



Full wwPDB EM Validation Report ⓘ

Nov 18, 2024 – 07:04 PM JST

PDB ID : 8XLS
EMDB ID : EMD-38457
Title : PSI-FCPI of the diatom *Thalassiosira pseudonana* CCMP1335
Authors : Kato, K.; Nakajima, Y.; Shen, J.R.; Nagao, R.
Deposited on : 2023-12-26
Resolution : 2.30 Å (reported)
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

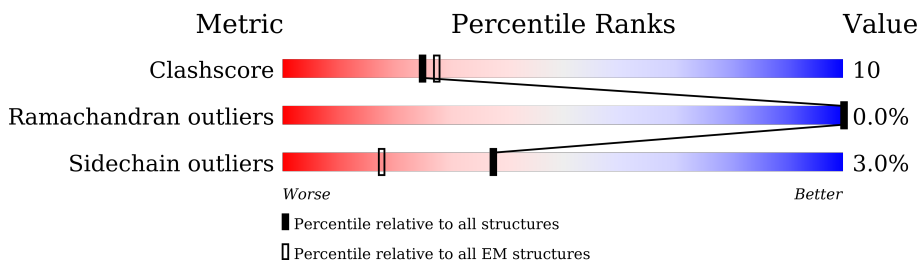
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	752	
2	B	733	
3	C	81	
4	D	139	
5	E	65	
6	F	185	
7	I	36	
8	J	41	

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Mol	Chain	Length	Quality of chain
9	L	148	
10	M	30	
11	W	188	
12	u	84	
13	1	221	
14	2	198	
15	3	196	
16	4	201	
17	5	194	

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
18	CL0	A	801	X	-	-	-
19	CLA	1	301	X	-	-	-
19	CLA	1	303	X	-	-	-
19	CLA	1	304	X	-	-	-
19	CLA	1	306	X	-	-	-
19	CLA	1	307	X	-	-	-
19	CLA	1	308	X	-	-	-
19	CLA	1	309	X	-	-	-
19	CLA	1	310	X	-	-	-
19	CLA	2	205	X	-	-	-
19	CLA	2	206	X	-	-	-
19	CLA	2	207	X	-	-	-
19	CLA	2	208	X	-	-	-
19	CLA	2	209	X	-	-	-
19	CLA	2	210	X	-	-	-
19	CLA	2	212	X	-	-	-
19	CLA	2	213	X	-	-	-
19	CLA	2	214	X	-	-	-
19	CLA	2	215	X	-	-	-
19	CLA	3	202	X	-	-	-
19	CLA	3	203	X	-	-	-
19	CLA	3	204	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	3	206	X	-	-	-
19	CLA	3	207	X	-	-	-
19	CLA	3	209	X	-	-	-
19	CLA	3	210	X	-	-	-
19	CLA	4	301	X	-	-	-
19	CLA	4	303	X	-	-	-
19	CLA	4	304	X	-	-	-
19	CLA	4	305	X	-	-	-
19	CLA	4	306	X	-	-	-
19	CLA	4	311	X	-	-	-
19	CLA	4	312	X	-	-	-
19	CLA	4	313	X	-	-	-
19	CLA	5	207	X	-	-	-
19	CLA	5	208	X	-	-	-
19	CLA	5	209	X	-	-	-
19	CLA	5	210	X	-	-	-
19	CLA	5	211	X	-	-	-
19	CLA	5	212	X	-	-	-
19	CLA	5	213	X	-	-	-
19	CLA	5	214	X	-	-	-
19	CLA	A	802	X	-	-	-
19	CLA	A	803	X	-	-	-
19	CLA	A	804	X	-	-	-
19	CLA	A	805	X	-	-	-
19	CLA	A	806	X	-	-	-
19	CLA	A	807	X	-	-	-
19	CLA	A	808	X	-	-	-
19	CLA	A	809	X	-	-	-
19	CLA	A	810	X	-	-	-
19	CLA	A	811	X	-	-	-
19	CLA	A	812	X	-	-	-
19	CLA	A	813	X	-	-	-
19	CLA	A	814	X	-	-	-
19	CLA	A	815	X	-	-	-
19	CLA	A	816	X	-	-	-
19	CLA	A	818	X	-	-	-
19	CLA	A	819	X	-	-	-
19	CLA	A	820	X	-	-	-
19	CLA	A	822	X	-	-	-
19	CLA	A	824	X	-	-	-
19	CLA	A	825	X	-	-	-
19	CLA	A	826	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	827	X	-	-	-
19	CLA	A	828	X	-	-	-
19	CLA	A	829	X	-	-	-
19	CLA	A	830	X	-	-	-
19	CLA	A	831	X	-	-	-
19	CLA	A	832	X	-	-	-
19	CLA	A	833	X	-	-	-
19	CLA	A	834	X	-	-	-
19	CLA	A	835	X	-	-	-
19	CLA	A	836	X	-	-	-
19	CLA	A	837	X	-	-	-
19	CLA	A	838	X	-	-	-
19	CLA	A	839	X	-	-	-
19	CLA	A	840	X	-	-	-
19	CLA	A	841	X	-	-	-
19	CLA	A	842	X	-	-	-
19	CLA	A	843	X	-	-	-
19	CLA	A	844	X	-	-	-
19	CLA	A	878	X	-	-	-
19	CLA	A	880	X	-	-	-
19	CLA	B	802	X	-	-	-
19	CLA	B	803	X	-	-	-
19	CLA	B	804	X	-	-	-
19	CLA	B	805	X	-	-	-
19	CLA	B	806	X	-	-	-
19	CLA	B	807	X	-	-	-
19	CLA	B	808	X	-	-	-
19	CLA	B	809	X	-	-	-
19	CLA	B	810	X	-	-	-
19	CLA	B	811	X	-	-	-
19	CLA	B	812	X	-	-	-
19	CLA	B	813	X	-	-	-
19	CLA	B	814	X	-	-	-
19	CLA	B	815	X	-	-	-
19	CLA	B	816	X	-	-	-
19	CLA	B	817	X	-	-	-
19	CLA	B	818	X	-	-	-
19	CLA	B	819	X	-	-	-
19	CLA	B	821	X	-	-	-
19	CLA	B	822	X	-	-	-
19	CLA	B	823	X	-	-	-
19	CLA	B	824	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	825	X	-	-	-
19	CLA	B	826	X	-	-	-
19	CLA	B	827	X	-	-	-
19	CLA	B	829	X	-	-	-
19	CLA	B	830	X	-	-	-
19	CLA	B	831	X	-	-	-
19	CLA	B	832	X	-	-	-
19	CLA	B	833	X	-	-	-
19	CLA	B	834	X	-	-	-
19	CLA	B	835	X	-	-	-
19	CLA	B	836	X	-	-	-
19	CLA	B	837	X	-	-	-
19	CLA	B	838	X	-	-	-
19	CLA	B	846	X	-	-	-
19	CLA	F	203	X	-	-	-
19	CLA	F	204	X	-	-	-
19	CLA	J	103	X	-	-	-
19	CLA	L	204	X	-	-	-
19	CLA	L	206	X	-	-	-
19	CLA	u	201	X	-	-	-
19	CLA	u	202	X	-	-	-
27	5X6	J	105	-	X	-	-

2 Entry composition i

There are 32 unique types of molecules in this entry. The entry contains 37637 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	741	5858	3828	994	1007	29	2	0

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	731	5835	3833	985	998	19	2	0

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	607	373	105	119	10	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	132	1050	671	181	195	3	1	0

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	61	494	312	88	94	0	0

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	161	1253	801	215	234	3	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	36	276	191	37	46	2	0	0

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	41	342	233	49	57	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	L	146	1106	728	182	194	2	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	M	30	228	152	35	39	2	0	0

- Molecule 11 is a protein called Photosystem I reaction center subunit Psa29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	W	122	912	576	144	188	4	0	0

- Molecule 12 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	u	76	380	228	76	76	0	0

- Molecule 13 is a protein called Fucoxanthin chlorophyll a/c-binding protein RedCAP.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	1	185	1413	902	235	262	14	0	0

- Molecule 14 is a protein called Fucoxanthin chl a/c light-harvesting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	2	167	1288	825	213	240	10	0	0

- Molecule 15 is a protein called Pt17531-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	3	164	1273	821	208	234	10	0	0

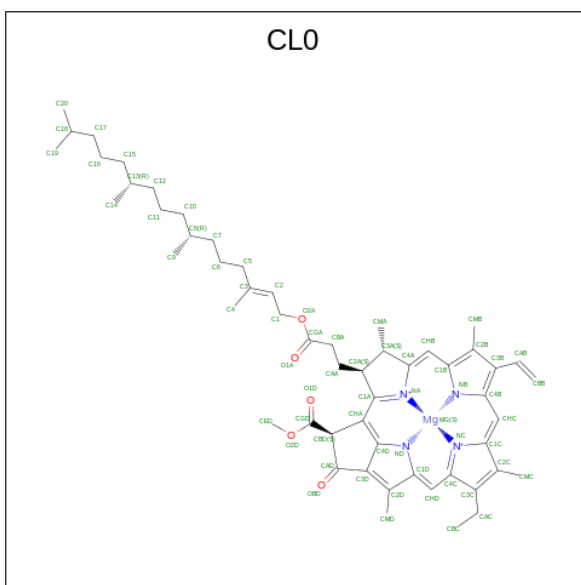
- Molecule 16 is a protein called Fucoxanthin chl a/c light-harvesting protein, major type.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	4	167	1289	834	210	237	8	0	0

- Molecule 17 is a protein called Fucoxanthin chlorophyll a/c-binding protein Lhcq8.

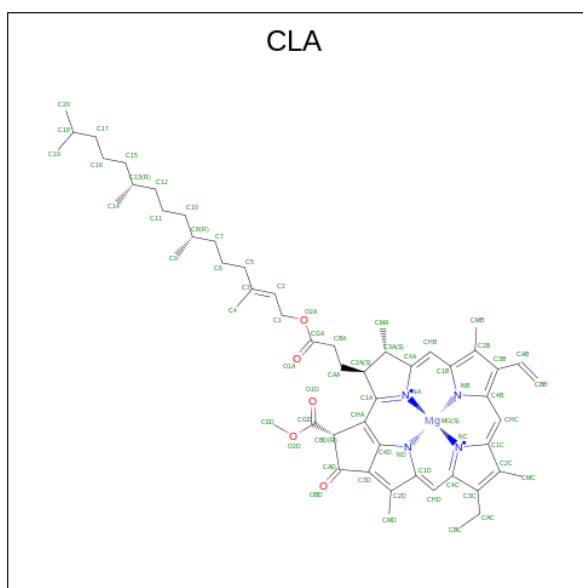
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	5	165	1285	833	204	240	8	0	0

- Molecule 18 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
18	A	1	65	55	1	4	5	0

- Molecule 19 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms				AltConf	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	A	1	50	40	1	4	5	0
19	A	1	50	40	1	4	5	0
19	A	1	49	39	1	4	5	0
19	A	1	54	44	1	4	5	0
19	A	1	54	44	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	54	44	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	49	39	1	4	5	0
19	A	1	51	41	1	4	5	0
19	A	1	59	49	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	60	50	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	A	1	54	44	1	4	5	0
19	A	1	45	35	1	4	5	0
19	A	1	51	41	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	47	37	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	45	35	1	4	5	0
19	B	1	55	45	1	4	5	0
19	B	1	59	49	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	45	35	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	54	44	1	4	5	0
19	B	1	56	46	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	45	35	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	58	48	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	B	1	60	50	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	47	37	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	F	1	55	45	1	4	5	0
19	F	1	45	35	1	4	5	0
19	J	1	45	35	1	4	5	0
19	L	1	65	55	1	4	5	0
19	L	1	45	35	1	4	5	0
19	L	1	60	50	1	4	5	0
19	u	1	55	45	1	4	5	0
19	u	1	45	35	1	4	5	0
19	1	1	65	55	1	4	5	0
19	1	1	65	55	1	4	5	0
19	1	1	65	55	1	4	5	0
19	1	1	51	41	1	4	5	0
19	1	1	55	45	1	4	5	0

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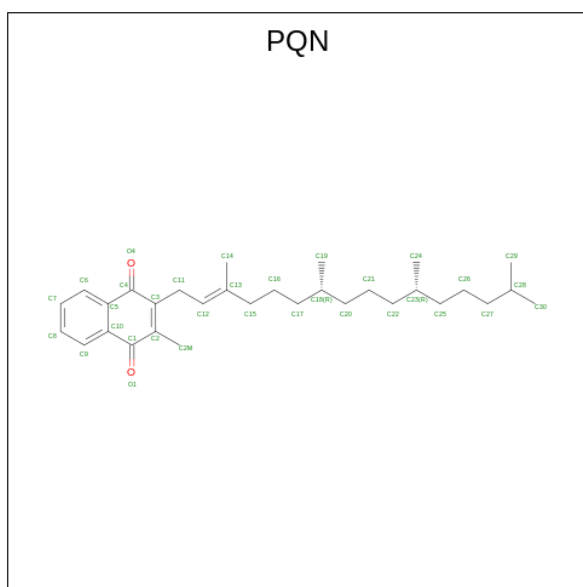
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	1	1	45	35	1	4	5	0
19	1	1	65	55	1	4	5	0
19	1	1	65	55	1	4	5	0
19	2	1	65	55	1	4	5	0
19	2	1	65	55	1	4	5	0
19	2	1	65	55	1	4	5	0
19	2	1	52	42	1	4	5	0
19	2	1	58	48	1	4	5	0
19	2	1	60	50	1	4	5	0
19	2	1	45	35	1	4	5	0
19	2	1	45	35	1	4	5	0
19	2	1	45	35	1	4	5	0
19	2	1	42	34	1	4	3	0
19	3	1	65	55	1	4	5	0
19	3	1	55	45	1	4	5	0
19	3	1	61	51	1	4	5	0
19	3	1	65	55	1	4	5	0
19	3	1	65	55	1	4	5	0
19	3	1	51	41	1	4	5	0
19	3	1	45	35	1	4	5	0
19	4	1	65	55	1	4	5	0

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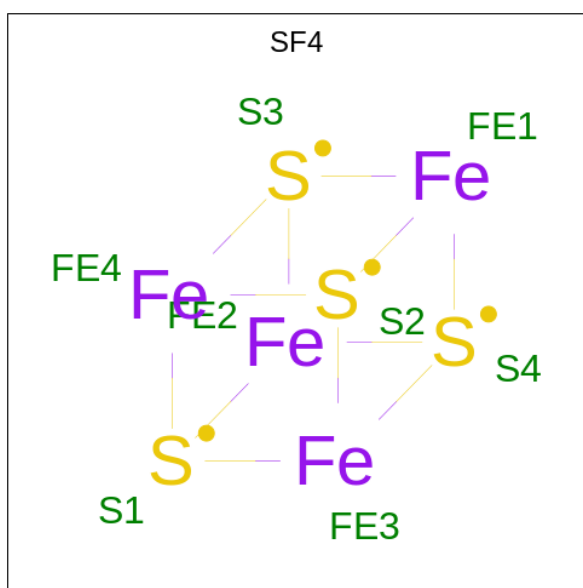
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	4	1	55	45	1	4	5	0
19	4	1	50	40	1	4	5	0
19	4	1	65	55	1	4	5	0
19	4	1	58	48	1	4	5	0
19	4	1	45	35	1	4	5	0
19	4	1	45	35	1	4	5	0
19	4	1	45	35	1	4	5	0
19	4	1	50	40	1	4	5	0
19	4	1	52	42	1	4	5	0
19	4	1	55	45	1	4	5	0
19	5	1	60	50	1	4	5	0
19	5	1	60	50	1	4	5	0
19	5	1	65	55	1	4	5	0
19	5	1	65	55	1	4	5	0
19	5	1	58	48	1	4	5	0
19	5	1	56	46	1	4	5	0
19	5	1	45	35	1	4	5	0
19	5	1	45	35	1	4	5	0
19	5	1	45	35	1	4	5	0
19	5	1	42	34	1	4	3	0

- Molecule 20 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			33	31	2	
20	B	1	Total	C	O	0
			33	31	2	

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



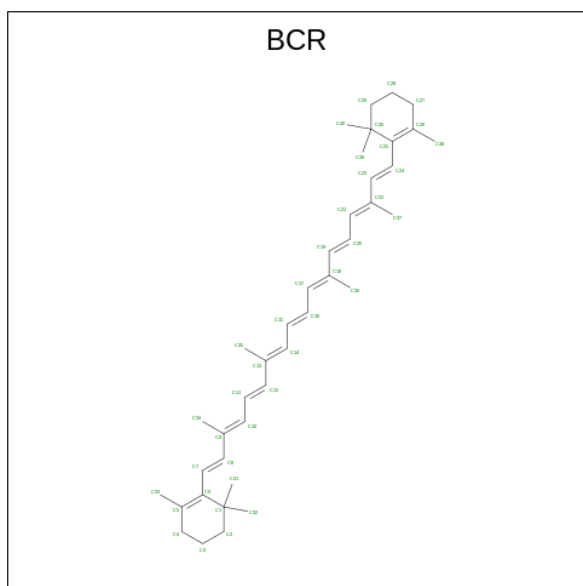
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	Fe	S	0
			8	4	4	
21	C	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
21	C	1	8	4	4	0

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



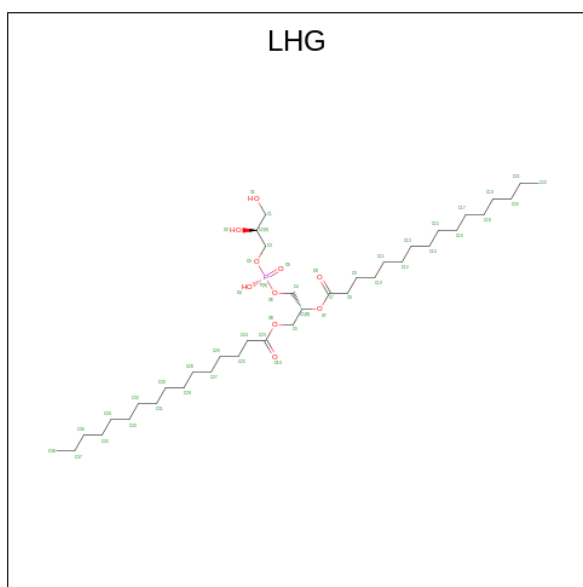
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms		AltConf
22	F	1	Total	C	0
			40	40	
22	F	1	Total	C	0
			40	40	
22	I	1	Total	C	0
			40	40	
22	I	1	Total	C	0
			40	40	
22	J	1	Total	C	0
			40	40	
22	L	1	Total	C	0
			40	40	
22	L	1	Total	C	0
			40	40	
22	M	1	Total	C	0
			40	40	
22	1	1	Total	C	0
			40	40	
22	1	1	Total	C	0
			40	40	

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



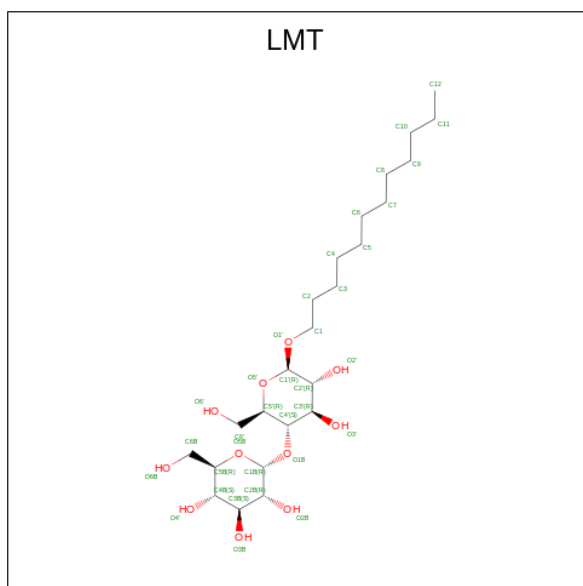
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			47	36	10	1	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
23	A	1	Total 49	C 38	O 10	P 1	0
23	B	1	Total 35	C 24	O 10	P 1	0
23	M	1	Total 41	C 30	O 10	P 1	0
23	1	1	Total 41	C 30	O 10	P 1	0
23	3	1	Total 34	C 23	O 10	P 1	0
23	4	1	Total 49	C 38	O 10	P 1	0

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

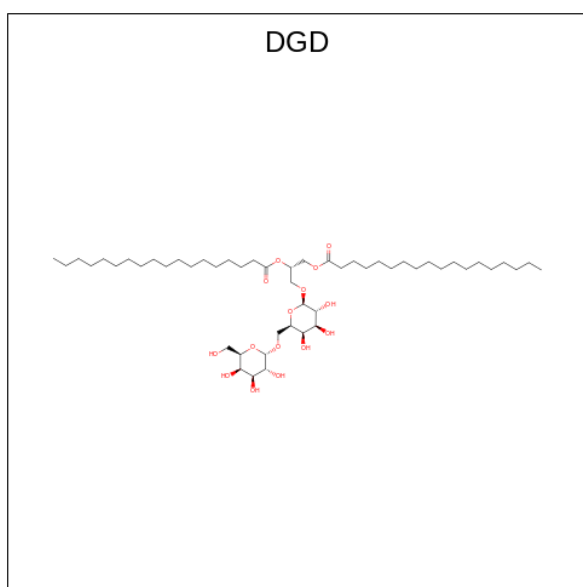


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	A	1	Total 35	C 24	O 11	0
24	1	1	Total 35	C 24	O 11	0
24	2	1	Total 35	C 24	O 11	0
24	3	1	Total 35	C 24	O 11	0

- Molecule 25 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

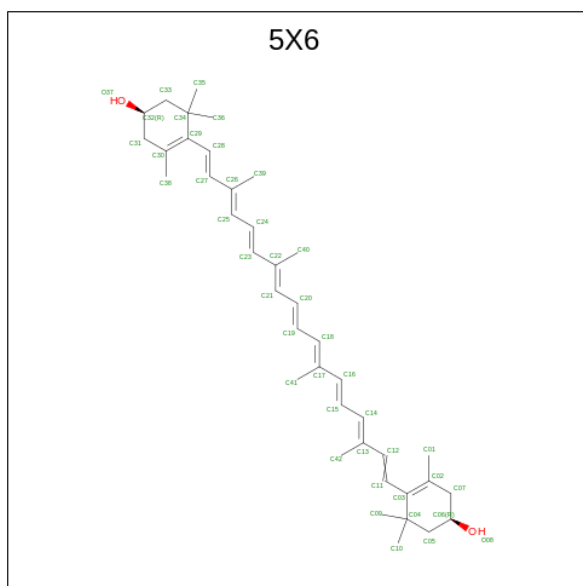
Mol	Chain	Residues	Atoms	AltConf
25	A	25	Total C 230 230	0
25	B	8	Total C 73 73	0
25	F	3	Total C 38 38	0
25	J	4	Total C 39 39	0
25	L	5	Total C 72 72	0
25	M	3	Total C 28 28	0
25	1	4	Total C 38 38	0
25	2	12	Total C 86 86	0
25	3	12	Total C 124 124	0
25	4	3	Total C 21 21	0
25	5	10	Total C 111 111	0

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



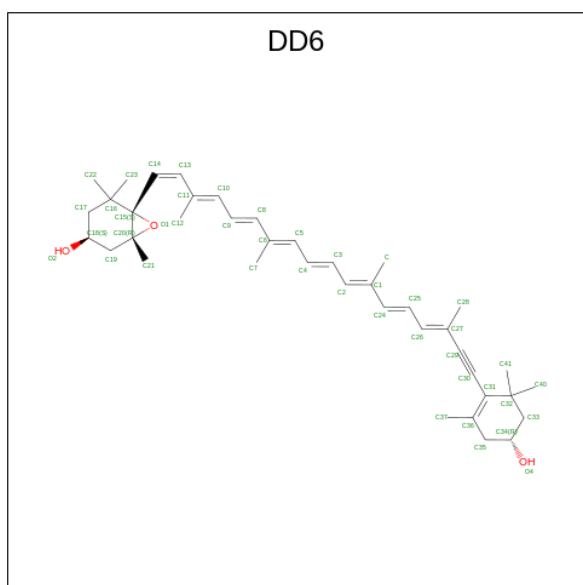
Mol	Chain	Residues	Atoms			AltConf
26	B	1	Total	C	O	0
			66	51	15	

- Molecule 27 is Zeaxanthin (three-letter code: 5X6) (formula: $C_{40}H_{56}O_2$).



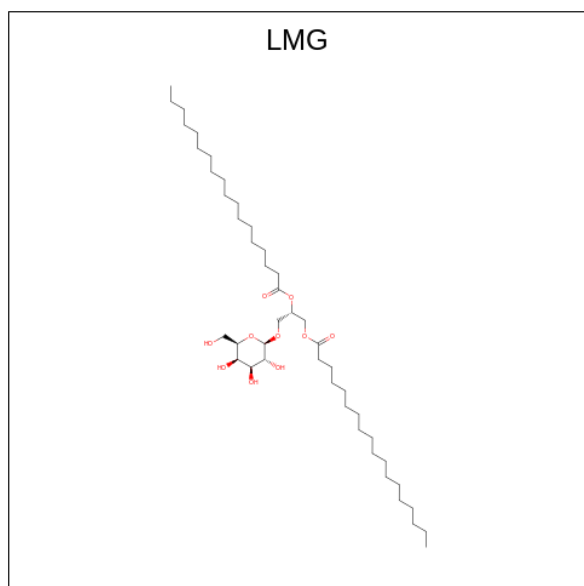
Mol	Chain	Residues	Atoms			AltConf
27	J	1	Total	C	O	0
			42	40	2	

- Molecule 28 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (three-letter code: DD6) (formula: $C_{40}H_{54}O_3$).



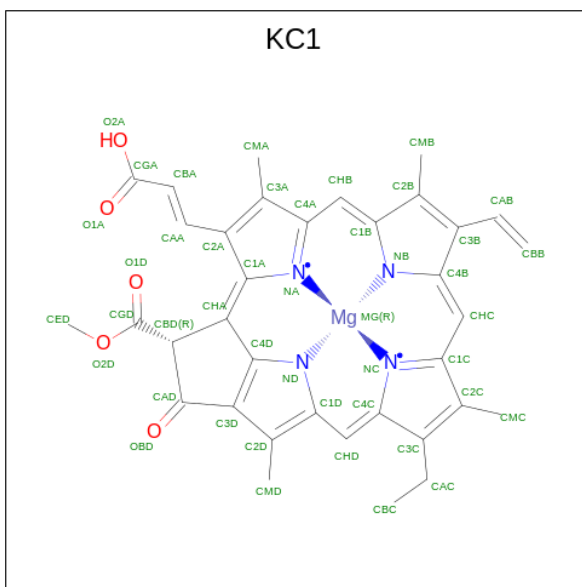
Mol	Chain	Residues	Atoms			AltConf
28	L	1	Total	C	O	0
			43	40	3	
28	1	1	Total	C	O	0
			43	40	3	
28	1	1	Total	C	O	0
			43	40	3	
28	1	1	Total	C	O	0
			43	40	3	
28	2	1	Total	C	O	0
			43	40	3	
28	3	1	Total	C	O	0
			43	40	3	
28	5	1	Total	C	O	0
			43	40	3	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



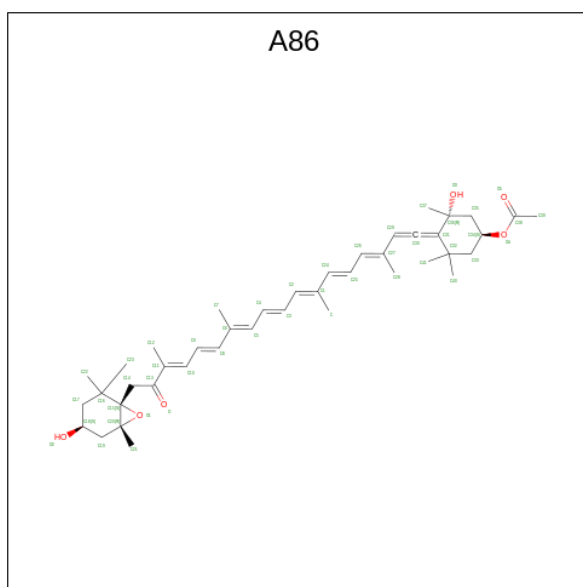
Mol	Chain	Residues	Atoms			AltConf
29	1	1	Total	C	O	0
			49	39	10	

- Molecule 30 is Chlorophyll c1 (three-letter code: KC1) (formula: $C_{35}H_{30}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
30	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 31 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (three-letter code: A86) (formula: C₄₂H₅₈O₆).



Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			48	42	6	
31	1	1	Total	C	O	0
			48	42	6	
31	2	1	Total	C	O	0
			48	42	6	
31	2	1	Total	C	O	0
			48	42	6	
31	2	1	Total	C	O	0
			48	42	6	
31	3	1	Total	C	O	0
			48	42	6	
31	3	1	Total	C	O	0
			48	42	6	
31	3	1	Total	C	O	0
			48	42	6	
31	4	1	Total	C	O	0
			48	42	6	
31	4	1	Total	C	O	0
			48	42	6	
31	4	1	Total	C	O	0
			48	42	6	
31	5	1	Total	C	O	0
			48	42	6	
31	5	1	Total	C	O	0
			48	42	6	
31	5	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	5	1	48	42	6	0

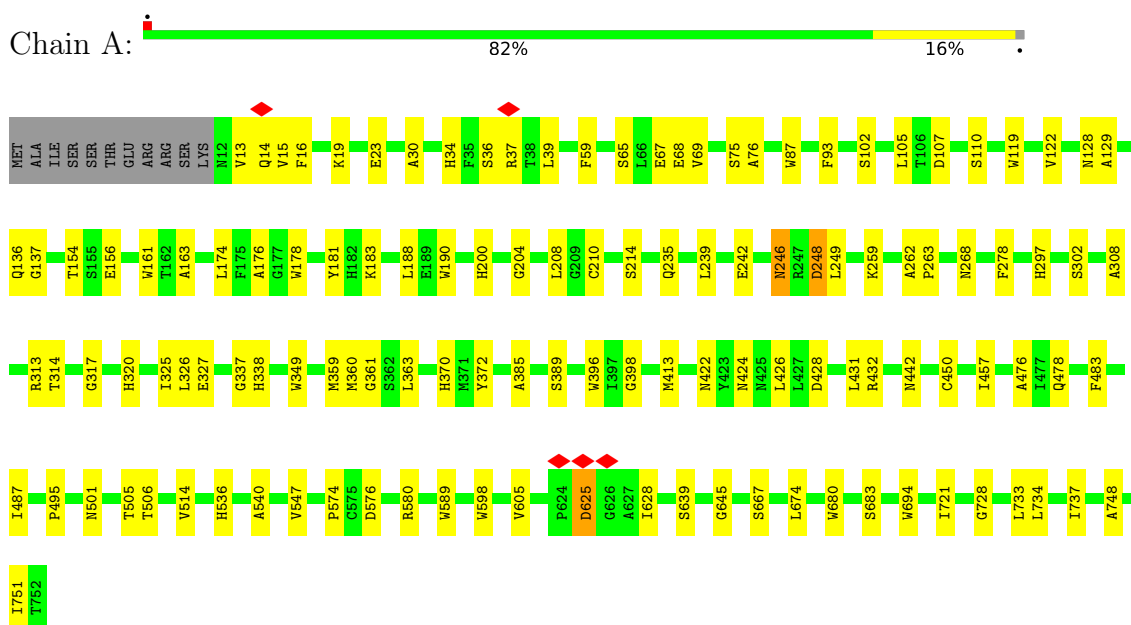
- Molecule 32 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
32	A	240	240	240	0
32	B	300	300	300	0
32	C	50	50	50	0
32	D	56	56	56	0
32	E	24	24	24	0
32	F	46	46	46	0
32	I	6	6	6	0
32	J	7	7	7	0
32	L	30	30	30	0
32	M	7	7	7	0
32	W	20	20	20	0
32	u	3	3	3	0
32	1	49	49	49	0
32	2	22	22	22	0
32	3	34	34	34	0
32	4	11	11	11	0
32	5	17	17	17	0

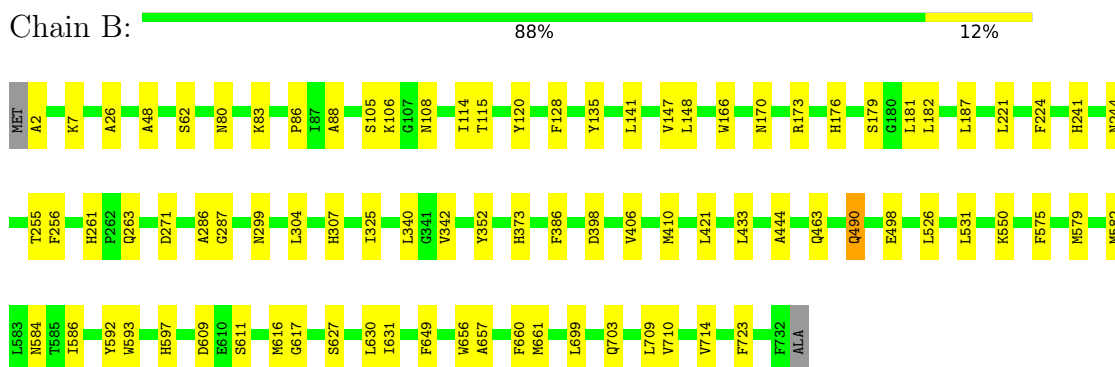
3 Residue-property plots i

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.

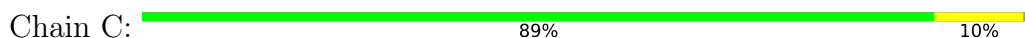
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center

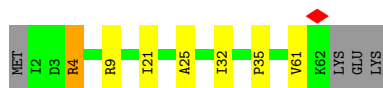
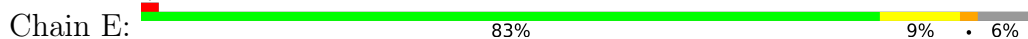




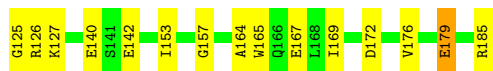
• Molecule 4: Photosystem I reaction center subunit II



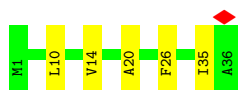
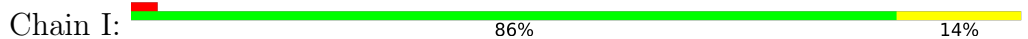
• Molecule 5: Photosystem I reaction center subunit IV



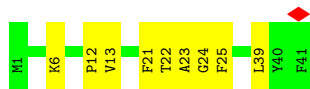
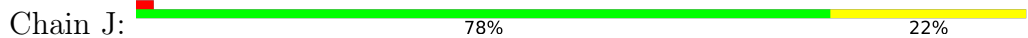
• Molecule 6: Photosystem I reaction center subunit III



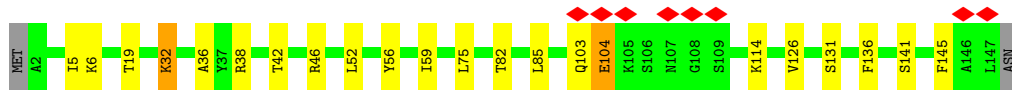
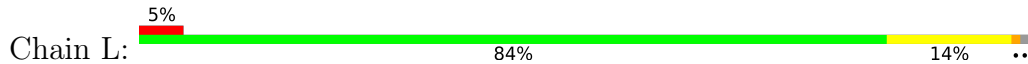
• Molecule 7: Photosystem I reaction center subunit VIII



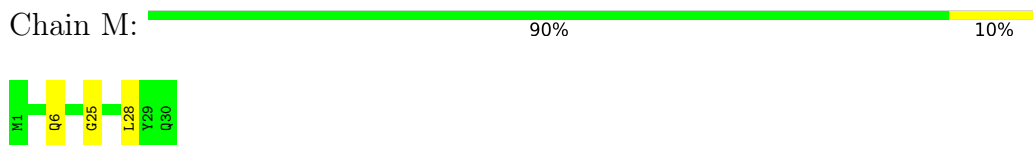
• Molecule 8: Photosystem I reaction center subunit IX



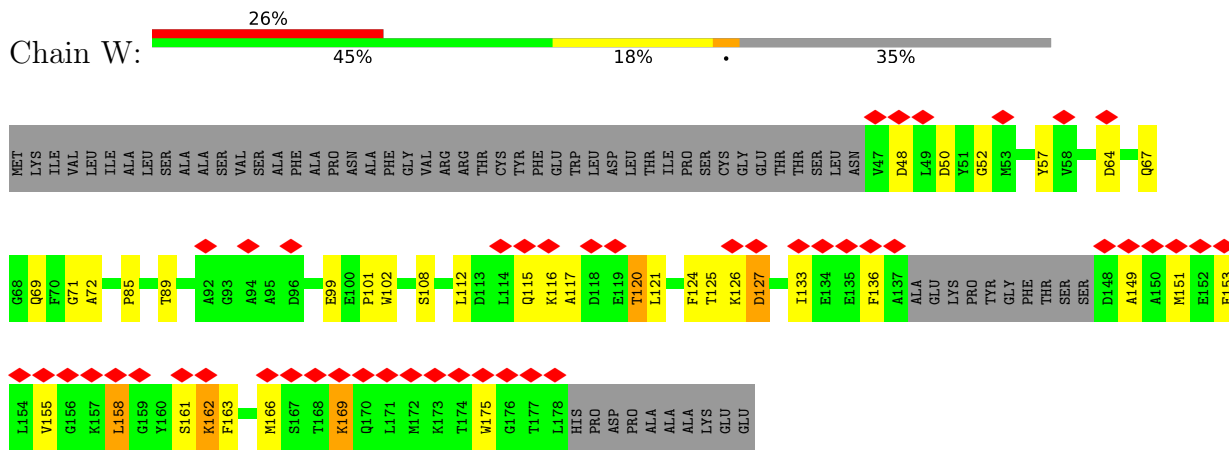
• Molecule 9: Photosystem I reaction center subunit XI



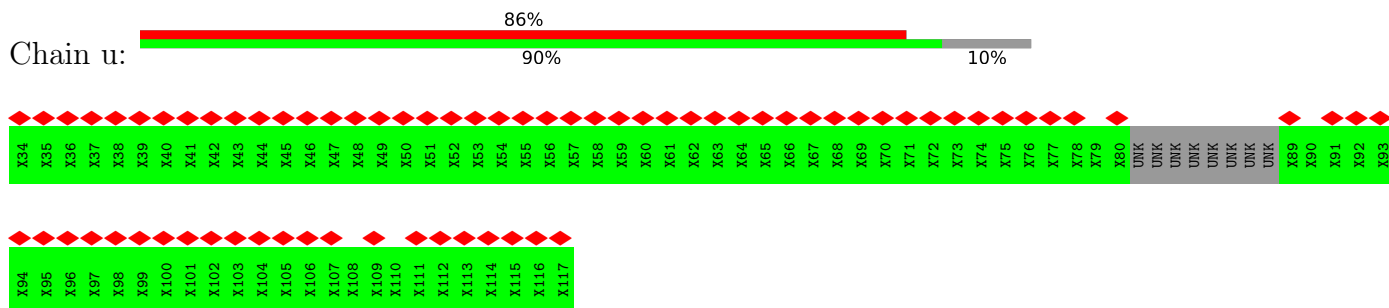
• Molecule 10: Photosystem I reaction center subunit XII



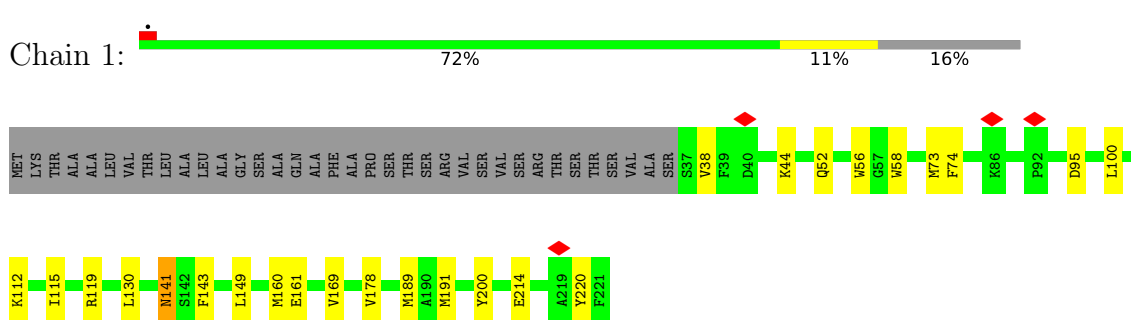
• Molecule 11: Photosystem I reaction center subunit Psa29



• Molecule 12: Unknown protein

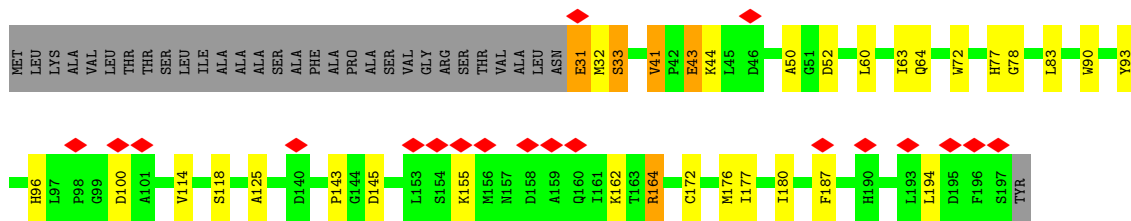


• Molecule 13: Fucoxanthin chlorophyll a/c-binding protein RedCAP

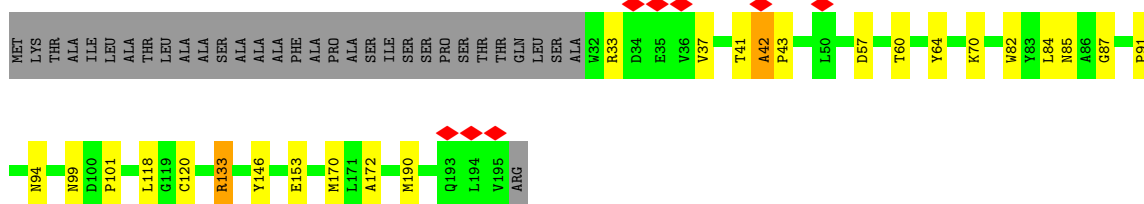


• Molecule 14: Fucoxanthin chl a/c light-harvesting protein

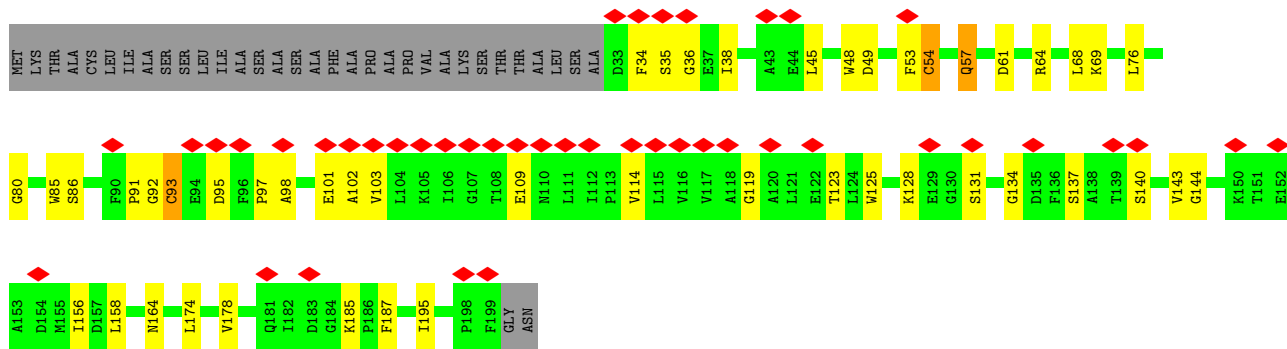




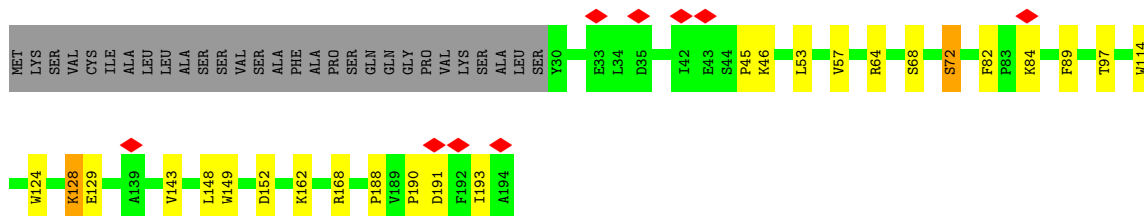
• Molecule 15: Pt17531-like protein



• Molecule 16: Fucoxanthin chl a/c light-harvesting protein, major type



• Molecule 17: Fucoxanthin chlorophyll a/c-binding protein Lhcq8



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	75667	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.097	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (\AA)	191.008, 191.008, 191.008	wwPDB
Map dimensions	254, 254, 254	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.752, 0.752, 0.752	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: DD6, BCR, LMG, A86, PQN, LHG, CL0, 5X6, LMT, CLA, DGD, SF4, KC1, UNL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/6056	0.49	0/8245
2	B	0.30	0/6045	0.49	0/8252
3	C	0.29	0/617	0.54	0/838
4	D	0.30	0/1077	0.56	0/1455
5	E	0.31	0/502	0.57	0/680
6	F	0.29	0/1282	0.50	0/1741
7	I	0.30	0/284	0.45	0/388
8	J	0.32	0/353	0.50	0/479
9	L	0.30	0/1134	0.51	0/1537
10	M	0.27	0/230	0.47	0/312
11	W	0.28	0/930	0.46	0/1255
13	1	0.28	0/1450	0.45	1/1974 (0.1%)
14	2	0.28	0/1321	0.47	0/1791
15	3	0.31	0/1306	0.50	0/1774
16	4	0.30	0/1326	0.48	0/1795
17	5	0.29	0/1324	0.47	0/1804
All	All	0.30	0/25237	0.49	1/34320 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
15	3	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	169	VAL	C-N-CA	-5.01	109.17	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	3	42	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5858	0	5684	89	0
2	B	5835	0	5649	76	0
3	C	607	0	586	7	0
4	D	1050	0	1039	18	0
5	E	494	0	488	4	0
6	F	1253	0	1252	21	0
7	I	276	0	287	6	0
8	J	342	0	340	8	0
9	L	1106	0	1128	17	0
10	M	228	0	249	3	0
11	W	912	0	863	24	0
12	u	380	0	81	0	0
13	1	1413	0	1365	14	0
14	2	1288	0	1253	25	0
15	3	1273	0	1231	20	0
16	4	1289	0	1235	37	0
17	5	1285	0	1239	17	0
18	A	65	0	72	5	0
19	1	476	0	483	34	0
19	2	542	0	503	38	0
19	3	407	0	400	31	0
19	4	585	0	517	35	0
19	5	541	0	498	24	0
19	A	2707	0	2766	164	0
19	B	2409	0	2542	136	0
19	F	100	0	82	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	J	45	0	33	3	0
19	L	170	0	164	12	0
19	u	100	0	80	0	0
20	A	33	0	46	2	0
20	B	33	0	46	2	0
21	A	8	0	0	0	0
21	C	16	0	0	0	0
22	1	80	0	112	7	0
22	A	200	0	280	11	0
22	B	200	0	280	18	0
22	F	80	0	112	7	0
22	I	80	0	112	10	0
22	J	40	0	56	3	0
22	L	80	0	112	5	0
22	M	40	0	56	4	0
23	1	41	0	52	6	0
23	3	34	0	38	2	0
23	4	49	0	73	6	0
23	A	96	0	141	10	0
23	B	35	0	40	1	0
23	M	41	0	55	3	0
24	1	35	0	43	4	0
24	2	35	0	43	1	0
24	3	35	0	46	1	0
24	A	35	0	45	0	0
25	1	38	0	0	1	0
25	2	86	0	0	0	0
25	3	124	0	0	0	0
25	4	21	0	0	0	0
25	5	111	0	0	0	0
25	A	230	0	0	0	0
25	B	73	0	0	0	0
25	F	38	0	0	0	0
25	J	39	0	0	0	0
25	L	72	0	0	0	0
25	M	28	0	0	0	0
26	B	66	0	96	9	0
27	J	42	0	0	0	0
28	1	129	0	0	0	0
28	2	43	0	0	0	0
28	3	43	0	0	1	0
28	5	43	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	L	43	0	0	0	0
29	1	49	0	71	0	0
30	1	45	0	0	0	0
30	2	45	0	0	0	0
30	3	135	0	0	2	0
30	4	90	0	0	0	0
31	1	96	0	0	2	0
31	2	144	0	0	2	0
31	3	144	0	0	1	0
31	4	144	0	0	5	0
31	5	192	0	0	4	0
32	1	49	0	0	0	0
32	2	22	0	0	1	0
32	3	34	0	0	2	0
32	4	11	0	0	1	0
32	5	17	0	0	0	0
32	A	240	0	0	0	0
32	B	300	0	0	11	0
32	C	50	0	0	1	0
32	D	56	0	0	0	0
32	E	24	0	0	0	0
32	F	46	0	0	2	0
32	I	6	0	0	0	0
32	J	7	0	0	0	0
32	L	30	0	0	0	0
32	M	7	0	0	0	0
32	W	20	0	0	1	0
32	u	3	0	0	0	0
All	All	37637	0	34064	725	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 (725) 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)
4:D:42:GLU:H	4:D:72:GLN:HE22	1.17	0.93
19:2:206:CLA:HHC	19:2:206:CLA:HBB1	1.56	0.88
1:A:87:TRP:HA	19:A:808:CLA:HBB2	1.56	0.84
1:A:313:ARG:NH1	1:A:317:GLY:O	2.11	0.81
19:A:804:CLA:HHC	19:A:804:CLA:HBB1	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:206:CLA:HHC	19:L:206:CLA:HBB1	1.64	0.80
19:4:309:CLA:HHC	19:4:309:CLA:HBB1	1.64	0.79
19:B:845:CLA:HBB1	19:B:845:CLA:HHC	1.63	0.79
16:4:137:SER:HA	16:4:143:VAL:HG23	1.64	0.77
4:D:116:ARG:NH1	4:D:123:ASN:OD1	2.18	0.76
19:B:811:CLA:HAA2	14:2:63:ILE:HD13	1.68	0.75
19:J:103:CLA:HHC	19:J:103:CLA:HBB1	1.67	0.75
9:L:38:ARG:O	9:L:46:ARG:NH2	2.20	0.74
22:M:102:BCR:H372	23:1:318:LHG:H172	1.70	0.74
19:A:804:CLA:HMA2	19:A:804:CLA:H12	1.70	0.74
19:2:205:CLA:H151	19:2:215:CLA:HBB2	1.69	0.74
19:B:804:CLA:H2	23:M:103:LHG:H161	1.69	0.74
19:B:809:CLA:H111	26:B:847:DGD:HBV1	1.68	0.74
19:A:822:CLA:HMB2	19:A:826:CLA:HMA3	1.70	0.74
19:A:824:CLA:HHC	19:A:824:CLA:HBB1	1.68	0.73
19:A:823:CLA:HMB2	19:A:824:CLA:H52	1.71	0.73
1:A:598:TRP:CH2	19:A:802:CLA:HAB	2.25	0.72
16:4:68:LEU:HD23	16:4:134:GLY:HA3	1.71	0.70
13:1:130:LEU:HB2	19:1:306:CLA:HBB1	1.73	0.70
16:4:86:SER:HB2	19:4:311:CLA:HMB1	1.74	0.70
14:2:164:ARG:HH21	19:2:210:CLA:H43	1.55	0.70
16:4:143:VAL:HG12	19:4:313:CLA:C4B	2.22	0.69
1:A:363:LEU:HD11	19:A:820:CLA:H71	1.73	0.69
19:A:817:CLA:HHC	19:A:817:CLA:HBB1	1.73	0.69
2:B:398:ASP:OD1	32:B:901:HOH:O	2.11	0.69
19:A:843:CLA:HHC	19:A:843:CLA:HBB1	1.73	0.68
19:B:804:CLA:H11	10:M:25:GLY:HA3	1.75	0.68
19:B:837:CLA:H12	22:B:844:BCR:H353	1.76	0.68
19:A:835:CLA:H171	19:L:203:CLA:HMB2	1.75	0.68
1:A:239:LEU:HD22	19:A:817:CLA:HED3	1.75	0.68
11:W:116:LYS:O	11:W:120:THR:OG1	2.13	0.67
19:4:311:CLA:HHC	19:4:311:CLA:HBB1	1.77	0.67
16:4:128:LYS:HD2	16:4:131:SER:HB2	1.78	0.66
6:F:126:ARG:NH1	6:F:167:GLU:OE2	2.22	0.66
19:5:212:CLA:H52	19:5:214:CLA:HBA1	1.76	0.66
2:B:80:ASN:HD21	2:B:83:LYS:HE3	1.61	0.65
19:3:209:CLA:H43	23:3:215:LHG:H122	1.78	0.65
19:A:821:CLA:HHC	19:A:821:CLA:HBB1	1.78	0.65
2:B:490:GLN:NE2	32:B:914:HOH:O	2.29	0.65
16:4:125:TRP:NE1	31:4:316:A86:O1	2.31	0.64
19:A:880:CLA:HED3	6:F:142:GLU:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:116:ARG:NH2	4:D:139:SER:O	2.26	0.64
16:4:85:TRP:HA	16:4:98:ALA:HB1	1.80	0.64
14:2:33:SER:HA	14:2:41:VAL:HG13	1.80	0.63
15:3:172:ALA:HA	19:3:210:CLA:HBB1	1.80	0.63
22:I:102:BCR:H403	22:I:102:BCR:H23C	1.80	0.63
1:A:349:TRP:HB3	19:A:806:CLA:HAC1	1.81	0.63
14:2:77:HIS:CE1	19:2:209:CLA:HMD1	2.33	0.63
2:B:181:LEU:HD11	19:B:813:CLA:H12	1.80	0.63
6:F:167:GLU:HG3	6:F:172:ASP:HB2	1.81	0.63
19:A:838:CLA:HBB1	19:A:838:CLA:HMB1	1.81	0.63
19:B:830:CLA:H43	22:F:201:BCR:HC22	1.80	0.63
1:A:598:TRP:HH2	19:A:802:CLA:HAB	1.63	0.62
23:M:103:LHG:HC41	13:1:52:GLN:HE22	1.64	0.62
14:2:114:VAL:HG11	19:2:207:CLA:HAA1	1.80	0.62
2:B:26:ALA:HB2	26:B:847:DGD:HB32	1.81	0.62
19:B:811:CLA:HAB	19:2:206:CLA:H162	1.81	0.62
1:A:102:SER:OG	1:A:156:GLU:OE1	2.18	0.62
19:A:880:CLA:HHC	19:A:880:CLA:HBB1	1.80	0.62
19:B:819:CLA:HMB2	19:B:822:CLA:HMA3	1.81	0.62
16:4:178:VAL:HG21	19:4:308:CLA:HBC3	1.80	0.62
2:B:307:HIS:HA	19:B:838:CLA:HMD1	1.81	0.62
11:W:67:GLN:HG2	11:W:72:ALA:H	1.64	0.61
19:A:806:CLA:H72	22:A:849:BCR:H23C	1.81	0.61
14:2:187:PHE:O	32:2:301:HOH:O	2.16	0.61
15:3:41:THR:HG22	15:3:42:ALA:H	1.64	0.61
2:B:7:LYS:HB3	7:I:35:ILE:HD11	1.82	0.61
4:D:9:PHE:O	4:D:52[B]:ARG:NE	2.32	0.61
19:A:841:CLA:H172	6:F:125:GLY:HA2	1.83	0.61
1:A:385:ALA:HA	1:A:748:ALA:HB1	1.83	0.61
19:A:878:CLA:HBC2	2:B:584:ASN:HB2	1.82	0.61
9:L:126:VAL:HG11	24:1:323:LMT:H12	1.83	0.61
3:C:2:SER:N	3:C:71:ALA:O	2.34	0.61
14:2:78:GLY:HA3	14:2:172:CYS:HB3	1.83	0.61
1:A:506:THR:HG23	19:A:836:CLA:HED3	1.84	0.60
2:B:241:HIS:O	2:B:263[B]:GLN:NE2	2.34	0.60
17:5:45:PRO:HD2	19:5:216:CLA:HMA3	1.83	0.60
19:4:301:CLA:O1A	32:4:401:HOH:O	2.16	0.60
19:A:815:CLA:HBA2	19:A:817:CLA:HMB3	1.83	0.60
9:L:36:ALA:HB2	19:L:203:CLA:HMD1	1.84	0.60
19:1:309:CLA:HHC	19:1:309:CLA:HBB1	1.84	0.60
14:2:125:ALA:HB1	19:2:207:CLA:H191	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:821:CLA:HBA2	22:B:852:BCR:H17C	1.83	0.60
19:B:829:CLA:HBB1	22:F:201:BCR:H323	1.84	0.59
6:F:185:ARG:O	32:F:301:HOH:O	2.17	0.59
2:B:108:ASN:OD1	32:B:902:HOH:O	2.17	0.59
19:1:303:CLA:HBA2	22:1:314:BCR:H362	1.84	0.59
1:A:424:ASN:HD22	1:A:432:ARG:HH12	1.49	0.59
19:A:878:CLA:H193	22:J:104:BCR:H362	1.85	0.59
2:B:224:PHE:HZ	22:B:840:BCR:H343	1.66	0.59
4:D:40:ILE:HG12	4:D:50:ILE:HG12	1.84	0.58
17:5:168:ARG:NH1	31:5:220:A86:O2	2.33	0.58
19:B:833:CLA:HMB1	19:B:833:CLA:HBB1	1.85	0.58
19:1:306:CLA:HED3	19:1:307:CLA:HBC2	1.86	0.58
19:2:205:CLA:H43	19:2:206:CLA:HBA1	1.85	0.58
11:W:112:LEU:HD11	11:W:117:ALA:HB2	1.86	0.58
19:B:805:CLA:HMB1	19:B:805:CLA:HBB1	1.84	0.58
11:W:121:LEU:O	11:W:125:THR:OG1	2.20	0.58
15:3:91:PRO:HD2	19:3:204:CLA:HMD1	1.84	0.58
23:A:853:LHG:H332	23:A:853:LHG:H161	1.86	0.57
11:W:158:LEU:HD12	11:W:162:LYS:HB2	1.86	0.57
19:A:843:CLA:H122	22:I:102:BCR:H19C	1.85	0.57
1:A:119:TRP:CD2	19:A:810:CLA:HED3	2.39	0.57
6:F:57:GLU:HG2	6:F:60:SER:HB3	1.85	0.57
19:B:811:CLA:H42	19:2:206:CLA:H51	1.87	0.57
16:4:195:ILE:HG22	19:4:312:CLA:HMB3	1.87	0.57
19:5:212:CLA:CGA	19:5:212:CLA:H3A	2.34	0.57
19:B:813:CLA:H141	19:B:818:CLA:HAB	1.85	0.57
19:A:832:CLA:HBA2	23:A:853:LHG:HC81	1.85	0.57
22:A:847:BCR:HC8	22:A:848:BCR:H383	1.86	0.57
2:B:48:ALA:HB3	10:M:28:LEU:HD21	1.87	0.57
19:A:834:CLA:H142	22:B:844:BCR:H15C	1.87	0.56
13:1:73:MET:HE3	19:1:307:CLA:HMC3	1.87	0.56
19:1:303:CLA:HMB1	19:1:303:CLA:HBB1	1.85	0.56
16:4:164:ASN:ND2	19:4:306:CLA:O1D	2.29	0.56
19:4:301:CLA:H193	23:4:317:LHG:H192	1.87	0.56
19:A:844:CLA:HBB1	19:A:844:CLA:HMB1	1.87	0.56
22:F:201:BCR:C10	19:F:203:CLA:HBB1	2.35	0.56
19:1:308:CLA:HHC	19:1:308:CLA:HBB1	1.88	0.56
16:4:57:GLN:NE2	16:4:61:ASP:OD2	2.36	0.56
19:4:303:CLA:HBD	19:4:303:CLA:HBA1	1.86	0.56
19:5:211:CLA:HHC	19:5:211:CLA:HBB1	1.87	0.56
19:A:834:CLA:HBB1	19:L:204:CLA:HBB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:843:CLA:H41	19:B:836:CLA:H43	1.88	0.56
19:A:820:CLA:H203	19:A:828:CLA:H3A	1.87	0.56
19:A:802:CLA:H122	22:B:844:BCR:H12C	1.88	0.56
23:A:853:LHG:H342	23:A:853:LHG:H191	1.88	0.56
2:B:299[B]:ASN:ND2	32:B:924:HOH:O	2.39	0.56
2:B:173:ARG:HB2	19:B:813:CLA:HBC2	1.87	0.56
1:A:501:ASN:HB2	19:A:837:CLA:HED2	1.87	0.56
13:1:200:TYR:HB2	19:1:310:CLA:H93	1.87	0.56
16:4:38:ILE:HD11	16:4:156:ILE:HG23	1.88	0.56
1:A:30:ALA:HB1	8:J:6:LYS:HD3	1.88	0.55
19:A:806:CLA:H51	19:A:814:CLA:H12	1.88	0.55
19:A:825:CLA:H52	22:A:851:BCR:H363	1.89	0.55
19:A:839:CLA:HBB1	19:A:839:CLA:HMB1	1.88	0.55
16:4:53:PHE:CD2	19:4:301:CLA:H2	2.42	0.55
19:4:309:CLA:HBB1	19:4:309:CLA:CHC	2.34	0.55
16:4:38:ILE:O	16:4:64:ARG:NH2	2.39	0.55
5:E:4:ARG:NH1	5:E:25:ALA:O	2.40	0.55
19:A:829:CLA:H18	19:A:878:CLA:H191	1.86	0.55
19:B:810:CLA:HMD3	22:I:101:BCR:H403	1.89	0.55
19:B:816:CLA:CHD	19:B:817:CLA:HBB2	2.36	0.55
11:W:127:ASP:OD1	11:W:127:ASP:N	2.39	0.55
1:A:589:TRP:CD1	19:A:831:CLA:HMD1	2.41	0.55
19:A:803:CLA:CGA	19:A:803:CLA:H3A	2.37	0.54
19:A:836:CLA:H2	22:A:851:BCR:H392	1.89	0.54
1:A:370:HIS:ND1	19:A:819:CLA:OBD	2.38	0.54
11:W:69:GLN:NE2	32:W:202:HOH:O	2.36	0.54
19:2:213:CLA:HHC	19:2:213:CLA:HBB1	1.89	0.54
9:L:103:GLN:OE1	9:L:114:LYS:NZ	2.41	0.54
19:3:206:CLA:H43	23:4:317:LHG:H132	1.89	0.54
4:D:85:ARG:HB2	4:D:95:LEU:HD11	1.88	0.54
19:1:310:CLA:HAB	22:1:311:BCR:H363	1.88	0.54
1:A:297:HIS:HB2	19:A:819:CLA:C1B	2.37	0.54
2:B:340:LEU:HD12	19:B:805:CLA:HED3	1.90	0.54
15:3:57:ASP:OD1	15:3:60:THR:OG1	2.22	0.54
19:A:808:CLA:H172	8:J:13:VAL:HG13	1.90	0.54
19:1:309:CLA:H152	23:1:318:LHG:H312	1.89	0.54
14:2:60:LEU:HD12	19:2:205:CLA:H12	1.89	0.54
19:1:310:CLA:H62	22:1:311:BCR:H371	1.89	0.54
19:A:813:CLA:HBB2	19:A:821:CLA:H52	1.90	0.54
14:2:145:ASP:HB2	19:2:210:CLA:HED2	1.90	0.54
2:B:166:TRP:CZ2	19:B:811:CLA:HMA1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:ILE:HG21	19:A:829:CLA:HMC2	1.90	0.53
18:A:801:CL0:CGD	18:A:801:CL0:H8	2.38	0.53
19:A:834:CLA:H91	19:B:803:CLA:H203	1.90	0.53
19:B:830:CLA:H122	6:F:117:ILE:HD11	1.89	0.53
4:D:11:THR:HB	4:D:50:ILE:HB	1.91	0.53
17:5:149:TRP:CE3	19:5:212:CLA:HAA2	2.43	0.53
13:1:189:MET:HG3	22:1:311:BCR:H15C	1.91	0.53
2:B:170:ASN:ND2	32:B:934:HOH:O	2.42	0.53
19:B:804:CLA:O1D	32:B:903:HOH:O	2.18	0.53
19:B:837:CLA:HBB1	19:B:837:CLA:HHC	1.90	0.53
19:2:208:CLA:HBC3	19:2:208:CLA:HHD	1.91	0.53
19:A:829:CLA:HBB1	19:A:829:CLA:HMB1	1.90	0.53
19:A:840:CLA:C3C	23:A:853:LHG:H331	2.39	0.53
19:A:820:CLA:HAB	19:A:820:CLA:H8	1.90	0.53
11:W:153:GLU:OE1	11:W:175:TRP:NE1	2.40	0.53
19:A:834:CLA:HMD3	19:A:839:CLA:H13	1.90	0.52
11:W:133:ILE:HG21	11:W:151:MET:HB2	1.89	0.52
14:2:90:TRP:CD1	19:2:207:CLA:HMD3	2.44	0.52
13:1:74:PHE:CD1	19:1:306:CLA:HMA1	2.44	0.52
16:4:174:LEU:HG	19:4:308:CLA:HBC2	1.91	0.52
19:5:209:CLA:HMB3	28:5:218:DD6:O1	2.10	0.52
19:A:803:CLA:H92	2:B:433:LEU:HD23	1.92	0.52
1:A:734:LEU:HD22	19:A:842:CLA:HMA1	1.92	0.52
19:A:807:CLA:H151	19:A:830:CLA:HBB2	1.91	0.52
15:3:91:PRO:O	32:3:301:HOH:O	2.19	0.52
19:B:807:CLA:H42	7:I:10:LEU:HD13	1.92	0.52
22:I:102:BCR:H281	19:L:203:CLA:CHD	2.40	0.52
2:B:261:HIS:HD1	2:B:263[A]:GLN:H	1.58	0.52
7:I:10:LEU:HD21	23:1:318:LHG:H151	1.92	0.52
2:B:342:VAL:HG21	19:B:824:CLA:H51	1.92	0.51
19:A:803:CLA:H91	19:A:804:CLA:H201	1.91	0.51
19:2:205:CLA:C15	19:2:215:CLA:HBB2	2.37	0.51
8:J:22:THR:HA	8:J:25:PHE:CE2	2.45	0.51
19:2:205:CLA:CGA	19:2:205:CLA:H3A	2.39	0.51
19:3:206:CLA:HMC2	23:4:317:LHG:H322	1.92	0.51
17:5:82:PHE:CD1	19:5:209:CLA:HHD	2.46	0.51
19:A:833:CLA:H171	22:L:205:BCR:H333	1.92	0.51
19:2:214:CLA:ND	24:2:220:LMT:H71	2.25	0.51
8:J:21:PHE:HA	19:J:103:CLA:HBB2	1.93	0.51
15:3:118:LEU:HD21	24:3:216:LMT:H111	1.93	0.51
19:3:206:CLA:HMB1	19:3:206:CLA:HBB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:592:TYR:CZ	19:B:833:CLA:HBC2	2.46	0.51
4:D:42:GLU:H	4:D:72:GLN:NE2	1.99	0.51
19:A:843:CLA:HMC2	19:B:836:CLA:H11	1.93	0.51
19:A:821:CLA:H51	19:A:821:CLA:C4B	2.40	0.50
15:3:170:MET:SD	19:3:202:CLA:HBB1	2.51	0.50
19:A:807:CLA:HBA2	19:A:807:CLA:HBD	1.93	0.50
6:F:120:TRP:CD1	6:F:157:GLY:HA3	2.46	0.50
19:A:841:CLA:HBB1	19:A:880:CLA:HMD1	1.94	0.50
19:3:206:CLA:H202	19:3:206:CLA:H71	1.93	0.50
1:A:674:LEU:HD11	2:B:616:MET:HB2	1.94	0.50
19:A:841:CLA:H102	19:B:829:CLA:H43	1.94	0.50
2:B:88:ALA:HB2	2:B:115:THR:HB	1.93	0.50
19:L:206:CLA:H2	19:L:206:CLA:H142	1.93	0.50
1:A:105:LEU:HD11	1:A:154:THR:HA	1.93	0.50
1:A:178:TRP:HB2	19:A:812:CLA:HMC3	1.94	0.50
19:A:821:CLA:HBB1	22:A:847:BCR:H14C	1.94	0.50
19:2:210:CLA:H71	31:2:216:A86:C26	2.42	0.50
19:A:804:CLA:H2	20:A:845:PQN:H222	1.93	0.50
19:A:823:CLA:HMB2	19:A:824:CLA:H12	1.94	0.50
19:A:833:CLA:H172	19:A:844:CLA:H193	1.92	0.50
19:A:809:CLA:HBA1	19:A:809:CLA:C4A	2.40	0.50
19:A:878:CLA:HBB1	19:A:878:CLA:HMB1	1.94	0.49
19:B:813:CLA:H42	22:B:841:BCR:H19C	1.94	0.49
19:B:819:CLA:H41	19:B:832:CLA:H171	1.93	0.49
16:4:91:PRO:HG2	19:4:310:CLA:C1D	2.41	0.49
19:A:814:CLA:HAA2	19:A:826:CLA:H52	1.94	0.49
4:D:28:LYS:HE2	4:D:59:TYR:HB3	1.95	0.49
22:I:102:BCR:HC32	23:M:103:LHG:H152	1.94	0.49
1:A:93[B]:PHE:CD2	1:A:163:ALA:HB1	2.47	0.49
14:2:180:ILE:HG22	19:2:213:CLA:HBC2	1.94	0.49
11:W:158:LEU:HD13	11:W:166:MET:SD	2.52	0.49
2:B:661:MET:HB2	19:B:803:CLA:C1C	2.42	0.49
5:E:9:ARG:NH2	6:F:179:GLU:HG3	2.26	0.49
1:A:161:TRP:CD1	19:A:817:CLA:HAA2	2.48	0.49
1:A:396:TRP:CD1	19:A:829:CLA:HAB	2.48	0.49
1:A:748:ALA:HA	1:A:751:ILE:HG12	1.95	0.49
19:B:812:CLA:H92	19:B:845:CLA:H72	1.93	0.49
19:B:823:CLA:HMA1	22:B:843:BCR:H14C	1.95	0.49
13:1:115:ILE:HD11	13:1:119:ARG:HG2	1.95	0.49
15:3:87:GLY:HA3	30:3:211:KC1:O1A	2.12	0.49
16:4:95:ASP:N	16:4:95:ASP:OD1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:880:CLA:HMC2	22:F:201:BCR:H381	1.95	0.49
2:B:261:HIS:HD1	2:B:263[B]:GLN:H	1.58	0.49
6:F:52:ARG:NH1	32:F:305:HOH:O	2.41	0.49
9:L:104:GLU:H	9:L:104:GLU:CD	2.15	0.48
19:A:806:CLA:HMB3	19:A:807:CLA:HAA2	1.95	0.48
19:A:834:CLA:H151	20:B:839:PQN:H202	1.94	0.48
16:4:114:VAL:HG11	19:4:303:CLA:HMB2	1.96	0.48
2:B:710:VAL:HG22	26:B:847:DGD:HAT2	1.95	0.48
20:B:839:PQN:H141	20:B:839:PQN:H161	1.57	0.48
15:3:84:LEU:HD12	19:3:204:CLA:HHD	1.94	0.48
19:5:213:CLA:HHC	19:5:216:CLA:HMD3	1.95	0.48
1:A:361:GLY:HA2	1:A:398:GLY:HA2	1.95	0.48
19:4:303:CLA:HAB	31:4:316:A86:C12	2.43	0.48
1:A:625:ASP:OD1	1:A:625:ASP:N	2.44	0.48
17:5:148:LEU:HD13	19:5:212:CLA:H42	1.96	0.48
19:A:822:CLA:CMB	19:A:826:CLA:HMA3	2.42	0.48
19:A:841:CLA:H41	22:F:201:BCR:H19C	1.95	0.48
19:B:810:CLA:H92	19:1:301:CLA:H8	1.96	0.48
19:4:301:CLA:H42	19:4:301:CLA:C2B	2.44	0.48
19:4:304:CLA:H3A	19:4:304:CLA:HBA2	1.63	0.48
17:5:114:TRP:HE1	31:5:219:A86:C9	2.27	0.48
19:5:213:CLA:C1D	19:5:214:CLA:HMD2	2.44	0.48
1:A:190:TRP:CZ2	19:A:811:CLA:HMA1	2.48	0.48
1:A:246:ASN:HD21	1:A:248:ASP:HB3	1.79	0.48
19:B:829:CLA:HBD	19:B:829:CLA:HAA1	1.96	0.48
1:A:34:HIS:NE2	19:A:812:CLA:O1A	2.47	0.48
1:A:574:PRO:HB3	1:A:721:ILE:HB	1.95	0.48
19:B:819:CLA:CMB	19:B:822:CLA:HMA3	2.42	0.48
4:D:83:ILE:HB	4:D:96:HIS:HB3	1.96	0.48
6:F:165:TRP:O	6:F:169:ILE:HG12	2.14	0.48
14:2:125:ALA:HB3	19:2:208:CLA:HBC2	1.94	0.48
19:2:206:CLA:HBB1	19:2:206:CLA:CHC	2.38	0.48
16:4:119:GLY:O	16:4:123:THR:HG23	2.13	0.48
1:A:200:HIS:CG	19:A:814:CLA:HMC2	2.48	0.47
22:A:851:BCR:H23C	22:A:851:BCR:H403	1.97	0.47
19:B:837:CLA:H112	19:B:837:CLA:H152	1.62	0.47
3:C:45:VAL:HG11	32:C:215:HOH:O	2.13	0.47
14:2:72:TRP:CE2	14:2:143:PRO:HA	2.49	0.47
1:A:424:ASN:ND2	1:A:432:ARG:HH12	2.10	0.47
19:A:827:CLA:HMA1	22:A:851:BCR:H15C	1.96	0.47
2:B:179:SER:HB3	2:B:287:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:703:GLN:HG3	26:B:847:DGD:HB22	1.95	0.47
1:A:359:MET:HG3	19:A:826:CLA:HBB	1.96	0.47
1:A:605:VAL:HG21	18:A:801:CL0:H69	1.96	0.47
19:A:818:CLA:CHD	19:A:819:CLA:HBB2	2.44	0.47
19:A:826:CLA:H142	19:A:826:CLA:H8	1.96	0.47
19:L:203:CLA:HMB3	19:L:204:CLA:HBC2	1.96	0.47
24:1:323:LMT:H72	19:5:208:CLA:HMD3	1.95	0.47
1:A:59:PHE:CD2	19:A:806:CLA:HMC2	2.49	0.47
1:A:210:CYS:HB3	1:A:302:SER:HB3	1.96	0.47
19:A:810:CLA:H112	19:A:810:CLA:H142	1.74	0.47
19:B:821:CLA:H71	19:B:821:CLA:H143	1.96	0.47
19:B:837:CLA:HAC2	22:B:844:BCR:H21C	1.96	0.47
11:W:169:LYS:H	11:W:169:LYS:HD2	1.79	0.47
19:1:310:CLA:HBB1	31:1:317:A86:C4	2.44	0.47
1:A:15:VAL:HG11	19:A:811:CLA:HAA2	1.95	0.47
19:A:878:CLA:HAA2	19:A:878:CLA:HBD	1.97	0.47
19:B:815:CLA:OBD	32:B:904:HOH:O	2.20	0.47
19:B:833:CLA:HMB2	19:B:835:CLA:HED1	1.95	0.47
19:1:306:CLA:HBA1	19:1:306:CLA:H3A	1.62	0.47
30:3:208:KC1:O1A	19:3:209:CLA:HMD1	2.14	0.47
1:A:396:TRP:HB3	19:A:829:CLA:HMC3	1.96	0.47
19:B:829:CLA:HBB1	19:B:829:CLA:HHC	1.96	0.47
3:C:46:GLU:HB2	11:W:72:ALA:HA	1.97	0.47
9:L:42:THR:O	9:L:46:ARG:HG3	2.15	0.47
11:W:99:GLU:OE2	15:3:133:ARG:NH2	2.40	0.47
15:3:64:TYR:OH	32:3:302:HOH:O	2.20	0.47
19:A:840:CLA:HHC	19:A:840:CLA:HBB1	1.96	0.47
2:B:550:LYS:O	32:B:905:HOH:O	2.21	0.47
2:B:657:ALA:O	2:B:660:PHE:HB2	2.15	0.47
6:F:25:GLU:N	6:F:29:LEU:O	2.48	0.47
19:A:827:CLA:H193	19:A:827:CLA:H161	1.75	0.47
19:A:844:CLA:H111	19:A:844:CLA:H72	1.78	0.47
1:A:349:TRP:CD1	19:A:826:CLA:H202	2.50	0.47
19:A:802:CLA:OBD	19:B:802:CLA:HMB3	2.15	0.47
19:A:816:CLA:CBB	22:A:847:BCR:H333	2.44	0.47
14:2:50:ALA:HA	14:2:162:LYS:HE3	1.96	0.47
14:2:96:HIS:HA	19:2:207:CLA:HMD1	1.97	0.47
17:5:68:SER:O	17:5:72:SER:OG	2.33	0.47
19:B:803:CLA:H13	22:I:101:BCR:H281	1.97	0.46
14:2:52:ASP:HB2	19:2:205:CLA:HED2	1.96	0.46
19:2:210:CLA:HBA2	19:2:210:CLA:H3A	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:TRP:CD2	19:A:817:CLA:HBA1	2.50	0.46
1:A:547:VAL:HG11	19:A:840:CLA:HMB3	1.96	0.46
1:A:667:SER:HB2	2:B:444:ALA:HB1	1.98	0.46
2:B:2:ALA:HA	2:B:7:LYS:HA	1.96	0.46
2:B:80:ASN:HD21	2:B:83:LYS:HB2	1.80	0.46
16:4:97:PRO:HB2	16:4:101:GLU:HB3	1.97	0.46
2:B:62:SER:HB2	2:B:141:LEU:HB2	1.97	0.46
19:B:811:CLA:H141	19:B:811:CLA:H162	1.82	0.46
19:B:811:CLA:H61	19:2:206:CLA:H93	1.97	0.46
19:B:808:CLA:H141	19:B:808:CLA:HBA2	1.98	0.46
19:B:810:CLA:HHC	19:B:810:CLA:HBB1	1.97	0.46
22:B:843:BCR:H15C	22:B:843:BCR:H351	1.80	0.46
19:B:845:CLA:HBB1	19:B:845:CLA:CHC	2.40	0.46
6:F:57:GLU:HG3	6:F:59:ASP:OD1	2.16	0.46
9:L:145:PHE:HA	19:5:210:CLA:H12	1.98	0.46
1:A:514:VAL:HG21	1:A:628:ILE:HD11	1.97	0.46
19:B:821:CLA:HMB2	22:B:852:BCR:H362	1.98	0.46
19:B:836:CLA:H41	19:B:836:CLA:H62	1.75	0.46
19:A:833:CLA:H41	19:A:833:CLA:H61	1.57	0.46
13:1:191:MET:HB3	19:1:303:CLA:HMC3	1.98	0.46
19:1:301:CLA:HMD2	19:1:309:CLA:HAC1	1.96	0.46
22:1:314:BCR:H15C	22:1:314:BCR:H351	1.82	0.46
19:A:804:CLA:O1A	23:A:852:LHG:H172	2.16	0.46
19:A:809:CLA:HMC3	19:A:810:CLA:HMD2	1.98	0.46
15:3:120:CYS:HB2	19:3:206:CLA:HMC3	1.97	0.46
2:B:340:LEU:HD11	19:B:805:CLA:H51	1.98	0.46
2:B:630:LEU:HD22	2:B:723:PHE:HA	1.96	0.46
19:B:837:CLA:H18	7:I:20:ALA:HB2	1.97	0.46
19:1:310:CLA:H41	19:1:310:CLA:H61	1.59	0.46
1:A:422:ASN:O	1:A:428:ASP:HB2	2.16	0.46
22:A:850:BCR:H20C	22:A:850:BCR:H361	1.77	0.46
9:L:126:VAL:HG11	24:1:323:LMT:C1	2.46	0.46
11:W:161:SER:HB2	11:W:162:LYS:HE3	1.97	0.46
19:5:212:CLA:HMC2	31:5:217:A86:C8	2.45	0.46
2:B:656:TRP:CE3	19:B:802:CLA:HMA1	2.51	0.45
19:B:832:CLA:HBA2	19:B:832:CLA:H3A	1.28	0.45
19:B:832:CLA:HMB1	22:B:843:BCR:HC32	1.97	0.45
4:D:32:THR:O	4:D:81:TYR:HA	2.16	0.45
19:2:206:CLA:H2	19:2:206:CLA:H61	1.68	0.45
19:3:204:CLA:HBA1	19:3:204:CLA:HBD	1.98	0.45
19:4:301:CLA:H43	31:4:315:A86:C29	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLY:O	1:A:208:LEU:HB2	2.16	0.45
19:A:841:CLA:HBB1	19:A:880:CLA:CMD	2.46	0.45
9:L:52:LEU:HA	9:L:131:SER:HB2	1.98	0.45
1:A:320:HIS:HB3	1:A:325:ILE:HD11	1.98	0.45
1:A:576:ASP:OD2	1:A:580:ARG:NH2	2.48	0.45
19:A:833:CLA:H2	19:L:203:CLA:H43	1.99	0.45
19:A:878:CLA:H13	19:A:878:CLA:H172	1.72	0.45
19:B:812:CLA:H121	19:B:812:CLA:H162	1.68	0.45
19:L:206:CLA:H142	19:L:206:CLA:H112	1.81	0.45
11:W:149:ALA:O	11:W:153:GLU:HG3	2.17	0.45
17:5:162:LYS:HD3	19:5:214:CLA:HAA2	1.98	0.45
1:A:457:ILE:HG22	19:A:835:CLA:HBC2	1.99	0.45
2:B:147:VAL:HG11	19:B:811:CLA:H193	1.99	0.45
2:B:286:ALA:HB2	19:B:819:CLA:HBC2	1.97	0.45
17:5:84:LYS:HG3	17:5:97:THR:HB	1.98	0.45
17:5:124:TRP:CE2	17:5:128:LYS:HD3	2.52	0.45
17:5:143:VAL:HG11	19:5:209:CLA:H172	1.99	0.45
17:5:190:PRO:HD2	17:5:193:ILE:HD11	1.98	0.45
2:B:182:LEU:HD21	19:B:813:CLA:H61	1.98	0.45
19:4:305:CLA:H91	19:4:305:CLA:H112	1.74	0.45
1:A:413:MET:HE1	1:A:431:LEU:HD11	1.99	0.45
1:A:536:HIS:CG	19:A:839:CLA:HED3	2.52	0.45
19:A:804:CLA:H8	19:A:804:CLA:H52	1.62	0.45
19:A:807:CLA:HBB	19:A:831:CLA:HAB	1.98	0.45
19:A:821:CLA:H41	19:A:821:CLA:H61	1.57	0.45
19:A:834:CLA:H162	19:A:834:CLA:H202	1.72	0.45
19:B:814:CLA:H152	19:B:814:CLA:H111	1.74	0.45
19:B:831:CLA:HBA2	19:B:832:CLA:HMB3	1.98	0.45
19:B:836:CLA:H151	9:L:85:LEU:HD11	1.98	0.45
19:1:308:CLA:HBC2	22:1:311:BCR:H342	1.98	0.45
19:3:203:CLA:HMD2	19:3:206:CLA:C4D	2.46	0.45
19:3:209:CLA:H11	23:3:215:LHG:H122	1.97	0.45
19:5:209:CLA:H18	19:5:212:CLA:HMD2	1.98	0.45
2:B:224:PHE:CZ	22:B:840:BCR:H343	2.49	0.45
19:B:807:CLA:H203	19:B:807:CLA:H162	1.70	0.45
19:2:210:CLA:H61	19:2:210:CLA:H41	1.63	0.45
1:A:13:VAL:HG21	1:A:314:THR:HB	1.99	0.45
23:A:853:LHG:H261	23:A:853:LHG:H131	1.98	0.45
19:1:303:CLA:HBC2	22:1:314:BCR:H21C	1.99	0.45
14:2:177:ILE:HD11	19:2:205:CLA:HAC1	1.98	0.45
19:3:206:CLA:C1C	23:4:317:LHG:H311	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LEU:O	1:A:338:HIS:HB2	2.17	0.45
19:A:813:CLA:H62	19:A:813:CLA:H41	1.74	0.45
19:5:208:CLA:HMD2	19:5:211:CLA:C1D	2.48	0.45
19:B:821:CLA:HBA2	19:B:821:CLA:H3A	1.82	0.44
13:1:149:LEU:HD13	13:1:160:MET:SD	2.57	0.44
19:1:310:CLA:H121	19:2:208:CLA:HMB3	1.99	0.44
14:2:176:MET:SD	19:2:205:CLA:HAB	2.57	0.44
19:4:306:CLA:H41	19:4:306:CLA:H61	1.70	0.44
1:A:580:ARG:HG3	3:C:49:VAL:HB	2.00	0.44
19:A:819:CLA:H93	19:A:837:CLA:HBA1	2.00	0.44
14:2:43:GLU:H	14:2:43:GLU:HG3	1.51	0.44
19:A:802:CLA:HAA2	19:A:802:CLA:HBD	1.98	0.44
19:A:839:CLA:H91	19:A:839:CLA:H112	1.75	0.44
2:B:406:VAL:O	2:B:410:MET:HG2	2.17	0.44
22:M:102:BCR:H20C	22:M:102:BCR:H361	1.80	0.44
13:1:56:TRP:HB2	13:1:58:TRP:CD1	2.52	0.44
19:B:835:CLA:HHC	19:B:835:CLA:HBB1	1.99	0.44
6:F:120:TRP:NE1	6:F:157:GLY:HA3	2.32	0.44
22:L:202:BCR:H20C	22:L:202:BCR:H361	1.88	0.44
2:B:176:HIS:CG	19:B:813:CLA:HMC2	2.52	0.44
19:B:816:CLA:HBA2	19:B:816:CLA:H3A	1.36	0.44
19:1:309:CLA:H92	19:1:309:CLA:H61	1.74	0.44
14:2:93:TYR:CZ	14:2:194:LEU:HB2	2.53	0.44
16:4:80:GLY:HA3	19:4:303:CLA:C1C	2.48	0.44
2:B:148:LEU:HD21	19:2:206:CLA:H201	2.00	0.44
1:A:67:GLU:HB2	1:A:188:LEU:HB2	2.00	0.44
19:B:804:CLA:HHC	19:B:806:CLA:OBD	2.18	0.44
19:B:808:CLA:O1A	19:B:825:CLA:HBD	2.18	0.44
15:3:99:ASN:N	15:3:99:ASN:HD22	2.15	0.44
16:4:93:CYS:HB3	19:4:310:CLA:HBB1	1.99	0.44
19:A:818:CLA:H3A	19:A:818:CLA:HBA2	1.64	0.44
19:B:812:CLA:HBA2	19:B:812:CLA:H3A	1.80	0.44
19:B:819:CLA:H112	19:B:819:CLA:H152	1.83	0.44
16:4:92:GLY:HA2	19:4:310:CLA:HMA3	1.99	0.44
1:A:36:SER:HB3	1:A:39:LEU:HB2	2.00	0.44
2:B:593:TRP:O	2:B:597:HIS:HD2	2.00	0.44
2:B:630:LEU:HD21	2:B:649:PHE:CD1	2.53	0.44
2:B:657:ALA:C	19:B:803:CLA:HAB	2.39	0.44
19:B:808:CLA:C1A	19:B:808:CLA:CGA	2.95	0.44
19:B:833:CLA:H2	19:B:833:CLA:H61	1.76	0.44
19:A:804:CLA:ND	8:J:12:PRO:HG3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:821:CLA:HMA1	19:B:838:CLA:CGD	2.48	0.43
26:B:847:DGD:HD2	32:B:1144:HOH:O	2.18	0.43
17:5:57:VAL:HG22	19:5:208:CLA:H11	2.00	0.43
1:A:487:ILE:HD13	19:A:836:CLA:HBB1	1.99	0.43
11:W:57:TYR:OH	11:W:64:ASP:OD1	2.35	0.43
23:1:318:LHG:H161	23:1:318:LHG:H131	1.84	0.43
1:A:129:ALA:N	1:A:137:GLY:O	2.49	0.43
1:A:683:SER:HB2	1:A:728:GLY:O	2.18	0.43
1:A:694:TRP:CZ2	20:A:845:PQN:H2M3	2.52	0.43
19:1:304:CLA:O1A	19:1:306:CLA:HAC1	2.19	0.43
19:1:310:CLA:HBA2	19:1:310:CLA:H12	1.83	0.43
19:5:210:CLA:H93	19:5:210:CLA:H112	1.80	0.43
19:A:880:CLA:H13	19:A:880:CLA:H172	1.85	0.43
23:B:842:LHG:H271	23:B:842:LHG:H302	1.47	0.43
26:B:847:DGD:HB91	26:B:847:DGD:HBW2	1.56	0.43
4:D:24:GLU:OE2	11:W:108:SER:HA	2.18	0.43
9:L:5:ILE:HG23	9:L:19:THR:HG22	2.00	0.43
23:4:317:LHG:H382	23:4:317:LHG:H301	2.01	0.43
16:4:178:VAL:HG21	19:4:308:CLA:CBC	2.46	0.43
1:A:450:CYS:SG	19:B:803:CLA:H12	2.58	0.43
19:A:834:CLA:C3B	19:A:835:CLA:HMB2	2.49	0.43
19:A:878:CLA:H152	19:A:878:CLA:H112	1.72	0.43
2:B:463:GLN:NE2	19:B:833:CLA:HMD1	2.34	0.43
2:B:699:LEU:HD22	2:B:703:GLN:NE2	2.34	0.43
19:B:804:CLA:HAA1	19:B:804:CLA:HBD	2.00	0.43
19:B:838:CLA:H91	19:B:838:CLA:H112	1.83	0.43
19:A:805:CLA:HBB1	19:A:806:CLA:CMB	2.48	0.43
19:A:834:CLA:HMA1	22:I:101:BCR:H282	2.01	0.43
19:B:838:CLA:HBA1	19:B:838:CLA:H3A	1.71	0.43
3:C:75:ARG:NH1	11:W:71:GLY:O	2.51	0.43
19:2:210:CLA:HMC2	31:2:216:A86:C25	2.49	0.43
1:A:75:SER:OG	1:A:181:TYR:HB2	2.18	0.43
1:A:680:TRP:CE3	18:A:801:CL0:H4	2.54	0.43
3:C:32:ASP:OD1	3:C:32:ASP:N	2.49	0.43
5:E:21:ILE:HD12	5:E:61:VAL:HG21	2.01	0.43
19:1:309:CLA:H192	19:1:309:CLA:H162	1.84	0.43
19:A:805:CLA:HMA2	19:A:812:CLA:HMD2	2.01	0.43
19:A:827:CLA:HBA2	19:A:827:CLA:H3A	1.78	0.43
19:A:841:CLA:H43	19:B:829:CLA:HAA2	2.00	0.43
8:J:24:GLY:HA3	19:J:103:CLA:CBB	2.48	0.43
9:L:32:LYS:NZ	15:3:133:ARG:HH21	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:303:CLA:H3A	19:1:303:CLA:HBA1	1.79	0.43
14:2:78:GLY:HA3	14:2:172:CYS:CB	2.48	0.43
19:2:205:CLA:H141	19:2:205:CLA:H161	1.76	0.43
19:2:207:CLA:H72	19:2:207:CLA:H111	1.83	0.43
16:4:69:LYS:HG3	31:4:316:A86:O2	2.19	0.43
17:5:64:ARG:NH2	17:5:129:GLU:OE1	2.44	0.43
17:5:188:PRO:O	31:5:217:A86:O3	2.37	0.43
19:A:844:CLA:H142	19:A:844:CLA:H112	1.86	0.43
19:B:814:CLA:H91	19:B:814:CLA:H112	1.64	0.43
19:3:206:CLA:H3A	19:3:206:CLA:HBA2	1.39	0.43
19:4:301:CLA:H3A	19:4:301:CLA:HBA2	1.63	0.43
19:A:814:CLA:H41	19:A:814:CLA:H61	1.79	0.42
19:B:807:CLA:H2	19:B:807:CLA:H62	1.81	0.42
19:B:808:CLA:HBD	19:B:808:CLA:HAA1	2.01	0.42
19:B:818:CLA:CGA	19:B:818:CLA:H3A	2.49	0.42
6:F:100:ARG:HG2	19:F:204:CLA:HMD2	2.01	0.42
19:1:306:CLA:HED2	19:1:307:CLA:HMD2	2.01	0.42
1:A:262:ALA:HB3	1:A:263:PRO:HD3	2.00	0.42
1:A:476:ALA:O	1:A:478:GLN:HG3	2.19	0.42
18:A:801:CL0:H72	18:A:801:CL0:H10	1.81	0.42
19:A:828:CLA:HED1	19:A:836:CLA:HAB	2.01	0.42
22:A:851:BCR:H20C	22:A:851:BCR:H361	1.84	0.42
2:B:114:ILE:O	19:B:808:CLA:HMD3	2.18	0.42
2:B:386:PHE:CE2	22:B:843:BCR:H373	2.53	0.42
19:B:820:CLA:C4C	22:B:840:BCR:H382	2.49	0.42
6:F:123:TRP:CH2	6:F:164:ALA:HA	2.54	0.42
19:F:204:CLA:HHC	19:F:204:CLA:HBB1	2.00	0.42
8:J:39:LEU:HD23	8:J:39:LEU:HA	1.88	0.42
9:L:56:TYR:HB2	9:L:131:SER:OG	2.20	0.42
19:1:304:CLA:HMC2	23:1:318:LHG:H311	2.01	0.42
1:A:122:VAL:HG21	19:A:810:CLA:HBB1	2.01	0.42
19:B:807:CLA:H12	7:I:14:VAL:HG21	2.01	0.42
19:B:812:CLA:H8	19:B:845:CLA:H52	2.01	0.42
19:3:206:CLA:H122	19:3:206:CLA:H161	1.74	0.42
19:4:306:CLA:H71	19:4:306:CLA:H111	1.80	0.42
1:A:76:ALA:HB1	19:A:806:CLA:HBB1	2.01	0.42
1:A:174:LEU:HD12	1:A:174:LEU:HA	1.87	0.42
2:B:373:HIS:HB2	19:B:825:CLA:C1B	2.49	0.42
19:B:806:CLA:H61	19:B:806:CLA:H41	1.59	0.42
14:2:44:LYS:NZ	14:2:64:GLN:O	2.45	0.42
19:A:842:CLA:H172	8:J:23:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:844:CLA:H61	19:3:207:CLA:C4D	2.50	0.42
2:B:304:LEU:HD11	19:B:822:CLA:HMC1	2.02	0.42
2:B:325:ILE:HD12	19:B:822:CLA:HMC2	2.02	0.42
2:B:703:GLN:HG3	26:B:847:DGD:HB41	2.01	0.42
6:F:127:LYS:HG2	6:F:153:ILE:HD13	2.01	0.42
13:1:141:ASN:HD22	13:1:143:PHE:H	1.68	0.42
13:1:220:TYR:OH	31:1:316:A86:O	2.29	0.42
19:1:307:CLA:HBB1	19:1:307:CLA:HMB1	2.00	0.42
19:3:206:CLA:H161	19:3:206:CLA:H203	1.80	0.42
2:B:579:MET:HG3	2:B:709:LEU:HD21	1.99	0.42
19:B:805:CLA:HBA1	19:B:805:CLA:H3A	1.61	0.42
19:B:831:CLA:HMD2	19:B:832:CLA:CHC	2.49	0.42
4:D:52[B]:ARG:CZ	4:D:52[B]:ARG:HB3	2.50	0.42
4:D:93:GLN:HA	11:W:124:PHE:CZ	2.54	0.42
5:E:32:ILE:HD11	5:E:35:PRO:HA	2.02	0.42
9:L:6:LYS:NZ	15:3:146:TYR:O	2.34	0.42
22:L:205:BCR:H11C	22:L:205:BCR:H341	1.90	0.42
19:3:204:CLA:C1A	19:3:204:CLA:CGA	2.97	0.42
1:A:14:GLN:HB2	1:A:16:PHE:CE2	2.55	0.42
19:A:818:CLA:C1D	19:A:818:CLA:H42	2.49	0.42
19:A:829:CLA:HBC3	23:A:852:LHG:H383	2.01	0.42
19:B:846:CLA:H42	22:F:205:BCR:H353	2.01	0.42
14:2:31:GLU:HB2	14:2:32:MET:H	1.62	0.42
19:2:207:CLA:HBA1	19:2:207:CLA:HBD	2.02	0.42
19:4:303:CLA:H41	19:4:303:CLA:H62	1.54	0.42
19:A:805:CLA:H92	19:A:805:CLA:H61	1.85	0.42
19:A:821:CLA:H3A	19:A:821:CLA:HBA2	1.32	0.42
19:B:808:CLA:HMB1	19:B:809:CLA:H42	2.01	0.42
19:B:822:CLA:HAA2	19:B:822:CLA:HBD	2.01	0.42
6:F:67:LYS:HE3	6:F:67:LYS:HB2	1.70	0.42
19:2:205:CLA:H41	19:2:205:CLA:H62	1.90	0.42
1:A:122:VAL:HB	19:B:830:CLA:HMD1	2.02	0.42
1:A:239:LEU:N	1:A:242:GLU:OE2	2.50	0.42
23:A:853:LHG:H252	23:A:853:LHG:H111	2.02	0.42
2:B:187:LEU:HG	19:B:815:CLA:CBB	2.50	0.42
2:B:255:THR:OG1	2:B:271:ASP:OD1	2.27	0.42
19:B:803:CLA:H121	19:B:803:CLA:H8	1.94	0.42
19:B:823:CLA:H52	19:B:823:CLA:H11	1.76	0.42
19:B:832:CLA:HHC	19:B:832:CLA:HBB1	2.02	0.42
6:F:42:LEU:HB2	6:F:77:PHE:CD1	2.55	0.42
19:A:820:CLA:H193	19:A:820:CLA:H161	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:834:CLA:HAA2	19:A:834:CLA:HBD	2.02	0.42
19:A:842:CLA:H91	19:A:842:CLA:H111	1.76	0.42
2:B:373:HIS:HE2	19:B:826:CLA:C1B	2.32	0.42
19:B:804:CLA:HMB2	22:M:102:BCR:H323	2.02	0.42
19:B:823:CLA:H3A	19:B:823:CLA:HBA2	1.65	0.42
22:L:205:BCR:H281	24:1:323:LMT:H62	2.01	0.42
19:L:206:CLA:H112	19:L:206:CLA:H72	1.86	0.42
19:3:202:CLA:HMC2	28:3:213:DD6:C25	2.50	0.42
19:3:206:CLA:CGA	23:4:317:LHG:H241	2.49	0.42
1:A:87:TRP:HA	19:A:808:CLA:CBB	2.40	0.41
1:A:639:SER:O	1:A:645:GLY:HA3	2.19	0.41
1:A:733:LEU:HD12	23:A:852:LHG:H331	2.02	0.41
18:A:801:CL0:H13	19:A:878:CLA:OBD	2.20	0.41
19:A:826:CLA:H111	19:A:826:CLA:H143	1.70	0.41
2:B:526:LEU:HD12	19:B:835:CLA:HED3	2.02	0.41
19:3:202:CLA:H18	19:3:202:CLA:H152	1.69	0.41
19:3:203:CLA:H12	16:4:48:TRP:CZ2	2.55	0.41
19:3:203:CLA:HED2	19:3:206:CLA:H42	2.02	0.41
16:4:76:LEU:HD23	16:4:76:LEU:HA	1.89	0.41
19:A:832:CLA:HMB2	19:A:833:CLA:C1D	2.50	0.41
2:B:373:HIS:HB2	19:B:825:CLA:CHB	2.50	0.41
13:1:178:VAL:HA	19:1:307:CLA:HMB2	2.00	0.41
19:A:806:CLA:H71	19:A:814:CLA:C2	2.50	0.41
19:A:824:CLA:HMA1	19:A:844:CLA:CBC	2.51	0.41
19:A:828:CLA:H2	19:A:828:CLA:H71	2.02	0.41
19:A:835:CLA:H92	19:A:835:CLA:H61	1.89	0.41
2:B:421:LEU:HG	2:B:531:LEU:HB2	2.02	0.41
19:B:804:CLA:H3A	19:B:804:CLA:HBA2	1.81	0.41
19:B:807:CLA:HBB1	19:B:807:CLA:H111	2.02	0.41
3:C:62:PHE:HD2	4:D:120:ILE:HG21	1.85	0.41
4:D:62:ARG:NH2	4:D:64:GLU:OE1	2.53	0.41
22:J:104:BCR:H11C	22:J:104:BCR:H341	1.91	0.41
22:L:205:BCR:H15C	22:L:205:BCR:H351	1.96	0.41
19:A:822:CLA:C4A	19:A:822:CLA:HBA2	2.50	0.41
19:A:841:CLA:H51	19:A:841:CLA:C4C	2.51	0.41
2:B:714:VAL:HG22	26:B:847:DGD:HAS1	2.03	0.41
19:B:826:CLA:H8	22:B:841:BCR:H21C	2.02	0.41
19:1:310:CLA:HMA1	19:1:310:CLA:H43	2.02	0.41
1:A:483:PHE:HE2	19:A:839:CLA:H42	1.85	0.41
1:A:501:ASN:ND2	19:A:818:CLA:OBD	2.48	0.41
19:A:804:CLA:HMB3	19:A:842:CLA:H42	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:LYS:HD3	2:B:106:LYS:HA	1.93	0.41
2:B:176:HIS:ND1	19:B:813:CLA:HMC2	2.36	0.41
19:B:812:CLA:C3D	19:B:813:CLA:HMC3	2.51	0.41
22:B:840:BCR:H20C	22:B:840:BCR:H361	1.97	0.41
9:L:59:ILE:HA	9:L:82:THR:OG1	2.21	0.41
19:2:213:CLA:HBA2	19:2:213:CLA:H3A	1.27	0.41
19:4:312:CLA:HBC2	17:5:89:PHE:CZ	2.55	0.41
17:5:53:LEU:HB2	19:5:207:CLA:O1A	2.21	0.41
1:A:65:SER:O	1:A:69:VAL:HG23	2.20	0.41
19:B:831:CLA:H122	19:B:831:CLA:H162	1.77	0.41
22:B:844:BCR:H15C	22:B:844:BCR:H351	1.94	0.41
4:D:93:GLN:NE2	11:W:52:GLY:HA3	2.36	0.41
19:F:203:CLA:HAA2	19:F:203:CLA:HBD	2.02	0.41
11:W:133:ILE:HG23	11:W:163:PHE:HZ	1.86	0.41
11:W:151:MET:O	11:W:155:VAL:HG22	2.20	0.41
16:4:49:ASP:OD2	16:4:54:CYS:N	2.49	0.41
16:4:57:GLN:HE21	16:4:57:GLN:HB2	1.62	0.41
16:4:97:PRO:O	16:4:102:ALA:HB2	2.20	0.41
1:A:19:LYS:HA	1:A:183:LYS:O	2.20	0.41
1:A:308:ALA:HB2	19:A:822:CLA:HBC2	2.02	0.41
1:A:337:GLY:O	1:A:426:LEU:HG	2.21	0.41
19:A:878:CLA:H61	19:A:878:CLA:H41	1.90	0.41
19:B:845:CLA:H71	19:B:845:CLA:H112	1.75	0.41
15:3:85:ASN:ND2	19:3:204:CLA:HED1	2.35	0.41
16:4:34:PHE:O	16:4:36:GLY:N	2.53	0.41
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.91	0.41
1:A:246:ASN:ND2	1:A:248:ASP:HB3	2.35	0.41
19:A:821:CLA:H51	19:A:821:CLA:NB	2.35	0.41
19:B:804:CLA:H93	22:M:102:BCR:HC8	2.03	0.41
19:B:826:CLA:C4A	19:B:826:CLA:HBA2	2.50	0.41
19:A:820:CLA:HBA2	19:A:820:CLA:H3A	1.69	0.41
19:A:825:CLA:HBB1	19:A:832:CLA:HMD2	2.03	0.41
19:A:834:CLA:HBB1	19:A:834:CLA:HHC	2.02	0.41
22:A:848:BCR:H20C	22:A:848:BCR:H361	1.77	0.41
2:B:128:PHE:CE2	19:B:814:CLA:HMA2	2.55	0.41
2:B:609:ASP:OD1	32:B:907:HOH:O	2.22	0.41
2:B:611:SER:O	2:B:617:GLY:HA3	2.21	0.41
2:B:627:SER:O	2:B:631:ILE:HG12	2.21	0.41
19:B:807:CLA:H92	19:B:807:CLA:HMC2	2.01	0.41
19:B:831:CLA:H41	19:B:831:CLA:H61	1.91	0.41
22:B:844:BCR:H24C	22:B:844:BCR:H371	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:F:205:BCR:H11C	22:F:205:BCR:H341	1.95	0.41
7:I:26:PHE:CD2	22:I:102:BCR:HC8	2.56	0.41
9:L:75:LEU:HG	9:L:136:PHE:CD1	2.56	0.41
19:L:204:CLA:HBA1	19:L:204:CLA:H3A	1.79	0.41
15:3:70:LYS:HD2	19:3:206:CLA:C3D	2.50	0.41
15:3:153:GLU:H	15:3:153:GLU:HG2	1.71	0.41
19:3:203:CLA:NA	19:3:206:CLA:H102	2.36	0.41
16:4:34:PHE:HB2	16:4:35:SER:H	1.71	0.41
16:4:144:GLY:O	19:4:313:CLA:HMA1	2.21	0.41
16:4:158:LEU:HB3	19:4:305:CLA:HMA1	2.02	0.41
19:4:309:CLA:HBB2	31:4:315:A86:C10	2.50	0.41
1:A:389:SER:HB2	19:A:829:CLA:HMA1	2.03	0.41
19:A:826:CLA:H162	19:A:826:CLA:H141	1.86	0.41
2:B:135:TYR:CZ	10:M:6:GLN:HB3	2.56	0.41
19:B:832:CLA:H41	19:B:832:CLA:H62	1.62	0.41
6:F:66:LEU:O	6:F:70:VAL:HG23	2.20	0.41
19:3:210:CLA:H3A	19:3:210:CLA:HBA2	1.68	0.41
16:4:185:LYS:HB3	16:4:187:PHE:O	2.20	0.41
19:5:210:CLA:C4A	19:5:210:CLA:HBA1	2.51	0.41
19:5:210:CLA:H142	19:5:210:CLA:H111	1.82	0.41
19:A:833:CLA:H112	19:A:833:CLA:H152	1.64	0.40
19:B:808:CLA:HBB1	19:B:808:CLA:H72	2.02	0.40
9:L:46:ARG:NH2	11:W:85:PRO:HB3	2.36	0.40
11:W:101:PRO:HD2	11:W:102:TRP:CZ3	2.56	0.40
16:4:45:LEU:HD23	16:4:45:LEU:HA	1.96	0.40
19:5:210:CLA:H61	19:5:210:CLA:H41	1.72	0.40
1:A:128:ASN:HB3	1:A:136:GLN:HB3	2.04	0.40
1:A:176:ALA:HB2	19:A:811:CLA:HBC2	2.03	0.40
1:A:495:PRO:HG3	1:A:505:THR:HA	2.02	0.40
19:A:843:CLA:HMC3	19:B:836:CLA:ND	2.36	0.40
2:B:80:ASN:ND2	2:B:83:LYS:HB2	2.36	0.40
2:B:187:LEU:HG	19:B:815:CLA:HBB2	2.02	0.40
19:B:804:CLA:H142	19:B:804:CLA:H111	1.75	0.40
19:B:812:CLA:C1A	19:B:812:CLA:CGA	2.99	0.40
19:B:828:CLA:C1C	19:B:838:CLA:H101	2.51	0.40
19:B:837:CLA:O2A	26:B:847:DGD:HBN1	2.21	0.40
6:F:45:SER:O	6:F:48:LYS:HG2	2.20	0.40
22:I:102:BCR:H20C	22:I:102:BCR:H361	1.82	0.40
13:1:191:MET:CB	19:1:303:CLA:HMC3	2.50	0.40
31:3:228:A86:C7	19:4:308:CLA:HAB	2.51	0.40
23:A:853:LHG:H242	23:A:853:LHG:HC62	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:I:102:BCR:H11C	22:I:102:BCR:H34I	1.96	0.40
19:1:308:CLA:HBB2	25:1:319:UNL:C26	2.51	0.40
19:1:309:CLA:H111	23:1:318:LHG:H301	2.04	0.40
19:4:301:CLA:H41	19:4:301:CLA:HBB1	2.04	0.40
19:A:822:CLA:H111	19:A:822:CLA:H152	1.87	0.40
19:A:839:CLA:CGA	19:A:839:CLA:C1A	2.99	0.40
2:B:221:LEU:HG	19:B:815:CLA:C3D	2.51	0.40
2:B:582:MET:O	2:B:586:ILE:HG12	2.20	0.40
19:B:833:CLA:H62	19:B:833:CLA:H92	1.88	0.40
22:J:104:BCR:H20C	22:J:104:BCR:H361	1.87	0.40
15:3:82:TRP:CE2	15:3:101:PRO:HG2	2.56	0.40
15:3:170:MET:HE3	19:3:202:CLA:HMC3	2.03	0.40
19:3:207:CLA:H101	19:3:207:CLA:H13	1.77	0.40
1:A:107:ASP:OD2	1:A:110:SER:OG	2.22	0.40
1:A:540:ALA:HB2	19:A:839:CLA:HMA1	2.03	0.40
2:B:86:PRO:HB3	2:B:120:TYR:CD2	2.57	0.40
2:B:244:ASN:OD1	32:B:906:HOH:O	2.21	0.40
19:B:808:CLA:H203	19:B:808:CLA:H161	1.82	0.40
4:D:32:THR:HA	4:D:56:ASN:O	2.21	0.40
19:L:206:CLA:C1D	19:L:206:CLA:H42	2.51	0.40
14:2:83:LEU:O	19:2:207:CLA:HMC3	2.22	0.40
16:4:93:CYS:SG	19:4:310:CLA:HBB1	2.62	0.40
19:5:209:CLA:H41	19:5:209:CLA:H62	1.68	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	A	741/752 (98%)	728 (98%)	13 (2%)	0	100	100
2	B	731/733 (100%)	716 (98%)	15 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	79/81 (98%)	78 (99%)	1 (1%)	0	100	100
4	D	131/139 (94%)	127 (97%)	4 (3%)	0	100	100
5	E	59/65 (91%)	58 (98%)	1 (2%)	0	100	100
6	F	159/185 (86%)	156 (98%)	3 (2%)	0	100	100
7	I	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
8	J	39/41 (95%)	39 (100%)	0	0	100	100
9	L	145/148 (98%)	144 (99%)	1 (1%)	0	100	100
10	M	28/30 (93%)	28 (100%)	0	0	100	100
11	W	118/188 (63%)	114 (97%)	4 (3%)	0	100	100
13	1	183/221 (83%)	180 (98%)	3 (2%)	0	100	100
14	2	165/198 (83%)	159 (96%)	6 (4%)	0	100	100
15	3	162/196 (83%)	158 (98%)	3 (2%)	1 (1%)	22	27
16	4	165/201 (82%)	158 (96%)	7 (4%)	0	100	100
17	5	163/194 (84%)	161 (99%)	2 (1%)	0	100	100
All	All	3102/3408 (91%)	3037 (98%)	64 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	3	43	PRO

