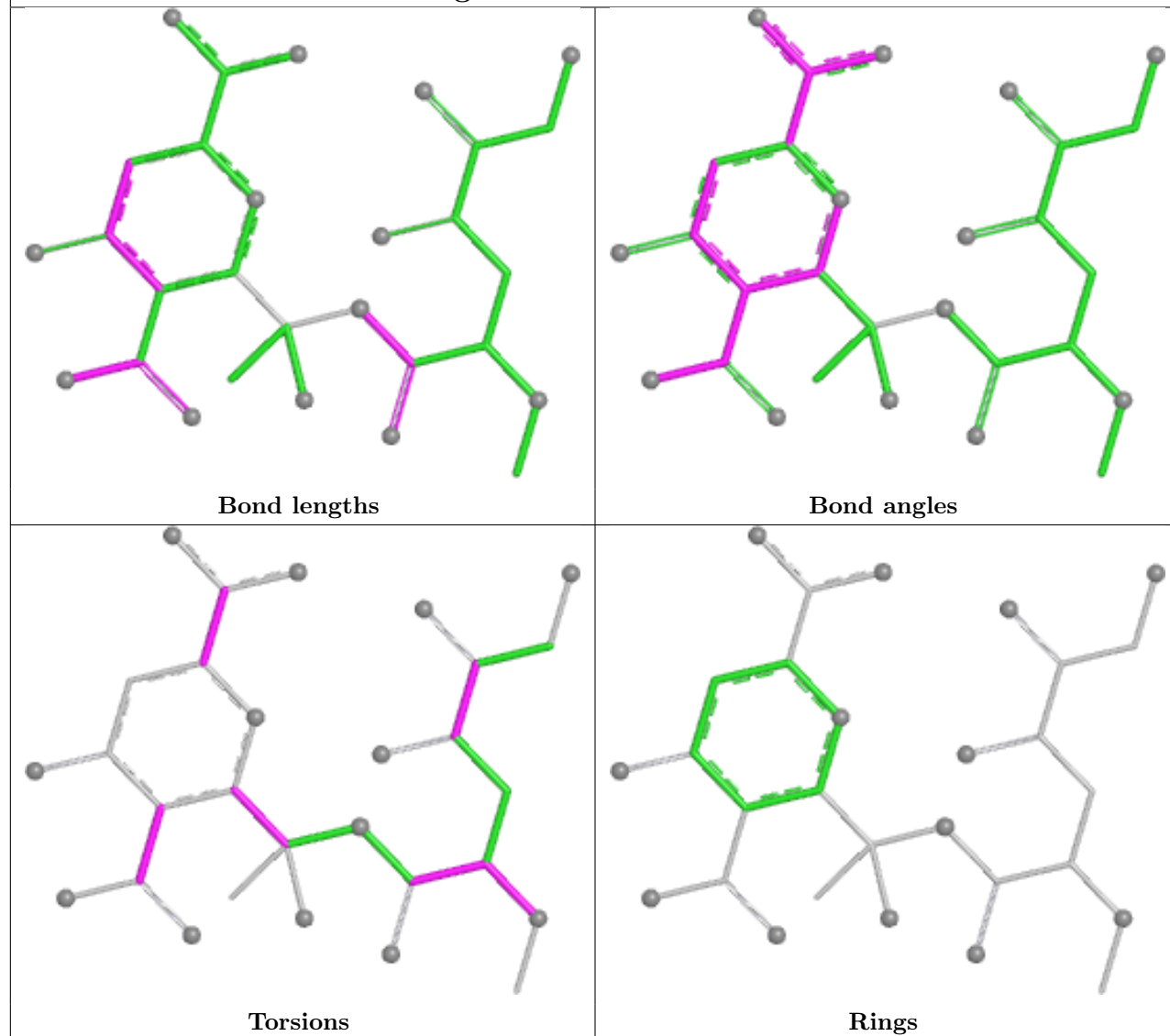
Ligand A1CIM DI 303



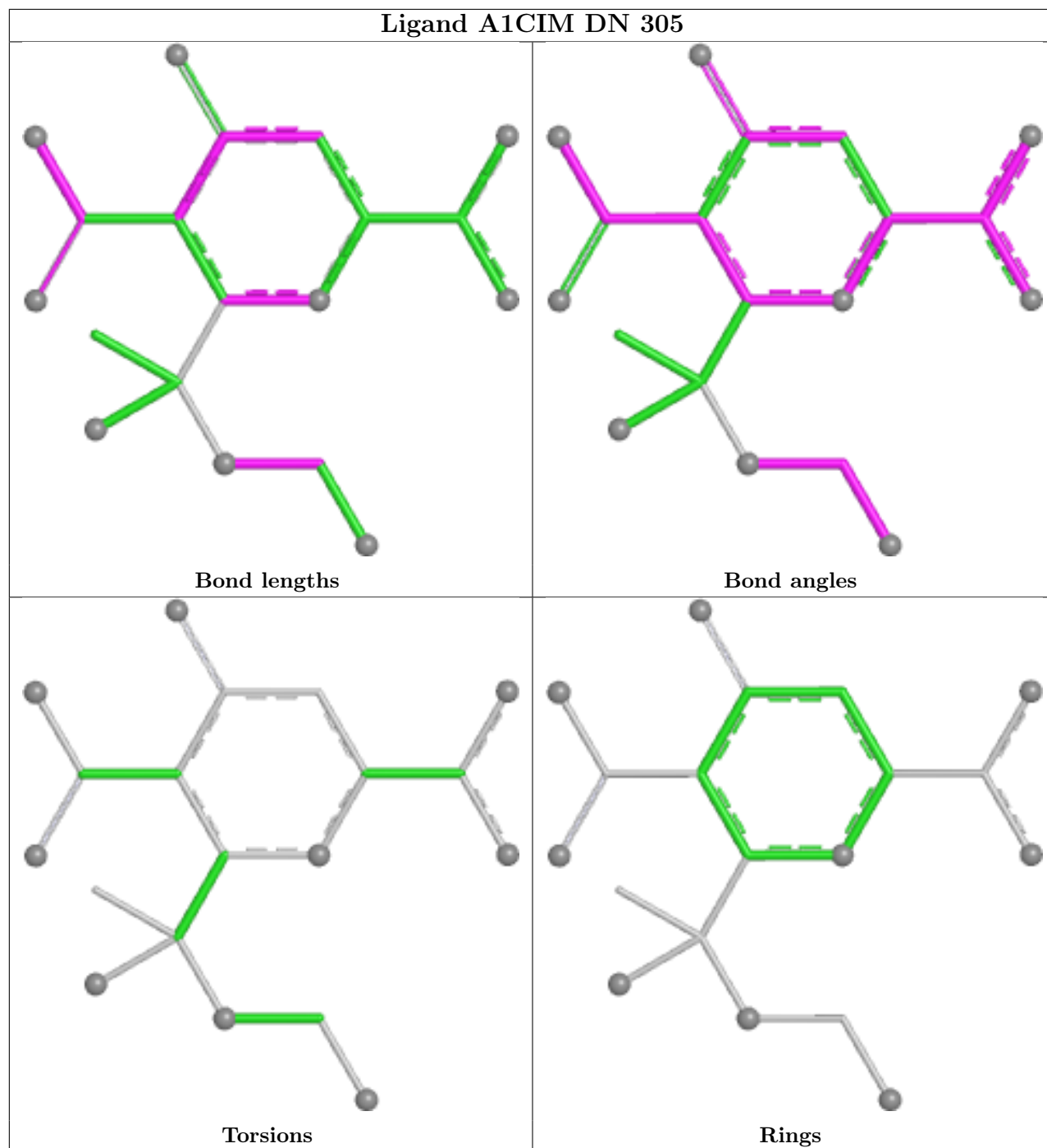
Ligand A1CIM DI 305



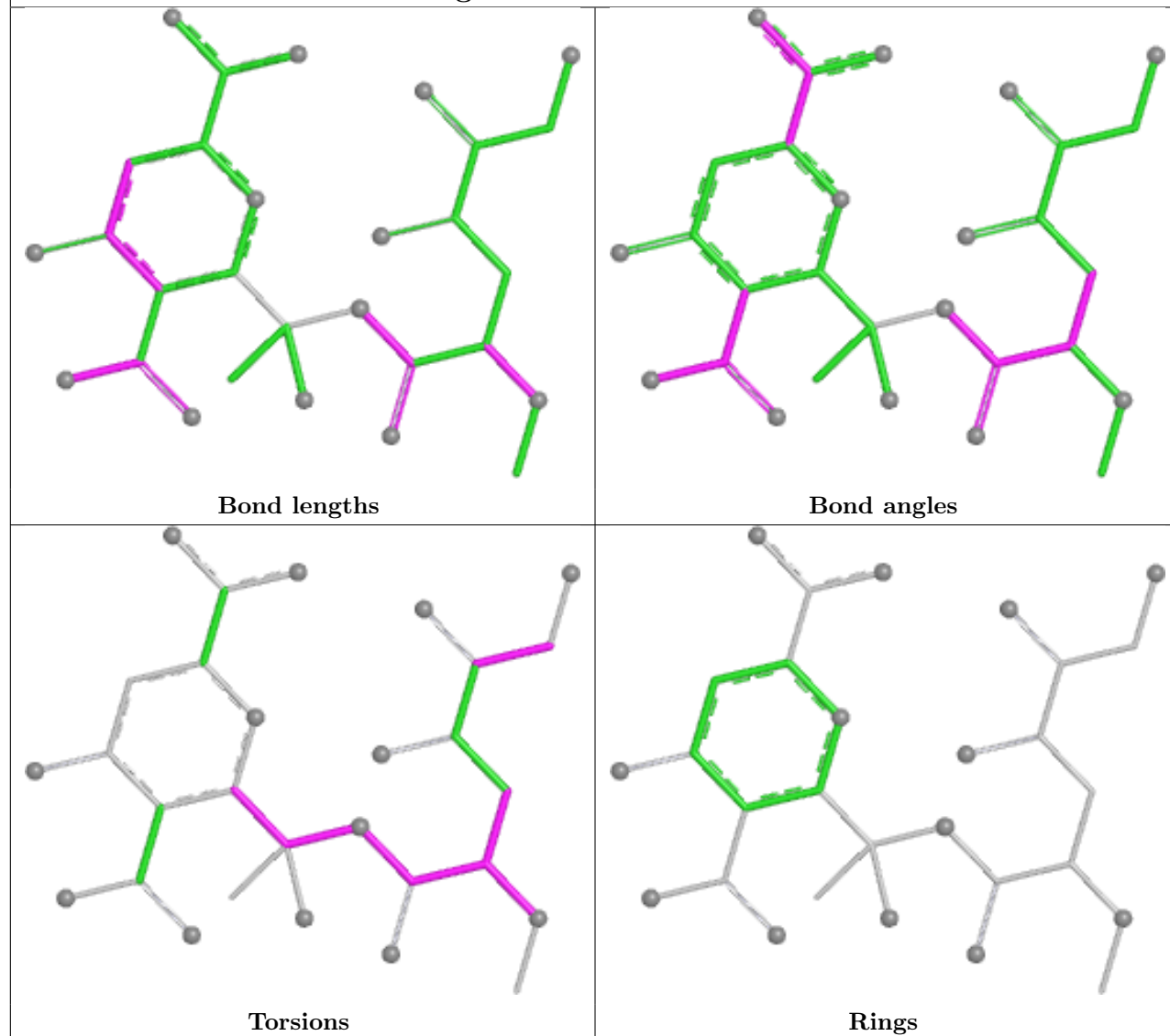
Ligand A1CIM DK 304



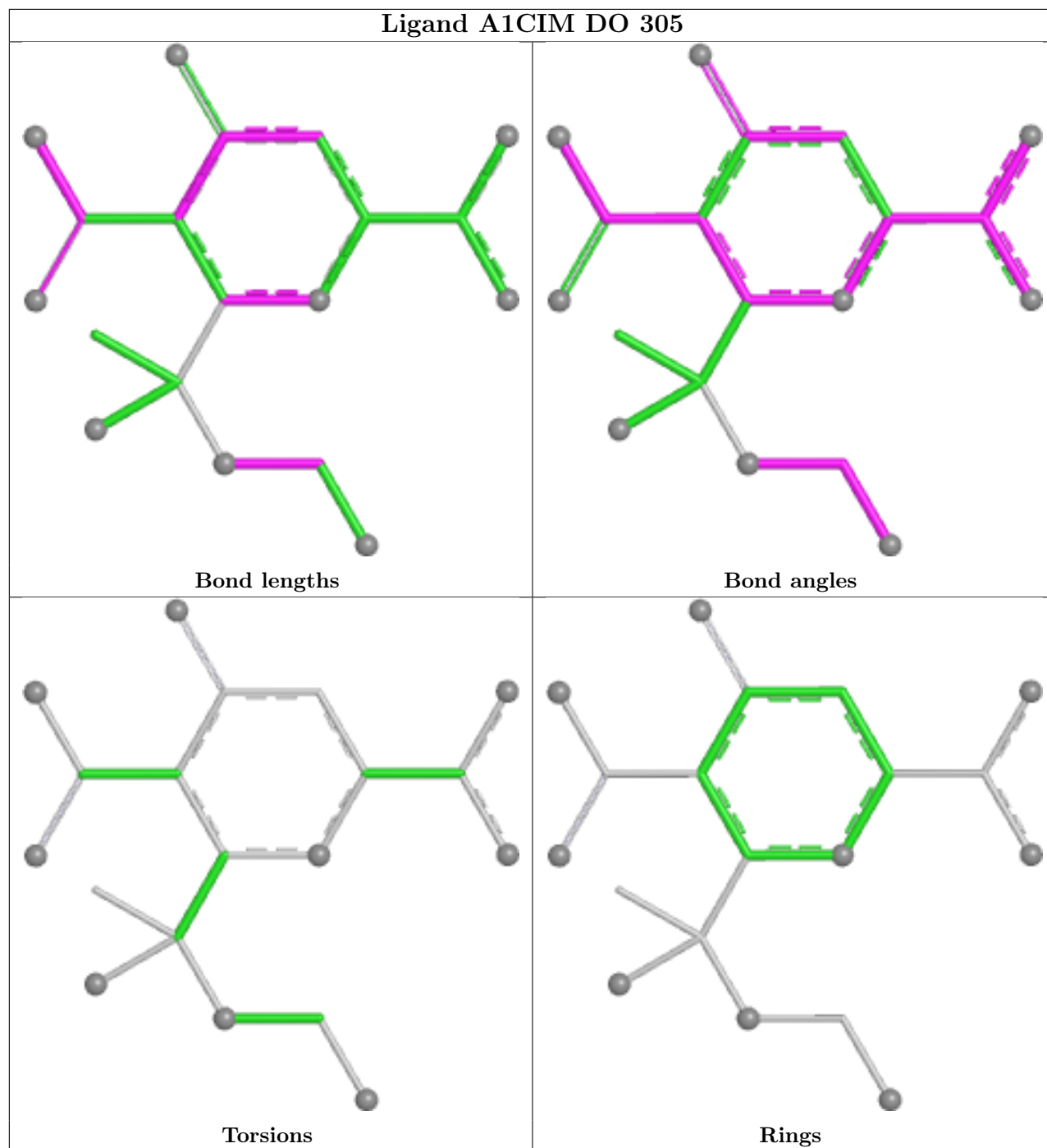
Ligand A1CIM DN 305



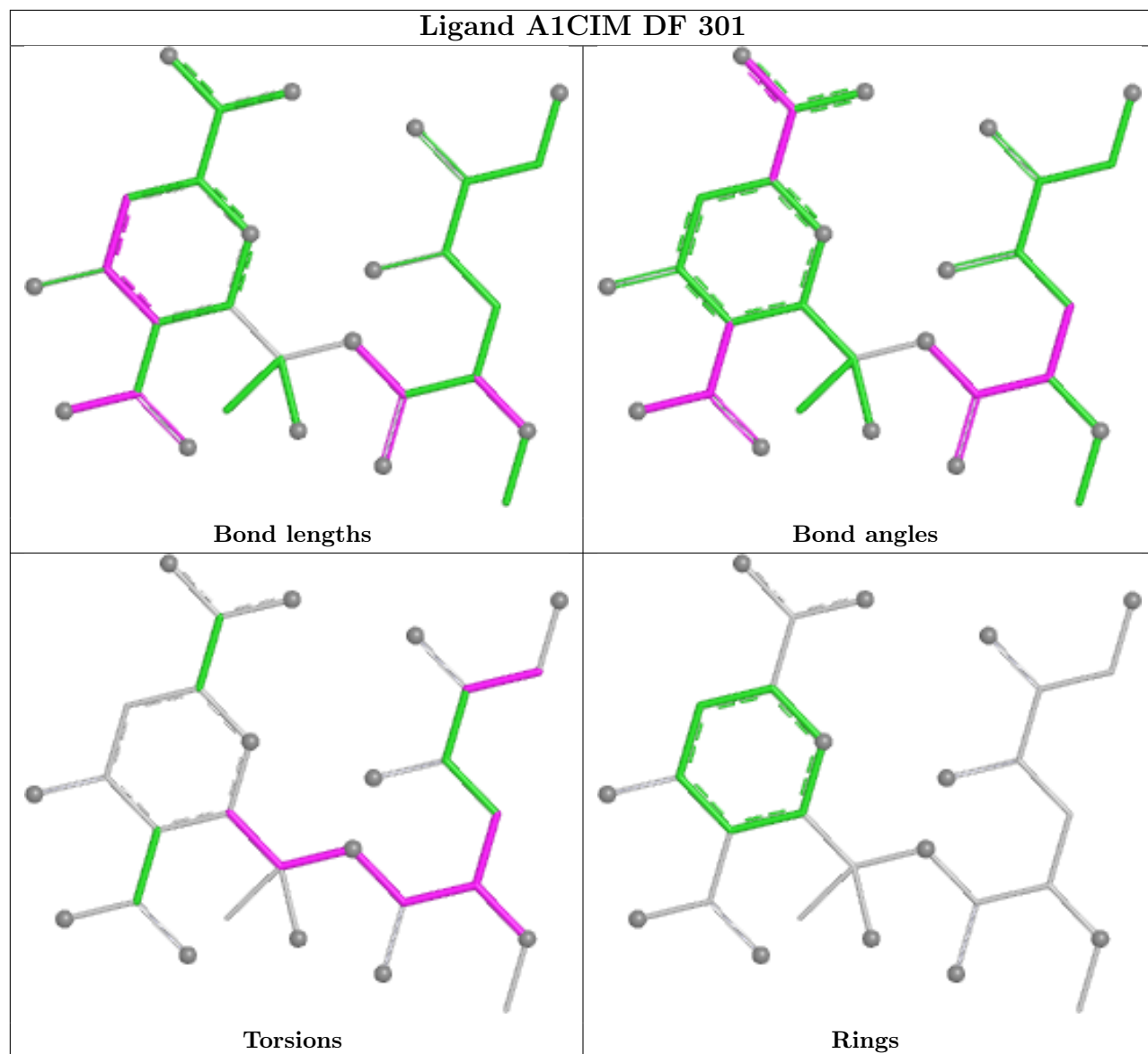
Ligand A1CIM DB 301



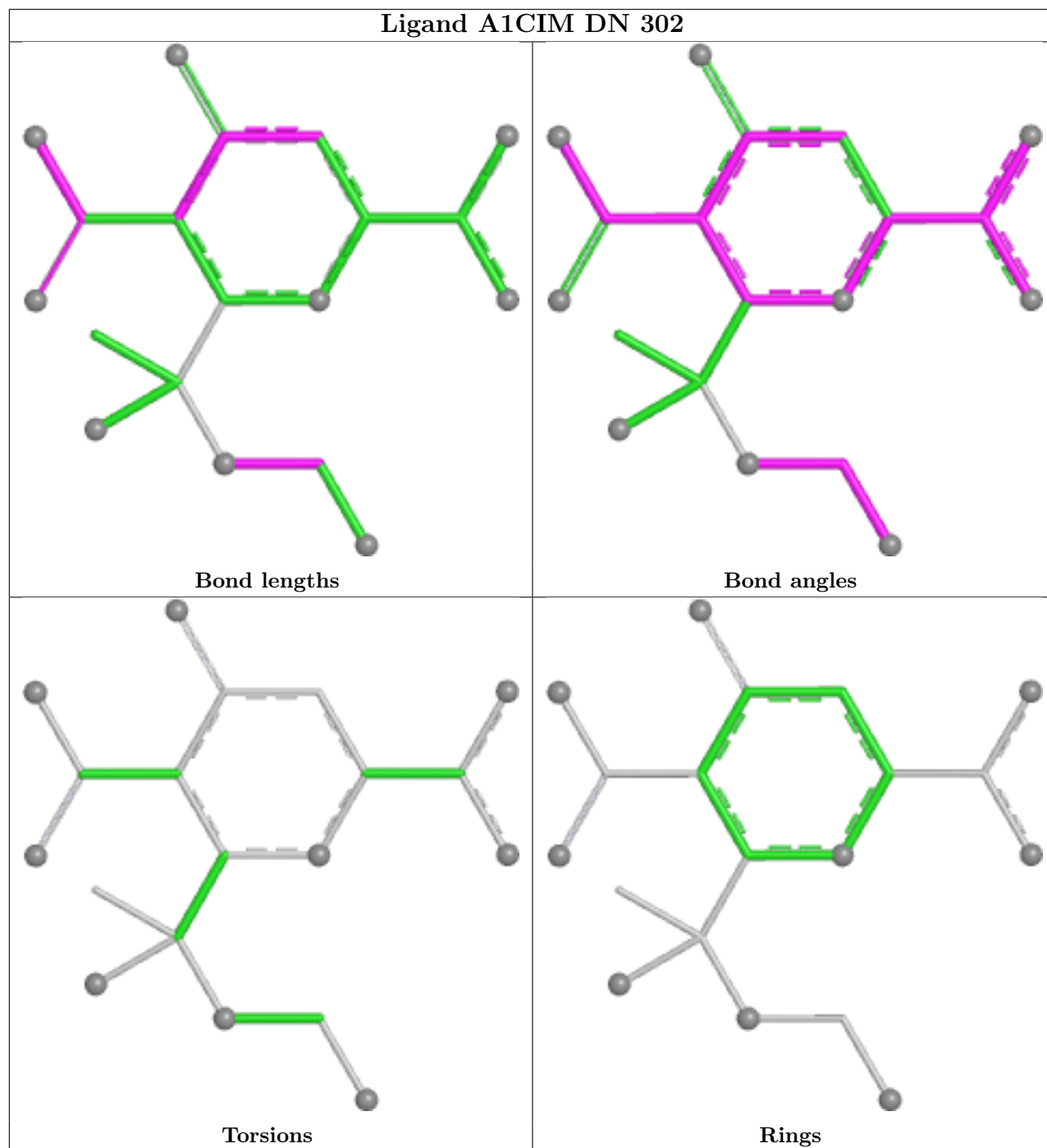
Ligand A1CIM DO 305



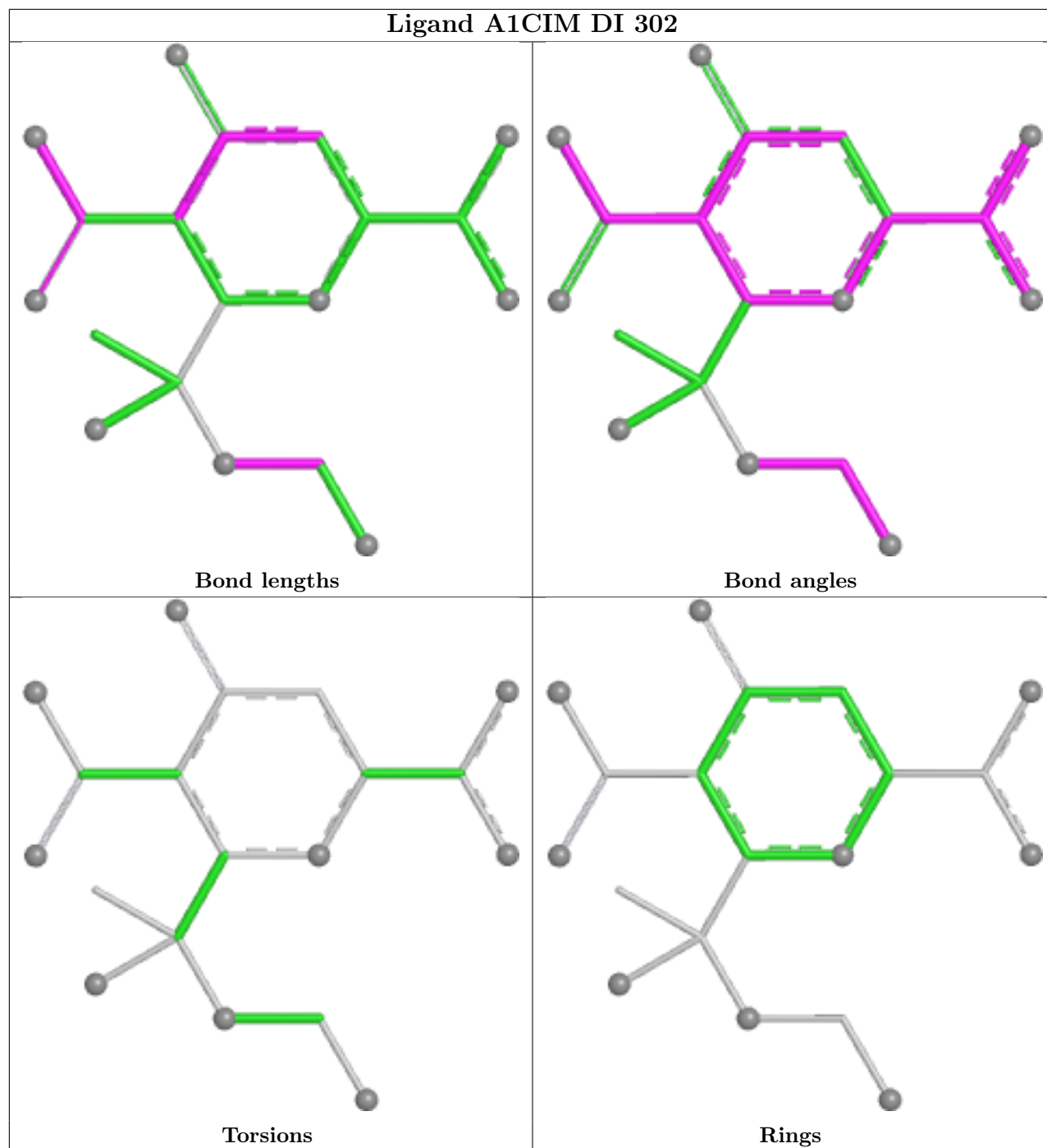
Ligand A1CIM DF 301



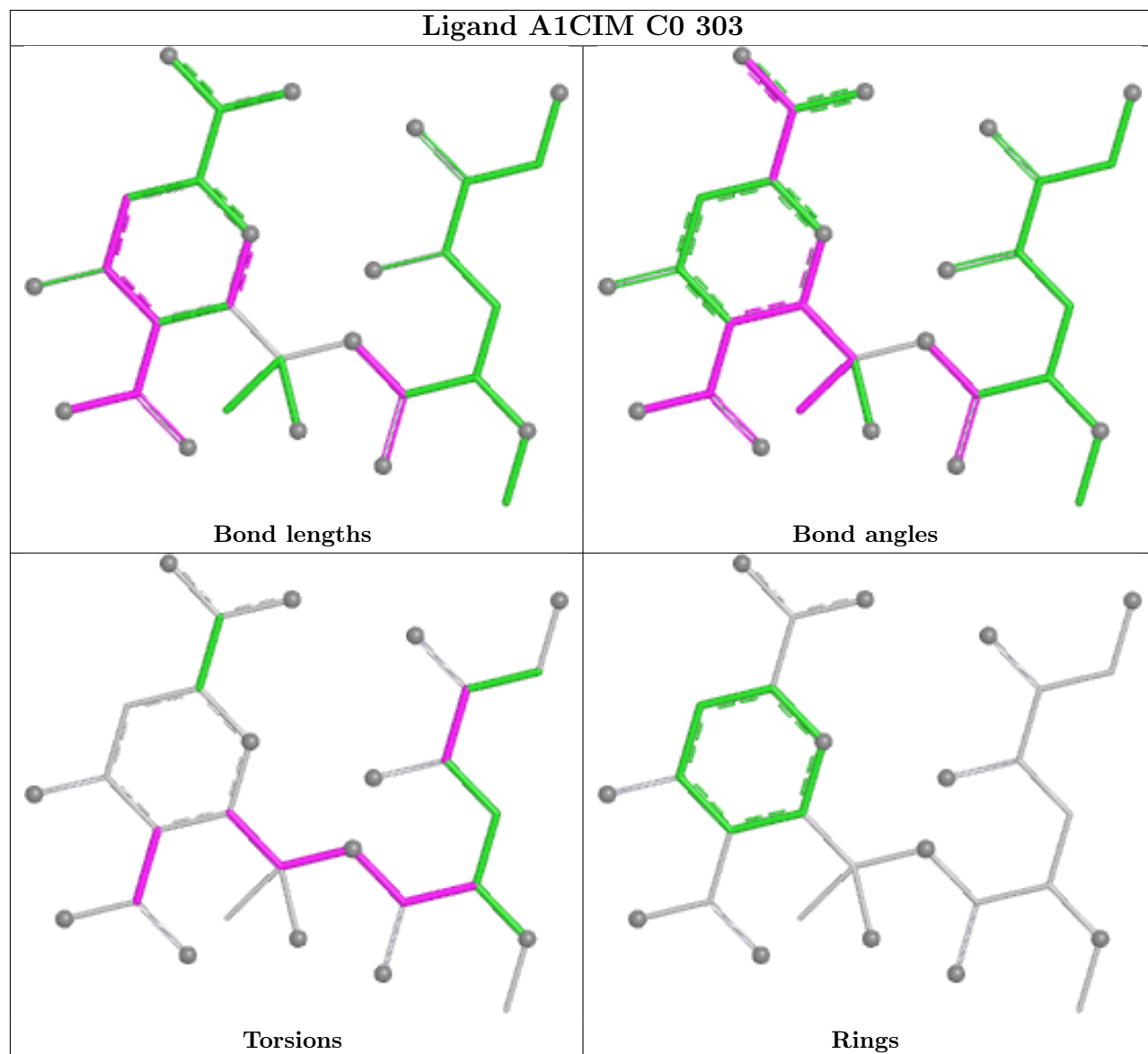
Ligand A1CIM DN 302



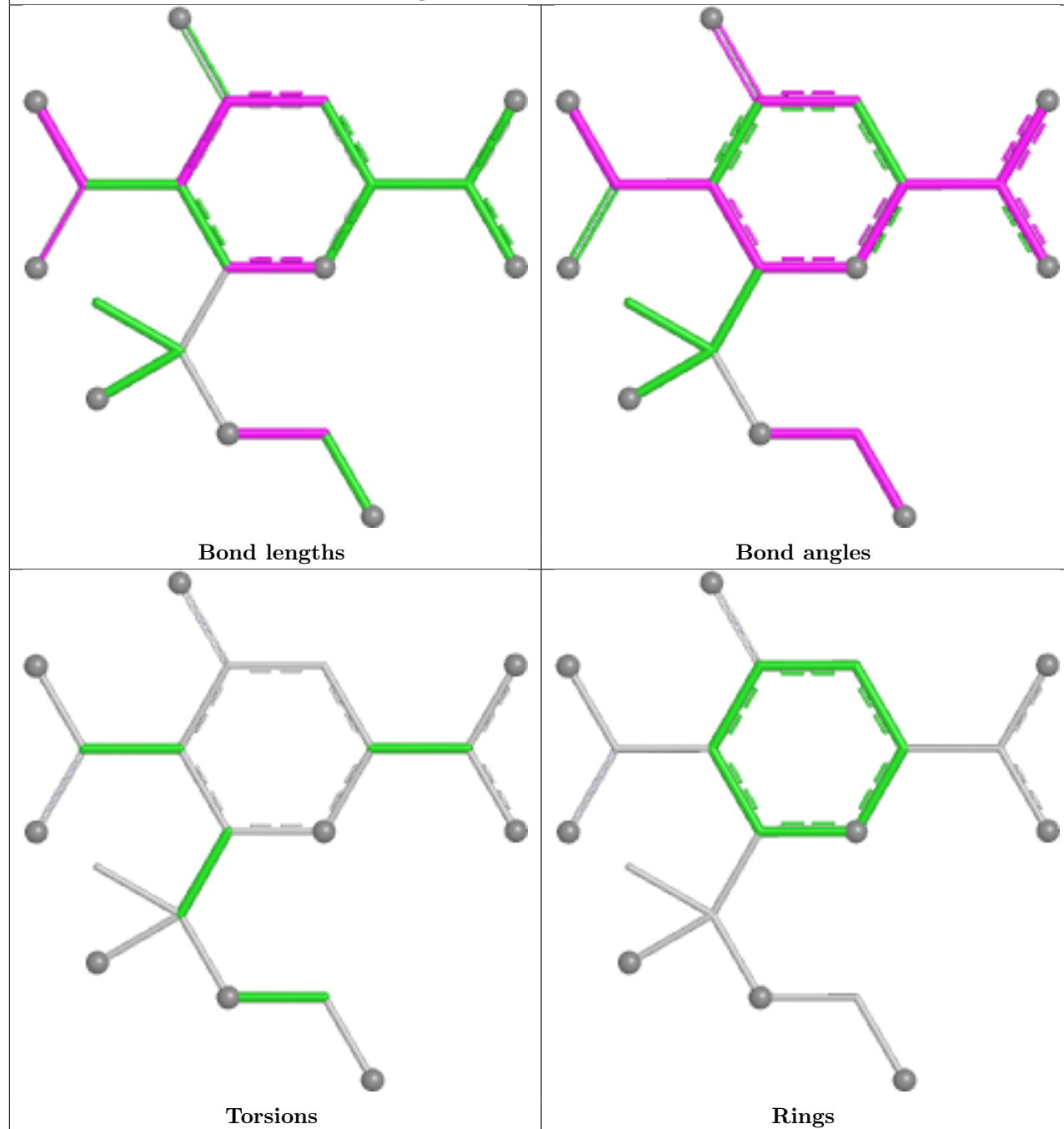
Ligand A1CIM DI 302



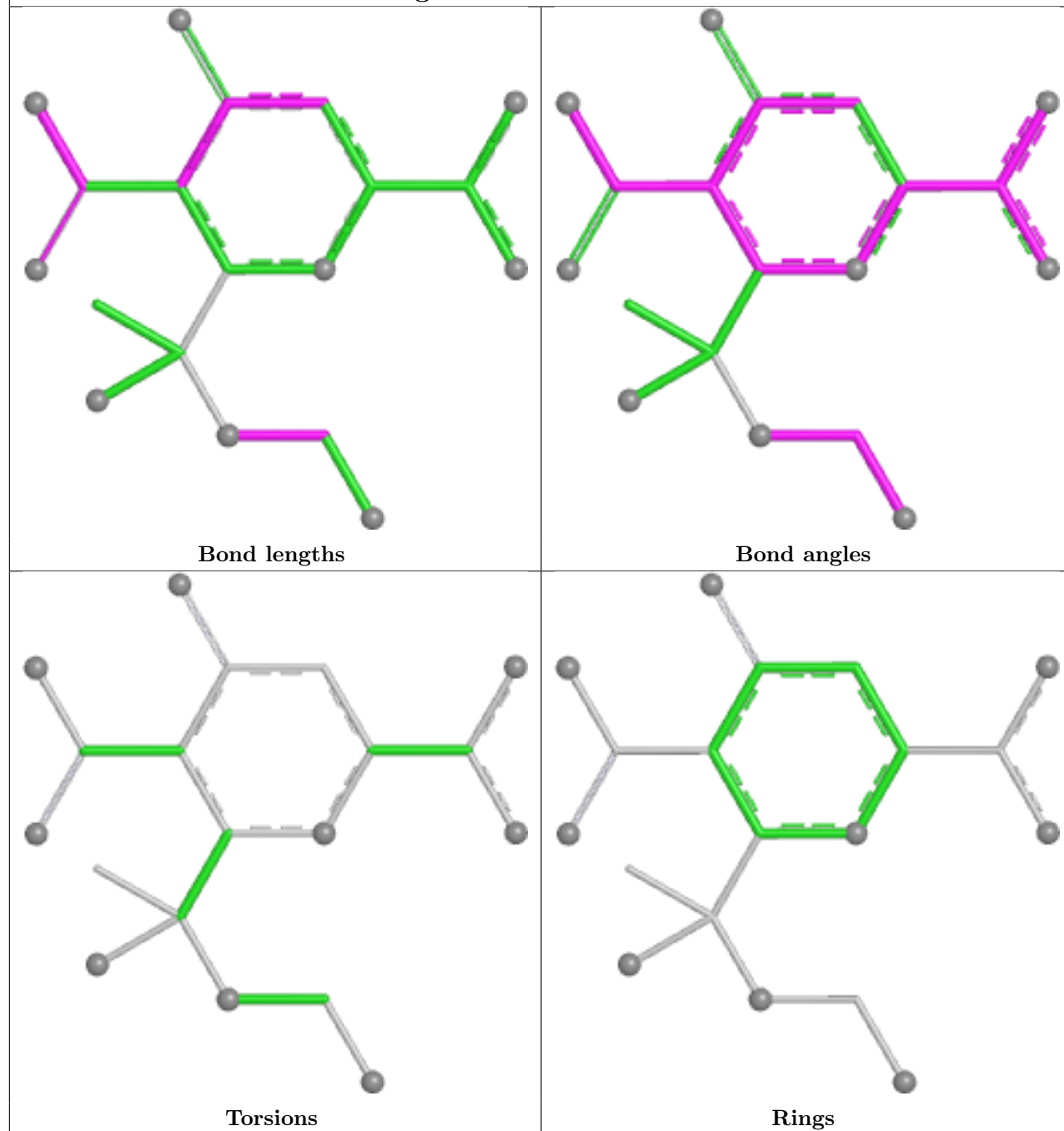
Ligand A1CIM C0 303



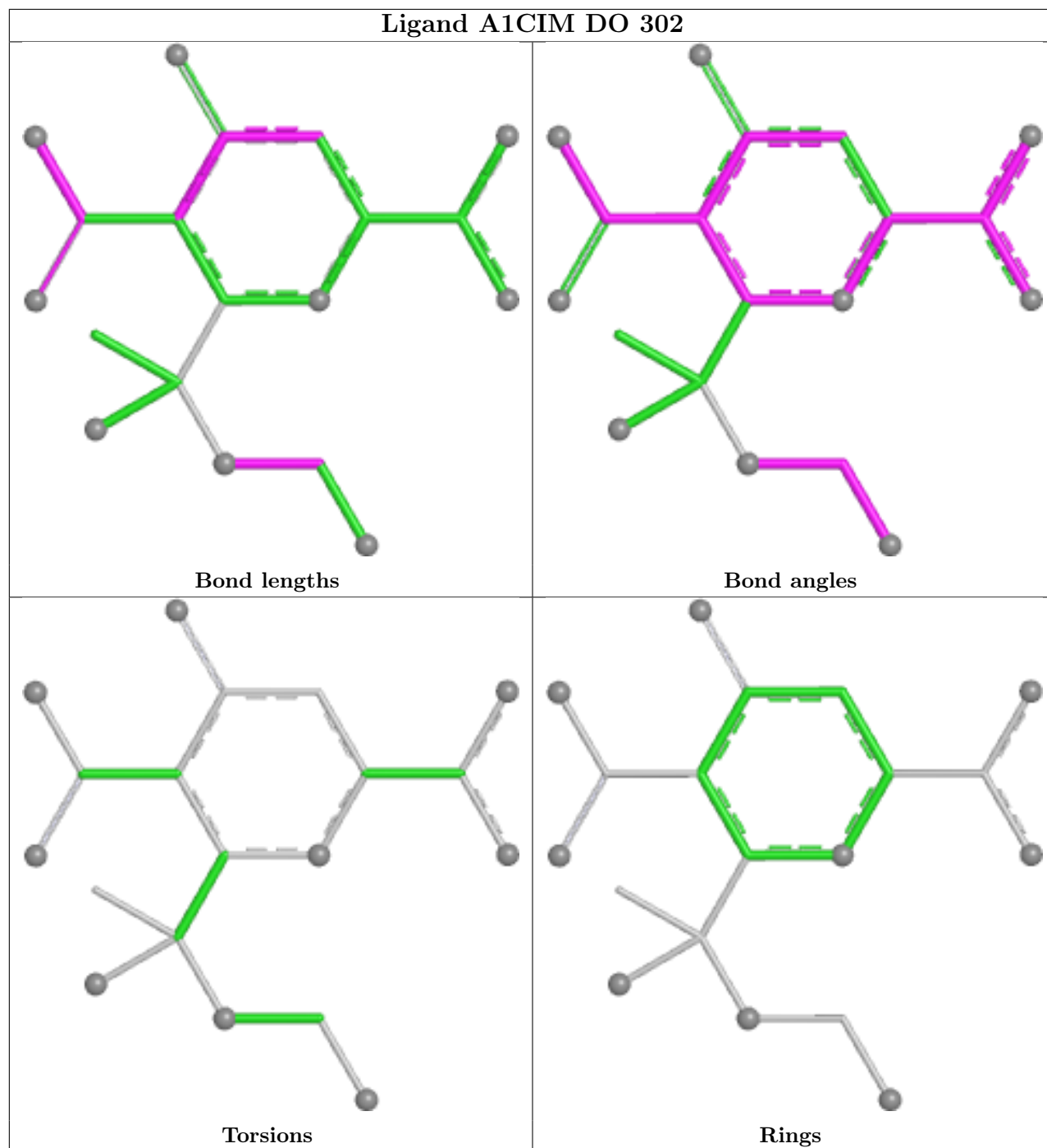
Ligand A1CIM DP 305



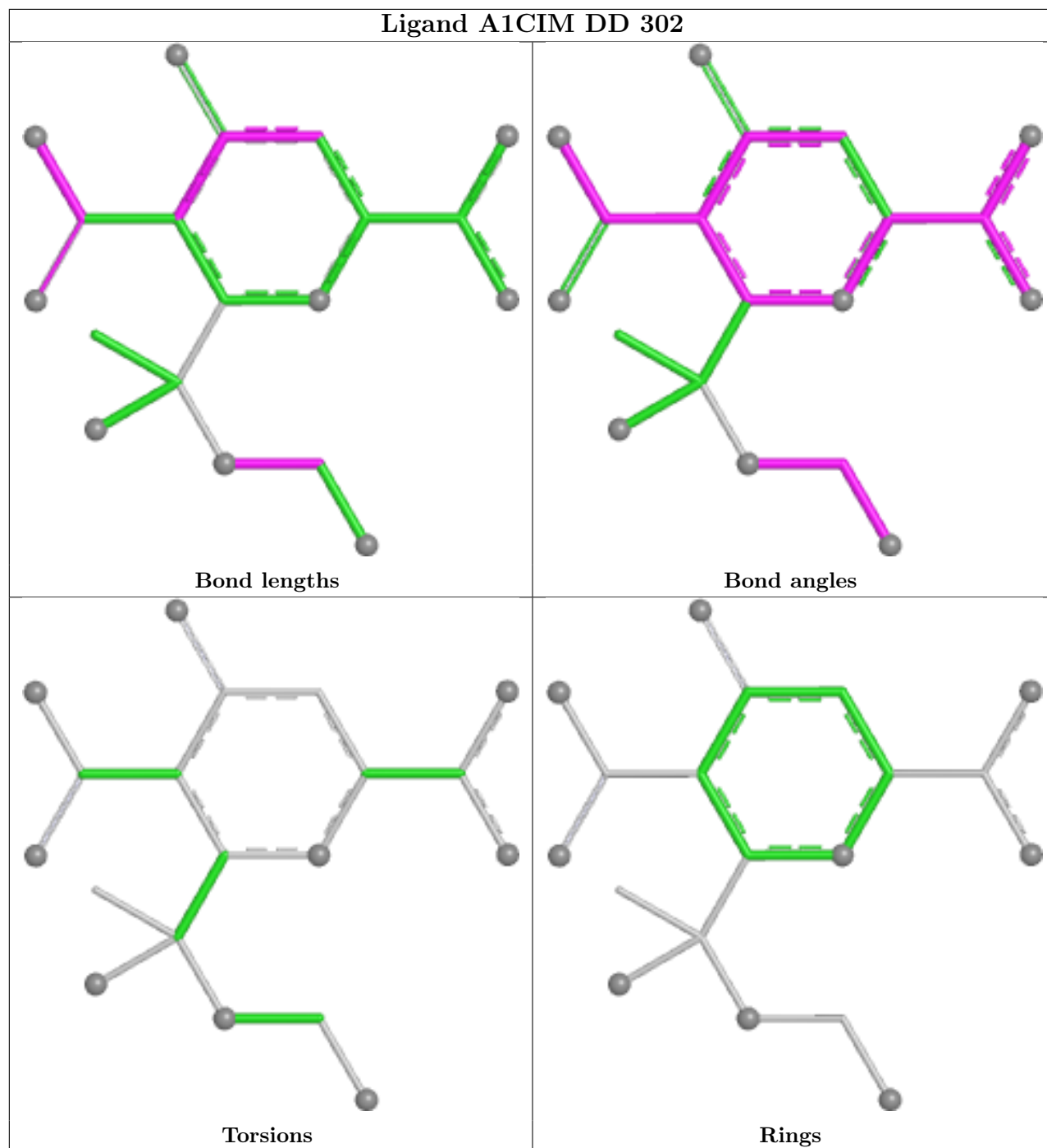
Ligand A1CIM DE 302



