



## Full wwPDB EM Validation Report ⓘ

Dec 19, 2022 – 02:05 am GMT

PDB ID : 7BLZ  
EMDB ID : EMD-12228  
Title : Red alga *C. merolae* Photosystem I  
Authors : Nelson, N.; Klaiman, D.; Hippler, M.  
Deposited on : 2021-01-19  
Resolution : 3.10 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](mailto: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.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

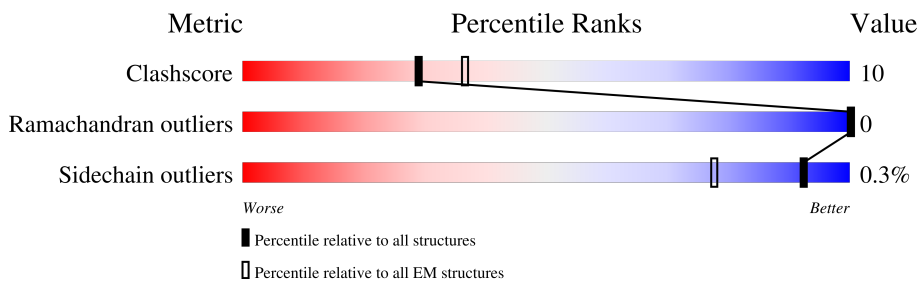
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



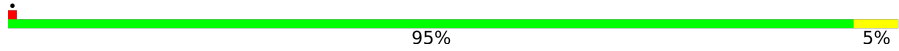


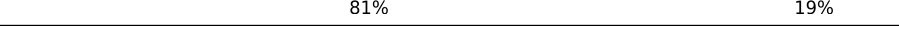

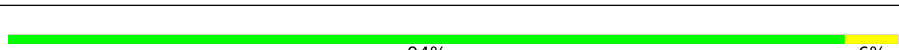

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	173	 87% 13%
2	2	179	 88% 12%
3	3	174	 80% 20%
4	A	743	 88% 12%
5	B	731	 87% 13%
6	C	80	 96% .
7	D	138	 96% .
8	E	61	 87% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	F	155	 95% 5%
10	I	31	 87% 13%
11	J	38	 89% 11%
12	K	54	 81% 19%
13	L	136	 88% 11%
14	M	27	 93% 7%
15	O	97	 94% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	1	601	X	-	-	-
16	CLA	1	602	X	-	-	-
16	CLA	1	603	X	-	-	-
16	CLA	1	604	X	-	-	-
16	CLA	1	605	X	-	-	-
16	CLA	1	606	X	-	-	-
16	CLA	1	607	X	-	-	-
16	CLA	1	608	X	-	-	-
16	CLA	1	609	X	-	-	-
16	CLA	1	610	X	-	-	-
16	CLA	1	611	X	-	-	-
16	CLA	2	601	X	-	-	-
16	CLA	2	602	X	-	-	-
16	CLA	2	603	X	-	-	-
16	CLA	2	604	X	-	-	-
16	CLA	2	605	X	-	-	-
16	CLA	2	606	X	-	-	-
16	CLA	2	607	X	-	-	-
16	CLA	2	608	X	-	-	-
16	CLA	2	609	X	-	-	-
16	CLA	2	610	X	-	-	-
16	CLA	2	611	X	-	-	-
16	CLA	2	612	X	-	-	-
16	CLA	2	613	X	-	-	-
16	CLA	3	203	X	-	-	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	3	204	X	-	-	-
16	CLA	3	205	X	-	-	-
16	CLA	3	206	X	-	-	-
16	CLA	3	207	X	-	-	-
16	CLA	3	208	X	-	-	-
16	CLA	3	209	X	-	-	-
16	CLA	3	210	X	-	-	-
16	CLA	3	211	X	-	-	-
16	CLA	3	212	X	-	-	-
16	CLA	3	213	X	-	-	-
16	CLA	3	214	X	-	-	-
16	CLA	A	802	X	-	-	-
16	CLA	A	803	X	-	-	-
16	CLA	A	804	X	-	-	-
16	CLA	A	805	X	-	-	-
16	CLA	A	806	X	-	-	-
16	CLA	A	807	X	-	-	-
16	CLA	A	808	X	-	-	-
16	CLA	A	809	X	-	-	-
16	CLA	A	810	X	-	-	-
16	CLA	A	811	X	-	-	-
16	CLA	A	812	X	-	-	-
16	CLA	A	813	X	-	-	-
16	CLA	A	814	X	-	-	-
16	CLA	A	815	X	-	-	-
16	CLA	A	816	X	-	-	-
16	CLA	A	817	X	-	-	-
16	CLA	A	818	X	-	-	-
16	CLA	A	819	X	-	-	-
16	CLA	A	820	X	-	-	-
16	CLA	A	821	X	-	-	-
16	CLA	A	822	X	-	-	-
16	CLA	A	823	X	-	-	-
16	CLA	A	824	X	-	-	-
16	CLA	A	825	X	-	-	-
16	CLA	A	826	X	-	-	-
16	CLA	A	827	X	-	-	-
16	CLA	A	828	X	-	-	-
16	CLA	A	829	X	-	-	-
16	CLA	A	830	X	-	-	-
16	CLA	A	831	X	-	-	-
16	CLA	A	832	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	A	833	X	-	-	-
16	CLA	A	834	X	-	-	-
16	CLA	A	835	X	-	-	-
16	CLA	A	836	X	-	-	-
16	CLA	A	837	X	-	-	-
16	CLA	A	838	X	-	-	-
16	CLA	A	839	X	-	-	-
16	CLA	A	854	X	-	-	-
16	CLA	A	855	X	-	-	-
16	CLA	A	856	X	-	-	-
16	CLA	B	801	X	-	-	-
16	CLA	B	802	X	-	-	-
16	CLA	B	803	X	-	-	-
16	CLA	B	804	X	-	-	-
16	CLA	B	805	X	-	-	-
16	CLA	B	806	X	-	-	-
16	CLA	B	807	X	-	-	-
16	CLA	B	808	X	-	-	-
16	CLA	B	809	X	-	-	-
16	CLA	B	810	X	-	-	-
16	CLA	B	811	X	-	-	-
16	CLA	B	812	X	-	-	-
16	CLA	B	813	X	-	-	-
16	CLA	B	814	X	-	-	-
16	CLA	B	815	X	-	-	-
16	CLA	B	816	X	-	-	-
16	CLA	B	817	X	-	-	-
16	CLA	B	818	X	-	-	-
16	CLA	B	819	X	-	-	-
16	CLA	B	820	X	-	-	-
16	CLA	B	821	X	-	-	-
16	CLA	B	822	X	-	-	-
16	CLA	B	823	X	-	-	-
16	CLA	B	824	X	-	-	-
16	CLA	B	825	X	-	-	-
16	CLA	B	826	X	-	-	-
16	CLA	B	827	X	-	-	-
16	CLA	B	828	X	-	-	-
16	CLA	B	829	X	-	-	-
16	CLA	B	830	X	-	-	-
16	CLA	B	831	X	-	-	-
16	CLA	B	832	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	CLA	B	833	X	-	-	-
16	CLA	B	834	X	-	-	-
16	CLA	B	835	X	-	-	-
16	CLA	B	836	X	-	-	-
16	CLA	B	837	X	-	-	-
16	CLA	B	838	X	-	-	-
16	CLA	F	201	X	-	-	-
16	CLA	F	202	X	-	-	-
16	CLA	F	204	X	-	-	-
16	CLA	F	205	X	-	-	-
16	CLA	I	101	X	-	-	-
16	CLA	I	102	X	-	-	-
16	CLA	J	102	X	-	-	-
16	CLA	K	101	X	-	-	-
16	CLA	K	102	X	-	-	-
16	CLA	L	201	X	-	-	-
16	CLA	L	203	X	-	-	-
16	CLA	L	204	X	-	-	-
16	CLA	L	205	X	-	-	-
16	CLA	O	201	X	-	-	-
16	CLA	O	202	X	-	-	-
16	CLA	O	203	X	-	-	-
16	CLA	O	204	X	-	-	-
17	C7Z	1	612	X	-	-	-
17	C7Z	1	614	X	-	-	-
17	C7Z	1	615	X	-	-	-
17	C7Z	1	616	X	-	-	-
17	C7Z	2	614	X	-	-	-
17	C7Z	2	615	X	-	-	-
17	C7Z	3	201	X	-	-	-
17	C7Z	3	215	X	-	-	-
17	C7Z	3	216	X	-	-	-
17	C7Z	3	217	X	-	-	-
17	C7Z	3	218	X	-	-	-
17	C7Z	A	843	X	-	-	-
17	C7Z	J	104	X	-	-	-
18	RRX	1	613	X	-	-	-
18	RRX	2	616	X	-	-	-
18	RRX	A	847	X	-	-	-
18	RRX	J	103	X	X	-	-
18	RRX	K	103	X	-	-	-
20	ERG	1	618	X	-	-	-

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
20	ERG	2	618	X	-	-	-
20	ERG	2	621	X	-	-	-
22	PGT	2	619	X	-	-	-
22	PGT	B	848	X	-	-	-
26	CL0	A	801	X	-	-	-

## 2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 68571 atoms, of which 34687 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 Similar to light harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	1	173	2734	906	1353	232	235	8	0	0

- Molecule 2 is a protein called Similar to chlorophyll a/b-binding protein, CP24.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	2	179	2780	906	1385	237	244	8	0	0

- Molecule 3 is a protein called Lhcr3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	3	174	2689	871	1348	226	237	7	0	0

- Molecule 4 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	A	743	11555	3802	5740	999	987	27	0	0

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	B	731	11464	3827	5645	982	991	19	0	0

- Molecule 6 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	C	80	1173	367	576	104	114	12	0	0



- Molecule 7 is a protein called Photosystem I p700 chlorophyll A apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	D	138	2187	694	1093	192	203	5	0	0

- Molecule 8 is a protein called Photosystem I iron-sulfur center subunit VII.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	E	61	1002	322	509	79	92		0	0

- Molecule 9 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	F	155	2513	816	1243	215	235	4	0	0

- Molecule 10 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	I	31	483	158	253	32	39	1	0	0

- Molecule 11 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	J	38	639	214	327	46	51	1	0	0

- Molecule 12 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	K	54	809	253	419	65	68	4	0	0

- Molecule 13 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	L	136	2096	682	1057	170	185	2	0	0

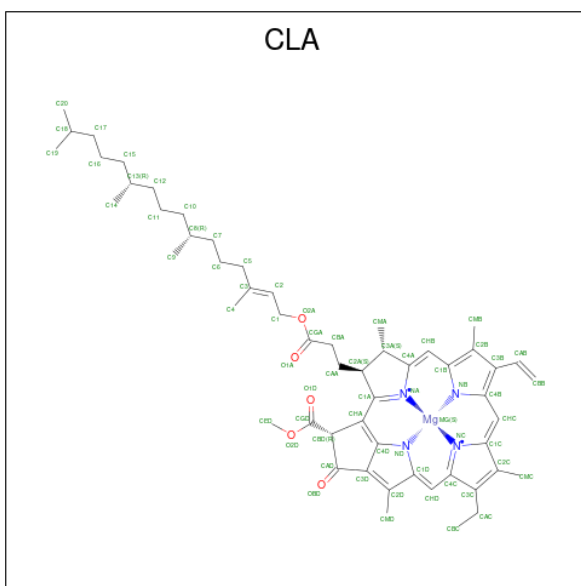
- Molecule 14 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
14	M	27	430	136	226	32	34	2	0	0

- Molecule 15 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
15	O	97	1489	505	742	113	129	0	0

- Molecule 16 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	Mg	N		O
16	1	1	1474	594	770	11	44	55	0
16	1	1	1474	594	770	11	44	55	0
16	1	1	1474	594	770	11	44	55	0
16	1	1	1474	594	770	11	44	55	0
16	1	1	1474	594	770	11	44	55	0
16	1	1	1474	594	770	11	44	55	0
16	1	1	1474	594	770	11	44	55	0
16	1	1	1474	594	770	11	44	55	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
16	1	1	Total 1474	C 594	H 770	Mg 11	N 44	O 55	0
16	1	1	Total 1474	C 594	H 770	Mg 11	N 44	O 55	0
16	1	1	Total 1474	C 594	H 770	Mg 11	N 44	O 55	0
16	2	1	Total 1781	C 713	H 938	Mg 13	N 52	O 65	0
16	2	1	Total 1781	C 713	H 938	Mg 13	N 52	O 65	0
16	2	1	Total 1781	C 713	H 938	Mg 13	N 52	O 65	0
16	2	1	Total 1781	C 713	H 938	Mg 13	N 52	O 65	0
16	2	1	Total 1781	C 713	H 938	Mg 13	N 52	O 65	0
16	2	1	Total 1781	C 713	H 938	Mg 13	N 52	O 65	0
16	2	1	Total 1781	C 713	H 938	Mg 13	N 52	O 65	0
16	2	1	Total 1781	C 713	H 938	Mg 13	N 52	O 65	0
16	2	1	Total 1781	C 713	H 938	Mg 13	N 52	O 65	0
16	2	1	Total 1781	C 713	H 938	Mg 13	N 52	O 65	0
16	2	1	Total 1781	C 713	H 938	Mg 13	N 52	O 65	0
16	2	1	Total 1781	C 713	H 938	Mg 13	N 52	O 65	0
16	2	1	Total 1781	C 713	H 938	Mg 13	N 52	O 65	0
16	2	1	Total 1781	C 713	H 938	Mg 13	N 52	O 65	0
16	2	1	Total 1781	C 713	H 938	Mg 13	N 52	O 65	0
16	3	1	Total 1547	C 629	H 798	Mg 12	N 48	O 60	0
16	3	1	Total 1547	C 629	H 798	Mg 12	N 48	O 60	0
16	3	1	Total 1547	C 629	H 798	Mg 12	N 48	O 60	0
16	3	1	Total 1547	C 629	H 798	Mg 12	N 48	O 60	0
16	3	1	Total 1547	C 629	H 798	Mg 12	N 48	O 60	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
16	3	1	Total 1547	C 629	H 798	Mg 12	N 48	O 60	0
16	3	1	Total 1547	C 629	H 798	Mg 12	N 48	O 60	0
16	3	1	Total 1547	C 629	H 798	Mg 12	N 48	O 60	0
16	3	1	Total 1547	C 629	H 798	Mg 12	N 48	O 60	0
16	3	1	Total 1547	C 629	H 798	Mg 12	N 48	O 60	0
16	3	1	Total 1547	C 629	H 798	Mg 12	N 48	O 60	0
16	3	1	Total 1547	C 629	H 798	Mg 12	N 48	O 60	0
16	A	1	Total 5649	C 2255	H 2984	Mg 41	N 164	O 205	0
16	A	1	Total 5649	C 2255	H 2984	Mg 41	N 164	O 205	0
16	A	1	Total 5649	C 2255	H 2984	Mg 41	N 164	O 205	0
16	A	1	Total 5649	C 2255	H 2984	Mg 41	N 164	O 205	0
16	A	1	Total 5649	C 2255	H 2984	Mg 41	N 164	O 205	0
16	A	1	Total 5649	C 2255	H 2984	Mg 41	N 164	O 205	0
16	A	1	Total 5649	C 2255	H 2984	Mg 41	N 164	O 205	0
16	A	1	Total 5649	C 2255	H 2984	Mg 41	N 164	O 205	0
16	A	1	Total 5649	C 2255	H 2984	Mg 41	N 164	O 205	0
16	A	1	Total 5649	C 2255	H 2984	Mg 41	N 164	O 205	0
16	A	1	Total 5649	C 2255	H 2984	Mg 41	N 164	O 205	0
16	A	1	Total 5649	C 2255	H 2984	Mg 41	N 164	O 205	0
16	A	1	Total 5649	C 2255	H 2984	Mg 41	N 164	O 205	0
16	A	1	Total 5649	C 2255	H 2984	Mg 41	N 164	O 205	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	Mg	N		O
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	Mg	N	O	
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	A	1	5649	2255	2984	41	164	205	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0
16	B	1	5202	2080	2742	38	152	190	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0

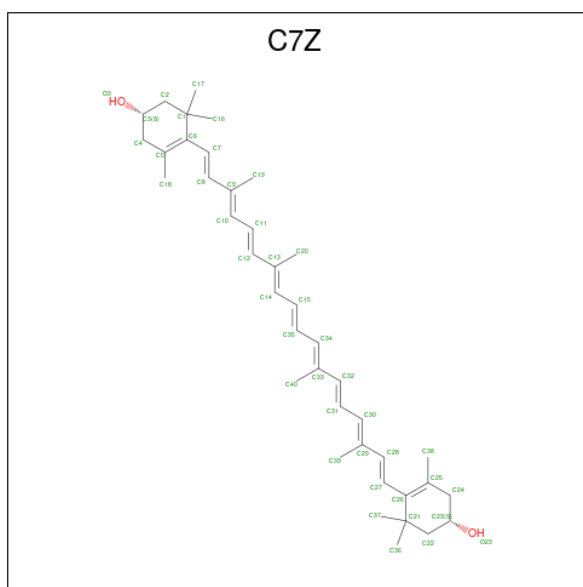
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	B	1	Total 5202	C 2080	H 2742	Mg 38	N 152	O 190	0
16	F	1	Total 536	C 216	H 280	Mg 4	N 16	O 20	0
16	F	1	Total 536	C 216	H 280	Mg 4	N 16	O 20	0
16	F	1	Total 536	C 216	H 280	Mg 4	N 16	O 20	0
16	F	1	Total 536	C 216	H 280	Mg 4	N 16	O 20	0
16	I	1	Total 276	C 110	H 146	Mg 2	N 8	O 10	0
16	I	1	Total 276	C 110	H 146	Mg 2	N 8	O 10	0
16	J	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	K	1	Total 275	C 110	H 145	Mg 2	N 8	O 10	0
16	K	1	Total 275	C 110	H 145	Mg 2	N 8	O 10	0
16	L	1	Total 551	C 220	H 291	Mg 4	N 16	O 20	0
16	L	1	Total 551	C 220	H 291	Mg 4	N 16	O 20	0
16	L	1	Total 551	C 220	H 291	Mg 4	N 16	O 20	0
16	L	1	Total 551	C 220	H 291	Mg 4	N 16	O 20	0
16	O	1	Total 548	C 220	H 288	Mg 4	N 16	O 20	0
16	O	1	Total 548	C 220	H 288	Mg 4	N 16	O 20	0
16	O	1	Total 548	C 220	H 288	Mg 4	N 16	O 20	0
16	O	1	Total 548	C 220	H 288	Mg 4	N 16	O 20	0

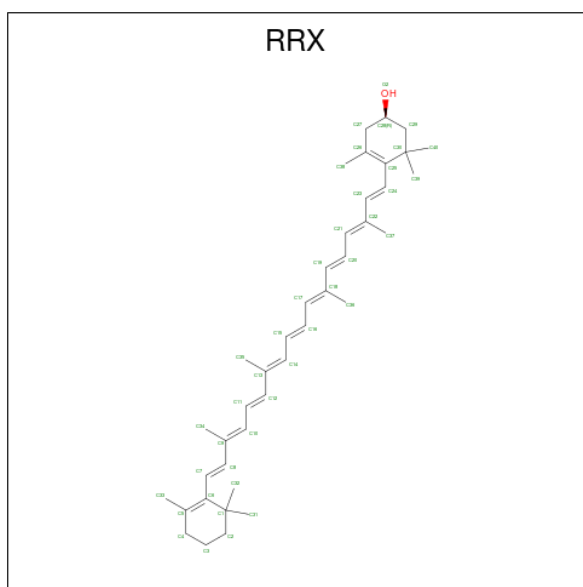
- Molecule 17 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).





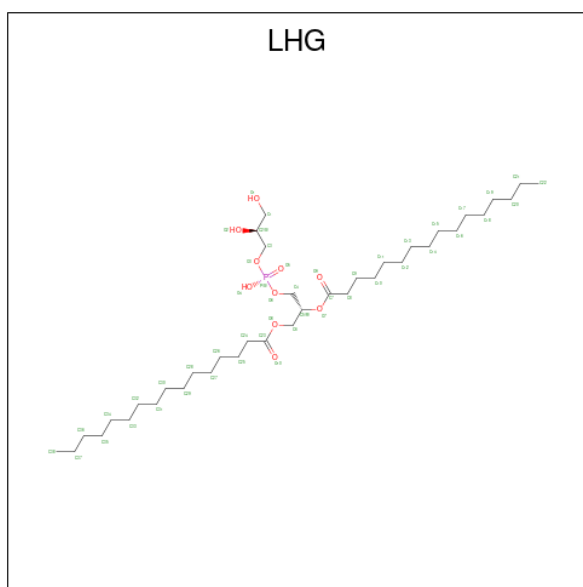
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
17	1	1	168	160	8	0
17	1	1	168	160	8	0
17	1	1	168	160	8	0
17	1	1	168	160	8	0
17	2	1	84	80	4	0
17	2	1	84	80	4	0
17	3	1	210	200	10	0
17	3	1	210	200	10	0
17	3	1	210	200	10	0
17	3	1	210	200	10	0
17	3	1	210	200	10	0
17	A	1	42	40	2	0
17	J	1	42	40	2	0

- Molecule 18 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C<sub>40</sub>H<sub>56</sub>O).



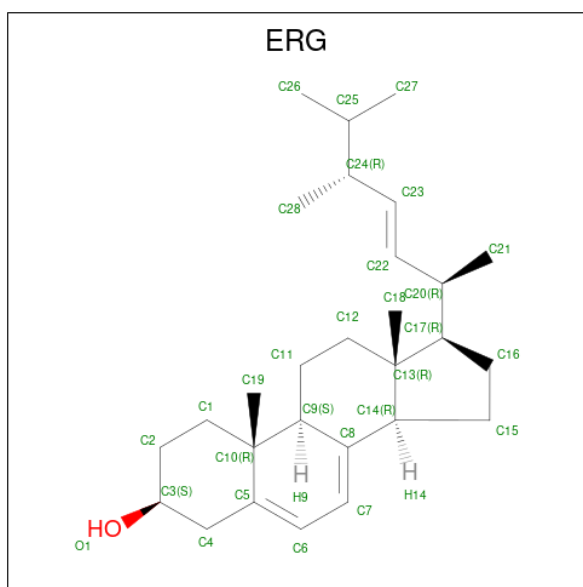
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
18	1	1	97	40	56	1	0
18	2	1	97	40	56	1	0
18	A	1	96	40	55	1	0
18	J	1	97	40	56	1	0
18	K	1	97	40	56	1	0

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



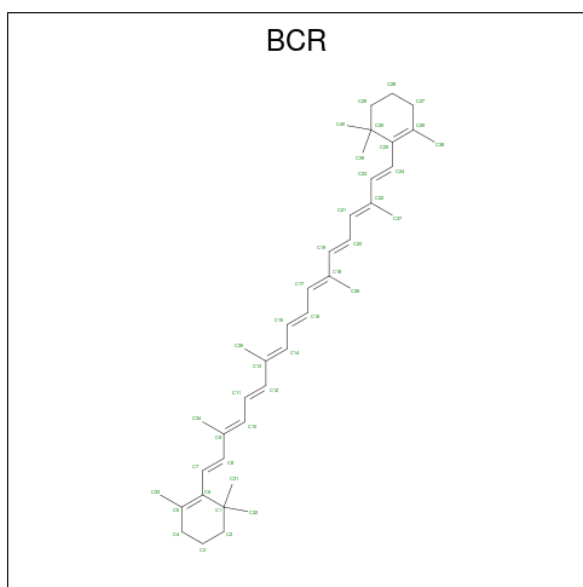
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
19	1	1	Total	C	H	O	P	0
			123	38	74	10	1	
19	2	1	Total	C	H	O	P	0
			123	38	74	10	1	
19	3	1	Total	C	H	O	P	0
			123	38	74	10	1	
19	A	1	Total	C	H	O	P	0
			246	76	148	20	2	
19	A	1	Total	C	H	O	P	0
			246	76	148	20	2	
19	B	1	Total	C	H	O	P	0
			108	34	63	10	1	

- Molecule 20 is ERGOSTEROL (three-letter code: ERG) (formula: C<sub>28</sub>H<sub>44</sub>O).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
20	1	1	67	28	38	1	0
20	2	1	134	56	76	2	0
20	2	1	134	56	76	2	0

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



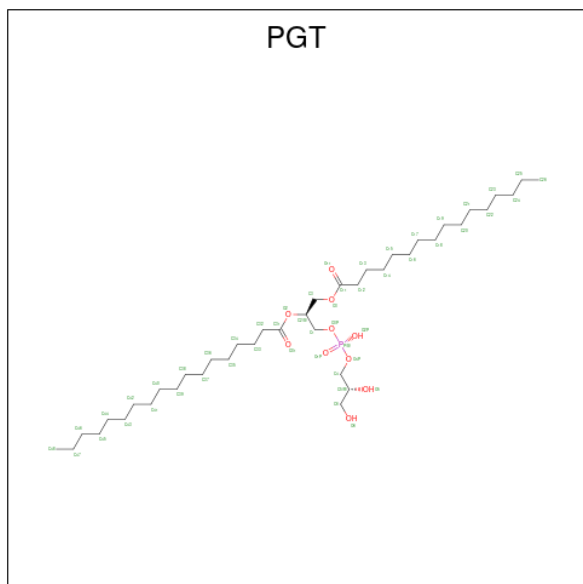
Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
21	2	1	93	40	53	0

*Continued on next page...*

*Continued from previous page...*

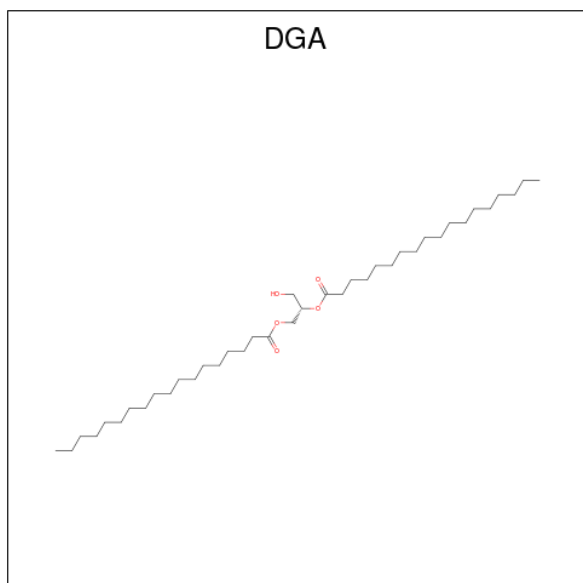
Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
21	A	1	460	200	260	0
21	A	1	460	200	260	0
21	A	1	460	200	260	0
21	A	1	460	200	260	0
21	A	1	460	200	260	0
21	B	1	733	320	413	0
21	B	1	733	320	413	0
21	B	1	733	320	413	0
21	B	1	733	320	413	0
21	B	1	733	320	413	0
21	B	1	733	320	413	0
21	B	1	733	320	413	0
21	B	1	733	320	413	0
21	B	1	733	320	413	0
21	F	1	184	80	104	0
21	F	1	184	80	104	0
21	I	1	91	40	51	0
21	K	1	91	40	51	0
21	L	1	276	120	156	0
21	L	1	276	120	156	0
21	L	1	276	120	156	0
21	O	1	92	40	52	0

- Molecule 22 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: C<sub>40</sub>H<sub>79</sub>O<sub>10</sub>P).



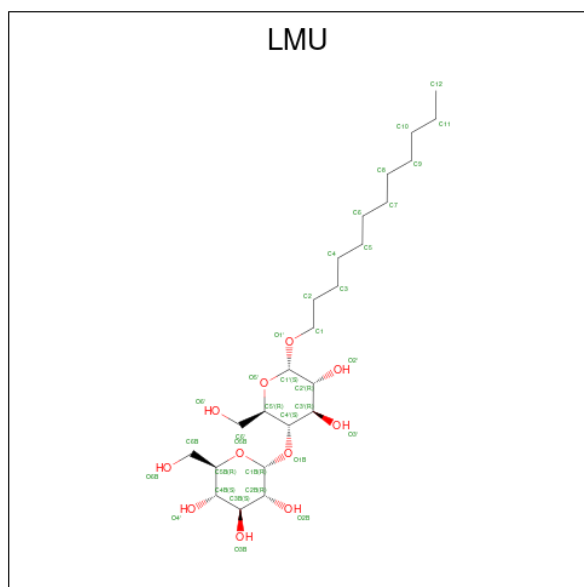
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
22	2	1	Total	C	H	O	P	0
			81	24	46	10	1	
22	B	1	Total	C	H	O	P	0
			81	24	46	10	1	

- Molecule 23 is DIACYL GLYCEROL (three-letter code: DGA) (formula: C<sub>39</sub>H<sub>76</sub>O<sub>5</sub>).



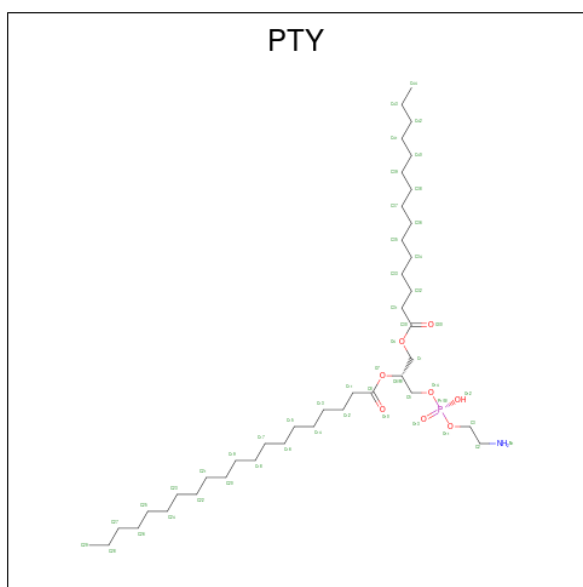
Mol	Chain	Residues	Atoms				AltConf
23	2	1	Total	C	H	O	0
			120	39	76	5	
23	J	1	Total	C	H	O	0
			120	39	76	5	

- Molecule 24 is DODECYL-ALPHA-D-MALTOSE (three-letter code: LMU) (formula:  $C_{24}H_{46}O_{11}$ ).



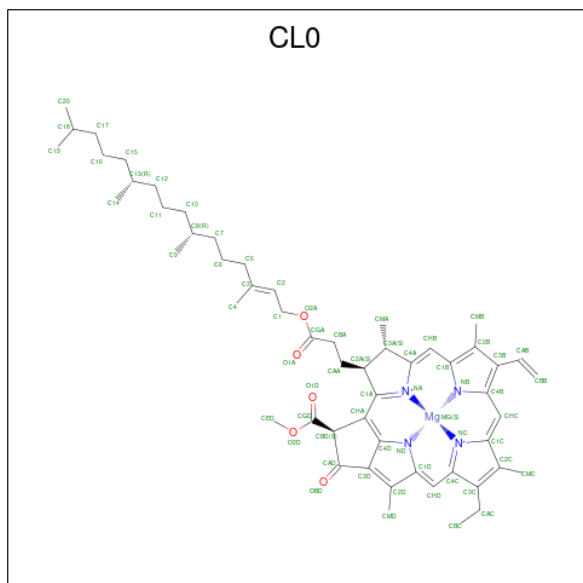
Mol	Chain	Residues	Atoms				AltConf
24	3	1	Total	C	H	O	0
			81	24	46	11	
24	A	1	Total	C	H	O	0
			81	24	46	11	

- Molecule 25 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula:  $C_{40}H_{80}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
25	3	1	258	80	158	2	16	2	0
25	3	1	258	80	158	2	16	2	0
25	A	1	113	37	66	1	8	1	0
25	L	1	129	40	79	1	8	1	0

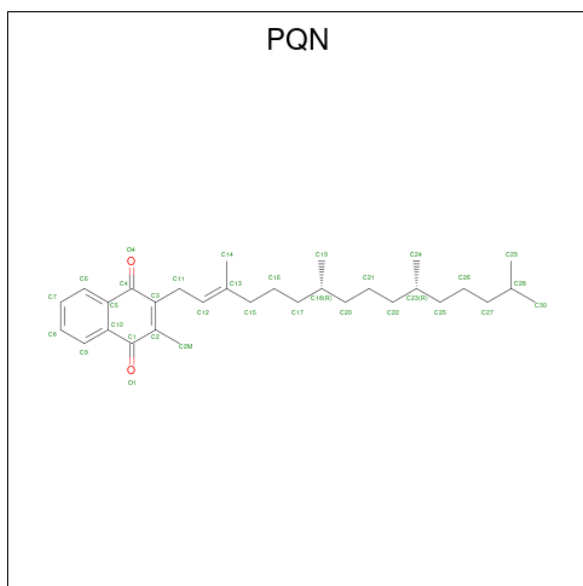
- Molecule 26 is CHLOROPHYLL A ISOMER (three-letter code: CLO) (formula:  $C_{55}H_{72}MgN_4O_5$ ).





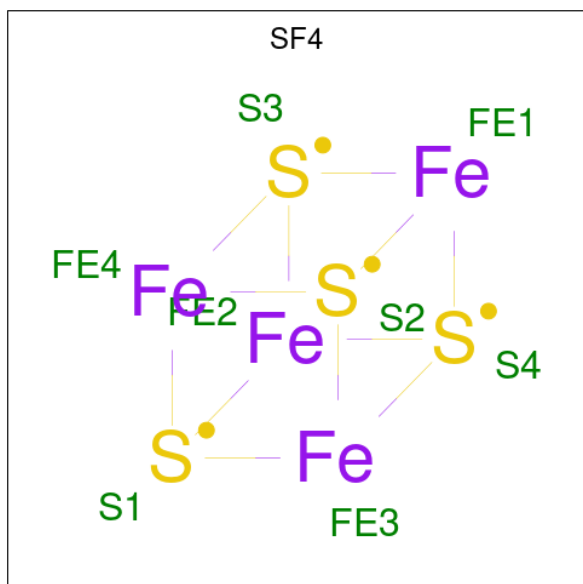
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	Mg	N		O
26	A	1	138	55	73	1	4	5	0

- Molecule 27 is PHYLLOQUINONE (three-letter code: PQN) (formula:  $C_{31}H_{46}O_2$ ).



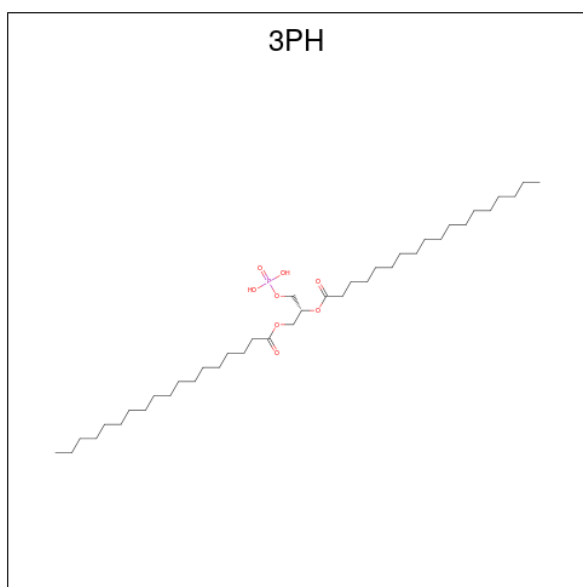
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
27	A	1	79	31	46	2	0
27	B	1	79	31	46	2	0

- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).



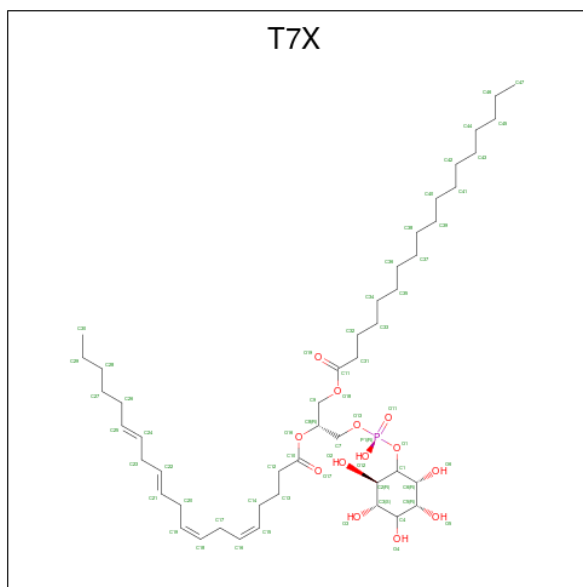
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
28	A	1	8	4	4	0
28	C	1	16	8	8	0
28	C	1	16	8	8	0

- Molecule 29 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula:  $C_{39}H_{77}O_8P$ ).



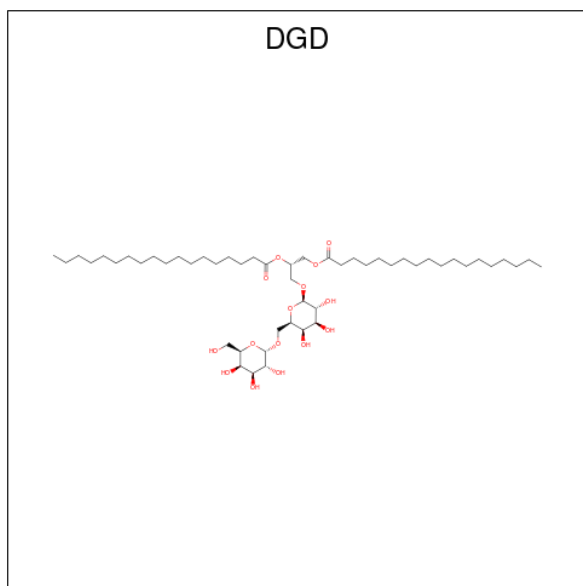
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
29	A	1	123	39	75	8	1	0
29	B	1	123	39	75	8	1	0
29	J	1	123	39	75	8	1	0

- Molecule 30 is Phosphatidylinositol (three-letter code: T7X) (formula:  $C_{47}H_{83}O_{13}P$ ).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	H	O		P
30	A	1	123	40	69	13	1	0

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
31	B	1	450	153	252	45	0
31	B	1	450	153	252	45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf
31	B	1	Total	C	H	O	0
			450	153	252	45	

- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
32	B	2	Total	Ca	0
			2	2	

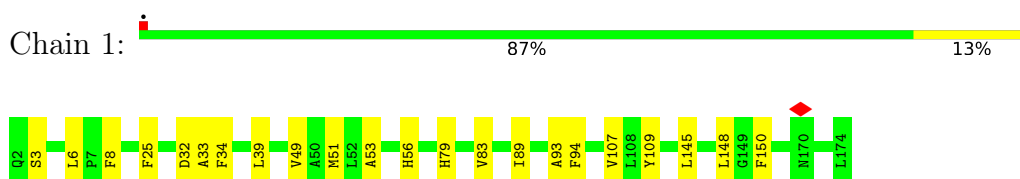
- Molecule 33 is water.

Mol	Chain	Residues	Atoms		AltConf
33	1	15	Total	O	0
			15	15	
33	2	8	Total	O	0
			8	8	
33	3	6	Total	O	0
			6	6	
33	A	79	Total	O	0
			79	79	
33	B	68	Total	O	0
			68	68	
33	C	24	Total	O	0
			24	24	
33	D	14	Total	O	0
			14	14	
33	E	11	Total	O	0
			11	11	
33	F	11	Total	O	0
			11	11	
33	J	2	Total	O	0
			2	2	
33	K	2	Total	O	0
			2	2	
33	L	2	Total	O	0
			2	2	
33	M	2	Total	O	0
			2	2	
33	O	5	Total	O	0
			5	5	

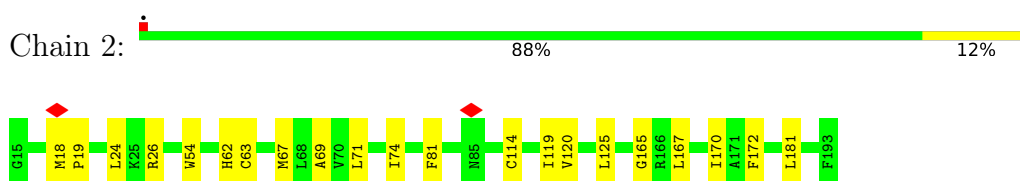
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

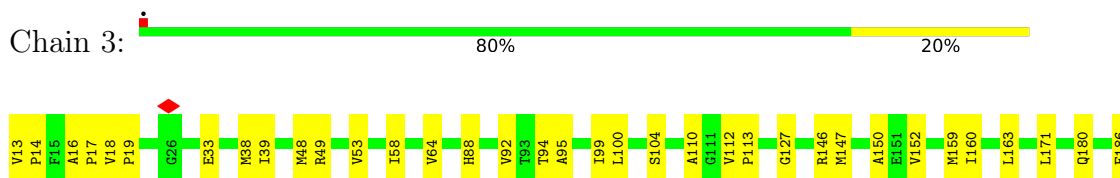
- Molecule 1: Similar to light harvesting protein



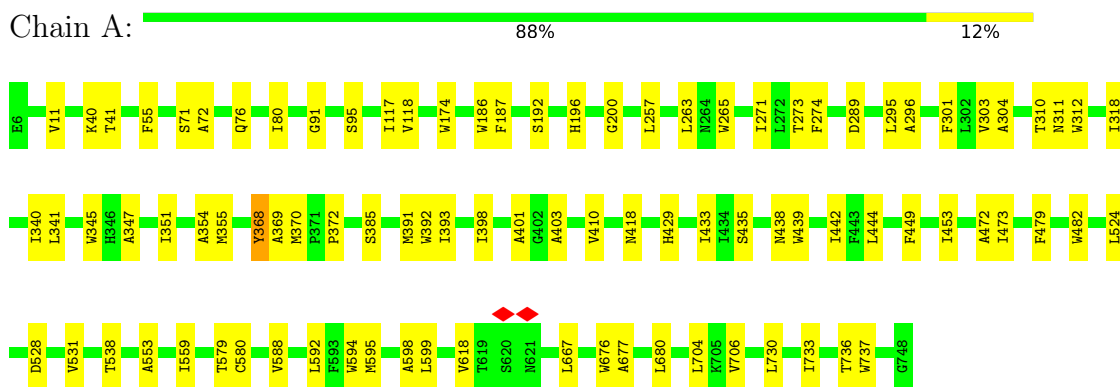
- Molecule 2: Similar to chlorophyll a/b-binding protein, CP24



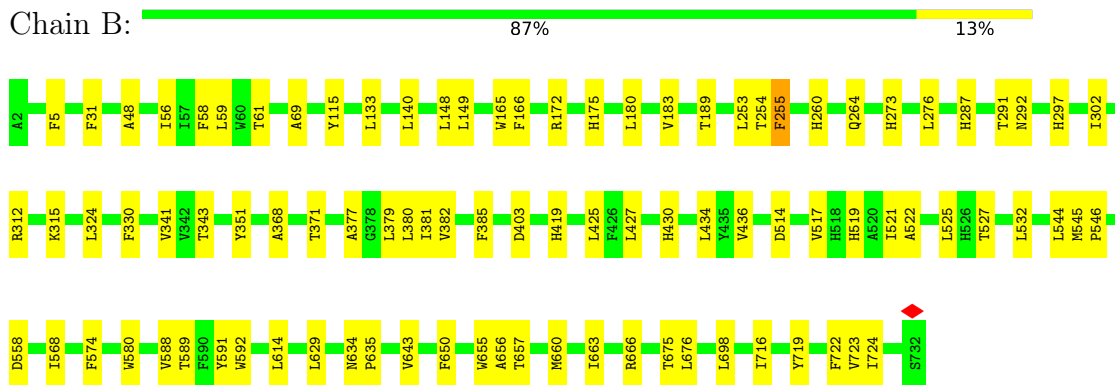
- Molecule 3: Lhcr3



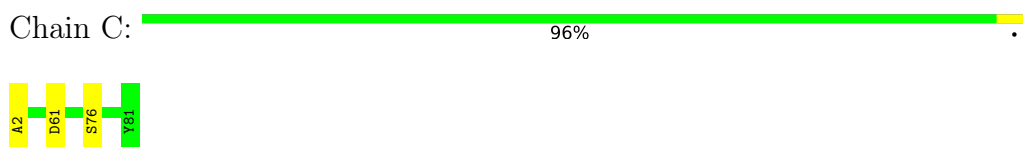
- Molecule 4: Photosystem I P700 chlorophyll a apoprotein A1



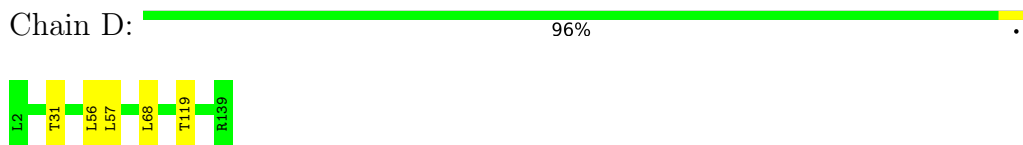
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A2



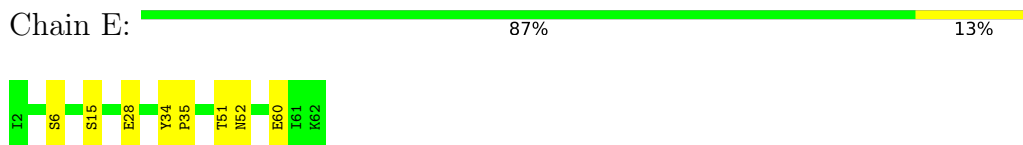
- Molecule 6: Photosystem I iron-sulfur center



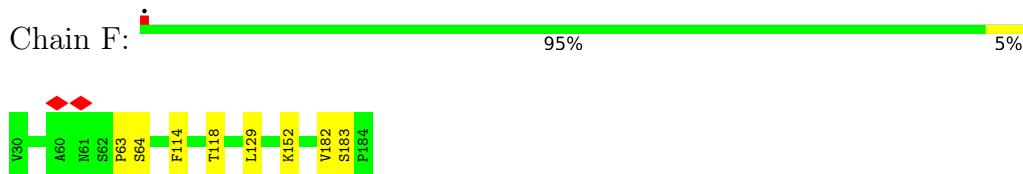
- Molecule 7: Photosystem I p700 chlorophyll A apoprotein A2



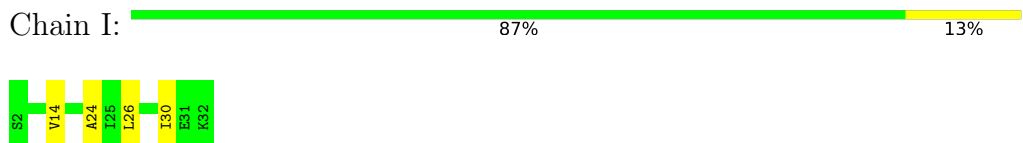
- Molecule 8: Photosystem I iron-sulfur center subunit VII




- Molecule 9: PSI-F



- Molecule 10: Photosystem I reaction center subunit VIII




- Molecule 11: Photosystem I reaction center subunit IX

Chain J:  89% 11%




- Molecule 12: PSI-K

Chain K:  81% 19%



- Molecule 13: Photosystem I reaction center subunit XI

Chain L:  88% 11%



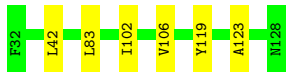
- Molecule 14: Photosystem I reaction center subunit XII

Chain M:  93% 7%



- Molecule 15: PsaO

Chain O:  94% 6%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128943	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 ( $e^-/\text{\AA}^2$ )	40.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.163	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0186	Depositor
Map size ( $\text{\AA}$ )	315.59998, 315.59998, 315.59998	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0519999, 1.0519999, 1.0519999	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, CLA, CL0, PTY, PGT, ERG, PQN, CA, 3PH, T7X, C7Z, DGA, DGD, SF4, RRX, LHG, LMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.28	0/1426	0.52	0/1927
2	2	0.27	0/1431	0.50	0/1931
3	3	0.25	0/1376	0.52	0/1867
4	A	0.26	0/6002	0.49	0/8179
5	B	0.25	0/6028	0.47	0/8236
6	C	0.24	0/607	0.53	0/822
7	D	0.25	0/1118	0.53	0/1509
8	E	0.24	0/502	0.50	0/680
9	F	0.25	0/1304	0.51	0/1772
10	I	0.25	0/235	0.44	0/321
11	J	0.26	0/321	0.47	0/437
12	K	0.25	0/394	0.46	0/534
13	L	0.26	0/1064	0.53	1/1448 (0.1%)
14	M	0.25	0/205	0.38	0/277
15	O	0.27	0/773	0.45	0/1061
All	All	0.26	0/22786	0.49	1/31001 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	93	MET	CG-SD-CE	-6.72	89.44	100.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1381	1353	1353	21	0
2	2	1395	1385	1385	21	0
3	3	1341	1348	1348	38	0
4	A	5815	5740	5740	88	0
5	B	5819	5645	5645	85	0
6	C	597	576	576	2	0
7	D	1094	1093	1093	3	0
8	E	493	509	509	6	0
9	F	1270	1243	1243	9	0
10	I	230	253	253	4	0
11	J	312	327	327	3	0
12	K	390	419	419	8	0
13	L	1039	1057	1057	15	0
14	M	204	226	226	2	0
15	O	747	742	742	8	0
16	1	704	770	759	36	0
16	2	843	938	928	42	0
16	3	749	798	786	49	0
16	A	2665	2984	2944	151	0
16	B	2460	2742	2705	132	0
16	F	256	280	276	13	0
16	I	130	146	144	9	0
16	J	65	73	71	3	0
16	K	130	145	144	6	0
16	L	260	291	287	14	0
16	O	260	288	284	13	0
17	1	168	0	0	7	0
17	2	84	0	0	0	0
17	3	210	0	0	11	0
17	A	42	0	0	0	0
17	J	42	0	0	0	0
18	1	41	56	56	10	0
18	2	41	56	56	2	0
18	A	41	55	56	2	0
18	J	41	56	56	2	0
18	K	41	56	56	4	0
19	1	49	74	74	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2	49	74	74	1	0
19	3	49	74	74	2	0
19	A	98	148	148	1	0
19	B	45	63	63	0	0
20	1	29	38	38	4	0
20	2	58	76	76	9	0
21	2	40	53	54	10	0
21	A	200	260	260	43	0
21	B	320	413	415	47	0
21	F	80	104	105	9	0
21	I	40	51	53	3	0
21	K	40	51	54	5	0
21	L	120	156	156	20	0
21	O	40	52	52	9	0
22	2	35	46	40	0	0
22	B	35	46	40	0	0
23	2	44	76	76	0	0
23	J	44	76	76	1	0
24	3	35	46	46	1	0
24	A	35	46	46	0	0
25	3	100	158	158	0	0
25	A	47	66	66	3	0
25	L	50	79	79	0	0
26	A	65	73	72	5	0
27	A	33	46	46	0	0
27	B	33	46	46	4	0
28	A	8	0	0	0	0
28	C	16	0	0	0	0
29	A	48	75	75	0	0
29	B	48	75	75	0	0
29	J	48	75	75	0	0
30	A	54	69	0	1	0
31	B	198	252	288	9	0
32	B	2	0	0	0	0
33	1	15	0	0	0	0
33	2	8	0	0	0	0
33	3	6	0	0	0	0
33	A	79	0	0	0	0
33	B	68	0	0	0	0
33	C	24	0	0	0	0
33	D	14	0	0	0	0
33	E	11	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	F	11	0	0	0	0
33	J	2	0	0	0	0
33	K	2	0	0	0	0
33	L	2	0	0	0	0
33	M	2	0	0	0	0
33	O	5	0	0	0	0
All	All	33884	34687	34524	699	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (699) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:621:ERG:C3	20:2:621:ERG:O1	1.70	1.39
20:2:618:ERG:O1	20:2:618:ERG:C3	1.70	1.37
20:1:618:ERG:C3	20:1:618:ERG:O1	1.70	1.36
16:A:854:CLA:HBB1	16:A:854:CLA:HMB1	1.36	1.04
16:A:828:CLA:HBB1	16:A:828:CLA:HMB1	1.37	1.01
16:B:827:CLA:HBB1	16:B:827:CLA:HMB1	1.44	1.00
16:A:802:CLA:HHC	16:A:802:CLA:HBB1	1.47	0.94
16:B:817:CLA:HBB1	16:B:817:CLA:HMB1	1.48	0.94
16:B:811:CLA:HHC	16:B:811:CLA:HBB1	1.51	0.92
16:A:837:CLA:HBB1	16:A:837:CLA:HMB1	1.51	0.91
16:A:822:CLA:HMB1	16:A:822:CLA:HBB1	1.53	0.90
4:A:392:TRP:CD1	16:A:827:CLA:HAB	2.08	0.89
16:B:836:CLA:HAB	27:B:839:PQN:H141	1.54	0.89
16:B:828:CLA:HBB1	16:B:828:CLA:HMB1	1.55	0.88
16:A:823:CLA:HMA1	16:O:201:CLA:HMC2	1.55	0.87
16:I:102:CLA:HHC	16:I:102:CLA:HBB1	1.56	0.87
16:A:819:CLA:HBB1	16:A:819:CLA:HMB1	1.56	0.86
16:A:834:CLA:HHC	16:A:834:CLA:HBB1	1.58	0.85
16:A:807:CLA:HBB1	16:A:807:CLA:HMB1	1.57	0.85
16:A:829:CLA:HBB1	16:A:829:CLA:HMB1	1.57	0.84
16:B:831:CLA:HMB1	16:B:831:CLA:HBB1	1.59	0.83
16:B:825:CLA:HMB1	16:B:825:CLA:HBB1	1.61	0.82
16:F:204:CLA:HBB1	16:F:204:CLA:HMB1	1.60	0.82
16:B:802:CLA:HHC	16:B:802:CLA:HBB1	1.60	0.82
16:2:606:CLA:HBB1	16:2:606:CLA:HMB1	1.61	0.81
16:A:821:CLA:HMB1	16:A:821:CLA:HBB1	1.62	0.81
16:B:834:CLA:HMB1	16:B:834:CLA:HBB1	1.62	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:819:CLA:H201	21:A:850:BCR:H352	1.62	0.80
16:B:818:CLA:HMB2	16:B:823:CLA:HMA3	1.63	0.79
4:A:265:TRP:CH2	16:A:816:CLA:HBB1	2.17	0.79
16:2:601:CLA:HHC	16:2:601:CLA:HBB1	1.65	0.79
16:B:833:CLA:HMB1	16:B:833:CLA:HBB1	1.65	0.78
5:B:656:ALA:HB3	16:B:801:CLA:HBB2	1.64	0.78
3:3:163:LEU:HD13	16:3:205:CLA:HBB2	1.67	0.77
21:B:840:BCR:HC8	21:B:840:BCR:H321	1.66	0.77
16:2:608:CLA:H43	16:2:608:CLA:HMB2	1.67	0.76
16:F:201:CLA:HMC2	21:F:203:BCR:H381	1.68	0.75
21:A:844:BCR:H383	21:A:844:BCR:H23C	1.69	0.75
16:2:602:CLA:HBB1	16:2:602:CLA:HMB1	1.68	0.75
16:A:835:CLA:HBB1	16:A:835:CLA:HMB1	1.70	0.74
21:B:847:BCR:H393	21:B:847:BCR:H23C	1.70	0.74
16:2:604:CLA:HBC2	16:2:613:CLA:HAB	1.68	0.73
21:A:845:BCR:H383	21:A:845:BCR:H23C	1.71	0.73
5:B:580:TRP:CH2	16:B:803:CLA:HAB	2.24	0.73
21:B:855:BCR:H403	21:B:855:BCR:H23C	1.70	0.72
16:A:837:CLA:H92	21:A:845:BCR:H10C	1.71	0.72
16:A:809:CLA:HHC	16:A:809:CLA:HBB1	1.71	0.72
16:1:611:CLA:HMB3	17:1:616:C7Z:C40	2.20	0.71
4:A:55:PHE:CD2	16:A:804:CLA:HMC2	2.25	0.71
21:B:855:BCR:HC8	21:B:855:BCR:H321	1.71	0.71
16:O:202:CLA:HHC	16:O:202:CLA:HBB1	1.73	0.71
16:3:213:CLA:HBB1	16:3:213:CLA:HMB1	1.73	0.71
16:A:826:CLA:HBB1	16:A:826:CLA:HMB1	1.72	0.71
16:B:813:CLA:HMB1	16:B:813:CLA:HBB1	1.73	0.71
16:B:810:CLA:HMB1	16:B:810:CLA:HBB1	1.73	0.70
16:A:855:CLA:CAD	16:B:804:CLA:HMB3	2.22	0.70
4:A:677:ALA:HB3	16:A:854:CLA:HBB2	1.73	0.69
16:A:854:CLA:HMB1	16:A:854:CLA:CBB	2.20	0.69
21:B:840:BCR:H383	21:B:840:BCR:H23C	1.75	0.69
21:B:844:BCR:H321	21:B:844:BCR:HC8	1.75	0.69
5:B:343:THR:HG23	5:B:377:ALA:HB2	1.74	0.68
21:L:207:BCR:H321	21:L:207:BCR:HC8	1.76	0.68
4:A:449:PHE:CZ	4:A:453:ILE:HD11	2.29	0.68
5:B:148:LEU:HD21	21:B:847:BCR:H333	1.76	0.68
16:3:214:CLA:HBC3	16:3:214:CLA:HHD	1.75	0.67
16:A:811:CLA:HMB1	16:A:811:CLA:HBB1	1.76	0.67
5:B:180:LEU:HD13	16:B:812:CLA:HBB	1.76	0.67
20:1:618:ERG:O1	20:1:618:ERG:C2	2.39	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:186:TRP:CZ2	16:A:809:CLA:HMA1	2.29	0.67
16:2:608:CLA:HBC2	16:2:608:CLA:HHD	1.77	0.67
5:B:650:PHE:CZ	21:B:845:BCR:H10C	2.29	0.67
16:L:203:CLA:HHC	16:L:203:CLA:HBB1	1.76	0.67
5:B:165:TRP:CZ2	16:B:810:CLA:HMA1	2.29	0.66
5:B:324:LEU:HD13	5:B:330:PHE:CD2	2.29	0.66
4:A:594:TRP:CH2	16:A:855:CLA:HAB	2.30	0.66
21:B:842:BCR:H383	21:B:842:BCR:H23C	1.78	0.66
21:A:857:BCR:H343	21:A:857:BCR:C33	2.26	0.66
16:A:825:CLA:HAB	21:A:846:BCR:H311	1.76	0.66
16:A:808:CLA:HAB	16:B:830:CLA:HMD2	1.76	0.66
26:A:801:CL0:H13	16:B:803:CLA:OBD	1.96	0.65
1:1:51:MET:HE2	16:1:607:CLA:HAB	1.78	0.65
20:2:621:ERG:O1	20:2:621:ERG:C2	2.38	0.65
4:A:559:ILE:HD11	4:A:579:THR:HG21	1.77	0.65
26:A:801:CL0:H15	26:A:801:CL0:H11	1.79	0.65
16:B:831:CLA:CHD	16:B:832:CLA:HAB	2.27	0.65
16:A:818:CLA:HBB1	16:A:818:CLA:HMB1	1.77	0.65
5:B:56:ILE:HG13	21:B:847:BCR:H332	1.79	0.65
26:A:801:CL0:H13	16:B:803:CLA:CAD	2.27	0.65
16:B:827:CLA:HMB1	16:B:827:CLA:CBB	2.25	0.65
16:A:812:CLA:HMA2	16:A:812:CLA:C2	2.28	0.64
16:A:828:CLA:HMB1	16:A:828:CLA:CBB	2.21	0.64
17:1:614:C7Z:C15	16:2:605:CLA:HAB	2.27	0.64
16:B:822:CLA:HAB	16:B:829:CLA:HMD2	1.79	0.64
16:B:835:CLA:H52	21:B:844:BCR:H10C	1.80	0.64
16:A:822:CLA:CAB	16:O:201:CLA:HMC3	2.28	0.64
16:A:827:CLA:O1D	16:A:828:CLA:HMA1	1.97	0.64
4:A:354:ALA:HB1	21:A:846:BCR:H10C	1.79	0.64
5:B:341:VAL:CG2	21:B:844:BCR:H362	2.28	0.64
16:1:602:CLA:HBB1	16:1:602:CLA:HMB1	1.79	0.64
4:A:435:SER:HB3	5:B:675:THR:HG22	1.79	0.64
21:I:103:BCR:H402	21:L:202:BCR:H361	1.80	0.64
16:2:612:CLA:HBC3	21:2:617:BCR:C10	2.27	0.63
21:L:202:BCR:H403	21:L:202:BCR:H23C	1.80	0.63
4:A:91:GLY:O	4:A:95:SER:OG	2.16	0.63
16:A:821:CLA:HBC2	21:A:857:BCR:H372	1.81	0.63
5:B:434:LEU:HD12	21:B:855:BCR:H383	1.79	0.63
4:A:370:MET:SD	16:A:826:CLA:HAB	2.39	0.63
16:A:802:CLA:HHC	16:A:802:CLA:CBB	2.26	0.63
21:A:857:BCR:H343	21:A:857:BCR:H332	1.80	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:53:VAL:HG21	3:3:127:GLY:HA3	1.80	0.63
17:3:201:C7Z:C14	16:3:207:CLA:HAB	2.28	0.63
16:A:855:CLA:OBD	16:B:804:CLA:HMB3	1.99	0.63
16:B:831:CLA:C4C	16:B:832:CLA:HAB	2.28	0.63
16:3:205:CLA:HMC1	16:3:208:CLA:CAB	2.29	0.62
9:F:63:PRO:O	9:F:64:SER:OG	2.14	0.62
16:1:610:CLA:HMD2	17:1:614:C7Z:C39	2.29	0.62
16:2:606:CLA:H43	16:A:806:CLA:HMD1	1.81	0.62
1:1:79:HIS:O	1:1:83:VAL:HG23	1.99	0.62
20:2:621:ERG:O1	20:2:621:ERG:C4	2.41	0.62
16:A:823:CLA:H41	16:A:823:CLA:H71	1.82	0.62
21:A:846:BCR:H403	21:A:846:BCR:H23C	1.81	0.62
4:A:479:PHE:CE2	16:A:836:CLA:H42	2.35	0.62
16:1:604:CLA:HHD	16:1:604:CLA:HBC2	1.80	0.62
4:A:296:ALA:CB	16:A:817:CLA:HBB1	2.31	0.61
16:A:825:CLA:H72	16:A:833:CLA:HAB	1.83	0.61
16:A:827:CLA:H193	16:B:803:CLA:H142	1.82	0.61
4:A:196:HIS:ND1	16:A:812:CLA:HMC2	2.16	0.60
16:B:837:CLA:HBB1	16:B:837:CLA:HHC	1.82	0.60
20:1:618:ERG:O1	20:1:618:ERG:C4	2.42	0.60
18:K:103:RRX:H36	18:K:103:RRX:H42	1.84	0.60
16:1:603:CLA:HMC2	18:1:613:RRX:H38	1.84	0.60
3:3:17:PRO:HG2	16:3:203:CLA:HMA3	1.82	0.60
16:A:823:CLA:HMA1	16:O:201:CLA:CMC	2.29	0.60
21:L:206:BCR:H23C	21:L:206:BCR:H392	1.83	0.60
16:1:601:CLA:HMC3	2:2:120:VAL:HG21	1.83	0.60
5:B:180:LEU:HD11	16:B:812:CLA:H12	1.83	0.60
5:B:183:VAL:CG2	16:B:819:CLA:HMC1	2.31	0.60
16:A:817:CLA:O1D	16:A:818:CLA:HMA1	2.01	0.59
16:B:811:CLA:H143	21:B:841:BCR:H322	1.83	0.59
16:A:811:CLA:O1D	16:A:812:CLA:HMC1	2.02	0.59
2:2:67:MET:SD	16:2:608:CLA:HAB	2.41	0.59
3:3:99:ILE:HG13	16:3:207:CLA:HMD3	1.84	0.59
16:3:207:CLA:HBB1	16:3:207:CLA:HHC	1.84	0.59
16:3:213:CLA:HAB	17:3:217:C7Z:C40	2.31	0.59
16:B:806:CLA:HMB1	16:B:806:CLA:HBB1	1.84	0.59
5:B:525:LEU:HD11	16:B:833:CLA:HBB1	1.84	0.59
12:K:36:LEU:HD13	21:K:104:BCR:H352	1.83	0.59
16:A:828:CLA:H43	21:A:844:BCR:H10C	1.85	0.59
13:L:50:ILE:HA	16:L:204:CLA:HED1	1.85	0.59
16:O:203:CLA:HMD3	21:O:205:BCR:H343	1.83	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2:612:CLA:HMB3	21:2:617:BCR:H362	1.85	0.58
16:3:211:CLA:C3D	16:3:212:CLA:HMA3	2.33	0.58
16:B:817:CLA:HMB1	16:B:817:CLA:CBB	2.29	0.58
21:O:205:BCR:H383	21:O:205:BCR:H23C	1.85	0.58
16:A:839:CLA:HMA2	21:L:202:BCR:H322	1.85	0.58
18:A:847:RRX:H36	18:A:847:RRX:H42	1.86	0.58
16:A:856:CLA:HAB	16:A:856:CLA:H111	1.86	0.58
5:B:368:ALA:HB1	16:B:826:CLA:HMA1	1.84	0.58
16:B:826:CLA:HBC3	31:B:846:DGD:HBS1	1.86	0.58
21:L:202:BCR:HC8	21:L:202:BCR:H311	1.84	0.58
16:3:205:CLA:HMC1	16:3:208:CLA:HAB	1.86	0.58
16:B:829:CLA:HAB	16:B:835:CLA:CBB	2.34	0.58
13:L:127:GLY:HA3	21:L:207:BCR:H312	1.85	0.58
16:I:101:CLA:HBC3	14:M:14:ALA:HB2	1.86	0.58
3:3:100:LEU:HD22	16:3:208:CLA:HMD2	1.84	0.57
16:A:822:CLA:HMB1	16:A:822:CLA:CBB	2.30	0.57
21:A:846:BCR:H311	21:A:846:BCR:HC8	1.85	0.57
4:A:736:THR:HG23	16:A:827:CLA:HBB2	1.85	0.57
16:B:811:CLA:HHC	16:B:811:CLA:CBB	2.30	0.57
1:1:51:MET:CE	16:1:607:CLA:HAB	2.33	0.57
5:B:59:LEU:HD22	16:I:101:CLA:H93	1.86	0.57
21:A:844:BCR:H321	21:A:844:BCR:HC8	1.87	0.57
5:B:61:THR:HG23	5:B:140:LEU:HD13	1.87	0.57
21:B:843:BCR:H311	21:B:843:BCR:HC8	1.87	0.57
16:2:605:CLA:HHC	16:2:605:CLA:HBB1	1.85	0.57
21:A:850:BCR:H403	21:A:850:BCR:H23C	1.87	0.57
5:B:255:PHE:CE2	16:B:816:CLA:HBB1	2.39	0.57
5:B:716:ILE:HD13	16:B:826:CLA:HMC2	1.85	0.57
16:B:810:CLA:HMB1	16:B:810:CLA:CBB	2.35	0.57
5:B:255:PHE:CD1	16:B:816:CLA:HMB2	2.40	0.57
16:B:826:CLA:O1D	16:B:827:CLA:HMA1	2.05	0.57
4:A:385:SER:HB3	16:A:827:CLA:HMA1	1.86	0.57
16:A:825:CLA:C4B	21:A:846:BCR:H342	2.35	0.56
5:B:656:ALA:C	16:B:801:CLA:HAB	2.26	0.56
20:2:618:ERG:O1	20:2:618:ERG:C4	2.42	0.56
1:1:49:VAL:HG12	18:1:613:RRX:H45	1.87	0.56
16:A:816:CLA:HBC3	16:A:816:CLA:HMC1	1.87	0.56
16:A:837:CLA:HMB1	16:A:837:CLA:CBB	2.31	0.56
4:A:76:GLN:OE1	4:A:80:ILE:HD11	2.05	0.56
16:B:821:CLA:HMB3	16:B:838:CLA:C1D	2.35	0.56
16:A:819:CLA:HMB1	16:A:819:CLA:CBB	2.33	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:842:BCR:H321	21:B:842:BCR:HC8	1.85	0.56
11:J:9:THR:O	11:J:13:VAL:HG22	2.05	0.56
16:2:612:CLA:CMB	21:2:617:BCR:H362	2.36	0.56
16:A:826:CLA:HMB1	16:A:826:CLA:CBB	2.35	0.56
25:A:852:PTY:C24	15:O:102:ILE:HD11	2.35	0.56
16:B:825:CLA:H143	21:B:843:BCR:C19	2.36	0.56
5:B:719:TYR:HB2	16:B:804:CLA:HED3	1.88	0.55
16:B:828:CLA:HMB1	16:B:828:CLA:CBB	2.33	0.55
4:A:118:VAL:HB	16:B:830:CLA:HMD1	1.86	0.55
21:L:202:BCR:HC8	21:L:202:BCR:H321	1.88	0.55
20:2:618:ERG:O1	20:2:618:ERG:C2	2.40	0.55
4:A:71:SER:O	4:A:72:ALA:HB3	2.06	0.55
16:F:204:CLA:HMB1	16:F:204:CLA:CBB	2.35	0.55
2:2:81:PHE:CE1	16:2:613:CLA:HMB3	2.41	0.55
16:A:822:CLA:HAB	16:O:201:CLA:HMC3	1.87	0.55
5:B:287:HIS:NE2	21:B:840:BCR:H352	2.21	0.55
16:B:808:CLA:C1A	16:B:808:CLA:CGA	2.84	0.55
16:F:201:CLA:HHC	16:F:201:CLA:HBB1	1.86	0.55
4:A:257:LEU:HD13	21:A:857:BCR:H322	1.89	0.55
16:B:808:CLA:HAB	16:B:809:CLA:HAA1	1.88	0.55
16:B:833:CLA:HMB1	16:B:833:CLA:CBB	2.36	0.55
3:3:112:VAL:HG22	16:3:209:CLA:HMA1	1.87	0.55
4:A:528:ASP:HA	4:A:531:VAL:HG12	1.89	0.55
21:B:845:BCR:H382	21:B:845:BCR:H23C	1.88	0.55
16:A:829:CLA:HMB1	16:A:829:CLA:CBB	2.33	0.55
16:B:815:CLA:C1D	16:B:816:CLA:HBB2	2.37	0.55
16:B:835:CLA:C5	21:B:844:BCR:H10C	2.37	0.55
16:A:825:CLA:CHC	21:A:846:BCR:H342	2.36	0.55
16:3:205:CLA:HMB1	16:3:205:CLA:HBB1	1.88	0.54
3:3:58:ILE:HD12	16:3:209:CLA:HMD3	1.90	0.54
19:A:842:LHG:H261	21:A:845:BCR:H341	1.90	0.54
31:B:850:DGD:HAF1	31:B:850:DGD:HAT1	1.90	0.54
4:A:200:GLY:HA3	16:A:812:CLA:HBB1	1.90	0.54
16:A:824:CLA:HMB1	16:A:824:CLA:HBB1	1.89	0.54
16:A:819:CLA:HMB3	12:K:41:CYS:SG	2.47	0.54
16:B:831:CLA:HMB1	16:B:831:CLA:CBB	2.35	0.54
20:2:621:ERG:H122	20:2:621:ERG:H212	1.88	0.54
16:A:830:CLA:HAB	16:A:837:CLA:CBB	2.38	0.54
5:B:287:HIS:CD2	21:B:840:BCR:H352	2.42	0.54
4:A:429:HIS:CE1	4:A:433:ILE:HD11	2.42	0.54
2:2:167:LEU:HD13	16:2:609:CLA:HBC1	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:203:CLA:O1A	16:O:203:CLA:H43	2.08	0.54
21:F:206:BCR:H392	21:F:206:BCR:H23C	1.90	0.54
21:L:207:BCR:H321	21:L:207:BCR:C8	2.37	0.54
16:B:802:CLA:CAB	21:F:206:BCR:H362	2.38	0.54
7:D:57:LEU:HD21	7:D:68:LEU:HD21	1.89	0.54
18:1:613:RRX:H36	18:1:613:RRX:C10	2.37	0.53
16:B:802:CLA:HHC	16:B:802:CLA:CBB	2.34	0.53
31:B:849:DGD:HAT1	16:I:102:CLA:H111	1.89	0.53
16:B:834:CLA:H93	16:B:834:CLA:CAB	2.38	0.53
16:2:602:CLA:HMB1	16:2:602:CLA:CBB	2.38	0.53
1:1:56:HIS:CD2	18:1:613:RRX:H54	2.43	0.53
16:3:213:CLA:HMB1	16:3:213:CLA:CBB	2.39	0.53
16:A:830:CLA:HAB	16:A:837:CLA:CAB	2.38	0.53
16:B:838:CLA:H2A	16:B:838:CLA:HED2	1.91	0.53
16:2:601:CLA:HHC	16:2:601:CLA:CBB	2.36	0.53
3:3:49:ARG:NH2	3:3:152:VAL:HG21	2.24	0.53
16:A:824:CLA:HMB1	16:A:824:CLA:CBB	2.39	0.53
4:A:303:VAL:O	16:A:821:CLA:HBC1	2.09	0.53
10:I:24:ALA:HB1	13:L:95:LEU:HD21	1.91	0.53
13:L:64:GLN:HB2	16:L:205:CLA:HMA1	1.91	0.53
21:F:206:BCR:HC8	21:F:206:BCR:H311	1.89	0.53
16:B:837:CLA:HMD2	27:B:839:PQN:H192	1.91	0.52
5:B:48:ALA:HB3	14:M:28:LEU:HD21	1.91	0.52
5:B:291:THR:HG22	5:B:292:ASN:H	1.73	0.52
16:B:825:CLA:HMB1	16:B:825:CLA:CBB	2.35	0.52
16:B:806:CLA:H192	16:B:812:CLA:HMD1	1.90	0.52
16:B:825:CLA:HMA3	21:B:844:BCR:H312	1.92	0.52
16:1:602:CLA:HMC2	18:1:613:RRX:H25	1.90	0.52
16:A:835:CLA:HMB1	16:A:835:CLA:CBB	2.38	0.52
16:A:839:CLA:H93	16:A:839:CLA:HBB1	1.92	0.52
16:B:821:CLA:CBB	21:B:843:BCR:H321	2.39	0.52
16:B:821:CLA:HBB1	21:B:843:BCR:H321	1.92	0.52
16:2:606:CLA:HMB1	16:2:606:CLA:CBB	2.37	0.52
16:2:607:CLA:HMB2	23:J:101:DGA:HAH1	1.92	0.52
18:2:616:RRX:H21	18:2:616:RRX:H11	1.92	0.52
5:B:522:ALA:HB2	16:B:834:CLA:HMA1	1.91	0.52
16:1:601:CLA:CMC	2:2:120:VAL:HG21	2.41	0.51
3:3:39:ILE:HD13	16:3:204:CLA:H42	1.92	0.51
16:A:807:CLA:HMB1	16:A:807:CLA:CBB	2.34	0.51
16:A:855:CLA:O1D	16:B:804:CLA:HBB1	2.10	0.51
15:O:42:LEU:CD2	21:O:205:BCR:H393	2.40	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:53:ALA:HB1	1:1:150:PHE:CE1	2.45	0.51
16:B:801:CLA:HBB1	16:B:801:CLA:HMB1	1.93	0.51
2:2:114:CYS:CB	16:2:607:CLA:HAB	2.40	0.51
4:A:192:SER:HA	4:A:310:THR:HG21	1.91	0.51
4:A:304:ALA:HB2	16:A:820:CLA:HBC2	1.93	0.51
4:A:347:ALA:HB1	21:A:845:BCR:H391	1.90	0.51
4:A:482:TRP:CH2	15:O:102:ILE:HD12	2.45	0.51
16:L:203:CLA:HHC	16:L:203:CLA:CBB	2.40	0.51
1:1:107:VAL:O	16:1:606:CLA:HMA2	2.11	0.51
16:3:203:CLA:HBC3	16:3:203:CLA:HHD	1.92	0.51
5:B:592:TRP:CD1	16:B:833:CLA:HBC2	2.45	0.51
13:L:21:ILE:HD11	16:L:201:CLA:C2D	2.40	0.51
21:L:202:BCR:H403	21:L:202:BCR:C23	2.41	0.51
18:1:613:RRX:H36	18:1:613:RRX:H42	1.92	0.51
3:3:99:ILE:CG1	16:3:207:CLA:HMD3	2.41	0.51
4:A:439:TRP:CZ2	16:L:201:CLA:HAB	2.45	0.51
16:B:801:CLA:H111	21:B:845:BCR:H362	1.92	0.51
16:I:102:CLA:HHC	16:I:102:CLA:CBB	2.35	0.51
4:A:296:ALA:HB2	16:A:817:CLA:HBB1	1.93	0.51
21:B:844:BCR:H23C	21:B:844:BCR:C38	2.41	0.51
16:1:607:CLA:HMB1	16:1:607:CLA:HBB1	1.91	0.51
5:B:315:LYS:N	5:B:403:ASP:OD2	2.44	0.51
16:A:805:CLA:C15	16:A:828:CLA:HBB2	2.40	0.51
5:B:698:LEU:HD11	16:B:837:CLA:HMD3	1.92	0.51
16:K:102:CLA:HMC2	18:K:103:RRX:H18	1.93	0.51
2:2:24:LEU:HD12	16:2:601:CLA:HMB3	1.92	0.51
20:2:618:ERG:C3	20:2:618:ERG:HO1	2.13	0.51
4:A:680:LEU:HB2	16:A:854:CLA:HMC3	1.92	0.51
4:A:345:TRP:NE1	16:A:824:CLA:H203	2.26	0.50
16:A:823:CLA:H42	21:A:845:BCR:H363	1.92	0.50
5:B:629:LEU:HD22	5:B:722:PHE:HA	1.94	0.50
3:3:104:SER:CB	16:3:209:CLA:HAB	2.40	0.50
5:B:273:HIS:ND1	16:B:816:CLA:HMB1	2.26	0.50
16:B:829:CLA:HAB	16:B:835:CLA:HBB2	1.93	0.50
10:I:14:VAL:HG21	16:I:101:CLA:H12	1.93	0.50
11:J:6:TYR:O	11:J:9:THR:HG22	2.11	0.50
4:A:403:ALA:HB2	4:A:588:VAL:HG11	1.92	0.50
1:1:3:SER:OG	1:1:6:LEU:O	2.25	0.50
2:2:18:MET:HB3	2:2:19:PRO:HD3	1.92	0.50
16:3:210:CLA:HMC2	17:3:215:C7Z:C11	2.42	0.50
16:3:214:CLA:H203	16:K:102:CLA:HAB	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:733:ILE:HG21	16:A:827:CLA:HMC2	1.93	0.50
5:B:580:TRP:HH2	16:B:803:CLA:HAB	1.75	0.50
3:3:64:VAL:HG21	17:3:215:C7Z:C20	2.42	0.50
3:3:171:LEU:HD22	16:3:213:CLA:HMD1	1.94	0.50
16:1:609:CLA:HHC	16:1:609:CLA:HBB1	1.93	0.50
4:A:347:ALA:HB1	21:A:845:BCR:C39	2.41	0.50
16:A:811:CLA:HBB1	16:A:819:CLA:H91	1.93	0.50
16:A:815:CLA:HBB1	16:A:815:CLA:HMB1	1.94	0.50
16:2:607:CLA:H93	16:2:607:CLA:H51	1.94	0.49
4:A:439:TRP:CE2	16:L:201:CLA:HAB	2.47	0.49
3:3:100:LEU:CD2	16:3:208:CLA:HMD2	2.42	0.49
25:A:852:PTY:C23	15:O:102:ILE:HD11	2.42	0.49
5:B:5:PHE:CD1	10:I:30:ILE:HG22	2.47	0.49
15:O:102:ILE:O	15:O:106:VAL:HG23	2.11	0.49
16:A:821:CLA:CAD	21:A:857:BCR:H393	2.42	0.49
5:B:341:VAL:HG21	21:B:844:BCR:H362	1.94	0.49
16:B:811:CLA:H141	16:B:819:CLA:H91	1.94	0.49
20:1:618:ERG:C3	20:1:618:ERG:HO1	2.13	0.49
2:2:181:LEU:HD22	16:2:611:CLA:HMD1	1.94	0.49
3:3:160:ILE:HG23	16:3:213:CLA:HMC3	1.94	0.49
16:F:202:CLA:CBB	16:F:202:CLA:HHC	2.42	0.49
15:O:119:TYR:O	15:O:123:ALA:HB3	2.12	0.49
16:2:606:CLA:HMB3	21:2:617:BCR:HC41	1.94	0.49
16:A:821:CLA:HMB1	16:A:821:CLA:CBB	2.40	0.49
16:B:828:CLA:H112	31:B:846:DGD:HBH2	1.95	0.49
16:B:830:CLA:HMB1	21:B:855:BCR:H373	1.95	0.49
9:F:114:PHE:CZ	9:F:118:THR:HG21	2.48	0.49
21:L:206:BCR:H331	21:L:206:BCR:HC8	1.93	0.49
16:O:202:CLA:HHC	16:O:202:CLA:CBB	2.42	0.49
16:3:205:CLA:HMB2	17:3:216:C7Z:C12	2.43	0.49
21:A:845:BCR:H383	21:A:845:BCR:C23	2.42	0.49
4:A:677:ALA:CB	16:A:854:CLA:HBB2	2.40	0.49
5:B:149:LEU:HD23	16:B:810:CLA:HBC1	1.93	0.49
16:B:801:CLA:HMB1	16:B:801:CLA:CBB	2.43	0.49
21:B:855:BCR:H351	21:B:855:BCR:H15C	1.69	0.49
16:A:832:CLA:H152	21:L:202:BCR:H343	1.95	0.49
16:F:202:CLA:HBC2	16:F:202:CLA:HHD	1.95	0.49
17:1:612:C7Z:C39	17:1:612:C7Z:C32	2.91	0.48
16:F:202:CLA:HBB2	21:F:203:BCR:HC41	1.95	0.48
16:2:609:CLA:C4D	16:2:610:CLA:HMA3	2.43	0.48
16:2:611:CLA:HMC1	16:2:611:CLA:HBC2	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:808:CLA:HAB	16:B:809:CLA:CAA	2.43	0.48
4:A:594:TRP:HH2	16:A:855:CLA:HAB	1.77	0.48
16:B:834:CLA:HMB1	16:B:834:CLA:CBB	2.40	0.48
3:3:180:GLN:HE21	16:3:213:CLA:HED1	1.78	0.48
4:A:369:ALA:HB1	16:A:826:CLA:HMC1	1.94	0.48
16:B:837:CLA:HBC3	21:B:845:BCR:C23	2.42	0.48
1:1:34:PHE:HB2	1:1:39:LEU:HD11	1.96	0.48
16:1:607:CLA:HMB1	16:1:607:CLA:CBB	2.43	0.48
4:A:11:VAL:HG11	16:A:809:CLA:HAA2	1.95	0.48
4:A:312:TRP:CZ2	21:A:850:BCR:H383	2.48	0.48
4:A:318:ILE:HG21	16:A:824:CLA:HAC1	1.96	0.48
4:A:372:PRO:HB3	16:A:818:CLA:HMA2	1.95	0.48
6:C:2:ALA:N	6:C:76:SER:HG	2.11	0.48
12:K:50:ILE:HG13	16:K:101:CLA:HMC3	1.95	0.48
16:L:201:CLA:HBB1	16:L:201:CLA:HMB1	1.95	0.48
2:2:71:LEU:HD11	16:2:613:CLA:HMC1	1.95	0.48
16:J:102:CLA:HHC	16:J:102:CLA:HBB1	1.96	0.48
16:3:204:CLA:HMC2	17:3:216:C7Z:C11	2.44	0.48
4:A:410:VAL:HG23	4:A:553:ALA:HB1	1.94	0.48
16:A:827:CLA:C1A	16:A:827:CLA:CGA	2.92	0.48
24:3:202:LMU:O5B	24:3:202:LMU:O3'	2.16	0.48
4:A:410:VAL:CG2	4:A:553:ALA:HB1	2.44	0.48
16:B:813:CLA:HMB1	16:B:813:CLA:CBB	2.42	0.48
16:A:805:CLA:H152	16:A:828:CLA:HBB2	1.96	0.47
16:B:816:CLA:HMD2	16:B:817:CLA:H202	1.94	0.47
16:B:834:CLA:HMC3	21:B:855:BCR:H401	1.95	0.47
4:A:706:VAL:HG21	16:A:856:CLA:HMB3	1.95	0.47
16:A:819:CLA:H203	21:A:844:BCR:H382	1.96	0.47
16:A:838:CLA:H42	16:A:854:CLA:H18	1.96	0.47
18:A:847:RRX:H36	18:A:847:RRX:C10	2.44	0.47
16:B:814:CLA:C1C	21:B:840:BCR:H393	2.43	0.47
4:A:704:LEU:HD22	16:B:802:CLA:HMD3	1.96	0.47
16:B:818:CLA:HMD2	16:B:822:CLA:C9	2.44	0.47
18:K:103:RRX:H36	18:K:103:RRX:C10	2.44	0.47
13:L:8:TYR:HA	13:L:18:ALA:HB2	1.95	0.47
16:2:605:CLA:HHC	16:2:605:CLA:CBB	2.43	0.47
16:B:827:CLA:H143	21:B:841:BCR:C17	2.44	0.47
7:D:31:THR:HG22	7:D:56:LEU:HD13	1.96	0.47
16:L:201:CLA:HMB1	16:L:201:CLA:CBB	2.44	0.47
4:A:677:ALA:O	16:A:854:CLA:HAB	2.15	0.47
5:B:312:ARG:HG3	5:B:312:ARG:HH11	1.79	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:L:202:BCR:H321	21:L:202:BCR:C8	2.43	0.47
8:E:51:THR:HG22	8:E:52:ASN:N	2.29	0.47
16:3:206:CLA:CGA	16:3:206:CLA:C1A	2.93	0.47
16:3:207:CLA:HHC	16:3:207:CLA:CBB	2.45	0.47
16:3:207:CLA:HMD2	17:3:218:C7Z:C34	2.45	0.47
4:A:257:LEU:HD22	21:A:857:BCR:H313	1.95	0.47
4:A:449:PHE:CE1	16:A:855:CLA:HMA1	2.50	0.47
16:A:809:CLA:HHC	16:A:809:CLA:CBB	2.42	0.47
16:A:836:CLA:H111	16:A:836:CLA:HMC2	1.97	0.47
16:A:854:CLA:O2A	5:B:425:LEU:HD23	2.15	0.47
5:B:175:HIS:NE2	16:B:819:CLA:HMD2	2.30	0.47
16:F:201:CLA:HHC	16:F:201:CLA:CBB	2.45	0.47
15:O:83:LEU:HB2	21:O:205:BCR:H313	1.96	0.47
16:O:204:CLA:C3A	16:O:204:CLA:CGA	2.92	0.47
21:O:205:BCR:H331	21:O:205:BCR:HC8	1.97	0.47
16:A:803:CLA:H43	16:A:810:CLA:HMC2	1.96	0.47
16:A:854:CLA:CGA	16:A:854:CLA:H3A	2.44	0.47
5:B:519:HIS:CE1	21:B:855:BCR:H393	2.50	0.47
10:I:26:LEU:O	10:I:30:ILE:HG23	2.15	0.47
16:B:808:CLA:HMB3	16:I:101:CLA:HMA1	1.97	0.47
16:2:608:CLA:HHH	16:2:608:CLA:CBC	2.45	0.47
16:A:816:CLA:HBC2	16:K:101:CLA:HMD3	1.97	0.46
21:A:857:BCR:C11	18:K:103:RRX:H19	2.45	0.46
16:O:203:CLA:HMA1	21:O:205:BCR:H362	1.97	0.46
16:2:611:CLA:HAC2	21:2:617:BCR:H363	1.96	0.46
21:2:617:BCR:H24C	21:2:617:BCR:H371	1.80	0.46
16:A:832:CLA:H171	16:L:204:CLA:HMB2	1.96	0.46
21:A:846:BCR:H311	21:A:846:BCR:C8	2.45	0.46
5:B:69:ALA:HB2	5:B:133:LEU:HB2	1.97	0.46
16:B:832:CLA:H3A	16:B:832:CLA:HBA2	1.62	0.46
1:1:107:VAL:HB	16:1:606:CLA:HMA1	1.97	0.46
5:B:175:HIS:ND1	16:B:812:CLA:HMC2	2.29	0.46
3:3:94:THR:HG23	3:3:95:ALA:N	2.30	0.46
3:3:146:ARG:NH1	3:3:150:ALA:HB2	2.30	0.46
16:A:832:CLA:H2A	16:A:832:CLA:HED2	1.97	0.46
5:B:655:TRP:CE3	16:B:804:CLA:HMA1	2.50	0.46
21:L:206:BCR:HC8	21:L:206:BCR:C33	2.46	0.46
4:A:444:LEU:HD23	30:A:851:T7X:C23	2.46	0.46
16:B:837:CLA:HHC	16:B:837:CLA:CBB	2.46	0.46
18:1:613:RRX:H25	18:1:613:RRX:H29	1.96	0.46
2:2:26:ARG:HH12	3:3:113:PRO:C	2.18	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:205:CLA:HMD2	16:3:209:CLA:C1D	2.46	0.46
16:A:804:CLA:CBB	16:A:804:CLA:HMB1	2.46	0.46
5:B:115:TYR:H	16:B:808:CLA:HMD1	1.81	0.46
5:B:260:HIS:O	5:B:264:GLN:N	2.46	0.46
21:B:855:BCR:HC8	21:B:855:BCR:C32	2.45	0.46
1:1:32:ASP:O	1:1:33:ALA:HB3	2.15	0.46
16:A:830:CLA:HMB1	16:A:830:CLA:HBB1	1.97	0.46
5:B:434:LEU:HD21	21:B:855:BCR:H372	1.98	0.46
16:F:202:CLA:HHC	16:F:202:CLA:HBB1	1.97	0.46
16:1:602:CLA:H62	16:1:603:CLA:HMA1	1.98	0.46
4:A:433:ILE:HG23	16:A:837:CLA:HBB2	1.97	0.46
5:B:419:HIS:CD2	16:B:829:CLA:HMB1	2.50	0.46
21:L:207:BCR:H351	21:L:207:BCR:H15C	1.74	0.46
2:2:54:TRP:CZ3	2:2:125:LEU:HD21	2.50	0.46
3:3:38:MET:SD	21:K:104:BCR:H312	2.56	0.46
4:A:730:LEU:HD22	16:A:838:CLA:HMA1	1.97	0.46
5:B:614:LEU:HD13	16:B:803:CLA:HMA2	1.98	0.46
16:B:818:CLA:HMD2	16:B:822:CLA:H92	1.98	0.46
5:B:517:VAL:HG21	5:B:591:TYR:HB2	1.97	0.45
17:1:614:C7Z:C12	17:1:614:C7Z:C19	2.94	0.45
16:3:203:CLA:HMC2	19:3:219:LHG:H141	1.97	0.45
4:A:355:MET:HG3	16:A:824:CLA:HBB	1.98	0.45
4:A:391:MET:HG3	4:A:599:LEU:CD1	2.47	0.45
16:A:804:CLA:HMB1	16:A:804:CLA:HBB1	1.98	0.45
1:1:8:PHE:CE2	2:2:120:VAL:HG13	2.52	0.45
16:1:602:CLA:HMB1	16:1:602:CLA:CBB	2.44	0.45
20:2:621:ERG:C3	20:2:621:ERG:HO1	2.13	0.45
16:A:808:CLA:HBB1	18:J:103:RRX:C8	2.47	0.45
16:A:813:CLA:HMC1	16:A:814:CLA:HMB3	1.98	0.45
21:A:844:BCR:H23C	21:A:844:BCR:C38	2.44	0.45
21:B:844:BCR:H321	21:B:844:BCR:C8	2.44	0.45
15:O:106:VAL:HG22	16:O:203:CLA:H93	1.99	0.45
4:A:71:SER:HB2	16:A:810:CLA:HMD3	1.99	0.45
4:A:438:ASN:ND2	5:B:676:LEU:HD11	2.30	0.45
21:A:845:BCR:H351	21:A:845:BCR:H15C	1.74	0.45
16:F:205:CLA:HMB2	21:F:206:BCR:H392	1.99	0.45
21:O:205:BCR:H351	21:O:205:BCR:H15C	1.72	0.45
3:3:163:LEU:HG	16:3:213:CLA:HBC2	1.99	0.45
16:A:820:CLA:HMB1	16:A:820:CLA:CBB	2.47	0.45
16:L:201:CLA:HHD	16:L:201:CLA:HBC3	1.98	0.45
1:1:89:ILE:HA	16:1:605:CLA:HED3	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:48:MET:HB3	16:3:204:CLA:HMA1	1.98	0.45
3:3:159:MET:SD	16:3:204:CLA:HAB	2.57	0.45
4:A:351:ILE:HD11	21:A:845:BCR:H24C	1.97	0.45
16:I:101:CLA:CBB	16:I:101:CLA:HMB1	2.46	0.45
4:A:524:LEU:HA	4:A:528:ASP:OD2	2.17	0.45
16:B:819:CLA:H152	16:B:819:CLA:HMC2	1.98	0.45
13:L:93:MET:HE1	21:L:206:BCR:H402	1.98	0.45
1:1:148:LEU:HG	16:1:602:CLA:HMC1	1.99	0.44
3:3:104:SER:CA	16:3:209:CLA:HAB	2.48	0.44
16:A:825:CLA:HAB	21:A:846:BCR:C8	2.47	0.44
21:I:103:BCR:H402	21:L:202:BCR:C36	2.46	0.44
4:A:618:VAL:HG13	4:A:618:VAL:O	2.17	0.44
16:A:809:CLA:H141	16:A:809:CLA:HMD2	1.98	0.44
5:B:546:PRO:O	9:F:182:VAL:HG21	2.17	0.44
6:C:61:ASP:OD2	8:E:15:SER:HA	2.18	0.44
9:F:114:PHE:CE1	9:F:118:THR:HG21	2.52	0.44
16:1:603:CLA:CBC	18:1:613:RRX:H44	2.47	0.44
16:1:609:CLA:HBC3	17:1:612:C7Z:C14	2.47	0.44
5:B:302:ILE:CG2	16:B:822:CLA:HED2	2.48	0.44
5:B:716:ILE:CD1	16:B:826:CLA:HMC2	2.45	0.44
16:2:603:CLA:HBB2	21:2:617:BCR:C15	2.47	0.44
16:A:816:CLA:HBC2	16:K:101:CLA:CMD	2.48	0.44
16:A:823:CLA:H142	16:A:830:CLA:HMC2	1.98	0.44
5:B:381:ILE:HG21	16:B:824:CLA:C3C	2.47	0.44
16:F:202:CLA:HBB2	21:F:203:BCR:HC31	2.00	0.44
21:A:846:BCR:H23C	21:A:846:BCR:C40	2.46	0.44
21:B:841:BCR:H351	21:B:841:BCR:H15C	1.83	0.44
16:1:608:CLA:H3A	16:1:608:CLA:H51	2.00	0.44
4:A:40:LYS:O	4:A:41:THR:HG23	2.17	0.44
5:B:253:LEU:HD11	16:B:814:CLA:HBC1	2.00	0.44
4:A:737:TRP:HA	16:A:827:CLA:HBB1	1.98	0.44
16:A:832:CLA:HHD	16:B:809:CLA:HBB2	2.00	0.44
16:A:836:CLA:H203	16:L:201:CLA:HMC2	2.00	0.44
21:A:850:BCR:H351	21:A:850:BCR:H15C	1.66	0.44
16:B:834:CLA:H92	16:B:835:CLA:HAC2	2.00	0.44
21:B:842:BCR:HC8	21:B:842:BCR:C32	2.48	0.44
16:3:211:CLA:CAD	16:3:212:CLA:HMA3	2.48	0.44
16:A:830:CLA:HMB1	16:A:830:CLA:CBB	2.47	0.44
1:1:93:ALA:O	1:1:94:PHE:HB3	2.18	0.43
16:1:609:CLA:HHC	16:1:609:CLA:CBB	2.48	0.43
3:3:13:VAL:N	3:3:14:PRO:CD	2.81	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:580:CYS:O	5:B:666:ARG:O	2.35	0.43
16:B:821:CLA:HBB	16:B:821:CLA:H43	1.99	0.43
16:B:829:CLA:HMC2	16:B:838:CLA:H143	2.00	0.43
3:3:53:VAL:HG21	3:3:127:GLY:CA	2.48	0.43
16:A:818:CLA:HMB1	16:A:818:CLA:CBB	2.46	0.43
5:B:527:THR:HG21	5:B:580:TRP:CZ2	2.53	0.43
16:B:806:CLA:HMB1	16:B:806:CLA:CBB	2.48	0.43
21:2:617:BCR:H373	17:3:201:C7Z:C35	2.47	0.43
4:A:354:ALA:N	4:A:401:ALA:HB2	2.34	0.43
3:3:18:VAL:CG2	3:3:19:PRO:HD3	2.48	0.43
16:3:213:CLA:HMD2	17:3:217:C7Z:C19	2.48	0.43
16:B:805:CLA:HBC2	31:B:846:DGD:HAH2	1.99	0.43
16:2:601:CLA:CBC	21:2:617:BCR:H382	2.49	0.43
21:A:846:BCR:H351	21:A:846:BCR:H15C	1.88	0.43
16:B:804:CLA:CBB	16:B:804:CLA:HMB1	2.48	0.43
16:B:809:CLA:H43	21:I:103:BCR:H342	2.00	0.43
21:F:203:BCR:H23C	21:F:203:BCR:H392	2.01	0.43
4:A:595:MET:CG	16:A:825:CLA:HBC1	2.49	0.43
5:B:544:LEU:HD23	5:B:568:ILE:CD1	2.48	0.43
16:B:821:CLA:HBB1	16:B:821:CLA:HHC	2.01	0.43
21:B:844:BCR:H351	21:B:844:BCR:H15C	1.72	0.43
7:D:119:THR:HG23	8:E:34:TYR:OH	2.19	0.43
21:L:206:BCR:H331	21:L:206:BCR:C8	2.48	0.43
1:1:145:LEU:HD22	16:1:608:CLA:HHD	2.00	0.43
2:2:69:ALA:HB1	2:2:172:PHE:CE1	2.53	0.43
16:A:815:CLA:HMB1	16:A:815:CLA:CBB	2.48	0.43
5:B:544:LEU:HD23	5:B:568:ILE:HD13	2.00	0.43
21:B:843:BCR:H383	21:B:843:BCR:H23C	2.00	0.43
21:L:206:BCR:H392	21:L:206:BCR:C23	2.49	0.43
5:B:545:MET:CE	5:B:558:ASP:HB2	2.49	0.43
4:A:271:ILE:HD12	16:A:814:CLA:HBC3	2.00	0.43
4:A:592:LEU:HD21	16:A:829:CLA:HBC1	2.00	0.43
5:B:148:LEU:CD2	21:B:847:BCR:H333	2.45	0.43
5:B:657:THR:O	5:B:660:MET:HB3	2.19	0.43
8:E:28:GLU:HB2	8:E:35:PRO:CB	2.48	0.43
1:1:49:VAL:CG1	18:1:613:RRX:H45	2.49	0.43
16:1:601:CLA:HBC2	2:2:120:VAL:HG23	2.00	0.43
16:1:610:CLA:HMB2	16:2:605:CLA:H171	2.01	0.43
16:3:209:CLA:H18	16:3:214:CLA:HMD2	2.00	0.43
4:A:117:ILE:CD1	11:J:30:ARG:HB3	2.48	0.43
16:A:828:CLA:C4	21:A:844:BCR:H10C	2.47	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:343:THR:HG21	5:B:380:LEU:HD12	2.00	0.43
5:B:656:ALA:CB	16:B:801:CLA:HBB2	2.43	0.43
16:B:816:CLA:HBA2	16:B:825:CLA:HBB2	2.00	0.43
2:2:63:CYS:HB3	2:2:165:GLY:HA3	2.00	0.42
16:2:602:CLA:H141	16:2:612:CLA:HAB	2.01	0.42
4:A:341:LEU:HD21	4:A:351:ILE:HD12	2.02	0.42
27:B:839:PQN:H142	21:B:845:BCR:H272	2.02	0.42
12:K:36:LEU:CD1	21:K:104:BCR:H352	2.50	0.42
13:L:5:ILE:HG23	13:L:19:THR:HG22	2.01	0.42
19:1:617:LHG:H222	2:2:119:ILE:HD13	2.01	0.42
16:2:609:CLA:C3D	16:2:610:CLA:HMA3	2.49	0.42
3:3:39:ILE:HD12	17:3:216:C7Z:C3	2.49	0.42
4:A:301:PHE:CE2	16:A:820:CLA:HAB	2.54	0.42
16:A:817:CLA:O2A	16:A:826:CLA:HBB2	2.18	0.42
16:2:601:CLA:HMC3	3:3:110:ALA:HB2	2.02	0.42
4:A:71:SER:O	4:A:72:ALA:CB	2.67	0.42
16:A:806:CLA:HMA1	16:A:807:CLA:HMB3	2.02	0.42
1:1:109:TYR:CE2	9:F:152:LYS:HA	2.54	0.42
3:3:18:VAL:HG22	3:3:19:PRO:HD3	2.00	0.42
3:3:104:SER:HB3	16:3:209:CLA:HAB	2.00	0.42
16:A:839:CLA:H141	13:L:88:ILE:HG22	2.02	0.42
16:A:839:CLA:HMD2	21:B:845:BCR:H383	2.01	0.42
16:B:804:CLA:HBB1	16:B:804:CLA:HMB1	2.02	0.42
2:2:114:CYS:HB3	16:2:607:CLA:HAB	2.01	0.42
4:A:196:HIS:CE1	16:A:812:CLA:HMC2	2.54	0.42
16:A:854:CLA:CGA	5:B:425:LEU:HA	2.50	0.42
9:F:63:PRO:O	9:F:64:SER:CB	2.68	0.42
16:1:603:CLA:HMD2	16:1:606:CLA:ND	2.35	0.42
3:3:186:PHE:H	16:3:213:CLA:HED2	1.84	0.42
4:A:538:THR:HB	4:A:598:ALA:HB2	2.02	0.42
16:A:830:CLA:HMA2	13:L:19:THR:HG21	2.01	0.42
5:B:31:PHE:CD2	16:B:806:CLA:HMC2	2.54	0.42
5:B:436:VAL:CG2	16:B:830:CLA:HMC3	2.50	0.42
16:L:203:CLA:CGA	16:L:203:CLA:C1A	2.97	0.42
21:O:205:BCR:H331	21:O:205:BCR:C8	2.49	0.42
1:1:25:PHE:CD2	16:1:601:CLA:HMD3	2.55	0.42
21:2:617:BCR:H15C	21:2:617:BCR:H351	1.75	0.42
5:B:663:ILE:HD12	16:B:801:CLA:HMC1	2.02	0.42
13:L:54:HIS:HA	13:L:57:PHE:CE2	2.55	0.42
4:A:295:LEU:HD22	16:A:814:CLA:HMC1	2.01	0.42
8:E:51:THR:CG2	8:E:52:ASN:N	2.83	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:102:CLA:HHC	16:J:102:CLA:CBB	2.49	0.42
16:1:610:CLA:CAD	16:2:605:CLA:HMA1	2.50	0.41
2:2:62:HIS:CE1	16:2:607:CLA:HMD1	2.55	0.41
18:2:616:RRX:H26	18:2:616:RRX:H22	1.97	0.41
5:B:371:THR:HG23	5:B:589:THR:HG21	2.02	0.41
5:B:521:ILE:HG12	5:B:588:VAL:HG22	2.01	0.41
16:B:803:CLA:HMB3	16:B:804:CLA:H18	2.01	0.41
9:F:114:PHE:CD2	9:F:114:PHE:C	2.91	0.41
16:J:102:CLA:HMA2	16:J:102:CLA:HBA2	2.02	0.41
12:K:32:ASP:HA	21:K:104:BCR:H332	2.02	0.41
16:1:608:CLA:CAD	16:1:609:CLA:HMA3	2.50	0.41
3:3:147:MET:HG3	16:3:210:CLA:HMA1	2.02	0.41
16:3:211:CLA:HMC3	19:3:219:LHG:C6	2.50	0.41
16:A:825:CLA:HAB	21:A:846:BCR:C31	2.48	0.41
5:B:254:THR:HG22	5:B:255:PHE:N	2.35	0.41
13:L:64:GLN:HB3	16:L:205:CLA:HMB3	2.02	0.41
4:A:667:LEU:HD13	16:A:808:CLA:HMC1	2.03	0.41
21:A:846:BCR:H24C	21:A:846:BCR:H371	1.95	0.41
16:I:101:CLA:HMB1	16:I:101:CLA:HBB1	2.02	0.41
5:B:382:VAL:HG12	5:B:574:PHE:CE1	2.56	0.41
12:K:9:ILE:HB	12:K:10:PRO:HD3	2.02	0.41
16:2:607:CLA:H62	16:2:607:CLA:H41	1.93	0.41
4:A:704:LEU:HD21	21:F:206:BCR:H342	2.02	0.41
26:A:801:CL0:CGD	26:A:801:CL0:H8	2.50	0.41
21:A:844:BCR:H351	21:A:844:BCR:H15C	1.79	0.41
5:B:189:THR:HG21	5:B:276:LEU:HB2	2.02	0.41
16:1:606:CLA:C19	16:1:611:CLA:HAB	2.50	0.41
2:2:74:ILE:HD12	19:2:622:LHG:H222	2.01	0.41
3:3:88:HIS:O	3:3:92:VAL:HB	2.20	0.41
16:A:805:CLA:HMB1	16:A:805:CLA:HBB1	2.02	0.41
21:A:850:BCR:H23C	21:A:850:BCR:C40	2.50	0.41
13:L:51:GLY:O	13:L:125:ALA:HA	2.20	0.41
13:L:93:MET:HB2	13:L:93:MET:HE3	1.97	0.41
4:A:442:ILE:HD11	21:B:845:BCR:H402	2.02	0.41
16:A:832:CLA:C15	21:L:202:BCR:H343	2.51	0.41
5:B:634:ASN:HB2	5:B:635:PRO:HD2	2.03	0.41
8:E:6:SER:OG	8:E:60:GLU:OE2	2.33	0.41
16:1:604:CLA:HAB	17:1:615:C7Z:C10	2.51	0.41
16:A:856:CLA:C1A	16:A:856:CLA:CGA	2.98	0.41
5:B:297:HIS:HB3	5:B:302:ILE:HD11	2.02	0.41
5:B:430:HIS:HB3	21:B:855:BCR:C24	2.51	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:202:CLA:H41	16:O:202:CLA:H71	2.02	0.41
1:1:148:LEU:HD11	16:1:602:CLA:HAC1	2.03	0.41
1:1:150:PHE:CE2	18:1:613:RRX:H42	2.56	0.41
16:1:607:CLA:H72	16:1:609:CLA:HMD1	2.02	0.41
16:3:207:CLA:H41	16:3:207:CLA:H61	1.76	0.41
16:3:210:CLA:HMB1	16:3:210:CLA:CBB	2.51	0.41
4:A:186:TRP:O	4:A:187:PHE:HB2	2.21	0.41
4:A:263:LEU:HD21	12:K:48:VAL:HG22	2.03	0.41
4:A:340:ILE:HD11	4:A:418:ASN:OD1	2.21	0.41
16:A:807:CLA:H122	18:J:103:RRX:H30	2.03	0.41
5:B:379:LEU:CD1	16:B:826:CLA:HMC1	2.51	0.41
5:B:385:PHE:CG	5:B:532:LEU:HB3	2.56	0.41
5:B:427:LEU:HD21	16:B:834:CLA:CMB	2.51	0.41
16:B:808:CLA:H202	16:B:826:CLA:H192	2.02	0.41
16:B:831:CLA:C1D	16:B:832:CLA:HAB	2.50	0.41
27:B:839:PQN:H142	21:B:845:BCR:C27	2.51	0.41
31:B:850:DGD:HD2	31:B:850:DGD:HAH1	2.03	0.41
12:K:21:VAL:HA	12:K:39:SER:HB3	2.02	0.41
13:L:5:ILE:HG22	13:L:17:LEU:HD22	2.03	0.41
3:3:16:ALA:O	3:3:19:PRO:HD2	2.20	0.41
3:3:99:ILE:HD11	16:3:207:CLA:HMD3	2.03	0.41
3:3:104:SER:HA	16:3:209:CLA:HAB	2.02	0.41
16:3:212:CLA:HAB	17:3:215:C7Z:C39	2.51	0.41
4:A:273:THR:OG1	4:A:289:ASP:OD1	2.39	0.41
4:A:368:TYR:CD1	4:A:368:TYR:C	2.93	0.41
4:A:676:TRP:CG	26:A:801:CL0:H5	2.55	0.41
16:A:837:CLA:H121	21:A:846:BCR:H372	2.03	0.41
25:A:852:PTY:C26	16:O:203:CLA:H141	2.51	0.41
5:B:58:PHE:HA	5:B:61:THR:HG22	2.03	0.41
16:1:601:CLA:H143	16:1:601:CLA:H111	1.97	0.40
4:A:174:TRP:HB2	16:A:810:CLA:HMC3	2.01	0.40
16:A:814:CLA:HMB1	16:A:814:CLA:CBB	2.51	0.40
16:A:814:CLA:HMB1	16:A:814:CLA:HBB1	2.02	0.40
5:B:166:PHE:O	5:B:172:ARG:NH2	2.54	0.40
16:B:805:CLA:CBC	31:B:846:DGD:HAH2	2.51	0.40
31:B:849:DGD:HA51	31:B:849:DGD:HA92	2.02	0.40
9:F:129:LEU:HD11	16:F:201:CLA:HMD1	2.03	0.40
2:2:170:ILE:HD11	16:2:602:CLA:HMC1	2.02	0.40
3:3:33:GLU:OE1	3:3:33:GLU:N	2.55	0.40
5:B:643:VAL:HG21	16:B:808:CLA:HAC1	2.02	0.40
16:B:812:CLA:HBB1	16:B:812:CLA:HMB1	2.02	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:817:CLA:H61	16:B:817:CLA:H41	1.85	0.40
16:1:610:CLA:H102	16:2:605:CLA:HBB1	2.04	0.40
4:A:472:ALA:O	4:A:473:ILE:C	2.59	0.40
16:A:818:CLA:HHD	21:A:844:BCR:H352	2.03	0.40
5:B:427:LEU:HD21	16:B:834:CLA:HMB3	2.03	0.40
16:B:821:CLA:CBB	16:B:838:CLA:HED1	2.51	0.40
16:B:830:CLA:HMB2	16:F:202:CLA:CAB	2.51	0.40
31:B:850:DGD:HAH2	31:B:850:DGD:HAV1	2.03	0.40
16:K:102:CLA:H72	21:K:104:BCR:H351	2.02	0.40
21:O:205:BCR:HC8	21:O:205:BCR:C33	2.52	0.40
4:A:393:ILE:HG23	16:A:805:CLA:H143	2.03	0.40
4:A:398:ILE:HG23	21:A:846:BCR:H343	2.03	0.40
16:A:821:CLA:H62	16:A:821:CLA:H41	1.81	0.40
16:A:830:CLA:HAB	16:A:837:CLA:HAB	2.03	0.40
5:B:723:VAL:HG13	5:B:724:ILE:N	2.36	0.40
9:F:182:VAL:O	9:F:183:SER:OG	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	171/173 (99%)	163 (95%)	8 (5%)	0	100	100
2	2	177/179 (99%)	167 (94%)	10 (6%)	0	100	100
3	3	172/174 (99%)	160 (93%)	12 (7%)	0	100	100
4	A	741/743 (100%)	714 (96%)	27 (4%)	0	100	100
5	B	729/731 (100%)	703 (96%)	26 (4%)	0	100	100
6	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
7	D	136/138 (99%)	128 (94%)	8 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	E	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
9	F	153/155 (99%)	144 (94%)	9 (6%)	0	100	100
10	I	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	J	36/38 (95%)	36 (100%)	0	0	100	100
12	K	52/54 (96%)	52 (100%)	0	0	100	100
13	L	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
14	M	25/27 (93%)	25 (100%)	0	0	100	100
15	O	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
All	All	2787/2817 (99%)	2668 (96%)	119 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	143/143 (100%)	143 (100%)	0	100	100
2	2	144/144 (100%)	144 (100%)	0	100	100
3	3	136/136 (100%)	136 (100%)	0	100	100
4	A	600/600 (100%)	597 (100%)	3 (0%)	88	94
5	B	598/598 (100%)	595 (100%)	3 (0%)	88	94
6	C	66/66 (100%)	66 (100%)	0	100	100
7	D	117/117 (100%)	117 (100%)	0	100	100
8	E	58/58 (100%)	58 (100%)	0	100	100
9	F	137/137 (100%)	137 (100%)	0	100	100
10	I	26/26 (100%)	26 (100%)	0	100	100
11	J	34/34 (100%)	34 (100%)	0	100	100
12	K	43/43 (100%)	42 (98%)	1 (2%)	50	77
13	L	109/109 (100%)	109 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	M	22/22 (100%)	22 (100%)	0	100	100
15	O	75/75 (100%)	75 (100%)	0	100	100
All	All	2308/2308 (100%)	2301 (100%)	7 (0%)	92	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	274	PHE
4	A	311	ASN
4	A	368	TYR
5	B	255	PHE
5	B	351	TYR
5	B	514	ASP
12	K	25	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	56	HIS
2	2	130	ASN
4	A	533	HIS
5	B	437	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 206 ligands modelled in this entry, 2 are monoatomic - leaving 204 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$
16	CLA	1	604	-	65,73,73	1.38	8 (12%)	76,113,113	1.90	15 (19%)
16	CLA	A	833	-	65,73,73	1.37	9 (13%)	76,113,113	1.91	16 (21%)
16	CLA	B	802	-	65,73,73	1.38	9 (13%)	76,113,113	1.92	14 (18%)
17	C7Z	J	104	-	43,43,43	5.40	26 (60%)	58,60,60	2.55	23 (39%)
16	CLA	F	205	9	65,73,73	1.38	8 (12%)	76,113,113	1.94	14 (18%)
21	BCR	2	617	-	41,41,41	1.90	5 (12%)	56,56,56	4.54	20 (35%)
21	BCR	L	207	-	41,41,41	1.85	4 (9%)	56,56,56	4.57	23 (41%)
16	CLA	3	204	3	63,71,73	1.39	9 (14%)	73,110,113	1.90	12 (16%)
16	CLA	L	204	-	65,73,73	1.38	9 (13%)	76,113,113	1.83	15 (19%)
16	CLA	A	831	-	65,73,73	1.38	9 (13%)	76,113,113	1.83	14 (18%)
16	CLA	1	610	-	65,73,73	1.36	9 (13%)	76,113,113	1.98	15 (19%)
17	C7Z	3	201	-	43,43,43	5.42	26 (60%)	58,60,60	2.37	20 (34%)
17	C7Z	3	217	-	43,43,43	5.36	25 (58%)	58,60,60	2.58	22 (37%)
16	CLA	3	209	3	65,73,73	1.37	10 (15%)	76,113,113	1.91	15 (19%)
16	CLA	A	836	-	65,73,73	1.37	9 (13%)	76,113,113	1.95	17 (22%)
16	CLA	B	810	-	65,73,73	1.36	8 (12%)	76,113,113	1.87	15 (19%)
16	CLA	I	101	-	65,73,73	1.35	8 (12%)	76,113,113	1.91	14 (18%)
16	CLA	A	807	-	65,73,73	1.36	8 (12%)	76,113,113	1.92	15 (19%)
16	CLA	2	609	-	65,73,73	1.36	9 (13%)	76,113,113	1.91	15 (19%)
16	CLA	B	805	-	65,73,73	1.36	9 (13%)	76,113,113	1.90	15 (19%)
16	CLA	B	831	33	65,73,73	1.36	8 (12%)	76,113,113	1.90	14 (18%)
16	CLA	B	820	-	65,73,73	1.37	9 (13%)	76,113,113	1.96	15 (19%)
21	BCR	F	206	-	41,41,41	1.86	4 (9%)	56,56,56	4.22	23 (41%)
16	CLA	3	211	-	65,73,73	1.37	9 (13%)	76,113,113	1.96	16 (21%)
21	BCR	A	844	-	41,41,41	1.86	4 (9%)	56,56,56	4.26	21 (37%)
16	CLA	A	827	-	65,73,73	1.36	9 (13%)	76,113,113	1.89	14 (18%)
31	DGD	B	846	-	67,67,67	1.19	7 (10%)	81,81,81	1.03	3 (3%)
19	LHG	2	622	16	48,48,48	0.40	0	51,54,54	1.06	4 (7%)
31	DGD	B	849	-	67,67,67	1.20	8 (11%)	81,81,81	1.04	5 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	A	856	-	65,73,73	1.35	8 (12%)	76,113,113	1.92	16 (21%)
16	CLA	B	833	-	65,73,73	1.36	9 (13%)	76,113,113	1.86	18 (23%)
16	CLA	A	839	33	65,73,73	1.38	9 (13%)	76,113,113	1.87	12 (15%)
16	CLA	2	606	-	65,73,73	1.36	9 (13%)	76,113,113	1.96	14 (18%)
16	CLA	A	826	-	65,73,73	1.36	9 (13%)	76,113,113	1.89	12 (15%)
21	BCR	B	847	-	41,41,41	1.88	4 (9%)	56,56,56	4.87	26 (46%)
16	CLA	B	826	-	65,73,73	1.37	9 (13%)	76,113,113	1.88	14 (18%)
30	T7X	A	851	-	54,54,61	0.88	4 (7%)	64,66,73	1.00	3 (4%)
17	C7Z	1	612	-	43,43,43	5.41	25 (58%)	58,60,60	2.10	16 (27%)
25	PTY	3	221	-	49,49,49	0.89	4 (8%)	52,54,54	0.98	2 (3%)
16	CLA	F	204	-	65,73,73	1.37	9 (13%)	76,113,113	1.82	14 (18%)
23	DGA	2	620	-	43,43,43	1.17	3 (6%)	45,45,45	1.16	3 (6%)
21	BCR	L	206	-	41,41,41	1.82	5 (12%)	56,56,56	4.49	19 (33%)
16	CLA	3	213	-	46,54,73	1.61	9 (19%)	53,90,113	2.17	13 (24%)
16	CLA	A	814	-	65,73,73	1.35	9 (13%)	76,113,113	1.97	17 (22%)
16	CLA	B	813	-	65,73,73	1.35	8 (12%)	76,113,113	1.88	15 (19%)
16	CLA	2	612	-	65,73,73	1.38	9 (13%)	76,113,113	1.85	15 (19%)
16	CLA	3	210	3	65,73,73	1.35	8 (12%)	76,113,113	2.17	18 (23%)
16	CLA	A	817	-	65,73,73	1.37	8 (12%)	76,113,113	1.87	16 (21%)
26	CL0	A	801	-	65,73,73	2.35	19 (29%)	76,113,113	2.48	23 (30%)
16	CLA	A	804	-	65,73,73	1.39	11 (16%)	76,113,113	1.91	18 (23%)
16	CLA	F	201	-	61,69,73	1.41	9 (14%)	71,108,113	1.81	14 (19%)
24	LMU	3	202	-	36,36,36	0.46	0	47,47,47	0.74	0
16	CLA	A	802	-	65,73,73	1.37	9 (13%)	76,113,113	2.00	14 (18%)
16	CLA	A	855	33	65,73,73	1.39	8 (12%)	76,113,113	1.76	13 (17%)
16	CLA	A	822	-	65,73,73	1.36	8 (12%)	76,113,113	1.89	16 (21%)
16	CLA	O	201	-	65,73,73	1.33	8 (12%)	76,113,113	2.01	17 (22%)
16	CLA	B	832	-	65,73,73	1.38	9 (13%)	76,113,113	1.92	16 (21%)
16	CLA	1	603	-	65,73,73	1.38	9 (13%)	76,113,113	1.92	18 (23%)
16	CLA	F	202	-	65,73,73	1.37	9 (13%)	76,113,113	2.12	20 (26%)
16	CLA	1	609	-	65,73,73	1.40	8 (12%)	76,113,113	1.81	14 (18%)
19	LHG	A	842	-	48,48,48	0.40	0	51,54,54	0.93	3 (5%)
25	PTY	A	852	-	45,45,49	0.92	4 (8%)	47,49,54	1.01	2 (4%)
21	BCR	B	841	-	41,41,41	1.79	4 (9%)	56,56,56	4.44	26 (46%)
16	CLA	2	610	19	65,73,73	1.38	9 (13%)	76,113,113	2.00	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	C7Z	2	615	-	43,43,43	5.41	26 (60%)	58,60,60	2.57	22 (37%)
21	BCR	F	203	-	41,41,41	1.83	4 (9%)	56,56,56	4.72	22 (39%)
16	CLA	2	603	-	65,73,73	1.37	11 (16%)	76,113,113	1.85	15 (19%)
16	CLA	A	805	-	65,73,73	1.34	8 (12%)	76,113,113	1.91	14 (18%)
16	CLA	A	820	33	65,73,73	1.38	10 (15%)	76,113,113	1.84	13 (17%)
21	BCR	A	857	-	41,41,41	1.85	4 (9%)	56,56,56	4.85	26 (46%)
16	CLA	3	203	-	65,73,73	1.37	9 (13%)	76,113,113	2.01	16 (21%)
16	CLA	O	203	-	65,73,73	1.39	9 (13%)	76,113,113	1.89	14 (18%)
16	CLA	1	606	-	65,73,73	1.35	9 (13%)	76,113,113	2.10	18 (23%)
16	CLA	L	205	-	65,73,73	1.35	9 (13%)	76,113,113	1.97	14 (18%)
28	SF4	C	102	6	0,12,12	-	-	-	-	-
16	CLA	B	817	-	65,73,73	1.36	9 (13%)	76,113,113	1.84	13 (17%)
16	CLA	A	824	33	65,73,73	1.38	10 (15%)	76,113,113	1.89	14 (18%)
16	CLA	B	824	-	65,73,73	1.34	7 (10%)	76,113,113	1.90	17 (22%)
19	LHG	3	219	-	48,48,48	0.41	0	51,54,54	0.93	3 (5%)
16	CLA	A	811	-	65,73,73	1.36	9 (13%)	76,113,113	1.88	15 (19%)
16	CLA	2	607	-	65,73,73	1.38	9 (13%)	76,113,113	1.82	11 (14%)
21	BCR	B	845	-	41,41,41	1.84	4 (9%)	56,56,56	4.44	19 (33%)
16	CLA	A	828	-	65,73,73	1.37	9 (13%)	76,113,113	1.80	14 (18%)
16	CLA	3	212	-	58,66,73	1.44	9 (15%)	67,104,113	2.09	17 (25%)
16	CLA	A	832	-	65,73,73	1.37	10 (15%)	76,113,113	1.88	15 (19%)
16	CLA	B	829	-	65,73,73	1.37	10 (15%)	76,113,113	1.88	14 (18%)
24	LMU	A	853	-	36,36,36	0.44	0	47,47,47	0.75	0
16	CLA	B	830	-	65,73,73	1.35	9 (13%)	76,113,113	1.83	15 (19%)
16	CLA	B	806	-	65,73,73	1.35	9 (13%)	76,113,113	1.89	16 (21%)
16	CLA	1	601	-	65,73,73	1.37	8 (12%)	76,113,113	1.87	15 (19%)
16	CLA	K	102	-	65,73,73	1.37	8 (12%)	76,113,113	1.85	13 (17%)
16	CLA	B	812	-	65,73,73	1.37	9 (13%)	76,113,113	1.92	17 (22%)
20	ERG	2	621	-	31,32,32	8.27	19 (61%)	47,50,50	2.95	18 (38%)
16	CLA	L	203	13	65,73,73	1.37	9 (13%)	76,113,113	1.86	15 (19%)
16	CLA	2	604	-	65,73,73	1.35	9 (13%)	76,113,113	1.99	17 (22%)
16	CLA	B	838	22	65,73,73	1.36	9 (13%)	76,113,113	1.93	17 (22%)
16	CLA	B	814	-	65,73,73	1.36	10 (15%)	76,113,113	1.88	14 (18%)
16	CLA	A	821	-	65,73,73	1.36	9 (13%)	76,113,113	1.98	19 (25%)
16	CLA	1	607	1	60,68,73	1.41	8 (13%)	70,107,113	1.95	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	A	809	-	65,73,73	1.38	9 (13%)	76,113,113	1.80	14 (18%)
16	CLA	B	835	-	65,73,73	1.37	9 (13%)	76,113,113	1.87	16 (21%)
16	CLA	B	809	5	65,73,73	1.35	9 (13%)	76,113,113	2.07	19 (25%)
28	SF4	C	101	6	0,12,12	-	-	-	-	-
16	CLA	1	611	-	65,73,73	1.38	9 (13%)	76,113,113	1.84	13 (17%)
23	DGA	J	101	-	43,43,43	1.15	3 (6%)	45,45,45	1.16	3 (6%)
17	C7Z	1	615	-	43,43,43	5.38	26 (60%)	58,60,60	2.45	19 (32%)
16	CLA	B	828	-	65,73,73	1.38	9 (13%)	76,113,113	1.83	13 (17%)
16	CLA	3	214	-	65,73,73	1.38	9 (13%)	76,113,113	1.92	15 (19%)
19	LHG	B	851	-	44,44,48	0.42	0	47,50,54	0.95	3 (6%)
16	CLA	2	608	-	65,73,73	1.39	8 (12%)	76,113,113	1.98	18 (23%)
16	CLA	A	808	4	65,73,73	1.38	9 (13%)	76,113,113	1.93	18 (23%)
16	CLA	A	823	-	65,73,73	1.36	8 (12%)	76,113,113	1.83	15 (19%)
20	ERG	2	618	-	31,32,32	8.30	18 (58%)	47,50,50	3.52	22 (46%)
27	PQN	B	839	-	34,34,34	0.46	0	42,45,45	1.00	2 (4%)
16	CLA	B	823	-	65,73,73	1.36	8 (12%)	76,113,113	1.83	14 (18%)
16	CLA	2	611	2	65,73,73	1.38	9 (13%)	76,113,113	1.91	16 (21%)
18	RRX	J	103	-	42,42,42	4.92	24 (57%)	57,58,58	3.14	30 (52%)
16	CLA	B	819	-	65,73,73	1.39	9 (13%)	76,113,113	1.93	14 (18%)
25	PTY	3	220	-	49,49,49	0.89	4 (8%)	52,54,54	1.06	2 (3%)
16	CLA	1	602	1	59,67,73	1.42	8 (13%)	68,105,113	2.07	16 (23%)
29	3PH	A	849	-	47,47,47	0.86	4 (8%)	51,52,52	1.07	2 (3%)
16	CLA	2	605	-	65,73,73	1.36	8 (12%)	76,113,113	1.88	16 (21%)
16	CLA	L	201	-	65,73,73	1.39	9 (13%)	76,113,113	1.83	16 (21%)
22	PGT	2	619	-	34,34,50	1.45	6 (17%)	37,40,56	1.03	2 (5%)
16	CLA	J	102	11	65,73,73	1.37	9 (13%)	76,113,113	2.06	17 (22%)
16	CLA	B	803	33	65,73,73	1.40	9 (13%)	76,113,113	1.79	15 (19%)
17	C7Z	2	614	-	43,43,43	5.39	26 (60%)	58,60,60	2.31	17 (29%)
21	BCR	B	843	-	41,41,41	1.84	4 (9%)	56,56,56	4.82	27 (48%)
18	RRX	A	847	-	42,42,42	4.98	25 (59%)	57,58,58	2.92	26 (45%)
18	RRX	1	613	-	42,42,42	4.96	25 (59%)	57,58,58	2.41	20 (35%)
16	CLA	B	821	-	65,73,73	1.39	9 (13%)	76,113,113	2.09	17 (22%)
16	CLA	I	102	-	65,73,73	1.36	8 (12%)	76,113,113	1.83	14 (18%)
18	RRX	K	103	-	42,42,42	4.99	26 (61%)	57,58,58	2.35	22 (38%)
16	CLA	1	605	-	65,73,73	1.37	9 (13%)	76,113,113	1.88	15 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	DGD	B	850	-	67,67,67	1.18	7 (10%)	81,81,81	1.04	3 (3%)
21	BCR	A	845	-	41,41,41	1.82	4 (9%)	56,56,56	5.62	29 (51%)
16	CLA	A	810	16	65,73,73	1.37	9 (13%)	76,113,113	1.99	16 (21%)
17	C7Z	3	215	-	43,43,43	5.42	26 (60%)	58,60,60	2.20	14 (24%)
16	CLA	O	204	-	65,73,73	1.37	9 (13%)	76,113,113	1.94	16 (21%)
16	CLA	A	829	-	65,73,73	1.37	8 (12%)	76,113,113	1.83	12 (15%)
16	CLA	A	816	-	65,73,73	1.40	8 (12%)	76,113,113	1.90	16 (21%)
16	CLA	A	830	-	65,73,73	1.40	9 (13%)	76,113,113	1.86	14 (18%)
16	CLA	B	808	-	65,73,73	1.37	10 (15%)	76,113,113	1.92	15 (19%)
21	BCR	I	103	-	41,41,41	1.81	4 (9%)	56,56,56	5.34	25 (44%)
16	CLA	A	806	-	65,73,73	1.37	8 (12%)	76,113,113	1.93	14 (18%)
16	CLA	B	816	-	65,73,73	1.39	10 (15%)	76,113,113	1.85	16 (21%)
16	CLA	A	815	-	65,73,73	1.37	9 (13%)	76,113,113	2.05	17 (22%)
16	CLA	1	608	19	65,73,73	1.38	8 (12%)	76,113,113	1.84	15 (19%)
16	CLA	3	206	-	65,73,73	1.36	9 (13%)	76,113,113	1.88	16 (21%)
16	CLA	A	812	-	65,73,73	1.35	8 (12%)	76,113,113	1.89	14 (18%)
16	CLA	B	815	-	55,63,73	1.48	9 (16%)	64,101,113	1.97	14 (21%)
21	BCR	B	855	-	41,41,41	1.85	4 (9%)	56,56,56	4.67	28 (50%)
17	C7Z	3	216	-	43,43,43	5.39	27 (62%)	58,60,60	3.47	24 (41%)
16	CLA	A	838	-	65,73,73	1.38	8 (12%)	76,113,113	1.88	16 (21%)
17	C7Z	3	218	-	43,43,43	5.38	26 (60%)	58,60,60	2.50	25 (43%)
21	BCR	B	840	-	41,41,41	1.83	4 (9%)	56,56,56	4.56	18 (32%)
16	CLA	B	825	-	65,73,73	1.38	9 (13%)	76,113,113	1.92	13 (17%)
21	BCR	O	205	-	41,41,41	1.83	4 (9%)	56,56,56	4.44	16 (28%)
25	PTY	L	208	-	49,49,49	0.89	4 (8%)	52,54,54	1.03	2 (3%)
16	CLA	A	835	-	65,73,73	1.36	8 (12%)	76,113,113	2.03	16 (21%)
16	CLA	2	613	-	65,73,73	1.38	9 (13%)	76,113,113	1.96	15 (19%)
16	CLA	B	801	-	65,73,73	1.36	8 (12%)	76,113,113	1.84	15 (19%)
16	CLA	3	205	-	65,73,73	1.35	7 (10%)	76,113,113	2.21	22 (28%)
21	BCR	A	850	-	41,41,41	1.88	4 (9%)	56,56,56	4.87	23 (41%)
17	C7Z	A	843	-	43,43,43	5.41	26 (60%)	58,60,60	2.24	18 (31%)
22	PGT	B	848	16	34,34,50	1.54	7 (20%)	37,40,56	1.06	2 (5%)
16	CLA	B	836	-	65,73,73	1.39	9 (13%)	76,113,113	1.87	13 (17%)
16	CLA	A	813	-	65,73,73	1.38	9 (13%)	76,113,113	1.87	14 (18%)
16	CLA	2	602	2	64,71,73	1.50	10 (15%)	74,110,113	1.89	15 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	CLA	B	834	-	65,73,73	1.36	9 (13%)	76,113,113	1.99	18 (23%)
16	CLA	O	202	-	65,73,73	1.36	8 (12%)	76,113,113	1.88	13 (17%)
16	CLA	A	819	-	65,73,73	1.37	10 (15%)	76,113,113	1.96	16 (21%)
20	ERG	1	618	-	31,32,32	8.17	18 (58%)	47,50,50	4.76	19 (40%)
21	BCR	B	844	-	41,41,41	1.82	4 (9%)	56,56,56	4.48	21 (37%)
27	PQN	A	840	-	34,34,34	0.44	0	42,45,45	1.30	4 (9%)
16	CLA	B	827	-	65,73,73	1.37	10 (15%)	76,113,113	1.80	15 (19%)
28	SF4	A	848	4,5	0,12,12	-	-	-	-	-
21	BCR	K	104	-	41,41,41	1.82	4 (9%)	56,56,56	4.15	26 (46%)
16	CLA	A	803	16	65,73,73	1.35	8 (12%)	76,113,113	1.99	16 (21%)
16	CLA	K	101	-	65,73,73	1.38	10 (15%)	76,113,113	1.88	17 (22%)
19	LHG	1	617	16	48,48,48	0.42	0	51,54,54	0.94	3 (5%)
16	CLA	3	208	-	65,73,73	1.36	8 (12%)	76,113,113	1.93	16 (21%)
29	3PH	B	854	-	47,47,47	0.87	4 (8%)	51,52,52	1.02	2 (3%)
29	3PH	J	105	-	47,47,47	0.88	3 (6%)	51,52,52	0.96	2 (3%)
16	CLA	B	837	-	65,73,73	1.37	8 (12%)	76,113,113	2.08	17 (22%)
16	CLA	A	837	-	65,73,73	1.37	9 (13%)	76,113,113	1.88	16 (21%)
17	C7Z	1	614	-	43,43,43	5.41	26 (60%)	58,60,60	2.32	17 (29%)
21	BCR	A	846	-	41,41,41	1.80	4 (9%)	56,56,56	4.48	25 (44%)
19	LHG	A	841	-	48,48,48	0.41	0	51,54,54	0.90	2 (3%)
16	CLA	B	818	33	65,73,73	1.38	9 (13%)	76,113,113	1.97	13 (17%)
16	CLA	3	207	-	62,70,73	1.39	8 (12%)	72,109,113	1.93	15 (20%)
21	BCR	B	842	-	41,41,41	1.87	4 (9%)	56,56,56	4.46	21 (37%)
16	CLA	2	601	-	65,73,73	1.38	9 (13%)	76,113,113	1.95	14 (18%)
16	CLA	B	807	-	65,73,73	1.33	7 (10%)	76,113,113	1.88	13 (17%)
16	CLA	A	825	-	65,73,73	1.39	9 (13%)	76,113,113	1.88	16 (21%)
21	BCR	L	202	-	41,41,41	1.75	4 (9%)	56,56,56	4.40	19 (33%)
16	CLA	B	822	-	65,73,73	1.40	8 (12%)	76,113,113	1.82	15 (19%)
17	C7Z	1	616	-	43,43,43	5.38	26 (60%)	58,60,60	2.79	22 (37%)
16	CLA	A	834	4	65,73,73	1.36	8 (12%)	76,113,113	1.88	16 (21%)
18	RRX	2	616	-	42,42,42	5.00	25 (59%)	57,58,58	2.37	24 (42%)
16	CLA	B	811	-	65,73,73	1.38	9 (13%)	76,113,113	1.85	14 (18%)
16	CLA	B	804	-	65,73,73	1.35	8 (12%)	76,113,113	1.92	16 (21%)
16	CLA	A	818	-	65,73,73	1.35	9 (13%)	76,113,113	2.17	18 (23%)
16	CLA	A	854	-	65,73,73	1.34	8 (12%)	76,113,113	1.79	13 (17%)

