



Full wwPDB EM Validation Report ⓘ

Sep 8, 2025 – 02:11 pm BST

PDB ID : 9GNW / pdb_00009gnw
EMDB ID : EMD-51482
Title : Universal PSII assembly intermediate
Authors : Fadeeva, M.; Klaiman, D.; Nelson, N.
Deposited on : 2024-09-04
Resolution : 2.93 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.dev126
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

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 2.93 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 24204 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 Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	0	0
			2635	1719	432	468	16		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3785	2480	630	665	10		

- Molecule 3 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	V	33	Total	C	N	O	S	0	0
			235	157	38	39	1		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3483	2282	581	607	13		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2766	1824	454	477	11		

- Molecule 6 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	76	Total	C	N	O	0	0
			621	404	102	115		

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			252	172	42	37	1		

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total	C	N	O	S	0	0
			503	334	76	92	1		

- Molecule 9 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	33	Total	C	N	O	S	0	0
			265	182	39	43	1		

- Molecule 10 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			265	181	40	44		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	42	LEU	GLN	conflict	UNP A0A1C8XRM8

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	207	43	47		

- Molecule 12 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	36	Total	C	N	O	0	0
			300	201	49	50		

- Molecule 13 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	31	Total	C	N	O	0	0
			235	161	33	41		

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total	C	N	O	S	0	0
			1819	1148	295	370	6		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	101	ASP	ASN	conflict	UNP A0A7S3QTM3
O	103	LYS	ARG	conflict	UNP A0A7S3QTM3
O	150	ASN	GLY	conflict	UNP A0A7S3QTM3
O	151	ASN	GLY	conflict	UNP A0A7S3QTM3
O	156	GLU	GLN	conflict	UNP A0A7S3QTM3
O	160	ASP	GLU	conflict	UNP A0A7S3QTM3
O	219	ALA	SER	conflict	UNP A0A7S3QTM3
O	220	THR	SER	conflict	UNP A0A7S3QTM3
O	226	ILE	VAL	conflict	UNP A0A7S3QTM3
O	240	LEU	VAL	conflict	UNP A0A7S3QTM3
O	244	SER	THR	conflict	UNP A0A7S3QTM3
O	248	GLY	SER	conflict	UNP A0A7S3QTM3
O	261	THR	ALA	conflict	UNP A0A7S3QTM3
O	272	SER	THR	conflict	UNP A0A7S3QTM3
O	285	ALA	SER	conflict	UNP A0A7S3QTM3

- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1453	923	243	286	1		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	96	GLN	GLU	conflict	UNP A0A9J4RF14
P	100	GLU	ASP	conflict	UNP A0A9J4RF14
P	107	GLU	ALA	conflict	UNP A0A9J4RF14
P	116	LEU	VAL	conflict	UNP A0A9J4RF14
P	119	VAL	ILE	conflict	UNP A0A9J4RF14
P	120	GLU	ALA	conflict	UNP A0A9J4RF14

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
P	121	ASP	GLN	conflict	UNP A0A9J4RF14
P	122	LYS	ASP	conflict	UNP A0A9J4RF14
P	123	SER	THR	conflict	UNP A0A9J4RF14
P	129	GLU	GLN	conflict	UNP A0A9J4RF14
P	130	ALA	ASP	conflict	UNP A0A9J4RF14
P	133	THR	SER	conflict	UNP A0A9J4RF14
P	147	LYS	ARG	conflict	UNP A0A9J4RF14
P	164	ARG	LYS	conflict	UNP A0A9J4RF14
P	167	ASN	SER	conflict	UNP A0A9J4RF14
P	191	THR	SER	conflict	UNP A0A9J4RF14

- Molecule 16 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PSII 6.1 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	45	Total	C	N	O	S	0	0
			335	217	54	63	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	104	GLY	-	expression tag	UNP A0A9J4RF15

- Molecule 18 is a protein called Photosystem II PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	X	33	Total	C	N	O	0	0
			225	148	36	41		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	81	VAL	THR	conflict	UNP A0A7S3VKF3

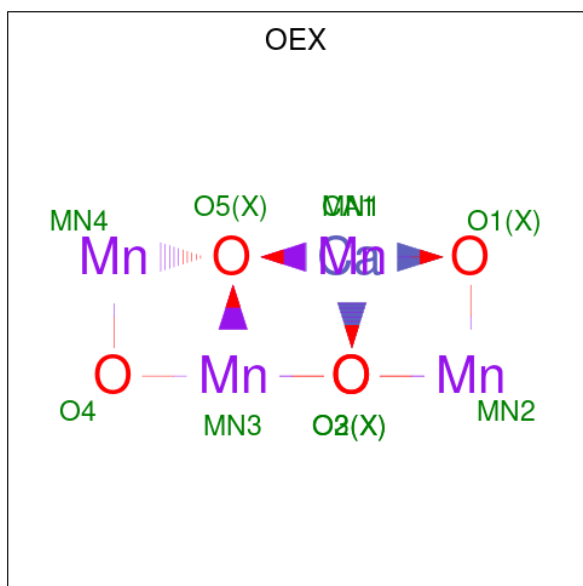
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0
			457	312	68	76	1		

- Molecule 20 is a protein called Photosystem II reaction center protein U, PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	28	Total	C	N	O	S	0	0
			235	141	46	47	1		

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				AltConf
21	A	1	Total	Ca	Mn	O	0
			10	1	4	5	

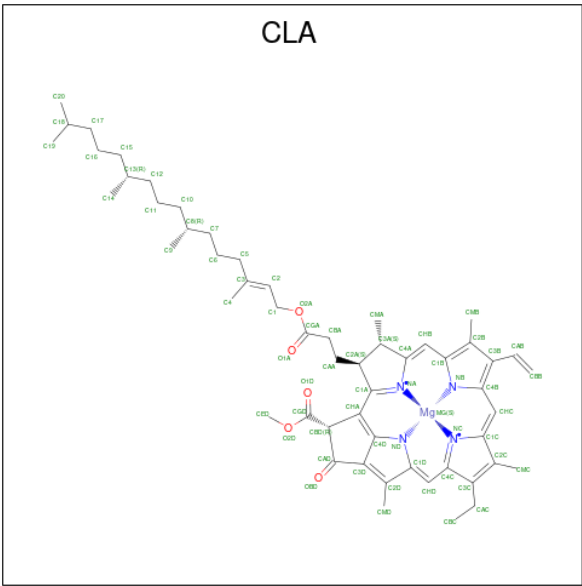
- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	Fe	0
			1	1	

- Molecule 23 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
23	A	2	Total	Cl	0
			2	2	

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

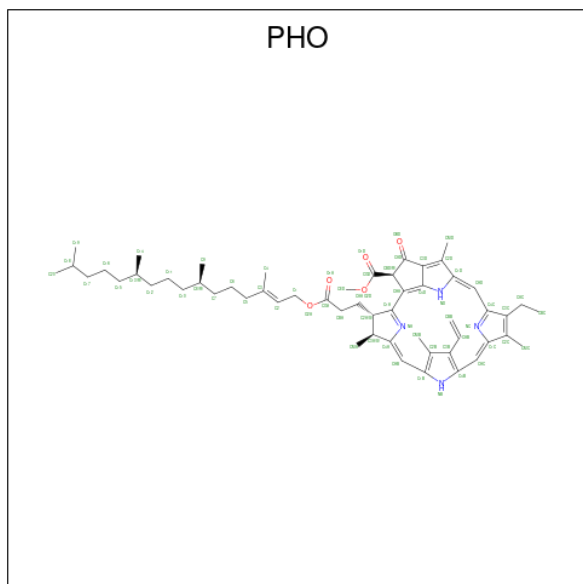
Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	C	1	Total 54	C 44	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	C	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	C	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0

Continued on next page...

Continued from previous page...

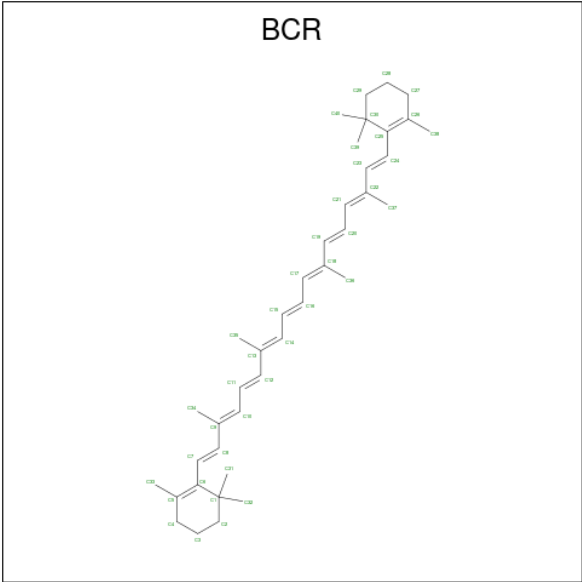
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
24	D	1	60	50	1	4	5	0

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



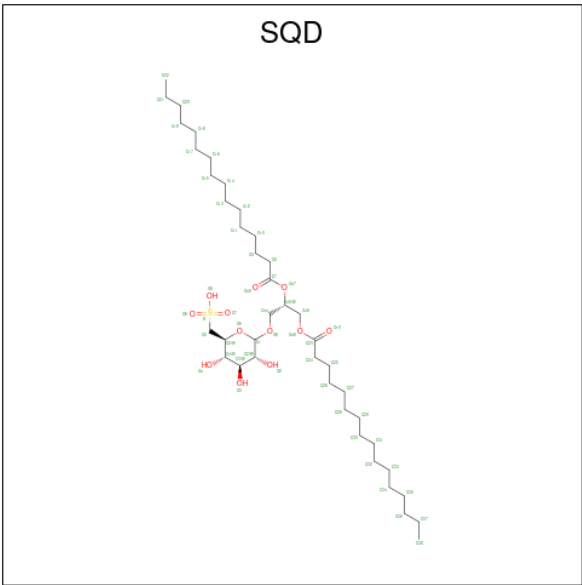
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
25	A	1	64	55	4	5	0
25	D	1	64	55	4	5	0

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



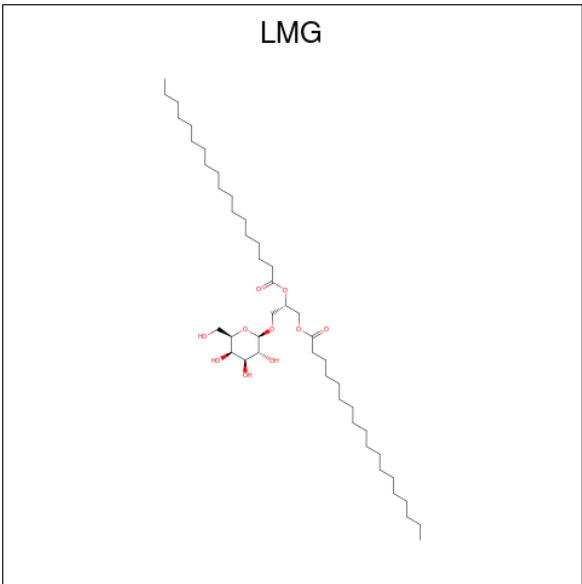
Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	C	1	Total C 40 40	0
26	D	1	Total C 40 40	0
26	J	1	Total C 40 40	0

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	O	S	0
			42	29	12	1	
27	M	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			34	24	10	

Continued on next page...

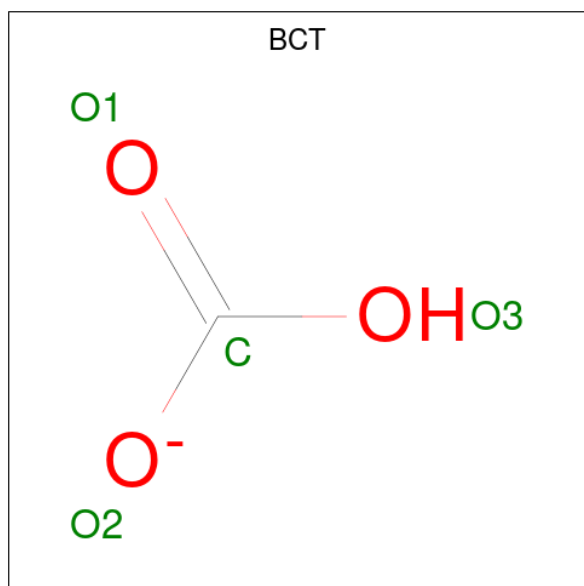
Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			37	27	10	
28	B	1	Total	C	O	0
			44	34	10	
28	C	1	Total	C	O	0
			40	30	10	
28	C	1	Total	C	O	0
			47	37	10	
28	C	1	Total	C	O	0
			33	24	9	
28	D	1	Total	C	O	0
			42	32	10	
28	H	1	Total	C	O	0
			48	38	10	

- Molecule 29 is SODIUM ION (CCD ID: NA) (formula: Na).

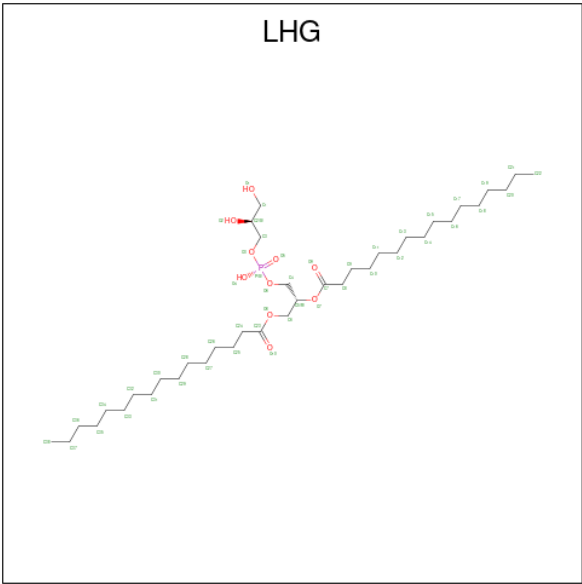
Mol	Chain	Residues	Atoms		AltConf
29	A	1	Total	Na	0
			1	1	

- Molecule 30 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



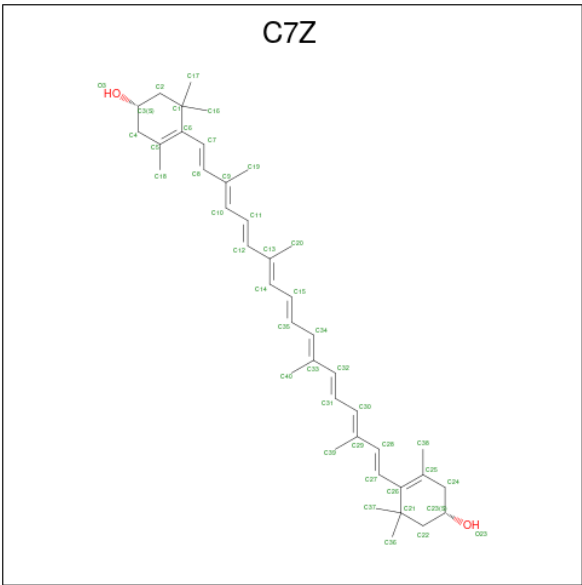
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			4	1	3	

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



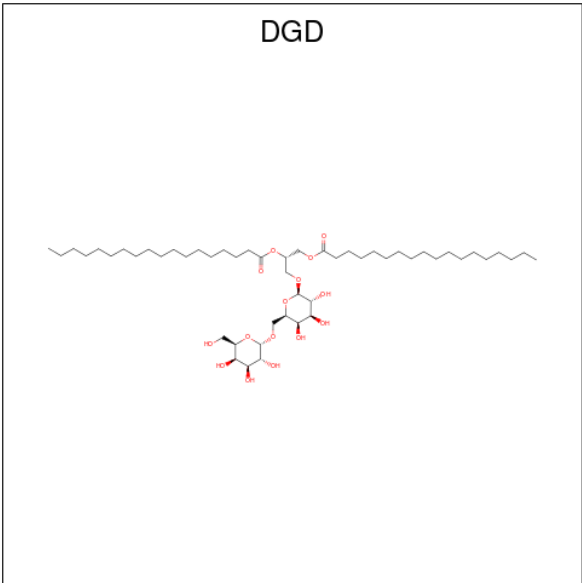
Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	O	P	0
			39	28	10	1	
31	D	1	Total	C	O	P	0
			44	33	10	1	
31	D	1	Total	C	O	P	0
			49	38	10	1	
31	D	1	Total	C	O	P	0
			39	28	10	1	
31	L	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 32 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
32	B	1	Total	C	O	0
			42	40	2	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



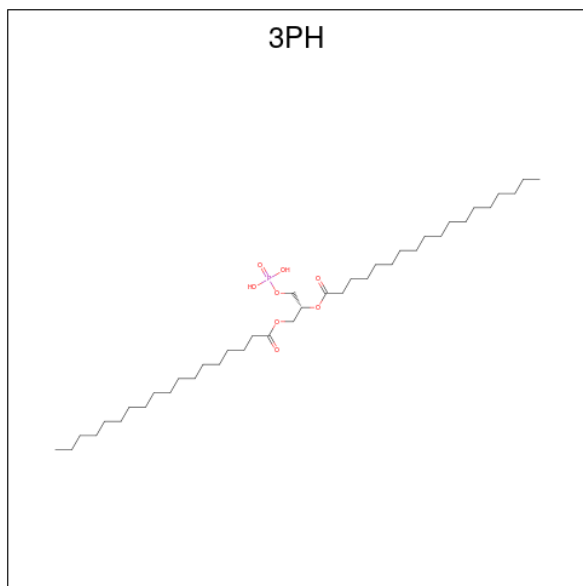
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			43	28	15	
33	C	1	Total	C	O	0
			44	29	15	

Continued on next page...

Continued from previous page...

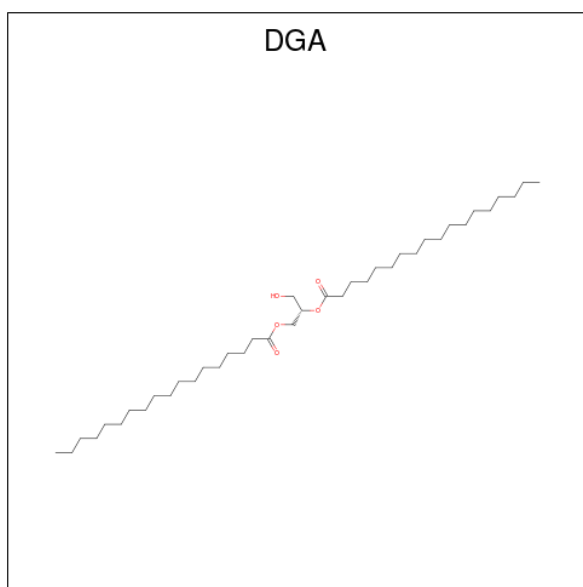
Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			53	38	15	
33	C	1	Total	C	O	0
			53	38	15	

- Molecule 34 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



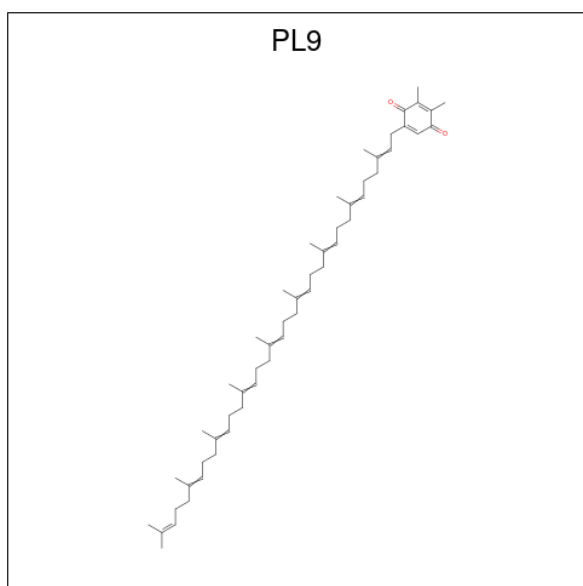
Mol	Chain	Residues	Atoms				AltConf
34	B	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 35 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			AltConf
35	B	1	Total	C	O	0
			37	32	5	

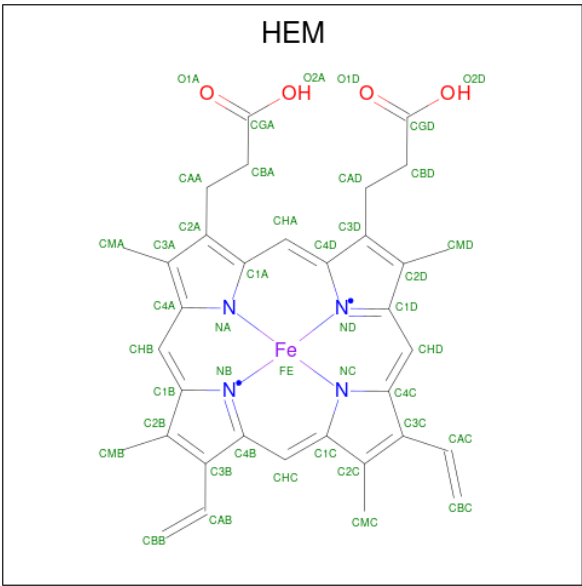
- Molecule 36 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms			AltConf
36	D	1	Total	C	O	0
			55	53	2	

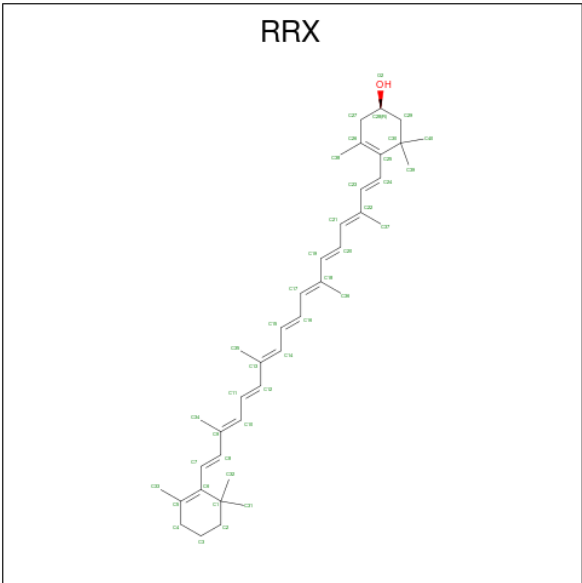
- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					AltConf
37	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).



Mol	Chain	Residues	Atoms			AltConf
38	H	1	Total	C	O	0
			41	40	1	

- Molecule 39 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
39	J	1	Total	C	O	0
			35	24	11	

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		AltConf
40	A	6	Total 6	O 6	0
40	B	3	Total 3	O 3	0
40	C	1	Total 1	O 1	0
40	D	1	Total 1	O 1	0

MolProbit failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	118340	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2250	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.028	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0047	Depositor
Map size (\AA)	193.5, 193.5, 193.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.645, 0.645, 0.645	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CSD	B	218	2	3,7,8	0.87	0	1,8,10	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CSD	B	218	2	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	218	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 77 ligands modelled in this entry, 4 are monoatomic - leaving 73 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
28	LMG	A	411	-	34,34,55	0.46	0	42,42,63	1.27	5 (11%)
24	CLA	C	513	-	55,63,73	1.48	8 (14%)	64,101,113	2.06	15 (23%)
28	LMG	C	501	-	40,40,55	0.76	2 (5%)	48,48,63	1.24	4 (8%)
38	RRX	H	101	-	42,42,42	5.02	26 (61%)	57,58,58	2.57	23 (40%)
28	LMG	D	409	-	42,42,55	0.77	2 (4%)	50,50,63	1.08	3 (6%)
24	CLA	C	503	-	65,73,73	1.36	7 (10%)	76,113,113	2.03	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LHG	D	410	-	38,38,48	0.43	0	41,44,54	1.20	4 (9%)
28	LMG	C	522	-	33,33,55	0.93	2 (6%)	40,40,63	1.10	2 (5%)
32	C7Z	B	519	-	43,43,43	5.30	27 (62%)	58,60,60	2.33	18 (31%)
24	CLA	B	505	-	65,73,73	1.35	7 (10%)	76,113,113	1.97	16 (21%)
27	SQD	A	410	-	41,42,54	0.87	0	50,53,65	1.01	2 (4%)
33	DGD	C	518	-	45,45,67	0.80	1 (2%)	59,59,81	1.11	4 (6%)
30	BCT	A	413	22	2,3,3	1.28	0	2,3,3	4.11	1 (50%)
35	DGA	B	523	-	36,36,43	1.17	3 (8%)	38,38,45	1.38	3 (7%)
39	LMU	J	102	-	36,36,36	0.39	0	47,47,47	0.77	2 (4%)
24	CLA	B	512	-	65,73,73	1.35	7 (10%)	76,113,113	1.99	15 (19%)
24	CLA	C	505	-	55,63,73	1.45	8 (14%)	64,101,113	2.21	17 (26%)
26	BCR	B	518	-	41,41,41	4.76	26 (63%)	56,56,56	2.24	19 (33%)
31	LHG	D	408	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
24	CLA	B	506	-	57,65,73	1.44	7 (12%)	66,103,113	2.07	17 (25%)
24	CLA	B	503	-	65,73,73	1.36	8 (12%)	76,113,113	1.96	17 (22%)
28	LMG	H	102	-	48,48,55	0.99	5 (10%)	56,56,63	1.13	2 (3%)
26	BCR	D	405	-	41,41,41	4.77	26 (63%)	56,56,56	2.20	19 (33%)
24	CLA	C	512	4	65,73,73	1.34	7 (10%)	76,113,113	2.05	19 (25%)
24	CLA	B	502	-	65,73,73	1.34	7 (10%)	76,113,113	1.97	16 (21%)
24	CLA	B	513	-	65,73,73	1.35	7 (10%)	76,113,113	2.02	16 (21%)
24	CLA	C	504	-	65,73,73	1.35	8 (12%)	76,113,113	1.98	18 (23%)
24	CLA	B	508	-	65,73,73	1.34	7 (10%)	76,113,113	1.97	17 (22%)
24	CLA	C	506	-	54,62,73	1.50	8 (14%)	62,99,113	2.15	16 (25%)
24	CLA	D	403	-	65,73,73	1.36	8 (12%)	76,113,113	1.89	14 (18%)
28	LMG	A	415	-	37,37,55	0.59	1 (2%)	45,45,63	1.07	3 (6%)
25	PHO	D	402	-	51,69,69	1.02	4 (7%)	47,99,99	1.21	6 (12%)
24	CLA	C	502	-	65,73,73	1.35	7 (10%)	76,113,113	1.99	17 (22%)
26	BCR	C	517	-	41,41,41	4.78	26 (63%)	56,56,56	2.38	19 (33%)
24	CLA	D	401	40	65,73,73	1.35	7 (10%)	76,113,113	2.05	19 (25%)
24	CLA	B	511	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	17 (22%)
24	CLA	B	514	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	18 (23%)
24	CLA	C	508	40	65,73,73	1.36	7 (10%)	76,113,113	2.00	14 (18%)
24	CLA	B	509	-	65,73,73	1.33	8 (12%)	76,113,113	2.00	18 (23%)
24	CLA	A	408	-	60,68,73	1.38	8 (13%)	70,107,113	2.22	20 (28%)
24	CLA	B	516	-	55,63,73	1.50	8 (14%)	64,101,113	2.04	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	DGD	B	521	-	44,44,67	0.86	1 (2%)	58,58,81	0.93	2 (3%)
27	SQD	M	101	-	41,42,54	0.87	0	50,53,65	0.93	2 (4%)
31	LHG	A	414	-	38,38,48	0.43	0	41,44,54	1.19	3 (7%)
24	CLA	B	507	40	65,73,73	1.35	8 (12%)	76,113,113	2.01	17 (22%)
26	BCR	A	409	-	41,41,41	4.79	26 (63%)	56,56,56	3.00	25 (44%)
31	LHG	D	407	-	43,43,48	0.42	0	46,49,54	1.05	3 (6%)
37	HEM	E	101	6,7	41,50,50	1.44	3 (7%)	45,82,82	1.28	7 (15%)
24	CLA	C	514	-	45,53,73	1.61	7 (15%)	52,89,113	2.21	14 (26%)
25	PHO	A	407	-	51,69,69	1.03	5 (9%)	47,99,99	1.19	5 (10%)
24	CLA	B	504	-	60,68,73	1.43	8 (13%)	70,107,113	2.09	16 (22%)
31	LHG	L	101	-	48,48,48	0.39	0	51,54,54	1.12	4 (7%)
24	CLA	A	405	-	65,73,73	1.34	7 (10%)	76,113,113	2.01	18 (23%)
24	CLA	B	515	-	65,73,73	1.33	8 (12%)	76,113,113	1.98	16 (21%)
26	BCR	B	517	-	41,41,41	4.74	25 (60%)	56,56,56	2.47	20 (35%)
24	CLA	A	406	40	65,73,73	1.36	8 (12%)	76,113,113	1.99	20 (26%)
24	CLA	C	509	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	18 (23%)
24	CLA	C	507	-	65,73,73	1.37	7 (10%)	76,113,113	1.97	17 (22%)
24	CLA	B	501	-	65,73,73	1.35	7 (10%)	76,113,113	2.02	18 (23%)
28	LMG	B	520	-	44,44,55	0.87	3 (6%)	52,52,63	1.14	2 (3%)
24	CLA	D	404	-	60,68,73	1.42	8 (13%)	70,107,113	2.12	14 (20%)
24	CLA	C	511	-	65,73,73	1.34	7 (10%)	76,113,113	2.06	16 (21%)
21	OEX	A	401	4,1	0,15,15	-	-	-	-	-
33	DGD	C	519	-	54,54,67	1.01	4 (7%)	68,68,81	1.21	5 (7%)
33	DGD	C	520	-	54,54,67	0.94	4 (7%)	68,68,81	1.16	5 (7%)
26	BCR	J	101	-	41,41,41	4.79	26 (63%)	56,56,56	2.39	20 (35%)
24	CLA	B	510	40	65,73,73	1.36	7 (10%)	76,113,113	1.97	15 (19%)
26	BCR	C	516	-	41,41,41	4.73	25 (60%)	56,56,56	2.40	22 (39%)
28	LMG	C	521	-	47,47,55	0.96	4 (8%)	55,55,63	1.09	3 (5%)
36	PL9	D	406	-	55,55,55	1.39	5 (9%)	68,69,69	1.52	13 (19%)
26	BCR	C	515	-	41,41,41	4.77	26 (63%)	56,56,56	2.23	20 (35%)
24	CLA	C	510	-	65,73,73	1.35	7 (10%)	76,113,113	1.99	18 (23%)
34	3PH	B	522	-	47,47,47	0.85	4 (8%)	51,52,52	1.15	2 (3%)

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
28	LMG	A	411	-	-	8/29/49/70	0/1/1/1
24	CLA	C	513	-	1/1/13/20	9/25/103/115	-
28	LMG	C	501	-	-	8/35/55/70	0/1/1/1
38	RRX	H	101	-	-	6/29/65/65	0/2/2/2
28	LMG	D	409	-	-	9/37/57/70	0/1/1/1
24	CLA	C	503	-	1/1/15/20	15/37/115/115	-
31	LHG	D	410	-	-	25/43/43/53	-
28	LMG	C	522	-	-	8/27/47/70	0/1/1/1
32	C7Z	B	519	-	-	12/29/67/67	0/2/2/2
24	CLA	B	505	-	1/1/15/20	15/37/115/115	-
27	SQD	A	410	-	-	8/37/57/69	0/1/1/1
33	DGD	C	518	-	-	6/33/73/95	0/2/2/2
35	DGA	B	523	-	-	24/38/38/45	-
39	LMU	J	102	-	-	6/21/61/61	0/2/2/2
24	CLA	B	512	-	1/1/15/20	15/37/115/115	-
24	CLA	C	505	-	1/1/13/20	9/25/103/115	-
26	BCR	B	518	-	-	13/29/63/63	0/2/2/2
31	LHG	D	408	-	-	26/53/53/53	-
24	CLA	B	506	-	1/1/13/20	7/28/106/115	-
24	CLA	B	503	-	1/1/15/20	21/37/115/115	-
28	LMG	H	102	-	-	13/43/63/70	0/1/1/1
26	BCR	D	405	-	-	8/29/63/63	0/2/2/2
24	CLA	C	512	4	1/1/15/20	13/37/115/115	-
24	CLA	B	502	-	1/1/15/20	14/37/115/115	-
24	CLA	B	513	-	1/1/15/20	18/37/115/115	-
24	CLA	C	504	-	1/1/15/20	15/37/115/115	-
24	CLA	B	508	-	1/1/15/20	15/37/115/115	-
24	CLA	C	506	-	1/1/12/20	12/24/102/115	-
24	CLA	D	403	-	1/1/15/20	13/37/115/115	-
28	LMG	A	415	-	-	4/32/52/70	0/1/1/1
25	PHO	D	402	-	-	7/37/103/103	0/5/6/6
24	CLA	C	502	-	1/1/15/20	18/37/115/115	-
26	BCR	C	517	-	-	10/29/63/63	0/2/2/2
24	CLA	D	401	40	1/1/15/20	21/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	511	-	1/1/15/20	16/37/115/115	-
24	CLA	B	514	-	1/1/15/20	17/37/115/115	-
24	CLA	C	508	40	1/1/15/20	12/37/115/115	-
24	CLA	B	509	-	1/1/15/20	15/37/115/115	-
24	CLA	A	408	-	1/1/14/20	15/31/109/115	-
24	CLA	B	516	-	1/1/13/20	13/25/103/115	-
33	DGD	B	521	-	-	14/32/72/95	0/2/2/2
27	SQD	M	101	-	-	14/37/57/69	0/1/1/1
31	LHG	A	414	-	-	26/43/43/53	-
24	CLA	B	507	40	1/1/15/20	24/37/115/115	-
26	BCR	A	409	-	-	13/29/63/63	0/2/2/2
31	LHG	D	407	-	-	23/48/48/53	-
37	HEM	E	101	6,7	-	2/12/54/54	-
24	CLA	C	514	-	1/1/11/20	7/13/91/115	-
25	PHO	A	407	-	-	13/37/103/103	0/5/6/6
24	CLA	B	504	-	1/1/14/20	18/31/109/115	-
31	LHG	L	101	-	-	30/53/53/53	-
24	CLA	A	405	-	1/1/15/20	14/37/115/115	-
24	CLA	B	515	-	1/1/15/20	18/37/115/115	-
26	BCR	B	517	-	-	10/29/63/63	0/2/2/2
24	CLA	A	406	40	1/1/15/20	13/37/115/115	-
24	CLA	C	509	-	1/1/15/20	15/37/115/115	-
24	CLA	C	507	-	1/1/15/20	18/37/115/115	-
24	CLA	B	501	-	1/1/15/20	16/37/115/115	-
28	LMG	B	520	-	-	9/39/59/70	0/1/1/1
24	CLA	D	404	-	1/1/14/20	14/31/109/115	-
24	CLA	C	511	-	1/1/15/20	16/37/115/115	-
33	DGD	C	520	-	-	9/42/82/95	0/2/2/2
33	DGD	C	519	-	-	16/42/82/95	0/2/2/2
26	BCR	J	101	-	-	11/29/63/63	0/2/2/2
24	CLA	B	510	40	1/1/15/20	19/37/115/115	-
26	BCR	C	516	-	-	9/29/63/63	0/2/2/2
28	LMG	C	521	-	-	9/42/62/70	0/1/1/1
36	PL9	D	406	-	-	8/53/73/73	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	C	515	-	-	13/29/63/63	0/2/2/2
24	CLA	C	510	-	1/1/15/20	9/37/115/115	-
34	3PH	B	522	-	-	25/49/49/49	-

All (571) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	519	C7Z	C25-C26	15.87	1.61	1.34
26	A	409	BCR	C26-C25	15.47	1.61	1.34
26	D	405	BCR	C26-C25	15.44	1.61	1.34
26	J	101	BCR	C26-C25	15.43	1.61	1.34
26	B	518	BCR	C26-C25	15.41	1.61	1.34
26	C	517	BCR	C26-C25	15.39	1.61	1.34
26	C	516	BCR	C26-C25	15.34	1.61	1.34
38	H	101	RRX	C26-C25	15.12	1.60	1.34
26	B	517	BCR	C26-C25	15.06	1.60	1.34
26	C	515	BCR	C26-C25	15.06	1.60	1.34
32	B	519	C7Z	C5-C6	14.79	1.60	1.34
38	H	101	RRX	C5-C6	14.11	1.58	1.34
26	J	101	BCR	C5-C6	14.06	1.58	1.34
26	A	409	BCR	C5-C6	14.04	1.58	1.34
26	C	515	BCR	C5-C6	14.00	1.58	1.34
26	C	517	BCR	C5-C6	13.99	1.58	1.34
26	B	518	BCR	C5-C6	13.90	1.58	1.34
26	D	405	BCR	C5-C6	13.81	1.58	1.34
26	B	517	BCR	C5-C6	13.66	1.58	1.34
26	C	516	BCR	C5-C6	13.58	1.58	1.34
32	B	519	C7Z	C24-C23	11.36	1.72	1.52
32	B	519	C7Z	C22-C23	-11.25	1.36	1.52
38	H	101	RRX	C29-C28	-10.70	1.36	1.52
32	B	519	C7Z	C2-C3	-10.06	1.37	1.52
32	B	519	C7Z	C4-C3	8.26	1.66	1.52
38	H	101	RRX	C27-C28	7.94	1.66	1.52
38	H	101	RRX	C30-C25	-7.34	1.43	1.53
26	B	517	BCR	C30-C25	-7.33	1.43	1.53
26	C	517	BCR	C30-C25	-7.17	1.43	1.53
26	C	515	BCR	C30-C25	-7.15	1.43	1.53
26	B	517	BCR	C1-C6	-7.11	1.44	1.53
26	D	405	BCR	C30-C25	-7.08	1.44	1.53
26	C	516	BCR	C1-C6	-7.04	1.44	1.53
26	C	516	BCR	C30-C25	-6.99	1.44	1.53
26	J	101	BCR	C1-C6	-6.98	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	518	BCR	C30-C25	-6.87	1.44	1.53
26	J	101	BCR	C30-C25	-6.81	1.44	1.53
38	H	101	RRX	C1-C6	-6.79	1.44	1.53
26	J	101	BCR	C2-C3	-6.78	1.35	1.52
26	A	409	BCR	C2-C3	-6.78	1.35	1.52
26	D	405	BCR	C1-C6	-6.77	1.44	1.53
26	A	409	BCR	C30-C25	-6.76	1.44	1.53
26	C	515	BCR	C1-C6	-6.74	1.44	1.53
26	C	517	BCR	C2-C3	-6.73	1.36	1.52
26	B	517	BCR	C2-C3	-6.71	1.36	1.52
38	H	101	RRX	C2-C3	-6.71	1.36	1.52
26	D	405	BCR	C2-C3	-6.71	1.36	1.52
26	B	518	BCR	C2-C3	-6.66	1.36	1.52
26	C	517	BCR	C1-C6	-6.63	1.44	1.53
26	C	515	BCR	C2-C3	-6.63	1.36	1.52
26	C	516	BCR	C2-C3	-6.55	1.36	1.52
26	A	409	BCR	C1-C6	-6.52	1.44	1.53
26	A	409	BCR	C29-C28	-6.50	1.36	1.52
26	B	518	BCR	C1-C6	-6.47	1.44	1.53
26	B	518	BCR	C29-C28	-6.47	1.36	1.52
26	C	517	BCR	C29-C28	-6.46	1.36	1.52
26	C	516	BCR	C29-C28	-6.44	1.36	1.52
26	J	101	BCR	C29-C28	-6.43	1.36	1.52
26	B	517	BCR	C29-C28	-6.42	1.36	1.52
26	C	515	BCR	C29-C28	-6.27	1.37	1.52
24	C	504	CLA	MG-NA	6.26	2.21	2.06
26	D	405	BCR	C29-C28	-6.26	1.37	1.52
24	C	508	CLA	MG-NA	6.26	2.21	2.06
24	B	516	CLA	MG-NA	6.24	2.21	2.06
24	B	504	CLA	MG-NA	6.24	2.21	2.06
24	C	506	CLA	MG-NA	6.23	2.21	2.06
24	B	510	CLA	MG-NA	6.21	2.21	2.06
24	C	512	CLA	MG-NA	6.21	2.21	2.06
24	C	507	CLA	MG-NA	6.20	2.21	2.06
24	B	501	CLA	MG-NA	6.16	2.20	2.06
24	C	509	CLA	MG-NA	6.15	2.20	2.06
24	C	514	CLA	MG-NA	6.15	2.20	2.06
24	C	513	CLA	MG-NA	6.15	2.20	2.06
24	D	404	CLA	MG-NA	6.15	2.20	2.06
24	C	503	CLA	MG-NA	6.13	2.20	2.06
24	B	514	CLA	MG-NA	6.13	2.20	2.06
24	A	406	CLA	MG-NA	6.12	2.20	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	503	CLA	MG-NA	6.12	2.20	2.06
24	C	502	CLA	MG-NA	6.11	2.20	2.06
24	B	508	CLA	MG-NA	6.11	2.20	2.06
24	B	507	CLA	MG-NA	6.11	2.20	2.06
24	B	502	CLA	MG-NA	6.08	2.20	2.06
24	B	511	CLA	MG-NA	6.07	2.20	2.06
24	A	408	CLA	MG-NA	6.05	2.20	2.06
24	D	403	CLA	MG-NA	6.05	2.20	2.06
24	B	515	CLA	MG-NA	6.04	2.20	2.06
24	B	513	CLA	MG-NA	6.03	2.20	2.06
24	C	510	CLA	MG-NA	6.03	2.20	2.06
24	C	511	CLA	MG-NA	6.02	2.20	2.06
24	C	505	CLA	MG-NA	6.02	2.20	2.06
24	B	505	CLA	MG-NA	6.00	2.20	2.06
24	B	509	CLA	MG-NA	6.00	2.20	2.06
24	B	506	CLA	MG-NA	5.98	2.20	2.06
24	B	512	CLA	MG-NA	5.96	2.20	2.06
24	D	401	CLA	MG-NA	5.96	2.20	2.06
24	A	405	CLA	MG-NA	5.93	2.20	2.06
32	B	519	C7Z	C12-C13	5.82	1.58	1.45
38	H	101	RRX	C19-C18	5.68	1.58	1.45
26	C	517	BCR	C12-C13	5.66	1.58	1.45
26	A	409	BCR	C12-C13	5.65	1.58	1.45
26	C	515	BCR	C12-C13	5.60	1.58	1.45
26	J	101	BCR	C12-C13	5.55	1.57	1.45
26	B	517	BCR	C12-C13	5.54	1.57	1.45
26	D	405	BCR	C12-C13	5.47	1.57	1.45
26	B	518	BCR	C12-C13	5.43	1.57	1.45
32	B	519	C7Z	C1-C6	-5.41	1.46	1.53
26	C	516	BCR	C12-C13	5.39	1.57	1.45
26	C	515	BCR	C8-C9	5.30	1.57	1.45
26	A	409	BCR	C8-C9	5.26	1.57	1.45
26	D	405	BCR	C8-C9	5.24	1.57	1.45
26	J	101	BCR	C8-C9	5.21	1.57	1.45
26	C	515	BCR	C29-C30	5.20	1.66	1.54
26	C	517	BCR	C8-C9	5.19	1.57	1.45
26	B	518	BCR	C8-C9	5.17	1.57	1.45
26	B	517	BCR	C8-C9	5.17	1.57	1.45
26	D	405	BCR	C29-C30	5.15	1.66	1.54
26	C	516	BCR	C8-C9	5.13	1.57	1.45
26	J	101	BCR	C29-C30	5.12	1.65	1.54
26	A	409	BCR	C23-C22	5.11	1.56	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	518	BCR	C23-C22	5.07	1.56	1.45
26	J	101	BCR	C23-C22	5.06	1.56	1.45
26	C	515	BCR	C23-C22	5.05	1.56	1.45
26	D	405	BCR	C23-C22	5.04	1.56	1.45
32	B	519	C7Z	C24-C25	-5.04	1.43	1.51
26	B	518	BCR	C29-C30	5.03	1.65	1.54
26	B	517	BCR	C29-C30	5.02	1.65	1.54
26	A	409	BCR	C29-C30	4.99	1.65	1.54
26	C	516	BCR	C29-C30	4.95	1.65	1.54
26	C	517	BCR	C23-C22	4.93	1.56	1.45
26	C	517	BCR	C29-C30	4.91	1.65	1.54
26	B	517	BCR	C23-C22	4.90	1.56	1.45
26	C	516	BCR	C23-C22	4.84	1.56	1.45
26	A	409	BCR	C15-C14	4.83	1.58	1.43
38	H	101	RRX	C8-C9	4.78	1.56	1.45
26	C	517	BCR	C15-C14	4.73	1.58	1.43
38	H	101	RRX	C12-C13	4.71	1.56	1.45
26	C	515	BCR	C15-C14	4.70	1.58	1.43
26	B	518	BCR	C15-C14	4.64	1.57	1.43
26	J	101	BCR	C15-C14	4.59	1.57	1.43
26	B	517	BCR	C15-C14	4.58	1.57	1.43
26	D	405	BCR	C15-C14	4.58	1.57	1.43
38	H	101	RRX	C2-C1	4.56	1.64	1.54
26	C	516	BCR	C15-C14	4.53	1.57	1.43
26	C	515	BCR	C19-C18	4.52	1.55	1.45
32	B	519	C7Z	C28-C29	4.47	1.55	1.45
26	C	517	BCR	C2-C1	4.45	1.64	1.54
36	D	406	PL9	C7-C3	-4.44	1.46	1.51
26	D	405	BCR	C2-C1	4.44	1.64	1.54
26	B	518	BCR	C19-C18	4.42	1.55	1.45
26	C	517	BCR	C19-C18	4.41	1.55	1.45
38	H	101	RRX	C27-C26	-4.40	1.44	1.51
38	H	101	RRX	C23-C22	4.38	1.55	1.45
26	C	516	BCR	C2-C1	4.38	1.64	1.54
26	D	405	BCR	C19-C18	4.37	1.55	1.45
26	J	101	BCR	C19-C18	4.36	1.55	1.45
26	B	517	BCR	C2-C1	4.36	1.64	1.54
26	B	518	BCR	C2-C1	4.34	1.64	1.54
32	B	519	C7Z	C31-C30	4.33	1.56	1.43
26	C	515	BCR	C2-C1	4.32	1.64	1.54
38	H	101	RRX	C24-C25	4.31	1.60	1.45
26	A	409	BCR	C19-C18	4.30	1.55	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J	101	BCR	C2-C1	4.29	1.64	1.54
26	B	517	BCR	C19-C18	4.29	1.55	1.45
38	H	101	RRX	C3-C4	4.28	1.65	1.52
26	C	515	BCR	C20-C21	4.26	1.56	1.43
33	C	518	DGD	O1G-C1A	4.25	1.45	1.33
26	D	405	BCR	C28-C27	4.25	1.65	1.52
26	B	518	BCR	C20-C21	4.24	1.56	1.43
33	B	521	DGD	O1G-C1A	4.23	1.45	1.33
26	A	409	BCR	C2-C1	4.23	1.63	1.54
38	H	101	RRX	C11-C10	4.22	1.56	1.43
26	C	516	BCR	C19-C18	4.20	1.55	1.45
26	C	517	BCR	C20-C21	4.19	1.56	1.43
26	J	101	BCR	C20-C21	4.18	1.56	1.43
26	A	409	BCR	C20-C21	4.15	1.56	1.43
26	C	515	BCR	C28-C27	4.14	1.65	1.52
33	C	519	DGD	O1G-C1A	4.14	1.45	1.33
24	B	513	CLA	MG-ND	-4.13	1.97	2.05
26	D	405	BCR	C20-C21	4.13	1.56	1.43
26	B	517	BCR	C20-C21	4.12	1.56	1.43
26	B	517	BCR	C28-C27	4.11	1.65	1.52
26	C	517	BCR	C28-C27	4.10	1.65	1.52
24	B	508	CLA	MG-ND	-4.10	1.97	2.05
24	C	513	CLA	MG-ND	-4.09	1.97	2.05
26	C	516	BCR	C28-C27	4.09	1.65	1.52
26	A	409	BCR	C28-C27	4.08	1.65	1.52
26	B	518	BCR	C28-C27	4.08	1.65	1.52
26	J	101	BCR	C28-C27	4.08	1.65	1.52
24	B	512	CLA	MG-ND	-4.07	1.97	2.05
32	B	519	C7Z	C32-C33	4.05	1.54	1.45
37	E	101	HEM	C3C-C2C	-4.05	1.34	1.40
24	C	510	CLA	MG-ND	-4.05	1.97	2.05
24	B	504	CLA	MG-ND	-4.04	1.97	2.05
24	B	503	CLA	MG-ND	-4.04	1.97	2.05
24	C	509	CLA	MG-ND	-4.03	1.97	2.05
33	C	520	DGD	O1G-C1A	4.02	1.45	1.33
24	D	403	CLA	MG-ND	-4.02	1.97	2.05
24	C	503	CLA	MG-ND	-4.01	1.97	2.05
26	C	516	BCR	C20-C21	4.01	1.55	1.43
36	D	406	PL9	C3-C4	-4.00	1.42	1.49
24	C	508	CLA	MG-ND	-3.99	1.97	2.05
32	B	519	C7Z	C4-C5	-3.98	1.44	1.51
24	B	516	CLA	MG-ND	-3.98	1.97	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	506	CLA	MG-ND	-3.98	1.97	2.05
24	C	507	CLA	MG-ND	-3.96	1.97	2.05
24	D	401	CLA	MG-ND	-3.96	1.97	2.05
24	A	406	CLA	MG-ND	-3.96	1.97	2.05
24	C	511	CLA	MG-ND	-3.96	1.97	2.05
24	B	507	CLA	MG-ND	-3.95	1.98	2.05
24	C	512	CLA	MG-ND	-3.95	1.98	2.05
24	B	515	CLA	MG-ND	-3.94	1.98	2.05
24	B	501	CLA	MG-ND	-3.94	1.98	2.05
24	B	514	CLA	MG-ND	-3.93	1.98	2.05
24	A	405	CLA	MG-ND	-3.93	1.98	2.05
24	D	404	CLA	MG-ND	-3.92	1.98	2.05
24	B	505	CLA	MG-ND	-3.92	1.98	2.05
24	B	510	CLA	MG-ND	-3.91	1.98	2.05
24	C	506	CLA	MG-ND	-3.91	1.98	2.05
26	C	516	BCR	C3-C4	3.91	1.64	1.52
38	H	101	RRX	C29-C30	3.90	1.67	1.54
24	C	514	CLA	MG-ND	-3.89	1.98	2.05
24	B	509	CLA	MG-ND	-3.88	1.98	2.05
38	H	101	RRX	C15-C14	3.87	1.55	1.43
26	B	518	BCR	C3-C4	3.86	1.64	1.52
26	C	515	BCR	C3-C4	3.85	1.64	1.52
26	B	517	BCR	C3-C4	3.84	1.64	1.52
24	B	511	CLA	MG-ND	-3.82	1.98	2.05
24	C	505	CLA	MG-ND	-3.81	1.98	2.05
24	C	504	CLA	MG-ND	-3.79	1.98	2.05
26	D	405	BCR	C3-C4	3.77	1.64	1.52
32	B	519	C7Z	C22-C21	3.77	1.66	1.54
26	A	409	BCR	C16-C17	3.76	1.55	1.43
26	J	101	BCR	C3-C4	3.76	1.64	1.52
24	C	502	CLA	MG-ND	-3.76	1.98	2.05
32	B	519	C7Z	C11-C10	3.76	1.55	1.43
24	D	401	CLA	C1C-NC	-3.75	1.32	1.37
26	C	517	BCR	C3-C4	3.73	1.64	1.52
26	A	409	BCR	C3-C4	3.73	1.64	1.52
38	H	101	RRX	C16-C17	3.72	1.55	1.43
32	B	519	C7Z	C15-C14	3.72	1.55	1.43
24	A	408	CLA	MG-ND	-3.72	1.98	2.05
26	A	409	BCR	C11-C10	3.71	1.55	1.43
24	B	502	CLA	MG-ND	-3.68	1.98	2.05
26	B	518	BCR	C16-C17	3.67	1.54	1.43
26	C	517	BCR	C11-C10	3.67	1.54	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	505	CLA	C1C-NC	-3.67	1.32	1.37
24	B	511	CLA	C1C-NC	-3.66	1.32	1.37
24	A	405	CLA	C1C-NC	-3.66	1.32	1.37
26	C	515	BCR	C16-C17	3.66	1.54	1.43
26	C	517	BCR	C16-C17	3.65	1.54	1.43
26	C	515	BCR	C11-C10	3.64	1.54	1.43
38	H	101	RRX	C20-C21	3.63	1.54	1.43
26	B	517	BCR	C11-C10	3.63	1.54	1.43
32	B	519	C7Z	C27-C26	3.62	1.58	1.45
24	C	509	CLA	C1C-NC	-3.60	1.32	1.37
26	D	405	BCR	C16-C17	3.60	1.54	1.43
26	J	101	BCR	C16-C17	3.60	1.54	1.43
24	C	505	CLA	C1C-NC	-3.59	1.32	1.37
37	E	101	HEM	C3C-CAC	3.59	1.55	1.47
26	J	101	BCR	C11-C10	3.58	1.54	1.43
24	A	406	CLA	C1C-NC	-3.58	1.32	1.37
24	C	503	CLA	C1C-NC	-3.58	1.32	1.37
26	B	517	BCR	C16-C17	3.58	1.54	1.43
24	B	506	CLA	C1C-NC	-3.57	1.32	1.37
24	B	512	CLA	C1C-NC	-3.57	1.32	1.37
24	B	510	CLA	C1C-NC	-3.57	1.32	1.37
24	B	504	CLA	C1C-NC	-3.56	1.32	1.37
26	D	405	BCR	C11-C10	3.56	1.54	1.43
26	A	409	BCR	C27-C26	-3.54	1.44	1.51
26	D	405	BCR	C24-C25	3.54	1.57	1.45
26	A	409	BCR	C24-C25	3.54	1.57	1.45
24	B	502	CLA	C1C-NC	-3.52	1.32	1.37
26	D	405	BCR	C4-C5	-3.52	1.44	1.51
26	B	518	BCR	C24-C25	3.52	1.57	1.45
24	C	510	CLA	C1C-NC	-3.52	1.32	1.37
24	C	507	CLA	C1C-NC	-3.51	1.32	1.37
24	B	507	CLA	C1C-NC	-3.50	1.32	1.37
26	B	518	BCR	C11-C10	3.50	1.54	1.43
24	C	512	CLA	C1C-NC	-3.50	1.32	1.37
24	C	514	CLA	C1C-NC	-3.50	1.32	1.37
35	B	523	DGA	OG2-CB1	3.50	1.44	1.34
24	D	404	CLA	C1C-NC	-3.50	1.32	1.37
24	B	501	CLA	C1C-NC	-3.50	1.32	1.37
32	B	519	C7Z	C2-C1	3.50	1.65	1.54
24	B	514	CLA	C1C-NC	-3.50	1.32	1.37
24	B	509	CLA	C1C-NC	-3.49	1.32	1.37
24	C	506	CLA	C1C-NC	-3.49	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J	101	BCR	C24-C25	3.49	1.57	1.45
32	B	519	C7Z	C35-C34	3.49	1.54	1.43
26	C	516	BCR	C16-C17	3.48	1.54	1.43
24	B	503	CLA	C1C-NC	-3.48	1.32	1.37
26	A	409	BCR	C4-C5	-3.48	1.44	1.51
26	C	515	BCR	C27-C26	-3.47	1.44	1.51
24	A	408	CLA	C1C-NC	-3.47	1.32	1.37
26	C	517	BCR	C4-C5	-3.46	1.44	1.51
24	C	502	CLA	C1C-NC	-3.46	1.32	1.37
26	C	517	BCR	C24-C25	3.45	1.57	1.45
24	C	511	CLA	C1C-NC	-3.45	1.32	1.37
26	C	516	BCR	C4-C5	-3.45	1.44	1.51
26	C	516	BCR	C11-C10	3.45	1.54	1.43
26	C	516	BCR	C24-C25	3.45	1.57	1.45
26	B	517	BCR	C27-C26	-3.43	1.44	1.51
26	C	516	BCR	C27-C26	-3.42	1.44	1.51
26	B	517	BCR	C24-C25	3.41	1.57	1.45
24	B	508	CLA	C1C-NC	-3.41	1.32	1.37
26	C	515	BCR	C24-C25	3.41	1.57	1.45
24	C	504	CLA	C1C-NC	-3.41	1.32	1.37
26	J	101	BCR	C4-C5	-3.40	1.44	1.51
26	C	517	BCR	C27-C26	-3.39	1.44	1.51
24	B	516	CLA	C1C-NC	-3.39	1.32	1.37
24	C	508	CLA	C1C-NC	-3.38	1.32	1.37
24	B	513	CLA	C1C-NC	-3.36	1.32	1.37
26	C	515	BCR	C4-C5	-3.36	1.44	1.51
26	B	518	BCR	C4-C5	-3.36	1.44	1.51
26	B	518	BCR	C27-C26	-3.35	1.44	1.51
26	B	517	BCR	C4-C5	-3.35	1.44	1.51
24	C	506	CLA	CBB-CAB	3.34	1.51	1.29
24	B	507	CLA	CBB-CAB	3.34	1.51	1.29
32	B	519	C7Z	C18-C5	3.34	1.56	1.50
24	D	404	CLA	CBB-CAB	3.34	1.51	1.29
26	J	101	BCR	C27-C26	-3.33	1.44	1.51
24	B	509	CLA	CBB-CAB	3.33	1.51	1.29
24	C	504	CLA	CBB-CAB	3.33	1.51	1.29
24	C	513	CLA	C1C-NC	-3.33	1.32	1.37
24	B	514	CLA	CBB-CAB	3.33	1.51	1.29
24	B	505	CLA	CBB-CAB	3.33	1.51	1.29
24	C	505	CLA	CBB-CAB	3.33	1.51	1.29
24	B	513	CLA	CBB-CAB	3.33	1.51	1.29
24	B	504	CLA	CBB-CAB	3.33	1.51	1.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	502	CLA	CBB-CAB	3.33	1.51	1.29
24	D	403	CLA	C1C-NC	-3.33	1.32	1.37
24	B	503	CLA	CBB-CAB	3.33	1.51	1.29
24	B	515	CLA	CBB-CAB	3.33	1.51	1.29
24	B	510	CLA	CBB-CAB	3.33	1.51	1.29
24	B	508	CLA	CBB-CAB	3.32	1.51	1.29
24	C	503	CLA	CBB-CAB	3.32	1.51	1.29
24	C	507	CLA	CBB-CAB	3.32	1.51	1.29
24	C	511	CLA	CBB-CAB	3.32	1.51	1.29
35	B	523	DGA	OG1-CA1	3.32	1.43	1.33
24	C	512	CLA	CBB-CAB	3.32	1.51	1.29
24	A	405	CLA	CBB-CAB	3.32	1.51	1.29
24	C	514	CLA	CBB-CAB	3.32	1.51	1.29
24	C	509	CLA	CBB-CAB	3.31	1.51	1.29
24	C	508	CLA	CBB-CAB	3.31	1.51	1.29
38	H	101	RRX	C7-C6	3.31	1.56	1.45
24	B	506	CLA	CBB-CAB	3.31	1.51	1.29
24	C	513	CLA	CBB-CAB	3.31	1.51	1.29
24	C	502	CLA	CBB-CAB	3.30	1.51	1.29
38	H	101	RRX	C17-C18	-3.29	1.31	1.35
24	A	406	CLA	CBB-CAB	3.29	1.51	1.29
28	B	520	LMG	C22-C21	-3.29	1.33	1.51
24	B	511	CLA	CBB-CAB	3.29	1.51	1.29
33	C	519	DGD	CAB-C9B	-3.29	1.33	1.51
24	B	515	CLA	C1C-NC	-3.29	1.32	1.37
24	B	516	CLA	CBB-CAB	3.28	1.51	1.29
24	D	401	CLA	CBB-CAB	3.28	1.51	1.29
24	B	501	CLA	CBB-CAB	3.28	1.51	1.29
28	C	522	LMG	C19-C18	-3.28	1.33	1.51
28	C	521	LMG	C19-C18	-3.28	1.33	1.51
24	A	408	CLA	CBB-CAB	3.28	1.51	1.29
24	B	512	CLA	CBB-CAB	3.27	1.51	1.29
33	C	519	DGD	CDB-CCB	-3.27	1.33	1.51
24	C	510	CLA	CBB-CAB	3.27	1.51	1.29
28	C	522	LMG	C22-C21	-3.27	1.33	1.51
33	C	520	DGD	CAA-C9A	-3.27	1.33	1.51
28	B	520	LMG	C19-C18	-3.26	1.33	1.51
28	H	102	LMG	C19-C18	-3.25	1.33	1.51
28	C	521	LMG	C40-C39	-3.25	1.33	1.51
24	D	403	CLA	CBB-CAB	3.24	1.50	1.29
28	C	521	LMG	C37-C36	-3.24	1.33	1.51
38	H	101	RRX	C4-C5	-3.23	1.44	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	409	LMG	C19-C18	-3.22	1.33	1.51
28	H	102	LMG	C40-C39	-3.22	1.33	1.51
26	D	405	BCR	C27-C26	-3.21	1.44	1.51
28	C	501	LMG	C19-C18	-3.20	1.33	1.51
28	H	102	LMG	C37-C36	-3.19	1.33	1.51
32	B	519	C7Z	C7-C6	3.18	1.56	1.45
32	B	519	C7Z	C21-C26	-3.17	1.49	1.53
36	D	406	PL9	C6-C1	-3.16	1.42	1.48
32	B	519	C7Z	C8-C9	3.13	1.52	1.45
24	B	516	CLA	C3B-C2B	-3.04	1.36	1.40
24	D	403	CLA	C3B-C2B	-3.02	1.36	1.40
37	E	101	HEM	CAB-C3B	2.94	1.55	1.47
24	C	513	CLA	C3B-C2B	-2.84	1.36	1.40
24	C	507	CLA	C3B-C2B	-2.82	1.36	1.40
24	B	501	CLA	C3B-C2B	-2.81	1.36	1.40
25	D	402	PHO	CAC-C3C	-2.81	1.47	1.52
26	A	409	BCR	C34-C9	2.80	1.56	1.50
25	A	407	PHO	CAC-C3C	-2.79	1.47	1.52
26	B	517	BCR	C34-C9	2.76	1.56	1.50
24	C	502	CLA	C3B-C2B	-2.73	1.36	1.40
24	B	510	CLA	C3B-C2B	-2.72	1.36	1.40
26	C	515	BCR	C34-C9	2.72	1.56	1.50
24	D	403	CLA	CHC-C1C	2.71	1.41	1.35
24	B	505	CLA	C3B-C2B	-2.69	1.36	1.40
24	C	508	CLA	C3B-C2B	-2.68	1.36	1.40
24	C	506	CLA	CHC-C1C	2.66	1.41	1.35
24	C	502	CLA	CHC-C1C	2.66	1.41	1.35
26	C	515	BCR	C7-C6	2.66	1.54	1.45
26	B	518	BCR	C34-C9	2.65	1.56	1.50
24	C	504	CLA	CHC-C1C	2.64	1.41	1.35
24	A	406	CLA	CHC-C1C	2.63	1.41	1.35
26	J	101	BCR	C34-C9	2.63	1.56	1.50
24	C	514	CLA	CHC-C1C	2.61	1.41	1.35
26	C	516	BCR	C34-C9	2.61	1.56	1.50
26	D	405	BCR	C34-C9	2.60	1.56	1.50
26	J	101	BCR	C7-C6	2.59	1.54	1.45
26	D	405	BCR	C7-C6	2.59	1.54	1.45
24	B	516	CLA	CHC-C1C	2.58	1.41	1.35
26	A	409	BCR	C7-C6	2.58	1.54	1.45
26	B	518	BCR	C7-C6	2.58	1.54	1.45
24	B	501	CLA	CHC-C1C	2.58	1.41	1.35
24	B	503	CLA	CHC-C1C	2.57	1.41	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	C3B-C2B	-2.56	1.36	1.40
24	D	404	CLA	C3B-C2B	-2.56	1.36	1.40
24	B	502	CLA	CHC-C1C	2.56	1.41	1.35
24	C	509	CLA	CHC-C1C	2.55	1.41	1.35
28	D	409	LMG	C37-C36	-2.55	1.33	1.51
26	C	517	BCR	C7-C6	2.55	1.54	1.45
24	B	509	CLA	CHC-C1C	2.55	1.41	1.35
24	B	508	CLA	CHC-C1C	2.54	1.41	1.35
24	B	510	CLA	CHC-C1C	2.54	1.41	1.35
24	C	511	CLA	CHC-C1C	2.53	1.41	1.35
24	B	513	CLA	CHC-C1C	2.53	1.41	1.35
26	B	517	BCR	C7-C6	2.52	1.54	1.45
26	C	516	BCR	C7-C6	2.52	1.54	1.45
24	C	513	CLA	CHC-C1C	2.52	1.41	1.35
24	B	515	CLA	C3B-C2B	-2.52	1.36	1.40
26	C	517	BCR	C34-C9	2.52	1.56	1.50
24	A	405	CLA	CHC-C1C	2.52	1.41	1.35
24	C	503	CLA	CHC-C1C	2.51	1.41	1.35
24	B	505	CLA	CHC-C1C	2.50	1.41	1.35
24	C	507	CLA	CHC-C1C	2.50	1.41	1.35
24	B	515	CLA	CHC-C1C	2.50	1.41	1.35
24	C	510	CLA	CHC-C1C	2.50	1.41	1.35
24	C	512	CLA	CHC-C1C	2.49	1.41	1.35
36	D	406	PL9	C53-C6	-2.48	1.45	1.50
24	B	507	CLA	CHC-C1C	2.48	1.41	1.35
26	C	516	BCR	C39-C30	-2.48	1.48	1.53
24	C	505	CLA	CHC-C1C	2.47	1.41	1.35
24	C	506	CLA	C3B-C2B	-2.47	1.36	1.40
24	D	404	CLA	CHC-C1C	2.47	1.41	1.35
24	B	512	CLA	CHC-C1C	2.46	1.41	1.35
24	B	511	CLA	CHC-C1C	2.46	1.41	1.35
24	B	504	CLA	CHC-C1C	2.46	1.41	1.35
24	B	514	CLA	CHC-C1C	2.46	1.41	1.35
24	C	508	CLA	CHC-C1C	2.45	1.41	1.35
24	D	401	CLA	CHC-C1C	2.45	1.41	1.35
24	B	506	CLA	CHC-C1C	2.45	1.41	1.35
24	A	406	CLA	C3B-C2B	-2.44	1.37	1.40
24	B	502	CLA	C3B-C2B	-2.43	1.37	1.40
24	A	408	CLA	CHC-C1C	2.42	1.41	1.35
34	B	522	3PH	O31-C31	2.42	1.40	1.33
26	C	517	BCR	C39-C30	-2.41	1.49	1.53
24	B	507	CLA	C3B-C2B	-2.40	1.37	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	504	CLA	C3B-C2B	-2.40	1.37	1.40
32	B	519	C7Z	C38-C25	2.40	1.54	1.50
24	B	511	CLA	C3B-C2B	-2.39	1.37	1.40
32	B	519	C7Z	C20-C13	2.38	1.55	1.50
26	J	101	BCR	C39-C30	-2.37	1.49	1.53
36	D	406	PL9	C52-C5	-2.37	1.45	1.50
24	B	506	CLA	C3B-C2B	-2.36	1.37	1.40
24	C	511	CLA	C3B-C2B	-2.35	1.37	1.40
26	C	515	BCR	C39-C30	-2.35	1.49	1.53
24	B	512	CLA	C3B-C2B	-2.32	1.37	1.40
38	H	101	RRX	C14-C13	-2.31	1.32	1.35
24	D	403	CLA	C3D-C4D	-2.30	1.39	1.44
26	C	516	BCR	C36-C18	2.30	1.55	1.50
24	B	503	CLA	C3D-C4D	-2.29	1.39	1.44
25	A	407	PHO	CMC-C2C	-2.29	1.46	1.51
24	B	508	CLA	C3B-C2B	-2.29	1.37	1.40
24	A	406	CLA	C3D-C4D	-2.29	1.39	1.44
26	A	409	BCR	C39-C30	-2.29	1.49	1.53
24	D	401	CLA	C3B-C2B	-2.28	1.37	1.40
26	B	518	BCR	C39-C30	-2.28	1.49	1.53
38	H	101	RRX	C34-C9	2.28	1.55	1.50
26	B	517	BCR	C39-C30	-2.28	1.49	1.53
24	A	405	CLA	C3B-C2B	-2.27	1.37	1.40
26	D	405	BCR	C39-C30	-2.27	1.49	1.53
26	C	515	BCR	C36-C18	2.27	1.55	1.50
25	D	402	PHO	CMC-C2C	-2.27	1.46	1.51
24	C	505	CLA	C3B-C2B	-2.25	1.37	1.40
24	B	509	CLA	C3B-C2B	-2.25	1.37	1.40
26	J	101	BCR	C36-C18	2.25	1.55	1.50
24	C	502	CLA	C3D-C4D	-2.25	1.39	1.44
24	C	504	CLA	C3B-C2B	-2.24	1.37	1.40
24	B	503	CLA	C3B-C2B	-2.24	1.37	1.40
24	C	510	CLA	C3D-C4D	-2.24	1.39	1.44
24	C	511	CLA	C3D-C4D	-2.23	1.39	1.44
32	B	519	C7Z	C40-C33	2.23	1.55	1.50
24	C	509	CLA	C3B-C2B	-2.23	1.37	1.40
26	B	517	BCR	C36-C18	2.22	1.55	1.50
24	A	408	CLA	C3D-C4D	-2.22	1.39	1.44
26	B	518	BCR	C36-C18	2.22	1.55	1.50
34	B	522	3PH	O21-C2	-2.22	1.41	1.46
26	D	405	BCR	C36-C18	2.21	1.55	1.50
24	D	401	CLA	C3D-C4D	-2.21	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	504	CLA	C3D-C4D	-2.21	1.39	1.44
24	A	405	CLA	C3D-C4D	-2.21	1.39	1.44
25	D	402	PHO	CMD-C2D	-2.21	1.46	1.51
24	C	509	CLA	C3D-C4D	-2.20	1.39	1.44
26	C	517	BCR	C36-C18	2.20	1.55	1.50
25	A	407	PHO	CMD-C2D	-2.20	1.46	1.51
34	B	522	3PH	O21-C21	2.19	1.40	1.34
24	B	508	CLA	C3D-C4D	-2.18	1.39	1.44
24	C	504	CLA	C3D-C4D	-2.18	1.39	1.44
24	B	505	CLA	C3D-C4D	-2.17	1.39	1.44
24	B	514	CLA	C3B-C2B	-2.17	1.37	1.40
24	C	512	CLA	C3D-C4D	-2.17	1.39	1.44
34	B	522	3PH	O31-C3	-2.17	1.40	1.45
26	D	405	BCR	C38-C26	2.17	1.54	1.50
24	B	506	CLA	C3D-C4D	-2.16	1.39	1.44
24	B	514	CLA	C3D-C4D	-2.16	1.39	1.44
24	B	512	CLA	C3D-C4D	-2.16	1.39	1.44
24	C	514	CLA	C3D-C4D	-2.15	1.39	1.44
24	C	506	CLA	C3D-C4D	-2.15	1.39	1.44
32	B	519	C7Z	C19-C9	2.15	1.55	1.50
24	B	511	CLA	C3D-C4D	-2.14	1.39	1.44
24	B	513	CLA	C3B-C2B	-2.14	1.37	1.40
24	B	516	CLA	C3D-C4D	-2.14	1.39	1.44
24	B	501	CLA	C3D-C4D	-2.13	1.39	1.44
24	B	502	CLA	C3D-C4D	-2.13	1.39	1.44
24	C	508	CLA	C3D-C4D	-2.12	1.39	1.44
24	C	507	CLA	C3D-C4D	-2.12	1.39	1.44
25	A	407	PHO	CMB-C2B	-2.12	1.46	1.51
24	D	404	CLA	C3D-C4D	-2.12	1.39	1.44
24	C	505	CLA	C3D-C4D	-2.12	1.39	1.44
25	D	402	PHO	CMB-C2B	-2.11	1.46	1.51
24	B	507	CLA	C1A-CHA	2.11	1.51	1.43
26	A	409	BCR	C36-C18	2.11	1.55	1.50
24	B	513	CLA	C3D-C4D	-2.10	1.39	1.44
24	C	512	CLA	C3B-C2B	-2.10	1.37	1.40
24	C	510	CLA	C3B-C2B	-2.10	1.37	1.40
24	B	507	CLA	C3D-C4D	-2.10	1.39	1.44
24	B	510	CLA	C3D-C4D	-2.10	1.39	1.44
24	C	503	CLA	C3D-C4D	-2.09	1.39	1.44
24	C	514	CLA	C3B-C2B	-2.08	1.37	1.40
24	B	509	CLA	C3D-C4D	-2.08	1.39	1.44
38	H	101	RRX	C33-C5	2.08	1.54	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	515	CLA	C3D-C4D	-2.08	1.39	1.44
24	A	408	CLA	C1A-CHA	2.07	1.51	1.43
26	A	409	BCR	C37-C22	2.07	1.55	1.50
24	C	513	CLA	C3D-C4D	-2.06	1.39	1.44
24	C	504	CLA	C1C-C2C	2.05	1.48	1.44
24	C	505	CLA	C1A-CHA	2.04	1.51	1.43
33	C	520	DGD	CDA-CCA	-2.04	1.33	1.49
24	B	504	CLA	C1A-CHA	2.04	1.51	1.43
28	H	102	LMG	C22-C21	-2.04	1.33	1.49
24	B	503	CLA	C1A-CHA	2.04	1.51	1.43
26	B	518	BCR	C38-C26	2.04	1.54	1.50
33	C	520	DGD	CAB-C9B	-2.04	1.33	1.49
24	A	406	CLA	C1A-CHA	2.03	1.51	1.43
25	A	407	PHO	C3B-C2B	-2.03	1.37	1.40
33	C	519	DGD	CGB-CFB	-2.03	1.33	1.49
26	J	101	BCR	C38-C26	2.03	1.54	1.50
24	A	408	CLA	C3B-C2B	-2.03	1.37	1.40
26	C	515	BCR	C38-C26	2.02	1.54	1.50
28	A	415	LMG	C37-C36	-2.02	1.33	1.49
28	B	520	LMG	C25-C24	-2.02	1.33	1.49
28	C	501	LMG	C22-C21	-2.02	1.33	1.49
28	C	521	LMG	C43-C42	-2.02	1.33	1.49
24	D	404	CLA	C1A-CHA	2.02	1.51	1.43
35	B	523	DGA	OG2-CG2	-2.02	1.41	1.46
26	C	517	BCR	C38-C26	2.01	1.54	1.50
24	B	515	CLA	C1A-CHA	2.01	1.51	1.43
24	B	516	CLA	C1B-NB	2.01	1.37	1.35
24	C	513	CLA	C1C-C2C	2.01	1.48	1.44
28	H	102	LMG	C43-C42	-2.01	1.33	1.49
24	C	506	CLA	C1A-CHA	2.01	1.51	1.43
24	B	509	CLA	C1A-CHA	2.00	1.51	1.43
24	D	403	CLA	C1C-C2C	2.00	1.48	1.44

