



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 08:45 PM JST

PDB ID : 8XKL / pdb_00008xkl
EMDB ID : EMD-38419
Title : Structure of ACPII-CCPII from cryptophyte algae
Authors : Li, X.Y.; Mao, Z.Y.; Shen, J.R.; Han, G.Y.
Deposited on : 2023-12-23
Resolution : 2.84 Å(reported)

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 : 1.8.5 (274361), CSD as541be (2020)
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

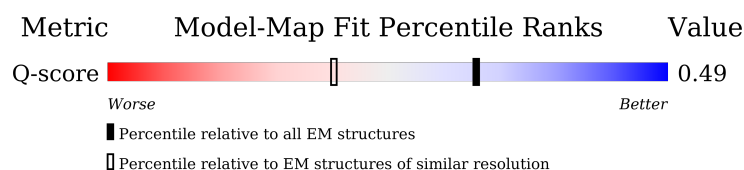
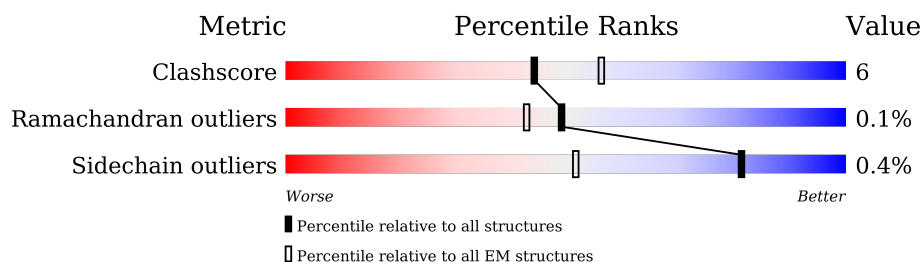
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.84 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	11884 (2.34 - 3.34)

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	0	226	
2	7	235	
3	8	217	
4	9	222	

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Mol	Chain	Length	Quality of chain
5	G	64	55% 100%
6	P	220	70% 9% 21%
7	p	218	6% 72% 14% 14%
8	s	285	42% 63% 8% 29%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 15357 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 ACPII-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	172	Total	C	N	O	S	0	0
			1308	845	225	229	9		

- Molecule 2 is a protein called ACPII-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	194	Total	C	N	O	S	0	0
			1472	946	256	262	8		

- Molecule 3 is a protein called ACPII-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	173	Total	C	N	O	S	0	0
			1362	899	222	238	3		

- Molecule 4 is a protein called ACPII-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	9	178	Total	C	N	O	S	0	0
			1371	885	230	247	9		

- Molecule 5 is a protein called Photosystem II reaction center protein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	64	Total	C	N	O	0	0
			320	192	64	64		

- Molecule 6 is a protein called ACPII-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	173	Total	C	N	O	S	0	0
			1344	878	221	237	8		

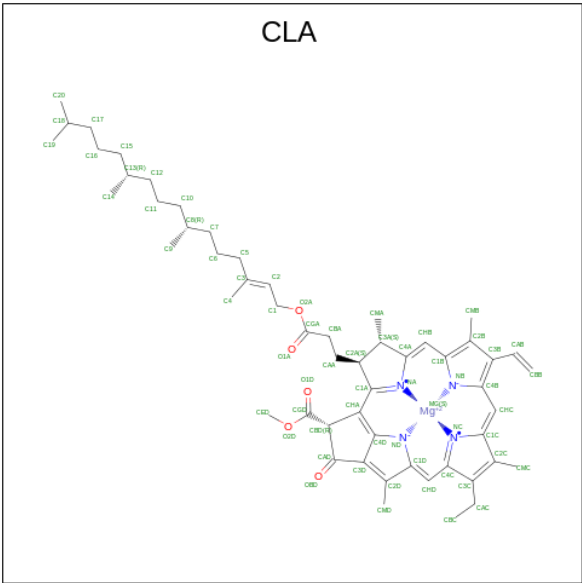
- Molecule 7 is a protein called ACPII-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	p	187	Total	C	N	O	S	0	0
			1471	956	243	267	5		

- Molecule 8 is a protein called CCPII-S.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	s	203	Total	C	N	O	S	0	0
			1563	1005	255	299	4		

- Molecule 9 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	0	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
9	0	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
9	0	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	0	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
9	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	0	1	Total 60	C 50	Mg 1	N 4	O 5	0
9	0	1	Total 41	C 33	Mg 1	N 4	O 3	0
9	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	0	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
9	7	1	Total 59	C 49	Mg 1	N 4	O 5	0
9	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
9	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
9	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
9	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
9	7	1	Total 41	C 33	Mg 1	N 4	O 3	0
9	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
9	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
9	8	1	Total 59	C 49	Mg 1	N 4	O 5	0
9	8	1	Total 50	C 40	Mg 1	N 4	O 5	0

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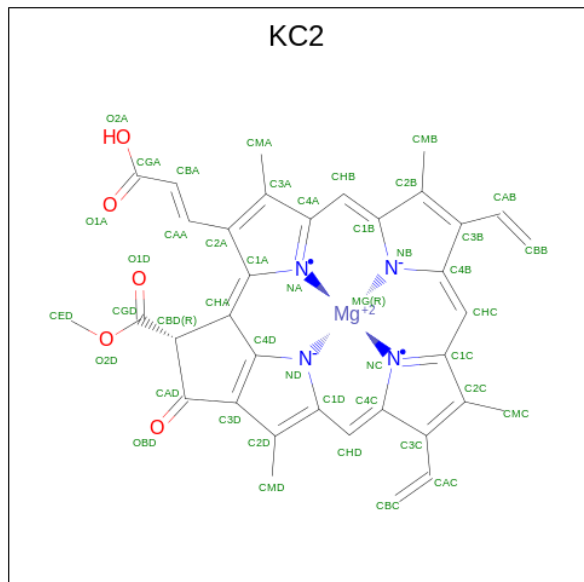
Mol	Chain	Residues	Atoms					AltConf
9	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	8	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	8	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
9	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
9	9	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
9	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	P	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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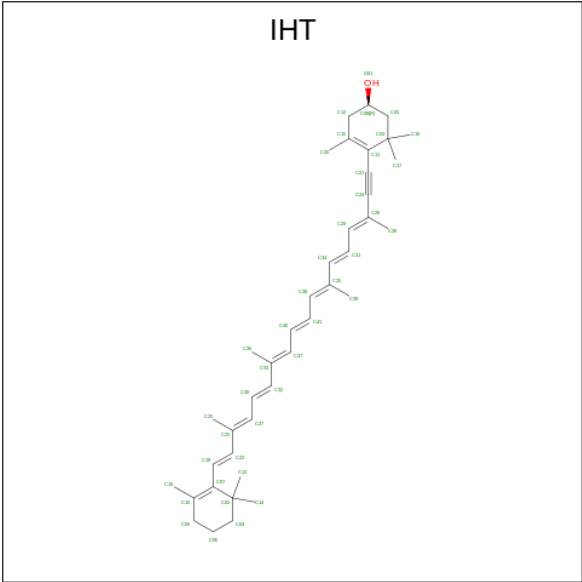
Mol	Chain	Residues	Atoms					AltConf
9	P	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
9	P	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	P	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	P	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	P	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
9	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
9	p	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
9	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	s	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
9	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 10 is Chlorophyll c2 (CCD ID: KC2) (formula: $C_{35}H_{28}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



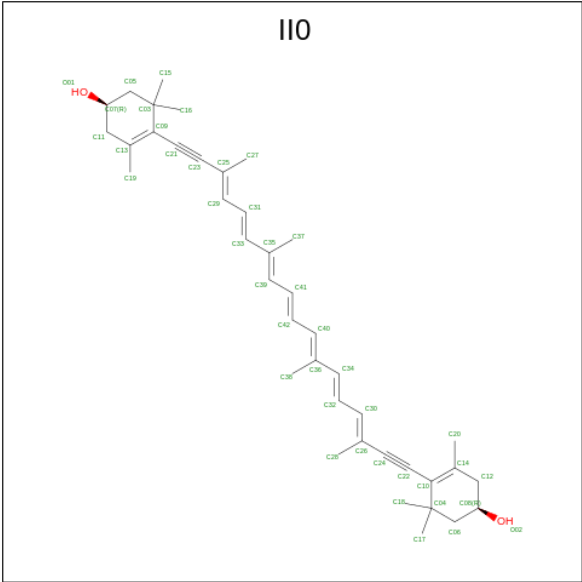
Mol	Chain	Residues	Atoms					AltConf
10	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	P	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	p	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 11 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-(2,6,6-trimethylcyclohexen-1-yl)octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: IHT) (formula: $C_{40}H_{54}O$).



Mol	Chain	Residues	Atoms			AltConf
11	0	1	Total	C	O	0
			41	40	1	
11	0	1	Total	C	O	0
			41	40	1	
11	7	1	Total	C	O	0
			41	40	1	
11	8	1	Total	C	O	0
			41	40	1	
11	p	1	Total	C	O	0
			41	40	1	

- Molecule 12 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E})-3,7,12,16-tetramethyl-18-[(4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-3,5,7,9,11,13,15-heptaen-1,17-diynyl]cyclohex-3-en-1-ol (CCD ID: II0) (formula: C₄₀H₅₂O₂).



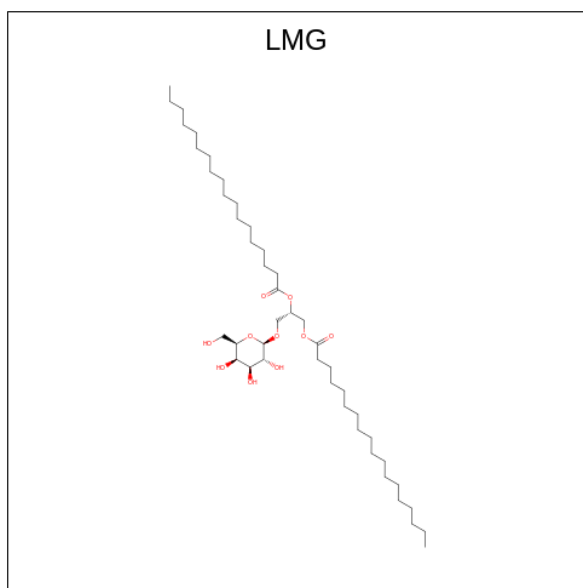
Mol	Chain	Residues	Atoms			AltConf
12	0	1	Total	C	O	0
			42	40	2	
12	0	1	Total	C	O	0
			42	40	2	
12	0	1	Total	C	O	0
			42	40	2	
12	7	1	Total	C	O	0
			42	40	2	
12	7	1	Total	C	O	0
			42	40	2	
12	7	1	Total	C	O	0
			42	40	2	
12	7	1	Total	C	O	0
			42	40	2	
12	8	1	Total	C	O	0
			42	40	2	
12	8	1	Total	C	O	0
			42	40	2	
12	8	1	Total	C	O	0
			42	40	2	
12	9	1	Total	C	O	0
			42	40	2	
12	9	1	Total	C	O	0
			42	40	2	
12	9	1	Total	C	O	0
			42	40	2	

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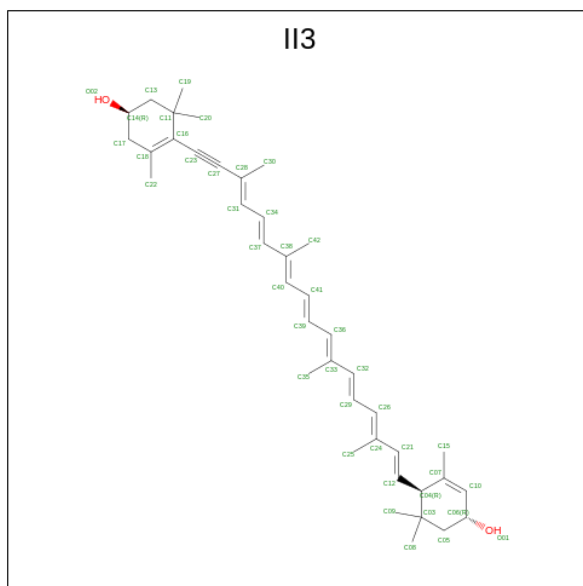
Mol	Chain	Residues	Atoms			AltConf
12	P	1	Total	C	O	0
			42	40	2	
12	P	1	Total	C	O	0
			42	40	2	
12	p	1	Total	C	O	0
			42	40	2	
12	p	1	Total	C	O	0
			42	40	2	
12	p	1	Total	C	O	0
			42	40	2	
12	p	1	Total	C	O	0
			42	40	2	

- Molecule 13 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



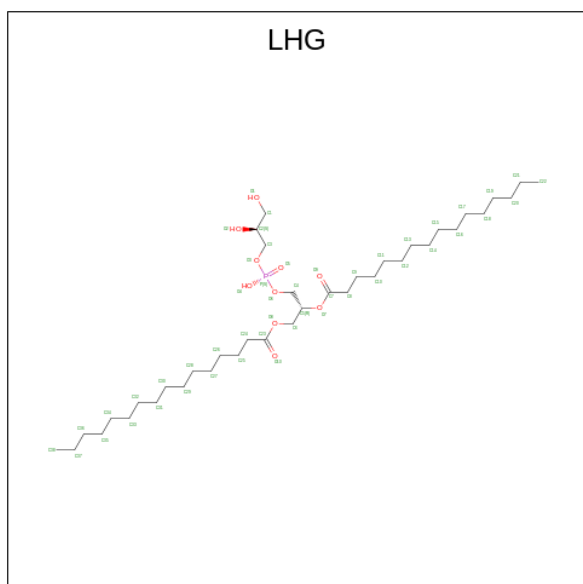
Mol	Chain	Residues	Atoms			AltConf
13	0	1	Total	C	O	0
			36	26	10	
13	8	1	Total	C	O	0
			36	26	10	
13	G	1	Total	C	O	0
			28	18	10	
13	G	1	Total	C	O	0
			28	18	10	

- Molecule 14 is (1 {R})-3,5,5-trimethyl-4-[(3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(1 {R},4 {R})-2,6,6-trimethyl-4-oxidanyl-cyclohex-2-en-1-yl]octadeca-3,5,7,9,11,13,15,17-octaen-1-ynyl]cyclohex-3-en-1-ol (CCD ID: II3) (formula: $C_{40}H_{54}O_2$).



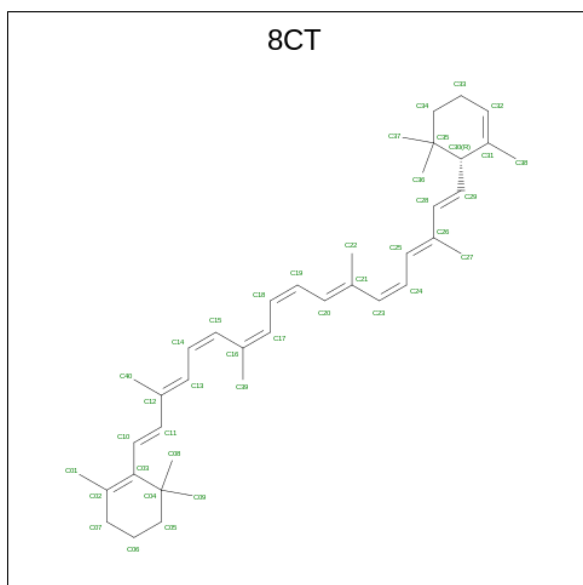
Mol	Chain	Residues	Atoms			AltConf
14	7	1	Total	C	O	0
			42	40	2	
14	P	1	Total	C	O	0
			42	40	2	

- Molecule 15 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



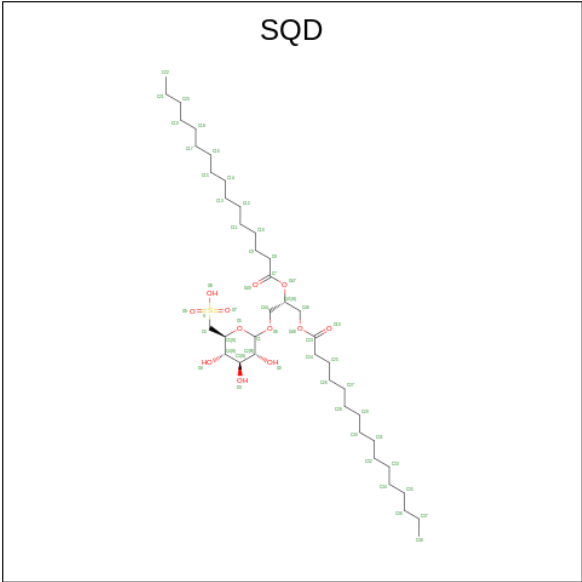
Mol	Chain	Residues	Atoms				AltConf
15	8	1	Total	C	O	P	0
			22	12	9	1	
15	s	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 16 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
16	9	1	Total	C	0
			40	40	
16	P	1	Total	C	0
			40	40	

- Molecule 17 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).

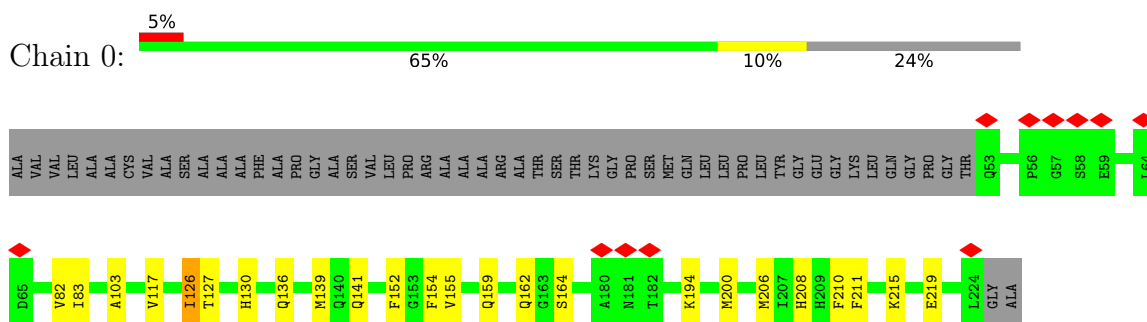


Mol	Chain	Residues	Atoms				AltConf
17	p	1	Total	C	O	S	0
			35	22	12	1	

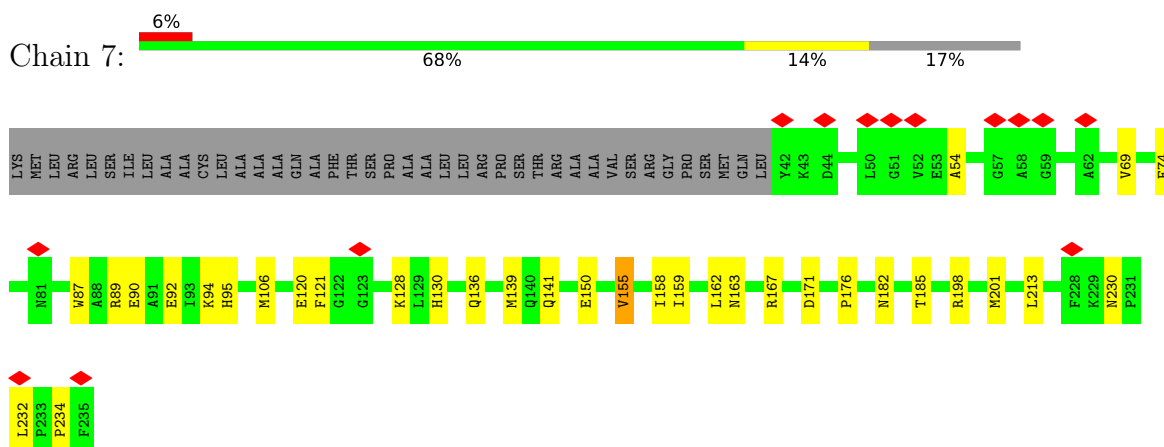
3 Residue-property plots [i](#)

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

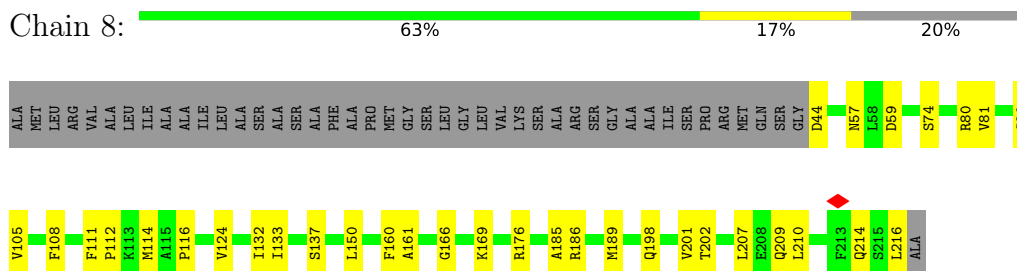
• Molecule 1: ACPII-4



• Molecule 2: ACPII-1

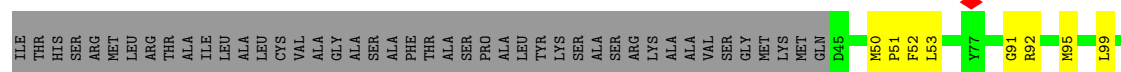


• Molecule 3: ACPII-2



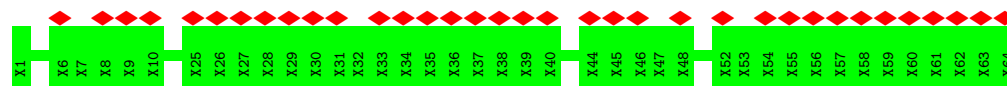
• Molecule 4: ACPII-3

Chain 9: 



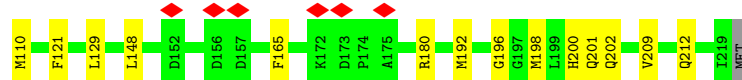
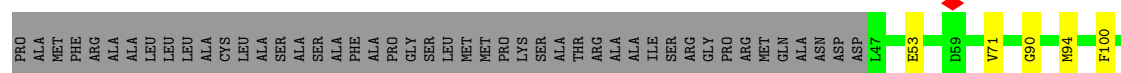
- Molecule 5: Photosystem II reaction center protein G

Chain G: 



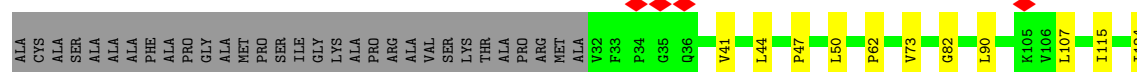
- Molecule 6: ACPII-6

Chain P: 



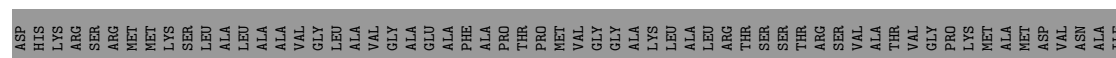
- Molecule 7: ACPII-5

Chain p: 



- Molecule 8: CCPII-S

Chain s: 



F161	A162	W163	K164	A170	D176	L177	D178	R179	A180	M181	M182	D183	P184	A185	R186	K195	S196	L197	G198	G199	A200	L201	D202	K203	T204	A205	V206	Y207	D208	E209	E210	D211	Q212	L213	L214	I215	L216	S217	D218	M219	E220	T221	F222	P223	E224	T225	E226	L227	G228	R229	R230	R231	V232	A233	Q234	A235
E236	A237	A238	G239	W240	F241	T242	G243	N244	P245	S246	F247	G248	K249	S250	L251	I252	E253	Y254	S255	E256	E257	T258	K259	K260	G261	M262	R263	E264	P265	G266	T267	V268	S269	I270	S271	A272	K273	E274	L275	A276	A277	L278	R279	A280	E281	A282	A283	K284	K285							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	610800	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.131	Depositor
Minimum map value	-0.417	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.266	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, IHT, KC2, CLA, LMG, II0, 8CT, LHG, II3

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	0	0.19	0/1339	0.29	0/1814
2	7	0.21	0/1507	0.34	0/2043
3	8	0.23	0/1399	0.29	0/1893
4	9	0.19	0/1404	0.24	0/1895
6	P	0.20	0/1380	0.27	0/1870
7	p	0.22	0/1510	0.30	0/2046
8	s	0.15	0/1603	0.31	0/2180
All	All	0.20	0/10142	0.29	0/13741

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1308	0	1323	19	0
2	7	1472	0	1473	23	0
3	8	1362	0	1348	25	0
4	9	1371	0	1370	16	0
5	G	320	0	70	0	0
6	P	1344	0	1329	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	p	1471	0	1445	26	0
8	s	1563	0	1540	21	0
9	0	582	0	469	13	0
9	7	582	0	469	17	0
9	8	547	0	456	14	0
9	9	548	0	456	13	0
9	G	45	0	33	2	0
9	P	442	0	364	10	0
9	p	547	0	456	13	0
9	s	110	0	105	6	0
10	0	45	0	0	0	0
10	7	45	0	0	0	0
10	8	45	0	0	0	0
10	P	90	0	0	0	0
10	p	45	0	0	0	0
11	0	82	0	0	0	0
11	7	41	0	0	0	0
11	8	41	0	0	0	0
11	p	41	0	0	0	0
12	0	126	0	0	1	0
12	7	168	0	0	1	0
12	8	168	0	0	2	0
12	9	126	0	0	0	0
12	P	84	0	0	0	0
12	p	210	0	0	0	0
13	0	36	0	42	0	0
13	8	36	0	42	2	0
13	G	56	0	52	0	0
14	7	42	0	0	0	0
14	P	42	0	0	0	0
15	8	22	0	20	0	0
15	s	37	0	44	2	0
16	9	40	0	0	0	0
16	P	40	0	0	0	0
17	p	35	0	34	4	0
All	All	15357	0	12940	180	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 6.

All (180) 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)
7:p:182:MET:HE1	9:p:304:CLA:HAB	1.65	0.77
3:8:90:GLY:HA3	3:8:185:ALA:HB1	1.69	0.74
7:p:82:GLY:HA3	7:p:178:SER:HB3	1.70	0.73
4:9:91:GLY:HA3	4:9:190:ALA:HB1	1.70	0.72
2:7:155:VAL:HG22	9:7:607:CLA:HMA1	1.72	0.72
2:7:90:GLU:HG2	2:7:158:ILE:HD11	1.75	0.69
6:P:192:MET:HE1	9:P:602:CLA:HAB	1.78	0.66
9:0:608:CLA:HBB1	9:0:608:CLA:H51	1.78	0.66
2:7:232:LEU:O	2:7:234:PRO:HD3	1.95	0.65
9:7:602:CLA:H2A	9:7:602:CLA:HED3	1.78	0.65
2:7:94:LYS:NZ	2:7:150:GLU:OE2	2.24	0.65
3:8:81:VAL:HG11	8:s:170:ALA:HB1	1.79	0.63
4:9:119:ALA:HB3	4:9:204:MET:HE1	1.80	0.63
9:9:606:CLA:HHC	9:9:606:CLA:HBB1	1.81	0.62
7:p:90:LEU:HB3	9:p:306:CLA:HMC2	1.81	0.62
2:7:150:GLU:HG2	9:7:607:CLA:NB	2.15	0.62
3:8:160:PHE:HA	4:9:52:PHE:HB3	1.81	0.61
4:9:211:PRO:O	4:9:213:GLU:N	2.32	0.61
1:0:130:HIS:ND1	1:0:139:MET:SD	2.73	0.60
6:P:201:GLN:HB3	6:P:212:GLN:HE22	1.66	0.60
2:7:89:ARG:NH1	2:7:92:GLU:OE1	2.35	0.60
8:s:284:LYS:HG3	8:s:285:LYS:HG2	1.83	0.60
9:0:603:CLA:HBC1	9:0:607:CLA:HBC2	1.82	0.60
2:7:69:VAL:O	2:7:89:ARG:NH2	2.35	0.60
1:0:154:PHE:HB2	9:0:607:CLA:HMA1	1.85	0.59
2:7:182:ASN:HD22	2:7:185:THR:H	1.51	0.59
3:8:201:VAL:HG23	3:8:202:THR:HG23	1.85	0.58
9:P:610:CLA:HBD	9:p:307:CLA:HBA1	1.86	0.57
7:p:107:LEU:HD13	7:p:192:TYR:HE1	1.70	0.57
8:s:93:HIS:CE1	9:s:302:CLA:H3A	2.40	0.57
2:7:141:GLN:HG2	9:7:605:CLA:ND	2.20	0.56
3:8:80:ARG:HB3	3:8:150:LEU:HD11	1.88	0.56
6:P:192:MET:HE1	9:P:602:CLA:HHC	1.86	0.56
6:P:196:GLY:O	6:P:200:HIS:ND1	2.30	0.56
6:P:180:ARG:HE	9:P:607:CLA:H43	1.68	0.56
9:7:612:CLA:HED2	9:7:612:CLA:H2A	1.87	0.56
7:p:115:ILE:HG13	9:p:306:CLA:HAA2	1.88	0.56
2:7:163:ASN:HB3	8:s:184:PRO:HB2	1.87	0.55
4:9:120:THR:HG23	4:9:204:MET:HE2	1.88	0.55
1:0:117:VAL:HG23	9:0:613:CLA:HBC3	1.88	0.55
3:8:112:PRO:HG2	3:8:114:MET:HE1	1.90	0.54
8:s:93:HIS:CE1	9:s:302:CLA:HAA1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:p:129:SER:HB3	9:p:309:CLA:HAB	1.90	0.53
6:P:53:GLU:OE1	7:p:146:LYS:NZ	2.41	0.53
3:8:108:PHE:HB2	3:8:111:PHE:HD2	1.74	0.53
2:7:167:ARG:NH1	2:7:171:ASP:O	2.39	0.53
6:P:90:GLY:O	6:P:94:MET:HB2	2.08	0.53
9:7:605:CLA:HBA1	9:8:611:CLA:HBD	1.91	0.53
9:8:603:CLA:H42	9:s:303:CLA:H91	1.91	0.52
4:9:173:SER:HB2	4:9:179:LEU:HD13	1.92	0.52
4:9:150:LEU:HD22	9:9:606:CLA:HMA1	1.92	0.51
7:p:142:THR:OG1	7:p:147:ARG:NH1	2.43	0.51
4:9:99:LEU:HB3	9:9:604:CLA:HMC2	1.92	0.51
3:8:132:ILE:HD12	9:8:606:CLA:HBC1	1.93	0.50
8:s:258:THR:HA	8:s:263:ARG:HH21	1.75	0.50
1:0:162:GLN:NE2	17:p:319:SQD:O9	2.45	0.50
8:s:87:LEU:HD21	9:s:302:CLA:C2D	2.42	0.50
3:8:166:GLY:HA2	3:8:169:LYS:HZ3	1.77	0.50
9:7:608:CLA:H2A	9:7:608:CLA:HED3	1.94	0.49
2:7:198:ARG:HA	2:7:201:MET:HE3	1.94	0.49
9:G:101:CLA:HHD	9:P:606:CLA:O1A	2.13	0.49
9:P:611:CLA:HED2	9:P:611:CLA:H2A	1.94	0.49
9:9:609:CLA:H43	17:p:319:SQD:H242	1.93	0.49
9:8:603:CLA:HAC1	9:8:606:CLA:HAB	1.94	0.49
7:p:47:PRO:HG2	7:p:50:LEU:HD12	1.94	0.49
4:9:191:ARG:HA	4:9:194:MET:HE3	1.95	0.48
3:8:102:VAL:HA	3:8:105:VAL:HG12	1.96	0.48
3:8:116:PRO:O	12:8:614:II0:O01	2.30	0.48
8:s:87:LEU:HD21	9:s:302:CLA:C1D	2.43	0.48
9:0:608:CLA:H2A	9:0:608:CLA:HED3	1.96	0.48
3:8:133:ILE:HD11	13:8:617:LMG:HC8	1.96	0.48
2:7:130:HIS:HD2	2:7:139:MET:HE2	1.77	0.48
1:0:159:GLN:HB3	1:0:164:SER:HB3	1.95	0.48
9:8:605:CLA:HBA2	9:9:610:CLA:HBD	1.96	0.48
4:9:171:ASN:ND2	8:s:117:GLY:O	2.47	0.48
7:p:124:ILE:HA	9:p:307:CLA:HBC3	1.96	0.48
1:0:103:ALA:HA	1:0:206:MET:HE1	1.96	0.48
1:0:152:PHE:HA	1:0:155:VAL:HG22	1.96	0.47
7:p:73:VAL:HG13	7:p:139:LEU:HD11	1.95	0.47
3:8:186:ARG:HA	3:8:189:MET:HE3	1.96	0.47
9:9:605:CLA:H3A	9:9:605:CLA:HBA2	1.43	0.47
1:0:155:VAL:HG21	7:p:62:PRO:HB2	1.96	0.47
8:s:158:VAL:O	8:s:161:PHE:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:s:113:TYR:O	8:s:117:GLY:N	2.49	0.46
9:0:612:CLA:H2A	9:0:612:CLA:O2D	2.15	0.46
3:8:44:ASP:N	3:8:44:ASP:OD1	2.48	0.46
9:p:304:CLA:HBA2	9:p:304:CLA:H3A	1.38	0.46
1:0:126:ILE:HD13	1:0:210:PHE:CD1	2.50	0.46
6:P:100:PHE:HD2	6:P:198:MET:HG3	1.80	0.46
9:9:607:CLA:H142	9:9:607:CLA:H111	1.70	0.46
1:0:155:VAL:HG23	7:p:44:LEU:HD21	1.97	0.46
2:7:128:LYS:HD3	2:7:234:PRO:HG2	1.98	0.46
1:0:82:VAL:HG23	1:0:83:ILE:HG12	1.98	0.46
2:7:120:GLU:HG2	2:7:136:GLN:HG3	1.98	0.46
9:0:601:CLA:H2A	9:0:601:CLA:HED3	1.98	0.46
9:8:605:CLA:HAB	12:8:619:II0:C42	2.46	0.46
9:p:307:CLA:HBA1	9:p:307:CLA:H3A	1.80	0.46
9:p:309:CLA:HAA2	8:s:108:VAL:HG21	1.98	0.46
2:7:155:VAL:O	2:7:159:ILE:HG13	2.16	0.46
9:8:602:CLA:HBA2	9:8:602:CLA:H3A	1.28	0.46
15:s:301:LHG:H121	15:s:301:LHG:HC91	1.73	0.46
9:7:602:CLA:H93	9:7:602:CLA:H61	1.76	0.45
4:9:168:ASP:N	4:9:168:ASP:OD1	2.48	0.45
9:7:603:CLA:HMA2	9:7:603:CLA:H11	1.98	0.45
9:9:602:CLA:H3A	9:9:602:CLA:HBA2	1.30	0.45
2:7:121:PHE:HD2	9:7:604:CLA:HED1	1.81	0.45
8:s:241:PHE:HB3	8:s:265:PRO:HG2	1.98	0.45
9:7:602:CLA:H62	9:7:602:CLA:H41	1.71	0.45
3:8:176:ARG:HG2	9:8:609:CLA:HED1	1.98	0.45
7:p:212:PHE:N	7:p:213:PRO:HD2	2.32	0.45
9:s:303:CLA:H161	9:s:303:CLA:H122	1.69	0.45
9:8:606:CLA:HBB1	9:8:606:CLA:HHC	1.99	0.45
7:p:142:THR:HG1	7:p:147:ARG:HH11	1.64	0.45
3:8:137:SER:CB	9:8:607:CLA:HAB	2.47	0.44
3:8:137:SER:HB3	9:8:607:CLA:HAB	1.99	0.44
3:8:161:ALA:HB3	4:9:51:PRO:HB2	1.99	0.44
3:8:198:GLN:HB3	3:8:209:GLN:HE22	1.83	0.44
8:s:142:TYR:CE2	8:s:144:PRO:HB3	2.52	0.44
9:7:606:CLA:H3A	9:7:606:CLA:HBA2	1.40	0.44
2:7:95:HIS:HB3	2:7:201:MET:SD	2.57	0.44
6:P:148:LEU:HD22	9:P:606:CLA:HMA1	1.99	0.44
7:p:188:MET:HE3	7:p:199:VAL:HG11	2.00	0.44
1:0:159:GLN:HA	1:0:162:GLN:HG2	1.99	0.44
6:P:121:PHE:CZ	6:P:129:LEU:HD11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:7:611:CLA:HAA1	9:7:613:CLA:C1C	2.48	0.44
4:9:92:ARG:HA	4:9:95:MET:HE3	2.00	0.43
9:P:602:CLA:H3A	9:P:602:CLA:HBA2	1.32	0.43
7:p:178:SER:O	7:p:182:MET:HG3	2.18	0.43
7:p:182:MET:HE1	9:p:304:CLA:CAB	2.41	0.43
2:7:54:ALA:HB3	2:7:74:PHE:HB2	2.00	0.43
2:7:176:PRO:O	12:7:614:II0:O01	2.37	0.43
8:s:183:ASP:HB3	8:s:186:ARG:HG3	1.99	0.43
9:9:607:CLA:CGA	9:9:607:CLA:H3A	2.49	0.43
1:0:215:LYS:HB3	1:0:219:GLU:HG3	2.01	0.43
9:7:605:CLA:HBA1	9:7:605:CLA:H3A	1.88	0.42
9:9:609:CLA:H11	17:p:319:SQD:H242	2.01	0.42
17:p:319:SQD:H122	17:p:319:SQD:H91	1.78	0.42
9:0:608:CLA:H91	9:0:608:CLA:H112	1.90	0.42
1:0:127:THR:HG21	1:0:211:PHE:HE1	1.84	0.42
6:P:110:MET:SD	6:P:110:MET:N	2.93	0.42
7:p:129:SER:CB	9:p:309:CLA:HAB	2.49	0.42
7:p:168:GLU:HG2	7:p:169:ARG:N	2.35	0.42
7:p:191:GLN:HB3	7:p:202:GLN:HE22	1.85	0.42
8:s:87:LEU:H	15:s:301:LHG:HC12	1.84	0.42
3:8:207:LEU:HD23	3:8:210:LEU:HD12	2.00	0.42
6:P:202:GLN:HE21	6:P:209:VAL:HG13	1.83	0.42
7:p:208:PRO:HB2	7:p:213:PRO:HD3	2.01	0.42
8:s:233:ALA:C	8:s:235:ALA:H	2.25	0.42
1:0:194:LYS:NZ	12:0:616:II0:O02	2.52	0.42
9:0:607:CLA:HMB1	9:9:609:CLA:H101	2.01	0.42
3:8:57:ASN:ND2	3:8:74:SER:O	2.47	0.42
9:P:604:CLA:H3A	9:P:604:CLA:HBA2	1.81	0.42
2:7:213:LEU:HG	9:7:612:CLA:HED3	2.02	0.42
9:7:602:CLA:HBA2	9:7:602:CLA:H3A	1.35	0.42
9:G:101:CLA:HBA2	9:G:101:CLA:H3A	1.72	0.41
3:8:94:MET:CE	9:8:608:CLA:HAB	2.50	0.41
7:p:132:GLU:HG3	9:p:309:CLA:NC	2.35	0.41
8:s:179:ARG:H	8:s:203:LYS:NZ	2.18	0.41
1:0:200:MET:SD	9:0:602:CLA:HAB	2.61	0.41
9:8:608:CLA:H2A	9:8:608:CLA:HED3	2.02	0.41
4:9:50:MET:HB2	4:9:53:LEU:HB2	2.01	0.41
2:7:87:TRP:HE3	2:7:162:LEU:HD11	1.85	0.41
9:7:611:CLA:HBD	9:7:611:CLA:HAA2	2.02	0.41
1:0:136:GLN:HG2	7:p:212:PHE:CE1	2.55	0.41
9:0:602:CLA:HBA2	9:0:602:CLA:H3A	1.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:230:ASN:OD1	2:7:230:ASN:N	2.53	0.41
3:8:59:ASP:OD1	3:8:59:ASP:N	2.53	0.41
6:P:165:PHE:HB3	9:P:607:CLA:HMD2	2.01	0.41
7:p:73:VAL:HG21	8:s:112:ALA:HB2	2.02	0.41
1:0:141:GLN:HE21	9:0:605:CLA:HMA3	1.86	0.41
7:p:159:LEU:HD13	9:p:310:CLA:H42	2.02	0.41
3:8:214:GLN:HE22	3:8:216:LEU:HB2	1.85	0.41
3:8:124:VAL:O	13:8:617:LMG:O3	2.34	0.41
4:9:171:ASN:HB2	8:s:113:TYR:OH	2.21	0.41
4:9:165:LEU:HD12	9:9:607:CLA:HMD2	2.03	0.41
1:0:208:HIS:HE1	9:0:612:CLA:NA	2.19	0.40
6:P:198:MET:HE3	6:P:209:VAL:HG11	2.01	0.40
9:9:607:CLA:HED3	9:9:607:CLA:HBD	1.86	0.40
9:8:606:CLA:HHC	9:8:606:CLA:CBB	2.52	0.40
8:s:179:ARG:H	8:s:203:LYS:HZ2	1.68	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	0	170/226 (75%)	167 (98%)	2 (1%)	1 (1%)	21	39
2	7	192/235 (82%)	183 (95%)	9 (5%)	0	100	100
3	8	171/217 (79%)	170 (99%)	1 (1%)	0	100	100
4	9	176/222 (79%)	172 (98%)	4 (2%)	0	100	100
6	P	171/220 (78%)	171 (100%)	0	0	100	100
7	p	185/218 (85%)	183 (99%)	2 (1%)	0	100	100
8	s	201/285 (70%)	180 (90%)	21 (10%)	0	100	100
All	All	1266/1623 (78%)	1226 (97%)	39 (3%)	1 (0%)	49	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	126	ILE

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	0	136/169 (80%)	136 (100%)	0	100	100
2	7	149/179 (83%)	147 (99%)	2 (1%)	61	79
3	8	139/167 (83%)	139 (100%)	0	100	100
4	9	143/175 (82%)	143 (100%)	0	100	100
6	P	141/174 (81%)	140 (99%)	1 (1%)	76	88
7	p	157/175 (90%)	156 (99%)	1 (1%)	78	89
8	s	159/219 (73%)	159 (100%)	0	100	100
All	All	1024/1258 (81%)	1020 (100%)	4 (0%)	81	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	7	106	MET
2	7	155	VAL
6	P	71	VAL
7	p	41	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	53	GLN
1	0	195	ASN
2	7	81	ASN
2	7	109	GLN
2	7	182	ASN
3	8	120	HIS

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Mol	Chain	Res	Type
3	8	131	GLN
3	8	198	GLN
3	8	209	GLN
4	9	104	GLN
4	9	209	GLN
6	P	89	HIS
6	P	131	GLN
6	P	212	GLN
6	P	215	ASN
7	p	49	ASN
7	p	158	ASN
7	p	202	GLN
7	p	205	ASN
7	p	210	ASN

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](#)

112 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	II0	7	616	-	39,43,43	2.76	4 (10%)	50,60,60	1.76	11 (22%)
12	II0	7	614	-	39,43,43	2.73	4 (10%)	50,60,60	1.75	10 (20%)
9	CLA	9	610	4	49,53,73	1.46	9 (18%)	59,89,113	1.49	5 (8%)
9	CLA	P	604	6	59,63,73	1.34	10 (16%)	71,101,113	1.41	6 (8%)
9	CLA	8	601	3	46,50,73	1.48	9 (19%)	55,85,113	1.47	4 (7%)
16	8CT	9	615	-	40,41,41	4.64	23 (57%)	50,56,56	2.87	20 (40%)
9	CLA	0	612	-	49,53,73	1.48	8 (16%)	59,89,113	1.46	6 (10%)
9	CLA	P	607	6	64,68,73	1.29	10 (15%)	77,107,113	1.33	5 (6%)
15	LHG	8	618	9	21,21,48	0.78	0	23,26,54	1.26	2 (8%)
9	CLA	8	609	15	45,49,73	1.51	10 (22%)	54,84,113	1.51	5 (9%)
11	IHT	7	618	-	40,42,42	2.01	2 (5%)	53,58,58	1.95	13 (24%)
10	KC2	7	610	2	49,53,53	1.77	11 (22%)	62,89,89	2.17	16 (25%)
9	CLA	0	613	1	49,53,73	1.49	10 (20%)	59,89,113	1.43	6 (10%)
9	CLA	8	602	3	63,67,73	1.29	9 (14%)	75,105,113	1.37	8 (10%)
12	II0	7	617	-	39,43,43	2.75	4 (10%)	50,60,60	1.72	10 (20%)
9	CLA	8	604	-	59,63,73	1.33	9 (15%)	71,101,113	1.38	7 (9%)
9	CLA	9	606	-	49,53,73	1.50	10 (20%)	59,89,113	1.35	5 (8%)
12	II0	9	612	-	39,43,43	2.73	4 (10%)	50,60,60	1.70	10 (20%)
9	CLA	9	602	4	63,67,73	1.30	10 (15%)	75,105,113	1.37	7 (9%)
9	CLA	0	604	1	59,63,73	1.36	10 (16%)	71,101,113	1.36	8 (11%)
9	CLA	8	605	3	64,68,73	1.29	9 (14%)	77,107,113	1.32	6 (7%)
9	CLA	P	601	6	46,50,73	1.49	9 (19%)	55,85,113	1.44	4 (7%)
9	CLA	8	611	3	49,53,73	1.46	10 (20%)	59,89,113	1.48	5 (8%)
12	II0	8	613	-	39,43,43	2.75	4 (10%)	50,60,60	1.77	10 (20%)
9	CLA	0	603	1	54,58,73	1.39	10 (18%)	65,95,113	1.42	6 (9%)
9	CLA	0	608	-	64,68,73	1.28	9 (14%)	77,107,113	1.34	6 (7%)
10	KC2	P	605	6	49,53,53	1.83	11 (22%)	62,89,89	2.11	15 (24%)
9	CLA	0	607	1	49,53,73	1.47	9 (18%)	59,89,113	1.37	6 (10%)
9	CLA	8	612	3	49,53,73	1.46	10 (20%)	59,89,113	1.41	5 (8%)
9	CLA	7	607	-	49,53,73	1.47	10 (20%)	59,89,113	1.40	5 (8%)
14	II3	P	613	-	40,43,43	2.00	2 (5%)	47,60,60	1.59	10 (21%)
9	CLA	s	303	8	69,73,73	1.27	9 (13%)	83,113,113	1.29	6 (7%)
9	CLA	P	606	6	49,53,73	1.48	8 (16%)	59,89,113	1.35	6 (10%)
12	II0	P	612	-	39,43,43	2.70	4 (10%)	50,60,60	1.77	10 (20%)
9	CLA	9	609	4	64,68,73	1.29	10 (15%)	77,107,113	1.34	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CLA	7	602	2	63,67,73	1.30	10 (15%)	75,105,113	1.32	6 (8%)
9	CLA	P	603	-	54,58,73	1.40	10 (18%)	65,95,113	1.47	7 (10%)
13	LMG	0	618	-	36,36,55	0.89	1 (2%)	44,44,63	1.29	6 (13%)
9	CLA	7	612	2	49,53,73	1.48	10 (20%)	59,89,113	1.42	4 (6%)
9	CLA	0	611	1	49,53,73	1.48	9 (18%)	59,89,113	1.42	5 (8%)
9	CLA	p	310	7	64,68,73	1.30	10 (15%)	77,107,113	1.35	5 (6%)
9	CLA	7	609	-	45,49,73	1.52	9 (20%)	54,84,113	1.50	6 (11%)
10	KC2	0	610	1	49,53,53	1.79	11 (22%)	62,89,89	2.21	18 (29%)
12	II0	9	614	-	39,43,43	2.71	4 (10%)	50,60,60	1.69	11 (22%)
9	CLA	9	608	-	45,49,73	1.49	9 (20%)	54,84,113	1.52	7 (12%)
9	CLA	7	605	-	54,58,73	1.40	9 (16%)	65,95,113	1.39	6 (9%)
16	8CT	P	615	-	40,41,41	4.66	23 (57%)	50,56,56	2.68	19 (38%)
12	II0	p	301	-	39,43,43	2.71	4 (10%)	50,60,60	1.79	11 (22%)
12	II0	8	619	-	39,43,43	2.74	4 (10%)	50,60,60	1.73	8 (16%)
9	CLA	7	606	2	49,53,73	1.46	8 (16%)	59,89,113	1.50	6 (10%)
9	CLA	9	604	4	59,63,73	1.36	10 (16%)	71,101,113	1.37	8 (11%)
9	CLA	p	314	7	49,53,73	1.47	10 (20%)	59,89,113	1.40	4 (6%)
12	II0	p	315	-	39,43,43	2.69	4 (10%)	50,60,60	1.75	12 (24%)
13	LMG	G	102	-	28,28,55	0.94	0	36,36,63	1.30	5 (13%)
9	CLA	7	603	2	54,58,73	1.38	9 (16%)	65,95,113	1.45	6 (9%)
9	CLA	8	606	3	49,53,73	1.47	9 (18%)	59,89,113	1.44	5 (8%)
9	CLA	p	309	7	49,53,73	1.48	10 (20%)	59,89,113	1.48	7 (11%)
12	II0	p	316	-	39,43,43	2.71	4 (10%)	50,60,60	1.60	10 (20%)
12	II0	p	317	-	39,43,43	2.74	4 (10%)	50,60,60	1.70	9 (18%)
12	II0	9	613	-	39,43,43	2.73	4 (10%)	50,60,60	1.74	9 (18%)
11	IHT	0	614	-	40,42,42	1.98	2 (5%)	53,58,58	1.79	13 (24%)
15	LHG	s	301	-	36,36,48	0.72	1 (2%)	39,42,54	1.24	4 (10%)
9	CLA	P	602	6	63,67,73	1.31	10 (15%)	75,105,113	1.32	8 (10%)
9	CLA	p	308	7	49,53,73	1.49	9 (18%)	59,89,113	1.46	6 (10%)
9	CLA	9	607	4	64,68,73	1.30	10 (15%)	77,107,113	1.32	5 (6%)
9	CLA	P	610	-	49,53,73	1.46	10 (20%)	59,89,113	1.51	7 (11%)
9	CLA	7	601	-	46,50,73	1.50	8 (17%)	55,85,113	1.42	4 (7%)
13	LMG	G	103	-	28,28,55	1.00	0	36,36,63	1.33	5 (13%)
9	CLA	p	307	7	64,68,73	1.29	9 (14%)	77,107,113	1.31	6 (7%)
12	II0	8	615	-	39,43,43	2.72	5 (12%)	50,60,60	1.84	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CLA	0	601	1	46,50,73	1.50	9 (19%)	55,85,113	1.45	4 (7%)
12	II0	P	614	-	39,43,43	2.74	4 (10%)	50,60,60	1.71	11 (22%)
12	II0	0	616	-	39,43,43	2.77	4 (10%)	50,60,60	1.75	12 (24%)
9	CLA	0	606	-	49,53,73	1.47	9 (18%)	59,89,113	1.39	5 (8%)
13	LMG	8	617	-	36,36,55	0.89	1 (2%)	44,44,63	1.30	6 (13%)
9	CLA	9	605	4	50,54,73	1.45	10 (20%)	60,90,113	1.39	4 (6%)
9	CLA	7	604	2	59,63,73	1.34	10 (16%)	71,101,113	1.42	7 (9%)
9	CLA	p	304	7	63,67,73	1.31	10 (15%)	75,105,113	1.30	9 (12%)
9	CLA	p	306	7	59,63,73	1.33	9 (15%)	71,101,113	1.39	6 (8%)
9	CLA	9	611	4	49,53,73	1.47	10 (20%)	59,89,113	1.44	5 (8%)
9	CLA	0	609	-	45,49,73	1.51	9 (20%)	54,84,113	1.48	7 (12%)
9	CLA	p	303	7	46,50,73	1.49	10 (21%)	55,85,113	1.45	4 (7%)
9	CLA	8	607	3	49,53,73	1.46	10 (20%)	59,89,113	1.43	5 (8%)
14	II3	7	615	-	40,43,43	1.99	2 (5%)	47,60,60	1.63	9 (19%)
10	KC2	p	312	7	49,53,53	1.80	11 (22%)	62,89,89	2.19	18 (29%)
9	CLA	p	305	-	54,58,73	1.41	10 (18%)	65,95,113	1.45	7 (10%)
12	II0	p	302	-	39,43,43	2.72	4 (10%)	50,60,60	1.76	11 (22%)
12	II0	0	615	-	39,43,43	2.70	4 (10%)	50,60,60	1.75	12 (24%)
9	CLA	P	608	-	45,49,73	1.50	10 (22%)	54,84,113	1.48	5 (9%)
9	CLA	9	601	4	46,50,73	1.48	10 (21%)	55,85,113	1.49	4 (7%)
11	IHT	0	617	-	40,42,42	1.99	3 (7%)	53,58,58	2.04	15 (28%)
12	II0	8	614	-	39,43,43	2.72	4 (10%)	50,60,60	1.69	8 (16%)
9	CLA	9	603	4	54,58,73	1.39	10 (18%)	65,95,113	1.46	6 (9%)
9	CLA	7	611	2	49,53,73	1.47	9 (18%)	59,89,113	1.46	5 (8%)
17	SQD	p	319	-	34,35,54	1.73	7 (20%)	43,46,65	1.60	7 (16%)
9	CLA	0	602	1	63,67,73	1.30	10 (15%)	75,105,113	1.32	7 (9%)
10	KC2	8	610	3	49,53,53	1.82	12 (24%)	62,89,89	2.21	17 (27%)
9	CLA	G	101	-	49,53,73	1.48	9 (18%)	59,89,113	1.43	5 (8%)
11	IHT	8	616	-	40,42,42	2.04	3 (7%)	53,58,58	2.03	15 (28%)
9	CLA	s	302	-	49,53,73	1.50	9 (18%)	59,89,113	1.50	7 (11%)
9	CLA	P	611	6	49,53,73	1.48	10 (20%)	59,89,113	1.46	6 (10%)
12	II0	0	619	-	39,43,43	2.68	4 (10%)	50,60,60	1.69	13 (26%)
9	CLA	8	603	3	54,58,73	1.40	10 (18%)	65,95,113	1.43	7 (10%)
9	CLA	8	608	3	64,68,73	1.29	9 (14%)	77,107,113	1.33	7 (9%)
12	II0	7	619	-	39,43,43	2.69	4 (10%)	50,60,60	1.67	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CLA	0	605	1	54,58,73	1.40	9 (16%)	65,95,113	1.38	5 (7%)
9	CLA	p	311	-	45,49,73	1.51	9 (20%)	54,84,113	1.47	7 (12%)
10	KC2	P	609	6	49,53,53	1.80	11 (22%)	62,89,89	2.18	17 (27%)
9	CLA	p	313	-	49,53,73	1.46	10 (20%)	59,89,113	1.49	5 (8%)
11	IHT	p	318	-	40,42,42	1.99	2 (5%)	53,58,58	1.81	11 (20%)
9	CLA	7	608	2	64,68,73	1.29	10 (15%)	77,107,113	1.34	6 (7%)
9	CLA	7	613	-	49,53,73	1.48	9 (18%)	59,89,113	1.43	5 (8%)

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
12	II0	7	616	-	-	5/21/67/67	0/2/2/2
12	II0	7	614	-	-	0/21/67/67	0/2/2/2
9	CLA	9	610	4	-	9/15/91/115	-
9	CLA	P	604	6	-	6/27/103/115	-
9	CLA	8	601	3	-	6/12/88/115	-
16	8CT	9	615	-	-	9/29/63/63	0/2/2/2
9	CLA	0	612	-	-	7/15/91/115	-
9	CLA	P	607	6	-	7/33/109/115	-
15	LHG	8	618	9	-	11/24/24/53	-
9	CLA	8	609	15	-	4/10/86/115	-
11	IHT	7	618	-	-	2/25/65/65	0/2/2/2
10	KC2	7	610	2	-	11/15/71/71	-
9	CLA	0	613	1	-	8/15/91/115	-
9	CLA	8	602	3	-	13/32/108/115	-
12	II0	7	617	-	-	4/21/67/67	0/2/2/2
9	CLA	8	604	-	-	3/27/103/115	-
9	CLA	9	606	-	-	1/15/91/115	-
12	II0	9	612	-	-	2/21/67/67	0/2/2/2
9	CLA	9	602	4	-	11/32/108/115	-
9	CLA	0	604	1	-	9/27/103/115	-
9	CLA	8	605	3	-	13/33/109/115	-
9	CLA	P	601	6	-	2/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	8	611	3	-	6/15/91/115	-
12	II0	8	613	-	-	0/21/67/67	0/2/2/2
9	CLA	0	603	1	-	5/21/97/115	-
9	CLA	0	608	-	-	11/33/109/115	-
10	KC2	P	605	6	-	10/15/71/71	-
9	CLA	0	607	1	-	2/15/91/115	-
9	CLA	8	612	3	-	8/15/91/115	-
9	CLA	7	607	-	-	9/15/91/115	-
14	II3	P	613	-	-	1/25/67/67	0/2/2/2
9	CLA	s	303	8	-	17/39/115/115	-
9	CLA	P	606	6	-	6/15/91/115	-
12	II0	P	612	-	-	0/21/67/67	0/2/2/2
9	CLA	9	609	4	-	9/33/109/115	-
9	CLA	7	602	2	-	12/32/108/115	-
9	CLA	P	603	-	-	3/21/97/115	-
13	LMG	0	618	-	-	10/31/51/70	0/1/1/1
9	CLA	7	612	2	-	7/15/91/115	-
9	CLA	0	611	1	-	9/15/91/115	-
9	CLA	p	310	7	-	9/33/109/115	-
9	CLA	7	609	-	-	3/10/86/115	-
10	KC2	0	610	1	-	11/15/71/71	-
12	II0	9	614	-	-	4/21/67/67	0/2/2/2
9	CLA	9	608	-	-	3/10/86/115	-
9	CLA	7	605	-	-	8/21/97/115	-
16	8CT	P	615	-	-	4/29/63/63	0/2/2/2
12	II0	p	301	-	-	2/21/67/67	0/2/2/2
12	II0	8	619	-	-	1/21/67/67	0/2/2/2
9	CLA	7	606	2	-	9/15/91/115	-
9	CLA	9	604	4	-	8/27/103/115	-
9	CLA	p	314	7	-	5/15/91/115	-
12	II0	p	315	-	-	1/21/67/67	0/2/2/2
13	LMG	G	102	-	-	9/23/43/70	0/1/1/1
9	CLA	7	603	2	-	8/21/97/115	-
9	CLA	8	606	3	-	2/15/91/115	-
9	CLA	p	309	7	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	II0	p	316	-	-	4/21/67/67	0/2/2/2
12	II0	p	317	-	-	5/21/67/67	0/2/2/2
12	II0	9	613	-	-	1/21/67/67	0/2/2/2
11	IHT	0	614	-	-	5/25/65/65	0/2/2/2
15	LHG	s	301	-	-	20/41/41/53	-
9	CLA	P	602	6	-	16/32/108/115	-
9	CLA	p	308	7	-	6/15/91/115	-
9	CLA	9	607	4	-	6/33/109/115	-
9	CLA	P	610	-	-	6/15/91/115	-
9	CLA	7	601	-	-	5/12/88/115	-
13	LMG	G	103	-	-	7/23/43/70	0/1/1/1
9	CLA	p	307	7	-	15/33/109/115	-
12	II0	8	615	-	-	3/21/67/67	0/2/2/2
9	CLA	0	601	1	-	7/12/88/115	-
12	II0	P	614	-	-	3/21/67/67	0/2/2/2
12	II0	0	616	-	-	4/21/67/67	0/2/2/2
9	CLA	0	606	-	-	7/15/91/115	-
13	LMG	8	617	-	-	10/31/51/70	0/1/1/1
9	CLA	9	605	4	-	7/17/93/115	-
9	CLA	7	604	2	-	5/27/103/115	-
9	CLA	p	304	7	-	14/32/108/115	-
9	CLA	p	306	7	-	11/27/103/115	-
9	CLA	9	611	4	-	6/15/91/115	-
9	CLA	0	609	-	-	4/10/86/115	-
9	CLA	p	303	7	-	8/12/88/115	-
9	CLA	8	607	3	-	5/15/91/115	-
14	II3	7	615	-	-	1/25/67/67	0/2/2/2
10	KC2	p	312	7	-	10/15/71/71	-
9	CLA	p	305	-	-	12/21/97/115	-
12	II0	p	302	-	-	1/21/67/67	0/2/2/2
12	II0	0	615	-	-	0/21/67/67	0/2/2/2
9	CLA	P	608	-	-	2/10/86/115	-
9	CLA	9	601	4	-	5/12/88/115	-
11	IHT	0	617	-	-	5/25/65/65	0/2/2/2
12	II0	8	614	-	-	0/21/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLA	9	603	4	-	6/21/97/115	-
9	CLA	7	611	2	-	7/15/91/115	-
17	SQD	p	319	-	-	19/30/50/69	0/1/1/1
9	CLA	0	602	1	-	13/32/108/115	-
10	KC2	8	610	3	-	9/15/71/71	-
9	CLA	G	101	-	-	9/15/91/115	-
11	IHT	8	616	-	-	1/25/65/65	0/2/2/2
9	CLA	s	302	-	-	5/15/91/115	-
9	CLA	P	611	6	-	7/15/91/115	-
12	II0	0	619	-	-	2/21/67/67	0/2/2/2
9	CLA	8	603	3	-	8/21/97/115	-
9	CLA	8	608	3	-	8/33/109/115	-
12	II0	7	619	-	-	2/21/67/67	0/2/2/2
9	CLA	0	605	1	-	9/21/97/115	-
9	CLA	p	311	-	-	5/10/86/115	-
10	KC2	P	609	6	-	12/15/71/71	-
9	CLA	p	313	-	-	8/15/91/115	-
11	IHT	p	318	-	-	0/25/65/65	0/2/2/2
9	CLA	7	608	2	-	10/33/109/115	-
9	CLA	7	613	-	-	9/15/91/115	-