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	A	603/611 (99%)	587 (97%)	16 (3%)	40	57
2	B	599/598 (100%)	593 (99%)	6 (1%)	73	85
3	C	70/70 (100%)	70 (100%)	0	100	100
4	D	112/118 (95%)	108 (96%)	4 (4%)	30	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	54/58 (93%)	53 (98%)	1 (2%)	52	69
6	F	133/153 (87%)	128 (96%)	5 (4%)	28	42
7	I	30/30 (100%)	30 (100%)	0	100	100
8	J	37/37 (100%)	37 (100%)	0	100	100
9	L	114/115 (99%)	111 (97%)	3 (3%)	41	58
10	M	23/23 (100%)	23 (100%)	0	100	100
11	W	91/144 (63%)	80 (88%)	11 (12%)	4	4
13	1	144/171 (84%)	136 (94%)	8 (6%)	17	26
14	2	135/157 (86%)	127 (94%)	8 (6%)	16	23
15	3	129/151 (85%)	124 (96%)	5 (4%)	27	41
16	4	129/152 (85%)	123 (95%)	6 (5%)	22	32
17	5	133/156 (85%)	128 (96%)	5 (4%)	28	42
All	All	2536/2744 (92%)	2458 (97%)	78 (3%)	37	51

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	37	ARG
1	A	68	GLU
1	A	214	SER
1	A	235	GLN
1	A	246	ASN
1	A	248	ASP
1	A	249	LEU
1	A	259	LYS
1	A	268	ASN
1	A	278	PHE
1	A	327	GLU
1	A	360	MET
1	A	372	TYR
1	A	442	ASN
1	A	625	ASP
2	B	105	SER
2	B	256	PHE
2	B	352	TYR
2	B	490	GLN
2	B	498	GLU

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Mol	Chain	Res	Type
2	B	575	PHE
4	D	52[A]	ARG
4	D	52[B]	ARG
4	D	58	LEU
4	D	86	ILE
5	E	4	ARG
6	F	30	THR
6	F	78	ASP
6	F	140	GLU
6	F	176	VAL
6	F	179	GLU
9	L	32	LYS
9	L	104	GLU
9	L	141	SER
11	W	48	ASP
11	W	50	ASP
11	W	89	THR
11	W	115	GLN
11	W	120	THR
11	W	126	LYS
11	W	127	ASP
11	W	136	PHE
11	W	158	LEU
11	W	162	LYS
11	W	169	LYS
13	1	38	VAL
13	1	44	LYS
13	1	95	ASP
13	1	100	LEU
13	1	112	LYS
13	1	141	ASN
13	1	161	GLU
13	1	214	GLU
14	2	31	GLU
14	2	33	SER
14	2	41	VAL
14	2	43	GLU
14	2	100	ASP
14	2	118	SER
14	2	155	LYS
14	2	164	ARG
15	3	33	ARG

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Mol	Chain	Res	Type
15	3	37	VAL
15	3	94	ASN
15	3	133	ARG
15	3	190	MET
16	4	54	CYS
16	4	57	GLN
16	4	93	CYS
16	4	103	VAL
16	4	109	GLU
16	4	140	SER
17	5	46	LYS
17	5	72	SER
17	5	128	LYS
17	5	152	ASP
17	5	191	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	ASN
1	A	321	ASN
1	A	424	ASN
1	A	630	HIS
1	A	715	GLN
2	B	80	ASN
2	B	241	HIS
2	B	490	GLN
2	B	597	HIS
4	D	72	GLN
5	E	20	GLN
6	F	103	HIS
8	J	5	GLN
11	W	73	GLN
11	W	115	GLN
13	1	126	ASN
13	1	141	ASN
14	2	91	GLN
14	2	96	HIS
15	3	99	ASN
16	4	75	GLN
17	5	180	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 296 ligands modelled in this entry, 89 are unknown - leaving 207 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
19	CLA	A	830	-	65,73,73	2.01	18 (27%)	76,113,113	2.67	26 (34%)
26	DGD	B	847	-	67,67,67	0.95	2 (2%)	81,81,81	1.36	10 (12%)
19	CLA	A	842	-	65,73,73	1.99	18 (27%)	76,113,113	2.71	28 (36%)
19	CLA	B	825	-	65,73,73	2.03	17 (26%)	76,113,113	2.65	30 (39%)
19	CLA	B	804	-	65,73,73	2.00	19 (29%)	76,113,113	2.79	29 (38%)
19	CLA	1	309	32	65,73,73	2.03	15 (23%)	76,113,113	2.74	31 (40%)
19	CLA	5	213	17	45,53,73	2.50	17 (37%)	52,89,113	3.22	23 (44%)
19	CLA	B	815	-	45,53,73	2.41	17 (37%)	52,89,113	3.25	24 (46%)
28	DD6	3	213	-	39,45,45	6.67	24 (61%)	52,67,67	6.89	25 (48%)
19	CLA	B	833	-	60,68,73	2.11	17 (28%)	70,107,113	2.79	25 (35%)
19	CLA	B	812	-	65,73,73	2.05	19 (29%)	76,113,113	2.67	27 (35%)
19	CLA	B	846	-	65,73,73	2.03	17 (26%)	76,113,113	2.74	26 (34%)
19	CLA	B	827	-	65,73,73	1.99	16 (24%)	76,113,113	2.76	28 (36%)
19	CLA	B	808	-	65,73,73	1.96	16 (24%)	76,113,113	2.74	29 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	SF4	C	101	3	0,12,12	-	-	-		
19	CLA	4	308	-	45,53,73	2.48	17 (37%)	52,89,113	3.31	23 (44%)
19	CLA	A	831	-	65,73,73	2.01	18 (27%)	76,113,113	2.71	28 (36%)
19	CLA	B	838	23	65,73,73	2.02	16 (24%)	76,113,113	2.71	28 (36%)
19	CLA	4	304	16	50,58,73	2.35	15 (30%)	58,95,113	3.24	30 (51%)
19	CLA	2	214	14	45,53,73	2.51	17 (37%)	52,89,113	3.21	24 (46%)
19	CLA	A	818	-	54,62,73	2.20	16 (29%)	62,99,113	3.00	25 (40%)
19	CLA	1	301	32	65,73,73	2.04	17 (26%)	76,113,113	2.76	29 (38%)
19	CLA	2	212	-	45,53,73	2.43	15 (33%)	52,89,113	3.30	24 (46%)
19	CLA	A	816	-	50,58,73	2.35	16 (32%)	58,95,113	3.08	30 (51%)
19	CLA	A	843	32	65,73,73	1.97	17 (26%)	76,113,113	2.67	26 (34%)
30	KC1	3	211	15	48,53,53	3.49	24 (50%)	55,89,89	3.78	32 (58%)
19	CLA	A	812	19	65,73,73	2.01	16 (24%)	76,113,113	2.75	27 (35%)
19	CLA	3	202	15	65,73,73	2.02	16 (24%)	76,113,113	2.71	28 (36%)
22	BCR	B	840	-	41,41,41	1.12	2 (4%)	56,56,56	1.13	5 (8%)
30	KC1	3	205	15	48,53,53	3.49	25 (52%)	55,89,89	3.63	29 (52%)
19	CLA	u	202	-	45,53,73	2.48	16 (35%)	52,89,113	3.24	23 (44%)
23	LHG	A	852	-	46,46,48	0.68	1 (2%)	49,52,54	1.23	5 (10%)
19	CLA	5	216	17	42,50,73	2.47	15 (35%)	48,85,113	3.35	25 (52%)
20	PQN	A	845	-	34,34,34	0.37	0	42,45,45	0.68	1 (2%)
19	CLA	B	823	32	56,64,73	2.14	18 (32%)	65,102,113	3.01	30 (46%)
30	KC1	4	302	-	48,53,53	3.43	20 (41%)	55,89,89	3.90	31 (56%)
19	CLA	B	819	32	65,73,73	2.02	18 (27%)	76,113,113	2.67	31 (40%)
19	CLA	B	813	-	65,73,73	2.03	17 (26%)	76,113,113	2.68	27 (35%)
19	CLA	A	832	-	60,68,73	2.09	17 (28%)	70,107,113	2.83	29 (41%)
19	CLA	B	831	32	65,73,73	2.04	17 (26%)	76,113,113	2.72	32 (42%)
19	CLA	A	817	32	49,57,73	2.34	15 (30%)	55,93,113	3.14	24 (43%)
19	CLA	A	802	32	65,73,73	2.02	18 (27%)	76,113,113	2.75	27 (35%)
21	SF4	C	102	3	0,12,12	-	-	-		
24	LMT	2	220	-	36,36,36	1.19	5 (13%)	47,47,47	0.94	2 (4%)
19	CLA	2	207	-	65,73,73	2.03	16 (24%)	76,113,113	2.77	28 (36%)
31	A86	3	212	-	44,50,50	3.94	23 (52%)	51,76,76	7.29	23 (45%)
19	CLA	A	822	32	65,73,73	2.06	17 (26%)	76,113,113	2.60	27 (35%)
19	CLA	1	304	13	65,73,73	1.99	16 (24%)	76,113,113	2.76	28 (36%)
31	A86	1	316	-	44,50,50	4.08	22 (50%)	51,76,76	7.66	17 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	A86	3	228	-	44,50,50	4.08	23 (52%)	51,76,76	7.23	16 (31%)
30	KC1	2	211	-	48,53,53	3.46	25 (52%)	55,89,89	3.84	31 (56%)
28	DD6	2	217	-	39,45,45	6.64	24 (61%)	52,67,67	6.73	26 (50%)
28	DD6	1	315	-	39,45,45	6.70	22 (56%)	52,67,67	6.74	27 (51%)
24	LMT	3	216	-	36,36,36	1.18	5 (13%)	47,47,47	1.06	2 (4%)
23	LHG	A	853	19	48,48,48	0.61	0	51,54,54	1.25	5 (9%)
19	CLA	B	817	-	59,67,73	2.14	18 (30%)	68,105,113	2.87	26 (38%)
19	CLA	A	809	1	65,73,73	2.03	18 (27%)	76,113,113	2.68	27 (35%)
31	A86	2	219	-	44,50,50	3.98	23 (52%)	51,76,76	7.48	19 (37%)
19	CLA	B	802	-	65,73,73	1.97	17 (26%)	76,113,113	2.74	29 (38%)
19	CLA	A	835	-	65,73,73	2.01	18 (27%)	76,113,113	2.72	25 (32%)
19	CLA	5	215	17	45,53,73	2.49	16 (35%)	52,89,113	3.21	23 (44%)
19	CLA	B	818	-	65,73,73	2.04	16 (24%)	76,113,113	2.71	27 (35%)
28	DD6	L	209	-	39,45,45	6.76	22 (56%)	52,67,67	6.72	26 (50%)
19	CLA	1	308	13	45,53,73	2.45	16 (35%)	52,89,113	3.19	23 (44%)
22	BCR	F	201	-	41,41,41	1.06	2 (4%)	56,56,56	1.11	5 (8%)
19	CLA	A	829	-	65,73,73	2.05	19 (29%)	76,113,113	2.73	29 (38%)
19	CLA	A	813	-	55,63,73	2.26	18 (32%)	64,101,113	2.93	28 (43%)
31	A86	2	216	-	44,50,50	4.04	23 (52%)	51,76,76	7.11	20 (39%)
22	BCR	B	843	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	7 (12%)
22	BCR	I	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.17	3 (5%)
19	CLA	B	828	-	45,53,73	2.44	15 (33%)	52,89,113	3.10	27 (51%)
19	CLA	4	311	32	50,58,73	2.39	17 (34%)	58,95,113	3.04	27 (46%)
19	CLA	B	809	2	65,73,73	1.97	16 (24%)	76,113,113	2.60	27 (35%)
19	CLA	A	838	-	51,59,73	2.29	18 (35%)	59,96,113	3.05	28 (47%)
30	KC1	4	307	16	48,53,53	3.45	24 (50%)	55,89,89	3.89	30 (54%)
19	CLA	A	819	-	54,62,73	2.24	18 (33%)	62,99,113	2.96	26 (41%)
19	CLA	A	823	-	49,57,73	2.36	19 (38%)	55,93,113	3.10	25 (45%)
19	CLA	B	820	-	45,53,73	2.48	16 (35%)	52,89,113	3.23	24 (46%)
19	CLA	A	841	-	65,73,73	2.00	17 (26%)	76,113,113	2.69	30 (39%)
31	A86	4	315	-	44,50,50	3.89	23 (52%)	51,76,76	7.58	20 (39%)
19	CLA	A	821	-	54,62,73	2.20	16 (29%)	62,99,113	3.03	28 (45%)
19	CLA	2	213	14	45,53,73	2.48	18 (40%)	52,89,113	3.20	25 (48%)
19	CLA	A	811	-	54,62,73	2.24	17 (31%)	62,99,113	2.98	26 (41%)
19	CLA	5	207	17	60,68,73	2.16	16 (26%)	70,107,113	2.82	29 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	A	850	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	6 (10%)
19	CLA	A	807	1	65,73,73	2.04	17 (26%)	76,113,113	2.77	30 (39%)
19	CLA	B	822	32	54,62,73	2.22	17 (31%)	62,99,113	2.88	26 (41%)
22	BCR	B	852	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	5 (8%)
19	CLA	F	203	-	55,63,73	2.20	15 (27%)	64,101,113	2.92	25 (39%)
19	CLA	B	834	-	65,73,73	2.04	17 (26%)	76,113,113	2.69	27 (35%)
22	BCR	1	314	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	6 (10%)
19	CLA	3	209	15	51,59,73	2.30	18 (35%)	59,96,113	3.11	27 (45%)
19	CLA	5	209	32	65,73,73	2.06	17 (26%)	76,113,113	2.69	27 (35%)
19	CLA	4	312	16	52,60,73	2.27	15 (28%)	60,97,113	3.05	26 (43%)
19	CLA	5	211	17	58,66,73	2.13	18 (31%)	67,104,113	2.89	26 (38%)
19	CLA	B	821	-	65,73,73	2.01	18 (27%)	76,113,113	2.66	30 (39%)
29	LMG	1	302	-	49,49,55	0.79	0	57,57,63	1.30	6 (10%)
19	CLA	A	878	32	65,73,73	1.99	16 (24%)	76,113,113	2.73	28 (36%)
19	CLA	A	827	32	65,73,73	2.00	17 (26%)	76,113,113	2.72	29 (38%)
22	BCR	I	102	-	41,41,41	1.05	2 (4%)	56,56,56	1.20	7 (12%)
22	BCR	L	205	-	41,41,41	1.13	2 (4%)	56,56,56	1.18	3 (5%)
19	CLA	B	807	-	65,73,73	2.00	16 (24%)	76,113,113	2.77	28 (36%)
19	CLA	3	207	15	65,73,73	2.05	17 (26%)	76,113,113	2.66	26 (34%)
19	CLA	J	103	8	45,53,73	2.44	16 (35%)	52,89,113	3.18	23 (44%)
22	BCR	B	844	-	41,41,41	1.10	3 (7%)	56,56,56	1.10	4 (7%)
22	BCR	M	102	-	41,41,41	1.16	2 (4%)	56,56,56	1.18	4 (7%)
19	CLA	2	210	14	60,68,73	2.11	17 (28%)	70,107,113	2.76	26 (37%)
19	CLA	2	215	-	42,50,73	2.48	15 (35%)	48,85,113	3.26	27 (56%)
19	CLA	2	208	14	52,60,73	2.30	16 (30%)	60,97,113	3.13	26 (43%)
19	CLA	B	830	-	58,66,73	2.14	17 (29%)	67,104,113	2.95	29 (43%)
19	CLA	1	306	-	51,59,73	2.31	16 (31%)	59,96,113	3.21	33 (55%)
23	LHG	3	215	-	33,33,48	0.75	1 (3%)	36,39,54	1.27	4 (11%)
19	CLA	L	204	32	45,53,73	2.42	17 (37%)	52,89,113	3.12	24 (46%)
22	BCR	J	104	-	41,41,41	1.15	2 (4%)	56,56,56	1.15	3 (5%)
19	CLA	B	803	-	65,73,73	1.98	16 (24%)	76,113,113	2.66	27 (35%)
19	CLA	3	203	15	55,63,73	2.20	16 (29%)	64,101,113	2.94	24 (37%)
19	CLA	3	210	32	45,53,73	2.47	17 (37%)	52,89,113	3.23	23 (44%)
19	CLA	A	880	32	65,73,73	1.99	17 (26%)	76,113,113	2.70	29 (38%)
19	CLA	A	803	-	65,73,73	2.02	18 (27%)	76,113,113	2.56	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	805	-	65,73,73	2.07	19 (29%)	76,113,113	2.75	25 (32%)
30	KC1	1	305	-	48,53,53	3.45	23 (47%)	55,89,89	3.82	30 (54%)
23	LHG	M	103	-	40,40,48	0.68	1 (2%)	43,46,54	1.29	6 (13%)
22	BCR	B	841	-	41,41,41	1.14	2 (4%)	56,56,56	1.17	5 (8%)
19	CLA	B	811	-	65,73,73	2.02	17 (26%)	76,113,113	2.74	29 (38%)
19	CLA	B	836	32	65,73,73	2.05	17 (26%)	76,113,113	2.60	27 (35%)
19	CLA	A	825	-	59,67,73	2.14	18 (30%)	68,105,113	2.80	29 (42%)
27	5X6	J	105	-	43,43,43	5.64	23 (53%)	58,60,60	4.79	31 (53%)
19	CLA	L	203	-	65,73,73	2.01	17 (26%)	76,113,113	2.80	27 (35%)
18	CL0	A	801	-	65,73,73	2.01	18 (27%)	76,113,113	2.63	32 (42%)
19	CLA	A	808	-	65,73,73	2.00	16 (24%)	76,113,113	2.74	24 (31%)
28	DD6	1	312	-	39,45,45	6.74	22 (56%)	52,67,67	6.74	25 (48%)
19	CLA	F	204	6	45,53,73	2.48	16 (35%)	52,89,113	3.15	24 (46%)
31	A86	4	314	-	44,50,50	4.02	23 (52%)	51,76,76	7.63	19 (37%)
19	CLA	B	835	-	47,55,73	2.34	17 (36%)	54,91,113	3.16	25 (46%)
19	CLA	3	204	32	61,69,73	2.14	17 (27%)	71,108,113	2.88	28 (39%)
22	BCR	1	311	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	5 (8%)
22	BCR	A	849	-	41,41,41	1.12	2 (4%)	56,56,56	1.15	5 (8%)
19	CLA	4	309	-	45,53,73	2.53	16 (35%)	52,89,113	3.21	22 (42%)
19	CLA	B	814	-	65,73,73	2.02	19 (29%)	76,113,113	2.73	27 (35%)
20	PQN	B	839	-	34,34,34	0.41	0	42,45,45	0.67	1 (2%)
31	A86	5	220	-	44,50,50	4.14	23 (52%)	51,76,76	8.03	19 (37%)
22	BCR	F	205	-	41,41,41	1.14	3 (7%)	56,56,56	1.22	6 (10%)
19	CLA	3	206	15	65,73,73	2.04	17 (26%)	76,113,113	2.71	26 (34%)
19	CLA	A	806	-	65,73,73	2.03	18 (27%)	76,113,113	2.80	28 (36%)
23	LHG	1	318	-	40,40,48	0.63	0	43,46,54	1.29	4 (9%)
19	CLA	4	306	23	58,66,73	2.18	16 (27%)	67,104,113	2.93	25 (37%)
31	A86	5	219	-	44,50,50	3.98	23 (52%)	51,76,76	7.34	19 (37%)
31	A86	2	218	-	44,50,50	3.99	22 (50%)	51,76,76	7.21	23 (45%)
28	DD6	1	313	-	39,45,45	6.66	22 (56%)	52,67,67	7.08	25 (48%)
19	CLA	B	832	32	65,73,73	2.05	17 (26%)	76,113,113	2.70	26 (34%)
19	CLA	2	205	14	65,73,73	2.06	17 (26%)	76,113,113	2.69	30 (39%)
19	CLA	A	805	19	56,64,73	2.16	16 (28%)	65,102,113	2.88	29 (44%)
19	CLA	2	209	14	58,66,73	2.14	17 (29%)	67,104,113	2.80	29 (43%)
22	BCR	L	202	-	41,41,41	1.08	2 (4%)	56,56,56	1.10	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	u	201	-	55,63,73	2.20	16 (29%)	64,101,113	2.95	28 (43%)
19	CLA	B	810	-	65,73,73	2.00	17 (26%)	76,113,113	4.68	28 (36%)
30	KC1	3	208	32	48,53,53	3.47	26 (54%)	55,89,89	3.76	31 (56%)
19	CLA	B	806	-	65,73,73	2.00	16 (24%)	76,113,113	2.65	26 (34%)
19	CLA	B	826	-	65,73,73	2.05	18 (27%)	76,113,113	3.96	30 (39%)
23	LHG	4	317	19	48,48,48	0.66	2 (4%)	51,54,54	1.24	6 (11%)
19	CLA	A	837	1	45,53,73	2.46	17 (37%)	52,89,113	3.17	23 (44%)
19	CLA	A	834	-	65,73,73	1.99	17 (26%)	76,113,113	2.68	26 (34%)
19	CLA	5	214	17	45,53,73	2.48	17 (37%)	52,89,113	3.19	22 (42%)
19	CLA	A	836	-	54,62,73	2.20	17 (31%)	62,99,113	2.91	31 (50%)
19	CLA	B	829	-	65,73,73	1.99	16 (24%)	76,113,113	2.70	25 (32%)
31	A86	5	217	-	44,50,50	3.99	23 (52%)	51,76,76	7.29	23 (45%)
19	CLA	2	206	-	65,73,73	2.03	18 (27%)	76,113,113	2.79	27 (35%)
19	CLA	A	824	-	51,59,73	2.29	17 (33%)	59,96,113	3.04	23 (38%)
19	CLA	L	206	9	60,68,73	2.12	17 (28%)	70,107,113	2.85	29 (41%)
22	BCR	A	851	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	7 (12%)
19	CLA	5	210	17	65,73,73	2.03	18 (27%)	76,113,113	2.75	28 (36%)
19	CLA	4	310	16	45,53,73	2.51	16 (35%)	52,89,113	3.28	21 (40%)
21	SF4	A	846	2,1	0,12,12	-	-	-	-	-
28	DD6	5	218	-	39,45,45	6.78	22 (56%)	52,67,67	6.34	26 (50%)
24	LMT	A	854	-	36,36,36	1.13	3 (8%)	47,47,47	1.16	4 (8%)
19	CLA	A	833	-	65,73,73	2.04	17 (26%)	76,113,113	2.66	28 (36%)
19	CLA	A	814	-	60,68,73	2.10	16 (26%)	70,107,113	2.82	29 (41%)
31	A86	4	316	-	44,50,50	4.10	23 (52%)	51,76,76	7.39	17 (33%)
19	CLA	B	837	-	65,73,73	1.99	17 (26%)	76,113,113	2.75	28 (36%)
22	BCR	A	848	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	5 (8%)
19	CLA	4	305	16	65,73,73	2.06	18 (27%)	76,113,113	2.60	28 (36%)
19	CLA	5	212	17	56,64,73	2.21	18 (32%)	65,102,113	4.99	33 (50%)
19	CLA	4	301	16	65,73,73	2.07	18 (27%)	76,113,113	2.72	27 (35%)
22	BCR	A	847	-	41,41,41	1.12	3 (7%)	56,56,56	1.22	5 (8%)
31	A86	3	214	-	44,50,50	3.94	23 (52%)	51,76,76	7.26	23 (45%)
19	CLA	A	820	-	65,73,73	2.04	16 (24%)	76,113,113	2.69	28 (36%)
19	CLA	A	844	23	65,73,73	2.01	18 (27%)	76,113,113	2.77	28 (36%)
19	CLA	A	839	-	65,73,73	2.04	19 (29%)	76,113,113	2.72	28 (36%)
19	CLA	1	310	13	65,73,73	2.08	19 (29%)	76,113,113	2.67	29 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	1	307	13	55,63,73	2.26	18 (32%)	64,101,113	5.06	29 (45%)
19	CLA	5	208	17	60,68,73	2.11	17 (28%)	70,107,113	2.78	27 (38%)
31	A86	1	317	-	44,50,50	3.98	23 (52%)	51,76,76	7.75	21 (41%)
19	CLA	A	840	-	47,55,73	2.38	16 (34%)	54,91,113	3.16	24 (44%)
19	CLA	B	816	-	55,63,73	2.17	16 (29%)	64,101,113	2.99	26 (40%)
31	A86	5	221	-	44,50,50	3.98	23 (52%)	51,76,76	7.77	17 (33%)
19	CLA	B	845	-	65,73,73	2.03	18 (27%)	76,113,113	2.76	26 (34%)
19	CLA	4	313	16	55,63,73	2.25	17 (30%)	64,101,113	2.96	27 (42%)
19	CLA	A	804	-	65,73,73	2.01	17 (26%)	76,113,113	2.75	30 (39%)
19	CLA	A	810	1	65,73,73	2.03	18 (27%)	76,113,113	2.68	28 (36%)
19	CLA	A	815	-	50,58,73	2.33	19 (38%)	58,95,113	3.02	27 (46%)
19	CLA	A	826	32	65,73,73	2.00	16 (24%)	76,113,113	2.76	26 (34%)
23	LHG	B	842	19	34,34,48	0.83	1 (2%)	37,40,54	1.21	4 (10%)
19	CLA	1	303	13	65,73,73	2.07	15 (23%)	76,113,113	2.66	28 (36%)
19	CLA	4	303	-	55,63,73	2.24	16 (29%)	64,101,113	3.05	27 (42%)
24	LMT	1	323	-	36,36,36	1.28	6 (16%)	47,47,47	1.11	3 (6%)
19	CLA	A	828	-	65,73,73	1.99	16 (24%)	76,113,113	2.75	28 (36%)
19	CLA	B	824	-	65,73,73	1.98	18 (27%)	76,113,113	2.80	28 (36%)

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
19	CLA	A	830	-	1/1/15/20	7/37/115/115	-
26	DGD	B	847	-	-	24/55/95/95	0/2/2/2
19	CLA	A	842	-	1/1/15/20	12/37/115/115	-
19	CLA	B	825	-	1/1/15/20	8/37/115/115	-
19	CLA	B	804	-	1/1/15/20	14/37/115/115	-
19	CLA	1	309	32	1/1/15/20	13/37/115/115	-
19	CLA	5	213	17	1/1/11/20	4/13/91/115	-
19	CLA	B	815	-	1/1/11/20	3/13/91/115	-
28	DD6	3	213	-	-	9/26/80/80	0/3/3/3
19	CLA	B	833	-	1/1/14/20	7/31/109/115	-
19	CLA	B	812	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	846	-	1/1/15/20	13/37/115/115	-
19	CLA	B	827	-	1/1/15/20	14/37/115/115	-
19	CLA	B	808	-	1/1/15/20	9/37/115/115	-
21	SF4	C	101	3	-	-	0/6/5/5
19	CLA	4	308	-	-	5/13/91/115	-
19	CLA	A	831	-	1/1/15/20	9/37/115/115	-
19	CLA	B	838	23	1/1/15/20	12/37/115/115	-
19	CLA	4	304	16	1/1/12/20	3/19/97/115	-
19	CLA	2	214	14	1/1/11/20	1/13/91/115	-
19	CLA	A	818	-	1/1/12/20	7/24/102/115	-
19	CLA	1	301	32	1/1/15/20	7/37/115/115	-
19	CLA	2	212	-	1/1/11/20	4/13/91/115	-
19	CLA	A	816	-	1/1/12/20	4/19/97/115	-
19	CLA	A	843	32	1/1/15/20	9/37/115/115	-
30	KC1	3	211	15	-	4/15/71/71	-
19	CLA	A	812	19	1/1/15/20	12/37/115/115	-
19	CLA	3	202	15	1/1/15/20	11/37/115/115	-
22	BCR	B	840	-	-	10/29/63/63	0/2/2/2
30	KC1	3	205	15	-	7/15/71/71	-
19	CLA	u	202	-	1/1/11/20	3/13/91/115	-
23	LHG	A	852	-	-	25/51/51/53	-
19	CLA	5	216	17	-	2/10/88/115	-
20	PQN	A	845	-	-	6/23/43/43	0/2/2/2
19	CLA	B	823	32	1/1/13/20	4/27/105/115	-
30	KC1	4	302	-	-	7/15/71/71	-
19	CLA	B	819	32	1/1/15/20	7/37/115/115	-
19	CLA	B	813	-	1/1/15/20	21/37/115/115	-
19	CLA	A	832	-	1/1/14/20	9/31/109/115	-
19	CLA	B	831	32	1/1/15/20	5/37/115/115	-
19	CLA	A	817	32	-	9/18/96/115	-
19	CLA	A	802	32	1/1/15/20	4/37/115/115	-
24	LMT	2	220	-	-	10/21/61/61	0/2/2/2
21	SF4	C	102	3	-	-	0/6/5/5
19	CLA	2	207	-	1/1/15/20	6/37/115/115	-
31	A86	3	212	-	-	6/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	822	32	1/1/15/20	8/37/115/115	-
19	CLA	1	304	13	1/1/15/20	10/37/115/115	-
31	A86	1	316	-	-	5/34/90/90	0/3/3/3
31	A86	3	228	-	-	8/34/90/90	0/3/3/3
30	KC1	2	211	-	-	7/15/71/71	-
28	DD6	2	217	-	-	8/26/80/80	0/3/3/3
28	DD6	1	315	-	-	11/26/80/80	0/3/3/3
24	LMT	3	216	-	-	8/21/61/61	0/2/2/2
23	LHG	A	853	19	-	28/53/53/53	-
19	CLA	B	817	-	1/1/13/20	5/30/108/115	-
19	CLA	A	809	1	1/1/15/20	8/37/115/115	-
31	A86	2	219	-	-	6/34/90/90	0/3/3/3
19	CLA	B	802	-	1/1/15/20	13/37/115/115	-
19	CLA	A	835	-	1/1/15/20	9/37/115/115	-
19	CLA	5	215	17	-	4/13/91/115	-
19	CLA	B	818	-	1/1/15/20	8/37/115/115	-
28	DD6	L	209	-	-	9/26/80/80	0/3/3/3
19	CLA	1	308	13	1/1/11/20	5/13/91/115	-
22	BCR	F	201	-	-	9/29/63/63	0/2/2/2
19	CLA	A	829	-	1/1/15/20	8/37/115/115	-
19	CLA	A	813	-	1/1/13/20	7/25/103/115	-
31	A86	2	216	-	-	5/34/90/90	0/3/3/3
22	BCR	B	843	-	-	6/29/63/63	0/2/2/2
22	BCR	I	101	-	-	3/29/63/63	0/2/2/2
19	CLA	B	828	-	-	1/13/91/115	-
19	CLA	4	311	32	1/1/12/20	6/19/97/115	-
19	CLA	B	809	2	1/1/15/20	8/37/115/115	-
19	CLA	A	838	-	1/1/12/20	2/21/99/115	-
30	KC1	4	307	16	-	5/15/71/71	-
19	CLA	A	819	-	1/1/12/20	10/24/102/115	-
19	CLA	A	823	-	-	3/18/96/115	-
19	CLA	B	820	-	-	2/13/91/115	-
19	CLA	A	841	-	1/1/15/20	7/37/115/115	-
31	A86	4	315	-	-	6/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	821	-	-	10/24/102/115	-
19	CLA	2	213	14	1/1/11/20	7/13/91/115	-
19	CLA	A	811	-	1/1/12/20	7/24/102/115	-
19	CLA	5	207	17	1/1/14/20	11/31/109/115	-
22	BCR	A	850	-	-	7/29/63/63	0/2/2/2
19	CLA	A	807	1	1/1/15/20	13/37/115/115	-
19	CLA	B	822	32	1/1/12/20	4/24/102/115	-
22	BCR	B	852	-	-	12/29/63/63	0/2/2/2
19	CLA	F	203	-	1/1/13/20	7/25/103/115	-
19	CLA	B	834	-	1/1/15/20	9/37/115/115	-
22	BCR	1	314	-	-	14/29/63/63	0/2/2/2
19	CLA	3	209	15	1/1/12/20	7/21/99/115	-
19	CLA	5	209	32	1/1/15/20	18/37/115/115	-
19	CLA	4	312	16	1/1/12/20	5/22/100/115	-
19	CLA	5	211	17	1/1/13/20	9/29/107/115	-
19	CLA	B	821	-	1/1/15/20	18/37/115/115	-
29	LMG	1	302	-	-	23/44/64/70	0/1/1/1
19	CLA	A	878	32	1/1/15/20	8/37/115/115	-
19	CLA	A	827	32	1/1/15/20	8/37/115/115	-
22	BCR	I	102	-	-	7/29/63/63	0/2/2/2
22	BCR	L	205	-	-	5/29/63/63	0/2/2/2
19	CLA	B	807	-	1/1/15/20	10/37/115/115	-
19	CLA	3	207	15	1/1/15/20	18/37/115/115	-
19	CLA	J	103	8	1/1/11/20	3/13/91/115	-
22	BCR	B	844	-	-	4/29/63/63	0/2/2/2
22	BCR	M	102	-	-	3/29/63/63	0/2/2/2
19	CLA	2	210	14	1/1/14/20	10/31/109/115	-
19	CLA	2	215	-	1/1/10/20	2/10/88/115	-
19	CLA	2	208	14	1/1/12/20	12/22/100/115	-
19	CLA	B	830	-	1/1/13/20	4/29/107/115	-
19	CLA	1	306	-	1/1/12/20	7/21/99/115	-
23	LHG	3	215	-	-	17/38/38/53	-
19	CLA	L	204	32	1/1/11/20	4/13/91/115	-
22	BCR	J	104	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	803	-	1/1/15/20	5/37/115/115	-
19	CLA	3	203	15	1/1/13/20	6/25/103/115	-
19	CLA	3	210	32	1/1/11/20	4/13/91/115	-
19	CLA	A	880	32	1/1/15/20	3/37/115/115	-
19	CLA	A	803	-	1/1/15/20	10/37/115/115	-
19	CLA	B	805	-	1/1/15/20	15/37/115/115	-
30	KC1	1	305	-	-	6/15/71/71	-
23	LHG	M	103	-	-	23/45/45/53	-
22	BCR	B	841	-	-	2/29/63/63	0/2/2/2
19	CLA	B	811	-	1/1/15/20	8/37/115/115	-
19	CLA	B	836	32	1/1/15/20	5/37/115/115	-
19	CLA	A	825	-	1/1/13/20	11/30/108/115	-
27	5X6	J	105	-	-	20/29/67/67	0/2/2/2
19	CLA	L	203	-	-	2/37/115/115	-
18	CL0	A	801	-	3/3/20/25	7/37/135/135	-
19	CLA	A	808	-	1/1/15/20	8/37/115/115	-
28	DD6	1	312	-	-	11/26/80/80	0/3/3/3
19	CLA	F	204	6	1/1/11/20	9/13/91/115	-
31	A86	4	314	-	-	6/34/90/90	0/3/3/3
19	CLA	B	835	-	1/1/11/20	2/16/94/115	-
19	CLA	3	204	32	1/1/14/20	10/33/111/115	-
22	BCR	1	311	-	-	8/29/63/63	0/2/2/2
22	BCR	A	849	-	-	7/29/63/63	0/2/2/2
19	CLA	4	309	-	-	2/13/91/115	-
19	CLA	B	814	-	1/1/15/20	11/37/115/115	-
20	PQN	B	839	-	-	9/23/43/43	0/2/2/2
31	A86	5	220	-	-	15/34/90/90	0/3/3/3
22	BCR	F	205	-	-	4/29/63/63	0/2/2/2
19	CLA	3	206	15	1/1/15/20	19/37/115/115	-
19	CLA	A	806	-	1/1/15/20	13/37/115/115	-
23	LHG	1	318	-	-	28/45/45/53	-
19	CLA	4	306	23	1/1/13/20	11/29/107/115	-
31	A86	5	219	-	-	3/34/90/90	0/3/3/3
31	A86	2	218	-	-	3/34/90/90	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	DD6	1	313	-	-	16/26/80/80	0/3/3/3
19	CLA	B	832	32	1/1/15/20	12/37/115/115	-
19	CLA	2	205	14	1/1/15/20	15/37/115/115	-
19	CLA	A	805	19	1/1/13/20	10/27/105/115	-
19	CLA	2	209	14	1/1/13/20	10/29/107/115	-
22	BCR	L	202	-	-	8/29/63/63	0/2/2/2
19	CLA	u	201	-	1/1/13/20	13/25/103/115	-
19	CLA	B	810	-	1/1/15/20	13/37/115/115	-
30	KC1	3	208	32	-	4/15/71/71	-
19	CLA	B	806	-	1/1/15/20	14/37/115/115	-
19	CLA	B	826	-	1/1/15/20	10/37/115/115	-
23	LHG	4	317	19	-	33/53/53/53	-
19	CLA	A	837	1	1/1/11/20	5/13/91/115	-
19	CLA	A	834	-	1/1/15/20	10/37/115/115	-
19	CLA	5	214	17	1/1/11/20	2/13/91/115	-
19	CLA	A	836	-	1/1/12/20	5/24/102/115	-
19	CLA	B	829	-	1/1/15/20	12/37/115/115	-
31	A86	5	217	-	-	6/34/90/90	0/3/3/3
19	CLA	2	206	-	1/1/15/20	9/37/115/115	-
19	CLA	A	824	-	1/1/12/20	5/21/99/115	-
19	CLA	L	206	9	1/1/14/20	6/31/109/115	-
22	BCR	A	851	-	-	7/29/63/63	0/2/2/2
19	CLA	5	210	17	1/1/15/20	12/37/115/115	-
19	CLA	4	310	16	-	3/13/91/115	-
21	SF4	A	846	2,1	-	-	0/6/5/5
28	DD6	5	218	-	-	10/26/80/80	0/3/3/3
24	LMT	A	854	-	-	8/21/61/61	0/2/2/2
19	CLA	A	833	-	1/1/15/20	9/37/115/115	-
19	CLA	A	814	-	1/1/14/20	6/31/109/115	-
31	A86	4	316	-	-	8/34/90/90	0/3/3/3
19	CLA	B	837	-	1/1/15/20	15/37/115/115	-
22	BCR	A	848	-	-	11/29/63/63	0/2/2/2
19	CLA	4	305	16	1/1/15/20	12/37/115/115	-
19	CLA	5	212	17	1/1/13/20	11/27/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	4	301	16	1/1/15/20	13/37/115/115	-
22	BCR	A	847	-	-	6/29/63/63	0/2/2/2
31	A86	3	214	-	-	3/34/90/90	0/3/3/3
19	CLA	A	820	-	1/1/15/20	11/37/115/115	-
19	CLA	A	844	23	1/1/15/20	9/37/115/115	-
19	CLA	A	839	-	1/1/15/20	10/37/115/115	-
19	CLA	1	310	13	1/1/15/20	12/37/115/115	-
19	CLA	1	307	13	1/1/13/20	7/25/103/115	-
19	CLA	5	208	17	1/1/14/20	10/31/109/115	-
31	A86	1	317	-	-	9/34/90/90	0/3/3/3
19	CLA	A	840	-	1/1/11/20	3/16/94/115	-
19	CLA	B	816	-	1/1/13/20	11/25/103/115	-
31	A86	5	221	-	-	7/34/90/90	0/3/3/3
19	CLA	B	845	-	-	9/37/115/115	-
19	CLA	4	313	16	1/1/13/20	5/25/103/115	-
19	CLA	A	804	-	1/1/15/20	12/37/115/115	-
19	CLA	A	810	1	1/1/15/20	6/37/115/115	-
19	CLA	A	815	-	1/1/12/20	3/19/97/115	-
19	CLA	A	826	32	1/1/15/20	15/37/115/115	-
23	LHG	B	842	19	-	21/39/39/53	-
19	CLA	1	303	13	1/1/15/20	13/37/115/115	-
19	CLA	4	303	-	1/1/13/20	6/25/103/115	-
24	LMT	1	323	-	-	12/21/61/61	0/2/2/2
19	CLA	A	828	-	1/1/15/20	14/37/115/115	-
19	CLA	B	824	-	1/1/15/20	4/37/115/115	-