All (890) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	408	CLA	C4A-NA-C1A	9.70	111.06	106.71
26	A	409	BCR	C7-C8-C9	-9.68	111.60	126.23
24	B	512	CLA	C4A-NA-C1A	9.65	111.05	106.71
24	D	404	CLA	C4A-NA-C1A	9.55	111.00	106.71
24	B	509	CLA	C4A-NA-C1A	9.44	110.95	106.71
24	B	513	CLA	C4A-NA-C1A	9.36	110.91	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	507	CLA	C4A-NA-C1A	9.30	110.89	106.71
24	C	505	CLA	C4A-NA-C1A	9.28	110.88	106.71
24	B	506	CLA	C4A-NA-C1A	9.20	110.84	106.71
24	A	405	CLA	C4A-NA-C1A	9.17	110.83	106.71
24	B	515	CLA	C4A-NA-C1A	9.14	110.81	106.71
24	C	503	CLA	C4A-NA-C1A	9.12	110.81	106.71
24	C	512	CLA	C4A-NA-C1A	9.11	110.80	106.71
24	C	508	CLA	C4A-NA-C1A	9.01	110.76	106.71
24	C	511	CLA	C4A-NA-C1A	9.01	110.76	106.71
24	C	514	CLA	C4A-NA-C1A	8.93	110.72	106.71
24	C	510	CLA	C4A-NA-C1A	8.91	110.71	106.71
24	B	510	CLA	C4A-NA-C1A	8.89	110.70	106.71
24	B	514	CLA	C4A-NA-C1A	8.89	110.70	106.71
24	C	513	CLA	C4A-NA-C1A	8.81	110.67	106.71
24	D	401	CLA	C4A-NA-C1A	8.78	110.65	106.71
24	B	501	CLA	C4A-NA-C1A	8.76	110.64	106.71
24	C	506	CLA	C4A-NA-C1A	8.75	110.64	106.71
24	B	502	CLA	C4A-NA-C1A	8.72	110.63	106.71
24	C	507	CLA	C4A-NA-C1A	8.69	110.61	106.71
24	B	508	CLA	C4A-NA-C1A	8.64	110.59	106.71
24	A	406	CLA	C4A-NA-C1A	8.63	110.59	106.71
24	B	511	CLA	C4A-NA-C1A	8.58	110.56	106.71
24	B	504	CLA	C4A-NA-C1A	8.58	110.56	106.71
24	B	503	CLA	C4A-NA-C1A	8.54	110.54	106.71
24	C	502	CLA	C4A-NA-C1A	8.44	110.50	106.71
26	A	409	BCR	C15-C14-C13	-8.39	115.34	127.31
24	B	505	CLA	C4A-NA-C1A	8.35	110.46	106.71
24	B	516	CLA	C4A-NA-C1A	8.33	110.45	106.71
24	C	504	CLA	C4A-NA-C1A	8.29	110.44	106.71
24	C	509	CLA	C4A-NA-C1A	8.01	110.31	106.71
38	H	101	RRX	C11-C10-C9	-7.90	116.03	127.31
24	D	403	CLA	C4A-NA-C1A	7.90	110.26	106.71
26	C	517	BCR	C7-C8-C9	-7.18	115.38	126.23
26	A	409	BCR	C20-C21-C22	-6.75	117.68	127.31
26	B	517	BCR	C33-C5-C6	-6.61	117.11	124.53
38	H	101	RRX	C20-C21-C22	-6.36	118.24	127.31
26	B	517	BCR	C15-C14-C13	-6.27	118.37	127.31
24	A	408	CLA	O2D-CGD-CBD	6.25	122.37	111.27
24	B	501	CLA	O2D-CGD-CBD	6.05	122.02	111.27
38	H	101	RRX	C15-C14-C13	-6.03	118.70	127.31
26	A	409	BCR	C33-C5-C6	-5.92	117.88	124.53
32	B	519	C7Z	C11-C10-C9	-5.91	118.88	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	O2D-CGD-CBD	5.91	121.76	111.27
24	C	502	CLA	CMD-C2D-C1D	5.89	135.09	124.71
26	B	517	BCR	C11-C10-C9	-5.77	119.08	127.31
24	A	405	CLA	O2A-C1-C2	5.71	123.65	108.64
24	C	511	CLA	CMD-C2D-C1D	5.63	134.64	124.71
26	C	515	BCR	C16-C17-C18	-5.63	119.27	127.31
24	C	512	CLA	CMD-C2D-C1D	5.63	134.63	124.71
24	B	507	CLA	CMD-C2D-C1D	5.61	134.61	124.71
24	D	401	CLA	CMD-C2D-C1D	5.60	134.58	124.71
24	D	404	CLA	O2D-CGD-CBD	5.59	121.20	111.27
24	C	509	CLA	O2A-C1-C2	5.59	123.32	108.64
24	B	506	CLA	CMD-C2D-C1D	5.58	134.55	124.71
24	B	512	CLA	O2D-CGD-CBD	5.56	121.15	111.27
24	C	509	CLA	O2D-CGD-CBD	5.55	121.14	111.27
24	B	514	CLA	O2A-C1-C2	5.54	123.20	108.64
24	C	503	CLA	O2A-C1-C2	5.53	123.17	108.64
24	B	505	CLA	CMD-C2D-C1D	5.52	134.45	124.71
24	C	502	CLA	O2D-CGD-CBD	5.52	121.07	111.27
24	C	513	CLA	O2D-CGD-CBD	5.50	121.04	111.27
26	A	409	BCR	C8-C9-C10	5.50	127.38	118.94
24	B	503	CLA	CMD-C2D-C1D	5.49	134.39	124.71
24	C	504	CLA	CMD-C2D-C1D	5.49	134.38	124.71
24	B	501	CLA	CMD-C2D-C1D	5.49	134.38	124.71
24	B	510	CLA	O2D-CGD-CBD	5.48	121.01	111.27
30	A	413	BCT	O2-C-O1	5.48	133.76	119.55
24	B	504	CLA	CMD-C2D-C1D	5.47	134.36	124.71
24	C	514	CLA	O2D-CGD-CBD	5.47	120.99	111.27
24	B	505	CLA	O2D-CGD-CBD	5.46	120.96	111.27
24	C	503	CLA	O2D-CGD-CBD	5.45	120.95	111.27
24	B	504	CLA	O2D-CGD-CBD	5.44	120.94	111.27
24	C	510	CLA	CMD-C2D-C1D	5.44	134.31	124.71
24	A	406	CLA	O2A-C1-C2	5.43	122.90	108.64
24	C	508	CLA	O2D-CGD-CBD	5.43	120.91	111.27
24	B	509	CLA	O2D-CGD-CBD	5.42	120.90	111.27
24	B	514	CLA	CMD-C2D-C1D	5.42	134.26	124.71
24	A	406	CLA	CMD-C2D-C1D	5.41	134.25	124.71
24	A	408	CLA	O2A-C1-C2	5.41	122.86	108.64
26	C	516	BCR	C15-C14-C13	-5.40	119.61	127.31
24	B	502	CLA	CMD-C2D-C1D	5.39	134.21	124.71
24	C	505	CLA	O2D-CGD-CBD	5.39	120.84	111.27
24	C	514	CLA	CMD-C2D-C1D	5.39	134.21	124.71
24	C	508	CLA	CMD-C2D-C1D	5.37	134.18	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	O2A-C1-C2	5.36	122.71	108.64
24	B	506	CLA	O2D-CGD-CBD	5.35	120.78	111.27
24	A	405	CLA	CMD-C2D-C1D	5.35	134.14	124.71
24	A	408	CLA	CMD-C2D-C1D	5.35	134.14	124.71
24	C	507	CLA	CMD-C2D-C1D	5.35	134.14	124.71
24	C	505	CLA	CMD-C2D-C1D	5.35	134.14	124.71
24	D	403	CLA	CMD-C2D-C1D	5.34	134.12	124.71
24	D	404	CLA	O2A-C1-C2	5.33	122.66	108.64
24	B	508	CLA	O2A-C1-C2	5.33	122.65	108.64
26	C	517	BCR	C20-C21-C22	-5.32	119.71	127.31
26	C	517	BCR	C11-C10-C9	-5.32	119.72	127.31
24	B	515	CLA	O2D-CGD-CBD	5.32	120.72	111.27
24	C	506	CLA	O2D-CGD-CBD	5.30	120.69	111.27
24	C	511	CLA	O2D-CGD-CBD	5.29	120.66	111.27
32	B	519	C7Z	C15-C14-C13	-5.28	119.77	127.31
24	D	401	CLA	O2A-C1-C2	5.28	122.52	108.64
24	C	506	CLA	CMD-C2D-C1D	5.28	134.02	124.71
24	B	513	CLA	CMD-C2D-C1D	5.27	134.00	124.71
24	B	505	CLA	O2A-C1-C2	5.24	122.40	108.64
24	B	507	CLA	O2A-C1-C2	5.23	122.38	108.64
24	C	511	CLA	O2A-C1-C2	5.23	122.37	108.64
24	D	404	CLA	CMD-C2D-C1D	5.22	133.92	124.71
24	B	509	CLA	CMD-C2D-C1D	5.20	133.87	124.71
26	J	101	BCR	C24-C23-C22	-5.19	118.39	126.23
24	C	504	CLA	O2A-C1-C2	5.18	122.24	108.64
24	C	507	CLA	O2A-C1-C2	5.18	122.24	108.64
26	J	101	BCR	C11-C10-C9	-5.16	119.95	127.31
24	B	516	CLA	CMD-C2D-C1D	5.16	133.80	124.71
24	C	512	CLA	O2D-CGD-CBD	5.16	120.43	111.27
24	B	511	CLA	CMD-C2D-C1D	5.15	133.80	124.71
24	B	515	CLA	CMD-C2D-C1D	5.15	133.78	124.71
24	B	501	CLA	O2A-C1-C2	5.14	122.15	108.64
24	A	406	CLA	O2D-CGD-CBD	5.13	120.38	111.27
24	B	511	CLA	O2D-CGD-CBD	5.13	120.38	111.27
26	J	101	BCR	C16-C17-C18	-5.12	120.00	127.31
24	C	509	CLA	CMD-C2D-C1D	5.12	133.74	124.71
24	C	508	CLA	O2A-C1-C2	5.12	122.08	108.64
26	C	516	BCR	C38-C26-C25	-5.11	118.79	124.53
24	B	502	CLA	O2D-CGD-CBD	5.07	120.28	111.27
24	B	513	CLA	O2A-C1-C2	5.07	121.96	108.64
24	B	510	CLA	CMD-C2D-C1D	5.07	133.64	124.71
26	A	409	BCR	C34-C9-C10	-5.06	115.83	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	O2D-CGD-CBD	5.06	120.26	111.27
24	D	403	CLA	O2A-C1-C2	5.05	121.92	108.64
24	B	508	CLA	O2D-CGD-CBD	5.05	120.25	111.27
24	B	503	CLA	O2D-CGD-CBD	5.04	120.23	111.27
24	C	512	CLA	O2A-C1-C2	5.04	121.87	108.64
26	C	516	BCR	C11-C10-C9	-5.03	120.14	127.31
24	B	504	CLA	O2A-C1-C2	5.03	121.85	108.64
26	A	409	BCR	C10-C11-C12	-5.02	107.54	123.22
26	J	101	BCR	C33-C5-C6	-5.02	118.89	124.53
24	B	516	CLA	O2D-CGD-CBD	5.01	120.17	111.27
24	C	507	CLA	O2D-CGD-CBD	5.00	120.15	111.27
24	C	503	CLA	CMD-C2D-C1D	4.99	133.50	124.71
24	B	511	CLA	O2A-C1-C2	4.99	121.74	108.64
26	C	515	BCR	C24-C23-C22	-4.99	118.70	126.23
24	C	506	CLA	O2A-C1-C2	4.99	121.74	108.64
24	D	403	CLA	O2D-CGD-CBD	4.98	120.13	111.27
24	B	516	CLA	O2A-C1-C2	4.98	121.74	108.64
24	B	507	CLA	O2D-CGD-CBD	4.97	120.10	111.27
24	B	509	CLA	O2A-C1-C2	4.93	121.60	108.64
26	C	516	BCR	C1-C6-C5	-4.93	115.67	122.61
24	B	513	CLA	O2D-CGD-CBD	4.93	120.03	111.27
24	B	512	CLA	CMD-C2D-C1D	4.93	133.39	124.71
24	C	513	CLA	CMD-C2D-C1D	4.91	133.36	124.71
26	D	405	BCR	C16-C17-C18	-4.90	120.32	127.31
26	B	517	BCR	C38-C26-C25	-4.90	119.03	124.53
24	B	514	CLA	O2D-CGD-CBD	4.89	119.96	111.27
32	B	519	C7Z	C35-C34-C33	-4.88	120.34	127.31
24	D	401	CLA	O2D-CGD-CBD	4.87	119.92	111.27
24	B	503	CLA	O2A-C1-C2	4.84	121.35	108.64
24	B	510	CLA	O2A-C1-C2	4.83	121.32	108.64
24	B	515	CLA	O2A-C1-C2	4.81	121.29	108.64
26	B	518	BCR	C38-C26-C25	-4.80	119.14	124.53
26	C	517	BCR	C16-C17-C18	-4.79	120.47	127.31
36	D	406	PL9	C7-C3-C4	4.78	120.76	116.88
24	B	508	CLA	CMD-C2D-C1D	4.77	133.13	124.71
26	B	518	BCR	C33-C5-C6	-4.77	119.18	124.53
26	J	101	BCR	C7-C8-C9	-4.75	119.06	126.23
26	B	518	BCR	C20-C21-C22	-4.74	120.54	127.31
26	J	101	BCR	C38-C26-C25	-4.74	119.20	124.53
26	C	517	BCR	C38-C26-C25	-4.73	119.21	124.53
28	B	520	LMG	O7-C10-C11	4.72	121.67	111.50
26	C	516	BCR	C16-C17-C18	-4.71	120.59	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	519	C7Z	C1-C6-C5	-4.68	116.02	122.61
24	C	502	CLA	O2A-C1-C2	4.67	120.91	108.64
26	B	518	BCR	C15-C14-C13	-4.67	120.65	127.31
24	C	510	CLA	O2A-C1-C2	4.66	120.88	108.64
24	A	405	CLA	O2D-CGD-CBD	4.65	119.53	111.27
26	C	516	BCR	C4-C5-C6	-4.63	116.01	122.73
26	J	101	BCR	C15-C14-C13	-4.56	120.80	127.31
32	B	519	C7Z	C18-C5-C6	-4.55	119.42	124.53
32	B	519	C7Z	C31-C30-C29	-4.53	120.84	127.31
28	C	501	LMG	O7-C10-C11	4.51	121.21	111.50
26	B	517	BCR	C7-C8-C9	-4.46	119.50	126.23
32	B	519	C7Z	C27-C28-C29	-4.45	119.51	126.23
26	B	518	BCR	C16-C17-C18	-4.43	120.99	127.31
26	C	515	BCR	C20-C21-C22	-4.43	120.99	127.31
31	D	410	LHG	O7-C7-C8	4.42	121.02	111.50
26	D	405	BCR	C20-C21-C22	-4.41	121.01	127.31
26	C	516	BCR	C33-C5-C6	-4.41	119.58	124.53
38	H	101	RRX	C24-C23-C22	-4.41	119.58	126.23
32	B	519	C7Z	C38-C25-C26	-4.40	119.59	124.53
38	H	101	RRX	C1-C6-C5	-4.37	116.45	122.61
32	B	519	C7Z	C7-C8-C9	-4.33	119.70	126.23
31	A	414	LHG	O7-C7-C8	4.31	120.80	111.50
33	C	518	DGD	O2G-C1B-C2B	4.30	120.78	111.50
24	B	512	CLA	O2A-C1-C2	4.30	119.95	108.64
28	A	411	LMG	O7-C10-C11	4.29	120.74	111.50
38	H	101	RRX	C16-C17-C18	-4.28	121.21	127.31
31	L	101	LHG	O7-C7-C8	4.27	120.71	111.50
28	C	522	LMG	O7-C10-C11	4.24	120.65	111.50
38	H	101	RRX	C4-C5-C6	-4.21	116.62	122.73
34	B	522	3PH	O21-C21-C22	4.21	120.57	111.50
35	B	523	DGA	OG2-CB1-CB2	4.18	120.51	111.50
38	H	101	RRX	C33-C5-C6	-4.18	119.84	124.53
26	J	101	BCR	C20-C21-C22	-4.17	121.36	127.31
28	H	102	LMG	O7-C10-C11	4.15	120.44	111.50
24	C	511	CLA	C1-C2-C3	-4.13	118.90	126.04
24	B	504	CLA	C1-C2-C3	-4.13	118.91	126.04
24	C	513	CLA	O2A-C1-C2	4.11	119.44	108.64
26	B	518	BCR	C24-C23-C22	-4.08	120.07	126.23
26	B	517	BCR	C4-C5-C6	-4.07	116.82	122.73
26	C	515	BCR	C27-C26-C25	-4.07	116.82	122.73
26	C	517	BCR	C24-C23-C22	-4.06	120.10	126.23
28	A	415	LMG	O7-C10-C11	4.06	120.24	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	405	BCR	C30-C25-C26	-4.05	116.91	122.61
33	C	519	DGD	O2G-C1B-C2B	4.04	120.20	111.50
24	D	401	CLA	C1-C2-C3	-4.00	119.13	126.04
31	D	408	LHG	O7-C7-C8	3.99	120.10	111.50
26	A	409	BCR	C11-C10-C9	3.99	133.00	127.31
28	C	521	LMG	O7-C10-C11	3.98	120.07	111.50
33	C	520	DGD	O2G-C1B-C2B	3.97	120.06	111.50
28	D	409	LMG	O7-C10-C11	3.96	120.03	111.50
24	B	502	CLA	O2A-C1-C2	3.96	119.03	108.64
33	B	521	DGD	O2G-C1B-C2B	3.91	119.93	111.50
31	D	407	LHG	O7-C7-C8	3.89	119.89	111.50
24	B	506	CLA	O2A-C1-C2	3.88	118.83	108.64
26	D	405	BCR	C33-C5-C6	-3.88	120.18	124.53
26	C	515	BCR	C7-C8-C9	-3.86	120.39	126.23
24	D	404	CLA	C1-C2-C3	-3.86	119.36	126.04
26	B	517	BCR	C16-C17-C18	-3.86	121.80	127.31
24	C	503	CLA	C1-C2-C3	-3.85	119.39	126.04
26	D	405	BCR	C27-C26-C25	-3.83	117.17	122.73
26	B	518	BCR	C4-C5-C6	-3.83	117.17	122.73
26	D	405	BCR	C15-C14-C13	-3.83	121.85	127.31
24	B	514	CLA	C1-C2-C3	-3.79	119.48	126.04
26	J	101	BCR	C1-C6-C5	-3.79	117.27	122.61
26	A	409	BCR	C12-C13-C14	3.78	124.75	118.94
35	B	523	DGA	CDB-CCB-CBB	-3.78	80.21	115.30
24	A	406	CLA	C1-C2-C3	-3.77	119.52	126.04
26	B	518	BCR	C11-C10-C9	-3.75	121.95	127.31
26	C	516	BCR	C7-C8-C9	-3.73	120.59	126.23
24	C	509	CLA	C1-C2-C3	-3.72	119.62	126.04
26	B	518	BCR	C1-C6-C5	-3.69	117.42	122.61
26	B	517	BCR	C30-C25-C26	-3.68	117.44	122.61
24	B	508	CLA	C1-C2-C3	-3.67	119.70	126.04
26	D	405	BCR	C38-C26-C25	-3.67	120.41	124.53
26	C	515	BCR	C1-C6-C5	-3.67	117.45	122.61
26	C	515	BCR	C15-C14-C13	-3.66	122.09	127.31
26	C	515	BCR	C38-C26-C25	-3.65	120.43	124.53
38	H	101	RRX	C38-C26-C25	-3.64	120.44	124.53
26	B	517	BCR	C27-C26-C25	-3.61	117.49	122.73
38	H	101	RRX	C30-C25-C26	-3.60	117.54	122.61
26	D	405	BCR	C1-C6-C5	-3.60	117.55	122.61
24	C	505	CLA	C1-C2-C3	-3.59	119.84	126.04
24	B	513	CLA	C1-C2-C3	-3.58	119.85	126.04
27	A	410	SQD	O7-S-C6	-3.58	102.69	106.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	515	BCR	C4-C5-C6	-3.57	117.55	122.73
26	C	517	BCR	C27-C26-C25	-3.57	117.56	122.73
26	B	517	BCR	C23-C24-C25	-3.56	117.20	127.20
26	A	409	BCR	C27-C26-C25	-3.55	117.58	122.73
26	C	516	BCR	C23-C24-C25	-3.53	117.29	127.20
26	C	515	BCR	C38-C26-C27	3.49	120.33	113.62
24	C	504	CLA	C1-C2-C3	-3.49	120.01	126.04
24	B	505	CLA	C1-C2-C3	-3.48	120.03	126.04
24	C	511	CLA	CHD-C1D-ND	-3.47	121.27	124.45
24	C	502	CLA	CHD-C1D-ND	-3.47	121.27	124.45
24	B	511	CLA	C1-C2-C3	-3.45	120.08	126.04
24	C	505	CLA	CHD-C1D-ND	-3.44	121.29	124.45
24	D	401	CLA	CHD-C1D-ND	-3.44	121.29	124.45
26	C	516	BCR	C27-C26-C25	-3.43	117.75	122.73
24	B	515	CLA	C1-C2-C3	-3.43	120.11	126.04
24	B	515	CLA	C2C-C1C-NC	3.40	113.16	109.97
24	B	502	CLA	CHD-C1D-ND	-3.40	121.33	124.45
24	B	516	CLA	C1-C2-C3	-3.36	120.24	126.04
24	C	512	CLA	C1-C2-C3	-3.36	120.24	126.04
24	C	512	CLA	CMA-C3A-C4A	3.35	120.77	111.77
24	B	513	CLA	CHD-C1D-ND	-3.34	121.38	124.45
24	C	510	CLA	CHD-C1D-ND	-3.34	121.39	124.45
26	C	515	BCR	C11-C10-C9	-3.33	122.55	127.31
24	B	506	CLA	CHD-C1D-ND	-3.33	121.40	124.45
24	B	516	CLA	C2C-C1C-NC	3.32	113.08	109.97
26	C	517	BCR	C4-C5-C6	-3.31	117.92	122.73
26	D	405	BCR	C4-C5-C6	-3.31	117.92	122.73
25	D	402	PHO	CMB-C2B-C3B	3.30	130.86	124.68
24	D	404	CLA	CHD-C1D-ND	-3.30	121.42	124.45
38	H	101	RRX	C29-C28-C27	3.30	114.81	110.30
24	D	403	CLA	C1-C2-C3	-3.30	120.34	126.04
26	C	515	BCR	C33-C5-C6	-3.29	120.83	124.53
24	B	516	CLA	CHD-C1D-ND	-3.29	121.43	124.45
26	D	405	BCR	C11-C10-C9	-3.28	122.62	127.31
24	C	506	CLA	C1-C2-C3	-3.28	120.37	126.04
24	C	510	CLA	C2C-C1C-NC	3.28	113.04	109.97
24	A	406	CLA	CHD-C1D-ND	-3.27	121.45	124.45
27	M	101	SQD	O7-S-C6	-3.27	103.06	106.94
24	C	508	CLA	C2C-C1C-NC	3.26	113.03	109.97
26	C	516	BCR	C20-C21-C22	-3.26	122.66	127.31
26	B	518	BCR	C8-C7-C6	-3.25	118.06	127.20
24	C	507	CLA	C2C-C1C-NC	3.25	113.02	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	516	BCR	C33-C5-C4	3.24	119.85	113.62
24	B	504	CLA	C2C-C1C-NC	3.24	113.01	109.97
24	A	408	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
24	C	502	CLA	C1-C2-C3	-3.24	120.44	126.04
26	C	517	BCR	C1-C6-C5	-3.24	118.05	122.61
36	D	406	PL9	C7-C3-C2	-3.23	119.05	123.30
24	A	408	CLA	C2C-C1C-NC	3.23	113.00	109.97
38	H	101	RRX	C8-C7-C6	-3.21	118.18	127.20
26	A	409	BCR	C4-C5-C6	-3.21	118.07	122.73
24	C	508	CLA	C1-C2-C3	-3.20	120.51	126.04
24	B	513	CLA	C2C-C1C-NC	3.20	112.97	109.97
24	B	501	CLA	C1-C2-C3	-3.19	120.53	126.04
24	C	513	CLA	C2C-C1C-NC	3.19	112.96	109.97
24	C	512	CLA	CHD-C1D-ND	-3.18	121.53	124.45
24	B	505	CLA	CHD-C1D-ND	-3.18	121.53	124.45
26	A	409	BCR	C23-C24-C25	-3.17	118.29	127.20
24	B	507	CLA	CHD-C1D-ND	-3.17	121.54	124.45
26	C	517	BCR	C15-C14-C13	-3.17	122.79	127.31
26	C	517	BCR	C30-C25-C26	-3.16	118.16	122.61
26	B	517	BCR	C38-C26-C27	3.16	119.69	113.62
24	B	514	CLA	CHD-C1D-ND	-3.15	121.56	124.45
24	C	514	CLA	CHD-C1D-ND	-3.15	121.56	124.45
26	D	405	BCR	C24-C23-C22	-3.15	121.47	126.23
26	D	405	BCR	C8-C7-C6	-3.15	118.36	127.20
26	D	405	BCR	C7-C8-C9	-3.15	121.48	126.23
26	C	517	BCR	C15-C16-C17	-3.12	117.08	123.47
24	B	511	CLA	CHD-C1D-ND	-3.12	121.59	124.45
24	D	403	CLA	CHD-C1D-ND	-3.11	121.59	124.45
24	B	510	CLA	C2C-C1C-NC	3.11	112.89	109.97
24	B	504	CLA	CMA-C3A-C4A	3.11	120.13	111.77
26	D	405	BCR	C33-C5-C4	3.10	119.58	113.62
24	C	504	CLA	CHD-C1D-ND	-3.10	121.60	124.45
26	A	409	BCR	C35-C13-C14	-3.09	118.60	122.92
24	C	512	CLA	C2C-C1C-NC	3.09	112.86	109.97
24	C	508	CLA	CHD-C1D-ND	-3.08	121.62	124.45
26	A	409	BCR	C16-C15-C14	-3.08	117.17	123.47
26	B	517	BCR	C15-C16-C17	-3.08	117.17	123.47
24	B	515	CLA	CHD-C1D-ND	-3.07	121.63	124.45
24	C	513	CLA	CHD-C1D-ND	-3.07	121.63	124.45
26	D	405	BCR	C23-C24-C25	-3.06	118.61	127.20
24	C	503	CLA	C2C-C1C-NC	3.05	112.83	109.97
36	D	406	PL9	C7-C8-C9	-3.05	121.71	126.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	510	CLA	CHD-C1D-ND	-3.04	121.66	124.45
24	B	509	CLA	C2D-C1D-ND	3.03	112.34	110.10
32	B	519	C7Z	C18-C5-C4	3.03	119.97	114.36
25	D	402	PHO	O1D-CGD-CBD	3.03	129.78	124.74
24	B	512	CLA	C2C-C1C-NC	3.03	112.81	109.97
24	D	401	CLA	C2C-C1C-NC	3.02	112.81	109.97
24	C	504	CLA	CMA-C3A-C4A	3.02	119.90	111.77
24	C	507	CLA	CHD-C1D-ND	-3.02	121.68	124.45
24	C	509	CLA	CMB-C2B-C3B	3.02	130.32	124.68
26	A	409	BCR	C1-C6-C5	-3.02	118.37	122.61
26	C	516	BCR	C8-C7-C6	-3.01	118.74	127.20
26	J	101	BCR	C38-C26-C27	3.00	119.39	113.62
24	C	511	CLA	C2C-C1C-NC	3.00	112.78	109.97
24	B	512	CLA	C1-C2-C3	-3.00	120.85	126.04
24	B	502	CLA	C2D-C1D-ND	2.99	112.31	110.10
24	B	510	CLA	C2D-C1D-ND	2.99	112.31	110.10
26	B	517	BCR	C1-C6-C5	-2.99	118.41	122.61
24	B	511	CLA	C2C-C1C-NC	2.99	112.77	109.97
33	C	519	DGD	C1D-O6D-C5D	2.98	119.54	113.69
28	A	411	LMG	C8-O7-C10	-2.98	110.45	117.79
24	B	514	CLA	C2C-C1C-NC	2.98	112.77	109.97
26	A	409	BCR	C38-C26-C25	-2.98	121.18	124.53
26	B	517	BCR	C21-C20-C19	-2.98	113.92	123.22
24	C	507	CLA	C1-C2-C3	-2.98	120.90	126.04
24	A	405	CLA	CHD-C1D-ND	-2.97	121.72	124.45
24	C	506	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
26	C	516	BCR	C21-C20-C19	-2.97	113.96	123.22
25	D	402	PHO	O2D-CGD-O1D	-2.97	118.04	123.84
24	B	509	CLA	C2C-C1C-NC	2.97	112.75	109.97
38	H	101	RRX	C23-C24-C25	-2.97	118.87	127.20
24	B	509	CLA	CHD-C1D-ND	-2.96	121.73	124.45
24	D	404	CLA	C2C-C1C-NC	2.96	112.75	109.97
24	B	510	CLA	C1-C2-C3	-2.96	120.93	126.04
24	C	503	CLA	C2D-C1D-ND	2.95	112.28	110.10
24	B	509	CLA	C1-C2-C3	-2.95	120.94	126.04
24	B	508	CLA	C2C-C1C-NC	2.95	112.73	109.97
24	B	507	CLA	C2C-C1C-NC	2.94	112.73	109.97
33	C	519	DGD	O1G-C1A-C2A	2.94	121.14	111.91
33	C	518	DGD	O1G-C1A-C2A	2.94	121.14	111.91
24	C	505	CLA	C2C-C1C-NC	2.94	112.73	109.97
24	B	502	CLA	C2C-C1C-NC	2.94	112.72	109.97
24	B	507	CLA	O2D-CGD-O1D	-2.93	118.11	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	509	CLA	C2C-C1C-NC	2.93	112.72	109.97
24	A	406	CLA	C2C-C1C-NC	2.93	112.72	109.97
24	C	509	CLA	CMB-C2B-C1B	-2.93	123.97	128.46
24	D	403	CLA	C2D-C1D-ND	2.93	112.26	110.10
31	D	410	LHG	O8-C23-C24	2.92	121.08	111.91
24	A	405	CLA	C2D-C1D-ND	2.92	112.26	110.10
24	B	510	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
26	C	517	BCR	C2-C1-C6	2.92	114.97	110.48
32	B	519	C7Z	C38-C25-C24	2.91	119.75	114.36
24	C	509	CLA	CHD-C1D-ND	-2.91	121.78	124.45
26	J	101	BCR	C29-C30-C25	2.91	114.96	110.48
24	C	514	CLA	C2C-C1C-NC	2.91	112.70	109.97
24	B	505	CLA	C2C-C1C-NC	2.91	112.70	109.97
24	B	505	CLA	C2D-C1D-ND	2.90	112.24	110.10
24	B	501	CLA	C2C-C1C-NC	2.90	112.69	109.97
24	C	504	CLA	C2D-C1D-ND	2.90	112.24	110.10
24	B	508	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
24	C	503	CLA	CHD-C1D-ND	-2.90	121.79	124.45
24	B	508	CLA	CMB-C2B-C3B	2.90	130.10	124.68
24	C	510	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	C	508	CLA	C1C-C2C-C3C	-2.90	103.91	106.96
24	B	513	CLA	C2D-C1D-ND	2.90	112.24	110.10
31	L	101	LHG	O8-C23-C24	2.90	121.00	111.91
24	B	506	CLA	C2C-C1C-NC	2.89	112.68	109.97
24	A	405	CLA	C1-C2-C3	-2.88	121.06	126.04
26	C	517	BCR	C33-C5-C4	2.88	119.15	113.62
32	B	519	C7Z	C8-C7-C6	-2.88	119.11	127.20
31	D	407	LHG	O8-C23-C24	2.88	120.95	111.91
24	B	512	CLA	CHD-C1D-ND	-2.88	121.81	124.45
25	A	407	PHO	CMB-C2B-C3B	2.88	130.06	124.68
24	B	512	CLA	C2D-C1D-ND	2.88	112.22	110.10
26	C	515	BCR	C30-C25-C26	-2.88	118.56	122.61
28	H	102	LMG	O8-C28-C29	2.88	120.93	111.91
24	B	502	CLA	O2A-CGA-CBA	2.87	120.91	111.91
24	B	511	CLA	C2D-C1D-ND	2.87	112.22	110.10
31	D	408	LHG	O8-C23-C24	2.87	120.91	111.91
24	C	511	CLA	C1C-C2C-C3C	-2.86	103.94	106.96
24	B	501	CLA	CMA-C3A-C4A	2.86	119.46	111.77
25	A	407	PHO	O2D-CGD-O1D	-2.86	118.25	123.84
24	D	401	CLA	O2A-CGA-CBA	2.86	120.88	111.91
26	D	405	BCR	C38-C26-C27	2.86	119.10	113.62
24	B	503	CLA	C1-C2-C3	-2.85	121.11	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	512	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
33	C	519	DGD	O6D-C5D-C6D	2.84	112.40	106.67
24	C	503	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
33	C	520	DGD	O1G-C1A-C2A	2.83	120.80	111.91
24	A	408	CLA	C2D-C1D-ND	2.83	112.19	110.10
24	B	513	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
38	H	101	RRX	C11-C12-C13	-2.82	118.48	126.42
24	B	501	CLA	C2D-C1D-ND	2.82	112.19	110.10
26	J	101	BCR	C30-C25-C26	-2.82	118.64	122.61
24	B	501	CLA	CHD-C1D-ND	-2.82	121.86	124.45
24	B	508	CLA	C2D-C1D-ND	2.82	112.18	110.10
26	A	409	BCR	C38-C26-C27	2.82	119.03	113.62
28	B	520	LMG	O8-C28-C29	2.81	120.74	111.91
24	A	408	CLA	CHD-C1D-ND	-2.81	121.87	124.45
24	C	513	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
24	C	506	CLA	C2D-C1D-ND	2.81	112.17	110.10
24	B	501	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
24	C	513	CLA	C2D-C1D-ND	2.81	112.17	110.10
24	D	404	CLA	O2D-CGD-O1D	-2.80	118.35	123.84
26	C	517	BCR	C33-C5-C6	-2.80	121.38	124.53
24	B	508	CLA	CHD-C1D-ND	-2.80	121.88	124.45
26	C	515	BCR	C33-C5-C4	2.80	118.99	113.62
24	B	503	CLA	C2C-C1C-NC	2.80	112.59	109.97
24	B	502	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
24	C	511	CLA	C2D-C1D-ND	2.79	112.16	110.10
24	B	503	CLA	CHD-C1D-ND	-2.79	121.89	124.45
24	D	404	CLA	C2D-C1D-ND	2.79	112.16	110.10
24	C	505	CLA	C2D-C1D-ND	2.78	112.15	110.10
24	C	505	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
24	A	408	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
24	B	515	CLA	C2D-C1D-ND	2.78	112.15	110.10
26	C	516	BCR	C15-C16-C17	-2.78	117.78	123.47
31	L	101	LHG	C5-O7-C7	-2.78	110.96	117.79
24	C	506	CLA	CHD-C1D-ND	-2.77	121.90	124.45
38	H	101	RRX	C35-C13-C14	-2.77	119.04	122.92
24	C	512	CLA	C2D-C1D-ND	2.77	112.15	110.10
24	C	506	CLA	C2C-C1C-NC	2.77	112.57	109.97
26	B	518	BCR	C33-C5-C4	2.77	118.93	113.62
24	B	505	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
24	C	514	CLA	C2D-C1D-ND	2.76	112.14	110.10
24	C	504	CLA	C2C-C1C-NC	2.76	112.56	109.97
38	H	101	RRX	C34-C9-C10	-2.76	119.06	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	517	BCR	C23-C24-C25	-2.76	119.46	127.20
24	B	514	CLA	C2D-C1D-ND	2.76	112.14	110.10
24	B	504	CLA	O2A-CGA-CBA	2.74	120.52	111.91
26	B	517	BCR	C20-C21-C22	-2.74	123.40	127.31
24	C	502	CLA	CMA-C3A-C4A	2.74	119.13	111.77
24	D	401	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
38	H	101	RRX	C7-C8-C9	-2.74	122.10	126.23
24	C	502	CLA	C2D-C1D-ND	2.73	112.12	110.10
31	A	414	LHG	C5-O7-C7	-2.73	111.08	117.79
26	B	518	BCR	C38-C26-C27	2.73	118.85	113.62
25	A	407	PHO	O1D-CGD-CBD	2.72	129.28	124.74
24	B	504	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
24	B	510	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
26	C	515	BCR	C16-C15-C14	-2.72	117.90	123.47
24	C	510	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
26	B	517	BCR	C8-C7-C6	-2.71	119.58	127.20
28	C	521	LMG	O8-C28-C29	2.71	120.41	111.91
24	B	501	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
36	D	406	PL9	C22-C23-C24	-2.71	121.14	127.66
24	D	403	CLA	O2A-CGA-CBA	2.71	120.40	111.91
24	B	508	CLA	CMA-C3A-C4A	2.70	119.03	111.77
24	B	504	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
24	D	403	CLA	C1D-ND-C4D	-2.70	104.42	106.33
24	C	507	CLA	C2D-C1D-ND	2.70	112.09	110.10
26	B	518	BCR	C23-C24-C25	-2.70	119.63	127.20
24	C	505	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
31	A	414	LHG	O8-C23-C24	2.69	120.35	111.91
24	A	408	CLA	CMB-C2B-C3B	2.69	129.71	124.68
24	A	406	CLA	C2D-C1D-ND	2.69	112.08	110.10
24	C	508	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
24	A	406	CLA	CMA-C3A-C4A	2.69	118.99	111.77
24	C	511	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
24	B	510	CLA	CMA-C3A-C4A	2.69	118.99	111.77
24	B	514	CLA	CMA-C3A-C4A	2.68	118.98	111.77
24	C	513	CLA	C1-C2-C3	-2.68	121.40	126.04
24	C	514	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
24	C	514	CLA	CMA-C3A-C4A	2.67	118.96	111.77
24	B	516	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
24	B	503	CLA	O2A-CGA-CBA	2.66	120.27	111.91
24	B	508	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
24	B	515	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
26	B	518	BCR	C27-C26-C25	-2.65	118.88	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	405	CLA	C2C-C1C-NC	2.65	112.46	109.97
24	A	408	CLA	CMA-C3A-C4A	2.65	118.91	111.77
24	B	507	CLA	C2D-C1D-ND	2.65	112.06	110.10
24	C	509	CLA	C2D-C1D-ND	2.65	112.06	110.10
24	B	508	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
24	C	514	CLA	CMB-C2B-C3B	2.65	129.64	124.68
24	A	406	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
24	C	507	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
24	D	404	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
33	C	520	DGD	O3G-C3G-C2G	-2.65	104.51	110.90
24	B	504	CLA	CHD-C1D-ND	-2.65	122.02	124.45
28	C	501	LMG	C7-O1-C1	-2.65	108.57	113.74
24	C	508	CLA	C2D-C1D-ND	2.64	112.05	110.10
24	C	502	CLA	C2C-C1C-NC	2.64	112.44	109.97
24	A	408	CLA	CAA-C2A-C3A	-2.64	105.56	112.78
24	A	408	CLA	C1-C2-C3	-2.64	121.48	126.04
24	B	503	CLA	CMB-C2B-C3B	2.63	129.61	124.68
24	C	510	CLA	CMB-C2B-C3B	2.63	129.61	124.68
26	J	101	BCR	C27-C26-C25	-2.63	118.91	122.73
24	C	512	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
24	D	401	CLA	CMB-C2B-C3B	2.63	129.59	124.68
24	B	514	CLA	C1-O2A-CGA	2.63	123.33	116.44
24	B	509	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
26	C	517	BCR	C21-C20-C19	-2.62	115.03	123.22
24	B	501	CLA	O2A-CGA-CBA	2.62	120.12	111.91
28	D	409	LMG	O8-C28-C29	2.62	120.12	111.91
24	B	512	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
26	B	518	BCR	C7-C8-C9	-2.61	122.29	126.23
24	C	513	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
32	B	519	C7Z	C28-C27-C26	-2.61	119.88	127.20
24	B	514	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
24	B	506	CLA	C2D-C1D-ND	2.60	112.02	110.10
24	B	505	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
26	B	517	BCR	C24-C23-C22	-2.60	122.31	126.23
26	A	409	BCR	C30-C25-C26	-2.59	118.96	122.61
24	B	504	CLA	CHA-C4D-ND	2.59	137.92	132.50
24	C	502	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
26	B	518	BCR	C15-C16-C17	-2.59	118.17	123.47
24	B	511	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
26	B	518	BCR	C29-C30-C25	2.59	114.46	110.48
24	B	503	CLA	CMA-C3A-C4A	2.58	118.72	111.77
24	C	503	CLA	CMA-C3A-C4A	2.58	118.72	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	513	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
35	B	523	DGA	OG1-CA1-CA2	2.58	120.00	111.91
24	B	506	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
34	B	522	3PH	O31-C31-C32	2.58	120.00	111.91
24	B	502	CLA	CMA-C3A-C4A	2.58	118.69	111.77
24	B	502	CLA	C1D-ND-C4D	-2.57	104.51	106.33
24	C	509	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
24	B	507	CLA	CHA-C4D-ND	2.57	137.87	132.50
24	C	503	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
24	B	507	CLA	C1-C2-C3	-2.56	121.61	126.04
26	D	405	BCR	C10-C11-C12	-2.56	115.22	123.22
24	C	514	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
24	B	503	CLA	CHA-C4D-ND	2.56	137.84	132.50
24	B	513	CLA	CMB-C2B-C3B	2.55	129.46	124.68
26	J	101	BCR	C4-C5-C6	-2.55	119.03	122.73
24	C	502	CLA	C1D-ND-C4D	-2.55	104.52	106.33
24	B	509	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
26	D	405	BCR	C16-C15-C14	-2.55	118.25	123.47
33	B	521	DGD	O1G-C1A-C2A	2.54	119.89	111.91
24	C	509	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
24	B	514	CLA	CMB-C2B-C3B	2.54	129.42	124.68
24	B	515	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
24	D	404	CLA	CMA-C3A-C4A	2.53	118.59	111.77
24	C	502	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
24	B	506	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
26	C	515	BCR	C8-C7-C6	-2.53	120.10	127.20
24	C	508	CLA	CMA-C3A-C4A	2.53	118.56	111.77
24	C	504	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
24	B	505	CLA	C1D-ND-C4D	-2.52	104.55	106.33
24	C	502	CLA	CMD-C2D-C3D	-2.52	121.83	127.61
38	H	101	RRX	C38-C26-C27	2.52	119.02	114.36
24	B	507	CLA	CMA-C3A-C4A	2.51	118.51	111.77
24	B	514	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
24	B	501	CLA	CHA-C4D-ND	2.50	137.73	132.50
32	B	519	C7Z	C15-C35-C34	-2.50	118.36	123.47
24	B	506	CLA	CHA-C4D-ND	2.49	137.72	132.50
24	D	403	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
24	C	506	CLA	CHA-C4D-ND	2.49	137.71	132.50
26	A	409	BCR	C29-C30-C25	2.49	114.31	110.48
24	B	507	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
26	J	101	BCR	C8-C7-C6	-2.49	120.22	127.20
32	B	519	C7Z	C4-C5-C6	-2.49	115.31	120.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	C1C-C2C-C3C	-2.48	104.34	106.96
26	A	409	BCR	C37-C22-C21	-2.48	119.44	122.92
36	D	406	PL9	C27-C28-C29	-2.48	121.69	127.66
24	D	401	CLA	C2D-C1D-ND	2.48	111.93	110.10
24	C	507	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
24	D	403	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
24	C	509	CLA	CHA-C4D-ND	2.48	137.68	132.50
24	A	408	CLA	C1D-ND-C4D	-2.48	104.58	106.33
24	C	505	CLA	CMB-C2B-C3B	2.47	129.31	124.68
24	C	512	CLA	CHA-C4D-ND	2.47	137.67	132.50
24	B	511	CLA	O2A-CGA-CBA	2.47	119.67	111.91
28	C	501	LMG	C8-O7-C10	-2.47	111.71	117.79
24	B	503	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
24	B	516	CLA	C2D-C1D-ND	2.46	111.92	110.10
24	C	511	CLA	O2A-CGA-CBA	2.46	119.64	111.91
24	C	511	CLA	CHA-C4D-ND	2.46	137.65	132.50
24	C	509	CLA	CMA-C3A-C4A	2.46	118.39	111.77
24	C	506	CLA	O2A-CGA-CBA	2.46	119.63	111.91
24	B	516	CLA	CHA-C4D-ND	2.46	137.64	132.50
24	C	508	CLA	CHA-C4D-ND	2.46	137.64	132.50
24	C	510	CLA	C2D-C1D-ND	2.46	111.92	110.10
24	D	403	CLA	CHA-C4D-ND	2.46	137.64	132.50
24	C	502	CLA	O2A-CGA-CBA	2.45	119.61	111.91
24	B	505	CLA	CHA-C4D-ND	2.45	137.63	132.50
24	C	504	CLA	CHA-C4D-ND	2.45	137.62	132.50
24	C	502	CLA	CHA-C4D-ND	2.45	137.61	132.50
24	C	505	CLA	CMA-C3A-C4A	2.44	118.34	111.77
24	C	506	CLA	CMA-C3A-C4A	2.44	118.33	111.77
28	A	411	LMG	O8-C28-C29	2.43	119.54	111.91
24	B	516	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
24	B	503	CLA	CMD-C2D-C3D	-2.43	122.02	127.61
24	B	506	CLA	CMA-C3A-C4A	2.43	118.30	111.77
24	B	514	CLA	CHA-C4D-ND	2.43	137.57	132.50
24	C	507	CLA	CHA-C4D-ND	2.43	137.57	132.50
26	B	518	BCR	C30-C25-C26	-2.42	119.20	122.61
24	B	511	CLA	CMB-C2B-C3B	2.42	129.21	124.68
24	C	504	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
24	D	403	CLA	C2C-C1C-NC	2.41	112.23	109.97
26	C	515	BCR	C23-C24-C25	-2.41	120.44	127.20
24	B	513	CLA	CHA-C4D-ND	2.41	137.53	132.50
39	J	102	LMU	C1B-O1B-C4'	-2.40	112.02	117.96
31	D	408	LHG	C5-O7-C7	-2.40	111.88	117.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	507	CLA	O2A-CGA-CBA	2.40	119.44	111.91
24	C	514	CLA	CHA-C4D-ND	2.40	137.52	132.50
24	B	503	CLA	C1C-C2C-C3C	-2.40	104.44	106.96
36	D	406	PL9	C20-C19-C21	2.39	119.29	115.27
24	A	405	CLA	CHA-C4D-ND	2.39	137.49	132.50
24	B	511	CLA	CMA-C3A-C4A	2.38	118.17	111.77
24	A	405	CLA	C1D-ND-C4D	-2.38	104.64	106.33
24	B	511	CLA	C1D-ND-C4D	-2.38	104.64	106.33
24	C	504	CLA	O2A-CGA-CBA	2.38	119.37	111.91
24	C	504	CLA	C1D-ND-C4D	-2.38	104.65	106.33
38	H	101	RRX	C20-C19-C18	-2.37	119.75	126.42
24	B	501	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
28	A	415	LMG	O8-C28-C29	2.37	119.35	111.91
24	D	404	CLA	CHA-C4D-ND	2.37	137.46	132.50
24	B	504	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
26	C	516	BCR	C30-C25-C26	-2.37	119.28	122.61
24	A	406	CLA	CHA-C4D-ND	2.37	137.46	132.50
24	D	401	CLA	CHA-C4D-ND	2.37	137.45	132.50
33	C	520	DGD	C2G-O2G-C1B	-2.37	111.97	117.79
24	B	510	CLA	CHA-C4D-ND	2.36	137.45	132.50
24	B	505	CLA	O2A-CGA-CBA	2.36	119.33	111.91
24	D	401	CLA	CMD-C2D-C3D	-2.36	122.18	127.61
24	C	505	CLA	CHA-C4D-ND	2.36	137.44	132.50
24	C	509	CLA	CAA-C2A-C3A	-2.36	106.31	112.78
24	A	405	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
24	C	503	CLA	CHA-C4D-ND	2.36	137.44	132.50
31	D	410	LHG	C5-O7-C7	-2.36	111.98	117.79
24	C	513	CLA	CHA-C4D-ND	2.36	137.43	132.50
26	J	101	BCR	C11-C12-C13	-2.36	119.80	126.42
24	B	502	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
24	B	515	CLA	CHA-C4D-ND	2.35	137.42	132.50
24	C	510	CLA	CHA-C4D-ND	2.35	137.41	132.50
24	A	406	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
25	D	402	PHO	C1-C2-C3	-2.35	121.99	126.04
24	C	512	CLA	CMB-C2B-C3B	2.34	129.05	124.68
24	B	512	CLA	CHA-C4D-ND	2.34	137.39	132.50
24	C	507	CLA	CMA-C3A-C4A	2.33	118.05	111.77
38	H	101	RRX	C15-C16-C17	-2.33	118.71	123.47
24	C	511	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
24	B	509	CLA	O2A-CGA-CBA	2.32	119.20	111.91
27	M	101	SQD	O3-C3-C2	-2.32	104.99	110.35
24	A	405	CLA	CMB-C2B-C3B	2.32	129.01	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	509	CLA	CHA-C4D-ND	2.32	137.34	132.50
24	A	405	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
24	B	506	CLA	CMD-C2D-C3D	-2.31	122.29	127.61
24	B	503	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
24	B	507	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
28	C	501	LMG	O8-C28-C29	2.31	119.16	111.91
24	B	511	CLA	CHA-C4D-ND	2.31	137.32	132.50
24	B	510	CLA	C1D-ND-C4D	-2.31	104.70	106.33
24	B	502	CLA	CHA-C4D-ND	2.30	137.32	132.50
37	E	101	HEM	CMC-C2C-C3C	2.30	128.99	124.68
24	B	511	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
24	C	512	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
24	B	507	CLA	CMB-C2B-C3B	2.30	128.98	124.68
24	D	401	CLA	CMA-C3A-C4A	2.30	117.95	111.77
24	C	512	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
24	B	505	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
24	C	504	CLA	CMB-C2B-C3B	2.29	128.97	124.68
27	A	410	SQD	O3-C3-C2	-2.29	105.06	110.35
24	B	503	CLA	CMB-C2B-C1B	-2.29	124.95	128.46
37	E	101	HEM	C4D-ND-C1D	2.29	107.44	105.07
37	E	101	HEM	CBA-CAA-C2A	-2.29	108.72	112.62
24	B	508	CLA	CHA-C4D-ND	2.28	137.28	132.50
26	C	517	BCR	C38-C26-C27	2.28	118.00	113.62
32	B	519	C7Z	C21-C26-C25	-2.28	119.40	122.61
24	B	508	CLA	C1D-ND-C4D	-2.28	104.72	106.33
24	A	408	CLA	O2A-CGA-CBA	2.27	119.04	111.91
24	A	406	CLA	CMB-C2B-C3B	2.27	128.92	124.68
24	A	406	CLA	C1D-ND-C4D	-2.27	104.72	106.33
28	C	521	LMG	C8-O7-C10	-2.27	112.21	117.79
24	B	516	CLA	O2A-CGA-CBA	2.27	119.02	111.91
24	C	509	CLA	O2A-CGA-CBA	2.26	119.01	111.91
24	B	507	CLA	O2A-CGA-CBA	2.26	119.00	111.91
26	J	101	BCR	C23-C24-C25	-2.26	120.86	127.20
24	D	403	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
24	C	510	CLA	O2A-CGA-CBA	2.25	118.98	111.91
24	B	511	CLA	CMB-C2B-C1B	-2.25	125.00	128.46
24	B	513	CLA	O2A-CGA-CBA	2.24	118.94	111.91
26	A	409	BCR	C1-C6-C7	2.24	122.12	115.78
24	B	512	CLA	O2A-CGA-CBA	2.24	118.93	111.91
36	D	406	PL9	O1-C4-C3	-2.24	118.26	120.72
26	A	409	BCR	C21-C20-C19	-2.23	116.25	123.22
24	C	514	CLA	C1D-ND-C4D	-2.23	104.75	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	401	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
24	A	408	CLA	CHA-C4D-ND	2.23	137.16	132.50
24	B	515	CLA	CMA-C3A-C4A	2.22	117.75	111.77
26	J	101	BCR	C33-C5-C4	2.22	117.89	113.62
24	B	512	CLA	CMA-C3A-C4A	2.22	117.74	111.77
37	E	101	HEM	C1B-NB-C4B	2.22	107.36	105.07
26	B	517	BCR	C35-C13-C14	-2.22	119.82	122.92
24	C	513	CLA	O2A-CGA-CBA	2.21	118.86	111.91
24	B	502	CLA	C1-C2-C3	-2.21	122.21	126.04
26	J	101	BCR	C16-C15-C14	-2.21	118.94	123.47
24	C	514	CLA	CMB-C2B-C1B	-2.21	125.06	128.46
24	B	512	CLA	CMB-C2B-C3B	2.21	128.82	124.68
24	B	504	CLA	CMB-C2B-C3B	2.21	128.81	124.68
26	A	409	BCR	C24-C23-C22	-2.21	122.90	126.23
24	C	512	CLA	O2A-CGA-CBA	2.21	118.83	111.91
24	D	401	CLA	C1D-ND-C4D	-2.20	104.77	106.33
24	C	503	CLA	C1-O2A-CGA	2.20	122.22	116.44
24	B	503	CLA	C2D-C1D-ND	2.20	111.72	110.10
24	B	506	CLA	O2A-CGA-CBA	2.20	118.81	111.91
24	C	509	CLA	CHA-C1A-NA	-2.20	121.36	126.40
24	C	510	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
24	D	401	CLA	C1-O2A-CGA	2.20	122.21	116.44
26	C	515	BCR	C20-C19-C18	-2.20	120.24	126.42
36	D	406	PL9	C37-C38-C39	-2.20	122.37	127.66
24	A	405	CLA	CMA-C3A-C4A	2.19	117.67	111.77
24	A	405	CLA	O2A-CGA-CBA	2.19	118.78	111.91
24	B	509	CLA	C1D-ND-C4D	-2.19	104.78	106.33
24	B	501	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
25	A	407	PHO	CMC-C2C-C3C	2.19	129.07	124.94
25	D	402	PHO	CMC-C2C-C3C	2.19	129.06	124.94
24	A	406	CLA	O2A-CGA-CBA	2.19	118.77	111.91
24	B	516	CLA	CHA-C1A-NA	-2.19	121.39	126.40
24	C	506	CLA	C1D-ND-C4D	-2.18	104.78	106.33
24	B	514	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
24	C	511	CLA	C1D-ND-C4D	-2.18	104.79	106.33
24	C	511	CLA	CMB-C2B-C3B	2.18	128.76	124.68
28	A	415	LMG	C8-O7-C10	-2.18	112.42	117.79
24	C	504	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
24	B	513	CLA	CMB-C2B-C1B	-2.18	125.12	128.46
24	C	507	CLA	CHA-C1A-NA	-2.18	121.41	126.40
24	B	514	CLA	C1D-ND-C4D	-2.18	104.79	106.33
26	A	409	BCR	C33-C5-C4	2.18	117.80	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	504	CLA	CHA-C1A-NA	-2.17	121.42	126.40
26	C	516	BCR	C11-C12-C13	-2.17	120.31	126.42
24	C	509	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
36	D	406	PL9	C12-C13-C14	-2.17	122.44	127.66
38	H	101	RRX	C33-C5-C4	2.17	117.78	113.62
24	C	510	CLA	CMA-C3A-C4A	2.17	117.59	111.77
24	C	510	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
24	D	401	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
32	B	519	C7Z	C11-C12-C13	-2.16	120.34	126.42
24	B	509	CLA	CMB-C2B-C3B	2.16	128.72	124.68
24	B	516	CLA	CMA-C3A-C4A	2.16	117.58	111.77
38	H	101	RRX	C8-C9-C10	2.16	122.26	118.94
24	C	514	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
24	B	506	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
24	B	515	CLA	CHA-C1A-NA	-2.16	121.45	126.40
25	D	402	PHO	O2A-CGA-O1A	-2.16	118.15	123.59
24	A	406	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
26	C	516	BCR	C37-C22-C23	2.15	121.47	118.08
24	D	401	CLA	C6-C5-C3	-2.15	107.81	113.45
24	A	408	CLA	CMB-C2B-C1B	-2.14	125.17	128.46
26	C	516	BCR	C1-C6-C7	2.14	121.84	115.78
26	B	517	BCR	C37-C22-C23	2.14	121.45	118.08
24	B	509	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
24	C	513	CLA	CMA-C3A-C4A	2.14	117.52	111.77
26	C	515	BCR	C36-C18-C17	-2.14	119.93	122.92
24	C	510	CLA	C1-C2-C3	-2.14	122.35	126.04
24	C	513	CLA	CHA-C1A-NA	-2.13	121.51	126.40
37	E	101	HEM	C4B-CHC-C1C	2.13	125.37	122.56
26	C	516	BCR	C24-C23-C22	-2.13	123.01	126.23
24	A	408	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
24	C	508	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
32	B	519	C7Z	C19-C9-C10	-2.13	119.94	122.92
24	C	505	CLA	O2A-CGA-CBA	2.12	118.57	111.91
24	C	503	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
24	B	502	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
26	B	518	BCR	C11-C12-C13	-2.12	120.47	126.42
24	C	508	CLA	CHA-C1A-NA	-2.12	121.55	126.40
24	B	514	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
24	C	502	CLA	O1D-CGD-CBD	-2.12	120.15	124.48
26	D	405	BCR	C20-C19-C18	-2.12	120.47	126.42
24	B	506	CLA	CMB-C2B-C3B	2.11	128.63	124.68
24	A	408	CLA	CMD-C2D-C3D	-2.11	122.75	127.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	507	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
24	C	503	CLA	C1D-ND-C4D	-2.11	104.84	106.33
38	H	101	RRX	C27-C26-C25	-2.11	116.16	120.85
28	C	522	LMG	C8-O7-C10	-2.10	112.61	117.79
24	B	508	CLA	C1-O2A-CGA	2.10	121.97	116.44
26	C	516	BCR	C16-C15-C14	-2.10	119.17	123.47
24	B	504	CLA	C2D-C1D-ND	2.10	111.65	110.10
24	C	512	CLA	C1D-ND-C4D	-2.10	104.84	106.33
24	A	405	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
24	C	503	CLA	CHA-C1A-NA	-2.10	121.59	126.40
24	C	505	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
31	D	407	LHG	C5-O7-C7	-2.10	112.63	117.79
24	B	513	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
24	C	506	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
24	A	406	CLA	CHA-C1A-NA	-2.09	121.61	126.40
26	C	515	BCR	C10-C11-C12	-2.09	116.69	123.22
31	D	410	LHG	O7-C7-O9	-2.09	118.65	123.70
24	B	501	CLA	C1D-ND-C4D	-2.09	104.85	106.33
26	B	517	BCR	C33-C5-C4	2.09	117.63	113.62
24	C	507	CLA	C1D-ND-C4D	-2.09	104.85	106.33
24	B	506	CLA	C1-O2A-CGA	2.09	121.92	116.44
24	C	513	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
24	A	406	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
24	C	512	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
24	B	507	CLA	C1-O2A-CGA	2.08	121.90	116.44
24	C	510	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
33	C	518	DGD	C2G-O2G-C1B	-2.08	112.68	117.79
24	D	404	CLA	O2A-CGA-CBA	2.07	118.42	111.91
28	A	411	LMG	O7-C10-O9	-2.07	118.70	123.70
24	C	505	CLA	C1D-ND-C4D	-2.07	104.87	106.33
24	B	512	CLA	C1D-ND-C4D	-2.07	104.87	106.33
24	C	504	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
31	L	101	LHG	O8-C23-O10	-2.06	118.39	123.59
26	A	409	BCR	C7-C6-C5	-2.06	116.47	121.46
24	B	510	CLA	O2A-CGA-CBA	2.06	118.37	111.91
36	D	406	PL9	C31-C32-C33	-2.06	105.11	111.88
24	B	509	CLA	CMA-C3A-C4A	2.06	117.30	111.77
24	B	505	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
36	D	406	PL9	O2-C1-C6	2.05	124.15	120.59
24	B	511	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
36	D	406	PL9	C40-C39-C41	2.05	118.72	115.27
25	A	407	PHO	C1-C2-C3	-2.05	122.50	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	E	101	HEM	C4C-CHD-C1D	2.05	125.26	122.56
37	E	101	HEM	CAD-CBD-CGD	-2.04	109.20	113.60
24	C	503	CLA	C6-C5-C3	-2.04	108.09	113.45
24	B	509	CLA	CHA-C1A-NA	-2.04	121.72	126.40
24	B	501	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
24	C	512	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
24	B	502	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
24	B	515	CLA	O2A-CGA-CBA	2.04	118.30	111.91
24	B	506	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
24	C	512	CLA	CHA-C1A-NA	-2.04	121.73	126.40
24	C	506	CLA	CMB-C2B-C3B	2.04	128.49	124.68
28	D	409	LMG	C8-O7-C10	-2.03	112.79	117.79
24	C	510	CLA	CHA-C1A-NA	-2.03	121.75	126.40
33	C	520	DGD	O1G-C1A-O1A	-2.03	118.47	123.59
24	B	508	CLA	O2A-CGA-CBA	2.03	118.27	111.91
24	D	404	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
26	C	516	BCR	C38-C26-C27	2.03	117.51	113.62
39	J	102	LMU	C1-O1'-C1'	-2.02	110.48	113.84
24	C	504	CLA	CHA-C1A-NA	-2.02	121.76	126.40
24	B	515	CLA	C1D-ND-C4D	-2.02	104.90	106.33
24	B	515	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
24	C	505	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
24	A	405	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
24	B	501	CLA	CHA-C1A-NA	-2.02	121.77	126.40
24	B	514	CLA	CHA-C1A-NA	-2.02	121.77	126.40
26	J	101	BCR	C37-C22-C21	-2.02	120.09	122.92
26	C	517	BCR	C37-C22-C21	-2.02	120.10	122.92
24	B	516	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
24	B	510	CLA	CHA-C1A-NA	-2.01	121.79	126.40
36	D	406	PL9	O2-C1-C2	-2.01	117.17	121.78
24	B	513	CLA	CHA-C1A-NA	-2.01	121.79	126.40
24	A	406	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
24	C	502	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
24	B	505	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
33	C	519	DGD	C3G-O3G-C1D	-2.01	109.81	113.74
24	A	408	CLA	C1-O2A-CGA	2.01	121.71	116.44
24	C	511	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
24	A	406	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
24	C	507	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
33	C	518	DGD	C3G-C2G-C1G	-2.00	107.05	111.79
24	A	405	CLA	CAC-C3C-C4C	2.00	127.41	124.81
24	B	507	CLA	C3D-C2D-C1D	-2.00	103.10	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	509	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
28	A	411	LMG	C9-C8-C7	-2.00	107.06	111.79