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
16	CLA	1	604	-	1/1/19/20	11/37/115/115	-
16	CLA	A	833	-	1/1/19/20	15/37/115/115	-
16	CLA	B	802	-	1/1/19/20	12/37/115/115	-
17	C7Z	J	104	-	1/1/12/26	6/29/67/67	0/2/2/2
16	CLA	F	205	9	1/1/19/20	17/37/115/115	-
21	BCR	2	617	-	-	8/29/63/63	0/2/2/2
21	BCR	L	207	-	-	8/29/63/63	0/2/2/2
16	CLA	3	204	3	1/1/18/20	8/35/113/115	-
16	CLA	L	204	-	1/1/19/20	21/37/115/115	-
16	CLA	A	831	-	1/1/19/20	13/37/115/115	-
16	CLA	1	610	-	1/1/19/20	11/37/115/115	-
17	C7Z	3	201	-	1/1/12/26	10/29/67/67	0/2/2/2
17	C7Z	3	217	-	1/1/12/26	11/29/67/67	0/2/2/2
16	CLA	3	209	3	1/1/19/20	17/37/115/115	-
16	CLA	A	836	-	1/1/19/20	9/37/115/115	-
16	CLA	B	810	-	1/1/19/20	11/37/115/115	-
16	CLA	I	101	-	1/1/19/20	12/37/115/115	-
16	CLA	A	807	-	1/1/19/20	14/37/115/115	-
16	CLA	2	609	-	1/1/19/20	17/37/115/115	-
16	CLA	B	805	-	1/1/19/20	14/37/115/115	-
16	CLA	B	831	33	1/1/19/20	15/37/115/115	-
16	CLA	B	820	-	1/1/19/20	14/37/115/115	-
21	BCR	F	206	-	-	10/29/63/63	0/2/2/2
16	CLA	3	211	-	1/1/19/20	17/37/115/115	-
21	BCR	A	844	-	-	6/29/63/63	0/2/2/2
16	CLA	A	827	-	1/1/19/20	15/37/115/115	-
31	DGD	B	846	-	-	20/55/95/95	0/2/2/2
19	LHG	2	622	16	-	30/53/53/53	-
31	DGD	B	849	-	-	16/55/95/95	0/2/2/2
16	CLA	A	856	-	1/1/19/20	13/37/115/115	-
16	CLA	B	833	-	1/1/19/20	15/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	839	33	1/1/19/20	12/37/115/115	-
16	CLA	2	606	-	1/1/19/20	15/37/115/115	-
16	CLA	A	826	-	1/1/19/20	13/37/115/115	-
21	BCR	B	847	-	-	15/29/63/63	0/2/2/2
16	CLA	B	826	-	1/1/19/20	17/37/115/115	-
30	T7X	A	851	-	-	19/49/73/80	0/1/1/1
17	C7Z	1	612	-	1/1/12/26	11/29/67/67	0/2/2/2
25	PTY	3	221	-	-	18/53/53/53	-
16	CLA	F	204	-	1/1/19/20	11/37/115/115	-
23	DGA	2	620	-	-	21/45/45/45	-
21	BCR	L	206	-	-	8/29/63/63	0/2/2/2
16	CLA	3	213	-	1/1/14/20	9/15/93/115	-
16	CLA	A	814	-	1/1/19/20	20/37/115/115	-
16	CLA	B	813	-	1/1/19/20	12/37/115/115	-
16	CLA	2	612	-	1/1/19/20	14/37/115/115	-
16	CLA	3	210	3	1/1/19/20	15/37/115/115	-
16	CLA	A	817	-	1/1/19/20	15/37/115/115	-
26	CL0	A	801	-	3/3/24/25	15/37/135/135	-
16	CLA	A	804	-	1/1/19/20	14/37/115/115	-
16	CLA	F	201	-	1/1/18/20	15/33/111/115	-
24	LMU	3	202	-	-	13/21/61/61	0/2/2/2
16	CLA	A	802	-	1/1/19/20	17/37/115/115	-
16	CLA	A	855	33	1/1/19/20	10/37/115/115	-
16	CLA	A	822	-	1/1/19/20	13/37/115/115	-
16	CLA	O	201	-	1/1/19/20	12/37/115/115	-
16	CLA	B	832	-	1/1/19/20	15/37/115/115	-
16	CLA	1	603	-	1/1/19/20	11/37/115/115	-
16	CLA	F	202	-	2/2/19/20	15/37/115/115	-
16	CLA	1	609	-	1/1/19/20	13/37/115/115	-
19	LHG	A	842	-	-	28/53/53/53	-
25	PTY	A	852	-	-	23/48/48/53	-
21	BCR	B	841	-	-	10/29/63/63	0/2/2/2
16	CLA	2	610	19	1/1/19/20	16/37/115/115	-
17	C7Z	2	615	-	1/1/12/26	8/29/67/67	0/2/2/2

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	F	203	-	-	8/29/63/63	0/2/2/2
16	CLA	2	603	-	1/1/19/20	9/37/115/115	-
16	CLA	A	805	-	1/1/19/20	18/37/115/115	-
16	CLA	A	820	33	1/1/19/20	13/37/115/115	-
21	BCR	A	857	-	-	9/29/63/63	0/2/2/2
16	CLA	3	203	-	1/1/19/20	15/37/115/115	-
16	CLA	O	203	-	1/1/19/20	17/37/115/115	-
16	CLA	1	606	-	1/1/19/20	17/37/115/115	-
16	CLA	L	205	-	1/1/19/20	13/37/115/115	-
28	SF4	C	102	6	-	-	0/6/5/5
16	CLA	B	817	-	1/1/19/20	7/37/115/115	-
16	CLA	A	824	33	1/1/19/20	14/37/115/115	-
16	CLA	B	824	-	1/1/19/20	15/37/115/115	-
19	LHG	3	219	-	-	32/53/53/53	-
16	CLA	A	811	-	1/1/19/20	10/37/115/115	-
16	CLA	2	607	-	1/1/19/20	12/37/115/115	-
21	BCR	B	845	-	-	12/29/63/63	0/2/2/2
16	CLA	A	828	-	1/1/19/20	7/37/115/115	-
16	CLA	3	212	-	1/1/17/20	12/29/107/115	-
16	CLA	A	832	-	1/1/19/20	10/37/115/115	-
16	CLA	B	829	-	1/1/19/20	12/37/115/115	-
24	LMU	A	853	-	-	7/21/61/61	0/2/2/2
16	CLA	B	830	-	1/1/19/20	14/37/115/115	-
16	CLA	B	806	-	1/1/19/20	11/37/115/115	-
16	CLA	1	601	-	1/1/19/20	16/37/115/115	-
16	CLA	K	102	-	1/1/19/20	15/37/115/115	-
16	CLA	B	812	-	1/1/19/20	20/37/115/115	-
20	ERG	2	621	-	5/5/15/15	4/13/71/71	0/4/4/4
16	CLA	L	203	13	1/1/19/20	12/37/115/115	-
16	CLA	2	604	-	1/1/19/20	10/37/115/115	-
16	CLA	B	838	22	1/1/19/20	13/37/115/115	-
16	CLA	B	814	-	1/1/19/20	12/37/115/115	-
16	CLA	A	821	-	1/1/19/20	13/37/115/115	-
16	CLA	1	607	1	1/1/18/20	12/31/109/115	-

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	809	-	1/1/19/20	17/37/115/115	-
16	CLA	B	835	-	1/1/19/20	14/37/115/115	-
16	CLA	B	809	5	1/1/19/20	17/37/115/115	-
28	SF4	C	101	6	-	-	0/6/5/5
16	CLA	1	611	-	1/1/19/20	13/37/115/115	-
23	DGA	J	101	-	-	17/45/45/45	-
17	C7Z	1	615	-	1/1/12/26	11/29/67/67	0/2/2/2
16	CLA	B	828	-	1/1/19/20	7/37/115/115	-
16	CLA	3	214	-	1/1/19/20	16/37/115/115	-
19	LHG	B	851	-	-	24/49/49/53	-
16	CLA	2	608	-	1/1/19/20	21/37/115/115	-
16	CLA	A	808	4	1/1/19/20	14/37/115/115	-
16	CLA	A	823	-	1/1/19/20	11/37/115/115	-
20	ERG	2	618	-	4/4/15/15	10/13/71/71	0/4/4/4
27	PQN	B	839	-	-	9/23/43/43	0/2/2/2
16	CLA	B	823	-	1/1/19/20	15/37/115/115	-
16	CLA	2	611	2	1/1/19/20	15/37/115/115	-
18	RRX	J	103	-	1/1/25/25	16/29/65/65	0/2/2/2
16	CLA	B	819	-	1/1/19/20	14/37/115/115	-
25	PTY	3	220	-	-	19/53/53/53	-
16	CLA	1	602	1	1/1/17/20	8/30/108/115	-
29	3PH	A	849	-	-	19/49/49/49	-
16	CLA	2	605	-	1/1/19/20	16/37/115/115	-
16	CLA	L	201	-	1/1/19/20	8/37/115/115	-
22	PGT	2	619	-	1/1/5/5	20/38/38/55	-
16	CLA	J	102	11	2/2/19/20	18/37/115/115	-
16	CLA	B	803	33	1/1/19/20	9/37/115/115	-
17	C7Z	2	614	-	1/1/12/26	10/29/67/67	0/2/2/2
21	BCR	B	843	-	-	9/29/63/63	0/2/2/2
18	RRX	A	847	-	1/1/24/25	13/29/65/65	0/2/2/2
18	RRX	1	613	-	1/1/25/25	20/29/65/65	0/2/2/2
16	CLA	B	821	-	2/2/19/20	13/37/115/115	-
16	CLA	I	102	-	1/1/19/20	14/37/115/115	-
18	RRX	K	103	-	1/1/25/25	16/29/65/65	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	1	605	-	1/1/19/20	14/37/115/115	-
31	DGD	B	850	-	-	18/55/95/95	0/2/2/2
21	BCR	A	845	-	-	11/29/63/63	0/2/2/2
16	CLA	A	810	16	1/1/19/20	11/37/115/115	-
17	C7Z	3	215	-	1/1/12/26	9/29/67/67	0/2/2/2
16	CLA	O	204	-	1/1/19/20	10/37/115/115	-
16	CLA	A	829	-	1/1/19/20	13/37/115/115	-
16	CLA	A	816	-	1/1/19/20	14/37/115/115	-
16	CLA	A	830	-	1/1/19/20	13/37/115/115	-
16	CLA	B	808	-	1/1/19/20	11/37/115/115	-
21	BCR	I	103	-	-	10/29/63/63	0/2/2/2
16	CLA	A	806	-	1/1/19/20	11/37/115/115	-
16	CLA	B	816	-	1/1/19/20	11/37/115/115	-
16	CLA	A	815	-	1/1/19/20	21/37/115/115	-
16	CLA	1	608	19	1/1/19/20	14/37/115/115	-
16	CLA	3	206	-	1/1/19/20	11/37/115/115	-
16	CLA	A	812	-	1/1/19/20	14/37/115/115	-
16	CLA	B	815	-	1/1/17/20	9/25/103/115	-
21	BCR	B	855	-	-	9/29/63/63	0/2/2/2
17	C7Z	3	216	-	1/1/12/26	9/29/67/67	0/2/2/2
16	CLA	A	838	-	1/1/19/20	6/37/115/115	-
17	C7Z	3	218	-	1/1/12/26	8/29/67/67	0/2/2/2
21	BCR	B	840	-	-	8/29/63/63	0/2/2/2
16	CLA	B	825	-	1/1/19/20	12/37/115/115	-
21	BCR	O	205	-	-	11/29/63/63	0/2/2/2
25	PTY	L	208	-	-	23/53/53/53	-
16	CLA	A	835	-	1/1/19/20	13/37/115/115	-
16	CLA	2	613	-	1/1/19/20	18/37/115/115	-
16	CLA	B	801	-	1/1/19/20	16/37/115/115	-
16	CLA	3	205	-	1/1/19/20	11/37/115/115	-
21	BCR	A	850	-	-	14/29/63/63	0/2/2/2
17	C7Z	A	843	-	1/1/12/26	12/29/67/67	0/2/2/2
22	PGT	B	848	16	1/1/5/5	21/38/38/55	-
16	CLA	B	836	-	1/1/19/20	13/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	813	-	1/1/19/20	16/37/115/115	-
16	CLA	2	602	2	1/1/19/20	13/35/113/115	-
16	CLA	B	834	-	1/1/19/20	14/37/115/115	-
16	CLA	O	202	-	1/1/19/20	11/37/115/115	-
16	CLA	A	819	-	1/1/19/20	17/37/115/115	-
20	ERG	1	618	-	6/6/15/15	3/13/71/71	0/4/4/4
21	BCR	B	844	-	-	7/29/63/63	0/2/2/2
27	PQN	A	840	-	-	10/23/43/43	0/2/2/2
16	CLA	B	827	-	1/1/19/20	12/37/115/115	-
28	SF4	A	848	4,5	-	-	0/6/5/5
21	BCR	K	104	-	-	14/29/63/63	0/2/2/2
16	CLA	A	803	16	1/1/19/20	13/37/115/115	-
16	CLA	K	101	-	1/1/19/20	16/37/115/115	-
19	LHG	1	617	16	-	29/53/53/53	-
16	CLA	3	208	-	1/1/19/20	14/37/115/115	-
29	3PH	B	854	-	-	28/49/49/49	-
29	3PH	J	105	-	-	20/49/49/49	-
16	CLA	B	837	-	1/1/19/20	15/37/115/115	-
16	CLA	A	837	-	1/1/19/20	17/37/115/115	-
17	C7Z	1	614	-	1/1/12/26	13/29/67/67	0/2/2/2
21	BCR	A	846	-	-	6/29/63/63	0/2/2/2
19	LHG	A	841	-	-	35/53/53/53	-
16	CLA	B	818	33	1/1/19/20	15/37/115/115	-
16	CLA	3	207	-	1/1/18/20	14/34/112/115	-
21	BCR	B	842	-	-	6/29/63/63	0/2/2/2
16	CLA	2	601	-	1/1/19/20	20/37/115/115	-
16	CLA	B	807	-	1/1/19/20	11/37/115/115	-
16	CLA	A	825	-	1/1/19/20	15/37/115/115	-
21	BCR	L	202	-	-	8/29/63/63	0/2/2/2
16	CLA	B	822	-	1/1/19/20	6/37/115/115	-
17	C7Z	1	616	-	1/1/12/26	7/29/67/67	0/2/2/2
16	CLA	A	834	4	1/1/19/20	14/37/115/115	-
18	RRX	2	616	-	1/1/25/25	13/29/65/65	0/2/2/2
16	CLA	B	811	-	1/1/19/20	8/37/115/115	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	804	-	1/1/19/20	13/37/115/115	-
16	CLA	A	818	-	1/1/19/20	14/37/115/115	-
16	CLA	A	854	-	1/1/19/20	11/37/115/115	-

All (1855) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	621	ERG	C1-C10	-24.95	1.06	1.54
20	2	618	ERG	C1-C10	-24.94	1.06	1.54
20	1	618	ERG	C1-C10	-24.51	1.07	1.54
20	2	618	ERG	C10-C9	-22.33	1.26	1.55
20	2	621	ERG	C10-C9	-21.86	1.26	1.55
20	1	618	ERG	C10-C9	-21.21	1.27	1.55
17	3	216	C7Z	C25-C26	16.04	1.62	1.34
17	3	215	C7Z	C25-C26	16.04	1.62	1.34
20	2	618	ERG	C10-C5	-16.03	1.21	1.52
18	2	616	RRX	C26-C25	15.96	1.62	1.34
17	1	612	C7Z	C25-C26	15.95	1.62	1.34
17	1	614	C7Z	C25-C26	15.94	1.62	1.34
20	2	621	ERG	C10-C5	-15.89	1.21	1.52
17	1	615	C7Z	C25-C26	15.89	1.62	1.34
17	A	843	C7Z	C25-C26	15.87	1.61	1.34
17	3	201	C7Z	C25-C26	15.87	1.61	1.34
17	2	614	C7Z	C25-C26	15.87	1.61	1.34
17	3	218	C7Z	C25-C26	15.72	1.61	1.34
17	1	616	C7Z	C25-C26	15.72	1.61	1.34
17	2	615	C7Z	C25-C26	15.67	1.61	1.34
17	J	104	C7Z	C25-C26	15.65	1.61	1.34
18	A	847	RRX	C26-C25	15.60	1.61	1.34
17	3	217	C7Z	C25-C26	15.59	1.61	1.34
20	1	618	ERG	C10-C5	-15.47	1.22	1.52
17	3	215	C7Z	C5-C6	15.35	1.61	1.34
17	1	614	C7Z	C5-C6	15.33	1.61	1.34
18	K	103	RRX	C26-C25	15.24	1.60	1.34
17	3	201	C7Z	C5-C6	15.21	1.60	1.34
17	2	615	C7Z	C5-C6	15.17	1.60	1.34
17	1	616	C7Z	C5-C6	15.13	1.60	1.34
17	2	614	C7Z	C5-C6	15.11	1.60	1.34
18	1	613	RRX	C5-C6	15.10	1.60	1.34
17	1	612	C7Z	C5-C6	15.10	1.60	1.34
17	3	217	C7Z	C5-C6	15.06	1.60	1.34
17	A	843	C7Z	C5-C6	15.05	1.60	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	J	103	RRX	C26-C25	15.03	1.60	1.34
17	3	218	C7Z	C5-C6	15.03	1.60	1.34
17	J	104	C7Z	C5-C6	15.00	1.60	1.34
17	3	216	C7Z	C5-C6	14.99	1.60	1.34
17	1	615	C7Z	C5-C6	14.91	1.60	1.34
18	1	613	RRX	C26-C25	14.84	1.60	1.34
18	J	103	RRX	C5-C6	14.84	1.60	1.34
18	A	847	RRX	C5-C6	14.72	1.59	1.34
18	K	103	RRX	C5-C6	14.71	1.59	1.34
18	2	616	RRX	C5-C6	14.69	1.59	1.34
20	2	618	ERG	C4-C3	-14.13	1.27	1.52
20	2	621	ERG	C4-C3	-14.11	1.27	1.52
20	1	618	ERG	C4-C3	-14.06	1.27	1.52
17	2	615	C7Z	C24-C23	12.06	1.73	1.52
17	1	616	C7Z	C24-C23	11.90	1.73	1.52
17	J	104	C7Z	C24-C23	11.90	1.73	1.52
17	3	218	C7Z	C24-C23	11.86	1.72	1.52
17	A	843	C7Z	C24-C23	11.84	1.72	1.52
17	3	201	C7Z	C24-C23	11.83	1.72	1.52
20	2	621	ERG	C2-C3	-11.81	1.23	1.51
17	1	615	C7Z	C24-C23	11.77	1.72	1.52
20	1	618	ERG	C2-C3	-11.76	1.23	1.51
17	1	614	C7Z	C24-C23	11.73	1.72	1.52
20	2	618	ERG	C2-C3	-11.70	1.23	1.51
17	3	215	C7Z	C24-C23	11.65	1.72	1.52
17	3	216	C7Z	C24-C23	11.60	1.72	1.52
17	2	614	C7Z	C24-C23	11.57	1.72	1.52
17	1	612	C7Z	C24-C23	11.52	1.72	1.52
17	3	217	C7Z	C24-C23	11.38	1.72	1.52
17	3	215	C7Z	C22-C23	-10.89	1.36	1.52
17	3	216	C7Z	C22-C23	-10.88	1.36	1.52
17	3	217	C7Z	C22-C23	-10.86	1.36	1.52
17	1	612	C7Z	C22-C23	-10.82	1.36	1.52
17	2	614	C7Z	C22-C23	-10.73	1.36	1.52
17	3	201	C7Z	C2-C3	-10.72	1.36	1.52
17	1	614	C7Z	C2-C3	-10.71	1.36	1.52
17	3	215	C7Z	C2-C3	-10.68	1.36	1.52
17	1	615	C7Z	C22-C23	-10.63	1.37	1.52
17	1	614	C7Z	C22-C23	-10.61	1.37	1.52
17	3	201	C7Z	C22-C23	-10.57	1.37	1.52
17	J	104	C7Z	C22-C23	-10.52	1.37	1.52
17	2	615	C7Z	C22-C23	-10.49	1.37	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	615	C7Z	C2-C3	-10.47	1.37	1.52
17	A	843	C7Z	C22-C23	-10.47	1.37	1.52
17	1	616	C7Z	C22-C23	-10.44	1.37	1.52
17	2	614	C7Z	C2-C3	-10.44	1.37	1.52
17	J	104	C7Z	C2-C3	-10.40	1.37	1.52
17	A	843	C7Z	C2-C3	-10.38	1.37	1.52
17	3	217	C7Z	C2-C3	-10.37	1.37	1.52
17	3	218	C7Z	C22-C23	-10.37	1.37	1.52
17	3	216	C7Z	C2-C3	-10.37	1.37	1.52
17	3	218	C7Z	C2-C3	-10.36	1.37	1.52
17	1	616	C7Z	C2-C3	-10.34	1.37	1.52
17	1	615	C7Z	C2-C3	-10.33	1.37	1.52
17	1	612	C7Z	C2-C3	-10.33	1.37	1.52
18	2	616	RRX	C29-C28	-10.11	1.37	1.52
20	1	618	ERG	C12-C13	10.07	1.72	1.54
18	A	847	RRX	C29-C28	-10.01	1.37	1.52
18	K	103	RRX	C29-C28	-9.78	1.38	1.52
18	J	103	RRX	C29-C28	-9.39	1.38	1.52
18	1	613	RRX	C29-C28	-9.14	1.39	1.52
20	2	618	ERG	O1-C3	9.10	1.70	1.43
20	1	618	ERG	O1-C3	9.10	1.70	1.43
20	2	621	ERG	O1-C3	9.08	1.70	1.43
26	A	801	CL0	MG-NA	8.92	2.27	2.06
20	1	618	ERG	C6-C5	8.73	1.54	1.33
20	2	618	ERG	C6-C5	8.72	1.54	1.33
20	2	621	ERG	C6-C5	8.72	1.53	1.33
17	A	843	C7Z	C4-C3	8.58	1.67	1.52
20	2	618	ERG	C12-C13	8.57	1.69	1.54
17	3	218	C7Z	C4-C3	8.56	1.67	1.52
17	1	616	C7Z	C4-C3	8.56	1.67	1.52
17	3	217	C7Z	C4-C3	8.55	1.67	1.52
17	J	104	C7Z	C4-C3	8.54	1.67	1.52
17	1	612	C7Z	C4-C3	8.51	1.67	1.52
17	1	615	C7Z	C4-C3	8.51	1.67	1.52
17	2	615	C7Z	C4-C3	8.49	1.67	1.52
17	3	216	C7Z	C4-C3	8.47	1.67	1.52
20	2	621	ERG	C12-C13	8.47	1.69	1.54
17	2	614	C7Z	C4-C3	8.44	1.66	1.52
17	3	201	C7Z	C4-C3	8.34	1.66	1.52
18	J	103	RRX	C27-C28	8.27	1.66	1.52
17	1	614	C7Z	C4-C3	8.23	1.66	1.52
18	1	613	RRX	C27-C28	8.21	1.66	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	215	C7Z	C4-C3	8.21	1.66	1.52
18	A	847	RRX	C27-C28	8.17	1.66	1.52
18	K	103	RRX	C27-C28	8.17	1.66	1.52
18	2	616	RRX	C27-C28	8.01	1.66	1.52
21	F	206	BCR	C10-C9	7.55	1.45	1.35
21	B	842	BCR	C10-C9	7.37	1.45	1.35
21	A	850	BCR	C10-C9	7.31	1.45	1.35
21	L	207	BCR	C10-C9	7.31	1.45	1.35
21	2	617	BCR	C10-C9	7.28	1.45	1.35
21	B	840	BCR	C10-C9	7.19	1.45	1.35
21	A	844	BCR	C10-C9	7.15	1.45	1.35
21	A	845	BCR	C10-C9	7.14	1.45	1.35
21	B	845	BCR	C10-C9	7.06	1.45	1.35
21	B	847	BCR	C10-C9	7.06	1.45	1.35
21	B	843	BCR	C10-C9	7.04	1.45	1.35
21	F	203	BCR	C10-C9	7.02	1.45	1.35
21	B	844	BCR	C10-C9	6.96	1.45	1.35
21	B	855	BCR	C10-C9	6.95	1.45	1.35
21	O	205	BCR	C10-C9	6.94	1.45	1.35
21	I	103	BCR	C10-C9	6.93	1.45	1.35
21	B	841	BCR	C10-C9	6.74	1.44	1.35
21	A	857	BCR	C10-C9	6.73	1.44	1.35
21	K	104	BCR	C10-C9	6.59	1.44	1.35
21	L	206	BCR	C10-C9	6.52	1.44	1.35
18	1	613	RRX	C2-C3	-6.52	1.36	1.52
18	J	103	RRX	C2-C3	-6.43	1.36	1.52
18	K	103	RRX	C2-C3	-6.41	1.36	1.52
21	L	202	BCR	C10-C9	6.40	1.44	1.35
18	2	616	RRX	C2-C3	-6.40	1.36	1.52
21	A	846	BCR	C10-C9	6.39	1.44	1.35
16	B	837	CLA	MG-NA	6.38	2.21	2.06
16	A	804	CLA	MG-NA	6.38	2.21	2.06
16	A	839	CLA	MG-NA	6.37	2.21	2.06
18	A	847	RRX	C2-C3	-6.37	1.36	1.52
16	B	821	CLA	MG-NA	6.36	2.21	2.06
16	1	609	CLA	MG-NA	6.36	2.21	2.06
16	A	815	CLA	MG-NA	6.35	2.21	2.06
16	3	203	CLA	MG-NA	6.35	2.21	2.06
16	3	205	CLA	MG-NA	6.35	2.21	2.06
16	O	203	CLA	MG-NA	6.35	2.21	2.06
16	B	825	CLA	MG-NA	6.33	2.21	2.06
16	1	605	CLA	MG-NA	6.33	2.21	2.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	822	CLA	MG-NA	6.33	2.21	2.06
16	2	603	CLA	MG-NA	6.32	2.21	2.06
16	A	831	CLA	MG-NA	6.32	2.21	2.06
16	A	830	CLA	MG-NA	6.31	2.21	2.06
16	B	838	CLA	MG-NA	6.31	2.21	2.06
16	A	837	CLA	MG-NA	6.30	2.21	2.06
16	B	803	CLA	MG-NA	6.30	2.21	2.06
16	B	836	CLA	MG-NA	6.30	2.21	2.06
16	L	203	CLA	MG-NA	6.30	2.21	2.06
16	A	824	CLA	MG-NA	6.30	2.21	2.06
16	A	836	CLA	MG-NA	6.30	2.21	2.06
16	A	816	CLA	MG-NA	6.29	2.21	2.06
16	B	816	CLA	MG-NA	6.29	2.21	2.06
20	2	618	ERG	C16-C17	-6.29	1.41	1.54
16	3	211	CLA	MG-NA	6.29	2.21	2.06
16	1	608	CLA	MG-NA	6.29	2.21	2.06
16	2	611	CLA	MG-NA	6.28	2.21	2.06
16	B	832	CLA	MG-NA	6.28	2.21	2.06
16	B	814	CLA	MG-NA	6.28	2.21	2.06
16	F	202	CLA	MG-NA	6.27	2.21	2.06
16	I	102	CLA	MG-NA	6.27	2.21	2.06
16	F	204	CLA	MG-NA	6.27	2.21	2.06
16	L	201	CLA	MG-NA	6.27	2.21	2.06
16	2	601	CLA	MG-NA	6.27	2.21	2.06
16	B	820	CLA	MG-NA	6.27	2.21	2.06
16	2	610	CLA	MG-NA	6.27	2.21	2.06
16	B	812	CLA	MG-NA	6.27	2.21	2.06
16	A	802	CLA	MG-NA	6.26	2.21	2.06
16	3	213	CLA	MG-NA	6.26	2.21	2.06
16	B	815	CLA	MG-NA	6.26	2.21	2.06
16	3	214	CLA	MG-NA	6.26	2.21	2.06
16	A	855	CLA	MG-NA	6.26	2.21	2.06
16	K	101	CLA	MG-NA	6.26	2.21	2.06
16	O	204	CLA	MG-NA	6.26	2.21	2.06
16	B	802	CLA	MG-NA	6.26	2.21	2.06
16	1	611	CLA	MG-NA	6.25	2.21	2.06
16	2	612	CLA	MG-NA	6.25	2.21	2.06
16	J	102	CLA	MG-NA	6.25	2.21	2.06
16	F	201	CLA	MG-NA	6.24	2.21	2.06
16	3	212	CLA	MG-NA	6.24	2.21	2.06
16	2	609	CLA	MG-NA	6.24	2.21	2.06
16	1	604	CLA	MG-NA	6.24	2.21	2.06

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	805	CLA	MG-NA	6.24	2.21	2.06
16	B	806	CLA	MG-NA	6.23	2.21	2.06
16	A	835	CLA	MG-NA	6.23	2.21	2.06
16	2	613	CLA	MG-NA	6.23	2.21	2.06
16	B	811	CLA	MG-NA	6.23	2.21	2.06
16	1	603	CLA	MG-NA	6.22	2.21	2.06
16	3	207	CLA	MG-NA	6.22	2.21	2.06
16	B	829	CLA	MG-NA	6.22	2.21	2.06
16	A	825	CLA	MG-NA	6.22	2.21	2.06
16	A	817	CLA	MG-NA	6.22	2.21	2.06
16	O	202	CLA	MG-NA	6.22	2.21	2.06
16	A	828	CLA	MG-NA	6.22	2.21	2.06
16	A	813	CLA	MG-NA	6.22	2.21	2.06
16	B	809	CLA	MG-NA	6.22	2.21	2.06
16	B	833	CLA	MG-NA	6.22	2.21	2.06
16	A	811	CLA	MG-NA	6.21	2.21	2.06
16	B	817	CLA	MG-NA	6.21	2.21	2.06
16	1	601	CLA	MG-NA	6.20	2.21	2.06
16	B	819	CLA	MG-NA	6.20	2.21	2.06
16	A	808	CLA	MG-NA	6.20	2.21	2.06
16	A	821	CLA	MG-NA	6.20	2.21	2.06
16	L	205	CLA	MG-NA	6.20	2.21	2.06
16	K	102	CLA	MG-NA	6.19	2.21	2.06
16	A	834	CLA	MG-NA	6.19	2.21	2.06
16	B	810	CLA	MG-NA	6.18	2.21	2.06
16	L	204	CLA	MG-NA	6.18	2.21	2.06
16	2	602	CLA	MG-NA	6.18	2.20	2.06
16	B	813	CLA	MG-NA	6.18	2.20	2.06
16	2	605	CLA	MG-NA	6.17	2.20	2.06
16	2	606	CLA	MG-NA	6.16	2.20	2.06
16	2	608	CLA	MG-NA	6.16	2.20	2.06
16	A	819	CLA	MG-NA	6.16	2.20	2.06
16	A	806	CLA	MG-NA	6.16	2.20	2.06
16	A	809	CLA	MG-NA	6.16	2.20	2.06
16	B	823	CLA	MG-NA	6.16	2.20	2.06
16	B	835	CLA	MG-NA	6.16	2.20	2.06
16	F	205	CLA	MG-NA	6.16	2.20	2.06
16	3	208	CLA	MG-NA	6.16	2.20	2.06
16	1	610	CLA	MG-NA	6.15	2.20	2.06
16	1	607	CLA	MG-NA	6.15	2.20	2.06
16	B	801	CLA	MG-NA	6.14	2.20	2.06
16	2	607	CLA	MG-NA	6.14	2.20	2.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	828	CLA	MG-NA	6.13	2.20	2.06
16	3	209	CLA	MG-NA	6.13	2.20	2.06
16	1	606	CLA	MG-NA	6.13	2.20	2.06
16	3	206	CLA	MG-NA	6.13	2.20	2.06
16	A	807	CLA	MG-NA	6.13	2.20	2.06
16	A	856	CLA	MG-NA	6.12	2.20	2.06
16	A	838	CLA	MG-NA	6.12	2.20	2.06
16	B	827	CLA	MG-NA	6.12	2.20	2.06
16	O	201	CLA	MG-NA	6.11	2.20	2.06
16	A	827	CLA	MG-NA	6.11	2.20	2.06
16	B	826	CLA	MG-NA	6.11	2.20	2.06
16	B	834	CLA	MG-NA	6.10	2.20	2.06
16	2	604	CLA	MG-NA	6.10	2.20	2.06
16	B	830	CLA	MG-NA	6.09	2.20	2.06
16	1	602	CLA	MG-NA	6.09	2.20	2.06
16	A	822	CLA	MG-NA	6.09	2.20	2.06
16	A	823	CLA	MG-NA	6.08	2.20	2.06
20	2	621	ERG	C16-C17	-6.08	1.41	1.54
16	A	805	CLA	MG-NA	6.08	2.20	2.06
16	A	814	CLA	MG-NA	6.07	2.20	2.06
16	A	826	CLA	MG-NA	6.07	2.20	2.06
16	3	210	CLA	MG-NA	6.06	2.20	2.06
16	A	833	CLA	MG-NA	6.05	2.20	2.06
16	A	820	CLA	MG-NA	6.05	2.20	2.06
16	A	810	CLA	MG-NA	6.05	2.20	2.06
16	B	807	CLA	MG-NA	6.05	2.20	2.06
21	2	617	BCR	C24-C23	6.05	1.51	1.33
16	A	803	CLA	MG-NA	6.04	2.20	2.06
16	A	829	CLA	MG-NA	6.04	2.20	2.06
20	2	621	ERG	C13-C14	-6.04	1.46	1.56
16	B	808	CLA	MG-NA	6.04	2.20	2.06
16	3	204	CLA	MG-NA	6.03	2.20	2.06
16	A	812	CLA	MG-NA	6.03	2.20	2.06
17	J	104	C7Z	C12-C13	6.03	1.58	1.45
16	I	101	CLA	MG-NA	6.03	2.20	2.06
16	B	831	CLA	MG-NA	6.03	2.20	2.06
16	B	818	CLA	MG-NA	6.02	2.20	2.06
16	A	832	CLA	MG-NA	6.01	2.20	2.06
16	B	824	CLA	MG-NA	5.99	2.20	2.06
16	A	818	CLA	MG-NA	5.98	2.20	2.06
21	B	842	BCR	C24-C23	5.97	1.51	1.33
16	B	804	CLA	MG-NA	5.96	2.20	2.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	612	C7Z	C12-C13	5.96	1.58	1.45
21	B	855	BCR	C24-C23	5.94	1.51	1.33
21	A	850	BCR	C24-C23	5.94	1.51	1.33
17	2	615	C7Z	C12-C13	5.94	1.58	1.45
21	B	845	BCR	C24-C23	5.94	1.51	1.33
21	A	844	BCR	C24-C23	5.92	1.51	1.33
21	L	207	BCR	C24-C23	5.92	1.51	1.33
21	B	844	BCR	C24-C23	5.91	1.50	1.33
17	3	201	C7Z	C12-C13	5.90	1.58	1.45
17	A	843	C7Z	C12-C13	5.89	1.58	1.45
21	F	206	BCR	C24-C23	5.87	1.50	1.33
21	O	205	BCR	C24-C23	5.86	1.50	1.33
18	K	103	RRX	C19-C18	5.86	1.58	1.45
21	B	843	BCR	C24-C23	5.84	1.50	1.33
21	I	103	BCR	C24-C23	5.83	1.50	1.33
21	K	104	BCR	C24-C23	5.83	1.50	1.33
21	A	857	BCR	C24-C23	5.82	1.50	1.33
18	1	613	RRX	C1-C6	-5.82	1.45	1.53
18	J	103	RRX	C19-C18	5.81	1.58	1.45
16	A	854	CLA	MG-NA	5.81	2.20	2.06
21	B	847	BCR	C24-C23	5.78	1.50	1.33
17	1	615	C7Z	C12-C13	5.77	1.58	1.45
21	B	840	BCR	C24-C23	5.77	1.50	1.33
17	1	616	C7Z	C12-C13	5.77	1.58	1.45
17	2	614	C7Z	C12-C13	5.76	1.58	1.45
17	3	215	C7Z	C12-C13	5.75	1.58	1.45
21	F	203	BCR	C24-C23	5.74	1.50	1.33
17	3	216	C7Z	C1-C6	-5.74	1.45	1.53
20	1	618	ERG	C16-C17	-5.72	1.42	1.54
18	2	616	RRX	C19-C18	5.72	1.58	1.45
17	3	218	C7Z	C12-C13	5.70	1.58	1.45
17	3	217	C7Z	C12-C13	5.68	1.58	1.45
21	A	845	BCR	C24-C23	5.68	1.50	1.33
17	1	614	C7Z	C12-C13	5.68	1.58	1.45
21	L	202	BCR	C24-C23	5.67	1.50	1.33
21	L	206	BCR	C24-C23	5.65	1.50	1.33
21	A	846	BCR	C24-C23	5.64	1.50	1.33
18	2	616	RRX	C1-C6	-5.64	1.46	1.53
18	J	103	RRX	C1-C6	-5.64	1.46	1.53
21	B	841	BCR	C24-C23	5.61	1.50	1.33
17	3	217	C7Z	C1-C6	-5.61	1.46	1.53
17	1	615	C7Z	C1-C6	-5.60	1.46	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	218	C7Z	C1-C6	-5.57	1.46	1.53
18	1	613	RRX	C19-C18	5.54	1.57	1.45
17	A	843	C7Z	C1-C6	-5.54	1.46	1.53
21	L	206	BCR	C11-C12	-5.53	1.20	1.34
18	A	847	RRX	C1-C6	-5.53	1.46	1.53
17	3	201	C7Z	C1-C6	-5.53	1.46	1.53
18	J	103	RRX	C30-C25	-5.50	1.46	1.53
17	2	615	C7Z	C1-C6	-5.50	1.46	1.53
17	1	616	C7Z	C1-C6	-5.49	1.46	1.53
17	2	614	C7Z	C1-C6	-5.48	1.46	1.53
17	1	612	C7Z	C1-C6	-5.47	1.46	1.53
17	3	216	C7Z	C12-C13	5.47	1.57	1.45
17	J	104	C7Z	C1-C6	-5.46	1.46	1.53
21	A	846	BCR	C11-C12	-5.42	1.20	1.34
18	K	103	RRX	C1-C6	-5.39	1.46	1.53
18	A	847	RRX	C30-C25	-5.38	1.46	1.53
18	A	847	RRX	C8-C9	5.38	1.57	1.45
18	A	847	RRX	C2-C1	5.38	1.66	1.54
17	1	614	C7Z	C1-C6	-5.36	1.46	1.53
18	A	847	RRX	C19-C18	5.34	1.57	1.45
26	A	801	CL0	CHC-C1C	5.33	1.48	1.35
18	J	103	RRX	C2-C1	5.30	1.66	1.54
18	2	616	RRX	C2-C1	5.29	1.66	1.54
21	A	844	BCR	C11-C12	-5.26	1.21	1.34
18	K	103	RRX	C2-C1	5.24	1.66	1.54
20	1	618	ERG	C13-C14	-5.24	1.47	1.56
21	A	857	BCR	C11-C12	-5.24	1.21	1.34
18	1	613	RRX	C8-C9	5.23	1.57	1.45
17	A	843	C7Z	C28-C29	5.23	1.57	1.45
20	2	618	ERG	C13-C14	-5.22	1.47	1.56
17	2	615	C7Z	C28-C29	5.22	1.57	1.45
21	B	841	BCR	C11-C12	-5.21	1.21	1.34
17	3	201	C7Z	C28-C29	5.20	1.57	1.45
17	3	216	C7Z	C28-C29	5.19	1.57	1.45
17	3	218	C7Z	C28-C29	5.17	1.57	1.45
20	2	618	ERG	C12-C11	-5.17	1.42	1.53
26	A	801	CL0	O2D-CGD	5.16	1.45	1.33
21	B	840	BCR	C11-C12	-5.15	1.21	1.34
21	B	847	BCR	C11-C12	-5.15	1.21	1.34
21	A	845	BCR	C11-C12	-5.15	1.21	1.34
17	3	215	C7Z	C28-C29	5.14	1.57	1.45
21	L	202	BCR	C11-C12	-5.13	1.21	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	103	RRX	C30-C25	-5.12	1.46	1.53
21	B	844	BCR	C11-C12	-5.12	1.21	1.34
17	1	616	C7Z	C28-C29	5.12	1.56	1.45
17	1	614	C7Z	C28-C29	5.12	1.56	1.45
17	1	612	C7Z	C28-C29	5.12	1.56	1.45
17	J	104	C7Z	C28-C29	5.11	1.56	1.45
21	B	855	BCR	C11-C12	-5.11	1.21	1.34
21	I	103	BCR	C11-C12	-5.11	1.21	1.34
17	2	614	C7Z	C28-C29	5.11	1.56	1.45
17	3	217	C7Z	C24-C25	-5.10	1.43	1.51
17	3	215	C7Z	C1-C6	-5.10	1.46	1.53
21	K	104	BCR	C11-C12	-5.08	1.21	1.34
21	F	203	BCR	C11-C12	-5.07	1.21	1.34
21	B	843	BCR	C11-C12	-5.07	1.21	1.34
17	1	612	C7Z	C32-C33	5.07	1.56	1.45
18	1	613	RRX	C12-C13	5.07	1.56	1.45
26	A	801	CL0	O2A-C1	5.07	1.60	1.46
18	1	613	RRX	C2-C1	5.07	1.65	1.54
18	K	103	RRX	C23-C22	5.06	1.56	1.45
17	2	615	C7Z	C32-C33	5.06	1.56	1.45
17	A	843	C7Z	C32-C33	5.05	1.56	1.45
17	1	615	C7Z	C28-C29	5.04	1.56	1.45
21	L	207	BCR	C11-C12	-5.04	1.21	1.34
21	O	205	BCR	C11-C12	-5.03	1.21	1.34
17	J	104	C7Z	C32-C33	5.00	1.56	1.45
18	K	103	RRX	C8-C9	5.00	1.56	1.45
18	2	616	RRX	C8-C9	4.99	1.56	1.45
17	3	201	C7Z	C32-C33	4.98	1.56	1.45
21	B	845	BCR	C11-C12	-4.97	1.21	1.34
21	A	850	BCR	C11-C12	-4.97	1.21	1.34
21	B	842	BCR	C11-C12	-4.96	1.21	1.34
18	J	103	RRX	C8-C9	4.96	1.56	1.45
21	2	617	BCR	C11-C12	-4.95	1.21	1.34
20	2	621	ERG	C12-C11	-4.93	1.42	1.53
17	1	616	C7Z	C32-C33	4.89	1.56	1.45
21	F	206	BCR	C11-C12	-4.88	1.22	1.34
18	K	103	RRX	C12-C13	4.88	1.56	1.45
17	1	614	C7Z	C32-C33	4.88	1.56	1.45
17	3	215	C7Z	C32-C33	4.87	1.56	1.45
18	A	847	RRX	C12-C13	4.86	1.56	1.45
17	3	217	C7Z	C28-C29	4.86	1.56	1.45
20	2	621	ERG	C7-C6	-4.83	1.27	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	613	RRX	C30-C25	-4.83	1.47	1.53
17	2	614	C7Z	C32-C33	4.83	1.56	1.45
17	3	218	C7Z	C32-C33	4.82	1.56	1.45
20	1	618	ERG	C13-C17	4.82	1.64	1.55
18	2	616	RRX	C30-C25	-4.78	1.47	1.53
18	1	613	RRX	C23-C22	4.78	1.56	1.45
17	1	615	C7Z	C32-C33	4.77	1.56	1.45
17	1	612	C7Z	C24-C25	-4.77	1.43	1.51
17	2	614	C7Z	C24-C25	-4.77	1.43	1.51
17	3	216	C7Z	C32-C33	4.77	1.56	1.45
17	1	612	C7Z	C31-C30	4.77	1.58	1.43
17	J	104	C7Z	C8-C9	4.75	1.56	1.45
26	A	801	CL0	C3B-C2B	4.73	1.46	1.40
17	3	218	C7Z	C24-C25	-4.72	1.43	1.51
20	2	618	ERG	C7-C6	-4.71	1.27	1.41
17	J	104	C7Z	C24-C25	-4.69	1.43	1.51
20	1	618	ERG	C7-C6	-4.68	1.27	1.41
17	1	616	C7Z	C24-C25	-4.68	1.43	1.51
18	2	616	RRX	C12-C13	4.66	1.56	1.45
17	3	216	C7Z	C24-C25	-4.66	1.43	1.51
17	3	201	C7Z	C24-C25	-4.65	1.43	1.51
26	A	801	CL0	CHD-C1D	4.64	1.47	1.38
17	1	614	C7Z	C24-C25	-4.64	1.43	1.51
17	A	843	C7Z	C24-C25	-4.64	1.43	1.51
18	J	103	RRX	C12-C13	4.63	1.55	1.45
18	1	613	RRX	C27-C26	-4.62	1.43	1.51
18	2	616	RRX	C23-C22	4.61	1.55	1.45
17	1	615	C7Z	C24-C25	-4.59	1.43	1.51
17	1	612	C7Z	C8-C9	4.58	1.55	1.45
17	A	843	C7Z	C31-C30	4.57	1.57	1.43
17	3	217	C7Z	C32-C33	4.56	1.55	1.45
17	3	215	C7Z	C24-C25	-4.55	1.44	1.51
17	3	201	C7Z	C31-C30	4.54	1.57	1.43
17	2	615	C7Z	C8-C9	4.53	1.55	1.45
17	2	615	C7Z	C31-C30	4.52	1.57	1.43
17	2	615	C7Z	C24-C25	-4.52	1.44	1.51
18	2	616	RRX	C20-C21	4.52	1.57	1.43
17	J	104	C7Z	C31-C30	4.51	1.57	1.43
18	A	847	RRX	C23-C22	4.50	1.55	1.45
26	A	801	CL0	C3C-C2C	4.50	1.46	1.36
18	K	103	RRX	C20-C21	4.48	1.57	1.43
21	K	104	BCR	C16-C17	-4.48	1.29	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	215	C7Z	C31-C30	4.48	1.57	1.43
17	3	201	C7Z	C8-C9	4.46	1.55	1.45
17	1	614	C7Z	C31-C30	4.46	1.57	1.43
17	1	616	C7Z	C8-C9	4.45	1.55	1.45
18	J	103	RRX	C27-C26	-4.45	1.44	1.51
17	A	843	C7Z	C8-C9	4.45	1.55	1.45
17	1	616	C7Z	C31-C30	4.43	1.57	1.43
18	J	103	RRX	C23-C22	4.42	1.55	1.45
17	3	216	C7Z	C31-C30	4.42	1.57	1.43
21	2	617	BCR	C16-C17	-4.42	1.29	1.43
18	1	613	RRX	C20-C21	4.42	1.57	1.43
31	B	846	DGD	O1G-C1A	4.42	1.46	1.33
17	2	614	C7Z	C31-C30	4.41	1.57	1.43
17	2	614	C7Z	C8-C9	4.40	1.55	1.45
17	3	215	C7Z	C8-C9	4.40	1.55	1.45
17	3	218	C7Z	C31-C30	4.40	1.57	1.43
17	J	104	C7Z	C11-C10	4.39	1.57	1.43
17	3	218	C7Z	C8-C9	4.39	1.55	1.45
17	3	217	C7Z	C8-C9	4.38	1.55	1.45
17	1	615	C7Z	C31-C30	4.37	1.57	1.43
21	B	847	BCR	C16-C17	-4.36	1.29	1.43
17	3	216	C7Z	C4-C5	-4.36	1.44	1.51
17	1	612	C7Z	C11-C10	4.36	1.56	1.43
17	1	614	C7Z	C11-C10	4.35	1.56	1.43
18	J	103	RRX	C20-C21	4.35	1.56	1.43
17	3	215	C7Z	C4-C5	-4.34	1.44	1.51
17	2	615	C7Z	C11-C10	4.30	1.56	1.43
18	1	613	RRX	C3-C4	4.30	1.66	1.52
17	1	615	C7Z	C4-C5	-4.30	1.44	1.51
31	B	849	DGD	O1G-C1A	4.30	1.45	1.33
31	B	850	DGD	O1G-C1A	4.29	1.45	1.33
18	A	847	RRX	C3-C4	4.29	1.66	1.52
20	1	618	ERG	C16-C15	4.28	1.65	1.54
17	1	614	C7Z	C4-C5	-4.28	1.44	1.51
18	2	616	RRX	C15-C14	4.28	1.56	1.43
17	A	843	C7Z	C11-C10	4.27	1.56	1.43
18	K	103	RRX	C3-C4	4.27	1.65	1.52
17	1	615	C7Z	C8-C9	4.27	1.55	1.45
18	J	103	RRX	C15-C14	4.27	1.56	1.43
17	2	614	C7Z	C4-C5	-4.27	1.44	1.51
21	B	855	BCR	C16-C17	-4.26	1.30	1.43
17	1	614	C7Z	C8-C9	4.26	1.55	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	201	C7Z	C11-C10	4.24	1.56	1.43
16	A	855	CLA	MG-ND	-4.24	1.97	2.05
20	2	618	ERG	C1-C2	4.23	1.62	1.53
21	O	205	BCR	C16-C17	-4.22	1.30	1.43
17	1	612	C7Z	C4-C5	-4.22	1.44	1.51
17	1	616	C7Z	C11-C10	4.22	1.56	1.43
17	J	104	C7Z	C4-C5	-4.21	1.44	1.51
21	A	846	BCR	C16-C17	-4.21	1.30	1.43
17	3	201	C7Z	C4-C5	-4.21	1.44	1.51
17	3	217	C7Z	C31-C30	4.21	1.56	1.43
18	2	616	RRX	C3-C4	4.20	1.65	1.52
17	3	217	C7Z	C4-C5	-4.20	1.44	1.51
17	1	616	C7Z	C4-C5	-4.20	1.44	1.51
21	B	843	BCR	C16-C17	-4.20	1.30	1.43
17	3	218	C7Z	C4-C5	-4.19	1.44	1.51
17	3	215	C7Z	C11-C10	4.19	1.56	1.43
17	2	614	C7Z	C11-C10	4.19	1.56	1.43
18	J	103	RRX	C3-C4	4.18	1.65	1.52
26	A	801	CL0	C3D-C4D	-4.18	1.34	1.44
17	1	615	C7Z	C11-C10	4.18	1.56	1.43
16	A	830	CLA	MG-ND	-4.17	1.97	2.05
17	3	217	C7Z	C11-C10	4.16	1.56	1.43
17	3	218	C7Z	C11-C10	4.15	1.56	1.43
18	K	103	RRX	C15-C14	4.15	1.56	1.43
17	A	843	C7Z	C4-C5	-4.14	1.44	1.51
18	K	103	RRX	C27-C26	-4.14	1.44	1.51
21	A	850	BCR	C16-C17	-4.13	1.30	1.43
20	2	618	ERG	C13-C17	4.12	1.62	1.55
17	2	615	C7Z	C4-C5	-4.11	1.44	1.51
17	3	216	C7Z	C8-C9	4.09	1.54	1.45
18	A	847	RRX	C15-C14	4.09	1.56	1.43
18	A	847	RRX	C20-C21	4.09	1.56	1.43
21	L	206	BCR	C16-C17	-4.08	1.30	1.43
16	B	801	CLA	MG-ND	-4.08	1.97	2.05
20	2	621	ERG	C16-C15	4.07	1.65	1.54
20	2	621	ERG	C13-C17	4.06	1.62	1.55
16	B	803	CLA	MG-ND	-4.06	1.97	2.05
16	B	828	CLA	MG-ND	-4.05	1.97	2.05
20	2	621	ERG	C1-C2	4.05	1.62	1.53
18	A	847	RRX	C27-C26	-4.05	1.44	1.51
16	B	823	CLA	MG-ND	-4.04	1.97	2.05
20	1	618	ERG	C1-C2	4.03	1.62	1.53

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	842	BCR	C16-C17	-4.02	1.31	1.43
26	A	801	CL0	CHD-C4C	4.02	1.48	1.39
16	A	819	CLA	MG-ND	-4.02	1.97	2.05
21	A	857	BCR	C16-C17	-4.02	1.31	1.43
16	A	828	CLA	MG-ND	-4.02	1.97	2.05
16	B	826	CLA	MG-ND	-4.01	1.97	2.05
21	A	845	BCR	C16-C17	-4.01	1.31	1.43
21	A	844	BCR	C16-C17	-4.01	1.31	1.43
16	A	826	CLA	MG-ND	-4.01	1.97	2.05
16	B	804	CLA	MG-ND	-4.01	1.97	2.05
16	B	825	CLA	MG-ND	-4.01	1.97	2.05
16	1	601	CLA	MG-ND	-4.00	1.97	2.05
17	A	843	C7Z	C15-C14	4.00	1.55	1.43
16	A	831	CLA	MG-ND	-4.00	1.97	2.05
18	1	613	RRX	C15-C14	4.00	1.55	1.43
17	3	216	C7Z	C11-C10	4.00	1.55	1.43
17	1	612	C7Z	C15-C14	4.00	1.55	1.43
16	B	816	CLA	MG-ND	-3.99	1.97	2.05
16	B	830	CLA	MG-ND	-3.99	1.97	2.05
16	B	822	CLA	MG-ND	-3.99	1.97	2.05
16	B	836	CLA	MG-ND	-3.98	1.97	2.05
16	B	812	CLA	MG-ND	-3.98	1.97	2.05
21	B	845	BCR	C16-C17	-3.98	1.31	1.43
18	A	847	RRX	C11-C10	3.98	1.55	1.43
17	J	104	C7Z	C15-C14	3.98	1.55	1.43
16	F	204	CLA	MG-ND	-3.98	1.97	2.05
16	B	821	CLA	MG-ND	-3.97	1.97	2.05
16	2	608	CLA	MG-ND	-3.97	1.97	2.05
16	A	822	CLA	MG-ND	-3.97	1.97	2.05
16	1	607	CLA	MG-ND	-3.97	1.97	2.05
16	A	827	CLA	MG-ND	-3.97	1.97	2.05
16	A	829	CLA	MG-ND	-3.96	1.97	2.05
20	2	618	ERG	C16-C15	3.96	1.64	1.54
16	A	839	CLA	MG-ND	-3.96	1.97	2.05
16	3	209	CLA	MG-ND	-3.95	1.97	2.05
16	A	825	CLA	MG-ND	-3.95	1.98	2.05
16	B	815	CLA	MG-ND	-3.95	1.98	2.05
16	B	820	CLA	MG-ND	-3.95	1.98	2.05
21	I	103	BCR	C16-C17	-3.95	1.31	1.43
16	B	833	CLA	MG-ND	-3.95	1.98	2.05
21	B	841	BCR	C16-C17	-3.95	1.31	1.43
16	A	813	CLA	MG-ND	-3.94	1.98	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	616	RRX	C27-C26	-3.94	1.44	1.51
21	F	203	BCR	C16-C17	-3.94	1.31	1.43
16	B	827	CLA	MG-ND	-3.94	1.98	2.05
16	2	607	CLA	MG-ND	-3.94	1.98	2.05
16	B	808	CLA	MG-ND	-3.94	1.98	2.05
16	A	804	CLA	MG-ND	-3.93	1.98	2.05
16	A	833	CLA	MG-ND	-3.93	1.98	2.05
16	B	819	CLA	MG-ND	-3.93	1.98	2.05
16	1	605	CLA	MG-ND	-3.93	1.98	2.05
16	A	810	CLA	MG-ND	-3.93	1.98	2.05
16	A	815	CLA	MG-ND	-3.93	1.98	2.05
16	B	817	CLA	MG-ND	-3.93	1.98	2.05
16	1	609	CLA	MG-ND	-3.92	1.98	2.05
16	A	835	CLA	MG-ND	-3.92	1.98	2.05
16	2	602	CLA	C3C-C4C	3.92	1.46	1.40
16	A	824	CLA	MG-ND	-3.92	1.98	2.05
16	A	820	CLA	MG-ND	-3.92	1.98	2.05
21	B	840	BCR	C16-C17	-3.91	1.31	1.43
16	2	601	CLA	MG-ND	-3.91	1.98	2.05
16	2	611	CLA	MG-ND	-3.91	1.98	2.05
16	3	203	CLA	MG-ND	-3.91	1.98	2.05
16	A	808	CLA	MG-ND	-3.91	1.98	2.05
16	3	205	CLA	MG-ND	-3.91	1.98	2.05
16	3	204	CLA	MG-ND	-3.91	1.98	2.05
16	3	214	CLA	MG-ND	-3.91	1.98	2.05
16	L	201	CLA	MG-ND	-3.91	1.98	2.05
16	A	821	CLA	MG-ND	-3.91	1.98	2.05
16	A	837	CLA	MG-ND	-3.91	1.98	2.05
16	2	606	CLA	MG-ND	-3.91	1.98	2.05
16	A	811	CLA	MG-ND	-3.90	1.98	2.05
16	B	829	CLA	MG-ND	-3.90	1.98	2.05
16	1	602	CLA	MG-ND	-3.90	1.98	2.05
16	2	603	CLA	MG-ND	-3.90	1.98	2.05
16	A	803	CLA	MG-ND	-3.90	1.98	2.05
16	A	802	CLA	MG-ND	-3.90	1.98	2.05
16	1	611	CLA	MG-ND	-3.90	1.98	2.05
16	A	834	CLA	MG-ND	-3.90	1.98	2.05
16	B	802	CLA	MG-ND	-3.90	1.98	2.05
16	B	813	CLA	MG-ND	-3.90	1.98	2.05
17	1	616	C7Z	C15-C14	3.89	1.55	1.43
21	L	202	BCR	C16-C17	-3.89	1.31	1.43
16	3	211	CLA	MG-ND	-3.89	1.98	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	3	210	CLA	MG-ND	-3.89	1.98	2.05
16	I	102	CLA	MG-ND	-3.89	1.98	2.05
16	K	101	CLA	MG-ND	-3.89	1.98	2.05
16	B	811	CLA	MG-ND	-3.89	1.98	2.05
16	A	812	CLA	MG-ND	-3.89	1.98	2.05
17	3	217	C7Z	C22-C21	3.88	1.67	1.54
16	A	814	CLA	MG-ND	-3.88	1.98	2.05
16	2	612	CLA	MG-ND	-3.88	1.98	2.05
16	A	856	CLA	MG-ND	-3.88	1.98	2.05
16	B	824	CLA	MG-ND	-3.88	1.98	2.05
16	A	805	CLA	MG-ND	-3.87	1.98	2.05
16	O	203	CLA	MG-ND	-3.87	1.98	2.05
16	1	603	CLA	MG-ND	-3.87	1.98	2.05
16	L	204	CLA	MG-ND	-3.87	1.98	2.05
16	B	835	CLA	MG-ND	-3.87	1.98	2.05
16	A	854	CLA	MG-ND	-3.87	1.98	2.05
16	L	203	CLA	MG-ND	-3.87	1.98	2.05
16	K	102	CLA	MG-ND	-3.87	1.98	2.05
16	2	613	CLA	MG-ND	-3.86	1.98	2.05
16	L	205	CLA	MG-ND	-3.86	1.98	2.05
16	B	810	CLA	MG-ND	-3.86	1.98	2.05
17	3	218	C7Z	C22-C21	3.86	1.66	1.54
16	B	809	CLA	MG-ND	-3.86	1.98	2.05
16	F	205	CLA	MG-ND	-3.86	1.98	2.05
20	1	618	ERG	C12-C11	-3.86	1.45	1.53
16	3	208	CLA	MG-ND	-3.86	1.98	2.05
16	B	814	CLA	MG-ND	-3.86	1.98	2.05
16	3	212	CLA	MG-ND	-3.86	1.98	2.05
16	B	838	CLA	MG-ND	-3.86	1.98	2.05
16	B	806	CLA	MG-ND	-3.85	1.98	2.05
16	B	832	CLA	MG-ND	-3.85	1.98	2.05
17	3	215	C7Z	C15-C14	3.85	1.55	1.43
16	B	834	CLA	MG-ND	-3.85	1.98	2.05
16	F	202	CLA	MG-ND	-3.84	1.98	2.05
16	3	206	CLA	MG-ND	-3.84	1.98	2.05
16	A	806	CLA	MG-ND	-3.84	1.98	2.05
18	1	613	RRX	C11-C10	3.84	1.55	1.43
16	B	807	CLA	MG-ND	-3.84	1.98	2.05
16	B	805	CLA	MG-ND	-3.84	1.98	2.05
17	2	614	C7Z	C22-C21	3.84	1.66	1.54
16	F	201	CLA	MG-ND	-3.84	1.98	2.05
16	1	608	CLA	MG-ND	-3.83	1.98	2.05

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	614	C7Z	C15-C14	3.83	1.55	1.43
16	1	604	CLA	MG-ND	-3.83	1.98	2.05
16	B	831	CLA	MG-ND	-3.83	1.98	2.05
16	J	102	CLA	MG-ND	-3.83	1.98	2.05
16	2	605	CLA	MG-ND	-3.83	1.98	2.05
17	1	612	C7Z	C22-C21	3.83	1.66	1.54
16	1	606	CLA	MG-ND	-3.82	1.98	2.05
16	2	609	CLA	MG-ND	-3.82	1.98	2.05
17	2	614	C7Z	C15-C14	3.82	1.55	1.43
17	A	843	C7Z	C22-C21	3.82	1.66	1.54
16	A	832	CLA	MG-ND	-3.82	1.98	2.05
16	3	213	CLA	MG-ND	-3.82	1.98	2.05
17	A	843	C7Z	C35-C34	3.82	1.55	1.43
16	A	823	CLA	MG-ND	-3.82	1.98	2.05
16	A	816	CLA	MG-ND	-3.81	1.98	2.05
17	J	104	C7Z	C35-C34	3.81	1.55	1.43
17	3	201	C7Z	C22-C21	3.81	1.66	1.54
17	2	615	C7Z	C35-C34	3.81	1.55	1.43
16	O	204	CLA	MG-ND	-3.81	1.98	2.05
17	3	216	C7Z	C15-C14	3.81	1.55	1.43
16	A	817	CLA	MG-ND	-3.80	1.98	2.05
16	A	809	CLA	MG-ND	-3.80	1.98	2.05
17	1	616	C7Z	C22-C21	3.80	1.66	1.54
16	A	838	CLA	MG-ND	-3.80	1.98	2.05
16	B	837	CLA	MG-ND	-3.80	1.98	2.05
16	1	610	CLA	MG-ND	-3.80	1.98	2.05
16	2	602	CLA	MG-ND	-3.80	1.98	2.05
17	1	615	C7Z	C15-C14	3.80	1.55	1.43
17	1	614	C7Z	C22-C21	3.79	1.66	1.54
16	A	807	CLA	MG-ND	-3.79	1.98	2.05
16	2	610	CLA	MG-ND	-3.79	1.98	2.05
16	O	201	CLA	MG-ND	-3.79	1.98	2.05
16	A	836	CLA	MG-ND	-3.79	1.98	2.05
21	B	844	BCR	C16-C17	-3.79	1.31	1.43
16	3	207	CLA	MG-ND	-3.78	1.98	2.05
16	B	818	CLA	MG-ND	-3.78	1.98	2.05
16	2	604	CLA	MG-ND	-3.78	1.98	2.05
17	2	615	C7Z	C15-C14	3.78	1.55	1.43
16	A	818	CLA	MG-ND	-3.77	1.98	2.05
17	3	201	C7Z	C15-C14	3.77	1.55	1.43
17	J	104	C7Z	C22-C21	3.77	1.66	1.54
17	3	216	C7Z	C22-C21	3.77	1.66	1.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	615	C7Z	C22-C21	3.76	1.66	1.54
18	2	616	RRX	C24-C25	3.76	1.58	1.45
17	3	217	C7Z	C15-C14	3.76	1.55	1.43
17	3	218	C7Z	C15-C14	3.75	1.55	1.43
16	I	101	CLA	MG-ND	-3.75	1.98	2.05
17	1	615	C7Z	C35-C34	3.75	1.55	1.43
21	F	206	BCR	C16-C17	-3.73	1.31	1.43
17	3	215	C7Z	C22-C21	3.72	1.66	1.54
21	L	207	BCR	C16-C17	-3.72	1.31	1.43
17	3	201	C7Z	C35-C34	3.72	1.55	1.43
17	3	216	C7Z	C27-C26	3.72	1.58	1.45
17	1	612	C7Z	C27-C26	3.71	1.58	1.45
17	2	615	C7Z	C27-C26	3.71	1.58	1.45
18	1	613	RRX	C29-C30	3.70	1.66	1.54
16	O	202	CLA	MG-ND	-3.70	1.98	2.05
17	3	201	C7Z	C27-C26	3.70	1.58	1.45
17	A	843	C7Z	C27-C26	3.68	1.58	1.45
18	2	616	RRX	C11-C10	3.68	1.54	1.43
17	2	615	C7Z	C22-C21	3.68	1.66	1.54
17	1	614	C7Z	C35-C34	3.67	1.54	1.43
17	3	218	C7Z	C27-C26	3.67	1.58	1.45
18	K	103	RRX	C11-C10	3.67	1.54	1.43
17	3	215	C7Z	C27-C26	3.66	1.58	1.45
18	K	103	RRX	C16-C17	3.66	1.54	1.43
17	J	104	C7Z	C27-C26	3.65	1.58	1.45
26	A	801	CL0	OBD-CAD	3.65	1.28	1.22
17	1	614	C7Z	C27-C26	3.64	1.58	1.45
17	1	616	C7Z	C27-C26	3.64	1.58	1.45
17	2	614	C7Z	C35-C34	3.64	1.54	1.43
17	3	215	C7Z	C35-C34	3.64	1.54	1.43
17	1	612	C7Z	C35-C34	3.63	1.54	1.43
17	2	614	C7Z	C27-C26	3.63	1.58	1.45
17	3	218	C7Z	C35-C34	3.60	1.54	1.43
17	3	215	C7Z	C2-C1	3.59	1.66	1.54
18	J	103	RRX	C16-C17	3.59	1.54	1.43
17	3	216	C7Z	C35-C34	3.59	1.54	1.43
17	1	615	C7Z	C27-C26	3.58	1.57	1.45
16	A	826	CLA	C1C-NC	-3.57	1.32	1.37
17	3	217	C7Z	C35-C34	3.57	1.54	1.43
17	3	218	C7Z	C2-C1	3.56	1.66	1.54
18	1	613	RRX	C16-C17	3.56	1.54	1.43
17	2	614	C7Z	C2-C1	3.54	1.65	1.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	J	103	RRX	C29-C30	3.54	1.65	1.54
17	1	616	C7Z	C35-C34	3.54	1.54	1.43
17	1	612	C7Z	C2-C1	3.54	1.65	1.54
17	1	615	C7Z	C2-C1	3.53	1.65	1.54
18	K	103	RRX	C24-C25	3.53	1.57	1.45
17	3	216	C7Z	C2-C1	3.52	1.65	1.54
18	J	103	RRX	C11-C10	3.52	1.54	1.43
17	J	104	C7Z	C2-C1	3.52	1.65	1.54
18	K	103	RRX	C29-C30	3.51	1.65	1.54
17	3	217	C7Z	C2-C1	3.51	1.65	1.54
17	2	615	C7Z	C2-C1	3.50	1.65	1.54
17	A	843	C7Z	C2-C1	3.50	1.65	1.54
16	A	812	CLA	C1C-NC	-3.50	1.32	1.37
16	B	802	CLA	C1C-NC	-3.49	1.32	1.37
17	1	616	C7Z	C2-C1	3.49	1.65	1.54
17	3	217	C7Z	C27-C26	3.49	1.57	1.45
17	3	201	C7Z	C2-C1	3.48	1.65	1.54
16	A	829	CLA	C1C-NC	-3.47	1.32	1.37
18	J	103	RRX	C24-C25	3.47	1.57	1.45
18	1	613	RRX	C24-C25	3.47	1.57	1.45
17	2	615	C7Z	C7-C6	3.47	1.57	1.45
26	A	801	CL0	C1D-ND	-3.47	1.33	1.37
17	1	612	C7Z	C7-C6	3.46	1.57	1.45
18	A	847	RRX	C24-C25	3.46	1.57	1.45
23	2	620	DGA	OG1-CA1	3.45	1.43	1.33
17	1	615	C7Z	C38-C25	3.45	1.56	1.50
16	B	825	CLA	C1C-NC	-3.45	1.32	1.37
16	B	828	CLA	C1C-NC	-3.44	1.32	1.37
17	3	217	C7Z	C38-C25	3.44	1.56	1.50
23	J	101	DGA	OG2-CB1	3.43	1.44	1.34
17	1	614	C7Z	C2-C1	3.43	1.65	1.54
23	2	620	DGA	OG2-CB1	3.43	1.44	1.34
17	A	843	C7Z	C7-C6	3.41	1.57	1.45
16	1	602	CLA	C1C-NC	-3.41	1.32	1.37
16	A	816	CLA	C1C-NC	-3.41	1.32	1.37
18	2	616	RRX	C16-C17	3.40	1.54	1.43
17	2	614	C7Z	C38-C25	3.40	1.56	1.50
17	3	201	C7Z	C38-C25	3.40	1.56	1.50
17	3	218	C7Z	C38-C25	3.39	1.56	1.50
17	1	616	C7Z	C7-C6	3.39	1.57	1.45
16	3	210	CLA	C1C-NC	-3.39	1.32	1.37
18	A	847	RRX	C16-C17	3.39	1.54	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	823	CLA	C1C-NC	-3.39	1.32	1.37
17	1	616	C7Z	C38-C25	3.39	1.56	1.50
16	B	802	CLA	CBB-CAB	3.39	1.51	1.29
17	1	614	C7Z	C38-C25	3.38	1.56	1.50
17	A	843	C7Z	C38-C25	3.38	1.56	1.50
16	B	831	CLA	C1C-NC	-3.38	1.32	1.37
17	3	201	C7Z	C7-C6	3.38	1.57	1.45
17	1	612	C7Z	C38-C25	3.38	1.56	1.50
16	2	608	CLA	C1C-NC	-3.38	1.32	1.37
16	2	602	CLA	C1C-C2C	3.37	1.48	1.42
17	J	104	C7Z	C38-C25	3.37	1.56	1.50
17	3	215	C7Z	C7-C6	3.37	1.57	1.45
17	2	614	C7Z	C7-C6	3.37	1.57	1.45
16	A	813	CLA	CBB-CAB	3.37	1.51	1.29
16	A	802	CLA	C1C-NC	-3.36	1.32	1.37
16	3	207	CLA	CBB-CAB	3.36	1.51	1.29
17	2	615	C7Z	C38-C25	3.36	1.56	1.50
16	B	809	CLA	CBB-CAB	3.36	1.51	1.29
17	3	218	C7Z	C7-C6	3.36	1.57	1.45
16	3	212	CLA	CBB-CAB	3.36	1.51	1.29
16	A	818	CLA	C1C-NC	-3.36	1.32	1.37
16	A	819	CLA	C1C-NC	-3.36	1.32	1.37
16	3	208	CLA	CBB-CAB	3.36	1.51	1.29
16	O	204	CLA	CBB-CAB	3.36	1.51	1.29
16	I	102	CLA	CBB-CAB	3.36	1.51	1.29
16	B	834	CLA	CBB-CAB	3.36	1.51	1.29
16	A	854	CLA	CBB-CAB	3.36	1.51	1.29
16	1	601	CLA	C1C-NC	-3.35	1.32	1.37
16	B	812	CLA	C1C-NC	-3.35	1.32	1.37
16	B	837	CLA	CBB-CAB	3.35	1.51	1.29
16	A	804	CLA	CBB-CAB	3.35	1.51	1.29
16	A	814	CLA	CBB-CAB	3.35	1.51	1.29
16	B	823	CLA	CBB-CAB	3.35	1.51	1.29
16	A	829	CLA	CBB-CAB	3.35	1.51	1.29
16	B	806	CLA	CBB-CAB	3.35	1.51	1.29
16	I	101	CLA	CBB-CAB	3.35	1.51	1.29
16	3	203	CLA	CBB-CAB	3.35	1.51	1.29
16	B	828	CLA	CBB-CAB	3.35	1.51	1.29
16	2	605	CLA	CBB-CAB	3.35	1.51	1.29
16	F	204	CLA	CBB-CAB	3.35	1.51	1.29
16	L	203	CLA	CBB-CAB	3.35	1.51	1.29
16	O	202	CLA	CBB-CAB	3.35	1.51	1.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	804	CLA	C1C-NC	-3.35	1.32	1.37
16	A	822	CLA	CBB-CAB	3.35	1.51	1.29
16	B	812	CLA	CBB-CAB	3.35	1.51	1.29
16	2	609	CLA	CBB-CAB	3.35	1.51	1.29
16	A	827	CLA	CBB-CAB	3.35	1.51	1.29
16	2	612	CLA	CBB-CAB	3.35	1.51	1.29
16	A	815	CLA	CBB-CAB	3.35	1.51	1.29
16	B	822	CLA	CBB-CAB	3.35	1.51	1.29
16	B	824	CLA	CBB-CAB	3.35	1.51	1.29
16	2	613	CLA	CBB-CAB	3.35	1.51	1.29
16	3	206	CLA	CBB-CAB	3.35	1.51	1.29
17	3	217	C7Z	C7-C6	3.34	1.57	1.45
16	L	201	CLA	CBB-CAB	3.34	1.51	1.29
16	2	601	CLA	CBB-CAB	3.34	1.51	1.29
16	1	606	CLA	CBB-CAB	3.34	1.51	1.29
16	3	213	CLA	CBB-CAB	3.34	1.51	1.29
16	A	807	CLA	CBB-CAB	3.34	1.51	1.29
16	B	838	CLA	CBB-CAB	3.34	1.51	1.29
16	3	211	CLA	CBB-CAB	3.34	1.51	1.29
16	B	803	CLA	CBB-CAB	3.34	1.51	1.29
16	A	810	CLA	CBB-CAB	3.34	1.51	1.29
16	B	805	CLA	CBB-CAB	3.34	1.51	1.29
16	1	611	CLA	CBB-CAB	3.34	1.51	1.29
16	A	821	CLA	CBB-CAB	3.34	1.51	1.29
16	K	101	CLA	CBB-CAB	3.34	1.51	1.29
16	1	608	CLA	CBB-CAB	3.34	1.51	1.29
16	B	818	CLA	CBB-CAB	3.34	1.51	1.29
16	A	836	CLA	CBB-CAB	3.34	1.51	1.29
16	2	608	CLA	CBB-CAB	3.34	1.51	1.29
16	I	101	CLA	C1C-NC	-3.34	1.32	1.37
16	A	856	CLA	CBB-CAB	3.34	1.51	1.29
16	B	830	CLA	CBB-CAB	3.33	1.51	1.29
16	2	607	CLA	CBB-CAB	3.33	1.51	1.29
16	A	805	CLA	CBB-CAB	3.33	1.51	1.29
16	J	102	CLA	CBB-CAB	3.33	1.51	1.29
16	3	209	CLA	CBB-CAB	3.33	1.51	1.29
16	A	806	CLA	CBB-CAB	3.33	1.51	1.29
16	B	826	CLA	CBB-CAB	3.33	1.51	1.29
16	1	605	CLA	CBB-CAB	3.33	1.51	1.29
16	B	815	CLA	CBB-CAB	3.33	1.51	1.29
17	3	215	C7Z	C38-C25	3.33	1.56	1.50
16	A	838	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)
16	B	819	CLA	CBB-CAB	3.33	1.51	1.29
16	2	603	CLA	CBB-CAB	3.33	1.51	1.29
16	1	609	CLA	CBB-CAB	3.33	1.51	1.29
16	3	205	CLA	C1C-NC	-3.33	1.32	1.37
16	A	811	CLA	C1C-NC	-3.33	1.32	1.37
16	3	204	CLA	CBB-CAB	3.33	1.51	1.29
16	2	611	CLA	CBB-CAB	3.33	1.51	1.29
16	B	820	CLA	CBB-CAB	3.33	1.51	1.29
16	A	832	CLA	CBB-CAB	3.33	1.51	1.29
16	1	604	CLA	CBB-CAB	3.33	1.51	1.29
16	2	604	CLA	CBB-CAB	3.33	1.51	1.29
16	2	610	CLA	CBB-CAB	3.33	1.51	1.29
16	A	828	CLA	CBB-CAB	3.33	1.51	1.29
16	A	830	CLA	C1C-NC	-3.33	1.32	1.37
16	3	205	CLA	CBB-CAB	3.33	1.51	1.29
16	A	830	CLA	CBB-CAB	3.33	1.51	1.29
16	B	807	CLA	CBB-CAB	3.33	1.51	1.29
16	1	607	CLA	CBB-CAB	3.33	1.51	1.29
16	3	214	CLA	CBB-CAB	3.33	1.51	1.29
16	B	801	CLA	CBB-CAB	3.33	1.51	1.29
16	B	808	CLA	C1C-NC	-3.33	1.32	1.37
16	B	811	CLA	CBB-CAB	3.33	1.51	1.29
16	A	831	CLA	CBB-CAB	3.33	1.51	1.29
16	2	606	CLA	CBB-CAB	3.33	1.51	1.29
16	B	817	CLA	CBB-CAB	3.33	1.51	1.29
16	B	810	CLA	CBB-CAB	3.33	1.51	1.29
16	A	803	CLA	CBB-CAB	3.33	1.51	1.29
16	B	836	CLA	CBB-CAB	3.33	1.51	1.29
16	B	829	CLA	CBB-CAB	3.33	1.51	1.29
16	L	204	CLA	CBB-CAB	3.33	1.51	1.29
16	A	820	CLA	CBB-CAB	3.32	1.51	1.29
16	1	602	CLA	CBB-CAB	3.32	1.51	1.29
16	F	205	CLA	CBB-CAB	3.32	1.51	1.29
16	1	610	CLA	CBB-CAB	3.32	1.51	1.29
16	A	802	CLA	CBB-CAB	3.32	1.51	1.29
16	O	201	CLA	CBB-CAB	3.32	1.51	1.29
16	B	833	CLA	CBB-CAB	3.32	1.51	1.29
16	O	203	CLA	CBB-CAB	3.32	1.51	1.29
16	1	601	CLA	CBB-CAB	3.32	1.51	1.29
16	A	834	CLA	CBB-CAB	3.32	1.51	1.29
16	B	835	CLA	CBB-CAB	3.32	1.51	1.29
16	F	205	CLA	C1C-NC	-3.32	1.32	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	811	CLA	CBB-CAB	3.32	1.51	1.29
16	B	814	CLA	CBB-CAB	3.32	1.51	1.29
16	1	603	CLA	CBB-CAB	3.32	1.51	1.29
16	2	602	CLA	CBB-CAB	3.32	1.51	1.29
16	A	855	CLA	CBB-CAB	3.32	1.51	1.29
16	A	809	CLA	CBB-CAB	3.32	1.51	1.29
16	A	839	CLA	CBB-CAB	3.32	1.51	1.29
16	B	833	CLA	C1C-NC	-3.31	1.32	1.37
16	A	812	CLA	CBB-CAB	3.31	1.51	1.29
16	A	825	CLA	CBB-CAB	3.31	1.51	1.29
16	A	818	CLA	CBB-CAB	3.31	1.51	1.29
16	B	832	CLA	CBB-CAB	3.31	1.51	1.29
16	A	833	CLA	CBB-CAB	3.31	1.51	1.29
17	J	104	C7Z	C7-C6	3.31	1.56	1.45
16	A	824	CLA	CBB-CAB	3.31	1.51	1.29
16	A	826	CLA	CBB-CAB	3.31	1.51	1.29
16	B	811	CLA	C1C-NC	-3.31	1.32	1.37
16	A	819	CLA	CBB-CAB	3.31	1.51	1.29
16	B	813	CLA	CBB-CAB	3.31	1.51	1.29
16	L	205	CLA	CBB-CAB	3.31	1.51	1.29
16	A	808	CLA	CBB-CAB	3.31	1.51	1.29
16	B	808	CLA	CBB-CAB	3.30	1.51	1.29
16	A	823	CLA	CBB-CAB	3.30	1.51	1.29
16	B	804	CLA	CBB-CAB	3.30	1.51	1.29
16	K	102	CLA	CBB-CAB	3.30	1.51	1.29
16	A	816	CLA	CBB-CAB	3.30	1.51	1.29
16	A	837	CLA	CBB-CAB	3.30	1.51	1.29
16	B	831	CLA	CBB-CAB	3.30	1.51	1.29
23	J	101	DGA	OG1-CA1	3.30	1.43	1.33
16	B	827	CLA	CBB-CAB	3.30	1.51	1.29
16	F	201	CLA	CBB-CAB	3.30	1.51	1.29
18	2	616	RRX	C29-C30	3.29	1.65	1.54
16	F	202	CLA	CBB-CAB	3.29	1.51	1.29
16	B	816	CLA	CBB-CAB	3.29	1.51	1.29
16	A	814	CLA	C1C-NC	-3.29	1.32	1.37
17	3	216	C7Z	C38-C25	3.29	1.56	1.50
16	B	821	CLA	CBB-CAB	3.28	1.51	1.29
16	3	210	CLA	CBB-CAB	3.28	1.51	1.29
16	B	825	CLA	CBB-CAB	3.28	1.51	1.29
16	A	810	CLA	C1C-NC	-3.28	1.32	1.37
16	3	204	CLA	C1C-NC	-3.28	1.32	1.37
16	B	827	CLA	C1C-NC	-3.28	1.32	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	835	CLA	CBB-CAB	3.28	1.51	1.29
16	A	806	CLA	C1C-NC	-3.28	1.32	1.37
16	A	820	CLA	C1C-NC	-3.28	1.32	1.37
16	B	819	CLA	C1C-NC	-3.28	1.32	1.37
17	1	615	C7Z	C7-C6	3.27	1.56	1.45
16	A	835	CLA	C1C-NC	-3.27	1.32	1.37
18	A	847	RRX	C29-C30	3.27	1.65	1.54
16	L	201	CLA	C1C-NC	-3.27	1.32	1.37
17	1	614	C7Z	C7-C6	3.27	1.56	1.45
16	A	803	CLA	C1C-NC	-3.26	1.32	1.37
16	3	209	CLA	C1C-NC	-3.26	1.32	1.37
16	B	830	CLA	C1C-NC	-3.26	1.32	1.37
16	3	214	CLA	C1C-NC	-3.26	1.32	1.37
16	I	102	CLA	C1C-NC	-3.25	1.32	1.37
16	B	826	CLA	C1C-NC	-3.25	1.32	1.37
16	2	607	CLA	C1C-NC	-3.25	1.32	1.37
26	A	801	CL0	MG-NC	3.25	2.14	2.06
16	B	824	CLA	C1C-NC	-3.24	1.33	1.37
16	K	102	CLA	C1C-NC	-3.24	1.33	1.37
31	B	846	DGD	CAB-C9B	-3.24	1.33	1.51
16	B	816	CLA	C1C-NC	-3.24	1.33	1.37
31	B	849	DGD	CAA-C9A	-3.24	1.33	1.51
16	2	612	CLA	C1C-NC	-3.24	1.33	1.37
31	B	849	DGD	CAB-C9B	-3.24	1.33	1.51
16	B	814	CLA	C1C-NC	-3.24	1.33	1.37
16	A	805	CLA	C1C-NC	-3.24	1.33	1.37
16	A	821	CLA	C1C-NC	-3.24	1.33	1.37
16	2	611	CLA	C1C-NC	-3.23	1.33	1.37
31	B	850	DGD	CGB-CFB	-3.23	1.33	1.51
31	B	849	DGD	CDA-CCA	-3.23	1.33	1.51
16	3	208	CLA	C1C-NC	-3.23	1.33	1.37
16	1	605	CLA	C1C-NC	-3.23	1.33	1.37
18	1	613	RRX	C7-C6	3.23	1.56	1.45
31	B	849	DGD	CDB-CCB	-3.23	1.33	1.51
16	A	817	CLA	CBB-CAB	3.23	1.50	1.29
16	A	832	CLA	C1C-NC	-3.23	1.33	1.37
31	B	846	DGD	CGB-CFB	-3.23	1.33	1.51
31	B	850	DGD	CAB-C9B	-3.22	1.33	1.51
31	B	849	DGD	CGB-CFB	-3.22	1.33	1.51
31	B	849	DGD	CGA-CFA	-3.22	1.33	1.51
16	F	204	CLA	C1C-NC	-3.22	1.33	1.37
16	A	828	CLA	C1C-NC	-3.22	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	836	CLA	C1C-NC	-3.22	1.33	1.37
16	F	202	CLA	C1C-NC	-3.21	1.33	1.37
16	2	606	CLA	C1C-NC	-3.21	1.33	1.37
16	L	204	CLA	C1C-NC	-3.21	1.33	1.37
16	1	603	CLA	C1C-NC	-3.21	1.33	1.37
16	2	602	CLA	C1C-NC	-3.21	1.33	1.37
16	A	822	CLA	C1C-NC	-3.21	1.33	1.37
16	3	213	CLA	C1C-NC	-3.21	1.33	1.37
16	B	809	CLA	C1C-NC	-3.21	1.33	1.37
16	B	817	CLA	C1C-NC	-3.20	1.33	1.37
16	B	818	CLA	C1C-NC	-3.20	1.33	1.37
31	B	850	DGD	CAA-C9A	-3.20	1.33	1.51
17	3	216	C7Z	C7-C6	3.20	1.56	1.45
16	1	610	CLA	C1C-NC	-3.20	1.33	1.37
16	A	839	CLA	C1C-NC	-3.20	1.33	1.37
16	B	810	CLA	C1C-NC	-3.20	1.33	1.37
16	L	203	CLA	C1C-NC	-3.19	1.33	1.37
16	B	807	CLA	C1C-NC	-3.19	1.33	1.37
16	O	202	CLA	C1C-NC	-3.19	1.33	1.37
31	B	846	DGD	CAA-C9A	-3.19	1.33	1.51
16	1	609	CLA	C1C-NC	-3.19	1.33	1.37
16	3	207	CLA	C1C-NC	-3.19	1.33	1.37
16	A	831	CLA	C1C-NC	-3.19	1.33	1.37
31	B	850	DGD	CDB-CCB	-3.18	1.33	1.51
16	A	807	CLA	C1C-NC	-3.18	1.33	1.37
16	B	821	CLA	C1C-NC	-3.18	1.33	1.37
18	J	103	RRX	C4-C5	-3.18	1.44	1.51
31	B	846	DGD	CDB-CCB	-3.18	1.33	1.51
16	3	206	CLA	C1C-NC	-3.18	1.33	1.37
16	A	838	CLA	C1C-NC	-3.18	1.33	1.37
16	B	822	CLA	C1C-NC	-3.18	1.33	1.37
31	B	850	DGD	CGA-CFA	-3.17	1.33	1.51
16	A	808	CLA	C1C-NC	-3.17	1.33	1.37
22	B	848	PGT	P-O3P	3.17	1.72	1.59
16	F	201	CLA	C1C-NC	-3.17	1.33	1.37
16	2	605	CLA	C1C-NC	-3.17	1.33	1.37
16	1	604	CLA	C1C-NC	-3.17	1.33	1.37
16	B	815	CLA	C1C-NC	-3.17	1.33	1.37
16	B	805	CLA	C1C-NC	-3.16	1.33	1.37
16	B	820	CLA	C1C-NC	-3.16	1.33	1.37
16	B	801	CLA	C1C-NC	-3.15	1.33	1.37
22	2	619	PGT	C3-C2	3.15	1.60	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	3	203	CLA	C1C-NC	-3.15	1.33	1.37
22	2	619	PGT	P-O3P	3.15	1.72	1.59
31	B	850	DGD	CDA-CCA	-3.15	1.33	1.51
31	B	846	DGD	CGA-CFA	-3.15	1.33	1.51
16	2	604	CLA	C1C-NC	-3.15	1.33	1.37
16	B	837	CLA	C1C-NC	-3.15	1.33	1.37
16	B	829	CLA	C1C-NC	-3.15	1.33	1.37
16	B	823	CLA	C1C-NC	-3.14	1.33	1.37
16	A	824	CLA	C1C-NC	-3.14	1.33	1.37
16	2	603	CLA	C1C-NC	-3.14	1.33	1.37
16	L	205	CLA	C1C-NC	-3.13	1.33	1.37
16	K	101	CLA	C1C-NC	-3.13	1.33	1.37
16	O	203	CLA	C1C-NC	-3.13	1.33	1.37
16	2	613	CLA	C1C-NC	-3.13	1.33	1.37
16	B	832	CLA	C1C-NC	-3.13	1.33	1.37
16	2	601	CLA	C1C-NC	-3.13	1.33	1.37
16	1	607	CLA	C1C-NC	-3.13	1.33	1.37
16	2	609	CLA	C1C-NC	-3.12	1.33	1.37
31	B	846	DGD	CDA-CCA	-3.12	1.34	1.51
16	B	838	CLA	C1C-NC	-3.12	1.33	1.37
16	1	611	CLA	C1C-NC	-3.12	1.33	1.37
18	2	616	RRX	C4-C5	-3.12	1.44	1.51
18	K	103	RRX	C21-C22	3.12	1.39	1.35
16	2	610	CLA	C1C-NC	-3.12	1.33	1.37
16	B	835	CLA	C1C-NC	-3.12	1.33	1.37
17	2	615	C7Z	C21-C26	-3.12	1.49	1.53
16	B	813	CLA	C1C-NC	-3.12	1.33	1.37
16	A	809	CLA	C1C-NC	-3.11	1.33	1.37
16	3	212	CLA	C1C-NC	-3.11	1.33	1.37
16	A	813	CLA	C1C-NC	-3.11	1.33	1.37
16	1	606	CLA	C1C-NC	-3.11	1.33	1.37
16	J	102	CLA	C1C-NC	-3.10	1.33	1.37
16	A	815	CLA	C1C-NC	-3.10	1.33	1.37
16	A	825	CLA	C1C-NC	-3.10	1.33	1.37
16	A	836	CLA	C1C-NC	-3.10	1.33	1.37
18	A	847	RRX	C4-C5	-3.09	1.44	1.51
18	K	103	RRX	C7-C6	3.09	1.56	1.45
16	1	608	CLA	C1C-NC	-3.08	1.33	1.37
16	A	804	CLA	C1C-NC	-3.08	1.33	1.37
16	O	204	CLA	C1C-NC	-3.08	1.33	1.37
16	A	856	CLA	C1C-NC	-3.07	1.33	1.37
18	J	103	RRX	C7-C6	3.06	1.56	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	616	RRX	C7-C6	3.06	1.56	1.45
16	A	817	CLA	C1C-NC	-3.06	1.33	1.37
16	A	833	CLA	C1C-NC	-3.06	1.33	1.37
16	A	834	CLA	C1C-NC	-3.05	1.33	1.37
16	A	854	CLA	CHC-C1C	3.05	1.42	1.35
17	J	104	C7Z	C21-C26	-3.04	1.49	1.53
16	B	803	CLA	C1C-NC	-3.04	1.33	1.37
16	3	211	CLA	C1C-NC	-3.04	1.33	1.37
17	3	218	C7Z	C21-C26	-3.04	1.49	1.53
18	K	103	RRX	C4-C5	-3.03	1.45	1.51
16	B	806	CLA	C1C-NC	-3.03	1.33	1.37
16	O	201	CLA	C1C-NC	-3.02	1.33	1.37
16	A	837	CLA	C1C-NC	-3.02	1.33	1.37
16	A	817	CLA	CHC-C1C	3.01	1.42	1.35
16	A	854	CLA	C1C-NC	-3.01	1.33	1.37
22	B	848	PGT	C1-C2	3.00	1.59	1.50
16	B	835	CLA	CHC-C1C	2.98	1.42	1.35
22	B	848	PGT	C3-C2	2.98	1.59	1.50
22	B	848	PGT	P-O4P	2.98	1.71	1.59
16	B	834	CLA	C1C-NC	-2.98	1.33	1.37
26	A	801	CL0	C3D-C2D	2.98	1.47	1.39
17	1	616	C7Z	C21-C26	-2.97	1.49	1.53
16	A	833	CLA	CHC-C1C	2.97	1.42	1.35
16	B	834	CLA	CHC-C1C	2.97	1.42	1.35
16	A	827	CLA	C1C-NC	-2.96	1.33	1.37
20	1	618	ERG	C11-C9	2.94	1.59	1.53
16	A	855	CLA	C1C-NC	-2.93	1.33	1.37
22	2	619	PGT	C1-C2	2.93	1.59	1.50
22	2	619	PGT	P-O4P	2.93	1.71	1.59
16	A	809	CLA	CHC-C1C	2.90	1.42	1.35
16	B	801	CLA	CHC-C1C	2.90	1.42	1.35
16	B	821	CLA	C3B-C2B	-2.90	1.36	1.40
18	A	847	RRX	C32-C1	2.90	1.59	1.53
16	A	827	CLA	CHC-C1C	2.89	1.42	1.35
16	F	201	CLA	CHC-C1C	2.88	1.42	1.35
16	A	807	CLA	CHC-C1C	2.88	1.42	1.35
16	O	204	CLA	CHC-C1C	2.87	1.42	1.35
17	1	615	C7Z	C21-C26	-2.87	1.49	1.53
16	A	855	CLA	C3B-C2B	-2.86	1.36	1.40
16	A	808	CLA	CHC-C1C	2.86	1.42	1.35
16	A	836	CLA	CHC-C1C	2.86	1.42	1.35
26	A	801	CL0	C4D-CHA	2.86	1.48	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	824	CLA	CHC-C1C	2.86	1.42	1.35
18	K	103	RRX	C32-C1	2.85	1.59	1.53
17	1	614	C7Z	C21-C26	-2.85	1.49	1.53
16	L	201	CLA	CHC-C1C	2.85	1.42	1.35
18	A	847	RRX	C7-C6	2.85	1.55	1.45
16	A	856	CLA	CHC-C1C	2.84	1.42	1.35
20	2	621	ERG	C9-C8	2.84	1.59	1.51
16	A	838	CLA	CHC-C1C	2.84	1.42	1.35
17	3	201	C7Z	C21-C26	-2.84	1.49	1.53
16	B	803	CLA	CHC-C1C	2.84	1.42	1.35
16	A	832	CLA	CHC-C1C	2.84	1.42	1.35
16	O	202	CLA	CHC-C1C	2.84	1.42	1.35
17	A	843	C7Z	C21-C26	-2.83	1.49	1.53
16	K	101	CLA	CHC-C1C	2.83	1.42	1.35
16	2	602	CLA	CHC-C1C	2.82	1.42	1.35
16	A	813	CLA	CHC-C1C	2.82	1.42	1.35
16	1	607	CLA	CHC-C1C	2.82	1.42	1.35
16	B	832	CLA	CHC-C1C	2.82	1.42	1.35
16	A	834	CLA	CHC-C1C	2.82	1.42	1.35
16	1	609	CLA	CHC-C1C	2.81	1.42	1.35
16	1	603	CLA	CHC-C1C	2.81	1.42	1.35
16	O	203	CLA	CHC-C1C	2.81	1.42	1.35
16	B	822	CLA	C3B-C2B	-2.81	1.36	1.40
16	1	608	CLA	CHC-C1C	2.81	1.42	1.35
16	B	815	CLA	CHC-C1C	2.81	1.42	1.35
18	2	616	RRX	C32-C1	2.81	1.59	1.53
16	1	604	CLA	CHC-C1C	2.80	1.42	1.35
16	O	201	CLA	CHC-C1C	2.80	1.42	1.35
16	2	612	CLA	CHC-C1C	2.80	1.42	1.35
16	A	828	CLA	CHC-C1C	2.80	1.42	1.35
16	A	822	CLA	CHC-C1C	2.79	1.42	1.35
16	A	837	CLA	CHC-C1C	2.79	1.42	1.35
16	2	604	CLA	CHC-C1C	2.79	1.42	1.35
16	B	822	CLA	CHC-C1C	2.79	1.42	1.35
16	B	830	CLA	CHC-C1C	2.79	1.42	1.35
16	2	610	CLA	CHC-C1C	2.79	1.42	1.35
18	1	613	RRX	C32-C1	2.79	1.59	1.53
16	B	811	CLA	CHC-C1C	2.78	1.42	1.35
16	J	102	CLA	CHC-C1C	2.78	1.42	1.35
16	L	204	CLA	CHC-C1C	2.78	1.42	1.35
16	3	206	CLA	CHC-C1C	2.78	1.42	1.35
16	3	209	CLA	CHC-C1C	2.78	1.42	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	823	CLA	CHC-C1C	2.78	1.42	1.35
16	B	813	CLA	CHC-C1C	2.78	1.42	1.35
16	2	601	CLA	C3B-C2B	-2.77	1.36	1.40
18	J	103	RRX	C32-C1	2.77	1.59	1.53
16	A	804	CLA	CHC-C1C	2.77	1.42	1.35
18	1	613	RRX	C4-C5	-2.77	1.45	1.51
16	B	805	CLA	CHC-C1C	2.76	1.42	1.35
16	A	855	CLA	CHC-C1C	2.76	1.42	1.35
16	B	833	CLA	CHC-C1C	2.76	1.42	1.35
16	3	212	CLA	CHC-C1C	2.76	1.42	1.35
16	3	214	CLA	CHC-C1C	2.76	1.42	1.35
16	3	211	CLA	CHC-C1C	2.76	1.42	1.35
16	A	810	CLA	CHC-C1C	2.76	1.42	1.35
16	B	838	CLA	CHC-C1C	2.76	1.42	1.35
16	2	607	CLA	CHC-C1C	2.76	1.42	1.35
16	B	821	CLA	CHC-C1C	2.76	1.42	1.35
16	3	204	CLA	CHC-C1C	2.76	1.42	1.35
16	A	816	CLA	CHC-C1C	2.75	1.42	1.35
16	I	102	CLA	CHC-C1C	2.75	1.42	1.35
16	2	609	CLA	CHC-C1C	2.75	1.42	1.35
16	B	832	CLA	C3B-C2B	-2.75	1.36	1.40
16	B	806	CLA	CHC-C1C	2.74	1.42	1.35
16	2	605	CLA	CHC-C1C	2.74	1.42	1.35
16	F	202	CLA	CHC-C1C	2.74	1.42	1.35
16	K	102	CLA	CHC-C1C	2.74	1.42	1.35
16	1	610	CLA	CHC-C1C	2.74	1.42	1.35
16	F	202	CLA	C3B-C2B	-2.74	1.36	1.40
16	A	815	CLA	CHC-C1C	2.74	1.42	1.35
16	A	824	CLA	CHC-C1C	2.74	1.42	1.35
16	B	818	CLA	CHC-C1C	2.74	1.42	1.35
16	2	611	CLA	CHC-C1C	2.73	1.42	1.35
16	2	608	CLA	CHC-C1C	2.73	1.42	1.35
16	3	203	CLA	CHC-C1C	2.73	1.42	1.35
16	2	613	CLA	CHC-C1C	2.73	1.42	1.35
16	B	820	CLA	CHC-C1C	2.73	1.42	1.35
16	B	818	CLA	C3B-C2B	-2.73	1.36	1.40
16	A	817	CLA	C3B-C2B	-2.73	1.36	1.40
16	A	820	CLA	C3B-C2B	-2.73	1.36	1.40
16	L	203	CLA	CHC-C1C	2.72	1.42	1.35
16	A	806	CLA	CHC-C1C	2.72	1.41	1.35
18	1	613	RRX	C21-C22	2.72	1.39	1.35
16	1	605	CLA	CHC-C1C	2.72	1.41	1.35