All (3113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	5	218	DD6	C10-C11	25.72	1.69	1.35
28	1	315	DD6	C10-C11	25.56	1.69	1.35
28	L	209	DD6	C10-C11	25.53	1.69	1.35
28	1	312	DD6	C10-C11	25.46	1.69	1.35
28	1	313	DD6	C10-C11	25.34	1.69	1.35
28	3	213	DD6	C10-C11	25.33	1.69	1.35
28	2	217	DD6	C10-C11	25.19	1.69	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1	312	DD6	C5-C6	17.93	1.59	1.35
28	5	218	DD6	C5-C6	17.92	1.59	1.35
28	L	209	DD6	C5-C6	17.89	1.59	1.35
28	1	313	DD6	C5-C6	17.41	1.58	1.35
28	3	213	DD6	C5-C6	17.39	1.58	1.35
28	1	315	DD6	C5-C6	17.37	1.58	1.35
28	2	217	DD6	C5-C6	17.08	1.58	1.35
27	J	105	5X6	C18-C17	14.86	1.55	1.35
31	2	216	A86	C14-C13	14.59	1.68	1.51
27	J	105	5X6	C14-C13	14.59	1.55	1.35
27	J	105	5X6	C21-C22	14.38	1.54	1.35
31	1	316	A86	C14-C13	14.10	1.68	1.51
31	1	317	A86	C14-C13	14.04	1.68	1.51
31	5	217	A86	C14-C13	14.03	1.68	1.51
31	3	212	A86	C14-C13	14.02	1.68	1.51
31	2	218	A86	C14-C13	13.99	1.68	1.51
31	2	219	A86	C14-C13	13.94	1.68	1.51
31	3	228	A86	C14-C13	13.93	1.68	1.51
31	4	315	A86	C14-C13	13.89	1.68	1.51
28	5	218	DD6	C36-C31	13.75	1.50	1.34
31	5	219	A86	C14-C13	13.72	1.67	1.51
31	5	220	A86	C14-C13	13.59	1.67	1.51
31	4	314	A86	C14-C13	13.58	1.67	1.51
27	J	105	5X6	C25-C26	13.58	1.53	1.35
31	4	316	A86	C14-C13	13.56	1.67	1.51
28	1	312	DD6	C36-C31	13.55	1.50	1.34
31	5	221	A86	C14-C13	13.41	1.67	1.51
28	L	209	DD6	C36-C31	13.36	1.49	1.34
28	3	213	DD6	C36-C31	13.34	1.49	1.34
31	3	214	A86	C14-C13	13.25	1.67	1.51
28	2	217	DD6	C36-C31	13.19	1.49	1.34
28	1	313	DD6	C36-C31	13.18	1.49	1.34
28	1	315	DD6	C36-C31	12.92	1.49	1.34
30	3	211	KC1	C1D-ND	9.88	1.44	1.35
30	4	307	KC1	C1D-ND	9.77	1.43	1.35
30	3	205	KC1	C1D-ND	9.75	1.43	1.35
30	3	208	KC1	C1D-ND	9.70	1.43	1.35
30	4	302	KC1	C1D-ND	9.56	1.43	1.35
30	2	211	KC1	C1D-ND	9.56	1.43	1.35
30	1	305	KC1	C1D-ND	9.53	1.43	1.35
31	5	220	A86	C30-C29	9.53	1.47	1.32
31	1	316	A86	C30-C29	9.07	1.47	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	228	A86	C30-C29	8.95	1.46	1.32
31	4	316	A86	C30-C29	8.94	1.46	1.32
31	3	214	A86	C30-C29	8.76	1.46	1.32
31	5	219	A86	C30-C29	8.69	1.46	1.32
31	2	219	A86	C30-C29	8.68	1.46	1.32
31	2	218	A86	C30-C29	8.67	1.46	1.32
31	2	216	A86	C30-C29	8.65	1.46	1.32
31	3	212	A86	C30-C29	8.63	1.46	1.32
28	2	217	DD6	C13-C11	-8.63	1.27	1.45
31	4	314	A86	C30-C29	8.62	1.46	1.32
31	5	217	A86	C30-C29	8.59	1.46	1.32
28	1	313	DD6	C13-C11	-8.51	1.27	1.45
31	1	317	A86	C30-C29	8.50	1.46	1.32
28	5	218	DD6	C2-C1	8.38	1.46	1.35
28	3	213	DD6	C13-C11	-8.37	1.28	1.45
28	3	213	DD6	C2-C1	8.36	1.46	1.35
28	L	209	DD6	C23-C16	8.34	1.70	1.53
28	1	312	DD6	C23-C16	8.32	1.70	1.53
28	L	209	DD6	C13-C11	-8.32	1.28	1.45
31	5	221	A86	C30-C29	8.32	1.45	1.32
31	4	315	A86	C30-C29	8.31	1.45	1.32
28	1	313	DD6	C23-C16	8.31	1.70	1.53
28	1	315	DD6	C23-C16	8.28	1.70	1.53
28	2	217	DD6	C23-C16	8.28	1.70	1.53
28	1	315	DD6	C13-C11	-8.28	1.28	1.45
28	3	213	DD6	C23-C16	8.24	1.69	1.53
28	5	218	DD6	C23-C16	8.20	1.69	1.53
28	1	312	DD6	C13-C11	-8.12	1.28	1.45
28	L	209	DD6	C2-C1	8.09	1.46	1.35
28	1	312	DD6	C2-C1	8.09	1.46	1.35
28	1	315	DD6	C2-C1	7.98	1.46	1.35
28	5	218	DD6	C13-C11	-7.90	1.29	1.45
28	1	313	DD6	C2-C1	7.89	1.46	1.35
28	2	217	DD6	C2-C1	7.84	1.46	1.35
27	J	105	5X6	C24-C23	7.83	1.54	1.34
30	3	205	KC1	C2A-C3A	7.82	1.53	1.37
28	1	313	DD6	C19-C20	7.76	1.63	1.52
28	5	218	DD6	C9-C10	7.74	1.67	1.43
27	J	105	5X6	C15-C16	7.64	1.54	1.34
28	L	209	DD6	C9-C10	7.63	1.67	1.43
28	1	312	DD6	C9-C10	7.57	1.66	1.43
31	3	228	A86	C4-C5	7.54	1.66	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	316	A86	C4-C5	7.53	1.66	1.43
31	5	220	A86	C4-C5	7.48	1.66	1.43
30	2	211	KC1	C2A-C3A	7.43	1.52	1.37
31	5	220	A86	C8-C6	7.43	1.61	1.45
28	1	312	DD6	C19-C20	7.43	1.62	1.52
31	4	314	A86	C4-C5	7.42	1.66	1.43
28	L	209	DD6	C19-C20	7.41	1.62	1.52
28	1	313	DD6	C9-C10	7.40	1.66	1.43
28	1	315	DD6	C19-C20	7.39	1.62	1.52
31	2	216	A86	C4-C5	7.38	1.66	1.43
30	4	302	KC1	C2A-C3A	7.37	1.52	1.37
30	1	305	KC1	C2A-C3A	7.37	1.52	1.37
31	5	221	A86	C4-C5	7.36	1.66	1.43
31	2	219	A86	C4-C5	7.35	1.66	1.43
31	4	314	A86	C8-C6	7.34	1.61	1.45
28	1	315	DD6	C9-C10	7.34	1.66	1.43
28	2	217	DD6	C9-C10	7.31	1.66	1.43
31	1	316	A86	C4-C5	7.31	1.66	1.43
31	4	316	A86	C8-C6	7.31	1.61	1.45
28	3	213	DD6	C9-C10	7.30	1.66	1.43
28	2	217	DD6	C19-C20	7.30	1.62	1.52
28	3	213	DD6	C24-C1	7.30	1.61	1.45
28	5	218	DD6	C24-C1	7.29	1.61	1.45
31	3	214	A86	C8-C6	7.28	1.61	1.45
28	1	315	DD6	C24-C1	7.26	1.61	1.45
31	5	217	A86	C4-C5	7.26	1.65	1.43
31	5	221	A86	C8-C6	7.25	1.61	1.45
28	3	213	DD6	C19-C20	7.23	1.62	1.52
30	3	208	KC1	C2A-C3A	7.23	1.51	1.37
27	J	105	5X6	C20-C19	7.23	1.54	1.36
31	3	214	A86	C4-C5	7.23	1.65	1.43
31	3	228	A86	C8-C6	7.21	1.61	1.45
31	2	218	A86	C4-C5	7.18	1.65	1.43
31	5	219	A86	C4-C5	7.17	1.65	1.43
31	1	317	A86	C4-C5	7.15	1.65	1.43
31	2	218	A86	C8-C6	7.14	1.61	1.45
28	L	209	DD6	C24-C1	7.14	1.61	1.45
30	4	307	KC1	C2A-C3A	7.12	1.51	1.37
27	J	105	5X6	C27-C28	7.12	1.54	1.33
31	2	219	A86	C8-C6	7.12	1.61	1.45
31	2	216	A86	C8-C6	7.11	1.61	1.45
31	4	315	A86	C4-C5	7.11	1.65	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	316	A86	C8-C6	7.10	1.61	1.45
28	5	218	DD6	C19-C20	7.10	1.62	1.52
28	2	217	DD6	C24-C1	7.05	1.61	1.45
27	J	105	5X6	C12-C11	7.05	1.54	1.33
31	3	212	A86	C4-C5	7.03	1.65	1.43
31	5	217	A86	C8-C6	7.01	1.61	1.45
31	1	317	A86	C8-C6	7.00	1.61	1.45
31	5	220	A86	C25-C26	6.99	1.65	1.43
27	J	105	5X6	C30-C29	6.97	1.46	1.34
31	3	228	A86	C25-C26	6.92	1.64	1.43
28	1	312	DD6	C24-C1	6.90	1.60	1.45
28	1	313	DD6	C24-C1	6.90	1.60	1.45
30	3	211	KC1	C2A-C3A	6.89	1.51	1.37
28	1	315	DD6	C30-C29	6.89	1.40	1.20
31	4	316	A86	C25-C26	6.88	1.64	1.43
31	3	212	A86	C8-C6	6.86	1.60	1.45
31	4	314	A86	C19-C20	6.85	1.61	1.52
31	5	219	A86	C19-C20	6.84	1.61	1.52
31	5	219	A86	C8-C6	6.80	1.60	1.45
31	3	228	A86	C19-C20	6.80	1.61	1.52
30	3	211	KC1	CBA-CAA	6.77	1.53	1.33
31	1	316	A86	C25-C26	6.75	1.64	1.43
28	L	209	DD6	C30-C29	6.73	1.39	1.20
31	1	316	A86	C19-C20	6.72	1.61	1.52
28	5	218	DD6	C30-C29	6.72	1.39	1.20
31	4	316	A86	C19-C20	6.70	1.61	1.52
28	1	312	DD6	C30-C29	6.70	1.39	1.20
30	3	205	KC1	CBA-CAA	6.70	1.53	1.33
31	4	315	A86	C8-C6	6.69	1.60	1.45
31	5	217	A86	C25-C26	6.69	1.64	1.43
28	1	313	DD6	C30-C29	6.68	1.39	1.20
31	3	214	A86	C25-C26	6.67	1.64	1.43
31	4	314	A86	C25-C26	6.66	1.64	1.43
30	3	208	KC1	CBA-CAA	6.63	1.53	1.33
31	1	317	A86	C19-C20	6.62	1.61	1.52
28	5	218	DD6	C21-C20	-6.62	1.41	1.51
31	2	218	A86	C25-C26	6.62	1.64	1.43
31	5	220	A86	C19-C20	6.62	1.61	1.52
28	L	209	DD6	C21-C20	-6.61	1.41	1.51
31	2	216	A86	C25-C26	6.58	1.63	1.43
19	1	307	CLA	C3B-C2B	6.58	1.49	1.40
28	3	213	DD6	C30-C29	6.57	1.39	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	2	211	KC1	CBA-CAA	6.56	1.52	1.33
28	2	217	DD6	C30-C29	6.56	1.39	1.20
31	3	214	A86	C19-C20	6.56	1.61	1.52
31	5	217	A86	C19-C20	6.55	1.61	1.52
31	1	317	A86	C25-C26	6.52	1.63	1.43
27	J	105	5X6	C02-C03	6.49	1.45	1.34
30	1	305	KC1	CBA-CAA	6.47	1.52	1.33
30	4	302	KC1	CBA-CAA	6.46	1.52	1.33
31	4	315	A86	C25-C26	6.46	1.63	1.43
31	2	219	A86	C25-C26	6.46	1.63	1.43
31	3	212	A86	C25-C26	6.46	1.63	1.43
31	5	219	A86	C25-C26	6.45	1.63	1.43
31	5	221	A86	C25-C26	6.44	1.63	1.43
28	1	312	DD6	C21-C20	-6.43	1.41	1.51
31	5	221	A86	C19-C20	6.41	1.61	1.52
30	4	307	KC1	CBA-CAA	6.40	1.52	1.33
19	A	813	CLA	C3B-C2B	6.40	1.49	1.40
28	3	213	DD6	C21-C20	-6.36	1.41	1.51
28	1	315	DD6	C21-C20	-6.36	1.41	1.51
19	B	833	CLA	C3B-C2B	6.36	1.49	1.40
19	A	839	CLA	C3B-C2B	6.32	1.49	1.40
19	2	205	CLA	C3B-C2B	6.32	1.49	1.40
19	A	838	CLA	C3B-C2B	6.30	1.49	1.40
31	3	212	A86	C19-C20	6.30	1.61	1.52
31	2	216	A86	C19-C20	6.30	1.61	1.52
31	4	315	A86	C19-C20	6.28	1.61	1.52
28	2	217	DD6	C21-C20	-6.28	1.42	1.51
28	1	313	DD6	C21-C20	-6.28	1.42	1.51
19	B	805	CLA	C3B-C2B	6.25	1.49	1.40
28	1	315	DD6	C30-C31	6.23	1.55	1.42
19	3	206	CLA	C3B-C2B	6.22	1.49	1.40
19	4	309	CLA	C3B-C2B	6.22	1.49	1.40
19	B	826	CLA	C3B-C2B	6.19	1.49	1.40
31	2	219	A86	C19-C20	6.17	1.60	1.52
19	3	204	CLA	C3B-C2B	6.16	1.48	1.40
19	A	826	CLA	C3B-C2B	6.16	1.48	1.40
31	2	218	A86	C19-C20	6.15	1.60	1.52
19	B	846	CLA	C3B-C2B	6.13	1.48	1.40
28	L	209	DD6	C30-C31	6.12	1.55	1.42
19	B	820	CLA	C3B-C2B	6.11	1.48	1.40
19	A	829	CLA	C3B-C2B	6.10	1.48	1.40
19	1	303	CLA	C3B-C2B	6.10	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	845	CLA	C3B-C2B	6.10	1.48	1.40
19	B	818	CLA	C3B-C2B	6.08	1.48	1.40
19	A	830	CLA	C3B-C2B	6.05	1.48	1.40
19	A	828	CLA	C3B-C2B	6.04	1.48	1.40
19	B	834	CLA	C3B-C2B	6.04	1.48	1.40
19	2	213	CLA	C3B-C2B	6.03	1.48	1.40
28	2	217	DD6	C30-C31	6.02	1.55	1.42
19	A	810	CLA	C3B-C2B	6.01	1.48	1.40
28	5	218	DD6	C30-C31	6.00	1.55	1.42
19	A	844	CLA	C3B-C2B	6.00	1.48	1.40
19	F	203	CLA	C3B-C2B	6.00	1.48	1.40
30	1	305	KC1	O2A-CGA	5.99	1.46	1.30
30	4	302	KC1	O2A-CGA	5.98	1.46	1.30
19	B	827	CLA	C3B-C2B	5.98	1.48	1.40
19	B	825	CLA	C3B-C2B	5.98	1.48	1.40
19	B	814	CLA	C3B-C2B	5.97	1.48	1.40
19	u	202	CLA	C3B-C2B	5.96	1.48	1.40
19	5	207	CLA	C3B-C2B	5.96	1.48	1.40
19	A	804	CLA	C3B-C2B	5.95	1.48	1.40
19	4	306	CLA	C3B-C2B	5.94	1.48	1.40
30	3	208	KC1	O2A-CGA	5.94	1.45	1.30
19	2	208	CLA	C3B-C2B	5.92	1.48	1.40
19	A	878	CLA	C3B-C2B	5.92	1.48	1.40
19	A	816	CLA	C3B-C2B	5.92	1.48	1.40
19	B	807	CLA	C3B-C2B	5.90	1.48	1.40
19	A	880	CLA	C3B-C2B	5.90	1.48	1.40
28	1	312	DD6	C30-C31	5.90	1.54	1.42
19	5	216	CLA	C3B-C2B	5.89	1.48	1.40
19	4	301	CLA	C3B-C2B	5.89	1.48	1.40
19	A	823	CLA	C3B-C2B	5.89	1.48	1.40
19	u	201	CLA	C3B-C2B	5.88	1.48	1.40
19	4	311	CLA	C3B-C2B	5.87	1.48	1.40
19	B	823	CLA	C3B-C2B	5.87	1.48	1.40
30	2	211	KC1	O2A-CGA	5.85	1.45	1.30
19	A	821	CLA	C3B-C2B	5.85	1.48	1.40
19	4	304	CLA	C3B-C2B	5.85	1.48	1.40
19	A	807	CLA	C3B-C2B	5.85	1.48	1.40
19	F	204	CLA	C3B-C2B	5.85	1.48	1.40
19	J	103	CLA	C3B-C2B	5.84	1.48	1.40
19	3	207	CLA	C3B-C2B	5.84	1.48	1.40
19	5	215	CLA	C3B-C2B	5.83	1.48	1.40
19	2	214	CLA	C3B-C2B	5.83	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	206	CLA	C3B-C2B	5.83	1.48	1.40
19	B	812	CLA	C3B-C2B	5.82	1.48	1.40
30	4	307	KC1	O2A-CGA	5.82	1.45	1.30
30	3	205	KC1	O2A-CGA	5.81	1.45	1.30
28	1	313	DD6	C30-C31	5.81	1.54	1.42
19	A	809	CLA	C3B-C2B	5.80	1.48	1.40
19	A	831	CLA	C3B-C2B	5.80	1.48	1.40
19	A	806	CLA	C3B-C2B	5.79	1.48	1.40
19	4	310	CLA	C3B-C2B	5.79	1.48	1.40
19	5	213	CLA	C3B-C2B	5.79	1.48	1.40
19	B	804	CLA	C3B-C2B	5.78	1.48	1.40
30	3	211	KC1	O2A-CGA	5.78	1.45	1.30
19	L	203	CLA	C3B-C2B	5.78	1.48	1.40
19	4	313	CLA	C3B-C2B	5.78	1.48	1.40
19	5	210	CLA	C3B-C2B	5.78	1.48	1.40
19	A	805	CLA	C3B-C2B	5.78	1.48	1.40
19	A	819	CLA	C3B-C2B	5.77	1.48	1.40
19	B	822	CLA	C3B-C2B	5.77	1.48	1.40
30	3	211	KC1	C3D-C2D	5.76	1.49	1.39
19	B	831	CLA	C3B-C2B	5.76	1.48	1.40
19	4	308	CLA	C3B-C2B	5.75	1.48	1.40
19	A	840	CLA	C3B-C2B	5.75	1.48	1.40
19	5	214	CLA	C3B-C2B	5.75	1.48	1.40
19	5	212	CLA	C3B-C2B	5.73	1.48	1.40
19	A	802	CLA	C3B-C2B	5.73	1.48	1.40
19	5	211	CLA	C3B-C2B	5.73	1.48	1.40
19	B	821	CLA	C3B-C2B	5.73	1.48	1.40
19	A	832	CLA	C3B-C2B	5.73	1.48	1.40
19	B	803	CLA	C3B-C2B	5.72	1.48	1.40
19	B	811	CLA	C3B-C2B	5.72	1.48	1.40
19	1	301	CLA	C3B-C2B	5.71	1.48	1.40
30	1	305	KC1	C3D-C2D	5.71	1.49	1.39
30	4	307	KC1	C3D-C2D	5.69	1.49	1.39
19	2	210	CLA	C3B-C2B	5.69	1.48	1.40
19	A	833	CLA	C3B-C2B	5.69	1.48	1.40
19	B	838	CLA	C3B-C2B	5.68	1.48	1.40
19	B	837	CLA	C3B-C2B	5.66	1.48	1.40
19	B	817	CLA	C3B-C2B	5.66	1.48	1.40
19	3	209	CLA	C3B-C2B	5.64	1.48	1.40
19	A	825	CLA	C3B-C2B	5.64	1.48	1.40
19	L	206	CLA	C3B-C2B	5.63	1.48	1.40
19	1	306	CLA	C3B-C2B	5.63	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	3	211	KC1	C3B-C2B	5.62	1.48	1.37
19	B	824	CLA	C3B-C2B	5.62	1.48	1.40
19	5	208	CLA	C3B-C2B	5.62	1.48	1.40
30	2	211	KC1	C3D-C2D	5.61	1.49	1.39
19	3	203	CLA	C3B-C2B	5.60	1.48	1.40
30	1	305	KC1	C3B-C2B	5.59	1.48	1.37
19	L	204	CLA	C3B-C2B	5.59	1.48	1.40
28	3	213	DD6	C30-C31	5.58	1.54	1.42
19	2	215	CLA	C3B-C2B	5.58	1.48	1.40
19	2	207	CLA	C3B-C2B	5.57	1.48	1.40
19	4	310	CLA	C3C-C2C	5.56	1.48	1.36
19	B	836	CLA	C3B-C2B	5.56	1.48	1.40
30	4	302	KC1	C3D-C2D	5.56	1.49	1.39
19	2	209	CLA	C3B-C2B	5.56	1.48	1.40
19	A	812	CLA	C3B-C2B	5.56	1.48	1.40
19	B	815	CLA	C3B-C2B	5.55	1.48	1.40
19	B	802	CLA	C3B-C2B	5.55	1.48	1.40
30	4	302	KC1	C3B-C2B	5.54	1.48	1.37
19	B	828	CLA	C3B-C2B	5.54	1.48	1.40
19	3	210	CLA	C3B-C2B	5.54	1.48	1.40
19	A	842	CLA	C3B-C2B	5.54	1.48	1.40
19	A	817	CLA	C3B-C2B	5.52	1.48	1.40
19	B	810	CLA	C3B-C2B	5.52	1.48	1.40
19	B	813	CLA	C3B-C2B	5.52	1.48	1.40
19	1	310	CLA	C3B-C2B	5.52	1.48	1.40
19	A	811	CLA	C3B-C2B	5.52	1.48	1.40
19	A	824	CLA	C3B-C2B	5.51	1.48	1.40
19	B	832	CLA	C3B-C2B	5.50	1.48	1.40
19	5	216	CLA	C3C-C2C	5.50	1.48	1.36
19	A	815	CLA	C3B-C2B	5.50	1.48	1.40
19	4	303	CLA	C3B-C2B	5.50	1.48	1.40
19	4	305	CLA	C3B-C2B	5.49	1.48	1.40
19	B	806	CLA	C3B-C2B	5.48	1.48	1.40
19	A	818	CLA	C3B-C2B	5.48	1.48	1.40
19	2	214	CLA	C3C-C2C	5.48	1.48	1.36
19	3	210	CLA	C3C-C2C	5.48	1.48	1.36
30	3	208	KC1	C3B-C2B	5.47	1.48	1.37
19	A	837	CLA	C3B-C2B	5.47	1.48	1.40
19	A	803	CLA	C3B-C2B	5.46	1.48	1.40
19	A	827	CLA	C3B-C2B	5.46	1.47	1.40
31	5	220	A86	C26-C27	5.46	1.43	1.35
19	A	814	CLA	C3B-C2B	5.46	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	835	CLA	C3B-C2B	5.46	1.47	1.40
19	1	309	CLA	CHC-C1C	5.45	1.49	1.35
19	2	212	CLA	C3B-C2B	5.45	1.47	1.40
19	5	214	CLA	C3C-C2C	5.45	1.48	1.36
19	4	303	CLA	C3C-C2C	5.45	1.48	1.36
19	4	312	CLA	C3B-C2B	5.44	1.47	1.40
19	A	820	CLA	C3B-C2B	5.44	1.47	1.40
19	4	306	CLA	C3C-C2C	5.44	1.48	1.36
19	5	209	CLA	C3C-C2C	5.44	1.48	1.36
30	3	205	KC1	C3B-C2B	5.44	1.48	1.37
28	5	218	DD6	C13-C14	5.42	1.44	1.32
30	4	307	KC1	C3B-C2B	5.42	1.48	1.37
19	B	808	CLA	C3B-C2B	5.42	1.47	1.40
19	1	308	CLA	C3C-C2C	5.42	1.48	1.36
19	A	808	CLA	C3B-C2B	5.41	1.47	1.40
19	u	202	CLA	C3C-C2C	5.41	1.48	1.36
18	A	801	CL0	C3B-C2B	5.40	1.47	1.40
30	2	211	KC1	C3B-C2B	5.40	1.48	1.37
19	5	215	CLA	C3C-C2C	5.40	1.48	1.36
19	A	824	CLA	C3C-C2C	5.39	1.48	1.36
19	A	810	CLA	C3C-C2C	5.39	1.48	1.36
19	4	312	CLA	C3C-C2C	5.38	1.48	1.36
19	A	834	CLA	C3B-C2B	5.38	1.47	1.40
19	1	304	CLA	C3C-C2C	5.37	1.48	1.36
28	1	312	DD6	C13-C14	5.37	1.44	1.32
30	4	307	KC1	C3C-C2C	5.37	1.48	1.36
19	2	212	CLA	C1D-ND	5.37	1.44	1.37
19	4	311	CLA	C3C-C2C	5.37	1.48	1.36
19	A	815	CLA	C3C-C2C	5.36	1.48	1.36
19	B	829	CLA	C3B-C2B	5.36	1.47	1.40
19	B	832	CLA	C3C-C2C	5.35	1.48	1.36
30	2	211	KC1	C3C-C2C	5.34	1.48	1.36
19	A	836	CLA	C3B-C2B	5.34	1.47	1.40
19	2	208	CLA	C3C-C2C	5.34	1.48	1.36
28	L	209	DD6	C13-C14	5.34	1.44	1.32
19	B	819	CLA	C3C-C2C	5.34	1.48	1.36
19	B	809	CLA	C3B-C2B	5.34	1.47	1.40
19	3	204	CLA	C3C-C2C	5.33	1.48	1.36
30	3	208	KC1	CHD-C4C	5.33	1.48	1.35
19	A	841	CLA	C3B-C2B	5.32	1.47	1.40
19	L	206	CLA	C3C-C2C	5.32	1.48	1.36
19	5	209	CLA	C3B-C2B	5.32	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	1	305	KC1	C1A-NA	-5.32	1.27	1.38
19	L	203	CLA	C3C-C2C	5.31	1.48	1.36
19	F	204	CLA	C3C-C2C	5.31	1.48	1.36
19	B	805	CLA	C3C-C2C	5.31	1.48	1.36
19	5	213	CLA	C3C-C2C	5.31	1.48	1.36
19	B	835	CLA	C3B-C2B	5.31	1.47	1.40
19	1	308	CLA	CHC-C1C	5.31	1.48	1.35
19	3	202	CLA	CHC-C1C	5.31	1.48	1.35
19	J	103	CLA	C3C-C2C	5.31	1.48	1.36
19	5	210	CLA	C3C-C2C	5.30	1.48	1.36
19	2	210	CLA	CHC-C1C	5.30	1.48	1.35
19	4	301	CLA	CHC-C1C	5.30	1.48	1.35
19	B	829	CLA	C3C-C2C	5.30	1.48	1.36
19	A	836	CLA	C3C-C2C	5.30	1.48	1.36
30	3	208	KC1	C3D-C2D	5.30	1.48	1.39
19	4	313	CLA	C3C-C2C	5.30	1.48	1.36
28	1	315	DD6	C13-C14	5.30	1.44	1.32
19	3	203	CLA	C3C-C2C	5.30	1.48	1.36
19	4	310	CLA	CHC-C1C	5.30	1.48	1.35
19	4	312	CLA	CHC-C1C	5.30	1.48	1.35
19	B	817	CLA	C3C-C2C	5.30	1.48	1.36
19	2	207	CLA	C3C-C2C	5.29	1.48	1.36
19	2	215	CLA	C3C-C2C	5.29	1.48	1.36
19	4	301	CLA	C3C-C2C	5.29	1.48	1.36
19	B	834	CLA	C3C-C2C	5.29	1.48	1.36
19	A	817	CLA	C3C-C2C	5.29	1.48	1.36
19	4	309	CLA	C3C-C2C	5.29	1.48	1.36
19	B	831	CLA	C3C-C2C	5.29	1.48	1.36
30	3	205	KC1	O2D-CGD	5.29	1.46	1.33
19	5	216	CLA	O2D-CGD	5.28	1.46	1.33
19	1	301	CLA	C3C-C2C	5.28	1.48	1.36
19	A	803	CLA	C3C-C2C	5.28	1.47	1.36
19	4	308	CLA	C3C-C2C	5.27	1.47	1.36
19	2	215	CLA	C1D-ND	5.27	1.44	1.37
19	B	811	CLA	C3C-C2C	5.27	1.47	1.36
19	5	207	CLA	C3C-C2C	5.26	1.47	1.36
30	3	205	KC1	C3D-C2D	5.26	1.48	1.39
19	4	310	CLA	C1D-ND	5.26	1.44	1.37
19	2	214	CLA	C1D-ND	5.26	1.44	1.37
30	3	211	KC1	C3C-C2C	5.26	1.47	1.36
19	2	212	CLA	C3C-C2C	5.26	1.47	1.36
19	B	815	CLA	C3C-C2C	5.26	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	827	CLA	C3C-C2C	5.25	1.47	1.36
30	3	208	KC1	C3C-C2C	5.25	1.47	1.36
19	A	840	CLA	C3C-C2C	5.25	1.47	1.36
19	A	835	CLA	C3C-C2C	5.25	1.47	1.36
19	A	822	CLA	C3C-C2C	5.25	1.47	1.36
19	1	309	CLA	C3C-C2C	5.24	1.47	1.36
30	3	211	KC1	CHD-C4C	5.24	1.48	1.35
19	B	812	CLA	C3C-C2C	5.24	1.47	1.36
19	A	817	CLA	O2D-CGD	5.24	1.46	1.33
19	1	308	CLA	C3B-C2B	5.24	1.47	1.40
19	4	305	CLA	C3C-C2C	5.24	1.47	1.36
19	A	878	CLA	C3C-C2C	5.24	1.47	1.36
19	4	305	CLA	O2D-CGD	5.24	1.46	1.33
19	B	810	CLA	C3C-C2C	5.23	1.47	1.36
19	1	304	CLA	C3B-C2B	5.23	1.47	1.40
19	B	819	CLA	C3B-C2B	5.23	1.47	1.40
19	A	814	CLA	C3C-C2C	5.23	1.47	1.36
19	A	841	CLA	C3C-C2C	5.23	1.47	1.36
19	A	843	CLA	C3B-C2B	5.23	1.47	1.40
30	4	307	KC1	CHD-C4C	5.23	1.48	1.35
19	A	842	CLA	C3C-C2C	5.23	1.47	1.36
19	B	828	CLA	C3C-C2C	5.23	1.47	1.36
19	B	833	CLA	C3C-C2C	5.23	1.47	1.36
19	B	823	CLA	C3C-C2C	5.23	1.47	1.36
19	B	820	CLA	C3C-C2C	5.22	1.47	1.36
19	u	202	CLA	CHC-C1C	5.22	1.48	1.35
19	4	304	CLA	C1D-ND	5.22	1.44	1.37
19	2	213	CLA	O2D-CGD	5.22	1.45	1.33
19	4	313	CLA	C1D-ND	5.22	1.44	1.37
19	A	813	CLA	C3C-C2C	5.22	1.47	1.36
19	4	309	CLA	C1D-ND	5.22	1.44	1.37
19	A	844	CLA	C3C-C2C	5.22	1.47	1.36
19	A	807	CLA	CHC-C1C	5.22	1.48	1.35
19	A	819	CLA	C3C-C2C	5.22	1.47	1.36
19	B	836	CLA	C3C-C2C	5.22	1.47	1.36
19	A	804	CLA	C3C-C2C	5.21	1.47	1.36
19	B	826	CLA	C3C-C2C	5.21	1.47	1.36
19	4	309	CLA	O2D-CGD	5.21	1.45	1.33
19	B	830	CLA	C3B-C2B	5.21	1.47	1.40
19	u	201	CLA	C3C-C2C	5.21	1.47	1.36
19	B	814	CLA	C3C-C2C	5.21	1.47	1.36
19	A	841	CLA	O2D-CGD	5.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	803	CLA	CHC-C1C	5.21	1.48	1.35
19	3	202	CLA	C3B-C2B	5.20	1.47	1.40
19	5	207	CLA	CHC-C1C	5.20	1.48	1.35
28	5	218	DD6	C3-C2	5.20	1.59	1.43
19	5	211	CLA	C3C-C2C	5.20	1.47	1.36
19	A	807	CLA	C3C-C2C	5.20	1.47	1.36
19	1	303	CLA	C3C-C2C	5.20	1.47	1.36
19	B	838	CLA	C3C-C2C	5.20	1.47	1.36
19	1	303	CLA	O2D-CGD	5.20	1.45	1.33
19	A	837	CLA	C3C-C2C	5.20	1.47	1.36
19	A	816	CLA	C3C-C2C	5.20	1.47	1.36
19	A	830	CLA	C3C-C2C	5.19	1.47	1.36
19	B	816	CLA	CHC-C1C	5.19	1.48	1.35
19	3	202	CLA	C3C-C2C	5.19	1.47	1.36
19	F	204	CLA	C1D-ND	5.19	1.44	1.37
19	4	303	CLA	C1D-ND	5.19	1.44	1.37
19	A	805	CLA	C3C-C2C	5.19	1.47	1.36
19	B	821	CLA	C3C-C2C	5.19	1.47	1.36
19	3	207	CLA	CHC-C1C	5.19	1.48	1.35
19	A	802	CLA	C3C-C2C	5.18	1.47	1.36
19	A	833	CLA	C3C-C2C	5.18	1.47	1.36
30	1	305	KC1	C3C-C2C	5.18	1.47	1.36
30	4	307	KC1	C1A-NA	-5.18	1.27	1.38
19	2	213	CLA	C3C-C2C	5.18	1.47	1.36
19	5	208	CLA	O2D-CGD	5.18	1.45	1.33
19	A	823	CLA	C3C-C2C	5.18	1.47	1.36
30	2	211	KC1	CHD-C4C	5.18	1.48	1.35
19	B	830	CLA	C3C-C2C	5.18	1.47	1.36
19	4	311	CLA	O2D-CGD	5.18	1.45	1.33
19	B	834	CLA	CHC-C1C	5.17	1.48	1.35
19	B	826	CLA	O2D-CGD	5.17	1.45	1.33
30	4	302	KC1	C1A-NA	-5.17	1.27	1.38
19	A	808	CLA	CHC-C1C	5.17	1.48	1.35
19	4	304	CLA	O2D-CGD	5.17	1.45	1.33
30	2	211	KC1	C1A-NA	-5.17	1.27	1.38
19	B	828	CLA	O2D-CGD	5.17	1.45	1.33
19	A	834	CLA	C3C-C2C	5.17	1.47	1.36
30	3	205	KC1	C3C-C2C	5.16	1.47	1.36
30	1	305	KC1	CHD-C4C	5.16	1.48	1.35
19	1	306	CLA	C3C-C2C	5.16	1.47	1.36
19	A	832	CLA	C3C-C2C	5.16	1.47	1.36
19	B	836	CLA	CHC-C1C	5.16	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	841	CLA	CHC-C1C	5.16	1.48	1.35
19	3	206	CLA	C3C-C2C	5.16	1.47	1.36
19	4	303	CLA	CHC-C1C	5.15	1.48	1.35
19	A	829	CLA	C3C-C2C	5.15	1.47	1.36
19	A	819	CLA	O2D-CGD	5.15	1.45	1.33
28	L	209	DD6	C3-C2	5.15	1.59	1.43
19	2	215	CLA	O2D-CGD	5.14	1.45	1.33
19	5	207	CLA	C1D-ND	5.14	1.44	1.37
19	5	213	CLA	C1D-ND	5.14	1.44	1.37
19	1	310	CLA	O2D-CGD	5.14	1.45	1.33
19	4	308	CLA	C1D-ND	5.14	1.44	1.37
28	1	313	DD6	C13-C14	5.14	1.43	1.32
19	F	203	CLA	C3C-C2C	5.14	1.47	1.36
19	1	306	CLA	CHC-C1C	5.13	1.48	1.35
19	A	826	CLA	C3C-C2C	5.13	1.47	1.36
19	A	831	CLA	C3C-C2C	5.13	1.47	1.36
19	A	811	CLA	C3C-C2C	5.13	1.47	1.36
19	A	843	CLA	C3C-C2C	5.13	1.47	1.36
19	B	816	CLA	C3B-C2B	5.13	1.47	1.40
19	A	822	CLA	CHC-C1C	5.13	1.48	1.35
19	B	819	CLA	O2D-CGD	5.13	1.45	1.33
30	3	205	KC1	CHD-C4C	5.13	1.48	1.35
19	4	304	CLA	CHC-C1C	5.13	1.48	1.35
19	A	830	CLA	O2D-CGD	5.13	1.45	1.33
19	A	819	CLA	CHC-C1C	5.13	1.48	1.35
19	A	838	CLA	C3C-C2C	5.12	1.47	1.36
19	A	810	CLA	CHC-C1C	5.12	1.48	1.35
19	3	210	CLA	CHC-C1C	5.12	1.48	1.35
19	1	310	CLA	C3C-C2C	5.12	1.47	1.36
19	B	821	CLA	O2D-CGD	5.12	1.45	1.33
19	A	839	CLA	C3C-C2C	5.12	1.47	1.36
19	B	813	CLA	C3C-C2C	5.12	1.47	1.36
19	A	816	CLA	CHC-C1C	5.12	1.48	1.35
19	A	823	CLA	O2D-CGD	5.12	1.45	1.33
19	A	825	CLA	C3C-C2C	5.12	1.47	1.36
19	B	817	CLA	CHC-C1C	5.12	1.48	1.35
19	u	202	CLA	C1D-ND	5.11	1.44	1.37
19	A	809	CLA	C3C-C2C	5.11	1.47	1.36
19	B	808	CLA	C3C-C2C	5.11	1.47	1.36
19	A	820	CLA	CHC-C1C	5.11	1.48	1.35
19	A	837	CLA	O2D-CGD	5.11	1.45	1.33
19	A	808	CLA	C3C-C2C	5.11	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	202	CLA	O2D-CGD	5.11	1.45	1.33
19	1	304	CLA	O2D-CGD	5.11	1.45	1.33
19	B	845	CLA	C3C-C2C	5.11	1.47	1.36
19	1	309	CLA	O2D-CGD	5.11	1.45	1.33
19	2	210	CLA	C3C-C2C	5.10	1.47	1.36
30	4	307	KC1	O2D-CGD	5.10	1.45	1.33
18	A	801	CL0	C3C-C2C	5.10	1.47	1.36
19	A	820	CLA	C3C-C2C	5.10	1.47	1.36
19	B	804	CLA	C3C-C2C	5.10	1.47	1.36
19	B	802	CLA	C3C-C2C	5.10	1.47	1.36
19	2	206	CLA	C3C-C2C	5.10	1.47	1.36
19	5	214	CLA	CHC-C1C	5.10	1.48	1.35
19	A	810	CLA	O2D-CGD	5.10	1.45	1.33
19	A	818	CLA	O2D-CGD	5.10	1.45	1.33
19	2	209	CLA	C3C-C2C	5.10	1.47	1.36
19	5	212	CLA	O2D-CGD	5.10	1.45	1.33
19	1	301	CLA	C1D-ND	5.10	1.44	1.37
19	1	310	CLA	CHC-C1C	5.10	1.48	1.35
19	A	806	CLA	CHC-C1C	5.10	1.48	1.35
19	2	214	CLA	CHC-C1C	5.10	1.48	1.35
19	4	313	CLA	O2D-CGD	5.10	1.45	1.33
19	2	205	CLA	C3C-C2C	5.10	1.47	1.36
19	J	103	CLA	O2D-CGD	5.10	1.45	1.33
19	4	311	CLA	CHC-C1C	5.09	1.48	1.35
19	5	215	CLA	O2D-CGD	5.09	1.45	1.33
19	A	821	CLA	C3C-C2C	5.09	1.47	1.36
19	B	835	CLA	C3C-C2C	5.09	1.47	1.36
19	5	212	CLA	CHC-C1C	5.09	1.48	1.35
19	A	812	CLA	C3C-C2C	5.09	1.47	1.36
19	A	816	CLA	O2D-CGD	5.09	1.45	1.33
19	A	837	CLA	C1D-ND	5.09	1.44	1.37
19	B	831	CLA	CHC-C1C	5.09	1.48	1.35
19	5	215	CLA	CHC-C1C	5.09	1.48	1.35
19	5	208	CLA	C3C-C2C	5.08	1.47	1.36
19	F	203	CLA	O2D-CGD	5.08	1.45	1.33
19	A	840	CLA	CHC-C1C	5.08	1.48	1.35
19	3	207	CLA	C3C-C2C	5.08	1.47	1.36
19	3	210	CLA	C1D-ND	5.08	1.44	1.37
19	B	837	CLA	C3C-C2C	5.08	1.47	1.36
19	3	203	CLA	CHC-C1C	5.08	1.48	1.35
19	B	811	CLA	CHC-C1C	5.08	1.48	1.35
28	1	315	DD6	C3-C2	5.07	1.59	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	820	CLA	CHC-C1C	5.07	1.48	1.35
19	B	807	CLA	C3C-C2C	5.07	1.47	1.36
19	2	207	CLA	CHC-C1C	5.07	1.48	1.35
19	B	818	CLA	O2D-CGD	5.07	1.45	1.33
19	4	301	CLA	O2D-CGD	5.07	1.45	1.33
19	L	203	CLA	CHC-C1C	5.07	1.48	1.35
19	5	212	CLA	C3C-C2C	5.07	1.47	1.36
19	1	307	CLA	C3C-C2C	5.07	1.47	1.36
19	A	833	CLA	C1D-ND	5.07	1.44	1.37
19	B	825	CLA	O2D-CGD	5.07	1.45	1.33
19	2	212	CLA	CHC-C1C	5.07	1.48	1.35
19	A	837	CLA	CHC-C1C	5.06	1.48	1.35
19	5	208	CLA	CHC-C1C	5.06	1.48	1.35
19	B	836	CLA	O2D-CGD	5.06	1.45	1.33
19	A	818	CLA	C3C-C2C	5.06	1.47	1.36
19	A	806	CLA	C3C-C2C	5.06	1.47	1.36
19	B	831	CLA	O2D-CGD	5.06	1.45	1.33
19	A	817	CLA	CHC-C1C	5.06	1.47	1.35
19	A	820	CLA	O2D-CGD	5.06	1.45	1.33
30	3	211	KC1	O2D-CGD	5.06	1.45	1.33
19	4	311	CLA	C1D-ND	5.06	1.44	1.37
19	5	213	CLA	O2D-CGD	5.06	1.45	1.33
19	4	312	CLA	O2D-CGD	5.06	1.45	1.33
19	A	802	CLA	CHC-C1C	5.06	1.47	1.35
19	B	846	CLA	O2D-CGD	5.06	1.45	1.33
30	3	208	KC1	C1A-NA	-5.05	1.28	1.38
19	4	306	CLA	CHC-C1C	5.05	1.47	1.35
19	1	306	CLA	O2D-CGD	5.05	1.45	1.33
19	A	833	CLA	O2D-CGD	5.05	1.45	1.33
19	2	209	CLA	O2D-CGD	5.05	1.45	1.33
19	B	806	CLA	C3C-C2C	5.05	1.47	1.36
19	1	307	CLA	O2D-CGD	5.05	1.45	1.33
19	1	310	CLA	C1D-ND	5.05	1.44	1.37
19	1	301	CLA	O2D-CGD	5.05	1.45	1.33
19	A	805	CLA	CHC-C1C	5.05	1.47	1.35
19	B	806	CLA	CHC-C1C	5.05	1.47	1.35
30	3	208	KC1	O2D-CGD	5.05	1.45	1.33
19	B	828	CLA	CHC-C1C	5.04	1.47	1.35
19	F	204	CLA	O2D-CGD	5.04	1.45	1.33
19	B	827	CLA	C3C-C2C	5.04	1.47	1.36
19	4	308	CLA	CHC-C1C	5.04	1.47	1.35
19	B	824	CLA	C3C-C2C	5.04	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	214	CLA	O2D-CGD	5.04	1.45	1.33
19	B	810	CLA	CHC-C1C	5.04	1.47	1.35
19	B	846	CLA	C3C-C2C	5.04	1.47	1.36
19	A	815	CLA	O2D-CGD	5.04	1.45	1.33
19	B	818	CLA	C3C-C2C	5.04	1.47	1.36
19	B	819	CLA	CHC-C1C	5.04	1.47	1.35
19	3	209	CLA	O2D-CGD	5.04	1.45	1.33
19	5	209	CLA	O2D-CGD	5.04	1.45	1.33
28	2	217	DD6	C13-C14	5.04	1.43	1.32
19	3	209	CLA	C3C-C2C	5.04	1.47	1.36
19	4	306	CLA	C1D-ND	5.04	1.44	1.37
19	2	205	CLA	O2D-CGD	5.04	1.45	1.33
19	A	807	CLA	O2D-CGD	5.03	1.45	1.33
19	B	820	CLA	C1D-ND	5.03	1.44	1.37
19	A	814	CLA	O2D-CGD	5.03	1.45	1.33
19	A	811	CLA	CHC-C1C	5.03	1.47	1.35
19	4	304	CLA	C3C-C2C	5.03	1.47	1.36
19	A	836	CLA	O2D-CGD	5.03	1.45	1.33
30	4	302	KC1	CHD-C4C	5.03	1.47	1.35
19	A	811	CLA	O2D-CGD	5.03	1.45	1.33
19	3	210	CLA	O2D-CGD	5.03	1.45	1.33
19	5	207	CLA	O2D-CGD	5.03	1.45	1.33
19	A	812	CLA	CHC-C1C	5.03	1.47	1.35
19	A	822	CLA	O2D-CGD	5.03	1.45	1.33
19	2	208	CLA	O2D-CGD	5.02	1.45	1.33
19	F	203	CLA	CHC-C1C	5.02	1.47	1.35
28	3	213	DD6	C13-C14	5.02	1.43	1.32
19	3	204	CLA	C1D-ND	5.02	1.44	1.37
19	4	305	CLA	CHC-C1C	5.02	1.47	1.35
19	1	304	CLA	CHC-C1C	5.02	1.47	1.35
19	B	815	CLA	CHC-C1C	5.02	1.47	1.35
19	A	825	CLA	O2D-CGD	5.02	1.45	1.33
19	2	208	CLA	CHC-C1C	5.02	1.47	1.35
19	A	813	CLA	CHC-C1C	5.02	1.47	1.35
19	4	306	CLA	O2D-CGD	5.02	1.45	1.33
19	A	824	CLA	CHC-C1C	5.02	1.47	1.35
19	L	204	CLA	CHC-C1C	5.02	1.47	1.35
30	2	211	KC1	O2D-CGD	5.01	1.45	1.33
19	u	201	CLA	CHC-C1C	5.01	1.47	1.35
19	A	829	CLA	O2D-CGD	5.01	1.45	1.33
19	F	204	CLA	CHC-C1C	5.01	1.47	1.35
19	5	215	CLA	C1D-ND	5.01	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	206	CLA	O2D-CGD	5.01	1.45	1.33
19	B	837	CLA	O2D-CGD	5.01	1.45	1.33
19	A	828	CLA	C3C-C2C	5.01	1.47	1.36
30	4	302	KC1	C3C-C2C	5.01	1.47	1.36
28	1	312	DD6	C3-C2	5.01	1.59	1.43
19	3	209	CLA	CHC-C1C	5.00	1.47	1.35
19	A	814	CLA	CHC-C1C	5.00	1.47	1.35
19	1	308	CLA	O2D-CGD	5.00	1.45	1.33
19	B	816	CLA	C3C-C2C	5.00	1.47	1.36
19	J	103	CLA	CHC-C1C	5.00	1.47	1.35
19	A	843	CLA	O2D-CGD	5.00	1.45	1.33
19	B	832	CLA	O2D-CGD	5.00	1.45	1.33
19	3	206	CLA	O2D-CGD	5.00	1.45	1.33
19	5	214	CLA	C1D-ND	5.00	1.43	1.37
19	L	204	CLA	C3C-C2C	5.00	1.47	1.36
19	B	825	CLA	C3C-C2C	5.00	1.47	1.36
19	B	832	CLA	CHC-C1C	4.99	1.47	1.35
30	4	302	KC1	O2D-CGD	4.99	1.45	1.33
19	u	202	CLA	O2D-CGD	4.99	1.45	1.33
19	A	832	CLA	CHC-C1C	4.99	1.47	1.35
19	3	203	CLA	O2D-CGD	4.99	1.45	1.33
30	1	305	KC1	O2D-CGD	4.99	1.45	1.33
19	B	809	CLA	O2D-CGD	4.99	1.45	1.33
19	A	828	CLA	CHC-C1C	4.99	1.47	1.35
19	B	807	CLA	CHC-C1C	4.99	1.47	1.35
19	4	308	CLA	O2D-CGD	4.98	1.45	1.33
19	A	805	CLA	O2D-CGD	4.98	1.45	1.33
19	2	215	CLA	CHC-C1C	4.98	1.47	1.35
19	L	204	CLA	O2D-CGD	4.98	1.45	1.33
19	A	830	CLA	CHC-C1C	4.98	1.47	1.35
19	B	822	CLA	C3C-C2C	4.98	1.47	1.36
30	3	211	KC1	C1A-NA	-4.98	1.28	1.38
19	B	805	CLA	O2D-CGD	4.98	1.45	1.33
19	5	216	CLA	CHC-C1C	4.98	1.47	1.35
19	4	310	CLA	O2D-CGD	4.98	1.45	1.33
19	5	210	CLA	O2D-CGD	4.98	1.45	1.33
19	A	827	CLA	CHC-C1C	4.97	1.47	1.35
19	B	829	CLA	CHC-C1C	4.97	1.47	1.35
19	2	210	CLA	O2D-CGD	4.97	1.45	1.33
19	2	213	CLA	C1D-ND	4.97	1.43	1.37
19	A	878	CLA	CHC-C1C	4.97	1.47	1.35
19	2	213	CLA	CHC-C1C	4.97	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	880	CLA	C3C-C2C	4.97	1.47	1.36
19	A	806	CLA	O2D-CGD	4.97	1.45	1.33
19	A	804	CLA	CHC-C1C	4.97	1.47	1.35
19	1	306	CLA	C1D-ND	4.96	1.43	1.37
19	B	812	CLA	CHC-C1C	4.96	1.47	1.35
28	3	213	DD6	C3-C2	4.96	1.58	1.43
19	A	842	CLA	O2D-CGD	4.96	1.45	1.33
19	B	838	CLA	O2D-CGD	4.96	1.45	1.33
19	5	213	CLA	CHC-C1C	4.96	1.47	1.35
19	A	816	CLA	C1D-ND	4.96	1.43	1.37
19	A	843	CLA	CHC-C1C	4.96	1.47	1.35
19	B	817	CLA	O2D-CGD	4.96	1.45	1.33
19	2	207	CLA	O2D-CGD	4.96	1.45	1.33
19	B	830	CLA	CHC-C1C	4.96	1.47	1.35
19	B	846	CLA	CHC-C1C	4.96	1.47	1.35
19	5	209	CLA	CHC-C1C	4.95	1.47	1.35
19	A	824	CLA	C1D-ND	4.95	1.43	1.37
19	3	204	CLA	O2D-CGD	4.95	1.45	1.33
19	3	204	CLA	CHC-C1C	4.95	1.47	1.35
19	A	880	CLA	O2D-CGD	4.95	1.45	1.33
19	A	808	CLA	O2D-CGD	4.95	1.45	1.33
19	1	307	CLA	CHC-C1C	4.95	1.47	1.35
19	A	813	CLA	O2D-CGD	4.95	1.45	1.33
19	B	822	CLA	CHC-C1C	4.94	1.47	1.35
19	B	816	CLA	O2D-CGD	4.94	1.45	1.33
19	3	209	CLA	C1D-ND	4.94	1.43	1.37
19	4	313	CLA	CHC-C1C	4.94	1.47	1.35
19	A	834	CLA	O2D-CGD	4.94	1.45	1.33
19	B	824	CLA	CHC-C1C	4.94	1.47	1.35
19	2	205	CLA	CHC-C1C	4.94	1.47	1.35
19	B	806	CLA	O2D-CGD	4.94	1.45	1.33
19	B	830	CLA	O2D-CGD	4.94	1.45	1.33
19	3	206	CLA	CHC-C1C	4.94	1.47	1.35
19	2	212	CLA	O2D-CGD	4.94	1.45	1.33
19	B	845	CLA	O2D-CGD	4.94	1.45	1.33
19	4	312	CLA	C1D-ND	4.94	1.43	1.37
19	A	828	CLA	O2D-CGD	4.93	1.45	1.33
19	A	803	CLA	O2D-CGD	4.93	1.45	1.33
19	5	211	CLA	O2D-CGD	4.93	1.45	1.33
19	B	821	CLA	CHC-C1C	4.93	1.47	1.35
19	B	805	CLA	CHC-C1C	4.93	1.47	1.35
31	5	221	A86	C9-C8	4.93	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	821	CLA	CHC-C1C	4.93	1.47	1.35
19	B	802	CLA	O2D-CGD	4.93	1.45	1.33
19	1	309	CLA	C3B-C2B	4.93	1.47	1.40
19	A	832	CLA	O2D-CGD	4.93	1.45	1.33
19	A	818	CLA	CHC-C1C	4.93	1.47	1.35
19	B	834	CLA	O2D-CGD	4.92	1.45	1.33
19	1	303	CLA	CHC-C1C	4.92	1.47	1.35
19	B	812	CLA	O2D-CGD	4.92	1.45	1.33
19	B	823	CLA	CHC-C1C	4.92	1.47	1.35
19	1	301	CLA	CHC-C1C	4.92	1.47	1.35
19	4	303	CLA	O2D-CGD	4.92	1.45	1.33
19	A	834	CLA	CHC-C1C	4.92	1.47	1.35
19	A	835	CLA	O2D-CGD	4.92	1.45	1.33
19	A	815	CLA	CHC-C1C	4.92	1.47	1.35
28	1	313	DD6	C3-C2	4.92	1.58	1.43
31	3	214	A86	C9-C8	4.92	1.47	1.34
19	A	838	CLA	O2D-CGD	4.92	1.45	1.33
19	2	209	CLA	CHC-C1C	4.91	1.47	1.35
18	A	801	CL0	O2D-CGD	4.91	1.45	1.33
19	A	838	CLA	CHC-C1C	4.91	1.47	1.35
18	A	801	CL0	CHC-C1C	4.91	1.47	1.35
19	B	835	CLA	O2D-CGD	4.91	1.45	1.33
19	2	214	CLA	O2D-CGD	4.91	1.45	1.33
19	A	818	CLA	C1D-ND	4.91	1.43	1.37
19	B	813	CLA	O2D-CGD	4.91	1.45	1.33
19	B	818	CLA	CHC-C1C	4.91	1.47	1.35
19	B	838	CLA	CHC-C1C	4.91	1.47	1.35
19	A	823	CLA	CHC-C1C	4.91	1.47	1.35
19	B	802	CLA	CHC-C1C	4.91	1.47	1.35
19	B	825	CLA	CHC-C1C	4.91	1.47	1.35
19	A	829	CLA	C1D-ND	4.91	1.43	1.37
19	B	817	CLA	C1D-ND	4.91	1.43	1.37
19	B	827	CLA	CHC-C1C	4.91	1.47	1.35
19	A	839	CLA	O2D-CGD	4.91	1.45	1.33
19	B	845	CLA	CHC-C1C	4.90	1.47	1.35
19	B	810	CLA	O2D-CGD	4.90	1.45	1.33
19	B	804	CLA	O2D-CGD	4.90	1.45	1.33
19	B	803	CLA	CHC-C1C	4.90	1.47	1.35
19	B	803	CLA	O2D-CGD	4.90	1.45	1.33
19	A	813	CLA	C1D-ND	4.89	1.43	1.37
19	B	806	CLA	C1D-ND	4.89	1.43	1.37
19	1	307	CLA	C1D-ND	4.89	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	829	CLA	CHC-C1C	4.89	1.47	1.35
19	B	803	CLA	C3C-C2C	4.88	1.47	1.36
19	B	833	CLA	CHC-C1C	4.88	1.47	1.35
19	A	821	CLA	O2D-CGD	4.88	1.45	1.33
19	2	206	CLA	C1D-ND	4.88	1.43	1.37
19	1	303	CLA	C1D-ND	4.88	1.43	1.37
19	B	812	CLA	C1D-ND	4.87	1.43	1.37
19	A	844	CLA	CHC-C1C	4.87	1.47	1.35
19	2	206	CLA	O2D-CGD	4.87	1.45	1.33
19	A	814	CLA	C1D-ND	4.87	1.43	1.37
19	A	833	CLA	CHC-C1C	4.87	1.47	1.35
19	1	308	CLA	C1D-ND	4.87	1.43	1.37
19	A	802	CLA	O2D-CGD	4.87	1.45	1.33
19	B	804	CLA	CHC-C1C	4.87	1.47	1.35
19	3	202	CLA	C1D-ND	4.87	1.43	1.37
19	A	822	CLA	C3B-C2B	4.86	1.47	1.40
28	2	217	DD6	C3-C2	4.86	1.58	1.43
31	3	228	A86	C9-C8	4.86	1.47	1.34
19	A	840	CLA	C1D-ND	4.86	1.43	1.37
19	B	814	CLA	CHC-C1C	4.86	1.47	1.35
19	B	807	CLA	O2D-CGD	4.86	1.45	1.33
19	A	812	CLA	C1D-ND	4.86	1.43	1.37
19	B	811	CLA	O2D-CGD	4.86	1.45	1.33
19	B	824	CLA	O2D-CGD	4.85	1.45	1.33
19	4	309	CLA	CHC-C1C	4.85	1.47	1.35
19	5	210	CLA	C1D-ND	4.85	1.43	1.37
19	B	837	CLA	CHC-C1C	4.85	1.47	1.35
19	A	824	CLA	O2D-CGD	4.85	1.45	1.33
19	B	813	CLA	C1D-ND	4.85	1.43	1.37
19	A	804	CLA	O2D-CGD	4.84	1.45	1.33
19	A	822	CLA	C1D-ND	4.84	1.43	1.37
19	A	880	CLA	CHC-C1C	4.84	1.47	1.35
19	A	836	CLA	CHC-C1C	4.84	1.47	1.35
19	A	826	CLA	CHC-C1C	4.84	1.47	1.35
19	A	827	CLA	O2D-CGD	4.84	1.45	1.33
19	L	206	CLA	CHC-C1C	4.84	1.47	1.35
19	B	813	CLA	CHC-C1C	4.84	1.47	1.35
19	B	833	CLA	O2D-CGD	4.84	1.45	1.33
19	A	809	CLA	CHC-C1C	4.83	1.47	1.35
19	A	815	CLA	C1D-ND	4.83	1.43	1.37
19	5	209	CLA	C1D-ND	4.83	1.43	1.37
19	A	839	CLA	CHC-C1C	4.83	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	832	CLA	C1D-ND	4.83	1.43	1.37
19	B	820	CLA	O2D-CGD	4.83	1.45	1.33
19	B	835	CLA	CHC-C1C	4.82	1.47	1.35
19	B	808	CLA	O2D-CGD	4.82	1.45	1.33
19	3	207	CLA	C1D-ND	4.81	1.43	1.37
31	5	220	A86	C9-C8	4.81	1.47	1.34
19	A	840	CLA	O2D-CGD	4.81	1.44	1.33
19	2	206	CLA	CHC-C1C	4.80	1.47	1.35
19	A	811	CLA	C1D-ND	4.80	1.43	1.37
19	5	216	CLA	C1D-ND	4.80	1.43	1.37
19	B	822	CLA	O2D-CGD	4.80	1.44	1.33
19	A	826	CLA	O2D-CGD	4.80	1.44	1.33
19	B	822	CLA	C1D-ND	4.80	1.43	1.37
19	B	815	CLA	O2D-CGD	4.79	1.44	1.33
19	A	831	CLA	O2D-CGD	4.79	1.44	1.33
19	A	820	CLA	C1D-ND	4.79	1.43	1.37
19	5	212	CLA	C1D-ND	4.79	1.43	1.37
19	A	817	CLA	C1D-ND	4.79	1.43	1.37
19	A	831	CLA	CHC-C1C	4.79	1.47	1.35
19	B	809	CLA	C3C-C2C	4.79	1.46	1.36
19	A	825	CLA	CHC-C1C	4.79	1.47	1.35
19	A	842	CLA	CHC-C1C	4.78	1.47	1.35
19	B	814	CLA	O2D-CGD	4.78	1.44	1.33
31	1	316	A86	C26-C27	4.78	1.42	1.35
19	A	835	CLA	CHC-C1C	4.78	1.47	1.35
19	3	203	CLA	C1D-ND	4.78	1.43	1.37
31	3	212	A86	C9-C8	4.77	1.46	1.34
31	2	219	A86	C9-C8	4.77	1.46	1.34
19	2	209	CLA	C1D-ND	4.77	1.43	1.37
19	A	878	CLA	O2D-CGD	4.77	1.44	1.33
31	3	228	A86	C26-C27	4.76	1.42	1.35
19	L	203	CLA	O2D-CGD	4.76	1.44	1.33
19	A	823	CLA	C1D-ND	4.76	1.43	1.37
19	B	809	CLA	CHC-C1C	4.76	1.47	1.35
19	u	201	CLA	C1D-ND	4.76	1.43	1.37
19	5	210	CLA	CHC-C1C	4.76	1.47	1.35
19	2	208	CLA	C1D-ND	4.76	1.43	1.37
19	1	309	CLA	C1D-ND	4.75	1.43	1.37
19	A	809	CLA	O2D-CGD	4.75	1.44	1.33
19	B	818	CLA	C1D-ND	4.75	1.43	1.37
19	u	201	CLA	O2D-CGD	4.75	1.44	1.33
30	2	211	KC1	CHC-C4B	4.75	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	812	CLA	O2D-CGD	4.75	1.44	1.33
19	4	301	CLA	C1D-ND	4.75	1.43	1.37
19	B	826	CLA	C1D-ND	4.75	1.43	1.37
19	B	829	CLA	C1D-ND	4.74	1.43	1.37
19	B	834	CLA	C1D-ND	4.74	1.43	1.37
19	B	816	CLA	C1D-ND	4.74	1.43	1.37
19	5	211	CLA	CHC-C1C	4.73	1.47	1.35
19	L	206	CLA	C1D-ND	4.73	1.43	1.37
19	B	823	CLA	O2D-CGD	4.73	1.44	1.33
19	A	828	CLA	C1D-ND	4.72	1.43	1.37
19	A	806	CLA	C1D-ND	4.72	1.43	1.37
31	1	317	A86	C9-C8	4.72	1.46	1.34
19	B	826	CLA	CHC-C1C	4.72	1.47	1.35
19	B	836	CLA	C1D-ND	4.71	1.43	1.37
19	B	805	CLA	C1D-ND	4.71	1.43	1.37
30	4	307	KC1	CHC-C4B	4.71	1.47	1.38
31	4	316	A86	C9-C8	4.71	1.46	1.34
30	3	211	KC1	CHC-C4B	4.71	1.47	1.38
19	J	103	CLA	C1D-ND	4.70	1.43	1.37
19	L	204	CLA	C1D-ND	4.70	1.43	1.37
19	B	810	CLA	C1D-ND	4.69	1.43	1.37
19	A	807	CLA	C1D-ND	4.69	1.43	1.37
19	B	846	CLA	C1D-ND	4.69	1.43	1.37
31	2	218	A86	C9-C8	4.69	1.46	1.34
19	B	838	CLA	C1D-ND	4.68	1.43	1.37
19	B	835	CLA	C1D-ND	4.68	1.43	1.37
19	B	829	CLA	O2D-CGD	4.68	1.44	1.33
30	3	205	KC1	C1A-NA	-4.68	1.28	1.38
19	A	819	CLA	C1D-ND	4.67	1.43	1.37
19	3	207	CLA	O2D-CGD	4.67	1.44	1.33
31	1	316	A86	C9-C8	4.66	1.46	1.34
30	3	211	KC1	OBD-CAD	4.66	1.28	1.22
19	B	808	CLA	CHC-C1C	4.66	1.46	1.35
19	A	808	CLA	C1D-ND	4.66	1.43	1.37
31	5	217	A86	C9-C8	4.65	1.46	1.34
19	A	826	CLA	C1D-ND	4.65	1.43	1.37
19	B	824	CLA	C1D-ND	4.65	1.43	1.37
19	4	305	CLA	C1D-ND	4.64	1.43	1.37
19	B	831	CLA	C1D-ND	4.64	1.43	1.37
19	B	845	CLA	C1D-ND	4.64	1.43	1.37
19	A	825	CLA	O2A-CGA	4.64	1.46	1.33
19	2	210	CLA	C1D-ND	4.64	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	832	CLA	C1D-ND	4.63	1.43	1.37
19	A	835	CLA	C1D-ND	4.63	1.43	1.37
31	5	219	A86	C9-C8	4.63	1.46	1.34
19	B	830	CLA	C1D-ND	4.63	1.43	1.37
19	5	211	CLA	C1D-ND	4.62	1.43	1.37
31	4	316	A86	C26-C27	4.62	1.41	1.35
19	B	815	CLA	C1D-ND	4.62	1.43	1.37
30	3	208	KC1	CHC-C4B	4.62	1.47	1.38
19	L	206	CLA	O2A-CGA	4.62	1.46	1.33
31	5	221	A86	C2-C1	4.61	1.41	1.35
30	3	205	KC1	CHC-C4B	4.61	1.47	1.38
19	A	844	CLA	O2D-CGD	4.60	1.44	1.33
19	A	880	CLA	C1D-ND	4.60	1.43	1.37
19	B	803	CLA	C1D-ND	4.60	1.43	1.37
19	F	203	CLA	C1D-ND	4.60	1.43	1.37
19	A	809	CLA	C1D-ND	4.60	1.43	1.37
19	A	825	CLA	C1D-ND	4.59	1.43	1.37
19	A	842	CLA	C1D-ND	4.59	1.43	1.37
19	A	834	CLA	C1D-ND	4.59	1.43	1.37
31	5	219	A86	C26-C27	4.59	1.41	1.35
30	3	205	KC1	CHB-C1B	4.59	1.47	1.38
19	1	310	CLA	CHD-C1D	4.59	1.47	1.38
31	2	216	A86	C9-C8	4.59	1.46	1.34
19	A	821	CLA	C1D-ND	4.59	1.43	1.37
31	1	316	A86	O4-C38	4.59	1.45	1.35
19	3	210	CLA	O2A-CGA	4.59	1.46	1.30
31	5	220	A86	C2-C1	4.58	1.41	1.35
19	5	208	CLA	C1D-ND	4.58	1.43	1.37
30	4	302	KC1	OBD-CAD	4.58	1.28	1.22
19	5	213	CLA	O2A-CGA	4.58	1.46	1.30
19	B	828	CLA	O2A-CGA	4.57	1.46	1.30
19	B	837	CLA	C1D-ND	4.57	1.43	1.37
19	4	309	CLA	O2A-CGA	4.57	1.46	1.30
19	B	820	CLA	O2A-CGA	4.57	1.46	1.30
19	A	816	CLA	O2A-CGA	4.56	1.46	1.33
30	3	208	KC1	OBD-CAD	4.56	1.28	1.22
19	4	310	CLA	O2A-CGA	4.56	1.46	1.30
19	2	207	CLA	C1D-ND	4.55	1.43	1.37
19	B	815	CLA	O2A-CGA	4.55	1.46	1.30
19	B	814	CLA	C1D-ND	4.55	1.43	1.37
19	4	311	CLA	CHD-C1D	4.54	1.47	1.38
31	4	314	A86	C9-C8	4.54	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	3	205	KC1	OBD-CAD	4.54	1.28	1.22
19	u	202	CLA	O2A-CGA	4.53	1.46	1.30
31	3	214	A86	C26-C27	4.53	1.41	1.35
31	5	217	A86	C17-C18	-4.53	1.45	1.52
19	J	103	CLA	O2A-CGA	4.53	1.46	1.30
19	A	805	CLA	C1D-ND	4.53	1.43	1.37
19	2	205	CLA	C1D-ND	4.53	1.43	1.37
19	A	839	CLA	C1D-ND	4.53	1.43	1.37
19	4	303	CLA	O2A-CGA	4.53	1.46	1.33
19	2	213	CLA	O2A-CGA	4.52	1.46	1.30
19	3	206	CLA	O2A-CGA	4.52	1.46	1.33
30	3	208	KC1	CHB-C1B	4.52	1.47	1.38
31	1	316	A86	C17-C18	-4.52	1.45	1.52
19	2	212	CLA	O2A-CGA	4.52	1.45	1.30
19	A	827	CLA	C1D-ND	4.51	1.43	1.37
19	B	821	CLA	C1D-ND	4.51	1.43	1.37
19	3	206	CLA	C1D-ND	4.51	1.43	1.37
30	2	211	KC1	OBD-CAD	4.51	1.28	1.22
31	2	218	A86	O4-C38	4.51	1.45	1.35
19	B	827	CLA	C1D-ND	4.51	1.43	1.37
19	B	818	CLA	CHD-C1D	4.51	1.47	1.38
19	A	844	CLA	C1D-ND	4.51	1.43	1.37
19	L	203	CLA	C1D-ND	4.51	1.43	1.37
19	5	215	CLA	CHD-C1D	4.50	1.47	1.38
31	5	219	A86	C17-C18	-4.50	1.45	1.52
31	4	316	A86	C2-C1	4.50	1.41	1.35
19	3	204	CLA	CHD-C1D	4.50	1.47	1.38
19	2	214	CLA	O2A-CGA	4.49	1.45	1.30
19	4	308	CLA	O2A-CGA	4.49	1.45	1.30
30	4	307	KC1	CHB-C1B	4.49	1.47	1.38
30	1	305	KC1	OBD-CAD	4.49	1.28	1.22
19	1	309	CLA	O2A-CGA	4.49	1.46	1.33
19	B	813	CLA	CHD-C1D	4.49	1.47	1.38
30	4	302	KC1	CHB-C1B	4.48	1.47	1.38
19	4	313	CLA	CHD-C1D	4.48	1.47	1.38
19	2	207	CLA	O2A-CGA	4.48	1.46	1.33
19	A	837	CLA	O2A-CGA	4.48	1.45	1.30
19	2	214	CLA	CHD-C1D	4.48	1.47	1.38
19	A	809	CLA	O2A-CGA	4.47	1.46	1.33
31	1	317	A86	C17-C18	-4.47	1.45	1.52
19	B	807	CLA	C1D-ND	4.47	1.43	1.37
19	A	810	CLA	C1D-ND	4.47	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	215	CLA	O2A-CGA	4.46	1.45	1.30
19	A	841	CLA	C1D-ND	4.46	1.43	1.37
19	B	808	CLA	C1D-ND	4.46	1.43	1.37
19	B	833	CLA	C1D-ND	4.45	1.43	1.37
31	4	314	A86	C17-C18	-4.45	1.45	1.52
19	A	817	CLA	O2A-CGA	4.45	1.46	1.33
31	3	212	A86	O4-C38	4.45	1.45	1.35
19	4	310	CLA	CHD-C1D	4.45	1.47	1.38
19	B	830	CLA	CHD-C1D	4.45	1.47	1.38
19	2	215	CLA	CHD-C1D	4.44	1.47	1.38
19	5	209	CLA	O2A-CGA	4.44	1.46	1.33
19	1	303	CLA	CHD-C1D	4.44	1.47	1.38
19	A	822	CLA	O2A-CGA	4.44	1.46	1.33
19	5	213	CLA	CHD-C1D	4.44	1.47	1.38
19	F	204	CLA	O2A-CGA	4.44	1.45	1.30
27	J	105	5X6	C27-C26	4.44	1.55	1.45
30	4	302	KC1	CHC-C4B	4.44	1.47	1.38
30	3	211	KC1	CHB-C1B	4.43	1.47	1.38
19	B	811	CLA	C1D-ND	4.43	1.43	1.37
19	F	204	CLA	CHD-C1D	4.43	1.47	1.38
31	4	315	A86	C9-C8	4.43	1.46	1.34
31	5	220	A86	O4-C38	4.43	1.45	1.35
19	1	303	CLA	O2A-CGA	4.43	1.46	1.33
19	L	204	CLA	O2A-CGA	4.43	1.45	1.30
19	3	207	CLA	CHD-C1D	4.43	1.47	1.38
19	A	806	CLA	O2A-CGA	4.42	1.46	1.33
19	A	878	CLA	C1D-ND	4.42	1.43	1.37
31	4	316	A86	O4-C38	4.42	1.45	1.35
19	B	809	CLA	C1D-ND	4.42	1.43	1.37
19	5	207	CLA	CHD-C1D	4.42	1.47	1.38
19	B	816	CLA	O2A-CGA	4.42	1.46	1.33
19	A	838	CLA	C1D-ND	4.42	1.43	1.37
19	A	813	CLA	O2A-CGA	4.42	1.46	1.33
31	2	218	A86	C26-C27	4.42	1.41	1.35
19	B	827	CLA	O2D-CGD	4.41	1.44	1.33
19	A	804	CLA	C1D-ND	4.41	1.43	1.37
19	B	833	CLA	O2A-CGA	4.41	1.46	1.33
30	1	305	KC1	CHC-C4B	4.40	1.46	1.38
19	B	823	CLA	C1D-ND	4.39	1.43	1.37
31	5	217	A86	C26-C27	4.39	1.41	1.35
19	B	829	CLA	O2A-CGA	4.39	1.46	1.33
18	A	801	CL0	O2A-CGA	4.39	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	308	CLA	O2A-CGA	4.39	1.45	1.30
19	4	309	CLA	CHD-C1D	4.38	1.46	1.38
19	5	207	CLA	O2A-CGA	4.38	1.46	1.33
19	5	209	CLA	CHD-C1D	4.38	1.46	1.38
19	A	802	CLA	C1D-ND	4.38	1.43	1.37
19	A	836	CLA	O2A-CGA	4.38	1.46	1.33
19	B	828	CLA	C1D-ND	4.37	1.43	1.37
19	1	304	CLA	C1D-ND	4.37	1.43	1.37
19	4	305	CLA	CHD-C1D	4.37	1.46	1.38
19	B	810	CLA	O2A-CGA	4.37	1.46	1.33
19	5	214	CLA	CHD-C1D	4.37	1.46	1.38
19	A	811	CLA	O2A-CGA	4.36	1.46	1.33
19	B	832	CLA	O2A-CGA	4.36	1.46	1.33
19	A	824	CLA	O2A-CGA	4.36	1.46	1.33
19	L	203	CLA	O2A-CGA	4.36	1.46	1.33
19	B	811	CLA	CHD-C1D	4.36	1.46	1.38
31	5	221	A86	C26-C27	4.36	1.41	1.35
19	5	212	CLA	O2A-CGA	4.35	1.46	1.33
31	5	220	A86	C17-C18	-4.35	1.46	1.52
19	3	210	CLA	CHD-C1D	4.35	1.46	1.38
19	3	202	CLA	CHD-C1D	4.35	1.46	1.38
19	A	825	CLA	CHD-C1D	4.34	1.46	1.38
31	1	317	A86	O4-C38	4.34	1.45	1.35
19	B	819	CLA	C1D-ND	4.34	1.43	1.37
19	1	309	CLA	CHD-C1D	4.34	1.46	1.38
19	A	802	CLA	CHD-C1D	4.34	1.46	1.38
19	B	828	CLA	CHD-C1D	4.34	1.46	1.38
19	A	823	CLA	O2A-CGA	4.34	1.46	1.33
19	5	214	CLA	O2A-CGA	4.34	1.45	1.30
19	A	830	CLA	C1D-ND	4.34	1.43	1.37
19	B	804	CLA	C1D-ND	4.34	1.43	1.37
19	B	822	CLA	O2A-CGA	4.34	1.46	1.33
19	A	811	CLA	CHD-C1D	4.33	1.46	1.38
19	4	301	CLA	CHD-C1D	4.33	1.46	1.38
19	B	825	CLA	C1D-ND	4.33	1.43	1.37
19	A	837	CLA	CHD-C1D	4.33	1.46	1.38
19	2	209	CLA	CHD-C1D	4.33	1.46	1.38
19	5	208	CLA	O2A-CGA	4.33	1.46	1.33
31	5	220	A86	C7-C6	4.33	1.59	1.50
19	B	817	CLA	O2A-CGA	4.33	1.46	1.33
19	3	209	CLA	O2A-CGA	4.33	1.46	1.33
19	A	808	CLA	O2A-CGA	4.32	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	804	CLA	O2A-CGA	4.32	1.46	1.33
31	4	314	A86	C2-C1	4.32	1.41	1.35
19	3	203	CLA	O2A-CGA	4.32	1.46	1.33
19	1	306	CLA	CHD-C1D	4.32	1.46	1.38
19	A	806	CLA	CHD-C1D	4.32	1.46	1.38
19	A	831	CLA	C1D-ND	4.32	1.43	1.37
19	B	836	CLA	CHD-C1D	4.32	1.46	1.38
31	3	228	A86	C7-C6	4.32	1.59	1.50
19	2	209	CLA	O2A-CGA	4.32	1.46	1.33
19	B	812	CLA	CHD-C1D	4.32	1.46	1.38
19	B	808	CLA	O2A-CGA	4.31	1.45	1.33
19	u	201	CLA	CHD-C1D	4.31	1.46	1.38
19	B	846	CLA	O2A-CGA	4.31	1.45	1.33
19	B	845	CLA	O2A-CGA	4.31	1.45	1.33
19	4	301	CLA	O2A-CGA	4.31	1.45	1.33
19	A	819	CLA	CHD-C1D	4.31	1.46	1.38
19	A	836	CLA	C1D-ND	4.31	1.43	1.37
19	B	838	CLA	CHD-C1D	4.31	1.46	1.38
19	3	207	CLA	O2A-CGA	4.31	1.45	1.33
19	4	308	CLA	CHD-C1D	4.31	1.46	1.38
19	4	304	CLA	O2A-CGA	4.31	1.45	1.33
19	A	807	CLA	CHD-C1D	4.30	1.46	1.38
19	A	817	CLA	CHD-C1D	4.30	1.46	1.38
19	B	812	CLA	O2A-CGA	4.30	1.45	1.33
31	4	314	A86	C26-C27	4.30	1.41	1.35
31	1	316	A86	C2-C1	4.29	1.41	1.35
19	A	820	CLA	CHD-C1D	4.29	1.46	1.38
19	A	842	CLA	O2A-CGA	4.29	1.45	1.33
31	2	216	A86	C7-C6	4.29	1.59	1.50
31	1	317	A86	C7-C6	4.29	1.59	1.50
19	1	307	CLA	O2A-CGA	4.29	1.45	1.33
19	A	838	CLA	O2A-CGA	4.29	1.45	1.33
31	2	216	A86	O4-C38	4.28	1.44	1.35
19	5	208	CLA	CHD-C1D	4.28	1.46	1.38
31	5	221	A86	O4-C38	4.28	1.44	1.35
19	B	834	CLA	CHD-C1D	4.28	1.46	1.38
31	3	214	A86	O4-C38	4.28	1.44	1.35
31	3	228	A86	C2-C1	4.28	1.41	1.35
19	A	839	CLA	O2A-CGA	4.28	1.45	1.33
19	A	833	CLA	CHD-C1D	4.27	1.46	1.38
19	4	312	CLA	O2A-CGA	4.27	1.45	1.33
31	5	219	A86	O4-C38	4.27	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	218	A86	C7-C6	4.27	1.59	1.50
19	A	815	CLA	CHD-C1D	4.27	1.46	1.38
19	B	816	CLA	CHD-C1D	4.26	1.46	1.38
19	F	203	CLA	CHD-C1D	4.26	1.46	1.38
31	2	218	A86	C17-C18	-4.26	1.46	1.52
31	5	217	A86	O4-C38	4.26	1.44	1.35
31	5	221	A86	C17-C18	-4.26	1.46	1.52
18	A	801	CL0	CHD-C1D	4.25	1.46	1.38
19	2	206	CLA	CHD-C1D	4.25	1.46	1.38
31	4	315	A86	C17-C18	-4.25	1.46	1.52
19	1	308	CLA	CHD-C1D	4.25	1.46	1.38
19	A	821	CLA	O2A-CGA	4.25	1.45	1.33
19	B	819	CLA	CHD-C1D	4.25	1.46	1.38
19	A	822	CLA	CHD-C1D	4.25	1.46	1.38
31	2	216	A86	C2-C1	4.25	1.41	1.35
19	4	303	CLA	CHD-C1D	4.25	1.46	1.38
19	u	201	CLA	O2A-CGA	4.25	1.45	1.33
30	1	305	KC1	CHB-C1B	4.25	1.46	1.38
19	1	301	CLA	O2A-CGA	4.25	1.45	1.33
19	B	819	CLA	O2A-CGA	4.24	1.45	1.33
19	A	805	CLA	CHD-C1D	4.24	1.46	1.38
19	A	820	CLA	O2A-CGA	4.24	1.45	1.33
19	4	311	CLA	O2A-CGA	4.24	1.45	1.33
31	2	219	A86	C26-C27	4.24	1.41	1.35
31	2	219	A86	C17-C18	-4.24	1.46	1.52
31	4	315	A86	C26-C27	4.24	1.41	1.35
19	B	835	CLA	O2A-CGA	4.24	1.45	1.33
19	1	304	CLA	CHD-C1D	4.24	1.46	1.38
31	3	214	A86	C17-C18	-4.24	1.46	1.52
19	4	306	CLA	O2A-CGA	4.24	1.45	1.33
19	B	830	CLA	O2A-CGA	4.24	1.45	1.33
30	3	211	KC1	C4D-ND	4.24	1.39	1.35
19	u	202	CLA	CHD-C1D	4.23	1.46	1.38
19	A	835	CLA	O2A-CGA	4.23	1.45	1.33
19	A	840	CLA	O2A-CGA	4.23	1.45	1.33
19	4	312	CLA	CHD-C1D	4.23	1.46	1.38
19	A	818	CLA	O2A-CGA	4.23	1.45	1.33
19	B	803	CLA	CHD-C1D	4.23	1.46	1.38
19	A	812	CLA	CHD-C1D	4.23	1.46	1.38
19	2	207	CLA	CHD-C1D	4.23	1.46	1.38
19	A	814	CLA	CHD-C1D	4.22	1.46	1.38
19	4	305	CLA	O2A-CGA	4.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	815	CLA	CHD-C1D	4.22	1.46	1.38
31	4	314	A86	C7-C6	4.22	1.59	1.50
19	B	805	CLA	CHD-C1D	4.22	1.46	1.38
19	A	829	CLA	O2A-CGA	4.22	1.45	1.33
19	2	210	CLA	O2A-CGA	4.22	1.45	1.33
19	A	878	CLA	O2A-CGA	4.22	1.45	1.33
19	3	209	CLA	CHD-C1D	4.22	1.46	1.38
19	B	821	CLA	O2A-CGA	4.22	1.45	1.33
18	A	801	CL0	C1D-ND	4.21	1.43	1.37
31	5	219	A86	C2-C1	4.21	1.41	1.35
19	A	831	CLA	O2A-CGA	4.21	1.45	1.33
19	A	843	CLA	C1D-ND	4.21	1.43	1.37
31	5	219	A86	C7-C6	4.21	1.59	1.50
19	B	814	CLA	O2A-CGA	4.21	1.45	1.33
19	1	310	CLA	O2A-CGA	4.21	1.45	1.33
31	2	219	A86	C7-C6	4.21	1.59	1.50
19	A	819	CLA	O2A-CGA	4.21	1.45	1.33
31	4	315	A86	C7-C6	4.21	1.59	1.50
19	4	313	CLA	O2A-CGA	4.20	1.45	1.33
19	B	832	CLA	CHD-C1D	4.20	1.46	1.38
19	B	822	CLA	CHD-C1D	4.20	1.46	1.38
19	2	205	CLA	O2A-CGA	4.20	1.45	1.33
19	A	827	CLA	O2A-CGA	4.20	1.45	1.33
19	B	831	CLA	O2A-CGA	4.20	1.45	1.33
31	4	316	A86	C10-C11	4.20	1.46	1.34
31	3	212	A86	C7-C6	4.20	1.59	1.50
19	B	820	CLA	CHD-C1D	4.20	1.46	1.38
19	A	813	CLA	CHD-C1D	4.20	1.46	1.38
19	B	811	CLA	O2A-CGA	4.20	1.45	1.33
19	1	310	CLA	CHD-C4C	4.20	1.48	1.39
19	A	803	CLA	C1D-ND	4.20	1.42	1.37
19	A	815	CLA	O2A-CGA	4.20	1.45	1.33
19	3	204	CLA	O2A-CGA	4.19	1.45	1.33
19	A	809	CLA	CHD-C1D	4.19	1.46	1.38
19	B	823	CLA	O2A-CGA	4.19	1.45	1.33
19	5	210	CLA	O2A-CGA	4.19	1.45	1.33
19	A	829	CLA	CHD-C1D	4.19	1.46	1.38
31	1	317	A86	C26-C27	4.19	1.41	1.35
19	1	306	CLA	O2A-CGA	4.19	1.45	1.33
19	2	208	CLA	O2A-CGA	4.18	1.45	1.33
19	2	205	CLA	CHD-C1D	4.18	1.46	1.38
19	B	826	CLA	O2A-CGA	4.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	210	CLA	CHD-C1D	4.18	1.46	1.38
31	2	218	A86	C2-C1	4.18	1.41	1.35
19	A	807	CLA	O2A-CGA	4.18	1.45	1.33
19	B	824	CLA	O2A-CGA	4.18	1.45	1.33
19	A	804	CLA	O2A-CGA	4.17	1.45	1.33
31	3	212	A86	C26-C27	4.17	1.41	1.35
19	A	840	CLA	CHD-C1D	4.16	1.46	1.38
19	B	836	CLA	O2A-CGA	4.16	1.45	1.33
19	4	304	CLA	CHD-C1D	4.16	1.46	1.38
19	A	824	CLA	CHD-C1D	4.16	1.46	1.38
31	4	316	A86	C19-C18	4.16	1.58	1.52
19	A	816	CLA	CHD-C1D	4.16	1.46	1.38
19	A	838	CLA	CHD-C1D	4.16	1.46	1.38
19	5	212	CLA	CHD-C1D	4.16	1.46	1.38
19	4	313	CLA	CHD-C4C	4.16	1.48	1.39
19	B	825	CLA	O2A-CGA	4.15	1.45	1.33
31	5	217	A86	C2-C1	4.15	1.41	1.35
19	A	823	CLA	CHD-C1D	4.15	1.46	1.38
19	F	203	CLA	O2A-CGA	4.15	1.45	1.33
30	2	211	KC1	C4D-ND	4.15	1.38	1.35
19	A	803	CLA	O2A-CGA	4.15	1.45	1.33
19	1	306	CLA	CHD-C4C	4.15	1.48	1.39
31	3	214	A86	C2-C1	4.15	1.41	1.35
31	5	221	A86	C5-C6	4.15	1.41	1.35
19	4	303	CLA	CHD-C4C	4.14	1.48	1.39
19	A	843	CLA	O2A-CGA	4.14	1.45	1.33
19	A	835	CLA	CHD-C1D	4.14	1.46	1.38
19	3	206	CLA	CHD-C1D	4.14	1.46	1.38
31	2	219	A86	O4-C38	4.14	1.44	1.35
31	3	228	A86	O4-C38	4.14	1.44	1.35
19	1	307	CLA	CHD-C4C	4.14	1.48	1.39
31	3	228	A86	C19-C18	4.14	1.58	1.52
19	1	301	CLA	CHD-C1D	4.14	1.46	1.38
31	4	314	A86	O4-C38	4.14	1.44	1.35
19	1	307	CLA	CHD-C1D	4.14	1.46	1.38
27	J	105	5X6	C12-C13	4.14	1.54	1.45
19	B	802	CLA	C1D-ND	4.14	1.42	1.37
19	1	304	CLA	O2A-CGA	4.13	1.45	1.33
19	A	836	CLA	CHD-C1D	4.13	1.46	1.38
19	2	214	CLA	CHD-C4C	4.13	1.48	1.39
19	B	835	CLA	CHD-C1D	4.13	1.46	1.38
19	B	831	CLA	CHD-C1D	4.13	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	307	KC1	OBD-CAD	4.13	1.28	1.22
31	4	314	A86	C10-C11	4.13	1.46	1.34
19	A	837	CLA	CHD-C4C	4.13	1.48	1.39
30	2	211	KC1	CHB-C1B	4.13	1.46	1.38
19	2	210	CLA	CHD-C1D	4.12	1.46	1.38
19	B	838	CLA	O2A-CGA	4.12	1.45	1.33
19	L	206	CLA	CHD-C1D	4.12	1.46	1.38
31	2	216	A86	C26-C27	4.12	1.41	1.35
19	B	817	CLA	CHD-C1D	4.12	1.46	1.38
19	3	203	CLA	CHD-C1D	4.12	1.46	1.38
19	B	807	CLA	O2A-CGA	4.12	1.45	1.33
19	A	802	CLA	O2A-CGA	4.12	1.45	1.33
19	A	826	CLA	O2A-CGA	4.12	1.45	1.33
19	B	806	CLA	O2A-CGA	4.12	1.45	1.33
19	A	834	CLA	CHD-C1D	4.11	1.46	1.38
19	L	204	CLA	CHD-C1D	4.11	1.46	1.38
19	4	306	CLA	CHD-C1D	4.11	1.46	1.38
19	B	806	CLA	CHD-C1D	4.11	1.46	1.38
19	3	210	CLA	CHD-C4C	4.11	1.48	1.39
19	A	818	CLA	CHD-C1D	4.11	1.46	1.38
19	5	216	CLA	CHD-C1D	4.11	1.46	1.38
19	B	809	CLA	O2A-CGA	4.11	1.45	1.33
19	2	208	CLA	CHD-C1D	4.11	1.46	1.38
31	2	219	A86	C2-C1	4.10	1.41	1.35
19	A	805	CLA	O2A-CGA	4.10	1.45	1.33
19	A	844	CLA	O2A-CGA	4.10	1.45	1.33
31	4	316	A86	C7-C6	4.10	1.59	1.50
19	B	813	CLA	O2A-CGA	4.10	1.45	1.33
19	B	827	CLA	CHD-C1D	4.10	1.46	1.38
31	5	221	A86	C7-C6	4.10	1.59	1.50
19	4	309	CLA	CHD-C4C	4.09	1.48	1.39
19	B	831	CLA	CHD-C4C	4.09	1.48	1.39
19	4	311	CLA	CHD-C4C	4.09	1.48	1.39
19	A	880	CLA	O2A-CGA	4.09	1.45	1.33
19	A	844	CLA	CHD-C1D	4.08	1.46	1.38
19	A	827	CLA	CHD-C1D	4.08	1.46	1.38
19	B	837	CLA	O2A-CGA	4.08	1.45	1.33
31	5	221	A86	C21-C20	4.08	1.58	1.51
19	5	214	CLA	CHD-C4C	4.08	1.48	1.39
19	B	804	CLA	CHD-C1D	4.08	1.46	1.38
19	B	826	CLA	CHD-C1D	4.08	1.46	1.38
19	F	204	CLA	CHD-C4C	4.08	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	211	CLA	CHD-C4C	4.08	1.48	1.39
19	B	830	CLA	CHD-C4C	4.08	1.48	1.39
19	5	211	CLA	CHD-C1D	4.07	1.46	1.38
19	A	841	CLA	CHD-C4C	4.07	1.48	1.39
19	5	208	CLA	CHD-C4C	4.07	1.48	1.39
19	A	833	CLA	O2A-CGA	4.07	1.45	1.33
19	A	839	CLA	CHD-C1D	4.07	1.46	1.38
19	A	831	CLA	CHD-C1D	4.07	1.46	1.38
19	A	812	CLA	CHD-C4C	4.06	1.48	1.39
19	A	843	CLA	CHD-C1D	4.06	1.46	1.38
31	4	315	A86	C21-C20	4.06	1.58	1.51
19	3	204	CLA	CHD-C4C	4.06	1.48	1.39
19	B	809	CLA	CHD-C1D	4.06	1.46	1.38
31	1	316	A86	C7-C6	4.06	1.59	1.50
19	B	805	CLA	O2A-CGA	4.05	1.45	1.33
19	A	803	CLA	CHD-C1D	4.05	1.46	1.38
19	A	812	CLA	O2A-CGA	4.05	1.45	1.33
31	5	217	A86	C7-C6	4.05	1.59	1.50
31	2	219	A86	C21-C20	4.05	1.58	1.51
31	4	316	A86	C9-C10	4.05	1.56	1.43
30	3	205	KC1	C4D-ND	4.04	1.38	1.35
19	2	212	CLA	CHD-C1D	4.04	1.46	1.38
19	A	832	CLA	CHD-C1D	4.04	1.46	1.38
19	A	810	CLA	CHD-C1D	4.04	1.46	1.38
19	5	212	CLA	CHD-C4C	4.04	1.48	1.39
19	A	841	CLA	CHD-C1D	4.04	1.46	1.38
19	4	310	CLA	CHD-C4C	4.04	1.48	1.39
19	A	880	CLA	CHD-C1D	4.03	1.46	1.38
19	B	827	CLA	O2A-CGA	4.03	1.45	1.33
31	2	218	A86	C21-C20	4.03	1.58	1.51
19	A	822	CLA	CHD-C4C	4.03	1.48	1.39
19	4	306	CLA	CHD-C4C	4.03	1.48	1.39
31	4	316	A86	C21-C20	4.02	1.58	1.51
19	B	807	CLA	CHD-C1D	4.02	1.46	1.38
19	5	213	CLA	CHD-C4C	4.02	1.48	1.39
19	4	305	CLA	CHD-C4C	4.02	1.48	1.39
19	A	808	CLA	CHD-C1D	4.02	1.46	1.38
19	B	818	CLA	CHD-C4C	4.02	1.48	1.39
19	A	842	CLA	CHD-C1D	4.02	1.46	1.38
31	4	315	A86	O4-C38	4.02	1.44	1.35
19	B	837	CLA	CHD-C1D	4.02	1.46	1.38
19	B	846	CLA	CHD-C1D	4.02	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	J	103	CLA	CHD-C1D	4.02	1.46	1.38
19	A	828	CLA	O2A-CGA	4.01	1.45	1.33
19	B	833	CLA	CHD-C1D	4.01	1.46	1.38
19	5	216	CLA	CHD-C4C	4.01	1.48	1.39
19	B	824	CLA	CHD-C1D	4.01	1.46	1.38
19	B	805	CLA	CHD-C4C	4.01	1.48	1.39
19	B	814	CLA	CHD-C1D	4.01	1.46	1.38
19	A	814	CLA	O2A-CGA	4.01	1.45	1.33
19	A	832	CLA	O2A-CGA	4.01	1.45	1.33
19	A	807	CLA	CHD-C4C	4.01	1.48	1.39
19	5	207	CLA	CHD-C4C	4.01	1.48	1.39
19	B	811	CLA	CHD-C4C	4.01	1.48	1.39
19	4	308	CLA	CHD-C4C	4.01	1.48	1.39
19	B	802	CLA	O2A-CGA	4.00	1.45	1.33
19	A	830	CLA	CHD-C1D	4.00	1.46	1.38
19	A	878	CLA	CHD-C1D	4.00	1.46	1.38
19	1	308	CLA	CHD-C4C	4.00	1.48	1.39
19	5	209	CLA	CHD-C4C	4.00	1.48	1.39
19	B	819	CLA	CHD-C4C	4.00	1.48	1.39
19	2	206	CLA	O2A-CGA	4.00	1.45	1.33
19	B	816	CLA	CHD-C4C	4.00	1.48	1.39
19	1	309	CLA	CHD-C4C	4.00	1.48	1.39
19	B	834	CLA	O2A-CGA	3.99	1.45	1.33
19	B	832	CLA	CHD-C4C	3.99	1.48	1.39
19	2	208	CLA	CHD-C4C	3.99	1.48	1.39
19	2	213	CLA	CHD-C1D	3.99	1.46	1.38
19	A	810	CLA	O2A-CGA	3.99	1.45	1.33
19	B	818	CLA	O2A-CGA	3.98	1.45	1.33
19	A	821	CLA	CHD-C1D	3.98	1.46	1.38
19	4	311	CLA	C3D-C2D	3.98	1.50	1.39
19	B	845	CLA	CHD-C1D	3.98	1.46	1.38
19	A	814	CLA	CHD-C4C	3.98	1.48	1.39
19	A	834	CLA	O2A-CGA	3.98	1.45	1.33
19	B	807	CLA	CHD-C4C	3.98	1.48	1.39
31	3	214	A86	C10-C11	3.98	1.46	1.34
31	4	316	A86	C5-C6	3.97	1.41	1.35
31	2	216	A86	C5-C6	3.97	1.41	1.35
19	B	825	CLA	CHD-C1D	3.97	1.46	1.38
19	A	816	CLA	CHD-C4C	3.96	1.48	1.39
19	5	211	CLA	O2A-CGA	3.96	1.44	1.33
19	A	825	CLA	CHD-C4C	3.96	1.48	1.39
19	3	202	CLA	CHD-C4C	3.96	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	841	CLA	O2A-CGA	3.96	1.44	1.33
19	2	210	CLA	CHD-C4C	3.96	1.48	1.39
19	5	215	CLA	CHD-C4C	3.96	1.48	1.39
19	A	833	CLA	CHD-C4C	3.96	1.48	1.39
31	3	212	A86	C21-C20	3.95	1.58	1.51
19	4	301	CLA	CHD-C4C	3.95	1.48	1.39
19	3	202	CLA	O2A-CGA	3.95	1.44	1.33
19	2	215	CLA	CHD-C4C	3.95	1.48	1.39
19	2	215	CLA	C3D-C2D	3.95	1.49	1.39
19	3	207	CLA	CHD-C4C	3.95	1.48	1.39
19	2	205	CLA	CHD-C4C	3.95	1.48	1.39
19	5	213	CLA	C3D-C2D	3.95	1.49	1.39
19	B	820	CLA	CHD-C4C	3.94	1.48	1.39
19	B	810	CLA	CHD-C1D	3.94	1.46	1.38
19	A	802	CLA	CHD-C4C	3.94	1.48	1.39
31	2	219	A86	C10-C11	3.94	1.46	1.34
19	B	838	CLA	C3D-C2D	3.94	1.49	1.39
19	B	836	CLA	CHD-C4C	3.94	1.48	1.39
31	4	314	A86	C9-C10	3.94	1.55	1.43
31	5	221	A86	C10-C11	3.94	1.46	1.34
19	B	802	CLA	CHD-C1D	3.94	1.46	1.38
19	A	819	CLA	CHD-C4C	3.94	1.48	1.39
31	5	220	A86	C21-C20	3.93	1.58	1.51
19	4	312	CLA	CHD-C4C	3.93	1.48	1.39
31	3	228	A86	C5-C6	3.93	1.41	1.35
31	3	212	A86	C17-C18	-3.92	1.46	1.52
31	3	214	A86	C21-C20	3.92	1.58	1.51
19	3	209	CLA	CHD-C4C	3.92	1.48	1.39
19	A	817	CLA	C3D-C2D	3.92	1.49	1.39
19	B	829	CLA	CHD-C1D	3.92	1.46	1.38
19	2	207	CLA	CHD-C4C	3.91	1.48	1.39
19	A	839	CLA	CHD-C4C	3.91	1.48	1.39
30	4	302	KC1	C4D-ND	3.91	1.38	1.35
19	B	835	CLA	CHD-C4C	3.91	1.48	1.39
19	u	202	CLA	CHD-C4C	3.91	1.48	1.39
19	A	806	CLA	CHD-C4C	3.91	1.48	1.39
19	A	804	CLA	CHD-C1D	3.90	1.46	1.38
19	A	820	CLA	CHD-C4C	3.90	1.48	1.39
19	A	830	CLA	O2A-CGA	3.90	1.44	1.33
19	A	815	CLA	CHD-C4C	3.90	1.48	1.39
19	2	205	CLA	C3D-C2D	3.90	1.49	1.39
19	B	838	CLA	CHD-C4C	3.90	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	823	CLA	CHD-C4C	3.90	1.48	1.39
19	B	821	CLA	CHD-C4C	3.90	1.48	1.39
19	B	834	CLA	CHD-C4C	3.89	1.48	1.39
19	3	202	CLA	C3D-C2D	3.89	1.49	1.39
30	4	307	KC1	C4D-ND	3.89	1.38	1.35
19	2	206	CLA	CHD-C4C	3.89	1.48	1.39
19	A	831	CLA	C3D-C2D	3.88	1.49	1.39
19	A	838	CLA	CHD-C4C	3.88	1.48	1.39
19	A	803	CLA	CHD-C4C	3.88	1.48	1.39
19	2	214	CLA	C3D-C2D	3.88	1.49	1.39
19	A	840	CLA	CHD-C4C	3.88	1.48	1.39
18	A	801	CL0	C3D-C2D	3.88	1.49	1.39
19	5	210	CLA	CHD-C4C	3.87	1.48	1.39
19	A	807	CLA	C3D-C2D	3.87	1.49	1.39
19	B	803	CLA	O2A-CGA	3.87	1.44	1.33
19	A	818	CLA	CHD-C4C	3.87	1.48	1.39
19	L	204	CLA	CHD-C4C	3.87	1.48	1.39
19	A	826	CLA	CHD-C1D	3.87	1.45	1.38
19	B	806	CLA	CHD-C4C	3.87	1.48	1.39
19	B	821	CLA	CHD-C1D	3.87	1.45	1.38
19	4	313	CLA	C3D-C2D	3.87	1.49	1.39
31	4	314	A86	C21-C20	3.86	1.57	1.51
19	L	206	CLA	C3D-C2D	3.86	1.49	1.39
19	A	810	CLA	CHD-C4C	3.86	1.48	1.39
19	A	832	CLA	CHD-C4C	3.86	1.48	1.39
19	1	303	CLA	CHD-C4C	3.85	1.48	1.39
19	B	815	CLA	CHD-C4C	3.85	1.48	1.39
30	3	208	KC1	C4D-ND	3.85	1.38	1.35
19	A	813	CLA	CHD-C4C	3.85	1.48	1.39
19	A	824	CLA	C3D-C2D	3.84	1.49	1.39
19	A	836	CLA	C3D-C2D	3.84	1.49	1.39
19	A	837	CLA	C3D-C2D	3.84	1.49	1.39
19	A	880	CLA	CHD-C4C	3.84	1.48	1.39
19	B	812	CLA	CHD-C4C	3.84	1.48	1.39
19	u	201	CLA	CHD-C4C	3.84	1.48	1.39
19	1	301	CLA	CHD-C4C	3.84	1.48	1.39
31	3	212	A86	C10-C11	3.84	1.45	1.34
19	2	209	CLA	CHD-C4C	3.84	1.48	1.39
19	5	215	CLA	C3D-C2D	3.84	1.49	1.39
19	A	830	CLA	C3D-C2D	3.84	1.49	1.39
19	B	817	CLA	CHD-C4C	3.84	1.48	1.39
19	B	812	CLA	C3D-C2D	3.84	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	802	CLA	C3D-C2D	3.83	1.49	1.39
19	5	212	CLA	C3D-C2D	3.83	1.49	1.39
19	B	826	CLA	CHD-C4C	3.83	1.48	1.39
19	4	309	CLA	C3D-C2D	3.83	1.49	1.39
19	A	831	CLA	CHD-C4C	3.83	1.48	1.39
19	B	830	CLA	C3D-C2D	3.83	1.49	1.39
19	B	803	CLA	CHD-C4C	3.83	1.48	1.39
30	3	205	KC1	CHC-C1C	3.83	1.48	1.39
19	1	304	CLA	CHD-C4C	3.83	1.48	1.39
19	B	822	CLA	CHD-C4C	3.82	1.48	1.39
19	L	203	CLA	CHD-C4C	3.82	1.48	1.39
19	A	811	CLA	C3D-C2D	3.82	1.49	1.39
19	A	823	CLA	CHD-C4C	3.82	1.48	1.39
19	A	805	CLA	CHD-C4C	3.82	1.47	1.39
19	F	203	CLA	CHD-C4C	3.81	1.47	1.39
19	5	208	CLA	C3D-C2D	3.81	1.49	1.39
19	A	804	CLA	CHD-C4C	3.81	1.47	1.39
31	5	220	A86	C9-C10	3.81	1.55	1.43
19	B	818	CLA	C3D-C2D	3.81	1.49	1.39
19	B	827	CLA	CHD-C4C	3.81	1.47	1.39
19	B	809	CLA	C3D-C2D	3.81	1.49	1.39
27	J	105	5X6	C23-C22	3.81	1.54	1.45
19	B	832	CLA	C3D-C2D	3.81	1.49	1.39
19	A	827	CLA	CHD-C4C	3.81	1.47	1.39
19	A	841	CLA	C3D-C2D	3.81	1.49	1.39
19	B	804	CLA	CHD-C4C	3.80	1.47	1.39
19	B	828	CLA	CHD-C4C	3.80	1.47	1.39
19	A	817	CLA	CHD-C4C	3.80	1.47	1.39
31	5	220	A86	C10-C11	3.80	1.45	1.34
19	2	206	CLA	C3D-C2D	3.80	1.49	1.39
19	A	820	CLA	C3D-C2D	3.80	1.49	1.39
19	A	822	CLA	C3D-C2D	3.80	1.49	1.39
19	B	834	CLA	C3D-C2D	3.80	1.49	1.39
19	B	846	CLA	CHD-C4C	3.80	1.47	1.39
31	3	228	A86	C21-C20	3.80	1.57	1.51
19	3	210	CLA	C3D-C2D	3.80	1.49	1.39
19	A	823	CLA	C3D-C2D	3.80	1.49	1.39
19	A	824	CLA	CHD-C4C	3.80	1.47	1.39
19	A	805	CLA	C3D-C2D	3.80	1.49	1.39
19	A	815	CLA	C3D-C2D	3.79	1.49	1.39
19	2	209	CLA	C3D-C2D	3.79	1.49	1.39
19	A	834	CLA	CHD-C4C	3.79	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	808	CLA	CHD-C1D	3.79	1.45	1.38
19	A	821	CLA	C3D-C2D	3.79	1.49	1.39
31	2	216	A86	C10-C11	3.79	1.45	1.34
19	B	835	CLA	C3D-C2D	3.79	1.49	1.39
19	A	829	CLA	CHD-C4C	3.79	1.47	1.39
19	A	825	CLA	C3D-C2D	3.78	1.49	1.39
19	A	803	CLA	C3D-C2D	3.78	1.49	1.39
19	2	213	CLA	C3D-C2D	3.78	1.49	1.39
19	B	823	CLA	CHD-C1D	3.78	1.45	1.38
19	4	304	CLA	CHD-C4C	3.78	1.47	1.39
19	B	826	CLA	C3D-C2D	3.78	1.49	1.39
19	B	822	CLA	C3D-C2D	3.78	1.49	1.39
19	3	209	CLA	C3D-C2D	3.78	1.49	1.39
19	A	836	CLA	CHD-C4C	3.77	1.47	1.39
31	5	221	A86	C9-C10	3.77	1.55	1.43
19	2	213	CLA	CHD-C4C	3.77	1.47	1.39
31	1	316	A86	C9-C10	3.77	1.55	1.43
19	1	303	CLA	C3D-C2D	3.77	1.49	1.39
19	3	206	CLA	CHD-C4C	3.77	1.47	1.39
19	B	828	CLA	C3D-C2D	3.77	1.49	1.39
19	4	310	CLA	OBD-CAD	3.77	1.29	1.22
19	A	844	CLA	CHD-C4C	3.77	1.47	1.39
22	A	850	BCR	C1-C6	-3.77	1.48	1.53
19	A	878	CLA	C3D-C2D	3.77	1.49	1.39
19	1	304	CLA	C3D-C2D	3.77	1.49	1.39
19	1	310	CLA	C3D-C2D	3.76	1.49	1.39
19	A	811	CLA	CHD-C4C	3.76	1.47	1.39
31	5	217	A86	C10-C11	3.76	1.45	1.34
31	3	228	A86	C10-C11	3.76	1.45	1.34
30	2	211	KC1	CHC-C1C	3.76	1.47	1.39
19	B	829	CLA	CHD-C4C	3.76	1.47	1.39
19	A	828	CLA	CHD-C1D	3.76	1.45	1.38
19	B	816	CLA	C3D-C2D	3.76	1.49	1.39
19	A	808	CLA	CHD-C4C	3.76	1.47	1.39
19	J	103	CLA	CHD-C4C	3.75	1.47	1.39
19	4	305	CLA	C3D-C2D	3.75	1.49	1.39
19	L	203	CLA	CHD-C1D	3.75	1.45	1.38
19	B	813	CLA	C3D-C2D	3.75	1.49	1.39
19	B	825	CLA	CHD-C4C	3.75	1.47	1.39
19	A	840	CLA	C3D-C2D	3.75	1.49	1.39
19	2	208	CLA	C3D-C2D	3.75	1.49	1.39
19	F	204	CLA	C3D-C2D	3.75	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	316	A86	C21-C20	3.75	1.57	1.51
31	1	317	A86	C21-C20	3.75	1.57	1.51
19	u	202	CLA	C3D-C2D	3.75	1.49	1.39
19	5	216	CLA	OBD-CAD	3.75	1.28	1.22
30	1	305	KC1	CHC-C1C	3.75	1.47	1.39
19	3	203	CLA	CHD-C4C	3.75	1.47	1.39
19	5	214	CLA	C3D-C2D	3.75	1.49	1.39
19	A	809	CLA	CHD-C4C	3.75	1.47	1.39
19	2	212	CLA	CHD-C4C	3.75	1.47	1.39
19	4	308	CLA	OBD-CAD	3.75	1.28	1.22
19	A	816	CLA	C3D-C2D	3.75	1.49	1.39
19	B	824	CLA	CHD-C4C	3.75	1.47	1.39
19	2	208	CLA	OBD-CAD	3.74	1.28	1.22
19	5	216	CLA	C3D-C2D	3.74	1.49	1.39
19	A	809	CLA	C3D-C2D	3.74	1.49	1.39
19	B	814	CLA	CHD-C4C	3.74	1.47	1.39
31	2	218	A86	C10-C11	3.74	1.45	1.34
30	1	305	KC1	C1B-NB	-3.74	1.33	1.37
19	A	835	CLA	C3D-C2D	3.73	1.49	1.39
19	2	210	CLA	C3D-C2D	3.73	1.49	1.39
19	L	206	CLA	CHD-C4C	3.73	1.47	1.39
19	A	821	CLA	CHD-C4C	3.73	1.47	1.39
19	A	835	CLA	CHD-C4C	3.73	1.47	1.39
19	B	819	CLA	C3D-C2D	3.73	1.49	1.39
30	4	307	KC1	CHC-C1C	3.73	1.47	1.39
19	4	301	CLA	C3D-C2D	3.73	1.49	1.39
19	3	207	CLA	C3D-C2D	3.72	1.49	1.39
19	4	308	CLA	C3D-C2D	3.72	1.49	1.39
19	3	203	CLA	C3D-C2D	3.72	1.49	1.39
31	1	316	A86	C10-C11	3.72	1.45	1.34
19	5	207	CLA	C3D-C2D	3.72	1.49	1.39
19	B	809	CLA	CHD-C4C	3.72	1.47	1.39
19	B	817	CLA	C3D-C2D	3.72	1.49	1.39
19	A	844	CLA	C3D-C2D	3.72	1.49	1.39
19	A	823	CLA	OBD-CAD	3.71	1.28	1.22
19	2	213	CLA	OBD-CAD	3.71	1.28	1.22
18	A	801	CL0	CHD-C4C	3.71	1.47	1.39
31	2	216	A86	C9-C10	3.71	1.55	1.43
19	4	306	CLA	C3D-C2D	3.71	1.49	1.39
19	A	880	CLA	C3D-C2D	3.71	1.49	1.39
19	2	214	CLA	OBD-CAD	3.71	1.28	1.22
19	B	806	CLA	C3D-C2D	3.71	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	813	CLA	CHD-C4C	3.71	1.47	1.39
19	A	830	CLA	CHD-C4C	3.71	1.47	1.39
19	2	209	CLA	OBD-CAD	3.71	1.28	1.22
19	A	813	CLA	C3D-C2D	3.71	1.49	1.39
31	5	220	A86	C5-C6	3.71	1.40	1.35
19	4	304	CLA	OBD-CAD	3.70	1.28	1.22
19	5	209	CLA	C3D-C2D	3.70	1.49	1.39
30	4	302	KC1	CHC-C1C	3.70	1.47	1.39
30	3	208	KC1	CHC-C1C	3.70	1.47	1.39
19	B	804	CLA	C3D-C2D	3.70	1.49	1.39
19	1	308	CLA	C3D-C2D	3.70	1.49	1.39
19	B	814	CLA	C3D-C2D	3.70	1.49	1.39
19	A	838	CLA	C3D-C2D	3.69	1.49	1.39
19	B	811	CLA	C3D-C2D	3.69	1.49	1.39
28	2	217	DD6	C35-C34	3.69	1.58	1.52
30	3	205	KC1	C1A-CHA	3.69	1.50	1.40
19	A	812	CLA	C3D-C2D	3.69	1.49	1.39
19	B	837	CLA	C3D-C2D	3.69	1.49	1.39
19	3	204	CLA	C3D-C2D	3.68	1.49	1.39
19	A	819	CLA	C3D-C2D	3.68	1.49	1.39
19	5	213	CLA	OBD-CAD	3.68	1.28	1.22
31	5	219	A86	C21-C20	3.68	1.57	1.51
19	A	833	CLA	C3D-C2D	3.68	1.49	1.39
19	B	805	CLA	C3D-C2D	3.68	1.49	1.39
31	2	216	A86	C21-C20	3.68	1.57	1.51
19	B	845	CLA	C3D-C2D	3.68	1.49	1.39
19	A	827	CLA	C3D-C2D	3.68	1.49	1.39
19	A	808	CLA	C3D-C2D	3.68	1.49	1.39
31	2	218	A86	C9-C10	3.68	1.54	1.43
19	5	211	CLA	C3D-C2D	3.67	1.49	1.39
19	B	831	CLA	C3D-C2D	3.67	1.49	1.39
19	A	804	CLA	C3D-C2D	3.67	1.49	1.39
19	4	309	CLA	OBD-CAD	3.67	1.28	1.22
19	u	202	CLA	OBD-CAD	3.67	1.28	1.22
19	3	206	CLA	C3D-C2D	3.67	1.49	1.39
19	B	825	CLA	C3D-C2D	3.67	1.49	1.39
19	B	846	CLA	C3D-C2D	3.66	1.49	1.39
22	J	104	BCR	C1-C6	-3.66	1.48	1.53
19	B	815	CLA	C3D-C2D	3.66	1.49	1.39
19	B	820	CLA	C3D-C2D	3.66	1.49	1.39
19	4	310	CLA	C3D-C2D	3.66	1.49	1.39
31	5	217	A86	C21-C20	3.65	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	212	CLA	OBD-CAD	3.65	1.28	1.22
19	1	309	CLA	C3D-C2D	3.65	1.49	1.39
19	A	843	CLA	C3D-C2D	3.65	1.49	1.39
19	A	839	CLA	C3D-C2D	3.65	1.49	1.39
19	A	814	CLA	C3D-C2D	3.65	1.49	1.39
19	L	203	CLA	C3D-C2D	3.65	1.49	1.39
19	2	207	CLA	C3D-C2D	3.65	1.49	1.39
19	4	304	CLA	C3D-C2D	3.65	1.49	1.39
19	4	312	CLA	C3D-C2D	3.65	1.49	1.39
19	4	312	CLA	OBD-CAD	3.65	1.28	1.22
31	2	219	A86	C9-C10	3.65	1.54	1.43
19	5	210	CLA	C3D-C2D	3.65	1.49	1.39
19	1	309	CLA	OBD-CAD	3.65	1.28	1.22
31	3	214	A86	C9-C10	3.65	1.54	1.43
19	A	826	CLA	C3D-C2D	3.64	1.49	1.39
19	A	828	CLA	CHD-C4C	3.64	1.47	1.39
31	3	228	A86	C9-C10	3.64	1.54	1.43
19	A	809	CLA	OBD-CAD	3.64	1.28	1.22
31	1	317	A86	C10-C11	3.64	1.45	1.34
19	A	842	CLA	CHD-C4C	3.64	1.47	1.39
30	1	305	KC1	C4B-NB	-3.64	1.33	1.37
31	4	315	A86	C2-C1	3.64	1.40	1.35
19	A	878	CLA	CHD-C4C	3.64	1.47	1.39
19	B	802	CLA	OBD-CAD	3.63	1.28	1.22
19	B	810	CLA	CHD-C4C	3.63	1.47	1.39
27	J	105	5X6	C19-C18	3.63	1.54	1.43
19	B	845	CLA	CHD-C4C	3.63	1.47	1.39
19	F	203	CLA	C3D-C2D	3.63	1.49	1.39
31	1	317	A86	C9-C10	3.63	1.54	1.43
19	A	828	CLA	C3D-C2D	3.63	1.49	1.39
27	J	105	5X6	C33-C32	3.62	1.57	1.52
19	B	836	CLA	C3D-C2D	3.62	1.49	1.39
30	3	211	KC1	CHC-C1C	3.62	1.47	1.39
19	B	807	CLA	C3D-C2D	3.62	1.49	1.39
19	B	808	CLA	C3D-C2D	3.61	1.49	1.39
19	B	802	CLA	C3D-C2D	3.61	1.49	1.39
19	4	313	CLA	OBD-CAD	3.61	1.28	1.22
19	A	843	CLA	CHD-C4C	3.61	1.47	1.39
19	3	210	CLA	OBD-CAD	3.61	1.28	1.22
19	A	829	CLA	C3D-C2D	3.61	1.49	1.39
19	4	311	CLA	OBD-CAD	3.60	1.28	1.22
19	B	833	CLA	CHD-C4C	3.60	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	302	KC1	C1B-NB	-3.60	1.33	1.37
19	1	310	CLA	OBD-CAD	3.60	1.28	1.22
19	B	833	CLA	C3D-C2D	3.60	1.49	1.39
19	4	305	CLA	OBD-CAD	3.60	1.28	1.22
19	B	803	CLA	C3D-C2D	3.60	1.48	1.39
31	3	212	A86	C9-C10	3.60	1.54	1.43
19	4	303	CLA	C3D-C2D	3.60	1.48	1.39
19	3	207	CLA	OBD-CAD	3.59	1.28	1.22
31	4	316	A86	C17-C18	-3.59	1.47	1.52
19	J	103	CLA	OBD-CAD	3.59	1.28	1.22
19	L	206	CLA	OBD-CAD	3.59	1.28	1.22
19	J	103	CLA	C3D-C2D	3.59	1.48	1.39
30	2	211	KC1	C1A-CHA	3.58	1.50	1.40
19	1	307	CLA	OBD-CAD	3.58	1.28	1.22
19	L	204	CLA	C3D-C2D	3.58	1.48	1.39
28	1	315	DD6	C35-C34	3.58	1.58	1.52
19	2	212	CLA	C3D-C2D	3.58	1.48	1.39
19	B	825	CLA	OBD-CAD	3.58	1.28	1.22
19	4	301	CLA	OBD-CAD	3.58	1.28	1.22
19	B	821	CLA	C3D-C2D	3.58	1.48	1.39
19	A	818	CLA	OBD-CAD	3.58	1.28	1.22
19	2	210	CLA	OBD-CAD	3.58	1.28	1.22
31	1	317	A86	C2-C1	3.58	1.40	1.35
19	B	837	CLA	CHD-C4C	3.58	1.47	1.39
19	2	207	CLA	OBD-CAD	3.57	1.28	1.22
19	A	840	CLA	OBD-CAD	3.57	1.28	1.22
30	3	205	KC1	C1B-NB	-3.56	1.33	1.37
31	1	317	A86	C19-C18	3.56	1.57	1.52
22	B	840	BCR	C1-C6	-3.55	1.48	1.53
31	4	314	A86	C5-C6	3.55	1.40	1.35
19	2	215	CLA	OBD-CAD	3.55	1.28	1.22
19	1	301	CLA	C3D-C2D	3.55	1.48	1.39
27	J	105	5X6	C16-C17	3.55	1.53	1.45
19	A	818	CLA	C3D-C2D	3.55	1.48	1.39
19	A	806	CLA	C3D-C2D	3.55	1.48	1.39
19	A	832	CLA	C3D-C2D	3.54	1.48	1.39
19	B	824	CLA	C3D-C2D	3.54	1.48	1.39
19	B	808	CLA	CHD-C4C	3.54	1.47	1.39
31	4	315	A86	C10-C11	3.54	1.44	1.34
31	5	219	A86	C10-C11	3.54	1.44	1.34
19	A	811	CLA	OBD-CAD	3.54	1.28	1.22
19	5	214	CLA	OBD-CAD	3.54	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	833	CLA	OBD-CAD	3.54	1.28	1.22
19	B	812	CLA	OBD-CAD	3.53	1.28	1.22
19	B	828	CLA	OBD-CAD	3.53	1.28	1.22
30	3	211	KC1	C1A-CHA	3.53	1.50	1.40
19	2	206	CLA	OBD-CAD	3.53	1.28	1.22
19	3	209	CLA	OBD-CAD	3.53	1.28	1.22
30	3	208	KC1	C1B-NB	-3.52	1.33	1.37
19	B	810	CLA	C3D-C2D	3.52	1.48	1.39
31	3	214	A86	C19-C18	3.52	1.57	1.52
19	5	215	CLA	OBD-CAD	3.52	1.28	1.22
19	B	819	CLA	OBD-CAD	3.52	1.28	1.22
19	A	826	CLA	CHD-C4C	3.51	1.47	1.39
30	4	302	KC1	C1A-CHA	3.51	1.50	1.40
19	A	810	CLA	C3D-C2D	3.51	1.48	1.39
19	B	829	CLA	C3D-C2D	3.51	1.48	1.39
19	B	802	CLA	CHD-C4C	3.50	1.47	1.39
19	B	816	CLA	OBD-CAD	3.50	1.28	1.22
19	B	832	CLA	OBD-CAD	3.50	1.28	1.22
19	1	306	CLA	C3D-C2D	3.50	1.48	1.39
30	2	211	KC1	C1B-NB	-3.50	1.33	1.37
19	5	209	CLA	OBD-CAD	3.50	1.28	1.22
19	A	819	CLA	OBD-CAD	3.50	1.28	1.22
19	B	822	CLA	OBD-CAD	3.50	1.28	1.22
19	A	841	CLA	OBD-CAD	3.50	1.28	1.22
19	B	823	CLA	C3D-C2D	3.49	1.48	1.39
19	5	212	CLA	OBD-CAD	3.49	1.28	1.22
27	J	105	5X6	C24-C25	3.49	1.54	1.43
30	3	211	KC1	C1B-NB	-3.49	1.33	1.37
19	A	817	CLA	OBD-CAD	3.49	1.28	1.22
19	1	307	CLA	C3D-C2D	3.49	1.48	1.39
19	u	201	CLA	C3D-C2D	3.48	1.48	1.39
19	A	842	CLA	C3D-C2D	3.48	1.48	1.39
31	2	216	A86	C19-C18	3.48	1.57	1.52
31	5	217	A86	C9-C10	3.48	1.54	1.43
30	4	302	KC1	C4B-NB	-3.48	1.33	1.37
30	4	307	KC1	C1B-NB	-3.47	1.33	1.37
31	2	216	A86	C17-C18	-3.47	1.47	1.52
31	3	214	A86	C7-C6	3.47	1.58	1.50
19	F	203	CLA	OBD-CAD	3.47	1.28	1.22
19	4	303	CLA	OBD-CAD	3.47	1.28	1.22
19	5	210	CLA	OBD-CAD	3.47	1.28	1.22
19	A	844	CLA	OBD-CAD	3.47	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	834	CLA	C3D-C2D	3.47	1.48	1.39
19	B	845	CLA	OBD-CAD	3.46	1.28	1.22
19	L	203	CLA	OBD-CAD	3.46	1.28	1.22
19	L	204	CLA	OBD-CAD	3.45	1.28	1.22
31	3	212	A86	C2-C1	3.45	1.40	1.35
27	J	105	5X6	C15-C14	3.45	1.54	1.43
19	A	813	CLA	OBD-CAD	3.45	1.28	1.22
19	B	813	CLA	OBD-CAD	3.45	1.28	1.22
19	5	211	CLA	OBD-CAD	3.45	1.28	1.22
19	B	827	CLA	C3D-C2D	3.45	1.48	1.39
19	3	202	CLA	OBD-CAD	3.44	1.28	1.22
19	A	815	CLA	OBD-CAD	3.44	1.28	1.22
31	5	220	A86	C25-C24	3.44	1.43	1.34
19	A	842	CLA	OBD-CAD	3.44	1.28	1.22
19	1	303	CLA	OBD-CAD	3.44	1.28	1.22
19	A	808	CLA	OBD-CAD	3.44	1.28	1.22
19	A	835	CLA	OBD-CAD	3.44	1.28	1.22
31	5	219	A86	C9-C10	3.44	1.54	1.43
31	5	219	A86	C5-C6	3.44	1.40	1.35
22	A	847	BCR	C1-C6	-3.43	1.49	1.53
30	1	305	KC1	C4D-ND	3.43	1.38	1.35
19	A	810	CLA	OBD-CAD	3.43	1.28	1.22
22	M	102	BCR	C1-C6	-3.43	1.49	1.53
19	1	301	CLA	OBD-CAD	3.42	1.28	1.22
30	3	208	KC1	C1A-CHA	3.42	1.49	1.40
19	A	822	CLA	C1B-NB	-3.42	1.32	1.35
19	B	821	CLA	OBD-CAD	3.41	1.28	1.22
19	4	306	CLA	OBD-CAD	3.41	1.28	1.22
19	A	837	CLA	OBD-CAD	3.41	1.28	1.22
19	B	814	CLA	OBD-CAD	3.41	1.28	1.22
19	A	821	CLA	OBD-CAD	3.41	1.28	1.22
19	u	201	CLA	OBD-CAD	3.40	1.28	1.22
19	B	820	CLA	OBD-CAD	3.40	1.28	1.22
19	2	205	CLA	OBD-CAD	3.40	1.28	1.22
19	A	816	CLA	OBD-CAD	3.40	1.28	1.22
19	B	836	CLA	OBD-CAD	3.40	1.28	1.22
19	1	308	CLA	OBD-CAD	3.40	1.28	1.22
19	3	203	CLA	OBD-CAD	3.40	1.28	1.22
28	3	213	DD6	C-C1	3.39	1.57	1.50
22	1	311	BCR	C1-C6	-3.39	1.49	1.53
19	B	826	CLA	OBD-CAD	3.38	1.28	1.22
19	F	204	CLA	OBD-CAD	3.38	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	204	CLA	OBD-CAD	3.38	1.28	1.22
19	A	805	CLA	OBD-CAD	3.38	1.28	1.22
19	B	831	CLA	OBD-CAD	3.38	1.28	1.22
31	4	314	A86	C19-C18	3.38	1.57	1.52
28	1	315	DD6	C-C1	3.37	1.57	1.50
31	4	315	A86	C9-C10	3.37	1.53	1.43
19	B	837	CLA	OBD-CAD	3.37	1.28	1.22
31	2	219	A86	C5-C6	3.36	1.40	1.35
19	B	805	CLA	OBD-CAD	3.36	1.28	1.22
19	A	804	CLA	OBD-CAD	3.36	1.28	1.22
19	B	804	CLA	OBD-CAD	3.36	1.28	1.22
19	A	826	CLA	OBD-CAD	3.36	1.28	1.22
31	1	317	A86	C5-C6	3.35	1.40	1.35
19	A	836	CLA	OBD-CAD	3.35	1.28	1.22
28	L	209	DD6	C-C1	3.35	1.57	1.50
22	F	205	BCR	C30-C25	-3.35	1.49	1.53
19	A	820	CLA	OBD-CAD	3.35	1.28	1.22
31	5	217	A86	C5-C6	3.35	1.40	1.35
27	J	105	5X6	C20-C21	3.35	1.53	1.43
19	A	803	CLA	OBD-CAD	3.35	1.28	1.22
19	B	818	CLA	OBD-CAD	3.34	1.28	1.22
31	3	212	A86	C19-C18	3.34	1.57	1.52
19	A	812	CLA	OBD-CAD	3.34	1.28	1.22
19	1	306	CLA	OBD-CAD	3.34	1.28	1.22
19	B	838	CLA	OBD-CAD	3.34	1.28	1.22
19	B	830	CLA	OBD-CAD	3.33	1.28	1.22
22	L	205	BCR	C1-C6	-3.33	1.49	1.53
18	A	801	CL0	OBD-CAD	3.33	1.28	1.22
31	5	221	A86	C19-C18	3.32	1.57	1.52
19	3	206	CLA	OBD-CAD	3.31	1.28	1.22
19	A	824	CLA	OBD-CAD	3.30	1.28	1.22
28	2	217	DD6	C-C1	3.30	1.57	1.50
31	4	316	A86	C25-C24	3.29	1.43	1.34
31	2	218	A86	C5-C6	3.29	1.40	1.35
19	A	827	CLA	OBD-CAD	3.29	1.28	1.22
19	5	207	CLA	OBD-CAD	3.29	1.28	1.22
19	A	806	CLA	OBD-CAD	3.29	1.28	1.22
28	L	209	DD6	O2-C18	3.28	1.53	1.43
28	1	315	DD6	O2-C18	3.28	1.53	1.43
31	4	315	A86	C19-C18	3.27	1.57	1.52
19	B	835	CLA	OBD-CAD	3.27	1.28	1.22
28	5	218	DD6	O2-C18	3.27	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	825	CLA	OBD-CAD	3.27	1.28	1.22
31	5	219	A86	C19-C18	3.27	1.57	1.52
31	1	316	A86	C5-C6	3.27	1.40	1.35
19	5	208	CLA	OBD-CAD	3.27	1.28	1.22
19	B	846	CLA	OBD-CAD	3.27	1.28	1.22
19	B	817	CLA	OBD-CAD	3.26	1.28	1.22
30	1	305	KC1	C1A-CHA	3.26	1.49	1.40
22	B	841	BCR	C1-C6	-3.26	1.49	1.53
19	B	807	CLA	OBD-CAD	3.25	1.28	1.22
19	A	831	CLA	OBD-CAD	3.25	1.28	1.22
28	1	312	DD6	C35-C34	3.25	1.57	1.52
28	1	313	DD6	O2-C18	3.25	1.53	1.43
28	3	213	DD6	O2-C18	3.25	1.53	1.43
28	5	218	DD6	C-C1	3.24	1.57	1.50
19	A	880	CLA	OBD-CAD	3.24	1.28	1.22
31	5	220	A86	C19-C18	3.24	1.57	1.52
19	B	811	CLA	OBD-CAD	3.23	1.28	1.22
27	J	105	5X6	C05-C06	3.22	1.57	1.52
30	3	205	KC1	C4B-NB	-3.22	1.33	1.37
22	F	201	BCR	C30-C25	-3.22	1.49	1.53
31	3	212	A86	C5-C6	3.22	1.40	1.35
22	M	102	BCR	C30-C25	-3.22	1.49	1.53
19	B	827	CLA	OBD-CAD	3.22	1.28	1.22
19	A	814	CLA	OBD-CAD	3.22	1.28	1.22
22	A	848	BCR	C1-C6	-3.21	1.49	1.53
19	A	822	CLA	OBD-CAD	3.21	1.28	1.22
19	1	304	CLA	OBD-CAD	3.21	1.28	1.22
19	B	823	CLA	OBD-CAD	3.21	1.28	1.22
22	B	841	BCR	C30-C25	-3.21	1.49	1.53
19	B	808	CLA	OBD-CAD	3.19	1.28	1.22
19	A	807	CLA	OBD-CAD	3.19	1.28	1.22
19	B	809	CLA	OBD-CAD	3.19	1.28	1.22
30	2	211	KC1	C4B-NB	-3.19	1.33	1.37
22	A	849	BCR	C1-C6	-3.18	1.49	1.53
19	B	829	CLA	OBD-CAD	3.18	1.28	1.22
28	1	312	DD6	O2-C18	3.17	1.52	1.43
30	4	307	KC1	C4B-NB	-3.17	1.33	1.37
28	5	218	DD6	C9-C8	3.16	1.42	1.34
28	2	217	DD6	O2-C18	3.16	1.52	1.43
19	B	815	CLA	OBD-CAD	3.16	1.27	1.22
30	3	211	KC1	C4B-NB	-3.16	1.33	1.37
31	2	218	A86	C19-C18	3.16	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	228	A86	C17-C18	-3.15	1.47	1.52
22	B	843	BCR	C1-C6	-3.15	1.49	1.53
19	A	834	CLA	OBD-CAD	3.15	1.27	1.22
28	1	312	DD6	C9-C8	3.15	1.42	1.34
19	A	839	CLA	OBD-CAD	3.15	1.27	1.22
22	B	852	BCR	C1-C6	-3.14	1.49	1.53
19	A	843	CLA	OBD-CAD	3.13	1.27	1.22
31	1	316	A86	C25-C24	3.13	1.42	1.34
19	A	829	CLA	OBD-CAD	3.13	1.27	1.22
31	3	228	A86	C25-C24	3.12	1.42	1.34
31	5	219	A86	C25-C24	3.12	1.42	1.34
19	A	828	CLA	OBD-CAD	3.12	1.27	1.22
27	J	105	5X6	C28-C29	3.11	1.56	1.45
19	B	803	CLA	OBD-CAD	3.11	1.27	1.22
22	I	101	BCR	C1-C6	-3.11	1.49	1.53
30	3	208	KC1	C4B-NB	-3.11	1.34	1.37
22	1	314	BCR	C30-C25	-3.11	1.49	1.53
22	F	205	BCR	C1-C6	-3.10	1.49	1.53
31	5	217	A86	C19-C18	3.10	1.56	1.52
22	B	844	BCR	C1-C6	-3.09	1.49	1.53
28	1	312	DD6	C-C1	3.08	1.57	1.50
31	2	219	A86	C19-C18	3.07	1.56	1.52
22	A	849	BCR	C30-C25	-3.05	1.49	1.53
30	4	307	KC1	C1A-CHA	3.05	1.48	1.40
28	1	313	DD6	C26-C27	-3.04	1.30	1.37
19	A	830	CLA	OBD-CAD	3.04	1.27	1.22
19	A	832	CLA	OBD-CAD	3.04	1.27	1.22
31	4	315	A86	C5-C6	3.04	1.39	1.35
31	5	220	A86	C24-C1	3.04	1.52	1.45
28	3	213	DD6	C35-C34	3.03	1.57	1.52
31	2	219	A86	C25-C24	3.02	1.42	1.34
28	L	209	DD6	C9-C8	3.02	1.42	1.34
22	1	314	BCR	C1-C6	-3.02	1.49	1.53
28	1	312	DD6	C26-C27	-3.02	1.30	1.37
19	B	810	CLA	OBD-CAD	3.01	1.27	1.22
31	3	214	A86	C25-C24	3.01	1.42	1.34
19	A	838	CLA	OBD-CAD	3.01	1.27	1.22
19	B	833	CLA	OBD-CAD	3.01	1.27	1.22
22	B	840	BCR	C30-C25	-3.00	1.49	1.53
31	1	316	A86	C19-C18	3.00	1.56	1.52
22	L	202	BCR	C1-C6	-3.00	1.49	1.53
28	1	313	DD6	C35-C34	3.00	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	806	CLA	OBD-CAD	3.00	1.27	1.22
28	2	217	DD6	C26-C27	-3.00	1.30	1.37
28	1	313	DD6	C-C1	2.99	1.57	1.50
22	A	851	BCR	C1-C6	-2.99	1.49	1.53
19	B	834	CLA	OBD-CAD	2.96	1.27	1.22
30	3	205	KC1	C4A-C3A	2.96	1.50	1.44
31	3	214	A86	C5-C6	2.96	1.39	1.35
22	L	205	BCR	C30-C25	-2.96	1.49	1.53
31	4	314	A86	C25-C24	2.95	1.42	1.34
30	3	211	KC1	C4A-C3A	2.94	1.50	1.44
28	L	209	DD6	C26-C27	-2.93	1.30	1.37
22	B	844	BCR	C30-C25	-2.92	1.49	1.53
22	J	104	BCR	C30-C25	-2.91	1.49	1.53
22	A	847	BCR	C30-C25	-2.90	1.49	1.53
31	5	219	A86	O-C13	-2.90	1.17	1.23
31	2	218	A86	C25-C24	2.90	1.42	1.34
31	2	216	A86	C25-C24	2.89	1.42	1.34
28	1	315	DD6	C9-C8	2.89	1.42	1.34
28	2	217	DD6	C9-C8	2.88	1.42	1.34
22	1	311	BCR	C30-C25	-2.87	1.49	1.53
31	5	217	A86	C25-C24	2.86	1.42	1.34
22	L	202	BCR	C30-C25	-2.86	1.49	1.53
22	I	102	BCR	C1-C6	-2.85	1.49	1.53
28	5	218	DD6	C35-C34	2.85	1.57	1.52
19	A	803	CLA	C1B-NB	-2.84	1.32	1.35
31	4	316	A86	C24-C1	2.84	1.52	1.45
31	5	219	A86	C24-C1	2.84	1.52	1.45
31	4	315	A86	C25-C24	2.83	1.41	1.34
24	2	220	LMT	O3'-C3'	-2.83	1.36	1.43
30	1	305	KC1	C4A-C3A	2.82	1.50	1.44
31	3	228	A86	C14-C15	2.82	1.58	1.52
19	A	878	CLA	OBD-CAD	2.82	1.27	1.22
22	A	848	BCR	C30-C25	-2.82	1.49	1.53
28	3	213	DD6	C9-C8	2.81	1.41	1.34
31	5	221	A86	C25-C24	2.81	1.41	1.34
24	1	323	LMT	O2B-C2B	-2.81	1.36	1.43
31	1	317	A86	C25-C24	2.80	1.41	1.34
22	B	843	BCR	C30-C25	-2.80	1.49	1.53
31	2	216	A86	C14-C15	2.80	1.58	1.52
28	L	209	DD6	C35-C34	2.78	1.57	1.52
19	B	825	CLA	C1B-NB	-2.77	1.32	1.35
28	1	313	DD6	C9-C8	2.77	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	3	208	KC1	C4A-C3A	2.76	1.49	1.44
27	J	105	5X6	C11-C03	2.76	1.54	1.45
30	2	211	KC1	CHB-C4A	-2.75	1.32	1.39
19	A	802	CLA	OBD-CAD	2.74	1.27	1.22
24	1	323	LMT	O3'-C3'	-2.73	1.36	1.43
19	1	309	CLA	C4B-CHC	2.73	1.48	1.41
28	3	213	DD6	C26-C27	-2.73	1.31	1.37
31	4	316	A86	C-C1	2.72	1.56	1.50
31	5	220	A86	C-C1	2.72	1.56	1.50
31	2	218	A86	C-C1	2.72	1.56	1.50
31	1	316	A86	C-C1	2.72	1.56	1.50
19	2	208	CLA	C4C-C3C	2.71	1.49	1.45
31	1	316	A86	C24-C1	2.71	1.51	1.45
19	5	209	CLA	C3D-C4D	-2.71	1.38	1.44
19	B	813	CLA	C4C-C3C	2.70	1.49	1.45
28	1	315	DD6	C26-C27	-2.70	1.31	1.37
19	B	833	CLA	C3D-C4D	-2.70	1.38	1.44
22	F	201	BCR	C1-C6	-2.70	1.50	1.53
19	A	834	CLA	C3D-C4D	-2.70	1.38	1.44
19	B	824	CLA	OBD-CAD	2.69	1.27	1.22
31	2	219	A86	C-C1	2.69	1.56	1.50
18	A	801	CL0	C3D-C4D	-2.68	1.38	1.44
31	2	216	A86	C-C1	2.68	1.56	1.50
19	B	829	CLA	C3D-C4D	-2.67	1.38	1.44
30	4	307	KC1	C4A-C3A	2.67	1.49	1.44
19	A	820	CLA	C3D-C4D	-2.67	1.38	1.44
19	1	310	CLA	C4D-CHA	2.67	1.47	1.38
26	B	847	DGD	O2G-C2G	-2.67	1.39	1.46
28	5	218	DD6	C26-C27	-2.67	1.31	1.37
31	4	314	A86	C-C1	2.67	1.56	1.50
31	4	315	A86	O-C13	-2.66	1.17	1.23
24	A	854	LMT	O3'-C3'	-2.66	1.36	1.43
31	3	228	A86	C-C1	2.66	1.56	1.50
31	2	218	A86	C14-C15	2.66	1.57	1.52
19	B	836	CLA	C4C-C3C	2.65	1.49	1.45
19	B	814	CLA	C1B-NB	-2.65	1.32	1.35
31	3	212	A86	C25-C24	2.65	1.41	1.34
26	B	847	DGD	O1G-C1G	-2.65	1.39	1.45
30	3	211	KC1	CHB-C4A	-2.65	1.33	1.39
19	5	213	CLA	C4C-C3C	2.64	1.49	1.45
19	1	308	CLA	C4B-CHC	2.64	1.48	1.41
19	B	822	CLA	C4D-CHA	2.64	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	220	A86	O-C13	-2.64	1.17	1.23
22	A	850	BCR	C30-C25	-2.64	1.50	1.53
24	2	220	LMT	O3B-C3B	-2.63	1.36	1.43
19	4	305	CLA	C4D-CHA	2.63	1.47	1.38
31	1	317	A86	C-C1	2.63	1.56	1.50
19	B	808	CLA	C1B-NB	-2.62	1.32	1.35
19	B	829	CLA	C1C-C2C	2.62	1.49	1.44
19	B	812	CLA	C4D-CHA	2.62	1.47	1.38
31	5	219	A86	C-C1	2.62	1.56	1.50
31	5	221	A86	O-C13	-2.61	1.17	1.23
22	I	101	BCR	C30-C25	-2.61	1.50	1.53
31	1	316	A86	C14-C15	2.61	1.57	1.52
19	A	813	CLA	C4D-CHA	2.61	1.47	1.38
19	A	844	CLA	C1B-NB	-2.61	1.32	1.35
19	u	201	CLA	C4C-C3C	2.60	1.49	1.45
31	5	217	A86	O-C13	-2.60	1.17	1.23
19	4	304	CLA	C1C-C2C	2.60	1.49	1.44
19	4	309	CLA	C4C-C3C	2.60	1.49	1.45
19	B	817	CLA	C3D-C4D	-2.60	1.38	1.44
31	4	314	A86	O-C13	-2.60	1.17	1.23
31	4	315	A86	C-C1	2.60	1.56	1.50
19	B	832	CLA	C1B-NB	-2.60	1.32	1.35
19	A	835	CLA	C3D-C4D	-2.59	1.38	1.44
19	A	878	CLA	C1B-NB	-2.59	1.32	1.35
19	B	805	CLA	C3D-C4D	-2.59	1.38	1.44
19	2	214	CLA	C4D-CHA	2.59	1.47	1.38
31	3	228	A86	C24-C1	2.59	1.51	1.45
19	5	213	CLA	C4D-CHA	2.59	1.47	1.38
19	A	825	CLA	C3D-C4D	-2.59	1.38	1.44
19	B	828	CLA	C3D-C4D	-2.59	1.38	1.44
19	A	805	CLA	C4D-CHA	2.59	1.47	1.38
31	5	221	A86	C-C1	2.58	1.56	1.50
19	A	826	CLA	C4D-CHA	2.58	1.47	1.38
31	5	217	A86	C-C1	2.58	1.56	1.50
19	A	838	CLA	C4D-CHA	2.58	1.47	1.38
19	A	825	CLA	C4D-CHA	2.58	1.47	1.38
19	B	829	CLA	C4B-CHC	2.58	1.48	1.41
30	4	307	KC1	CHB-C4A	-2.58	1.33	1.39
19	B	820	CLA	C4D-CHA	2.58	1.47	1.38
19	B	809	CLA	C1B-NB	-2.58	1.32	1.35
19	u	202	CLA	C4B-CHC	2.57	1.48	1.41
19	A	822	CLA	C4D-CHA	2.57	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	826	CLA	C1B-CHB	2.57	1.48	1.41
31	2	219	A86	C14-C15	2.57	1.57	1.52
19	1	303	CLA	C4D-CHA	2.57	1.47	1.38
19	2	215	CLA	C4D-CHA	2.56	1.47	1.38
19	A	832	CLA	C3D-C4D	-2.56	1.38	1.44
19	B	827	CLA	C4D-CHA	2.56	1.47	1.38
19	L	203	CLA	C3D-C4D	-2.56	1.38	1.44
19	4	308	CLA	C1C-C2C	2.56	1.49	1.44
19	A	807	CLA	C3D-C4D	-2.56	1.38	1.44
30	3	205	KC1	CHB-C4A	-2.56	1.33	1.39
19	4	309	CLA	C4D-CHA	2.56	1.47	1.38
19	A	835	CLA	C4C-C3C	2.56	1.49	1.45
19	2	213	CLA	C4D-CHA	2.56	1.47	1.38
19	B	833	CLA	C4D-CHA	2.55	1.47	1.38
19	5	208	CLA	C3D-C4D	-2.55	1.38	1.44
19	A	815	CLA	C4D-CHA	2.55	1.47	1.38
19	A	822	CLA	C3D-C4D	-2.55	1.38	1.44
19	B	845	CLA	C4B-CHC	2.55	1.48	1.41
31	1	316	A86	O-C13	-2.55	1.17	1.23
19	A	802	CLA	C3D-C4D	-2.55	1.38	1.44
19	A	804	CLA	C3D-C4D	-2.55	1.38	1.44
19	5	216	CLA	C4D-CHA	2.55	1.47	1.38
19	B	813	CLA	C4D-CHA	2.54	1.47	1.38
19	1	307	CLA	C4D-CHA	2.54	1.47	1.38
19	5	212	CLA	C4D-CHA	2.54	1.47	1.38
19	B	809	CLA	C4D-CHA	2.54	1.47	1.38
24	3	216	LMT	O3'-C3'	-2.54	1.37	1.43
19	A	803	CLA	C4D-CHA	2.54	1.47	1.38
19	A	833	CLA	C4D-CHA	2.54	1.47	1.38
31	3	214	A86	C24-C1	2.54	1.51	1.45
19	B	825	CLA	C4D-CHA	2.54	1.47	1.38
19	B	834	CLA	C4D-CHA	2.54	1.47	1.38
19	2	208	CLA	C4D-CHA	2.54	1.47	1.38
19	u	201	CLA	C3D-C4D	-2.54	1.38	1.44
19	A	836	CLA	C4D-CHA	2.53	1.47	1.38
19	A	809	CLA	C1B-NB	-2.53	1.32	1.35
19	A	823	CLA	C4D-CHA	2.53	1.47	1.38
31	3	212	A86	C-C1	2.53	1.56	1.50
19	A	820	CLA	C4D-CHA	2.53	1.47	1.38
19	F	203	CLA	C4D-CHA	2.53	1.47	1.38
19	u	202	CLA	C1C-C2C	2.53	1.49	1.44
19	A	809	CLA	C4D-CHA	2.53	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	209	CLA	C4C-C3C	2.53	1.49	1.45
19	A	811	CLA	C4D-CHA	2.53	1.47	1.38
19	B	829	CLA	C4D-CHA	2.53	1.47	1.38
19	3	204	CLA	C4D-CHA	2.53	1.47	1.38
24	1	323	LMT	O1'-C1'	-2.53	1.35	1.40
19	B	821	CLA	C3D-C4D	-2.52	1.38	1.44
19	2	206	CLA	C3D-C4D	-2.52	1.38	1.44
19	B	828	CLA	C4D-CHA	2.52	1.47	1.38
19	A	812	CLA	C4D-CHA	2.52	1.47	1.38
31	2	216	A86	O-C13	-2.52	1.18	1.23
19	3	203	CLA	C1B-NB	-2.52	1.33	1.35
19	A	843	CLA	C1B-NB	-2.52	1.33	1.35
19	B	806	CLA	C3D-C4D	-2.52	1.38	1.44
19	B	836	CLA	C4D-CHA	2.52	1.47	1.38
19	1	301	CLA	C4D-CHA	2.51	1.47	1.38
19	F	204	CLA	C4D-CHA	2.51	1.47	1.38
19	B	804	CLA	C4D-CHA	2.51	1.47	1.38
19	4	313	CLA	C4D-CHA	2.51	1.47	1.38
19	A	838	CLA	C3D-C4D	-2.51	1.38	1.44
19	A	824	CLA	C4D-CHA	2.51	1.47	1.38
19	5	216	CLA	C4C-C3C	2.51	1.49	1.45
19	B	838	CLA	C4D-CHA	2.51	1.47	1.38
19	B	835	CLA	C4D-CHA	2.51	1.47	1.38
28	L	209	DD6	C4-C5	2.51	1.51	1.43
19	A	807	CLA	C4D-CHA	2.51	1.47	1.38
19	2	205	CLA	C3D-C4D	-2.51	1.38	1.44
19	A	841	CLA	C3D-C4D	-2.51	1.38	1.44
19	B	834	CLA	C3D-C4D	-2.51	1.38	1.44
19	A	819	CLA	C4B-CHC	2.51	1.48	1.41
19	4	311	CLA	C4B-CHC	2.51	1.48	1.41
19	A	878	CLA	C1C-C2C	2.50	1.49	1.44
19	3	206	CLA	C4D-CHA	2.50	1.47	1.38
19	2	212	CLA	C4D-CHA	2.50	1.47	1.38
19	5	212	CLA	C3D-C4D	-2.50	1.38	1.44
31	3	228	A86	O-C13	-2.50	1.18	1.23
19	A	835	CLA	C4D-CHA	2.50	1.47	1.38
19	A	814	CLA	C3D-C4D	-2.50	1.38	1.44
19	B	815	CLA	C4D-CHA	2.50	1.47	1.38
19	A	841	CLA	C4B-CHC	2.50	1.47	1.41
19	A	831	CLA	C4D-CHA	2.50	1.47	1.38
19	5	207	CLA	C4D-CHA	2.50	1.47	1.38
31	4	316	A86	O-C13	-2.50	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	218	A86	C24-C1	2.50	1.51	1.45
19	A	841	CLA	C4D-CHA	2.50	1.47	1.38
19	A	816	CLA	C3D-C4D	-2.50	1.38	1.44
19	B	824	CLA	C4D-CHA	2.50	1.47	1.38
19	A	827	CLA	C3D-C4D	-2.50	1.38	1.44
19	A	843	CLA	C3D-C4D	-2.50	1.38	1.44
19	5	215	CLA	C4D-CHA	2.50	1.47	1.38
19	A	843	CLA	C1B-CHB	2.49	1.47	1.41
19	A	837	CLA	C4D-CHA	2.49	1.47	1.38
19	A	813	CLA	C3D-C4D	-2.49	1.38	1.44
19	B	818	CLA	C4D-CHA	2.49	1.47	1.38
19	A	816	CLA	C4D-CHA	2.49	1.47	1.38
31	3	212	A86	O-C13	-2.49	1.18	1.23
31	3	212	A86	C14-C15	2.49	1.57	1.52
19	B	831	CLA	C3D-C4D	-2.49	1.38	1.44
19	1	304	CLA	C3D-C4D	-2.49	1.38	1.44
19	A	840	CLA	C1C-C2C	2.49	1.49	1.44
19	5	211	CLA	C4D-CHA	2.49	1.47	1.38
18	A	801	CL0	C4D-CHA	2.49	1.47	1.38
19	B	828	CLA	C1C-C2C	2.49	1.49	1.44
19	2	209	CLA	C4D-CHA	2.49	1.47	1.38
19	A	821	CLA	C1C-C2C	2.49	1.49	1.44
19	B	810	CLA	C3D-C4D	-2.49	1.38	1.44
19	B	846	CLA	C4D-CHA	2.49	1.47	1.38
19	4	304	CLA	C4D-CHA	2.49	1.47	1.38
30	2	211	KC1	C1C-C2C	2.49	1.49	1.44
19	B	830	CLA	C4D-CHA	2.49	1.47	1.38
19	3	202	CLA	C1C-C2C	2.49	1.49	1.44
19	1	308	CLA	C4D-CHA	2.48	1.47	1.38
19	4	311	CLA	C4D-CHA	2.48	1.47	1.38
19	B	813	CLA	C3D-C4D	-2.48	1.38	1.44
19	B	827	CLA	C1C-C2C	2.48	1.49	1.44
19	B	827	CLA	C3D-C4D	-2.48	1.38	1.44
28	5	218	DD6	C4-C5	2.48	1.51	1.43
19	3	209	CLA	C4D-CHA	2.48	1.47	1.38
24	3	216	LMT	O2B-C2B	-2.48	1.37	1.43
31	2	216	A86	C24-C1	2.48	1.51	1.45
19	u	201	CLA	C4D-CHA	2.48	1.47	1.38
19	3	202	CLA	C1B-NB	-2.48	1.33	1.35
19	L	204	CLA	C4D-CHA	2.48	1.47	1.38
19	A	810	CLA	C4D-CHA	2.48	1.47	1.38
19	B	808	CLA	C3D-C4D	-2.48	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	840	CLA	C3D-C4D	-2.48	1.38	1.44
19	B	824	CLA	C3D-C4D	-2.48	1.38	1.44
19	A	829	CLA	C3D-C4D	-2.48	1.38	1.44
30	1	305	KC1	CHB-C4A	-2.48	1.33	1.39
19	2	210	CLA	C4B-CHC	2.48	1.47	1.41
19	4	304	CLA	C4B-CHC	2.48	1.47	1.41
19	B	811	CLA	C3D-C4D	-2.48	1.38	1.44
19	2	215	CLA	C4B-CHC	2.48	1.47	1.41
19	A	818	CLA	C4D-CHA	2.47	1.47	1.38
19	4	310	CLA	C3D-C4D	-2.47	1.38	1.44
19	B	815	CLA	C3D-C4D	-2.47	1.38	1.44
19	A	819	CLA	C4D-CHA	2.47	1.47	1.38
19	u	202	CLA	C4D-CHA	2.47	1.47	1.38
30	4	302	KC1	C4A-C3A	2.47	1.49	1.44
19	4	306	CLA	C4D-CHA	2.47	1.47	1.38
19	J	103	CLA	C4B-CHC	2.47	1.47	1.41
19	3	202	CLA	C4D-CHA	2.47	1.47	1.38
19	3	207	CLA	C4D-CHA	2.47	1.47	1.38
28	1	312	DD6	C4-C5	2.47	1.51	1.43
19	3	206	CLA	C1C-C2C	2.47	1.49	1.44
19	A	809	CLA	C4B-NB	-2.47	1.33	1.35
31	1	317	A86	C14-C15	2.47	1.57	1.52
31	5	217	A86	C14-C15	2.47	1.57	1.52
19	A	806	CLA	C3D-C4D	-2.47	1.38	1.44
19	A	844	CLA	C4D-CHA	2.47	1.47	1.38
31	2	218	A86	O-C13	-2.47	1.18	1.23
30	2	211	KC1	C4A-C3A	2.47	1.49	1.44
19	3	202	CLA	C4B-CHC	2.47	1.47	1.41
24	1	323	LMT	O2'-C2'	-2.47	1.37	1.43
30	4	307	KC1	C4C-C3C	2.46	1.49	1.45
19	L	204	CLA	C3D-C4D	-2.46	1.38	1.44
19	2	212	CLA	C4B-CHC	2.46	1.47	1.41
19	A	840	CLA	C4D-CHA	2.46	1.47	1.38
19	2	210	CLA	C4D-CHA	2.46	1.47	1.38
19	5	211	CLA	C4C-C3C	2.46	1.49	1.45
19	1	308	CLA	C1C-C2C	2.46	1.49	1.44
19	4	305	CLA	C1B-NB	-2.46	1.33	1.35
19	B	806	CLA	C4D-CHA	2.46	1.47	1.38
19	B	832	CLA	C4B-CHC	2.46	1.47	1.41
19	A	808	CLA	C4D-CHA	2.46	1.47	1.38
19	A	802	CLA	C1B-NB	-2.46	1.33	1.35
19	A	821	CLA	C4D-CHA	2.46	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	207	CLA	C3D-C4D	-2.46	1.38	1.44
19	3	207	CLA	C4B-CHC	2.46	1.47	1.41
19	B	826	CLA	C3D-C4D	-2.46	1.38	1.44
19	2	213	CLA	C1C-C2C	2.46	1.49	1.44
19	5	208	CLA	C4D-CHA	2.46	1.47	1.38
19	1	309	CLA	C4D-CHA	2.46	1.47	1.38
19	A	830	CLA	C4D-CHA	2.46	1.47	1.38
30	4	302	KC1	CHB-C4A	-2.46	1.33	1.39
19	B	816	CLA	C4D-CHA	2.46	1.47	1.38
19	L	204	CLA	C1C-C2C	2.46	1.49	1.44
19	A	819	CLA	C4C-C3C	2.46	1.49	1.45
19	4	306	CLA	C4B-CHC	2.45	1.47	1.41
19	4	303	CLA	C4D-CHA	2.45	1.47	1.38
19	5	209	CLA	C4D-CHA	2.45	1.47	1.38
19	B	825	CLA	C1C-C2C	2.45	1.49	1.44
19	5	214	CLA	C4C-C3C	2.45	1.49	1.45
31	5	219	A86	C14-C15	2.45	1.57	1.52
19	A	808	CLA	C1C-C2C	2.45	1.49	1.44
19	4	301	CLA	C4D-CHA	2.45	1.47	1.38
19	J	103	CLA	C1C-C2C	2.45	1.49	1.44
19	B	837	CLA	C3D-C4D	-2.45	1.38	1.44
19	1	310	CLA	C3D-C4D	-2.45	1.38	1.44
19	2	214	CLA	C3D-C4D	-2.45	1.38	1.44
19	B	826	CLA	C1B-NB	-2.45	1.33	1.35
19	A	810	CLA	C3D-C4D	-2.45	1.38	1.44
19	1	309	CLA	C3D-C4D	-2.45	1.38	1.44
19	B	810	CLA	C1C-C2C	2.45	1.49	1.44
19	A	829	CLA	C4D-CHA	2.45	1.47	1.38
19	A	827	CLA	C1C-C2C	2.45	1.49	1.44
19	B	832	CLA	C4D-CHA	2.45	1.47	1.38
19	B	820	CLA	C3D-C4D	-2.45	1.38	1.44
19	1	310	CLA	C4C-C3C	2.44	1.49	1.45
30	3	208	KC1	CHB-C4A	-2.44	1.33	1.39
19	L	206	CLA	C3D-C4D	-2.44	1.38	1.44
19	B	823	CLA	C3D-C4D	-2.44	1.38	1.44
19	B	808	CLA	C4D-CHA	2.44	1.47	1.38
19	B	807	CLA	C4D-CHA	2.44	1.47	1.38
19	1	309	CLA	C1C-C2C	2.44	1.49	1.44
19	A	840	CLA	C4B-CHC	2.44	1.47	1.41
19	1	301	CLA	C3D-C4D	-2.44	1.38	1.44
19	F	203	CLA	C3D-C4D	-2.44	1.38	1.44
19	A	826	CLA	C3D-C4D	-2.44	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	851	BCR	C30-C25	-2.44	1.50	1.53
19	2	205	CLA	C4D-CHA	2.44	1.47	1.38
19	4	310	CLA	C4D-CHA	2.44	1.47	1.38
19	A	815	CLA	C3D-C4D	-2.44	1.38	1.44
19	4	312	CLA	C4C-C3C	2.44	1.49	1.45
19	5	214	CLA	C4D-CHA	2.44	1.47	1.38
19	B	819	CLA	C1B-NB	-2.43	1.33	1.35
19	2	215	CLA	C3D-C4D	-2.43	1.38	1.44
19	B	802	CLA	C4D-CHA	2.43	1.47	1.38
19	B	807	CLA	C3D-C4D	-2.43	1.38	1.44
19	B	805	CLA	C4D-CHA	2.43	1.47	1.38
19	2	207	CLA	C3D-C4D	-2.43	1.38	1.44
19	A	804	CLA	C4D-CHA	2.43	1.47	1.38
19	A	821	CLA	C4B-CHC	2.43	1.47	1.41
19	A	827	CLA	C4D-CHA	2.43	1.47	1.38
19	A	839	CLA	C4D-CHA	2.43	1.47	1.38
19	2	206	CLA	C4D-CHA	2.43	1.47	1.38
19	A	818	CLA	C3D-C4D	-2.43	1.38	1.44
19	B	817	CLA	C4B-CHC	2.43	1.47	1.41
19	B	835	CLA	C1B-NB	-2.43	1.33	1.35
19	B	837	CLA	C4B-CHC	2.43	1.47	1.41
19	A	808	CLA	C3D-C4D	-2.43	1.38	1.44
19	B	846	CLA	C3D-C4D	-2.43	1.38	1.44
24	A	854	LMT	O2B-C2B	-2.42	1.37	1.43
19	A	824	CLA	C4B-CHC	2.42	1.47	1.41
30	3	211	KC1	CAA-C2A	2.42	1.54	1.46
19	B	834	CLA	C4B-CHC	2.42	1.47	1.41
19	A	880	CLA	C4D-CHA	2.42	1.47	1.38
31	5	217	A86	C24-C1	2.42	1.51	1.45
19	A	843	CLA	C4B-CHC	2.42	1.47	1.41
19	5	210	CLA	C3D-C4D	-2.42	1.38	1.44
19	A	804	CLA	C4B-CHC	2.42	1.47	1.41
19	B	826	CLA	C4D-CHA	2.42	1.47	1.38
19	B	810	CLA	C4D-CHA	2.42	1.47	1.38
19	A	828	CLA	C4D-CHA	2.42	1.47	1.38
19	B	817	CLA	C4D-CHA	2.42	1.47	1.38
19	A	810	CLA	C1B-CHB	2.42	1.47	1.41
19	4	308	CLA	C4B-CHC	2.42	1.47	1.41
19	4	308	CLA	C4D-CHA	2.42	1.47	1.38
19	B	845	CLA	C1C-C2C	2.42	1.49	1.44
19	B	834	CLA	C1B-NB	-2.42	1.33	1.35
19	A	811	CLA	C3D-C4D	-2.42	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	305	CLA	C4C-C3C	2.42	1.49	1.45
19	A	832	CLA	C4D-CHA	2.42	1.47	1.38
19	A	811	CLA	C1C-C2C	2.42	1.49	1.44
19	A	839	CLA	C3D-C4D	-2.42	1.38	1.44
19	B	810	CLA	C4B-CHC	2.42	1.47	1.41
19	A	829	CLA	C1B-NB	-2.42	1.33	1.35
19	5	211	CLA	C3D-C4D	-2.42	1.38	1.44
19	4	311	CLA	C4C-C3C	2.42	1.49	1.45
19	A	805	CLA	C3D-C4D	-2.41	1.38	1.44
19	B	831	CLA	C4D-CHA	2.41	1.47	1.38
19	1	306	CLA	C4D-CHA	2.41	1.47	1.38
19	5	210	CLA	C4D-CHA	2.41	1.47	1.38
22	B	852	BCR	C30-C25	-2.41	1.50	1.53
19	A	843	CLA	C4D-CHA	2.41	1.47	1.38
19	4	312	CLA	C1C-C2C	2.41	1.49	1.44
19	B	824	CLA	C4B-CHC	2.41	1.47	1.41
19	A	878	CLA	C4D-CHA	2.41	1.47	1.38
19	4	310	CLA	C4B-CHC	2.41	1.47	1.41
31	1	317	A86	C24-C1	2.41	1.51	1.45
31	4	316	A86	C35-C34	2.41	1.56	1.51
19	F	204	CLA	C3D-C4D	-2.41	1.38	1.44
19	3	207	CLA	C3D-C4D	-2.41	1.38	1.44
19	L	206	CLA	C4D-CHA	2.41	1.47	1.38
19	F	203	CLA	C1B-CHB	2.41	1.47	1.41
19	A	824	CLA	C3D-C4D	-2.41	1.38	1.44
19	4	303	CLA	C1C-C2C	2.40	1.49	1.44
19	4	312	CLA	C4B-CHC	2.40	1.47	1.41
19	1	301	CLA	C1B-CHB	2.40	1.47	1.41
19	A	812	CLA	C3D-C4D	-2.40	1.38	1.44
19	B	827	CLA	C4C-C3C	2.40	1.49	1.45
19	B	837	CLA	C4D-CHA	2.40	1.46	1.38
19	B	809	CLA	C3D-C4D	-2.40	1.38	1.44
19	B	819	CLA	C4D-CHA	2.40	1.46	1.38
19	L	203	CLA	C1C-C2C	2.40	1.49	1.44
30	3	211	KC1	C4C-C3C	2.40	1.49	1.45
19	B	818	CLA	C3D-C4D	-2.40	1.38	1.44
19	J	103	CLA	C4D-CHA	2.40	1.46	1.38
19	A	839	CLA	C1B-CHB	2.40	1.47	1.41
19	B	845	CLA	C3D-C4D	-2.40	1.38	1.44
19	5	214	CLA	C3D-C4D	-2.40	1.38	1.44
19	A	831	CLA	C1B-CHB	2.40	1.47	1.41
19	A	809	CLA	C3D-C4D	-2.40	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	214	A86	O-C13	-2.40	1.18	1.23
19	A	811	CLA	C1B-CHB	2.40	1.47	1.41
19	1	304	CLA	C4D-CHA	2.40	1.46	1.38
19	5	207	CLA	C4B-CHC	2.40	1.47	1.41
19	A	839	CLA	C1C-C2C	2.39	1.49	1.44
19	2	212	CLA	C1B-CHB	2.39	1.47	1.41
19	B	825	CLA	C3D-C4D	-2.39	1.38	1.44
19	A	833	CLA	C1B-CHB	2.39	1.47	1.41
19	B	836	CLA	C3D-C4D	-2.39	1.38	1.44
19	1	307	CLA	C1B-NB	-2.39	1.33	1.35
19	1	306	CLA	C4B-CHC	2.39	1.47	1.41
19	B	846	CLA	C4B-CHC	2.39	1.47	1.41
19	B	832	CLA	C3D-C4D	-2.39	1.38	1.44
31	4	314	A86	C14-C15	2.39	1.57	1.52
19	A	833	CLA	C3D-C4D	-2.39	1.38	1.44
19	A	810	CLA	C1C-C2C	2.39	1.49	1.44
19	B	814	CLA	C4D-CHA	2.39	1.46	1.38
19	4	301	CLA	C3D-C4D	-2.39	1.38	1.44
19	2	209	CLA	C4B-CHC	2.39	1.47	1.41
19	4	304	CLA	C3D-C4D	-2.39	1.38	1.44
19	A	820	CLA	C4B-CHC	2.39	1.47	1.41
19	B	845	CLA	C4D-CHA	2.39	1.46	1.38
19	1	307	CLA	C3D-C4D	-2.38	1.38	1.44
19	4	301	CLA	C4B-CHC	2.38	1.47	1.41
19	3	210	CLA	C4B-CHC	2.38	1.47	1.41
19	4	312	CLA	C4D-CHA	2.38	1.46	1.38
31	3	214	A86	C14-C15	2.38	1.57	1.52
19	1	308	CLA	C3D-C4D	-2.38	1.38	1.44
19	A	802	CLA	C4D-CHA	2.38	1.46	1.38
19	A	842	CLA	C4D-CHA	2.38	1.46	1.38
19	3	204	CLA	C1C-C2C	2.38	1.49	1.44
19	4	306	CLA	C1C-C2C	2.38	1.49	1.44
19	2	215	CLA	C1C-C2C	2.38	1.49	1.44
19	B	838	CLA	C3D-C4D	-2.38	1.38	1.44
19	A	814	CLA	C4D-CHA	2.38	1.46	1.38
19	1	307	CLA	C1B-CHB	2.38	1.47	1.41
19	A	817	CLA	C3D-C4D	-2.38	1.38	1.44
19	2	208	CLA	C3D-C4D	-2.38	1.38	1.44
19	A	823	CLA	C3D-C4D	-2.38	1.38	1.44
30	3	205	KC1	C4C-C3C	2.38	1.49	1.45
19	B	820	CLA	C4B-CHC	2.37	1.47	1.41
19	B	819	CLA	C3D-C4D	-2.37	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	213	CLA	C4B-CHC	2.37	1.47	1.41
19	5	215	CLA	C4B-CHC	2.37	1.47	1.41
19	A	817	CLA	C4B-CHC	2.37	1.47	1.41
19	L	206	CLA	C1C-NC	-2.37	1.34	1.37
19	A	844	CLA	C1B-CHB	2.37	1.47	1.41
19	4	309	CLA	C1B-CHB	2.37	1.47	1.41
19	A	828	CLA	C1C-NC	-2.37	1.34	1.37
19	A	817	CLA	C4D-CHA	2.37	1.46	1.38
19	B	823	CLA	C4D-CHA	2.37	1.46	1.38
19	2	208	CLA	C4B-CHC	2.37	1.47	1.41
19	A	831	CLA	C3D-C4D	-2.37	1.38	1.44
19	B	804	CLA	C1B-NB	-2.37	1.33	1.35
19	4	306	CLA	C3D-C4D	-2.37	1.38	1.44
19	A	802	CLA	C1C-C2C	2.37	1.49	1.44
28	2	217	DD6	C35-C36	2.37	1.54	1.51
19	F	204	CLA	C4B-CHC	2.37	1.47	1.41
19	A	812	CLA	C1C-C2C	2.37	1.49	1.44
19	2	213	CLA	C1B-CHB	2.37	1.47	1.41
19	A	839	CLA	C4C-C3C	2.37	1.49	1.45
30	3	208	KC1	C4C-C3C	2.37	1.49	1.45
19	B	804	CLA	C4C-C3C	2.37	1.49	1.45
19	4	310	CLA	C1C-C2C	2.37	1.49	1.44
30	3	205	KC1	C2A-C1A	2.37	1.51	1.44
19	A	802	CLA	C4B-CHC	2.37	1.47	1.41
30	3	205	KC1	C1C-C2C	2.37	1.49	1.44
19	A	834	CLA	C1C-NC	-2.37	1.34	1.37
19	1	303	CLA	C3D-C4D	-2.36	1.38	1.44
19	A	811	CLA	C4B-CHC	2.36	1.47	1.41
19	A	828	CLA	C4B-CHC	2.36	1.47	1.41
19	B	816	CLA	C3D-C4D	-2.36	1.38	1.44
19	2	212	CLA	C1C-C2C	2.36	1.49	1.44
19	3	206	CLA	C3D-C4D	-2.36	1.38	1.44
31	2	219	A86	O-C13	-2.36	1.18	1.23
19	B	816	CLA	C4B-CHC	2.36	1.47	1.41
19	3	206	CLA	C4B-CHC	2.36	1.47	1.41
19	B	831	CLA	C1C-C2C	2.36	1.49	1.44
19	A	806	CLA	C4D-CHA	2.36	1.46	1.38
19	B	807	CLA	C1B-NB	-2.36	1.33	1.35
19	B	815	CLA	C4C-C3C	2.36	1.49	1.45
19	3	207	CLA	C1C-C2C	2.36	1.49	1.44
19	B	814	CLA	C3D-C4D	-2.36	1.38	1.44
31	2	219	A86	C24-C1	2.36	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	815	CLA	C1C-C2C	2.36	1.49	1.44
19	B	835	CLA	C3D-C4D	-2.36	1.38	1.44
19	3	203	CLA	C4D-CHA	2.36	1.46	1.38
19	4	309	CLA	C4B-CHC	2.36	1.47	1.41
19	B	835	CLA	C1B-CHB	2.36	1.47	1.41
19	A	820	CLA	C1C-C2C	2.35	1.49	1.44
28	1	315	DD6	C4-C5	2.35	1.50	1.43
19	A	830	CLA	C3D-C4D	-2.35	1.38	1.44
19	L	203	CLA	C1B-CHB	2.35	1.47	1.41
19	A	819	CLA	C3D-C4D	-2.35	1.38	1.44
19	4	308	CLA	C3D-C4D	-2.35	1.38	1.44
19	A	830	CLA	C1B-NB	-2.35	1.33	1.35
19	2	207	CLA	C4B-CHC	2.35	1.47	1.41
19	B	825	CLA	C1B-CHB	2.35	1.47	1.41
19	3	204	CLA	C1B-CHB	2.35	1.47	1.41
19	A	828	CLA	C3D-C4D	-2.35	1.38	1.44
19	5	212	CLA	C4B-CHC	2.35	1.47	1.41
19	B	806	CLA	C1C-C2C	2.35	1.49	1.44
19	4	309	CLA	C1C-C2C	2.35	1.49	1.44
19	A	808	CLA	C4B-CHC	2.35	1.47	1.41
19	A	842	CLA	C1C-NC	-2.35	1.34	1.37
19	1	306	CLA	C3D-C4D	-2.35	1.38	1.44
19	5	211	CLA	C1B-NB	-2.35	1.33	1.35
19	A	836	CLA	C3D-C4D	-2.35	1.38	1.44
19	5	216	CLA	C1C-C2C	2.35	1.49	1.44
19	B	836	CLA	C1B-NB	-2.35	1.33	1.35
19	A	810	CLA	C4B-CHC	2.35	1.47	1.41
19	A	813	CLA	C4B-CHC	2.35	1.47	1.41
19	A	816	CLA	C4B-CHC	2.34	1.47	1.41
19	B	835	CLA	C4B-CHC	2.34	1.47	1.41
31	5	221	A86	C24-C1	2.34	1.51	1.45
19	5	215	CLA	C3D-C4D	-2.34	1.38	1.44
19	B	837	CLA	C1B-NB	-2.34	1.33	1.35
19	A	837	CLA	C4B-CHC	2.34	1.47	1.41
19	B	820	CLA	C1B-CHB	2.34	1.47	1.41
31	3	214	A86	C-C1	2.34	1.55	1.50
19	A	842	CLA	C3D-C4D	-2.34	1.38	1.44
19	3	210	CLA	C4D-CHA	2.34	1.46	1.38
19	B	811	CLA	C1C-C2C	2.34	1.49	1.44
19	L	204	CLA	C4B-CHC	2.34	1.47	1.41
19	B	811	CLA	C4D-CHA	2.34	1.46	1.38
19	5	209	CLA	C1B-NB	-2.34	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	880	CLA	C3D-C4D	-2.34	1.38	1.44
19	A	834	CLA	C4D-CHA	2.34	1.46	1.38
23	B	842	LHG	P-O6	2.34	1.68	1.59
19	4	308	CLA	C1B-NB	-2.34	1.33	1.35
19	A	844	CLA	C3D-C4D	-2.33	1.38	1.44
19	B	802	CLA	C1C-C2C	2.33	1.49	1.44
19	5	214	CLA	C4B-CHC	2.33	1.47	1.41
30	3	208	KC1	C1C-C2C	2.33	1.49	1.44
31	1	317	A86	O-C13	-2.33	1.18	1.23
28	1	312	DD6	C35-C36	2.33	1.54	1.51
19	2	205	CLA	C1B-CHB	2.33	1.47	1.41
19	A	804	CLA	C1B-NB	-2.33	1.33	1.35
19	A	813	CLA	C1B-CHB	2.33	1.47	1.41
19	B	813	CLA	C4B-NB	-2.33	1.33	1.35
31	2	216	A86	O4-C34	-2.33	1.40	1.46
19	J	103	CLA	C1B-CHB	2.33	1.47	1.41
19	5	215	CLA	C1B-CHB	2.33	1.47	1.41
19	5	210	CLA	C1B-NB	-2.33	1.33	1.35
19	5	216	CLA	C3D-C4D	-2.33	1.38	1.44
19	B	806	CLA	C4B-CHC	2.33	1.47	1.41
19	B	822	CLA	C4C-C3C	2.33	1.49	1.45
19	F	203	CLA	C4B-CHC	2.33	1.47	1.41
19	B	817	CLA	C1B-NB	-2.33	1.33	1.35
19	B	832	CLA	C1C-C2C	2.33	1.49	1.44
19	B	803	CLA	C4B-CHC	2.33	1.47	1.41
23	4	317	LHG	O7-C5	-2.33	1.40	1.46
19	B	828	CLA	C4B-CHC	2.32	1.47	1.41
28	2	217	DD6	O1-C20	2.32	1.49	1.46
31	4	315	A86	C24-C1	2.32	1.50	1.45
19	4	303	CLA	C4B-CHC	2.32	1.47	1.41
19	1	303	CLA	C4C-C3C	2.32	1.49	1.45
19	2	206	CLA	C4B-CHC	2.32	1.47	1.41
19	A	821	CLA	C3D-C4D	-2.32	1.38	1.44
19	L	203	CLA	C4B-CHC	2.32	1.47	1.41
19	2	206	CLA	C1B-CHB	2.32	1.47	1.41
19	4	309	CLA	C3D-C4D	-2.32	1.38	1.44
19	B	833	CLA	C1C-C2C	2.32	1.49	1.44
19	B	833	CLA	C4B-CHC	2.32	1.47	1.41
19	B	821	CLA	C4D-CHA	2.32	1.46	1.38
19	B	802	CLA	C4B-CHC	2.32	1.47	1.41
19	2	210	CLA	C1C-C2C	2.32	1.49	1.44
19	B	825	CLA	C4B-CHC	2.32	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	837	CLA	C1C-C2C	2.32	1.49	1.44
19	5	210	CLA	C1B-CHB	2.32	1.47	1.41
19	L	204	CLA	C1B-CHB	2.32	1.47	1.41
19	3	210	CLA	C1C-C2C	2.32	1.49	1.44
19	B	817	CLA	C1C-C2C	2.32	1.49	1.44
19	J	103	CLA	C3D-C4D	-2.31	1.38	1.44
19	B	808	CLA	C1B-CHB	2.31	1.47	1.41
19	A	837	CLA	C4C-C3C	2.31	1.49	1.45
19	2	214	CLA	C4B-CHC	2.31	1.47	1.41
31	5	221	A86	O4-C34	-2.31	1.40	1.46
19	B	820	CLA	C4C-C3C	2.31	1.49	1.45
19	3	204	CLA	C4B-CHC	2.31	1.47	1.41
19	2	209	CLA	C1C-C2C	2.31	1.49	1.44
24	1	323	LMT	O3B-C3B	-2.31	1.37	1.43
19	4	313	CLA	C3D-C4D	-2.31	1.39	1.44
19	5	208	CLA	C4C-C3C	2.31	1.49	1.45
19	A	815	CLA	C1B-CHB	2.31	1.47	1.41
19	B	803	CLA	C4D-CHA	2.31	1.46	1.38
19	A	826	CLA	C1C-C2C	2.31	1.49	1.44
19	A	838	CLA	C1B-CHB	2.31	1.47	1.41
18	A	801	CL0	C1B-CHB	2.31	1.47	1.41
19	A	808	CLA	C1B-NB	-2.31	1.33	1.35
28	3	213	DD6	C4-C5	2.31	1.50	1.43
19	1	301	CLA	C4B-CHC	2.31	1.47	1.41
19	A	809	CLA	C1C-C2C	2.31	1.49	1.44
18	A	801	CL0	C1C-C2C	2.31	1.49	1.44
19	4	305	CLA	C1C-C2C	2.31	1.49	1.44
19	4	312	CLA	C3D-C4D	-2.31	1.39	1.44
19	A	834	CLA	C1B-CHB	2.31	1.47	1.41
19	B	805	CLA	C4C-C3C	2.31	1.49	1.45
19	2	213	CLA	C3D-C4D	-2.31	1.39	1.44
19	A	832	CLA	C4B-CHC	2.31	1.47	1.41
19	B	805	CLA	C1C-NC	-2.31	1.34	1.37
19	A	812	CLA	C4B-CHC	2.31	1.47	1.41
19	A	838	CLA	C1B-NB	-2.30	1.33	1.35
19	A	806	CLA	C1B-CHB	2.30	1.47	1.41
19	B	845	CLA	C1B-CHB	2.30	1.47	1.41
19	A	807	CLA	C4B-CHC	2.30	1.47	1.41
28	1	315	DD6	O1-C20	2.30	1.49	1.46
19	A	878	CLA	C3D-C4D	-2.30	1.39	1.44
19	4	311	CLA	C3D-C4D	-2.30	1.39	1.44
19	3	209	CLA	C3D-C4D	-2.30	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	838	CLA	C1C-C2C	2.30	1.49	1.44
28	2	217	DD6	C4-C5	2.30	1.50	1.43
19	A	832	CLA	C1B-CHB	2.30	1.47	1.41
19	A	831	CLA	C4C-C3C	2.30	1.49	1.45
19	A	829	CLA	C1C-C2C	2.30	1.49	1.44
19	B	838	CLA	C1B-CHB	2.30	1.47	1.41
19	B	802	CLA	C1B-NB	-2.30	1.33	1.35
19	2	207	CLA	C1B-CHB	2.30	1.47	1.41
19	A	822	CLA	C4B-CHC	2.30	1.47	1.41
19	A	818	CLA	C4B-CHC	2.29	1.47	1.41
19	A	837	CLA	C1C-C2C	2.29	1.49	1.44
19	A	803	CLA	C3D-C4D	-2.29	1.39	1.44
19	2	210	CLA	C3D-C4D	-2.29	1.39	1.44
31	4	315	A86	C14-C15	2.29	1.57	1.52
19	L	203	CLA	C4D-CHA	2.29	1.46	1.38
19	B	812	CLA	C3D-C4D	-2.29	1.39	1.44
24	2	220	LMT	O2'-C2'	-2.29	1.37	1.43
19	2	205	CLA	C1B-NB	-2.29	1.33	1.35
19	B	827	CLA	C1B-CHB	2.29	1.47	1.41
19	A	803	CLA	C4B-CHC	2.29	1.47	1.41
19	A	842	CLA	C1B-CHB	2.29	1.47	1.41
24	A	854	LMT	O3B-C3B	-2.29	1.37	1.43
30	1	305	KC1	C4C-C3C	2.29	1.49	1.45
19	u	201	CLA	C4B-CHC	2.29	1.47	1.41
19	5	215	CLA	C1C-C2C	2.29	1.49	1.44
31	1	317	A86	C35-C34	2.29	1.55	1.51
19	A	806	CLA	C4B-CHC	2.29	1.47	1.41
19	A	828	CLA	C1B-CHB	2.29	1.47	1.41
19	5	213	CLA	C4B-CHC	2.29	1.47	1.41
31	5	219	A86	O4-C34	-2.29	1.40	1.46
19	A	805	CLA	C4B-CHC	2.29	1.47	1.41
19	B	810	CLA	C1C-NC	-2.29	1.34	1.37
30	3	208	KC1	CAA-C2A	2.28	1.53	1.46
19	4	313	CLA	C1B-CHB	2.28	1.47	1.41
19	4	306	CLA	C4C-C3C	2.28	1.49	1.45
19	u	202	CLA	C1B-CHB	2.28	1.47	1.41
19	5	213	CLA	C1B-NB	-2.28	1.33	1.35
19	2	207	CLA	C4D-CHA	2.28	1.46	1.38
19	2	205	CLA	C4C-C3C	2.28	1.49	1.45
19	A	827	CLA	C4C-C3C	2.28	1.49	1.45
19	B	811	CLA	C4B-CHC	2.28	1.47	1.41
19	1	301	CLA	C4C-C3C	2.28	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	830	CLA	C4B-CHC	2.28	1.47	1.41
19	3	202	CLA	C3D-C4D	-2.28	1.39	1.44
19	A	817	CLA	C1C-C2C	2.28	1.49	1.44
19	B	836	CLA	C4B-CHC	2.28	1.47	1.41
19	1	304	CLA	C4B-CHC	2.28	1.47	1.41
19	A	836	CLA	C4B-CHC	2.28	1.47	1.41
19	5	216	CLA	C4B-CHC	2.28	1.47	1.41
19	A	806	CLA	C1C-C2C	2.27	1.49	1.44
19	3	210	CLA	C3D-C4D	-2.27	1.39	1.44
19	4	313	CLA	C4C-C3C	2.27	1.49	1.45
19	3	204	CLA	C4C-C3C	2.27	1.49	1.45
19	A	880	CLA	C1B-CHB	2.27	1.47	1.41
19	B	808	CLA	C1C-C2C	2.27	1.49	1.44
19	L	206	CLA	C4B-CHC	2.27	1.47	1.41
19	B	807	CLA	C4B-CHC	2.27	1.47	1.41
19	3	203	CLA	C3D-C4D	-2.27	1.39	1.44
19	B	828	CLA	C4C-C3C	2.27	1.48	1.45
19	3	204	CLA	C3D-C4D	-2.27	1.39	1.44
19	B	820	CLA	C1C-C2C	2.27	1.49	1.44
19	B	805	CLA	C1C-C2C	2.27	1.49	1.44
19	B	826	CLA	C1C-NC	-2.27	1.34	1.37
19	A	827	CLA	C4B-CHC	2.27	1.47	1.41
19	2	207	CLA	C1C-C2C	2.26	1.48	1.44
19	3	207	CLA	C1B-CHB	2.26	1.47	1.41
19	A	826	CLA	C4B-CHC	2.26	1.47	1.41
19	B	838	CLA	C4C-C3C	2.26	1.48	1.45
19	A	830	CLA	C1B-CHB	2.26	1.47	1.41
19	B	804	CLA	C3D-C4D	-2.26	1.39	1.44
31	4	315	A86	O4-C34	-2.26	1.40	1.46
19	B	813	CLA	C1B-CHB	2.26	1.47	1.41
19	B	846	CLA	C1B-CHB	2.26	1.47	1.41
19	2	205	CLA	C1C-C2C	2.26	1.48	1.44
19	A	878	CLA	C4B-CHC	2.26	1.47	1.41
19	B	815	CLA	C4B-CHC	2.26	1.47	1.41
31	4	314	A86	C24-C1	2.26	1.50	1.45
19	A	806	CLA	C4C-C3C	2.26	1.48	1.45
19	B	802	CLA	C1B-CHB	2.26	1.47	1.41
19	A	814	CLA	C4B-CHC	2.26	1.47	1.41
19	4	303	CLA	C4C-C3C	2.26	1.48	1.45
19	B	833	CLA	C1B-NB	-2.26	1.33	1.35
19	3	203	CLA	C1C-C2C	2.26	1.48	1.44
19	B	822	CLA	C3D-C4D	-2.26	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	833	CLA	C4B-NB	-2.26	1.33	1.35
19	B	803	CLA	C1C-NC	-2.26	1.34	1.37
19	A	832	CLA	C1C-C2C	2.26	1.48	1.44
19	3	203	CLA	C4B-CHC	2.26	1.47	1.41
19	2	214	CLA	C1C-C2C	2.26	1.48	1.44
19	B	810	CLA	C1B-CHB	2.26	1.47	1.41
30	3	211	KC1	C1C-C2C	2.26	1.48	1.44
19	B	814	CLA	C1B-CHB	2.26	1.47	1.41
19	A	816	CLA	C4C-C3C	2.26	1.48	1.45
19	5	212	CLA	C1B-NB	-2.26	1.33	1.35
19	B	818	CLA	C4B-CHC	2.26	1.47	1.41
19	A	805	CLA	C1B-CHB	2.25	1.47	1.41
19	B	806	CLA	C1B-CHB	2.25	1.47	1.41
24	3	216	LMT	O3B-C3B	-2.25	1.37	1.43
19	A	836	CLA	C1B-NB	-2.25	1.33	1.35
19	5	207	CLA	C1C-C2C	2.25	1.48	1.44
19	A	837	CLA	C1B-NB	-2.25	1.33	1.35
19	B	824	CLA	C1B-CHB	2.25	1.47	1.41
19	4	301	CLA	C1C-C2C	2.25	1.48	1.44
19	4	305	CLA	C4B-CHC	2.25	1.47	1.41
19	A	825	CLA	C4B-CHC	2.25	1.47	1.41
19	A	824	CLA	C1B-CHB	2.25	1.47	1.41
19	B	834	CLA	C1C-C2C	2.25	1.48	1.44
19	3	206	CLA	C4C-C3C	2.25	1.48	1.45
19	A	880	CLA	C4B-CHC	2.25	1.47	1.41
19	1	304	CLA	C1C-NC	-2.25	1.34	1.37
24	3	216	LMT	O4'-C4B	-2.25	1.37	1.43
28	3	213	DD6	C22-C16	-2.25	1.49	1.53
31	2	219	A86	O4-C34	-2.25	1.41	1.46
19	4	311	CLA	C1C-C2C	2.25	1.48	1.44
19	B	816	CLA	C1C-C2C	2.24	1.48	1.44
19	1	301	CLA	C1C-C2C	2.24	1.48	1.44
19	u	201	CLA	C1B-CHB	2.24	1.47	1.41
19	A	842	CLA	C1B-NB	-2.24	1.33	1.35
19	3	207	CLA	C4C-C3C	2.24	1.48	1.45
19	B	831	CLA	C4B-CHC	2.24	1.47	1.41
19	B	826	CLA	C4C-C3C	2.24	1.48	1.45
19	A	817	CLA	C1B-CHB	2.24	1.47	1.41
19	5	208	CLA	C4B-CHC	2.24	1.47	1.41
19	4	308	CLA	C4C-C3C	2.24	1.48	1.45
19	2	205	CLA	C4B-CHC	2.24	1.47	1.41
19	A	815	CLA	C1B-NB	-2.24	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	831	CLA	C1C-C2C	2.24	1.48	1.44
18	A	801	CL0	C4B-CHC	2.24	1.47	1.41
19	B	816	CLA	C4C-C3C	2.24	1.48	1.45
19	A	829	CLA	C4B-CHC	2.24	1.47	1.41
30	1	305	KC1	C1C-C2C	2.24	1.48	1.44
19	A	823	CLA	C1C-C2C	2.24	1.48	1.44
19	B	802	CLA	C3D-C4D	-2.24	1.39	1.44
19	A	824	CLA	C4C-C3C	2.23	1.48	1.45
19	B	803	CLA	C3D-C4D	-2.23	1.39	1.44
19	B	830	CLA	C1C-C2C	2.23	1.48	1.44
19	2	215	CLA	C4C-C3C	2.23	1.48	1.45
19	B	822	CLA	C4B-CHC	2.23	1.47	1.41
19	A	837	CLA	C3D-C4D	-2.23	1.39	1.44
19	B	830	CLA	C1B-CHB	2.23	1.47	1.41
19	1	310	CLA	C4B-CHC	2.23	1.47	1.41
19	A	832	CLA	C1B-NB	-2.23	1.33	1.35
19	A	803	CLA	C1C-C2C	2.23	1.48	1.44
19	4	305	CLA	C3D-C4D	-2.23	1.39	1.44
19	B	815	CLA	C1B-CHB	2.23	1.47	1.41
31	3	228	A86	O4-C34	-2.23	1.41	1.46
19	B	831	CLA	C1B-NB	-2.23	1.33	1.35
19	A	823	CLA	C1B-CHB	2.23	1.47	1.41
19	F	203	CLA	C1C-C2C	2.23	1.48	1.44
19	B	838	CLA	C4B-CHC	2.23	1.47	1.41
19	B	812	CLA	C4B-CHC	2.23	1.47	1.41
19	A	842	CLA	C4C-C3C	2.22	1.48	1.45
19	L	206	CLA	C1B-NB	-2.22	1.33	1.35
19	B	819	CLA	C4B-CHC	2.22	1.47	1.41
19	2	208	CLA	C1C-C2C	2.22	1.48	1.44
19	5	214	CLA	C1B-CHB	2.22	1.47	1.41
19	B	830	CLA	C4B-CHC	2.22	1.47	1.41
19	F	204	CLA	C1B-CHB	2.22	1.47	1.41
31	3	214	A86	O4-C34	-2.22	1.41	1.46
19	A	814	CLA	C1C-C2C	2.22	1.48	1.44
31	3	212	A86	C35-C34	2.22	1.55	1.51
19	A	820	CLA	C1B-NB	-2.22	1.33	1.35
19	A	813	CLA	C1C-C2C	2.22	1.48	1.44
19	5	212	CLA	C1C-C2C	2.22	1.48	1.44
28	3	213	DD6	O1-C20	2.22	1.49	1.46
19	B	830	CLA	C3D-C4D	-2.22	1.39	1.44
19	B	805	CLA	C4B-CHC	2.22	1.47	1.41
28	L	209	DD6	C22-C16	-2.22	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	818	CLA	C1B-CHB	2.22	1.47	1.41
19	B	827	CLA	C4B-CHC	2.22	1.47	1.41
19	B	836	CLA	C1B-CHB	2.22	1.47	1.41
19	B	836	CLA	C1C-C2C	2.22	1.48	1.44
19	B	809	CLA	C4C-C3C	2.22	1.48	1.45
19	A	842	CLA	C4B-CHC	2.22	1.47	1.41
19	B	821	CLA	C4B-CHC	2.22	1.47	1.41
19	5	209	CLA	C1B-CHB	2.22	1.47	1.41
19	B	845	CLA	C4C-C3C	2.21	1.48	1.45
19	B	834	CLA	C1B-CHB	2.21	1.47	1.41
30	4	307	KC1	C3B-C4B	2.21	1.50	1.46
19	4	306	CLA	C1B-CHB	2.21	1.47	1.41
19	B	826	CLA	C1B-CHB	2.21	1.47	1.41
19	B	809	CLA	C1B-CHB	2.21	1.47	1.41
19	4	310	CLA	C1B-CHB	2.21	1.47	1.41
19	B	832	CLA	C4C-C3C	2.21	1.48	1.45
19	B	824	CLA	C1C-C2C	2.21	1.48	1.44
18	A	801	CL0	C1B-NB	-2.21	1.33	1.35
19	B	822	CLA	C1B-NB	-2.21	1.33	1.35
19	A	836	CLA	C4C-C3C	2.21	1.48	1.45
19	A	812	CLA	C4C-C3C	2.21	1.48	1.45
19	A	802	CLA	C4B-NB	-2.21	1.33	1.35
19	A	814	CLA	C1B-NB	-2.21	1.33	1.35
31	5	217	A86	O4-C34	-2.21	1.41	1.46
19	2	206	CLA	C1C-C2C	2.21	1.48	1.44
19	A	815	CLA	C4B-CHC	2.21	1.47	1.41
19	A	843	CLA	C1C-C2C	2.20	1.48	1.44
19	2	209	CLA	C3D-C4D	-2.20	1.39	1.44
19	A	835	CLA	C1C-NC	-2.20	1.34	1.37
19	A	831	CLA	C1B-NB	-2.20	1.33	1.35
19	5	215	CLA	C4C-C3C	2.20	1.48	1.45
31	5	220	A86	C14-C15	2.20	1.57	1.52
19	A	814	CLA	C1B-CHB	2.20	1.47	1.41
19	A	833	CLA	C1B-NB	-2.20	1.33	1.35
19	B	813	CLA	C1C-C2C	2.20	1.48	1.44
24	2	220	LMT	O2B-C2B	-2.20	1.37	1.43
19	A	802	CLA	C1B-CHB	2.20	1.47	1.41
19	A	823	CLA	C4B-CHC	2.20	1.47	1.41
19	B	833	CLA	C1B-CHB	2.20	1.47	1.41
19	u	202	CLA	C4C-C3C	2.20	1.48	1.45
19	B	802	CLA	C1C-NC	-2.19	1.34	1.37
19	B	808	CLA	C4B-CHC	2.19	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	2	217	DD6	C22-C16	-2.19	1.49	1.53
19	A	835	CLA	C4B-NB	-2.19	1.33	1.35
19	2	210	CLA	C4B-NB	-2.19	1.33	1.35
19	B	804	CLA	C1B-CHB	2.19	1.47	1.41
19	B	811	CLA	C1B-CHB	2.19	1.47	1.41
19	A	839	CLA	C1B-NB	-2.19	1.33	1.35
19	4	310	CLA	C4C-C3C	2.19	1.48	1.45
19	A	839	CLA	C4B-NB	-2.19	1.33	1.35
19	A	841	CLA	C1C-C2C	2.19	1.48	1.44
19	2	209	CLA	C4C-C3C	2.19	1.48	1.45
19	5	207	CLA	C1B-CHB	2.19	1.47	1.41
19	A	822	CLA	C4C-C3C	2.19	1.48	1.45
19	A	834	CLA	C4C-C3C	2.19	1.48	1.45
19	1	303	CLA	C1B-CHB	2.19	1.47	1.41
30	2	211	KC1	C2A-C1A	2.19	1.51	1.44
19	A	815	CLA	C4C-C3C	2.19	1.48	1.45
19	F	204	CLA	C1C-C2C	2.19	1.48	1.44
19	4	313	CLA	C4B-CHC	2.19	1.47	1.41
19	B	829	CLA	C4C-C3C	2.19	1.48	1.45
19	B	823	CLA	C1B-CHB	2.19	1.47	1.41
19	F	204	CLA	C4C-C3C	2.19	1.48	1.45
19	B	822	CLA	C1B-CHB	2.19	1.47	1.41
19	3	209	CLA	C4B-CHC	2.19	1.47	1.41
23	4	317	LHG	P-O6	2.18	1.68	1.59
24	2	220	LMT	O4'-C4B	-2.18	1.37	1.43
19	1	308	CLA	C4C-C3C	2.18	1.48	1.45
19	B	809	CLA	C4B-CHC	2.18	1.47	1.41
30	1	305	KC1	C2A-C1A	2.18	1.51	1.44
19	4	308	CLA	C1B-CHB	2.18	1.47	1.41
19	B	805	CLA	C4B-NB	-2.18	1.33	1.35
19	3	209	CLA	C4C-C3C	2.18	1.48	1.45
19	B	846	CLA	C1C-NC	-2.18	1.34	1.37
19	2	214	CLA	C1B-CHB	2.18	1.47	1.41
19	A	818	CLA	C4C-C3C	2.18	1.48	1.45
19	A	825	CLA	C1B-CHB	2.18	1.47	1.41
19	2	208	CLA	C1B-CHB	2.18	1.47	1.41
19	A	835	CLA	C4B-CHC	2.18	1.47	1.41
19	A	805	CLA	C1C-C2C	2.18	1.48	1.44
19	2	212	CLA	C3D-C4D	-2.18	1.39	1.44
19	A	819	CLA	C1C-C2C	2.18	1.48	1.44
19	A	844	CLA	C1C-C2C	2.18	1.48	1.44
23	3	215	LHG	O7-C5	-2.17	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	845	CLA	C1C-NC	-2.17	1.34	1.37
31	4	314	A86	O4-C34	-2.17	1.41	1.46
19	A	804	CLA	C1C-C2C	2.17	1.48	1.44
31	3	212	A86	C24-C1	2.17	1.50	1.45
19	B	823	CLA	C4C-C3C	2.17	1.48	1.45
19	A	840	CLA	C1B-CHB	2.17	1.47	1.41
19	A	819	CLA	C1B-NB	-2.17	1.33	1.35
19	A	829	CLA	C4C-C3C	2.17	1.48	1.45
19	A	810	CLA	C1C-NC	-2.17	1.34	1.37
19	B	807	CLA	C1B-CHB	2.17	1.47	1.41
19	A	830	CLA	C4C-C3C	2.17	1.48	1.45
23	A	852	LHG	O7-C5	-2.17	1.41	1.46
19	A	802	CLA	C4C-C3C	2.17	1.48	1.45
19	B	821	CLA	C1C-C2C	2.17	1.48	1.44
19	2	209	CLA	C1B-NB	-2.17	1.33	1.35
19	5	211	CLA	C4B-CHC	2.17	1.47	1.41
19	A	807	CLA	C1B-CHB	2.17	1.47	1.41
19	5	213	CLA	C3D-C4D	-2.17	1.39	1.44
19	A	844	CLA	C4B-CHC	2.17	1.47	1.41
19	A	834	CLA	C4B-CHC	2.17	1.47	1.41
19	B	823	CLA	C4B-NB	-2.17	1.33	1.35
19	A	836	CLA	C1B-CHB	2.17	1.47	1.41
19	A	823	CLA	C1C-NC	-2.17	1.34	1.37
19	B	815	CLA	C1C-NC	-2.17	1.34	1.37
19	1	306	CLA	C1D-C2D	2.17	1.49	1.45
19	A	820	CLA	C4C-C3C	2.17	1.48	1.45
19	A	809	CLA	C4B-CHC	2.16	1.47	1.41
19	B	835	CLA	C1C-C2C	2.16	1.48	1.44
19	3	206	CLA	C1B-CHB	2.16	1.47	1.41
28	3	213	DD6	C29-C27	-2.16	1.38	1.42
19	A	813	CLA	C4C-C3C	2.16	1.48	1.45
19	B	837	CLA	C1C-NC	-2.16	1.34	1.37
19	A	834	CLA	C1C-C2C	2.16	1.48	1.44
19	B	822	CLA	C1C-C2C	2.16	1.48	1.44
19	4	303	CLA	C3D-C4D	-2.16	1.39	1.44
19	A	807	CLA	C1C-C2C	2.16	1.48	1.44
19	5	216	CLA	C1B-CHB	2.16	1.47	1.41
19	A	841	CLA	C4C-C3C	2.16	1.48	1.45
19	A	829	CLA	C4B-NB	-2.16	1.33	1.35
19	A	829	CLA	C1B-CHB	2.16	1.47	1.41
19	2	215	CLA	C1B-CHB	2.16	1.47	1.41
19	A	825	CLA	C1C-C2C	2.16	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	812	CLA	C1B-CHB	2.16	1.47	1.41
19	A	822	CLA	C1C-C2C	2.16	1.48	1.44
19	A	838	CLA	C4B-CHC	2.16	1.47	1.41
19	B	803	CLA	C1B-NB	-2.16	1.33	1.35
19	A	831	CLA	C4B-CHC	2.16	1.47	1.41
19	2	209	CLA	C1B-CHB	2.15	1.47	1.41
19	B	810	CLA	C1B-NB	-2.15	1.33	1.35
19	A	844	CLA	C4C-C3C	2.15	1.48	1.45
18	A	801	CL0	C4C-C3C	2.15	1.48	1.45
19	B	830	CLA	C4C-C3C	2.15	1.48	1.45
19	A	821	CLA	C1B-CHB	2.15	1.47	1.41
19	B	831	CLA	C4C-C3C	2.15	1.48	1.45
19	B	835	CLA	C4C-C3C	2.15	1.48	1.45
19	u	201	CLA	C1C-C2C	2.15	1.48	1.44
19	A	880	CLA	C1B-NB	-2.15	1.33	1.35
19	A	880	CLA	C1C-C2C	2.15	1.48	1.44
19	A	818	CLA	C1C-C2C	2.15	1.48	1.44
28	1	313	DD6	C4-C5	2.15	1.50	1.43
19	A	806	CLA	C4B-NB	-2.15	1.33	1.35
19	B	812	CLA	C1B-CHB	2.15	1.47	1.41
19	5	209	CLA	C1C-C2C	2.15	1.48	1.44
19	B	813	CLA	C4B-CHC	2.15	1.47	1.41
19	B	816	CLA	C1B-CHB	2.14	1.47	1.41
19	3	207	CLA	C1B-NB	-2.14	1.33	1.35
19	5	209	CLA	C4B-CHC	2.14	1.47	1.41
19	1	307	CLA	C4C-C3C	2.14	1.48	1.45
19	A	835	CLA	C1B-NB	-2.14	1.33	1.35
19	3	209	CLA	C1B-CHB	2.14	1.46	1.41
19	L	204	CLA	C4C-C3C	2.14	1.48	1.45
19	B	815	CLA	C1C-C2C	2.14	1.48	1.44
19	1	310	CLA	C1B-NB	-2.14	1.33	1.35
19	A	808	CLA	C1B-CHB	2.14	1.46	1.41
19	B	803	CLA	C4C-C3C	2.14	1.48	1.45
19	A	844	CLA	C1C-NC	-2.14	1.34	1.37
19	1	303	CLA	C4B-CHC	2.14	1.46	1.41
19	1	306	CLA	C1C-C2C	2.14	1.48	1.44
30	2	211	KC1	CAA-C2A	2.14	1.53	1.46
19	5	214	CLA	C1C-C2C	2.14	1.48	1.44
19	3	209	CLA	C1B-NB	-2.14	1.33	1.35
19	4	301	CLA	C1B-CHB	2.14	1.46	1.41
19	B	805	CLA	C1B-CHB	2.14	1.46	1.41
19	3	210	CLA	C1B-CHB	2.14	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	2	217	DD6	C29-C27	-2.14	1.38	1.42
19	2	214	CLA	C4C-C3C	2.14	1.48	1.45
19	B	812	CLA	C1C-C2C	2.14	1.48	1.44
28	5	218	DD6	C22-C16	-2.13	1.49	1.53
30	4	307	KC1	C1D-CHD	2.13	1.46	1.41
19	L	203	CLA	C4C-C3C	2.13	1.48	1.45
19	B	823	CLA	C1C-C2C	2.13	1.48	1.44
19	2	210	CLA	C1B-CHB	2.13	1.46	1.41
19	5	213	CLA	C1C-C2C	2.13	1.48	1.44
19	A	816	CLA	C1B-CHB	2.13	1.46	1.41
19	A	838	CLA	C4C-C3C	2.13	1.48	1.45
19	A	824	CLA	C1C-NC	-2.13	1.34	1.37
24	3	216	LMT	O2'-C2'	-2.13	1.38	1.43
23	M	103	LHG	O7-C5	-2.13	1.41	1.46
28	1	312	DD6	C22-C16	-2.13	1.49	1.53
19	A	803	CLA	C4C-C3C	2.13	1.48	1.45
19	B	825	CLA	C4C-C3C	2.13	1.48	1.45
19	A	835	CLA	C1C-C2C	2.13	1.48	1.44
19	A	840	CLA	C4C-C3C	2.13	1.48	1.45
19	5	214	CLA	C1B-NB	-2.13	1.33	1.35
19	B	826	CLA	C4B-CHC	2.13	1.46	1.41
19	4	301	CLA	C4C-C3C	2.13	1.48	1.45
19	1	306	CLA	C4C-C3C	2.13	1.48	1.45
19	A	809	CLA	C1C-NC	-2.12	1.34	1.37
19	A	829	CLA	C1C-NC	-2.12	1.34	1.37
19	4	305	CLA	C1B-CHB	2.12	1.46	1.41
19	A	807	CLA	C1B-NB	-2.12	1.33	1.35
19	3	209	CLA	C4B-NB	-2.12	1.33	1.35
19	B	814	CLA	C4B-CHC	2.12	1.46	1.41
19	A	833	CLA	C1C-C2C	2.12	1.48	1.44
19	B	829	CLA	C1B-CHB	2.12	1.46	1.41
19	5	208	CLA	C1C-C2C	2.12	1.48	1.44
19	A	823	CLA	C1B-NB	-2.12	1.33	1.35
19	A	821	CLA	C1B-NB	-2.12	1.33	1.35
19	1	307	CLA	C1C-NC	-2.12	1.34	1.37
19	B	804	CLA	C1C-C2C	2.12	1.48	1.44
19	1	304	CLA	C4C-C3C	2.12	1.48	1.45
19	B	826	CLA	C4B-NB	-2.11	1.33	1.35
19	B	819	CLA	C1C-C2C	2.11	1.48	1.44
19	B	817	CLA	C1C-NC	-2.11	1.34	1.37
19	B	845	CLA	C1B-NB	-2.11	1.33	1.35
19	A	838	CLA	C1C-C2C	2.11	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	813	CLA	C4B-NB	-2.11	1.33	1.35
19	4	304	CLA	C1B-CHB	2.11	1.46	1.41
19	B	823	CLA	C4B-CHC	2.11	1.46	1.41
19	A	811	CLA	C1B-NB	-2.11	1.33	1.35
28	3	213	DD6	C35-C36	2.11	1.54	1.51
19	5	211	CLA	C1C-NC	-2.11	1.34	1.37
19	A	807	CLA	C4C-C3C	2.11	1.48	1.45
19	B	819	CLA	C4C-C3C	2.11	1.48	1.45
19	L	204	CLA	C1B-NB	-2.11	1.33	1.35
19	A	839	CLA	C4B-CHC	2.10	1.46	1.41
19	B	818	CLA	C4C-C3C	2.10	1.48	1.45
19	4	303	CLA	C1B-CHB	2.10	1.46	1.41
19	A	830	CLA	C1C-C2C	2.10	1.48	1.44
19	A	805	CLA	C1B-NB	-2.10	1.33	1.35
19	B	814	CLA	C4B-NB	-2.10	1.33	1.35
19	A	832	CLA	C4C-C3C	2.10	1.48	1.45
19	1	308	CLA	C1B-CHB	2.10	1.46	1.41
19	A	828	CLA	C1C-C2C	2.10	1.48	1.44
30	3	208	KC1	C1D-CHD	2.10	1.46	1.41
19	L	203	CLA	C1B-NB	-2.10	1.33	1.35
19	3	209	CLA	C1C-C2C	2.10	1.48	1.44
19	B	811	CLA	C1B-NB	-2.10	1.33	1.35
19	3	204	CLA	C1B-NB	-2.10	1.33	1.35
31	5	221	A86	C14-C15	2.10	1.56	1.52
30	2	211	KC1	C1D-CHD	2.10	1.46	1.41
19	B	812	CLA	C4C-C3C	2.10	1.48	1.45
19	2	206	CLA	C1C-NC	-2.10	1.34	1.37
19	A	804	CLA	C1C-NC	-2.10	1.34	1.37
19	1	301	CLA	C1B-NB	-2.10	1.33	1.35
19	A	841	CLA	C1B-CHB	2.10	1.46	1.41
19	A	836	CLA	C1C-C2C	2.10	1.48	1.44
19	5	211	CLA	C1C-C2C	2.10	1.48	1.44
19	B	837	CLA	C1B-CHB	2.10	1.46	1.41
19	1	304	CLA	C1B-NB	-2.10	1.33	1.35
19	B	814	CLA	C1C-NC	-2.10	1.34	1.37
19	4	311	CLA	C1B-CHB	2.09	1.46	1.41
30	3	211	KC1	C1D-CHD	2.09	1.46	1.41
19	4	311	CLA	C1B-NB	-2.09	1.33	1.35
31	4	316	A86	C14-C15	2.09	1.56	1.52
19	A	838	CLA	C1C-NC	-2.09	1.34	1.37
19	B	812	CLA	C1C-NC	-2.09	1.34	1.37
19	4	301	CLA	C1B-NB	-2.09	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	210	CLA	C4B-CHC	2.09	1.46	1.41
19	A	826	CLA	C4C-C3C	2.09	1.48	1.45
19	A	823	CLA	C4C-C3C	2.09	1.48	1.45
19	A	819	CLA	C1B-CHB	2.09	1.46	1.41
19	1	310	CLA	C1B-CHB	2.09	1.46	1.41
19	A	813	CLA	C1C-NC	-2.09	1.34	1.37
19	B	807	CLA	C1C-C2C	2.09	1.48	1.44
19	A	825	CLA	C4C-C3C	2.09	1.48	1.45
19	B	814	CLA	C1C-C2C	2.09	1.48	1.44
19	A	815	CLA	C1C-NC	-2.09	1.34	1.37
19	B	821	CLA	C1B-CHB	2.08	1.46	1.41
19	B	823	CLA	C1C-NC	-2.08	1.34	1.37
19	2	207	CLA	C4C-C3C	2.08	1.48	1.45
19	B	818	CLA	C1B-CHB	2.08	1.46	1.41
19	2	206	CLA	C4C-C3C	2.08	1.48	1.45
19	3	203	CLA	C1B-CHB	2.08	1.46	1.41
24	1	323	LMT	O5'-C5'	-2.08	1.39	1.44
19	5	208	CLA	C1B-NB	-2.08	1.33	1.35
19	5	210	CLA	C1C-NC	-2.08	1.34	1.37
19	A	839	CLA	C1C-NC	-2.08	1.34	1.37
19	3	206	CLA	C1B-NB	-2.08	1.33	1.35
19	2	214	CLA	C1D-C2D	2.07	1.49	1.45
19	A	803	CLA	C4B-NB	-2.07	1.33	1.35
19	B	804	CLA	C4B-NB	-2.07	1.33	1.35
19	A	825	CLA	C1B-NB	-2.07	1.33	1.35
19	B	806	CLA	C4C-C3C	2.07	1.48	1.45
19	3	210	CLA	C4C-C3C	2.07	1.48	1.45
28	1	313	DD6	C29-C27	-2.07	1.38	1.42
19	A	824	CLA	C1C-C2C	2.07	1.48	1.44
19	1	307	CLA	C1C-C2C	2.07	1.48	1.44
19	u	202	CLA	C3D-C4D	-2.07	1.39	1.44
19	4	301	CLA	C1D-C2D	2.07	1.49	1.45
19	A	833	CLA	C4B-CHC	2.07	1.46	1.41
19	B	846	CLA	C1B-NB	-2.07	1.33	1.35
19	B	834	CLA	C4C-C3C	2.07	1.48	1.45
19	2	213	CLA	C1C-NC	-2.07	1.34	1.37
28	L	209	DD6	C41-C32	-2.07	1.49	1.53
18	A	801	CL0	C4B-NB	-2.07	1.33	1.35
19	A	810	CLA	C4C-C3C	2.07	1.48	1.45
19	L	206	CLA	C4C-C3C	2.07	1.48	1.45
19	A	815	CLA	C4B-NB	-2.07	1.33	1.35
19	A	804	CLA	C1B-CHB	2.07	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	846	CLA	C1C-C2C	2.07	1.48	1.44
19	B	824	CLA	C1C-NC	-2.07	1.34	1.37
19	A	842	CLA	C4B-NB	-2.06	1.33	1.35
22	I	102	BCR	C30-C25	-2.06	1.50	1.53
30	3	205	KC1	C1D-CHD	2.06	1.46	1.41
19	B	821	CLA	C1B-NB	-2.06	1.33	1.35
19	A	819	CLA	C1C-NC	-2.06	1.34	1.37
30	3	208	KC1	C1B-C2B	2.06	1.49	1.45
19	J	103	CLA	C1B-NB	-2.06	1.33	1.35
19	B	812	CLA	C1B-NB	-2.06	1.33	1.35
19	A	833	CLA	C4C-C3C	2.06	1.48	1.45
19	5	212	CLA	C1B-CHB	2.06	1.46	1.41
19	A	880	CLA	C4C-C3C	2.06	1.48	1.45
19	5	210	CLA	C4C-C3C	2.06	1.48	1.45
19	A	823	CLA	C4B-NB	-2.06	1.33	1.35
19	A	811	CLA	C4C-C3C	2.06	1.48	1.45
30	3	208	KC1	C2A-C1A	2.06	1.50	1.44
19	B	819	CLA	C1C-NC	-2.06	1.34	1.37
19	B	821	CLA	C1C-NC	-2.05	1.34	1.37
19	B	805	CLA	C1B-NB	-2.05	1.33	1.35
30	3	205	KC1	CAA-C2A	2.05	1.52	1.46
19	B	821	CLA	C4C-C3C	2.05	1.48	1.45
19	A	827	CLA	C1C-NC	-2.05	1.34	1.37
19	A	830	CLA	C4B-NB	-2.05	1.33	1.35
28	1	313	DD6	C22-C16	-2.05	1.49	1.53
19	A	843	CLA	C1C-NC	-2.05	1.34	1.37
19	B	817	CLA	C1B-CHB	2.05	1.46	1.41
19	5	212	CLA	C4C-C3C	2.05	1.48	1.45
19	A	827	CLA	C1B-CHB	2.05	1.46	1.41
19	1	307	CLA	C4B-CHC	2.05	1.46	1.41
19	2	210	CLA	C4C-C3C	2.05	1.48	1.45
19	B	812	CLA	C4B-NB	-2.04	1.33	1.35
19	A	878	CLA	C1B-CHB	2.04	1.46	1.41
19	3	202	CLA	C1B-CHB	2.04	1.46	1.41
19	5	211	CLA	C1B-CHB	2.04	1.46	1.41
19	1	309	CLA	C4C-C3C	2.04	1.48	1.45
19	A	837	CLA	C1B-CHB	2.04	1.46	1.41
19	5	207	CLA	C4C-C3C	2.04	1.48	1.45
19	5	213	CLA	C1B-CHB	2.04	1.46	1.41
19	2	213	CLA	C4C-C3C	2.04	1.48	1.45
19	B	824	CLA	C1B-NB	-2.04	1.33	1.35
19	5	210	CLA	C1C-C2C	2.04	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	313	CLA	C1C-C2C	2.04	1.48	1.44
28	5	218	DD6	C35-C36	2.04	1.54	1.51
28	1	315	DD6	C22-C16	-2.04	1.49	1.53
19	A	810	CLA	C1B-NB	-2.04	1.33	1.35
19	5	208	CLA	C1B-CHB	2.03	1.46	1.41
22	A	847	BCR	C33-C5	-2.03	1.47	1.50
19	A	825	CLA	C1C-NC	-2.03	1.34	1.37
19	B	830	CLA	C1C-NC	-2.03	1.34	1.37
19	A	816	CLA	C1B-NB	-2.03	1.33	1.35
19	B	814	CLA	C4C-C3C	2.03	1.48	1.45
19	A	803	CLA	C1C-NC	-2.03	1.34	1.37
30	4	307	KC1	CAA-C2A	2.03	1.52	1.46
19	3	210	CLA	C1D-C2D	2.03	1.49	1.45
19	A	822	CLA	C1C-NC	-2.03	1.34	1.37
19	B	817	CLA	C4C-C3C	2.03	1.48	1.45
19	B	831	CLA	C1B-CHB	2.03	1.46	1.41
19	5	212	CLA	C4B-NB	-2.03	1.33	1.35
19	B	804	CLA	C4B-CHC	2.02	1.46	1.41
19	B	832	CLA	C1B-CHB	2.02	1.46	1.41
19	A	831	CLA	C1C-NC	-2.02	1.34	1.37
19	1	310	CLA	C1C-NC	-2.02	1.34	1.37
19	B	824	CLA	C4B-NB	-2.02	1.33	1.35
19	B	819	CLA	C1B-CHB	2.02	1.46	1.41
19	2	213	CLA	C1B-NB	-2.02	1.33	1.35
19	B	818	CLA	C1B-NB	-2.02	1.33	1.35
30	2	211	KC1	C4C-C3C	2.02	1.48	1.45
22	B	844	BCR	C38-C26	-2.02	1.47	1.50
19	A	809	CLA	C1B-CHB	2.01	1.46	1.41
19	4	313	CLA	C1D-C2D	2.01	1.49	1.45
19	4	305	CLA	C1C-NC	-2.01	1.34	1.37
31	5	220	A86	O4-C34	-2.01	1.41	1.46
19	1	310	CLA	C1D-C2D	2.01	1.49	1.45
19	B	811	CLA	C4C-C3C	2.01	1.48	1.45
19	B	804	CLA	C1C-NC	-2.01	1.34	1.37
19	A	841	CLA	C1B-NB	-2.01	1.33	1.35
19	L	206	CLA	C1B-CHB	2.01	1.46	1.41
22	F	205	BCR	C33-C5	-2.01	1.47	1.50
19	A	806	CLA	C1C-NC	-2.00	1.34	1.37
19	2	206	CLA	C1B-NB	-2.00	1.33	1.35
19	1	310	CLA	C1C-C2C	2.00	1.48	1.44