All (35) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	406	CLA	ND
24	A	408	CLA	ND
24	B	501	CLA	ND
24	B	502	CLA	ND
24	B	503	CLA	ND
24	B	504	CLA	ND
24	B	505	CLA	ND
24	B	506	CLA	ND
24	B	507	CLA	ND
24	B	508	CLA	ND
24	B	509	CLA	ND
24	B	510	CLA	ND
24	B	511	CLA	ND
24	B	512	CLA	ND
24	B	513	CLA	ND
24	B	514	CLA	ND
24	B	515	CLA	ND
24	B	516	CLA	ND
24	C	502	CLA	ND
24	C	503	CLA	ND
24	C	504	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	507	CLA	ND
24	C	508	CLA	ND
24	C	509	CLA	ND
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	C	514	CLA	ND
24	D	401	CLA	ND
24	D	403	CLA	ND
24	D	404	CLA	ND

All (974) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	405	CLA	C1A-C2A-CAA-CBA
24	A	405	CLA	C3A-C2A-CAA-CBA
24	A	406	CLA	C1A-C2A-CAA-CBA
24	A	406	CLA	CHA-CBD-CGD-O1D
24	A	406	CLA	CHA-CBD-CGD-O2D
24	A	408	CLA	C1A-C2A-CAA-CBA
24	A	408	CLA	CHA-CBD-CGD-O1D
24	A	408	CLA	CHA-CBD-CGD-O2D
24	A	408	CLA	C2-C3-C5-C6
24	A	408	CLA	C4-C3-C5-C6
24	B	501	CLA	C2-C1-O2A-CGA
24	B	501	CLA	CHA-CBD-CGD-O2D
24	B	502	CLA	CHA-CBD-CGD-O1D
24	B	502	CLA	CHA-CBD-CGD-O2D
24	B	503	CLA	CBD-CGD-O2D-CED
24	B	504	CLA	CHA-CBD-CGD-O1D
24	B	504	CLA	CHA-CBD-CGD-O2D
24	B	504	CLA	CAD-CBD-CGD-O1D
24	B	504	CLA	C6-C7-C8-C9
24	B	505	CLA	C4-C3-C5-C6
24	B	506	CLA	CHA-CBD-CGD-O1D
24	B	506	CLA	CHA-CBD-CGD-O2D
24	B	506	CLA	CBD-CGD-O2D-CED
24	B	507	CLA	C1A-C2A-CAA-CBA
24	B	507	CLA	C3A-C2A-CAA-CBA
24	B	507	CLA	CAD-CBD-CGD-O1D
24	B	507	CLA	CAD-CBD-CGD-O2D
24	B	508	CLA	C1A-C2A-CAA-CBA
24	B	508	CLA	C3A-C2A-CAA-CBA
24	B	508	CLA	CBD-CGD-O2D-CED
24	B	508	CLA	C2-C3-C5-C6
24	B	508	CLA	C4-C3-C5-C6
24	B	509	CLA	C1A-C2A-CAA-CBA
24	B	509	CLA	C3A-C2A-CAA-CBA
24	B	509	CLA	CHA-CBD-CGD-O1D
24	B	509	CLA	CBD-CGD-O2D-CED
24	B	509	CLA	C4-C3-C5-C6
24	B	510	CLA	CHA-CBD-CGD-O1D
24	B	510	CLA	CHA-CBD-CGD-O2D
24	B	511	CLA	CHA-CBD-CGD-O1D
24	B	511	CLA	CHA-CBD-CGD-O2D
24	B	511	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	B	512	CLA	C1A-C2A-CAA-CBA
24	B	512	CLA	C3A-C2A-CAA-CBA
24	B	512	CLA	C2-C1-O2A-CGA
24	B	514	CLA	C1A-C2A-CAA-CBA
24	B	514	CLA	C3A-C2A-CAA-CBA
24	B	514	CLA	CBD-CGD-O2D-CED
24	C	502	CLA	CBD-CGD-O2D-CED
24	C	502	CLA	C2-C3-C5-C6
24	C	502	CLA	C4-C3-C5-C6
24	C	503	CLA	CHA-CBD-CGD-O1D
24	C	503	CLA	CHA-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CBD-CGD-O2D-CED
24	C	505	CLA	CHA-CBD-CGD-O1D
24	C	505	CLA	CHA-CBD-CGD-O2D
24	C	506	CLA	CHA-CBD-CGD-O1D
24	C	506	CLA	CHA-CBD-CGD-O2D
24	C	506	CLA	CAD-CBD-CGD-O1D
24	C	506	CLA	CAD-CBD-CGD-O2D
24	C	507	CLA	C2-C1-O2A-CGA
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	507	CLA	CAD-CBD-CGD-O1D
24	C	507	CLA	CBD-CGD-O2D-CED
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	C2-C3-C5-C6
24	C	508	CLA	C4-C3-C5-C6
24	C	509	CLA	CBD-CGD-O2D-CED
24	C	510	CLA	CHA-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O2D
24	C	512	CLA	CHA-CBD-CGD-O1D
24	C	512	CLA	CHA-CBD-CGD-O2D
24	C	512	CLA	CBD-CGD-O2D-CED
24	C	513	CLA	C2-C1-O2A-CGA
24	C	514	CLA	C1A-C2A-CAA-CBA
24	C	514	CLA	C3A-C2A-CAA-CBA
24	C	514	CLA	C2A-CAA-CBA-CGA
24	C	514	CLA	CBD-CGD-O2D-CED
24	D	401	CLA	C1A-C2A-CAA-CBA
24	D	401	CLA	C3A-C2A-CAA-CBA
24	D	401	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	D	401	CLA	CHA-CBD-CGD-O2D
24	D	404	CLA	C1A-C2A-CAA-CBA
24	D	404	CLA	C3A-C2A-CAA-CBA
25	D	402	PHO	C3A-C2A-CAA-CBA
26	A	409	BCR	C5-C6-C7-C8
26	A	409	BCR	C11-C12-C13-C14
26	A	409	BCR	C11-C12-C13-C35
26	A	409	BCR	C17-C18-C19-C20
26	A	409	BCR	C36-C18-C19-C20
26	B	517	BCR	C11-C12-C13-C14
26	B	517	BCR	C11-C12-C13-C35
26	B	517	BCR	C17-C18-C19-C20
26	B	517	BCR	C36-C18-C19-C20
26	B	517	BCR	C21-C22-C23-C24
26	B	517	BCR	C37-C22-C23-C24
26	B	518	BCR	C7-C8-C9-C10
26	B	518	BCR	C7-C8-C9-C34
26	B	518	BCR	C9-C10-C11-C12
26	B	518	BCR	C17-C18-C19-C20
26	B	518	BCR	C36-C18-C19-C20
26	B	518	BCR	C19-C20-C21-C22
26	C	515	BCR	C7-C8-C9-C10
26	C	515	BCR	C7-C8-C9-C34
26	C	515	BCR	C11-C12-C13-C14
26	C	515	BCR	C11-C12-C13-C35
26	C	515	BCR	C17-C18-C19-C20
26	C	516	BCR	C17-C18-C19-C20
26	C	516	BCR	C36-C18-C19-C20
26	C	516	BCR	C19-C20-C21-C22
26	C	517	BCR	C7-C8-C9-C10
26	C	517	BCR	C7-C8-C9-C34
26	D	405	BCR	C19-C20-C21-C22
26	D	405	BCR	C23-C24-C25-C30
26	J	101	BCR	C11-C12-C13-C14
26	J	101	BCR	C11-C12-C13-C35
27	A	410	SQD	O5-C5-C6-S
27	M	101	SQD	O5-C1-O6-C44
28	A	411	LMG	C11-C10-O7-C8
28	B	520	LMG	O9-C10-O7-C8
28	B	520	LMG	C11-C10-O7-C8
28	C	521	LMG	O7-C8-C9-O8
31	A	414	LHG	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	A	414	LHG	C4-O6-P-O3
31	A	414	LHG	C4-O6-P-O4
31	A	414	LHG	C4-O6-P-O5
31	D	407	LHG	C1-C2-C3-O3
31	D	408	LHG	O1-C1-C2-O2
31	D	408	LHG	O1-C1-C2-C3
31	D	408	LHG	C1-C2-C3-O3
31	D	408	LHG	C4-O6-P-O5
31	D	410	LHG	C2-C3-O3-P
31	D	410	LHG	C3-O3-P-O4
31	L	101	LHG	O1-C1-C2-C3
31	L	101	LHG	C3-O3-P-O5
31	L	101	LHG	C3-O3-P-O6
31	L	101	LHG	C4-O6-P-O3
31	L	101	LHG	C4-O6-P-O4
31	L	101	LHG	C4-O6-P-O5
32	B	519	C7Z	C21-C26-C27-C28
32	B	519	C7Z	C7-C8-C9-C19
32	B	519	C7Z	C7-C8-C9-C10
32	B	519	C7Z	C11-C12-C13-C20
32	B	519	C7Z	C11-C12-C13-C14
32	B	519	C7Z	C31-C32-C33-C34
32	B	519	C7Z	C31-C32-C33-C40
33	B	521	DGD	O6E-C1E-O5D-C6D
33	C	520	DGD	O6D-C1D-O3G-C3G
34	B	522	3PH	C1-O11-P-O14
34	B	522	3PH	C2-C1-O11-P
34	B	522	3PH	C22-C21-O21-C2
35	B	523	DGA	CB2-CB1-OG2-CG2
35	B	523	DGA	OB1-CB1-OG2-CG2
36	D	406	PL9	C37-C38-C39-C41
38	H	101	RRX	C37-C22-C23-C24
38	H	101	RRX	C21-C22-C23-C24
24	A	405	CLA	O1D-CGD-O2D-CED
24	A	405	CLA	CBD-CGD-O2D-CED
24	A	408	CLA	CBD-CGD-O2D-CED
24	B	502	CLA	CBD-CGD-O2D-CED
24	B	505	CLA	CBD-CGD-O2D-CED
24	B	507	CLA	CBD-CGD-O2D-CED
24	B	513	CLA	CBD-CGD-O2D-CED
24	B	515	CLA	CBD-CGD-O2D-CED
24	B	516	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	C	503	CLA	CBD-CGD-O2D-CED
24	C	505	CLA	CBD-CGD-O2D-CED
24	C	511	CLA	CBD-CGD-O2D-CED
24	D	403	CLA	CBD-CGD-O2D-CED
24	B	510	CLA	O1A-CGA-O2A-C1
24	D	401	CLA	O1A-CGA-O2A-C1
28	A	411	LMG	O10-C28-O8-C9
24	B	505	CLA	O1D-CGD-O2D-CED
24	B	506	CLA	O1D-CGD-O2D-CED
24	B	513	CLA	O1D-CGD-O2D-CED
24	B	503	CLA	O1D-CGD-O2D-CED
24	B	508	CLA	O1D-CGD-O2D-CED
24	B	511	CLA	O1D-CGD-O2D-CED
24	C	504	CLA	O1D-CGD-O2D-CED
24	C	509	CLA	O1D-CGD-O2D-CED
24	C	512	CLA	O1D-CGD-O2D-CED
24	B	501	CLA	CBA-CGA-O2A-C1
24	B	510	CLA	CBA-CGA-O2A-C1
24	D	401	CLA	CBA-CGA-O2A-C1
28	A	411	LMG	C29-C28-O8-C9
24	B	501	CLA	CBD-CGD-O2D-CED
24	B	510	CLA	CBD-CGD-O2D-CED
24	B	512	CLA	CBD-CGD-O2D-CED
24	C	508	CLA	CBD-CGD-O2D-CED
24	D	404	CLA	CBD-CGD-O2D-CED
24	B	501	CLA	O1A-CGA-O2A-C1
24	C	506	CLA	O1A-CGA-O2A-C1
28	C	521	LMG	O10-C28-O8-C9
24	B	514	CLA	O1D-CGD-O2D-CED
24	C	507	CLA	O1D-CGD-O2D-CED
24	B	509	CLA	O1D-CGD-O2D-CED
24	C	502	CLA	O1D-CGD-O2D-CED
24	C	505	CLA	O1D-CGD-O2D-CED
24	C	514	CLA	O1D-CGD-O2D-CED
28	A	411	LMG	O9-C10-O7-C8
28	C	521	LMG	O9-C10-O7-C8
31	D	410	LHG	O9-C7-O7-C5
34	B	522	3PH	O22-C21-O21-C2
24	A	408	CLA	C3-C5-C6-C7
24	B	502	CLA	C3-C5-C6-C7
24	B	504	CLA	C3-C5-C6-C7
24	C	505	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	C	513	CLA	C3-C5-C6-C7
25	D	402	PHO	C3-C5-C6-C7
24	B	502	CLA	CBA-CGA-O2A-C1
33	C	518	DGD	C2A-C1A-O1G-C1G
34	B	522	3PH	C32-C31-O31-C3
31	D	410	LHG	C8-C7-O7-C5
24	B	502	CLA	O1D-CGD-O2D-CED
24	B	507	CLA	O1D-CGD-O2D-CED
24	B	503	CLA	C4-C3-C5-C6
24	B	503	CLA	C2-C3-C5-C6
24	B	505	CLA	C2-C3-C5-C6
24	B	509	CLA	C2-C3-C5-C6
24	C	513	CLA	CBD-CGD-O2D-CED
24	B	506	CLA	C2A-CAA-CBA-CGA
24	C	506	CLA	C2A-CAA-CBA-CGA
28	B	520	LMG	C17-C18-C19-C20
28	C	501	LMG	C17-C18-C19-C20
28	C	521	LMG	C35-C36-C37-C38
28	C	522	LMG	C17-C18-C19-C20
28	D	409	LMG	C17-C18-C19-C20
28	H	102	LMG	C35-C36-C37-C38
28	H	102	LMG	C38-C39-C40-C41
33	C	519	DGD	CBB-CCB-CDB-CEB
24	B	515	CLA	C3-C5-C6-C7
24	B	512	CLA	CBA-CGA-O2A-C1
24	C	506	CLA	CBA-CGA-O2A-C1
24	C	513	CLA	CBA-CGA-O2A-C1
28	B	520	LMG	C29-C28-O8-C9
28	C	521	LMG	C29-C28-O8-C9
31	D	410	LHG	C13-C14-C15-C16
24	B	515	CLA	O1D-CGD-O2D-CED
24	C	511	CLA	O1D-CGD-O2D-CED
24	D	403	CLA	O1D-CGD-O2D-CED
24	B	502	CLA	O1A-CGA-O2A-C1
33	C	518	DGD	O1A-C1A-O1G-C1G
31	D	407	LHG	C11-C12-C13-C14
24	C	503	CLA	O1D-CGD-O2D-CED
26	A	409	BCR	C19-C20-C21-C22
26	C	515	BCR	C13-C14-C15-C16
26	C	517	BCR	C13-C14-C15-C16
24	A	406	CLA	CBD-CGD-O2D-CED
24	C	506	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	A	414	LHG	O2-C2-C3-O3
24	C	510	CLA	CBA-CGA-O2A-C1
33	B	521	DGD	C2A-C1A-O1G-C1G
28	B	520	LMG	O10-C28-O8-C9
34	B	522	3PH	O32-C31-O31-C3
28	C	521	LMG	C11-C10-O7-C8
31	D	407	LHG	C28-C29-C30-C31
31	D	410	LHG	C11-C12-C13-C14
24	B	516	CLA	O1D-CGD-O2D-CED
24	C	513	CLA	O1A-CGA-O2A-C1
33	B	521	DGD	O1A-C1A-O1G-C1G
24	B	502	CLA	C4-C3-C5-C6
24	C	504	CLA	C4-C3-C5-C6
24	D	404	CLA	C4-C3-C5-C6
24	B	502	CLA	C2-C3-C5-C6
24	C	504	CLA	C2-C3-C5-C6
24	D	404	CLA	C2-C3-C5-C6
24	A	406	CLA	C2A-CAA-CBA-CGA
24	A	408	CLA	C2A-CAA-CBA-CGA
24	B	512	CLA	O1A-CGA-O2A-C1
36	D	406	PL9	C39-C41-C42-C43
24	C	507	CLA	CBA-CGA-O2A-C1
24	A	408	CLA	O1D-CGD-O2D-CED
27	M	101	SQD	C8-C7-O47-C45
24	B	512	CLA	O1D-CGD-O2D-CED
24	D	404	CLA	O1D-CGD-O2D-CED
24	B	510	CLA	O1D-CGD-O2D-CED
31	D	410	LHG	C1-C2-C3-O3
31	L	101	LHG	C1-C2-C3-O3
24	C	507	CLA	O1A-CGA-O2A-C1
24	C	510	CLA	O1A-CGA-O2A-C1
24	A	406	CLA	CBA-CGA-O2A-C1
24	B	507	CLA	CBA-CGA-O2A-C1
24	B	510	CLA	C13-C15-C16-C17
26	B	517	BCR	C9-C10-C11-C12
24	B	515	CLA	C5-C6-C7-C8
24	B	503	CLA	C15-C16-C17-C18
24	B	513	CLA	C5-C6-C7-C8
31	D	407	LHG	O2-C2-C3-O3
31	D	408	LHG	O2-C2-C3-O3
28	C	522	LMG	C2-C1-O1-C7
33	B	521	DGD	C2E-C1E-O5D-C6D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	A	406	CLA	C11-C12-C13-C14
24	B	503	CLA	C14-C13-C15-C16
24	B	510	CLA	C14-C13-C15-C16
24	B	511	CLA	C11-C12-C13-C14
24	B	515	CLA	C6-C7-C8-C9
24	C	502	CLA	C11-C10-C8-C9
24	C	512	CLA	C11-C10-C8-C9
25	A	407	PHO	C6-C7-C8-C9
24	B	501	CLA	O1D-CGD-O2D-CED
35	B	523	DGA	CBB-CAB-CB9-CB8
24	B	501	CLA	C8-C10-C11-C12
26	A	409	BCR	C37-C22-C23-C24
26	C	515	BCR	C36-C18-C19-C20
26	C	516	BCR	C7-C8-C9-C34
26	C	517	BCR	C36-C18-C19-C20
26	C	517	BCR	C37-C22-C23-C24
26	D	405	BCR	C37-C22-C23-C24
26	J	101	BCR	C37-C22-C23-C24
32	B	519	C7Z	C27-C28-C29-C39
38	H	101	RRX	C7-C8-C9-C34
26	A	409	BCR	C21-C22-C23-C24
26	C	516	BCR	C7-C8-C9-C10
26	C	517	BCR	C17-C18-C19-C20
26	D	405	BCR	C21-C22-C23-C24
26	J	101	BCR	C21-C22-C23-C24
32	B	519	C7Z	C27-C28-C29-C30
38	H	101	RRX	C7-C8-C9-C10
39	J	102	LMU	O5B-C5B-C6B-O6B
28	A	415	LMG	C11-C10-O7-C8
31	A	414	LHG	C23-C24-C25-C26
24	B	507	CLA	C15-C16-C17-C18
24	B	512	CLA	C15-C16-C17-C18
24	C	507	CLA	C15-C16-C17-C18
24	B	505	CLA	C15-C16-C17-C18
24	B	508	CLA	C15-C16-C17-C18
24	B	515	CLA	C15-C16-C17-C18
24	C	502	CLA	C10-C11-C12-C13
24	D	401	CLA	C15-C16-C17-C18
28	C	522	LMG	C10-C11-C12-C13
24	B	501	CLA	C10-C11-C12-C13
24	B	502	CLA	C13-C15-C16-C17
24	B	504	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	B	508	CLA	C13-C15-C16-C17
24	B	511	CLA	C13-C15-C16-C17
24	B	514	CLA	C13-C15-C16-C17
24	C	502	CLA	C8-C10-C11-C12
24	C	504	CLA	C15-C16-C17-C18
24	D	404	CLA	C10-C11-C12-C13
31	D	407	LHG	O1-C1-C2-O2
28	B	520	LMG	C10-C11-C12-C13
31	D	410	LHG	C7-C8-C9-C10
31	L	101	LHG	C7-C8-C9-C10
35	B	523	DGA	CA1-CA2-CA3-CA4
39	J	102	LMU	C4B-C5B-C6B-O6B
24	A	405	CLA	C15-C16-C17-C18
24	B	503	CLA	C5-C6-C7-C8
24	B	510	CLA	C15-C16-C17-C18
24	B	512	CLA	C13-C15-C16-C17
24	B	513	CLA	C10-C11-C12-C13
31	L	101	LHG	C11-C10-C9-C8
27	M	101	SQD	O49-C7-O47-C45
24	B	509	CLA	C2-C1-O2A-CGA
24	B	515	CLA	C2-C1-O2A-CGA
24	B	516	CLA	C2-C1-O2A-CGA
24	D	404	CLA	C2-C1-O2A-CGA
24	A	408	CLA	C8-C10-C11-C12
24	B	507	CLA	C5-C6-C7-C8
31	D	410	LHG	C23-C24-C25-C26
37	E	101	HEM	C3D-CAD-CBD-CGD
24	A	408	CLA	C11-C10-C8-C7
26	A	409	BCR	C13-C14-C15-C16
26	C	515	BCR	C15-C16-C17-C18
26	C	515	BCR	C19-C20-C21-C22
26	C	517	BCR	C15-C16-C17-C18
26	C	517	BCR	C19-C20-C21-C22
24	A	405	CLA	C2A-CAA-CBA-CGA
24	C	502	CLA	C2A-CAA-CBA-CGA
24	C	508	CLA	O1D-CGD-O2D-CED
24	A	408	CLA	C10-C11-C12-C13
24	B	511	CLA	C15-C16-C17-C18
24	A	406	CLA	O1A-CGA-O2A-C1
24	B	507	CLA	O1A-CGA-O2A-C1
24	B	508	CLA	C5-C6-C7-C8
28	D	409	LMG	C35-C36-C37-C38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	D	410	LHG	O2-C2-C3-O3
31	L	101	LHG	O2-C2-C3-O3
28	A	415	LMG	O9-C10-O7-C8
24	D	404	CLA	C8-C10-C11-C12
24	B	510	CLA	C5-C6-C7-C8
24	B	510	CLA	C10-C11-C12-C13
24	B	511	CLA	C8-C10-C11-C12
24	C	502	CLA	C15-C16-C17-C18
24	C	511	CLA	C15-C16-C17-C18
31	D	407	LHG	C3-O3-P-O6
31	D	408	LHG	C3-O3-P-O6
31	D	408	LHG	C4-O6-P-O3
31	D	410	LHG	C3-O3-P-O6
31	D	410	LHG	C4-O6-P-O3
31	L	101	LHG	C23-C24-C25-C26
24	C	511	CLA	CBA-CGA-O2A-C1
36	D	406	PL9	C37-C38-C39-C40
27	M	101	SQD	C7-C8-C9-C10
24	C	513	CLA	O1D-CGD-O2D-CED
31	A	414	LHG	C1-C2-C3-O3
33	C	519	DGD	C9B-CAB-CBB-CCB
24	B	509	CLA	C5-C6-C7-C8
24	C	502	CLA	C16-C17-C18-C20
33	C	519	DGD	C2A-C1A-O1G-C1G
24	C	509	CLA	C5-C6-C7-C8
24	C	511	CLA	C13-C15-C16-C17
26	A	409	BCR	C15-C16-C17-C18
28	B	520	LMG	C28-C29-C30-C31
31	L	101	LHG	C13-C14-C15-C16
24	D	404	CLA	C3-C5-C6-C7
31	L	101	LHG	C26-C27-C28-C29
33	C	520	DGD	C2A-C3A-C4A-C5A
24	B	513	CLA	CBA-CGA-O2A-C1
24	D	404	CLA	CBA-CGA-O2A-C1
34	B	522	3PH	C3-C2-O21-C21
35	B	523	DGA	CB1-CB2-CB3-CB4
35	B	523	DGA	CA6-CA7-CA8-CA9
39	J	102	LMU	C6-C7-C8-C9
31	A	414	LHG	O7-C5-C6-O8
34	B	522	3PH	C29-C2A-C2B-C2C
24	C	508	CLA	C8-C10-C11-C12
24	C	506	CLA	O1D-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	A	414	LHG	C28-C29-C30-C31
24	B	505	CLA	C11-C12-C13-C14
24	C	512	CLA	C6-C7-C8-C9
24	C	506	CLA	C5-C6-C7-C8
28	D	409	LMG	C13-C14-C15-C16
31	A	414	LHG	C25-C26-C27-C28
31	D	407	LHG	C13-C14-C15-C16
33	C	519	DGD	O1A-C1A-O1G-C1G
26	B	518	BCR	C11-C12-C13-C35
26	D	405	BCR	C36-C18-C19-C20
34	B	522	3PH	C39-C3A-C3B-C3C
31	D	407	LHG	O1-C1-C2-C3
31	D	410	LHG	O1-C1-C2-C3
26	B	518	BCR	C11-C12-C13-C14
26	D	405	BCR	C17-C18-C19-C20
24	B	507	CLA	C8-C10-C11-C12
31	D	408	LHG	C7-C8-C9-C10
31	D	410	LHG	C10-C11-C12-C13
35	B	523	DGA	CB3-CB4-CB5-CB6
35	B	523	DGA	CB5-CB6-CB7-CB8
24	B	516	CLA	C6-C7-C8-C9
24	B	516	CLA	C6-C7-C8-C10
33	C	518	DGD	C2G-C1G-O1G-C1A
27	M	101	SQD	C24-C25-C26-C27
31	L	101	LHG	C11-C12-C13-C14
24	B	516	CLA	C5-C6-C7-C8
24	C	511	CLA	O1A-CGA-O2A-C1
24	C	504	CLA	CBA-CGA-O2A-C1
33	C	520	DGD	C2A-C1A-O1G-C1G
28	H	102	LMG	C16-C17-C18-C19
31	A	414	LHG	C11-C10-C9-C8
24	A	406	CLA	O1D-CGD-O2D-CED
24	B	510	CLA	C3A-C2A-CAA-CBA
34	B	522	3PH	C2B-C2C-C2D-C2E
27	A	410	SQD	C11-C10-C9-C8
31	L	101	LHG	C34-C35-C36-C37
31	A	414	LHG	C31-C32-C33-C34
25	A	407	PHO	C2-C3-C5-C6
31	D	410	LHG	C14-C15-C16-C17
31	A	414	LHG	O1-C1-C2-O2
31	L	101	LHG	O1-C1-C2-O2
31	A	414	LHG	C26-C27-C28-C29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	D	408	LHG	C13-C14-C15-C16
35	B	523	DGA	CB9-CAB-CBB-CCB
24	B	513	CLA	O1A-CGA-O2A-C1
24	D	404	CLA	O1A-CGA-O2A-C1
33	C	520	DGD	O1A-C1A-O1G-C1G
28	C	501	LMG	O9-C10-O7-C8
24	A	405	CLA	C2-C1-O2A-CGA
24	A	408	CLA	C2-C1-O2A-CGA
24	B	507	CLA	C2-C1-O2A-CGA
24	B	513	CLA	C2-C1-O2A-CGA
24	B	514	CLA	C2-C1-O2A-CGA
24	C	503	CLA	C2-C1-O2A-CGA
24	C	508	CLA	C2-C1-O2A-CGA
24	C	510	CLA	C2-C1-O2A-CGA
24	D	401	CLA	C2-C1-O2A-CGA
28	B	520	LMG	C11-C12-C13-C14
24	C	512	CLA	C10-C11-C12-C13
34	B	522	3PH	C3A-C3B-C3C-C3D
31	D	408	LHG	C23-C24-C25-C26
24	B	516	CLA	C3-C5-C6-C7
26	A	409	BCR	C1-C6-C7-C8
26	B	517	BCR	C23-C24-C25-C26
26	B	518	BCR	C1-C6-C7-C8
26	B	518	BCR	C23-C24-C25-C26
26	C	516	BCR	C1-C6-C7-C8
26	J	101	BCR	C5-C6-C7-C8
26	J	101	BCR	C23-C24-C25-C26
32	B	519	C7Z	C1-C6-C7-C8
32	B	519	C7Z	C25-C26-C27-C28
28	D	409	LMG	C12-C13-C14-C15
24	B	505	CLA	CBA-CGA-O2A-C1
24	A	405	CLA	C13-C15-C16-C17
24	B	513	CLA	C13-C15-C16-C17
24	C	509	CLA	C13-C15-C16-C17
28	C	501	LMG	C11-C10-O7-C8
31	A	414	LHG	C24-C25-C26-C27
31	D	408	LHG	C28-C29-C30-C31
31	D	408	LHG	C33-C34-C35-C36
24	C	504	CLA	O1A-CGA-O2A-C1
31	L	101	LHG	C33-C34-C35-C36
24	B	503	CLA	C8-C10-C11-C12
24	B	510	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	B	504	CLA	C4-C3-C5-C6
25	A	407	PHO	C4-C3-C5-C6
24	A	405	CLA	C11-C12-C13-C15
24	B	503	CLA	C6-C7-C8-C10
24	B	505	CLA	C11-C12-C13-C15
24	B	515	CLA	C6-C7-C8-C10
24	C	502	CLA	C11-C10-C8-C7
24	C	512	CLA	C6-C7-C8-C10
25	A	407	PHO	C11-C10-C8-C7
24	C	508	CLA	C13-C15-C16-C17
24	D	401	CLA	C8-C10-C11-C12
34	B	522	3PH	C31-C32-C33-C34
24	B	516	CLA	CBA-CGA-O2A-C1
24	B	512	CLA	C10-C11-C12-C13
24	C	508	CLA	C15-C16-C17-C18
33	B	521	DGD	C3A-C4A-C5A-C6A
31	D	408	LHG	C9-C10-C11-C12
31	D	408	LHG	C34-C35-C36-C37
33	C	519	DGD	CCB-CDB-CEB-CFB
24	B	509	CLA	C8-C10-C11-C12
24	C	503	CLA	C8-C10-C11-C12
31	D	408	LHG	C11-C12-C13-C14
24	C	508	CLA	C5-C6-C7-C8
28	H	102	LMG	C33-C34-C35-C36
24	B	501	CLA	C13-C15-C16-C17
27	M	101	SQD	C2-C1-O6-C44
24	B	505	CLA	C8-C10-C11-C12
27	A	410	SQD	C28-C29-C30-C31
24	A	405	CLA	C11-C12-C13-C14
24	A	408	CLA	C11-C10-C8-C9
24	B	503	CLA	C6-C7-C8-C9
24	B	513	CLA	C11-C12-C13-C14
24	C	502	CLA	C6-C7-C8-C9
24	C	509	CLA	C11-C12-C13-C14
24	C	511	CLA	C6-C7-C8-C9
24	C	511	CLA	C11-C10-C8-C9
24	D	401	CLA	C14-C13-C15-C16
25	A	407	PHO	C11-C10-C8-C9
33	B	521	DGD	C2A-C3A-C4A-C5A
24	C	507	CLA	C3-C5-C6-C7
24	B	502	CLA	C2A-CAA-CBA-CGA
24	D	404	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	B	505	CLA	O1A-CGA-O2A-C1
24	B	504	CLA	C1A-C2A-CAA-CBA
24	B	510	CLA	C1A-C2A-CAA-CBA
24	C	502	CLA	C1A-C2A-CAA-CBA
24	C	504	CLA	C1A-C2A-CAA-CBA
24	C	502	CLA	C16-C17-C18-C19
31	D	407	LHG	C27-C28-C29-C30
24	B	503	CLA	C13-C15-C16-C17
33	C	519	DGD	C3A-C4A-C5A-C6A
24	B	504	CLA	C10-C11-C12-C13
31	D	407	LHG	C7-C8-C9-C10
31	L	101	LHG	C31-C32-C33-C34
34	B	522	3PH	C27-C28-C29-C2A
35	B	523	DGA	CAB-CBB-CCB-CDB
31	A	414	LHG	C33-C34-C35-C36
35	B	523	DGA	CA2-CA3-CA4-CA5
24	C	504	CLA	C8-C10-C11-C12
24	C	509	CLA	C8-C10-C11-C12
31	D	407	LHG	C4-C5-C6-O8
33	C	520	DGD	O6E-C5E-C6E-O5E
24	D	401	CLA	C13-C15-C16-C17
28	A	415	LMG	C8-C7-O1-C1
33	C	519	DGD	C5D-C6D-O5D-C1E
31	D	408	LHG	C11-C10-C9-C8
24	B	516	CLA	O1A-CGA-O2A-C1
28	C	522	LMG	O6-C1-O1-C7
27	A	410	SQD	C24-C25-C26-C27
28	D	409	LMG	O6-C5-C6-O5
33	C	519	DGD	O6D-C5D-C6D-O5D
36	D	406	PL9	C40-C39-C41-C42
24	C	505	CLA	CBA-CGA-O2A-C1
24	C	512	CLA	CBA-CGA-O2A-C1
24	B	502	CLA	C15-C16-C17-C18
24	B	507	CLA	C13-C15-C16-C17
31	D	410	LHG	C17-C18-C19-C20
27	M	101	SQD	C46-C45-O47-C7
33	C	518	DGD	O6E-C5E-C6E-O5E
24	B	503	CLA	C2A-CAA-CBA-CGA
24	B	507	CLA	C2A-CAA-CBA-CGA
24	B	514	CLA	C15-C16-C17-C18
31	A	414	LHG	C34-C35-C36-C37
24	C	502	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	A	405	CLA	C16-C17-C18-C19
24	C	502	CLA	O1A-CGA-O2A-C1
31	D	410	LHG	C11-C10-C9-C8
24	B	501	CLA	C5-C6-C7-C8
33	B	521	DGD	C2D-C1D-O3G-C3G
33	C	520	DGD	C2D-C1D-O3G-C3G
31	D	410	LHG	C18-C19-C20-C21
33	C	519	DGD	O1G-C1G-C2G-O2G
24	A	406	CLA	C11-C10-C8-C7
24	B	503	CLA	C11-C12-C13-C15
24	B	504	CLA	C2-C3-C5-C6
24	B	504	CLA	C6-C7-C8-C10
24	B	504	CLA	C11-C10-C8-C7
24	B	513	CLA	C11-C10-C8-C7
24	B	513	CLA	C11-C12-C13-C15
24	C	502	CLA	C6-C7-C8-C10
24	C	509	CLA	C11-C12-C13-C15
24	C	511	CLA	C6-C7-C8-C10
24	C	511	CLA	C11-C10-C8-C7
24	C	511	CLA	C12-C13-C15-C16
24	C	512	CLA	C11-C10-C8-C7
24	D	401	CLA	C12-C13-C15-C16
24	D	403	CLA	C11-C12-C13-C15
25	A	407	PHO	C3-C5-C6-C7
24	B	507	CLA	C14-C13-C15-C16
24	B	513	CLA	C11-C10-C8-C9
24	B	514	CLA	C6-C7-C8-C9
24	C	511	CLA	C14-C13-C15-C16
24	D	403	CLA	C11-C12-C13-C14
31	D	407	LHG	C23-C24-C25-C26
24	B	515	CLA	C8-C10-C11-C12
26	B	517	BCR	C7-C8-C9-C34
26	B	518	BCR	C37-C22-C23-C24
26	B	517	BCR	C7-C8-C9-C10
26	B	518	BCR	C21-C22-C23-C24
26	C	517	BCR	C21-C22-C23-C24
26	J	101	BCR	C7-C8-C9-C10
31	A	414	LHG	C30-C31-C32-C33
34	B	522	3PH	C25-C26-C27-C28
24	B	507	CLA	C16-C17-C18-C20
24	C	512	CLA	C3-C5-C6-C7
24	B	515	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	C	510	CLA	C13-C15-C16-C17
24	C	505	CLA	O1A-CGA-O2A-C1
24	B	503	CLA	CBA-CGA-O2A-C1
24	B	514	CLA	CAA-CBA-CGA-O2A
24	C	507	CLA	C3A-C2A-CAA-CBA
26	C	516	BCR	C9-C10-C11-C12
24	B	511	CLA	C5-C6-C7-C8
31	A	414	LHG	C24-C23-O8-C6
28	A	411	LMG	O1-C7-C8-C9
28	C	521	LMG	C7-C8-C9-O8
28	H	102	LMG	C7-C8-C9-O8
31	A	414	LHG	C4-C5-C6-O8
31	D	408	LHG	C4-C5-C6-O8
33	B	521	DGD	C1G-C2G-C3G-O3G
35	B	523	DGA	OG1-CG1-CG2-CG3
24	C	512	CLA	O1A-CGA-O2A-C1
33	C	520	DGD	O6D-C5D-C6D-O5D
24	B	504	CLA	C5-C6-C7-C8
31	D	410	LHG	O6-C4-C5-O7
24	B	511	CLA	CBA-CGA-O2A-C1
24	B	515	CLA	CBA-CGA-O2A-C1
35	B	523	DGA	CBB-CCB-CDB-CEB
28	A	411	LMG	O1-C7-C8-O7
28	H	102	LMG	O7-C8-C9-O8
31	D	407	LHG	C35-C36-C37-C38
34	B	522	3PH	C24-C25-C26-C27
35	B	523	DGA	CG1-CG2-CG3-OXT
24	B	503	CLA	C2-C1-O2A-CGA
25	A	407	PHO	C13-C15-C16-C17
24	B	515	CLA	C11-C12-C13-C14
24	C	503	CLA	C14-C13-C15-C16
28	C	522	LMG	C15-C16-C17-C18
31	D	408	LHG	C19-C20-C21-C22
25	D	402	PHO	C2A-CAA-CBA-CGA
24	B	514	CLA	C3-C5-C6-C7
26	C	515	BCR	C23-C24-C25-C30
26	C	516	BCR	C5-C6-C7-C8
26	D	405	BCR	C5-C6-C7-C8
25	A	407	PHO	C10-C11-C12-C13
31	D	408	LHG	C25-C26-C27-C28
33	C	519	DGD	C6B-C7B-C8B-C9B
35	B	523	DGA	CB7-CB8-CB9-CAB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	A	405	CLA	C8-C10-C11-C12
39	J	102	LMU	C9-C10-C11-C12
24	A	405	CLA	C16-C17-C18-C20
24	C	504	CLA	C16-C17-C18-C19
31	A	414	LHG	O6-C4-C5-C6
31	D	407	LHG	O6-C4-C5-C6
24	B	507	CLA	C12-C13-C15-C16
24	B	508	CLA	C6-C7-C8-C10
24	B	508	CLA	C11-C12-C13-C15
24	B	514	CLA	C6-C7-C8-C10
24	B	515	CLA	C11-C12-C13-C15
24	C	503	CLA	C12-C13-C15-C16
35	B	523	DGA	OG2-CG2-CG3-OXT
32	B	519	C7Z	C9-C10-C11-C12
34	B	522	3PH	C1-O11-P-O13
24	B	513	CLA	C3-C5-C6-C7
24	B	507	CLA	C16-C17-C18-C19
28	H	102	LMG	C36-C37-C38-C39
33	C	518	DGD	C1B-C2B-C3B-C4B
24	B	514	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	C	507	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
35	B	523	DGA	CG1-CG2-OG2-CB1
24	C	508	CLA	C16-C17-C18-C19
28	H	102	LMG	C32-C33-C34-C35
31	D	407	LHG	C31-C32-C33-C34
28	A	415	LMG	O6-C1-O1-C7
31	D	407	LHG	C34-C35-C36-C37
31	A	414	LHG	O6-C4-C5-O7
31	D	407	LHG	O6-C4-C5-O7
31	L	101	LHG	O6-C4-C5-O7
34	B	522	3PH	C32-C33-C34-C35
24	B	501	CLA	CHA-CBD-CGD-O1D
24	B	505	CLA	CHA-CBD-CGD-O1D
24	B	509	CLA	CHA-CBD-CGD-O2D
24	B	512	CLA	CHA-CBD-CGD-O1D
24	B	512	CLA	CHA-CBD-CGD-O2D
24	B	513	CLA	CHA-CBD-CGD-O1D
34	B	522	3PH	C2A-C2B-C2C-C2D
24	B	503	CLA	O1A-CGA-O2A-C1
31	D	407	LHG	O7-C5-C6-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	L	101	LHG	O7-C5-C6-O8
24	B	515	CLA	O1A-CGA-O2A-C1
31	L	101	LHG	C10-C11-C12-C13
24	C	503	CLA	C3-C5-C6-C7
24	B	511	CLA	O1A-CGA-O2A-C1
31	A	414	LHG	O10-C23-O8-C6
33	B	521	DGD	O1B-C1B-O2G-C2G
33	C	520	DGD	O1B-C1B-O2G-C2G
24	B	501	CLA	C11-C12-C13-C14
24	B	508	CLA	C11-C12-C13-C14
24	C	507	CLA	C11-C12-C13-C14
24	D	401	CLA	C2A-CAA-CBA-CGA
26	C	515	BCR	C37-C22-C23-C24
26	J	101	BCR	C7-C8-C9-C34
26	C	515	BCR	C21-C22-C23-C24
24	C	507	CLA	C1A-C2A-CAA-CBA
24	B	503	CLA	C16-C17-C18-C19
24	C	512	CLA	C2-C1-O2A-CGA
26	D	405	BCR	C9-C10-C11-C12
31	D	407	LHG	C4-O6-P-O3
31	A	414	LHG	C2-C3-O3-P
31	D	407	LHG	C3-O3-P-O5
31	D	408	LHG	C3-O3-P-O5
31	D	408	LHG	C4-O6-P-O4
31	D	410	LHG	C4-O6-P-O5
24	C	510	CLA	C8-C10-C11-C12
24	B	509	CLA	CBA-CGA-O2A-C1
31	D	410	LHG	O6-C4-C5-C6
31	L	101	LHG	O6-C4-C5-C6
24	B	505	CLA	CAD-CBD-CGD-O1D
24	B	509	CLA	CAD-CBD-CGD-O1D
24	B	512	CLA	CAD-CBD-CGD-O1D
24	C	505	CLA	CAD-CBD-CGD-O1D
27	M	101	SQD	C5-C6-S-O9
24	B	502	CLA	CAA-CBA-CGA-O2A
28	H	102	LMG	O7-C10-C11-C12
24	D	401	CLA	C3-C5-C6-C7
24	C	504	CLA	C16-C17-C18-C20
24	B	503	CLA	C12-C13-C15-C16
24	B	507	CLA	C6-C7-C8-C10
24	B	510	CLA	C12-C13-C15-C16
24	B	515	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	D	401	CLA	C11-C12-C13-C15
33	B	521	DGD	C1A-C2A-C3A-C4A
33	B	521	DGD	C2B-C1B-O2G-C2G
31	L	101	LHG	O8-C23-C24-C25
35	B	523	DGA	CB2-CB3-CB4-CB5
31	D	408	LHG	O7-C5-C6-O8
33	B	521	DGD	O2G-C2G-C3G-O3G
35	B	523	DGA	OG1-CG1-CG2-OG2
33	B	521	DGD	C2G-C3G-O3G-C1D
24	B	509	CLA	O1A-CGA-O2A-C1
28	C	501	LMG	C29-C28-O8-C9
24	A	406	CLA	C11-C10-C8-C9
24	B	504	CLA	C11-C10-C8-C9
24	B	508	CLA	C6-C7-C8-C9
24	B	514	CLA	C14-C13-C15-C16
24	D	403	CLA	C14-C13-C15-C16
28	C	501	LMG	O10-C28-O8-C9
24	B	510	CLA	C16-C17-C18-C19
35	B	523	DGA	CB6-CB7-CB8-CB9
28	A	411	LMG	C28-C29-C30-C31
24	B	516	CLA	CAA-CBA-CGA-O2A
24	C	509	CLA	C3-C5-C6-C7
24	C	507	CLA	C16-C17-C18-C20
31	L	101	LHG	C28-C29-C30-C31
24	B	505	CLA	C16-C17-C18-C20
28	D	409	LMG	C31-C32-C33-C34
24	B	514	CLA	C10-C11-C12-C13
28	B	520	LMG	C9-C8-O7-C10
24	B	510	CLA	C2-C1-O2A-CGA
24	B	511	CLA	C2-C1-O2A-CGA
27	M	101	SQD	C23-C24-C25-C26
24	A	405	CLA	CAA-CBA-CGA-O2A
28	D	409	LMG	C10-C11-C12-C13
34	B	522	3PH	C1-O11-P-O12
24	C	509	CLA	CBA-CGA-O2A-C1
31	D	410	LHG	C9-C10-C11-C12
31	D	407	LHG	C26-C27-C28-C29
24	C	503	CLA	C16-C17-C18-C20
33	C	519	DGD	C2D-C1D-O3G-C3G
39	J	102	LMU	C1-C2-C3-C4
24	B	511	CLA	C10-C11-C12-C13
31	D	407	LHG	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	A	414	LHG	C3-O3-P-O6
25	D	402	PHO	CHA-CBD-CGD-O2D
33	C	519	DGD	O1G-C1G-C2G-C3G
33	C	519	DGD	C4D-C5D-C6D-O5D
24	B	501	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C12-C13-C15
24	B	503	CLA	C11-C12-C13-C14
24	D	401	CLA	C11-C12-C13-C14
33	C	520	DGD	C2B-C1B-O2G-C2G
24	A	406	CLA	C10-C11-C12-C13
24	B	503	CLA	C3-C5-C6-C7
31	D	410	LHG	C25-C26-C27-C28
34	B	522	3PH	C28-C29-C2A-C2B
31	D	410	LHG	O1-C1-C2-O2
35	B	523	DGA	CA5-CA6-CA7-CA8
39	J	102	LMU	C5-C6-C7-C8
24	C	509	CLA	O1A-CGA-O2A-C1
26	J	101	BCR	C9-C10-C11-C12
26	J	101	BCR	C15-C16-C17-C18
38	H	101	RRX	C15-C16-C17-C18
27	M	101	SQD	C25-C26-C27-C28
24	D	401	CLA	C16-C17-C18-C19
24	B	513	CLA	C4-C3-C5-C6
36	D	406	PL9	C30-C29-C31-C32
36	D	406	PL9	C13-C14-C16-C17
28	C	522	LMG	O9-C10-O7-C8
31	L	101	LHG	C9-C10-C11-C12
24	C	509	CLA	C10-C11-C12-C13
35	B	523	DGA	CA9-CAA-CBA-CCA
24	B	507	CLA	C6-C7-C8-C9
24	C	507	CLA	C11-C10-C8-C9
24	C	510	CLA	C11-C10-C8-C9
24	B	510	CLA	C16-C17-C18-C20
26	A	409	BCR	C11-C10-C9-C34
31	L	101	LHG	C4-C5-C6-O8
24	B	511	CLA	C16-C17-C18-C19
24	C	507	CLA	C16-C17-C18-C19
31	L	101	LHG	C24-C25-C26-C27
24	B	503	CLA	C1A-C2A-CAA-CBA
24	B	506	CLA	C6-C7-C8-C10
25	A	407	PHO	C6-C7-C8-C10
25	D	402	PHO	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	B	504	CLA	O1A-CGA-O2A-C1
27	M	101	SQD	O47-C7-C8-C9
24	C	503	CLA	C13-C15-C16-C17
24	D	401	CLA	C5-C6-C7-C8
34	B	522	3PH	C2C-C2D-C2E-C2F
24	B	514	CLA	C16-C17-C18-C20
26	A	409	BCR	C11-C10-C9-C8
28	H	102	LMG	C30-C31-C32-C33
24	C	503	CLA	C16-C17-C18-C19
28	D	409	LMG	C11-C12-C13-C14
36	D	406	PL9	C38-C39-C41-C42
31	L	101	LHG	C35-C36-C37-C38
24	C	502	CLA	C11-C12-C13-C14
24	B	501	CLA	C3-C5-C6-C7
31	L	101	LHG	C2-C3-O3-P
24	D	403	CLA	CAA-CBA-CGA-O2A
31	L	101	LHG	C30-C31-C32-C33
26	C	517	BCR	C23-C24-C25-C30
26	J	101	BCR	C13-C14-C15-C16
24	C	511	CLA	C2-C3-C5-C6
24	B	504	CLA	CBA-CGA-O2A-C1
31	D	407	LHG	C12-C13-C14-C15
26	C	515	BCR	C9-C10-C11-C12
24	B	514	CLA	CAA-CBA-CGA-O1A
24	D	403	CLA	C15-C16-C17-C18
24	A	408	CLA	C11-C12-C13-C15
24	C	514	CLA	CAA-CBA-CGA-O2A
24	C	503	CLA	C4-C3-C5-C6
28	C	501	LMG	C31-C32-C33-C34
34	B	522	3PH	O21-C21-C22-C23
24	B	501	CLA	C14-C13-C15-C16
24	B	502	CLA	C14-C13-C15-C16
24	B	505	CLA	C11-C10-C8-C9
24	B	506	CLA	C6-C7-C8-C9
24	B	515	CLA	C11-C10-C8-C9
25	D	402	PHO	C6-C7-C8-C9
24	A	406	CLA	C3A-C2A-CAA-CBA
24	B	504	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	C	509	CLA	CAD-CBD-CGD-O2D
24	C	511	CLA	CAD-CBD-CGD-O2D
25	A	407	PHO	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	H	101	RRX	C19-C20-C21-C22
24	C	504	CLA	C2-C1-O2A-CGA
31	D	408	LHG	C30-C31-C32-C33
24	B	511	CLA	C4-C3-C5-C6
24	B	513	CLA	C16-C17-C18-C20
28	C	521	LMG	O7-C10-C11-C12
27	A	410	SQD	C10-C11-C12-C13
24	C	514	CLA	CAA-CBA-CGA-O1A
25	A	407	PHO	O2A-C1-C2-C3
24	B	512	CLA	C8-C10-C11-C12
24	B	507	CLA	CAA-CBA-CGA-O2A
33	C	519	DGD	O2G-C1B-C2B-C3B
24	D	401	CLA	C16-C17-C18-C20
24	B	505	CLA	CHA-CBD-CGD-O2D
24	B	507	CLA	CHA-CBD-CGD-O1D
24	B	507	CLA	CHA-CBD-CGD-O2D
24	B	513	CLA	CHA-CBD-CGD-O2D
24	B	515	CLA	CHA-CBD-CGD-O1D
24	B	515	CLA	CHA-CBD-CGD-O2D
24	B	516	CLA	CHA-CBD-CGD-O1D
24	B	516	CLA	CHA-CBD-CGD-O2D
24	D	403	CLA	CHA-CBD-CGD-O2D
26	B	518	BCR	C15-C16-C17-C18
24	C	511	CLA	C4-C3-C5-C6
28	A	411	LMG	C31-C32-C33-C34
31	D	408	LHG	C32-C33-C34-C35
27	A	410	SQD	C25-C26-C27-C28
24	C	506	CLA	CAA-CBA-CGA-O2A
25	A	407	PHO	CHA-CBD-CGD-O1D
25	D	402	PHO	CHA-CBD-CGD-O1D
31	D	410	LHG	C24-C23-O8-C6
28	C	501	LMG	O7-C10-C11-C12
35	B	523	DGA	CA7-CA8-CA9-CAA
31	D	408	LHG	C2-C3-O3-P
33	C	519	DGD	O1B-C1B-C2B-C3B
27	M	101	SQD	C4-C5-C6-S
27	M	101	SQD	C5-C6-S-O8
24	C	509	CLA	CAA-CBA-CGA-O2A
24	C	513	CLA	CAA-CBA-CGA-O2A
34	B	522	3PH	O22-C21-C22-C23
28	H	102	LMG	C12-C13-C14-C15
24	C	511	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	C	521	LMG	O9-C10-C11-C12
28	C	501	LMG	C16-C17-C18-C19
24	B	514	CLA	C2A-CAA-CBA-CGA
36	D	406	PL9	C15-C14-C16-C17
34	B	522	3PH	O31-C31-C32-C33
28	H	102	LMG	C40-C41-C42-C43
31	A	414	LHG	C3-O3-P-O5
28	C	522	LMG	C11-C10-O7-C8
28	C	522	LMG	O7-C10-C11-C12
26	C	516	BCR	C23-C24-C25-C30
35	B	523	DGA	CA4-CA5-CA6-CA7
24	B	504	CLA	CAA-CBA-CGA-O2A
24	B	509	CLA	CAA-CBA-CGA-O2A
24	B	516	CLA	C2A-CAA-CBA-CGA
24	B	507	CLA	CAA-CBA-CGA-O1A
24	D	403	CLA	CAD-CBD-CGD-O1D
27	M	101	SQD	O5-C5-C6-S
24	C	506	CLA	CAA-CBA-CGA-O1A
24	C	509	CLA	CAA-CBA-CGA-O1A
24	C	504	CLA	CAA-CBA-CGA-O2A
24	B	510	CLA	C11-C12-C13-C14
24	C	509	CLA	C14-C13-C15-C16
24	D	401	CLA	C11-C10-C8-C9
24	D	403	CLA	C6-C7-C8-C9
24	D	403	CLA	C11-C10-C8-C9
31	D	408	LHG	C15-C16-C17-C18
37	E	101	HEM	CAA-CBA-CGA-O2A
28	H	102	LMG	C14-C15-C16-C17
24	B	508	CLA	CAA-CBA-CGA-O2A
24	D	404	CLA	CAA-CBA-CGA-O2A
28	D	409	LMG	O7-C10-C11-C12
24	C	513	CLA	CAA-CBA-CGA-O1A
24	B	501	CLA	C11-C12-C13-C15
24	B	511	CLA	C11-C12-C13-C15
24	B	513	CLA	C2-C3-C5-C6
24	C	510	CLA	C6-C7-C8-C10
24	D	401	CLA	C11-C10-C8-C7
24	D	403	CLA	C11-C10-C8-C7
27	A	410	SQD	O47-C7-C8-C9
33	B	521	DGD	O2G-C1B-C2B-C3B
33	C	518	DGD	O2G-C1B-C2B-C3B
27	A	410	SQD	O49-C7-C8-C9