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	825	CLA	CHC-C1C	2.72	1.41	1.35
26	A	801	CL0	C4B-CHC	2.72	1.48	1.41
16	1	606	CLA	CHC-C1C	2.71	1.41	1.35
16	2	603	CLA	CHC-C1C	2.71	1.41	1.35
16	A	825	CLA	C3B-C2B	-2.71	1.36	1.40
16	F	204	CLA	CHC-C1C	2.71	1.41	1.35
16	B	837	CLA	C3B-C2B	-2.71	1.36	1.40
16	B	803	CLA	C3B-C2B	-2.71	1.36	1.40
16	3	207	CLA	CHC-C1C	2.71	1.41	1.35
16	B	836	CLA	C3B-C2B	-2.70	1.36	1.40
16	B	816	CLA	CHC-C1C	2.70	1.41	1.35
16	B	810	CLA	CHC-C1C	2.70	1.41	1.35
16	3	211	CLA	C3B-C2B	-2.70	1.36	1.40
16	B	814	CLA	CHC-C1C	2.70	1.41	1.35
16	B	819	CLA	CHC-C1C	2.70	1.41	1.35
16	B	819	CLA	C3B-C2B	-2.69	1.36	1.40
16	A	823	CLA	CHC-C1C	2.69	1.41	1.35
16	A	839	CLA	CHC-C1C	2.69	1.41	1.35
16	B	826	CLA	CHC-C1C	2.69	1.41	1.35
26	A	801	CL0	C1B-CHB	2.69	1.48	1.41
16	B	807	CLA	CHC-C1C	2.69	1.41	1.35
16	A	835	CLA	CHC-C1C	2.69	1.41	1.35
16	B	808	CLA	C3B-C2B	-2.69	1.36	1.40
17	3	217	C7Z	C21-C26	-2.68	1.50	1.53
16	A	820	CLA	CHC-C1C	2.68	1.41	1.35
16	A	838	CLA	C1B-NB	2.68	1.37	1.35
16	B	827	CLA	CHC-C1C	2.68	1.41	1.35
16	B	817	CLA	CHC-C1C	2.68	1.41	1.35
16	B	808	CLA	CHC-C1C	2.68	1.41	1.35
16	A	832	CLA	C3B-C2B	-2.68	1.36	1.40
17	3	215	C7Z	C21-C26	-2.68	1.50	1.53
16	B	829	CLA	C3B-C2B	-2.68	1.36	1.40
16	2	613	CLA	C1B-NB	2.67	1.37	1.35
16	2	610	CLA	C3B-C2B	-2.67	1.36	1.40
16	I	101	CLA	CHC-C1C	2.67	1.41	1.35
16	3	208	CLA	CHC-C1C	2.67	1.41	1.35
17	2	614	C7Z	C21-C26	-2.67	1.50	1.53
16	B	809	CLA	CHC-C1C	2.67	1.41	1.35
16	A	831	CLA	CHC-C1C	2.66	1.41	1.35
16	A	803	CLA	CHC-C1C	2.66	1.41	1.35
16	1	611	CLA	CHC-C1C	2.66	1.41	1.35
16	3	213	CLA	CHC-C1C	2.66	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	802	CLA	CHC-C1C	2.66	1.41	1.35
16	B	837	CLA	CHC-C1C	2.65	1.41	1.35
16	B	819	CLA	C1B-NB	2.65	1.37	1.35
16	A	809	CLA	C3B-C2B	-2.65	1.36	1.40
16	A	821	CLA	CHC-C1C	2.64	1.41	1.35
16	2	601	CLA	CHC-C1C	2.64	1.41	1.35
16	1	611	CLA	C3B-C2B	-2.64	1.36	1.40
16	A	838	CLA	C3B-C2B	-2.64	1.36	1.40
16	A	819	CLA	CHC-C1C	2.64	1.41	1.35
16	1	601	CLA	CHC-C1C	2.63	1.41	1.35
16	F	205	CLA	CHC-C1C	2.63	1.41	1.35
16	K	101	CLA	C3B-C2B	-2.63	1.36	1.40
16	B	829	CLA	CHC-C1C	2.63	1.41	1.35
16	A	814	CLA	CHC-C1C	2.63	1.41	1.35
16	A	826	CLA	CHC-C1C	2.62	1.41	1.35
16	A	830	CLA	CHC-C1C	2.62	1.41	1.35
16	B	831	CLA	CHC-C1C	2.62	1.41	1.35
16	1	602	CLA	CHC-C1C	2.62	1.41	1.35
16	L	205	CLA	CHC-C1C	2.62	1.41	1.35
16	A	818	CLA	CHC-C1C	2.61	1.41	1.35
16	A	805	CLA	CHC-C1C	2.61	1.41	1.35
16	B	816	CLA	C3B-C2B	-2.61	1.36	1.40
16	B	836	CLA	CHC-C1C	2.61	1.41	1.35
16	2	610	CLA	C1B-NB	2.61	1.37	1.35
16	L	201	CLA	C1B-NB	2.61	1.37	1.35
16	L	204	CLA	C1B-NB	2.61	1.37	1.35
16	A	811	CLA	CHC-C1C	2.61	1.41	1.35
16	2	606	CLA	CHC-C1C	2.60	1.41	1.35
16	A	829	CLA	CHC-C1C	2.60	1.41	1.35
16	B	802	CLA	C3B-C2B	-2.60	1.36	1.40
16	2	607	CLA	C3B-C2B	-2.59	1.36	1.40
16	3	209	CLA	C3B-C2B	-2.59	1.36	1.40
20	1	618	ERG	C9-C8	2.59	1.58	1.51
16	2	613	CLA	C3B-C2B	-2.59	1.36	1.40
16	A	809	CLA	C1B-NB	2.59	1.37	1.35
16	A	812	CLA	CHC-C1C	2.58	1.41	1.35
16	A	834	CLA	C3B-C2B	-2.58	1.36	1.40
16	3	205	CLA	CHC-C1C	2.58	1.41	1.35
17	3	216	C7Z	C21-C26	-2.58	1.50	1.53
16	F	201	CLA	C3B-C2B	-2.57	1.36	1.40
20	2	618	ERG	C9-C8	2.57	1.58	1.51
16	A	810	CLA	C3B-C2B	-2.57	1.36	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	J	103	RRX	C35-C13	2.57	1.56	1.50
16	F	205	CLA	C3B-C2B	-2.57	1.36	1.40
16	K	102	CLA	C1B-NB	2.56	1.37	1.35
16	F	205	CLA	C1B-NB	2.56	1.37	1.35
16	1	604	CLA	C3B-C2B	-2.56	1.36	1.40
16	B	805	CLA	C3B-C2B	-2.56	1.36	1.40
16	B	818	CLA	C1B-NB	2.55	1.37	1.35
16	B	812	CLA	CHC-C1C	2.55	1.41	1.35
16	1	603	CLA	C3B-C2B	-2.55	1.36	1.40
26	A	801	CL0	C1C-NC	-2.55	1.34	1.37
29	J	105	3PH	O31-C31	2.55	1.40	1.33
16	A	824	CLA	C3B-C2B	-2.54	1.36	1.40
16	2	612	CLA	C3B-C2B	-2.54	1.36	1.40
16	B	802	CLA	CHC-C1C	2.54	1.41	1.35
16	B	831	CLA	C1B-NB	2.54	1.37	1.35
16	1	608	CLA	C3B-C2B	-2.54	1.36	1.40
16	3	210	CLA	CHC-C1C	2.53	1.41	1.35
16	B	834	CLA	C1C-C2C	2.53	1.49	1.44
16	B	820	CLA	C3B-C2B	-2.53	1.36	1.40
18	K	103	RRX	C35-C13	2.52	1.56	1.50
16	L	204	CLA	C3B-C2B	-2.52	1.36	1.40
16	1	609	CLA	C3B-C2B	-2.52	1.36	1.40
16	O	203	CLA	C1B-NB	2.52	1.37	1.35
16	A	816	CLA	C3B-C2B	-2.52	1.36	1.40
16	B	804	CLA	CHC-C1C	2.52	1.41	1.35
25	A	852	PTY	O7-C6	-2.51	1.40	1.46
16	A	831	CLA	C3B-C2B	-2.51	1.36	1.40
29	B	854	3PH	O21-C2	-2.51	1.40	1.46
16	J	102	CLA	C3B-C2B	-2.50	1.36	1.40
16	K	102	CLA	C3B-C2B	-2.50	1.36	1.40
16	L	203	CLA	C3B-C2B	-2.50	1.36	1.40
16	A	813	CLA	C3B-C2B	-2.49	1.36	1.40
17	3	201	C7Z	C20-C13	2.49	1.56	1.50
16	B	828	CLA	C3B-C2B	-2.49	1.36	1.40
16	I	102	CLA	C3B-C2B	-2.49	1.36	1.40
16	O	203	CLA	C3B-C2B	-2.49	1.36	1.40
16	B	822	CLA	C1B-NB	2.49	1.37	1.35
16	A	806	CLA	C3B-C2B	-2.49	1.36	1.40
16	B	825	CLA	CHC-C1C	2.48	1.41	1.35
16	A	854	CLA	C1C-C2C	2.48	1.49	1.44
17	A	843	C7Z	C20-C13	2.48	1.56	1.50
16	2	608	CLA	C1B-NB	2.48	1.37	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	1	612	C7Z	C20-C13	2.48	1.56	1.50
17	3	217	C7Z	C20-C13	2.48	1.56	1.50
17	1	615	C7Z	C20-C13	2.47	1.56	1.50
16	A	802	CLA	C3B-C2B	-2.47	1.36	1.40
16	2	602	CLA	C1B-NB	2.47	1.37	1.35
25	3	220	PTY	O7-C6	-2.47	1.40	1.46
16	B	804	CLA	C3B-C2B	-2.47	1.36	1.40
29	B	854	3PH	O31-C31	2.46	1.40	1.33
17	J	104	C7Z	C20-C13	2.46	1.56	1.50
16	2	603	CLA	C3B-C2B	-2.46	1.37	1.40
16	O	202	CLA	C3B-C2B	-2.46	1.37	1.40
17	2	614	C7Z	C20-C13	2.46	1.56	1.50
17	3	216	C7Z	C20-C13	2.46	1.56	1.50
16	2	605	CLA	C3B-C2B	-2.45	1.37	1.40
17	2	615	C7Z	C20-C13	2.45	1.55	1.50
16	A	839	CLA	C3B-C2B	-2.45	1.37	1.40
16	B	811	CLA	C3B-C2B	-2.45	1.37	1.40
16	B	803	CLA	C1B-NB	2.45	1.37	1.35
17	1	616	C7Z	C20-C13	2.45	1.55	1.50
16	1	605	CLA	C3B-C2B	-2.45	1.37	1.40
18	1	613	RRX	C35-C13	2.44	1.55	1.50
16	A	830	CLA	C3B-C2B	-2.44	1.37	1.40
16	1	604	CLA	C1B-NB	2.44	1.37	1.35
16	O	202	CLA	C1B-NB	2.44	1.37	1.35
16	1	610	CLA	C3B-C2B	-2.44	1.37	1.40
17	3	217	C7Z	C18-C5	2.44	1.54	1.50
17	1	614	C7Z	C20-C13	2.44	1.55	1.50
16	1	603	CLA	C1B-NB	2.43	1.37	1.35
17	3	218	C7Z	C20-C13	2.43	1.55	1.50
16	B	814	CLA	C3B-C2B	-2.43	1.37	1.40
16	I	101	CLA	C1B-NB	2.43	1.37	1.35
16	A	808	CLA	C3B-C2B	-2.43	1.37	1.40
29	A	849	3PH	O21-C2	-2.43	1.40	1.46
16	A	829	CLA	C3B-C2B	-2.43	1.37	1.40
16	B	812	CLA	C1B-NB	2.43	1.37	1.35
17	1	616	C7Z	C18-C5	2.43	1.54	1.50
22	B	848	PGT	O2-C31	2.43	1.41	1.34
16	3	203	CLA	C3B-C2B	-2.43	1.37	1.40
16	O	204	CLA	C1B-NB	2.43	1.37	1.35
16	F	201	CLA	C1C-C2C	2.42	1.49	1.44
25	L	208	PTY	O4-C30	2.42	1.40	1.33
16	3	207	CLA	C3B-C2B	-2.42	1.37	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	830	CLA	C3B-C2B	-2.42	1.37	1.40
17	3	215	C7Z	C18-C5	2.42	1.54	1.50
16	K	101	CLA	C1B-NB	2.42	1.37	1.35
16	B	828	CLA	CHC-C1C	2.42	1.41	1.35
16	1	601	CLA	C3B-C2B	-2.42	1.37	1.40
16	B	835	CLA	C3B-C2B	-2.42	1.37	1.40
16	2	611	CLA	C1B-NB	2.41	1.37	1.35
16	A	816	CLA	C1B-NB	2.41	1.37	1.35
25	A	852	PTY	O4-C30	2.41	1.40	1.33
29	A	849	3PH	O31-C31	2.41	1.40	1.33
16	3	213	CLA	C1B-NB	2.41	1.37	1.35
16	A	820	CLA	C1B-NB	2.41	1.37	1.35
17	2	614	C7Z	C18-C5	2.41	1.54	1.50
16	B	835	CLA	C1C-C2C	2.41	1.49	1.44
16	A	833	CLA	C3B-C2B	-2.41	1.37	1.40
16	A	819	CLA	C1B-NB	2.41	1.37	1.35
17	1	614	C7Z	C18-C5	2.41	1.54	1.50
16	A	823	CLA	C3B-C2B	-2.41	1.37	1.40
17	J	104	C7Z	C18-C5	2.41	1.54	1.50
17	3	218	C7Z	C18-C5	2.41	1.54	1.50
25	3	220	PTY	O4-C30	2.41	1.40	1.33
16	1	606	CLA	C3B-C2B	-2.41	1.37	1.40
18	2	616	RRX	C35-C13	2.41	1.55	1.50
16	A	836	CLA	C3B-C2B	-2.40	1.37	1.40
16	B	825	CLA	C1B-NB	2.40	1.37	1.35
16	1	610	CLA	C1B-NB	2.40	1.37	1.35
16	I	101	CLA	C3B-C2B	-2.40	1.37	1.40
17	A	843	C7Z	C18-C5	2.40	1.54	1.50
17	1	612	C7Z	C21-C26	-2.40	1.50	1.53
16	2	611	CLA	C3B-C2B	-2.40	1.37	1.40
17	1	615	C7Z	C18-C5	2.40	1.54	1.50
16	O	201	CLA	C1C-C2C	2.40	1.49	1.44
16	O	203	CLA	C1C-C2C	2.40	1.49	1.44
29	J	105	3PH	O21-C2	-2.39	1.40	1.46
16	A	822	CLA	C1B-NB	2.39	1.37	1.35
16	2	608	CLA	C3B-C2B	-2.39	1.37	1.40
16	B	810	CLA	C3B-C2B	-2.39	1.37	1.40
16	1	611	CLA	C1B-NB	2.39	1.37	1.35
16	A	835	CLA	C1B-NB	2.39	1.37	1.35
16	A	809	CLA	C1C-C2C	2.39	1.49	1.44
16	B	811	CLA	C1B-NB	2.38	1.37	1.35
16	B	810	CLA	C1B-NB	2.38	1.37	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	826	CLA	C3B-C2B	-2.38	1.37	1.40
25	3	221	PTY	O4-C30	2.38	1.40	1.33
16	A	856	CLA	C3B-C2B	-2.38	1.37	1.40
16	A	804	CLA	C3B-C2B	-2.38	1.37	1.40
16	A	808	CLA	C1B-NB	2.38	1.37	1.35
16	1	609	CLA	C1B-NB	2.38	1.37	1.35
16	3	214	CLA	C3B-C2B	-2.38	1.37	1.40
16	A	806	CLA	C1B-NB	2.37	1.37	1.35
16	2	606	CLA	C1B-NB	2.37	1.37	1.35
16	B	807	CLA	C3B-C2B	-2.36	1.37	1.40
17	3	216	C7Z	C18-C5	2.36	1.54	1.50
16	B	821	CLA	C1B-NB	2.36	1.37	1.35
16	1	607	CLA	C3B-C2B	-2.36	1.37	1.40
16	3	204	CLA	C3B-C2B	-2.36	1.37	1.40
16	O	201	CLA	C1B-NB	2.36	1.37	1.35
16	A	826	CLA	C3B-C2B	-2.36	1.37	1.40
16	B	815	CLA	C1C-C2C	2.36	1.49	1.44
16	A	823	CLA	C1B-NB	2.35	1.37	1.35
16	A	817	CLA	C1C-C2C	2.35	1.49	1.44
16	2	612	CLA	C1B-NB	2.35	1.37	1.35
16	F	201	CLA	C1B-NB	2.35	1.37	1.35
16	1	607	CLA	C1C-C2C	2.35	1.49	1.44
16	3	206	CLA	C3B-C2B	-2.35	1.37	1.40
16	B	802	CLA	C1B-NB	2.35	1.37	1.35
30	A	851	T7X	O18-C11	2.35	1.40	1.33
17	3	201	C7Z	C18-C5	2.34	1.54	1.50
16	J	102	CLA	C1B-NB	2.34	1.37	1.35
16	3	214	CLA	C1B-NB	2.34	1.37	1.35
16	F	204	CLA	C1B-NB	2.34	1.37	1.35
16	A	836	CLA	C1B-NB	2.34	1.37	1.35
17	3	215	C7Z	C20-C13	2.34	1.55	1.50
18	A	847	RRX	C35-C13	2.34	1.55	1.50
16	B	804	CLA	C1B-NB	2.34	1.37	1.35
16	A	827	CLA	C1C-C2C	2.34	1.49	1.44
16	B	835	CLA	C1B-NB	2.34	1.37	1.35
16	2	609	CLA	C3B-C2B	-2.33	1.37	1.40
16	B	815	CLA	C3B-C2B	-2.33	1.37	1.40
16	B	801	CLA	C1C-C2C	2.33	1.49	1.44
16	3	210	CLA	C3B-C2B	-2.33	1.37	1.40
16	L	205	CLA	C3B-C2B	-2.33	1.37	1.40
16	B	820	CLA	C1B-NB	2.33	1.37	1.35
16	L	201	CLA	C1C-C2C	2.32	1.49	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	2	609	CLA	C1B-NB	2.32	1.37	1.35
16	A	811	CLA	C1B-NB	2.32	1.37	1.35
17	2	615	C7Z	C18-C5	2.32	1.54	1.50
16	B	801	CLA	C3B-C2B	-2.32	1.37	1.40
16	B	805	CLA	C1B-NB	2.32	1.37	1.35
16	A	807	CLA	C1B-NB	2.32	1.37	1.35
25	L	208	PTY	O7-C6	-2.32	1.40	1.46
16	F	204	CLA	C1C-C2C	2.32	1.49	1.44
16	A	837	CLA	C1C-C2C	2.31	1.49	1.44
16	3	204	CLA	C1B-NB	2.31	1.37	1.35
16	A	828	CLA	C3B-C2B	-2.31	1.37	1.40
16	3	209	CLA	C1B-NB	2.31	1.37	1.35
16	F	202	CLA	C1B-NB	2.31	1.37	1.35
16	1	608	CLA	C1B-NB	2.31	1.37	1.35
16	O	204	CLA	C3B-C2B	-2.31	1.37	1.40
16	L	201	CLA	C3B-C2B	-2.31	1.37	1.40
16	A	807	CLA	C1C-C2C	2.30	1.49	1.44
16	3	211	CLA	C1B-NB	2.30	1.37	1.35
16	A	833	CLA	C1C-C2C	2.30	1.49	1.44
30	A	851	T7X	O16-C8	-2.30	1.40	1.46
16	B	803	CLA	C1C-C2C	2.29	1.49	1.44
16	A	815	CLA	C3B-C2B	-2.29	1.37	1.40
16	A	837	CLA	C1B-NB	2.29	1.37	1.35
16	F	202	CLA	C1C-C2C	2.29	1.49	1.44
17	1	612	C7Z	C18-C5	2.29	1.54	1.50
16	B	832	CLA	C1B-NB	2.29	1.37	1.35
16	L	203	CLA	C1B-NB	2.28	1.37	1.35
16	2	613	CLA	C1C-C2C	2.28	1.49	1.44
16	1	610	CLA	C1C-C2C	2.28	1.49	1.44
16	1	602	CLA	C1B-NB	2.28	1.37	1.35
16	O	204	CLA	C1C-C2C	2.28	1.49	1.44
25	L	208	PTY	O7-C8	2.28	1.40	1.34
16	A	827	CLA	C3B-C2B	-2.28	1.37	1.40
20	2	618	ERG	C14-C8	2.28	1.57	1.51
16	2	604	CLA	C1B-NB	2.27	1.37	1.35
16	A	821	CLA	C1B-NB	2.27	1.37	1.35
16	1	609	CLA	C1C-C2C	2.27	1.49	1.44
16	2	607	CLA	C1B-NB	2.27	1.37	1.35
16	A	836	CLA	C1C-C2C	2.27	1.49	1.44
16	A	802	CLA	C1B-NB	2.27	1.37	1.35
16	K	101	CLA	C1C-C2C	2.27	1.49	1.44
25	3	221	PTY	O7-C8	2.27	1.40	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	3	206	CLA	C1B-NB	2.27	1.37	1.35
16	A	856	CLA	C1C-C2C	2.26	1.48	1.44
16	2	605	CLA	C1B-NB	2.26	1.37	1.35
16	B	809	CLA	C3B-C2B	-2.26	1.37	1.40
16	L	205	CLA	C1B-NB	2.26	1.37	1.35
16	2	604	CLA	C1C-C2C	2.25	1.48	1.44
16	A	818	CLA	C1B-NB	2.25	1.37	1.35
16	1	605	CLA	C1B-NB	2.25	1.37	1.35
16	A	829	CLA	C1B-NB	2.25	1.37	1.35
16	A	803	CLA	C3B-C2B	-2.25	1.37	1.40
16	2	605	CLA	C1C-C2C	2.25	1.48	1.44
16	A	838	CLA	C1C-C2C	2.25	1.48	1.44
16	B	808	CLA	C1B-NB	2.25	1.37	1.35
16	A	805	CLA	C1B-NB	2.25	1.37	1.35
16	2	604	CLA	C3B-C2B	-2.25	1.37	1.40
16	J	102	CLA	C1C-C2C	2.25	1.48	1.44
16	A	814	CLA	C1B-NB	2.25	1.37	1.35
16	A	815	CLA	C1B-NB	2.24	1.37	1.35
16	3	205	CLA	C1A-CHA	2.24	1.52	1.43
16	A	805	CLA	C3B-C2B	-2.24	1.37	1.40
16	B	813	CLA	C1B-NB	2.24	1.37	1.35
16	B	824	CLA	C3B-C2B	-2.24	1.37	1.40
16	A	815	CLA	C1C-C2C	2.24	1.48	1.44
20	2	621	ERG	C14-C8	2.24	1.57	1.51
16	A	831	CLA	C1B-NB	2.24	1.37	1.35
29	J	105	3PH	O21-C21	2.23	1.40	1.34
16	B	822	CLA	C1C-C2C	2.23	1.48	1.44
16	2	611	CLA	C1C-C2C	2.23	1.48	1.44
16	A	812	CLA	C3B-C2B	-2.23	1.37	1.40
17	1	615	C7Z	C40-C33	2.23	1.55	1.50
16	B	806	CLA	C1C-C2C	2.23	1.48	1.44
16	A	830	CLA	C1C-C2C	2.23	1.48	1.44
16	3	203	CLA	C1C-C2C	2.22	1.48	1.44
16	3	203	CLA	C1B-NB	2.22	1.37	1.35
16	A	813	CLA	C1B-NB	2.22	1.37	1.35
16	3	210	CLA	C1B-NB	2.22	1.37	1.35
16	1	603	CLA	C1C-C2C	2.22	1.48	1.44
16	A	817	CLA	C1B-NB	2.22	1.37	1.35
16	A	830	CLA	C1B-NB	2.22	1.37	1.35
16	L	204	CLA	C1C-C2C	2.21	1.48	1.44
16	B	838	CLA	C1C-C2C	2.21	1.48	1.44
16	B	827	CLA	C3B-C2B	-2.21	1.37	1.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	825	CLA	C3B-C2B	-2.21	1.37	1.40
16	B	806	CLA	C1B-NB	2.21	1.37	1.35
16	B	826	CLA	C1B-NB	2.21	1.37	1.35
16	B	837	CLA	C1B-NB	2.21	1.37	1.35
16	A	808	CLA	C1C-C2C	2.20	1.48	1.44
16	3	213	CLA	C1C-C2C	2.20	1.48	1.44
16	A	822	CLA	C3B-C2B	-2.20	1.37	1.40
16	B	823	CLA	C3B-C2B	-2.20	1.37	1.40
16	B	834	CLA	C1B-NB	2.20	1.37	1.35
18	2	616	RRX	C21-C22	2.20	1.38	1.35
16	B	838	CLA	C1B-NB	2.19	1.37	1.35
17	3	216	C7Z	C10-C9	-2.19	1.32	1.35
16	B	805	CLA	C1C-C2C	2.19	1.48	1.44
16	A	804	CLA	C1C-C2C	2.19	1.48	1.44
31	B	849	DGD	O3G-C1D	2.19	1.43	1.40
16	A	819	CLA	C3B-C2B	-2.19	1.37	1.40
16	2	601	CLA	C1B-NB	2.19	1.37	1.35
16	B	821	CLA	C1C-C2C	2.19	1.48	1.44
16	2	610	CLA	C1C-C2C	2.19	1.48	1.44
16	B	817	CLA	C3B-C2B	-2.19	1.37	1.40
16	A	830	CLA	C1A-CHA	2.19	1.52	1.43
16	O	202	CLA	C1C-C2C	2.19	1.48	1.44
16	B	816	CLA	C1B-NB	2.19	1.37	1.35
16	3	211	CLA	C1C-C2C	2.19	1.48	1.44
16	2	602	CLA	C3B-C2B	-2.19	1.37	1.40
16	1	602	CLA	C1C-C2C	2.19	1.48	1.44
16	B	812	CLA	C3B-C2B	-2.19	1.37	1.40
16	1	606	CLA	C1B-NB	2.19	1.37	1.35
16	2	601	CLA	C1C-C2C	2.18	1.48	1.44
20	2	621	ERG	C11-C9	2.18	1.57	1.53
16	1	611	CLA	C1C-C2C	2.18	1.48	1.44
16	B	824	CLA	C1C-C2C	2.18	1.48	1.44
16	2	606	CLA	C3B-C2B	-2.18	1.37	1.40
16	B	833	CLA	C3B-C2B	-2.18	1.37	1.40
16	B	828	CLA	C1B-NB	2.18	1.37	1.35
16	3	208	CLA	C3B-C2B	-2.18	1.37	1.40
16	A	812	CLA	C1B-NB	2.18	1.37	1.35
25	3	221	PTY	O7-C6	-2.18	1.41	1.46
16	1	605	CLA	C1A-CHA	2.18	1.52	1.43
25	3	220	PTY	O7-C8	2.18	1.40	1.34
16	3	203	CLA	C1A-CHA	2.18	1.52	1.43
16	3	213	CLA	C3B-C2B	-2.18	1.37	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	854	CLA	C3B-C2B	-2.18	1.37	1.40
16	A	814	CLA	C3B-C2B	-2.17	1.37	1.40
16	L	203	CLA	C1C-C2C	2.17	1.48	1.44
16	B	817	CLA	C1A-CHA	2.17	1.52	1.43
16	3	211	CLA	C1A-CHA	2.17	1.52	1.43
16	I	101	CLA	C1C-C2C	2.17	1.48	1.44
16	A	835	CLA	C3B-C2B	-2.17	1.37	1.40
16	B	836	CLA	C1B-NB	2.17	1.37	1.35
16	A	831	CLA	C1C-C2C	2.17	1.48	1.44
16	B	823	CLA	C1C-C2C	2.17	1.48	1.44
16	1	608	CLA	C1C-C2C	2.17	1.48	1.44
16	1	605	CLA	C1C-C2C	2.17	1.48	1.44
16	B	827	CLA	C1B-NB	2.17	1.37	1.35
16	B	825	CLA	C1A-CHA	2.17	1.52	1.43
16	A	822	CLA	C1C-C2C	2.17	1.48	1.44
16	B	815	CLA	C1B-NB	2.17	1.37	1.35
16	I	102	CLA	C1B-NB	2.17	1.37	1.35
16	1	602	CLA	C3B-C2B	-2.16	1.37	1.40
16	A	839	CLA	C1B-NB	2.16	1.37	1.35
16	2	612	CLA	C1C-C2C	2.16	1.48	1.44
18	A	847	RRX	C21-C22	2.16	1.38	1.35
16	B	832	CLA	C1C-C2C	2.16	1.48	1.44
29	A	849	3PH	O21-C21	2.16	1.40	1.34
16	A	803	CLA	C1A-CHA	2.16	1.52	1.43
16	A	824	CLA	C1B-NB	2.16	1.37	1.35
16	A	834	CLA	C1C-C2C	2.16	1.48	1.44
16	A	813	CLA	C1C-C2C	2.16	1.48	1.44
16	A	821	CLA	C3B-C2B	-2.16	1.37	1.40
16	2	611	CLA	C1A-CHA	2.16	1.52	1.43
16	A	818	CLA	C3B-C2B	-2.15	1.37	1.40
16	B	831	CLA	C3B-C2B	-2.15	1.37	1.40
16	A	855	CLA	C1C-C2C	2.15	1.48	1.44
16	2	609	CLA	C1C-C2C	2.15	1.48	1.44
16	2	603	CLA	C1B-NB	2.15	1.37	1.35
30	A	851	T7X	O18-C9	-2.15	1.40	1.45
16	F	204	CLA	C3B-C2B	-2.15	1.37	1.40
17	J	104	C7Z	C40-C33	2.15	1.55	1.50
16	B	817	CLA	C1C-C2C	2.15	1.48	1.44
16	B	833	CLA	C1C-C2C	2.15	1.48	1.44
16	2	607	CLA	C1C-C2C	2.15	1.48	1.44
17	3	215	C7Z	C40-C33	2.14	1.55	1.50
16	A	806	CLA	C1C-C2C	2.14	1.48	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	801	CL0	C1D-C2D	2.14	1.49	1.45
16	A	810	CLA	C1B-NB	2.14	1.37	1.35
16	2	613	CLA	C1A-CHA	2.14	1.52	1.43
16	B	820	CLA	C1C-C2C	2.14	1.48	1.44
16	3	212	CLA	C1C-C2C	2.14	1.48	1.44
29	B	854	3PH	O21-C21	2.14	1.40	1.34
16	B	817	CLA	C1B-NB	2.14	1.37	1.35
16	A	814	CLA	C1C-C2C	2.13	1.48	1.44
16	A	802	CLA	C1A-CHA	2.13	1.52	1.43
16	B	812	CLA	C1A-CHA	2.13	1.52	1.43
16	A	839	CLA	C1A-CHA	2.13	1.52	1.43
25	A	852	PTY	O7-C8	2.13	1.40	1.34
16	A	819	CLA	C1C-C2C	2.13	1.48	1.44
20	2	621	ERG	C4-C5	2.13	1.56	1.51
16	3	208	CLA	C1B-NB	2.13	1.37	1.35
16	A	821	CLA	C1C-C2C	2.13	1.48	1.44
16	B	812	CLA	C1C-C2C	2.13	1.48	1.44
16	I	102	CLA	C1C-C2C	2.13	1.48	1.44
16	A	837	CLA	C3B-C2B	-2.13	1.37	1.40
17	1	614	C7Z	C40-C33	2.13	1.55	1.50
16	3	204	CLA	C1C-C2C	2.13	1.48	1.44
16	A	856	CLA	C1A-CHA	2.13	1.51	1.43
16	A	823	CLA	C1C-C2C	2.13	1.48	1.44
16	A	825	CLA	C1C-C2C	2.13	1.48	1.44
30	A	851	T7X	O16-C10	2.13	1.40	1.34
16	B	829	CLA	CHD-C1D	2.12	1.42	1.38
16	A	812	CLA	C1A-CHA	2.12	1.51	1.43
16	A	835	CLA	C1C-C2C	2.12	1.48	1.44
16	3	206	CLA	C1C-C2C	2.12	1.48	1.44
29	A	849	3PH	O31-C3	-2.12	1.40	1.45
17	A	843	C7Z	C40-C33	2.12	1.55	1.50
16	A	828	CLA	C1C-C2C	2.12	1.48	1.44
16	B	811	CLA	C1C-C2C	2.12	1.48	1.44
16	B	810	CLA	C1C-C2C	2.12	1.48	1.44
16	3	212	CLA	C3B-C2B	-2.12	1.37	1.40
16	F	204	CLA	C1A-CHA	2.12	1.51	1.43
16	2	606	CLA	C1A-CHA	2.12	1.51	1.43
16	3	213	CLA	C1A-CHA	2.12	1.51	1.43
16	3	208	CLA	C1C-C2C	2.12	1.48	1.44
16	B	815	CLA	C1A-CHA	2.11	1.51	1.43
22	B	848	PGT	C4-C5	2.11	1.58	1.51
16	B	803	CLA	C1A-CHA	2.11	1.51	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	816	CLA	CHD-C1D	2.11	1.42	1.38
16	2	612	CLA	C1A-CHA	2.11	1.51	1.43
17	3	218	C7Z	C40-C33	2.11	1.55	1.50
16	2	601	CLA	C1A-CHA	2.11	1.51	1.43
20	1	618	ERG	C4-C5	2.11	1.56	1.51
23	J	101	DGA	OG2-CG2	-2.11	1.41	1.46
17	2	614	C7Z	C40-C33	2.11	1.55	1.50
16	A	839	CLA	C1C-C2C	2.11	1.48	1.44
16	A	802	CLA	C1C-C2C	2.11	1.48	1.44
16	A	810	CLA	C1C-C2C	2.11	1.48	1.44
16	A	833	CLA	C1B-NB	2.11	1.37	1.35
16	A	804	CLA	C1B-NB	2.11	1.37	1.35
16	A	827	CLA	C1A-CHA	2.11	1.51	1.43
25	3	220	PTY	O4-C1	-2.10	1.40	1.45
16	3	209	CLA	C1A-CHA	2.10	1.51	1.43
16	3	212	CLA	C1B-NB	2.10	1.37	1.35
16	A	828	CLA	C1B-NB	2.10	1.37	1.35
16	3	209	CLA	C1C-C2C	2.10	1.48	1.44
16	A	815	CLA	C1A-CHA	2.10	1.51	1.43
22	2	619	PGT	O2-C31	2.10	1.40	1.34
16	3	212	CLA	C1A-CHA	2.10	1.51	1.43
16	A	824	CLA	C1C-C2C	2.10	1.48	1.44
16	3	207	CLA	C1C-C2C	2.10	1.48	1.44
16	B	819	CLA	C3D-C4D	-2.10	1.39	1.44
17	3	216	C7Z	C40-C33	2.10	1.55	1.50
16	2	607	CLA	C1A-CHA	2.10	1.51	1.43
16	2	606	CLA	C1C-C2C	2.10	1.48	1.44
16	B	813	CLA	C1C-C2C	2.10	1.48	1.44
16	A	826	CLA	C1B-NB	2.10	1.37	1.35
23	2	620	DGA	OG2-CG2	-2.09	1.41	1.46
16	J	102	CLA	C1A-CHA	2.09	1.51	1.43
16	1	606	CLA	C1C-C2C	2.09	1.48	1.44
16	1	604	CLA	C1C-C2C	2.09	1.48	1.44
16	A	819	CLA	C1A-CHA	2.09	1.51	1.43
16	B	830	CLA	C1C-C2C	2.09	1.48	1.44
16	B	818	CLA	C1C-C2C	2.09	1.48	1.44
16	B	828	CLA	C3D-C4D	-2.09	1.39	1.44
16	A	807	CLA	C3B-C2B	-2.09	1.37	1.40
16	3	207	CLA	C1B-NB	2.09	1.37	1.35
16	A	825	CLA	C1A-CHA	2.09	1.51	1.43
16	B	829	CLA	C1B-NB	2.09	1.37	1.35
16	B	838	CLA	C1A-CHA	2.09	1.51	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	834	CLA	C1A-CHA	2.09	1.51	1.43
16	A	832	CLA	C1B-NB	2.08	1.37	1.35
16	B	826	CLA	C1A-CHA	2.08	1.51	1.43
21	2	617	BCR	C1-C6	-2.08	1.50	1.53
16	B	833	CLA	C1B-NB	2.08	1.37	1.35
16	B	816	CLA	C3D-C4D	-2.08	1.39	1.44
16	B	809	CLA	C1B-NB	2.08	1.37	1.35
16	B	825	CLA	C1C-C2C	2.08	1.48	1.44
16	2	604	CLA	C1A-CHA	2.08	1.51	1.43
16	A	854	CLA	C1B-NB	2.08	1.37	1.35
16	3	214	CLA	C1C-C2C	2.08	1.48	1.44
16	A	837	CLA	C1A-CHA	2.08	1.51	1.43
16	B	801	CLA	C1A-CHA	2.08	1.51	1.43
16	B	836	CLA	CHD-C1D	2.08	1.42	1.38
17	3	201	C7Z	C40-C33	2.07	1.55	1.50
17	1	616	C7Z	C40-C33	2.07	1.55	1.50
16	F	205	CLA	C1A-CHA	2.07	1.51	1.43
16	A	813	CLA	C1A-CHA	2.07	1.51	1.43
25	L	208	PTY	O4-C1	-2.07	1.40	1.45
16	1	610	CLA	C1A-CHA	2.07	1.51	1.43
16	A	804	CLA	C1A-CHA	2.07	1.51	1.43
17	2	615	C7Z	C40-C33	2.07	1.55	1.50
29	B	854	3PH	O31-C3	-2.07	1.40	1.45
16	B	831	CLA	C1C-C2C	2.06	1.48	1.44
16	A	826	CLA	C3D-C4D	-2.06	1.39	1.44
16	B	806	CLA	C3B-C2B	-2.06	1.37	1.40
16	B	821	CLA	C1A-CHA	2.06	1.51	1.43
16	3	205	CLA	C3B-C2B	-2.06	1.37	1.40
16	3	210	CLA	C1C-C2C	2.06	1.48	1.44
16	A	825	CLA	C1B-NB	2.06	1.37	1.35
16	A	818	CLA	CHD-C1D	2.06	1.42	1.38
16	1	601	CLA	C1A-CHA	2.06	1.51	1.43
16	1	611	CLA	C1A-CHA	2.06	1.51	1.43
22	B	848	PGT	C32-C31	2.06	1.56	1.50
16	B	808	CLA	C1A-CHA	2.05	1.51	1.43
16	A	821	CLA	C1A-CHA	2.05	1.51	1.43
16	B	806	CLA	C1A-CHA	2.05	1.51	1.43
16	B	836	CLA	C3D-C4D	-2.05	1.39	1.44
16	A	811	CLA	C1C-C2C	2.05	1.48	1.44
16	B	814	CLA	C1B-NB	2.05	1.37	1.35
16	B	807	CLA	C1C-C2C	2.05	1.48	1.44
16	L	203	CLA	C1A-CHA	2.05	1.51	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	O	201	CLA	C3B-C2B	-2.05	1.37	1.40
16	K	102	CLA	C1C-C2C	2.05	1.48	1.44
16	B	813	CLA	C3B-C2B	-2.05	1.37	1.40
16	B	828	CLA	CHD-C1D	2.05	1.42	1.38
16	B	834	CLA	C1A-CHA	2.05	1.51	1.43
25	A	852	PTY	O4-C1	-2.05	1.40	1.45
16	3	204	CLA	C3D-C4D	-2.05	1.39	1.44
16	B	805	CLA	C1A-CHA	2.05	1.51	1.43
16	A	828	CLA	C3D-C4D	-2.05	1.39	1.44
16	A	818	CLA	C3D-C4D	-2.05	1.39	1.44
16	A	810	CLA	C1A-CHA	2.04	1.51	1.43
16	2	609	CLA	C1A-CHA	2.04	1.51	1.43
16	B	804	CLA	C1A-CHA	2.04	1.51	1.43
16	B	833	CLA	C1A-CHA	2.04	1.51	1.43
16	L	205	CLA	C1A-CHA	2.04	1.51	1.43
16	2	603	CLA	C1C-C2C	2.04	1.48	1.44
16	B	809	CLA	C1A-CHA	2.04	1.51	1.43
16	B	823	CLA	C1A-CHA	2.04	1.51	1.43
16	F	202	CLA	C1A-CHA	2.04	1.51	1.43
16	A	811	CLA	CHD-C1D	2.04	1.42	1.38
16	B	820	CLA	C1A-CHA	2.04	1.51	1.43
16	B	819	CLA	C1C-C2C	2.04	1.48	1.44
16	B	835	CLA	C3D-C4D	-2.04	1.39	1.44
16	A	814	CLA	C1A-CHA	2.04	1.51	1.43
16	B	834	CLA	C3B-C2B	-2.04	1.37	1.40
16	A	826	CLA	C1A-CHA	2.04	1.51	1.43
16	B	830	CLA	C1B-NB	2.04	1.37	1.35
16	O	203	CLA	C3D-C4D	-2.04	1.39	1.44
25	3	221	PTY	O4-C1	-2.04	1.40	1.45
16	A	820	CLA	C1C-C2C	2.04	1.48	1.44
21	L	206	BCR	C12-C13	-2.04	1.41	1.45
16	3	206	CLA	C1A-CHA	2.03	1.51	1.43
16	B	829	CLA	C1C-C2C	2.03	1.48	1.44
16	B	827	CLA	C1C-C2C	2.03	1.48	1.44
16	B	814	CLA	C1A-CHA	2.03	1.51	1.43
16	3	214	CLA	C1A-CHA	2.03	1.51	1.43
16	B	809	CLA	C1C-C2C	2.03	1.48	1.44
16	2	602	CLA	C3D-C4D	-2.03	1.39	1.44
16	A	803	CLA	C1B-NB	2.02	1.37	1.35
16	A	808	CLA	C3D-C4D	-2.02	1.39	1.44
18	K	103	RRX	C17-C18	2.02	1.38	1.35
16	F	201	CLA	C1A-CHA	2.02	1.51	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	829	CLA	C3D-C4D	-2.02	1.39	1.44
16	1	601	CLA	C1B-NB	2.02	1.37	1.35
16	B	811	CLA	C3D-C4D	-2.02	1.39	1.44
16	B	802	CLA	C1A-CHA	2.02	1.51	1.43
16	A	809	CLA	C3D-C4D	-2.02	1.39	1.44
16	A	833	CLA	C3D-C4D	-2.02	1.39	1.44
16	A	819	CLA	C3D-C4D	-2.02	1.39	1.44
16	A	804	CLA	CHD-C1D	2.02	1.42	1.38
16	2	608	CLA	C3D-C4D	-2.02	1.39	1.44
16	A	836	CLA	C1A-CHA	2.02	1.51	1.43
16	B	826	CLA	C1C-C2C	2.02	1.48	1.44
22	2	619	PGT	C4-C5	2.02	1.58	1.51
16	A	824	CLA	C1A-CHA	2.01	1.51	1.43
16	A	805	CLA	C1A-CHA	2.01	1.51	1.43
16	2	603	CLA	C3D-C4D	-2.01	1.39	1.44
16	A	832	CLA	CHD-C1D	2.01	1.42	1.38
26	A	801	CL0	C1C-C2C	2.01	1.48	1.44
16	A	816	CLA	C1A-CHA	2.01	1.51	1.43
16	B	814	CLA	C1C-C2C	2.01	1.48	1.44
16	O	204	CLA	C1A-CHA	2.01	1.51	1.43
20	2	618	ERG	C4-C5	2.01	1.56	1.51
16	1	606	CLA	C1A-CHA	2.01	1.51	1.43
16	A	829	CLA	C3D-C4D	-2.01	1.39	1.44
16	B	830	CLA	C3D-C4D	-2.01	1.39	1.44
16	B	816	CLA	C1C-C2C	2.01	1.48	1.44
16	2	610	CLA	C1A-CHA	2.01	1.51	1.43
16	B	808	CLA	C3D-C4D	-2.01	1.39	1.44
16	B	837	CLA	C1A-CHA	2.01	1.51	1.43
16	A	804	CLA	C3D-C4D	-2.01	1.39	1.44
16	2	603	CLA	CHD-C1D	2.01	1.42	1.38
16	A	827	CLA	C1B-NB	2.01	1.37	1.35
16	A	824	CLA	C3D-C4D	-2.01	1.39	1.44
16	A	831	CLA	C1A-CHA	2.01	1.51	1.43
16	A	820	CLA	C3D-C4D	-2.01	1.39	1.44
16	K	101	CLA	C3D-C4D	-2.01	1.39	1.44
16	B	838	CLA	C3B-C2B	-2.00	1.37	1.40
16	A	820	CLA	C1A-CHA	2.00	1.51	1.43
16	A	832	CLA	C3D-C4D	-2.00	1.39	1.44
16	1	607	CLA	C1A-CHA	2.00	1.51	1.43
16	K	101	CLA	C1A-CHA	2.00	1.51	1.43
16	A	832	CLA	C1C-C2C	2.00	1.48	1.44
16	B	818	CLA	CHD-C1D	2.00	1.42	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	855	CLA	C3D-C4D	-2.00	1.39	1.44
16	B	832	CLA	C1A-CHA	2.00	1.51	1.43
16	L	204	CLA	C1A-CHA	2.00	1.51	1.43
16	L	205	CLA	CHD-C1D	2.00	1.42	1.38
16	B	808	CLA	C1C-C2C	2.00	1.48	1.44
16	A	811	CLA	C3B-C2B	-2.00	1.37	1.40
16	B	802	CLA	C3D-C4D	-2.00	1.39	1.44
16	3	209	CLA	C3D-C4D	-2.00	1.39	1.44
16	B	827	CLA	C3D-C4D	-2.00	1.39	1.44
16	L	201	CLA	C1A-CHA	2.00	1.51	1.43
16	B	827	CLA	CHD-C1D	2.00	1.42	1.38
16	1	603	CLA	C3D-C4D	-2.00	1.39	1.44
16	B	814	CLA	CHD-C1D	2.00	1.42	1.38
16	2	603	CLA	C1A-CHA	2.00	1.51	1.43

All (3037) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	K	104	BCR	C10-C11-C12	18.18	179.96	123.22
20	1	618	ERG	C18-C13-C12	-18.17	81.89	110.59
21	B	842	BCR	C10-C11-C12	17.98	179.32	123.22
21	O	205	BCR	C10-C11-C12	17.86	178.94	123.22
21	L	202	BCR	C10-C11-C12	17.78	178.71	123.22
21	B	843	BCR	C10-C11-C12	17.76	178.64	123.22
21	B	844	BCR	C10-C11-C12	17.75	178.62	123.22
21	B	845	BCR	C10-C11-C12	17.74	178.57	123.22
21	B	855	BCR	C10-C11-C12	17.64	178.26	123.22
21	A	850	BCR	C10-C11-C12	17.60	178.14	123.22
21	I	103	BCR	C10-C11-C12	17.54	177.96	123.22
21	B	841	BCR	C10-C11-C12	17.43	177.60	123.22
21	2	617	BCR	C10-C11-C12	17.41	177.55	123.22
21	A	846	BCR	C10-C11-C12	17.31	177.23	123.22
21	A	844	BCR	C10-C11-C12	17.14	176.70	123.22
21	B	840	BCR	C10-C11-C12	17.11	176.61	123.22
21	L	207	BCR	C10-C11-C12	16.96	176.13	123.22
21	L	206	BCR	C10-C11-C12	16.70	175.32	123.22
21	B	843	BCR	C16-C15-C14	16.69	157.66	123.47
21	A	857	BCR	C10-C11-C12	16.42	174.45	123.22
21	F	203	BCR	C10-C11-C12	16.25	173.94	123.22
21	A	845	BCR	C10-C11-C12	16.14	173.59	123.22
21	F	206	BCR	C10-C11-C12	15.88	172.76	123.22
21	B	847	BCR	C10-C11-C12	15.78	172.45	123.22

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	845	BCR	C32-C1-C6	-15.21	85.63	110.30
21	F	203	BCR	C11-C10-C9	14.98	148.69	127.31
21	A	845	BCR	C31-C1-C6	-14.92	86.10	110.30
21	I	103	BCR	C32-C1-C6	-14.83	86.24	110.30
21	F	203	BCR	C21-C20-C19	14.80	169.40	123.22
21	I	103	BCR	C31-C1-C6	-14.57	86.67	110.30
21	F	206	BCR	C21-C20-C19	14.53	168.57	123.22
21	B	855	BCR	C16-C15-C14	14.53	153.24	123.47
21	B	847	BCR	C16-C15-C14	14.31	152.78	123.47
21	B	840	BCR	C11-C10-C9	14.24	147.64	127.31
20	1	618	ERG	C18-C13-C17	-14.08	85.46	111.71
21	O	205	BCR	C21-C20-C19	14.05	167.06	123.22
21	L	207	BCR	C16-C15-C14	13.93	152.01	123.47
21	A	850	BCR	C16-C15-C14	13.90	151.95	123.47
21	A	845	BCR	C11-C10-C9	13.88	147.11	127.31
21	L	202	BCR	C21-C20-C19	13.74	166.09	123.22
20	2	618	ERG	C15-C14-C8	-13.71	99.66	120.44
21	B	845	BCR	C21-C20-C19	13.69	165.94	123.22
21	B	840	BCR	C21-C20-C19	13.68	165.90	123.22
21	B	842	BCR	C16-C15-C14	13.59	151.30	123.47
21	O	205	BCR	C16-C15-C14	13.52	151.18	123.47
21	L	206	BCR	C11-C10-C9	13.47	146.54	127.31
21	A	846	BCR	C21-C20-C19	13.39	164.99	123.22
21	I	103	BCR	C21-C20-C19	13.26	164.58	123.22
21	B	844	BCR	C16-C15-C14	13.00	150.11	123.47
21	A	857	BCR	C21-C20-C19	12.83	163.26	123.22
21	B	847	BCR	C11-C10-C9	12.79	145.56	127.31
21	A	850	BCR	C21-C20-C19	12.62	162.59	123.22
21	B	844	BCR	C21-C20-C19	12.56	162.41	123.22
21	A	845	BCR	C21-C20-C19	12.45	162.07	123.22
21	2	617	BCR	C16-C15-C14	12.37	148.82	123.47
21	B	840	BCR	C16-C15-C14	12.32	148.70	123.47
21	A	844	BCR	C16-C15-C14	12.27	148.62	123.47
21	L	207	BCR	C21-C20-C19	12.23	161.38	123.22
21	B	843	BCR	C21-C20-C19	12.22	161.34	123.22
21	L	207	BCR	C20-C19-C18	12.20	160.70	126.42
21	A	850	BCR	C20-C19-C18	12.18	160.64	126.42
21	A	846	BCR	C16-C15-C14	12.18	148.43	123.47
21	L	206	BCR	C21-C20-C19	12.13	161.08	123.22
21	A	845	BCR	C16-C15-C14	12.06	148.17	123.47
21	L	202	BCR	C11-C12-C13	11.98	160.06	126.42
21	B	855	BCR	C11-C10-C9	11.97	144.39	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	I	103	BCR	C16-C15-C14	11.93	147.91	123.47
17	3	216	C7Z	C35-C34-C33	-11.87	110.37	127.31
21	A	844	BCR	C20-C19-C18	11.80	159.58	126.42
21	B	841	BCR	C16-C15-C14	11.66	147.37	123.47
16	3	205	CLA	C4A-NA-C1A	11.64	111.94	106.71
21	A	857	BCR	C20-C19-C18	11.64	159.12	126.42
20	1	618	ERG	C12-C13-C17	11.62	133.97	116.57
21	L	206	BCR	C16-C15-C14	11.48	147.00	123.47
21	B	841	BCR	C20-C19-C18	11.44	158.56	126.42
21	B	847	BCR	C8-C7-C6	11.43	159.30	127.20
21	A	844	BCR	C21-C20-C19	11.36	158.68	123.22
21	L	206	BCR	C20-C19-C18	11.33	158.26	126.42
21	2	617	BCR	C11-C10-C9	11.25	143.36	127.31
21	L	202	BCR	C16-C15-C14	11.21	146.44	123.47
21	B	841	BCR	C21-C20-C19	11.11	157.88	123.22
21	B	844	BCR	C20-C19-C18	11.11	157.62	126.42
21	A	857	BCR	C16-C15-C14	11.07	146.15	123.47
21	I	103	BCR	C11-C12-C13	11.03	157.41	126.42
21	A	857	BCR	C11-C10-C9	11.03	143.05	127.31
20	2	621	ERG	C15-C14-C8	-11.00	103.78	120.44
21	A	845	BCR	C20-C19-C18	10.92	157.10	126.42
16	3	210	CLA	C4A-NA-C1A	10.84	111.58	106.71
21	L	206	BCR	C11-C12-C13	10.82	156.82	126.42
21	B	843	BCR	C20-C19-C18	10.80	156.77	126.42
21	F	203	BCR	C11-C12-C13	10.75	156.61	126.42
21	2	617	BCR	C11-C12-C13	10.72	156.52	126.42
16	1	606	CLA	C4A-NA-C1A	10.70	111.52	106.71
21	F	206	BCR	C16-C15-C14	10.70	145.40	123.47
16	A	818	CLA	C4A-NA-C1A	10.66	111.50	106.71
21	B	845	BCR	C16-C15-C14	10.47	144.93	123.47
16	B	804	CLA	C4A-NA-C1A	10.46	111.41	106.71
21	F	203	BCR	C16-C15-C14	10.46	144.89	123.47
21	B	845	BCR	C20-C19-C18	10.44	155.75	126.42
21	B	840	BCR	C20-C19-C18	10.37	155.56	126.42
21	B	847	BCR	C11-C12-C13	10.35	155.49	126.42
21	L	207	BCR	C11-C10-C9	10.34	142.07	127.31
21	A	850	BCR	C11-C12-C13	10.32	155.40	126.42
16	B	809	CLA	C4A-NA-C1A	10.30	111.33	106.71
21	A	846	BCR	C20-C19-C18	10.29	155.32	126.42
16	B	821	CLA	C4A-NA-C1A	10.23	111.31	106.71
21	L	202	BCR	C20-C19-C18	10.21	155.10	126.42
21	A	846	BCR	C11-C12-C13	10.18	155.00	126.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	J	102	CLA	C4A-NA-C1A	10.15	111.27	106.71
21	O	205	BCR	C20-C19-C18	10.13	154.89	126.42
21	B	842	BCR	C11-C10-C9	10.10	141.73	127.31
21	B	844	BCR	C11-C10-C9	10.05	141.66	127.31
16	2	606	CLA	C4A-NA-C1A	10.04	111.22	106.71
16	F	202	CLA	C4A-NA-C1A	10.04	111.22	106.71
16	1	610	CLA	C4A-NA-C1A	10.02	111.21	106.71
21	B	844	BCR	C11-C12-C13	10.02	154.56	126.42
21	A	850	BCR	C11-C10-C9	9.98	141.56	127.31
16	B	825	CLA	C4A-NA-C1A	9.95	111.18	106.71
16	A	812	CLA	C4A-NA-C1A	9.94	111.18	106.71
16	3	203	CLA	C4A-NA-C1A	9.94	111.17	106.71
21	L	207	BCR	C11-C12-C13	9.89	154.19	126.42
21	B	842	BCR	C21-C20-C19	9.88	154.04	123.22
21	B	841	BCR	C11-C10-C9	9.87	141.39	127.31
16	A	815	CLA	C4A-NA-C1A	9.86	111.14	106.71
21	B	845	BCR	C11-C10-C9	9.85	141.36	127.31
16	2	604	CLA	C4A-NA-C1A	9.84	111.13	106.71
16	2	611	CLA	C4A-NA-C1A	9.83	111.13	106.71
16	2	610	CLA	C4A-NA-C1A	9.82	111.12	106.71
16	B	837	CLA	C4A-NA-C1A	9.82	111.12	106.71
16	A	803	CLA	C4A-NA-C1A	9.81	111.12	106.71
21	B	842	BCR	C20-C19-C18	9.81	153.96	126.42
16	O	201	CLA	C4A-NA-C1A	9.80	111.11	106.71
16	2	613	CLA	C4A-NA-C1A	9.79	111.11	106.71
21	A	845	BCR	C11-C12-C13	9.77	153.86	126.42
16	A	835	CLA	C4A-NA-C1A	9.69	111.06	106.71
21	B	855	BCR	C21-C20-C19	9.68	153.44	123.22
16	A	802	CLA	C4A-NA-C1A	9.68	111.06	106.71
21	F	206	BCR	C20-C19-C18	9.67	153.59	126.42
21	B	841	BCR	C11-C12-C13	9.65	153.54	126.42
16	L	205	CLA	C4A-NA-C1A	9.65	111.04	106.71
16	B	831	CLA	C4A-NA-C1A	9.64	111.04	106.71
16	A	826	CLA	C4A-NA-C1A	9.62	111.03	106.71
16	3	211	CLA	C4A-NA-C1A	9.62	111.03	106.71
16	A	820	CLA	C4A-NA-C1A	9.62	111.03	106.71
16	B	802	CLA	C4A-NA-C1A	9.60	111.02	106.71
16	F	205	CLA	C4A-NA-C1A	9.60	111.02	106.71
16	A	805	CLA	C4A-NA-C1A	9.59	111.02	106.71
17	3	216	C7Z	C11-C10-C9	-9.54	113.69	127.31
16	B	808	CLA	C4A-NA-C1A	9.54	111.00	106.71
16	3	213	CLA	C4A-NA-C1A	9.54	110.99	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	605	CLA	C4A-NA-C1A	9.51	110.98	106.71
17	3	216	C7Z	C31-C30-C29	-9.50	113.75	127.31
16	3	212	CLA	C4A-NA-C1A	9.50	110.98	106.71
16	A	810	CLA	C4A-NA-C1A	9.48	110.97	106.71
16	B	820	CLA	C4A-NA-C1A	9.47	110.96	106.71
21	B	847	BCR	C20-C19-C18	9.44	152.93	126.42
16	A	819	CLA	C4A-NA-C1A	9.42	110.94	106.71
16	A	814	CLA	C4A-NA-C1A	9.41	110.94	106.71
16	B	812	CLA	C4A-NA-C1A	9.41	110.94	106.71
16	A	811	CLA	C4A-NA-C1A	9.37	110.92	106.71
16	A	821	CLA	C4A-NA-C1A	9.36	110.92	106.71
16	B	818	CLA	C4A-NA-C1A	9.35	110.91	106.71
21	O	205	BCR	C11-C12-C13	9.34	152.65	126.42
21	B	843	BCR	C11-C12-C13	9.34	152.64	126.42
16	A	839	CLA	C4A-NA-C1A	9.33	110.90	106.71
21	B	855	BCR	C20-C19-C18	9.30	152.55	126.42
16	B	807	CLA	C4A-NA-C1A	9.30	110.89	106.71
20	2	618	ERG	C14-C13-C17	9.29	109.63	99.72
16	3	209	CLA	C4A-NA-C1A	9.29	110.88	106.71
16	2	609	CLA	C4A-NA-C1A	9.28	110.88	106.71
16	3	206	CLA	C4A-NA-C1A	9.26	110.87	106.71
16	B	817	CLA	C4A-NA-C1A	9.24	110.86	106.71
16	1	602	CLA	C4A-NA-C1A	9.24	110.86	106.71
16	2	607	CLA	C4A-NA-C1A	9.24	110.86	106.71
16	B	833	CLA	C4A-NA-C1A	9.23	110.86	106.71
16	B	834	CLA	C4A-NA-C1A	9.21	110.84	106.71
16	1	611	CLA	C4A-NA-C1A	9.20	110.84	106.71
16	I	101	CLA	C4A-NA-C1A	9.19	110.84	106.71
16	A	854	CLA	C4A-NA-C1A	9.18	110.83	106.71
16	B	826	CLA	C4A-NA-C1A	9.18	110.83	106.71
16	A	856	CLA	C4A-NA-C1A	9.17	110.83	106.71
16	A	829	CLA	C4A-NA-C1A	9.17	110.83	106.71
16	B	805	CLA	C4A-NA-C1A	9.17	110.83	106.71
16	F	204	CLA	C4A-NA-C1A	9.16	110.82	106.71
16	3	214	CLA	C4A-NA-C1A	9.15	110.82	106.71
21	B	840	BCR	C11-C12-C13	9.13	152.07	126.42
16	K	101	CLA	C4A-NA-C1A	9.12	110.81	106.71
16	A	827	CLA	C4A-NA-C1A	9.11	110.80	106.71
21	F	203	BCR	C20-C19-C18	9.10	151.99	126.42
16	A	822	CLA	C4A-NA-C1A	9.09	110.79	106.71
16	B	801	CLA	C4A-NA-C1A	9.08	110.79	106.71
21	I	103	BCR	C11-C10-C9	9.08	140.26	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	814	CLA	C4A-NA-C1A	9.08	110.79	106.71
16	1	604	CLA	C4A-NA-C1A	9.05	110.78	106.71
16	B	824	CLA	C4A-NA-C1A	9.05	110.77	106.71
16	O	204	CLA	C4A-NA-C1A	9.04	110.77	106.71
16	A	823	CLA	C4A-NA-C1A	9.04	110.77	106.71
16	2	601	CLA	C4A-NA-C1A	9.02	110.76	106.71
16	A	825	CLA	C4A-NA-C1A	9.02	110.76	106.71
16	1	601	CLA	C4A-NA-C1A	9.01	110.76	106.71
21	2	617	BCR	C23-C22-C21	9.01	132.77	118.94
16	O	202	CLA	C4A-NA-C1A	8.99	110.75	106.71
16	A	824	CLA	C4A-NA-C1A	8.96	110.73	106.71
16	3	204	CLA	C4A-NA-C1A	8.94	110.73	106.71
16	A	838	CLA	C4A-NA-C1A	8.94	110.73	106.71
16	B	819	CLA	C4A-NA-C1A	8.94	110.72	106.71
16	B	828	CLA	C4A-NA-C1A	8.94	110.72	106.71
16	A	830	CLA	C4A-NA-C1A	8.93	110.72	106.71
21	K	104	BCR	C20-C19-C18	8.92	151.49	126.42
16	O	203	CLA	C4A-NA-C1A	8.92	110.72	106.71
16	A	836	CLA	C4A-NA-C1A	8.92	110.72	106.71
16	K	102	CLA	C4A-NA-C1A	8.90	110.71	106.71
16	B	836	CLA	C4A-NA-C1A	8.89	110.70	106.71
16	2	612	CLA	C4A-NA-C1A	8.89	110.70	106.71
21	I	103	BCR	C2-C1-C6	-8.89	96.80	110.48
16	B	823	CLA	C4A-NA-C1A	8.88	110.70	106.71
16	A	813	CLA	C4A-NA-C1A	8.87	110.69	106.71
16	L	203	CLA	C4A-NA-C1A	8.87	110.69	106.71
16	A	807	CLA	C4A-NA-C1A	8.86	110.69	106.71
21	O	205	BCR	C11-C10-C9	8.86	139.95	127.31
16	3	208	CLA	C4A-NA-C1A	8.84	110.68	106.71
16	A	809	CLA	C4A-NA-C1A	8.83	110.67	106.71
16	B	810	CLA	C4A-NA-C1A	8.82	110.67	106.71
16	B	806	CLA	C4A-NA-C1A	8.81	110.67	106.71
16	L	204	CLA	C4A-NA-C1A	8.81	110.67	106.71
16	1	607	CLA	C4A-NA-C1A	8.80	110.66	106.71
16	A	816	CLA	C4A-NA-C1A	8.77	110.65	106.71
16	B	835	CLA	C4A-NA-C1A	8.77	110.65	106.71
16	B	811	CLA	C4A-NA-C1A	8.76	110.64	106.71
16	B	815	CLA	C4A-NA-C1A	8.76	110.64	106.71
16	A	831	CLA	C4A-NA-C1A	8.76	110.64	106.71
21	K	104	BCR	C12-C13-C14	8.74	132.35	118.94
16	B	813	CLA	C4A-NA-C1A	8.72	110.63	106.71
21	B	843	BCR	C11-C10-C9	8.72	139.75	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	618	ERG	C14-C13-C17	8.71	109.01	99.72
21	B	847	BCR	C21-C20-C19	8.71	150.40	123.22
16	3	207	CLA	C4A-NA-C1A	8.71	110.62	106.71
17	1	616	C7Z	C15-C14-C13	-8.70	114.89	127.31
16	A	806	CLA	C4A-NA-C1A	8.70	110.62	106.71
16	A	832	CLA	C4A-NA-C1A	8.70	110.62	106.71
16	F	201	CLA	C4A-NA-C1A	8.69	110.61	106.71
21	B	842	BCR	C11-C12-C13	8.68	150.81	126.42
16	2	605	CLA	C4A-NA-C1A	8.68	110.61	106.71
16	1	608	CLA	C4A-NA-C1A	8.67	110.60	106.71
16	B	803	CLA	C4A-NA-C1A	8.67	110.60	106.71
21	A	845	BCR	C2-C1-C6	-8.66	97.14	110.48
16	2	608	CLA	C4A-NA-C1A	8.66	110.60	106.71
16	B	838	CLA	C4A-NA-C1A	8.66	110.60	106.71
16	1	603	CLA	C4A-NA-C1A	8.61	110.58	106.71
16	2	603	CLA	C4A-NA-C1A	8.61	110.58	106.71
16	A	808	CLA	C4A-NA-C1A	8.60	110.57	106.71
16	B	830	CLA	C4A-NA-C1A	8.58	110.56	106.71
21	K	104	BCR	C21-C20-C19	8.58	149.99	123.22
16	L	201	CLA	C4A-NA-C1A	8.57	110.56	106.71
16	B	822	CLA	C4A-NA-C1A	8.53	110.54	106.71
16	A	834	CLA	C4A-NA-C1A	8.48	110.52	106.71
16	B	832	CLA	C4A-NA-C1A	8.46	110.51	106.71
16	2	602	CLA	C4A-NA-C1A	8.45	110.50	106.71
16	1	609	CLA	C4A-NA-C1A	8.44	110.50	106.71
16	A	833	CLA	C4A-NA-C1A	8.39	110.48	106.71
16	B	827	CLA	C4A-NA-C1A	8.38	110.47	106.71
16	A	837	CLA	C4A-NA-C1A	8.37	110.47	106.71
16	B	829	CLA	C4A-NA-C1A	8.32	110.45	106.71
16	I	102	CLA	C4A-NA-C1A	8.30	110.44	106.71
16	A	828	CLA	C4A-NA-C1A	8.22	110.40	106.71
16	A	804	CLA	C4A-NA-C1A	8.17	110.38	106.71
21	A	857	BCR	C34-C9-C10	-8.12	111.55	122.92
21	2	617	BCR	C37-C22-C21	-8.07	111.62	122.92
16	A	817	CLA	C4A-NA-C1A	8.07	110.33	106.71
21	A	857	BCR	C11-C12-C13	8.06	149.07	126.42
21	A	857	BCR	C34-C9-C8	8.03	130.73	118.08
21	B	855	BCR	C11-C12-C13	8.00	148.88	126.42
21	A	844	BCR	C11-C12-C13	7.95	148.76	126.42
20	1	618	ERG	C15-C14-C8	-7.95	108.40	120.44
16	B	816	CLA	C4A-NA-C1A	7.94	110.27	106.71
26	A	801	CL0	C4A-NA-C1A	7.93	110.27	106.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	201	C7Z	C11-C10-C9	-7.72	116.30	127.31
17	J	104	C7Z	C15-C14-C13	-7.62	116.44	127.31
16	A	855	CLA	C4A-NA-C1A	7.61	110.13	106.71
21	2	617	BCR	C19-C18-C17	7.60	130.60	118.94
17	2	615	C7Z	C35-C34-C33	-7.60	116.47	127.31
21	A	850	BCR	C30-C25-C26	-7.57	111.96	122.61
21	A	844	BCR	C11-C10-C9	7.56	138.10	127.31
26	A	801	CL0	CMD-C2D-C1D	7.52	137.96	124.71
17	1	615	C7Z	C7-C8-C9	-7.45	114.98	126.23
17	1	616	C7Z	C31-C30-C29	-7.41	116.74	127.31
20	2	618	ERG	C19-C10-C9	-7.39	98.61	111.03
21	2	617	BCR	C21-C20-C19	7.32	146.08	123.22
20	2	621	ERG	C19-C10-C9	-7.31	98.74	111.03
18	J	103	RRX	C35-C13-C14	-7.30	112.69	122.92
20	1	618	ERG	C13-C17-C20	-7.25	110.08	119.43
21	A	857	BCR	C1-C6-C5	-7.19	112.48	122.61
18	A	847	RRX	C11-C10-C9	-7.14	117.12	127.31
17	2	614	C7Z	C35-C34-C33	-7.12	117.15	127.31
21	B	845	BCR	C12-C13-C14	7.10	129.84	118.94
20	1	618	ERG	C18-C13-C14	-7.09	98.75	110.24
21	B	847	BCR	C27-C26-C25	-7.04	112.52	122.73
17	3	217	C7Z	C35-C34-C33	-7.00	117.32	127.31
17	1	616	C7Z	C35-C34-C33	-6.96	117.38	127.31
18	J	103	RRX	C12-C13-C14	6.95	129.60	118.94
18	1	613	RRX	C30-C25-C26	-6.93	112.85	122.61
21	2	617	BCR	C20-C19-C18	6.92	145.85	126.42
21	A	857	BCR	C28-C27-C26	-6.88	101.78	114.08
21	K	104	BCR	C35-C13-C14	-6.84	113.34	122.92
18	A	847	RRX	C1-C6-C5	-6.81	113.02	122.61
21	I	103	BCR	C20-C19-C18	6.79	145.48	126.42
17	3	217	C7Z	C27-C28-C29	-6.77	116.00	126.23
21	B	845	BCR	C11-C12-C13	6.76	145.40	126.42
18	J	103	RRX	C16-C15-C14	-6.71	109.72	123.47
21	A	846	BCR	C11-C10-C9	6.69	136.86	127.31
18	K	103	RRX	C30-C25-C26	-6.60	113.32	122.61
17	J	104	C7Z	C31-C30-C29	-6.59	117.91	127.31
21	B	847	BCR	C30-C25-C26	-6.57	113.35	122.61
21	B	855	BCR	C19-C18-C17	6.56	129.00	118.94
17	3	218	C7Z	C31-C30-C29	-6.52	118.00	127.31
20	2	621	ERG	C19-C10-C1	-6.51	99.15	109.43
17	1	616	C7Z	C27-C28-C29	-6.49	116.43	126.23
21	A	850	BCR	C1-C6-C5	-6.47	113.50	122.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	615	C7Z	C31-C30-C29	-6.43	118.14	127.31
17	2	615	C7Z	C38-C25-C26	-6.38	117.36	124.53
18	A	847	RRX	C19-C18-C17	-6.38	109.15	118.94
16	A	810	CLA	O2D-CGD-CBD	6.34	122.53	111.27
17	1	615	C7Z	C31-C30-C29	-6.30	118.32	127.31
17	1	614	C7Z	C31-C30-C29	-6.29	118.33	127.31
21	B	843	BCR	C15-C14-C13	-6.29	118.33	127.31
21	F	203	BCR	C19-C18-C17	6.28	128.58	118.94
18	A	847	RRX	C8-C9-C10	6.25	128.54	118.94
21	A	845	BCR	C28-C27-C26	-6.25	102.92	114.08
17	2	614	C7Z	C31-C30-C29	-6.23	118.42	127.31
18	2	616	RRX	C15-C14-C13	-6.19	118.47	127.31
16	2	601	CLA	O2D-CGD-CBD	6.17	122.23	111.27
26	A	801	CL0	C2D-C1D-ND	6.15	114.64	110.10
18	A	847	RRX	C20-C21-C22	-6.12	118.58	127.31
17	1	614	C7Z	C35-C34-C33	-6.10	118.61	127.31
21	K	104	BCR	C19-C18-C17	6.09	128.28	118.94
17	3	215	C7Z	C15-C14-C13	-6.08	118.63	127.31
16	A	807	CLA	O2D-CGD-CBD	6.04	122.00	111.27
17	3	216	C7Z	C27-C28-C29	-6.02	117.14	126.23
17	1	616	C7Z	C11-C10-C9	-6.00	118.74	127.31
16	B	819	CLA	O2D-CGD-CBD	6.00	121.92	111.27
17	3	201	C7Z	C18-C5-C6	-5.96	117.84	124.53
16	B	838	CLA	O2D-CGD-CBD	5.96	121.85	111.27
16	3	210	CLA	CMA-C3A-C4A	5.96	127.78	111.77
17	A	843	C7Z	C31-C30-C29	-5.94	118.84	127.31
16	A	834	CLA	O2D-CGD-CBD	5.92	121.78	111.27
17	3	216	C7Z	C35-C15-C14	-5.91	111.36	123.47
16	B	837	CLA	CMD-C2D-C1D	5.89	135.10	124.71
18	J	103	RRX	C11-C10-C9	-5.89	118.91	127.31
21	K	104	BCR	C30-C25-C26	-5.88	114.33	122.61
20	1	618	ERG	C12-C13-C14	5.87	116.58	107.27
17	3	217	C7Z	C31-C30-C29	-5.87	118.94	127.31
16	3	211	CLA	O2D-CGD-CBD	5.86	121.68	111.27
17	3	218	C7Z	C11-C10-C9	-5.84	118.97	127.31
17	3	215	C7Z	C31-C30-C29	-5.83	118.98	127.31
16	1	604	CLA	O2D-CGD-CBD	5.83	121.62	111.27
21	K	104	BCR	C16-C15-C14	5.82	135.40	123.47
17	3	215	C7Z	C38-C25-C26	-5.82	118.00	124.53
16	B	819	CLA	CMD-C2D-C1D	5.80	134.94	124.71
16	A	818	CLA	CMA-C3A-C4A	5.79	127.34	111.77
16	O	203	CLA	CMD-C2D-C1D	5.76	134.86	124.71

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	613	RRX	C35-C13-C14	-5.76	114.86	122.92
17	3	216	C7Z	C7-C8-C9	-5.74	117.56	126.23
16	B	805	CLA	O2D-CGD-CBD	5.74	121.46	111.27
20	1	618	ERG	C14-C8-C9	-5.74	106.02	114.66
21	B	845	BCR	C35-C13-C14	-5.73	114.89	122.92
16	A	835	CLA	O2D-CGD-CBD	5.73	121.45	111.27
16	F	202	CLA	CMA-C3A-C4A	5.72	127.15	111.77
16	A	830	CLA	O2D-CGD-CBD	5.71	121.42	111.27
16	1	602	CLA	O2D-CGD-CBD	5.69	121.38	111.27
16	A	804	CLA	CMD-C2D-C1D	5.68	134.73	124.71
16	B	829	CLA	CMD-C2D-C1D	5.68	134.72	124.71
16	2	608	CLA	O2D-CGD-CBD	5.67	121.34	111.27
16	3	207	CLA	CMD-C2D-C1D	5.67	134.70	124.71
16	A	817	CLA	O2D-CGD-CBD	5.66	121.33	111.27
16	A	815	CLA	CMD-C2D-C1D	5.65	134.68	124.71
16	A	819	CLA	O2D-CGD-CBD	5.65	121.31	111.27
16	B	818	CLA	O2A-C1-C2	5.65	123.47	108.64
17	1	612	C7Z	C38-C25-C26	-5.64	118.20	124.53
21	A	845	BCR	C32-C1-C31	5.63	125.81	108.53
16	B	813	CLA	O2D-CGD-CBD	5.63	121.27	111.27
16	B	808	CLA	O2D-CGD-CBD	5.60	121.22	111.27
17	1	614	C7Z	C7-C8-C9	-5.59	117.80	126.23
16	F	202	CLA	O2D-CGD-CBD	5.58	121.19	111.27
16	A	817	CLA	CMD-C2D-C1D	5.58	134.55	124.71
21	F	206	BCR	C11-C12-C13	5.58	142.09	126.42
16	B	806	CLA	CMD-C2D-C1D	5.58	134.54	124.71
21	K	104	BCR	C27-C26-C25	-5.56	114.65	122.73
16	3	204	CLA	CMD-C2D-C1D	5.56	134.51	124.71
16	B	816	CLA	CMD-C2D-C1D	5.55	134.49	124.71
16	2	602	CLA	CMD-C2D-C1D	5.55	134.49	124.71
16	B	818	CLA	CMD-C2D-C1D	5.54	134.47	124.71
21	A	850	BCR	C4-C5-C6	-5.54	114.69	122.73
16	A	823	CLA	CMD-C2D-C1D	5.53	134.46	124.71
26	A	801	CL0	C2C-C1C-NC	5.52	115.15	109.97
16	B	835	CLA	CMD-C2D-C1D	5.52	134.44	124.71
17	3	217	C7Z	C38-C25-C26	-5.52	118.33	124.53
21	F	206	BCR	C12-C13-C14	5.52	127.41	118.94
17	3	218	C7Z	C15-C14-C13	-5.52	119.44	127.31
17	1	614	C7Z	C15-C14-C13	-5.51	119.44	127.31
16	B	821	CLA	O2D-CGD-CBD	5.50	121.05	111.27
21	I	103	BCR	C32-C1-C31	5.49	125.38	108.53
16	2	613	CLA	O2D-CGD-CBD	5.49	121.03	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	F	203	BCR	C28-C27-C26	-5.49	104.28	114.08
16	A	813	CLA	CMD-C2D-C1D	5.48	134.38	124.71
16	3	208	CLA	CMD-C2D-C1D	5.48	134.38	124.71
16	L	204	CLA	CMD-C2D-C1D	5.48	134.37	124.71
16	3	206	CLA	CMD-C2D-C1D	5.48	134.37	124.71
16	B	806	CLA	O2D-CGD-CBD	5.48	121.00	111.27
16	2	603	CLA	CMD-C2D-C1D	5.48	134.37	124.71
16	A	819	CLA	CMD-C2D-C1D	5.47	134.36	124.71
16	B	832	CLA	CMD-C2D-C1D	5.47	134.35	124.71
16	L	205	CLA	CMD-C2D-C1D	5.47	134.35	124.71
16	A	808	CLA	O2D-CGD-CBD	5.47	120.99	111.27
16	A	838	CLA	O2D-CGD-CBD	5.47	120.98	111.27
16	2	604	CLA	O2D-CGD-CBD	5.47	120.98	111.27
16	A	806	CLA	O2D-CGD-CBD	5.47	120.98	111.27
16	3	212	CLA	CMD-C2D-C1D	5.47	134.34	124.71
16	A	856	CLA	O2D-CGD-CBD	5.46	120.98	111.27
16	2	612	CLA	CMD-C2D-C1D	5.46	134.33	124.71
16	A	806	CLA	CMD-C2D-C1D	5.46	134.33	124.71
16	B	811	CLA	CMD-C2D-C1D	5.45	134.32	124.71
16	B	837	CLA	O2D-CGD-CBD	5.45	120.95	111.27
16	A	822	CLA	O2D-CGD-CBD	5.44	120.94	111.27
16	B	835	CLA	O2D-CGD-CBD	5.44	120.93	111.27
16	A	818	CLA	CMD-C2D-C1D	5.42	134.27	124.71
17	3	216	C7Z	C38-C25-C26	-5.42	118.45	124.53
16	O	204	CLA	CMD-C2D-C1D	5.41	134.25	124.71
16	A	832	CLA	CMD-C2D-C1D	5.41	134.25	124.71
16	3	213	CLA	CMD-C2D-C1D	5.41	134.24	124.71
16	A	836	CLA	CMD-C2D-C1D	5.41	134.24	124.71
21	L	202	BCR	C11-C10-C9	5.40	135.02	127.31
16	B	826	CLA	CMD-C2D-C1D	5.40	134.23	124.71
16	3	203	CLA	CMD-C2D-C1D	5.40	134.22	124.71
16	3	214	CLA	CMD-C2D-C1D	5.39	134.22	124.71
16	L	203	CLA	CMD-C2D-C1D	5.39	134.21	124.71
16	B	829	CLA	O2D-CGD-CBD	5.39	120.84	111.27
17	1	615	C7Z	C27-C28-C29	-5.38	118.10	126.23
16	L	201	CLA	CMD-C2D-C1D	5.38	134.19	124.71
21	A	846	BCR	C34-C9-C10	-5.38	115.39	122.92
16	A	834	CLA	CMD-C2D-C1D	5.36	134.17	124.71
16	2	606	CLA	CMD-C2D-C1D	5.36	134.16	124.71
18	J	103	RRX	C15-C16-C17	5.36	134.45	123.47
16	O	201	CLA	CMD-C2D-C1D	5.36	134.15	124.71
16	B	834	CLA	O2D-CGD-CBD	5.35	120.78	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	816	CLA	O2D-CGD-CBD	5.35	120.77	111.27
16	B	805	CLA	CMD-C2D-C1D	5.35	134.14	124.71
16	I	101	CLA	CMD-C2D-C1D	5.34	134.13	124.71
16	A	810	CLA	CMD-C2D-C1D	5.34	134.13	124.71
16	A	831	CLA	CMD-C2D-C1D	5.34	134.13	124.71
16	1	603	CLA	CMD-C2D-C1D	5.34	134.13	124.71
16	2	605	CLA	CMD-C2D-C1D	5.34	134.12	124.71
16	O	202	CLA	CMD-C2D-C1D	5.33	134.11	124.71
16	A	833	CLA	CMD-C2D-C1D	5.33	134.11	124.71
16	3	205	CLA	CMD-C2D-C1D	5.33	134.11	124.71
18	A	847	RRX	C38-C26-C25	-5.33	118.54	124.53
16	A	816	CLA	CMD-C2D-C1D	5.33	134.11	124.71
17	A	843	C7Z	C27-C28-C29	-5.33	118.18	126.23
16	B	814	CLA	CMD-C2D-C1D	5.33	134.10	124.71
16	A	828	CLA	CMD-C2D-C1D	5.33	134.10	124.71
16	A	803	CLA	CMD-C2D-C1D	5.33	134.10	124.71
17	2	614	C7Z	C38-C25-C26	-5.32	118.55	124.53
16	A	802	CLA	O2D-CGD-CBD	5.32	120.72	111.27
16	B	831	CLA	O2D-CGD-CBD	5.32	120.72	111.27
16	B	820	CLA	CMD-C2D-C1D	5.32	134.08	124.71
17	J	104	C7Z	C27-C28-C29	-5.31	118.20	126.23
16	B	824	CLA	CMD-C2D-C1D	5.31	134.08	124.71
16	A	804	CLA	O2A-C1-C2	5.31	122.60	108.64
16	A	816	CLA	O2D-CGD-CBD	5.31	120.70	111.27
16	1	604	CLA	CMD-C2D-C1D	5.31	134.07	124.71
16	A	814	CLA	O2D-CGD-CBD	5.30	120.69	111.27
18	J	103	RRX	C38-C26-C25	-5.30	118.58	124.53
16	B	834	CLA	CMD-C2D-C1D	5.30	134.04	124.71
16	A	832	CLA	O2D-CGD-CBD	5.29	120.68	111.27
16	1	602	CLA	CMD-C2D-C1D	5.28	134.02	124.71
16	2	610	CLA	CMD-C2D-C1D	5.28	134.01	124.71
16	A	826	CLA	O2D-CGD-CBD	5.28	120.65	111.27
16	1	610	CLA	CMD-C2D-C1D	5.28	134.01	124.71
16	F	205	CLA	O2D-CGD-CBD	5.27	120.64	111.27
16	2	608	CLA	CMD-C2D-C1D	5.27	134.01	124.71
16	B	809	CLA	CMA-C3A-C4A	5.27	125.94	111.77
16	B	838	CLA	CMD-C2D-C1D	5.26	133.99	124.71
16	3	212	CLA	O2D-CGD-CBD	5.26	120.62	111.27
17	3	216	C7Z	C31-C32-C33	-5.26	111.64	126.42
16	1	606	CLA	O2D-CGD-CBD	5.26	120.61	111.27
16	3	210	CLA	CMD-C2D-C1D	5.26	133.98	124.71
16	2	601	CLA	CMD-C2D-C1D	5.26	133.98	124.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	837	CLA	CMD-C2D-C1D	5.26	133.98	124.71
16	B	802	CLA	CMD-C2D-C1D	5.26	133.97	124.71
16	A	805	CLA	CMD-C2D-C1D	5.25	133.97	124.71
16	2	609	CLA	CMD-C2D-C1D	5.25	133.97	124.71
16	A	822	CLA	CMD-C2D-C1D	5.25	133.97	124.71
16	B	809	CLA	CMD-C2D-C1D	5.25	133.97	124.71
16	1	611	CLA	CMD-C2D-C1D	5.25	133.97	124.71
18	2	616	RRX	C11-C10-C9	-5.25	119.82	127.31
16	A	808	CLA	CMD-C2D-C1D	5.24	133.94	124.71
16	B	837	CLA	CMA-C3A-C4A	5.23	125.83	111.77
16	J	102	CLA	CMA-C3A-C4A	5.22	125.81	111.77
16	K	101	CLA	O2D-CGD-CBD	5.22	120.55	111.27
16	1	609	CLA	CMD-C2D-C1D	5.22	133.92	124.71
17	1	614	C7Z	C18-C5-C6	-5.22	118.66	124.53
16	A	809	CLA	CMD-C2D-C1D	5.22	133.92	124.71
16	B	803	CLA	CMD-C2D-C1D	5.22	133.91	124.71
16	2	613	CLA	CMD-C2D-C1D	5.22	133.91	124.71
16	B	808	CLA	CMD-C2D-C1D	5.22	133.91	124.71
16	K	102	CLA	CMD-C2D-C1D	5.22	133.91	124.71
16	2	611	CLA	CMD-C2D-C1D	5.21	133.90	124.71
16	3	210	CLA	O2D-CGD-CBD	5.21	120.53	111.27
20	2	618	ERG	C12-C13-C14	5.21	115.53	107.27
16	B	832	CLA	O2A-C1-C2	5.21	122.32	108.64
16	B	821	CLA	CMA-C3A-C4A	5.20	125.76	111.77
16	A	816	CLA	O2A-C1-C2	5.20	122.31	108.64
16	B	807	CLA	CMD-C2D-C1D	5.20	133.88	124.71
16	B	836	CLA	CMD-C2D-C1D	5.20	133.87	124.71
16	A	824	CLA	CMD-C2D-C1D	5.20	133.87	124.71
16	K	101	CLA	CMD-C2D-C1D	5.19	133.87	124.71
16	A	820	CLA	CMD-C2D-C1D	5.19	133.87	124.71
16	A	811	CLA	CMD-C2D-C1D	5.19	133.87	124.71
17	3	218	C7Z	C35-C34-C33	-5.19	119.91	127.31
16	J	102	CLA	O2D-CGD-CBD	5.19	120.48	111.27
16	B	825	CLA	O2D-CGD-CBD	5.18	120.47	111.27
17	1	615	C7Z	C1-C6-C5	-5.18	115.32	122.61
16	B	822	CLA	CMD-C2D-C1D	5.17	133.82	124.71
16	3	203	CLA	O2D-CGD-CBD	5.17	120.45	111.27
16	B	810	CLA	CMD-C2D-C1D	5.17	133.82	124.71
16	F	205	CLA	CMD-C2D-C1D	5.16	133.81	124.71
17	1	612	C7Z	C32-C33-C34	5.16	126.86	118.94
16	A	838	CLA	CMD-C2D-C1D	5.15	133.79	124.71
16	A	814	CLA	CMD-C2D-C1D	5.15	133.79	124.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	3	211	CLA	CMD-C2D-C1D	5.15	133.79	124.71
16	1	608	CLA	CMD-C2D-C1D	5.15	133.79	124.71
26	A	801	CL0	O2A-CGA-O1A	-5.15	110.61	123.59
16	A	803	CLA	O2D-CGD-CBD	5.14	120.41	111.27
16	1	601	CLA	CMD-C2D-C1D	5.14	133.78	124.71
16	3	209	CLA	CMD-C2D-C1D	5.14	133.78	124.71
16	1	603	CLA	O2D-CGD-CBD	5.14	120.41	111.27
16	I	102	CLA	O2D-CGD-CBD	5.14	120.40	111.27
16	3	214	CLA	O2D-CGD-CBD	5.14	120.40	111.27
16	A	831	CLA	O2D-CGD-CBD	5.14	120.39	111.27
26	A	801	CL0	C1C-C2C-C3C	-5.13	101.56	106.96
16	J	102	CLA	CMD-C2D-C1D	5.13	133.76	124.71
16	A	836	CLA	O2D-CGD-CBD	5.13	120.38	111.27
16	B	832	CLA	O2D-CGD-CBD	5.13	120.38	111.27
16	B	828	CLA	CMD-C2D-C1D	5.12	133.74	124.71
16	A	833	CLA	O2A-C1-C2	5.12	122.10	108.64
16	B	821	CLA	CMD-C2D-C1D	5.12	133.73	124.71
16	B	827	CLA	CMD-C2D-C1D	5.11	133.72	124.71
16	B	813	CLA	CMD-C2D-C1D	5.11	133.72	124.71
18	J	103	RRX	C19-C18-C17	-5.11	111.10	118.94
16	A	827	CLA	CMD-C2D-C1D	5.11	133.71	124.71
16	A	835	CLA	CMD-C2D-C1D	5.11	133.71	124.71
16	B	836	CLA	O2D-CGD-CBD	5.10	120.34	111.27
16	A	825	CLA	CMD-C2D-C1D	5.10	133.69	124.71
17	3	218	C7Z	C21-C26-C25	-5.09	115.44	122.61
16	B	818	CLA	O2D-CGD-CBD	5.09	120.31	111.27
20	2	621	ERG	C1-C10-C9	5.09	118.82	108.28
16	A	813	CLA	O2D-CGD-CBD	5.08	120.30	111.27
16	A	829	CLA	CMD-C2D-C1D	5.08	133.67	124.71
16	B	810	CLA	O2D-CGD-CBD	5.08	120.30	111.27
16	A	821	CLA	CMD-C2D-C1D	5.08	133.66	124.71
16	A	820	CLA	O2D-CGD-CBD	5.07	120.28	111.27
16	A	833	CLA	O2D-CGD-CBD	5.07	120.27	111.27
16	F	204	CLA	O2D-CGD-CBD	5.07	120.27	111.27
16	B	820	CLA	O2D-CGD-CBD	5.06	120.26	111.27
16	A	809	CLA	O2D-CGD-CBD	5.06	120.26	111.27
16	I	102	CLA	CMD-C2D-C1D	5.05	133.62	124.71
16	I	101	CLA	O2D-CGD-CBD	5.05	120.25	111.27
18	K	103	RRX	C1-C6-C5	-5.05	115.50	122.61
17	A	843	C7Z	C7-C8-C9	-5.05	118.61	126.23
16	A	808	CLA	O2A-C1-C2	5.05	121.90	108.64
17	A	843	C7Z	C21-C26-C25	-5.04	115.51	122.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	817	CLA	CMD-C2D-C1D	5.04	133.60	124.71
16	B	824	CLA	O2D-CGD-CBD	5.04	120.22	111.27
16	2	612	CLA	O2D-CGD-CBD	5.04	120.22	111.27
16	1	607	CLA	CMD-C2D-C1D	5.04	133.59	124.71
16	3	204	CLA	O2D-CGD-CBD	5.04	120.22	111.27
16	2	610	CLA	O2D-CGD-CBD	5.03	120.21	111.27
16	F	202	CLA	CMD-C2D-C1D	5.03	133.58	124.71
16	A	837	CLA	O2D-CGD-CBD	5.03	120.21	111.27
16	A	807	CLA	CMD-C2D-C1D	5.02	133.56	124.71
16	B	812	CLA	O2D-CGD-CBD	5.02	120.19	111.27
16	A	855	CLA	O2D-CGD-CBD	5.02	120.19	111.27
16	B	831	CLA	CMD-C2D-C1D	5.02	133.56	124.71
16	3	208	CLA	O2D-CGD-CBD	5.02	120.18	111.27
16	B	814	CLA	O2D-CGD-CBD	5.01	120.18	111.27
16	2	607	CLA	O2D-CGD-CBD	5.01	120.18	111.27
16	O	201	CLA	O2D-CGD-CBD	5.01	120.17	111.27
16	B	807	CLA	O2D-CGD-CBD	5.01	120.16	111.27
16	A	805	CLA	O2D-CGD-CBD	5.00	120.16	111.27
16	A	830	CLA	CMD-C2D-C1D	5.00	133.53	124.71
16	1	607	CLA	O2D-CGD-CBD	4.99	120.14	111.27
16	B	826	CLA	O2D-CGD-CBD	4.99	120.14	111.27
16	3	206	CLA	O2D-CGD-CBD	4.99	120.13	111.27
16	A	812	CLA	O2D-CGD-CBD	4.98	120.13	111.27
18	J	103	RRX	C30-C25-C26	-4.98	115.59	122.61
16	2	605	CLA	O2A-C1-C2	4.98	121.72	108.64
16	A	806	CLA	O2A-C1-C2	4.97	121.71	108.64
21	B	842	BCR	C1-C6-C7	4.97	129.85	115.78
16	1	606	CLA	CMA-C3A-C4A	4.97	125.14	111.77
16	2	606	CLA	O2D-CGD-CBD	4.97	120.10	111.27
16	2	602	CLA	O2D-CGD-CBD	4.97	120.10	111.27
16	A	812	CLA	CMD-C2D-C1D	4.96	133.46	124.71
17	J	104	C7Z	C21-C26-C25	-4.96	115.62	122.61
21	F	206	BCR	C19-C18-C17	4.96	126.56	118.94
17	3	218	C7Z	C7-C8-C9	-4.96	118.74	126.23
18	K	103	RRX	C11-C10-C9	-4.96	120.23	127.31
27	A	840	PQN	C14-C13-C15	4.96	123.61	115.27
16	3	207	CLA	O2D-CGD-CBD	4.96	120.08	111.27
16	3	213	CLA	O2D-CGD-CBD	4.96	120.08	111.27
16	O	202	CLA	O2D-CGD-CBD	4.96	120.08	111.27
16	1	605	CLA	CMD-C2D-C1D	4.95	133.44	124.71
16	A	815	CLA	O2D-CGD-CBD	4.95	120.06	111.27
16	1	606	CLA	CMD-C2D-C1D	4.94	133.43	124.71

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	2	604	CLA	CMD-C2D-C1D	4.94	133.43	124.71
16	1	601	CLA	O2D-CGD-CBD	4.94	120.05	111.27
16	K	102	CLA	O2D-CGD-CBD	4.94	120.05	111.27
17	2	614	C7Z	C18-C5-C6	-4.94	118.98	124.53
16	A	826	CLA	CMD-C2D-C1D	4.94	133.41	124.71
16	1	607	CLA	O2A-C1-C2	4.94	121.61	108.64
16	A	839	CLA	O2A-C1-C2	4.93	121.59	108.64
20	2	618	ERG	C1-C10-C9	4.93	118.49	108.28
21	F	206	BCR	C33-C5-C6	-4.93	119.00	124.53
21	B	843	BCR	C34-C9-C10	-4.93	116.02	122.92
16	A	856	CLA	CMD-C2D-C1D	4.92	133.39	124.71
17	1	615	C7Z	C38-C25-C26	-4.92	119.00	124.53
16	B	802	CLA	O2D-CGD-CBD	4.92	120.01	111.27
22	B	848	PGT	O2-C31-C32	4.92	122.09	111.50
21	F	206	BCR	C34-C9-C10	-4.91	116.04	122.92
16	A	827	CLA	O2D-CGD-CBD	4.91	119.99	111.27
16	B	830	CLA	CMD-C2D-C1D	4.91	133.36	124.71
16	A	802	CLA	CMD-C2D-C1D	4.90	133.35	124.71
17	1	612	C7Z	C1-C6-C5	-4.90	115.72	122.61
16	L	205	CLA	O2D-CGD-CBD	4.89	119.96	111.27
16	B	823	CLA	CMD-C2D-C1D	4.89	133.33	124.71
16	1	605	CLA	O2D-CGD-CBD	4.88	119.95	111.27
16	B	833	CLA	O2D-CGD-CBD	4.88	119.95	111.27
21	A	850	BCR	C30-C25-C24	4.88	129.59	115.78
16	A	818	CLA	O2D-CGD-CBD	4.88	119.94	111.27
17	2	614	C7Z	C27-C28-C29	-4.87	118.87	126.23
16	2	607	CLA	CMD-C2D-C1D	4.87	133.30	124.71
21	K	104	BCR	C11-C12-C13	4.87	140.10	126.42
16	B	828	CLA	O2D-CGD-CBD	4.87	119.92	111.27
26	A	801	CL0	C3D-C2D-C1D	-4.86	99.20	105.83
16	B	815	CLA	CMD-C2D-C1D	4.86	133.27	124.71
18	2	616	RRX	C16-C17-C18	-4.85	120.38	127.31
21	B	843	BCR	C28-C27-C26	-4.85	105.42	114.08
22	2	619	PGT	O2-C31-C32	4.85	121.95	111.50
16	O	203	CLA	O2D-CGD-CBD	4.84	119.87	111.27
16	2	609	CLA	O2A-C1-C2	4.84	121.36	108.64
16	2	603	CLA	O2D-CGD-CBD	4.84	119.86	111.27
17	3	217	C7Z	C11-C10-C9	-4.84	120.41	127.31
16	A	821	CLA	O2A-C1-C2	4.83	121.32	108.64
16	A	839	CLA	CMD-C2D-C1D	4.83	133.22	124.71
16	B	815	CLA	O2D-CGD-CBD	4.82	119.83	111.27
20	2	618	ERG	C19-C10-C1	-4.81	101.83	109.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	855	BCR	C30-C25-C26	-4.80	115.85	122.61
16	B	804	CLA	CMD-C2D-C1D	4.80	133.17	124.71
18	A	847	RRX	C16-C17-C18	4.80	134.16	127.31
16	L	201	CLA	O2D-CGD-CBD	4.80	119.79	111.27
16	2	604	CLA	O2A-C1-C2	4.80	121.24	108.64
16	B	812	CLA	CMD-C2D-C1D	4.78	133.14	124.71
21	A	850	BCR	C29-C30-C25	-4.78	103.13	110.48
21	L	202	BCR	C34-C9-C10	-4.77	116.24	122.92
16	A	818	CLA	O2A-C1-C2	4.77	121.17	108.64
21	K	104	BCR	C36-C18-C17	-4.76	116.25	122.92
17	1	614	C7Z	C27-C28-C29	-4.76	119.04	126.23
16	1	608	CLA	O2D-CGD-CBD	4.76	119.73	111.27
16	F	201	CLA	CMD-C2D-C1D	4.76	133.10	124.71
16	A	835	CLA	O2A-C1-C2	4.74	121.10	108.64
16	A	829	CLA	O2D-CGD-CBD	4.74	119.69	111.27
16	B	810	CLA	O2A-C1-C2	4.74	121.08	108.64
21	B	842	BCR	C1-C6-C5	-4.73	115.94	122.61
16	3	212	CLA	O2A-C1-C2	4.73	121.08	108.64
16	3	209	CLA	O2D-CGD-CBD	4.73	119.68	111.27
20	2	621	ERG	C14-C13-C17	4.73	104.77	99.72
16	B	833	CLA	CMD-C2D-C1D	4.73	133.05	124.71
16	B	809	CLA	O2D-CGD-CBD	4.73	119.67	111.27
17	3	201	C7Z	C7-C8-C9	-4.73	119.09	126.23
16	L	203	CLA	O2D-CGD-CBD	4.71	119.65	111.27
16	F	201	CLA	O2D-CGD-CBD	4.71	119.64	111.27
18	J	103	RRX	C7-C8-C9	-4.71	119.12	126.23
16	2	608	CLA	CAC-C3C-C4C	4.70	130.91	124.81
16	B	801	CLA	O2D-CGD-CBD	4.70	119.62	111.27
16	B	831	CLA	O2A-C1-C2	4.70	120.98	108.64
16	A	810	CLA	O2A-C1-C2	4.69	120.97	108.64
16	1	609	CLA	O2D-CGD-CBD	4.69	119.61	111.27
17	3	218	C7Z	C1-C6-C5	-4.69	116.00	122.61
18	1	613	RRX	C29-C28-C27	4.68	116.72	110.30
17	3	201	C7Z	C31-C30-C29	-4.68	120.63	127.31
16	A	838	CLA	O2A-C1-C2	4.67	120.92	108.64
16	2	611	CLA	O2D-CGD-CBD	4.66	119.55	111.27
17	J	104	C7Z	C18-C5-C6	-4.65	119.30	124.53
17	1	612	C7Z	C7-C8-C9	-4.64	119.22	126.23
16	B	803	CLA	O2A-C1-C2	4.64	120.84	108.64
21	A	846	BCR	C30-C25-C26	-4.64	116.07	122.61
18	K	103	RRX	C33-C5-C6	-4.64	119.32	124.53
21	O	205	BCR	C34-C9-C10	-4.64	116.43	122.92

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	847	BCR	C30-C25-C24	4.64	128.90	115.78
17	2	615	C7Z	C15-C14-C13	-4.64	120.69	127.31
18	1	613	RRX	C33-C5-C6	-4.64	119.32	124.53
16	A	855	CLA	CMD-C2D-C1D	4.63	132.88	124.71
16	B	830	CLA	O2D-CGD-CBD	4.63	119.50	111.27
18	2	616	RRX	C20-C21-C22	-4.63	120.71	127.31
16	1	611	CLA	O2D-CGD-CBD	4.63	119.49	111.27
26	A	801	CL0	O2D-CGD-CBD	4.63	119.49	111.27
16	3	203	CLA	O2A-C1-C2	4.63	120.79	108.64
21	B	841	BCR	C34-C9-C10	-4.62	116.45	122.92
21	B	855	BCR	C1-C6-C7	4.62	128.85	115.78
16	2	609	CLA	O2D-CGD-CBD	4.62	119.48	111.27
18	K	103	RRX	C4-C5-C6	-4.61	116.04	122.73
17	3	201	C7Z	C35-C34-C33	-4.61	120.73	127.31
17	3	216	C7Z	C32-C33-C34	4.61	126.01	118.94
16	2	610	CLA	CMA-C3A-C4A	4.60	124.14	111.77
21	A	845	BCR	C3-C4-C5	-4.60	105.86	114.08
17	3	216	C7Z	C18-C5-C6	-4.59	119.37	124.53
21	L	202	BCR	C28-C27-C26	-4.59	105.88	114.08
16	A	839	CLA	O2D-CGD-CBD	4.59	119.42	111.27
18	J	103	RRX	C20-C19-C18	-4.59	113.53	126.42
16	A	821	CLA	O2D-CGD-CBD	4.59	119.42	111.27
17	3	215	C7Z	C35-C34-C33	-4.58	120.77	127.31
16	1	610	CLA	O2A-C1-C2	4.57	120.64	108.64
16	B	804	CLA	O2D-CGD-CBD	4.57	119.38	111.27
21	F	206	BCR	C35-C13-C14	-4.56	116.53	122.92
16	L	204	CLA	O2D-CGD-CBD	4.56	119.37	111.27
17	J	104	C7Z	C11-C12-C13	-4.55	113.63	126.42
21	B	841	BCR	C27-C26-C25	-4.55	116.12	122.73
16	B	801	CLA	CMD-C2D-C1D	4.54	132.72	124.71
21	B	842	BCR	C37-C22-C21	-4.53	116.58	122.92
20	2	621	ERG	C7-C6-C5	-4.52	115.26	123.20
20	2	618	ERG	C19-C10-C5	-4.52	101.02	108.34
16	A	825	CLA	O2D-CGD-CBD	4.52	119.29	111.27
16	A	815	CLA	O2A-C1-C2	4.52	120.50	108.64
18	J	103	RRX	C23-C22-C21	-4.51	112.02	118.94
25	L	208	PTY	O7-C8-C11	4.51	121.22	111.50
16	O	204	CLA	O2A-C1-C2	4.51	120.48	108.64
16	A	837	CLA	O2A-C1-C2	4.50	120.47	108.64
17	A	843	C7Z	C18-C5-C6	-4.50	119.47	124.53
16	A	804	CLA	O2D-CGD-CBD	4.50	119.26	111.27
16	2	610	CLA	O2A-C1-C2	4.50	120.46	108.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	811	CLA	O2A-C1-C2	4.50	120.46	108.64
17	1	615	C7Z	C18-C5-C6	-4.50	119.48	124.53
16	B	838	CLA	O2A-C1-C2	4.49	120.44	108.64
16	B	823	CLA	O2D-CGD-CBD	4.49	119.25	111.27
16	B	821	CLA	O2A-C1-C2	4.49	120.43	108.64
17	3	217	C7Z	C15-C14-C13	-4.49	120.91	127.31
21	B	843	BCR	C19-C18-C17	4.48	125.82	118.94
18	1	613	RRX	C38-C26-C25	-4.48	119.50	124.53
16	B	809	CLA	O2A-C1-C2	4.47	120.39	108.64
16	A	854	CLA	CMD-C2D-C1D	4.47	132.59	124.71
16	A	814	CLA	O2A-C1-C2	4.47	120.37	108.64
17	1	614	C7Z	C38-C25-C26	-4.46	119.52	124.53
16	B	825	CLA	CMD-C2D-C1D	4.46	132.58	124.71
16	B	834	CLA	O2A-C1-C2	4.46	120.36	108.64
16	2	613	CLA	O2A-C1-C2	4.46	120.36	108.64
17	3	217	C7Z	C1-C6-C5	-4.46	116.33	122.61
21	B	842	BCR	C23-C22-C21	4.46	125.78	118.94
18	A	847	RRX	C36-C18-C19	4.44	125.08	118.08
21	L	202	BCR	C19-C18-C17	4.44	125.76	118.94
16	1	610	CLA	O2D-CGD-CBD	4.44	119.15	111.27
16	I	102	CLA	O2A-C1-C2	4.44	120.29	108.64
16	2	602	CLA	O2A-C1-C2	4.42	120.26	108.64
16	A	836	CLA	O2A-C1-C2	4.42	120.26	108.64
16	A	824	CLA	O2D-CGD-CBD	4.42	119.12	111.27
16	1	602	CLA	O2A-C1-C2	4.42	120.25	108.64
16	3	205	CLA	O2D-CGD-CBD	4.41	119.10	111.27
19	2	622	LHG	O7-C7-C8	4.41	121.00	111.50
16	F	204	CLA	CMD-C2D-C1D	4.40	132.47	124.71
16	A	823	CLA	O2D-CGD-CBD	4.39	119.07	111.27
21	L	206	BCR	C12-C13-C14	-4.39	112.20	118.94
17	3	217	C7Z	C7-C8-C9	-4.39	119.60	126.23
26	A	801	CL0	O2A-C1-C2	4.39	120.17	108.64
21	A	857	BCR	C7-C6-C5	4.39	132.09	121.46
16	A	825	CLA	O2A-C1-C2	4.39	120.16	108.64
16	A	829	CLA	O2A-C1-C2	4.38	120.16	108.64
16	1	611	CLA	O2A-C1-C2	4.38	120.14	108.64
16	A	807	CLA	O2A-C1-C2	4.38	120.14	108.64
17	J	104	C7Z	C35-C34-C33	-4.37	121.07	127.31
16	3	205	CLA	CAA-C2A-C1A	4.37	126.30	111.97
21	B	847	BCR	C29-C30-C25	-4.37	103.75	110.48
16	2	611	CLA	O2A-C1-C2	4.36	120.10	108.64
16	O	204	CLA	O2D-CGD-CBD	4.36	119.01	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	841	BCR	C30-C25-C26	-4.36	116.47	122.61
21	A	846	BCR	C30-C25-C24	4.35	128.09	115.78
18	J	103	RRX	C16-C17-C18	4.35	133.51	127.31
25	3	221	PTY	O7-C8-C11	4.34	120.86	111.50
16	B	827	CLA	O2D-CGD-CBD	4.34	118.98	111.27
31	B	849	DGD	O2G-C1B-C2B	4.34	120.86	111.50
21	B	847	BCR	C38-C26-C27	4.34	121.96	113.62
17	2	615	C7Z	C11-C10-C9	-4.34	121.11	127.31
17	3	216	C7Z	C1-C6-C5	-4.34	116.50	122.61
16	A	832	CLA	O2A-C1-C2	4.33	120.01	108.64
17	3	216	C7Z	C40-C33-C34	-4.32	116.87	122.92
16	A	824	CLA	O2A-C1-C2	4.32	120.00	108.64
23	2	620	DGA	OG2-CB1-CB2	4.32	120.82	111.50
16	A	811	CLA	O2D-CGD-CBD	4.32	118.95	111.27
31	B	850	DGD	O2G-C1B-C2B	4.32	120.80	111.50
21	B	847	BCR	C15-C14-C13	-4.32	121.15	127.31
16	3	204	CLA	O2A-C1-C2	4.31	119.97	108.64
21	A	844	BCR	C30-C25-C26	-4.31	116.54	122.61
16	I	101	CLA	O2A-C1-C2	4.31	119.96	108.64
16	L	203	CLA	O2A-C1-C2	4.29	119.92	108.64
26	A	801	CL0	O2A-CGA-CBA	4.29	125.37	111.91
16	B	826	CLA	O2A-C1-C2	4.29	119.90	108.64
16	B	828	CLA	O2A-C1-C2	4.28	119.89	108.64
25	3	220	PTY	O7-C8-C11	4.28	120.73	111.50
16	B	808	CLA	O2A-C1-C2	4.28	119.88	108.64
21	F	203	BCR	C36-C18-C17	-4.28	116.93	122.92
18	1	613	RRX	C20-C21-C22	-4.28	121.20	127.31
16	2	608	CLA	O2A-C1-C2	4.27	119.84	108.64
20	2	618	ERG	C18-C13-C12	-4.26	103.86	110.59
16	B	817	CLA	O2D-CGD-CBD	4.25	118.82	111.27
16	B	812	CLA	O2A-C1-C2	4.25	119.81	108.64
16	B	823	CLA	O2A-C1-C2	4.24	119.79	108.64
16	2	601	CLA	O2A-C1-C2	4.24	119.77	108.64
21	O	205	BCR	C19-C18-C17	4.22	125.42	118.94
21	A	857	BCR	C4-C5-C6	-4.22	116.60	122.73
16	B	822	CLA	O2D-CGD-CBD	4.22	118.77	111.27
16	B	807	CLA	O2A-C1-C2	4.22	119.72	108.64
16	A	811	CLA	O2A-C1-C2	4.22	119.72	108.64
21	A	857	BCR	C27-C26-C25	-4.21	116.61	122.73
17	2	615	C7Z	C1-C6-C5	-4.21	116.68	122.61
16	O	203	CLA	O2A-C1-C2	4.20	119.67	108.64
18	A	847	RRX	C15-C14-C13	-4.20	121.32	127.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	820	CLA	O2A-C1-C2	4.19	119.66	108.64
20	2	618	ERG	C7-C6-C5	-4.19	115.84	123.20
18	A	847	RRX	C15-C16-C17	-4.19	114.89	123.47
21	A	846	BCR	C40-C30-C25	4.19	117.10	110.30
17	3	217	C7Z	C18-C5-C6	-4.19	119.83	124.53
17	3	215	C7Z	C27-C28-C29	-4.19	119.91	126.23
16	2	606	CLA	O2A-C1-C2	4.19	119.64	108.64
16	B	811	CLA	O2D-CGD-CBD	4.18	118.69	111.27
16	A	803	CLA	O2A-C1-C2	4.18	119.61	108.64
21	B	845	BCR	C37-C22-C21	-4.17	117.08	122.92
16	F	204	CLA	O2A-C1-C2	4.16	119.58	108.64
16	A	822	CLA	O2A-C1-C2	4.16	119.58	108.64
17	1	616	C7Z	C18-C5-C6	-4.16	119.86	124.53
20	2	621	ERG	C19-C10-C5	-4.15	101.62	108.34
21	L	207	BCR	C34-C9-C10	-4.15	117.11	122.92
16	L	201	CLA	O2A-C1-C2	4.15	119.55	108.64
16	L	204	CLA	O2A-C1-C2	4.15	119.54	108.64
21	B	847	BCR	C37-C22-C23	4.15	124.61	118.08
16	B	833	CLA	O2A-C1-C2	4.14	119.52	108.64
18	1	613	RRX	C7-C8-C9	-4.13	119.99	126.23
16	B	835	CLA	O2A-C1-C2	4.13	119.49	108.64
16	3	214	CLA	O2A-C1-C2	4.13	119.48	108.64
16	O	202	CLA	O2A-C1-C2	4.12	119.48	108.64
16	L	205	CLA	O2A-C1-C2	4.12	119.47	108.64
17	3	201	C7Z	C27-C28-C29	-4.12	120.01	126.23
21	L	207	BCR	C30-C25-C26	-4.12	116.81	122.61
21	F	206	BCR	C37-C22-C21	-4.11	117.16	122.92
26	A	801	CL0	CHD-C1D-ND	-4.11	120.67	124.45
16	3	207	CLA	O2A-C1-C2	4.11	119.44	108.64
16	A	856	CLA	O2A-C1-C2	4.10	119.41	108.64
21	I	103	BCR	C37-C22-C21	-4.10	117.18	122.92
16	A	828	CLA	O2D-CGD-CBD	4.10	118.55	111.27
21	I	103	BCR	C34-C9-C10	-4.10	117.18	122.92
16	A	813	CLA	O2A-C1-C2	4.09	119.39	108.64
21	B	855	BCR	C1-C6-C5	-4.09	116.85	122.61
16	B	816	CLA	O2A-C1-C2	4.09	119.38	108.64
16	A	854	CLA	O2D-CGD-CBD	4.08	118.52	111.27
16	A	831	CLA	O2A-C1-C2	4.08	119.36	108.64
16	1	604	CLA	O2A-C1-C2	4.08	119.35	108.64
17	1	612	C7Z	C18-C5-C6	-4.07	119.95	124.53
16	F	202	CLA	O2A-C1-C2	4.07	119.33	108.64
21	B	847	BCR	C19-C18-C17	4.07	125.18	118.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	103	RRX	C20-C21-C22	-4.07	121.50	127.31
16	B	819	CLA	O2A-C1-C2	4.06	119.31	108.64
17	3	215	C7Z	C11-C10-C9	-4.06	121.52	127.31
16	B	802	CLA	O2A-C1-C2	4.05	119.28	108.64
17	2	615	C7Z	C18-C5-C6	-4.04	119.99	124.53
19	1	617	LHG	O7-C7-C8	4.04	120.22	111.50
16	B	815	CLA	O2A-C1-C2	4.04	119.24	108.64
21	B	845	BCR	C34-C9-C10	-4.03	117.27	122.92
21	2	617	BCR	C36-C18-C17	-4.03	117.28	122.92
16	F	205	CLA	O2A-C1-C2	4.03	119.22	108.64
16	1	606	CLA	O2A-C1-C2	4.02	119.21	108.64
16	1	603	CLA	O2A-C1-C2	4.02	119.20	108.64
21	L	207	BCR	C27-C26-C25	-4.02	116.90	122.73
17	3	201	C7Z	C38-C25-C26	-4.01	120.02	124.53
21	A	845	BCR	C27-C26-C25	-4.01	116.91	122.73
21	B	855	BCR	C30-C25-C24	4.01	127.12	115.78
16	B	829	CLA	O2A-C1-C2	4.01	119.17	108.64
16	2	605	CLA	O2D-CGD-CBD	4.00	118.38	111.27
17	1	616	C7Z	C1-C6-C5	-4.00	116.98	122.61
18	2	616	RRX	C30-C25-C26	-3.99	116.99	122.61
16	3	208	CLA	O2A-C1-C2	3.99	119.13	108.64
16	3	209	CLA	O2A-C1-C2	3.99	119.13	108.64
16	B	836	CLA	O2A-C1-C2	3.99	119.12	108.64
16	3	211	CLA	O2A-C1-C2	3.99	119.12	108.64
17	1	612	C7Z	C40-C33-C34	-3.98	117.34	122.92
17	3	218	C7Z	C38-C25-C26	-3.98	120.06	124.53
16	A	802	CLA	C1-O2A-CGA	3.97	126.87	116.44
16	A	854	CLA	O2A-C1-C2	3.96	119.05	108.64
21	2	617	BCR	C36-C18-C19	-3.96	111.84	118.08
16	J	102	CLA	O2A-C1-C2	3.95	119.02	108.64
16	3	210	CLA	O2A-C1-C2	3.95	119.01	108.64
16	A	855	CLA	O2A-C1-C2	3.93	118.97	108.64
17	1	616	C7Z	C21-C26-C25	-3.93	117.08	122.61
17	3	218	C7Z	C18-C5-C6	-3.93	120.12	124.53
16	A	819	CLA	O2A-C1-C2	3.92	118.94	108.64
21	A	850	BCR	C33-C5-C4	3.92	121.15	113.62
17	1	616	C7Z	C38-C25-C26	-3.92	120.13	124.53
16	A	834	CLA	O2A-C1-C2	3.92	118.94	108.64
16	K	102	CLA	O2A-C1-C2	3.92	118.93	108.64
23	J	101	DGA	OG2-CB1-CB2	3.91	119.94	111.50
21	A	845	BCR	C4-C5-C6	-3.91	117.06	122.73
17	1	615	C7Z	C35-C15-C14	-3.91	115.47	123.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	854	3PH	O21-C21-C22	3.90	119.90	111.50
25	A	852	PTY	O7-C8-C11	3.89	119.89	111.50
21	F	206	BCR	C8-C9-C10	3.89	124.91	118.94
20	2	621	ERG	C6-C7-C8	-3.89	114.42	122.07
16	A	827	CLA	O2A-C1-C2	3.88	118.84	108.64
21	L	207	BCR	C37-C22-C21	-3.88	117.49	122.92
16	K	101	CLA	O2A-C1-C2	3.88	118.83	108.64
16	A	802	CLA	O2A-C1-C2	3.88	118.82	108.64
29	A	849	3PH	O21-C21-C22	3.87	119.85	111.50
16	1	608	CLA	O2A-C1-C2	3.87	118.80	108.64
21	A	844	BCR	C34-C9-C10	-3.86	117.51	122.92
17	1	612	C7Z	C11-C10-C9	-3.86	121.80	127.31
21	B	842	BCR	C34-C9-C10	-3.86	117.52	122.92
21	B	844	BCR	C3-C4-C5	-3.86	107.19	114.08
16	B	817	CLA	O2A-C1-C2	3.85	118.75	108.64
16	B	825	CLA	CMA-C3A-C4A	3.84	122.10	111.77
21	F	206	BCR	C28-C27-C26	-3.84	107.22	114.08
16	2	603	CLA	O2A-C1-C2	3.84	118.72	108.64
21	A	857	BCR	C8-C7-C6	3.84	137.97	127.20
16	B	827	CLA	O2A-C1-C2	3.83	118.71	108.64
21	B	855	BCR	C36-C18-C17	-3.83	117.56	122.92
17	2	615	C7Z	C22-C23-C24	3.83	115.55	110.30
16	3	206	CLA	O2A-C1-C2	3.82	118.68	108.64
21	A	845	BCR	C33-C5-C4	3.82	120.96	113.62
17	A	843	C7Z	C11-C10-C9	-3.82	121.86	127.31
16	2	607	CLA	O2A-C1-C2	3.82	118.66	108.64
17	2	615	C7Z	C21-C26-C25	-3.80	117.25	122.61
16	B	813	CLA	O2A-C1-C2	3.80	118.63	108.64
30	A	851	T7X	O16-C10-C12	3.80	119.70	111.50
16	B	837	CLA	O2A-C1-C2	3.80	118.62	108.64
16	A	823	CLA	O2A-C1-C2	3.79	118.61	108.64
16	A	833	CLA	C1-O2A-CGA	3.79	126.38	116.44
16	A	828	CLA	O2A-C1-C2	3.78	118.58	108.64
17	1	614	C7Z	C21-C26-C25	-3.78	117.29	122.61
16	1	609	CLA	CMA-C3A-C4A	3.78	121.93	111.77
17	2	615	C7Z	C7-C8-C9	-3.78	120.53	126.23
19	3	219	LHG	O7-C7-C8	3.78	119.64	111.50
18	J	103	RRX	C36-C18-C19	3.77	124.02	118.08
21	B	843	BCR	C37-C22-C23	3.77	124.01	118.08
21	K	104	BCR	C15-C14-C13	3.77	132.68	127.31
21	B	845	BCR	C33-C5-C6	-3.76	120.30	124.53
21	2	617	BCR	C34-C9-C10	-3.76	117.66	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	O	201	CLA	C2D-C1D-ND	3.76	112.87	110.10
18	K	103	RRX	C36-C18-C19	3.75	123.99	118.08
21	B	843	BCR	C30-C25-C26	-3.75	117.33	122.61
17	A	843	C7Z	C1-C6-C5	-3.75	117.33	122.61
21	A	846	BCR	C3-C4-C5	-3.75	107.39	114.08
21	I	103	BCR	C3-C4-C5	-3.74	107.39	114.08
18	2	616	RRX	C33-C5-C4	3.74	120.80	113.62
16	B	814	CLA	O2A-C1-C2	3.73	118.45	108.64
16	A	802	CLA	O2A-CGA-CBA	3.73	123.62	111.91
18	A	847	RRX	C4-C5-C6	-3.73	117.31	122.73
16	O	201	CLA	CMA-C3A-C4A	3.73	121.80	111.77
18	J	103	RRX	C15-C14-C13	3.73	132.63	127.31
21	B	840	BCR	C19-C18-C17	3.73	124.66	118.94
21	F	203	BCR	C33-C5-C6	-3.73	120.34	124.53
17	3	217	C7Z	C31-C32-C33	-3.73	115.95	126.42
21	A	850	BCR	C40-C30-C25	3.72	116.34	110.30
17	J	104	C7Z	C38-C25-C26	-3.72	120.35	124.53
16	A	827	CLA	C1-C2-C3	-3.71	119.62	126.04
21	A	845	BCR	C34-C9-C8	3.71	123.92	118.08
16	1	601	CLA	O2A-C1-C2	3.71	118.38	108.64
21	B	855	BCR	C3-C4-C5	-3.70	107.46	114.08
17	1	615	C7Z	C31-C32-C33	-3.70	116.01	126.42
18	K	103	RRX	C15-C14-C13	-3.70	122.03	127.31
21	B	842	BCR	C12-C13-C14	3.70	124.61	118.94
16	3	205	CLA	C2A-C1A-CHA	3.70	130.32	123.86
21	K	104	BCR	C11-C10-C9	3.70	132.58	127.31
16	A	812	CLA	O2A-C1-C2	3.69	118.33	108.64
16	O	203	CLA	CMA-C3A-C4A	3.68	121.67	111.77
17	J	104	C7Z	C1-C6-C5	-3.68	117.43	122.61
17	2	615	C7Z	C27-C28-C29	-3.67	120.70	126.23
17	3	216	C7Z	C39-C29-C30	-3.67	117.79	122.92
18	A	847	RRX	C33-C5-C4	3.66	120.66	113.62
18	2	616	RRX	C12-C13-C14	3.66	124.56	118.94
19	A	841	LHG	O7-C7-C8	3.66	119.39	111.50
26	A	801	CL0	C1D-ND-C4D	-3.66	103.74	106.33
17	1	612	C7Z	C15-C14-C13	-3.66	122.09	127.31
17	3	201	C7Z	C21-C26-C25	-3.65	117.47	122.61
21	A	844	BCR	C33-C5-C6	-3.65	120.43	124.53
17	A	843	C7Z	C38-C25-C26	-3.64	120.44	124.53
16	3	203	CLA	CMA-C3A-C4A	3.64	121.56	111.77
18	K	103	RRX	C37-C22-C21	-3.64	117.82	122.92
16	B	803	CLA	O2D-CGD-CBD	3.63	117.73	111.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	609	CLA	O2A-C1-C2	3.63	118.18	108.64
16	A	824	CLA	CMA-C3A-C4A	3.63	121.53	111.77
21	B	855	BCR	C33-C5-C4	3.63	120.58	113.62
18	K	103	RRX	C38-C26-C25	-3.63	120.45	124.53
19	A	842	LHG	O7-C7-C8	3.62	119.31	111.50
21	B	841	BCR	C34-C9-C8	3.62	123.78	118.08
17	3	216	C7Z	C11-C12-C13	-3.62	116.25	126.42
18	J	103	RRX	C4-C5-C6	-3.61	117.48	122.73
16	B	822	CLA	O2A-C1-C2	3.61	118.12	108.64
21	A	857	BCR	C36-C18-C17	-3.61	117.87	122.92
16	3	205	CLA	O2A-C1-C2	3.61	118.11	108.64
21	A	857	BCR	C30-C25-C24	3.61	125.98	115.78
21	B	855	BCR	C15-C14-C13	-3.60	122.17	127.31
21	B	840	BCR	C1-C6-C7	3.60	125.97	115.78
16	A	817	CLA	O2A-C1-C2	3.60	118.09	108.64
21	B	845	BCR	C30-C25-C26	-3.60	117.55	122.61
16	A	835	CLA	CMA-C3A-C4A	3.59	121.43	111.77
18	1	613	RRX	C11-C10-C9	-3.59	122.18	127.31
19	B	851	LHG	O7-C7-C8	3.59	119.24	111.50
20	2	621	ERG	C1-C10-C5	3.58	115.30	108.75
16	B	825	CLA	O2A-C1-C2	3.57	118.03	108.64
21	2	617	BCR	C1-C6-C5	-3.57	117.58	122.61
20	2	618	ERG	C14-C8-C7	-3.56	117.37	124.38
29	J	105	3PH	O21-C21-C22	3.56	119.18	111.50
16	B	802	CLA	C2C-C1C-NC	3.56	113.31	109.97
21	K	104	BCR	C33-C5-C6	-3.56	120.53	124.53
16	B	818	CLA	C1-O2A-CGA	3.55	125.75	116.44
21	I	103	BCR	C30-C25-C26	-3.55	117.62	122.61
21	A	857	BCR	C12-C13-C14	-3.55	113.50	118.94
17	J	104	C7Z	C20-C13-C14	-3.55	117.96	122.92
16	B	825	CLA	C2C-C1C-NC	3.54	113.29	109.97
16	B	834	CLA	O2A-CGA-CBA	3.54	123.01	111.91
20	2	618	ERG	C18-C13-C14	-3.54	104.51	110.24
18	1	613	RRX	C36-C18-C17	-3.53	117.98	122.92
18	2	616	RRX	C33-C5-C6	-3.53	120.56	124.53
16	A	836	CLA	CMA-C3A-C4A	3.53	121.26	111.77
21	F	203	BCR	C27-C26-C25	-3.51	117.64	122.73
16	3	205	CLA	C3A-C2A-C1A	3.51	106.59	101.34
17	1	615	C7Z	C8-C9-C10	3.51	124.32	118.94
16	B	805	CLA	O2A-C1-C2	3.50	117.84	108.64
18	A	847	RRX	C35-C13-C14	-3.50	118.02	122.92
17	3	215	C7Z	C18-C5-C6	-3.50	120.60	124.53

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	801	CLA	O2A-C1-C2	3.49	117.80	108.64
18	J	103	RRX	C33-C5-C6	-3.49	120.61	124.53
31	B	846	DGD	O2G-C1B-C2B	3.48	119.01	111.50
21	L	206	BCR	C30-C25-C24	3.48	125.63	115.78
21	K	104	BCR	C34-C9-C10	-3.48	118.05	122.92
18	A	847	RRX	C24-C23-C22	-3.48	120.98	126.23
21	2	617	BCR	C4-C5-C6	-3.47	117.69	122.73
17	2	614	C7Z	C11-C10-C9	-3.46	122.37	127.31
21	A	846	BCR	C33-C5-C6	-3.46	120.65	124.53
17	J	104	C7Z	C12-C13-C14	3.45	124.23	118.94
21	L	206	BCR	C34-C9-C8	3.45	123.51	118.08
17	1	616	C7Z	C11-C12-C13	-3.45	116.74	126.42
18	2	616	RRX	C4-C5-C6	-3.45	117.73	122.73
21	O	205	BCR	C28-C27-C26	-3.44	107.93	114.08
21	B	847	BCR	C23-C22-C21	-3.44	113.66	118.94
21	I	103	BCR	C27-C26-C25	-3.44	117.73	122.73
21	A	844	BCR	C33-C5-C4	3.44	120.23	113.62
21	A	846	BCR	C34-C9-C8	3.44	123.50	118.08
21	F	206	BCR	C33-C5-C4	3.44	120.22	113.62
17	A	843	C7Z	C11-C12-C13	-3.44	116.75	126.42
18	K	103	RRX	C38-C26-C27	3.44	120.73	114.36
16	B	830	CLA	O2A-C1-C2	3.44	117.67	108.64
16	A	815	CLA	CMA-C3A-C4A	3.44	121.02	111.77
18	J	103	RRX	C29-C28-C27	3.44	115.01	110.30
21	F	203	BCR	C12-C13-C14	-3.44	113.67	118.94
20	2	618	ERG	C1-C10-C5	3.44	115.04	108.75
16	A	833	CLA	O2A-CGA-CBA	3.43	122.69	111.91
18	J	103	RRX	C11-C12-C13	-3.43	116.77	126.42
16	J	102	CLA	CMA-C3A-C2A	3.43	127.67	113.83
21	L	202	BCR	C34-C9-C8	3.41	123.45	118.08
16	A	809	CLA	O2A-C1-C2	3.41	117.59	108.64
21	B	841	BCR	C1-C6-C5	-3.40	117.83	122.61
21	A	845	BCR	C35-C13-C12	3.39	123.43	118.08
21	F	206	BCR	C11-C10-C9	3.39	132.15	127.31
16	A	823	CLA	CHD-C1D-ND	-3.39	121.33	124.45
16	1	603	CLA	C2D-C1D-ND	3.39	112.60	110.10
21	A	857	BCR	C3-C4-C5	-3.39	108.03	114.08
18	K	103	RRX	C35-C13-C14	-3.39	118.18	122.92
17	1	616	C7Z	C31-C32-C33	-3.38	116.92	126.42
21	B	843	BCR	C36-C18-C17	-3.38	118.19	122.92
21	B	842	BCR	C35-C13-C14	-3.37	118.20	122.92
16	B	821	CLA	CMA-C3A-C2A	3.37	127.42	113.83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	847	RRX	C34-C9-C8	-3.36	112.78	118.08
21	B	844	BCR	C34-C9-C10	-3.36	118.22	122.92
21	B	842	BCR	C32-C1-C6	3.36	115.74	110.30
21	A	857	BCR	C19-C18-C17	3.35	124.08	118.94
21	L	202	BCR	C36-C18-C17	-3.35	118.23	122.92
21	A	844	BCR	C36-C18-C17	-3.35	118.24	122.92
17	1	615	C7Z	C18-C5-C4	3.34	120.54	114.36
20	2	618	ERG	C6-C7-C8	-3.34	115.50	122.07
16	B	828	CLA	C2C-C1C-NC	3.33	113.09	109.97
16	3	212	CLA	CMA-C3A-C4A	3.33	120.73	111.77
17	2	615	C7Z	C31-C32-C33	-3.33	117.05	126.42
18	2	616	RRX	C2-C1-C6	3.32	115.59	110.48
21	B	842	BCR	C33-C5-C4	3.32	119.98	113.62
21	L	207	BCR	C30-C25-C24	3.31	125.14	115.78
21	B	840	BCR	C36-C18-C17	-3.30	118.30	122.92
17	2	614	C7Z	C35-C15-C14	-3.30	116.72	123.47
21	B	842	BCR	C3-C4-C5	-3.30	108.19	114.08
17	3	201	C7Z	C20-C13-C14	-3.30	118.30	122.92
27	A	840	PQN	C15-C13-C12	-3.30	114.45	121.12
16	3	210	CLA	C2C-C1C-NC	3.29	113.06	109.97
17	2	614	C7Z	C1-C6-C5	-3.29	117.98	122.61
21	B	844	BCR	C1-C6-C7	3.29	125.09	115.78
18	1	613	RRX	C27-C26-C25	-3.28	113.53	120.85
21	B	842	BCR	C4-C5-C6	-3.28	117.97	122.73
21	B	841	BCR	C3-C4-C5	-3.27	108.23	114.08
16	O	204	CLA	CMA-C3A-C4A	3.27	120.57	111.77
16	B	806	CLA	O2A-C1-C2	3.27	117.23	108.64
21	B	845	BCR	C19-C18-C17	3.27	123.96	118.94
17	3	218	C7Z	C27-C28-C29	-3.26	121.31	126.23
18	A	847	RRX	C7-C8-C9	3.26	131.16	126.23
17	1	616	C7Z	C20-C13-C14	-3.26	118.36	122.92
16	B	836	CLA	C2C-C1C-NC	3.25	113.02	109.97
17	3	215	C7Z	C18-C5-C4	3.25	120.38	114.36
16	1	610	CLA	C2D-C1D-ND	3.25	112.50	110.10
21	B	855	BCR	C37-C22-C21	-3.25	118.37	122.92
16	1	607	CLA	C2D-C1D-ND	3.24	112.49	110.10
16	B	837	CLA	C2C-C1C-NC	3.24	113.00	109.97
16	B	818	CLA	O2A-CGA-CBA	3.23	122.05	111.91
18	2	616	RRX	C11-C12-C13	-3.23	117.35	126.42
16	1	602	CLA	C1-C2-C3	-3.23	120.46	126.04
21	K	104	BCR	C37-C22-C23	3.23	123.16	118.08
17	3	201	C7Z	C19-C9-C10	-3.22	118.41	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	615	C7Z	C21-C26-C25	-3.22	118.08	122.61
16	B	837	CLA	CMA-C3A-C2A	3.22	126.81	113.83
21	A	845	BCR	C19-C18-C17	3.22	123.88	118.94
16	A	821	CLA	C2D-C1D-ND	3.22	112.47	110.10
17	2	615	C7Z	C40-C33-C34	-3.21	118.42	122.92
21	B	843	BCR	C33-C5-C6	-3.21	120.92	124.53
21	F	206	BCR	C1-C6-C5	-3.21	118.09	122.61
17	1	615	C7Z	C19-C9-C10	-3.21	118.43	122.92
21	A	857	BCR	C23-C22-C21	3.21	123.86	118.94
16	A	830	CLA	O2A-C1-C2	3.20	117.04	108.64
16	B	836	CLA	CMA-C3A-C4A	3.20	120.37	111.77
16	B	812	CLA	O2A-CGA-CBA	3.20	121.94	111.91
21	F	206	BCR	C23-C22-C21	3.19	123.84	118.94
21	B	843	BCR	C27-C26-C25	-3.19	118.11	122.73
18	J	103	RRX	C1-C6-C5	-3.18	118.13	122.61
21	B	841	BCR	C28-C27-C26	-3.18	108.40	114.08
21	2	617	BCR	C16-C17-C18	3.18	131.85	127.31
20	2	621	ERG	C17-C20-C22	3.18	116.31	110.27
16	O	204	CLA	C1-O2A-CGA	3.18	124.78	116.44
16	F	202	CLA	C1-C2-C3	-3.18	120.55	126.04
21	B	844	BCR	C33-C5-C6	-3.17	120.96	124.53
16	3	207	CLA	C1-C2-C3	-3.17	120.56	126.04
21	I	103	BCR	C33-C5-C6	-3.17	120.97	124.53
16	3	213	CLA	CMA-C3A-C4A	3.17	120.29	111.77
21	2	617	BCR	C33-C5-C4	3.17	119.70	113.62
21	K	104	BCR	C38-C26-C27	3.17	119.70	113.62
17	3	215	C7Z	C8-C7-C6	-3.17	118.31	127.20
16	A	819	CLA	C2C-C1C-NC	3.16	112.94	109.97
16	A	835	CLA	C2C-C1C-NC	3.16	112.94	109.97
21	B	845	BCR	C27-C26-C25	-3.16	118.14	122.73
21	B	855	BCR	C33-C5-C6	-3.16	120.98	124.53
17	A	843	C7Z	C38-C25-C24	3.16	120.21	114.36
21	A	850	BCR	C34-C9-C10	-3.16	118.50	122.92
18	2	616	RRX	C38-C26-C25	-3.16	120.98	124.53
21	F	206	BCR	C1-C6-C7	3.16	124.71	115.78
16	A	811	CLA	C2C-C1C-NC	3.15	112.93	109.97
17	3	216	C7Z	C19-C9-C10	-3.15	118.51	122.92
18	1	613	RRX	C1-C6-C5	-3.15	118.17	122.61
17	2	614	C7Z	C15-C14-C13	-3.15	122.81	127.31
17	2	614	C7Z	C8-C7-C6	-3.15	118.35	127.20
16	A	805	CLA	O2A-C1-C2	3.15	116.91	108.64
21	O	205	BCR	C36-C18-C17	-3.15	118.51	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	809	CLA	CMA-C3A-C2A	3.15	126.52	113.83
21	B	843	BCR	C33-C5-C4	3.14	119.65	113.62
16	2	611	CLA	CMA-C3A-C4A	3.14	120.21	111.77
16	B	822	CLA	CMA-C3A-C4A	3.14	120.21	111.77
21	A	846	BCR	C33-C5-C4	3.14	119.65	113.62
18	J	103	RRX	C20-C21-C22	3.14	131.79	127.31
16	B	811	CLA	CMA-C3A-C4A	3.14	120.20	111.77
21	B	841	BCR	C19-C18-C17	3.14	123.75	118.94
16	I	102	CLA	C1-C2-C3	-3.13	120.63	126.04
17	A	843	C7Z	C15-C35-C34	-3.12	117.07	123.47
16	A	805	CLA	O2A-CGA-CBA	3.12	121.71	111.91
17	J	104	C7Z	C38-C25-C24	3.12	120.14	114.36
21	A	844	BCR	C37-C22-C23	3.12	123.00	118.08
17	1	616	C7Z	C38-C25-C24	3.11	120.12	114.36
16	2	606	CLA	C2C-C1C-NC	3.10	112.88	109.97
17	3	216	C7Z	C20-C13-C14	-3.10	118.58	122.92
21	K	104	BCR	C28-C27-C26	-3.10	108.53	114.08
16	A	802	CLA	C2C-C1C-NC	3.10	112.88	109.97
18	1	613	RRX	C37-C22-C21	-3.10	118.58	122.92
17	A	843	C7Z	C35-C34-C33	-3.10	122.89	127.31
17	1	612	C7Z	C28-C27-C26	-3.10	118.50	127.20
16	B	835	CLA	C2D-C1D-ND	3.10	112.39	110.10
16	A	828	CLA	O2A-CGA-CBA	3.10	121.63	111.91
16	B	834	CLA	C2D-C1D-ND	3.10	112.39	110.10
21	B	843	BCR	C1-C6-C5	-3.10	118.25	122.61
18	J	103	RRX	C33-C5-C4	3.09	119.55	113.62
21	A	845	BCR	C36-C18-C17	-3.09	118.60	122.92
21	B	844	BCR	C37-C22-C21	-3.09	118.60	122.92
21	A	846	BCR	C28-C27-C26	-3.09	108.56	114.08
18	2	616	RRX	C36-C18-C17	-3.09	118.60	122.92
16	A	825	CLA	C2C-C1C-NC	3.09	112.86	109.97
16	A	831	CLA	C2C-C1C-NC	3.08	112.86	109.97
21	L	207	BCR	C3-C4-C5	-3.08	108.57	114.08
16	F	204	CLA	C2D-C1D-ND	3.08	112.38	110.10
16	1	602	CLA	C2D-C1D-ND	3.08	112.38	110.10
16	2	609	CLA	CMA-C3A-C4A	3.08	120.05	111.77
16	2	613	CLA	CMA-C3A-C4A	3.08	120.04	111.77
20	1	618	ERG	C2-C3-C4	3.08	114.52	110.31
16	1	610	CLA	C1-O2A-CGA	3.08	124.52	116.44
18	J	103	RRX	C23-C24-C25	-3.08	118.56	127.20
16	1	610	CLA	CMA-C3A-C4A	3.08	120.04	111.77
16	A	803	CLA	C2C-C1C-NC	3.07	112.85	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	F	203	BCR	C30-C25-C24	3.07	124.46	115.78
16	B	812	CLA	C2C-C1C-NC	3.06	112.84	109.97
16	A	839	CLA	C2C-C1C-NC	3.06	112.84	109.97
21	A	845	BCR	C12-C13-C14	-3.06	114.24	118.94
16	A	811	CLA	CMA-C3A-C4A	3.06	120.00	111.77
16	B	816	CLA	C2C-C1C-NC	3.06	112.84	109.97
26	A	801	CL0	CMC-C2C-C1C	3.06	129.69	125.04
16	F	202	CLA	CMA-C3A-C2A	3.06	126.16	113.83
18	1	613	RRX	C35-C13-C12	3.05	122.89	118.08
16	A	826	CLA	C2C-C1C-NC	3.05	112.83	109.97
21	B	855	BCR	C29-C28-C27	3.05	118.19	111.38
17	1	616	C7Z	C12-C13-C14	3.05	123.62	118.94
21	B	847	BCR	C34-C9-C10	-3.05	118.65	122.92
21	L	202	BCR	C30-C25-C24	3.04	124.39	115.78
16	B	832	CLA	C1-O2A-CGA	3.04	124.42	116.44
21	B	843	BCR	C1-C6-C7	3.04	124.37	115.78
16	O	202	CLA	CMA-C3A-C4A	3.04	119.94	111.77
18	1	613	RRX	C16-C17-C18	-3.03	122.98	127.31
16	A	824	CLA	C2C-C1C-NC	3.03	112.81	109.97
18	A	847	RRX	C34-C9-C10	-3.03	118.68	122.92
16	3	211	CLA	CMA-C3A-C4A	3.03	119.91	111.77
21	B	855	BCR	C32-C1-C6	3.03	115.21	110.30
16	A	854	CLA	CHD-C1D-ND	-3.03	121.67	124.45
16	B	833	CLA	C2D-C1D-ND	3.03	112.33	110.10
21	L	206	BCR	C27-C26-C25	-3.03	118.34	122.73
23	2	620	DGA	CDB-CCB-CBB	-3.02	99.07	114.42
16	1	605	CLA	CMA-C3A-C4A	3.02	119.89	111.77
21	B	843	BCR	C16-C17-C18	3.02	131.62	127.31
17	3	218	C7Z	C38-C25-C24	3.02	119.95	114.36
17	3	217	C7Z	C35-C15-C14	-3.02	117.29	123.47
16	A	818	CLA	C2C-C1C-NC	3.02	112.80	109.97
16	B	801	CLA	C2D-C1D-ND	3.02	112.33	110.10
16	B	801	CLA	CHD-C1D-ND	-3.02	121.68	124.45
16	A	830	CLA	C2C-C1C-NC	3.01	112.80	109.97
21	B	855	BCR	C16-C17-C18	3.01	131.61	127.31
16	B	802	CLA	CMA-C3A-C4A	3.01	119.87	111.77
16	A	811	CLA	C1-C2-C3	-3.01	120.84	126.04
16	1	604	CLA	CMA-C3A-C4A	3.00	119.85	111.77
16	B	820	CLA	CMA-C3A-C4A	3.00	119.84	111.77
16	1	605	CLA	C2D-C1D-ND	3.00	112.32	110.10
17	J	104	C7Z	C19-C9-C8	3.00	122.81	118.08
16	A	810	CLA	CHD-C1D-ND	-3.00	121.70	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F	202	CLA	C2D-C1D-ND	3.00	112.31	110.10
21	B	842	BCR	C7-C6-C5	-3.00	114.20	121.46
21	K	104	BCR	C30-C25-C24	3.00	124.26	115.78
16	2	607	CLA	C2C-C1C-NC	3.00	112.78	109.97
16	B	824	CLA	O2A-C1-C2	2.99	116.50	108.64
16	A	802	CLA	CMA-C3A-C4A	2.99	119.82	111.77
21	A	844	BCR	C1-C6-C7	2.99	124.25	115.78
16	1	602	CLA	C2C-C1C-NC	2.99	112.78	109.97
16	A	855	CLA	C2C-C1C-NC	2.99	112.77	109.97
16	3	210	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
16	B	831	CLA	C2C-C1C-NC	2.99	112.77	109.97
16	3	214	CLA	CMA-C3A-C4A	2.99	119.81	111.77
16	A	826	CLA	O2A-C1-C2	2.99	116.49	108.64
20	2	621	ERG	C18-C13-C12	-2.99	105.87	110.59
16	L	205	CLA	CMA-C3A-C4A	2.99	119.80	111.77
21	B	855	BCR	C7-C6-C5	-2.98	114.23	121.46
21	L	207	BCR	C38-C26-C27	2.98	119.35	113.62
16	F	201	CLA	C2D-C1D-ND	2.98	112.30	110.10
16	3	205	CLA	C2C-C1C-NC	2.98	112.77	109.97
16	2	605	CLA	C2D-C1D-ND	2.98	112.30	110.10
16	O	201	CLA	CMC-C2C-C1C	2.98	129.58	125.04
16	B	824	CLA	CMA-C3A-C4A	2.98	119.78	111.77
16	B	821	CLA	C2C-C1C-NC	2.98	112.76	109.97
18	K	103	RRX	C33-C5-C4	2.98	119.34	113.62
16	L	203	CLA	C2C-C1C-NC	2.98	112.76	109.97
17	3	201	C7Z	C12-C13-C14	2.98	123.51	118.94
21	F	203	BCR	C23-C22-C21	2.98	123.51	118.94
21	A	846	BCR	C27-C26-C25	-2.98	118.41	122.73
16	B	829	CLA	C2C-C1C-NC	2.98	112.76	109.97
16	B	838	CLA	C1-C2-C3	-2.98	120.90	126.04
21	B	855	BCR	C36-C18-C19	-2.97	113.39	118.08
17	3	216	C7Z	C18-C5-C4	2.97	119.86	114.36
16	L	205	CLA	C2C-C1C-NC	2.97	112.75	109.97
16	B	814	CLA	C5-C3-C2	2.97	127.13	121.12
21	B	855	BCR	C4-C5-C6	-2.97	118.42	122.73
21	I	103	BCR	C38-C26-C27	2.97	119.31	113.62
16	A	818	CLA	C1-O2A-CGA	2.96	124.22	116.44
16	1	606	CLA	CMA-C3A-C2A	2.96	125.78	113.83
16	3	213	CLA	C2C-C1C-NC	2.96	112.75	109.97
16	B	827	CLA	O2A-CGA-CBA	2.96	121.20	111.91
16	F	201	CLA	O2A-C1-C2	2.96	116.41	108.64
16	A	854	CLA	C2D-C1D-ND	2.96	112.28	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	611	CLA	C2C-C1C-NC	2.96	112.74	109.97
16	O	201	CLA	C1D-ND-C4D	-2.96	104.23	106.33
16	A	812	CLA	C2C-C1C-NC	2.95	112.74	109.97
16	B	826	CLA	C2C-C1C-NC	2.95	112.74	109.97
21	A	857	BCR	C33-C5-C4	2.95	119.28	113.62
16	B	804	CLA	C2C-C1C-NC	2.95	112.74	109.97
16	I	101	CLA	C2D-C1D-ND	2.95	112.28	110.10
21	A	850	BCR	C15-C14-C13	-2.95	123.10	127.31
16	2	611	CLA	C2D-C1D-ND	2.95	112.28	110.10
20	1	618	ERG	C15-C14-C13	2.95	106.83	104.21
17	1	616	C7Z	C8-C7-C6	-2.94	118.93	127.20
18	J	103	RRX	C37-C22-C23	2.94	122.72	118.08
16	2	613	CLA	C2C-C1C-NC	2.94	112.73	109.97
17	3	216	C7Z	C28-C29-C30	2.94	123.46	118.94
16	1	605	CLA	O2A-C1-C2	2.94	116.37	108.64
16	O	201	CLA	O2A-C1-C2	2.94	116.37	108.64
16	2	604	CLA	C2D-C1D-ND	2.94	112.27	110.10
16	A	856	CLA	C1-C2-C3	-2.94	120.96	126.04
16	3	203	CLA	C2D-C1D-ND	2.94	112.27	110.10
16	A	838	CLA	C1-O2A-CGA	2.93	124.14	116.44
16	2	605	CLA	CHD-C1D-ND	-2.93	121.76	124.45
20	2	618	ERG	C12-C13-C17	-2.93	112.18	116.57
21	A	857	BCR	C24-C25-C26	-2.93	114.36	121.46
16	F	205	CLA	C2C-C1C-NC	2.93	112.72	109.97
16	A	818	CLA	CHD-C1D-ND	-2.93	121.76	124.45
16	1	605	CLA	C2C-C1C-NC	2.93	112.72	109.97
21	B	840	BCR	C33-C5-C6	-2.93	121.24	124.53
16	A	814	CLA	CMA-C3A-C4A	2.93	119.64	111.77
16	B	810	CLA	C2C-C1C-NC	2.93	112.71	109.97
16	K	102	CLA	C2C-C1C-NC	2.93	112.71	109.97
18	2	616	RRX	C23-C22-C21	2.93	123.43	118.94
16	2	611	CLA	C2C-C1C-NC	2.92	112.71	109.97
21	2	617	BCR	C20-C21-C22	2.92	131.48	127.31
21	B	841	BCR	C38-C26-C27	2.92	119.23	113.62
17	3	217	C7Z	C18-C5-C4	2.92	119.77	114.36
21	A	845	BCR	C34-C9-C10	-2.92	118.83	122.92
16	2	603	CLA	C2C-C1C-NC	2.92	112.71	109.97
17	3	218	C7Z	C28-C27-C26	-2.92	119.01	127.20
16	B	827	CLA	C2C-C1C-NC	2.92	112.70	109.97
21	K	104	BCR	C33-C5-C4	2.92	119.22	113.62
16	A	804	CLA	C1-O2A-CGA	2.92	124.09	116.44
16	2	601	CLA	C2C-C1C-NC	2.92	112.70	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	3	207	CLA	C2C-C1C-NC	2.92	112.70	109.97
16	B	804	CLA	C6-C5-C3	-2.92	105.81	113.45
16	2	601	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
21	B	840	BCR	C34-C9-C10	-2.91	118.85	122.92
21	B	844	BCR	C38-C26-C25	2.91	127.79	124.53
16	B	819	CLA	CMA-C3A-C4A	2.90	119.58	111.77
16	1	606	CLA	C2C-C1C-NC	2.90	112.69	109.97
16	3	209	CLA	CMA-C3A-C4A	2.90	119.58	111.77
18	J	103	RRX	C30-C25-C24	2.90	123.99	115.78
16	A	817	CLA	O2A-CGA-CBA	2.90	121.01	111.91
16	1	611	CLA	C1-C2-C3	-2.90	121.03	126.04
16	A	820	CLA	O2A-C1-C2	2.90	116.26	108.64
16	A	815	CLA	C2C-C1C-NC	2.90	112.69	109.97
16	K	101	CLA	CMA-C3A-C4A	2.90	119.56	111.77
16	B	828	CLA	C1C-C2C-C3C	-2.90	103.91	106.96
16	I	101	CLA	C1C-C2C-C3C	-2.90	103.91	106.96
16	B	818	CLA	C2C-C1C-NC	2.90	112.69	109.97
16	B	819	CLA	C2C-C1C-NC	2.90	112.69	109.97
16	B	817	CLA	C2C-C1C-NC	2.90	112.69	109.97
21	O	205	BCR	C16-C17-C18	2.90	131.44	127.31
16	B	830	CLA	C6-C5-C3	-2.89	105.86	113.45
16	A	839	CLA	CMA-C3A-C4A	2.89	119.55	111.77
16	A	817	CLA	CHD-C1D-ND	-2.89	121.80	124.45
21	B	841	BCR	C37-C22-C23	2.89	122.64	118.08
21	B	841	BCR	C23-C24-C25	-2.89	119.08	127.20
16	A	810	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
16	3	203	CLA	C2C-C1C-NC	2.89	112.68	109.97
16	A	829	CLA	C2C-C1C-NC	2.89	112.68	109.97
16	B	812	CLA	C2D-C1D-ND	2.89	112.23	110.10
16	F	204	CLA	C2C-C1C-NC	2.89	112.68	109.97
16	A	820	CLA	C2C-C1C-NC	2.89	112.68	109.97
17	3	201	C7Z	C38-C25-C24	2.89	119.70	114.36
21	A	846	BCR	C19-C18-C17	2.89	123.37	118.94
16	1	601	CLA	CMA-C3A-C4A	2.89	119.53	111.77
16	3	214	CLA	C2C-C1C-NC	2.89	112.67	109.97
16	A	805	CLA	C2C-C1C-NC	2.89	112.67	109.97
21	A	846	BCR	C1-C6-C7	2.88	123.94	115.78
21	L	207	BCR	C37-C22-C23	2.88	122.62	118.08
26	A	801	CL0	CHB-C4A-NA	2.88	128.50	124.51
16	A	821	CLA	C2C-C1C-NC	2.88	112.67	109.97
16	B	830	CLA	CHD-C1D-ND	-2.87	121.81	124.45
17	3	216	C7Z	C21-C26-C25	-2.87	118.56	122.61