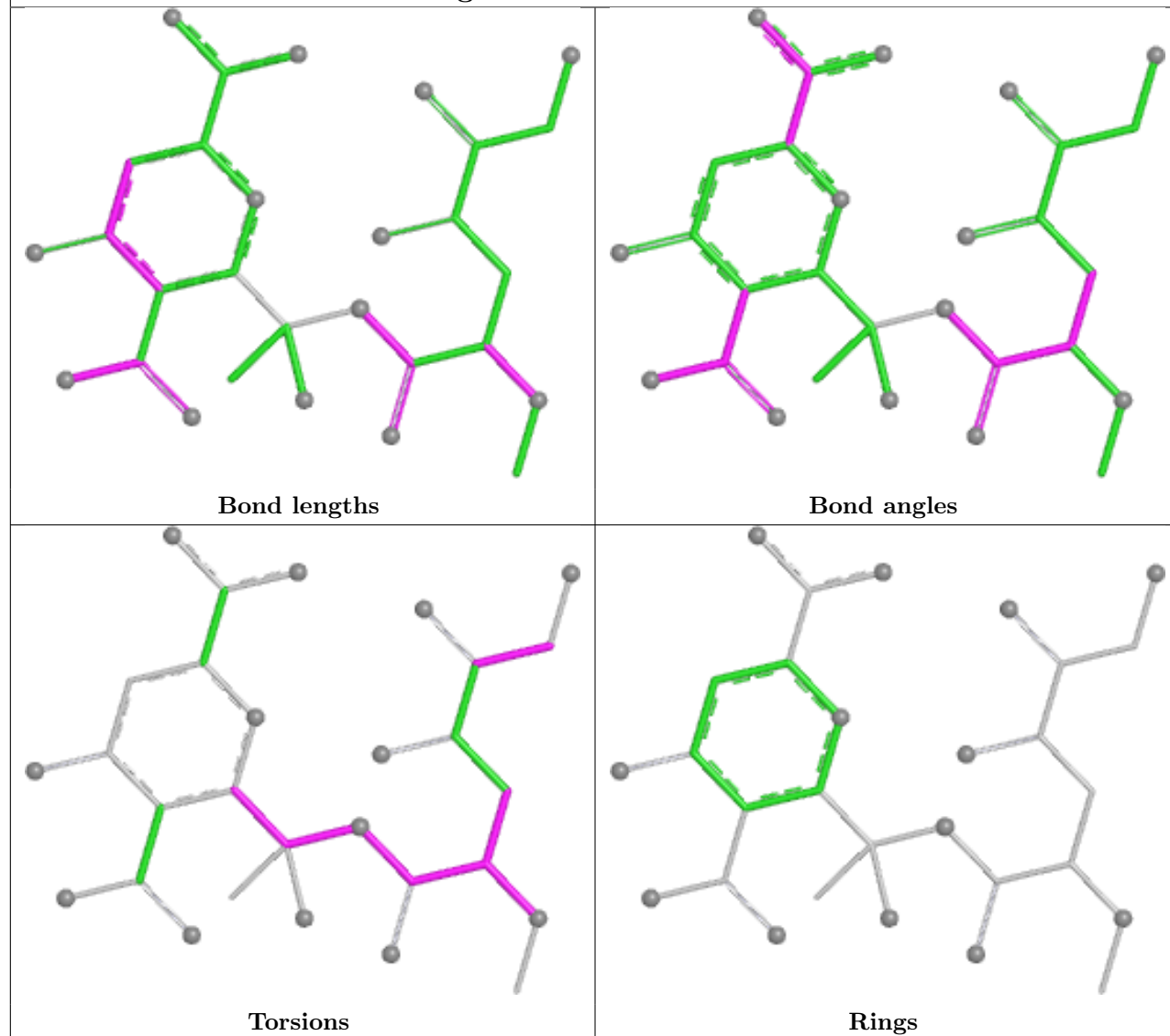
Ligand A1CIM DO 302



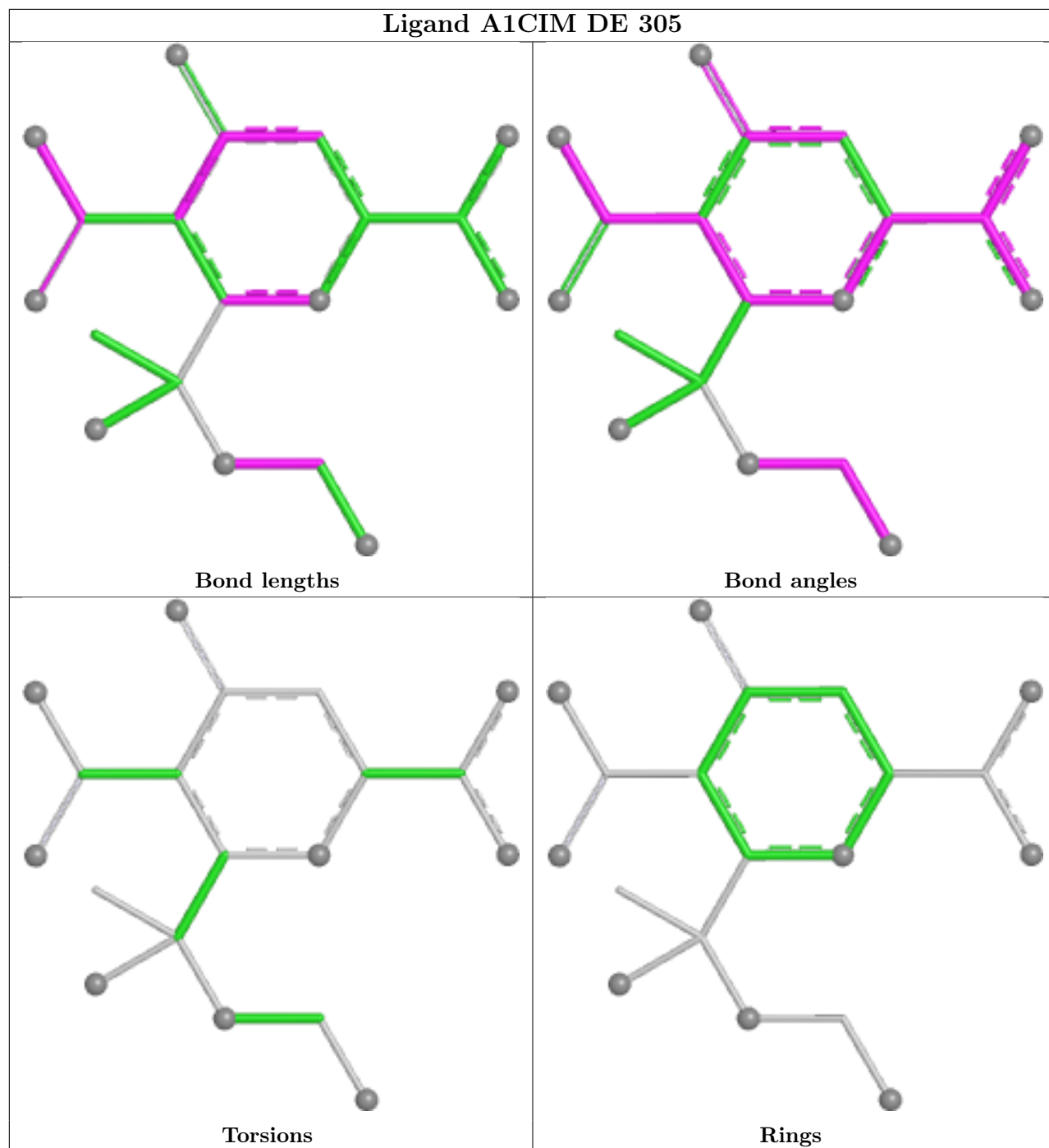
Ligand A1CIM DD 302



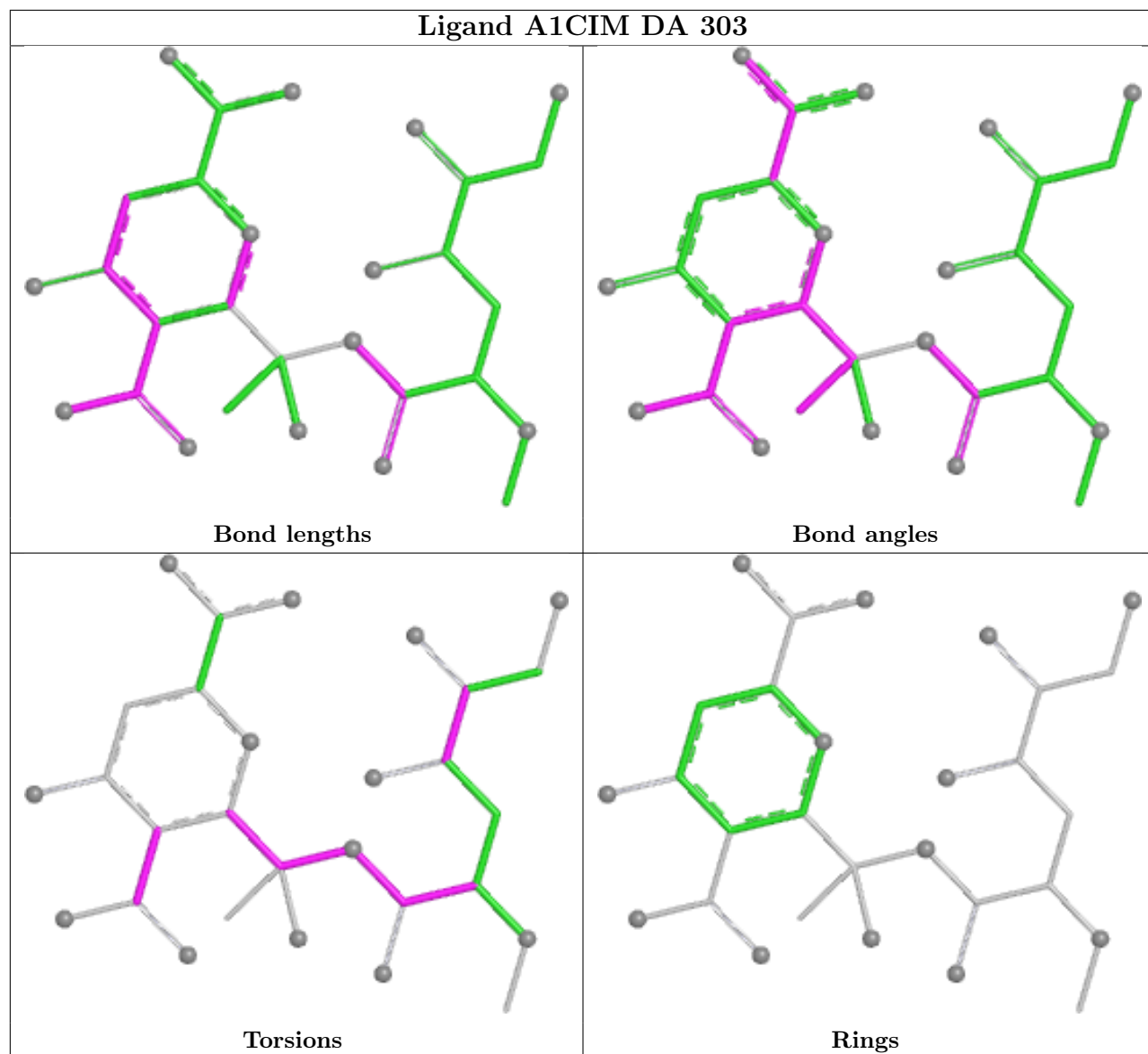
Ligand A1CIM DL 301



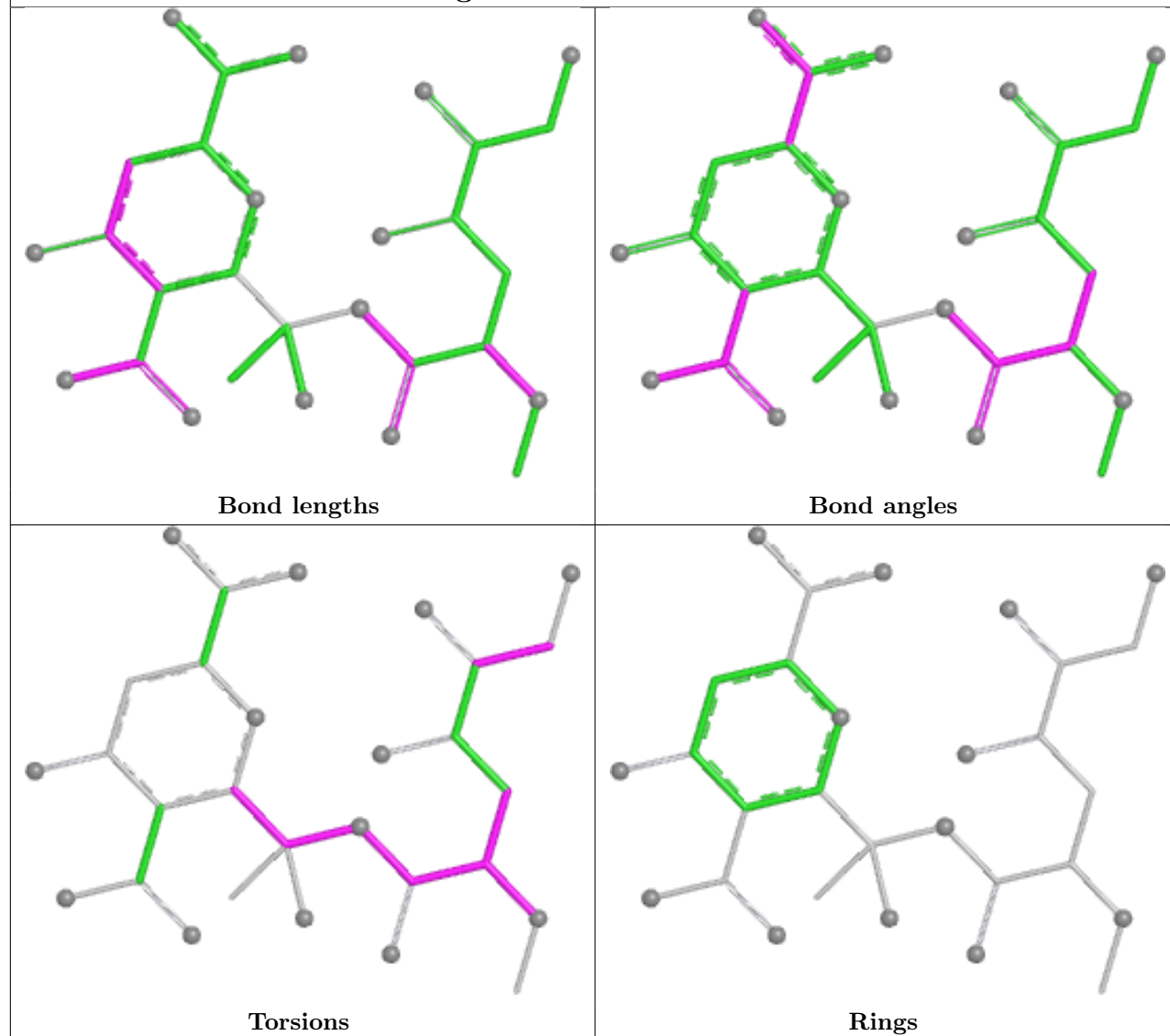
Ligand A1CIM DE 305



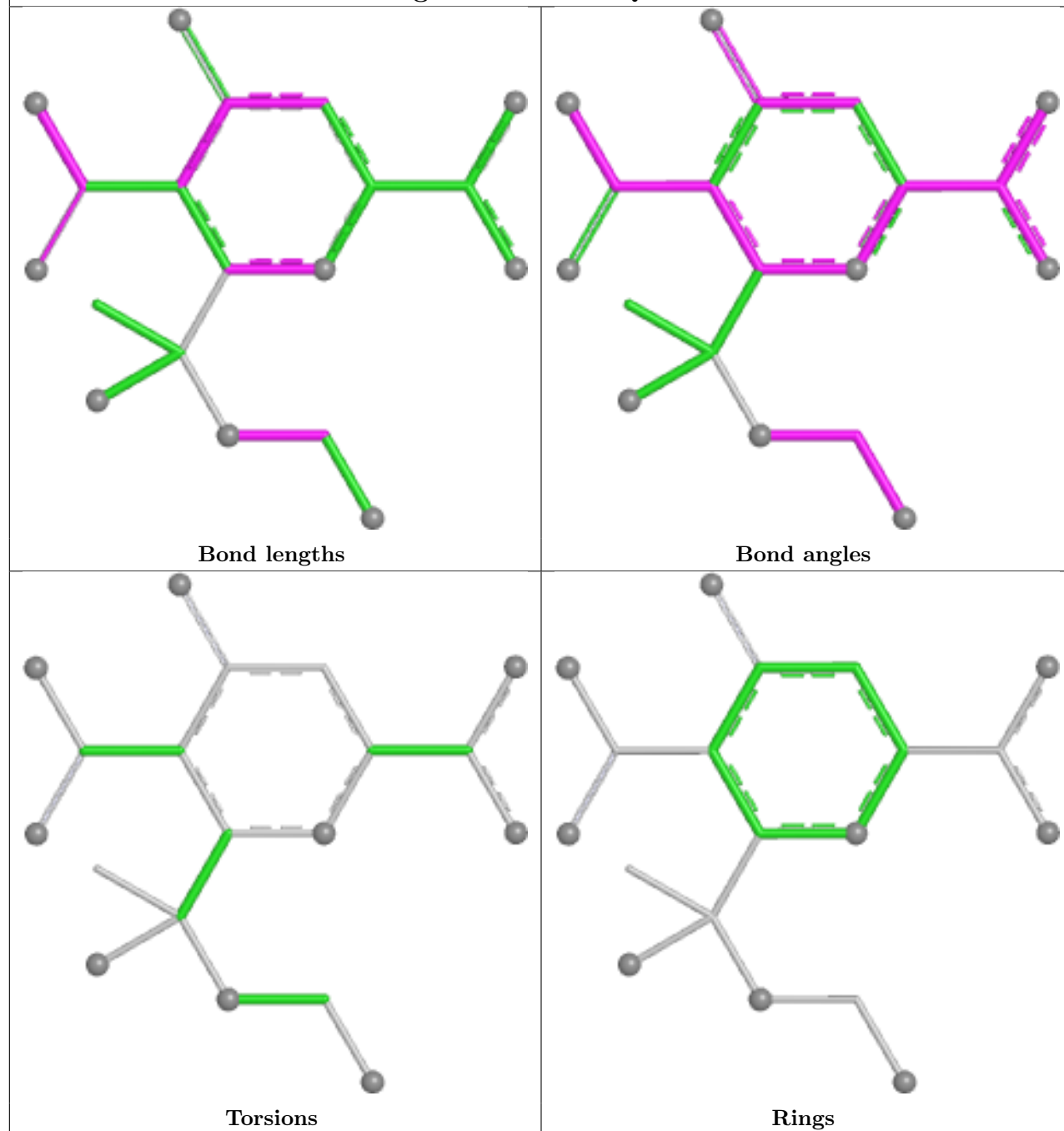
Ligand A1CIM DA 303



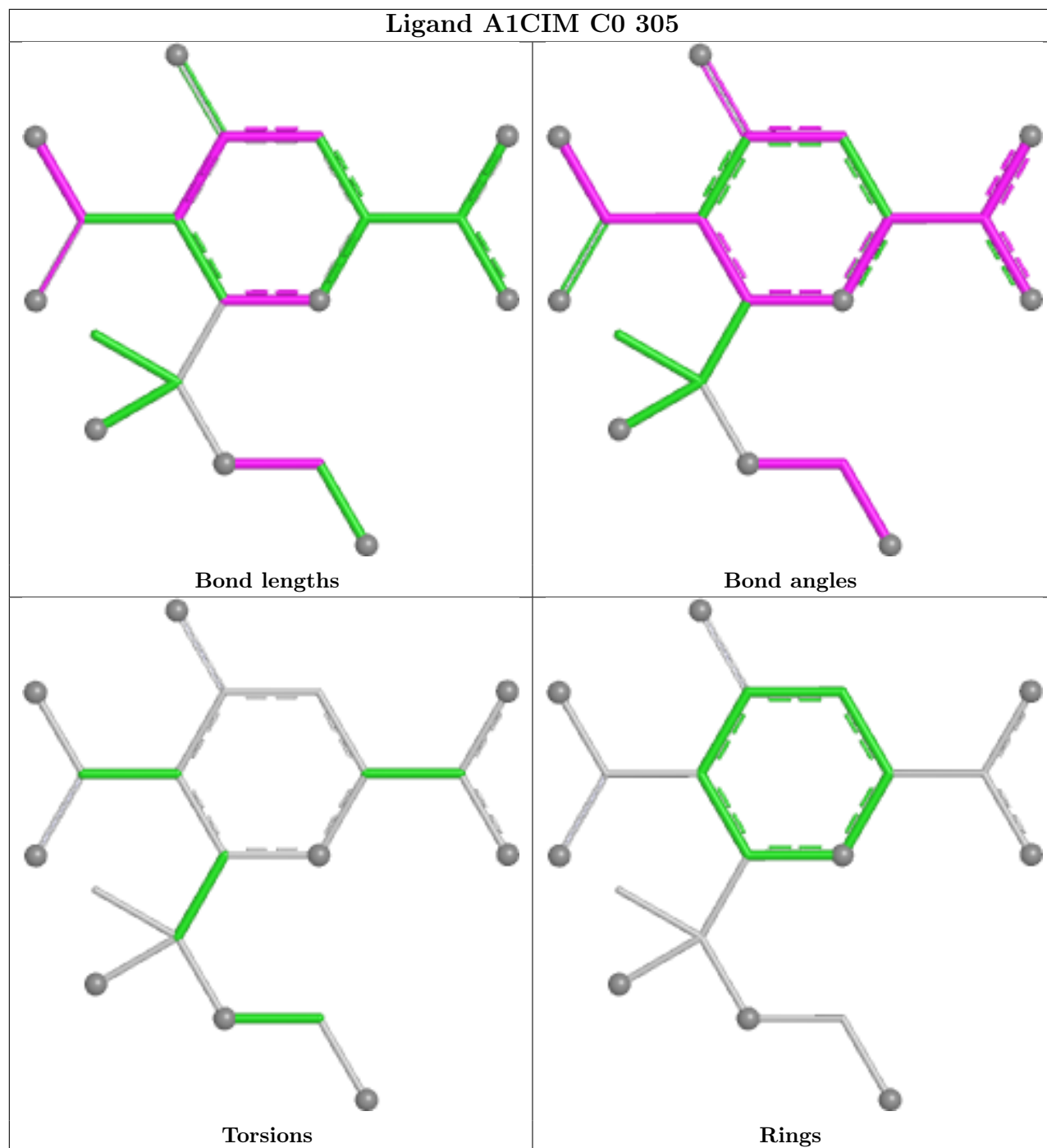
Ligand A1CIM DP 301



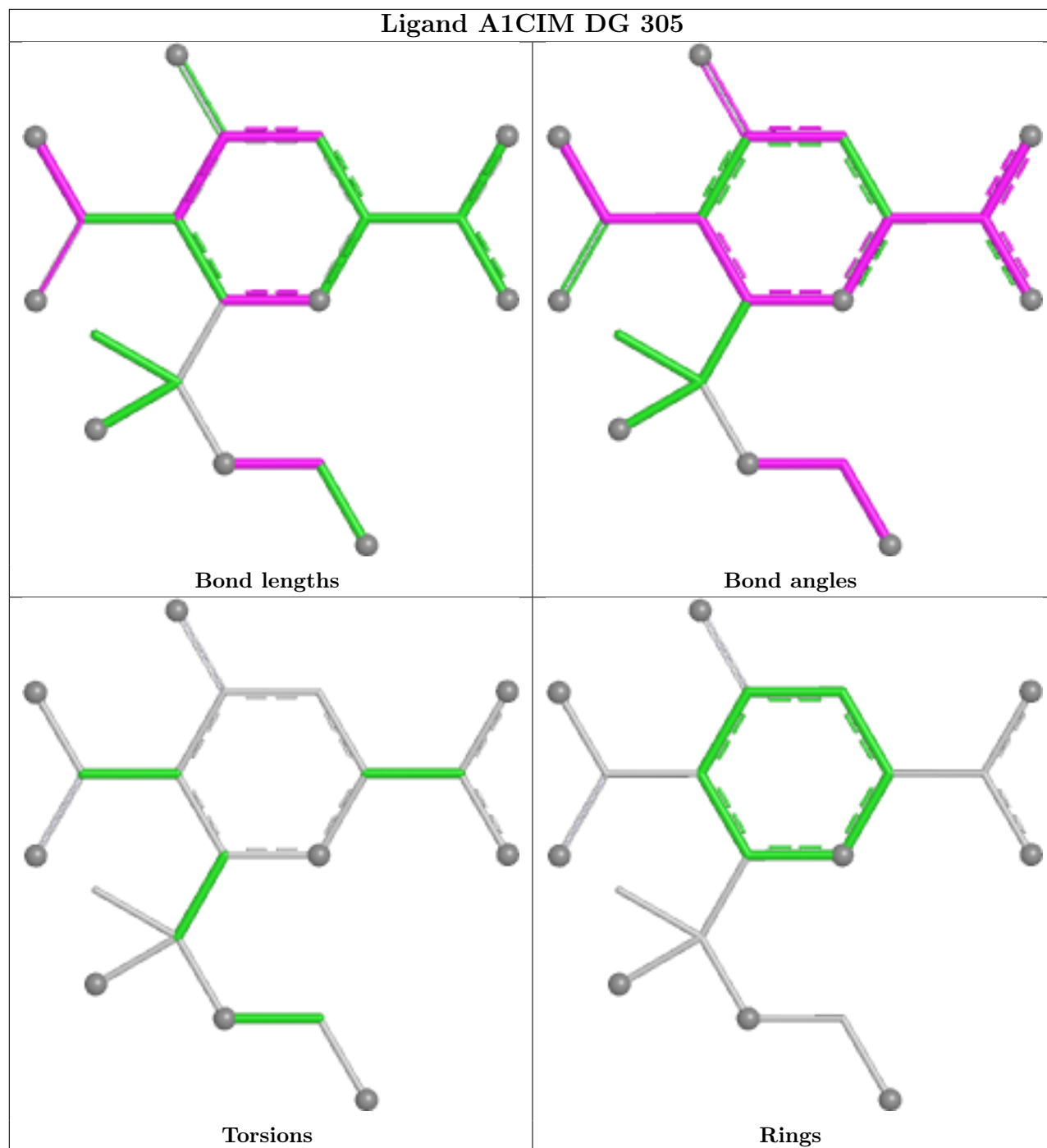
Ligand A1CIM DQ 305



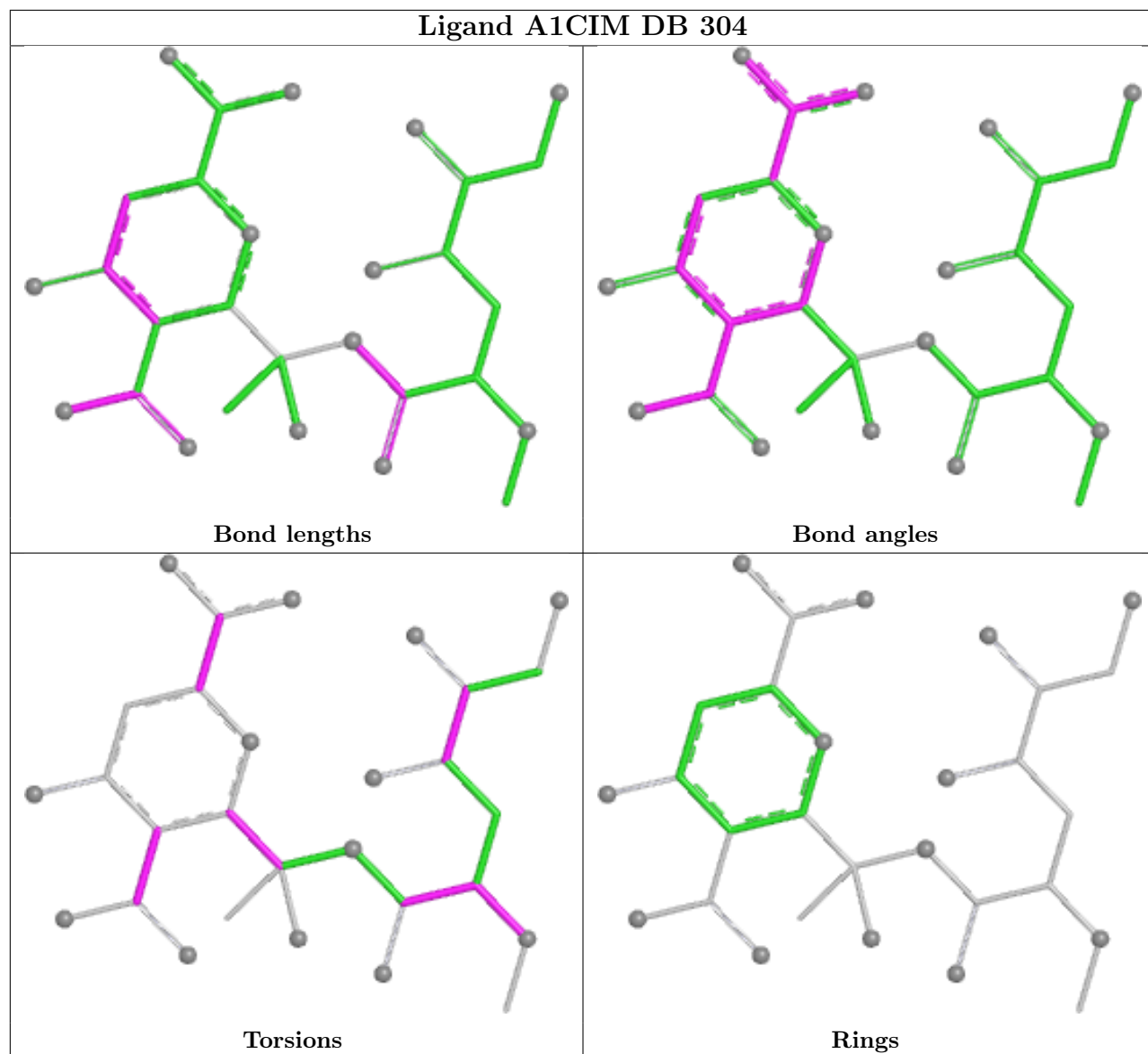
Ligand A1CIM C0 305



Ligand A1CIM DG 305



Ligand A1CIM DB 304



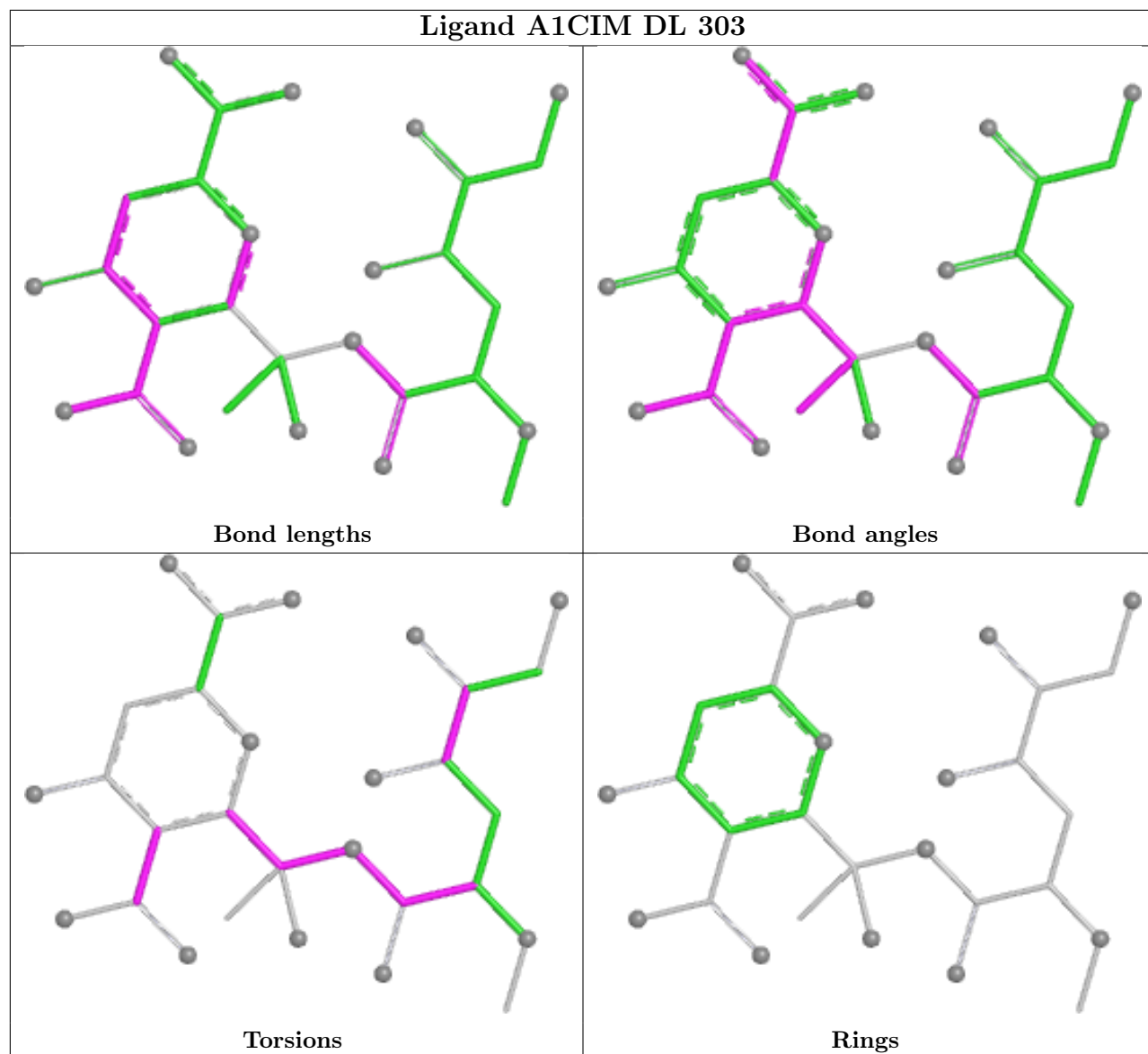
Bond lengths

Bond angles

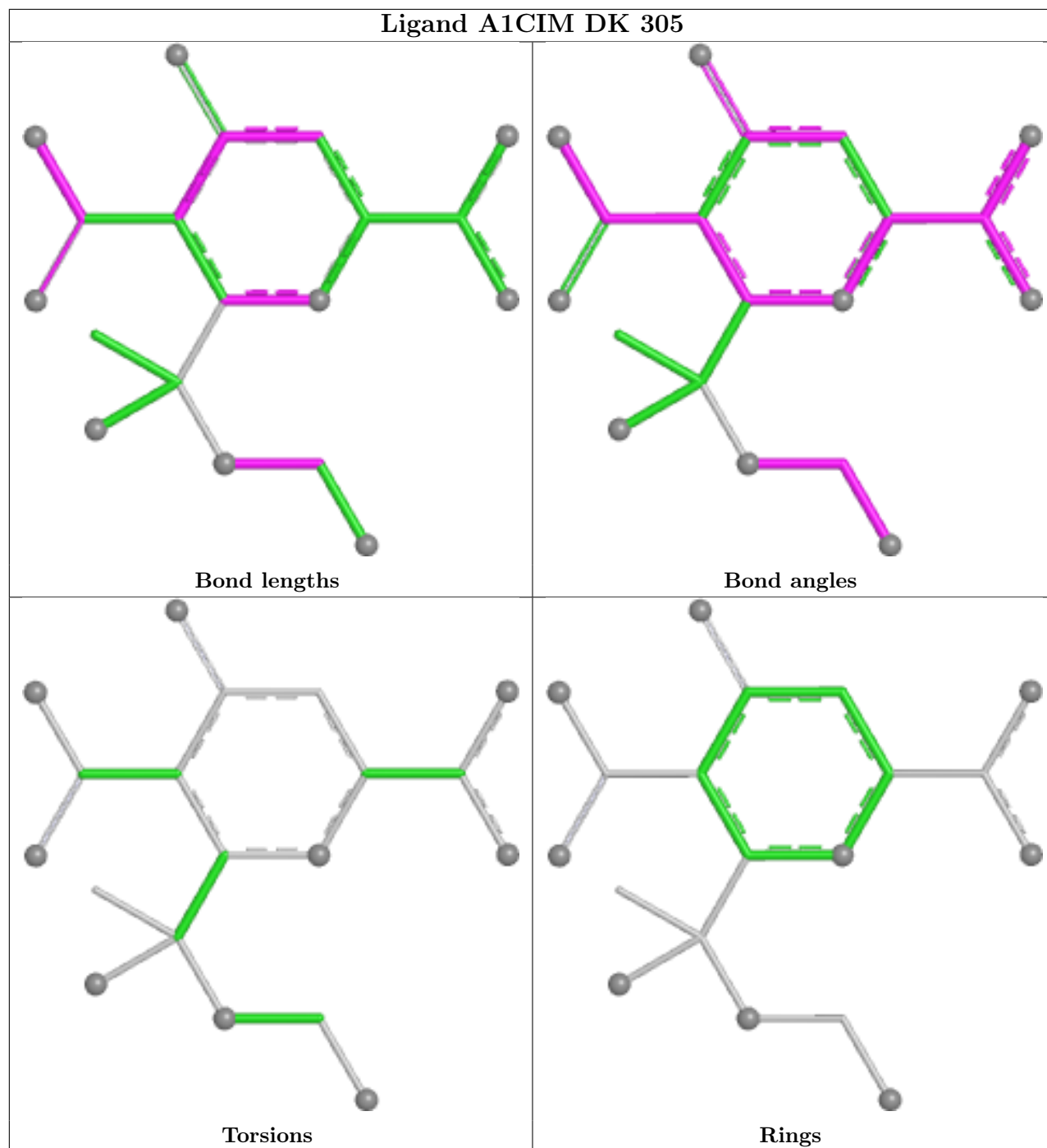
Torsions

Rings

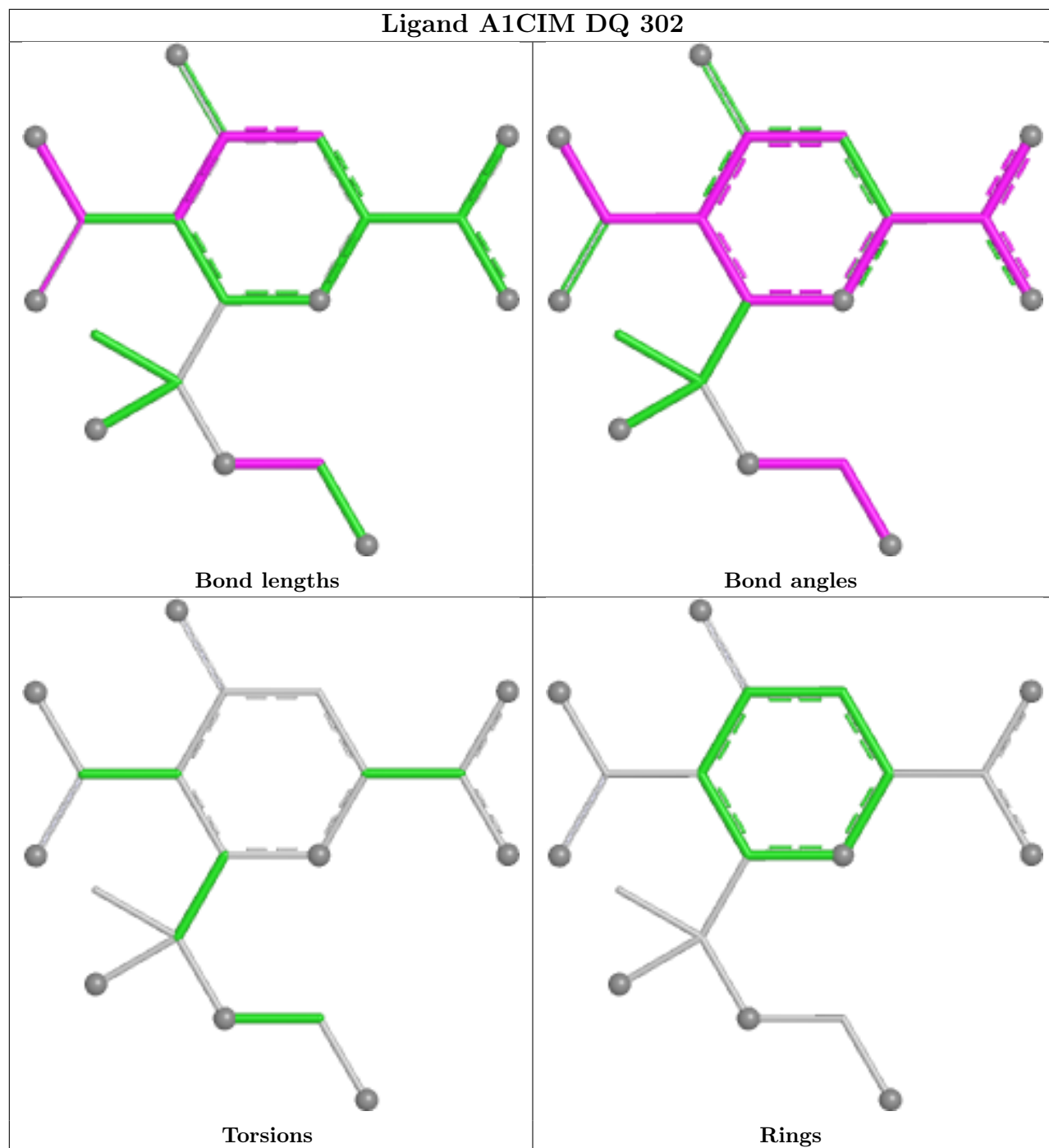
Ligand A1CIM DL 303



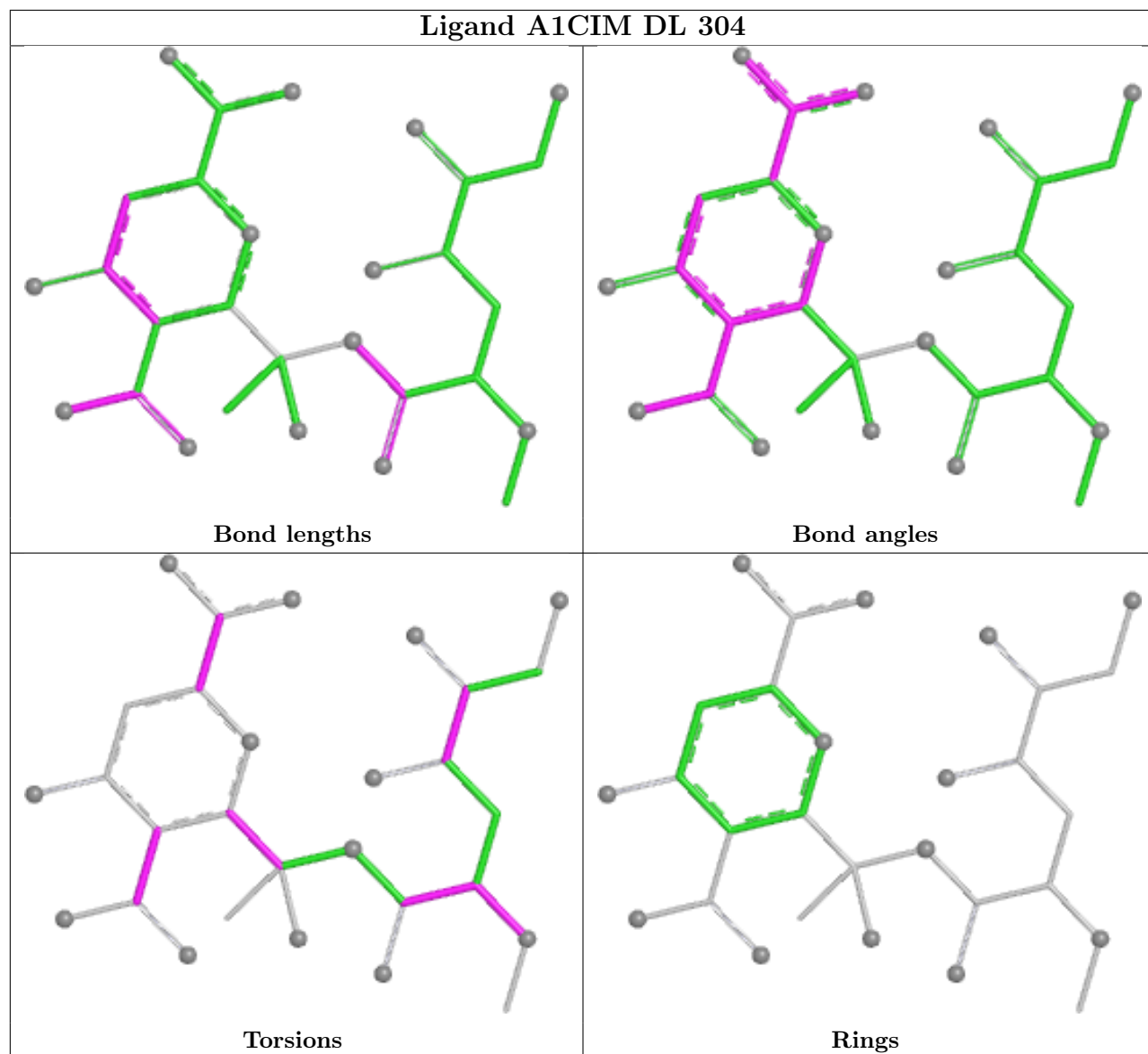