Continued on next page...

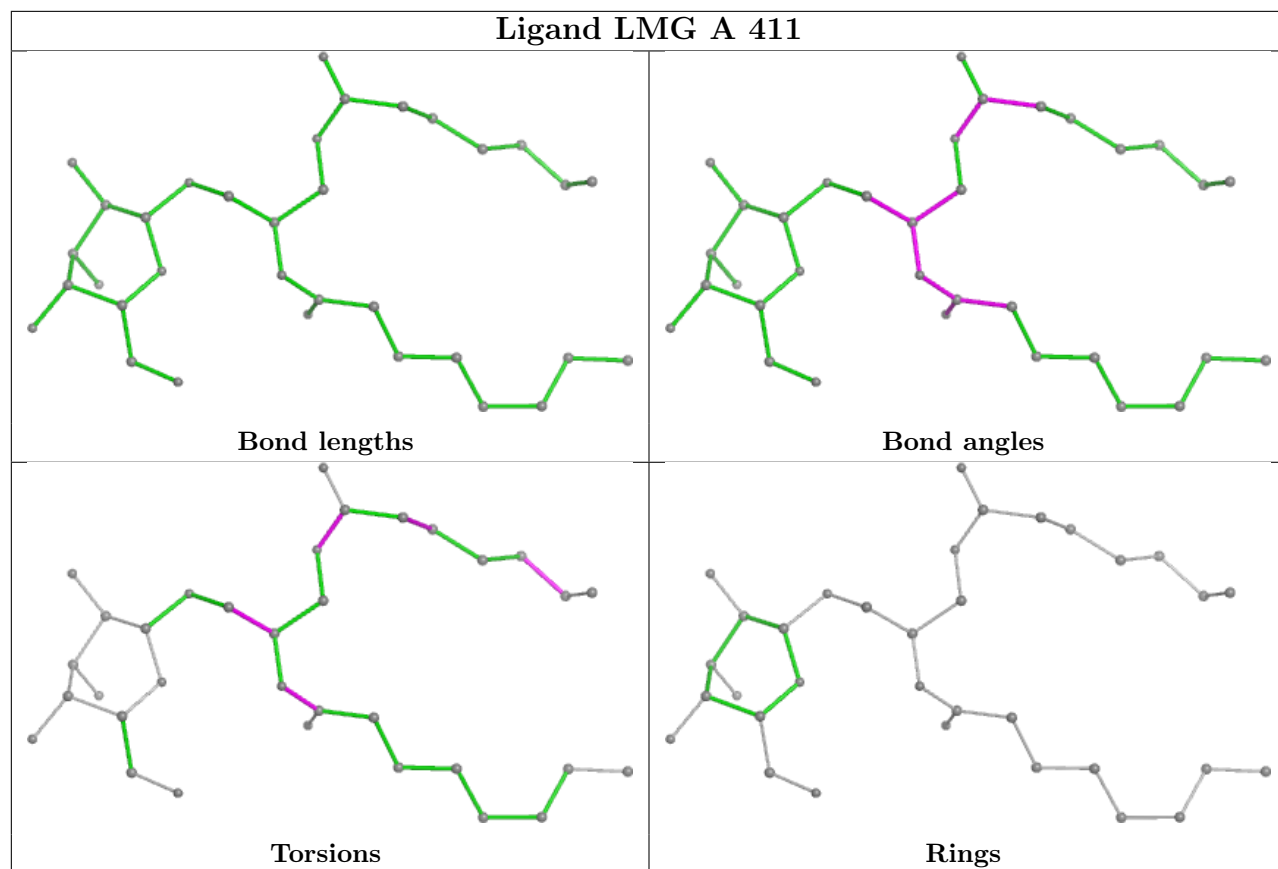
Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	B	522	3PH	O32-C31-C32-C33
33	C	519	DGD	O6D-C1D-O3G-C3G
25	A	407	PHO	C15-C16-C17-C18
24	C	504	CLA	CAA-CBA-CGA-O1A
24	B	508	CLA	CAA-CBA-CGA-O1A
24	B	512	CLA	C2A-CAA-CBA-CGA
24	D	403	CLA	C4-C3-C5-C6
24	C	505	CLA	CAA-CBA-CGA-O2A

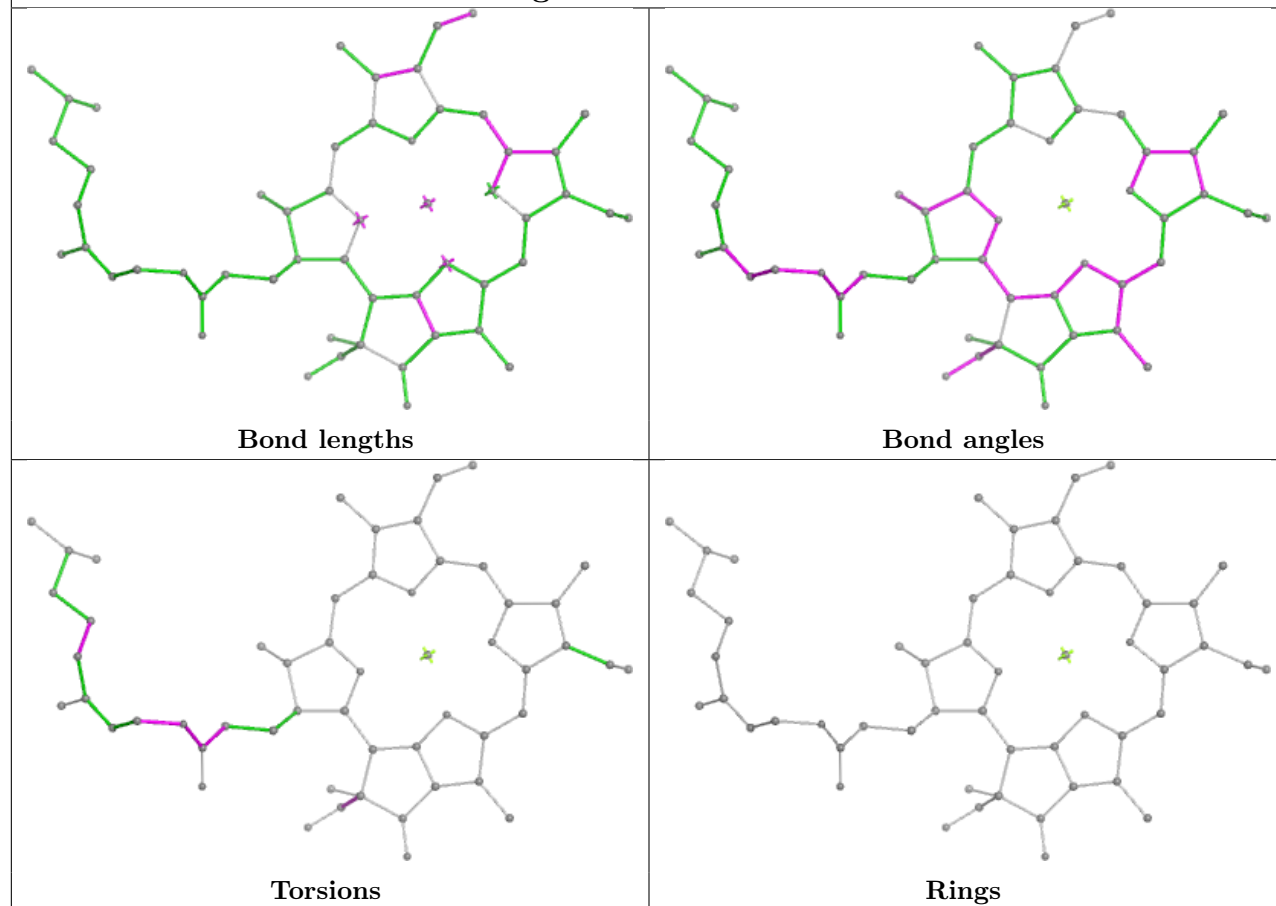
There are no ring outliers.

No monomer is involved in short contacts.

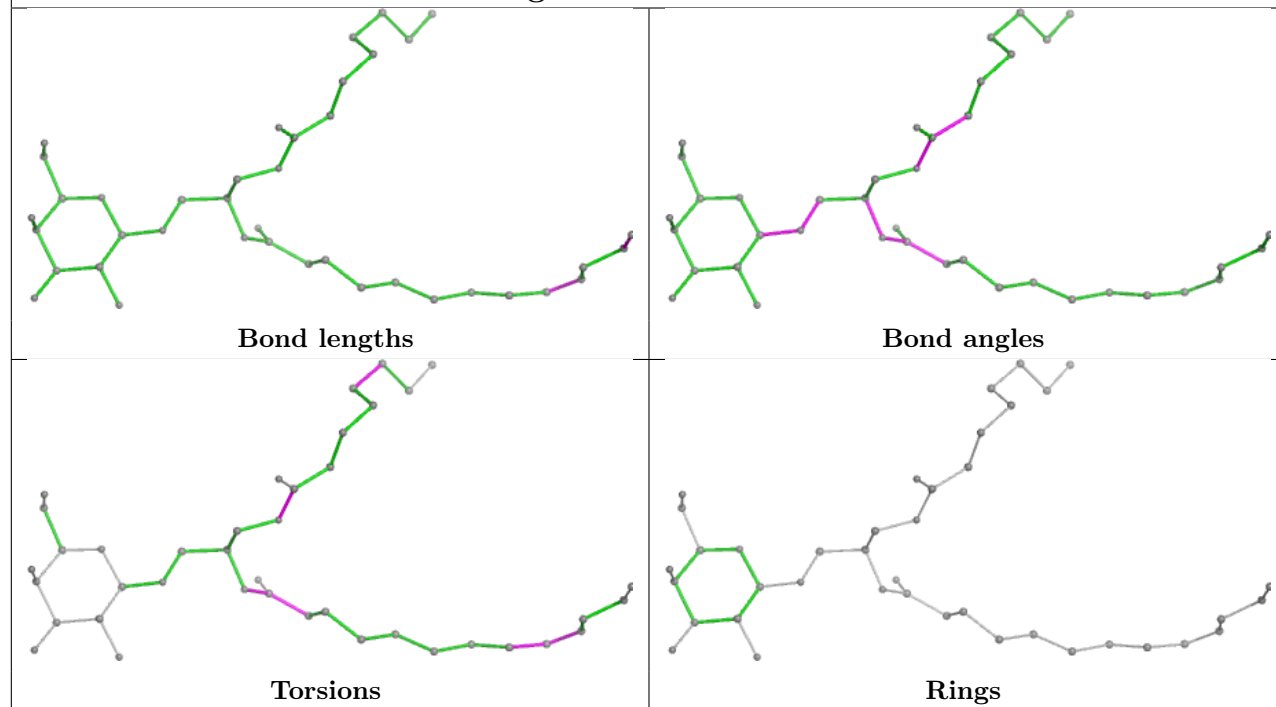
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

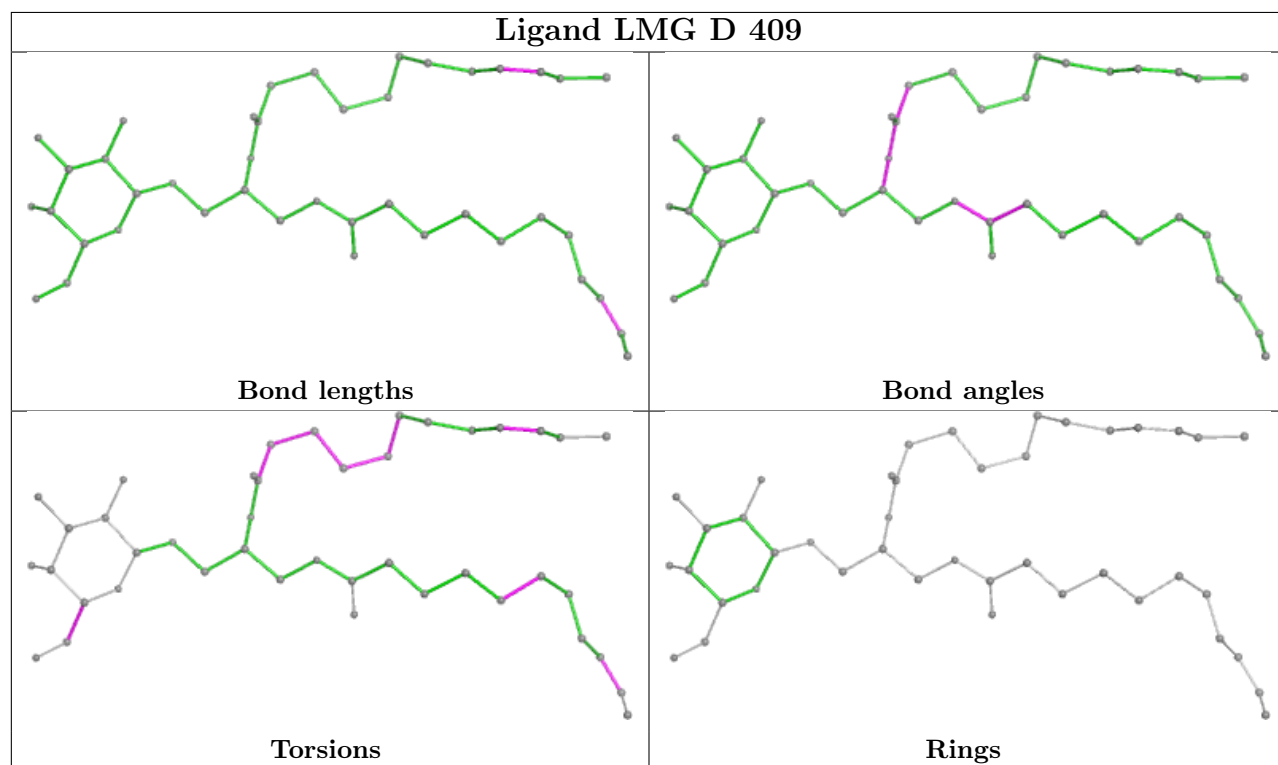
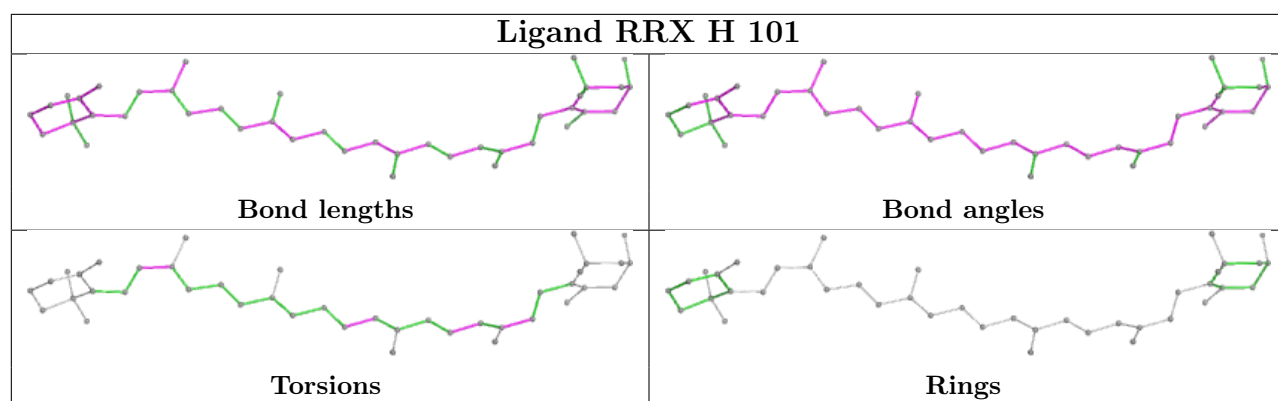


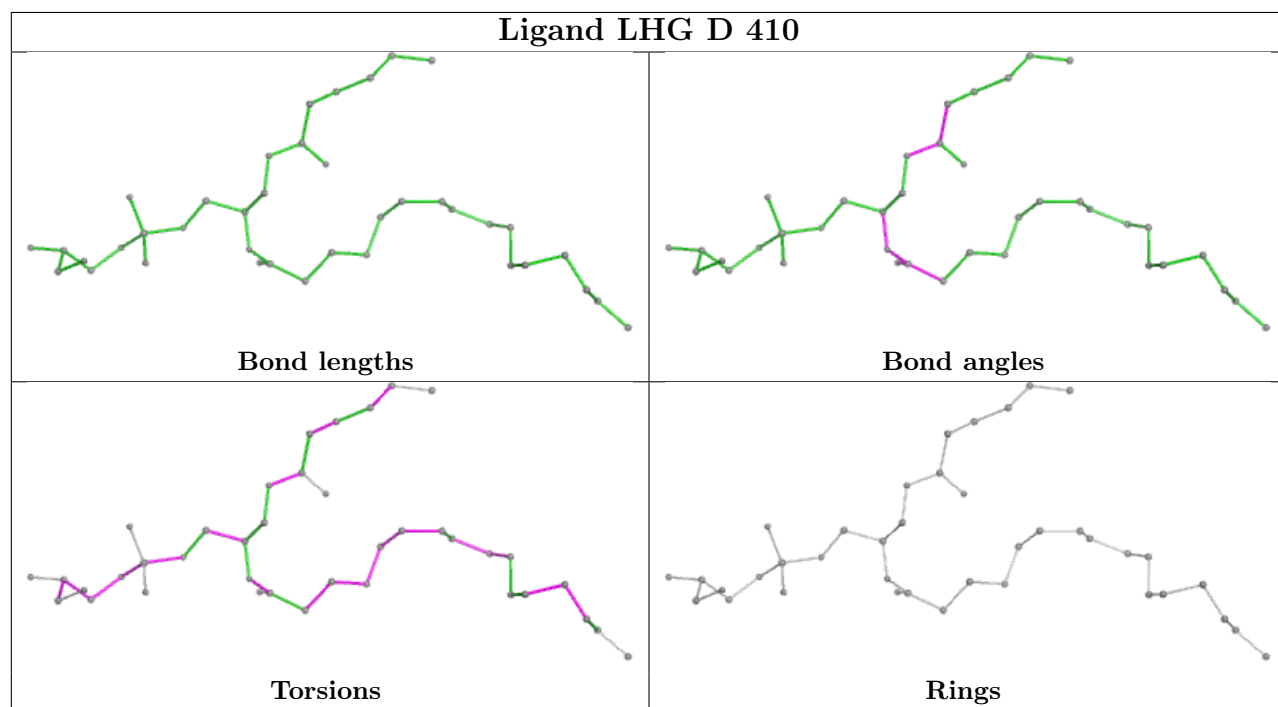
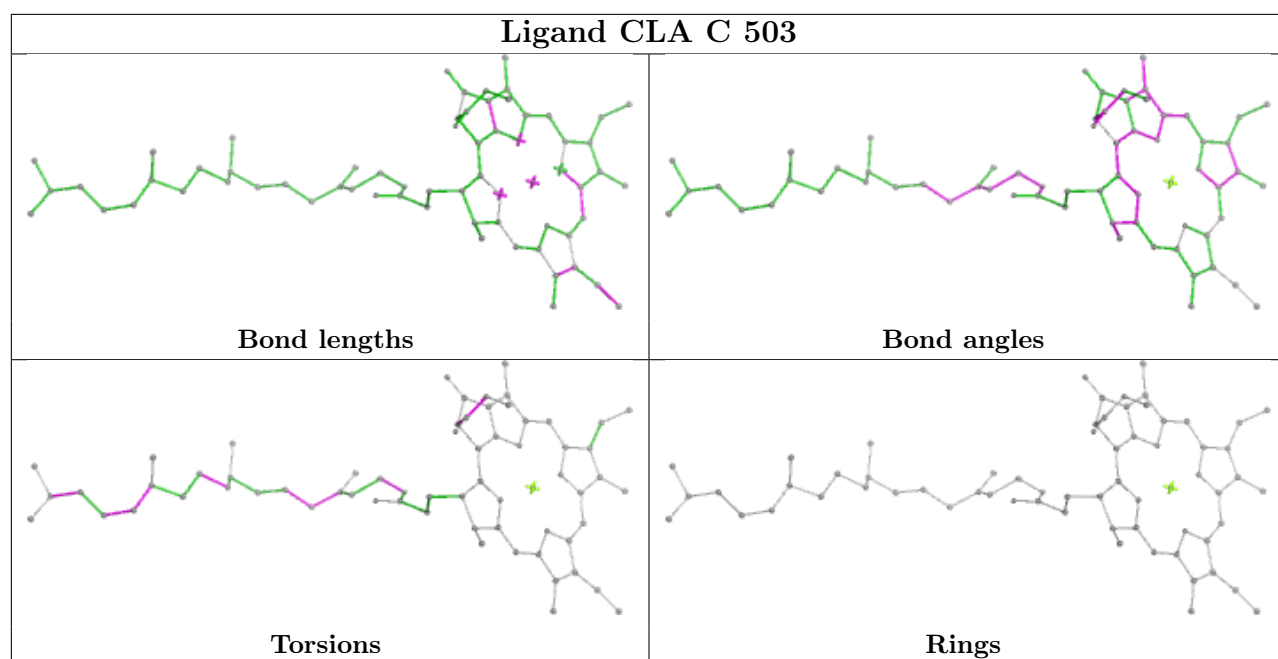
Ligand CLA C 513

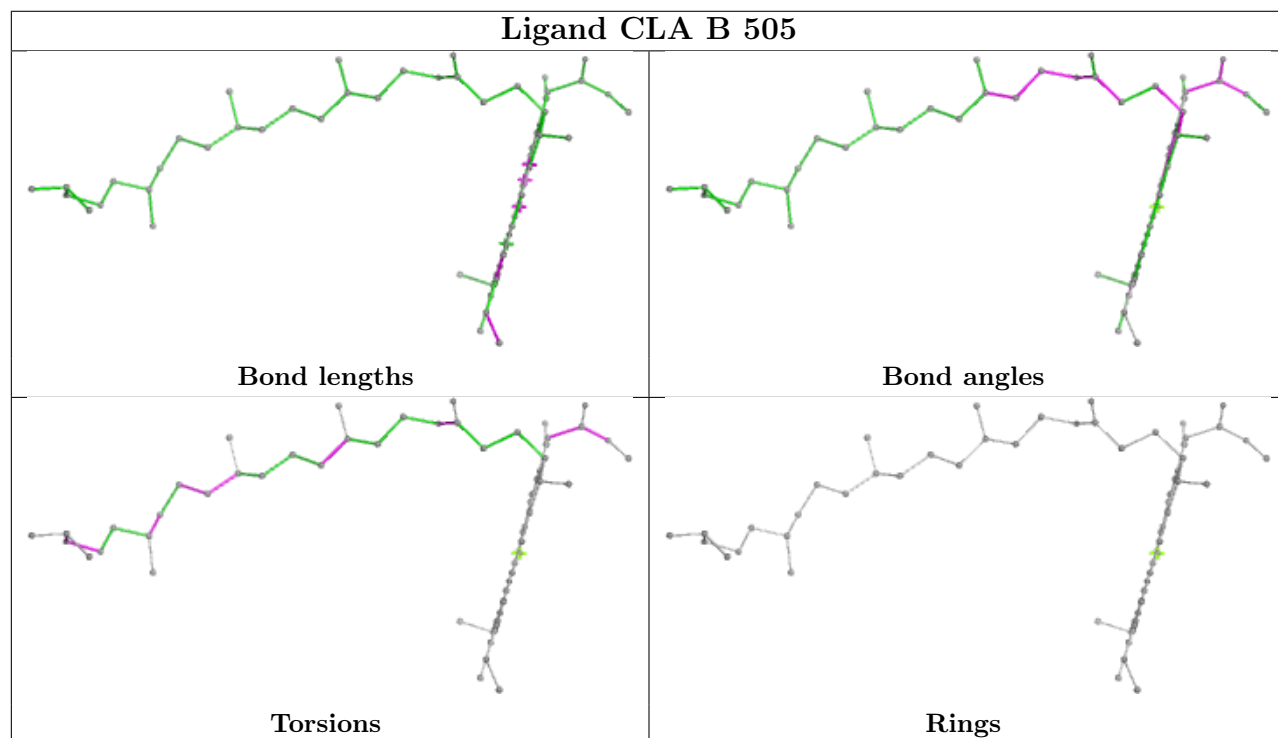
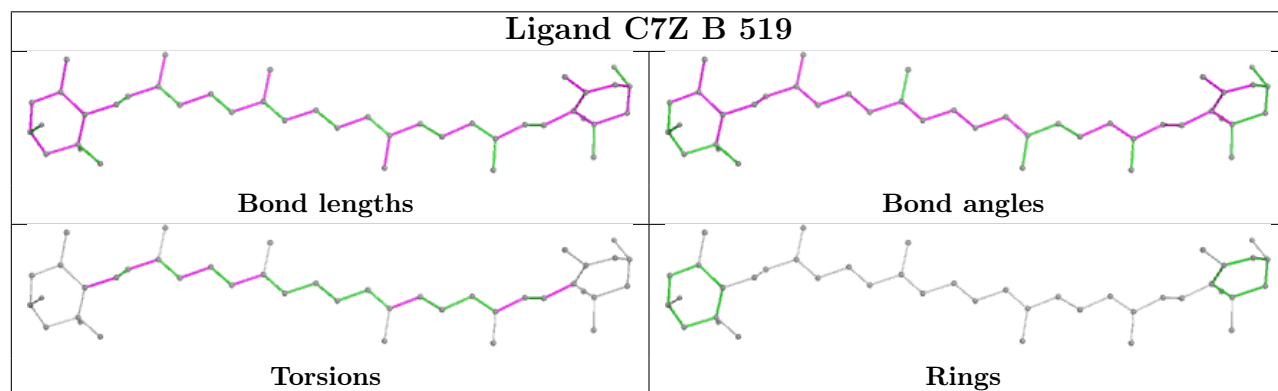
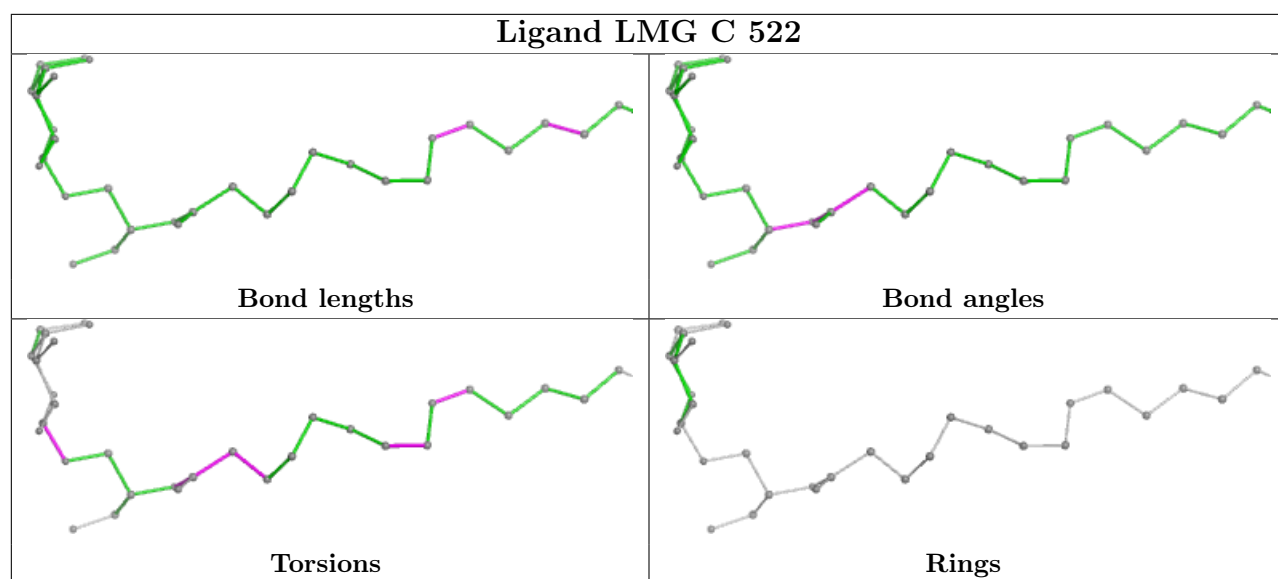


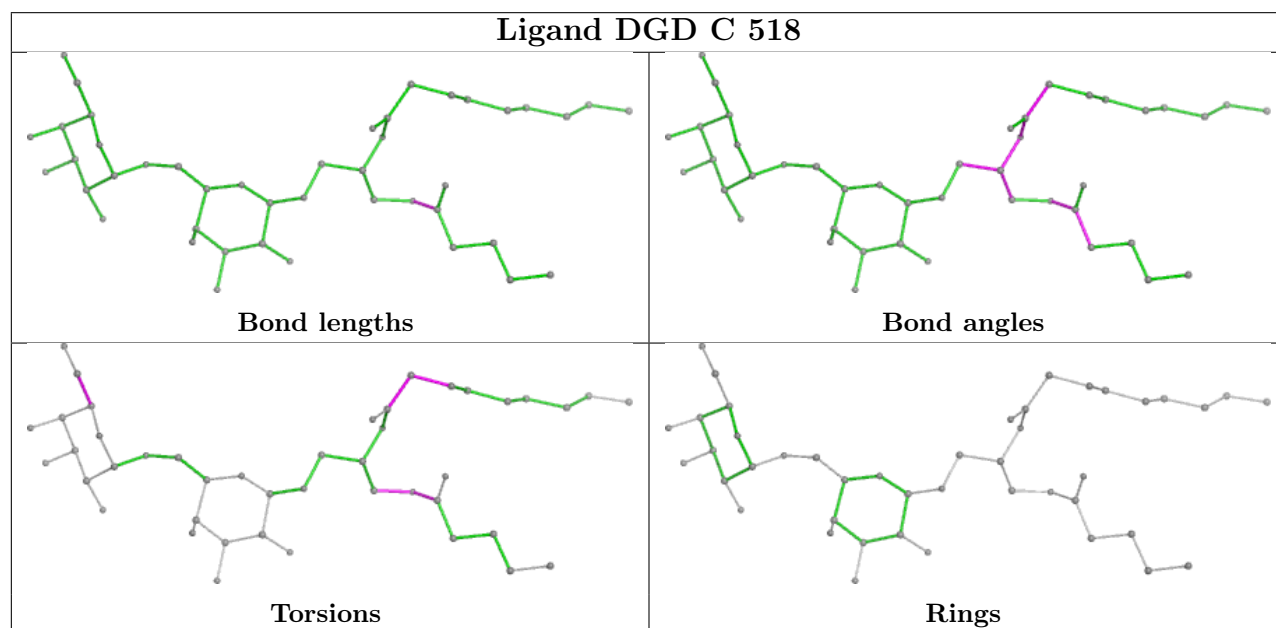
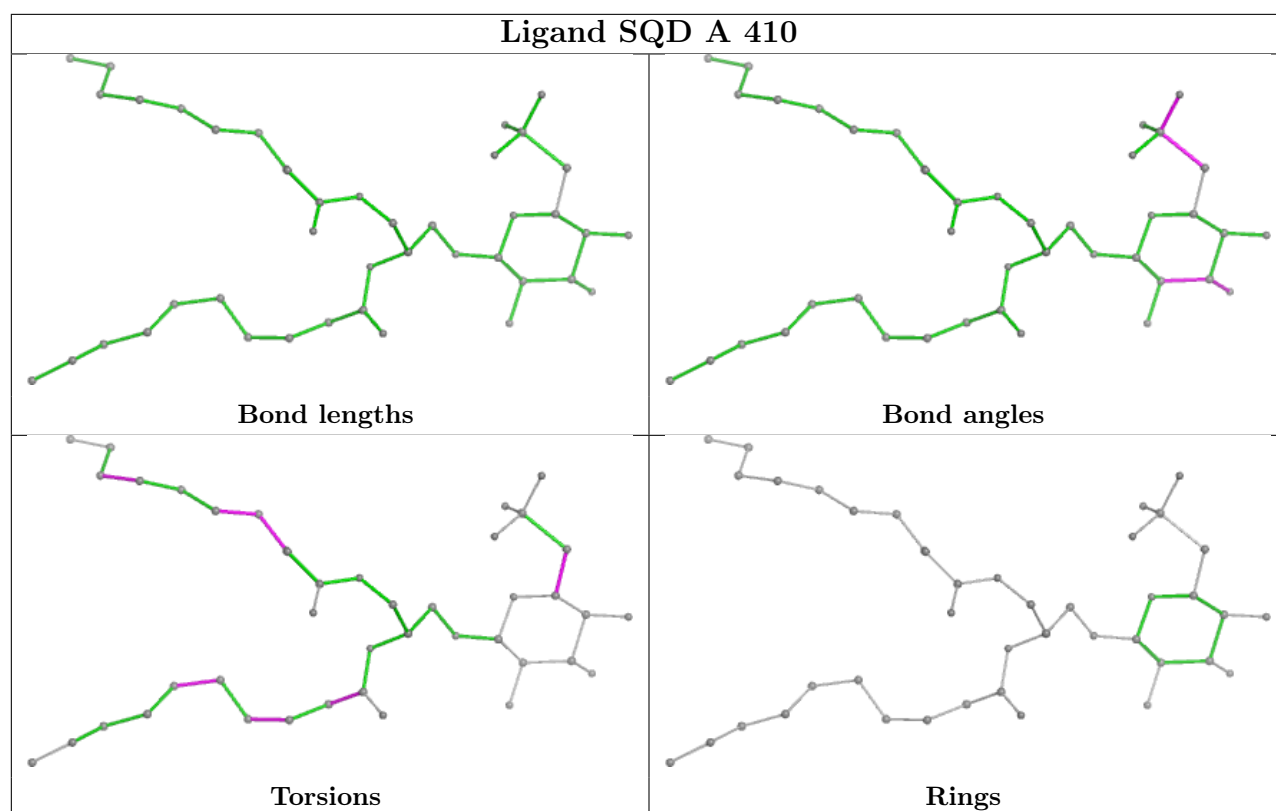
Ligand LMG C 501