All (878) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	9	615	8CT	C02-C03	13.96	1.58	1.34
16	P	615	8CT	C02-C03	13.88	1.58	1.34
16	P	615	8CT	C32-C31	13.81	1.59	1.32
16	9	615	8CT	C32-C31	13.63	1.59	1.32
12	0	616	II0	C24-C26	-8.78	1.25	1.42
12	7	617	II0	C23-C25	-8.75	1.25	1.42
12	7	616	II0	C23-C25	-8.73	1.25	1.42
12	9	612	II0	C23-C25	-8.72	1.25	1.42
12	P	614	II0	C23-C25	-8.71	1.25	1.42
12	8	613	II0	C24-C26	-8.70	1.25	1.42
12	8	614	II0	C24-C26	-8.70	1.25	1.42
12	7	614	II0	C23-C25	-8.69	1.25	1.42
12	7	616	II0	C24-C26	-8.68	1.25	1.42
12	9	613	II0	C24-C26	-8.68	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	p	317	II0	C23-C25	-8.68	1.25	1.42
12	9	612	II0	C24-C26	-8.65	1.25	1.42
12	8	619	II0	C24-C26	-8.65	1.25	1.42
12	8	613	II0	C23-C25	-8.65	1.25	1.42
12	p	301	II0	C24-C26	-8.65	1.25	1.42
11	8	616	IHT	C24-C26	-8.63	1.25	1.42
11	p	318	IHT	C24-C26	-8.62	1.26	1.42
11	7	618	IHT	C24-C26	-8.62	1.26	1.42
12	p	316	II0	C24-C26	-8.62	1.26	1.42
14	7	615	II3	C27-C28	-8.61	1.26	1.42
12	9	614	II0	C23-C25	-8.60	1.26	1.42
14	P	613	II3	C27-C28	-8.59	1.26	1.42
12	0	616	II0	C23-C25	-8.59	1.26	1.42
12	9	614	II0	C24-C26	-8.58	1.26	1.42
12	8	619	II0	C23-C25	-8.58	1.26	1.42
11	0	617	IHT	C24-C26	-8.57	1.26	1.42
11	0	614	IHT	C24-C26	-8.56	1.26	1.42
12	9	613	II0	C23-C25	-8.56	1.26	1.42
12	0	615	II0	C24-C26	-8.56	1.26	1.42
12	7	617	II0	C24-C26	-8.55	1.26	1.42
12	8	615	II0	C24-C26	-8.54	1.26	1.42
12	P	614	II0	C24-C26	-8.53	1.26	1.42
12	7	614	II0	C24-C26	-8.51	1.26	1.42
12	7	619	II0	C24-C26	-8.51	1.26	1.42
12	p	315	II0	C23-C25	-8.50	1.26	1.42
12	P	612	II0	C24-C26	-8.50	1.26	1.42
12	8	615	II0	C23-C25	-8.50	1.26	1.42
12	p	301	II0	C23-C25	-8.49	1.26	1.42
12	p	302	II0	C24-C26	-8.49	1.26	1.42
12	P	612	II0	C23-C25	-8.48	1.26	1.42
12	p	317	II0	C24-C26	-8.48	1.26	1.42
12	p	302	II0	C23-C25	-8.44	1.26	1.42
12	p	315	II0	C24-C26	-8.42	1.26	1.42
12	7	619	II0	C23-C25	-8.41	1.26	1.42
12	0	619	II0	C24-C26	-8.41	1.26	1.42
12	p	316	II0	C23-C25	-8.41	1.26	1.42
12	0	615	II0	C23-C25	-8.40	1.26	1.42
12	0	619	II0	C23-C25	-8.40	1.26	1.42
16	P	615	8CT	C34-C35	-8.40	1.36	1.54
12	8	614	II0	C23-C25	-8.37	1.26	1.42
16	9	615	8CT	C34-C35	-8.27	1.37	1.54
12	0	616	II0	C22-C10	-8.05	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	7	618	IHT	C21-C11	-7.99	1.25	1.42
12	8	619	II0	C22-C10	-7.96	1.25	1.42
12	P	614	II0	C21-C09	-7.94	1.25	1.42
12	9	613	II0	C22-C10	-7.94	1.25	1.42
12	7	616	II0	C22-C10	-7.94	1.25	1.42
12	p	302	II0	C22-C10	-7.93	1.25	1.42
12	7	617	II0	C21-C09	-7.92	1.25	1.42
12	7	614	II0	C21-C09	-7.90	1.25	1.42
12	7	617	II0	C22-C10	-7.90	1.25	1.42
12	p	317	II0	C21-C09	-7.89	1.25	1.42
12	7	616	II0	C21-C09	-7.89	1.25	1.42
11	8	616	IHT	C21-C11	-7.88	1.25	1.42
12	8	614	II0	C22-C10	-7.88	1.25	1.42
11	0	614	IHT	C21-C11	-7.87	1.25	1.42
12	p	301	II0	C22-C10	-7.87	1.25	1.42
11	p	318	IHT	C21-C11	-7.86	1.25	1.42
12	8	613	II0	C22-C10	-7.84	1.26	1.42
12	8	613	II0	C21-C09	-7.84	1.26	1.42
12	9	614	II0	C21-C09	-7.84	1.26	1.42
12	8	619	II0	C21-C09	-7.84	1.26	1.42
12	p	316	II0	C22-C10	-7.84	1.26	1.42
12	p	301	II0	C21-C09	-7.83	1.26	1.42
12	9	612	II0	C21-C09	-7.83	1.26	1.42
12	p	317	II0	C22-C10	-7.82	1.26	1.42
12	0	619	II0	C22-C10	-7.81	1.26	1.42
12	P	612	II0	C21-C09	-7.81	1.26	1.42
14	7	615	II3	C23-C16	-7.81	1.26	1.42
12	7	614	II0	C22-C10	-7.81	1.26	1.42
12	9	612	II0	C22-C10	-7.80	1.26	1.42
14	P	613	II3	C23-C16	-7.80	1.26	1.42
12	0	616	II0	C21-C09	-7.79	1.26	1.42
12	0	615	II0	C22-C10	-7.79	1.26	1.42
11	0	617	IHT	C21-C11	-7.78	1.26	1.42
12	8	615	II0	C22-C10	-7.78	1.26	1.42
12	9	614	II0	C22-C10	-7.77	1.26	1.42
12	P	614	II0	C22-C10	-7.77	1.26	1.42
12	7	619	II0	C22-C10	-7.77	1.26	1.42
12	9	613	II0	C21-C09	-7.77	1.26	1.42
12	P	612	II0	C22-C10	-7.75	1.26	1.42
12	0	615	II0	C21-C09	-7.74	1.26	1.42
12	p	315	II0	C21-C09	-7.74	1.26	1.42
12	8	615	II0	C21-C09	-7.72	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	p	315	II0	C22-C10	-7.71	1.26	1.42
12	7	619	II0	C21-C09	-7.67	1.26	1.42
12	8	614	II0	C21-C09	-7.64	1.26	1.42
12	p	316	II0	C21-C09	-7.64	1.26	1.42
12	p	302	II0	C21-C09	-7.59	1.26	1.42
12	0	619	II0	C21-C09	-7.59	1.26	1.42
16	P	615	8CT	C05-C06	-6.41	1.36	1.52
16	9	615	8CT	C05-C06	-6.37	1.36	1.52
16	P	615	8CT	C15-C16	6.29	1.59	1.45
16	9	615	8CT	C15-C16	6.22	1.59	1.45
16	P	615	8CT	C28-C26	6.22	1.59	1.45
16	9	615	8CT	C28-C26	6.09	1.59	1.45
16	9	615	8CT	C04-C03	-5.83	1.45	1.53
16	P	615	8CT	C04-C03	-5.73	1.45	1.53
16	P	615	8CT	C23-C21	5.72	1.58	1.45
16	9	615	8CT	C23-C21	5.62	1.58	1.45
10	P	605	KC2	CHD-C4C	5.20	1.49	1.38
16	9	615	8CT	C34-C33	5.14	1.64	1.52
16	P	615	8CT	C34-C33	5.14	1.64	1.52
10	7	610	KC2	CHD-C4C	5.10	1.48	1.38
10	0	610	KC2	CHD-C4C	5.09	1.48	1.38
10	P	609	KC2	CHD-C4C	5.09	1.48	1.38
10	p	312	KC2	CHD-C4C	5.02	1.48	1.38
10	8	610	KC2	CHD-C4C	4.99	1.48	1.38
16	P	615	8CT	C05-C04	4.97	1.65	1.54
16	9	615	8CT	C05-C04	4.95	1.65	1.54
16	9	615	8CT	C06-C07	4.69	1.67	1.52
10	8	610	KC2	MG-ND	-4.68	1.96	2.05
10	0	610	KC2	MG-ND	-4.59	1.96	2.05
16	P	615	8CT	C06-C07	4.57	1.66	1.52
10	P	605	KC2	MG-ND	-4.56	1.96	2.05
17	p	319	SQD	O48-C23	4.56	1.46	1.33
10	P	609	KC2	MG-ND	-4.54	1.96	2.05
10	p	312	KC2	MG-ND	-4.50	1.96	2.05
10	7	610	KC2	MG-ND	-4.41	1.97	2.05
16	P	615	8CT	C19-C20	4.41	1.57	1.43
10	8	610	KC2	MG-NB	-4.40	1.97	2.05
10	P	605	KC2	MG-NB	-4.39	1.97	2.05
16	9	615	8CT	C19-C20	4.31	1.56	1.43
10	0	610	KC2	MG-NB	-4.27	1.97	2.05
10	p	312	KC2	MG-NB	-4.21	1.97	2.05
10	P	609	KC2	MG-NB	-4.20	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	7	610	KC2	MG-NB	-4.11	1.97	2.05
10	0	610	KC2	CHC-C1C	4.08	1.48	1.39
10	p	312	KC2	CHC-C1C	4.08	1.48	1.39
10	P	609	KC2	CHC-C1C	4.08	1.48	1.39
10	P	605	KC2	CHC-C1C	4.05	1.48	1.39
16	P	615	8CT	C24-C25	4.05	1.56	1.43
16	9	615	8CT	C24-C25	4.04	1.56	1.43
10	P	605	KC2	CHC-C4B	4.02	1.46	1.38
10	0	610	KC2	CHC-C4B	4.01	1.46	1.38
10	p	312	KC2	CHC-C4B	3.97	1.46	1.38
10	7	610	KC2	CHC-C1C	3.97	1.48	1.39
10	P	609	KC2	CHC-C4B	3.96	1.46	1.38
10	8	610	KC2	CHC-C1C	3.90	1.48	1.39
9	P	606	CLA	C1D-ND	3.84	1.42	1.37
9	7	613	CLA	C1D-ND	3.82	1.42	1.37
9	s	302	CLA	C1D-ND	3.80	1.42	1.37
16	P	615	8CT	C14-C13	3.78	1.55	1.43
10	7	610	KC2	CHC-C4B	3.77	1.45	1.38
10	8	610	KC2	CHC-C4B	3.76	1.45	1.38
9	s	303	CLA	C1D-ND	3.76	1.42	1.37
9	0	611	CLA	C1D-ND	3.75	1.42	1.37
9	0	612	CLA	C1D-ND	3.75	1.42	1.37
9	0	601	CLA	C1D-ND	3.74	1.42	1.37
16	9	615	8CT	C14-C13	3.73	1.55	1.43
9	7	601	CLA	C1D-ND	3.71	1.42	1.37
9	0	609	CLA	C1D-ND	3.71	1.42	1.37
9	0	606	CLA	C1D-ND	3.68	1.42	1.37
9	9	605	CLA	C1D-ND	3.68	1.42	1.37
9	7	609	CLA	C1D-ND	3.67	1.42	1.37
9	P	607	CLA	C1D-ND	3.66	1.42	1.37
9	p	314	CLA	C1D-ND	3.65	1.42	1.37
9	7	604	CLA	C1D-ND	3.65	1.42	1.37
16	P	615	8CT	C11-C12	3.65	1.53	1.45
9	9	609	CLA	C1D-ND	3.64	1.42	1.37
9	7	612	CLA	C1D-ND	3.64	1.42	1.37
9	0	608	CLA	C1D-ND	3.64	1.42	1.37
9	0	604	CLA	C1D-ND	3.63	1.42	1.37
9	9	607	CLA	C1D-ND	3.63	1.42	1.37
9	9	604	CLA	C1D-ND	3.61	1.42	1.37
16	9	615	8CT	C11-C12	3.60	1.53	1.45
9	p	308	CLA	C1D-ND	3.60	1.42	1.37
9	p	309	CLA	C1D-ND	3.59	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	604	CLA	C1D-ND	3.59	1.42	1.37
9	P	611	CLA	C1D-ND	3.58	1.42	1.37
9	9	601	CLA	C1D-ND	3.58	1.42	1.37
9	0	613	CLA	C1D-ND	3.57	1.42	1.37
9	0	605	CLA	C1D-ND	3.57	1.42	1.37
9	p	304	CLA	C1D-ND	3.56	1.42	1.37
9	7	605	CLA	C1D-ND	3.56	1.42	1.37
9	P	603	CLA	C1D-ND	3.56	1.42	1.37
9	p	305	CLA	C1D-ND	3.55	1.42	1.37
9	9	611	CLA	C1D-ND	3.54	1.42	1.37
9	p	307	CLA	C1D-ND	3.53	1.42	1.37
9	8	609	CLA	C1D-ND	3.52	1.42	1.37
9	G	101	CLA	C1D-ND	3.52	1.42	1.37
9	p	306	CLA	C1D-ND	3.52	1.42	1.37
9	0	607	CLA	C1D-ND	3.52	1.42	1.37
9	8	607	CLA	C1D-ND	3.52	1.42	1.37
9	9	606	CLA	C1D-ND	3.52	1.42	1.37
9	P	602	CLA	C1D-ND	3.51	1.42	1.37
9	p	311	CLA	C1D-ND	3.51	1.42	1.37
9	7	611	CLA	C1D-ND	3.51	1.42	1.37
9	0	603	CLA	C1D-ND	3.50	1.42	1.37
9	p	310	CLA	C1D-ND	3.50	1.42	1.37
9	8	602	CLA	C4D-ND	-3.50	1.32	1.37
9	P	608	CLA	C1D-ND	3.50	1.42	1.37
9	8	603	CLA	C1D-ND	3.50	1.42	1.37
16	P	615	8CT	C28-C29	3.49	1.40	1.32
9	0	602	CLA	C1D-ND	3.47	1.42	1.37
9	8	611	CLA	C1D-ND	3.46	1.42	1.37
9	7	603	CLA	C1D-ND	3.46	1.42	1.37
10	P	605	KC2	CHD-C1D	3.46	1.47	1.39
9	9	603	CLA	C1D-ND	3.45	1.42	1.37
9	p	303	CLA	C1D-ND	3.44	1.42	1.37
9	9	602	CLA	C1D-ND	3.44	1.42	1.37
9	9	602	CLA	C4D-ND	-3.44	1.33	1.37
9	8	606	CLA	C1D-ND	3.44	1.42	1.37
9	9	610	CLA	C1D-ND	3.44	1.42	1.37
9	8	608	CLA	C1D-ND	3.43	1.42	1.37
9	8	612	CLA	C1D-ND	3.43	1.42	1.37
9	7	608	CLA	C1D-ND	3.43	1.42	1.37
9	8	605	CLA	C1D-ND	3.42	1.42	1.37
9	9	608	CLA	C1D-ND	3.42	1.42	1.37
9	7	607	CLA	C1D-ND	3.42	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	s	302	CLA	C4D-ND	-3.41	1.33	1.37
9	8	601	CLA	C1D-ND	3.41	1.42	1.37
9	s	303	CLA	C4B-NB	3.40	1.42	1.37
9	7	606	CLA	C1D-ND	3.40	1.42	1.37
9	P	604	CLA	C1D-ND	3.39	1.42	1.37
16	9	615	8CT	C28-C29	3.39	1.40	1.32
9	P	601	CLA	C1D-ND	3.39	1.42	1.37
10	0	610	KC2	CHD-C1D	3.37	1.47	1.39
9	p	313	CLA	C1D-ND	3.36	1.41	1.37
9	7	602	CLA	C1D-ND	3.34	1.41	1.37
17	p	319	SQD	O47-C7	3.33	1.43	1.34
9	8	608	CLA	C4D-ND	-3.33	1.33	1.37
17	p	319	SQD	O5-C1	3.33	1.50	1.41
9	P	610	CLA	C1D-ND	3.33	1.41	1.37
9	7	607	CLA	C4D-ND	-3.30	1.33	1.37
9	9	606	CLA	C4B-NB	3.30	1.41	1.37
9	7	603	CLA	C4D-ND	-3.30	1.33	1.37
9	p	305	CLA	C4D-ND	-3.30	1.33	1.37
9	0	612	CLA	C4B-NB	3.30	1.41	1.37
9	7	602	CLA	C4D-ND	-3.30	1.33	1.37
10	P	609	KC2	CHD-C1D	3.30	1.46	1.39
10	7	610	KC2	CHD-C1D	3.30	1.46	1.39
9	P	602	CLA	C4D-ND	-3.29	1.33	1.37
17	p	319	SQD	O47-C45	-3.29	1.38	1.46
9	8	603	CLA	C4D-ND	-3.29	1.33	1.37
9	9	606	CLA	C3B-C4B	3.28	1.50	1.42
9	8	602	CLA	C1D-ND	3.27	1.41	1.37
9	9	607	CLA	C4D-ND	-3.27	1.33	1.37
9	G	101	CLA	C4B-NB	3.27	1.41	1.37
9	0	613	CLA	C4B-NB	3.26	1.41	1.37
9	8	611	CLA	C4D-ND	-3.25	1.33	1.37
16	9	615	8CT	C35-C30	3.25	1.65	1.56
9	7	606	CLA	C4D-ND	-3.24	1.33	1.37
9	7	601	CLA	C4B-NB	3.24	1.41	1.37
9	7	608	CLA	C4D-ND	-3.24	1.33	1.37
16	9	615	8CT	C01-C02	3.24	1.56	1.50
9	P	604	CLA	C4D-ND	-3.23	1.33	1.37
9	9	608	CLA	C4D-ND	-3.23	1.33	1.37
10	p	312	KC2	CHD-C1D	3.23	1.46	1.39
9	8	609	CLA	C4D-ND	-3.22	1.33	1.37
9	9	603	CLA	C4D-ND	-3.22	1.33	1.37
9	p	309	CLA	C4D-ND	-3.22	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	p	311	CLA	C4D-ND	-3.22	1.33	1.37
9	0	604	CLA	C4B-NB	3.21	1.41	1.37
9	p	304	CLA	C4D-ND	-3.21	1.33	1.37
9	7	612	CLA	C4B-NB	3.21	1.41	1.37
10	8	610	KC2	CHD-C1D	3.21	1.46	1.39
9	P	601	CLA	C4D-ND	-3.21	1.33	1.37
9	0	607	CLA	C4B-NB	3.20	1.41	1.37
9	7	604	CLA	C4D-ND	-3.20	1.33	1.37
9	0	601	CLA	C4B-NB	3.20	1.41	1.37
9	8	604	CLA	C4D-ND	-3.19	1.33	1.37
9	9	604	CLA	C4B-NB	3.19	1.41	1.37
9	p	306	CLA	C4D-ND	-3.19	1.33	1.37
9	p	303	CLA	C4D-ND	-3.18	1.33	1.37
9	7	613	CLA	C4B-NB	3.18	1.41	1.37
9	P	610	CLA	C4D-ND	-3.18	1.33	1.37
9	p	310	CLA	C4D-ND	-3.18	1.33	1.37
9	7	605	CLA	C4D-ND	-3.17	1.33	1.37
9	0	603	CLA	C4D-ND	-3.17	1.33	1.37
9	0	605	CLA	C4B-NB	3.16	1.41	1.37
9	9	604	CLA	C4D-ND	-3.16	1.33	1.37
9	7	609	CLA	C4B-NB	3.16	1.41	1.37
9	9	605	CLA	C4B-NB	3.16	1.41	1.37
9	8	606	CLA	C4D-ND	-3.16	1.33	1.37
9	P	611	CLA	C4B-NB	3.15	1.41	1.37
9	8	601	CLA	C4D-ND	-3.15	1.33	1.37
9	7	611	CLA	C4D-ND	-3.15	1.33	1.37
16	9	615	8CT	C30-C29	3.15	1.54	1.50
9	P	608	CLA	C4D-ND	-3.15	1.33	1.37
16	P	615	8CT	C35-C30	3.14	1.65	1.56
9	8	607	CLA	C4D-ND	-3.14	1.33	1.37
9	9	609	CLA	C4D-ND	-3.14	1.33	1.37
9	P	606	CLA	C4B-NB	3.14	1.41	1.37
9	0	611	CLA	C4B-NB	3.14	1.41	1.37
9	P	603	CLA	C4D-ND	-3.13	1.33	1.37
9	0	609	CLA	C4B-NB	3.13	1.41	1.37
16	P	615	8CT	C01-C02	3.13	1.56	1.50
9	p	314	CLA	C4B-NB	3.13	1.41	1.37
9	7	612	CLA	C4D-ND	-3.13	1.33	1.37
9	8	605	CLA	C4D-ND	-3.12	1.33	1.37
9	9	610	CLA	C4D-ND	-3.12	1.33	1.37
9	p	313	CLA	C4D-ND	-3.12	1.33	1.37
9	8	605	CLA	C4B-NB	3.12	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	0	602	CLA	C4D-ND	-3.12	1.33	1.37
9	0	608	CLA	C4D-ND	-3.12	1.33	1.37
9	8	606	CLA	C4B-NB	3.12	1.41	1.37
9	p	308	CLA	C4D-ND	-3.11	1.33	1.37
9	9	606	CLA	C4D-ND	-3.11	1.33	1.37
9	8	612	CLA	C4D-ND	-3.10	1.33	1.37
9	9	611	CLA	C4D-ND	-3.10	1.33	1.37
9	p	307	CLA	C4D-ND	-3.10	1.33	1.37
9	0	606	CLA	C4B-NB	3.09	1.41	1.37
9	7	609	CLA	C4D-ND	-3.09	1.33	1.37
9	P	604	CLA	C4B-NB	3.08	1.41	1.37
16	P	615	8CT	C30-C29	3.08	1.54	1.50
9	G	101	CLA	C4D-ND	-3.07	1.33	1.37
9	0	604	CLA	C4D-ND	-3.06	1.33	1.37
9	p	311	CLA	C4B-NB	3.06	1.41	1.37
9	s	303	CLA	C4D-ND	-3.06	1.33	1.37
9	7	605	CLA	C4B-NB	3.05	1.41	1.37
9	p	314	CLA	C4D-ND	-3.05	1.33	1.37
9	0	607	CLA	C4D-ND	-3.04	1.33	1.37
9	0	606	CLA	C4D-ND	-3.04	1.33	1.37
9	7	601	CLA	C4D-ND	-3.03	1.33	1.37
9	P	611	CLA	C4D-ND	-3.02	1.33	1.37
9	P	603	CLA	C4B-NB	3.02	1.41	1.37
9	9	601	CLA	C4D-ND	-3.02	1.33	1.37
9	9	601	CLA	C4B-NB	3.02	1.41	1.37
9	0	603	CLA	C4B-NB	3.02	1.41	1.37
9	0	609	CLA	C4D-ND	-3.02	1.33	1.37
9	8	612	CLA	C4B-NB	3.02	1.41	1.37
9	p	305	CLA	C4B-NB	3.02	1.41	1.37
9	0	602	CLA	C4B-NB	3.02	1.41	1.37
9	8	609	CLA	C4B-NB	3.01	1.41	1.37
9	0	613	CLA	C4D-ND	-3.01	1.33	1.37
16	P	615	8CT	C18-C17	3.01	1.52	1.43
9	0	604	CLA	C3B-C4B	3.01	1.49	1.42
9	0	611	CLA	C4D-ND	-3.00	1.33	1.37
9	7	613	CLA	C4D-ND	-2.99	1.33	1.37
9	9	611	CLA	C4B-NB	2.99	1.41	1.37
9	P	608	CLA	C4B-NB	2.99	1.41	1.37
16	9	615	8CT	C18-C17	2.99	1.52	1.43
9	P	607	CLA	C4D-ND	-2.98	1.33	1.37
9	p	303	CLA	C4B-NB	2.98	1.41	1.37
9	s	302	CLA	C4B-NB	2.97	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	p	308	CLA	C4B-NB	2.97	1.41	1.37
9	9	604	CLA	C3B-C4B	2.97	1.49	1.42
9	P	602	CLA	C4B-NB	2.97	1.41	1.37
9	p	304	CLA	C4B-NB	2.97	1.41	1.37
9	9	605	CLA	C4D-ND	-2.96	1.33	1.37
9	0	605	CLA	C4D-ND	-2.95	1.33	1.37
9	0	608	CLA	C4B-NB	2.95	1.41	1.37
9	P	606	CLA	C4D-ND	-2.95	1.33	1.37
9	p	307	CLA	C4B-NB	2.95	1.41	1.37
9	P	607	CLA	C4B-NB	2.94	1.41	1.37
9	0	612	CLA	C4D-ND	-2.92	1.33	1.37
9	p	310	CLA	C4B-NB	2.92	1.41	1.37
9	P	601	CLA	C4B-NB	2.92	1.41	1.37
9	0	601	CLA	C4D-ND	-2.92	1.33	1.37
9	8	601	CLA	C4B-NB	2.91	1.41	1.37
9	0	601	CLA	C3B-C4B	2.90	1.49	1.42
9	9	608	CLA	C4B-NB	2.90	1.41	1.37
9	9	609	CLA	C4B-NB	2.90	1.41	1.37
16	P	615	8CT	C07-C02	-2.89	1.45	1.51
16	P	615	8CT	C10-C03	2.89	1.55	1.45
9	9	607	CLA	C4B-NB	2.89	1.41	1.37
9	p	309	CLA	C4B-NB	2.89	1.41	1.37
10	8	610	KC2	C4B-NB	-2.89	1.34	1.37
9	7	608	CLA	C4B-NB	2.88	1.41	1.37
9	8	604	CLA	C4B-NB	2.88	1.41	1.37
9	7	611	CLA	C4B-NB	2.87	1.41	1.37
16	9	615	8CT	C10-C03	2.87	1.55	1.45
9	7	607	CLA	C4B-NB	2.87	1.41	1.37
9	p	313	CLA	C4B-NB	2.86	1.41	1.37
9	9	603	CLA	C4B-NB	2.86	1.41	1.37
9	8	608	CLA	C4B-NB	2.86	1.41	1.37
9	0	606	CLA	C3B-C4B	2.85	1.49	1.42
10	7	610	KC2	CBA-CGA	-2.85	1.41	1.48
9	7	601	CLA	C3B-C4B	2.85	1.49	1.42
9	s	303	CLA	C3B-C4B	2.84	1.49	1.42
9	9	610	CLA	C4B-NB	2.84	1.41	1.37
9	8	603	CLA	C4B-NB	2.84	1.41	1.37
9	8	606	CLA	C3B-C4B	2.83	1.49	1.42
9	7	604	CLA	C4B-NB	2.83	1.41	1.37
9	P	610	CLA	C4B-NB	2.83	1.41	1.37
10	P	605	KC2	CBA-CGA	-2.82	1.42	1.48
9	9	605	CLA	C3B-C4B	2.82	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	7	609	CLA	C3B-C4B	2.81	1.49	1.42
9	p	304	CLA	C3B-C4B	2.81	1.49	1.42
9	7	602	CLA	C4B-NB	2.80	1.41	1.37
10	P	605	KC2	C4B-NB	-2.80	1.34	1.37
9	0	602	CLA	C3B-C4B	2.80	1.49	1.42
9	P	611	CLA	C3B-C4B	2.80	1.49	1.42
9	p	311	CLA	C3B-C4B	2.79	1.49	1.42
9	0	607	CLA	C3B-C4B	2.79	1.49	1.42
9	P	603	CLA	C3B-C4B	2.79	1.49	1.42
9	P	602	CLA	C3B-C4B	2.78	1.49	1.42
10	p	312	KC2	CBA-CGA	-2.78	1.42	1.48
9	7	606	CLA	C4B-NB	2.78	1.41	1.37
10	P	609	KC2	CBA-CGA	-2.78	1.42	1.48
9	p	306	CLA	C4B-NB	2.78	1.41	1.37
10	0	610	KC2	CBA-CGA	-2.77	1.42	1.48
9	8	607	CLA	C3B-C4B	2.77	1.49	1.42
9	0	612	CLA	C3B-C4B	2.77	1.49	1.42
10	8	610	KC2	CBA-CGA	-2.77	1.42	1.48
9	9	601	CLA	C3B-C4B	2.77	1.49	1.42
9	7	607	CLA	C3B-C4B	2.76	1.49	1.42
9	p	309	CLA	C3B-C4B	2.76	1.49	1.42
9	G	101	CLA	C3B-C4B	2.76	1.49	1.42
9	0	613	CLA	C3B-C4B	2.76	1.49	1.42
9	0	609	CLA	C3B-C4B	2.76	1.49	1.42
9	p	310	CLA	C3B-C4B	2.76	1.49	1.42
9	P	606	CLA	C3B-C4B	2.75	1.49	1.42
9	8	607	CLA	C4B-NB	2.74	1.41	1.37
9	7	612	CLA	C3B-C4B	2.74	1.49	1.42
16	9	615	8CT	C07-C02	-2.74	1.45	1.51
9	9	602	CLA	C4B-NB	2.73	1.41	1.37
9	7	613	CLA	C3B-C4B	2.72	1.49	1.42
9	P	604	CLA	C3B-C4B	2.72	1.49	1.42
9	7	603	CLA	C4B-NB	2.72	1.41	1.37
9	0	603	CLA	C3B-C4B	2.71	1.49	1.42
9	8	609	CLA	C3B-C4B	2.71	1.49	1.42
9	P	601	CLA	C3B-C4B	2.71	1.49	1.42
9	9	608	CLA	C3B-C4B	2.70	1.49	1.42
9	p	313	CLA	C3B-C4B	2.70	1.49	1.42
10	7	610	KC2	C4B-NB	-2.70	1.34	1.37
9	7	604	CLA	C3B-C4B	2.70	1.49	1.42
9	7	602	CLA	C3B-C4B	2.70	1.49	1.42
9	9	609	CLA	C3B-C4B	2.69	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	p	305	CLA	C3B-C4B	2.69	1.49	1.42
9	0	608	CLA	C3B-C4B	2.69	1.49	1.42
9	0	611	CLA	C3B-C4B	2.69	1.49	1.42
9	P	607	CLA	C3B-C4B	2.68	1.49	1.42
9	9	607	CLA	C3B-C4B	2.67	1.49	1.42
9	7	601	CLA	C1B-C2B	2.67	1.49	1.43
9	p	303	CLA	C3B-C4B	2.67	1.49	1.42
9	8	604	CLA	C3B-C4B	2.67	1.49	1.42
9	P	608	CLA	C3B-C4B	2.67	1.49	1.42
9	0	605	CLA	C3B-C4B	2.66	1.49	1.42
9	8	601	CLA	C3B-C4B	2.66	1.49	1.42
9	7	608	CLA	C3B-C4B	2.66	1.49	1.42
9	P	606	CLA	C1B-C2B	2.66	1.49	1.43
9	8	611	CLA	C4B-NB	2.65	1.41	1.37
9	8	605	CLA	C3B-C4B	2.65	1.49	1.42
9	9	611	CLA	C3B-C4B	2.64	1.49	1.42
9	9	602	CLA	C3B-C4B	2.64	1.48	1.42
9	7	606	CLA	C1B-C2B	2.64	1.49	1.43
9	p	314	CLA	C3B-C4B	2.63	1.48	1.42
9	9	610	CLA	C3B-C4B	2.63	1.48	1.42
9	P	610	CLA	C3B-C4B	2.63	1.48	1.42
9	8	612	CLA	C3B-C4B	2.62	1.48	1.42
10	P	609	KC2	C4B-NB	-2.62	1.34	1.37
9	p	307	CLA	C1B-C2B	2.62	1.49	1.43
9	0	601	CLA	C1B-C2B	2.62	1.49	1.43
9	s	302	CLA	C3B-C4B	2.62	1.48	1.42
10	p	312	KC2	C4B-NB	-2.61	1.34	1.37
9	0	612	CLA	C1B-C2B	2.61	1.49	1.43
9	G	101	CLA	C1B-C2B	2.61	1.49	1.43
9	8	603	CLA	C3B-C4B	2.61	1.48	1.42
9	0	611	CLA	C1B-C2B	2.61	1.49	1.43
9	8	608	CLA	C3B-C4B	2.60	1.48	1.42
9	8	602	CLA	C4B-NB	2.60	1.41	1.37
9	0	609	CLA	C1B-C2B	2.60	1.49	1.43
9	8	611	CLA	C3B-C4B	2.60	1.48	1.42
9	7	603	CLA	C3B-C4B	2.60	1.48	1.42
9	0	605	CLA	C1B-C2B	2.60	1.49	1.43
9	p	307	CLA	C3B-C4B	2.60	1.48	1.42
9	p	308	CLA	C3B-C4B	2.60	1.48	1.42
9	p	306	CLA	C3B-C4B	2.60	1.48	1.42
9	s	303	CLA	C1B-C2B	2.59	1.49	1.43
9	7	609	CLA	C1B-C2B	2.59	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	p	314	CLA	C1B-C2B	2.59	1.49	1.43
9	P	608	CLA	C1B-C2B	2.58	1.49	1.43
12	8	615	II0	C13-C09	-2.58	1.32	1.34
9	9	603	CLA	C3B-C4B	2.58	1.48	1.42
9	0	603	CLA	C1B-C2B	2.58	1.49	1.43
9	7	611	CLA	C3B-C4B	2.57	1.48	1.42
9	9	611	CLA	C1B-C2B	2.57	1.49	1.43
9	7	613	CLA	C1B-C2B	2.57	1.49	1.43
11	8	616	IHT	C02-C07	-2.56	1.50	1.53
9	9	605	CLA	C1B-C2B	2.56	1.49	1.43
10	0	610	KC2	C4B-NB	-2.56	1.34	1.37
9	0	613	CLA	C1B-C2B	2.55	1.49	1.43
9	7	605	CLA	C3B-C4B	2.55	1.48	1.42
9	7	603	CLA	C1B-C2B	2.54	1.49	1.43
9	p	311	CLA	C1B-C2B	2.53	1.49	1.43
9	p	305	CLA	C1B-C2B	2.53	1.49	1.43
9	0	602	CLA	C1B-C2B	2.53	1.49	1.43
9	p	306	CLA	C1B-C2B	2.53	1.49	1.43
9	7	612	CLA	C1B-C2B	2.52	1.49	1.43
9	9	610	CLA	C1B-C2B	2.52	1.49	1.43
9	8	609	CLA	C1B-C2B	2.52	1.49	1.43
9	8	611	CLA	C1B-C2B	2.52	1.49	1.43
9	0	606	CLA	C1B-C2B	2.52	1.49	1.43
9	7	611	CLA	C1B-C2B	2.51	1.49	1.43
9	9	601	CLA	C1B-C2B	2.51	1.49	1.43
9	9	607	CLA	C1B-C2B	2.51	1.49	1.43
9	8	601	CLA	C1B-C2B	2.51	1.49	1.43
9	P	601	CLA	C1B-C2B	2.51	1.49	1.43
9	8	605	CLA	C1B-C2B	2.50	1.49	1.43
9	p	303	CLA	C1B-C2B	2.50	1.49	1.43
9	0	607	CLA	C1B-C2B	2.50	1.49	1.43
9	9	603	CLA	C1B-C2B	2.48	1.49	1.43
9	7	602	CLA	C1B-C2B	2.48	1.49	1.43
9	7	604	CLA	C1B-C2B	2.47	1.49	1.43
9	9	609	CLA	C1B-C2B	2.47	1.49	1.43
9	P	602	CLA	C1B-C2B	2.47	1.49	1.43
9	s	302	CLA	MG-NB	-2.47	2.00	2.05
9	9	602	CLA	C1B-C2B	2.47	1.49	1.43
9	P	603	CLA	C1B-C2B	2.47	1.49	1.43
9	p	313	CLA	C1B-C2B	2.46	1.49	1.43
9	P	607	CLA	C1B-C2B	2.46	1.49	1.43
9	8	612	CLA	C1B-C2B	2.46	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	p	310	CLA	C1B-C2B	2.46	1.49	1.43
9	7	608	CLA	C1B-C2B	2.46	1.49	1.43
9	8	602	CLA	C3B-C4B	2.46	1.48	1.42
9	0	608	CLA	C1B-C2B	2.45	1.49	1.43
9	P	611	CLA	C1B-C2B	2.45	1.49	1.43
9	7	606	CLA	C3B-C4B	2.44	1.48	1.42
9	8	604	CLA	C1B-C2B	2.44	1.49	1.43
9	8	602	CLA	MG-NB	-2.44	2.01	2.05
9	p	308	CLA	C1B-C2B	2.43	1.49	1.43
9	8	606	CLA	C1B-C2B	2.43	1.49	1.43
9	7	605	CLA	C1B-C2B	2.43	1.49	1.43
9	p	309	CLA	C1B-C2B	2.43	1.49	1.43
9	P	601	CLA	MG-NB	-2.42	2.01	2.05
9	7	607	CLA	C1B-C2B	2.42	1.48	1.43
9	9	608	CLA	C1B-C2B	2.41	1.48	1.43
9	7	602	CLA	MG-NB	-2.41	2.01	2.05
9	8	603	CLA	MG-NB	-2.40	2.01	2.05
9	8	601	CLA	MG-NB	-2.40	2.01	2.05
9	P	610	CLA	C1B-C2B	2.40	1.48	1.43
9	p	304	CLA	C1B-C2B	2.40	1.48	1.43
11	0	617	IHT	C02-C07	-2.40	1.50	1.53
9	8	607	CLA	C1B-C2B	2.39	1.48	1.43
9	p	313	CLA	MG-NB	-2.39	2.01	2.05
9	8	603	CLA	C1B-C2B	2.39	1.48	1.43
16	9	615	8CT	C33-C32	-2.39	1.43	1.50
9	7	611	CLA	MG-NB	-2.38	2.01	2.05
9	P	604	CLA	C1B-C2B	2.38	1.48	1.43
9	9	602	CLA	MG-NB	-2.38	2.01	2.05
9	p	303	CLA	MG-NB	-2.38	2.01	2.05
9	P	610	CLA	MG-NB	-2.38	2.01	2.05
9	p	308	CLA	MG-NB	-2.38	2.01	2.05
9	9	604	CLA	C1B-C2B	2.38	1.48	1.43
10	8	610	KC2	C4A-C3A	-2.38	1.40	1.44
9	0	604	CLA	C1B-C2B	2.38	1.48	1.43
9	s	302	CLA	C1B-C2B	2.37	1.48	1.43
9	8	608	CLA	C1B-C2B	2.37	1.48	1.43
9	8	608	CLA	MG-NB	-2.37	2.01	2.05
10	8	610	KC2	C1D-ND	-2.36	1.34	1.37
9	9	608	CLA	MG-NB	-2.36	2.01	2.05
9	p	305	CLA	CMD-C2D	-2.35	1.45	1.50
10	8	610	KC2	C1C-C2C	-2.35	1.40	1.44
9	8	609	CLA	MG-NB	-2.35	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	p	312	KC2	C4A-C3A	-2.35	1.40	1.44
9	9	610	CLA	MG-NB	-2.35	2.01	2.05
9	8	611	CLA	MG-NB	-2.34	2.01	2.05
9	0	609	CLA	MG-NB	-2.34	2.01	2.05
9	7	606	CLA	MG-NB	-2.34	2.01	2.05
9	8	605	CLA	CMB-C2B	-2.33	1.45	1.50
9	9	603	CLA	MG-NB	-2.33	2.01	2.05
9	p	304	CLA	CHC-C1C	2.33	1.43	1.38
9	7	603	CLA	MG-NB	-2.33	2.01	2.05
9	p	309	CLA	MG-NB	-2.32	2.01	2.05
9	9	607	CLA	MG-NB	-2.32	2.01	2.05
9	p	307	CLA	CMB-C2B	-2.32	1.45	1.50
16	P	615	8CT	C33-C32	-2.32	1.44	1.50
9	p	306	CLA	MG-NB	-2.31	2.01	2.05
9	p	311	CLA	MG-NB	-2.31	2.01	2.05
9	8	602	CLA	C1B-C2B	2.31	1.48	1.43
9	8	604	CLA	MG-NB	-2.31	2.01	2.05
9	7	605	CLA	CMB-C2B	-2.31	1.45	1.50
9	P	610	CLA	CMD-C2D	-2.30	1.45	1.50
9	9	611	CLA	MG-NB	-2.29	2.01	2.05
9	7	607	CLA	MG-NB	-2.29	2.01	2.05
9	9	604	CLA	CHC-C1C	2.29	1.43	1.38
9	p	308	CLA	CMB-C2B	-2.29	1.46	1.50
9	P	608	CLA	MG-NB	-2.29	2.01	2.05
9	7	608	CLA	MG-NB	-2.28	2.01	2.05
9	7	605	CLA	MG-NB	-2.28	2.01	2.05
9	0	603	CLA	MG-NB	-2.27	2.01	2.05
13	8	617	LMG	O7-C8	-2.27	1.40	1.46
10	7	610	KC2	C4A-C3A	-2.27	1.40	1.44
9	9	609	CLA	MG-NB	-2.27	2.01	2.05
13	0	618	LMG	O7-C8	-2.26	1.40	1.46
9	8	605	CLA	MG-NB	-2.26	2.01	2.05
9	0	605	CLA	CMB-C2B	-2.26	1.46	1.50
9	P	602	CLA	MG-NB	-2.26	2.01	2.05
9	p	310	CLA	MG-NB	-2.26	2.01	2.05
9	P	602	CLA	CHC-C1C	2.26	1.43	1.38
9	9	606	CLA	CHC-C1C	2.26	1.43	1.38
9	7	607	CLA	CMD-C2D	-2.26	1.46	1.50
9	8	611	CLA	CMD-C2D	-2.26	1.46	1.50
9	7	604	CLA	MG-NB	-2.25	2.01	2.05
9	8	608	CLA	CMB-C2B	-2.25	1.46	1.50
9	0	613	CLA	MG-NB	-2.25	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	9	601	CLA	MG-NB	-2.25	2.01	2.05
9	P	604	CLA	MG-NB	-2.25	2.01	2.05
9	p	305	CLA	MG-NB	-2.25	2.01	2.05
9	P	611	CLA	MG-NB	-2.25	2.01	2.05
9	0	611	CLA	MG-NB	-2.25	2.01	2.05
9	P	603	CLA	CMD-C2D	-2.24	1.46	1.50
9	7	609	CLA	MG-NB	-2.24	2.01	2.05
9	0	602	CLA	MG-NB	-2.24	2.01	2.05
15	s	301	LHG	O7-C5	-2.23	1.41	1.46
10	7	610	KC2	C1C-C2C	-2.23	1.40	1.44
9	0	608	CLA	MG-NB	-2.23	2.01	2.05
9	8	601	CLA	CMD-C2D	-2.23	1.46	1.50
9	9	606	CLA	C1B-C2B	2.22	1.48	1.43
9	G	101	CLA	MG-NB	-2.22	2.01	2.05
9	9	606	CLA	MG-NB	-2.22	2.01	2.05
9	8	612	CLA	MG-NB	-2.21	2.01	2.05
9	8	607	CLA	MG-NB	-2.21	2.01	2.05
9	P	603	CLA	MG-NB	-2.21	2.01	2.05
9	8	609	CLA	CMD-C2D	-2.21	1.46	1.50
9	p	306	CLA	CMD-C2D	-2.21	1.46	1.50
9	9	606	CLA	CMD-C2D	-2.21	1.46	1.50
9	7	612	CLA	MG-NB	-2.21	2.01	2.05
9	8	606	CLA	MG-NB	-2.20	2.01	2.05
9	8	602	CLA	CMD-C2D	-2.20	1.46	1.50
9	0	607	CLA	MG-NB	-2.20	2.01	2.05
9	p	304	CLA	CMD-C2D	-2.20	1.46	1.50
9	0	613	CLA	CHC-C1C	2.20	1.43	1.38
9	8	602	CLA	CMB-C2B	-2.20	1.46	1.50
9	p	307	CLA	CMD-C2D	-2.20	1.46	1.50
9	8	606	CLA	CMB-C2B	-2.20	1.46	1.50
9	s	303	CLA	CHC-C1C	2.19	1.43	1.38
9	0	604	CLA	CHC-C1C	2.19	1.43	1.38
10	p	312	KC2	C1C-C2C	-2.19	1.40	1.44
9	7	606	CLA	CMD-C2D	-2.19	1.46	1.50
9	7	609	CLA	CMD-C2D	-2.19	1.46	1.50
9	P	608	CLA	CMD-C2D	-2.19	1.46	1.50
9	p	307	CLA	MG-NB	-2.19	2.01	2.05
9	0	606	CLA	MG-NB	-2.19	2.01	2.05
10	P	605	KC2	C4A-C3A	-2.18	1.40	1.44
9	P	607	CLA	MG-NB	-2.18	2.01	2.05
10	P	605	KC2	C1D-ND	-2.18	1.35	1.37
9	P	607	CLA	CMB-C2B	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	7	601	CLA	MG-NB	-2.18	2.01	2.05
9	p	309	CLA	CHC-C1C	2.18	1.42	1.38
9	7	604	CLA	CMD-C2D	-2.18	1.46	1.50
9	0	608	CLA	CMB-C2B	-2.18	1.46	1.50
9	9	606	CLA	CMB-C2B	-2.17	1.46	1.50
9	P	604	CLA	CMD-C2D	-2.17	1.46	1.50
9	0	602	CLA	CMD-C2D	-2.17	1.46	1.50
9	8	602	CLA	CMC-C2C	-2.17	1.46	1.50
9	G	101	CLA	CMD-C2D	-2.17	1.46	1.50
10	P	609	KC2	C1D-ND	-2.17	1.35	1.37
10	P	609	KC2	C4A-C3A	-2.17	1.40	1.44
9	P	603	CLA	CHC-C1C	2.17	1.42	1.38
9	0	602	CLA	CHC-C1C	2.17	1.42	1.38
9	7	609	CLA	CHC-C1C	2.17	1.42	1.38
17	p	319	SQD	C24-C23	2.17	1.59	1.51
9	7	603	CLA	CMD-C2D	-2.17	1.46	1.50
9	P	606	CLA	CHC-C1C	2.16	1.42	1.38
9	7	607	CLA	CMB-C2B	-2.16	1.46	1.50
9	0	605	CLA	MG-NB	-2.16	2.01	2.05
9	8	608	CLA	CMC-C2C	-2.16	1.46	1.50
9	9	601	CLA	CMD-C2D	-2.16	1.46	1.50
9	p	314	CLA	MG-NB	-2.16	2.01	2.05
9	8	612	CLA	CMB-C2B	-2.16	1.46	1.50
9	p	310	CLA	CMB-C2B	-2.16	1.46	1.50
9	p	304	CLA	MG-NB	-2.16	2.01	2.05
9	9	608	CLA	CMD-C2D	-2.16	1.46	1.50
9	8	606	CLA	CMD-C2D	-2.16	1.46	1.50
9	0	603	CLA	CMD-C2D	-2.16	1.46	1.50
9	9	604	CLA	MG-NB	-2.15	2.01	2.05
10	p	312	KC2	C1D-ND	-2.15	1.35	1.37
9	7	608	CLA	CMB-C2B	-2.15	1.46	1.50
9	P	606	CLA	CMD-C2D	-2.15	1.46	1.50
9	7	613	CLA	MG-NB	-2.15	2.01	2.05
9	7	612	CLA	CHC-C1C	2.15	1.42	1.38
9	p	310	CLA	CMD-C2D	-2.15	1.46	1.50
9	8	607	CLA	CMD-C2D	-2.15	1.46	1.50
9	9	605	CLA	MG-NB	-2.15	2.01	2.05
9	P	604	CLA	CMB-C2B	-2.15	1.46	1.50
9	9	609	CLA	CMB-C2B	-2.14	1.46	1.50
9	8	603	CLA	CMD-C2D	-2.14	1.46	1.50
9	9	607	CLA	CMB-C2B	-2.14	1.46	1.50
9	p	309	CLA	CMC-C2C	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	s	302	CLA	CHC-C1C	2.14	1.42	1.38
9	P	601	CLA	CMD-C2D	-2.14	1.46	1.50
10	P	605	KC2	C1C-C2C	-2.14	1.40	1.44
9	8	612	CLA	CMD-C2D	-2.14	1.46	1.50
9	8	607	CLA	CHC-C1C	2.14	1.42	1.38
9	9	603	CLA	CMB-C2B	-2.14	1.46	1.50
9	P	604	CLA	CMC-C2C	-2.14	1.46	1.50
9	7	612	CLA	CMB-C2B	-2.14	1.46	1.50
9	0	601	CLA	CHC-C1C	2.14	1.42	1.38
9	9	603	CLA	CMD-C2D	-2.14	1.46	1.50
9	0	601	CLA	MG-NB	-2.13	2.01	2.05
9	9	605	CLA	CHC-C1C	2.13	1.42	1.38
9	0	612	CLA	CHC-C1C	2.13	1.42	1.38
9	7	604	CLA	CMC-C2C	-2.13	1.46	1.50
9	p	303	CLA	CMD-C2D	-2.13	1.46	1.50
9	p	308	CLA	CMD-C2D	-2.13	1.46	1.50
9	0	607	CLA	CHC-C1C	2.13	1.42	1.38
9	p	304	CLA	CMB-C2B	-2.13	1.46	1.50
9	7	608	CLA	CMD-C2D	-2.13	1.46	1.50
9	9	610	CLA	CMD-C2D	-2.13	1.46	1.50
9	0	611	CLA	CHC-C1C	2.13	1.42	1.38
9	0	612	CLA	MG-NB	-2.13	2.01	2.05
9	p	309	CLA	CMD-C2D	-2.13	1.46	1.50
9	p	310	CLA	CHC-C1C	2.12	1.42	1.38
9	8	612	CLA	CMC-C2C	-2.12	1.46	1.50
9	0	604	CLA	CMB-C2B	-2.12	1.46	1.50
9	P	611	CLA	CMD-C2D	-2.12	1.46	1.50
9	0	604	CLA	CMD-C2D	-2.12	1.46	1.50
9	0	609	CLA	CMD-C2D	-2.12	1.46	1.50
9	0	604	CLA	MG-NB	-2.12	2.01	2.05
9	8	609	CLA	CHC-C1C	2.12	1.42	1.38
9	p	310	CLA	CMC-C2C	-2.12	1.46	1.50
9	p	313	CLA	CMB-C2B	-2.12	1.46	1.50
10	P	609	KC2	C1C-C2C	-2.12	1.40	1.44
9	P	607	CLA	CMD-C2D	-2.12	1.46	1.50
9	p	313	CLA	CMD-C2D	-2.12	1.46	1.50
9	8	601	CLA	CMB-C2B	-2.12	1.46	1.50
9	8	601	CLA	CMC-C2C	-2.12	1.46	1.50
9	P	610	CLA	CMB-C2B	-2.12	1.46	1.50
9	8	608	CLA	CMD-C2D	-2.12	1.46	1.50
9	P	602	CLA	CMC-C2C	-2.12	1.46	1.50
9	p	311	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	P	602	CLA	CMD-C2D	-2.11	1.46	1.50
17	p	319	SQD	O9-S	2.11	1.51	1.45
9	7	611	CLA	CMD-C2D	-2.11	1.46	1.50
9	s	302	CLA	CMB-C2B	-2.11	1.46	1.50
9	9	609	CLA	CMD-C2D	-2.11	1.46	1.50
9	8	604	CLA	CMD-C2D	-2.11	1.46	1.50
9	8	607	CLA	CMB-C2B	-2.11	1.46	1.50
9	p	311	CLA	CHC-C1C	2.11	1.42	1.38
9	9	604	CLA	CMB-C2B	-2.11	1.46	1.50
9	7	602	CLA	CMC-C2C	-2.11	1.46	1.50
9	0	609	CLA	CHC-C1C	2.11	1.42	1.38
9	0	607	CLA	CMD-C2D	-2.11	1.46	1.50
9	p	306	CLA	CMC-C2C	-2.11	1.46	1.50
9	9	602	CLA	CMC-C2C	-2.10	1.46	1.50
9	9	602	CLA	CMD-C2D	-2.10	1.46	1.50
9	P	608	CLA	CMB-C2B	-2.10	1.46	1.50
9	7	601	CLA	CHC-C1C	2.10	1.42	1.38
9	0	606	CLA	CMD-C2D	-2.10	1.46	1.50
9	7	611	CLA	CMB-C2B	-2.10	1.46	1.50
9	9	604	CLA	CMD-C2D	-2.10	1.46	1.50
9	0	605	CLA	CMD-C2D	-2.10	1.46	1.50
9	p	306	CLA	CMB-C2B	-2.10	1.46	1.50
9	p	303	CLA	CMB-C2B	-2.10	1.46	1.50
9	8	605	CLA	CMC-C2C	-2.10	1.46	1.50
9	7	608	CLA	CMC-C2C	-2.10	1.46	1.50
9	0	613	CLA	CMB-C2B	-2.10	1.46	1.50
9	8	611	CLA	CMB-C2B	-2.10	1.46	1.50
9	p	314	CLA	CHC-C1C	2.10	1.42	1.38
9	8	605	CLA	CMD-C2D	-2.10	1.46	1.50
9	8	609	CLA	CMB-C2B	-2.10	1.46	1.50
9	P	608	CLA	CHC-C1C	2.10	1.42	1.38
9	7	602	CLA	CMD-C2D	-2.09	1.46	1.50
9	0	607	CLA	CMB-C2B	-2.09	1.46	1.50
9	p	309	CLA	CMB-C2B	-2.09	1.46	1.50
9	9	609	CLA	CHC-C1C	2.09	1.42	1.38
9	8	604	CLA	CMB-C2B	-2.09	1.46	1.50
9	s	303	CLA	MG-NB	-2.09	2.01	2.05
9	p	305	CLA	CHC-C1C	2.09	1.42	1.38
9	9	611	CLA	CMB-C2B	-2.09	1.46	1.50
9	P	603	CLA	CMB-C2B	-2.09	1.46	1.50
9	7	612	CLA	CMD-C2D	-2.09	1.46	1.50
9	8	603	CLA	CMB-C2B	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	9	607	CLA	CMD-C2D	-2.09	1.46	1.50
9	P	602	CLA	CMB-C2B	-2.09	1.46	1.50
9	s	303	CLA	CMD-C2D	-2.09	1.46	1.50
9	9	602	CLA	CMB-C2B	-2.09	1.46	1.50
9	p	314	CLA	CMD-C2D	-2.08	1.46	1.50
10	8	610	KC2	C1B-NB	-2.08	1.35	1.37
9	0	613	CLA	CMD-C2D	-2.08	1.46	1.50
9	8	603	CLA	CMC-C2C	-2.08	1.46	1.50
9	9	611	CLA	CMD-C2D	-2.08	1.46	1.50
9	P	607	CLA	CHC-C1C	2.08	1.42	1.38
9	7	607	CLA	CHC-C1C	2.08	1.42	1.38
9	P	611	CLA	CMC-C2C	-2.08	1.46	1.50
9	7	602	CLA	CMB-C2B	-2.08	1.46	1.50
9	7	605	CLA	CMD-C2D	-2.08	1.46	1.50
9	0	608	CLA	CMD-C2D	-2.08	1.46	1.50
9	0	611	CLA	CMD-C2D	-2.08	1.46	1.50
9	7	613	CLA	CHC-C1C	2.08	1.42	1.38
9	7	607	CLA	CMC-C2C	-2.08	1.46	1.50
9	8	604	CLA	CMC-C2C	-2.08	1.46	1.50
9	0	608	CLA	CHC-C1C	2.08	1.42	1.38
9	p	313	CLA	CMC-C2C	-2.08	1.46	1.50
9	0	612	CLA	CMB-C2B	-2.07	1.46	1.50
9	p	305	CLA	CMC-C2C	-2.07	1.46	1.50
9	9	601	CLA	CHC-C1C	2.07	1.42	1.38
9	7	606	CLA	CMB-C2B	-2.07	1.46	1.50
9	P	611	CLA	CMB-C2B	-2.07	1.46	1.50
9	p	304	CLA	CMC-C2C	-2.07	1.46	1.50
9	p	305	CLA	CMB-C2B	-2.07	1.46	1.50
9	P	611	CLA	CHC-C1C	2.07	1.42	1.38
9	8	611	CLA	CMC-C2C	-2.07	1.46	1.50
9	9	607	CLA	CHC-C1C	2.07	1.42	1.38
9	0	603	CLA	CHC-C1C	2.07	1.42	1.38
9	G	101	CLA	CHC-C1C	2.07	1.42	1.38
9	9	608	CLA	CMB-C2B	-2.07	1.46	1.50
9	0	601	CLA	CMB-C2B	-2.06	1.46	1.50
9	9	604	CLA	CMC-C2C	-2.06	1.46	1.50
9	P	606	CLA	MG-NB	-2.06	2.01	2.05
9	8	612	CLA	CHC-C1C	2.06	1.42	1.38
9	9	607	CLA	CMC-C2C	-2.06	1.46	1.50
10	0	610	KC2	C4A-C3A	-2.06	1.40	1.44
9	9	611	CLA	CHC-C1C	2.06	1.42	1.38
9	7	604	CLA	CMB-C2B	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	7	608	CLA	CHC-C1C	2.06	1.42	1.38
9	9	608	CLA	CHC-C1C	2.06	1.42	1.38
9	9	602	CLA	CHC-C1C	2.06	1.42	1.38
9	7	604	CLA	CHC-C1C	2.06	1.42	1.38
10	0	610	KC2	C1C-C2C	-2.06	1.40	1.44
9	8	607	CLA	CMC-C2C	-2.06	1.46	1.50
9	9	605	CLA	CMB-C2B	-2.05	1.46	1.50
9	9	605	CLA	CMD-C2D	-2.05	1.46	1.50
9	9	610	CLA	CMB-C2B	-2.05	1.46	1.50
9	P	601	CLA	CMB-C2B	-2.05	1.46	1.50
10	7	610	KC2	C1D-ND	-2.05	1.35	1.37
9	P	608	CLA	CMC-C2C	-2.05	1.46	1.50
9	0	606	CLA	CHC-C1C	2.05	1.42	1.38
9	7	613	CLA	CMD-C2D	-2.05	1.46	1.50
9	7	603	CLA	CMB-C2B	-2.05	1.46	1.50
9	9	610	CLA	CMC-C2C	-2.05	1.46	1.50
9	0	602	CLA	CMB-C2B	-2.05	1.46	1.50
9	0	604	CLA	CMC-C2C	-2.04	1.46	1.50
9	7	613	CLA	CMB-C2B	-2.04	1.46	1.50
9	7	605	CLA	CMC-C2C	-2.04	1.46	1.50
9	8	609	CLA	CMC-C2C	-2.04	1.46	1.50
9	9	603	CLA	CMC-C2C	-2.04	1.46	1.50
9	9	606	CLA	CMC-C2C	-2.04	1.46	1.50
9	p	303	CLA	CMC-C2C	-2.04	1.46	1.50
9	0	603	CLA	CMB-C2B	-2.04	1.46	1.50
9	P	603	CLA	CMC-C2C	-2.04	1.46	1.50
17	p	319	SQD	O7-S	2.04	1.51	1.45
9	0	601	CLA	CMD-C2D	-2.04	1.46	1.50
9	0	603	CLA	CMC-C2C	-2.03	1.46	1.50
9	s	303	CLA	CMB-C2B	-2.03	1.46	1.50
9	G	101	CLA	CMC-C2C	-2.03	1.46	1.50
9	9	611	CLA	CMC-C2C	-2.03	1.46	1.50
9	p	307	CLA	CMC-C2C	-2.03	1.46	1.50
9	9	601	CLA	CMB-C2B	-2.03	1.46	1.50
9	p	311	CLA	CMB-C2B	-2.03	1.46	1.50
9	0	606	CLA	CMB-C2B	-2.03	1.46	1.50
9	P	610	CLA	CMC-C2C	-2.03	1.46	1.50
9	0	609	CLA	CMB-C2B	-2.03	1.46	1.50
9	8	606	CLA	CMC-C2C	-2.03	1.46	1.50
9	P	607	CLA	CMC-C2C	-2.03	1.46	1.50
9	p	308	CLA	CMC-C2C	-2.03	1.46	1.50
9	7	611	CLA	CHC-C1C	2.03	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	0	602	CLA	CMC-C2C	-2.02	1.46	1.50
9	p	314	CLA	CMB-C2B	-2.02	1.46	1.50
9	7	612	CLA	CMC-C2C	-2.02	1.46	1.50
9	7	601	CLA	CMD-C2D	-2.02	1.46	1.50
9	s	302	CLA	CMD-C2D	-2.02	1.46	1.50
9	P	604	CLA	CHC-C1C	2.02	1.42	1.38
10	0	610	KC2	C1D-ND	-2.02	1.35	1.37
9	0	605	CLA	CHC-C1C	2.02	1.42	1.38
9	p	313	CLA	CHC-C1C	2.02	1.42	1.38
9	P	601	CLA	CHC-C1C	2.02	1.42	1.38
9	8	603	CLA	CHC-C1C	2.02	1.42	1.38
9	9	601	CLA	CMC-C2C	-2.02	1.46	1.50
9	9	605	CLA	CMC-C2C	-2.02	1.46	1.50
9	7	603	CLA	CMC-C2C	-2.01	1.46	1.50
9	8	611	CLA	MG-ND	-2.01	2.01	2.05
9	P	610	CLA	MG-ND	-2.01	2.01	2.05
9	9	603	CLA	CHC-C1C	2.01	1.42	1.38
9	0	611	CLA	CMB-C2B	-2.01	1.46	1.50
9	7	602	CLA	CHC-C1C	2.01	1.42	1.38
9	0	613	CLA	CMC-C2C	-2.01	1.46	1.50
9	7	609	CLA	CMB-C2B	-2.00	1.46	1.50
9	p	303	CLA	CHC-C1C	2.00	1.42	1.38
9	9	609	CLA	CMC-C2C	-2.00	1.46	1.50
9	p	314	CLA	CMC-C2C	-2.00	1.46	1.50