Ligand A1CIM DK 305



Ligand A1CIM DQ 302



Ligand A1CIM DL 304



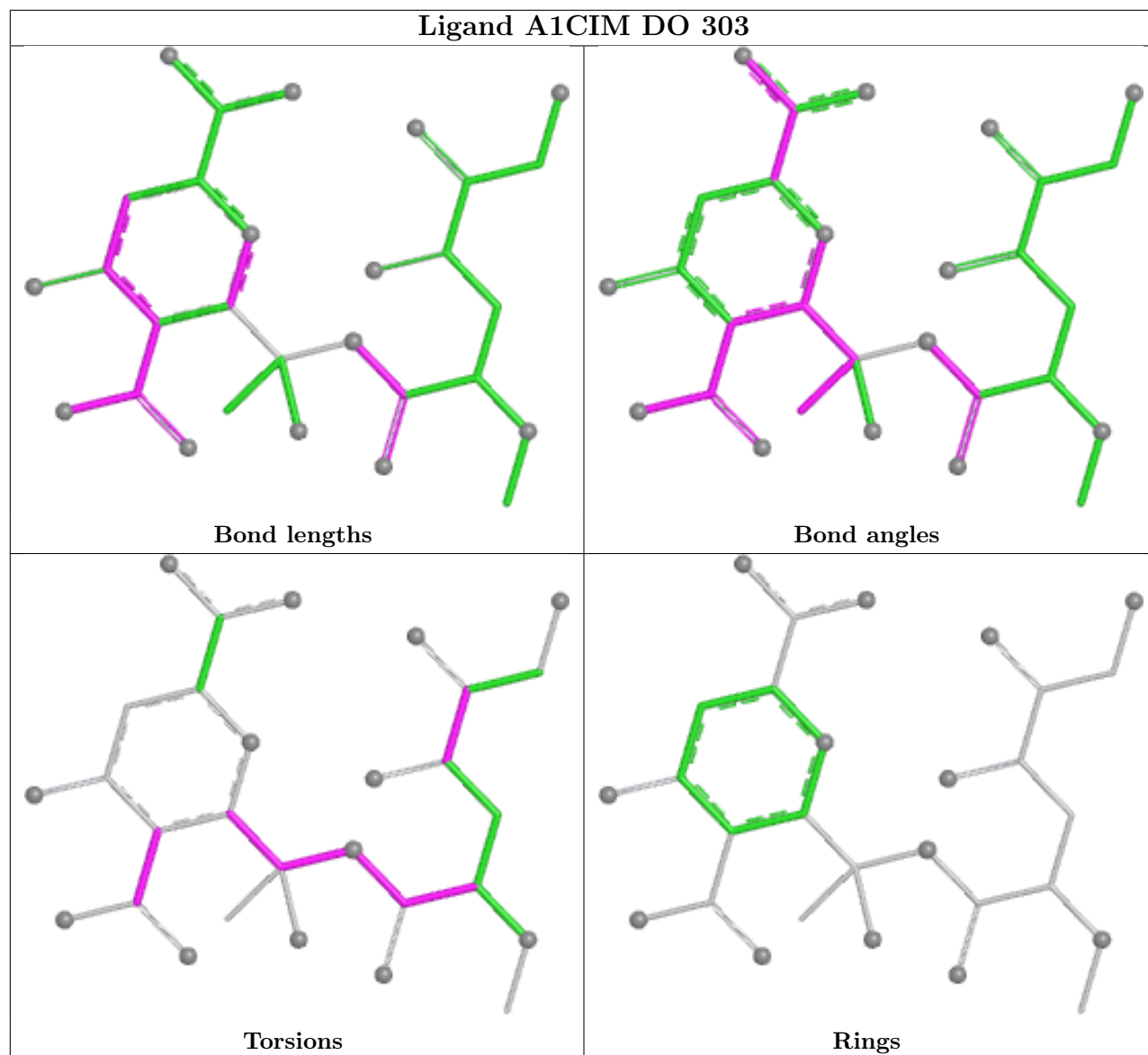
Bond lengths

Bond angles

Torsions

Rings

Ligand A1CIM DO 303



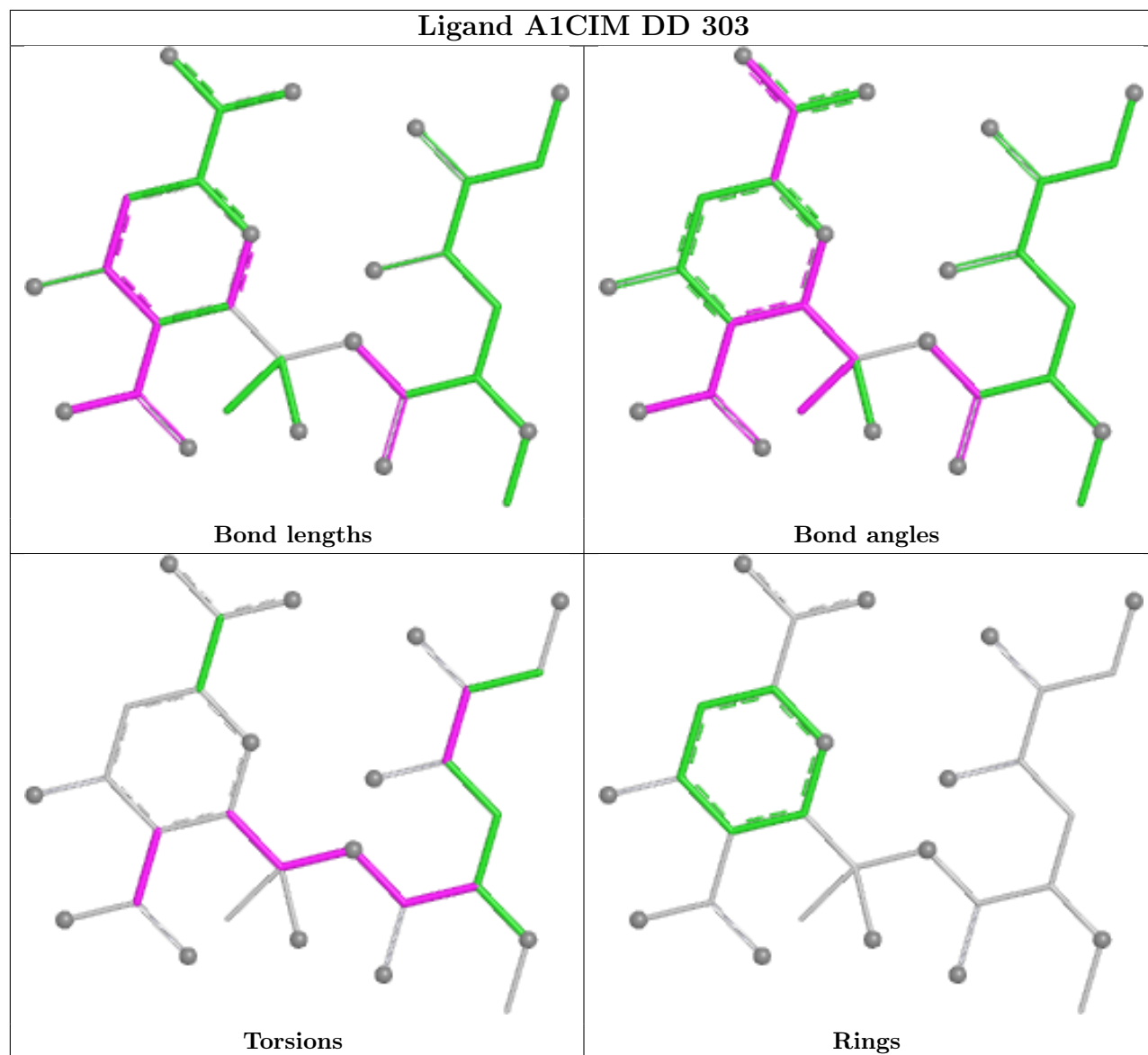
Bond lengths

Bond angles

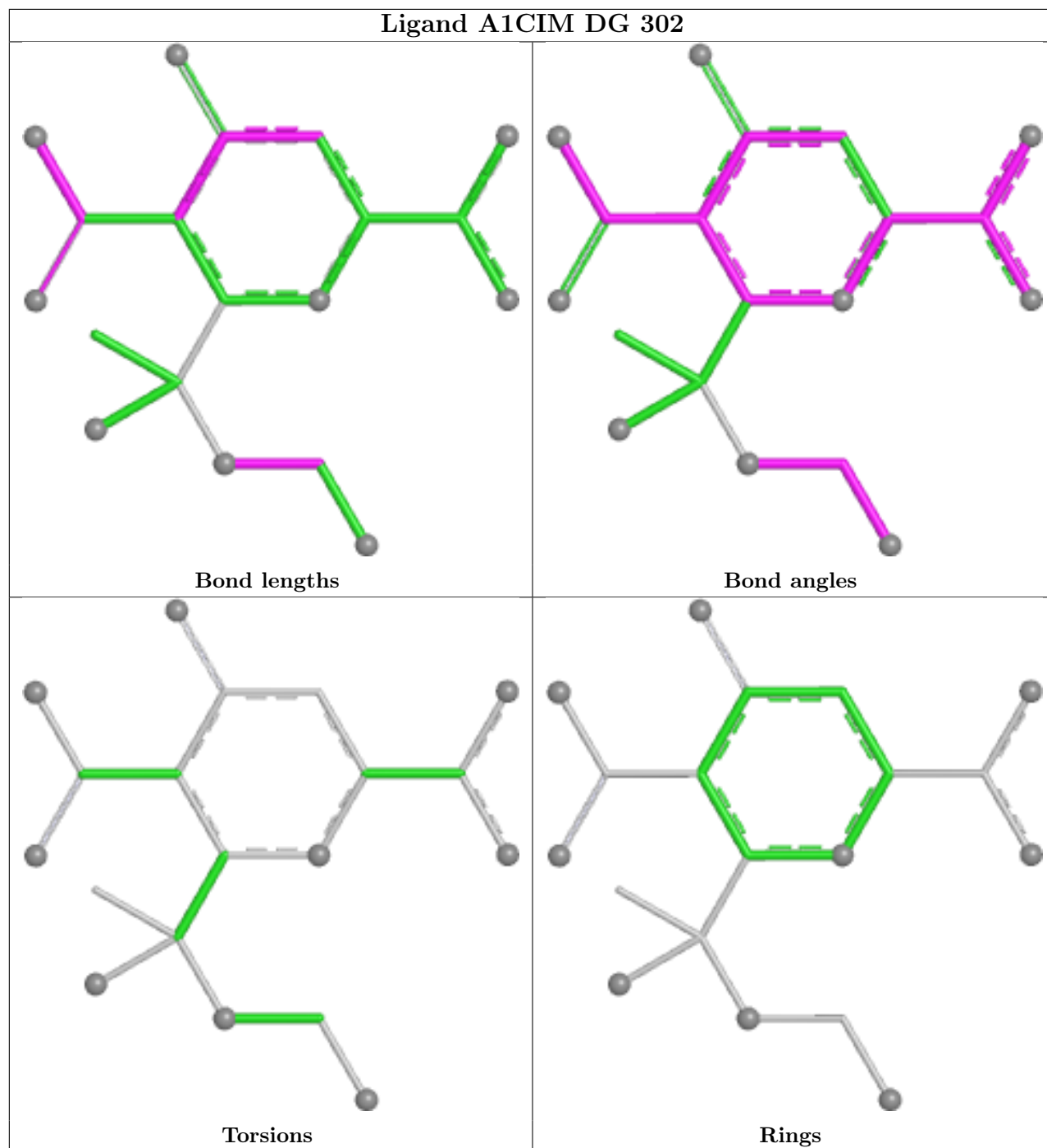
Torsions

Rings

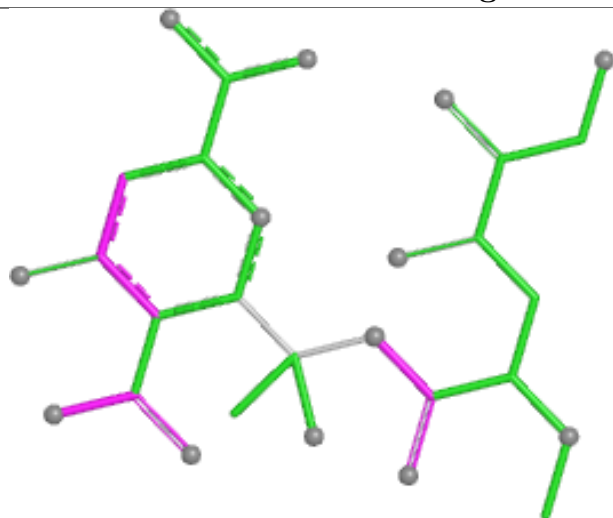
Ligand A1CIM DD 303



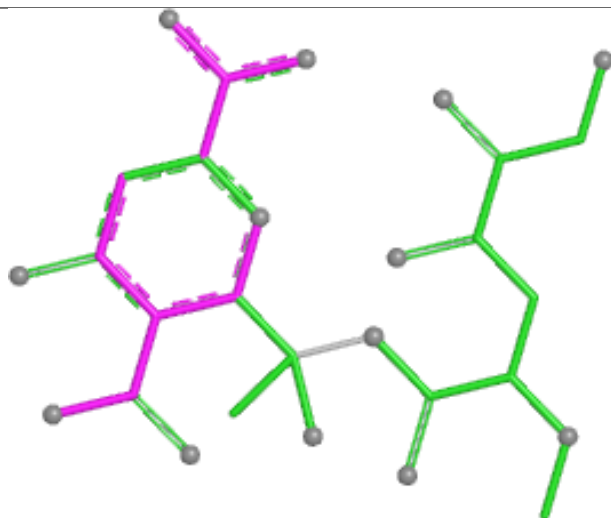
Ligand A1CIM DG 302



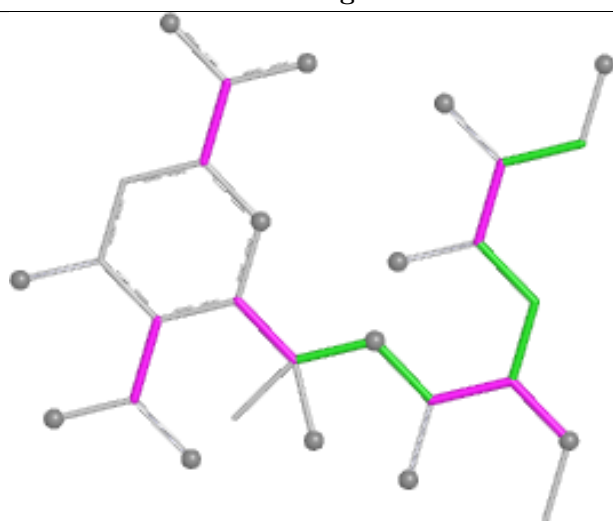
Ligand A1CIM DP 304



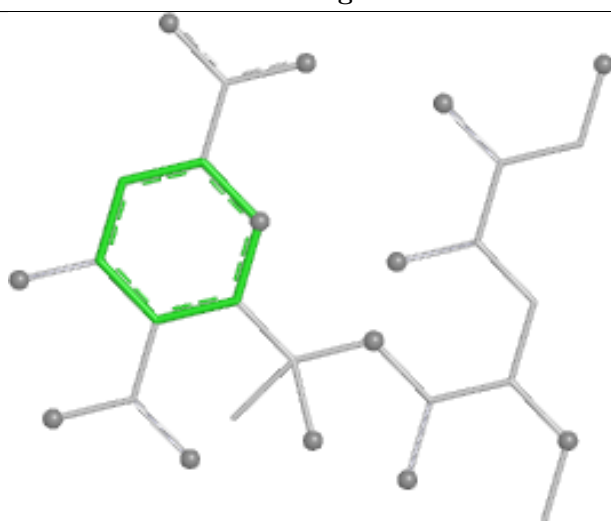
Bond lengths



Bond angles

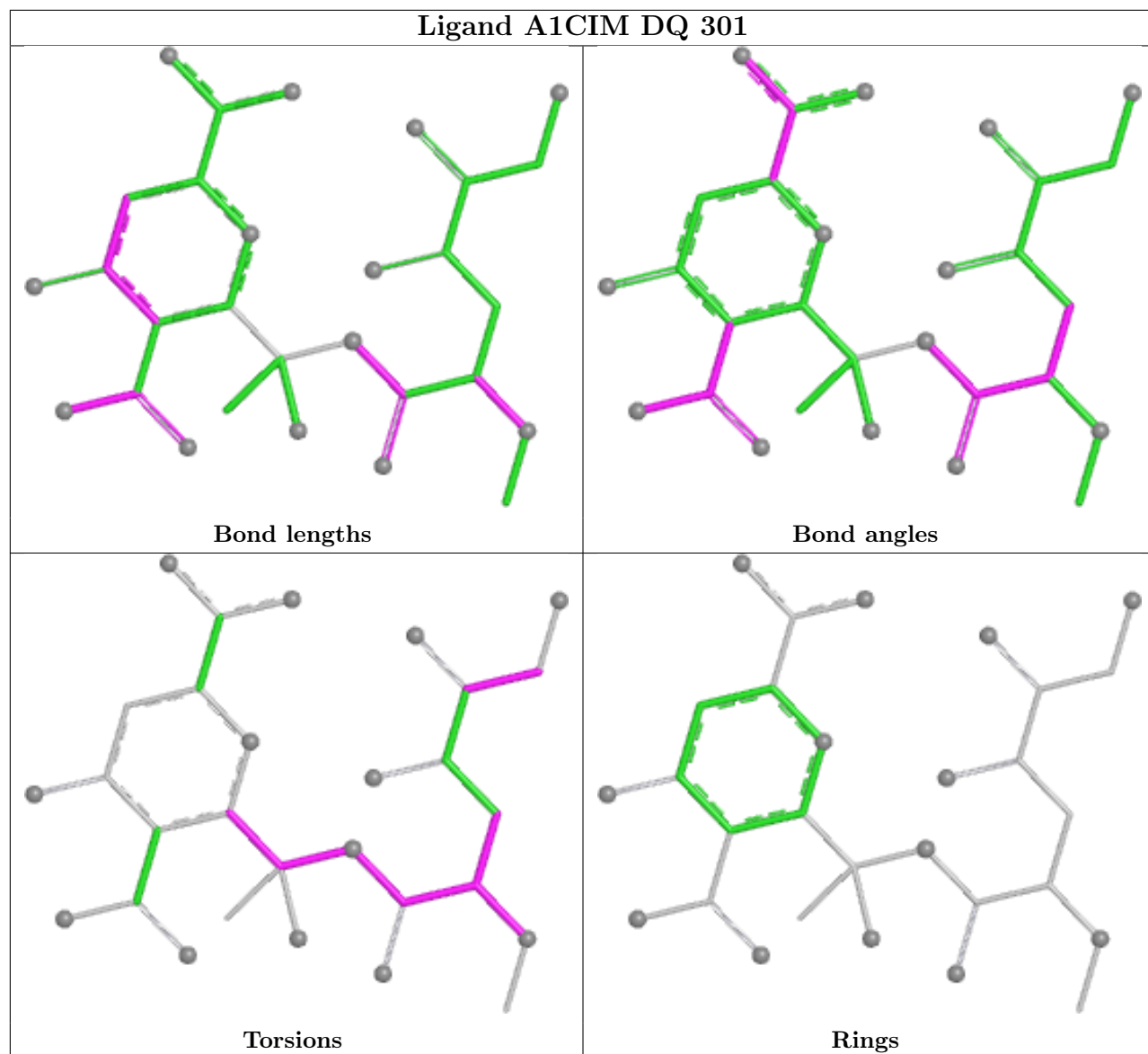


Torsions

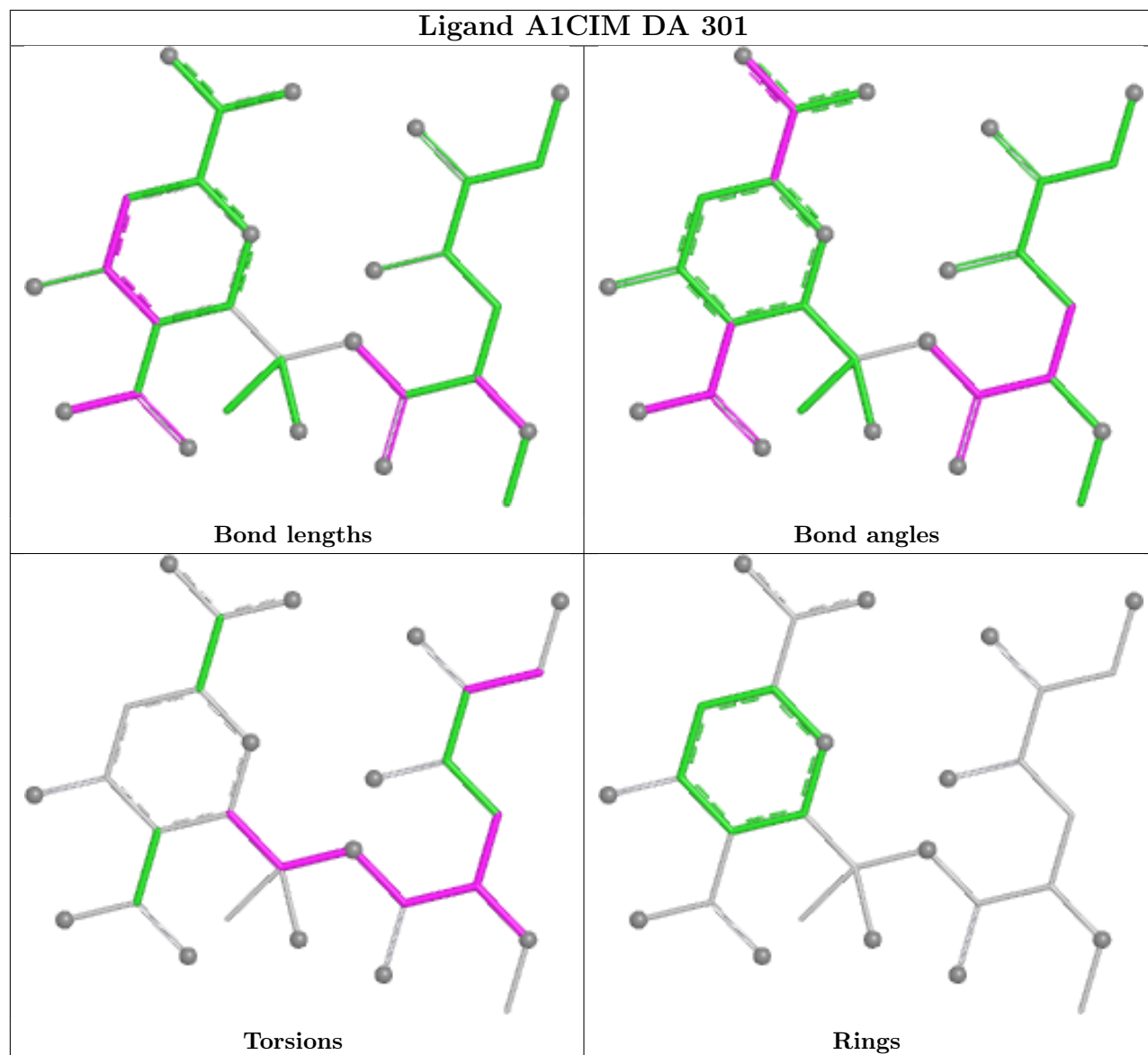


Rings

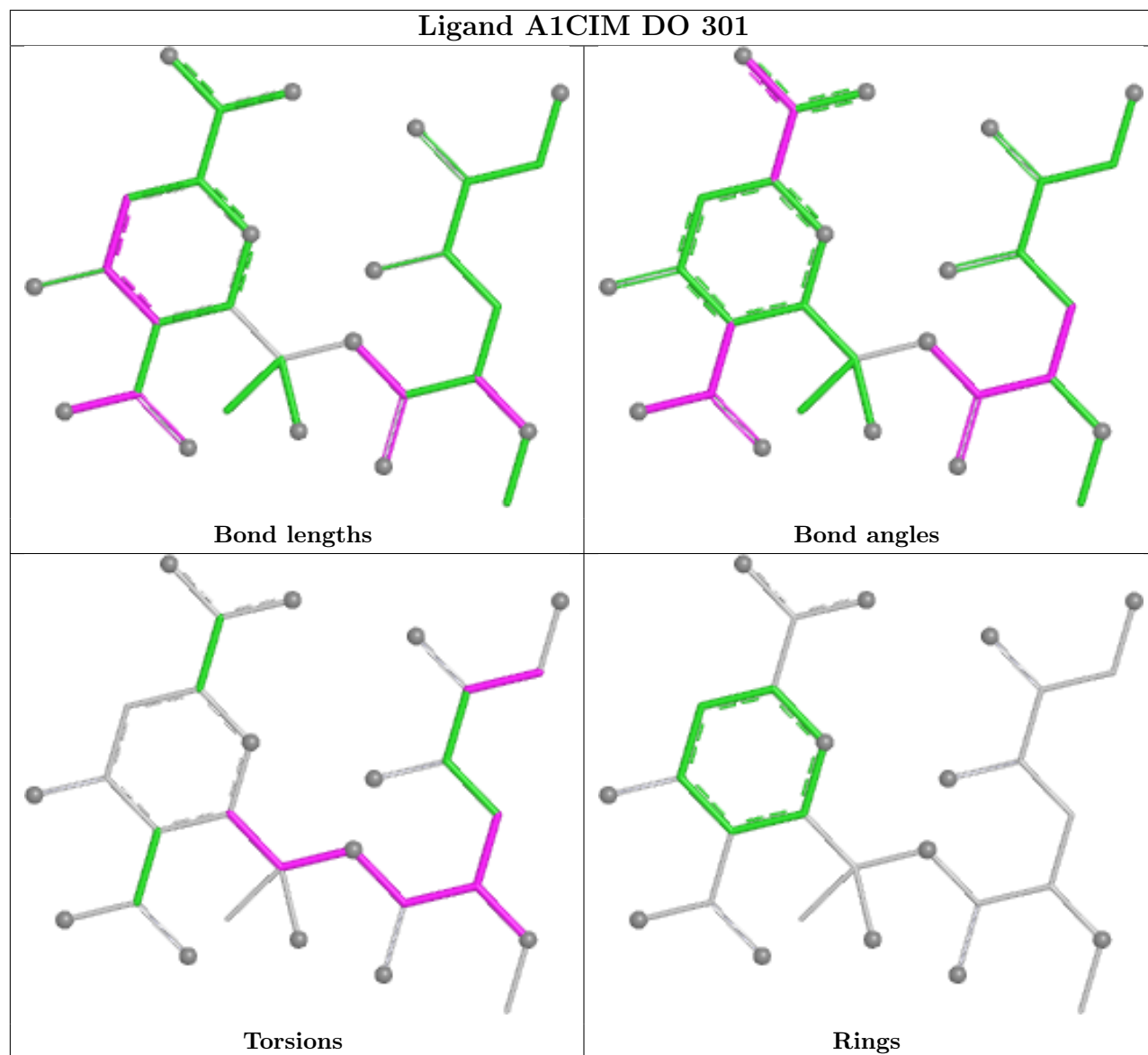
Ligand A1CIM DQ 301



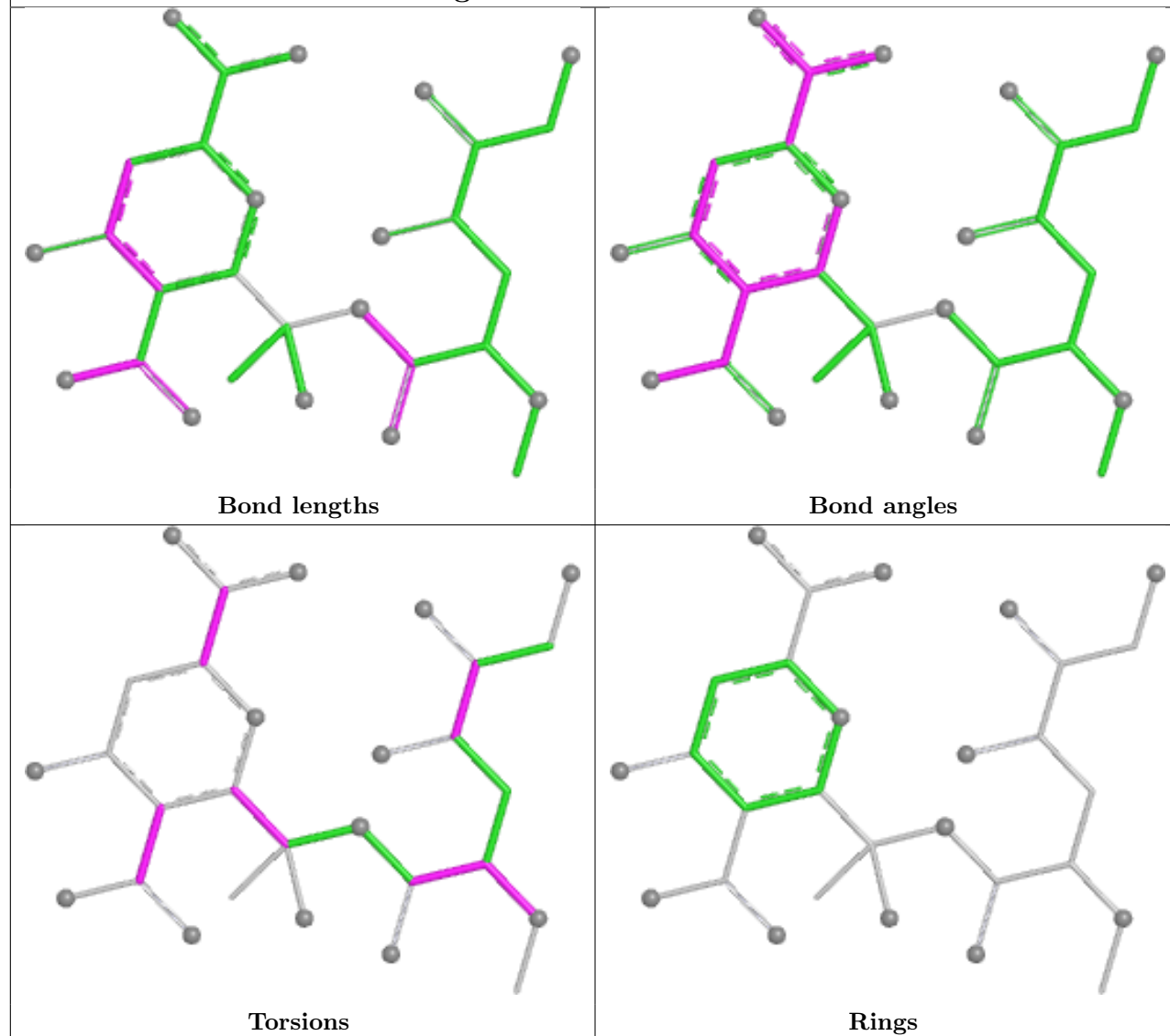