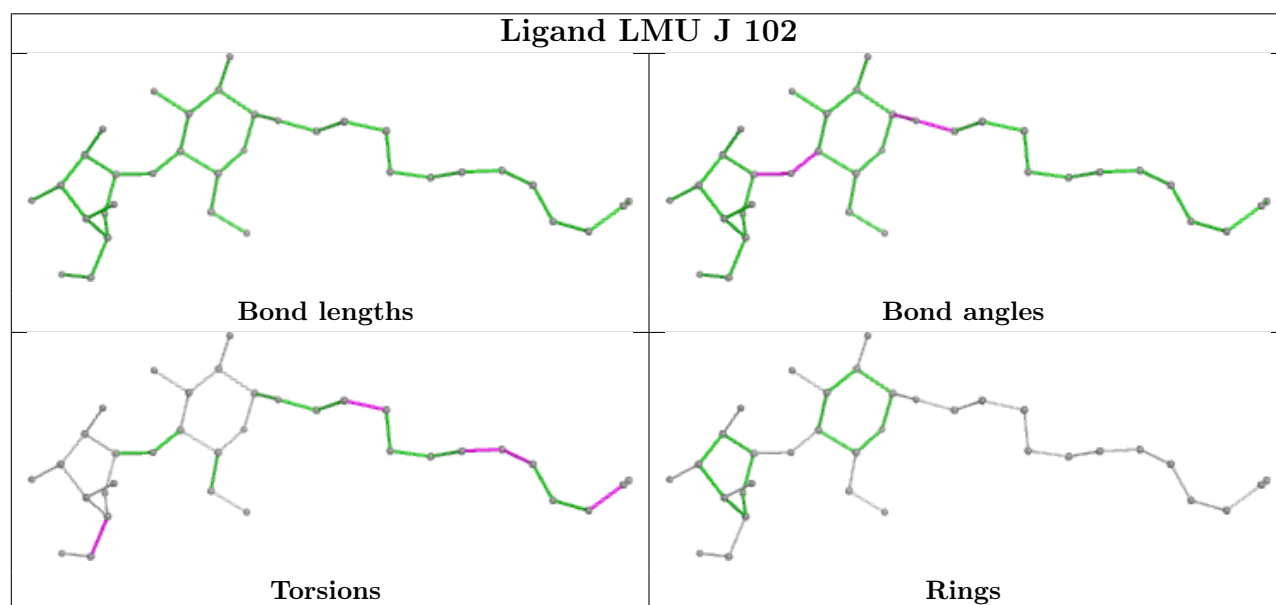
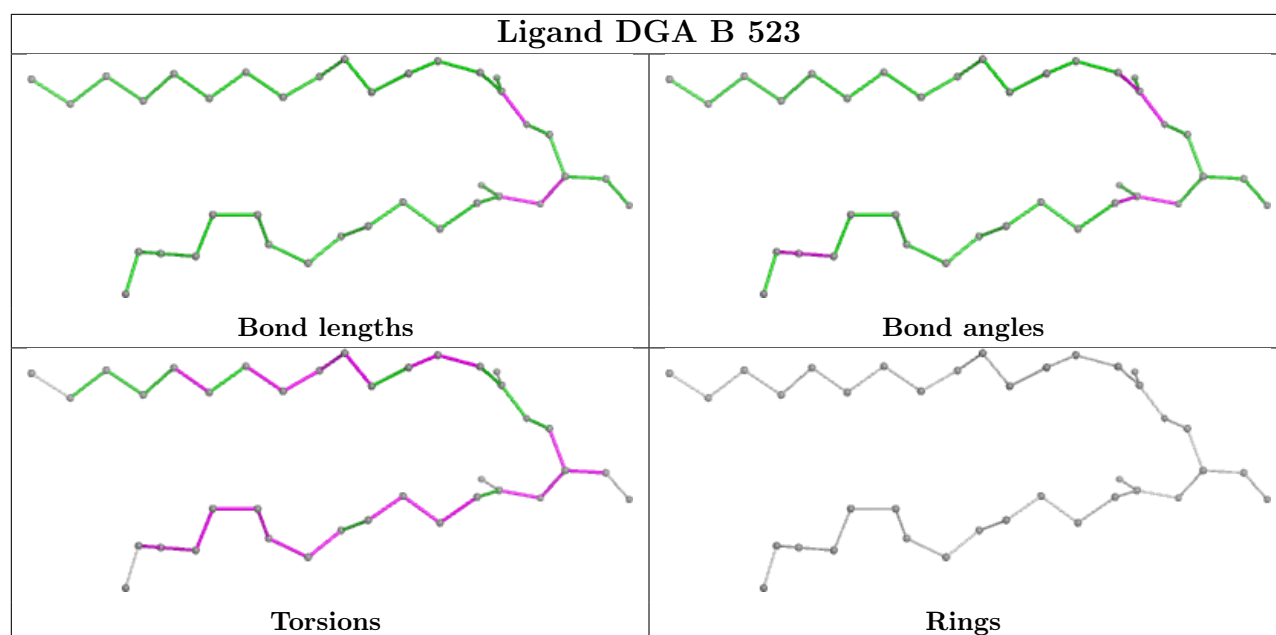


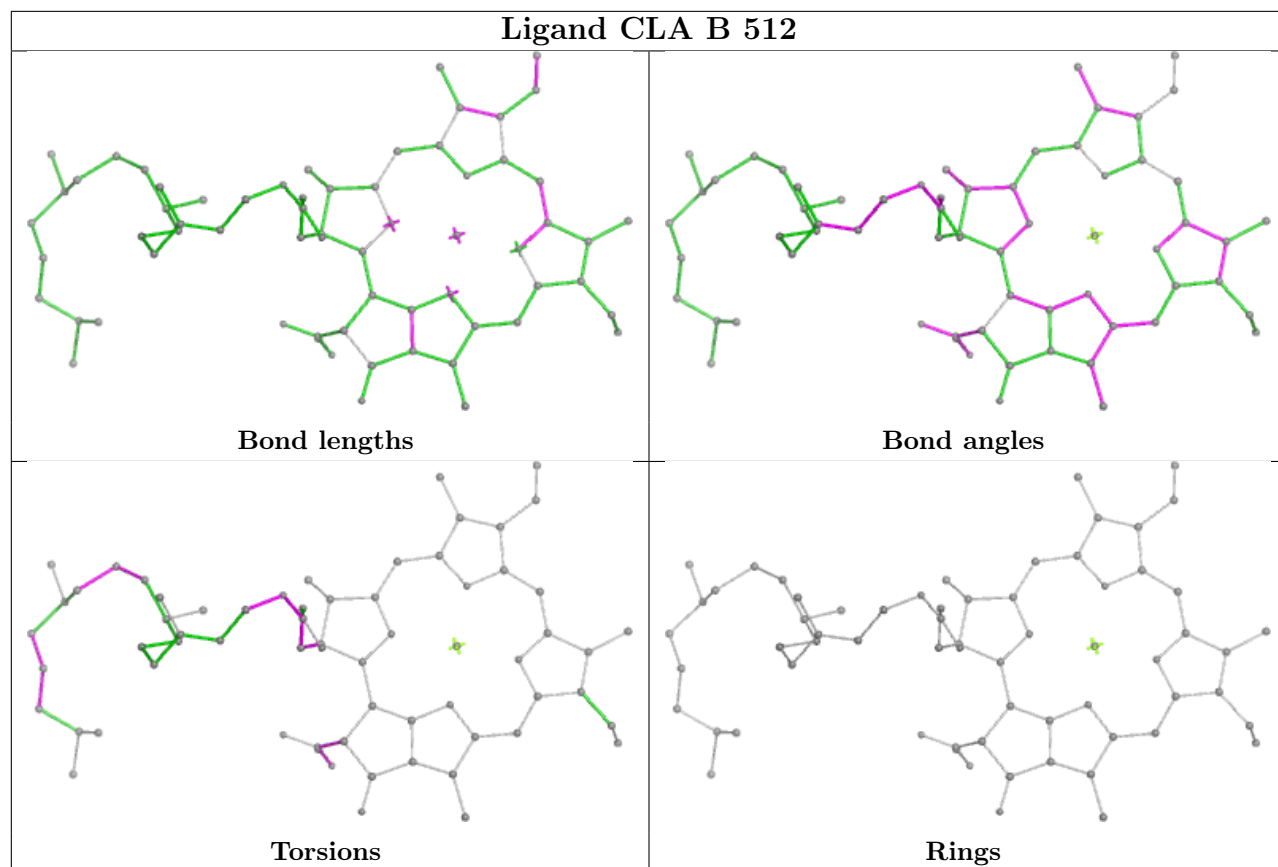




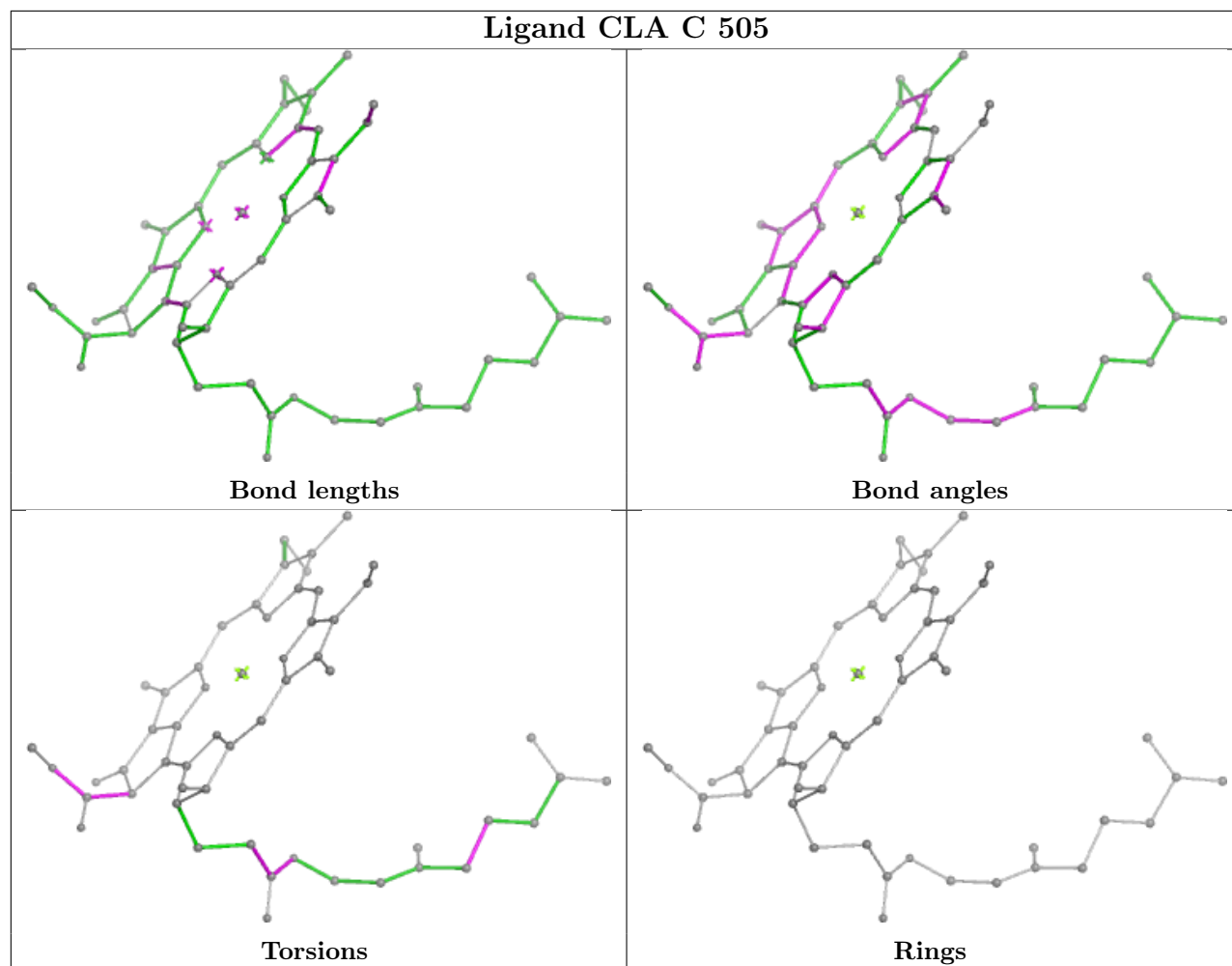




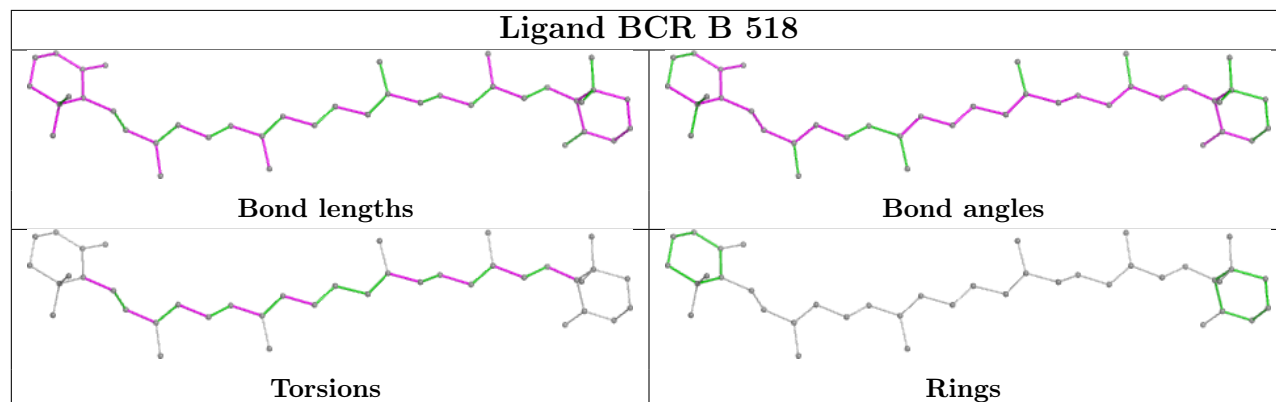


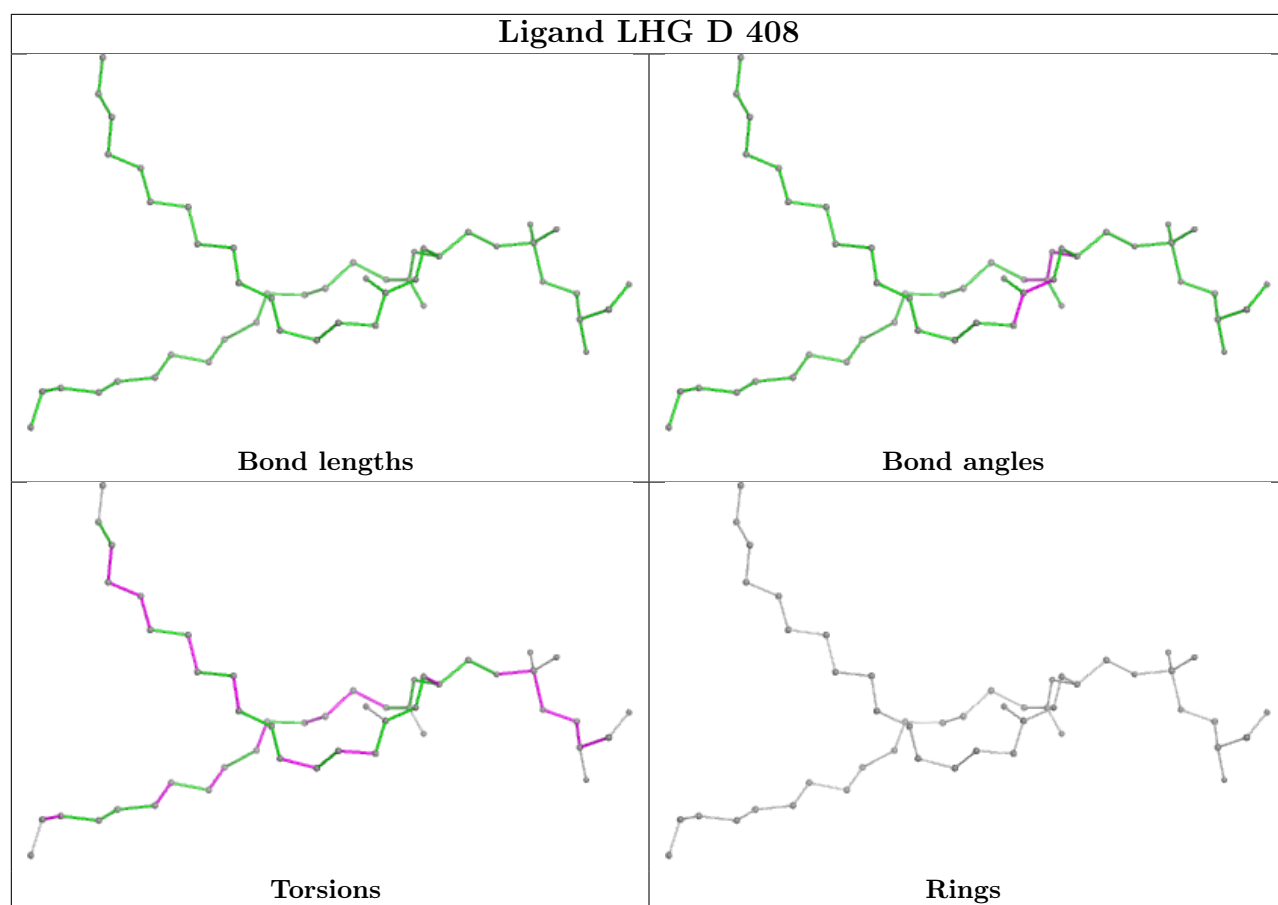


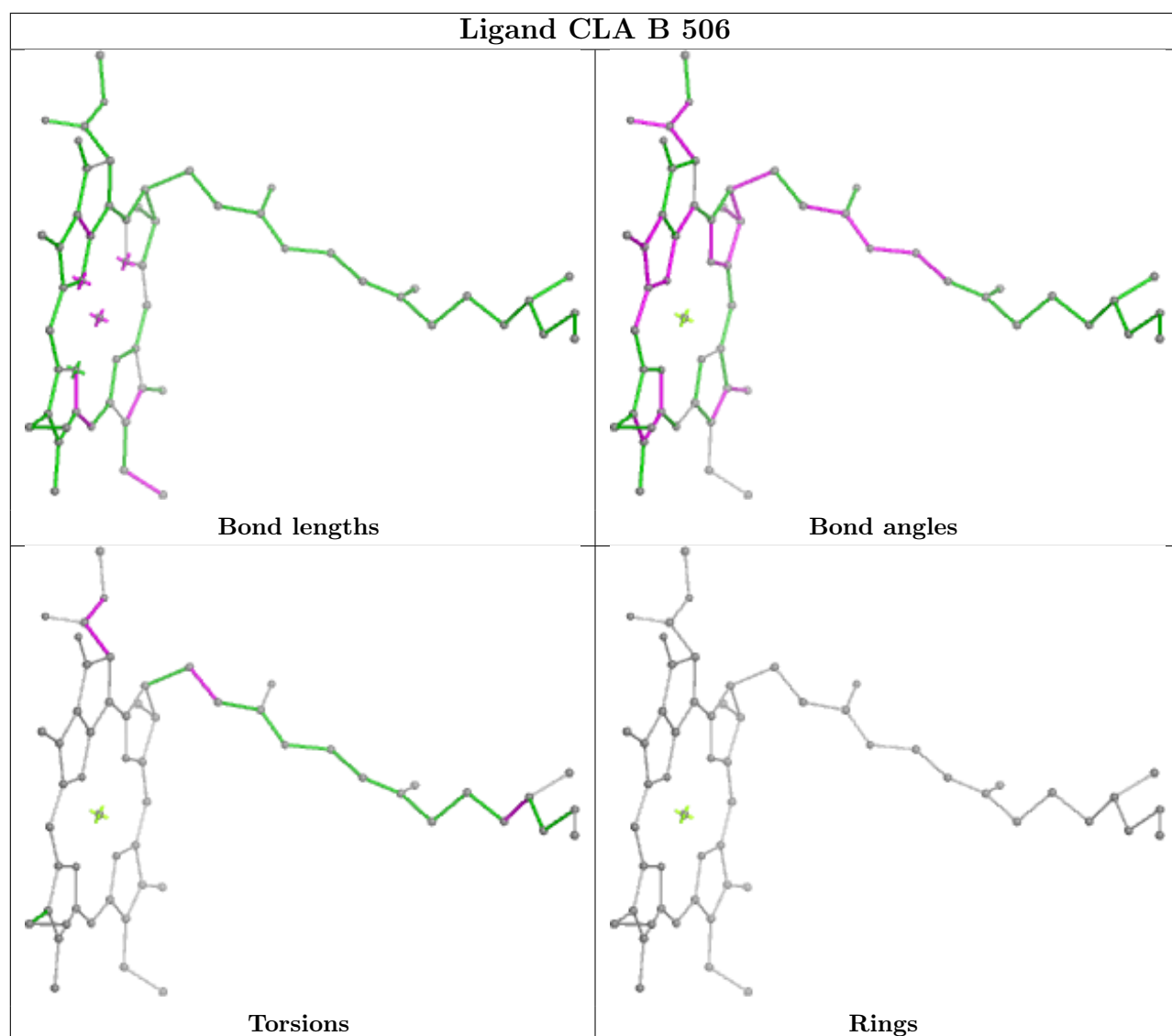
Ligand CLA C 505

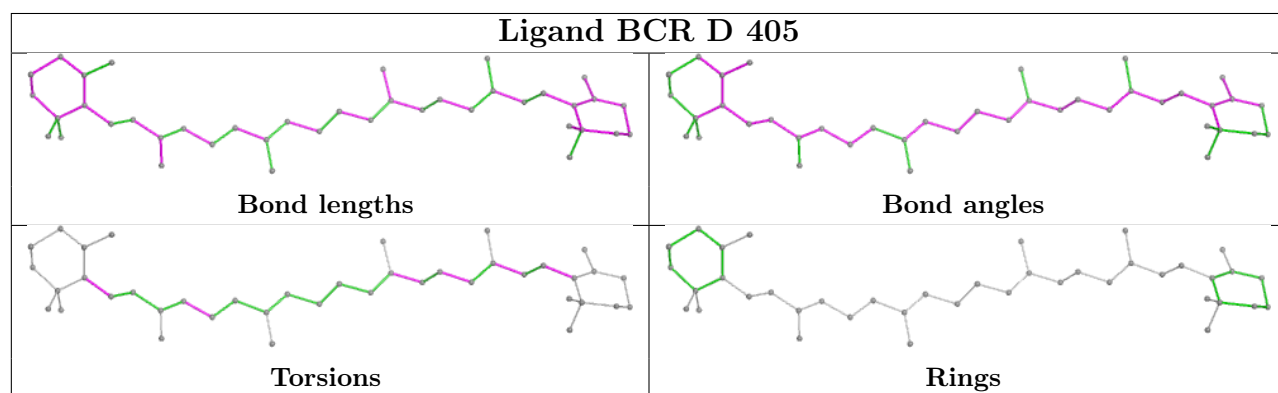
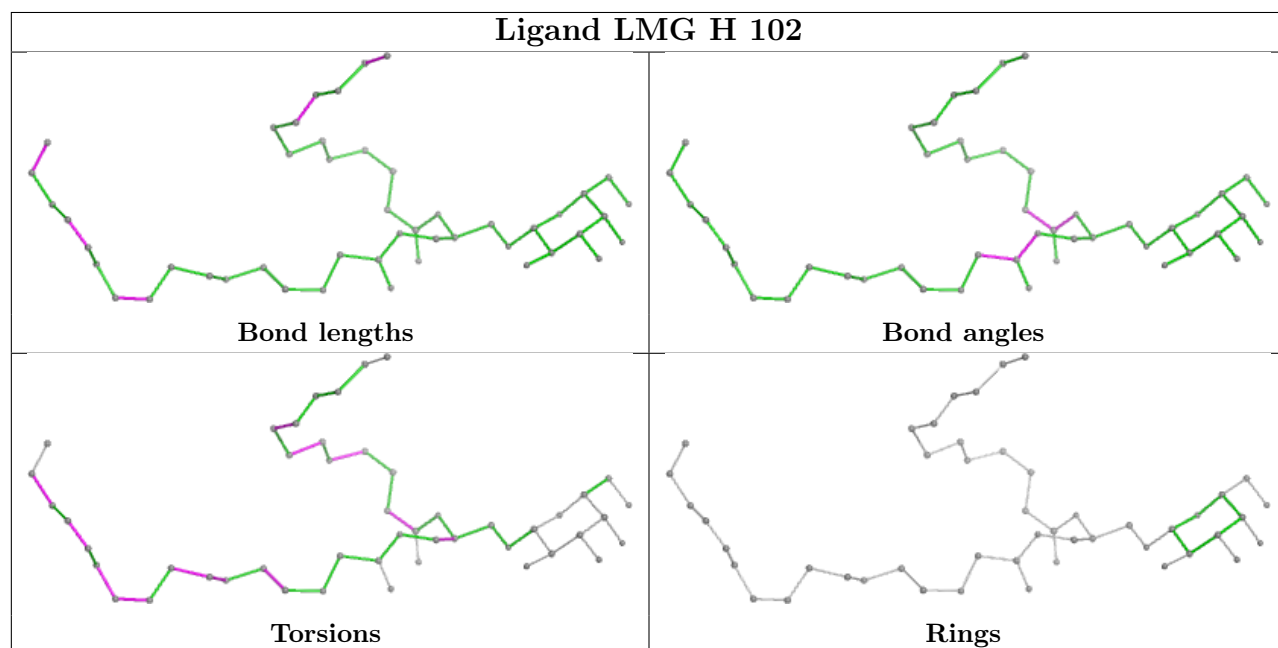
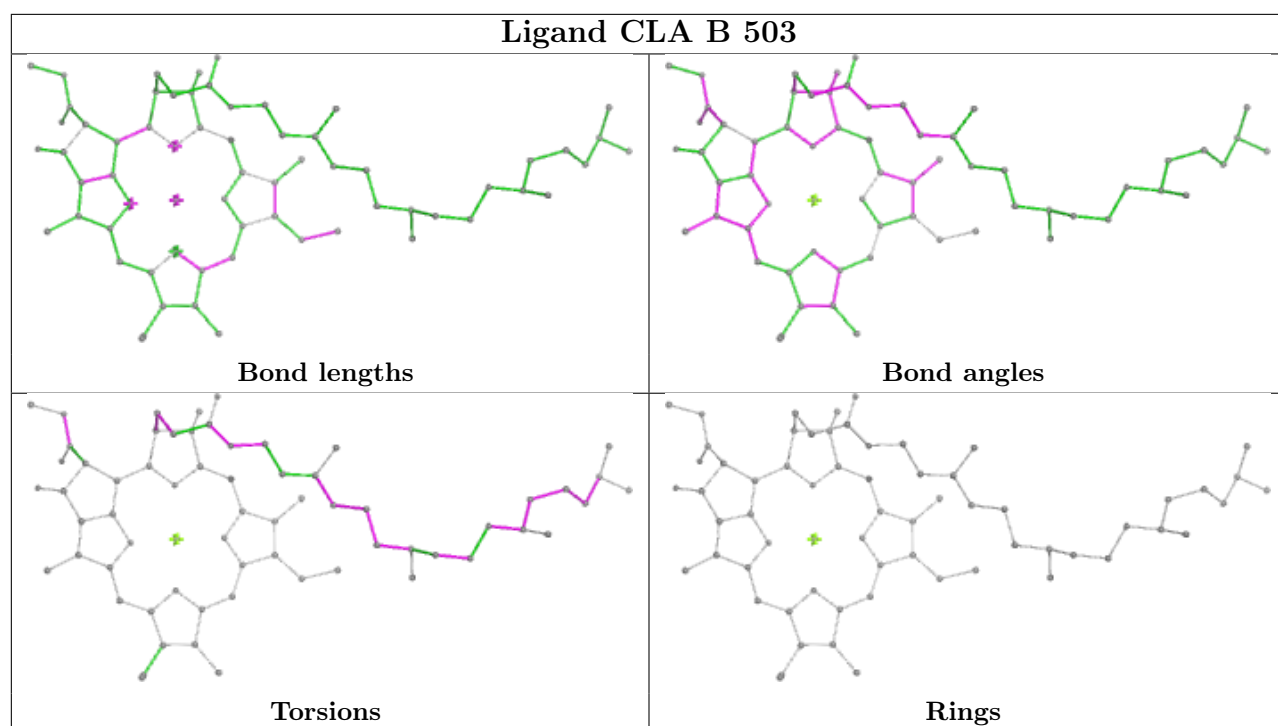


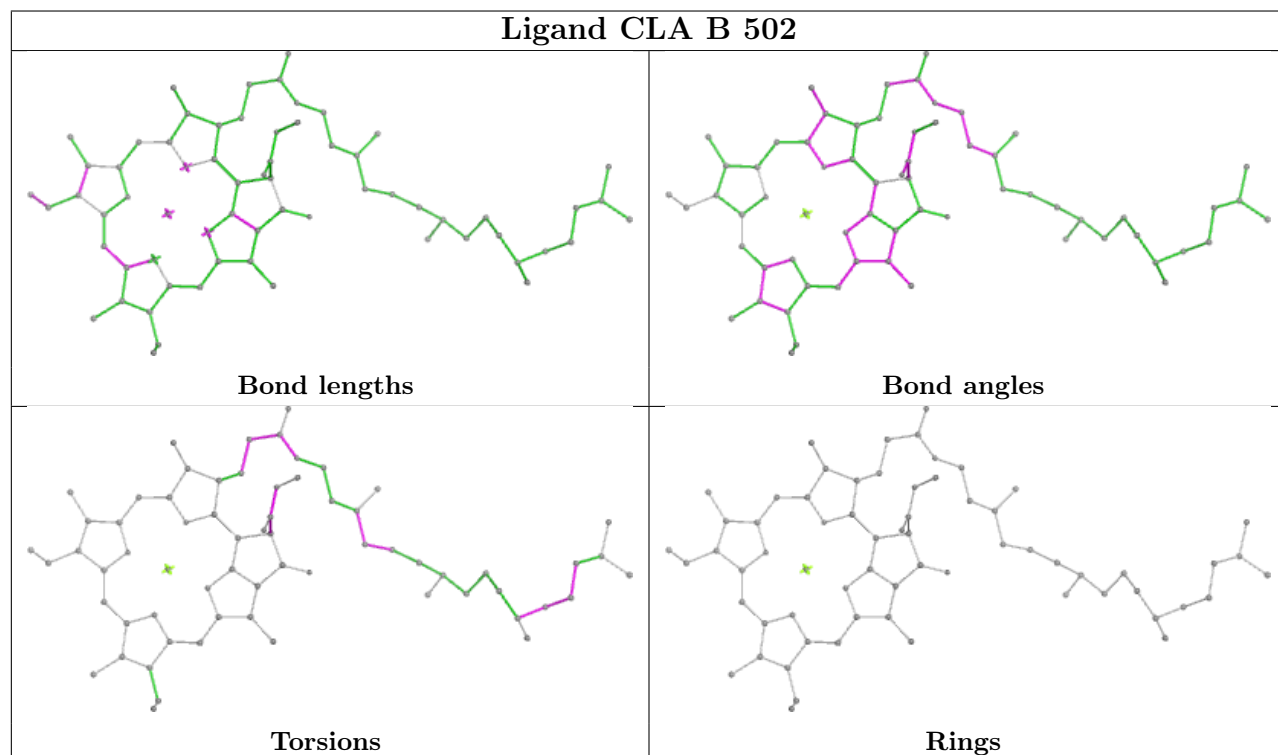
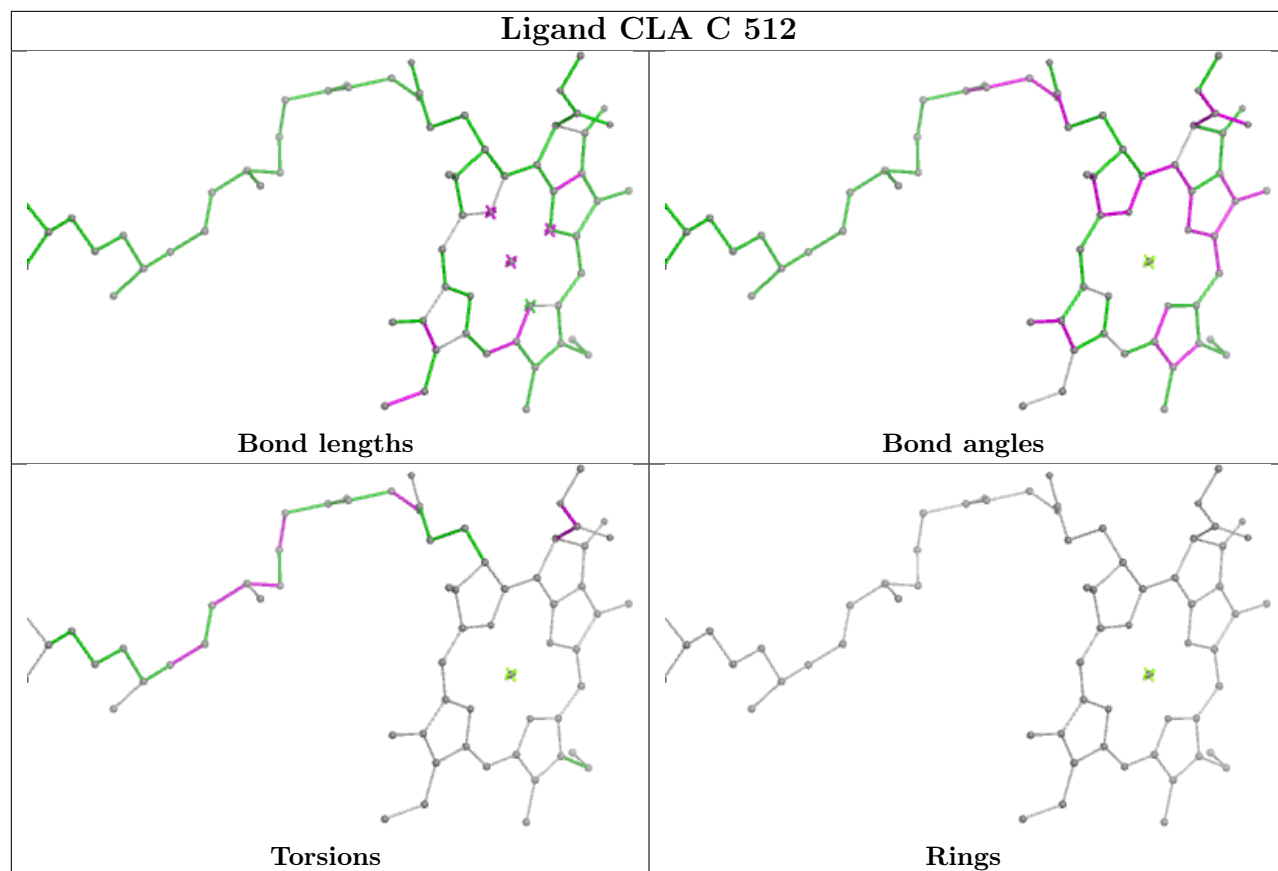
Ligand BCR B 518

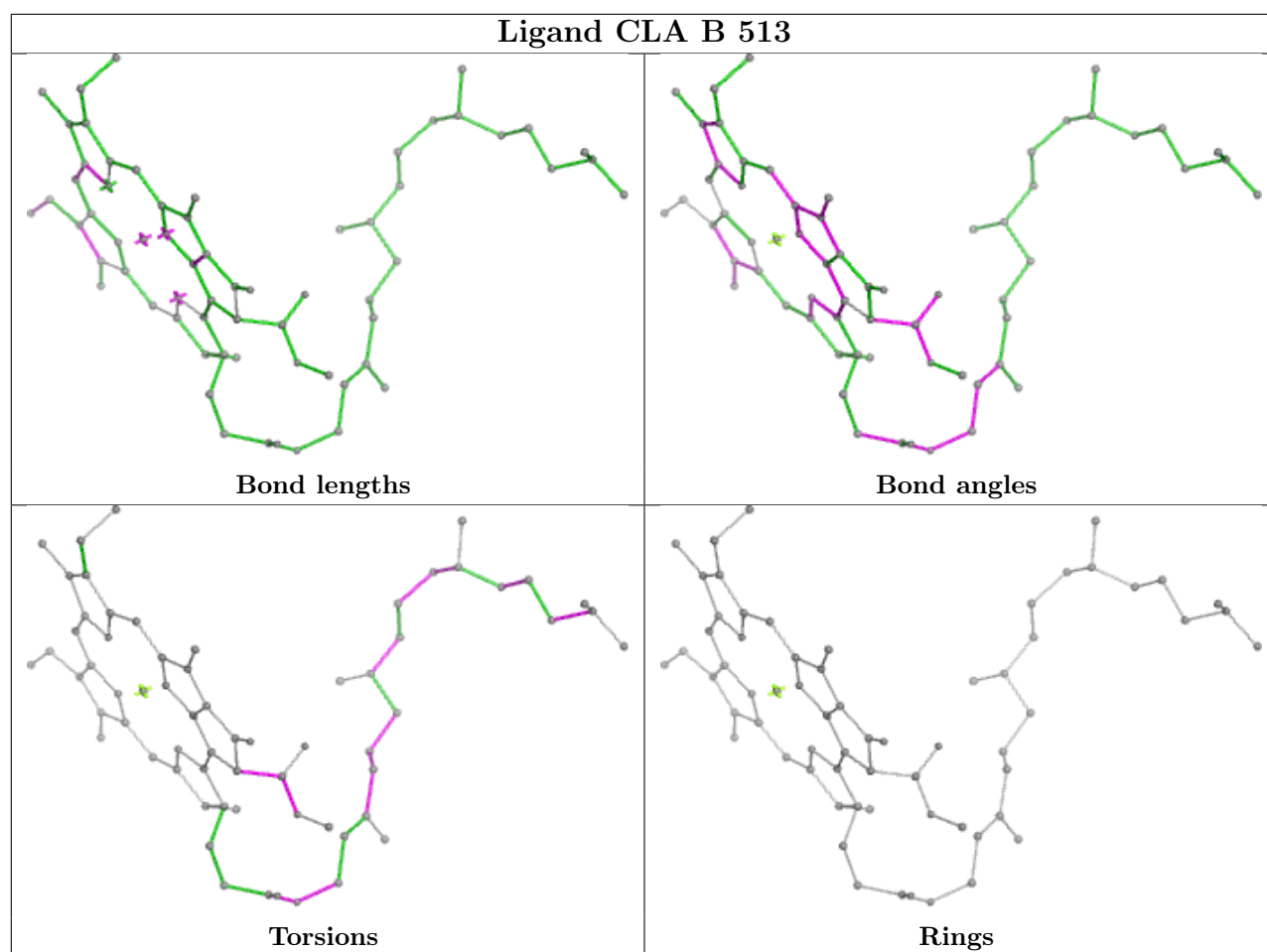




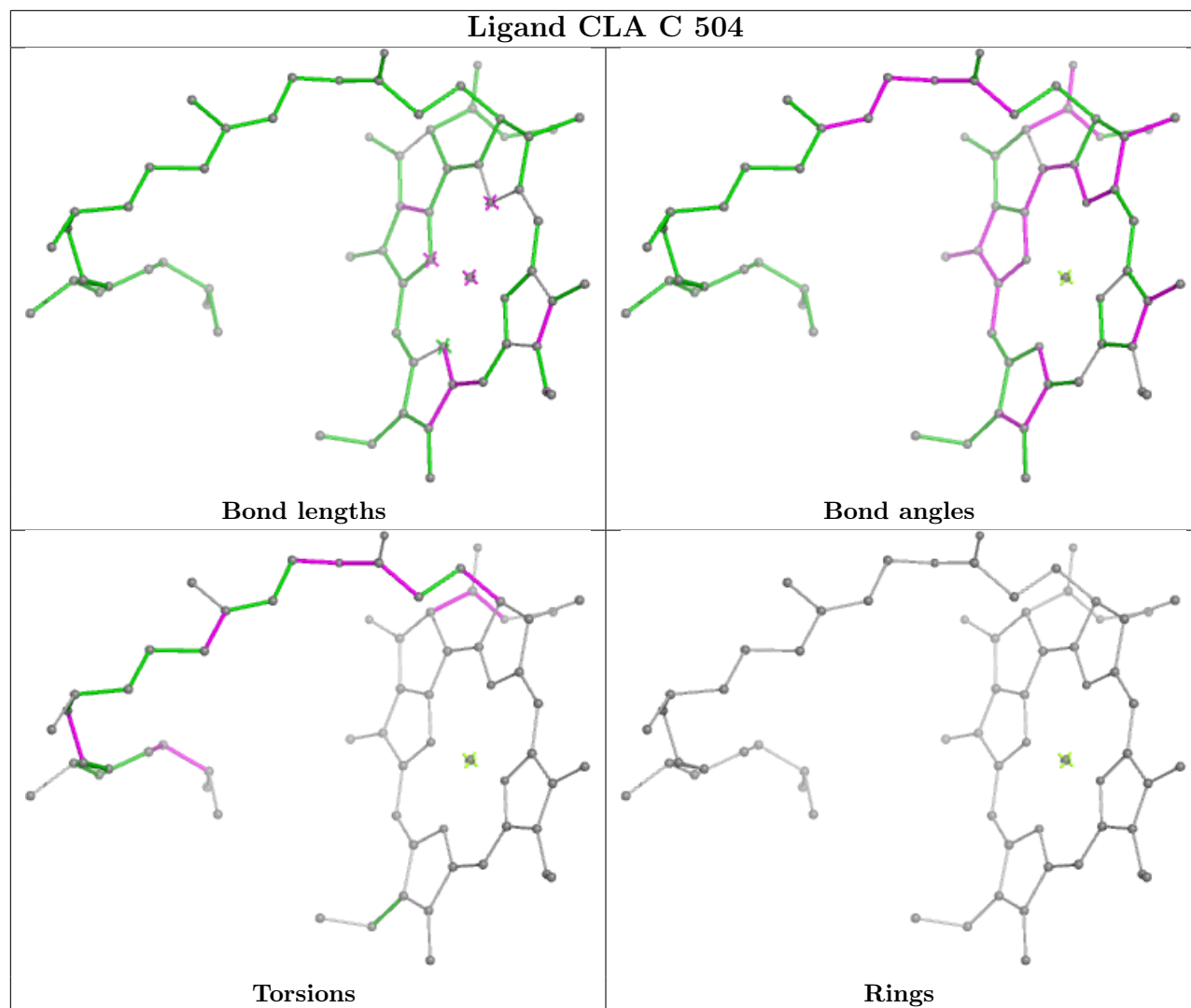




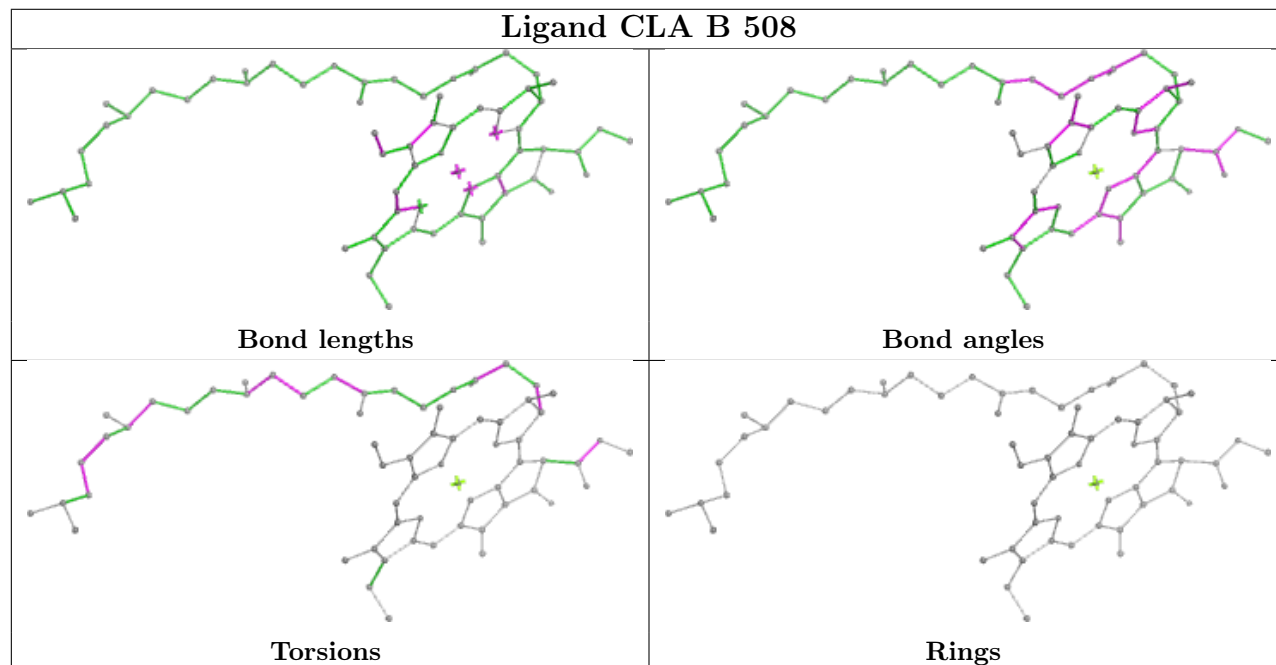




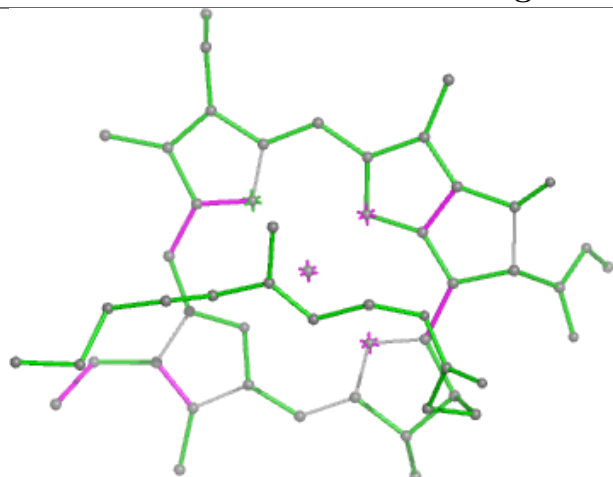
Ligand CLA C 504



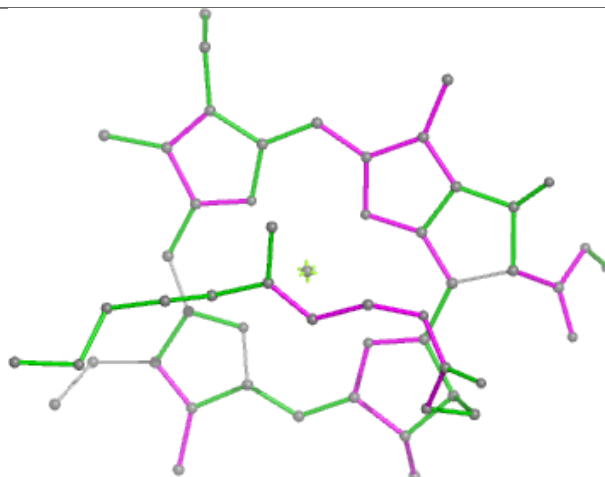
Ligand CLA B 508



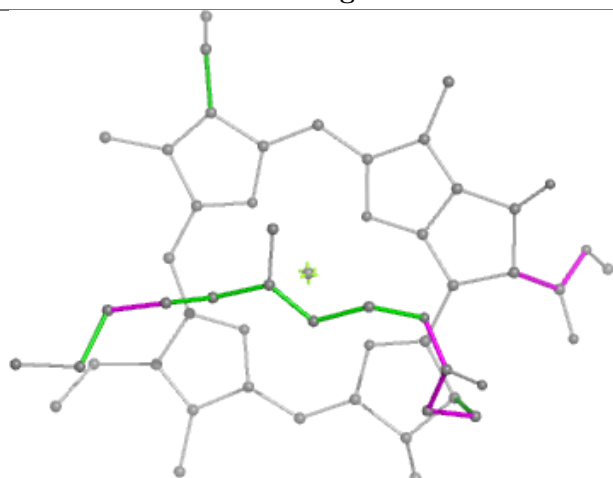
Ligand CLA C 506



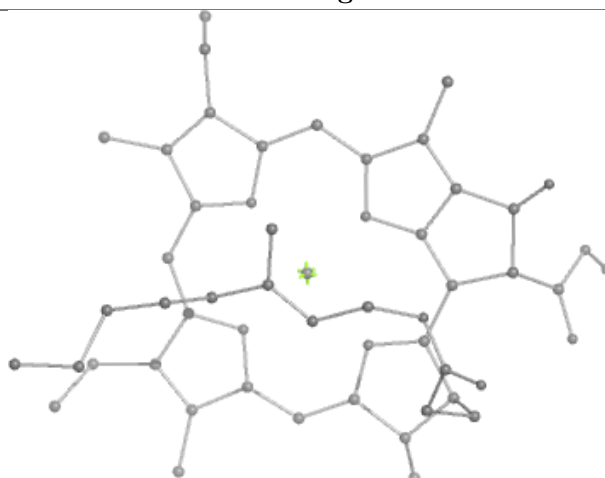
Bond lengths



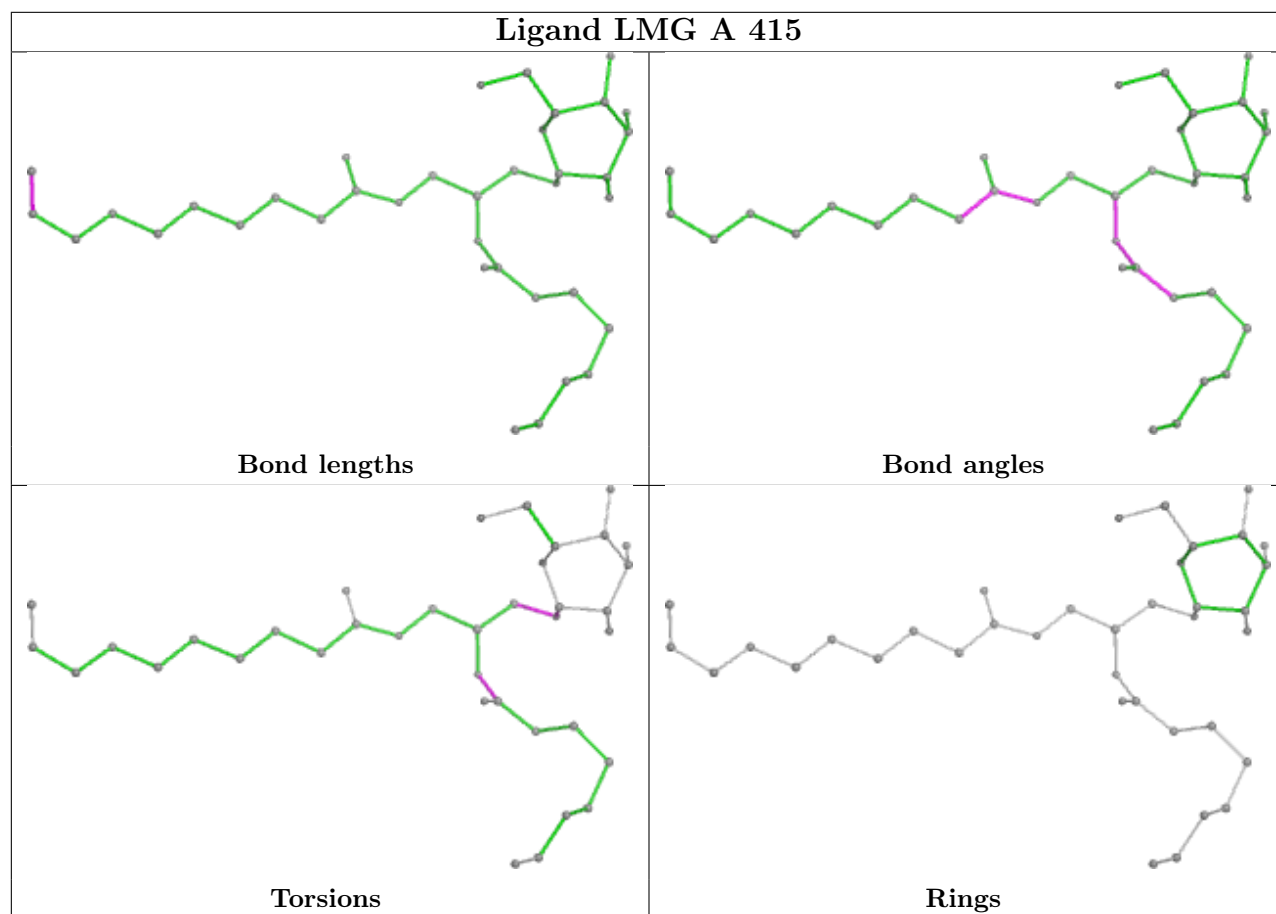
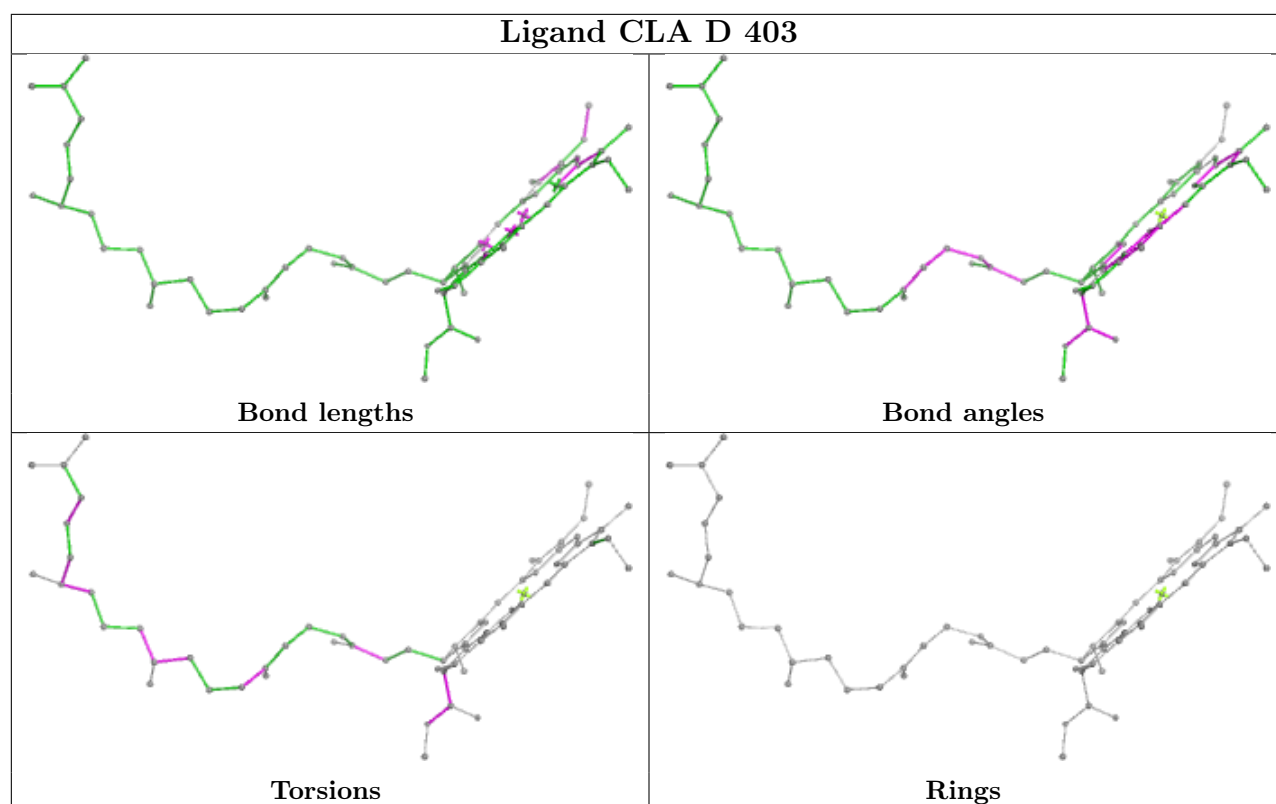
Bond angles