All (881) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	9	615	8CT	C33-C32-C31	-8.64	116.57	124.85
16	P	615	8CT	C33-C32-C31	-8.01	117.17	124.85
10	0	610	KC2	CHB-C1B-NB	7.41	131.26	124.45
10	8	610	KC2	CHC-C4B-NB	7.14	131.02	124.45
10	8	610	KC2	CHB-C1B-NB	7.13	131.01	124.45
10	p	312	KC2	CHB-C1B-NB	7.07	130.95	124.45
9	7	604	CLA	C4A-NA-C1A	6.98	109.85	106.71
10	7	610	KC2	CHB-C1B-NB	6.95	130.84	124.45
9	8	611	CLA	C4A-NA-C1A	6.95	109.83	106.71
10	P	609	KC2	CHB-C1B-NB	6.94	130.84	124.45
10	P	605	KC2	CHB-C1B-NB	6.92	130.82	124.45
9	7	606	CLA	C4A-NA-C1A	6.86	109.79	106.71
16	9	615	8CT	C18-C17-C16	-6.85	117.54	127.31
9	p	306	CLA	C4A-NA-C1A	6.84	109.78	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	9	603	CLA	C4A-NA-C1A	6.84	109.78	106.71
9	9	609	CLA	C4A-NA-C1A	6.83	109.78	106.71
9	7	608	CLA	C4A-NA-C1A	6.82	109.77	106.71
9	0	608	CLA	C4A-NA-C1A	6.81	109.77	106.71
9	p	310	CLA	C4A-NA-C1A	6.80	109.76	106.71
9	7	611	CLA	C4A-NA-C1A	6.78	109.75	106.71
9	9	601	CLA	C4A-NA-C1A	6.77	109.75	106.71
9	9	607	CLA	C4A-NA-C1A	6.76	109.74	106.71
10	0	610	KC2	CHC-C4B-NB	6.74	130.65	124.45
16	9	615	8CT	C04-C03-C02	-6.73	113.13	122.61
9	P	607	CLA	C4A-NA-C1A	6.72	109.73	106.71
9	8	606	CLA	C4A-NA-C1A	6.72	109.73	106.71
10	P	609	KC2	CHC-C4B-NB	6.71	130.62	124.45
9	9	610	CLA	C4A-NA-C1A	6.70	109.72	106.71
9	P	604	CLA	C4A-NA-C1A	6.69	109.71	106.71
9	8	605	CLA	C4A-NA-C1A	6.67	109.70	106.71
9	0	605	CLA	C4A-NA-C1A	6.62	109.68	106.71
9	0	612	CLA	C4A-NA-C1A	6.62	109.68	106.71
9	p	307	CLA	C4A-NA-C1A	6.60	109.67	106.71
9	7	603	CLA	C4A-NA-C1A	6.59	109.67	106.71
9	8	601	CLA	C4A-NA-C1A	6.58	109.66	106.71
9	P	610	CLA	C4A-NA-C1A	6.56	109.66	106.71
9	p	309	CLA	C4A-NA-C1A	6.56	109.65	106.71
9	P	603	CLA	C4A-NA-C1A	6.56	109.65	106.71
9	s	303	CLA	C4A-NA-C1A	6.56	109.65	106.71
9	0	603	CLA	C4A-NA-C1A	6.53	109.64	106.71
9	7	613	CLA	C4A-NA-C1A	6.53	109.64	106.71
9	p	314	CLA	C4A-NA-C1A	6.52	109.64	106.71
9	G	101	CLA	C4A-NA-C1A	6.52	109.64	106.71
9	8	609	CLA	C4A-NA-C1A	6.50	109.63	106.71
9	8	608	CLA	C4A-NA-C1A	6.49	109.62	106.71
16	P	615	8CT	C14-C13-C12	-6.49	118.05	127.31
10	7	610	KC2	CHC-C4B-NB	6.48	130.41	124.45
9	9	611	CLA	C4A-NA-C1A	6.47	109.62	106.71
9	8	604	CLA	C4A-NA-C1A	6.45	109.61	106.71
9	9	604	CLA	C4A-NA-C1A	6.43	109.60	106.71
9	9	605	CLA	C4A-NA-C1A	6.41	109.59	106.71
9	0	601	CLA	C4A-NA-C1A	6.40	109.58	106.71
9	p	303	CLA	C4A-NA-C1A	6.39	109.58	106.71
9	0	611	CLA	C4A-NA-C1A	6.38	109.57	106.71
9	0	602	CLA	C4A-NA-C1A	6.37	109.57	106.71
9	7	609	CLA	C4A-NA-C1A	6.37	109.57	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	605	KC2	CHC-C4B-NB	6.37	130.30	124.45
9	7	612	CLA	C4A-NA-C1A	6.36	109.57	106.71
9	9	602	CLA	C4A-NA-C1A	6.36	109.56	106.71
9	p	313	CLA	C4A-NA-C1A	6.35	109.56	106.71
9	7	607	CLA	C4A-NA-C1A	6.33	109.55	106.71
9	9	608	CLA	C4A-NA-C1A	6.32	109.55	106.71
9	7	601	CLA	C4A-NA-C1A	6.30	109.54	106.71
9	p	308	CLA	C4A-NA-C1A	6.29	109.54	106.71
9	P	608	CLA	C4A-NA-C1A	6.29	109.53	106.71
9	8	602	CLA	C4A-NA-C1A	6.27	109.53	106.71
9	P	601	CLA	C4A-NA-C1A	6.27	109.53	106.71
10	p	312	KC2	CHC-C4B-NB	6.25	130.20	124.45
9	8	612	CLA	C4A-NA-C1A	6.23	109.51	106.71
9	7	605	CLA	C4A-NA-C1A	6.22	109.50	106.71
9	7	602	CLA	C4A-NA-C1A	6.18	109.49	106.71
9	0	609	CLA	C4A-NA-C1A	6.15	109.47	106.71
9	0	607	CLA	C4A-NA-C1A	6.11	109.45	106.71
9	P	611	CLA	C4A-NA-C1A	6.10	109.45	106.71
9	0	606	CLA	C4A-NA-C1A	6.09	109.44	106.71
9	8	607	CLA	C4A-NA-C1A	6.08	109.44	106.71
9	p	305	CLA	C4A-NA-C1A	6.05	109.43	106.71
9	0	613	CLA	C4A-NA-C1A	6.00	109.40	106.71
9	8	603	CLA	C4A-NA-C1A	5.98	109.40	106.71
9	0	604	CLA	C4A-NA-C1A	5.97	109.39	106.71
9	p	311	CLA	C4A-NA-C1A	5.93	109.37	106.71
9	P	606	CLA	C4A-NA-C1A	5.91	109.36	106.71
9	P	602	CLA	C4A-NA-C1A	5.86	109.34	106.71
9	p	304	CLA	C4A-NA-C1A	5.86	109.34	106.71
9	9	606	CLA	C4A-NA-C1A	5.74	109.29	106.71
11	0	617	IHT	C40-C37-C33	-5.66	119.23	127.31
9	s	302	CLA	C4A-NA-C1A	5.63	109.23	106.71
16	P	615	8CT	C18-C17-C16	-5.57	119.36	127.31
16	9	615	8CT	C14-C13-C12	-5.34	119.68	127.31
11	0	617	IHT	C41-C38-C35	-5.30	119.75	127.31
10	p	312	KC2	O2D-CGD-CBD	5.28	120.65	111.27
16	9	615	8CT	C07-C02-C03	-5.24	115.12	122.73
11	8	616	IHT	C18-C22-C23	-5.23	118.33	126.23
12	9	613	II0	C42-C40-C36	-5.20	119.89	127.31
12	0	615	II0	C42-C40-C36	-5.18	119.92	127.31
11	7	618	IHT	C41-C38-C35	-5.10	120.03	127.31
11	p	318	IHT	C41-C38-C35	-5.10	120.04	127.31
12	p	317	II0	C42-C40-C36	-5.06	120.09	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	9	615	8CT	C01-C02-C03	-5.04	118.87	124.53
12	8	615	II0	C03-C09-C13	-5.00	115.57	122.63
16	9	615	8CT	C24-C25-C26	-4.97	120.21	127.31
12	P	612	II0	C41-C39-C35	-4.96	120.23	127.31
10	P	605	KC2	O2D-CGD-CBD	4.95	120.07	111.27
16	P	615	8CT	C24-C25-C26	-4.92	120.29	127.31
12	p	315	II0	C41-C39-C35	-4.91	120.31	127.31
11	8	616	IHT	C30-C27-C23	-4.87	120.37	127.31
12	8	614	II0	C42-C40-C36	-4.86	120.38	127.31
10	7	610	KC2	O2D-CGD-CBD	4.82	119.84	111.27
11	8	616	IHT	C41-C38-C35	-4.81	120.45	127.31
10	P	609	KC2	O2D-CGD-CBD	4.73	119.67	111.27
12	7	616	II0	C42-C40-C36	-4.72	120.57	127.31
12	7	614	II0	C41-C39-C35	-4.72	120.58	127.31
10	0	610	KC2	CHD-C1D-ND	4.72	129.25	124.26
10	P	609	KC2	CHD-C1D-ND	4.70	129.24	124.26
10	0	610	KC2	O2D-CGD-CBD	4.70	119.62	111.27
11	7	618	IHT	C30-C27-C23	-4.68	120.64	127.31
11	0	614	IHT	C41-C38-C35	-4.66	120.66	127.31
16	P	615	8CT	C04-C03-C02	-4.66	116.05	122.61
10	p	312	KC2	CHD-C1D-ND	4.66	129.19	124.26
12	p	301	II0	C41-C39-C35	-4.63	120.71	127.31
12	8	613	II0	C41-C39-C35	-4.61	120.73	127.31
16	P	615	8CT	C10-C11-C12	-4.60	119.28	126.23
12	0	616	II0	C41-C39-C35	-4.59	120.76	127.31
11	0	614	IHT	C19-C10-C07	-4.57	119.39	124.53
11	0	617	IHT	C18-C22-C23	-4.53	119.39	126.23
16	P	615	8CT	C01-C02-C03	-4.53	119.44	124.53
16	P	615	8CT	C07-C02-C03	-4.53	116.16	122.73
12	9	612	II0	C41-C39-C35	-4.52	120.86	127.31
11	7	618	IHT	C18-C22-C23	-4.48	119.46	126.23
12	7	617	II0	C42-C40-C36	-4.48	120.92	127.31
12	8	619	II0	C42-C40-C36	-4.47	120.93	127.31
11	0	617	IHT	C19-C10-C07	-4.47	119.51	124.53
10	7	610	KC2	CHD-C1D-ND	4.45	128.97	124.26
12	8	615	II0	C42-C40-C36	-4.44	120.97	127.31
12	7	616	II0	C41-C39-C35	-4.44	120.98	127.31
12	p	302	II0	C42-C40-C36	-4.42	121.00	127.31
12	p	301	II0	C42-C40-C36	-4.41	121.02	127.31
10	8	610	KC2	CHD-C1D-ND	4.33	128.84	124.26
11	8	616	IHT	C19-C10-C07	-4.32	119.68	124.53
15	s	301	LHG	O4-P-O5	4.16	132.83	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	8	618	LHG	O4-P-O5	4.16	132.81	112.24
10	P	605	KC2	C4B-CHC-C1C	-4.14	117.12	126.06
12	8	619	II0	C41-C39-C35	-4.14	121.40	127.31
14	7	615	II3	C39-C36-C33	-4.10	121.46	127.31
10	8	610	KC2	C4B-CHC-C1C	-4.10	117.22	126.06
12	8	613	II0	C42-C40-C36	-4.09	121.48	127.31
17	p	319	SQD	O47-C7-C8	4.07	120.27	111.50
10	P	609	KC2	C4B-CHC-C1C	-4.04	117.33	126.06
12	0	619	II0	C42-C40-C36	-4.02	121.57	127.31
12	p	302	II0	C20-C14-C10	-4.00	118.92	124.35
12	9	614	II0	C42-C40-C36	-3.98	121.64	127.31
11	8	616	IHT	C40-C37-C33	-3.97	121.64	127.31
10	0	610	KC2	C4B-CHC-C1C	-3.97	117.50	126.06
10	p	312	KC2	C1D-CHD-C4C	-3.96	116.95	126.34
11	p	318	IHT	C18-C22-C23	-3.95	120.27	126.23
10	P	605	KC2	CHD-C1D-ND	3.94	128.43	124.26
10	8	610	KC2	O1D-CGD-CBD	-3.92	116.46	124.48
10	7	610	KC2	C4B-CHC-C1C	-3.91	117.61	126.06
12	P	614	II0	C42-C40-C36	-3.91	121.73	127.31
14	P	613	II3	C39-C36-C33	-3.90	121.75	127.31
12	7	616	II0	C20-C14-C10	-3.88	119.07	124.35
10	0	610	KC2	C1D-CHD-C4C	-3.88	117.13	126.34
12	0	616	II0	C42-C40-C36	-3.88	121.78	127.31
10	p	312	KC2	C4B-CHC-C1C	-3.85	117.76	126.06
10	7	610	KC2	C1D-CHD-C4C	-3.82	117.27	126.34
10	P	605	KC2	C1D-CHD-C4C	-3.82	117.28	126.34
12	7	617	II0	C41-C39-C35	-3.82	121.86	127.31
10	P	609	KC2	C1D-CHD-C4C	-3.82	117.28	126.34
12	8	619	II0	C20-C14-C10	-3.81	119.17	124.35
16	P	615	8CT	C19-C20-C21	-3.80	121.88	127.31
12	p	302	II0	C41-C39-C35	-3.79	121.90	127.31
12	8	615	II0	C19-C13-C11	3.79	121.38	114.36
12	p	315	II0	C19-C13-C09	-3.76	119.25	124.35
12	p	301	II0	C19-C13-C09	-3.74	119.26	124.35
12	p	316	II0	C42-C40-C36	-3.73	121.98	127.31
14	P	613	II3	C22-C18-C16	-3.73	119.29	124.35
12	p	302	II0	C03-C09-C13	-3.72	117.39	122.63
11	p	318	IHT	C19-C10-C07	-3.70	120.37	124.53
16	9	615	8CT	C19-C20-C21	-3.70	122.03	127.31
12	8	613	II0	C19-C13-C09	-3.70	119.33	124.35
10	8	610	KC2	CHC-C4B-C3B	-3.69	118.94	125.26
12	8	613	II0	C20-C14-C10	-3.69	119.34	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	0	614	IHT	C20-C15-C11	-3.69	119.34	124.35
17	p	319	SQD	O7-S-C6	3.68	111.31	106.94
11	7	618	IHT	C40-C37-C33	-3.67	122.08	127.31
12	8	615	II0	C20-C14-C10	-3.66	119.37	124.35
12	P	614	II0	C19-C13-C09	-3.66	119.38	124.35
10	8	610	KC2	C1D-CHD-C4C	-3.65	117.68	126.34
17	p	319	SQD	O9-S-O7	-3.64	101.36	113.95
12	7	619	II0	C42-C40-C36	-3.63	122.13	127.31
12	0	615	II0	C19-C13-C09	-3.59	119.47	124.35
12	7	619	II0	C20-C14-C10	-3.59	119.47	124.35
12	9	614	II0	C41-C39-C35	-3.58	122.21	127.31
12	9	612	II0	C20-C14-C10	-3.57	119.50	124.35
12	0	616	II0	C20-C14-C10	-3.55	119.52	124.35
12	P	612	II0	C20-C14-C10	-3.54	119.53	124.35
10	P	605	KC2	C1D-ND-C4D	3.54	108.85	106.33
16	9	615	8CT	C11-C10-C03	-3.54	117.26	127.20
14	7	615	II3	C41-C40-C38	-3.52	122.28	127.31
10	P	609	KC2	CHC-C4B-C3B	-3.50	119.27	125.26
12	8	615	II0	C41-C39-C35	-3.50	122.31	127.31
10	7	610	KC2	CHC-C4B-C3B	-3.49	119.28	125.26
12	0	619	II0	C03-C09-C13	-3.49	117.70	122.63
11	0	617	IHT	C20-C15-C11	-3.49	119.61	124.35
12	P	612	II0	C19-C13-C09	-3.49	119.61	124.35
11	0	617	IHT	C30-C27-C23	-3.48	122.35	127.31
12	7	619	II0	C41-C39-C35	-3.48	122.35	127.31
12	9	612	II0	C42-C40-C36	-3.47	122.36	127.31
12	9	613	II0	C19-C13-C09	-3.46	119.64	124.35
12	7	614	II0	C19-C13-C09	-3.45	119.66	124.35
16	P	615	8CT	C01-C02-C07	3.45	120.24	113.62
12	P	614	II0	C41-C39-C35	-3.44	122.39	127.31
11	8	616	IHT	C20-C15-C11	-3.44	119.68	124.35
14	7	615	II3	C22-C18-C16	-3.43	119.68	124.35
11	7	618	IHT	C19-C10-C07	-3.42	120.69	124.53
10	0	610	KC2	CHC-C4B-C3B	-3.41	119.43	125.26
12	p	315	II0	C42-C40-C36	-3.41	122.45	127.31
12	9	614	II0	C19-C13-C09	-3.39	119.74	124.35
11	p	318	IHT	C20-C15-C11	-3.39	119.74	124.35
17	p	319	SQD	O48-C23-C24	3.39	120.26	111.38
10	0	610	KC2	CHB-C1B-C2B	-3.38	118.38	125.48
10	0	610	KC2	C1A-NA-C4A	-3.38	105.19	106.71
12	7	614	II0	C42-C40-C36	-3.37	122.50	127.31
11	0	614	IHT	C40-C37-C33	-3.37	122.50	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	7	618	IHT	C06-C09-C10	-3.35	108.09	114.08
9	P	610	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
12	9	613	II0	C06-C08-C12	-3.35	105.72	110.30
12	9	612	II0	C19-C13-C09	-3.35	119.80	124.35
12	p	315	II0	C20-C14-C10	-3.35	119.80	124.35
10	p	312	KC2	CHB-C1B-C2B	-3.34	118.47	125.48
12	8	614	II0	C20-C14-C10	-3.34	119.81	124.35
12	p	316	II0	C19-C13-C09	-3.34	119.82	124.35
12	P	614	II0	C20-C14-C12	3.33	120.53	114.36
12	P	612	II0	C42-C40-C36	-3.33	122.56	127.31
12	7	614	II0	C20-C14-C10	-3.32	119.83	124.35
12	7	619	II0	C19-C13-C09	-3.32	119.84	124.35
9	9	604	CLA	C3B-C4B-NB	-3.31	107.44	110.52
12	8	619	II0	C19-C13-C09	-3.30	119.86	124.35
16	9	615	8CT	C35-C30-C31	3.30	117.32	111.42
9	8	603	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
10	7	610	KC2	CHB-C1B-C2B	-3.27	118.61	125.48
12	0	619	II0	C20-C14-C10	-3.27	119.90	124.35
9	9	609	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
11	p	318	IHT	C40-C37-C33	-3.27	122.65	127.31
17	p	319	SQD	O9-S-C6	3.26	110.82	106.94
12	0	616	II0	C19-C13-C11	3.24	120.36	114.36
9	p	305	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
12	p	317	II0	C41-C39-C35	-3.24	122.69	127.31
10	8	610	KC2	CHB-C1B-C2B	-3.23	118.70	125.48
9	p	308	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
9	7	604	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
12	p	317	II0	C19-C13-C09	-3.23	119.96	124.35
11	7	618	IHT	C20-C15-C11	-3.22	119.97	124.35
9	0	604	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
9	8	602	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
9	p	313	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
10	p	312	KC2	CHC-C4B-C3B	-3.20	119.78	125.26
12	p	315	II0	C05-C07-C11	-3.20	105.92	110.30
9	P	603	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
12	7	617	II0	C19-C13-C11	3.19	120.26	114.36
10	8	610	KC2	C1D-ND-C4D	3.18	108.60	106.33
9	0	612	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
9	P	611	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
12	7	616	II0	C19-C13-C09	-3.18	120.03	124.35
11	0	614	IHT	C18-C22-C23	-3.18	121.44	126.23
10	P	605	KC2	C2D-C1D-ND	-3.17	108.11	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	8	615	II0	C07-C11-C13	-3.17	105.55	111.85
12	0	619	II0	C19-C13-C11	3.16	120.22	114.36
9	0	608	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
10	0	610	KC2	C1D-ND-C4D	3.15	108.58	106.33
12	9	613	II0	C20-C14-C10	-3.15	120.06	124.35
10	P	609	KC2	CHB-C1B-C2B	-3.15	118.87	125.48
12	p	301	II0	C06-C08-C12	-3.15	105.99	110.30
12	7	617	II0	C20-C14-C10	-3.14	120.08	124.35
9	0	604	CLA	C3B-C4B-NB	-3.13	107.61	110.52
10	8	610	KC2	O2D-CGD-CBD	3.13	116.83	111.27
9	9	606	CLA	C3B-C4B-NB	-3.13	107.61	110.52
9	P	604	CLA	C3B-C4B-NB	-3.13	107.61	110.52
12	0	616	II0	C41-C42-C40	-3.13	117.07	123.47
12	9	614	II0	C20-C14-C10	-3.13	120.10	124.35
12	8	614	II0	C19-C13-C09	-3.12	120.11	124.35
9	p	305	CLA	C1-C2-C3	-3.12	121.70	126.75
12	0	615	II0	C20-C14-C10	-3.12	120.11	124.35
9	8	607	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
10	P	605	KC2	CHC-C4B-C3B	-3.11	119.94	125.26
9	9	602	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
9	P	604	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
12	p	316	II0	C41-C39-C35	-3.09	122.89	127.31
9	8	604	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
12	8	614	II0	C06-C08-C12	-3.08	106.09	110.30
12	8	614	II0	C41-C39-C35	-3.08	122.92	127.31
12	9	614	II0	C05-C07-C11	-3.07	106.11	110.30
9	8	609	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
14	7	615	II3	C29-C26-C24	-3.05	122.95	127.31
12	P	612	II0	C05-C07-C11	-3.04	106.14	110.30
12	P	612	II0	C06-C08-C12	-3.04	106.14	110.30
9	0	613	CLA	C3B-C4B-NB	-3.04	107.69	110.52
9	9	604	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
9	7	605	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
9	p	310	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
10	P	605	KC2	CHB-C1B-C2B	-3.03	119.13	125.48
12	7	614	II0	C06-C08-C12	-3.02	106.16	110.30
9	7	612	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
9	P	601	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
16	9	615	8CT	C10-C11-C12	-3.02	121.68	126.23
12	0	615	II0	C41-C39-C35	-3.02	123.01	127.31
12	7	617	II0	C19-C13-C09	-3.01	120.25	124.35
12	8	614	II0	C05-C07-C11	-3.01	106.19	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	s	302	CLA	C3B-C4B-NB	-3.00	107.73	110.52
12	7	619	II0	C05-C07-C11	-3.00	106.20	110.30
9	9	610	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
9	8	603	CLA	C3B-C4B-NB	-3.00	107.73	110.52
9	8	605	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
10	7	610	KC2	C1D-ND-C4D	3.00	108.46	106.33
12	p	317	II0	C20-C14-C10	-2.99	120.28	124.35
9	p	303	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
9	0	601	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
9	7	608	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
9	P	602	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
9	8	608	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
11	p	318	IHT	C30-C27-C23	-2.97	123.07	127.31
12	9	613	II0	C42-C41-C39	-2.97	117.39	123.47
9	0	603	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
9	0	602	CLA	C3B-C4B-NB	-2.96	107.77	110.52
9	8	601	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
16	9	615	8CT	C18-C19-C20	-2.96	117.41	123.47
9	P	607	CLA	C3B-C4B-NB	-2.96	107.77	110.52
10	p	312	KC2	C1D-ND-C4D	2.96	108.44	106.33
10	P	609	KC2	C1D-ND-C4D	2.95	108.43	106.33
13	G	103	LMG	O6-C1-O1	-2.95	102.99	109.97
12	7	617	II0	C06-C08-C12	-2.95	106.27	110.30
12	8	613	II0	C05-C07-C11	-2.95	106.27	110.30
10	0	610	KC2	C2D-C1D-ND	-2.94	108.26	110.23
11	7	618	IHT	C20-C15-C12	2.94	119.80	114.36
9	8	606	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
9	7	607	CLA	C3B-C4B-NB	-2.94	107.79	110.52
12	p	315	II0	C06-C08-C12	-2.94	106.28	110.30
9	p	306	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
16	9	615	8CT	C01-C02-C07	2.93	119.24	113.62
12	0	616	II0	C19-C13-C09	-2.92	120.38	124.35
9	8	611	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
9	9	611	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
9	7	603	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
10	8	610	KC2	O2D-CGD-O1D	-2.92	118.13	123.84
11	0	617	IHT	C19-C10-C09	2.92	119.22	113.62
9	P	610	CLA	C3B-C4B-NB	-2.91	107.81	110.52
9	p	304	CLA	C3B-C4B-NB	-2.91	107.81	110.52
12	0	619	II0	C19-C13-C09	-2.91	120.40	124.35
9	9	608	CLA	CAA-C2A-C3A	-2.90	109.32	116.10
12	p	301	II0	C20-C14-C10	-2.90	120.41	124.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	p	304	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
12	0	619	II0	C41-C39-C35	-2.90	123.17	127.31
9	P	608	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
12	p	316	II0	C20-C14-C10	-2.90	120.41	124.35
10	p	312	KC2	C1A-NA-C4A	-2.89	105.41	106.71
9	9	602	CLA	C3B-C4B-NB	-2.89	107.83	110.52
9	p	310	CLA	C3B-C4B-NB	-2.89	107.83	110.52
9	0	613	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
9	7	607	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
9	s	303	CLA	C3B-C4B-NB	-2.88	107.84	110.52
9	7	602	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
9	s	303	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
9	P	602	CLA	C3B-C4B-NB	-2.88	107.84	110.52
11	8	616	IHT	C19-C10-C09	2.88	119.15	113.62
9	s	302	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
9	9	603	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
9	p	314	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
12	p	317	II0	C20-C14-C12	2.87	119.67	114.36
9	s	302	CLA	CHB-C1B-NB	2.86	127.29	124.26
12	7	616	II0	C19-C13-C11	2.86	119.66	114.36
9	8	612	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
12	p	302	II0	C19-C13-C09	-2.86	120.46	124.35
12	P	614	II0	C20-C14-C10	-2.86	120.47	124.35
12	p	302	II0	C19-C13-C11	2.86	119.65	114.36
9	9	608	CLA	C3B-C4B-NB	-2.85	107.87	110.52
9	9	601	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
13	8	617	LMG	O6-C1-O1	-2.85	103.22	109.97
12	9	612	II0	C05-C07-C11	-2.85	106.41	110.30
17	p	319	SQD	O8-S-C6	2.85	110.28	105.74
9	9	605	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
9	P	603	CLA	C3B-C4B-NB	-2.84	107.88	110.52
9	0	602	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
10	7	610	KC2	C2D-C1D-ND	-2.83	108.34	110.23
9	8	607	CLA	C3B-C4B-NB	-2.83	107.89	110.52
9	9	609	CLA	C3B-C4B-NB	-2.83	107.89	110.52
10	8	610	KC2	C2D-C1D-ND	-2.82	108.34	110.23
12	0	616	II0	C20-C14-C12	2.82	119.58	114.36
12	7	619	II0	C06-C08-C12	-2.82	106.44	110.30
11	8	616	IHT	C05-C08-C12	-2.82	106.44	110.30
9	p	311	CLA	C3B-C4B-NB	-2.82	107.90	110.52
9	0	606	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
9	p	309	CLA	C3B-C4B-NB	-2.81	107.91	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	8	610	KC2	C1A-NA-C4A	-2.81	105.44	106.71
9	P	608	CLA	C3B-C4B-NB	-2.81	107.91	110.52
10	P	609	KC2	C1A-NA-C4A	-2.80	105.44	106.71
9	7	602	CLA	C3B-C4B-NB	-2.80	107.91	110.52
16	9	615	8CT	C35-C30-C29	-2.80	109.16	112.70
9	0	611	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
9	0	609	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
9	P	607	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
9	G	101	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
12	8	615	II0	C32-C34-C36	-2.80	118.56	126.42
9	p	313	CLA	C3B-C4B-NB	-2.80	107.92	110.52
11	p	318	IHT	C20-C15-C12	2.79	119.53	114.36
12	p	316	II0	C05-C07-C11	-2.79	106.48	110.30
9	7	604	CLA	C3B-C4B-NB	-2.79	107.93	110.52
9	P	611	CLA	C3B-C4B-NB	-2.79	107.93	110.52
14	P	613	II3	C39-C41-C40	-2.79	117.76	123.47
9	7	609	CLA	C3B-C4B-NB	-2.79	107.93	110.52
9	0	605	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
9	9	601	CLA	C3B-C4B-NB	-2.79	107.93	110.52
9	8	609	CLA	C3B-C4B-NB	-2.78	107.94	110.52
9	7	611	CLA	C3B-C4B-NB	-2.77	107.94	110.52
12	p	317	II0	C32-C34-C36	-2.77	118.62	126.42
9	7	606	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
9	P	601	CLA	C3B-C4B-NB	-2.77	107.95	110.52
16	P	615	8CT	C40-C12-C13	-2.77	119.05	122.92
12	8	613	II0	C06-C08-C12	-2.77	106.52	110.30
12	9	612	II0	C06-C08-C12	-2.77	106.52	110.30
14	7	615	II3	C05-C06-C10	-2.76	108.60	111.74
9	0	609	CLA	C3B-C4B-NB	-2.76	107.95	110.52
11	0	614	IHT	C30-C27-C23	-2.76	123.37	127.31
9	8	608	CLA	C3B-C4B-NB	-2.76	107.96	110.52
9	9	605	CLA	C3B-C4B-NB	-2.75	107.96	110.52
16	P	615	8CT	C35-C30-C31	2.75	116.35	111.42
9	p	311	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
9	p	306	CLA	C3B-C4B-NB	-2.75	107.97	110.52
9	7	609	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
13	0	618	LMG	O6-C1-O1	-2.74	103.48	109.97
9	7	608	CLA	C3B-C4B-NB	-2.74	107.97	110.52
9	8	604	CLA	C3B-C4B-NB	-2.74	107.98	110.52
12	0	619	II0	C06-C08-C12	-2.74	106.56	110.30
9	9	606	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
10	p	312	KC2	CHD-C4C-NC	2.73	128.34	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	0	608	CLA	C3B-C4B-NB	-2.73	107.99	110.52
9	8	602	CLA	C3B-C4B-NB	-2.72	107.99	110.52
13	G	103	LMG	O1-C1-C2	-2.72	104.05	108.30
9	7	601	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
11	p	318	IHT	C31-C34-C35	-2.71	118.80	126.42
10	7	610	KC2	C1A-NA-C4A	-2.71	105.49	106.71
9	p	305	CLA	C3B-C4B-NB	-2.71	108.00	110.52
9	7	613	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
9	p	303	CLA	C3B-C4B-NB	-2.71	108.00	110.52
9	0	607	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
9	7	612	CLA	C3B-C4B-NB	-2.70	108.01	110.52
9	7	611	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
9	0	601	CLA	C3B-C4B-NB	-2.70	108.01	110.52
9	9	610	CLA	C3B-C4B-NB	-2.70	108.01	110.52
10	p	312	KC2	CBD-CHA-C1A	2.70	133.91	128.88
11	7	618	IHT	C19-C10-C09	2.69	118.79	113.62
12	p	301	II0	C05-C07-C11	-2.69	106.62	110.30
9	9	608	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
9	P	603	CLA	C1-C2-C3	-2.69	122.41	126.75
12	p	302	II0	C32-C30-C26	-2.68	118.79	126.58
16	P	615	8CT	C18-C19-C20	-2.68	117.98	123.47
9	9	607	CLA	C3B-C4B-NB	-2.68	108.03	110.52
9	9	611	CLA	C3B-C4B-NB	-2.67	108.03	110.52
10	P	605	KC2	CBD-CHA-C1A	2.67	133.86	128.88
10	7	610	KC2	O1D-CGD-CBD	-2.67	119.02	124.48
9	7	609	CLA	CAA-C2A-C3A	-2.67	109.87	116.10
9	9	602	CLA	C1-C2-C3	-2.67	121.43	126.04
9	9	603	CLA	C3B-C4B-NB	-2.67	108.04	110.52
9	8	605	CLA	C3B-C4B-NB	-2.66	108.04	110.52
12	P	614	II0	C04-C10-C14	-2.66	118.87	122.63
12	9	614	II0	C06-C08-C12	-2.66	106.66	110.30
11	0	614	IHT	C05-C08-C12	-2.66	106.66	110.30
9	9	607	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
10	P	609	KC2	C2D-C1D-ND	-2.65	108.45	110.23
12	7	614	II0	C05-C07-C11	-2.65	106.68	110.30
15	8	618	LHG	O8-C23-C24	2.65	120.22	111.91
12	7	619	II0	C20-C14-C12	2.64	119.25	114.36
15	s	301	LHG	O8-C23-C24	2.64	120.20	111.91
9	8	608	CLA	CHB-C4A-NA	2.64	128.16	124.51
10	7	610	KC2	CBD-CHA-C1A	2.64	133.80	128.88
9	9	603	CLA	CHB-C4A-NA	2.63	128.16	124.51
9	P	607	CLA	CHB-C4A-NA	2.63	128.16	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	p	312	KC2	C2D-C1D-ND	-2.63	108.47	110.23
10	8	610	KC2	CBD-CHA-C1A	2.63	133.79	128.88
9	p	308	CLA	C3B-C4B-NB	-2.63	108.07	110.52
9	8	612	CLA	C3B-C4B-NB	-2.63	108.07	110.52
9	0	602	CLA	CHB-C4A-NA	2.63	128.15	124.51
10	P	609	KC2	O1D-CGD-CBD	-2.63	119.11	124.48
12	P	614	II0	C05-C07-C11	-2.63	106.71	110.30
9	0	608	CLA	CHB-C4A-NA	2.62	128.14	124.51
9	0	612	CLA	C3B-C4B-NB	-2.62	108.09	110.52
14	P	613	II3	C05-C06-C10	-2.61	108.77	111.74
9	p	311	CLA	CAA-C2A-C3A	-2.61	110.00	116.10
9	P	604	CLA	CHB-C4A-NA	2.61	128.12	124.51
10	0	610	KC2	CHD-C4C-NC	2.60	128.15	124.20
12	0	616	II0	C31-C29-C25	-2.60	119.03	126.58
9	8	611	CLA	CHB-C4A-NA	2.60	128.10	124.51
12	8	614	II0	C42-C41-C39	-2.59	118.17	123.47
13	G	102	LMG	O6-C1-O1	-2.59	103.84	109.97
9	0	612	CLA	CHB-C4A-NA	2.59	128.09	124.51
16	9	615	8CT	C39-C16-C17	-2.59	119.30	122.92
12	8	619	II0	C19-C13-C11	2.59	119.15	114.36
12	p	317	II0	C19-C13-C11	2.58	119.14	114.36
16	9	615	8CT	C13-C14-C15	-2.58	115.15	123.22
15	s	301	LHG	C11-C10-C9	-2.58	101.31	114.42
9	8	601	CLA	C3B-C4B-NB	-2.58	108.12	110.52
9	p	309	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
9	7	606	CLA	CHB-C4A-NA	2.58	128.08	124.51
9	7	601	CLA	C3B-C4B-NB	-2.58	108.12	110.52
12	0	615	II0	C05-C07-C11	-2.58	106.78	110.30
12	0	615	II0	C06-C08-C12	-2.58	106.78	110.30
9	9	610	CLA	CHB-C4A-NA	2.58	128.07	124.51
9	p	309	CLA	CHB-C4A-NA	2.57	128.07	124.51
9	7	604	CLA	CHB-C4A-NA	2.57	128.07	124.51
9	8	611	CLA	C3B-C4B-NB	-2.57	108.13	110.52
12	0	616	II0	C31-C33-C35	-2.57	119.20	126.42
9	9	607	CLA	CHB-C4A-NA	2.57	128.06	124.51
12	9	613	II0	C05-C07-C11	-2.57	106.79	110.30
9	0	611	CLA	C3B-C4B-NB	-2.57	108.14	110.52
9	7	611	CLA	CHB-C4A-NA	2.56	128.06	124.51
9	p	307	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
12	P	614	II0	C31-C29-C25	-2.56	119.16	126.58
11	0	617	IHT	C05-C08-C12	-2.54	106.82	110.30
9	0	603	CLA	C3B-C4B-NB	-2.54	108.16	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	P	615	8CT	C11-C10-C03	-2.54	120.06	127.20
11	0	617	IHT	C20-C15-C12	2.54	119.06	114.36
9	7	605	CLA	C3B-C4B-NB	-2.54	108.16	110.52
9	P	610	CLA	CHB-C4A-NA	2.54	128.02	124.51
9	p	310	CLA	CHB-C4A-NA	2.53	128.02	124.51
16	P	615	8CT	C14-C15-C16	-2.53	119.30	126.42
9	9	601	CLA	CHB-C4A-NA	2.53	128.01	124.51
9	9	609	CLA	CHB-C4A-NA	2.53	128.01	124.51
12	0	615	II0	C20-C14-C12	2.53	119.04	114.36
9	8	606	CLA	C3B-C4B-NB	-2.53	108.17	110.52
12	7	614	II0	C19-C13-C11	2.53	119.03	114.36
9	p	306	CLA	CHB-C4A-NA	2.53	128.00	124.51
9	0	609	CLA	CAA-C2A-C3A	-2.52	110.21	116.10
12	7	614	II0	C08-C12-C14	-2.52	106.83	111.85
9	s	303	CLA	CHB-C4A-NA	2.52	128.00	124.51
10	P	609	KC2	CHD-C4C-NC	2.52	128.03	124.20
11	p	318	IHT	C31-C29-C26	-2.52	119.27	126.58
9	P	603	CLA	CHB-C4A-NA	2.52	127.99	124.51
9	7	613	CLA	C3B-C4B-NB	-2.52	108.18	110.52
9	9	604	CLA	CHB-C4A-NA	2.52	127.99	124.51
12	p	316	II0	C20-C14-C12	2.51	119.01	114.36
12	P	612	II0	C31-C33-C35	-2.51	119.36	126.42
10	P	609	KC2	O2D-CGD-O1D	-2.51	118.93	123.84
9	8	601	CLA	CHB-C4A-NA	2.51	127.98	124.51
9	7	603	CLA	CHB-C4A-NA	2.51	127.98	124.51
9	0	606	CLA	C3B-C4B-NB	-2.51	108.19	110.52
9	7	608	CLA	CHB-C4A-NA	2.51	127.98	124.51
9	8	605	CLA	CHB-C4A-NA	2.51	127.98	124.51
12	7	614	II0	C20-C14-C12	2.51	119.00	114.36
12	8	619	II0	C20-C14-C12	2.50	119.00	114.36
9	P	606	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
14	P	613	II3	C25-C24-C21	2.50	122.01	118.08
9	7	609	CLA	CHB-C4A-NA	2.49	127.96	124.51
9	9	611	CLA	CHB-C4A-NA	2.49	127.96	124.51
9	p	304	CLA	CHB-C4A-NA	2.49	127.96	124.51
12	p	317	II0	C42-C41-C39	-2.49	118.38	123.47
9	G	101	CLA	C3B-C4B-NB	-2.49	108.21	110.52
9	p	313	CLA	CHB-C4A-NA	2.49	127.95	124.51
12	0	616	II0	C06-C08-C12	2.49	113.71	110.30
12	p	302	II0	C20-C14-C12	2.48	118.95	114.36
12	9	614	II0	C08-C12-C14	-2.48	106.92	111.85
9	7	613	CLA	CHB-C4A-NA	2.48	127.94	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	p	314	CLA	CHB-C4A-NA	2.48	127.94	124.51
9	9	608	CLA	CHB-C4A-NA	2.48	127.94	124.51
9	p	307	CLA	C3B-C4B-NB	-2.48	108.22	110.52
9	7	603	CLA	C1-C2-C3	-2.47	122.75	126.75
9	9	602	CLA	CHB-C4A-NA	2.47	127.93	124.51
9	8	602	CLA	CHB-C4A-NA	2.47	127.93	124.51
9	8	606	CLA	CHB-C4A-NA	2.47	127.93	124.51
9	0	607	CLA	C3B-C4B-NB	-2.47	108.22	110.52
12	8	619	II0	C05-C07-C11	-2.47	106.93	110.30
9	8	609	CLA	CAA-C2A-C3A	-2.47	110.34	116.10
10	p	312	KC2	C1A-C2A-C3A	-2.46	105.16	107.11
12	8	615	II0	C06-C08-C12	-2.46	106.94	110.30
9	8	604	CLA	CHB-C4A-NA	2.46	127.91	124.51
9	0	601	CLA	CHB-C4A-NA	2.46	127.91	124.51
9	8	602	CLA	C1-C2-C3	-2.45	121.80	126.04
9	0	613	CLA	CHB-C4A-NA	2.45	127.90	124.51
10	P	605	KC2	O1D-CGD-CBD	-2.45	119.47	124.48
9	8	612	CLA	CHB-C4A-NA	2.45	127.90	124.51
9	G	101	CLA	CHB-C4A-NA	2.45	127.89	124.51
12	0	616	II0	C03-C09-C13	-2.44	119.19	122.63
9	9	605	CLA	CHB-C4A-NA	2.44	127.89	124.51
14	7	615	II3	C13-C14-C17	2.43	113.63	110.30
13	8	617	LMG	O3-C3-C2	-2.43	104.74	110.35
9	8	607	CLA	CHB-C4A-NA	2.42	127.86	124.51
12	9	614	II0	C31-C29-C25	-2.42	119.55	126.58
9	7	612	CLA	CHB-C4A-NA	2.42	127.86	124.51
9	0	603	CLA	CHB-C4A-NA	2.41	127.85	124.51
13	G	102	LMG	O1-C7-C8	-2.41	105.07	110.90
11	0	617	IHT	C31-C34-C35	-2.41	119.64	126.42
9	7	602	CLA	CHB-C4A-NA	2.41	127.85	124.51
11	0	614	IHT	C20-C15-C12	2.41	118.82	114.36
9	P	611	CLA	CHB-C4A-NA	2.41	127.84	124.51
14	P	613	II3	C26-C29-C32	-2.40	115.72	123.22
13	G	103	LMG	O3-C3-C2	-2.40	104.80	110.35
9	7	601	CLA	CHB-C4A-NA	2.40	127.83	124.51
9	0	605	CLA	C3B-C4B-NB	-2.40	108.29	110.52
10	P	605	KC2	CHD-C4C-NC	2.40	127.84	124.20
9	8	603	CLA	CHB-C4A-NA	2.40	127.83	124.51
9	8	609	CLA	CHB-C4A-NA	2.40	127.83	124.51
13	0	618	LMG	O3-C3-C2	-2.40	104.81	110.35
13	G	103	LMG	O1-C7-C8	-2.39	105.13	110.90
11	8	616	IHT	C31-C29-C26	-2.39	119.64	126.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	p	316	II0	C08-C12-C14	-2.39	107.10	111.85
9	9	606	CLA	CHB-C1B-NB	2.39	126.78	124.26
12	0	615	II0	C42-C41-C39	-2.38	118.59	123.47
10	P	605	KC2	C1B-CHB-C4A	-2.38	120.91	126.06
13	0	618	LMG	O1-C7-C8	-2.38	105.15	110.90
10	p	312	KC2	O1D-CGD-CBD	-2.38	119.61	124.48
12	p	317	II0	C38-C36-C40	-2.38	119.59	122.92
9	0	605	CLA	CHB-C4A-NA	2.38	127.80	124.51
12	9	614	II0	C31-C33-C35	-2.38	119.73	126.42
9	0	604	CLA	CHB-C4A-NA	2.38	127.80	124.51
13	G	103	LMG	O2-C2-C1	-2.38	104.27	110.05
11	0	617	IHT	C31-C29-C26	-2.38	119.67	126.58
16	9	615	8CT	C10-C03-C02	-2.38	115.70	121.46
10	7	610	KC2	O2D-CGD-O1D	-2.38	119.19	123.84
9	0	611	CLA	CHB-C4A-NA	2.37	127.79	124.51
9	7	607	CLA	CHB-C4A-NA	2.37	127.79	124.51
16	P	615	8CT	C27-C26-C25	-2.37	119.60	122.92
12	p	301	II0	C31-C29-C25	-2.37	119.70	126.58
9	0	612	CLA	O2D-CGD-CBD	2.37	115.48	111.27
10	7	610	KC2	C1B-CHB-C4A	-2.37	120.95	126.06
9	p	305	CLA	CHB-C4A-NA	2.37	127.78	124.51
11	8	616	IHT	C31-C34-C35	-2.36	119.78	126.42
9	P	602	CLA	CHB-C4A-NA	2.36	127.78	124.51
12	P	614	II0	C31-C33-C35	-2.36	119.78	126.42
12	7	617	II0	C03-C09-C13	-2.36	119.30	122.63
9	9	603	CLA	C1-C2-C3	-2.35	122.94	126.75
11	8	616	IHT	C41-C40-C37	-2.35	118.65	123.47
12	P	612	II0	C37-C35-C39	-2.35	119.62	122.92
13	8	617	LMG	O2-C2-C1	-2.35	104.33	110.05
9	7	606	CLA	C3B-C4B-NB	-2.35	108.33	110.52
10	7	610	KC2	CHD-C4C-NC	2.35	127.77	124.20
12	0	615	II0	C08-C12-C14	-2.35	107.17	111.85
13	G	102	LMG	O3-C3-C2	-2.35	104.92	110.35
14	P	613	II3	C31-C34-C37	-2.34	115.91	123.22
9	9	604	CLA	CHB-C1B-NB	2.34	126.73	124.26
12	0	619	II0	C20-C14-C12	2.34	118.69	114.36
12	7	616	II0	C31-C29-C25	-2.33	119.80	126.58
9	p	308	CLA	CHB-C4A-NA	2.33	127.74	124.51
13	0	618	LMG	O2-C2-C1	-2.33	104.39	110.05
12	0	619	II0	C18-C04-C10	-2.33	106.77	110.47
12	P	612	II0	C31-C29-C25	-2.32	119.83	126.58
9	0	609	CLA	CHB-C4A-NA	2.32	127.72	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	P	601	CLA	CHB-C4A-NA	2.31	127.70	124.51
13	G	102	LMG	O1-C1-C2	-2.31	104.70	108.30
9	p	303	CLA	CHB-C4A-NA	2.30	127.70	124.51
12	7	619	II0	C31-C29-C25	-2.30	119.89	126.58
14	7	615	II3	C22-C18-C17	2.30	118.62	114.36
9	0	606	CLA	CHB-C4A-NA	2.30	127.69	124.51
9	0	604	CLA	CHB-C1B-NB	2.30	126.69	124.26
12	p	301	II0	C20-C14-C12	2.30	118.61	114.36
16	9	615	8CT	C30-C31-C32	-2.29	118.65	121.47
9	0	607	CLA	CHB-C4A-NA	2.29	127.68	124.51
9	7	604	CLA	O2D-CGD-CBD	2.29	115.34	111.27
9	p	311	CLA	CHB-C4A-NA	2.29	127.68	124.51
10	0	610	KC2	O1D-CGD-CBD	-2.28	119.81	124.48
11	p	318	IHT	C19-C10-C09	2.28	118.00	113.62
12	0	619	II0	C08-C12-C14	-2.28	107.31	111.85
16	9	615	8CT	C27-C26-C25	-2.28	119.73	122.92
9	P	602	CLA	C1-C2-C3	-2.28	122.10	126.04
9	P	603	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
10	8	610	KC2	C1B-CHB-C4A	-2.28	121.15	126.06
13	8	617	LMG	O1-C7-C8	-2.28	105.41	110.90
14	7	615	II3	C39-C41-C40	-2.28	118.81	123.47
9	0	603	CLA	C1-C2-C3	-2.27	123.08	126.75
9	P	608	CLA	CAA-C2A-C3A	-2.27	110.80	116.10
9	P	608	CLA	CHB-C4A-NA	2.27	127.65	124.51
9	7	605	CLA	CHD-C1D-ND	-2.27	122.37	124.45
10	8	610	KC2	CHD-C4C-NC	2.27	127.65	124.20
14	P	613	II3	C22-C18-C17	2.27	118.55	114.36
9	7	606	CLA	CHC-C4B-NB	2.26	126.65	124.26
9	P	604	CLA	CHB-C1B-NB	2.26	126.65	124.26
12	p	315	II0	C19-C13-C11	2.26	118.55	114.36
12	7	616	II0	C31-C33-C35	-2.26	120.07	126.42
13	8	617	LMG	O7-C10-O9	-2.25	118.25	123.70
9	p	307	CLA	CHB-C4A-NA	2.25	127.62	124.51
12	9	614	II0	C20-C14-C12	2.25	118.52	114.36
12	P	614	II0	C08-C12-C14	-2.25	107.38	111.85
11	0	617	IHT	C22-C18-C07	-2.24	120.90	127.20
11	0	614	IHT	C31-C29-C26	-2.24	120.07	126.58
9	0	613	CLA	CHB-C1B-NB	2.24	126.63	124.26
9	7	604	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
15	s	301	LHG	C27-C26-C25	-2.24	103.08	114.42
12	7	617	II0	C31-C33-C35	-2.24	120.14	126.42
9	p	314	CLA	C3B-C4B-NB	-2.23	108.44	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	p	302	II0	C38-C36-C40	-2.23	119.79	122.92
12	9	613	II0	C41-C39-C35	-2.23	124.12	127.31
13	8	617	LMG	O1-C1-C2	-2.23	104.83	108.30
10	0	610	KC2	O2D-CGD-O1D	-2.22	119.49	123.84
12	P	612	II0	C19-C13-C11	2.22	118.47	114.36
9	7	605	CLA	CHB-C4A-NA	2.22	127.59	124.51
11	0	614	IHT	C19-C10-C09	2.22	117.89	113.62
9	p	309	CLA	CHB-C1B-NB	2.22	126.61	124.26
9	0	607	CLA	O2A-CGA-O1A	-2.22	117.77	123.30
9	7	603	CLA	C3B-C4B-NB	-2.22	108.46	110.52
12	7	616	II0	C20-C14-C12	2.21	118.45	114.36
12	7	617	II0	C42-C41-C39	-2.21	118.95	123.47
12	p	315	II0	C41-C42-C40	-2.21	118.96	123.47
9	9	610	CLA	O2A-CGA-O1A	-2.20	117.81	123.30
12	9	614	II0	C19-C13-C11	2.20	118.44	114.36
10	P	609	KC2	C1A-C2A-C3A	-2.20	105.37	107.11
12	9	612	II0	C32-C30-C26	-2.20	120.19	126.58
10	0	610	KC2	C1B-CHB-C4A	-2.20	121.31	126.06
9	P	606	CLA	CAA-CBA-CGA	-2.20	106.67	112.51
9	9	606	CLA	CHB-C4A-NA	2.20	127.55	124.51
14	P	613	II3	C30-C28-C27	2.20	121.19	116.84
9	0	604	CLA	O2D-CGD-CBD	2.20	115.17	111.27
9	s	303	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
12	8	615	II0	C19-C13-C09	-2.19	121.37	124.35
9	9	609	CLA	O2D-CGD-CBD	2.19	115.17	111.27
10	0	610	KC2	CBD-CHA-C1A	2.19	132.97	128.88
12	p	316	II0	C32-C30-C26	-2.19	120.22	126.58
10	p	312	KC2	C1B-CHB-C4A	-2.19	121.33	126.06
12	9	613	II0	C19-C13-C11	2.19	118.41	114.36
9	9	602	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
10	p	312	KC2	O2D-CGD-O1D	-2.19	119.56	123.84
12	p	301	II0	C31-C33-C35	-2.19	120.27	126.42
16	P	615	8CT	C04-C03-C10	2.19	121.96	115.78
10	0	610	KC2	C1A-C2A-C3A	-2.19	105.38	107.11
11	0	617	IHT	C41-C40-C37	-2.18	119.00	123.47
9	p	308	CLA	CHB-C1B-NB	2.18	126.57	124.26
11	0	617	IHT	C39-C35-C38	-2.18	119.87	122.92
9	0	609	CLA	CHB-C1B-NB	2.18	126.56	124.26
9	8	603	CLA	CHB-C1B-NB	2.18	126.56	124.26
11	0	617	IHT	C36-C33-C37	-2.18	119.87	122.92
17	p	319	SQD	C4-C3-C2	2.17	114.62	110.82
12	8	613	II0	C19-C13-C11	2.17	118.38	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	8	608	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
12	p	301	II0	C19-C13-C11	2.17	118.37	114.36
9	p	309	CLA	CMB-C2B-C1B	-2.17	122.07	125.37
9	0	604	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
9	8	605	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
9	p	304	CLA	CHD-C1D-ND	-2.16	122.47	124.45
9	0	608	CLA	CHD-C1D-ND	-2.15	122.47	124.45
9	p	304	CLA	CHB-C1B-NB	2.15	126.53	124.26
10	p	312	KC2	CHB-C4A-C3A	-2.15	121.62	124.98
12	9	612	II0	C41-C42-C40	-2.15	119.08	123.47
13	0	618	LMG	O1-C1-C2	-2.15	104.95	108.30
12	0	615	II0	C38-C36-C40	-2.14	119.92	122.92
12	p	301	II0	C08-C12-C14	-2.14	107.59	111.85
9	8	602	CLA	O2D-CGD-CBD	2.14	115.07	111.27
12	p	302	II0	C31-C29-C25	-2.14	120.37	126.58
9	p	313	CLA	O2A-CGA-O1A	-2.14	117.97	123.30
9	8	603	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
9	8	604	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
12	p	315	II0	C37-C35-C39	-2.13	119.93	122.92
16	P	615	8CT	C39-C16-C17	-2.13	119.94	122.92
9	8	611	CLA	O2A-CGA-O1A	-2.13	117.99	123.30
9	s	302	CLA	CHB-C4A-NA	2.13	127.46	124.51
9	9	604	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
9	p	305	CLA	CHB-C1B-NB	2.13	126.51	124.26
12	p	316	II0	C29-C31-C33	-2.13	116.58	123.22
9	8	608	CLA	CHD-C1D-ND	-2.12	122.50	124.45
12	p	315	II0	C20-C14-C12	2.12	118.29	114.36
9	9	608	CLA	CMA-C3A-C2A	-2.12	111.14	116.10
12	0	616	II0	C32-C30-C26	-2.12	120.42	126.58
9	P	602	CLA	CHD-C1D-ND	-2.12	122.50	124.45
9	0	608	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
12	9	612	II0	C20-C14-C12	2.12	118.28	114.36
9	P	611	CLA	CHB-C1B-NB	2.12	126.50	124.26
12	P	614	II0	C19-C13-C11	2.12	118.28	114.36
11	8	616	IHT	C22-C18-C07	-2.12	121.25	127.20
9	p	306	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
9	P	602	CLA	CHB-C1B-NB	2.12	126.50	124.26
12	9	612	II0	C19-C13-C11	2.12	118.28	114.36
11	8	616	IHT	C25-C23-C27	-2.12	119.96	122.92
9	7	602	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
11	7	618	IHT	C25-C23-C27	-2.11	119.96	122.92
12	8	613	II0	C41-C42-C40	-2.11	119.14	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	0	614	IHT	C31-C34-C35	-2.11	120.48	126.42
9	7	602	CLA	CHD-C1D-ND	-2.11	122.51	124.45
12	7	616	II0	C41-C42-C40	-2.11	119.15	123.47
9	P	604	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
12	8	613	II0	C20-C14-C12	2.11	118.26	114.36
10	8	610	KC2	CHB-C4A-C3A	-2.11	121.68	124.98
9	7	608	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
9	9	608	CLA	CHB-C1B-NB	2.11	126.49	124.26
9	p	305	CLA	CHD-C1D-ND	-2.11	122.52	124.45
9	8	602	CLA	CHD-C1D-ND	-2.11	122.52	124.45
12	7	616	II0	C42-C41-C39	-2.11	119.16	123.47
9	8	604	CLA	CHB-C1B-NB	2.10	126.48	124.26
9	p	311	CLA	CMA-C3A-C2A	-2.10	111.19	116.10
12	7	619	II0	C19-C13-C11	2.10	118.25	114.36
9	p	310	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
12	9	613	II0	C20-C14-C12	2.10	118.25	114.36
9	P	606	CLA	CHD-C1D-ND	-2.10	122.53	124.45
14	7	615	II3	C25-C24-C21	2.09	121.38	118.08
12	7	616	II0	C32-C30-C26	-2.09	120.50	126.58
9	s	303	CLA	CHB-C1B-NB	2.09	126.47	124.26
11	0	614	IHT	C22-C18-C07	-2.09	121.32	127.20
11	7	618	IHT	C39-C35-C38	-2.09	119.99	122.92
12	8	619	II0	C32-C30-C26	-2.09	120.52	126.58
9	0	609	CLA	CMA-C3A-C2A	-2.09	111.22	116.10
9	0	602	CLA	C1-C2-C3	-2.09	122.43	126.04
12	7	619	II0	C37-C35-C39	-2.09	120.00	122.92
9	p	307	CLA	CHD-C1D-ND	-2.09	122.54	124.45
11	p	318	IHT	C41-C40-C37	-2.09	119.20	123.47
13	0	618	LMG	C1-O6-C5	-2.09	109.59	113.69
14	P	613	II3	C42-C38-C37	2.09	121.36	118.08
13	G	102	LMG	O2-C2-C1	-2.08	104.98	110.05
11	7	618	IHT	C41-C40-C37	-2.08	119.20	123.47
9	8	603	CLA	CHD-C1D-ND	-2.08	122.54	124.45
9	p	307	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
10	P	605	KC2	O2D-CGD-O1D	-2.08	119.77	123.84
12	0	615	II0	C32-C30-C26	-2.08	120.55	126.58
9	s	302	CLA	CMB-C2B-C1B	-2.08	122.20	125.37
9	p	304	CLA	C1-C2-C3	-2.08	122.45	126.04
9	8	608	CLA	CHB-C1B-NB	2.08	126.45	124.26
10	P	609	KC2	C1B-CHB-C4A	-2.08	121.58	126.06
12	0	619	II0	C32-C30-C26	-2.07	120.56	126.58
11	7	618	IHT	C05-C08-C12	2.07	113.14	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	0	602	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
9	7	603	CLA	CMB-C2B-C1B	-2.07	122.22	125.37
9	P	607	CLA	CHB-C1B-NB	2.07	126.45	124.26
16	9	615	8CT	C40-C12-C13	-2.07	120.03	122.92
11	8	616	IHT	C20-C15-C12	2.07	118.18	114.36
9	0	607	CLA	CHD-C1D-ND	-2.06	122.56	124.45
9	9	607	CLA	CHB-C1B-NB	2.06	126.44	124.26
9	p	304	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
10	P	609	KC2	C2A-C3A-C4A	2.06	108.02	106.49
9	P	606	CLA	CHB-C4A-NA	2.06	127.36	124.51
9	P	603	CLA	CHB-C1B-NB	2.06	126.43	124.26
9	9	609	CLA	CHB-C1B-NB	2.06	126.43	124.26
9	0	604	CLA	C1-C2-C3	-2.05	122.49	126.04
9	9	603	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
9	8	612	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
12	7	617	II0	C20-C14-C12	2.05	118.16	114.36
12	p	315	II0	C32-C34-C36	-2.05	120.66	126.42
9	P	610	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
9	0	612	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
12	8	615	II0	C18-C04-C10	-2.05	107.21	110.47
9	8	604	CLA	CMB-C2B-C1B	-2.05	122.25	125.37
9	P	610	CLA	CHB-C1B-NB	2.05	126.42	124.26
9	7	604	CLA	CHB-C1B-NB	2.04	126.42	124.26
12	0	619	II0	C06-C04-C10	2.04	113.75	109.62
9	P	610	CLA	O2D-CGD-CBD	2.04	114.89	111.27
9	P	602	CLA	O2D-CGD-CBD	2.04	114.89	111.27
9	7	606	CLA	CMB-C2B-C1B	-2.04	122.27	125.37
9	7	605	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
12	8	613	II0	C37-C35-C39	-2.04	120.07	122.92
9	9	604	CLA	CHD-C1D-ND	-2.04	122.58	124.45
9	0	606	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
9	0	603	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
9	s	302	CLA	CHC-C4B-NB	2.03	126.41	124.26
9	7	607	CLA	O2A-CGA-O1A	-2.03	118.23	123.30
9	7	608	CLA	CHD-C1D-ND	-2.03	122.59	124.45
9	P	606	CLA	C2D-C1D-ND	-2.03	108.61	110.10
9	G	101	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
9	7	611	CLA	CHC-C4B-NB	2.03	126.41	124.26
9	8	605	CLA	CHD-C1D-ND	-2.03	122.59	124.45
9	7	609	CLA	CHB-C1B-NB	2.02	126.40	124.26
12	0	615	II0	C32-C34-C36	-2.02	120.73	126.42
12	7	614	II0	C07-C11-C13	-2.02	107.83	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	7	613	CLA	O2A-CGA-O1A	-2.02	118.26	123.30
9	8	606	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
9	0	611	CLA	CHB-C1B-NB	2.02	126.39	124.26
9	p	311	CLA	CHB-C1B-NB	2.02	126.39	124.26
12	p	302	II0	C31-C33-C35	-2.02	120.75	126.42
12	7	619	II0	C04-C06-C08	-2.02	109.09	113.64
12	8	614	II0	C19-C13-C11	2.02	118.09	114.36
11	0	614	IHT	C39-C35-C38	-2.01	120.10	122.92
11	8	616	IHT	C06-C09-C10	-2.01	110.48	114.08
9	p	308	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
12	0	619	II0	C30-C32-C34	-2.01	116.94	123.22
9	p	309	CLA	O2A-CGA-O1A	-2.01	118.28	123.30
9	p	304	CLA	O2D-CGD-CBD	2.01	114.84	111.27
9	P	611	CLA	CHD-C1D-ND	-2.01	122.61	124.45
9	9	604	CLA	O2D-CGD-CBD	2.01	114.84	111.27
12	p	315	II0	C31-C33-C35	-2.01	120.77	126.42
10	0	610	KC2	O2A-CGA-O1A	-2.01	118.50	122.67
9	8	602	CLA	CHB-C1B-NB	2.01	126.38	124.26
9	8	607	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
16	P	615	8CT	C35-C30-C29	-2.00	110.17	112.70
9	9	602	CLA	CHB-C1B-NB	2.00	126.38	124.26
9	p	306	CLA	CHB-C1B-NB	2.00	126.38	124.26
9	0	613	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
9	0	602	CLA	CHD-C1D-ND	-2.00	122.61	124.45
12	p	316	II0	C06-C08-C12	-2.00	107.56	110.30
9	0	605	CLA	CHD-C1D-ND	-2.00	122.62	124.45
9	9	611	CLA	O2A-CGA-O1A	-2.00	118.31	123.30

There are no chirality outliers.

All (734) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	0	602	CLA	C1A-C2A-CAA-CBA
9	0	602	CLA	C3A-C2A-CAA-CBA
9	0	602	CLA	CHA-CBD-CGD-O1D
9	0	602	CLA	CHA-CBD-CGD-O2D
9	0	603	CLA	C1A-C2A-CAA-CBA
9	0	605	CLA	CBD-CGD-O2D-CED
9	0	611	CLA	CHA-CBD-CGD-O1D
9	0	611	CLA	CHA-CBD-CGD-O2D
9	0	612	CLA	CBD-CGD-O2D-CED
9	0	613	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
9	7	601	CLA	C4B-C3B-CAB-CBB
9	7	602	CLA	C1A-C2A-CAA-CBA
9	7	602	CLA	C3A-C2A-CAA-CBA
9	7	602	CLA	CBD-CGD-O2D-CED
9	7	603	CLA	C1A-C2A-CAA-CBA
9	7	603	CLA	C3A-C2A-CAA-CBA
9	7	605	CLA	C1A-C2A-CAA-CBA
9	7	605	CLA	C3A-C2A-CAA-CBA
9	7	605	CLA	CBD-CGD-O2D-CED
9	7	606	CLA	C1A-C2A-CAA-CBA
9	7	606	CLA	C3A-C2A-CAA-CBA
9	7	607	CLA	C1A-C2A-CAA-CBA
9	7	607	CLA	C3A-C2A-CAA-CBA
9	7	608	CLA	C2B-C3B-CAB-CBB
9	7	608	CLA	C4B-C3B-CAB-CBB
9	7	609	CLA	C4B-C3B-CAB-CBB
9	7	611	CLA	CBD-CGD-O2D-CED
9	7	611	CLA	O1D-CGD-O2D-CED
9	7	612	CLA	C4B-C3B-CAB-CBB
9	7	612	CLA	CBD-CGD-O2D-CED
9	7	613	CLA	CBD-CGD-O2D-CED
9	8	602	CLA	C1A-C2A-CAA-CBA
9	8	602	CLA	C3A-C2A-CAA-CBA
9	8	602	CLA	CHA-CBD-CGD-O1D
9	8	602	CLA	CHA-CBD-CGD-O2D
9	8	603	CLA	C1A-C2A-CAA-CBA
9	8	603	CLA	C3A-C2A-CAA-CBA
9	8	603	CLA	CHA-CBD-CGD-O1D
9	8	603	CLA	CHA-CBD-CGD-O2D
9	8	609	CLA	C4B-C3B-CAB-CBB
9	8	611	CLA	C1A-C2A-CAA-CBA
9	8	611	CLA	C3A-C2A-CAA-CBA
9	8	611	CLA	CBD-CGD-O2D-CED
9	8	612	CLA	CBD-CGD-O2D-CED
9	9	601	CLA	CBD-CGD-O2D-CED
9	9	602	CLA	C1A-C2A-CAA-CBA
9	9	602	CLA	C3A-C2A-CAA-CBA
9	9	604	CLA	CHA-CBD-CGD-O1D
9	9	604	CLA	CHA-CBD-CGD-O2D
9	9	605	CLA	C3A-C2A-CAA-CBA
9	9	605	CLA	C4B-C3B-CAB-CBB
9	9	607	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	9	610	CLA	CHA-CBD-CGD-O1D
9	9	610	CLA	CHA-CBD-CGD-O2D
9	G	101	CLA	C1A-C2A-CAA-CBA
9	G	101	CLA	CHA-CBD-CGD-O1D
9	G	101	CLA	CHA-CBD-CGD-O2D
9	P	602	CLA	C1A-C2A-CAA-CBA
9	P	602	CLA	C3A-C2A-CAA-CBA
9	P	610	CLA	CHA-CBD-CGD-O1D
9	P	610	CLA	CHA-CBD-CGD-O2D
9	p	304	CLA	C1A-C2A-CAA-CBA
9	p	304	CLA	C3A-C2A-CAA-CBA
9	p	304	CLA	C2B-C3B-CAB-CBB
9	p	304	CLA	C4B-C3B-CAB-CBB
9	p	306	CLA	CHA-CBD-CGD-O1D
9	p	306	CLA	CHA-CBD-CGD-O2D
9	p	307	CLA	C1A-C2A-CAA-CBA
9	p	307	CLA	C3A-C2A-CAA-CBA
9	p	307	CLA	CHA-CBD-CGD-O1D
9	p	307	CLA	CHA-CBD-CGD-O2D
9	p	307	CLA	CBD-CGD-O2D-CED
9	p	308	CLA	C2B-C3B-CAB-CBB
9	p	308	CLA	C4B-C3B-CAB-CBB
9	p	309	CLA	C1A-C2A-CAA-CBA
9	p	313	CLA	C1A-C2A-CAA-CBA
9	p	313	CLA	C3A-C2A-CAA-CBA
9	p	313	CLA	CHA-CBD-CGD-O1D
9	p	313	CLA	CHA-CBD-CGD-O2D
9	s	302	CLA	C1A-C2A-CAA-CBA
9	s	302	CLA	C3A-C2A-CAA-CBA
9	s	302	CLA	CBD-CGD-O2D-CED
9	s	303	CLA	C4B-C3B-CAB-CBB
10	0	610	KC2	C1A-C2A-CAA-CBA
10	0	610	KC2	C2B-C3B-CAB-CBB
10	0	610	KC2	C4B-C3B-CAB-CBB
10	0	610	KC2	C2C-C3C-CAC-CBC
10	0	610	KC2	C4C-C3C-CAC-CBC
10	0	610	KC2	C2A-CAA-CBA-CGA
10	0	610	KC2	CAA-CBA-CGA-O2A
10	7	610	KC2	C1A-C2A-CAA-CBA
10	7	610	KC2	C2B-C3B-CAB-CBB
10	7	610	KC2	C4B-C3B-CAB-CBB
10	7	610	KC2	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
10	7	610	KC2	CBD-CGD-O2D-CED
10	8	610	KC2	C1A-C2A-CAA-CBA
10	8	610	KC2	C3A-C2A-CAA-CBA
10	8	610	KC2	C2B-C3B-CAB-CBB
10	P	605	KC2	C1A-C2A-CAA-CBA
10	P	605	KC2	C2B-C3B-CAB-CBB
10	P	605	KC2	C4B-C3B-CAB-CBB
10	P	605	KC2	C2C-C3C-CAC-CBC
10	P	605	KC2	C4C-C3C-CAC-CBC
10	P	605	KC2	CBD-CGD-O2D-CED
10	P	609	KC2	C1A-C2A-CAA-CBA
10	P	609	KC2	C2B-C3B-CAB-CBB
10	P	609	KC2	C4B-C3B-CAB-CBB
10	P	609	KC2	C2C-C3C-CAC-CBC
10	P	609	KC2	C4C-C3C-CAC-CBC
10	P	609	KC2	CAA-CBA-CGA-O2A
10	p	312	KC2	C2B-C3B-CAB-CBB
10	p	312	KC2	C4B-C3B-CAB-CBB
10	p	312	KC2	C2C-C3C-CAC-CBC
10	p	312	KC2	C4C-C3C-CAC-CBC
11	0	614	IHT	C30-C32-C33-C36
11	0	614	IHT	C30-C32-C33-C37
11	0	617	IHT	C30-C32-C33-C36
11	0	617	IHT	C30-C32-C33-C37
11	0	617	IHT	C33-C37-C40-C41
12	0	619	II0	C26-C30-C32-C34
12	7	616	II0	C09-C21-C23-C25
12	7	617	II0	C31-C33-C35-C37
12	7	617	II0	C31-C33-C35-C39
12	9	614	II0	C31-C33-C35-C37
12	9	614	II0	C31-C33-C35-C39
12	P	614	II0	C31-C33-C35-C37
12	P	614	II0	C31-C33-C35-C39
12	p	301	II0	C31-C33-C35-C37
12	p	301	II0	C31-C33-C35-C39
12	p	316	II0	C09-C21-C23-C25
12	p	317	II0	C32-C34-C36-C38
12	p	317	II0	C32-C34-C36-C40
13	G	102	LMG	C11-C10-O7-C8
14	P	613	II3	C16-C23-C27-C28
15	8	618	LHG	O1-C1-C2-C3
15	8	618	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
15	s	301	LHG	C3-O3-P-O4
15	s	301	LHG	C4-O6-P-O5
15	s	301	LHG	O9-C7-O7-C5
15	s	301	LHG	C8-C7-O7-C5
16	9	615	8CT	C12-C13-C14-C15
16	9	615	8CT	C22-C21-C23-C24
16	P	615	8CT	C04-C03-C10-C11
17	p	319	SQD	O5-C1-O6-C44
17	p	319	SQD	C8-C7-O47-C45
17	p	319	SQD	C5-C6-S-O7
17	p	319	SQD	C5-C6-S-O8
17	p	319	SQD	C5-C6-S-O9
9	0	611	CLA	O1D-CGD-O2D-CED
9	7	601	CLA	O1D-CGD-O2D-CED
9	7	613	CLA	O1D-CGD-O2D-CED
9	9	601	CLA	O1D-CGD-O2D-CED
9	9	607	CLA	O1D-CGD-O2D-CED
10	P	605	KC2	O1D-CGD-O2D-CED
9	0	605	CLA	O1D-CGD-O2D-CED
9	s	302	CLA	O1D-CGD-O2D-CED
10	7	610	KC2	O1D-CGD-O2D-CED
9	0	611	CLA	CBD-CGD-O2D-CED
9	0	613	CLA	CBD-CGD-O2D-CED
9	7	601	CLA	CBD-CGD-O2D-CED
9	8	609	CLA	CBD-CGD-O2D-CED
9	p	311	CLA	CBD-CGD-O2D-CED
9	p	313	CLA	CBD-CGD-O2D-CED
10	8	610	KC2	CBD-CGD-O2D-CED
9	p	307	CLA	O1D-CGD-O2D-CED
9	7	612	CLA	O1D-CGD-O2D-CED
9	8	612	CLA	O1D-CGD-O2D-CED
9	0	601	CLA	CBD-CGD-O2D-CED
9	0	608	CLA	CBD-CGD-O2D-CED
9	7	604	CLA	CBD-CGD-O2D-CED
9	7	606	CLA	CBD-CGD-O2D-CED
9	7	608	CLA	CBD-CGD-O2D-CED
9	8	601	CLA	CBD-CGD-O2D-CED
9	9	603	CLA	CBD-CGD-O2D-CED
9	P	606	CLA	CBD-CGD-O2D-CED
9	P	610	CLA	CBD-CGD-O2D-CED
9	P	611	CLA	CBD-CGD-O2D-CED
17	p	319	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
9	7	602	CLA	O1D-CGD-O2D-CED
9	7	605	CLA	O1D-CGD-O2D-CED
9	0	612	CLA	O1D-CGD-O2D-CED
9	8	611	CLA	O1D-CGD-O2D-CED
13	G	102	LMG	O9-C10-O7-C8
17	p	319	SQD	O49-C7-O47-C45
9	0	602	CLA	C3-C5-C6-C7
9	9	609	CLA	C3-C5-C6-C7
9	8	608	CLA	CBD-CGD-O2D-CED
10	7	610	KC2	CAA-CBA-CGA-O1A
9	p	303	CLA	CBD-CGD-O2D-CED
9	p	310	CLA	CBD-CGD-O2D-CED
9	p	314	CLA	CBD-CGD-O2D-CED
9	s	303	CLA	C2A-CAA-CBA-CGA
9	s	303	CLA	C3-C5-C6-C7
17	p	319	SQD	C24-C23-O48-C46
9	p	313	CLA	O1D-CGD-O2D-CED
9	0	613	CLA	O1D-CGD-O2D-CED
10	0	610	KC2	CAA-CBA-CGA-O1A
10	P	609	KC2	CAA-CBA-CGA-O1A
9	7	607	CLA	CBD-CGD-O2D-CED
9	P	602	CLA	CBD-CGD-O2D-CED
9	0	604	CLA	C3-C5-C6-C7
9	8	602	CLA	CBD-CGD-O2D-CED
9	8	607	CLA	CBD-CGD-O2D-CED
9	9	610	CLA	CBD-CGD-O2D-CED
10	P	609	KC2	CBD-CGD-O2D-CED
9	8	609	CLA	O1D-CGD-O2D-CED
9	p	311	CLA	O1D-CGD-O2D-CED
10	8	610	KC2	CAA-CBA-CGA-O2A
9	0	613	CLA	C2A-CAA-CBA-CGA
15	s	301	LHG	C28-C29-C30-C31
13	G	102	LMG	O6-C1-O1-C7
9	p	305	CLA	CBA-CGA-O2A-C1
9	0	601	CLA	O1D-CGD-O2D-CED
10	8	610	KC2	CAA-CBA-CGA-O1A
9	7	608	CLA	O1D-CGD-O2D-CED
9	P	606	CLA	O1D-CGD-O2D-CED
9	P	610	CLA	O1D-CGD-O2D-CED
15	8	618	LHG	C1-C2-C3-O3
9	8	603	CLA	O1A-CGA-O2A-C1
9	p	305	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	8	601	CLA	O1D-CGD-O2D-CED
9	0	605	CLA	CBA-CGA-O2A-C1
9	7	603	CLA	CBA-CGA-O2A-C1
9	8	603	CLA	CBA-CGA-O2A-C1
9	s	303	CLA	CBA-CGA-O2A-C1
9	7	604	CLA	O1D-CGD-O2D-CED
11	0	617	IHT	C23-C27-C30-C32
17	p	319	SQD	C2-C1-O6-C44
9	0	608	CLA	O1D-CGD-O2D-CED
9	P	611	CLA	O1D-CGD-O2D-CED
9	0	611	CLA	C2A-CAA-CBA-CGA
12	7	616	II0	C31-C33-C35-C37
16	9	615	8CT	C14-C15-C16-C39
9	P	607	CLA	C8-C10-C11-C12
9	P	607	CLA	C10-C11-C12-C13
9	p	310	CLA	C8-C10-C11-C12
13	0	618	LMG	C10-C11-C12-C13
15	8	618	LHG	C23-C24-C25-C26
9	8	608	CLA	C8-C10-C11-C12
9	7	606	CLA	O1D-CGD-O2D-CED
10	8	610	KC2	O1D-CGD-O2D-CED
9	9	607	CLA	C10-C11-C12-C13
9	P	602	CLA	C6-C7-C8-C10
9	0	605	CLA	O1A-CGA-O2A-C1
9	s	303	CLA	O1A-CGA-O2A-C1
11	0	614	IHT	C23-C27-C30-C32
9	9	603	CLA	O1D-CGD-O2D-CED
9	7	603	CLA	O1A-CGA-O2A-C1
9	0	604	CLA	CBD-CGD-O2D-CED
13	0	618	LMG	O6-C1-O1-C7
9	p	306	CLA	C5-C6-C7-C8
9	0	602	CLA	C5-C6-C7-C8
9	7	608	CLA	C8-C10-C11-C12
9	s	303	CLA	C13-C15-C16-C17
15	s	301	LHG	C3-O3-P-O6
9	8	608	CLA	O1D-CGD-O2D-CED
9	p	304	CLA	CBD-CGD-O2D-CED
15	s	301	LHG	C23-C24-C25-C26
9	p	314	CLA	O1D-CGD-O2D-CED
9	0	602	CLA	C4-C3-C5-C6
9	P	611	CLA	C2A-CAA-CBA-CGA
9	p	307	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
12	0	616	II0	C35-C39-C41-C42
12	0	616	II0	C36-C40-C42-C41
12	p	316	II0	C36-C40-C42-C41
12	p	317	II0	C26-C30-C32-C34
10	P	609	KC2	C2A-CAA-CBA-CGA
10	p	312	KC2	C2A-CAA-CBA-CGA
17	p	319	SQD	C44-C45-O47-C7
9	p	303	CLA	O1D-CGD-O2D-CED
9	p	310	CLA	O1D-CGD-O2D-CED
15	8	618	LHG	C24-C25-C26-C27
13	0	618	LMG	C28-C29-C30-C31
13	0	618	LMG	C2-C1-O1-C7
13	G	102	LMG	O7-C8-C9-O8
9	7	608	CLA	C11-C12-C13-C14
9	p	310	CLA	C11-C12-C13-C14
15	s	301	LHG	C24-C25-C26-C27
10	P	605	KC2	CAA-CBA-CGA-O1A
10	p	312	KC2	CAA-CBA-CGA-O2A
16	9	615	8CT	C14-C15-C16-C17
16	9	615	8CT	C20-C21-C23-C24
13	8	617	LMG	C14-C15-C16-C17
9	0	601	CLA	C4B-C3B-CAB-CBB
9	0	607	CLA	C4B-C3B-CAB-CBB
9	0	609	CLA	C4B-C3B-CAB-CBB
9	0	612	CLA	C4B-C3B-CAB-CBB
9	7	605	CLA	C4B-C3B-CAB-CBB
9	7	607	CLA	C4B-C3B-CAB-CBB
9	9	609	CLA	C4B-C3B-CAB-CBB
9	G	101	CLA	C4B-C3B-CAB-CBB
9	P	604	CLA	C4B-C3B-CAB-CBB
9	P	608	CLA	C4B-C3B-CAB-CBB
9	p	303	CLA	C4B-C3B-CAB-CBB
9	p	305	CLA	C4B-C3B-CAB-CBB
9	p	311	CLA	C4B-C3B-CAB-CBB
9	0	608	CLA	C11-C12-C13-C14
9	0	608	CLA	C11-C12-C13-C15
9	8	608	CLA	C10-C11-C12-C13
17	p	319	SQD	C11-C10-C9-C8
17	p	319	SQD	C7-C8-C9-C10
9	7	608	CLA	C10-C11-C12-C13
15	s	301	LHG	C27-C28-C29-C30
9	0	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
15	s	301	LHG	C11-C10-C9-C8
9	0	603	CLA	C3A-C2A-CAA-CBA
9	9	603	CLA	C3A-C2A-CAA-CBA
9	P	603	CLA	C3A-C2A-CAA-CBA
9	p	305	CLA	C3A-C2A-CAA-CBA
9	p	307	CLA	C8-C10-C11-C12
15	s	301	LHG	C30-C31-C32-C33
17	p	319	SQD	C11-C12-C13-C14
9	p	310	CLA	C11-C12-C13-C15
9	p	305	CLA	CBD-CGD-O2D-CED
9	7	605	CLA	CBA-CGA-O2A-C1
10	p	312	KC2	CAA-CBA-CGA-O1A
15	8	618	LHG	O1-C1-C2-O2
9	0	601	CLA	C2B-C3B-CAB-CBB
9	0	607	CLA	C2B-C3B-CAB-CBB
9	0	612	CLA	C2B-C3B-CAB-CBB
9	0	613	CLA	C2B-C3B-CAB-CBB
9	7	601	CLA	C2B-C3B-CAB-CBB
9	7	605	CLA	C2B-C3B-CAB-CBB
9	7	607	CLA	C2B-C3B-CAB-CBB
9	7	609	CLA	C2B-C3B-CAB-CBB
9	7	612	CLA	C2B-C3B-CAB-CBB
9	8	609	CLA	C2B-C3B-CAB-CBB
9	9	605	CLA	C2B-C3B-CAB-CBB
9	9	609	CLA	C2B-C3B-CAB-CBB
9	G	101	CLA	C2B-C3B-CAB-CBB
9	P	604	CLA	C2B-C3B-CAB-CBB
9	P	608	CLA	C2B-C3B-CAB-CBB
9	p	303	CLA	C2B-C3B-CAB-CBB
9	p	305	CLA	C2B-C3B-CAB-CBB
9	p	311	CLA	C2B-C3B-CAB-CBB
9	s	303	CLA	C2B-C3B-CAB-CBB
9	p	307	CLA	O1A-CGA-O2A-C1
11	0	614	IHT	C02-C07-C18-C22
11	0	614	IHT	C10-C07-C18-C22
11	7	618	IHT	C02-C07-C18-C22
11	7	618	IHT	C10-C07-C18-C22
16	9	615	8CT	C04-C03-C10-C11
9	7	607	CLA	O1D-CGD-O2D-CED
9	8	602	CLA	CBA-CGA-O2A-C1
9	P	602	CLA	CBA-CGA-O2A-C1
9	p	304	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	9	604	CLA	C5-C6-C7-C8
9	7	602	CLA	C4-C3-C5-C6
9	9	602	CLA	C4-C3-C5-C6
9	0	603	CLA	O1A-CGA-O2A-C1
9	7	605	CLA	O1A-CGA-O2A-C1
9	P	602	CLA	O1A-CGA-O2A-C1
9	7	602	CLA	C5-C6-C7-C8
9	7	608	CLA	C11-C12-C13-C15
9	p	314	CLA	C2A-CAA-CBA-CGA
9	P	602	CLA	O1D-CGD-O2D-CED
15	s	301	LHG	C25-C26-C27-C28
9	8	607	CLA	O1D-CGD-O2D-CED
13	8	617	LMG	C30-C31-C32-C33
10	7	610	KC2	C2C-C3C-CAC-CBC
9	8	608	CLA	C11-C12-C13-C15
9	9	607	CLA	C11-C12-C13-C15
9	0	608	CLA	C8-C10-C11-C12
9	9	610	CLA	O1D-CGD-O2D-CED
10	7	610	KC2	C4C-C3C-CAC-CBC
10	8	610	KC2	C4B-C3B-CAB-CBB
9	0	606	CLA	CBD-CGD-O2D-CED
9	8	602	CLA	O1A-CGA-O2A-C1
9	p	304	CLA	O1A-CGA-O2A-C1
17	p	319	SQD	O47-C45-C46-O48
13	0	618	LMG	O6-C5-C6-O5
9	8	602	CLA	O1D-CGD-O2D-CED
9	0	602	CLA	C2-C3-C5-C6
12	0	616	II0	C10-C22-C24-C26
12	8	615	II0	C09-C21-C23-C25
12	9	613	II0	C10-C22-C24-C26
12	9	614	II0	C09-C21-C23-C25
12	P	614	II0	C10-C22-C24-C26
12	p	316	II0	C10-C22-C24-C26
12	p	317	II0	C09-C21-C23-C25
9	P	602	CLA	C6-C7-C8-C9
9	s	303	CLA	C6-C7-C8-C9
9	p	306	CLA	C2A-CAA-CBA-CGA
9	0	612	CLA	C1A-C2A-CAA-CBA
9	7	612	CLA	C1A-C2A-CAA-CBA
9	8	612	CLA	C1A-C2A-CAA-CBA
9	9	603	CLA	C1A-C2A-CAA-CBA
9	9	605	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	9	610	CLA	C1A-C2A-CAA-CBA
9	9	611	CLA	C1A-C2A-CAA-CBA
9	P	603	CLA	C1A-C2A-CAA-CBA
9	p	305	CLA	C1A-C2A-CAA-CBA
9	p	314	CLA	C1A-C2A-CAA-CBA
9	8	608	CLA	C11-C12-C13-C14
15	8	618	LHG	C4-O6-P-O3
9	7	602	CLA	CBA-CGA-O2A-C1
9	7	602	CLA	C2-C3-C5-C6
13	G	103	LMG	O1-C7-C8-C9
15	s	301	LHG	C4-C5-C6-O8
9	0	602	CLA	C11-C12-C13-C14
9	0	602	CLA	CBA-CGA-O2A-C1
13	8	617	LMG	O6-C5-C6-O5
15	s	301	LHG	C32-C33-C34-C35
13	G	103	LMG	O6-C5-C6-O5
10	8	610	KC2	C2A-CAA-CBA-CGA
9	p	310	CLA	C10-C11-C12-C13
9	p	313	CLA	C2A-CAA-CBA-CGA
9	0	604	CLA	O1D-CGD-O2D-CED
9	7	604	CLA	C5-C6-C7-C8
13	G	102	LMG	O1-C7-C8-O7
9	P	602	CLA	C11-C12-C13-C14
9	0	602	CLA	O1A-CGA-O2A-C1
9	7	602	CLA	O1A-CGA-O2A-C1
9	p	304	CLA	C11-C10-C8-C7
9	p	307	CLA	C11-C10-C8-C7
9	s	303	CLA	C6-C7-C8-C10
9	p	306	CLA	C3-C5-C6-C7
9	8	605	CLA	C6-C7-C8-C9
9	9	609	CLA	C6-C7-C8-C9
9	P	602	CLA	C11-C10-C8-C9
9	p	307	CLA	C11-C10-C8-C9
9	s	303	CLA	C11-C12-C13-C14
9	8	604	CLA	C2A-CAA-CBA-CGA
9	9	604	CLA	C2A-CAA-CBA-CGA
16	9	615	8CT	C10-C11-C12-C40
13	0	618	LMG	C32-C33-C34-C35
9	0	605	CLA	C4B-C3B-CAB-CBB
9	7	613	CLA	C4B-C3B-CAB-CBB
9	8	605	CLA	C4B-C3B-CAB-CBB
9	8	612	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
9	9	601	CLA	C4B-C3B-CAB-CBB
9	9	608	CLA	C4B-C3B-CAB-CBB
9	9	611	CLA	C4B-C3B-CAB-CBB
9	P	602	CLA	C4B-C3B-CAB-CBB
9	P	607	CLA	C4B-C3B-CAB-CBB
9	P	611	CLA	C4B-C3B-CAB-CBB
9	p	306	CLA	C4B-C3B-CAB-CBB
9	p	307	CLA	C4B-C3B-CAB-CBB
13	G	103	LMG	C28-C29-C30-C31
9	9	602	CLA	CBA-CGA-O2A-C1
13	8	617	LMG	C29-C28-O8-C9
9	9	603	CLA	CBA-CGA-O2A-C1
9	9	610	CLA	C3A-C2A-CAA-CBA
9	G	101	CLA	C3A-C2A-CAA-CBA
9	p	309	CLA	C3A-C2A-CAA-CBA
13	0	618	LMG	O1-C7-C8-C9
13	8	617	LMG	O1-C7-C8-C9
13	8	617	LMG	C7-C8-C9-O8
13	G	102	LMG	O1-C7-C8-C9
13	G	102	LMG	C7-C8-C9-O8
17	p	319	SQD	C44-C45-C46-O48
9	7	602	CLA	C11-C12-C13-C14
9	0	604	CLA	C5-C6-C7-C8
13	G	103	LMG	C29-C30-C31-C32
13	G	103	LMG	C29-C28-O8-C9
15	s	301	LHG	C31-C32-C33-C34
9	0	609	CLA	C2B-C3B-CAB-CBB
9	8	605	CLA	C2B-C3B-CAB-CBB
9	9	601	CLA	C2B-C3B-CAB-CBB
9	9	608	CLA	C2B-C3B-CAB-CBB
9	P	607	CLA	C2B-C3B-CAB-CBB
9	P	611	CLA	C2B-C3B-CAB-CBB
9	p	306	CLA	C2B-C3B-CAB-CBB
13	8	617	LMG	O1-C7-C8-O7
13	G	103	LMG	O1-C7-C8-O7
15	s	301	LHG	O7-C5-C6-O8
9	9	607	CLA	C11-C12-C13-C14
13	8	617	LMG	C32-C33-C34-C35
9	7	603	CLA	C2-C1-O2A-CGA
9	8	605	CLA	C2-C1-O2A-CGA
9	p	304	CLA	O1D-CGD-O2D-CED
15	s	301	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
9	0	601	CLA	C1A-C2A-CAA-CBA
9	8	601	CLA	C1A-C2A-CAA-CBA
9	9	601	CLA	C1A-C2A-CAA-CBA
9	p	303	CLA	C1A-C2A-CAA-CBA
12	7	616	II0	C31-C33-C35-C39
9	p	305	CLA	O1D-CGD-O2D-CED
9	0	606	CLA	O1D-CGD-O2D-CED
9	8	605	CLA	C6-C7-C8-C10
9	8	605	CLA	C11-C10-C8-C7
9	9	609	CLA	C6-C7-C8-C10
9	P	602	CLA	C11-C10-C8-C7
9	s	303	CLA	C11-C12-C13-C15
9	0	608	CLA	C5-C6-C7-C8
12	8	619	II0	C26-C30-C32-C34
9	0	603	CLA	CAD-CBD-CGD-O2D
9	0	606	CLA	CAD-CBD-CGD-O2D
9	7	603	CLA	CAD-CBD-CGD-O2D
9	7	607	CLA	CAD-CBD-CGD-O2D
9	P	603	CLA	CAD-CBD-CGD-O2D
9	p	311	CLA	CAD-CBD-CGD-O2D
9	0	604	CLA	C2A-CAA-CBA-CGA
10	0	610	KC2	CBD-CGD-O2D-CED
9	0	605	CLA	CHA-CBD-CGD-O1D
9	0	605	CLA	CHA-CBD-CGD-O2D
9	7	613	CLA	CHA-CBD-CGD-O1D
9	8	608	CLA	CHA-CBD-CGD-O1D
9	8	611	CLA	CHA-CBD-CGD-O1D
9	8	611	CLA	CHA-CBD-CGD-O2D
9	p	304	CLA	CHA-CBD-CGD-O1D
9	p	304	CLA	CHA-CBD-CGD-O2D
9	p	305	CLA	CHA-CBD-CGD-O1D
10	7	610	KC2	CHA-CBD-CGD-O2D
10	P	609	KC2	CHA-CBD-CGD-O1D
10	p	312	KC2	CHA-CBD-CGD-O2D
9	9	602	CLA	O1A-CGA-O2A-C1
9	9	603	CLA	O1A-CGA-O2A-C1
11	8	616	IHT	C11-C21-C24-C26
12	0	616	II0	C09-C21-C23-C25
12	7	616	II0	C10-C22-C24-C26
12	7	617	II0	C09-C21-C23-C25
12	7	617	II0	C10-C22-C24-C26
12	7	619	II0	C09-C21-C23-C25