Ligand A1CIM DA 301



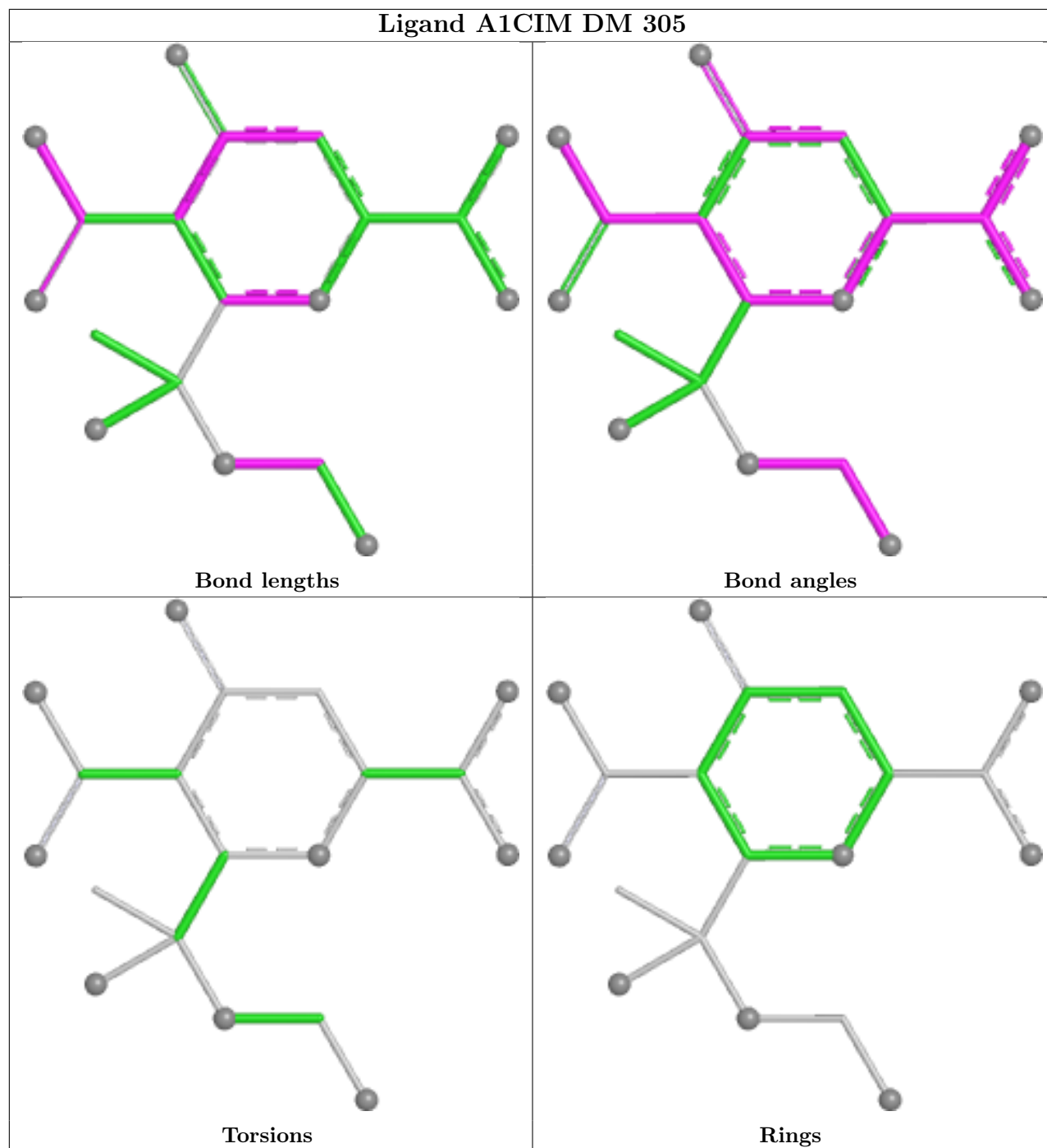
Ligand A1CIM DO 301



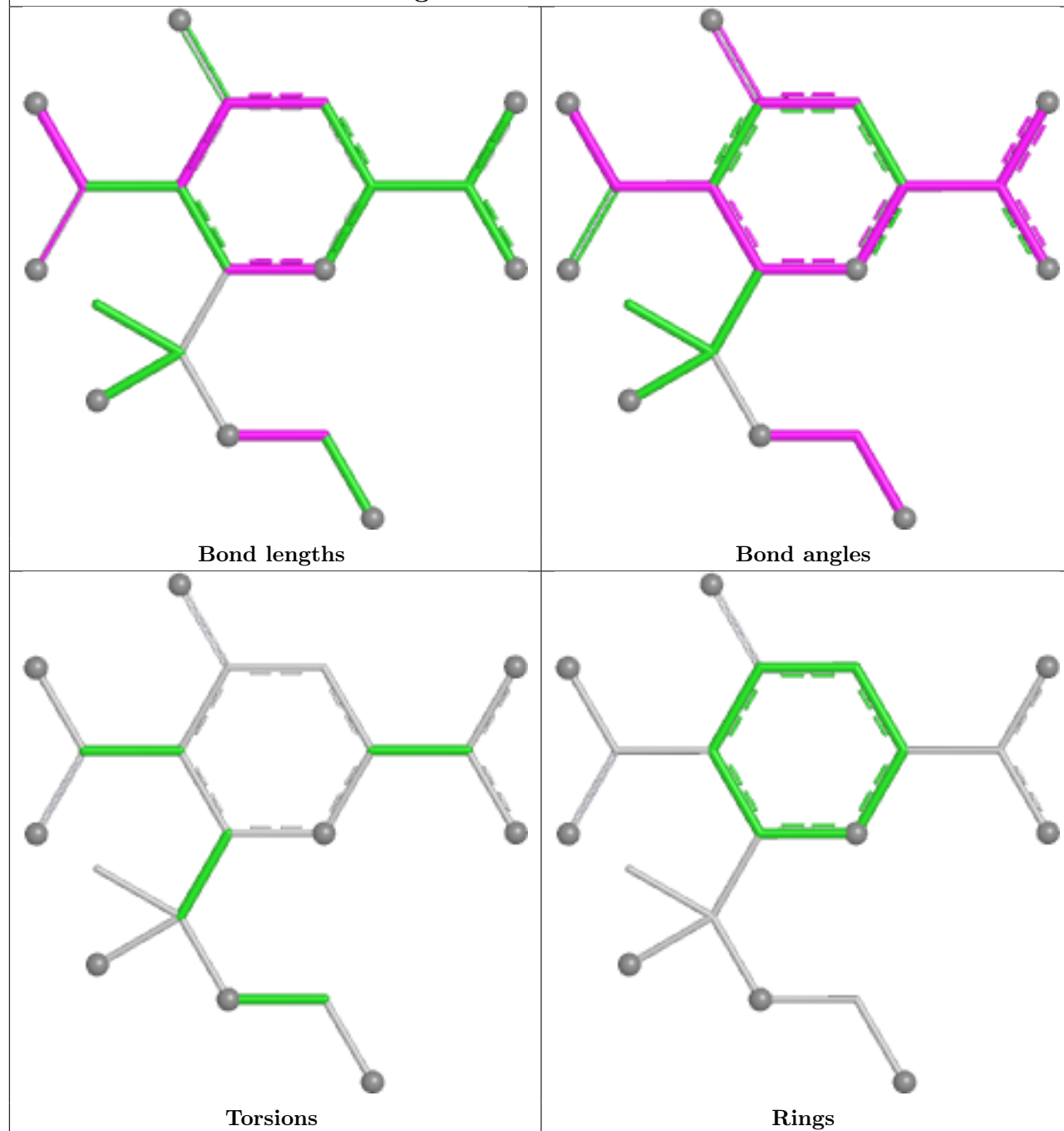
Ligand A1CIM DG 304



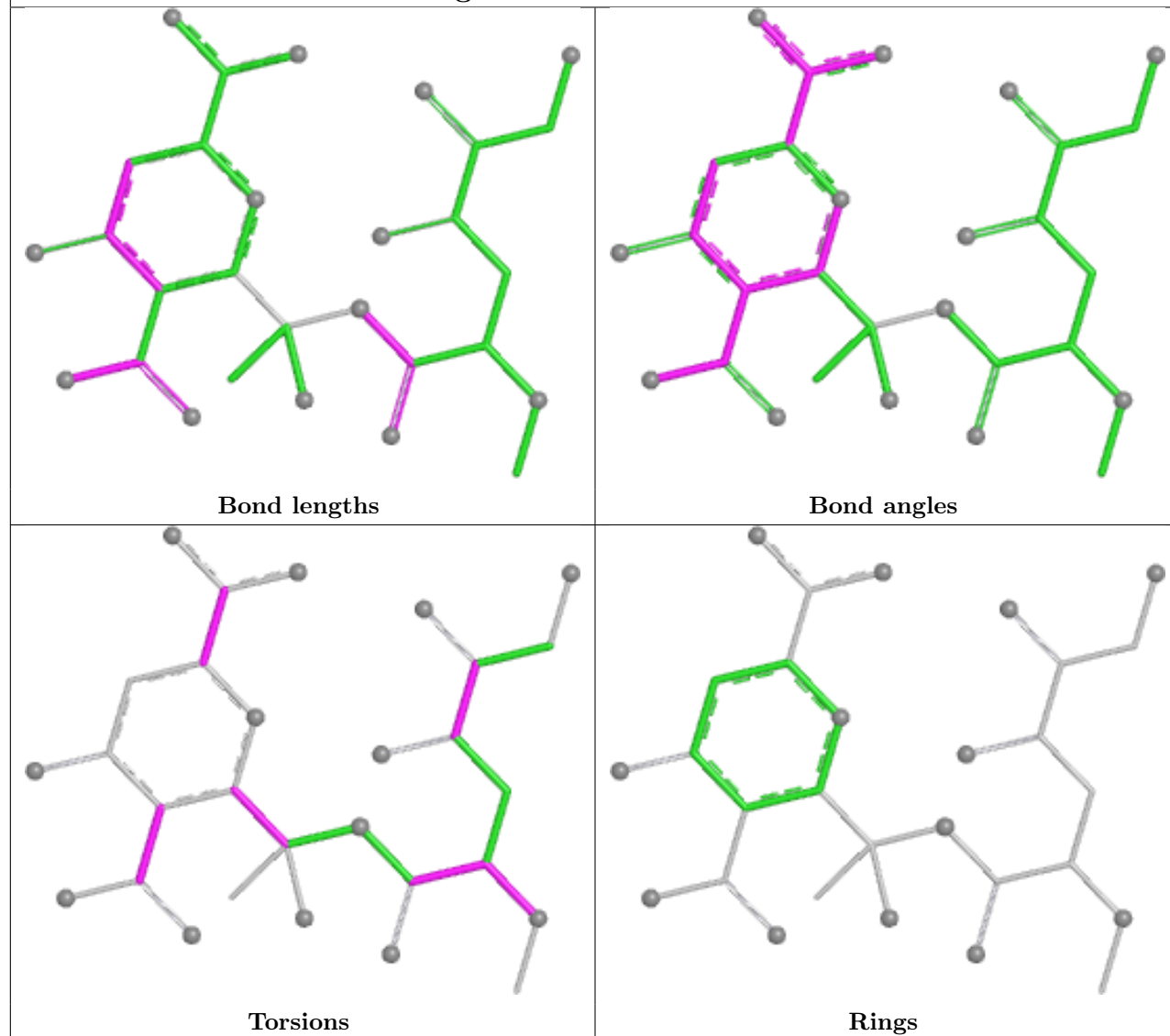
Ligand A1CIM DM 305



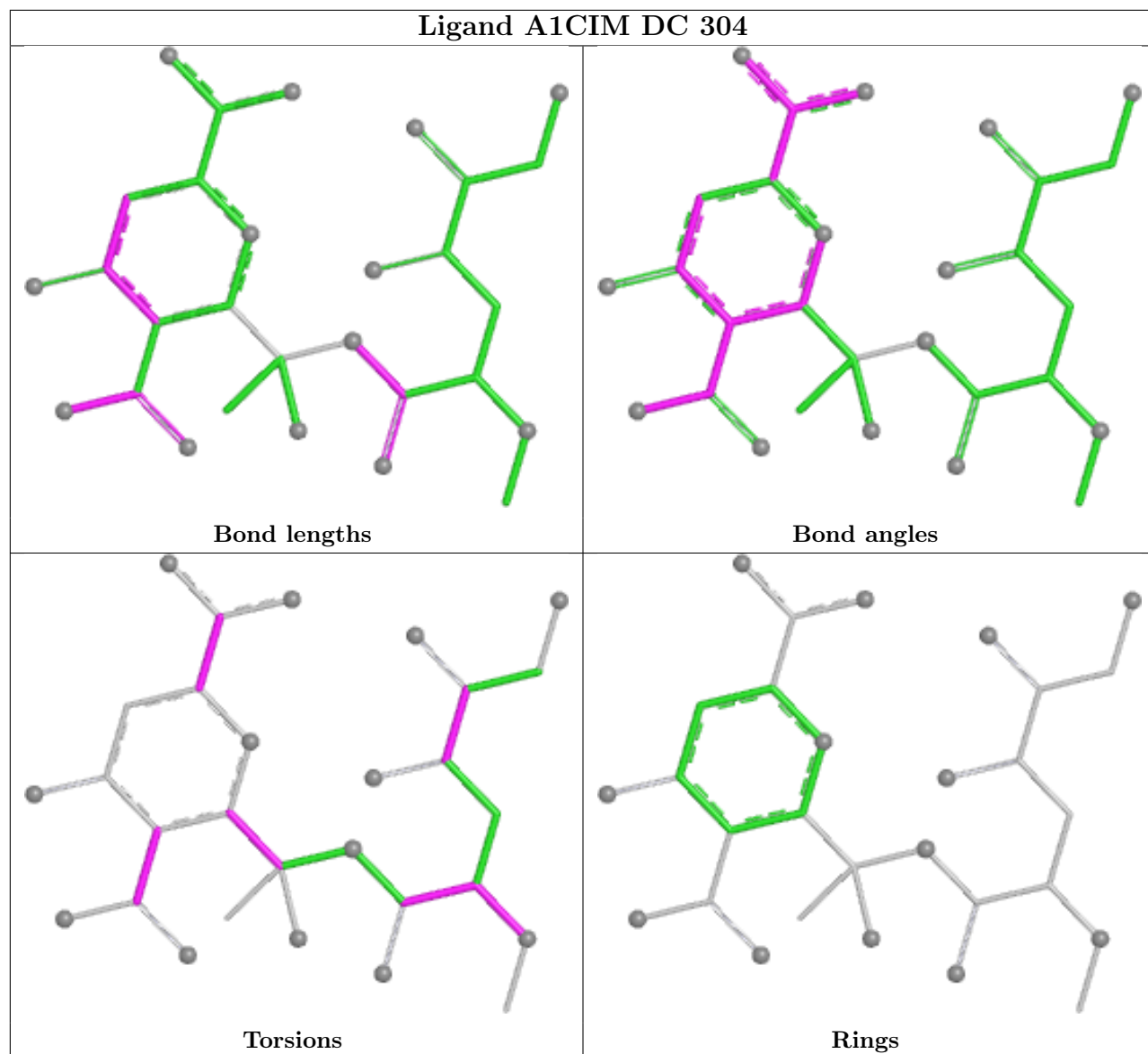
Ligand A1CIM DB 305



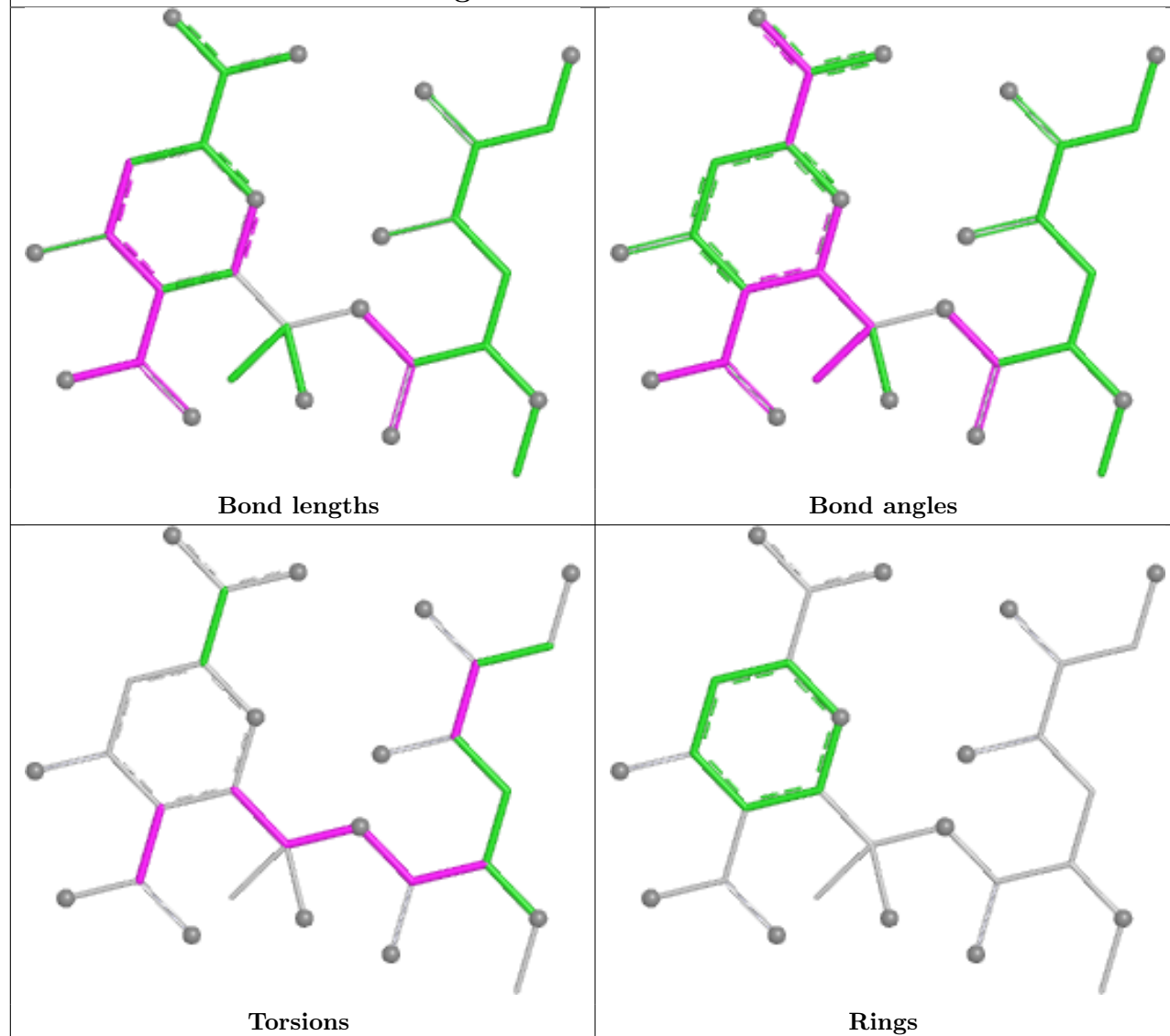
Ligand A1CIM DA 304



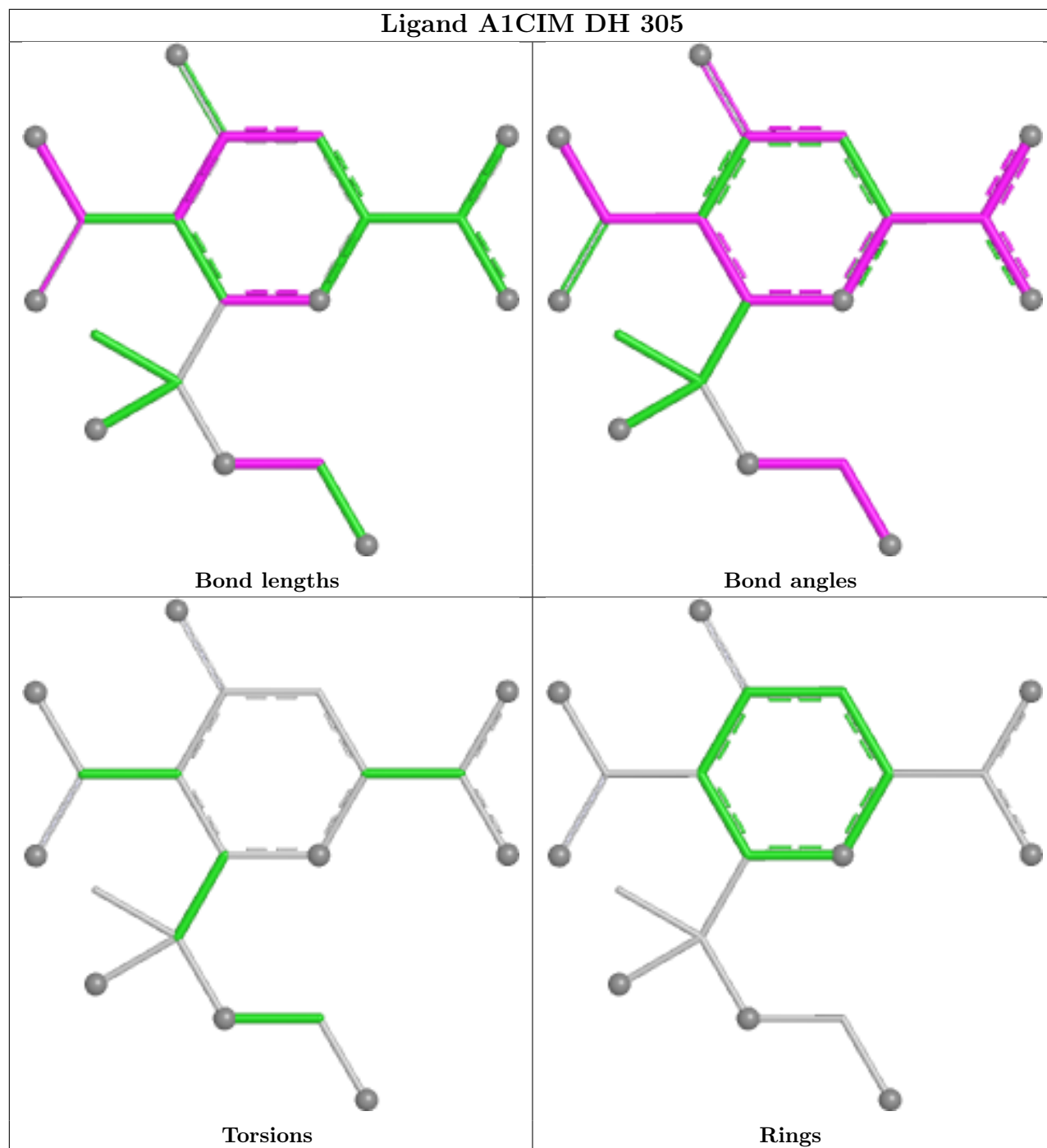
Ligand A1CIM DC 304



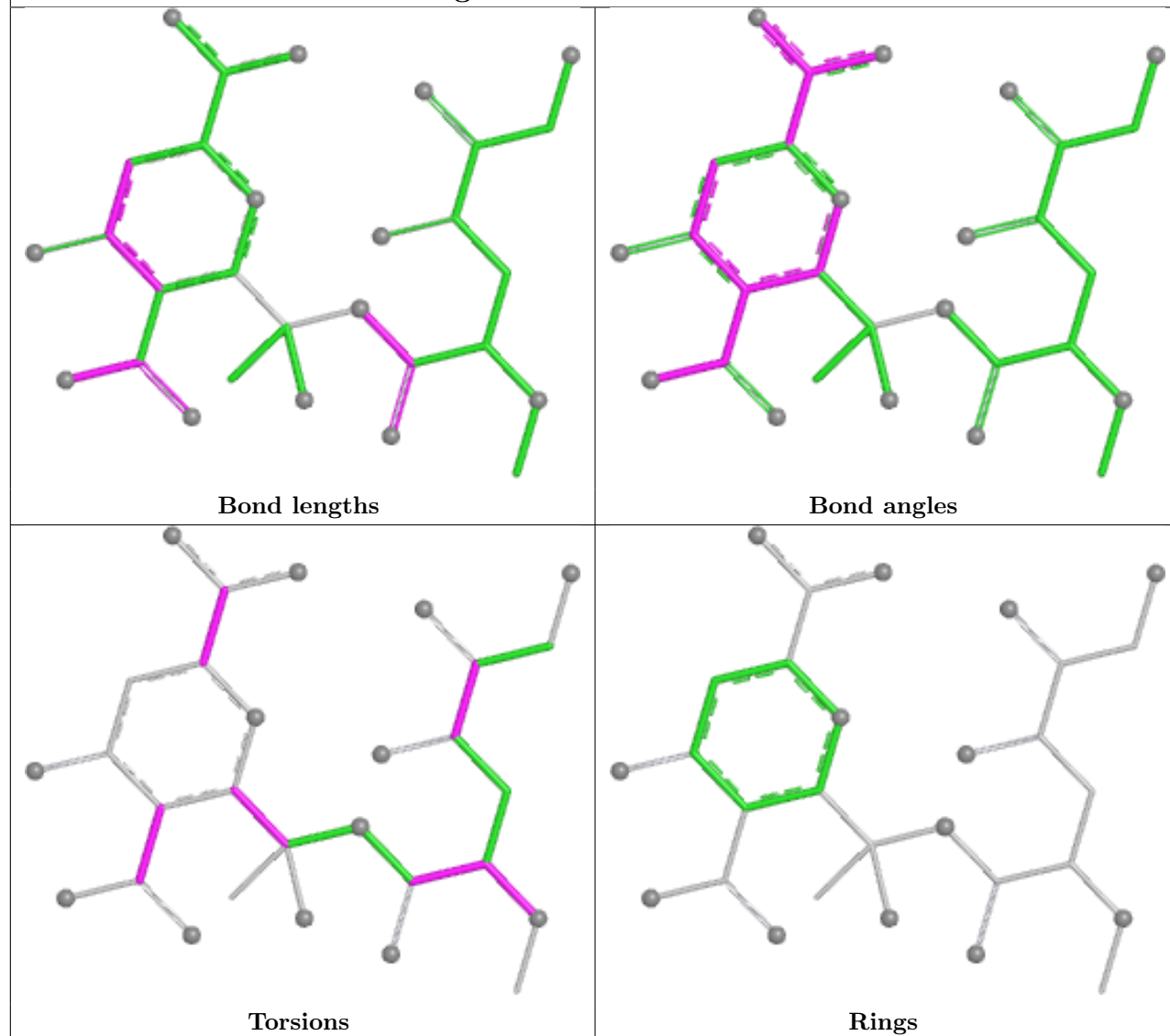
Ligand A1CIM DK 303

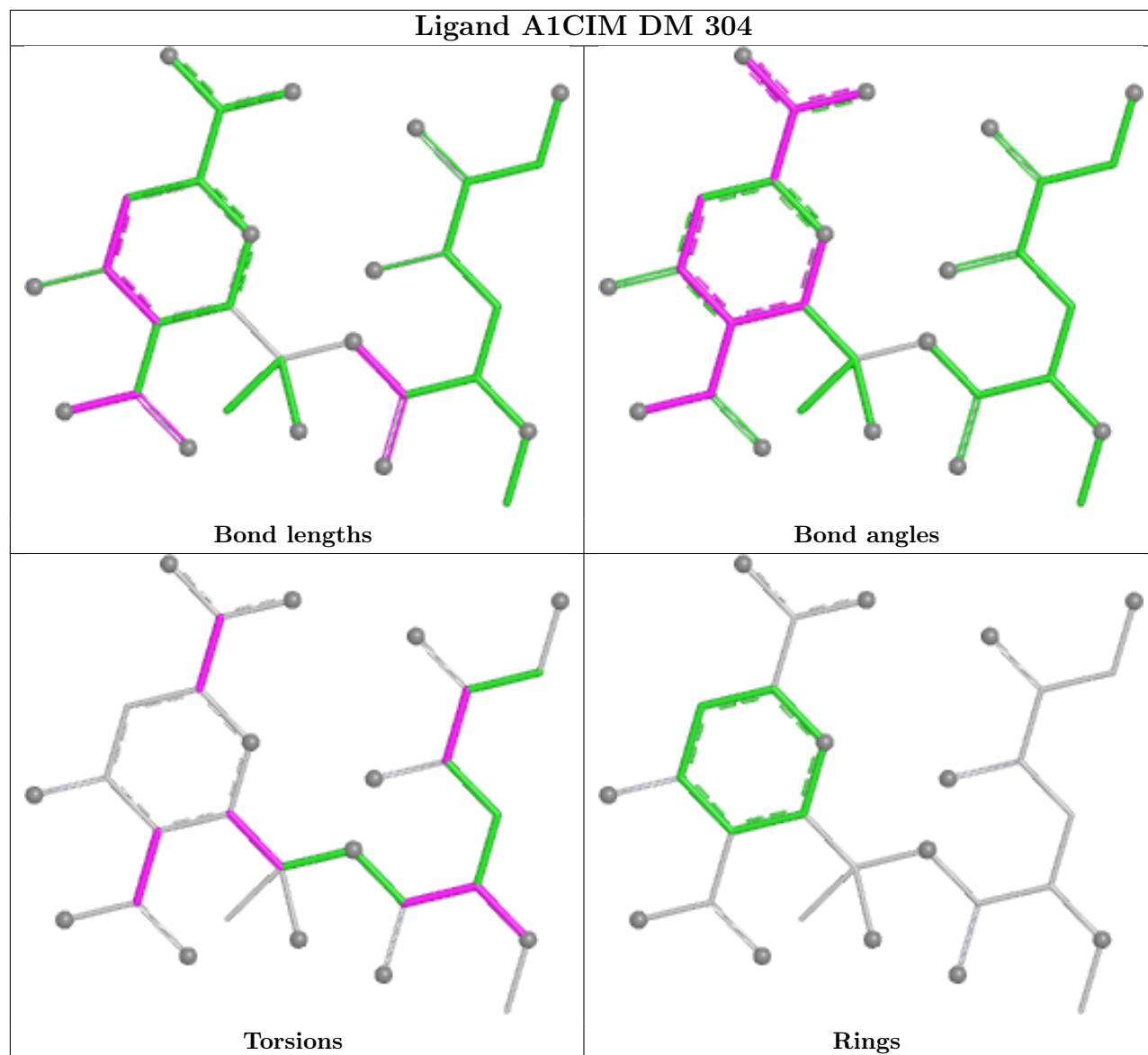


Ligand A1CIM DH 305

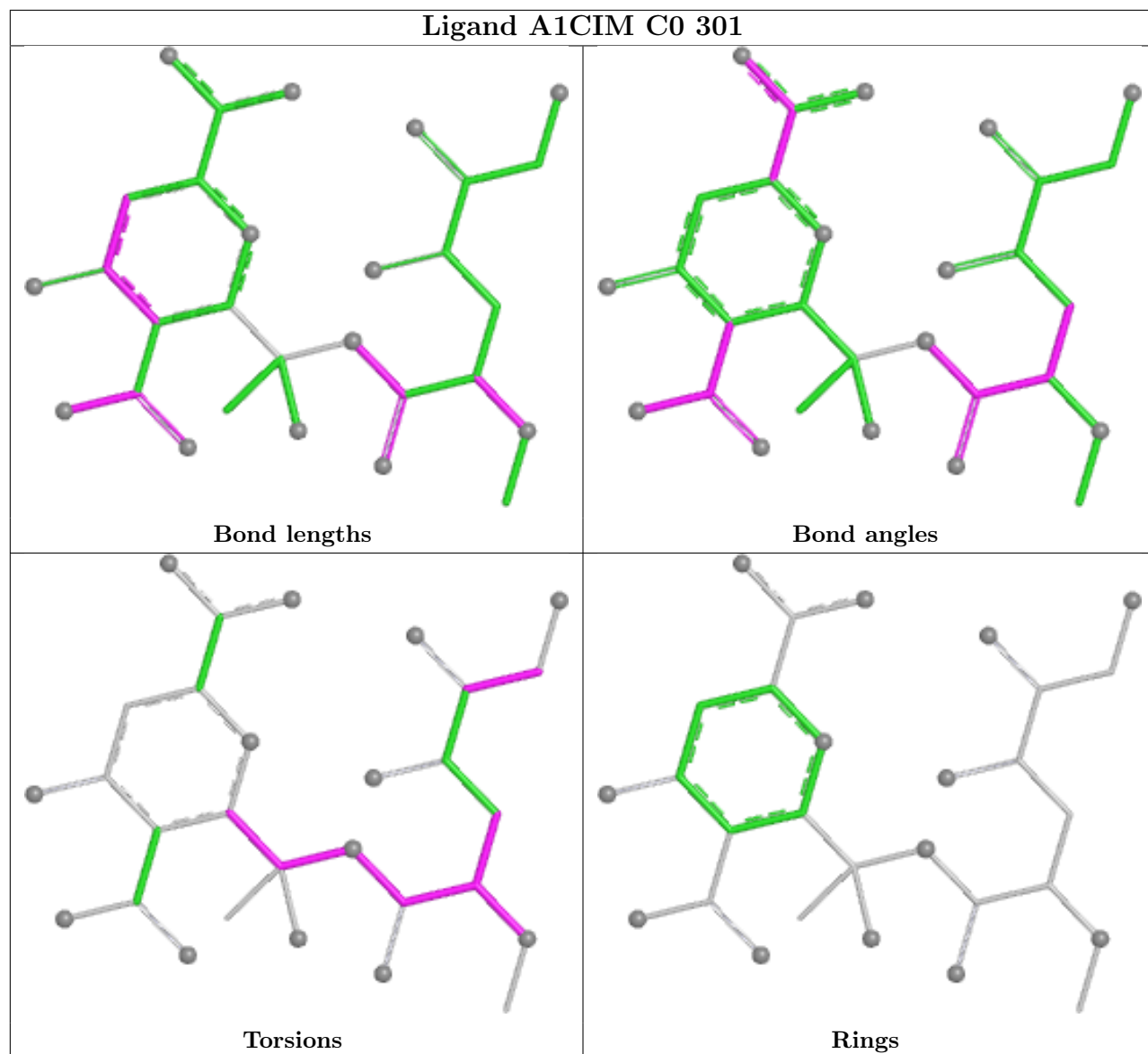


Ligand A1CIM DN 304

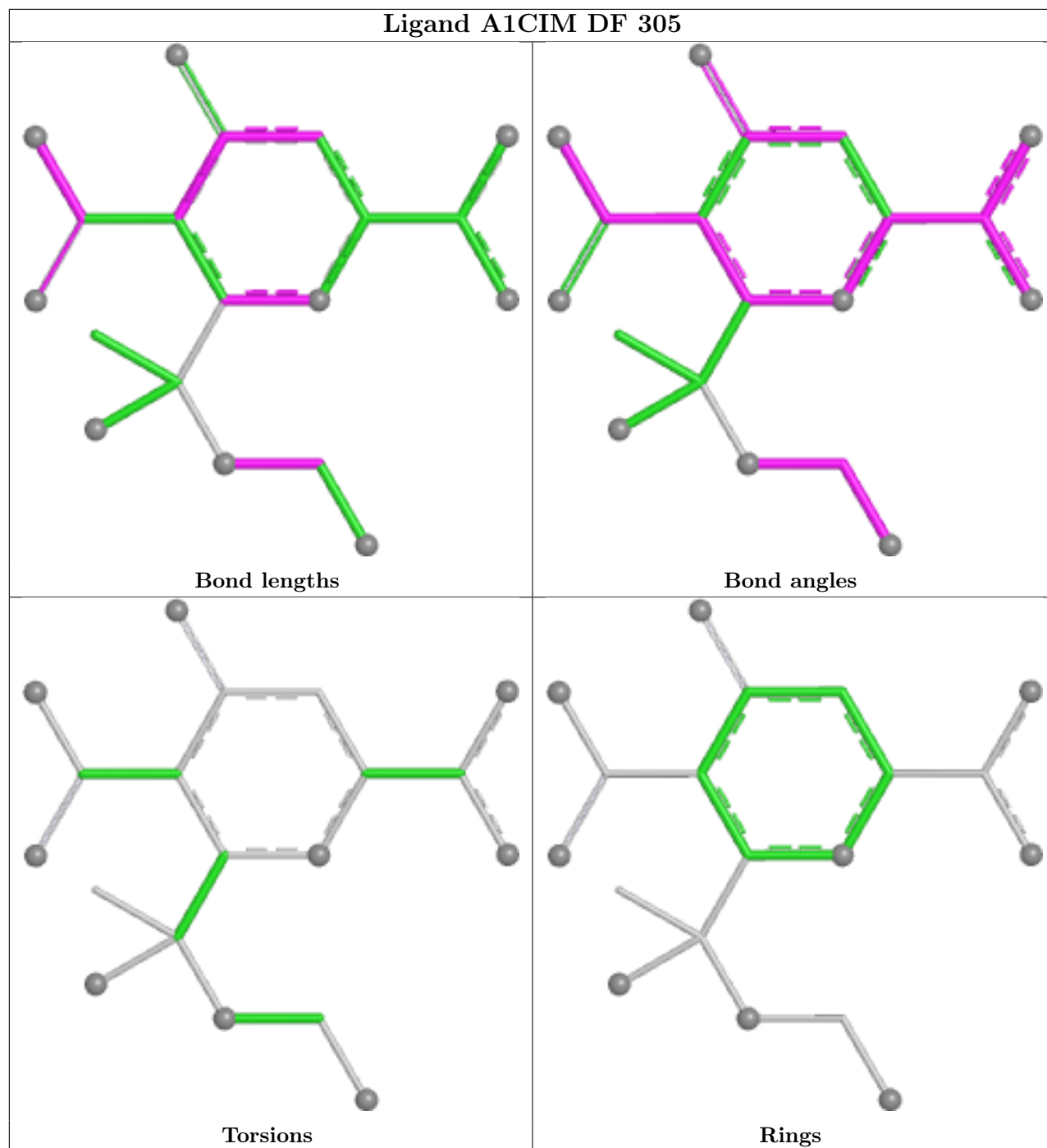




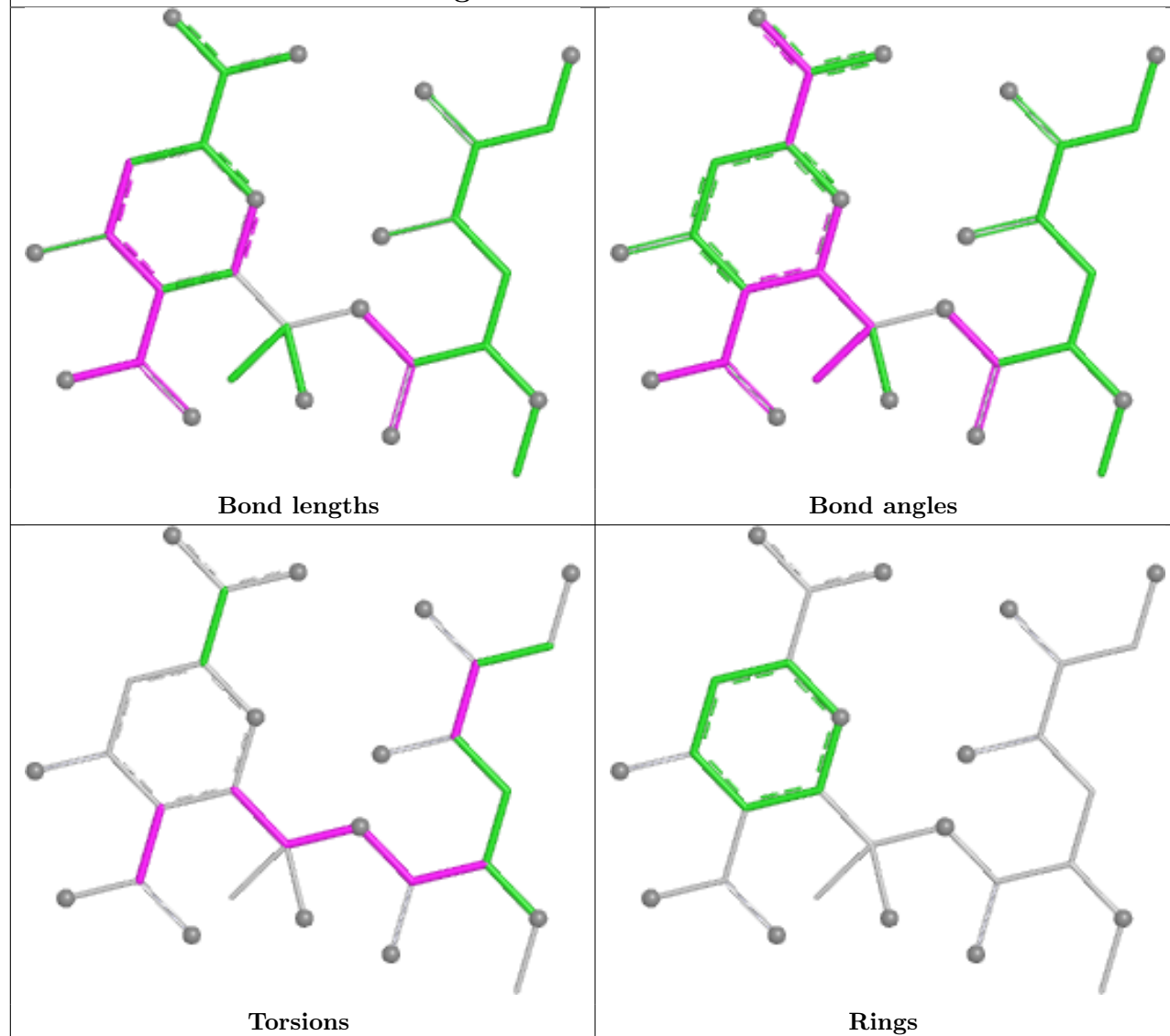
Ligand A1CIM C0 301



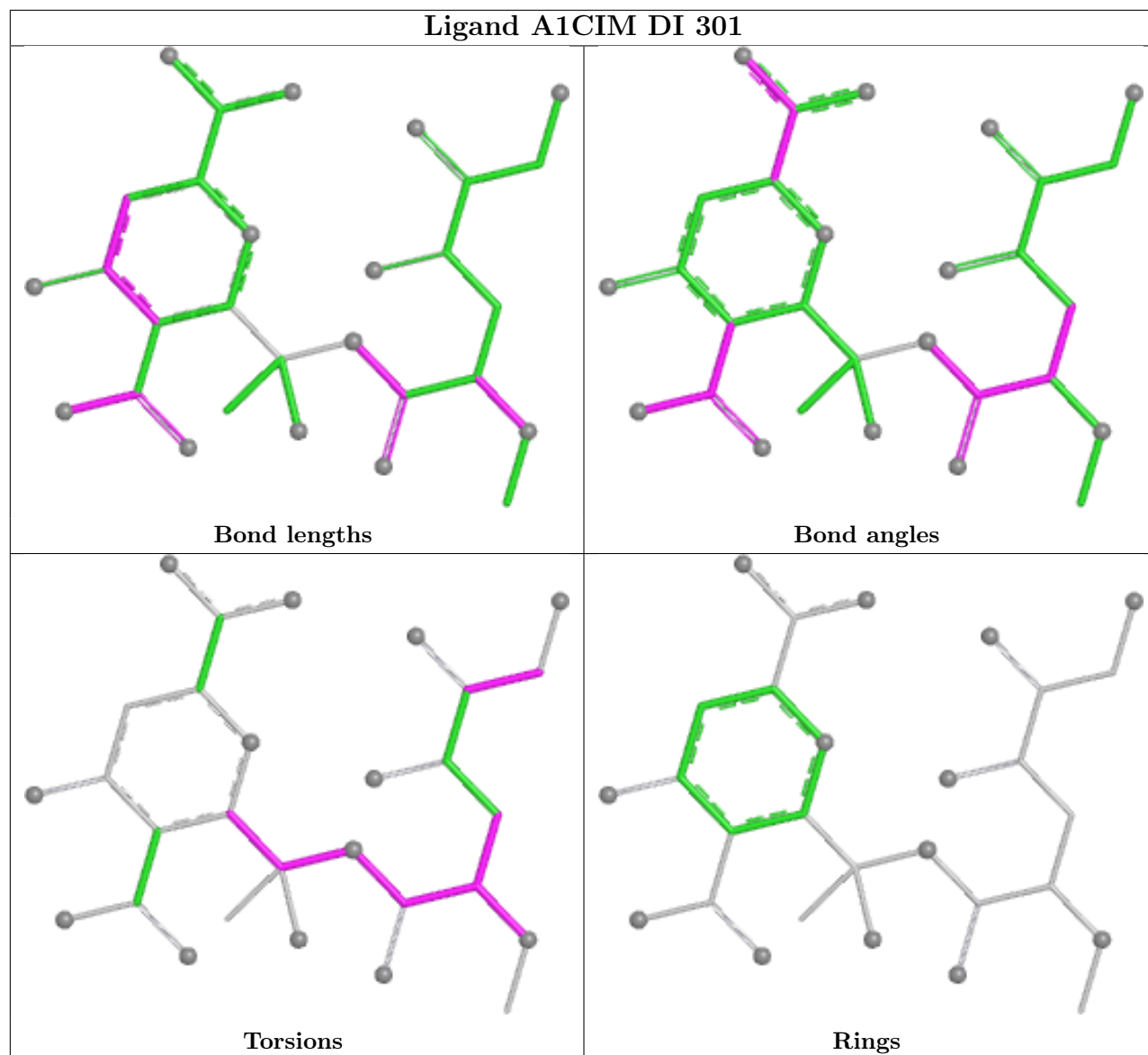