All (4640) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	5	220	A86	O1-C20-C19	52.11	152.53	113.38
31	5	221	A86	O1-C20-C19	51.07	151.75	113.38
31	1	317	A86	O1-C20-C19	49.95	150.91	113.38
31	4	314	A86	O1-C20-C19	49.86	150.84	113.38
31	1	316	A86	O1-C20-C19	49.82	150.80	113.38
31	4	315	A86	O1-C20-C19	49.01	150.20	113.38
31	4	316	A86	O1-C20-C19	48.54	149.84	113.38
31	2	219	A86	O1-C20-C19	47.77	149.27	113.38
31	3	228	A86	O1-C20-C19	47.76	149.26	113.38
31	5	217	A86	O1-C20-C19	47.52	149.08	113.38
31	3	212	A86	O1-C20-C19	46.76	148.50	113.38
31	5	219	A86	O1-C20-C19	46.49	148.31	113.38
31	2	216	A86	O1-C20-C19	46.12	148.03	113.38
31	2	218	A86	O1-C20-C19	46.01	147.95	113.38
31	3	214	A86	O1-C20-C19	45.65	147.68	113.38
28	3	213	DD6	O1-C20-C19	31.44	137.00	113.38
28	1	315	DD6	O1-C20-C19	30.60	136.37	113.38
28	1	313	DD6	O1-C20-C19	30.18	136.06	113.38
28	1	312	DD6	O1-C20-C19	28.66	134.91	113.38
28	2	217	DD6	O1-C20-C19	28.58	134.85	113.38
28	L	209	DD6	O1-C20-C19	28.36	134.68	113.38
28	5	218	DD6	O1-C20-C19	25.61	132.62	113.38
19	B	810	CLA	C4-C3-C5	-21.16	79.67	115.27
19	1	307	CLA	C4-C3-C5	-21.14	79.72	115.27
19	5	212	CLA	C4-C3-C5	-20.93	80.07	115.27
19	5	212	CLA	C5-C3-C2	19.10	159.76	121.12
19	1	307	CLA	C5-C3-C2	18.74	159.03	121.12
28	2	217	DD6	C28-C27-C29	18.69	153.86	116.84
28	1	313	DD6	C28-C27-C29	18.37	153.22	116.84
19	B	810	CLA	C5-C3-C2	18.34	158.22	121.12
19	B	826	CLA	O2A-CGA-O1A	-18.12	77.85	123.59
28	3	213	DD6	C28-C27-C29	17.77	152.03	116.84
28	1	312	DD6	C28-C27-C29	17.71	151.91	116.84
28	5	218	DD6	C28-C27-C29	17.54	151.57	116.84
19	B	810	CLA	C4-C3-C2	-17.53	78.70	123.68
19	1	307	CLA	C4-C3-C2	-17.28	79.34	123.68
28	L	209	DD6	C28-C27-C29	17.13	150.77	116.84
19	5	212	CLA	C4-C3-C2	-17.12	79.75	123.68
28	1	315	DD6	C28-C27-C29	15.20	146.95	116.84
19	B	826	CLA	O2A-CGA-CBA	14.83	158.44	111.91
28	1	312	DD6	C29-C30-C31	-14.33	139.13	175.43
28	1	313	DD6	C29-C30-C31	-13.86	140.33	175.43
28	3	213	DD6	C29-C30-C31	-13.82	140.43	175.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	313	DD6	C37-C36-C31	-13.41	106.12	124.35
28	L	209	DD6	C29-C30-C31	-13.16	142.10	175.43
28	5	218	DD6	C29-C30-C31	-13.05	142.37	175.43
28	1	315	DD6	C3-C2-C1	-13.00	108.76	127.31
28	L	209	DD6	C37-C36-C31	-12.05	107.97	124.35
28	5	218	DD6	C37-C36-C31	-12.00	108.04	124.35
28	1	312	DD6	C37-C36-C31	-11.74	108.40	124.35
30	4	302	KC1	CMA-C3A-C4A	-11.70	107.22	125.04
28	3	213	DD6	C37-C36-C31	-11.65	108.52	124.35
28	3	213	DD6	C13-C11-C10	-11.45	101.37	118.94
27	J	105	5X6	C38-C30-C29	-11.33	111.81	124.53
28	1	315	DD6	C37-C36-C31	-11.29	109.00	124.35
30	2	211	KC1	CMA-C3A-C4A	-11.29	107.85	125.04
30	4	307	KC1	CMA-C3A-C4A	-11.20	107.98	125.04
28	2	217	DD6	C29-C30-C31	-11.13	147.25	175.43
19	B	826	CLA	O1A-CGA-CBA	-11.05	80.61	123.73
28	L	209	DD6	C9-C10-C11	-11.04	111.56	127.31
27	J	105	5X6	C19-C18-C17	-10.99	111.62	127.31
31	3	214	A86	C17-C16-C15	10.98	120.36	109.16
28	1	312	DD6	C12-C11-C10	-10.78	107.83	122.92
31	5	217	A86	C21-C20-C19	-10.72	102.22	114.28
31	3	212	A86	C17-C16-C15	10.66	120.04	109.16
30	3	208	KC1	CMA-C3A-C4A	-10.61	108.88	125.04
31	2	219	A86	C17-C16-C15	10.51	119.88	109.16
28	2	217	DD6	C37-C36-C31	-10.44	110.16	124.35
30	1	305	KC1	CMA-C3A-C4A	-10.24	109.44	125.04
30	2	211	KC1	C2A-C3A-C4A	-10.19	98.93	106.49
19	L	203	CLA	C1D-ND-C4D	-10.17	99.11	106.33
31	4	315	A86	C17-C16-C15	10.06	119.43	109.16
31	5	220	A86	O1-C20-C21	-10.02	103.05	115.06
19	4	308	CLA	C1D-ND-C4D	-9.94	99.27	106.33
28	5	218	DD6	C3-C2-C1	-9.94	113.12	127.31
28	1	313	DD6	C12-C11-C10	-9.94	109.00	122.92
19	2	212	CLA	C1D-ND-C4D	-9.87	99.33	106.33
28	2	217	DD6	C4-C5-C6	-9.85	113.25	127.31
31	5	221	A86	C21-C20-C19	-9.84	103.21	114.28
30	3	211	KC1	CMA-C3A-C4A	-9.84	110.06	125.04
27	J	105	5X6	C20-C21-C22	-9.82	113.29	127.31
30	3	205	KC1	C2A-C3A-C4A	-9.78	99.23	106.49
27	J	105	5X6	C24-C25-C26	-9.78	113.35	127.31
19	5	216	CLA	C1D-ND-C4D	-9.77	99.39	106.33
28	1	315	DD6	C13-C11-C10	-9.75	103.97	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	310	CLA	C1D-ND-C4D	-9.74	99.41	106.33
19	2	208	CLA	C1D-ND-C4D	-9.73	99.42	106.33
28	3	213	DD6	C3-C2-C1	-9.72	113.44	127.31
19	B	816	CLA	C1D-ND-C4D	-9.71	99.44	106.33
19	u	202	CLA	C1D-ND-C4D	-9.68	99.46	106.33
19	4	309	CLA	C1D-ND-C4D	-9.65	99.48	106.33
19	A	821	CLA	C1D-ND-C4D	-9.64	99.49	106.33
19	B	810	CLA	C1D-ND-C4D	-9.63	99.49	106.33
19	A	808	CLA	C1D-ND-C4D	-9.63	99.50	106.33
30	1	305	KC1	C2A-C3A-C4A	-9.60	99.36	106.49
19	A	817	CLA	C1D-ND-C4D	-9.60	99.51	106.33
30	4	302	KC1	C2A-C3A-C4A	-9.58	99.38	106.49
31	1	317	A86	C17-C16-C15	9.56	118.91	109.16
28	1	312	DD6	C3-C2-C1	-9.55	113.67	127.31
31	1	317	A86	O1-C20-C21	-9.54	103.62	115.06
19	4	303	CLA	C1D-ND-C4D	-9.54	99.56	106.33
19	A	806	CLA	C1D-ND-C4D	-9.53	99.56	106.33
19	A	818	CLA	C1D-ND-C4D	-9.53	99.57	106.33
28	1	313	DD6	C-C1-C2	-9.52	109.59	122.92
19	3	209	CLA	C1D-ND-C4D	-9.51	99.58	106.33
30	3	208	KC1	C2A-C3A-C4A	-9.51	99.43	106.49
31	2	218	A86	C17-C16-C15	9.51	118.86	109.16
19	5	215	CLA	C1D-ND-C4D	-9.49	99.59	106.33
19	4	304	CLA	C1D-ND-C4D	-9.49	99.60	106.33
28	1	313	DD6	C3-C2-C1	-9.49	113.77	127.31
19	2	207	CLA	C1D-ND-C4D	-9.49	99.60	106.33
19	1	309	CLA	C1D-ND-C4D	-9.48	99.60	106.33
19	2	213	CLA	C1D-ND-C4D	-9.47	99.61	106.33
19	4	301	CLA	C1D-ND-C4D	-9.46	99.62	106.33
19	B	823	CLA	C1D-ND-C4D	-9.44	99.63	106.33
28	1	313	DD6	C9-C10-C11	-9.44	113.84	127.31
28	1	315	DD6	C-C1-C2	-9.44	109.70	122.92
31	1	316	A86	O1-C20-C21	-9.44	103.75	115.06
19	1	307	CLA	C1D-ND-C4D	-9.44	99.63	106.33
31	5	220	A86	C21-C20-C19	-9.42	103.68	114.28
28	1	313	DD6	C4-C5-C6	-9.42	113.87	127.31
19	A	842	CLA	C1D-ND-C4D	-9.42	99.65	106.33
19	3	210	CLA	C1D-ND-C4D	-9.41	99.65	106.33
19	J	103	CLA	C1D-ND-C4D	-9.41	99.65	106.33
19	B	846	CLA	C1D-ND-C4D	-9.41	99.65	106.33
19	1	301	CLA	C1D-ND-C4D	-9.40	99.65	106.33
28	2	217	DD6	C13-C11-C10	-9.38	104.54	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	815	CLA	C1D-ND-C4D	-9.38	99.67	106.33
19	B	807	CLA	C1D-ND-C4D	-9.38	99.67	106.33
19	4	306	CLA	C1D-ND-C4D	-9.37	99.68	106.33
19	3	203	CLA	C1D-ND-C4D	-9.36	99.68	106.33
19	1	306	CLA	C1D-ND-C4D	-9.36	99.68	106.33
31	2	216	A86	C17-C16-C15	9.34	118.69	109.16
19	4	312	CLA	C1D-ND-C4D	-9.34	99.70	106.33
19	B	820	CLA	C1D-ND-C4D	-9.33	99.71	106.33
19	B	837	CLA	C1D-ND-C4D	-9.32	99.71	106.33
19	A	823	CLA	C1D-ND-C4D	-9.31	99.72	106.33
30	4	307	KC1	C2A-C3A-C4A	-9.31	99.58	106.49
19	B	819	CLA	C1D-ND-C4D	-9.30	99.73	106.33
19	B	805	CLA	C1D-ND-C4D	-9.29	99.74	106.33
19	A	840	CLA	C1D-ND-C4D	-9.29	99.74	106.33
28	2	217	DD6	C7-C6-C5	-9.29	109.91	122.92
30	3	211	KC1	C2A-C3A-C4A	-9.28	99.60	106.49
19	B	845	CLA	C1D-ND-C4D	-9.28	99.75	106.33
28	1	312	DD6	C4-C5-C6	-9.28	114.07	127.31
19	B	830	CLA	C1D-ND-C4D	-9.27	99.75	106.33
31	5	221	A86	O1-C20-C21	-9.26	103.95	115.06
19	5	214	CLA	C1D-ND-C4D	-9.25	99.76	106.33
19	A	828	CLA	C1D-ND-C4D	-9.25	99.77	106.33
31	1	316	A86	C17-C16-C15	9.24	118.59	109.16
31	4	314	A86	O1-C20-C21	-9.23	103.99	115.06
19	1	304	CLA	C1D-ND-C4D	-9.23	99.78	106.33
28	L	209	DD6	C4-C5-C6	-9.23	114.14	127.31
19	B	814	CLA	C1D-ND-C4D	-9.22	99.78	106.33
19	B	811	CLA	C1D-ND-C4D	-9.22	99.79	106.33
19	1	308	CLA	C1D-ND-C4D	-9.22	99.79	106.33
19	A	810	CLA	C1D-ND-C4D	-9.21	99.79	106.33
28	1	315	DD6	C29-C30-C31	-9.21	152.12	175.43
19	2	214	CLA	C1D-ND-C4D	-9.20	99.80	106.33
31	2	218	A86	C21-C20-C19	-9.20	103.93	114.28
28	1	313	DD6	C13-C11-C10	-9.19	104.83	118.94
19	4	313	CLA	C1D-ND-C4D	-9.19	99.81	106.33
31	4	315	A86	O1-C20-C21	-9.18	104.06	115.06
19	A	814	CLA	C1D-ND-C4D	-9.16	99.83	106.33
19	A	816	CLA	C1D-ND-C4D	-9.16	99.83	106.33
19	B	832	CLA	C1D-ND-C4D	-9.16	99.83	106.33
19	2	210	CLA	C1D-ND-C4D	-9.16	99.83	106.33
28	1	312	DD6	C-C1-C2	-9.15	110.10	122.92
27	J	105	5X6	C15-C14-C13	-9.15	114.26	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	819	CLA	C1D-ND-C4D	-9.14	99.84	106.33
19	2	215	CLA	C1D-ND-C4D	-9.14	99.84	106.33
19	A	811	CLA	C1D-ND-C4D	-9.14	99.84	106.33
28	L	209	DD6	C12-C11-C10	-9.13	110.13	122.92
28	5	218	DD6	C9-C10-C11	-9.13	114.29	127.31
19	A	843	CLA	C1D-ND-C4D	-9.11	99.86	106.33
28	5	218	DD6	C7-C6-C5	-9.11	110.16	122.92
19	B	829	CLA	C1D-ND-C4D	-9.11	99.86	106.33
28	1	313	DD6	C7-C6-C5	-9.10	110.17	122.92
31	4	316	A86	O1-C20-C21	-9.10	104.15	115.06
31	4	314	A86	C21-C20-C19	-9.09	104.05	114.28
19	A	880	CLA	C1D-ND-C4D	-9.09	99.87	106.33
19	2	209	CLA	C1D-ND-C4D	-9.09	99.88	106.33
28	2	217	DD6	C12-C11-C10	-9.08	110.20	122.92
19	A	827	CLA	C1D-ND-C4D	-9.08	99.89	106.33
31	5	219	A86	C17-C16-C15	9.07	118.42	109.16
28	2	217	DD6	C3-C2-C1	-9.07	114.37	127.31
19	3	202	CLA	C1D-ND-C4D	-9.06	99.90	106.33
28	L	209	DD6	C3-C2-C1	-9.05	114.39	127.31
19	B	831	CLA	C1D-ND-C4D	-9.05	99.90	106.33
31	5	219	A86	C25-C26-C27	-9.04	114.41	127.31
19	2	206	CLA	C1D-ND-C4D	-9.04	99.91	106.33
19	A	839	CLA	C1D-ND-C4D	-9.03	99.92	106.33
19	L	204	CLA	C1D-ND-C4D	-9.03	99.92	106.33
19	L	206	CLA	C1D-ND-C4D	-9.03	99.92	106.33
19	5	210	CLA	C1D-ND-C4D	-9.01	99.93	106.33
31	3	228	A86	C21-C20-C19	-9.01	104.14	114.28
19	5	213	CLA	C1D-ND-C4D	-9.01	99.94	106.33
19	A	844	CLA	C1D-ND-C4D	-9.01	99.94	106.33
19	3	206	CLA	C1D-ND-C4D	-9.00	99.94	106.33
19	5	211	CLA	C1D-ND-C4D	-9.00	99.94	106.33
27	J	105	5X6	C01-C02-C03	-9.00	114.43	124.53
19	F	204	CLA	C1D-ND-C4D	-8.98	99.95	106.33
19	B	817	CLA	C1D-ND-C4D	-8.98	99.96	106.33
19	A	832	CLA	C1D-ND-C4D	-8.97	99.96	106.33
19	2	205	CLA	C1D-ND-C4D	-8.97	99.96	106.33
19	B	804	CLA	C1D-ND-C4D	-8.95	99.97	106.33
19	5	207	CLA	C1D-ND-C4D	-8.95	99.98	106.33
19	A	836	CLA	C1D-ND-C4D	-8.94	99.98	106.33
19	u	201	CLA	C1D-ND-C4D	-8.94	99.99	106.33
31	3	212	A86	O1-C20-C21	-8.92	104.37	115.06
19	A	833	CLA	C1D-ND-C4D	-8.91	100.00	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	821	CLA	C1D-ND-C4D	-8.89	100.02	106.33
19	B	806	CLA	C1D-ND-C4D	-8.89	100.02	106.33
19	B	835	CLA	C1D-ND-C4D	-8.89	100.02	106.33
31	5	219	A86	C21-C20-C19	-8.88	104.29	114.28
19	A	830	CLA	C1D-ND-C4D	-8.88	100.03	106.33
19	A	804	CLA	C1D-ND-C4D	-8.87	100.03	106.33
19	3	204	CLA	C1D-ND-C4D	-8.87	100.04	106.33
28	L	209	DD6	C7-C6-C5	-8.86	110.51	122.92
19	B	827	CLA	C1D-ND-C4D	-8.86	100.04	106.33
19	A	813	CLA	C1D-ND-C4D	-8.86	100.04	106.33
19	B	812	CLA	C1D-ND-C4D	-8.85	100.05	106.33
19	A	824	CLA	C1D-ND-C4D	-8.84	100.05	106.33
19	A	807	CLA	C1D-ND-C4D	-8.83	100.06	106.33
19	5	209	CLA	C1D-ND-C4D	-8.82	100.07	106.33
31	1	316	A86	C21-C20-C19	-8.82	104.36	114.28
19	A	834	CLA	C1D-ND-C4D	-8.81	100.08	106.33
19	1	303	CLA	C1D-ND-C4D	-8.81	100.08	106.33
28	L	209	DD6	C-C1-C2	-8.80	110.60	122.92
19	A	841	CLA	C1D-ND-C4D	-8.79	100.09	106.33
28	5	218	DD6	C12-C11-C10	-8.78	110.62	122.92
19	F	203	CLA	C1D-ND-C4D	-8.78	100.10	106.33
19	A	812	CLA	C1D-ND-C4D	-8.77	100.10	106.33
28	1	315	DD6	C7-C6-C5	-8.76	110.65	122.92
19	A	802	CLA	C1D-ND-C4D	-8.76	100.11	106.33
19	4	311	CLA	C1D-ND-C4D	-8.74	100.12	106.33
19	5	212	CLA	C1D-ND-C4D	-8.74	100.13	106.33
19	A	828	CLA	C2D-C1D-ND	8.74	116.54	110.10
19	B	824	CLA	C1D-ND-C4D	-8.73	100.14	106.33
19	B	803	CLA	C1D-ND-C4D	-8.72	100.14	106.33
19	B	802	CLA	C1D-ND-C4D	-8.71	100.15	106.33
19	B	836	CLA	C1D-ND-C4D	-8.70	100.15	106.33
19	A	837	CLA	C1D-ND-C4D	-8.70	100.16	106.33
19	B	834	CLA	C1D-ND-C4D	-8.69	100.16	106.33
30	3	211	KC1	CMA-C3A-C2A	-8.68	107.04	128.30
30	4	307	KC1	CMA-C3A-C2A	-8.68	107.05	128.30
31	1	317	A86	C21-C20-C19	-8.67	104.52	114.28
19	1	310	CLA	C1D-ND-C4D	-8.67	100.18	106.33
19	A	815	CLA	C1D-ND-C4D	-8.67	100.18	106.33
19	A	825	CLA	C1D-ND-C4D	-8.66	100.18	106.33
19	3	207	CLA	C1D-ND-C4D	-8.66	100.18	106.33
19	A	831	CLA	C1D-ND-C4D	-8.65	100.19	106.33
19	A	829	CLA	C1D-ND-C4D	-8.65	100.19	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	203	CLA	C2D-C1D-ND	8.65	116.48	110.10
28	5	218	DD6	C-C1-C2	-8.65	110.81	122.92
19	B	808	CLA	C1D-ND-C4D	-8.63	100.20	106.33
19	2	212	CLA	C2D-C1D-ND	8.63	116.46	110.10
19	B	828	CLA	C1D-ND-C4D	-8.61	100.22	106.33
19	B	825	CLA	C1D-ND-C4D	-8.61	100.22	106.33
30	3	205	KC1	CMA-C3A-C4A	-8.61	111.93	125.04
19	A	826	CLA	C1D-ND-C4D	-8.60	100.23	106.33
19	A	878	CLA	C1D-ND-C4D	-8.59	100.23	106.33
28	1	312	DD6	C7-C6-C5	-8.59	110.90	122.92
19	4	305	CLA	C1D-ND-C4D	-8.57	100.25	106.33
19	5	208	CLA	C1D-ND-C4D	-8.57	100.25	106.33
28	1	315	DD6	C8-C6-C5	-8.56	105.81	118.94
31	5	220	A86	C33-C32-C31	8.55	117.52	109.21
31	4	315	A86	C21-C20-C19	-8.53	104.68	114.28
19	A	820	CLA	C1D-ND-C4D	-8.53	100.27	106.33
31	2	219	A86	C21-C20-C19	-8.53	104.68	114.28
19	B	813	CLA	C1D-ND-C4D	-8.53	100.28	106.33
19	B	838	CLA	C1D-ND-C4D	-8.50	100.30	106.33
19	A	835	CLA	C1D-ND-C4D	-8.50	100.30	106.33
19	B	826	CLA	C1D-ND-C4D	-8.48	100.31	106.33
31	2	219	A86	O1-C20-C21	-8.48	104.90	115.06
31	4	316	A86	C21-C20-C19	-8.44	104.79	114.28
19	u	202	CLA	C2D-C1D-ND	8.42	116.31	110.10
28	3	213	DD6	C12-C11-C10	-8.42	111.13	122.92
19	A	805	CLA	C1D-ND-C4D	-8.41	100.36	106.33
31	3	214	A86	O1-C20-C21	-8.38	105.02	115.06
28	2	217	DD6	C9-C10-C11	-8.37	115.37	127.31
19	A	809	CLA	C1D-ND-C4D	-8.36	100.39	106.33
28	5	218	DD6	C4-C5-C6	-8.35	115.39	127.31
19	B	833	CLA	C1D-ND-C4D	-8.34	100.41	106.33
19	2	208	CLA	C2D-C1D-ND	8.32	116.24	110.10
31	2	216	A86	C21-C20-C19	-8.29	104.95	114.28
19	A	821	CLA	C2D-C1D-ND	8.29	116.22	110.10
19	B	823	CLA	C2D-C1D-ND	8.27	116.20	110.10
28	3	213	DD6	C8-C6-C5	-8.26	106.27	118.94
19	B	818	CLA	C1D-ND-C4D	-8.26	100.47	106.33
19	5	216	CLA	C2D-C1D-ND	8.22	116.16	110.10
19	A	808	CLA	C2D-C1D-ND	8.21	116.15	110.10
19	B	824	CLA	C2D-C1D-ND	8.21	116.15	110.10
19	3	203	CLA	C2D-C1D-ND	8.19	116.14	110.10
19	2	213	CLA	C2D-C1D-ND	8.19	116.14	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	810	CLA	C2D-C1D-ND	8.18	116.14	110.10
19	B	816	CLA	C2D-C1D-ND	8.18	116.13	110.10
19	A	838	CLA	C1D-ND-C4D	-8.17	100.53	106.33
19	4	308	CLA	C2D-C1D-ND	8.17	116.12	110.10
19	B	837	CLA	C2D-C1D-ND	8.16	116.11	110.10
19	A	878	CLA	C2D-C1D-ND	8.15	116.11	110.10
19	B	846	CLA	C2D-C1D-ND	8.14	116.11	110.10
19	B	822	CLA	C1D-ND-C4D	-8.13	100.56	106.33
31	2	218	A86	C33-C32-C31	8.13	117.11	109.21
28	1	315	DD6	C12-C11-C10	-8.13	111.53	122.92
19	A	818	CLA	C2D-C1D-ND	8.12	116.09	110.10
31	3	228	A86	O1-C20-C21	-8.11	105.34	115.06
19	4	309	CLA	C2D-C1D-ND	8.06	116.04	110.10
19	A	826	CLA	C2D-C1D-ND	8.04	116.03	110.10
19	A	880	CLA	C2D-C1D-ND	8.03	116.02	110.10
19	A	803	CLA	C1D-ND-C4D	-8.03	100.63	106.33
19	B	804	CLA	C2D-C1D-ND	8.03	116.02	110.10
19	A	842	CLA	C2D-C1D-ND	8.02	116.02	110.10
28	1	313	DD6	C8-C6-C5	-8.02	106.64	118.94
19	A	822	CLA	C1D-ND-C4D	-8.01	100.64	106.33
28	1	312	DD6	C9-C10-C11	-8.01	115.88	127.31
19	B	807	CLA	C2D-C1D-ND	7.99	115.99	110.10
19	J	103	CLA	C2D-C1D-ND	7.99	115.99	110.10
19	B	802	CLA	C2D-C1D-ND	7.98	115.99	110.10
19	A	844	CLA	C2D-C1D-ND	7.98	115.98	110.10
19	4	303	CLA	C2D-C1D-ND	7.97	115.98	110.10
19	4	312	CLA	C2D-C1D-ND	7.97	115.98	110.10
19	4	306	CLA	C2D-C1D-ND	7.97	115.98	110.10
19	L	206	CLA	C2D-C1D-ND	7.97	115.98	110.10
19	A	817	CLA	C2D-C1D-ND	7.96	115.97	110.10
19	3	209	CLA	C2D-C1D-ND	7.96	115.97	110.10
28	3	213	DD6	C4-C5-C6	-7.95	115.96	127.31
19	A	840	CLA	C2D-C1D-ND	7.95	115.96	110.10
31	3	214	A86	C33-C32-C31	7.94	116.93	109.21
19	A	830	CLA	C2D-C1D-ND	7.92	115.94	110.10
28	3	213	DD6	C7-C6-C5	-7.91	111.84	122.92
19	B	815	CLA	C2D-C1D-ND	7.90	115.92	110.10
28	2	217	DD6	C32-C31-C36	-7.89	111.49	122.63
19	5	215	CLA	C2D-C1D-ND	7.88	115.91	110.10
19	2	210	CLA	C2D-C1D-ND	7.87	115.91	110.10
19	A	823	CLA	C2D-C1D-ND	7.87	115.90	110.10
19	5	213	CLA	C2D-C1D-ND	7.85	115.89	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	206	CLA	C2D-C1D-ND	7.85	115.89	110.10
19	A	811	CLA	C2D-C1D-ND	7.85	115.89	110.10
19	A	836	CLA	C2D-C1D-ND	7.82	115.86	110.10
19	F	203	CLA	C2D-C1D-ND	7.81	115.86	110.10
19	A	843	CLA	C2D-C1D-ND	7.81	115.86	110.10
19	B	829	CLA	C2D-C1D-ND	7.80	115.86	110.10
19	A	813	CLA	C2D-C1D-ND	7.80	115.85	110.10
19	1	308	CLA	C2D-C1D-ND	7.80	115.85	110.10
19	1	301	CLA	C2D-C1D-ND	7.80	115.85	110.10
28	2	217	DD6	C-C1-C2	-7.79	112.01	122.92
19	2	206	CLA	C2D-C1D-ND	7.79	115.84	110.10
19	5	211	CLA	C2D-C1D-ND	7.78	115.84	110.10
28	1	315	DD6	C32-C31-C36	-7.78	111.65	122.63
19	B	820	CLA	C2D-C1D-ND	7.78	115.83	110.10
19	B	845	CLA	C2D-C1D-ND	7.77	115.83	110.10
19	4	304	CLA	C2D-C1D-ND	7.75	115.82	110.10
19	B	814	CLA	C2D-C1D-ND	7.75	115.82	110.10
30	2	211	KC1	C2B-C1B-NB	7.73	115.80	110.10
19	A	804	CLA	C2D-C1D-ND	7.73	115.80	110.10
19	A	819	CLA	C2D-C1D-ND	7.71	115.79	110.10
19	B	835	CLA	C2D-C1D-ND	7.71	115.79	110.10
19	1	307	CLA	C2D-C1D-ND	7.71	115.78	110.10
30	3	208	KC1	CMA-C3A-C2A	-7.71	109.43	128.30
19	B	806	CLA	C2D-C1D-ND	7.70	115.78	110.10
19	B	832	CLA	C2D-C1D-ND	7.70	115.78	110.10
19	4	301	CLA	C2D-C1D-ND	7.70	115.78	110.10
28	2	217	DD6	C24-C1-C2	-7.69	107.14	118.94
30	4	302	KC1	C2B-C1B-NB	7.69	115.77	110.10
19	4	310	CLA	C2D-C1D-ND	7.69	115.77	110.10
19	A	839	CLA	C2D-C1D-ND	7.68	115.77	110.10
27	J	105	5X6	C12-C13-C14	-7.68	107.16	118.94
19	A	833	CLA	C2D-C1D-ND	7.68	115.76	110.10
19	A	802	CLA	C2D-C1D-ND	7.67	115.76	110.10
19	3	210	CLA	C2D-C1D-ND	7.67	115.76	110.10
19	B	830	CLA	C2D-C1D-ND	7.66	115.75	110.10
19	2	209	CLA	C2D-C1D-ND	7.66	115.75	110.10
19	2	205	CLA	C2D-C1D-ND	7.66	115.75	110.10
31	2	216	A86	O1-C20-C21	-7.65	105.89	115.06
19	A	841	CLA	C2D-C1D-ND	7.65	115.74	110.10
19	1	304	CLA	C2D-C1D-ND	7.65	115.74	110.10
19	3	204	CLA	C2D-C1D-ND	7.65	115.74	110.10
19	A	827	CLA	C2D-C1D-ND	7.65	115.74	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	5	217	A86	C17-C16-C15	7.64	116.95	109.16
18	A	801	CL0	C1D-ND-C4D	-7.64	100.91	106.33
31	5	219	A86	O1-C20-C21	-7.63	105.92	115.06
19	A	806	CLA	C2D-C1D-ND	7.62	115.72	110.10
19	B	819	CLA	C2D-C1D-ND	7.62	115.72	110.10
31	4	314	A86	C4-C5-C6	-7.62	116.44	127.31
19	2	207	CLA	C2D-C1D-ND	7.62	115.72	110.10
19	5	210	CLA	C2D-C1D-ND	7.61	115.71	110.10
19	B	808	CLA	C2D-C1D-ND	7.61	115.71	110.10
19	B	803	CLA	C2D-C1D-ND	7.61	115.71	110.10
19	B	809	CLA	C1D-ND-C4D	-7.58	100.95	106.33
19	B	825	CLA	C2D-C1D-ND	7.57	115.69	110.10
19	A	816	CLA	C2D-C1D-ND	7.57	115.69	110.10
19	3	202	CLA	C2D-C1D-ND	7.57	115.68	110.10
19	B	827	CLA	C2D-C1D-ND	7.56	115.68	110.10
19	A	831	CLA	C2D-C1D-ND	7.56	115.67	110.10
19	B	812	CLA	C2D-C1D-ND	7.55	115.67	110.10
30	4	302	KC1	CMA-C3A-C2A	-7.53	109.86	128.30
19	A	837	CLA	C2D-C1D-ND	7.53	115.65	110.10
19	B	817	CLA	C2D-C1D-ND	7.53	115.65	110.10
19	A	805	CLA	C2D-C1D-ND	7.52	115.65	110.10
19	A	803	CLA	C2D-C1D-ND	7.52	115.65	110.10
19	A	824	CLA	C2D-C1D-ND	7.51	115.64	110.10
31	3	214	A86	C21-C20-C19	-7.50	105.84	114.28
19	B	805	CLA	C2D-C1D-ND	7.50	115.63	110.10
19	A	807	CLA	C2D-C1D-ND	7.50	115.63	110.10
30	1	305	KC1	C2B-C1B-NB	7.50	115.63	110.10
19	5	212	CLA	C2D-C1D-ND	7.49	115.62	110.10
28	1	312	DD6	C13-C11-C10	-7.48	107.46	118.94
28	3	213	DD6	C-C1-C2	-7.48	112.44	122.92
19	B	833	CLA	C2D-C1D-ND	7.47	115.61	110.10
19	A	829	CLA	C2D-C1D-ND	7.46	115.61	110.10
19	B	834	CLA	C2D-C1D-ND	7.46	115.60	110.10
19	1	309	CLA	C2D-C1D-ND	7.46	115.60	110.10
19	B	813	CLA	C2D-C1D-ND	7.45	115.59	110.10
19	4	313	CLA	C2D-C1D-ND	7.45	115.59	110.10
19	1	306	CLA	C2D-C1D-ND	7.44	115.59	110.10
19	A	809	CLA	C2D-C1D-ND	7.44	115.59	110.10
19	A	815	CLA	C2D-C1D-ND	7.43	115.58	110.10
19	5	214	CLA	C2D-C1D-ND	7.43	115.58	110.10
28	1	315	DD6	C9-C10-C11	-7.42	116.72	127.31
19	A	814	CLA	C2D-C1D-ND	7.42	115.57	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	204	CLA	C2D-C1D-ND	7.42	115.57	110.10
31	3	212	A86	C21-C20-C19	-7.41	105.94	114.28
19	B	831	CLA	C2D-C1D-ND	7.41	115.56	110.10
19	A	810	CLA	C2D-C1D-ND	7.40	115.56	110.10
19	A	812	CLA	C2D-C1D-ND	7.39	115.55	110.10
19	A	835	CLA	C2D-C1D-ND	7.38	115.54	110.10
28	1	315	DD6	C4-C5-C6	-7.38	116.78	127.31
19	B	811	CLA	C2D-C1D-ND	7.34	115.52	110.10
30	1	305	KC1	C1A-C2A-C3A	-7.34	101.29	107.11
19	B	826	CLA	C2D-C1D-ND	7.34	115.51	110.10
19	2	215	CLA	C2D-C1D-ND	7.33	115.51	110.10
19	B	836	CLA	C2D-C1D-ND	7.30	115.49	110.10
30	4	307	KC1	C1A-C2A-C3A	-7.30	101.32	107.11
19	2	214	CLA	C2D-C1D-ND	7.29	115.47	110.10
31	2	216	A86	C33-C32-C31	7.26	116.27	109.21
19	B	821	CLA	C2D-C1D-ND	7.25	115.45	110.10
19	1	303	CLA	C2D-C1D-ND	7.25	115.45	110.10
19	A	832	CLA	C2D-C1D-ND	7.24	115.44	110.10
19	5	208	CLA	C2D-C1D-ND	7.24	115.44	110.10
28	1	313	DD6	C24-C1-C2	-7.23	107.84	118.94
19	B	822	CLA	C2D-C1D-ND	7.23	115.43	110.10
27	J	105	5X6	C42-C13-C14	-7.22	112.81	122.92
19	4	305	CLA	C2D-C1D-ND	7.22	115.43	110.10
30	3	205	KC1	C2B-C1B-NB	7.22	115.42	110.10
19	A	826	CLA	O2D-CGD-CBD	7.22	124.10	111.27
19	A	834	CLA	C2D-C1D-ND	7.20	115.41	110.10
19	B	838	CLA	C2D-C1D-ND	7.20	115.41	110.10
19	4	311	CLA	C2D-C1D-ND	7.19	115.41	110.10
19	1	306	CLA	CMD-C2D-C1D	7.18	137.37	124.71
19	F	204	CLA	C2D-C1D-ND	7.17	115.39	110.10
19	5	207	CLA	C2D-C1D-ND	7.17	115.39	110.10
19	B	818	CLA	C2D-C1D-ND	7.14	115.37	110.10
19	A	825	CLA	C2D-C1D-ND	7.14	115.37	110.10
30	3	211	KC1	C2B-C1B-NB	7.14	115.37	110.10
19	5	209	CLA	C2D-C1D-ND	7.13	115.36	110.10
19	B	803	CLA	CHD-C1D-ND	-7.13	117.90	124.45
19	B	828	CLA	C2D-C1D-ND	7.13	115.36	110.10
19	3	207	CLA	C2D-C1D-ND	7.12	115.35	110.10
19	4	310	CLA	CMD-C2D-C1D	7.10	137.23	124.71
19	A	820	CLA	C2D-C1D-ND	7.09	115.33	110.10
31	4	316	A86	C33-C32-C31	7.08	116.09	109.21
19	u	201	CLA	CMD-C2D-C1D	7.07	137.18	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	217	DD6	C8-C6-C5	-7.07	108.10	118.94
19	4	303	CLA	CMD-C2D-C1D	7.03	137.10	124.71
28	3	213	DD6	C9-C10-C11	-7.02	117.29	127.31
19	4	308	CLA	CHD-C1D-ND	-7.01	118.01	124.45
27	J	105	5X6	C27-C26-C25	-7.01	108.19	118.94
19	1	307	CLA	CMD-C2D-C1D	7.01	137.06	124.71
31	2	219	A86	C33-C32-C31	7.01	116.02	109.21
31	5	219	A86	C4-C5-C6	-6.99	117.33	127.31
19	B	803	CLA	CMD-C2D-C1D	6.99	137.03	124.71
19	B	809	CLA	C2D-C1D-ND	6.99	115.25	110.10
31	4	314	A86	C33-C32-C31	6.99	116.00	109.21
19	4	304	CLA	CMD-C2D-C1D	6.98	137.02	124.71
19	1	301	CLA	CMD-C2D-C1D	6.98	137.01	124.71
31	2	218	A86	O1-C20-C21	-6.98	106.70	115.06
31	1	317	A86	C33-C32-C31	6.97	115.99	109.21
19	A	838	CLA	C2D-C1D-ND	6.97	115.24	110.10
19	1	310	CLA	C2D-C1D-ND	6.96	115.24	110.10
19	3	210	CLA	CHD-C1D-ND	-6.96	118.06	124.45
30	2	211	KC1	CMA-C3A-C2A	-6.94	111.30	128.30
30	4	307	KC1	C2B-C1B-NB	6.94	115.22	110.10
19	A	814	CLA	CMD-C2D-C1D	6.93	136.93	124.71
30	1	305	KC1	CMA-C3A-C2A	-6.93	111.33	128.30
19	A	806	CLA	CMD-C2D-C1D	6.93	136.93	124.71
19	u	201	CLA	C2D-C1D-ND	6.93	115.21	110.10
19	B	804	CLA	O2D-CGD-CBD	6.93	123.58	111.27
19	4	310	CLA	CHD-C1D-ND	-6.93	118.09	124.45
30	3	211	KC1	C1A-C2A-C3A	-6.90	101.63	107.11
19	F	203	CLA	CMD-C2D-C1D	6.90	136.87	124.71
19	B	818	CLA	CMD-C2D-C1D	6.88	136.84	124.71
19	1	310	CLA	CMD-C2D-C1D	6.88	136.84	124.71
31	2	219	A86	C3-C2-C1	-6.88	117.50	127.31
19	A	834	CLA	CMD-C2D-C1D	6.88	136.83	124.71
19	B	817	CLA	CMD-C2D-C1D	6.87	136.83	124.71
27	J	105	5X6	C28-C27-C26	-6.87	115.85	126.23
19	4	312	CLA	CMD-C2D-C1D	6.87	136.82	124.71
19	A	822	CLA	C2D-C1D-ND	6.86	115.16	110.10
19	B	827	CLA	O2D-CGD-CBD	6.84	123.42	111.27
19	B	816	CLA	CHD-C1D-ND	-6.84	118.17	124.45
19	A	829	CLA	CMD-C2D-C1D	6.84	136.77	124.71
27	J	105	5X6	C19-C20-C21	-6.84	109.47	123.47
30	3	208	KC1	C2B-C1B-NB	6.84	115.14	110.10
19	4	304	CLA	CHD-C1D-ND	-6.83	118.17	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	818	CLA	CMD-C2D-C1D	6.83	136.74	124.71
19	5	211	CLA	CMD-C2D-C1D	6.82	136.74	124.71
28	3	213	DD6	C32-C31-C36	-6.81	113.02	122.63
19	2	208	CLA	CHD-C1D-ND	-6.80	118.21	124.45
19	4	308	CLA	CMD-C2D-C1D	6.80	136.69	124.71
19	B	824	CLA	CMD-C2D-C1D	6.78	136.66	124.71
19	1	306	CLA	CHD-C1D-ND	-6.78	118.22	124.45
31	5	220	A86	C17-C16-C15	6.78	116.08	109.16
31	5	221	A86	C33-C32-C31	6.77	115.80	109.21
19	B	829	CLA	CMD-C2D-C1D	6.77	136.65	124.71
19	F	204	CLA	CMD-C2D-C1D	6.76	136.62	124.71
19	2	214	CLA	CHD-C1D-ND	-6.74	118.26	124.45
19	5	210	CLA	CMD-C2D-C1D	6.74	136.59	124.71
27	J	105	5X6	C39-C26-C25	-6.73	113.49	122.92
30	4	302	KC1	C1A-C2A-C3A	-6.72	101.78	107.11
19	B	831	CLA	CHD-C1D-ND	-6.72	118.28	124.45
19	2	214	CLA	CMD-C2D-C1D	6.72	136.55	124.71
19	B	820	CLA	CMD-C2D-C1D	6.71	136.54	124.71
30	3	208	KC1	C1A-C2A-C3A	-6.71	101.79	107.11
19	5	214	CLA	CMD-C2D-C1D	6.70	136.52	124.71
19	B	810	CLA	CMD-C2D-C1D	6.70	136.52	124.71
19	4	301	CLA	CMD-C2D-C1D	6.69	136.51	124.71
19	4	312	CLA	CHD-C1D-ND	-6.69	118.31	124.45
19	5	209	CLA	CMD-C2D-C1D	6.68	136.49	124.71
19	B	831	CLA	CMD-C2D-C1D	6.68	136.49	124.71
19	B	807	CLA	CMD-C2D-C1D	6.66	136.46	124.71
19	A	813	CLA	CMD-C2D-C1D	6.66	136.46	124.71
19	A	833	CLA	CMD-C2D-C1D	6.66	136.46	124.71
19	A	835	CLA	CMD-C2D-C1D	6.66	136.45	124.71
27	J	105	5X6	C11-C12-C13	-6.66	116.17	126.23
30	2	211	KC1	CHB-C4A-C3A	-6.66	114.58	124.98
19	A	825	CLA	CMD-C2D-C1D	6.65	136.44	124.71
19	B	827	CLA	CMD-C2D-C1D	6.65	136.44	124.71
19	A	820	CLA	CMD-C2D-C1D	6.65	136.44	124.71
19	3	210	CLA	CMD-C2D-C1D	6.65	136.43	124.71
19	4	301	CLA	CHD-C1D-ND	-6.63	118.36	124.45
19	J	103	CLA	CMD-C2D-C1D	6.63	136.40	124.71
19	A	808	CLA	CMD-C2D-C1D	6.63	136.39	124.71
19	A	812	CLA	O2D-CGD-CBD	6.62	123.04	111.27
19	2	206	CLA	O2D-CGD-CBD	6.62	123.03	111.27
30	2	211	KC1	C3A-C4A-NA	6.61	117.79	110.57
19	A	802	CLA	CHD-C1D-ND	-6.61	118.38	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	807	CLA	CHD-C1D-ND	-6.61	118.38	124.45
19	B	832	CLA	CMD-C2D-C1D	6.61	136.37	124.71
19	A	806	CLA	CHD-C1D-ND	-6.60	118.39	124.45
19	A	812	CLA	CMD-C2D-C1D	6.60	136.34	124.71
30	3	205	KC1	C1A-C2A-C3A	-6.59	101.89	107.11
19	A	824	CLA	CMD-C2D-C1D	6.58	136.31	124.71
31	5	221	A86	C3-C2-C1	-6.57	117.93	127.31
19	B	813	CLA	CMD-C2D-C1D	6.57	136.30	124.71
19	3	204	CLA	CMD-C2D-C1D	6.57	136.29	124.71
19	2	207	CLA	CMD-C2D-C1D	6.55	136.26	124.71
19	B	821	CLA	CMD-C2D-C1D	6.55	136.26	124.71
19	4	303	CLA	CHD-C1D-ND	-6.55	118.43	124.45
19	1	308	CLA	CMD-C2D-C1D	6.55	136.26	124.71
19	5	207	CLA	CMD-C2D-C1D	6.55	136.26	124.71
19	B	830	CLA	CHD-C1D-ND	-6.53	118.45	124.45
19	3	209	CLA	CHD-C1D-ND	-6.53	118.45	124.45
31	3	214	A86	C3-C2-C1	-6.53	117.99	127.31
19	5	211	CLA	CHD-C1D-ND	-6.53	118.45	124.45
19	1	309	CLA	CMD-C2D-C1D	6.53	136.22	124.71
19	A	840	CLA	CMD-C2D-C1D	6.52	136.21	124.71
19	A	819	CLA	CMD-C2D-C1D	6.52	136.21	124.71
19	1	307	CLA	CHD-C1D-ND	-6.52	118.46	124.45
19	B	805	CLA	CMD-C2D-C1D	6.52	136.20	124.71
19	B	835	CLA	CMD-C2D-C1D	6.52	136.20	124.71
19	B	818	CLA	CHD-C1D-ND	-6.51	118.47	124.45
19	2	212	CLA	CMD-C2D-C1D	6.51	136.18	124.71
19	A	838	CLA	CMD-C2D-C1D	6.50	136.18	124.71
19	2	208	CLA	CMD-C2D-C1D	6.50	136.17	124.71
31	5	217	A86	O1-C20-C21	-6.50	107.27	115.06
19	A	829	CLA	CHD-C1D-ND	-6.49	118.49	124.45
19	4	313	CLA	CMD-C2D-C1D	6.49	136.15	124.71
19	A	841	CLA	CMD-C2D-C1D	6.47	136.12	124.71
19	A	826	CLA	CMD-C2D-C1D	6.47	136.12	124.71
19	L	204	CLA	CMD-C2D-C1D	6.46	136.10	124.71
19	5	208	CLA	CMD-C2D-C1D	6.46	136.10	124.71
19	B	819	CLA	CHD-C1D-ND	-6.46	118.52	124.45
31	5	220	A86	C36-C31-C32	-6.46	113.28	119.70
19	4	311	CLA	CMD-C2D-C1D	6.46	136.09	124.71
18	A	801	CL0	C2D-C1D-ND	6.45	114.86	110.10
19	4	309	CLA	CMD-C2D-C1D	6.45	136.07	124.71
30	2	211	KC1	C3B-C2B-C1B	-6.44	100.92	107.08
30	1	305	KC1	C3B-C2B-C1B	-6.44	100.93	107.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	810	CLA	CMD-C2D-C1D	6.44	136.06	124.71
19	A	814	CLA	CHD-C1D-ND	-6.44	118.54	124.45
19	A	808	CLA	CHD-C1D-ND	-6.43	118.55	124.45
19	2	206	CLA	CMD-C2D-C1D	6.43	136.04	124.71
19	B	816	CLA	CMD-C2D-C1D	6.43	136.04	124.71
19	B	832	CLA	CHD-C1D-ND	-6.43	118.55	124.45
19	A	832	CLA	CMD-C2D-C1D	6.43	136.04	124.71
19	1	303	CLA	CHD-C1D-ND	-6.43	118.55	124.45
19	3	203	CLA	CHD-C1D-ND	-6.42	118.56	124.45
19	A	816	CLA	CMD-C2D-C1D	6.41	136.02	124.71
19	1	303	CLA	CMD-C2D-C1D	6.41	136.01	124.71
19	3	207	CLA	CMD-C2D-C1D	6.41	136.01	124.71
31	4	314	A86	C17-C16-C15	6.41	115.70	109.16
19	B	837	CLA	CMD-C2D-C1D	6.41	136.00	124.71
19	A	835	CLA	CHD-C1D-ND	-6.40	118.57	124.45
19	B	823	CLA	CMD-C2D-C1D	6.39	135.98	124.71
19	B	834	CLA	CMD-C2D-C1D	6.39	135.98	124.71
19	B	824	CLA	O2D-CGD-CBD	6.39	122.63	111.27
30	1	305	KC1	C3A-C4A-NA	6.39	117.55	110.57
19	3	206	CLA	CMD-C2D-C1D	6.39	135.97	124.71
28	L	209	DD6	C13-C11-C10	-6.38	109.15	118.94
19	B	830	CLA	O2D-CGD-CBD	6.38	122.61	111.27
27	J	105	5X6	C16-C17-C18	-6.38	109.15	118.94
19	B	815	CLA	CMD-C2D-C1D	6.38	135.96	124.71
19	B	806	CLA	CMD-C2D-C1D	6.38	135.95	124.71
19	A	818	CLA	CHD-C1D-ND	-6.38	118.59	124.45
19	B	805	CLA	CHD-C1D-ND	-6.37	118.60	124.45
19	2	215	CLA	CMD-C2D-C1D	6.37	135.94	124.71
19	B	823	CLA	CHD-C1D-ND	-6.37	118.60	124.45
19	4	306	CLA	CHD-C1D-ND	-6.37	118.60	124.45
19	5	213	CLA	CMD-C2D-C1D	6.37	135.94	124.71
19	A	841	CLA	CHD-C1D-ND	-6.37	118.60	124.45
19	A	805	CLA	O2D-CGD-CBD	6.36	122.58	111.27
19	1	308	CLA	C4A-NA-C1A	-6.36	103.85	106.71
19	5	213	CLA	CHD-C1D-ND	-6.36	118.61	124.45
19	B	828	CLA	CMD-C2D-C1D	6.36	135.92	124.71
19	B	845	CLA	CMD-C2D-C1D	6.36	135.92	124.71
19	2	207	CLA	CHD-C1D-ND	-6.36	118.61	124.45
19	5	209	CLA	CHD-C1D-ND	-6.35	118.62	124.45
19	B	817	CLA	CHD-C1D-ND	-6.35	118.62	124.45
19	B	846	CLA	CMD-C2D-C1D	6.35	135.90	124.71
19	A	825	CLA	CHD-C1D-ND	-6.34	118.63	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	819	CLA	CMD-C2D-C1D	6.34	135.88	124.71
19	2	213	CLA	CMD-C2D-C1D	6.34	135.88	124.71
19	A	812	CLA	CHD-C1D-ND	-6.33	118.64	124.45
19	4	306	CLA	CMD-C2D-C1D	6.33	135.87	124.71
19	F	203	CLA	CHD-C1D-ND	-6.33	118.64	124.45
19	u	202	CLA	CMD-C2D-C1D	6.33	135.86	124.71
28	5	218	DD6	C12-C11-C13	-6.32	108.11	118.08
19	5	216	CLA	CMD-C2D-C1D	6.32	135.86	124.71
19	A	811	CLA	CHD-C1D-ND	-6.32	118.64	124.45
19	1	309	CLA	CHD-C1D-ND	-6.32	118.65	124.45
19	1	304	CLA	CHD-C1D-ND	-6.31	118.65	124.45
19	1	310	CLA	CHD-C1D-ND	-6.31	118.65	124.45
31	3	214	A86	C20-C19-C18	-6.31	100.27	112.75
19	A	839	CLA	CMD-C2D-C1D	6.31	135.83	124.71
28	L	209	DD6	C24-C1-C2	-6.30	109.27	118.94
19	B	804	CLA	CHD-C1D-ND	-6.30	118.67	124.45
19	4	313	CLA	CHD-C1D-ND	-6.30	118.67	124.45
28	L	209	DD6	C8-C6-C5	-6.30	109.28	118.94
19	B	815	CLA	CHD-C1D-ND	-6.29	118.67	124.45
19	B	820	CLA	CHD-C1D-ND	-6.29	118.67	124.45
19	B	804	CLA	CMD-C2D-C1D	6.29	135.81	124.71
19	3	207	CLA	CHD-C1D-ND	-6.29	118.67	124.45
19	A	807	CLA	CMD-C2D-C1D	6.29	135.79	124.71
19	4	311	CLA	CHD-C1D-ND	-6.29	118.68	124.45
19	A	837	CLA	CMD-C2D-C1D	6.28	135.78	124.71
19	3	203	CLA	CMD-C2D-C1D	6.28	135.78	124.71
27	J	105	5X6	C41-C17-C18	-6.27	114.13	122.92
19	A	842	CLA	CMD-C2D-C1D	6.27	135.77	124.71
19	B	812	CLA	CMD-C2D-C1D	6.27	135.76	124.71
19	5	215	CLA	CMD-C2D-C1D	6.27	135.76	124.71
19	A	827	CLA	CMD-C2D-C1D	6.26	135.75	124.71
30	2	211	KC1	C1A-C2A-C3A	-6.26	102.14	107.11
19	F	204	CLA	CHD-C1D-ND	-6.26	118.70	124.45
30	4	307	KC1	C3A-C4A-NA	6.25	117.39	110.57
19	B	815	CLA	O2D-CGD-CBD	6.25	122.37	111.27
19	u	202	CLA	CHD-C1D-ND	-6.24	118.72	124.45
19	5	214	CLA	CHD-C1D-ND	-6.24	118.72	124.45
19	4	305	CLA	CMD-C2D-C1D	6.24	135.72	124.71
30	3	205	KC1	C3A-C4A-NA	6.24	117.38	110.57
19	A	822	CLA	CMD-C2D-C1D	6.24	135.70	124.71
19	B	834	CLA	CHD-C1D-ND	-6.23	118.72	124.45
19	B	814	CLA	CHD-C1D-ND	-6.23	118.73	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	817	CLA	CHD-C1D-ND	-6.23	118.73	124.45
19	1	301	CLA	CHD-C1D-ND	-6.23	118.73	124.45
19	5	210	CLA	CHD-C1D-ND	-6.22	118.73	124.45
19	B	814	CLA	CMD-C2D-C1D	6.22	135.68	124.71
19	A	880	CLA	CHD-C1D-ND	-6.22	118.74	124.45
19	L	204	CLA	CHD-C1D-ND	-6.22	118.74	124.45
19	A	844	CLA	O2D-CGD-CBD	6.22	122.32	111.27
19	B	829	CLA	CHD-C1D-ND	-6.22	118.74	124.45
19	A	827	CLA	CHD-C1D-ND	-6.21	118.74	124.45
19	A	802	CLA	CMD-C2D-C1D	6.21	135.66	124.71
19	B	811	CLA	CHD-C1D-ND	-6.21	118.75	124.45
19	5	212	CLA	CMD-C2D-C1D	6.20	135.64	124.71
30	3	205	KC1	CHB-C4A-C3A	-6.20	115.29	124.98
19	A	831	CLA	O2D-CGD-CBD	6.19	122.28	111.27
19	A	810	CLA	CHD-C1D-ND	-6.19	118.76	124.45
19	5	215	CLA	CHD-C1D-ND	-6.19	118.77	124.45
19	A	811	CLA	CMD-C2D-C1D	6.19	135.62	124.71
19	B	822	CLA	O2D-CGD-CBD	6.19	122.26	111.27
19	2	215	CLA	CHD-C1D-ND	-6.19	118.77	124.45
19	L	206	CLA	O2D-CGD-CBD	6.18	122.26	111.27
19	A	823	CLA	CMD-C2D-C1D	6.18	135.61	124.71
19	5	207	CLA	CHD-C1D-ND	-6.18	118.77	124.45
19	2	212	CLA	CHD-C4C-C3C	-6.18	115.76	124.84
19	5	208	CLA	CHD-C1D-ND	-6.18	118.78	124.45
19	L	203	CLA	CHD-C1D-ND	-6.17	118.78	124.45
19	5	216	CLA	CHD-C1D-ND	-6.17	118.78	124.45
28	1	312	DD6	C24-C1-C2	-6.17	109.47	118.94
19	A	808	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
19	3	206	CLA	CHD-C1D-ND	-6.17	118.78	124.45
19	B	822	CLA	CMD-C2D-C1D	6.17	135.59	124.71
19	A	823	CLA	CHD-C1D-ND	-6.17	118.78	124.45
30	4	302	KC1	C3B-C2B-C1B	-6.16	101.19	107.08
19	A	837	CLA	CHD-C1D-ND	-6.16	118.79	124.45
19	A	826	CLA	CHD-C4C-C3C	-6.16	115.79	124.84
19	A	807	CLA	CHD-C1D-ND	-6.15	118.80	124.45
19	A	817	CLA	CMD-C2D-C1D	6.14	135.54	124.71
19	u	202	CLA	CHD-C4C-C3C	-6.14	115.81	124.84
19	1	304	CLA	CMD-C2D-C1D	6.14	135.53	124.71
19	B	808	CLA	O2D-CGD-CBD	6.13	122.17	111.27
19	B	838	CLA	O2D-CGD-CBD	6.13	122.17	111.27
19	4	309	CLA	CHD-C1D-ND	-6.13	118.82	124.45
19	A	816	CLA	CHD-C1D-ND	-6.13	118.82	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	815	CLA	CMD-C2D-C1D	6.13	135.51	124.71
30	1	305	KC1	CHB-C4A-C3A	-6.13	115.41	124.98
19	A	804	CLA	CMD-C2D-C1D	6.12	135.51	124.71
19	4	312	CLA	C4A-NA-C1A	-6.12	103.95	106.71
19	A	819	CLA	CHD-C1D-ND	-6.12	118.83	124.45
19	A	833	CLA	CHD-C1D-ND	-6.12	118.83	124.45
27	J	105	5X6	C27-C28-C29	-6.11	110.03	127.20
19	3	209	CLA	CMD-C2D-C1D	6.11	135.49	124.71
19	B	810	CLA	CHD-C4C-C3C	-6.11	115.85	124.84
19	A	878	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
19	A	828	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
19	A	828	CLA	CMD-C2D-C1D	6.11	135.47	124.71
19	A	805	CLA	CMD-C2D-C1D	6.10	135.47	124.71
19	A	828	CLA	CHD-C1D-ND	-6.10	118.85	124.45
19	2	207	CLA	O2D-CGD-CBD	6.10	122.11	111.27
19	B	826	CLA	CMD-C2D-C1D	6.10	135.47	124.71
19	A	840	CLA	CHD-C1D-ND	-6.10	118.85	124.45
30	4	302	KC1	CHB-C4A-C3A	-6.09	115.46	124.98
19	3	202	CLA	CMD-C2D-C1D	6.09	135.45	124.71
19	L	206	CLA	CMD-C2D-C1D	6.09	135.45	124.71
19	A	809	CLA	CMD-C2D-C1D	6.09	135.45	124.71
19	2	212	CLA	CHD-C1D-ND	-6.09	118.86	124.45
19	B	846	CLA	CHD-C1D-ND	-6.09	118.86	124.45
30	3	208	KC1	C3A-C4A-NA	6.09	117.22	110.57
30	4	307	KC1	C1A-NA-C4A	-6.09	103.97	106.71
19	A	821	CLA	O2D-CGD-CBD	6.09	122.09	111.27
19	3	202	CLA	CHD-C1D-ND	-6.08	118.86	124.45
19	A	844	CLA	CMD-C2D-C1D	6.07	135.42	124.71
19	3	204	CLA	CHD-C1D-ND	-6.07	118.88	124.45
19	1	308	CLA	CHD-C1D-ND	-6.06	118.88	124.45
19	B	808	CLA	CMD-C2D-C1D	6.06	135.40	124.71
19	4	303	CLA	O2D-CGD-CBD	6.06	122.04	111.27
19	A	821	CLA	CHD-C1D-ND	-6.06	118.89	124.45
19	B	824	CLA	CHD-C1D-ND	-6.06	118.89	124.45
19	B	808	CLA	CHD-C4C-C3C	-6.05	115.94	124.84
30	3	211	KC1	C3A-C4A-NA	6.05	117.17	110.57
19	B	828	CLA	CHD-C1D-ND	-6.05	118.90	124.45
28	1	312	DD6	C8-C6-C5	-6.04	109.67	118.94
19	B	811	CLA	CMD-C2D-C1D	6.04	135.36	124.71
19	B	833	CLA	CMD-C2D-C1D	6.04	135.35	124.71
19	B	823	CLA	O2D-CGD-CBD	6.03	121.99	111.27
31	5	221	A86	C17-C16-C15	6.03	115.32	109.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	824	CLA	CHD-C1D-ND	-6.03	118.91	124.45
19	B	835	CLA	CHD-C1D-ND	-6.03	118.91	124.45
19	B	836	CLA	CMD-C2D-C1D	6.02	135.33	124.71
19	A	843	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
30	3	205	KC1	C3B-C2B-C1B	-6.01	101.33	107.08
19	A	832	CLA	CHD-C1D-ND	-6.01	118.93	124.45
19	A	844	CLA	CHD-C1D-ND	-6.01	118.93	124.45
28	1	315	DD6	C35-C36-C31	-6.01	106.93	120.57
19	B	824	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
19	B	809	CLA	CMD-C2D-C1D	6.00	135.28	124.71
19	B	812	CLA	CHD-C1D-ND	-6.00	118.94	124.45
19	2	210	CLA	CMD-C2D-C1D	6.00	135.28	124.71
19	B	821	CLA	CHD-C1D-ND	-5.99	118.95	124.45
19	u	201	CLA	CHD-C1D-ND	-5.99	118.95	124.45
19	4	304	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
19	A	880	CLA	CMD-C2D-C1D	5.99	135.26	124.71
19	B	802	CLA	CHD-C4C-C3C	-5.98	116.04	124.84
19	A	839	CLA	CHD-C1D-ND	-5.98	118.95	124.45
30	4	302	KC1	C3A-C4A-NA	5.98	117.10	110.57
30	4	307	KC1	CHB-C4A-C3A	-5.97	115.65	124.98
28	5	218	DD6	C32-C31-C36	-5.97	114.20	122.63
19	B	810	CLA	CHD-C1D-ND	-5.97	118.97	124.45
19	2	212	CLA	O2D-CGD-CBD	5.97	121.88	111.27
19	A	821	CLA	CMD-C2D-C1D	5.97	135.23	124.71
28	5	218	DD6	C8-C6-C5	-5.96	109.79	118.94
19	B	845	CLA	O2D-CGD-CBD	5.96	121.86	111.27
19	B	837	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
31	3	214	A86	C36-C31-C32	-5.95	113.79	119.70
19	B	833	CLA	CHD-C1D-ND	-5.95	118.98	124.45
19	B	811	CLA	O2D-CGD-CBD	5.95	121.85	111.27
31	2	219	A86	C25-C26-C27	-5.95	118.81	127.31
19	5	212	CLA	CHD-C1D-ND	-5.95	118.99	124.45
19	2	213	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
19	L	203	CLA	CMD-C2D-C1D	5.94	135.19	124.71
27	J	105	5X6	C23-C22-C21	-5.94	109.82	118.94
30	3	211	KC1	CHB-C4A-C3A	-5.94	115.70	124.98
19	A	832	CLA	O2D-CGD-CBD	5.94	121.82	111.27
19	A	821	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
19	A	814	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
19	2	213	CLA	CHD-C1D-ND	-5.93	119.00	124.45
19	2	210	CLA	CHD-C1D-ND	-5.93	119.01	124.45
19	A	835	CLA	C4A-NA-C1A	-5.92	104.04	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	813	CLA	CHD-C1D-ND	-5.92	119.01	124.45
19	A	820	CLA	CHD-C1D-ND	-5.92	119.01	124.45
31	5	219	A86	C36-C31-C32	-5.92	113.82	119.70
19	J	103	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
19	4	305	CLA	CHD-C1D-ND	-5.92	119.02	124.45
19	3	206	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
28	1	312	DD6	C-C1-C24	-5.91	108.76	118.08
19	B	809	CLA	C2C-C1C-NC	5.91	115.51	109.97
19	B	825	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
19	A	836	CLA	CHD-C1D-ND	-5.90	119.03	124.45
19	A	842	CLA	CHD-C1D-ND	-5.90	119.03	124.45
28	5	218	DD6	C21-C20-C15	-5.90	112.37	122.26
30	3	211	KC1	C3B-C2B-C1B	-5.89	101.45	107.08
19	B	830	CLA	CMD-C2D-C1D	5.88	135.08	124.71
19	A	817	CLA	CHD-C4C-C3C	-5.88	116.19	124.84
30	3	208	KC1	CHB-C4A-C3A	-5.88	115.79	124.98
19	2	210	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
19	2	209	CLA	CHD-C1D-ND	-5.87	119.06	124.45
19	A	813	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
19	A	838	CLA	CHD-C1D-ND	-5.87	119.06	124.45
19	B	806	CLA	CHD-C1D-ND	-5.87	119.06	124.45
19	3	210	CLA	CHD-C4C-C3C	-5.87	116.22	124.84
19	2	206	CLA	CHD-C1D-ND	-5.86	119.06	124.45
19	A	831	CLA	C2C-C1C-NC	5.86	115.46	109.97
19	A	843	CLA	CMD-C2D-C1D	5.86	135.04	124.71
19	A	815	CLA	CHD-C1D-ND	-5.86	119.07	124.45
19	B	827	CLA	CHD-C1D-ND	-5.86	119.07	124.45
19	J	103	CLA	CHD-C1D-ND	-5.86	119.07	124.45
19	B	833	CLA	C4A-NA-C1A	-5.85	104.07	106.71
19	5	210	CLA	C2C-C1C-NC	5.85	115.46	109.97
19	B	820	CLA	O2D-CGD-CBD	5.85	121.67	111.27
19	B	822	CLA	CHD-C1D-ND	-5.85	119.08	124.45
19	B	818	CLA	O2D-CGD-CBD	5.85	121.67	111.27
27	J	105	5X6	C40-C22-C21	-5.85	114.73	122.92
19	3	202	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
19	A	809	CLA	O2D-CGD-CBD	5.85	121.66	111.27
19	A	813	CLA	CHD-C1D-ND	-5.84	119.09	124.45
18	A	801	CL0	CMD-C2D-C1D	5.84	135.00	124.71
19	A	822	CLA	C4A-NA-C1A	-5.84	104.08	106.71
19	A	828	CLA	O2D-CGD-CBD	5.83	121.63	111.27
19	1	309	CLA	CHD-C4C-C3C	-5.83	116.28	124.84
19	A	804	CLA	CHD-C1D-ND	-5.82	119.10	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	209	DD6	C14-C13-C11	-5.81	116.51	125.53
19	B	838	CLA	CHD-C1D-ND	-5.81	119.11	124.45
19	A	844	CLA	CHD-C4C-C3C	-5.81	116.31	124.84
31	4	316	A86	C4-C5-C6	-5.80	119.03	127.31
30	3	211	KC1	C1A-NA-C4A	-5.79	104.10	106.71
19	B	806	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
19	B	802	CLA	CHD-C1D-ND	-5.79	119.14	124.45
19	A	802	CLA	C4A-NA-C1A	-5.79	104.10	106.71
19	B	829	CLA	C4A-NA-C1A	-5.79	104.10	106.71
19	A	835	CLA	O2D-CGD-CBD	5.79	121.55	111.27
19	B	813	CLA	O2D-CGD-CBD	5.79	121.55	111.27
19	B	838	CLA	CMD-C2D-C1D	5.78	134.91	124.71
19	B	802	CLA	CMD-C2D-C1D	5.78	134.91	124.71
30	3	208	KC1	C3B-C2B-C1B	-5.78	101.56	107.08
19	L	206	CLA	CHD-C1D-ND	-5.77	119.15	124.45
19	A	804	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
28	1	313	DD6	C32-C31-C36	-5.77	114.49	122.63
19	A	805	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
19	A	811	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
19	B	845	CLA	CHD-C1D-ND	-5.76	119.16	124.45
19	4	309	CLA	C2C-C1C-NC	5.76	115.36	109.97
31	2	218	A86	C4-C5-C6	-5.76	119.10	127.31
19	B	834	CLA	CHD-C4C-C3C	-5.75	116.38	124.84
19	3	204	CLA	O2D-CGD-CBD	5.75	121.49	111.27
19	A	827	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
19	B	817	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
19	1	306	CLA	C4A-NA-C1A	-5.75	104.12	106.71
19	A	810	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
19	B	830	CLA	C4A-NA-C1A	-5.74	104.12	106.71
19	B	846	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
31	1	317	A86	C4-C5-C6	-5.74	119.12	127.31
19	2	207	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
19	3	203	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
19	B	845	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
19	F	203	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
19	5	213	CLA	C4A-NA-C1A	-5.73	104.13	106.71
19	2	209	CLA	CMD-C2D-C1D	5.73	134.81	124.71
28	2	217	DD6	C12-C11-C13	-5.73	109.06	118.08
19	A	809	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
28	1	312	DD6	C32-C31-C36	-5.72	114.55	122.63
19	B	832	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
19	4	313	CLA	O2D-CGD-CBD	5.72	121.42	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	306	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
19	B	805	CLA	O2D-CGD-CBD	5.70	121.41	111.27
19	B	829	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
19	A	840	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
19	4	310	CLA	O2D-CGD-CBD	5.70	121.39	111.27
19	A	878	CLA	CHD-C1D-ND	-5.69	119.22	124.45
19	3	207	CLA	O2D-CGD-CBD	5.69	121.38	111.27
19	4	308	CLA	CHD-C4C-C3C	-5.69	116.48	124.84
19	5	213	CLA	C2C-C1C-NC	5.69	115.30	109.97
19	A	830	CLA	CMD-C2D-C1D	5.69	134.73	124.71
19	B	813	CLA	C2C-C1C-NC	5.68	115.30	109.97
19	L	204	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
19	A	880	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
19	A	839	CLA	C2C-C1C-NC	5.68	115.29	109.97
19	A	878	CLA	CMD-C2D-C1D	5.68	134.72	124.71
19	B	837	CLA	CHD-C1D-ND	-5.68	119.24	124.45
19	A	822	CLA	CHD-C1D-ND	-5.67	119.24	124.45
19	1	308	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
19	A	836	CLA	CMD-C2D-C1D	5.66	134.69	124.71
19	5	211	CLA	C2C-C1C-NC	5.66	115.28	109.97
19	A	819	CLA	C4A-NA-C1A	-5.66	104.16	106.71
31	5	221	A86	C4-C5-C6	-5.66	119.23	127.31
19	B	825	CLA	CMD-C2D-C1D	5.66	134.69	124.71
19	B	814	CLA	O2D-CGD-CBD	5.66	121.32	111.27
19	B	812	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
19	A	805	CLA	CHD-C1D-ND	-5.66	119.25	124.45
19	A	841	CLA	CHD-C4C-C3C	-5.66	116.53	124.84
19	1	301	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
18	A	801	CL0	C2C-C1C-NC	5.65	115.27	109.97
19	4	310	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
19	A	830	CLA	CHD-C1D-ND	-5.65	119.27	124.45
19	3	209	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
19	2	208	CLA	O2D-CGD-CBD	5.64	121.30	111.27
19	B	820	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
19	5	216	CLA	C2C-C1C-NC	5.64	115.25	109.97
19	L	203	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
19	B	838	CLA	CHD-C4C-C3C	-5.64	116.56	124.84
19	4	301	CLA	C4A-NA-C1A	-5.63	104.17	106.71
19	B	814	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
31	5	220	A86	C3-C2-C1	-5.63	119.27	127.31
19	A	806	CLA	O2D-CGD-CBD	5.63	121.27	111.27
19	2	206	CLA	C2C-C1C-NC	5.63	115.25	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	215	CLA	O2D-CGD-CBD	5.63	121.27	111.27
19	A	823	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
19	B	835	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
19	A	824	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
31	2	216	A86	C20-C19-C18	-5.62	101.64	112.75
19	B	835	CLA	C2C-C1C-NC	5.61	115.23	109.97
19	2	214	CLA	O2D-CGD-CBD	5.61	121.23	111.27
19	1	301	CLA	C2C-C1C-NC	5.61	115.22	109.97
19	B	818	CLA	C2C-C1C-NC	5.61	115.22	109.97
19	A	834	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
19	A	820	CLA	CHD-C4C-C3C	-5.60	116.60	124.84
19	B	833	CLA	CHD-C4C-C3C	-5.60	116.60	124.84
19	3	204	CLA	CHD-C4C-C3C	-5.60	116.60	124.84
19	2	205	CLA	CHD-C1D-ND	-5.60	119.31	124.45
19	A	802	CLA	O2D-CGD-CBD	5.60	121.21	111.27
19	B	838	CLA	C2C-C1C-NC	5.60	115.22	109.97
18	A	801	CL0	O2D-CGD-CBD	5.60	121.21	111.27
19	A	834	CLA	CHD-C1D-ND	-5.60	119.31	124.45
19	A	809	CLA	C2C-C1C-NC	5.59	115.21	109.97
19	A	825	CLA	C2C-C1C-NC	5.59	115.21	109.97
19	B	826	CLA	C2C-C1C-NC	5.59	115.21	109.97
19	B	845	CLA	C2C-C1C-NC	5.59	115.21	109.97
19	u	201	CLA	C2C-C1C-NC	5.59	115.21	109.97
19	A	831	CLA	CMD-C2D-C1D	5.59	134.56	124.71
19	5	207	CLA	CHD-C4C-C3C	-5.59	116.63	124.84
19	A	832	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
19	5	208	CLA	C4A-NA-C1A	-5.58	104.20	106.71
19	A	842	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
30	1	305	KC1	O2D-CGD-CBD	5.57	121.16	111.27
19	A	842	CLA	C2C-C1C-NC	5.56	115.19	109.97
19	4	311	CLA	C4A-NA-C1A	-5.55	104.21	106.71
30	3	205	KC1	C3C-C4C-NC	5.55	115.10	109.88
28	L	209	DD6	C32-C31-C36	-5.54	114.81	122.63
19	2	215	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
19	A	807	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
19	B	828	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
31	4	315	A86	C4-C5-C6	-5.54	119.41	127.31
19	B	823	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
30	4	307	KC1	C3B-C2B-C1B	-5.54	101.79	107.08
19	2	205	CLA	CMD-C2D-C1D	5.53	134.46	124.71
19	B	804	CLA	C2C-C1C-NC	5.53	115.16	109.97
19	A	833	CLA	CHD-C4C-C3C	-5.53	116.71	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	206	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
19	4	313	CLA	C2C-C1C-NC	5.53	115.15	109.97
19	A	835	CLA	C2C-C1C-NC	5.53	115.15	109.97
19	L	203	CLA	O2D-CGD-CBD	5.52	121.08	111.27
19	A	834	CLA	C2C-C1C-NC	5.52	115.14	109.97
19	A	837	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
19	A	818	CLA	CHD-C4C-C3C	-5.51	116.73	124.84
28	L	209	DD6	C7-C6-C8	-5.51	109.39	118.08
19	A	804	CLA	C4A-NA-C1A	-5.51	104.23	106.71
19	3	203	CLA	C4A-NA-C1A	-5.51	104.23	106.71
19	B	807	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
19	5	210	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
19	A	829	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
19	A	837	CLA	O2D-CGD-CBD	5.50	121.05	111.27
30	1	305	KC1	C1A-NA-C4A	-5.50	104.23	106.71
19	F	204	CLA	O2D-CGD-CBD	5.50	121.04	111.27
19	B	808	CLA	C2C-C1C-NC	5.50	115.12	109.97
19	A	830	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
19	B	838	CLA	C4A-NA-C1A	-5.49	104.24	106.71
19	A	831	CLA	CHD-C1D-ND	-5.49	119.41	124.45
19	5	212	CLA	CHD-C4C-C3C	-5.49	116.78	124.84
19	B	827	CLA	C2C-C1C-NC	5.49	115.11	109.97
19	A	809	CLA	CHD-C1D-ND	-5.48	119.42	124.45
19	2	206	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
19	2	208	CLA	C2C-C1C-NC	5.48	115.11	109.97
19	4	303	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
19	A	816	CLA	O2D-CGD-CBD	5.48	121.00	111.27
19	B	837	CLA	C2C-C1C-NC	5.47	115.10	109.97
19	A	815	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
19	B	822	CLA	C2C-C1C-NC	5.47	115.09	109.97
30	3	205	KC1	CMA-C3A-C2A	-5.46	114.92	128.30
19	A	837	CLA	C4A-NA-C1A	-5.46	104.25	106.71
28	5	218	DD6	C-C1-C24	-5.46	109.47	118.08
19	B	809	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
19	A	826	CLA	C2C-C1C-NC	5.46	115.08	109.97
19	B	833	CLA	C2C-C1C-NC	5.45	115.08	109.97
19	A	838	CLA	O2D-CGD-CBD	5.45	120.95	111.27
19	A	838	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
19	3	204	CLA	C2C-C1C-NC	5.44	115.07	109.97
19	B	835	CLA	O2D-CGD-CBD	5.44	120.94	111.27
19	A	878	CLA	C2C-C1C-NC	5.44	115.07	109.97
19	B	811	CLA	CHD-C4C-C3C	-5.44	116.84	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	215	CLA	CHD-C4C-C3C	-5.44	116.85	124.84
19	4	312	CLA	CHD-C4C-C3C	-5.43	116.85	124.84
19	5	215	CLA	C2C-C1C-NC	5.43	115.06	109.97
31	3	212	A86	O4-C38-C39	5.43	121.08	111.09
19	A	844	CLA	C2C-C1C-NC	5.43	115.06	109.97
19	A	843	CLA	CHD-C1D-ND	-5.43	119.47	124.45
19	B	826	CLA	CHD-C1D-ND	-5.43	119.47	124.45
19	B	813	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
19	A	807	CLA	O2D-CGD-CBD	5.42	120.91	111.27
19	3	209	CLA	C2C-C1C-NC	5.42	115.05	109.97
19	2	205	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
19	3	202	CLA	C4A-NA-C1A	-5.42	104.27	106.71
19	3	210	CLA	C4A-NA-C1A	-5.42	104.27	106.71
19	5	216	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
19	A	803	CLA	CHD-C1D-ND	-5.41	119.48	124.45
19	4	306	CLA	C2C-C1C-NC	5.41	115.04	109.97
19	A	840	CLA	O2D-CGD-CBD	5.41	120.88	111.27
19	A	824	CLA	O2D-CGD-CBD	5.41	120.87	111.27
19	A	806	CLA	C4A-NA-C1A	-5.40	104.28	106.71
19	A	802	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
19	4	308	CLA	C4A-NA-C1A	-5.40	104.28	106.71
19	B	831	CLA	C4A-NA-C1A	-5.39	104.28	106.71
28	3	213	DD6	C24-C1-C2	-5.39	110.67	118.94
19	A	806	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
19	A	827	CLA	O2D-CGD-CBD	5.38	120.83	111.27
19	B	825	CLA	C2C-C1C-NC	5.38	115.01	109.97
19	B	816	CLA	CHD-C4C-C3C	-5.38	116.94	124.84
19	B	804	CLA	CHD-C4C-C3C	-5.38	116.94	124.84
19	5	208	CLA	CHD-C4C-C3C	-5.38	116.94	124.84
19	B	810	CLA	O2D-CGD-CBD	5.37	120.82	111.27
28	1	313	DD6	C7-C6-C8	-5.37	109.62	118.08
19	A	842	CLA	O2D-CGD-CBD	5.37	120.81	111.27
19	1	303	CLA	C2C-C1C-NC	5.37	115.00	109.97
19	A	819	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
30	3	205	KC1	CMD-C2D-C1D	5.37	136.72	128.46
19	4	308	CLA	O2D-CGD-CBD	5.37	120.81	111.27
19	4	301	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
19	5	214	CLA	C4A-NA-C1A	-5.36	104.30	106.71
19	A	839	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
19	A	838	CLA	C2C-C1C-NC	5.36	114.99	109.97
19	1	307	CLA	C2C-C1C-NC	5.36	114.99	109.97
19	A	816	CLA	CHD-C4C-C3C	-5.36	116.97	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	306	CLA	C4A-NA-C1A	-5.35	104.30	106.71
19	L	206	CLA	C2C-C1C-NC	5.35	114.99	109.97
19	2	209	CLA	CHD-C4C-C3C	-5.35	116.97	124.84
19	5	214	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
19	3	206	CLA	C2C-C1C-NC	5.35	114.98	109.97
19	3	207	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
19	A	820	CLA	C4A-NA-C1A	-5.35	104.30	106.71
19	4	310	CLA	C4A-NA-C1A	-5.35	104.30	106.71
19	B	808	CLA	CHD-C1D-ND	-5.35	119.54	124.45
19	A	811	CLA	C2C-C1C-NC	5.34	114.98	109.97
19	A	825	CLA	CHD-C4C-C3C	-5.34	116.98	124.84
19	1	309	CLA	C4A-NA-C1A	-5.34	104.31	106.71
18	A	801	CL0	CHD-C4C-C3C	-5.34	116.99	124.84
19	4	313	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
19	2	214	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
19	B	827	CLA	CHD-C4C-C3C	-5.34	117.00	124.84
19	A	803	CLA	C4A-NA-C1A	-5.33	104.31	106.71
19	1	304	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
19	B	831	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
19	5	209	CLA	C2C-C1C-NC	5.33	114.96	109.97
19	B	821	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
19	4	309	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
19	A	804	CLA	O2D-CGD-CBD	5.32	120.73	111.27
19	B	820	CLA	C2C-C1C-NC	5.32	114.96	109.97
19	B	836	CLA	C2C-C1C-NC	5.32	114.96	109.97
19	A	833	CLA	C2C-C1C-NC	5.32	114.96	109.97
19	u	201	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
19	B	826	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
19	A	815	CLA	C2C-C1C-NC	5.32	114.95	109.97
19	4	305	CLA	C2C-C1C-NC	5.32	114.95	109.97
19	A	836	CLA	C4A-NA-C1A	-5.32	104.32	106.71
19	B	811	CLA	C4A-NA-C1A	-5.32	104.32	106.71
19	A	812	CLA	C2C-C1C-NC	5.31	114.95	109.97
19	B	814	CLA	C2C-C1C-NC	5.31	114.95	109.97
19	B	815	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
19	A	823	CLA	C2C-C1C-NC	5.31	114.95	109.97
19	A	818	CLA	C2C-C1C-NC	5.30	114.94	109.97
19	5	208	CLA	C2C-C1C-NC	5.30	114.94	109.97
31	3	228	A86	C36-C31-C32	-5.30	114.44	119.70
19	4	305	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
19	2	205	CLA	C2C-C1C-NC	5.29	114.93	109.97
19	5	214	CLA	O2D-CGD-CBD	5.29	120.68	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	209	CLA	O2D-CGD-CBD	5.29	120.67	111.27
19	B	822	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
19	A	803	CLA	CMD-C2D-C1D	5.29	134.04	124.71
19	A	812	CLA	C4A-NA-C1A	-5.29	104.33	106.71
19	A	836	CLA	C2C-C1C-NC	5.29	114.92	109.97
28	1	315	DD6	C7-C6-C8	-5.29	109.75	118.08
31	1	316	A86	C33-C32-C31	5.29	114.35	109.21
19	B	802	CLA	C2C-C1C-NC	5.28	114.92	109.97
19	2	208	CLA	C4A-NA-C1A	-5.28	104.33	106.71
19	B	819	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
19	A	822	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
19	A	812	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
19	3	209	CLA	O2D-CGD-CBD	5.27	120.63	111.27
19	A	832	CLA	C2C-C1C-NC	5.27	114.91	109.97
31	1	317	A86	O4-C38-C39	5.27	120.78	111.09
19	3	207	CLA	C4A-NA-C1A	-5.26	104.34	106.71
31	3	228	A86	C3-C2-C1	-5.26	119.81	127.31
19	B	805	CLA	C2C-C1C-NC	5.25	114.89	109.97
31	5	219	A86	C4-C3-C2	-5.25	112.72	123.47
19	4	311	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
30	4	302	KC1	O2D-CGD-CBD	5.25	120.60	111.27
19	2	215	CLA	O2D-CGD-CBD	5.25	120.60	111.27
19	F	204	CLA	CHD-C4C-C3C	-5.25	117.13	124.84
19	A	828	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
19	F	203	CLA	C2C-C1C-NC	5.25	114.89	109.97
19	5	207	CLA	O2D-CGD-CBD	5.24	120.59	111.27
19	B	807	CLA	O2D-CGD-CBD	5.24	120.58	111.27
31	5	220	A86	C4-C5-C6	-5.24	119.83	127.31
19	A	813	CLA	C2C-C1C-NC	5.23	114.87	109.97
19	A	837	CLA	C2C-C1C-NC	5.23	114.87	109.97
31	1	316	A86	O4-C38-C39	5.23	120.71	111.09
19	A	880	CLA	C2C-C1C-NC	5.23	114.87	109.97
19	A	826	CLA	CHD-C1D-ND	-5.23	119.65	124.45
19	A	815	CLA	O2D-CGD-CBD	5.23	120.56	111.27
19	A	829	CLA	C4A-NA-C1A	-5.22	104.36	106.71
19	1	304	CLA	C2C-C1C-NC	5.22	114.87	109.97
19	5	207	CLA	C4A-NA-C1A	-5.22	104.36	106.71
19	B	824	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
19	B	836	CLA	CHD-C1D-ND	-5.21	119.66	124.45
19	A	804	CLA	C2C-C1C-NC	5.21	114.85	109.97
19	A	823	CLA	O2D-CGD-CBD	5.21	120.52	111.27
19	B	805	CLA	CHD-C4C-C3C	-5.21	117.19	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	803	CLA	CHD-C4C-C3C	-5.21	117.19	124.84
19	B	828	CLA	O2D-CGD-CBD	5.21	120.52	111.27
31	3	214	A86	C4-C5-C6	-5.20	119.89	127.31
19	A	835	CLA	CHD-C4C-C3C	-5.20	117.19	124.84
31	1	316	A86	C3-C2-C1	-5.20	119.89	127.31
19	A	802	CLA	C2C-C1C-NC	5.20	114.84	109.97
19	A	824	CLA	C2C-C1C-NC	5.20	114.84	109.97
19	B	833	CLA	O2D-CGD-CBD	5.20	120.50	111.27
19	5	216	CLA	C4A-NA-C1A	-5.20	104.37	106.71
30	2	211	KC1	C3C-C4C-NC	5.19	114.77	109.88
30	4	307	KC1	C2A-C1A-NA	5.19	117.72	109.40
19	2	214	CLA	C4A-NA-C1A	-5.18	104.38	106.71
19	u	201	CLA	O2D-CGD-CBD	5.18	120.47	111.27
19	L	203	CLA	C2C-C1C-NC	5.18	114.82	109.97
19	u	202	CLA	O2D-CGD-CBD	5.17	120.46	111.27
19	1	307	CLA	CHD-C4C-C3C	-5.17	117.24	124.84
19	B	815	CLA	C4A-NA-C1A	-5.17	104.38	106.71
19	B	815	CLA	C2C-C1C-NC	5.17	114.81	109.97
31	5	217	A86	O4-C38-C39	5.17	120.59	111.09
30	4	302	KC1	C3C-C4C-NC	5.17	114.74	109.88
19	A	836	CLA	CHD-C4C-C3C	-5.17	117.25	124.84
19	A	831	CLA	CHD-C4C-C3C	-5.16	117.25	124.84
19	B	816	CLA	C4A-NA-C1A	-5.16	104.39	106.71
19	5	209	CLA	CHD-C4C-C3C	-5.15	117.27	124.84
19	5	213	CLA	CHD-C4C-C3C	-5.15	117.27	124.84
19	A	827	CLA	C2C-C1C-NC	5.15	114.80	109.97
19	B	836	CLA	CHD-C4C-C3C	-5.15	117.27	124.84
27	J	105	5X6	C20-C19-C18	-5.15	112.93	123.47
31	1	316	A86	C36-C31-C32	-5.14	114.59	119.70
19	5	210	CLA	O2D-CGD-CBD	5.14	120.40	111.27
19	A	829	CLA	C2C-C1C-NC	5.14	114.79	109.97
30	4	307	KC1	C3C-C4C-NC	5.14	114.71	109.88
19	2	213	CLA	C2C-C1C-NC	5.13	114.78	109.97
19	A	807	CLA	C4A-NA-C1A	-5.13	104.40	106.71
19	B	834	CLA	C4A-NA-C1A	-5.13	104.40	106.71
19	L	204	CLA	C2C-C1C-NC	5.13	114.78	109.97
19	B	818	CLA	CHD-C4C-C3C	-5.13	117.31	124.84
28	1	313	DD6	C21-C20-C15	-5.12	113.67	122.26
19	B	812	CLA	C2C-C1C-NC	5.12	114.77	109.97
31	3	228	A86	C4-C5-C6	-5.12	120.00	127.31
19	F	204	CLA	C2C-C1C-NC	5.12	114.77	109.97
19	2	206	CLA	C4A-NA-C1A	-5.12	104.41	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	806	CLA	C2C-C1C-NC	5.12	114.77	109.97
19	2	212	CLA	C2C-C1C-NC	5.11	114.76	109.97
31	3	212	A86	C25-C26-C27	-5.11	120.02	127.31
19	A	815	CLA	C4A-NA-C1A	-5.11	104.41	106.71
19	B	825	CLA	CHD-C1D-ND	-5.11	119.76	124.45
30	3	208	KC1	C3C-C4C-NC	5.10	114.68	109.88
19	1	303	CLA	CHD-C4C-C3C	-5.10	117.34	124.84
19	A	822	CLA	C2C-C1C-NC	5.10	114.75	109.97
19	A	843	CLA	C2C-C1C-NC	5.10	114.75	109.97
19	5	211	CLA	C4A-NA-C1A	-5.10	104.42	106.71
19	B	807	CLA	C2C-C1C-NC	5.09	114.74	109.97
19	B	834	CLA	C2C-C1C-NC	5.09	114.74	109.97
31	3	212	A86	C20-C19-C18	-5.09	102.68	112.75
19	A	805	CLA	C2C-C1C-NC	5.09	114.74	109.97
19	5	214	CLA	C2C-C1C-NC	5.09	114.74	109.97
19	A	841	CLA	C4A-NA-C1A	-5.08	104.42	106.71
19	1	306	CLA	CHD-C4C-C3C	-5.08	117.38	124.84
19	A	810	CLA	C2C-C1C-NC	5.08	114.73	109.97
19	J	103	CLA	C2C-C1C-NC	5.07	114.72	109.97
28	L	209	DD6	C12-C11-C13	-5.07	110.09	118.08
30	1	305	KC1	C2A-C1A-NA	5.07	117.53	109.40
19	A	830	CLA	C2C-C1C-NC	5.06	114.72	109.97
19	4	304	CLA	C2C-C1C-NC	5.06	114.71	109.97
30	1	305	KC1	C3C-C4C-NC	5.06	114.64	109.88
30	1	305	KC1	CMD-C2D-C1D	5.06	136.23	128.46
31	5	220	A86	O4-C38-C39	5.04	120.36	111.09
19	A	838	CLA	C4A-NA-C1A	-5.04	104.44	106.71
19	B	830	CLA	CHD-C4C-C3C	-5.04	117.44	124.84
19	4	303	CLA	C2C-C1C-NC	5.03	114.69	109.97
18	A	801	CL0	CHD-C1D-ND	-5.03	119.83	124.45
19	B	816	CLA	O2D-CGD-CBD	5.03	120.20	111.27
19	B	828	CLA	C2C-C1C-NC	5.03	114.68	109.97
19	B	846	CLA	C2C-C1C-NC	5.03	114.68	109.97
19	B	817	CLA	C4A-NA-C1A	-5.03	104.45	106.71
28	2	217	DD6	C35-C36-C31	-5.02	109.17	120.57
19	B	803	CLA	CHD-C4C-C3C	-5.02	117.46	124.84
19	B	809	CLA	CHD-C1D-ND	-5.02	119.84	124.45
30	3	208	KC1	C1A-NA-C4A	-5.02	104.45	106.71
19	B	813	CLA	C4A-NA-C1A	-5.02	104.45	106.71
19	u	201	CLA	C4A-NA-C1A	-5.02	104.45	106.71
31	2	218	A86	O4-C38-C39	5.02	120.32	111.09
27	J	105	5X6	C25-C24-C23	-5.02	107.56	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	817	CLA	O2D-CGD-CBD	5.01	120.17	111.27
19	B	830	CLA	C2C-C1C-NC	5.01	114.67	109.97
19	F	204	CLA	C4A-NA-C1A	-5.01	104.45	106.71
19	B	824	CLA	C4A-NA-C1A	-5.00	104.46	106.71
30	3	211	KC1	C2A-C1A-NA	5.00	117.42	109.40
31	2	216	A86	O4-C38-C39	5.00	120.28	111.09
30	2	211	KC1	CHD-C4C-C3C	-4.99	115.96	125.33
19	5	211	CLA	CHD-C4C-C3C	-4.99	117.50	124.84
19	B	821	CLA	C2C-C1C-NC	4.98	114.64	109.97
19	B	807	CLA	C4A-NA-C1A	-4.98	104.47	106.71
19	B	823	CLA	C2C-C1C-NC	4.98	114.63	109.97
31	4	316	A86	O4-C38-C39	4.97	120.24	111.09
19	B	811	CLA	C2C-C1C-NC	4.97	114.63	109.97
31	4	315	A86	O4-C38-C39	4.97	120.22	111.09
19	A	839	CLA	O2D-CGD-CBD	4.96	120.09	111.27
19	A	840	CLA	C2C-C1C-NC	4.96	114.62	109.97
19	2	215	CLA	C2C-C1C-NC	4.96	114.62	109.97
19	3	210	CLA	C2C-C1C-NC	4.96	114.62	109.97
28	1	312	DD6	C7-C6-C8	-4.96	110.27	118.08
19	2	205	CLA	C4A-NA-C1A	-4.96	104.48	106.71
19	5	209	CLA	C4A-NA-C1A	-4.96	104.48	106.71
19	A	821	CLA	C2C-C1C-NC	4.96	114.62	109.97
19	B	806	CLA	C2C-C1C-NC	4.95	114.61	109.97
19	B	834	CLA	O2D-CGD-CBD	4.95	120.07	111.27
19	2	209	CLA	C2C-C1C-NC	4.95	114.61	109.97
31	4	315	A86	C20-C19-C18	-4.95	102.95	112.75
19	1	304	CLA	O2D-CGD-CBD	4.94	120.05	111.27
19	B	825	CLA	O2D-CGD-CBD	4.94	120.05	111.27
19	A	843	CLA	O2D-CGD-CBD	4.94	120.04	111.27
19	3	210	CLA	O2D-CGD-CBD	4.93	120.04	111.27
19	1	310	CLA	CHD-C4C-C3C	-4.93	117.60	124.84
28	1	313	DD6	C12-C11-C13	-4.93	110.31	118.08
19	2	210	CLA	C2C-C1C-NC	4.92	114.58	109.97
19	B	832	CLA	O2D-CGD-CBD	4.92	120.00	111.27
19	A	878	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
28	1	312	DD6	C12-C11-C13	-4.91	110.34	118.08
19	A	807	CLA	C2C-C1C-NC	4.91	114.57	109.97
19	2	212	CLA	C3D-C2D-C1D	-4.91	99.14	105.83
30	3	208	KC1	CMD-C2D-C1D	4.90	136.00	128.46
19	A	841	CLA	C2C-C1C-NC	4.90	114.57	109.97
19	B	845	CLA	C4A-NA-C1A	-4.90	104.50	106.71
19	u	202	CLA	C2C-C1C-NC	4.90	114.56	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	819	CLA	C2C-C1C-NC	4.90	114.56	109.97
19	B	821	CLA	C4A-NA-C1A	-4.89	104.51	106.71
19	4	301	CLA	O2D-CGD-CBD	4.89	119.96	111.27
30	3	211	KC1	C3C-C4C-NC	4.89	114.48	109.88
19	u	202	CLA	C4A-NA-C1A	-4.89	104.51	106.71
19	A	878	CLA	O2D-CGD-CBD	4.89	119.95	111.27
31	4	315	A86	C33-C32-C31	4.88	113.96	109.21
19	4	311	CLA	C2C-C1C-NC	4.88	114.55	109.97
19	4	304	CLA	C4A-NA-C1A	-4.88	104.51	106.71
19	B	846	CLA	O2D-CGD-CBD	4.88	119.94	111.27
31	4	314	A86	O4-C38-C39	4.88	120.06	111.09
19	A	826	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
19	1	310	CLA	C4A-NA-C1A	-4.87	104.52	106.71
19	3	207	CLA	C2C-C1C-NC	4.87	114.54	109.97
19	A	816	CLA	C4A-NA-C1A	-4.87	104.52	106.71
19	1	310	CLA	C2C-C1C-NC	4.86	114.53	109.97
19	2	214	CLA	C2C-C1C-NC	4.86	114.53	109.97
19	A	808	CLA	C4A-NA-C1A	-4.86	104.52	106.71
19	4	312	CLA	C2C-C1C-NC	4.86	114.53	109.97
28	L	209	DD6	C-C1-C24	-4.86	110.42	118.08
28	1	313	DD6	C-C1-C24	-4.85	110.43	118.08
19	B	818	CLA	C4A-NA-C1A	-4.85	104.52	106.71
30	4	302	KC1	CHD-C4C-C3C	-4.85	116.22	125.33
19	B	828	CLA	C4A-NA-C1A	-4.85	104.53	106.71
19	L	206	CLA	C4A-NA-C1A	-4.85	104.53	106.71
28	2	217	DD6	C21-C20-C15	-4.85	114.13	122.26
19	2	207	CLA	C2C-C1C-NC	4.85	114.51	109.97
19	5	207	CLA	C2C-C1C-NC	4.85	114.51	109.97
19	B	832	CLA	C4A-NA-C1A	-4.84	104.53	106.71
19	B	836	CLA	C4A-NA-C1A	-4.84	104.53	106.71
30	3	211	KC1	CMD-C2D-C1D	4.84	135.91	128.46
19	B	831	CLA	C2C-C1C-NC	4.84	114.51	109.97
19	3	203	CLA	C2C-C1C-NC	4.84	114.51	109.97
19	4	308	CLA	C2C-C1C-NC	4.84	114.51	109.97
19	A	814	CLA	O2D-CGD-CBD	4.84	119.88	111.27
30	4	307	KC1	CMD-C2D-C1D	4.84	135.91	128.46
19	B	832	CLA	C2C-C1C-NC	4.84	114.51	109.97
19	1	310	CLA	O2D-CGD-CBD	4.84	119.86	111.27
31	5	219	A86	O4-C38-C39	4.84	119.98	111.09
30	3	205	KC1	CHD-C4C-C3C	-4.83	116.25	125.33
19	B	817	CLA	O2D-CGD-CBD	4.83	119.85	111.27
19	A	820	CLA	O2D-CGD-CBD	4.83	119.84	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	817	CLA	C2C-C1C-NC	4.82	114.49	109.97
19	3	204	CLA	C1-C2-C3	-4.82	117.71	126.04
19	F	203	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
31	4	315	A86	C12-C11-C13	4.81	124.10	116.02
19	B	829	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
28	1	312	DD6	O1-C20-C21	-4.80	109.30	115.06
19	B	809	CLA	C4A-NA-C1A	-4.80	104.55	106.71
31	3	214	A86	O4-C38-C39	4.80	119.92	111.09
19	B	824	CLA	C2C-C1C-NC	4.80	114.47	109.97
19	B	837	CLA	O2D-CGD-CBD	4.80	119.79	111.27
31	3	228	A86	O4-C38-C39	4.78	119.88	111.09
19	B	833	CLA	C3D-C2D-C1D	-4.77	99.31	105.83
19	4	305	CLA	C4A-NA-C1A	-4.77	104.56	106.71
19	3	206	CLA	C4A-NA-C1A	-4.77	104.56	106.71
30	3	208	KC1	C2A-C1A-NA	4.77	117.05	109.40
19	B	803	CLA	C2C-C1C-NC	4.76	114.43	109.97
30	4	307	KC1	O2D-CGD-CBD	4.76	119.73	111.27
19	A	817	CLA	C3D-C4D-ND	4.76	117.94	110.24
19	3	203	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
19	2	208	CLA	CHD-C4C-C3C	-4.75	117.86	124.84
19	L	203	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
19	A	878	CLA	C4A-NA-C1A	-4.75	104.57	106.71
19	1	301	CLA	O2D-CGD-CBD	4.75	119.70	111.27
19	B	819	CLA	C3D-C4D-ND	4.74	117.91	110.24
19	4	311	CLA	O2D-CGD-CBD	4.74	119.69	111.27
19	A	814	CLA	C4A-NA-C1A	-4.74	104.57	106.71
19	4	303	CLA	C4A-NA-C1A	-4.74	104.57	106.71
19	B	820	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
30	4	302	KC1	C2A-C1A-NA	4.74	117.00	109.40
19	2	210	CLA	O2D-CGD-CBD	4.73	119.68	111.27
19	A	818	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
19	L	203	CLA	C3D-C4D-ND	4.73	117.89	110.24
27	J	105	5X6	C15-C16-C17	-4.73	113.13	126.42
19	4	306	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
19	2	208	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
19	A	880	CLA	C4A-NA-C1A	-4.72	104.58	106.71
19	B	819	CLA	C4A-NA-C1A	-4.72	104.58	106.71
19	A	835	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
28	2	217	DD6	C7-C6-C8	-4.71	110.65	118.08
19	A	813	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
19	A	803	CLA	C2C-C1C-NC	4.71	114.39	109.97
19	B	806	CLA	C3D-C2D-C1D	-4.71	99.40	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	215	CLA	C4A-NA-C1A	-4.71	104.59	106.71
19	3	202	CLA	C1-C2-C3	-4.71	117.90	126.04
19	1	304	CLA	C3D-C4D-ND	4.71	117.85	110.24
19	B	811	CLA	C3D-C4D-ND	4.71	117.85	110.24
19	2	210	CLA	C4A-NA-C1A	-4.71	104.59	106.71
19	4	312	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
19	A	806	CLA	C3D-C4D-ND	4.70	117.85	110.24
19	A	805	CLA	C4A-NA-C1A	-4.70	104.59	106.71
19	A	831	CLA	C4A-NA-C1A	-4.70	104.59	106.71
31	5	217	A86	C33-C32-C31	4.70	113.78	109.21
19	1	309	CLA	C3D-C4D-ND	4.70	117.85	110.24
19	5	216	CLA	O2D-CGD-CBD	4.70	119.62	111.27
19	A	810	CLA	C4A-NA-C1A	-4.70	104.59	106.71
19	B	835	CLA	C4A-NA-C1A	-4.70	104.59	106.71
19	1	308	CLA	O2D-CGD-CBD	4.70	119.62	111.27
19	A	833	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
19	A	829	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
19	B	829	CLA	C2C-C1C-NC	4.70	114.37	109.97
19	5	212	CLA	C2C-C1C-NC	4.70	114.37	109.97
19	1	304	CLA	C4A-NA-C1A	-4.70	104.59	106.71
19	L	206	CLA	C3D-C2D-C1D	-4.69	99.42	105.83
19	u	202	CLA	C3D-C2D-C1D	-4.69	99.42	105.83
19	A	824	CLA	C4A-NA-C1A	-4.69	104.60	106.71
19	A	880	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
28	1	313	DD6	O1-C20-C21	-4.69	109.44	115.06
19	A	816	CLA	C2C-C1C-NC	4.69	114.37	109.97
19	A	840	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
19	2	207	CLA	C3D-C4D-ND	4.69	117.82	110.24
19	4	301	CLA	C3D-C4D-ND	4.69	117.82	110.24
19	A	817	CLA	C4A-NA-C1A	-4.68	104.60	106.71
19	B	816	CLA	C3D-C4D-ND	4.68	117.81	110.24
31	3	212	A86	C36-C31-C32	-4.68	115.05	119.70
19	B	810	CLA	C4A-NA-C1A	-4.68	104.60	106.71
19	2	206	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
19	4	310	CLA	C2C-C1C-NC	4.68	114.36	109.97
19	4	310	CLA	C3D-C4D-ND	4.68	117.81	110.24
19	B	823	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
19	B	806	CLA	C4A-NA-C1A	-4.68	104.60	106.71
19	4	308	CLA	C3D-C4D-ND	4.68	117.80	110.24
19	B	830	CLA	C3D-C4D-ND	4.67	117.80	110.24
19	B	846	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
31	2	219	A86	C20-C19-C18	-4.67	103.51	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	837	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
19	2	213	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
19	B	804	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
19	2	205	CLA	O2D-CGD-CBD	4.66	119.55	111.27
19	B	807	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
19	A	840	CLA	C4A-NA-C1A	-4.66	104.61	106.71
19	A	844	CLA	C4A-NA-C1A	-4.66	104.61	106.71
19	A	842	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
19	J	103	CLA	O2D-CGD-CBD	4.66	119.54	111.27
19	4	303	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
19	A	820	CLA	C2C-C1C-NC	4.65	114.33	109.97
19	A	808	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
19	A	818	CLA	O2D-CGD-CBD	4.65	119.53	111.27
19	2	209	CLA	O2D-CGD-CBD	4.65	119.53	111.27
30	4	302	KC1	CMD-C2D-C1D	4.65	135.61	128.46
19	3	210	CLA	C3D-C4D-ND	4.65	117.76	110.24
19	4	309	CLA	O2D-CGD-CBD	4.65	119.53	111.27
19	B	813	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
30	2	211	KC1	C1A-NA-C4A	-4.65	104.62	106.71
31	5	221	A86	O4-C38-C39	4.64	119.63	111.09
19	A	832	CLA	C4A-NA-C1A	-4.64	104.62	106.71
19	4	309	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
19	4	312	CLA	O2D-CGD-CBD	4.64	119.50	111.27
19	B	805	CLA	C3D-C4D-ND	4.64	117.74	110.24
19	B	803	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
19	B	834	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
19	A	834	CLA	C4A-NA-C1A	-4.63	104.62	106.71
19	4	308	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
19	1	309	CLA	O2D-CGD-CBD	4.63	119.49	111.27
19	B	810	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
19	B	816	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
19	5	216	CLA	C3D-C4D-ND	4.63	117.72	110.24
28	3	213	DD6	C7-C6-C8	-4.62	110.79	118.08
19	B	817	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
19	A	802	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
19	1	306	CLA	C2C-C1C-NC	4.62	114.30	109.97
19	5	215	CLA	C4A-NA-C1A	-4.62	104.63	106.71
19	2	214	CLA	C3D-C4D-ND	4.62	117.71	110.24
31	2	218	A86	C20-C19-C18	-4.62	103.62	112.75
19	2	213	CLA	C4A-NA-C1A	-4.62	104.63	106.71
19	3	203	CLA	O2D-CGD-CBD	4.62	119.47	111.27
19	A	844	CLA	C3D-C2D-C1D	-4.61	99.53	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	5	219	A86	C-C1-C24	4.61	125.34	118.08
19	B	802	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
19	3	204	CLA	C4A-NA-C1A	-4.61	104.63	106.71
19	4	313	CLA	C4A-NA-C1A	-4.60	104.64	106.71
19	2	215	CLA	C3D-C4D-ND	4.60	117.68	110.24
19	5	215	CLA	C3D-C4D-ND	4.60	117.68	110.24
19	B	835	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
19	A	819	CLA	C2C-C1C-NC	4.60	114.28	109.97
19	5	211	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
28	1	315	DD6	C-C1-C24	-4.60	110.83	118.08
19	4	304	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
19	A	821	CLA	C3D-C4D-ND	4.60	117.67	110.24
19	5	212	CLA	C4A-NA-C1A	-4.59	104.64	106.71
28	1	315	DD6	C33-C34-C35	4.59	116.59	110.30
19	4	301	CLA	C2C-C1C-NC	4.59	114.27	109.97
19	5	213	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
19	1	307	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
19	5	214	CLA	C3D-C4D-ND	4.59	117.66	110.24
19	5	210	CLA	C3D-C2D-C1D	-4.58	99.57	105.83
19	A	837	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
19	B	832	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
19	A	815	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
28	L	209	DD6	O1-C20-C21	-4.58	109.56	115.06
19	B	816	CLA	C2C-C1C-NC	4.58	114.27	109.97
19	A	807	CLA	CAA-C2A-C3A	-4.58	100.23	112.78
30	3	208	KC1	CHD-C4C-C3C	-4.58	116.73	125.33
19	A	808	CLA	C2C-C1C-NC	4.58	114.26	109.97
19	3	202	CLA	C2C-C1C-NC	4.58	114.26	109.97
19	2	208	CLA	C3D-C4D-ND	4.58	117.65	110.24
28	5	218	DD6	C24-C1-C2	-4.58	111.92	118.94
19	1	308	CLA	C3D-C2D-C1D	-4.58	99.59	105.83
19	A	811	CLA	C3D-C2D-C1D	-4.58	99.59	105.83
19	3	204	CLA	C3D-C2D-C1D	-4.58	99.59	105.83
19	B	817	CLA	C2C-C1C-NC	4.58	114.26	109.97
19	B	820	CLA	C4A-NA-C1A	-4.58	104.65	106.71
19	2	207	CLA	C4A-NA-C1A	-4.58	104.65	106.71
19	1	301	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
30	2	211	KC1	CMD-C2D-C1D	4.57	135.49	128.46
27	J	105	5X6	C14-C15-C16	-4.57	108.95	123.22
19	A	804	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
31	4	314	A86	C4-C3-C2	-4.57	114.12	123.47
19	A	821	CLA	C3D-C2D-C1D	-4.57	99.60	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	819	CLA	O2D-CGD-CBD	4.57	119.38	111.27
19	5	216	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
19	A	814	CLA	C2C-C1C-NC	4.56	114.24	109.97
19	3	206	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
19	B	815	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
19	B	822	CLA	C4A-NA-C1A	-4.55	104.66	106.71
19	2	213	CLA	O2D-CGD-CBD	4.55	119.35	111.27
19	B	802	CLA	C3C-C4C-NC	4.54	115.67	110.57
31	5	217	A86	C4-C5-C6	-4.54	120.82	127.31
19	A	841	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
19	B	812	CLA	O2D-CGD-CBD	4.54	119.34	111.27
19	5	215	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
19	4	309	CLA	C3D-C4D-ND	4.54	117.58	110.24
28	1	312	DD6	C21-C20-C15	-4.54	114.65	122.26
31	1	317	A86	C3-C2-C1	-4.54	120.83	127.31
19	B	837	CLA	C4A-NA-C1A	-4.54	104.67	106.71
19	A	808	CLA	O2D-CGD-CBD	4.54	119.33	111.27
19	B	805	CLA	C4A-NA-C1A	-4.54	104.67	106.71
19	3	209	CLA	C3D-C4D-ND	4.53	117.57	110.24
19	A	834	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
19	4	313	CLA	C3D-C4D-ND	4.53	117.57	110.24
19	A	805	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
19	B	807	CLA	C3D-C4D-ND	4.53	117.57	110.24
19	A	808	CLA	C3D-C4D-ND	4.53	117.57	110.24
18	A	801	CL0	C4A-NA-C1A	-4.53	104.67	106.71
19	B	812	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
19	1	306	CLA	C3D-C4D-ND	4.53	117.56	110.24
19	B	845	CLA	C3D-C4D-ND	4.52	117.56	110.24
19	1	308	CLA	C2C-C1C-NC	4.52	114.21	109.97
31	1	317	A86	C25-C26-C27	-4.52	120.85	127.31
19	4	310	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
19	B	832	CLA	C3D-C4D-ND	4.52	117.55	110.24
19	J	103	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
31	2	219	A86	O4-C38-C39	4.52	119.40	111.09
19	A	823	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
19	A	826	CLA	C3C-C4C-NC	4.52	115.64	110.57
19	3	209	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
19	A	827	CLA	C3D-C2D-C1D	-4.52	99.67	105.83
19	A	810	CLA	C3D-C4D-ND	4.51	117.54	110.24
19	3	202	CLA	C3D-C4D-ND	4.51	117.54	110.24
19	A	824	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
19	A	822	CLA	O2D-CGD-CBD	4.51	119.28	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	823	CLA	C3D-C4D-ND	4.51	117.53	110.24
19	A	812	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
28	3	213	DD6	C-C1-C24	-4.51	110.98	118.08
19	4	301	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
19	B	831	CLA	C3D-C4D-ND	4.50	117.52	110.24
19	L	204	CLA	C4A-NA-C1A	-4.50	104.68	106.71
19	F	203	CLA	O2D-CGD-CBD	4.49	119.25	111.27
19	1	306	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
19	A	830	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
19	A	814	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
19	3	210	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
19	F	203	CLA	C4A-NA-C1A	-4.49	104.69	106.71
31	3	228	A86	C17-C16-C15	4.49	113.74	109.16
19	A	814	CLA	C3D-C4D-ND	4.49	117.50	110.24
19	B	827	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
19	L	204	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
19	u	201	CLA	C3D-C4D-ND	4.48	117.49	110.24
19	A	820	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
19	A	809	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
19	B	808	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
19	1	307	CLA	C3D-C4D-ND	4.48	117.48	110.24
19	A	813	CLA	O2D-CGD-CBD	4.48	119.23	111.27
19	B	814	CLA	C3D-C4D-ND	4.48	117.48	110.24
19	B	818	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
28	5	218	DD6	C13-C11-C10	-4.47	112.08	118.94
19	B	826	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
19	A	819	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
19	B	815	CLA	C3D-C4D-ND	4.47	117.47	110.24
19	A	811	CLA	O2D-CGD-CBD	4.47	119.20	111.27
19	B	805	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
19	B	831	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
19	2	205	CLA	C3D-C4D-ND	4.46	117.45	110.24
30	1	305	KC1	CHD-C4C-C3C	-4.46	116.96	125.33
19	A	817	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
19	A	836	CLA	C3D-C4D-ND	4.46	117.45	110.24
19	B	826	CLA	O2D-CGD-CBD	4.46	119.19	111.27
19	A	878	CLA	C3C-C4C-NC	4.46	115.57	110.57
19	A	836	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
19	B	809	CLA	O2D-CGD-CBD	4.45	119.18	111.27
19	A	816	CLA	C3D-C4D-ND	4.45	117.44	110.24
19	A	828	CLA	C2C-C1C-NC	4.45	114.14	109.97
19	B	826	CLA	C4A-NA-C1A	-4.45	104.71	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	5	220	A86	C9-C10-C11	-4.45	113.53	126.61
19	A	839	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
19	A	830	CLA	O2D-CGD-CBD	4.45	119.17	111.27
19	A	819	CLA	C3D-C4D-ND	4.45	117.43	110.24
28	1	315	DD6	C21-C20-C15	-4.45	114.81	122.26
19	B	820	CLA	C3D-C4D-ND	4.45	117.43	110.24
19	A	832	CLA	C3D-C4D-ND	4.44	117.43	110.24
19	4	303	CLA	C3D-C4D-ND	4.44	117.43	110.24
28	5	218	DD6	C7-C6-C8	-4.44	111.07	118.08
19	A	807	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
19	A	825	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
19	A	825	CLA	C3D-C4D-ND	4.44	117.42	110.24
19	B	808	CLA	C4A-NA-C1A	-4.44	104.71	106.71
19	4	306	CLA	O2D-CGD-CBD	4.44	119.16	111.27
19	B	810	CLA	C3D-C4D-ND	4.44	117.42	110.24
19	A	811	CLA	C4A-NA-C1A	-4.44	104.71	106.71
19	B	822	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
19	A	821	CLA	C4A-NA-C1A	-4.44	104.71	106.71
19	3	202	CLA	O2D-CGD-CBD	4.44	119.15	111.27
19	A	803	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
19	2	209	CLA	C3D-C4D-ND	4.44	117.41	110.24
19	5	212	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
30	4	302	KC1	C1A-NA-C4A	-4.44	104.71	106.71
19	B	845	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
19	A	816	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
19	4	304	CLA	C3D-C4D-ND	4.43	117.41	110.24
19	4	311	CLA	C3D-C4D-ND	4.43	117.41	110.24
19	F	204	CLA	C3D-C4D-ND	4.43	117.40	110.24
19	4	306	CLA	C3D-C4D-ND	4.43	117.40	110.24
19	A	822	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
30	2	211	KC1	C2A-C1A-NA	4.42	116.50	109.40
19	B	814	CLA	C4A-NA-C1A	-4.42	104.72	106.71
19	4	313	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
19	A	827	CLA	C3D-C4D-ND	4.42	117.39	110.24
19	A	842	CLA	C3D-C4D-ND	4.42	117.38	110.24
19	3	203	CLA	C3D-C4D-ND	4.41	117.38	110.24
31	5	219	A86	C20-C19-C18	-4.41	104.02	112.75
19	4	312	CLA	C3D-C4D-ND	4.41	117.37	110.24
19	2	215	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
19	2	214	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
19	A	839	CLA	C4A-NA-C1A	-4.41	104.72	106.71
19	2	213	CLA	C3D-C4D-ND	4.41	117.37	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	843	CLA	C3D-C4D-ND	4.41	117.37	110.24
31	3	228	A86	C25-C26-C27	-4.40	121.03	127.31
31	5	220	A86	C25-C26-C27	-4.40	121.03	127.31
19	B	828	CLA	C3D-C4D-ND	4.40	117.36	110.24
19	u	202	CLA	C3D-C4D-ND	4.40	117.36	110.24
19	A	840	CLA	C3D-C4D-ND	4.40	117.36	110.24
19	L	204	CLA	C3D-C4D-ND	4.40	117.36	110.24
19	B	838	CLA	C3D-C4D-ND	4.40	117.36	110.24
19	A	806	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
19	2	210	CLA	C3D-C4D-ND	4.40	117.35	110.24
19	5	207	CLA	C3D-C4D-ND	4.40	117.35	110.24
31	1	316	A86	C12-C11-C13	4.40	123.41	116.02
19	B	810	CLA	C2C-C1C-NC	4.40	114.09	109.97
19	5	209	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
19	A	843	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
19	1	301	CLA	C4A-NA-C1A	-4.39	104.73	106.71
19	B	821	CLA	C3D-C4D-ND	4.39	117.34	110.24
19	B	825	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
19	B	812	CLA	C3D-C4D-ND	4.39	117.34	110.24
19	3	209	CLA	C4A-NA-C1A	-4.39	104.73	106.71
19	A	804	CLA	C1-C2-C3	-4.39	118.45	126.04
19	1	303	CLA	C3D-C4D-ND	4.38	117.33	110.24
30	3	205	KC1	O2D-CGD-CBD	4.38	119.06	111.27
19	2	210	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
31	5	221	A86	C40-C32-C31	-4.38	106.55	110.47
19	A	839	CLA	C3D-C4D-ND	4.38	117.32	110.24
19	J	103	CLA	C3D-C4D-ND	4.38	117.32	110.24
19	B	802	CLA	O2D-CGD-CBD	4.38	119.05	111.27
19	A	811	CLA	C3D-C4D-ND	4.38	117.32	110.24
19	5	208	CLA	C3D-C2D-C1D	-4.37	99.86	105.83
19	B	846	CLA	C3D-C4D-ND	4.37	117.31	110.24
19	A	818	CLA	C4A-NA-C1A	-4.37	104.74	106.71
19	B	835	CLA	C3D-C4D-ND	4.37	117.31	110.24
19	5	214	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
19	1	304	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
31	4	316	A86	C25-C26-C27	-4.37	121.07	127.31
19	B	809	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
31	4	315	A86	C3-C2-C1	-4.37	121.08	127.31
31	5	219	A86	C24-C1-C2	-4.36	112.24	118.94
19	B	846	CLA	C4A-NA-C1A	-4.36	104.74	106.71
19	1	303	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
19	B	814	CLA	C3D-C2D-C1D	-4.36	99.88	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	205	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
19	4	304	CLA	O2D-CGD-CBD	4.36	119.02	111.27
19	A	838	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
19	A	813	CLA	C4A-NA-C1A	-4.36	104.75	106.71
19	A	807	CLA	C3D-C4D-ND	4.36	117.29	110.24
19	A	802	CLA	C3C-C4C-NC	4.36	115.46	110.57
19	L	206	CLA	C3D-C4D-ND	4.36	117.28	110.24
19	B	825	CLA	C4A-NA-C1A	-4.36	104.75	106.71
19	B	817	CLA	C3D-C4D-ND	4.35	117.28	110.24
19	5	209	CLA	C3D-C4D-ND	4.35	117.28	110.24
19	5	207	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
19	B	831	CLA	O2D-CGD-CBD	4.35	119.00	111.27
19	F	204	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
19	1	303	CLA	O2D-CGD-CBD	4.34	118.98	111.27
30	3	205	KC1	C2A-C1A-NA	4.34	116.36	109.40
19	5	213	CLA	C3D-C4D-ND	4.34	117.25	110.24
19	B	836	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
19	5	210	CLA	C1C-C2C-C3C	-4.33	102.40	106.96
19	J	103	CLA	C4A-NA-C1A	-4.33	104.76	106.71
30	3	205	KC1	CBA-CAA-C2A	-4.33	108.75	125.27
19	B	837	CLA	C3D-C4D-ND	4.33	117.24	110.24
19	A	841	CLA	O2D-CGD-CBD	4.33	118.96	111.27
19	A	809	CLA	C1C-C2C-C3C	-4.33	102.40	106.96
19	A	831	CLA	C3D-C4D-ND	4.33	117.24	110.24
23	3	215	LHG	O4-P-O5	4.33	133.64	112.24
19	B	823	CLA	C3D-C4D-ND	4.33	117.24	110.24
19	A	818	CLA	C3D-C4D-ND	4.33	117.24	110.24
19	A	834	CLA	C3D-C4D-ND	4.33	117.24	110.24
31	1	316	A86	C4-C5-C6	-4.33	121.14	127.31
19	A	831	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
19	A	830	CLA	C3D-C4D-ND	4.32	117.23	110.24
19	A	825	CLA	C4A-NA-C1A	-4.32	104.76	106.71
19	1	308	CLA	C3D-C4D-ND	4.32	117.23	110.24
19	A	830	CLA	C4A-NA-C1A	-4.32	104.77	106.71
19	A	820	CLA	C3D-C4D-ND	4.32	117.22	110.24
19	A	880	CLA	C3D-C4D-ND	4.32	117.22	110.24
19	A	832	CLA	C3D-C2D-C1D	-4.32	99.94	105.83
19	B	828	CLA	C3D-C2D-C1D	-4.32	99.94	105.83
30	3	208	KC1	O2D-CGD-CBD	4.32	118.94	111.27
19	1	301	CLA	C3D-C4D-ND	4.31	117.22	110.24
19	B	819	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
19	3	206	CLA	C3D-C4D-ND	4.31	117.21	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	1	316	A86	C25-C26-C27	-4.31	121.16	127.31
19	A	824	CLA	C3D-C4D-ND	4.30	117.20	110.24
26	B	847	DGD	O3G-C3G-C2G	-4.30	100.51	110.90
19	A	828	CLA	C3C-C4C-NC	4.30	115.40	110.57
31	4	316	A86	C36-C31-C32	-4.30	115.42	119.70
19	5	208	CLA	C3D-C4D-ND	4.30	117.20	110.24
19	A	843	CLA	C3C-C4C-NC	4.30	115.40	110.57
19	2	207	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
19	2	212	CLA	C3D-C4D-ND	4.30	117.19	110.24
19	1	310	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
19	B	808	CLA	C3C-C4C-NC	4.30	115.39	110.57
23	M	103	LHG	O4-P-O5	4.30	133.48	112.24
19	1	310	CLA	C3D-C4D-ND	4.30	117.19	110.24
31	1	317	A86	C12-C11-C13	4.30	123.24	116.02
19	4	305	CLA	C3D-C4D-ND	4.29	117.19	110.24
28	1	315	DD6	O1-C20-C21	-4.29	109.91	115.06
30	4	307	KC1	CHD-C4C-C3C	-4.29	117.27	125.33
19	5	211	CLA	C3D-C4D-ND	4.29	117.18	110.24
19	4	311	CLA	C3D-C2D-C1D	-4.29	99.97	105.83
19	3	202	CLA	C3D-C2D-C1D	-4.29	99.97	105.83
19	A	841	CLA	C3D-C4D-ND	4.29	117.18	110.24
28	3	213	DD6	C21-C20-C15	-4.29	115.07	122.26
19	5	210	CLA	C3D-C4D-ND	4.29	117.17	110.24
19	A	827	CLA	C4A-NA-C1A	-4.28	104.78	106.71
31	2	218	A86	C12-C11-C13	4.28	123.21	116.02
19	A	844	CLA	C3D-C4D-ND	4.28	117.16	110.24
19	A	802	CLA	C3D-C4D-ND	4.28	117.16	110.24
19	B	829	CLA	C3C-C4C-NC	4.28	115.37	110.57
19	B	838	CLA	C3D-C2D-C1D	-4.28	100.00	105.83
19	B	834	CLA	C3D-C4D-ND	4.27	117.15	110.24
19	2	206	CLA	C3D-C4D-ND	4.27	117.15	110.24
19	B	836	CLA	C3D-C4D-ND	4.27	117.15	110.24
19	5	212	CLA	C3D-C4D-ND	4.27	117.14	110.24
19	5	213	CLA	O2D-CGD-CBD	4.27	118.86	111.27
19	3	207	CLA	C3D-C4D-ND	4.27	117.14	110.24
19	2	209	CLA	C3D-C2D-C1D	-4.27	100.01	105.83
19	A	831	CLA	C1-C2-C3	-4.27	118.67	126.04
19	5	210	CLA	C4A-NA-C1A	-4.26	104.79	106.71
19	B	804	CLA	C3D-C4D-ND	4.26	117.13	110.24
31	2	218	A86	C36-C31-C32	-4.26	115.47	119.70
19	A	834	CLA	O2D-CGD-CBD	4.26	118.83	111.27
19	A	839	CLA	C1C-C2C-C3C	-4.25	102.49	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	825	CLA	O2D-CGD-CBD	4.25	118.82	111.27
31	3	212	A86	C33-C32-C31	4.25	113.34	109.21
19	A	812	CLA	C3D-C4D-ND	4.25	117.11	110.24
19	4	304	CLA	C1D-CHD-C4C	-4.24	116.90	126.06
19	A	804	CLA	C3D-C4D-ND	4.24	117.09	110.24
19	5	211	CLA	C1-C2-C3	-4.24	118.72	126.04
19	B	830	CLA	C3D-C2D-C1D	-4.23	100.05	105.83
30	3	211	KC1	O2D-CGD-CBD	4.23	118.79	111.27
30	4	307	KC1	CHC-C1C-C2C	-4.23	118.37	124.98
19	1	309	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
19	1	307	CLA	C4A-NA-C1A	-4.23	104.80	106.71
19	A	837	CLA	C3D-C4D-ND	4.23	117.08	110.24
19	A	806	CLA	C1-O2A-CGA	4.23	127.54	116.44
19	3	207	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
30	3	211	KC1	CHD-C4C-C3C	-4.23	117.39	125.33
19	5	211	CLA	O2D-CGD-CBD	4.23	118.78	111.27
19	B	818	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
19	A	835	CLA	C3D-C4D-ND	4.22	117.07	110.24
19	4	305	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
19	B	826	CLA	C3D-C4D-ND	4.22	117.07	110.24
28	2	217	DD6	C-C1-C24	-4.22	111.43	118.08
19	B	825	CLA	C3C-C4C-NC	4.22	115.30	110.57
19	A	815	CLA	C3D-C4D-ND	4.22	117.06	110.24
19	1	306	CLA	CMA-C3A-C4A	-4.22	100.44	111.77
19	1	309	CLA	C1-C2-C3	-4.21	118.75	126.04
23	A	853	LHG	O4-P-O5	4.21	133.07	112.24
19	B	802	CLA	C4A-NA-C1A	-4.21	104.81	106.71
19	A	833	CLA	C3D-C4D-ND	4.21	117.04	110.24
27	J	105	5X6	C41-C17-C16	-4.20	111.46	118.08
19	B	845	CLA	C3C-C4C-NC	4.20	115.28	110.57
18	A	801	CL0	C1C-C2C-C3C	-4.20	102.54	106.96
19	B	803	CLA	C3D-C4D-ND	4.20	117.03	110.24
19	B	806	CLA	C3D-C4D-ND	4.20	117.03	110.24
28	L	209	DD6	C33-C32-C31	4.19	118.12	109.62
19	B	809	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
31	5	219	A86	C33-C32-C31	4.19	113.28	109.21
19	4	309	CLA	C4A-NA-C1A	-4.19	104.82	106.71
19	u	201	CLA	C3D-C2D-C1D	-4.18	100.12	105.83
19	J	103	CLA	C3C-C4C-NC	4.18	115.26	110.57
19	A	810	CLA	C3D-C2D-C1D	-4.18	100.13	105.83
19	1	303	CLA	C4A-NA-C1A	-4.17	104.83	106.71
19	5	208	CLA	O2D-CGD-CBD	4.17	118.68	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	829	CLA	C3D-C4D-ND	4.17	116.98	110.24
19	A	831	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
19	B	812	CLA	C4A-NA-C1A	-4.17	104.83	106.71
31	2	219	A86	C4-C5-C6	-4.17	121.36	127.31
30	3	211	KC1	CHC-C1C-C2C	-4.17	118.47	124.98
19	B	829	CLA	O2D-CGD-CBD	4.16	118.67	111.27
19	B	821	CLA	C3D-C2D-C1D	-4.16	100.15	105.83
19	B	827	CLA	C4A-NA-C1A	-4.16	104.83	106.71
19	A	838	CLA	C3D-C4D-ND	4.16	116.96	110.24
19	4	306	CLA	C1-C2-C3	-4.15	118.86	126.04
19	B	836	CLA	O2D-CGD-CBD	4.15	118.65	111.27
23	1	318	LHG	O4-P-O5	4.15	132.76	112.24
23	4	317	LHG	O4-P-O5	4.15	132.75	112.24
19	2	206	CLA	C1C-C2C-C3C	-4.15	102.60	106.96
27	J	105	5X6	C24-C23-C22	-4.14	114.78	126.42
19	3	204	CLA	C3D-C4D-ND	4.14	116.94	110.24
19	3	206	CLA	C3C-C4C-NC	4.14	115.22	110.57
23	A	852	LHG	O4-P-O5	4.14	132.72	112.24
30	4	302	KC1	CHC-C1C-C2C	-4.14	118.52	124.98
30	2	211	KC1	O2D-CGD-CBD	4.13	118.61	111.27
31	4	314	A86	C36-C31-C32	-4.13	115.60	119.70
19	u	202	CLA	C3C-C4C-NC	4.13	115.20	110.57
19	B	824	CLA	C3C-C4C-NC	4.12	115.20	110.57
19	B	811	CLA	C3D-C2D-C1D	-4.12	100.20	105.83
30	4	307	KC1	C2C-C1C-NC	4.12	115.07	110.57
19	B	827	CLA	C3D-C4D-ND	4.12	116.90	110.24
19	B	818	CLA	C3D-C4D-ND	4.12	116.90	110.24
19	1	309	CLA	C2C-C1C-NC	4.12	113.83	109.97
19	A	825	CLA	C1C-C2C-C3C	-4.11	102.63	106.96
19	A	804	CLA	C3C-C4C-NC	4.11	115.18	110.57
19	F	203	CLA	C3D-C4D-ND	4.11	116.89	110.24
19	A	813	CLA	C3D-C4D-ND	4.11	116.88	110.24
19	A	827	CLA	C3C-C4C-NC	4.10	115.17	110.57
18	A	801	CL0	CAA-C2A-C3A	-4.10	101.54	112.78
19	B	825	CLA	C3D-C4D-ND	4.10	116.87	110.24
19	B	833	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
19	A	828	CLA	C3D-C4D-ND	4.09	116.86	110.24
19	B	813	CLA	C3D-C4D-ND	4.09	116.86	110.24
19	B	808	CLA	C3D-C4D-ND	4.09	116.86	110.24
19	4	306	CLA	C1D-CHD-C4C	-4.09	117.24	126.06
19	B	808	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
19	B	802	CLA	C3D-C4D-ND	4.08	116.84	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	301	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
30	3	208	KC1	CHC-C1C-C2C	-4.08	118.61	124.98
19	A	844	CLA	C3C-C4C-NC	4.08	115.14	110.57
19	A	813	CLA	C3C-C4C-NC	4.07	115.14	110.57
19	B	827	CLA	C3C-C4C-NC	4.07	115.14	110.57
19	A	836	CLA	O2D-CGD-CBD	4.07	118.50	111.27
19	2	209	CLA	C4A-NA-C1A	-4.07	104.88	106.71
31	4	316	A86	C17-C16-C15	4.07	113.31	109.16
19	A	824	CLA	C3C-C4C-NC	4.07	115.13	110.57
19	4	311	CLA	C1-C2-C3	-4.06	120.17	126.75
19	4	309	CLA	C1C-C2C-C3C	-4.06	102.68	106.96
18	A	801	CL0	C3D-C4D-ND	4.06	116.81	110.24
31	4	316	A86	C41-C32-C31	-4.06	106.83	110.47
30	3	205	KC1	CHC-C1C-C2C	-4.06	118.63	124.98
23	B	842	LHG	O4-P-O5	4.06	132.32	112.24
19	A	829	CLA	O2D-CGD-CBD	4.06	118.48	111.27
19	A	880	CLA	O2D-CGD-CBD	4.06	118.48	111.27
19	A	878	CLA	C1D-CHD-C4C	-4.06	117.30	126.06
19	A	810	CLA	O2D-CGD-CBD	4.06	118.48	111.27
19	A	805	CLA	C3D-C4D-ND	4.06	116.80	110.24
19	3	206	CLA	O2D-CGD-CBD	4.06	118.47	111.27
19	A	842	CLA	C3C-C4C-NC	4.05	115.11	110.57
19	L	203	CLA	C3C-C4C-NC	4.05	115.11	110.57
19	B	812	CLA	C1-C2-C3	-4.05	119.05	126.04
19	A	807	CLA	O2A-CGA-CBA	4.04	124.58	111.91
18	A	801	CL0	C3D-C2D-C1D	-4.04	100.32	105.83
19	u	201	CLA	C1-C2-C3	-4.03	119.07	126.04
19	3	209	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
19	4	306	CLA	C3C-C4C-NC	4.03	115.09	110.57
19	A	832	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
19	B	811	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
30	3	205	KC1	C2C-C1C-NC	4.03	114.97	110.57
19	2	213	CLA	C3C-C4C-NC	4.03	115.09	110.57
31	4	316	A86	C35-C34-C33	4.02	116.90	109.88
19	B	802	CLA	C1D-CHD-C4C	-4.02	117.38	126.06
28	L	209	DD6	C35-C36-C31	-4.02	111.44	120.57
19	A	809	CLA	C3D-C4D-ND	4.02	116.74	110.24
19	A	810	CLA	C3C-C4C-NC	4.01	115.07	110.57
19	A	822	CLA	C3D-C4D-ND	4.01	116.73	110.24
19	A	829	CLA	C3D-C4D-ND	4.01	116.73	110.24
19	4	309	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
19	1	304	CLA	C4-C3-C5	4.00	122.01	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	810	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
31	2	219	A86	C36-C31-C32	-4.00	115.73	119.70
30	3	211	KC1	C2C-C1C-NC	4.00	114.94	110.57
19	A	812	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
19	A	823	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
19	A	823	CLA	C4A-NA-C1A	-3.99	104.91	106.71
19	2	212	CLA	C1D-CHD-C4C	-3.99	117.44	126.06
19	B	808	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
19	A	843	CLA	C4A-NA-C1A	-3.99	104.91	106.71
19	B	835	CLA	C1C-C2C-C3C	-3.99	102.77	106.96
30	3	208	KC1	C2C-C1C-NC	3.99	114.92	110.57
19	5	216	CLA	C3C-C4C-NC	3.98	115.04	110.57
19	A	878	CLA	C3D-C4D-ND	3.98	116.68	110.24
18	A	801	CL0	C3C-C4C-NC	3.98	115.04	110.57
31	1	317	A86	C20-C19-C18	-3.98	104.87	112.75
19	L	204	CLA	O2D-CGD-CBD	3.98	118.34	111.27
19	A	878	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
19	B	833	CLA	C3D-C4D-ND	3.98	116.68	110.24
28	3	213	DD6	C21-C20-C19	-3.98	109.80	114.28
19	5	213	CLA	C1D-CHD-C4C	-3.98	117.48	126.06
19	A	811	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
19	2	208	CLA	CAC-C3C-C4C	3.97	129.96	124.81
19	B	837	CLA	C3C-C4C-NC	3.97	115.02	110.57
19	B	837	CLA	C1C-C2C-C3C	-3.97	102.79	106.96
19	B	838	CLA	C1C-C2C-C3C	-3.97	102.79	106.96
19	B	833	CLA	C3C-C4C-NC	3.96	115.01	110.57
19	3	209	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
19	5	215	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
19	2	205	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
19	B	804	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
19	4	304	CLA	C3C-C4C-NC	3.95	115.00	110.57
19	B	823	CLA	C4A-NA-C1A	-3.94	104.93	106.71
28	1	312	DD6	C35-C36-C31	-3.94	111.62	120.57
31	5	217	A86	C36-C31-C32	-3.94	115.79	119.70
19	B	809	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
19	B	830	CLA	C1C-C2C-C3C	-3.94	102.82	106.96
19	A	821	CLA	C3C-C4C-NC	3.94	114.99	110.57
19	2	212	CLA	C3C-C4C-NC	3.94	114.99	110.57
19	4	304	CLA	O2A-CGA-CBA	3.94	124.26	111.91
19	A	819	CLA	CAC-C3C-C4C	3.94	129.92	124.81
19	A	808	CLA	C3C-C4C-NC	3.94	114.98	110.57
19	B	827	CLA	C1-C2-C3	-3.94	119.24	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	208	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
19	A	834	CLA	C1D-CHD-C4C	-3.93	117.57	126.06
19	A	833	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
28	5	218	DD6	C15-C14-C13	-3.93	117.68	125.99
19	B	813	CLA	C3C-C4C-NC	3.93	114.98	110.57
19	3	210	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
19	A	834	CLA	C3C-C4C-NC	3.93	114.98	110.57
19	B	822	CLA	C3D-C4D-ND	3.93	116.59	110.24
30	4	307	KC1	C4B-C3B-C2B	-3.93	103.53	106.75
19	A	838	CLA	C1-C2-C3	-3.92	119.26	126.04
19	3	204	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
19	B	819	CLA	O2D-CGD-CBD	3.92	118.23	111.27
19	B	828	CLA	C3C-C4C-NC	3.91	114.96	110.57
19	A	841	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
19	3	204	CLA	C1D-CHD-C4C	-3.91	117.62	126.06
19	5	211	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
19	B	836	CLA	C3C-C4C-NC	3.91	114.95	110.57
31	3	212	A86	C4-C5-C6	-3.90	121.74	127.31
19	B	802	CLA	C1-C2-C3	-3.90	119.30	126.04
19	A	837	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
19	1	304	CLA	C1-C2-C3	-3.90	119.30	126.04
19	A	803	CLA	C3D-C4D-ND	3.90	116.54	110.24
30	4	302	KC1	C4B-C3B-C2B	-3.90	103.55	106.75
19	A	831	CLA	C3C-C4C-NC	3.89	114.94	110.57
19	B	806	CLA	C3C-C4C-NC	3.89	114.94	110.57
19	4	305	CLA	O2D-CGD-CBD	3.89	118.19	111.27
19	2	208	CLA	C1-C2-C3	-3.89	119.31	126.04
19	A	811	CLA	C3C-C4C-NC	3.89	114.93	110.57
19	A	830	CLA	C1-C2-C3	-3.88	119.33	126.04
19	A	815	CLA	C3C-C4C-NC	3.88	114.93	110.57
19	2	210	CLA	C3C-C4C-NC	3.88	114.93	110.57
19	B	814	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
19	B	824	CLA	C3D-C4D-ND	3.88	116.52	110.24
28	1	313	DD6	C35-C36-C31	-3.88	111.77	120.57
19	B	807	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
19	B	846	CLA	C1-C2-C3	-3.88	119.34	126.04
19	1	303	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
19	5	214	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
19	5	215	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
19	A	809	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
19	A	812	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
19	4	304	CLA	C1C-C2C-C3C	-3.86	102.89	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	809	CLA	C4A-NA-C1A	-3.86	104.97	106.71
19	B	812	CLA	C3C-C4C-NC	3.86	114.90	110.57
19	B	817	CLA	C3C-C4C-NC	3.86	114.90	110.57
19	B	804	CLA	C4A-NA-C1A	-3.86	104.97	106.71
19	B	838	CLA	C3C-C4C-NC	3.86	114.90	110.57
19	1	307	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
19	4	303	CLA	CAA-C2A-C3A	-3.86	102.22	112.78
19	B	831	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
19	4	313	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
19	1	308	CLA	C3C-C4C-NC	3.86	114.89	110.57
19	L	204	CLA	C3C-C4C-NC	3.85	114.89	110.57
19	A	805	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
30	2	211	KC1	C1C-C2C-C3C	-3.85	102.91	106.96
31	4	315	A86	C3-C4-C5	-3.85	115.59	123.47
28	3	213	DD6	O1-C20-C21	-3.85	110.45	115.06
19	A	844	CLA	C1-C2-C3	-3.85	119.39	126.04
19	2	215	CLA	C1D-CHD-C4C	-3.84	117.77	126.06
19	5	216	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
19	B	825	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
19	L	204	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
19	A	880	CLA	C1-C2-C3	-3.84	119.40	126.04
19	3	204	CLA	C3C-C4C-NC	3.84	114.88	110.57
31	5	220	A86	C9-C8-C6	-3.84	115.64	126.42
19	1	307	CLA	C3B-C4B-NB	3.84	114.17	109.21
19	A	838	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
19	A	880	CLA	C3C-C4C-NC	3.83	114.87	110.57
19	F	203	CLA	C3C-C4C-NC	3.83	114.87	110.57
19	5	212	CLA	O2D-CGD-CBD	3.83	118.07	111.27
19	A	818	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
19	5	216	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
19	A	836	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
28	L	209	DD6	C21-C20-C15	-3.82	115.85	122.26
19	B	821	CLA	O2D-CGD-CBD	3.82	118.06	111.27
19	2	213	CLA	C1D-CHD-C4C	-3.82	117.81	126.06
19	A	828	CLA	C4A-NA-C1A	-3.82	104.99	106.71
31	3	212	A86	C12-C11-C13	3.82	122.44	116.02
19	F	204	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
19	A	844	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
19	2	209	CLA	C1D-CHD-C4C	-3.82	117.82	126.06
19	A	819	CLA	C3C-C4C-NC	3.82	114.85	110.57
19	F	203	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
19	A	821	CLA	C1C-C2C-C3C	-3.81	102.95	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	304	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
19	L	206	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
19	A	880	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
19	4	310	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
19	L	203	CLA	C4A-NA-C1A	-3.81	104.99	106.71
19	2	212	CLA	C4A-NA-C1A	-3.81	104.99	106.71
19	B	834	CLA	C3C-C4C-NC	3.81	114.84	110.57
30	4	302	KC1	CBA-CAA-C2A	-3.81	110.75	125.27
19	B	809	CLA	C3D-C4D-ND	3.81	116.40	110.24
19	B	810	CLA	C3C-C4C-NC	3.81	114.84	110.57
19	A	880	CLA	C1D-CHD-C4C	-3.81	117.85	126.06
19	B	823	CLA	CAA-C2A-C3A	-3.81	102.36	112.78
19	5	213	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
19	B	827	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
30	3	205	KC1	C1A-NA-C4A	-3.80	105.00	106.71
19	B	827	CLA	O2D-CGD-O1D	-3.80	116.40	123.84
19	F	203	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
19	3	203	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
19	A	817	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
19	A	826	CLA	C3D-C4D-ND	3.80	116.38	110.24
19	B	803	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
19	4	308	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
19	B	845	CLA	C1C-C2C-C3C	-3.80	102.97	106.96
19	2	208	CLA	C3C-C4C-NC	3.79	114.82	110.57
19	A	838	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
19	B	826	CLA	C3C-C4C-NC	3.79	114.82	110.57
19	u	202	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
31	5	217	A86	C4-C3-C2	-3.79	115.72	123.47
19	A	814	CLA	C3C-C4C-NC	3.78	114.81	110.57
19	A	810	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
19	u	201	CLA	C3C-C4C-NC	3.78	114.81	110.57
31	5	219	A86	C12-C11-C13	3.78	122.38	116.02
19	2	210	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
19	A	840	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
19	B	820	CLA	C3C-C4C-NC	3.78	114.81	110.57
19	A	818	CLA	C3C-C4C-NC	3.77	114.80	110.57
19	B	824	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
19	F	204	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
19	5	207	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
31	4	316	A86	C4-C3-C2	-3.77	115.75	123.47
19	A	816	CLA	C1-C2-C3	-3.77	120.65	126.75
19	B	822	CLA	C1C-C2C-C3C	-3.77	102.99	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	203	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
19	A	820	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
19	A	833	CLA	O2D-CGD-CBD	3.77	117.96	111.27
19	A	827	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
19	4	303	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
19	A	829	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
19	B	805	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
19	1	306	CLA	C4-C3-C5	3.76	120.29	115.98
19	1	307	CLA	O2D-CGD-CBD	3.76	117.95	111.27
19	A	829	CLA	C3B-C4B-NB	3.76	114.07	109.21
19	B	815	CLA	C3C-C4C-NC	3.76	114.78	110.57
19	B	813	CLA	C1C-C2C-C3C	-3.76	103.01	106.96
19	2	214	CLA	C1C-C2C-C3C	-3.76	103.01	106.96
30	1	305	KC1	CHC-C1C-C2C	-3.75	119.11	124.98
19	A	809	CLA	C3C-C4C-NC	3.75	114.78	110.57
19	1	306	CLA	C1D-CHD-C4C	-3.75	117.96	126.06
19	4	313	CLA	C1D-CHD-C4C	-3.75	117.96	126.06
19	A	803	CLA	C3C-C4C-NC	3.75	114.78	110.57
19	A	835	CLA	C3C-C4C-NC	3.75	114.78	110.57
19	B	822	CLA	C3C-C4C-NC	3.75	114.78	110.57
30	3	211	KC1	C1C-C2C-C3C	-3.75	103.01	106.96
19	A	807	CLA	C3C-C4C-NC	3.75	114.78	110.57
19	A	830	CLA	C3C-C4C-NC	3.75	114.77	110.57
19	L	206	CLA	C1D-CHD-C4C	-3.75	117.98	126.06
19	A	813	CLA	C1D-CHD-C4C	-3.75	117.98	126.06
19	5	207	CLA	C1D-CHD-C4C	-3.74	117.98	126.06
19	B	815	CLA	C1D-CHD-C4C	-3.74	117.98	126.06
19	4	308	CLA	C3C-C4C-NC	3.74	114.77	110.57
28	1	315	DD6	C24-C1-C2	-3.74	113.20	118.94
19	4	306	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
19	A	825	CLA	C3C-C4C-NC	3.74	114.76	110.57
19	A	840	CLA	C3C-C4C-NC	3.74	114.76	110.57
19	3	202	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
19	A	805	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
19	B	825	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
19	5	215	CLA	C3C-C4C-NC	3.73	114.75	110.57
30	3	211	KC1	C4B-C3B-C2B	-3.73	103.69	106.75
19	2	206	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
19	B	836	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
19	B	802	CLA	CAA-C2A-C3A	-3.72	102.58	112.78
19	B	837	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
19	A	829	CLA	C1D-CHD-C4C	-3.72	118.03	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	831	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
19	A	826	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
19	J	103	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
19	B	826	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
19	A	815	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
19	B	806	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
19	4	304	CLA	CMC-C2C-C1C	3.71	130.69	125.04
30	3	208	KC1	C1C-C2C-C3C	-3.71	103.05	106.96
19	B	804	CLA	C3C-C4C-NC	3.71	114.73	110.57
19	B	814	CLA	C3C-C4C-NC	3.71	114.73	110.57
19	A	834	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
19	B	826	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
19	5	211	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
19	2	206	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
19	3	206	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
19	A	816	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
19	5	210	CLA	C3B-C4B-NB	3.70	114.00	109.21
19	4	313	CLA	C1-C2-C3	-3.70	119.64	126.04
19	A	808	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
19	1	301	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
19	A	844	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
19	B	836	CLA	CAC-C3C-C4C	3.70	129.60	124.81
19	B	832	CLA	C3C-C4C-NC	3.69	114.71	110.57
19	B	819	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
19	B	821	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
19	4	303	CLA	C1D-CHD-C4C	-3.69	118.09	126.06
19	A	844	CLA	C3B-C4B-NB	3.69	113.98	109.21
19	A	818	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
19	1	306	CLA	O2D-CGD-CBD	3.69	117.82	111.27
19	B	835	CLA	C3C-C4C-NC	3.69	114.71	110.57
19	2	215	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
30	2	211	KC1	C2C-C1C-NC	3.69	114.60	110.57
19	A	843	CLA	C1D-CHD-C4C	-3.69	118.11	126.06
28	3	213	DD6	C35-C36-C31	-3.69	112.20	120.57
30	3	208	KC1	C4B-C3B-C2B	-3.68	103.73	106.75
19	3	202	CLA	C3C-C4C-NC	3.68	114.70	110.57
19	4	305	CLA	C3C-C4C-NC	3.68	114.70	110.57
19	2	206	CLA	C1-C2-C3	-3.68	119.67	126.04
19	A	837	CLA	C1D-CHD-C4C	-3.68	118.11	126.06
19	A	817	CLA	C3C-C4C-NC	3.68	114.70	110.57
19	3	210	CLA	C1D-CHD-C4C	-3.68	118.11	126.06
31	1	317	A86	C36-C31-C32	-3.68	116.04	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	206	CLA	C3C-C4C-NC	3.68	114.70	110.57
19	2	213	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
19	3	207	CLA	C3C-C4C-NC	3.68	114.70	110.57
19	2	214	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
19	B	820	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
31	3	212	A86	C41-C32-C31	-3.68	107.18	110.47
19	4	305	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
19	5	212	CLA	C1D-CHD-C4C	-3.67	118.13	126.06
19	B	811	CLA	C1-C2-C3	-3.67	119.69	126.04
19	A	815	CLA	C1D-CHD-C4C	-3.67	118.13	126.06
19	B	823	CLA	C1C-C2C-C3C	-3.67	103.09	106.96
31	2	216	A86	C26-C25-C24	-3.67	111.76	123.22
19	A	839	CLA	C3C-C4C-NC	3.67	114.69	110.57
19	J	103	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
30	2	211	KC1	CBA-CAA-C2A	-3.67	111.28	125.27
19	B	809	CLA	C1-C2-C3	-3.67	119.70	126.04
19	2	205	CLA	C1D-CHD-C4C	-3.66	118.15	126.06
28	L	209	DD6	C15-C14-C13	3.66	133.74	125.99
19	5	209	CLA	C1C-C2C-C3C	-3.66	103.10	106.96
19	B	826	CLA	C1-C2-C3	-3.66	119.71	126.04
19	B	821	CLA	C3C-C4C-NC	3.66	114.68	110.57
19	2	212	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
31	5	217	A86	C20-C19-C18	-3.66	105.50	112.75
19	1	303	CLA	C1-C2-C3	-3.66	119.71	126.04
19	A	842	CLA	C4A-NA-C1A	-3.66	105.06	106.71
19	B	828	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
19	A	817	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
19	A	835	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
19	A	822	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
19	A	805	CLA	C3C-C4C-NC	3.66	114.67	110.57
19	A	838	CLA	C3C-C4C-NC	3.65	114.67	110.57
19	2	207	CLA	C3C-C4C-NC	3.65	114.67	110.57
19	A	828	CLA	C1D-CHD-C4C	-3.65	118.18	126.06
19	B	834	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
19	5	208	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
19	B	817	CLA	C1-C2-C3	-3.65	119.73	126.04
19	3	206	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
19	B	846	CLA	C3C-C4C-NC	3.65	114.66	110.57
30	2	211	KC1	CHC-C1C-C2C	-3.64	119.29	124.98
31	2	216	A86	C12-C11-C13	3.64	122.14	116.02
19	5	213	CLA	C3C-C4C-NC	3.64	114.66	110.57
19	A	804	CLA	C1C-C2C-C3C	-3.64	103.13	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	833	CLA	C3B-C4B-NB	3.64	113.91	109.21
19	B	845	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
19	1	309	CLA	C3C-C4C-NC	3.64	114.65	110.57
19	A	806	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
19	A	830	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
19	B	820	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
19	u	201	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
19	5	209	CLA	C3C-C4C-NC	3.63	114.64	110.57
19	B	832	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
19	A	836	CLA	C3C-C4C-NC	3.63	114.64	110.57
19	B	807	CLA	C3C-C4C-NC	3.63	114.64	110.57
19	B	836	CLA	C1-C2-C3	-3.62	119.77	126.04
19	A	823	CLA	C3C-C4C-NC	3.62	114.64	110.57
19	B	823	CLA	C3C-C4C-NC	3.62	114.64	110.57
19	2	205	CLA	C3C-C4C-NC	3.62	114.64	110.57
19	A	814	CLA	C1D-CHD-C4C	-3.62	118.24	126.06
19	A	826	CLA	O2D-CGD-O1D	-3.62	116.75	123.84
19	5	210	CLA	C1D-CHD-C4C	-3.62	118.24	126.06
19	B	817	CLA	C1D-CHD-C4C	-3.62	118.24	126.06
31	2	216	A86	C34-O4-C38	-3.62	111.15	117.90
19	A	803	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
19	B	805	CLA	C3C-C4C-NC	3.62	114.63	110.57
31	3	228	A86	C33-C32-C31	3.62	112.73	109.21
19	B	804	CLA	C3B-C4B-NB	3.62	113.89	109.21
31	5	217	A86	C25-C26-C27	-3.62	122.14	127.31
19	5	212	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
19	A	807	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
19	1	303	CLA	C3B-C4B-NB	3.62	113.89	109.21
19	4	310	CLA	C3C-C4C-NC	3.62	114.63	110.57
31	4	315	A86	C25-C26-C27	-3.62	122.15	127.31
19	4	308	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
19	A	839	CLA	C3B-C4B-NB	3.62	113.89	109.21
19	3	209	CLA	C3C-C4C-NC	3.61	114.62	110.57
19	B	812	CLA	C1D-CHD-C4C	-3.61	118.26	126.06
19	4	312	CLA	C3C-C4C-NC	3.61	114.62	110.57
22	F	205	BCR	C2-C1-C6	3.61	116.04	110.48
19	B	832	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
19	B	846	CLA	C1D-CHD-C4C	-3.61	118.28	126.06
30	1	305	KC1	CBA-CAA-C2A	-3.61	111.53	125.27
19	B	806	CLA	O2D-CGD-CBD	3.60	117.67	111.27
19	B	846	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
19	2	209	CLA	C1C-C2C-C3C	-3.60	103.17	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	838	CLA	C1-C2-C3	-3.60	119.81	126.04
19	A	812	CLA	C3C-C4C-NC	3.60	114.61	110.57
19	A	833	CLA	C3C-C4C-NC	3.60	114.61	110.57
19	2	206	CLA	C3C-C4C-NC	3.60	114.61	110.57
19	A	822	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
19	1	306	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
19	B	814	CLA	C3B-C4B-NB	3.60	113.86	109.21
19	A	822	CLA	C3C-C4C-NC	3.60	114.60	110.57
19	A	841	CLA	C1D-CHD-C4C	-3.59	118.30	126.06
19	A	830	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
19	A	820	CLA	C3C-C4C-NC	3.59	114.60	110.57
19	B	806	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
19	A	823	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
19	A	842	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
19	A	808	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
19	1	309	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
19	3	203	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
19	B	827	CLA	C3B-C4B-NB	3.59	113.85	109.21
19	1	309	CLA	CAA-C2A-C3A	-3.58	102.96	112.78
19	B	802	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
27	J	105	5X6	C12-C11-C03	-3.58	117.14	127.20
19	4	312	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
19	A	833	CLA	C1-C2-C3	-3.58	119.85	126.04
19	1	310	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
19	B	830	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
19	1	308	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
19	B	838	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
19	B	816	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
19	2	209	CLA	C4-C3-C5	3.57	121.28	115.27
19	3	203	CLA	C3C-C4C-NC	3.57	114.58	110.57
19	1	303	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
19	3	207	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
30	4	307	KC1	CBA-CAA-C2A	-3.57	111.65	125.27
30	3	205	KC1	C1C-C2C-C3C	-3.57	103.20	106.96
19	5	212	CLA	C1-C2-C3	-3.57	119.87	126.04
19	5	211	CLA	C3B-C4B-NB	3.57	113.83	109.21
19	A	831	CLA	C3B-C4B-NB	3.57	113.83	109.21
19	B	806	CLA	C1-C2-C3	-3.57	119.87	126.04
30	1	305	KC1	C2C-C1C-NC	3.57	114.47	110.57
19	B	809	CLA	C3C-C4C-NC	3.57	114.57	110.57
19	2	207	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
19	1	301	CLA	C3C-C4C-NC	3.56	114.57	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	307	CLA	CAC-C3C-C4C	3.56	129.43	124.81
19	A	806	CLA	C1D-CHD-C4C	-3.56	118.37	126.06
19	3	202	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
31	5	217	A86	C12-C11-C13	3.56	122.00	116.02
19	B	821	CLA	O2A-CGA-CBA	3.56	123.08	111.91
19	A	833	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
19	A	826	CLA	C3B-C4B-NB	3.56	113.81	109.21
19	A	878	CLA	C3B-C4B-NB	3.56	113.81	109.21
19	5	213	CLA	C3B-C4B-NB	3.56	113.81	109.21
19	B	827	CLA	C1D-CHD-C4C	-3.56	118.39	126.06
19	B	829	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
31	2	219	A86	C25-C24-C1	-3.55	116.43	126.42
19	A	807	CLA	C1-C2-C3	-3.55	119.90	126.04
19	A	813	CLA	C3B-C4B-NB	3.55	113.80	109.21
19	4	303	CLA	C3C-C4C-NC	3.55	114.56	110.57
19	B	831	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
19	A	833	CLA	C4A-NA-C1A	-3.55	105.11	106.71
19	A	829	CLA	C3C-C4C-NC	3.55	114.55	110.57
19	A	832	CLA	C1D-CHD-C4C	-3.55	118.40	126.06
19	1	306	CLA	C1-C2-C3	-3.55	119.91	126.04
19	A	805	CLA	C1-C2-C3	-3.55	119.91	126.04
31	2	219	A86	C12-C11-C13	3.55	121.98	116.02
19	A	838	CLA	C3B-C4B-NB	3.54	113.79	109.21
31	2	218	A86	C41-C32-C31	-3.54	107.30	110.47
19	A	835	CLA	C1D-CHD-C4C	-3.54	118.41	126.06
30	4	302	KC1	C2C-C1C-NC	3.54	114.44	110.57
31	1	316	A86	C20-C19-C18	-3.54	105.74	112.75
19	A	842	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
19	A	826	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
19	1	310	CLA	CAC-C3C-C4C	3.54	129.40	124.81
19	A	840	CLA	C1D-CHD-C4C	-3.54	118.43	126.06
19	B	826	CLA	C3B-C4B-NB	3.54	113.78	109.21
28	2	217	DD6	C15-C14-C13	-3.53	118.52	125.99
19	B	811	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
19	B	811	CLA	C3C-C4C-NC	3.53	114.53	110.57
19	A	832	CLA	C3C-C4C-NC	3.53	114.53	110.57
19	B	812	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
19	A	804	CLA	C1D-CHD-C4C	-3.53	118.45	126.06
19	5	209	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
19	1	303	CLA	C3C-C4C-NC	3.52	114.52	110.57
19	u	201	CLA	CAC-C3C-C4C	3.52	129.38	124.81
19	A	821	CLA	C1D-CHD-C4C	-3.52	118.47	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	828	CLA	C4C-C3C-C2C	-3.52	101.77	106.90
19	A	813	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
19	2	209	CLA	C3C-C4C-NC	3.51	114.51	110.57
19	A	839	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
19	A	806	CLA	C3C-C4C-NC	3.51	114.51	110.57
19	5	211	CLA	C3C-C4C-NC	3.51	114.51	110.57
19	2	210	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
19	3	209	CLA	C3B-C4B-NB	3.51	113.75	109.21
19	4	309	CLA	C3C-C4C-NC	3.51	114.50	110.57
19	5	210	CLA	C3C-C4C-NC	3.51	114.50	110.57
19	A	837	CLA	C3C-C4C-NC	3.50	114.50	110.57
19	B	835	CLA	C1D-CHD-C4C	-3.50	118.50	126.06
19	4	305	CLA	C1D-CHD-C4C	-3.50	118.52	126.06
19	2	207	CLA	C1D-CHD-C4C	-3.50	118.52	126.06
19	4	311	CLA	C1D-CHD-C4C	-3.49	118.52	126.06
19	A	830	CLA	C3B-C4B-NB	3.49	113.73	109.21
19	1	310	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
19	A	802	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
19	A	811	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
19	5	209	CLA	CAC-C3C-C4C	3.49	129.34	124.81
19	3	206	CLA	C3B-C4B-NB	3.49	113.72	109.21
30	4	302	KC1	CAA-CBA-CGA	-3.49	109.33	127.26
30	3	205	KC1	C4B-C3B-C2B	-3.49	103.89	106.75
19	1	307	CLA	C1D-CHD-C4C	-3.49	118.54	126.06
19	B	804	CLA	C1D-CHD-C4C	-3.48	118.54	126.06
19	u	202	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
19	B	833	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
19	B	816	CLA	CAC-C3C-C4C	3.48	129.32	124.81
28	1	315	DD6	C21-C20-C19	-3.48	110.37	114.28
19	u	201	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
19	B	811	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
19	B	814	CLA	C1D-CHD-C4C	-3.47	118.56	126.06
31	1	317	A86	C40-C32-C31	-3.47	107.37	110.47
28	2	217	DD6	C33-C34-C35	3.47	115.05	110.30
19	5	214	CLA	C3C-C4C-NC	3.47	114.46	110.57
19	4	310	CLA	C1C-C2C-C3C	-3.46	103.31	106.96
19	1	304	CLA	C3C-C4C-NC	3.46	114.45	110.57
19	B	836	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
19	B	834	CLA	C1D-CHD-C4C	-3.46	118.59	126.06
19	A	826	CLA	C4A-NA-C1A	-3.46	105.15	106.71
19	A	802	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
30	4	302	KC1	CAA-C2A-C1A	-3.45	108.87	124.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	5	217	A86	C10-C9-C8	-3.45	112.45	123.22
19	4	311	CLA	C3C-C4C-NC	3.45	114.44	110.57
19	1	304	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
19	B	810	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
19	A	843	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
28	2	217	DD6	O1-C20-C21	-3.45	110.93	115.06
19	L	203	CLA	C1D-CHD-C4C	-3.44	118.63	126.06
19	L	204	CLA	C3B-C4B-NB	3.44	113.66	109.21
31	3	214	A86	C25-C26-C27	-3.44	122.40	127.31
19	2	205	CLA	C3B-C4B-NB	3.44	113.66	109.21
19	2	208	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
19	5	214	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
19	B	813	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
19	B	825	CLA	C3B-C4B-NB	3.44	113.65	109.21
19	1	307	CLA	C3C-C4C-NC	3.44	114.42	110.57
19	2	215	CLA	C3C-C4C-NC	3.43	114.42	110.57
19	L	204	CLA	C1D-CHD-C4C	-3.43	118.66	126.06
19	B	815	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
19	B	803	CLA	C4A-NA-C1A	-3.43	105.17	106.71
18	A	801	CL0	C1D-CHD-C4C	-3.42	118.67	126.06
19	4	311	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
19	5	212	CLA	CMB-C2B-C3B	3.42	131.07	124.68
19	1	303	CLA	CAC-C3C-C4C	3.42	129.25	124.81
19	4	301	CLA	C3C-C4C-NC	3.42	114.40	110.57
19	B	829	CLA	CAC-C3C-C4C	3.42	129.24	124.81
19	B	822	CLA	C1D-CHD-C4C	-3.41	118.69	126.06
18	A	801	CL0	O2A-CGA-CBA	3.41	122.62	111.91
19	A	824	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
19	B	818	CLA	C3B-C4B-NB	3.41	113.62	109.21
19	B	819	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
19	A	819	CLA	C1D-CHD-C4C	-3.41	118.71	126.06
31	2	218	A86	C4-C3-C2	-3.40	116.50	123.47
19	B	805	CLA	C3B-C4B-NB	3.40	113.61	109.21
31	2	219	A86	C40-C32-C31	-3.40	107.43	110.47
31	4	314	A86	C26-C25-C24	-3.40	112.61	123.22
19	B	812	CLA	C3B-C4B-NB	3.40	113.60	109.21
19	5	212	CLA	C3C-C4C-NC	3.40	114.38	110.57
19	B	823	CLA	C1D-CHD-C4C	-3.40	118.73	126.06
19	A	807	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
30	1	305	KC1	C4B-C3B-C2B	-3.39	103.97	106.75
19	A	820	CLA	C3B-C4B-NB	3.39	113.59	109.21