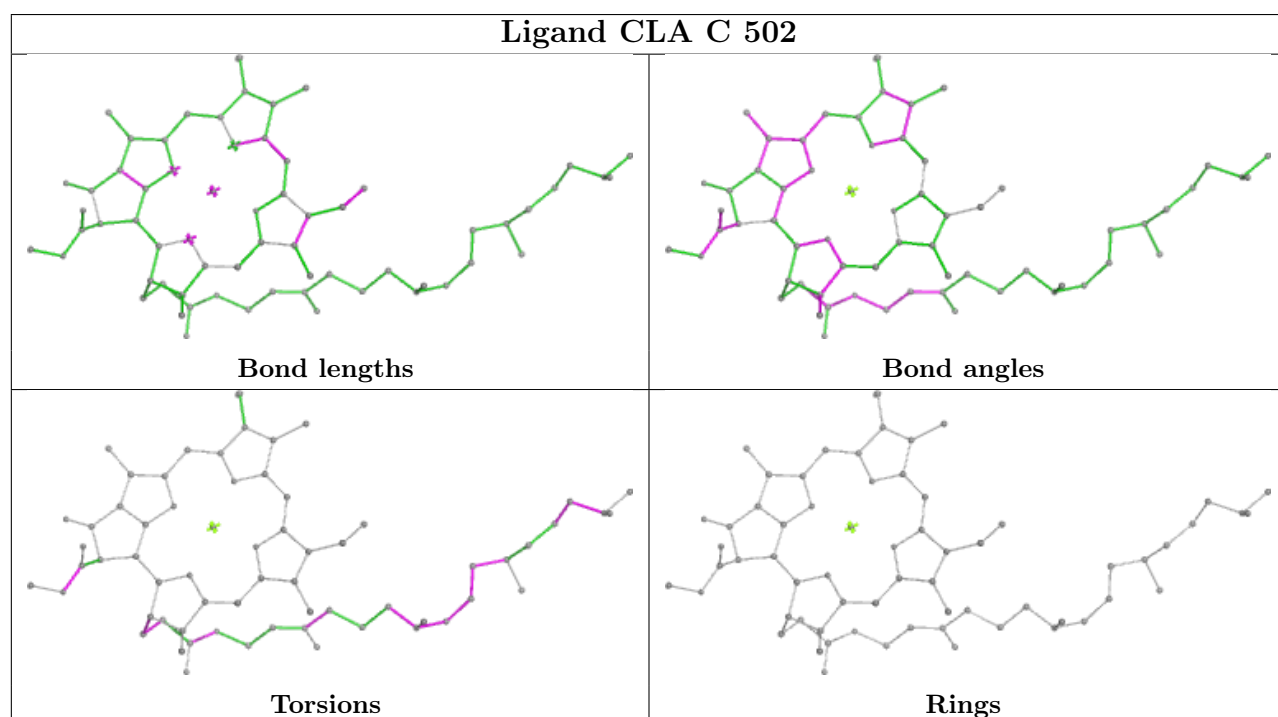
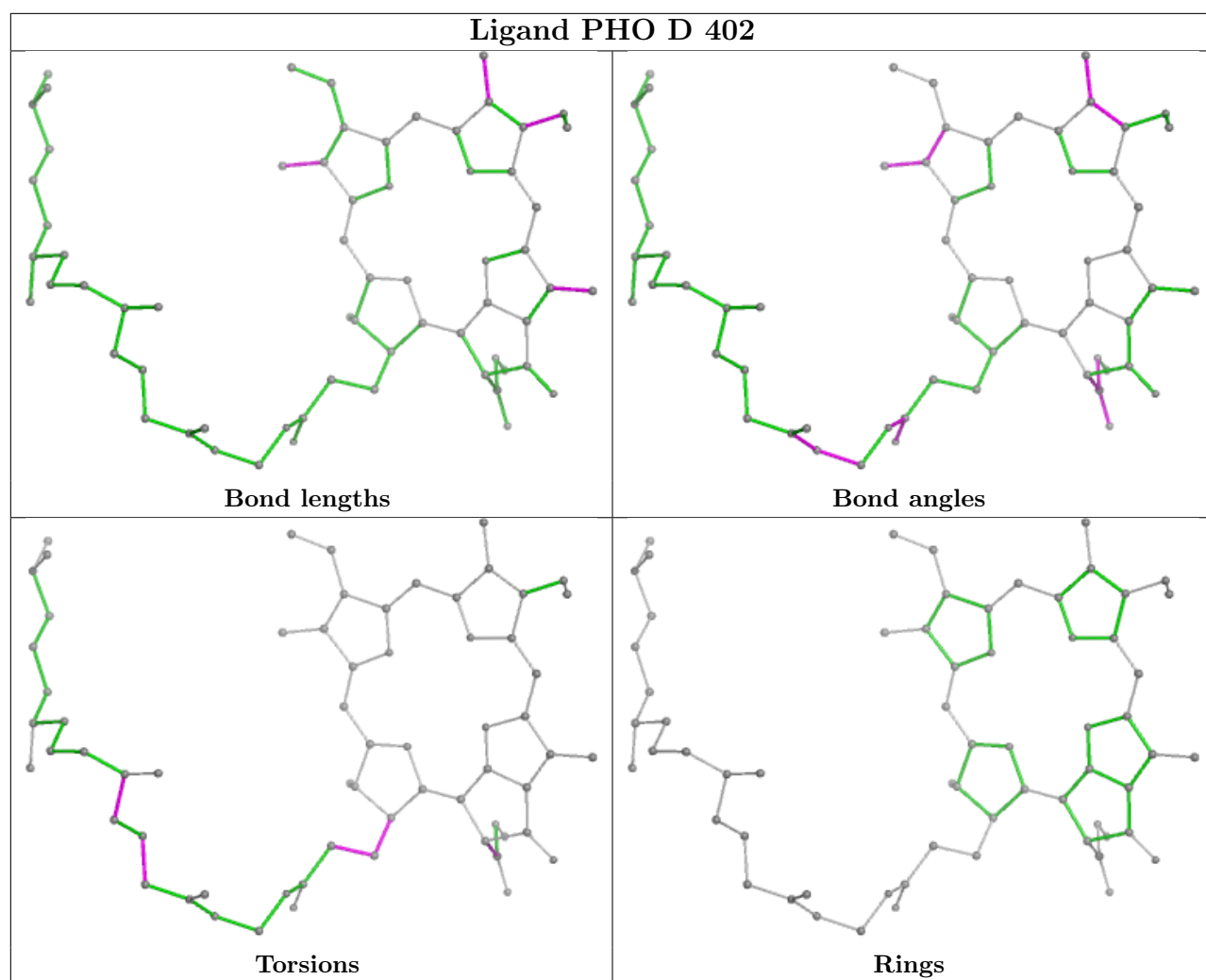


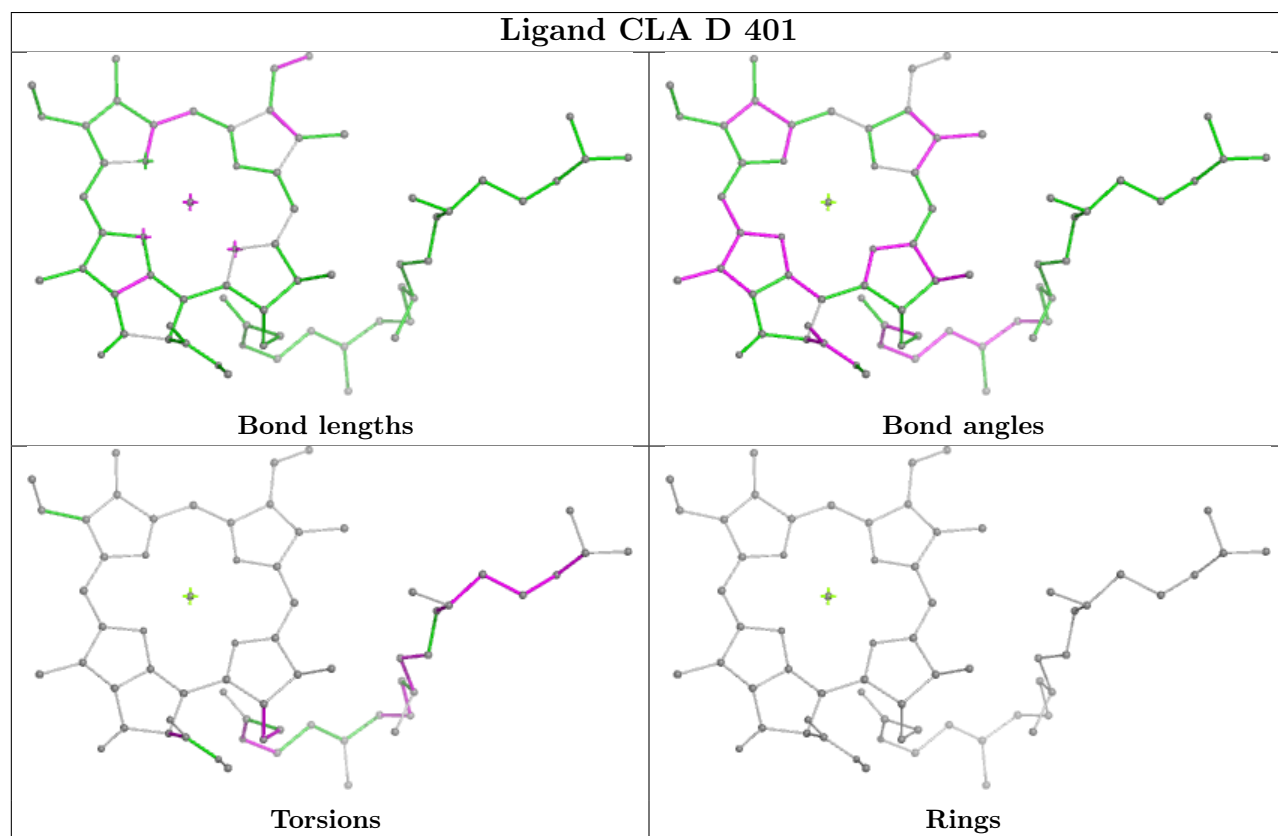
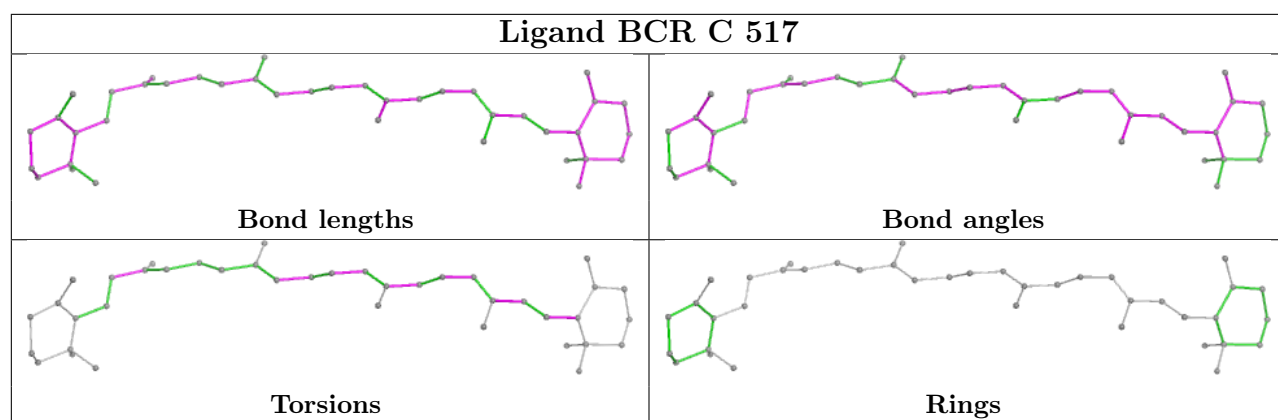
Torsions

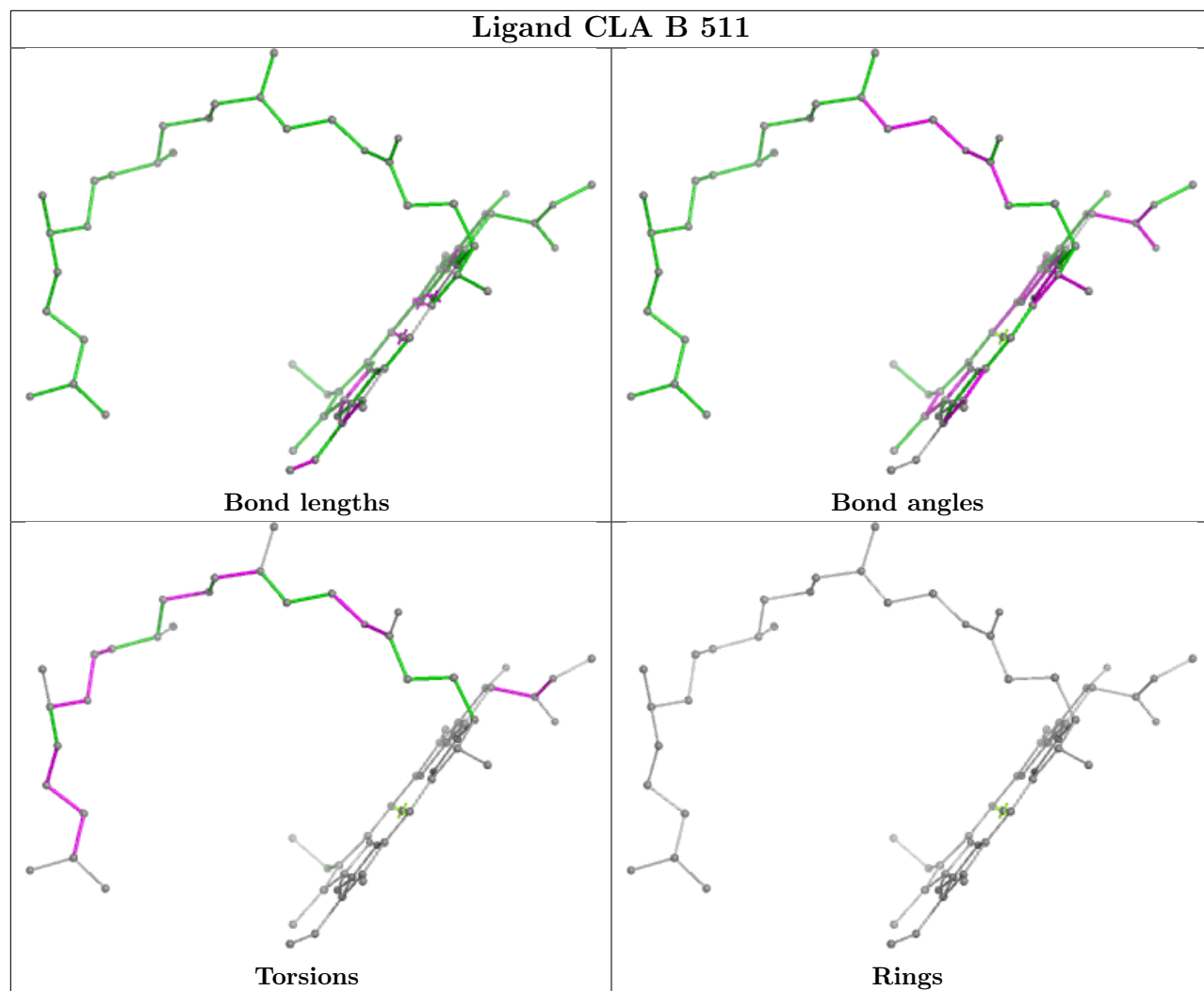


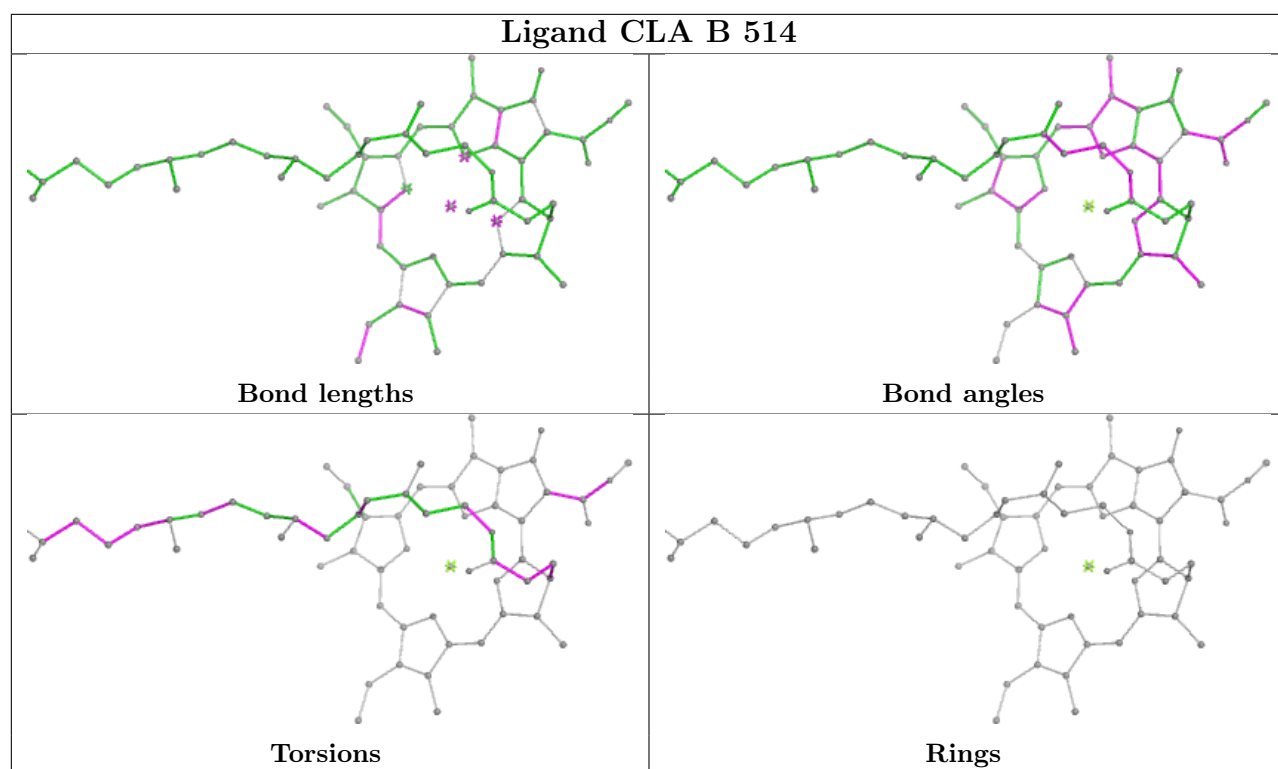
Rings

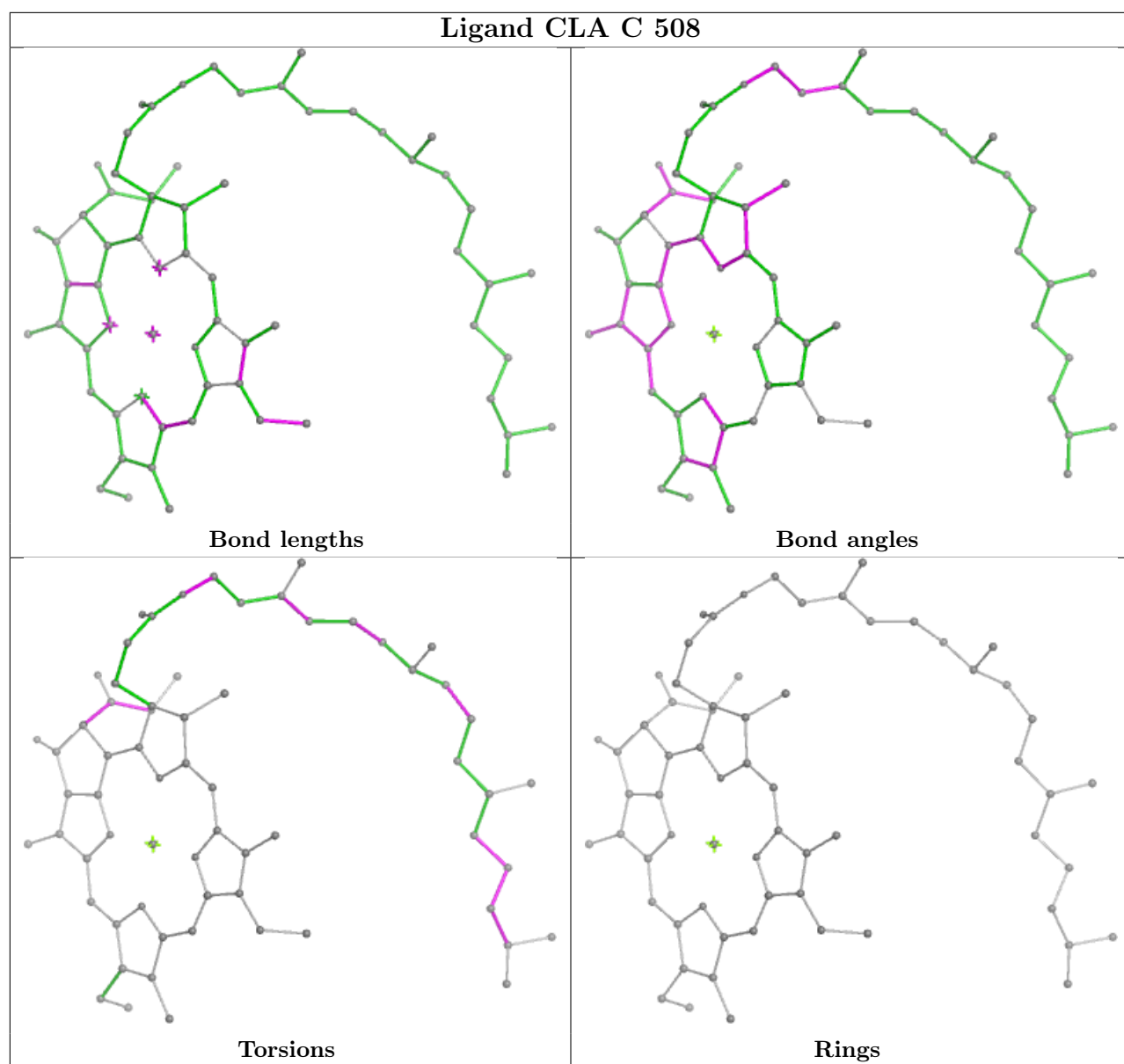


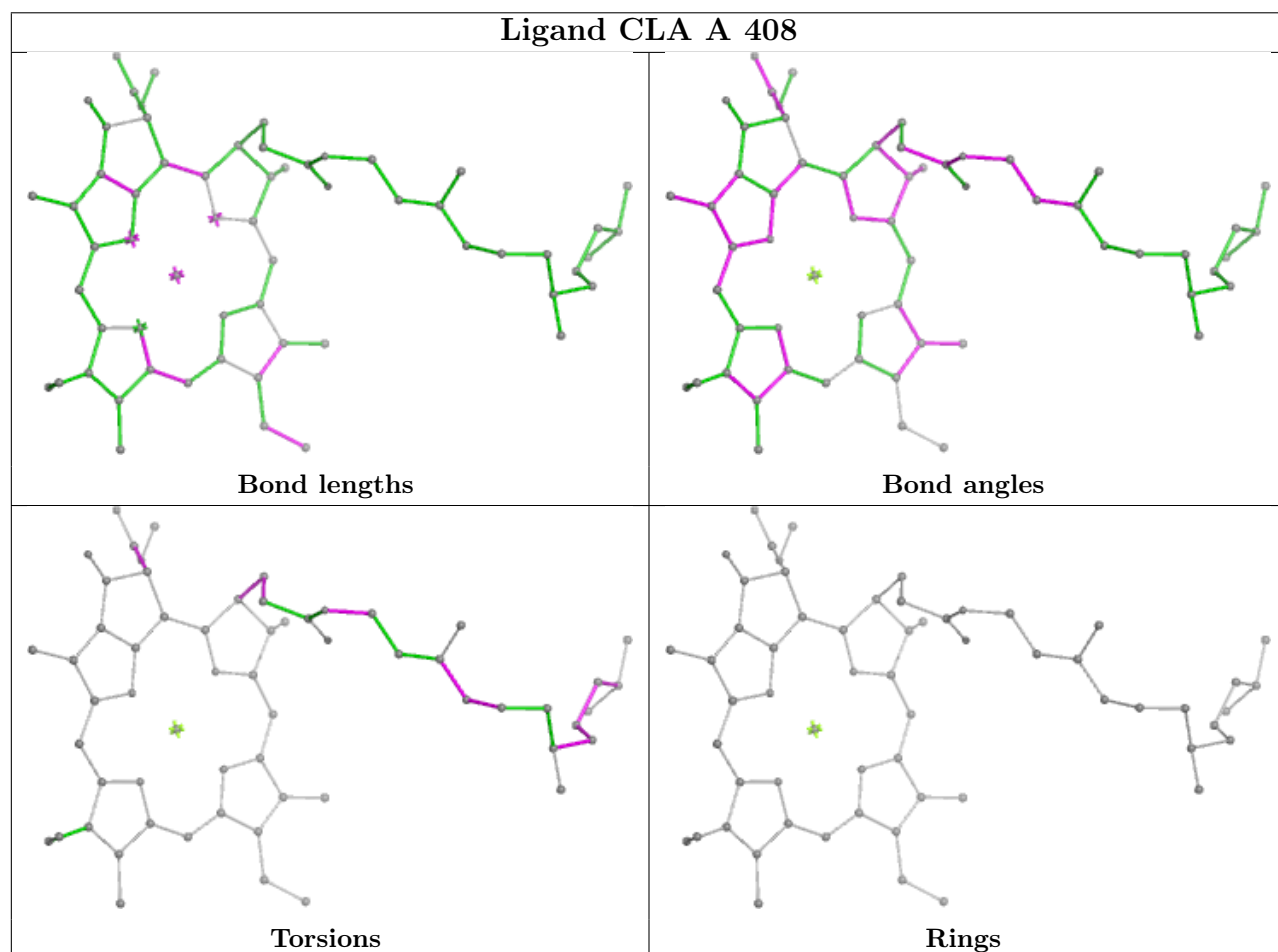
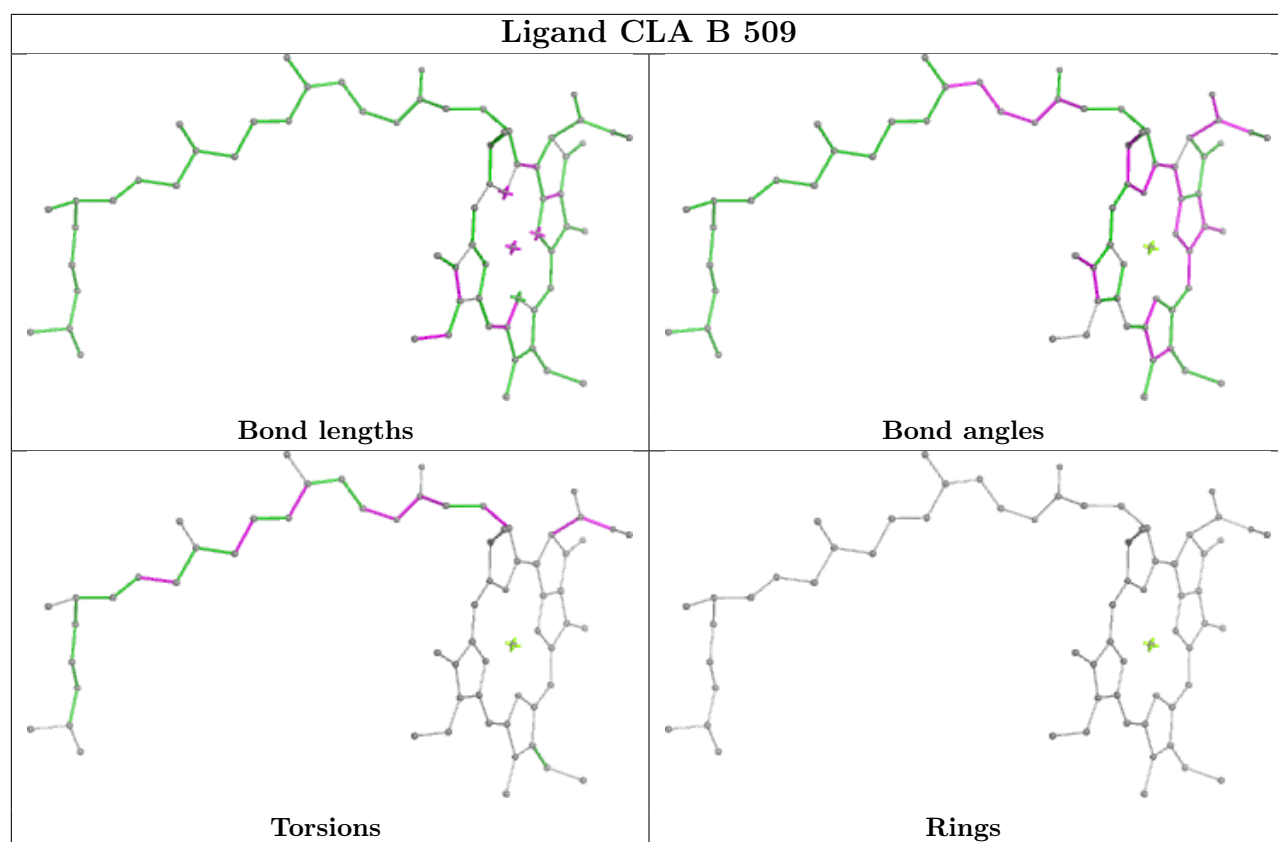




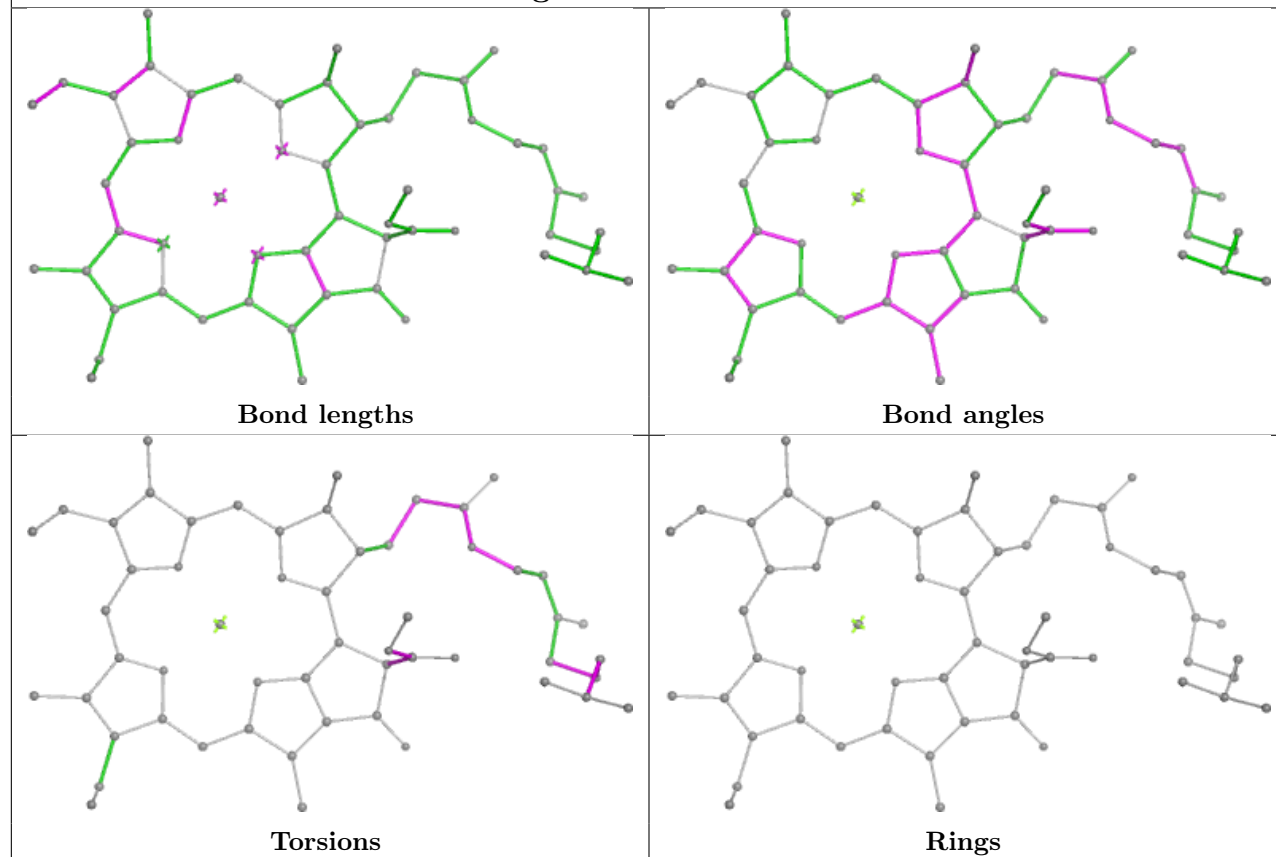




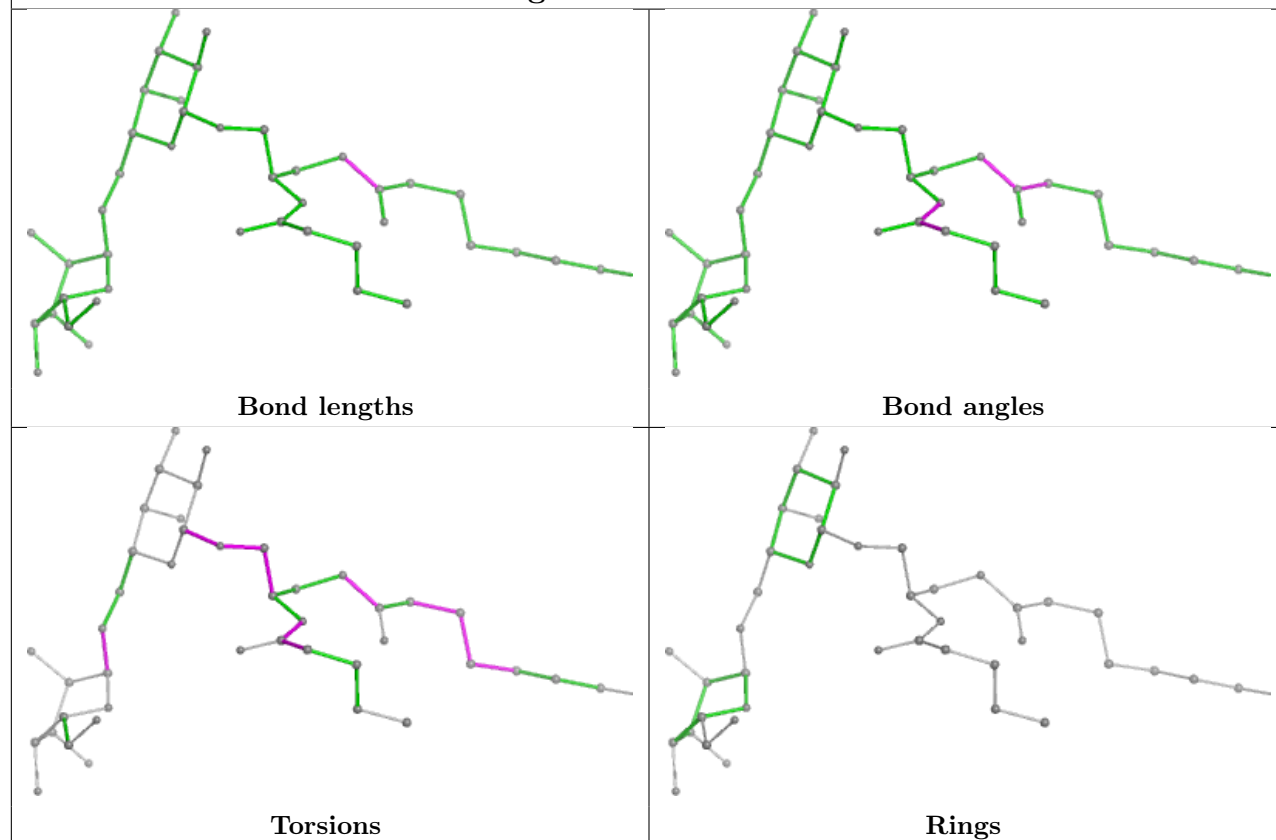


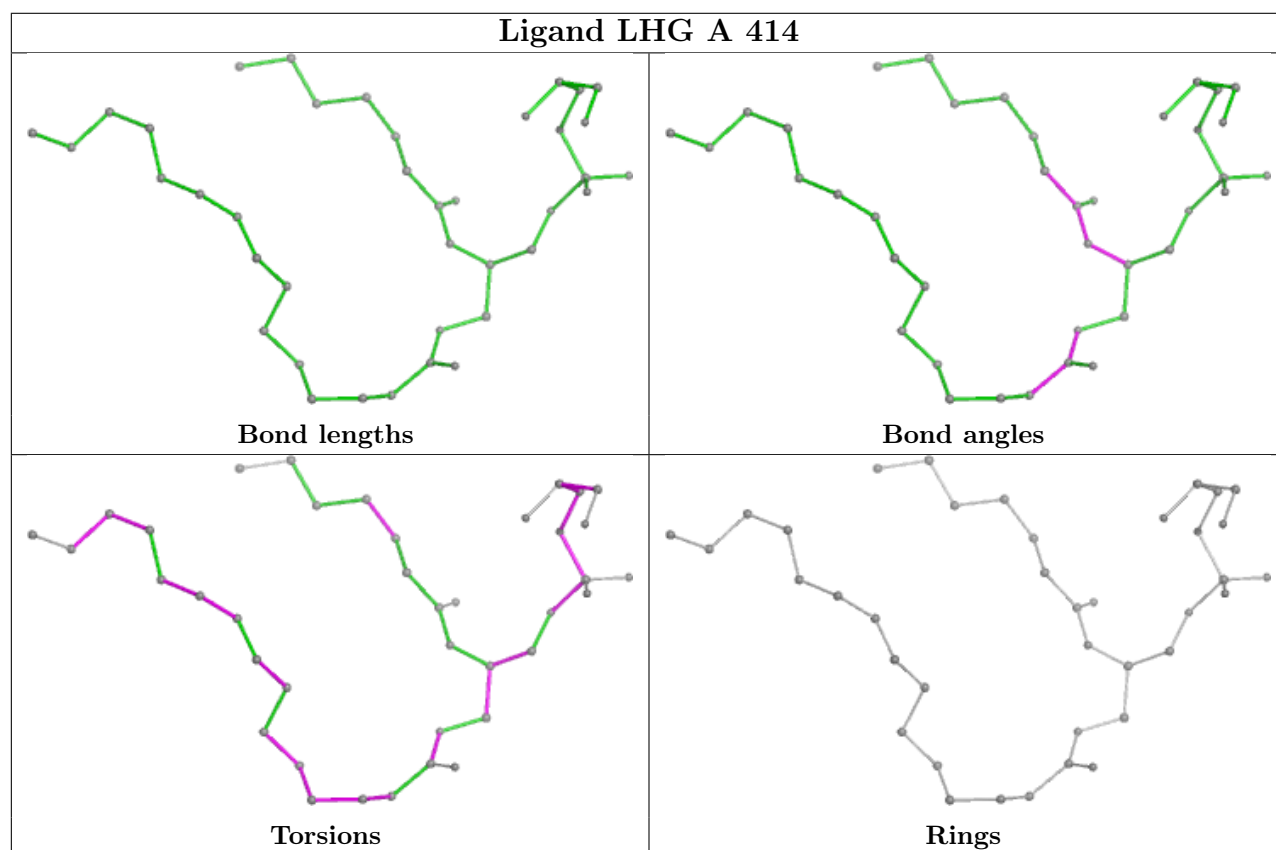
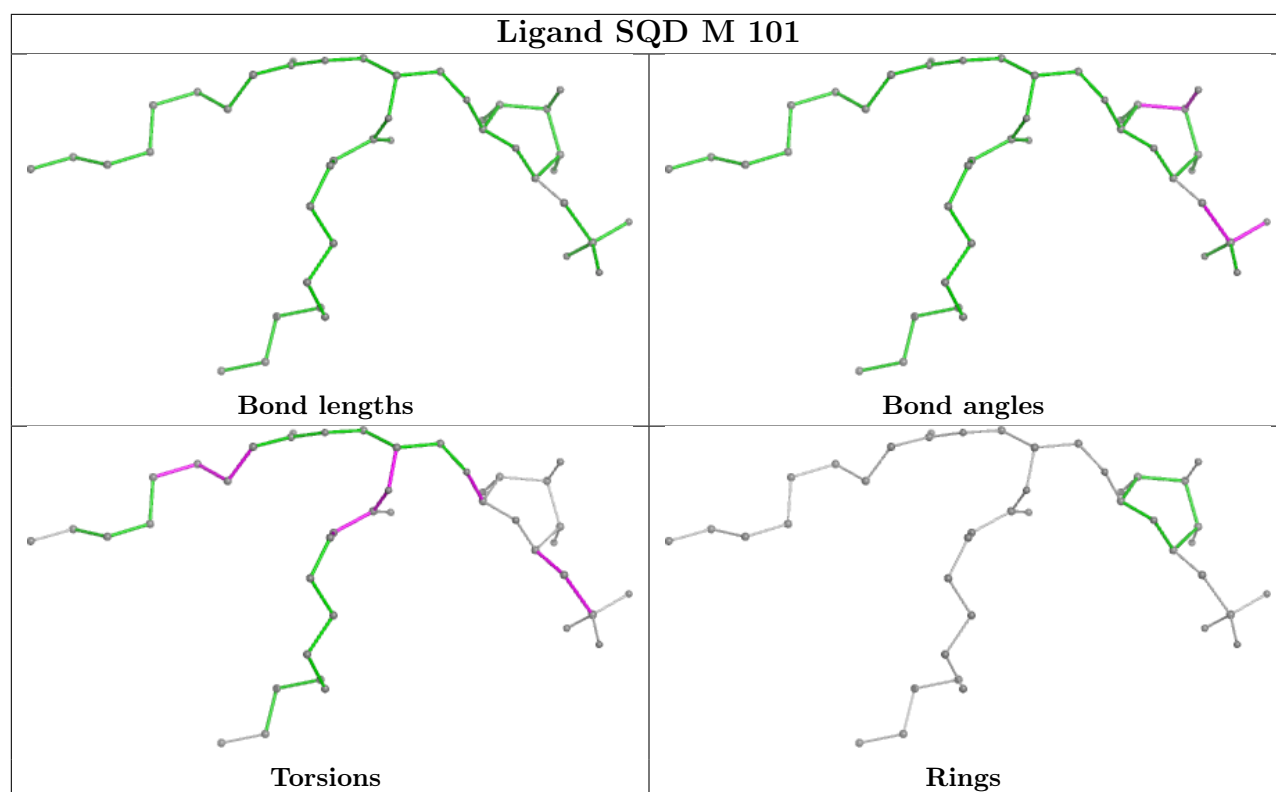


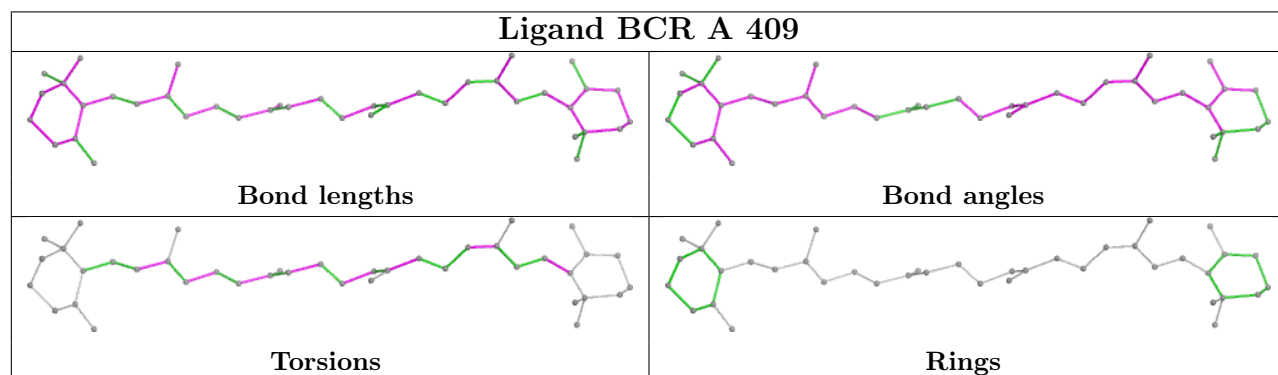
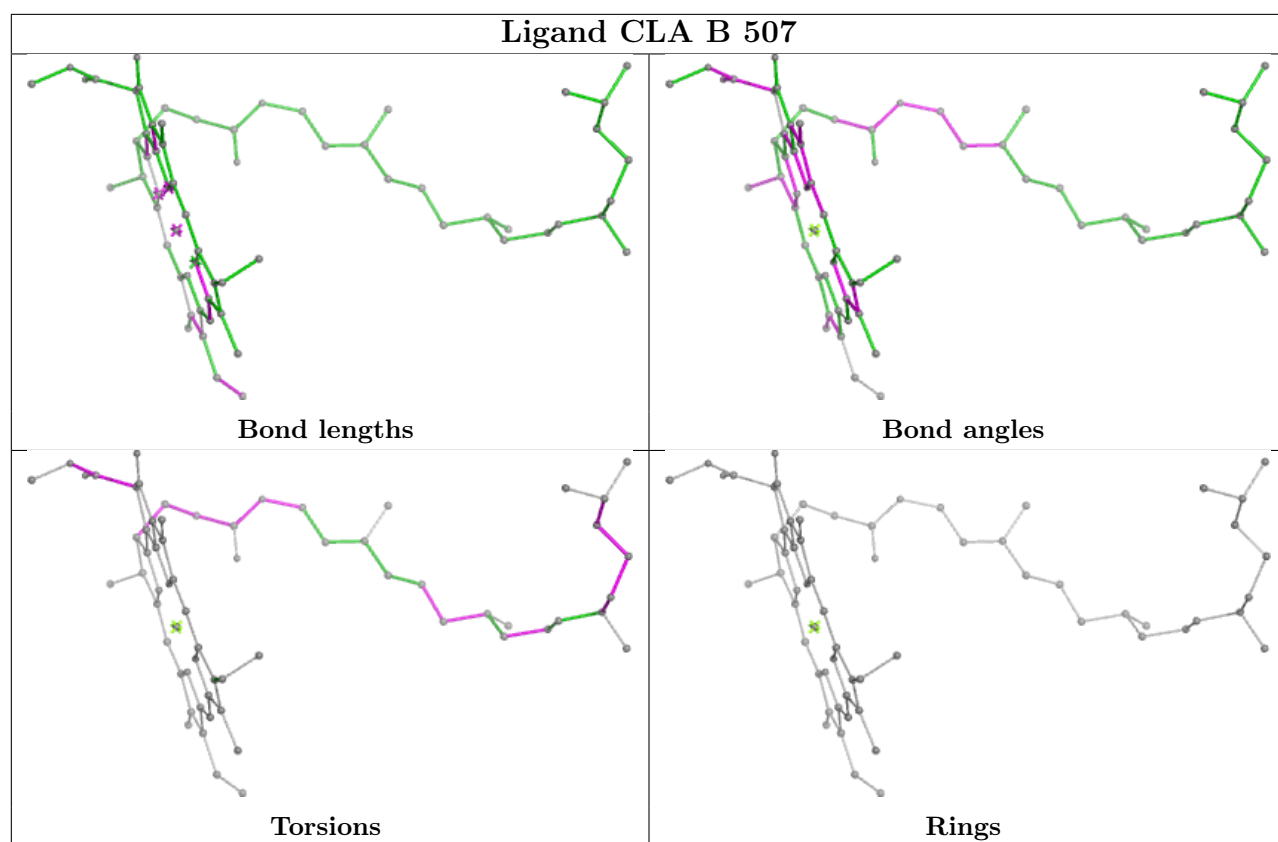
Ligand CLA B 516