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	3	210	CLA	CMA-C3A-C2A	2.87	125.42	113.83
16	I	101	CLA	CHD-C1D-ND	-2.87	121.81	124.45
16	F	205	CLA	CMA-C3A-C4A	2.87	119.49	111.77
16	B	818	CLA	CHD-C1D-ND	-2.87	121.82	124.45
16	A	825	CLA	C5-C3-C2	2.87	126.92	121.12
16	B	808	CLA	C1-C2-C3	-2.87	121.09	126.04
21	A	844	BCR	C1-C6-C5	-2.86	118.58	122.61
17	2	615	C7Z	C32-C33-C34	2.86	123.33	118.94
16	A	821	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
16	A	804	CLA	C1-C2-C3	-2.86	121.10	126.04
16	B	824	CLA	CHD-C1D-ND	-2.86	121.83	124.45
16	1	602	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
16	3	205	CLA	CMA-C3A-C4A	2.86	119.45	111.77
16	I	101	CLA	C2C-C1C-NC	2.86	112.65	109.97
18	K	103	RRX	C16-C17-C18	-2.85	123.24	127.31
21	I	103	BCR	C33-C5-C4	2.85	119.10	113.62
16	1	603	CLA	O2A-CGA-CBA	2.85	120.86	111.91
16	B	814	CLA	C2C-C1C-NC	2.85	112.64	109.97
23	J	101	DGA	CDB-CCB-CBB	-2.85	99.96	114.42
16	1	601	CLA	C2C-C1C-NC	2.85	112.64	109.97
16	F	202	CLA	C2C-C1C-NC	2.85	112.64	109.97
16	B	815	CLA	C2D-C1D-ND	2.85	112.20	110.10
16	3	208	CLA	C2C-C1C-NC	2.85	112.64	109.97
17	1	615	C7Z	C10-C11-C12	-2.84	114.34	123.22
16	B	832	CLA	C1-C2-C3	-2.84	121.12	126.04
20	2	618	ERG	C2-C3-C4	2.84	114.20	110.31
16	B	819	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
16	O	201	CLA	CHD-C1D-ND	-2.84	121.85	124.45
16	2	608	CLA	C2C-C1C-NC	2.84	112.63	109.97
16	3	208	CLA	O2A-CGA-CBA	2.84	120.81	111.91
16	2	605	CLA	C2C-C1C-NC	2.84	112.63	109.97
17	3	218	C7Z	C18-C5-C4	2.83	119.61	114.36
16	B	829	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
16	O	204	CLA	O2A-CGA-CBA	2.83	120.80	111.91
16	3	212	CLA	C2C-C1C-NC	2.83	112.62	109.97
16	2	608	CLA	CAC-C3C-C2C	-2.83	122.69	127.53
16	B	833	CLA	C2C-C1C-NC	2.83	112.62	109.97
21	B	841	BCR	C23-C22-C21	-2.83	114.61	118.94
16	B	825	CLA	C2D-C1D-ND	2.83	112.19	110.10
16	B	813	CLA	C2C-C1C-NC	2.82	112.62	109.97
16	A	806	CLA	C2C-C1C-NC	2.82	112.62	109.97
16	A	837	CLA	C1-C2-C3	-2.82	121.17	126.04

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	J	104	C7Z	C18-C5-C4	2.82	119.57	114.36
16	1	610	CLA	C1C-C2C-C3C	-2.82	104.00	106.96
16	A	837	CLA	C2C-C1C-NC	2.81	112.61	109.97
16	B	811	CLA	C1-C2-C3	-2.81	121.18	126.04
16	A	813	CLA	CHD-C1D-ND	-2.81	121.87	124.45
16	1	608	CLA	C2C-C1C-NC	2.81	112.61	109.97
16	A	812	CLA	C2D-C1D-ND	2.81	112.17	110.10
16	B	812	CLA	CMA-C3A-C4A	2.81	119.33	111.77
16	L	204	CLA	CHD-C1D-ND	-2.81	121.87	124.45
16	2	609	CLA	C2C-C1C-NC	2.81	112.60	109.97
16	B	838	CLA	C2C-C1C-NC	2.81	112.60	109.97
17	1	616	C7Z	C18-C5-C4	2.81	119.56	114.36
16	J	102	CLA	O2A-CGA-CBA	2.81	120.72	111.91
25	L	208	PTY	O4-C30-C31	2.81	120.72	111.91
16	B	820	CLA	C2C-C1C-NC	2.81	112.60	109.97
17	A	843	C7Z	C18-C5-C4	2.81	119.55	114.36
21	A	857	BCR	C37-C22-C21	-2.80	119.00	122.92
16	B	834	CLA	C5-C3-C2	2.80	126.78	121.12
21	B	844	BCR	C39-C30-C25	-2.80	105.76	110.30
21	K	104	BCR	C3-C4-C5	-2.80	109.08	114.08
20	1	618	ERG	C14-C8-C7	-2.80	118.87	124.38
16	B	829	CLA	CHD-C1D-ND	-2.80	121.88	124.45
16	2	602	CLA	O2A-CGA-CBA	2.80	120.68	111.91
16	B	820	CLA	CHD-C1D-ND	-2.80	121.89	124.45
16	A	807	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
21	B	840	BCR	C1-C6-C5	-2.79	118.68	122.61
21	O	205	BCR	C15-C14-C13	-2.79	123.32	127.31
16	L	201	CLA	CHD-C1D-ND	-2.79	121.89	124.45
16	O	204	CLA	C2D-C1D-ND	2.79	112.16	110.10
16	A	832	CLA	C1-O2A-CGA	2.79	123.77	116.44
21	A	846	BCR	C12-C13-C14	-2.79	114.66	118.94
16	B	807	CLA	C2D-C1D-ND	2.79	112.16	110.10
21	B	843	BCR	C23-C24-C25	-2.79	119.37	127.20
21	L	202	BCR	C33-C5-C6	-2.78	121.40	124.53
16	A	809	CLA	C2D-C1D-ND	2.78	112.15	110.10
21	L	207	BCR	C15-C14-C13	-2.78	123.34	127.31
16	2	612	CLA	O2A-C1-C2	2.78	115.94	108.64
16	B	808	CLA	C2C-C1C-NC	2.78	112.58	109.97
18	1	613	RRX	C30-C29-C28	2.78	119.92	113.64
16	3	206	CLA	C2C-C1C-NC	2.78	112.57	109.97
16	2	606	CLA	CMA-C3A-C4A	2.78	119.23	111.77
16	A	835	CLA	C1-C2-C3	-2.78	121.24	126.04

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	802	CLA	C2D-C1D-ND	2.77	112.15	110.10
16	B	822	CLA	C2C-C1C-NC	2.77	112.57	109.97
16	A	814	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
16	1	608	CLA	CMA-C3A-C4A	2.77	119.22	111.77
16	A	805	CLA	C1-O2A-CGA	2.77	123.71	116.44
17	3	217	C7Z	C24-C25-C26	-2.77	114.68	120.85
16	B	835	CLA	CHD-C1D-ND	-2.77	121.91	124.45
16	A	814	CLA	C2C-C1C-NC	2.76	112.56	109.97
16	A	828	CLA	C2C-C1C-NC	2.76	112.56	109.97
16	3	206	CLA	CHD-C1D-ND	-2.76	121.92	124.45
16	3	211	CLA	C2C-C1C-NC	2.76	112.56	109.97
16	3	211	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
16	2	612	CLA	C2C-C1C-NC	2.76	112.56	109.97
17	3	218	C7Z	C22-C23-C24	2.76	114.08	110.30
16	2	612	CLA	C5-C3-C2	2.76	126.69	121.12
21	B	842	BCR	C16-C17-C18	2.76	131.24	127.31
26	A	801	CL0	C1-C2-C3	-2.76	121.28	126.04
16	2	613	CLA	C2D-C1D-ND	2.75	112.13	110.10
16	B	820	CLA	O2A-CGA-CBA	2.75	120.55	111.91
21	L	206	BCR	C34-C9-C10	-2.75	119.06	122.92
16	3	214	CLA	CHD-C1D-ND	-2.75	121.92	124.45
21	L	206	BCR	C30-C25-C26	-2.75	118.74	122.61
16	A	815	CLA	O2A-CGA-CBA	2.75	120.54	111.91
16	A	834	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
16	B	803	CLA	C2C-C1C-NC	2.75	112.55	109.97
16	3	204	CLA	CHD-C1D-ND	-2.75	121.93	124.45
16	3	204	CLA	C2C-C1C-NC	2.75	112.54	109.97
16	A	813	CLA	C2C-C1C-NC	2.75	112.54	109.97
16	B	809	CLA	C2C-C1C-NC	2.75	112.54	109.97
16	A	819	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
17	1	614	C7Z	C39-C29-C30	-2.74	119.08	122.92
16	B	826	CLA	O2A-CGA-CBA	2.74	120.52	111.91
16	3	207	CLA	CHD-C1D-ND	-2.74	121.93	124.45
21	L	206	BCR	C36-C18-C17	-2.74	119.08	122.92
16	A	807	CLA	C2D-C1D-ND	2.74	112.12	110.10
16	B	810	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
16	K	101	CLA	C2C-C1C-NC	2.73	112.53	109.97
16	A	836	CLA	CHD-C1D-ND	-2.73	121.94	124.45
21	L	202	BCR	C27-C26-C25	-2.73	118.76	122.73
16	A	825	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
16	A	822	CLA	C2D-C1D-ND	2.73	112.12	110.10
16	B	835	CLA	C1D-ND-C4D	-2.73	104.39	106.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	604	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
21	B	841	BCR	C12-C13-C14	-2.73	114.75	118.94
16	B	811	CLA	CHD-C1D-ND	-2.73	121.94	124.45
20	1	618	ERG	C11-C12-C13	2.73	117.46	112.78
16	O	203	CLA	C2C-C1C-NC	2.73	112.53	109.97
16	B	804	CLA	C2D-C1D-ND	2.73	112.11	110.10
16	B	832	CLA	CMA-C3A-C4A	2.73	119.10	111.77
17	3	215	C7Z	C1-C6-C5	-2.73	118.78	122.61
16	O	201	CLA	C1-C2-C3	-2.73	121.33	126.04
16	1	610	CLA	C5-C3-C2	2.72	126.63	121.12
16	B	803	CLA	C2D-C1D-ND	2.72	112.11	110.10
16	O	203	CLA	CHD-C1D-ND	-2.72	121.95	124.45
16	L	205	CLA	O2A-CGA-CBA	2.72	120.46	111.91
16	3	208	CLA	CHD-C1D-ND	-2.72	121.95	124.45
16	L	205	CLA	CHD-C1D-ND	-2.72	121.95	124.45
16	B	807	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
16	A	838	CLA	C2D-C1D-ND	2.72	112.11	110.10
16	A	830	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
16	A	814	CLA	CHD-C1D-ND	-2.72	121.95	124.45
21	F	203	BCR	C38-C26-C27	2.72	118.84	113.62
16	A	823	CLA	C2D-C1D-ND	2.72	112.11	110.10
16	B	838	CLA	O2A-CGA-CBA	2.72	120.44	111.91
16	A	803	CLA	C1-C2-C3	-2.72	121.34	126.04
16	B	806	CLA	C2C-C1C-NC	2.72	112.52	109.97
18	2	616	RRX	C8-C7-C6	-2.71	119.58	127.20
16	A	816	CLA	CMA-C3A-C4A	2.71	119.06	111.77
16	A	806	CLA	C1-O2A-CGA	2.71	123.56	116.44
16	A	820	CLA	C1-O2A-CGA	2.71	123.56	116.44
16	K	101	CLA	O2A-CGA-CBA	2.71	120.42	111.91
16	1	609	CLA	C2C-C1C-NC	2.71	112.51	109.97
16	B	807	CLA	C2C-C1C-NC	2.71	112.51	109.97
16	B	819	CLA	CMD-C2D-C3D	-2.71	121.38	127.61
21	A	850	BCR	C16-C17-C18	2.71	131.18	127.31
16	B	836	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
16	A	806	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
16	A	821	CLA	C1-O2A-CGA	2.71	123.55	116.44
16	2	604	CLA	C1-O2A-CGA	2.71	123.55	116.44
18	A	847	RRX	C7-C6-C5	-2.71	114.90	121.46
20	1	618	ERG	C16-C17-C13	2.71	107.11	103.84
16	1	603	CLA	C1D-ND-C4D	-2.71	104.41	106.33
21	A	845	BCR	C29-C30-C25	2.71	114.65	110.48
21	A	850	BCR	C36-C18-C17	-2.71	119.13	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	831	CLA	C2D-C1D-ND	2.71	112.10	110.10
17	J	104	C7Z	C39-C29-C30	-2.70	119.14	122.92
21	B	844	BCR	C7-C6-C5	-2.70	114.91	121.46
16	A	803	CLA	CHD-C1D-ND	-2.70	121.97	124.45
16	3	205	CLA	C2D-C1D-ND	2.70	112.09	110.10
16	1	609	CLA	O2A-CGA-CBA	2.70	120.39	111.91
16	2	601	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
16	O	201	CLA	C6-C5-C3	-2.70	106.37	113.45
21	A	850	BCR	C1-C6-C7	2.70	123.42	115.78
16	A	833	CLA	CHD-C1D-ND	-2.70	121.97	124.45
18	A	847	RRX	C33-C5-C6	-2.70	121.50	124.53
17	1	616	C7Z	C39-C29-C30	-2.70	119.14	122.92
16	1	604	CLA	C2C-C1C-NC	2.70	112.50	109.97
16	A	815	CLA	CHD-C1D-ND	-2.69	121.98	124.45
16	A	838	CLA	CHD-C1D-ND	-2.69	121.98	124.45
17	3	217	C7Z	C21-C26-C25	-2.69	118.82	122.61
16	A	832	CLA	CHD-C1D-ND	-2.69	121.98	124.45
18	2	616	RRX	C24-C23-C22	-2.69	122.17	126.23
21	B	843	BCR	C37-C22-C21	-2.69	119.15	122.92
16	A	826	CLA	OBD-CAD-C3D	-2.69	122.04	128.52
16	1	610	CLA	C2C-C1C-NC	2.69	112.49	109.97
16	A	827	CLA	C2D-C1D-ND	2.69	112.08	110.10
16	J	102	CLA	C2C-C1C-NC	2.69	112.49	109.97
16	B	809	CLA	CHD-C1D-ND	-2.69	121.99	124.45
16	2	604	CLA	CMA-C3A-C4A	2.68	118.99	111.77
27	B	839	PQN	C11-C12-C13	-2.68	122.33	126.79
20	2	618	ERG	C13-C17-C20	-2.68	115.97	119.43
16	A	819	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
21	K	104	BCR	C23-C22-C21	-2.68	114.83	118.94
16	L	204	CLA	C2C-C1C-NC	2.68	112.48	109.97
16	O	202	CLA	CHD-C1D-ND	-2.68	121.99	124.45
21	L	207	BCR	C8-C9-C10	2.68	123.05	118.94
16	1	607	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
16	2	606	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
16	B	837	CLA	CHD-C1D-ND	-2.68	121.99	124.45
16	1	603	CLA	C2C-C1C-NC	2.68	112.48	109.97
16	B	838	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
16	1	606	CLA	C2A-C3A-C4A	2.68	106.19	101.87
17	1	612	C7Z	C31-C30-C29	-2.67	123.49	127.31
16	B	834	CLA	CHD-C1D-ND	-2.67	122.00	124.45
16	A	806	CLA	CHD-C1D-ND	-2.67	122.00	124.45
16	3	213	CLA	C2D-C1D-ND	2.67	112.07	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	805	CLA	C2D-C1D-ND	2.67	112.07	110.10
16	B	825	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
16	A	826	CLA	C2D-C1D-ND	2.67	112.07	110.10
16	1	606	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
17	J	104	C7Z	C22-C23-C24	2.67	113.95	110.30
25	3	220	PTY	O4-C30-C31	2.67	120.27	111.91
16	B	804	CLA	C1-O2A-CGA	2.66	123.43	116.44
16	1	604	CLA	CHD-C1D-ND	-2.66	122.01	124.45
16	3	210	CLA	C2D-C1D-ND	2.66	112.07	110.10
18	A	847	RRX	C2-C1-C6	2.66	114.58	110.48
16	B	816	CLA	C1-C2-C3	-2.66	121.44	126.04
21	A	850	BCR	C37-C22-C21	-2.66	119.20	122.92
21	F	206	BCR	C36-C18-C17	-2.66	119.20	122.92
16	A	803	CLA	O2A-CGA-CBA	2.66	120.25	111.91
21	F	203	BCR	C33-C5-C4	2.66	118.72	113.62
16	O	204	CLA	CHD-C1D-ND	-2.66	122.01	124.45
16	B	827	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
16	B	832	CLA	C2C-C1C-NC	2.66	112.46	109.97
16	L	201	CLA	C2D-C1D-ND	2.66	112.06	110.10
16	A	835	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
16	A	835	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
16	B	813	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
16	B	837	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
16	B	819	CLA	CHD-C1D-ND	-2.65	122.02	124.45
16	B	805	CLA	C2D-C1D-ND	2.65	112.06	110.10
16	A	831	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
16	B	809	CLA	C2D-C1D-ND	2.65	112.06	110.10
16	A	822	CLA	C2C-C1C-NC	2.65	112.45	109.97
16	2	610	CLA	CHD-C1D-ND	-2.65	122.02	124.45
17	3	216	C7Z	C8-C7-C6	-2.65	119.77	127.20
16	A	815	CLA	C2D-C1D-ND	2.65	112.05	110.10
16	B	806	CLA	CHD-C1D-ND	-2.65	122.02	124.45
16	B	816	CLA	CHD-C1D-ND	-2.65	122.02	124.45
21	K	104	BCR	C29-C30-C25	-2.65	106.41	110.48
18	2	616	RRX	C30-C25-C24	2.65	123.26	115.78
17	1	616	C7Z	C7-C8-C9	-2.64	122.24	126.23
16	A	803	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
16	A	856	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
16	2	602	CLA	C1-C2-C3	-2.64	121.47	126.04
21	B	847	BCR	C31-C1-C6	-2.64	106.01	110.30
20	1	618	ERG	C19-C10-C1	-2.64	105.26	109.43
16	A	826	CLA	O2D-CGD-O1D	-2.64	118.68	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	2	615	C7Z	C21-C26-C27	2.64	123.25	115.78
16	A	855	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
21	A	845	BCR	C40-C30-C25	-2.64	106.02	110.30
16	A	814	CLA	C2D-C1D-ND	2.64	112.05	110.10
16	1	602	CLA	O2A-CGA-CBA	2.64	120.19	111.91
17	2	614	C7Z	C7-C8-C9	-2.64	122.25	126.23
16	A	808	CLA	C1-O2A-CGA	2.64	123.37	116.44
16	2	602	CLA	C2C-C1C-NC	2.64	112.44	109.97
21	K	104	BCR	C23-C24-C25	-2.64	119.80	127.20
16	B	817	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
16	B	806	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
21	B	847	BCR	C16-C17-C18	2.63	131.07	127.31
21	B	844	BCR	C33-C5-C4	2.63	118.68	113.62
16	J	102	CLA	C2D-C1D-ND	2.63	112.04	110.10
16	1	605	CLA	C5-C3-C2	2.63	126.44	121.12
16	B	831	CLA	CHD-C1D-ND	-2.63	122.04	124.45
16	A	835	CLA	C2D-C1D-ND	2.63	112.04	110.10
16	B	824	CLA	C2D-C1D-ND	2.63	112.04	110.10
16	A	821	CLA	C1-C2-C3	-2.63	121.49	126.04
16	A	815	CLA	C1-C2-C3	-2.63	121.49	126.04
16	A	805	CLA	CHD-C1D-ND	-2.63	122.04	124.45
16	O	202	CLA	C2C-C1C-NC	2.63	112.44	109.97
16	B	804	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
18	2	616	RRX	C7-C8-C9	-2.63	122.26	126.23
21	B	842	BCR	C31-C1-C6	-2.63	106.04	110.30
17	1	615	C7Z	C7-C6-C5	-2.62	115.11	121.46
16	2	601	CLA	C2D-C1D-ND	2.62	112.04	110.10
16	A	806	CLA	C1-C2-C3	-2.62	121.51	126.04
16	B	837	CLA	CMD-C2D-C3D	-2.62	121.59	127.61
16	3	210	CLA	C5-C3-C2	2.62	126.41	121.12
17	J	104	C7Z	C8-C9-C10	-2.62	114.93	118.94
16	B	830	CLA	O2A-CGA-CBA	2.61	120.11	111.91
16	B	834	CLA	CMC-C2C-C1C	2.61	129.02	125.04
21	K	104	BCR	C8-C7-C6	-2.61	119.86	127.20
16	L	201	CLA	C2C-C1C-NC	2.61	112.42	109.97
16	2	603	CLA	C5-C3-C2	2.61	126.41	121.12
16	A	829	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
17	2	615	C7Z	C18-C5-C4	2.61	119.20	114.36
16	I	101	CLA	O2A-CGA-CBA	2.61	120.11	111.91
18	A	847	RRX	C30-C25-C26	-2.61	118.93	122.61
16	B	806	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
21	L	206	BCR	C19-C18-C17	2.61	122.94	118.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	823	CLA	CMB-C2B-C3B	2.61	129.56	124.68
16	A	856	CLA	CMB-C2B-C3B	2.61	129.56	124.68
16	1	606	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
21	L	202	BCR	C30-C25-C26	-2.61	118.94	122.61
21	B	855	BCR	C38-C26-C25	-2.60	121.60	124.53
16	A	805	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
16	A	832	CLA	C2C-C1C-NC	2.60	112.41	109.97
16	A	856	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
16	A	834	CLA	CHD-C1D-ND	-2.60	122.06	124.45
16	F	204	CLA	C1-C2-C3	-2.60	121.54	126.04
16	A	814	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
16	A	838	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
16	B	808	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
17	2	614	C7Z	C40-C33-C34	-2.60	119.28	122.92
16	3	209	CLA	C2C-C1C-NC	2.60	112.41	109.97
16	A	811	CLA	CHD-C1D-ND	-2.60	122.06	124.45
16	B	820	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
17	3	216	C7Z	C15-C35-C34	2.60	128.80	123.47
21	A	850	BCR	C19-C18-C17	2.60	122.93	118.94
16	B	805	CLA	C2C-C1C-NC	2.60	112.41	109.97
16	B	805	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
16	1	605	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
16	A	810	CLA	C2D-C1D-ND	2.59	112.02	110.10
21	B	847	BCR	C8-C9-C10	2.59	122.92	118.94
20	1	618	ERG	C6-C7-C8	-2.59	116.96	122.07
16	B	818	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
16	1	602	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
16	O	203	CLA	CMD-C2D-C3D	-2.59	121.65	127.61
31	B	849	DGD	O1G-C1A-C2A	2.59	120.04	111.91
16	A	811	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
16	2	608	CLA	C2D-C1D-ND	2.59	112.01	110.10
16	A	856	CLA	C2D-C1D-ND	2.59	112.01	110.10
16	2	610	CLA	C2C-C1C-NC	2.59	112.40	109.97
16	1	607	CLA	CHD-C1D-ND	-2.59	122.07	124.45
16	A	820	CLA	CHD-C1D-ND	-2.59	122.07	124.45
16	A	806	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
16	I	102	CLA	C2C-C1C-NC	2.59	112.39	109.97
16	B	835	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
16	A	804	CLA	C2C-C1C-NC	2.59	112.39	109.97
16	A	818	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
18	2	616	RRX	C1-C6-C5	-2.58	118.97	122.61
20	2	621	ERG	C20-C22-C23	-2.58	117.65	125.67

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	837	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
16	B	829	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
16	3	208	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
16	3	206	CLA	C2D-C1D-ND	2.58	112.01	110.10
16	B	823	CLA	C2C-C1C-NC	2.58	112.39	109.97
16	A	829	CLA	C2D-C1D-ND	2.58	112.01	110.10
16	A	836	CLA	C2D-C1D-ND	2.58	112.00	110.10
17	1	612	C7Z	C18-C5-C4	2.58	119.13	114.36
30	A	851	T7X	O18-C11-C31	2.58	120.00	111.91
16	A	836	CLA	C2C-C1C-NC	2.58	112.39	109.97
17	3	217	C7Z	C38-C25-C24	2.58	119.13	114.36
19	2	622	LHG	C5-O7-C7	-2.58	111.45	117.79
16	L	204	CLA	C2D-C1D-ND	2.58	112.00	110.10
21	L	206	BCR	C35-C13-C12	2.58	122.14	118.08
16	3	203	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
16	B	811	CLA	C2C-C1C-NC	2.57	112.38	109.97
17	2	615	C7Z	C39-C29-C30	-2.57	119.32	122.92
16	2	605	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
21	B	843	BCR	C38-C26-C27	2.57	118.56	113.62
16	1	611	CLA	C2D-C1D-ND	2.57	112.00	110.10
16	A	837	CLA	CHD-C1D-ND	-2.57	122.09	124.45
16	B	807	CLA	CHD-C1D-ND	-2.57	122.09	124.45
16	A	855	CLA	CHA-C1A-NA	-2.57	120.51	126.40
21	2	617	BCR	C30-C25-C24	2.57	123.05	115.78
16	A	830	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
16	A	808	CLA	C2D-C1D-ND	2.57	112.00	110.10
16	A	832	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
17	3	218	C7Z	C39-C29-C30	-2.56	119.33	122.92
16	2	604	CLA	CHD-C1D-ND	-2.56	122.10	124.45
16	A	816	CLA	C2C-C1C-NC	2.56	112.37	109.97
16	B	830	CLA	CMA-C3A-C4A	2.56	118.66	111.77
16	B	803	CLA	CHD-C1D-ND	-2.56	122.10	124.45
16	A	808	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
16	A	818	CLA	CMA-C3A-C2A	2.56	124.16	113.83
16	3	208	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
17	3	216	C7Z	C8-C9-C10	2.56	122.87	118.94
16	B	831	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
16	A	817	CLA	C2D-C1D-ND	2.56	111.99	110.10
16	A	822	CLA	CHD-C1D-ND	-2.56	122.10	124.45
20	2	621	ERG	C14-C8-C7	-2.56	119.34	124.38
16	A	819	CLA	CBA-CAA-C2A	2.56	121.41	113.86
16	3	205	CLA	CHA-C4D-ND	2.56	137.85	132.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	I	103	BCR	C36-C18-C17	-2.56	119.34	122.92
16	I	101	CLA	C1D-ND-C4D	-2.56	104.52	106.33
29	A	849	3PH	O31-C31-C32	2.56	119.93	111.91
21	B	843	BCR	C34-C9-C8	2.56	122.11	118.08
16	3	206	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
16	A	824	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
16	B	816	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
31	B	850	DGD	O1G-C1A-C2A	2.56	119.93	111.91
16	A	809	CLA	CHD-C1D-ND	-2.56	122.11	124.45
22	2	619	PGT	O2-C31-O31	-2.56	117.53	123.70
16	A	822	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
16	B	805	CLA	CMA-C3A-C4A	2.55	118.64	111.77
16	1	608	CLA	C5-C3-C2	2.55	126.29	121.12
16	3	204	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
16	A	804	CLA	CHA-C4D-ND	2.55	137.84	132.50
16	3	211	CLA	C2D-C1D-ND	2.55	111.98	110.10
21	B	841	BCR	C33-C5-C4	2.55	118.52	113.62
16	B	815	CLA	C1-C2-C3	-2.55	121.63	126.04
16	O	204	CLA	C2C-C1C-NC	2.55	112.36	109.97
16	A	814	CLA	O2A-CGA-CBA	2.55	119.91	111.91
16	F	204	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
16	3	207	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
16	A	827	CLA	CMB-C2B-C3B	2.55	129.44	124.68
16	A	828	CLA	C1-O2A-CGA	2.54	123.12	116.44
19	2	622	LHG	O8-C23-C24	2.54	119.89	111.91
16	B	832	CLA	CHD-C1D-ND	-2.54	122.12	124.45
16	F	205	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
16	L	205	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
17	3	215	C7Z	C7-C8-C9	-2.54	122.39	126.23
16	B	833	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
17	1	614	C7Z	C38-C25-C24	2.54	119.06	114.36
16	1	606	CLA	C2D-C1D-ND	2.54	111.98	110.10
18	2	616	RRX	C19-C18-C17	2.54	122.84	118.94
21	B	840	BCR	C7-C6-C5	-2.54	115.31	121.46
16	B	838	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
16	A	810	CLA	O1D-CGD-CBD	-2.54	119.29	124.48
16	A	835	CLA	CHD-C1D-ND	-2.54	122.12	124.45
16	2	608	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
16	A	802	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
16	B	801	CLA	CMB-C2B-C3B	2.54	129.43	124.68
21	B	845	BCR	C33-C5-C4	2.54	118.49	113.62
17	3	217	C7Z	C8-C7-C6	-2.54	120.08	127.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	815	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
16	B	808	CLA	O2A-CGA-CBA	2.54	119.86	111.91
16	A	802	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
16	B	817	CLA	C2D-C1D-ND	2.53	111.97	110.10
16	O	202	CLA	C2D-C1D-ND	2.53	111.97	110.10
16	B	831	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
16	B	828	CLA	O2A-CGA-CBA	2.53	119.86	111.91
16	L	203	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
16	L	204	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
16	1	603	CLA	OBD-CAD-C3D	-2.53	122.43	128.52
16	3	205	CLA	CMB-C2B-C3B	2.53	129.41	124.68
16	B	827	CLA	CHD-C1D-ND	-2.53	122.13	124.45
16	O	201	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
16	1	610	CLA	C1D-ND-C4D	-2.53	104.54	106.33
16	A	816	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
25	A	852	PTY	O4-C30-C31	2.53	119.84	111.91
16	B	810	CLA	CHD-C1D-ND	-2.53	122.13	124.45
16	2	603	CLA	O2A-CGA-CBA	2.53	119.84	111.91
16	B	816	CLA	O2A-CGA-CBA	2.52	119.83	111.91
16	B	837	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
16	2	602	CLA	CHD-C1D-ND	-2.52	122.14	124.45
16	B	826	CLA	CHD-C1D-ND	-2.52	122.14	124.45
17	1	615	C7Z	C38-C25-C24	2.52	119.03	114.36
16	A	855	CLA	CHA-C4D-ND	2.52	137.77	132.50
16	1	611	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
16	3	213	CLA	CHD-C1D-ND	-2.52	122.14	124.45
16	B	829	CLA	CMD-C2D-C3D	-2.52	121.82	127.61
16	A	825	CLA	C2D-C1D-ND	2.52	111.96	110.10
16	K	101	CLA	C2D-C1D-ND	2.52	111.96	110.10
16	3	214	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
16	3	208	CLA	C1-O2A-CGA	2.52	123.05	116.44
16	2	613	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
16	A	804	CLA	CHD-C1D-ND	-2.52	122.14	124.45
16	B	814	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
16	A	839	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
22	B	848	PGT	O2-C31-O31	-2.51	117.63	123.70
20	1	618	ERG	C7-C6-C5	-2.51	118.79	123.20
21	B	847	BCR	C28-C27-C26	-2.51	109.59	114.08
16	B	837	CLA	C1-C2-C3	-2.51	121.69	126.04
16	A	834	CLA	C2C-C1C-NC	2.51	112.33	109.97
16	A	821	CLA	CHD-C1D-ND	-2.51	122.15	124.45
29	B	854	3PH	O31-C31-C32	2.51	119.79	111.91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	602	CLA	C1D-ND-C4D	-2.51	104.55	106.33
16	A	823	CLA	C2C-C1C-NC	2.51	112.32	109.97
16	A	829	CLA	CHD-C1D-ND	-2.51	122.15	124.45
23	J	101	DGA	OG1-CA1-CA2	2.51	119.78	111.91
21	B	841	BCR	C4-C5-C6	-2.51	119.09	122.73
16	B	820	CLA	C2D-C1D-ND	2.51	111.95	110.10
16	B	803	CLA	O2A-CGA-CBA	2.51	119.78	111.91
16	3	213	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
17	J	104	C7Z	C2-C3-C4	2.51	113.73	110.30
16	2	606	CLA	C2D-C1D-ND	2.51	111.95	110.10
16	A	817	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
16	2	603	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
16	A	807	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
16	A	837	CLA	O2A-CGA-CBA	2.51	119.77	111.91
21	B	855	BCR	C34-C9-C8	2.51	122.02	118.08
16	A	837	CLA	C2D-C1D-ND	2.50	111.95	110.10
20	2	621	ERG	C2-C3-C4	2.50	113.74	110.31
16	B	824	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
16	2	613	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
21	I	103	BCR	C28-C27-C26	-2.50	109.61	114.08
16	1	606	CLA	CHA-C4D-ND	2.50	137.73	132.50
16	A	827	CLA	CHD-C1D-ND	-2.50	122.16	124.45
16	I	102	CLA	C2D-C1D-ND	2.50	111.94	110.10
16	2	610	CLA	CMA-C3A-C2A	2.50	123.90	113.83
29	J	105	3PH	O31-C31-C32	2.50	119.74	111.91
18	1	613	RRX	C38-C26-C27	2.50	118.98	114.36
16	O	203	CLA	CHA-C4D-ND	2.50	137.72	132.50
16	A	825	CLA	CHD-C1D-ND	-2.50	122.16	124.45
16	2	611	CLA	C1C-C2C-C3C	-2.49	104.33	106.96
16	K	102	CLA	CHD-C1D-ND	-2.49	122.16	124.45
16	B	837	CLA	CHA-C4D-ND	2.49	137.71	132.50
16	B	828	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
18	J	103	RRX	C2-C1-C6	2.49	114.32	110.48
16	A	807	CLA	C2C-C1C-NC	2.49	112.31	109.97
16	1	604	CLA	C2D-C1D-ND	2.49	111.94	110.10
16	I	102	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
16	1	601	CLA	CHD-C1D-ND	-2.49	122.17	124.45
16	K	102	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
16	3	205	CLA	O2A-CGA-CBA	2.49	119.72	111.91
16	3	211	CLA	CHA-C4D-ND	2.49	137.71	132.50
21	B	840	BCR	C3-C4-C5	-2.49	109.63	114.08
16	A	831	CLA	CHD-C1D-ND	-2.49	122.17	124.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	828	CLA	CHD-C1D-ND	-2.49	122.17	124.45
16	B	834	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
16	B	815	CLA	C2C-C1C-NC	2.49	112.30	109.97
16	3	203	CLA	CHA-C4D-ND	2.49	137.70	132.50
16	2	609	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
16	A	802	CLA	CHD-C1D-ND	-2.49	122.17	124.45
19	B	851	LHG	C5-O7-C7	-2.49	111.67	117.79
16	3	212	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
16	B	814	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
16	B	810	CLA	C2D-C1D-ND	2.49	111.94	110.10
16	B	809	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
17	2	614	C7Z	C38-C25-C24	2.49	118.96	114.36
16	1	601	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
16	J	102	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
16	3	207	CLA	C4-C3-C5	2.48	119.45	115.27
16	A	804	CLA	CMD-C2D-C3D	-2.48	121.90	127.61
16	A	816	CLA	O2A-CGA-CBA	2.48	119.70	111.91
16	B	834	CLA	CMB-C2B-C3B	2.48	129.33	124.68
16	B	815	CLA	O2A-CGA-CBA	2.48	119.70	111.91
16	B	824	CLA	CAA-C2A-C1A	-2.48	103.84	111.97
16	A	813	CLA	C2D-C1D-ND	2.48	111.93	110.10
21	A	844	BCR	C19-C18-C17	2.48	122.75	118.94
16	A	827	CLA	C2C-C1C-NC	2.48	112.30	109.97
16	B	821	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
16	A	810	CLA	O2A-CGA-CBA	2.48	119.70	111.91
16	3	210	CLA	CHD-C1D-ND	-2.48	122.17	124.45
21	B	847	BCR	C35-C13-C12	2.48	121.99	118.08
17	1	612	C7Z	C15-C35-C34	-2.48	118.39	123.47
17	A	843	C7Z	C39-C29-C30	-2.48	119.45	122.92
16	1	601	CLA	C2D-C1D-ND	2.48	111.93	110.10
16	A	834	CLA	CHA-C4D-ND	2.48	137.69	132.50
16	2	607	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
16	A	833	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
16	A	828	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
16	B	813	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
16	B	816	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
16	B	819	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
16	B	802	CLA	C2D-C1D-ND	2.48	111.93	110.10
16	B	830	CLA	C2D-C1D-ND	2.48	111.93	110.10
16	A	832	CLA	C1-C2-C3	-2.48	121.76	126.04
16	O	203	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
16	3	209	CLA	O2A-CGA-CBA	2.48	119.68	111.91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	834	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
16	A	830	CLA	CHA-C4D-ND	2.47	137.68	132.50
16	3	205	CLA	CBA-CAA-C2A	2.47	121.16	113.86
17	2	615	C7Z	C23-C24-C25	2.47	116.78	111.85
16	A	856	CLA	CHD-C1D-ND	-2.47	122.18	124.45
19	A	841	LHG	O8-C23-C24	2.47	119.66	111.91
16	1	608	CLA	CHD-C1D-ND	-2.47	122.19	124.45
16	A	854	CLA	C1-O2A-CGA	2.47	122.92	116.44
16	3	203	CLA	C1-C2-C3	-2.47	121.78	126.04
16	1	607	CLA	C2C-C1C-NC	2.47	112.28	109.97
16	1	606	CLA	O2A-CGA-CBA	2.47	119.65	111.91
31	B	846	DGD	O1G-C1A-C2A	2.47	119.65	111.91
16	B	806	CLA	CHA-C4D-ND	2.47	137.66	132.50
16	A	833	CLA	C2D-C1D-ND	2.47	111.92	110.10
16	L	203	CLA	C2D-C1D-ND	2.47	111.92	110.10
16	3	203	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
16	A	856	CLA	C2C-C1C-NC	2.46	112.28	109.97
16	A	808	CLA	CHD-C1D-ND	-2.46	122.19	124.45
16	B	821	CLA	C2D-C1D-ND	2.46	111.92	110.10
16	2	604	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
20	2	618	ERG	C13-C14-C8	2.46	118.26	113.48
16	A	812	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
16	1	610	CLA	CHD-C1D-ND	-2.46	122.19	124.45
16	B	819	CLA	CHA-C4D-ND	2.46	137.65	132.50
16	B	814	CLA	CMA-C3A-C4A	2.46	118.39	111.77
16	J	102	CLA	CHA-C4D-ND	2.46	137.65	132.50
26	A	801	CL0	CMB-C2B-C3B	2.46	129.28	124.68
17	3	215	C7Z	C28-C27-C26	-2.46	120.29	127.20
16	I	101	CLA	C1-C2-C3	-2.46	121.79	126.04
16	1	603	CLA	CHD-C1D-ND	-2.46	122.19	124.45
16	B	821	CLA	CHA-C4D-ND	2.46	137.65	132.50
16	A	836	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
17	1	615	C7Z	C2-C3-C4	2.46	113.67	110.30
16	3	214	CLA	C2D-C1D-ND	2.46	111.92	110.10
16	A	855	CLA	CHD-C1D-ND	-2.46	122.19	124.45
16	B	802	CLA	CHD-C1D-ND	-2.46	122.19	124.45
16	A	803	CLA	CHA-C4D-ND	2.46	137.64	132.50
16	A	829	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
16	F	205	CLA	C2D-C1D-ND	2.46	111.92	110.10
16	A	810	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
16	B	814	CLA	CHD-C1D-ND	-2.46	122.20	124.45
16	B	801	CLA	O2A-CGA-CBA	2.46	119.61	111.91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F	202	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
16	B	815	CLA	C1-O2A-CGA	2.45	122.89	116.44
16	B	810	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
16	L	203	CLA	CHD-C1D-ND	-2.45	122.20	124.45
16	L	201	CLA	CMA-C3A-C4A	2.45	118.37	111.77
16	A	839	CLA	CHA-C4D-ND	2.45	137.63	132.50
16	O	202	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
16	2	612	CLA	CHA-C4D-ND	2.45	137.62	132.50
16	2	609	CLA	CHD-C1D-ND	-2.45	122.20	124.45
16	3	210	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
16	3	204	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
16	3	212	CLA	CHD-C1D-ND	-2.45	122.20	124.45
16	2	601	CLA	CHA-C4D-ND	2.45	137.62	132.50
17	2	614	C7Z	C39-C29-C30	-2.45	119.50	122.92
16	2	609	CLA	C2D-C1D-ND	2.45	111.91	110.10
16	3	204	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
16	B	836	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
16	O	204	CLA	C1D-ND-C4D	-2.45	104.60	106.33
16	A	808	CLA	C2C-C1C-NC	2.44	112.26	109.97
16	A	804	CLA	O2A-CGA-CBA	2.44	119.58	111.91
16	1	611	CLA	CHD-C1D-ND	-2.44	122.21	124.45
16	3	207	CLA	CMD-C2D-C3D	-2.44	121.99	127.61
16	B	803	CLA	CHA-C4D-ND	2.44	137.61	132.50
23	2	620	DGA	OG1-CA1-CA2	2.44	119.57	111.91
16	A	813	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
16	1	603	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
16	A	820	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
21	L	207	BCR	C33-C5-C6	-2.44	121.79	124.53
16	2	606	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
16	B	829	CLA	C5-C3-C2	2.44	126.06	121.12
16	F	205	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
16	A	831	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
16	1	607	CLA	C1D-ND-C4D	-2.44	104.60	106.33
16	B	808	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
16	A	821	CLA	CMA-C3A-C4A	2.44	118.33	111.77
17	1	615	C7Z	C28-C27-C26	-2.44	120.35	127.20
16	A	830	CLA	C2D-C1D-ND	2.44	111.90	110.10
16	A	820	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
16	A	815	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	B	849	DGD	C3G-O3G-C1D	2.44	118.50	113.74
16	2	610	CLA	C1-O2A-CGA	2.44	122.83	116.44
16	B	826	CLA	C2D-C1D-ND	2.44	111.90	110.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	2	604	CLA	C2C-C1C-NC	2.43	112.25	109.97
18	J	103	RRX	C21-C20-C19	2.43	130.81	123.22
16	2	605	CLA	O2A-CGA-CBA	2.43	119.55	111.91
16	A	803	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
16	1	606	CLA	CHD-C1D-ND	-2.43	122.22	124.45
16	B	813	CLA	O2A-CGA-CBA	2.43	119.55	111.91
21	F	206	BCR	C36-C18-C19	-2.43	114.24	118.08
16	J	102	CLA	C1-C2-C3	-2.43	121.83	126.04
16	B	822	CLA	CHD-C1D-ND	-2.43	122.22	124.45
16	3	212	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
16	2	602	CLA	C2D-C1D-ND	2.43	111.90	110.10
16	A	821	CLA	C1D-ND-C4D	-2.43	104.61	106.33
18	A	847	RRX	C10-C11-C12	2.43	130.80	123.22
16	A	820	CLA	CHA-C4D-ND	2.43	137.58	132.50
16	3	212	CLA	C2D-C1D-ND	2.43	111.89	110.10
16	B	802	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
16	A	855	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
17	2	615	C7Z	C28-C27-C26	-2.43	120.38	127.20
21	A	844	BCR	C29-C30-C25	-2.43	106.74	110.48
17	3	215	C7Z	C20-C13-C14	-2.43	119.52	122.92
16	A	836	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
16	K	101	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
21	B	844	BCR	C19-C18-C17	2.43	122.67	118.94
17	2	615	C7Z	C20-C13-C14	-2.43	119.52	122.92
16	B	805	CLA	C1C-C2C-C3C	-2.43	104.41	106.96
16	A	818	CLA	C1-C2-C3	-2.42	121.85	126.04
16	A	816	CLA	C2D-C1D-ND	2.42	111.89	110.10
16	1	608	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
16	B	829	CLA	CHA-C4D-ND	2.42	137.57	132.50
16	B	838	CLA	CHA-C4D-ND	2.42	137.57	132.50
16	B	832	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
16	3	209	CLA	CHA-C4D-ND	2.42	137.57	132.50
16	F	201	CLA	O2A-CGA-CBA	2.42	119.52	111.91
16	B	815	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
16	J	102	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
16	3	206	CLA	C1-C2-C3	-2.42	121.85	126.04
16	B	838	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
16	2	612	CLA	C4-C3-C2	-2.42	117.46	123.68
16	B	822	CLA	C2D-C1D-ND	2.42	111.89	110.10
16	2	607	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
16	B	817	CLA	CHA-C4D-ND	2.42	137.56	132.50
16	B	825	CLA	O2A-CGA-CBA	2.42	119.50	111.91

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	838	CLA	C2D-C1D-ND	2.42	111.89	110.10
16	A	825	CLA	CHA-C4D-ND	2.42	137.56	132.50
16	L	203	CLA	CHA-C4D-ND	2.42	137.56	132.50
16	2	604	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
16	2	611	CLA	CHD-C1D-ND	-2.42	122.23	124.45
26	A	801	CL0	C4-C3-C5	2.42	119.34	115.27
16	A	826	CLA	CHA-C4D-ND	2.42	137.56	132.50
16	3	211	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
16	B	808	CLA	C2D-C1D-ND	2.42	111.89	110.10
16	3	207	CLA	CHA-C4D-ND	2.42	137.56	132.50
21	B	841	BCR	C36-C18-C17	-2.42	119.54	122.92
16	2	607	CLA	CHA-C4D-ND	2.42	137.56	132.50
21	O	205	BCR	C32-C1-C6	-2.42	106.38	110.30
16	B	835	CLA	C1C-C2C-C3C	-2.42	104.42	106.96
19	A	842	LHG	O8-C23-C24	2.42	119.49	111.91
16	B	820	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
16	2	603	CLA	CHA-C4D-ND	2.42	137.55	132.50
16	B	825	CLA	CHA-C4D-ND	2.42	137.55	132.50
16	A	824	CLA	CHA-C4D-ND	2.42	137.55	132.50
16	B	823	CLA	CHA-C4D-ND	2.42	137.55	132.50
16	B	807	CLA	O2D-CGD-O1D	-2.42	119.12	123.84
17	2	614	C7Z	C28-C27-C26	-2.41	120.42	127.20
16	A	819	CLA	CHA-C4D-ND	2.41	137.55	132.50
16	A	825	CLA	O2A-CGA-CBA	2.41	119.48	111.91
16	F	201	CLA	C2C-C1C-NC	2.41	112.23	109.97
17	2	614	C7Z	C18-C5-C4	2.41	118.83	114.36
16	B	836	CLA	CHA-C4D-ND	2.41	137.55	132.50
16	1	608	CLA	C2D-C1D-ND	2.41	111.88	110.10
17	3	201	C7Z	C28-C27-C26	-2.41	120.42	127.20
16	1	609	CLA	CHA-C4D-ND	2.41	137.55	132.50
16	B	818	CLA	CHA-C4D-ND	2.41	137.55	132.50
16	B	805	CLA	CHD-C1D-ND	-2.41	122.24	124.45
16	A	833	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
17	3	216	C7Z	C2-C3-C4	2.41	113.61	110.30
16	B	823	CLA	O2A-CGA-CBA	2.41	119.48	111.91
16	B	804	CLA	CHA-C4D-ND	2.41	137.54	132.50
16	B	816	CLA	CMD-C2D-C3D	-2.41	122.07	127.61
16	B	825	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
19	1	617	LHG	C5-O7-C7	-2.41	111.85	117.79
16	B	832	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
16	A	813	CLA	CHA-C4D-ND	2.41	137.54	132.50
16	K	101	CLA	O2D-CGD-O1D	-2.41	119.13	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	844	BCR	C27-C26-C25	-2.41	119.23	122.73
16	2	610	CLA	C2D-C1D-ND	2.41	111.88	110.10
16	B	803	CLA	OBD-CAD-C3D	-2.41	122.72	128.52
16	B	818	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
21	L	206	BCR	C24-C25-C26	-2.41	115.63	121.46
16	2	613	CLA	CHD-C1D-ND	-2.41	122.24	124.45
16	A	819	CLA	CHD-C1D-ND	-2.41	122.24	124.45
16	A	828	CLA	CHD-C1D-ND	-2.41	122.24	124.45
16	B	812	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
18	2	616	RRX	C8-C9-C10	2.41	122.64	118.94
16	2	605	CLA	C1D-ND-C4D	-2.41	104.62	106.33
16	2	609	CLA	C1-C2-C3	-2.41	121.88	126.04
16	A	831	CLA	CHA-C4D-ND	2.41	137.53	132.50
17	3	201	C7Z	C8-C9-C10	2.41	122.63	118.94
17	3	218	C7Z	C2-C3-C4	2.40	113.60	110.30
16	2	613	CLA	CHA-C4D-ND	2.40	137.53	132.50
16	K	102	CLA	CMA-C3A-C4A	2.40	118.23	111.77
16	B	826	CLA	C1C-C2C-C3C	-2.40	104.43	106.96
16	B	808	CLA	CHA-C4D-ND	2.40	137.53	132.50
16	A	820	CLA	O2A-CGA-CBA	2.40	119.45	111.91
16	3	207	CLA	C2D-C1D-ND	2.40	111.87	110.10
16	2	603	CLA	CHD-C1D-ND	-2.40	122.25	124.45
21	B	840	BCR	C33-C5-C4	2.40	118.23	113.62
18	J	103	RRX	C38-C26-C27	2.40	118.80	114.36
16	B	832	CLA	O2A-CGA-CBA	2.40	119.44	111.91
16	A	805	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
16	2	601	CLA	CMA-C3A-C4A	2.40	118.22	111.77
21	L	207	BCR	C28-C27-C26	-2.40	109.79	114.08
19	3	219	LHG	C5-O7-C7	-2.40	111.89	117.79
16	3	207	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
16	A	809	CLA	C1D-ND-C4D	-2.40	104.63	106.33
16	A	813	CLA	C1-C2-C3	-2.40	121.90	126.04
16	A	827	CLA	CHA-C4D-ND	2.40	137.51	132.50
16	L	204	CLA	CMA-C3A-C4A	2.40	118.21	111.77
16	K	102	CLA	CHA-C4D-ND	2.39	137.51	132.50
16	F	205	CLA	CHD-C1D-ND	-2.39	122.25	124.45
16	B	815	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
16	B	816	CLA	CHA-C4D-ND	2.39	137.50	132.50
16	B	824	CLA	O2A-CGA-CBA	2.39	119.42	111.91
16	3	212	CLA	CHA-C4D-ND	2.39	137.50	132.50
21	K	104	BCR	C35-C13-C12	-2.39	114.31	118.08
17	1	614	C7Z	C40-C33-C34	-2.39	119.57	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	824	CLA	C1-C2-C3	-2.39	121.91	126.04
21	B	855	BCR	C40-C30-C25	2.39	114.18	110.30
16	B	802	CLA	C1C-C2C-C3C	-2.39	104.44	106.96
17	3	217	C7Z	C11-C12-C13	-2.39	119.70	126.42
21	B	844	BCR	C15-C14-C13	-2.39	123.90	127.31
16	B	834	CLA	C1D-ND-C4D	-2.39	104.64	106.33
16	B	835	CLA	CHA-C4D-ND	2.39	137.50	132.50
16	A	817	CLA	CMD-C2D-C3D	-2.39	122.12	127.61
16	B	818	CLA	CMD-C2D-C3D	-2.39	122.12	127.61
16	K	102	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
16	K	101	CLA	CHA-C4D-ND	2.39	137.49	132.50
16	1	607	CLA	O2A-CGA-CBA	2.39	119.40	111.91
16	2	612	CLA	CHD-C1D-ND	-2.39	122.26	124.45
16	O	202	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
16	A	827	CLA	C1C-C2C-C3C	-2.39	104.45	106.96
16	A	832	CLA	CHA-C4D-ND	2.39	137.49	132.50
16	A	856	CLA	O2A-CGA-CBA	2.39	119.40	111.91
21	B	845	BCR	C34-C9-C8	2.39	121.84	118.08
16	2	608	CLA	CHA-C4D-ND	2.38	137.49	132.50
16	B	808	CLA	CHD-C1D-ND	-2.38	122.26	124.45
16	3	213	CLA	CHA-C4D-ND	2.38	137.49	132.50
16	3	214	CLA	CHA-C4D-ND	2.38	137.49	132.50
16	2	602	CLA	CHA-C4D-ND	2.38	137.48	132.50
17	1	614	C7Z	C28-C27-C26	-2.38	120.51	127.20
16	A	816	CLA	CHD-C1D-ND	-2.38	122.27	124.45
16	A	810	CLA	CHA-C4D-ND	2.38	137.48	132.50
16	A	804	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
16	A	809	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
16	1	602	CLA	CHD-C1D-ND	-2.38	122.27	124.45
20	2	621	ERG	C18-C13-C14	-2.38	106.39	110.24
17	J	104	C7Z	C31-C32-C33	-2.38	119.73	126.42
16	2	609	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
18	1	613	RRX	C24-C25-C26	-2.38	115.70	121.46
16	B	826	CLA	CHA-C4D-ND	2.38	137.48	132.50
16	F	201	CLA	C1C-C2C-C3C	-2.38	104.45	106.96
16	A	813	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
16	A	805	CLA	CHA-C4D-ND	2.38	137.47	132.50
16	2	601	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
16	L	203	CLA	O2A-CGA-CBA	2.38	119.37	111.91
16	A	814	CLA	CMB-C2B-C3B	2.38	129.13	124.68
16	B	824	CLA	C1C-C2C-C3C	-2.38	104.46	106.96
16	B	805	CLA	CHA-C4D-ND	2.38	137.47	132.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	835	CLA	C2C-C1C-NC	2.38	112.20	109.97
16	1	607	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
21	A	846	BCR	C24-C25-C26	-2.38	115.71	121.46
17	2	615	C7Z	C11-C12-C13	-2.38	119.74	126.42
16	F	204	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
16	L	205	CLA	CHA-C4D-ND	2.37	137.47	132.50
16	A	818	CLA	CMD-C2D-C3D	-2.37	122.15	127.61
16	2	602	CLA	O2D-CGD-O1D	-2.37	119.19	123.84
16	2	612	CLA	C2D-C1D-ND	2.37	111.85	110.10
16	A	828	CLA	CHA-C4D-ND	2.37	137.47	132.50
16	B	822	CLA	CHA-C4D-ND	2.37	137.47	132.50
16	1	611	CLA	CHA-C4D-ND	2.37	137.47	132.50
16	B	802	CLA	CHA-C4D-ND	2.37	137.47	132.50
16	A	807	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
16	2	610	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
16	A	807	CLA	CHA-C4D-ND	2.37	137.46	132.50
30	A	851	T7X	C12-C13-C14	-2.37	109.00	113.23
16	3	209	CLA	C2D-C1D-ND	2.37	111.85	110.10
16	3	204	CLA	O2A-CGA-CBA	2.37	119.35	111.91
16	A	818	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
16	3	204	CLA	CHA-C4D-ND	2.37	137.46	132.50
16	3	205	CLA	C1C-C2C-C3C	-2.37	104.46	106.96
16	B	833	CLA	C5-C3-C2	2.37	125.91	121.12
16	2	611	CLA	CHA-C4D-ND	2.37	137.46	132.50
16	A	819	CLA	CAA-C2A-C3A	2.37	119.26	112.78
16	A	807	CLA	CHD-C1D-ND	-2.37	122.28	124.45
16	K	101	CLA	CHD-C1D-ND	-2.37	122.28	124.45
16	A	802	CLA	CHA-C4D-ND	2.37	137.45	132.50
16	A	837	CLA	CHA-C4D-ND	2.37	137.45	132.50
16	A	854	CLA	C1D-ND-C4D	-2.37	104.65	106.33
21	F	206	BCR	C30-C25-C26	-2.37	119.28	122.61
16	A	806	CLA	CMA-C3A-C4A	2.37	118.13	111.77
31	B	849	DGD	O3G-C1D-C2D	2.37	112.00	108.30
16	A	812	CLA	CHA-C4D-ND	2.37	137.45	132.50
16	B	823	CLA	C1C-C2C-C3C	-2.37	104.47	106.96
16	2	608	CLA	C5-C3-C2	2.37	125.90	121.12
16	A	834	CLA	C1-C2-C3	-2.37	121.95	126.04
16	A	833	CLA	CHA-C4D-ND	2.37	137.45	132.50
16	A	819	CLA	C2D-C1D-ND	2.37	111.85	110.10
16	1	608	CLA	CHA-C4D-ND	2.36	137.44	132.50
21	A	857	BCR	C38-C26-C27	2.36	118.16	113.62
16	A	815	CLA	CMD-C2D-C3D	-2.36	122.18	127.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	617	BCR	C24-C25-C26	-2.36	115.74	121.46
16	A	838	CLA	CMA-C3A-C4A	2.36	118.12	111.77
17	1	616	C7Z	C22-C23-C24	2.36	113.54	110.30
16	B	832	CLA	CHA-C4D-ND	2.36	137.44	132.50
18	A	847	RRX	C35-C13-C12	2.36	121.80	118.08
16	A	825	CLA	C4-C3-C2	-2.36	117.62	123.68
16	B	814	CLA	CHA-C4D-ND	2.36	137.44	132.50
21	F	203	BCR	C1-C6-C5	-2.36	119.29	122.61
16	L	205	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
16	B	804	CLA	O2A-C1-C2	2.36	114.84	108.64
16	1	601	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
16	B	833	CLA	CHA-C4D-ND	2.36	137.44	132.50
16	B	801	CLA	OBD-CAD-C3D	-2.36	122.84	128.52
16	2	606	CLA	CHA-C4D-ND	2.36	137.43	132.50
16	B	806	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
16	1	603	CLA	C1-O2A-CGA	2.36	122.63	116.44
16	A	821	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
16	B	822	CLA	O2A-CGA-CBA	2.36	119.31	111.91
16	I	102	CLA	C1C-C2C-C3C	-2.36	104.48	106.96
16	2	609	CLA	CHA-C4D-ND	2.36	137.43	132.50
16	B	828	CLA	C1-O2A-CGA	2.36	122.63	116.44
16	A	803	CLA	CMB-C2B-C3B	2.36	129.09	124.68
16	B	828	CLA	CHA-C4D-ND	2.35	137.43	132.50
16	A	804	CLA	C1C-C2C-C3C	-2.35	104.48	106.96
17	A	843	C7Z	C2-C3-C4	2.35	113.53	110.30
20	2	618	ERG	C20-C22-C23	-2.35	118.37	125.67
21	B	843	BCR	C30-C25-C24	2.35	122.44	115.78
16	A	834	CLA	C2D-C1D-ND	2.35	111.84	110.10
16	A	810	CLA	C1-O2A-CGA	2.35	122.61	116.44
16	1	603	CLA	CHA-C4D-ND	2.35	137.42	132.50
16	B	832	CLA	C2D-C1D-ND	2.35	111.84	110.10
16	A	832	CLA	C1C-C2C-C3C	-2.35	104.48	106.96
16	B	811	CLA	CHA-C4D-ND	2.35	137.42	132.50
16	B	838	CLA	CMA-C3A-C4A	2.35	118.09	111.77
16	A	809	CLA	CHA-C4D-ND	2.35	137.42	132.50
16	B	815	CLA	CHA-C4D-ND	2.35	137.41	132.50
16	A	830	CLA	C4-C3-C2	-2.35	117.65	123.68
16	A	810	CLA	C2C-C1C-NC	2.35	112.17	109.97
16	A	838	CLA	C1D-ND-C4D	-2.35	104.67	106.33
16	F	201	CLA	CHD-C1D-ND	-2.35	122.30	124.45
21	A	850	BCR	C38-C26-C25	-2.35	121.89	124.53
21	O	205	BCR	C37-C22-C21	-2.35	119.64	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	838	CLA	C2C-C1C-NC	2.35	112.17	109.97
16	2	610	CLA	CHA-C4D-ND	2.35	137.41	132.50
16	B	813	CLA	CHA-C4D-ND	2.35	137.41	132.50
16	2	612	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
16	O	204	CLA	C1C-C2C-C3C	-2.34	104.49	106.96
16	B	811	CLA	CMD-C2D-C3D	-2.34	122.22	127.61
16	A	819	CLA	CMD-C2D-C3D	-2.34	122.22	127.61
16	2	607	CLA	C2D-C1D-ND	2.34	111.83	110.10
16	2	603	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
16	1	605	CLA	CHA-C4D-ND	2.34	137.40	132.50
16	3	210	CLA	CHA-C4D-ND	2.34	137.40	132.50
16	B	806	CLA	C2D-C1D-ND	2.34	111.83	110.10
16	2	602	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
16	B	816	CLA	OBD-CAD-C3D	-2.34	122.89	128.52
21	F	203	BCR	C30-C25-C26	-2.34	119.32	122.61
16	B	812	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
16	B	812	CLA	CHA-C4D-ND	2.34	137.39	132.50
16	I	101	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
16	A	816	CLA	C1-O2A-CGA	2.34	122.58	116.44
21	A	844	BCR	C4-C5-C6	-2.34	119.34	122.73
16	2	610	CLA	C1C-C2C-C3C	-2.34	104.50	106.96
16	B	807	CLA	O2A-CGA-CBA	2.34	119.24	111.91
16	B	818	CLA	C2D-C1D-ND	2.34	111.83	110.10
16	B	837	CLA	C2D-C1D-ND	2.34	111.83	110.10
16	B	813	CLA	CHD-C1D-ND	-2.34	122.31	124.45
16	A	808	CLA	CAA-C2A-C1A	-2.34	104.32	111.97
26	A	801	CL0	C4D-C3D-CAD	2.33	110.85	108.10
16	B	833	CLA	C4-C3-C2	-2.33	117.69	123.68
16	B	827	CLA	CHA-C4D-ND	2.33	137.38	132.50
16	A	817	CLA	CHA-C4D-ND	2.33	137.38	132.50
16	3	208	CLA	CHA-C4D-ND	2.33	137.38	132.50
16	B	814	CLA	C2D-C1D-ND	2.33	111.82	110.10
21	B	841	BCR	C35-C13-C12	2.33	121.75	118.08
16	B	824	CLA	CHA-C4D-ND	2.33	137.38	132.50
16	2	601	CLA	CHD-C1D-ND	-2.33	122.31	124.45
16	I	102	CLA	CHD-C1D-ND	-2.33	122.31	124.45
16	B	810	CLA	CMA-C3A-C4A	2.33	118.04	111.77
16	B	803	CLA	C1C-C2C-C3C	-2.33	104.50	106.96
16	2	609	CLA	C1-O2A-CGA	2.33	122.56	116.44
16	B	809	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
16	A	832	CLA	C2D-C1D-ND	2.33	111.82	110.10
16	3	212	CLA	O2A-CGA-CBA	2.33	119.22	111.91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	O	201	CLA	C3D-C2D-C1D	-2.33	102.65	105.83
16	3	208	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
16	I	102	CLA	CHA-C4D-ND	2.33	137.37	132.50
16	1	610	CLA	CHA-C4D-ND	2.33	137.37	132.50
16	O	202	CLA	CHA-C4D-ND	2.33	137.37	132.50
16	1	609	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
16	F	202	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
17	3	215	C7Z	C39-C29-C30	-2.33	119.66	122.92
16	1	605	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
16	A	856	CLA	CHA-C4D-ND	2.33	137.37	132.50
16	A	839	CLA	C2D-C1D-ND	2.33	111.82	110.10
16	1	603	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
16	B	807	CLA	CHA-C4D-ND	2.33	137.37	132.50
16	1	607	CLA	CHA-C4D-ND	2.33	137.37	132.50
16	A	812	CLA	C1-C2-C3	-2.33	122.02	126.04
16	B	802	CLA	C1-C2-C3	-2.33	122.02	126.04
16	L	201	CLA	C5-C3-C2	2.33	125.82	121.12
16	B	821	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
16	O	203	CLA	C2D-C1D-ND	2.33	111.82	110.10
16	A	822	CLA	CHA-C4D-ND	2.33	137.36	132.50
16	B	820	CLA	CHA-C4D-ND	2.33	137.36	132.50
16	A	829	CLA	CHA-C4D-ND	2.32	137.36	132.50
16	B	803	CLA	CHA-C1A-NA	-2.32	121.08	126.40
16	A	824	CLA	CHD-C1D-ND	-2.32	122.32	124.45
16	A	817	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
17	3	218	C7Z	C31-C32-C33	-2.32	119.89	126.42
16	1	601	CLA	CHA-C4D-ND	2.32	137.36	132.50
16	2	602	CLA	CHC-C1C-C2C	-2.32	124.25	129.77
16	B	830	CLA	C2C-C1C-NC	2.32	112.14	109.97
16	B	822	CLA	C1C-C2C-C3C	-2.32	104.52	106.96
16	L	204	CLA	CHA-C4D-ND	2.32	137.35	132.50
16	A	836	CLA	CHA-C4D-ND	2.32	137.35	132.50
16	A	837	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
16	B	807	CLA	C1D-ND-C4D	-2.32	104.69	106.33
16	A	804	CLA	C7-C6-C5	2.32	119.65	113.36
16	A	806	CLA	C2D-C1D-ND	2.32	111.81	110.10
16	2	604	CLA	C1D-ND-C4D	-2.32	104.69	106.33
16	3	206	CLA	CHA-C4D-ND	2.32	137.34	132.50
16	A	808	CLA	CHA-C4D-ND	2.31	137.34	132.50
16	A	811	CLA	CHA-C4D-ND	2.31	137.34	132.50
21	L	207	BCR	C16-C17-C18	2.31	130.61	127.31
17	3	217	C7Z	C27-C26-C25	-2.31	115.86	121.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	839	CLA	O2A-CGA-CBA	2.31	119.17	111.91
16	L	203	CLA	CMA-C3A-C4A	2.31	117.99	111.77
16	3	209	CLA	CHD-C1D-ND	-2.31	122.33	124.45
16	3	213	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
16	1	605	CLA	C1-O2A-CGA	2.31	122.51	116.44
16	A	834	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
16	2	603	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
16	1	608	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
16	L	201	CLA	C1C-C2C-C3C	-2.31	104.53	106.96
16	A	820	CLA	C2D-C1D-ND	2.31	111.81	110.10
16	F	202	CLA	CHA-C4D-ND	2.31	137.33	132.50
16	2	605	CLA	C5-C3-C2	2.31	125.78	121.12
17	3	201	C7Z	C22-C23-C24	2.31	113.46	110.30
16	L	205	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
16	3	214	CLA	C1C-C2C-C3C	-2.30	104.53	106.96
16	F	202	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
16	2	603	CLA	C2D-C1D-ND	2.30	111.80	110.10
16	A	833	CLA	CMD-C2D-C3D	-2.30	122.31	127.61
21	F	203	BCR	C36-C18-C19	-2.30	114.45	118.08
16	F	201	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
16	2	606	CLA	C5-C3-C2	2.30	125.77	121.12
16	B	836	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
16	F	205	CLA	CHA-C4D-ND	2.30	137.31	132.50
16	A	810	CLA	CMA-C3A-C4A	2.30	117.96	111.77
16	B	805	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
16	B	809	CLA	CHA-C4D-ND	2.30	137.31	132.50
16	O	203	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
16	2	612	CLA	CMA-C3A-C4A	2.30	117.95	111.77
16	B	823	CLA	C2D-C1D-ND	2.30	111.80	110.10
16	2	606	CLA	CHD-C1D-ND	-2.30	122.34	124.45
16	2	608	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
16	L	204	CLA	O2A-CGA-CBA	2.30	119.12	111.91
21	A	845	BCR	C33-C5-C6	-2.30	121.95	124.53
21	B	855	BCR	C31-C1-C6	-2.30	106.57	110.30
16	A	827	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
16	A	823	CLA	CMA-C3A-C4A	2.30	117.94	111.77
16	A	838	CLA	C1C-C2C-C3C	-2.30	104.54	106.96
16	F	205	CLA	O2A-CGA-CBA	2.30	119.11	111.91
16	A	816	CLA	CHA-C4D-ND	2.29	137.30	132.50
16	B	801	CLA	CHA-C4D-ND	2.29	137.30	132.50
16	B	819	CLA	O1D-CGD-CBD	-2.29	119.79	124.48
17	1	614	C7Z	C8-C7-C6	-2.29	120.76	127.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	808	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
16	B	834	CLA	CHA-C4D-ND	2.29	137.29	132.50
16	A	825	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
16	O	201	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
16	B	812	CLA	C16-C15-C13	-2.29	108.51	115.92
16	A	838	CLA	C1-C2-C3	-2.29	122.08	126.04
21	F	206	BCR	C30-C25-C24	2.29	122.26	115.78
16	A	832	CLA	C5-C3-C2	2.29	125.75	121.12
16	B	833	CLA	O2A-CGA-CBA	2.29	119.09	111.91
21	A	850	BCR	C38-C26-C27	2.29	118.02	113.62
16	B	806	CLA	O2A-CGA-CBA	2.29	119.09	111.91
16	L	203	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
16	2	611	CLA	C1-O2A-CGA	2.29	122.45	116.44
16	A	814	CLA	CHA-C4D-ND	2.29	137.28	132.50
17	3	218	C7Z	C24-C25-C26	-2.29	115.75	120.85
16	B	810	CLA	CHA-C4D-ND	2.29	137.28	132.50
17	1	612	C7Z	C38-C25-C24	2.29	118.59	114.36
16	B	834	CLA	CBA-CAA-C2A	2.29	120.61	113.86
21	L	207	BCR	C1-C6-C7	2.29	122.25	115.78
16	A	806	CLA	CHA-C4D-ND	2.29	137.28	132.50
16	L	201	CLA	CHA-C4D-ND	2.29	137.28	132.50
16	B	835	CLA	CMD-C2D-C3D	-2.29	122.36	127.61
16	A	806	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
16	F	201	CLA	CHA-C4D-ND	2.28	137.28	132.50
16	B	810	CLA	C1-C2-C3	-2.28	122.09	126.04
16	B	832	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
17	1	614	C7Z	C18-C5-C4	2.28	118.59	114.36
16	A	818	CLA	CHA-C4D-ND	2.28	137.28	132.50
16	2	612	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
16	A	817	CLA	C1D-ND-C4D	-2.28	104.71	106.33
16	A	829	CLA	O2A-CGA-CBA	2.28	119.07	111.91
21	B	843	BCR	C4-C5-C6	-2.28	119.42	122.73
16	A	835	CLA	CHA-C4D-ND	2.28	137.26	132.50
16	A	836	CLA	C6-C5-C3	-2.28	107.48	113.45
16	3	212	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
17	3	218	C7Z	C11-C12-C13	-2.28	120.02	126.42
18	K	103	RRX	C2-C1-C6	2.28	113.99	110.48
17	1	615	C7Z	C20-C13-C12	2.28	121.67	118.08
16	A	803	CLA	C2D-C1D-ND	2.28	111.78	110.10
16	B	823	CLA	CHA-C1A-NA	-2.28	121.19	126.40
21	B	845	BCR	C1-C6-C5	-2.28	119.41	122.61
17	3	217	C7Z	C2-C3-C4	2.27	113.42	110.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	3	214	CLA	CAC-C3C-C4C	2.27	127.76	124.81
16	A	825	CLA	CMA-C3A-C4A	2.27	117.88	111.77
21	B	844	BCR	C16-C17-C18	2.27	130.55	127.31
16	2	604	CLA	CHA-C4D-ND	2.27	137.25	132.50
16	F	204	CLA	CHA-C4D-ND	2.27	137.25	132.50
19	A	842	LHG	C5-O7-C7	-2.27	112.20	117.79
16	A	854	CLA	C1C-C2C-C3C	-2.27	104.57	106.96
16	A	831	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
21	L	202	BCR	C38-C26-C27	2.27	117.97	113.62
16	A	809	CLA	C4-C3-C2	-2.27	117.86	123.68
16	A	804	CLA	CHA-C1A-NA	-2.27	121.21	126.40
16	A	813	CLA	CMA-C3A-C4A	2.27	117.86	111.77
16	A	813	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
19	B	851	LHG	O8-C23-C24	2.27	119.02	111.91
16	3	209	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
17	3	201	C7Z	C1-C6-C5	-2.27	119.42	122.61
16	1	602	CLA	O1D-CGD-CBD	-2.27	119.85	124.48
16	3	212	CLA	CMB-C2B-C3B	2.27	128.92	124.68
16	F	201	CLA	C1D-ND-C4D	-2.26	104.73	106.33
16	A	838	CLA	CHA-C4D-ND	2.26	137.24	132.50
25	3	221	PTY	O4-C30-C31	2.26	119.01	111.91
16	A	809	CLA	C2C-C1C-NC	2.26	112.09	109.97
17	2	614	C7Z	C10-C11-C12	-2.26	116.15	123.22
21	A	844	BCR	C34-C9-C8	2.26	121.64	118.08
16	L	205	CLA	C2D-C1D-ND	2.26	111.77	110.10
16	B	833	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
16	L	204	CLA	C1-C2-C3	-2.26	122.13	126.04
16	B	808	CLA	CMA-C3A-C4A	2.26	117.85	111.77
16	A	823	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
16	3	206	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
16	L	204	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
16	A	828	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
16	B	809	CLA	C2A-C3A-C4A	2.26	105.52	101.87
21	L	206	BCR	C31-C1-C6	-2.26	106.64	110.30
17	3	201	C7Z	C15-C14-C13	-2.26	124.09	127.31
16	B	809	CLA	O2A-CGA-CBA	2.26	118.99	111.91
16	A	823	CLA	C1D-ND-C4D	-2.26	104.73	106.33
16	A	833	CLA	C1D-ND-C4D	-2.26	104.73	106.33
16	1	608	CLA	O2A-CGA-CBA	2.26	118.99	111.91
16	A	807	CLA	C1D-ND-C4D	-2.26	104.73	106.33
16	A	855	CLA	OBD-CAD-C3D	-2.25	123.09	128.52
16	3	211	CLA	O1D-CGD-CBD	-2.25	119.87	124.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	102	CLA	O2A-CGA-CBA	2.25	118.98	111.91
16	3	208	CLA	C2D-C1D-ND	2.25	111.76	110.10
16	2	605	CLA	CHA-C4D-ND	2.25	137.21	132.50
17	1	612	C7Z	C2-C3-C4	2.25	113.39	110.30
26	A	801	CL0	C3D-C4D-ND	2.25	113.88	110.24
17	1	614	C7Z	C20-C13-C14	-2.25	119.77	122.92
16	K	101	CLA	C1-C2-C3	-2.25	122.15	126.04
16	3	206	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
16	1	604	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
16	B	821	CLA	CHA-C1A-NA	-2.25	121.24	126.40
18	K	103	RRX	C21-C20-C19	2.25	130.24	123.22
16	J	102	CLA	CHD-C1D-ND	-2.25	122.39	124.45
16	1	604	CLA	CHA-C4D-ND	2.25	137.21	132.50
16	A	821	CLA	CHA-C4D-ND	2.25	137.21	132.50
16	A	832	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
16	2	607	CLA	CHD-C1D-ND	-2.25	122.39	124.45
16	3	203	CLA	O2A-CGA-CBA	2.25	118.97	111.91
18	A	847	RRX	C23-C24-C25	-2.25	120.89	127.20
16	A	822	CLA	C1D-ND-C4D	-2.25	104.74	106.33
16	K	102	CLA	C2D-C1D-ND	2.25	111.76	110.10
21	L	207	BCR	C36-C18-C17	-2.25	119.78	122.92
16	B	831	CLA	CHA-C4D-ND	2.25	137.20	132.50
16	B	826	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
16	B	817	CLA	CHD-C1D-ND	-2.24	122.39	124.45
16	O	204	CLA	CHA-C4D-ND	2.24	137.19	132.50
16	A	826	CLA	C1-C2-C3	-2.24	122.16	126.04
16	1	602	CLA	CHA-C4D-ND	2.24	137.19	132.50
16	B	813	CLA	C2D-C1D-ND	2.24	111.76	110.10
16	A	812	CLA	O2A-CGA-CBA	2.24	118.94	111.91
16	A	835	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
16	B	804	CLA	O2A-CGA-CBA	2.24	118.94	111.91
16	B	838	CLA	CHD-C1D-ND	-2.24	122.39	124.45
16	1	606	CLA	C1-O2A-CGA	2.24	122.32	116.44
16	A	811	CLA	C2D-C1D-ND	2.24	111.75	110.10
16	F	202	CLA	CHA-C1A-NA	-2.24	121.27	126.40
16	2	612	CLA	C1C-C2C-C3C	-2.24	104.60	106.96
16	F	205	CLA	C5-C3-C2	2.24	125.64	121.12
16	3	208	CLA	CMA-C3A-C4A	2.24	117.78	111.77
16	A	811	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
16	A	807	CLA	C1-O2A-CGA	2.24	122.31	116.44
20	2	621	ERG	C10-C5-C6	-2.23	118.65	122.58
16	2	604	CLA	O1D-CGD-CBD	-2.23	119.91	124.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	837	CLA	C2A-C3A-C4A	2.23	105.48	101.87
17	3	201	C7Z	C35-C15-C14	-2.23	118.90	123.47
16	A	831	CLA	O2A-CGA-CBA	2.23	118.92	111.91
16	B	811	CLA	C2D-C1D-ND	2.23	111.75	110.10
16	A	821	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
16	B	837	CLA	CHA-C1A-NA	-2.23	121.29	126.40
16	A	824	CLA	C2D-C1D-ND	2.23	111.75	110.10
16	B	836	CLA	CHD-C1D-ND	-2.23	122.40	124.45
16	2	608	CLA	CHD-C1D-ND	-2.23	122.41	124.45
21	A	844	BCR	C2-C1-C6	-2.23	107.05	110.48
16	B	831	CLA	O2A-CGA-CBA	2.23	118.90	111.91
16	B	820	CLA	C1-C2-C3	-2.23	122.19	126.04
16	B	824	CLA	C2C-C1C-NC	2.23	112.06	109.97
20	1	618	ERG	C12-C11-C9	2.23	118.20	112.60
16	B	829	CLA	CMA-C3A-C4A	2.23	117.76	111.77
16	F	204	CLA	CMA-C3A-C4A	2.23	117.76	111.77
16	O	203	CLA	O2A-CGA-CBA	2.23	118.89	111.91
16	B	821	CLA	O2A-CGA-CBA	2.22	118.89	111.91
16	1	609	CLA	C2D-C1D-ND	2.22	111.74	110.10
16	F	204	CLA	CHA-C1A-NA	-2.22	121.31	126.40
16	I	102	CLA	CMA-C3A-C4A	2.22	117.75	111.77
26	A	801	CL0	O2D-CGD-O1D	-2.22	119.49	123.84
16	2	608	CLA	C1-O2A-CGA	2.22	122.28	116.44
16	A	830	CLA	C5-C3-C2	2.22	125.61	121.12
16	O	202	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
17	1	616	C7Z	C19-C9-C10	-2.22	119.81	122.92
16	1	603	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
16	A	836	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
16	O	204	CLA	C5-C3-C2	2.22	125.61	121.12
16	A	809	CLA	C1C-C2C-C3C	-2.22	104.62	106.96
17	3	218	C7Z	C19-C9-C10	-2.22	119.82	122.92
16	3	214	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
17	A	843	C7Z	C31-C32-C33	-2.22	120.19	126.42
16	2	611	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
16	L	204	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
16	O	202	CLA	C1D-ND-C4D	-2.22	104.76	106.33
16	B	801	CLA	C1C-C2C-C3C	-2.22	104.63	106.96
16	A	837	CLA	CHA-C1A-NA	-2.22	121.32	126.40
16	1	609	CLA	CHD-C1D-ND	-2.22	122.42	124.45
16	A	815	CLA	O2D-CGD-O1D	-2.22	119.51	123.84
16	B	815	CLA	CHD-C1D-ND	-2.21	122.42	124.45
16	A	834	CLA	CMD-C2D-C3D	-2.21	122.52	127.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	816	CLA	CHA-C1A-NA	-2.21	121.33	126.40
21	I	103	BCR	C37-C22-C23	2.21	121.56	118.08
16	1	606	CLA	C5-C3-C2	2.21	125.59	121.12
16	B	830	CLA	CHA-C4D-ND	2.21	137.13	132.50
16	A	822	CLA	C1C-C2C-C3C	-2.21	104.63	106.96
16	B	813	CLA	C1-C2-C3	-2.21	122.22	126.04
16	O	204	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
16	B	821	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
16	B	826	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
16	1	604	CLA	CAC-C3C-C4C	2.21	127.68	124.81
16	1	609	CLA	C1C-C2C-C3C	-2.21	104.63	106.96
16	I	101	CLA	CHA-C4D-ND	2.21	137.12	132.50
16	O	201	CLA	C2C-C1C-NC	2.21	112.04	109.97
19	3	219	LHG	O8-C23-C24	2.21	118.84	111.91
21	B	842	BCR	C33-C5-C6	-2.21	122.05	124.53
16	A	826	CLA	C1C-C2C-C3C	-2.21	104.64	106.96
17	2	615	C7Z	C8-C7-C6	-2.21	121.01	127.20
16	B	823	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
21	B	847	BCR	C35-C13-C14	-2.20	119.83	122.92
16	A	808	CLA	C1D-ND-C4D	-2.20	104.77	106.33
21	A	846	BCR	C7-C6-C5	-2.20	116.12	121.46
31	B	850	DGD	O2G-C1B-O1B	-2.20	118.38	123.70
16	1	601	CLA	C5-C3-C2	2.20	125.58	121.12
16	B	814	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
16	3	206	CLA	CMA-C3A-C4A	2.20	117.69	111.77
16	B	819	CLA	O2A-CGA-CBA	2.20	118.82	111.91
21	B	844	BCR	C34-C9-C8	2.20	121.55	118.08
18	J	103	RRX	C1-C6-C7	2.20	122.00	115.78
16	1	611	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
16	B	831	CLA	C1D-ND-C4D	-2.20	104.77	106.33
16	B	828	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
16	A	816	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
16	B	811	CLA	C1C-C2C-C3C	-2.20	104.65	106.96
16	A	817	CLA	C2C-C1C-NC	2.20	112.03	109.97
17	J	104	C7Z	C15-C35-C34	-2.19	118.98	123.47
16	2	612	CLA	C1-O2A-CGA	2.19	122.20	116.44
16	L	203	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
16	F	201	CLA	C1-O2A-CGA	2.19	122.20	116.44
18	1	613	RRX	C1-C6-C7	2.19	121.98	115.78
18	J	103	RRX	C27-C26-C25	-2.19	115.96	120.85
21	L	202	BCR	C35-C13-C12	2.19	121.53	118.08
16	3	205	CLA	O2D-CGD-O1D	-2.19	119.55	123.84

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	605	CLA	CHA-C1A-NA	-2.19	121.38	126.40
16	3	211	CLA	C1-C2-C3	-2.19	122.25	126.04
21	B	845	BCR	C16-C17-C18	2.19	130.44	127.31
16	1	604	CLA	C1C-C2C-C3C	-2.19	104.65	106.96
16	2	610	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
21	F	203	BCR	C24-C25-C26	-2.19	116.16	121.46
18	2	616	RRX	C35-C13-C14	-2.19	119.86	122.92
16	A	835	CLA	C1-O2A-CGA	2.19	122.19	116.44
16	F	202	CLA	C1D-ND-C4D	-2.19	104.78	106.33
16	B	806	CLA	CMB-C2B-C3B	2.19	128.77	124.68
16	A	810	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
16	B	823	CLA	CHD-C1D-ND	-2.19	122.44	124.45
16	B	826	CLA	CMA-C3A-C4A	2.19	117.65	111.77
18	K	103	RRX	C30-C25-C24	2.19	121.97	115.78
20	2	618	ERG	C14-C8-C9	2.19	117.95	114.66
16	3	206	CLA	O2A-CGA-CBA	2.19	118.77	111.91
16	1	605	CLA	CHD-C1D-ND	-2.18	122.45	124.45
18	K	103	RRX	C39-C30-C25	-2.18	106.76	110.30
16	A	803	CLA	CMA-C3A-C4A	2.18	117.64	111.77
16	2	606	CLA	O2A-CGA-CBA	2.18	118.76	111.91
16	2	606	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
16	B	808	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
16	A	833	CLA	C2C-C1C-NC	2.18	112.02	109.97
16	2	613	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
21	B	847	BCR	C39-C30-C25	2.18	113.83	110.30
16	B	804	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
16	A	823	CLA	C1-O2A-CGA	2.18	122.15	116.44
17	3	218	C7Z	C20-C13-C14	-2.18	119.88	122.92
16	3	203	CLA	CHD-C1D-ND	-2.18	122.45	124.45
16	A	823	CLA	CHA-C4D-ND	2.18	137.05	132.50
21	B	844	BCR	C30-C25-C26	-2.18	119.55	122.61
16	A	815	CLA	CHA-C1A-NA	-2.17	121.42	126.40
16	A	803	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
21	B	840	BCR	C31-C1-C6	-2.17	106.77	110.30
16	3	203	CLA	C3D-C2D-C1D	-2.17	102.86	105.83
16	1	605	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
16	K	102	CLA	C1-C2-C3	-2.17	122.29	126.04
16	A	821	CLA	C4-C3-C5	2.17	118.92	115.27
16	3	209	CLA	CBA-CAA-C2A	2.17	120.27	113.86
16	B	801	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
16	B	832	CLA	CHA-C1A-NA	-2.17	121.43	126.40
16	B	801	CLA	C2C-C1C-NC	2.17	112.00	109.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	604	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
16	B	821	CLA	C1-C2-C3	-2.17	122.29	126.04
16	A	804	CLA	C2D-C1D-ND	2.17	111.70	110.10
16	A	831	CLA	CMA-C3A-C4A	2.17	117.60	111.77
16	B	801	CLA	CHA-C1A-NA	-2.17	121.43	126.40
16	B	834	CLA	C1C-C2C-C3C	-2.17	104.68	106.96
16	A	830	CLA	CHA-C1A-NA	-2.17	121.43	126.40
16	A	827	CLA	O2A-CGA-CBA	2.17	118.71	111.91
16	A	854	CLA	CHA-C4D-ND	2.17	137.03	132.50
16	A	823	CLA	C1C-C2C-C3C	-2.17	104.68	106.96
16	3	208	CLA	CMB-C2B-C3B	2.17	128.73	124.68
21	B	843	BCR	C35-C13-C14	-2.17	119.89	122.92
17	1	614	C7Z	C31-C32-C33	-2.17	120.33	126.42
16	A	812	CLA	C1C-C2C-C3C	-2.17	104.68	106.96
16	B	812	CLA	CAC-C3C-C4C	2.17	127.62	124.81
17	3	217	C7Z	C40-C33-C34	-2.17	119.89	122.92
16	A	839	CLA	CHA-C1A-NA	-2.16	121.44	126.40
21	I	103	BCR	C35-C13-C12	2.16	121.49	118.08
27	A	840	PQN	C12-C11-C3	-2.16	106.21	112.05
21	L	206	BCR	C40-C30-C25	2.16	113.81	110.30
16	A	830	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
16	2	603	CLA	CHA-C1A-NA	-2.16	121.44	126.40
16	A	837	CLA	C5-C3-C2	2.16	125.50	121.12
16	A	834	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
16	A	822	CLA	O2A-CGA-CBA	2.16	118.69	111.91
16	B	830	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
21	A	857	BCR	C35-C13-C12	2.16	121.48	118.08
16	A	808	CLA	O2A-CGA-CBA	2.16	118.69	111.91
16	B	805	CLA	O2A-CGA-CBA	2.16	118.69	111.91
16	A	817	CLA	C1C-C2C-C3C	-2.16	104.68	106.96
16	B	824	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
21	A	846	BCR	C36-C18-C17	-2.16	119.90	122.92
18	1	613	RRX	C12-C13-C14	2.16	122.26	118.94
16	1	609	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
17	3	216	C7Z	C38-C25-C24	2.16	118.36	114.36
16	A	812	CLA	CAC-C3C-C4C	2.16	127.61	124.81
16	1	607	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
16	A	824	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
21	B	843	BCR	C12-C13-C14	2.16	122.25	118.94
16	3	209	CLA	C1C-C2C-C3C	-2.16	104.69	106.96
16	A	814	CLA	C4-C3-C2	-2.16	118.14	123.68
17	1	614	C7Z	C11-C12-C13	-2.16	120.36	126.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	820	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
16	L	201	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
16	3	213	CLA	CMD-C2D-C3D	-2.16	122.66	127.61
16	A	815	CLA	C1D-ND-C4D	-2.16	104.80	106.33
21	B	847	BCR	C36-C18-C17	-2.15	119.91	122.92
16	B	817	CLA	C1-O2A-CGA	2.15	122.10	116.44
16	B	813	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
16	2	604	CLA	C1-C2-C3	-2.15	122.32	126.04
16	2	602	CLA	C1D-ND-C4D	-2.15	104.81	106.33
16	A	828	CLA	C2D-C1D-ND	2.15	111.69	110.10
16	A	836	CLA	C5-C3-C2	2.15	125.47	121.12
16	L	201	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
16	A	839	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
26	A	801	CL0	CED-O2D-CGD	2.15	120.80	115.94
16	A	820	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
16	3	204	CLA	C2D-C1D-ND	2.15	111.69	110.10
16	B	833	CLA	C1-O2A-CGA	2.15	122.08	116.44
21	I	103	BCR	C32-C1-C2	2.15	117.50	108.91
16	2	601	CLA	O2A-CGA-CBA	2.15	118.64	111.91
16	K	102	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
16	B	813	CLA	CMB-C2B-C3B	2.15	128.69	124.68
16	O	201	CLA	CHA-C4D-ND	2.15	136.99	132.50
16	B	827	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
16	A	819	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
16	2	609	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
16	A	804	CLA	CMA-C3A-C4A	2.14	117.54	111.77
16	B	816	CLA	CMA-C3A-C4A	2.14	117.54	111.77
17	3	217	C7Z	C39-C29-C28	2.14	121.45	118.08
16	A	837	CLA	CMB-C2B-C3B	2.14	128.69	124.68
20	2	618	ERG	C10-C5-C6	-2.14	118.81	122.58
16	3	210	CLA	O2A-CGA-CBA	2.14	118.63	111.91
16	O	204	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
16	3	211	CLA	O2A-CGA-CBA	2.14	118.62	111.91
16	B	817	CLA	C1-C2-C3	-2.14	122.34	126.04
17	3	218	C7Z	C40-C33-C34	-2.14	119.93	122.92
16	L	203	CLA	C1-C2-C3	-2.14	122.34	126.04
17	J	104	C7Z	C24-C25-C26	-2.14	116.08	120.85
16	2	610	CLA	C5-C3-C2	2.14	125.45	121.12
16	F	202	CLA	C5-C3-C2	2.14	125.45	121.12
17	J	104	C7Z	C40-C33-C34	-2.14	119.93	122.92
16	B	833	CLA	CHA-C1A-NA	-2.14	121.50	126.40
16	A	803	CLA	CHA-C1A-NA	-2.14	121.50	126.40

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	1	608	CLA	C4-C3-C2	-2.14	118.19	123.68
16	B	823	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
16	1	610	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
16	B	827	CLA	C1-O2A-CGA	2.14	122.05	116.44
16	B	805	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
16	2	611	CLA	O2A-CGA-CBA	2.14	118.61	111.91
17	1	616	C7Z	C2-C3-C4	2.14	113.23	110.30
16	B	804	CLA	CHD-C1D-ND	-2.14	122.49	124.45
16	B	813	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
16	A	856	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
16	B	838	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
16	F	202	CLA	CHD-C1D-ND	-2.13	122.49	124.45
17	1	612	C7Z	C27-C28-C29	-2.13	123.01	126.23
16	B	808	CLA	CMD-C2D-C3D	-2.13	122.70	127.61
16	A	856	CLA	CMA-C3A-C4A	2.13	117.51	111.77
16	B	835	CLA	C5-C3-C2	2.13	125.43	121.12
16	A	808	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
16	A	834	CLA	CMB-C2B-C3B	2.13	128.66	124.68
16	B	802	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
16	B	836	CLA	O2A-CGA-CBA	2.13	118.59	111.91
16	A	811	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
16	B	838	CLA	CMB-C2B-C3B	2.13	128.66	124.68
16	A	836	CLA	C1D-ND-C4D	-2.13	104.82	106.33
16	A	810	CLA	C1D-ND-C4D	-2.13	104.82	106.33
16	K	101	CLA	C1D-ND-C4D	-2.13	104.82	106.33
16	A	855	CLA	O2A-CGA-CBA	2.13	118.58	111.91
18	K	103	RRX	C34-C9-C10	-2.13	119.94	122.92
16	L	205	CLA	C1-C2-C3	-2.12	122.37	126.04
20	2	618	ERG	C17-C20-C22	-2.12	106.22	110.27
16	K	101	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
21	A	845	BCR	C15-C14-C13	-2.12	124.28	127.31
16	B	824	CLA	CMB-C2B-C3B	2.12	128.65	124.68
17	3	201	C7Z	C39-C29-C30	-2.12	119.95	122.92
16	I	101	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
16	A	824	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
16	B	806	CLA	CBA-CAA-C2A	2.12	120.13	113.86
16	B	837	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
16	A	807	CLA	CBA-CAA-C2A	2.12	120.12	113.86
16	A	828	CLA	CHA-C1A-NA	-2.12	121.54	126.40
16	A	835	CLA	CHA-C1A-NA	-2.12	121.54	126.40
17	1	616	C7Z	C28-C29-C30	2.12	122.19	118.94
16	A	832	CLA	O2A-CGA-CBA	2.12	118.56	111.91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	830	CLA	CHD-C1D-ND	-2.12	122.51	124.45
16	2	605	CLA	C1-O2A-CGA	2.12	122.00	116.44
16	A	809	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
16	A	822	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
21	B	855	BCR	C34-C9-C10	-2.12	119.95	122.92
16	B	817	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
16	3	205	CLA	C5-C3-C2	2.12	125.40	121.12
16	2	608	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
21	A	844	BCR	C15-C14-C13	-2.12	124.29	127.31
16	B	830	CLA	C1D-ND-C4D	-2.12	104.83	106.33
16	B	830	CLA	C1C-C2C-C3C	-2.12	104.73	106.96
16	B	822	CLA	CHA-C1A-NA	-2.12	121.55	126.40
16	A	818	CLA	C2D-C1D-ND	2.12	111.66	110.10
21	O	205	BCR	C34-C9-C8	2.11	121.41	118.08
16	3	205	CLA	CHA-C1A-NA	-2.11	121.56	126.40
16	2	608	CLA	CMA-C3A-C4A	2.11	117.45	111.77
18	J	103	RRX	C34-C9-C10	-2.11	119.97	122.92
16	B	804	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
18	K	103	RRX	C35-C13-C12	2.11	121.40	118.08
21	A	846	BCR	C1-C6-C5	-2.11	119.64	122.61
16	A	818	CLA	C2A-C3A-C4A	2.11	105.27	101.87
16	B	833	CLA	CHD-C1D-ND	-2.11	122.52	124.45
16	2	605	CLA	CMD-C2D-C3D	-2.11	122.77	127.61
20	2	621	ERG	C12-C13-C17	2.11	119.72	116.57
16	B	824	CLA	C1D-ND-C4D	-2.11	104.84	106.33
16	3	203	CLA	CHA-C1A-NA	-2.11	121.57	126.40
16	B	836	CLA	CAC-C3C-C4C	2.11	127.54	124.81
16	2	608	CLA	O2A-CGA-CBA	2.11	118.52	111.91
21	L	202	BCR	C12-C13-C14	-2.11	115.71	118.94
16	A	802	CLA	CHA-C1A-NA	-2.11	121.58	126.40
17	1	615	C7Z	C39-C29-C30	-2.11	119.97	122.92
16	1	604	CLA	C1D-ND-C4D	-2.11	104.84	106.33
16	B	833	CLA	C1D-ND-C4D	-2.11	104.84	106.33
16	O	203	CLA	C1D-ND-C4D	-2.11	104.84	106.33
21	A	846	BCR	C4-C5-C6	-2.11	119.67	122.73
16	B	831	CLA	C1-O2A-CGA	2.11	121.97	116.44
21	A	845	BCR	C23-C24-C25	-2.11	121.29	127.20
16	F	201	CLA	CMA-C3A-C4A	2.11	117.43	111.77
17	J	104	C7Z	C28-C27-C26	-2.10	121.29	127.20
18	K	103	RRX	C19-C18-C17	-2.10	115.71	118.94
18	2	616	RRX	C37-C22-C21	-2.10	119.98	122.92
27	B	839	PQN	C14-C13-C15	2.10	118.81	115.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F	204	CLA	O2A-CGA-CBA	2.10	118.51	111.91
16	3	213	CLA	CHA-C1A-NA	-2.10	121.58	126.40
16	3	205	CLA	CMB-C2B-C1B	-2.10	125.23	128.46
16	A	833	CLA	CMB-C2B-C3B	2.10	128.61	124.68
16	3	206	CLA	C1-O2A-CGA	2.10	121.96	116.44
16	A	808	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
16	B	810	CLA	C1D-ND-C4D	-2.10	104.84	106.33
16	A	824	CLA	CHA-C1A-NA	-2.10	121.59	126.40
16	B	821	CLA	C2A-C3A-C4A	2.10	105.26	101.87
21	B	845	BCR	C38-C26-C27	2.10	117.65	113.62
16	B	810	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
16	A	811	CLA	CMB-C2B-C3B	2.10	128.61	124.68
16	B	835	CLA	C1-O2A-CGA	2.10	121.95	116.44
17	3	217	C7Z	C28-C27-C26	-2.10	121.31	127.20
16	1	603	CLA	C5-C3-C2	2.10	125.36	121.12
21	B	840	BCR	C30-C25-C26	-2.10	119.66	122.61
16	3	209	CLA	CHA-C1A-NA	-2.10	121.60	126.40
20	2	621	ERG	C9-C8-C7	-2.10	114.22	119.90
21	A	857	BCR	C30-C25-C26	-2.09	119.66	122.61
16	A	821	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
16	B	821	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
16	B	809	CLA	C1-O2A-CGA	2.09	121.94	116.44
16	A	831	CLA	CHA-C1A-NA	-2.09	121.60	126.40
16	A	822	CLA	CMA-C3A-C4A	2.09	117.39	111.77
16	A	819	CLA	OBD-CAD-C3D	-2.09	123.49	128.52
16	1	611	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
16	B	827	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
16	A	811	CLA	O2A-CGA-CBA	2.09	118.47	111.91
16	A	837	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
16	1	603	CLA	C4-C3-C2	-2.09	118.32	123.68
16	B	809	CLA	C1D-ND-C4D	-2.09	104.85	106.33
16	3	210	CLA	C1-O2A-CGA	2.09	121.92	116.44
21	L	207	BCR	C33-C5-C4	2.09	117.62	113.62
16	1	606	CLA	C1D-ND-C4D	-2.09	104.85	106.33
16	A	805	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
16	B	810	CLA	O2A-CGA-CBA	2.09	118.45	111.91
17	3	201	C7Z	C40-C33-C34	-2.09	120.00	122.92
20	1	618	ERG	C1-C10-C9	2.09	112.60	108.28
16	A	822	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
16	B	802	CLA	C1D-ND-C4D	-2.08	104.85	106.33
16	3	211	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
16	B	812	CLA	CHA-C1A-NA	-2.08	121.62	126.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	3	209	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
16	A	818	CLA	O2A-CGA-CBA	2.08	118.45	111.91
16	1	607	CLA	CHA-C1A-NA	-2.08	121.63	126.40
16	3	205	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
16	B	827	CLA	C2D-C1D-ND	2.08	111.64	110.10
16	A	854	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
16	A	814	CLA	C1-C2-C3	-2.08	122.44	126.04
16	B	809	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
16	2	613	CLA	C1D-ND-C4D	-2.08	104.86	106.33
16	3	210	CLA	C1D-ND-C4D	-2.08	104.86	106.33
16	1	608	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
16	3	210	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
16	A	808	CLA	CMA-C3A-C4A	2.08	117.36	111.77
16	B	809	CLA	CHA-C1A-NA	-2.08	121.64	126.40
26	A	801	CL0	CMD-C2D-C3D	-2.08	122.83	127.61
31	B	849	DGD	O6D-C5D-C6D	2.08	110.86	106.67
18	K	103	RRX	C20-C19-C18	2.08	132.25	126.42
16	1	602	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
16	B	816	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
16	B	822	CLA	CMD-C2D-C3D	-2.08	122.84	127.61
21	B	840	BCR	C15-C14-C13	-2.08	124.35	127.31
16	B	804	CLA	C7-C6-C5	2.08	119.00	113.36
16	A	826	CLA	C1-O2A-CGA	2.08	121.89	116.44
17	3	218	C7Z	C8-C7-C6	-2.08	121.37	127.20
16	2	601	CLA	CMD-C2D-C3D	-2.08	122.84	127.61
16	B	834	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
16	A	838	CLA	CMD-C2D-C3D	-2.07	122.84	127.61
21	F	203	BCR	C34-C9-C8	2.07	121.34	118.08
16	2	610	CLA	C1D-ND-C4D	-2.07	104.86	106.33
16	B	807	CLA	CMD-C2D-C3D	-2.07	122.84	127.61
16	A	814	CLA	C1D-ND-C4D	-2.07	104.86	106.33
17	1	612	C7Z	C4-C5-C6	-2.07	116.23	120.85
18	1	613	RRX	C37-C22-C23	2.07	121.34	118.08
16	J	102	CLA	C2A-C3A-C4A	2.07	105.21	101.87
31	B	846	DGD	O5D-C6D-C5D	2.07	112.88	109.05
27	A	840	PQN	C2M-C2-C3	-2.07	121.02	124.40
16	A	835	CLA	O2A-CGA-CBA	2.07	118.40	111.91
16	B	831	CLA	C1-C2-C3	-2.07	122.46	126.04
16	A	823	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
16	B	834	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
16	1	603	CLA	CMA-C3A-C4A	2.07	117.33	111.77
16	B	824	CLA	C1-C2-C3	-2.07	122.47	126.04

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	F	204	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
16	2	605	CLA	C1-C2-C3	-2.06	122.47	126.04
16	A	819	CLA	O2A-CGA-CBA	2.06	118.39	111.91
16	F	202	CLA	O2A-CGA-CBA	2.06	118.39	111.91
16	A	815	CLA	C1-O2A-CGA	2.06	121.86	116.44
16	A	807	CLA	CAA-C2A-C1A	-2.06	105.21	111.97
16	B	815	CLA	C1D-ND-C4D	-2.06	104.87	106.33
21	A	844	BCR	C12-C13-C14	-2.06	115.78	118.94
16	A	838	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
16	A	816	CLA	C1D-ND-C4D	-2.06	104.87	106.33
21	L	202	BCR	C24-C25-C26	-2.06	116.47	121.46
16	B	838	CLA	CHA-C1A-NA	-2.06	121.68	126.40
16	2	608	CLA	C1D-ND-C4D	-2.06	104.87	106.33
16	A	812	CLA	CHD-C1D-ND	-2.06	122.56	124.45
16	A	856	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
16	A	805	CLA	C1D-ND-C4D	-2.06	104.87	106.33
21	I	103	BCR	C12-C13-C14	-2.06	115.78	118.94
16	F	202	CLA	OBD-CAD-C3D	-2.06	123.57	128.52
16	B	835	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
16	3	205	CLA	OBD-CAD-C3D	-2.06	123.57	128.52
16	2	604	CLA	CMC-C2C-C1C	2.06	128.17	125.04
16	B	817	CLA	CHA-C1A-NA	-2.06	121.69	126.40
16	B	820	CLA	CHA-C1A-NA	-2.06	121.69	126.40
21	A	845	BCR	C32-C1-C2	2.06	117.13	108.91
16	A	821	CLA	O2A-CGA-CBA	2.06	118.36	111.91
16	B	830	CLA	CMB-C2B-C3B	2.06	128.52	124.68
16	B	835	CLA	O2A-CGA-CBA	2.05	118.35	111.91
16	A	829	CLA	C1-O2A-CGA	2.05	121.83	116.44
19	2	622	LHG	O7-C7-O9	-2.05	118.74	123.70
21	2	617	BCR	C15-C14-C13	-2.05	124.38	127.31
20	2	618	ERG	C9-C8-C7	-2.05	114.34	119.90
16	L	201	CLA	O2A-CGA-CBA	2.05	118.34	111.91
21	I	103	BCR	C31-C1-C2	2.05	117.11	108.91
16	F	202	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
16	A	823	CLA	O2A-CGA-CBA	2.05	118.34	111.91
16	1	611	CLA	CHA-C1A-NA	-2.05	121.70	126.40
16	A	833	CLA	C1-C2-C3	-2.05	122.50	126.04
16	B	804	CLA	C1D-ND-C4D	-2.05	104.88	106.33
16	A	816	CLA	C1C-C2C-C3C	-2.05	104.80	106.96
16	F	205	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
16	B	828	CLA	CMA-C3A-C4A	2.05	117.28	111.77
16	3	212	CLA	CHA-C1A-NA	-2.05	121.71	126.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	836	CLA	C1-C2-C3	-2.05	122.50	126.04
16	B	814	CLA	CHA-C1A-NA	-2.05	121.71	126.40
16	3	207	CLA	C1D-ND-C4D	-2.05	104.88	106.33
16	3	212	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
16	L	203	CLA	CHA-C1A-NA	-2.05	121.71	126.40
16	B	803	CLA	C2A-C1A-CHA	2.05	127.44	123.86
16	A	814	CLA	CMD-C2D-C3D	-2.04	122.91	127.61
17	A	843	C7Z	C1-C6-C7	2.04	121.56	115.78
16	A	827	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
16	A	855	CLA	C2A-C1A-CHA	2.04	127.43	123.86
16	3	203	CLA	CMD-C2D-C3D	-2.04	122.91	127.61
16	B	825	CLA	CHA-C1A-NA	-2.04	121.72	126.40
16	3	205	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
16	B	806	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
16	J	102	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
16	1	609	CLA	CHA-C1A-NA	-2.04	121.72	126.40
17	A	843	C7Z	C24-C25-C26	-2.04	116.30	120.85
16	2	607	CLA	O2A-CGA-CBA	2.04	118.31	111.91
16	2	611	CLA	C1D-ND-C4D	-2.04	104.89	106.33
16	L	204	CLA	C1D-ND-C4D	-2.04	104.89	106.33
26	A	801	CL0	C3C-C4C-NC	2.04	112.86	110.57
16	3	211	CLA	CHA-C1A-NA	-2.04	121.72	126.40
16	2	611	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
21	B	841	BCR	C31-C1-C6	-2.04	106.99	110.30
16	A	836	CLA	O2A-CGA-CBA	2.04	118.31	111.91
16	2	613	CLA	O2A-CGA-CBA	2.04	118.31	111.91
16	2	613	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
16	A	809	CLA	CMA-C3A-C4A	2.04	117.25	111.77
16	B	811	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
16	1	610	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
16	B	829	CLA	CHA-C1A-NA	-2.04	121.73	126.40
16	2	603	CLA	OBD-CAD-C3D	-2.04	123.62	128.52
16	3	210	CLA	CBC-CAC-C3C	-2.04	106.82	112.43
21	B	841	BCR	C33-C5-C6	-2.04	122.24	124.53
16	L	201	CLA	C1D-ND-C4D	-2.04	104.89	106.33
16	3	212	CLA	CMA-C3A-C2A	2.04	122.04	113.83
16	B	812	CLA	C3D-C2D-C1D	-2.03	103.05	105.83
16	3	211	CLA	CHD-C1D-ND	-2.03	122.58	124.45
16	3	207	CLA	CHA-C1A-NA	-2.03	121.74	126.40
16	3	208	CLA	C1-C2-C3	-2.03	122.53	126.04
16	A	834	CLA	C11-C12-C13	-2.03	109.35	115.92
18	A	847	RRX	C37-C22-C21	-2.03	120.08	122.92

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	101	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
16	B	827	CLA	CHA-C1A-NA	-2.03	121.74	126.40
21	B	841	BCR	C29-C30-C25	-2.03	107.35	110.48
18	A	847	RRX	C36-C18-C17	2.03	125.77	122.92
16	A	854	CLA	CMC-C2C-C1C	2.03	128.13	125.04
21	L	206	BCR	C28-C27-C26	-2.03	110.45	114.08
16	B	812	CLA	CHD-C1D-ND	-2.03	122.59	124.45
16	L	201	CLA	C1-O2A-CGA	2.03	121.77	116.44
21	A	845	BCR	C31-C1-C2	2.03	117.02	108.91
16	B	834	CLA	CMD-C2D-C3D	-2.03	122.95	127.61
16	1	601	CLA	CMD-C2D-C3D	-2.03	122.95	127.61
16	O	201	CLA	CMB-C2B-C3B	2.03	128.47	124.68
21	L	207	BCR	C7-C6-C5	-2.03	116.55	121.46
16	B	826	CLA	CHA-C1A-NA	-2.03	121.76	126.40
19	1	617	LHG	O8-C23-C24	2.02	118.26	111.91
21	A	845	BCR	C38-C26-C27	2.02	117.50	113.62
16	A	808	CLA	C5-C3-C2	2.02	125.21	121.12
16	A	822	CLA	C5-C3-C2	2.02	125.21	121.12
16	B	822	CLA	C5-C3-C2	2.02	125.21	121.12
16	A	828	CLA	C1-C2-C3	-2.02	122.54	126.04
16	1	601	CLA	CMB-C2B-C3B	2.02	128.46	124.68
16	2	609	CLA	O2A-CGA-CBA	2.02	118.26	111.91
16	A	831	CLA	C2D-C1D-ND	2.02	111.59	110.10
17	3	218	C7Z	C15-C35-C34	-2.02	119.33	123.47
16	B	801	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
16	A	817	CLA	OBD-CAD-C3D	-2.02	123.66	128.52
16	1	602	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
16	B	806	CLA	CHA-C1A-NA	-2.02	121.77	126.40
16	2	604	CLA	C5-C3-C2	2.02	125.20	121.12
16	A	825	CLA	C1-O2A-CGA	2.02	121.74	116.44
16	B	825	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
16	J	102	CLA	C1D-ND-C4D	-2.02	104.90	106.33
16	B	803	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
21	A	846	BCR	C29-C30-C25	-2.02	107.38	110.48
16	B	822	CLA	C1-O2A-CGA	2.02	121.73	116.44
16	B	809	CLA	CMB-C2B-C3B	2.02	128.45	124.68
16	1	601	CLA	CHA-C1A-NA	-2.02	121.78	126.40
16	A	825	CLA	CHA-C1A-NA	-2.02	121.78	126.40
16	B	833	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
16	K	101	CLA	CHA-C1A-NA	-2.01	121.78	126.40
16	B	811	CLA	C1D-ND-C4D	-2.01	104.90	106.33
21	O	205	BCR	C8-C9-C10	2.01	122.03	118.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	3	214	CLA	C1-C2-C3	-2.01	122.56	126.04
16	A	817	CLA	CHA-C1A-NA	-2.01	121.79	126.40
21	A	850	BCR	C29-C28-C27	2.01	115.87	111.38
16	2	605	CLA	CHA-C1A-NA	-2.01	121.79	126.40
21	B	847	BCR	C36-C18-C19	-2.01	114.91	118.08
16	2	610	CLA	O2A-CGA-CBA	2.01	118.22	111.91
16	A	818	CLA	C1D-ND-C4D	-2.01	104.91	106.33
16	B	805	CLA	C1D-ND-C4D	-2.01	104.91	106.33
16	B	829	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
16	1	606	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
16	A	804	CLA	CMC-C2C-C1C	2.01	128.10	125.04
16	A	821	CLA	C4-C3-C2	-2.01	118.53	123.68
16	B	812	CLA	CMC-C2C-C1C	2.01	128.09	125.04
16	I	102	CLA	CMD-C2D-C3D	-2.01	123.00	127.61
16	B	833	CLA	OBD-CAD-C3D	-2.01	123.69	128.52
17	3	218	C7Z	C4-C5-C6	-2.01	116.38	120.85
16	A	813	CLA	CHA-C1A-NA	-2.01	121.81	126.40
16	2	602	CLA	CMA-C3A-C4A	2.01	117.16	111.77
16	A	812	CLA	C1D-ND-C4D	-2.00	104.91	106.33
16	B	819	CLA	C1D-ND-C4D	-2.00	104.91	106.33
16	A	854	CLA	CMB-C2B-C3B	2.00	128.43	124.68
16	B	803	CLA	CMD-C2D-C3D	-2.00	123.00	127.61
21	F	206	BCR	C3-C4-C5	-2.00	110.50	114.08
16	3	214	CLA	O2A-CGA-CBA	2.00	118.19	111.91
16	B	827	CLA	CMA-C3A-C4A	2.00	117.15	111.77
16	3	213	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
18	2	616	RRX	C20-C19-C18	-2.00	120.79	126.42
16	2	611	CLA	CHA-C1A-NA	-2.00	121.82	126.40
16	3	206	CLA	C1D-ND-C4D	-2.00	104.91	106.33
21	F	203	BCR	C37-C22-C21	-2.00	120.12	122.92
16	A	816	CLA	CAC-C3C-C4C	2.00	127.41	124.81

All (173) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	1	601	CLA	ND
16	1	602	CLA	ND
16	1	603	CLA	ND
16	1	604	CLA	ND
16	1	605	CLA	ND
16	1	606	CLA	ND
16	1	607	CLA	ND

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
16	1	608	CLA	ND
16	1	609	CLA	ND
16	1	610	CLA	ND
16	1	611	CLA	ND
16	2	601	CLA	ND
16	2	602	CLA	ND
16	2	603	CLA	ND
16	2	604	CLA	ND
16	2	605	CLA	ND
16	2	606	CLA	ND
16	2	607	CLA	ND
16	2	608	CLA	ND
16	2	609	CLA	ND
16	2	610	CLA	ND
16	2	611	CLA	ND
16	2	612	CLA	ND
16	2	613	CLA	ND
16	3	203	CLA	ND
16	3	204	CLA	ND
16	3	205	CLA	ND
16	3	206	CLA	ND
16	3	207	CLA	ND
16	3	208	CLA	ND
16	3	209	CLA	ND
16	3	210	CLA	ND
16	3	211	CLA	ND
16	3	212	CLA	ND
16	3	213	CLA	ND
16	3	214	CLA	ND
16	A	802	CLA	ND
16	A	803	CLA	ND
16	A	804	CLA	ND
16	A	805	CLA	ND
16	A	806	CLA	ND
16	A	807	CLA	ND
16	A	808	CLA	ND
16	A	809	CLA	ND
16	A	810	CLA	ND
16	A	811	CLA	ND
16	A	812	CLA	ND
16	A	813	CLA	ND
16	A	814	CLA	ND

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
16	A	815	CLA	ND
16	A	816	CLA	ND
16	A	817	CLA	ND
16	A	818	CLA	ND
16	A	819	CLA	ND
16	A	820	CLA	ND
16	A	821	CLA	ND
16	A	822	CLA	ND
16	A	823	CLA	ND
16	A	824	CLA	ND
16	A	825	CLA	ND
16	A	826	CLA	ND
16	A	827	CLA	ND
16	A	828	CLA	ND
16	A	829	CLA	ND
16	A	830	CLA	ND
16	A	831	CLA	ND
16	A	832	CLA	ND
16	A	833	CLA	ND
16	A	834	CLA	ND
16	A	835	CLA	ND
16	A	836	CLA	ND
16	A	837	CLA	ND
16	A	838	CLA	ND
16	A	839	CLA	ND
16	A	854	CLA	ND
16	A	855	CLA	ND
16	A	856	CLA	ND
16	B	801	CLA	ND
16	B	802	CLA	ND
16	B	803	CLA	ND
16	B	804	CLA	ND
16	B	805	CLA	ND
16	B	806	CLA	ND
16	B	807	CLA	ND
16	B	808	CLA	ND
16	B	809	CLA	ND
16	B	810	CLA	ND
16	B	811	CLA	ND
16	B	812	CLA	ND
16	B	813	CLA	ND
16	B	814	CLA	ND

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
16	B	815	CLA	ND
16	B	816	CLA	ND
16	B	817	CLA	ND
16	B	818	CLA	ND
16	B	819	CLA	ND
16	B	820	CLA	ND
16	B	821	CLA	C3A
16	B	821	CLA	ND
16	B	822	CLA	ND
16	B	823	CLA	ND
16	B	824	CLA	ND
16	B	825	CLA	ND
16	B	826	CLA	ND
16	B	827	CLA	ND
16	B	828	CLA	ND
16	B	829	CLA	ND
16	B	830	CLA	ND
16	B	831	CLA	ND
16	B	832	CLA	ND
16	B	833	CLA	ND
16	B	834	CLA	ND
16	B	835	CLA	ND
16	B	836	CLA	ND
16	B	837	CLA	ND
16	B	838	CLA	ND
16	F	201	CLA	ND
16	F	202	CLA	C3A
16	F	202	CLA	ND
16	F	204	CLA	ND
16	F	205	CLA	ND
16	I	101	CLA	ND
16	I	102	CLA	ND
16	J	102	CLA	C3A
16	J	102	CLA	ND
16	K	101	CLA	ND
16	K	102	CLA	ND
16	L	201	CLA	ND
16	L	203	CLA	ND
16	L	204	CLA	ND
16	L	205	CLA	ND
16	O	201	CLA	ND
16	O	202	CLA	ND

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
16	O	203	CLA	ND
16	O	204	CLA	ND
17	1	612	C7Z	C3
17	1	614	C7Z	C3
17	1	615	C7Z	C3
17	1	616	C7Z	C3
17	2	614	C7Z	C3
17	2	615	C7Z	C3
17	3	201	C7Z	C3
17	3	215	C7Z	C3
17	3	216	C7Z	C3
17	3	217	C7Z	C3
17	3	218	C7Z	C3
17	A	843	C7Z	C3
17	J	104	C7Z	C3
18	1	613	RRX	C28
18	2	616	RRX	C28
18	A	847	RRX	C28
18	J	103	RRX	C28
18	K	103	RRX	C28
20	1	618	ERG	C20
20	1	618	ERG	C10
20	1	618	ERG	C9
20	1	618	ERG	C13
20	1	618	ERG	C24
20	1	618	ERG	C14
20	2	618	ERG	C20
20	2	618	ERG	C9
20	2	618	ERG	C14
20	2	618	ERG	C24
20	2	621	ERG	C20
20	2	621	ERG	C9
20	2	621	ERG	C24
20	2	621	ERG	C10
20	2	621	ERG	C14
22	2	619	PGT	C5
22	B	848	PGT	C5
26	A	801	CL0	NA
26	A	801	CL0	NC
26	A	801	CL0	ND