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Mol	Chain	Res	Type	Atoms
12	7	619	II0	C10-C22-C24-C26
12	8	615	II0	C10-C22-C24-C26
12	9	612	II0	C09-C21-C23-C25
12	9	612	II0	C10-C22-C24-C26
12	9	614	II0	C10-C22-C24-C26
12	p	302	II0	C09-C21-C23-C25
12	p	315	II0	C10-C22-C24-C26
14	7	615	II3	C16-C23-C27-C28
9	8	605	CLA	C11-C10-C8-C9
9	8	605	CLA	C8-C10-C11-C12
9	7	604	CLA	C2A-CAA-CBA-CGA
13	G	102	LMG	O10-C28-O8-C9
16	P	615	8CT	C10-C11-C12-C40
16	9	615	8CT	C10-C11-C12-C13
16	P	615	8CT	C10-C11-C12-C13
11	0	617	IHT	C35-C38-C41-C40
15	8	618	LHG	C3-O3-P-O6
9	9	602	CLA	C2-C3-C5-C6
9	0	604	CLA	C4B-C3B-CAB-CBB
9	0	606	CLA	C4B-C3B-CAB-CBB
9	8	601	CLA	C4B-C3B-CAB-CBB
9	9	604	CLA	C4B-C3B-CAB-CBB
9	P	601	CLA	C4B-C3B-CAB-CBB
15	8	618	LHG	C3-O3-P-O4
15	8	618	LHG	C4-O6-P-O5
9	9	605	CLA	C2A-CAA-CBA-CGA
9	0	604	CLA	C6-C7-C8-C10
9	8	603	CLA	CAD-CBD-CGD-O1D
9	p	305	CLA	CAD-CBD-CGD-O1D
15	8	618	LHG	O6-C4-C5-C6
9	8	602	CLA	C11-C10-C8-C7
9	9	609	CLA	C11-C10-C8-C7
9	7	603	CLA	CBD-CGD-O2D-CED
9	P	604	CLA	C2A-CAA-CBA-CGA
9	9	605	CLA	CAA-CBA-CGA-O2A
13	0	618	LMG	O1-C7-C8-O7
13	8	617	LMG	O7-C8-C9-O8
9	0	602	CLA	C2B-C3B-CAB-CBB
9	0	605	CLA	C2B-C3B-CAB-CBB
9	0	608	CLA	C2B-C3B-CAB-CBB
9	0	611	CLA	C2B-C3B-CAB-CBB
9	7	613	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
9	8	601	CLA	C2B-C3B-CAB-CBB
9	8	607	CLA	C2B-C3B-CAB-CBB
9	8	612	CLA	C2B-C3B-CAB-CBB
9	9	604	CLA	C2B-C3B-CAB-CBB
9	9	610	CLA	C2B-C3B-CAB-CBB
9	9	611	CLA	C2B-C3B-CAB-CBB
9	P	601	CLA	C2B-C3B-CAB-CBB
9	P	602	CLA	C2B-C3B-CAB-CBB
9	p	307	CLA	C2B-C3B-CAB-CBB
9	s	303	CLA	C10-C11-C12-C13
9	8	602	CLA	C2A-CAA-CBA-CGA
9	P	602	CLA	C2A-CAA-CBA-CGA
9	p	305	CLA	C2-C1-O2A-CGA
15	s	301	LHG	C4-O6-P-O3
9	8	602	CLA	C11-C10-C8-C9
9	9	609	CLA	C11-C10-C8-C9
9	p	304	CLA	C11-C10-C8-C9
9	7	606	CLA	C4C-C3C-CAC-CBC
9	7	606	CLA	C2C-C3C-CAC-CBC
13	G	102	LMG	C29-C28-O8-C9
9	0	602	CLA	C4B-C3B-CAB-CBB
9	0	608	CLA	C4B-C3B-CAB-CBB
9	0	611	CLA	C4B-C3B-CAB-CBB
9	8	603	CLA	C4B-C3B-CAB-CBB
9	8	607	CLA	C4B-C3B-CAB-CBB
9	9	610	CLA	C4B-C3B-CAB-CBB
9	P	604	CLA	C5-C6-C7-C8
9	G	101	CLA	C2A-CAA-CBA-CGA
9	p	306	CLA	C3A-C2A-CAA-CBA
9	0	611	CLA	CAA-CBA-CGA-O1A
9	7	603	CLA	O1D-CGD-O2D-CED
9	8	605	CLA	CAA-CBA-CGA-O2A
12	p	317	II0	C10-C22-C24-C26
9	s	303	CLA	C12-C13-C15-C16
9	7	613	CLA	CAA-CBA-CGA-O1A
17	p	319	SQD	O48-C23-C24-C25
9	0	605	CLA	CAA-CBA-CGA-O2A
9	P	610	CLA	CAA-CBA-CGA-O1A
9	P	610	CLA	CAA-CBA-CGA-O2A
9	9	607	CLA	C2A-CAA-CBA-CGA
10	0	610	KC2	C3A-C2A-CAA-CBA
10	7	610	KC2	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
10	P	605	KC2	C3A-C2A-CAA-CBA
10	P	609	KC2	C3A-C2A-CAA-CBA
10	p	312	KC2	C3A-C2A-CAA-CBA
9	P	604	CLA	C6-C7-C8-C10
9	0	611	CLA	CAA-CBA-CGA-O2A
9	0	604	CLA	C2B-C3B-CAB-CBB
9	0	606	CLA	C2B-C3B-CAB-CBB
9	8	602	CLA	C2B-C3B-CAB-CBB
9	P	606	CLA	C2B-C3B-CAB-CBB
9	9	611	CLA	O1D-CGD-O2D-CED
9	0	608	CLA	C10-C11-C12-C13
9	7	602	CLA	C3-C5-C6-C7
13	0	618	LMG	C29-C30-C31-C32
9	7	613	CLA	CAA-CBA-CGA-O2A
9	9	602	CLA	C2A-CAA-CBA-CGA
9	9	611	CLA	CBD-CGD-O2D-CED
9	p	313	CLA	C2C-C3C-CAC-CBC
9	P	611	CLA	CAA-CBA-CGA-O1A
12	7	616	II0	C26-C30-C32-C34
12	p	316	II0	C25-C29-C31-C33
17	p	319	SQD	C45-C44-O6-C1
9	7	611	CLA	CAA-CBA-CGA-O2A
9	P	607	CLA	C11-C12-C13-C15
17	p	319	SQD	C9-C10-C11-C12
9	7	607	CLA	CAA-CBA-CGA-O2A
9	9	610	CLA	C2A-CAA-CBA-CGA
9	7	611	CLA	C4B-C3B-CAB-CBB
9	8	602	CLA	C4B-C3B-CAB-CBB
9	P	606	CLA	C4B-C3B-CAB-CBB
17	p	319	SQD	C12-C13-C14-C15
9	8	612	CLA	CAA-CBA-CGA-O2A
9	8	605	CLA	C11-C12-C13-C15
9	7	611	CLA	CAA-CBA-CGA-O1A
9	0	612	CLA	CAA-CBA-CGA-O2A
9	7	607	CLA	CAA-CBA-CGA-O1A
9	7	612	CLA	CAA-CBA-CGA-O2A
9	0	606	CLA	CAA-CBA-CGA-O2A
9	0	613	CLA	CAD-CBD-CGD-O2D
9	7	609	CLA	CAD-CBD-CGD-O2D
9	8	601	CLA	CAD-CBD-CGD-O2D
9	8	607	CLA	CAD-CBD-CGD-O2D
9	8	612	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
9	9	606	CLA	CAD-CBD-CGD-O2D
9	9	608	CLA	CAD-CBD-CGD-O2D
9	P	606	CLA	CAD-CBD-CGD-O2D
9	s	302	CLA	CAD-CBD-CGD-O2D
10	P	605	KC2	CAD-CBD-CGD-O2D
9	7	602	CLA	C2A-CAA-CBA-CGA
9	0	613	CLA	CAA-CBA-CGA-O2A
9	p	309	CLA	CAA-CBA-CGA-O2A
9	p	306	CLA	CAA-CBA-CGA-O2A
9	9	602	CLA	C11-C12-C13-C14
12	8	615	II0	C32-C34-C36-C40
9	0	613	CLA	CAA-CBA-CGA-O1A
9	9	609	CLA	O2A-C1-C2-C3
9	0	612	CLA	CAA-CBA-CGA-O1A
9	0	601	CLA	CHA-CBD-CGD-O1D
9	0	601	CLA	CHA-CBD-CGD-O2D
9	0	608	CLA	CHA-CBD-CGD-O1D
9	0	608	CLA	CHA-CBD-CGD-O2D
9	0	609	CLA	CHA-CBD-CGD-O1D
9	0	609	CLA	CHA-CBD-CGD-O2D
9	7	606	CLA	CHA-CBD-CGD-O1D
9	7	608	CLA	CHA-CBD-CGD-O1D
9	7	608	CLA	CHA-CBD-CGD-O2D
9	7	611	CLA	CHA-CBD-CGD-O1D
9	7	611	CLA	CHA-CBD-CGD-O2D
9	7	613	CLA	CHA-CBD-CGD-O2D
9	8	605	CLA	CHA-CBD-CGD-O1D
9	8	605	CLA	CHA-CBD-CGD-O2D
9	8	608	CLA	CHA-CBD-CGD-O2D
9	9	602	CLA	CHA-CBD-CGD-O1D
9	9	602	CLA	CHA-CBD-CGD-O2D
9	9	605	CLA	CHA-CBD-CGD-O1D
9	9	611	CLA	CHA-CBD-CGD-O1D
9	P	602	CLA	CHA-CBD-CGD-O1D
9	P	602	CLA	CHA-CBD-CGD-O2D
9	P	607	CLA	CHA-CBD-CGD-O1D
9	P	607	CLA	CHA-CBD-CGD-O2D
9	p	303	CLA	CHA-CBD-CGD-O1D
9	p	303	CLA	CHA-CBD-CGD-O2D
9	p	305	CLA	CHA-CBD-CGD-O2D
9	p	308	CLA	CHA-CBD-CGD-O2D
9	p	310	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
9	p	310	CLA	CHA-CBD-CGD-O2D
9	p	314	CLA	CHA-CBD-CGD-O1D
9	s	303	CLA	CHA-CBD-CGD-O1D
9	s	303	CLA	CHA-CBD-CGD-O2D
10	0	610	KC2	CHA-CBD-CGD-O1D
10	P	609	KC2	CHA-CBD-CGD-O2D
10	p	312	KC2	CHA-CBD-CGD-O1D
9	7	606	CLA	CAA-CBA-CGA-O2A
9	0	606	CLA	CAA-CBA-CGA-O1A
9	7	612	CLA	CAA-CBA-CGA-O1A
9	8	612	CLA	CAA-CBA-CGA-O1A
9	p	309	CLA	CAA-CBA-CGA-O1A
9	s	303	CLA	CAA-CBA-CGA-O2A
13	0	618	LMG	C15-C16-C17-C18
9	p	308	CLA	O1D-CGD-O2D-CED
9	p	304	CLA	C11-C12-C13-C14
9	P	611	CLA	CAA-CBA-CGA-O2A
9	P	606	CLA	C1A-C2A-CAA-CBA
9	p	306	CLA	C1A-C2A-CAA-CBA
9	p	307	CLA	CAA-CBA-CGA-O2A
9	p	310	CLA	C2A-CAA-CBA-CGA
15	s	301	LHG	O10-C23-C24-C25
9	8	606	CLA	CAA-CBA-CGA-O2A
13	8	617	LMG	O9-C10-C11-C12
9	P	604	CLA	CAA-CBA-CGA-O2A
9	p	308	CLA	CAA-CBA-CGA-O2A
9	p	304	CLA	C2A-CAA-CBA-CGA
9	p	306	CLA	CAA-CBA-CGA-O1A
9	7	606	CLA	CAA-CBA-CGA-O1A
9	G	101	CLA	CAA-CBA-CGA-O2A
15	s	301	LHG	C29-C30-C31-C32
9	7	613	CLA	CAD-CBD-CGD-O1D
9	8	605	CLA	CAD-CBD-CGD-O1D
9	p	303	CLA	CAD-CBD-CGD-O1D
9	s	303	CLA	CAA-CBA-CGA-O1A
9	8	604	CLA	CAA-CBA-CGA-O2A
9	9	604	CLA	CAA-CBA-CGA-O2A
13	G	103	LMG	O8-C28-C29-C30
9	p	308	CLA	CAA-CBA-CGA-O1A
9	7	601	CLA	C3A-C2A-CAA-CBA
9	9	602	CLA	C11-C10-C8-C7
16	9	615	8CT	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
16	P	615	8CT	C28-C29-C30-C31
9	8	606	CLA	CAA-CBA-CGA-O1A
12	0	619	II0	C32-C34-C36-C40
9	7	604	CLA	CAA-CBA-CGA-O2A
9	9	604	CLA	CAA-CBA-CGA-O1A
9	0	604	CLA	CAA-CBA-CGA-O2A
9	9	609	CLA	CAA-CBA-CGA-O2A
9	p	307	CLA	CAA-CBA-CGA-O1A
9	G	101	CLA	CAA-CBA-CGA-O1A
9	8	604	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

54 monomers are involved in 91 short contacts:

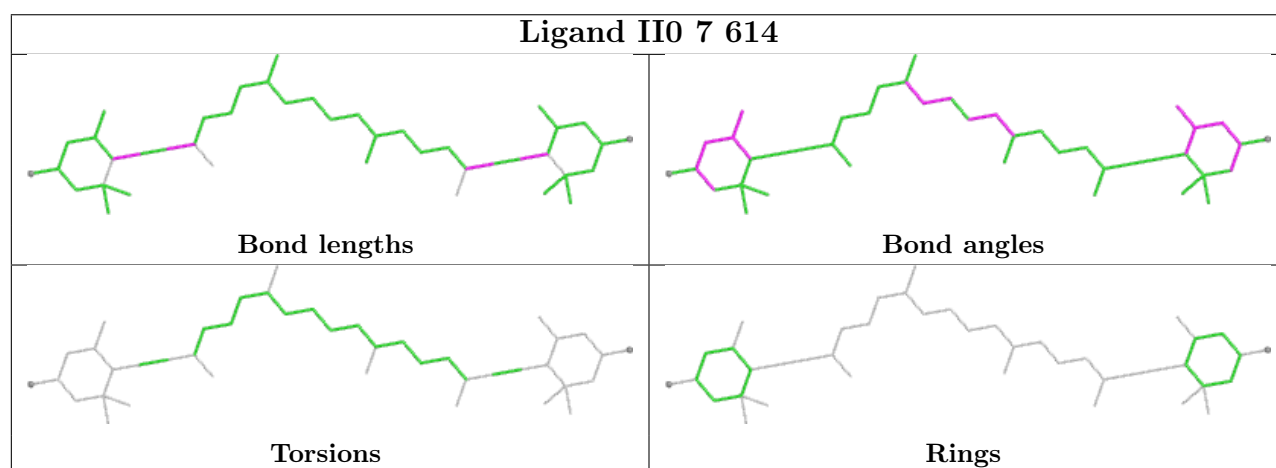
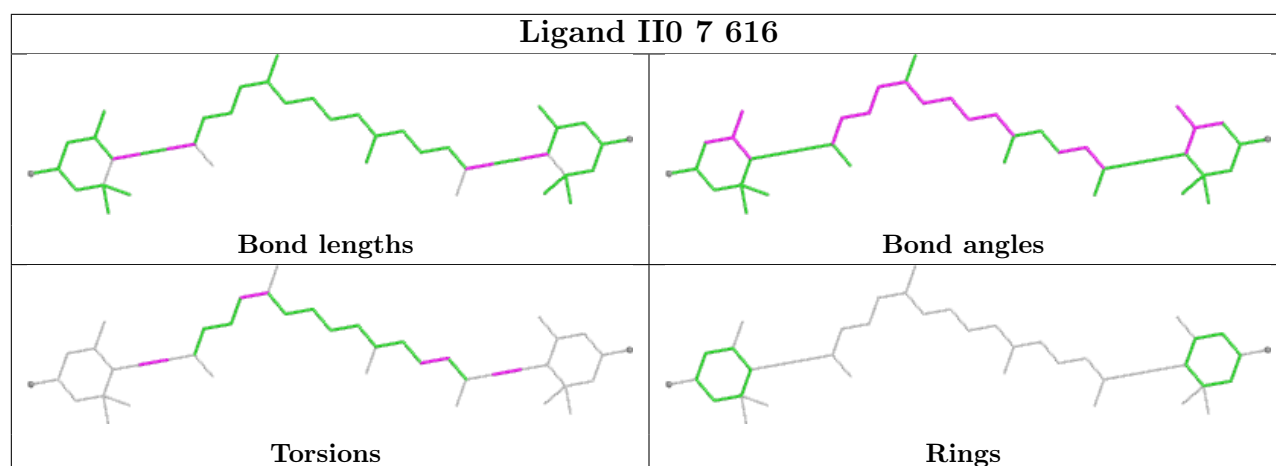
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	7	614	II0	1	0
9	9	610	CLA	1	0
9	P	604	CLA	1	0
9	0	612	CLA	2	0
9	P	607	CLA	2	0
9	8	609	CLA	1	0
9	0	613	CLA	1	0
9	8	602	CLA	1	0
9	9	606	CLA	2	0
9	9	602	CLA	1	0
9	8	605	CLA	2	0
9	8	611	CLA	1	0
9	0	603	CLA	1	0
9	0	608	CLA	3	0
9	0	607	CLA	3	0
9	7	607	CLA	2	0
9	s	303	CLA	2	0
9	P	606	CLA	2	0
9	9	609	CLA	3	0
9	7	602	CLA	4	0
9	7	612	CLA	2	0
9	p	310	CLA	1	0
9	7	605	CLA	3	0
12	8	619	II0	1	0
9	7	606	CLA	1	0
9	9	604	CLA	1	0
9	7	603	CLA	1	0

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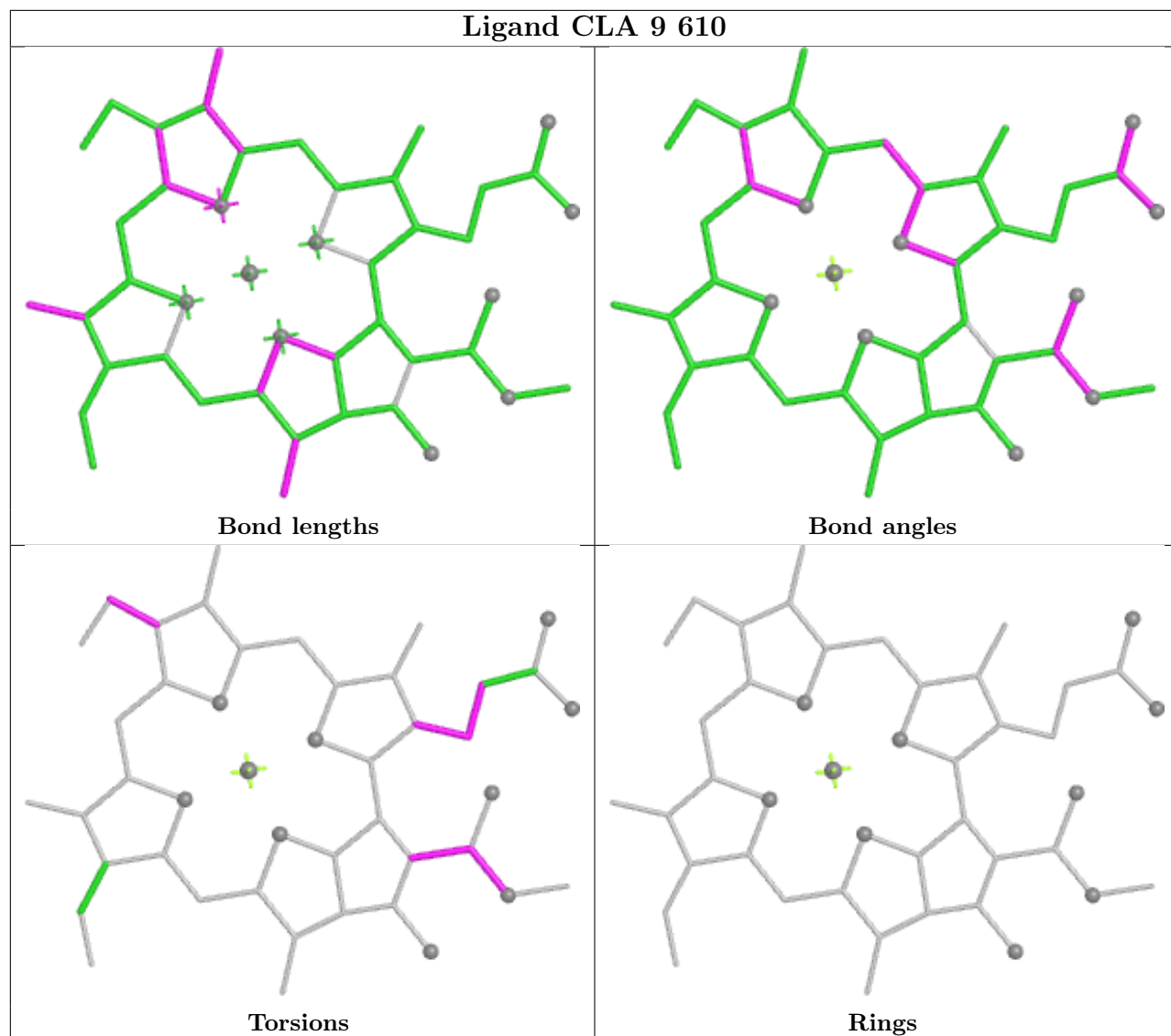
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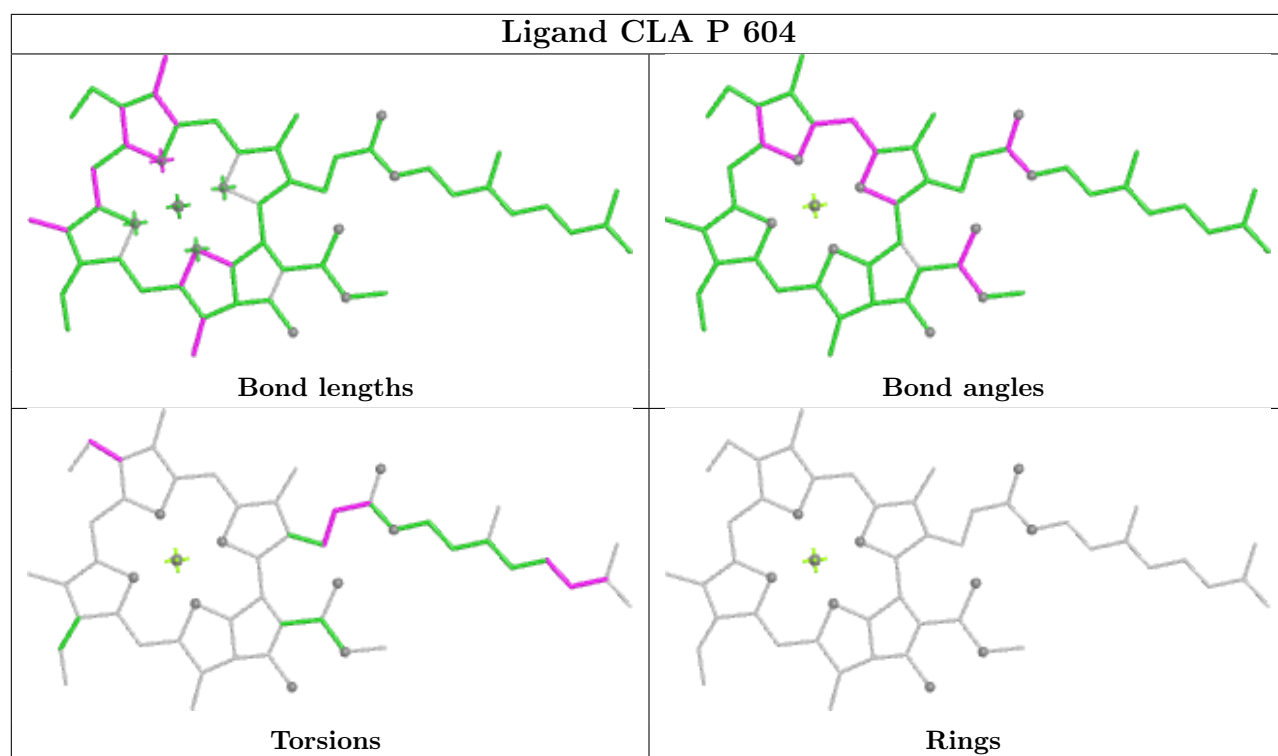
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	8	606	CLA	4	0
9	p	309	CLA	4	0
15	s	301	LHG	2	0
9	P	602	CLA	3	0
9	9	607	CLA	4	0
9	P	610	CLA	1	0
9	p	307	CLA	3	0
9	0	601	CLA	1	0
12	0	616	II0	1	0
13	8	617	LMG	2	0
9	9	605	CLA	1	0
9	7	604	CLA	1	0
9	p	304	CLA	3	0
9	p	306	CLA	2	0
9	8	607	CLA	2	0
12	8	614	II0	1	0
9	7	611	CLA	2	0
17	p	319	SQD	4	0
9	0	602	CLA	2	0
9	G	101	CLA	2	0
9	s	302	CLA	4	0
9	P	611	CLA	1	0
9	8	603	CLA	2	0
9	8	608	CLA	2	0
9	0	605	CLA	1	0
9	7	608	CLA	1	0
9	7	613	CLA	1	0

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

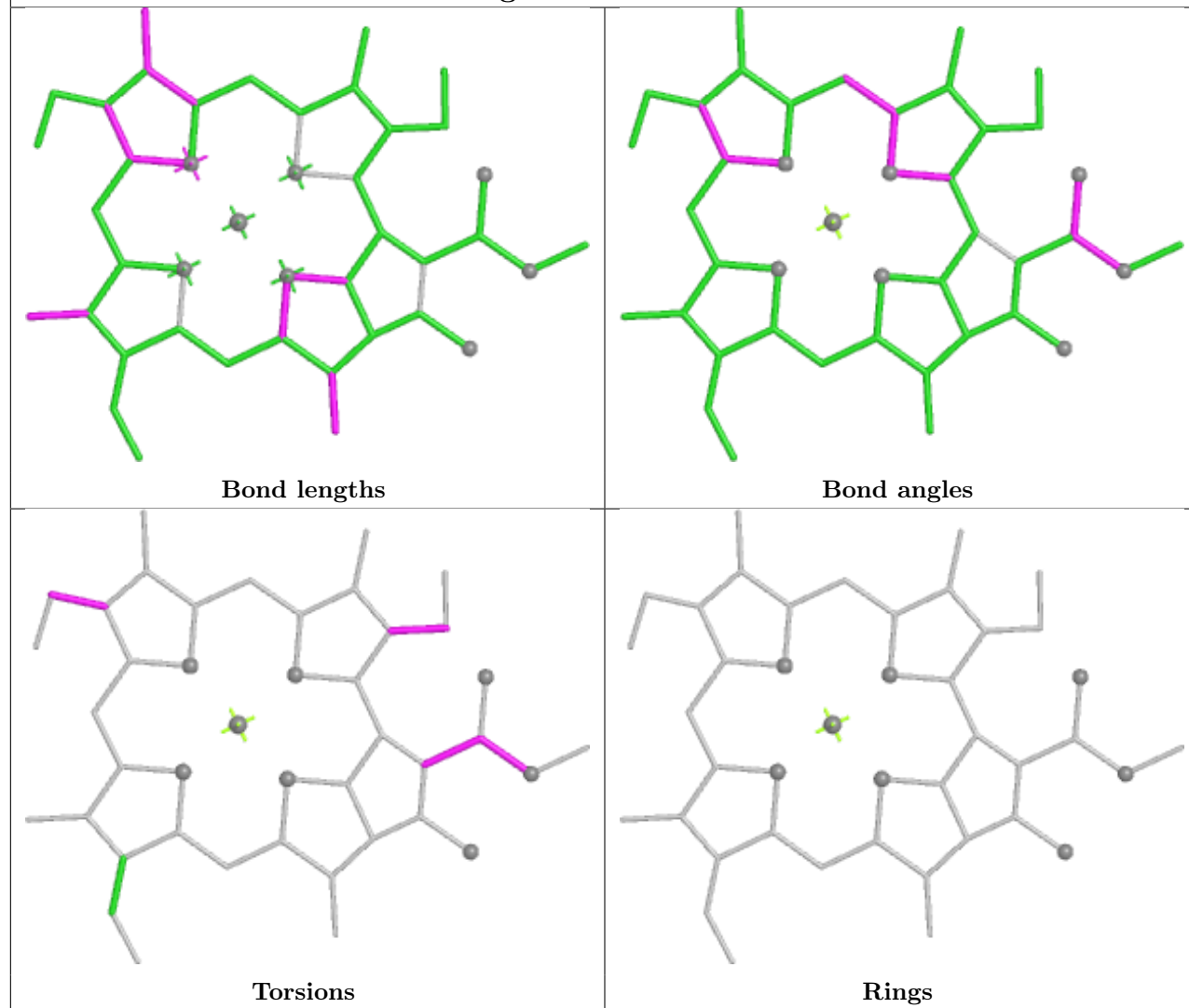


Ligand CLA 9 610

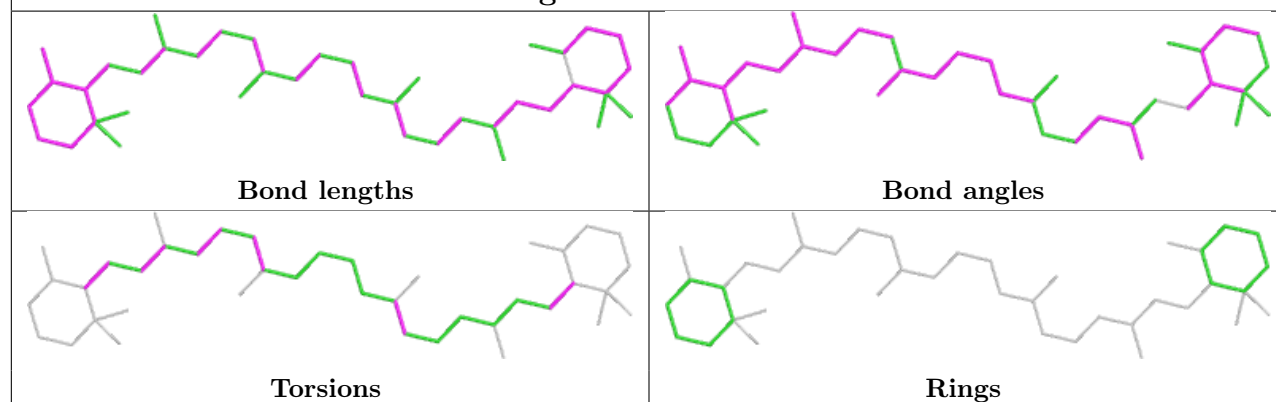




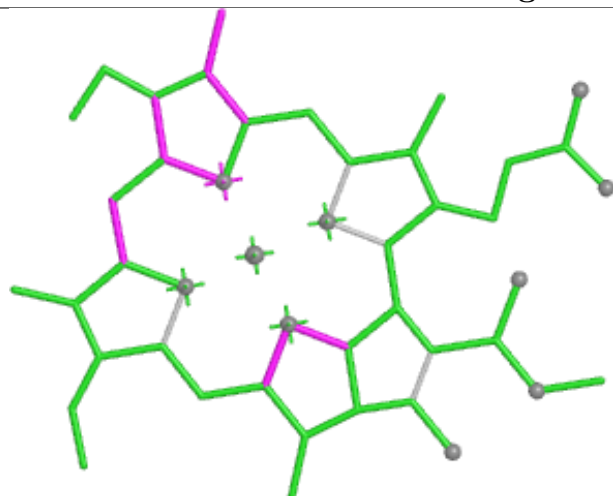
Ligand CLA 8 601



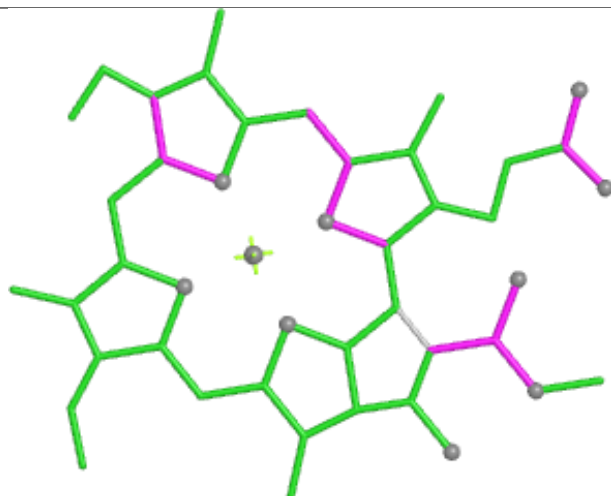
Ligand 8CT 9 615



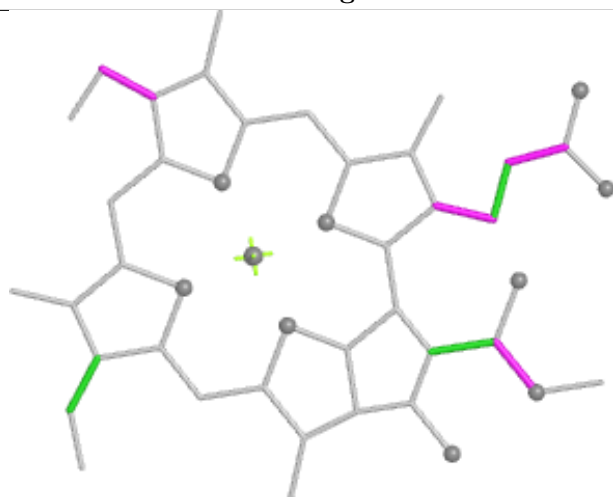
Ligand CLA 0 612



Bond lengths



Bond angles

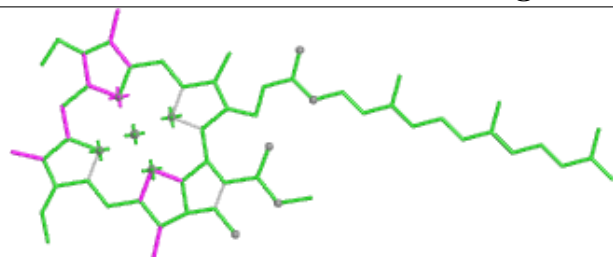


Torsions

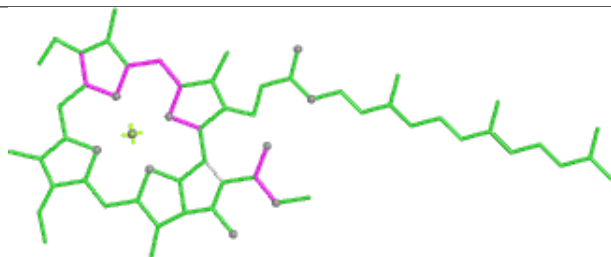


Rings

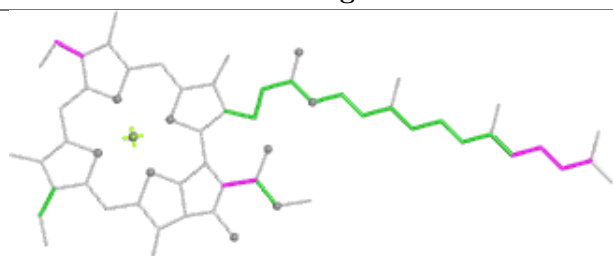
Ligand CLA P 607



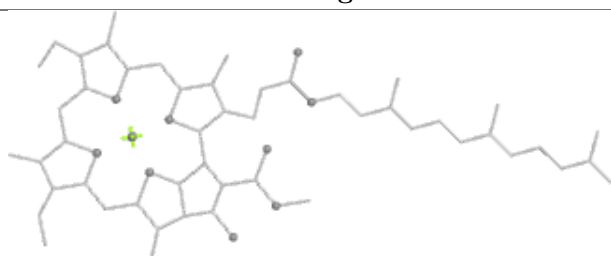
Bond lengths



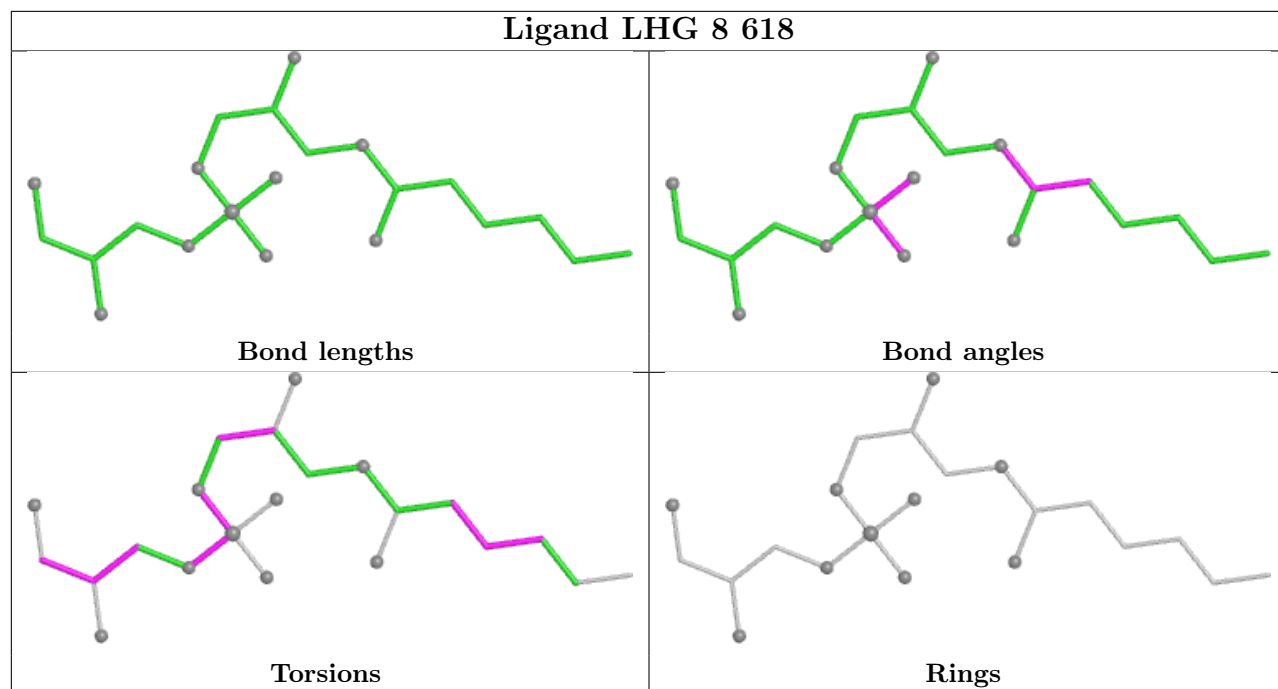
Bond angles



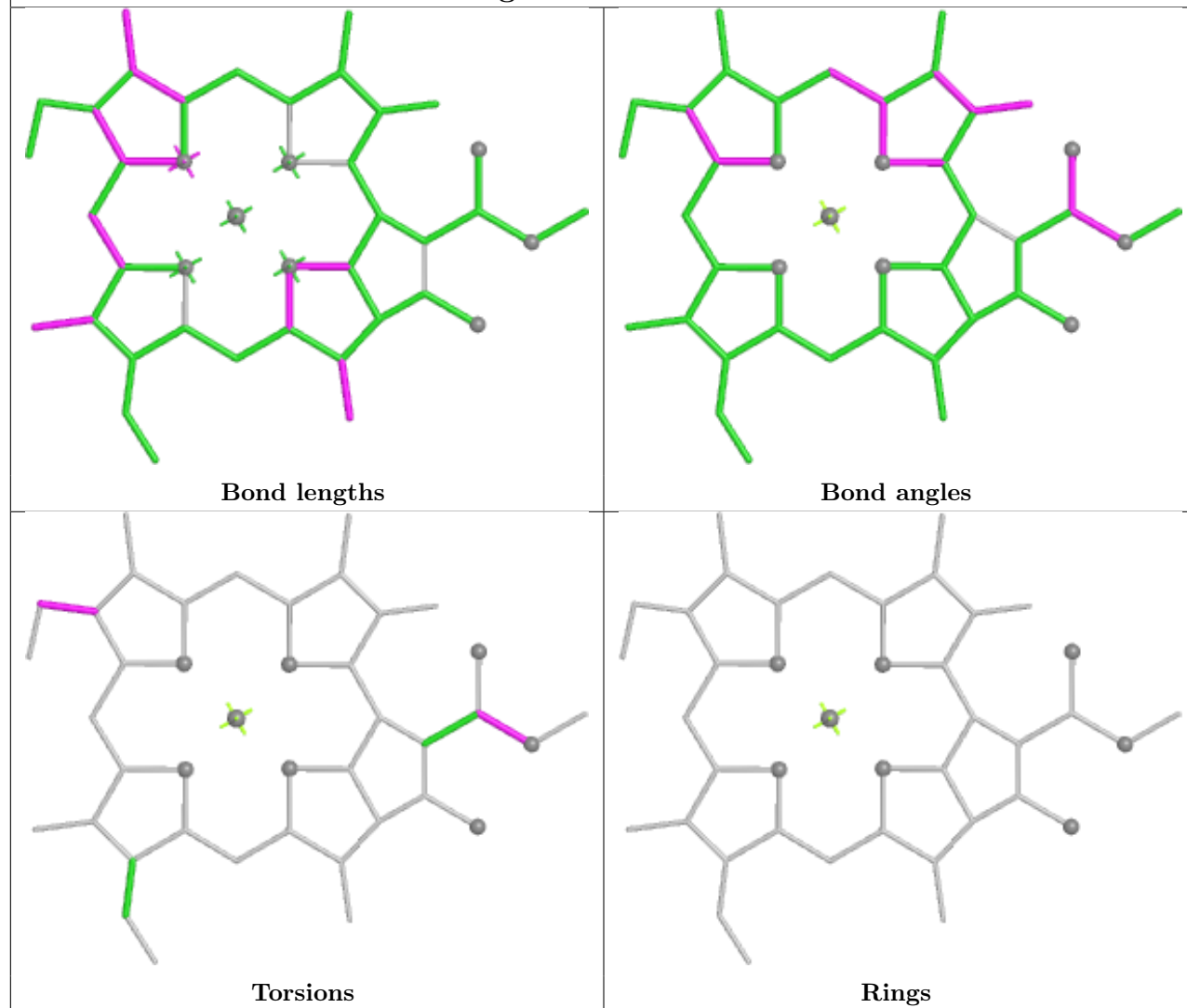
Torsions



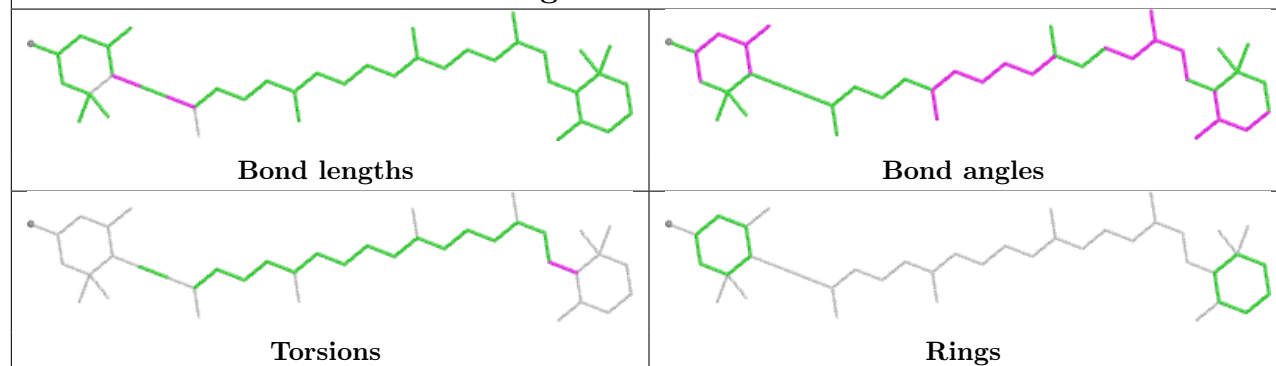
Rings



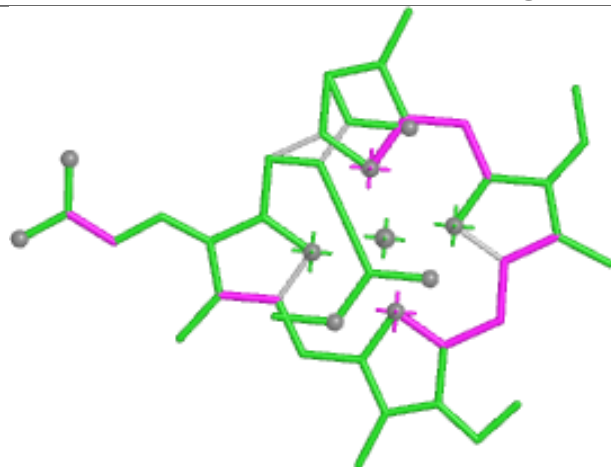
Ligand CLA 8 609



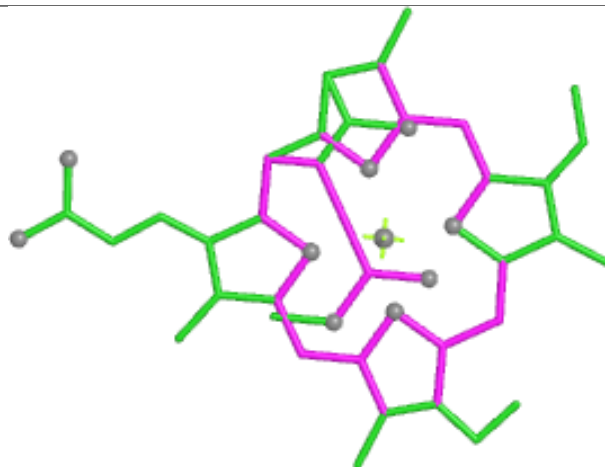
Ligand IHT 7 618



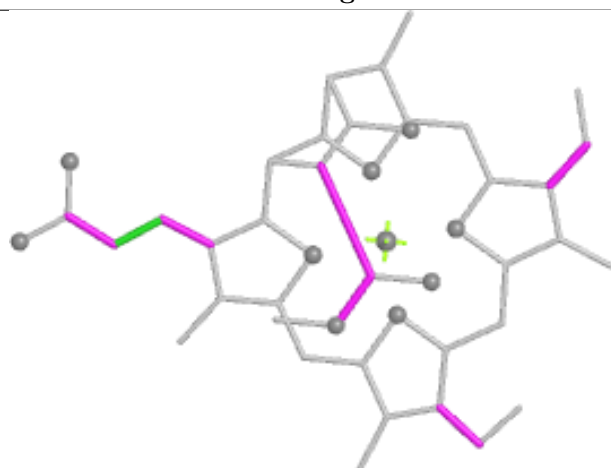
Ligand KC2 7 610



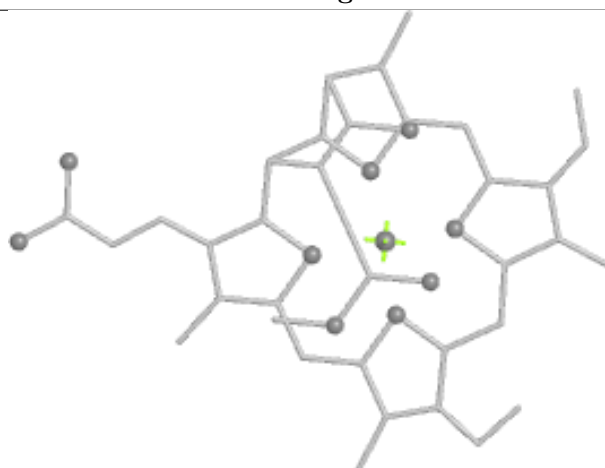
Bond lengths



Bond angles

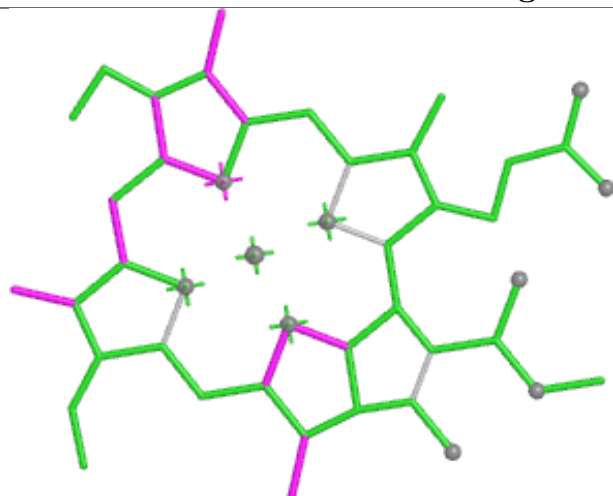


Torsions

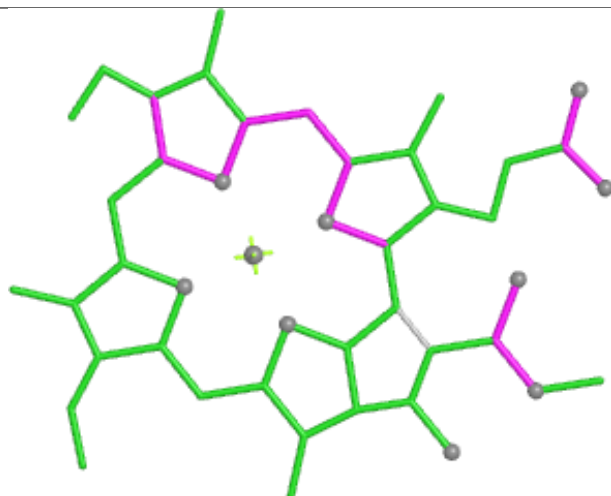


Rings

Ligand CLA 0 613



Bond lengths



Bond angles

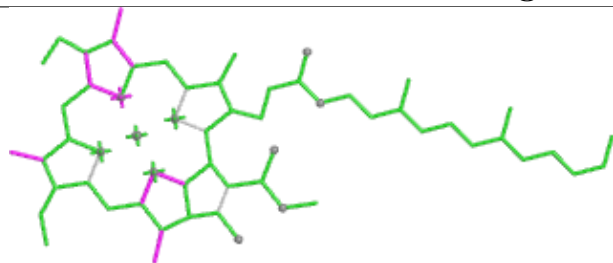


Torsions

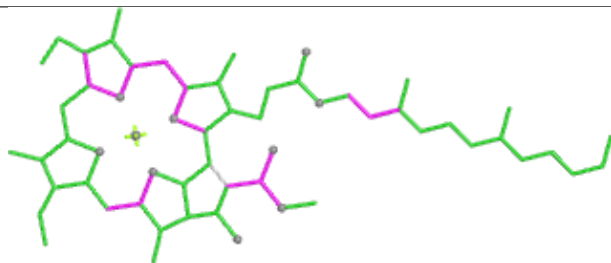


Rings

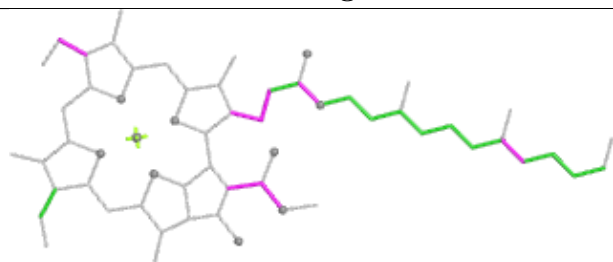
Ligand CLA 8 602



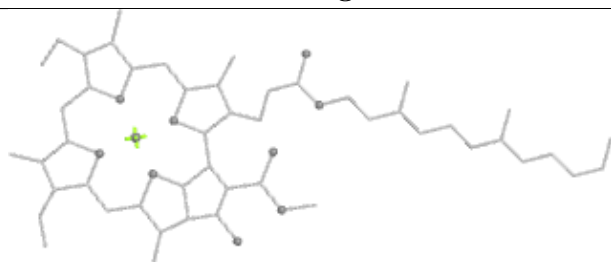
Bond lengths



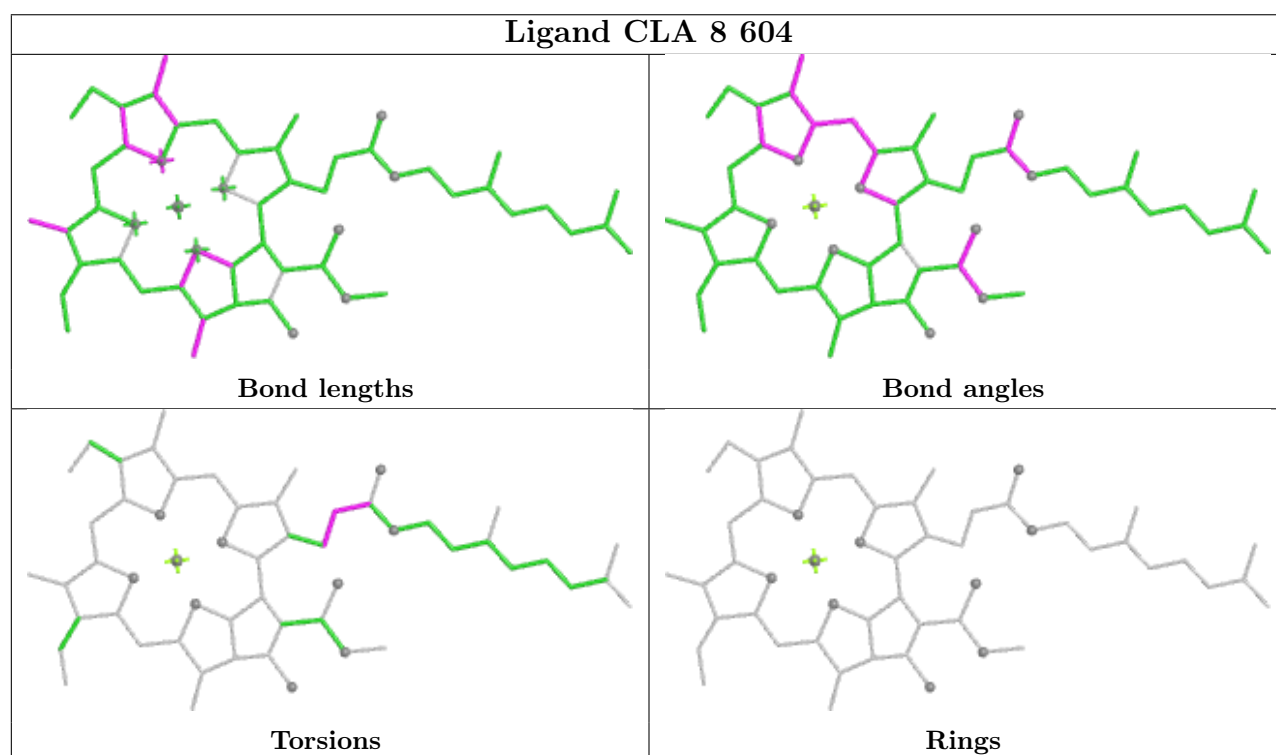
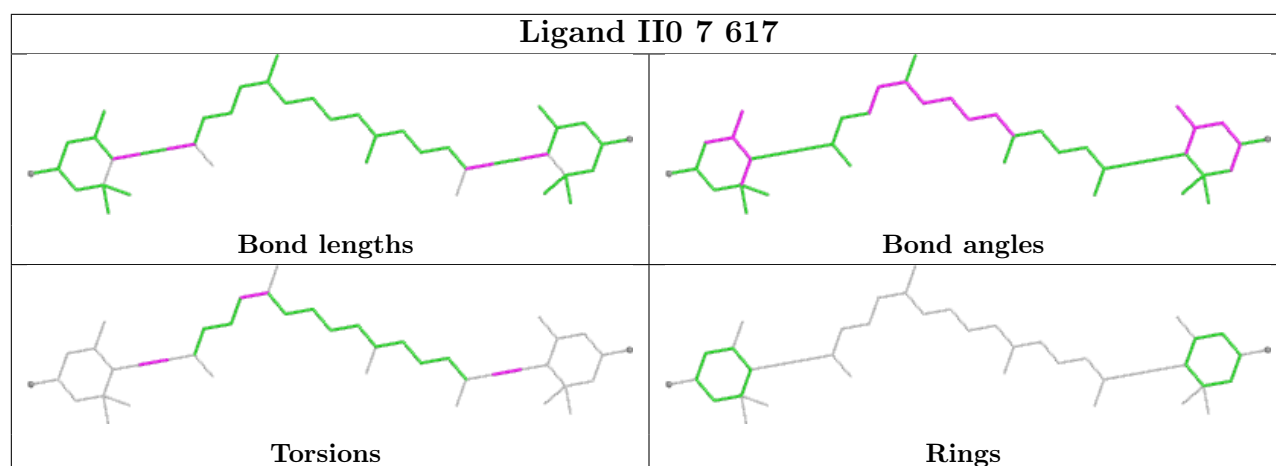
Bond angles