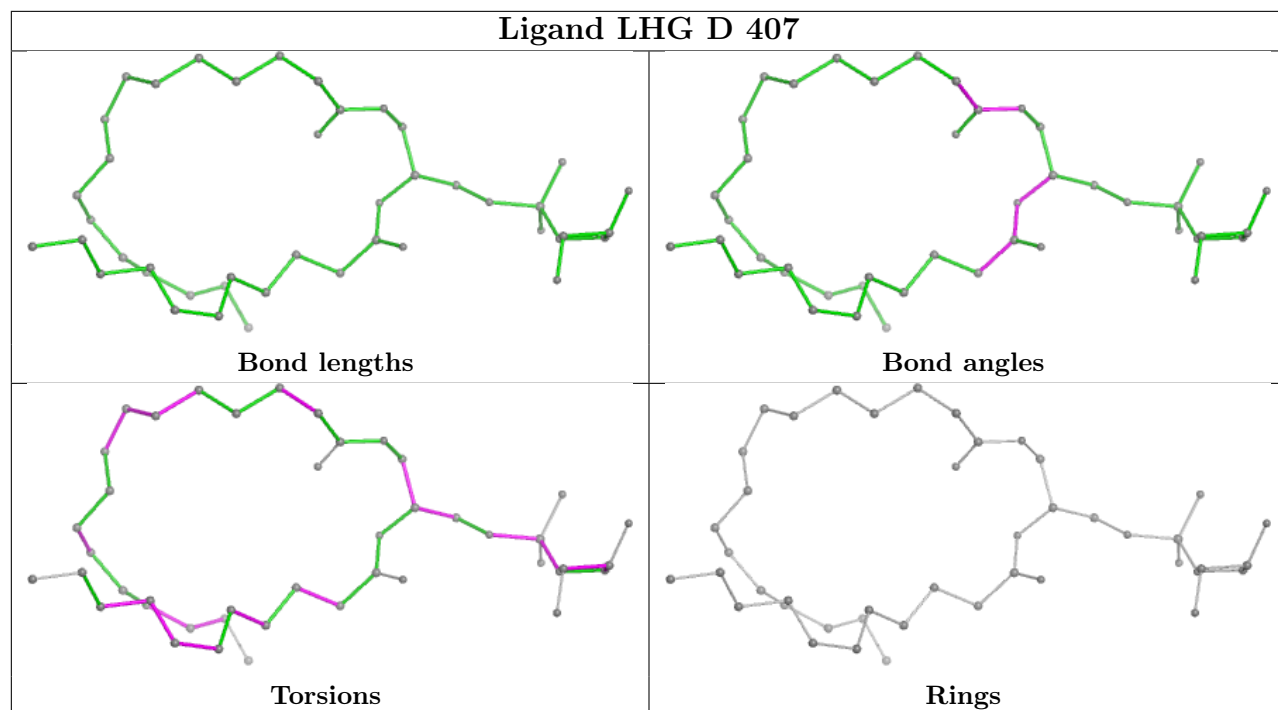


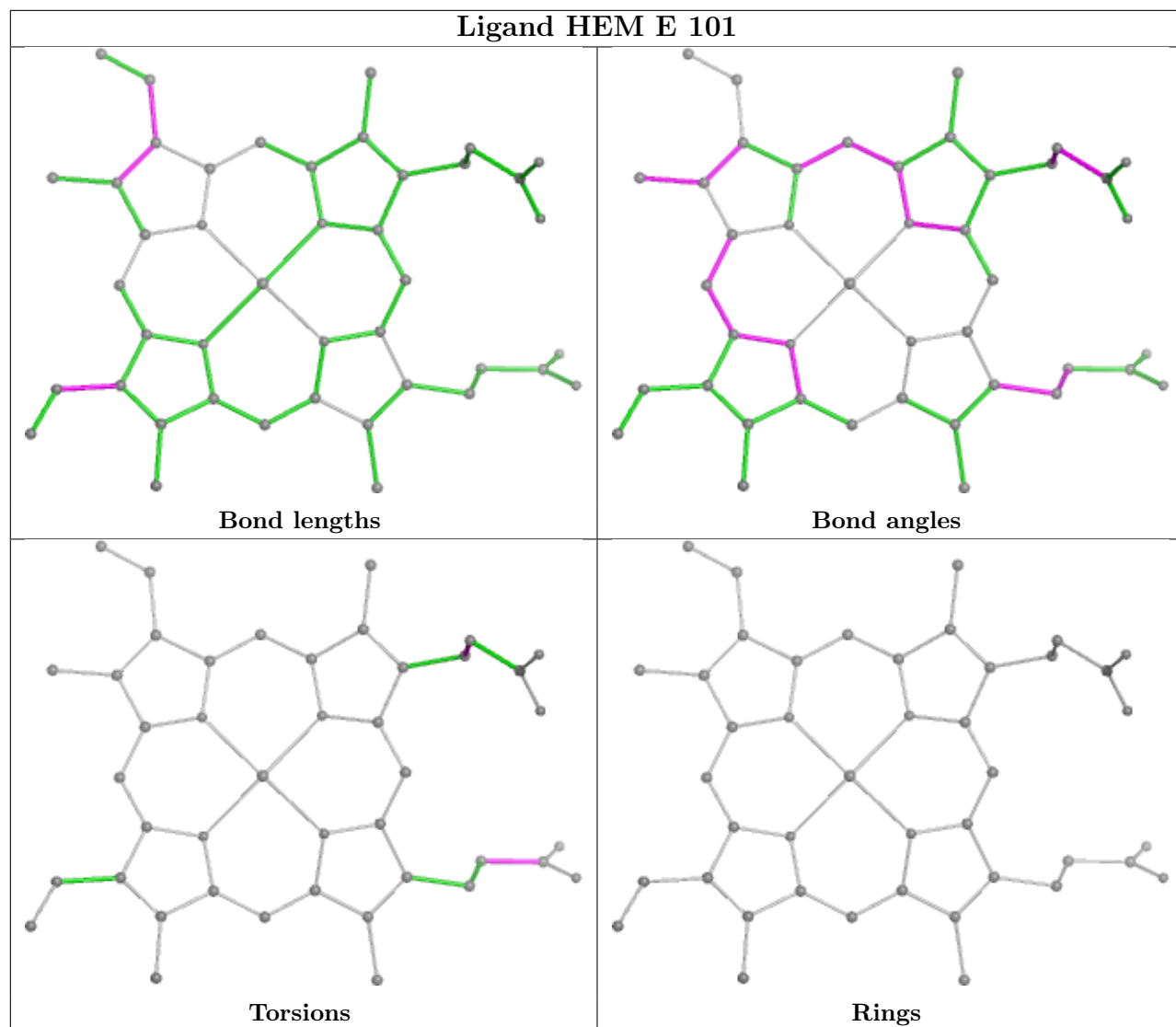
Ligand DGD B 521

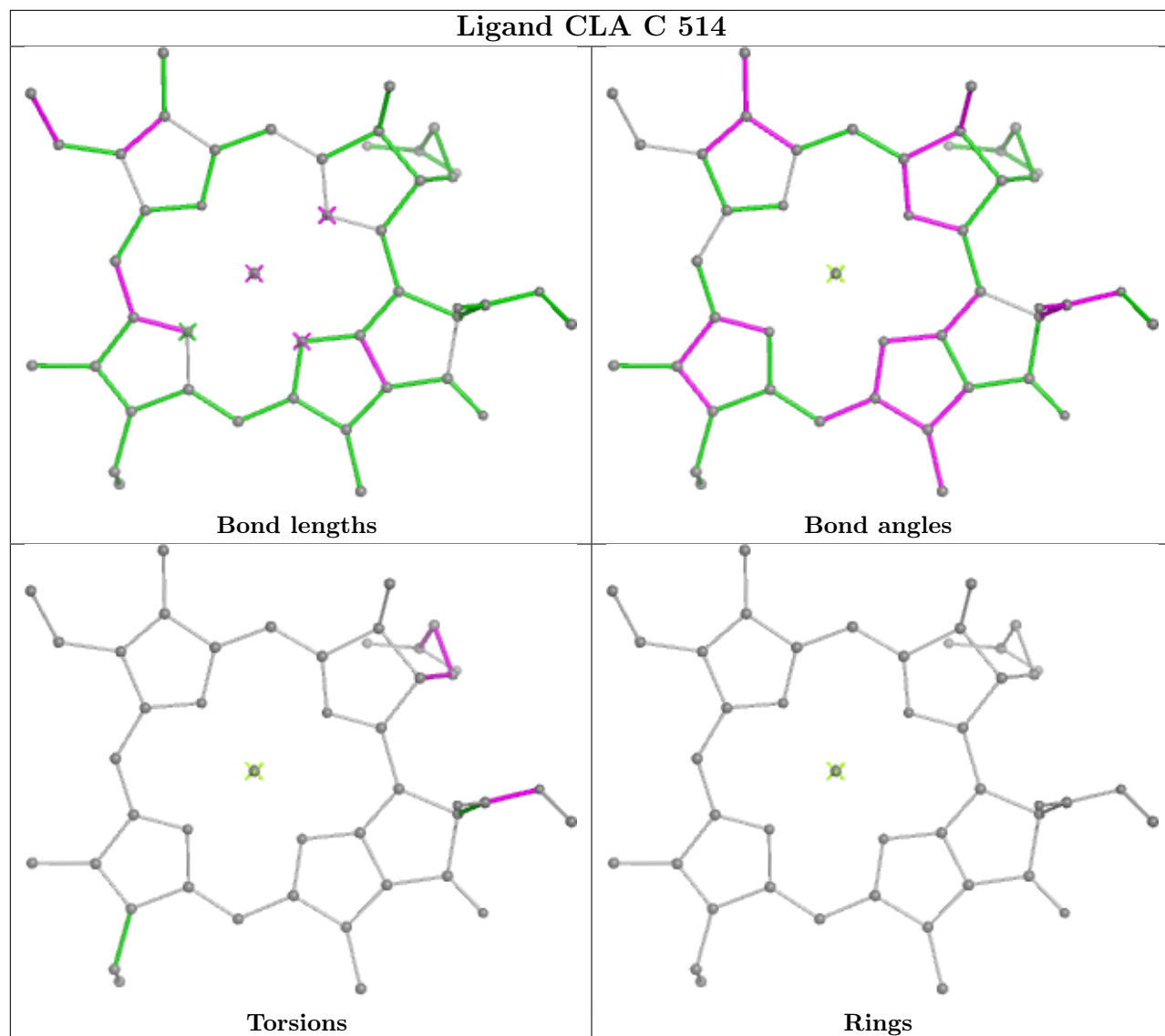


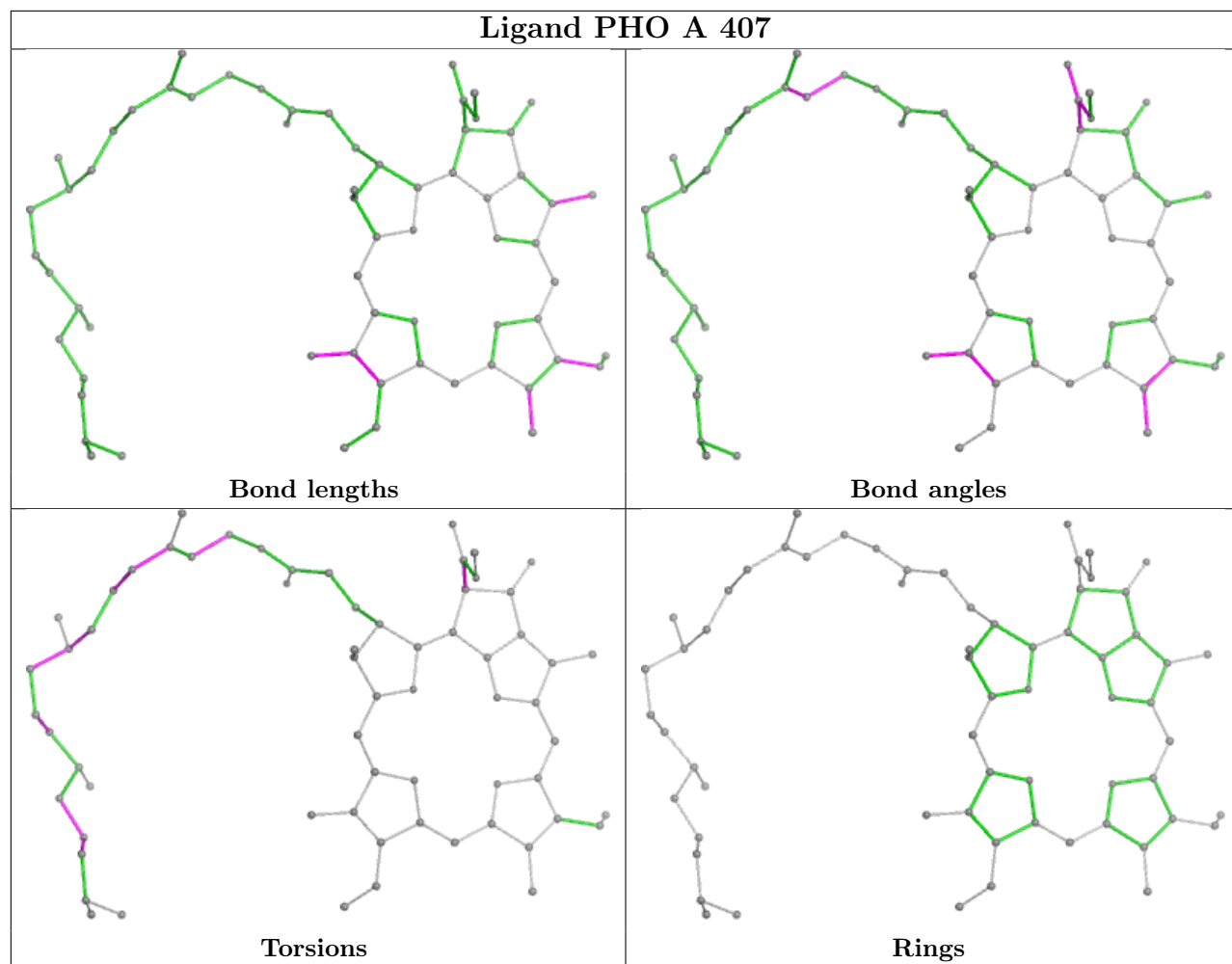


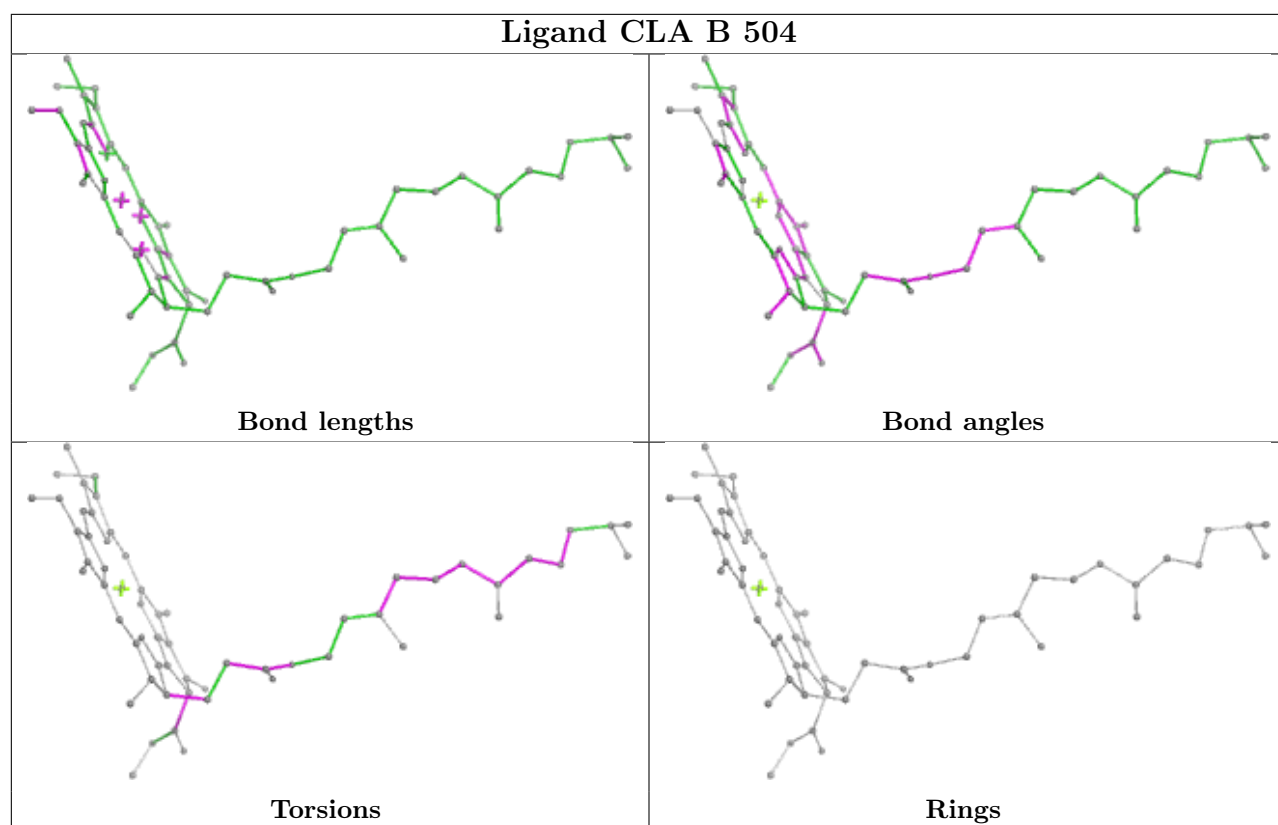


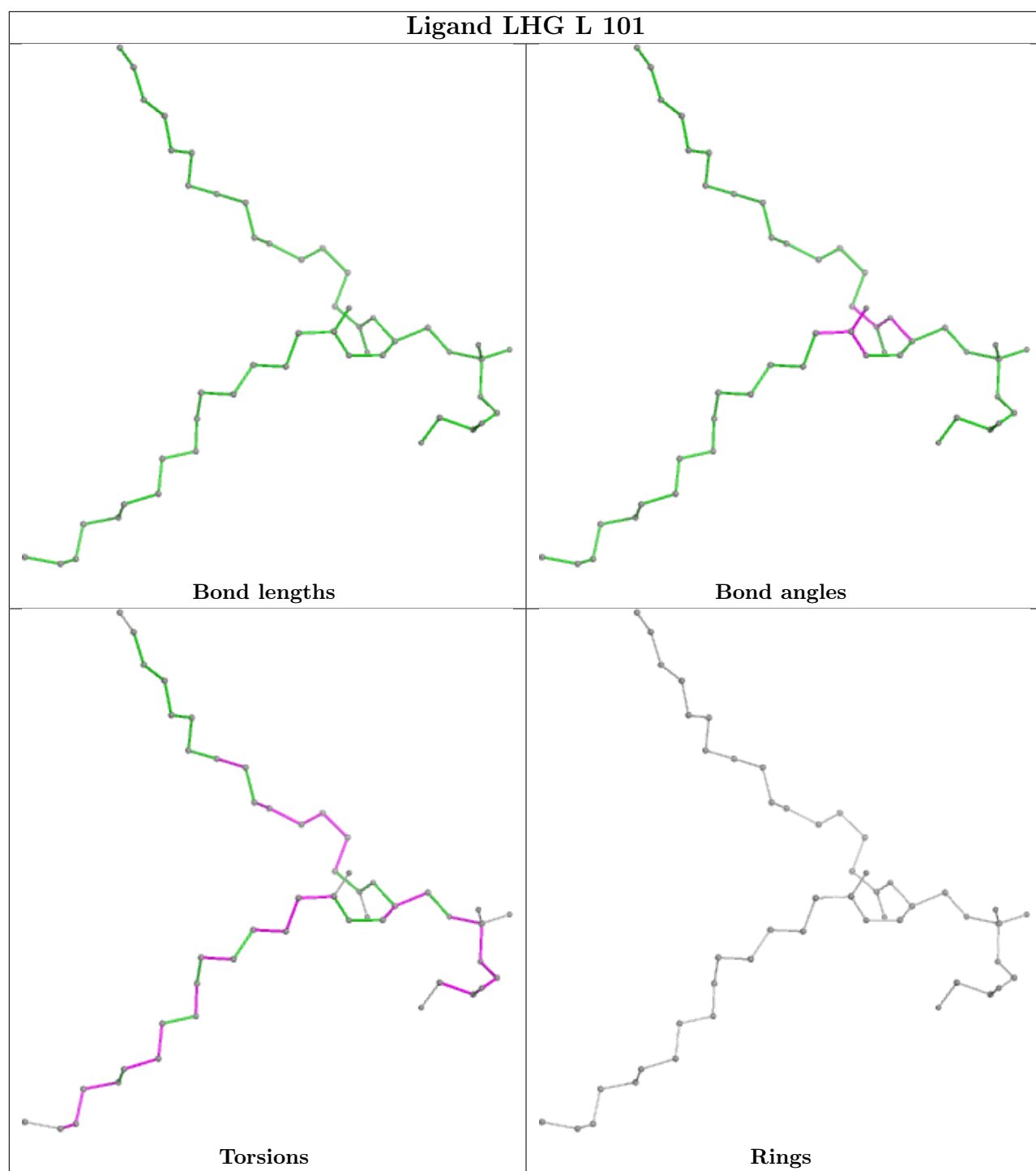




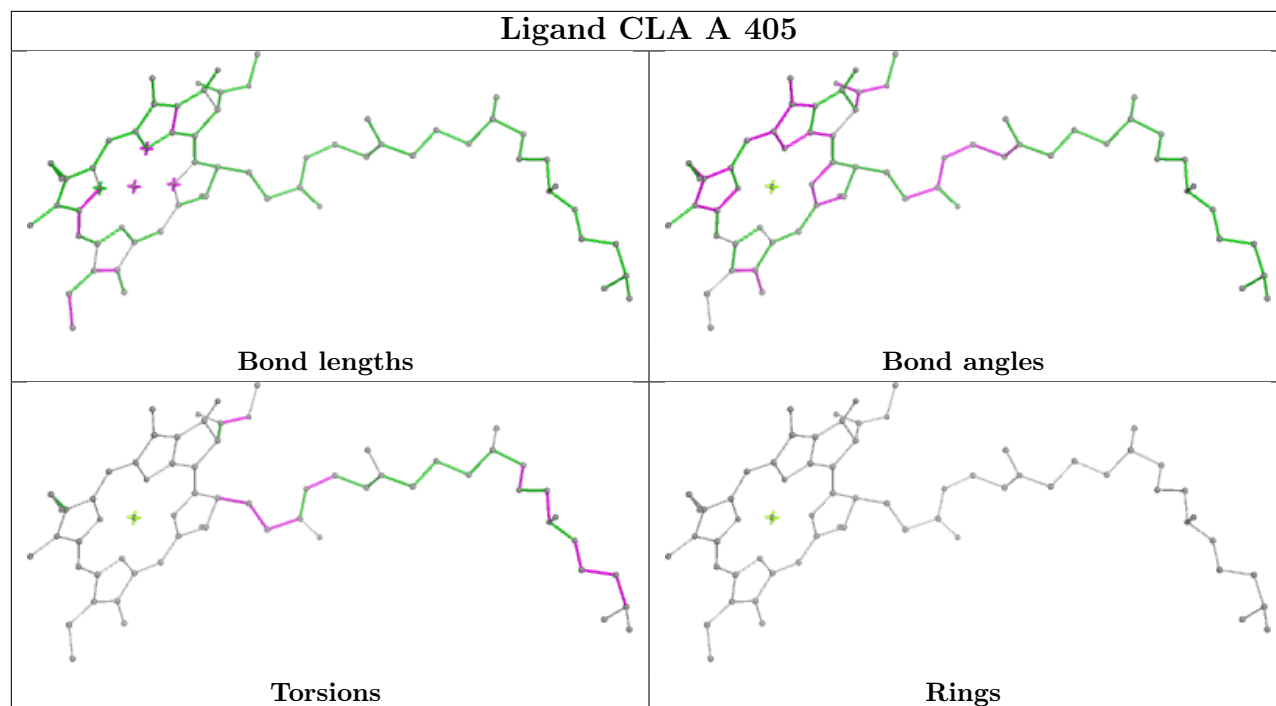




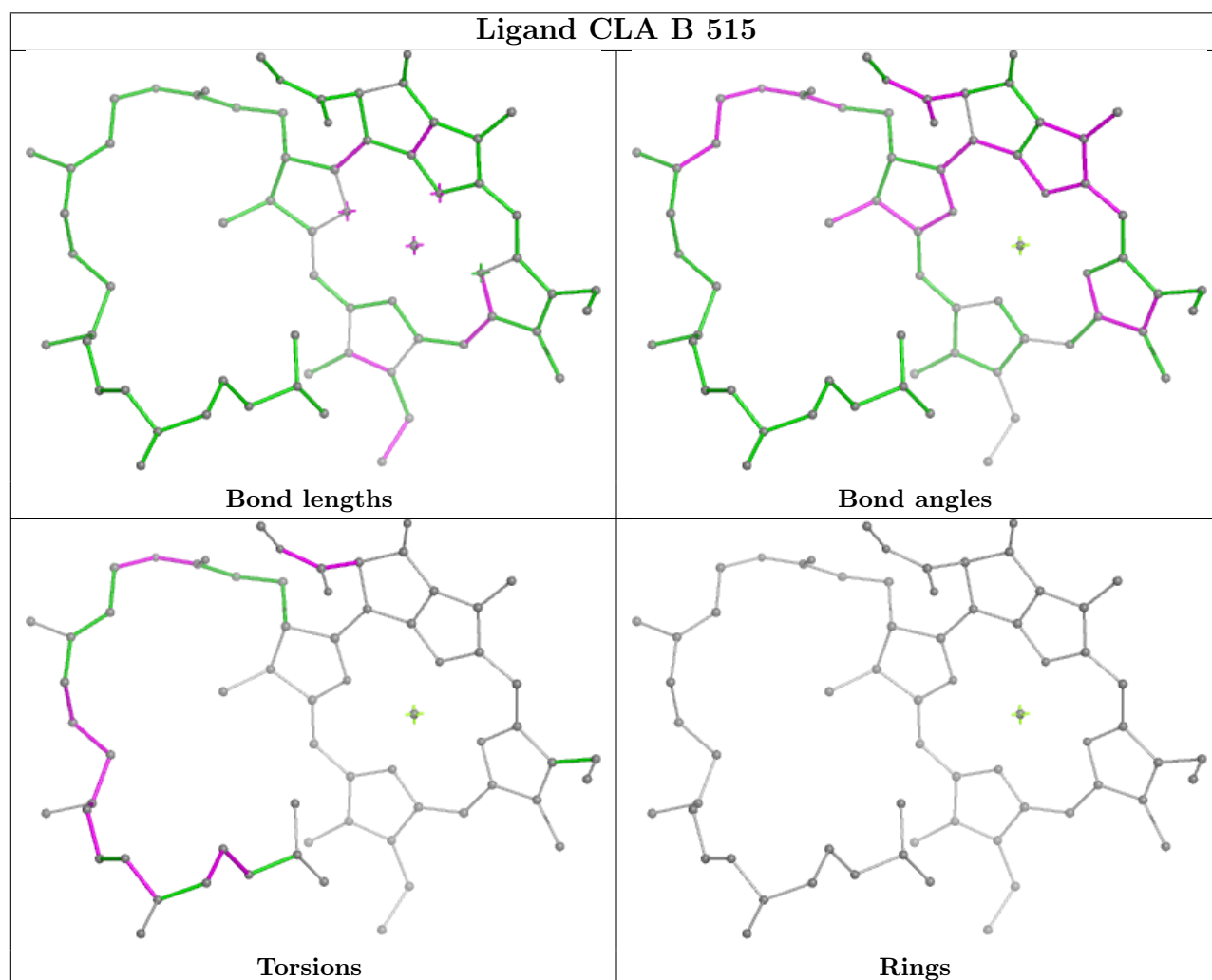


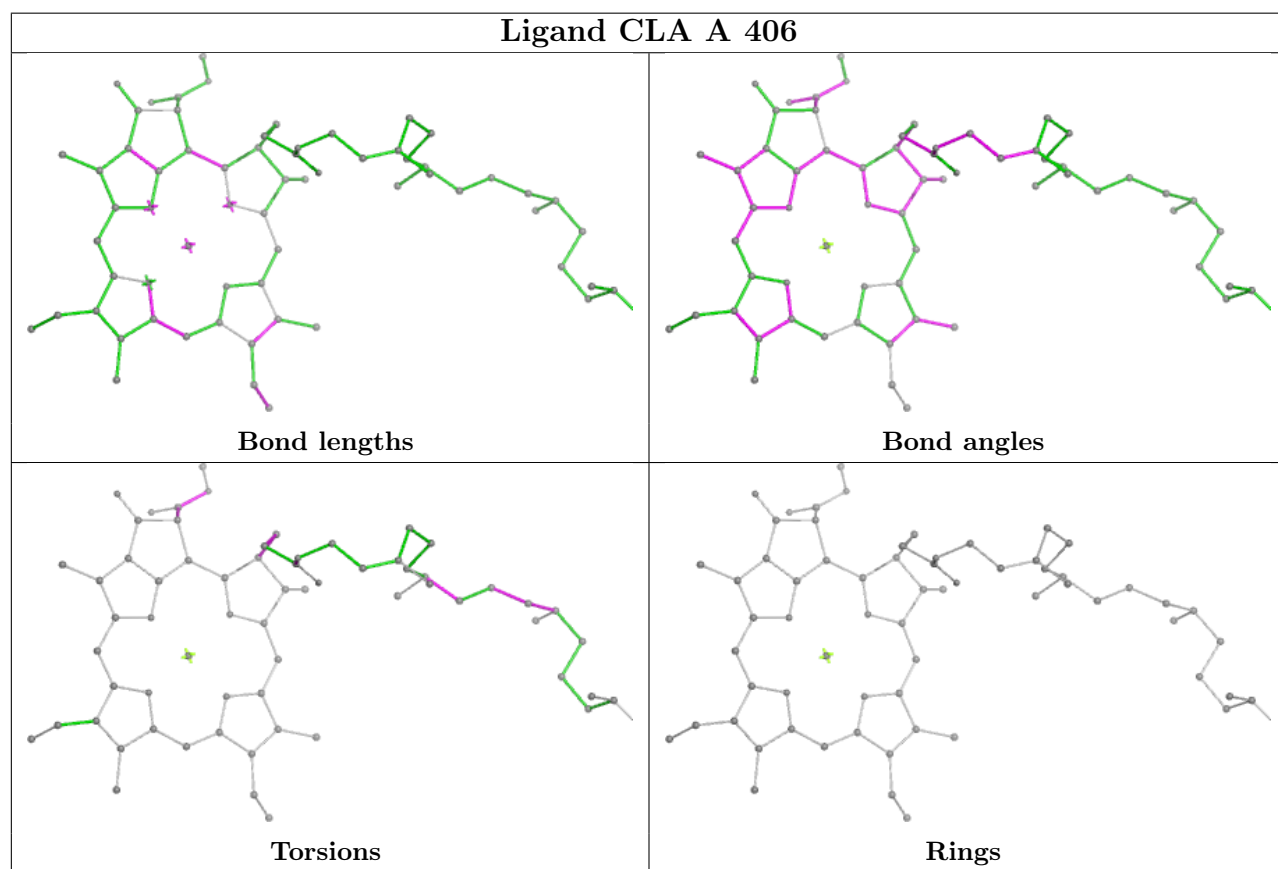
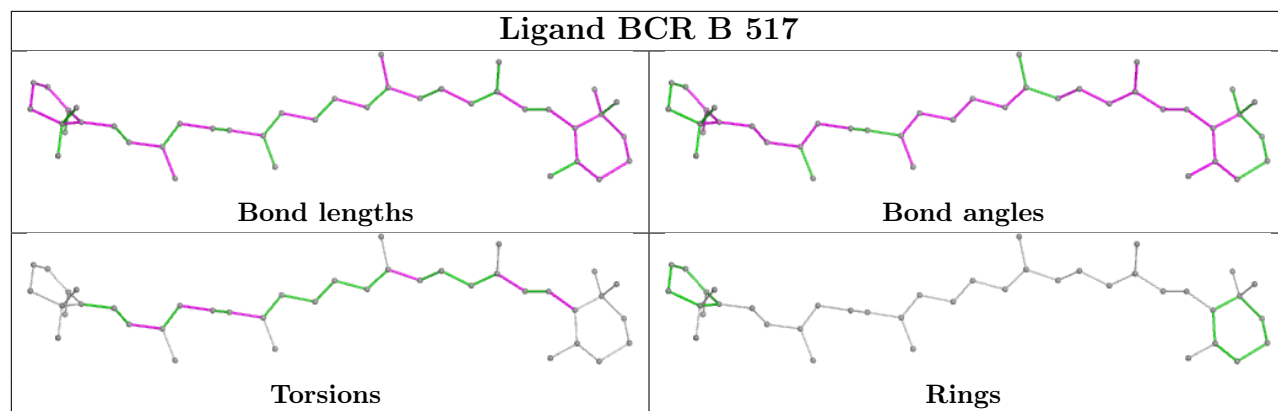


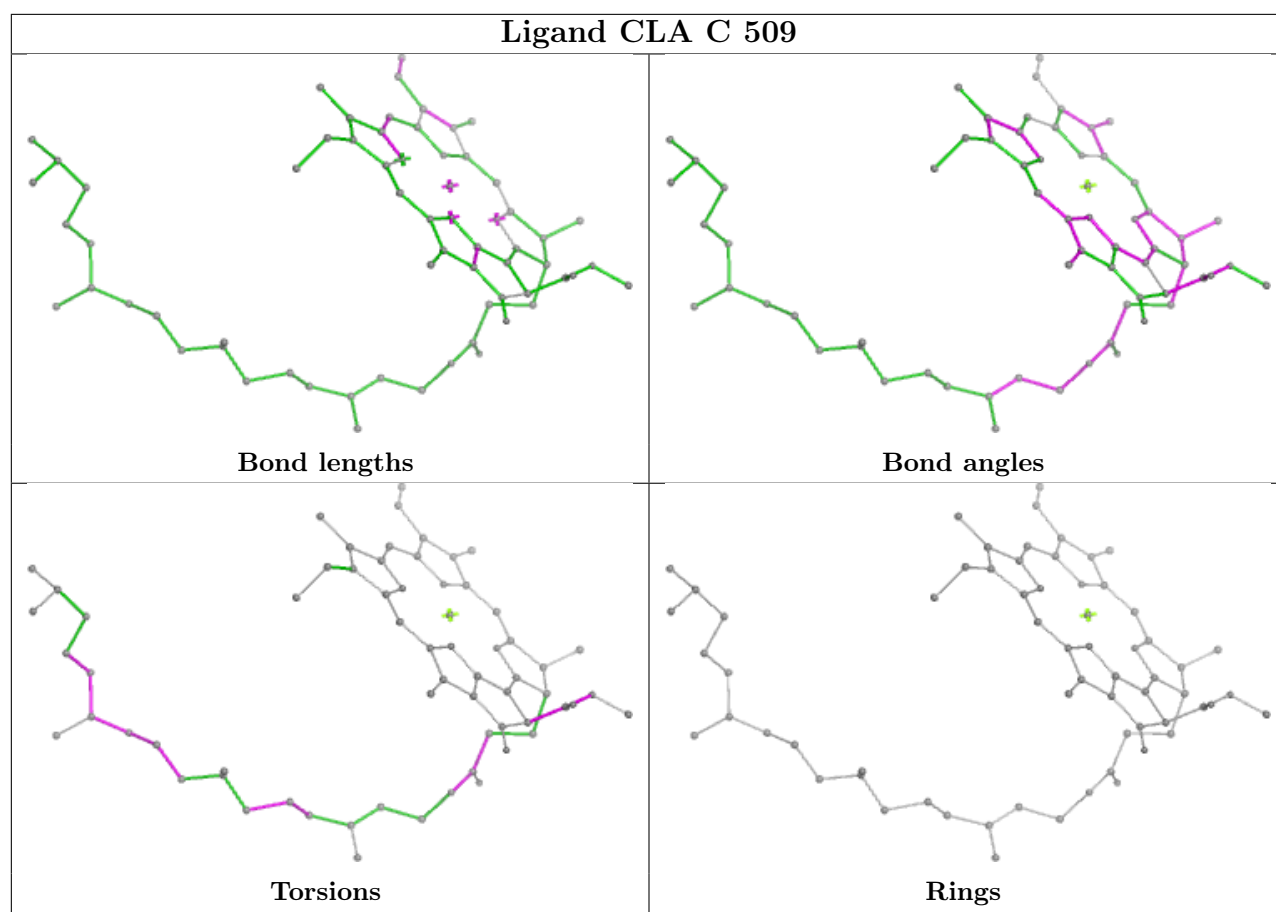
Ligand CLA A 405

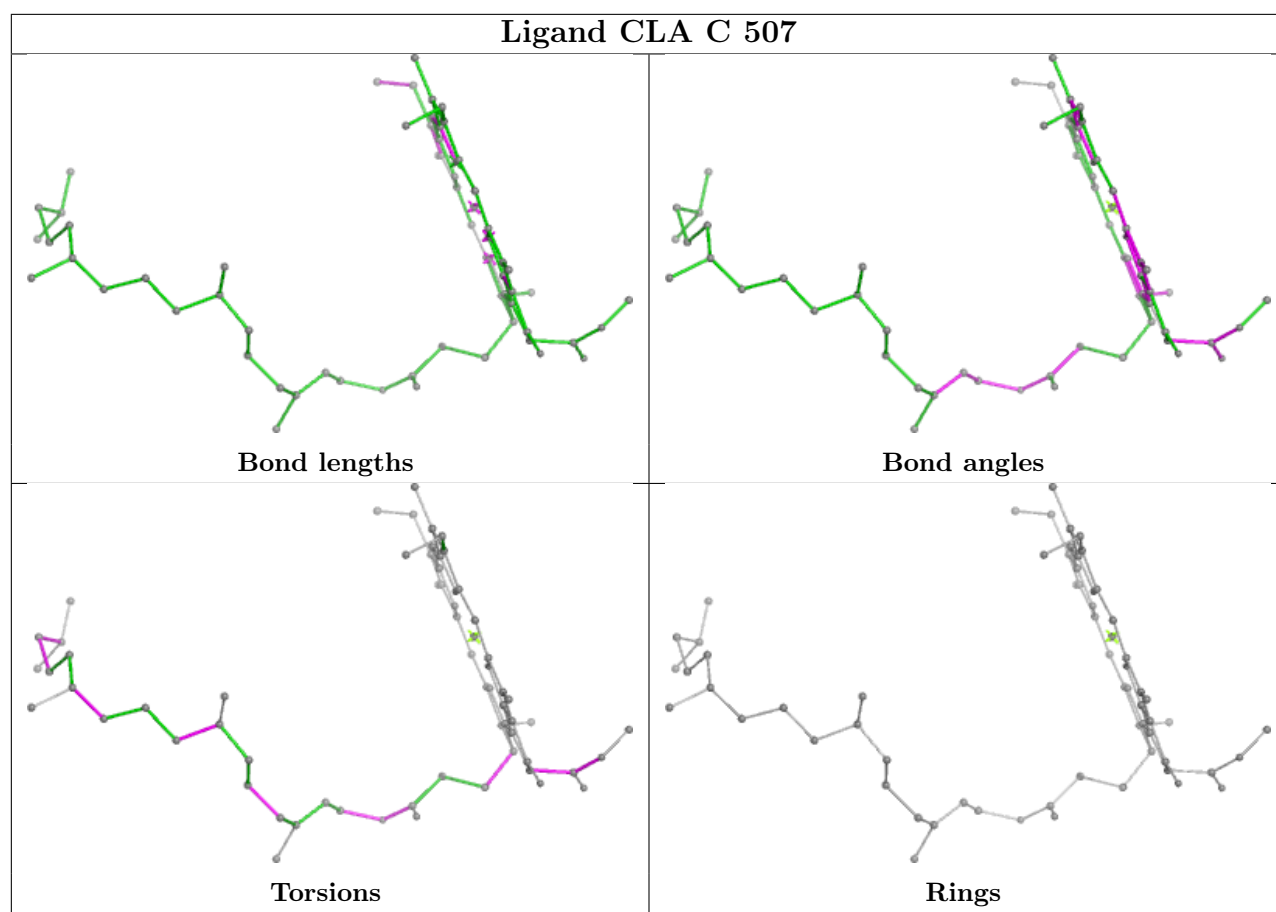


Ligand CLA B 515

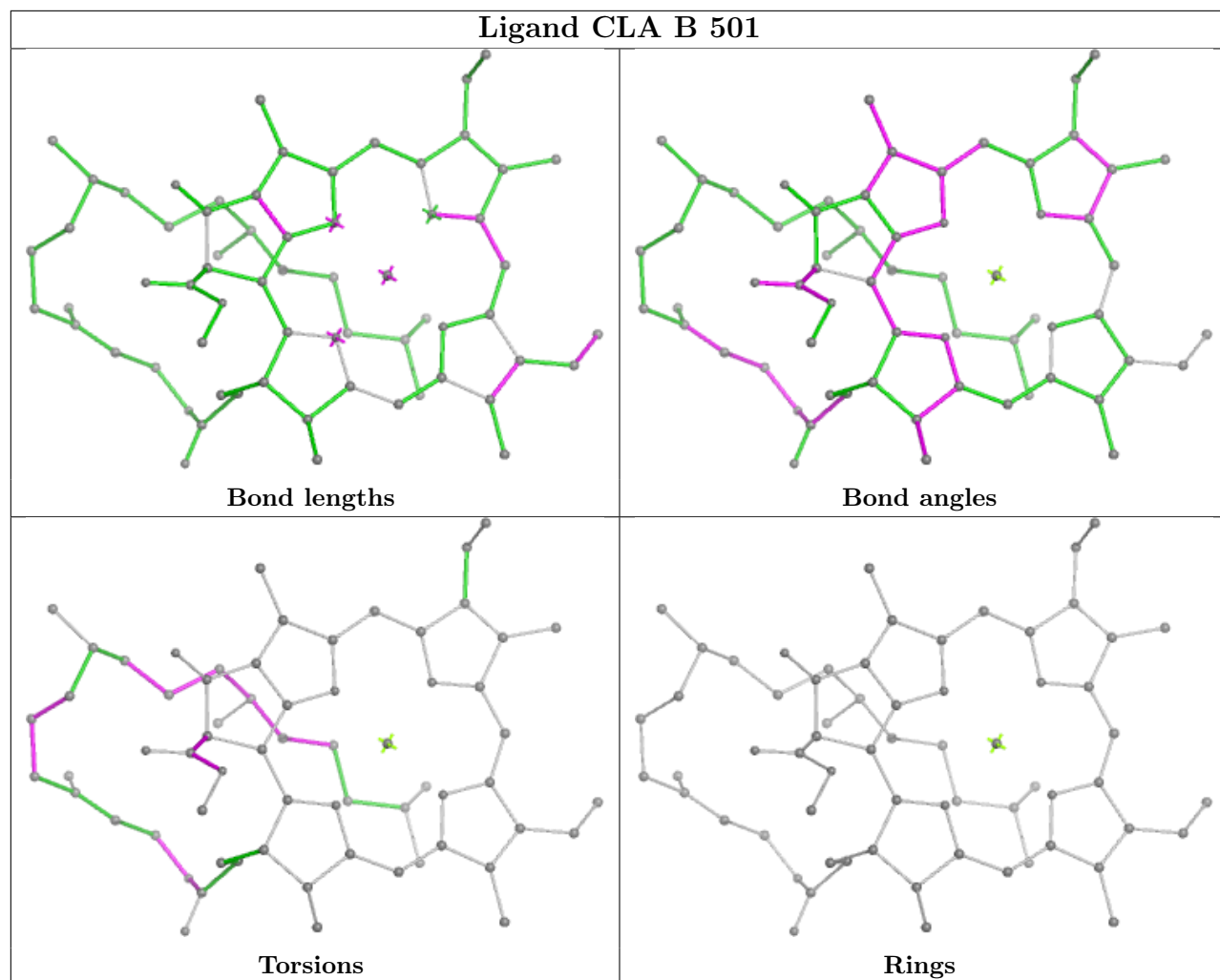


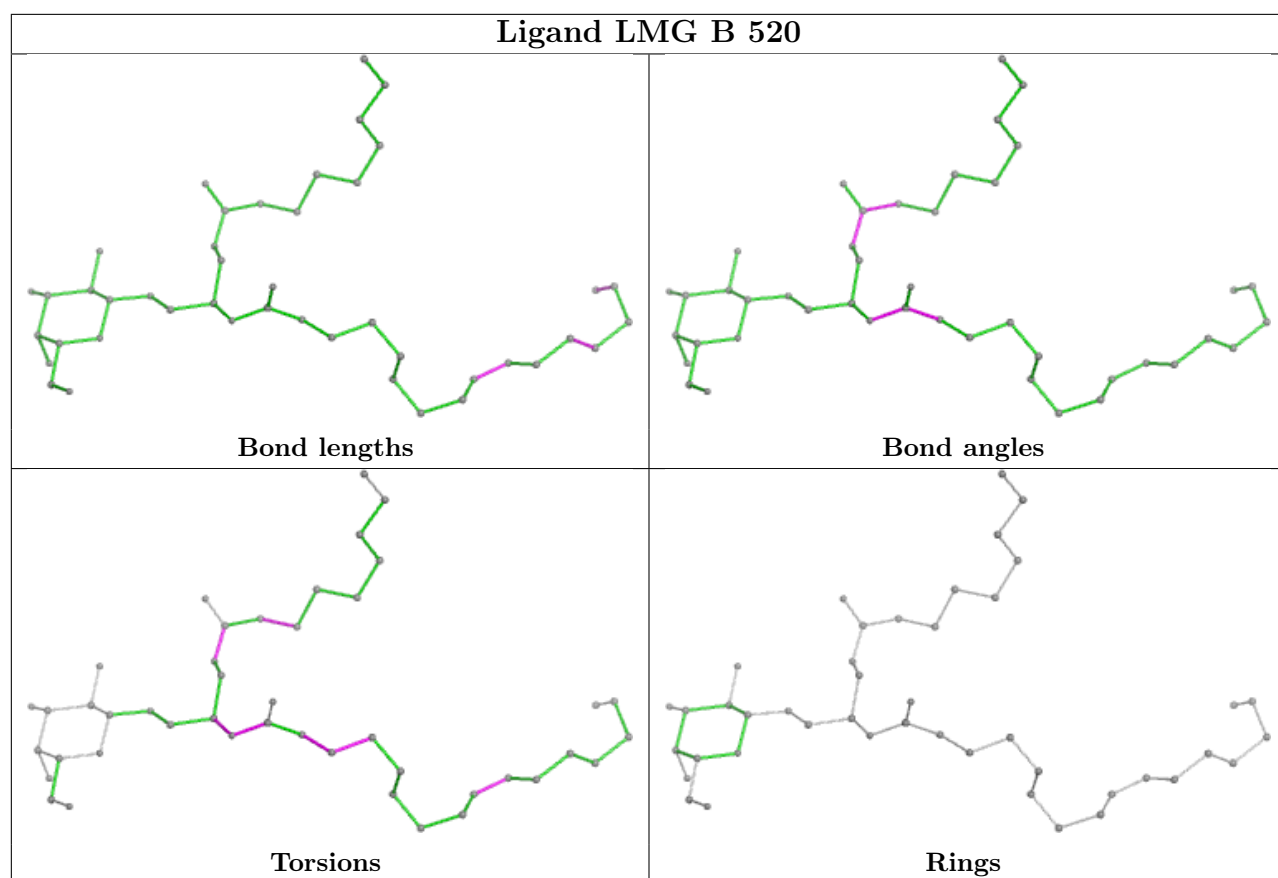


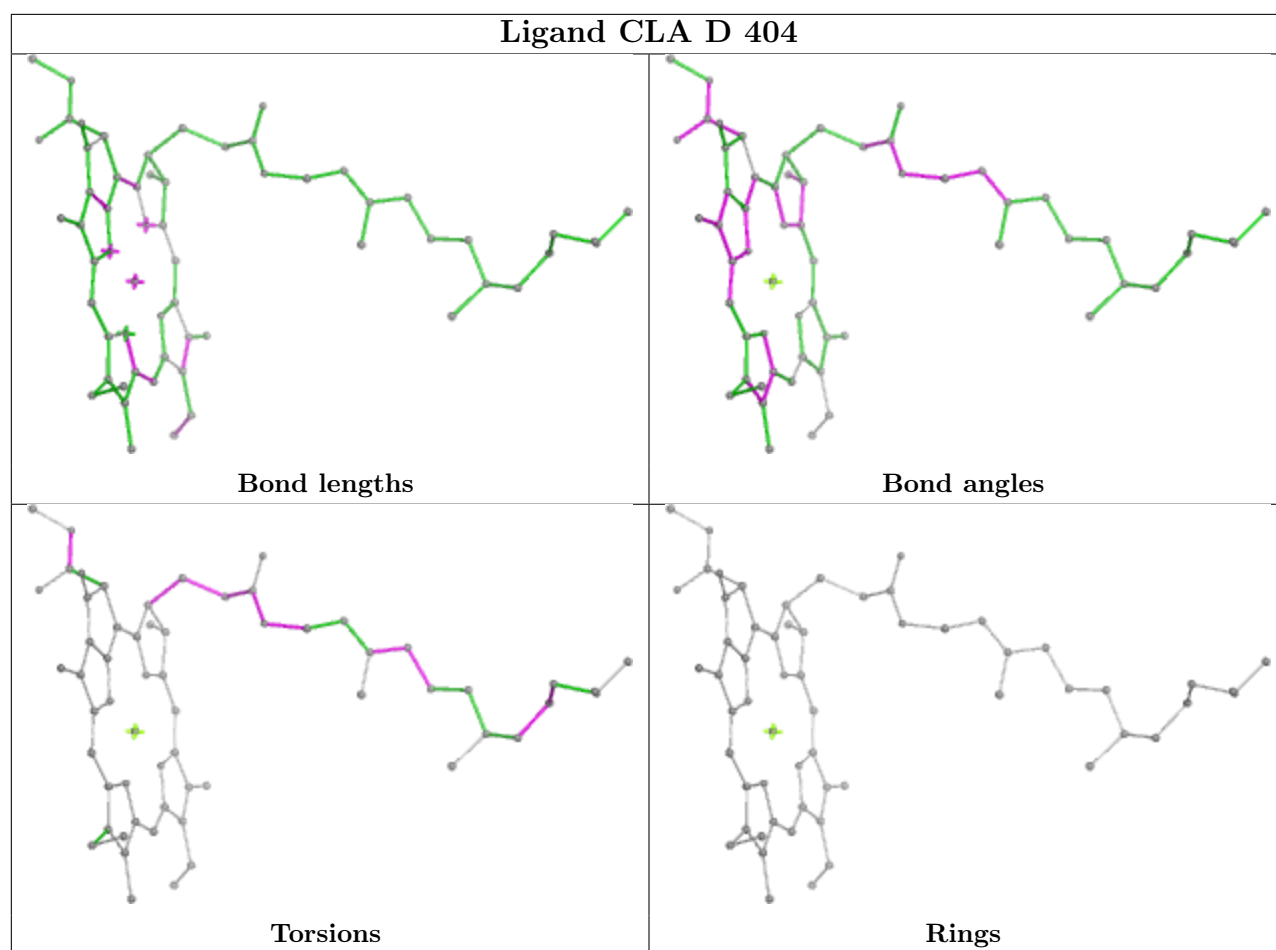




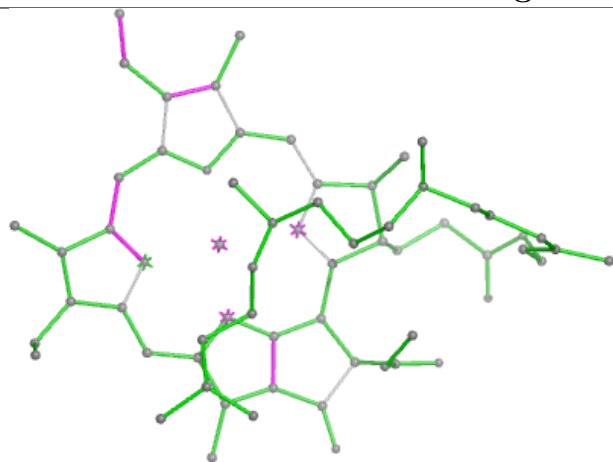
Ligand CLA B 501



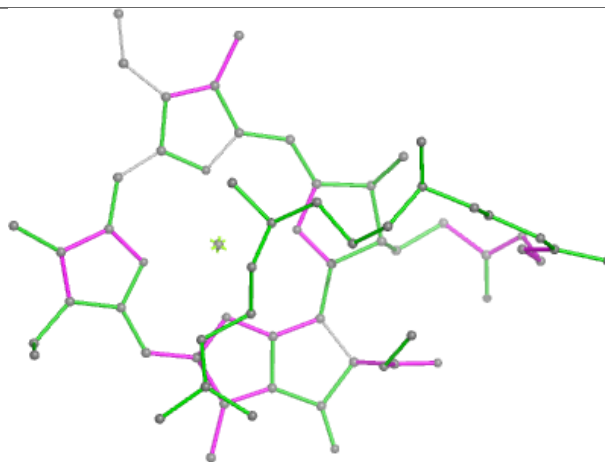




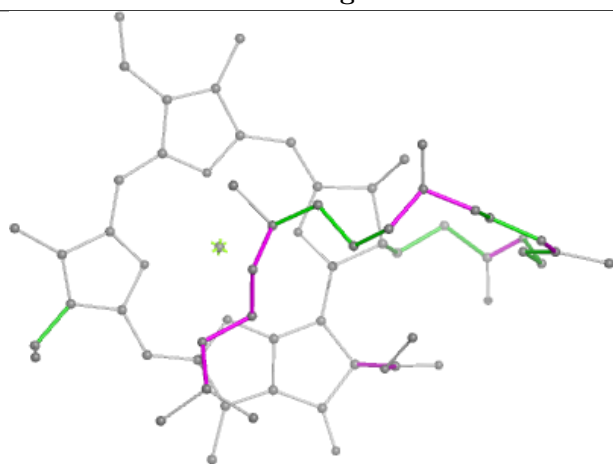
Ligand CLA C 511



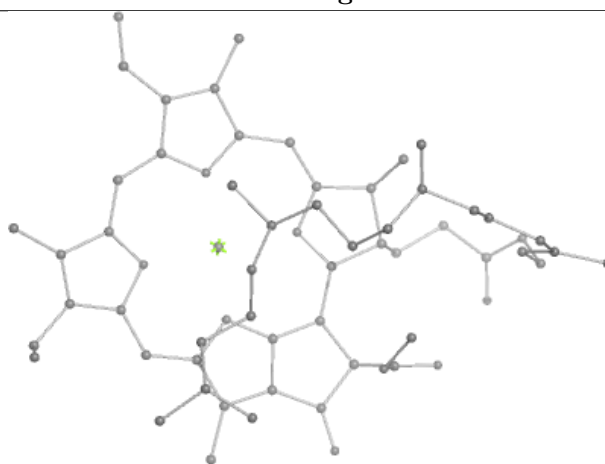
Bond lengths



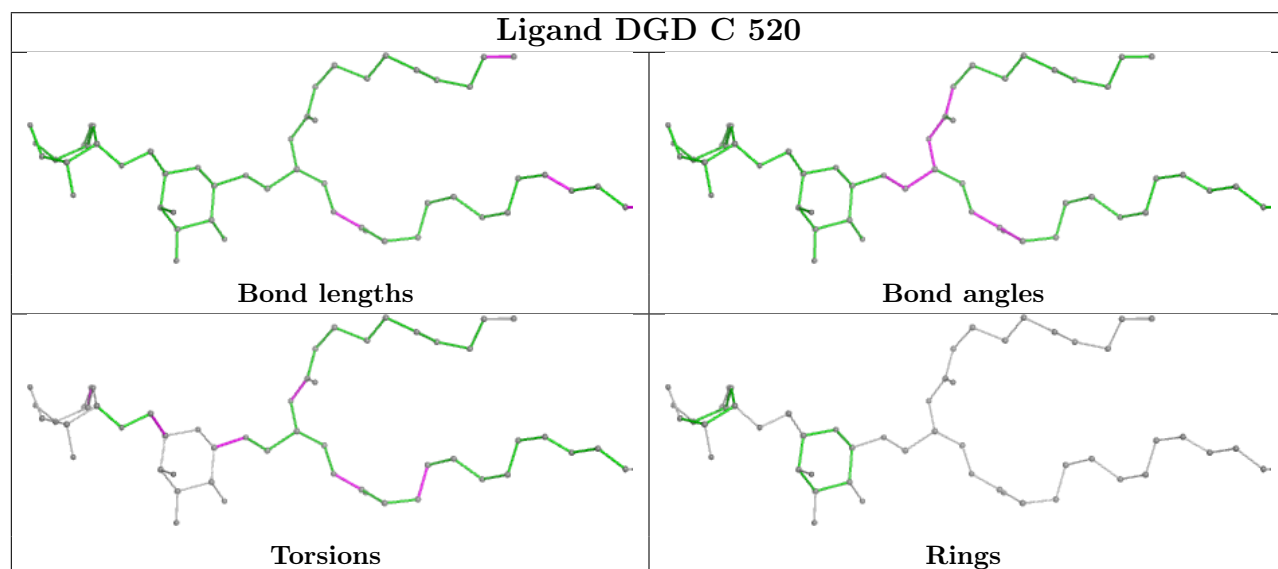
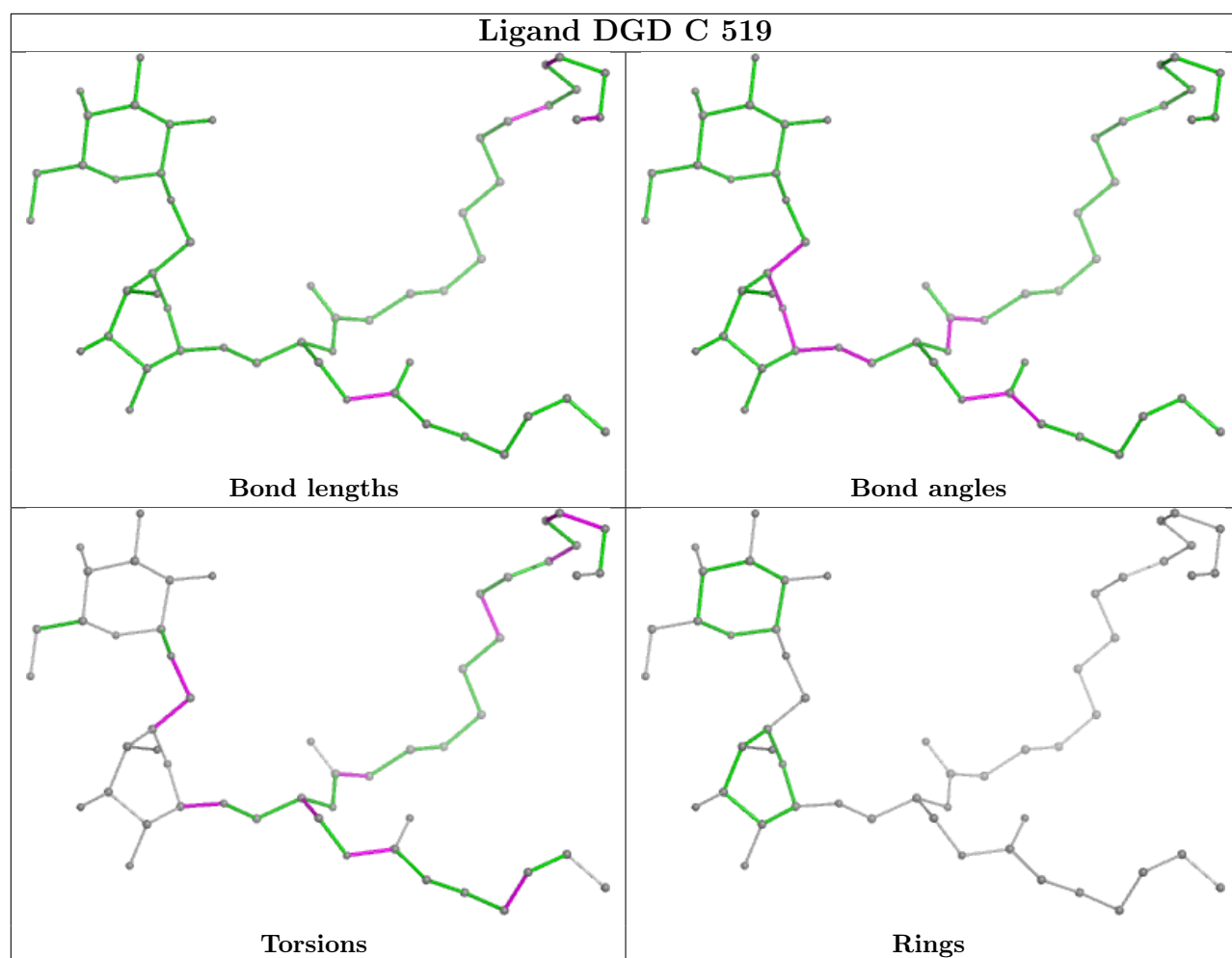
Bond angles



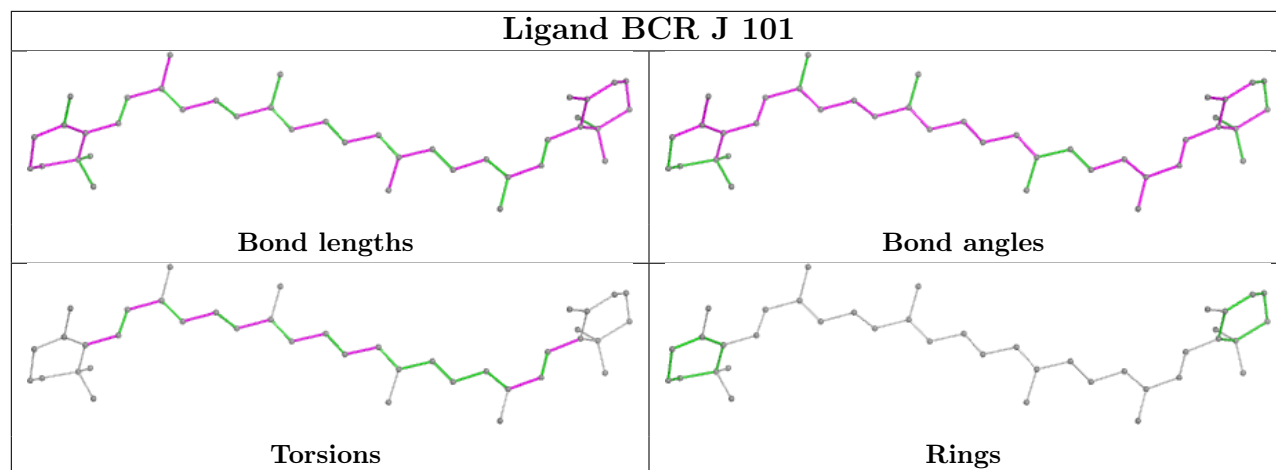
Torsions



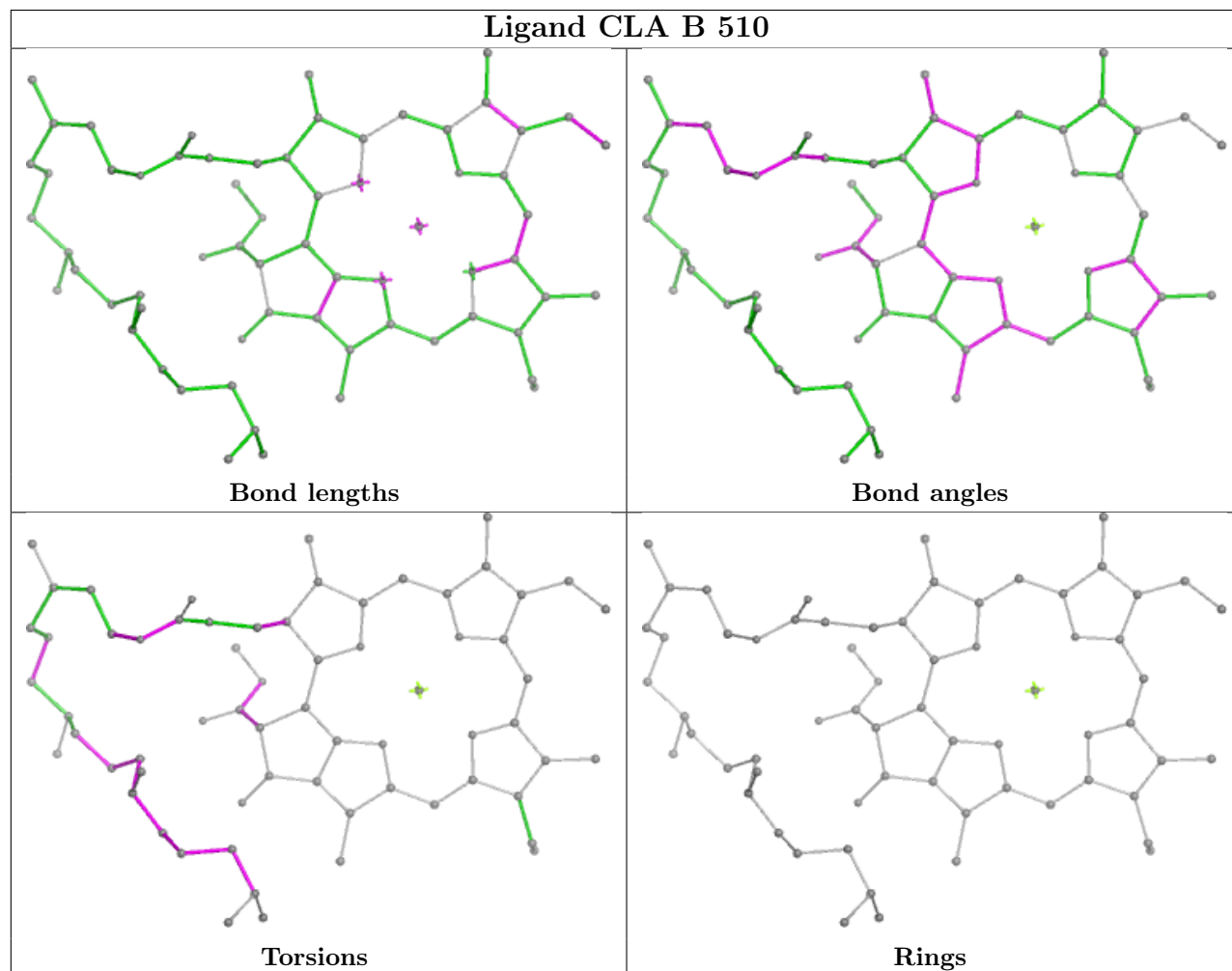
Rings

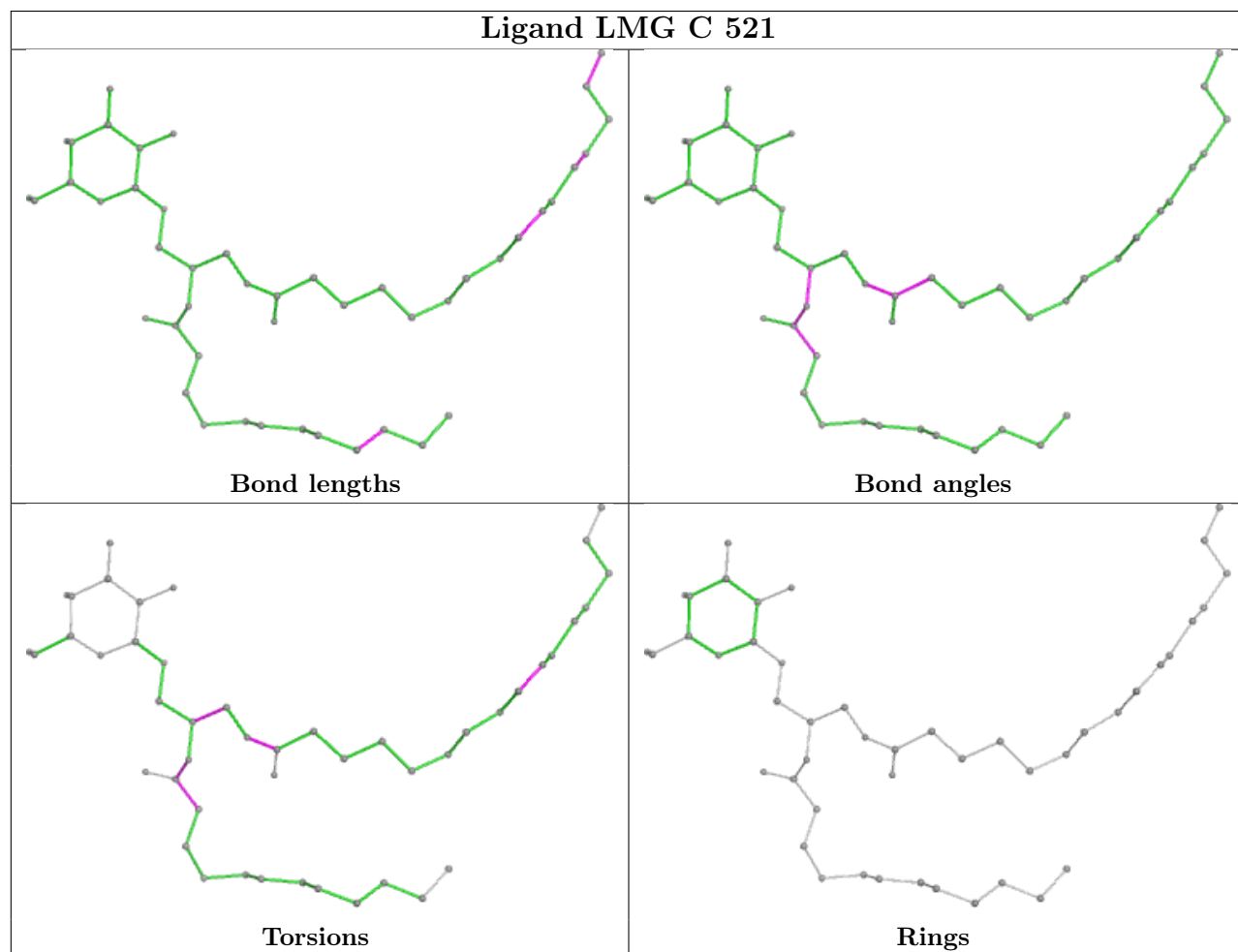
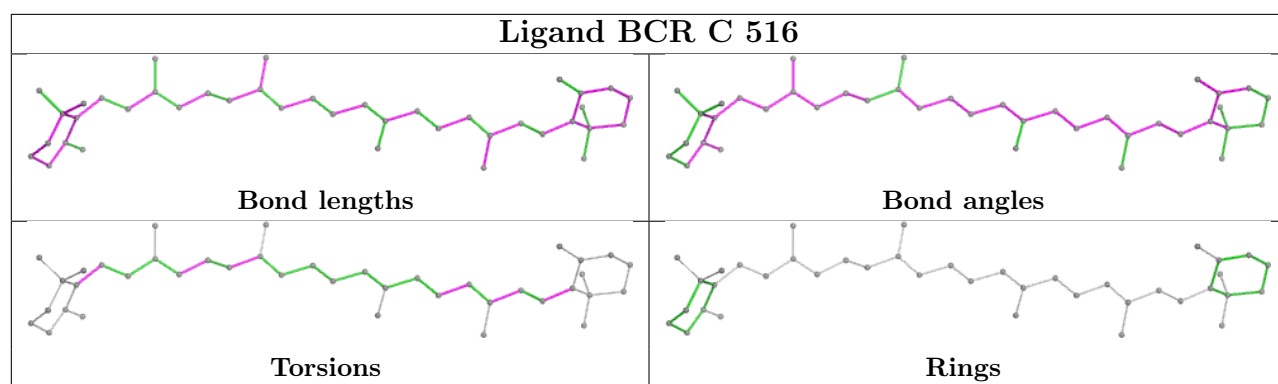