19	A	825	CLA	C1D-CHD-C4C	-3.39	118.74	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	823	CLA	C3B-C4B-NB	3.39	113.59	109.21
19	A	807	CLA	C3B-C4B-NB	3.39	113.59	109.21
19	A	803	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
19	A	816	CLA	C3B-C4B-NB	3.39	113.59	109.21
19	A	819	CLA	O2A-CGA-CBA	3.39	122.54	111.91
19	B	819	CLA	C3C-C4C-NC	3.39	114.37	110.57
19	5	216	CLA	C3B-C4B-NB	3.39	113.59	109.21
19	A	832	CLA	C1-C2-C3	-3.39	120.19	126.04
19	4	313	CLA	C3B-C4B-NB	3.39	113.59	109.21
19	B	822	CLA	C3B-C4B-NB	3.39	113.59	109.21
30	4	307	KC1	C1C-C2C-C3C	-3.39	103.40	106.96
19	4	312	CLA	C1-C2-C3	-3.39	120.19	126.04
19	4	313	CLA	C3C-C4C-NC	3.38	114.37	110.57
31	3	212	A86	C3-C2-C1	-3.38	122.49	127.31
19	A	810	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
19	B	805	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
19	3	210	CLA	C3C-C4C-NC	3.37	114.35	110.57
28	1	315	DD6	C12-C11-C13	-3.37	112.77	118.08
19	A	809	CLA	C3B-C4B-NB	3.37	113.56	109.21
19	4	304	CLA	C1-C2-C3	-3.37	121.30	126.75
19	A	836	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
19	4	312	CLA	C1D-CHD-C4C	-3.37	118.80	126.06
19	2	208	CLA	C1D-CHD-C4C	-3.37	118.80	126.06
19	A	827	CLA	CAA-C2A-C3A	-3.36	103.57	112.78
19	F	204	CLA	C3C-C4C-NC	3.36	114.34	110.57
19	A	816	CLA	C3C-C4C-NC	3.36	114.34	110.57
19	3	207	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
19	A	812	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
19	A	815	CLA	C3B-C4B-NB	3.36	113.55	109.21
30	2	211	KC1	CAA-CBA-CGA	-3.36	110.00	127.26
19	B	821	CLA	C1D-CHD-C4C	-3.35	118.82	126.06
19	A	814	CLA	C1C-C2C-C3C	-3.35	103.43	106.96
19	A	809	CLA	CAA-C2A-C3A	-3.35	103.59	112.78
19	A	827	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
19	B	807	CLA	C1D-CHD-C4C	-3.35	118.83	126.06
31	3	214	A86	C3-C4-C5	-3.35	116.61	123.47
19	2	205	CLA	C1-C2-C3	-3.35	120.25	126.04
19	2	209	CLA	CAC-C3C-C4C	3.35	129.16	124.81
19	B	830	CLA	C3C-C4C-NC	3.35	114.33	110.57
19	B	831	CLA	C3C-C4C-NC	3.35	114.33	110.57
19	A	814	CLA	C1-C2-C3	-3.35	120.25	126.04
19	4	301	CLA	C1C-C2C-C3C	-3.35	103.44	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	818	CLA	C3C-C4C-NC	3.34	114.32	110.57
19	B	828	CLA	C1D-CHD-C4C	-3.34	118.84	126.06
31	3	228	A86	C9-C8-C6	-3.34	117.03	126.42
30	2	211	KC1	CHD-C4C-NC	3.34	129.27	124.20
19	B	809	CLA	C3B-C4B-NB	3.34	113.53	109.21
19	A	841	CLA	C3C-C4C-NC	3.34	114.32	110.57
31	2	219	A86	C35-C34-C33	3.34	115.70	109.88
19	B	824	CLA	C1-C2-C3	-3.34	120.27	126.04
19	B	823	CLA	C3B-C4B-NB	3.34	113.53	109.21
30	1	305	KC1	CAA-CBA-CGA	-3.34	110.11	127.26
19	B	803	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
30	3	211	KC1	CBA-CAA-C2A	-3.34	112.55	125.27
19	A	824	CLA	C4-C3-C5	3.34	119.80	115.98
19	1	306	CLA	CAC-C3C-C4C	3.33	129.14	124.81
19	A	878	CLA	C4-C3-C5	3.33	120.88	115.27
19	A	819	CLA	C4C-C3C-C2C	-3.33	102.04	106.90
19	3	204	CLA	C3B-C4B-NB	3.33	113.52	109.21
30	3	211	KC1	CAC-C3C-C4C	3.33	129.13	124.81
28	1	315	DD6	C15-C14-C13	-3.33	118.96	125.99
19	B	817	CLA	C1C-C2C-C3C	-3.32	103.46	106.96
30	1	305	KC1	C1C-C2C-C3C	-3.32	103.46	106.96
19	B	837	CLA	C1-C2-C3	-3.32	120.30	126.04
19	3	210	CLA	CHD-C4C-NC	3.32	129.43	124.20
19	A	810	CLA	C3B-C4B-NB	3.32	113.50	109.21
19	A	824	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
19	4	301	CLA	C1D-CHD-C4C	-3.31	118.91	126.06
19	A	810	CLA	O2A-CGA-CBA	3.31	122.30	111.91
31	5	221	A86	C9-C8-C6	-3.31	117.11	126.42
19	A	820	CLA	C1C-C2C-C3C	-3.31	103.48	106.96
19	B	817	CLA	CAA-C2A-C3A	-3.31	103.72	112.78
19	B	816	CLA	C1C-C2C-C3C	-3.30	103.48	106.96
19	A	802	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
19	A	803	CLA	CMB-C2B-C3B	3.30	130.85	124.68
19	B	803	CLA	C3C-C4C-NC	3.30	114.27	110.57
19	3	206	CLA	CMC-C2C-C1C	3.30	130.06	125.04
30	3	208	KC1	CAC-C3C-C4C	3.30	129.09	124.81
31	4	315	A86	C36-C31-C32	-3.30	116.42	119.70
19	A	811	CLA	C1-C2-C3	-3.29	120.35	126.04
19	B	816	CLA	C3C-C4C-NC	3.29	114.26	110.57
31	3	214	A86	C7-C6-C5	-3.29	118.31	122.92
19	B	837	CLA	C4-C3-C5	3.29	120.80	115.27
19	B	846	CLA	C3B-C4B-NB	3.29	113.46	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	217	DD6	C37-C36-C35	-3.29	108.27	114.36
19	5	208	CLA	C3C-C4C-NC	3.28	114.25	110.57
19	A	820	CLA	CAC-C3C-C4C	3.28	129.07	124.81
19	5	207	CLA	C3C-C4C-NC	3.28	114.25	110.57
19	A	803	CLA	CAA-C2A-C3A	-3.28	103.80	112.78
19	1	308	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
31	5	221	A86	C25-C26-C27	-3.28	122.64	127.31
19	B	826	CLA	CAC-C3C-C4C	3.27	129.06	124.81
19	2	207	CLA	CAA-C2A-C3A	-3.27	103.81	112.78
19	B	833	CLA	C3B-C4B-NB	3.27	113.44	109.21
19	1	306	CLA	CAA-C2A-C3A	-3.27	103.82	112.78
19	1	306	CLA	O2A-CGA-CBA	3.27	122.16	111.91
31	3	212	A86	C4-C3-C2	-3.27	116.78	123.47
19	A	816	CLA	C1C-C2C-C3C	-3.26	103.52	106.96
19	B	818	CLA	C1D-CHD-C4C	-3.26	119.02	126.06
19	1	301	CLA	C4-C3-C5	3.26	120.76	115.27
28	3	213	DD6	C12-C11-C13	-3.26	112.94	118.08
19	B	833	CLA	CMB-C2B-C3B	3.26	130.78	124.68
19	A	844	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
19	B	832	CLA	C4-C3-C5	3.26	120.75	115.27
19	A	824	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
28	1	313	DD6	C21-C20-C19	-3.26	110.61	114.28
19	A	821	CLA	CMC-C2C-C1C	3.26	130.00	125.04
19	A	812	CLA	CAA-C2A-C3A	-3.25	103.86	112.78
19	B	829	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
19	5	208	CLA	C3B-C4B-NB	3.25	113.42	109.21
19	B	807	CLA	C3B-C4B-NB	3.25	113.41	109.21
19	1	310	CLA	C3B-C4B-NB	3.25	113.41	109.21
19	B	802	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
19	A	822	CLA	C1-C2-C3	-3.25	120.42	126.04
19	5	207	CLA	O2A-CGA-CBA	3.25	122.10	111.91
19	5	214	CLA	C3B-C4B-NB	3.25	113.41	109.21
19	B	845	CLA	CAC-C3C-C4C	3.24	129.01	124.81
19	B	803	CLA	C1-C2-C3	-3.24	120.44	126.04
19	B	824	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
19	B	820	CLA	C3B-C4B-NB	3.24	113.40	109.21
19	B	830	CLA	C3B-C4B-NB	3.24	113.40	109.21
19	A	817	CLA	O2A-CGA-CBA	3.24	122.07	111.91
19	B	803	CLA	O2D-CGD-CBD	3.24	117.02	111.27
28	1	315	DD6	C37-C36-C35	-3.24	108.36	114.36
19	B	810	CLA	CHD-C4C-NC	3.24	129.30	124.20
26	B	847	DGD	O6D-C1D-O3G	-3.24	102.31	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	5	217	A86	C3-C2-C1	-3.24	122.69	127.31
19	B	835	CLA	C3B-C4B-NB	3.24	113.39	109.21
19	5	209	CLA	C4-C3-C5	3.23	120.71	115.27
19	B	804	CLA	CAC-C3C-C4C	3.23	129.00	124.81
19	A	810	CLA	C1-C2-C3	-3.23	120.45	126.04
19	B	805	CLA	C1-O2A-CGA	3.23	124.92	116.44
19	B	830	CLA	C1-C2-C3	-3.23	120.45	126.04
19	2	214	CLA	C3B-C4B-NB	3.23	113.38	109.21
19	F	203	CLA	C3B-C4B-NB	3.23	113.38	109.21
31	1	317	A86	C4-C3-C2	-3.23	116.87	123.47
19	B	804	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
19	A	842	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
19	4	303	CLA	C3B-C4B-NB	3.22	113.37	109.21
27	J	105	5X6	C28-C29-C30	-3.22	113.66	121.46
19	A	811	CLA	C3B-C4B-NB	3.22	113.37	109.21
19	u	201	CLA	C3B-C4B-NB	3.22	113.37	109.21
19	A	802	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
30	4	302	KC1	CBC-CAC-C3C	-3.21	103.57	112.43
31	3	214	A86	C9-C8-C6	-3.21	117.39	126.42
19	B	814	CLA	C1-C2-C3	-3.21	120.48	126.04
28	1	313	DD6	C37-C36-C35	-3.21	108.41	114.36
31	2	218	A86	C26-C25-C24	-3.21	113.20	123.22
28	1	315	DD6	C3-C4-C5	-3.21	116.90	123.47
19	A	806	CLA	C3B-C4B-NB	3.21	113.36	109.21
19	A	829	CLA	C1-C2-C3	-3.21	120.50	126.04
19	2	212	CLA	CHD-C4C-NC	3.21	129.25	124.20
22	M	102	BCR	C15-C16-C17	-3.20	116.91	123.47
19	A	826	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
19	1	306	CLA	CMA-C3A-C2A	-3.20	100.90	113.83
19	A	805	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
30	4	302	KC1	C4C-C3C-C2C	-3.20	102.23	106.90
19	L	203	CLA	C3B-C4B-NB	3.20	113.35	109.21
19	5	209	CLA	C3B-C4B-NB	3.20	113.34	109.21
19	A	830	CLA	CAC-C3C-C4C	3.19	128.96	124.81
19	B	804	CLA	C1-C2-C3	-3.19	120.52	126.04
19	A	808	CLA	CHD-C4C-NC	3.19	129.24	124.20
19	B	825	CLA	CMC-C2C-C1C	3.19	129.90	125.04
19	A	843	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
19	B	813	CLA	C3B-C4B-NB	3.19	113.33	109.21
19	2	210	CLA	C1-C2-C3	-3.19	120.53	126.04
31	3	228	A86	C34-O4-C38	-3.19	111.95	117.90
19	B	825	CLA	C1-C2-C3	-3.19	120.53	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	209	CLA	C3B-C4B-NB	3.19	113.33	109.21
18	A	801	CL0	O2D-CGD-O1D	-3.19	117.61	123.84
30	4	302	KC1	CHD-C4C-NC	3.19	129.04	124.20
19	B	829	CLA	C1C-C2C-C3C	-3.19	103.61	106.96
19	2	214	CLA	C3C-C4C-NC	3.19	114.14	110.57
19	A	819	CLA	C1-C2-C3	-3.18	120.54	126.04
19	A	835	CLA	CAC-C3C-C4C	3.18	128.94	124.81
31	1	317	A86	C35-C34-C33	3.18	115.42	109.88
19	B	823	CLA	CMB-C2B-C3B	3.18	130.62	124.68
19	B	831	CLA	C3B-C4B-NB	3.18	113.31	109.21
31	1	317	A86	C10-C9-C8	-3.17	113.31	123.22
30	2	211	KC1	CAA-C2A-C1A	-3.17	110.16	124.75
19	B	824	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
19	A	806	CLA	C4-C3-C5	3.17	120.60	115.27
19	A	836	CLA	O2A-CGA-CBA	3.17	121.84	111.91
19	B	808	CLA	C3B-C4B-NB	3.17	113.30	109.21
19	B	836	CLA	C4C-C3C-C2C	-3.16	102.28	106.90
31	1	316	A86	C3-C4-C5	-3.16	117.00	123.47
30	4	307	KC1	C4C-C3C-C2C	-3.16	102.29	106.90
19	A	843	CLA	C4-C3-C5	3.16	120.58	115.27
19	A	816	CLA	CAC-C3C-C4C	3.16	128.91	124.81
19	2	207	CLA	C3B-C4B-NB	3.16	113.29	109.21
19	4	309	CLA	C3B-C4B-NB	3.15	113.29	109.21
19	2	205	CLA	CAC-C3C-C4C	3.15	128.90	124.81
19	B	805	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
19	B	821	CLA	C3B-C4B-NB	3.15	113.28	109.21
19	A	819	CLA	C3B-C4B-NB	3.15	113.28	109.21
31	1	317	A86	C41-C32-C31	-3.15	107.66	110.47
19	A	813	CLA	CMB-C2B-C3B	3.14	130.56	124.68
19	B	815	CLA	CAC-C3C-C4C	3.14	128.89	124.81
19	5	211	CLA	CAC-C3C-C4C	3.14	128.89	124.81
19	4	305	CLA	C3B-C4B-NB	3.14	113.27	109.21
19	B	808	CLA	O2A-CGA-CBA	3.14	121.76	111.91
19	3	207	CLA	CMC-C2C-C1C	3.14	129.82	125.04
19	3	207	CLA	CAC-C3C-C4C	3.14	128.88	124.81
19	4	313	CLA	CHC-C1C-C2C	-3.14	118.04	126.72
19	A	841	CLA	CHD-C4C-NC	3.14	129.15	124.20
19	A	835	CLA	C3B-C4B-NB	3.14	113.27	109.21
31	2	218	A86	C40-C32-C31	-3.14	107.67	110.47
30	4	302	KC1	CAC-C3C-C4C	3.14	128.88	124.81
19	A	839	CLA	O2A-CGA-CBA	3.14	121.75	111.91
19	B	815	CLA	O2D-CGD-O1D	-3.14	117.71	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	203	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
19	F	203	CLA	C1-C2-C3	-3.13	120.62	126.04
19	3	206	CLA	CMB-C2B-C3B	3.13	130.54	124.68
19	A	805	CLA	C3B-C4B-NB	3.13	113.26	109.21
19	B	831	CLA	CMB-C2B-C3B	3.13	130.54	124.68
19	B	818	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
24	1	323	LMT	C3B-C4B-C5B	-3.13	104.66	110.24
19	L	206	CLA	C1-C2-C3	-3.13	120.64	126.04
19	F	204	CLA	C3B-C4B-NB	3.13	113.25	109.21
19	2	213	CLA	C3B-C4B-NB	3.13	113.25	109.21
19	A	813	CLA	C4C-C3C-C2C	-3.12	102.34	106.90
19	L	206	CLA	C3B-C4B-NB	3.12	113.25	109.21
19	B	809	CLA	CHC-C1C-C2C	-3.12	118.08	126.72
31	3	212	A86	C7-C6-C8	3.12	123.00	118.08
19	3	210	CLA	C3B-C4B-NB	3.12	113.25	109.21
30	4	307	KC1	CAA-CBA-CGA	-3.12	111.22	127.26
19	5	207	CLA	CHD-C4C-NC	3.12	129.12	124.20
31	2	219	A86	C3-C4-C5	-3.12	117.08	123.47
19	A	812	CLA	CMC-C2C-C1C	3.12	129.79	125.04
19	A	838	CLA	O2A-CGA-CBA	3.12	121.69	111.91
19	B	824	CLA	O2A-CGA-CBA	3.12	121.69	111.91
19	B	822	CLA	CAC-C3C-C4C	3.12	128.85	124.81
19	3	207	CLA	C3B-C4B-NB	3.11	113.24	109.21
19	B	846	CLA	CAC-C3C-C4C	3.11	128.85	124.81
19	1	309	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
19	3	202	CLA	CMC-C2C-C1C	3.11	129.78	125.04
19	A	813	CLA	CAC-C3C-C4C	3.11	128.84	124.81
19	A	842	CLA	C3B-C4B-NB	3.11	113.23	109.21
19	2	208	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
19	A	817	CLA	CHD-C4C-NC	3.11	129.10	124.20
19	B	815	CLA	C4C-C3C-C2C	-3.10	102.37	106.90
31	5	220	A86	C40-C32-C31	-3.10	107.69	110.47
19	B	817	CLA	C4C-C3C-C2C	-3.10	102.37	106.90
19	B	804	CLA	O2A-CGA-CBA	3.10	121.64	111.91
19	B	803	CLA	CAC-C3C-C4C	3.10	128.84	124.81
19	5	208	CLA	C4-C3-C5	3.10	120.49	115.27
19	A	825	CLA	C3B-C4B-NB	3.10	113.22	109.21
31	3	214	A86	C41-C32-C31	-3.10	107.70	110.47
19	3	207	CLA	O2A-CGA-CBA	3.10	121.62	111.91
28	5	218	DD6	C37-C36-C35	-3.09	108.62	114.36
19	1	309	CLA	CHD-C4C-NC	3.09	129.08	124.20
19	2	212	CLA	C3B-C4B-NB	3.09	113.21	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	211	CLA	CHC-C1C-C2C	-3.09	118.17	126.72
19	4	308	CLA	C3B-C4B-NB	3.09	113.21	109.21
22	A	848	BCR	C11-C10-C9	-3.09	122.90	127.31
19	1	308	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
19	5	213	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
19	A	824	CLA	C3B-C4B-NB	3.09	113.20	109.21
19	A	814	CLA	CHD-C4C-NC	3.09	129.07	124.20
19	A	836	CLA	C3B-C4B-NB	3.08	113.20	109.21
19	B	822	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
19	2	206	CLA	CBC-CAC-C3C	-3.08	103.93	112.43
19	4	308	CLA	CMB-C2B-C3B	3.08	130.44	124.68
31	4	315	A86	C10-C9-C8	-3.08	113.60	123.22
19	2	208	CLA	C3B-C4B-NB	3.08	113.19	109.21
19	1	306	CLA	CBC-CAC-C3C	-3.08	103.94	112.43
31	4	315	A86	C34-O4-C38	-3.08	112.16	117.90
19	B	827	CLA	CAC-C3C-C4C	3.08	128.81	124.81
19	3	202	CLA	CHD-C4C-NC	3.08	129.06	124.20
19	A	802	CLA	C3B-C4B-NB	3.08	113.19	109.21
19	B	821	CLA	CAA-CBA-CGA	-3.08	104.25	113.25
19	A	839	CLA	CAC-C3C-C4C	3.08	128.81	124.81
31	2	216	A86	C36-C31-C32	-3.08	116.64	119.70
19	1	303	CLA	CHC-C1C-C2C	-3.08	118.21	126.72
19	1	301	CLA	C3B-C4B-NB	3.08	113.19	109.21
19	1	307	CLA	CHC-C1C-C2C	-3.07	118.22	126.72
19	A	804	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
19	1	306	CLA	C3C-C4C-NC	3.07	114.02	110.57
19	B	803	CLA	C3B-C4B-NB	3.07	113.18	109.21
19	B	824	CLA	C3B-C4B-NB	3.07	113.18	109.21
19	A	825	CLA	CHC-C1C-C2C	-3.07	118.23	126.72
28	L	209	DD6	C37-C36-C35	-3.07	108.67	114.36
19	A	818	CLA	C3B-C4B-NB	3.07	113.18	109.21
19	A	835	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
19	B	805	CLA	CAC-C3C-C4C	3.06	128.79	124.81
19	A	828	CLA	C3B-C4B-NB	3.06	113.17	109.21
19	5	208	CLA	CBC-CAC-C3C	-3.06	103.98	112.43
19	u	202	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
19	1	301	CLA	O2A-CGA-CBA	3.06	121.52	111.91
19	1	310	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
22	A	849	BCR	C2-C1-C6	3.06	115.19	110.48
19	3	206	CLA	C4-C3-C5	3.06	120.42	115.27
19	5	210	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
18	A	801	CL0	C3B-C4B-NB	3.06	113.16	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	203	CLA	C1-C2-C3	-3.06	120.75	126.04
19	5	213	CLA	CAC-C3C-C4C	3.06	128.78	124.81
19	B	817	CLA	O2A-CGA-CBA	3.06	121.50	111.91
19	A	834	CLA	C1-C2-C3	-3.06	120.76	126.04
30	4	307	KC1	CAC-C3C-C4C	3.06	128.78	124.81
19	A	833	CLA	C4-C3-C5	3.06	120.41	115.27
19	A	827	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
19	A	880	CLA	CMC-C2C-C1C	3.05	129.69	125.04
19	B	838	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
19	A	802	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
19	B	817	CLA	C3B-C4B-NB	3.05	113.16	109.21
19	5	207	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
19	B	835	CLA	CAC-C3C-C4C	3.05	128.77	124.81
19	A	834	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
19	B	810	CLA	C3B-C4B-NB	3.05	113.15	109.21
19	3	203	CLA	CHD-C4C-NC	3.05	129.01	124.20
19	A	838	CLA	CAC-C3C-C4C	3.05	128.77	124.81
19	4	311	CLA	O2A-CGA-CBA	3.05	121.48	111.91
19	B	804	CLA	CMC-C2C-C1C	3.05	129.68	125.04
31	5	217	A86	C26-C25-C24	-3.05	113.71	123.22
19	5	210	CLA	CAA-C2A-C3A	-3.05	104.44	112.78
18	A	801	CL0	CMA-C3A-C2A	-3.04	101.55	113.83
19	B	823	CLA	C4-C3-C5	3.04	120.39	115.27
19	A	831	CLA	CHC-C1C-C2C	-3.04	118.30	126.72
31	2	216	A86	C10-C9-C8	-3.04	113.72	123.22
19	B	836	CLA	C3B-C4B-NB	3.04	113.14	109.21
19	A	837	CLA	C3B-C4B-NB	3.04	113.14	109.21
19	B	834	CLA	C3B-C4B-NB	3.04	113.14	109.21
19	B	802	CLA	C3B-C4B-NB	3.04	113.14	109.21
19	5	207	CLA	C3B-C4B-NB	3.04	113.14	109.21
19	B	825	CLA	CAC-C3C-C4C	3.04	128.75	124.81
19	A	844	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
31	2	216	A86	C4-C5-C6	-3.04	122.97	127.31
19	2	210	CLA	CMC-C2C-C1C	3.04	129.66	125.04
19	B	846	CLA	CMB-C2B-C3B	3.04	130.36	124.68
19	A	803	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
19	B	813	CLA	C4C-C3C-C2C	-3.03	102.47	106.90
19	u	202	CLA	CHD-C4C-NC	3.03	128.98	124.20
19	B	845	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
19	A	834	CLA	CAC-C3C-C4C	3.03	128.74	124.81
31	4	314	A86	C9-C8-C6	-3.03	117.90	126.42
19	A	802	CLA	CMB-C2B-C3B	3.03	130.34	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	810	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
19	B	812	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
19	A	838	CLA	CHC-C1C-C2C	-3.03	118.35	126.72
31	4	316	A86	C3-C2-C1	-3.02	122.99	127.31
19	B	822	CLA	CHC-C1C-C2C	-3.02	118.36	126.72
19	4	311	CLA	CAC-C3C-C4C	3.02	128.73	124.81
19	A	840	CLA	O2A-CGA-CBA	3.02	121.39	111.91
19	B	845	CLA	C4-C3-C5	3.02	120.35	115.27
31	5	220	A86	C41-C32-C31	-3.02	107.77	110.47
19	B	835	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
19	1	303	CLA	CMB-C2B-C3B	3.02	130.33	124.68
19	4	301	CLA	C3B-C4B-NB	3.02	113.11	109.21
19	3	202	CLA	O2A-CGA-CBA	3.02	121.38	111.91
30	3	211	KC1	CAA-C2A-C1A	-3.02	110.87	124.75
19	B	820	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
19	A	809	CLA	CBC-CAC-C3C	-3.02	104.11	112.43
19	2	215	CLA	C3B-C4B-NB	3.02	113.11	109.21
19	A	839	CLA	C4-C3-C5	3.02	120.34	115.27
19	A	805	CLA	CHD-C4C-NC	3.02	128.96	124.20
19	B	815	CLA	C3B-C4B-NB	3.02	113.11	109.21
19	B	838	CLA	C3B-C4B-NB	3.02	113.11	109.21
19	B	826	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
24	A	854	LMT	C3'-C4'-C5'	-3.01	104.02	110.93
19	A	832	CLA	C3B-C4B-NB	3.01	113.11	109.21
19	3	203	CLA	C3B-C4B-NB	3.01	113.11	109.21
19	B	809	CLA	CBC-CAC-C3C	-3.01	104.13	112.43
19	A	839	CLA	CMC-C2C-C1C	3.01	129.62	125.04
19	J	103	CLA	C3B-C4B-NB	3.01	113.10	109.21
19	B	838	CLA	C4-C3-C5	3.01	120.33	115.27
19	A	838	CLA	C4-C3-C5	3.01	119.42	115.98
19	B	845	CLA	CMC-C2C-C1C	3.01	129.62	125.04
19	A	831	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
19	B	835	CLA	CHC-C1C-C2C	-3.01	118.41	126.72
19	B	846	CLA	CHD-C4C-NC	3.01	128.94	124.20
19	A	826	CLA	CAC-C3C-C4C	3.01	128.71	124.81
19	J	103	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
19	2	207	CLA	CMC-C2C-C1C	3.00	129.61	125.04
19	5	215	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
19	4	304	CLA	CHD-C4C-NC	3.00	128.93	124.20
19	A	805	CLA	CMC-C2C-C1C	3.00	129.61	125.04
19	4	304	CLA	CBC-CAC-C3C	-3.00	104.16	112.43
19	B	803	CLA	CHC-C1C-C2C	-3.00	118.42	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	835	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
19	B	805	CLA	CMB-C2B-C3B	3.00	130.29	124.68
19	B	816	CLA	CMC-C2C-C1C	3.00	129.61	125.04
19	A	840	CLA	C3B-C4B-NB	3.00	113.09	109.21
19	A	824	CLA	C1-C2-C3	-3.00	120.86	126.04
19	L	203	CLA	C2A-C1A-CHA	-3.00	118.62	123.86
19	2	207	CLA	CHD-C4C-NC	3.00	128.92	124.20
28	5	218	DD6	C35-C36-C31	-2.99	113.77	120.57
19	A	842	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
19	A	840	CLA	CMC-C2C-C1C	2.99	129.60	125.04
19	5	209	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
19	A	826	CLA	C1-C2-C3	-2.99	120.87	126.04
30	1	305	KC1	C4C-C3C-C2C	-2.99	102.54	106.90
30	3	205	KC1	C4C-C3C-C2C	-2.99	102.54	106.90
19	1	308	CLA	CAA-C2A-C3A	-2.99	104.59	112.78
22	J	104	BCR	C11-C10-C9	-2.99	123.04	127.31
19	B	818	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
19	5	208	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
19	u	201	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
19	5	210	CLA	C4-C3-C5	2.99	120.30	115.27
19	A	802	CLA	CAC-C3C-C4C	2.99	128.69	124.81
19	B	803	CLA	O2A-CGA-CBA	2.99	121.28	111.91
19	B	815	CLA	CHC-C1C-C2C	-2.99	118.46	126.72
19	A	834	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
19	B	810	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
19	4	306	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
30	4	302	KC1	C1C-C2C-C3C	-2.98	103.82	106.96
19	A	824	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
19	1	304	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
19	3	206	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
19	1	301	CLA	CHD-C4C-NC	2.98	128.90	124.20
19	A	821	CLA	CHD-C4C-NC	2.98	128.90	124.20
19	5	216	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
19	A	836	CLA	CAC-C3C-C4C	2.98	128.67	124.81
19	A	817	CLA	C3B-C4B-NB	2.98	113.06	109.21
19	B	837	CLA	CHD-C4C-NC	2.97	128.89	124.20
19	B	804	CLA	O2A-C1-C2	2.97	116.45	108.64
19	A	880	CLA	C3B-C4B-NB	2.97	113.06	109.21
19	5	212	CLA	CAC-C3C-C4C	2.97	128.67	124.81
19	A	814	CLA	C3B-C4B-NB	2.97	113.05	109.21
19	2	215	CLA	CHD-C4C-NC	2.97	128.88	124.20
19	L	206	CLA	CHC-C1C-C2C	-2.97	118.51	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	214	CLA	CHC-C1C-C2C	-2.97	118.51	126.72
19	B	845	CLA	C3B-C4B-NB	2.97	113.05	109.21
19	4	305	CLA	CAC-C3C-C4C	2.97	128.66	124.81
19	3	209	CLA	C1-C2-C3	-2.97	120.91	126.04
19	A	815	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
31	1	316	A86	C10-C9-C8	-2.97	113.96	123.22
19	A	804	CLA	O2A-CGA-CBA	2.97	121.22	111.91
19	L	206	CLA	C4C-C3C-C2C	-2.97	102.58	106.90
19	2	207	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
19	4	305	CLA	CHC-C1C-C2C	-2.96	118.52	126.72
19	2	210	CLA	CHD-C4C-NC	2.96	128.87	124.20
19	A	830	CLA	CMB-C2B-C3B	2.96	130.22	124.68
19	A	835	CLA	C1-C2-C3	-2.96	120.92	126.04
19	A	823	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
19	B	826	CLA	CMB-C2B-C3B	2.96	130.22	124.68
19	4	304	CLA	O2A-CGA-O1A	-2.96	116.12	123.59
31	5	221	A86	C36-C31-C32	-2.96	116.76	119.70
19	4	311	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
19	B	838	CLA	CHC-C1C-C2C	-2.96	118.54	126.72
19	L	203	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
19	A	814	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
19	A	878	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
19	B	811	CLA	C3B-C4B-NB	2.96	113.03	109.21
19	5	215	CLA	C3B-C4B-NB	2.96	113.03	109.21
30	3	208	KC1	CAA-CBA-CGA	-2.96	112.07	127.26
19	A	812	CLA	CAC-C3C-C4C	2.96	128.65	124.81
19	2	214	CLA	CHD-C4C-NC	2.96	128.86	124.20
19	5	208	CLA	CAC-C3C-C4C	2.95	128.64	124.81
19	2	210	CLA	CAC-C3C-C4C	2.95	128.64	124.81
31	2	218	A86	C3-C2-C1	-2.95	123.09	127.31
19	4	311	CLA	C3B-C4B-NB	2.95	113.03	109.21
22	1	311	BCR	C15-C16-C17	-2.95	117.43	123.47
22	1	314	BCR	C15-C16-C17	-2.95	117.43	123.47
19	A	835	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
31	4	314	A86	C12-C11-C13	2.95	120.98	116.02
19	2	213	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
19	A	811	CLA	CBC-CAC-C3C	-2.95	104.30	112.43
19	A	834	CLA	C3B-C4B-NB	2.95	113.02	109.21
19	5	216	CLA	CAC-C3C-C4C	2.95	128.63	124.81
19	1	309	CLA	O2A-CGA-CBA	2.95	121.16	111.91
19	B	833	CLA	O2A-CGA-CBA	2.95	121.16	111.91
19	5	214	CLA	C4C-C3C-C2C	-2.95	102.60	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	832	CLA	CHD-C4C-NC	2.95	128.85	124.20
19	3	207	CLA	CAA-C2A-C3A	-2.95	104.71	112.78
19	B	804	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
19	5	212	CLA	CHD-C4C-NC	2.95	128.84	124.20
19	B	813	CLA	O2A-CGA-CBA	2.95	121.15	111.91
19	4	310	CLA	CHD-C4C-NC	2.94	128.84	124.20
30	4	307	KC1	CAA-C2A-C1A	-2.94	111.22	124.75
19	A	809	CLA	C4-C3-C5	2.94	120.22	115.27
19	5	209	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
19	B	828	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
19	2	209	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
19	B	805	CLA	C4-C3-C5	2.94	120.22	115.27
19	A	822	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
19	A	829	CLA	CAC-C3C-C4C	2.94	128.62	124.81
19	3	204	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
19	5	214	CLA	CAC-C3C-C4C	2.94	128.62	124.81
19	3	209	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
19	2	206	CLA	C3B-C4B-NB	2.94	113.01	109.21
19	B	818	CLA	CMB-C2B-C3B	2.94	130.18	124.68
31	3	212	A86	C-C1-C24	2.94	122.71	118.08
19	4	310	CLA	C3B-C4B-NB	2.94	113.01	109.21
30	1	305	KC1	CAA-C2A-C1A	-2.94	111.24	124.75
19	1	310	CLA	C3C-C4C-NC	2.94	113.86	110.57
19	3	209	CLA	CHD-C4C-NC	2.94	128.83	124.20
19	B	832	CLA	CMB-C2B-C3B	2.93	130.17	124.68
19	A	832	CLA	CHD-C4C-NC	2.93	128.83	124.20
19	B	805	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
19	B	819	CLA	O2A-CGA-CBA	2.93	121.10	111.91
19	A	843	CLA	C3B-C4B-NB	2.93	113.00	109.21
19	3	203	CLA	C1-C2-C3	-2.93	120.98	126.04
19	B	829	CLA	C1-O2A-CGA	2.93	124.13	116.44
19	F	204	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
30	3	205	KC1	CHD-C4C-NC	2.93	128.65	124.20
19	2	213	CLA	CHD-C4C-NC	2.93	128.81	124.20
19	A	815	CLA	C1-C2-C3	-2.92	122.02	126.75
19	5	208	CLA	CHD-C4C-NC	2.92	128.81	124.20
19	B	826	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
19	B	846	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
19	2	214	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
19	A	839	CLA	CMB-C2B-C3B	2.92	130.14	124.68
19	B	820	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
19	A	827	CLA	O2D-CGD-O1D	-2.92	118.13	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	307	CLA	CMB-C2B-C3B	2.92	130.14	124.68
19	A	816	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
19	B	816	CLA	CHD-C4C-NC	2.92	128.80	124.20
19	A	809	CLA	CMB-C2B-C3B	2.92	130.14	124.68
19	2	205	CLA	CMB-C2B-C3B	2.92	130.14	124.68
19	A	808	CLA	CMC-C2C-C1C	2.92	129.48	125.04
19	A	818	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
19	B	802	CLA	CMA-C3A-C4A	-2.92	103.94	111.77
23	1	318	LHG	O8-C23-C24	2.92	121.06	111.91
19	A	843	CLA	CAC-C3C-C4C	2.92	128.59	124.81
19	B	813	CLA	CAC-C3C-C4C	2.92	128.59	124.81
19	1	301	CLA	CHC-C1C-C2C	-2.92	118.66	126.72
19	A	820	CLA	CHD-C4C-NC	2.92	128.80	124.20
19	A	878	CLA	CMB-C2B-C3B	2.91	130.13	124.68
19	4	310	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
19	1	309	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
19	A	823	CLA	CHD-C4C-NC	2.91	128.79	124.20
19	4	309	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
19	A	812	CLA	C3B-C4B-NB	2.91	112.97	109.21
19	A	830	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
19	A	809	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
19	F	204	CLA	CAC-C3C-C4C	2.91	128.59	124.81
19	3	204	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
19	A	809	CLA	CHD-C4C-NC	2.91	128.79	124.20
19	A	841	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
19	B	834	CLA	CMB-C2B-C3B	2.91	130.12	124.68
19	2	205	CLA	O2A-C1-C2	2.91	116.28	108.64
19	A	803	CLA	C4-C3-C5	2.91	120.16	115.27
19	B	824	CLA	CHD-C4C-NC	2.91	128.79	124.20
19	2	208	CLA	C4-C3-C5	2.91	120.16	115.27
19	A	820	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
19	B	831	CLA	C4-C3-C5	2.91	120.16	115.27
19	A	828	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
19	B	819	CLA	C1-C2-C3	-2.91	121.02	126.04
19	B	837	CLA	CMC-C2C-C1C	2.91	129.46	125.04
19	A	832	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
19	A	840	CLA	CHD-C4C-NC	2.90	128.78	124.20
19	4	305	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
19	B	834	CLA	O2A-CGA-CBA	2.90	121.02	111.91
19	B	835	CLA	CBC-CAC-C3C	-2.90	104.43	112.43
19	A	829	CLA	CMB-C2B-C3B	2.90	130.11	124.68
19	B	806	CLA	C4C-C3C-C2C	-2.90	102.67	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	833	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
19	A	837	CLA	CHD-C4C-NC	2.90	128.77	124.20
19	B	827	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
19	B	834	CLA	CHD-C4C-NC	2.90	128.77	124.20
19	A	842	CLA	CAC-C3C-C4C	2.90	128.57	124.81
19	A	838	CLA	CMB-C2B-C3B	2.90	130.10	124.68
28	3	213	DD6	C10-C9-C8	-2.90	114.17	123.22
19	u	202	CLA	C3B-C4B-NB	2.90	112.96	109.21
19	A	803	CLA	O2D-CGD-CBD	2.90	116.42	111.27
19	A	819	CLA	C1C-C2C-C3C	-2.90	103.91	106.96
24	1	323	LMT	C3'-C4'-C5'	-2.90	104.28	110.93
19	B	808	CLA	CMC-C2C-C1C	2.90	129.45	125.04
19	B	823	CLA	C4C-C3C-C2C	-2.90	102.68	106.90
19	4	311	CLA	C4C-C3C-C2C	-2.90	102.68	106.90
19	2	208	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
19	4	301	CLA	CMB-C2B-C3B	2.89	130.09	124.68
19	B	832	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
19	B	838	CLA	CMC-C2C-C1C	2.89	129.44	125.04
19	5	212	CLA	C3B-C4B-NB	2.89	112.95	109.21
19	B	838	CLA	O2A-CGA-CBA	2.89	120.98	111.91
31	4	315	A86	C26-C25-C24	-2.89	114.20	123.22
30	3	208	KC1	CHD-C4C-NC	2.89	128.59	124.20
19	5	210	CLA	CHD-C4C-NC	2.89	128.75	124.20
19	A	815	CLA	CAC-C3C-C4C	2.89	128.56	124.81
19	B	832	CLA	C3B-C4B-NB	2.89	112.94	109.21
19	4	308	CLA	CHD-C4C-NC	2.89	128.75	124.20
19	A	827	CLA	C3B-C4B-NB	2.89	112.94	109.21
19	2	206	CLA	CHC-C1C-C2C	-2.89	118.74	126.72
31	2	218	A86	C-C1-C24	2.88	122.62	118.08
19	A	818	CLA	CAC-C3C-C4C	2.88	128.55	124.81
19	B	818	CLA	CAC-C3C-C4C	2.88	128.55	124.81
19	5	216	CLA	CMB-C2B-C3B	2.88	130.07	124.68
19	B	806	CLA	O2A-CGA-CBA	2.88	120.95	111.91
19	4	306	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
19	B	803	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
19	B	820	CLA	CAC-C3C-C4C	2.88	128.55	124.81
19	B	812	CLA	CHC-C1C-C2C	-2.88	118.75	126.72
19	A	826	CLA	CMC-C2C-C1C	2.88	129.42	125.04
19	B	827	CLA	CMC-C2C-C1C	2.88	129.42	125.04
19	A	818	CLA	C1-C2-C3	-2.88	121.07	126.04
19	B	846	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
19	A	822	CLA	C4C-C3C-C2C	-2.88	102.70	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	828	CLA	CHD-C4C-NC	2.88	128.74	124.20
19	A	807	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
19	B	808	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
19	A	841	CLA	C3B-C4B-NB	2.87	112.92	109.21
19	4	306	CLA	C4-C3-C5	2.87	120.10	115.27
22	A	848	BCR	C7-C8-C9	-2.87	121.89	126.23
19	B	806	CLA	CHD-C4C-NC	2.87	128.73	124.20
19	B	809	CLA	CAC-C3C-C4C	2.87	128.54	124.81
30	3	205	KC1	CAA-CBA-CGA	-2.87	112.50	127.26
19	A	815	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
19	B	814	CLA	CMC-C2C-C1C	2.87	129.41	125.04
19	B	830	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
19	A	843	CLA	C1-C2-C3	-2.87	121.08	126.04
19	4	304	CLA	C3B-C4B-NB	2.87	112.92	109.21
19	5	213	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
19	A	828	CLA	C4-C3-C5	2.87	120.10	115.27
28	2	217	DD6	C21-C20-C19	-2.87	111.05	114.28
19	B	836	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
19	B	820	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
19	1	310	CLA	CBA-CAA-C2A	-2.87	105.39	113.86
19	A	844	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
19	u	201	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
19	B	803	CLA	C4-C3-C5	2.87	120.09	115.27
19	2	210	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
19	1	303	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
19	1	304	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
19	1	306	CLA	CMC-C2C-C1C	2.86	129.40	125.04
19	B	825	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
19	F	203	CLA	CHD-C4C-NC	2.86	128.72	124.20
19	A	816	CLA	CHC-C1C-C2C	-2.86	118.80	126.72
19	A	825	CLA	CAC-C3C-C4C	2.86	128.53	124.81
19	B	835	CLA	CHD-C4C-NC	2.86	128.72	124.20
19	2	212	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
19	2	214	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
30	2	211	KC1	C4B-C3B-C2B	-2.86	104.40	106.75
19	A	816	CLA	O2A-CGA-CBA	2.86	120.89	111.91
19	B	828	CLA	C3B-C4B-NB	2.86	112.91	109.21
30	3	208	KC1	CAA-C2A-C1A	-2.86	111.60	124.75
19	A	826	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
19	5	215	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
19	F	203	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
19	L	206	CLA	O2A-CGA-CBA	2.86	120.88	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	817	CLA	CHD-C4C-NC	2.86	128.71	124.20
19	3	204	CLA	CBC-CAC-C3C	-2.86	104.55	112.43
19	B	824	CLA	O1D-CGD-CBD	-2.86	118.64	124.48
19	B	814	CLA	CHD-C4C-NC	2.86	128.71	124.20
19	4	301	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
31	5	220	A86	C28-C27-C26	-2.85	118.92	122.92
19	B	829	CLA	C6-C7-C8	-2.85	106.69	115.92
19	u	201	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
19	1	304	CLA	O2A-CGA-CBA	2.85	120.86	111.91
19	B	846	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
19	B	818	CLA	O2A-CGA-CBA	2.85	120.86	111.91
19	5	207	CLA	CMC-C2C-C1C	2.85	129.38	125.04
19	A	829	CLA	CHD-C4C-NC	2.85	128.70	124.20
19	B	820	CLA	CMB-C2B-C3B	2.85	130.01	124.68
31	5	220	A86	C34-O4-C38	-2.85	112.58	117.90
19	A	807	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
19	A	830	CLA	CMC-C2C-C1C	2.85	129.38	125.04
19	5	212	CLA	CMC-C2C-C1C	2.85	129.38	125.04
19	A	811	CLA	CHD-C4C-NC	2.85	128.69	124.20
19	B	802	CLA	C4-C3-C5	2.85	120.06	115.27
19	F	203	CLA	CBC-CAC-C3C	-2.85	104.58	112.43
19	B	816	CLA	C3B-C4B-NB	2.85	112.89	109.21
19	B	834	CLA	C1-C2-C3	-2.85	121.11	126.04
19	4	306	CLA	C3B-C4B-NB	2.85	112.89	109.21
19	3	203	CLA	CMC-C2C-C1C	2.85	129.38	125.04
19	A	821	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
19	A	839	CLA	CBC-CAC-C3C	-2.85	104.58	112.43
19	1	304	CLA	CAA-C2A-C3A	-2.85	104.98	112.78
19	A	816	CLA	CHD-C4C-NC	2.85	128.69	124.20
19	B	821	CLA	CHC-C1C-C2C	-2.85	118.85	126.72
19	A	878	CLA	CAA-C2A-C3A	-2.85	104.98	112.78
19	A	839	CLA	CHC-C1C-C2C	-2.85	118.85	126.72
31	3	212	A86	C3-C4-C5	-2.85	117.64	123.47
19	B	821	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
19	5	207	CLA	CMB-C2B-C3B	2.84	130.00	124.68
19	A	833	CLA	CHD-C4C-NC	2.84	128.68	124.20
30	3	208	KC1	CBA-CAA-C2A	-2.84	114.44	125.27
19	3	206	CLA	CAC-C3C-C4C	2.84	128.49	124.81
19	B	805	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
19	2	207	CLA	CAC-C3C-C4C	2.84	128.49	124.81
22	A	851	BCR	C15-C16-C17	-2.84	117.66	123.47
19	A	829	CLA	CMC-C2C-C1C	2.84	129.36	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	305	CLA	C1-C2-C3	-2.84	121.14	126.04
19	B	827	CLA	C4-C3-C5	2.84	120.04	115.27
19	B	811	CLA	C2A-C1A-CHA	-2.84	118.90	123.86
19	B	819	CLA	CHC-C1C-C2C	-2.84	118.88	126.72
19	B	819	CLA	C3B-C4B-NB	2.83	112.88	109.21
19	2	205	CLA	CMC-C2C-C1C	2.83	129.35	125.04
19	B	808	CLA	CHD-C4C-NC	2.83	128.67	124.20
30	1	305	KC1	O2D-CGD-O1D	-2.83	118.30	123.84
19	4	308	CLA	CMC-C2C-C1C	2.83	129.35	125.04
19	A	836	CLA	C4-C3-C5	2.83	120.03	115.27
19	2	215	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
19	B	806	CLA	CMC-C2C-C1C	2.83	129.35	125.04
19	A	836	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
19	B	831	CLA	CHD-C4C-NC	2.83	128.66	124.20
19	3	202	CLA	CBC-CAC-C3C	-2.83	104.63	112.43
19	B	825	CLA	CMB-C2B-C3B	2.83	129.97	124.68
19	B	823	CLA	CHD-C4C-NC	2.83	128.66	124.20
19	4	303	CLA	CHD-C4C-NC	2.83	128.66	124.20
19	B	834	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
31	1	317	A86	C26-C25-C24	-2.83	114.39	123.22
19	A	821	CLA	O2A-CGA-CBA	2.83	120.77	111.91
19	A	818	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
19	A	819	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
30	3	205	KC1	CAC-C3C-C4C	2.82	128.47	124.81
31	5	221	A86	C9-C10-C11	-2.82	118.31	126.61
19	A	813	CLA	CHD-C4C-NC	2.82	128.65	124.20
19	A	831	CLA	C4-C3-C5	2.82	120.02	115.27
19	2	207	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
19	B	832	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
19	A	811	CLA	CMC-C2C-C1C	2.82	129.34	125.04
19	A	837	CLA	CHC-C1C-C2C	-2.82	118.92	126.72
22	B	843	BCR	C15-C14-C13	-2.82	123.29	127.31
19	4	301	CLA	CHD-C4C-NC	2.82	128.65	124.20
28	1	312	DD6	C37-C36-C35	-2.82	109.13	114.36
19	5	212	CLA	CED-O2D-CGD	2.82	122.31	115.94
19	B	816	CLA	C4-C3-C5	2.82	120.01	115.27
19	B	820	CLA	CHD-C4C-NC	2.82	128.64	124.20
19	A	830	CLA	C4-C3-C5	2.82	120.01	115.27
19	A	804	CLA	C3B-C4B-NB	2.82	112.85	109.21
19	B	837	CLA	C3B-C4B-NB	2.82	112.85	109.21
19	B	835	CLA	CMC-C2C-C1C	2.82	129.33	125.04
19	A	880	CLA	CHD-C4C-NC	2.82	128.64	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	212	CLA	O2A-CGA-CBA	2.82	120.75	111.91
19	A	821	CLA	C3B-C4B-NB	2.82	112.85	109.21
19	B	806	CLA	C3B-C4B-NB	2.82	112.85	109.21
19	4	313	CLA	CHD-C4C-NC	2.81	128.64	124.20
19	A	827	CLA	C4-C3-C5	2.81	120.01	115.27
19	B	832	CLA	C1-C2-C3	-2.81	121.17	126.04
19	4	309	CLA	CAC-C3C-C4C	2.81	128.46	124.81
19	5	208	CLA	O2A-CGA-CBA	2.81	120.73	111.91
31	3	228	A86	C12-C11-C13	2.81	120.75	116.02
19	4	312	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
19	A	841	CLA	CMC-C2C-C1C	2.81	129.32	125.04
19	B	814	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
19	A	836	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
19	B	804	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
19	B	822	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
19	3	206	CLA	CHD-C4C-NC	2.81	128.63	124.20
23	4	317	LHG	O8-C23-C24	2.81	120.73	111.91
19	A	810	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
19	A	803	CLA	CAC-C3C-C4C	2.81	128.46	124.81
19	5	213	CLA	CMB-C2B-C3B	2.81	129.94	124.68
19	B	833	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
19	1	306	CLA	C3B-C4B-NB	2.81	112.84	109.21
19	L	204	CLA	CMC-C2C-C1C	2.81	129.31	125.04
22	B	840	BCR	C7-C8-C9	-2.81	121.99	126.23
19	B	814	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
19	B	807	CLA	CMC-C2C-C1C	2.81	129.31	125.04
19	B	823	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
19	1	304	CLA	C7-C6-C5	-2.81	105.74	113.36
19	B	813	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
19	A	838	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
30	3	208	KC1	C4C-C3C-C2C	-2.80	102.81	106.90
19	L	204	CLA	CHD-C4C-NC	2.80	128.62	124.20
19	B	807	CLA	CHD-C4C-NC	2.80	128.62	124.20
19	5	209	CLA	O2A-CGA-CBA	2.80	120.70	111.91
19	2	205	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
19	B	811	CLA	CHD-C4C-NC	2.80	128.62	124.20
19	A	811	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
19	B	812	CLA	C4-C3-C5	2.80	119.98	115.27
19	A	821	CLA	CAC-C3C-C4C	2.80	128.44	124.81
19	B	816	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
19	B	834	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
19	A	828	CLA	C1C-C2C-C3C	-2.80	104.01	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	814	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
30	2	211	KC1	CBC-CAC-C3C	-2.80	104.72	112.43
19	B	837	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
18	A	801	CL0	CHC-C1C-C2C	-2.80	118.98	126.72
19	5	215	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
19	B	809	CLA	CHD-C4C-NC	2.80	128.61	124.20
31	4	314	A86	C40-C32-C31	-2.80	107.97	110.47
19	2	206	CLA	CHD-C4C-NC	2.80	128.61	124.20
19	A	878	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
19	A	813	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
31	5	217	A86	C-C1-C24	2.79	122.48	118.08
23	A	853	LHG	O8-C23-C24	2.79	120.68	111.91
19	1	306	CLA	CHD-C4C-NC	2.79	128.61	124.20
19	1	308	CLA	CAC-C3C-C4C	2.79	128.44	124.81
19	A	880	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
19	J	103	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
28	1	313	DD6	C15-C14-C13	-2.79	120.09	125.99
19	B	808	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
19	3	204	CLA	CMC-C2C-C1C	2.79	129.29	125.04
19	A	834	CLA	O2A-CGA-CBA	2.79	120.67	111.91
19	A	843	CLA	CHD-C4C-NC	2.79	128.60	124.20
19	B	821	CLA	C1-C2-C3	-2.79	121.22	126.04
19	J	103	CLA	CHD-C4C-NC	2.79	128.60	124.20
19	B	831	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
19	5	211	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
19	1	308	CLA	CHD-C4C-NC	2.79	128.60	124.20
19	A	812	CLA	C4-C3-C5	2.79	119.96	115.27
19	A	841	CLA	C4-C3-C5	2.79	119.96	115.27
19	A	830	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
19	2	206	CLA	CAC-C3C-C4C	2.79	128.43	124.81
19	B	829	CLA	O2A-CGA-CBA	2.79	120.65	111.91
19	3	204	CLA	CAC-C3C-C4C	2.79	128.42	124.81
19	A	820	CLA	CBC-CAC-C3C	-2.79	104.75	112.43
19	B	816	CLA	CHC-C1C-C2C	-2.78	119.02	126.72
19	A	822	CLA	C3B-C4B-NB	2.78	112.81	109.21
19	L	206	CLA	CHD-C4C-NC	2.78	128.59	124.20
19	3	203	CLA	CMB-C2B-C3B	2.78	129.89	124.68
19	4	310	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
19	A	878	CLA	C1-C2-C3	-2.78	121.23	126.04
19	A	840	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
19	3	202	CLA	CAC-C3C-C4C	2.78	128.42	124.81
30	3	211	KC1	CAA-CBA-CGA	-2.78	112.96	127.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	303	CLA	CBC-CAC-C3C	-2.78	104.76	112.43
19	B	821	CLA	CAC-C3C-C4C	2.78	128.42	124.81
19	A	818	CLA	C4-C3-C5	2.78	119.95	115.27
19	A	843	CLA	CHC-C1C-C2C	-2.78	119.03	126.72
19	A	880	CLA	CHC-C1C-C2C	-2.78	119.03	126.72
23	M	103	LHG	O8-C23-C24	2.78	120.63	111.91
19	B	819	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
19	A	878	CLA	O2A-CGA-CBA	2.78	120.62	111.91
19	4	301	CLA	CHC-C1C-C2C	-2.78	119.04	126.72
19	A	808	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
19	B	811	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
19	4	303	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
19	B	812	CLA	CHD-C4C-NC	2.77	128.57	124.20
19	B	827	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
19	A	878	CLA	CHD-C4C-NC	2.77	128.57	124.20
19	A	804	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
19	A	805	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
31	4	314	A86	C20-C19-C18	-2.77	107.26	112.75
19	4	310	CLA	CMB-C2B-C3B	2.77	129.87	124.68
19	B	812	CLA	CAC-C3C-C4C	2.77	128.41	124.81
19	A	812	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
19	B	838	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
19	L	203	CLA	O2A-CGA-CBA	2.77	120.60	111.91
31	2	218	A86	C7-C6-C8	2.77	122.44	118.08
19	A	880	CLA	O2A-CGA-CBA	2.77	120.60	111.91
19	4	306	CLA	CMB-C2B-C3B	2.77	129.86	124.68
19	A	844	CLA	C4-C3-C5	2.77	119.93	115.27
19	F	203	CLA	O2A-CGA-CBA	2.77	120.60	111.91
19	5	210	CLA	C1-C2-C3	-2.77	121.25	126.04
19	A	826	CLA	CHD-C4C-NC	2.77	128.57	124.20
19	5	212	CLA	CHC-C1C-C2C	-2.77	119.06	126.72
19	A	832	CLA	CHC-C1C-C2C	-2.77	119.06	126.72
19	A	831	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
19	A	806	CLA	CHD-C4C-NC	2.77	128.57	124.20
19	B	808	CLA	CAA-C2A-C3A	-2.77	105.20	112.78
19	3	207	CLA	C4C-C3C-C2C	-2.77	102.87	106.90
19	2	212	CLA	CMC-C2C-C1C	2.77	129.25	125.04
19	4	305	CLA	C4-C3-C5	2.77	119.92	115.27
19	1	308	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
19	B	837	CLA	O2A-CGA-CBA	2.76	120.58	111.91
19	5	214	CLA	CHD-C4C-NC	2.76	128.56	124.20
19	A	829	CLA	C4C-C3C-C2C	-2.76	102.87	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	1	305	KC1	CHD-C4C-NC	2.76	128.39	124.20
19	A	806	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
20	B	839	PQN	C11-C3-C4	-2.76	115.55	118.50
28	5	218	DD6	C14-C13-C11	2.76	129.82	125.53
19	B	827	CLA	O2A-CGA-CBA	2.76	120.58	111.91
19	B	818	CLA	C4-C3-C5	2.76	119.92	115.27
19	A	878	CLA	CMC-C2C-C1C	2.76	129.24	125.04
23	B	842	LHG	O8-C23-C24	2.76	120.57	111.91
19	4	303	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
19	A	813	CLA	O2A-CGA-CBA	2.76	120.57	111.91
19	A	832	CLA	CBC-CAC-C3C	-2.76	104.82	112.43
19	B	822	CLA	CBC-CAC-C3C	-2.76	104.82	112.43
19	4	310	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
19	B	833	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
19	A	840	CLA	CAC-C3C-C4C	2.76	128.39	124.81
19	B	838	CLA	CHD-C4C-NC	2.76	128.55	124.20
19	4	311	CLA	CMB-C2B-C3B	2.75	129.83	124.68
26	B	847	DGD	C1D-C2D-C3D	-2.75	104.26	110.00
19	B	819	CLA	CHD-C4C-NC	2.75	128.54	124.20
19	A	844	CLA	CHD-C4C-NC	2.75	128.54	124.20
19	B	830	CLA	C4-C3-C5	2.75	119.90	115.27
19	B	825	CLA	CHD-C4C-NC	2.75	128.54	124.20
19	u	201	CLA	O2A-CGA-CBA	2.75	120.55	111.91
19	B	835	CLA	O2A-CGA-CBA	2.75	120.54	111.91
19	4	306	CLA	O2A-CGA-CBA	2.75	120.54	111.91
30	3	211	KC1	CBC-CAC-C3C	-2.75	104.85	112.43
19	A	817	CLA	CHC-C1C-C2C	-2.75	119.11	126.72
19	1	304	CLA	CHD-C4C-NC	2.75	128.54	124.20
22	I	102	BCR	C29-C30-C25	2.75	114.71	110.48
19	1	310	CLA	CHD-C4C-NC	2.75	128.54	124.20
19	A	821	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
18	A	801	CL0	CMC-C2C-C1C	2.75	129.22	125.04
19	B	838	CLA	CAC-C3C-C4C	2.75	128.38	124.81
19	4	304	CLA	CAC-C3C-C4C	2.75	128.38	124.81
19	B	802	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
19	A	810	CLA	CHD-C4C-NC	2.75	128.53	124.20
19	A	842	CLA	C4-C3-C5	2.75	119.89	115.27
19	A	830	CLA	CED-O2D-CGD	2.75	122.15	115.94
19	2	213	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
19	4	309	CLA	CMB-C2B-C3B	2.75	129.81	124.68
19	4	308	CLA	C4C-C3C-C2C	-2.75	102.90	106.90
19	B	830	CLA	CHC-C1C-C2C	-2.75	119.13	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	828	CLA	CMB-C2B-C3B	2.75	129.81	124.68
19	5	207	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
19	A	817	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
19	A	827	CLA	CAC-C3C-C4C	2.74	128.37	124.81
19	2	207	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
19	A	832	CLA	CMC-C2C-C1C	2.74	129.22	125.04
30	3	211	KC1	C4C-C3C-C2C	-2.74	102.90	106.90
19	A	807	CLA	CHD-C4C-NC	2.74	128.53	124.20
19	4	312	CLA	CHD-C4C-NC	2.74	128.53	124.20
19	A	823	CLA	CBC-CAC-C3C	-2.74	104.87	112.43
19	B	804	CLA	O1D-CGD-CBD	-2.74	118.88	124.48
30	1	305	KC1	CAC-C3C-C4C	2.74	128.37	124.81
19	B	806	CLA	C4-C3-C5	2.74	119.88	115.27
19	1	301	CLA	C1-C2-C3	-2.74	121.30	126.04
22	1	314	BCR	C15-C14-C13	-2.74	123.40	127.31
19	A	824	CLA	O2A-CGA-CBA	2.74	120.50	111.91
19	A	803	CLA	CHC-C1C-C2C	-2.74	119.14	126.72
22	F	201	BCR	C27-C26-C25	2.74	126.71	122.73
19	B	816	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
31	3	214	A86	C34-O4-C38	-2.74	112.79	117.90
19	A	806	CLA	CAC-C3C-C4C	2.74	128.36	124.81
19	A	803	CLA	C3B-C4B-NB	2.74	112.75	109.21
19	2	209	CLA	CHD-C4C-NC	2.74	128.52	124.20
19	B	833	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
22	A	851	BCR	C33-C5-C6	-2.74	121.45	124.53
19	L	204	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
19	3	204	CLA	CHD-C4C-NC	2.74	128.51	124.20
19	1	307	CLA	C1-O2A-CGA	2.74	123.62	116.44
19	A	819	CLA	C4-C3-C5	2.73	119.87	115.27
19	3	202	CLA	C4-C3-C5	2.73	119.87	115.27
19	A	829	CLA	C4-C3-C5	2.73	119.87	115.27
19	B	808	CLA	C4-C3-C5	2.73	119.87	115.27
19	F	204	CLA	CHD-C4C-NC	2.73	128.51	124.20
19	A	822	CLA	CAC-C3C-C4C	2.73	128.35	124.81
19	A	805	CLA	C4-C3-C5	2.73	119.87	115.27
19	F	203	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
19	A	807	CLA	O2A-CGA-O1A	-2.73	116.70	123.59
19	B	808	CLA	C1-C2-C3	-2.73	121.32	126.04
19	B	825	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
19	A	809	CLA	C1-O2A-CGA	2.73	123.60	116.44
19	A	820	CLA	CMB-C2B-C3B	2.73	129.78	124.68
19	4	303	CLA	CHC-C1C-C2C	-2.73	119.18	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	216	CLA	CHC-C1C-C2C	-2.73	119.18	126.72
19	B	824	CLA	CMB-C2B-C3B	2.73	129.78	124.68
30	4	302	KC1	CHB-C1B-NB	-2.73	121.95	124.45
30	3	205	KC1	CMB-C2B-C1B	2.73	129.52	124.71
19	3	206	CLA	CHC-C1C-C2C	-2.72	119.18	126.72
19	A	840	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
19	5	207	CLA	CAC-C3C-C4C	2.72	128.34	124.81
19	B	812	CLA	O2A-CGA-CBA	2.72	120.45	111.91
19	A	829	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
19	A	823	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
19	3	204	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
19	1	309	CLA	CAC-C3C-C4C	2.72	128.34	124.81
19	2	205	CLA	CHD-C4C-NC	2.72	128.49	124.20
19	3	207	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
28	5	218	DD6	C25-C24-C1	-2.72	118.78	126.42
19	3	210	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
19	1	310	CLA	CAA-C2A-C3A	-2.72	105.34	112.78
28	L	209	DD6	C41-C32-C31	-2.72	106.15	110.47
31	5	221	A86	C41-C32-C31	-2.72	108.04	110.47
23	A	852	LHG	O8-C23-C24	2.72	120.43	111.91
18	A	801	CL0	CAC-C3C-C4C	2.72	128.33	124.81
19	A	827	CLA	CHC-C1C-C2C	-2.72	119.21	126.72
28	3	213	DD6	C37-C36-C35	-2.72	109.32	114.36
19	2	212	CLA	CHC-C1C-C2C	-2.72	119.21	126.72
31	4	316	A86	C25-C24-C1	-2.72	118.79	126.42
19	A	838	CLA	CHD-C4C-NC	2.71	128.48	124.20
19	4	309	CLA	CHD-C4C-NC	2.71	128.48	124.20
19	3	209	CLA	O2A-CGA-CBA	2.71	120.43	111.91
19	A	820	CLA	CHC-C1C-C2C	-2.71	119.22	126.72
19	A	811	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
19	A	828	CLA	CHC-C1C-C2C	-2.71	119.22	126.72
19	2	205	CLA	C1-O2A-CGA	2.71	123.56	116.44
19	5	215	CLA	CAC-C3C-C4C	2.71	128.33	124.81
19	2	215	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
19	2	215	CLA	CAC-C3C-C4C	2.71	128.33	124.81
19	A	831	CLA	CAC-C3C-C4C	2.71	128.33	124.81
19	B	807	CLA	CHC-C1C-C2C	-2.71	119.22	126.72
31	3	212	A86	C8-C6-C5	-2.71	114.78	118.94
19	B	825	CLA	CBC-CAC-C3C	-2.71	104.96	112.43
19	1	303	CLA	CAA-C2A-C3A	-2.71	105.36	112.78
19	A	837	CLA	CMC-C2C-C1C	2.71	129.16	125.04
19	B	817	CLA	CHC-C1C-C2C	-2.71	119.23	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	301	CLA	CAC-C3C-C4C	2.71	128.32	124.81
19	A	841	CLA	CED-O2D-CGD	2.71	122.06	115.94
19	A	841	CLA	O2A-CGA-CBA	2.71	120.40	111.91
19	2	206	CLA	CMC-C2C-C1C	2.71	129.16	125.04
31	3	228	A86	C9-C10-C11	-2.71	118.65	126.61
19	A	813	CLA	C1-C2-C3	-2.71	121.36	126.04
19	A	817	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
19	A	814	CLA	CHC-C1C-C2C	-2.70	119.24	126.72
19	A	837	CLA	CAC-C3C-C4C	2.70	128.32	124.81
19	4	301	CLA	C1-C2-C3	-2.70	121.37	126.04
19	2	209	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
19	A	818	CLA	CHD-C4C-NC	2.70	128.46	124.20
28	2	217	DD6	C41-C32-C31	-2.70	106.17	110.47
19	B	806	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
19	A	837	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
19	B	809	CLA	C4-C3-C5	2.70	119.81	115.27
19	A	804	CLA	CHD-C4C-NC	2.70	128.46	124.20
19	B	829	CLA	CMC-C2C-C1C	2.70	129.15	125.04
19	A	807	CLA	C4-C3-C5	2.70	119.81	115.27
19	B	806	CLA	CAC-C3C-C4C	2.70	128.31	124.81
19	A	830	CLA	CHD-C4C-NC	2.69	128.45	124.20
19	B	807	CLA	CBC-CAC-C3C	-2.69	105.00	112.43
19	B	808	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
19	A	806	CLA	CMC-C2C-C1C	2.69	129.14	125.04
19	4	301	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
19	A	825	CLA	O2A-CGA-CBA	2.69	120.35	111.91
19	A	844	CLA	CAC-C3C-C4C	2.69	128.30	124.81
19	B	837	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
19	A	835	CLA	O2A-CGA-CBA	2.69	120.35	111.91
19	A	830	CLA	O2A-CGA-CBA	2.69	120.35	111.91
19	u	202	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
19	4	306	CLA	CHD-C4C-NC	2.69	128.44	124.20
30	2	211	KC1	C4C-C3C-C2C	-2.69	102.98	106.90
19	1	306	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
19	4	311	CLA	CHD-C4C-NC	2.69	128.44	124.20
19	A	827	CLA	CHD-C4C-NC	2.69	128.44	124.20
19	A	833	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
19	A	839	CLA	C1-C2-C3	-2.68	121.40	126.04
19	L	203	CLA	CHC-C1C-C2C	-2.68	119.30	126.72
19	3	209	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
19	2	207	CLA	CBA-CAA-C2A	2.68	121.78	113.86
19	A	804	CLA	CAC-C3C-C4C	2.68	128.29	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	202	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
19	1	307	CLA	CMC-C2C-C1C	2.68	129.12	125.04
19	3	209	CLA	C4-C3-C5	2.68	119.05	115.98
19	A	825	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
19	B	810	CLA	O2A-CGA-CBA	2.68	120.32	111.91
19	5	209	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
19	L	204	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
31	3	212	A86	C24-C1-C2	-2.68	114.83	118.94
19	A	821	CLA	CBC-CAC-C3C	-2.68	105.05	112.43
19	B	831	CLA	CAA-C2A-C3A	-2.68	105.45	112.78
19	B	812	CLA	CMB-C2B-C3B	2.68	129.69	124.68
19	3	202	CLA	C4C-C3C-C2C	-2.68	103.00	106.90
30	2	211	KC1	CMC-C2C-C1C	2.68	129.11	125.04
19	B	836	CLA	O2A-CGA-CBA	2.68	120.30	111.91
19	A	834	CLA	CHD-C4C-NC	2.68	128.42	124.20
19	B	845	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
19	1	307	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
19	A	842	CLA	O2A-CGA-CBA	2.67	120.30	111.91
19	A	802	CLA	C4-C3-C5	2.67	119.77	115.27
19	2	208	CLA	CMB-C2B-C3B	2.67	129.68	124.68
19	A	878	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
19	4	303	CLA	O2A-CGA-CBA	2.67	120.29	111.91
31	3	212	A86	C26-C25-C24	-2.67	114.88	123.22
19	F	204	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
22	A	847	BCR	C33-C5-C6	-2.67	121.53	124.53
19	A	809	CLA	CMC-C2C-C1C	2.67	129.11	125.04
19	2	213	CLA	CAC-C3C-C4C	2.67	128.27	124.81
22	F	205	BCR	C3-C4-C5	-2.67	109.31	114.08
19	1	310	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
19	4	309	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
19	4	312	CLA	C3B-C4B-NB	2.67	112.66	109.21
19	B	846	CLA	CMC-C2C-C1C	2.66	129.10	125.04
19	A	880	CLA	CMB-C2B-C3B	2.66	129.66	124.68
19	B	810	CLA	CMC-C2C-C1C	2.66	129.09	125.04
31	3	214	A86	O1-C15-C14	-2.66	107.87	113.21
19	2	206	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
31	3	214	A86	C12-C11-C13	2.66	120.49	116.02
19	B	845	CLA	O2A-CGA-CBA	2.66	120.25	111.91
19	B	811	CLA	CMA-C3A-C2A	-2.66	103.10	113.83
19	5	215	CLA	CHD-C4C-NC	2.66	128.39	124.20
19	4	313	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
19	A	827	CLA	C1-C2-C3	-2.66	121.45	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	210	CLA	CBC-CAC-C3C	-2.66	105.10	112.43
31	1	317	A86	C7-C6-C8	2.66	122.26	118.08
31	4	314	A86	C41-C32-C31	-2.66	108.09	110.47
19	A	808	CLA	O2A-CGA-CBA	2.66	120.25	111.91
23	1	318	LHG	C11-C10-C9	-2.66	100.94	114.42
19	A	821	CLA	C4-C3-C5	2.66	119.74	115.27
19	4	313	CLA	CAC-C3C-C4C	2.66	128.26	124.81
19	4	304	CLA	C4C-C3C-C2C	-2.66	103.03	106.90
19	2	214	CLA	CBC-CAC-C3C	-2.65	105.11	112.43
19	B	804	CLA	CMB-C2B-C3B	2.65	129.64	124.68
26	B	847	DGD	O5D-C6D-C5D	-2.65	104.14	109.05
27	J	105	5X6	C11-C03-C02	-2.65	115.04	121.46
19	B	805	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
19	B	816	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
19	B	822	CLA	C4-C3-C5	2.65	119.73	115.27
19	L	206	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
19	A	840	CLA	CHC-C1C-C2C	-2.65	119.39	126.72
19	B	811	CLA	CMC-C2C-C1C	2.65	129.07	125.04
19	B	826	CLA	CAA-C2A-C3A	-2.65	105.52	112.78
19	B	833	CLA	CHD-C4C-NC	2.65	128.38	124.20
19	1	304	CLA	C3B-C4B-NB	2.65	112.63	109.21
19	B	807	CLA	O2A-CGA-CBA	2.65	120.22	111.91
19	B	834	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
19	A	806	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
18	A	801	CL0	C4C-C3C-C2C	-2.65	103.04	106.90
19	1	303	CLA	O2A-CGA-CBA	2.65	120.21	111.91
19	2	207	CLA	O2A-CGA-CBA	2.65	120.21	111.91
19	3	203	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
19	B	835	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
19	A	832	CLA	CMB-C2B-C3B	2.64	129.62	124.68
19	A	810	CLA	CED-O2D-CGD	2.64	121.91	115.94
19	A	814	CLA	C4-C3-C5	2.64	119.71	115.27
22	A	848	BCR	C33-C5-C6	-2.64	121.56	124.53
19	B	818	CLA	CHD-C4C-NC	2.64	128.36	124.20
19	1	310	CLA	O2A-CGA-CBA	2.64	120.19	111.91
19	A	839	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
19	B	812	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
19	L	206	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
19	4	308	CLA	CHC-C1C-C2C	-2.64	119.43	126.72
19	2	205	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
19	B	830	CLA	CAC-C3C-C4C	2.64	128.23	124.81
30	3	211	KC1	CMB-C2B-C1B	2.64	129.36	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	816	CLA	CMB-C2B-C3B	2.63	129.61	124.68
19	A	808	CLA	C3B-C4B-NB	2.63	112.61	109.21
19	A	805	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
19	A	839	CLA	CHD-C4C-NC	2.63	128.35	124.20
19	A	826	CLA	O1D-CGD-CBD	-2.63	119.10	124.48
19	4	313	CLA	CBC-CAC-C3C	-2.63	105.18	112.43
19	A	820	CLA	C1-C2-C3	-2.63	121.49	126.04
19	B	811	CLA	C4-C3-C5	2.63	119.70	115.27
19	1	301	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
19	A	839	CLA	O2A-CGA-O1A	-2.63	116.96	123.59
19	4	312	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
19	A	818	CLA	O2A-CGA-CBA	2.63	120.16	111.91
19	B	831	CLA	CMC-C2C-C1C	2.63	129.04	125.04
19	3	207	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
19	5	208	CLA	CMC-C2C-C1C	2.63	129.04	125.04
19	B	828	CLA	CHD-C4C-NC	2.63	128.34	124.20
19	B	821	CLA	C4-C3-C5	2.63	119.69	115.27
19	1	310	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
19	F	203	CLA	CAC-C3C-C4C	2.63	128.22	124.81
30	3	208	KC1	CMB-C2B-C1B	2.63	129.34	124.71
19	L	203	CLA	CHD-C4C-NC	2.62	128.34	124.20
19	1	307	CLA	CHD-C4C-NC	2.62	128.34	124.20
19	A	843	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
19	B	824	CLA	CHC-C1C-C2C	-2.62	119.47	126.72
19	B	845	CLA	CHC-C1C-C2C	-2.62	119.47	126.72
19	B	828	CLA	CHC-C1C-C2C	-2.62	119.47	126.72
31	3	212	A86	C9-C8-C6	-2.62	119.06	126.42
19	3	210	CLA	CMC-C2C-C1C	2.62	129.03	125.04
19	5	212	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
19	A	814	CLA	CAC-C3C-C4C	2.62	128.21	124.81
19	L	204	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
22	J	104	BCR	C33-C5-C6	-2.62	121.59	124.53
19	5	214	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
19	L	203	CLA	CMC-C2C-C1C	2.62	129.02	125.04
31	2	218	A86	C10-C9-C8	-2.62	115.05	123.22
31	2	216	A86	C24-C1-C2	-2.62	114.93	118.94
19	B	836	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
19	3	207	CLA	CHD-C4C-NC	2.61	128.32	124.20
19	B	823	CLA	O1D-CGD-CBD	-2.61	119.14	124.48
19	B	824	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
19	A	811	CLA	CAC-C3C-C4C	2.61	128.20	124.81
19	2	210	CLA	CHC-C1C-C2C	-2.61	119.49	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	824	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
19	1	309	CLA	CMC-C2C-C1C	2.61	129.02	125.04
22	M	102	BCR	C15-C14-C13	-2.61	123.58	127.31
26	B	847	DGD	CDB-CCB-CBB	-2.61	101.16	114.42
19	B	830	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
19	B	814	CLA	CAC-C3C-C4C	2.61	128.20	124.81
19	A	880	CLA	CAC-C3C-C4C	2.61	128.20	124.81
19	B	804	CLA	CHD-C4C-NC	2.61	128.32	124.20
19	A	823	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
19	A	806	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
19	A	802	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
19	B	815	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
31	3	214	A86	C-C1-C2	-2.61	119.27	122.92
19	B	814	CLA	C4-C3-C5	2.61	119.66	115.27
19	A	825	CLA	C1-O2A-CGA	2.61	123.29	116.44
19	B	818	CLA	C1-C2-C3	-2.61	121.53	126.04
19	A	838	CLA	CBC-CAC-C3C	-2.61	105.24	112.43
19	A	820	CLA	CMC-C2C-C1C	2.61	129.01	125.04
19	B	821	CLA	CHD-C4C-NC	2.61	128.31	124.20
19	A	810	CLA	CAC-C3C-C4C	2.61	128.19	124.81
19	B	845	CLA	CHD-C4C-NC	2.60	128.31	124.20
19	A	833	CLA	CMC-C2C-C1C	2.60	129.00	125.04
19	F	203	CLA	CMC-C2C-C1C	2.60	129.00	125.04
19	A	828	CLA	O2A-CGA-CBA	2.60	120.08	111.91
19	B	807	CLA	C4C-C3C-C2C	-2.60	103.10	106.90
19	A	822	CLA	CHD-C4C-NC	2.60	128.31	124.20
19	A	809	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
19	B	819	CLA	C2A-C1A-CHA	-2.60	119.31	123.86
19	A	837	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
19	A	817	CLA	CMC-C2C-C1C	2.60	129.00	125.04
19	B	830	CLA	O1D-CGD-CBD	-2.60	119.16	124.48
18	A	801	CL0	CMA-C3A-C4A	-2.60	104.78	111.77
19	2	212	CLA	O1D-CGD-CBD	-2.60	119.17	124.48
19	B	833	CLA	CMC-C2C-C1C	2.60	129.00	125.04
19	A	844	CLA	CBC-CAC-C3C	-2.60	105.27	112.43
19	B	807	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
19	2	214	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
19	3	203	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
30	3	208	KC1	CMC-C2C-C1C	2.60	128.99	125.04
19	L	203	CLA	CBC-CAC-C3C	-2.60	105.28	112.43
19	5	207	CLA	C4-C3-C5	2.60	119.64	115.27
19	A	812	CLA	CHD-C4C-NC	2.60	128.29	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	834	CLA	C2A-C1A-CHA	-2.60	119.32	123.86
19	2	206	CLA	C4C-C3C-C2C	-2.59	103.11	106.90
19	B	802	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
19	B	811	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
19	B	831	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
19	A	827	CLA	O2A-CGA-CBA	2.59	120.05	111.91
19	A	824	CLA	CHD-C4C-NC	2.59	128.29	124.20
30	3	208	KC1	O2D-CGD-O1D	-2.59	118.77	123.84
19	3	203	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
19	B	819	CLA	CMB-C2B-C3B	2.59	129.53	124.68
19	A	818	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
19	B	828	CLA	CMC-C2C-C1C	2.59	128.98	125.04
19	B	822	CLA	C1-C2-C3	-2.59	121.56	126.04
19	3	204	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
22	B	844	BCR	C27-C26-C25	2.59	126.49	122.73
19	B	823	CLA	C1-C2-C3	-2.59	121.57	126.04
19	B	802	CLA	CHD-C4C-NC	2.59	128.28	124.20
31	4	315	A86	C41-C32-C31	-2.59	108.16	110.47
19	A	832	CLA	C4C-C3C-C2C	-2.59	103.13	106.90
22	J	104	BCR	C27-C26-C25	2.59	126.49	122.73
19	B	823	CLA	CAC-C3C-C4C	2.59	128.17	124.81
19	1	310	CLA	CHB-C4A-NA	2.59	128.09	124.51
19	A	843	CLA	CMC-C2C-C1C	2.59	128.98	125.04
19	B	802	CLA	O2A-CGA-CBA	2.59	120.02	111.91
19	A	829	CLA	C1-O2A-CGA	2.58	123.23	116.44
19	A	815	CLA	CHD-C4C-NC	2.58	128.28	124.20
19	B	818	CLA	CMC-C2C-C1C	2.58	128.97	125.04
30	3	211	KC1	CHD-C4C-NC	2.58	128.12	124.20
19	B	838	CLA	CBC-CAC-C3C	-2.58	105.31	112.43
31	5	220	A86	C-C1-C2	-2.58	119.31	122.92
19	L	206	CLA	CAC-C3C-C4C	2.58	128.16	124.81
19	B	837	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
19	4	303	CLA	C1-C2-C3	-2.58	121.58	126.04
19	B	803	CLA	CHD-C4C-NC	2.58	128.27	124.20
19	B	813	CLA	CMC-C2C-C1C	2.58	128.97	125.04
19	A	802	CLA	O2A-CGA-CBA	2.58	120.01	111.91
19	A	812	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
28	1	312	DD6	C15-C14-C13	-2.58	120.54	125.99
19	A	824	CLA	CAC-C3C-C4C	2.58	128.16	124.81
19	B	824	CLA	C4-C3-C5	2.58	119.61	115.27
19	3	202	CLA	C3B-C4B-NB	2.58	112.54	109.21
19	B	812	CLA	CMC-C2C-C1C	2.58	128.96	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	2	218	A86	O1-C15-C14	-2.58	108.04	113.21
19	B	830	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
28	L	209	DD6	C20-C19-C18	-2.58	107.65	112.75
19	B	803	CLA	CAA-C2A-C3A	-2.58	105.73	112.78
24	A	854	LMT	O5'-C1'-O1'	-2.57	103.88	109.97
24	A	854	LMT	O5B-C5B-C4B	2.57	114.37	109.69
19	A	811	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
19	A	833	CLA	CED-O2D-CGD	2.57	121.76	115.94
19	2	213	CLA	CMC-C2C-C1C	2.57	128.96	125.04
22	B	852	BCR	C24-C23-C22	-2.57	122.35	126.23
22	1	311	BCR	C15-C14-C13	-2.57	123.64	127.31
19	5	210	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
19	A	844	CLA	CMB-C2B-C3B	2.57	129.49	124.68
19	B	809	CLA	CMC-C2C-C1C	2.57	128.95	125.04
19	1	310	CLA	CBC-CAC-C3C	-2.57	105.35	112.43
19	A	822	CLA	CMB-C2B-C3B	2.57	129.49	124.68
19	A	825	CLA	CHD-C4C-NC	2.57	128.25	124.20
19	B	846	CLA	O2A-CGA-CBA	2.57	119.97	111.91
19	B	830	CLA	C2A-C1A-CHA	-2.57	119.37	123.86
19	A	815	CLA	C5-C3-C4	2.57	120.28	114.60
31	5	219	A86	C34-O4-C38	-2.57	113.11	117.90
19	B	816	CLA	C1-C2-C3	-2.57	121.60	126.04
19	A	811	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
19	A	815	CLA	O2A-CGA-CBA	2.57	119.97	111.91
19	B	817	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
19	1	308	CLA	CHC-C1C-C2C	-2.57	119.62	126.72
19	2	208	CLA	O2A-CGA-CBA	2.57	119.96	111.91
19	4	301	CLA	O2A-CGA-CBA	2.57	119.96	111.91
19	A	827	CLA	CMC-C2C-C1C	2.57	128.95	125.04
19	2	209	CLA	CMC-C2C-C1C	2.57	128.95	125.04
19	4	305	CLA	CHD-C4C-NC	2.57	128.25	124.20
19	3	206	CLA	O2A-CGA-CBA	2.56	119.96	111.91
19	1	308	CLA	CMC-C2C-C1C	2.56	128.94	125.04
19	A	810	CLA	CMB-C2B-C3B	2.56	129.47	124.68
19	L	204	CLA	CAC-C3C-C4C	2.56	128.13	124.81
19	B	834	CLA	CBC-CAC-C3C	-2.56	105.37	112.43
19	2	210	CLA	CMB-C2B-C3B	2.56	129.47	124.68
19	A	808	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
19	A	842	CLA	CHD-C4C-NC	2.56	128.24	124.20
19	B	836	CLA	CMB-C2B-C3B	2.56	129.47	124.68
19	1	306	CLA	CED-O2D-CGD	2.56	121.72	115.94
19	B	830	CLA	O2A-CGA-CBA	2.56	119.94	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	840	BCR	C24-C23-C22	-2.56	122.37	126.23
19	2	205	CLA	CAA-C2A-C3A	-2.56	105.78	112.78
19	B	830	CLA	CHD-C4C-NC	2.56	128.23	124.20
19	B	834	CLA	C4-C3-C5	2.56	119.57	115.27
19	4	313	CLA	C4-C3-C5	2.55	119.57	115.27
19	5	209	CLA	C1-O2A-CGA	2.55	123.15	116.44
22	F	205	BCR	C27-C26-C25	2.55	126.44	122.73
19	B	808	CLA	O1D-CGD-CBD	-2.55	119.26	124.48
19	B	802	CLA	CMA-C3A-C2A	-2.55	103.53	113.83
19	A	814	CLA	CMC-C2C-C1C	2.55	128.93	125.04
19	A	842	CLA	CMB-C2B-C3B	2.55	129.45	124.68
22	A	850	BCR	C7-C8-C9	-2.55	122.38	126.23
19	A	810	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
22	L	205	BCR	C27-C26-C25	2.55	126.44	122.73
19	A	834	CLA	CBC-CAC-C3C	-2.55	105.40	112.43
19	1	310	CLA	CMC-C2C-C1C	2.55	128.92	125.04
19	A	805	CLA	CBC-CAC-C3C	-2.55	105.40	112.43
19	B	828	CLA	CAC-C3C-C4C	2.55	128.12	124.81
19	B	810	CLA	C2A-C1A-CHA	-2.55	119.40	123.86
19	5	210	CLA	C4C-C3C-C2C	-2.55	103.18	106.90
19	B	824	CLA	CAC-C3C-C4C	2.55	128.12	124.81
19	B	803	CLA	O2A-CGA-O1A	-2.55	117.16	123.59
31	2	216	A86	C8-C6-C5	-2.55	115.03	118.94
19	A	808	CLA	C4-C3-C5	2.55	119.56	115.27
19	4	313	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
19	A	829	CLA	O2A-CGA-CBA	2.55	119.90	111.91
19	4	304	CLA	CAA-C2A-C3A	-2.55	105.81	112.78
19	A	803	CLA	CED-O2D-CGD	2.55	121.69	115.94
19	A	820	CLA	O2A-CGA-CBA	2.55	119.89	111.91
19	3	209	CLA	CBC-CAC-C3C	-2.54	105.42	112.43
19	B	821	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
19	4	303	CLA	CAC-C3C-C4C	2.54	128.11	124.81
19	A	806	CLA	C2A-C1A-CHA	-2.54	119.41	123.86
19	1	310	CLA	CMB-C2B-C3B	2.54	129.44	124.68
19	2	206	CLA	CMB-C2B-C3B	2.54	129.43	124.68
19	5	208	CLA	C4C-C3C-C2C	-2.54	103.19	106.90
19	A	839	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
19	B	823	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
30	2	211	KC1	CMB-C2B-C1B	2.54	129.19	124.71
19	4	304	CLA	CHC-C1C-C2C	-2.54	119.69	126.72
19	B	823	CLA	O2A-CGA-CBA	2.54	119.88	111.91
22	A	847	BCR	C15-C16-C17	-2.54	118.27	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	306	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	1	301	CLA	CMC-C2C-C1C	2.54	128.91	125.04
19	A	844	CLA	O2A-CGA-CBA	2.54	119.87	111.91
19	A	832	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
19	5	211	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
19	B	808	CLA	CAC-C3C-C4C	2.54	128.10	124.81
19	B	827	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
19	2	212	CLA	CBC-CAC-C3C	-2.53	105.44	112.43
19	A	819	CLA	CHD-C4C-NC	2.53	128.20	124.20
19	A	809	CLA	C4C-C3C-C2C	-2.53	103.20	106.90
19	A	814	CLA	C2A-C1A-CHA	-2.53	119.43	123.86
19	4	312	CLA	CMB-C2B-C3B	2.53	129.42	124.68
22	A	847	BCR	C11-C10-C9	-2.53	123.70	127.31
23	4	317	LHG	C11-C10-C9	-2.53	101.57	114.42
19	3	210	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
19	L	206	CLA	CBC-CAC-C3C	-2.53	105.45	112.43
19	A	817	CLA	CAC-C3C-C4C	2.53	128.09	124.81
19	A	825	CLA	C6-C7-C8	-2.53	107.75	115.92
30	4	302	KC1	CMB-C2B-C1B	2.53	129.17	124.71
19	5	207	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
22	I	101	BCR	C16-C15-C14	-2.53	118.30	123.47
19	3	202	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
19	5	212	CLA	CAA-C2A-C3A	-2.53	105.86	112.78
19	B	833	CLA	C1-C2-C3	-2.53	121.67	126.04
19	B	815	CLA	CHD-C4C-NC	2.52	128.18	124.20
19	1	301	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
19	B	805	CLA	CHD-C4C-NC	2.52	128.18	124.20
19	B	807	CLA	CMB-C2B-C3B	2.52	129.40	124.68
19	5	209	CLA	O1D-CGD-CBD	-2.52	119.33	124.48
19	1	304	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
31	5	221	A86	C12-C11-C13	2.52	120.25	116.02
19	A	832	CLA	C4-C3-C5	2.52	119.51	115.27
19	B	829	CLA	CHD-C4C-NC	2.52	128.17	124.20
19	B	816	CLA	O2A-CGA-CBA	2.52	119.81	111.91
19	u	201	CLA	CHD-C4C-NC	2.52	128.17	124.20
19	4	309	CLA	CMC-C2C-C1C	2.52	128.87	125.04
19	B	813	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
22	M	102	BCR	C27-C26-C25	2.51	126.38	122.73
30	4	307	KC1	CHD-C4C-NC	2.51	128.02	124.20
19	B	811	CLA	CBC-CAC-C3C	-2.51	105.50	112.43
19	1	306	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
19	A	813	CLA	O2D-CGD-O1D	-2.51	118.92	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	831	CLA	C1-C2-C3	-2.51	121.70	126.04
19	3	209	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
19	B	826	CLA	CHD-C4C-NC	2.51	128.16	124.20
19	4	304	CLA	CAA-C2A-C1A	-2.51	103.75	111.97
19	A	808	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
19	B	813	CLA	CHD-C4C-NC	2.51	128.15	124.20
19	B	822	CLA	CHD-C4C-NC	2.51	128.15	124.20
19	B	832	CLA	O2A-CGA-CBA	2.51	119.77	111.91
19	B	817	CLA	CMB-C2B-C3B	2.51	129.37	124.68
19	3	207	CLA	CMB-C2B-C3B	2.51	129.37	124.68
19	A	833	CLA	CAC-C3C-C4C	2.51	128.06	124.81
19	B	809	CLA	CED-O2D-CGD	2.51	121.60	115.94
30	3	208	KC1	CBC-CAC-C3C	-2.50	105.53	112.43
19	A	806	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
22	A	849	BCR	C27-C26-C25	2.50	126.36	122.73
19	1	307	CLA	CBC-CAC-C3C	-2.50	105.53	112.43
19	A	831	CLA	CMC-C2C-C1C	2.50	128.85	125.04
19	B	804	CLA	C4-C3-C5	2.50	119.48	115.27
19	B	832	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	L	205	BCR	C7-C8-C9	-2.50	122.46	126.23
19	A	821	CLA	CHC-C1C-C2C	-2.50	119.81	126.72
19	2	212	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
19	4	312	CLA	CAC-C3C-C4C	2.50	128.05	124.81
22	1	311	BCR	C33-C5-C6	-2.50	121.72	124.53
19	B	824	CLA	CBC-CAC-C3C	-2.50	105.55	112.43
19	2	215	CLA	CBC-CAC-C3C	-2.49	105.55	112.43
19	u	201	CLA	CMC-C2C-C1C	2.49	128.83	125.04
19	L	203	CLA	CAC-C3C-C4C	2.49	128.04	124.81
19	A	823	CLA	CAC-C3C-C4C	2.49	128.04	124.81
19	u	202	CLA	CMB-C2B-C3B	2.49	129.34	124.68
22	F	205	BCR	C24-C23-C22	-2.49	122.47	126.23
31	3	214	A86	C4-C3-C2	-2.49	118.38	123.47
19	1	303	CLA	CHD-C4C-NC	2.49	128.12	124.20
19	1	306	CLA	CMB-C2B-C3B	2.49	129.33	124.68
19	A	805	CLA	O2A-CGA-CBA	2.49	119.71	111.91
19	4	308	CLA	CAC-C3C-C4C	2.49	128.04	124.81
19	1	309	CLA	O2A-C1-C2	2.49	115.17	108.64
31	1	316	A86	C7-C6-C8	2.49	121.99	118.08
31	5	217	A86	C19-C18-C17	-2.49	105.97	110.77
19	A	839	CLA	C2A-C1A-CHA	-2.49	119.51	123.86
19	B	809	CLA	C4C-C3C-C2C	-2.48	103.28	106.90
19	1	307	CLA	C1-C2-C3	-2.48	121.75	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	804	CLA	CMB-C2B-C3B	2.48	129.32	124.68
19	B	828	CLA	CMB-C2B-C3B	2.48	129.32	124.68
19	A	831	CLA	CBC-CAC-C3C	-2.48	105.58	112.43
19	2	207	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
19	3	204	CLA	CMB-C2B-C3B	2.48	129.32	124.68
19	A	832	CLA	O2A-CGA-CBA	2.48	119.69	111.91
19	L	206	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
31	5	221	A86	C26-C25-C24	-2.48	115.47	123.22
19	A	841	CLA	C4C-C3C-C2C	-2.48	103.28	106.90
19	A	836	CLA	CHD-C4C-NC	2.48	128.11	124.20
19	2	208	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
19	4	303	CLA	CMC-C2C-C1C	2.48	128.81	125.04
19	2	209	CLA	CAA-C2A-C3A	-2.48	105.99	112.78
22	L	205	BCR	C11-C10-C9	-2.48	123.77	127.31
19	B	821	CLA	CMA-C3A-C4A	-2.48	105.11	111.77
19	1	309	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
31	1	317	A86	C-C1-C24	2.48	121.98	118.08
19	B	803	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
19	B	837	CLA	CAC-C3C-C4C	2.48	128.02	124.81
19	B	833	CLA	C4-C3-C5	2.47	119.43	115.27
19	B	822	CLA	CMC-C2C-C1C	2.47	128.81	125.04
19	B	804	CLA	CBC-CAC-C3C	-2.47	105.62	112.43
19	2	213	CLA	CMB-C2B-C3B	2.47	129.30	124.68
19	B	834	CLA	CAC-C3C-C4C	2.47	128.02	124.81
19	A	808	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
19	B	830	CLA	CBC-CAC-C3C	-2.47	105.62	112.43
24	3	216	LMT	C1'-O5'-C5'	-2.47	108.84	113.69
30	3	205	KC1	CMC-C2C-C1C	2.47	128.80	125.04
19	B	829	CLA	CHC-C1C-C2C	-2.47	119.90	126.72
31	2	216	A86	C41-C32-C31	-2.47	108.26	110.47
19	A	843	CLA	C2A-C1A-CHA	-2.47	119.55	123.86
28	3	213	DD6	C25-C24-C1	-2.47	119.49	126.42
19	5	214	CLA	CMB-C2B-C3B	2.47	129.29	124.68
19	A	843	CLA	O2A-CGA-CBA	2.46	119.64	111.91
19	3	203	CLA	CAC-C3C-C4C	2.46	128.01	124.81
19	5	209	CLA	CHD-C4C-NC	2.46	128.09	124.20
19	A	823	CLA	CMB-C2B-C3B	2.46	129.28	124.68
31	4	316	A86	C9-C8-C6	-2.46	119.50	126.42
19	4	312	CLA	C4-C3-C5	2.46	119.41	115.27
19	1	306	CLA	C4C-C3C-C2C	-2.46	103.31	106.90
19	A	841	CLA	C1-C2-C3	-2.46	121.79	126.04
23	3	215	LHG	O8-C23-C24	2.46	119.63	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	840	CLA	CMB-C2B-C3B	2.46	129.28	124.68
19	B	813	CLA	CMB-C2B-C3B	2.46	129.28	124.68
19	A	825	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
19	L	204	CLA	CBC-CAC-C3C	-2.46	105.65	112.43
19	A	834	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
19	A	821	CLA	CMB-C2B-C3B	2.46	129.28	124.68
22	A	851	BCR	C28-C27-C26	-2.46	109.69	114.08
19	A	807	CLA	CBC-CAC-C3C	-2.46	105.66	112.43
19	5	213	CLA	CHD-C4C-NC	2.46	128.07	124.20
19	5	216	CLA	CHD-C4C-NC	2.46	128.07	124.20
22	F	201	BCR	C30-C25-C26	-2.46	119.16	122.61
19	A	832	CLA	CAC-C3C-C4C	2.45	128.00	124.81
19	5	211	CLA	C4-C3-C5	2.45	119.40	115.27
19	L	206	CLA	CMB-C2B-C3B	2.45	129.27	124.68
19	1	309	CLA	CHC-C1C-C2C	-2.45	119.94	126.72
19	A	834	CLA	C4-C3-C5	2.45	119.39	115.27
23	A	853	LHG	C11-C10-C9	-2.45	101.98	114.42
19	A	835	CLA	CMB-C2B-C3B	2.45	129.26	124.68
19	2	210	CLA	C3B-C4B-NB	2.45	112.38	109.21
19	A	831	CLA	O2A-CGA-CBA	2.45	119.59	111.91
19	2	209	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
19	B	808	CLA	O2A-CGA-O1A	-2.45	117.41	123.59
22	L	202	BCR	C24-C23-C22	-2.45	122.54	126.23
19	B	807	CLA	C1-O2A-CGA	2.45	122.87	116.44
31	5	219	A86	C9-C8-C6	-2.45	119.54	126.42
19	B	810	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
19	A	815	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
23	M	103	LHG	C11-C10-C9	-2.45	102.01	114.42
31	5	217	A86	C7-C6-C8	2.45	121.93	118.08
19	1	301	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
19	A	828	CLA	CAC-C3C-C4C	2.45	127.98	124.81
19	A	835	CLA	CAA-C2A-C3A	-2.45	106.08	112.78
19	B	825	CLA	C4-C3-C5	2.44	119.38	115.27
22	A	848	BCR	C24-C23-C22	-2.44	122.54	126.23
19	A	804	CLA	CMC-C2C-C1C	2.44	128.76	125.04
19	1	308	CLA	CMB-C2B-C3B	2.44	129.25	124.68
19	A	802	CLA	CMC-C2C-C1C	2.44	128.76	125.04
19	A	836	CLA	CBC-CAC-C3C	-2.44	105.70	112.43
19	B	810	CLA	CHC-C1C-C2C	-2.44	119.97	126.72
19	A	840	CLA	CBC-CAC-C3C	-2.44	105.71	112.43
19	5	207	CLA	CBC-CAC-C3C	-2.44	105.71	112.43
19	A	803	CLA	O2A-CGA-CBA	2.44	119.56	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	831	CLA	CBC-CAC-C3C	-2.44	105.71	112.43
19	u	202	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
19	1	301	CLA	CAA-C2A-C3A	-2.44	106.11	112.78
30	1	305	KC1	CBC-CAC-C3C	-2.44	105.72	112.43
19	B	814	CLA	CBC-CAC-C3C	-2.44	105.72	112.43
19	u	201	CLA	C4-C3-C5	2.43	119.37	115.27
19	B	815	CLA	C2A-C1A-CHA	-2.43	119.60	123.86
19	B	826	CLA	C2A-C1A-CHA	-2.43	119.60	123.86
19	B	821	CLA	C2A-C1A-CHA	-2.43	119.60	123.86
19	1	304	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
19	A	817	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
19	4	313	CLA	O2A-CGA-CBA	2.43	119.53	111.91
19	4	304	CLA	CMB-C2B-C3B	2.43	129.22	124.68
19	A	803	CLA	CHD-C4C-NC	2.43	128.03	124.20
19	2	206	CLA	C4-C3-C5	2.43	119.36	115.27
19	F	204	CLA	CMC-C2C-C1C	2.43	128.74	125.04
19	1	310	CLA	CED-O2D-CGD	2.43	121.43	115.94
19	B	807	CLA	CAC-C3C-C4C	2.43	127.96	124.81
19	B	845	CLA	CMB-C2B-C3B	2.43	129.22	124.68
19	B	836	CLA	CED-O2D-CGD	2.43	121.43	115.94
19	A	835	CLA	CHD-C4C-NC	2.43	128.03	124.20
19	F	203	CLA	CMB-C2B-C3B	2.43	129.22	124.68
19	1	301	CLA	CAC-C3C-C4C	2.42	127.95	124.81
19	F	204	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
30	3	205	KC1	CED-O2D-CGD	2.42	121.42	115.94
19	A	826	CLA	CGD-CBD-CAD	-2.42	102.89	110.73
19	B	813	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
22	B	841	BCR	C15-C16-C17	-2.42	118.51	123.47
19	3	209	CLA	CAC-C3C-C4C	2.42	127.95	124.81
19	A	829	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
30	3	211	KC1	CMC-C2C-C1C	2.42	128.72	125.04
22	B	843	BCR	C15-C16-C17	-2.42	118.52	123.47
19	B	845	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
19	2	205	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
19	A	811	CLA	O2A-CGA-CBA	2.42	119.50	111.91
19	A	808	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
31	2	219	A86	C28-C27-C26	-2.42	119.54	122.92
19	B	818	CLA	C11-C10-C8	-2.42	108.11	115.92
19	A	807	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
19	B	811	CLA	CMB-C2B-C3B	2.42	129.20	124.68
28	1	315	DD6	C25-C26-C27	-2.41	119.57	126.58
19	B	814	CLA	O2A-CGA-CBA	2.41	119.48	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	801	CL0	CBC-CAC-C3C	-2.41	105.78	112.43
19	4	303	CLA	CHB-C4A-NA	2.41	127.85	124.51
19	L	204	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
19	4	303	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
19	B	814	CLA	CMB-C2B-C3B	2.41	129.19	124.68
19	A	828	CLA	C1-C2-C3	-2.41	121.87	126.04
19	A	807	CLA	CMC-C2C-C1C	2.41	128.71	125.04
19	A	841	CLA	CAC-C3C-C4C	2.41	127.94	124.81
19	A	838	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
19	2	209	CLA	O2A-CGA-CBA	2.41	119.46	111.91
19	5	207	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
19	A	813	CLA	CMC-C2C-C1C	2.41	128.70	125.04
19	A	833	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
19	5	210	CLA	CMC-C2C-C1C	2.41	128.70	125.04
19	B	834	CLA	CMC-C2C-C1C	2.40	128.70	125.04
19	L	204	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
19	2	209	CLA	CHB-C4A-NA	2.40	127.84	124.51
19	A	825	CLA	CMC-C2C-C1C	2.40	128.70	125.04
19	A	811	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
19	5	215	CLA	CMC-C2C-C1C	2.40	128.70	125.04
30	4	302	KC1	O2D-CGD-O1D	-2.40	119.14	123.84
31	2	216	A86	C7-C6-C8	2.40	121.86	118.08
19	2	214	CLA	CAC-C3C-C4C	2.40	127.93	124.81
19	4	311	CLA	C5-C3-C4	2.40	119.91	114.60
19	5	211	CLA	CHD-C4C-NC	2.40	127.99	124.20
19	B	818	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
19	3	204	CLA	C4-C3-C5	2.40	119.31	115.27
23	A	852	LHG	C11-C10-C9	-2.40	102.24	114.42
22	B	844	BCR	C8-C7-C6	-2.40	120.46	127.20
19	A	836	CLA	C1-O2A-CGA	2.40	122.74	116.44
19	A	880	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
19	A	809	CLA	O1D-CGD-CBD	-2.40	119.58	124.48
19	A	826	CLA	O2A-CGA-CBA	2.40	119.44	111.91
19	A	880	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
19	A	822	CLA	C1-O2A-CGA	2.40	122.73	116.44
19	5	215	CLA	CMB-C2B-C3B	2.40	129.16	124.68
29	1	302	LMG	C38-C37-C36	-2.40	102.26	114.42
19	A	803	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	4	310	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
19	5	211	CLA	CMC-C2C-C1C	2.40	128.69	125.04
19	B	828	CLA	CHB-C4A-NA	2.40	127.82	124.51
19	A	823	CLA	CMC-C2C-C1C	2.39	128.69	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	824	CLA	CMC-C2C-C1C	2.39	128.69	125.04
31	2	218	A86	C34-O4-C38	-2.39	113.44	117.90
19	B	807	CLA	C11-C10-C8	-2.39	108.18	115.92
31	5	217	A86	C41-C32-C31	-2.39	108.33	110.47
19	B	805	CLA	CMC-C2C-C1C	2.39	128.68	125.04
19	3	209	CLA	CMC-C2C-C1C	2.39	128.68	125.04
18	A	801	CL0	CHD-C4C-NC	2.39	127.97	124.20
19	B	827	CLA	CMB-C2B-C3B	2.39	129.15	124.68
19	4	308	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
19	A	807	CLA	CMB-C2B-C3B	2.39	129.15	124.68
19	4	313	CLA	CMB-C2B-C3B	2.39	129.15	124.68
19	B	818	CLA	C4C-C3C-C2C	-2.39	103.42	106.90
19	B	819	CLA	C4-C3-C5	2.39	119.29	115.27
31	5	220	A86	C12-C11-C10	-2.39	117.65	123.42
19	5	210	CLA	CAC-C3C-C4C	2.39	127.91	124.81
19	A	818	CLA	CMC-C2C-C1C	2.39	128.67	125.04
19	2	206	CLA	CAA-C2A-C1A	-2.39	104.15	111.97
19	B	829	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
19	A	837	CLA	CBC-CAC-C3C	-2.39	105.85	112.43
19	5	208	CLA	CMB-C2B-C3B	2.39	129.14	124.68
30	4	307	KC1	C2A-C1A-CHA	-2.39	119.55	127.44
19	J	103	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
30	4	307	KC1	CMB-C2B-C1B	2.38	128.91	124.71
19	1	303	CLA	CHB-C4A-NA	2.38	127.81	124.51
19	A	837	CLA	CMB-C2B-C3B	2.38	129.13	124.68
19	B	825	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
19	A	825	CLA	CBC-CAC-C3C	-2.38	105.87	112.43
19	L	203	CLA	CMB-C2B-C3B	2.38	129.13	124.68
19	1	309	CLA	CBC-CAC-C3C	-2.38	105.87	112.43
22	1	311	BCR	C27-C26-C25	2.38	126.18	122.73
19	A	841	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
19	A	816	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
19	4	312	CLA	O2A-CGA-CBA	2.37	119.35	111.91
19	A	825	CLA	CAA-C2A-C3A	-2.37	106.29	112.78
19	B	803	CLA	CMB-C2B-C3B	2.37	129.11	124.68
19	5	208	CLA	CED-O2D-CGD	2.37	121.29	115.94
18	A	801	CL0	C2A-C1A-CHA	-2.37	119.72	123.86
22	A	851	BCR	C15-C14-C13	-2.37	123.93	127.31
19	A	804	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
19	B	825	CLA	O2A-CGA-CBA	2.37	119.33	111.91
19	A	821	CLA	O1D-CGD-CBD	-2.37	119.64	124.48
19	1	307	CLA	CAA-C2A-C3A	-2.37	106.30	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	312	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
19	5	213	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
22	A	847	BCR	C15-C14-C13	-2.37	123.93	127.31
31	3	212	A86	C35-C34-C33	2.36	114.00	109.88
19	A	827	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
19	B	802	CLA	CMC-C2C-C1C	2.36	128.64	125.04
19	4	305	CLA	O2A-CGA-CBA	2.36	119.32	111.91
19	A	817	CLA	CBC-CAC-C3C	-2.36	105.92	112.43
19	A	838	CLA	CBA-CAA-C2A	-2.36	106.89	113.86
19	L	206	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
19	5	214	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
22	B	841	BCR	C27-C26-C25	2.36	126.16	122.73
31	4	314	A86	C7-C6-C5	-2.36	119.62	122.92
19	B	806	CLA	CED-O2D-CGD	2.36	121.27	115.94
19	B	810	CLA	CAC-C3C-C4C	2.36	127.87	124.81
19	A	804	CLA	CAA-CBA-CGA	-2.36	106.37	113.25
19	5	211	CLA	CBC-CAC-C3C	-2.36	105.94	112.43
19	3	210	CLA	CAC-C3C-C4C	2.35	127.86	124.81
23	B	842	LHG	C11-C10-C9	-2.35	102.47	114.42
19	A	813	CLA	C4-C3-C5	2.35	119.23	115.27
19	A	823	CLA	O2A-CGA-CBA	2.35	119.29	111.91
19	4	305	CLA	CMB-C2B-C3B	2.35	129.08	124.68
19	2	205	CLA	O2A-CGA-CBA	2.35	119.29	111.91
19	B	836	CLA	C4-C3-C5	2.35	119.23	115.27
22	F	201	BCR	C24-C23-C22	-2.35	122.68	126.23
19	A	814	CLA	C1-O2A-CGA	2.35	122.61	116.44
22	1	311	BCR	C8-C7-C6	-2.35	120.60	127.20
19	2	209	CLA	C1-O2A-CGA	2.35	122.61	116.44
19	B	810	CLA	C11-C10-C8	-2.35	108.33	115.92
31	2	216	A86	C-C1-C24	2.35	121.77	118.08
19	A	815	CLA	CMC-C2C-C1C	2.35	128.61	125.04
19	A	812	CLA	O1D-CGD-CBD	-2.35	119.69	124.48
19	3	210	CLA	CBC-CAC-C3C	-2.35	105.97	112.43
19	2	214	CLA	CMB-C2B-C3B	2.34	129.06	124.68
19	4	311	CLA	O2D-CGD-O1D	-2.34	119.25	123.84
19	B	830	CLA	CMC-C2C-C1C	2.34	128.61	125.04
19	1	308	CLA	C3B-C4B-NB	2.34	112.24	109.21
19	2	214	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	1	310	CLA	C4-C3-C5	2.34	119.21	115.27
19	A	819	CLA	CMB-C2B-C3B	2.34	129.06	124.68
19	2	205	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
19	4	309	CLA	CBC-CAC-C3C	-2.34	105.98	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	830	CLA	CMB-C2B-C3B	2.34	129.06	124.68
19	A	816	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
19	3	204	CLA	CBA-CAA-C2A	2.34	120.77	113.86
19	2	208	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
29	1	302	LMG	C40-C39-C38	-2.34	102.55	114.42
19	5	209	CLA	C1-C2-C3	-2.34	122.00	126.04
19	5	213	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	A	809	CLA	O2A-CGA-CBA	2.34	119.24	111.91
19	u	201	CLA	CMB-C2B-C3B	2.34	129.05	124.68
22	A	850	BCR	C33-C5-C6	-2.34	121.91	124.53
19	A	805	CLA	CHB-C4A-NA	2.34	127.74	124.51
19	B	810	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
19	B	829	CLA	O2A-C1-C2	2.34	114.77	108.64
19	u	201	CLA	O2A-C1-C2	2.34	114.77	108.64
28	1	312	DD6	C33-C32-C31	2.34	114.35	109.62
19	4	304	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
19	4	313	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
22	I	102	BCR	C15-C16-C17	-2.33	118.70	123.47
28	3	213	DD6	C3-C4-C5	-2.33	118.70	123.47
19	A	842	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
24	1	323	LMT	O5'-C1'-O1'	-2.33	104.45	109.97
19	J	103	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
31	2	218	A86	C25-C26-C27	-2.33	123.98	127.31
30	4	307	KC1	O2D-CGD-O1D	-2.33	119.28	123.84
19	A	878	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
19	A	836	CLA	CMA-C3A-C4A	-2.33	105.52	111.77
19	B	821	CLA	CMB-C2B-C3B	2.33	129.03	124.68
19	B	803	CLA	CED-O2D-CGD	2.33	121.20	115.94
19	A	831	CLA	C2A-C1A-CHA	-2.32	119.79	123.86
19	A	825	CLA	CED-O2D-CGD	2.32	121.19	115.94
19	1	307	CLA	CED-O2D-CGD	2.32	121.19	115.94
19	A	816	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
19	B	827	CLA	CHD-C4C-NC	2.32	127.86	124.20
19	A	816	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
19	B	831	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
19	4	304	CLA	C5-C3-C4	2.32	119.73	114.60
19	5	212	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	B	840	BCR	C27-C26-C25	2.32	126.10	122.73
19	B	828	CLA	CED-O2D-CGD	2.32	121.19	115.94
19	B	819	CLA	CED-O2D-CGD	2.32	121.19	115.94
19	B	831	CLA	CAC-C3C-C4C	2.32	127.82	124.81
19	A	810	CLA	C4-C3-C5	2.32	119.17	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	205	CLA	CAA-C2A-C1A	-2.32	104.38	111.97
19	B	831	CLA	C2A-C1A-CHA	-2.32	119.81	123.86
19	B	819	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
19	B	831	CLA	O2A-CGA-CBA	2.32	119.18	111.91
23	3	215	LHG	C11-C10-C9	-2.32	102.67	114.42
19	B	818	CLA	CBC-CAC-C3C	-2.31	106.05	112.43
19	2	215	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
19	A	817	CLA	CED-O2D-CGD	2.31	121.16	115.94
19	A	831	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
19	4	301	CLA	C2A-C1A-CHA	-2.31	119.83	123.86
19	4	309	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
19	A	803	CLA	C1-C2-C3	-2.31	122.06	126.04
18	A	801	CL0	C1-C2-C3	-2.31	122.06	126.04
19	1	303	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
19	5	212	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
19	A	838	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
19	B	813	CLA	C4-C3-C5	2.30	119.15	115.27
19	u	202	CLA	CMC-C2C-C1C	2.30	128.55	125.04
19	A	878	CLA	CHA-C1A-NA	-2.30	121.13	126.40
28	5	218	DD6	C23-C16-C17	-2.30	104.98	108.98
19	2	215	CLA	CMC-C2C-C1C	2.30	128.54	125.04
19	A	807	CLA	CAC-C3C-C4C	2.30	127.80	124.81
19	A	841	CLA	C6-C7-C8	-2.30	108.48	115.92
19	B	834	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
19	A	806	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
19	4	312	CLA	CMC-C2C-C1C	2.30	128.54	125.04
19	A	818	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
19	F	204	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
19	F	204	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
19	B	846	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
19	B	832	CLA	CAC-C3C-C4C	2.30	127.79	124.81
19	A	820	CLA	CED-O2D-CGD	2.30	121.13	115.94
19	5	210	CLA	CMB-C2B-C3B	2.30	128.97	124.68
19	A	812	CLA	C1-O2A-CGA	2.29	122.47	116.44
22	I	102	BCR	C3-C4-C5	-2.29	109.98	114.08
19	B	814	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
19	A	839	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
31	3	228	A86	C26-C25-C24	-2.29	116.06	123.22
19	A	842	CLA	C1-C2-C3	-2.29	122.08	126.04
19	5	211	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
19	2	210	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
19	5	216	CLA	O2D-CGD-O1D	-2.29	119.36	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	830	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
19	1	308	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
19	3	210	CLA	CMB-C2B-C3B	2.29	128.96	124.68
19	A	834	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
30	3	211	KC1	C2A-C1A-CHA	-2.29	119.88	127.44
30	3	211	KC1	CED-O2D-CGD	2.29	121.11	115.94
19	3	206	CLA	CMA-C3A-C4A	-2.29	105.63	111.77
30	1	305	KC1	CHB-C1B-NB	-2.29	122.35	124.45
19	3	203	CLA	C4-C3-C5	2.29	119.11	115.27
19	2	210	CLA	CBC-CAC-C3C	-2.28	106.13	112.43
19	A	841	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
19	A	831	CLA	CHD-C4C-NC	2.28	127.80	124.20
19	5	213	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
31	2	219	A86	C7-C6-C8	2.28	121.67	118.08
19	B	811	CLA	CAC-C3C-C4C	2.28	127.77	124.81
24	2	220	LMT	C3'-C4'-C5'	-2.28	105.69	110.93
19	5	216	CLA	CAA-C2A-C3A	-2.28	108.56	114.26
19	B	805	CLA	CHB-C4A-NA	2.28	127.67	124.51
30	4	302	KC1	C2A-C1A-CHA	-2.28	119.90	127.44
19	A	803	CLA	CMC-C2C-C1C	2.28	128.51	125.04
19	A	828	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
19	2	205	CLA	CBC-CAC-C3C	-2.28	106.15	112.43
31	1	317	A86	C3-C4-C5	-2.28	118.81	123.47
19	A	819	CLA	CMC-C2C-C1C	2.28	128.51	125.04
19	3	206	CLA	C1-O2A-CGA	2.28	122.42	116.44
19	4	305	CLA	CMC-C2C-C1C	2.28	128.51	125.04
19	B	819	CLA	CMA-C3A-C4A	-2.28	105.66	111.77
19	B	829	CLA	C3B-C4B-NB	2.27	112.15	109.21
31	3	214	A86	C9-C10-C11	-2.27	119.92	126.61
19	A	802	CLA	C1-C2-C3	-2.27	122.11	126.04
19	B	831	CLA	CHB-C4A-NA	2.27	127.66	124.51
19	B	811	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
19	A	810	CLA	C2A-C1A-CHA	-2.27	119.88	123.86
29	1	302	LMG	O6-C1-O1	-2.27	104.59	109.97
19	B	836	CLA	CMC-C2C-C1C	2.27	128.50	125.04
22	A	850	BCR	C11-C10-C9	-2.27	124.07	127.31
19	B	811	CLA	O2A-CGA-CBA	2.27	119.03	111.91
19	F	204	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
19	A	831	CLA	CMA-C3A-C2A	-2.27	104.67	113.83
19	A	805	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
19	3	209	CLA	CMB-C2B-C3B	2.27	128.92	124.68
19	3	209	CLA	CHB-C4A-NA	2.27	127.65	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	207	CLA	O1D-CGD-CBD	-2.27	119.85	124.48
27	J	105	5X6	C42-C13-C12	-2.27	114.51	118.08
19	B	802	CLA	CHB-C4A-NA	2.27	127.65	124.51
19	1	304	CLA	C2A-C1A-CHA	-2.27	119.90	123.86
19	5	209	CLA	CAA-C2A-C3A	-2.27	106.58	112.78
22	B	843	BCR	C33-C5-C6	-2.26	121.98	124.53
19	A	805	CLA	CAC-C3C-C4C	2.26	127.75	124.81
19	4	306	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
19	4	305	CLA	C1-O2A-CGA	2.26	122.38	116.44
19	B	836	CLA	CHD-C4C-NC	2.26	127.77	124.20
19	B	831	CLA	C11-C10-C8	-2.26	108.61	115.92
30	3	208	KC1	O2A-CGA-O1A	-2.26	117.97	122.67
19	1	301	CLA	CMB-C2B-C3B	2.26	128.91	124.68
31	4	314	A86	C24-C1-C2	-2.26	115.47	118.94
19	A	803	CLA	CBC-CAC-C3C	-2.26	106.20	112.43
23	1	318	LHG	C18-C17-C16	-2.26	102.95	114.42
22	B	843	BCR	C35-C13-C14	-2.26	119.76	122.92
19	5	210	CLA	CHB-C4A-NA	2.26	127.63	124.51
19	A	812	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
19	B	809	CLA	O2A-CGA-CBA	2.25	118.98	111.91
19	A	814	CLA	O2A-CGA-CBA	2.25	118.98	111.91
19	B	835	CLA	CMB-C2B-C3B	2.25	128.90	124.68
19	B	823	CLA	C4-C3-C2	-2.25	117.90	123.68
19	A	823	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
27	J	105	5X6	C04-C03-C11	2.25	122.15	115.78
31	5	219	A86	C10-C9-C8	-2.25	116.19	123.22
19	A	843	CLA	C4-C3-C2	-2.25	117.90	123.68
19	B	845	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
28	1	315	DD6	C10-C9-C8	-2.25	116.19	123.22
19	A	819	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
22	B	844	BCR	C33-C5-C6	-2.25	122.00	124.53
31	5	217	A86	C40-C32-C31	-2.25	108.46	110.47
22	B	841	BCR	C15-C14-C13	-2.25	124.10	127.31
23	A	852	LHG	C27-C26-C25	-2.25	103.01	114.42
19	B	827	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
24	A	854	LMT	C1'-C2'-C3'	2.25	114.68	110.00
23	M	103	LHG	C20-C19-C18	-2.25	103.02	114.42
18	A	801	CL0	CHB-C4A-NA	2.25	127.62	124.51
19	3	207	CLA	O1D-CGD-CBD	-2.25	119.89	124.48
19	2	212	CLA	CAC-C3C-C4C	2.25	127.72	124.81
23	A	852	LHG	C18-C17-C16	-2.24	103.03	114.42
19	A	827	CLA	CHB-C4A-NA	2.24	127.61	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	205	KC1	CHB-C1B-NB	-2.24	122.39	124.45
19	A	802	CLA	CHA-C1A-NA	-2.24	121.26	126.40
23	4	317	LHG	C27-C26-C25	-2.24	103.04	114.42
19	B	836	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
22	1	314	BCR	C35-C13-C14	-2.24	119.78	122.92
19	L	203	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
23	4	317	LHG	C20-C19-C18	-2.24	103.05	114.42
19	A	828	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
24	2	220	LMT	C1'-O5'-C5'	-2.24	109.29	113.69
19	B	807	CLA	C1-C2-C3	-2.24	122.17	126.04
22	I	102	BCR	C2-C1-C6	2.24	113.93	110.48
19	A	841	CLA	CHB-C4A-NA	2.24	127.61	124.51
19	A	842	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
23	A	853	LHG	C5-O7-C7	-2.24	112.28	117.79
19	3	210	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
19	1	304	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	I	102	BCR	C11-C10-C9	-2.24	124.12	127.31
19	A	836	CLA	C2A-C1A-CHA	-2.24	119.95	123.86
19	A	822	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
22	B	843	BCR	C27-C26-C25	2.24	125.98	122.73
19	F	203	CLA	C4-C3-C5	2.23	119.03	115.27
22	B	852	BCR	C16-C15-C14	-2.23	118.90	123.47
28	2	217	DD6	C10-C9-C8	-2.23	116.25	123.22
19	A	838	CLA	CMC-C2C-C1C	2.23	128.44	125.04
19	4	313	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
19	A	838	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
22	B	843	BCR	C21-C20-C19	-2.23	116.26	123.22
24	3	216	LMT	C3'-C4'-C5'	-2.23	105.82	110.93
19	B	815	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
19	J	103	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
22	A	850	BCR	C20-C21-C22	-2.23	124.13	127.31
19	B	828	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
19	5	216	CLA	CMC-C2C-C1C	2.23	128.43	125.04
19	B	837	CLA	CBC-CAC-C3C	-2.23	106.30	112.43
19	B	822	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
19	1	309	CLA	CHB-C4A-NA	2.23	127.59	124.51
19	5	210	CLA	CGD-CBD-CAD	-2.22	103.53	110.73
19	B	838	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
19	J	103	CLA	CMB-C2B-C3B	2.22	128.84	124.68
22	A	849	BCR	C33-C5-C6	-2.22	122.03	124.53
19	A	813	CLA	CBC-CAC-C3C	-2.22	106.30	112.43
26	B	847	DGD	O2G-C1B-O1B	-2.22	118.33	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	836	CLA	CMB-C2B-C3B	2.22	128.84	124.68
19	B	821	CLA	CMA-C3A-C2A	-2.22	104.87	113.83
19	2	213	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
19	B	819	CLA	CHB-C4A-NA	2.22	127.58	124.51
19	A	837	CLA	O2A-CGA-CBA	2.22	121.16	114.03
19	B	817	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
19	2	208	CLA	CHB-C4A-NA	2.22	127.58	124.51
19	B	828	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
19	F	204	CLA	CMB-C2B-C3B	2.22	128.83	124.68
19	B	826	CLA	CMC-C2C-C1C	2.22	128.41	125.04
19	A	815	CLA	CMB-C2B-C3B	2.22	128.82	124.68
19	B	838	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
19	A	814	CLA	CHB-C4A-NA	2.22	127.58	124.51
19	1	303	CLA	CMC-C2C-C1C	2.22	128.41	125.04
22	B	852	BCR	C28-C27-C26	-2.22	110.12	114.08
19	B	823	CLA	CHB-C4A-NA	2.22	127.58	124.51
19	A	880	CLA	C4-C3-C5	2.21	119.00	115.27
19	5	209	CLA	CMC-C2C-C1C	2.21	128.41	125.04
19	2	209	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
30	4	307	KC1	CED-O2D-CGD	2.21	120.94	115.94
19	A	844	CLA	CMC-C2C-C1C	2.21	128.41	125.04
19	4	305	CLA	CHB-C4A-NA	2.21	127.57	124.51
19	3	207	CLA	C4-C3-C5	2.21	118.99	115.27
19	B	821	CLA	CBC-CAC-C3C	-2.21	106.33	112.43
19	1	301	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
19	B	824	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
19	B	807	CLA	C2A-C1A-CHA	-2.21	120.00	123.86
19	B	804	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
19	A	808	CLA	CMB-C2B-C3B	2.21	128.81	124.68
19	B	837	CLA	CMB-C2B-C3B	2.21	128.81	124.68
19	A	822	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
22	A	849	BCR	C15-C16-C17	-2.21	118.95	123.47
19	A	835	CLA	C2A-C1A-CHA	-2.21	120.00	123.86
22	L	202	BCR	C27-C26-C25	2.21	125.94	122.73
19	A	836	CLA	CHB-C4A-NA	2.21	127.56	124.51
19	A	833	CLA	CMB-C2B-C3B	2.20	128.80	124.68
19	A	815	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
19	4	305	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
19	B	825	CLA	CED-O2D-CGD	2.20	120.92	115.94
19	A	807	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
19	B	826	CLA	CED-O2D-CGD	2.20	120.92	115.94
19	B	828	CLA	O1D-CGD-CBD	-2.20	119.98	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	802	CLA	CAC-C3C-C4C	2.20	127.67	124.81
19	B	820	CLA	CMC-C2C-C1C	2.20	128.39	125.04
19	A	822	CLA	O2A-CGA-CBA	2.20	118.81	111.91
30	1	305	KC1	CMC-C2C-C1C	2.20	128.39	125.04
22	1	314	BCR	C27-C26-C25	2.20	125.92	122.73
19	2	210	CLA	C4-C3-C5	2.20	118.97	115.27
19	B	823	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
27	J	105	5X6	C10-C04-C03	2.20	113.86	110.30
19	L	203	CLA	C4-C3-C5	2.20	118.97	115.27
19	B	832	CLA	CMC-C2C-C1C	2.20	128.38	125.04
19	A	844	CLA	C2A-C1A-CHA	-2.20	120.02	123.86
19	A	826	CLA	C4-C3-C5	2.20	118.97	115.27
19	3	204	CLA	O2A-CGA-CBA	2.19	118.80	111.91
19	A	822	CLA	CBC-CAC-C3C	-2.19	106.38	112.43
19	A	820	CLA	C2A-C3A-C4A	-2.19	98.33	101.87
19	5	212	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
19	B	807	CLA	C4-C3-C5	2.19	118.96	115.27
19	5	212	CLA	O2A-C1-C2	2.19	114.40	108.64
19	A	816	CLA	CMC-C2C-C1C	2.19	128.38	125.04
19	4	301	CLA	C4-C3-C5	2.19	118.96	115.27
19	2	213	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
31	5	219	A86	C19-C18-C17	-2.19	106.54	110.77
19	B	808	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
31	4	316	A86	C12-C11-C13	2.19	119.70	116.02
19	B	817	CLA	CED-O2D-CGD	2.19	120.89	115.94
31	4	314	A86	C25-C26-C27	-2.19	124.19	127.31
30	2	211	KC1	O2D-CGD-O1D	-2.19	119.56	123.84
19	B	816	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
19	4	303	CLA	CMB-C2B-C3B	2.19	128.77	124.68
19	A	836	CLA	CMC-C2C-C1C	2.19	128.37	125.04
19	4	313	CLA	CMC-C2C-C1C	2.19	128.37	125.04
31	5	217	A86	C23-C16-C22	-2.19	104.15	107.37
19	4	308	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
19	B	833	CLA	CAC-C3C-C4C	2.18	127.64	124.81
19	4	306	CLA	CAC-C3C-C4C	2.18	127.64	124.81
31	4	315	A86	C-C1-C24	2.18	121.52	118.08
19	B	813	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
19	A	825	CLA	C2A-C1A-CHA	-2.18	120.04	123.86
23	3	215	LHG	C27-C26-C25	-2.18	103.35	114.42
19	A	832	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
19	A	821	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
19	B	819	CLA	CBC-CAC-C3C	-2.18	106.42	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	802	CLA	CHD-C4C-NC	2.18	127.64	124.20
19	A	816	CLA	CHB-C4A-NA	2.18	127.53	124.51
19	4	312	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
19	A	805	CLA	CMB-C2B-C3B	2.18	128.75	124.68
19	2	212	CLA	CHB-C4A-NA	2.18	127.52	124.51
19	A	880	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
23	A	853	LHG	C27-C26-C25	-2.18	103.37	114.42
22	1	314	BCR	C33-C5-C6	-2.18	122.08	124.53
19	B	822	CLA	CMB-C2B-C3B	2.17	128.75	124.68
19	B	819	CLA	CAA-C2A-C3A	-2.17	106.82	112.78
19	B	823	CLA	CAA-C2A-C1A	-2.17	104.85	111.97
19	1	309	CLA	C2A-C1A-CHA	-2.17	120.06	123.86
19	A	806	CLA	O2A-CGA-CBA	2.17	118.73	111.91
19	A	835	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
19	5	207	CLA	C1-C2-C3	-2.17	122.28	126.04
19	A	878	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
30	2	211	KC1	CHB-C4A-NA	2.17	127.63	124.20
19	A	820	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
19	2	215	CLA	CMB-C2B-C3B	2.17	128.74	124.68
19	5	207	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
30	3	208	KC1	C2A-C1A-CHA	-2.17	120.27	127.44
19	4	312	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
19	A	836	CLA	CED-O2D-CGD	2.17	120.84	115.94
19	u	202	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
19	2	208	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
19	2	215	CLA	CHB-C4A-NA	2.17	127.51	124.51
19	B	802	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
19	B	828	CLA	CBC-CAC-C3C	-2.16	106.46	112.43
19	4	306	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
19	B	808	CLA	CMB-C2B-C3B	2.16	128.72	124.68
19	5	211	CLA	CMB-C2B-C3B	2.16	128.72	124.68
19	4	311	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
19	A	802	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
22	A	851	BCR	C10-C11-C12	-2.16	116.47	123.22
22	B	852	BCR	C27-C26-C25	2.16	125.87	122.73
19	B	827	CLA	CBC-CAC-C3C	-2.16	106.47	112.43
19	A	814	CLA	CMB-C2B-C3B	2.16	128.72	124.68
19	B	836	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
31	2	218	A86	C19-C18-C17	-2.16	106.60	110.77
19	B	822	CLA	O2A-CGA-CBA	2.16	118.69	111.91
19	5	215	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
19	5	216	CLA	CHB-C4A-NA	2.16	127.50	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	829	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
19	B	833	CLA	C2A-C1A-CHA	-2.16	120.09	123.86
19	B	846	CLA	C2A-C1A-CHA	-2.15	120.09	123.86
31	1	316	A86	C25-C24-C1	-2.15	120.36	126.42
19	A	813	CLA	C1-O2A-CGA	2.15	122.10	116.44
19	B	828	CLA	C2A-C1A-CHA	-2.15	120.09	123.86
22	A	851	BCR	C35-C13-C12	2.15	121.47	118.08
19	A	804	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
19	B	819	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
19	A	804	CLA	CBC-CAC-C3C	-2.15	106.50	112.43
19	B	824	CLA	OBD-CAD-C3D	-2.15	123.34	128.52
19	3	202	CLA	CMB-C2B-C3B	2.15	128.70	124.68
19	2	215	CLA	CED-O2D-CGD	2.15	120.80	115.94
18	A	801	CL0	C1-O2A-CGA	2.15	122.08	116.44
19	4	308	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
19	2	207	CLA	C4-C3-C5	2.15	118.89	115.27
19	2	206	CLA	O2A-CGA-CBA	2.15	118.65	111.91
30	3	208	KC1	CHB-C1B-NB	-2.15	122.48	124.45
18	A	801	CL0	CGD-CBD-CAD	-2.15	103.78	110.73
19	A	821	CLA	C1-C2-C3	-2.15	122.33	126.04
22	B	843	BCR	C29-C30-C25	2.14	113.78	110.48
19	A	804	CLA	CAA-C2A-C3A	-2.14	106.91	112.78
19	B	803	CLA	CMC-C2C-C1C	2.14	128.30	125.04
19	B	821	CLA	CMC-C2C-C1C	2.14	128.30	125.04
19	u	201	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
29	1	302	LMG	O3-C3-C2	-2.14	105.39	110.35
19	2	215	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
19	3	206	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
19	J	103	CLA	CMC-C2C-C1C	2.14	128.30	125.04
19	2	215	CLA	CAA-C2A-C3A	-2.14	108.91	114.26
19	1	310	CLA	C1-C2-C3	-2.14	122.34	126.04
19	A	820	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
30	3	205	KC1	O2D-CGD-O1D	-2.14	119.65	123.84
19	5	209	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
19	4	304	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
19	5	208	CLA	C1-C2-C3	-2.14	122.34	126.04
31	4	316	A86	C20-C19-C18	-2.14	108.52	112.75
19	A	831	CLA	CMB-C2B-C3B	2.14	128.68	124.68
19	A	819	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
19	A	833	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
28	1	312	DD6	C40-C32-C31	-2.14	107.07	110.47
19	A	833	CLA	O2D-CGD-O1D	-2.14	119.66	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	825	CLA	CHB-C4A-NA	2.14	127.47	124.51
19	4	305	CLA	CED-O2D-CGD	2.14	120.77	115.94
19	u	201	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
19	A	812	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
19	B	826	CLA	CHB-C4A-NA	2.14	127.47	124.51
20	A	845	PQN	C11-C3-C4	-2.14	116.22	118.50
19	A	810	CLA	CAA-CBA-CGA	-2.14	107.01	113.25
19	5	216	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
19	2	210	CLA	O2A-CGA-CBA	2.13	118.61	111.91
19	4	301	CLA	CMC-C2C-C1C	2.13	128.29	125.04
19	4	301	CLA	C11-C12-C13	-2.13	109.02	115.92
19	A	805	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
31	3	214	A86	C25-C24-C1	-2.13	120.42	126.42
19	A	806	CLA	CMB-C2B-C3B	2.13	128.67	124.68
19	1	309	CLA	C4-C3-C5	2.13	118.86	115.27
19	2	209	CLA	CMB-C2B-C3B	2.13	128.67	124.68
22	A	847	BCR	C27-C26-C25	2.13	125.83	122.73
19	2	215	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
19	A	832	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
30	2	211	KC1	CAC-C3C-C4C	2.13	127.57	124.81
19	B	810	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
19	1	304	CLA	CMB-C2B-C3B	2.13	128.66	124.68
22	B	852	BCR	C33-C5-C6	-2.13	122.14	124.53
22	I	101	BCR	C33-C5-C6	-2.13	122.14	124.53
19	A	815	CLA	CHB-C4A-NA	2.13	127.46	124.51
19	A	822	CLA	CMA-C3A-C4A	-2.13	106.05	111.77
19	A	836	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
19	2	214	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
19	B	809	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
19	A	826	CLA	CMB-C2B-C3B	2.13	128.66	124.68
19	1	307	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
19	B	835	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
19	B	813	CLA	CHB-C4A-NA	2.13	127.45	124.51
19	1	303	CLA	C4-C3-C5	2.13	118.85	115.27
19	5	207	CLA	C1-O2A-CGA	2.13	122.02	116.44
30	1	305	KC1	C2A-C1A-CHA	-2.12	120.42	127.44
19	5	214	CLA	CMC-C2C-C1C	2.12	128.27	125.04
19	A	814	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
19	B	845	CLA	C1-C2-C3	-2.12	122.37	126.04
19	3	207	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
19	2	212	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
19	B	819	CLA	CAC-C3C-C4C	2.12	127.56	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	313	DD6	C40-C32-C31	-2.12	107.10	110.47
22	M	102	BCR	C24-C23-C22	-2.12	123.03	126.23
19	A	830	CLA	CMA-C3A-C2A	-2.12	105.28	113.83
22	F	205	BCR	C38-C26-C25	-2.12	122.15	124.53
19	A	836	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
30	3	211	KC1	O2D-CGD-O1D	-2.12	119.70	123.84
19	2	213	CLA	CHB-C4A-NA	2.12	127.44	124.51
19	A	807	CLA	C2A-C1A-CHA	-2.12	120.16	123.86
19	F	203	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
22	I	102	BCR	C33-C5-C6	-2.12	122.15	124.53
19	A	834	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
19	3	202	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
19	4	311	CLA	CMC-C2C-C1C	2.12	128.26	125.04
19	A	828	CLA	OBD-CAD-C3D	-2.11	123.43	128.52
22	F	201	BCR	C38-C26-C27	-2.11	109.55	113.62
19	A	813	CLA	C2A-C1A-CHA	-2.11	120.16	123.86
30	3	211	KC1	CHB-C1B-NB	-2.11	122.51	124.45
31	4	315	A86	C7-C6-C8	2.11	121.41	118.08
27	J	105	5X6	C39-C26-C27	-2.11	114.75	118.08
19	B	812	CLA	CHB-C4A-NA	2.11	127.43	124.51
19	A	813	CLA	CHB-C4A-NA	2.11	127.43	124.51
19	B	827	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
19	B	821	CLA	CHB-C4A-NA	2.11	127.43	124.51
19	1	303	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
19	A	810	CLA	CMC-C2C-C1C	2.11	128.25	125.04
19	A	816	CLA	C5-C3-C4	2.11	119.25	114.60
19	B	802	CLA	C1B-CHB-C4A	-2.11	125.95	130.12
19	B	838	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
19	1	304	CLA	CAC-C3C-C4C	2.10	127.54	124.81
19	A	841	CLA	CMB-C2B-C3B	2.10	128.61	124.68
19	1	309	CLA	C3B-C4B-NB	2.10	111.93	109.21
19	A	814	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
31	5	217	A86	O1-C15-C14	-2.10	108.99	113.21
19	A	821	CLA	CHB-C4A-NA	2.10	127.42	124.51
19	B	825	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
19	4	301	CLA	C16-C15-C13	-2.10	109.13	115.92
19	B	825	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
22	B	840	BCR	C33-C5-C6	-2.10	122.17	124.53
19	2	208	CLA	CMC-C2C-C1C	2.10	128.23	125.04
19	B	812	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
19	A	827	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
19	B	815	CLA	CMC-C2C-C1C	2.10	128.23	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	837	CLA	CHB-C4A-NA	2.10	127.41	124.51
19	2	213	CLA	CED-O2D-CGD	2.10	120.68	115.94
19	1	301	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
23	B	842	LHG	C27-C26-C25	-2.10	103.79	114.42
19	3	202	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
30	4	307	KC1	CHC-C4B-NB	-2.09	122.53	124.45
19	L	204	CLA	CMB-C2B-C3B	2.09	128.60	124.68
19	A	880	CLA	C11-C10-C8	-2.09	109.15	115.92
22	F	201	BCR	C33-C5-C6	-2.09	122.18	124.53
19	5	211	CLA	O2A-CGA-CBA	2.09	118.48	111.91
19	5	207	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
19	A	825	CLA	CMB-C2B-C3B	2.09	128.59	124.68
19	4	310	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
19	B	817	CLA	CHB-C4A-NA	2.09	127.41	124.51
30	1	305	KC1	CMB-C2B-C1B	2.09	128.40	124.71
19	A	844	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
31	2	216	A86	C40-C32-C31	-2.09	108.60	110.47
19	4	306	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
19	A	810	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
18	A	801	CL0	O2A-CGA-O1A	-2.09	118.32	123.59
19	B	825	CLA	C11-C12-C13	-2.09	109.17	115.92
19	A	828	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
19	3	210	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
22	A	850	BCR	C28-C27-C26	-2.09	110.35	114.08
31	5	221	A86	C20-C19-C18	-2.09	108.62	112.75
19	1	303	CLA	O2D-CGD-O1D	-2.09	119.76	123.84
19	1	309	CLA	CED-O2D-CGD	2.09	120.65	115.94
19	A	827	CLA	CMB-C2B-C3B	2.09	128.58	124.68
19	A	842	CLA	C2A-C1A-CHA	-2.08	120.21	123.86
19	A	829	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
19	2	205	CLA	CED-O2D-CGD	2.08	120.65	115.94
19	A	811	CLA	CMB-C2B-C3B	2.08	128.57	124.68
19	5	212	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
19	B	829	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
19	A	836	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
31	3	228	A86	O1-C15-C14	-2.08	109.04	113.21
23	M	103	LHG	C27-C26-C25	-2.08	103.87	114.42
19	A	878	CLA	CBC-CAC-C3C	-2.08	106.70	112.43
19	B	808	CLA	C2A-C1A-CHA	-2.08	120.23	123.86
19	B	831	CLA	CMA-C3A-C2A	-2.08	105.45	113.83
19	A	833	CLA	O2A-CGA-CBA	2.08	118.42	111.91
22	B	841	BCR	C11-C10-C9	-2.07	124.35	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	823	CLA	CBC-CAC-C3C	-2.07	106.71	112.43
19	B	813	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
19	A	804	CLA	C4-C3-C5	2.07	118.76	115.27
22	L	202	BCR	C33-C5-C6	-2.07	122.20	124.53
19	A	812	CLA	CMB-C2B-C3B	2.07	128.55	124.68
19	B	817	CLA	CMC-C2C-C1C	2.07	128.19	125.04
19	A	841	CLA	CMA-C3A-C4A	-2.07	106.22	111.77
29	1	302	LMG	O2-C2-C1	-2.07	105.03	110.05
30	4	302	KC1	O1D-CGD-CBD	-2.07	120.26	124.48
31	2	218	A86	C24-C1-C2	-2.07	115.77	118.94
19	B	820	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
19	B	826	CLA	CAA-CBA-CGA	2.06	119.28	113.25
19	A	809	CLA	CHB-C4A-NA	2.06	127.36	124.51
19	B	837	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
28	1	312	DD6	C23-C16-C15	-2.06	104.48	110.05
19	5	208	CLA	C7-C6-C5	-2.06	107.76	113.36
18	A	801	CL0	C4-C3-C5	2.06	118.74	115.27
31	3	212	A86	C22-C16-C17	-2.06	105.40	108.98
19	A	880	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
19	A	823	CLA	CHB-C4A-NA	2.06	127.36	124.51
19	4	304	CLA	C2A-C3A-C4A	-2.06	98.54	101.87
19	B	830	CLA	CHB-C4A-NA	2.06	127.36	124.51
19	J	103	CLA	CHB-C4A-NA	2.06	127.36	124.51
19	2	209	CLA	CED-O2D-CGD	2.06	120.59	115.94
28	1	313	DD6	C3-C4-C5	-2.06	119.26	123.47
19	B	835	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
19	5	210	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
19	B	826	CLA	C4-C3-C5	2.06	118.73	115.27
26	B	847	DGD	C5B-C4B-C3B	-2.06	103.99	114.42
19	B	815	CLA	CMB-C2B-C3B	2.06	128.52	124.68
31	3	214	A86	C8-C6-C5	2.06	122.09	118.94
19	A	819	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
19	A	820	CLA	O2A-C1-C2	2.05	114.03	108.64
19	A	842	CLA	CMC-C2C-C1C	2.05	128.17	125.04
19	B	820	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
30	4	302	KC1	CHB-C4A-NA	2.05	127.44	124.20
19	A	804	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
19	A	829	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
19	A	843	CLA	CMA-C3A-C2A	-2.05	105.54	113.83
31	1	316	A86	C-C1-C2	-2.05	120.05	122.92
22	B	841	BCR	C8-C7-C6	-2.05	121.44	127.20
19	B	806	CLA	O2A-CGA-O1A	-2.05	118.41	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	216	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
19	A	832	CLA	CHB-C4A-NA	2.05	127.35	124.51
19	3	206	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
19	2	214	CLA	CMC-C2C-C1C	2.05	128.16	125.04
19	4	305	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
19	A	844	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
26	B	847	DGD	C3D-C4D-C5D	-2.05	106.58	110.24
19	5	215	CLA	CHB-C4A-NA	2.05	127.35	124.51
29	1	302	LMG	C42-C41-C40	-2.05	104.02	114.42
19	4	311	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
19	u	202	CLA	CHB-C4A-NA	2.05	127.34	124.51
19	A	833	CLA	CHB-C4A-NA	2.05	127.34	124.51
19	A	829	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
19	2	209	CLA	CBC-CAC-C3C	-2.05	106.79	112.43
19	5	213	CLA	CED-O2D-CGD	2.05	120.57	115.94
19	A	880	CLA	O2D-CGD-O1D	-2.05	119.84	123.84
19	1	309	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
19	B	831	CLA	C11-C12-C13	-2.05	109.31	115.92
19	A	840	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
30	2	211	KC1	CHB-C1B-C2B	-2.04	121.19	125.48
28	5	218	DD6	C21-C20-C19	-2.04	111.98	114.28
26	B	847	DGD	CFB-CEB-CDB	-2.04	104.05	114.42
31	4	314	A86	C34-O4-C38	-2.04	114.09	117.90
22	I	101	BCR	C8-C7-C6	-2.04	121.46	127.20
22	B	840	BCR	C15-C16-C17	-2.04	119.29	123.47
19	B	814	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
19	A	816	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
19	A	828	CLA	CMC-C2C-C1C	2.04	128.15	125.04
19	3	209	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
28	5	218	DD6	C33-C32-C31	2.04	113.76	109.62
19	B	809	CLA	C1-O2A-CGA	2.04	121.80	116.44
19	A	842	CLA	CHB-C4A-NA	2.04	127.33	124.51
19	L	206	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
19	A	827	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
19	B	838	CLA	CMB-C2B-C3B	2.04	128.49	124.68
22	A	849	BCR	C8-C7-C6	-2.04	121.48	127.20
19	1	306	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
19	A	841	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
19	1	309	CLA	CBA-CAA-C2A	2.04	119.88	113.86
22	1	314	BCR	C2-C1-C6	2.04	113.62	110.48
19	B	819	CLA	CMC-C2C-C1C	2.04	128.14	125.04
22	A	850	BCR	C27-C26-C25	2.04	125.69	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	831	CLA	CMA-C3A-C4A	-2.04	106.30	111.77
19	B	837	CLA	CMA-C3A-C4A	-2.03	106.30	111.77
31	5	219	A86	C40-C32-C31	-2.03	108.65	110.47
19	A	834	CLA	O2D-CGD-O1D	-2.03	119.86	123.84
19	B	804	CLA	C2A-C1A-CHA	-2.03	120.30	123.86
31	2	216	A86	O1-C15-C14	-2.03	109.13	113.21
19	A	818	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
19	L	206	CLA	CHB-C4A-NA	2.03	127.32	124.51
19	A	806	CLA	O2A-C1-C2	2.03	113.97	108.64
19	u	202	CLA	O2A-CGA-CBA	2.03	120.55	114.03
19	A	805	CLA	C2A-C1A-CHA	-2.03	120.31	123.86
19	B	816	CLA	CHB-C4A-NA	2.03	127.32	124.51
19	B	846	CLA	CHB-C4A-NA	2.03	127.32	124.51
19	A	842	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
19	B	806	CLA	C2A-C1A-CHA	-2.03	120.32	123.86
19	3	204	CLA	C11-C12-C13	-2.03	109.37	115.92
30	2	211	KC1	C2A-C1A-CHA	-2.03	120.74	127.44
31	4	315	A86	C4-C3-C2	-2.02	119.33	123.47
22	F	205	BCR	C35-C13-C14	-2.02	120.09	122.92
22	B	844	BCR	C10-C11-C12	-2.02	116.91	123.22
19	A	816	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
31	5	220	A86	C7-C6-C5	-2.02	120.09	122.92
19	A	804	CLA	CMA-C3A-C4A	-2.02	106.35	111.77
31	2	219	A86	O1-C15-C14	-2.02	109.16	113.21
22	A	848	BCR	C27-C26-C25	2.02	125.66	122.73
19	2	213	CLA	O2A-CGA-CBA	2.02	120.51	114.03
19	B	809	CLA	CMB-C2B-C3B	2.02	128.45	124.68
19	A	824	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
22	I	102	BCR	C27-C26-C25	2.02	125.66	122.73
19	2	207	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
19	B	806	CLA	CHB-C4A-NA	2.01	127.30	124.51
30	3	205	KC1	O2A-CGA-O1A	-2.01	118.48	122.67
19	3	203	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
30	3	211	KC1	O2A-CGA-O1A	-2.01	118.48	122.67
26	B	847	DGD	CAB-C9B-C8B	-2.01	104.20	114.42
19	A	814	CLA	CED-O2D-CGD	2.01	120.49	115.94
19	1	306	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
19	4	311	CLA	CED-O2D-CGD	2.01	120.49	115.94
19	B	832	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
19	2	210	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
19	1	301	CLA	C11-C10-C8	-2.01	109.42	115.92
19	B	812	CLA	O2A-CGA-O1A	-2.01	118.52	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	M	103	LHG	C18-C17-C16	-2.01	104.22	114.42
19	B	832	CLA	CHB-C4A-NA	2.01	127.29	124.51
23	4	317	LHG	C18-C17-C16	-2.01	104.22	114.42
19	L	206	CLA	CMC-C2C-C1C	2.01	128.10	125.04
19	2	207	CLA	CMB-C2B-C3B	2.01	128.44	124.68
19	1	306	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
19	3	202	CLA	CED-O2D-CGD	2.01	120.48	115.94
19	u	201	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
22	A	851	BCR	C2-C1-C6	2.01	113.57	110.48
31	5	217	A86	C24-C1-C2	-2.01	115.86	118.94
30	4	307	KC1	CAB-C3B-C4B	2.00	129.74	124.90
19	B	820	CLA	O1D-CGD-CBD	-2.00	120.38	124.48
19	A	822	CLA	C2A-C1A-CHA	-2.00	120.36	123.86
19	5	212	CLA	C2A-C1A-CHA	-2.00	120.36	123.86
19	B	811	CLA	CMA-C3A-C4A	-2.00	106.39	111.77
19	A	815	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
19	A	807	CLA	O2A-C1-C2	2.00	113.90	108.64
19	B	825	CLA	CHA-C1A-NA	-2.00	121.81	126.40
19	5	208	CLA	C2A-C1A-CHA	-2.00	120.36	123.86