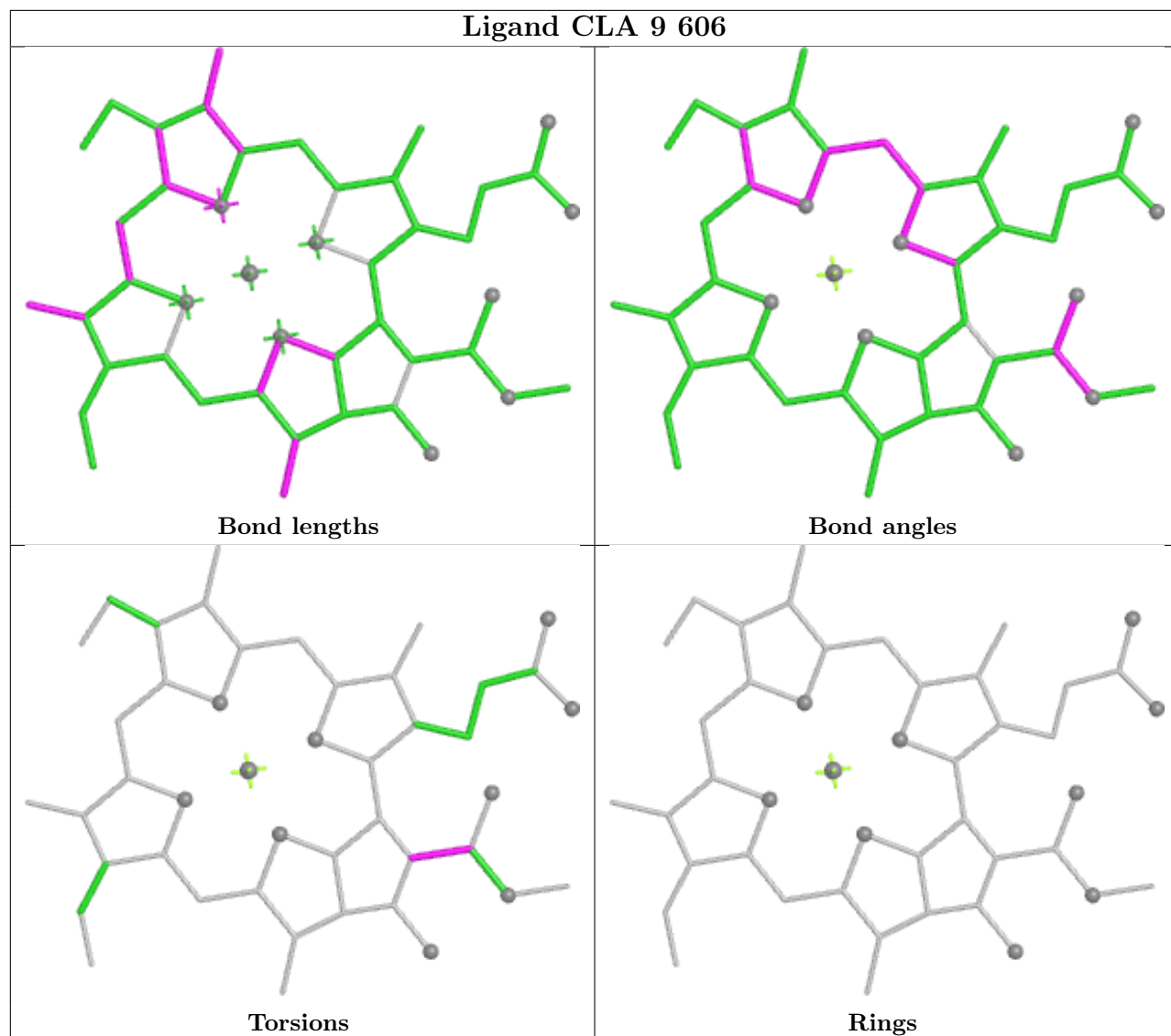
Torsions



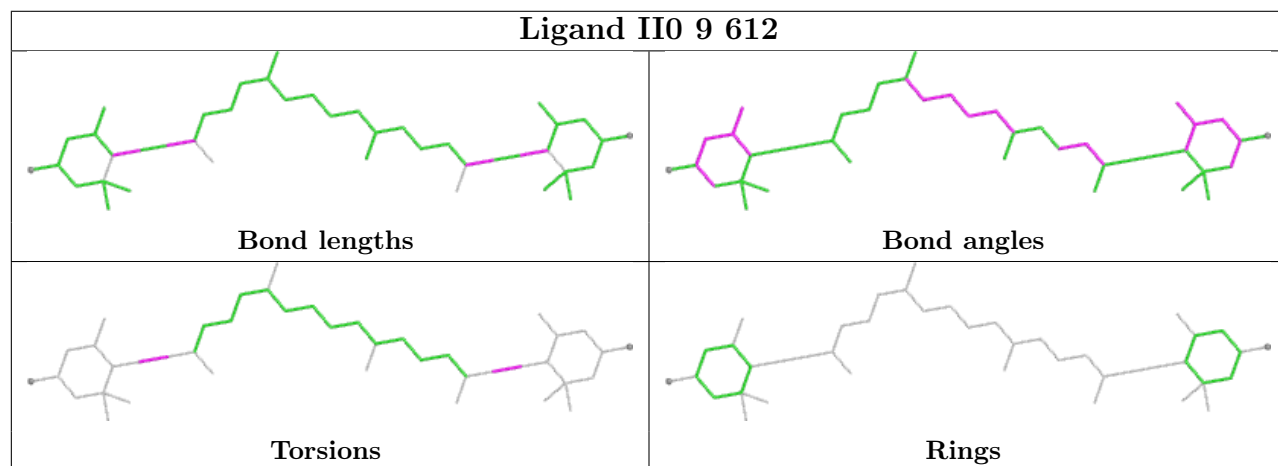
Rings



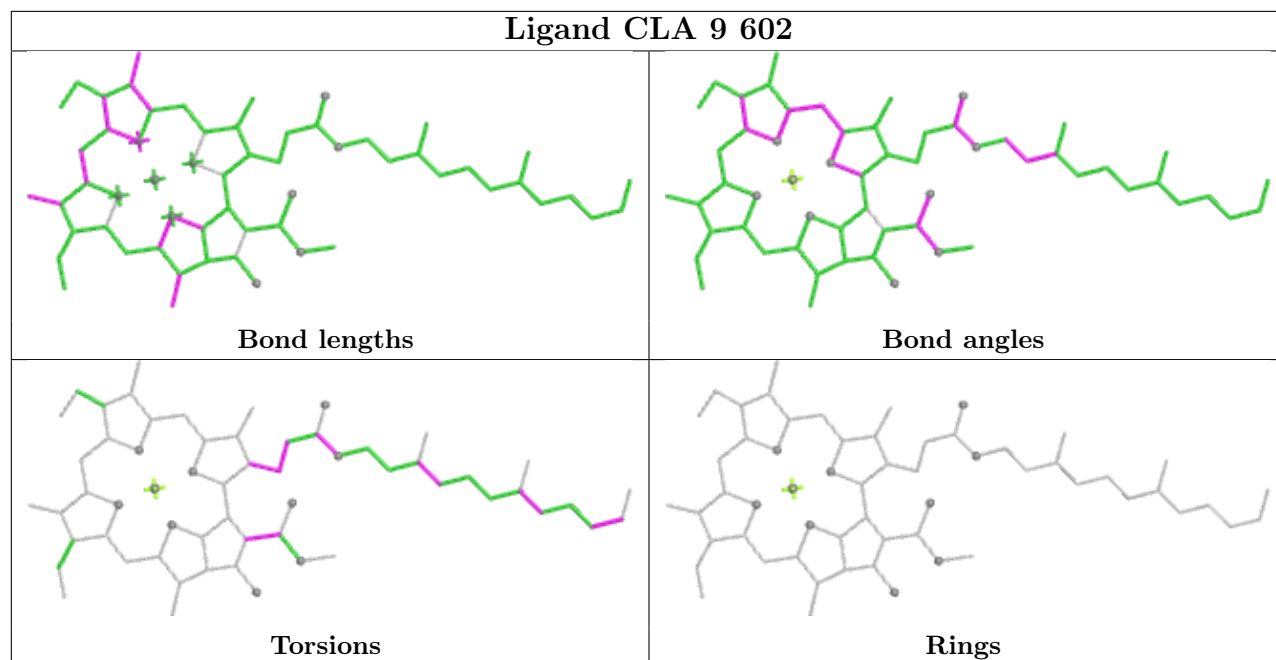
Ligand CLA 9 606



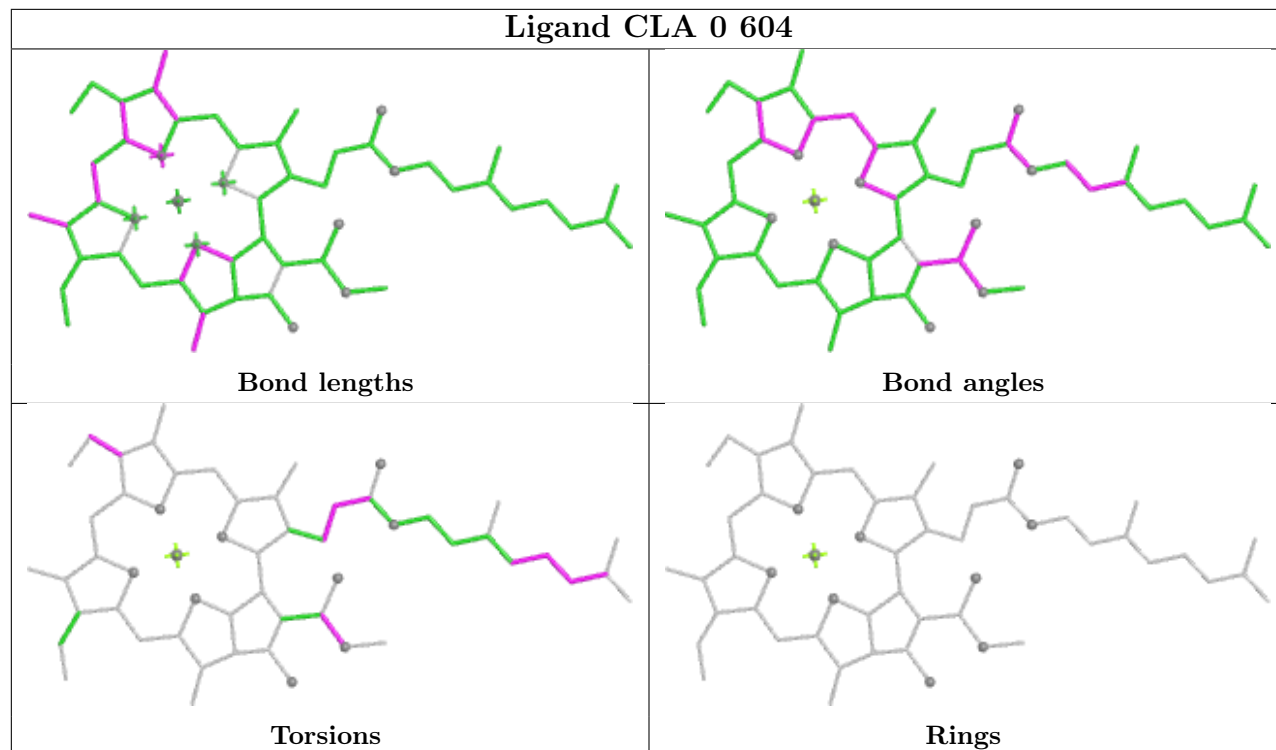
Ligand II0 9 612



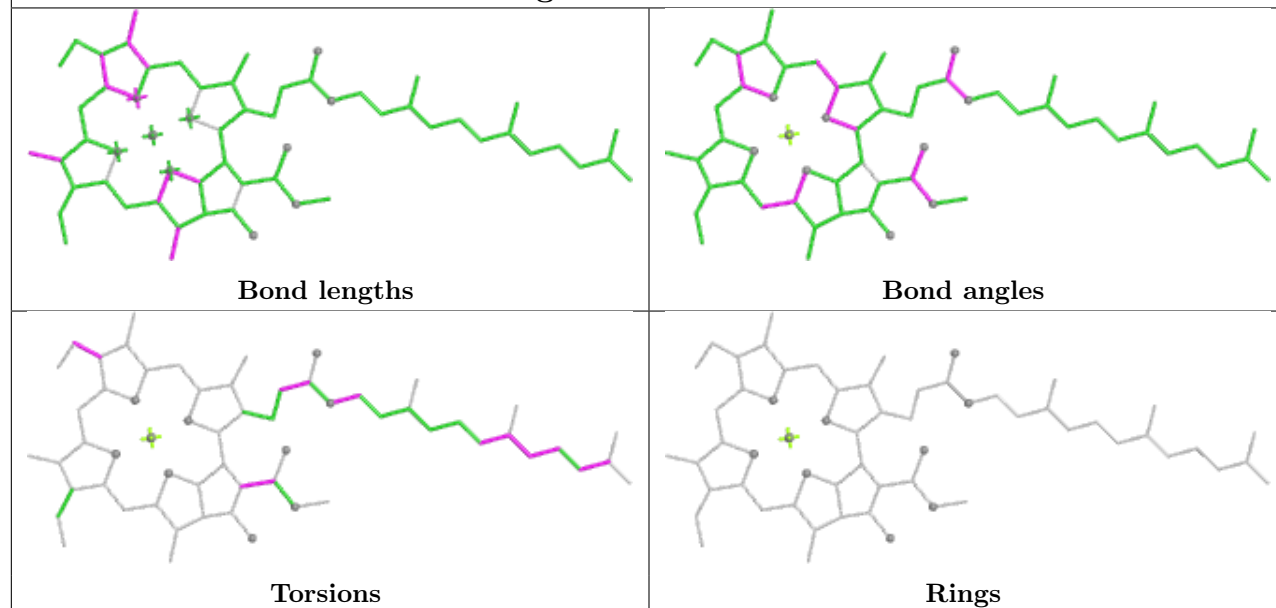
Ligand CLA 9 602



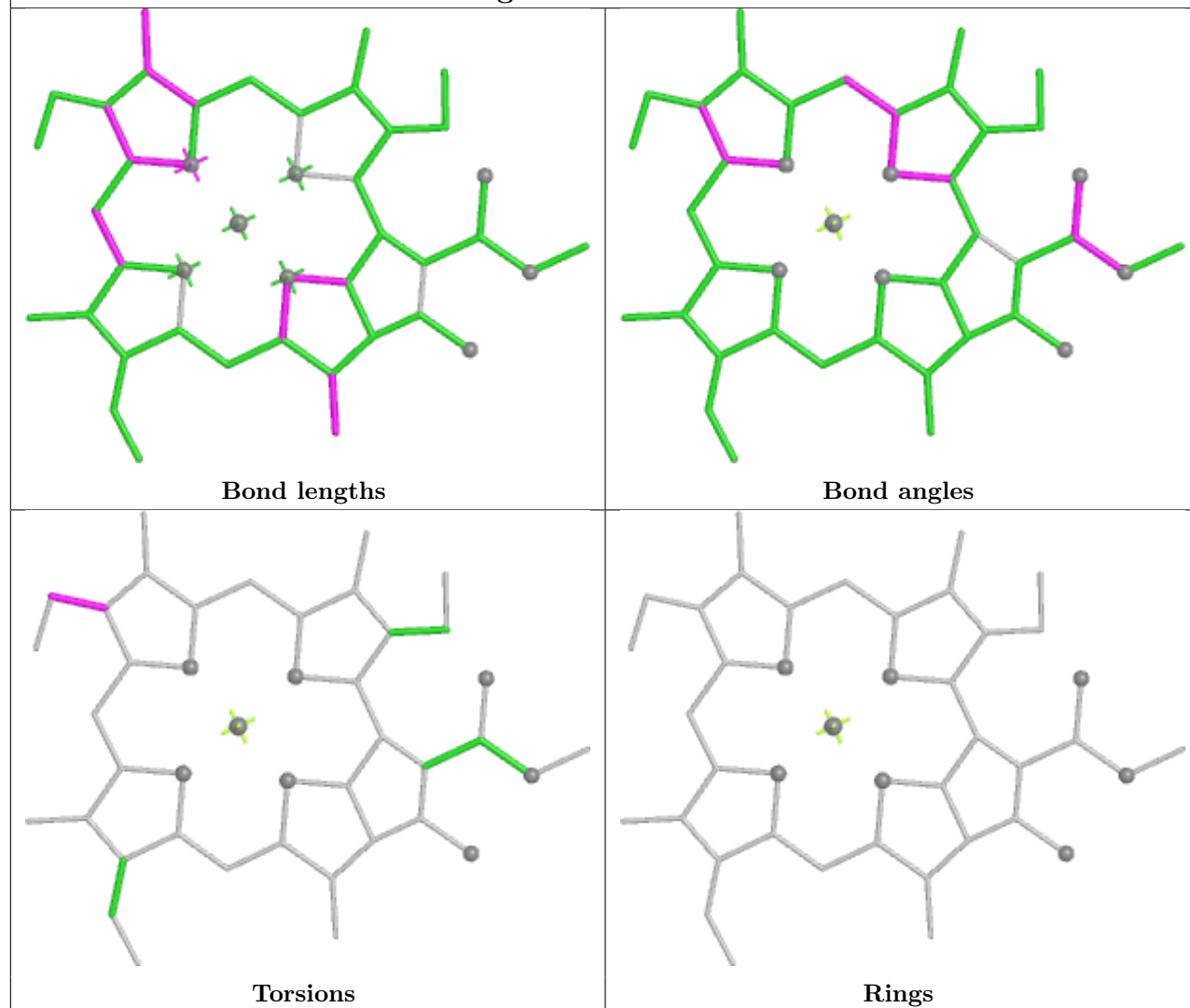
Ligand CLA 0 604



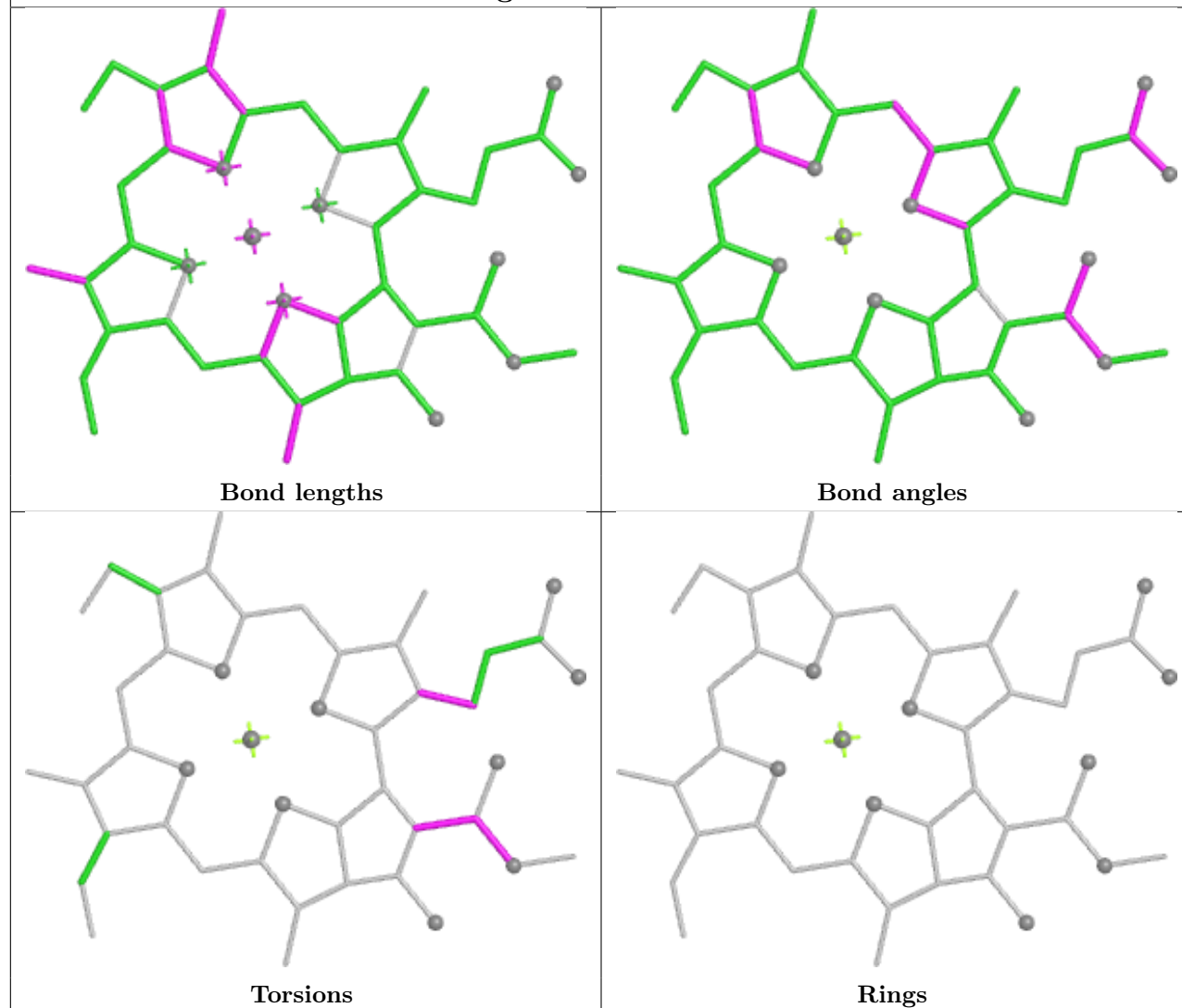
Ligand CLA 8 605



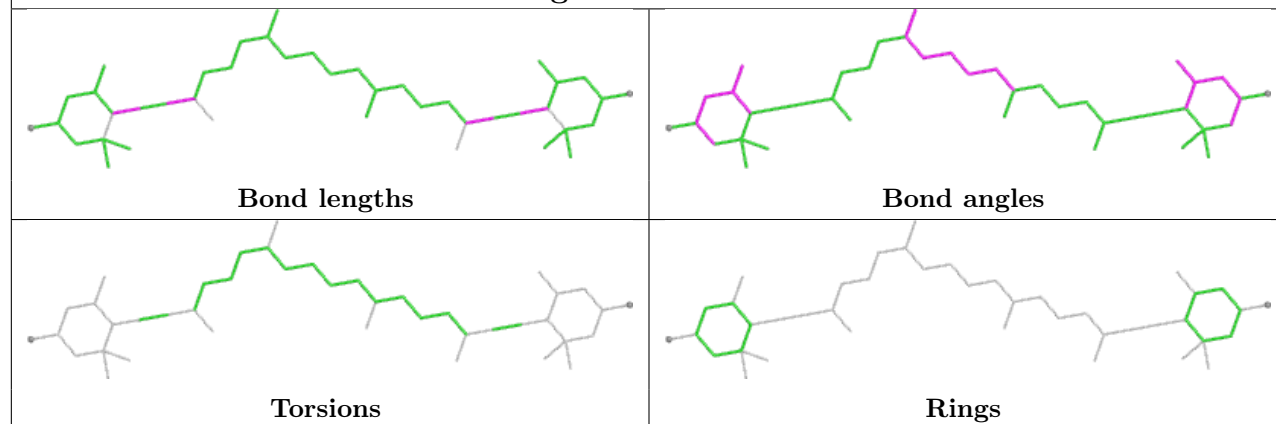
Ligand CLA P 601



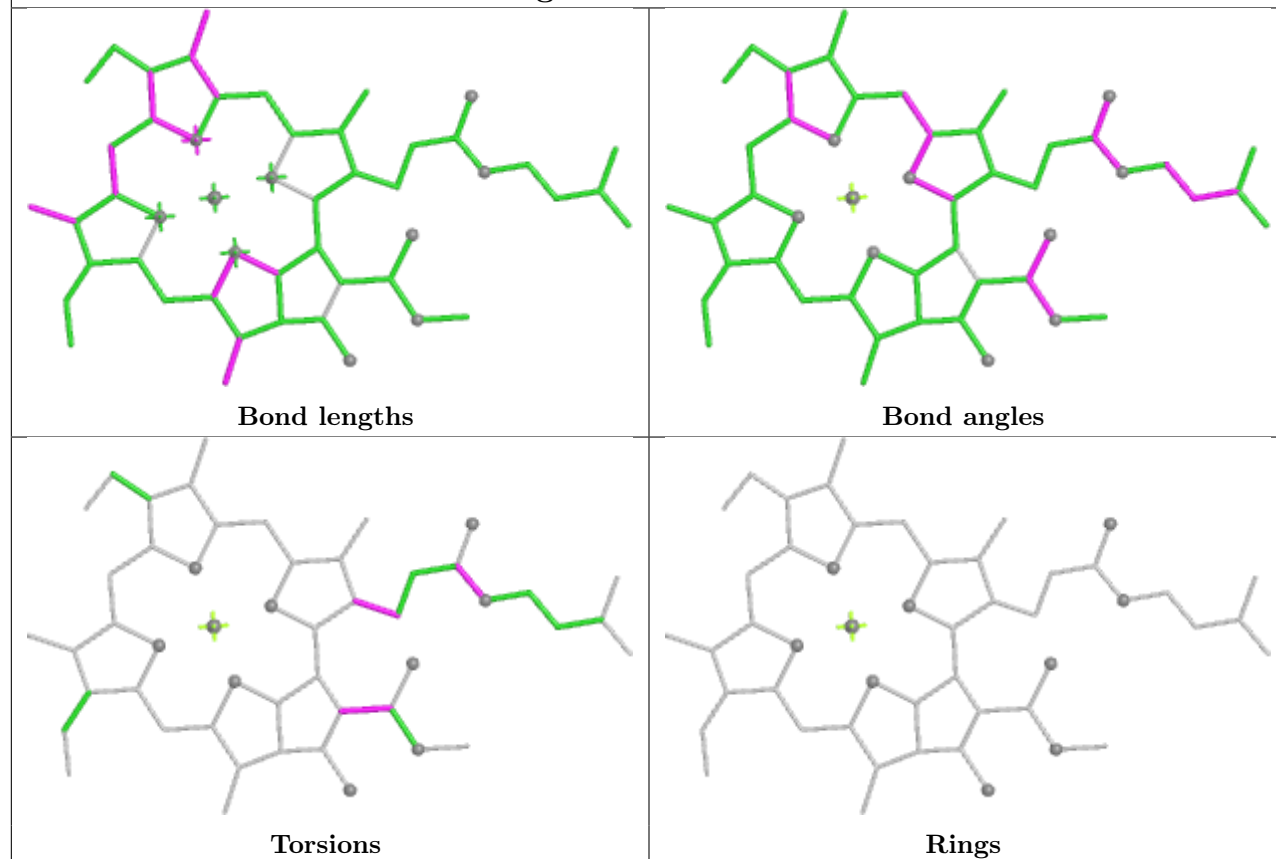
Ligand CLA 8 611



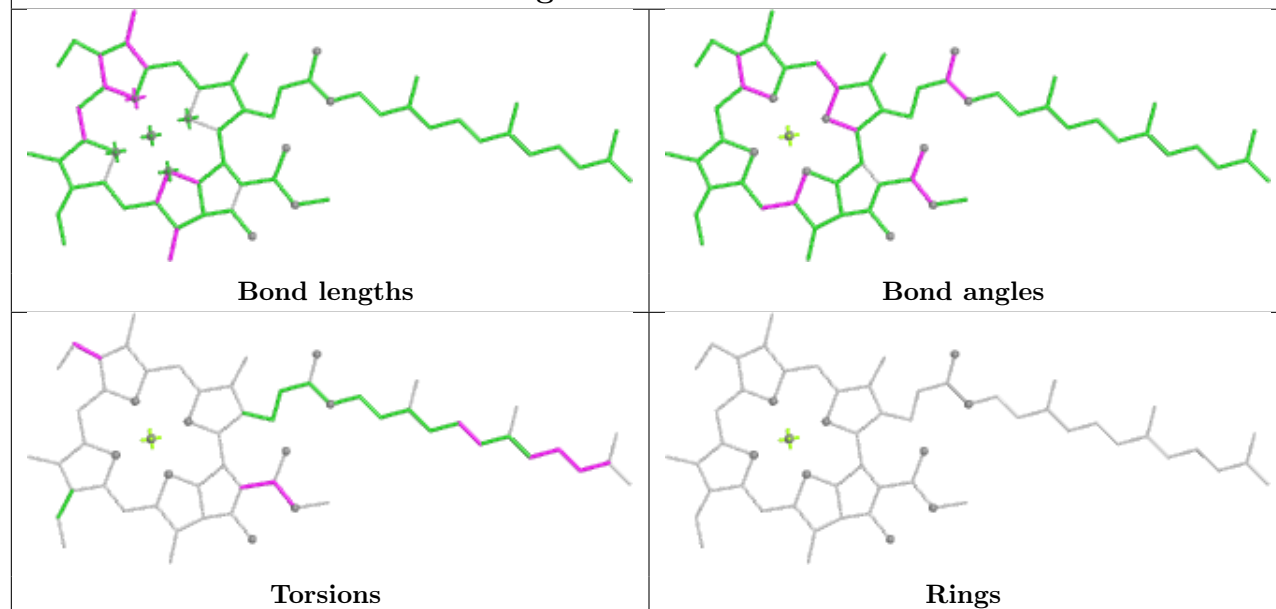
Ligand II0 8 613



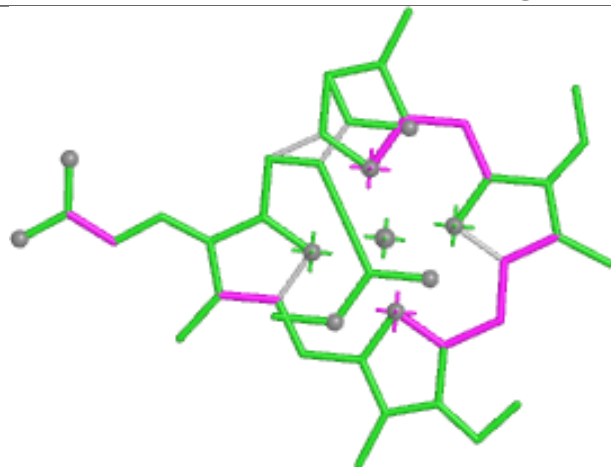
Ligand CLA 0 603



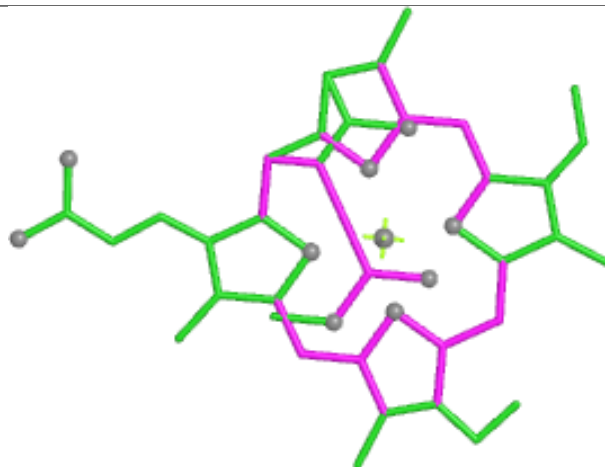
Ligand CLA 0 608



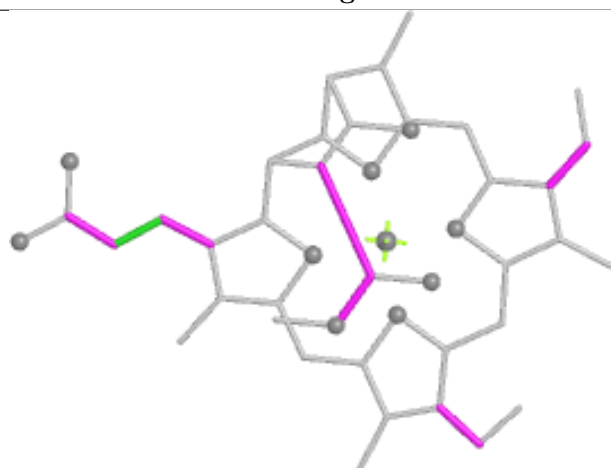
Ligand KC2 P 605



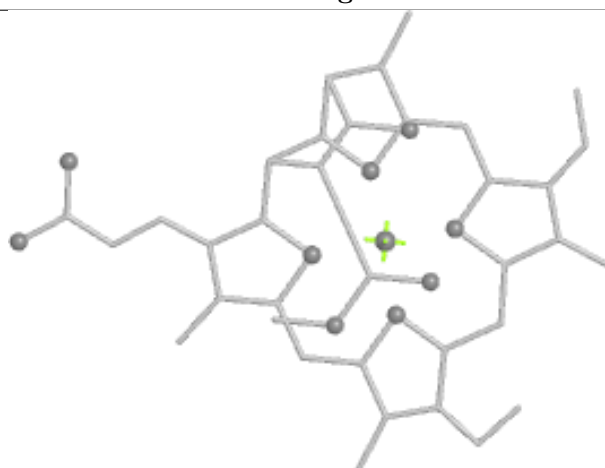
Bond lengths



Bond angles

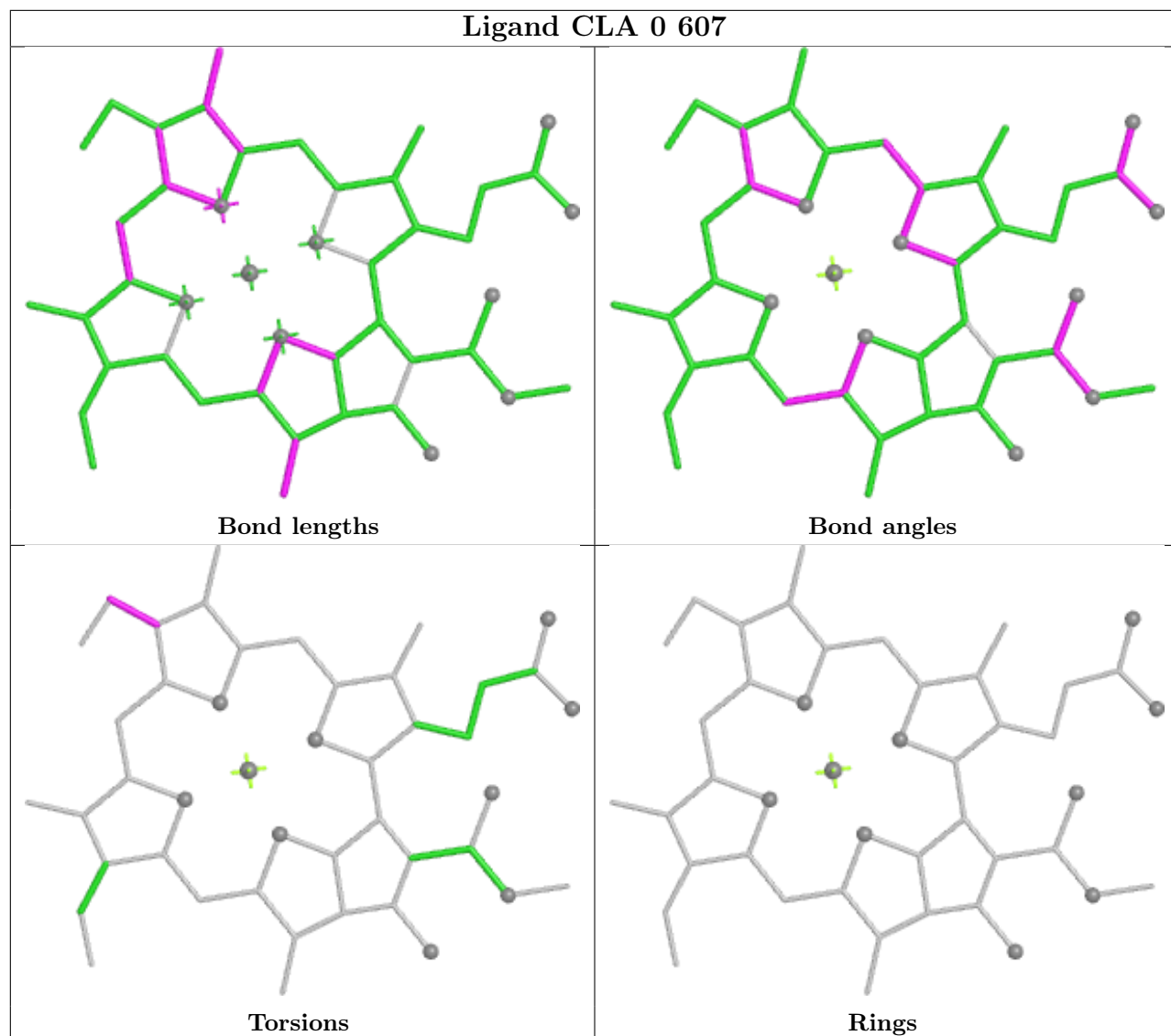


Torsions

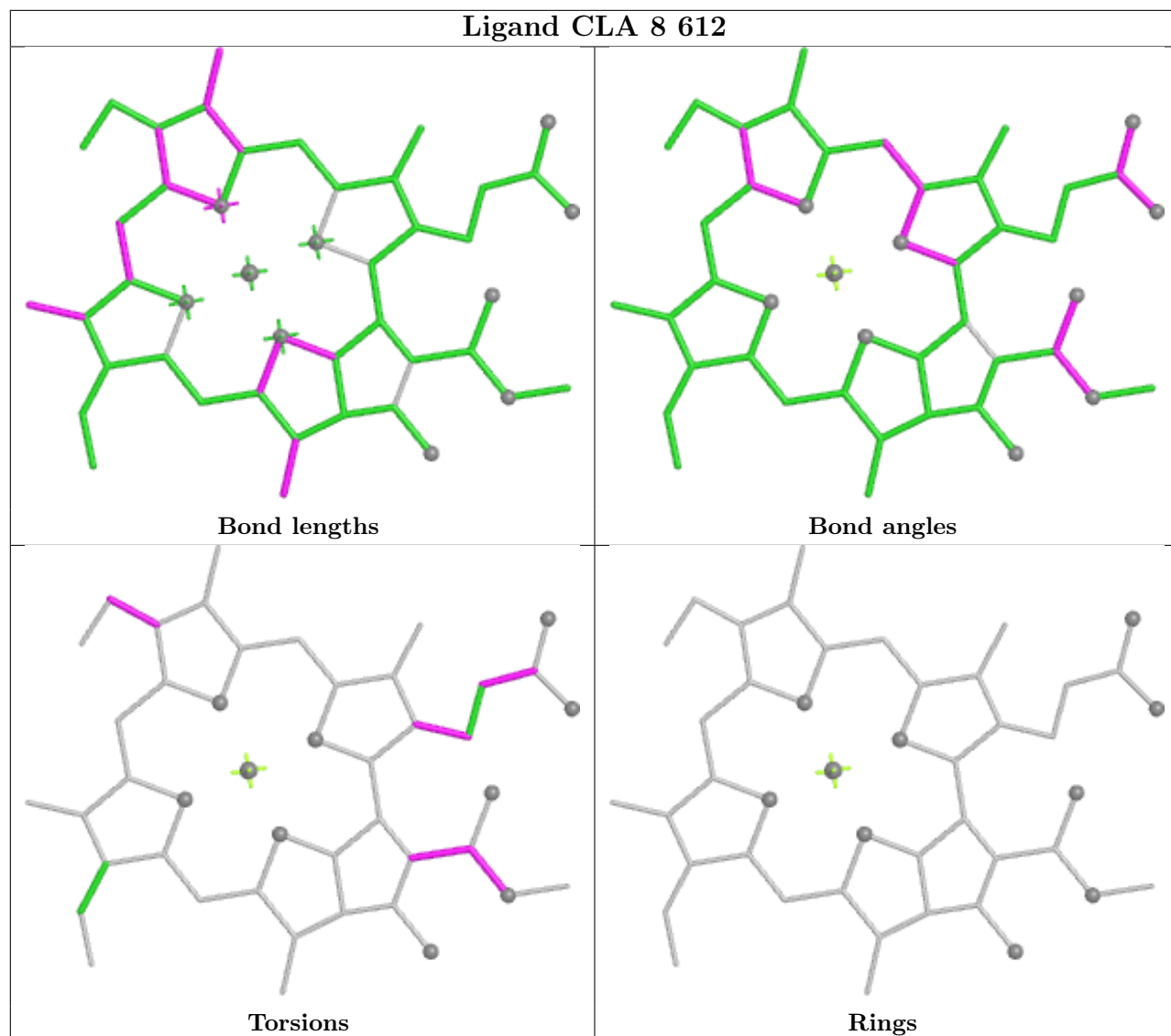


Rings

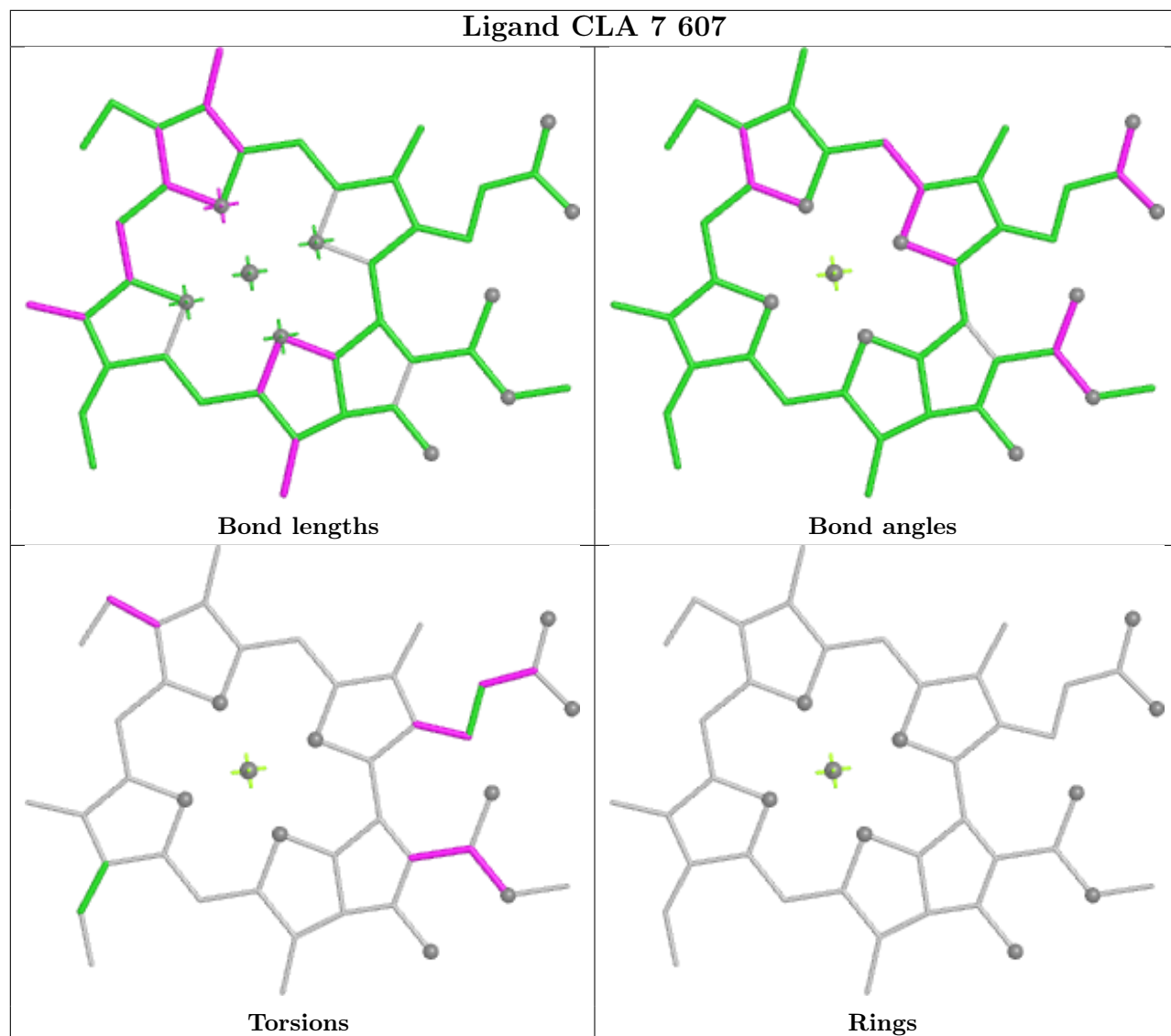
Ligand CLA 0 607



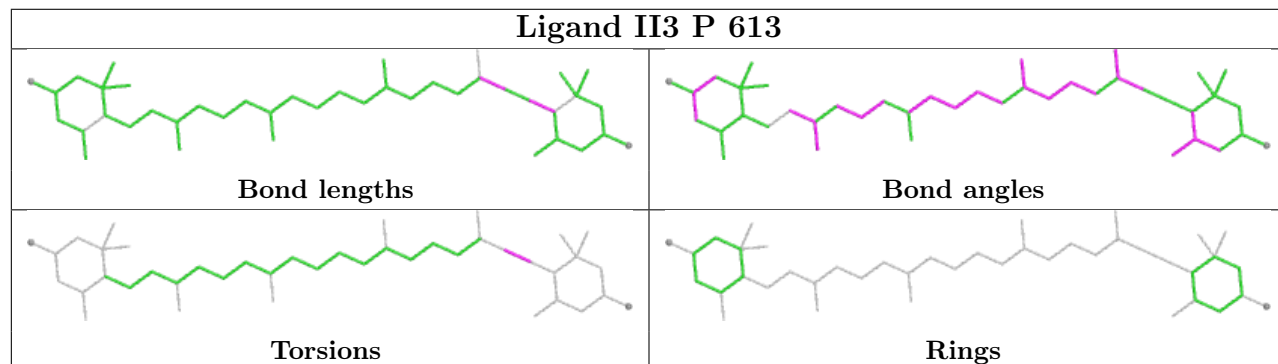
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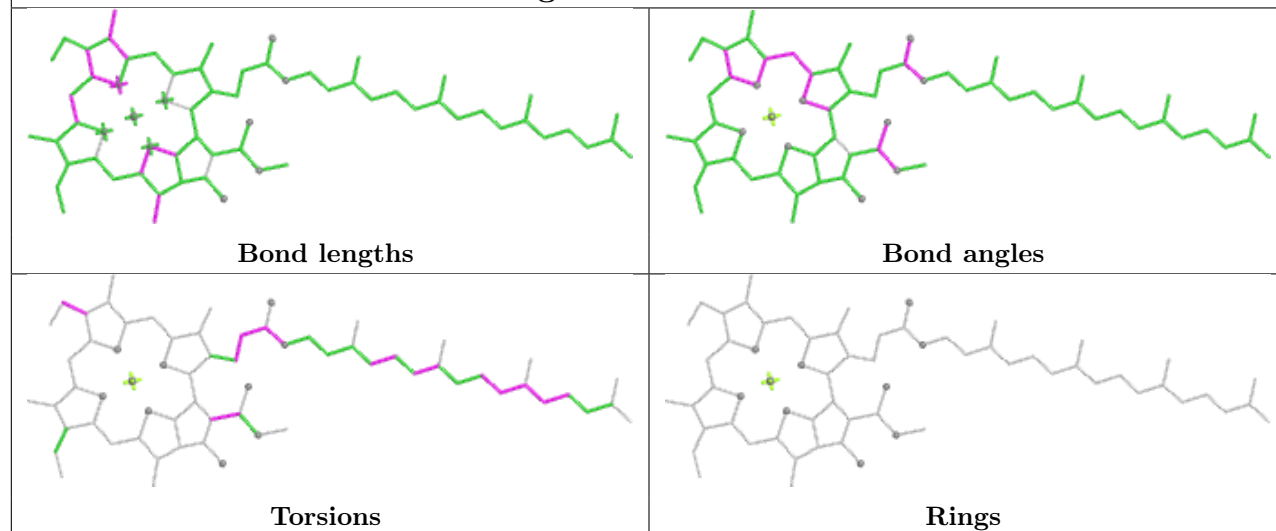
Ligand CLA 7 607



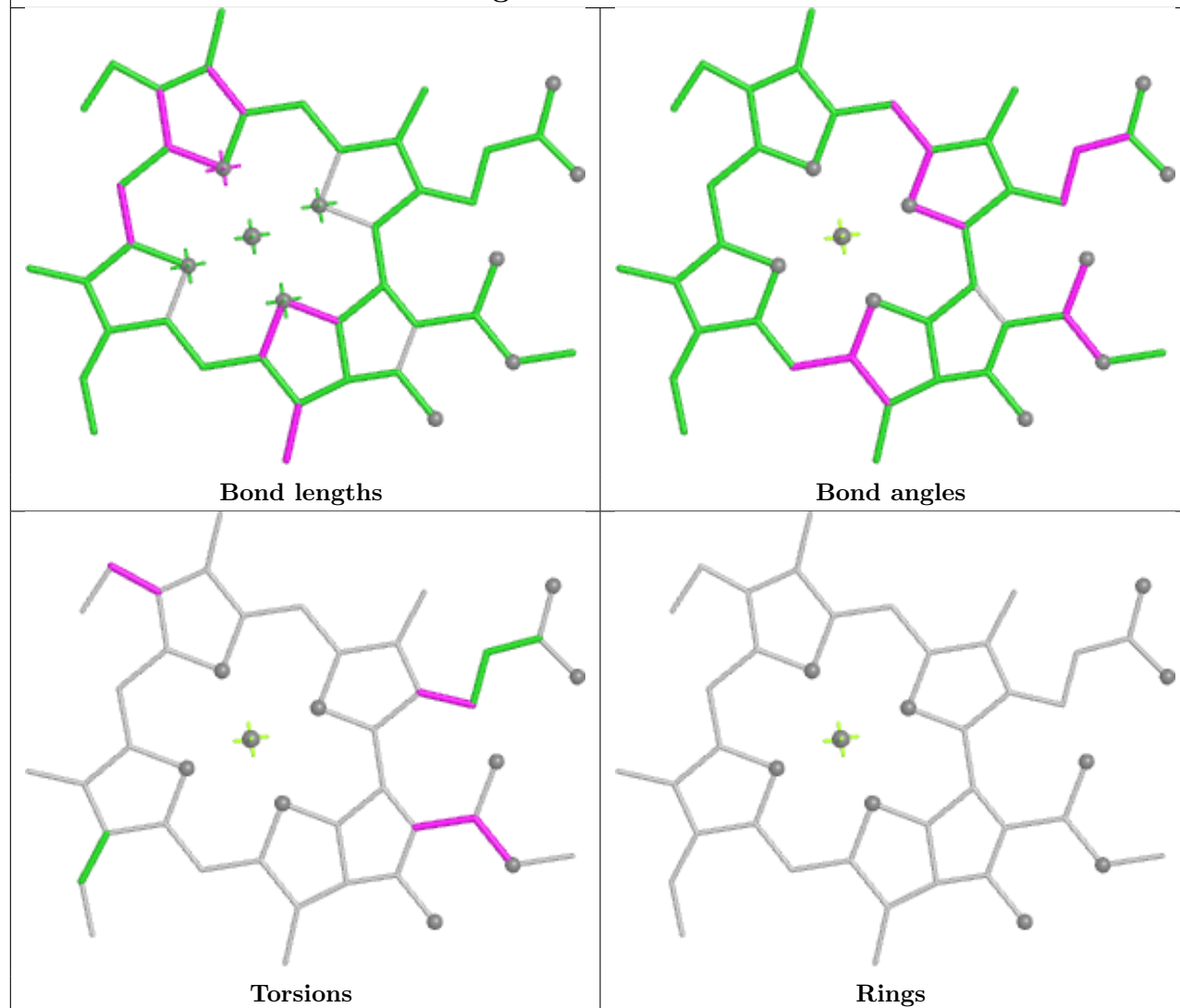
Ligand II3 P 613



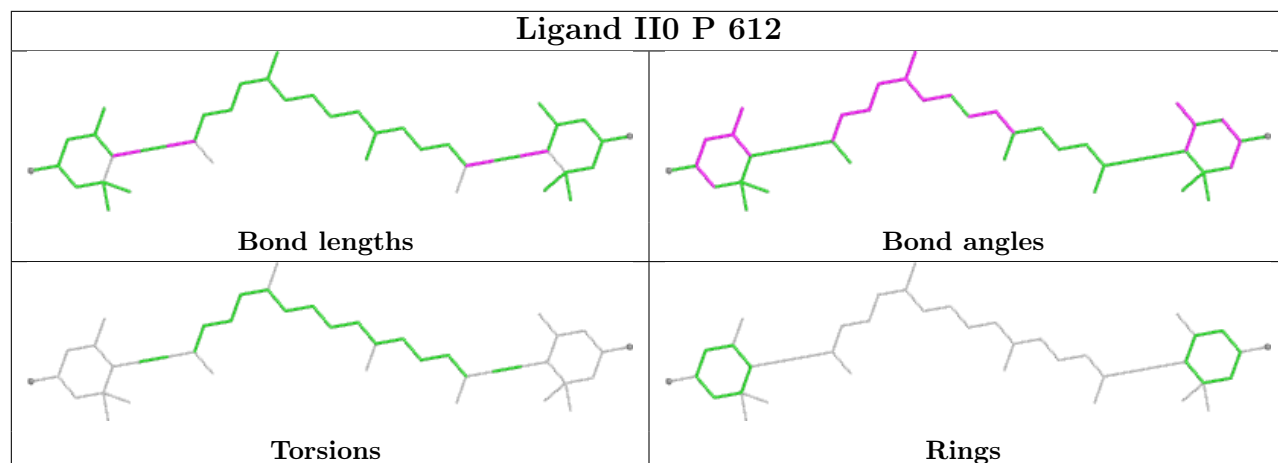
Ligand CLA s 303



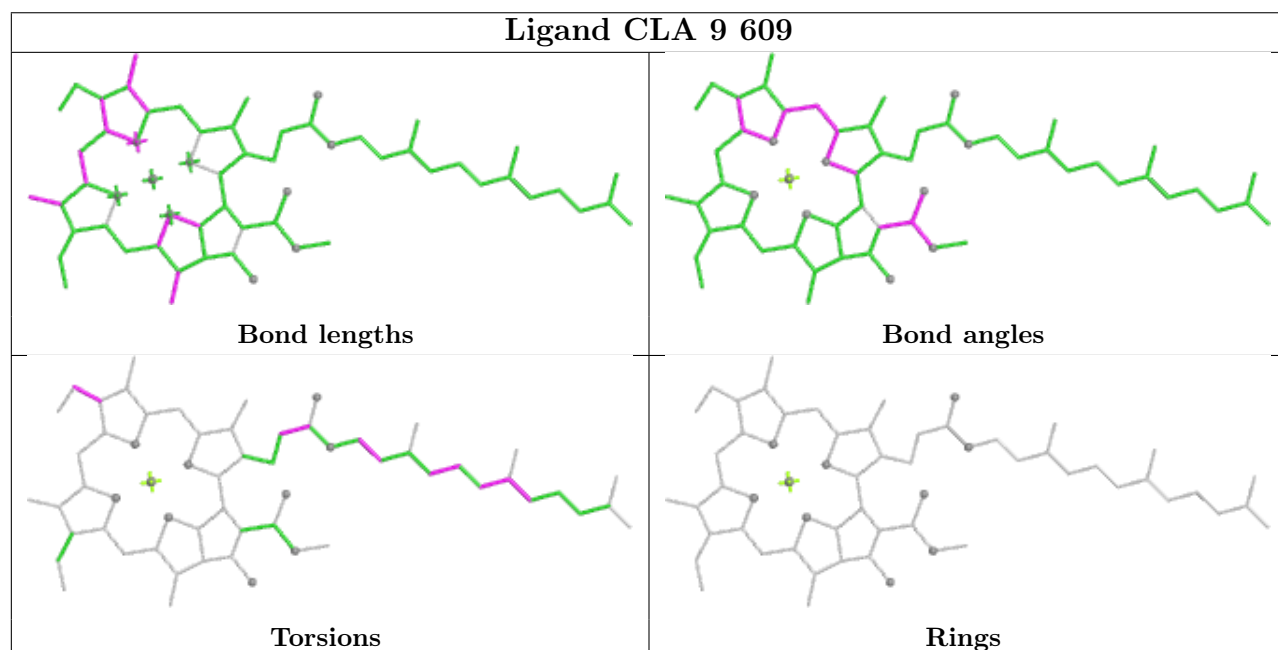
Ligand CLA P 606



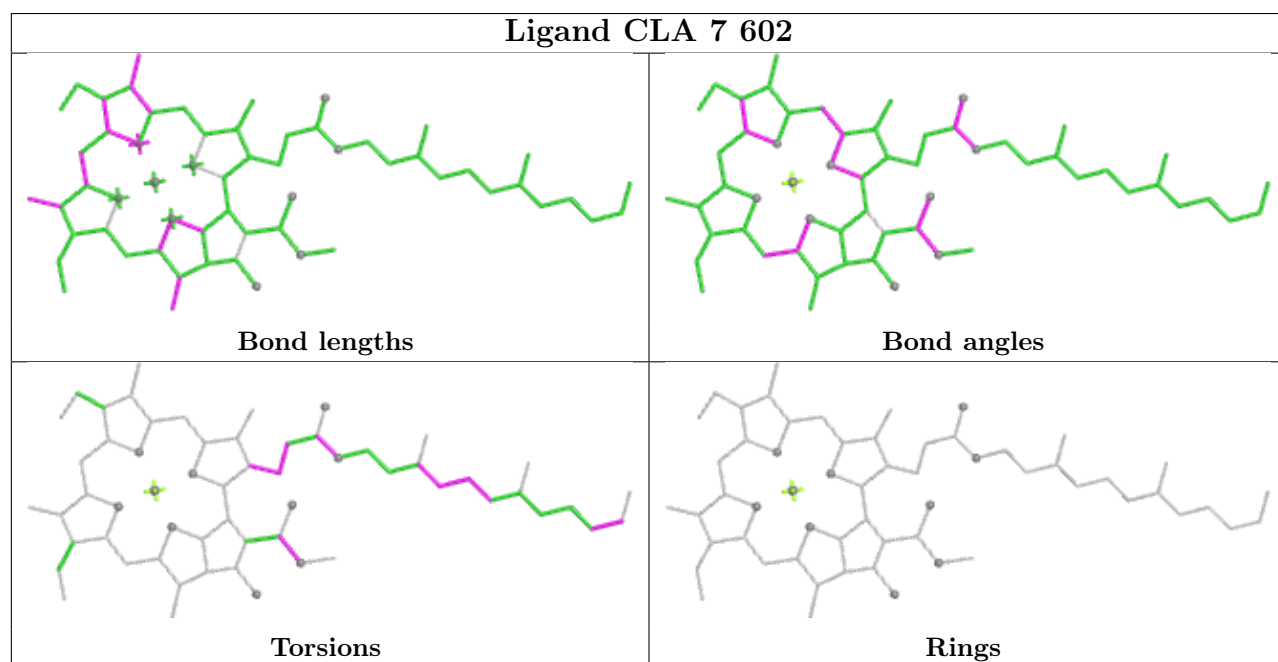
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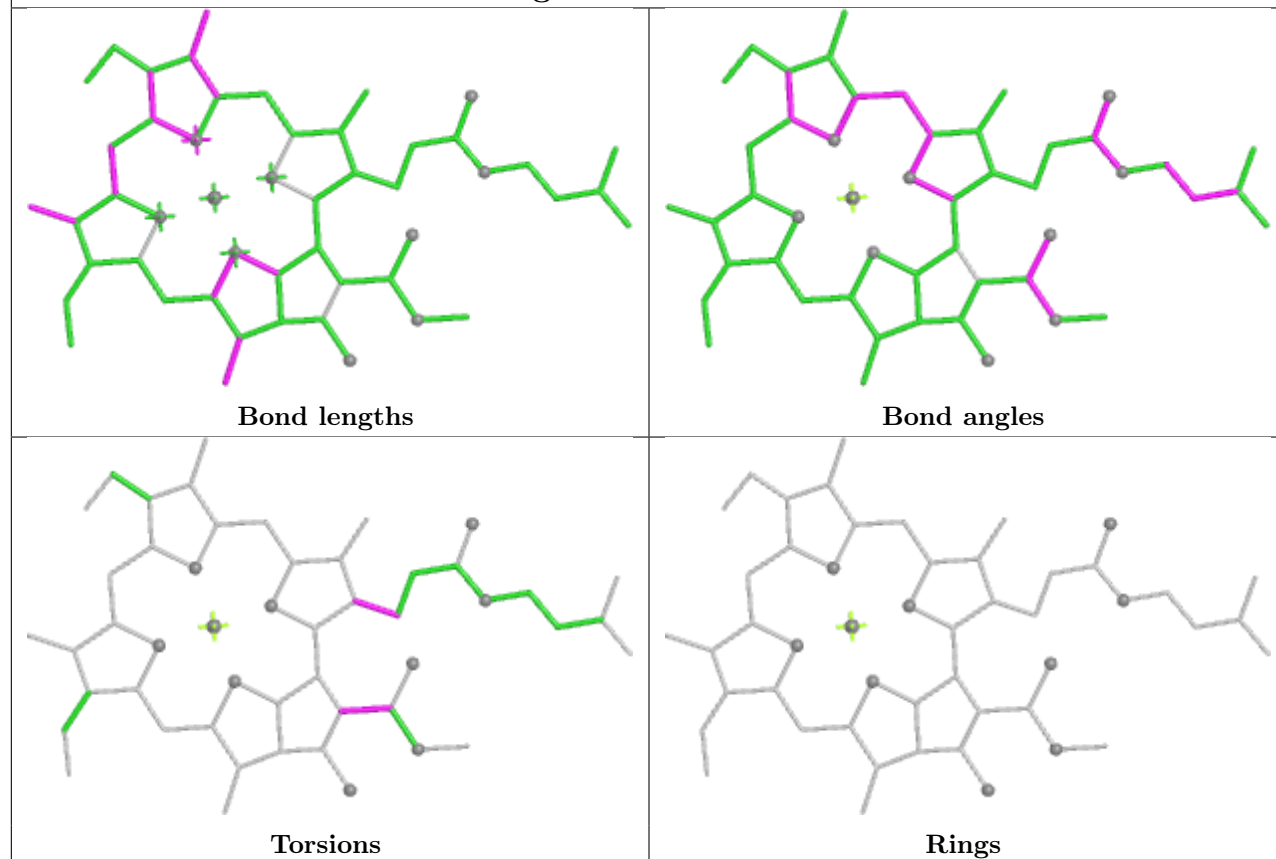
Ligand CLA 9 609



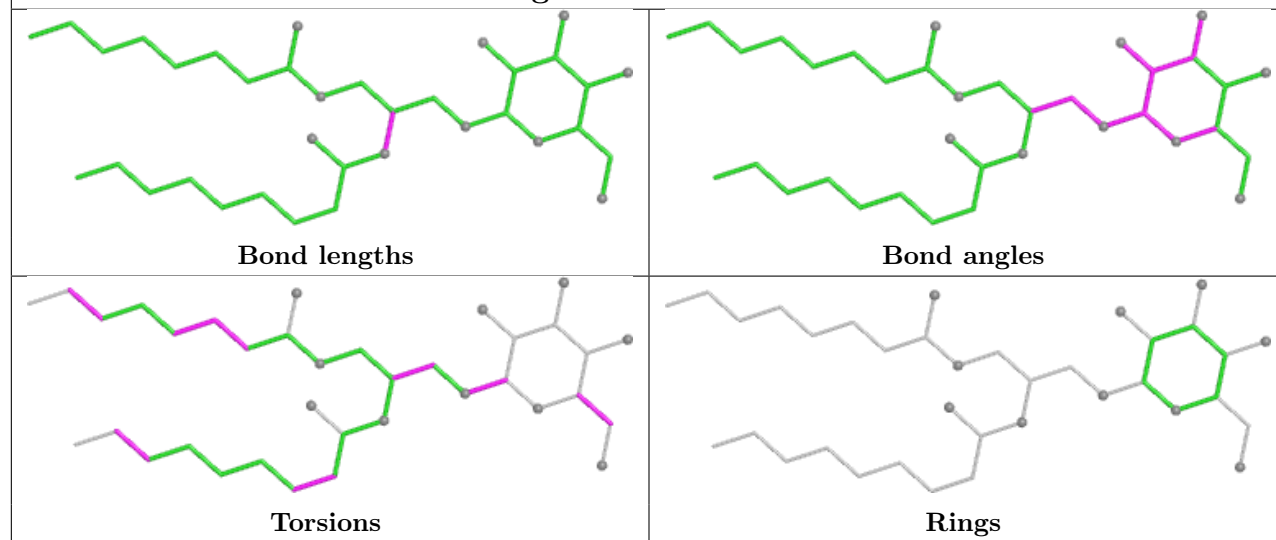
Ligand CLA 7 602



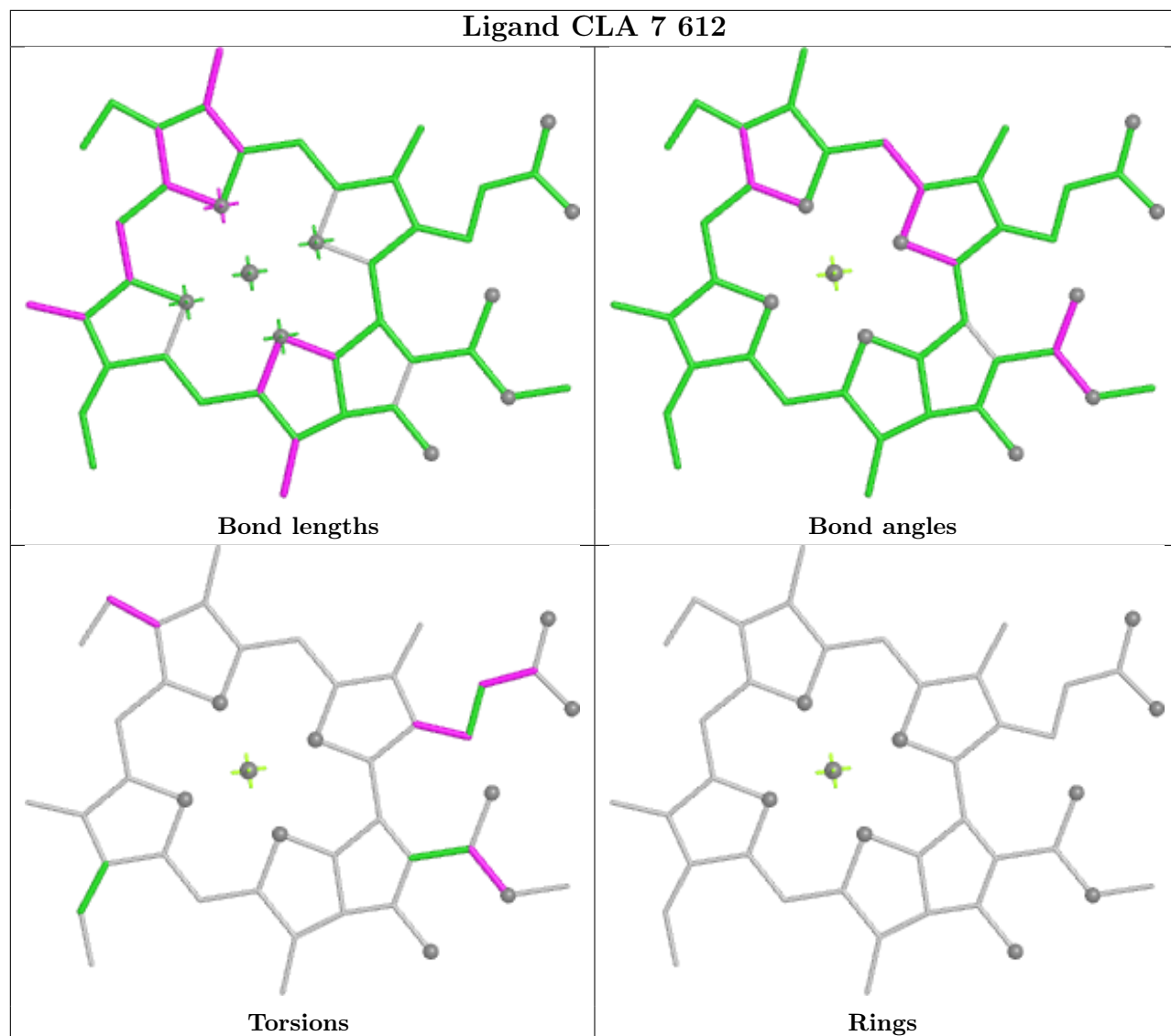
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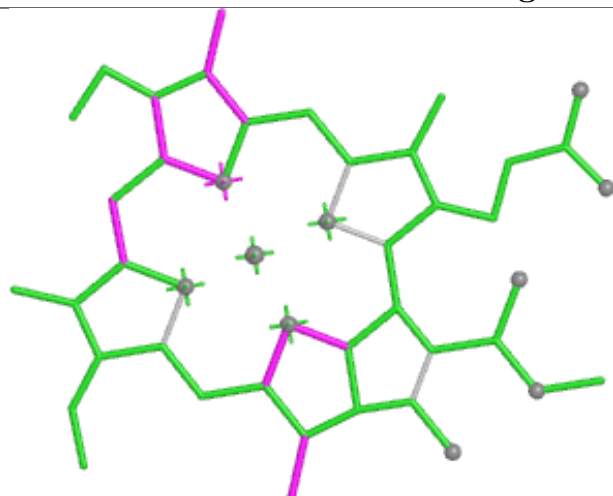
Ligand LMG 0 618