All (2730) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	1	601	CLA	CHA-CBD-CGD-O1D
16	1	601	CLA	CHA-CBD-CGD-O2D
16	1	601	CLA	CBD-CGD-O2D-CED
16	1	604	CLA	CHA-CBD-CGD-O1D
16	1	604	CLA	CHA-CBD-CGD-O2D
16	1	605	CLA	CBD-CGD-O2D-CED
16	1	606	CLA	C3A-C2A-CAA-CBA
16	1	606	CLA	CHA-CBD-CGD-O1D
16	1	606	CLA	CHA-CBD-CGD-O2D
16	1	606	CLA	CBD-CGD-O2D-CED
16	1	607	CLA	CBD-CGD-O2D-CED
16	1	609	CLA	CBD-CGD-O2D-CED
16	1	610	CLA	C2A-CAA-CBA-CGA
16	1	610	CLA	CBD-CGD-O2D-CED
16	1	611	CLA	C2-C1-O2A-CGA
16	1	611	CLA	CBD-CGD-O2D-CED
16	2	601	CLA	CHA-CBD-CGD-O1D
16	2	601	CLA	CHA-CBD-CGD-O2D
16	2	605	CLA	C2A-CAA-CBA-CGA
16	2	605	CLA	CBD-CGD-O2D-CED
16	2	607	CLA	CHA-CBD-CGD-O1D
16	2	607	CLA	CHA-CBD-CGD-O2D
16	2	608	CLA	C2C-C3C-CAC-CBC
16	2	608	CLA	C4C-C3C-CAC-CBC
16	2	609	CLA	C3A-C2A-CAA-CBA
16	2	609	CLA	CHA-CBD-CGD-O1D
16	2	609	CLA	CBD-CGD-O2D-CED
16	2	610	CLA	C2-C1-O2A-CGA
16	2	610	CLA	CHA-CBD-CGD-O1D
16	2	610	CLA	CHA-CBD-CGD-O2D
16	2	610	CLA	CBD-CGD-O2D-CED
16	2	611	CLA	C1A-C2A-CAA-CBA
16	2	611	CLA	C3A-C2A-CAA-CBA
16	2	611	CLA	CHA-CBD-CGD-O1D
16	2	611	CLA	CHA-CBD-CGD-O2D
16	2	611	CLA	CBD-CGD-O2D-CED
16	2	613	CLA	C2-C1-O2A-CGA
16	2	613	CLA	CBD-CGD-O2D-CED
16	3	205	CLA	C1A-C2A-CAA-CBA
16	3	205	CLA	C2-C1-O2A-CGA
16	3	207	CLA	CBD-CGD-O2D-CED
16	3	210	CLA	C1A-C2A-CAA-CBA
16	3	210	CLA	C3A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	3	211	CLA	C1A-C2A-CAA-CBA
16	3	211	CLA	C3A-C2A-CAA-CBA
16	3	211	CLA	C2-C1-O2A-CGA
16	3	212	CLA	CHA-CBD-CGD-O1D
16	3	212	CLA	CHA-CBD-CGD-O2D
16	3	212	CLA	CBD-CGD-O2D-CED
16	A	802	CLA	CBA-CGA-O2A-C1
16	A	802	CLA	O1A-CGA-O2A-C1
16	A	802	CLA	CHA-CBD-CGD-O1D
16	A	802	CLA	CHA-CBD-CGD-O2D
16	A	803	CLA	C1A-C2A-CAA-CBA
16	A	803	CLA	C3A-C2A-CAA-CBA
16	A	803	CLA	CHA-CBD-CGD-O1D
16	A	803	CLA	CHA-CBD-CGD-O2D
16	A	804	CLA	C2-C1-O2A-CGA
16	A	804	CLA	CAD-CBD-CGD-O1D
16	A	804	CLA	CAD-CBD-CGD-O2D
16	A	804	CLA	CBD-CGD-O2D-CED
16	A	806	CLA	C2-C1-O2A-CGA
16	A	807	CLA	C3A-C2A-CAA-CBA
16	A	808	CLA	CBD-CGD-O2D-CED
16	A	809	CLA	CHA-CBD-CGD-O1D
16	A	809	CLA	CBD-CGD-O2D-CED
16	A	810	CLA	C1A-C2A-CAA-CBA
16	A	811	CLA	CBD-CGD-O2D-CED
16	A	814	CLA	CHA-CBD-CGD-O1D
16	A	814	CLA	CHA-CBD-CGD-O2D
16	A	814	CLA	CAD-CBD-CGD-O1D
16	A	815	CLA	C1A-C2A-CAA-CBA
16	A	815	CLA	CBD-CGD-O2D-CED
16	A	816	CLA	C2-C3-C5-C6
16	A	816	CLA	C4-C3-C5-C6
16	A	817	CLA	C3A-C2A-CAA-CBA
16	A	817	CLA	CBD-CGD-O2D-CED
16	A	817	CLA	C11-C10-C8-C9
16	A	818	CLA	C1A-C2A-CAA-CBA
16	A	818	CLA	C3A-C2A-CAA-CBA
16	A	819	CLA	C3A-C2A-CAA-CBA
16	A	819	CLA	C2-C1-O2A-CGA
16	A	820	CLA	C2A-CAA-CBA-CGA
16	A	820	CLA	CHA-CBD-CGD-O1D
16	A	820	CLA	CHA-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	821	CLA	C1A-C2A-CAA-CBA
16	A	821	CLA	C3A-C2A-CAA-CBA
16	A	821	CLA	C2-C1-O2A-CGA
16	A	822	CLA	C2-C1-O2A-CGA
16	A	822	CLA	CBD-CGD-O2D-CED
16	A	823	CLA	CHA-CBD-CGD-O1D
16	A	823	CLA	CHA-CBD-CGD-O2D
16	A	824	CLA	C1A-C2A-CAA-CBA
16	A	824	CLA	C3A-C2A-CAA-CBA
16	A	826	CLA	CBD-CGD-O2D-CED
16	A	827	CLA	CHA-CBD-CGD-O1D
16	A	827	CLA	CBD-CGD-O2D-CED
16	A	828	CLA	O1A-CGA-O2A-C1
16	A	830	CLA	C1A-C2A-CAA-CBA
16	A	831	CLA	CBD-CGD-O2D-CED
16	A	832	CLA	CHA-CBD-CGD-O1D
16	A	832	CLA	CHA-CBD-CGD-O2D
16	A	832	CLA	CBD-CGD-O2D-CED
16	A	833	CLA	CBD-CGD-O2D-CED
16	A	834	CLA	CHA-CBD-CGD-O1D
16	A	834	CLA	CHA-CBD-CGD-O2D
16	A	837	CLA	C2-C1-O2A-CGA
16	A	837	CLA	CHA-CBD-CGD-O1D
16	A	837	CLA	CHA-CBD-CGD-O2D
16	A	839	CLA	O2A-C1-C2-C3
16	A	854	CLA	CHA-CBD-CGD-O1D
16	A	854	CLA	CHA-CBD-CGD-O2D
16	A	855	CLA	CBD-CGD-O2D-CED
16	A	855	CLA	C6-C7-C8-C9
16	A	856	CLA	CBD-CGD-O2D-CED
16	B	801	CLA	CHA-CBD-CGD-O1D
16	B	801	CLA	CHA-CBD-CGD-O2D
16	B	801	CLA	CBD-CGD-O2D-CED
16	B	802	CLA	CBD-CGD-O2D-CED
16	B	804	CLA	CBD-CGD-O2D-CED
16	B	806	CLA	C3A-C2A-CAA-CBA
16	B	807	CLA	C2A-CAA-CBA-CGA
16	B	808	CLA	CHA-CBD-CGD-O1D
16	B	808	CLA	CHA-CBD-CGD-O2D
16	B	809	CLA	C3A-C2A-CAA-CBA
16	B	813	CLA	CBD-CGD-O2D-CED
16	B	813	CLA	C2-C3-C5-C6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	813	CLA	C4-C3-C5-C6
16	B	814	CLA	C1A-C2A-CAA-CBA
16	B	814	CLA	CBD-CGD-O2D-CED
16	B	815	CLA	CBD-CGD-O2D-CED
16	B	817	CLA	C1A-C2A-CAA-CBA
16	B	817	CLA	C3A-C2A-CAA-CBA
16	B	817	CLA	C4-C3-C5-C6
16	B	818	CLA	CHA-CBD-CGD-O1D
16	B	818	CLA	CHA-CBD-CGD-O2D
16	B	819	CLA	C1A-C2A-CAA-CBA
16	B	819	CLA	CHA-CBD-CGD-O1D
16	B	819	CLA	CHA-CBD-CGD-O2D
16	B	821	CLA	C1A-C2A-CAA-CBA
16	B	821	CLA	C3A-C2A-CAA-CBA
16	B	821	CLA	CBD-CGD-O2D-CED
16	B	826	CLA	C1A-C2A-CAA-CBA
16	B	826	CLA	C3A-C2A-CAA-CBA
16	B	826	CLA	CHA-CBD-CGD-O1D
16	B	826	CLA	CHA-CBD-CGD-O2D
16	B	827	CLA	C1A-C2A-CAA-CBA
16	B	827	CLA	C3A-C2A-CAA-CBA
16	B	830	CLA	CHA-CBD-CGD-O1D
16	B	830	CLA	CHA-CBD-CGD-O2D
16	B	832	CLA	C3A-C2A-CAA-CBA
16	B	832	CLA	C2-C1-O2A-CGA
16	B	832	CLA	CBD-CGD-O2D-CED
16	B	834	CLA	C1A-C2A-CAA-CBA
16	B	834	CLA	C3A-C2A-CAA-CBA
16	B	834	CLA	CBD-CGD-O2D-CED
16	B	835	CLA	C2-C1-O2A-CGA
16	B	835	CLA	CBD-CGD-O2D-CED
16	B	836	CLA	C2A-CAA-CBA-CGA
16	B	837	CLA	C1A-C2A-CAA-CBA
16	B	837	CLA	C3A-C2A-CAA-CBA
16	B	837	CLA	CBD-CGD-O2D-CED
16	F	202	CLA	C1A-C2A-CAA-CBA
16	F	204	CLA	CBD-CGD-O2D-CED
16	J	102	CLA	C1A-C2A-CAA-CBA
16	J	102	CLA	C3A-C2A-CAA-CBA
16	J	102	CLA	CHA-CBD-CGD-O1D
16	J	102	CLA	CHA-CBD-CGD-O2D
16	K	101	CLA	CBD-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	K	102	CLA	C1A-C2A-CAA-CBA
16	K	102	CLA	C3A-C2A-CAA-CBA
16	L	204	CLA	C2-C1-O2A-CGA
16	L	204	CLA	CBD-CGD-O2D-CED
16	L	205	CLA	C1A-C2A-CAA-CBA
16	L	205	CLA	CBD-CGD-O2D-CED
16	O	202	CLA	CHA-CBD-CGD-O1D
16	O	202	CLA	CHA-CBD-CGD-O2D
16	O	203	CLA	CBD-CGD-O2D-CED
16	O	204	CLA	C3A-C2A-CAA-CBA
16	O	204	CLA	CHA-CBD-CGD-O1D
16	O	204	CLA	CHA-CBD-CGD-O2D
16	O	204	CLA	CBD-CGD-O2D-CED
17	1	612	C7Z	C7-C8-C9-C19
17	1	612	C7Z	C7-C8-C9-C10
17	1	612	C7Z	C31-C32-C33-C34
17	1	612	C7Z	C31-C32-C33-C40
17	1	612	C7Z	C27-C28-C29-C30
17	1	614	C7Z	C21-C26-C27-C28
17	1	614	C7Z	C25-C26-C27-C28
17	1	614	C7Z	C7-C8-C9-C19
17	1	614	C7Z	C9-C10-C11-C12
17	1	614	C7Z	C31-C32-C33-C34
17	1	614	C7Z	C31-C32-C33-C40
17	1	614	C7Z	C27-C28-C29-C30
17	1	614	C7Z	C27-C28-C29-C39
17	1	615	C7Z	C7-C8-C9-C19
17	1	615	C7Z	C7-C8-C9-C10
17	1	615	C7Z	C27-C28-C29-C30
17	1	615	C7Z	C27-C28-C29-C39
17	2	614	C7Z	C7-C8-C9-C19
17	2	614	C7Z	C7-C8-C9-C10
17	2	614	C7Z	C31-C32-C33-C34
17	2	614	C7Z	C31-C32-C33-C40
17	2	615	C7Z	C21-C26-C27-C28
17	2	615	C7Z	C25-C26-C27-C28
17	2	615	C7Z	C7-C8-C9-C19
17	3	215	C7Z	C11-C12-C13-C20
17	3	215	C7Z	C11-C12-C13-C14
17	3	216	C7Z	C25-C26-C27-C28
17	3	216	C7Z	C7-C8-C9-C19
17	3	216	C7Z	C7-C8-C9-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
17	3	217	C7Z	C25-C26-C27-C28
17	3	217	C7Z	C9-C10-C11-C12
17	3	218	C7Z	C7-C8-C9-C19
17	3	218	C7Z	C7-C8-C9-C10
17	A	843	C7Z	C1-C6-C7-C8
17	A	843	C7Z	C5-C6-C7-C8
17	A	843	C7Z	C21-C26-C27-C28
17	A	843	C7Z	C7-C8-C9-C19
17	A	843	C7Z	C7-C8-C9-C10
17	A	843	C7Z	C9-C10-C11-C12
17	A	843	C7Z	C13-C14-C15-C35
17	J	104	C7Z	C9-C10-C11-C12
17	J	104	C7Z	C27-C28-C29-C30
17	J	104	C7Z	C27-C28-C29-C39
18	1	613	RRX	C36-C18-C19-C20
18	1	613	RRX	C17-C18-C19-C20
18	1	613	RRX	C7-C8-C9-C10
18	1	613	RRX	C7-C8-C9-C34
18	1	613	RRX	C1-C6-C7-C8
18	1	613	RRX	C5-C6-C7-C8
18	2	616	RRX	C36-C18-C19-C20
18	2	616	RRX	C17-C18-C19-C20
18	A	847	RRX	C37-C22-C23-C24
18	A	847	RRX	C21-C22-C23-C24
18	J	103	RRX	C37-C22-C23-C24
18	J	103	RRX	C21-C22-C23-C24
18	J	103	RRX	C19-C20-C21-C22
18	J	103	RRX	C36-C18-C19-C20
18	J	103	RRX	C15-C16-C17-C18
18	J	103	RRX	C11-C12-C13-C14
18	J	103	RRX	C11-C12-C13-C35
18	J	103	RRX	C7-C8-C9-C10
18	J	103	RRX	C7-C8-C9-C34
18	J	103	RRX	C1-C6-C7-C8
18	K	103	RRX	C9-C10-C11-C12
19	1	617	LHG	O1-C1-C2-C3
19	1	617	LHG	C1-C2-C3-O3
19	1	617	LHG	O2-C2-C3-O3
19	1	617	LHG	C3-O3-P-O4
19	1	617	LHG	C3-O3-P-O5
19	1	617	LHG	C8-C7-O7-C5
19	2	622	LHG	C1-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	2	622	LHG	C3-O3-P-O5
19	3	219	LHG	C3-O3-P-O4
19	3	219	LHG	C3-O3-P-O5
19	3	219	LHG	C3-O3-P-O6
19	3	219	LHG	O7-C5-C6-O8
19	3	219	LHG	C8-C7-O7-C5
19	A	841	LHG	O2-C2-C3-O3
19	A	841	LHG	C4-O6-P-O5
19	A	842	LHG	O1-C1-C2-C3
19	A	842	LHG	C1-C2-C3-O3
19	A	842	LHG	C3-O3-P-O6
19	B	851	LHG	O1-C1-C2-C3
19	B	851	LHG	C4-O6-P-O3
19	B	851	LHG	O7-C5-C6-O8
19	B	851	LHG	C8-C7-O7-C5
20	2	618	ERG	C16-C17-C20-C21
20	2	618	ERG	C23-C24-C25-C26
20	2	618	ERG	C28-C24-C25-C27
20	2	621	ERG	C13-C17-C20-C22
21	2	617	BCR	C1-C6-C7-C8
21	2	617	BCR	C5-C6-C7-C8
21	A	845	BCR	C5-C6-C7-C8
21	A	845	BCR	C9-C10-C11-C12
21	A	845	BCR	C10-C11-C12-C13
21	A	845	BCR	C11-C12-C13-C14
21	A	845	BCR	C11-C12-C13-C35
21	A	846	BCR	C11-C10-C9-C8
21	A	846	BCR	C11-C10-C9-C34
21	A	850	BCR	C1-C6-C7-C8
21	A	850	BCR	C5-C6-C7-C8
21	A	850	BCR	C11-C10-C9-C8
21	A	850	BCR	C11-C10-C9-C34
21	A	850	BCR	C9-C10-C11-C12
21	A	850	BCR	C10-C11-C12-C13
21	A	857	BCR	C1-C6-C7-C8
21	A	857	BCR	C5-C6-C7-C8
21	A	857	BCR	C11-C10-C9-C8
21	A	857	BCR	C11-C10-C9-C34
21	A	857	BCR	C10-C11-C12-C13
21	A	857	BCR	C11-C12-C13-C14
21	A	857	BCR	C11-C12-C13-C35
21	B	840	BCR	C11-C10-C9-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	B	840	BCR	C11-C10-C9-C34
21	B	840	BCR	C9-C10-C11-C12
21	B	840	BCR	C10-C11-C12-C13
21	B	840	BCR	C11-C12-C13-C14
21	B	840	BCR	C11-C12-C13-C35
21	B	840	BCR	C23-C24-C25-C26
21	B	841	BCR	C1-C6-C7-C8
21	B	841	BCR	C5-C6-C7-C8
21	B	841	BCR	C11-C10-C9-C8
21	B	841	BCR	C11-C10-C9-C34
21	B	841	BCR	C10-C11-C12-C13
21	B	841	BCR	C11-C12-C13-C14
21	B	841	BCR	C11-C12-C13-C35
21	B	841	BCR	C23-C24-C25-C26
21	B	842	BCR	C10-C11-C12-C13
21	B	843	BCR	C11-C10-C9-C8
21	B	843	BCR	C11-C10-C9-C34
21	B	843	BCR	C10-C11-C12-C13
21	B	844	BCR	C11-C10-C9-C8
21	B	844	BCR	C11-C10-C9-C34
21	B	844	BCR	C10-C11-C12-C13
21	B	845	BCR	C10-C11-C12-C13
21	B	847	BCR	C1-C6-C7-C8
21	B	847	BCR	C5-C6-C7-C8
21	B	847	BCR	C11-C10-C9-C8
21	B	847	BCR	C11-C10-C9-C34
21	B	847	BCR	C10-C11-C12-C13
21	B	847	BCR	C11-C12-C13-C14
21	B	847	BCR	C11-C12-C13-C35
21	B	855	BCR	C11-C10-C9-C8
21	B	855	BCR	C11-C10-C9-C34
21	B	855	BCR	C9-C10-C11-C12
21	B	855	BCR	C10-C11-C12-C13
21	B	855	BCR	C11-C12-C13-C14
21	B	855	BCR	C11-C12-C13-C35
21	F	203	BCR	C10-C11-C12-C13
21	F	203	BCR	C21-C22-C23-C24
21	F	206	BCR	C7-C8-C9-C10
21	F	206	BCR	C10-C11-C12-C13
21	F	206	BCR	C21-C22-C23-C24
21	I	103	BCR	C5-C6-C7-C8
21	I	103	BCR	C11-C10-C9-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	I	103	BCR	C11-C10-C9-C34
21	I	103	BCR	C10-C11-C12-C13
21	I	103	BCR	C17-C18-C19-C20
21	I	103	BCR	C36-C18-C19-C20
21	K	104	BCR	C11-C10-C9-C8
21	K	104	BCR	C11-C10-C9-C34
21	K	104	BCR	C10-C11-C12-C13
21	K	104	BCR	C23-C24-C25-C26
21	K	104	BCR	C23-C24-C25-C30
21	L	202	BCR	C11-C10-C9-C8
21	L	202	BCR	C11-C10-C9-C34
21	L	202	BCR	C21-C22-C23-C24
21	L	202	BCR	C37-C22-C23-C24
21	L	206	BCR	C11-C10-C9-C8
21	L	206	BCR	C11-C10-C9-C34
21	L	206	BCR	C10-C11-C12-C13
21	L	206	BCR	C11-C12-C13-C14
21	L	206	BCR	C11-C12-C13-C35
21	L	207	BCR	C11-C10-C9-C8
21	L	207	BCR	C11-C10-C9-C34
21	L	207	BCR	C10-C11-C12-C13
21	O	205	BCR	C11-C10-C9-C8
21	O	205	BCR	C11-C10-C9-C34
21	O	205	BCR	C10-C11-C12-C13
22	2	619	PGT	C4-O4P-P-O2P
22	2	619	PGT	C4-C5-C6-O6
22	B	848	PGT	C1-O3P-P-O2P
22	B	848	PGT	C4-O4P-P-O1P
23	2	620	DGA	OB1-CB1-OG2-CG2
23	2	620	DGA	OG2-CG2-CG3-OXT
23	J	101	DGA	CB2-CB1-OG2-CG2
24	3	202	LMU	O5'-C1'-O1'-C1
24	A	853	LMU	C2'-C1'-O1'-C1
24	A	853	LMU	O5'-C1'-O1'-C1
25	3	220	PTY	N1-C2-C3-O11
25	3	220	PTY	C5-O14-P1-O13
25	A	852	PTY	C11-C8-O7-C6
25	L	208	PTY	C5-O14-P1-O12
29	A	849	3PH	C1-O11-P-O13
29	A	849	3PH	C1-O11-P-O14
30	A	851	T7X	C7-O13-P1-O12
30	A	851	T7X	C12-C10-O16-C8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	B	849	DGD	C2B-C1B-O2G-C2G
31	B	849	DGD	O1B-C1B-O2G-C2G
31	B	849	DGD	O6D-C1D-O3G-C3G
31	B	850	DGD	O1B-C1B-O2G-C2G
31	B	850	DGD	C2D-C1D-O3G-C3G
31	B	850	DGD	O6D-C1D-O3G-C3G
16	1	601	CLA	O1D-CGD-O2D-CED
16	1	605	CLA	O1D-CGD-O2D-CED
16	1	609	CLA	O1D-CGD-O2D-CED
16	1	610	CLA	O1D-CGD-O2D-CED
16	2	607	CLA	O1D-CGD-O2D-CED
16	2	609	CLA	O1D-CGD-O2D-CED
16	2	611	CLA	O1D-CGD-O2D-CED
16	3	208	CLA	O1D-CGD-O2D-CED
16	3	212	CLA	O1D-CGD-O2D-CED
16	F	201	CLA	O1D-CGD-O2D-CED
16	L	203	CLA	O1D-CGD-O2D-CED
16	O	201	CLA	O1D-CGD-O2D-CED
16	B	804	CLA	C5-C6-C7-C8
16	1	603	CLA	O1D-CGD-O2D-CED
16	1	607	CLA	O1D-CGD-O2D-CED
16	1	611	CLA	O1D-CGD-O2D-CED
16	2	605	CLA	O1D-CGD-O2D-CED
16	2	606	CLA	O1D-CGD-O2D-CED
16	3	207	CLA	O1D-CGD-O2D-CED
16	A	826	CLA	O1D-CGD-O2D-CED
16	A	833	CLA	O1D-CGD-O2D-CED
16	A	856	CLA	O1D-CGD-O2D-CED
16	B	801	CLA	O1D-CGD-O2D-CED
16	B	804	CLA	O1D-CGD-O2D-CED
16	B	831	CLA	O1D-CGD-O2D-CED
16	O	204	CLA	O1D-CGD-O2D-CED
16	1	603	CLA	CBD-CGD-O2D-CED
16	2	603	CLA	CBD-CGD-O2D-CED
16	2	606	CLA	CBD-CGD-O2D-CED
16	2	607	CLA	CBD-CGD-O2D-CED
16	3	204	CLA	CBD-CGD-O2D-CED
16	3	208	CLA	CBD-CGD-O2D-CED
16	3	211	CLA	CBD-CGD-O2D-CED
16	3	213	CLA	CBD-CGD-O2D-CED
16	3	214	CLA	CBD-CGD-O2D-CED
16	A	803	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	806	CLA	CBD-CGD-O2D-CED
16	A	812	CLA	CBD-CGD-O2D-CED
16	A	820	CLA	CBD-CGD-O2D-CED
16	A	821	CLA	CBD-CGD-O2D-CED
16	A	829	CLA	CBD-CGD-O2D-CED
16	A	836	CLA	CBD-CGD-O2D-CED
16	B	807	CLA	CBD-CGD-O2D-CED
16	B	809	CLA	CBD-CGD-O2D-CED
16	B	818	CLA	CBD-CGD-O2D-CED
16	B	820	CLA	CBD-CGD-O2D-CED
16	B	824	CLA	CBD-CGD-O2D-CED
16	B	826	CLA	CBD-CGD-O2D-CED
16	B	828	CLA	CBD-CGD-O2D-CED
16	B	831	CLA	CBD-CGD-O2D-CED
16	B	838	CLA	CBD-CGD-O2D-CED
16	F	201	CLA	CBD-CGD-O2D-CED
16	J	102	CLA	CBD-CGD-O2D-CED
16	L	203	CLA	CBD-CGD-O2D-CED
16	O	201	CLA	CBD-CGD-O2D-CED
16	O	202	CLA	CBD-CGD-O2D-CED
16	1	603	CLA	O1A-CGA-O2A-C1
16	1	608	CLA	O1A-CGA-O2A-C1
16	2	610	CLA	O1A-CGA-O2A-C1
16	3	203	CLA	O1A-CGA-O2A-C1
16	3	208	CLA	O1A-CGA-O2A-C1
16	3	211	CLA	O1A-CGA-O2A-C1
16	A	833	CLA	O1A-CGA-O2A-C1
16	B	805	CLA	O1A-CGA-O2A-C1
16	B	811	CLA	O1A-CGA-O2A-C1
16	B	818	CLA	O1A-CGA-O2A-C1
16	B	820	CLA	O1A-CGA-O2A-C1
16	B	832	CLA	O1A-CGA-O2A-C1
16	B	836	CLA	O1A-CGA-O2A-C1
16	O	204	CLA	O1A-CGA-O2A-C1
16	3	204	CLA	O1D-CGD-O2D-CED
16	3	213	CLA	O1D-CGD-O2D-CED
16	A	809	CLA	O1D-CGD-O2D-CED
16	A	821	CLA	O1D-CGD-O2D-CED
16	A	829	CLA	O1D-CGD-O2D-CED
16	B	807	CLA	O1D-CGD-O2D-CED
16	B	826	CLA	O1D-CGD-O2D-CED
16	K	101	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
24	3	202	LMU	O5B-C1B-O1B-C4'
16	1	606	CLA	O1D-CGD-O2D-CED
16	2	613	CLA	O1D-CGD-O2D-CED
16	3	211	CLA	O1D-CGD-O2D-CED
16	A	808	CLA	O1D-CGD-O2D-CED
16	A	817	CLA	O1D-CGD-O2D-CED
16	A	822	CLA	O1D-CGD-O2D-CED
16	A	827	CLA	O1D-CGD-O2D-CED
16	A	832	CLA	O1D-CGD-O2D-CED
16	B	802	CLA	O1D-CGD-O2D-CED
16	B	813	CLA	O1D-CGD-O2D-CED
16	B	815	CLA	O1D-CGD-O2D-CED
16	B	818	CLA	O1D-CGD-O2D-CED
16	B	820	CLA	O1D-CGD-O2D-CED
16	B	821	CLA	O1D-CGD-O2D-CED
16	B	835	CLA	O1D-CGD-O2D-CED
16	B	837	CLA	O1D-CGD-O2D-CED
16	F	204	CLA	O1D-CGD-O2D-CED
16	L	204	CLA	O1D-CGD-O2D-CED
16	1	603	CLA	CBA-CGA-O2A-C1
16	1	608	CLA	CBA-CGA-O2A-C1
16	3	203	CLA	CBA-CGA-O2A-C1
16	3	208	CLA	CBA-CGA-O2A-C1
16	3	211	CLA	CBA-CGA-O2A-C1
16	A	833	CLA	CBA-CGA-O2A-C1
16	B	811	CLA	CBA-CGA-O2A-C1
16	B	818	CLA	CBA-CGA-O2A-C1
16	B	820	CLA	CBA-CGA-O2A-C1
23	J	101	DGA	CA2-CA1-OG1-CG1
25	3	220	PTY	C31-C30-O4-C1
16	1	608	CLA	CBD-CGD-O2D-CED
16	2	601	CLA	CBD-CGD-O2D-CED
16	2	608	CLA	CBD-CGD-O2D-CED
16	A	802	CLA	CBD-CGD-O2D-CED
16	A	805	CLA	CBD-CGD-O2D-CED
16	A	814	CLA	CBD-CGD-O2D-CED
16	A	818	CLA	CBD-CGD-O2D-CED
16	A	819	CLA	CBD-CGD-O2D-CED
16	A	825	CLA	CBD-CGD-O2D-CED
16	A	834	CLA	CBD-CGD-O2D-CED
16	A	838	CLA	CBD-CGD-O2D-CED
16	A	854	CLA	CBD-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	808	CLA	CBD-CGD-O2D-CED
16	B	810	CLA	CBD-CGD-O2D-CED
16	B	822	CLA	CBD-CGD-O2D-CED
16	B	836	CLA	CBD-CGD-O2D-CED
16	F	202	CLA	CBD-CGD-O2D-CED
16	1	607	CLA	O1A-CGA-O2A-C1
16	1	611	CLA	O1A-CGA-O2A-C1
16	2	611	CLA	O1A-CGA-O2A-C1
16	3	210	CLA	O1A-CGA-O2A-C1
16	A	805	CLA	O1A-CGA-O2A-C1
16	A	809	CLA	O1A-CGA-O2A-C1
16	A	811	CLA	O1A-CGA-O2A-C1
16	A	819	CLA	O1A-CGA-O2A-C1
16	A	820	CLA	O1A-CGA-O2A-C1
16	A	821	CLA	O1A-CGA-O2A-C1
16	B	807	CLA	O1A-CGA-O2A-C1
16	B	809	CLA	O1A-CGA-O2A-C1
16	B	813	CLA	O1A-CGA-O2A-C1
16	B	814	CLA	O1A-CGA-O2A-C1
16	B	815	CLA	O1A-CGA-O2A-C1
16	B	816	CLA	O1A-CGA-O2A-C1
16	B	821	CLA	O1A-CGA-O2A-C1
16	B	831	CLA	O1A-CGA-O2A-C1
16	F	201	CLA	O1A-CGA-O2A-C1
16	F	204	CLA	O1A-CGA-O2A-C1
16	I	102	CLA	O1A-CGA-O2A-C1
16	L	201	CLA	O1A-CGA-O2A-C1
16	L	204	CLA	O1A-CGA-O2A-C1
16	L	205	CLA	O1A-CGA-O2A-C1
16	O	202	CLA	O1A-CGA-O2A-C1
23	J	101	DGA	OA1-CA1-OG1-CG1
25	3	220	PTY	O30-C30-O4-C1
25	L	208	PTY	O30-C30-O4-C1
16	2	610	CLA	O1D-CGD-O2D-CED
16	A	831	CLA	O1D-CGD-O2D-CED
16	A	855	CLA	O1D-CGD-O2D-CED
16	B	814	CLA	O1D-CGD-O2D-CED
16	B	834	CLA	O1D-CGD-O2D-CED
16	L	205	CLA	O1D-CGD-O2D-CED
16	A	804	CLA	O1D-CGD-O2D-CED
16	A	811	CLA	O1D-CGD-O2D-CED
16	B	832	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	O	203	CLA	O1D-CGD-O2D-CED
16	A	824	CLA	CBD-CGD-O2D-CED
16	B	805	CLA	CBD-CGD-O2D-CED
16	B	812	CLA	CBD-CGD-O2D-CED
16	1	603	CLA	C8-C10-C11-C12
16	A	825	CLA	C8-C10-C11-C12
16	A	803	CLA	O1D-CGD-O2D-CED
16	A	815	CLA	O1D-CGD-O2D-CED
16	B	828	CLA	O1D-CGD-O2D-CED
16	B	838	CLA	O1D-CGD-O2D-CED
19	1	617	LHG	O9-C7-O7-C5
19	3	219	LHG	O9-C7-O7-C5
19	B	851	LHG	O9-C7-O7-C5
23	J	101	DGA	OB1-CB1-OG2-CG2
25	3	221	PTY	O10-C8-O7-C6
25	A	852	PTY	O10-C8-O7-C6
30	A	851	T7X	O17-C10-O16-C8
16	O	201	CLA	O1A-CGA-O2A-C1
16	3	213	CLA	O1A-CGA-O2A-C1
16	1	603	CLA	C3-C5-C6-C7
16	1	604	CLA	C3-C5-C6-C7
16	1	607	CLA	C3-C5-C6-C7
16	1	611	CLA	C3-C5-C6-C7
16	2	605	CLA	C3-C5-C6-C7
16	2	606	CLA	C3-C5-C6-C7
16	A	808	CLA	C3-C5-C6-C7
16	A	812	CLA	C3-C5-C6-C7
16	A	813	CLA	C3-C5-C6-C7
16	A	814	CLA	C3-C5-C6-C7
16	A	819	CLA	C3-C5-C6-C7
16	A	830	CLA	C3-C5-C6-C7
16	A	834	CLA	C3-C5-C6-C7
16	A	835	CLA	C3-C5-C6-C7
16	A	838	CLA	C3-C5-C6-C7
16	A	839	CLA	C3-C5-C6-C7
16	A	855	CLA	C3-C5-C6-C7
16	B	808	CLA	C3-C5-C6-C7
16	B	812	CLA	C3-C5-C6-C7
16	B	821	CLA	C3-C5-C6-C7
16	B	823	CLA	C3-C5-C6-C7
16	B	829	CLA	C3-C5-C6-C7
16	B	835	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	836	CLA	C3-C5-C6-C7
16	L	204	CLA	C3-C5-C6-C7
16	L	205	CLA	C3-C5-C6-C7
16	O	203	CLA	C3-C5-C6-C7
16	1	607	CLA	CBA-CGA-O2A-C1
16	2	610	CLA	CBA-CGA-O2A-C1
16	2	611	CLA	CBA-CGA-O2A-C1
16	2	612	CLA	CBA-CGA-O2A-C1
16	A	811	CLA	CBA-CGA-O2A-C1
16	A	820	CLA	CBA-CGA-O2A-C1
16	A	821	CLA	CBA-CGA-O2A-C1
16	A	827	CLA	CBA-CGA-O2A-C1
16	A	828	CLA	CBA-CGA-O2A-C1
16	B	805	CLA	CBA-CGA-O2A-C1
16	B	813	CLA	CBA-CGA-O2A-C1
16	B	814	CLA	CBA-CGA-O2A-C1
16	B	815	CLA	CBA-CGA-O2A-C1
16	B	816	CLA	CBA-CGA-O2A-C1
16	B	821	CLA	CBA-CGA-O2A-C1
16	B	832	CLA	CBA-CGA-O2A-C1
16	B	836	CLA	CBA-CGA-O2A-C1
16	I	101	CLA	CBA-CGA-O2A-C1
16	I	102	CLA	CBA-CGA-O2A-C1
16	L	201	CLA	CBA-CGA-O2A-C1
16	L	204	CLA	CBA-CGA-O2A-C1
16	L	205	CLA	CBA-CGA-O2A-C1
16	O	202	CLA	CBA-CGA-O2A-C1
16	O	204	CLA	CBA-CGA-O2A-C1
25	L	208	PTY	C31-C30-O4-C1
23	2	620	DGA	CB2-CB1-OG2-CG2
25	3	221	PTY	C11-C8-O7-C6
31	B	850	DGD	C2B-C1B-O2G-C2G
16	3	214	CLA	O1D-CGD-O2D-CED
16	A	803	CLA	O1A-CGA-O2A-C1
22	2	619	PGT	O11-C11-O3-C3
16	3	213	CLA	CBA-CGA-O2A-C1
16	A	814	CLA	C4-C3-C5-C6
16	B	833	CLA	C4-C3-C5-C6
16	B	817	CLA	C2-C3-C5-C6
16	B	833	CLA	C2-C3-C5-C6
16	2	612	CLA	CBD-CGD-O2D-CED
16	3	203	CLA	CBD-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	3	210	CLA	CBD-CGD-O2D-CED
16	3	212	CLA	C2A-CAA-CBA-CGA
16	A	802	CLA	C2A-CAA-CBA-CGA
16	A	834	CLA	C2A-CAA-CBA-CGA
16	B	809	CLA	C2A-CAA-CBA-CGA
16	F	202	CLA	C2A-CAA-CBA-CGA
16	B	802	CLA	O1A-CGA-O2A-C1
31	B	846	DGD	CBA-CCA-CDA-CEA
31	B	846	DGD	CEA-CFA-CGA-CHA
31	B	846	DGD	CBB-CCB-CDB-CEB
31	B	850	DGD	CBA-CCA-CDA-CEA
31	B	850	DGD	CEA-CFA-CGA-CHA
31	B	850	DGD	CBB-CCB-CDB-CEB
16	1	606	CLA	C3-C5-C6-C7
16	1	610	CLA	C3-C5-C6-C7
16	2	609	CLA	C3-C5-C6-C7
16	3	209	CLA	C3-C5-C6-C7
16	3	211	CLA	C3-C5-C6-C7
16	A	807	CLA	C3-C5-C6-C7
16	A	828	CLA	C3-C5-C6-C7
16	B	803	CLA	C3-C5-C6-C7
16	B	818	CLA	C3-C5-C6-C7
16	B	819	CLA	C3-C5-C6-C7
16	I	102	CLA	C3-C5-C6-C7
16	1	609	CLA	CBA-CGA-O2A-C1
16	1	611	CLA	CBA-CGA-O2A-C1
16	2	607	CLA	CBA-CGA-O2A-C1
16	2	613	CLA	CBA-CGA-O2A-C1
16	3	210	CLA	CBA-CGA-O2A-C1
16	A	804	CLA	CBA-CGA-O2A-C1
16	A	805	CLA	CBA-CGA-O2A-C1
16	A	809	CLA	CBA-CGA-O2A-C1
16	A	813	CLA	CBA-CGA-O2A-C1
16	A	819	CLA	CBA-CGA-O2A-C1
16	A	825	CLA	CBA-CGA-O2A-C1
16	B	802	CLA	CBA-CGA-O2A-C1
16	B	804	CLA	CBA-CGA-O2A-C1
16	B	807	CLA	CBA-CGA-O2A-C1
16	B	809	CLA	CBA-CGA-O2A-C1
16	B	828	CLA	CBA-CGA-O2A-C1
16	B	831	CLA	CBA-CGA-O2A-C1
16	F	201	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	F	204	CLA	CBA-CGA-O2A-C1
16	K	102	CLA	CBA-CGA-O2A-C1
16	J	102	CLA	O1D-CGD-O2D-CED
16	A	807	CLA	CBD-CGD-O2D-CED
16	F	205	CLA	CBD-CGD-O2D-CED
16	A	806	CLA	O1D-CGD-O2D-CED
16	A	836	CLA	O1D-CGD-O2D-CED
16	B	824	CLA	O1D-CGD-O2D-CED
19	2	622	LHG	O9-C7-O7-C5
16	1	609	CLA	O1A-CGA-O2A-C1
16	2	607	CLA	O1A-CGA-O2A-C1
16	2	609	CLA	O1A-CGA-O2A-C1
16	2	612	CLA	O1A-CGA-O2A-C1
16	2	613	CLA	O1A-CGA-O2A-C1
16	A	813	CLA	O1A-CGA-O2A-C1
16	A	825	CLA	O1A-CGA-O2A-C1
16	B	804	CLA	O1A-CGA-O2A-C1
16	B	819	CLA	O1A-CGA-O2A-C1
16	B	824	CLA	O1A-CGA-O2A-C1
16	B	828	CLA	O1A-CGA-O2A-C1
16	B	829	CLA	O1A-CGA-O2A-C1
16	K	102	CLA	O1A-CGA-O2A-C1
29	B	854	3PH	O32-C31-O31-C3
22	2	619	PGT	C12-C11-O3-C3
16	O	202	CLA	O1D-CGD-O2D-CED
17	1	615	C7Z	C33-C34-C35-C15
18	1	613	RRX	C15-C16-C17-C18
18	J	103	RRX	C9-C10-C11-C12
21	A	857	BCR	C9-C10-C11-C12
21	B	841	BCR	C9-C10-C11-C12
21	B	844	BCR	C9-C10-C11-C12
21	B	847	BCR	C9-C10-C11-C12
21	L	207	BCR	C19-C20-C21-C22
21	O	205	BCR	C9-C10-C11-C12
24	3	202	LMU	O5B-C5B-C6B-O6B
16	A	810	CLA	CBD-CGD-O2D-CED
16	B	816	CLA	CBD-CGD-O2D-CED
19	2	622	LHG	O2-C2-C3-O3
19	A	842	LHG	O2-C2-C3-O3
16	B	813	CLA	C3-C5-C6-C7
16	K	101	CLA	C3-C5-C6-C7
16	1	604	CLA	CBA-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	2	609	CLA	CBA-CGA-O2A-C1
16	A	803	CLA	CBA-CGA-O2A-C1
16	A	824	CLA	CBA-CGA-O2A-C1
16	B	810	CLA	CBA-CGA-O2A-C1
16	B	824	CLA	CBA-CGA-O2A-C1
16	B	829	CLA	CBA-CGA-O2A-C1
16	O	201	CLA	CBA-CGA-O2A-C1
16	O	203	CLA	CBA-CGA-O2A-C1
19	1	617	LHG	C24-C23-O8-C6
29	B	854	3PH	C32-C31-O31-C3
16	1	601	CLA	O1A-CGA-O2A-C1
16	1	604	CLA	O1A-CGA-O2A-C1
16	A	827	CLA	O1A-CGA-O2A-C1
16	A	830	CLA	O1A-CGA-O2A-C1
16	I	101	CLA	O1A-CGA-O2A-C1
16	2	603	CLA	O1D-CGD-O2D-CED
16	B	809	CLA	O1D-CGD-O2D-CED
19	2	622	LHG	C8-C7-O7-C5
16	B	823	CLA	CBD-CGD-O2D-CED
16	B	830	CLA	CBD-CGD-O2D-CED
19	2	622	LHG	C11-C12-C13-C14
19	A	842	LHG	C11-C10-C9-C8
16	B	809	CLA	C3-C5-C6-C7
16	L	201	CLA	C3-C5-C6-C7
16	1	601	CLA	CBA-CGA-O2A-C1
16	A	830	CLA	CBA-CGA-O2A-C1
16	B	819	CLA	CBA-CGA-O2A-C1
16	A	805	CLA	O1D-CGD-O2D-CED
24	3	202	LMU	C4B-C5B-C6B-O6B
19	2	622	LHG	C2-C3-O3-P
16	A	804	CLA	O1A-CGA-O2A-C1
16	A	824	CLA	O1A-CGA-O2A-C1
16	J	102	CLA	C13-C15-C16-C17
16	3	207	CLA	C4-C3-C5-C6
16	A	821	CLA	C4-C3-C5-C6
27	A	840	PQN	C14-C13-C15-C16
16	3	207	CLA	C2-C3-C5-C6
16	A	821	CLA	C2-C3-C5-C6
27	A	840	PQN	C12-C13-C15-C16
16	2	601	CLA	C2A-CAA-CBA-CGA
16	A	811	CLA	C2A-CAA-CBA-CGA
16	A	835	CLA	C2A-CAA-CBA-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	810	CLA	O1A-CGA-O2A-C1
16	O	203	CLA	O1A-CGA-O2A-C1
16	A	820	CLA	O1D-CGD-O2D-CED
16	1	604	CLA	C2C-C3C-CAC-CBC
16	B	806	CLA	CBA-CGA-O2A-C1
22	B	848	PGT	C34-C35-C36-C37
19	A	841	LHG	C31-C32-C33-C34
16	1	608	CLA	O1D-CGD-O2D-CED
16	A	812	CLA	O1D-CGD-O2D-CED
19	A	841	LHG	C8-C7-O7-C5
22	2	619	PGT	C32-C31-O2-C2
16	A	834	CLA	O1D-CGD-O2D-CED
16	2	611	CLA	C2C-C3C-CAC-CBC
16	A	819	CLA	O1D-CGD-O2D-CED
19	A	841	LHG	C1-C2-C3-O3
22	B	848	PGT	O4P-C4-C5-C6
19	1	617	LHG	O10-C23-O8-C6
16	A	802	CLA	C3-C5-C6-C7
16	A	854	CLA	C3-C5-C6-C7
16	A	814	CLA	O1D-CGD-O2D-CED
16	F	202	CLA	O1D-CGD-O2D-CED
16	2	603	CLA	CBA-CGA-O2A-C1
16	3	204	CLA	CBA-CGA-O2A-C1
16	3	207	CLA	CBA-CGA-O2A-C1
16	3	212	CLA	CBA-CGA-O2A-C1
16	A	806	CLA	CBA-CGA-O2A-C1
16	A	807	CLA	CBA-CGA-O2A-C1
16	A	812	CLA	CBA-CGA-O2A-C1
16	A	815	CLA	CBA-CGA-O2A-C1
16	A	818	CLA	CBA-CGA-O2A-C1
16	A	834	CLA	CBA-CGA-O2A-C1
16	A	838	CLA	CBA-CGA-O2A-C1
16	A	839	CLA	CBA-CGA-O2A-C1
16	B	837	CLA	CBA-CGA-O2A-C1
16	K	101	CLA	CBA-CGA-O2A-C1
19	2	622	LHG	C24-C23-O8-C6
16	A	804	CLA	C5-C6-C7-C8
16	2	602	CLA	CBD-CGD-O2D-CED
16	B	810	CLA	O1D-CGD-O2D-CED
17	J	104	C7Z	C29-C30-C31-C32
21	L	207	BCR	C9-C10-C11-C12
16	A	820	CLA	C15-C16-C17-C18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	1	604	CLA	C8-C10-C11-C12
16	A	807	CLA	C8-C10-C11-C12
16	A	837	CLA	C15-C16-C17-C18
19	B	851	LHG	C7-C8-C9-C10
24	3	202	LMU	C2'-C1'-O1'-C1
31	B	849	DGD	C2D-C1D-O3G-C3G
19	A	842	LHG	O7-C5-C6-O8
16	A	812	CLA	O1A-CGA-O2A-C1
16	K	101	CLA	O1A-CGA-O2A-C1
16	2	607	CLA	C4-C3-C5-C6
16	2	607	CLA	C2-C3-C5-C6
16	A	814	CLA	C2-C3-C5-C6
16	1	602	CLA	C6-C7-C8-C9
16	1	604	CLA	C6-C7-C8-C9
16	1	606	CLA	C14-C13-C15-C16
16	1	611	CLA	C6-C7-C8-C9
16	2	601	CLA	C6-C7-C8-C9
16	2	604	CLA	C6-C7-C8-C9
16	2	606	CLA	C11-C12-C13-C14
16	2	610	CLA	C11-C10-C8-C9
16	3	203	CLA	C14-C13-C15-C16
16	3	208	CLA	C11-C10-C8-C9
16	3	211	CLA	C6-C7-C8-C9
16	3	214	CLA	C11-C12-C13-C14
16	A	807	CLA	C6-C7-C8-C9
16	A	809	CLA	C6-C7-C8-C9
16	A	809	CLA	C11-C12-C13-C14
16	A	813	CLA	C6-C7-C8-C9
16	A	814	CLA	C11-C10-C8-C9
16	A	837	CLA	C11-C10-C8-C9
16	B	802	CLA	C6-C7-C8-C9
16	B	803	CLA	C6-C7-C8-C9
16	B	808	CLA	C6-C7-C8-C9
16	B	821	CLA	C6-C7-C8-C9
16	B	832	CLA	C6-C7-C8-C9
16	B	836	CLA	C6-C7-C8-C9
16	F	201	CLA	C6-C7-C8-C9
16	F	205	CLA	C6-C7-C8-C9
16	K	101	CLA	C11-C12-C13-C14
16	K	102	CLA	C11-C12-C13-C14
26	A	801	CL0	C11-C12-C13-C14
16	A	838	CLA	O1D-CGD-O2D-CED

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	854	CLA	O1D-CGD-O2D-CED
17	1	612	C7Z	C27-C28-C29-C39
17	1	614	C7Z	C11-C12-C13-C20
17	1	615	C7Z	C31-C32-C33-C40
17	1	616	C7Z	C27-C28-C29-C39
17	2	614	C7Z	C27-C28-C29-C39
17	2	615	C7Z	C27-C28-C29-C39
17	3	215	C7Z	C7-C8-C9-C19
17	3	215	C7Z	C27-C28-C29-C39
17	3	216	C7Z	C11-C12-C13-C20
17	3	217	C7Z	C11-C12-C13-C20
17	3	217	C7Z	C27-C28-C29-C39
17	3	218	C7Z	C27-C28-C29-C39
17	A	843	C7Z	C11-C12-C13-C20
17	A	843	C7Z	C27-C28-C29-C39
18	2	616	RRX	C11-C12-C13-C35
18	A	847	RRX	C7-C8-C9-C34
18	K	103	RRX	C11-C12-C13-C35
18	K	103	RRX	C7-C8-C9-C34
21	A	844	BCR	C11-C12-C13-C35
21	A	846	BCR	C7-C8-C9-C34
21	A	850	BCR	C7-C8-C9-C34
21	B	844	BCR	C37-C22-C23-C24
21	B	847	BCR	C7-C8-C9-C34
21	F	203	BCR	C37-C22-C23-C24
21	F	206	BCR	C7-C8-C9-C34
21	F	206	BCR	C37-C22-C23-C24
17	1	614	C7Z	C11-C12-C13-C14
17	1	615	C7Z	C31-C32-C33-C34
17	2	614	C7Z	C27-C28-C29-C30
17	2	615	C7Z	C27-C28-C29-C30
17	3	215	C7Z	C27-C28-C29-C30
17	3	216	C7Z	C11-C12-C13-C14
17	3	217	C7Z	C11-C12-C13-C14
17	3	217	C7Z	C27-C28-C29-C30
17	3	218	C7Z	C27-C28-C29-C30
17	A	843	C7Z	C11-C12-C13-C14
18	2	616	RRX	C11-C12-C13-C14
18	A	847	RRX	C7-C8-C9-C10
18	K	103	RRX	C7-C8-C9-C10
21	A	844	BCR	C11-C12-C13-C14
21	A	846	BCR	C7-C8-C9-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	A	850	BCR	C7-C8-C9-C10
21	B	844	BCR	C21-C22-C23-C24
21	B	847	BCR	C7-C8-C9-C10
19	A	842	LHG	C8-C7-O7-C5
16	3	214	CLA	C2C-C3C-CAC-CBC
16	3	204	CLA	O1A-CGA-O2A-C1
16	3	207	CLA	O1A-CGA-O2A-C1
16	A	838	CLA	O1A-CGA-O2A-C1
16	1	608	CLA	C5-C6-C7-C8
16	A	806	CLA	C8-C10-C11-C12
16	A	813	CLA	C8-C10-C11-C12
16	A	820	CLA	C8-C10-C11-C12
16	B	836	CLA	O1D-CGD-O2D-CED
16	A	833	CLA	C3-C5-C6-C7
16	A	837	CLA	CBA-CGA-O2A-C1
16	B	830	CLA	CBA-CGA-O2A-C1
16	2	607	CLA	C13-C15-C16-C17
16	3	206	CLA	C8-C10-C11-C12
16	A	802	CLA	C8-C10-C11-C12
16	A	821	CLA	C13-C15-C16-C17
16	A	823	CLA	C8-C10-C11-C12
16	B	810	CLA	C8-C10-C11-C12
16	B	820	CLA	C13-C15-C16-C17
16	B	825	CLA	C5-C6-C7-C8
16	J	102	CLA	C8-C10-C11-C12
19	2	622	LHG	C7-C8-C9-C10
19	A	841	LHG	C23-C24-C25-C26
23	2	620	DGA	CA1-CA2-CA3-CA4
16	A	802	CLA	O1D-CGD-O2D-CED
16	B	822	CLA	O1D-CGD-O2D-CED
16	1	603	CLA	C13-C15-C16-C17
16	A	814	CLA	C8-C10-C11-C12
16	A	816	CLA	C10-C11-C12-C13
16	A	833	CLA	C13-C15-C16-C17
16	B	816	CLA	C5-C6-C7-C8
16	B	835	CLA	C8-C10-C11-C12
16	B	838	CLA	C15-C16-C17-C18
16	F	201	CLA	C10-C11-C12-C13
16	I	101	CLA	C8-C10-C11-C12
16	K	102	CLA	C13-C15-C16-C17
16	L	203	CLA	C8-C10-C11-C12
16	A	825	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	A	842	LHG	O1-C1-C2-O2
16	2	603	CLA	O1A-CGA-O2A-C1
16	A	807	CLA	O1A-CGA-O2A-C1
16	A	818	CLA	O1A-CGA-O2A-C1
16	A	834	CLA	O1A-CGA-O2A-C1
16	A	839	CLA	O1A-CGA-O2A-C1
19	3	219	LHG	C23-C24-C25-C26
19	B	851	LHG	C23-C24-C25-C26
23	2	620	DGA	CB1-CB2-CB3-CB4
23	J	101	DGA	CB1-CB2-CB3-CB4
22	B	848	PGT	C36-C37-C38-C39
24	A	853	LMU	C4'-C5'-C6'-O6'
16	1	606	CLA	C8-C10-C11-C12
16	3	209	CLA	C8-C10-C11-C12
16	A	815	CLA	C3-C5-C6-C7
16	3	214	CLA	CBA-CGA-O2A-C1
16	A	829	CLA	CBA-CGA-O2A-C1
16	A	816	CLA	C2C-C3C-CAC-CBC
16	2	601	CLA	O1D-CGD-O2D-CED
16	2	608	CLA	O1D-CGD-O2D-CED
16	A	818	CLA	O1D-CGD-O2D-CED
16	2	605	CLA	C2-C1-O2A-CGA
16	2	609	CLA	C2-C1-O2A-CGA
16	A	824	CLA	C2-C1-O2A-CGA
16	A	827	CLA	C2-C1-O2A-CGA
16	B	814	CLA	C2-C1-O2A-CGA
16	B	821	CLA	C2-C1-O2A-CGA
16	F	205	CLA	C2-C1-O2A-CGA
16	O	203	CLA	C2-C1-O2A-CGA
16	2	613	CLA	C8-C10-C11-C12
16	B	836	CLA	C10-C11-C12-C13
29	A	849	3PH	C31-C32-C33-C34
16	3	210	CLA	C5-C6-C7-C8
16	B	820	CLA	C5-C6-C7-C8
16	A	824	CLA	O1D-CGD-O2D-CED
16	1	605	CLA	C11-C12-C13-C15
16	A	809	CLA	C11-C12-C13-C15
16	A	815	CLA	C11-C10-C8-C7
16	L	204	CLA	C6-C7-C8-C10
16	O	203	CLA	C6-C7-C8-C10
16	A	809	CLA	C3-C5-C6-C7
16	B	833	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	806	CLA	O1A-CGA-O2A-C1
19	2	622	LHG	O10-C23-O8-C6
17	1	615	C7Z	C29-C30-C31-C32
17	3	201	C7Z	C9-C10-C11-C12
17	3	216	C7Z	C9-C10-C11-C12
17	3	218	C7Z	C29-C30-C31-C32
21	I	103	BCR	C9-C10-C11-C12
21	L	206	BCR	C9-C10-C11-C12
16	1	603	CLA	C2A-CAA-CBA-CGA
16	A	815	CLA	C2A-CAA-CBA-CGA
16	B	818	CLA	C2A-CAA-CBA-CGA
16	B	805	CLA	O1D-CGD-O2D-CED
16	B	808	CLA	O1D-CGD-O2D-CED
16	2	601	CLA	C8-C10-C11-C12
16	2	603	CLA	C5-C6-C7-C8
16	A	806	CLA	O1A-CGA-O2A-C1
31	B	849	DGD	O6E-C1E-O5D-C6D
16	3	203	CLA	C8-C10-C11-C12
16	A	825	CLA	C15-C16-C17-C18
16	A	837	CLA	C5-C6-C7-C8
16	B	818	CLA	C8-C10-C11-C12
16	F	204	CLA	C8-C10-C11-C12
21	2	617	BCR	C10-C11-C12-C13
21	A	844	BCR	C10-C11-C12-C13
21	A	846	BCR	C10-C11-C12-C13
19	A	841	LHG	O9-C7-O7-C5
22	2	619	PGT	O31-C31-O2-C2
16	3	206	CLA	C3-C5-C6-C7
16	A	831	CLA	C3-C5-C6-C7
16	1	611	CLA	C15-C16-C17-C18
16	3	209	CLA	C13-C15-C16-C17
16	3	212	CLA	C8-C10-C11-C12
16	A	806	CLA	C5-C6-C7-C8
16	A	812	CLA	C8-C10-C11-C12
16	A	831	CLA	C5-C6-C7-C8
16	B	801	CLA	C13-C15-C16-C17
16	B	803	CLA	C8-C10-C11-C12
16	B	810	CLA	C5-C6-C7-C8
16	B	819	CLA	C15-C16-C17-C18
16	I	101	CLA	C5-C6-C7-C8
30	A	851	T7X	C31-C11-O18-C9
16	3	212	CLA	O1A-CGA-O2A-C1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	815	CLA	O1A-CGA-O2A-C1
16	B	837	CLA	O1A-CGA-O2A-C1
16	1	603	CLA	C5-C6-C7-C8
16	1	607	CLA	C8-C10-C11-C12
16	A	810	CLA	C13-C15-C16-C17
16	A	821	CLA	C8-C10-C11-C12
16	A	822	CLA	C5-C6-C7-C8
16	A	838	CLA	C13-C15-C16-C17
16	L	204	CLA	C8-C10-C11-C12
16	A	829	CLA	O1A-CGA-O2A-C1
25	3	220	PTY	C11-C8-O7-C6
16	1	606	CLA	C5-C6-C7-C8
16	1	608	CLA	C8-C10-C11-C12
16	2	601	CLA	C13-C15-C16-C17
16	2	604	CLA	C10-C11-C12-C13
16	A	827	CLA	C13-C15-C16-C17
16	A	839	CLA	C8-C10-C11-C12
16	O	201	CLA	C13-C15-C16-C17
19	1	617	LHG	C3-O3-P-O6
19	2	622	LHG	C3-O3-P-O6
19	2	622	LHG	C4-O6-P-O3
19	A	841	LHG	C4-O6-P-O3
25	A	852	PTY	C3-O11-P1-O14
25	L	208	PTY	C5-O14-P1-O11
30	A	851	T7X	C7-O13-P1-O1
16	A	806	CLA	C3-C5-C6-C7
16	A	817	CLA	C3-C5-C6-C7
26	A	801	CL0	C3-C5-C6-C7
20	2	618	ERG	C28-C24-C25-C26
16	1	610	CLA	CBA-CGA-O2A-C1
31	B	850	DGD	C2A-C1A-O1G-C1G
16	2	612	CLA	O1D-CGD-O2D-CED
16	B	812	CLA	O1D-CGD-O2D-CED
16	I	102	CLA	CBD-CGD-O2D-CED
16	3	208	CLA	C8-C10-C11-C12
16	A	816	CLA	C5-C6-C7-C8
16	A	825	CLA	C5-C6-C7-C8
16	A	837	CLA	O1A-CGA-O2A-C1
16	B	830	CLA	O1A-CGA-O2A-C1
24	A	853	LMU	C4B-C5B-C6B-O6B
31	B	850	DGD	O6D-C5D-C6D-O5D
19	A	841	LHG	C7-C8-C9-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	3	203	CLA	O1D-CGD-O2D-CED
19	A	842	LHG	O9-C7-O7-C5
25	3	220	PTY	O10-C8-O7-C6
16	A	805	CLA	C8-C10-C11-C12
16	A	816	CLA	C2A-CAA-CBA-CGA
16	B	816	CLA	C2A-CAA-CBA-CGA
16	B	827	CLA	C2A-CAA-CBA-CGA
16	B	832	CLA	C2A-CAA-CBA-CGA
16	B	837	CLA	C2A-CAA-CBA-CGA
16	I	101	CLA	C2A-CAA-CBA-CGA
16	3	203	CLA	C16-C17-C18-C20
16	A	816	CLA	C3-C5-C6-C7
16	B	827	CLA	C3-C5-C6-C7
16	A	814	CLA	CBA-CGA-O2A-C1
16	A	823	CLA	CBA-CGA-O2A-C1
19	B	851	LHG	C24-C23-O8-C6
31	B	846	DGD	C2A-C1A-O1G-C1G
16	2	610	CLA	C8-C10-C11-C12
23	J	101	DGA	CB9-CAB-CBB-CCB
17	2	614	C7Z	C29-C30-C31-C32
19	2	622	LHG	C23-C24-C25-C26
19	2	622	LHG	C13-C14-C15-C16
23	J	101	DGA	CB7-CB8-CB9-CAB
16	3	210	CLA	O1D-CGD-O2D-CED
29	B	854	3PH	C22-C21-O21-C2
16	1	610	CLA	C8-C10-C11-C12
21	A	845	BCR	C11-C10-C9-C34
21	B	845	BCR	C11-C10-C9-C34
16	B	802	CLA	C3-C5-C6-C7
16	B	824	CLA	C3-C5-C6-C7
16	O	201	CLA	C3-C5-C6-C7
23	2	620	DGA	CA4-CA5-CA6-CA7
23	2	620	DGA	CA5-CA6-CA7-CA8
24	A	853	LMU	O1'-C1-C2-C3
29	J	105	3PH	C29-C2A-C2B-C2C
30	A	851	T7X	C35-C36-C37-C38
16	A	826	CLA	C16-C17-C18-C19
16	B	815	CLA	C6-C7-C8-C9
16	B	836	CLA	C16-C17-C18-C20
16	2	601	CLA	CBA-CGA-O2A-C1
16	J	102	CLA	CBA-CGA-O2A-C1
19	2	622	LHG	C28-C29-C30-C31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	A	841	LHG	C9-C10-C11-C12
24	3	202	LMU	C6-C7-C8-C9
25	A	852	PTY	C33-C34-C35-C36
30	A	851	T7X	C7-C8-O16-C10
16	A	807	CLA	O1D-CGD-O2D-CED
29	B	854	3PH	O22-C21-O21-C2
16	2	608	CLA	C8-C10-C11-C12
16	B	831	CLA	C5-C6-C7-C8
23	2	620	DGA	CAA-CBA-CCA-CDA
31	B	850	DGD	C2A-C3A-C4A-C5A
16	3	214	CLA	O1A-CGA-O2A-C1
19	A	842	LHG	C25-C26-C27-C28
25	3	220	PTY	C35-C36-C37-C38
29	A	849	3PH	C29-C2A-C2B-C2C
16	F	205	CLA	O1D-CGD-O2D-CED
16	2	611	CLA	C13-C15-C16-C17
22	B	848	PGT	O4P-C4-C5-O5
19	3	219	LHG	C28-C29-C30-C31
19	1	617	LHG	C7-C8-C9-C10
21	A	845	BCR	C11-C10-C9-C8
21	B	845	BCR	C11-C10-C9-C8
31	B	849	DGD	C2E-C1E-O5D-C6D
16	A	808	CLA	CBA-CGA-O2A-C1
16	A	822	CLA	CBA-CGA-O2A-C1
16	B	835	CLA	CBA-CGA-O2A-C1
19	2	622	LHG	C25-C26-C27-C28
19	A	842	LHG	C26-C27-C28-C29
22	2	619	PGT	C40-C41-C42-C43
22	B	848	PGT	C38-C39-C40-C41
16	A	823	CLA	O1A-CGA-O2A-C1
16	2	606	CLA	C16-C17-C18-C20
16	3	208	CLA	C16-C17-C18-C19
16	A	815	CLA	C16-C17-C18-C20
16	B	834	CLA	C16-C17-C18-C20
16	L	205	CLA	C16-C17-C18-C20
27	B	839	PQN	C26-C27-C28-C30
16	B	816	CLA	O1D-CGD-O2D-CED
19	A	841	LHG	C16-C17-C18-C19
19	B	851	LHG	C33-C34-C35-C36
22	B	848	PGT	C32-C33-C34-C35
16	2	613	CLA	C11-C12-C13-C14
16	3	204	CLA	C11-C10-C8-C9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	3	212	CLA	C6-C7-C8-C9
16	A	809	CLA	C11-C10-C8-C9
16	A	815	CLA	C11-C10-C8-C9
16	A	839	CLA	C6-C7-C8-C9
16	F	204	CLA	C11-C12-C13-C14
16	O	203	CLA	C6-C7-C8-C9
19	1	617	LHG	C28-C29-C30-C31
19	A	841	LHG	C11-C12-C13-C14
22	2	619	PGT	C42-C43-C44-C45
22	2	619	PGT	C39-C40-C41-C42
25	3	221	PTY	C18-C19-C20-C21
31	B	846	DGD	C3A-C4A-C5A-C6A
16	A	855	CLA	C8-C10-C11-C12
16	3	209	CLA	C2A-CAA-CBA-CGA
30	A	851	T7X	O19-C11-O18-C9
17	1	616	C7Z	C7-C8-C9-C19
17	3	201	C7Z	C7-C8-C9-C19
17	3	217	C7Z	C7-C8-C9-C19
21	A	850	BCR	C11-C12-C13-C35
21	F	203	BCR	C11-C12-C13-C35
21	L	202	BCR	C11-C12-C13-C35
21	L	207	BCR	C11-C12-C13-C35
17	1	614	C7Z	C7-C8-C9-C10
17	1	616	C7Z	C7-C8-C9-C10
17	2	615	C7Z	C7-C8-C9-C10
17	3	201	C7Z	C7-C8-C9-C10
17	3	215	C7Z	C7-C8-C9-C10
17	3	217	C7Z	C7-C8-C9-C10
18	J	103	RRX	C17-C18-C19-C20
21	A	850	BCR	C11-C12-C13-C14
21	F	203	BCR	C11-C12-C13-C14
16	2	601	CLA	C3-C5-C6-C7
16	2	604	CLA	C3-C5-C6-C7
23	2	620	DGA	CB5-CB6-CB7-CB8
23	J	101	DGA	CCA-CDA-CEA-CFA
23	J	101	DGA	CCB-CDB-CEB-CFB
19	A	842	LHG	C23-C24-C25-C26
22	2	619	PGT	C37-C38-C39-C40
23	2	620	DGA	CA2-CA3-CA4-CA5
23	2	620	DGA	CA6-CA7-CA8-CA9
25	3	220	PTY	C37-C38-C39-C40
16	1	610	CLA	C16-C17-C18-C19

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	2	606	CLA	C16-C17-C18-C19
16	A	826	CLA	C16-C17-C18-C20
16	L	204	CLA	C16-C17-C18-C19
27	B	839	PQN	C26-C27-C28-C29
16	A	812	CLA	C13-C15-C16-C17
29	B	854	3PH	C3B-C3C-C3D-C3E
31	B	850	DGD	C4D-C5D-C6D-O5D
20	2	618	ERG	C16-C17-C20-C22
16	1	604	CLA	C4C-C3C-CAC-CBC
16	2	611	CLA	C4C-C3C-CAC-CBC
19	A	842	LHG	C34-C35-C36-C37
25	3	220	PTY	C11-C12-C13-C14
25	3	220	PTY	C22-C23-C24-C25
16	2	603	CLA	C8-C10-C11-C12
16	A	832	CLA	C15-C16-C17-C18
16	B	834	CLA	C13-C15-C16-C17
16	B	837	CLA	C10-C11-C12-C13
16	B	838	CLA	C5-C6-C7-C8
16	1	610	CLA	O1A-CGA-O2A-C1
19	A	842	LHG	C13-C14-C15-C16
19	A	842	LHG	C28-C29-C30-C31
25	L	208	PTY	C22-C23-C24-C25
29	B	854	3PH	C29-C2A-C2B-C2C
16	1	609	CLA	C3A-C2A-CAA-CBA
16	2	603	CLA	C3A-C2A-CAA-CBA
16	3	214	CLA	C3A-C2A-CAA-CBA
16	A	802	CLA	C3A-C2A-CAA-CBA
16	A	805	CLA	C3A-C2A-CAA-CBA
16	A	808	CLA	C3A-C2A-CAA-CBA
16	A	815	CLA	C3A-C2A-CAA-CBA
16	A	831	CLA	C3A-C2A-CAA-CBA
16	A	835	CLA	C3A-C2A-CAA-CBA
16	B	802	CLA	C3A-C2A-CAA-CBA
16	B	823	CLA	C3A-C2A-CAA-CBA
16	B	833	CLA	C3A-C2A-CAA-CBA
16	L	205	CLA	C3A-C2A-CAA-CBA
16	O	201	CLA	C3A-C2A-CAA-CBA
16	3	210	CLA	C13-C15-C16-C17
24	3	202	LMU	C2-C1-O1'-C1'
19	A	841	LHG	C26-C27-C28-C29
19	B	851	LHG	C24-C25-C26-C27
16	A	810	CLA	O1D-CGD-O2D-CED

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	B	850	DGD	O1A-C1A-O1G-C1G
16	A	815	CLA	C16-C17-C18-C19
16	B	834	CLA	C16-C17-C18-C19
16	L	204	CLA	C16-C17-C18-C20
29	A	849	3PH	C24-C25-C26-C27
16	2	602	CLA	C3-C5-C6-C7
16	2	610	CLA	C3-C5-C6-C7
16	A	823	CLA	C3-C5-C6-C7
16	B	832	CLA	C3-C5-C6-C7
19	2	622	LHG	C33-C34-C35-C36
16	B	837	CLA	C4-C3-C5-C6
16	A	820	CLA	C2-C3-C5-C6
16	A	827	CLA	C2-C3-C5-C6
16	B	837	CLA	C2-C3-C5-C6
29	A	849	3PH	C22-C21-O21-C2
22	B	848	PGT	C12-C11-O3-C3
20	2	621	ERG	C22-C23-C24-C28
16	1	605	CLA	C2A-CAA-CBA-CGA
19	1	617	LHG	O1-C1-C2-O2
16	A	834	CLA	C8-C10-C11-C12
30	A	851	T7X	C41-C42-C43-C44
16	J	102	CLA	O1A-CGA-O2A-C1
19	B	851	LHG	O10-C23-O8-C6
16	1	610	CLA	C16-C17-C18-C20
16	B	831	CLA	C16-C17-C18-C19
16	B	836	CLA	C16-C17-C18-C19
23	2	620	DGA	CB7-CB8-CB9-CAB
23	J	101	DGA	CA4-CA5-CA6-CA7
16	1	602	CLA	C3-C5-C6-C7
16	2	613	CLA	C3-C5-C6-C7
16	A	814	CLA	O1A-CGA-O2A-C1
31	B	846	DGD	O1A-C1A-O1G-C1G
16	A	802	CLA	C15-C16-C17-C18
16	B	805	CLA	C13-C15-C16-C17
16	B	817	CLA	C10-C11-C12-C13
29	A	849	3PH	O22-C21-O21-C2
16	2	604	CLA	C2-C1-O2A-CGA
16	3	209	CLA	C2-C1-O2A-CGA
16	3	212	CLA	C2-C1-O2A-CGA
16	A	808	CLA	C2-C1-O2A-CGA
16	A	855	CLA	C2-C1-O2A-CGA
16	B	818	CLA	C2-C1-O2A-CGA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	825	CLA	C2-C1-O2A-CGA
16	B	833	CLA	C2-C1-O2A-CGA
16	F	202	CLA	C2-C1-O2A-CGA
23	2	620	DGA	CEA-CFA-CGA-CHA
16	A	856	CLA	C5-C6-C7-C8
16	2	601	CLA	O1A-CGA-O2A-C1
16	A	808	CLA	O1A-CGA-O2A-C1
16	A	822	CLA	O1A-CGA-O2A-C1
19	A	842	LHG	C11-C12-C13-C14
16	A	822	CLA	C3-C5-C6-C7
16	B	815	CLA	C3-C5-C6-C7
17	1	612	C7Z	C21-C26-C27-C28
17	1	612	C7Z	C25-C26-C27-C28
17	1	614	C7Z	C5-C6-C7-C8
17	1	615	C7Z	C5-C6-C7-C8
17	1	616	C7Z	C25-C26-C27-C28
17	2	614	C7Z	C21-C26-C27-C28
17	2	614	C7Z	C25-C26-C27-C28
17	3	201	C7Z	C25-C26-C27-C28
17	3	215	C7Z	C1-C6-C7-C8
17	3	215	C7Z	C25-C26-C27-C28
17	3	217	C7Z	C5-C6-C7-C8
17	3	217	C7Z	C21-C26-C27-C28
17	3	218	C7Z	C21-C26-C27-C28
17	A	843	C7Z	C25-C26-C27-C28
17	J	104	C7Z	C5-C6-C7-C8
17	J	104	C7Z	C25-C26-C27-C28
18	1	613	RRX	C23-C24-C25-C26
18	2	616	RRX	C23-C24-C25-C26
18	A	847	RRX	C5-C6-C7-C8
18	J	103	RRX	C23-C24-C25-C26
18	J	103	RRX	C5-C6-C7-C8
18	K	103	RRX	C23-C24-C25-C26
18	K	103	RRX	C1-C6-C7-C8
21	A	844	BCR	C23-C24-C25-C26
21	A	845	BCR	C1-C6-C7-C8
21	A	845	BCR	C23-C24-C25-C26
21	B	840	BCR	C23-C24-C25-C30
21	B	841	BCR	C23-C24-C25-C30
21	B	842	BCR	C23-C24-C25-C26
21	B	843	BCR	C23-C24-C25-C26
21	B	843	BCR	C23-C24-C25-C30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	B	845	BCR	C1-C6-C7-C8
21	B	845	BCR	C5-C6-C7-C8
21	B	845	BCR	C23-C24-C25-C26
21	B	845	BCR	C23-C24-C25-C30
21	F	203	BCR	C1-C6-C7-C8
21	F	203	BCR	C5-C6-C7-C8
21	I	103	BCR	C1-C6-C7-C8
21	I	103	BCR	C23-C24-C25-C26
21	I	103	BCR	C23-C24-C25-C30
21	K	104	BCR	C5-C6-C7-C8
21	L	206	BCR	C1-C6-C7-C8
21	L	206	BCR	C5-C6-C7-C8
21	O	205	BCR	C1-C6-C7-C8
21	O	205	BCR	C5-C6-C7-C8
21	O	205	BCR	C23-C24-C25-C26
21	O	205	BCR	C23-C24-C25-C30
19	A	841	LHG	C25-C26-C27-C28
16	A	831	CLA	CBA-CGA-O2A-C1
31	B	849	DGD	C2A-C1A-O1G-C1G
16	1	601	CLA	C15-C16-C17-C18
16	3	211	CLA	C8-C10-C11-C12
16	B	809	CLA	C13-C15-C16-C17
16	B	812	CLA	C8-C10-C11-C12
16	L	201	CLA	C8-C10-C11-C12
16	L	205	CLA	C10-C11-C12-C13
16	O	201	CLA	C8-C10-C11-C12
23	2	620	DGA	CA8-CA9-CAA-CBA
23	J	101	DGA	CAA-CBA-CCA-CDA
25	3	220	PTY	C31-C32-C33-C34
25	L	208	PTY	C11-C12-C13-C14
16	B	835	CLA	O1A-CGA-O2A-C1
16	K	102	CLA	CBD-CGD-O2D-CED
23	J	101	DGA	CB5-CB6-CB7-CB8
16	B	827	CLA	C15-C16-C17-C18
19	3	219	LHG	C32-C33-C34-C35
16	A	827	CLA	C4-C3-C5-C6
16	1	602	CLA	C6-C7-C8-C10
16	2	613	CLA	C11-C12-C13-C15
16	3	204	CLA	C11-C10-C8-C7
16	3	207	CLA	C11-C10-C8-C7
16	3	214	CLA	C11-C12-C13-C15
16	A	807	CLA	C11-C12-C13-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	820	CLA	C11-C12-C13-C15
16	A	822	CLA	C11-C10-C8-C7
16	A	833	CLA	C6-C7-C8-C10
16	B	806	CLA	C6-C7-C8-C10
16	K	101	CLA	C11-C12-C13-C15
26	A	801	CL0	C11-C12-C13-C15
27	A	840	PQN	C21-C22-C23-C25
16	A	811	CLA	C3-C5-C6-C7
16	F	205	CLA	C3-C5-C6-C7
31	B	849	DGD	O1A-C1A-O1G-C1G
16	3	208	CLA	C16-C17-C18-C20
16	B	815	CLA	C6-C7-C8-C10
16	L	205	CLA	C16-C17-C18-C19
16	1	605	CLA	CBA-CGA-O2A-C1
16	3	209	CLA	CBA-CGA-O2A-C1
16	A	810	CLA	CBA-CGA-O2A-C1
16	B	826	CLA	CBA-CGA-O2A-C1
19	2	622	LHG	C29-C30-C31-C32
16	B	801	CLA	C2A-CAA-CBA-CGA
16	2	607	CLA	C10-C11-C12-C13
16	L	204	CLA	C13-C15-C16-C17
29	B	854	3PH	C3D-C3E-C3F-C3G
16	2	612	CLA	C2C-C3C-CAC-CBC
25	A	852	PTY	C38-C39-C40-C41
29	J	105	3PH	C3D-C3E-C3F-C3G
31	B	846	DGD	C6A-C7A-C8A-C9A
31	B	846	DGD	C2G-C1G-O1G-C1A
16	3	214	CLA	C4C-C3C-CAC-CBC
19	1	617	LHG	C13-C14-C15-C16
16	B	809	CLA	C5-C6-C7-C8
16	B	823	CLA	O1D-CGD-O2D-CED
16	B	830	CLA	O1D-CGD-O2D-CED
29	B	854	3PH	C27-C28-C29-C2A
21	A	850	BCR	C18-C19-C20-C21
21	L	207	BCR	C18-C19-C20-C21
22	B	848	PGT	C42-C43-C44-C45
23	J	101	DGA	CB3-CB4-CB5-CB6
16	A	839	CLA	C13-C15-C16-C17
16	B	813	CLA	C15-C16-C17-C18
16	B	817	CLA	C8-C10-C11-C12
16	B	830	CLA	C5-C6-C7-C8
24	A	853	LMU	O5B-C5B-C6B-O6B

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
24	A	853	LMU	O5'-C5'-C6'-O6'
25	L	208	PTY	O10-C8-O7-C6
29	J	105	3PH	O21-C2-C3-O31
19	A	842	LHG	C29-C30-C31-C32
16	A	820	CLA	C4-C3-C5-C6
16	A	856	CLA	C4-C3-C5-C6
16	A	856	CLA	C2-C3-C5-C6
16	L	204	CLA	C2-C3-C5-C6
16	A	816	CLA	C4C-C3C-CAC-CBC
25	3	221	PTY	C16-C17-C18-C19
16	1	601	CLA	C6-C7-C8-C9
16	1	605	CLA	C11-C12-C13-C14
16	3	207	CLA	C11-C10-C8-C9
16	A	816	CLA	C6-C7-C8-C9
16	A	818	CLA	C11-C12-C13-C14
16	A	828	CLA	C6-C7-C8-C9
16	A	833	CLA	C6-C7-C8-C9
16	A	836	CLA	C6-C7-C8-C9
16	B	806	CLA	C6-C7-C8-C9
16	B	816	CLA	C6-C7-C8-C9
16	I	102	CLA	C11-C10-C8-C9
16	L	204	CLA	C6-C7-C8-C9
27	A	840	PQN	C21-C22-C23-C24
16	A	833	CLA	C10-C11-C12-C13
16	J	102	CLA	C3-C5-C6-C7
16	A	812	CLA	C2A-CAA-CBA-CGA
16	A	823	CLA	C2A-CAA-CBA-CGA
16	B	815	CLA	C2A-CAA-CBA-CGA
18	1	613	RRX	C37-C22-C23-C24
16	A	815	CLA	C13-C15-C16-C17
16	B	810	CLA	C10-C11-C12-C13
16	F	202	CLA	C2C-C3C-CAC-CBC
17	1	616	C7Z	C27-C28-C29-C30
16	1	602	CLA	C1A-C2A-CAA-CBA
16	1	606	CLA	C1A-C2A-CAA-CBA
16	1	608	CLA	C1A-C2A-CAA-CBA
16	1	609	CLA	C1A-C2A-CAA-CBA
16	2	603	CLA	C1A-C2A-CAA-CBA
16	2	608	CLA	C1A-C2A-CAA-CBA
16	2	609	CLA	C1A-C2A-CAA-CBA
16	2	610	CLA	C1A-C2A-CAA-CBA
16	3	209	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	3	213	CLA	C1A-C2A-CAA-CBA
16	3	214	CLA	C1A-C2A-CAA-CBA
16	A	802	CLA	C1A-C2A-CAA-CBA
16	A	805	CLA	C1A-C2A-CAA-CBA
16	A	807	CLA	C1A-C2A-CAA-CBA
16	A	808	CLA	C1A-C2A-CAA-CBA
16	A	809	CLA	C1A-C2A-CAA-CBA
16	A	814	CLA	C1A-C2A-CAA-CBA
16	A	817	CLA	C1A-C2A-CAA-CBA
16	A	819	CLA	C1A-C2A-CAA-CBA
16	A	822	CLA	C1A-C2A-CAA-CBA
16	A	831	CLA	C1A-C2A-CAA-CBA
16	A	835	CLA	C1A-C2A-CAA-CBA
16	B	802	CLA	C1A-C2A-CAA-CBA
16	B	806	CLA	C1A-C2A-CAA-CBA
16	B	809	CLA	C1A-C2A-CAA-CBA
16	B	810	CLA	C1A-C2A-CAA-CBA
16	B	820	CLA	C1A-C2A-CAA-CBA
16	B	823	CLA	C1A-C2A-CAA-CBA
16	B	829	CLA	C1A-C2A-CAA-CBA
16	B	830	CLA	C1A-C2A-CAA-CBA
16	B	832	CLA	C1A-C2A-CAA-CBA
16	B	833	CLA	C1A-C2A-CAA-CBA
16	B	835	CLA	C1A-C2A-CAA-CBA
16	B	838	CLA	C1A-C2A-CAA-CBA
16	K	101	CLA	C1A-C2A-CAA-CBA
16	L	201	CLA	C1A-C2A-CAA-CBA
16	O	201	CLA	C1A-C2A-CAA-CBA
16	O	202	CLA	C1A-C2A-CAA-CBA
16	O	204	CLA	C1A-C2A-CAA-CBA
16	B	831	CLA	C16-C17-C18-C20
25	L	208	PTY	C11-C8-O7-C6
22	B	848	PGT	C39-C40-C41-C42
23	2	620	DGA	CB9-CAB-CBB-CCB
21	A	846	BCR	C9-C10-C11-C12
16	1	601	CLA	C10-C11-C12-C13
16	B	826	CLA	C5-C6-C7-C8
16	O	203	CLA	C13-C15-C16-C17
27	A	840	PQN	C15-C16-C17-C18
22	2	619	PGT	C4-O4P-P-O3P
22	B	848	PGT	C1-O3P-P-O4P
22	B	848	PGT	C4-O4P-P-O3P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	831	CLA	O1A-CGA-O2A-C1
20	2	618	ERG	C23-C24-C25-C27
16	B	830	CLA	C13-C15-C16-C17
16	L	205	CLA	C8-C10-C11-C12
16	2	606	CLA	CBA-CGA-O2A-C1
19	1	617	LHG	O6-C4-C5-C6
19	3	219	LHG	O6-C4-C5-C6
22	B	848	PGT	O3P-C1-C2-C3
16	2	602	CLA	O1D-CGD-O2D-CED
19	3	219	LHG	C11-C12-C13-C14
29	A	849	3PH	C23-C24-C25-C26
16	3	203	CLA	C16-C17-C18-C19
26	A	801	CL0	C16-C17-C18-C19
19	A	842	LHG	C30-C31-C32-C33
25	3	221	PTY	C22-C23-C24-C25
16	1	608	CLA	C13-C15-C16-C17
29	B	854	3PH	C37-C38-C39-C3A
31	B	849	DGD	O6E-C5E-C6E-O5E
16	L	204	CLA	C4-C3-C5-C6
16	O	203	CLA	C4-C3-C5-C6
19	A	841	LHG	C30-C31-C32-C33
31	B	849	DGD	C6A-C7A-C8A-C9A
16	A	803	CLA	C13-C15-C16-C17
19	3	219	LHG	C11-C10-C9-C8
23	J	101	DGA	CA6-CA7-CA8-CA9
16	1	605	CLA	O1A-CGA-O2A-C1
19	B	851	LHG	C28-C29-C30-C31
16	1	608	CLA	C3-C5-C6-C7
19	3	219	LHG	C4-C5-C6-O8
19	A	842	LHG	C4-C5-C6-O8
29	J	105	3PH	C1-C2-C3-O31
31	B	846	DGD	O1G-C1G-C2G-C3G
31	B	849	DGD	C1G-C2G-C3G-O3G
16	3	210	CLA	C15-C16-C17-C18
16	A	829	CLA	C5-C6-C7-C8
19	2	622	LHG	C18-C19-C20-C21
20	1	618	ERG	C17-C20-C22-C23
20	2	621	ERG	C17-C20-C22-C23
20	2	621	ERG	C22-C23-C24-C25
31	B	849	DGD	C2G-C3G-O3G-C1D
29	J	105	3PH	C3F-C3G-C3H-C3I
16	A	810	CLA	O1A-CGA-O2A-C1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	1	601	CLA	C3-C5-C6-C7
16	B	804	CLA	C15-C16-C17-C18
22	B	848	PGT	C43-C44-C45-C46
29	J	105	3PH	C25-C26-C27-C28
31	B	846	DGD	C2B-C3B-C4B-C5B
19	B	851	LHG	O1-C1-C2-O2
22	2	619	PGT	O5-C5-C6-O6
19	A	841	LHG	C28-C29-C30-C31
25	3	220	PTY	C24-C25-C26-C27
16	B	826	CLA	O1A-CGA-O2A-C1
22	2	619	PGT	C31-C32-C33-C34
31	B	850	DGD	O6E-C5E-C6E-O5E
23	2	620	DGA	CDB-CEB-CFB-CGB
16	A	804	CLA	C16-C17-C18-C19
16	1	602	CLA	CBA-CGA-O2A-C1
16	O	201	CLA	C5-C6-C7-C8
16	B	837	CLA	C8-C10-C11-C12
16	F	204	CLA	C13-C15-C16-C17
16	O	202	CLA	C5-C6-C7-C8
16	B	801	CLA	C2-C1-O2A-CGA
16	B	819	CLA	C2-C1-O2A-CGA
29	B	854	3PH	C34-C35-C36-C37
27	A	840	PQN	C13-C15-C16-C17
16	2	606	CLA	C8-C10-C11-C12
16	B	806	CLA	C15-C16-C17-C18
25	A	852	PTY	C31-C30-O4-C1
16	3	209	CLA	O1A-CGA-O2A-C1
30	A	851	T7X	C40-C41-C42-C43
16	3	211	CLA	C15-C16-C17-C18
16	A	834	CLA	C5-C6-C7-C8
16	B	819	CLA	C8-C10-C11-C12
29	J	105	3PH	C3B-C3C-C3D-C3E
31	B	849	DGD	C3B-C4B-C5B-C6B
30	A	851	T7X	C12-C13-C14-C15
27	B	839	PQN	C13-C15-C16-C17
16	3	205	CLA	C5-C6-C7-C8
16	A	835	CLA	C13-C15-C16-C17
19	3	219	LHG	C13-C14-C15-C16
19	3	219	LHG	C31-C32-C33-C34
16	2	613	CLA	C15-C16-C17-C18
24	3	202	LMU	C1-C2-C3-C4
16	A	813	CLA	C13-C15-C16-C17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	824	CLA	C8-C10-C11-C12
16	1	601	CLA	C6-C7-C8-C10
16	1	609	CLA	C6-C7-C8-C10
16	2	602	CLA	C11-C10-C8-C7
16	2	605	CLA	C11-C10-C8-C7
16	2	609	CLA	C6-C7-C8-C10
16	3	203	CLA	C12-C13-C15-C16
16	A	802	CLA	C11-C12-C13-C15
16	A	803	CLA	C6-C7-C8-C10
16	A	805	CLA	C11-C12-C13-C15
16	A	813	CLA	C6-C7-C8-C10
16	A	814	CLA	C6-C7-C8-C10
16	A	816	CLA	C6-C7-C8-C10
16	A	818	CLA	C6-C7-C8-C10
16	A	818	CLA	C11-C12-C13-C15
16	A	819	CLA	C11-C12-C13-C15
16	A	821	CLA	C11-C10-C8-C7
16	A	823	CLA	C6-C7-C8-C10
16	A	827	CLA	C6-C7-C8-C10
16	A	828	CLA	C6-C7-C8-C10
16	A	829	CLA	C6-C7-C8-C10
16	A	834	CLA	C6-C7-C8-C10
16	A	855	CLA	C6-C7-C8-C10
16	B	802	CLA	C6-C7-C8-C10
16	B	805	CLA	C11-C12-C13-C15
16	B	807	CLA	C11-C12-C13-C15
16	B	808	CLA	C6-C7-C8-C10
16	B	814	CLA	C11-C12-C13-C15
16	B	816	CLA	C6-C7-C8-C10
16	B	820	CLA	C11-C10-C8-C7
16	B	823	CLA	C11-C12-C13-C15
16	B	830	CLA	C11-C10-C8-C7
16	B	837	CLA	C11-C10-C8-C7
16	F	201	CLA	C6-C7-C8-C10
16	F	201	CLA	C11-C10-C8-C7
16	I	102	CLA	C11-C10-C8-C7
16	I	102	CLA	C12-C13-C15-C16
16	O	203	CLA	C2-C3-C5-C6
26	A	801	CL0	C6-C7-C8-C10
26	A	801	CL0	C11-C10-C8-C7
27	B	839	PQN	C16-C17-C18-C20
31	B	846	DGD	CAA-CBA-CCA-CDA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	1	601	CLA	C11-C10-C8-C9
16	2	605	CLA	C11-C10-C8-C9
16	2	608	CLA	C6-C7-C8-C9
16	2	609	CLA	C6-C7-C8-C9
16	A	802	CLA	C6-C7-C8-C9
16	A	802	CLA	C11-C12-C13-C14
16	A	803	CLA	C6-C7-C8-C9
16	A	804	CLA	C11-C10-C8-C9
16	A	814	CLA	C6-C7-C8-C9
16	A	818	CLA	C6-C7-C8-C9
16	A	819	CLA	C11-C12-C13-C14
16	A	823	CLA	C6-C7-C8-C9
16	A	825	CLA	C11-C10-C8-C9
16	A	827	CLA	C6-C7-C8-C9
16	A	831	CLA	C6-C7-C8-C9
16	B	807	CLA	C11-C12-C13-C14
16	B	823	CLA	C11-C10-C8-C9
16	B	823	CLA	C11-C12-C13-C14
16	B	830	CLA	C11-C10-C8-C9
16	B	837	CLA	C11-C10-C8-C9
16	F	201	CLA	C11-C10-C8-C9
16	I	102	CLA	C14-C13-C15-C16
26	A	801	CL0	C6-C7-C8-C9
26	A	801	CL0	C11-C10-C8-C9
27	A	840	PQN	C19-C18-C20-C21
27	B	839	PQN	C16-C17-C18-C19
27	B	839	PQN	C19-C18-C20-C21
19	1	617	LHG	C31-C32-C33-C34
16	1	606	CLA	CBA-CGA-O2A-C1
16	A	836	CLA	CBA-CGA-O2A-C1
19	3	219	LHG	C24-C23-O8-C6
16	A	836	CLA	C15-C16-C17-C18
16	1	606	CLA	C2A-CAA-CBA-CGA
16	3	204	CLA	C2A-CAA-CBA-CGA
23	J	101	DGA	CEB-CFB-CGB-CHB
16	2	606	CLA	O1A-CGA-O2A-C1
18	2	616	RRX	C37-C22-C23-C24
21	B	843	BCR	C11-C12-C13-C35
20	2	618	ERG	C21-C20-C22-C23
18	2	616	RRX	C21-C22-C23-C24
18	2	616	RRX	C7-C8-C9-C10
16	B	818	CLA	C15-C16-C17-C18

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	1	617	LHG	C9-C10-C11-C12
16	A	817	CLA	CBA-CGA-O2A-C1
16	B	822	CLA	CBA-CGA-O2A-C1
26	A	801	CL0	CBA-CGA-O2A-C1
16	2	613	CLA	C10-C11-C12-C13
16	B	812	CLA	C15-C16-C17-C18
26	A	801	CL0	C8-C10-C11-C12
29	J	105	3PH	C22-C23-C24-C25
16	B	820	CLA	C16-C17-C18-C19
22	B	848	PGT	O11-C11-O3-C3
16	A	854	CLA	C13-C15-C16-C17
22	2	619	PGT	O3P-C1-C2-C3
25	L	208	PTY	C12-C13-C14-C15
16	B	826	CLA	CAA-CBA-CGA-O2A
29	B	854	3PH	C2C-C2D-C2E-C2F
29	B	854	3PH	C3E-C3F-C3G-C3H
16	K	102	CLA	O1D-CGD-O2D-CED
16	2	610	CLA	C5-C6-C7-C8
16	1	602	CLA	O1A-CGA-O2A-C1
16	I	102	CLA	O1D-CGD-O2D-CED
16	A	833	CLA	C16-C17-C18-C19
26	A	801	CL0	C16-C17-C18-C20
25	A	852	PTY	C11-C12-C13-C14
19	1	617	LHG	C2-C3-O3-P
16	2	605	CLA	C3A-C2A-CAA-CBA
16	3	209	CLA	C3A-C2A-CAA-CBA
16	A	812	CLA	C3A-C2A-CAA-CBA
16	A	830	CLA	C3A-C2A-CAA-CBA
16	B	814	CLA	C3A-C2A-CAA-CBA
16	F	202	CLA	C3A-C2A-CAA-CBA
16	A	856	CLA	C8-C10-C11-C12
19	A	842	LHG	C18-C19-C20-C21
16	B	812	CLA	CBA-CGA-O2A-C1
16	F	205	CLA	CBA-CGA-O2A-C1
19	1	617	LHG	C18-C19-C20-C21
16	2	602	CLA	C5-C6-C7-C8
16	B	803	CLA	C10-C11-C12-C13
16	L	203	CLA	C13-C15-C16-C17
19	B	851	LHG	C4-C5-C6-O8
23	2	620	DGA	CA9-CAA-CBA-CCA
19	1	617	LHG	C23-C24-C25-C26
16	1	607	CLA	O2A-C1-C2-C3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	1	609	CLA	C2C-C3C-CAC-CBC
16	B	820	CLA	C3-C5-C6-C7
27	B	839	PQN	C20-C21-C22-C23
16	A	833	CLA	C16-C17-C18-C20
16	2	612	CLA	C4C-C3C-CAC-CBC
16	A	830	CLA	C15-C16-C17-C18
16	I	102	CLA	C8-C10-C11-C12
30	A	851	T7X	C16-C17-C18-C19
16	B	822	CLA	O1A-CGA-O2A-C1
25	A	852	PTY	O30-C30-O4-C1
16	A	826	CLA	C3-C5-C6-C7
16	K	102	CLA	C3-C5-C6-C7
16	B	804	CLA	C2A-CAA-CBA-CGA
16	I	102	CLA	C2A-CAA-CBA-CGA
16	A	854	CLA	C5-C6-C7-C8
19	1	617	LHG	O6-C4-C5-O7
22	2	619	PGT	O3P-C1-C2-O2
16	1	606	CLA	O1A-CGA-O2A-C1
16	A	804	CLA	C16-C17-C18-C20
16	B	812	CLA	CAA-CBA-CGA-O2A
19	A	842	LHG	C33-C34-C35-C36
16	A	836	CLA	O1A-CGA-O2A-C1
19	1	617	LHG	O7-C5-C6-O8
19	A	841	LHG	O7-C5-C6-O8
31	B	849	DGD	O2G-C2G-C3G-O3G
16	A	815	CLA	CAA-CBA-CGA-O2A
19	2	622	LHG	C35-C36-C37-C38
19	B	851	LHG	C29-C30-C31-C32
17	1	612	C7Z	C29-C30-C31-C32
16	F	202	CLA	C16-C17-C18-C20
16	2	604	CLA	C15-C16-C17-C18
16	A	811	CLA	C5-C6-C7-C8
16	1	601	CLA	C2-C1-O2A-CGA
16	A	812	CLA	C2-C1-O2A-CGA
16	1	605	CLA	C11-C10-C8-C9
16	1	610	CLA	C6-C7-C8-C9
16	2	611	CLA	C11-C10-C8-C9
16	2	612	CLA	C11-C12-C13-C14
16	A	810	CLA	C6-C7-C8-C9
16	A	813	CLA	C11-C12-C13-C14
16	A	832	CLA	C6-C7-C8-C9
16	B	805	CLA	C11-C12-C13-C14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	820	CLA	C11-C10-C8-C9
16	B	820	CLA	C11-C12-C13-C14
16	I	101	CLA	C11-C12-C13-C14
16	J	102	CLA	C6-C7-C8-C9
16	K	101	CLA	C11-C10-C8-C9
16	K	102	CLA	C11-C10-C8-C9
16	B	833	CLA	CBD-CGD-O2D-CED
16	2	607	CLA	C8-C10-C11-C12
16	3	203	CLA	C15-C16-C17-C18
16	B	833	CLA	C13-C15-C16-C17
25	L	208	PTY	C6-C5-O14-P1
26	A	801	CL0	O1A-CGA-O2A-C1
16	A	855	CLA	C2A-CAA-CBA-CGA
16	3	207	CLA	C8-C10-C11-C12
19	A	841	LHG	C19-C20-C21-C22
16	B	834	CLA	CAA-CBA-CGA-O2A
18	2	616	RRX	C7-C8-C9-C34
29	J	105	3PH	C36-C37-C38-C39
17	A	843	C7Z	C27-C28-C29-C30
18	K	103	RRX	C11-C12-C13-C14
21	L	202	BCR	C11-C12-C13-C14
25	3	220	PTY	C41-C42-C43-C44
24	3	202	LMU	C9-C10-C11-C12
25	L	208	PTY	C39-C40-C41-C42
16	A	817	CLA	O1A-CGA-O2A-C1
16	A	819	CLA	C16-C17-C18-C20
16	A	813	CLA	CBD-CGD-O2D-CED
27	A	840	PQN	C18-C20-C21-C22
25	3	221	PTY	C36-C37-C38-C39
19	2	622	LHG	O6-C4-C5-C6
25	3	221	PTY	O14-C5-C6-C1
29	B	854	3PH	O11-C1-C2-C3
29	J	105	3PH	O11-C1-C2-C3
16	3	205	CLA	CAA-CBA-CGA-O2A
16	1	601	CLA	C11-C10-C8-C7
16	1	604	CLA	C6-C7-C8-C10
16	2	601	CLA	C11-C12-C13-C15
16	2	605	CLA	C12-C13-C15-C16
16	2	606	CLA	C11-C12-C13-C15
16	2	610	CLA	C11-C10-C8-C7
16	2	611	CLA	C11-C10-C8-C7
16	3	208	CLA	C11-C10-C8-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	808	CLA	C11-C12-C13-C15
16	A	813	CLA	C11-C12-C13-C15
16	A	814	CLA	C11-C10-C8-C7
16	A	817	CLA	C6-C7-C8-C10
16	A	817	CLA	C11-C10-C8-C7
16	A	824	CLA	C11-C10-C8-C7
16	A	825	CLA	C11-C10-C8-C7
16	A	825	CLA	C11-C12-C13-C15
16	A	831	CLA	C6-C7-C8-C10
16	A	835	CLA	C11-C12-C13-C15
16	A	839	CLA	C6-C7-C8-C10
16	A	856	CLA	C11-C12-C13-C15
16	B	801	CLA	C11-C10-C8-C7
16	B	803	CLA	C11-C12-C13-C15
16	B	809	CLA	C6-C7-C8-C10
16	B	812	CLA	C6-C7-C8-C10
16	B	819	CLA	C12-C13-C15-C16
16	B	821	CLA	C6-C7-C8-C10
16	B	829	CLA	C11-C12-C13-C15
16	B	836	CLA	C6-C7-C8-C10
16	F	204	CLA	C6-C7-C8-C10
16	I	101	CLA	C11-C12-C13-C15
16	J	102	CLA	C6-C7-C8-C10
16	K	102	CLA	C11-C10-C8-C7
16	K	102	CLA	C11-C12-C13-C15
16	L	201	CLA	C12-C13-C15-C16
16	L	204	CLA	C11-C12-C13-C15
27	A	840	PQN	C17-C18-C20-C21
27	B	839	PQN	C17-C18-C20-C21
23	J	101	DGA	CA9-CAA-CBA-CCA
16	B	832	CLA	C5-C6-C7-C8
18	1	613	RRX	C9-C10-C11-C12
21	K	104	BCR	C15-C16-C17-C18
21	L	202	BCR	C9-C10-C11-C12
16	B	820	CLA	C16-C17-C18-C20
19	2	622	LHG	C26-C27-C28-C29
21	F	206	BCR	C11-C10-C9-C34
31	B	850	DGD	C3B-C4B-C5B-C6B
16	3	203	CLA	C2C-C3C-CAC-CBC
16	1	606	CLA	C10-C11-C12-C13
16	B	811	CLA	C8-C10-C11-C12
16	B	825	CLA	C8-C10-C11-C12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	2	602	CLA	CAD-CBD-CGD-O2D
16	2	613	CLA	CAD-CBD-CGD-O2D
16	3	203	CLA	CAD-CBD-CGD-O2D
16	3	213	CLA	CAD-CBD-CGD-O2D
16	B	820	CLA	CAD-CBD-CGD-O2D
16	B	838	CLA	CAD-CBD-CGD-O2D
16	K	101	CLA	CAD-CBD-CGD-O2D
16	K	102	CLA	CAD-CBD-CGD-O2D
16	L	205	CLA	CAD-CBD-CGD-O2D
16	A	819	CLA	C13-C15-C16-C17
16	A	831	CLA	C4-C3-C5-C6
19	B	851	LHG	C31-C32-C33-C34
22	2	619	PGT	C35-C36-C37-C38
19	1	617	LHG	C35-C36-C37-C38
19	A	841	LHG	C4-C5-C6-O8
22	B	848	PGT	C5-C4-O4P-P
25	A	852	PTY	C6-C5-O14-P1
16	F	205	CLA	O1A-CGA-O2A-C1
19	A	841	LHG	O6-C4-C5-O7
19	B	851	LHG	O6-C4-C5-O7
22	B	848	PGT	O3P-C1-C2-O2
16	B	832	CLA	C8-C10-C11-C12
16	B	828	CLA	C3-C5-C6-C7
16	A	814	CLA	C10-C11-C12-C13
16	F	202	CLA	C16-C17-C18-C19
31	B	849	DGD	C2A-C3A-C4A-C5A
16	2	604	CLA	CHA-CBD-CGD-O1D
16	2	608	CLA	CHA-CBD-CGD-O1D
16	2	608	CLA	CHA-CBD-CGD-O2D
16	2	612	CLA	CHA-CBD-CGD-O1D
16	2	612	CLA	CHA-CBD-CGD-O2D
16	3	206	CLA	CHA-CBD-CGD-O1D
16	3	206	CLA	CHA-CBD-CGD-O2D
16	3	214	CLA	CHA-CBD-CGD-O1D
16	A	807	CLA	CHA-CBD-CGD-O1D
16	A	807	CLA	CHA-CBD-CGD-O2D
16	A	809	CLA	CHA-CBD-CGD-O2D
16	A	810	CLA	CHA-CBD-CGD-O1D
16	A	810	CLA	CHA-CBD-CGD-O2D
16	A	812	CLA	CHA-CBD-CGD-O1D
16	A	812	CLA	CHA-CBD-CGD-O2D
16	A	826	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	826	CLA	CHA-CBD-CGD-O2D
16	A	827	CLA	CHA-CBD-CGD-O2D
16	A	830	CLA	CHA-CBD-CGD-O1D
16	A	839	CLA	CHA-CBD-CGD-O1D
16	A	856	CLA	CHA-CBD-CGD-O1D
16	B	804	CLA	CHA-CBD-CGD-O1D
16	B	804	CLA	CHA-CBD-CGD-O2D
16	B	805	CLA	CHA-CBD-CGD-O1D
16	B	805	CLA	CHA-CBD-CGD-O2D
16	B	812	CLA	CHA-CBD-CGD-O1D
16	B	812	CLA	CHA-CBD-CGD-O2D
16	L	203	CLA	CHA-CBD-CGD-O1D
16	B	802	CLA	C8-C10-C11-C12
16	2	603	CLA	C3-C5-C6-C7
16	A	804	CLA	C3-C5-C6-C7
16	B	812	CLA	O1A-CGA-O2A-C1
19	3	219	LHG	O10-C23-O8-C6
25	3	221	PTY	C39-C40-C41-C42
19	3	219	LHG	C10-C11-C12-C13
25	L	208	PTY	O4-C1-C6-O7
31	B	846	DGD	O2G-C2G-C3G-O3G
19	2	622	LHG	C15-C16-C17-C18
29	A	849	3PH	C39-C3A-C3B-C3C
19	3	219	LHG	O1-C1-C2-O2
16	B	831	CLA	C3-C5-C6-C7
16	B	827	CLA	C4-C3-C5-C6
25	L	208	PTY	C24-C25-C26-C27
16	1	601	CLA	C8-C10-C11-C12
16	2	601	CLA	C11-C12-C13-C14
16	2	608	CLA	C11-C10-C8-C9
16	A	817	CLA	C6-C7-C8-C9
16	A	824	CLA	C11-C12-C13-C14
16	A	826	CLA	C14-C13-C15-C16
16	B	801	CLA	C11-C10-C8-C9
16	B	803	CLA	C11-C12-C13-C14
16	B	812	CLA	C6-C7-C8-C9
16	B	812	CLA	C11-C12-C13-C14
16	B	814	CLA	C6-C7-C8-C9
16	B	816	CLA	C11-C10-C8-C9
16	L	204	CLA	C11-C12-C13-C14
16	A	813	CLA	O1D-CGD-O2D-CED
16	1	602	CLA	C11-C12-C13-C14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	A	801	CL0	CBD-CGD-O2D-CED
17	3	201	C7Z	C11-C12-C13-C20
21	A	844	BCR	C36-C18-C19-C20
24	3	202	LMU	C5'-C4'-O1B-C1B
25	L	208	PTY	C32-C33-C34-C35
19	2	622	LHG	C12-C13-C14-C15
25	L	208	PTY	C14-C15-C16-C17
17	3	201	C7Z	C11-C12-C13-C14
25	A	852	PTY	C39-C40-C41-C42
16	2	602	CLA	C1A-C2A-CAA-CBA
16	3	208	CLA	C1A-C2A-CAA-CBA
16	A	812	CLA	C1A-C2A-CAA-CBA
16	A	832	CLA	C1A-C2A-CAA-CBA
16	O	203	CLA	C1A-C2A-CAA-CBA
29	B	854	3PH	C21-C22-C23-C24
16	A	805	CLA	C16-C17-C18-C19
16	2	606	CLA	C15-C16-C17-C18
16	F	205	CLA	C8-C10-C11-C12
16	2	608	CLA	C2-C1-O2A-CGA
16	A	830	CLA	C2-C1-O2A-CGA
16	B	809	CLA	C2-C1-O2A-CGA
16	B	831	CLA	C2-C1-O2A-CGA
18	A	847	RRX	C9-C10-C11-C12
16	O	202	CLA	C13-C15-C16-C17
25	3	220	PTY	C5-O14-P1-O11
19	B	851	LHG	C26-C27-C28-C29
16	B	831	CLA	C4-C3-C5-C6
16	A	810	CLA	C3-C5-C6-C7
19	3	219	LHG	C2-C3-O3-P
19	A	842	LHG	C5-C4-O6-P
26	A	801	CL0	O1D-CGD-O2D-CED
24	3	202	LMU	C3'-C4'-O1B-C1B
19	2	622	LHG	C3-O3-P-O4
19	2	622	LHG	C4-O6-P-O4
19	A	841	LHG	C4-O6-P-O4
19	A	842	LHG	C3-O3-P-O5
19	B	851	LHG	C4-O6-P-O4
22	2	619	PGT	C4-O4P-P-O1P
22	B	848	PGT	C1-O3P-P-O1P
22	B	848	PGT	C4-O4P-P-O2P
25	A	852	PTY	C3-O11-P1-O13
25	L	208	PTY	C5-O14-P1-O13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
30	A	851	T7X	C7-O13-P1-O11
16	A	825	CLA	C16-C17-C18-C19
16	A	829	CLA	C16-C17-C18-C20
19	2	622	LHG	C9-C10-C11-C12
19	A	841	LHG	O6-C4-C5-C6
19	1	617	LHG	C26-C27-C28-C29
16	A	817	CLA	C15-C16-C17-C18
31	B	849	DGD	C1A-C2A-C3A-C4A
16	A	839	CLA	C2A-CAA-CBA-CGA
16	B	807	CLA	C3-C5-C6-C7
20	1	618	ERG	C16-C17-C20-C21
16	A	812	CLA	CAD-CBD-CGD-O1D
16	B	812	CLA	CAD-CBD-CGD-O1D
25	A	852	PTY	C2-C3-O11-P1
16	1	609	CLA	C4C-C3C-CAC-CBC
19	A	841	LHG	C27-C28-C29-C30
29	B	854	3PH	C25-C26-C27-C28
16	2	602	CLA	C16-C17-C18-C20
16	1	608	CLA	C11-C10-C8-C7
16	2	602	CLA	C11-C12-C13-C15
16	2	608	CLA	C11-C12-C13-C15
16	3	211	CLA	C11-C12-C13-C15
16	A	806	CLA	C11-C12-C13-C15
16	A	808	CLA	C11-C10-C8-C7
16	A	817	CLA	C11-C12-C13-C15
16	A	826	CLA	C11-C10-C8-C7
16	A	830	CLA	C11-C12-C13-C15
16	A	835	CLA	C11-C10-C8-C7
16	A	837	CLA	C11-C10-C8-C7
16	A	837	CLA	C12-C13-C15-C16
16	A	854	CLA	C11-C10-C8-C7
16	B	801	CLA	C6-C7-C8-C10
16	B	806	CLA	C11-C12-C13-C15
16	B	810	CLA	C11-C12-C13-C15
16	B	814	CLA	C6-C7-C8-C10
16	B	816	CLA	C11-C10-C8-C7
16	B	818	CLA	C11-C10-C8-C7
16	B	819	CLA	C3A-C2A-CAA-CBA
16	B	825	CLA	C11-C12-C13-C15
16	B	830	CLA	C11-C12-C13-C15
16	B	832	CLA	C6-C7-C8-C10
16	B	838	CLA	C6-C7-C8-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	F	201	CLA	C11-C12-C13-C15
16	F	205	CLA	C6-C7-C8-C10
19	2	622	LHG	O6-C4-C5-O7
25	3	221	PTY	O14-C5-C6-O7
29	J	105	3PH	O11-C1-C2-O21
31	B	846	DGD	O6E-C5E-C6E-O5E
29	B	854	3PH	C32-C33-C34-C35
31	B	846	DGD	C7A-C8A-C9A-CAA
29	J	105	3PH	C3A-C3B-C3C-C3D
22	2	619	PGT	O2-C2-C3-O3
19	3	219	LHG	C24-C25-C26-C27
29	B	854	3PH	C2B-C2C-C2D-C2E
20	2	618	ERG	C17-C20-C22-C23
16	A	835	CLA	C5-C6-C7-C8
19	3	219	LHG	C35-C36-C37-C38
16	3	210	CLA	C10-C11-C12-C13
16	1	607	CLA	C11-C10-C8-C9
16	2	605	CLA	C14-C13-C15-C16
16	2	606	CLA	C6-C7-C8-C9
16	3	206	CLA	C6-C7-C8-C9
16	A	814	CLA	C11-C12-C13-C14
16	A	824	CLA	C11-C10-C8-C9
16	A	825	CLA	C11-C12-C13-C14
16	A	835	CLA	C11-C12-C13-C14
16	A	856	CLA	C11-C12-C13-C14
16	B	819	CLA	C14-C13-C15-C16
16	B	827	CLA	C6-C7-C8-C9
16	F	204	CLA	C6-C7-C8-C9
16	K	101	CLA	C6-C7-C8-C9
16	L	201	CLA	C14-C13-C15-C16
16	A	805	CLA	C16-C17-C18-C20
16	A	819	CLA	C16-C17-C18-C19
16	A	834	CLA	C16-C17-C18-C19
29	B	854	3PH	C22-C23-C24-C25
29	J	105	3PH	C26-C27-C28-C29
18	1	613	RRX	C18-C19-C20-C21
18	1	613	RRX	C10-C11-C12-C13
18	A	847	RRX	C18-C19-C20-C21
18	A	847	RRX	C10-C11-C12-C13
18	K	103	RRX	C18-C19-C20-C21
18	K	103	RRX	C10-C11-C12-C13
21	2	617	BCR	C18-C19-C20-C21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	A	857	BCR	C18-C19-C20-C21
21	B	847	BCR	C18-C19-C20-C21
21	B	855	BCR	C18-C19-C20-C21
21	K	104	BCR	C18-C19-C20-C21
16	2	602	CLA	C8-C10-C11-C12
16	3	208	CLA	C5-C6-C7-C8
16	A	806	CLA	C13-C15-C16-C17
19	A	842	LHG	C15-C16-C17-C18
19	3	219	LHG	O2-C2-C3-O3
16	A	831	CLA	C2-C3-C5-C6
16	B	827	CLA	C2-C3-C5-C6
16	3	207	CLA	C3-C5-C6-C7
25	3	220	PTY	C12-C11-C8-O7
25	3	221	PTY	C37-C38-C39-C40
16	B	826	CLA	C2A-CAA-CBA-CGA
16	1	610	CLA	C2-C1-O2A-CGA
16	A	818	CLA	C2-C1-O2A-CGA
16	A	832	CLA	C2-C1-O2A-CGA
16	B	813	CLA	C2-C1-O2A-CGA
16	F	204	CLA	C2-C1-O2A-CGA
16	K	101	CLA	C2-C1-O2A-CGA
16	K	102	CLA	C2-C1-O2A-CGA
19	1	617	LHG	C19-C20-C21-C22
19	A	842	LHG	C35-C36-C37-C38
29	J	105	3PH	C1-O11-P-O12
29	B	854	3PH	C2D-C2E-C2F-C2G
19	3	219	LHG	O6-C4-C5-O7
29	B	854	3PH	O11-C1-C2-O21
16	A	855	CLA	C16-C17-C18-C20
16	2	611	CLA	C8-C10-C11-C12
20	1	618	ERG	C20-C22-C23-C24
17	3	216	C7Z	C21-C26-C27-C28
16	B	831	CLA	C2-C3-C5-C6
19	3	219	LHG	C34-C35-C36-C37
16	A	829	CLA	C15-C16-C17-C18
16	L	204	CLA	C5-C6-C7-C8
16	B	834	CLA	C10-C11-C12-C13
16	B	811	CLA	C2A-CAA-CBA-CGA
21	2	617	BCR	C16-C17-C18-C19
21	F	206	BCR	C11-C10-C9-C8
25	3	220	PTY	C20-C21-C22-C23
19	3	219	LHG	C4-O6-P-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	A	841	LHG	C3-O3-P-O6
19	B	851	LHG	C3-O3-P-O6
25	A	852	PTY	C5-O14-P1-O11
25	L	208	PTY	C3-O11-P1-O14
25	A	852	PTY	C34-C35-C36-C37
22	2	619	PGT	C1-C2-C3-O3
19	3	219	LHG	C26-C27-C28-C29
16	1	611	CLA	C6-C7-C8-C10
16	2	608	CLA	C6-C7-C8-C10
16	2	612	CLA	C11-C12-C13-C15
16	3	206	CLA	C6-C7-C8-C10
16	A	809	CLA	C11-C10-C8-C7
16	B	812	CLA	C11-C12-C13-C15
16	B	812	CLA	C12-C13-C15-C16
16	K	101	CLA	C11-C10-C8-C7
19	3	219	LHG	C30-C31-C32-C33
22	B	848	PGT	O2-C31-C32-C33
16	1	609	CLA	C6-C7-C8-C9
16	2	602	CLA	C11-C10-C8-C9
16	2	602	CLA	C11-C12-C13-C14
16	A	805	CLA	C11-C12-C13-C14
16	A	829	CLA	C6-C7-C8-C9
16	A	834	CLA	C6-C7-C8-C9
16	B	801	CLA	C6-C7-C8-C9
16	B	804	CLA	C11-C12-C13-C14
16	B	806	CLA	C11-C12-C13-C14
16	B	814	CLA	C11-C12-C13-C14
16	B	824	CLA	C14-C13-C15-C16
16	B	825	CLA	C11-C12-C13-C14
16	B	829	CLA	C11-C12-C13-C14
16	B	830	CLA	C11-C12-C13-C14
21	B	845	BCR	C9-C10-C11-C12
21	K	104	BCR	C9-C10-C11-C12
16	A	825	CLA	C16-C17-C18-C20
16	A	832	CLA	C16-C17-C18-C19
16	B	833	CLA	O1D-CGD-O2D-CED
16	B	838	CLA	O1A-CGA-O2A-C1
16	A	829	CLA	C16-C17-C18-C19
16	B	807	CLA	C16-C17-C18-C20
16	O	203	CLA	C16-C17-C18-C20
29	B	854	3PH	C28-C29-C2A-C2B
19	A	841	LHG	C2-C3-O3-P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	A	842	LHG	C2-C3-O3-P
16	1	603	CLA	C10-C11-C12-C13
21	K	104	BCR	C7-C8-C9-C10
19	A	841	LHG	C13-C14-C15-C16
16	B	834	CLA	O1A-CGA-O2A-C1
16	A	822	CLA	C16-C17-C18-C19
16	B	834	CLA	CBA-CGA-O2A-C1
16	A	809	CLA	C2C-C3C-CAC-CBC
19	1	617	LHG	C11-C12-C13-C14
19	A	841	LHG	C10-C11-C12-C13
16	B	834	CLA	C15-C16-C17-C18
16	2	605	CLA	O1A-CGA-O2A-C1
16	2	605	CLA	CBA-CGA-O2A-C1
16	3	205	CLA	C2A-CAA-CBA-CGA
17	3	215	C7Z	C29-C30-C31-C32
18	2	616	RRX	C19-C20-C21-C22
18	A	847	RRX	C13-C14-C15-C16
19	2	622	LHG	C17-C18-C19-C20
16	B	827	CLA	C8-C10-C11-C12
21	L	202	BCR	C10-C11-C12-C13
20	2	618	ERG	C13-C17-C20-C21
20	2	618	ERG	C13-C17-C20-C22
22	2	619	PGT	C33-C34-C35-C36
16	B	824	CLA	C16-C17-C18-C20
16	B	805	CLA	C3-C5-C6-C7
29	A	849	3PH	C2D-C2E-C2F-C2G
16	F	202	CLA	C13-C15-C16-C17
16	A	816	CLA	CBD-CGD-O2D-CED
30	A	851	T7X	C43-C44-C45-C46
16	A	818	CLA	C2-C3-C5-C6
16	B	814	CLA	C5-C6-C7-C8
16	B	828	CLA	C8-C10-C11-C12
16	O	204	CLA	C15-C16-C17-C18
16	B	804	CLA	CAA-CBA-CGA-O2A
16	1	605	CLA	C2-C1-O2A-CGA
16	3	204	CLA	C2-C1-O2A-CGA
16	B	805	CLA	C2-C1-O2A-CGA
16	B	824	CLA	C2-C1-O2A-CGA
16	2	602	CLA	C16-C17-C18-C19
16	K	102	CLA	C5-C6-C7-C8
16	A	807	CLA	C2A-CAA-CBA-CGA
29	A	849	3PH	O21-C2-C3-O31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
31	B	846	DGD	O1G-C1G-C2G-O2G
24	3	202	LMU	C3-C4-C5-C6
16	3	205	CLA	C3A-C2A-CAA-CBA
16	B	812	CLA	C3A-C2A-CAA-CBA
16	3	205	CLA	C11-C12-C13-C14
16	3	214	CLA	C6-C7-C8-C9
16	A	816	CLA	C11-C10-C8-C9
16	A	819	CLA	C6-C7-C8-C9
16	A	839	CLA	C11-C12-C13-C14
16	B	802	CLA	C14-C13-C15-C16
16	B	832	CLA	C11-C12-C13-C14
16	B	835	CLA	C11-C12-C13-C14
16	O	204	CLA	C6-C7-C8-C9
17	1	612	C7Z	C40-C33-C34-C35
17	1	615	C7Z	C11-C10-C9-C19
17	1	616	C7Z	C40-C33-C34-C35
17	2	615	C7Z	C20-C13-C14-C15
17	3	201	C7Z	C20-C13-C14-C15
17	3	216	C7Z	C20-C13-C14-C15
18	1	613	RRX	C20-C21-C22-C37
18	1	613	RRX	C16-C17-C18-C36
18	1	613	RRX	C35-C13-C14-C15
18	2	616	RRX	C16-C17-C18-C36
18	A	847	RRX	C20-C21-C22-C37
18	A	847	RRX	C35-C13-C14-C15
18	J	103	RRX	C35-C13-C14-C15
18	K	103	RRX	C20-C21-C22-C37
18	K	103	RRX	C35-C13-C14-C15
18	K	103	RRX	C11-C10-C9-C34
19	1	617	LHG	C4-C5-C6-O8
21	2	617	BCR	C16-C17-C18-C36
21	2	617	BCR	C20-C21-C22-C37
21	A	850	BCR	C16-C17-C18-C36
21	B	842	BCR	C35-C13-C14-C15
21	B	842	BCR	C20-C21-C22-C37
21	B	843	BCR	C16-C17-C18-C36
21	B	845	BCR	C35-C13-C14-C15
21	B	845	BCR	C16-C17-C18-C36
21	B	847	BCR	C35-C13-C14-C15
21	B	847	BCR	C16-C17-C18-C36
21	B	855	BCR	C16-C17-C18-C36
21	F	206	BCR	C35-C13-C14-C15