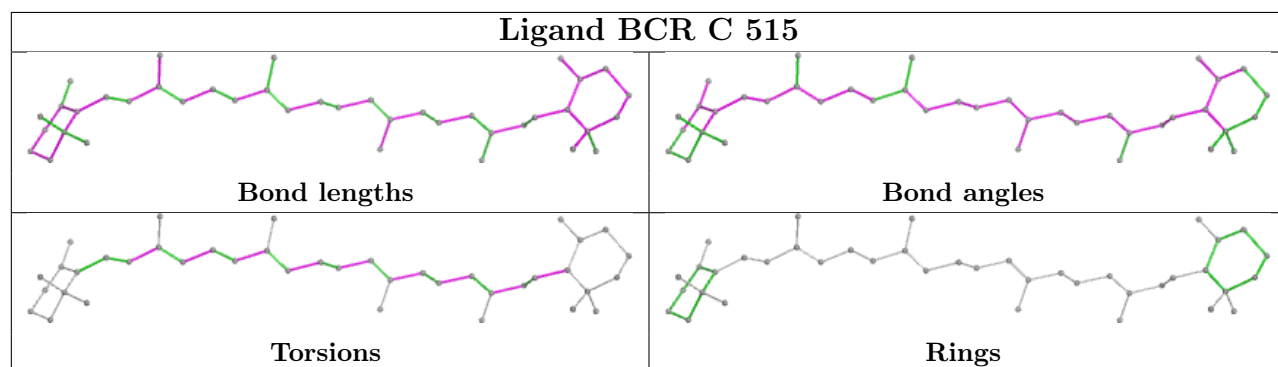
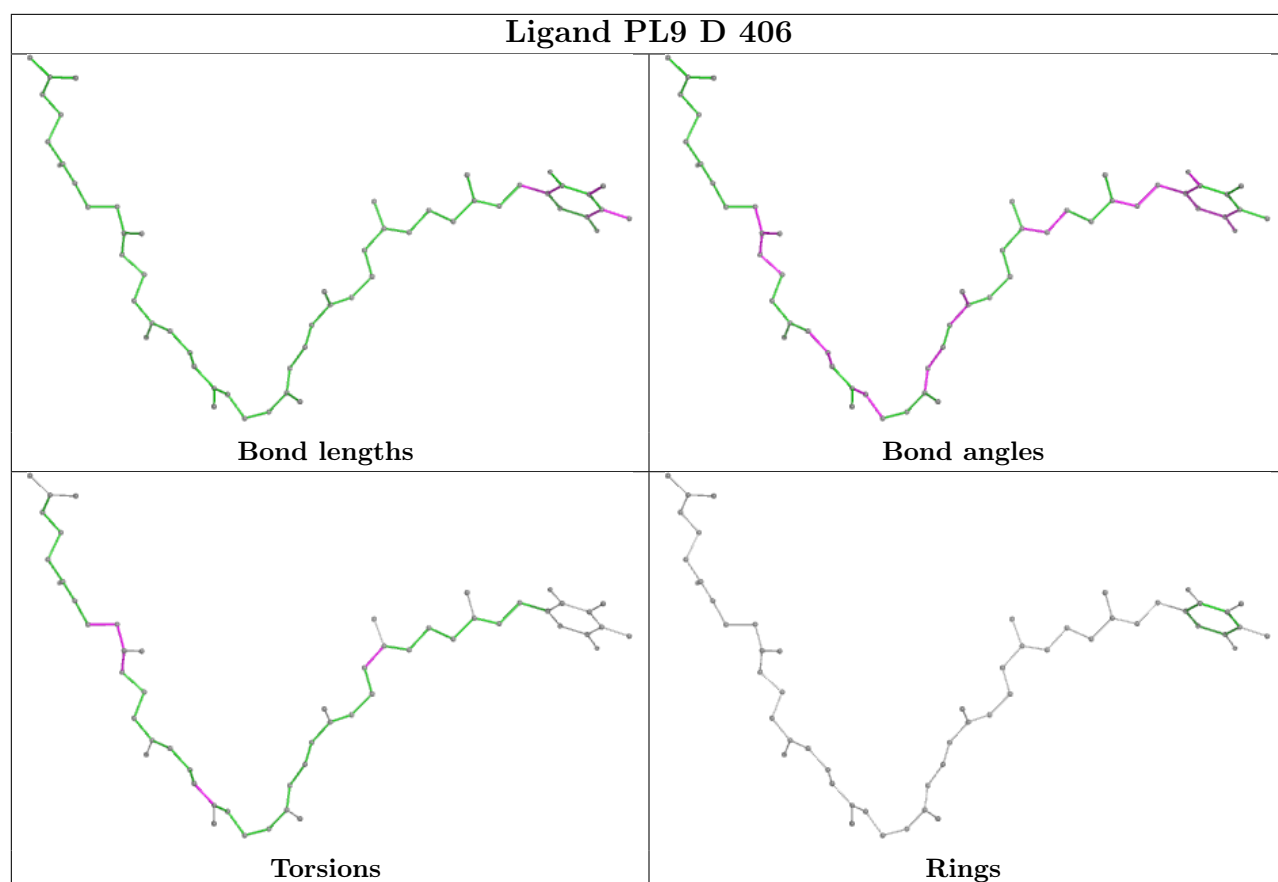
Ligand BCR J 101



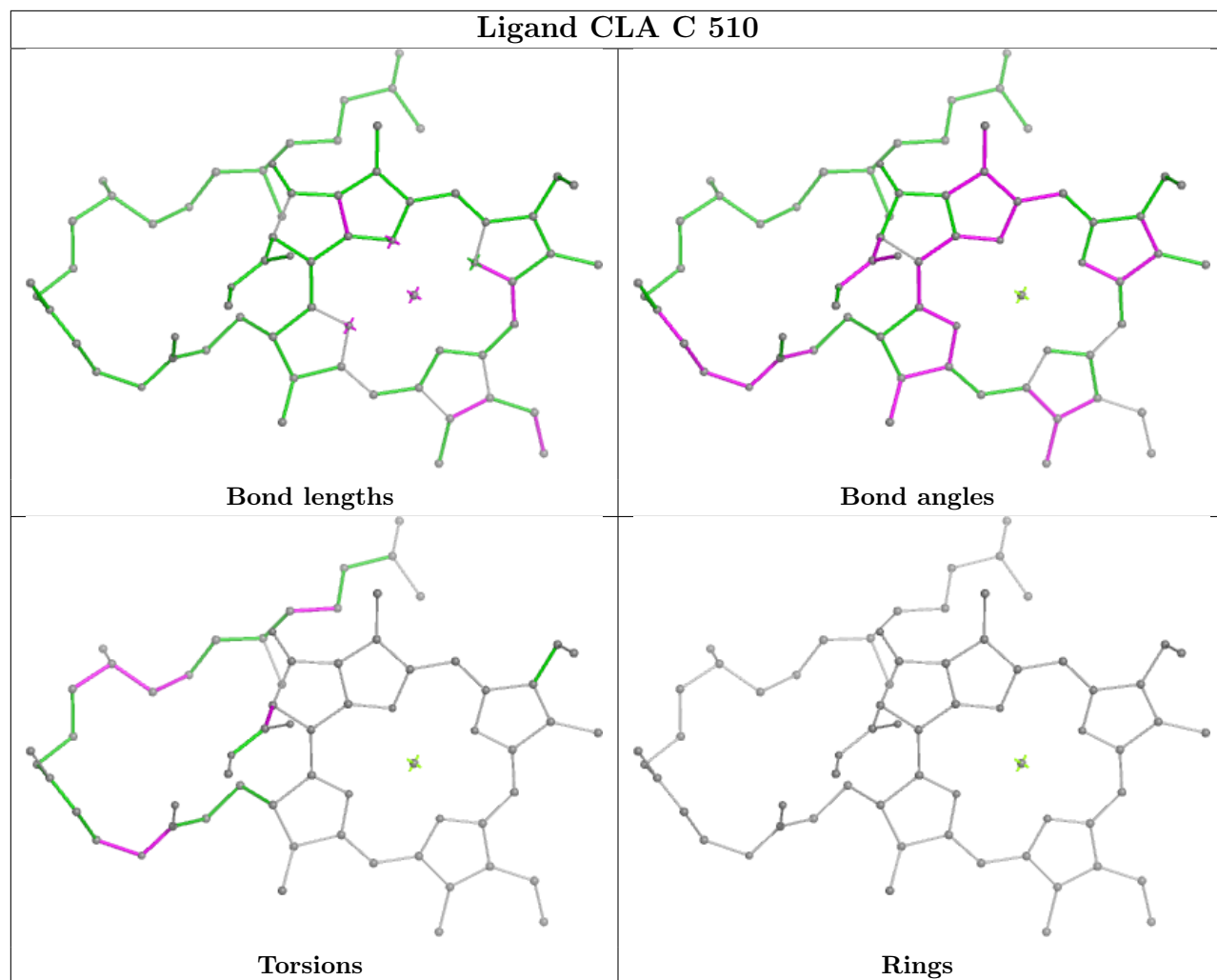
Ligand CLA B 510



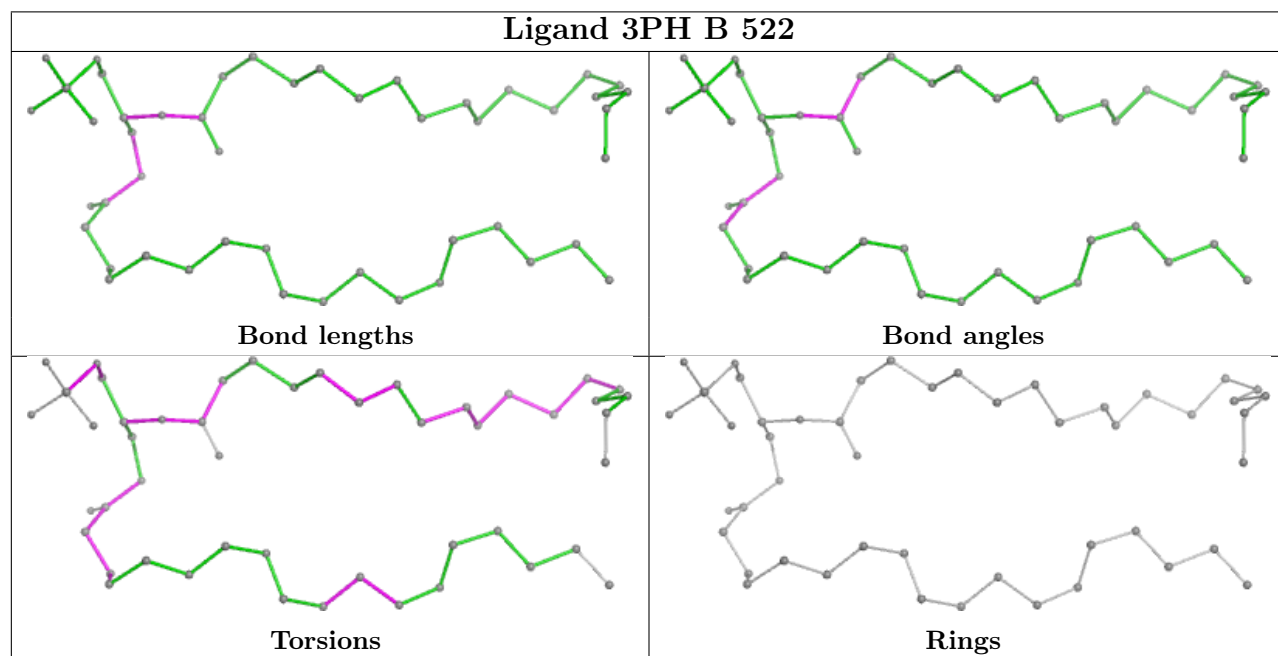




Ligand CLA C 510



Ligand 3PH B 522



4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

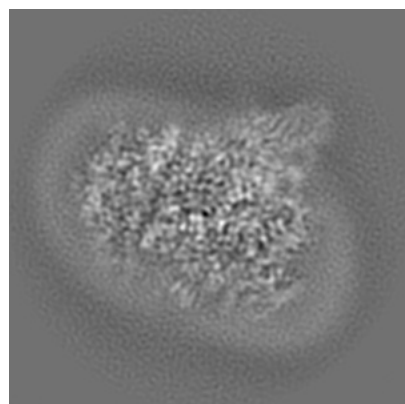
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51482. These allow visual inspection of the internal detail of the map and identification of artifacts.

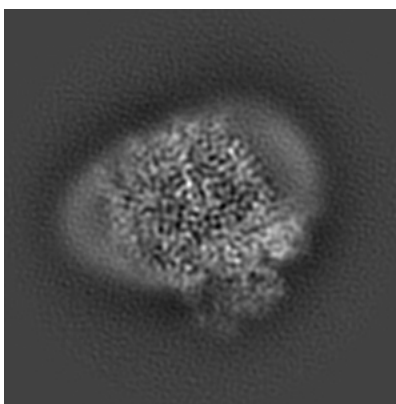
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections [i](#)

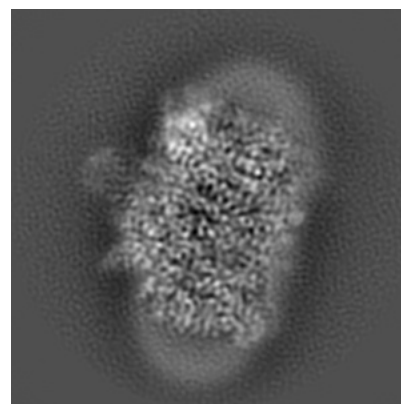
5.1.1 Primary map



X

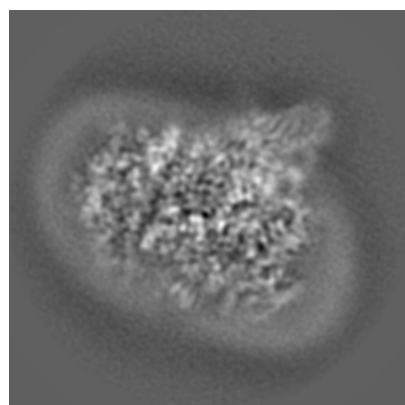


Y

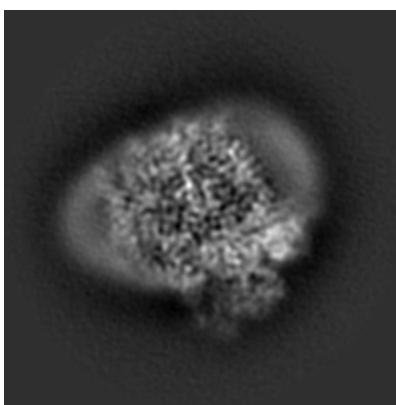


Z

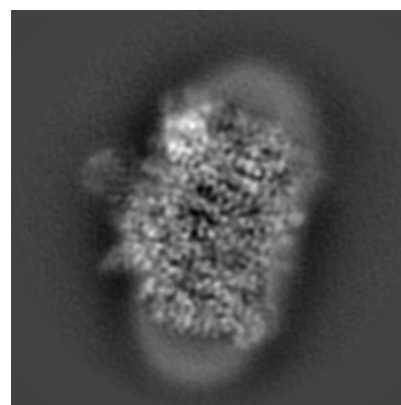
5.1.2 Raw map



X



Y

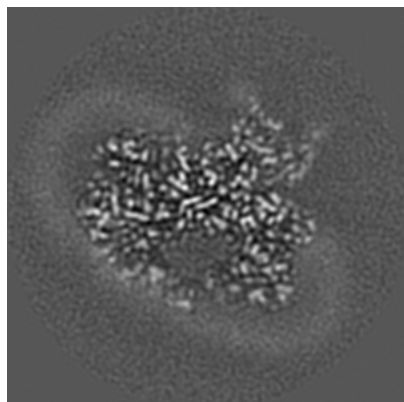


Z

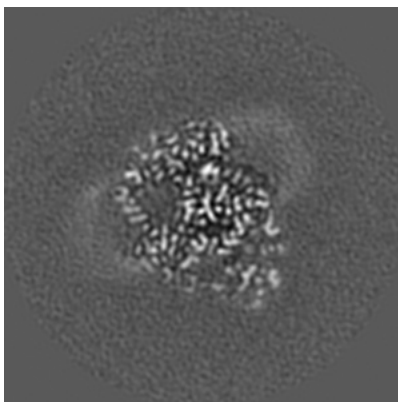
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

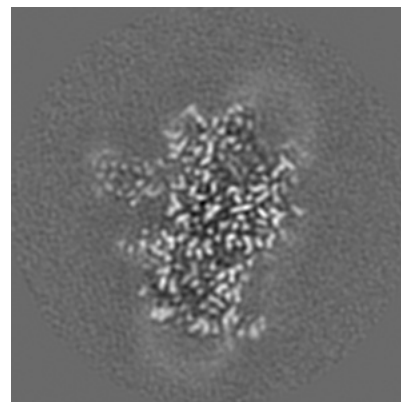
5.2.1 Primary map



X Index: 150

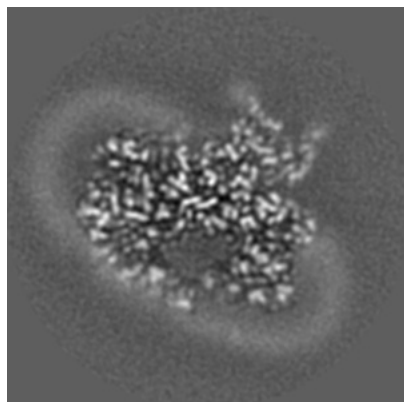


Y Index: 150

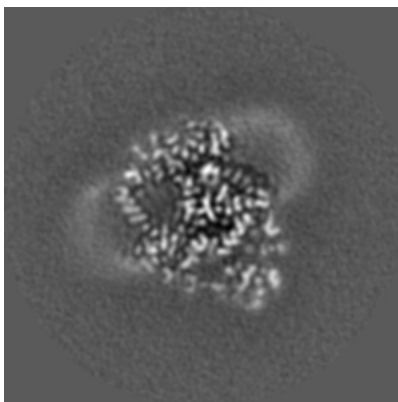


Z Index: 150

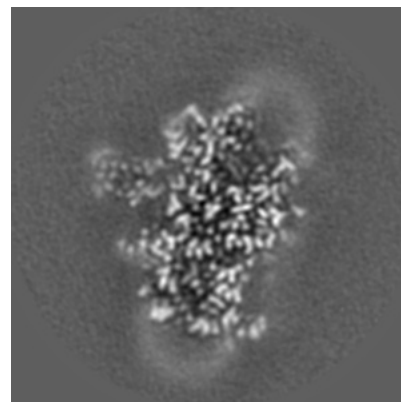
5.2.2 Raw map



X Index: 150



Y Index: 150

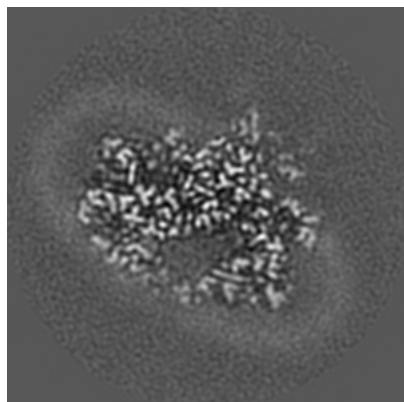


Z Index: 150

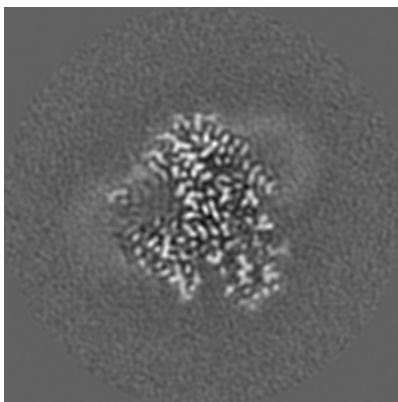
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

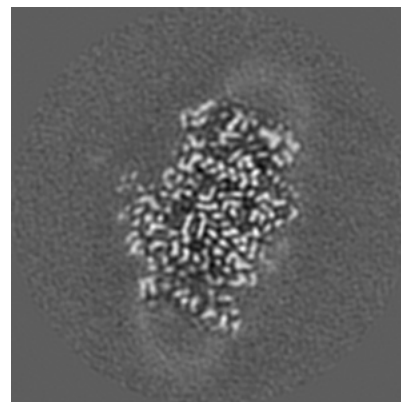
5.3.1 Primary map



X Index: 154

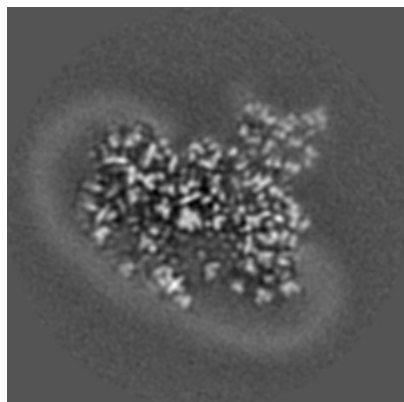


Y Index: 143

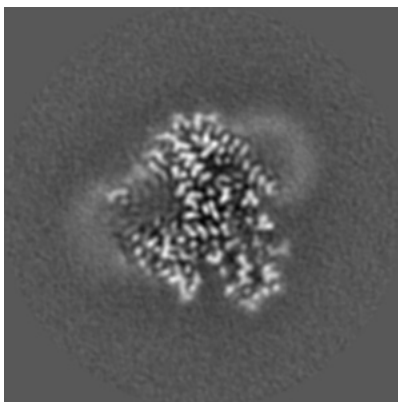


Z Index: 137

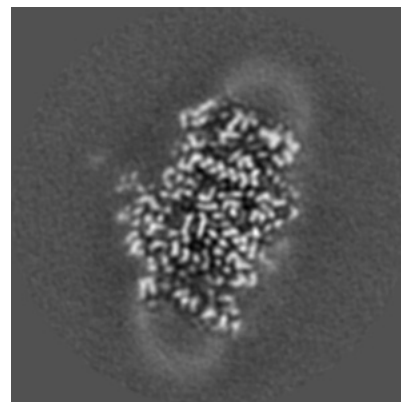
5.3.2 Raw map



X Index: 142



Y Index: 143

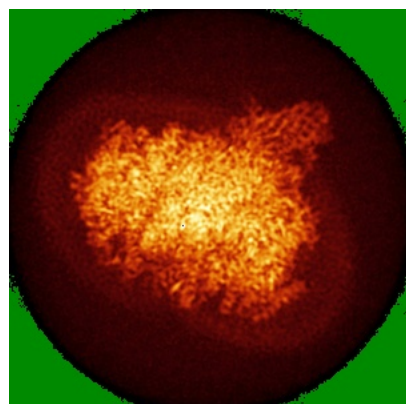


Z Index: 137

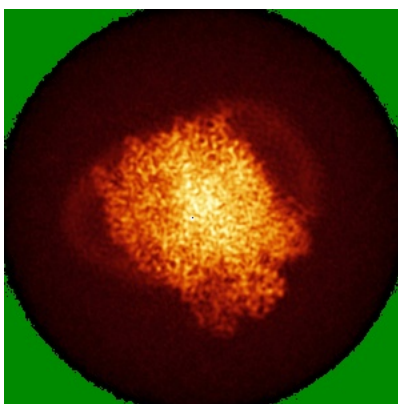
The images above show the largest variance slices of the map in three orthogonal directions.

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

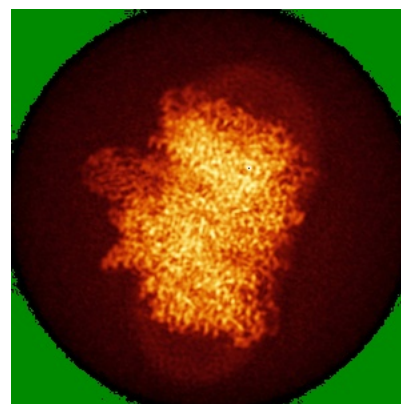
5.4.1 Primary map



X

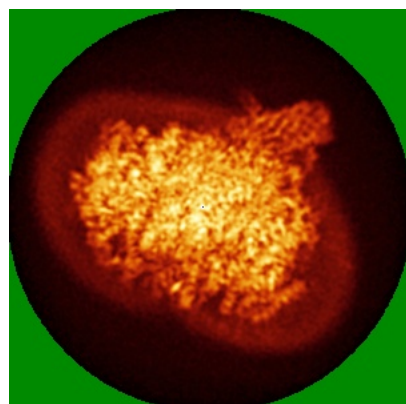


Y

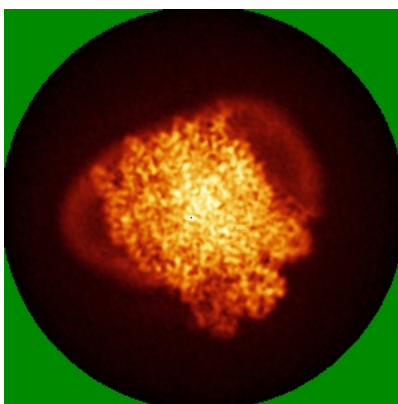


Z

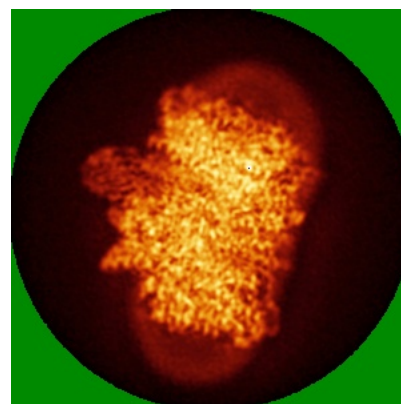
5.4.2 Raw map



X



Y

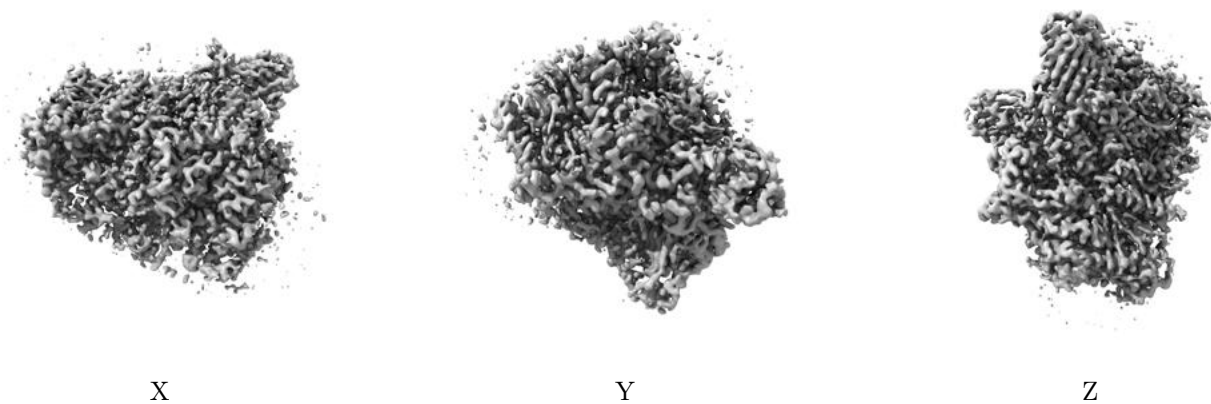


Z

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.

5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0047. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

5.5.2 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.

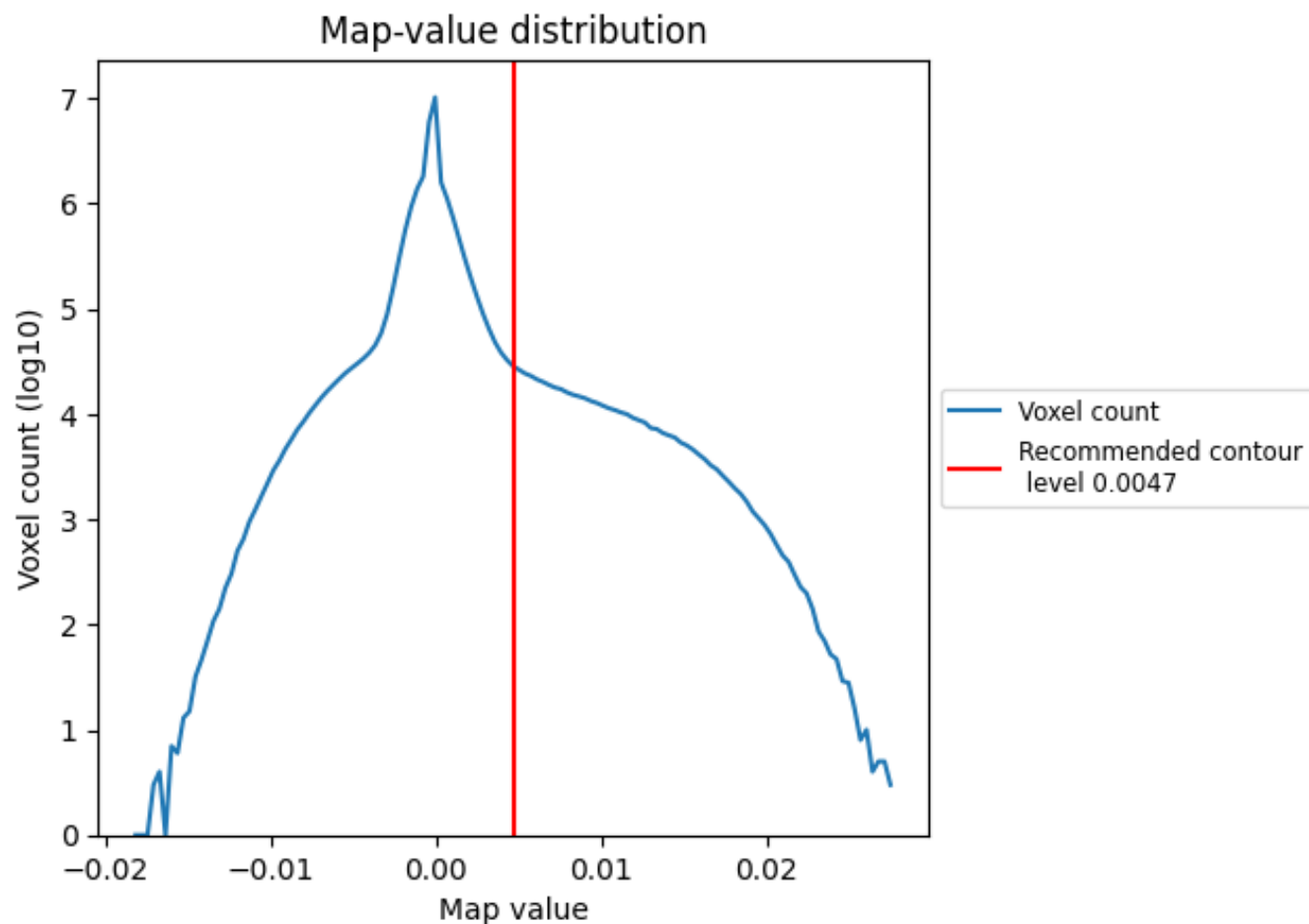
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

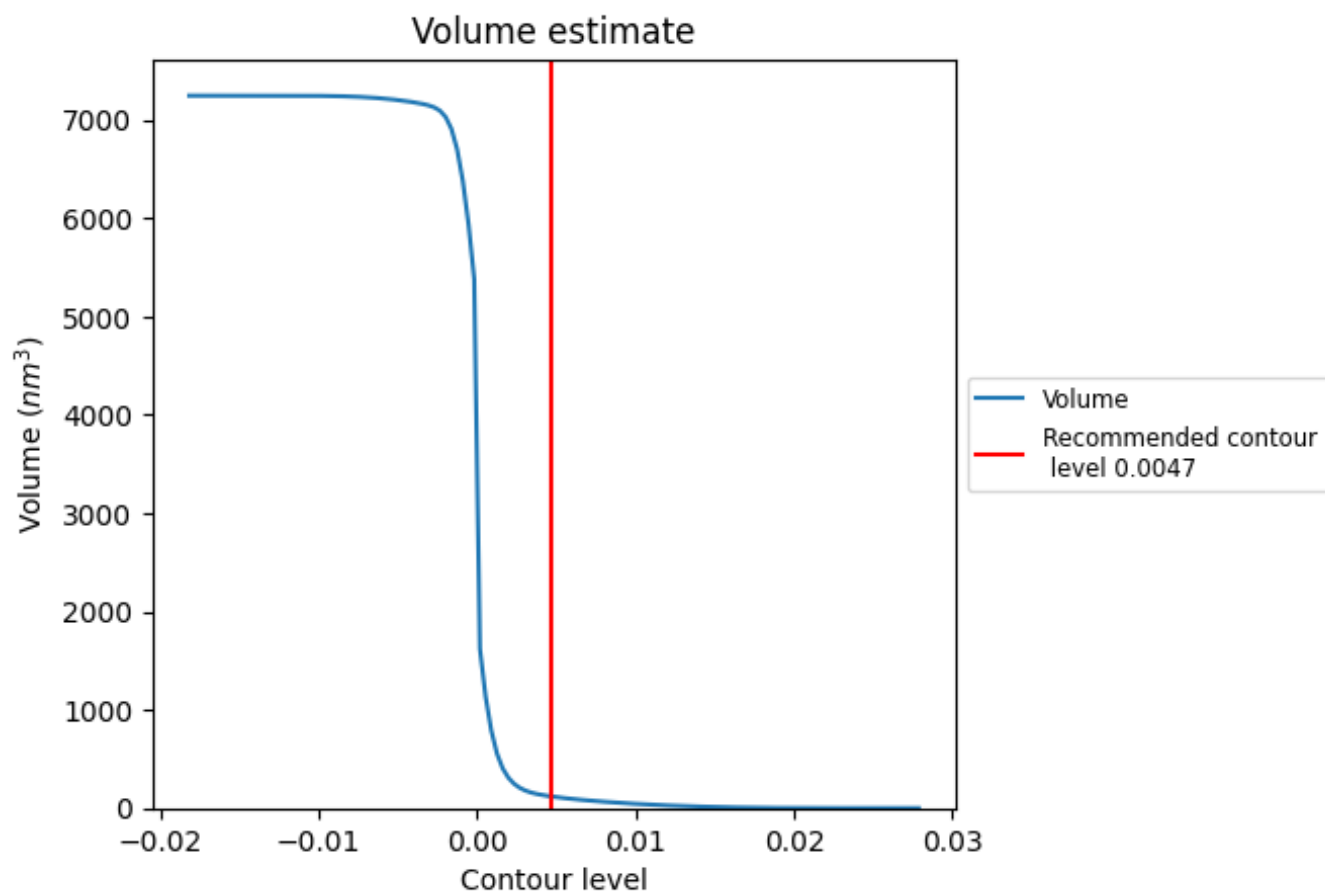
This section contains the results of statistical analysis of the map.

6.1 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.

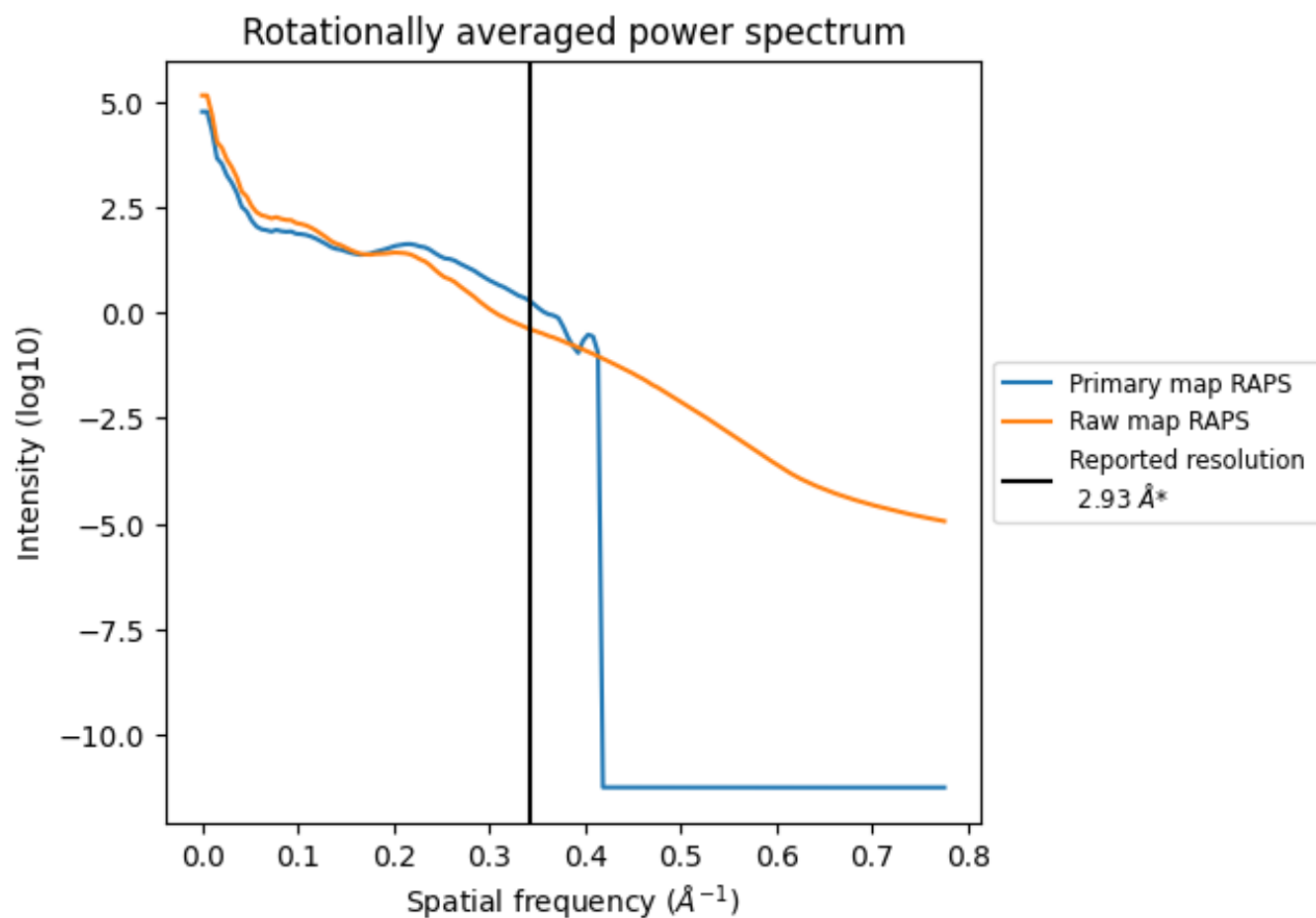
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm³; this corresponds to an approximate mass of 107 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.

6.3 Rotationally averaged power spectrum ⓘ

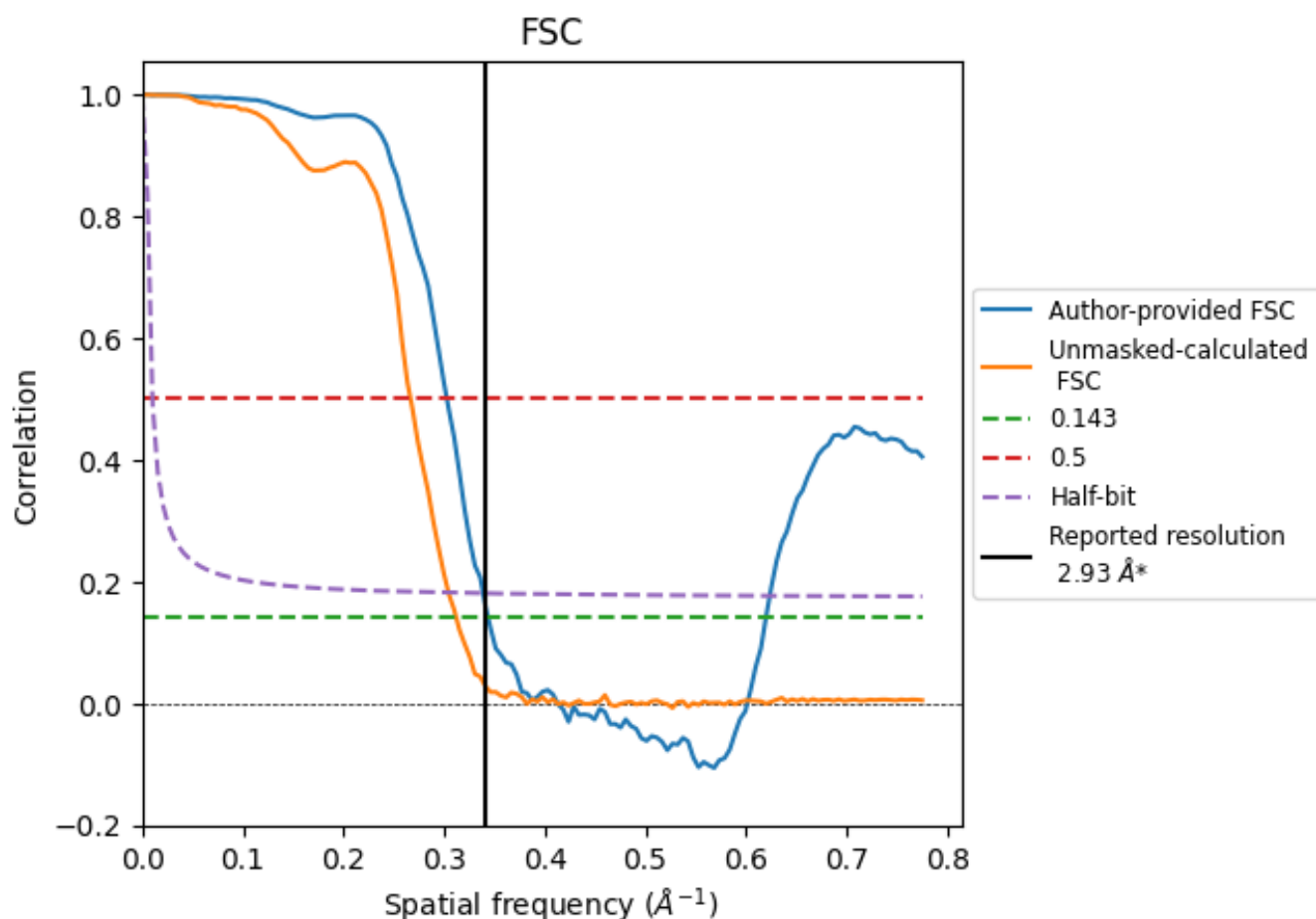


*Reported resolution corresponds to spatial frequency of 0.341 Å⁻¹

7 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.

7.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.341 \AA^{-1}

7.2 Resolution estimates [i](#)

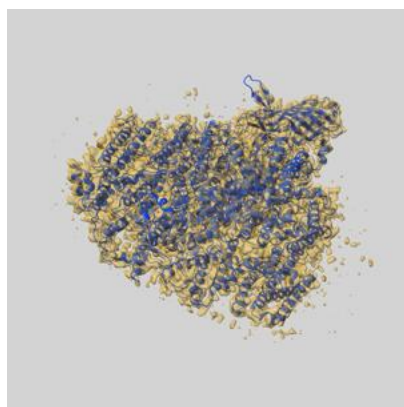
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	2.91	3.30	2.95
Unmasked-calculated*	3.21	3.75	3.28

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

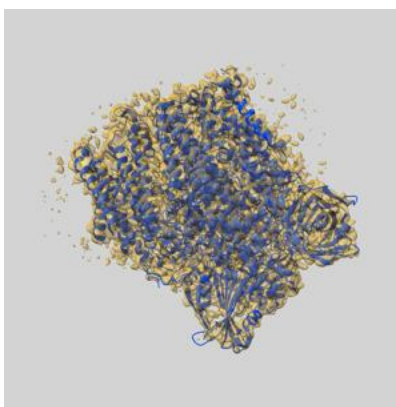
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51482 and PDB model 9GNW. Per-residue inclusion information can be found in section ?? on page ??.

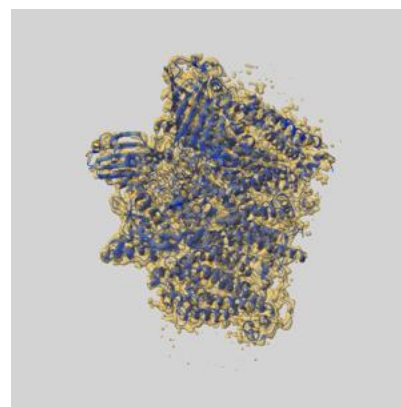
8.1 Map-model overlay [i](#)



X



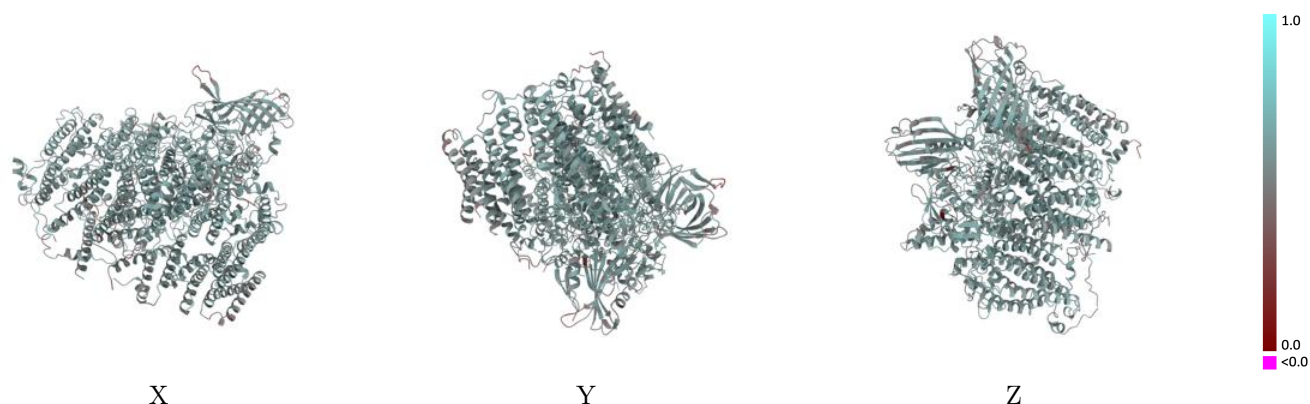
Y



Z

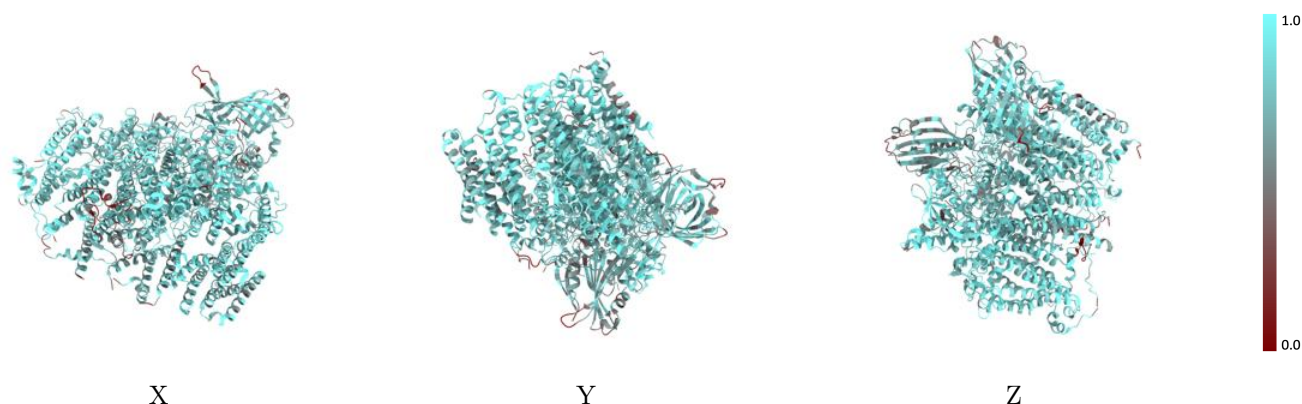
The images above show the 3D surface view of the map at the recommended contour level 0.0047 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



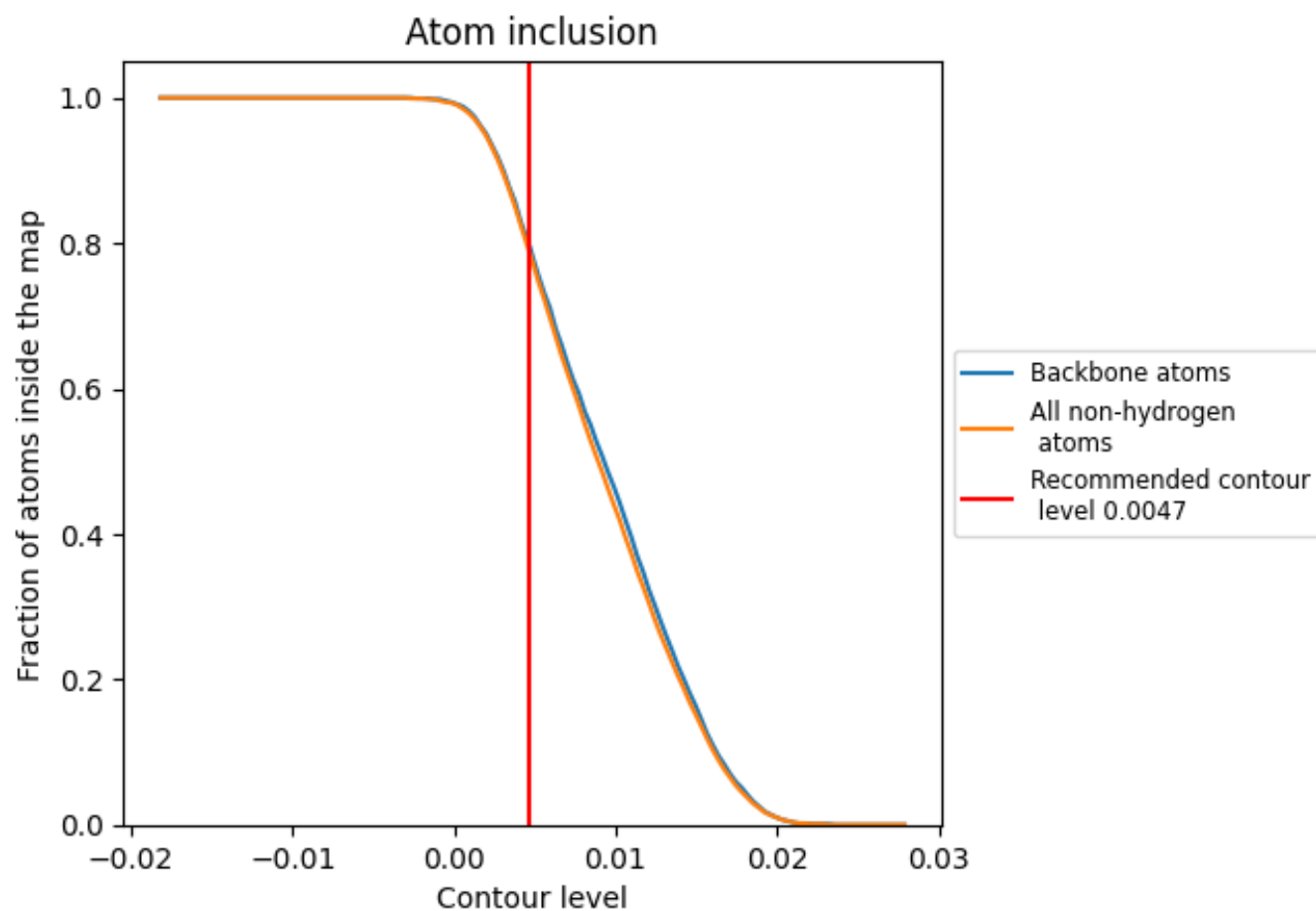
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 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 (0.0047).











































8.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0047) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7850	 0.5690
A	 0.7720	 0.5710
B	 0.8280	 0.5800
C	 0.8450	 0.5850
D	 0.8440	 0.5940
E	 0.8120	 0.5530
F	 0.7850	 0.5490
H	 0.8020	 0.5590
I	 0.8740	 0.5830
J	 0.7080	 0.5580
K	 0.8120	 0.5530
L	 0.8280	 0.5780
M	 0.6450	 0.5220
O	 0.7270	 0.5420
P	 0.5960	 0.5350
T	 0.7560	 0.5580
U	 0.6040	 0.4710
V	 0.7470	 0.5420
W	 0.5480	 0.5110
X	 0.7200	 0.5210
Z	 0.7280	 0.5050