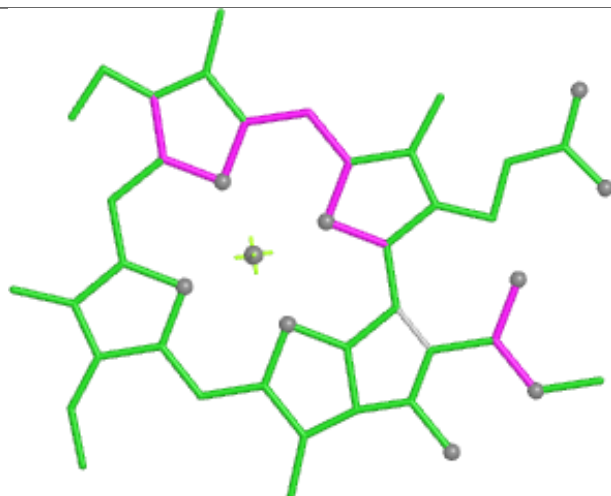
Ligand CLA 7 612



Ligand CLA 0 611



Bond lengths



Bond angles

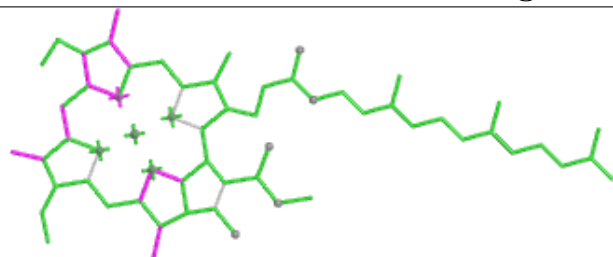


Torsions

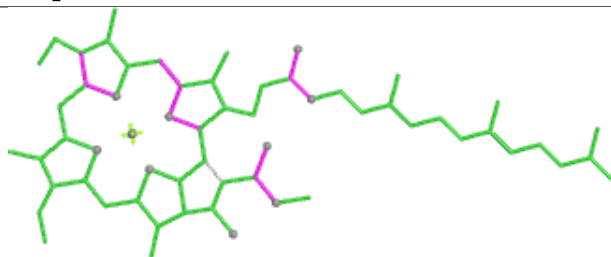


Rings

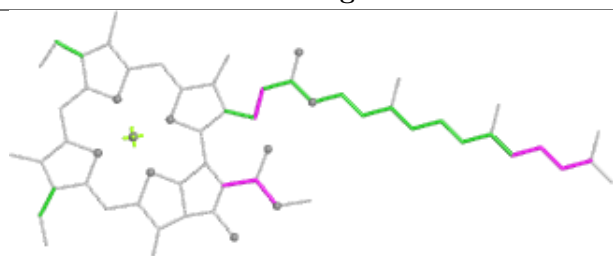
Ligand CLA p 310



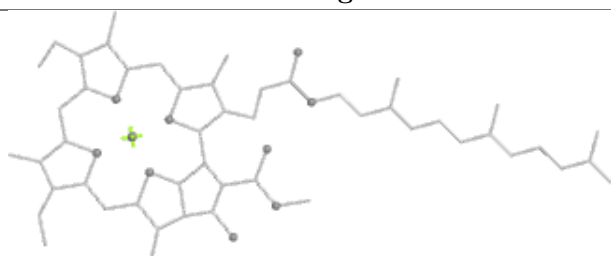
Bond lengths



Bond angles

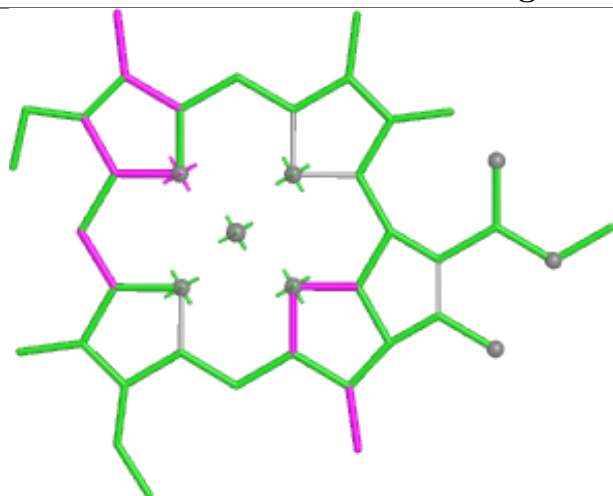


Torsions

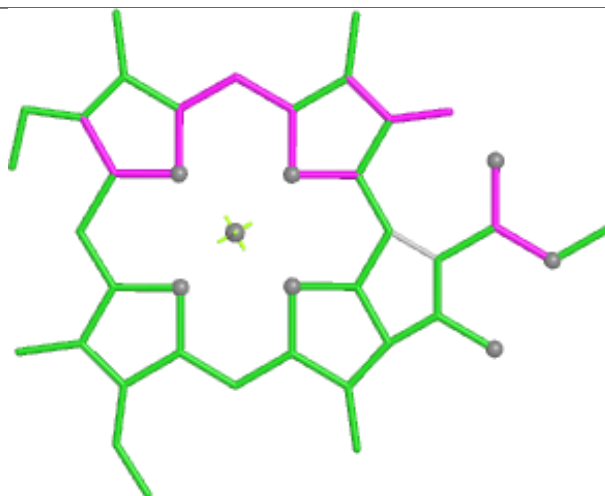


Rings

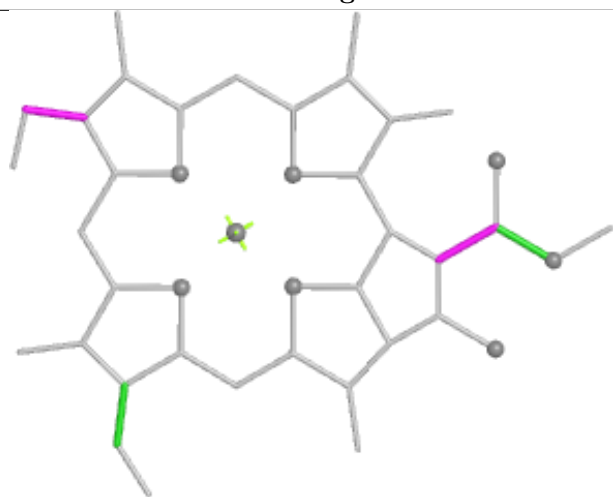
Ligand CLA 7 609



Bond lengths



Bond angles

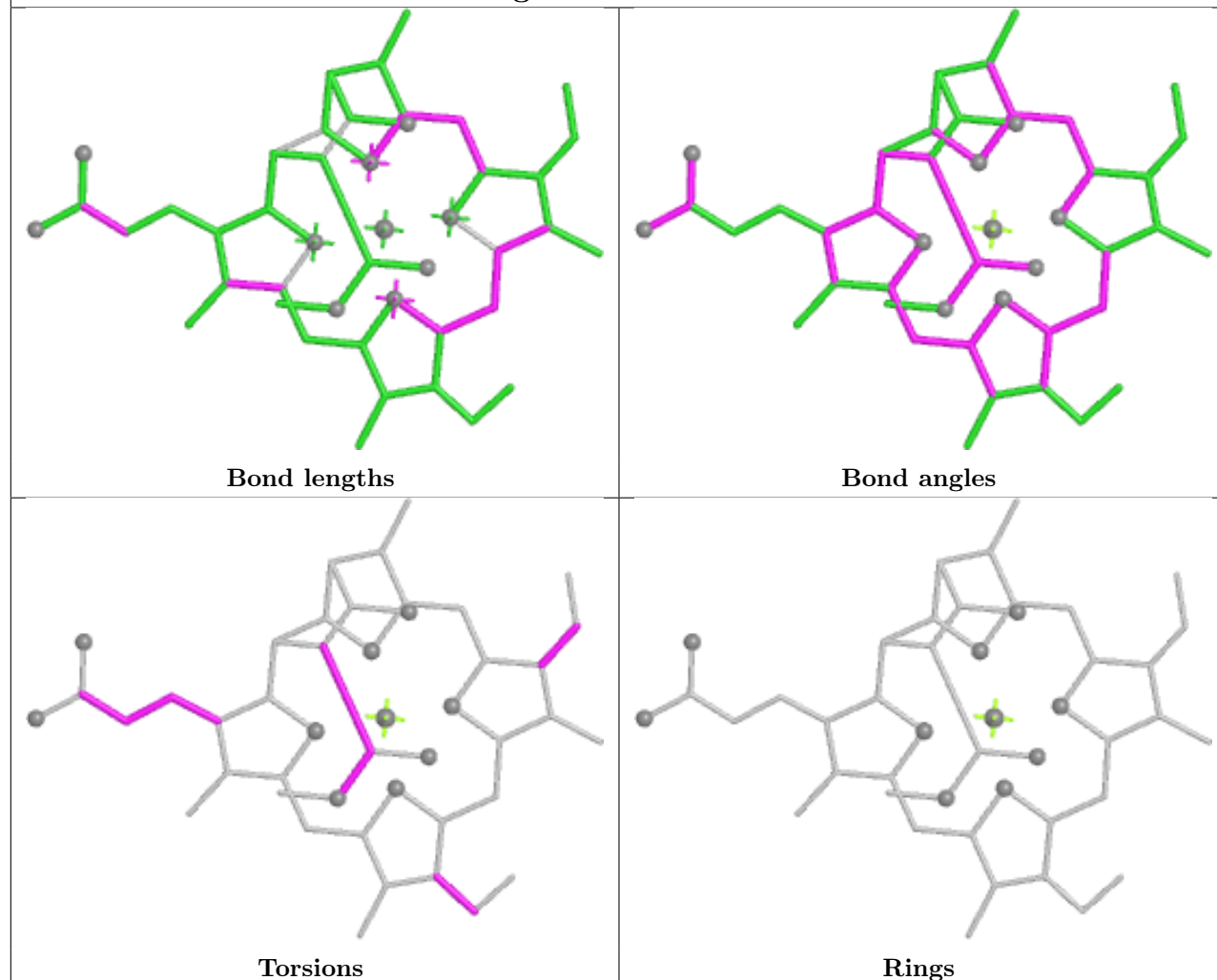


Torsions

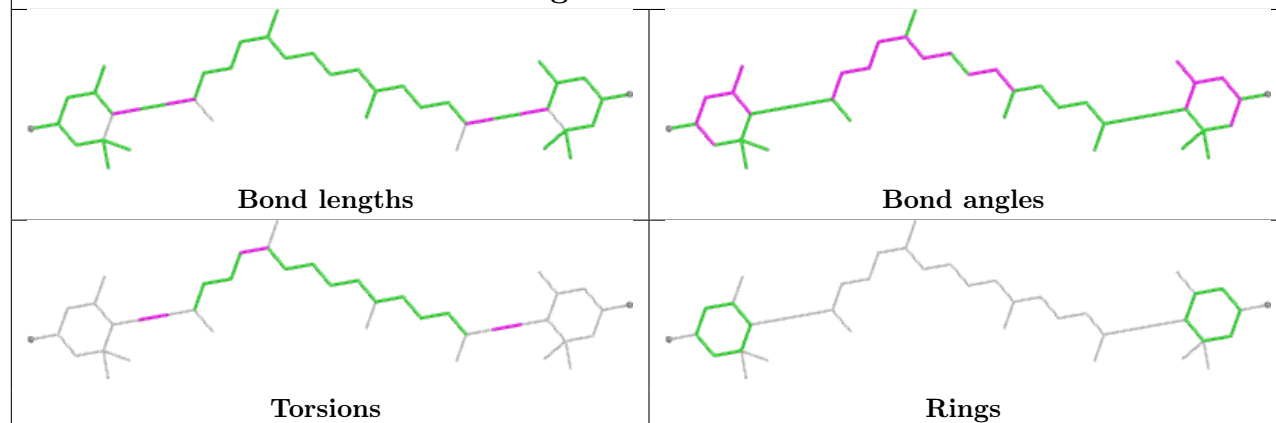


Rings

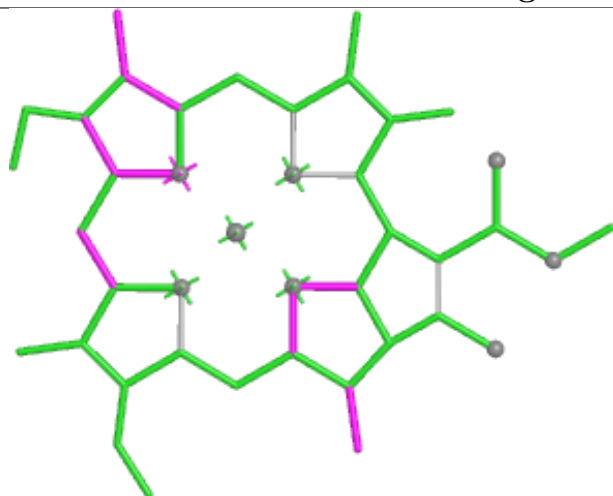
Ligand KC2 0 610



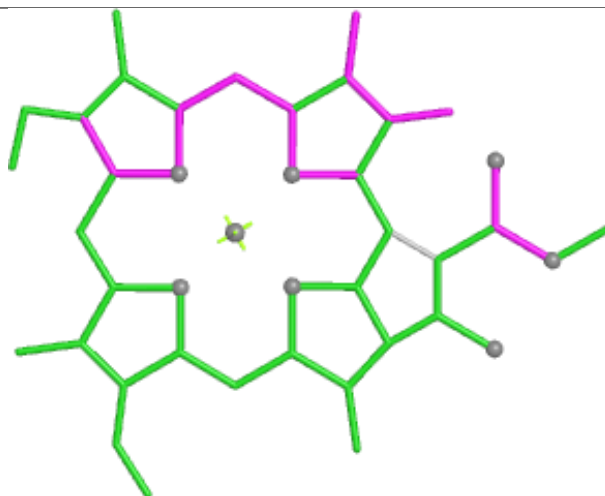
Ligand II0 9 614



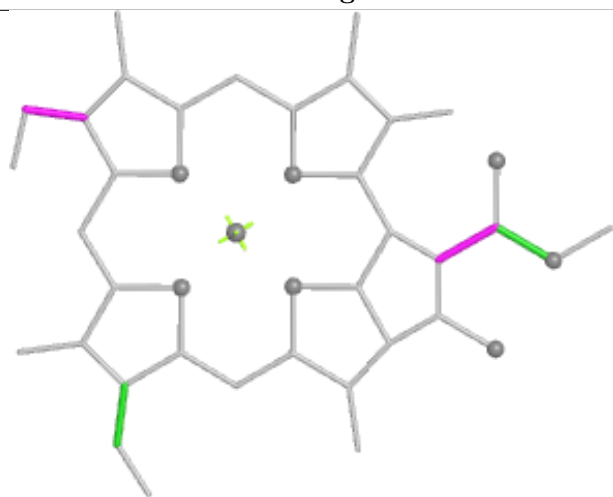
Ligand CLA 9 608



Bond lengths



Bond angles

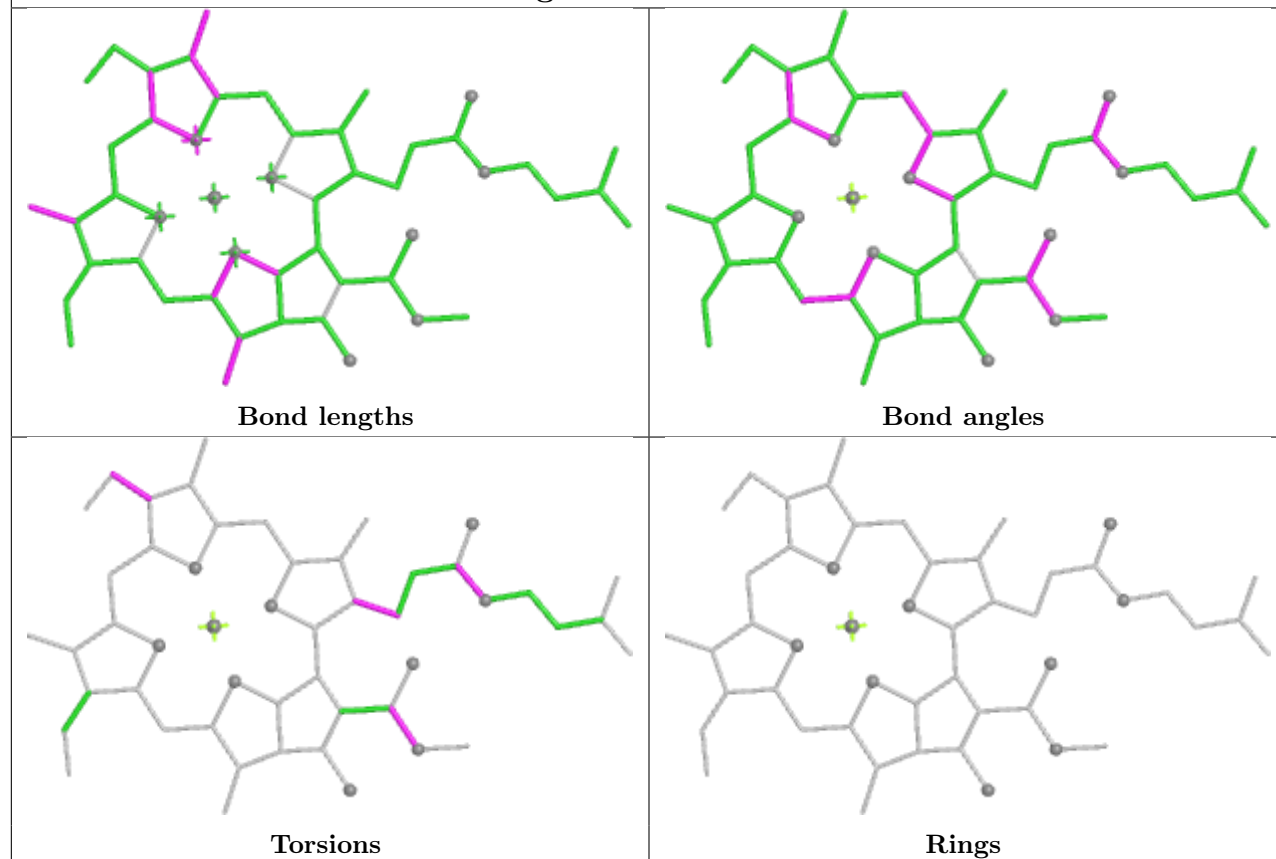


Torsions

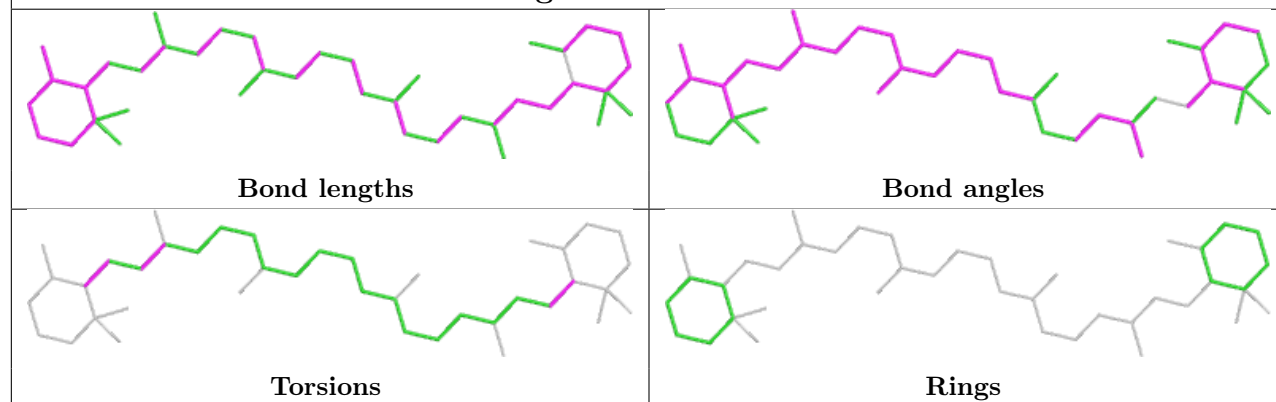


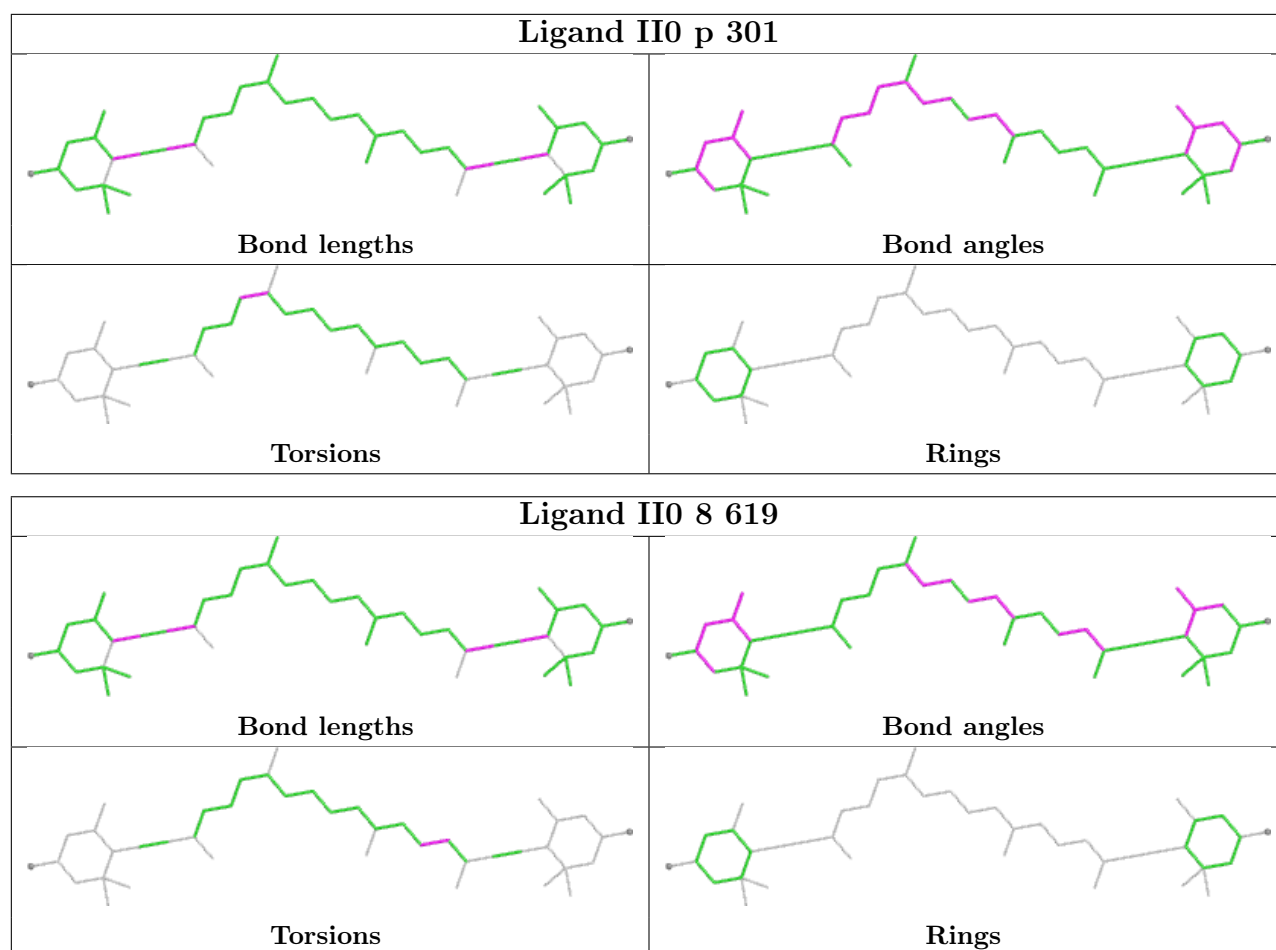
Rings

Ligand CLA 7 605

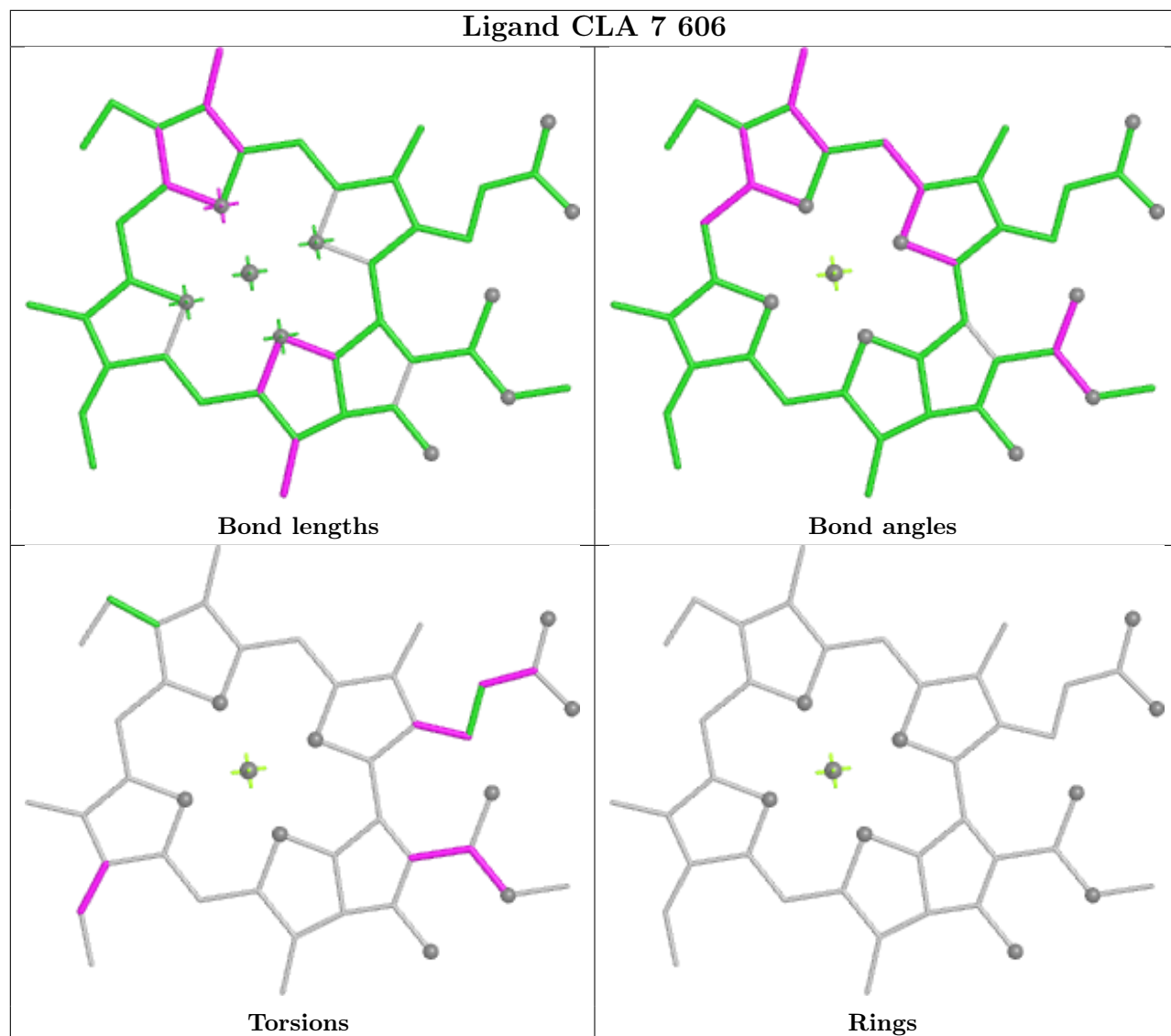


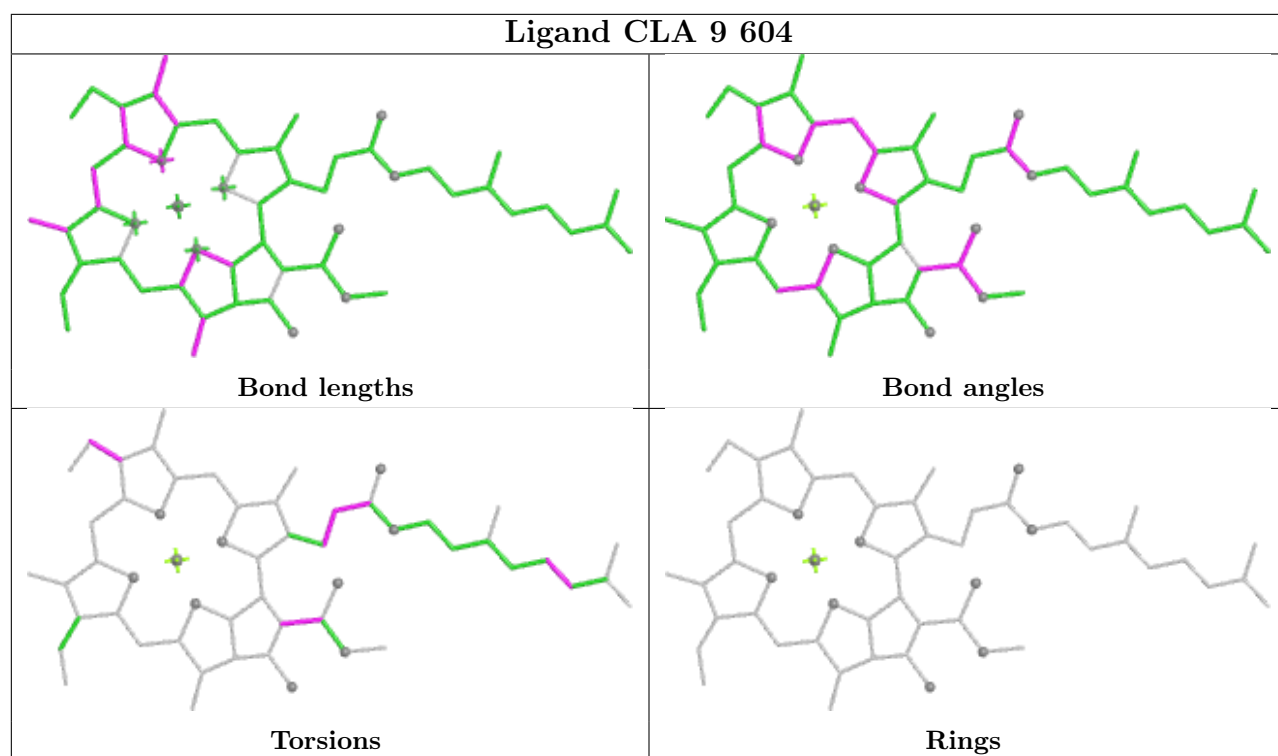
Ligand 8CT P 615



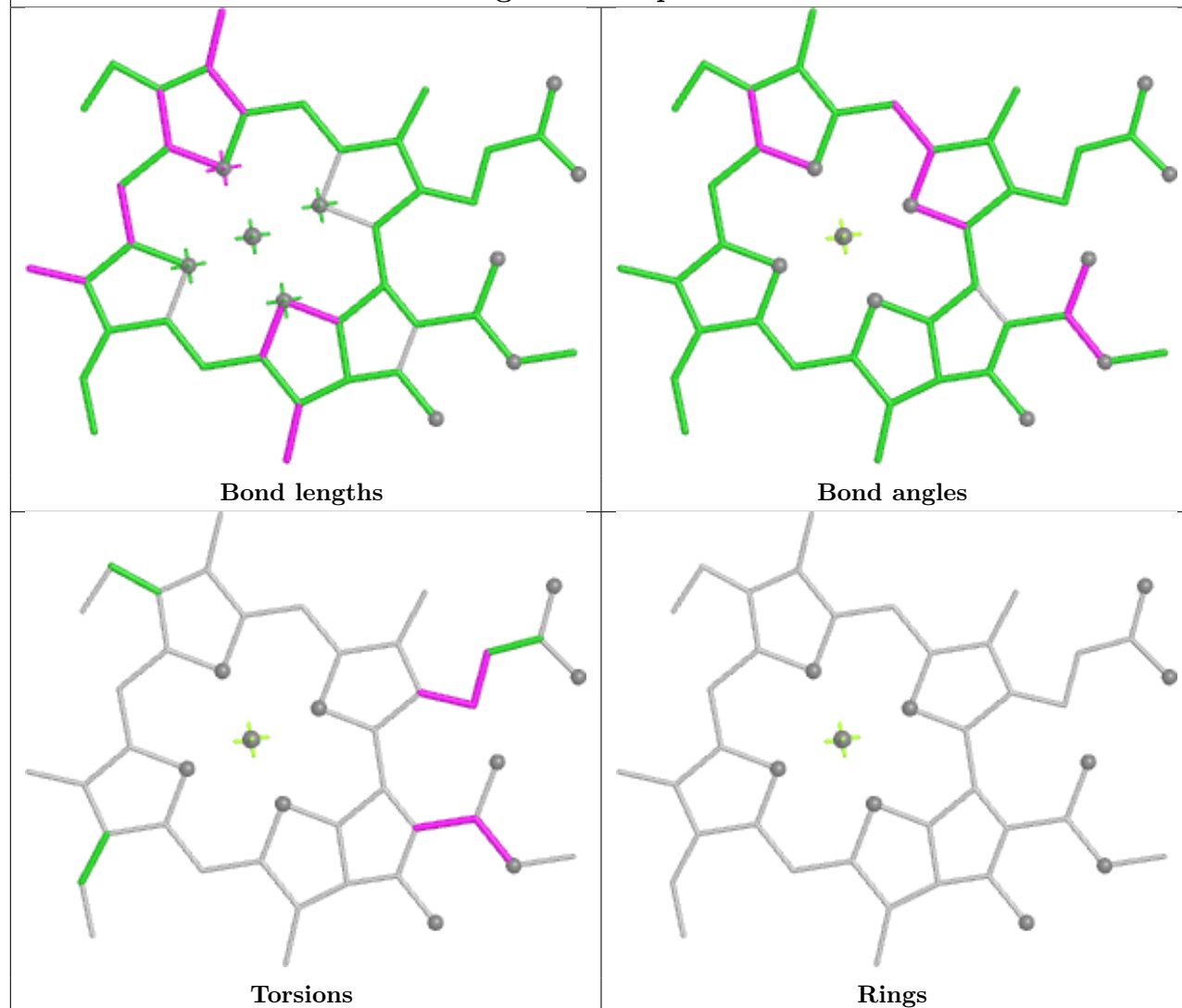


Ligand CLA 7 606

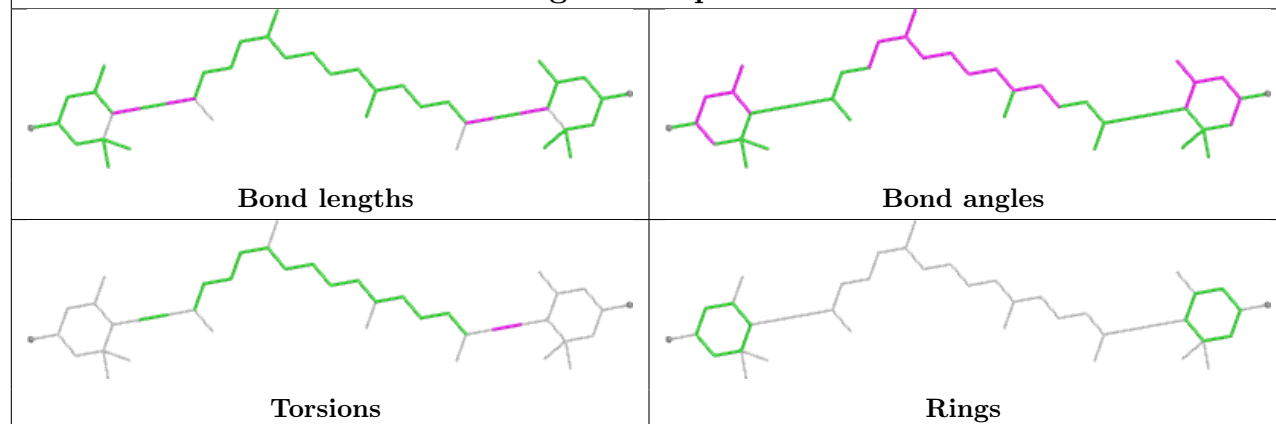


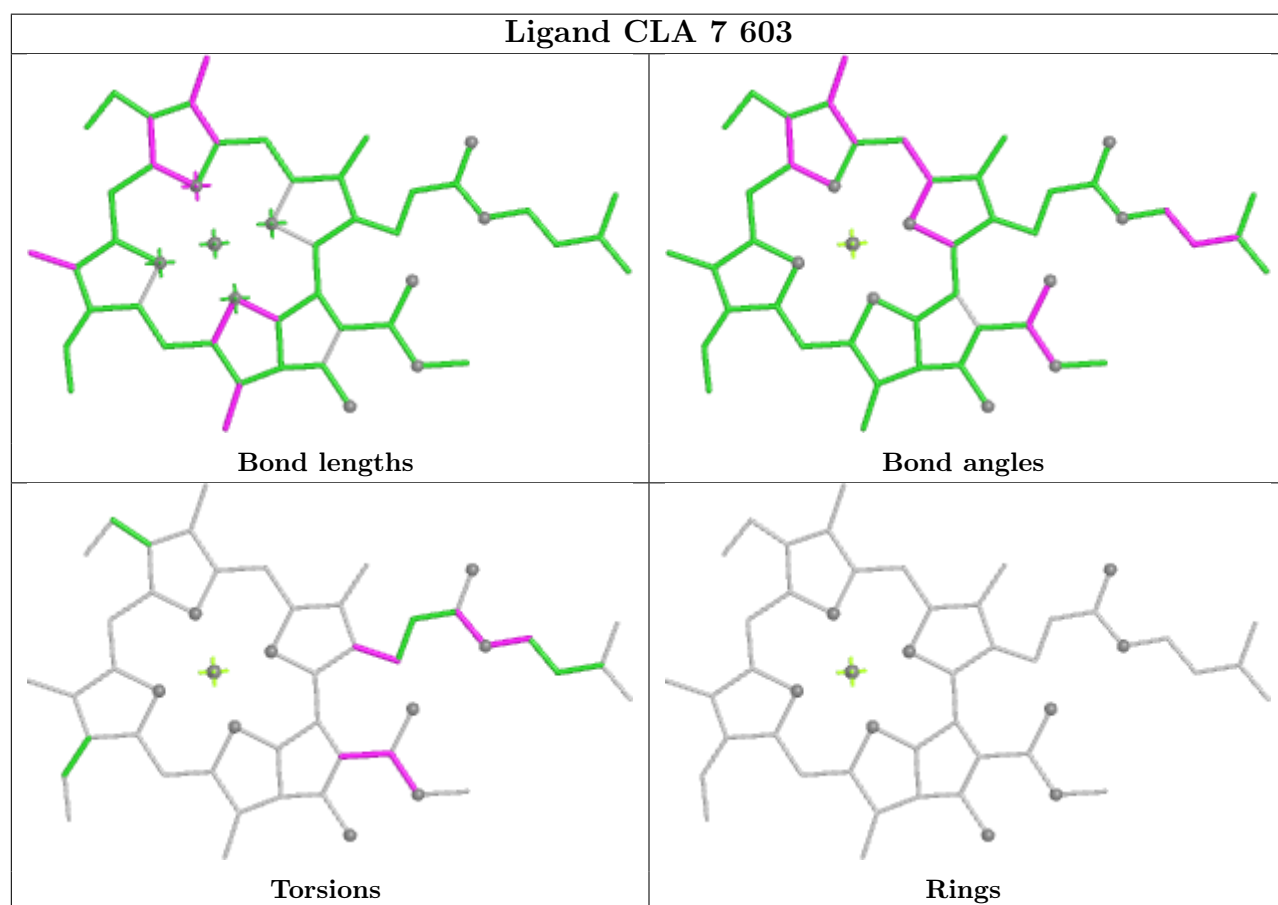
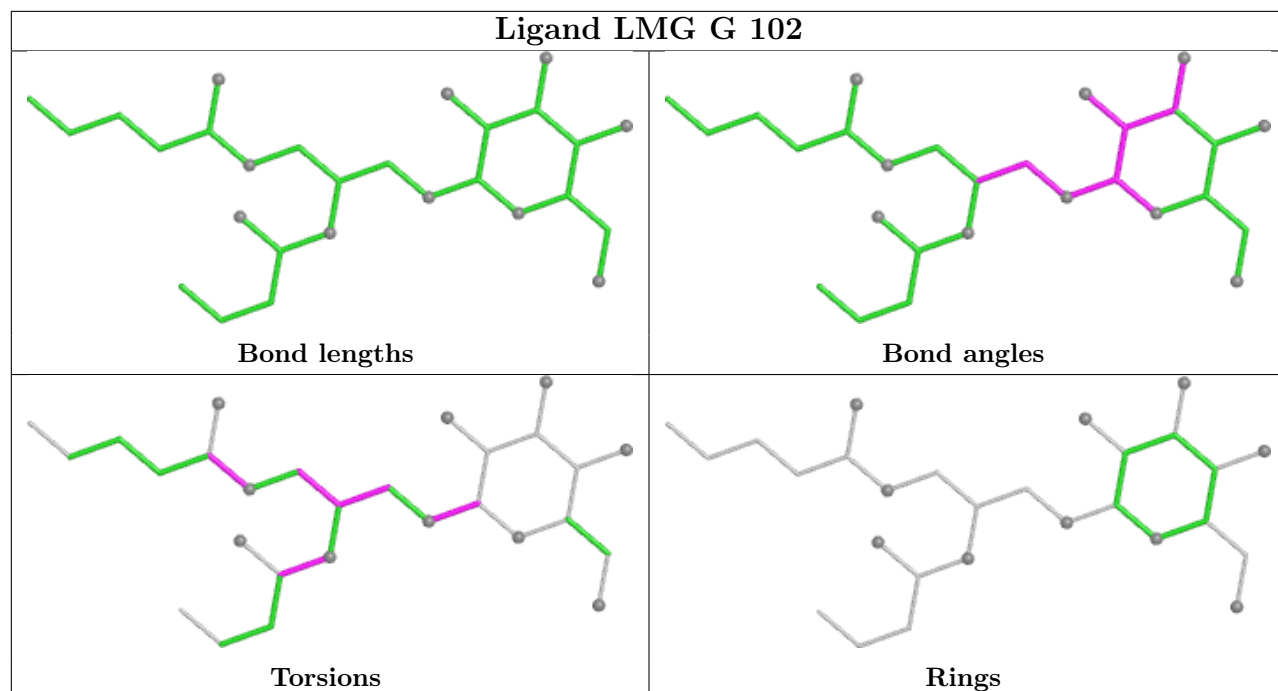


Ligand CLA p 314

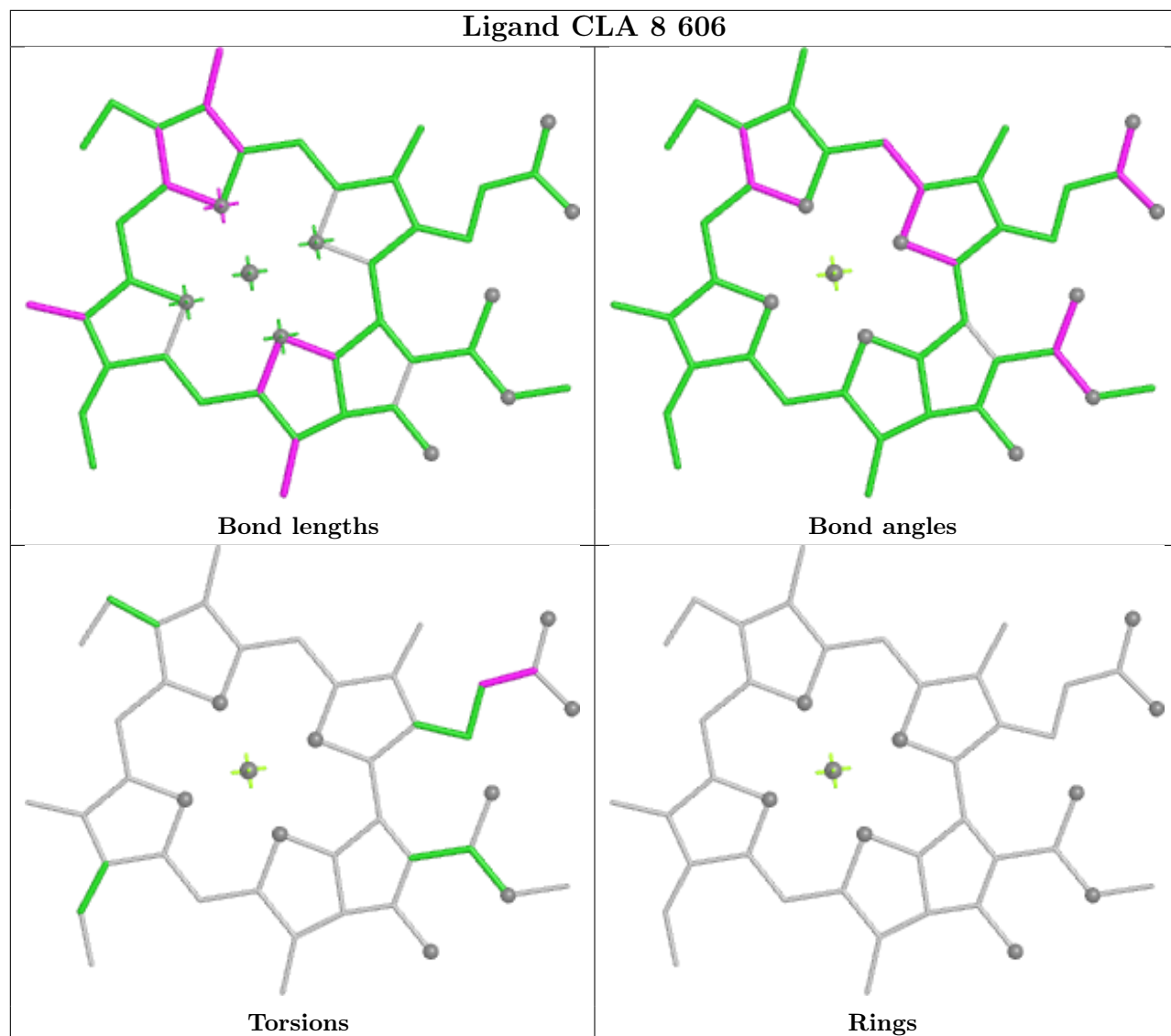


Ligand II0 p 315

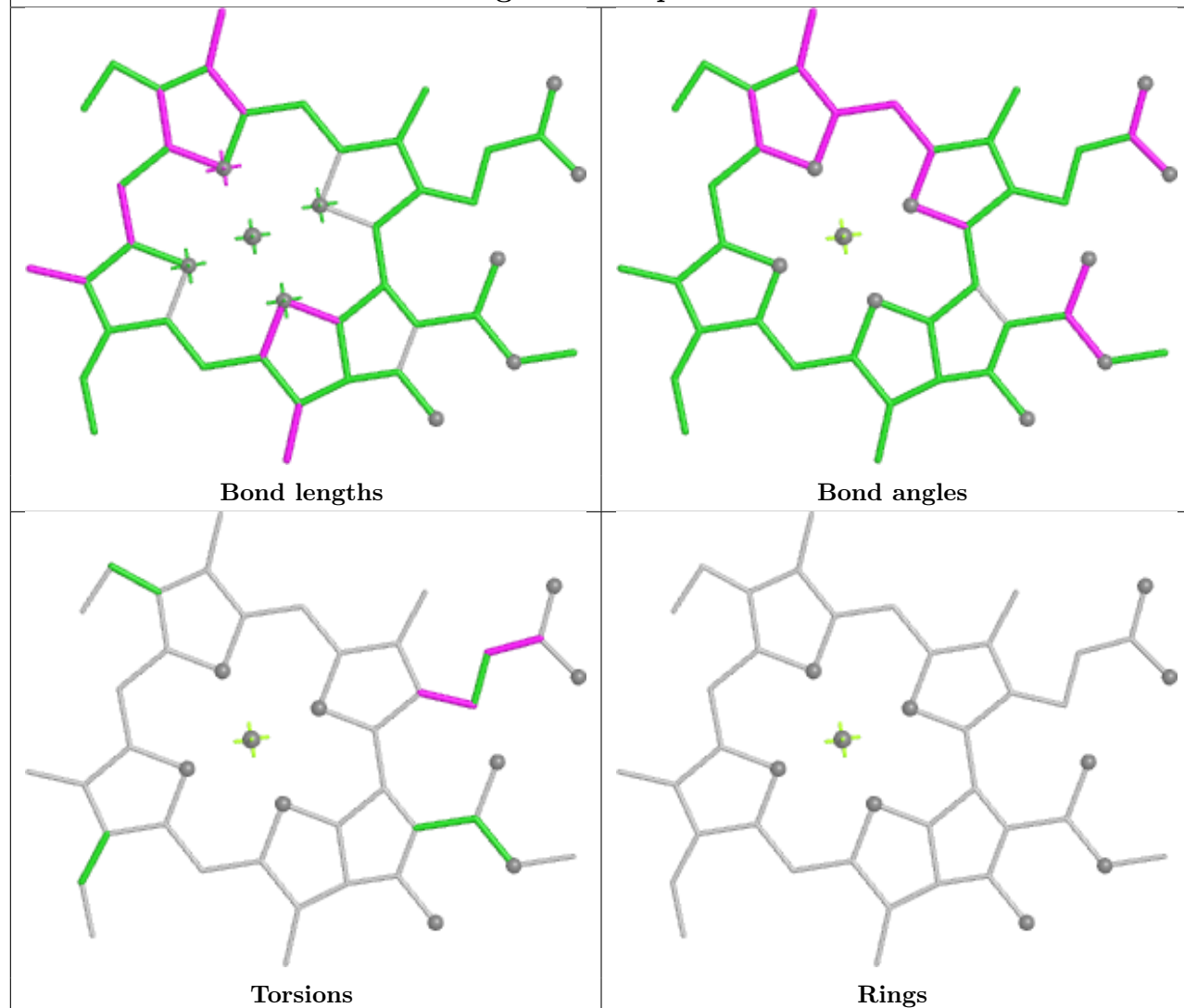




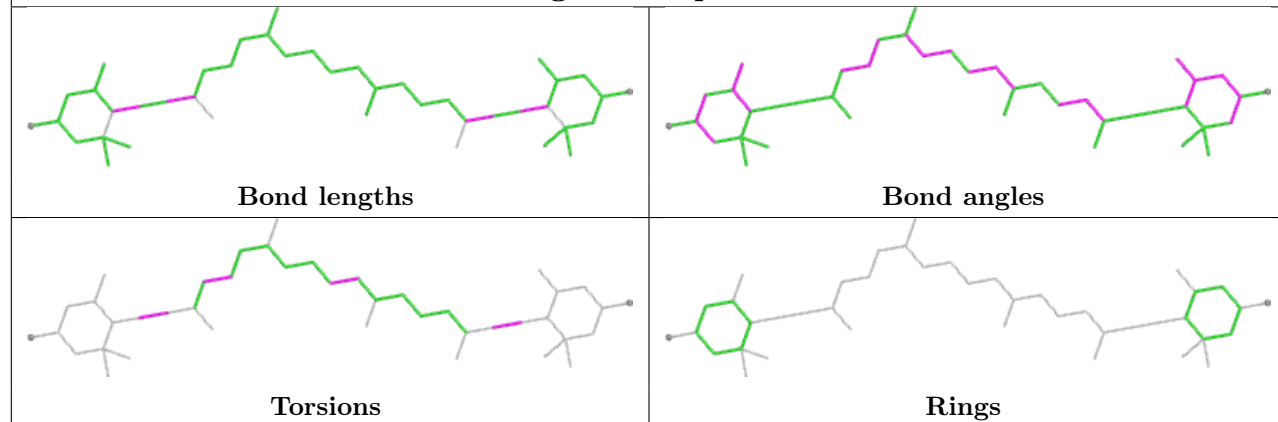
Ligand CLA 8 606

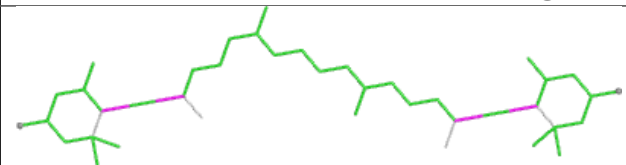
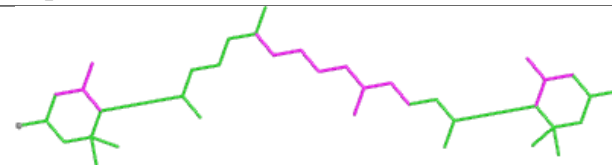
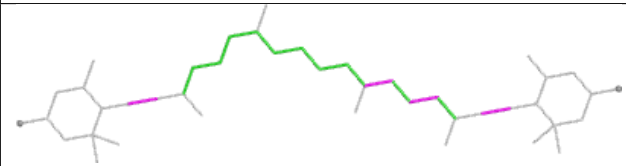
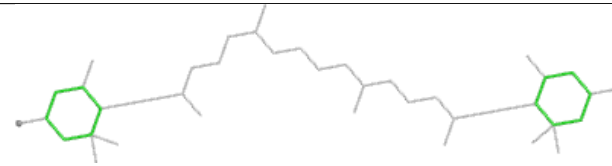


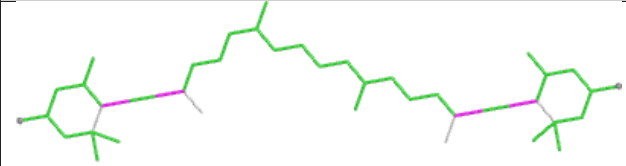
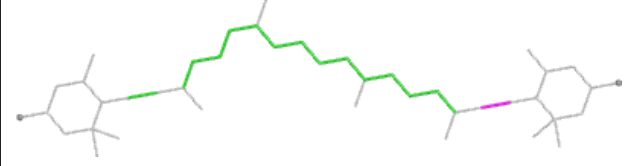
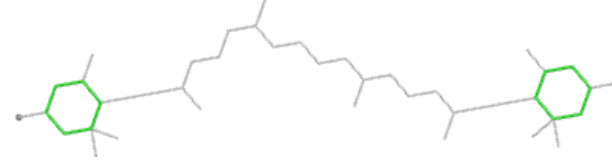
Ligand CLA p 309

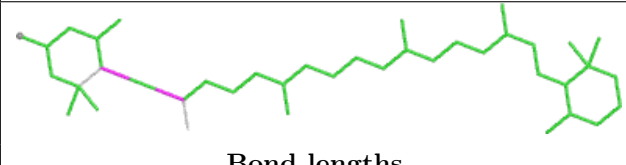
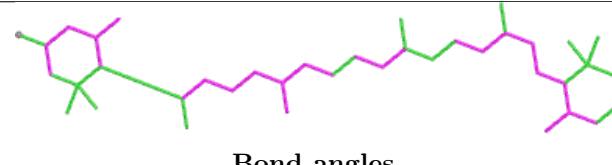
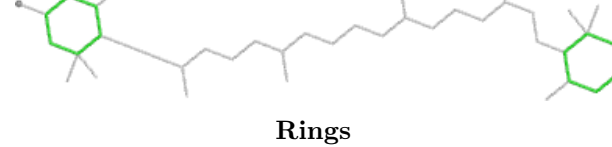


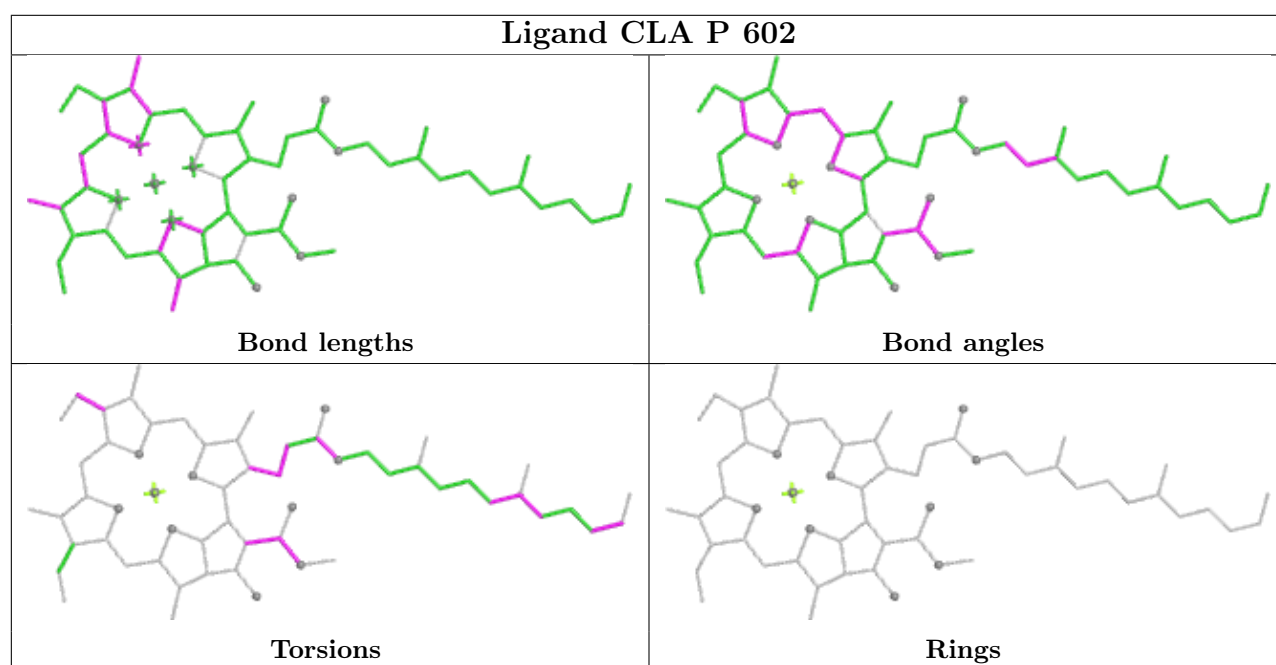
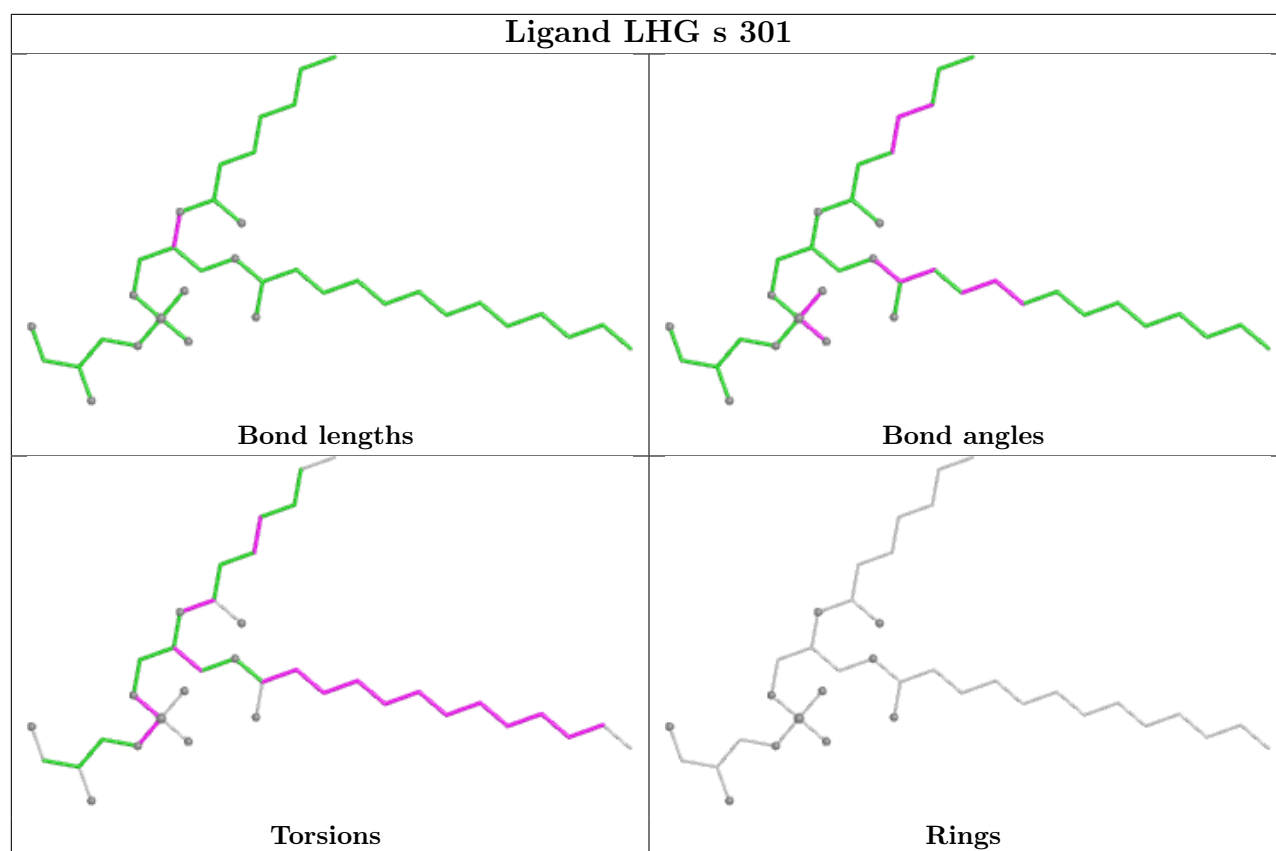
Ligand II0 p 316



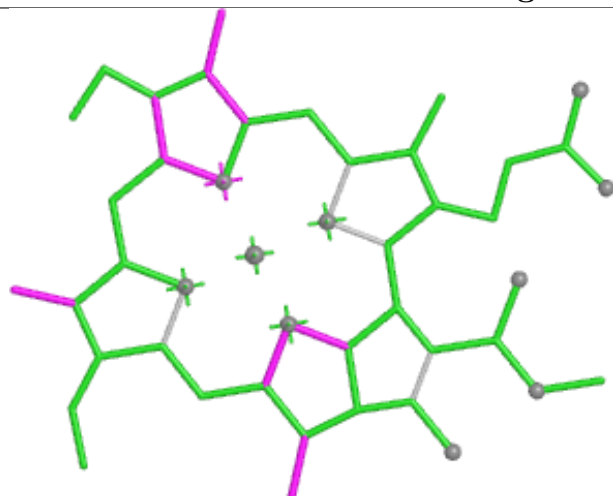
Ligand II0 p 317	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand II0 9 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

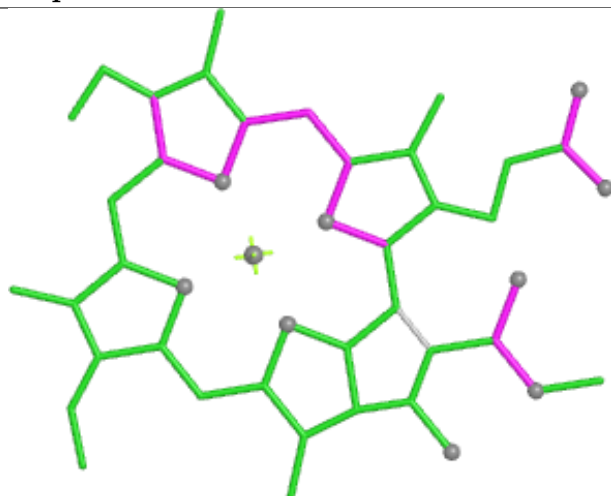
Ligand IHT 0 614	
	
Bond lengths	Bond angles
	
Torsions	Rings



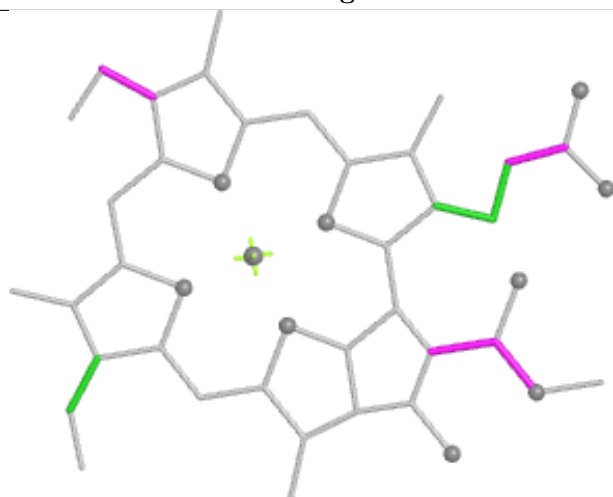
Ligand CLA p 308



Bond lengths



Bond angles

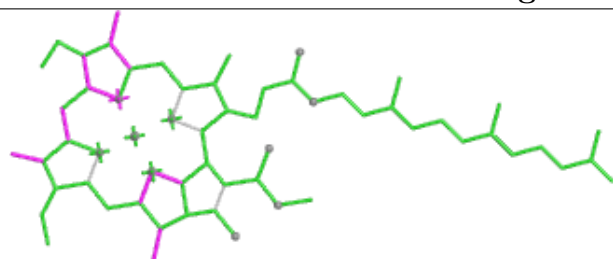


Torsions

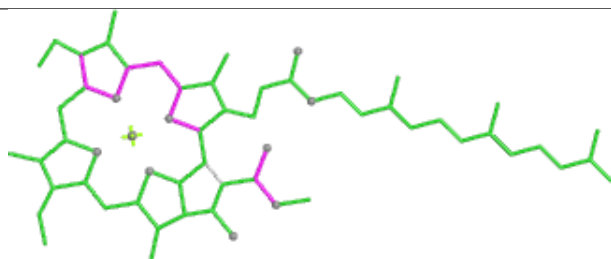


Rings

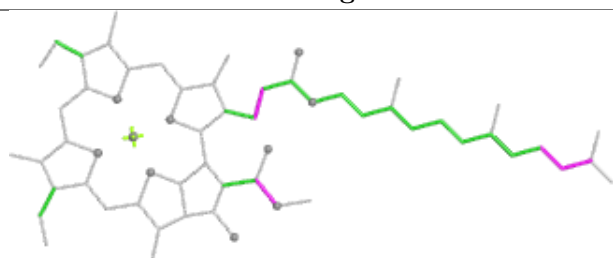
Ligand CLA 9 607



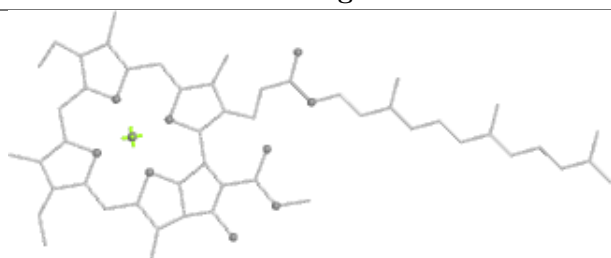
Bond lengths



Bond angles

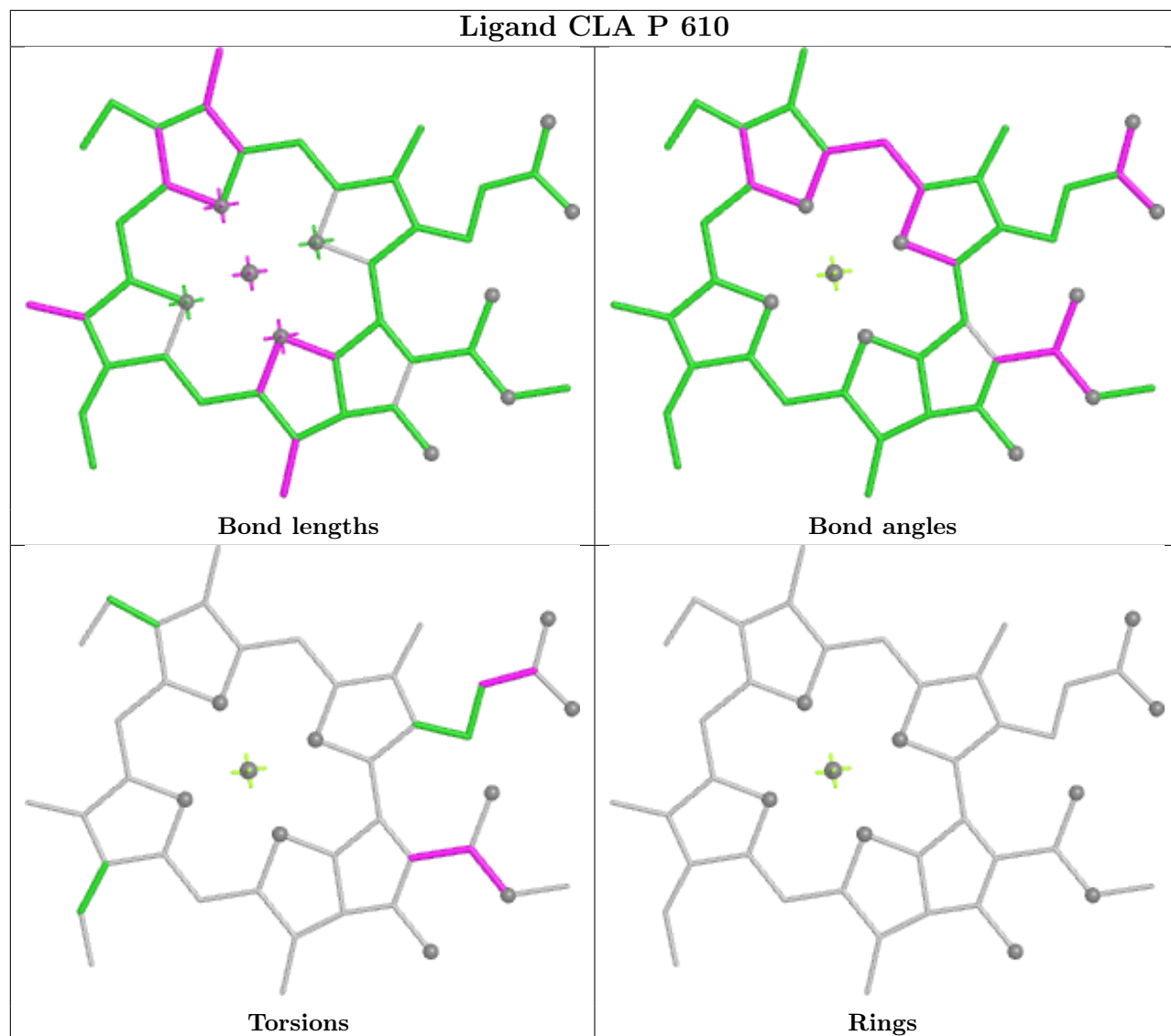


Torsions

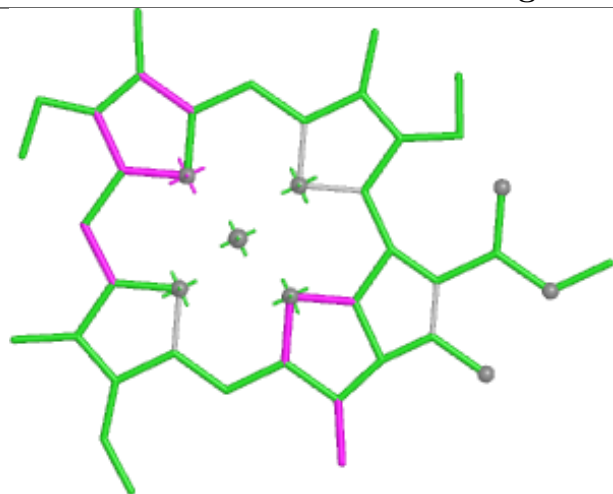


Rings

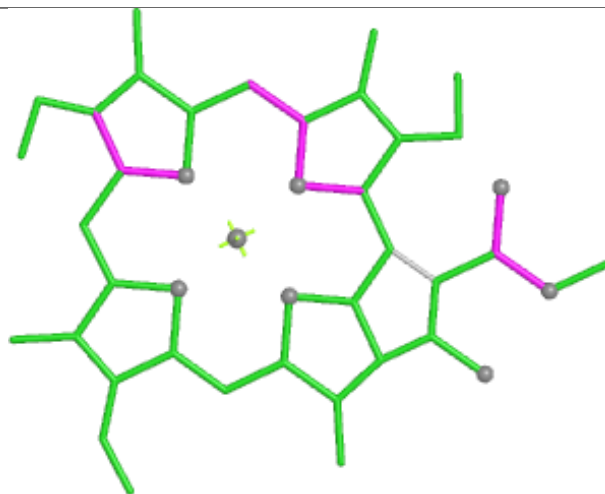
Ligand CLA P 610



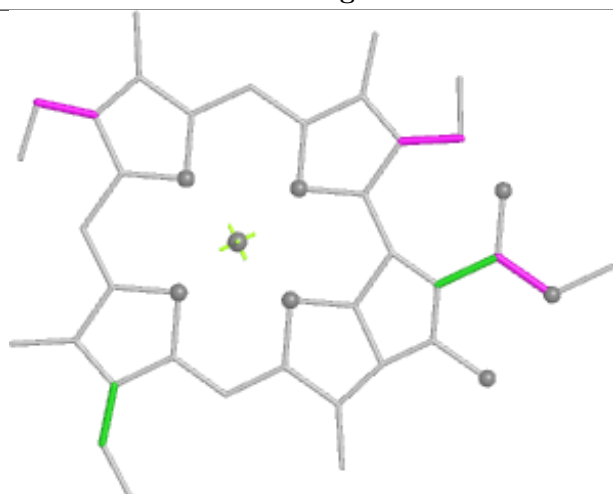
Ligand CLA 7 601



Bond lengths



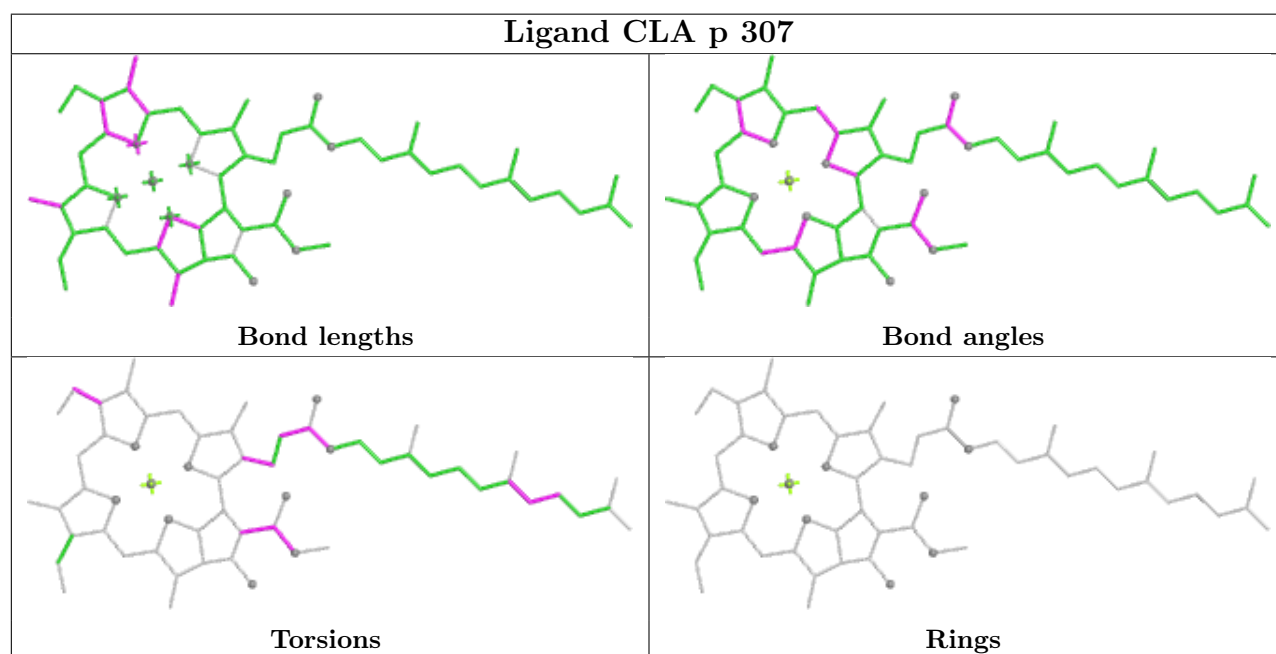
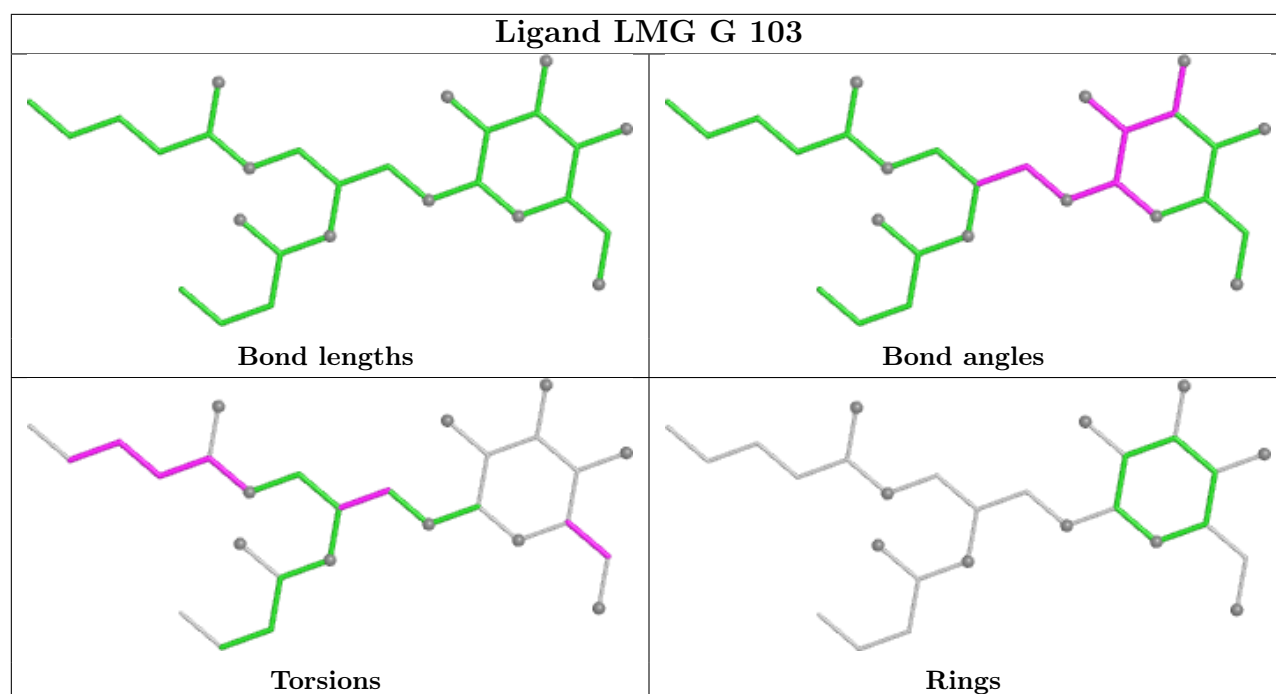
Bond angles



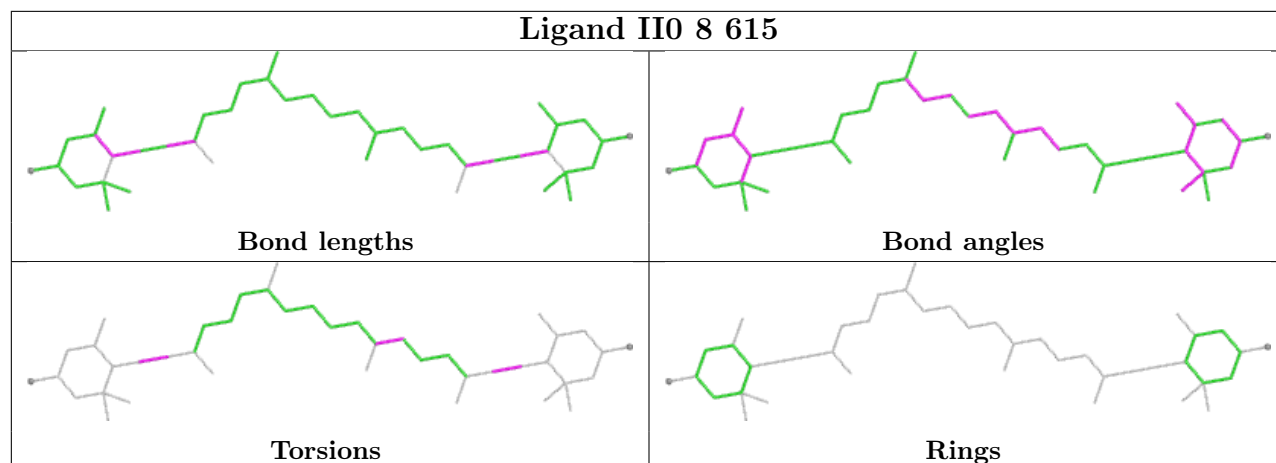
Torsions



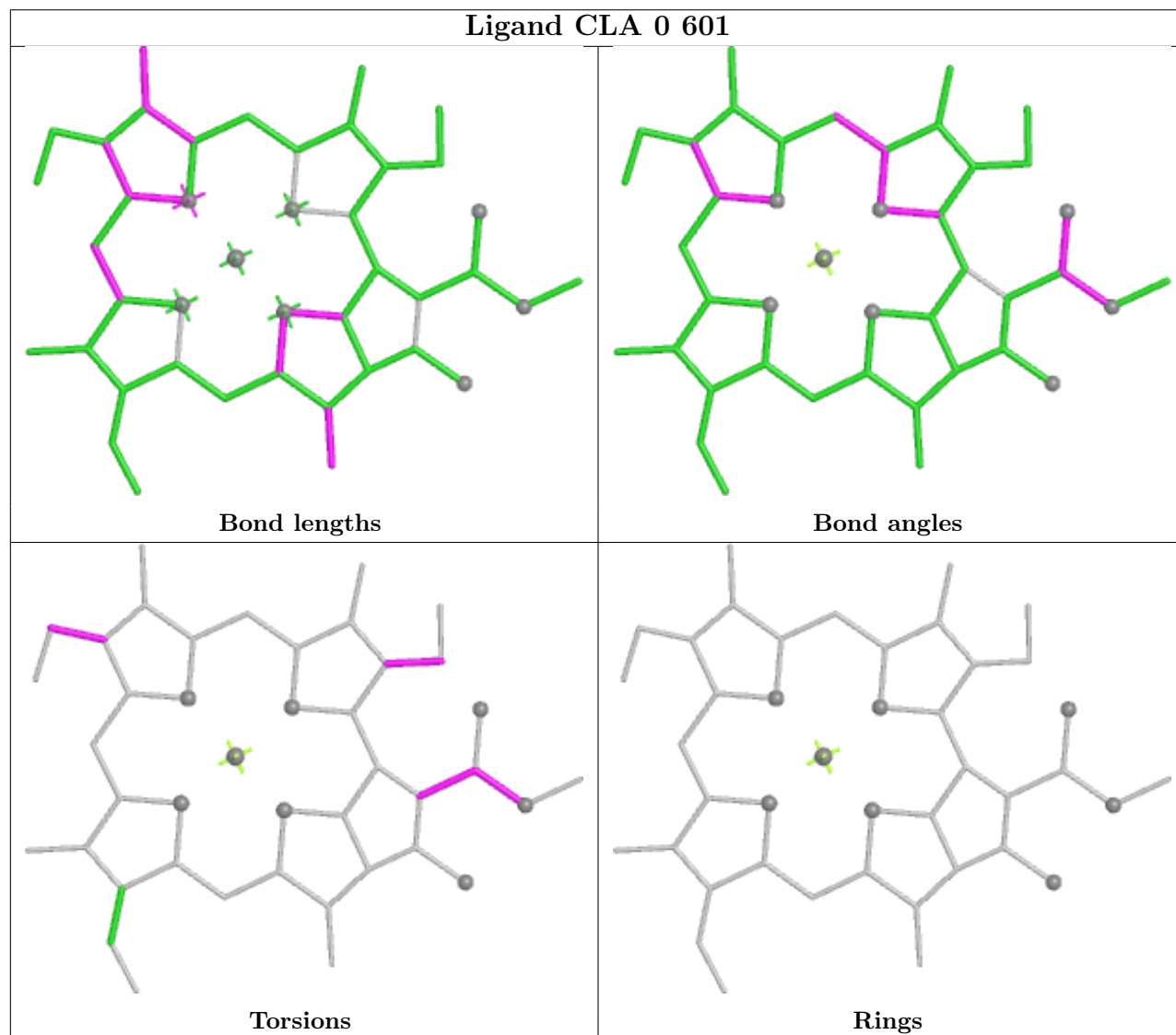
Rings

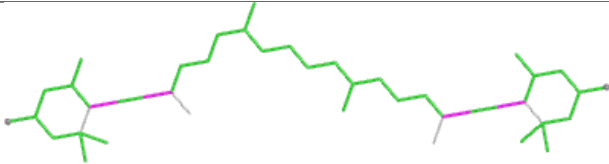
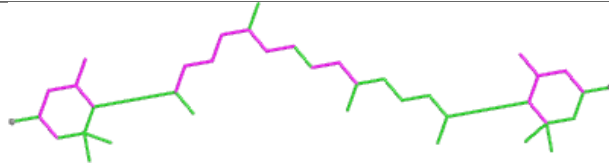
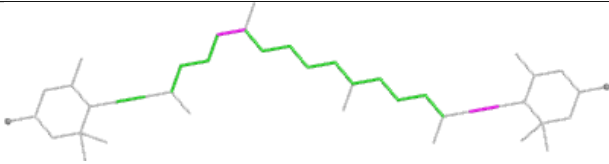
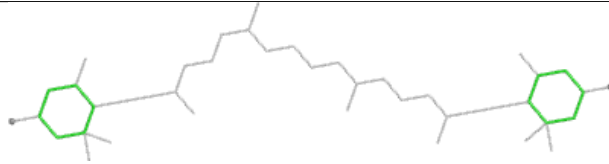


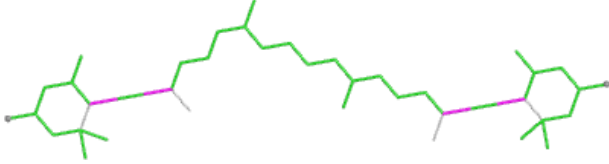
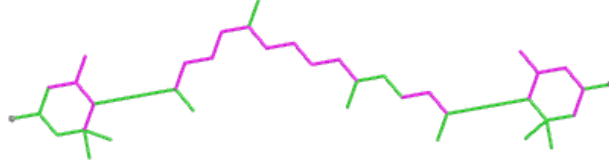
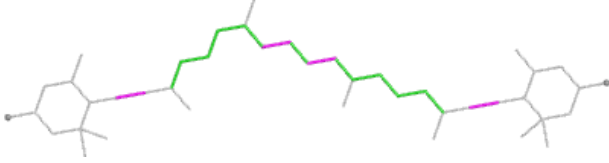
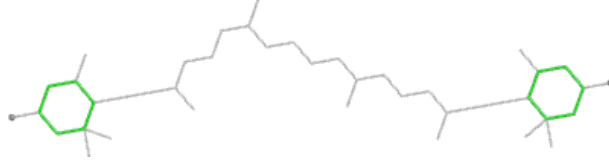
Ligand II0 8 615



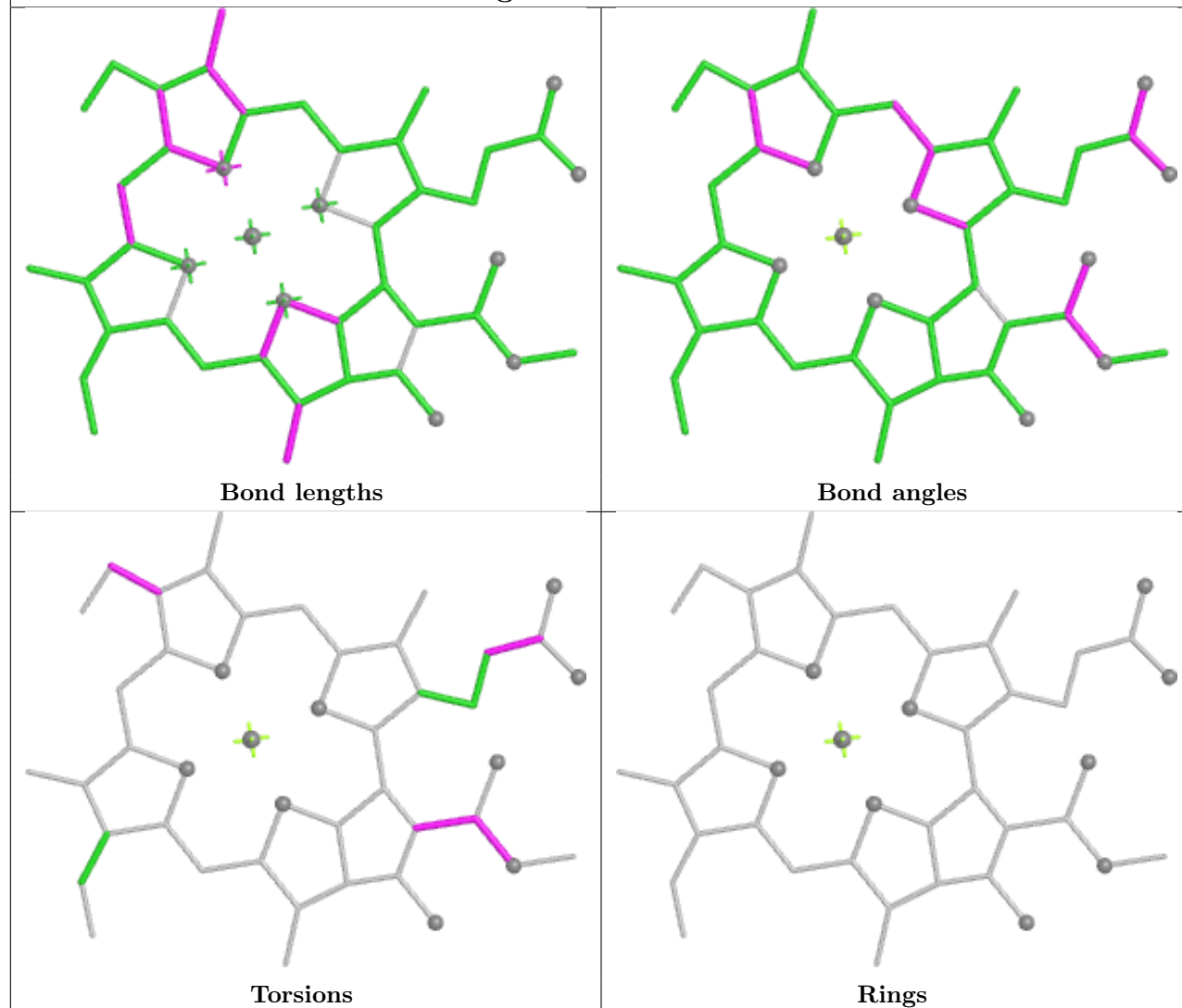
Ligand CLA 0 601



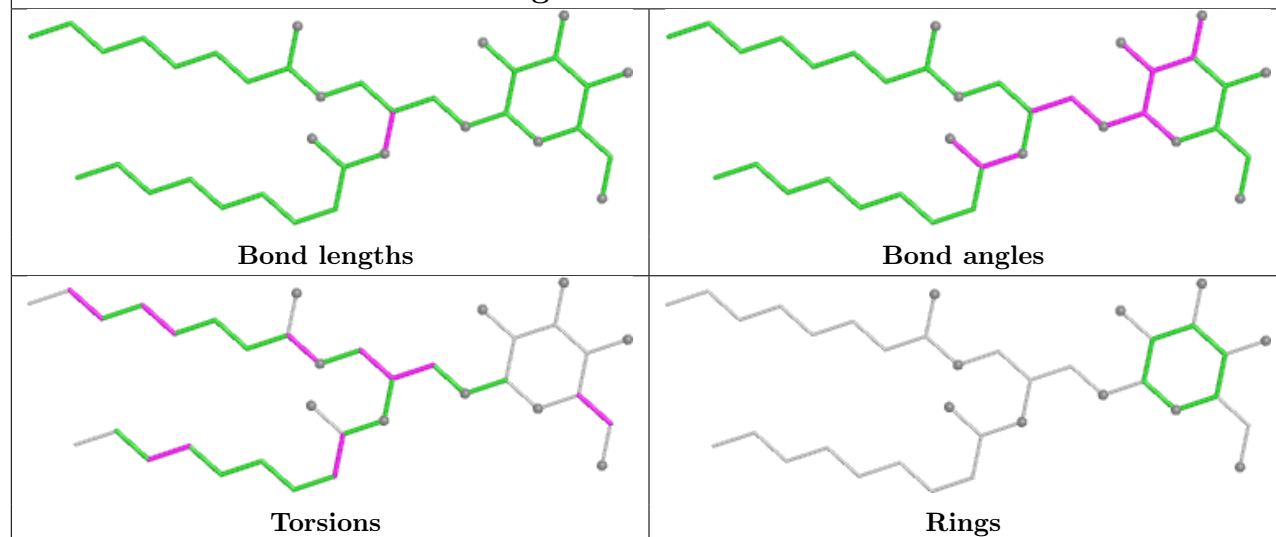
Ligand II0 P 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand II0 O 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