Ligand A1CIM DF 305



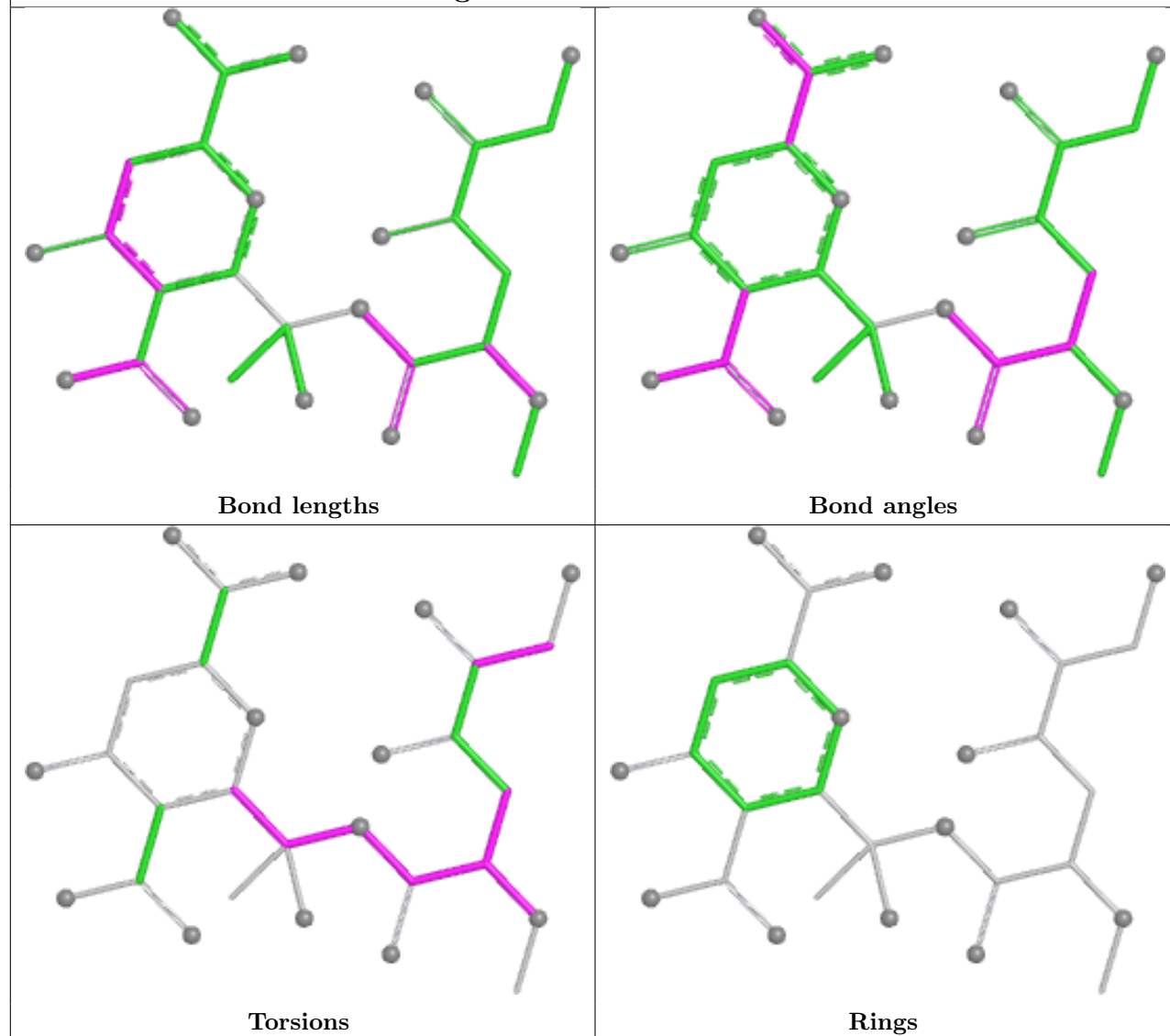
Ligand A1CIM DG 303



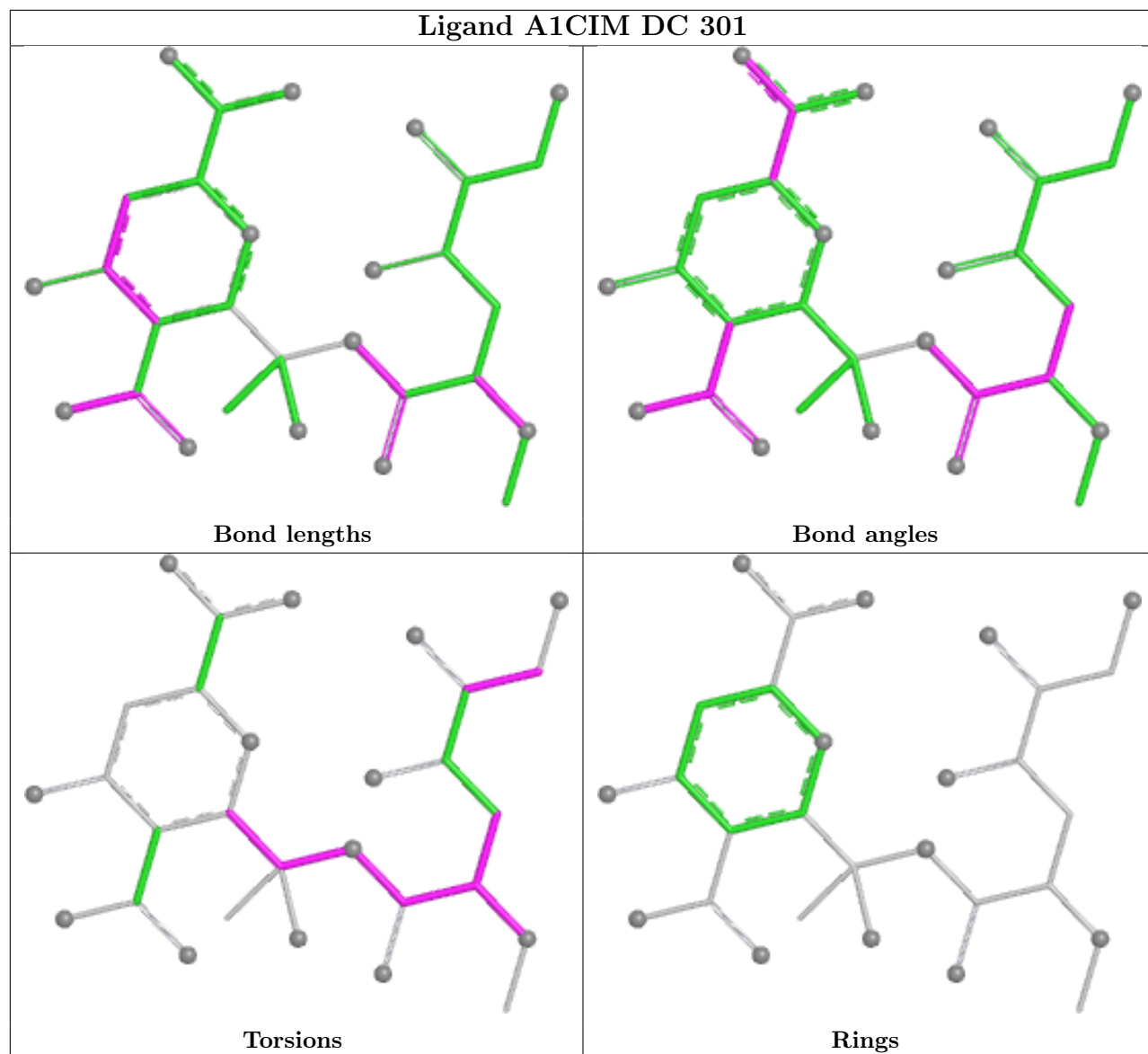
Ligand A1CIM DI 301



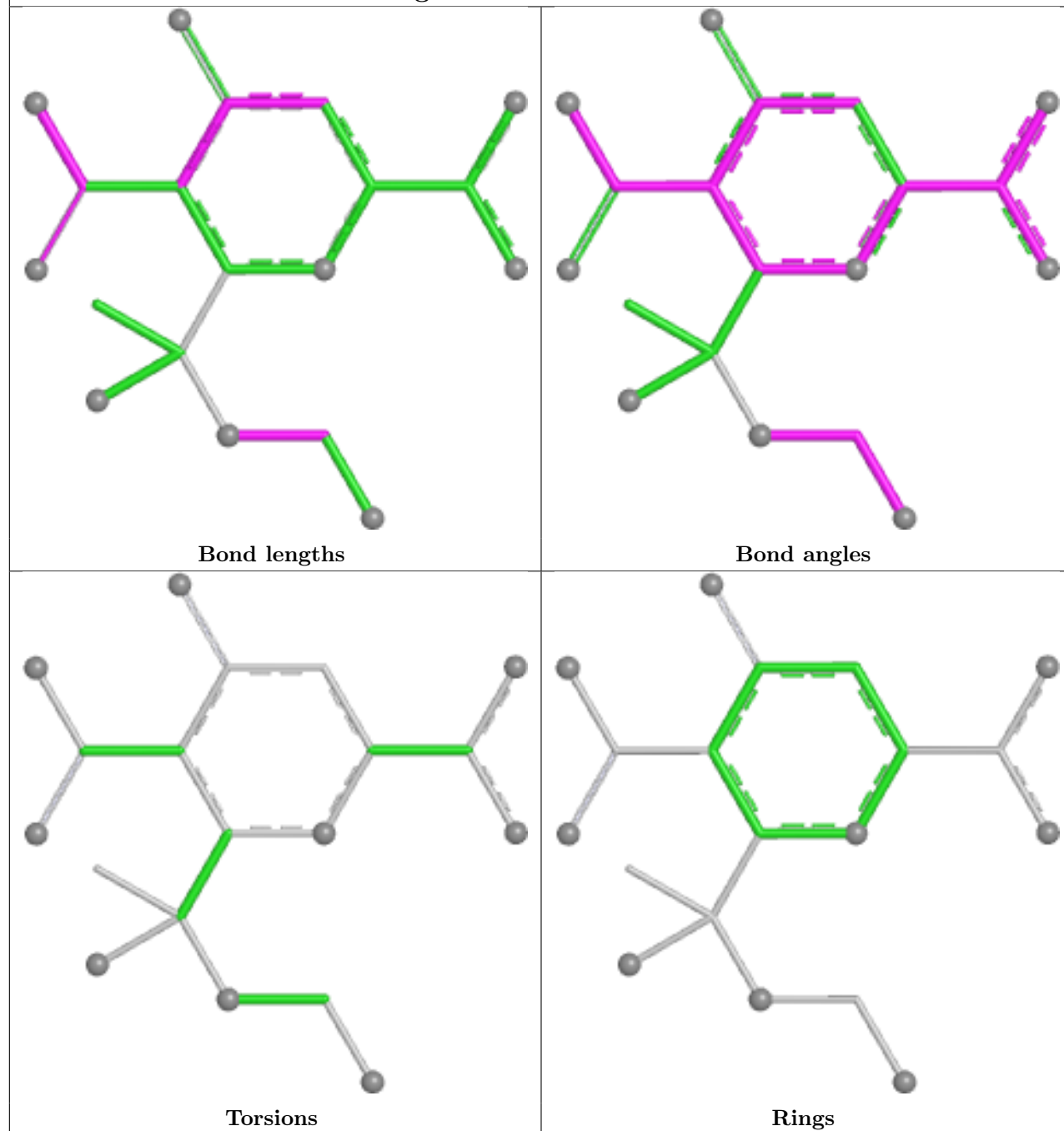
Ligand A1CIM DK 301



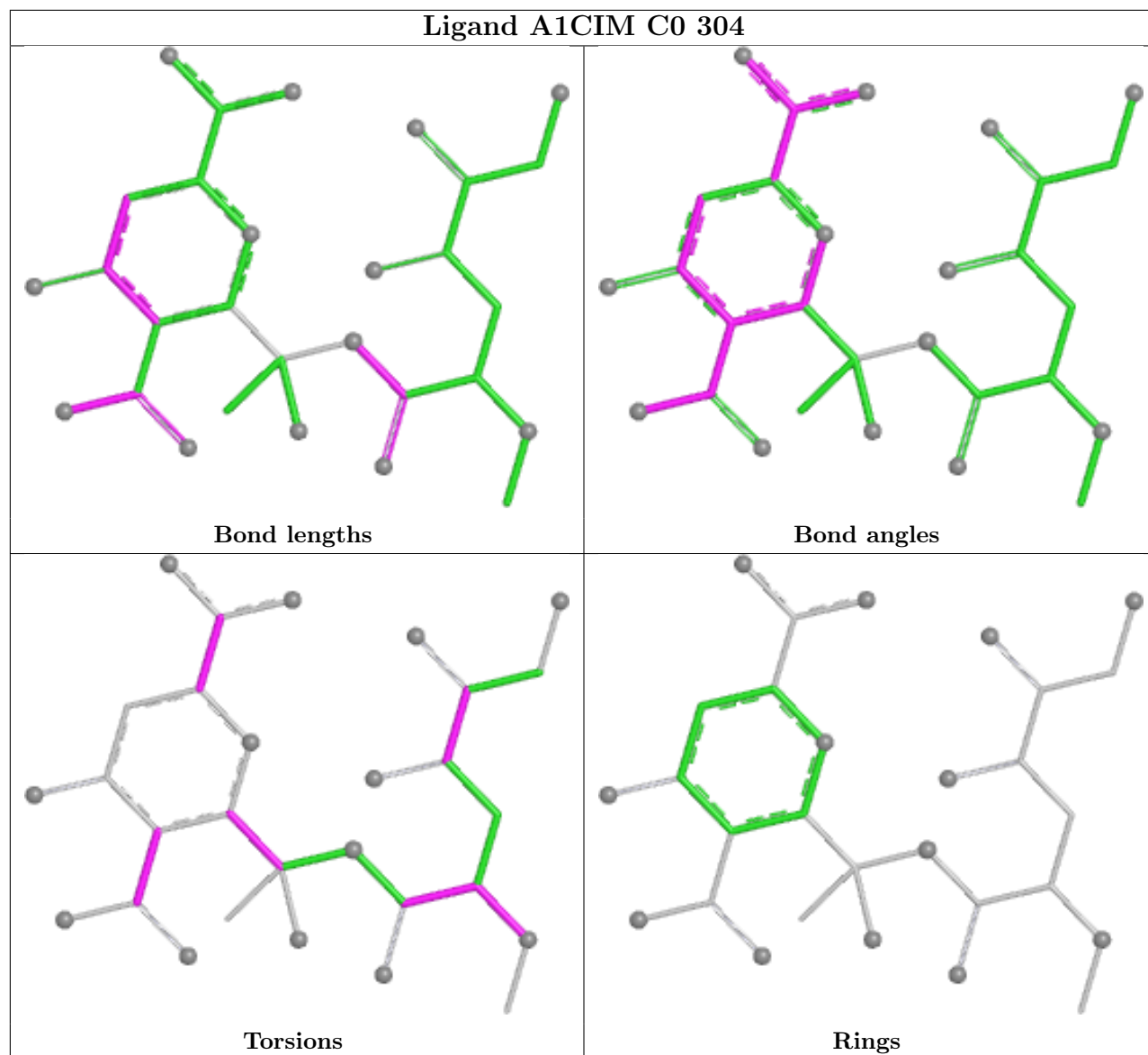
Ligand A1CIM DC 301



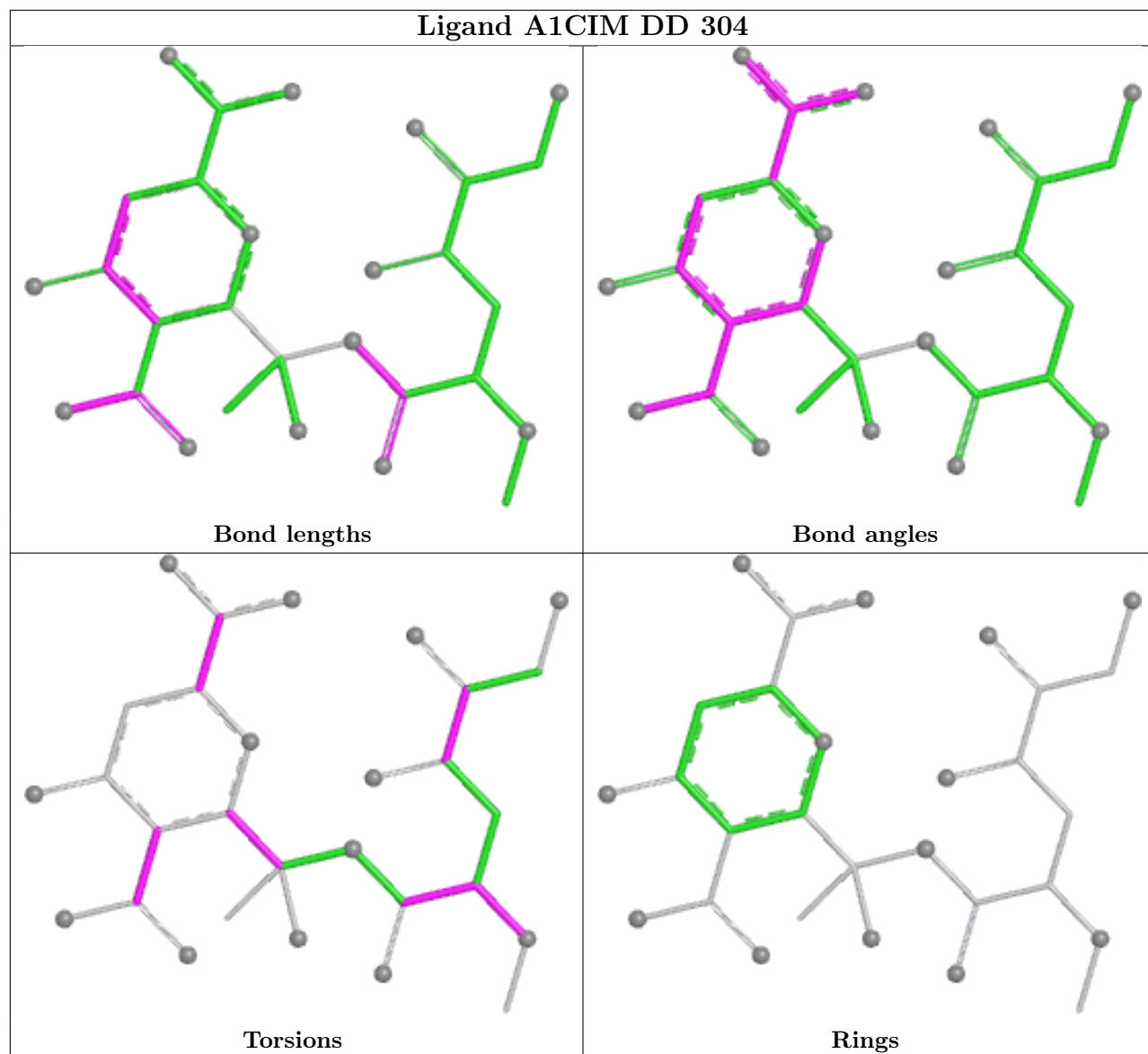
Ligand A1CIM DP 302



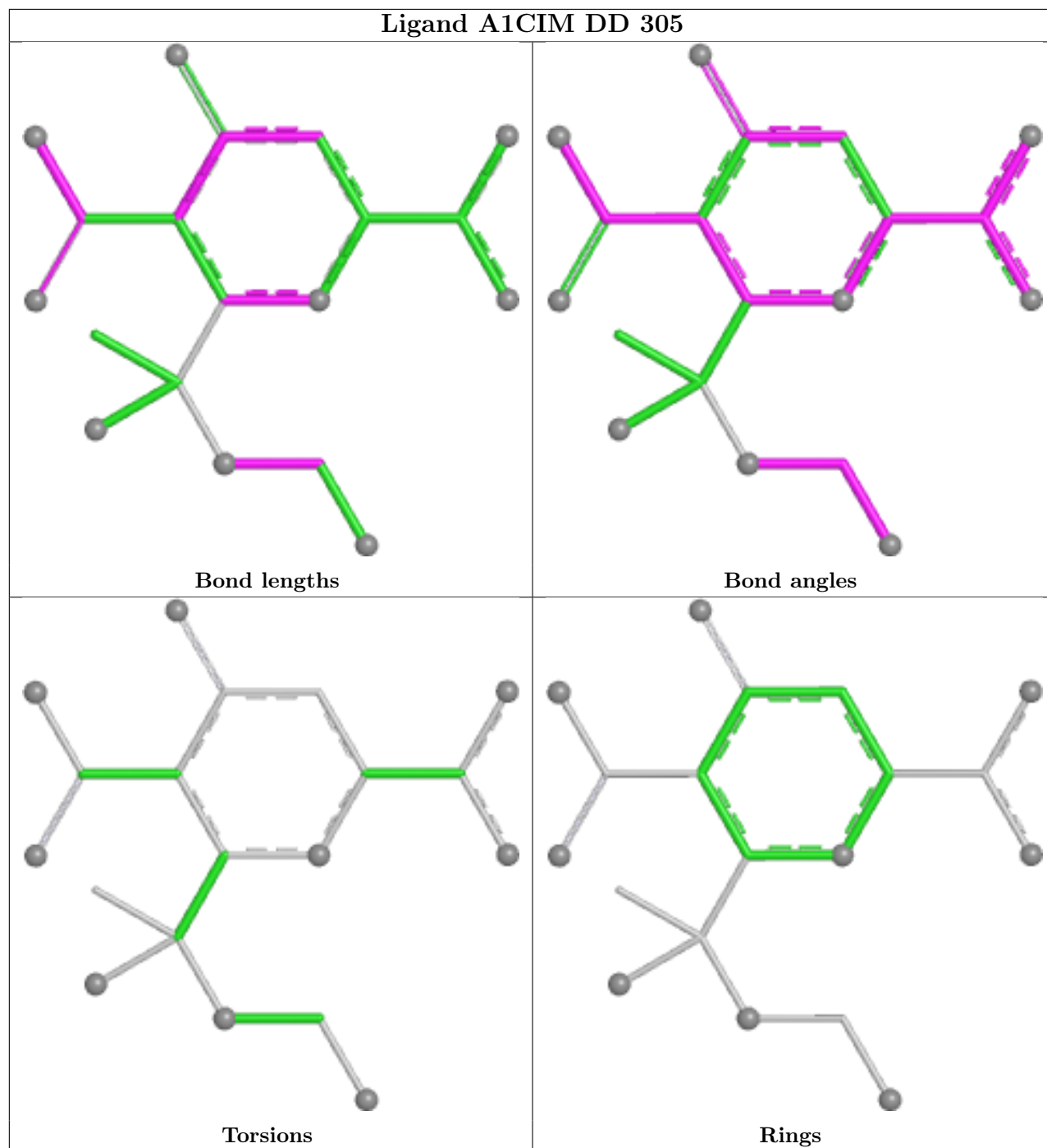
Ligand A1CIM C0 304



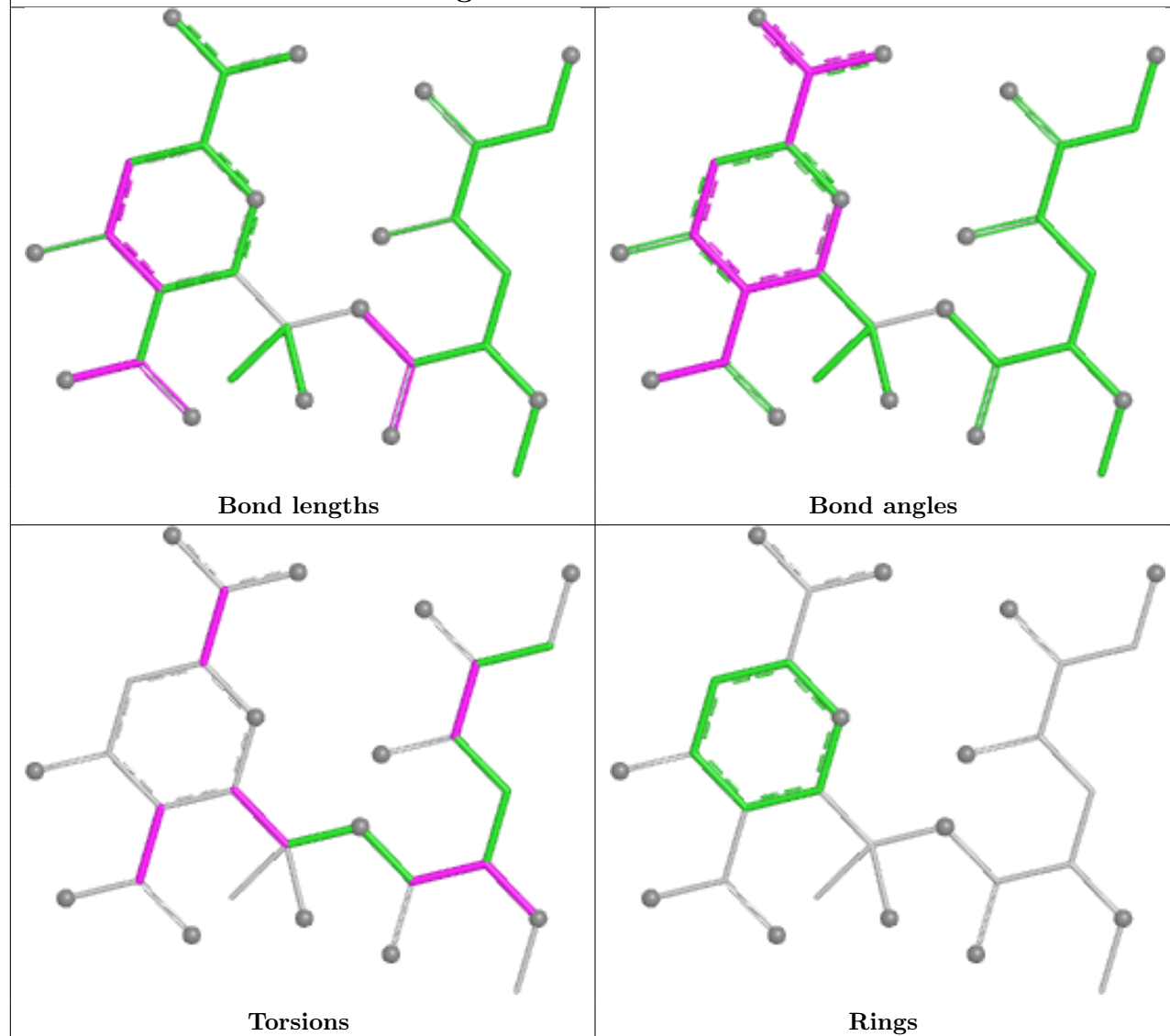
Ligand A1CIM DD 304



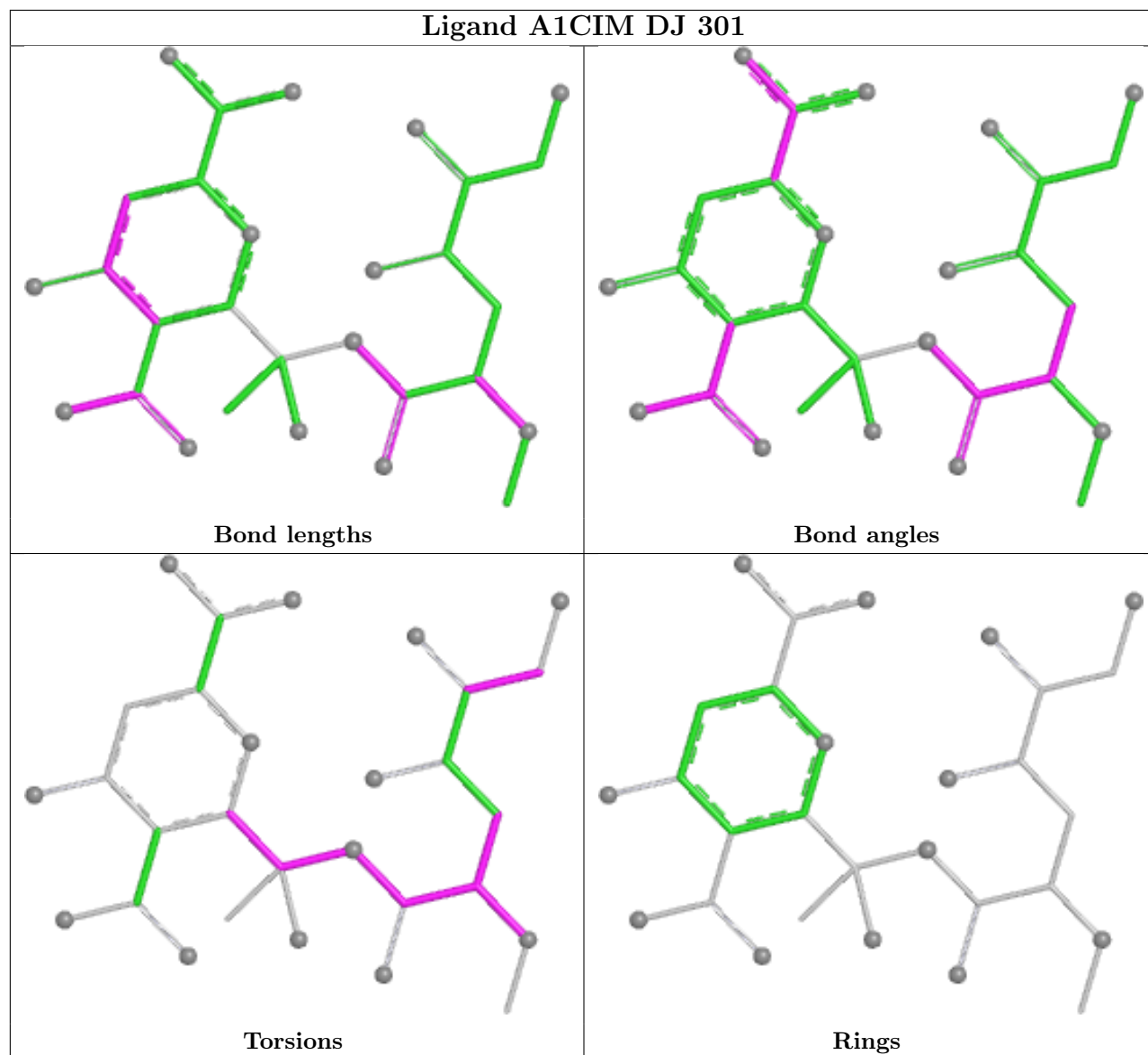
Ligand A1CIM DD 305



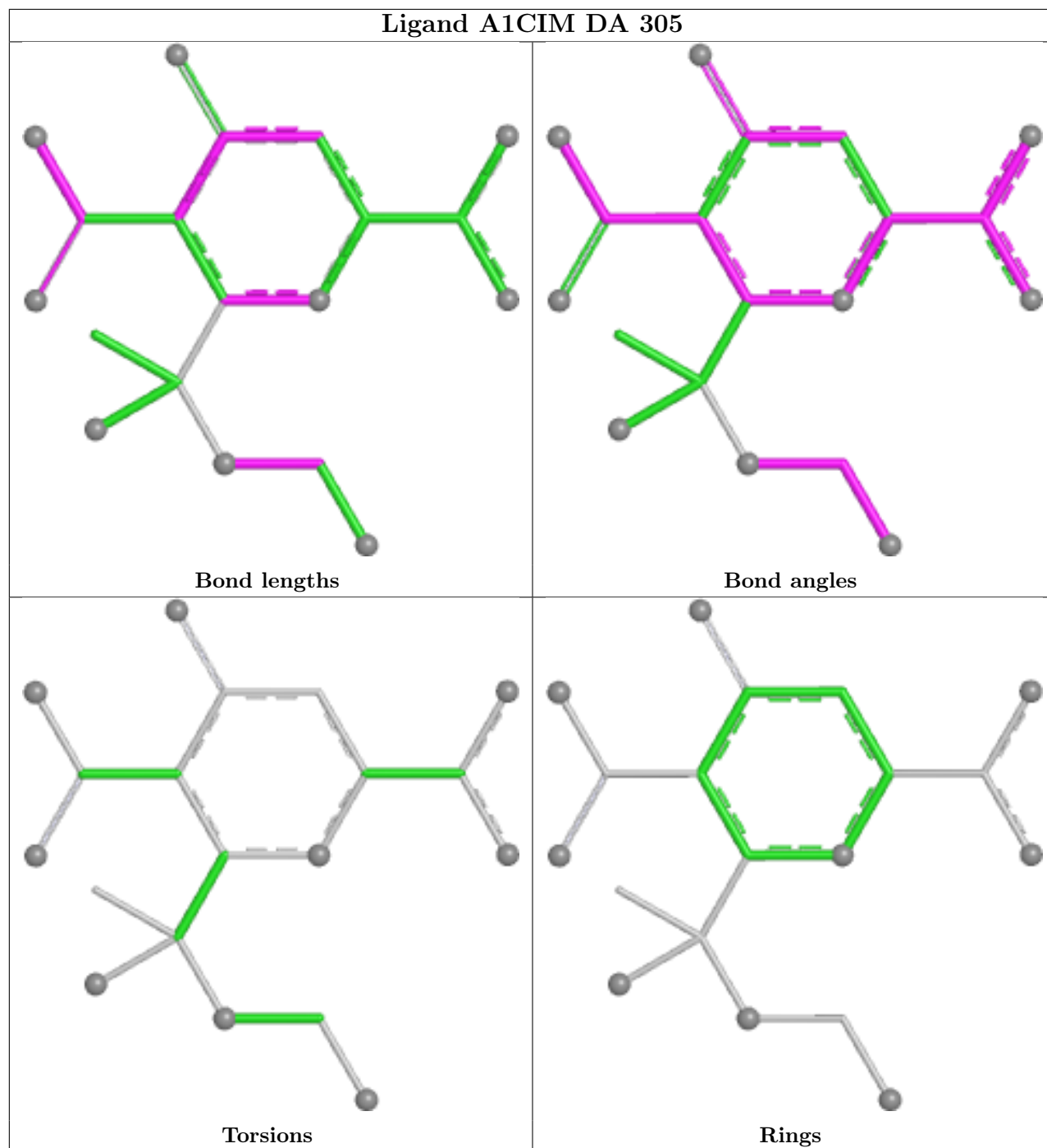
Ligand A1CIM DE 304



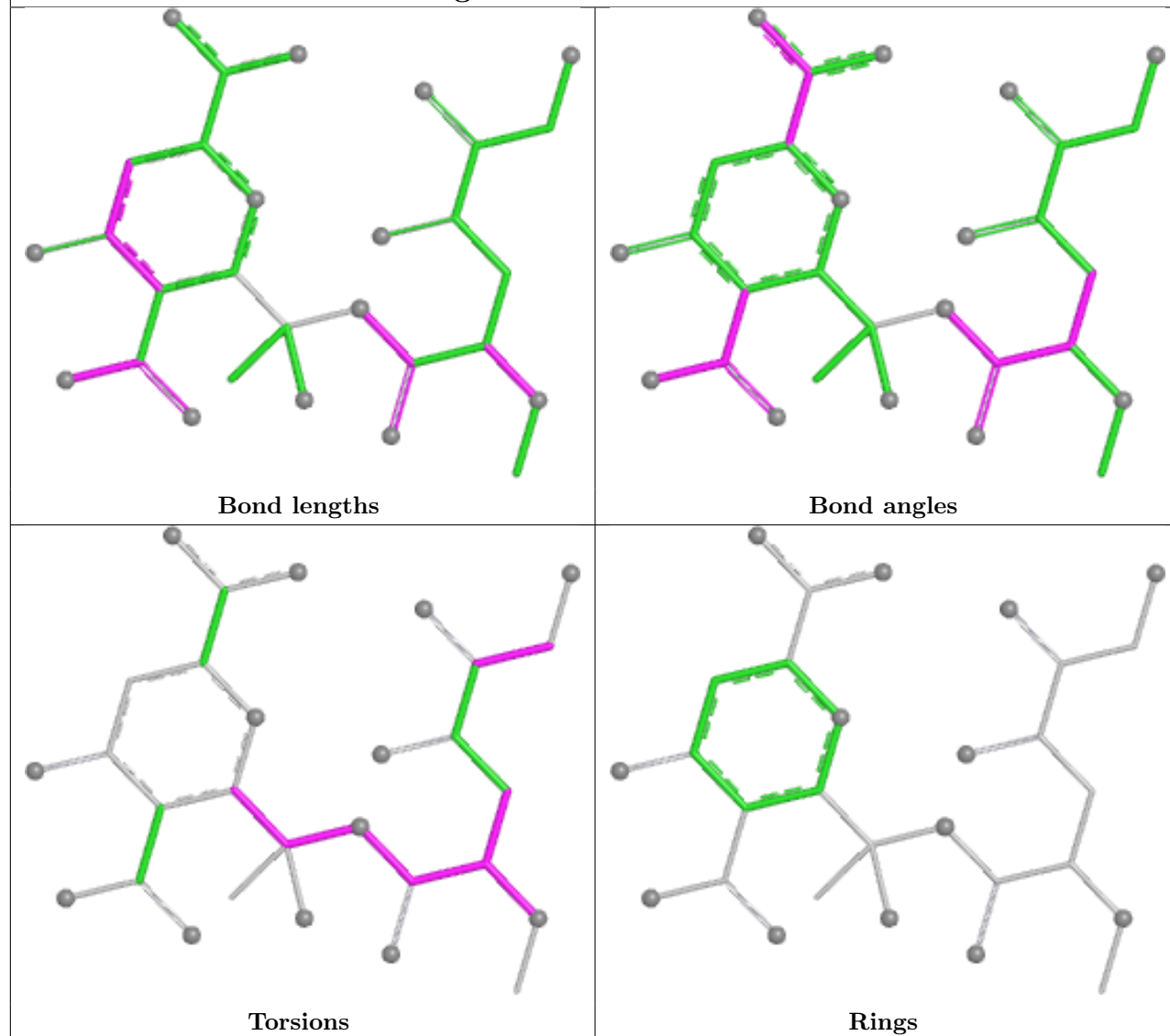
Ligand A1CIM DJ 301



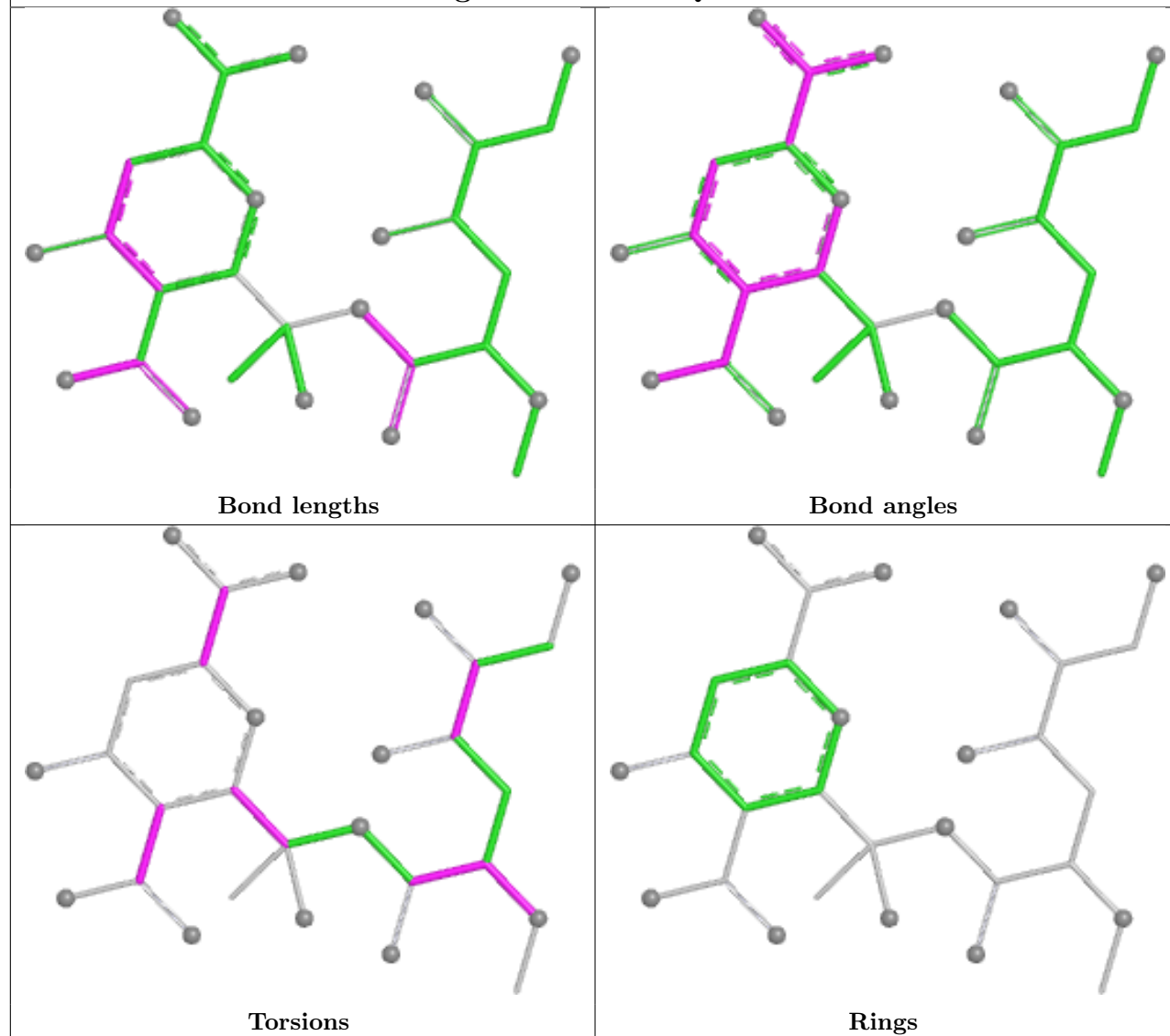
Ligand A1CIM DA 305



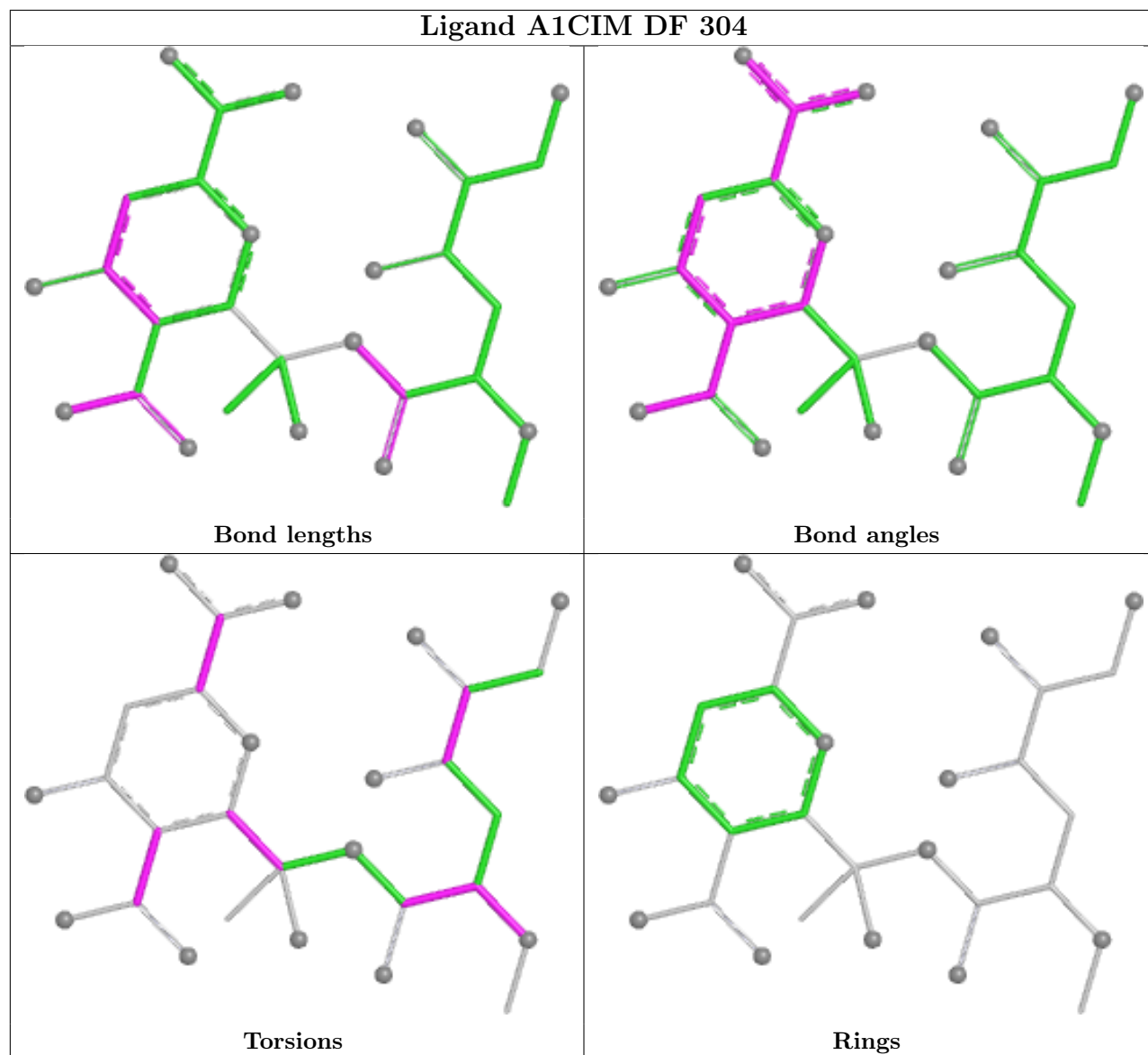
Ligand A1CIM DN 301