All (129) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	801	CL0	NA
18	A	801	CL0	ND
18	A	801	CL0	NC
19	A	802	CLA	ND
19	A	803	CLA	ND
19	A	804	CLA	ND
19	A	805	CLA	ND
19	A	806	CLA	ND
19	A	807	CLA	ND
19	A	808	CLA	ND
19	A	809	CLA	ND
19	A	810	CLA	ND
19	A	811	CLA	ND
19	A	812	CLA	ND
19	A	813	CLA	ND
19	A	814	CLA	ND
19	A	815	CLA	ND
19	A	816	CLA	ND
19	A	818	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	819	CLA	ND
19	A	820	CLA	ND
19	A	822	CLA	ND
19	A	824	CLA	ND
19	A	825	CLA	ND
19	A	826	CLA	ND
19	A	827	CLA	ND
19	A	828	CLA	ND
19	A	829	CLA	ND
19	A	830	CLA	ND
19	A	831	CLA	ND
19	A	832	CLA	ND
19	A	833	CLA	ND
19	A	834	CLA	ND
19	A	835	CLA	ND
19	A	836	CLA	ND
19	A	837	CLA	ND
19	A	838	CLA	ND
19	A	839	CLA	ND
19	A	840	CLA	ND
19	A	841	CLA	ND
19	A	842	CLA	ND
19	A	843	CLA	ND
19	A	844	CLA	ND
19	A	878	CLA	ND
19	A	880	CLA	ND
19	B	802	CLA	ND
19	B	803	CLA	ND
19	B	804	CLA	ND
19	B	805	CLA	ND
19	B	806	CLA	ND
19	B	807	CLA	ND
19	B	808	CLA	ND
19	B	809	CLA	ND
19	B	810	CLA	ND
19	B	811	CLA	ND
19	B	812	CLA	ND
19	B	813	CLA	ND
19	B	814	CLA	ND
19	B	815	CLA	ND
19	B	816	CLA	ND
19	B	817	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	818	CLA	ND
19	B	819	CLA	ND
19	B	821	CLA	ND
19	B	822	CLA	ND
19	B	823	CLA	ND
19	B	824	CLA	ND
19	B	825	CLA	ND
19	B	826	CLA	ND
19	B	827	CLA	ND
19	B	829	CLA	ND
19	B	830	CLA	ND
19	B	831	CLA	ND
19	B	832	CLA	ND
19	B	833	CLA	ND
19	B	834	CLA	ND
19	B	835	CLA	ND
19	B	836	CLA	ND
19	B	837	CLA	ND
19	B	838	CLA	ND
19	B	846	CLA	ND
19	F	203	CLA	ND
19	F	204	CLA	ND
19	J	103	CLA	ND
19	L	204	CLA	ND
19	L	206	CLA	ND
19	u	201	CLA	ND
19	u	202	CLA	ND
19	1	301	CLA	ND
19	1	303	CLA	ND
19	1	304	CLA	ND
19	1	306	CLA	ND
19	1	307	CLA	ND
19	1	308	CLA	ND
19	1	309	CLA	ND
19	1	310	CLA	ND
19	2	205	CLA	ND
19	2	206	CLA	ND
19	2	207	CLA	ND
19	2	208	CLA	ND
19	2	209	CLA	ND
19	2	210	CLA	ND
19	2	212	CLA	ND