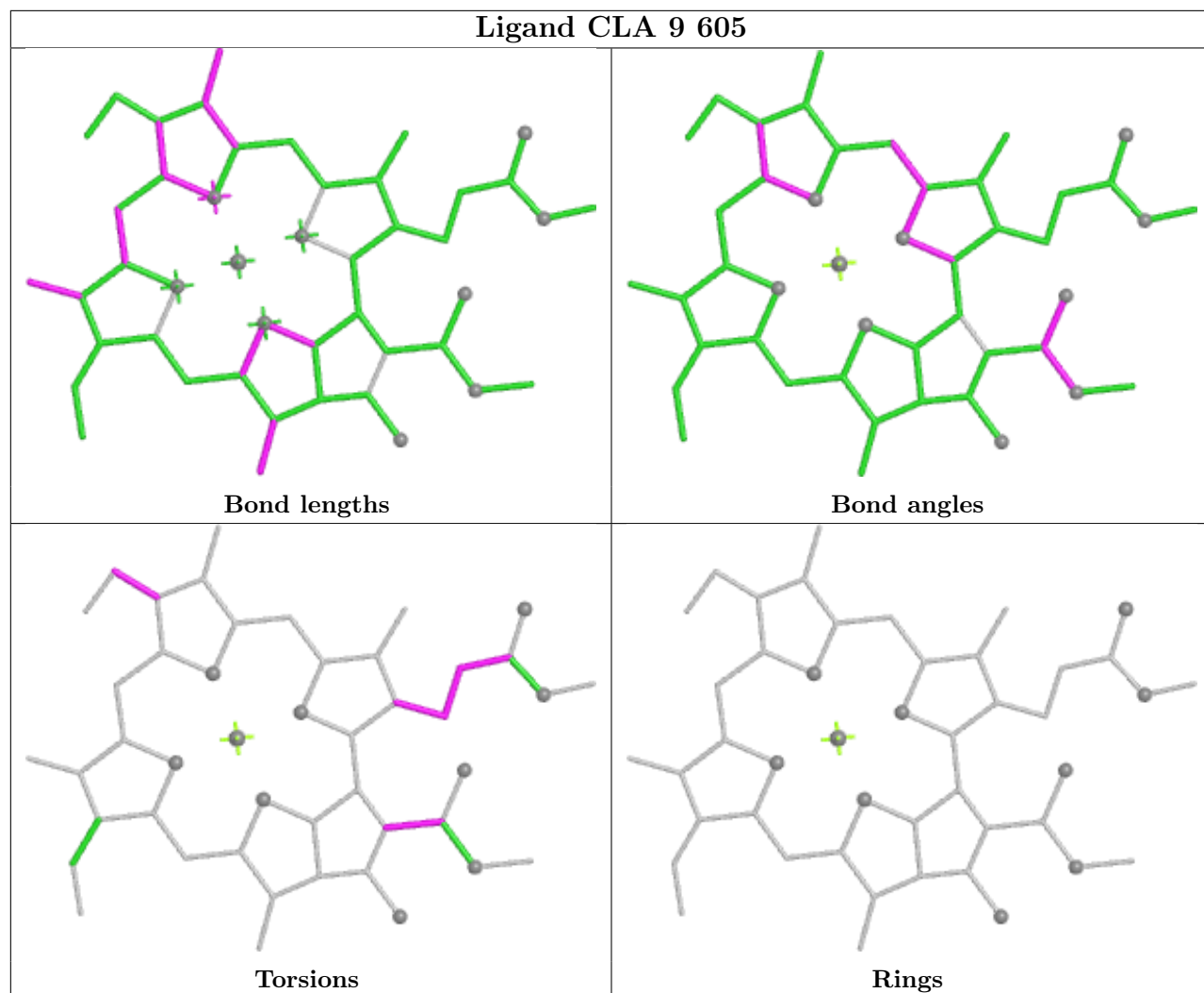
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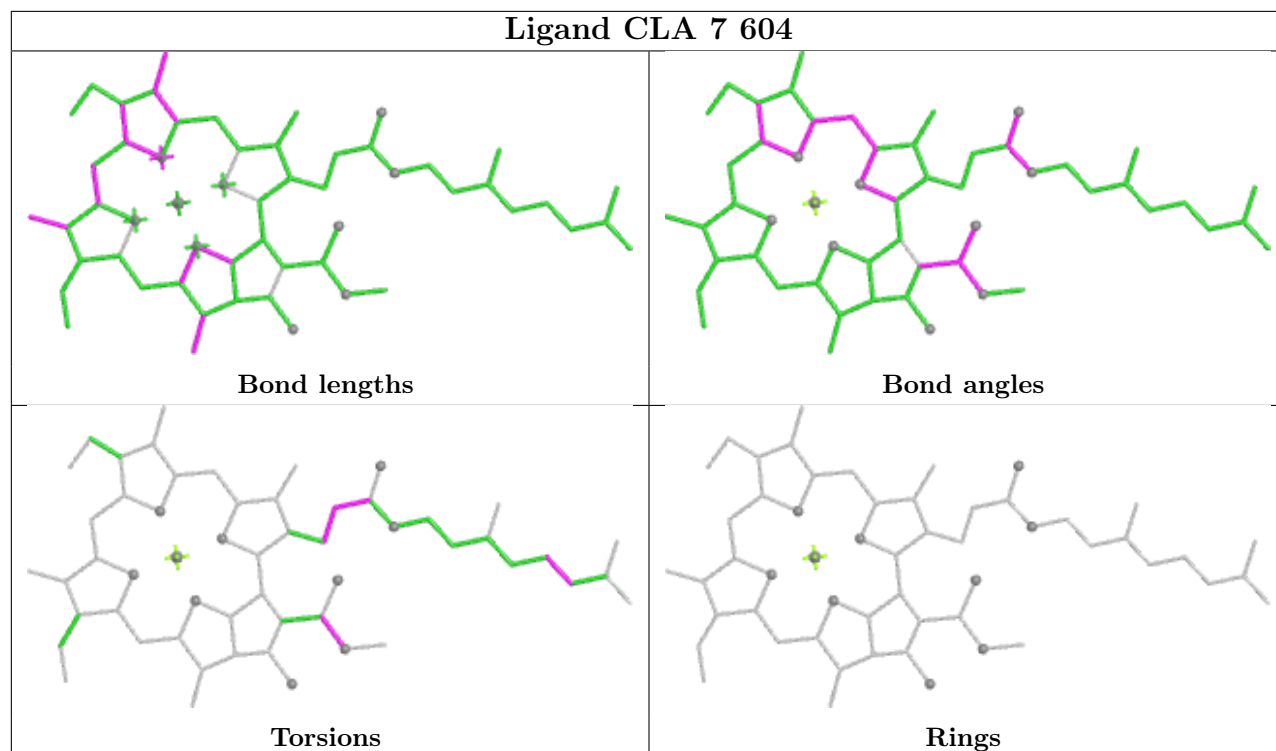
Ligand LMG 8 617



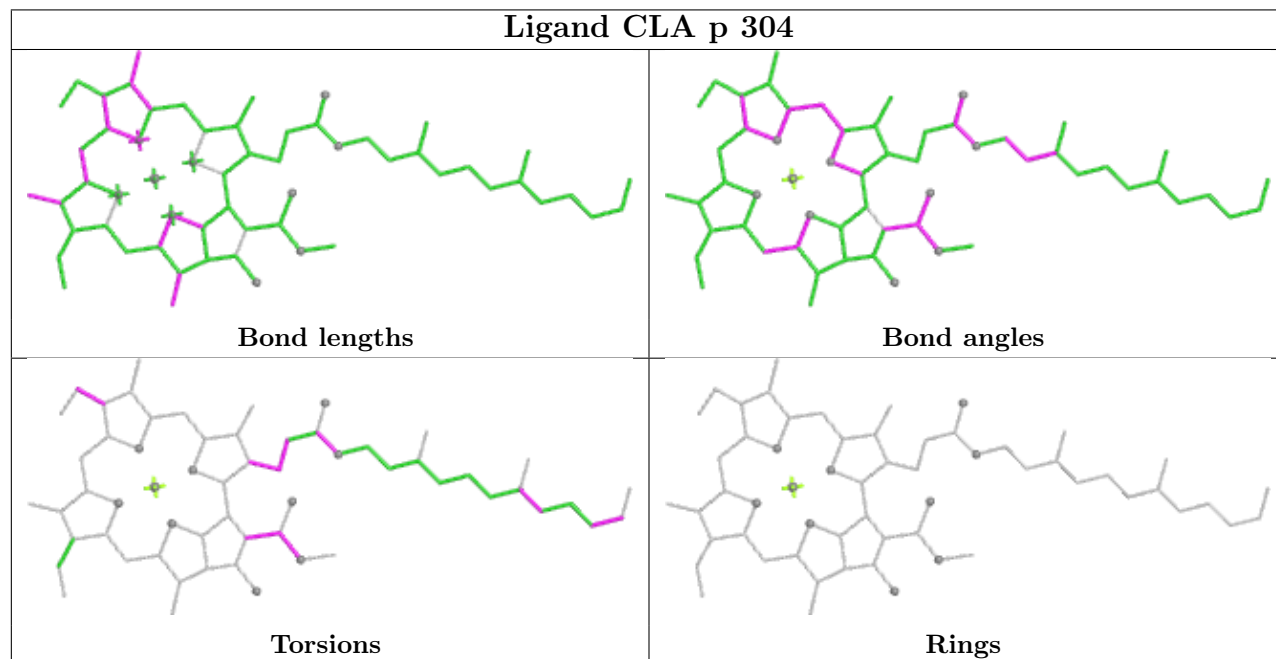
Ligand CLA 9 605

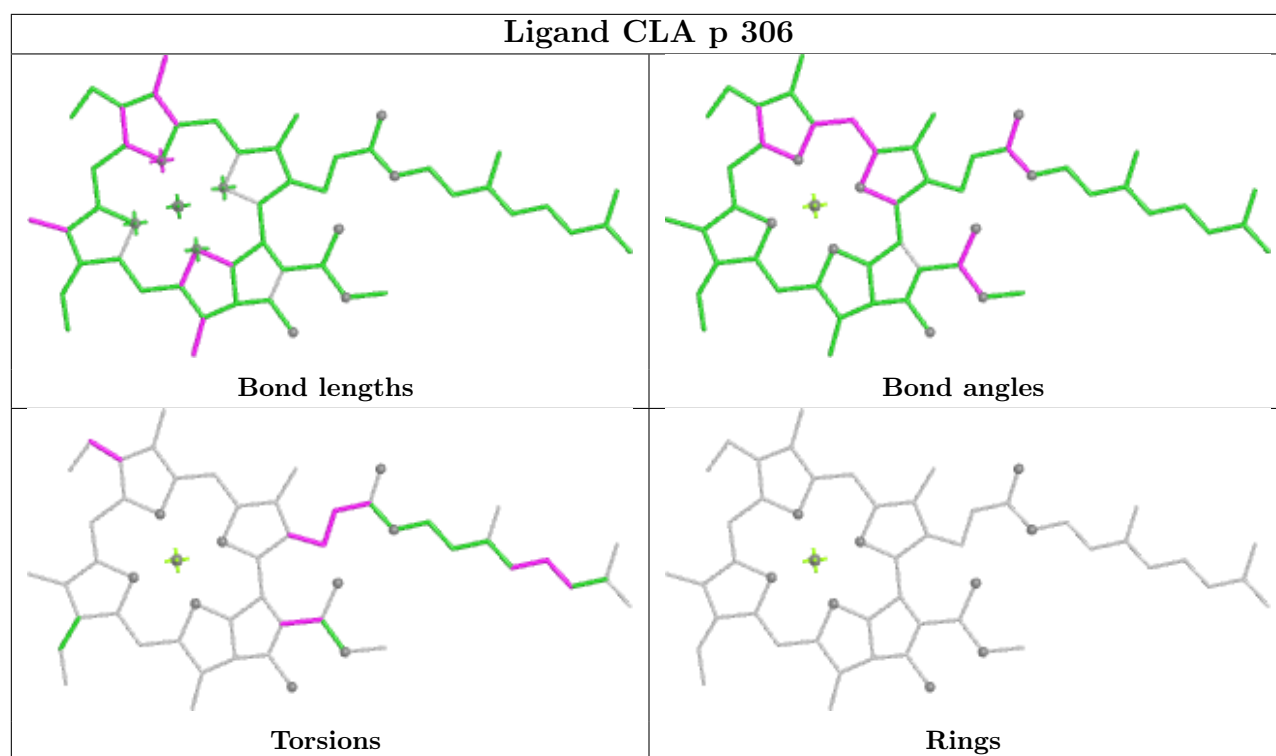


Ligand CLA 7 604

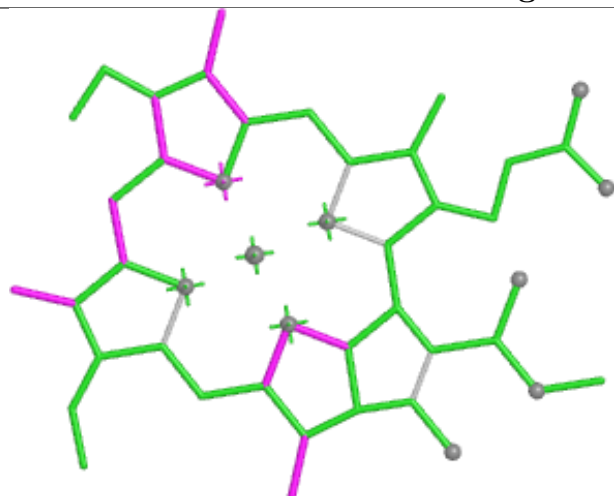


Ligand CLA p 304

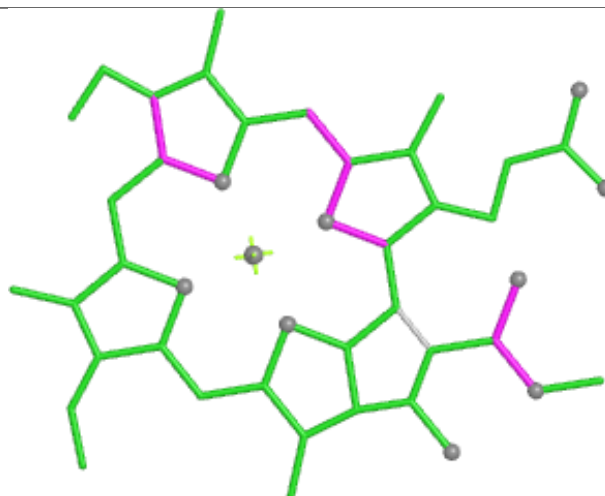




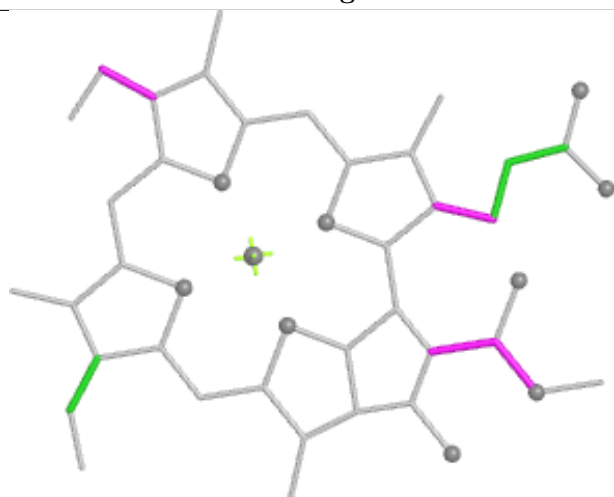
Ligand CLA 9 611



Bond lengths



Bond angles

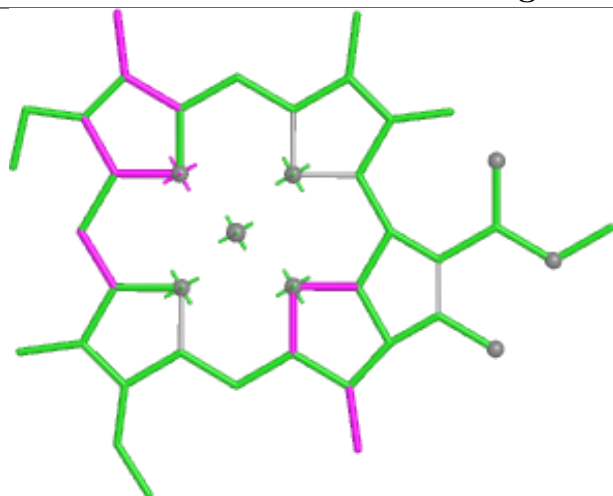


Torsions

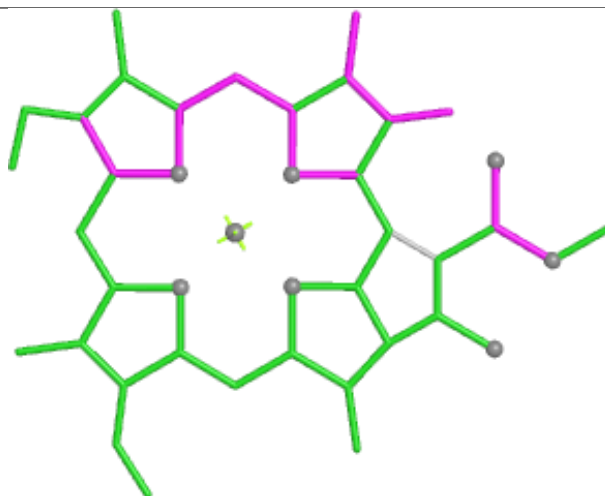


Rings

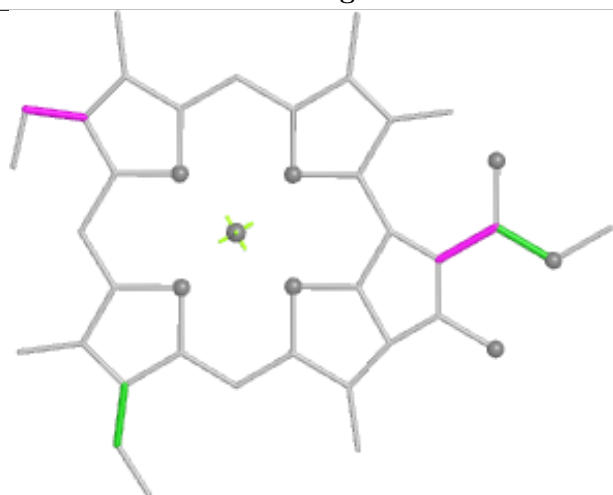
Ligand CLA 0 609



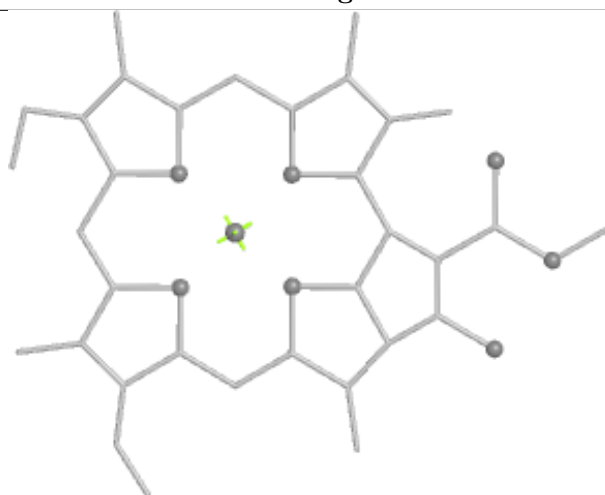
Bond lengths



Bond angles

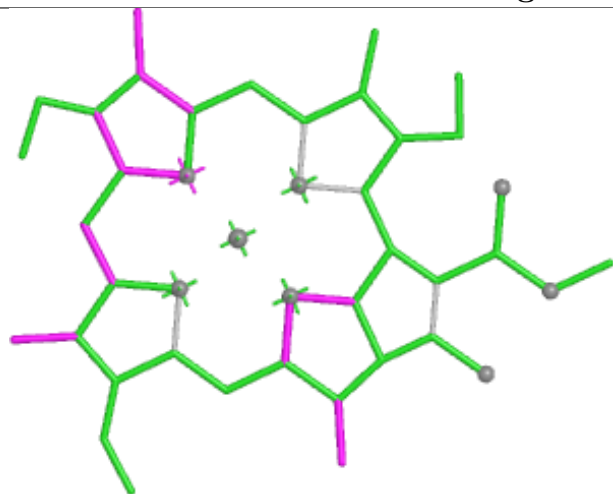


Torsions

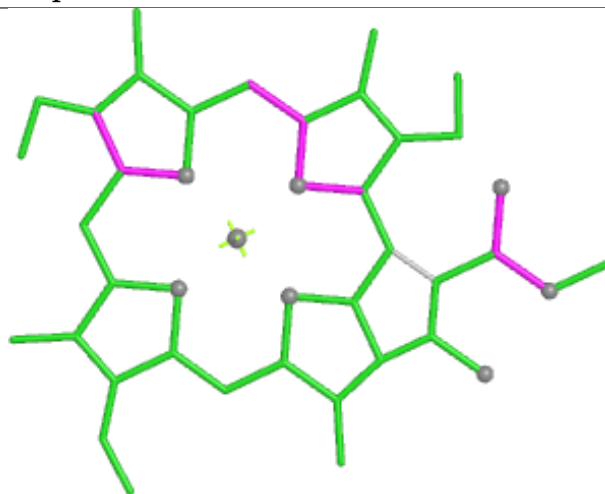


Rings

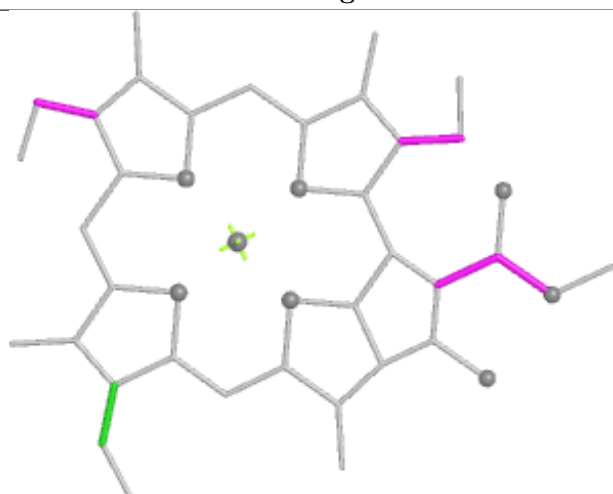
Ligand CLA p 303



Bond lengths



Bond angles

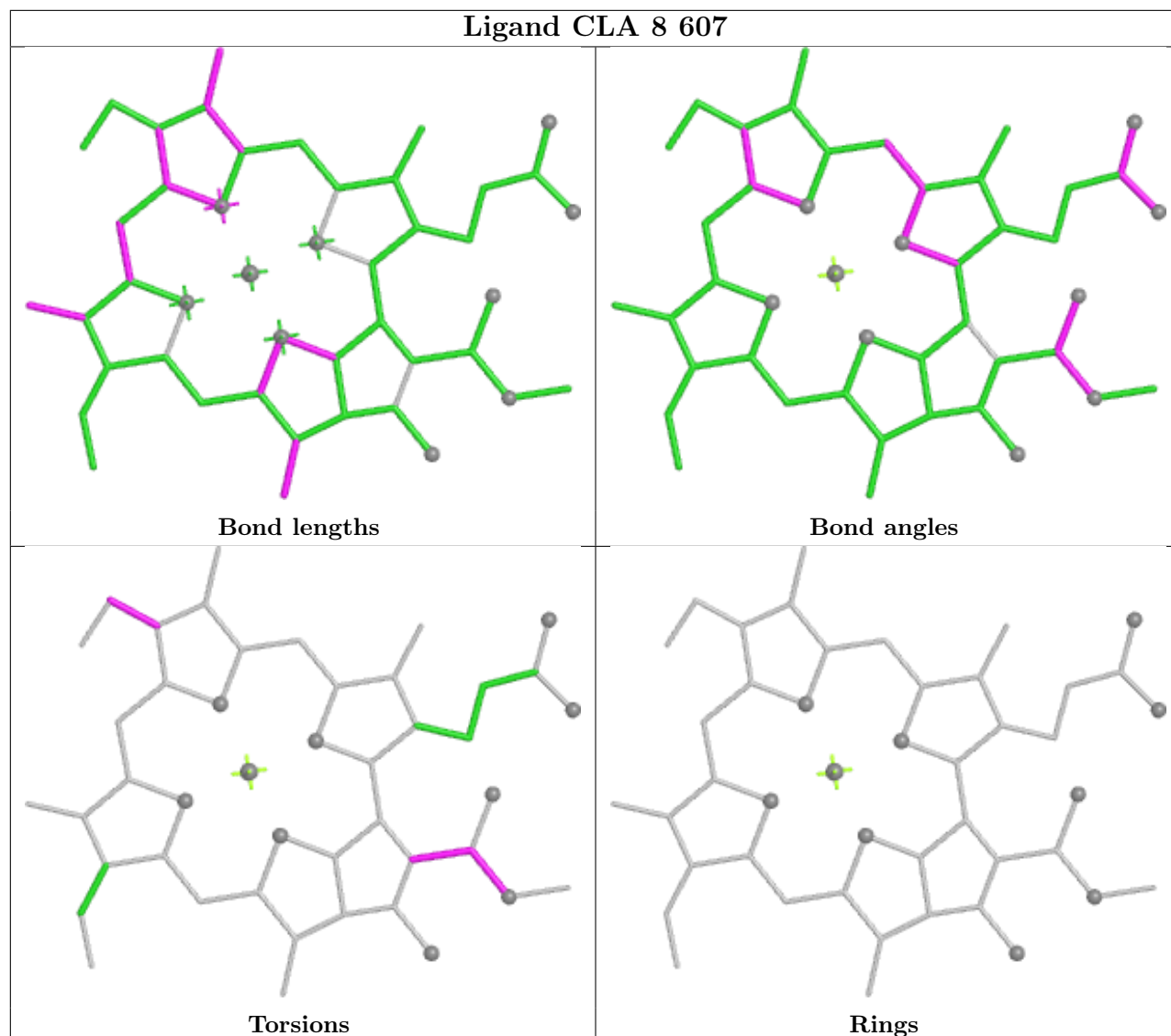


Torsions

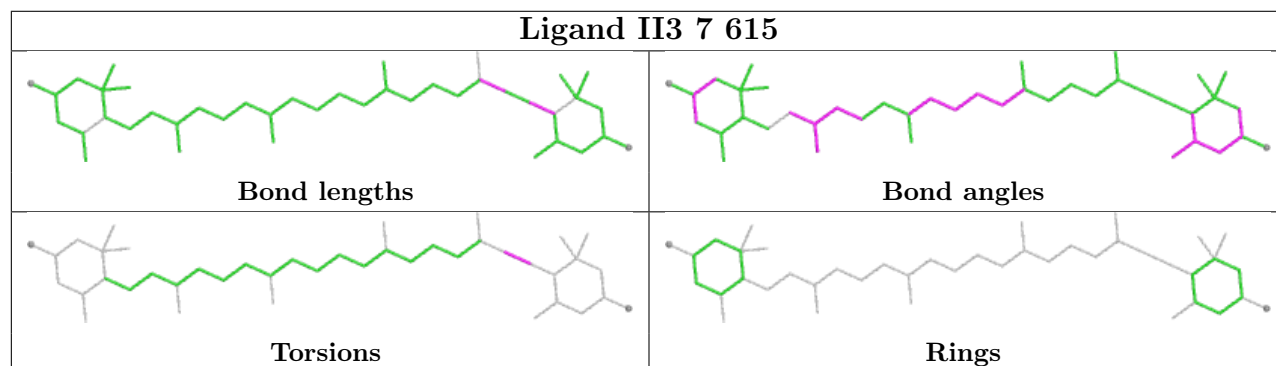


Rings

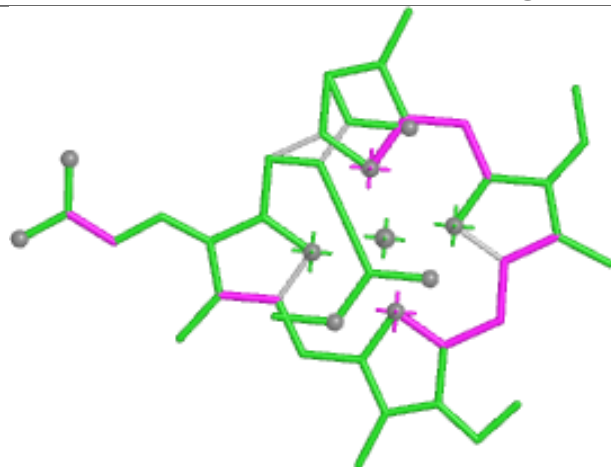
Ligand CLA 8 607



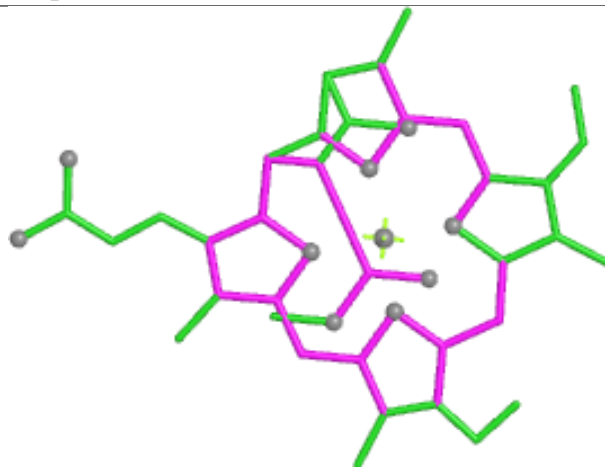
Ligand II3 7 615



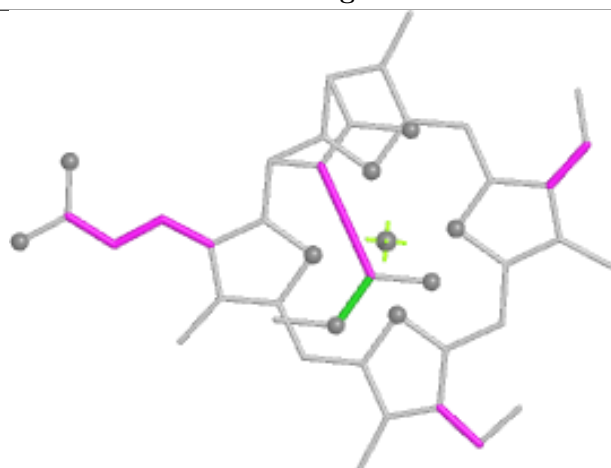
Ligand KC2 p 312



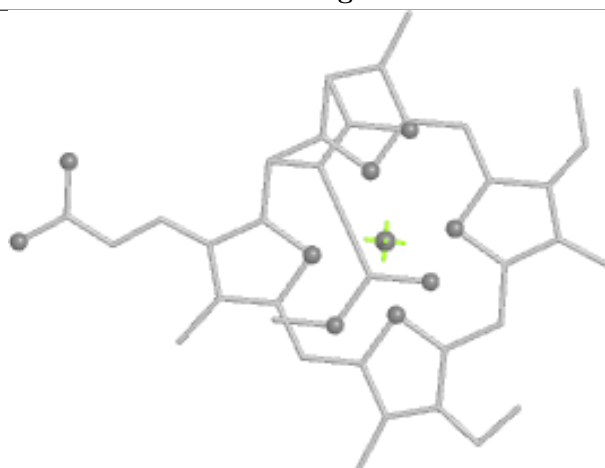
Bond lengths



Bond angles

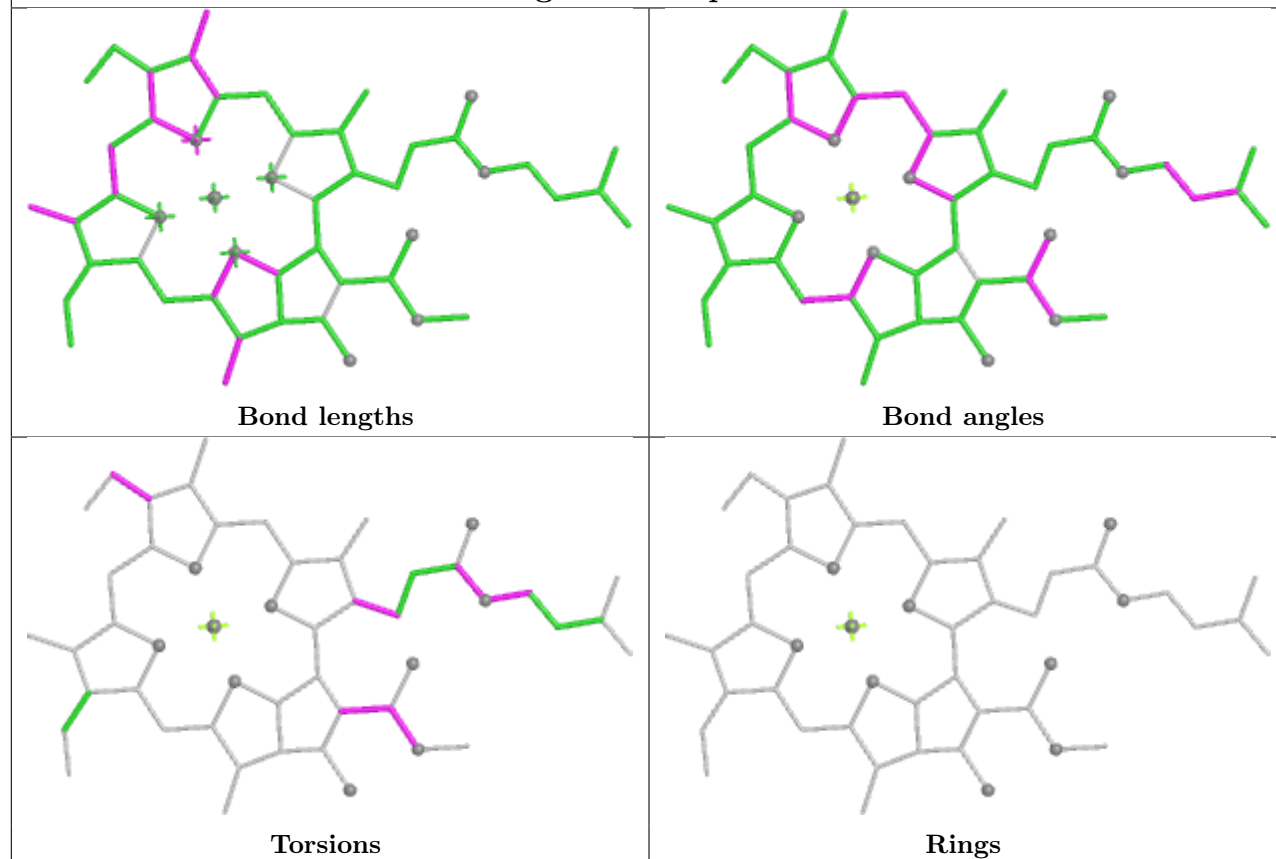


Torsions

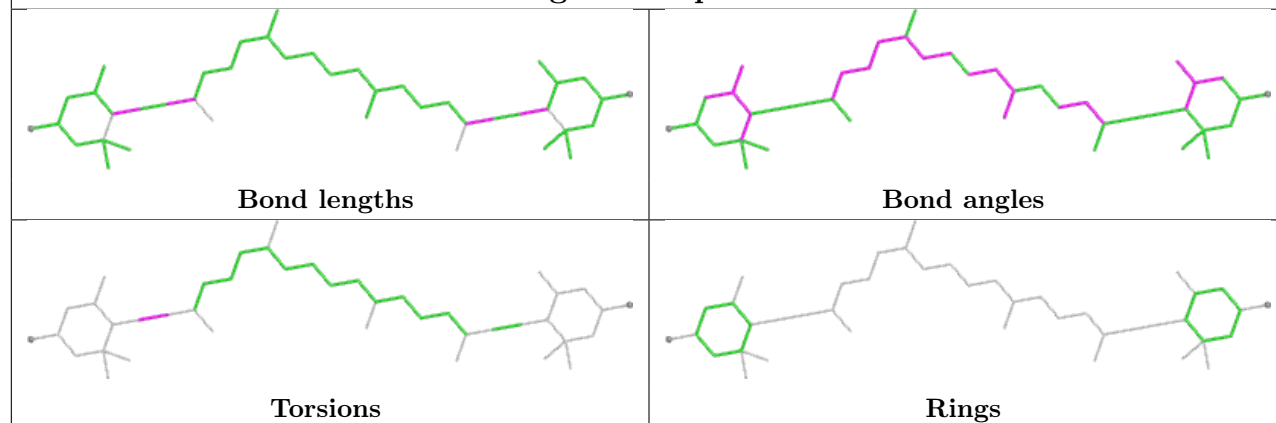


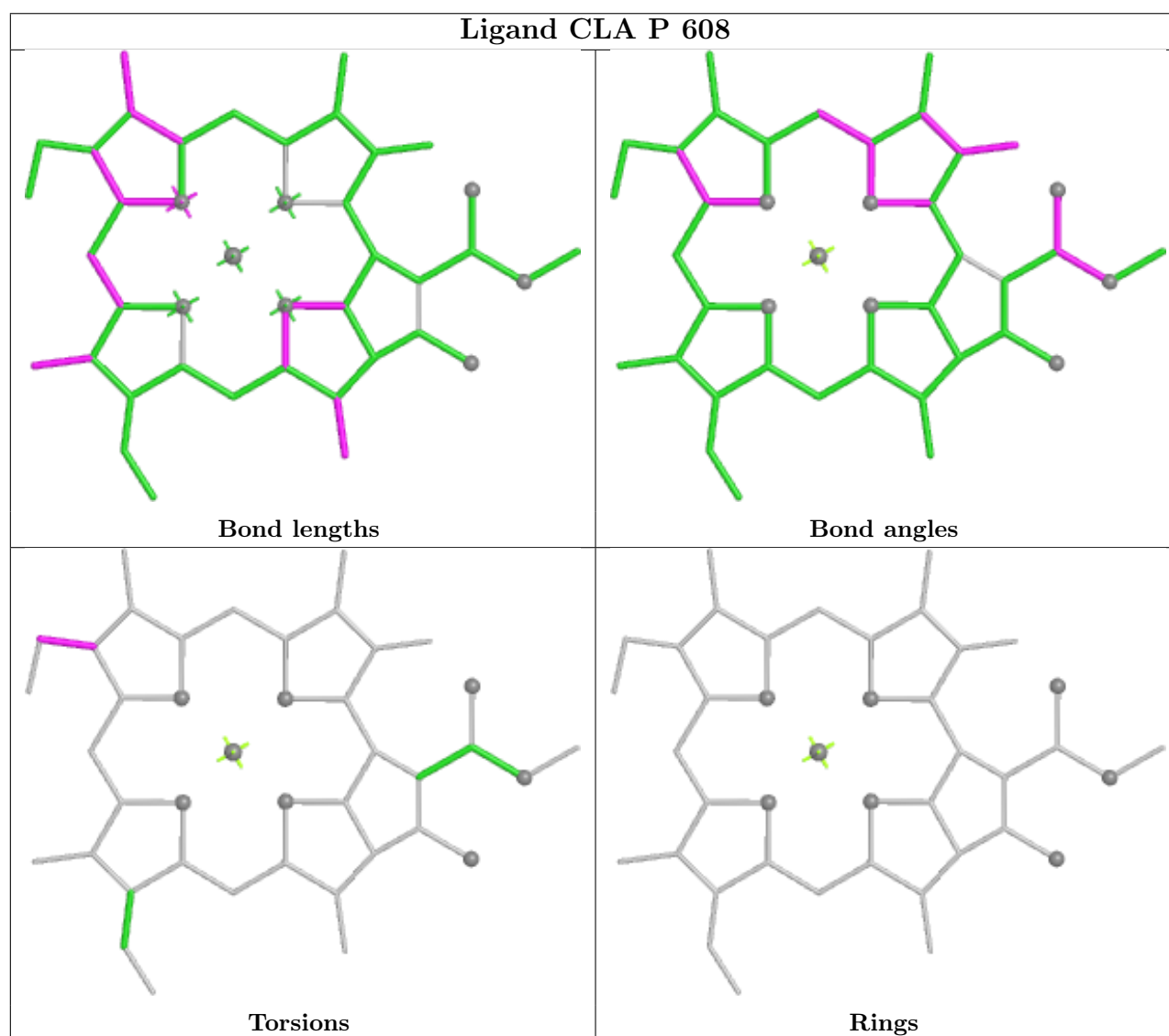
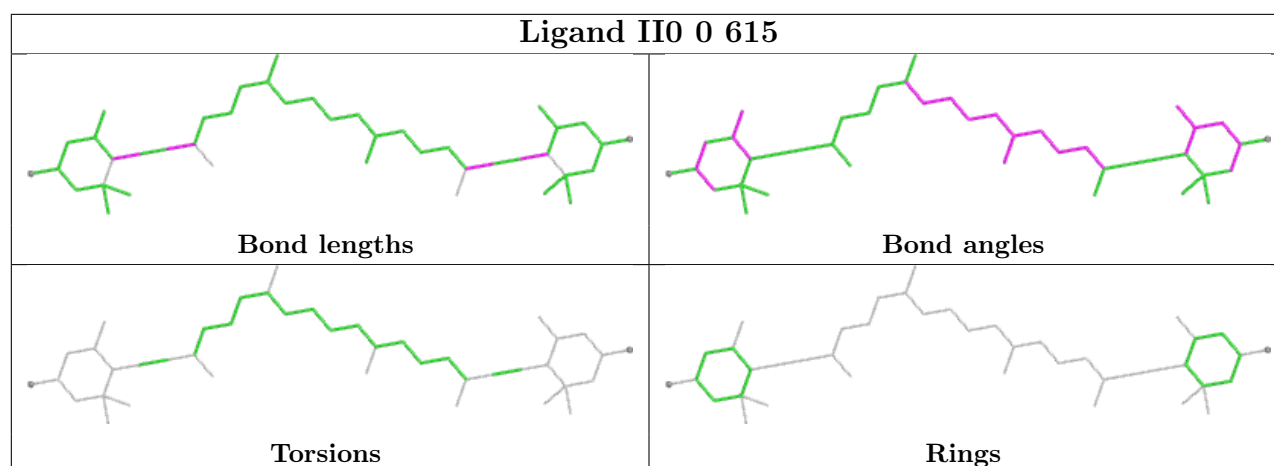
Rings

Ligand CLA p 305

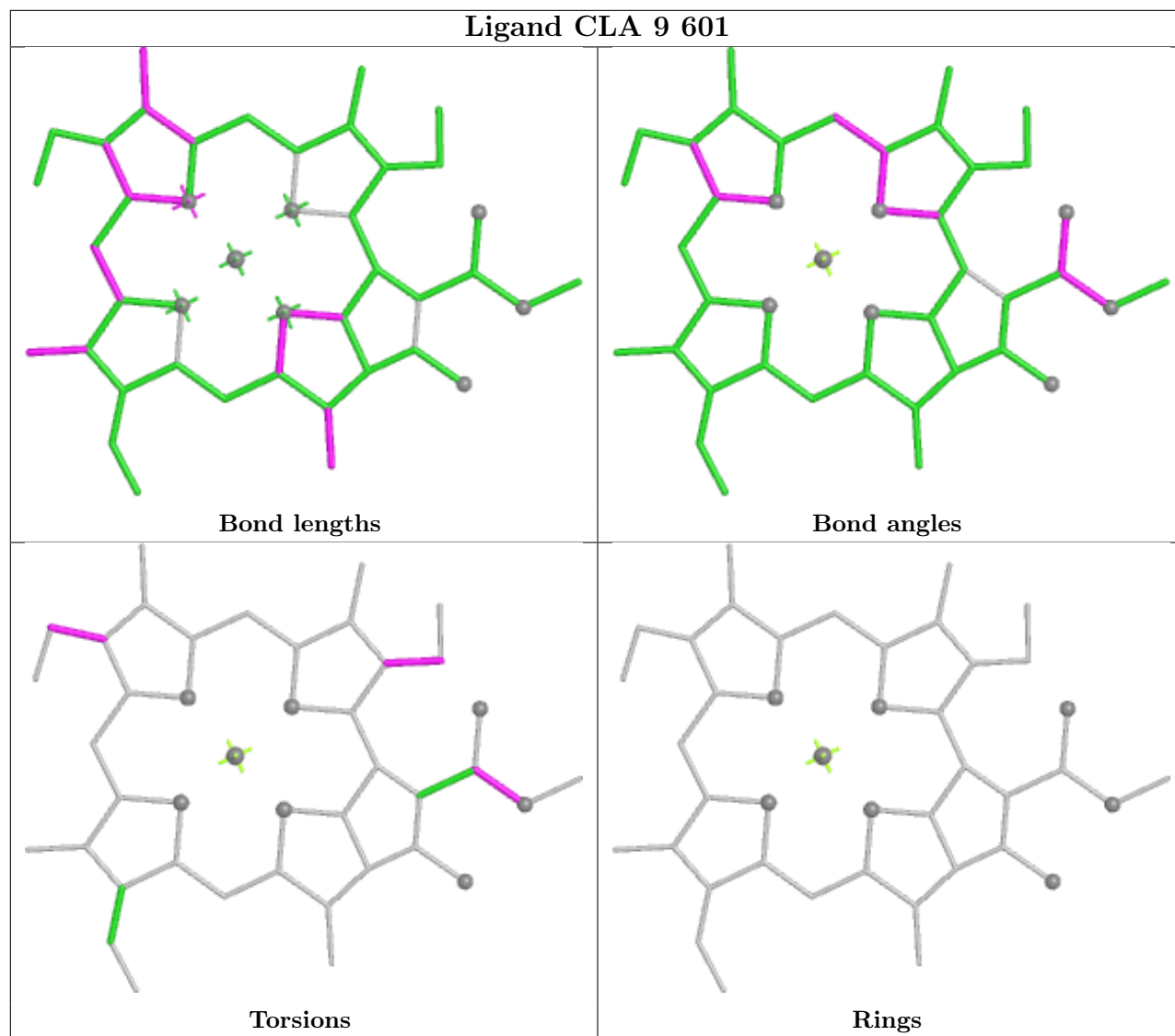


Ligand II0 p 302

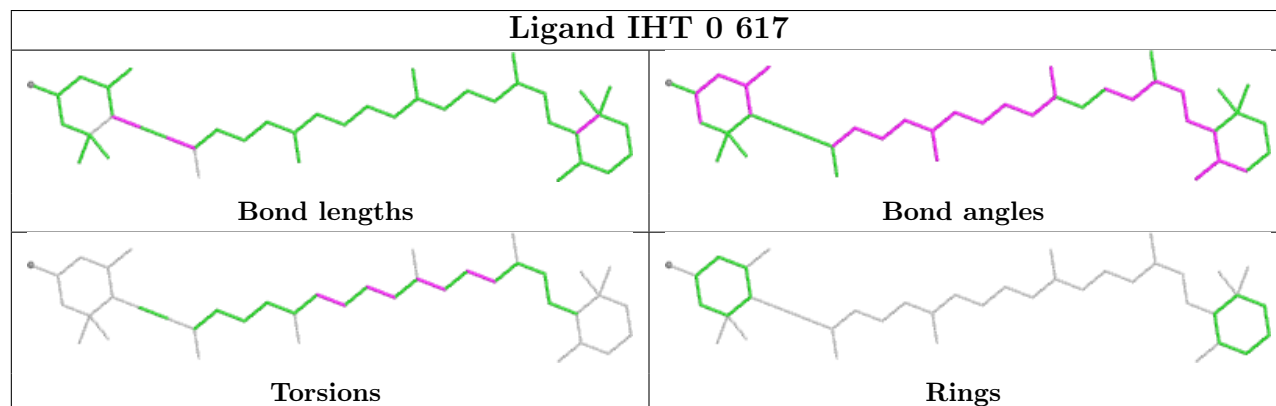


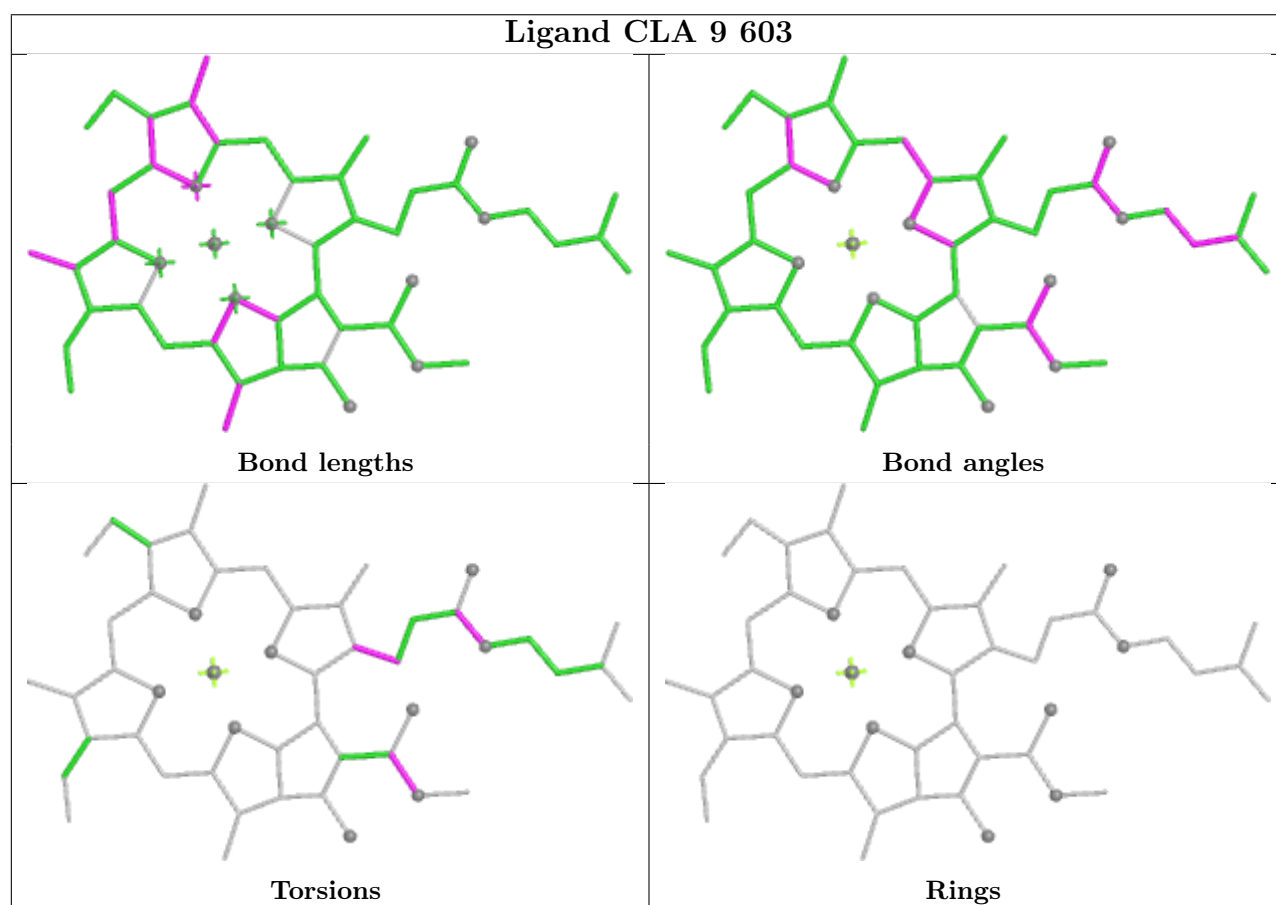
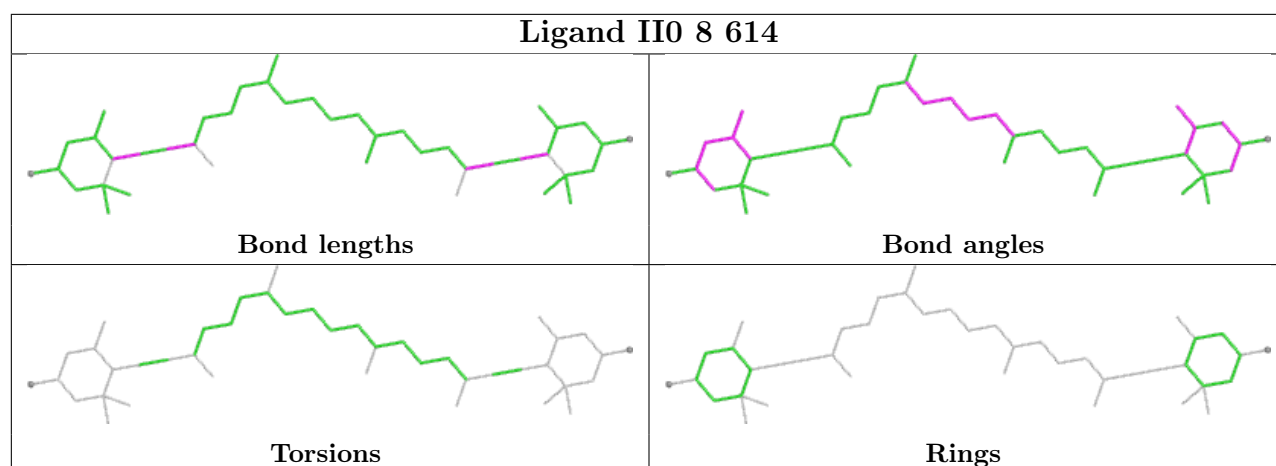


Ligand CLA 9 601

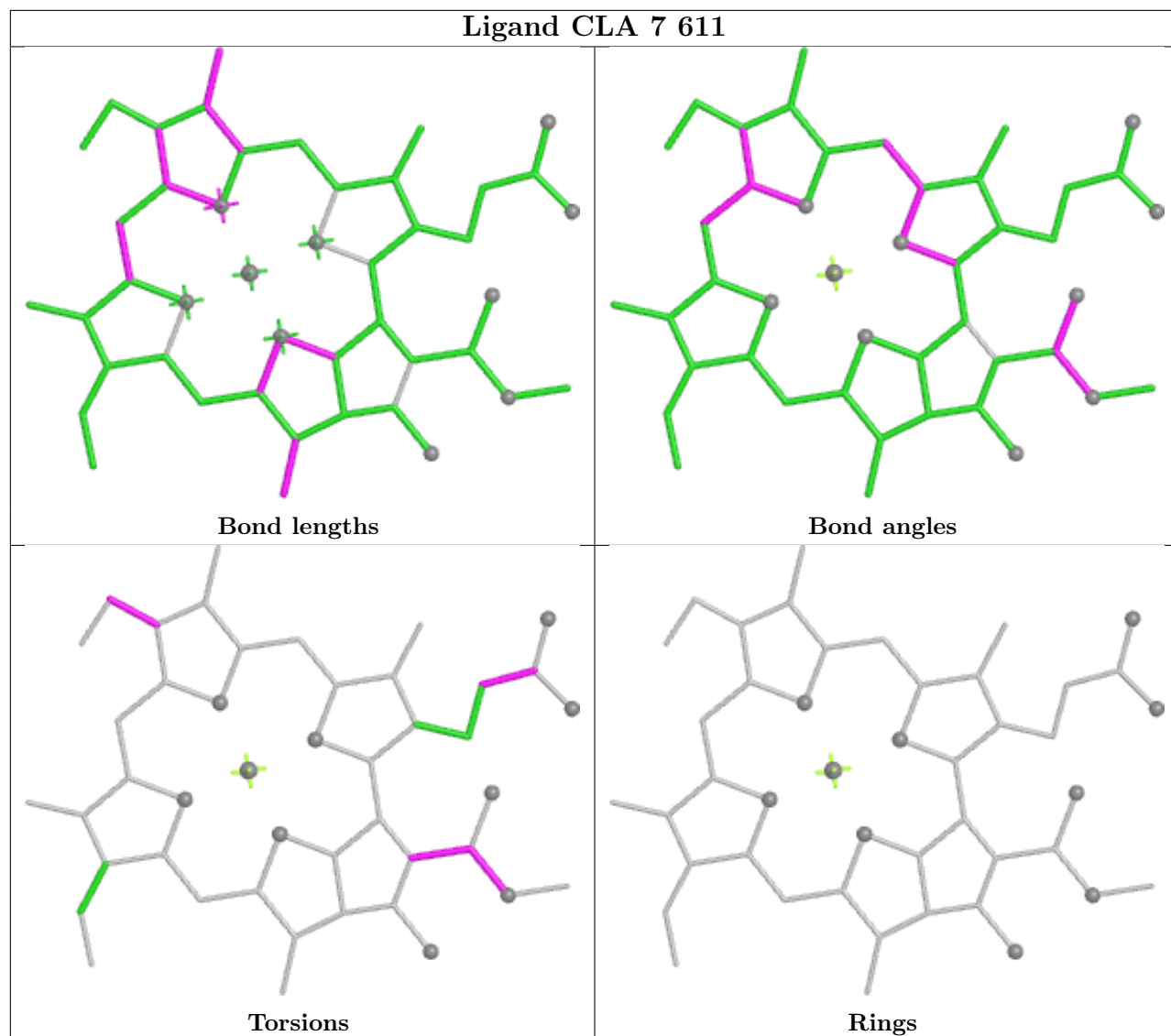


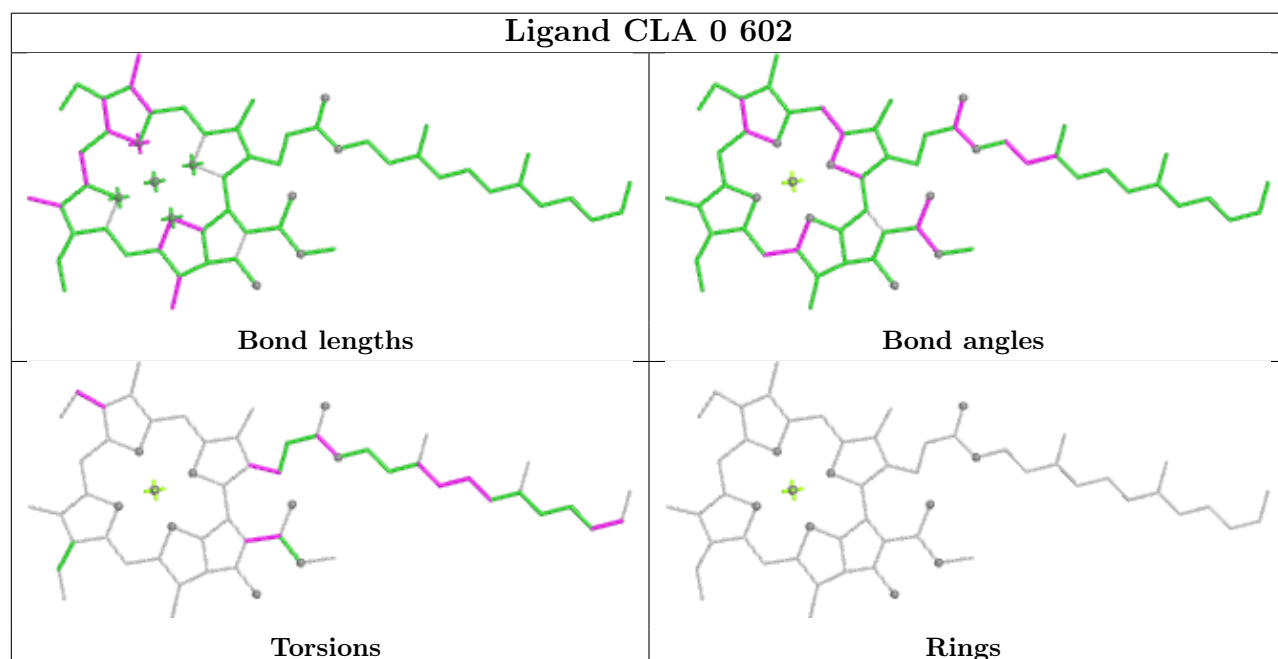
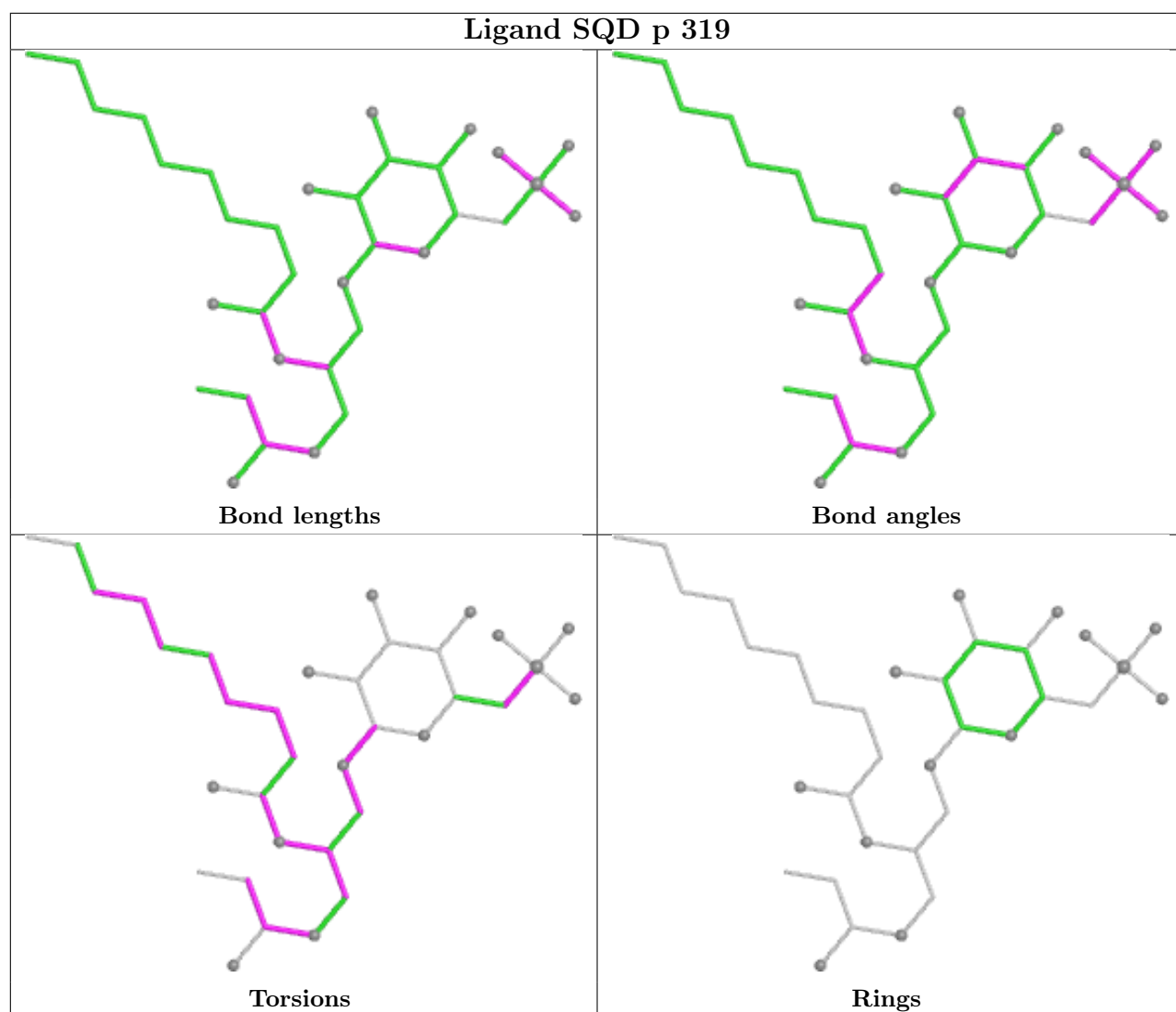
Ligand IHT 0 617