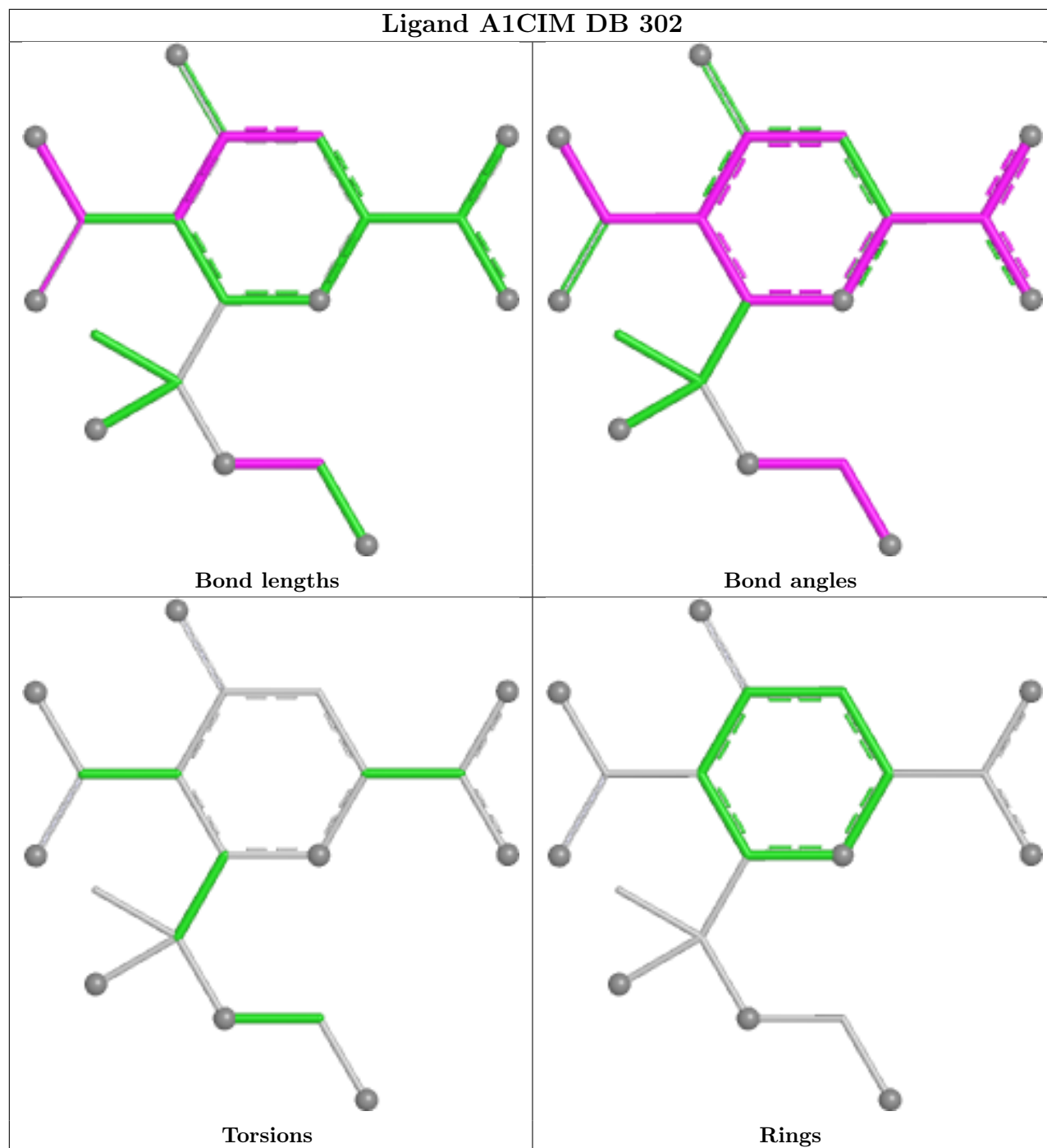
Ligand A1CIM DQ 304



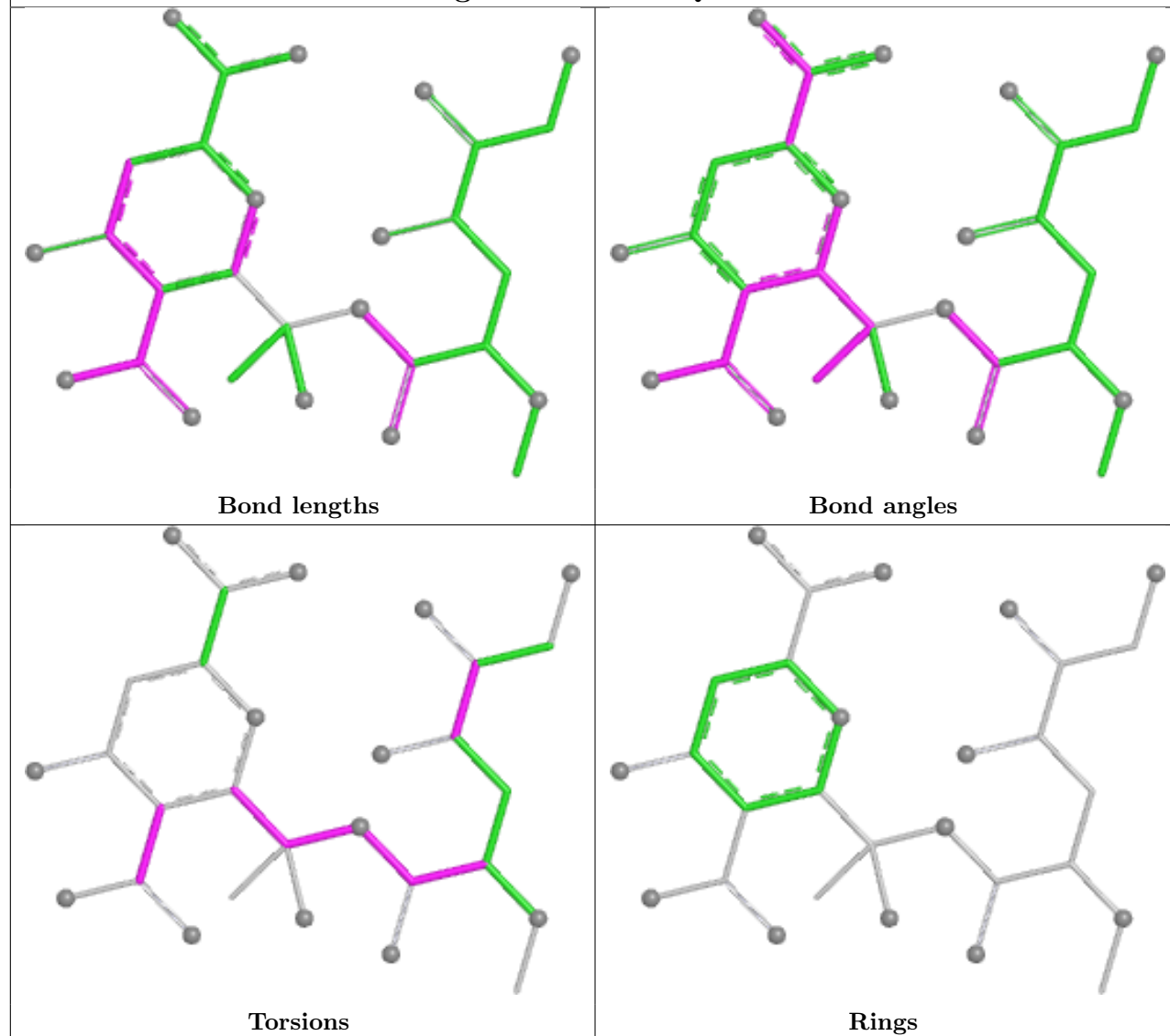
Ligand A1CIM DF 304

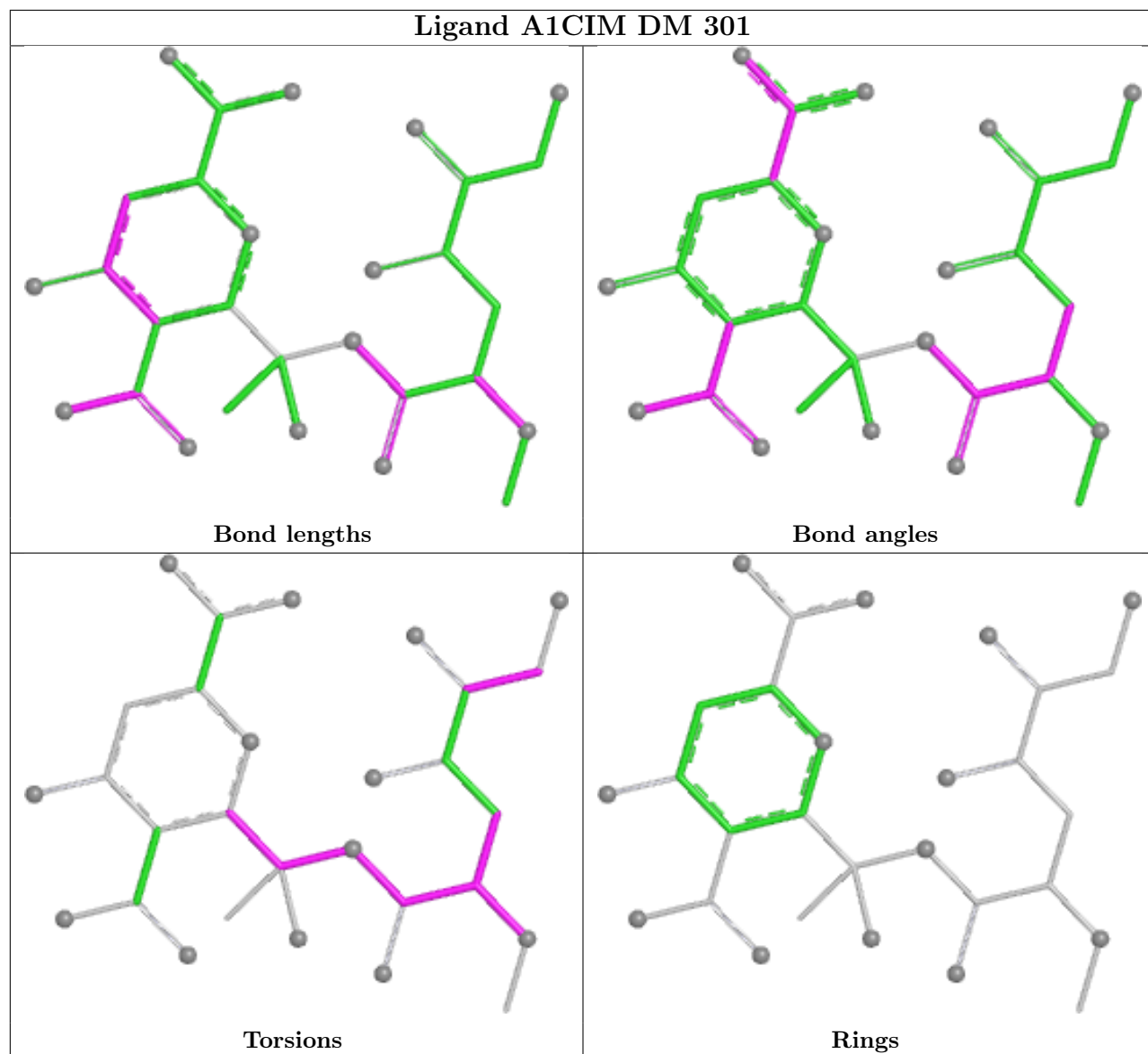


Ligand A1CIM DB 302

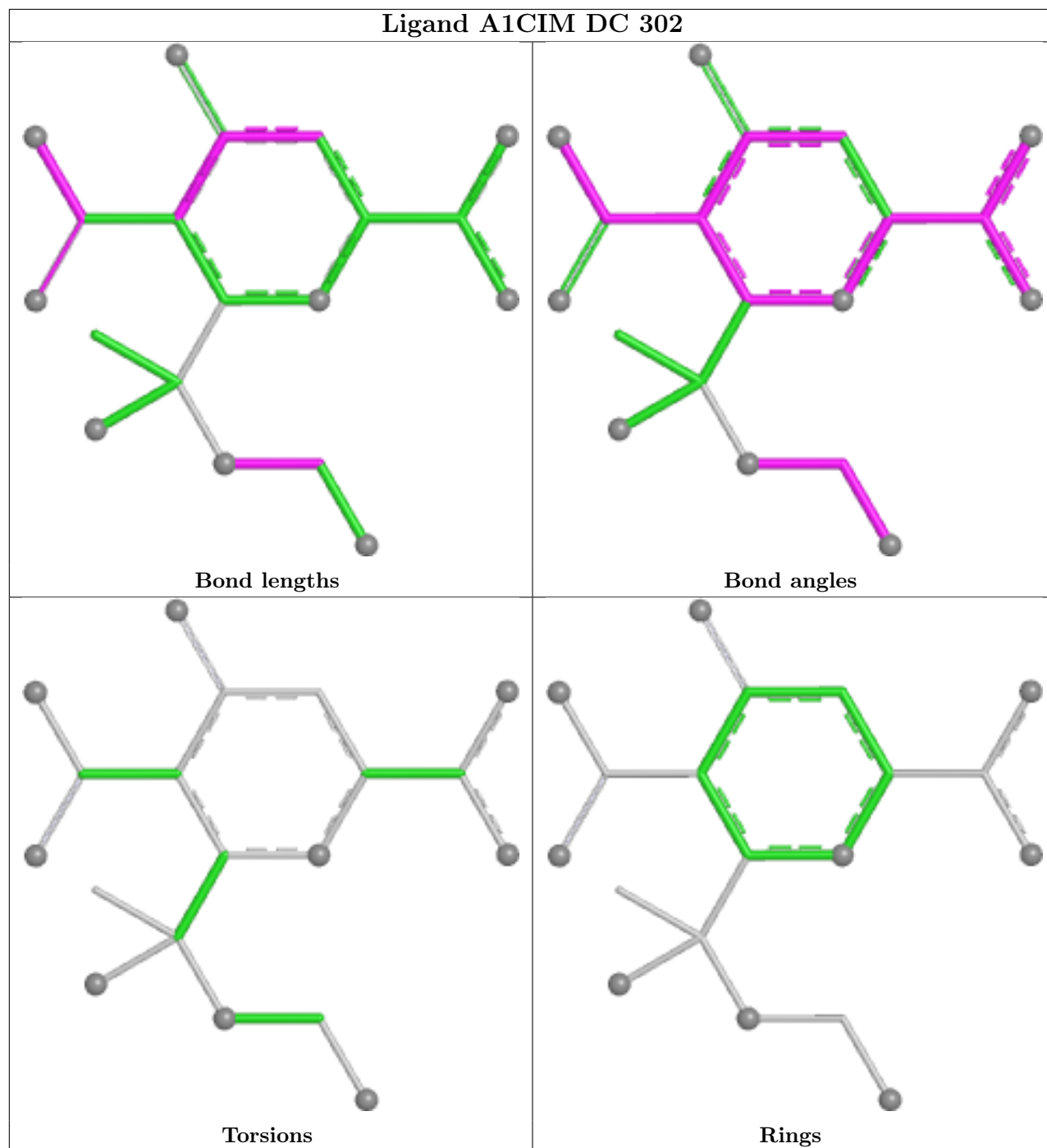


Ligand A1CIM DQ 303

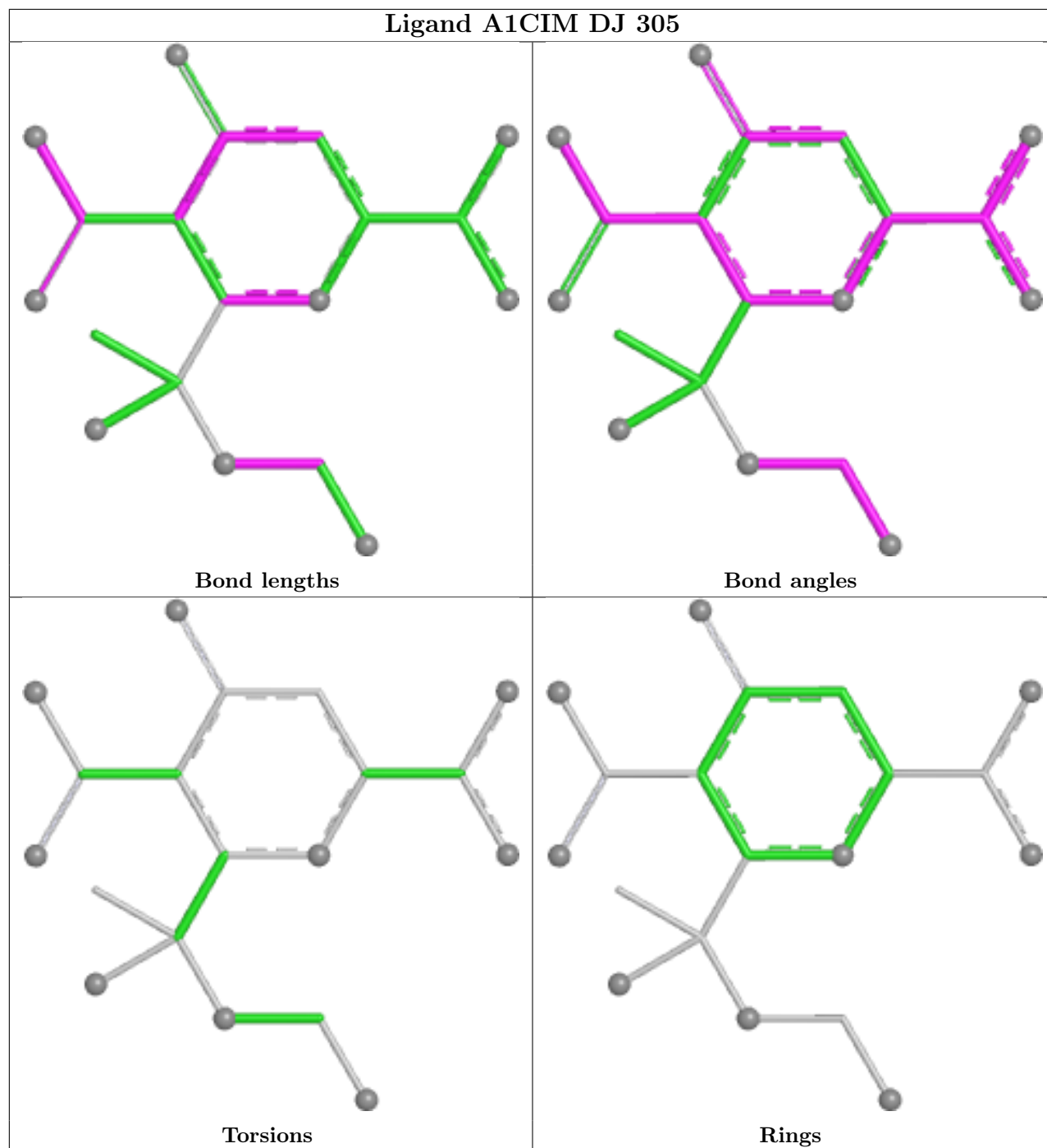




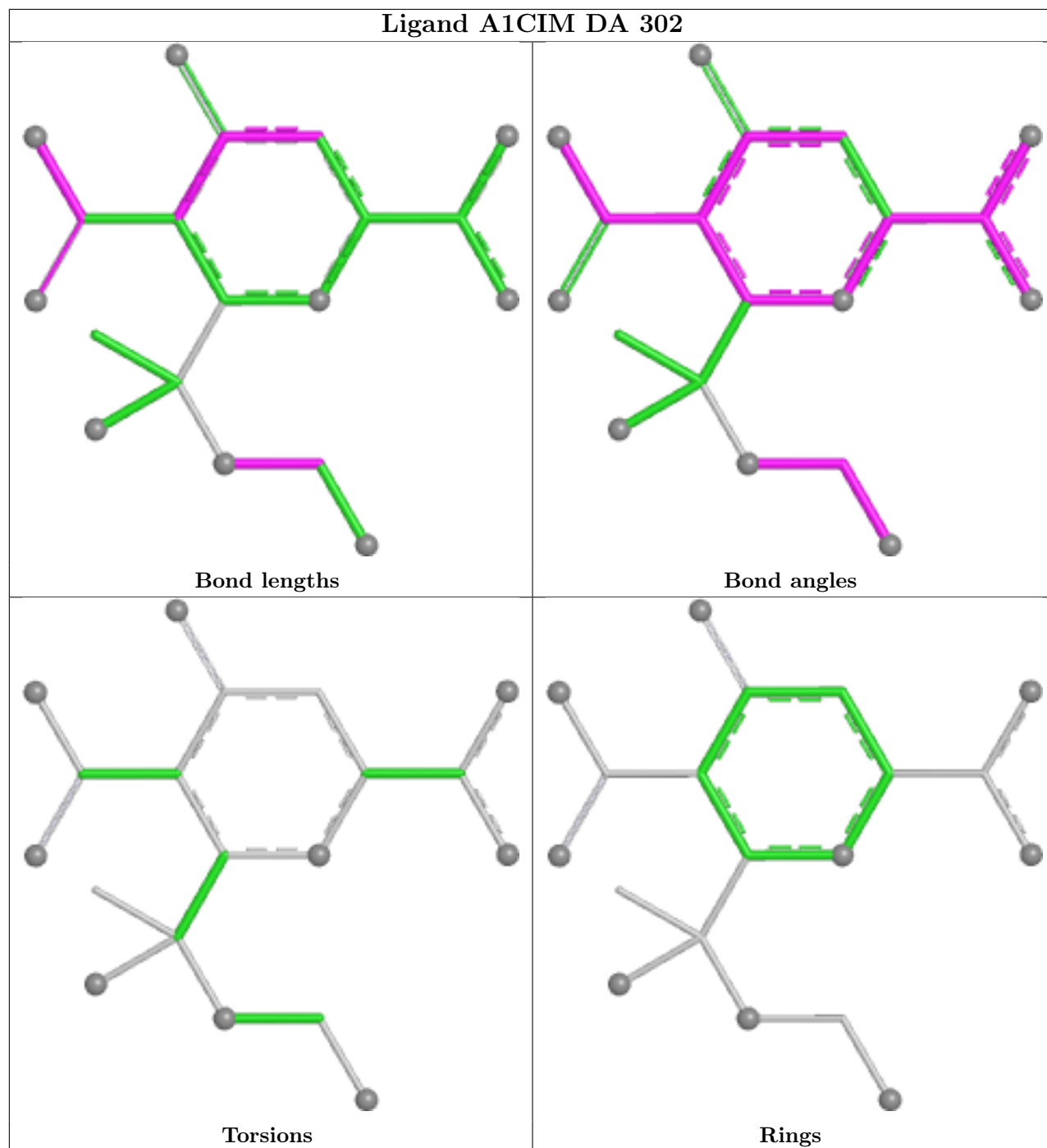
Ligand A1CIM DC 302



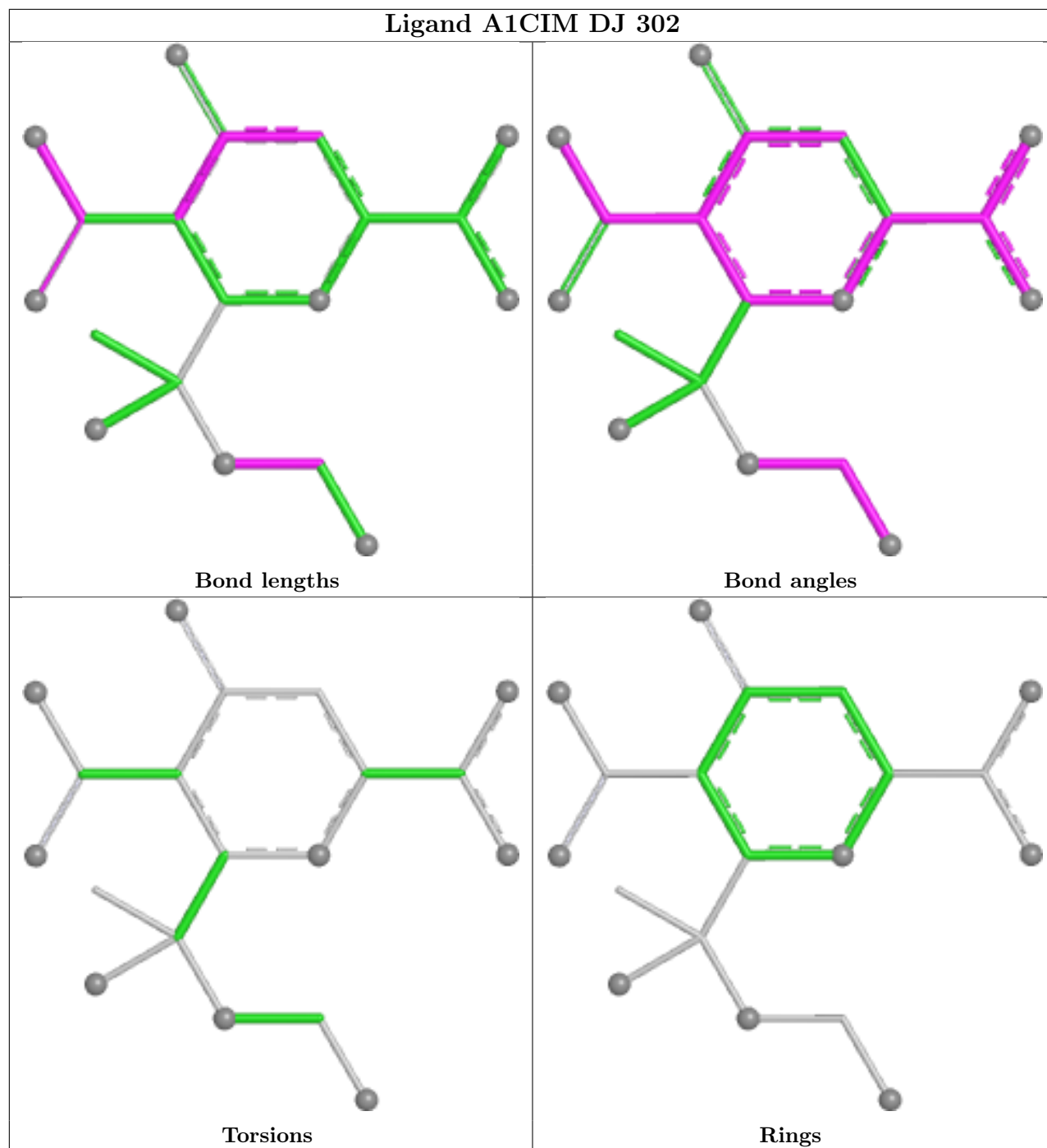
Ligand A1CIM DJ 305



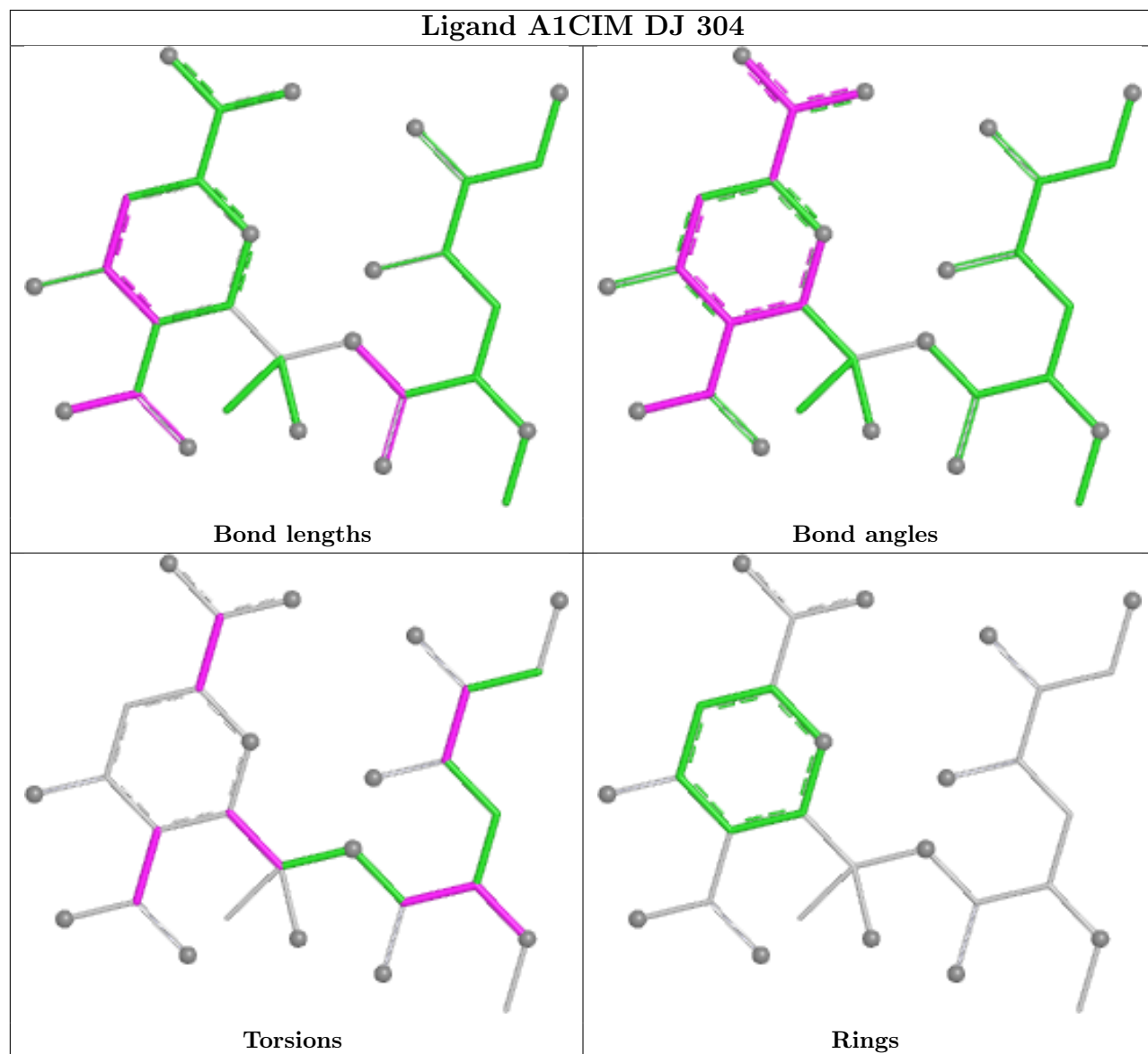
Ligand A1CIM DA 302



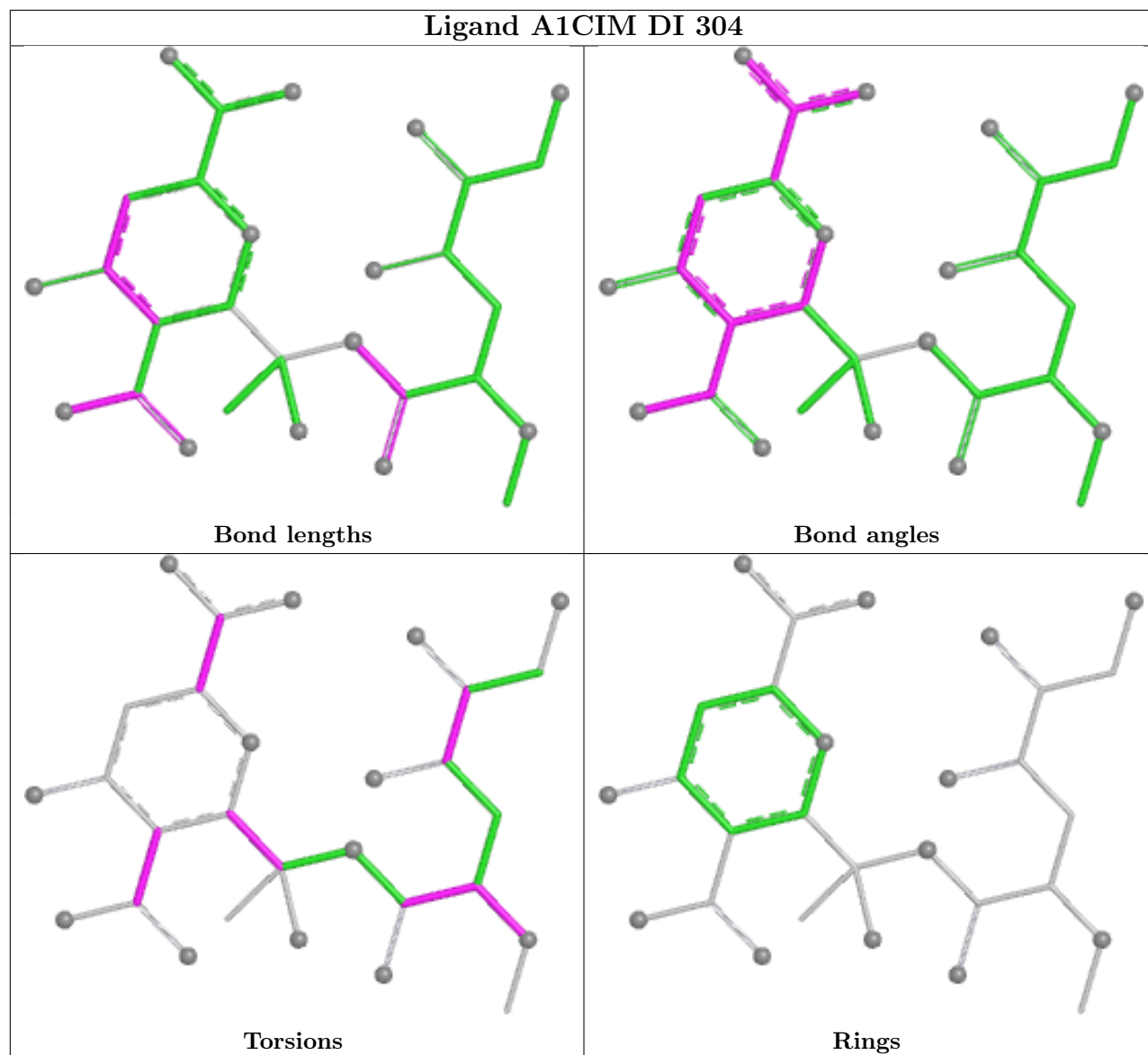
Ligand A1CIM DJ 302



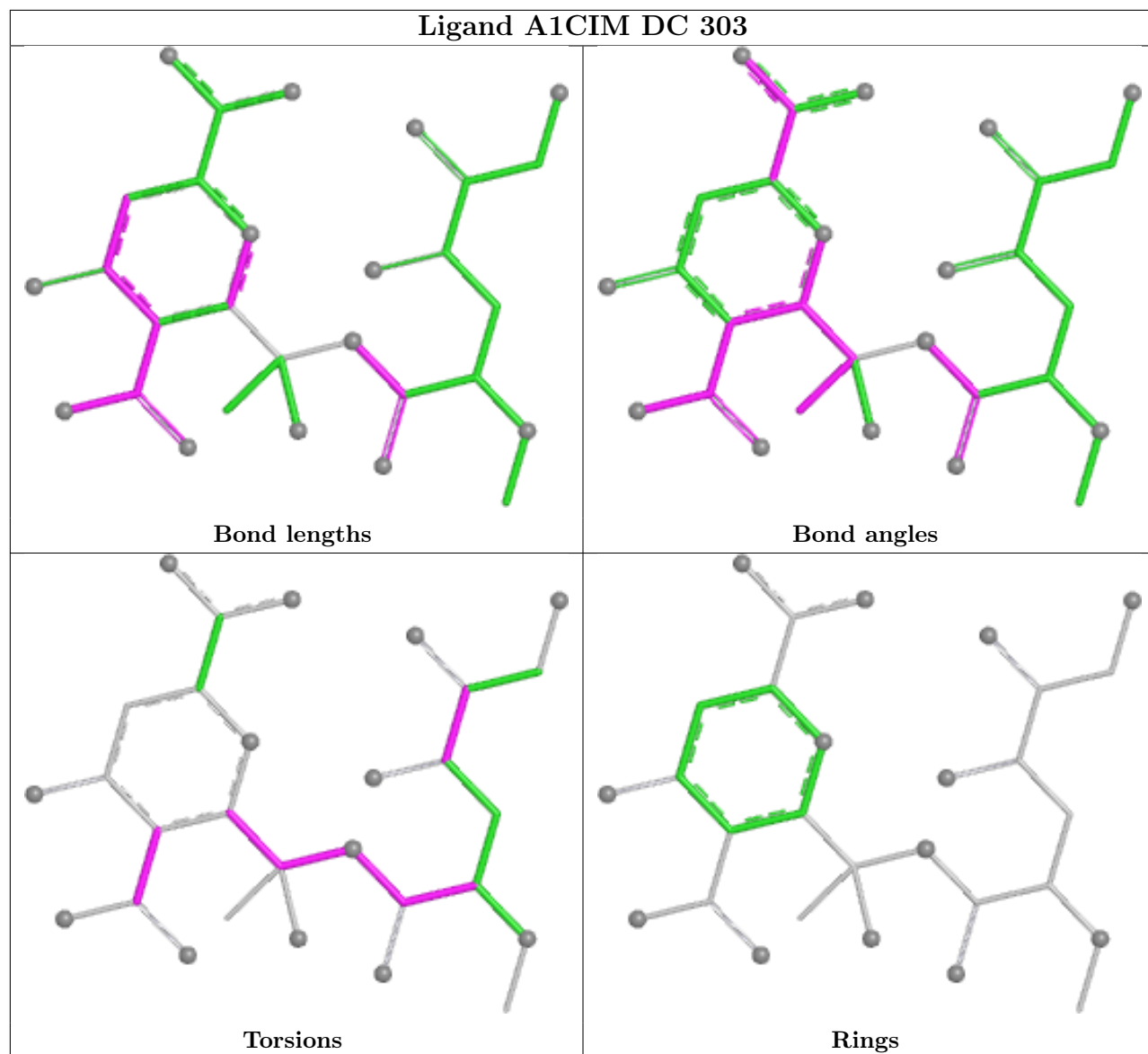
Ligand A1CIM DJ 304



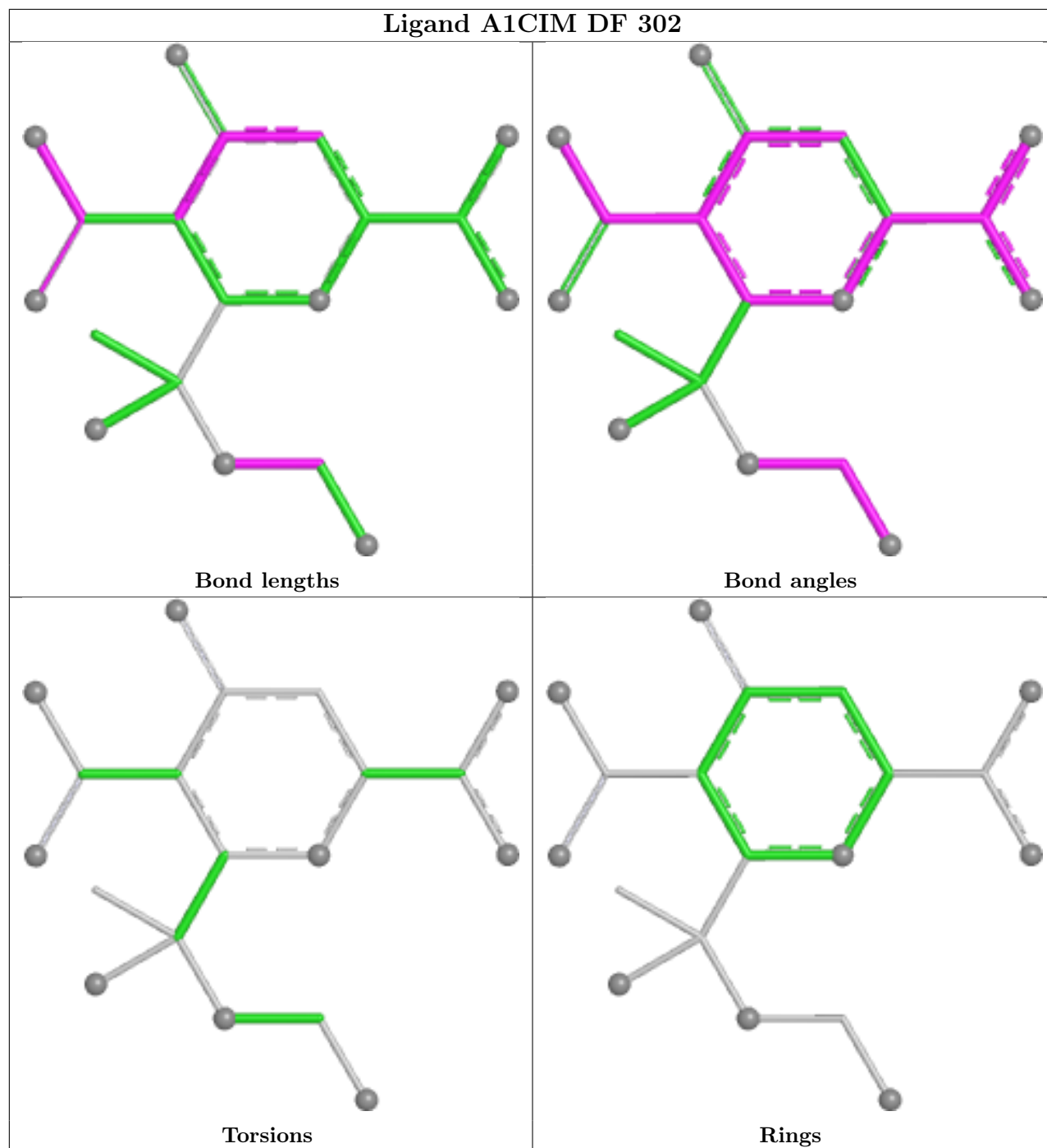
Ligand A1CIM DI 304

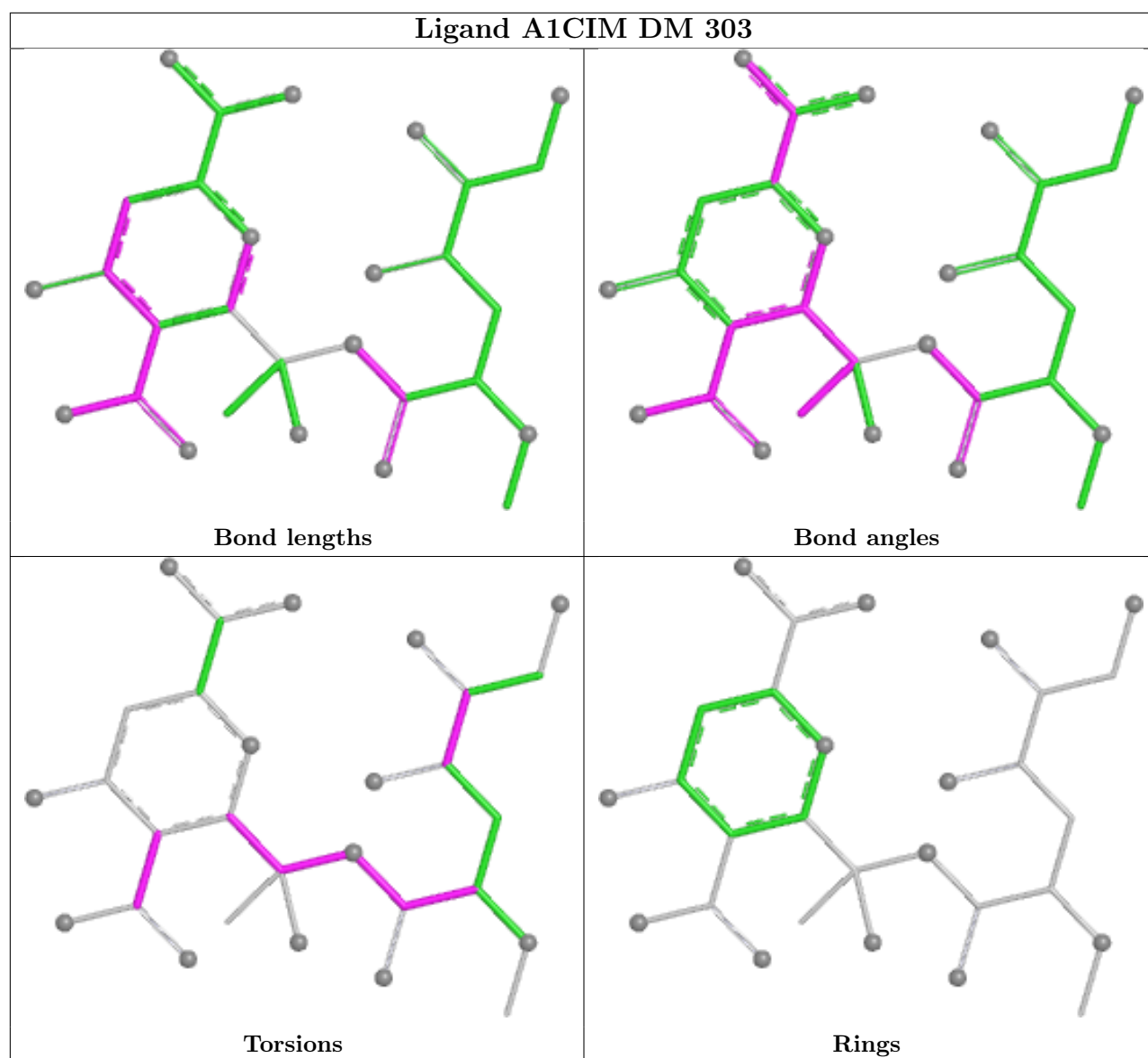


Ligand A1CIM DC 303