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	K	104	BCR	C35-C13-C14-C15
21	O	205	BCR	C16-C17-C18-C36
16	K	101	CLA	C2A-CAA-CBA-CGA
16	A	817	CLA	C13-C15-C16-C17
16	A	834	CLA	C16-C17-C18-C20
16	A	815	CLA	O2A-C1-C2-C3
21	K	104	BCR	C36-C18-C19-C20
25	L	208	PTY	C19-C20-C21-C22
30	A	851	T7X	C34-C35-C36-C37
25	3	221	PTY	C1-C6-O7-C8
16	1	609	CLA	C5-C6-C7-C8
16	B	805	CLA	C15-C16-C17-C18
16	A	818	CLA	C4-C3-C5-C6
16	2	605	CLA	C1A-C2A-CAA-CBA
16	2	613	CLA	C1A-C2A-CAA-CBA
16	B	811	CLA	C1A-C2A-CAA-CBA
16	B	812	CLA	C1A-C2A-CAA-CBA
16	B	825	CLA	C1A-C2A-CAA-CBA
16	F	205	CLA	C1A-C2A-CAA-CBA
19	3	219	LHG	C19-C20-C21-C22
16	1	603	CLA	C6-C7-C8-C10
16	1	606	CLA	C12-C13-C15-C16
16	2	609	CLA	C11-C12-C13-C15
16	3	209	CLA	C11-C12-C13-C15
16	3	210	CLA	C11-C10-C8-C7
16	3	211	CLA	C6-C7-C8-C10
16	A	804	CLA	C11-C10-C8-C7
16	A	811	CLA	C6-C7-C8-C10
16	A	826	CLA	C11-C12-C13-C15
16	A	835	CLA	C6-C7-C8-C10
16	A	837	CLA	C6-C7-C8-C10
16	B	804	CLA	C11-C12-C13-C15
16	B	807	CLA	C11-C10-C8-C7
16	B	819	CLA	C6-C7-C8-C10
16	B	822	CLA	C12-C13-C15-C16
16	B	823	CLA	C11-C10-C8-C7
16	B	823	CLA	C12-C13-C15-C16
16	B	824	CLA	C11-C10-C8-C7
16	B	826	CLA	C11-C12-C13-C15
16	B	831	CLA	C11-C10-C8-C7
16	F	205	CLA	C11-C12-C13-C15
16	J	102	CLA	C11-C12-C13-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	1	611	CLA	C10-C11-C12-C13
16	B	824	CLA	C13-C15-C16-C17
18	1	613	RRX	C13-C14-C15-C16
30	A	851	T7X	C18-C19-C20-C21
29	J	105	3PH	C2B-C2C-C2D-C2E
16	1	604	CLA	C2A-CAA-CBA-CGA
16	1	609	CLA	C2A-CAA-CBA-CGA
16	A	837	CLA	C2A-CAA-CBA-CGA
16	F	201	CLA	C2A-CAA-CBA-CGA
16	A	804	CLA	C13-C15-C16-C17
16	A	832	CLA	C5-C6-C7-C8
16	B	809	CLA	C10-C11-C12-C13
16	A	813	CLA	C15-C16-C17-C18
16	B	838	CLA	CBA-CGA-O2A-C1
25	3	220	PTY	C33-C34-C35-C36
24	3	202	LMU	C2B-C1B-O1B-C4'
16	A	830	CLA	C13-C15-C16-C17
16	B	828	CLA	C5-C6-C7-C8
17	1	612	C7Z	C32-C33-C34-C35
17	1	615	C7Z	C11-C10-C9-C8
17	1	616	C7Z	C32-C33-C34-C35
17	2	615	C7Z	C12-C13-C14-C15
17	3	201	C7Z	C12-C13-C14-C15
17	3	216	C7Z	C12-C13-C14-C15
18	1	613	RRX	C20-C21-C22-C23
18	1	613	RRX	C16-C17-C18-C19
18	1	613	RRX	C12-C13-C14-C15
18	2	616	RRX	C16-C17-C18-C19
18	A	847	RRX	C20-C21-C22-C23
18	A	847	RRX	C12-C13-C14-C15
18	J	103	RRX	C12-C13-C14-C15
18	K	103	RRX	C20-C21-C22-C23
18	K	103	RRX	C12-C13-C14-C15
18	K	103	RRX	C11-C10-C9-C8
21	2	617	BCR	C20-C21-C22-C23
21	A	850	BCR	C16-C17-C18-C19
21	B	842	BCR	C12-C13-C14-C15
21	B	842	BCR	C20-C21-C22-C23
21	B	843	BCR	C16-C17-C18-C19
21	B	845	BCR	C12-C13-C14-C15
21	B	845	BCR	C16-C17-C18-C19
21	B	847	BCR	C12-C13-C14-C15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	B	847	BCR	C16-C17-C18-C19
21	F	206	BCR	C12-C13-C14-C15
21	K	104	BCR	C12-C13-C14-C15
21	O	205	BCR	C16-C17-C18-C19
16	2	605	CLA	C13-C15-C16-C17
17	2	614	C7Z	C9-C10-C11-C12
17	3	217	C7Z	C13-C14-C15-C35
17	3	218	C7Z	C9-C10-C11-C12
18	2	616	RRX	C9-C10-C11-C12
19	2	622	LHG	C34-C35-C36-C37
23	2	620	DGA	CAB-CBB-CCB-CDB
16	A	814	CLA	C5-C6-C7-C8
29	B	854	3PH	C33-C34-C35-C36
16	B	829	CLA	O1D-CGD-O2D-CED
16	A	816	CLA	O1D-CGD-O2D-CED
16	A	819	CLA	C4-C3-C5-C6
16	B	807	CLA	C4-C3-C5-C6
16	B	808	CLA	C4-C3-C5-C6
16	B	824	CLA	C4-C3-C5-C6
16	A	829	CLA	C2-C1-O2A-CGA
16	B	838	CLA	C2-C1-O2A-CGA
16	I	101	CLA	C2-C1-O2A-CGA
16	L	201	CLA	C2-C1-O2A-CGA
26	A	801	CL0	CAA-CBA-CGA-O2A
16	2	608	CLA	C14-C13-C15-C16
16	3	210	CLA	C6-C7-C8-C9
16	B	801	CLA	C14-C13-C15-C16
16	B	805	CLA	C6-C7-C8-C9
16	B	825	CLA	C6-C7-C8-C9
16	L	203	CLA	C6-C7-C8-C9
31	B	846	DGD	O6D-C5D-C6D-O5D
16	F	202	CLA	C4C-C3C-CAC-CBC
16	A	809	CLA	C4C-C3C-CAC-CBC
25	A	852	PTY	C17-C18-C19-C20
16	A	830	CLA	C2A-CAA-CBA-CGA
16	A	803	CLA	C16-C17-C18-C19
17	3	201	C7Z	C21-C26-C27-C28
17	3	218	C7Z	C1-C6-C7-C8
21	A	845	BCR	C23-C24-C25-C30
21	B	844	BCR	C23-C24-C25-C26
16	2	605	CLA	C15-C16-C17-C18
25	L	208	PTY	C31-C32-C33-C34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
25	L	208	PTY	C12-C11-C8-O7
31	B	846	DGD	C1G-C2G-C3G-O3G
16	B	835	CLA	C5-C6-C7-C8
19	3	219	LHG	O1-C1-C2-C3
17	3	201	C7Z	C29-C30-C31-C32
18	K	103	RRX	C13-C14-C15-C16
21	F	203	BCR	C9-C10-C11-C12
16	A	826	CLA	C4-C3-C5-C6
16	B	805	CLA	C4-C3-C5-C6
16	J	102	CLA	C4-C3-C5-C6
16	3	214	CLA	C15-C16-C17-C18
16	A	825	CLA	C10-C11-C12-C13
16	F	205	CLA	C5-C6-C7-C8
19	1	617	LHG	C16-C17-C18-C19
16	B	821	CLA	C16-C17-C18-C20
16	B	834	CLA	C3-C5-C6-C7
16	B	815	CLA	C5-C6-C7-C8
16	O	203	CLA	C8-C10-C11-C12
29	A	849	3PH	O11-C1-C2-O21
16	2	604	CLA	C5-C6-C7-C8
16	B	808	CLA	C8-C10-C11-C12
16	3	206	CLA	C15-C16-C17-C18
19	B	851	LHG	O6-C4-C5-C6
29	A	849	3PH	O11-C1-C2-C3
16	A	813	CLA	C4-C3-C5-C6
16	O	201	CLA	C4-C3-C5-C6
16	2	601	CLA	C6-C7-C8-C10
16	2	608	CLA	C11-C10-C8-C7
16	A	824	CLA	C11-C12-C13-C15
16	B	825	CLA	C6-C7-C8-C10
17	1	614	C7Z	C13-C14-C15-C35
31	B	850	DGD	C5A-C6A-C7A-C8A
25	A	852	PTY	C35-C36-C37-C38
16	B	826	CLA	CAA-CBA-CGA-O1A
16	2	608	CLA	C3-C5-C6-C7
16	B	827	CLA	CAA-CBA-CGA-O2A
16	J	102	CLA	CAA-CBA-CGA-O2A
19	A	841	LHG	C33-C34-C35-C36
16	B	833	CLA	C2A-CAA-CBA-CGA
16	F	205	CLA	C10-C11-C12-C13
16	A	822	CLA	C16-C17-C18-C20
16	3	214	CLA	C10-C11-C12-C13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	828	CLA	CAA-CBA-CGA-O2A
16	B	823	CLA	CAA-CBA-CGA-O2A
16	B	829	CLA	CBD-CGD-O2D-CED
16	2	601	CLA	C4-C3-C5-C6
16	A	805	CLA	C4-C3-C5-C6
16	A	815	CLA	C4-C3-C5-C6
16	A	833	CLA	C4-C3-C5-C6
16	B	812	CLA	C4-C3-C5-C6
16	2	601	CLA	C10-C11-C12-C13
16	A	837	CLA	C8-C10-C11-C12
16	B	836	CLA	C8-C10-C11-C12
25	3	221	PTY	C40-C41-C42-C43
16	B	824	CLA	C16-C17-C18-C19
19	A	841	LHG	O7-C7-C8-C9
19	A	841	LHG	O8-C23-C24-C25
16	1	602	CLA	C11-C10-C8-C9
16	1	608	CLA	C11-C10-C8-C9
16	2	608	CLA	C11-C12-C13-C14
16	3	203	CLA	C6-C7-C8-C9
16	3	209	CLA	C11-C12-C13-C14
16	3	211	CLA	C11-C12-C13-C14
16	A	806	CLA	C11-C12-C13-C14
16	A	808	CLA	C11-C10-C8-C9
16	A	817	CLA	C11-C12-C13-C14
16	A	826	CLA	C11-C10-C8-C9
16	A	830	CLA	C11-C12-C13-C14
16	A	831	CLA	C11-C12-C13-C14
16	A	835	CLA	C11-C10-C8-C9
16	A	837	CLA	C14-C13-C15-C16
16	A	854	CLA	C11-C10-C8-C9
16	A	855	CLA	C14-C13-C15-C16
16	B	809	CLA	C6-C7-C8-C9
16	B	810	CLA	C11-C12-C13-C14
16	B	818	CLA	C11-C10-C8-C9
16	B	823	CLA	C14-C13-C15-C16
16	B	824	CLA	C11-C10-C8-C9
16	B	829	CLA	C6-C7-C8-C9
16	B	838	CLA	C6-C7-C8-C9
16	F	201	CLA	C11-C12-C13-C14
16	J	102	CLA	C11-C12-C13-C14
27	A	840	PQN	C24-C23-C25-C26
16	A	805	CLA	C3-C5-C6-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	B	851	LHG	C15-C16-C17-C18
16	2	601	CLA	C3A-C2A-CAA-CBA
16	B	811	CLA	C3A-C2A-CAA-CBA
16	B	825	CLA	C3A-C2A-CAA-CBA
16	F	205	CLA	C3A-C2A-CAA-CBA
16	2	612	CLA	CAA-CBA-CGA-O2A
16	2	613	CLA	CAA-CBA-CGA-O2A
16	3	208	CLA	CAA-CBA-CGA-O2A
29	A	849	3PH	O21-C21-C22-C23
29	B	854	3PH	C38-C39-C3A-C3B
16	2	604	CLA	CAD-CBD-CGD-O2D
16	2	608	CLA	CAD-CBD-CGD-O2D
16	3	214	CLA	CAD-CBD-CGD-O2D
16	A	805	CLA	CAD-CBD-CGD-O2D
16	A	856	CLA	CAD-CBD-CGD-O2D
16	B	802	CLA	CAD-CBD-CGD-O2D
16	B	813	CLA	CAD-CBD-CGD-O2D
16	B	817	CLA	CAD-CBD-CGD-O2D
16	I	102	CLA	CAD-CBD-CGD-O2D
16	L	204	CLA	CAD-CBD-CGD-O2D
16	A	818	CLA	C15-C16-C17-C18
16	A	829	CLA	C13-C15-C16-C17
16	B	816	CLA	C8-C10-C11-C12
16	A	811	CLA	C2-C1-O2A-CGA
16	2	606	CLA	CAA-CBA-CGA-O2A
16	A	833	CLA	CAA-CBA-CGA-O2A
16	B	811	CLA	CAA-CBA-CGA-O2A
16	K	101	CLA	CAA-CBA-CGA-O2A
16	B	812	CLA	CAA-CBA-CGA-O1A
16	1	607	CLA	C4-C3-C5-C6
16	B	826	CLA	C4-C3-C5-C6
25	A	852	PTY	C30-C31-C32-C33
16	B	826	CLA	C13-C15-C16-C17
16	A	819	CLA	C2-C3-C5-C6
16	B	808	CLA	C2-C3-C5-C6
16	1	607	CLA	CAA-CBA-CGA-O2A
16	2	601	CLA	CAA-CBA-CGA-O2A
16	A	808	CLA	CAA-CBA-CGA-O2A
16	A	822	CLA	CAA-CBA-CGA-O2A
16	B	803	CLA	CAA-CBA-CGA-O2A
25	3	221	PTY	O4-C30-C31-C32
21	A	844	BCR	C17-C18-C19-C20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	A	845	BCR	C21-C22-C23-C24
21	K	104	BCR	C17-C18-C19-C20
21	L	207	BCR	C11-C12-C13-C14
25	L	208	PTY	C37-C38-C39-C40
16	A	837	CLA	C13-C15-C16-C17
16	B	810	CLA	C13-C15-C16-C17
16	2	609	CLA	CAA-CBA-CGA-O2A
16	I	101	CLA	CAA-CBA-CGA-O2A
19	3	219	LHG	O7-C7-C8-C9
19	B	851	LHG	O8-C23-C24-C25
16	2	609	CLA	O2A-C1-C2-C3
16	2	613	CLA	O2A-C1-C2-C3
16	3	211	CLA	O2A-C1-C2-C3
16	A	827	CLA	O2A-C1-C2-C3
16	B	821	CLA	O2A-C1-C2-C3
23	2	620	DGA	CFA-CGA-CHA-CIA
23	2	620	DGA	CFB-CGB-CHB-CIB
16	1	601	CLA	C13-C15-C16-C17
16	3	206	CLA	CAA-CBA-CGA-O2A
16	L	203	CLA	CAA-CBA-CGA-O2A
29	J	105	3PH	O21-C21-C22-C23
16	B	834	CLA	CAA-CBA-CGA-O1A
16	1	605	CLA	CHA-CBD-CGD-O1D
16	1	605	CLA	CHA-CBD-CGD-O2D
16	1	608	CLA	CHA-CBD-CGD-O1D
16	1	608	CLA	CHA-CBD-CGD-O2D
16	2	604	CLA	CHA-CBD-CGD-O2D
16	2	609	CLA	CHA-CBD-CGD-O2D
16	3	207	CLA	CHA-CBD-CGD-O1D
16	3	207	CLA	CHA-CBD-CGD-O2D
16	3	209	CLA	CHA-CBD-CGD-O1D
16	3	209	CLA	CHA-CBD-CGD-O2D
16	3	210	CLA	CHA-CBD-CGD-O1D
16	3	210	CLA	CHA-CBD-CGD-O2D
16	A	813	CLA	CHA-CBD-CGD-O1D
16	A	815	CLA	CHA-CBD-CGD-O1D
16	A	815	CLA	CHA-CBD-CGD-O2D
16	A	819	CLA	CHA-CBD-CGD-O2D
16	A	824	CLA	CHA-CBD-CGD-O1D
16	A	824	CLA	CHA-CBD-CGD-O2D
16	A	830	CLA	CHA-CBD-CGD-O2D
16	A	836	CLA	CHA-CBD-CGD-O1D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	A	836	CLA	CHA-CBD-CGD-O2D
16	A	839	CLA	CHA-CBD-CGD-O2D
16	A	856	CLA	CHA-CBD-CGD-O2D
16	B	806	CLA	CHA-CBD-CGD-O2D
16	B	809	CLA	CHA-CBD-CGD-O2D
16	B	823	CLA	CHA-CBD-CGD-O1D
16	B	823	CLA	CHA-CBD-CGD-O2D
16	B	825	CLA	CHA-CBD-CGD-O2D
16	B	833	CLA	CHA-CBD-CGD-O1D
16	B	833	CLA	CHA-CBD-CGD-O2D
16	F	201	CLA	CHA-CBD-CGD-O1D
16	F	201	CLA	CHA-CBD-CGD-O2D
16	F	205	CLA	CHA-CBD-CGD-O1D
16	F	205	CLA	CHA-CBD-CGD-O2D
16	I	101	CLA	CHA-CBD-CGD-O2D
16	L	203	CLA	CHA-CBD-CGD-O2D
16	O	203	CLA	CHA-CBD-CGD-O1D
16	O	203	CLA	CHA-CBD-CGD-O2D
16	B	835	CLA	CAA-CBA-CGA-O2A
16	B	826	CLA	C2-C3-C5-C6
16	J	102	CLA	C2-C3-C5-C6
16	O	201	CLA	C2-C3-C5-C6
31	B	846	DGD	CDA-CEA-CFA-CGA
21	B	855	BCR	C16-C17-C18-C19
19	A	841	LHG	C11-C10-C9-C8
25	A	852	PTY	C36-C37-C38-C39
16	3	209	CLA	C16-C17-C18-C20
16	3	211	CLA	C16-C17-C18-C19
29	B	854	3PH	O31-C31-C32-C33
16	2	612	CLA	C5-C6-C7-C8
16	A	815	CLA	C15-C16-C17-C18
16	F	204	CLA	C5-C6-C7-C8
19	A	841	LHG	C34-C35-C36-C37
19	1	617	LHG	O8-C23-C24-C25
19	A	842	LHG	O8-C23-C24-C25
16	3	205	CLA	C16-C17-C18-C20
16	F	201	CLA	C8-C10-C11-C12
23	2	620	DGA	CBB-CAB-CB9-CB8
16	1	605	CLA	CAA-CBA-CGA-O2A
16	B	809	CLA	CAA-CBA-CGA-O2A
16	1	607	CLA	C2-C3-C5-C6
16	2	608	CLA	C12-C13-C15-C16

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	2	612	CLA	C11-C10-C8-C7
16	2	613	CLA	C6-C7-C8-C10
16	A	814	CLA	C11-C12-C13-C15
16	B	813	CLA	C11-C10-C8-C7
16	B	829	CLA	C11-C10-C8-C7
16	L	203	CLA	C12-C13-C15-C16
16	B	833	CLA	CAA-CBA-CGA-O2A
16	1	611	CLA	C11-C12-C13-C14
16	A	805	CLA	C11-C10-C8-C9
16	A	808	CLA	C11-C12-C13-C14
16	A	826	CLA	C11-C12-C13-C14
16	A	835	CLA	C6-C7-C8-C9
16	A	856	CLA	C11-C10-C8-C9
16	B	813	CLA	C11-C10-C8-C9
16	B	818	CLA	C14-C13-C15-C16
16	B	822	CLA	C14-C13-C15-C16
16	B	825	CLA	C11-C10-C8-C9
16	B	827	CLA	C11-C12-C13-C14
16	B	831	CLA	C11-C10-C8-C9
16	B	838	CLA	C14-C13-C15-C16
16	F	205	CLA	C11-C12-C13-C14
16	O	202	CLA	C11-C12-C13-C14
29	B	854	3PH	C2A-C2B-C2C-C2D
25	A	852	PTY	C16-C17-C18-C19
25	3	221	PTY	C31-C30-O4-C1
25	3	221	PTY	O30-C30-O4-C1
16	3	209	CLA	C10-C11-C12-C13
16	A	809	CLA	C8-C10-C11-C12
16	A	805	CLA	C2A-CAA-CBA-CGA
16	3	207	CLA	CAA-CBA-CGA-O2A
16	3	209	CLA	CAA-CBA-CGA-O2A
16	A	828	CLA	CAA-CBA-CGA-O1A
16	B	823	CLA	CAA-CBA-CGA-O1A
16	I	101	CLA	CAA-CBA-CGA-O1A
19	A	841	LHG	O9-C7-C8-C9
16	A	854	CLA	C16-C17-C18-C20
16	A	837	CLA	C2-C3-C5-C6
16	3	213	CLA	CAA-CBA-CGA-O2A
18	1	613	RRX	C21-C22-C23-C24
21	B	843	BCR	C11-C12-C13-C14
29	A	849	3PH	C32-C31-O31-C3
16	2	601	CLA	C1A-C2A-CAA-CBA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	3	203	CLA	C1A-C2A-CAA-CBA
16	A	813	CLA	C1A-C2A-CAA-CBA
16	A	837	CLA	C1A-C2A-CAA-CBA
16	B	803	CLA	C1A-C2A-CAA-CBA
16	A	811	CLA	C16-C17-C18-C19
16	A	836	CLA	C16-C17-C18-C19
19	A	841	LHG	O10-C23-C24-C25
29	A	849	3PH	O22-C21-C22-C23
16	1	608	CLA	C2-C1-O2A-CGA
29	A	849	3PH	C2C-C2D-C2E-C2F
16	2	606	CLA	C10-C11-C12-C13
16	2	610	CLA	C13-C15-C16-C17
16	B	821	CLA	C8-C10-C11-C12
16	1	607	CLA	CAA-CBA-CGA-O1A
16	2	601	CLA	CAA-CBA-CGA-O1A
16	3	208	CLA	CAA-CBA-CGA-O1A
19	B	851	LHG	O10-C23-C24-C25
23	J	101	DGA	OG1-CG1-CG2-CG3
25	L	208	PTY	O4-C1-C6-C5
16	A	825	CLA	CAA-CBA-CGA-O2A
16	B	829	CLA	C2A-CAA-CBA-CGA
29	J	105	3PH	C32-C33-C34-C35
16	A	803	CLA	C16-C17-C18-C20
16	2	612	CLA	CAA-CBA-CGA-O1A
16	A	808	CLA	CAA-CBA-CGA-O1A
16	A	833	CLA	CAA-CBA-CGA-O1A
16	B	811	CLA	CAA-CBA-CGA-O1A
16	K	101	CLA	CAA-CBA-CGA-O1A
16	1	609	CLA	C10-C11-C12-C13
16	3	205	CLA	C10-C11-C12-C13
16	3	211	CLA	C10-C11-C12-C13
16	F	202	CLA	C15-C16-C17-C18
16	B	801	CLA	C3-C5-C6-C7
16	1	605	CLA	CAA-CBA-CGA-O1A
16	3	207	CLA	CAA-CBA-CGA-O1A
16	3	209	CLA	CAA-CBA-CGA-O1A
16	B	835	CLA	CAA-CBA-CGA-O1A
25	3	220	PTY	C19-C20-C21-C22
19	A	841	LHG	C3-O3-P-O5
25	3	221	PTY	C5-O14-P1-O13
16	3	206	CLA	CAA-CBA-CGA-O1A
16	A	822	CLA	CAA-CBA-CGA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
19	3	219	LHG	O9-C7-C8-C9
29	B	854	3PH	O32-C31-C32-C33
16	2	608	CLA	CAA-CBA-CGA-O2A
25	L	208	PTY	C36-C37-C38-C39
21	A	850	BCR	C23-C24-C25-C26
21	F	206	BCR	C23-C24-C25-C26
16	L	203	CLA	CAA-CBA-CGA-O1A
19	A	842	LHG	O10-C23-C24-C25
29	J	105	3PH	O22-C21-C22-C23
31	B	846	DGD	CFB-CGB-CHB-CIB
16	A	823	CLA	CAA-CBA-CGA-O2A
16	A	854	CLA	CAA-CBA-CGA-O2A
25	A	852	PTY	C18-C19-C20-C21
16	A	809	CLA	C2A-CAA-CBA-CGA
16	2	606	CLA	CAA-CBA-CGA-O1A
16	A	815	CLA	CAA-CBA-CGA-O1A
25	3	221	PTY	O30-C30-C31-C32
16	2	605	CLA	CAA-CBA-CGA-O2A
16	2	609	CLA	CAA-CBA-CGA-O1A
16	3	205	CLA	CAA-CBA-CGA-O1A
16	A	833	CLA	C2-C3-C5-C6
29	J	105	3PH	C27-C28-C29-C2A
31	B	846	DGD	CDB-CEB-CFB-CGB
16	3	213	CLA	CAD-CBD-CGD-O1D
16	A	813	CLA	CAD-CBD-CGD-O1D
16	B	803	CLA	CAD-CBD-CGD-O1D
16	B	835	CLA	CAD-CBD-CGD-O1D
16	I	101	CLA	CAD-CBD-CGD-O1D
25	3	220	PTY	C2-C3-O11-P1
16	B	801	CLA	O1A-CGA-O2A-C1
16	2	613	CLA	CAA-CBA-CGA-O1A
16	L	204	CLA	C10-C11-C12-C13
16	1	606	CLA	C6-C7-C8-C9
16	2	609	CLA	C11-C12-C13-C14
16	3	206	CLA	C11-C10-C8-C9
16	3	208	CLA	C6-C7-C8-C9
16	3	210	CLA	C11-C10-C8-C9
16	A	823	CLA	C11-C10-C8-C9
16	B	826	CLA	C11-C12-C13-C14
16	B	829	CLA	C11-C10-C8-C9
16	F	202	CLA	C6-C7-C8-C9
16	L	203	CLA	C14-C13-C15-C16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	B	830	CLA	C15-C16-C17-C18
16	F	202	CLA	C10-C11-C12-C13
29	A	849	3PH	O32-C31-O31-C3
16	2	611	CLA	CAA-CBA-CGA-O2A
16	B	801	CLA	CAA-CBA-CGA-O2A
16	B	808	CLA	CAA-CBA-CGA-O2A
16	B	831	CLA	CAA-CBA-CGA-O2A
16	A	815	CLA	C8-C10-C11-C12
16	B	837	CLA	C2C-C3C-CAC-CBC
16	A	802	CLA	CAA-CBA-CGA-O2A
16	A	805	CLA	CAA-CBA-CGA-O2A
16	L	204	CLA	CAA-CBA-CGA-O2A
30	A	851	T7X	O16-C10-C12-C13
31	B	850	DGD	O1G-C1A-C2A-C3A
16	3	205	CLA	C4-C3-C5-C6
30	A	851	T7X	C44-C45-C46-C47
16	1	605	CLA	C11-C10-C8-C7
16	1	606	CLA	C6-C7-C8-C10
16	1	611	CLA	C11-C12-C13-C15
16	2	604	CLA	C6-C7-C8-C10
16	2	607	CLA	C6-C7-C8-C10
16	2	613	CLA	C12-C13-C15-C16
16	3	206	CLA	C11-C10-C8-C7
16	3	214	CLA	C11-C10-C8-C7
16	A	805	CLA	C11-C10-C8-C7
16	A	807	CLA	C6-C7-C8-C10
16	A	810	CLA	C3A-C2A-CAA-CBA
16	A	820	CLA	C11-C10-C8-C7
16	A	827	CLA	C11-C12-C13-C15
16	A	829	CLA	C11-C12-C13-C15
16	B	806	CLA	C11-C10-C8-C7
16	B	818	CLA	C12-C13-C15-C16
16	B	824	CLA	C2-C3-C5-C6
16	B	824	CLA	C12-C13-C15-C16
16	B	825	CLA	C11-C10-C8-C7
16	B	827	CLA	C11-C12-C13-C15
16	B	832	CLA	C11-C12-C13-C15
16	B	833	CLA	C11-C10-C8-C7
16	B	835	CLA	C11-C12-C13-C15
16	B	837	CLA	C12-C13-C15-C16
16	B	838	CLA	C12-C13-C15-C16
16	L	203	CLA	C6-C7-C8-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
16	O	202	CLA	C11-C12-C13-C15
31	B	850	DGD	C1B-C2B-C3B-C4B
31	B	850	DGD	O1A-C1A-C2A-C3A
16	2	610	CLA	CAA-CBA-CGA-O2A
16	3	212	CLA	CAA-CBA-CGA-O2A
16	A	835	CLA	CAA-CBA-CGA-O2A
16	I	102	CLA	CAA-CBA-CGA-O2A
25	A	852	PTY	C32-C33-C34-C35
29	A	849	3PH	C35-C36-C37-C38
29	J	105	3PH	C2C-C2D-C2E-C2F
21	O	205	BCR	C17-C18-C19-C20
16	A	802	CLA	CAA-CBA-CGA-O1A
16	B	809	CLA	CAA-CBA-CGA-O1A
16	B	833	CLA	CAA-CBA-CGA-O1A
16	3	203	CLA	CAA-CBA-CGA-O2A
16	A	816	CLA	CAA-CBA-CGA-O2A
25	3	221	PTY	C15-C16-C17-C18
16	F	202	CLA	C5-C6-C7-C8
16	3	212	CLA	CAA-CBA-CGA-O1A
16	3	213	CLA	CAA-CBA-CGA-O1A
16	B	801	CLA	CAA-CBA-CGA-O1A
25	A	852	PTY	C37-C38-C39-C40
16	1	611	CLA	C13-C15-C16-C17
16	B	819	CLA	C5-C6-C7-C8
16	L	205	CLA	C15-C16-C17-C18
16	O	203	CLA	C5-C6-C7-C8
16	B	836	CLA	CAA-CBA-CGA-O2A
25	A	852	PTY	C12-C11-C8-O7
16	2	610	CLA	CAA-CBA-CGA-O1A
16	A	827	CLA	C16-C17-C18-C20
16	2	608	CLA	C15-C16-C17-C18
16	A	821	CLA	C15-C16-C17-C18
16	B	804	CLA	C13-C15-C16-C17
27	B	839	PQN	C25-C26-C27-C28
29	B	854	3PH	C31-C32-C33-C34
16	B	831	CLA	CAA-CBA-CGA-O1A
16	I	102	CLA	CAA-CBA-CGA-O1A
16	L	204	CLA	CAA-CBA-CGA-O1A
30	A	851	T7X	O17-C10-C12-C13
16	A	856	CLA	CAA-CBA-CGA-O2A
29	B	854	3PH	O21-C21-C22-C23

There are no ring outliers.

181 monomers are involved in 586 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	1	604	CLA	2	0
16	A	833	CLA	1	0
16	B	802	CLA	4	0
16	F	205	CLA	1	0
21	2	617	BCR	10	0
21	L	207	BCR	4	0
16	3	204	CLA	4	0
16	L	204	CLA	2	0
16	1	610	CLA	4	0
17	3	201	C7Z	2	0
17	3	217	C7Z	2	0
16	3	209	CLA	8	0
16	A	836	CLA	3	0
16	B	810	CLA	4	0
16	I	101	CLA	6	0
16	A	807	CLA	4	0
16	2	609	CLA	3	0
16	B	805	CLA	2	0
16	B	831	CLA	5	0
21	F	206	BCR	5	0
16	3	211	CLA	3	0
21	A	844	BCR	8	0
16	A	827	CLA	8	0
31	B	846	DGD	4	0
19	2	622	LHG	1	0
31	B	849	DGD	2	0
16	A	856	CLA	3	0
16	B	833	CLA	4	0
16	A	839	CLA	4	0
16	2	606	CLA	4	0
16	A	826	CLA	5	0
21	B	847	BCR	4	0
16	B	826	CLA	7	0
30	A	851	T7X	1	0
17	1	612	C7Z	2	0
16	F	204	CLA	2	0
21	L	206	BCR	6	0
16	3	213	CLA	9	0
16	A	814	CLA	5	0
16	B	813	CLA	2	0
16	2	612	CLA	4	0
16	3	210	CLA	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	817	CLA	4	0
26	A	801	CLO	5	0
16	A	804	CLA	3	0
16	F	201	CLA	4	0
24	3	202	LMU	1	0
16	A	802	CLA	2	0
16	A	855	CLA	6	0
16	A	822	CLA	4	0
16	O	201	CLA	4	0
16	B	832	CLA	4	0
16	1	603	CLA	4	0
16	F	202	CLA	6	0
16	1	609	CLA	5	0
19	A	842	LHG	1	0
25	A	852	PTY	3	0
21	B	841	BCR	3	0
16	2	610	CLA	2	0
21	F	203	BCR	4	0
16	2	603	CLA	1	0
16	A	805	CLA	4	0
16	A	820	CLA	3	0
21	A	857	BCR	7	0
16	3	203	CLA	3	0
16	O	203	CLA	5	0
16	1	606	CLA	4	0
16	L	205	CLA	2	0
16	B	817	CLA	4	0
16	A	824	CLA	5	0
16	B	824	CLA	1	0
19	3	219	LHG	2	0
16	A	811	CLA	3	0
16	2	607	CLA	6	0
21	B	845	BCR	8	0
16	A	828	CLA	7	0
16	3	212	CLA	3	0
16	A	832	CLA	5	0
16	B	829	CLA	5	0
16	B	830	CLA	5	0
16	B	806	CLA	4	0
16	1	601	CLA	5	0
16	K	102	CLA	3	0
16	B	812	CLA	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	2	621	ERG	5	0
16	L	203	CLA	3	0
16	2	604	CLA	1	0
16	B	838	CLA	4	0
16	B	814	CLA	2	0
16	A	821	CLA	6	0
16	1	607	CLA	5	0
16	A	809	CLA	5	0
16	B	835	CLA	5	0
16	B	809	CLA	4	0
16	1	611	CLA	2	0
23	J	101	DGA	1	0
17	1	615	C7Z	1	0
16	B	828	CLA	3	0
16	3	214	CLA	3	0
16	2	608	CLA	4	0
16	A	808	CLA	3	0
16	A	823	CLA	5	0
20	2	618	ERG	4	0
27	B	839	PQN	4	0
16	B	823	CLA	1	0
16	2	611	CLA	3	0
18	J	103	RRX	2	0
16	B	819	CLA	4	0
16	1	602	CLA	6	0
16	2	605	CLA	6	0
16	L	201	CLA	7	0
16	J	102	CLA	3	0
16	B	803	CLA	7	0
21	B	843	BCR	5	0
18	A	847	RRX	2	0
18	1	613	RRX	10	0
16	B	821	CLA	6	0
16	I	102	CLA	3	0
18	K	103	RRX	4	0
16	1	605	CLA	1	0
31	B	850	DGD	3	0
21	A	845	BCR	9	0
16	A	810	CLA	3	0
17	3	215	C7Z	3	0
16	O	204	CLA	1	0
16	A	829	CLA	3	0

*Continued on next page...*



*Continued from previous page...*

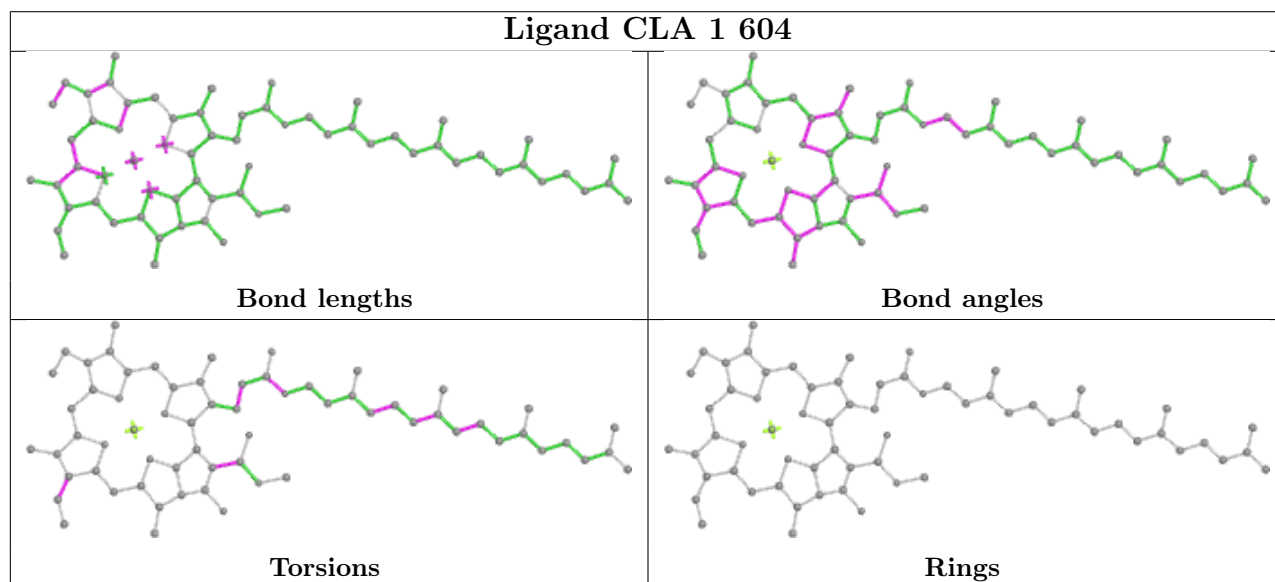
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	816	CLA	4	0
16	A	830	CLA	7	0
16	B	808	CLA	7	0
21	I	103	BCR	3	0
16	A	806	CLA	2	0
16	B	816	CLA	6	0
16	A	815	CLA	2	0
16	1	608	CLA	3	0
16	3	206	CLA	1	0
16	A	812	CLA	5	0
16	B	815	CLA	1	0
21	B	855	BCR	10	0
17	3	216	C7Z	3	0
16	A	838	CLA	2	0
17	3	218	C7Z	1	0
21	B	840	BCR	5	0
16	B	825	CLA	5	0
21	O	205	BCR	9	0
16	A	835	CLA	2	0
16	2	613	CLA	3	0
16	B	801	CLA	7	0
16	3	205	CLA	6	0
21	A	850	BCR	5	0
16	B	836	CLA	1	0
16	A	813	CLA	1	0
16	2	602	CLA	4	0
16	B	834	CLA	8	0
16	O	202	CLA	3	0
16	A	819	CLA	6	0
20	1	618	ERG	4	0
21	B	844	BCR	9	0
16	B	827	CLA	4	0
21	K	104	BCR	5	0
16	A	803	CLA	1	0
16	K	101	CLA	3	0
19	1	617	LHG	1	0
16	3	208	CLA	4	0
16	B	837	CLA	5	0
16	A	837	CLA	8	0
17	1	614	C7Z	3	0
21	A	846	BCR	14	0
16	B	818	CLA	3	0

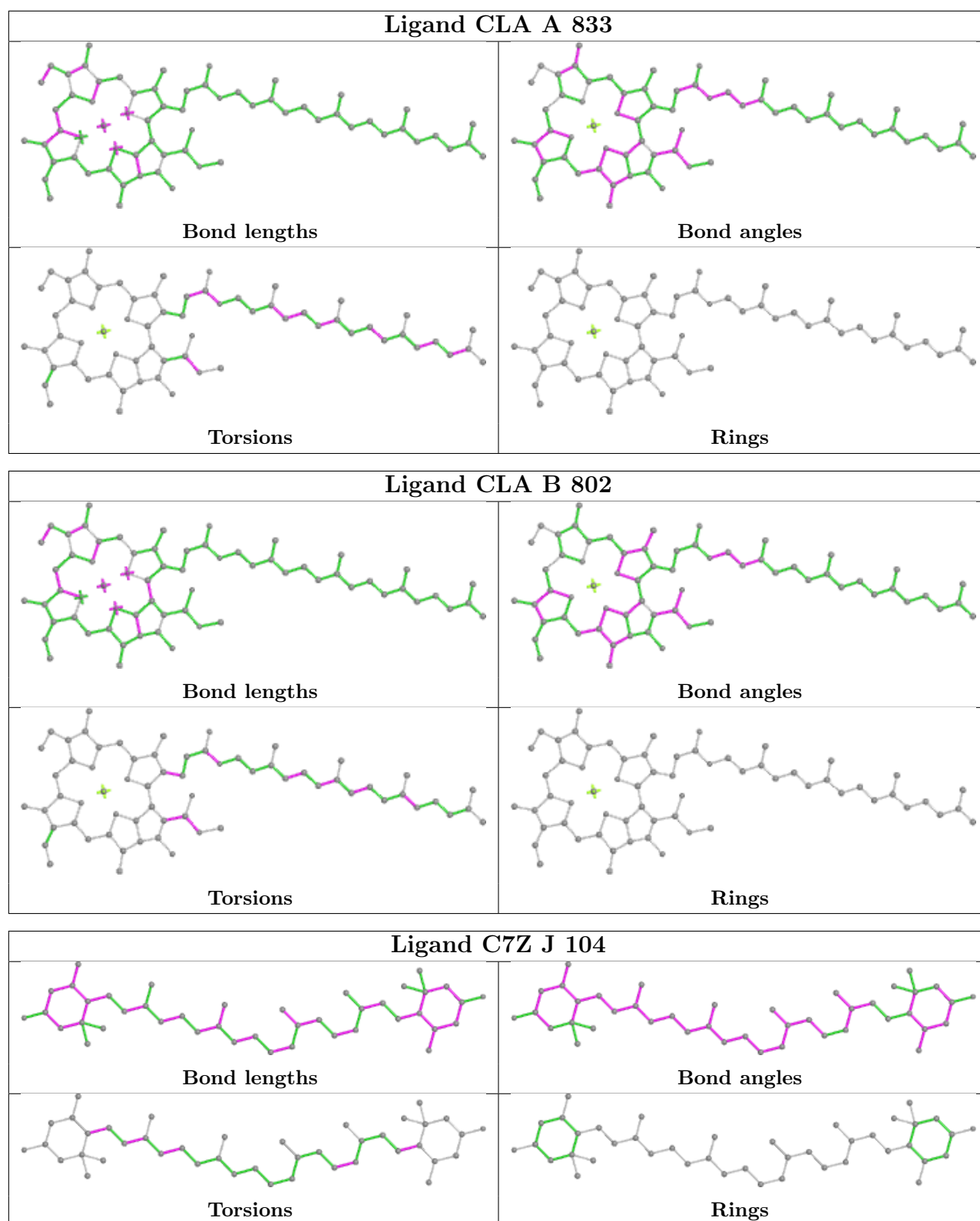
*Continued on next page...*

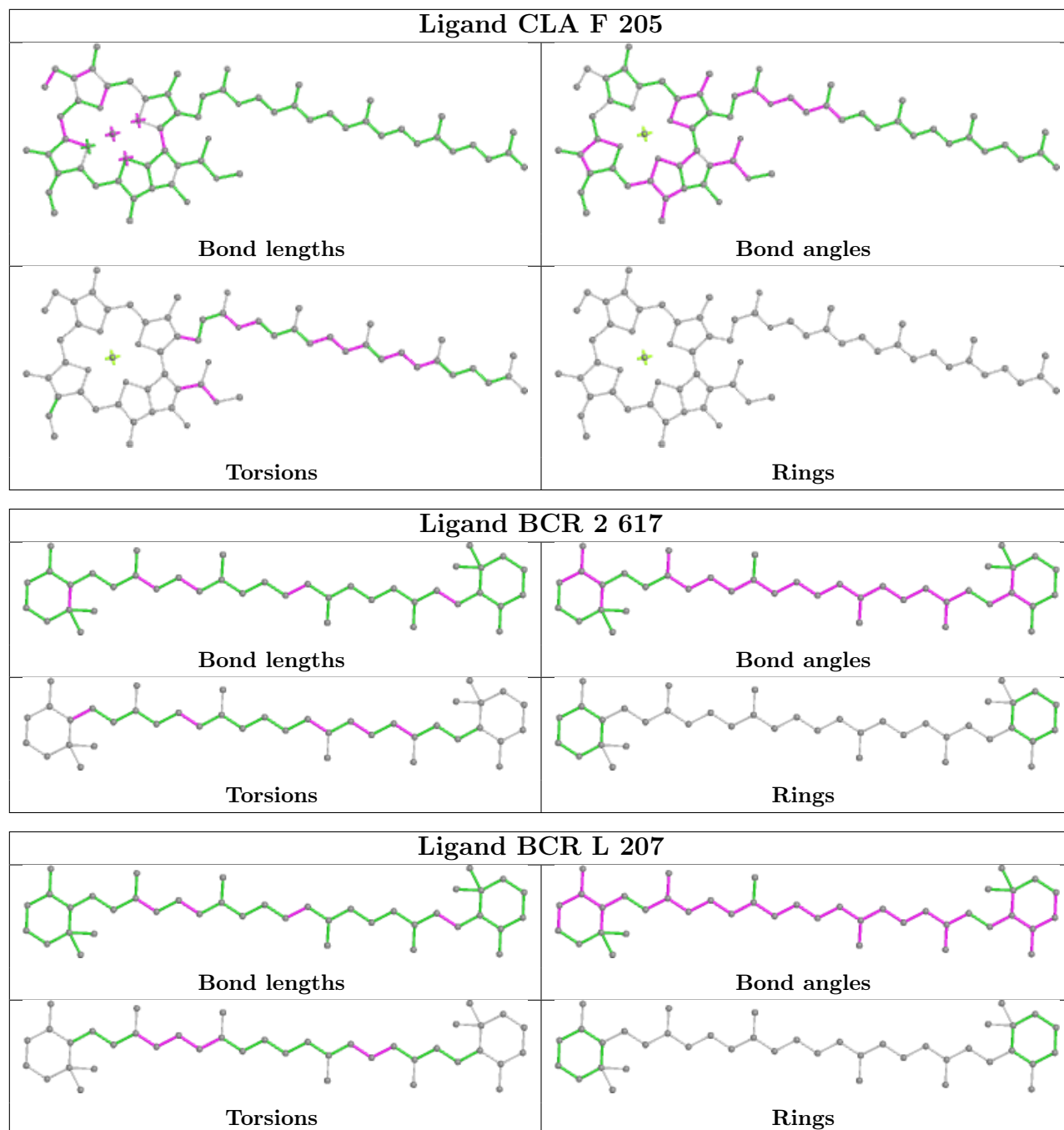
Continued from previous page...

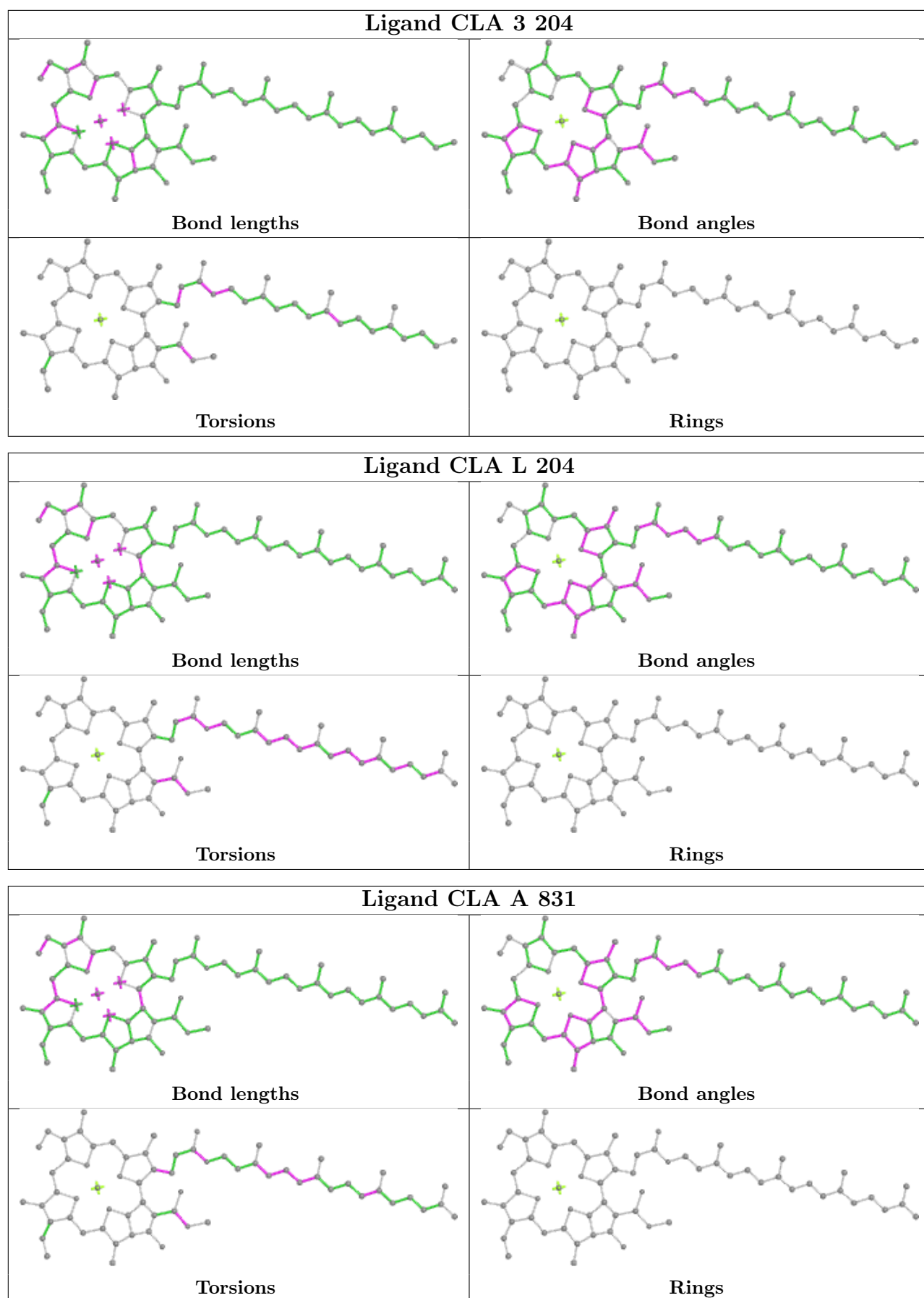
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	3	207	CLA	8	0
21	B	842	BCR	3	0
16	2	601	CLA	5	0
16	A	825	CLA	7	0
21	L	202	BCR	10	0
16	B	822	CLA	4	0
17	1	616	C7Z	1	0
16	A	834	CLA	1	0
18	2	616	RRX	2	0
16	B	811	CLA	4	0
16	B	804	CLA	8	0
16	A	818	CLA	5	0
16	A	854	CLA	10	0

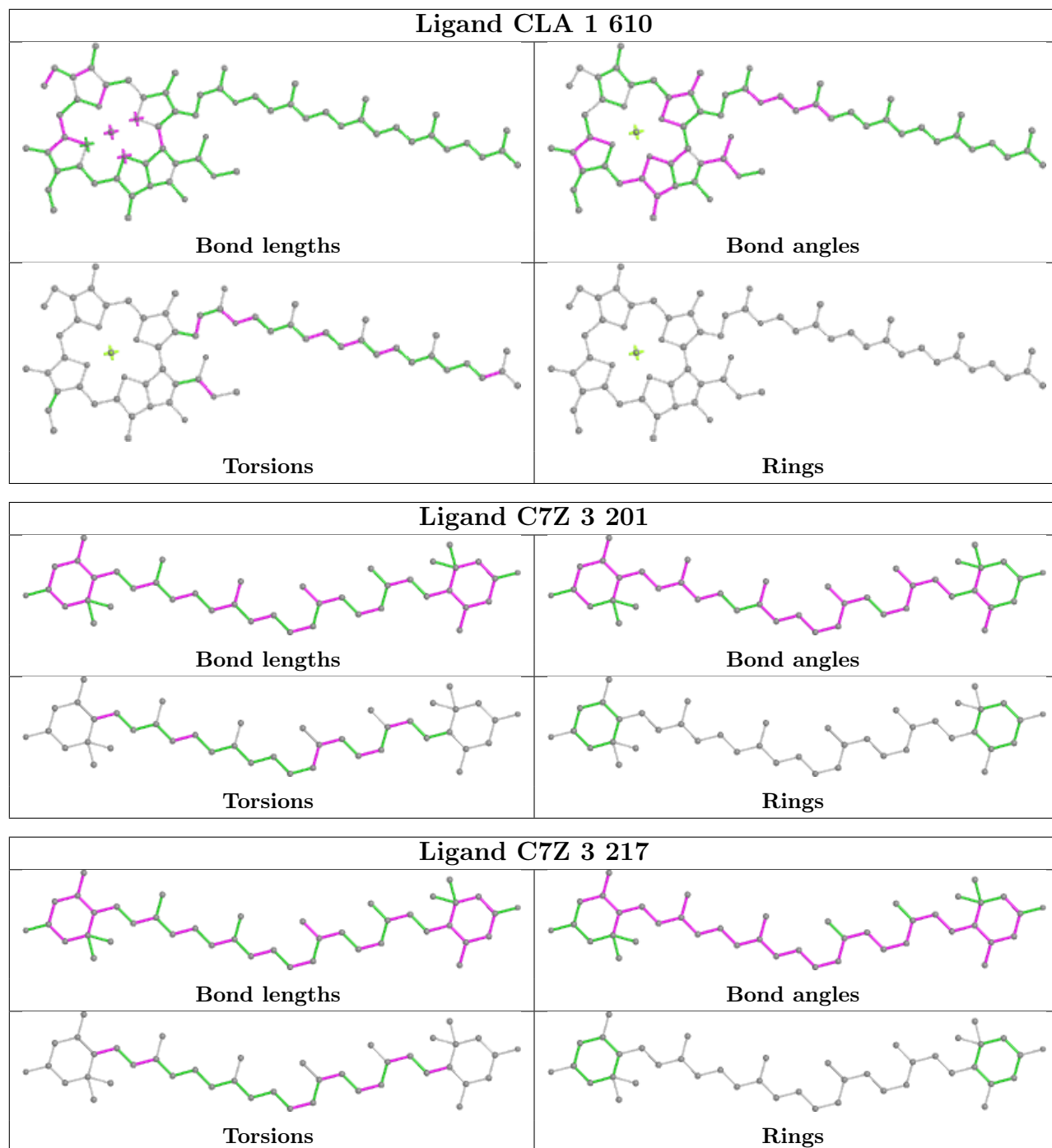
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

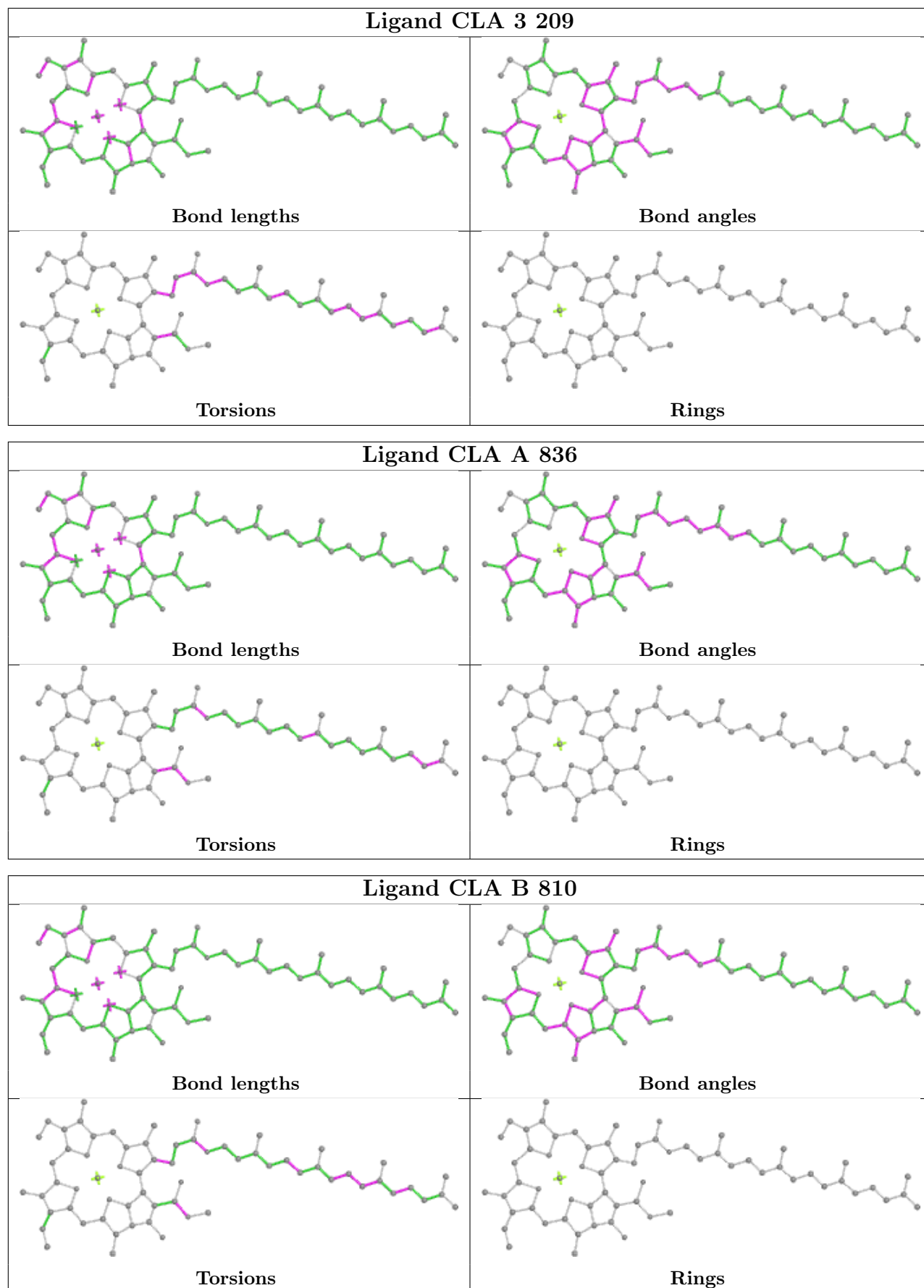


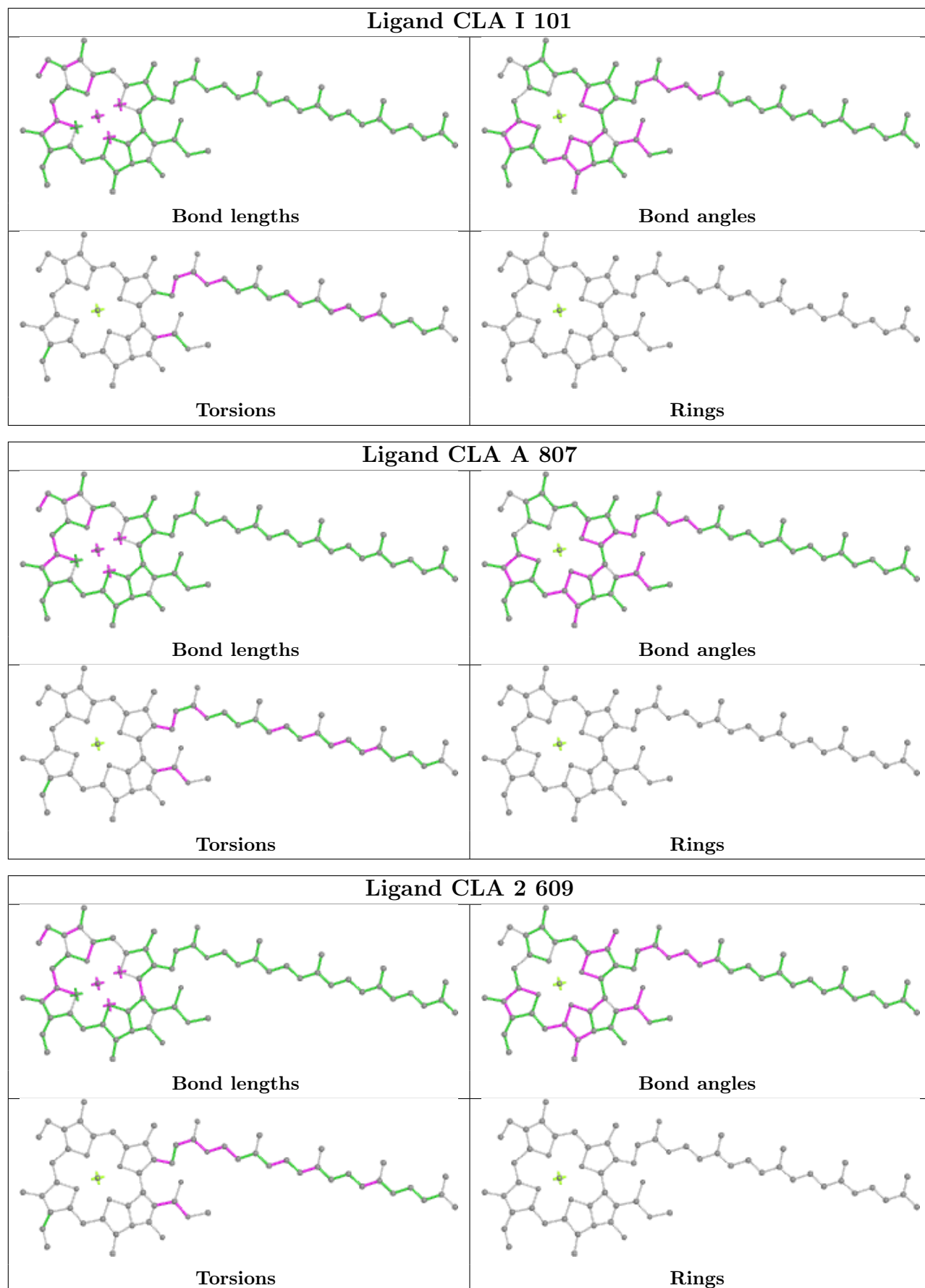




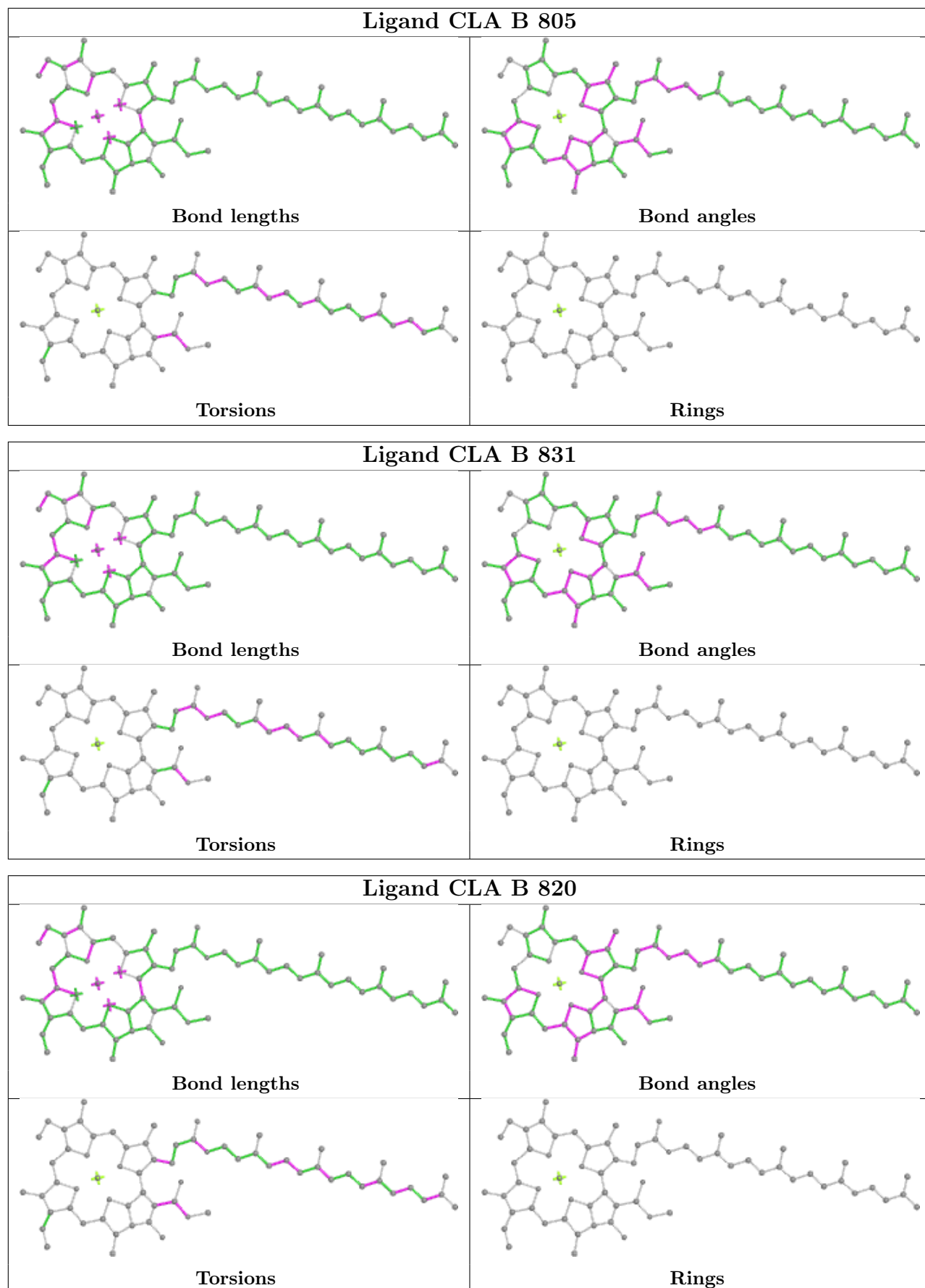


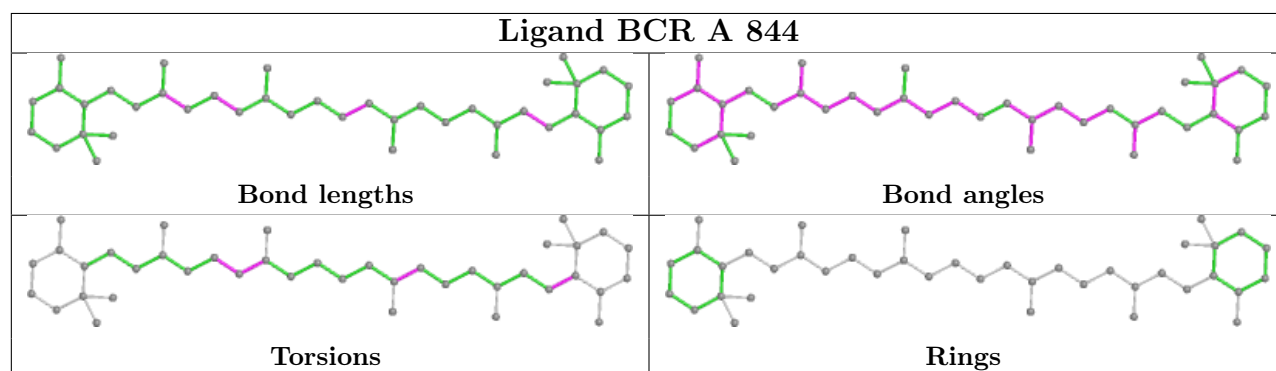
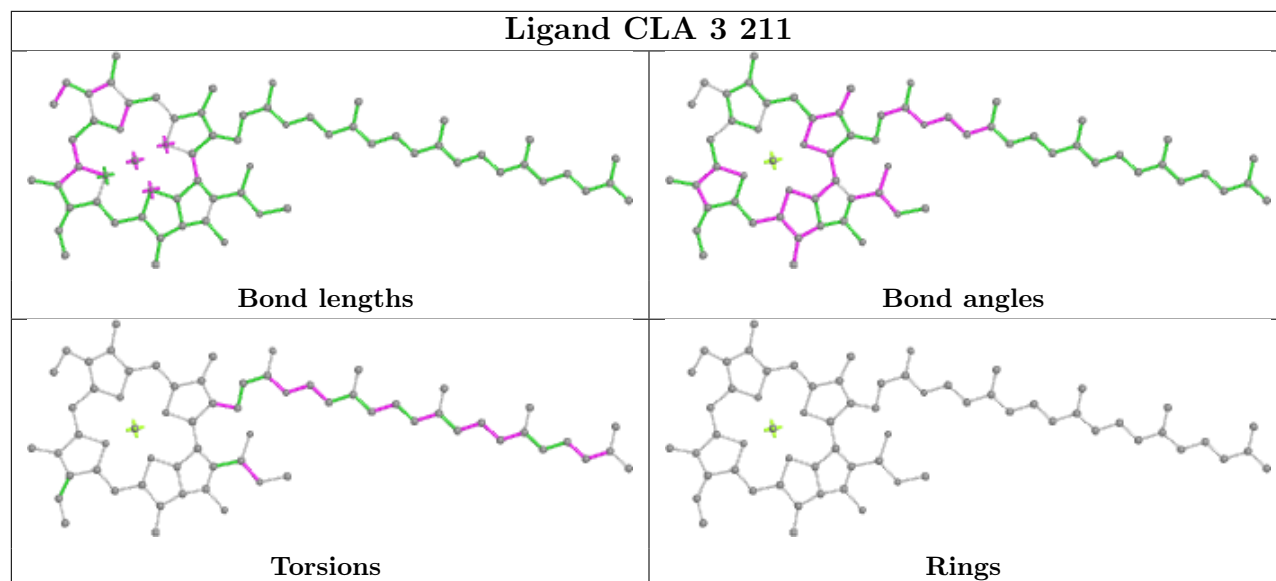
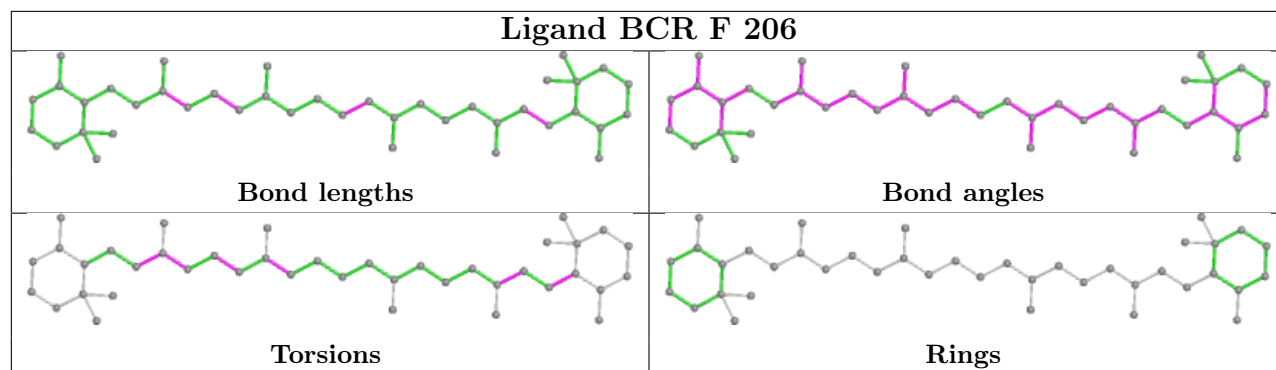


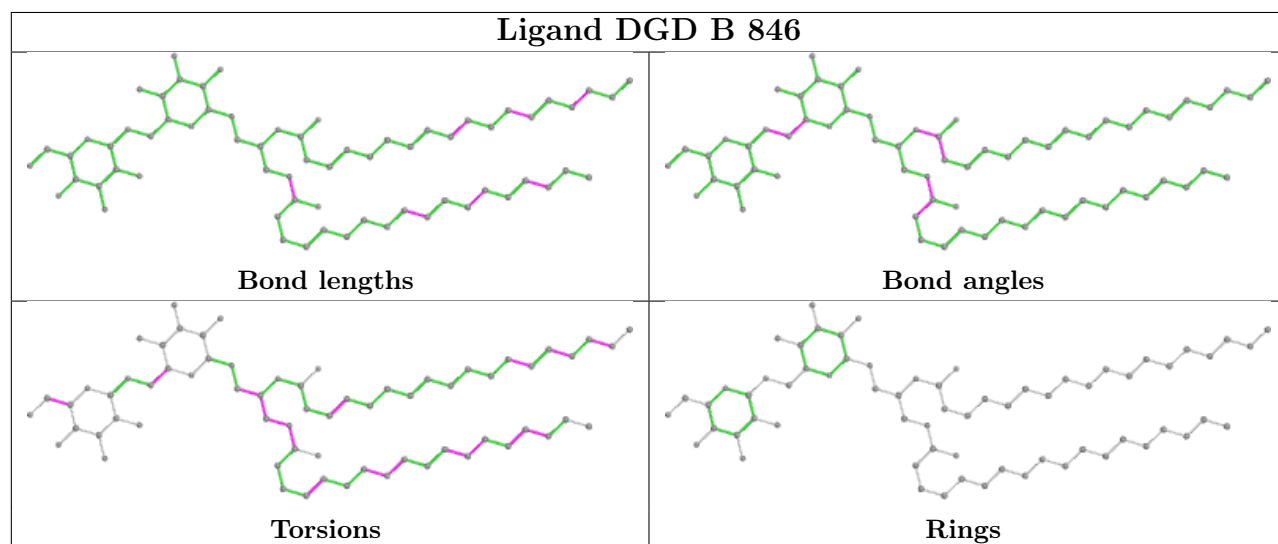
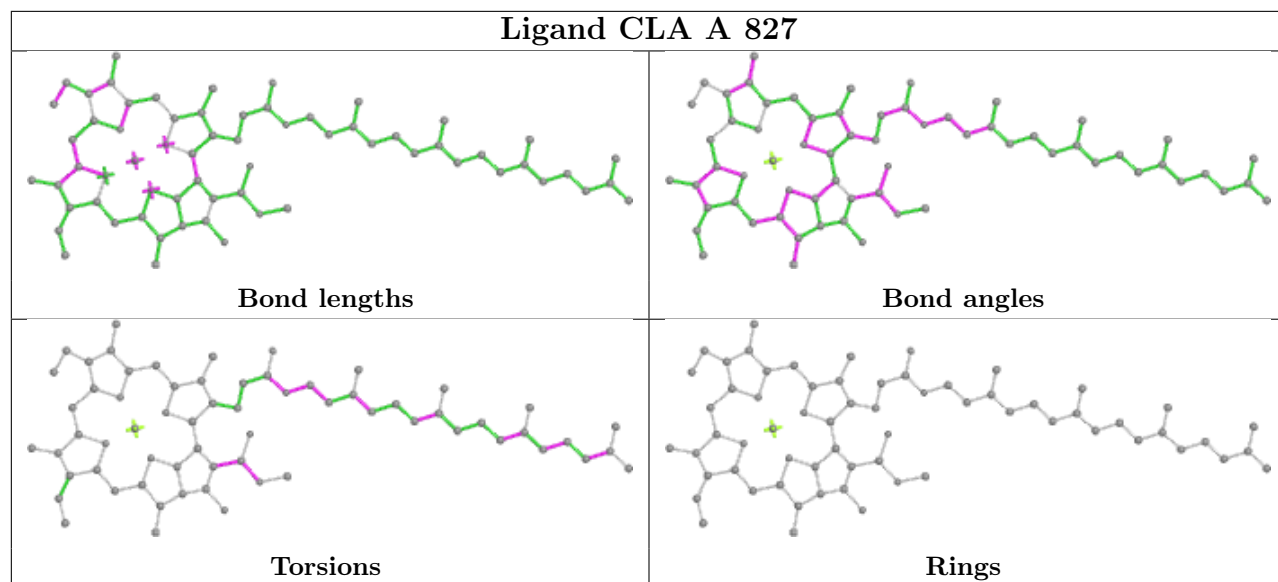


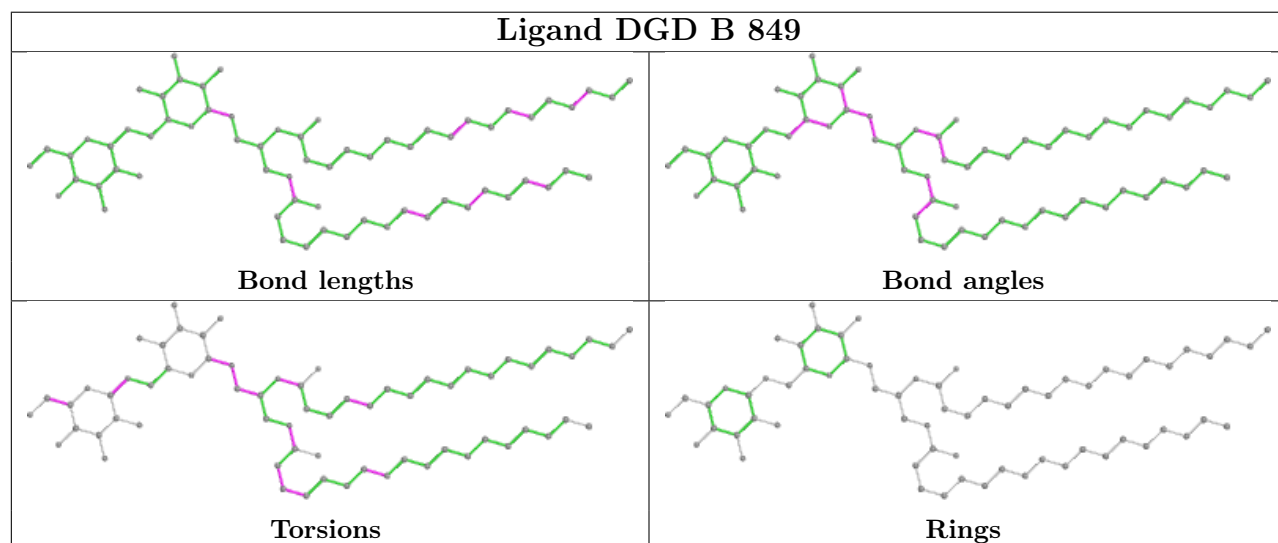
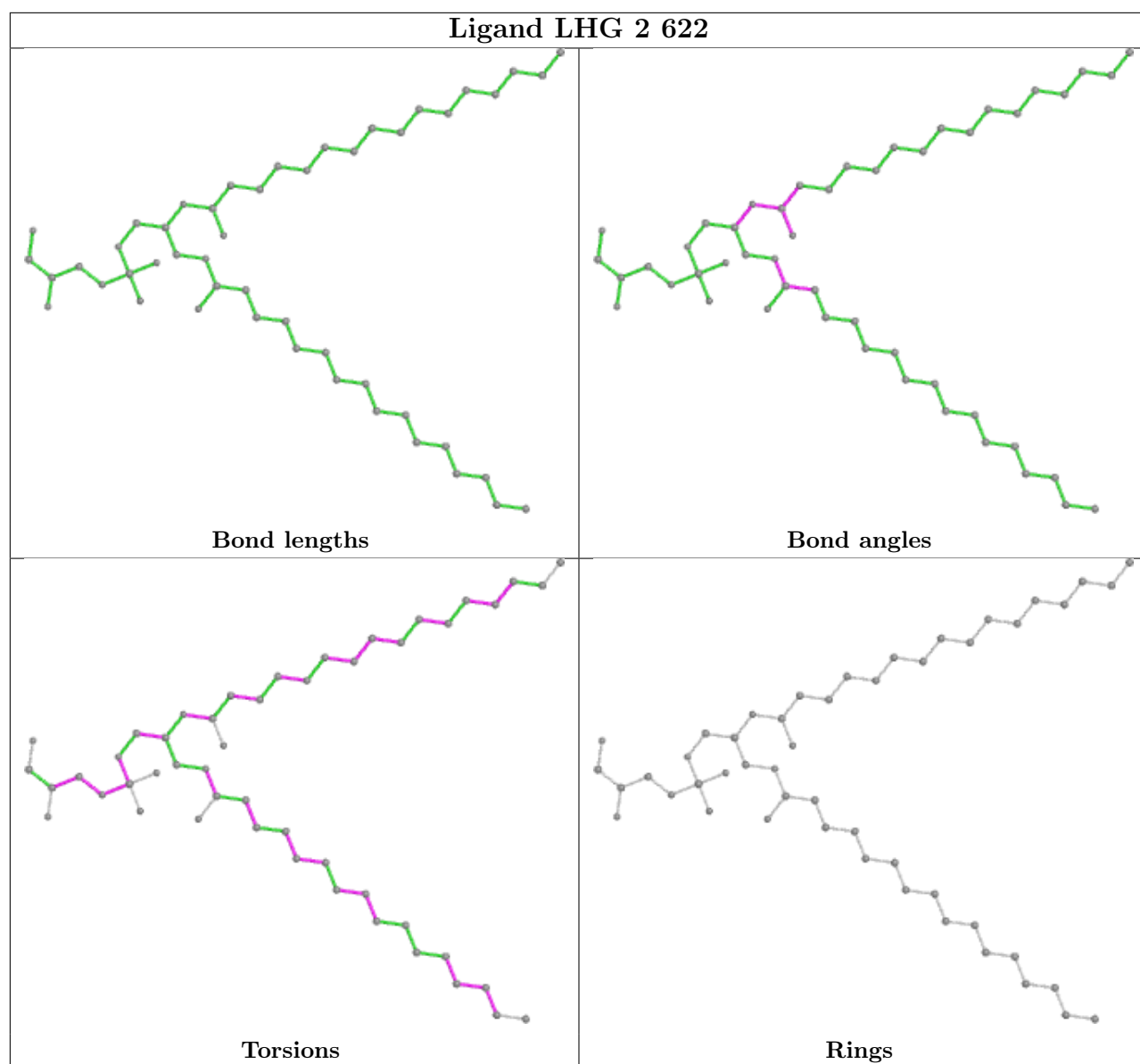


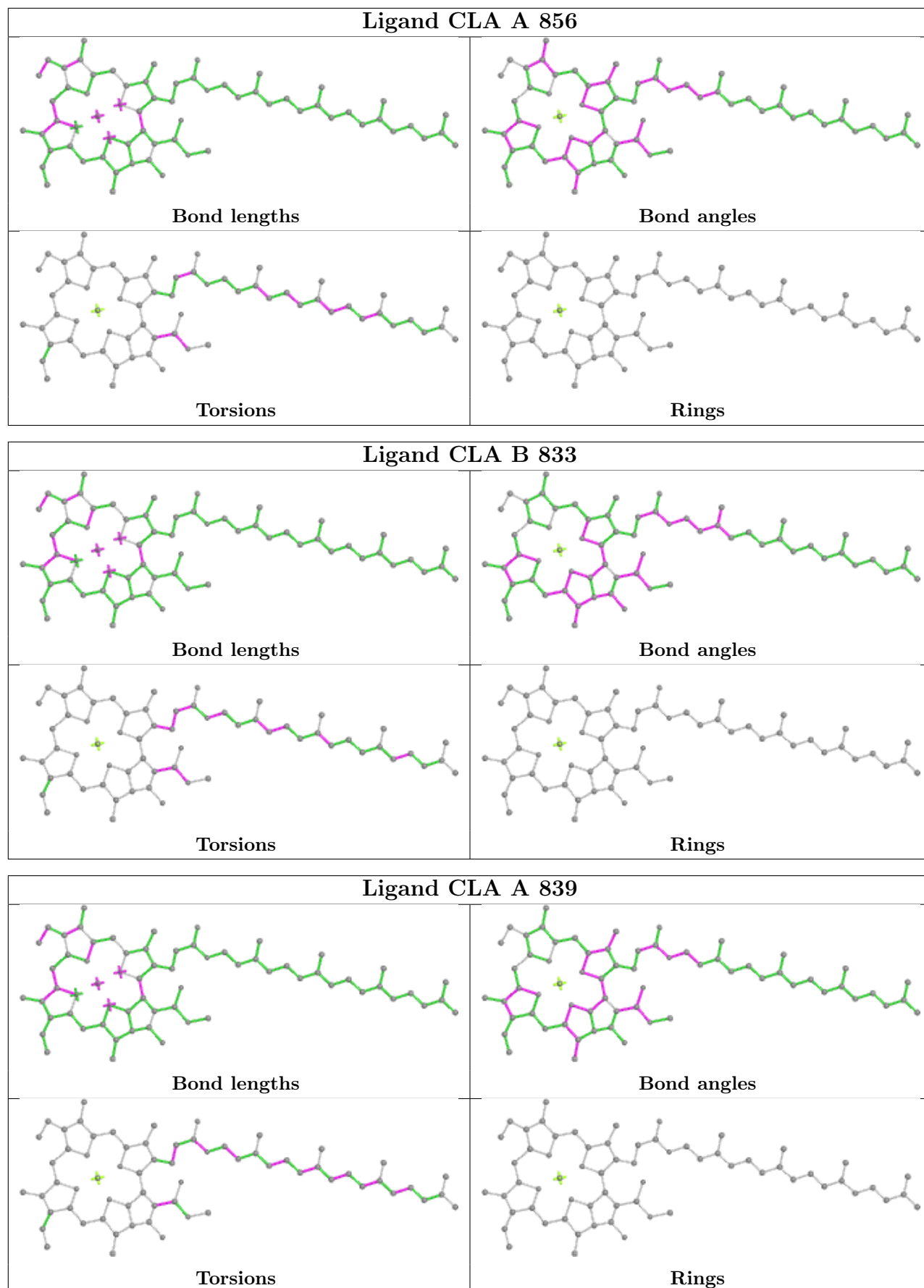


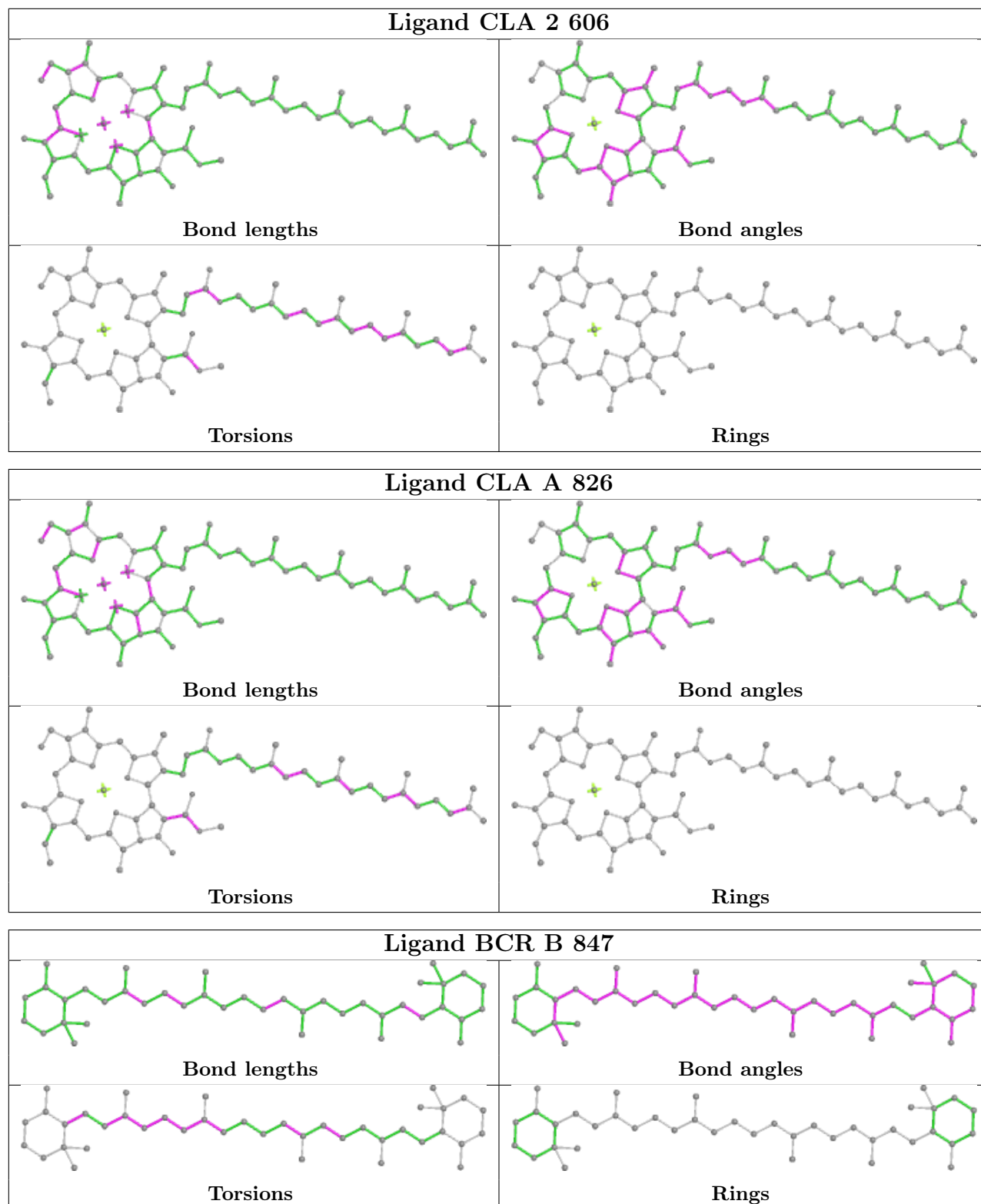


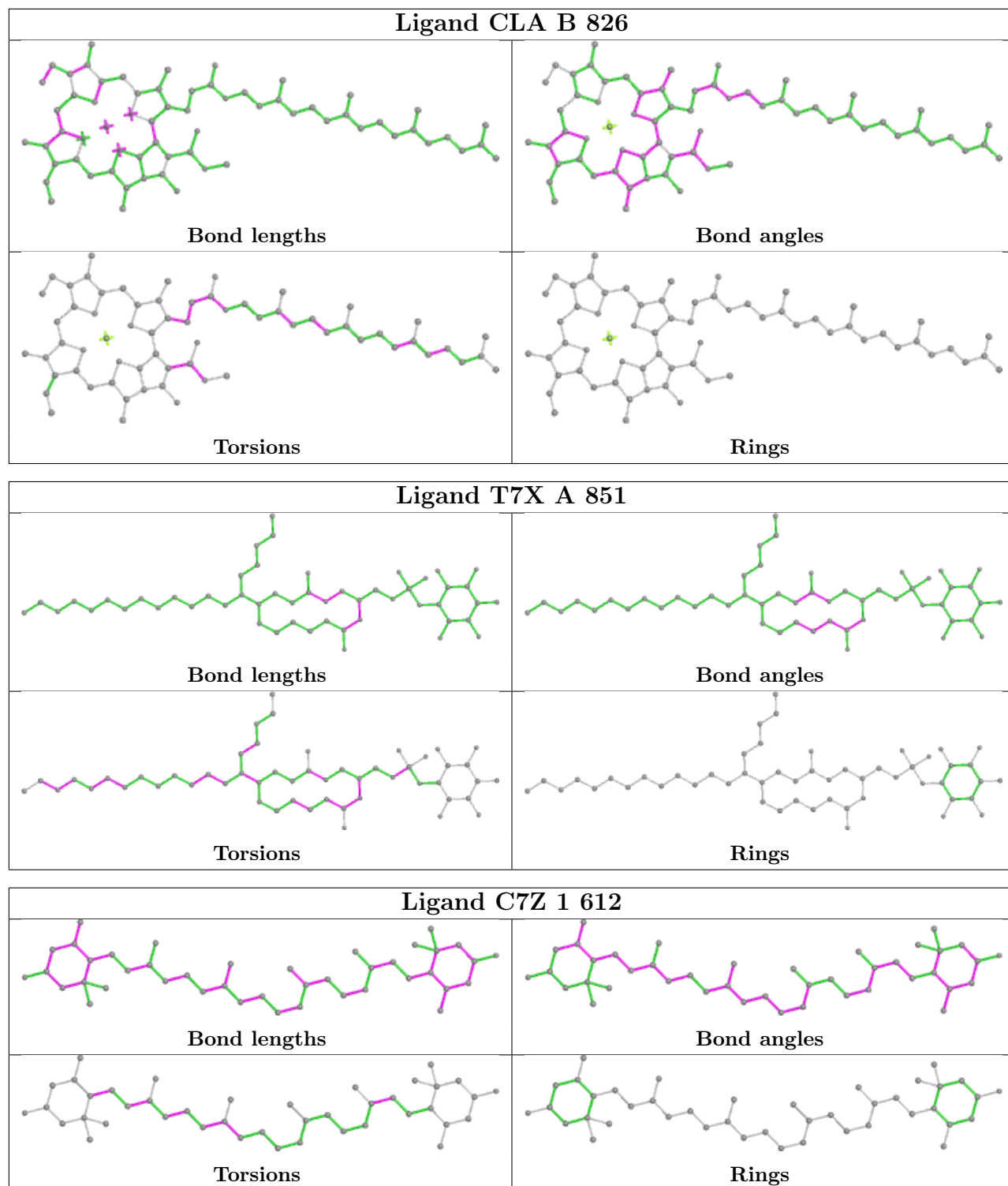


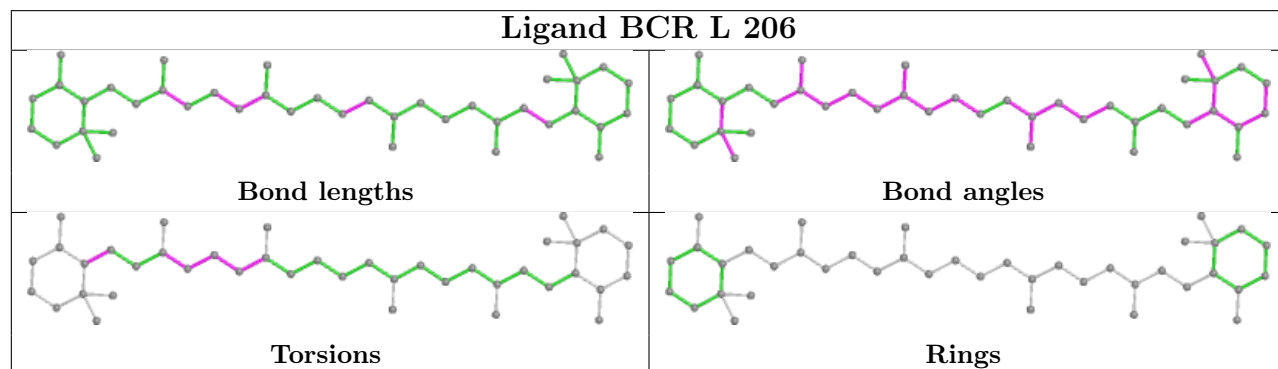
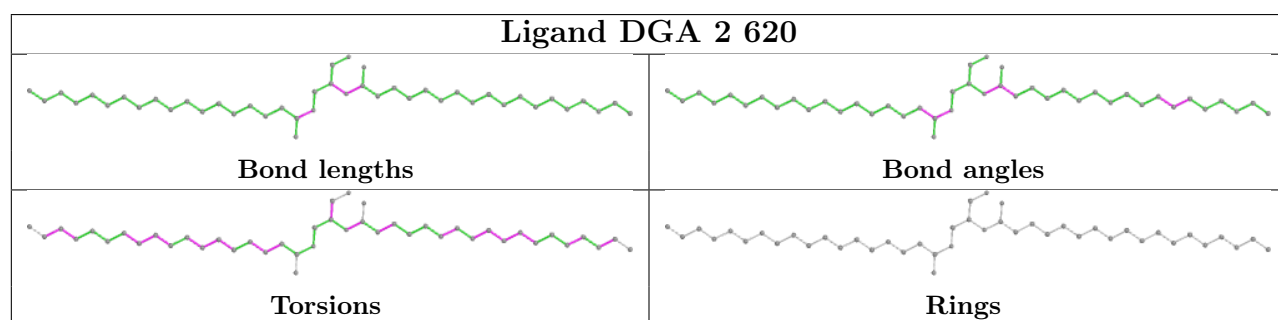
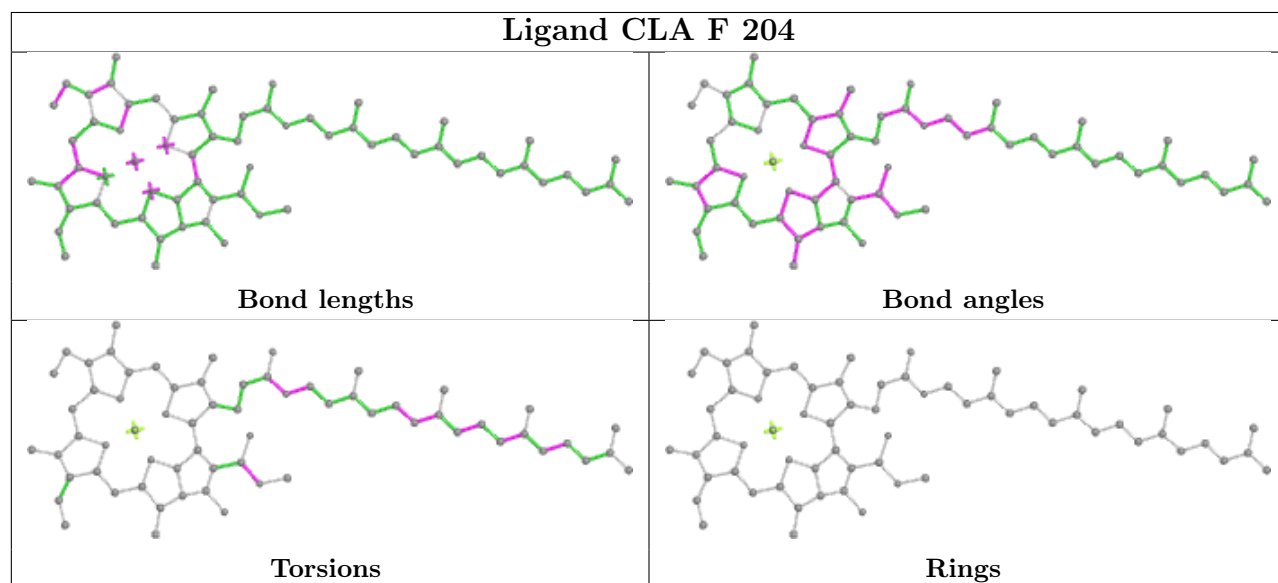
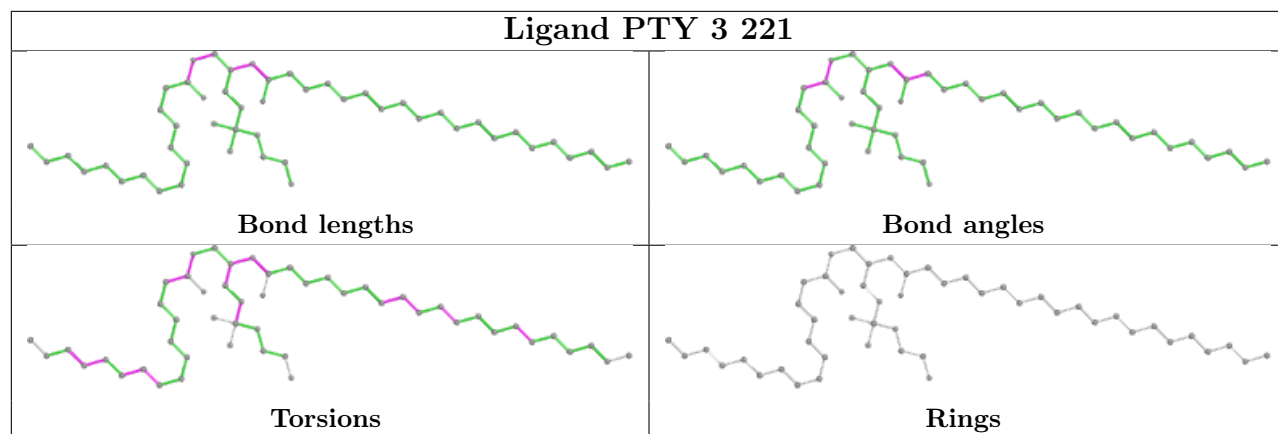






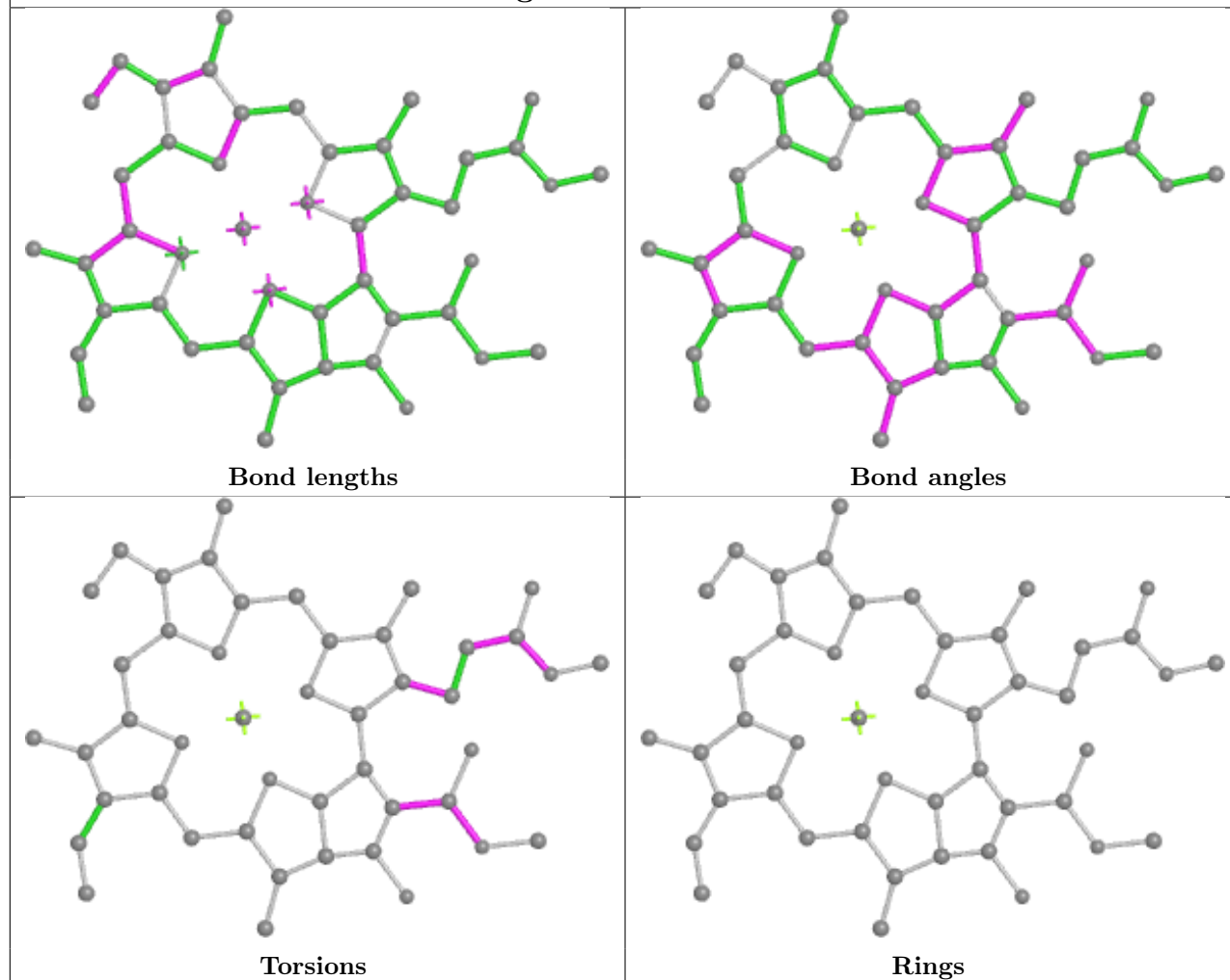




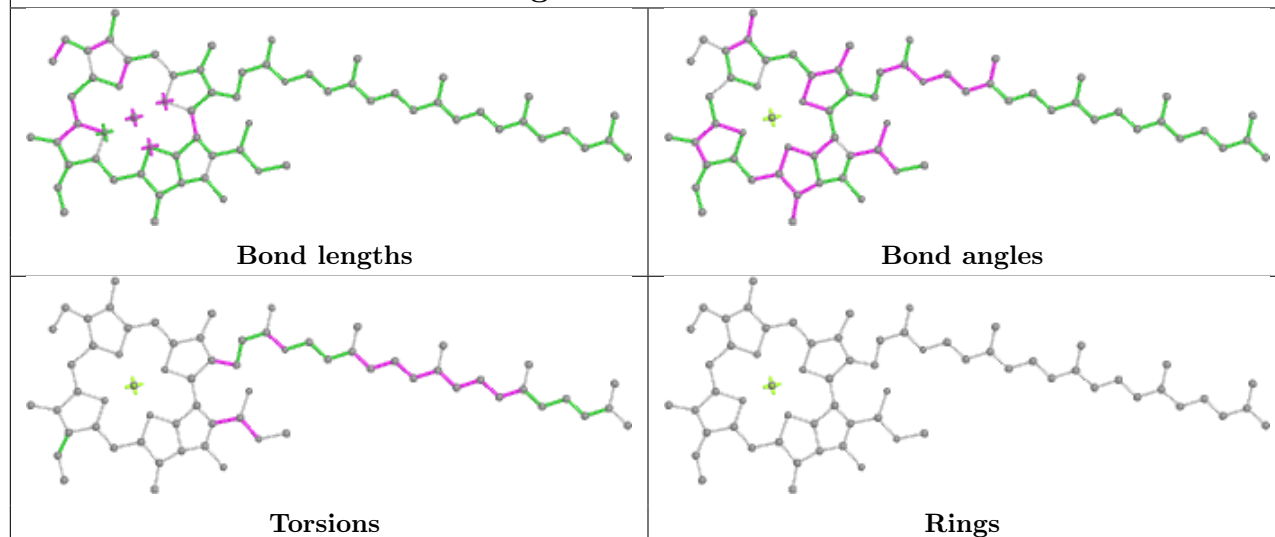


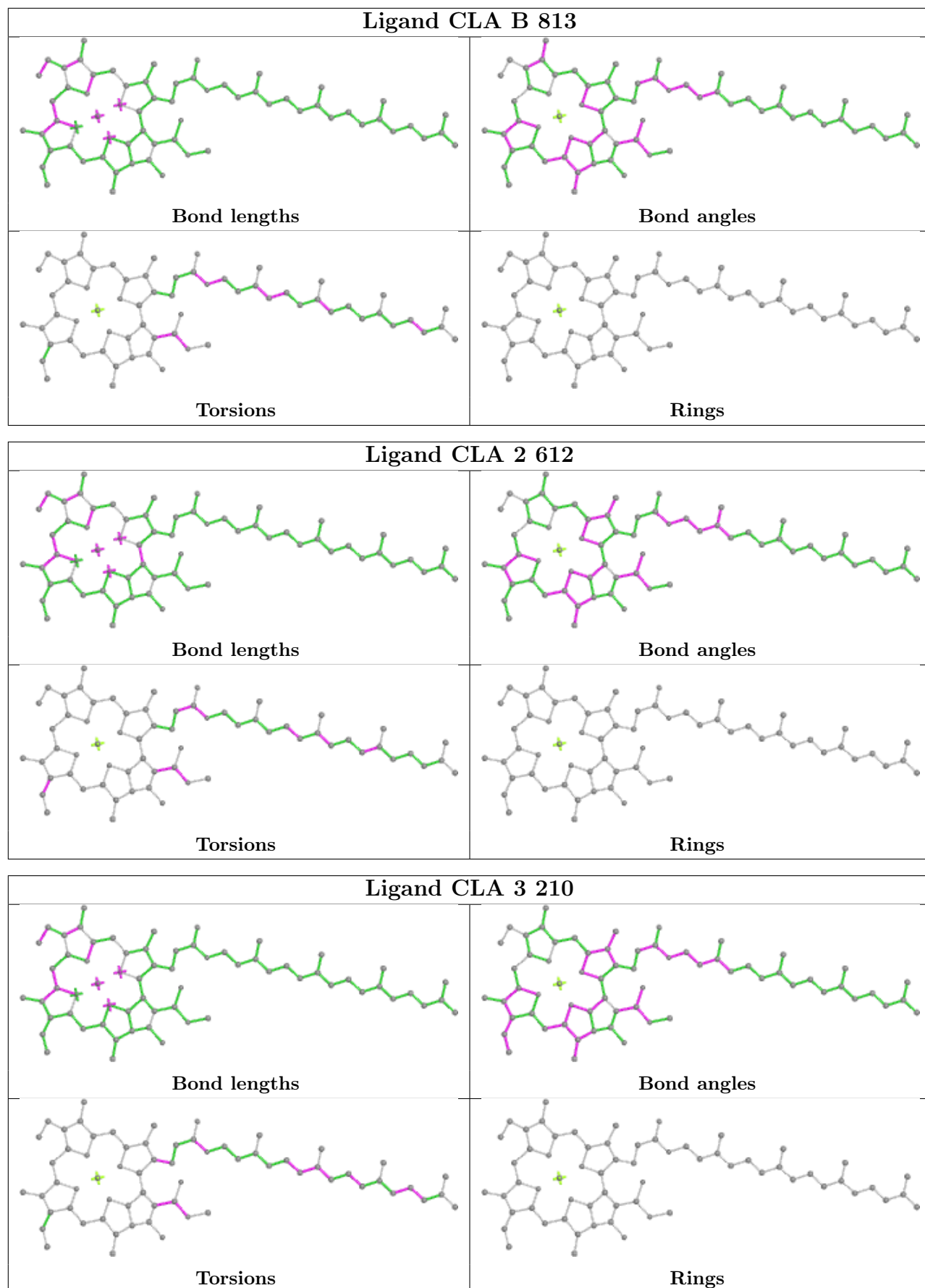


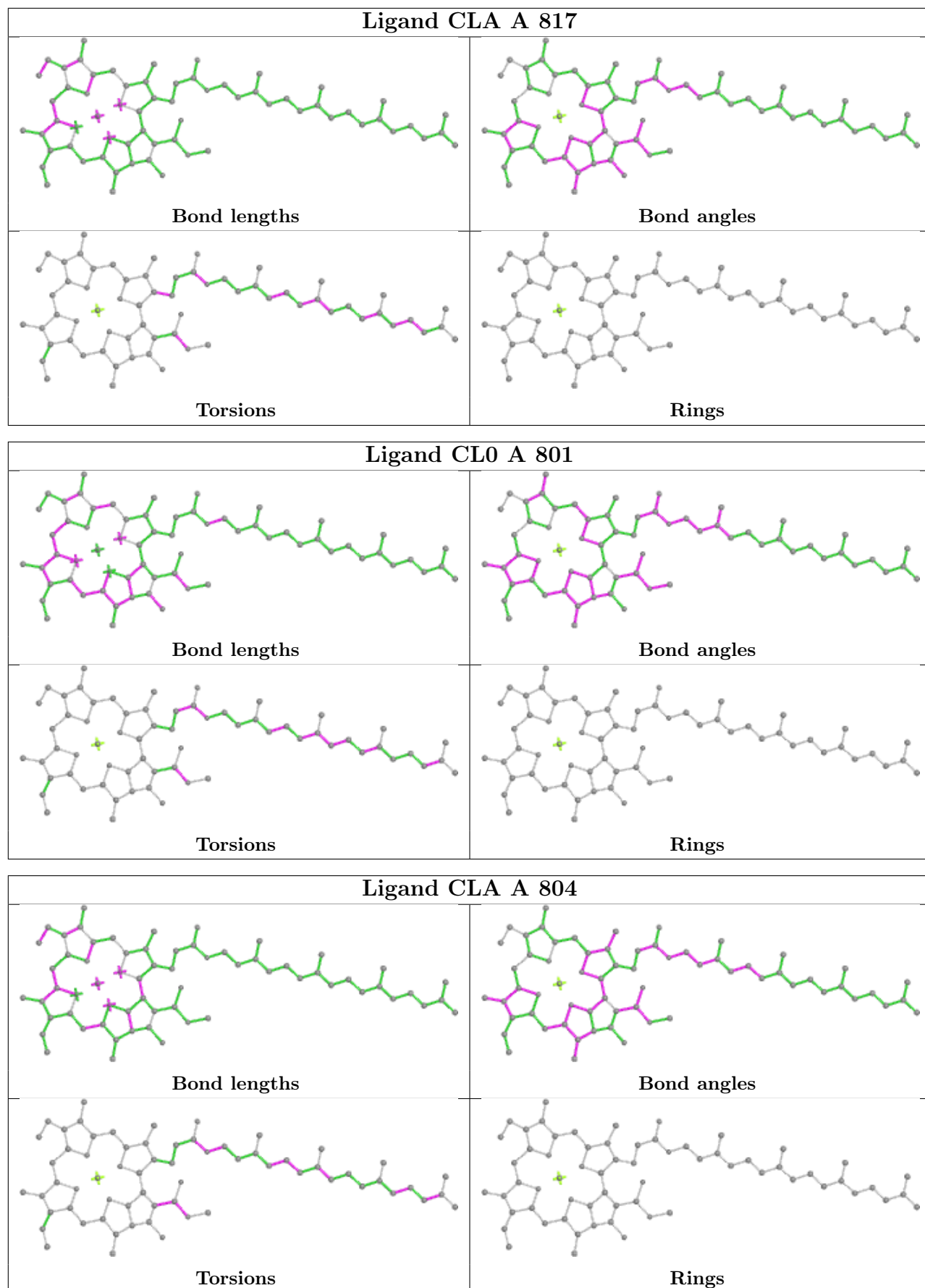
## Ligand CLA 3 213

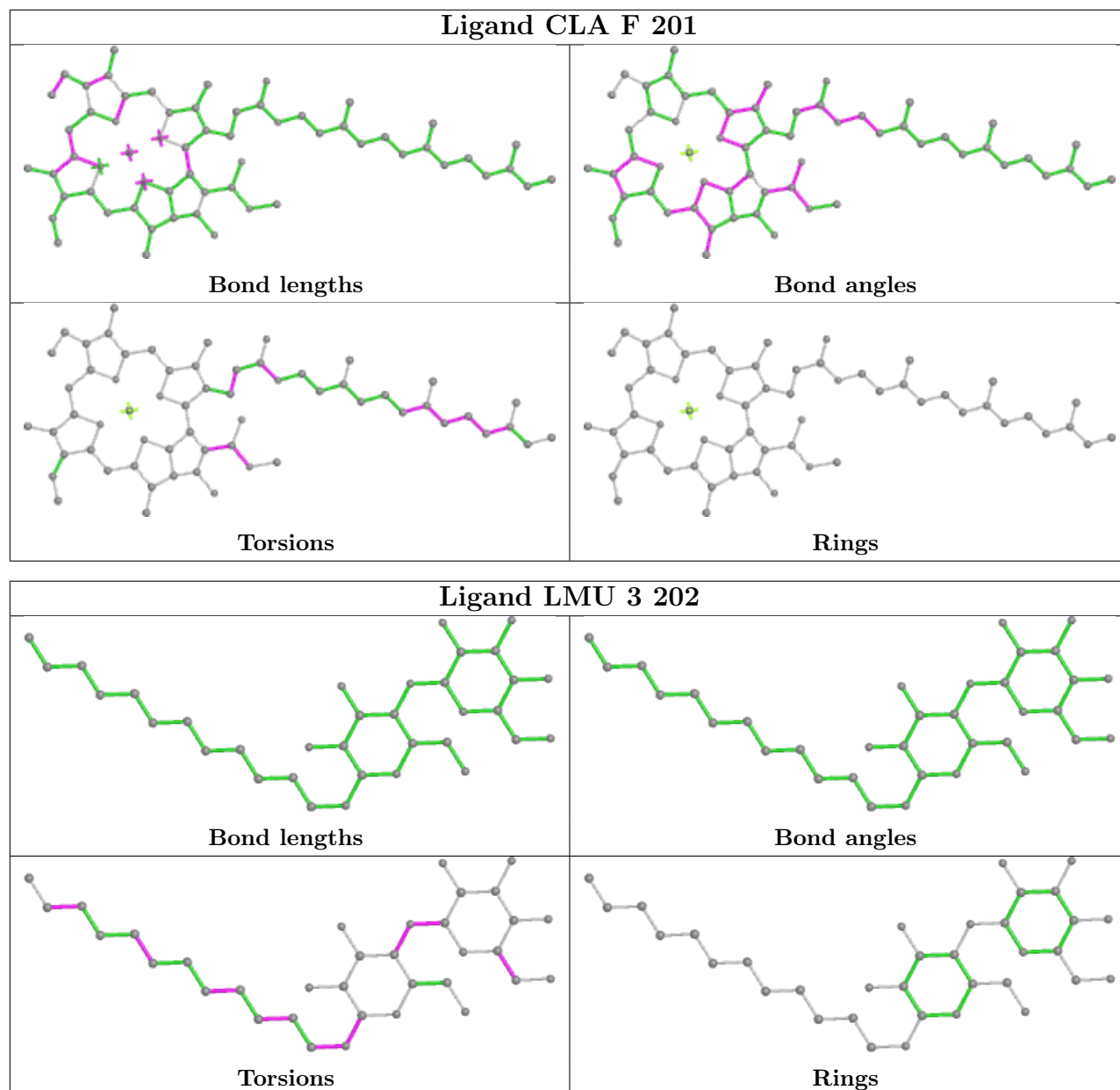


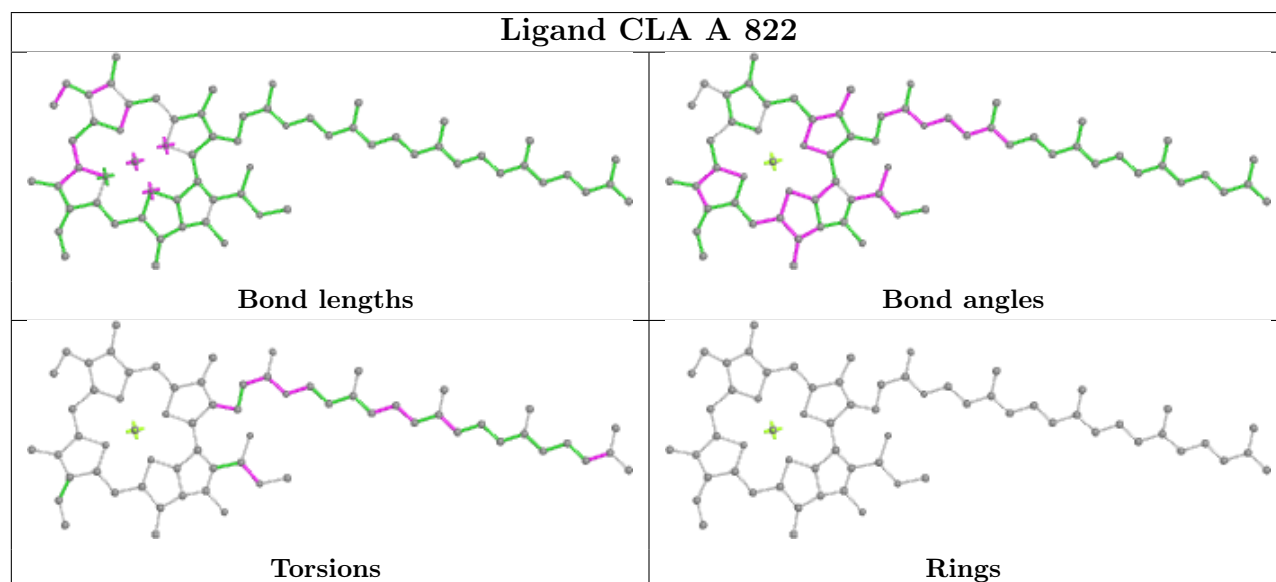
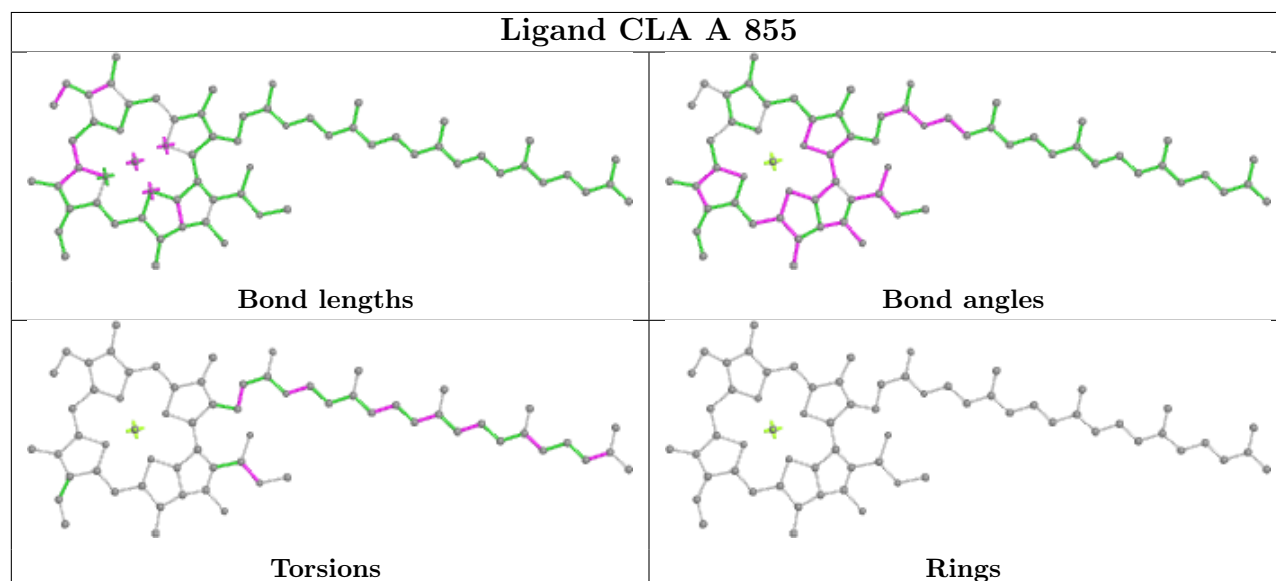
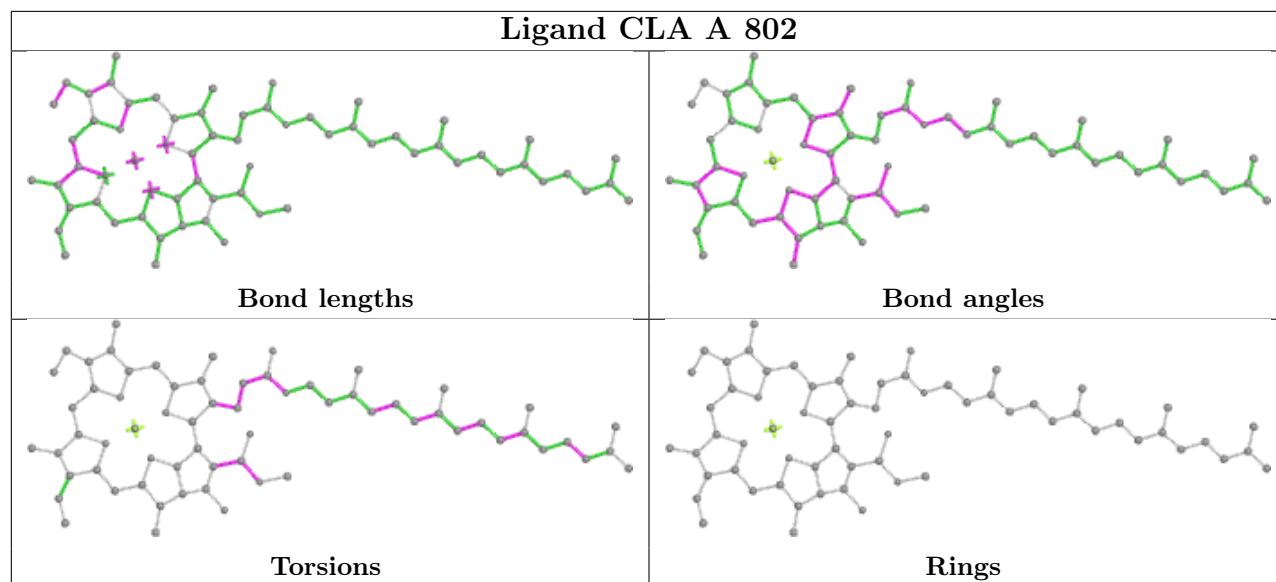
## Ligand CLA A 814

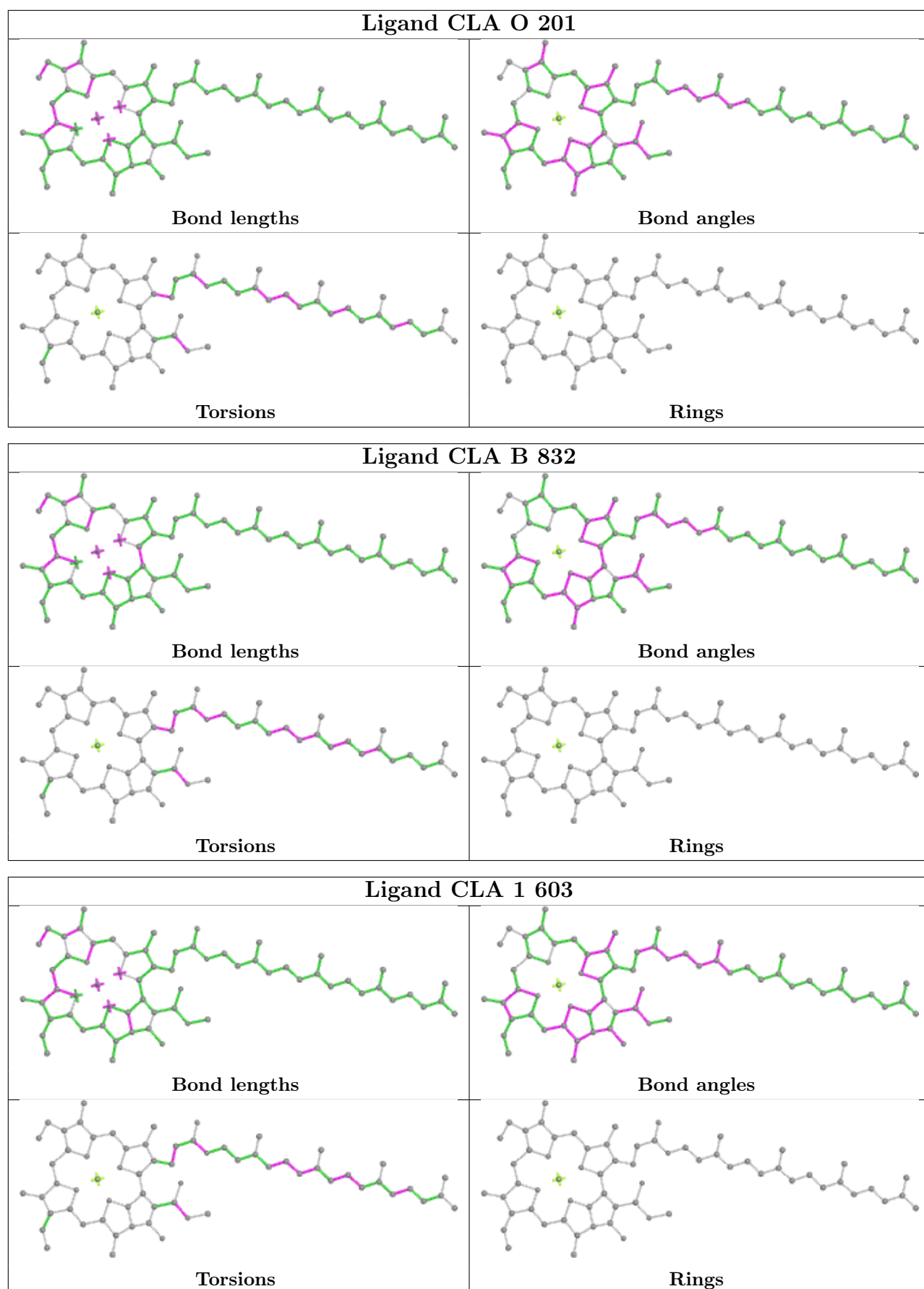


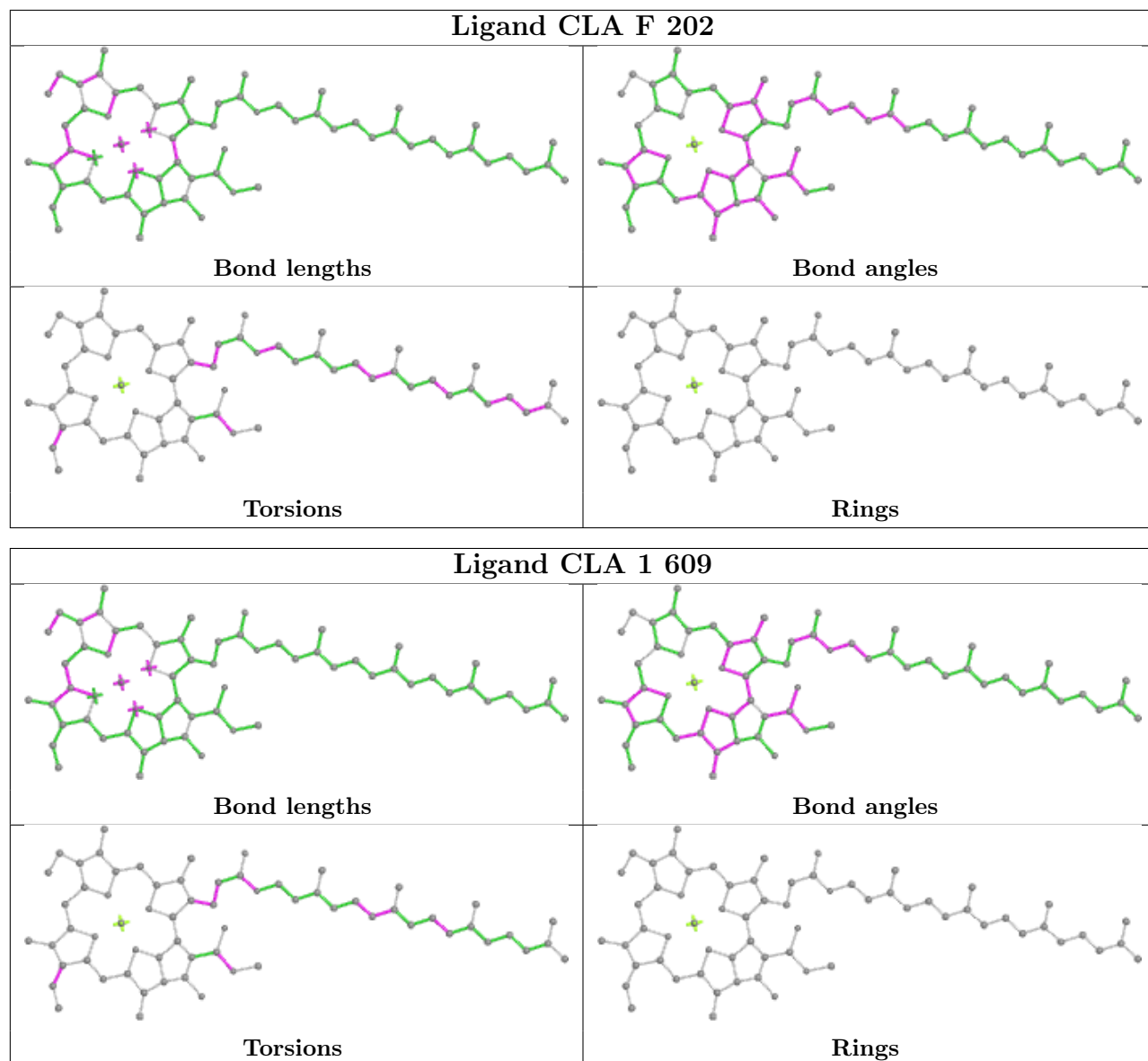


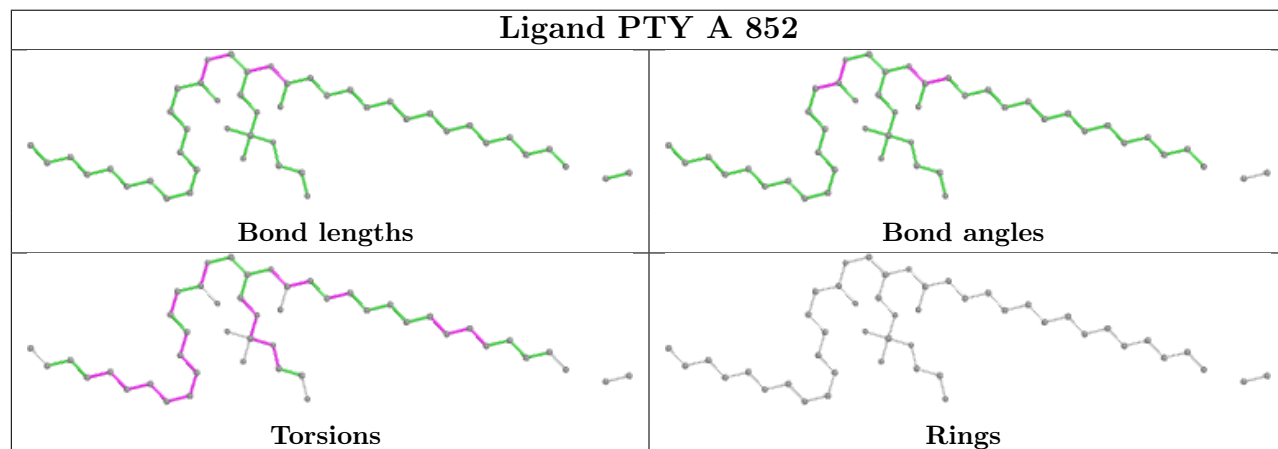
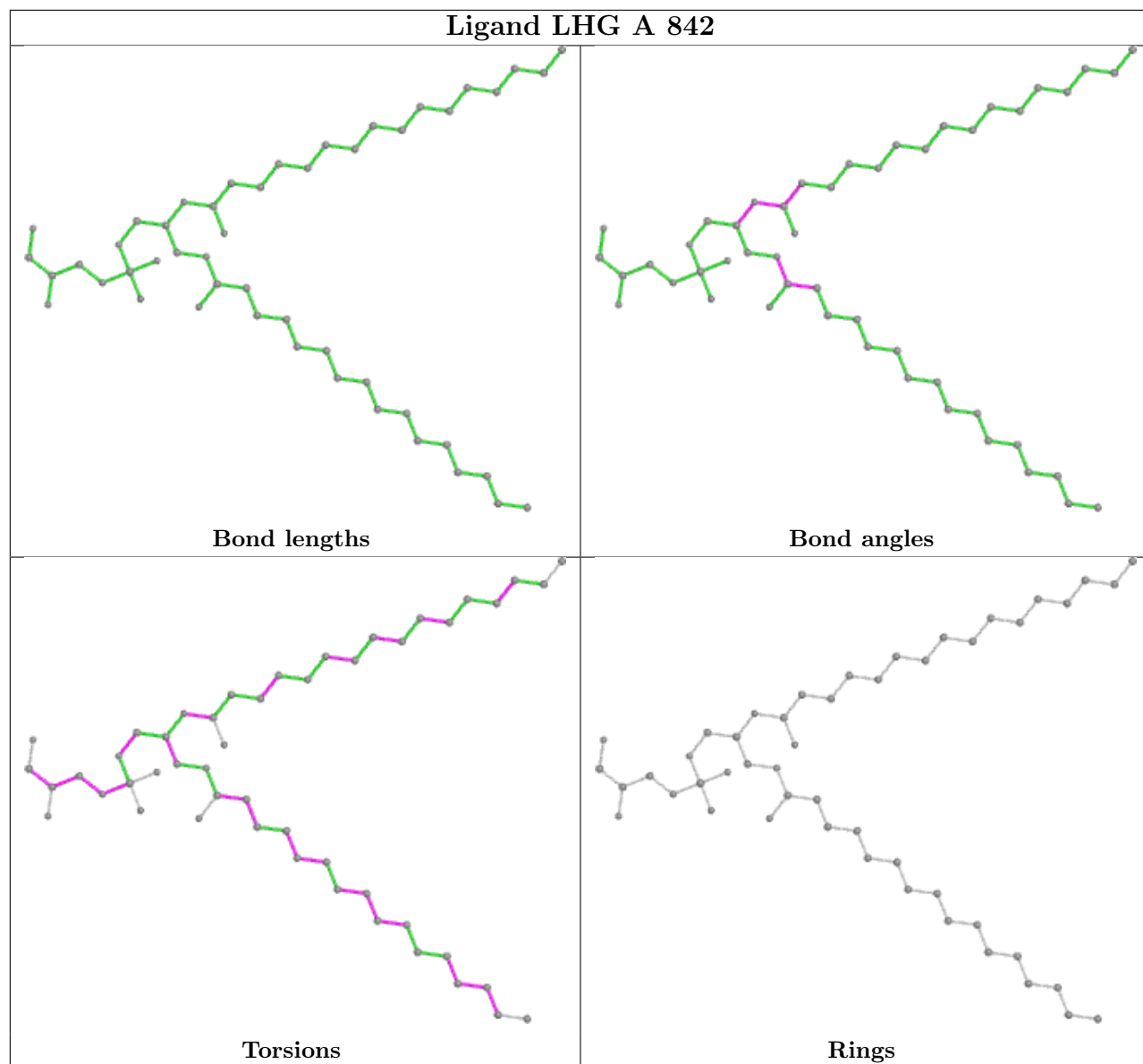