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Mol	Chain	Res	Type	Atom
19	2	213	CLA	ND
19	2	214	CLA	ND
19	2	215	CLA	ND
19	3	202	CLA	ND
19	3	203	CLA	ND
19	3	204	CLA	ND
19	3	206	CLA	ND
19	3	207	CLA	ND
19	3	209	CLA	ND
19	3	210	CLA	ND
19	4	301	CLA	ND
19	4	303	CLA	ND
19	4	304	CLA	ND
19	4	305	CLA	ND
19	4	306	CLA	ND
19	4	311	CLA	ND
19	4	312	CLA	ND
19	4	313	CLA	ND
19	5	207	CLA	ND
19	5	208	CLA	ND
19	5	209	CLA	ND
19	5	210	CLA	ND
19	5	211	CLA	ND
19	5	212	CLA	ND
19	5	213	CLA	ND
19	5	214	CLA	ND

All (1800) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	805	CLA	C3A-C2A-CAA-CBA
19	A	806	CLA	C1A-C2A-CAA-CBA
19	A	806	CLA	C3A-C2A-CAA-CBA
19	A	806	CLA	C2-C1-O2A-CGA
19	A	807	CLA	C1A-C2A-CAA-CBA
19	A	808	CLA	C2-C3-C5-C6
19	A	808	CLA	C4-C3-C5-C6
19	A	813	CLA	C2-C3-C5-C6
19	A	813	CLA	C4-C3-C5-C6
19	A	817	CLA	C1A-C2A-CAA-CBA
19	A	817	CLA	C3A-C2A-CAA-CBA
19	A	817	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	A	817	CLA	CHA-CBD-CGD-O1D
19	A	817	CLA	CHA-CBD-CGD-O2D
19	A	819	CLA	C3A-C2A-CAA-CBA
19	A	820	CLA	C1A-C2A-CAA-CBA
19	A	820	CLA	C3A-C2A-CAA-CBA
19	A	821	CLA	C3A-C2A-CAA-CBA
19	A	821	CLA	C2A-CAA-CBA-CGA
19	A	824	CLA	C2-C3-C5-C6
19	A	824	CLA	C4-C3-C5-C6
19	A	825	CLA	CHA-CBD-CGD-O1D
19	A	825	CLA	CHA-CBD-CGD-O2D
19	A	831	CLA	CHA-CBD-CGD-O1D
19	A	831	CLA	CHA-CBD-CGD-O2D
19	A	835	CLA	CHA-CBD-CGD-O1D
19	A	835	CLA	CHA-CBD-CGD-O2D
19	A	836	CLA	C4-C3-C5-C6
19	A	837	CLA	CHA-CBD-CGD-O1D
19	A	837	CLA	CHA-CBD-CGD-O2D
19	A	841	CLA	CHA-CBD-CGD-O1D
19	A	841	CLA	CHA-CBD-CGD-O2D
19	A	842	CLA	C4-C3-C5-C6
19	A	878	CLA	C2-C3-C5-C6
19	A	878	CLA	C4-C3-C5-C6
19	B	802	CLA	CHA-CBD-CGD-O1D
19	B	805	CLA	C3A-C2A-CAA-CBA
19	B	806	CLA	C2-C3-C5-C6
19	B	806	CLA	C4-C3-C5-C6
19	B	808	CLA	CHA-CBD-CGD-O2D
19	B	811	CLA	C14-C13-C15-C16
19	B	815	CLA	CHA-CBD-CGD-O1D
19	B	815	CLA	CHA-CBD-CGD-O2D
19	B	816	CLA	C1A-C2A-CAA-CBA
19	B	816	CLA	C3A-C2A-CAA-CBA
19	B	816	CLA	C2-C3-C5-C6
19	B	816	CLA	C4-C3-C5-C6
19	B	821	CLA	C3A-C2A-CAA-CBA
19	B	823	CLA	CHA-CBD-CGD-O2D
19	B	827	CLA	CHA-CBD-CGD-O1D
19	B	827	CLA	CHA-CBD-CGD-O2D
19	B	832	CLA	C1A-C2A-CAA-CBA
19	B	832	CLA	C3A-C2A-CAA-CBA
19	B	846	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	B	846	CLA	C3A-C2A-CAA-CBA
19	F	204	CLA	C1A-C2A-CAA-CBA
19	F	204	CLA	C3A-C2A-CAA-CBA
19	1	301	CLA	C2A-CAA-CBA-CGA
19	1	306	CLA	C2-C3-C5-C6
19	1	306	CLA	C4-C3-C5-C6
19	1	307	CLA	C2-C3-C5-C6
19	1	308	CLA	C1A-C2A-CAA-CBA
19	1	309	CLA	C1A-C2A-CAA-CBA
19	1	309	CLA	C2-C3-C5-C6
19	1	309	CLA	C4-C3-C5-C6
19	1	310	CLA	CBA-CGA-O2A-C1
19	1	310	CLA	O1A-CGA-O2A-C1
19	1	310	CLA	C2-C3-C5-C6
19	1	310	CLA	C4-C3-C5-C6
19	2	205	CLA	C1A-C2A-CAA-CBA
19	2	207	CLA	C1A-C2A-CAA-CBA
19	2	207	CLA	C3A-C2A-CAA-CBA
19	2	208	CLA	C1A-C2A-CAA-CBA
19	2	208	CLA	C3A-C2A-CAA-CBA
19	2	210	CLA	C1A-C2A-CAA-CBA
19	2	210	CLA	C3A-C2A-CAA-CBA
19	2	210	CLA	CHA-CBD-CGD-O1D
19	2	210	CLA	CHA-CBD-CGD-O2D
19	2	210	CLA	C2-C3-C5-C6
19	2	210	CLA	C4-C3-C5-C6
19	2	212	CLA	CHA-CBD-CGD-O1D
19	2	212	CLA	CHA-CBD-CGD-O2D
19	2	213	CLA	C1A-C2A-CAA-CBA
19	2	213	CLA	C3A-C2A-CAA-CBA
19	2	215	CLA	CHA-CBD-CGD-O1D
19	2	215	CLA	CHA-CBD-CGD-O2D
19	3	204	CLA	C1A-C2A-CAA-CBA
19	3	204	CLA	C3A-C2A-CAA-CBA
19	3	204	CLA	CHA-CBD-CGD-O1D
19	3	204	CLA	CHA-CBD-CGD-O2D
19	3	206	CLA	C1A-C2A-CAA-CBA
19	3	206	CLA	C3A-C2A-CAA-CBA
19	3	207	CLA	C1A-C2A-CAA-CBA
19	3	207	CLA	C3A-C2A-CAA-CBA
19	3	209	CLA	C2-C3-C5-C6
19	3	209	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	3	210	CLA	C1A-C2A-CAA-CBA
19	4	301	CLA	C1A-C2A-CAA-CBA
19	4	301	CLA	C3A-C2A-CAA-CBA
19	4	303	CLA	C1A-C2A-CAA-CBA
19	4	304	CLA	C1A-C2A-CAA-CBA
19	4	304	CLA	C3A-C2A-CAA-CBA
19	4	305	CLA	CHA-CBD-CGD-O1D
19	4	305	CLA	CHA-CBD-CGD-O2D
19	4	306	CLA	C2-C3-C5-C6
19	4	306	CLA	C4-C3-C5-C6
19	4	311	CLA	CHA-CBD-CGD-O1D
19	4	311	CLA	CHA-CBD-CGD-O2D
19	5	207	CLA	C3A-C2A-CAA-CBA
19	5	207	CLA	C6-C7-C8-C9
19	5	209	CLA	C4-C3-C5-C6
19	5	212	CLA	C2-C3-C5-C6
19	5	216	CLA	CHA-CBD-CGD-O1D
19	5	216	CLA	CHA-CBD-CGD-O2D
20	B	839	PQN	C12-C13-C15-C16
20	B	839	PQN	C14-C13-C15-C16
22	A	847	BCR	C37-C22-C23-C24
22	A	847	BCR	C22-C23-C24-C25
22	A	848	BCR	C35-C13-C14-C15
22	A	848	BCR	C20-C21-C22-C37
22	A	848	BCR	C21-C22-C23-C24
22	A	848	BCR	C23-C24-C25-C30
22	A	849	BCR	C37-C22-C23-C24
22	A	850	BCR	C22-C23-C24-C25
22	A	851	BCR	C1-C6-C7-C8
22	A	851	BCR	C37-C22-C23-C24
22	A	851	BCR	C22-C23-C24-C25
22	A	851	BCR	C23-C24-C25-C26
22	A	851	BCR	C23-C24-C25-C30
22	B	840	BCR	C7-C8-C9-C10
22	B	840	BCR	C7-C8-C9-C34
22	B	840	BCR	C18-C19-C20-C21
22	B	840	BCR	C21-C22-C23-C24
22	B	840	BCR	C37-C22-C23-C24
22	B	852	BCR	C20-C21-C22-C23
22	B	852	BCR	C20-C21-C22-C37
22	B	852	BCR	C21-C22-C23-C24
22	B	852	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	F	201	BCR	C20-C21-C22-C37
22	F	201	BCR	C21-C22-C23-C24
22	I	102	BCR	C7-C8-C9-C34
22	I	102	BCR	C21-C22-C23-C24
22	I	102	BCR	C37-C22-C23-C24
22	I	102	BCR	C23-C24-C25-C26
22	I	102	BCR	C23-C24-C25-C30
22	J	104	BCR	C5-C6-C7-C8
22	J	104	BCR	C6-C7-C8-C9
22	J	104	BCR	C7-C8-C9-C10
22	J	104	BCR	C7-C8-C9-C34
22	J	104	BCR	C21-C22-C23-C24
22	L	202	BCR	C20-C21-C22-C23
22	L	205	BCR	C7-C8-C9-C34
22	M	102	BCR	C21-C22-C23-C24
22	M	102	BCR	C37-C22-C23-C24
22	1	311	BCR	C7-C8-C9-C34
22	1	311	BCR	C37-C22-C23-C24
22	1	314	BCR	C1-C6-C7-C8
22	1	314	BCR	C20-C21-C22-C37
22	1	314	BCR	C21-C22-C23-C24
23	A	852	LHG	O1-C1-C2-O2
23	A	852	LHG	O1-C1-C2-C3
23	A	852	LHG	C3-O3-P-O5
23	A	852	LHG	C3-O3-P-O6
23	A	853	LHG	C3-O3-P-O5
23	B	842	LHG	O1-C1-C2-C3
23	B	842	LHG	O2-C2-C3-O3
23	M	103	LHG	O1-C1-C2-C3
23	M	103	LHG	O2-C2-C3-O3
23	M	103	LHG	C3-O3-P-O5
23	M	103	LHG	C4-O6-P-O3
23	M	103	LHG	C4-O6-P-O5
23	1	318	LHG	O1-C1-C2-C3
23	1	318	LHG	C4-O6-P-O5
23	1	318	LHG	O9-C7-O7-C5
23	1	318	LHG	C8-C7-O7-C5
23	3	215	LHG	C3-O3-P-O4
23	3	215	LHG	C3-O3-P-O5
23	3	215	LHG	C4-O6-P-O5
23	3	215	LHG	C8-C7-O7-C5
23	4	317	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
23	4	317	LHG	O1-C1-C2-C3
23	4	317	LHG	C3-O3-P-O4
23	4	317	LHG	C3-O3-P-O6
23	4	317	LHG	C4-O6-P-O5
23	4	317	LHG	O7-C5-C6-O8
24	A	854	LMT	O5'-C1'-O1'-C1
24	1	323	LMT	C2'-C1'-O1'-C1
24	1	323	LMT	O5'-C1'-O1'-C1
24	1	323	LMT	C2-C1-O1'-C1'
24	2	220	LMT	O5'-C1'-O1'-C1
27	J	105	5X6	C16-C17-C18-C19
27	J	105	5X6	C15-C16-C17-C18
27	J	105	5X6	C15-C16-C17-C41
27	J	105	5X6	C25-C26-C27-C28
27	J	105	5X6	C24-C25-C26-C39
27	J	105	5X6	C03-C11-C12-C13
27	J	105	5X6	C12-C13-C14-C15
27	J	105	5X6	C27-C28-C29-C34
27	J	105	5X6	C27-C28-C29-C30
27	J	105	5X6	C20-C21-C22-C40
27	J	105	5X6	C21-C22-C23-C24
28	L	209	DD6	C-C1-C2-C3
28	L	209	DD6	C9-C10-C11-C12
28	L	209	DD6	C10-C11-C13-C14
28	L	209	DD6	C4-C5-C6-C7
28	L	209	DD6	C5-C6-C8-C9
28	1	312	DD6	C-C1-C2-C3
28	1	312	DD6	C2-C1-C24-C25
28	1	312	DD6	C9-C10-C11-C13
28	1	312	DD6	C4-C5-C6-C7
28	1	312	DD6	C7-C6-C8-C9
28	1	313	DD6	C-C1-C2-C3
28	1	313	DD6	C-C1-C24-C25
28	1	313	DD6	C2-C1-C24-C25
28	1	313	DD6	C9-C10-C11-C13
28	1	313	DD6	C10-C11-C13-C14
28	1	313	DD6	C12-C11-C13-C14
28	1	313	DD6	C4-C5-C6-C7
28	1	315	DD6	C-C1-C2-C3
28	1	315	DD6	C-C1-C24-C25
28	1	315	DD6	C2-C1-C24-C25
28	1	315	DD6	C9-C10-C11-C13

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Mol	Chain	Res	Type	Atoms
28	1	315	DD6	C4-C5-C6-C7
28	2	217	DD6	C-C1-C2-C3
28	2	217	DD6	C-C1-C24-C25
28	2	217	DD6	C9-C10-C11-C12
28	2	217	DD6	C4-C5-C6-C7
28	2	217	DD6	C5-C6-C8-C9
28	3	213	DD6	C-C1-C2-C3
28	3	213	DD6	C-C1-C24-C25
28	3	213	DD6	C9-C10-C11-C12
28	3	213	DD6	C10-C11-C13-C14
28	3	213	DD6	C12-C11-C13-C14
28	3	213	DD6	C13-C14-C15-C20
28	3	213	DD6	C13-C14-C15-O1
28	3	213	DD6	C4-C5-C6-C7
28	3	213	DD6	C7-C6-C8-C9
28	5	218	DD6	C-C1-C2-C3
28	5	218	DD6	C-C1-C24-C25
28	5	218	DD6	C9-C10-C11-C12
28	5	218	DD6	C10-C11-C13-C14
28	5	218	DD6	C13-C14-C15-O1
28	5	218	DD6	C4-C5-C6-C7
29	1	302	LMG	O6-C1-O1-C7
29	1	302	LMG	O7-C8-C9-O8
30	1	305	KC1	C2A-CAA-CBA-CGA
30	1	305	KC1	CHA-CBD-CGD-O1D
30	1	305	KC1	CHA-CBD-CGD-O2D
30	2	211	KC1	C2B-C3B-CAB-CBB
30	2	211	KC1	C4B-C3B-CAB-CBB
30	3	205	KC1	C2A-CAA-CBA-CGA
30	3	205	KC1	CAA-CBA-CGA-O1A
30	3	208	KC1	C1A-C2A-CAA-CBA
30	3	208	KC1	C2A-CAA-CBA-CGA
30	3	211	KC1	C1A-C2A-CAA-CBA
30	4	302	KC1	C2B-C3B-CAB-CBB
30	4	302	KC1	C2A-CAA-CBA-CGA
30	4	302	KC1	CHA-CBD-CGD-O1D
30	4	302	KC1	CHA-CBD-CGD-O2D
30	4	307	KC1	C3A-C2A-CAA-CBA
30	4	307	KC1	C2A-CAA-CBA-CGA
31	1	317	A86	C1-C2-C3-C4
31	1	317	A86	C28-C27-C29-C30
31	2	216	A86	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
31	2	216	A86	C39-C38-O4-C34
31	2	216	A86	C3-C4-C5-C6
31	2	218	A86	C39-C38-O4-C34
31	2	219	A86	C-C1-C24-C25
31	2	219	A86	C2-C1-C24-C25
31	3	212	A86	C5-C6-C8-C9
31	3	212	A86	C7-C6-C8-C9
31	3	228	A86	C-C1-C24-C25
31	3	228	A86	C2-C1-C24-C25
31	4	315	A86	C-C1-C24-C25
31	4	315	A86	C2-C1-C24-C25
31	4	315	A86	C24-C25-C26-C27
31	4	316	A86	C11-C10-C9-C8
31	4	316	A86	C24-C25-C26-C27
31	5	217	A86	C39-C38-O4-C34
31	5	217	A86	O5-C38-O4-C34
31	5	220	A86	C-C1-C24-C25
31	5	220	A86	C13-C14-C15-O1
31	5	220	A86	C39-C38-O4-C34
31	5	220	A86	O5-C38-O4-C34
31	1	317	A86	C39-C38-O4-C34
19	B	802	CLA	CBD-CGD-O2D-CED
19	4	305	CLA	CBD-CGD-O2D-CED
30	2	211	KC1	CBD-CGD-O2D-CED
19	A	843	CLA	O1A-CGA-O2A-C1
24	A	854	LMT	O5B-C1B-O1B-C4'
31	1	317	A86	O5-C38-O4-C34
19	A	843	CLA	CBA-CGA-O2A-C1
19	2	210	CLA	CBA-CGA-O2A-C1
23	A	853	LHG	C24-C23-O8-C6
19	B	821	CLA	CBD-CGD-O2D-CED
31	3	212	A86	C39-C38-O4-C34
19	A	815	CLA	O1A-CGA-O2A-C1
19	B	810	CLA	O1A-CGA-O2A-C1
19	B	826	CLA	O1A-CGA-O2A-C1
19	2	210	CLA	O1A-CGA-O2A-C1
19	5	212	CLA	O1A-CGA-O2A-C1
23	A	853	LHG	O10-C23-O8-C6
30	3	205	KC1	CAA-CBA-CGA-O2A
31	3	212	A86	O5-C38-O4-C34
19	A	811	CLA	CBD-CGD-O2D-CED
19	B	837	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	F	204	CLA	CBD-CGD-O2D-CED
19	2	208	CLA	CBD-CGD-O2D-CED
23	3	215	LHG	O9-C7-O7-C5
19	A	821	CLA	O1A-CGA-O2A-C1
19	A	804	CLA	C3-C5-C6-C7
19	A	825	CLA	C3-C5-C6-C7
19	A	827	CLA	C3-C5-C6-C7
19	A	832	CLA	C3-C5-C6-C7
19	A	833	CLA	C3-C5-C6-C7
19	B	823	CLA	C3-C5-C6-C7
19	u	201	CLA	C3-C5-C6-C7
19	2	210	CLA	C3-C5-C6-C7
19	3	203	CLA	C3-C5-C6-C7
19	3	206	CLA	C3-C5-C6-C7
19	3	207	CLA	C3-C5-C6-C7
20	B	839	PQN	C13-C15-C16-C17
19	B	810	CLA	CBA-CGA-O2A-C1
19	5	212	CLA	CBA-CGA-O2A-C1
31	4	315	A86	C39-C38-O4-C34
19	1	307	CLA	CBD-CGD-O2D-CED
19	5	210	CLA	CBD-CGD-O2D-CED
31	1	316	A86	C39-C38-O4-C34
31	1	316	A86	O5-C38-O4-C34
31	2	216	A86	O5-C38-O4-C34
31	2	218	A86	O5-C38-O4-C34
19	2	208	CLA	C3-C5-C6-C7
19	B	837	CLA	C4-C3-C5-C6
19	2	209	CLA	C4-C3-C5-C6
19	4	303	CLA	C4-C3-C5-C6
19	A	836	CLA	C2-C3-C5-C6
19	A	842	CLA	C2-C3-C5-C6
19	B	810	CLA	C2-C3-C5-C6
19	5	209	CLA	C2-C3-C5-C6
19	A	824	CLA	C2A-CAA-CBA-CGA
19	B	810	CLA	C2A-CAA-CBA-CGA
19	B	822	CLA	C2A-CAA-CBA-CGA
19	B	832	CLA	C2A-CAA-CBA-CGA
19	B	837	CLA	C2A-CAA-CBA-CGA
19	F	204	CLA	C2A-CAA-CBA-CGA
19	2	208	CLA	C2A-CAA-CBA-CGA
19	3	206	CLA	C2A-CAA-CBA-CGA
23	B	842	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
19	A	819	CLA	C3-C5-C6-C7
19	A	821	CLA	C3-C5-C6-C7
19	A	843	CLA	C3-C5-C6-C7
19	B	832	CLA	C3-C5-C6-C7
19	2	206	CLA	C3-C5-C6-C7
19	A	813	CLA	CBA-CGA-O2A-C1
19	A	815	CLA	CBA-CGA-O2A-C1
19	A	821	CLA	CBA-CGA-O2A-C1
19	A	836	CLA	CBA-CGA-O2A-C1
19	B	804	CLA	CBA-CGA-O2A-C1
19	B	837	CLA	CBA-CGA-O2A-C1
19	4	306	CLA	CBA-CGA-O2A-C1
23	M	103	LHG	C24-C23-O8-C6
19	A	836	CLA	O1A-CGA-O2A-C1
23	M	103	LHG	O10-C23-O8-C6
28	L	209	DD6	C1-C2-C3-C4
28	1	312	DD6	C3-C4-C5-C6
28	1	313	DD6	C24-C25-C26-C27
19	5	208	CLA	CBD-CGD-O2D-CED
23	1	318	LHG	O2-C2-C3-O3
23	3	215	LHG	O2-C2-C3-O3
23	4	317	LHG	O2-C2-C3-O3
19	A	810	CLA	C3-C5-C6-C7
19	A	822	CLA	C3-C5-C6-C7
19	B	822	CLA	C3-C5-C6-C7
19	B	837	CLA	C3-C5-C6-C7
19	1	301	CLA	C3-C5-C6-C7
19	A	820	CLA	CBA-CGA-O2A-C1
19	A	825	CLA	CBA-CGA-O2A-C1
19	1	303	CLA	CBA-CGA-O2A-C1
31	2	219	A86	C39-C38-O4-C34
19	A	813	CLA	O1A-CGA-O2A-C1
24	3	216	LMT	O5B-C5B-C6B-O6B
26	B	847	DGD	O6E-C5E-C6E-O5E
19	u	201	CLA	CBD-CGD-O2D-CED
23	A	853	LHG	C32-C33-C34-C35
24	1	323	LMT	O5'-C5'-C6'-O6'
19	A	803	CLA	C3-C5-C6-C7
19	B	803	CLA	C3-C5-C6-C7
19	B	808	CLA	C3-C5-C6-C7
30	2	211	KC1	CAA-CBA-CGA-O2A
30	3	211	KC1	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	A	825	CLA	O1A-CGA-O2A-C1
19	B	804	CLA	O1A-CGA-O2A-C1
19	B	837	CLA	O1A-CGA-O2A-C1
19	1	303	CLA	O1A-CGA-O2A-C1
19	4	306	CLA	O1A-CGA-O2A-C1
19	A	821	CLA	C4-C3-C5-C6
19	A	833	CLA	C4-C3-C5-C6
19	B	832	CLA	C4-C3-C5-C6
19	1	304	CLA	C4-C3-C5-C6
19	3	206	CLA	C4-C3-C5-C6
19	5	210	CLA	C4-C3-C5-C6
24	2	220	LMT	C4'-C5'-C6'-O6'
19	A	821	CLA	C2-C3-C5-C6
19	A	833	CLA	C2-C3-C5-C6
19	B	832	CLA	C2-C3-C5-C6
19	1	304	CLA	C2-C3-C5-C6
19	3	206	CLA	C2-C3-C5-C6
19	5	210	CLA	C2-C3-C5-C6
19	B	836	CLA	C2A-CAA-CBA-CGA
19	u	202	CLA	C2A-CAA-CBA-CGA
19	4	311	CLA	C2A-CAA-CBA-CGA
19	A	820	CLA	O1A-CGA-O2A-C1
19	A	805	CLA	CBA-CGA-O2A-C1
19	B	825	CLA	CBA-CGA-O2A-C1
23	B	842	LHG	C24-C23-O8-C6
23	4	317	LHG	C32-C33-C34-C35
19	4	305	CLA	O1D-CGD-O2D-CED
30	3	211	KC1	CAA-CBA-CGA-O1A
30	4	302	KC1	CAA-CBA-CGA-O1A
24	A	854	LMT	C4'-C5'-C6'-O6'
19	B	802	CLA	O1D-CGD-O2D-CED
30	2	211	KC1	O1D-CGD-O2D-CED
23	B	842	LHG	C1-C2-C3-O3
23	M	103	LHG	C1-C2-C3-O3
23	4	317	LHG	C1-C2-C3-O3
19	A	805	CLA	O1A-CGA-O2A-C1
19	B	812	CLA	C3-C5-C6-C7
19	B	816	CLA	CBA-CGA-O2A-C1
19	B	818	CLA	CBA-CGA-O2A-C1
19	B	826	CLA	CBA-CGA-O2A-C1
19	B	827	CLA	CBA-CGA-O2A-C1
19	2	208	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	4	305	CLA	CBA-CGA-O2A-C1
28	1	313	DD6	C1-C2-C3-C4
28	1	315	DD6	C24-C25-C26-C27
31	4	314	A86	C11-C10-C9-C8
19	A	810	CLA	C13-C15-C16-C17
19	B	816	CLA	O1A-CGA-O2A-C1
24	1	323	LMT	C4'-C5'-C6'-O6'
24	3	216	LMT	C4B-C5B-C6B-O6B
23	A	852	LHG	C29-C30-C31-C32
30	2	211	KC1	CAA-CBA-CGA-O1A
30	4	302	KC1	CAA-CBA-CGA-O2A
30	4	307	KC1	CAA-CBA-CGA-O1A
23	3	215	LHG	O6-C4-C5-O7
26	B	847	DGD	C4E-C5E-C6E-O5E
19	A	835	CLA	C13-C15-C16-C17
19	B	810	CLA	C13-C15-C16-C17
19	B	819	CLA	C10-C11-C12-C13
19	B	827	CLA	O1A-CGA-O2A-C1
19	2	208	CLA	O1A-CGA-O2A-C1
19	A	807	CLA	C6-C7-C8-C9
19	A	826	CLA	C11-C12-C13-C14
19	A	828	CLA	C6-C7-C8-C9
19	B	804	CLA	C11-C12-C13-C14
19	B	821	CLA	C14-C13-C15-C16
19	B	827	CLA	C11-C12-C13-C14
19	B	837	CLA	C11-C10-C8-C9
19	1	303	CLA	C14-C13-C15-C16
19	2	205	CLA	C11-C10-C8-C9
19	2	206	CLA	C11-C10-C8-C9
19	3	206	CLA	C11-C10-C8-C9
19	4	301	CLA	C6-C7-C8-C9
19	4	305	CLA	C14-C13-C15-C16
19	5	209	CLA	C6-C7-C8-C9
19	B	845	CLA	C2A-CAA-CBA-CGA
19	5	213	CLA	C2A-CAA-CBA-CGA
22	F	205	BCR	C37-C22-C23-C24
22	I	101	BCR	C37-C22-C23-C24
22	L	202	BCR	C7-C8-C9-C34
22	L	205	BCR	C37-C22-C23-C24
22	1	314	BCR	C37-C22-C23-C24
28	2	217	DD6	C12-C11-C13-C14
28	2	217	DD6	C7-C6-C8-C9