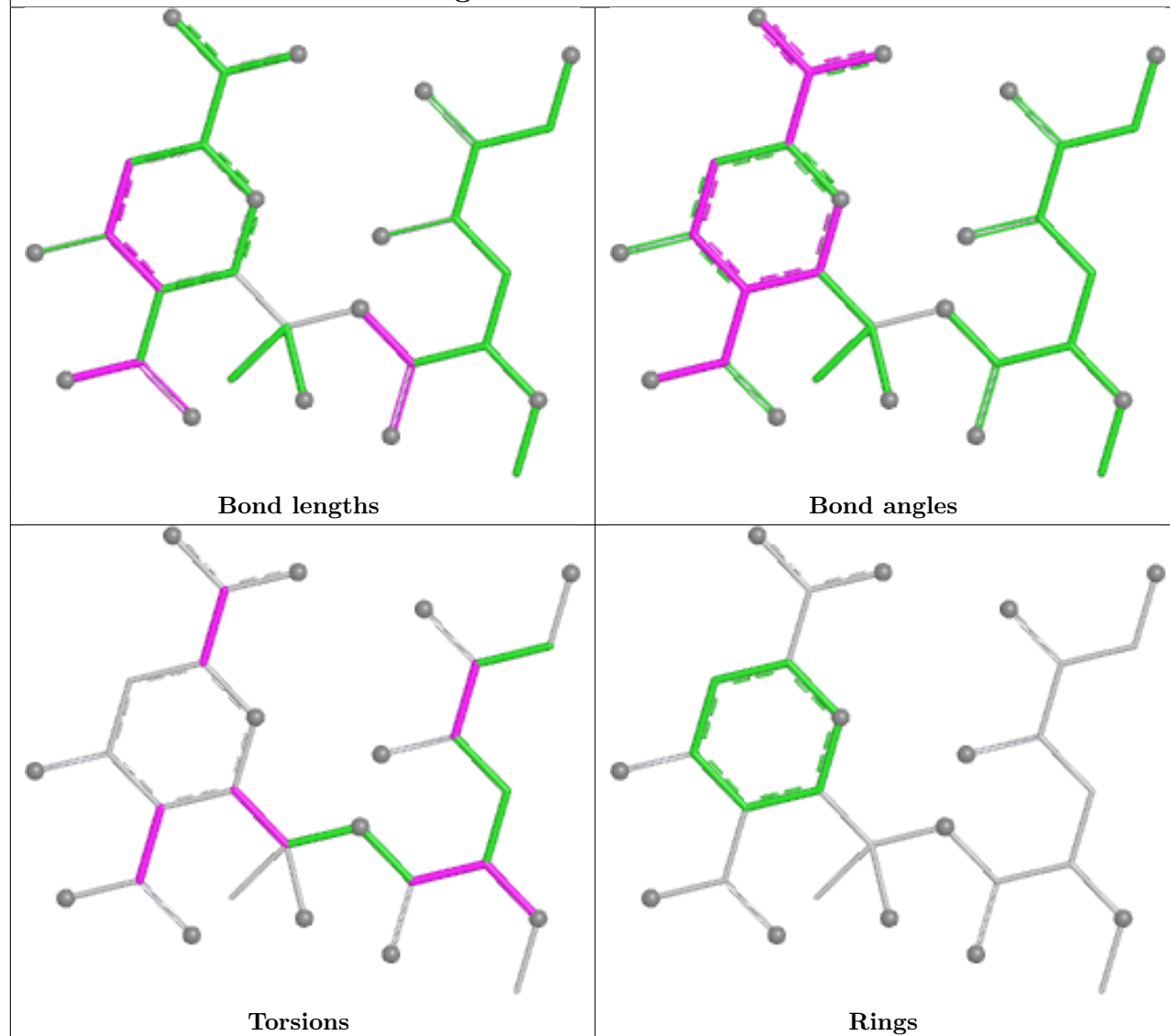


Ligand A1CIM DF 302

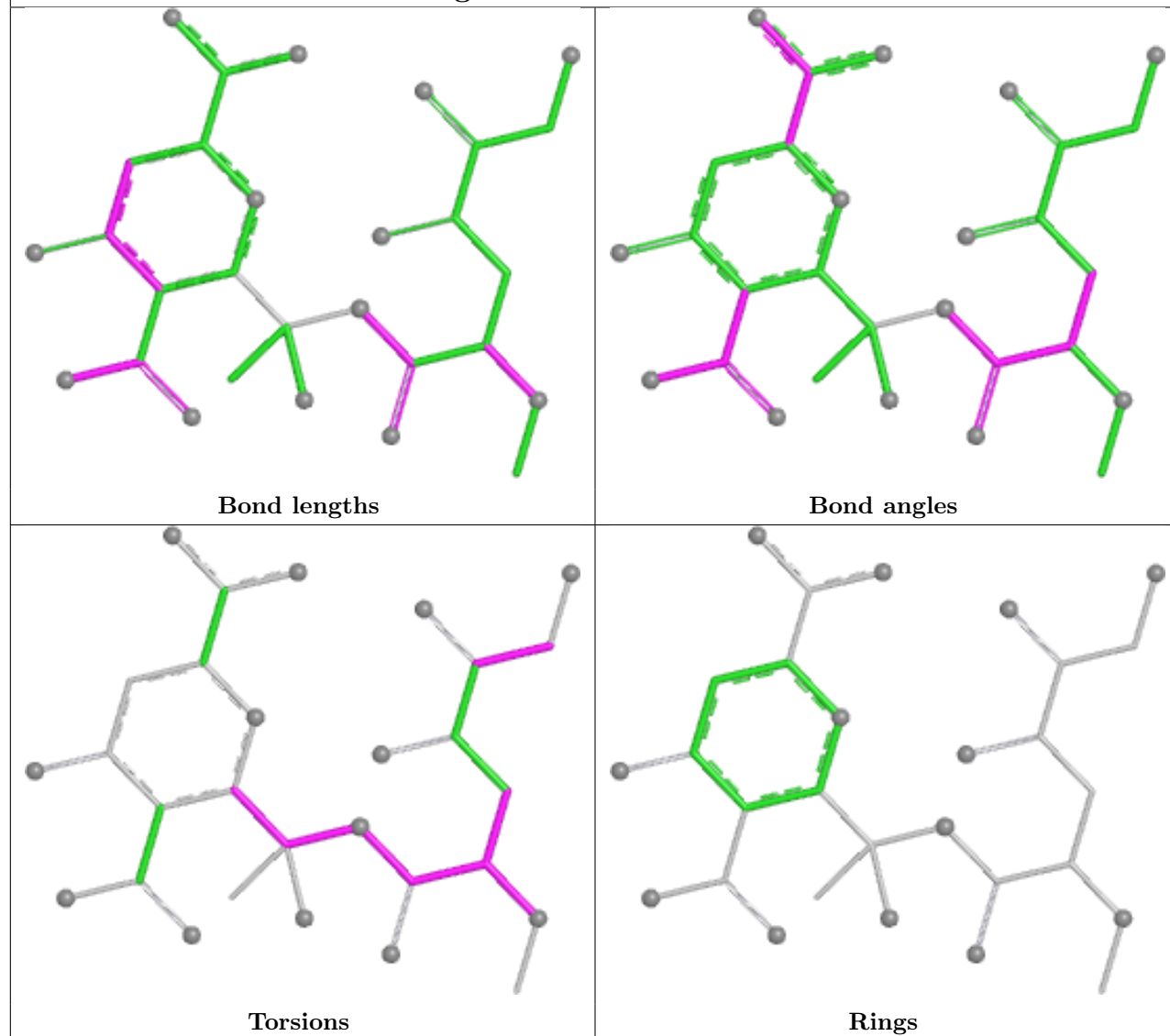




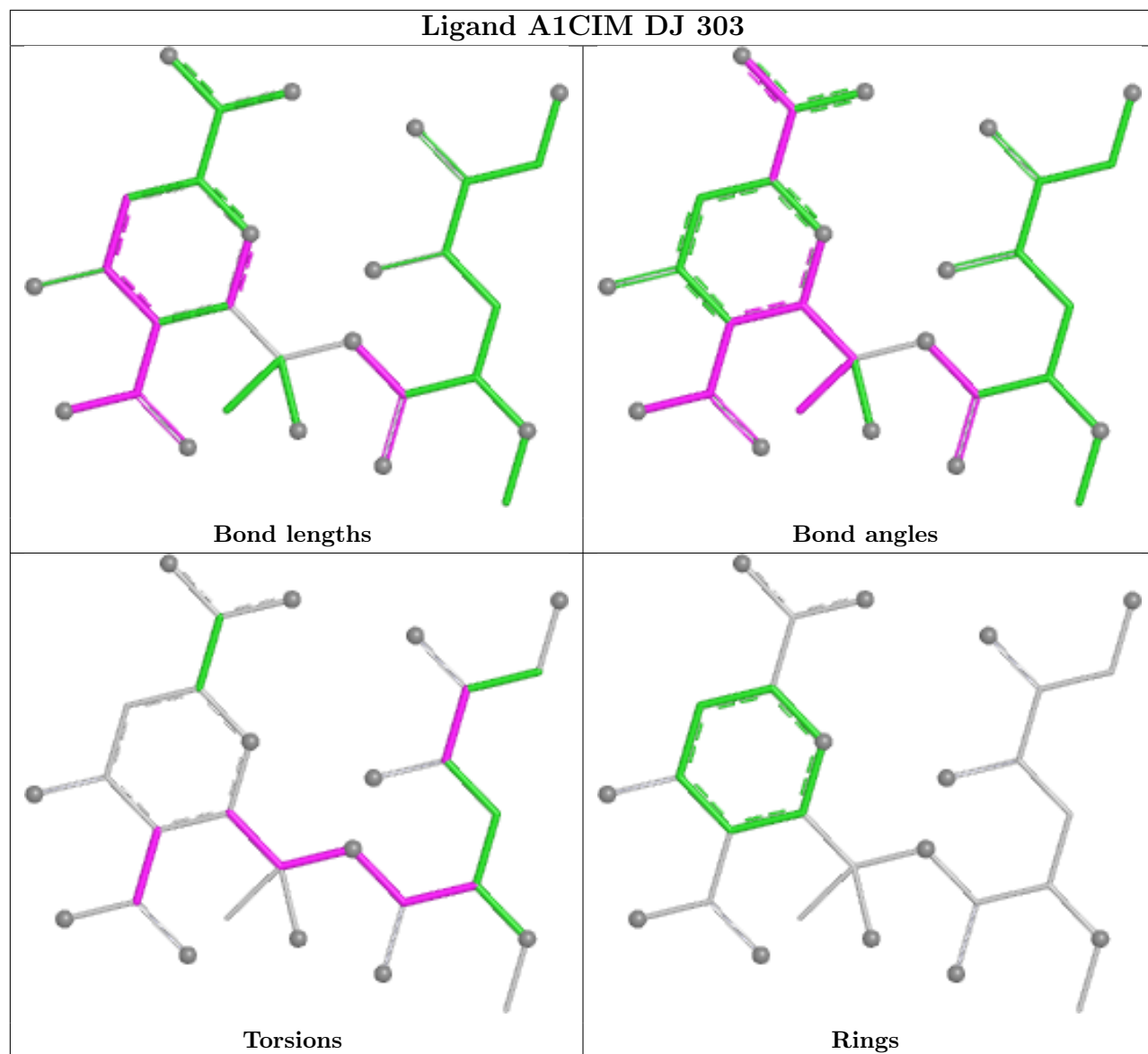
Ligand A1CIM DO 304



Ligand A1CIM DH 301



Ligand A1CIM DJ 303



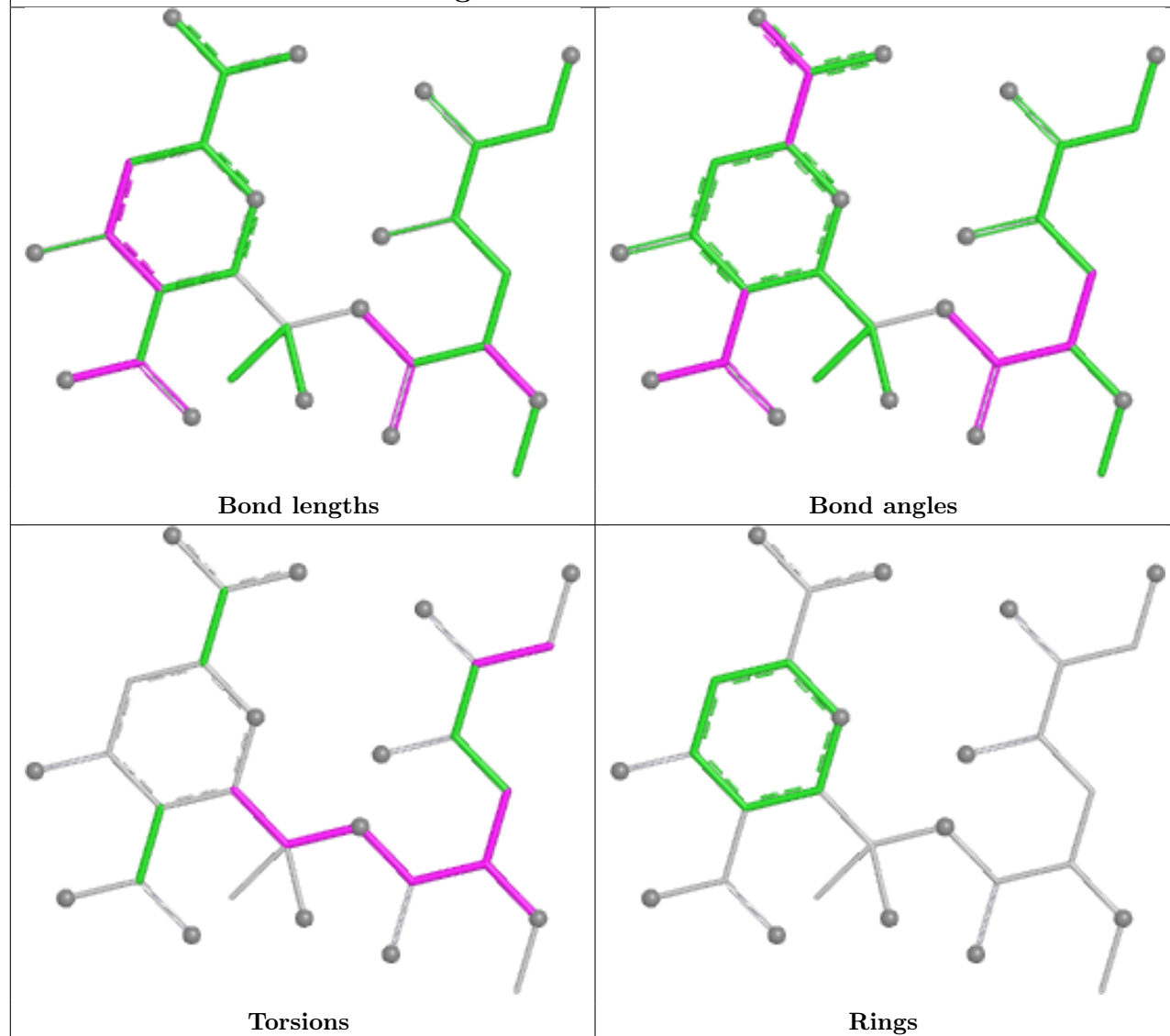
Bond lengths

Bond angles

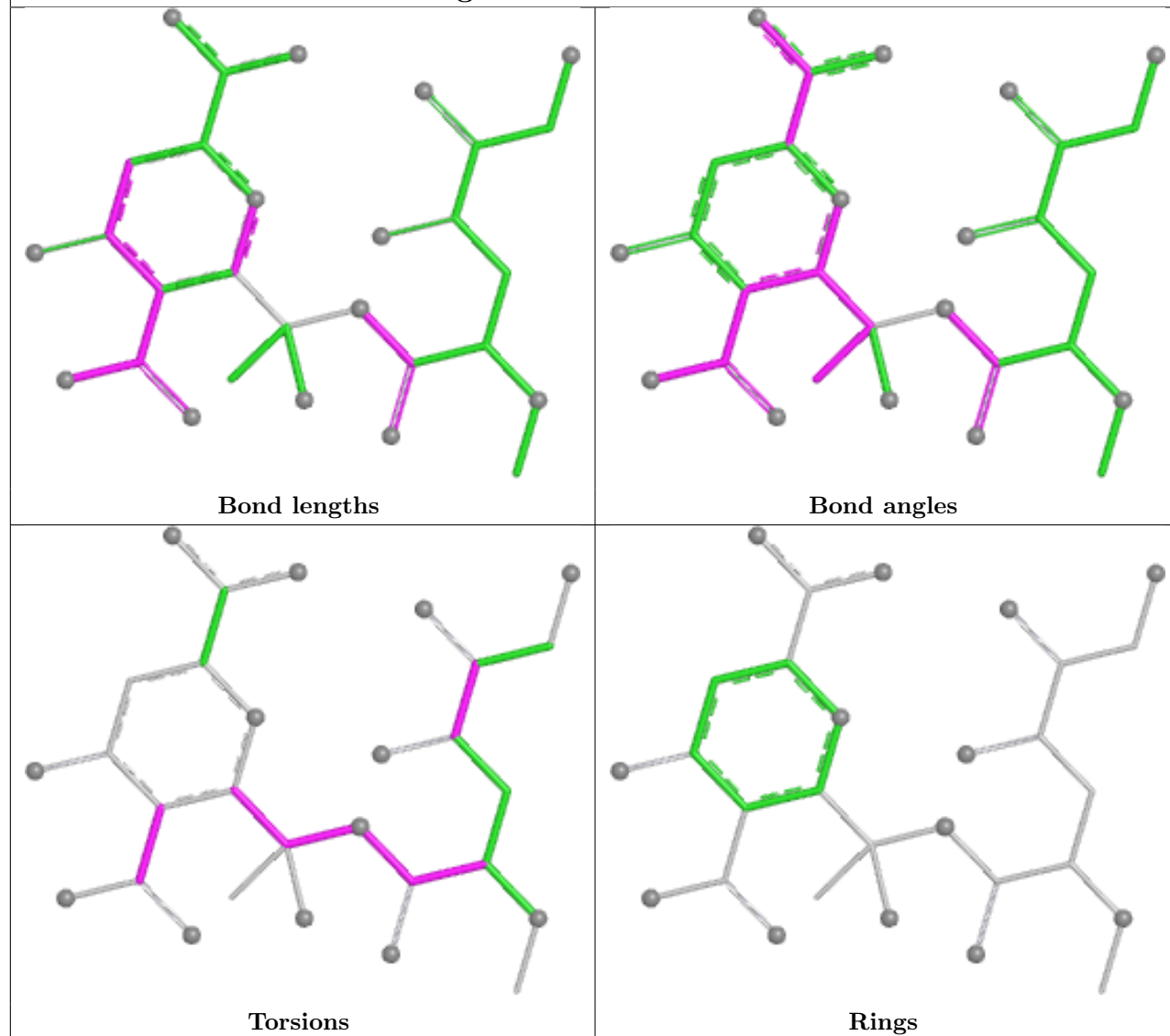
Torsions

Rings

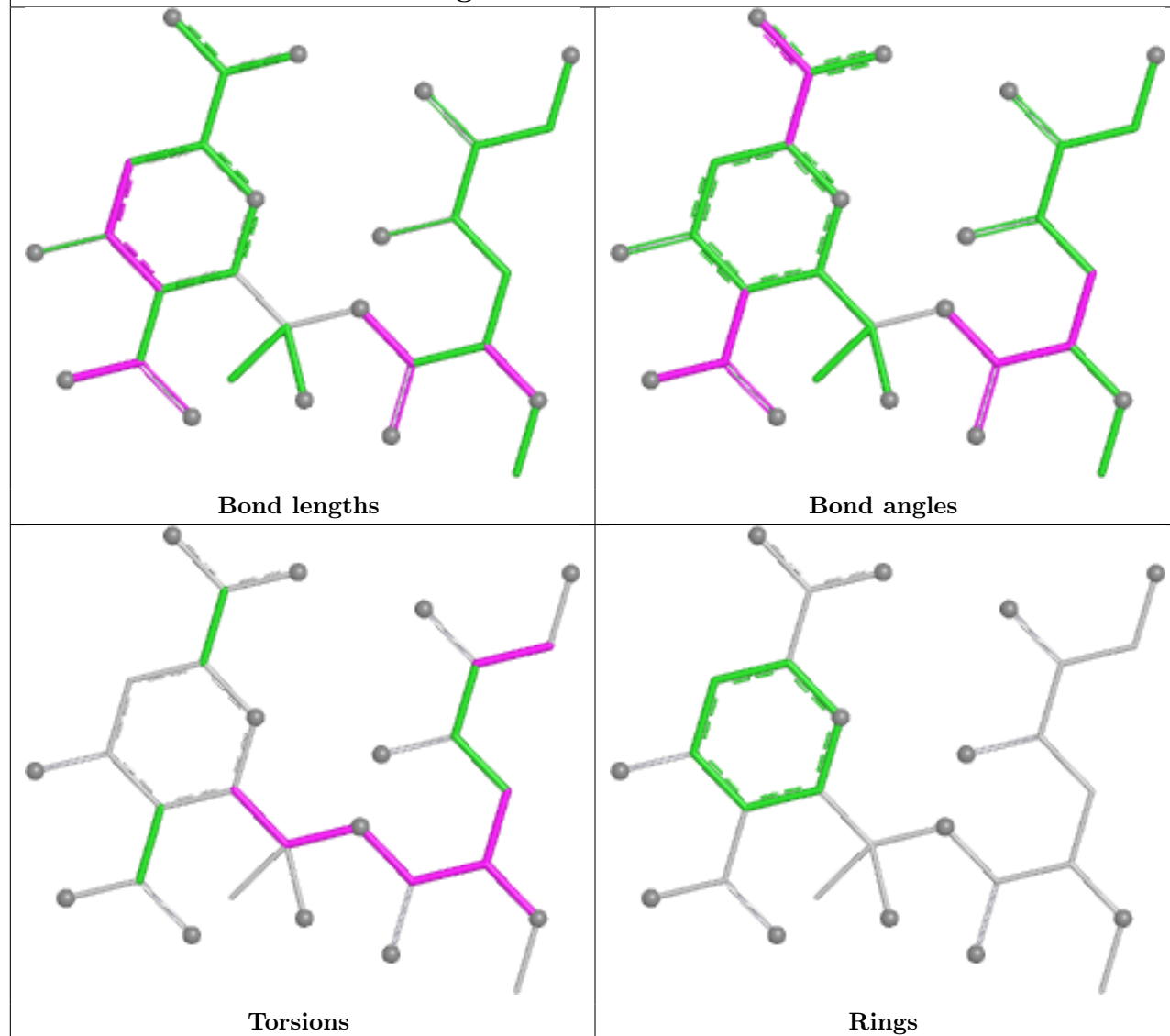
Ligand A1CIM DD 301



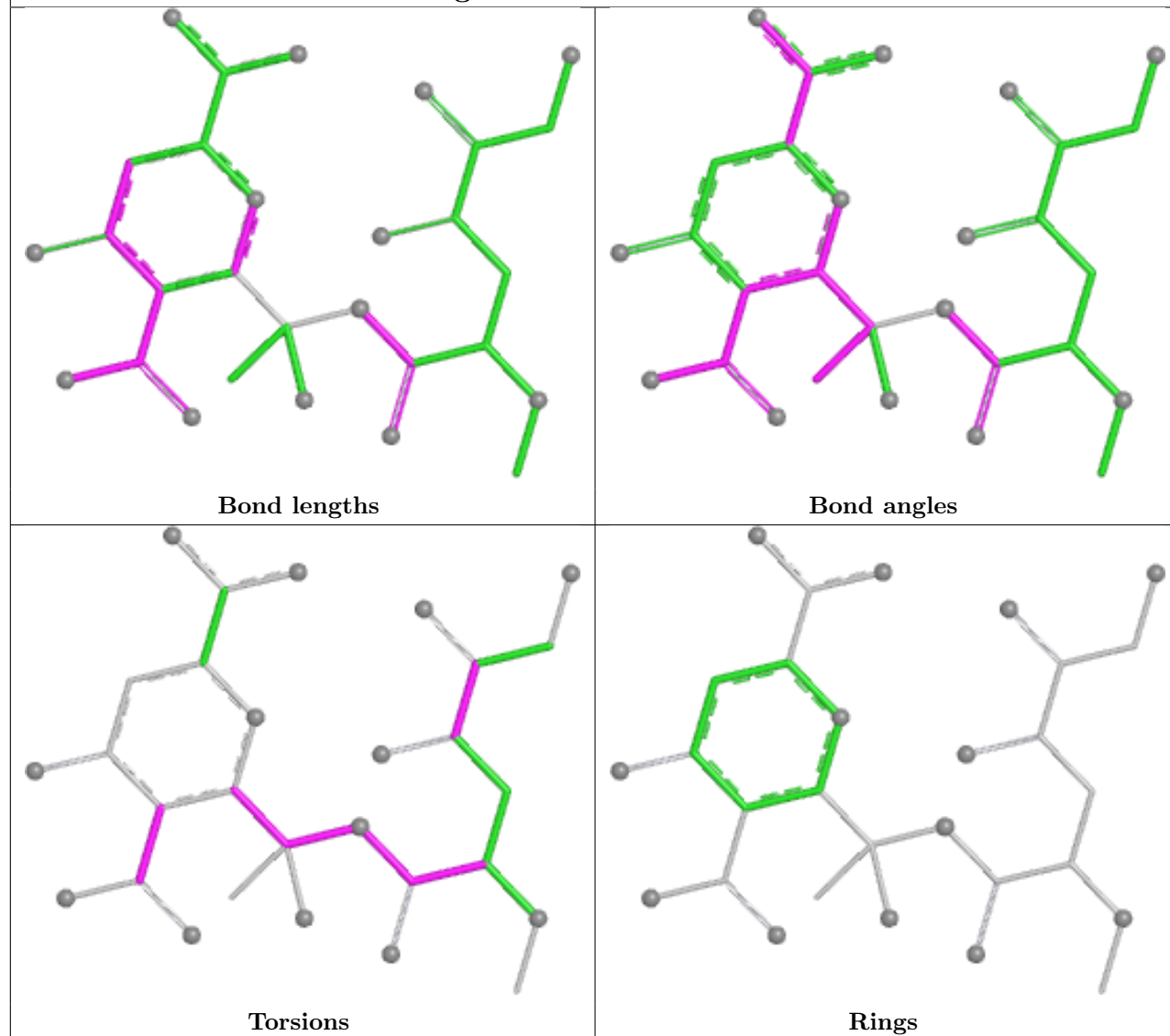
Ligand A1CIM DF 303



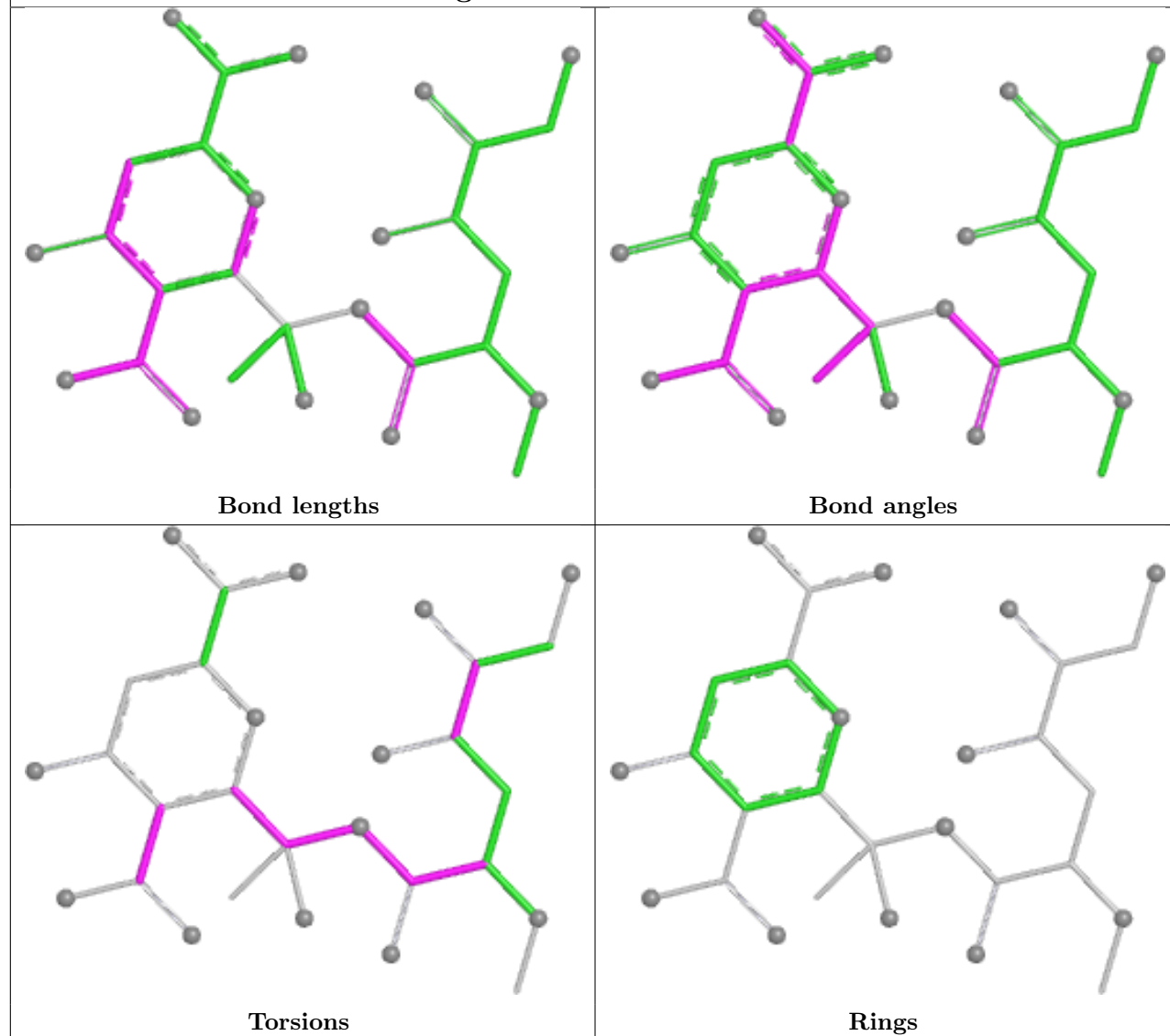
Ligand A1CIM DE 301

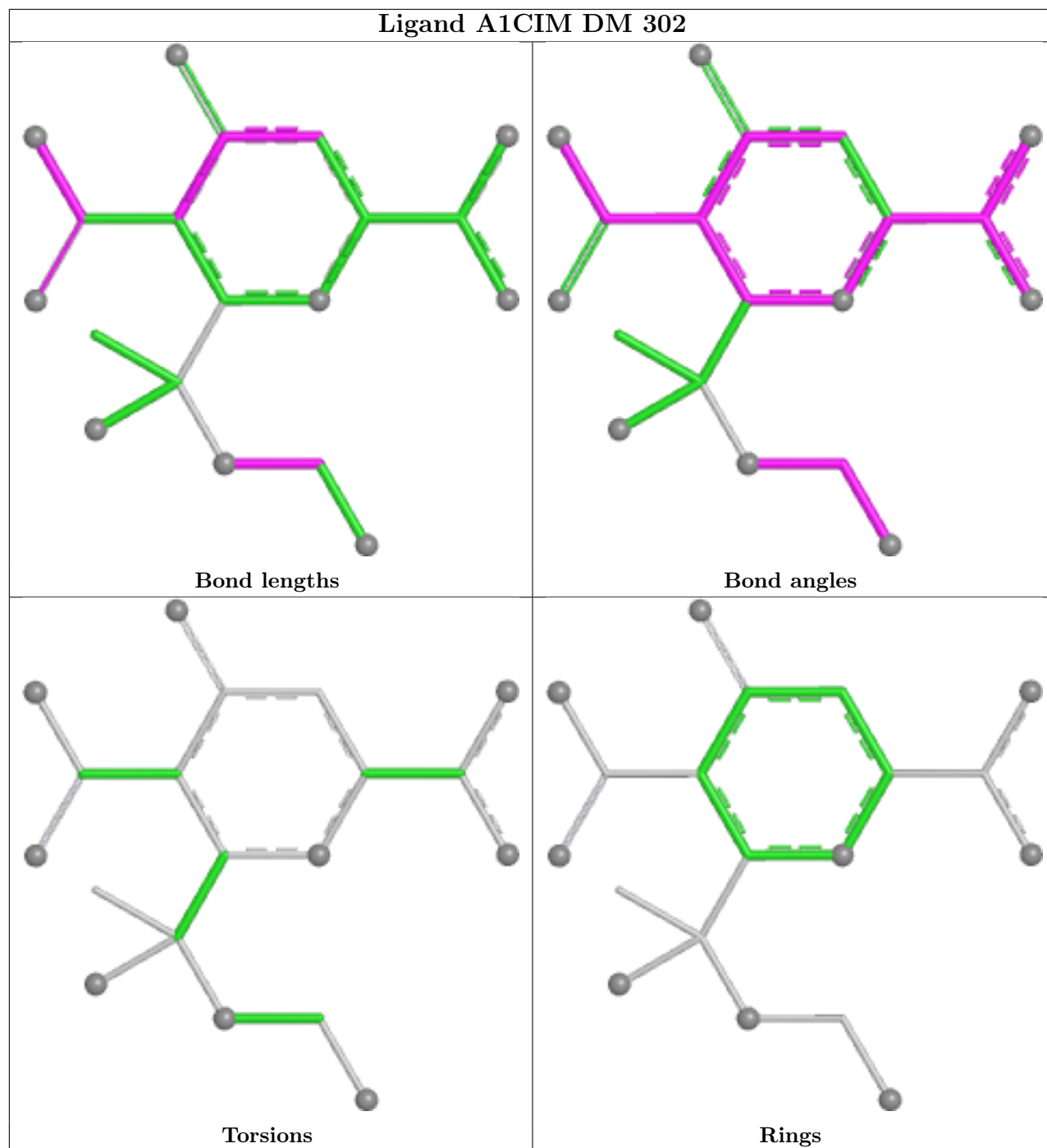


Ligand A1CIM DH 303

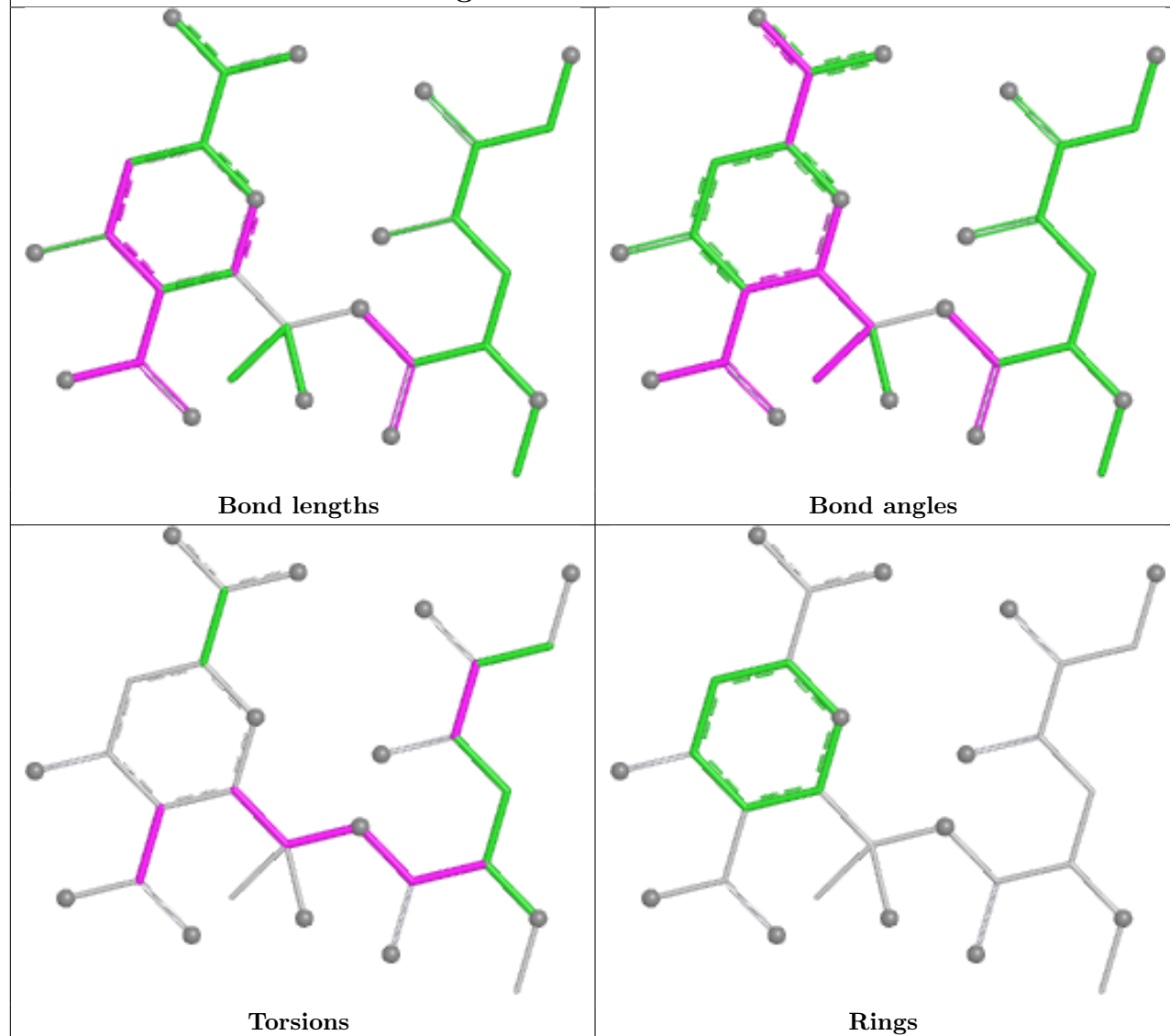


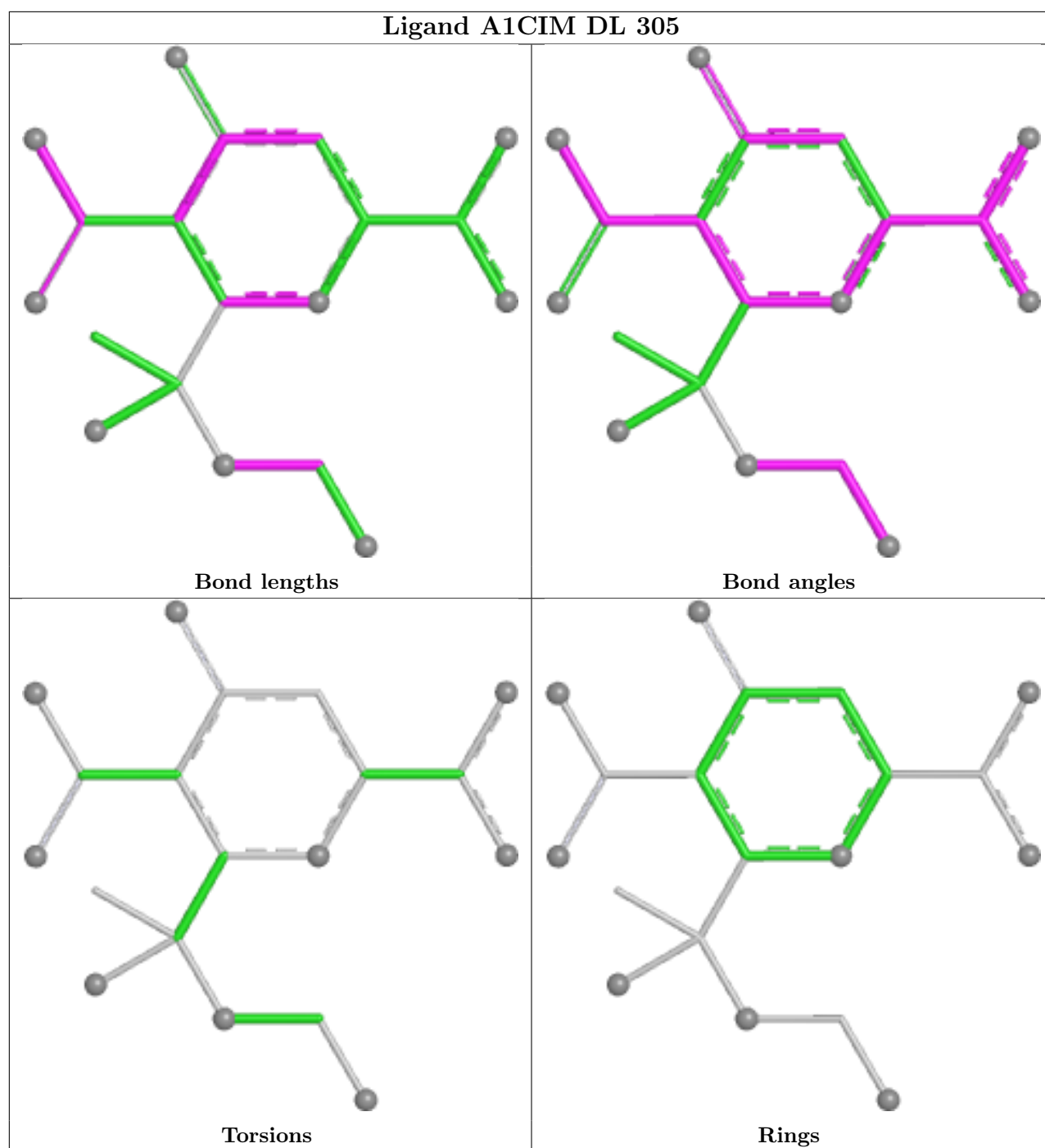
Ligand A1CIM DP 303





Ligand A1CIM DE 303





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.