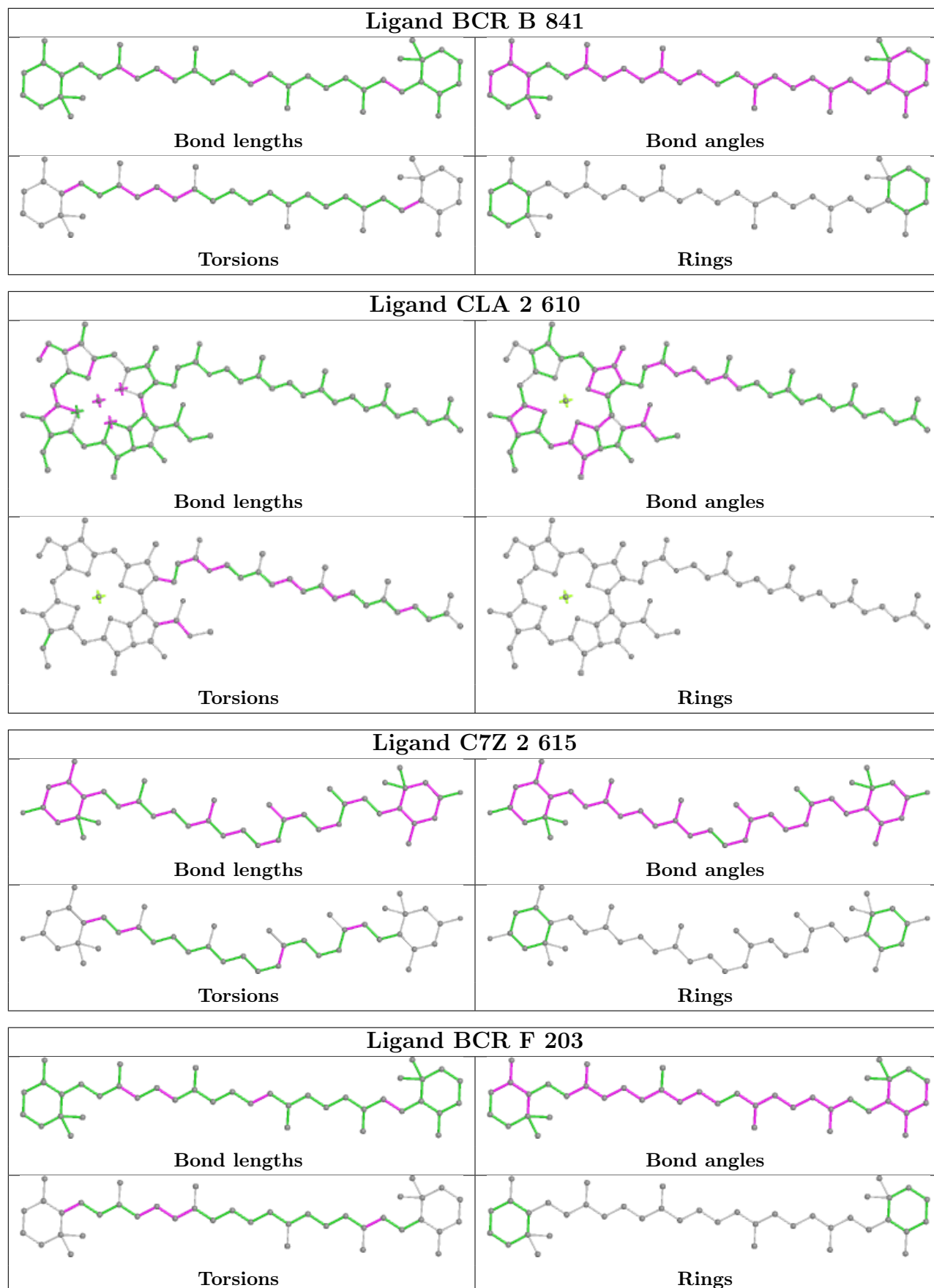


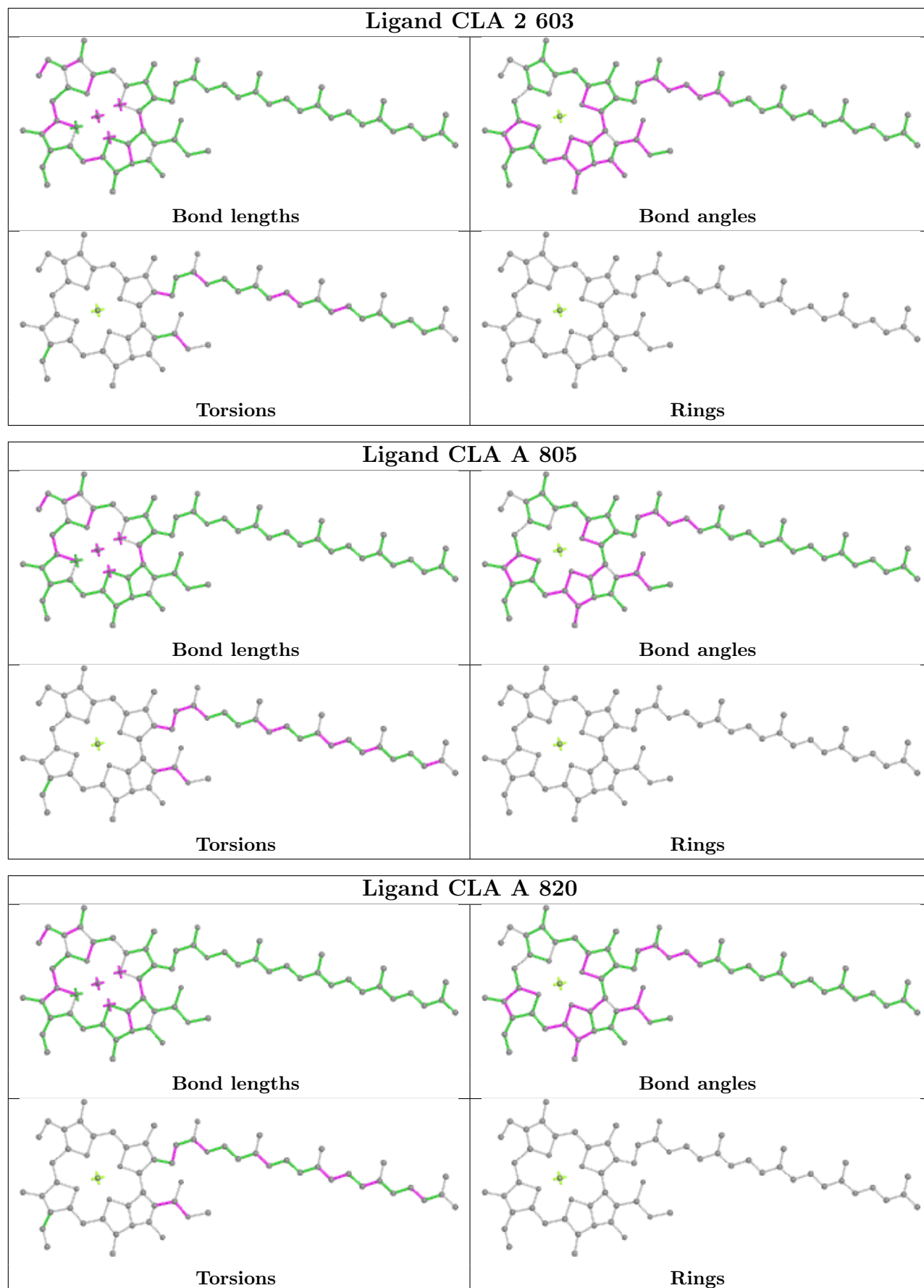


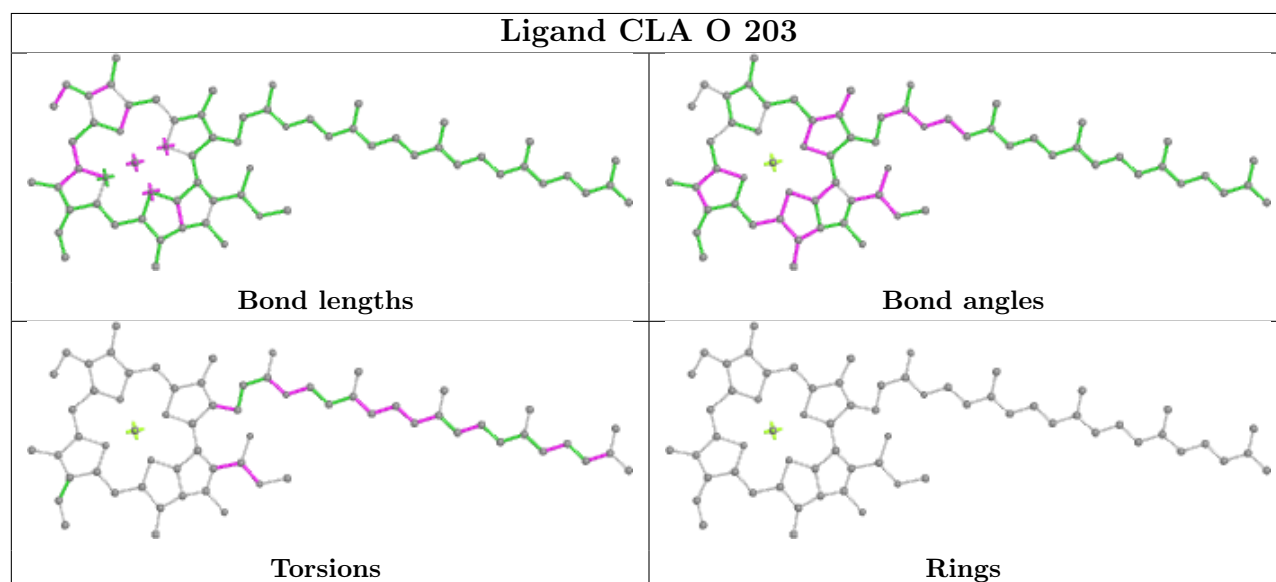
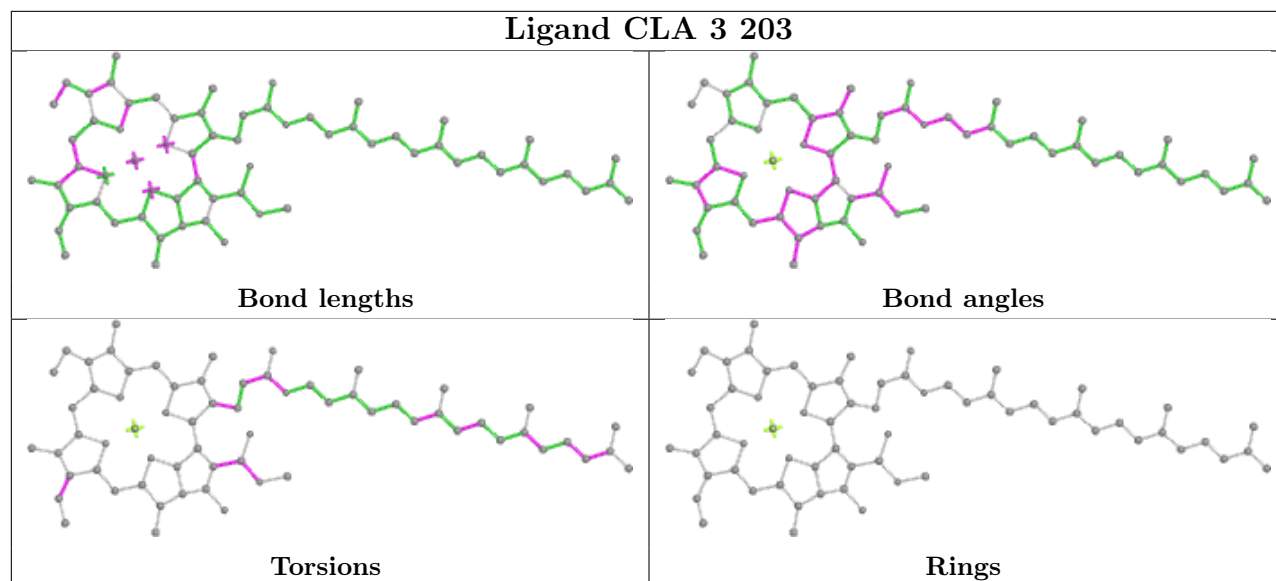
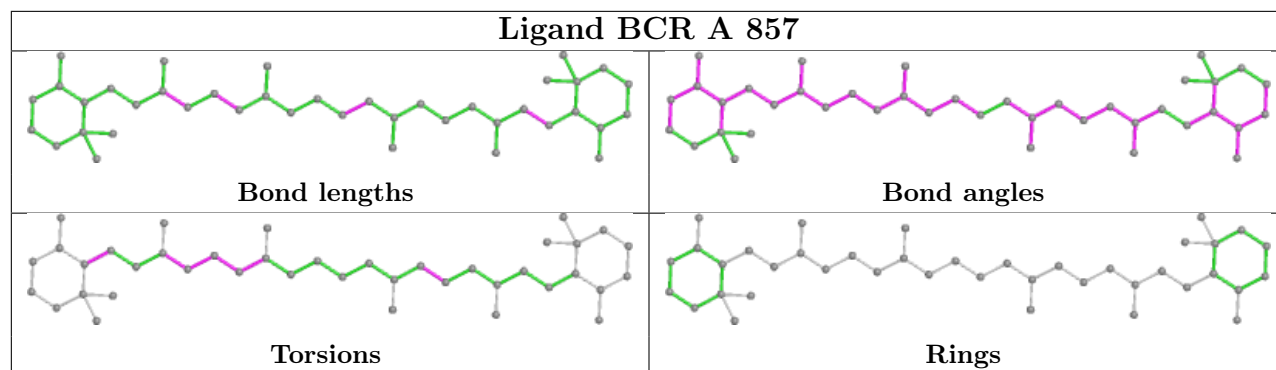


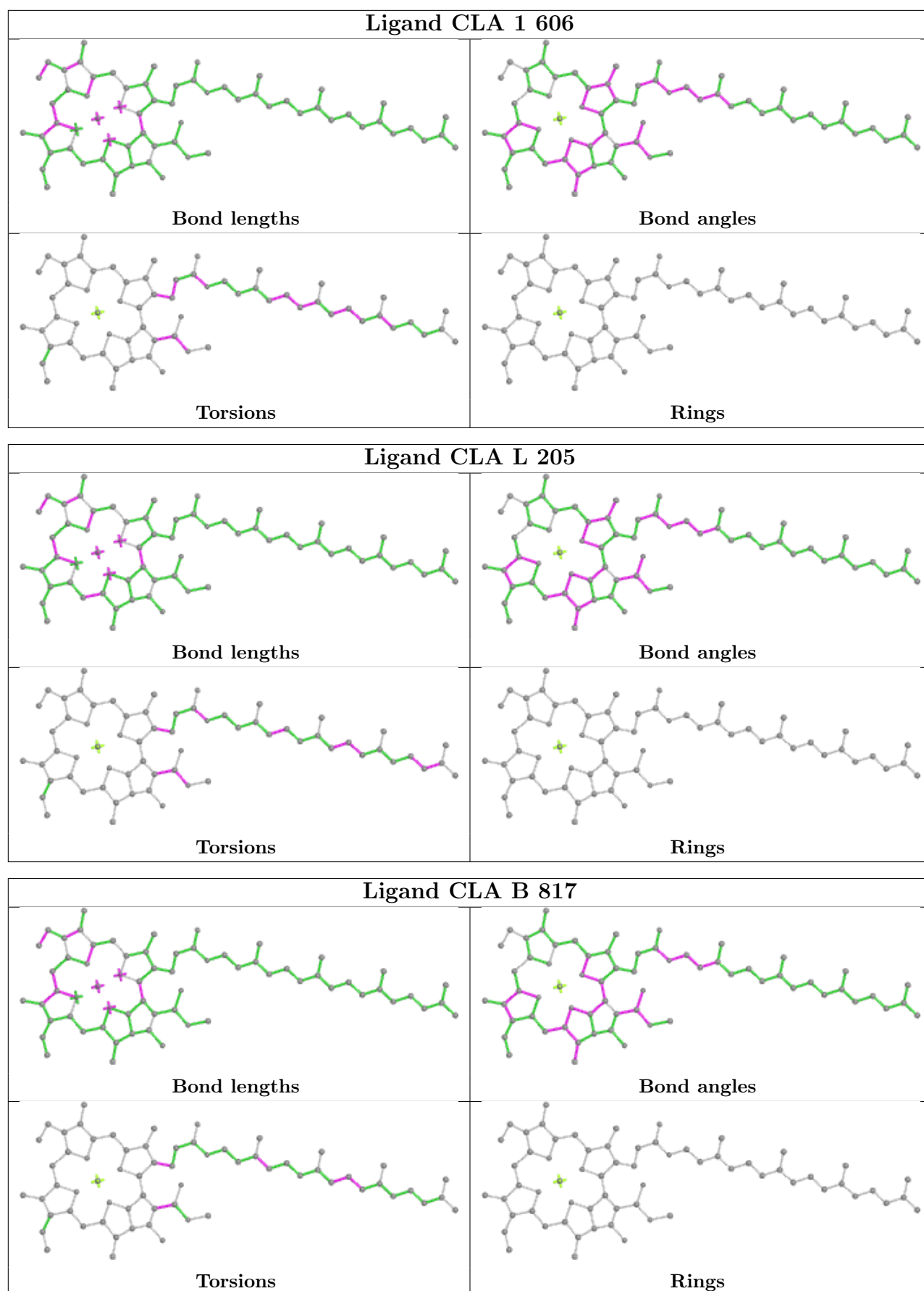


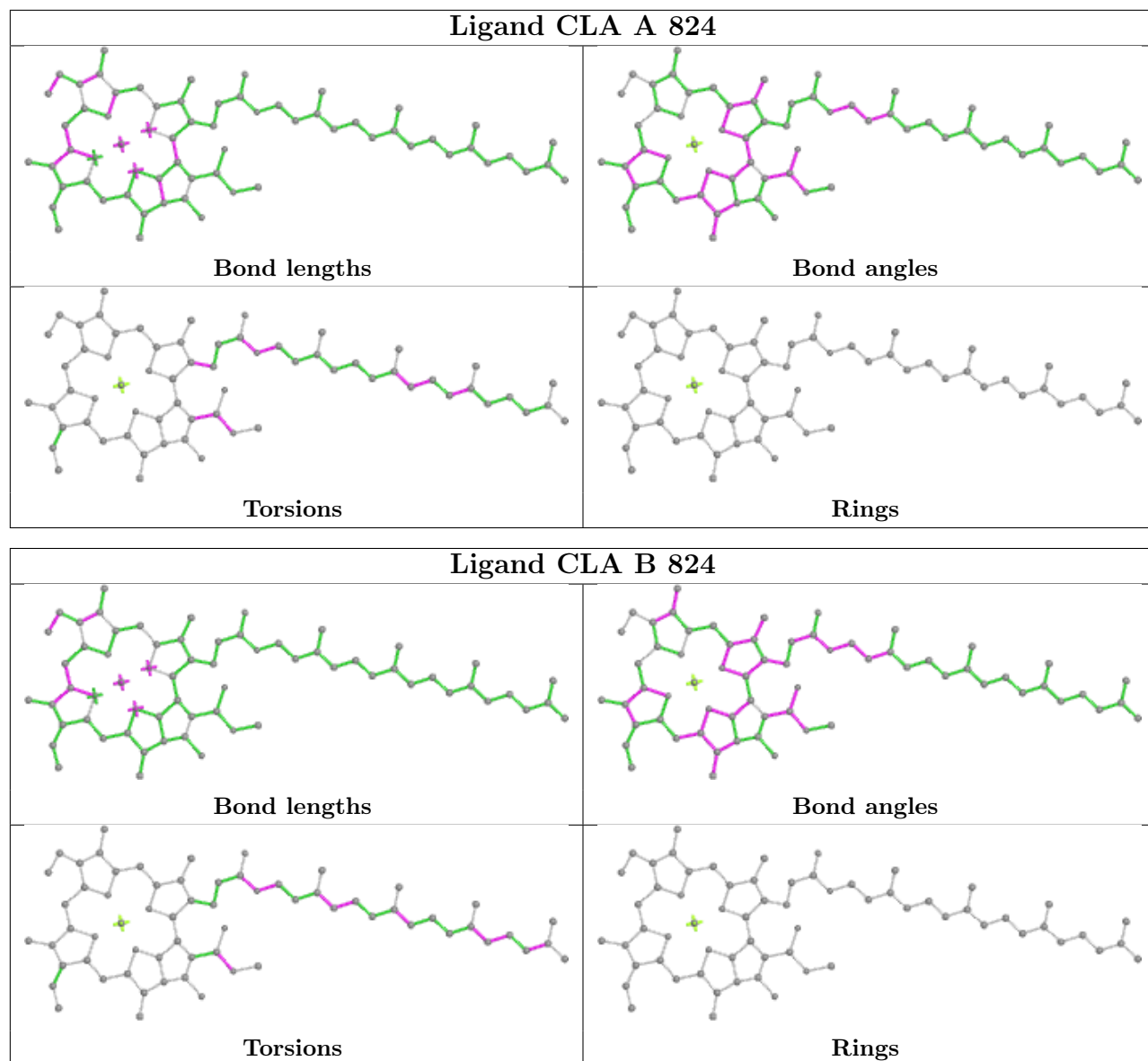


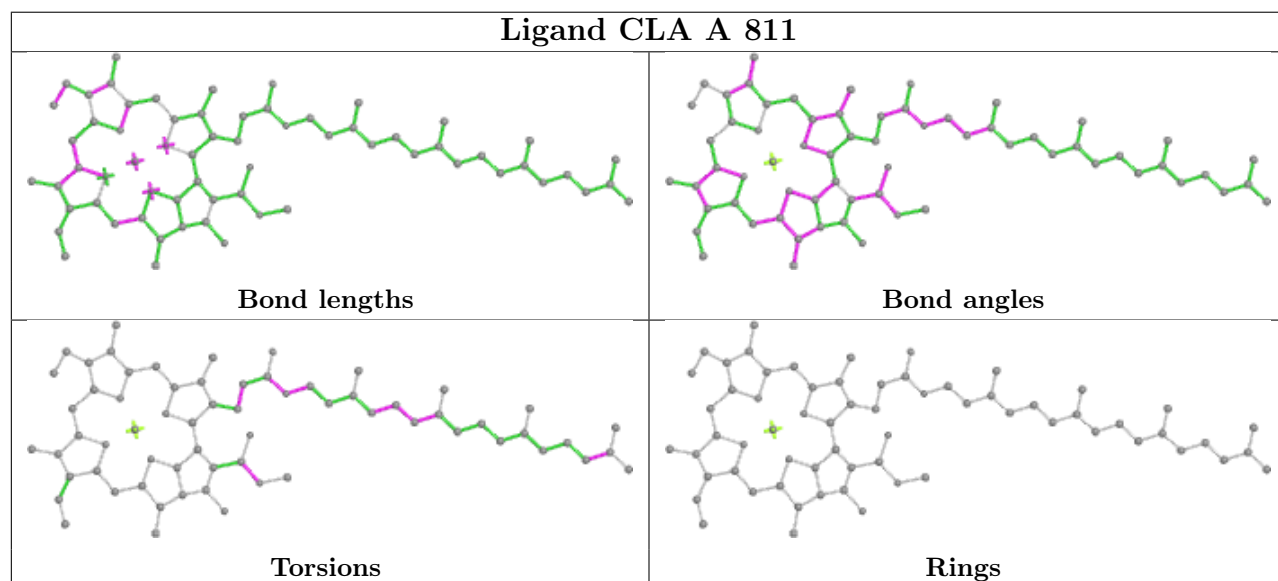
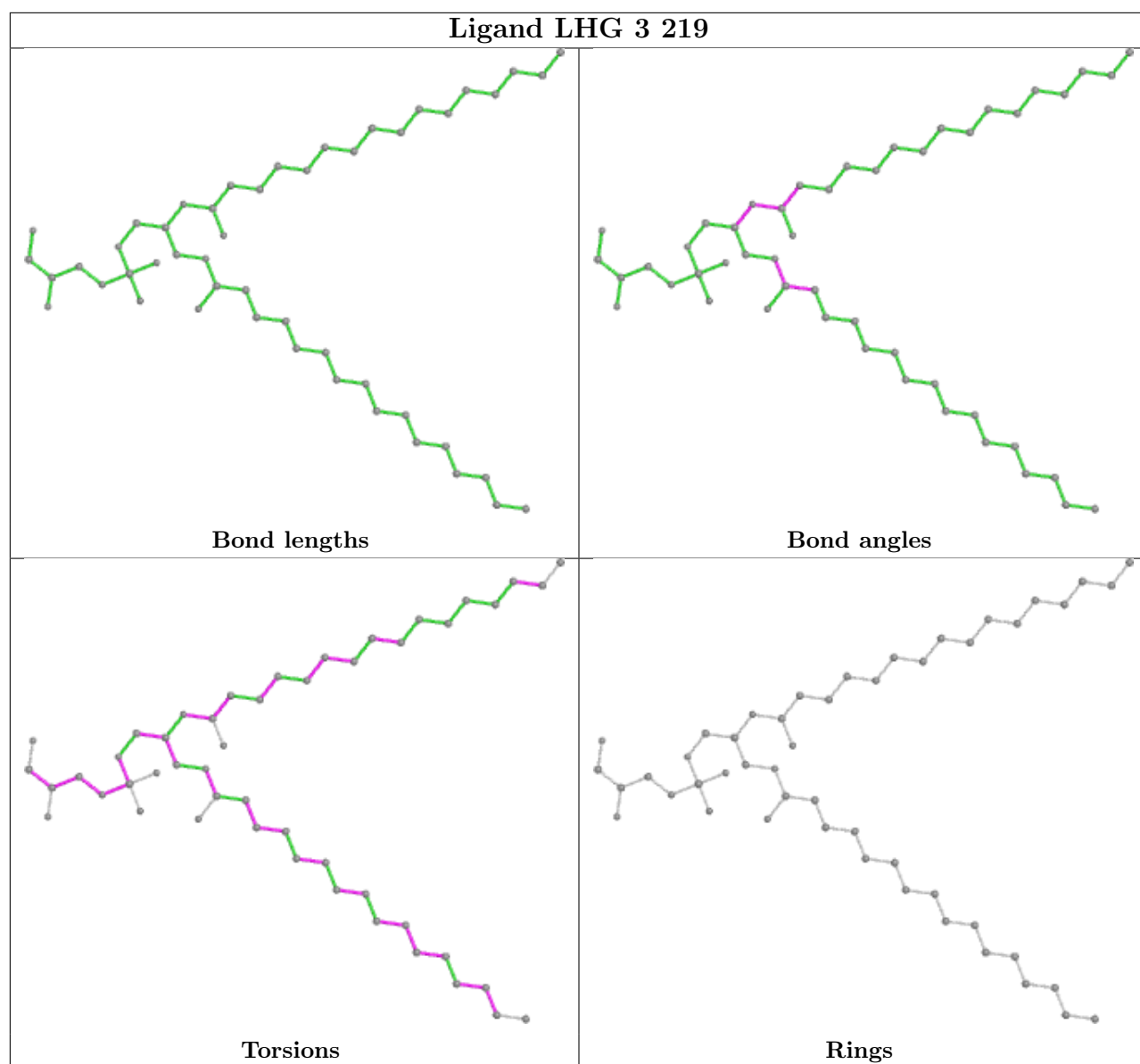


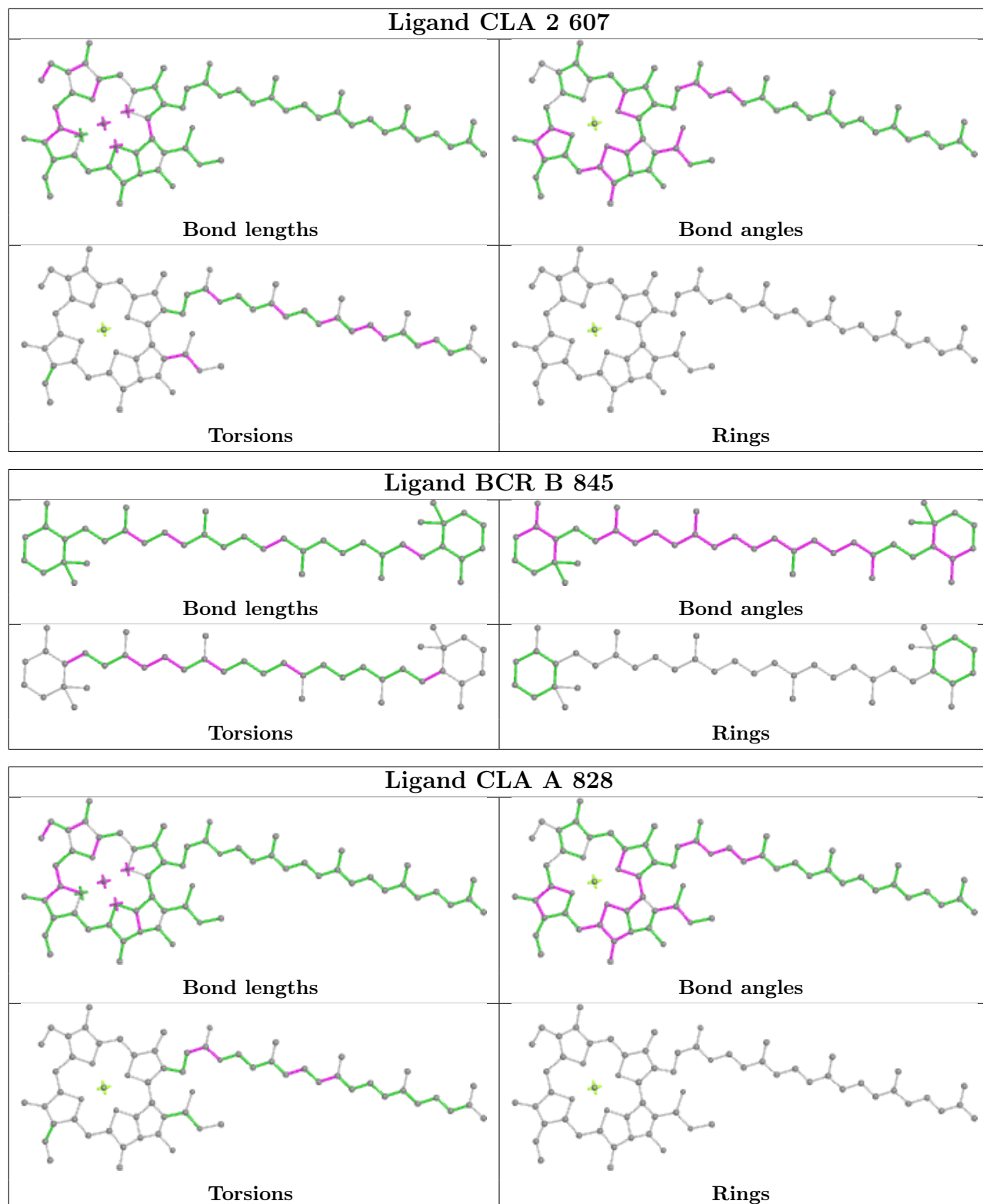


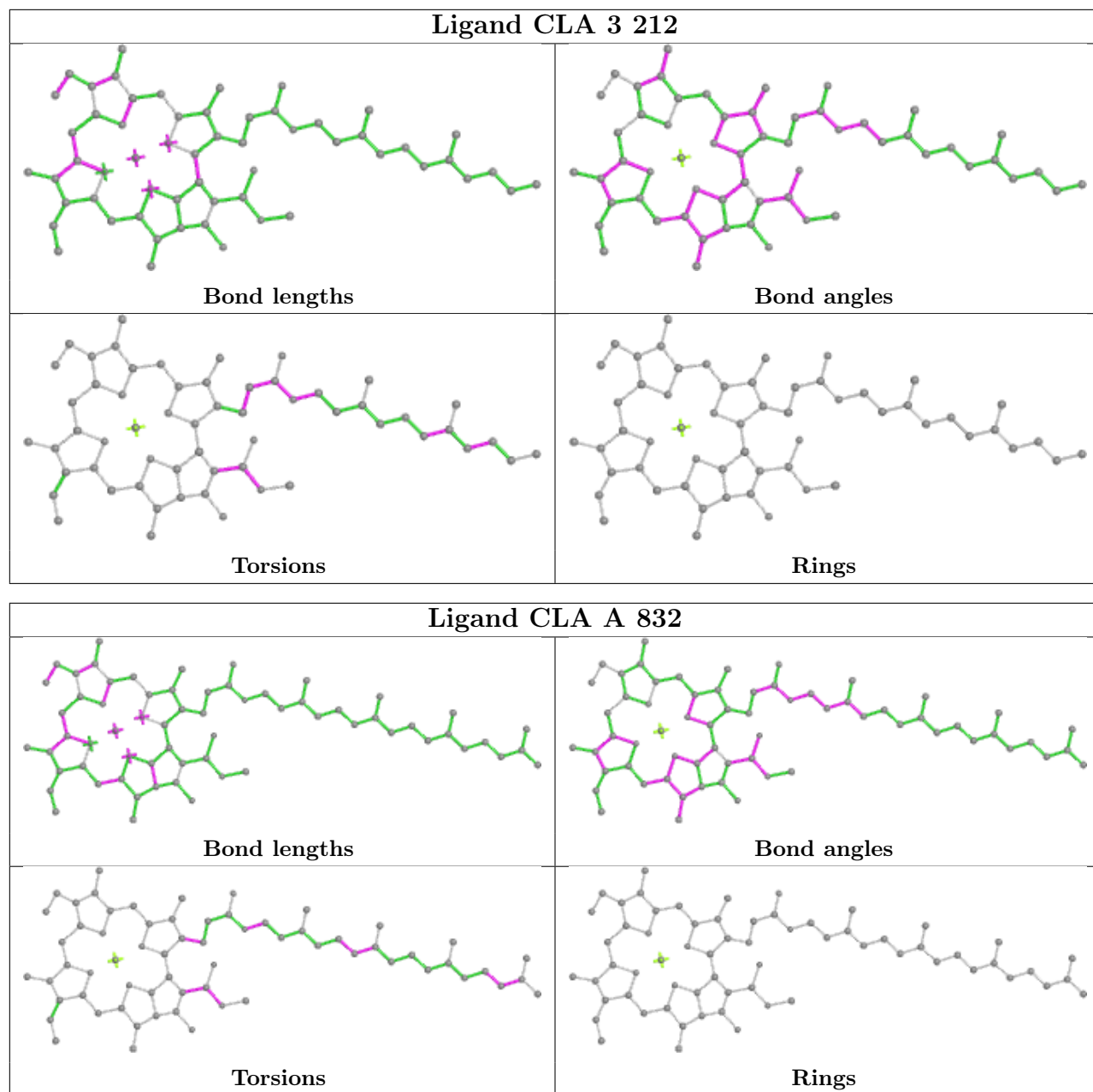




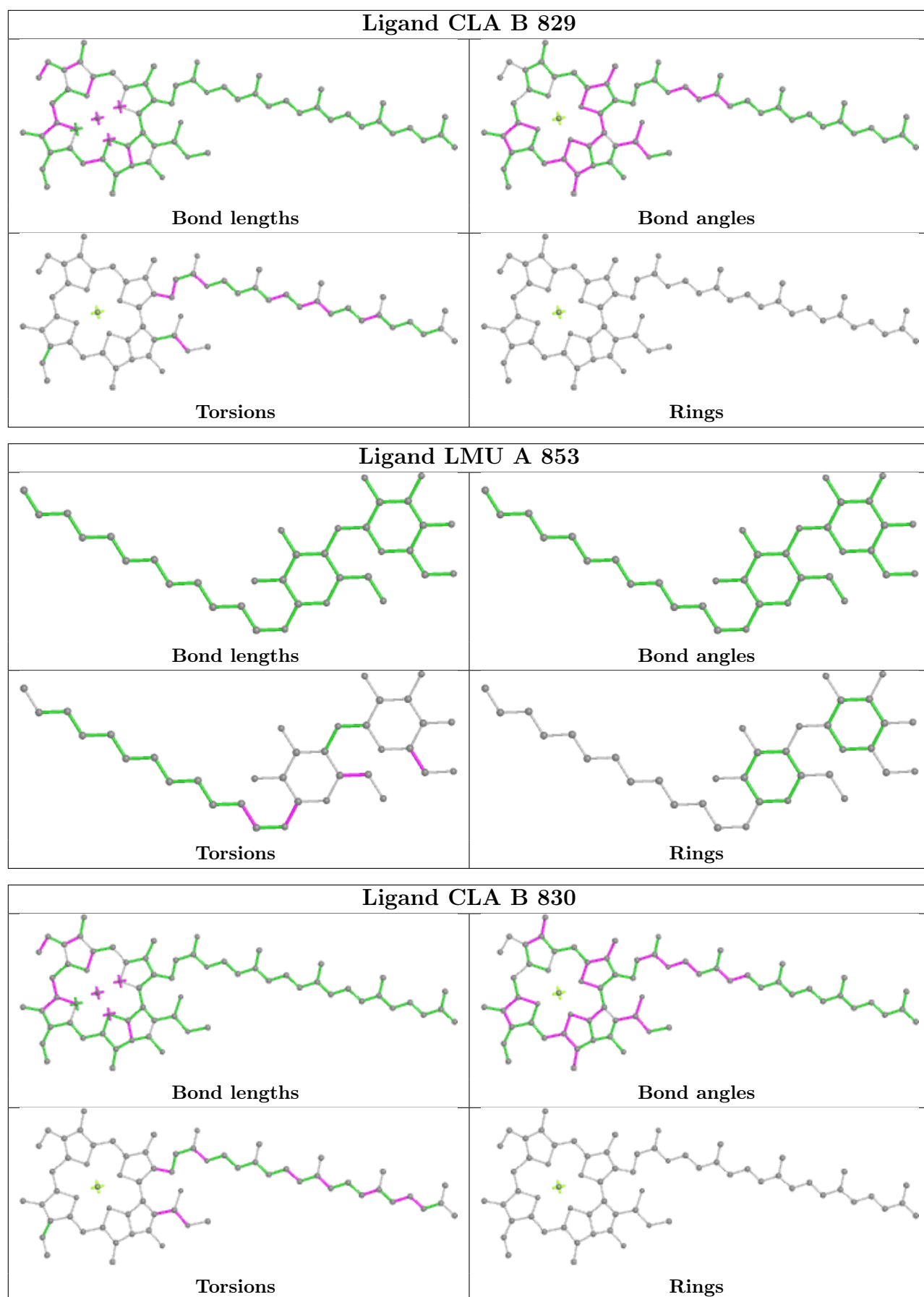


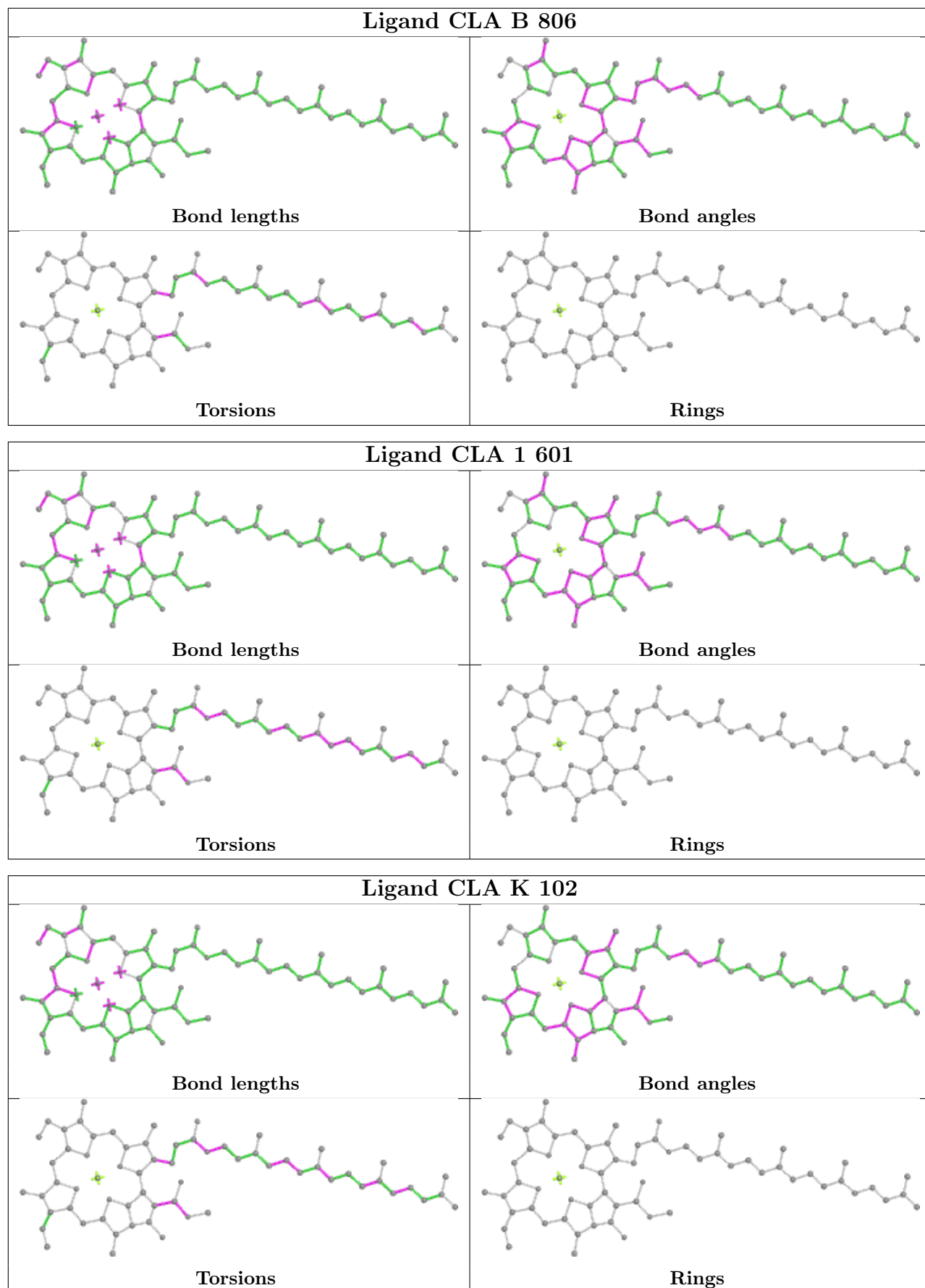


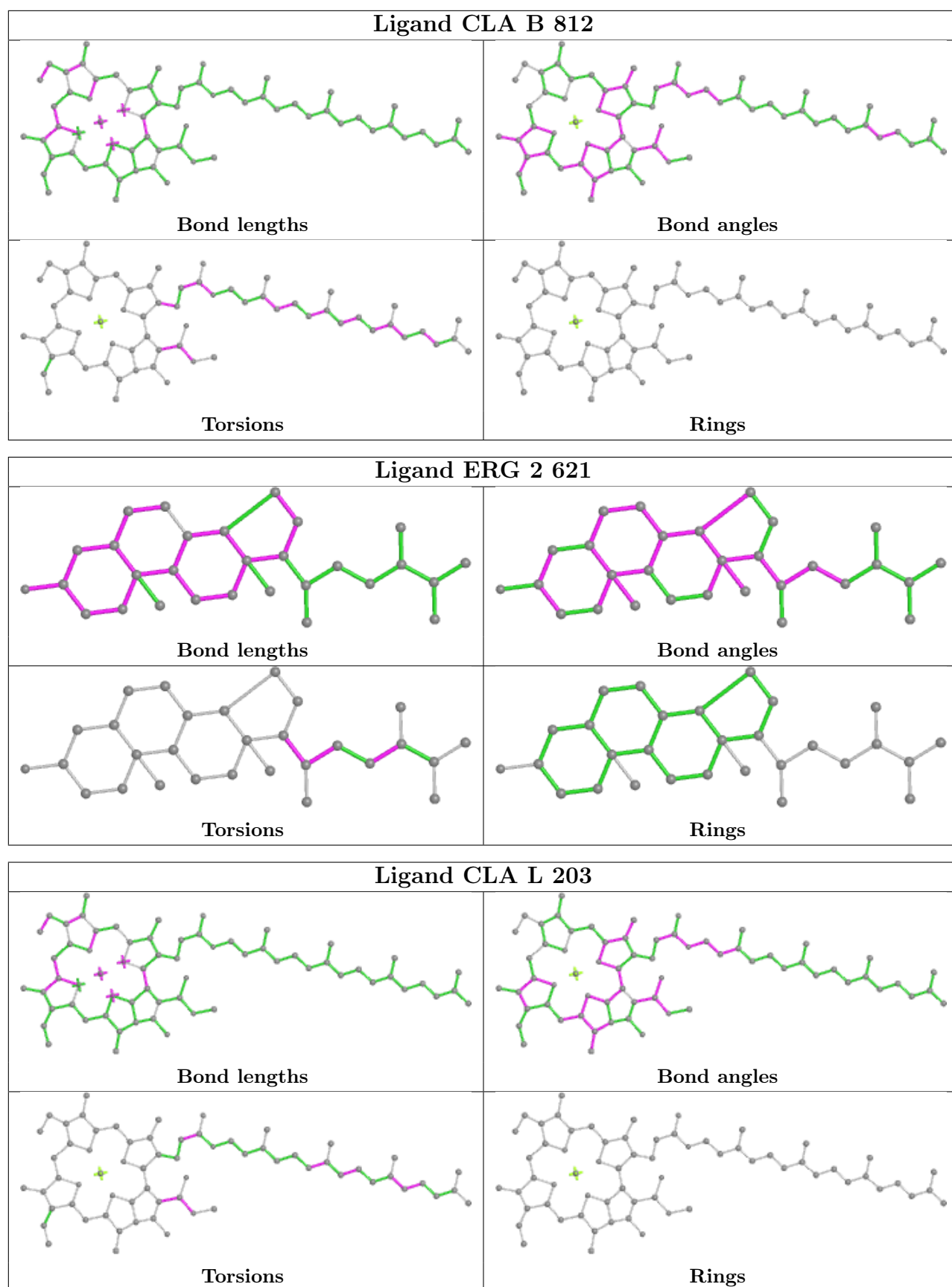


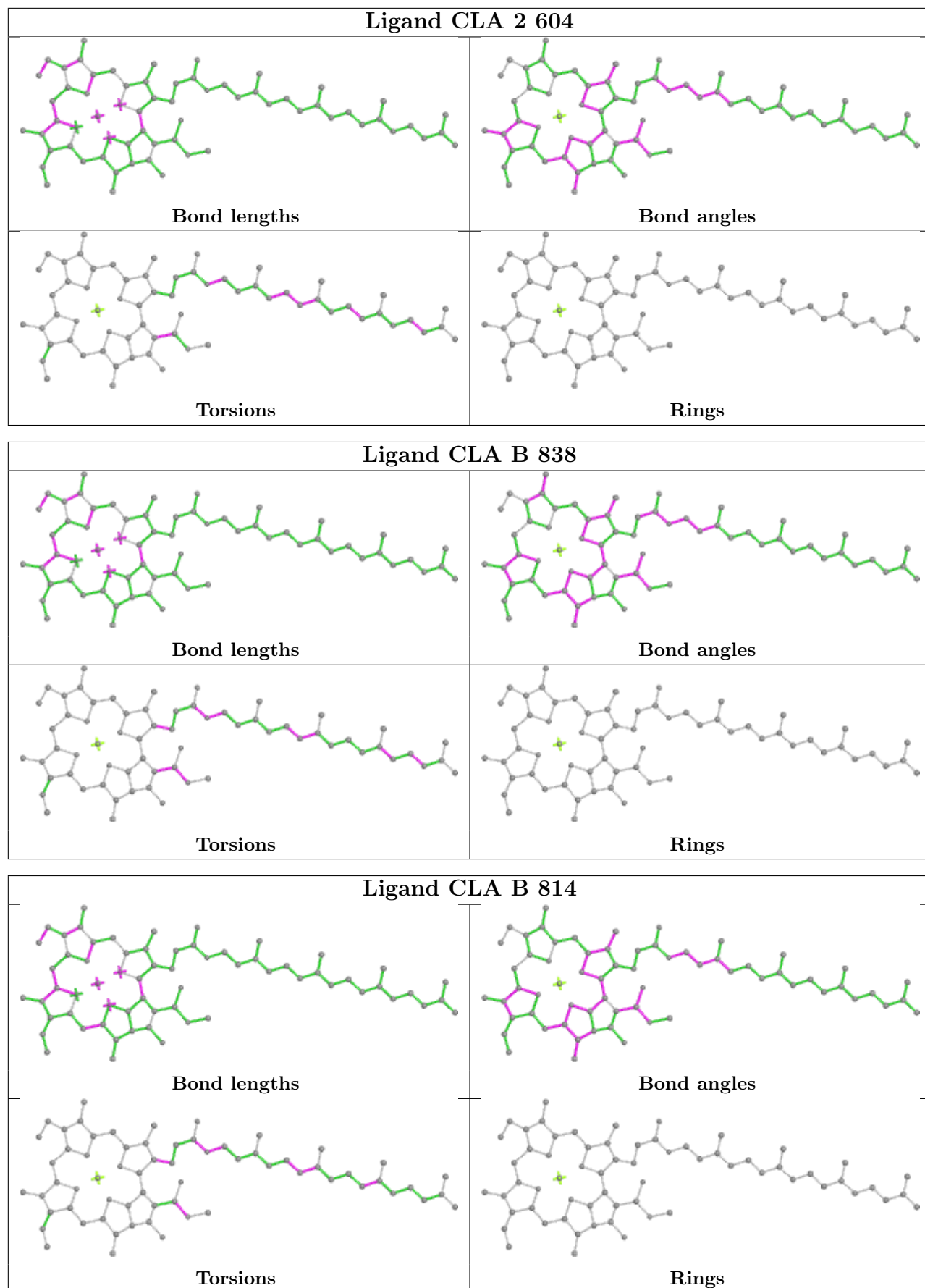


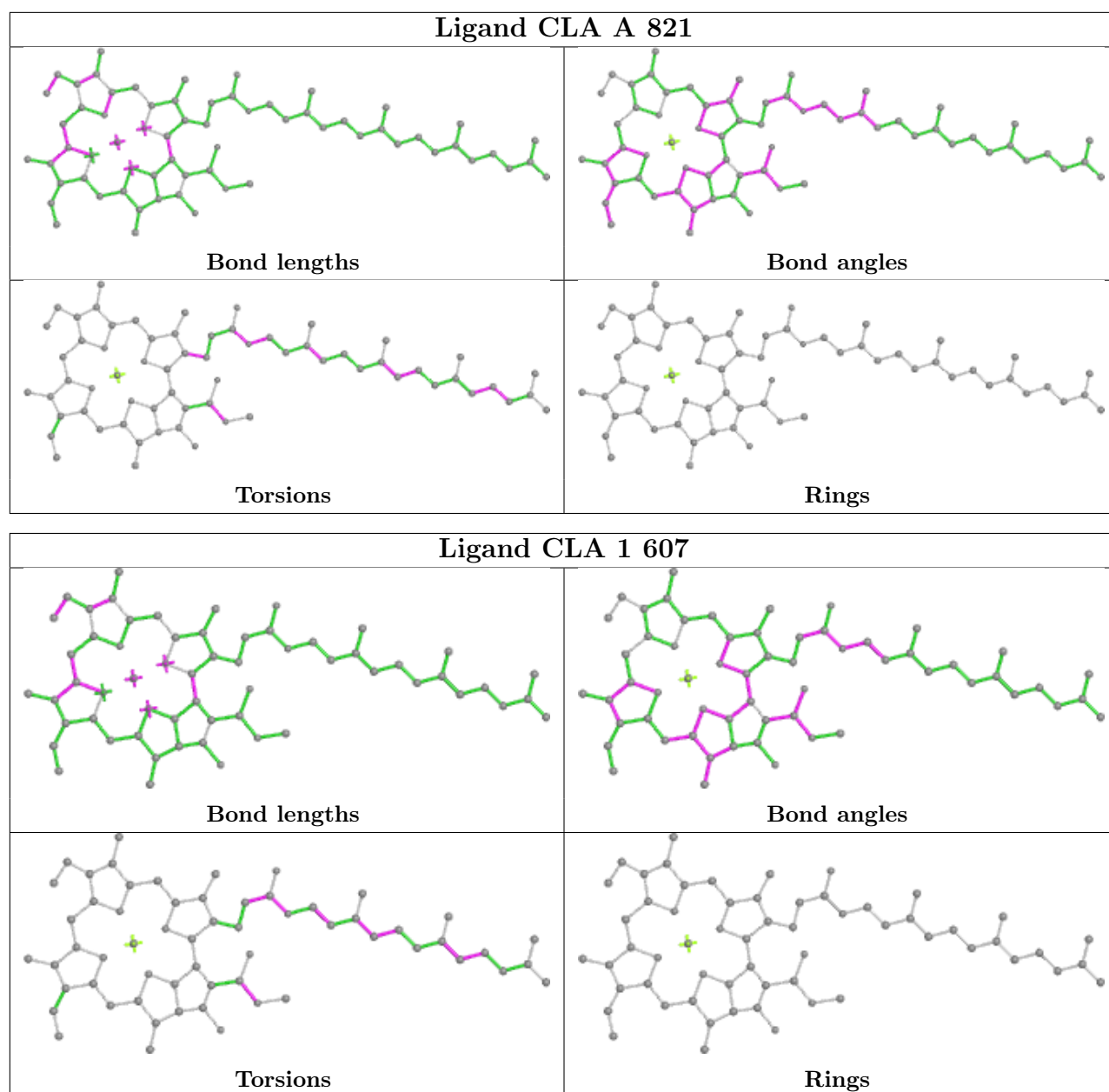


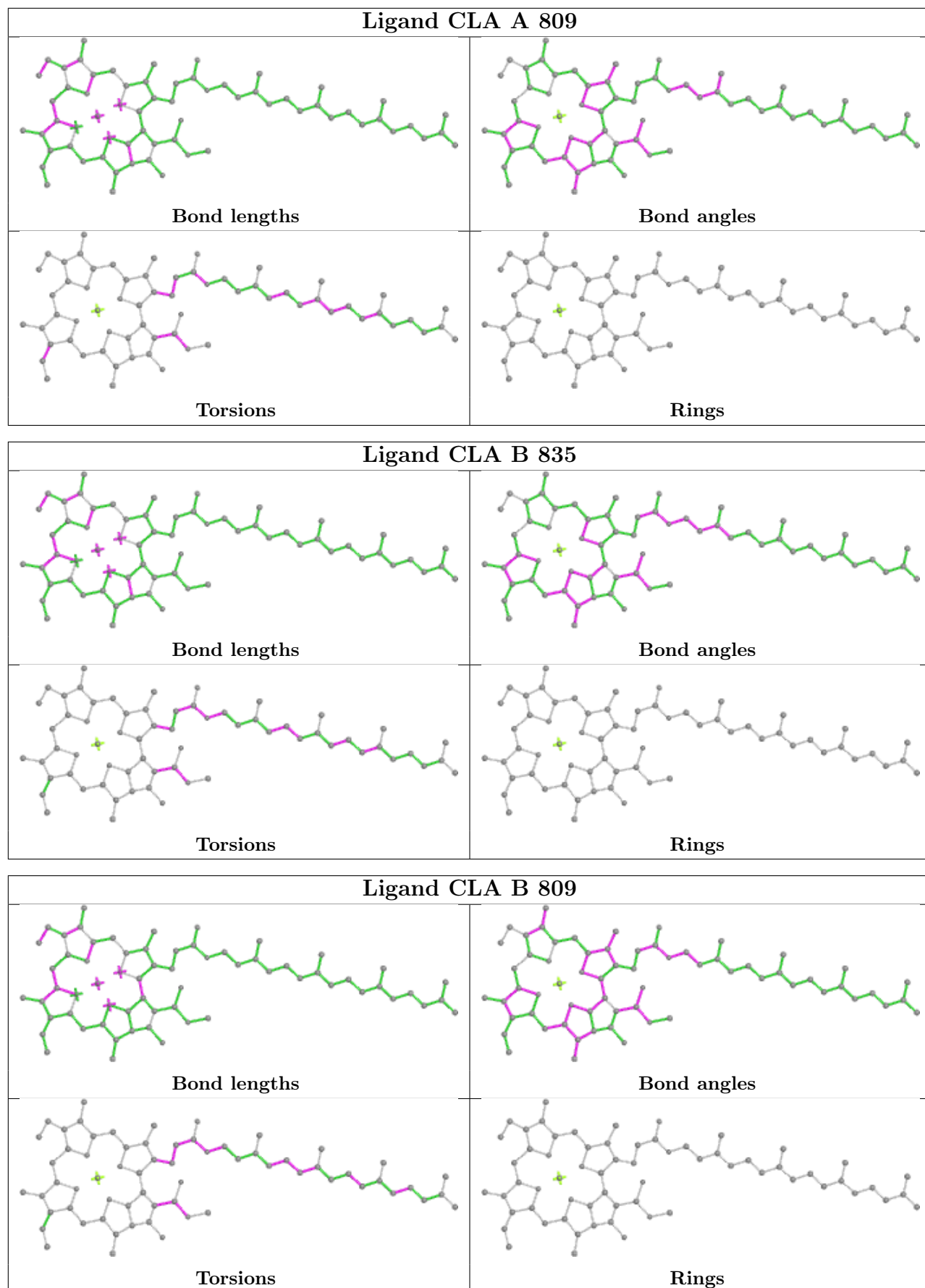


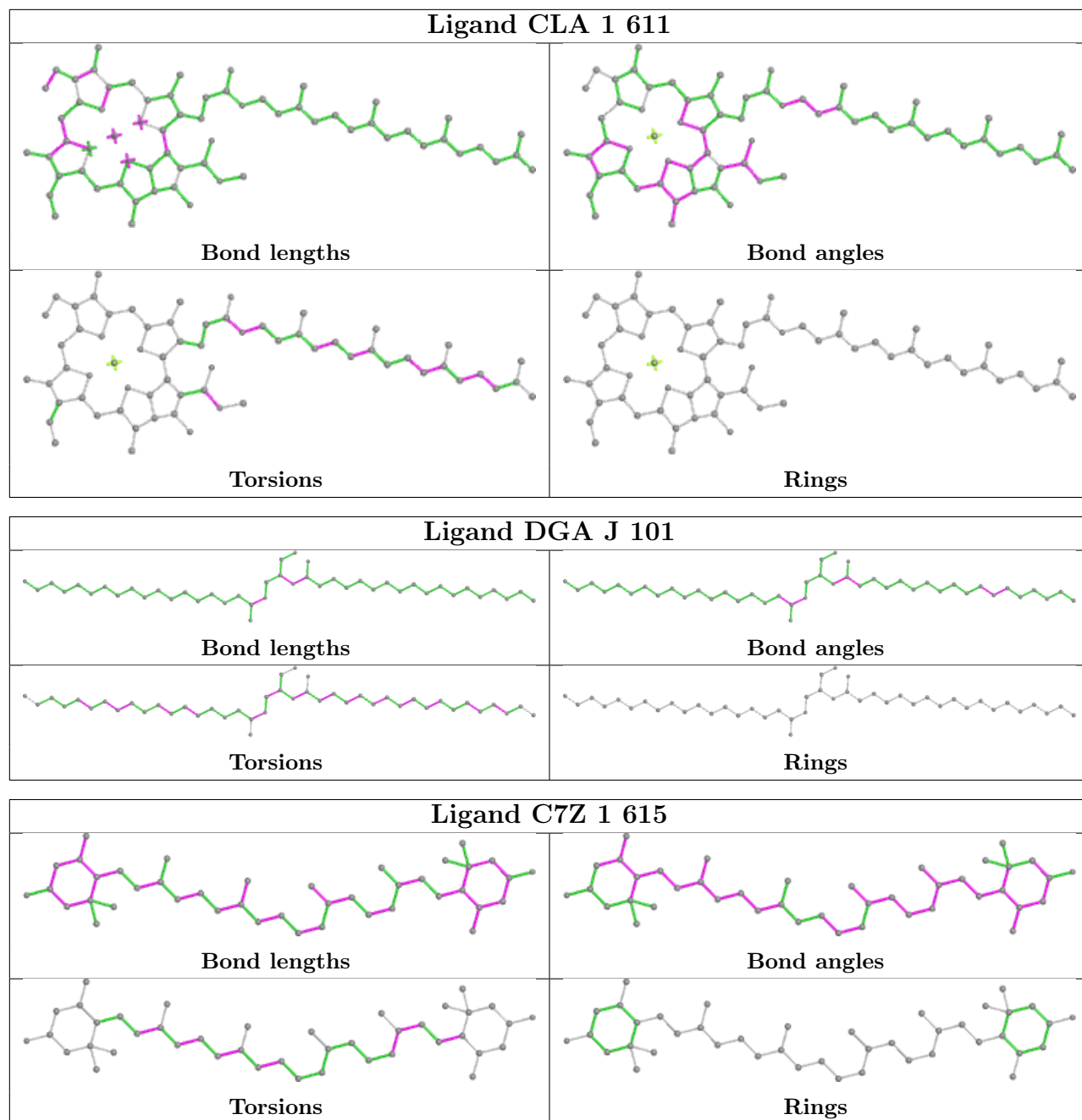


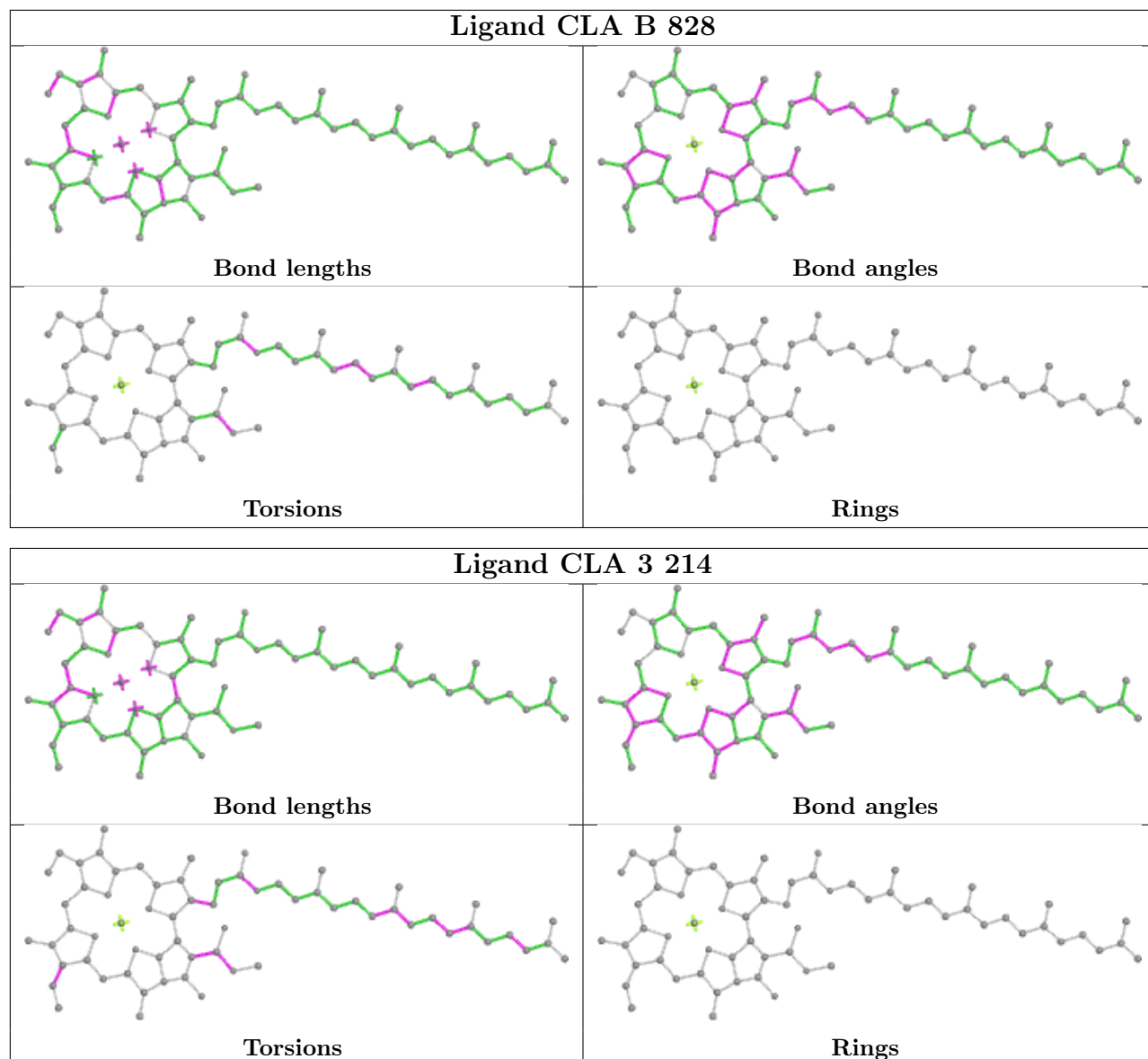




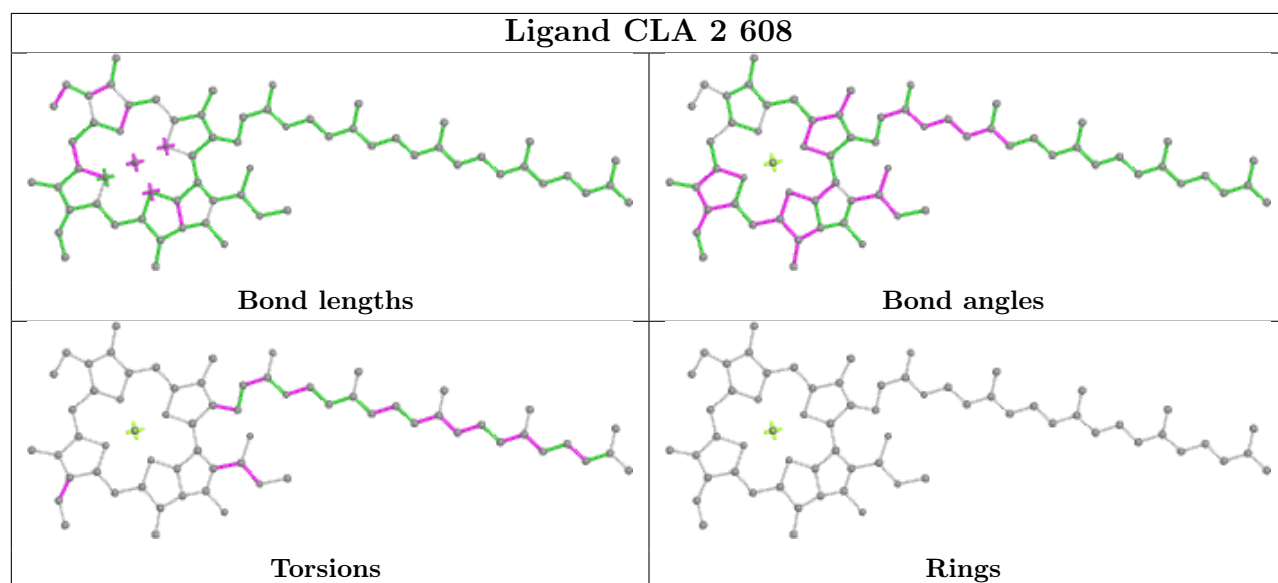
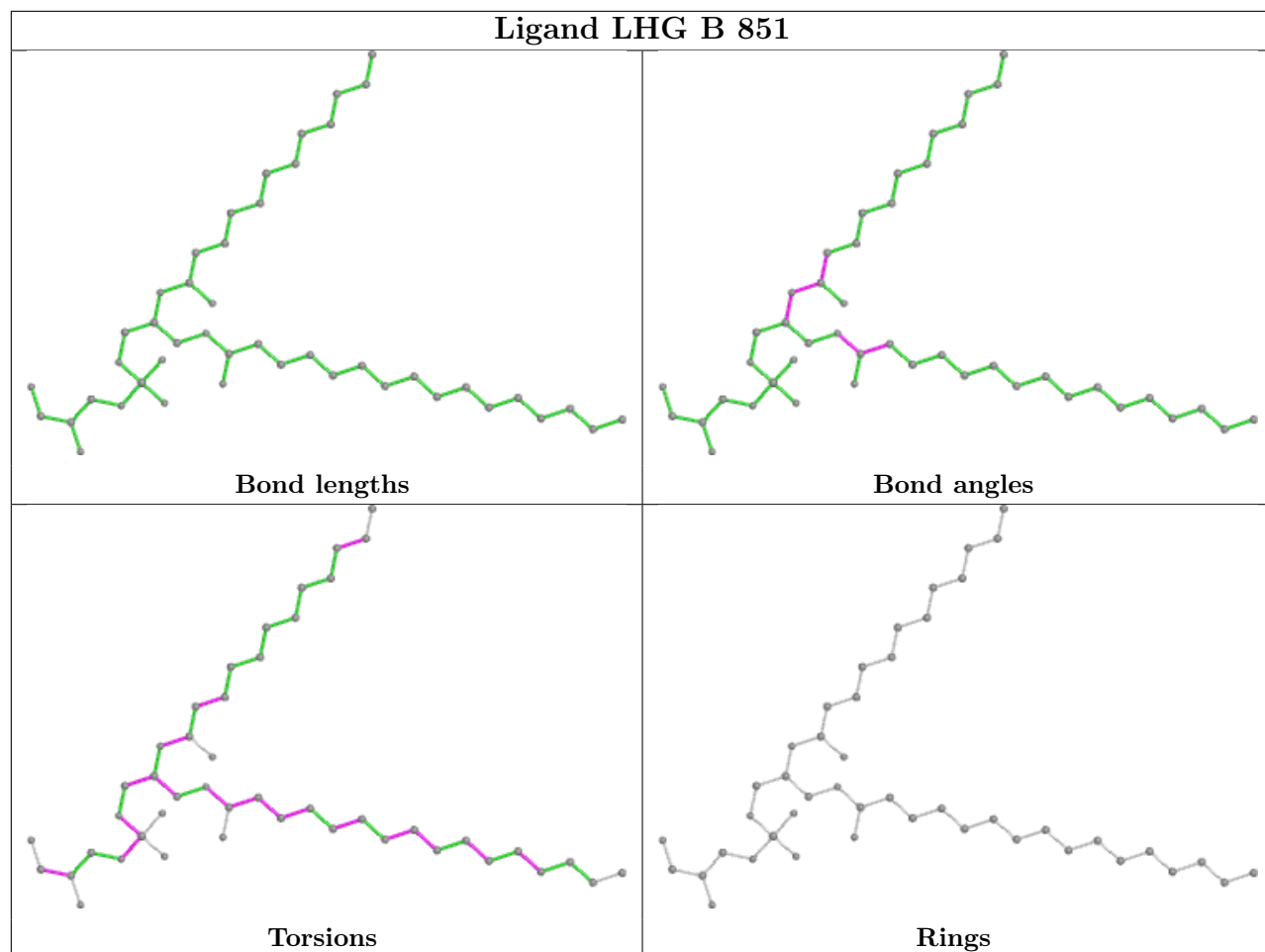


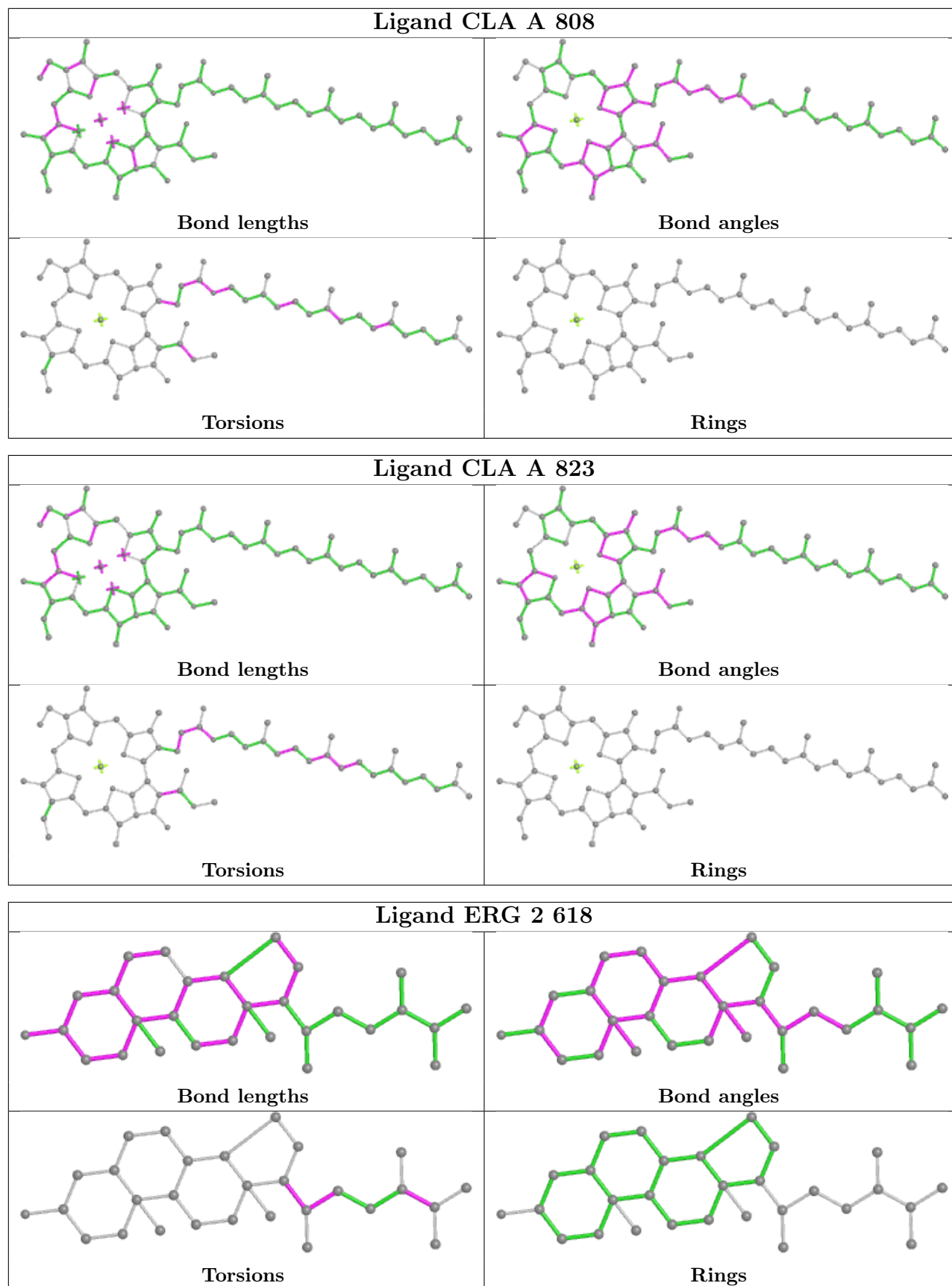


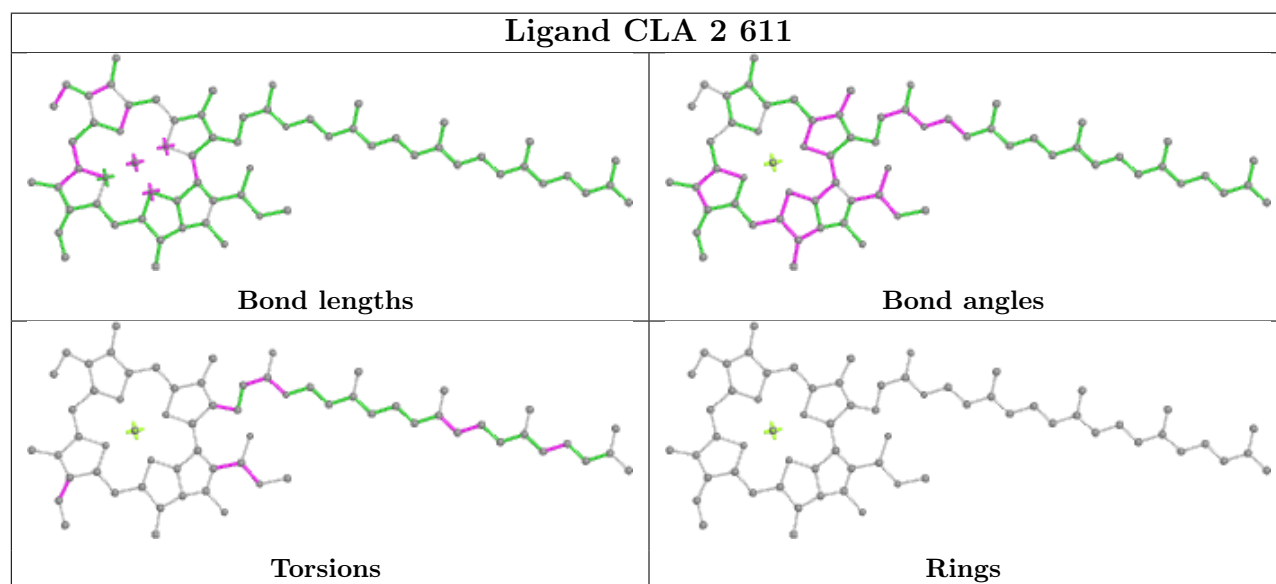
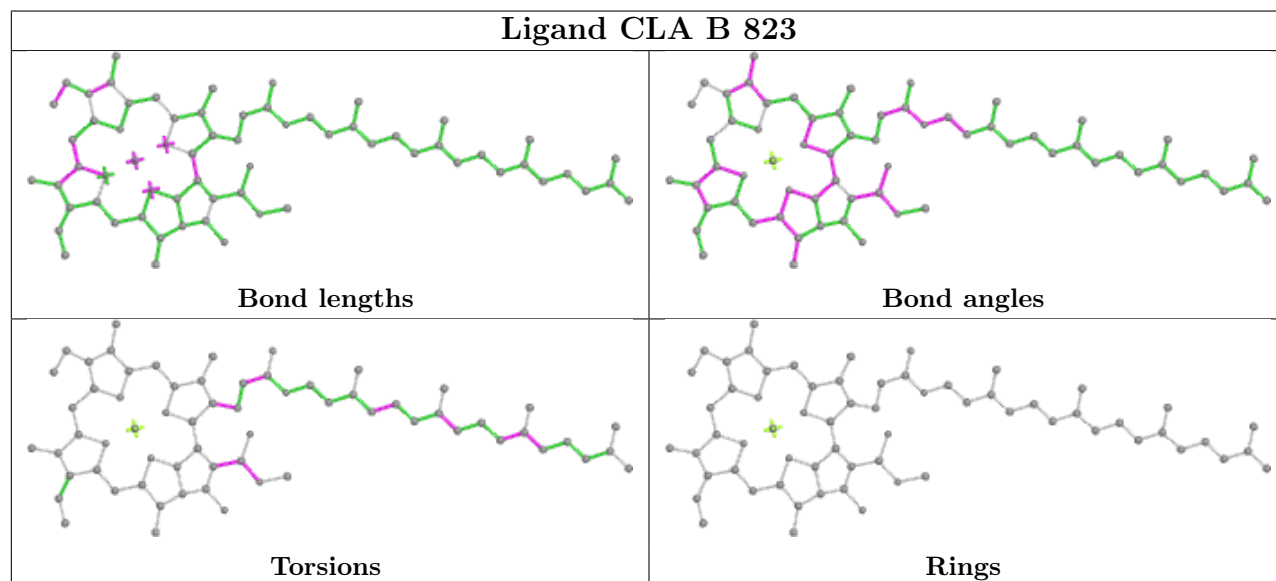
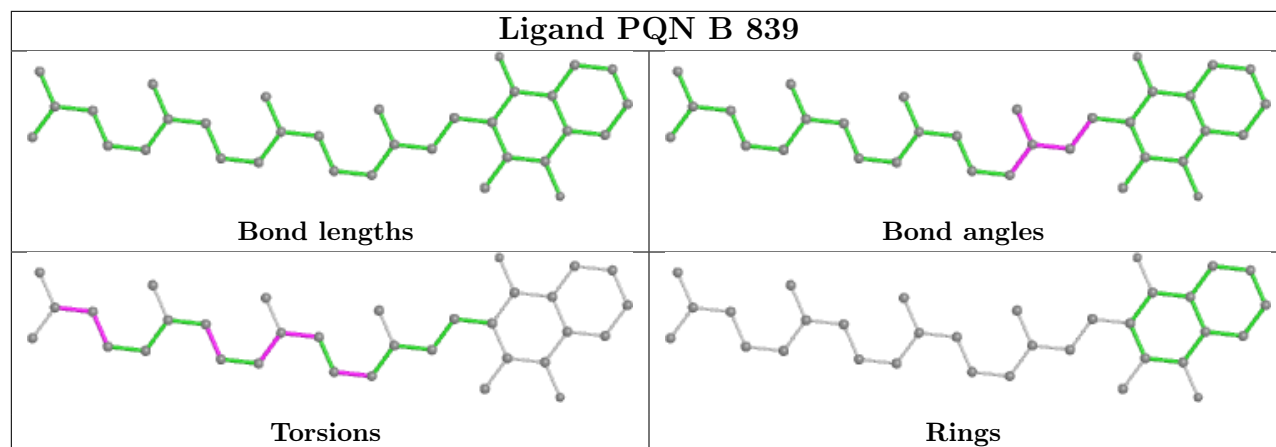


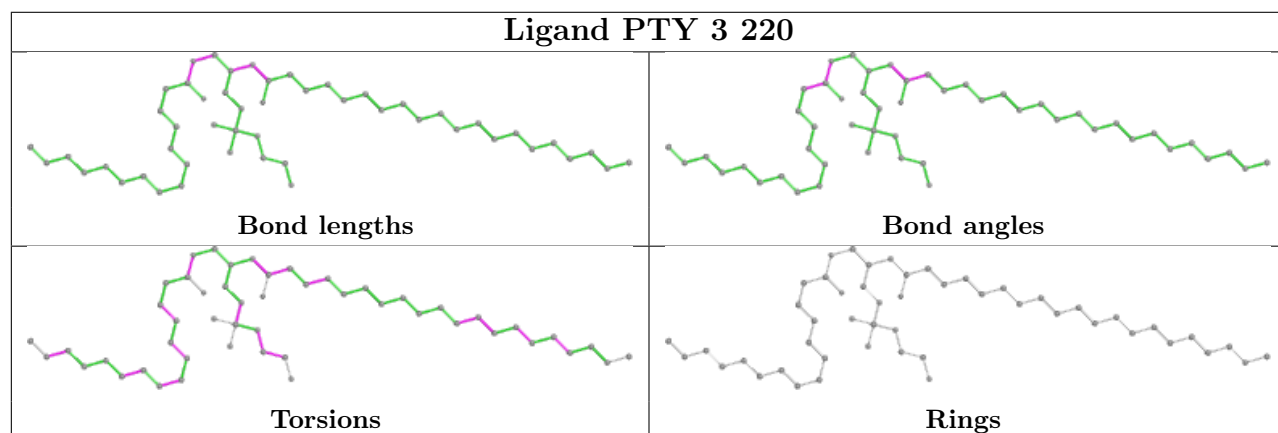
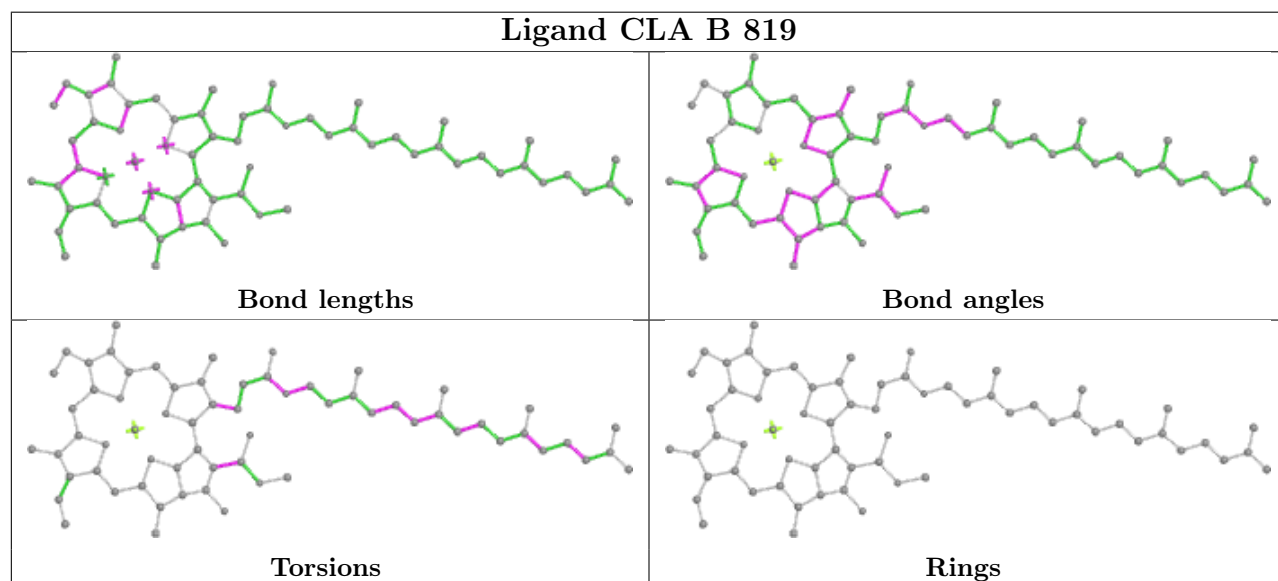
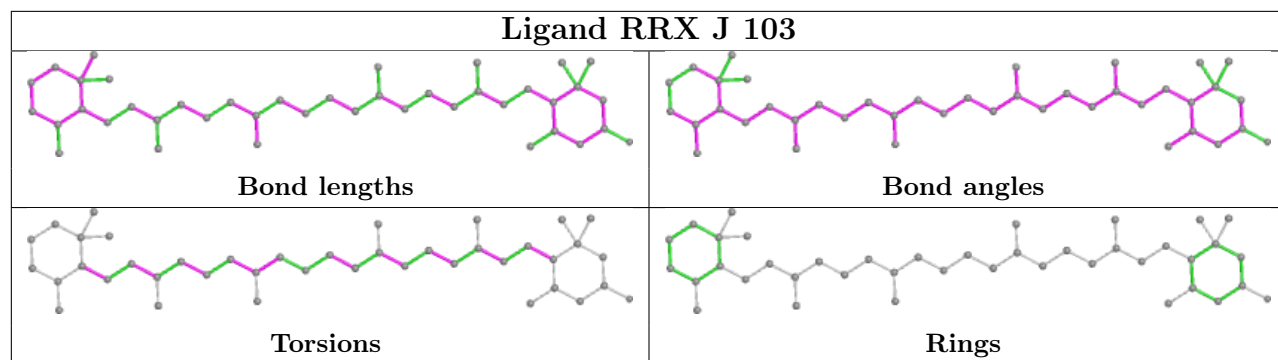


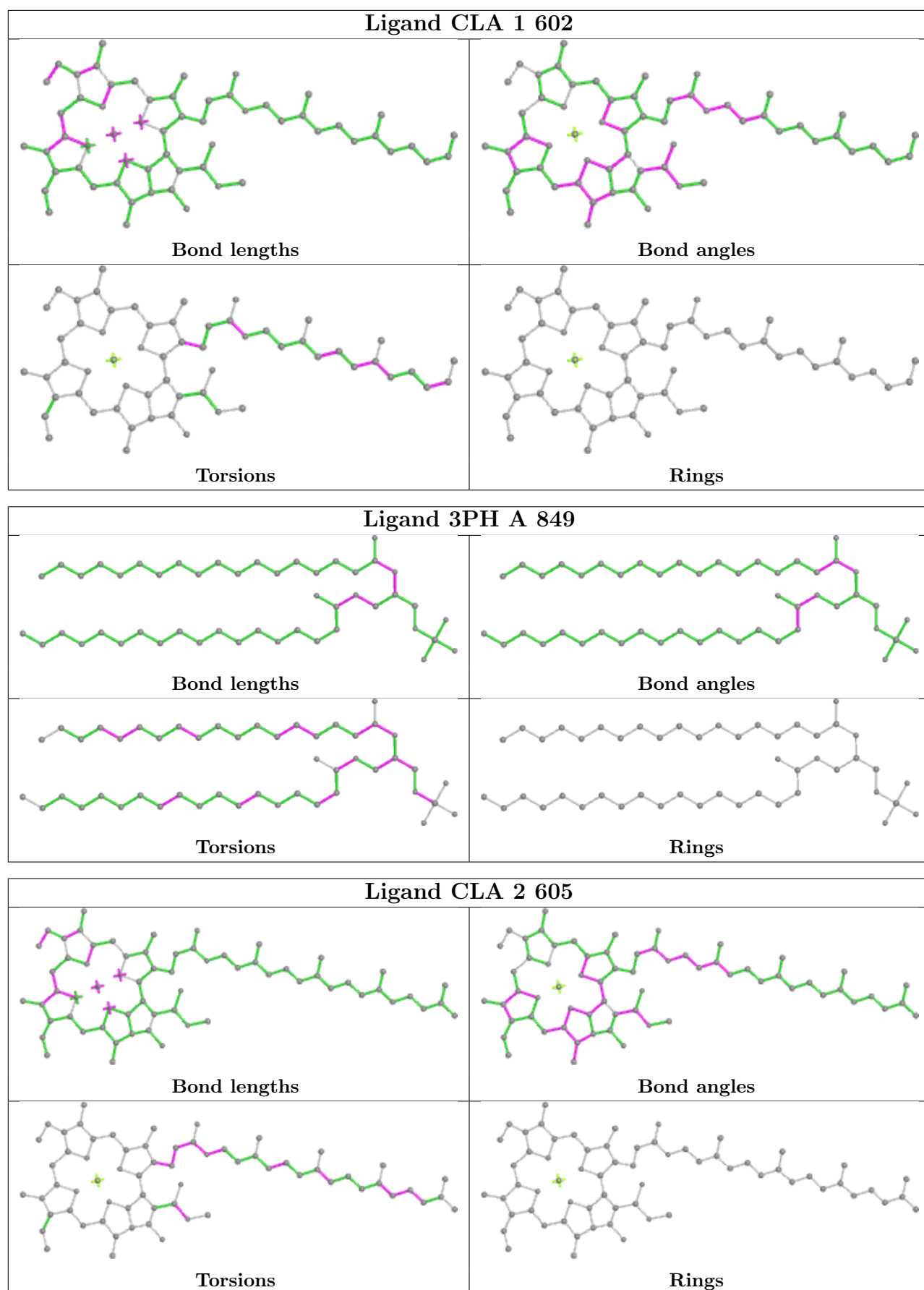


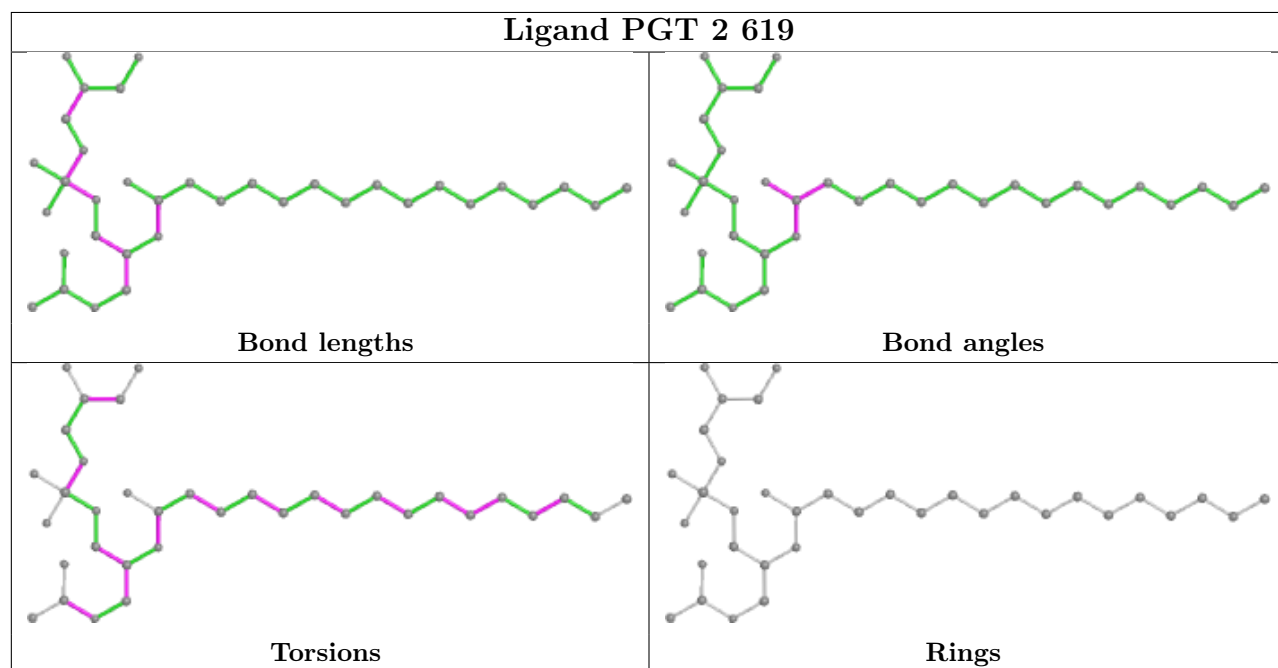
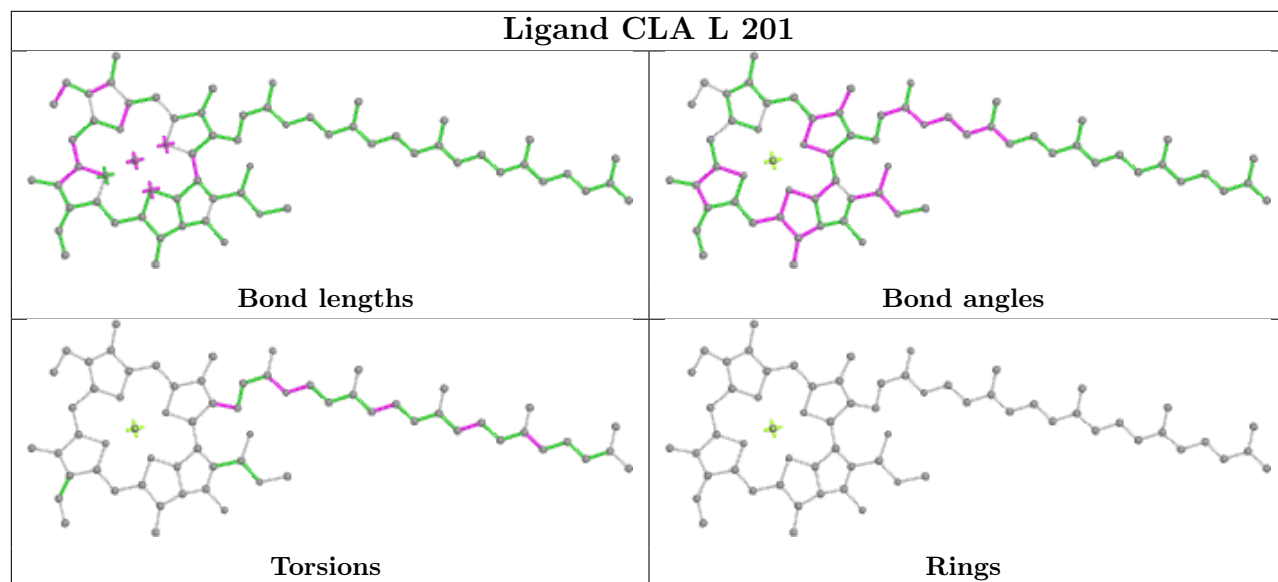


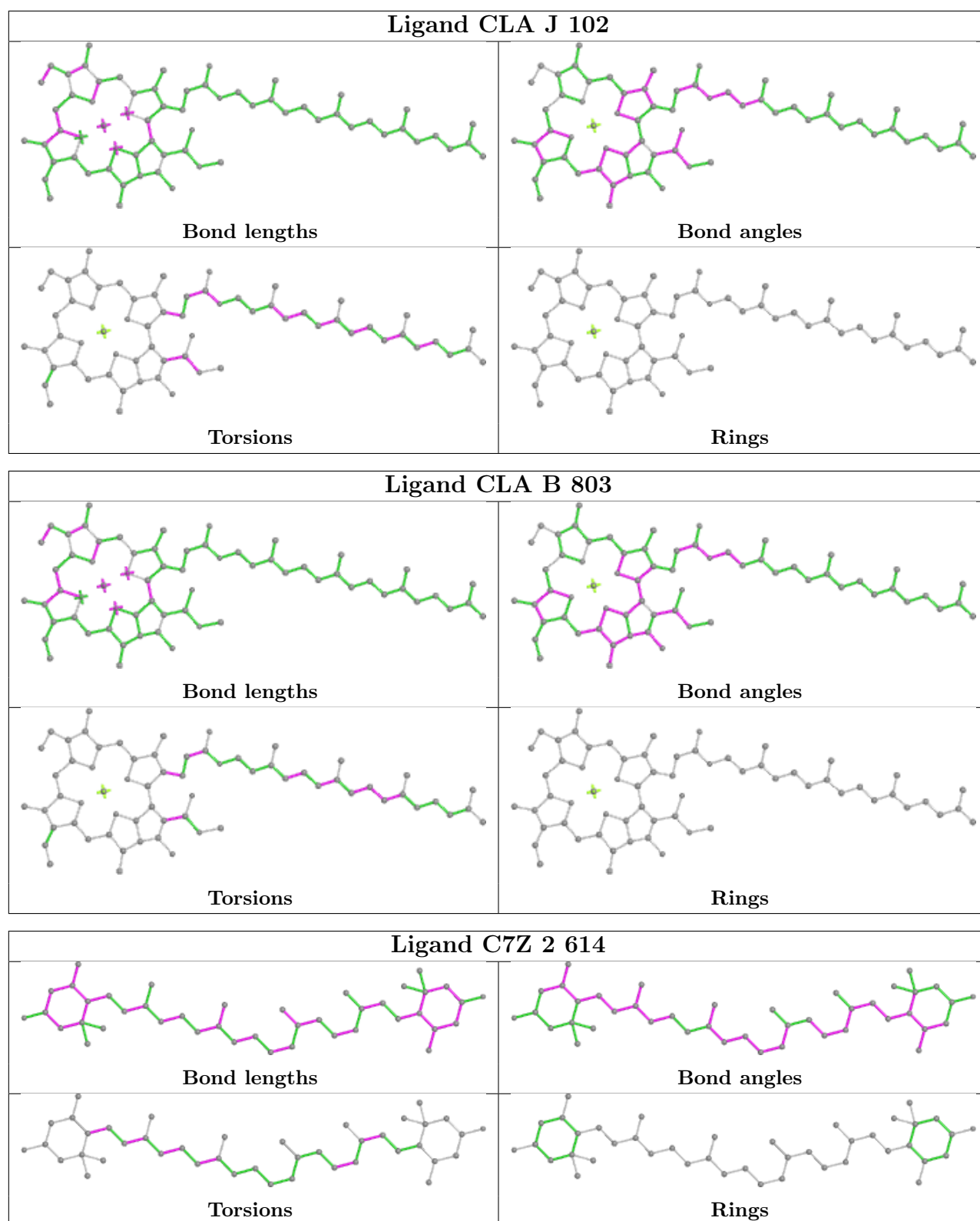


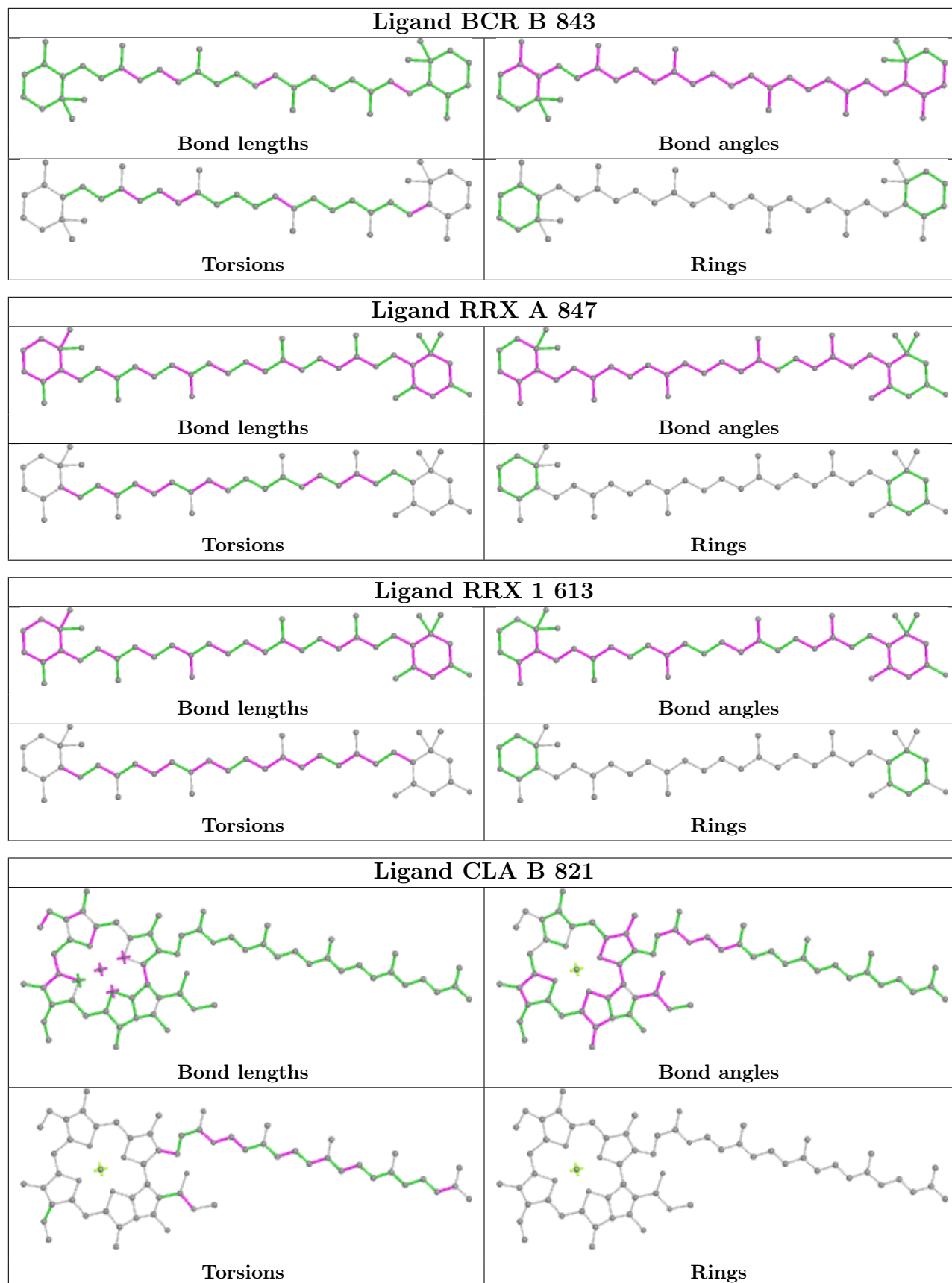




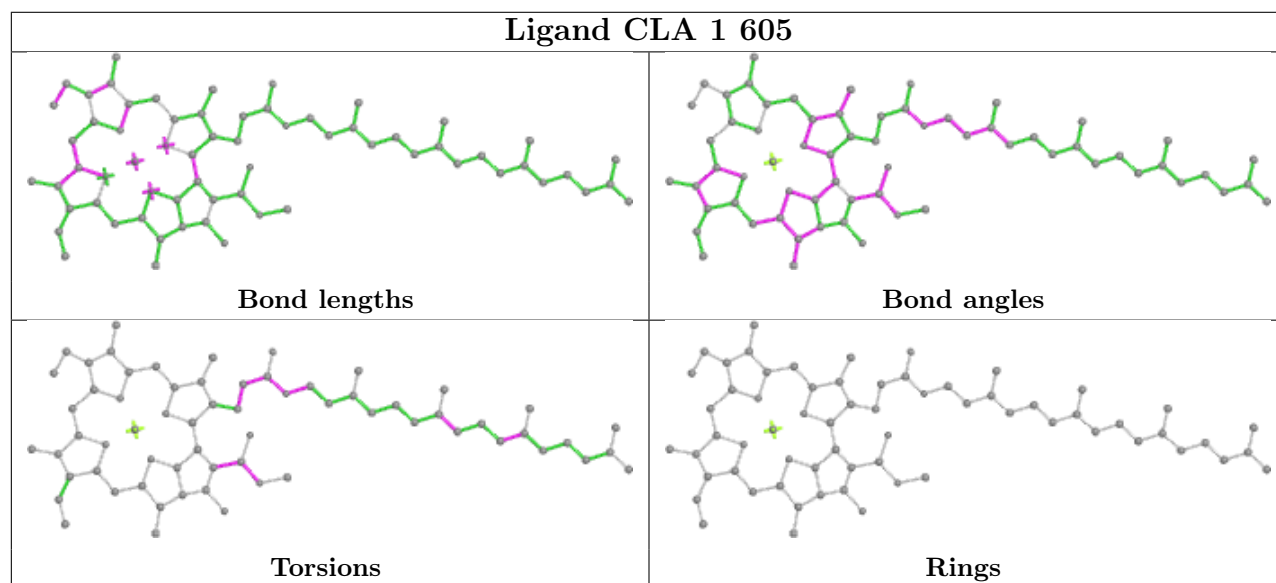
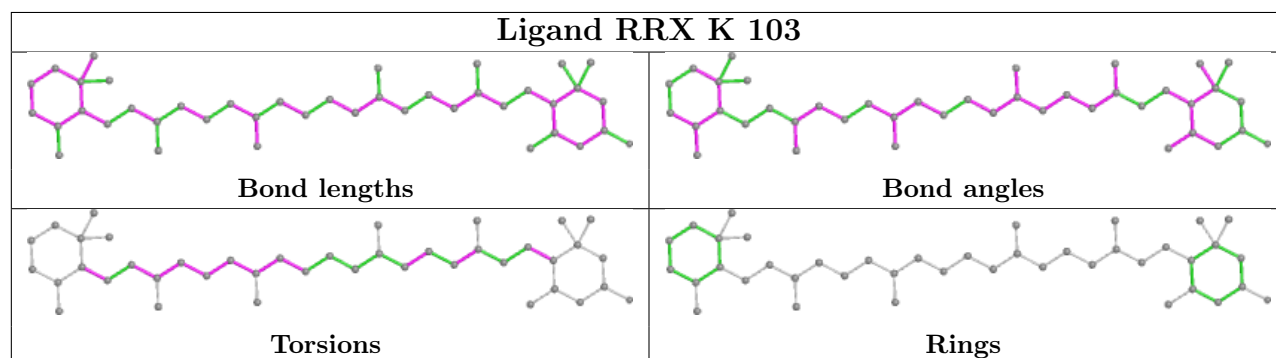
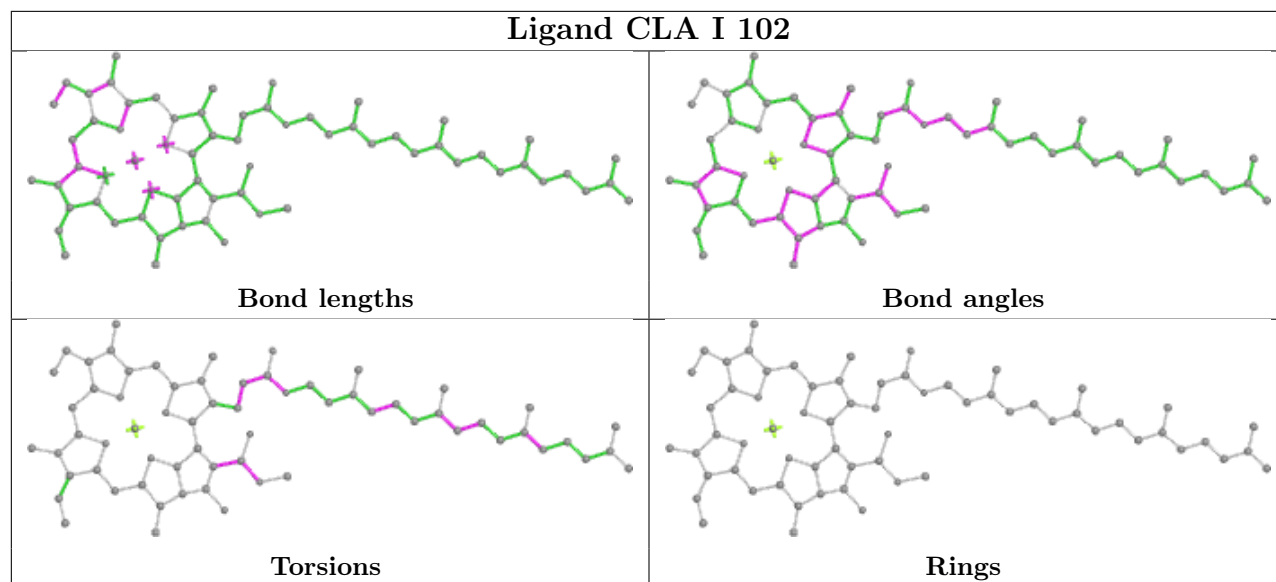


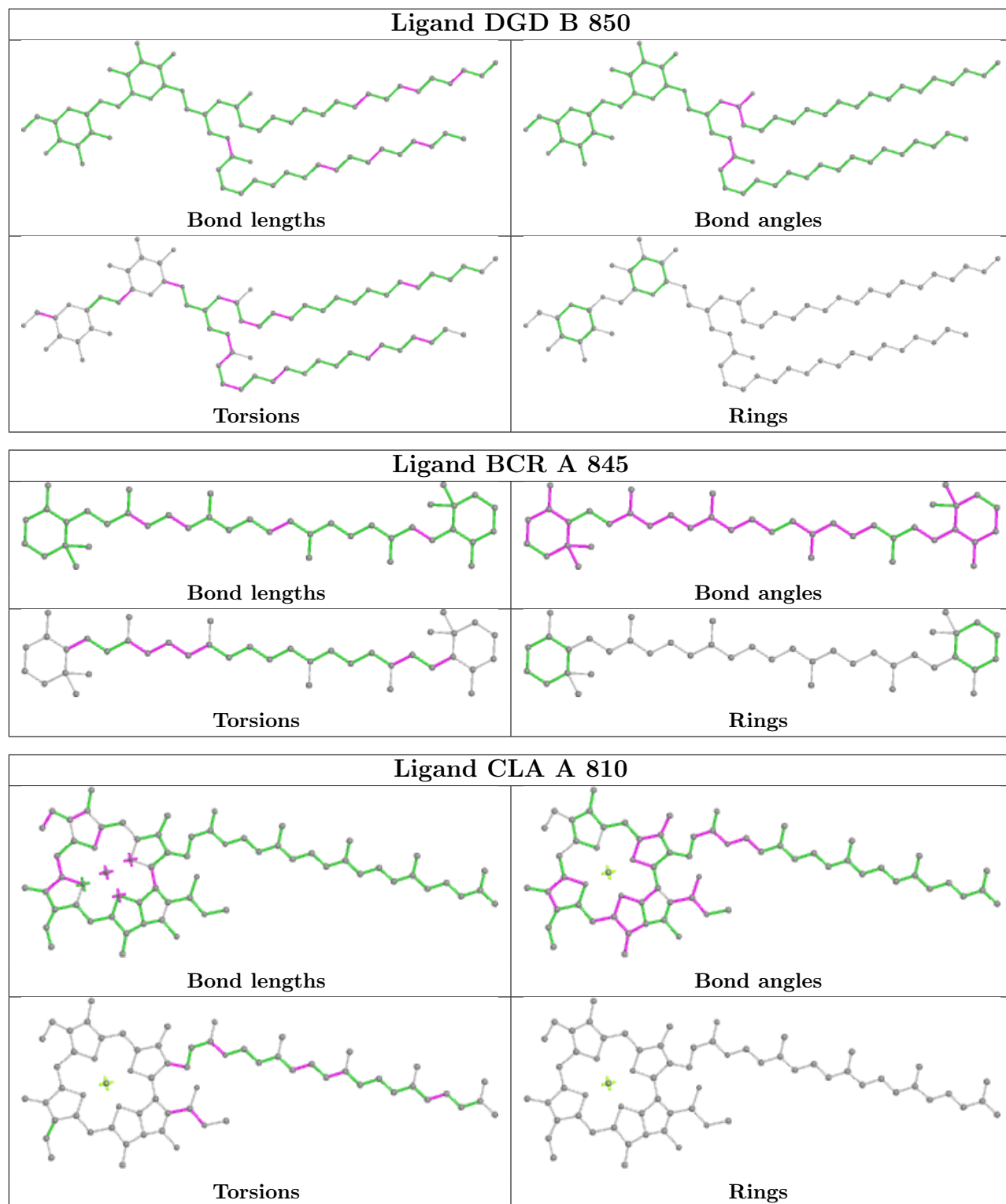


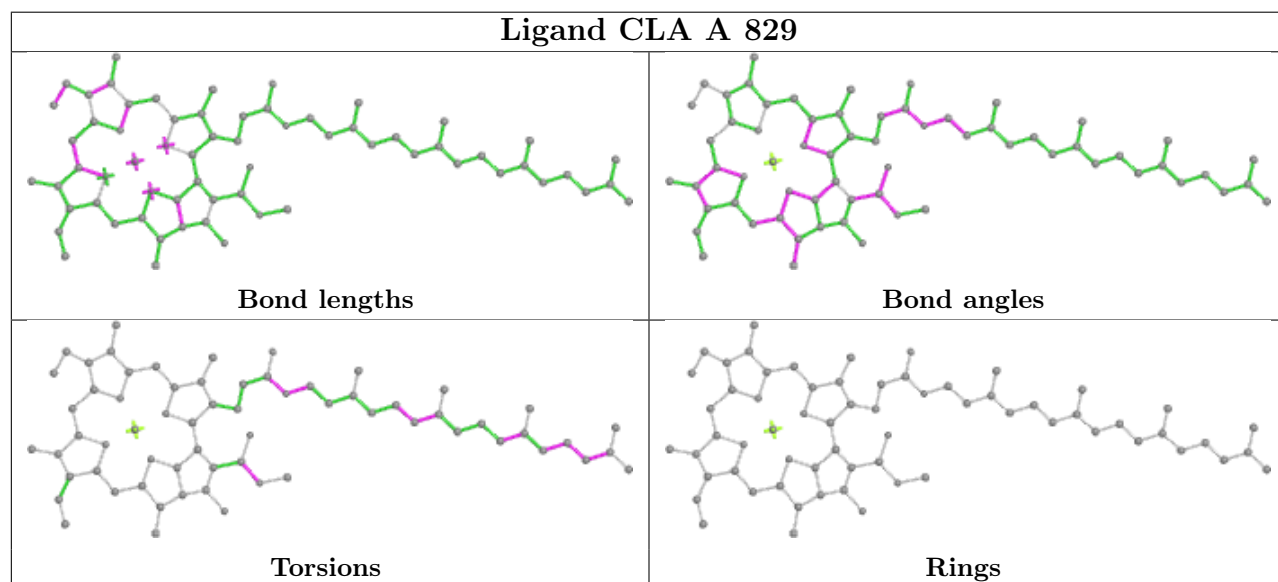
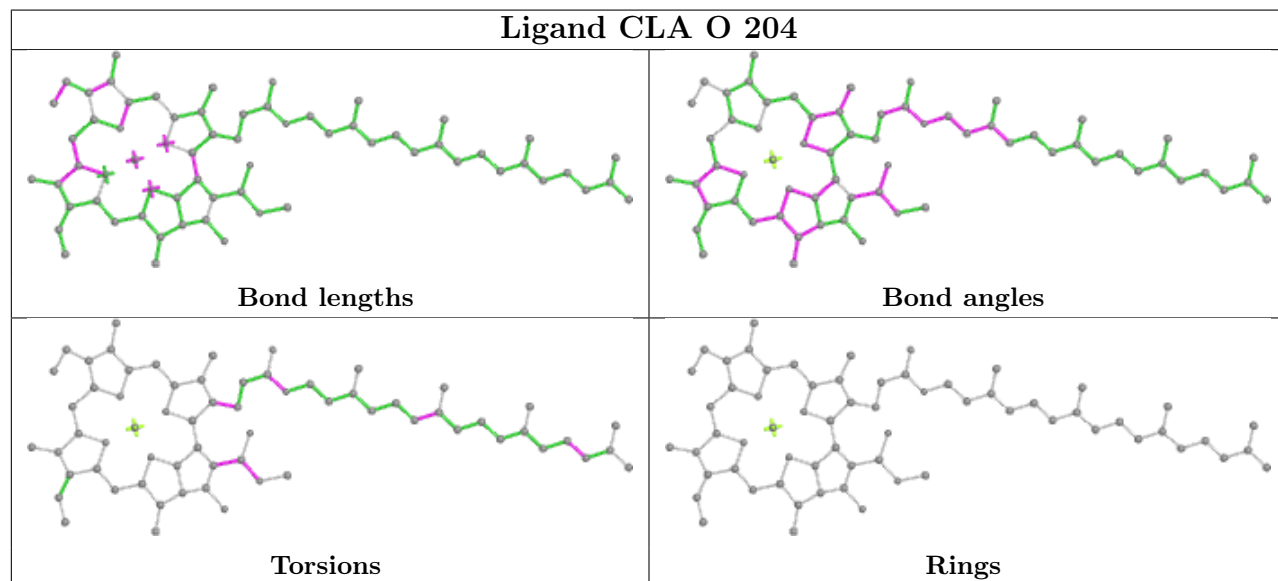
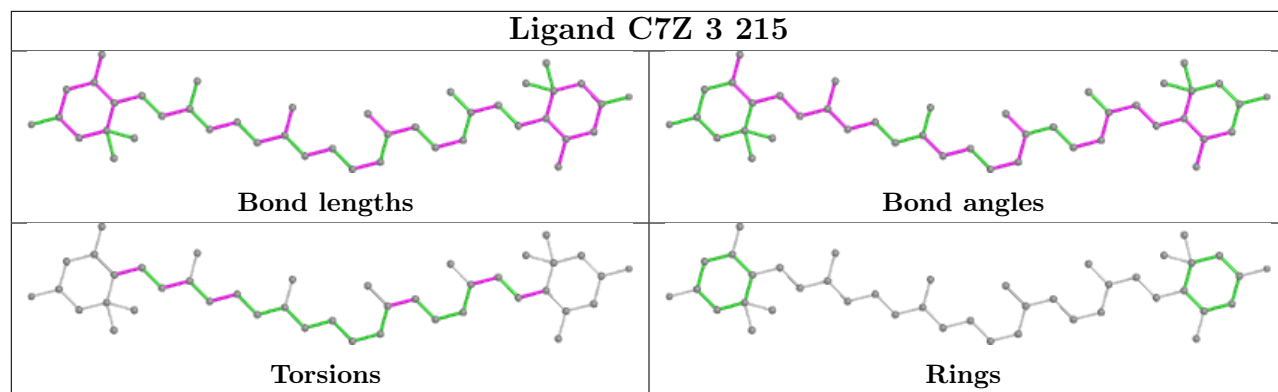


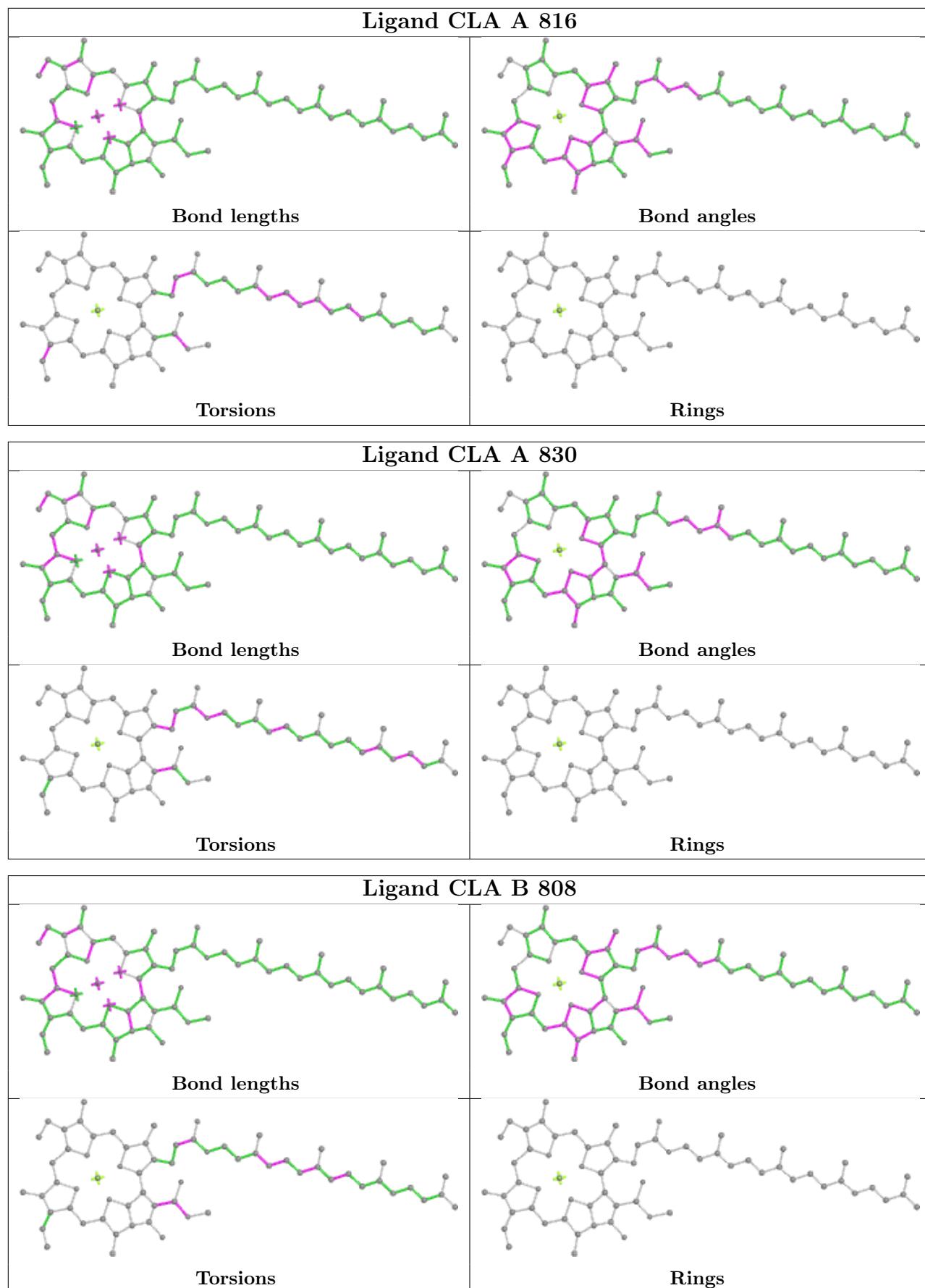


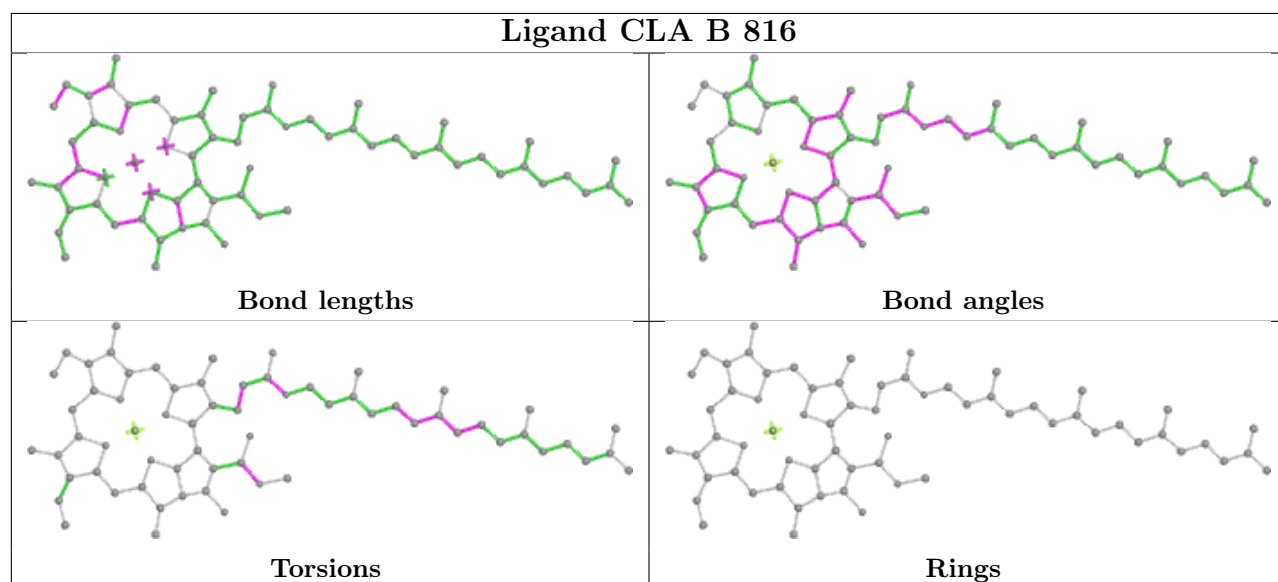
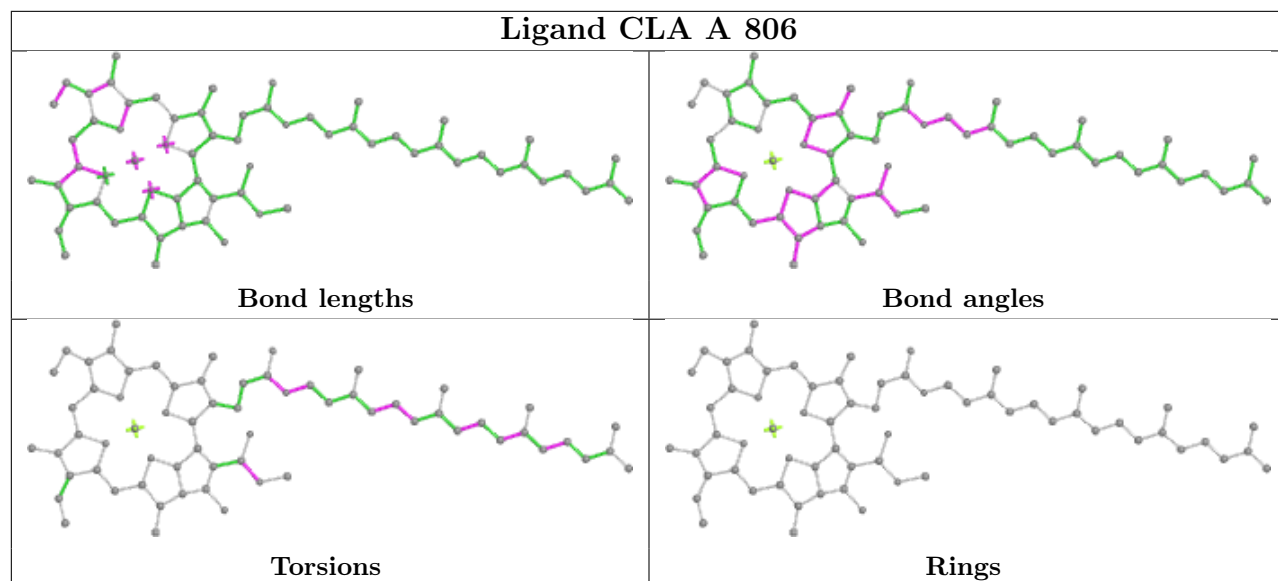
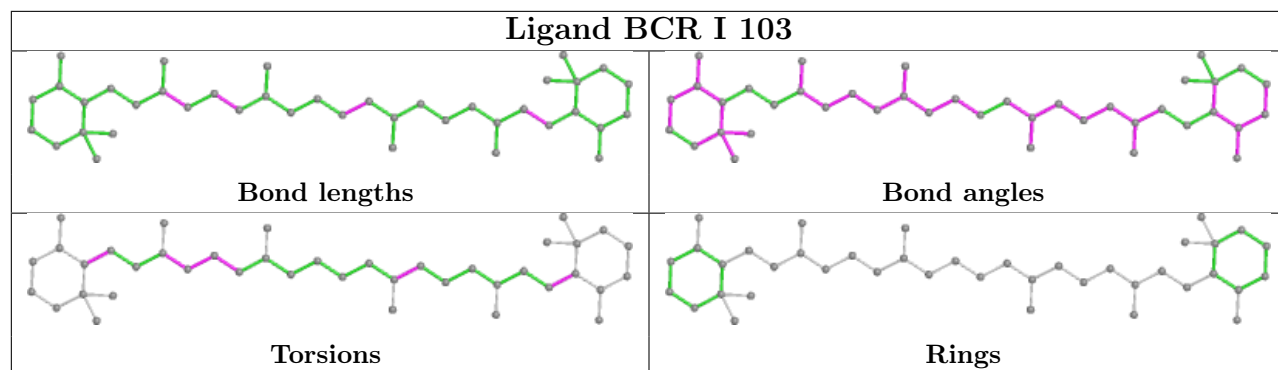