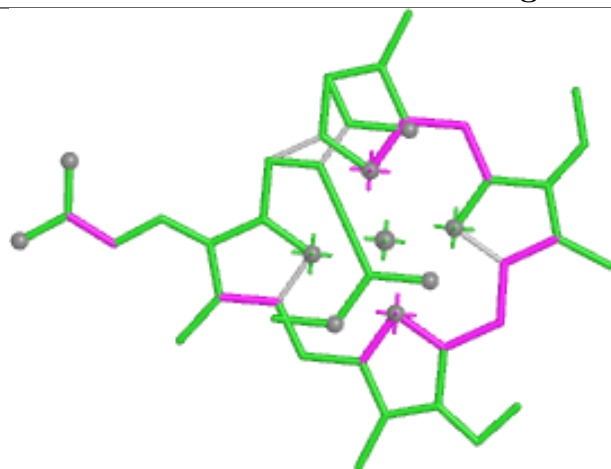


Ligand CLA 7 611

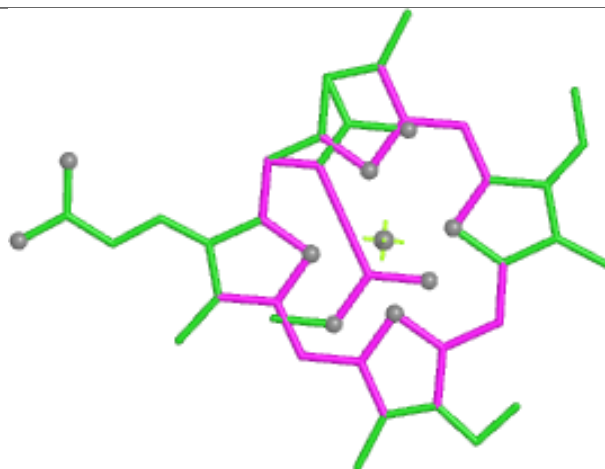




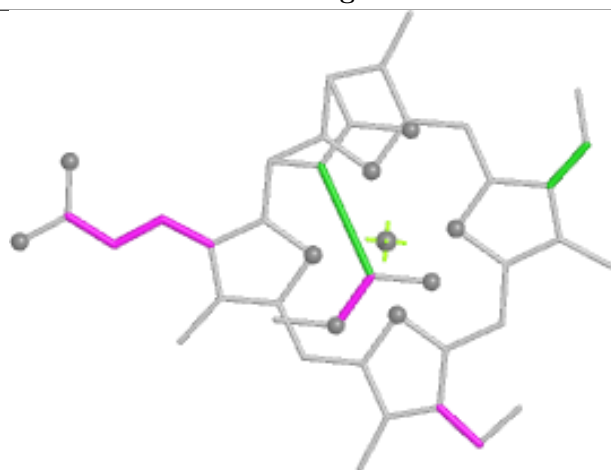
Ligand KC2 8 610



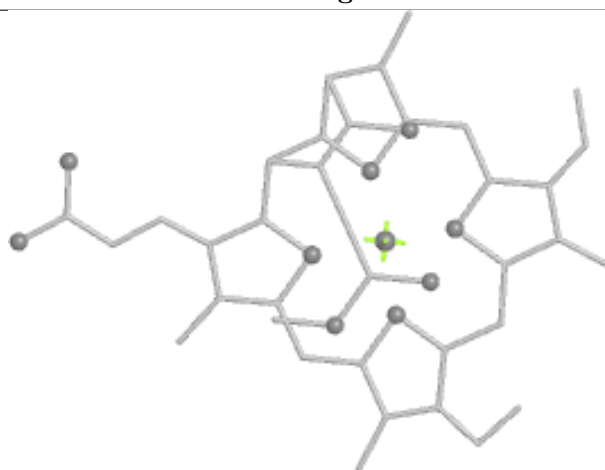
Bond lengths



Bond angles

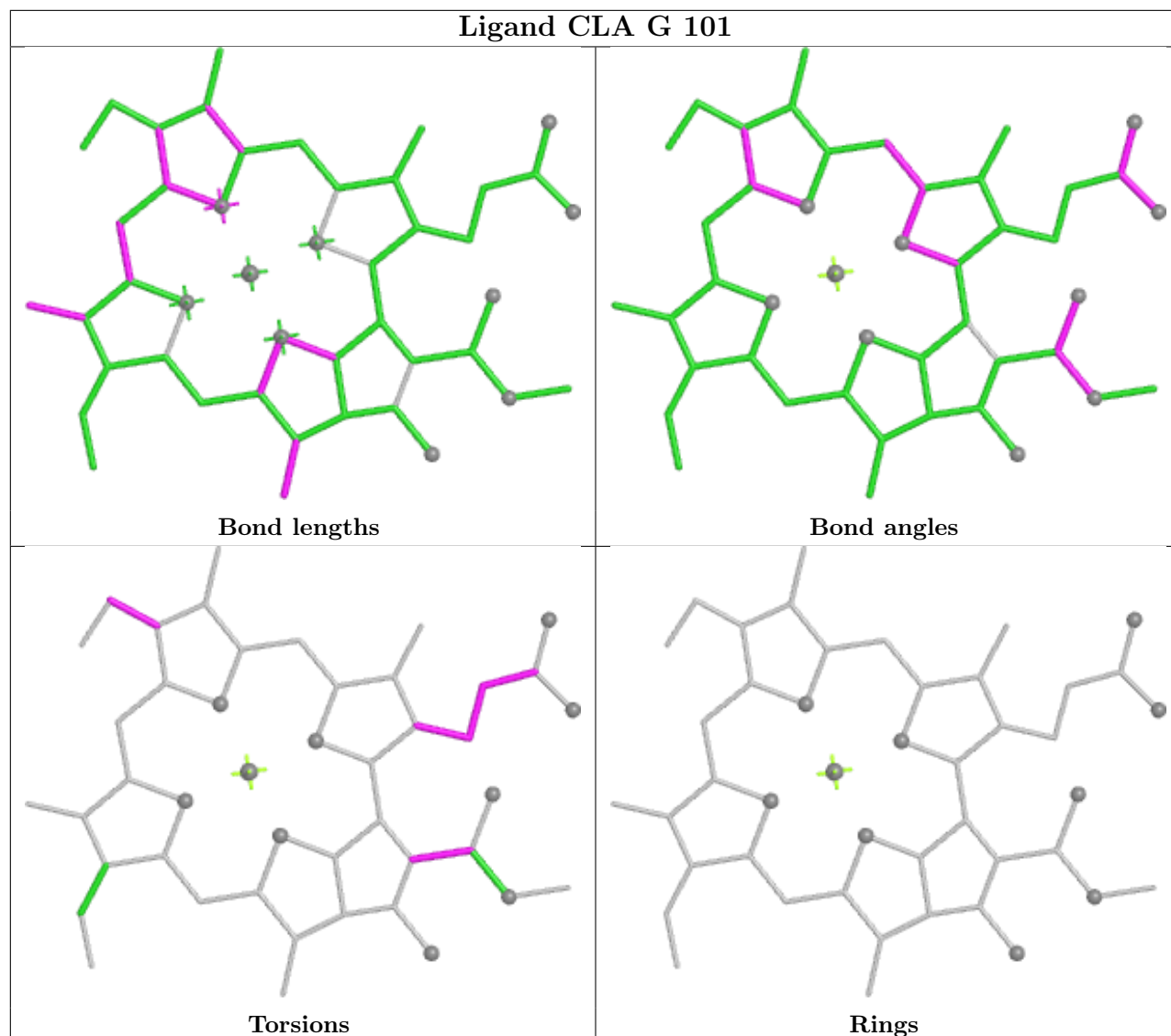


Torsions

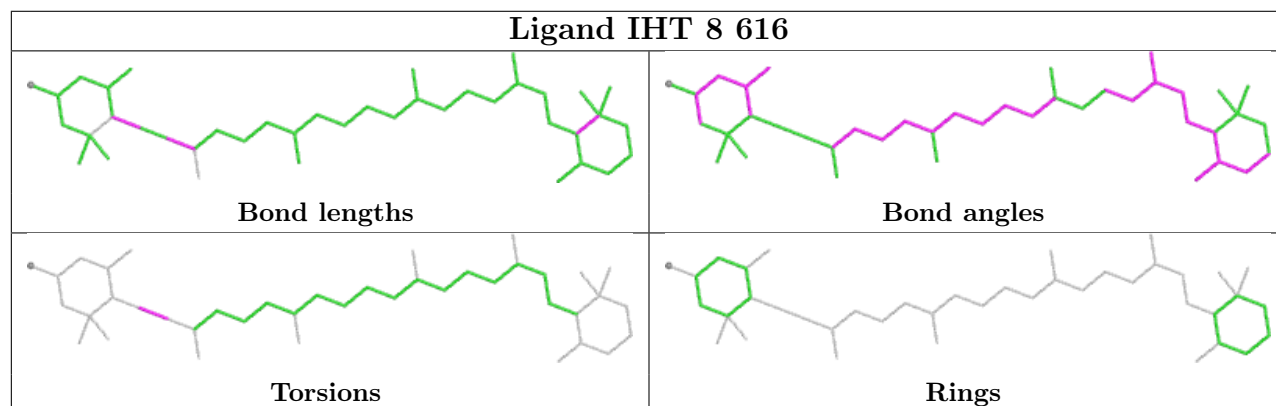


Rings

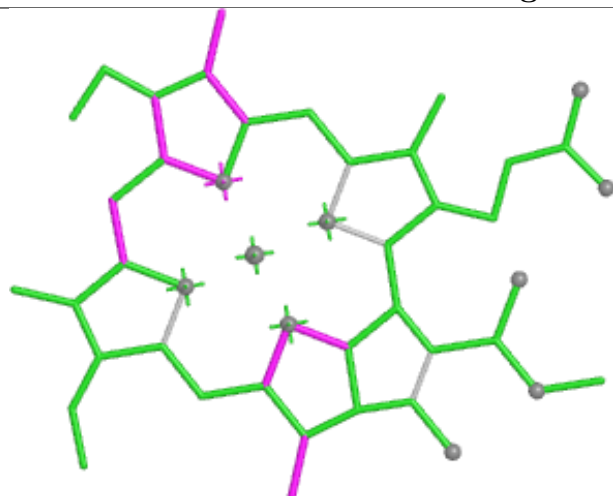
Ligand CLA G 101



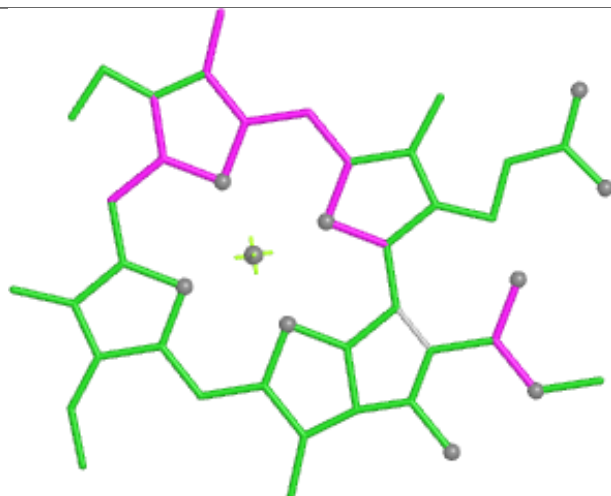
Ligand IHT 8 616



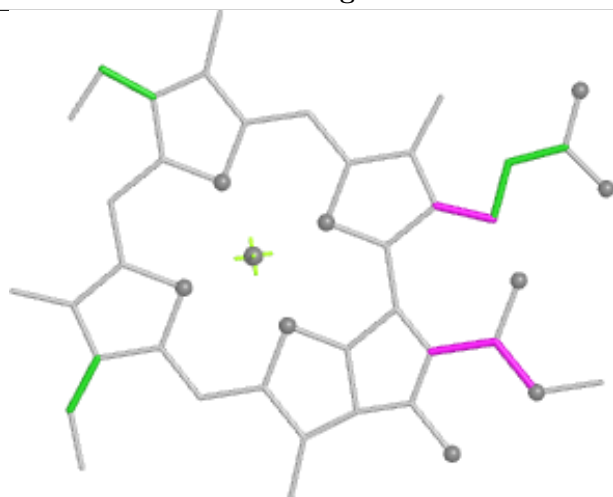
Ligand CLA s 302



Bond lengths



Bond angles

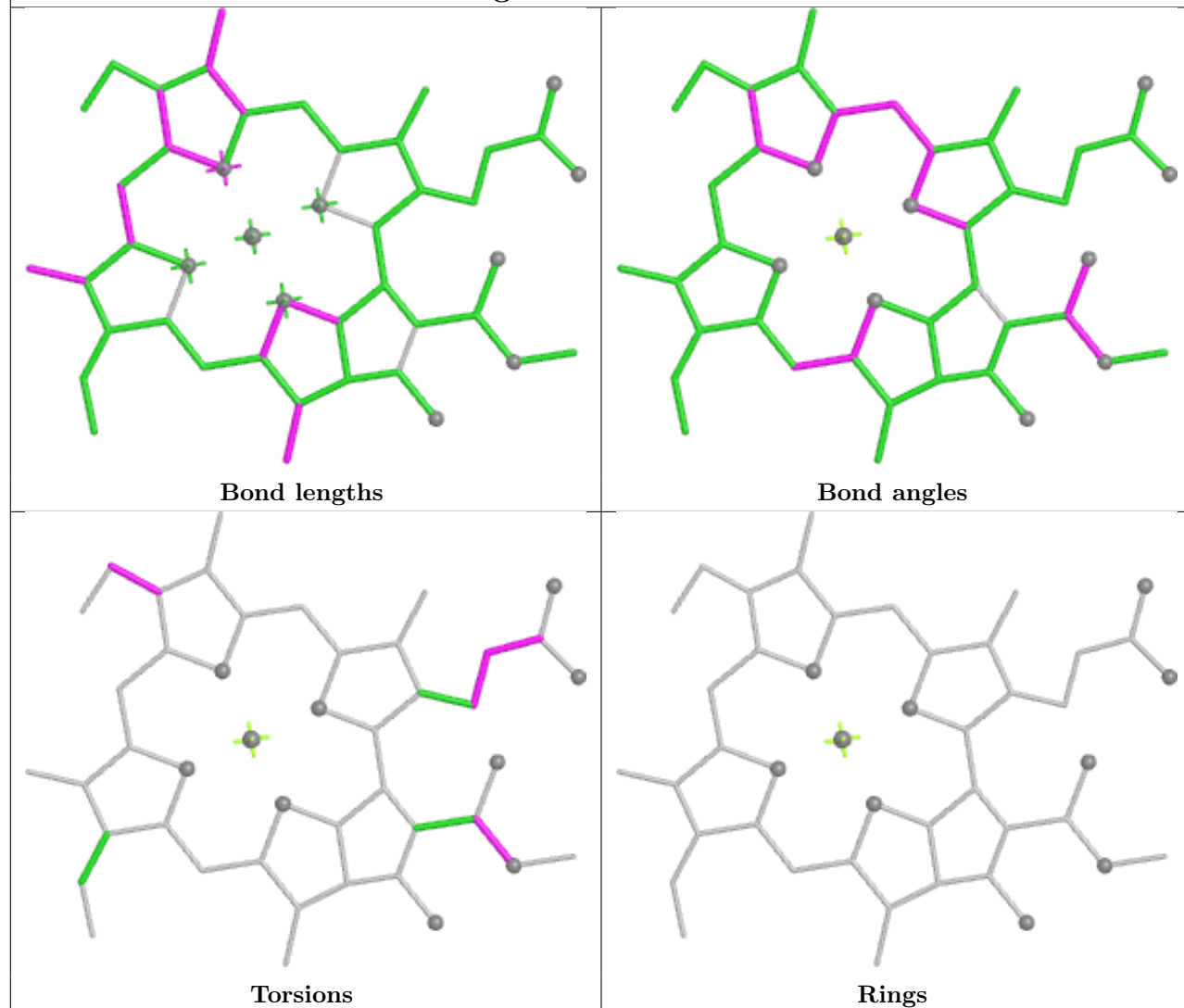


Torsions

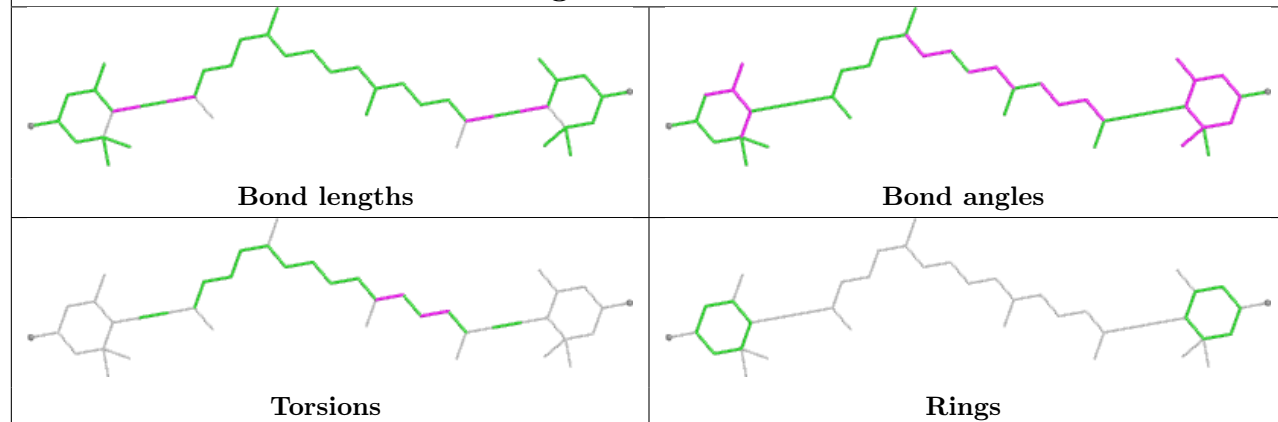


Rings

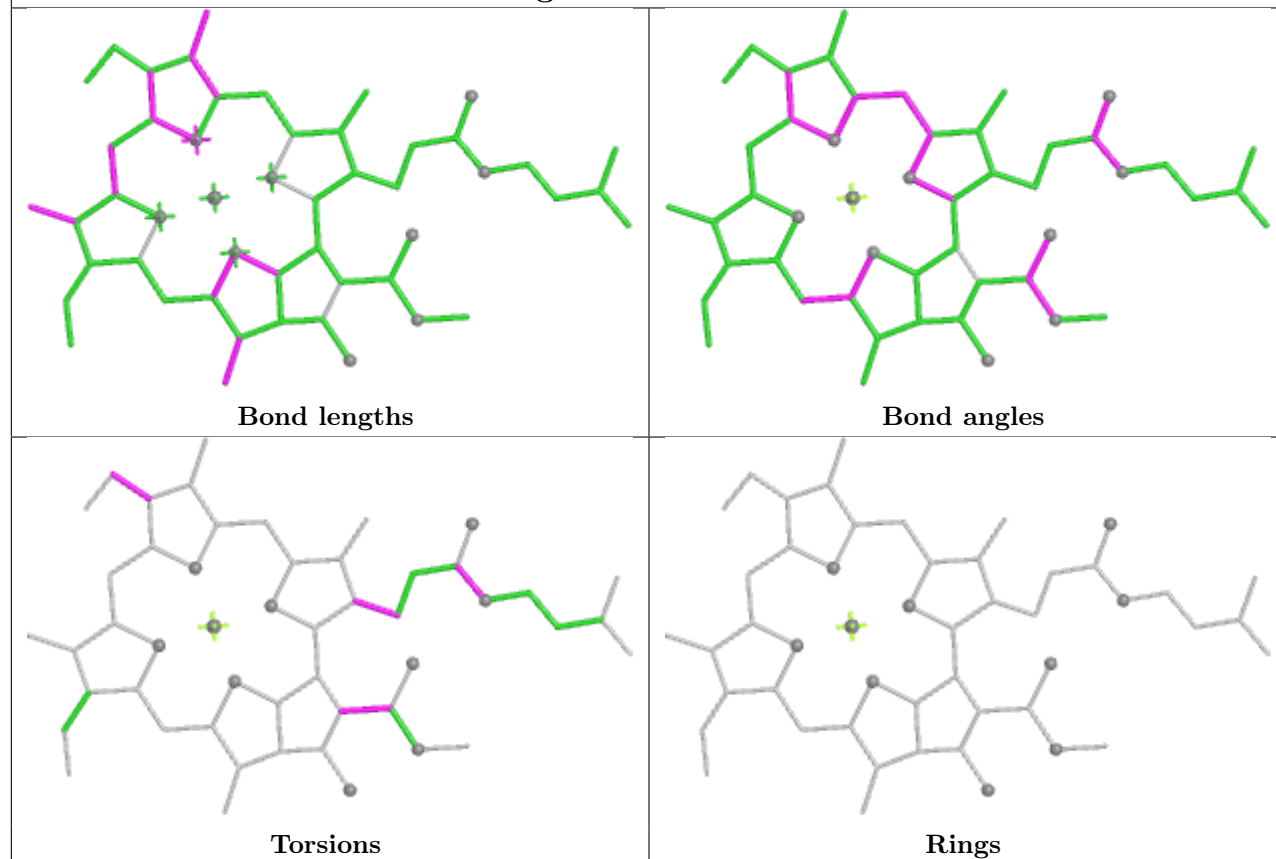
Ligand CLA P 611



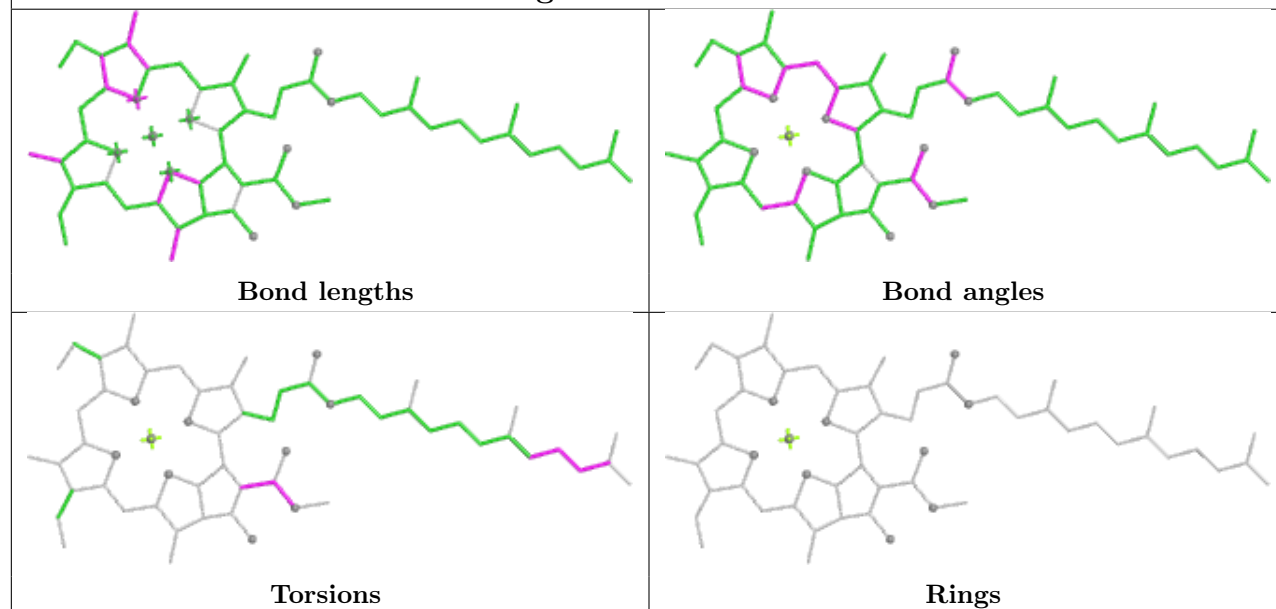
Ligand II0 0 619

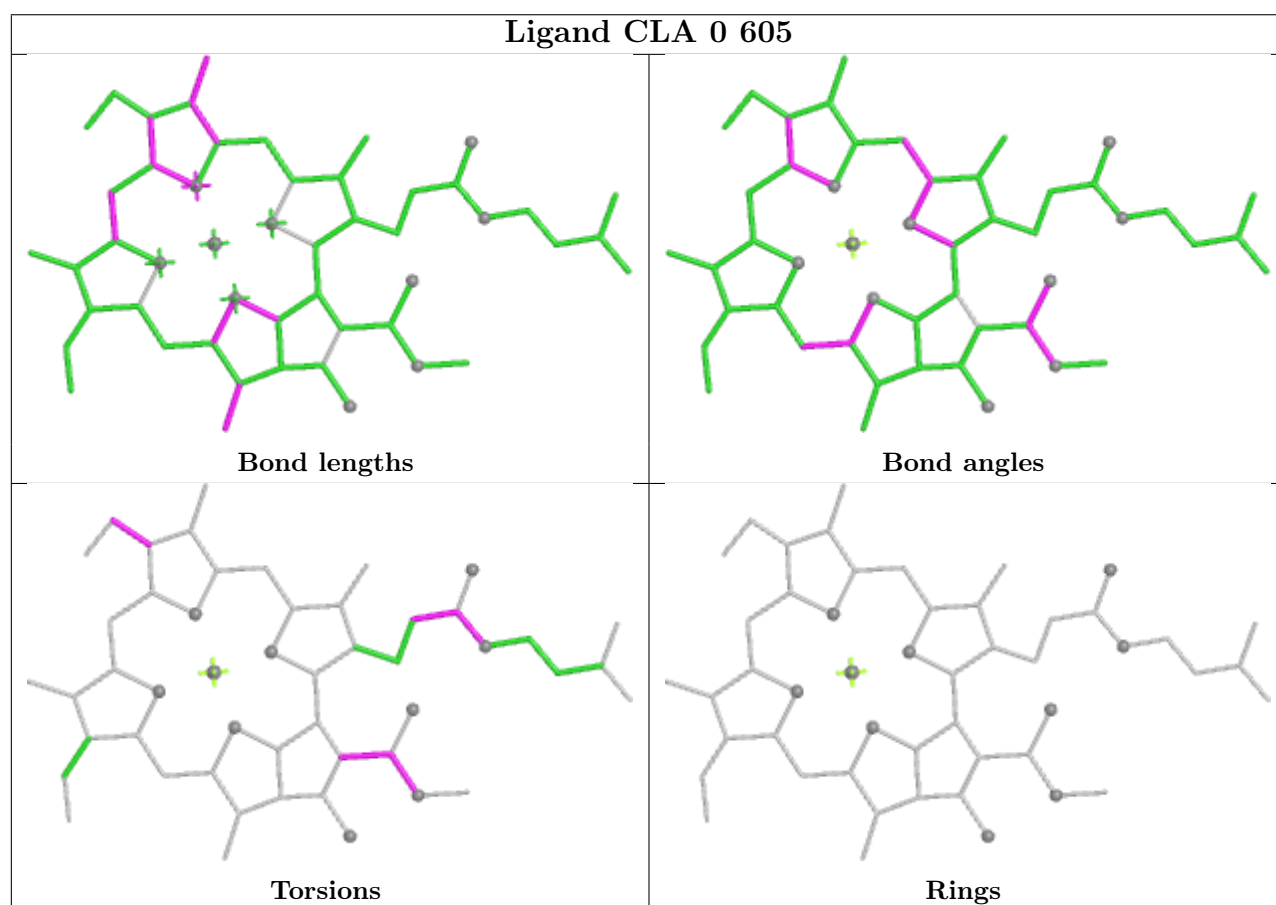
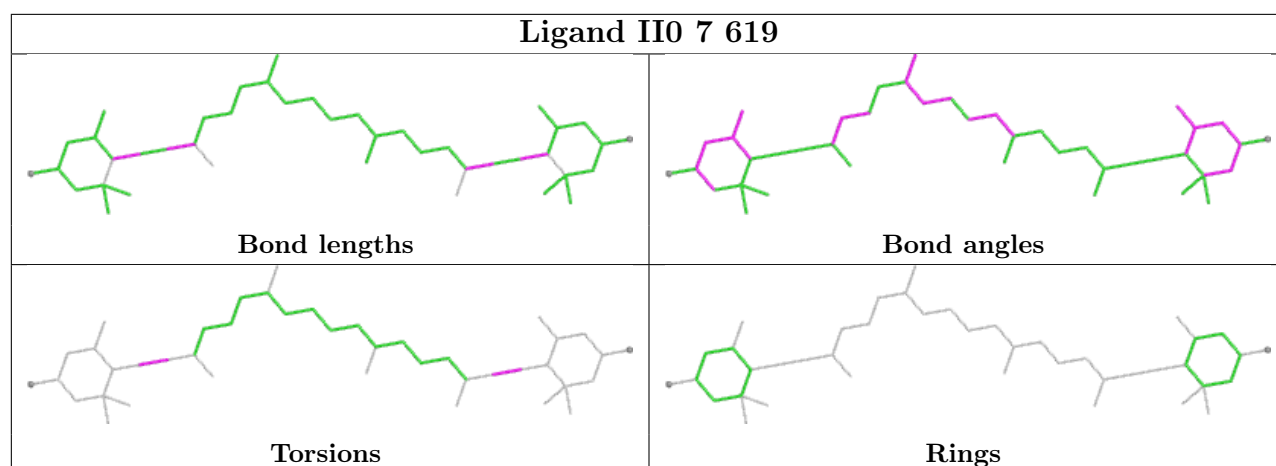


Ligand CLA 8 603

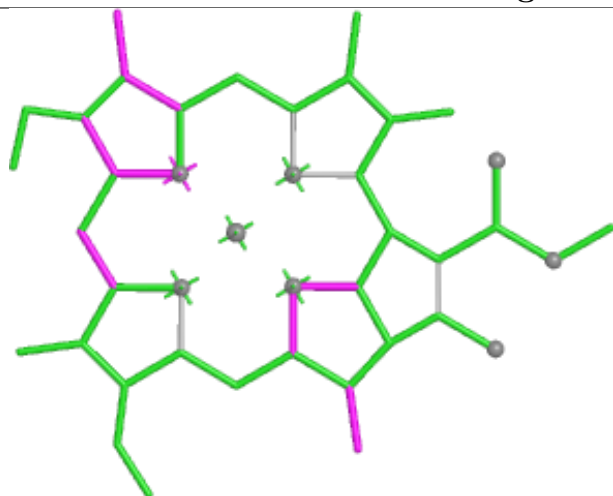


Ligand CLA 8 608

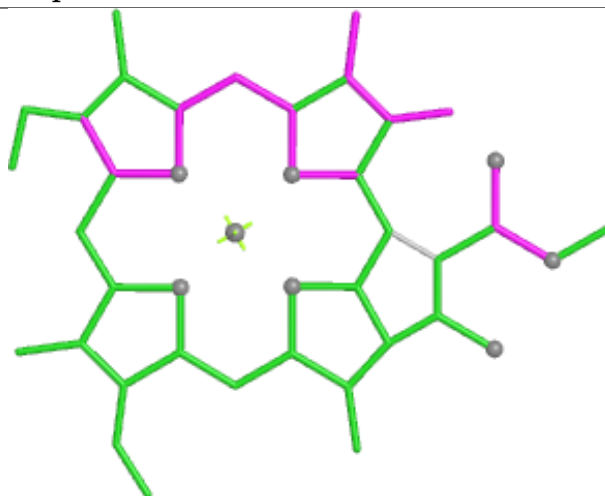




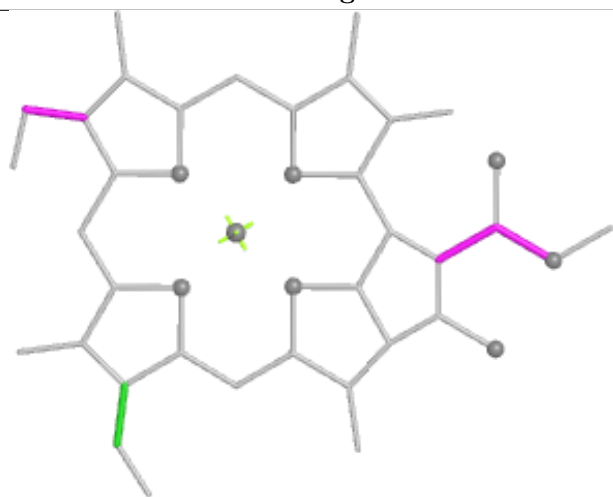
Ligand CLA p 311



Bond lengths



Bond angles

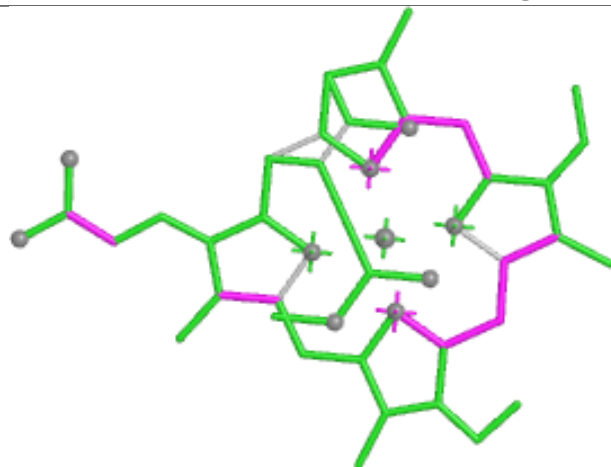


Torsions

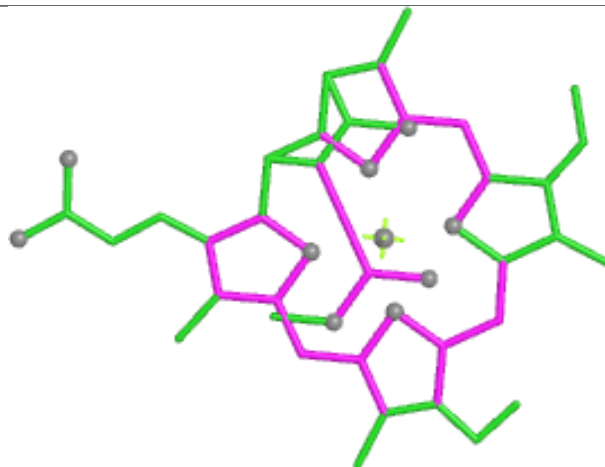


Rings

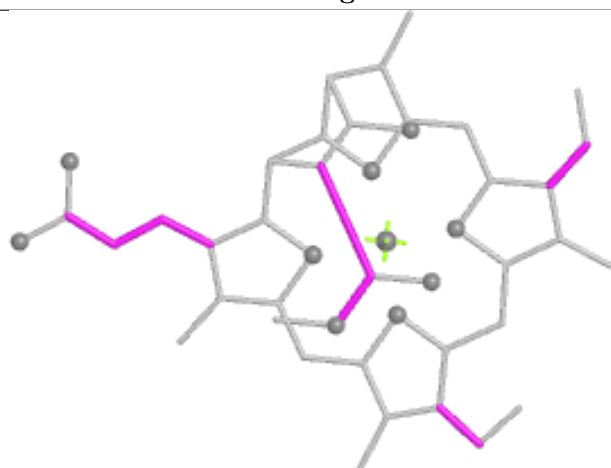
Ligand KC2 P 609



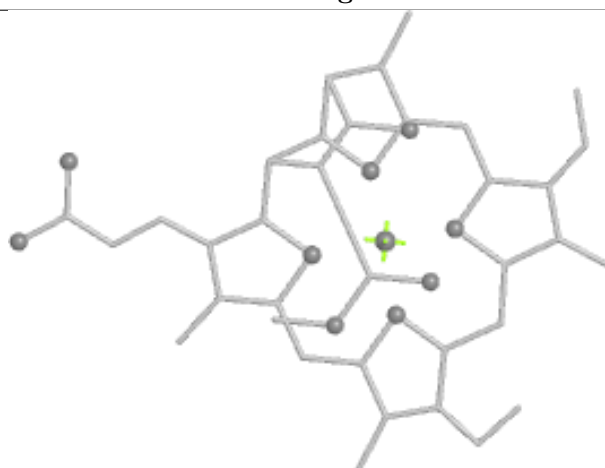
Bond lengths



Bond angles

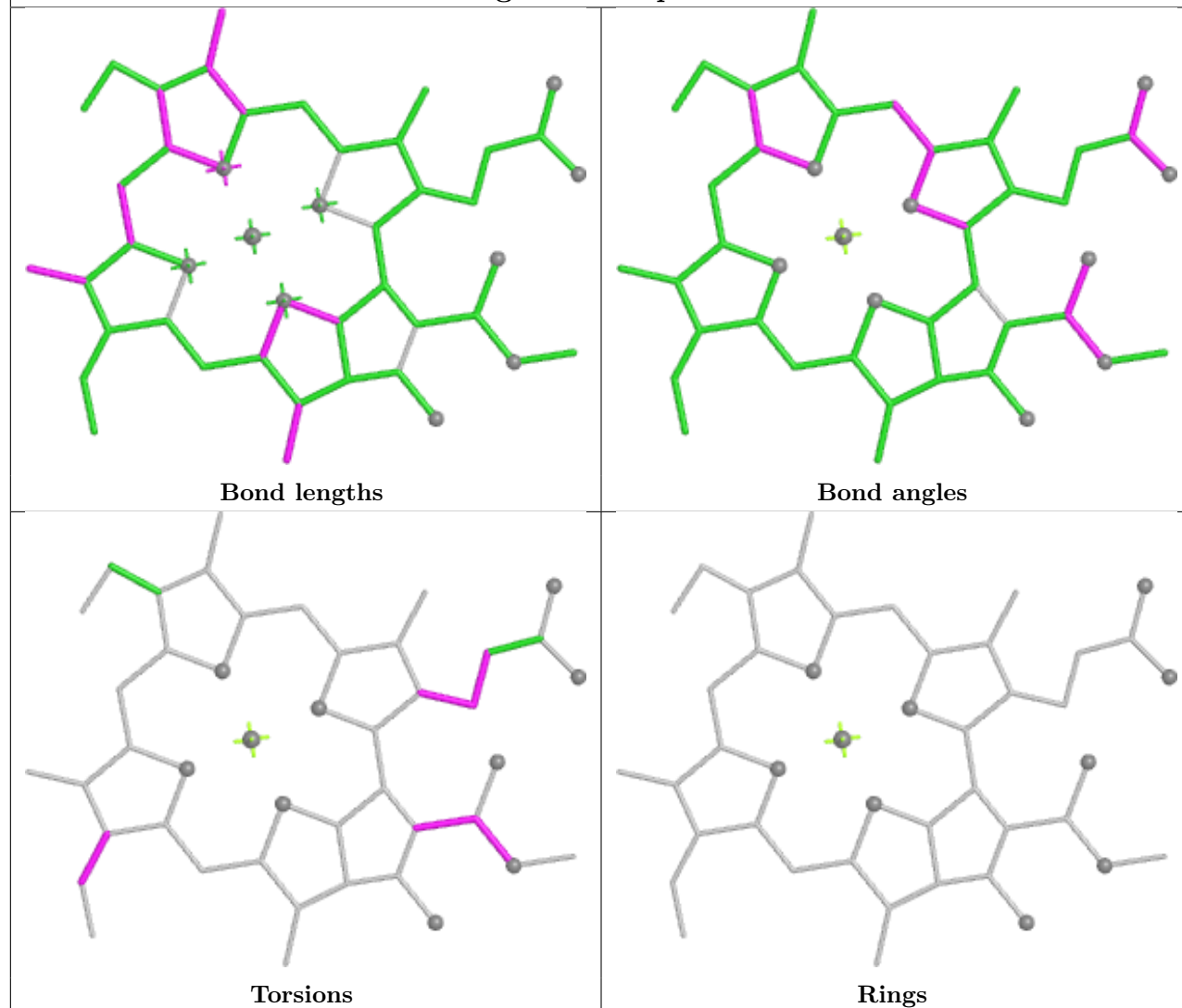


Torsions

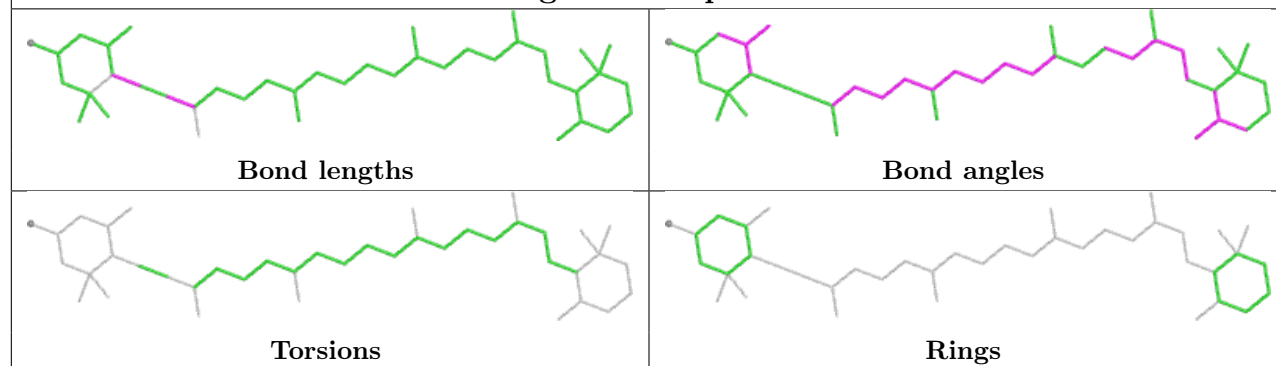


Rings

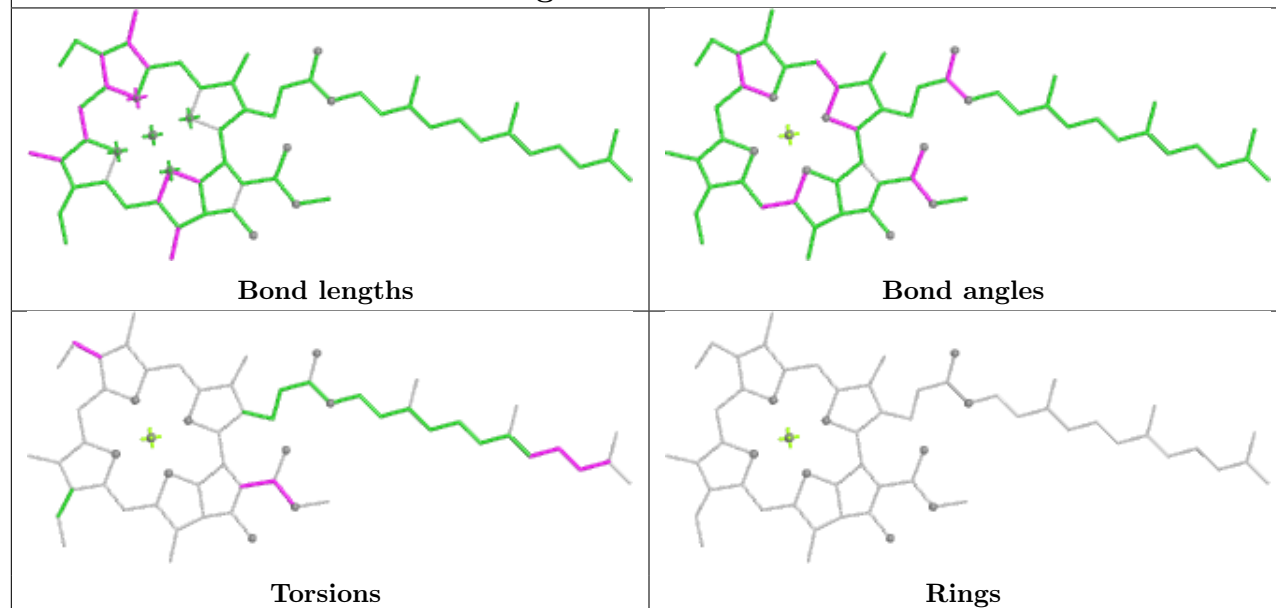
Ligand CLA p 313



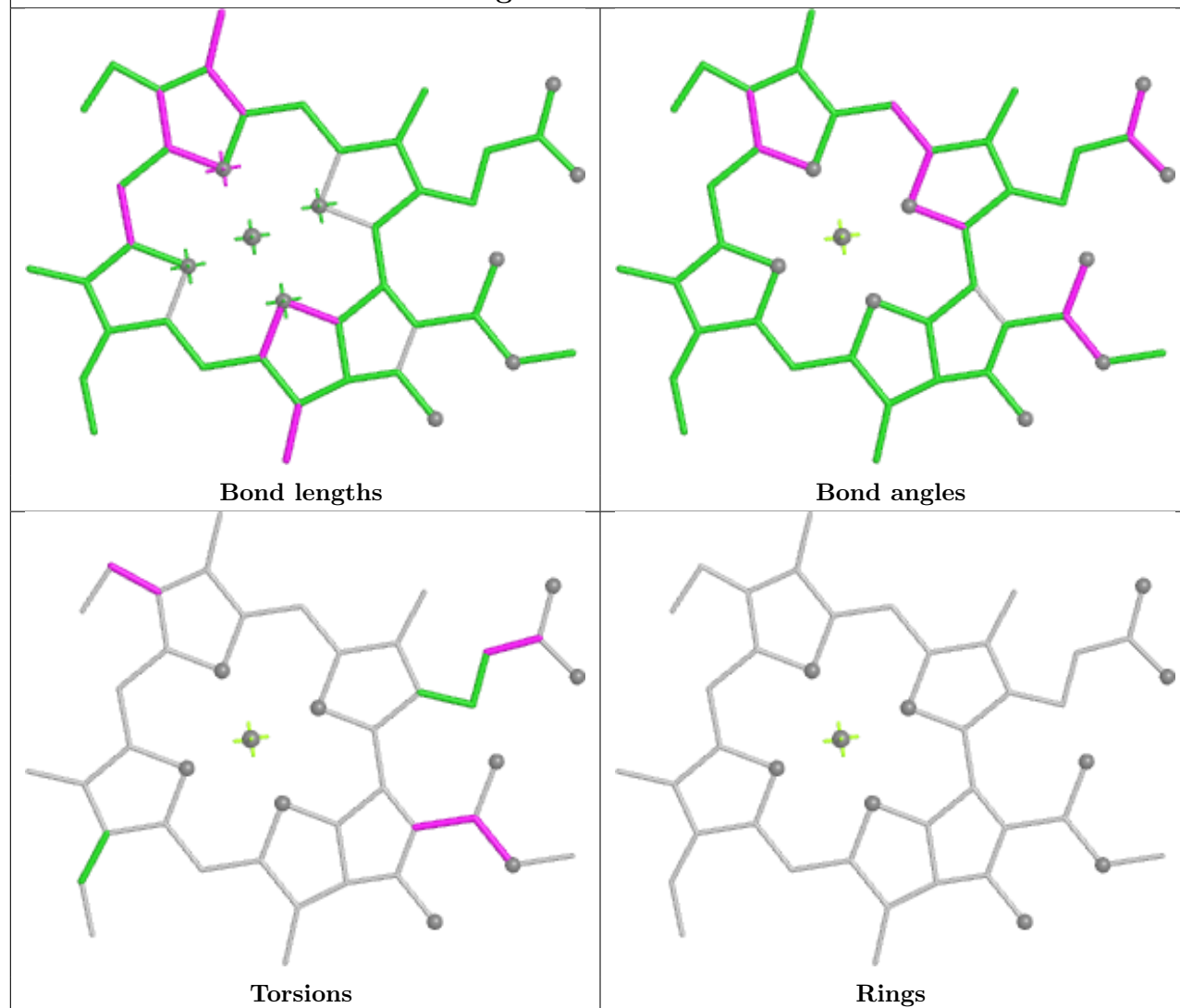
Ligand IHT p 318



Ligand CLA 7 608



Ligand CLA 7 613



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

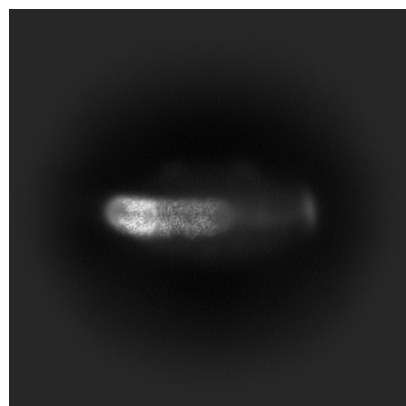
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38419. These allow visual inspection of the internal detail of the map and identification of artifacts.

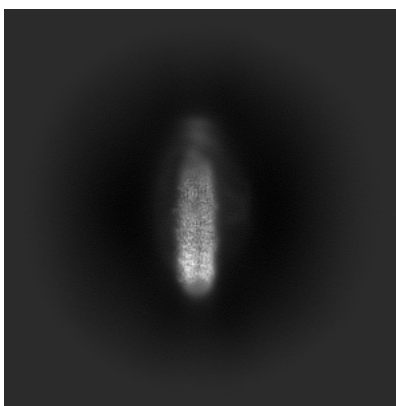
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

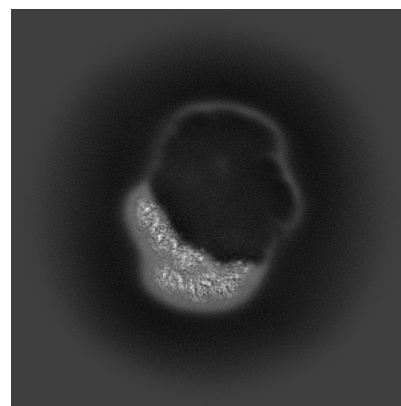
6.1.1 Primary map



X

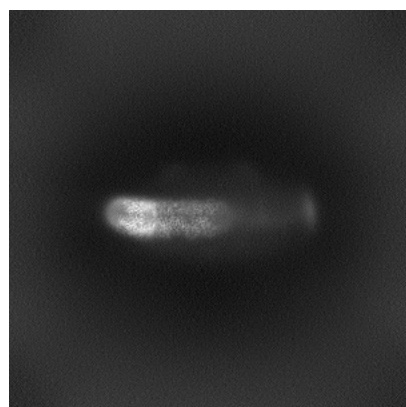


Y

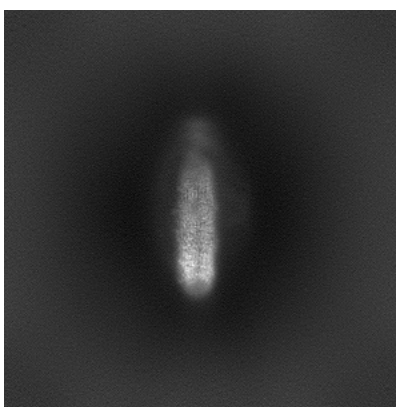


Z

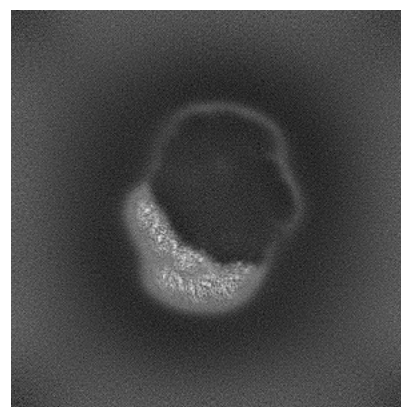
6.1.2 Raw map



X



Y

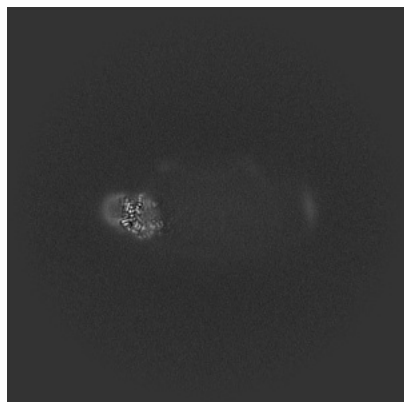


Z

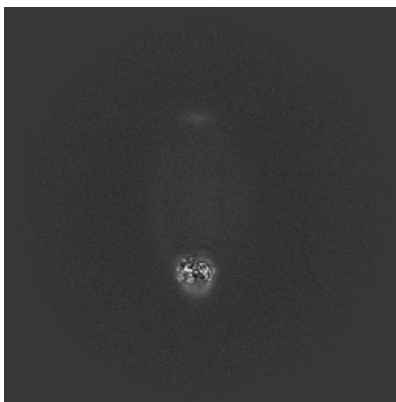
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

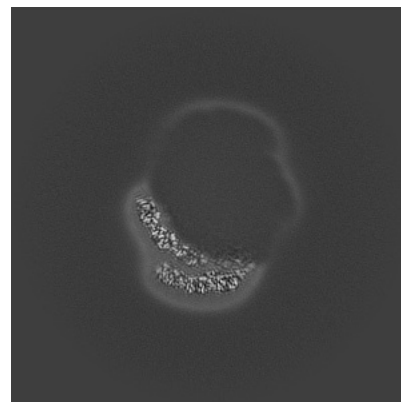
6.2.1 Primary map



X Index: 256



Y Index: 256

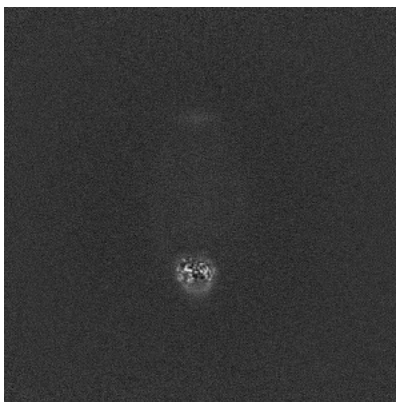


Z Index: 256

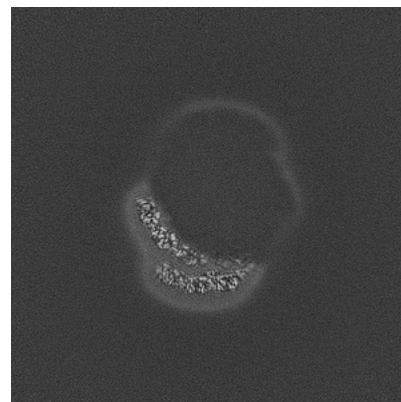
6.2.2 Raw map



X Index: 256



Y Index: 256

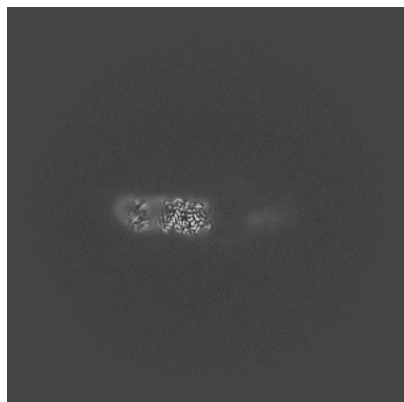


Z Index: 256

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

6.3 Largest variance slices [i](#)

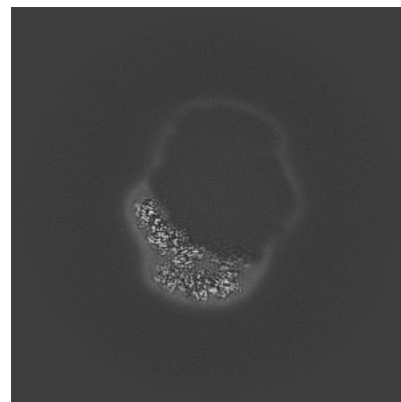
6.3.1 Primary map



X Index: 188



Y Index: 159

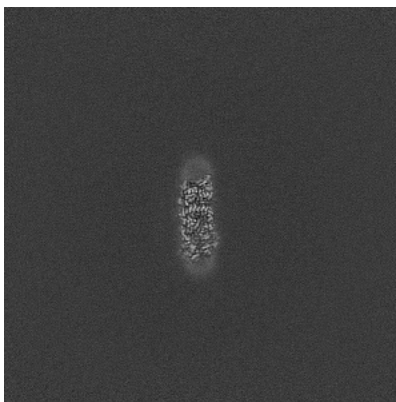


Z Index: 237

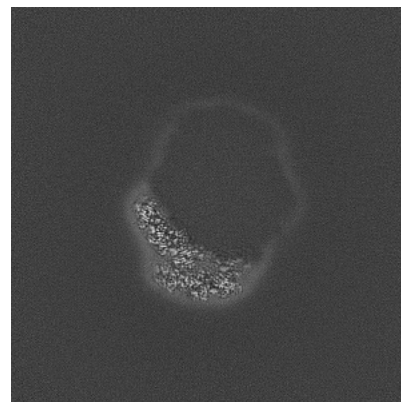
6.3.2 Raw map



X Index: 189



Y Index: 159

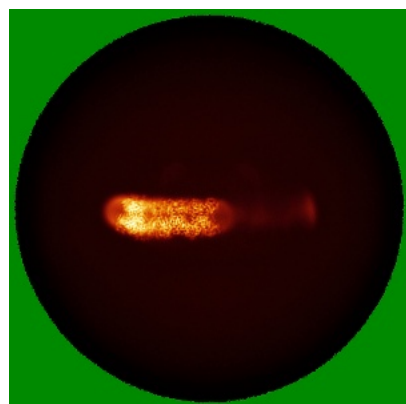


Z Index: 236

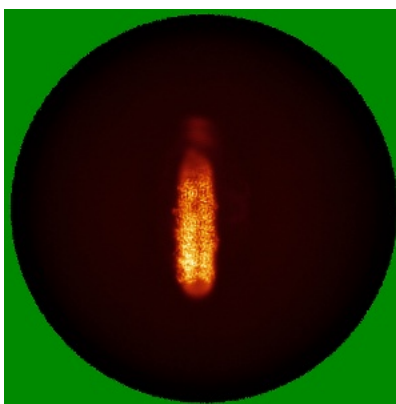
The images above show the largest variance slices of the map in three orthogonal directions.

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

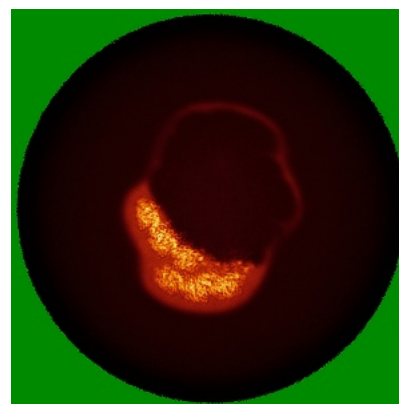
6.4.1 Primary map



X

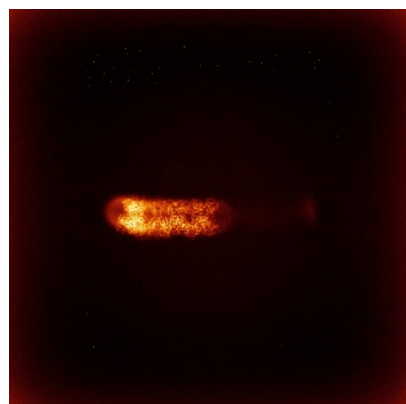


Y

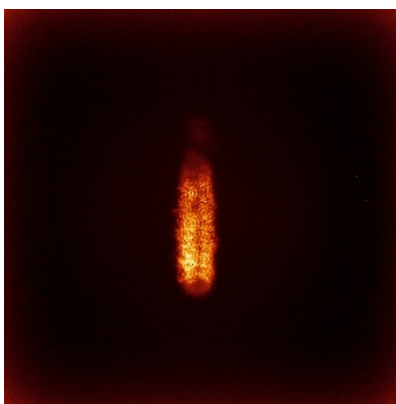


Z

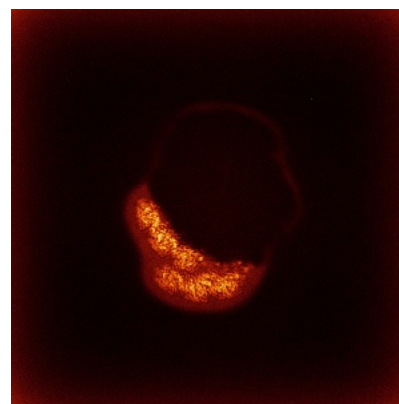
6.4.2 Raw map



X



Y

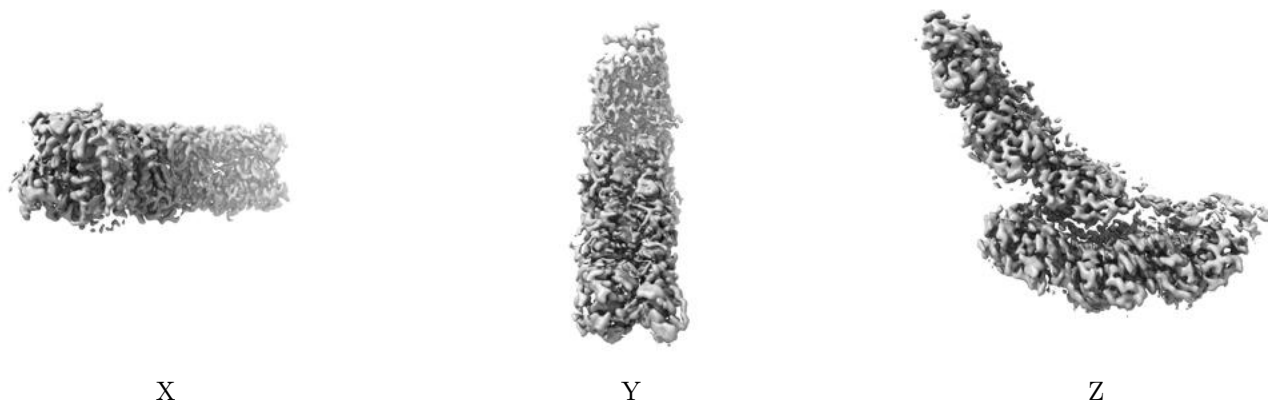


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.266. 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



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.

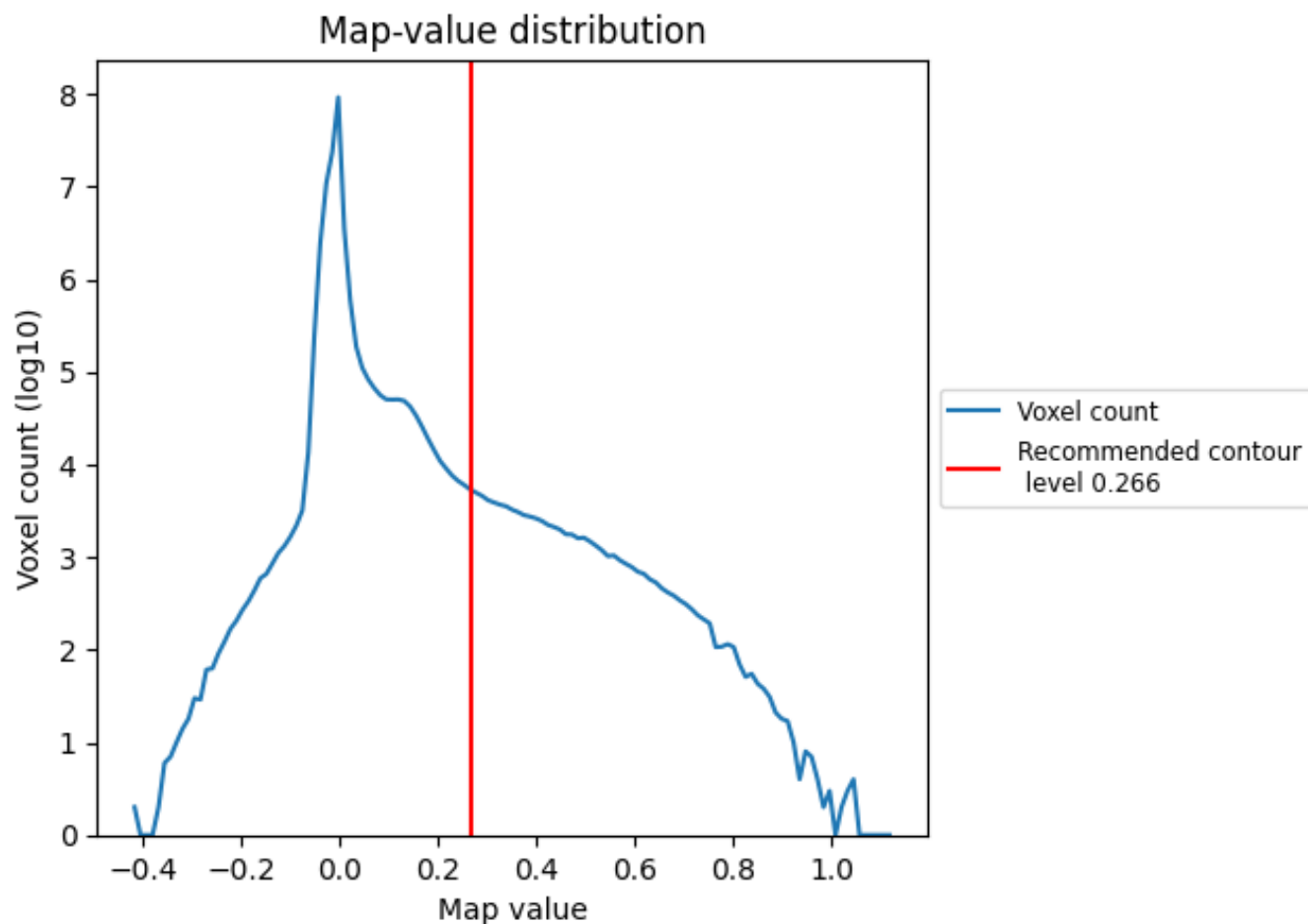
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

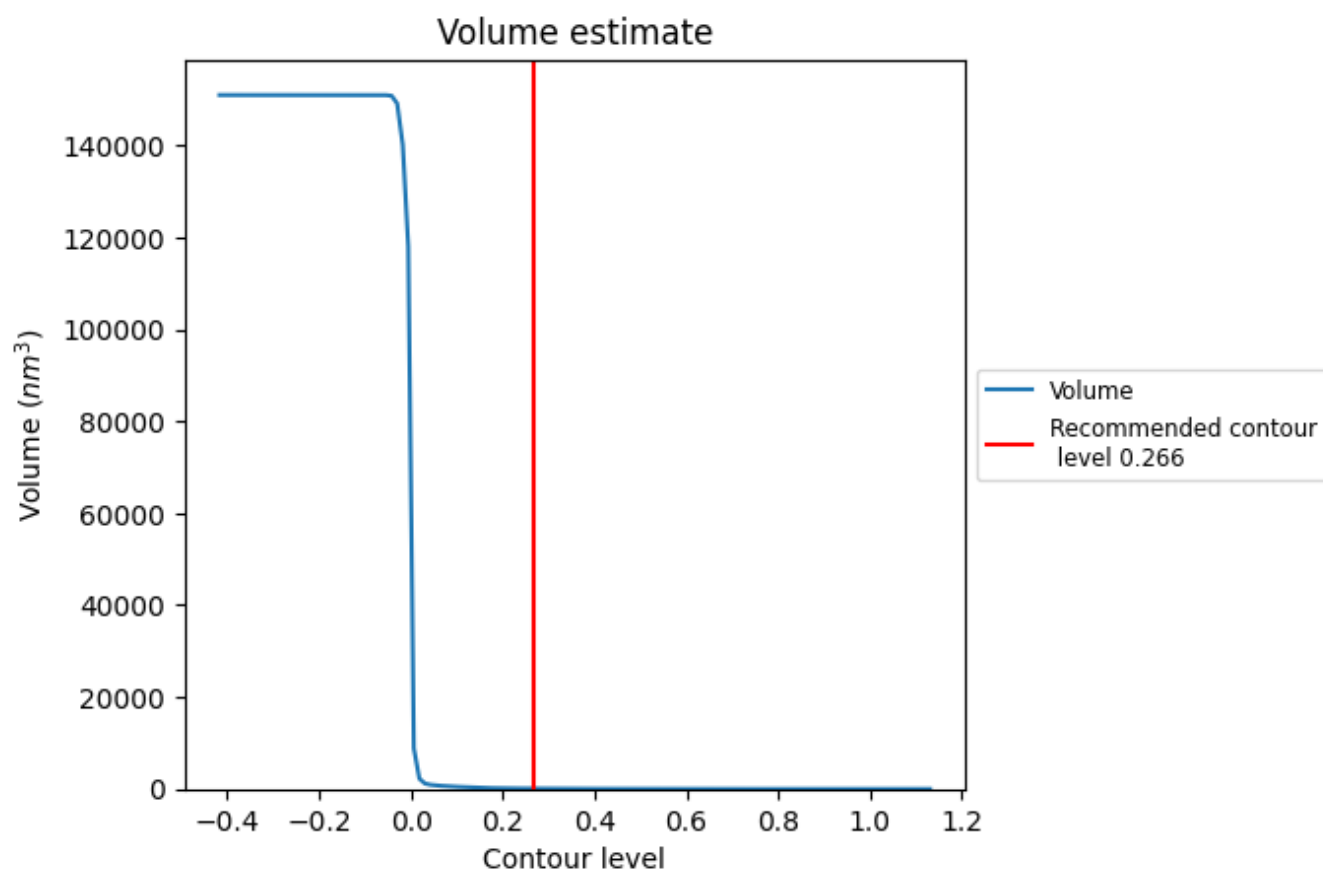
This section contains the results of statistical analysis of the map.

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.

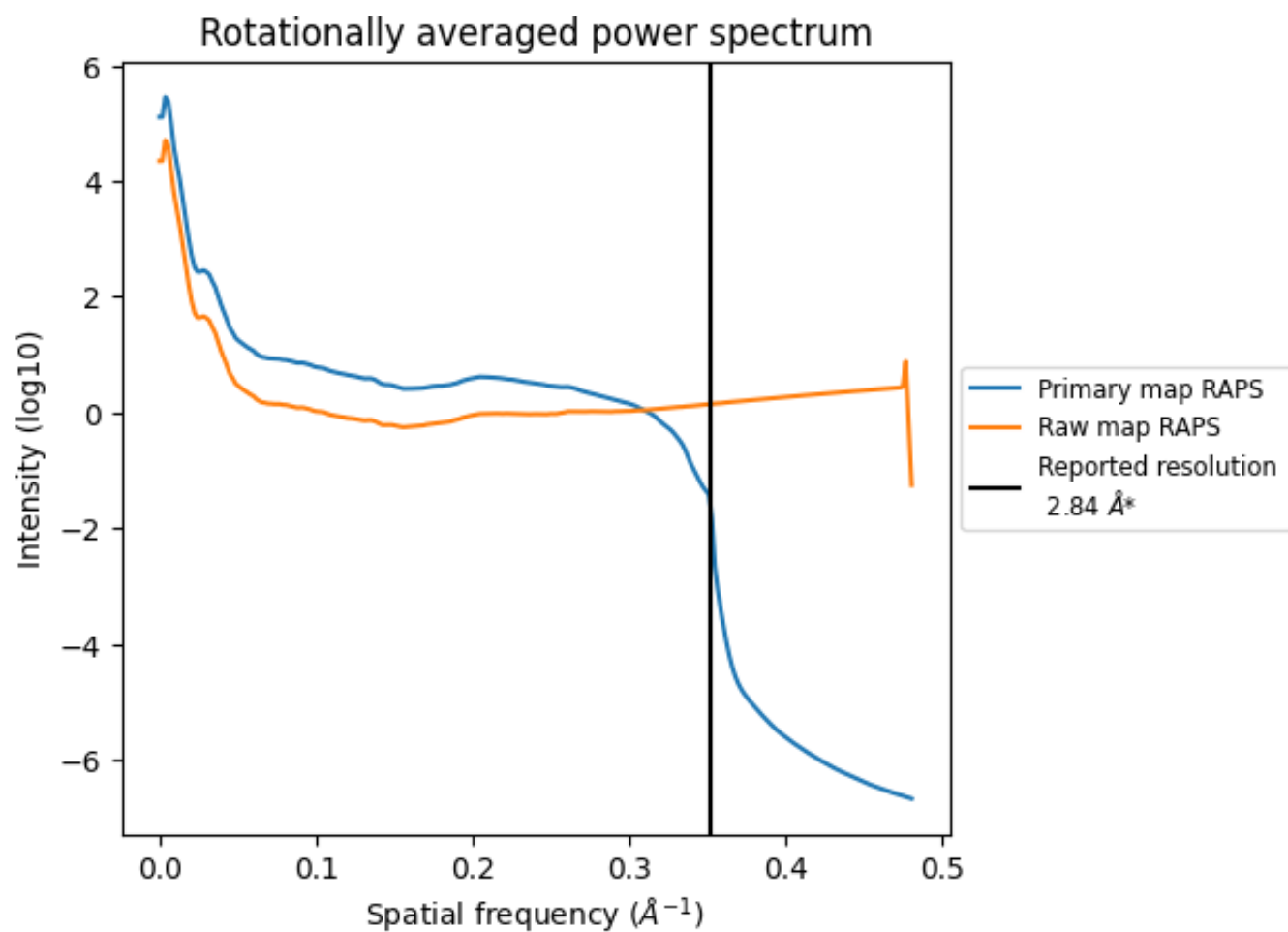
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm^3 ; this corresponds to an approximate mass of 76 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 ⓘ

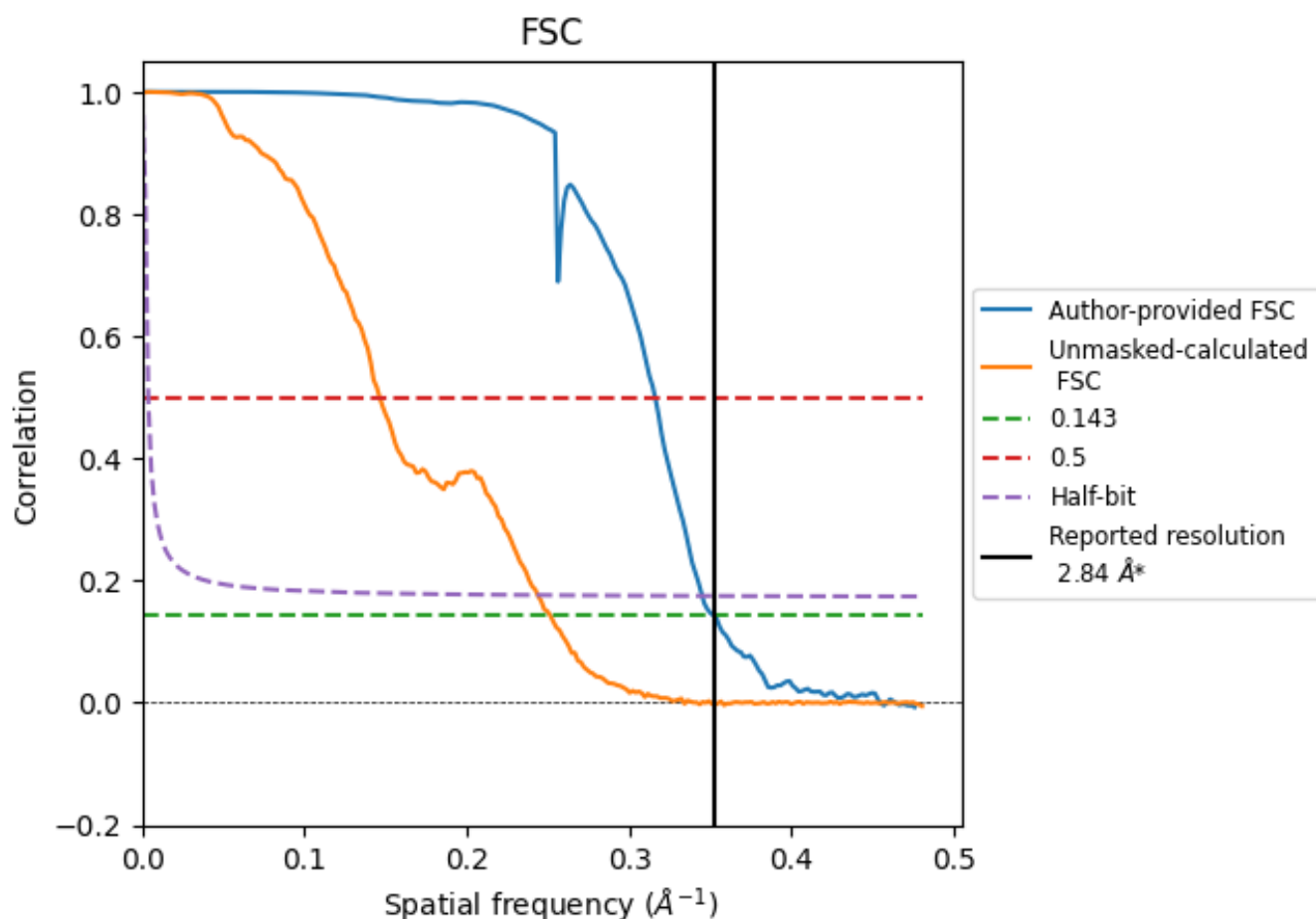


*Reported resolution corresponds to spatial frequency of 0.352 $\text{\AA}^{-1}$

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 0.352 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

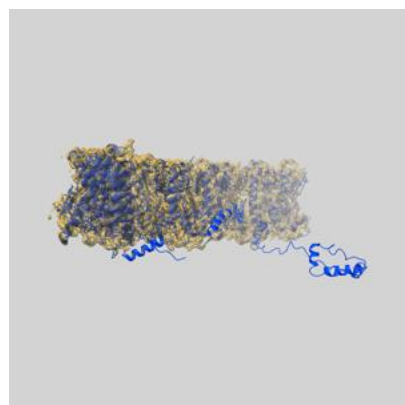
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.16	2.90
Unmasked-calculated*	3.98	6.83	4.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 2.84 by more than 10 %

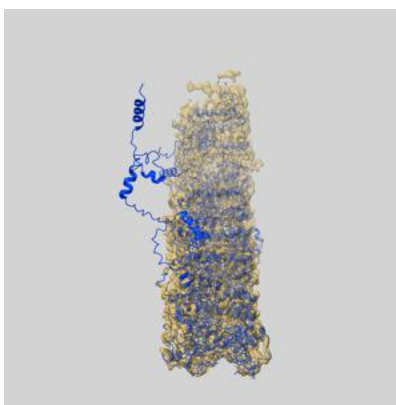
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38419 and PDB model 8XKL. Per-residue inclusion information can be found in section 3 on page 16.

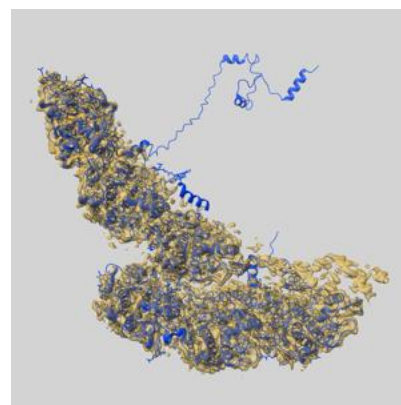
9.1 Map-model overlay [i](#)



X



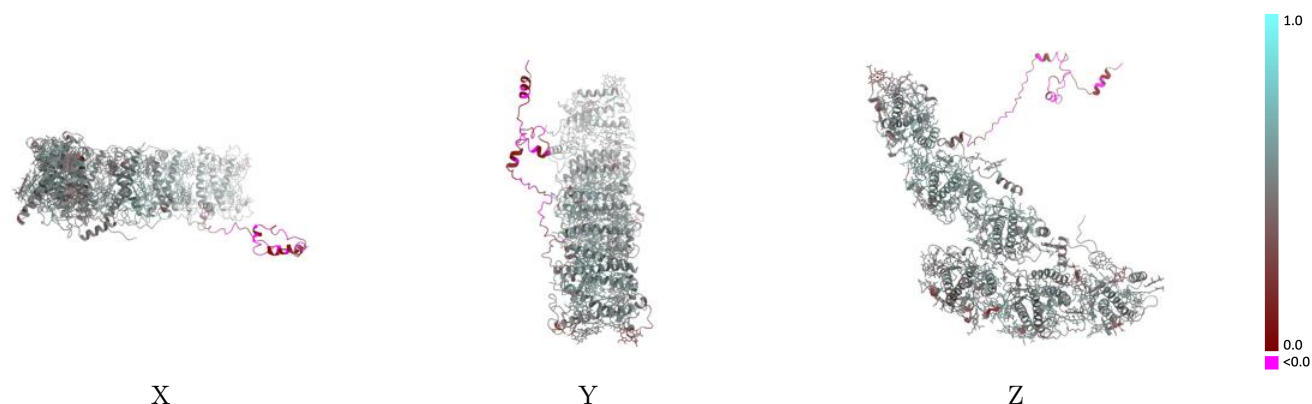
Y



Z

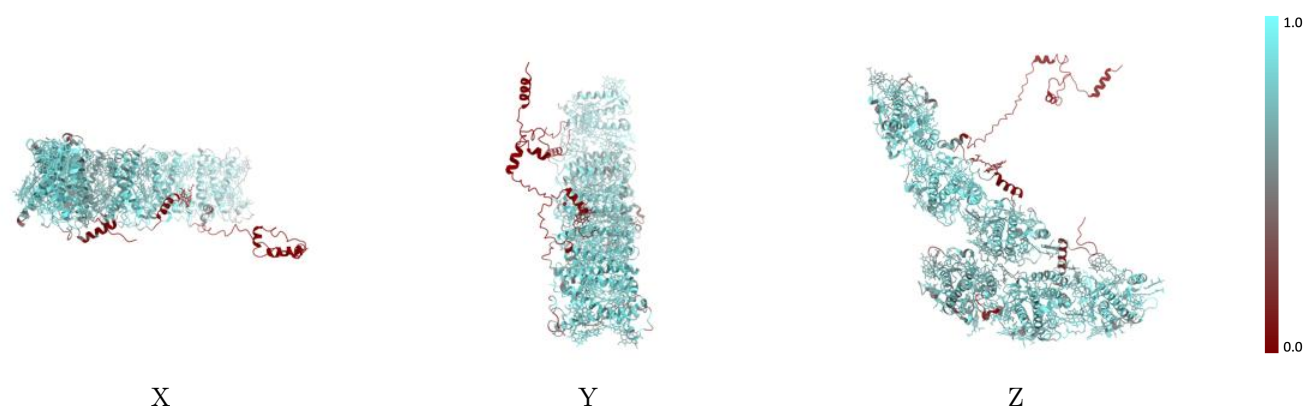
The images above show the 3D surface view of the map at the recommended contour level 0.266 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



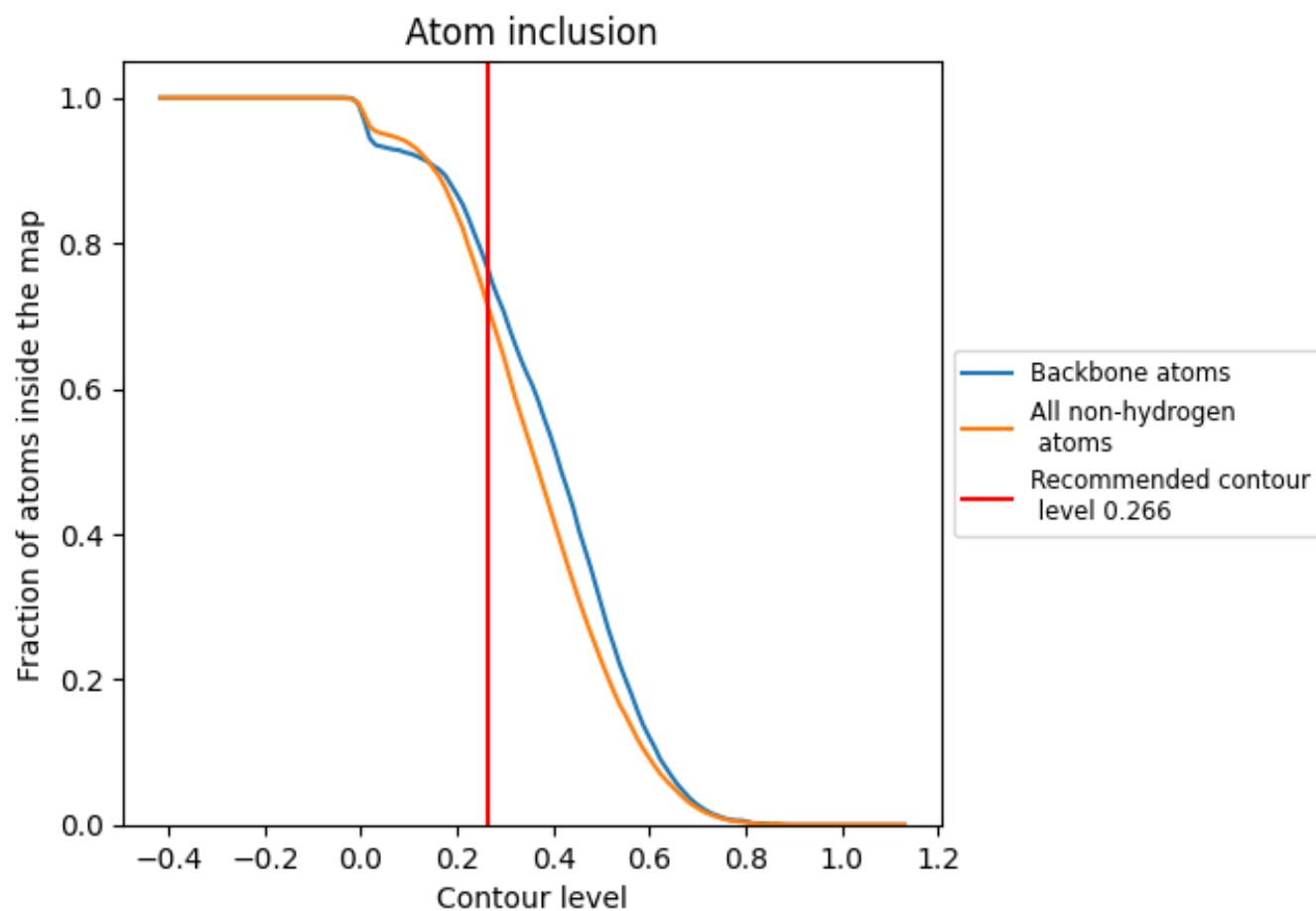
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.266).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 71% 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 (0.266) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7090	0.4900
0	0.7050	0.4920
7	0.7430	0.5020
8	0.8400	0.5470
9	0.7770	0.5340
G	0.4410	0.4780
P	0.7690	0.4930
p	0.7700	0.5160
s	0.3310	0.3040

1.0

0.0

<0.0