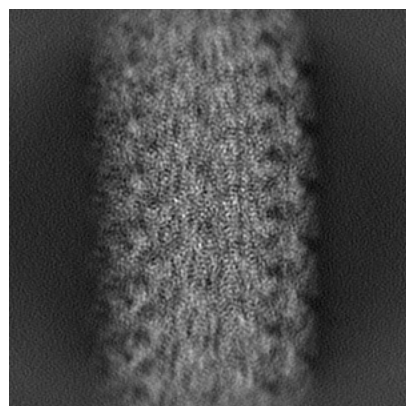
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71673. These allow visual inspection of the internal detail of the map and identification of artifacts.

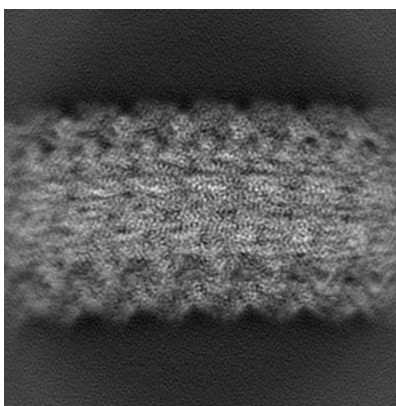
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

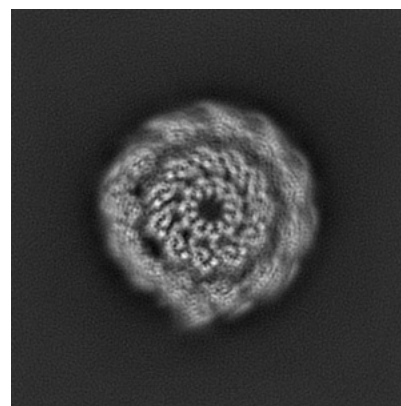
6.1.1 Primary map



X

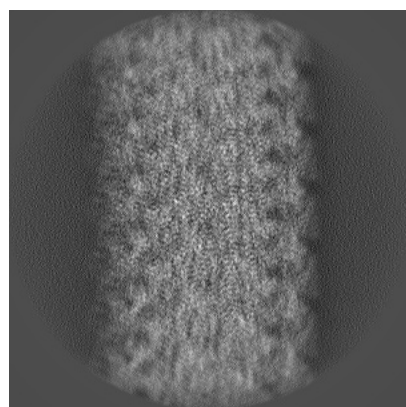


Y

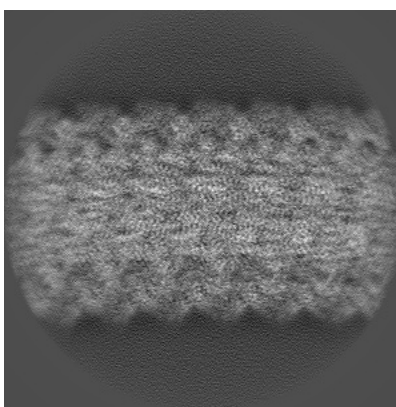


Z

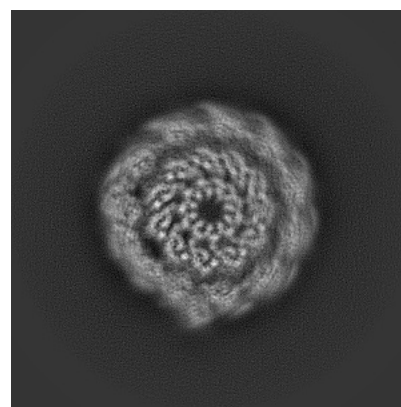
6.1.2 Raw map



X



Y

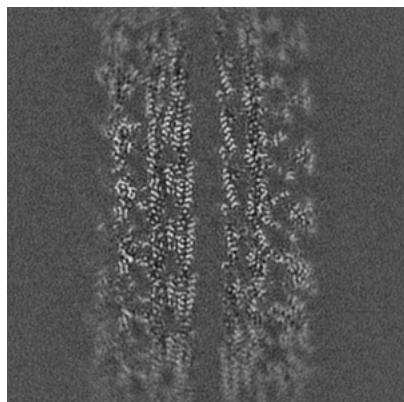


Z

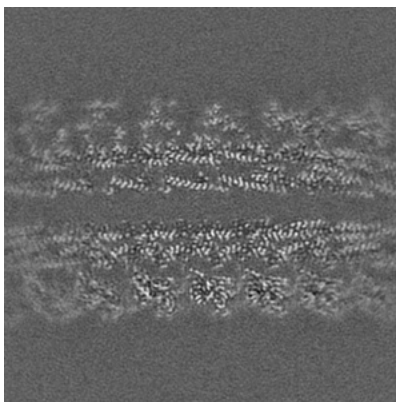
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

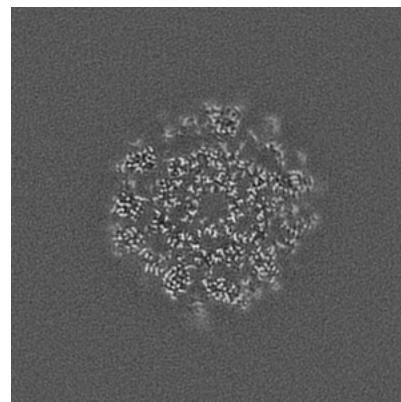
6.2.1 Primary map



X Index: 224

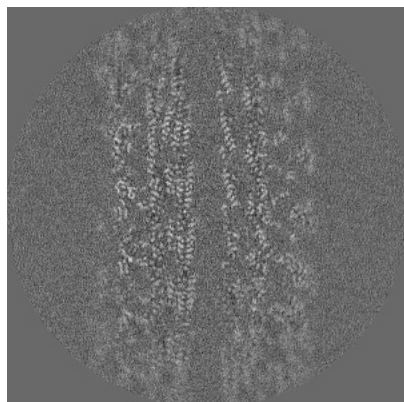


Y Index: 224

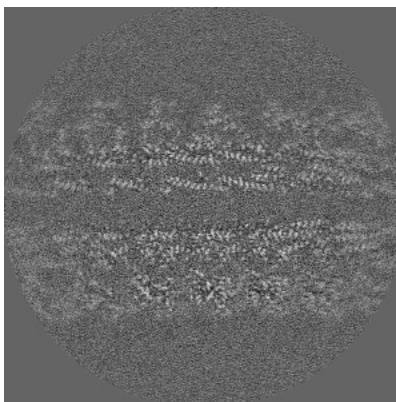


Z Index: 224

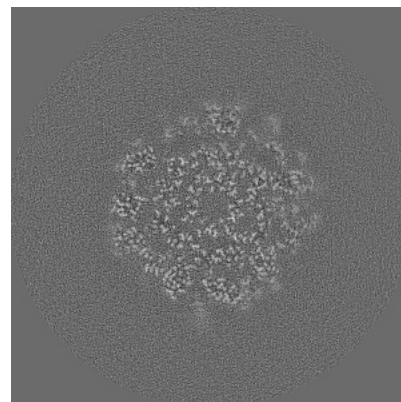
6.2.2 Raw map



X Index: 224



Y Index: 224

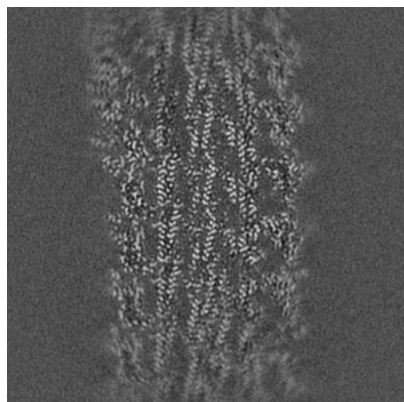


Z Index: 224

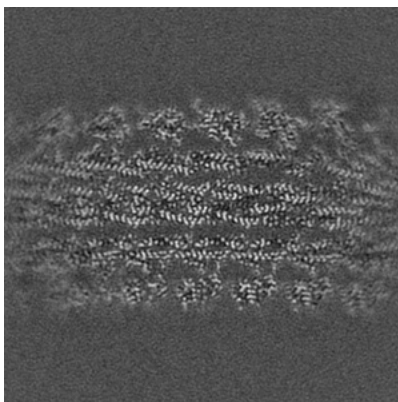
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

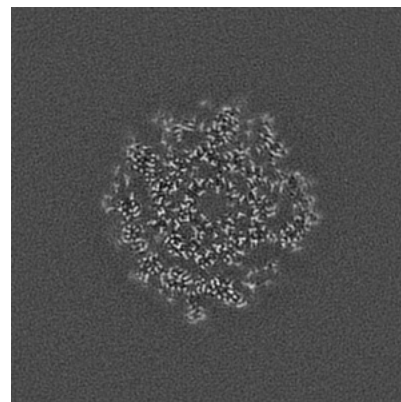
6.3.1 Primary map



X Index: 193

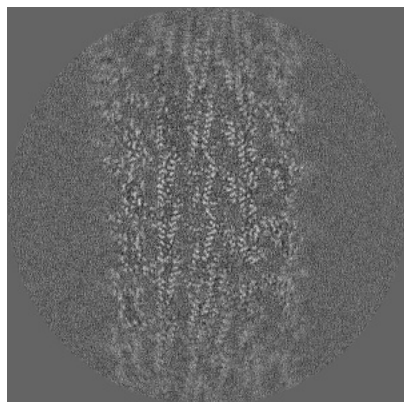


Y Index: 198

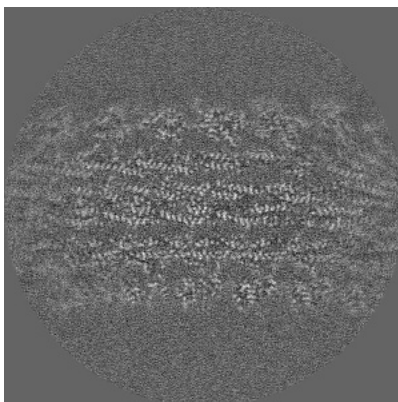


Z Index: 234

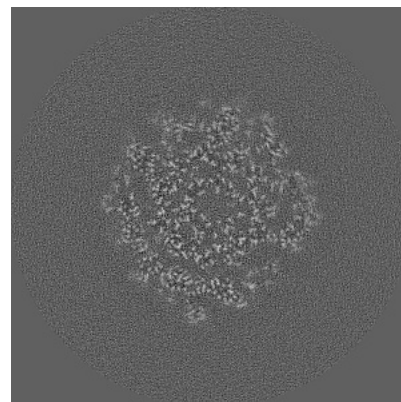
6.3.2 Raw map



X Index: 193



Y Index: 198

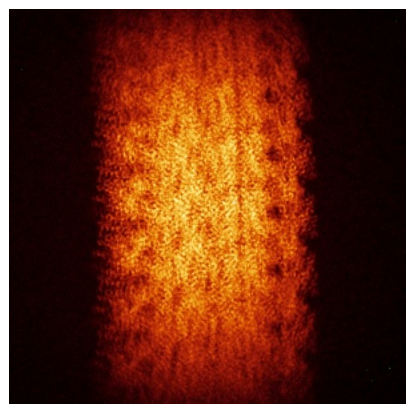


Z Index: 234

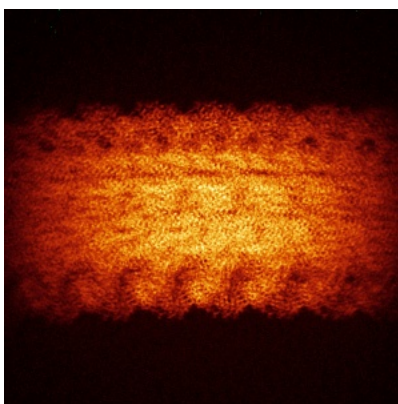
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

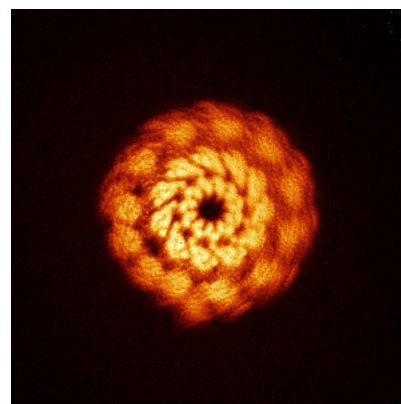
6.4.1 Primary map



X

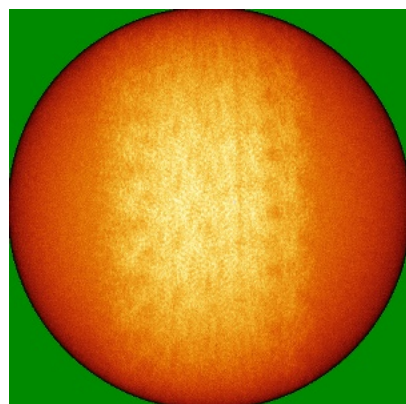


Y

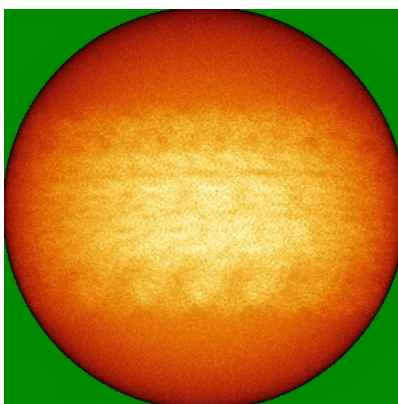


Z

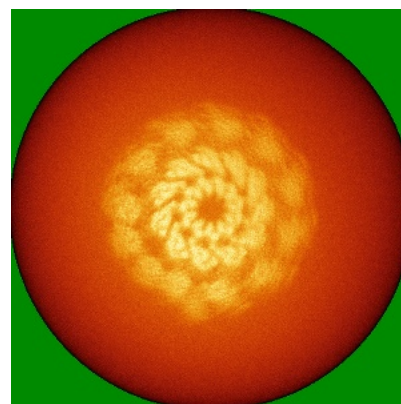
6.4.2 Raw map



X



Y

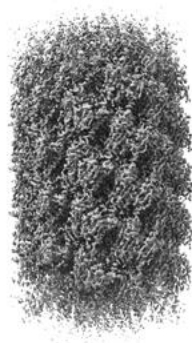


Z

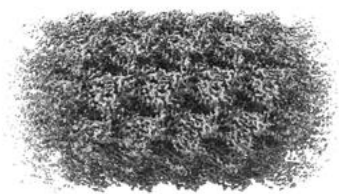
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



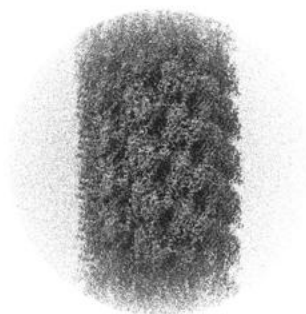
Y



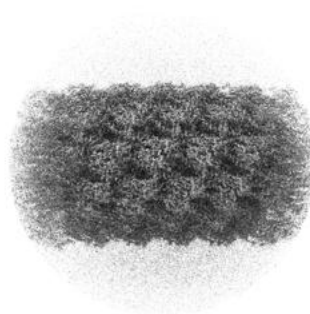
Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

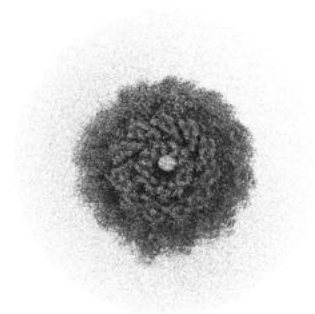
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

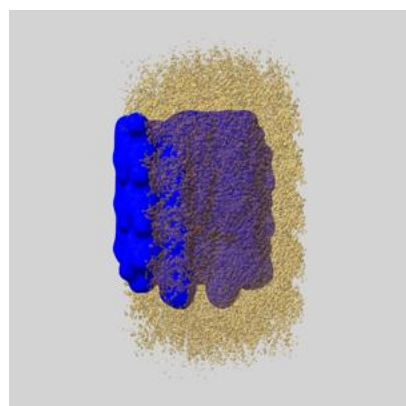
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

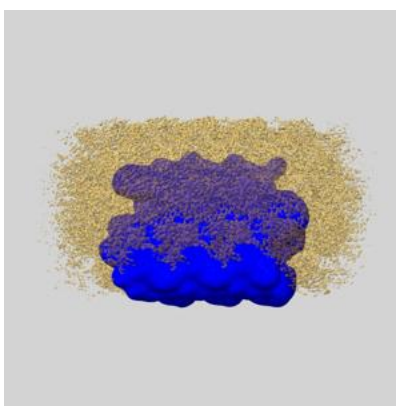
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

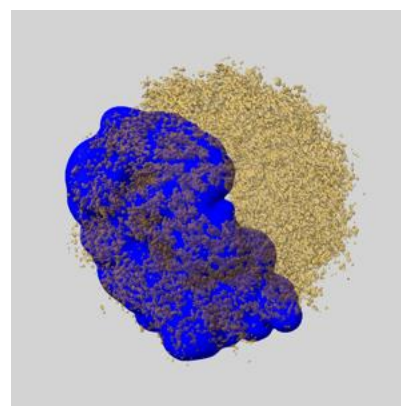
6.6.1 emd_71673_msk_1.map [i](#)



X



Y

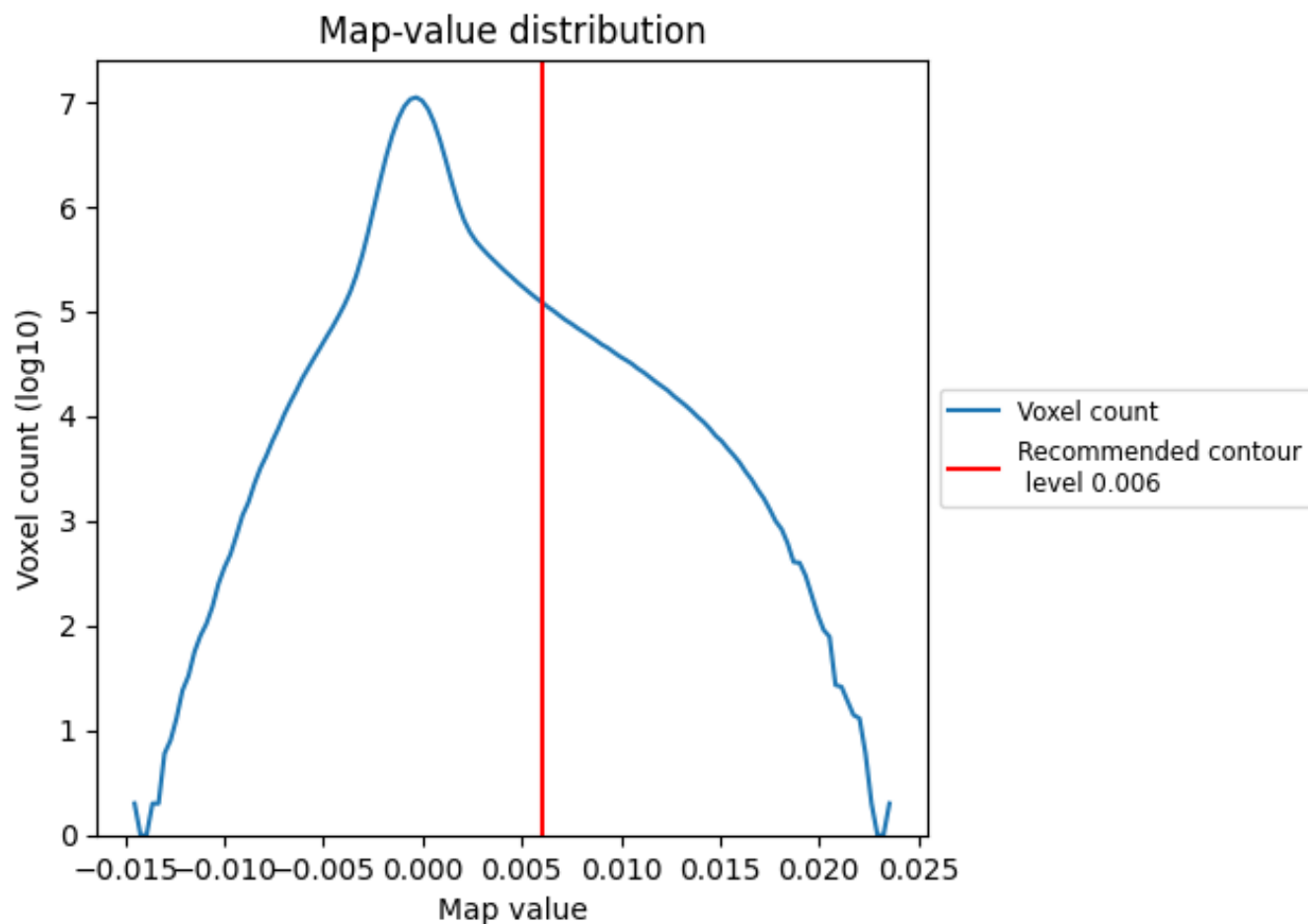


Z

7 Map analysis [i](#)

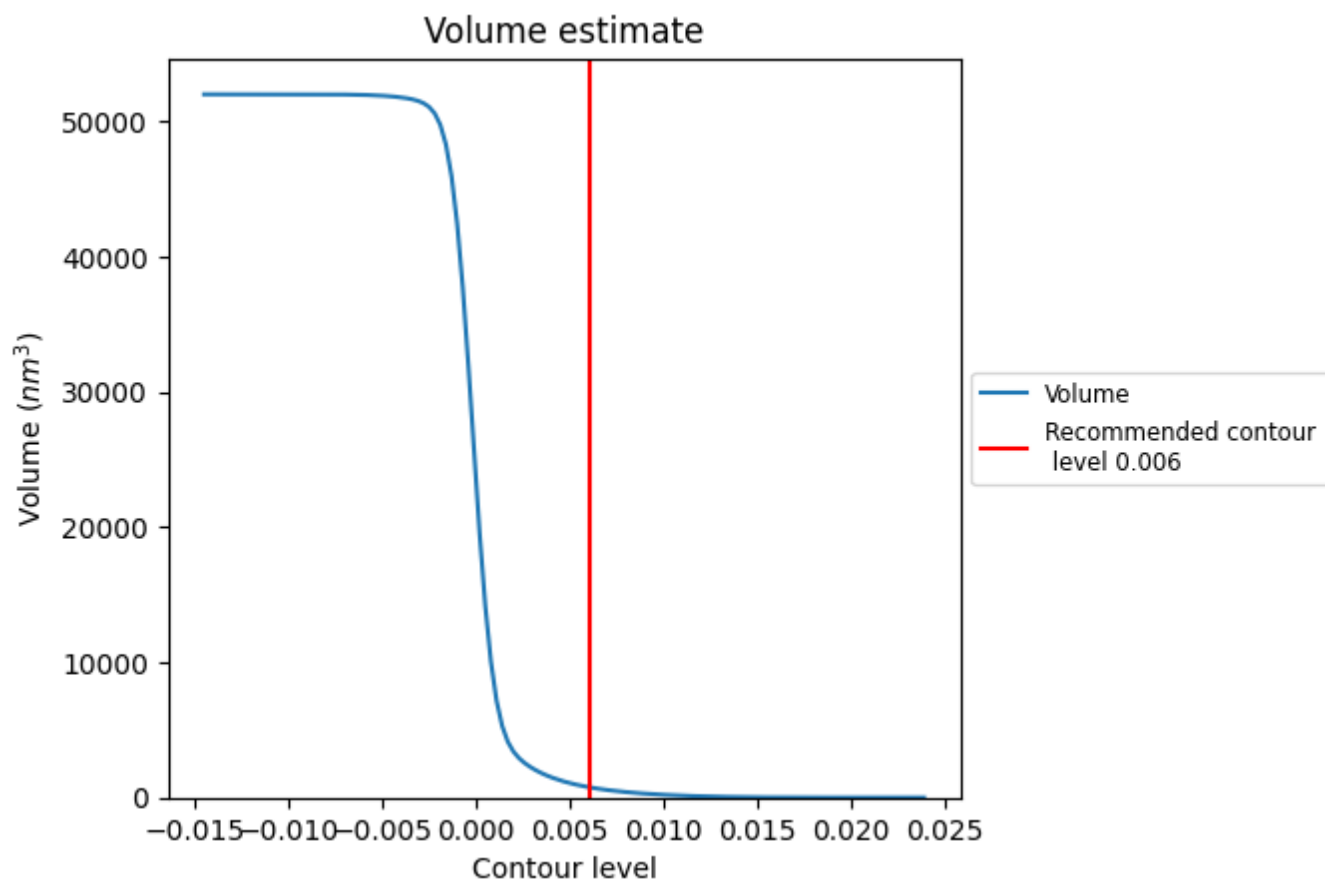
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

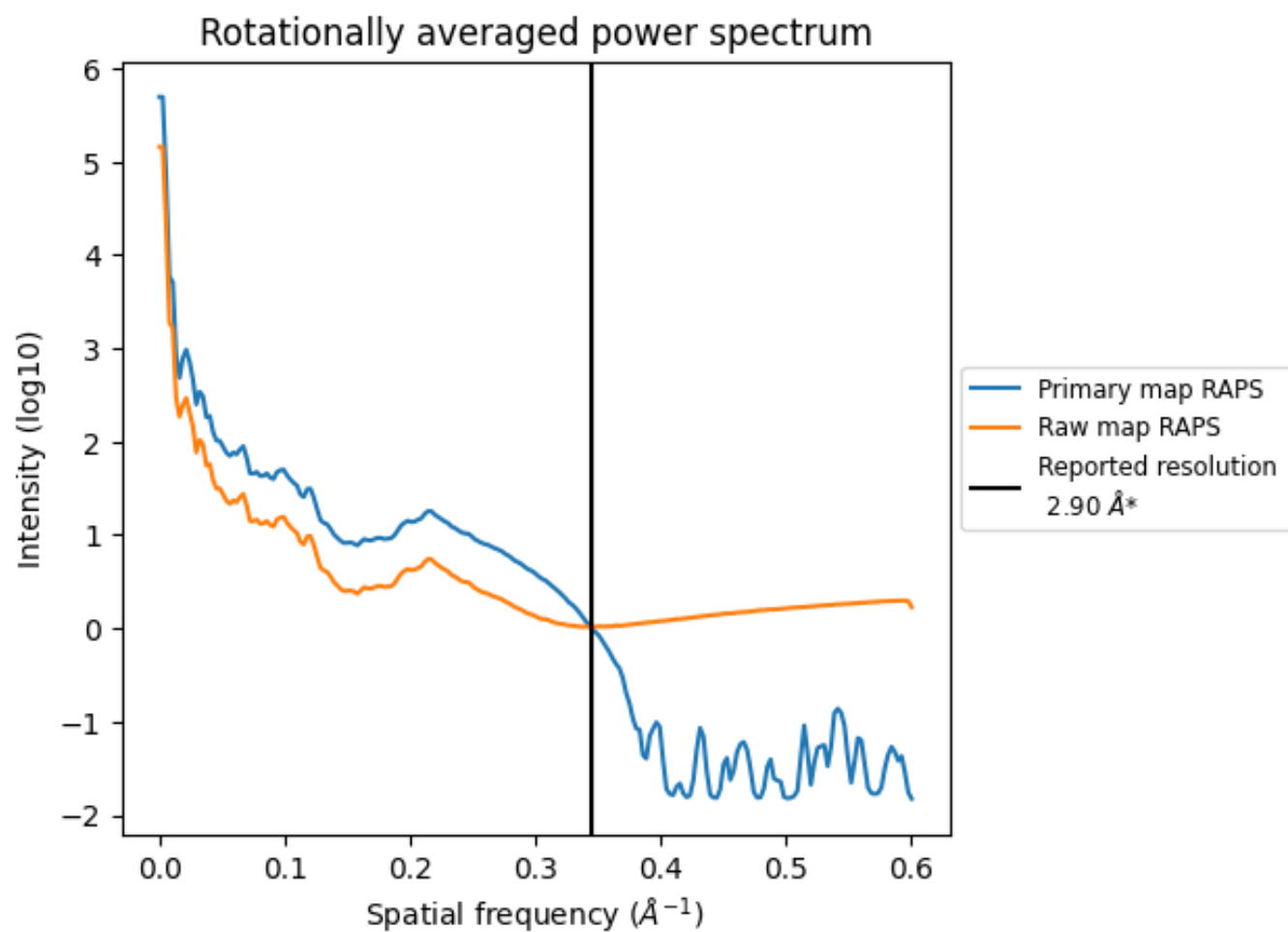
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 766 nm³; this corresponds to an approximate mass of 692 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

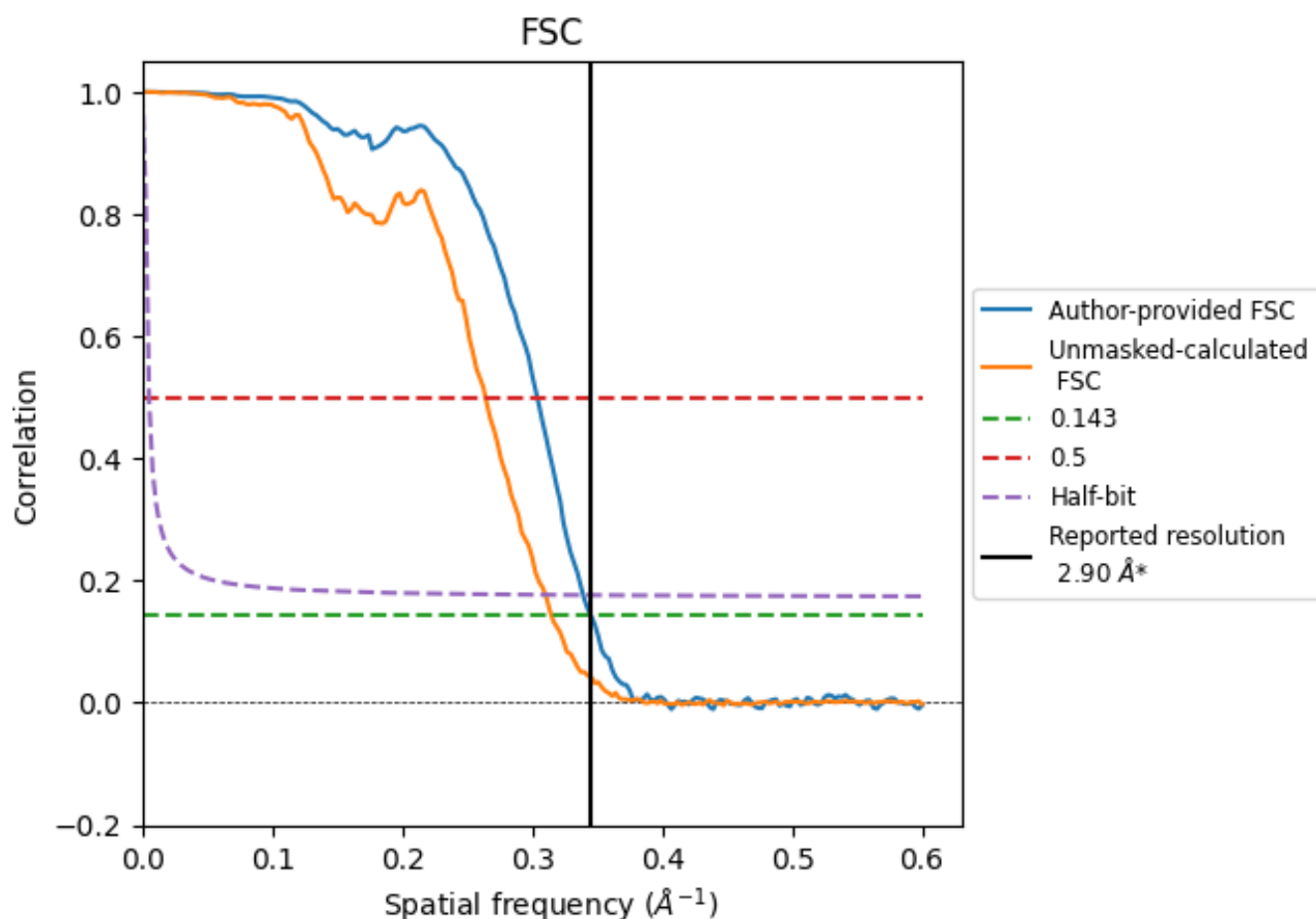


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

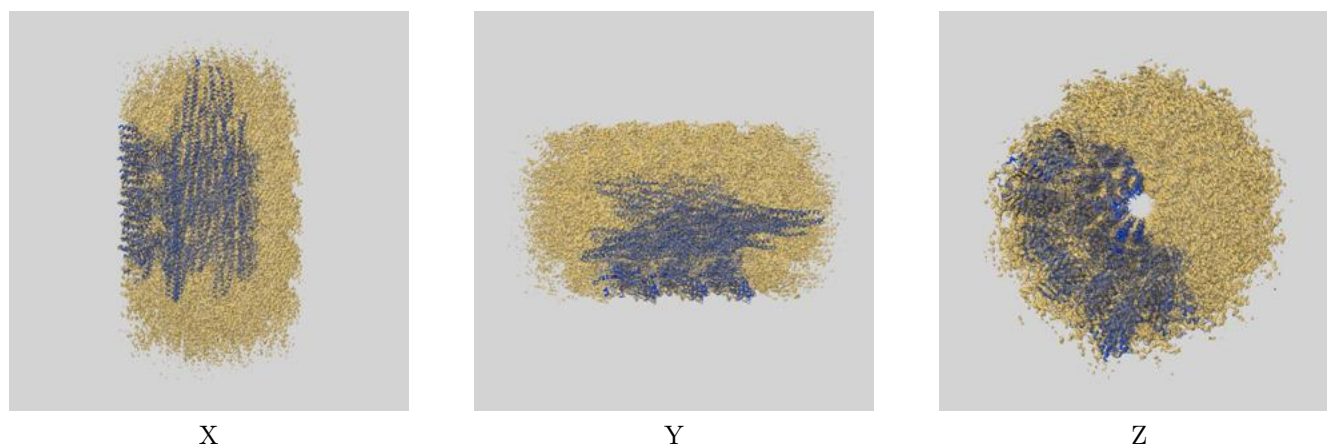
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.29	2.95
Unmasked-calculated*	3.18	3.79	3.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

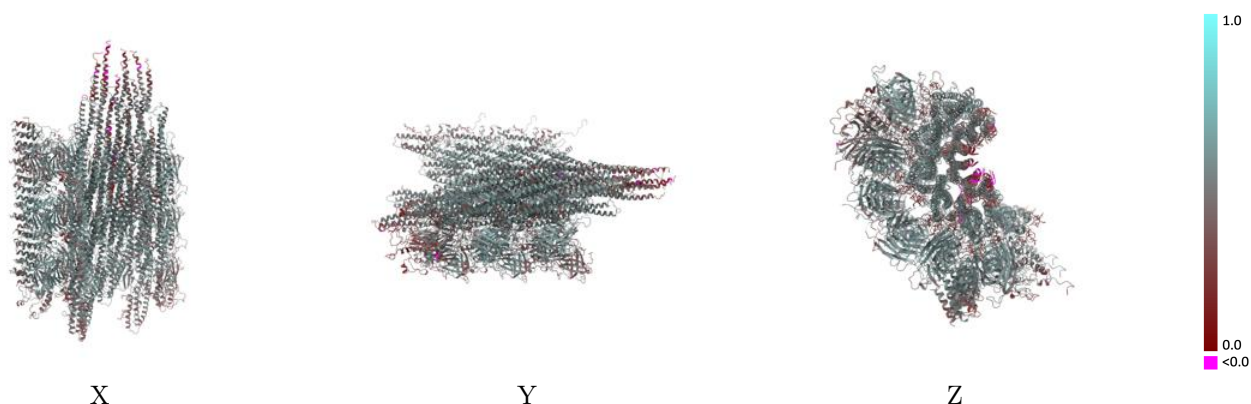
This section contains information regarding the fit between EMDB map EMD-71673 and PDB model 9PIN. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



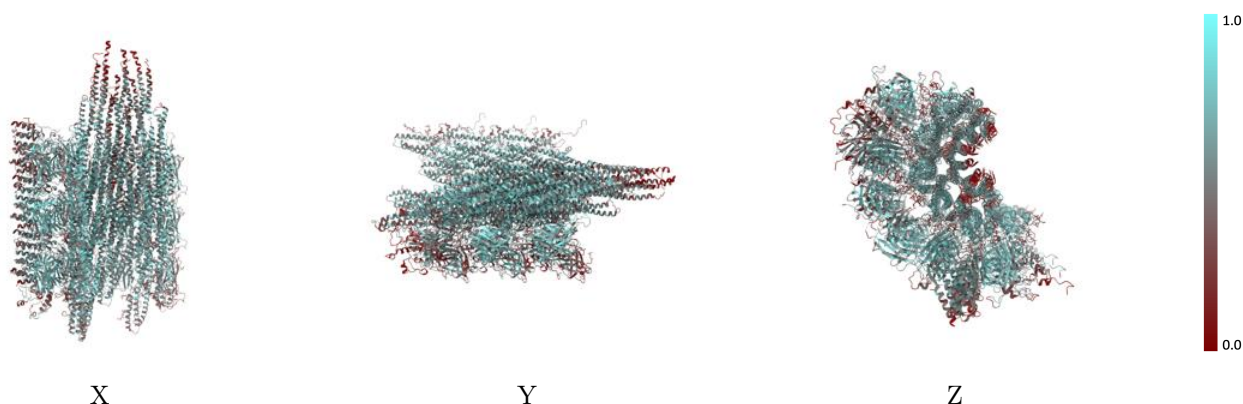
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



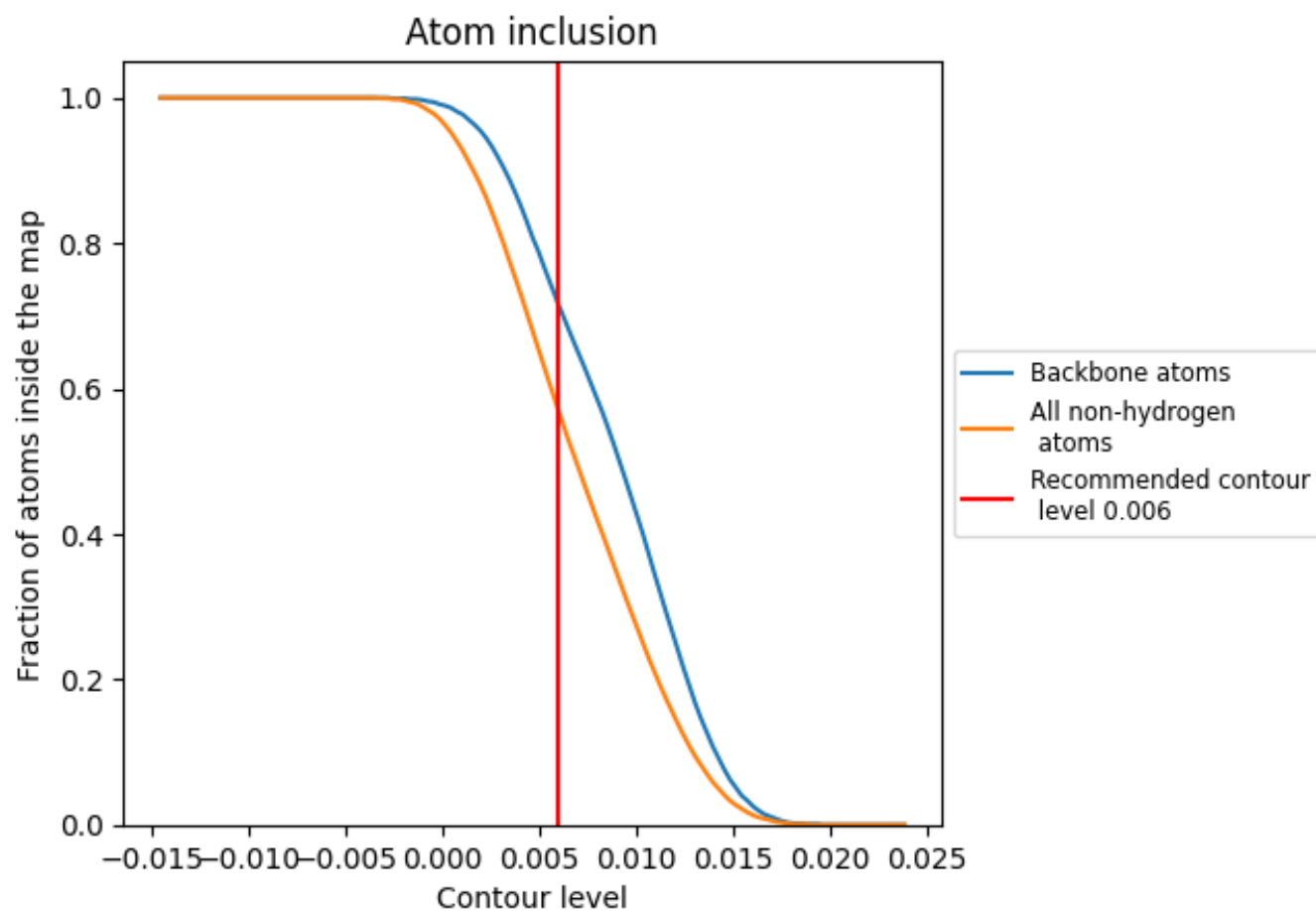
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5700	 0.4940
A0	 0.5330	 0.4770
A3	 0.6490	 0.5540
A4	 0.6250	 0.5530
A5	 0.5730	 0.5030
A6	 0.5460	 0.4960
A7	 0.6530	 0.5540
A8	 0.5950	 0.5210
A9	 0.5290	 0.4740
BA	 0.5950	 0.5190
BI	 0.6860	 0.5680
BJ	 0.6400	 0.5410
BK	 0.6370	 0.5450
BL	 0.5050	 0.4730
BM	 0.6340	 0.5400
BN	 0.6210	 0.5270
BQ	 0.5490	 0.4960
BR	 0.3150	 0.3420
BS	 0.5330	 0.4720
C0	 0.5900	 0.5020
DA	 0.6210	 0.5160
DB	 0.5900	 0.5040
DC	 0.5910	 0.4940
DD	 0.5690	 0.4640
DE	 0.6130	 0.5030
DF	 0.5300	 0.4680
DG	 0.5310	 0.4610
DH	 0.6200	 0.5110
DI	 0.6050	 0.5050
DJ	 0.6130	 0.5120
DK	 0.5320	 0.4670
DL	 0.6010	 0.4830
DM	 0.6070	 0.4820
DN	 0.5120	 0.4440
DO	 0.5770	 0.4860



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
DP	 0.6150	 0.5060
DQ	 0.5750	 0.4740
E	 0.5280	 0.5140
F	 0.4940	 0.4940
G	 0.3270	 0.3980
P2	 0.5590	 0.5350
P3	 0.5290	 0.5080
P4	 0.4340	 0.4570