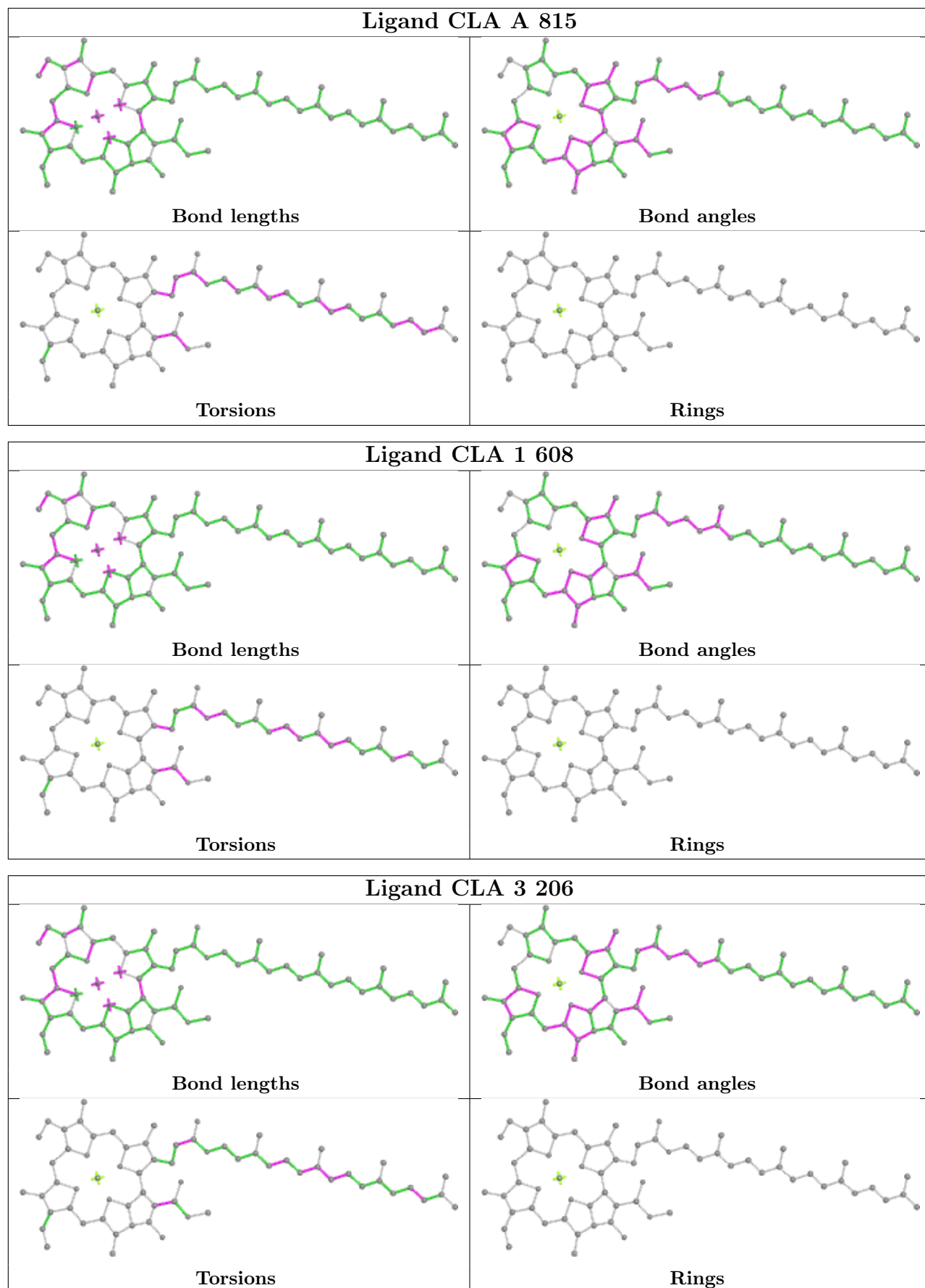


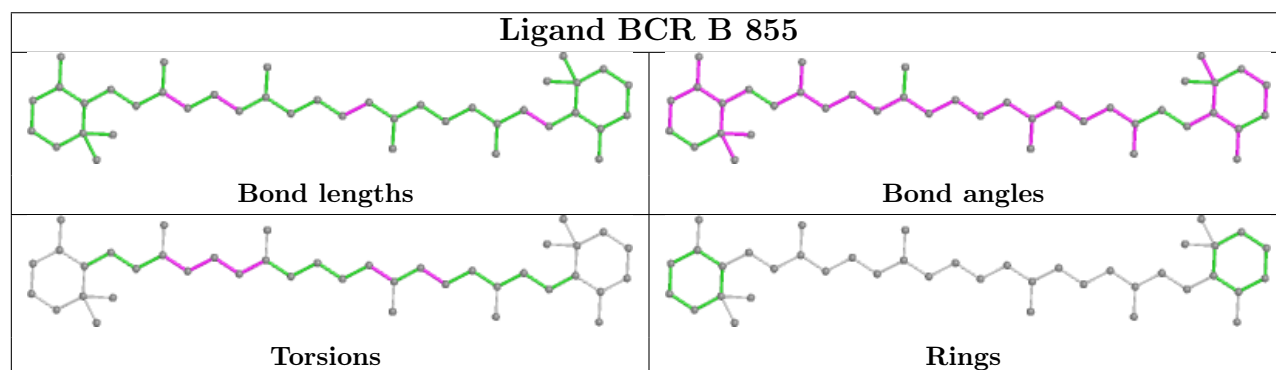
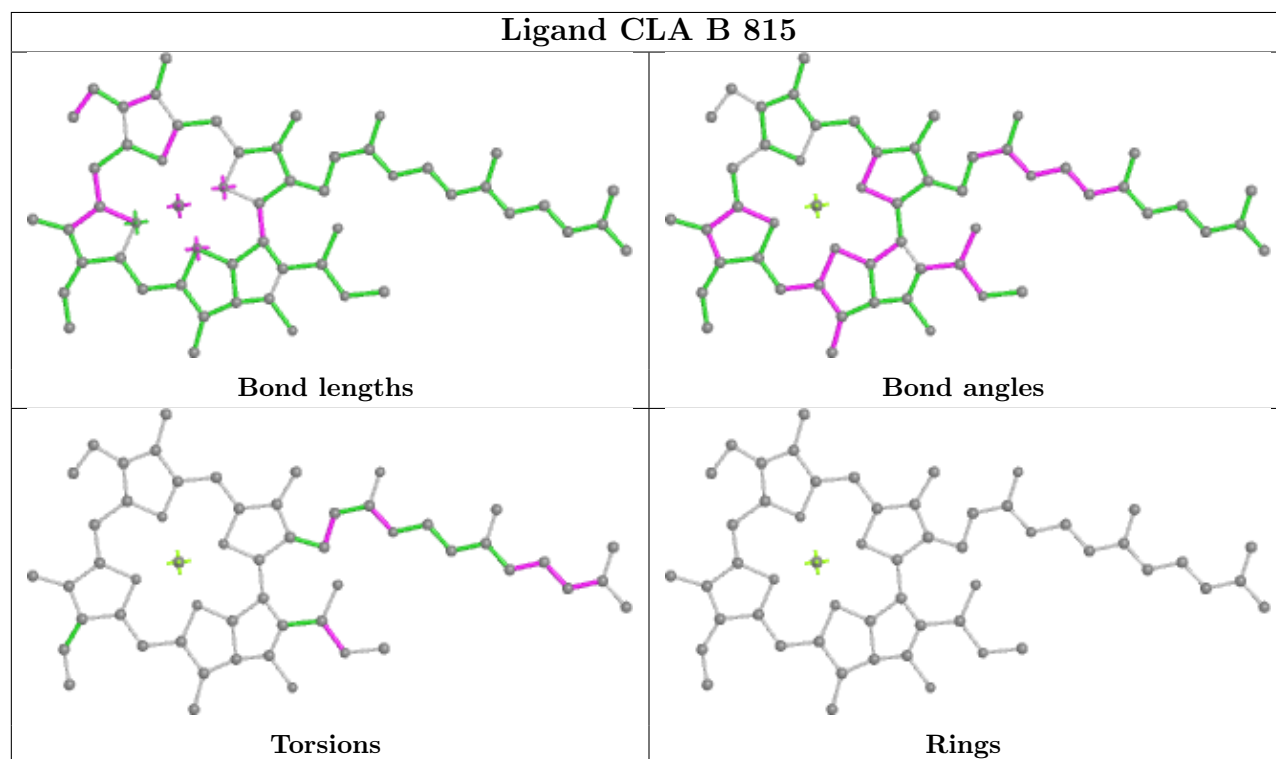
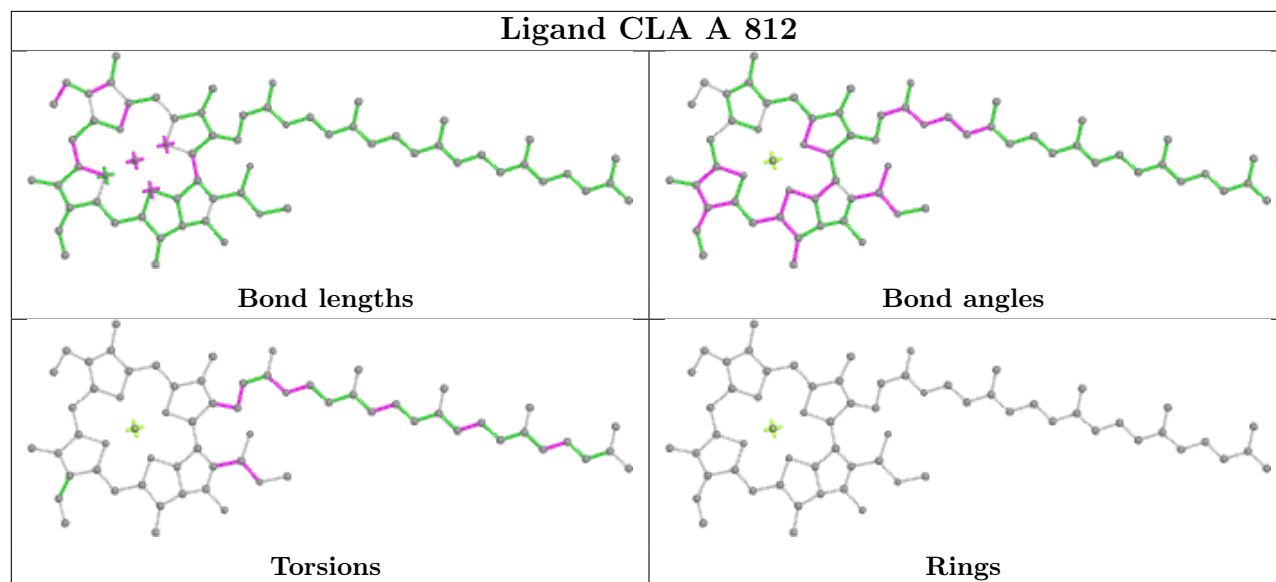


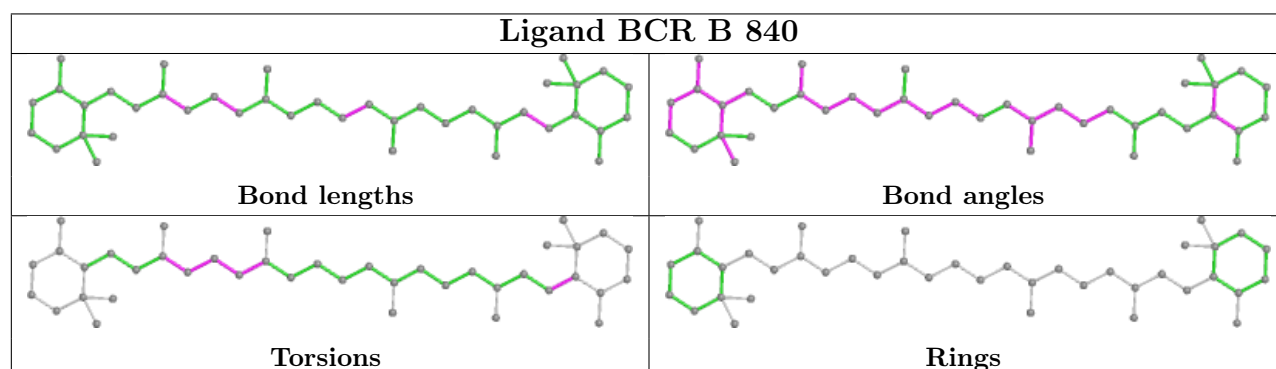
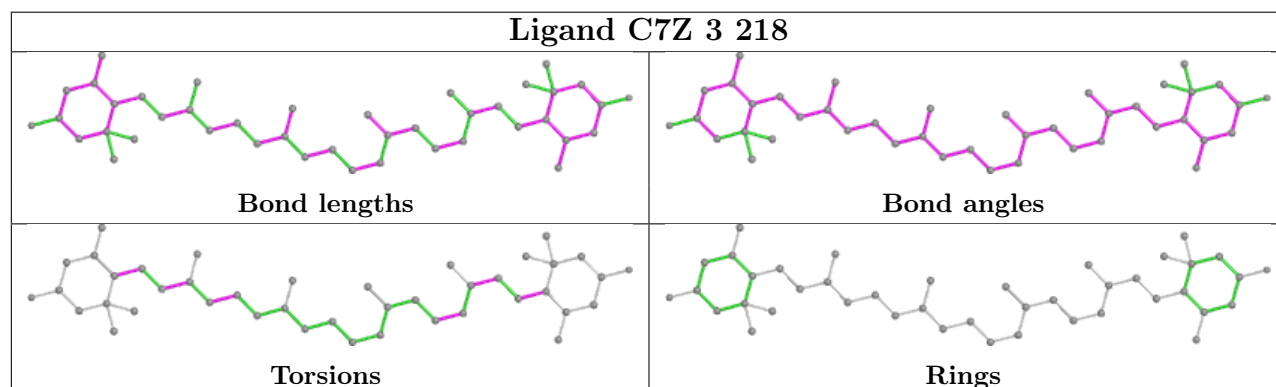
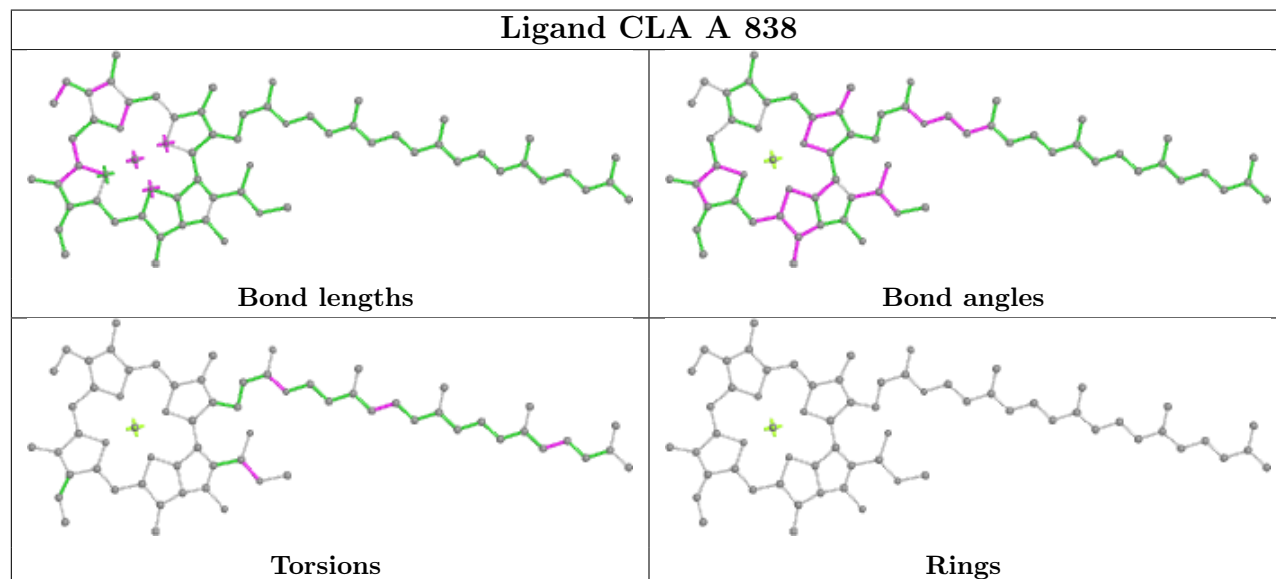
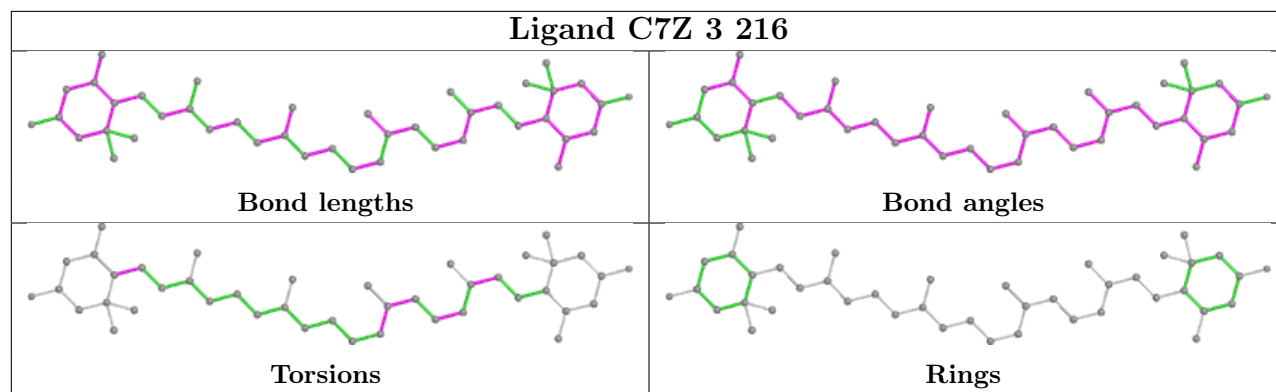




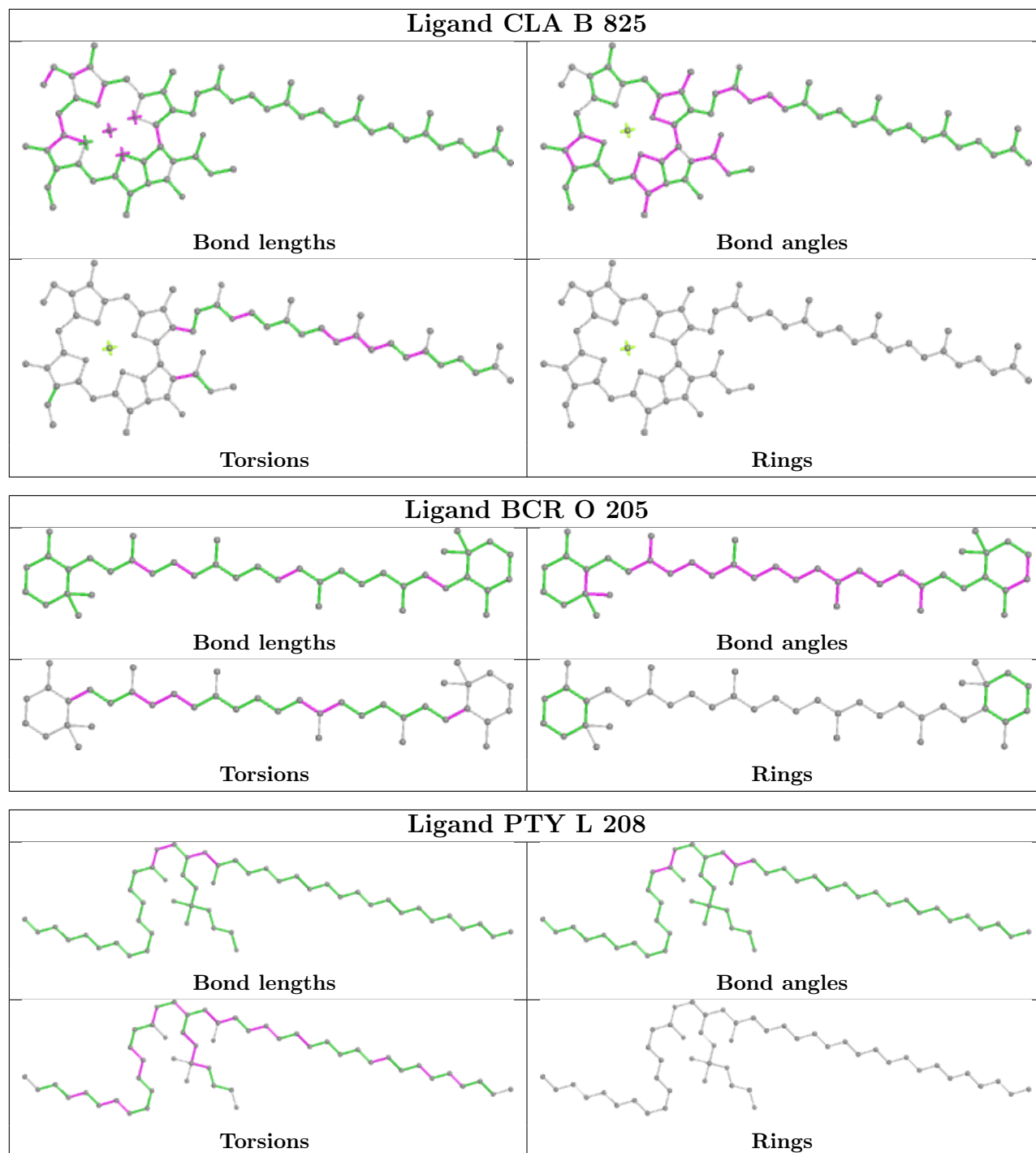


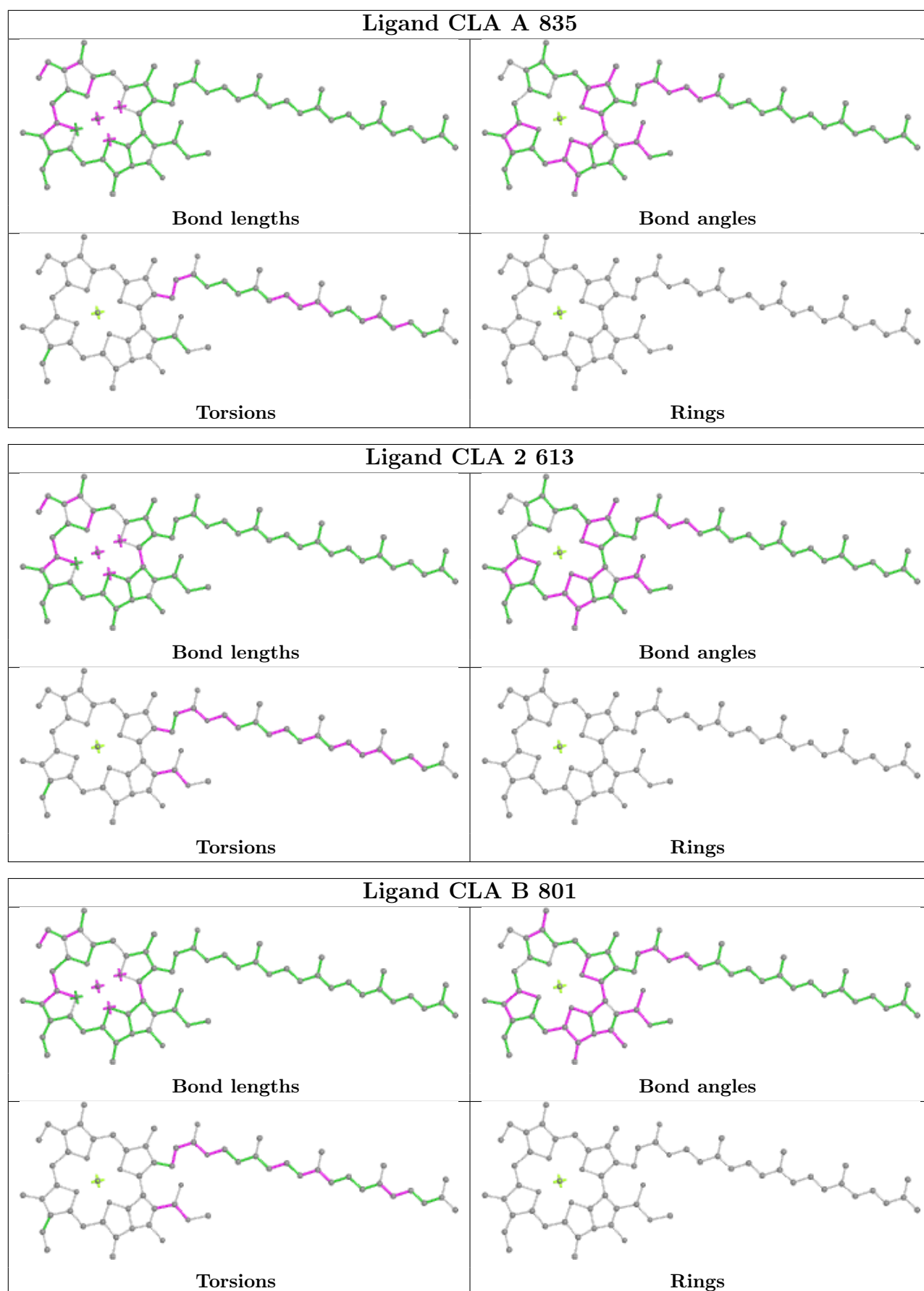


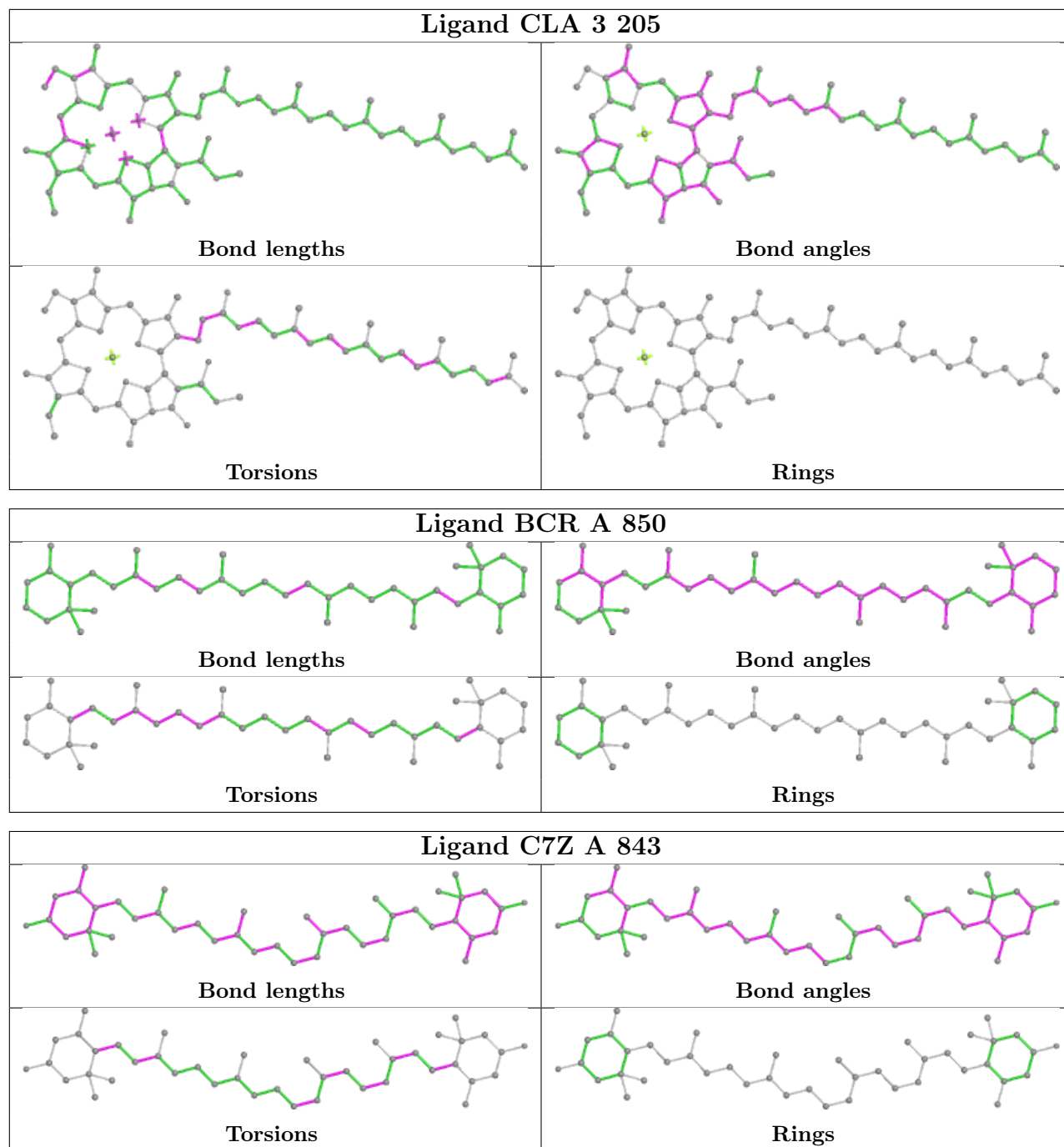


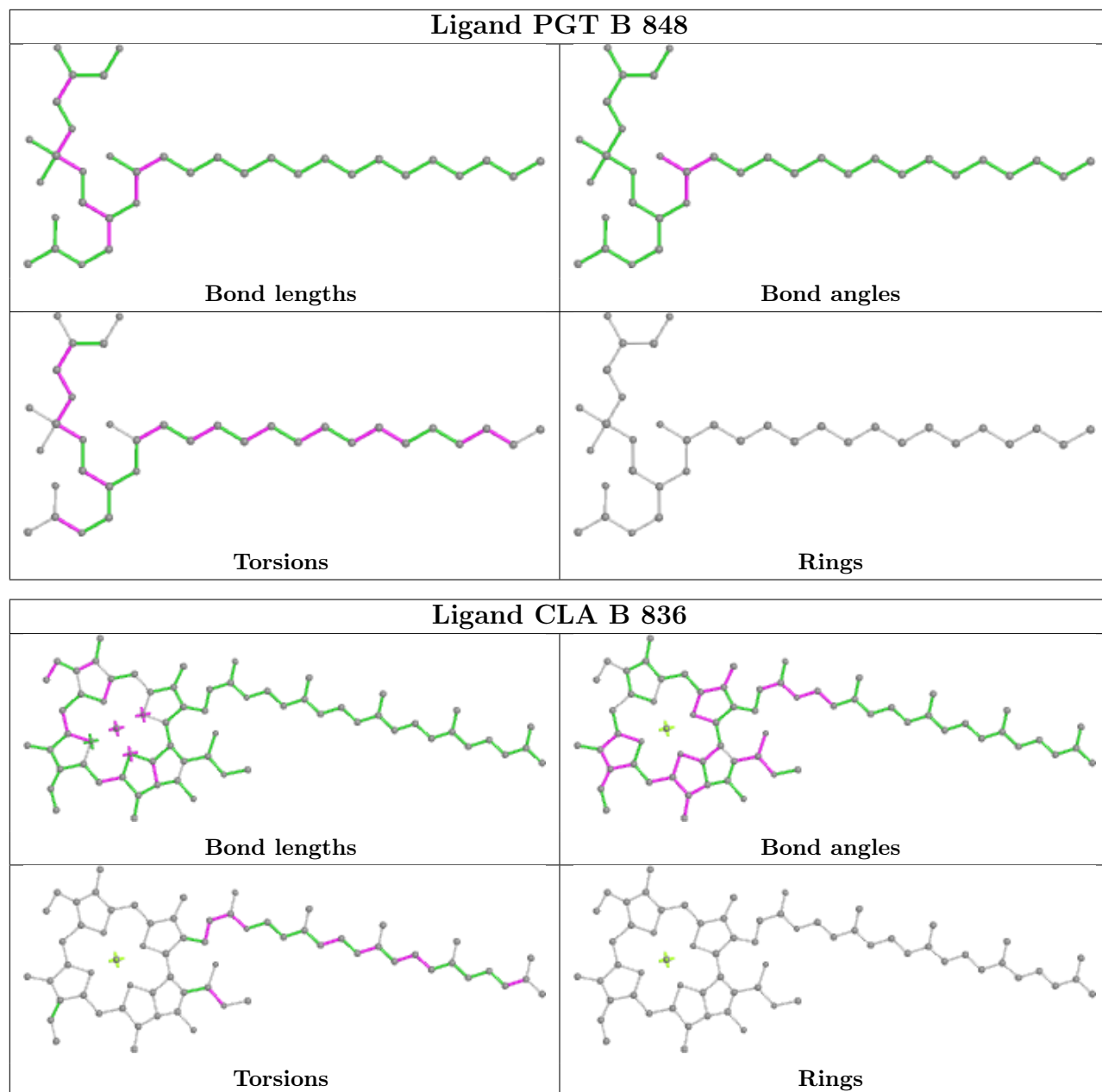


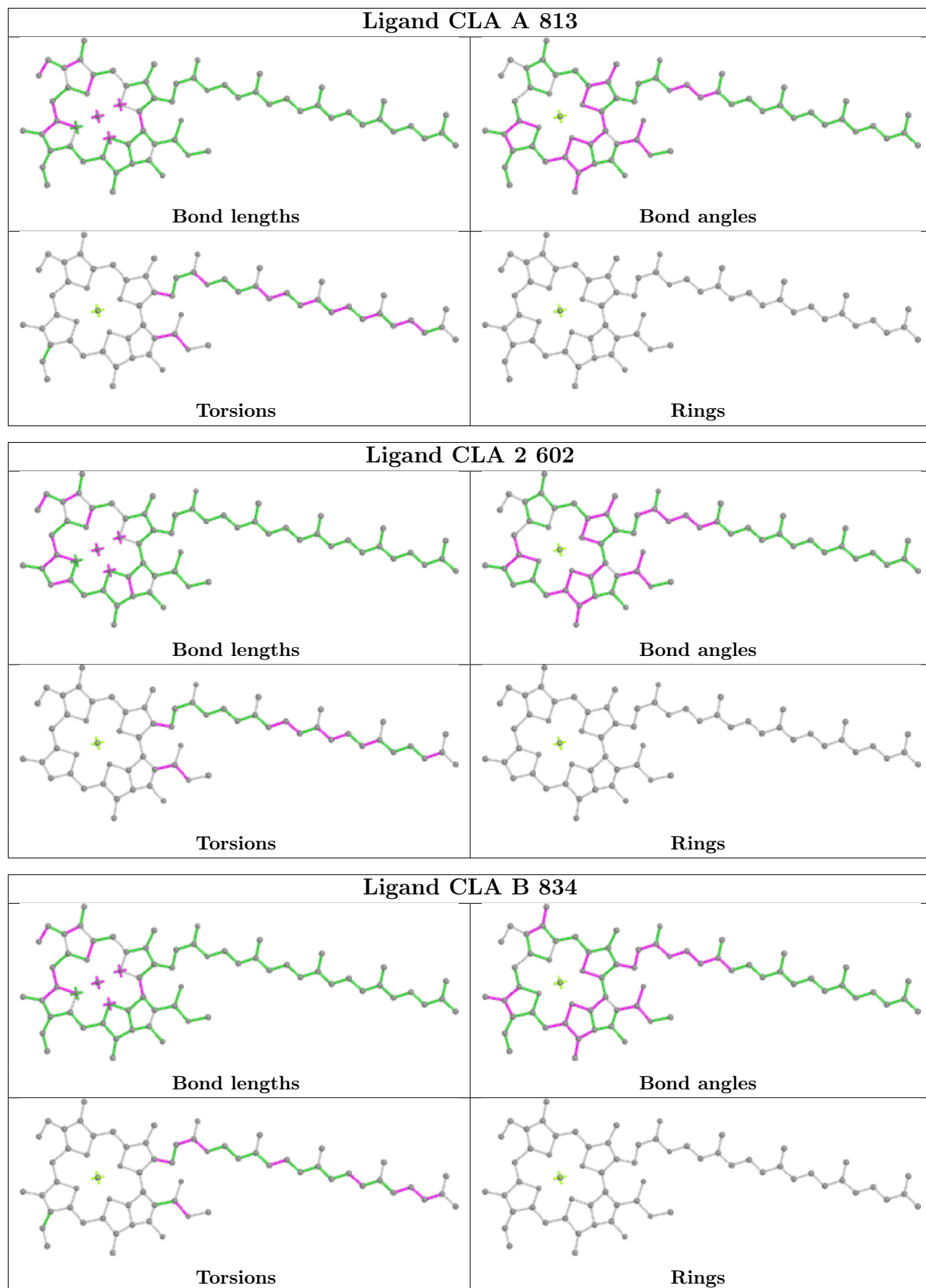


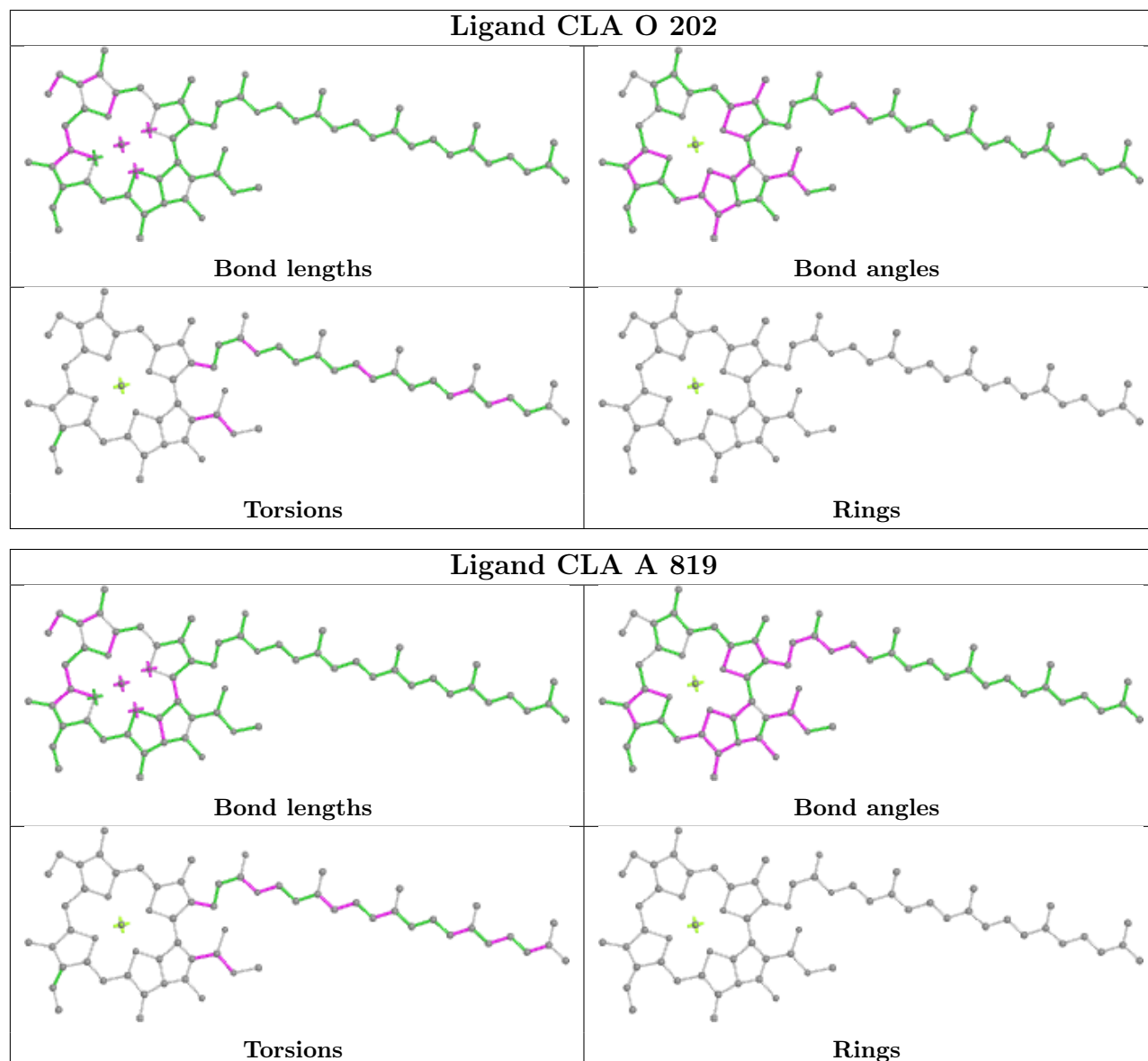


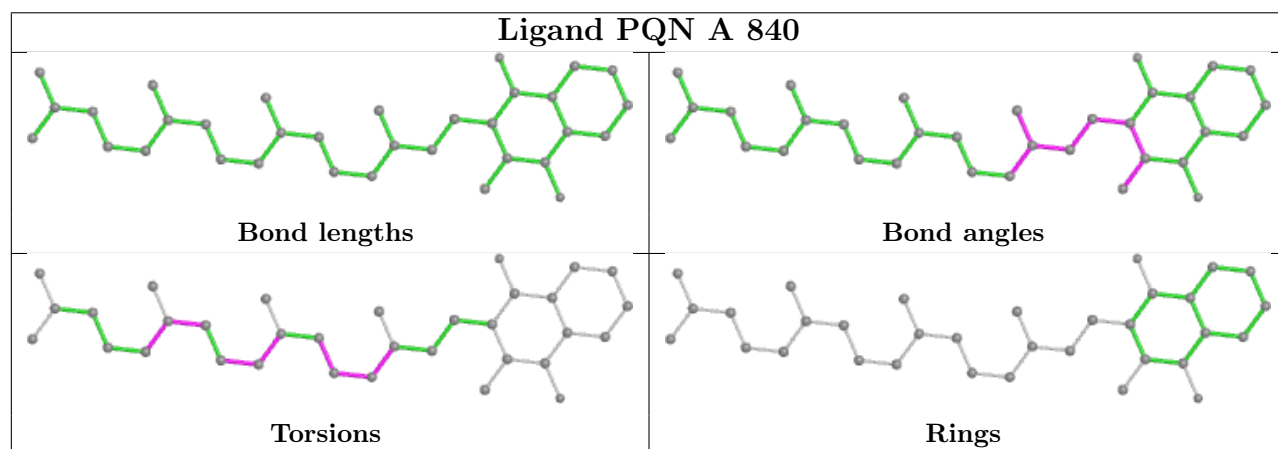
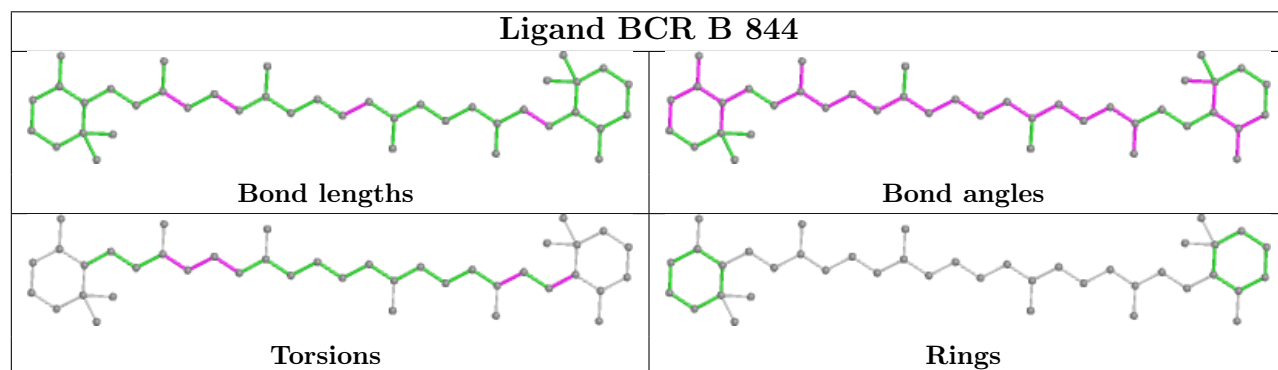
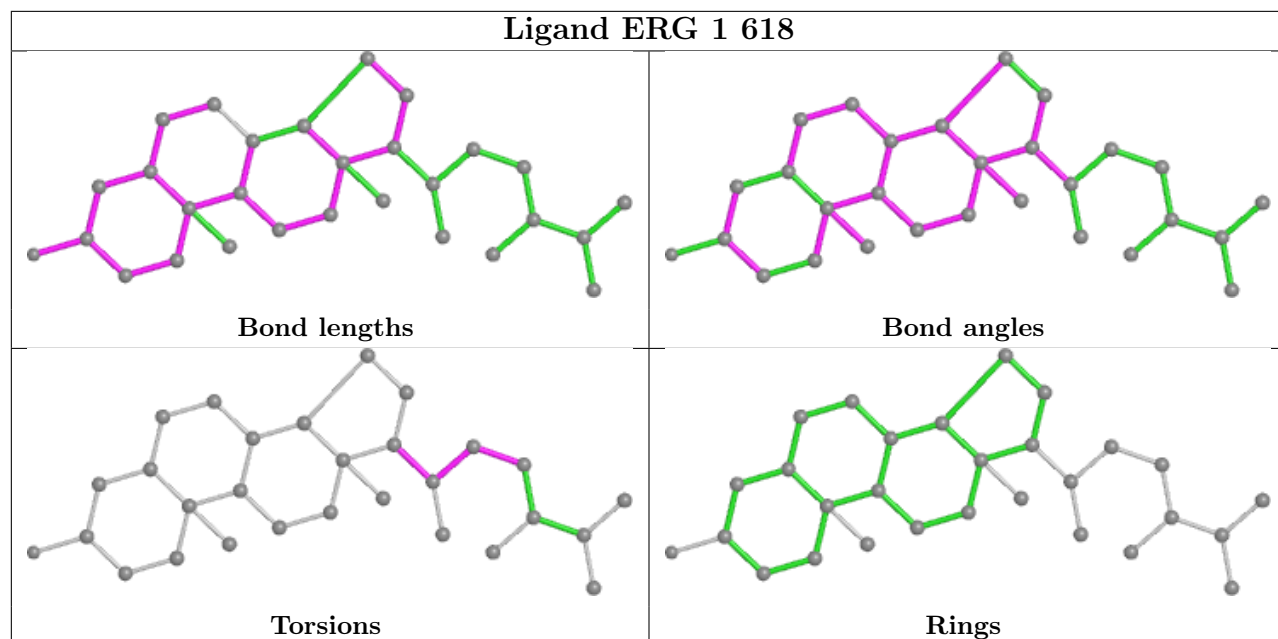


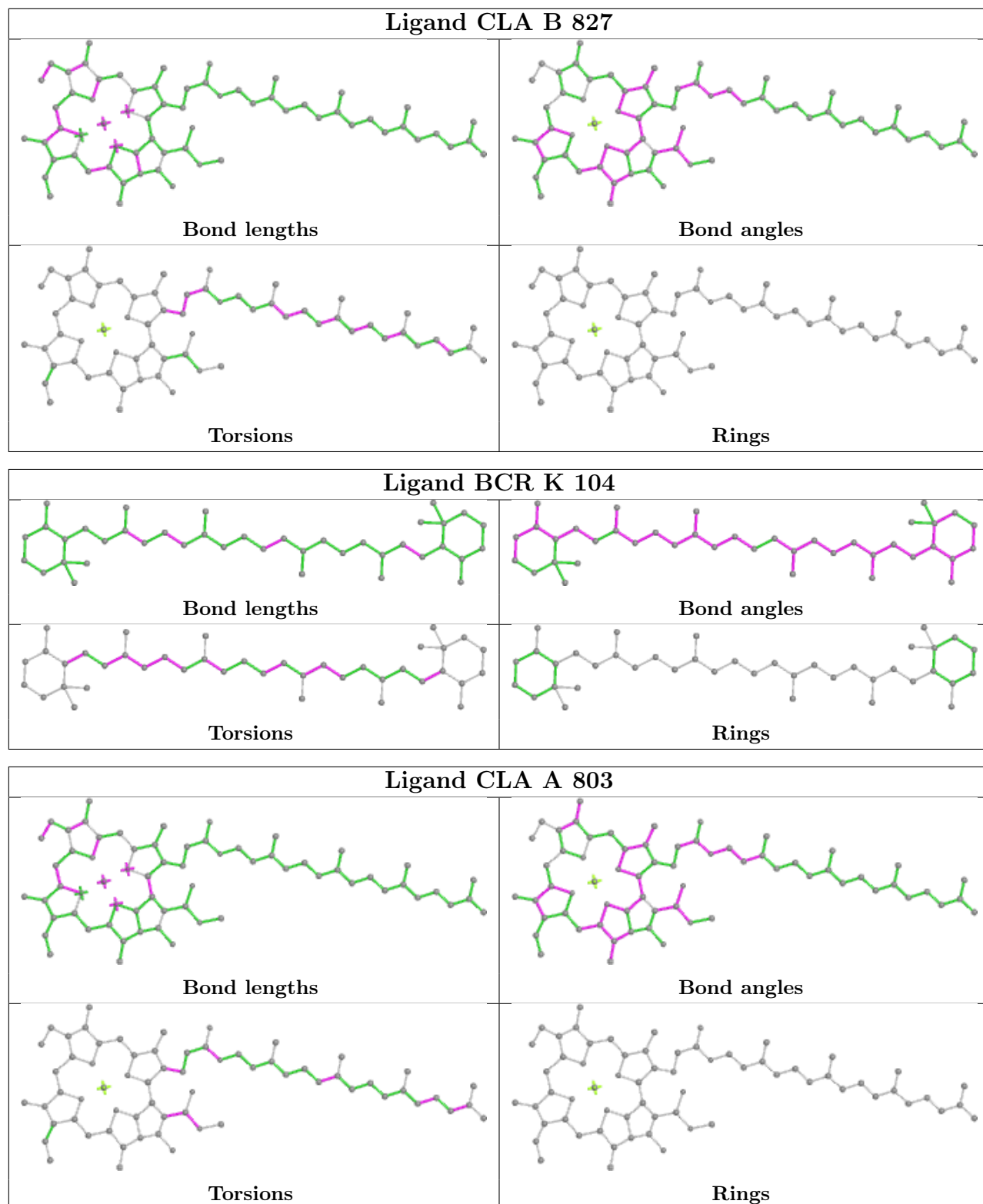




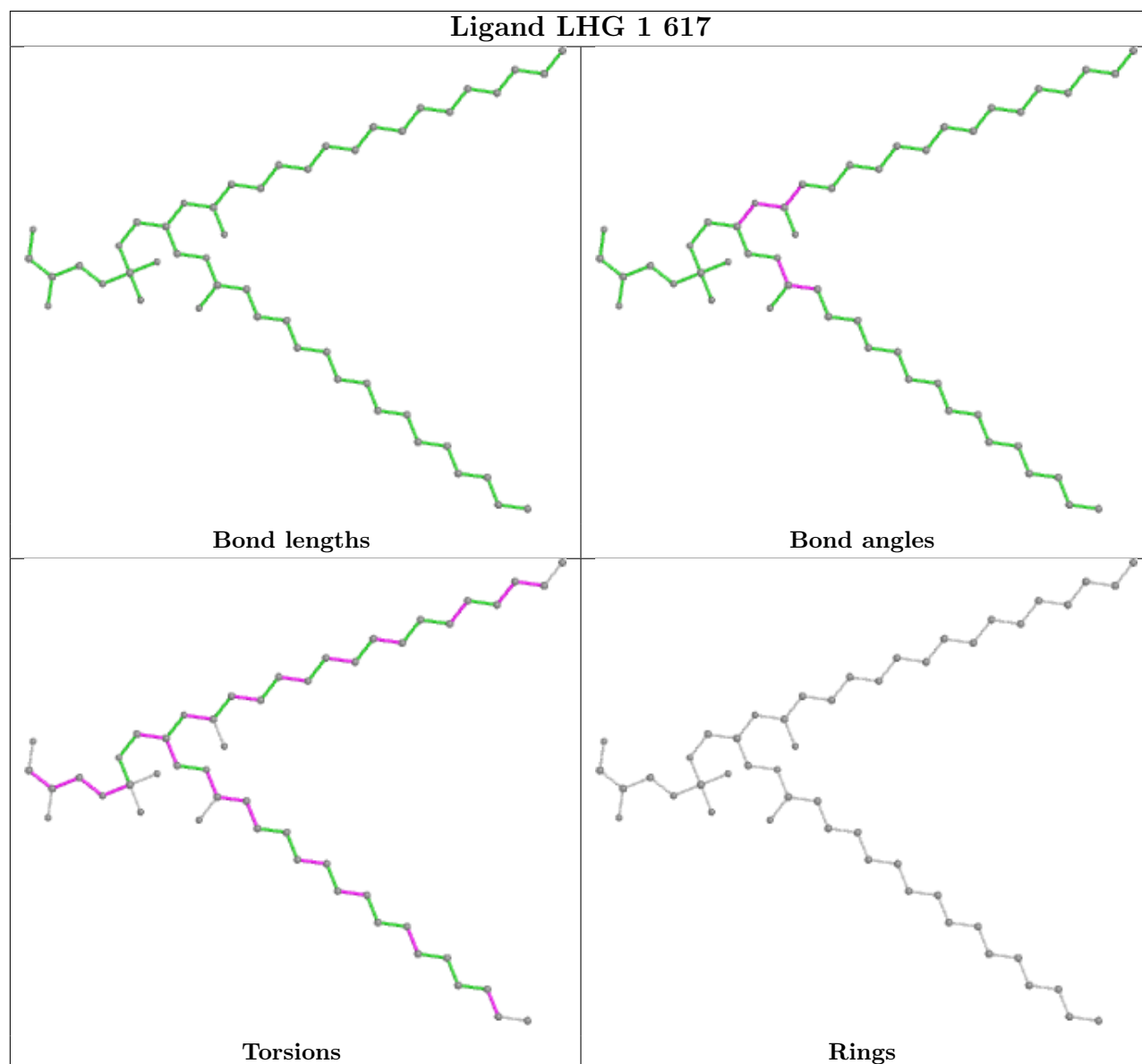
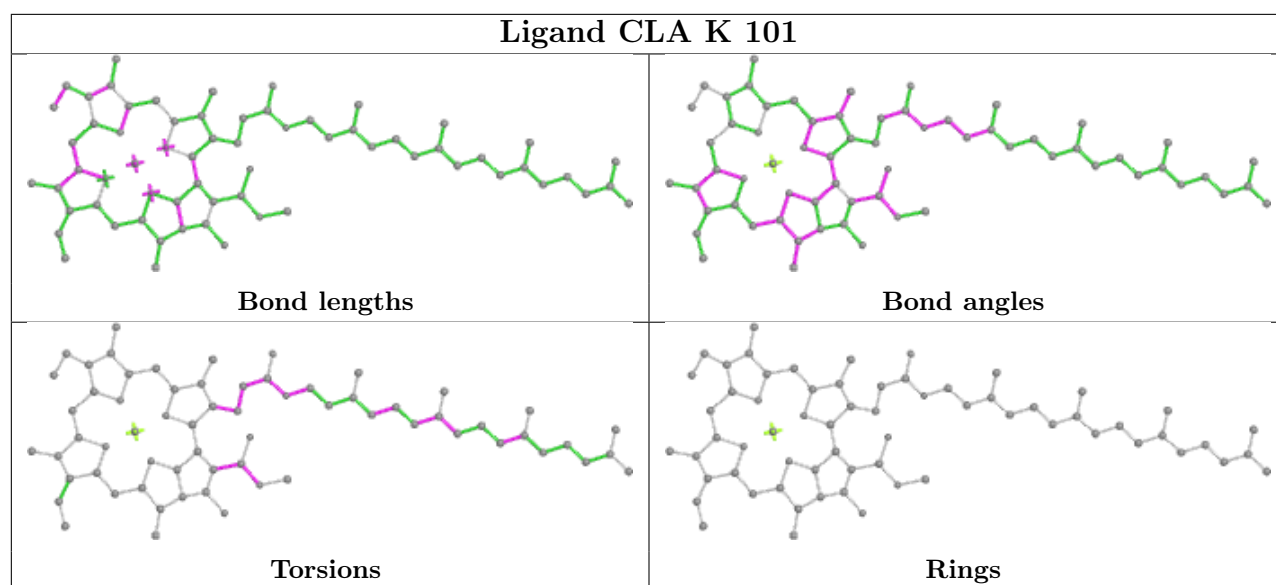


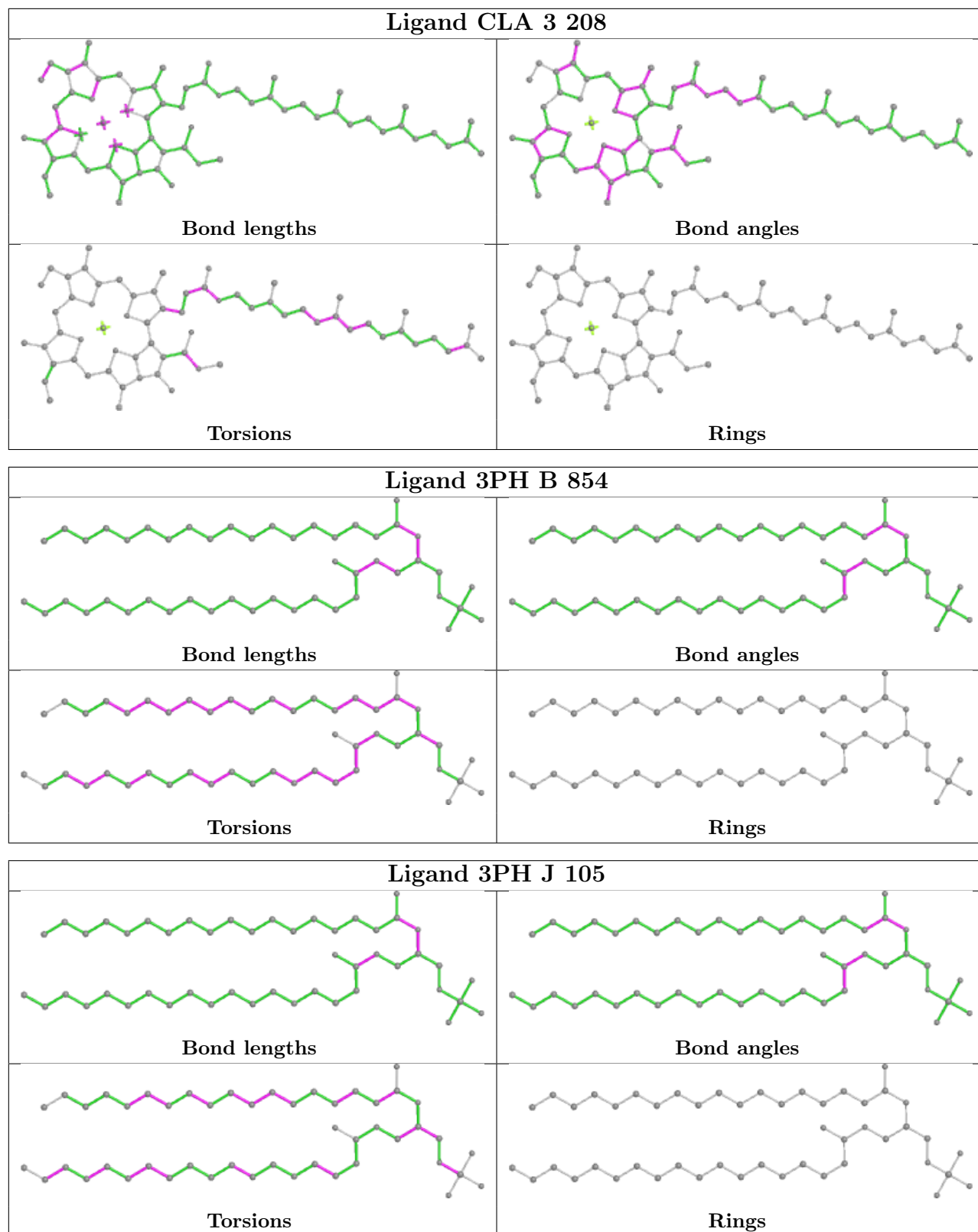


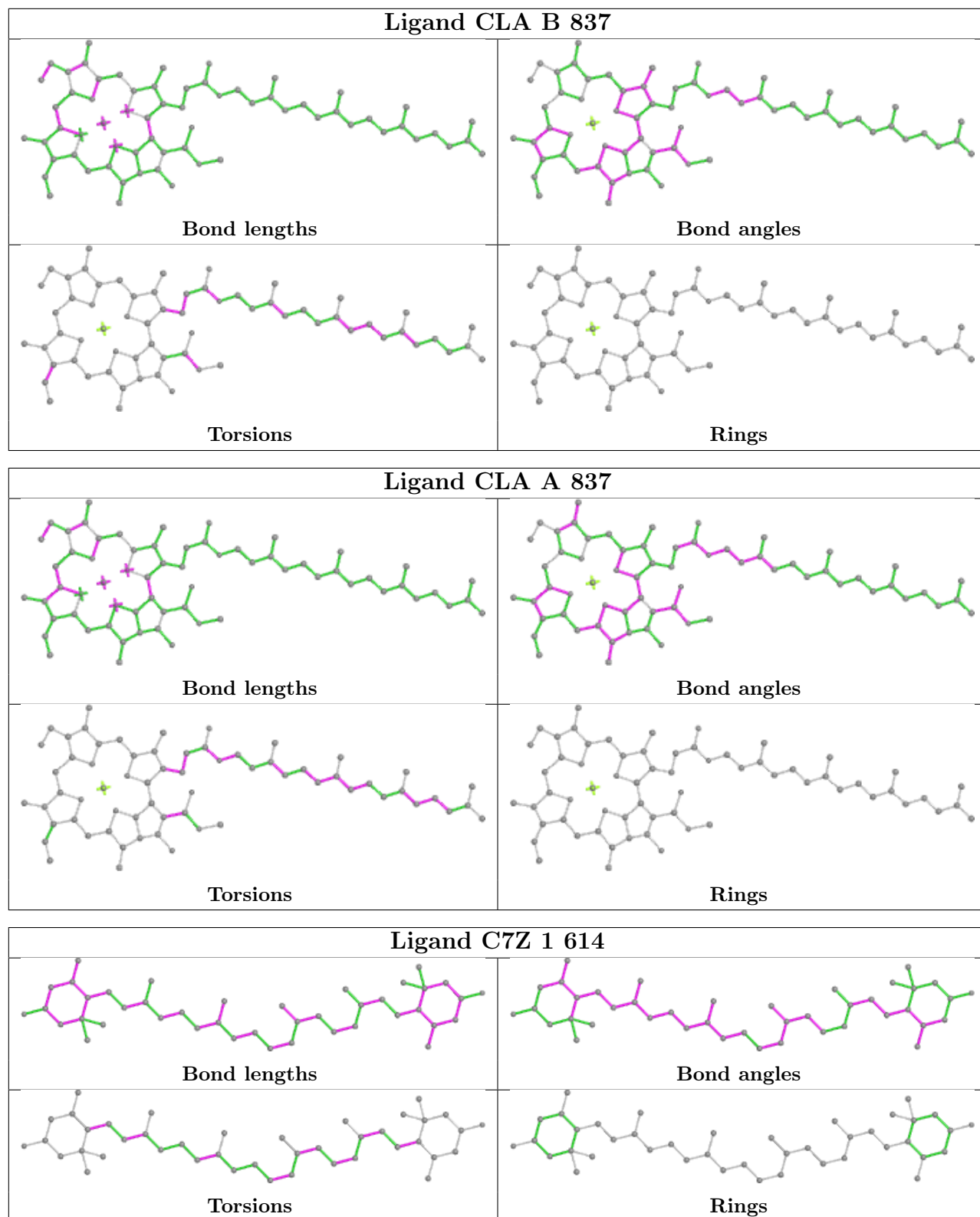


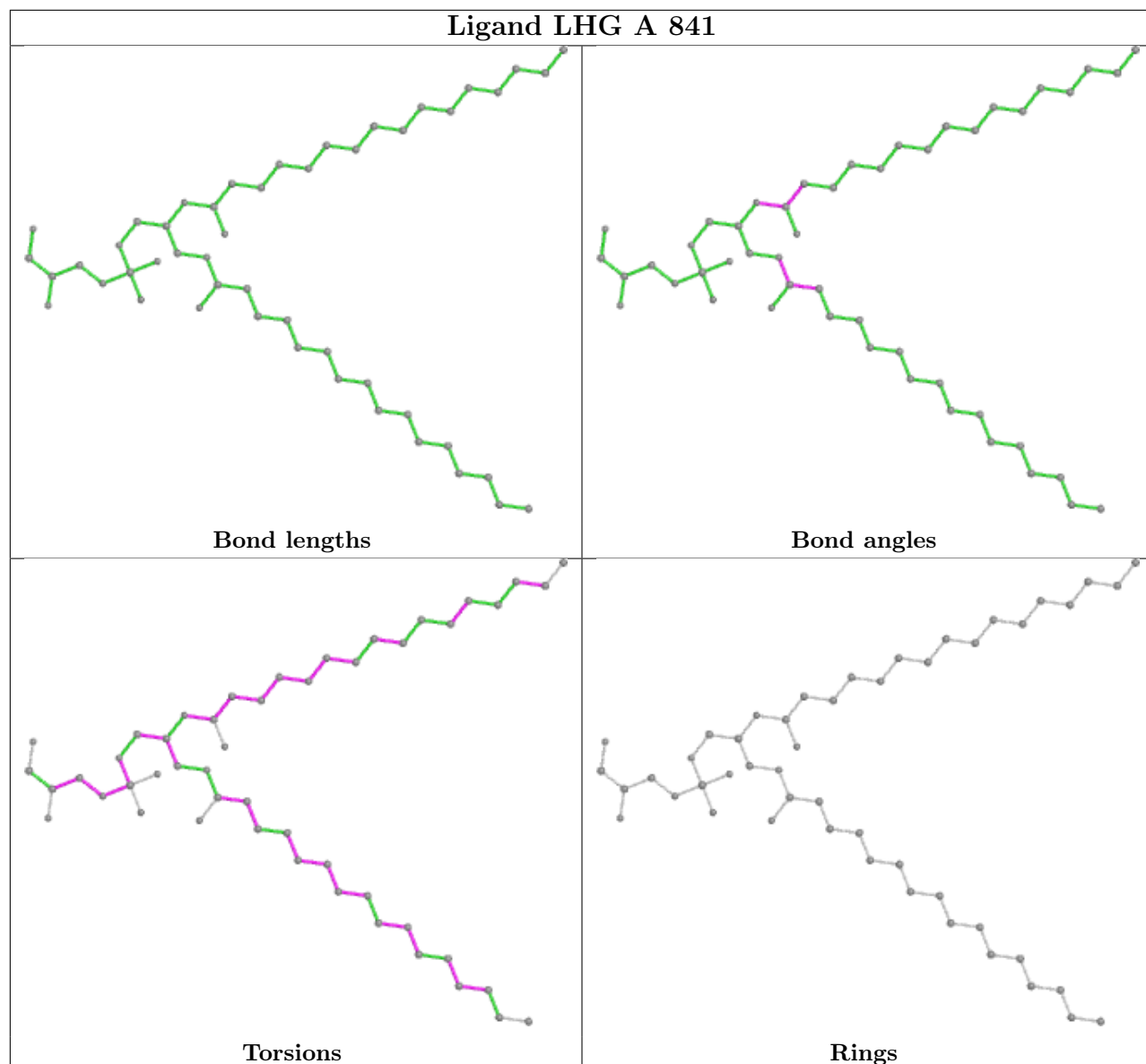
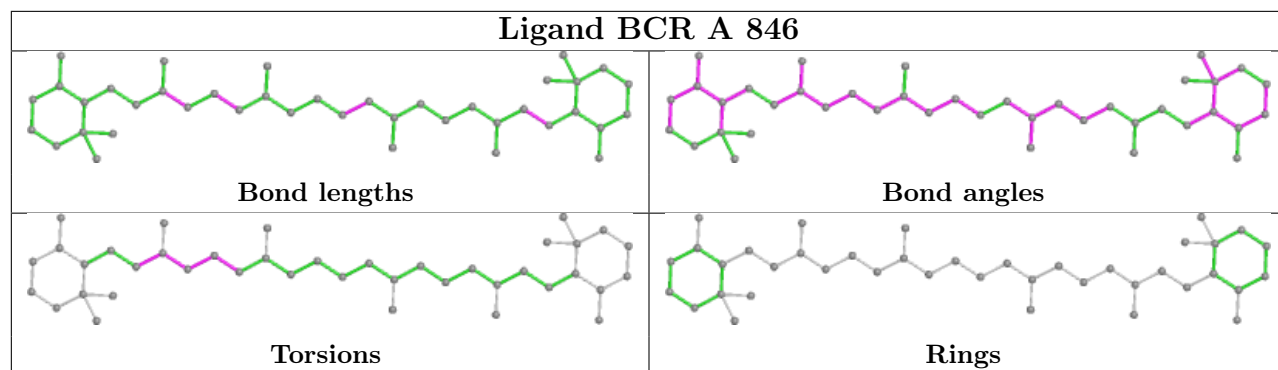


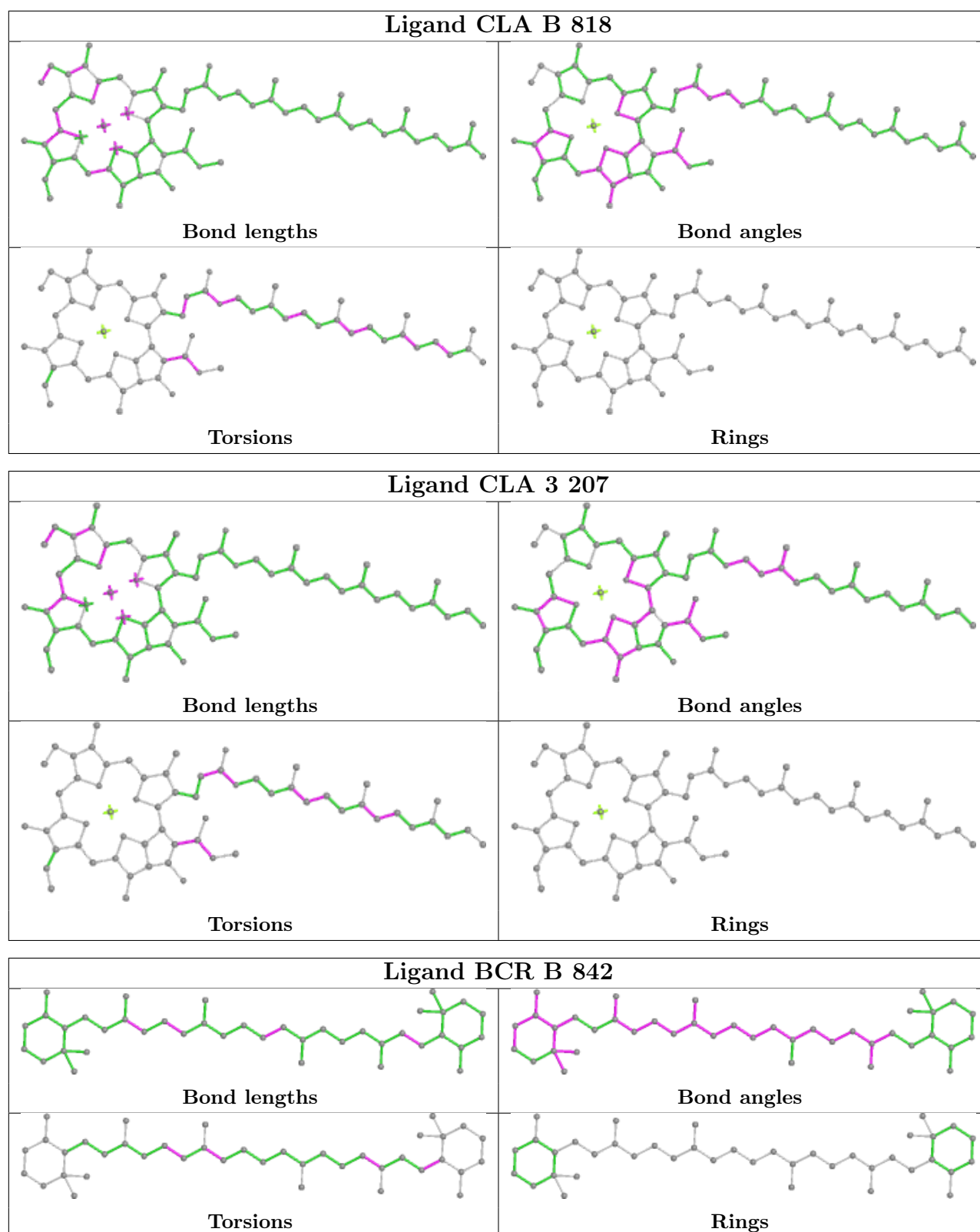


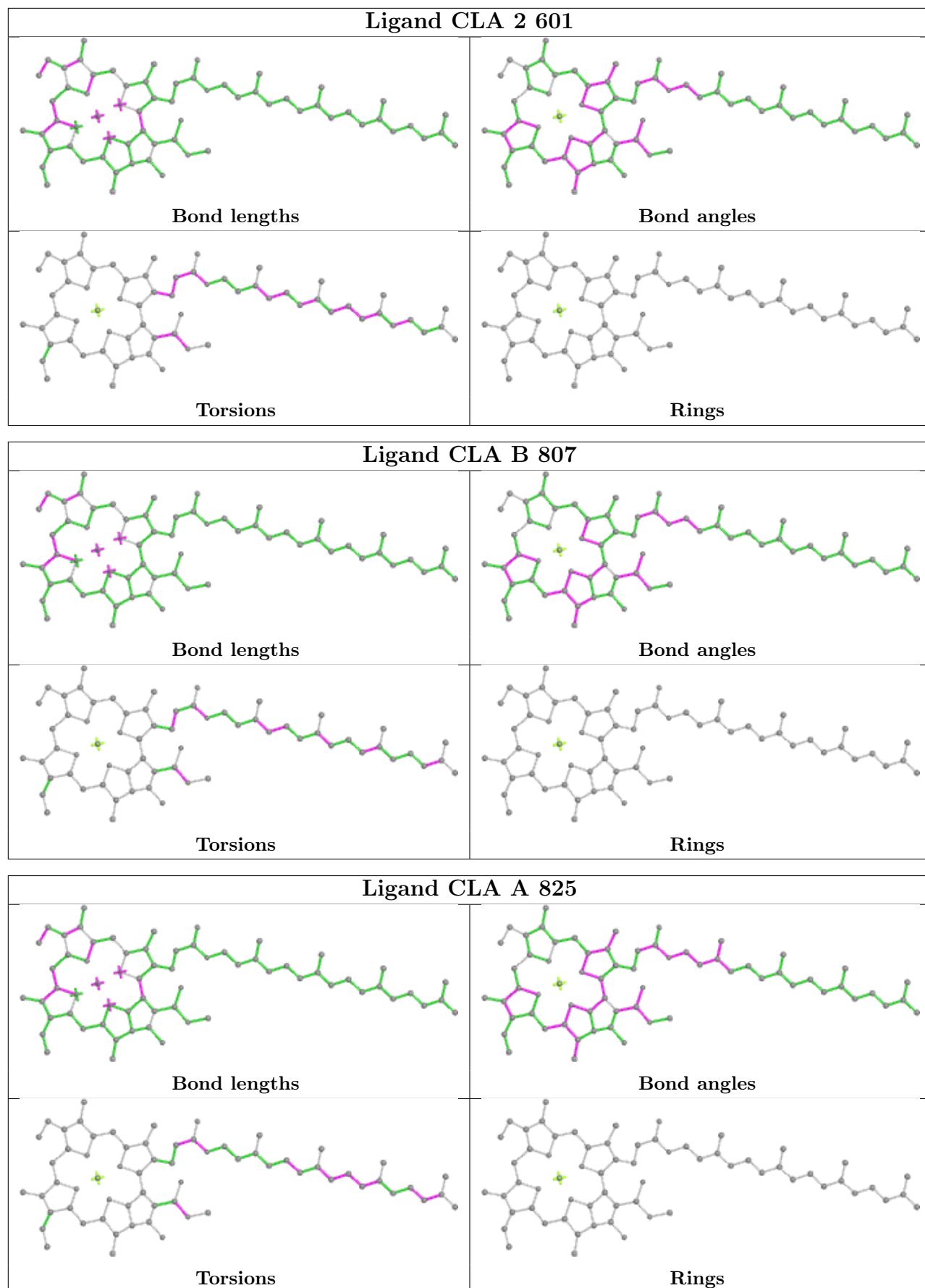


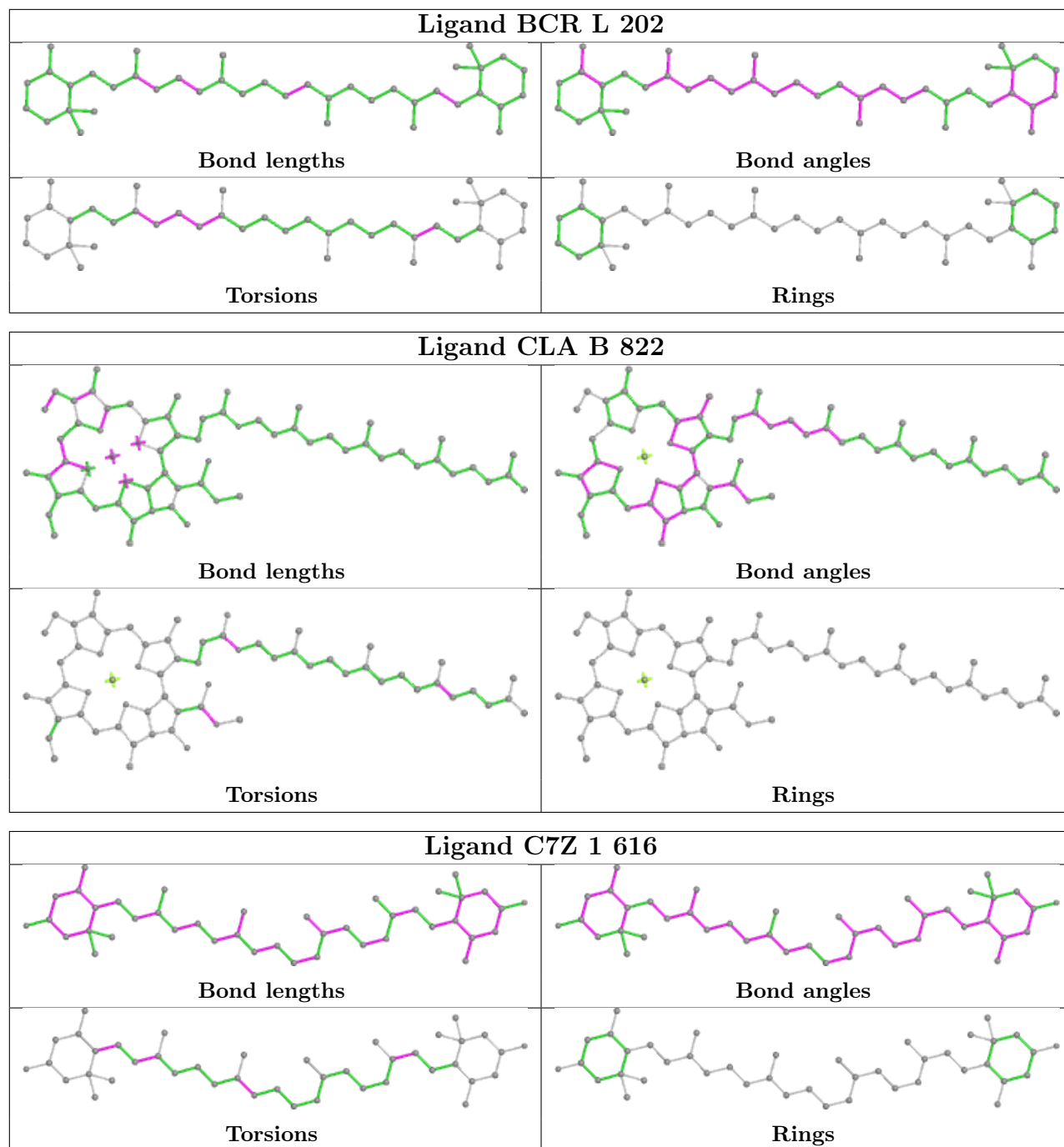


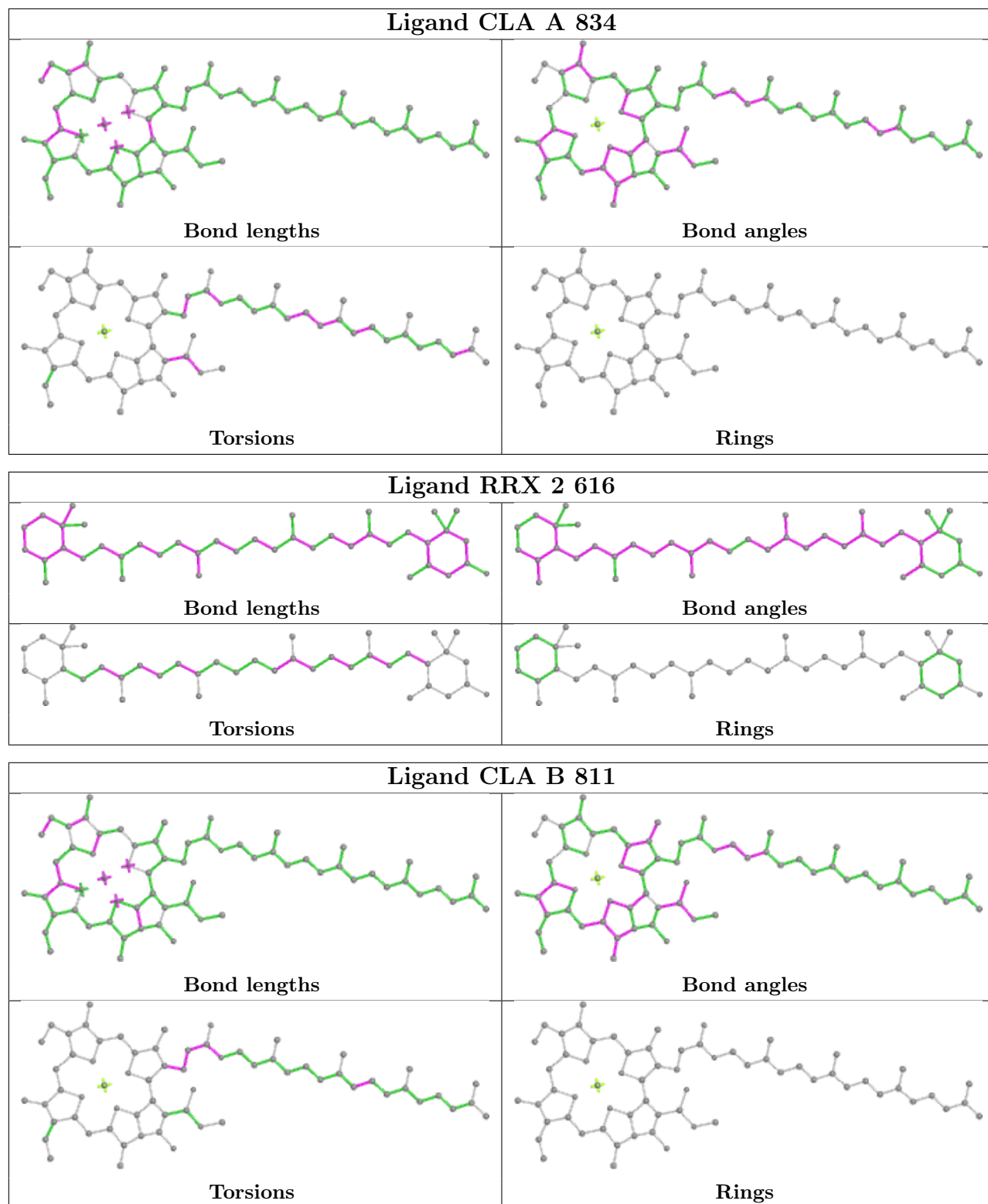




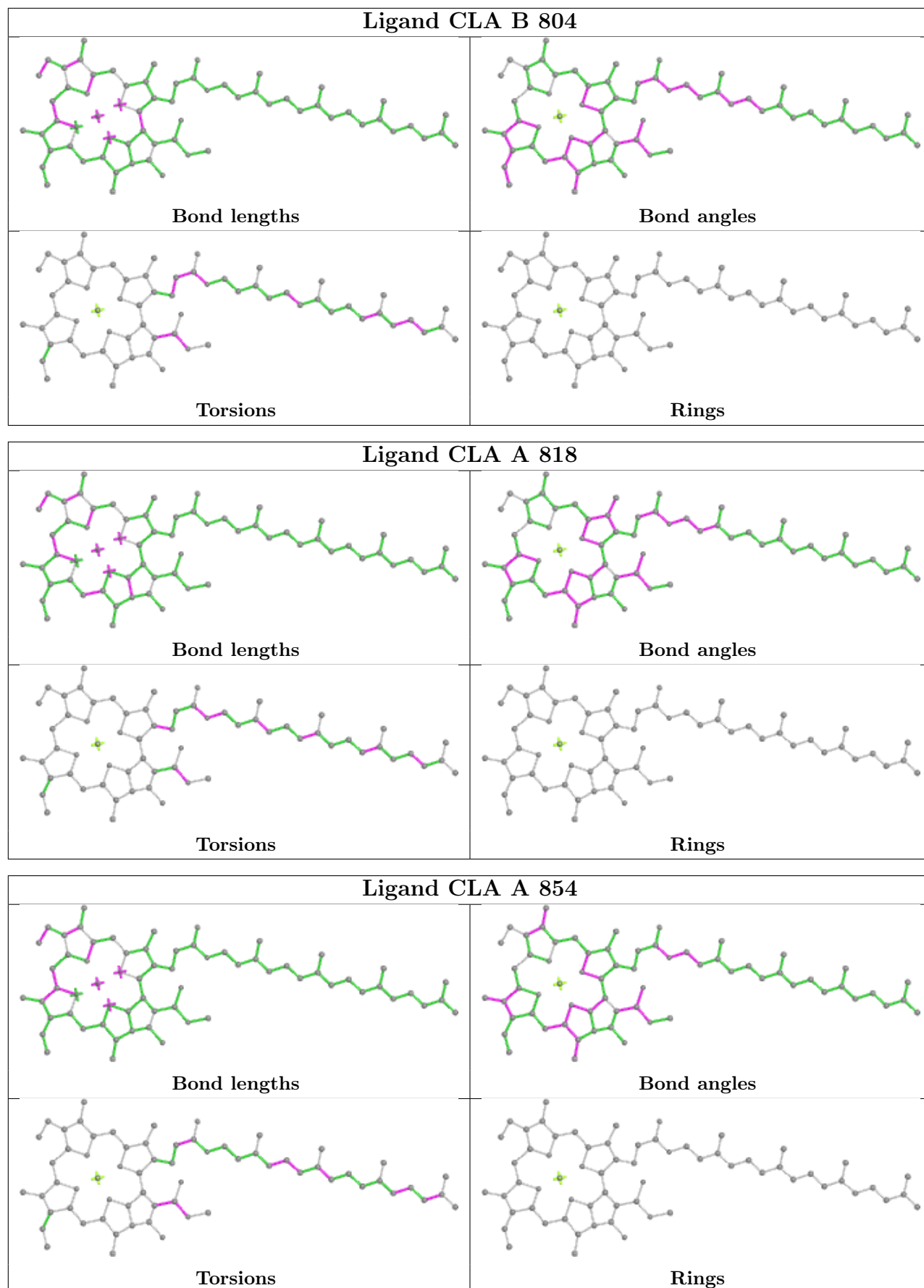












## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

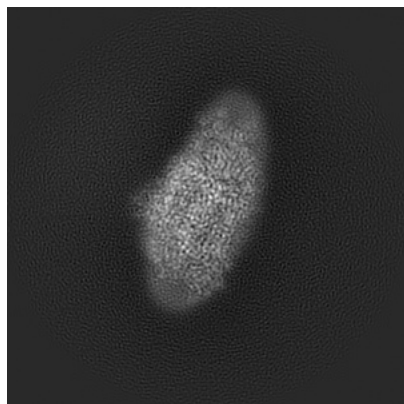
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12228. These allow visual inspection of the internal detail of the map and identification of artifacts.

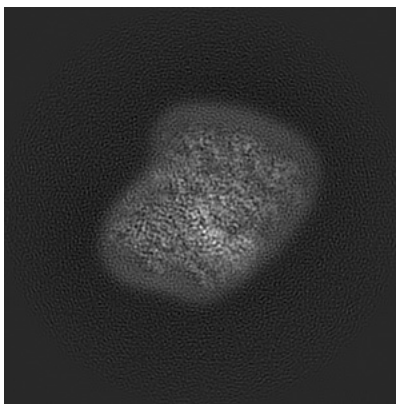
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

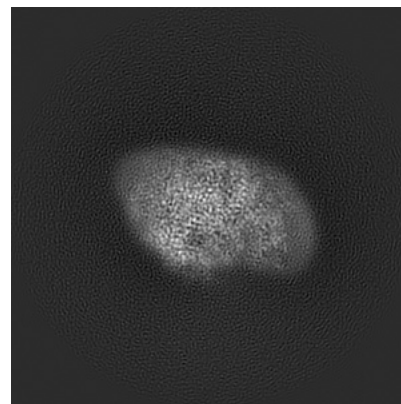
#### 6.1.1 Primary map



X

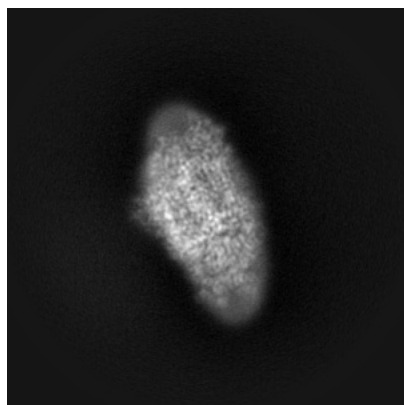


Y

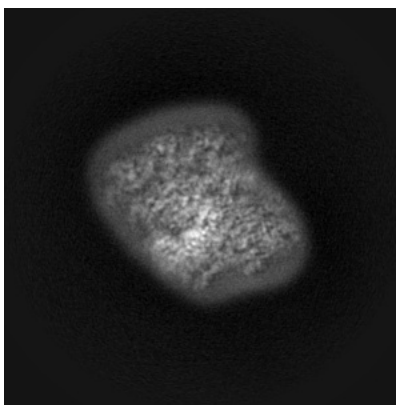


Z

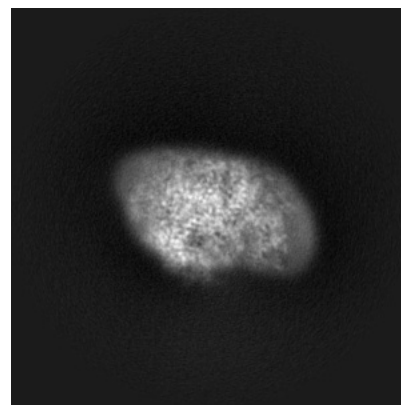
#### 6.1.2 Raw map



X



Y

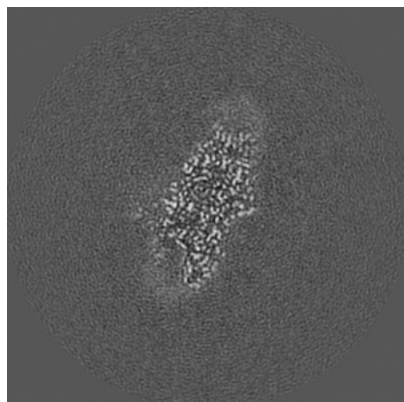


Z

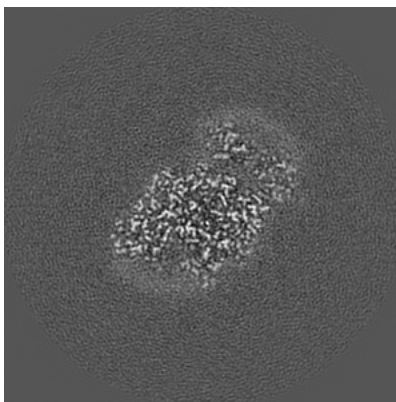
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

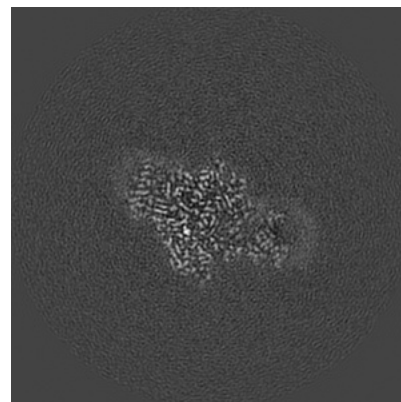
### 6.2.1 Primary map



X Index: 150

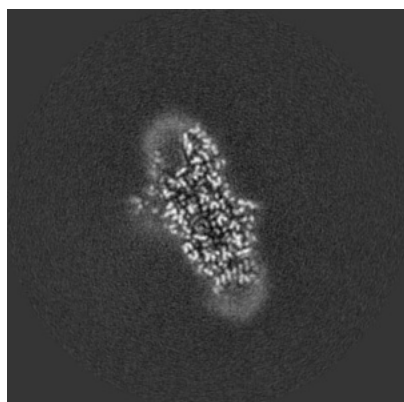


Y Index: 150

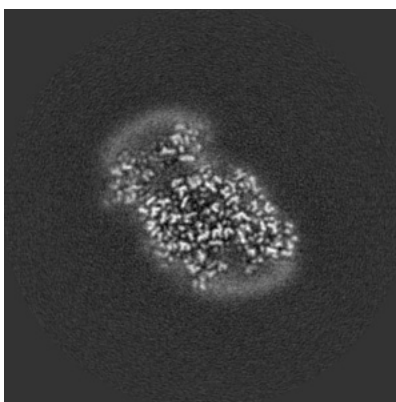


Z Index: 150

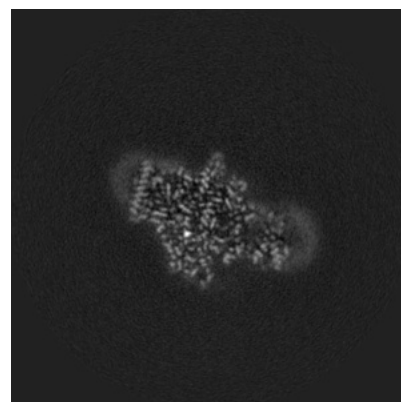
### 6.2.2 Raw map



X Index: 150



Y Index: 150

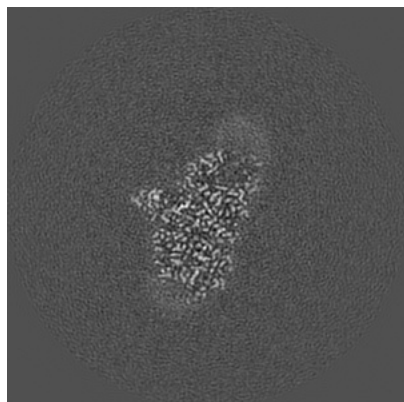


Z Index: 150

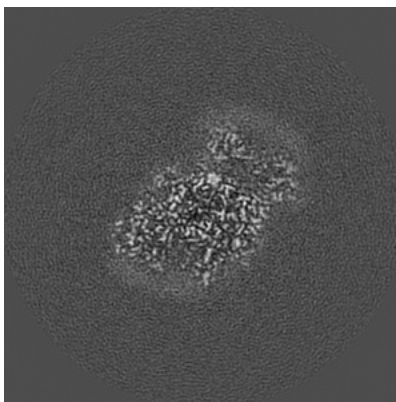
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

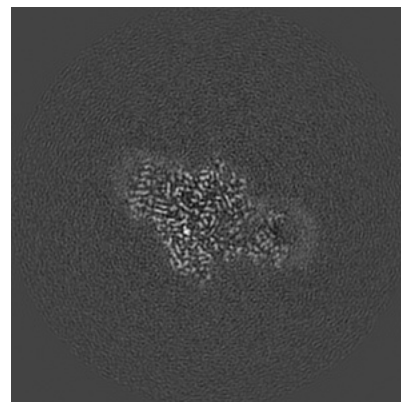
### 6.3.1 Primary map



X Index: 130

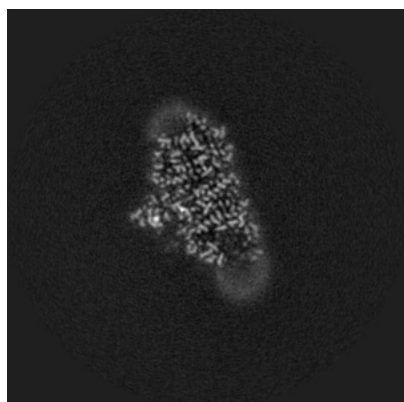


Y Index: 151

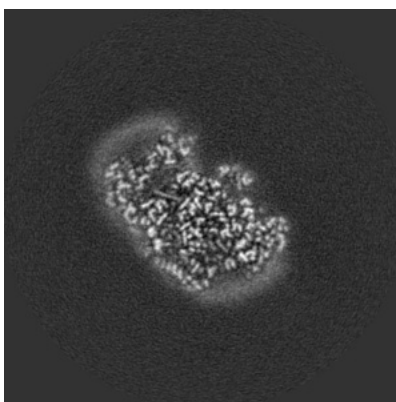


Z Index: 150

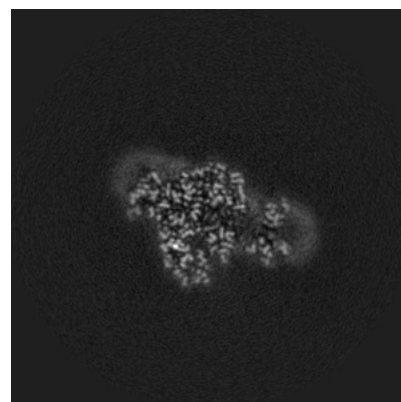
### 6.3.2 Raw map



X Index: 130



Y Index: 158

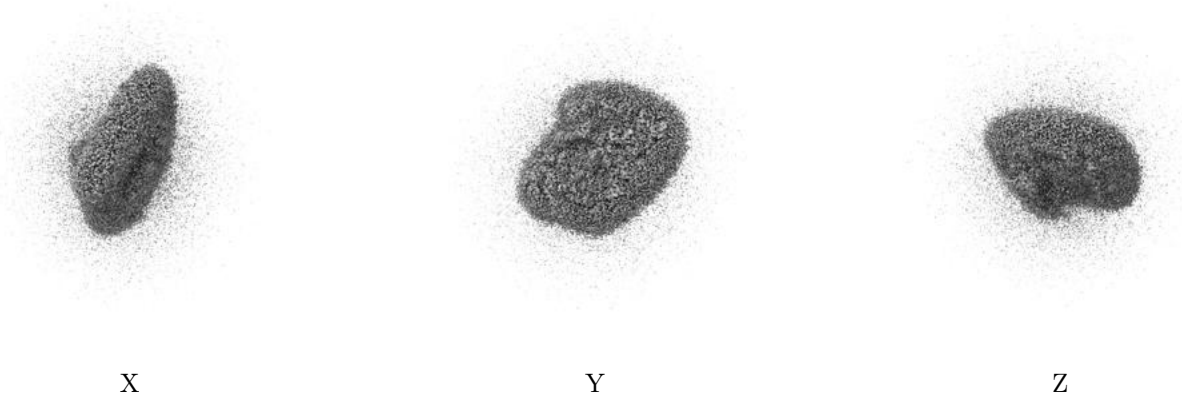


Z Index: 144

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

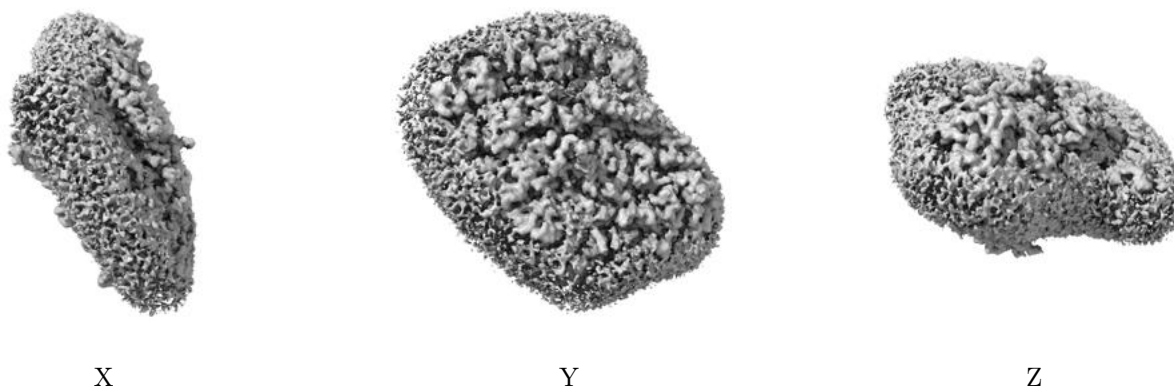
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0186. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



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

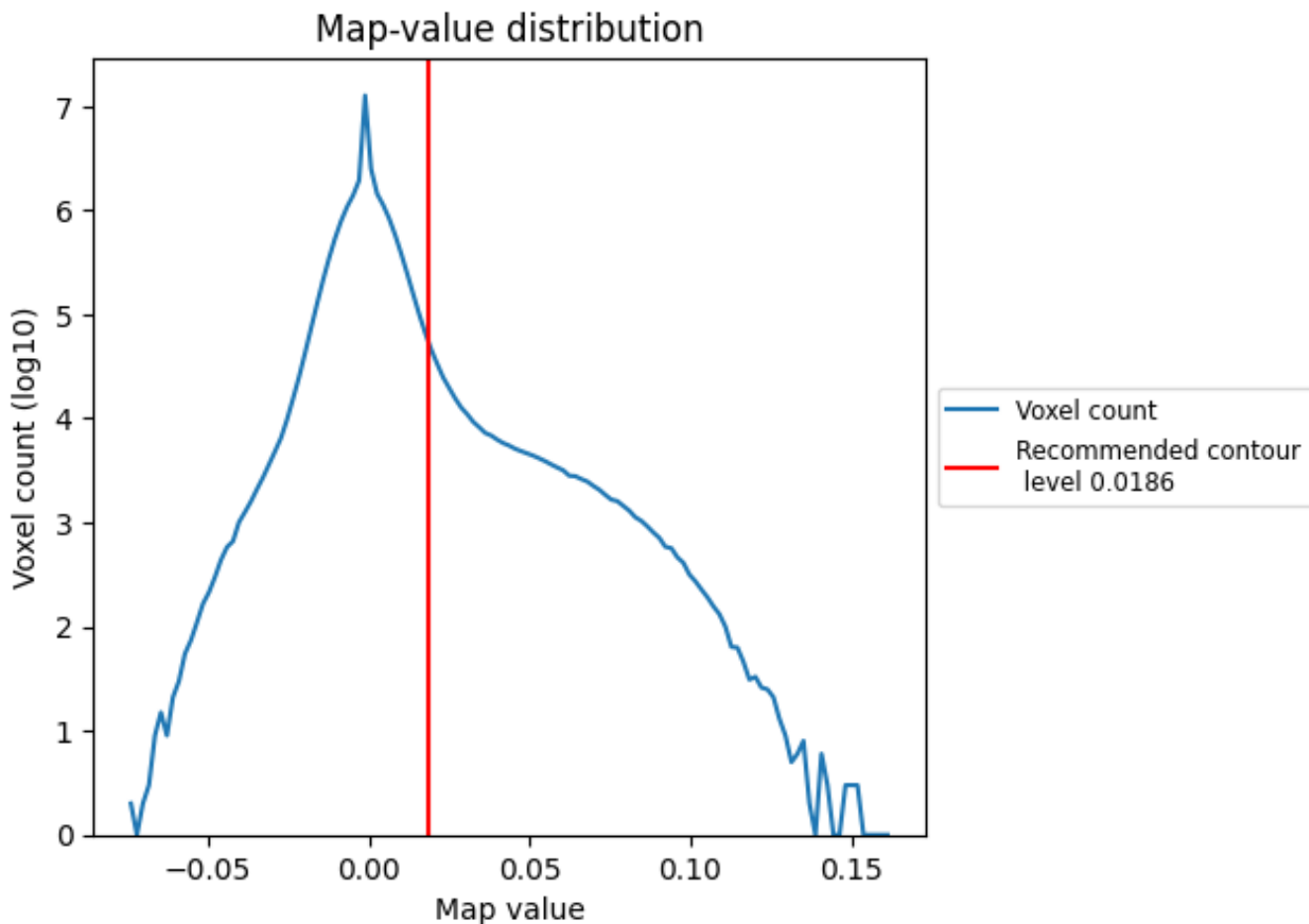
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

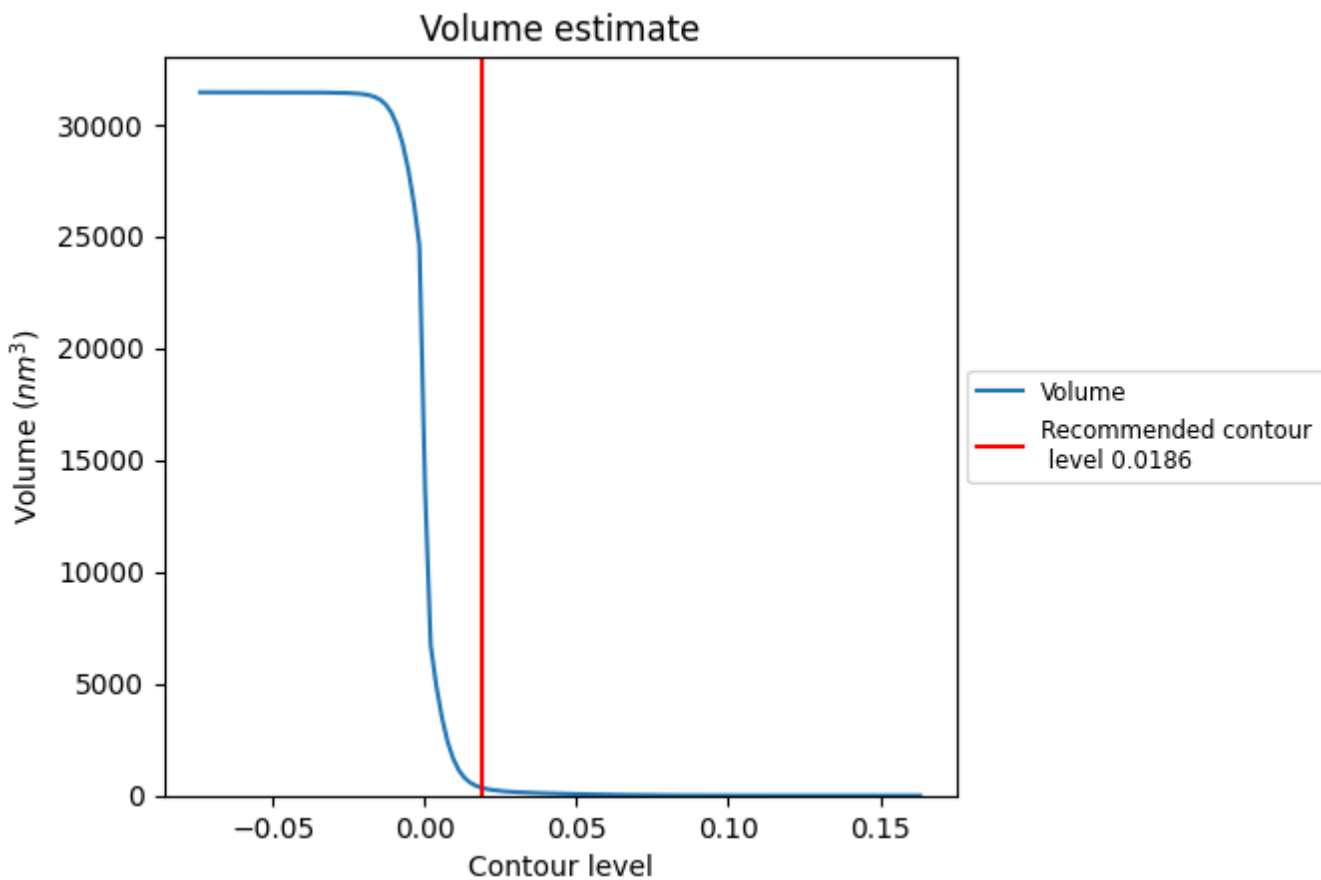
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

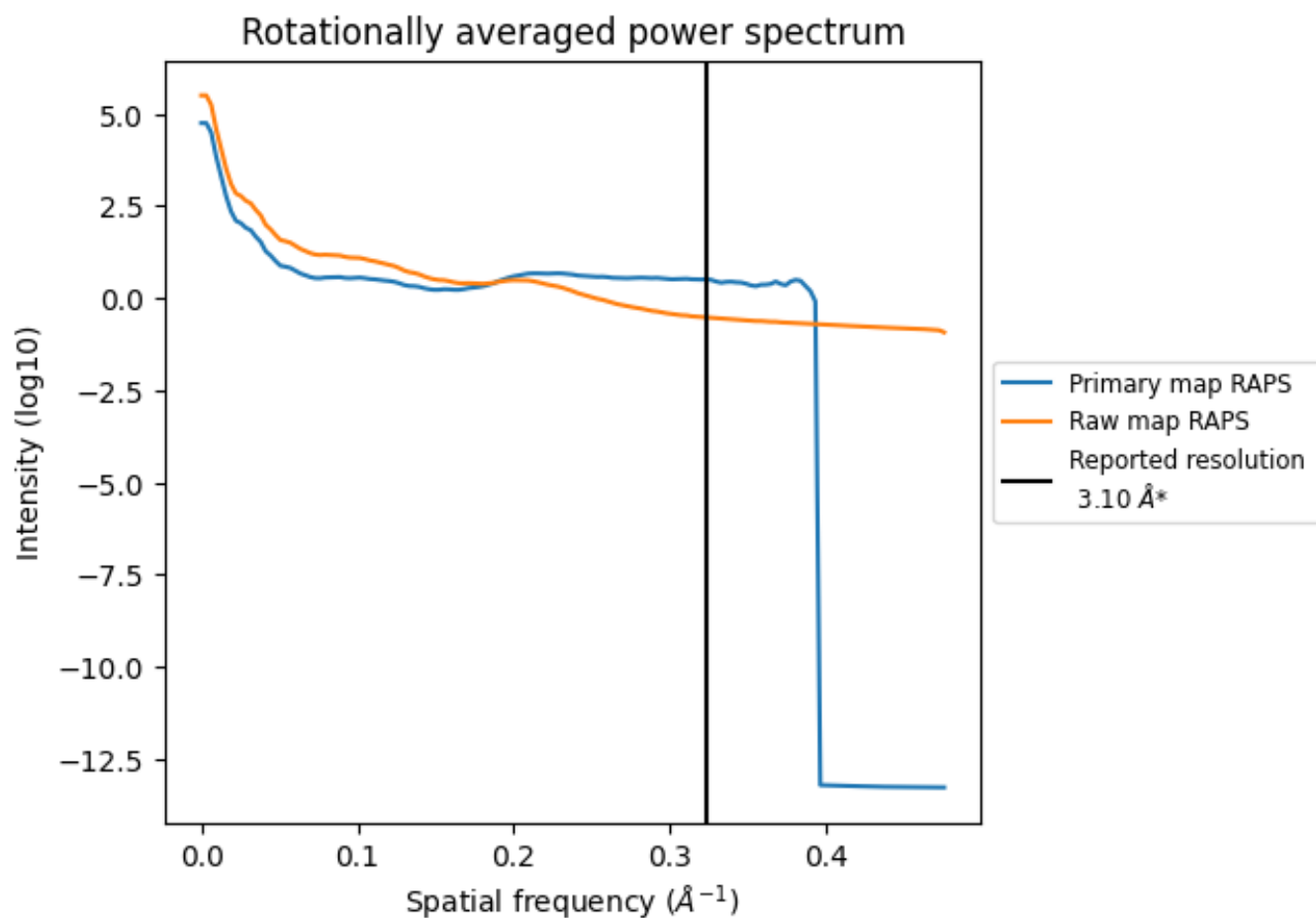


The volume at the recommended contour level is 355  $\text{nm}^3$ ; this corresponds to an approximate mass of 321 kDa.

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



### 7.3 Rotationally averaged power spectrum [i](#)

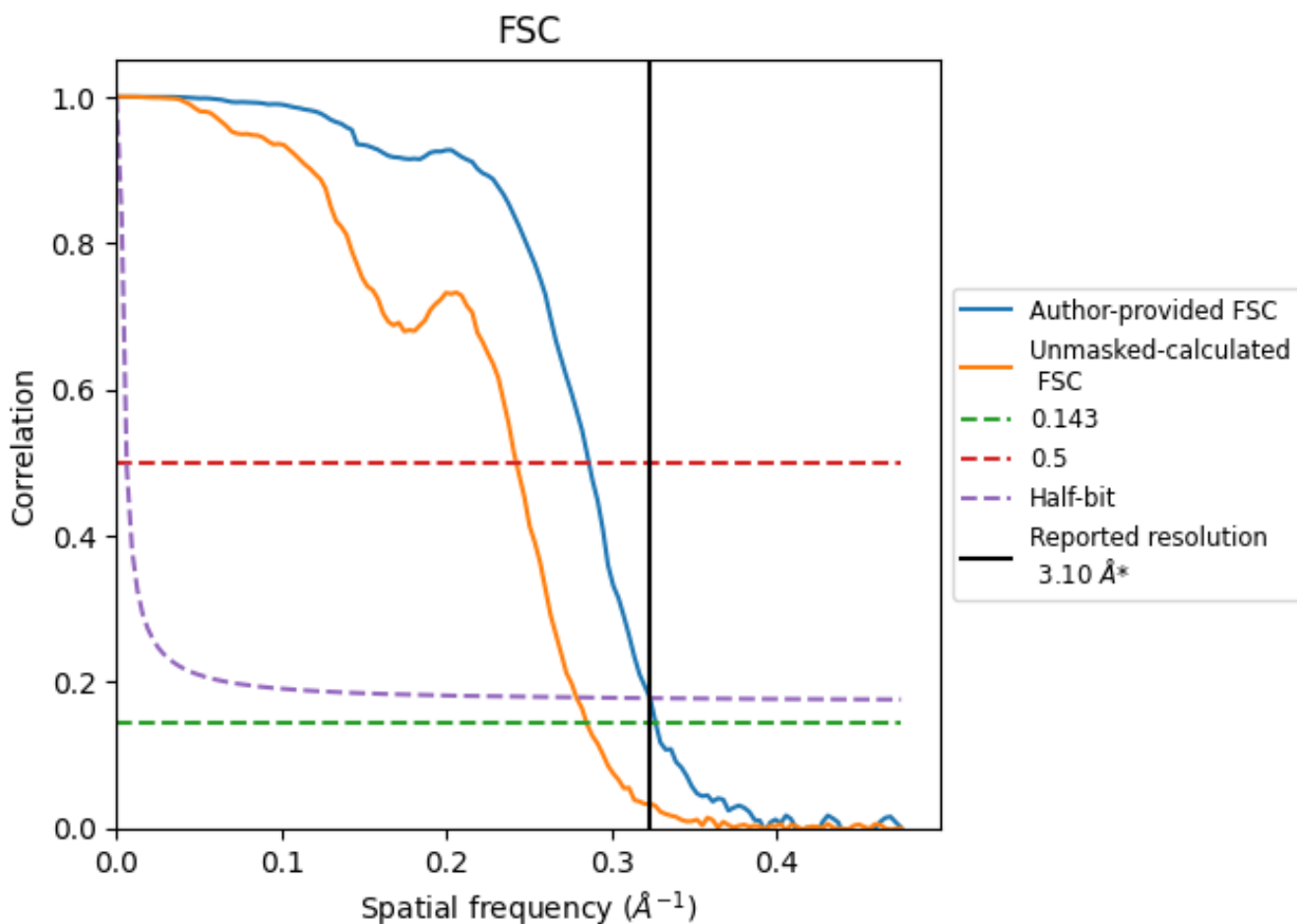


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.50	3.09
Unmasked-calculated*	3.51	4.13	3.59

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.51 differs from the reported value 3.1 by more than 10 %

## 9 Map-model fit [i](#)

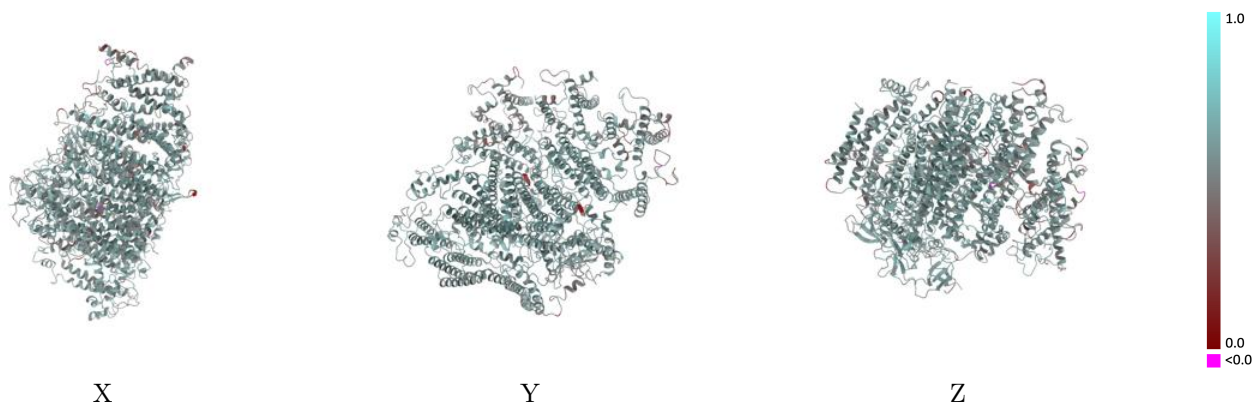
This section contains information regarding the fit between EMDB map EMD-12228 and PDB model 7BLZ. Per-residue inclusion information can be found in section [3](#) on page [29](#).

### 9.1 Map-model overlay [i](#)



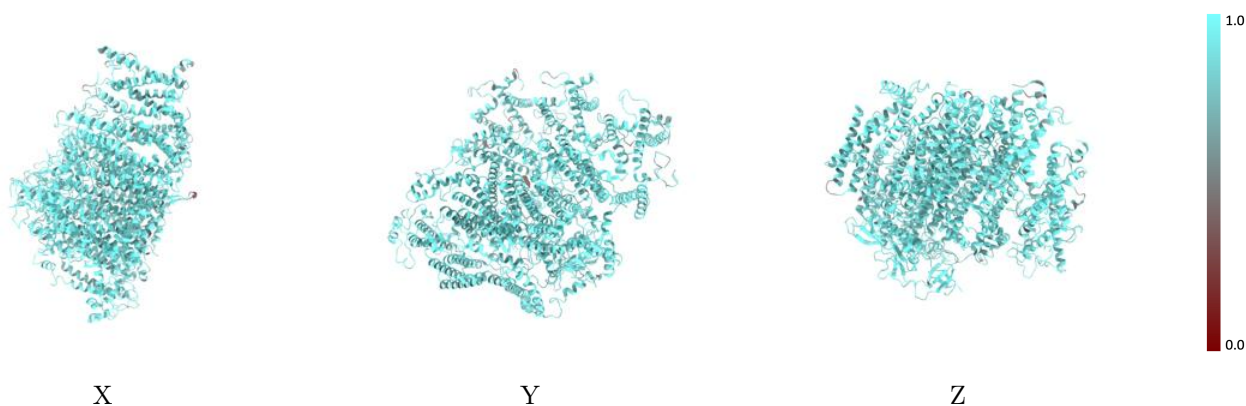
The images above show the 3D surface view of the map at the recommended contour level 0.0186 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



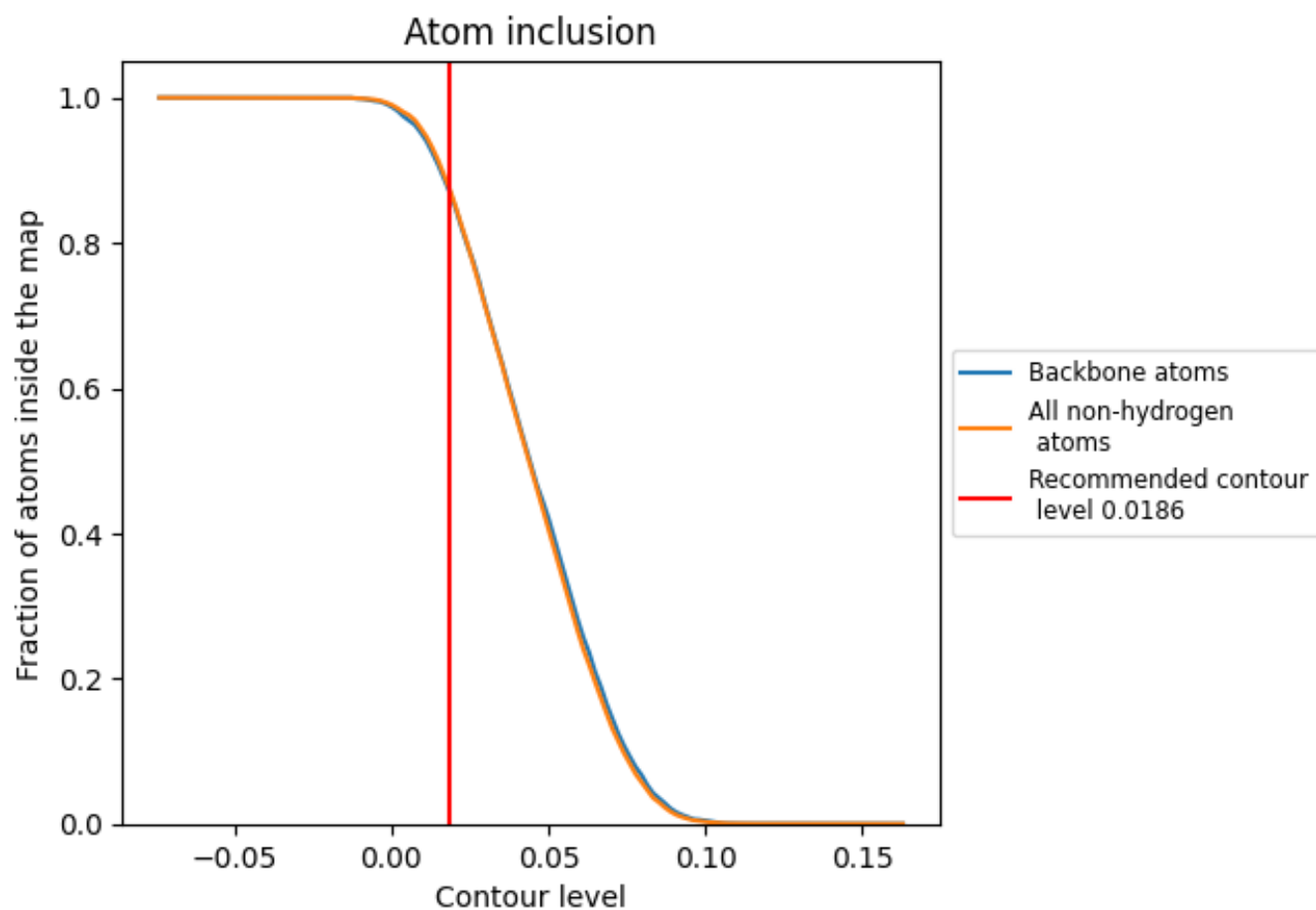
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0186).

































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0186) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.5470
1	 0.8140	 0.4800
2	 0.8132	 0.4930
3	 0.7951	 0.4820
A	 0.9136	 0.5800
B	 0.9075	 0.5710
C	 0.9566	 0.5860
D	 0.9216	 0.5680
E	 0.9134	 0.5640
F	 0.8732	 0.5450
I	 0.8772	 0.5500
J	 0.8237	 0.5150
K	 0.8228	 0.5260
L	 0.8478	 0.5200
M	 0.8719	 0.5430
O	 0.8451	 0.5130