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Mol	Chain	Res	Type	Atoms
28	5	218	DD6	C12-C11-C13-C14
28	5	218	DD6	C7-C6-C8-C9
31	1	317	A86	C-C1-C24-C25
31	4	316	A86	C7-C6-C8-C9
31	5	221	A86	C-C1-C24-C25
22	A	847	BCR	C21-C22-C23-C24
22	L	205	BCR	C7-C8-C9-C10
28	1	312	DD6	C10-C11-C13-C14
28	1	313	DD6	C5-C6-C8-C9
31	4	314	A86	C5-C6-C8-C9
31	4	316	A86	C2-C1-C24-C25
31	4	316	A86	C5-C6-C8-C9
31	5	220	A86	C2-C1-C24-C25
23	B	842	LHG	C23-C24-C25-C26
26	B	847	DGD	C1A-C2A-C3A-C4A
19	B	818	CLA	O1A-CGA-O2A-C1
19	4	305	CLA	O1A-CGA-O2A-C1
23	B	842	LHG	O10-C23-O8-C6
19	A	833	CLA	C10-C11-C12-C13
19	A	834	CLA	C15-C16-C17-C18
19	B	806	CLA	C5-C6-C7-C8
19	2	206	CLA	C13-C15-C16-C17
20	B	839	PQN	C23-C25-C26-C27
19	A	825	CLA	CBD-CGD-O2D-CED
19	4	306	CLA	C2C-C3C-CAC-CBC
19	3	207	CLA	CBA-CGA-O2A-C1
19	A	820	CLA	C15-C16-C17-C18
19	A	839	CLA	C5-C6-C7-C8
19	A	839	CLA	C13-C15-C16-C17
19	B	804	CLA	C10-C11-C12-C13
19	B	807	CLA	C15-C16-C17-C18
19	B	813	CLA	C15-C16-C17-C18
19	B	827	CLA	C5-C6-C7-C8
19	B	831	CLA	C15-C16-C17-C18
19	4	305	CLA	C8-C10-C11-C12
19	5	209	CLA	C13-C15-C16-C17
23	4	317	LHG	C7-C8-C9-C10
24	A	854	LMT	O5'-C5'-C6'-O6'
19	A	826	CLA	C10-C11-C12-C13
19	A	826	CLA	C13-C15-C16-C17
19	A	826	CLA	C15-C16-C17-C18
19	A	832	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	A	878	CLA	C10-C11-C12-C13
19	B	806	CLA	C10-C11-C12-C13
19	B	810	CLA	C10-C11-C12-C13
19	B	816	CLA	C5-C6-C7-C8
19	B	829	CLA	C13-C15-C16-C17
19	1	307	CLA	C5-C6-C7-C8
19	1	310	CLA	C5-C6-C7-C8
19	1	310	CLA	C8-C10-C11-C12
19	1	310	CLA	C13-C15-C16-C17
19	3	206	CLA	C13-C15-C16-C17
19	4	305	CLA	C10-C11-C12-C13
19	5	207	CLA	C5-C6-C7-C8
19	5	209	CLA	C5-C6-C7-C8
20	A	845	PQN	C23-C25-C26-C27
23	1	318	LHG	C7-C8-C9-C10
24	2	220	LMT	O5'-C5'-C6'-O6'
19	2	207	CLA	C15-C16-C17-C18
30	4	307	KC1	CAA-CBA-CGA-O2A
19	A	815	CLA	C2-C1-O2A-CGA
19	F	203	CLA	C2-C1-O2A-CGA
31	5	221	A86	C39-C38-O4-C34
19	A	810	CLA	C8-C10-C11-C12
19	B	804	CLA	C8-C10-C11-C12
19	B	821	CLA	C10-C11-C12-C13
19	L	206	CLA	C10-C11-C12-C13
19	2	205	CLA	C13-C15-C16-C17
19	B	816	CLA	CBD-CGD-O2D-CED
19	A	833	CLA	C8-C10-C11-C12
19	B	804	CLA	C5-C6-C7-C8
19	1	303	CLA	C8-C10-C11-C12
19	A	820	CLA	C12-C13-C15-C16
19	A	878	CLA	C11-C10-C8-C7
19	B	821	CLA	C11-C10-C8-C7
19	5	211	CLA	C6-C7-C8-C10
19	A	807	CLA	C3-C5-C6-C7
19	B	804	CLA	C3-C5-C6-C7
19	B	816	CLA	C3-C5-C6-C7
19	5	209	CLA	C3-C5-C6-C7
28	1	313	DD6	C11-C10-C9-C8
31	1	317	A86	C3-C4-C5-C6
19	u	201	CLA	CBA-CGA-O2A-C1
19	2	213	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	3	207	CLA	C2A-CAA-CBA-CGA
19	A	811	CLA	O1D-CGD-O2D-CED
19	B	821	CLA	O1D-CGD-O2D-CED
19	A	812	CLA	C8-C10-C11-C12
19	A	827	CLA	C13-C15-C16-C17
19	A	843	CLA	C5-C6-C7-C8
19	B	814	CLA	C8-C10-C11-C12
19	1	309	CLA	C5-C6-C7-C8
19	2	206	CLA	C8-C10-C11-C12
24	3	216	LMT	C5'-C4'-O1B-C1B
19	A	842	CLA	CBD-CGD-O2D-CED
19	A	829	CLA	C15-C16-C17-C18
19	B	837	CLA	O1D-CGD-O2D-CED
22	B	852	BCR	C18-C19-C20-C21
22	J	104	BCR	C10-C11-C12-C13
22	1	314	BCR	C18-C19-C20-C21
27	J	105	5X6	C22-C23-C24-C25
19	1	303	CLA	C3-C5-C6-C7
19	5	210	CLA	C3-C5-C6-C7
19	A	826	CLA	C8-C10-C11-C12
19	A	833	CLA	C5-C6-C7-C8
19	B	811	CLA	C10-C11-C12-C13
19	B	827	CLA	C8-C10-C11-C12
19	1	301	CLA	C5-C6-C7-C8
19	1	304	CLA	C15-C16-C17-C18
20	A	845	PQN	C20-C21-C22-C23
29	1	302	LMG	C29-C28-O8-C9
19	B	825	CLA	O1A-CGA-O2A-C1
19	B	821	CLA	C15-C16-C17-C18
19	3	207	CLA	O1A-CGA-O2A-C1
19	B	810	CLA	C5-C6-C7-C8
19	1	309	CLA	C8-C10-C11-C12
23	B	842	LHG	C3-O3-P-O6
23	M	103	LHG	C3-O3-P-O6
23	3	215	LHG	C3-O3-P-O6
23	4	317	LHG	C4-O6-P-O3
19	4	303	CLA	C3-C5-C6-C7
19	1	306	CLA	CBA-CGA-O2A-C1
19	5	211	CLA	CBA-CGA-O2A-C1
31	4	315	A86	O5-C38-O4-C34
19	A	804	CLA	C5-C6-C7-C8
19	A	828	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	B	811	CLA	C13-C15-C16-C17
19	B	827	CLA	C10-C11-C12-C13
19	5	210	CLA	C8-C10-C11-C12
19	4	312	CLA	C3-C5-C6-C7
19	F	204	CLA	O1D-CGD-O2D-CED
19	1	307	CLA	O1D-CGD-O2D-CED
19	2	208	CLA	O1D-CGD-O2D-CED
23	3	215	LHG	C1-C2-C3-O3
19	B	836	CLA	C4-C3-C5-C6
19	B	816	CLA	C2A-CAA-CBA-CGA
19	3	203	CLA	C2A-CAA-CBA-CGA
19	A	839	CLA	C3-C5-C6-C7
19	1	309	CLA	C3-C5-C6-C7
19	A	842	CLA	CBA-CGA-O2A-C1
19	B	824	CLA	C13-C15-C16-C17
23	1	318	LHG	C28-C29-C30-C31
22	A	848	BCR	C16-C17-C18-C36
22	A	849	BCR	C20-C21-C22-C37
22	A	850	BCR	C20-C21-C22-C37
22	A	851	BCR	C35-C13-C14-C15
22	B	840	BCR	C35-C13-C14-C15
22	B	841	BCR	C16-C17-C18-C36
22	B	844	BCR	C20-C21-C22-C37
22	B	852	BCR	C35-C13-C14-C15
22	F	201	BCR	C35-C13-C14-C15
22	I	102	BCR	C35-C13-C14-C15
22	J	104	BCR	C20-C21-C22-C37
22	L	202	BCR	C16-C17-C18-C36
22	L	202	BCR	C20-C21-C22-C37
24	1	323	LMT	O5B-C5B-C6B-O6B
23	A	852	LHG	C11-C12-C13-C14
23	B	842	LHG	C9-C10-C11-C12
23	4	317	LHG	C9-C10-C11-C12
23	4	317	LHG	C27-C28-C29-C30
23	4	317	LHG	C33-C34-C35-C36
29	1	302	LMG	C29-C30-C31-C32
30	3	211	KC1	C2A-CAA-CBA-CGA
23	M	103	LHG	C9-C10-C11-C12
23	4	317	LHG	C31-C32-C33-C34
26	B	847	DGD	C4A-C5A-C6A-C7A
26	B	847	DGD	C5A-C6A-C7A-C8A
19	B	819	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	M	103	LHG	C23-C24-C25-C26
23	A	853	LHG	C27-C28-C29-C30
23	A	853	LHG	C30-C31-C32-C33
23	4	317	LHG	C11-C12-C13-C14
26	B	847	DGD	C5B-C6B-C7B-C8B
19	5	210	CLA	O1D-CGD-O2D-CED
23	A	852	LHG	C16-C17-C18-C19
23	4	317	LHG	C28-C29-C30-C31
19	3	207	CLA	CBD-CGD-O2D-CED
22	A	850	BCR	C20-C21-C22-C23
22	B	840	BCR	C12-C13-C14-C15
22	F	201	BCR	C16-C17-C18-C19
22	1	311	BCR	C20-C21-C22-C23
22	1	314	BCR	C20-C21-C22-C23
28	1	313	DD6	C24-C1-C2-C3
28	1	313	DD6	C4-C5-C6-C8
23	A	852	LHG	C27-C28-C29-C30
23	B	842	LHG	C26-C27-C28-C29
26	B	847	DGD	C3A-C4A-C5A-C6A
26	B	847	DGD	C7B-C8B-C9B-CAB
19	A	842	CLA	O1A-CGA-O2A-C1
19	A	809	CLA	C4-C3-C5-C6
19	A	826	CLA	C4-C3-C5-C6
19	A	834	CLA	C4-C3-C5-C6
19	A	844	CLA	C4-C3-C5-C6
19	B	807	CLA	C4-C3-C5-C6
19	B	833	CLA	C4-C3-C5-C6
19	1	307	CLA	C4-C3-C5-C6
24	3	216	LMT	C7-C8-C9-C10
29	1	302	LMG	C32-C33-C34-C35
19	A	809	CLA	C2-C3-C5-C6
19	B	837	CLA	C2-C3-C5-C6
19	A	827	CLA	C14-C13-C15-C16
19	A	831	CLA	C14-C13-C15-C16
19	B	821	CLA	C11-C10-C8-C9
19	1	309	CLA	C6-C7-C8-C9
19	3	207	CLA	C11-C12-C13-C14
19	A	818	CLA	C5-C6-C7-C8
23	1	318	LHG	C9-C10-C11-C12
30	1	305	KC1	CAA-CBA-CGA-O1A
30	1	305	KC1	CAA-CBA-CGA-O2A
19	A	829	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	A	830	CLA	C2A-CAA-CBA-CGA
19	u	201	CLA	O1A-CGA-O2A-C1
22	A	850	BCR	C37-C22-C23-C24
22	F	201	BCR	C37-C22-C23-C24
27	J	105	5X6	C11-C12-C13-C42
28	1	315	DD6	C12-C11-C13-C14
28	1	315	DD6	C7-C6-C8-C9
31	4	314	A86	C7-C6-C8-C9
31	4	316	A86	C-C1-C24-C25
29	1	302	LMG	C41-C42-C43-C44
23	A	853	LHG	O1-C1-C2-C3
22	A	850	BCR	C21-C22-C23-C24
28	L	209	DD6	C2-C1-C24-C25
19	1	310	CLA	C3-C5-C6-C7
23	A	853	LHG	C18-C19-C20-C21
23	4	317	LHG	C10-C11-C12-C13
26	B	847	DGD	CAB-CBB-CCB-CDB
23	B	842	LHG	C11-C10-C9-C8
23	1	318	LHG	C16-C17-C18-C19
23	4	317	LHG	C12-C13-C14-C15
24	1	323	LMT	C7-C8-C9-C10
24	3	216	LMT	C3'-C4'-O1B-C1B
19	A	835	CLA	C16-C17-C18-C20
19	A	880	CLA	C16-C17-C18-C19
19	B	821	CLA	C16-C17-C18-C19
19	B	838	CLA	C16-C17-C18-C20
19	A	830	CLA	C13-C15-C16-C17
19	A	880	CLA	C15-C16-C17-C18
19	B	811	CLA	C15-C16-C17-C18
23	B	842	LHG	C24-C25-C26-C27
23	A	852	LHG	C34-C35-C36-C37
31	2	219	A86	O5-C38-O4-C34
19	A	827	CLA	C8-C10-C11-C12
19	1	306	CLA	O1A-CGA-O2A-C1
19	5	211	CLA	O1A-CGA-O2A-C1
23	4	317	LHG	C14-C15-C16-C17
19	A	804	CLA	CBA-CGA-O2A-C1
19	A	839	CLA	CBA-CGA-O2A-C1
19	5	208	CLA	O1D-CGD-O2D-CED
19	A	804	CLA	C3A-C2A-CAA-CBA
19	B	838	CLA	C3A-C2A-CAA-CBA
19	1	308	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	1	309	CLA	C3A-C2A-CAA-CBA
19	4	303	CLA	C3A-C2A-CAA-CBA
31	1	316	A86	C24-C25-C26-C27
23	B	842	LHG	C28-C29-C30-C31
19	B	821	CLA	C16-C17-C18-C20
23	A	852	LHG	C24-C25-C26-C27
24	2	220	LMT	C1-C2-C3-C4
19	A	822	CLA	C4-C3-C5-C6
19	B	829	CLA	C4-C3-C5-C6
19	A	822	CLA	C2-C3-C5-C6
19	A	832	CLA	C2-C3-C5-C6
19	A	834	CLA	C2-C3-C5-C6
19	A	844	CLA	C2-C3-C5-C6
19	B	807	CLA	C2-C3-C5-C6
19	2	209	CLA	C2-C3-C5-C6
26	B	847	DGD	C2B-C1B-O2G-C2G
19	A	835	CLA	CBD-CGD-O2D-CED
29	1	302	LMG	C16-C17-C18-C19
23	1	318	LHG	O1-C1-C2-O2
23	M	103	LHG	C26-C27-C28-C29
24	1	323	LMT	C5-C6-C7-C8
19	A	820	CLA	C16-C17-C18-C20
19	B	824	CLA	C16-C17-C18-C19
19	B	810	CLA	C3-C5-C6-C7
19	A	839	CLA	O1A-CGA-O2A-C1
23	A	853	LHG	C7-C8-C9-C10
29	1	302	LMG	O6-C5-C6-O5
23	A	852	LHG	C26-C27-C28-C29
23	4	317	LHG	C24-C25-C26-C27
19	A	829	CLA	C2-C1-O2A-CGA
19	B	829	CLA	C2-C1-O2A-CGA
19	3	206	CLA	C2-C1-O2A-CGA
19	2	205	CLA	C5-C6-C7-C8
29	1	302	LMG	C28-C29-C30-C31
22	A	848	BCR	C1-C6-C7-C8
22	A	848	BCR	C5-C6-C7-C8
22	A	848	BCR	C23-C24-C25-C26
22	A	850	BCR	C23-C24-C25-C26
22	A	850	BCR	C23-C24-C25-C30
22	A	851	BCR	C5-C6-C7-C8
22	B	843	BCR	C23-C24-C25-C26
22	B	843	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
22	B	852	BCR	C23-C24-C25-C26
22	B	852	BCR	C23-C24-C25-C30
22	J	104	BCR	C1-C6-C7-C8
22	1	311	BCR	C1-C6-C7-C8
22	1	311	BCR	C5-C6-C7-C8
22	1	314	BCR	C5-C6-C7-C8
27	J	105	5X6	C02-C03-C11-C12
27	J	105	5X6	C04-C03-C11-C12
19	B	819	CLA	CBA-CGA-O2A-C1
26	B	847	DGD	CEB-CFB-CGB-CHB
31	3	228	A86	C39-C38-O4-C34
19	3	207	CLA	C5-C6-C7-C8
23	M	103	LHG	C24-C25-C26-C27
29	1	302	LMG	C38-C39-C40-C41
19	A	832	CLA	C4-C3-C5-C6
19	B	827	CLA	C4-C3-C5-C6
19	B	830	CLA	C4-C3-C5-C6
19	A	807	CLA	C11-C10-C8-C7
19	A	808	CLA	C12-C13-C15-C16
19	A	826	CLA	C2-C3-C5-C6
19	A	826	CLA	C11-C12-C13-C15
19	A	827	CLA	C12-C13-C15-C16
19	A	831	CLA	C12-C13-C15-C16
19	B	806	CLA	C11-C10-C8-C7
19	B	813	CLA	C12-C13-C15-C16
19	B	819	CLA	C11-C10-C8-C7
19	B	829	CLA	C2-C3-C5-C6
19	B	831	CLA	C12-C13-C15-C16
19	B	833	CLA	C2-C3-C5-C6
19	B	845	CLA	C11-C10-C8-C7
19	3	207	CLA	C11-C12-C13-C15
19	4	305	CLA	C12-C13-C15-C16
20	B	839	PQN	C16-C17-C18-C20
19	A	804	CLA	O1A-CGA-O2A-C1
19	A	805	CLA	C5-C6-C7-C8
28	1	312	DD6	C24-C25-C26-C27
28	1	313	DD6	C3-C4-C5-C6
28	1	315	DD6	C1-C2-C3-C4
19	A	806	CLA	CBA-CGA-O2A-C1
19	A	824	CLA	CBA-CGA-O2A-C1
19	A	829	CLA	CBA-CGA-O2A-C1
19	4	311	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	1	302	LMG	C15-C16-C17-C18
19	u	201	CLA	C2A-CAA-CBA-CGA
19	A	839	CLA	C15-C16-C17-C18
19	B	845	CLA	C10-C11-C12-C13
24	2	220	LMT	C2-C3-C4-C5
19	B	834	CLA	C13-C15-C16-C17
19	4	306	CLA	C4C-C3C-CAC-CBC
30	3	205	KC1	C2B-C3B-CAB-CBB
19	B	805	CLA	C3-C5-C6-C7
23	1	318	LHG	C11-C10-C9-C8
26	B	847	DGD	CBA-CCA-CDA-CEA
26	B	847	DGD	C6B-C7B-C8B-C9B
19	A	831	CLA	CBA-CGA-O2A-C1
19	3	203	CLA	C6-C7-C8-C9
19	5	210	CLA	C15-C16-C17-C18
24	1	323	LMT	C6-C7-C8-C9
23	B	842	LHG	C7-C8-C9-C10
23	4	317	LHG	C23-C24-C25-C26
23	A	853	LHG	C11-C10-C9-C8
30	3	205	KC1	C4B-C3B-CAB-CBB
30	4	302	KC1	C4B-C3B-CAB-CBB
30	4	307	KC1	C4B-C3B-CAB-CBB
19	B	836	CLA	C5-C6-C7-C8
19	2	206	CLA	C10-C11-C12-C13
19	A	834	CLA	CBD-CGD-O2D-CED
19	B	838	CLA	CBD-CGD-O2D-CED
19	1	303	CLA	CBD-CGD-O2D-CED
23	3	215	LHG	C24-C25-C26-C27
23	A	853	LHG	C16-C17-C18-C19
26	B	847	DGD	C3B-C4B-C5B-C6B
19	B	819	CLA	O1A-CGA-O2A-C1
19	B	810	CLA	C4-C3-C5-C6
19	5	208	CLA	C4-C3-C5-C6
19	5	212	CLA	C4-C3-C5-C6
19	B	827	CLA	C2-C3-C5-C6
19	B	836	CLA	C2-C3-C5-C6
19	4	303	CLA	C2-C3-C5-C6
19	A	807	CLA	C11-C10-C8-C9
19	A	808	CLA	C14-C13-C15-C16
19	A	820	CLA	C14-C13-C15-C16
19	B	804	CLA	C6-C7-C8-C9
19	B	819	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
19	1	309	CLA	C11-C12-C13-C14
19	2	210	CLA	C6-C7-C8-C9
19	5	211	CLA	C6-C7-C8-C9
20	B	839	PQN	C16-C17-C18-C19
19	B	833	CLA	C3-C5-C6-C7
19	A	802	CLA	C2A-CAA-CBA-CGA
19	A	818	CLA	C2A-CAA-CBA-CGA
19	A	843	CLA	C2A-CAA-CBA-CGA
19	L	204	CLA	C2A-CAA-CBA-CGA
19	5	207	CLA	C2A-CAA-CBA-CGA
19	A	809	CLA	CBA-CGA-O2A-C1
19	F	203	CLA	CBA-CGA-O2A-C1
19	2	205	CLA	C8-C10-C11-C12
19	A	804	CLA	C1A-C2A-CAA-CBA
19	A	805	CLA	C1A-C2A-CAA-CBA
19	A	810	CLA	C1A-C2A-CAA-CBA
19	A	812	CLA	C1A-C2A-CAA-CBA
19	A	818	CLA	C1A-C2A-CAA-CBA
19	A	819	CLA	C1A-C2A-CAA-CBA
19	A	821	CLA	C1A-C2A-CAA-CBA
19	B	805	CLA	C1A-C2A-CAA-CBA
19	B	821	CLA	C1A-C2A-CAA-CBA
19	B	825	CLA	C1A-C2A-CAA-CBA
19	B	838	CLA	C1A-C2A-CAA-CBA
19	1	307	CLA	C1A-C2A-CAA-CBA
19	3	202	CLA	C1A-C2A-CAA-CBA
19	5	207	CLA	C1A-C2A-CAA-CBA
19	5	210	CLA	C1A-C2A-CAA-CBA
19	3	203	CLA	C6-C7-C8-C10
22	A	847	BCR	C15-C16-C17-C18
19	A	803	CLA	C15-C16-C17-C18
19	A	825	CLA	C5-C6-C7-C8
19	B	818	CLA	C10-C11-C12-C13
19	B	813	CLA	CBA-CGA-O2A-C1
19	5	209	CLA	CBA-CGA-O2A-C1
23	A	853	LHG	O6-C4-C5-C6
23	3	215	LHG	O6-C4-C5-C6
19	u	201	CLA	O1D-CGD-O2D-CED
19	A	827	CLA	C15-C16-C17-C18
19	B	812	CLA	C5-C6-C7-C8
19	A	834	CLA	C16-C17-C18-C19
19	A	811	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	806	CLA	C4-C3-C5-C6
19	B	826	CLA	C4-C3-C5-C6
24	A	854	LMT	C11-C10-C9-C8
19	5	212	CLA	C5-C6-C7-C8
19	A	806	CLA	O1A-CGA-O2A-C1
19	A	809	CLA	O1A-CGA-O2A-C1
19	A	824	CLA	O1A-CGA-O2A-C1
19	A	829	CLA	O1A-CGA-O2A-C1
19	B	813	CLA	O1A-CGA-O2A-C1
23	4	317	LHG	C30-C31-C32-C33
19	B	807	CLA	C2A-CAA-CBA-CGA
19	u	201	CLA	C6-C7-C8-C9
26	B	847	DGD	CAA-CBA-CCA-CDA
23	1	318	LHG	C29-C30-C31-C32
26	B	847	DGD	CFA-CGA-CHA-CIA
23	3	215	LHG	C9-C10-C11-C12
24	2	220	LMT	O5B-C5B-C6B-O6B
19	F	203	CLA	O1A-CGA-O2A-C1
23	M	103	LHG	C27-C28-C29-C30
19	A	818	CLA	C6-C7-C8-C9
23	M	103	LHG	O1-C1-C2-O2
19	A	831	CLA	O1A-CGA-O2A-C1
19	4	311	CLA	O1A-CGA-O2A-C1
19	A	836	CLA	C6-C7-C8-C9
23	A	852	LHG	C28-C29-C30-C31
26	B	847	DGD	CDA-CEA-CFA-CGA
22	B	844	BCR	C16-C17-C18-C36
19	A	820	CLA	C4-C3-C5-C6
19	B	821	CLA	C4-C3-C5-C6
19	5	209	CLA	O1A-CGA-O2A-C1
19	1	304	CLA	CBA-CGA-O2A-C1
19	A	828	CLA	C8-C10-C11-C12
29	1	302	LMG	C42-C43-C44-C45
19	B	821	CLA	C8-C10-C11-C12
19	B	833	CLA	C5-C6-C7-C8
19	3	204	CLA	C10-C11-C12-C13
19	A	843	CLA	C2-C1-O2A-CGA
19	1	303	CLA	C2-C1-O2A-CGA
19	B	816	CLA	O1D-CGD-O2D-CED
19	B	833	CLA	CBA-CGA-O2A-C1
19	3	202	CLA	CBA-CGA-O2A-C1
19	5	208	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	813	CLA	C16-C17-C18-C19
24	3	216	LMT	C5-C6-C7-C8
23	A	852	LHG	O2-C2-C3-O3
23	1	318	LHG	C23-C24-C25-C26
19	5	209	CLA	C10-C11-C12-C13
24	A	854	LMT	C2'-C1'-O1'-C1
27	J	105	5X6	C24-C25-C26-C27
28	1	315	DD6	C4-C5-C6-C8
19	A	811	CLA	O1A-CGA-O2A-C1
31	5	221	A86	O5-C38-O4-C34
19	A	811	CLA	C4-C3-C5-C6
19	A	830	CLA	C4-C3-C5-C6
19	B	805	CLA	C13-C15-C16-C17
19	A	806	CLA	C11-C12-C13-C15
19	A	807	CLA	C11-C12-C13-C15
19	A	812	CLA	C6-C7-C8-C10
19	A	820	CLA	C2-C3-C5-C6
19	A	828	CLA	C11-C10-C8-C7
19	A	842	CLA	C12-C13-C15-C16
19	B	802	CLA	C11-C10-C8-C7
19	B	804	CLA	C6-C7-C8-C10
19	B	821	CLA	C2-C3-C5-C6
19	B	821	CLA	C12-C13-C15-C16
19	B	826	CLA	C2-C3-C5-C6
19	B	837	CLA	C11-C10-C8-C7
19	1	301	CLA	C11-C10-C8-C7
19	1	309	CLA	C11-C12-C13-C15
19	2	206	CLA	C11-C10-C8-C7
19	3	206	CLA	C11-C10-C8-C7
19	3	206	CLA	C12-C13-C15-C16
19	5	207	CLA	C11-C10-C8-C7
19	5	209	CLA	C6-C7-C8-C10
19	L	206	CLA	C3-C5-C6-C7
19	A	825	CLA	C11-C12-C13-C14
19	A	803	CLA	C14-C13-C15-C16
19	A	806	CLA	C11-C12-C13-C14
19	A	807	CLA	C11-C12-C13-C14
19	A	808	CLA	C11-C10-C8-C9
19	A	812	CLA	C6-C7-C8-C9
19	A	812	CLA	C14-C13-C15-C16
19	A	828	CLA	C11-C10-C8-C9
19	B	813	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	B	832	CLA	C14-C13-C15-C16
19	1	301	CLA	C11-C10-C8-C9
20	A	845	PQN	C19-C18-C20-C21
19	A	812	CLA	CBA-CGA-O2A-C1
19	3	204	CLA	CBA-CGA-O2A-C1
23	1	318	LHG	C24-C23-O8-C6
19	A	809	CLA	C2A-CAA-CBA-CGA
19	B	804	CLA	C2A-CAA-CBA-CGA
19	1	304	CLA	O1A-CGA-O2A-C1
28	1	313	DD6	C7-C6-C8-C9
22	A	849	BCR	C21-C22-C23-C24
22	1	314	BCR	C11-C12-C13-C14
19	B	810	CLA	C15-C16-C17-C18
19	B	829	CLA	CBA-CGA-O2A-C1
19	5	208	CLA	C8-C10-C11-C12
23	1	318	LHG	C26-C27-C28-C29
19	B	833	CLA	O1A-CGA-O2A-C1
19	A	809	CLA	CBD-CGD-O2D-CED
23	1	318	LHG	O6-C4-C5-C6
23	4	317	LHG	O6-C4-C5-C6
19	B	802	CLA	C3-C5-C6-C7
19	B	834	CLA	C3-C5-C6-C7
19	A	816	CLA	CBA-CGA-O2A-C1
19	B	807	CLA	CBA-CGA-O2A-C1
19	A	806	CLA	C2-C3-C5-C6
19	A	811	CLA	C2-C3-C5-C6
19	A	830	CLA	C2-C3-C5-C6
23	1	318	LHG	C10-C11-C12-C13
19	A	810	CLA	C10-C11-C12-C13
19	A	825	CLA	O1D-CGD-O2D-CED
19	B	831	CLA	C3-C5-C6-C7
18	A	801	CL0	C16-C17-C18-C20
19	A	811	CLA	C6-C7-C8-C9
19	3	206	CLA	C8-C10-C11-C12
19	4	308	CLA	C2A-CAA-CBA-CGA
19	2	207	CLA	CBA-CGA-O2A-C1
23	3	215	LHG	C7-C8-C9-C10
19	A	807	CLA	C3A-C2A-CAA-CBA
19	A	818	CLA	C3A-C2A-CAA-CBA
19	A	822	CLA	C3A-C2A-CAA-CBA
19	B	804	CLA	C3A-C2A-CAA-CBA
19	B	812	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	B	826	CLA	C3A-C2A-CAA-CBA
19	u	201	CLA	C3A-C2A-CAA-CBA
19	2	205	CLA	C3A-C2A-CAA-CBA
19	3	210	CLA	C3A-C2A-CAA-CBA
24	3	216	LMT	C2-C3-C4-C5
31	2	219	A86	O-C13-C14-C15
31	3	228	A86	O-C13-C14-C15
31	4	314	A86	O-C13-C14-C15
23	3	215	LHG	C23-C24-C25-C26
29	1	302	LMG	C14-C15-C16-C17
19	A	880	CLA	C16-C17-C18-C20
19	4	313	CLA	CBA-CGA-O2A-C1
19	2	209	CLA	C5-C6-C7-C8
23	1	318	LHG	C4-C5-C6-O8
19	A	812	CLA	C13-C15-C16-C17
19	B	806	CLA	C3-C5-C6-C7
19	A	835	CLA	O1D-CGD-O2D-CED
19	A	814	CLA	C4-C3-C5-C6
19	A	834	CLA	C16-C17-C18-C20
19	3	210	CLA	CBD-CGD-O2D-CED
23	A	853	LHG	C31-C32-C33-C34
19	B	818	CLA	C2A-CAA-CBA-CGA
23	B	842	LHG	O1-C1-C2-O2
23	A	852	LHG	C25-C26-C27-C28
19	A	812	CLA	O1A-CGA-O2A-C1
19	3	202	CLA	O1A-CGA-O2A-C1
19	3	204	CLA	O1A-CGA-O2A-C1
19	B	824	CLA	C16-C17-C18-C20
19	u	201	CLA	C6-C7-C8-C10
19	A	844	CLA	C15-C16-C17-C18
19	B	825	CLA	CBD-CGD-O2D-CED
19	B	812	CLA	C13-C15-C16-C17
19	B	807	CLA	O1A-CGA-O2A-C1
19	5	208	CLA	O1A-CGA-O2A-C1
31	4	316	A86	C39-C38-O4-C34
29	1	302	LMG	O1-C7-C8-O7
19	1	303	CLA	C10-C11-C12-C13
19	A	821	CLA	C6-C7-C8-C9
23	1	318	LHG	C12-C13-C14-C15
23	A	852	LHG	C8-C7-O7-C5
19	A	820	CLA	C16-C17-C18-C19
19	A	835	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
19	B	838	CLA	C16-C17-C18-C19
19	5	210	CLA	C10-C11-C12-C13
23	1	318	LHG	C1-C2-C3-O3
19	2	209	CLA	C10-C11-C12-C13
23	A	853	LHG	C28-C29-C30-C31
19	A	835	CLA	C2-C1-O2A-CGA
19	B	838	CLA	C2-C1-O2A-CGA
19	u	201	CLA	C2-C1-O2A-CGA
19	1	306	CLA	C2-C1-O2A-CGA
19	1	309	CLA	C2-C1-O2A-CGA
19	5	212	CLA	C2-C1-O2A-CGA
19	A	842	CLA	C14-C13-C15-C16
19	B	808	CLA	C11-C10-C8-C9
19	B	810	CLA	C6-C7-C8-C9
19	2	205	CLA	C14-C13-C15-C16
19	3	202	CLA	C14-C13-C15-C16
19	3	206	CLA	C6-C7-C8-C9
19	3	207	CLA	C14-C13-C15-C16
26	B	847	DGD	CEA-CFA-CGA-CHA
19	B	826	CLA	C5-C6-C7-C8
19	B	829	CLA	C15-C16-C17-C18
19	A	816	CLA	O1A-CGA-O2A-C1
23	3	215	LHG	C26-C27-C28-C29
19	2	205	CLA	C2A-CAA-CBA-CGA
19	4	310	CLA	C2A-CAA-CBA-CGA
19	A	843	CLA	C16-C17-C18-C20
22	A	847	BCR	C1-C6-C7-C8
22	A	847	BCR	C5-C6-C7-C8
22	A	849	BCR	C1-C6-C7-C8
22	A	849	BCR	C5-C6-C7-C8
22	B	843	BCR	C1-C6-C7-C8
22	B	843	BCR	C5-C6-C7-C8
22	L	202	BCR	C23-C24-C25-C26
22	L	205	BCR	C23-C24-C25-C26
22	L	205	BCR	C23-C24-C25-C30
22	1	314	BCR	C23-C24-C25-C30
19	A	819	CLA	CAA-CBA-CGA-O2A
28	L	209	DD6	C12-C11-C13-C14
23	B	842	LHG	C29-C30-C31-C32
19	A	842	CLA	O1D-CGD-O2D-CED
19	A	814	CLA	C10-C11-C12-C13
19	B	817	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	4	313	CLA	C3-C5-C6-C7
29	1	302	LMG	C34-C35-C36-C37
19	4	301	CLA	C15-C16-C17-C18
19	2	207	CLA	O1A-CGA-O2A-C1
19	A	842	CLA	C5-C6-C7-C8
19	A	803	CLA	C12-C13-C15-C16
19	A	808	CLA	C11-C10-C8-C7
19	B	811	CLA	C12-C13-C15-C16
19	B	813	CLA	C6-C7-C8-C10
19	B	832	CLA	C12-C13-C15-C16
19	B	846	CLA	C11-C10-C8-C7
19	4	301	CLA	C12-C13-C15-C16
19	5	207	CLA	C6-C7-C8-C10
20	A	845	PQN	C17-C18-C20-C21
20	B	839	PQN	C21-C22-C23-C25
28	5	218	DD6	C11-C10-C9-C8
31	1	316	A86	C3-C4-C5-C6
31	5	220	A86	C1-C2-C3-C4
31	5	220	A86	C24-C25-C26-C27
19	A	826	CLA	C16-C17-C18-C20
19	A	829	CLA	C10-C11-C12-C13
19	1	303	CLA	C5-C6-C7-C8
19	B	829	CLA	O1A-CGA-O2A-C1
19	4	313	CLA	O1A-CGA-O2A-C1
19	A	837	CLA	C2A-CAA-CBA-CGA
22	F	201	BCR	C16-C17-C18-C36
22	1	311	BCR	C20-C21-C22-C37
27	J	105	5X6	C42-C13-C14-C15
28	1	315	DD6	C9-C10-C11-C12
29	1	302	LMG	C40-C41-C42-C43
19	B	813	CLA	C16-C17-C18-C20
19	B	805	CLA	C10-C11-C12-C13
19	5	207	CLA	C8-C10-C11-C12
19	A	807	CLA	CBA-CGA-O2A-C1
19	3	206	CLA	CBA-CGA-O2A-C1
19	3	204	CLA	C12-C13-C15-C16
19	A	839	CLA	C8-C10-C11-C12
19	A	808	CLA	CAD-CBD-CGD-O2D
19	A	878	CLA	CAD-CBD-CGD-O2D
19	B	813	CLA	CAD-CBD-CGD-O2D
19	B	814	CLA	CAD-CBD-CGD-O2D
19	B	824	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	L	204	CLA	CAD-CBD-CGD-O2D
19	1	309	CLA	CAD-CBD-CGD-O2D
19	2	208	CLA	CAD-CBD-CGD-O2D
19	2	213	CLA	CAD-CBD-CGD-O2D
19	3	207	CLA	CAD-CBD-CGD-O2D
23	1	318	LHG	C6-C5-O7-C7
30	3	205	KC1	CAD-CBD-CGD-O2D
31	5	217	A86	C28-C27-C29-C30
19	B	826	CLA	C13-C15-C16-C17
19	F	203	CLA	C5-C6-C7-C8
22	1	314	BCR	C22-C23-C24-C25
19	A	838	CLA	CBA-CGA-O2A-C1
19	B	814	CLA	CBA-CGA-O2A-C1
24	1	323	LMT	C9-C10-C11-C12
23	4	317	LHG	C4-C5-C6-O8
29	1	302	LMG	O1-C7-C8-C9
19	A	831	CLA	CBD-CGD-O2D-CED
19	5	213	CLA	CBD-CGD-O2D-CED
23	A	853	LHG	C14-C15-C16-C17
23	1	318	LHG	O6-C4-C5-O7
23	4	317	LHG	O6-C4-C5-O7
19	A	841	CLA	C15-C16-C17-C18
19	3	202	CLA	C3-C5-C6-C7
19	A	807	CLA	CAA-CBA-CGA-O2A
19	B	846	CLA	C2A-CAA-CBA-CGA
22	L	202	BCR	C14-C15-C16-C17
23	1	318	LHG	O10-C23-O8-C6
19	A	806	CLA	CHA-CBD-CGD-O1D
19	A	806	CLA	CHA-CBD-CGD-O2D
19	A	826	CLA	CHA-CBD-CGD-O1D
19	A	826	CLA	CHA-CBD-CGD-O2D
19	B	802	CLA	CHA-CBD-CGD-O2D
19	B	805	CLA	CHA-CBD-CGD-O1D
19	B	808	CLA	CHA-CBD-CGD-O1D
19	B	823	CLA	CHA-CBD-CGD-O1D
19	4	306	CLA	CHA-CBD-CGD-O1D
19	5	215	CLA	CHA-CBD-CGD-O1D
19	3	210	CLA	O1D-CGD-O2D-CED
22	A	848	BCR	C16-C17-C18-C19
28	2	217	DD6	C9-C10-C11-C13
20	B	839	PQN	C18-C20-C21-C22
23	A	853	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
18	A	801	CL0	C15-C16-C17-C18
19	5	208	CLA	C2-C3-C5-C6
19	A	834	CLA	C10-C11-C12-C13
19	A	833	CLA	C14-C13-C15-C16
19	B	837	CLA	C14-C13-C15-C16
19	3	206	CLA	O1A-CGA-O2A-C1
24	2	220	LMT	O1'-C1-C2-C3
29	1	302	LMG	C18-C19-C20-C21
19	B	814	CLA	O1A-CGA-O2A-C1
22	J	104	BCR	C37-C22-C23-C24
22	1	314	BCR	C11-C12-C13-C35
28	1	312	DD6	C12-C11-C13-C14
19	3	207	CLA	C10-C11-C12-C13
31	1	317	A86	C2-C1-C24-C25
31	5	221	A86	C2-C1-C24-C25
19	4	313	CLA	C1A-C2A-CAA-CBA
19	5	215	CLA	C1A-C2A-CAA-CBA
19	B	845	CLA	C2-C1-O2A-CGA
19	2	205	CLA	C2-C1-O2A-CGA
19	A	819	CLA	CBA-CGA-O2A-C1
23	A	853	LHG	C3-O3-P-O6
19	2	208	CLA	C2C-C3C-CAC-CBC
23	4	317	LHG	C2-C3-O3-P
19	B	830	CLA	C2-C3-C5-C6
19	B	817	CLA	C2C-C3C-CAC-CBC
19	A	838	CLA	O1A-CGA-O2A-C1
23	A	853	LHG	C4-O6-P-O4
23	B	842	LHG	C3-O3-P-O5
23	B	842	LHG	C4-O6-P-O5
23	M	103	LHG	C4-O6-P-O4
23	4	317	LHG	C3-O3-P-O5
23	4	317	LHG	C4-O6-P-O4
18	A	801	CL0	C16-C17-C18-C19
26	B	847	DGD	C1B-C2B-C3B-C4B
19	5	210	CLA	CBA-CGA-O2A-C1
23	A	852	LHG	O10-C23-O8-C6
19	A	806	CLA	CAD-CBD-CGD-O1D
19	B	805	CLA	CAD-CBD-CGD-O1D
19	3	209	CLA	CAD-CBD-CGD-O1D
19	5	215	CLA	CAD-CBD-CGD-O1D
30	1	305	KC1	CAD-CBD-CGD-O1D
31	1	317	A86	C26-C27-C29-C30

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Mol	Chain	Res	Type	Atoms
19	5	209	CLA	C8-C10-C11-C12
19	A	828	CLA	C3-C5-C6-C7
19	5	212	CLA	C3-C5-C6-C7
19	B	805	CLA	CBA-CGA-O2A-C1
19	A	803	CLA	C11-C10-C8-C7
19	A	828	CLA	C12-C13-C15-C16
19	A	833	CLA	C12-C13-C15-C16
19	A	834	CLA	C11-C12-C13-C15
19	A	841	CLA	C11-C10-C8-C7
19	B	802	CLA	C12-C13-C15-C16
19	B	804	CLA	C11-C12-C13-C15
19	B	809	CLA	C11-C12-C13-C15
19	B	827	CLA	C11-C12-C13-C15
19	B	834	CLA	C6-C7-C8-C10
19	B	837	CLA	C12-C13-C15-C16
19	1	303	CLA	C12-C13-C15-C16
19	1	304	CLA	C12-C13-C15-C16
19	4	301	CLA	C11-C10-C8-C7
23	A	853	LHG	O6-C4-C5-O7
31	3	214	A86	C24-C25-C26-C27
23	A	853	LHG	C35-C36-C37-C38
19	B	837	CLA	C8-C10-C11-C12
19	B	813	CLA	C2C-C3C-CAC-CBC
31	3	228	A86	O5-C38-O4-C34
19	A	827	CLA	C10-C11-C12-C13
29	1	302	LMG	C7-C8-C9-O8
23	1	318	LHG	O7-C5-C6-O8
19	A	807	CLA	O1A-CGA-O2A-C1
19	A	808	CLA	C10-C11-C12-C13
19	3	206	CLA	C5-C6-C7-C8
19	F	203	CLA	C3-C5-C6-C7
31	4	316	A86	O5-C38-O4-C34
19	A	819	CLA	O1A-CGA-O2A-C1
19	A	832	CLA	O1A-CGA-O2A-C1
19	1	303	CLA	O1D-CGD-O2D-CED
19	A	805	CLA	C4-C3-C5-C6
19	B	813	CLA	C4-C3-C5-C6
31	5	220	A86	C13-C14-C15-C20
19	B	802	CLA	C11-C10-C8-C9
19	B	821	CLA	C6-C7-C8-C9
19	B	846	CLA	C11-C10-C8-C9
19	1	304	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	1	310	CLA	C11-C10-C8-C9
19	4	301	CLA	C14-C13-C15-C16
20	B	839	PQN	C21-C22-C23-C24
19	3	207	CLA	O1D-CGD-O2D-CED
19	A	822	CLA	CBD-CGD-O2D-CED
19	A	817	CLA	O1A-CGA-O2A-C1
19	B	834	CLA	O1A-CGA-O2A-C1
19	5	210	CLA	O1A-CGA-O2A-C1
19	B	808	CLA	C10-C11-C12-C13
19	B	846	CLA	C8-C10-C11-C12
19	5	211	CLA	C5-C6-C7-C8
31	5	219	A86	C1-C24-C25-C26
31	5	220	A86	C1-C24-C25-C26
19	A	831	CLA	O1D-CGD-O2D-CED
19	4	301	CLA	C8-C10-C11-C12
29	1	302	LMG	O10-C28-O8-C9
26	B	847	DGD	CDB-CEB-CFB-CGB
20	A	845	PQN	C26-C27-C28-C29
23	4	317	LHG	C13-C14-C15-C16
19	B	838	CLA	C15-C16-C17-C18
24	3	216	LMT	O1'-C1-C2-C3
19	A	818	CLA	C3-C5-C6-C7
23	A	852	LHG	C32-C33-C34-C35
19	B	813	CLA	C13-C15-C16-C17
19	B	846	CLA	C13-C15-C16-C17
20	A	845	PQN	C26-C27-C28-C30
19	A	819	CLA	C5-C6-C7-C8
23	M	103	LHG	C11-C12-C13-C14
19	A	817	CLA	C1-C2-C3-C4
19	A	823	CLA	C1-C2-C3-C4
19	A	829	CLA	C3-C5-C6-C7
19	B	831	CLA	C13-C15-C16-C17
19	A	878	CLA	C2A-CAA-CBA-CGA
19	3	202	CLA	C2A-CAA-CBA-CGA
19	3	204	CLA	C2A-CAA-CBA-CGA
23	A	852	LHG	O9-C7-O7-C5
19	B	805	CLA	O1A-CGA-O2A-C1
19	A	817	CLA	CBA-CGA-O2A-C1
19	A	832	CLA	CBA-CGA-O2A-C1
19	A	834	CLA	O1D-CGD-O2D-CED
19	3	207	CLA	C2-C1-O2A-CGA
19	3	209	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	5	207	CLA	C2-C1-O2A-CGA
23	1	318	LHG	C2-C3-O3-P
19	B	830	CLA	O1A-CGA-O2A-C1
23	4	317	LHG	O10-C23-O8-C6
22	B	844	BCR	C1-C6-C7-C8
22	B	844	BCR	C5-C6-C7-C8
22	I	101	BCR	C1-C6-C7-C8
22	I	101	BCR	C5-C6-C7-C8
22	L	202	BCR	C23-C24-C25-C30
22	1	314	BCR	C23-C24-C25-C26
19	B	813	CLA	C2-C3-C5-C6
23	1	318	LHG	C15-C16-C17-C18
19	B	817	CLA	C4C-C3C-CAC-CBC
19	B	803	CLA	C16-C17-C18-C19
22	B	843	BCR	C11-C10-C9-C8
28	1	312	DD6	C4-C5-C6-C8
19	B	817	CLA	CAA-CBA-CGA-O2A
23	A	853	LHG	C4-O6-P-O3
23	B	842	LHG	C4-O6-P-O3
23	3	215	LHG	C4-O6-P-O3
19	3	204	CLA	C14-C13-C15-C16
19	B	838	CLA	O1D-CGD-O2D-CED
29	1	302	LMG	C11-C12-C13-C14
23	A	852	LHG	C15-C16-C17-C18
19	4	312	CLA	C4-C3-C5-C6
19	A	812	CLA	C12-C13-C15-C16
19	B	810	CLA	C6-C7-C8-C10
19	2	205	CLA	CAA-CBA-CGA-O2A
19	A	803	CLA	C11-C10-C8-C9
19	A	841	CLA	C11-C10-C8-C9
19	A	878	CLA	C11-C10-C8-C9
19	B	802	CLA	C14-C13-C15-C16
19	1	304	CLA	C14-C13-C15-C16
19	2	209	CLA	C6-C7-C8-C9
19	4	301	CLA	C11-C10-C8-C9
19	5	207	CLA	C11-C10-C8-C9
22	F	201	BCR	C13-C14-C15-C16
27	J	105	5X6	C13-C14-C15-C16
27	J	105	5X6	C23-C24-C25-C26
28	L	209	DD6	C24-C25-C26-C27
31	3	212	A86	C11-C10-C9-C8
31	4	315	A86	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
31	5	217	A86	C11-C10-C9-C8
19	A	826	CLA	C16-C17-C18-C19
19	B	808	CLA	C16-C17-C18-C20
24	A	854	LMT	C7-C8-C9-C10
19	B	822	CLA	C5-C6-C7-C8
29	1	302	LMG	C31-C32-C33-C34
22	M	102	BCR	C7-C8-C9-C34
19	A	814	CLA	C2-C3-C5-C6
19	B	846	CLA	C2-C3-C5-C6
19	B	830	CLA	CBA-CGA-O2A-C1
19	L	203	CLA	CBA-CGA-O2A-C1
19	3	203	CLA	CBA-CGA-O2A-C1
23	M	103	LHG	C10-C11-C12-C13
23	A	853	LHG	C29-C30-C31-C32
22	F	201	BCR	C10-C11-C12-C13
22	L	202	BCR	C18-C19-C20-C21
27	J	105	5X6	C14-C15-C16-C17
23	A	853	LHG	C15-C16-C17-C18
19	A	804	CLA	C4-C3-C5-C6
19	B	846	CLA	C4-C3-C5-C6
18	A	801	CL0	C13-C15-C16-C17
19	A	831	CLA	C5-C6-C7-C8
19	3	202	CLA	CBD-CGD-O2D-CED
19	B	820	CLA	CAA-CBA-CGA-O1A
19	A	817	CLA	C2-C1-O2A-CGA
19	A	844	CLA	C2-C1-O2A-CGA
19	B	802	CLA	C2-C1-O2A-CGA
19	B	812	CLA	C2-C1-O2A-CGA
19	B	837	CLA	C2-C1-O2A-CGA
19	2	209	CLA	C2-C1-O2A-CGA
19	4	301	CLA	C2-C1-O2A-CGA
19	5	209	CLA	C2-C1-O2A-CGA
19	A	842	CLA	C8-C10-C11-C12
19	L	203	CLA	O1A-CGA-O2A-C1
19	F	204	CLA	CAA-CBA-CGA-O1A
19	5	212	CLA	C2A-CAA-CBA-CGA
24	2	220	LMT	C6-C7-C8-C9
19	B	813	CLA	C4C-C3C-CAC-CBC
19	4	310	CLA	C3A-C2A-CAA-CBA
19	A	823	CLA	O2A-C1-C2-C3
31	4	314	A86	C24-C25-C26-C27
31	5	217	A86	O-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
19	L	204	CLA	CAA-CBA-CGA-O1A
19	B	808	CLA	C4-C3-C5-C6
19	5	211	CLA	C8-C10-C11-C12
19	A	805	CLA	C6-C7-C8-C9
19	A	832	CLA	C6-C7-C8-C9
19	A	842	CLA	C11-C10-C8-C9
19	B	814	CLA	C11-C10-C8-C9
19	B	818	CLA	C6-C7-C8-C9
19	B	823	CLA	C6-C7-C8-C9
19	B	826	CLA	C14-C13-C15-C16
19	B	832	CLA	C6-C7-C8-C9
19	B	845	CLA	C11-C10-C8-C9
19	4	306	CLA	C6-C7-C8-C9
19	4	301	CLA	C16-C17-C18-C20
19	B	834	CLA	CBA-CGA-O2A-C1
23	A	852	LHG	C31-C32-C33-C34
19	4	301	CLA	C10-C11-C12-C13
22	B	840	BCR	C16-C17-C18-C36
22	F	205	BCR	C35-C13-C14-C15
31	3	214	A86	C4-C5-C6-C7
31	3	228	A86	C-C1-C2-C3
31	5	219	A86	C25-C26-C27-C28
31	5	220	A86	C25-C26-C27-C28
31	5	220	A86	C4-C5-C6-C7
31	5	221	A86	C4-C5-C6-C7
19	5	213	CLA	CAA-CBA-CGA-O1A
19	1	310	CLA	C2A-CAA-CBA-CGA
19	5	210	CLA	C2A-CAA-CBA-CGA
19	5	208	CLA	C10-C11-C12-C13
19	B	803	CLA	C16-C17-C18-C20
19	B	807	CLA	C16-C17-C18-C20
19	B	829	CLA	O2A-C1-C2-C3
24	1	323	LMT	C3-C4-C5-C6
19	B	818	CLA	C3-C5-C6-C7
19	B	836	CLA	C3-C5-C6-C7
19	1	304	CLA	C13-C15-C16-C17
19	4	309	CLA	CAA-CBA-CGA-O1A
19	B	802	CLA	C4-C3-C5-C6
19	B	814	CLA	C4-C3-C5-C6
19	B	834	CLA	C4-C3-C5-C6
19	B	845	CLA	C4-C3-C5-C6
19	L	206	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	u	201	CLA	C1A-C2A-CAA-CBA
19	4	306	CLA	C1A-C2A-CAA-CBA
19	4	310	CLA	C1A-C2A-CAA-CBA
19	4	311	CLA	C1A-C2A-CAA-CBA
19	5	208	CLA	C11-C12-C13-C14
19	A	833	CLA	C11-C12-C13-C15
19	B	805	CLA	C11-C12-C13-C15
19	B	806	CLA	C6-C7-C8-C10
19	B	808	CLA	C11-C10-C8-C7
19	B	846	CLA	C12-C13-C15-C16
19	L	206	CLA	C11-C10-C8-C7
19	1	304	CLA	C11-C12-C13-C15
19	3	202	CLA	C12-C13-C15-C16
19	5	209	CLA	C11-C12-C13-C15
19	B	832	CLA	O1A-CGA-O2A-C1
19	B	820	CLA	CAA-CBA-CGA-O2A
19	B	832	CLA	CBA-CGA-O2A-C1
19	B	807	CLA	C13-C15-C16-C17
23	A	852	LHG	C17-C18-C19-C20
23	M	103	LHG	C19-C20-C21-C22
23	M	103	LHG	C5-C4-O6-P
23	4	317	LHG	C5-C4-O6-P
19	A	810	CLA	C2A-CAA-CBA-CGA
19	B	825	CLA	C2A-CAA-CBA-CGA
19	5	209	CLA	C15-C16-C17-C18
19	F	204	CLA	CAA-CBA-CGA-O2A
19	J	103	CLA	CAA-CBA-CGA-O1A
30	2	211	KC1	C3A-C2A-CAA-CBA
30	3	205	KC1	C3A-C2A-CAA-CBA
19	A	844	CLA	C16-C17-C18-C19
19	4	306	CLA	C8-C10-C11-C12
19	5	213	CLA	CAA-CBA-CGA-O2A
19	A	809	CLA	O1D-CGD-O2D-CED
19	2	212	CLA	CAA-CBA-CGA-O1A
19	A	822	CLA	O1D-CGD-O2D-CED
19	A	841	CLA	C13-C15-C16-C17
19	A	844	CLA	C13-C15-C16-C17
19	B	802	CLA	C5-C6-C7-C8
19	5	211	CLA	CBD-CGD-O2D-CED
22	F	205	BCR	C12-C13-C14-C15
31	2	218	A86	C13-C14-C15-C16
31	2	219	A86	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
31	3	214	A86	C4-C5-C6-C8
31	3	228	A86	C24-C1-C2-C3
31	4	314	A86	C13-C14-C15-C16
31	5	217	A86	C13-C14-C15-C16
31	5	219	A86	C25-C26-C27-C29
31	5	220	A86	C25-C26-C27-C29
31	5	220	A86	C4-C5-C6-C8
31	5	221	A86	C13-C14-C15-C16
31	5	221	A86	C4-C5-C6-C8
19	J	103	CLA	CAA-CBA-CGA-O2A
23	A	853	LHG	O7-C5-C6-O8
31	1	317	A86	C11-C10-C9-C8
19	2	212	CLA	CAA-CBA-CGA-O2A
19	5	214	CLA	CAA-CBA-CGA-O1A
19	B	829	CLA	C10-C11-C12-C13
19	A	806	CLA	C10-C11-C12-C13
19	3	203	CLA	O1A-CGA-O2A-C1
19	B	825	CLA	C4-C3-C5-C6
19	F	203	CLA	C4-C3-C5-C6
19	1	303	CLA	C4-C3-C5-C6
19	A	812	CLA	C2-C1-O2A-CGA
19	A	816	CLA	C2-C1-O2A-CGA
19	A	825	CLA	C2-C1-O2A-CGA
19	A	832	CLA	C2-C1-O2A-CGA
19	1	307	CLA	C2-C1-O2A-CGA
19	B	808	CLA	C2-C3-C5-C6
19	B	834	CLA	C2-C3-C5-C6
19	4	312	CLA	C2-C3-C5-C6
19	A	814	CLA	C8-C10-C11-C12
19	4	309	CLA	CAA-CBA-CGA-O2A
23	1	318	LHG	C25-C26-C27-C28
19	4	301	CLA	C3-C5-C6-C7
19	A	822	CLA	C2A-CAA-CBA-CGA
18	A	801	CL0	O1A-CGA-O2A-C1
22	A	849	BCR	C23-C24-C25-C30
22	B	840	BCR	C1-C6-C7-C8
22	B	852	BCR	C1-C6-C7-C8
22	B	852	BCR	C5-C6-C7-C8
22	F	205	BCR	C1-C6-C7-C8
22	1	311	BCR	C23-C24-C25-C30
23	B	842	LHG	C4-C5-C6-O8
22	A	848	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	A	802	CLA	C4-C3-C5-C6
19	A	828	CLA	C4-C3-C5-C6
19	1	301	CLA	C4-C3-C5-C6
19	2	208	CLA	C4-C3-C5-C6
19	3	202	CLA	C4-C3-C5-C6
19	5	207	CLA	C4-C3-C5-C6
19	5	211	CLA	C4-C3-C5-C6
19	A	805	CLA	C2-C3-C5-C6
19	B	814	CLA	C2-C3-C5-C6
19	B	845	CLA	C2-C3-C5-C6
19	1	308	CLA	CAA-CBA-CGA-O2A
22	B	852	BCR	C14-C15-C16-C17
19	A	841	CLA	C16-C17-C18-C20
19	B	814	CLA	C16-C17-C18-C20
19	2	207	CLA	C3-C5-C6-C7
19	2	213	CLA	CAA-CBA-CGA-O2A
23	A	852	LHG	C10-C11-C12-C13
19	2	213	CLA	CAA-CBA-CGA-O1A
19	4	308	CLA	CAA-CBA-CGA-O2A
23	A	853	LHG	C24-C25-C26-C27
19	A	825	CLA	C4-C3-C5-C6
19	B	831	CLA	C4-C3-C5-C6
19	A	828	CLA	C2-C3-C5-C6
19	F	203	CLA	C2-C3-C5-C6
19	L	204	CLA	CAA-CBA-CGA-O2A
22	1	314	BCR	C9-C10-C11-C12
19	4	305	CLA	C16-C17-C18-C19
31	2	216	A86	C35-C34-O4-C38
19	B	835	CLA	CAA-CBA-CGA-O2A
23	A	853	LHG	O8-C23-C24-C25
26	B	847	DGD	O2G-C1B-C2B-C3B
23	A	852	LHG	C13-C14-C15-C16
22	1	314	BCR	C16-C17-C18-C36
23	4	317	LHG	C17-C18-C19-C20
19	A	826	CLA	CAA-CBA-CGA-O2A
19	B	813	CLA	CAA-CBA-CGA-O2A
19	u	201	CLA	CAA-CBA-CGA-O2A
19	B	821	CLA	C5-C6-C7-C8
19	A	804	CLA	C2-C3-C5-C6
19	L	206	CLA	C2-C3-C5-C6
19	2	208	CLA	C2-C3-C5-C6
19	1	310	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
23	A	853	LHG	C17-C18-C19-C20
19	A	828	CLA	C14-C13-C15-C16
19	A	834	CLA	C11-C12-C13-C14
19	B	805	CLA	C11-C12-C13-C14
19	B	806	CLA	C11-C10-C8-C9
19	B	809	CLA	C11-C12-C13-C14
19	B	834	CLA	C6-C7-C8-C9
19	A	802	CLA	C3A-C2A-CAA-CBA
19	B	811	CLA	C3A-C2A-CAA-CBA
19	B	813	CLA	C3A-C2A-CAA-CBA
19	B	819	CLA	C3A-C2A-CAA-CBA
19	5	212	CLA	C3A-C2A-CAA-CBA
19	A	830	CLA	O1A-CGA-O2A-C1
19	A	807	CLA	CAD-CBD-CGD-O2D
19	A	816	CLA	CAD-CBD-CGD-O2D
19	A	819	CLA	CAD-CBD-CGD-O2D
19	A	823	CLA	CAD-CBD-CGD-O2D
19	A	827	CLA	CAD-CBD-CGD-O2D
19	A	832	CLA	CAD-CBD-CGD-O2D
19	A	844	CLA	CAD-CBD-CGD-O2D
19	B	833	CLA	CAD-CBD-CGD-O2D
19	B	846	CLA	CAD-CBD-CGD-O2D
19	J	103	CLA	CAD-CBD-CGD-O2D
19	1	308	CLA	CAD-CBD-CGD-O2D
19	2	209	CLA	CAD-CBD-CGD-O2D
19	4	303	CLA	CAD-CBD-CGD-O2D
19	4	308	CLA	CAD-CBD-CGD-O2D
19	B	813	CLA	C5-C6-C7-C8
19	A	842	CLA	C2A-CAA-CBA-CGA
19	4	304	CLA	CBD-CGD-O2D-CED
19	B	846	CLA	C2-C1-O2A-CGA
19	A	837	CLA	CAA-CBA-CGA-O2A
19	B	838	CLA	CAA-CBA-CGA-O2A
19	3	207	CLA	CAA-CBA-CGA-O2A
19	5	209	CLA	CAA-CBA-CGA-O2A
22	A	848	BCR	C22-C23-C24-C25
19	B	845	CLA	O1A-CGA-O2A-C1
23	1	318	LHG	C11-C12-C13-C14
19	B	812	CLA	C4-C3-C5-C6
19	A	837	CLA	CAA-CBA-CGA-O1A
19	1	308	CLA	CAA-CBA-CGA-O1A
19	B	825	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	1	301	CLA	C2-C3-C5-C6
19	5	211	CLA	C2-C3-C5-C6
19	B	803	CLA	CAA-CBA-CGA-O2A
19	3	206	CLA	CAA-CBA-CGA-O2A
22	1	311	BCR	C21-C22-C23-C24
28	1	312	DD6	C13-C14-C15-O1
28	1	313	DD6	C13-C14-C15-O1
31	5	220	A86	C12-C11-C13-O
19	4	308	CLA	CAA-CBA-CGA-O1A
19	B	809	CLA	CAA-CBA-CGA-O2A
24	A	854	LMT	C5'-C4'-O1B-C1B
19	A	826	CLA	O2A-C1-C2-C3
19	4	313	CLA	O2A-C1-C2-C3
18	A	801	CL0	CBA-CGA-O2A-C1
19	A	843	CLA	C10-C11-C12-C13
19	A	843	CLA	C16-C17-C18-C19
19	5	208	CLA	C11-C12-C13-C15
19	A	803	CLA	CHA-CBD-CGD-O1D
19	A	803	CLA	CHA-CBD-CGD-O2D
19	A	804	CLA	CHA-CBD-CGD-O1D
19	A	804	CLA	CHA-CBD-CGD-O2D
19	A	812	CLA	CHA-CBD-CGD-O1D
19	A	812	CLA	CHA-CBD-CGD-O2D
19	A	828	CLA	CHA-CBD-CGD-O1D
19	B	804	CLA	CHA-CBD-CGD-O2D
19	B	805	CLA	CHA-CBD-CGD-O2D
19	B	809	CLA	CHA-CBD-CGD-O1D
19	B	809	CLA	CHA-CBD-CGD-O2D
19	B	813	CLA	CHA-CBD-CGD-O2D
19	B	821	CLA	CHA-CBD-CGD-O2D
19	B	822	CLA	CHA-CBD-CGD-O2D
19	B	828	CLA	CHA-CBD-CGD-O2D
19	F	204	CLA	CHA-CBD-CGD-O1D
19	F	204	CLA	CHA-CBD-CGD-O2D
19	u	202	CLA	CHA-CBD-CGD-O1D
19	2	205	CLA	CHA-CBD-CGD-O1D
19	2	205	CLA	CHA-CBD-CGD-O2D
19	2	206	CLA	CHA-CBD-CGD-O2D
19	2	213	CLA	CHA-CBD-CGD-O2D
19	3	209	CLA	CHA-CBD-CGD-O1D
19	4	306	CLA	CHA-CBD-CGD-O2D
19	4	308	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	4	312	CLA	CHA-CBD-CGD-O1D
19	4	312	CLA	CHA-CBD-CGD-O2D
19	5	215	CLA	CHA-CBD-CGD-O2D
30	3	208	KC1	CHA-CBD-CGD-O1D
30	3	208	KC1	CHA-CBD-CGD-O2D
19	A	802	CLA	C2-C3-C5-C6
19	B	838	CLA	C10-C11-C12-C13
19	A	839	CLA	CAA-CBA-CGA-O2A
19	B	807	CLA	CAA-CBA-CGA-O2A
24	1	323	LMT	C4B-C5B-C6B-O6B
19	5	209	CLA	C2A-CAA-CBA-CGA
19	5	214	CLA	CAA-CBA-CGA-O2A
31	5	220	A86	C10-C11-C13-O
19	A	830	CLA	C15-C16-C17-C18
19	A	830	CLA	CBA-CGA-O2A-C1
19	B	845	CLA	CBA-CGA-O2A-C1
19	B	814	CLA	CAA-CBA-CGA-O2A
19	A	803	CLA	C4-C3-C5-C6
19	3	207	CLA	C12-C13-C15-C16
19	A	844	CLA	C16-C17-C18-C20
19	A	814	CLA	CAA-CBA-CGA-O2A
19	A	844	CLA	C3-C5-C6-C7
19	B	805	CLA	C11-C10-C8-C9
19	B	806	CLA	C11-C12-C13-C14
19	B	827	CLA	C6-C7-C8-C9
19	B	846	CLA	C14-C13-C15-C16
19	5	209	CLA	C11-C12-C13-C14
23	M	103	LHG	O8-C23-C24-C25
29	1	302	LMG	O7-C10-C11-C12
19	A	819	CLA	C2A-CAA-CBA-CGA
19	1	306	CLA	C2A-CAA-CBA-CGA
19	B	835	CLA	CAA-CBA-CGA-O1A
19	A	840	CLA	CAA-CBA-CGA-O2A
19	A	878	CLA	CBD-CGD-O2D-CED
19	1	310	CLA	CAA-CBA-CGA-O1A
22	B	841	BCR	C21-C22-C23-C24
31	3	228	A86	C5-C6-C8-C9
19	A	822	CLA	C1A-C2A-CAA-CBA
19	B	804	CLA	C1A-C2A-CAA-CBA
19	B	812	CLA	C1A-C2A-CAA-CBA
19	B	813	CLA	C1A-C2A-CAA-CBA
19	B	826	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	1	306	CLA	C1A-C2A-CAA-CBA
19	2	214	CLA	C1A-C2A-CAA-CBA
19	A	814	CLA	CAA-CBA-CGA-O1A
19	B	838	CLA	CAA-CBA-CGA-O1A
19	u	201	CLA	CAA-CBA-CGA-O1A
23	M	103	LHG	O10-C23-C24-C25
19	B	826	CLA	CAA-CBA-CGA-O2A
19	3	209	CLA	CAA-CBA-CGA-O2A
19	A	818	CLA	C2-C1-O2A-CGA
26	B	847	DGD	C8A-C9A-CAA-CBA
19	2	206	CLA	CBA-CGA-O2A-C1
19	A	826	CLA	CAA-CBA-CGA-O1A
19	B	809	CLA	CAA-CBA-CGA-O1A
19	B	813	CLA	CAA-CBA-CGA-O1A
19	2	209	CLA	CAA-CBA-CGA-O2A
19	A	813	CLA	C2A-CAA-CBA-CGA
19	A	819	CLA	CAA-CBA-CGA-O1A
19	B	809	CLA	C4-C3-C5-C6
19	A	813	CLA	CAA-CBA-CGA-O2A
19	5	212	CLA	CAA-CBA-CGA-O2A
23	B	842	LHG	O9-C7-O7-C5
19	B	803	CLA	CAA-CBA-CGA-O1A
23	A	852	LHG	O10-C23-C24-C25
19	2	206	CLA	O1A-CGA-O2A-C1
24	2	220	LMT	C2'-C1'-O1'-C1
19	B	814	CLA	C15-C16-C17-C18
23	A	853	LHG	C4-O6-P-O5
23	M	103	LHG	C3-O3-P-O4
19	3	206	CLA	O1D-CGD-O2D-CED
19	3	207	CLA	CAA-CBA-CGA-O1A
19	5	209	CLA	CAA-CBA-CGA-O1A
19	B	805	CLA	CAA-CBA-CGA-O2A
23	3	215	LHG	C27-C28-C29-C30
22	A	849	BCR	C23-C24-C25-C26
22	B	840	BCR	C5-C6-C7-C8
26	B	847	DGD	CFB-CGB-CHB-CIB
19	B	806	CLA	C8-C10-C11-C12
19	3	206	CLA	CAA-CBA-CGA-O1A
19	A	804	CLA	CAA-CBA-CGA-O2A
19	4	305	CLA	C15-C16-C17-C18
24	2	220	LMT	C3-C4-C5-C6
19	A	807	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	B	852	BCR	C19-C20-C21-C22
19	A	821	CLA	CAD-CBD-CGD-O1D
19	A	828	CLA	CAD-CBD-CGD-O1D
19	A	840	CLA	CAD-CBD-CGD-O1D
19	B	809	CLA	CAD-CBD-CGD-O1D
19	B	827	CLA	CAD-CBD-CGD-O1D
19	B	838	CLA	CAD-CBD-CGD-O1D
19	u	202	CLA	CAD-CBD-CGD-O1D
31	1	316	A86	C26-C27-C29-C30
19	A	829	CLA	CAA-CBA-CGA-O2A
19	A	809	CLA	C11-C10-C8-C9
19	A	839	CLA	C6-C7-C8-C9
19	B	806	CLA	C6-C7-C8-C9
19	B	811	CLA	C6-C7-C8-C9
19	B	813	CLA	C14-C13-C15-C16
19	B	818	CLA	C11-C10-C8-C9
19	2	209	CLA	CBA-CGA-O2A-C1
19	A	828	CLA	CAA-CBA-CGA-O2A
19	1	309	CLA	CBD-CGD-O2D-CED
19	A	803	CLA	CAA-CBA-CGA-O2A
19	A	805	CLA	CAA-CBA-CGA-O2A
19	B	834	CLA	CAA-CBA-CGA-O2A
23	A	852	LHG	O8-C23-C24-C25
19	A	835	CLA	C5-C6-C7-C8
19	B	814	CLA	CAA-CBA-CGA-O1A
19	3	209	CLA	CAA-CBA-CGA-O1A
19	2	205	CLA	C4-C3-C5-C6
19	B	829	CLA	C5-C6-C7-C8
18	A	801	CL0	C12-C13-C15-C16
19	A	804	CLA	C11-C10-C8-C7
19	B	802	CLA	C2-C3-C5-C6
19	B	805	CLA	C11-C10-C8-C7
19	B	806	CLA	C11-C12-C13-C15
19	B	811	CLA	C11-C10-C8-C7
19	B	818	CLA	C11-C10-C8-C7
19	B	827	CLA	C6-C7-C8-C10
19	B	837	CLA	C11-C12-C13-C15
19	1	303	CLA	C6-C7-C8-C10
19	2	205	CLA	C11-C10-C8-C7
19	3	202	CLA	C2-C3-C5-C6
19	B	807	CLA	CAA-CBA-CGA-O1A
19	B	806	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	B	829	CLA	CAA-CBA-CGA-O2A
22	B	843	BCR	C7-C8-C9-C10
22	F	201	BCR	C7-C8-C9-C10
22	I	102	BCR	C7-C8-C9-C10
28	5	218	DD6	C2-C1-C24-C25
31	3	212	A86	C2-C1-C24-C25
19	A	840	CLA	CAA-CBA-CGA-O1A
19	B	829	CLA	CAA-CBA-CGA-O1A
19	2	209	CLA	CAA-CBA-CGA-O1A
19	L	206	CLA	CAA-CBA-CGA-O2A
19	B	825	CLA	O1D-CGD-O2D-CED
19	2	205	CLA	C15-C16-C17-C18
26	B	847	DGD	CBB-CCB-CDB-CEB
19	A	805	CLA	CAA-CBA-CGA-O1A
19	A	813	CLA	CAA-CBA-CGA-O1A
19	A	828	CLA	CAA-CBA-CGA-O1A
19	A	839	CLA	CAA-CBA-CGA-O1A
19	B	806	CLA	CAA-CBA-CGA-O1A
19	5	212	CLA	CAA-CBA-CGA-O1A
19	B	815	CLA	CAA-CBA-CGA-O2A
19	B	810	CLA	CAA-CBA-CGA-O2A
19	B	832	CLA	C5-C6-C7-C8
19	3	202	CLA	C8-C10-C11-C12
19	B	817	CLA	C2A-CAA-CBA-CGA

There are no ring outliers.

179 monomers are involved in 527 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	830	CLA	1	0
26	B	847	DGD	9	0
19	A	842	CLA	4	0
19	B	825	CLA	3	0
19	B	804	CLA	9	0
19	1	309	CLA	6	0
19	5	213	CLA	2	0
19	B	815	CLA	4	0
28	3	213	DD6	1	0
19	B	833	CLA	6	0
19	B	812	CLA	6	0
19	B	846	CLA	1	0
19	B	808	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	4	308	CLA	4	0
19	A	831	CLA	2	0
19	B	838	CLA	5	0
19	4	304	CLA	1	0
19	2	214	CLA	1	0
19	A	818	CLA	4	0
19	1	301	CLA	2	0
19	A	816	CLA	1	0
19	A	843	CLA	5	0
30	3	211	KC1	1	0
19	A	812	CLA	3	0
19	3	202	CLA	4	0
22	B	840	BCR	4	0
23	A	852	LHG	3	0
19	5	216	CLA	2	0
20	A	845	PQN	2	0
19	B	823	CLA	3	0
19	B	819	CLA	5	0
19	B	813	CLA	8	0
19	A	832	CLA	3	0
19	B	831	CLA	4	0
19	A	817	CLA	5	0
19	A	802	CLA	5	0
24	2	220	LMT	1	0
19	2	207	CLA	7	0
19	A	822	CLA	5	0
19	1	304	CLA	2	0
31	1	316	A86	1	0
31	3	228	A86	1	0
24	3	216	LMT	1	0
23	A	853	LHG	7	0
19	B	817	CLA	1	0
19	A	809	CLA	2	0
19	B	802	CLA	2	0
19	A	835	CLA	4	0
19	B	818	CLA	2	0
19	1	308	CLA	3	0
22	F	201	BCR	5	0
19	A	829	CLA	7	0
19	A	813	CLA	2	0
31	2	216	A86	2	0
22	B	843	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	I	101	BCR	3	0
19	B	828	CLA	1	0
19	4	311	CLA	2	0
19	B	809	CLA	2	0
19	A	838	CLA	1	0
19	A	819	CLA	4	0
19	A	823	CLA	2	0
19	B	820	CLA	1	0
19	A	841	CLA	7	0
31	4	315	A86	2	0
19	A	821	CLA	7	0
19	2	213	CLA	3	0
19	A	811	CLA	3	0
19	5	207	CLA	1	0
22	A	850	BCR	1	0
19	A	807	CLA	4	0
19	B	822	CLA	5	0
22	B	852	BCR	2	0
19	F	203	CLA	2	0
22	1	314	BCR	3	0
19	3	209	CLA	3	0
19	5	209	CLA	5	0
19	4	312	CLA	2	0
19	5	211	CLA	2	0
19	B	821	CLA	5	0
19	A	878	CLA	9	0
19	A	827	CLA	3	0
22	I	102	BCR	7	0
22	L	205	BCR	4	0
19	B	807	CLA	6	0
19	3	207	CLA	2	0
19	J	103	CLA	3	0
22	B	844	BCR	6	0
22	M	102	BCR	4	0
19	2	210	CLA	6	0
19	2	215	CLA	2	0
19	2	208	CLA	3	0
19	B	830	CLA	3	0
19	1	306	CLA	6	0
23	3	215	LHG	2	0
19	L	204	CLA	3	0
22	J	104	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	803	CLA	6	0
19	3	203	CLA	4	0
19	3	210	CLA	2	0
19	A	880	CLA	6	0
19	A	803	CLA	3	0
19	B	805	CLA	4	0
23	M	103	LHG	3	0
22	B	841	BCR	2	0
19	B	811	CLA	7	0
19	B	836	CLA	5	0
19	A	825	CLA	2	0
19	L	203	CLA	5	0
18	A	801	CL0	5	0
19	A	808	CLA	3	0
19	F	204	CLA	2	0
19	B	835	CLA	3	0
19	3	204	CLA	5	0
22	1	311	BCR	4	0
22	A	849	BCR	1	0
19	4	309	CLA	3	0
19	B	814	CLA	3	0
20	B	839	PQN	2	0
31	5	220	A86	1	0
22	F	205	BCR	2	0
19	3	206	CLA	14	0
19	A	806	CLA	8	0
23	1	318	LHG	6	0
19	4	306	CLA	3	0
31	5	219	A86	1	0
19	B	832	CLA	7	0
19	2	205	CLA	10	0
19	A	805	CLA	3	0
19	2	209	CLA	1	0
22	L	202	BCR	1	0
19	B	810	CLA	3	0
30	3	208	KC1	1	0
19	B	806	CLA	2	0
19	B	826	CLA	3	0
23	4	317	LHG	6	0
19	A	837	CLA	2	0
19	A	834	CLA	10	0
19	5	214	CLA	3	0

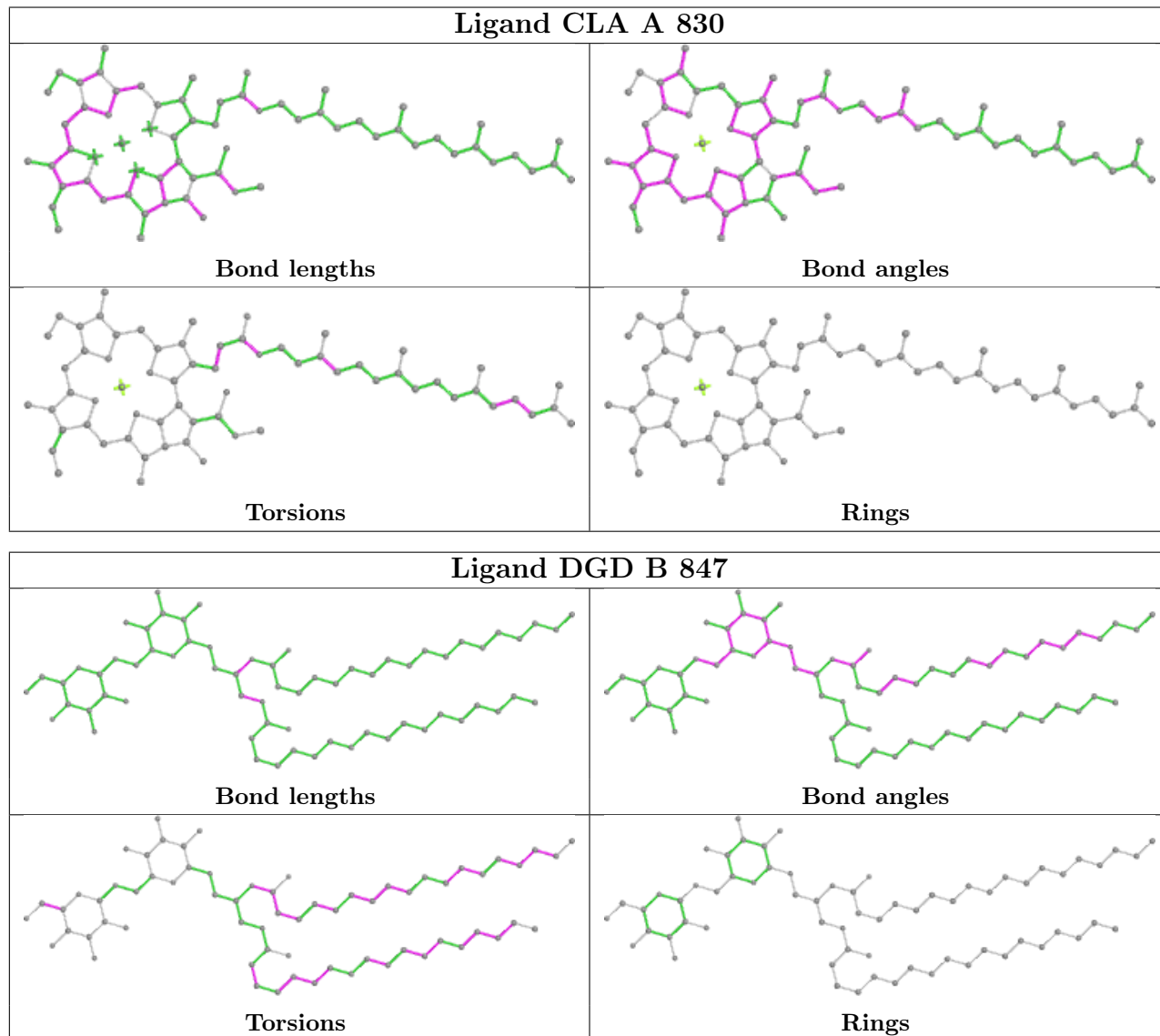
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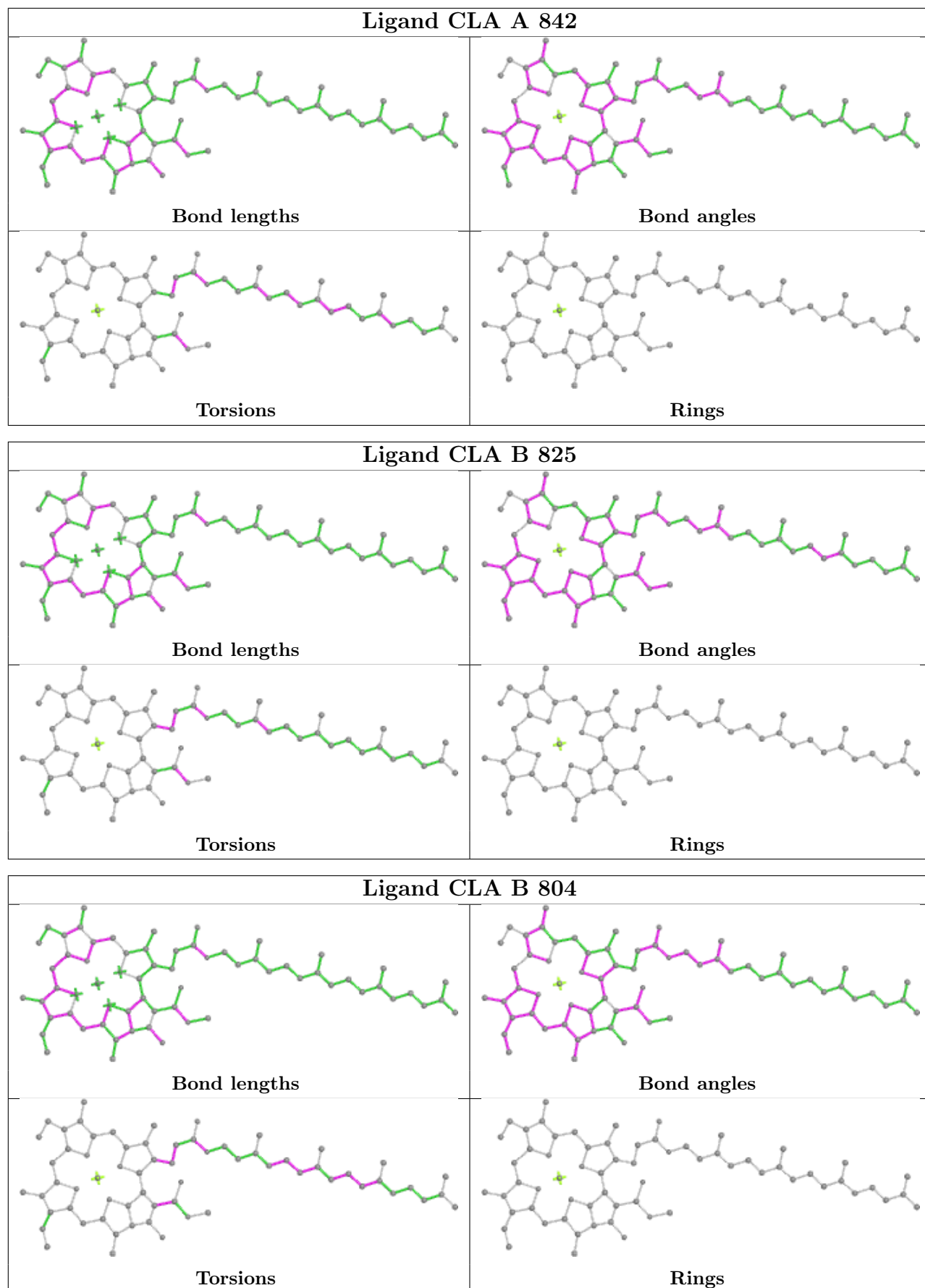
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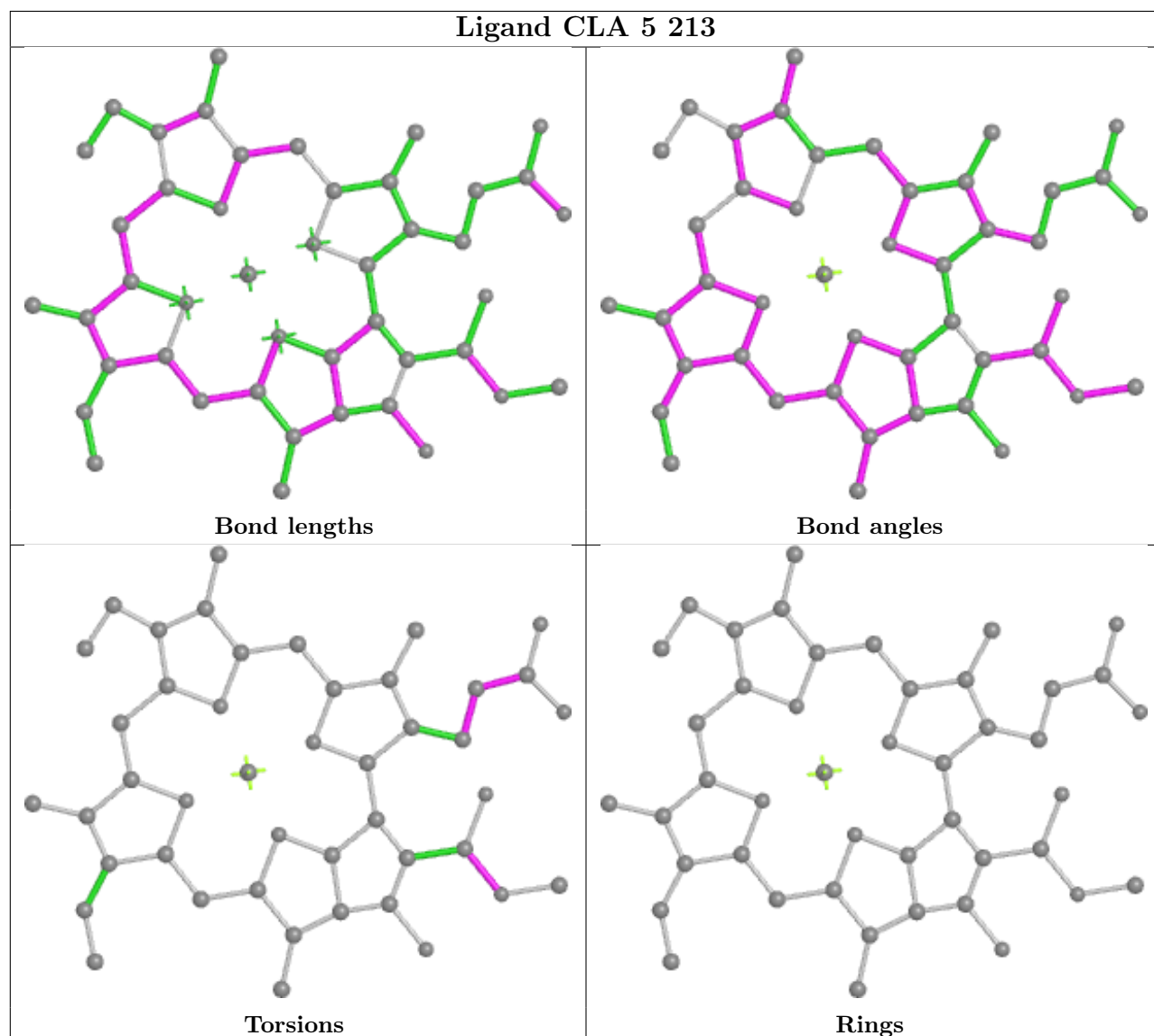
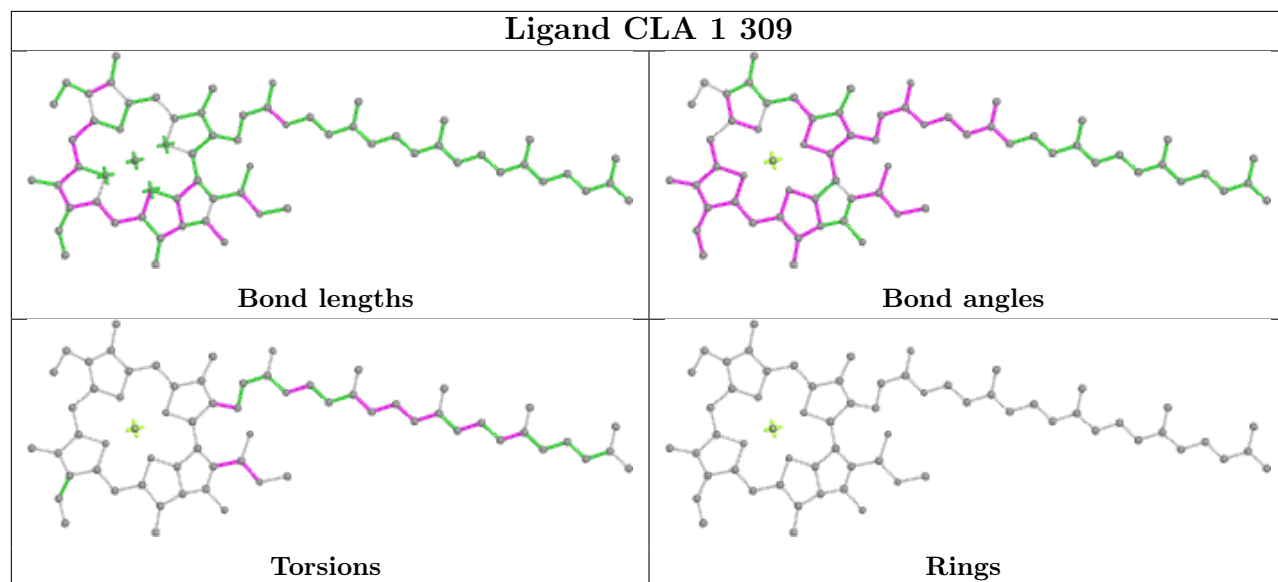
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	836	CLA	4	0
19	B	829	CLA	5	0
31	5	217	A86	2	0
19	2	206	CLA	8	0
19	A	824	CLA	4	0
19	L	206	CLA	5	0
22	A	851	BCR	5	0
19	5	210	CLA	5	0
19	4	310	CLA	4	0
28	5	218	DD6	1	0
19	A	833	CLA	6	0
19	A	814	CLA	5	0
31	4	316	A86	3	0
19	B	837	CLA	6	0
22	A	848	BCR	2	0
19	4	305	CLA	2	0
19	5	212	CLA	6	0
19	4	301	CLA	7	0
22	A	847	BCR	3	0
19	A	820	CLA	5	0
19	A	844	CLA	6	0
19	A	839	CLA	7	0
19	1	310	CLA	8	0
19	1	307	CLA	5	0
19	5	208	CLA	3	0
31	1	317	A86	1	0
19	A	840	CLA	3	0
19	B	816	CLA	2	0
19	B	845	CLA	5	0
19	4	313	CLA	2	0
19	A	804	CLA	8	0
19	A	810	CLA	4	0
19	A	815	CLA	1	0
19	A	826	CLA	8	0
23	B	842	LHG	1	0
19	1	303	CLA	6	0
19	4	303	CLA	5	0
24	1	323	LMT	4	0
19	A	828	CLA	3	0
19	B	824	CLA	1	0

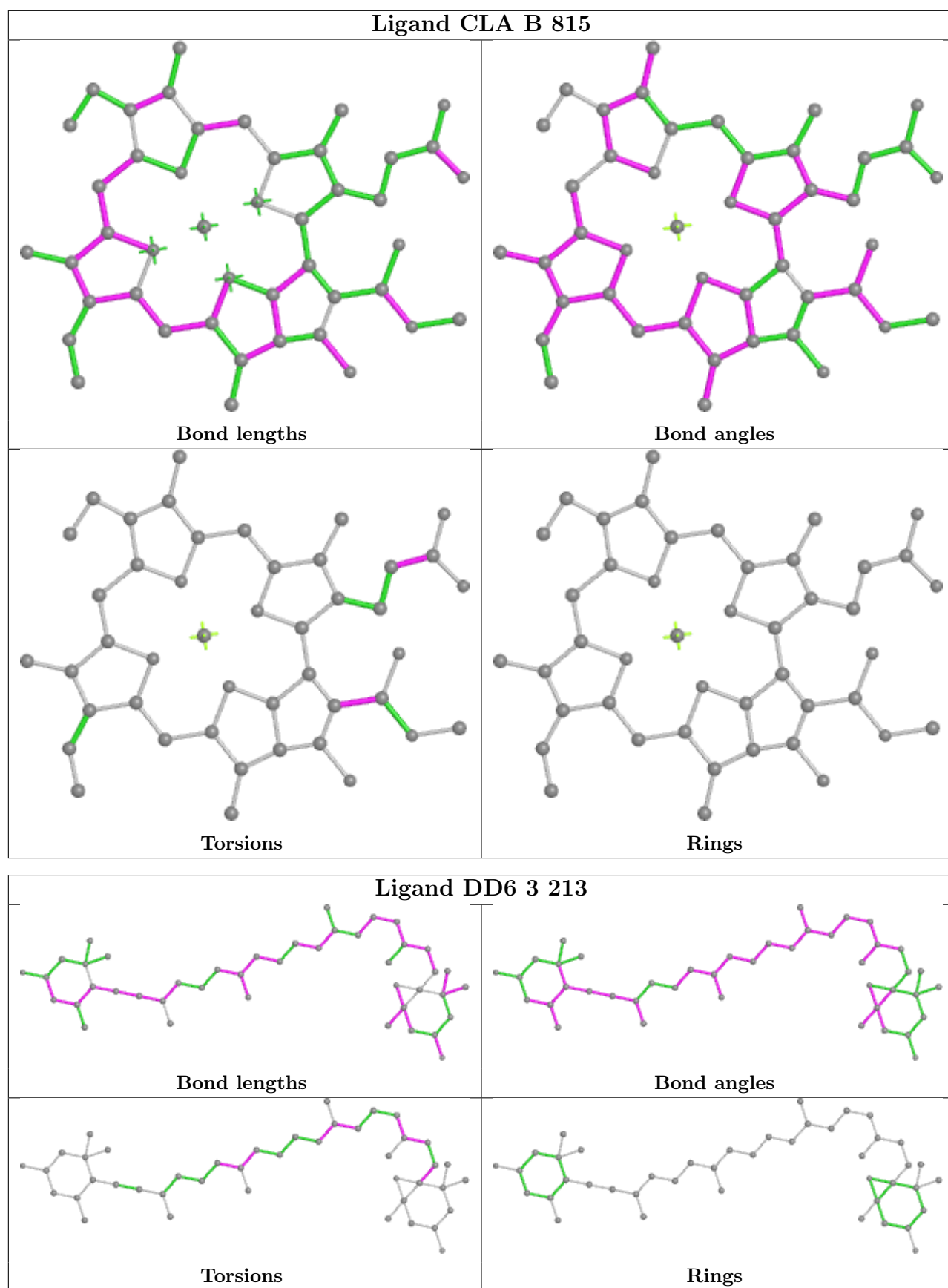
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

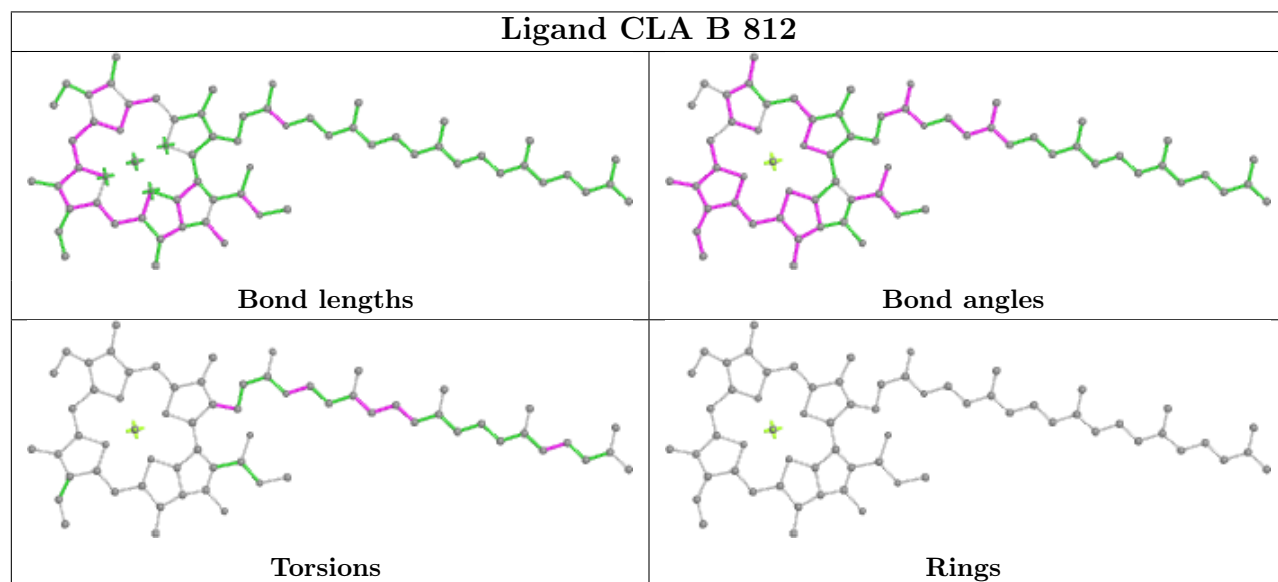
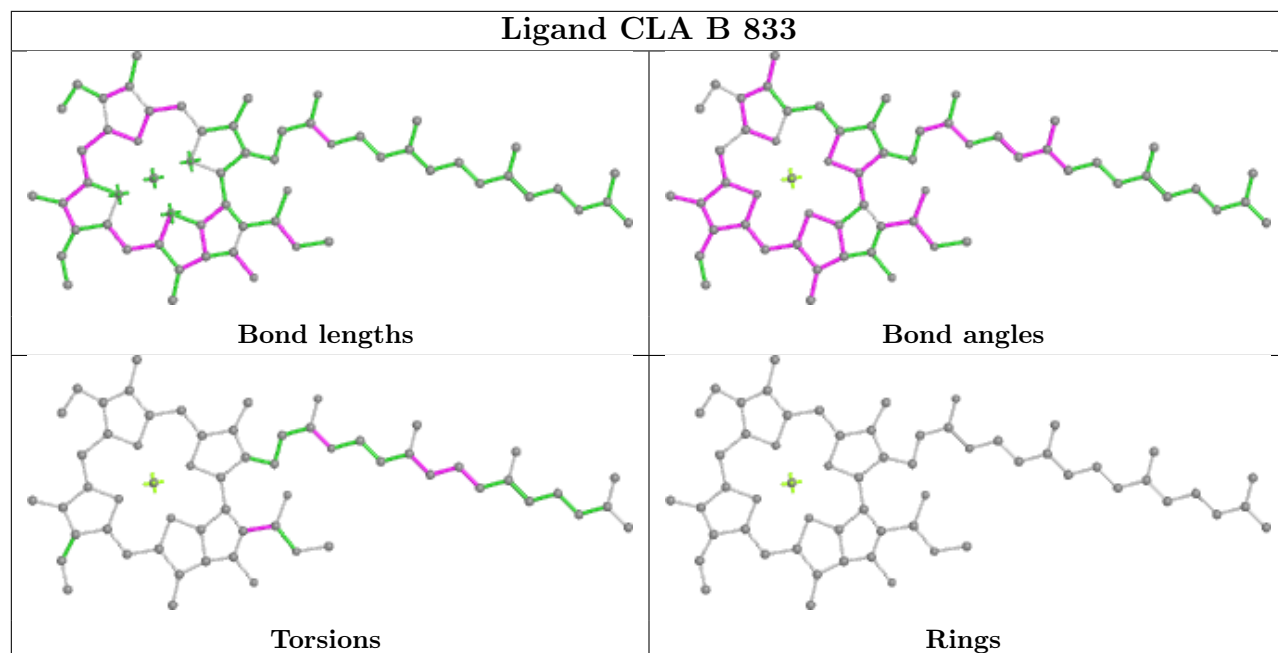
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

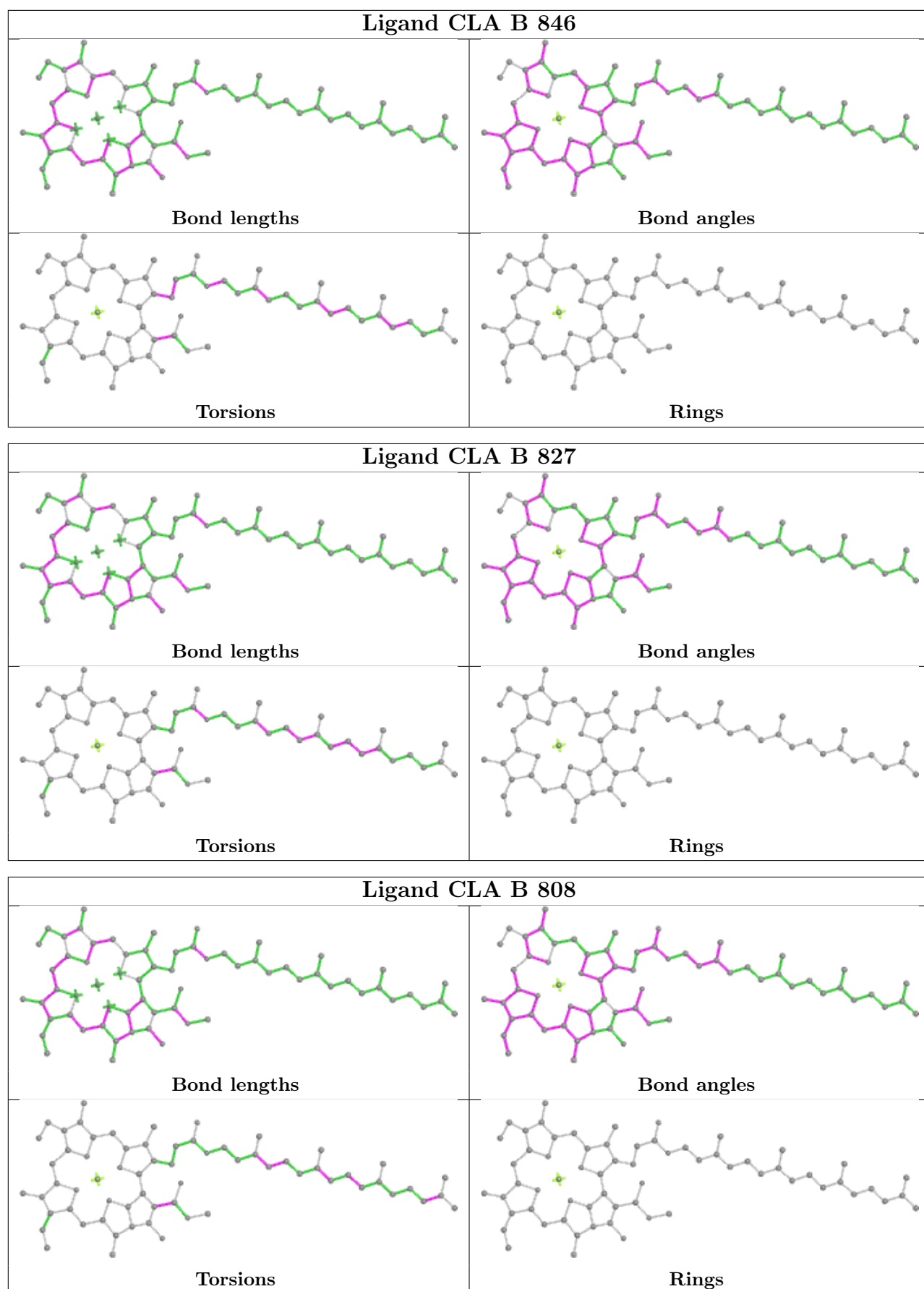


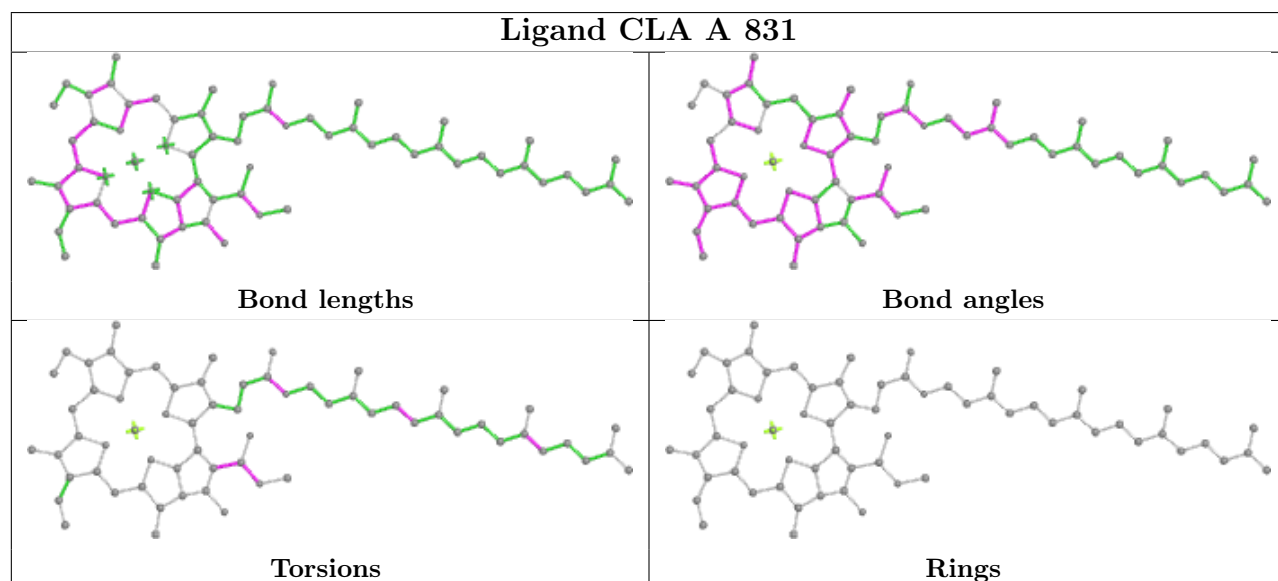
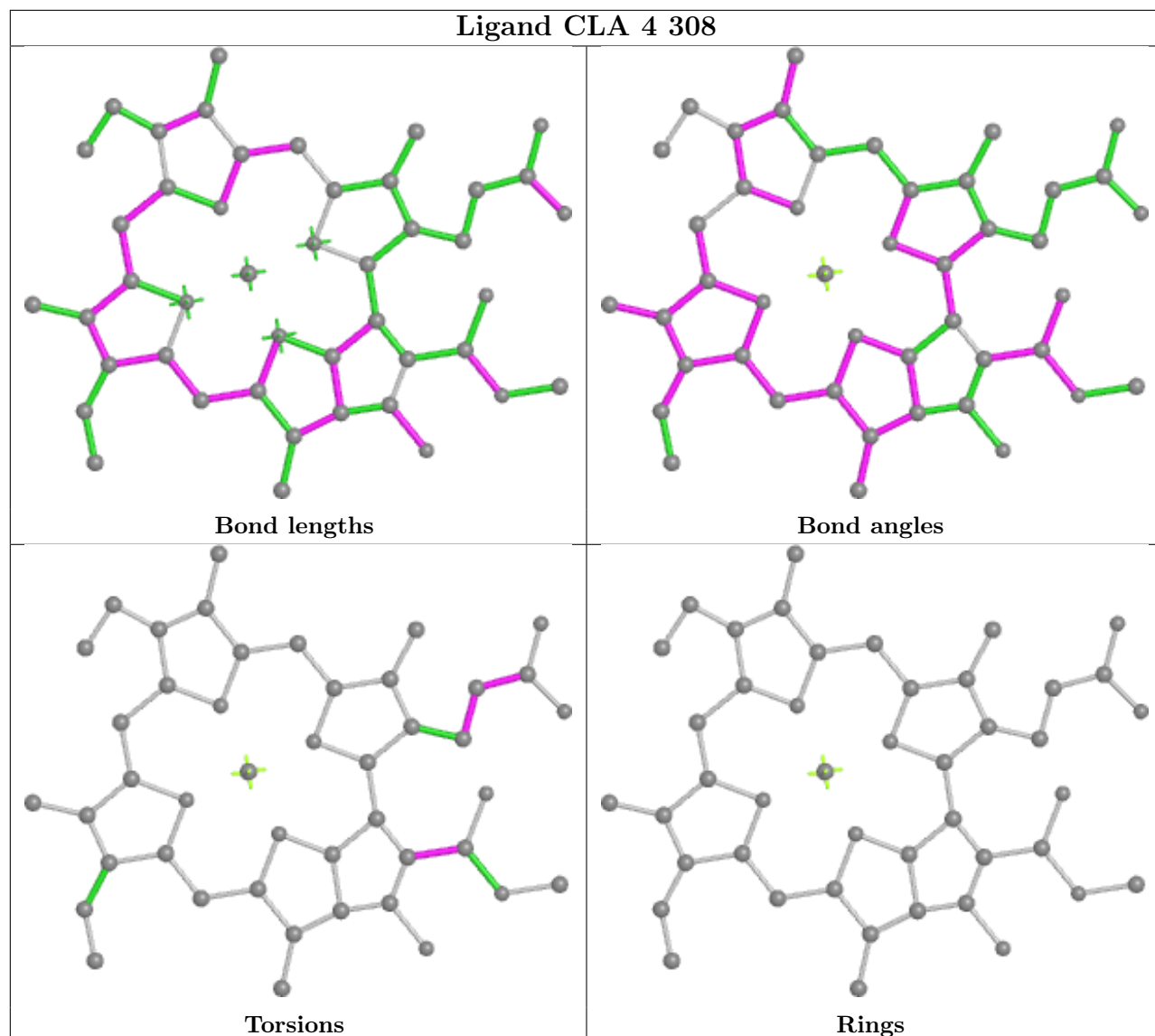


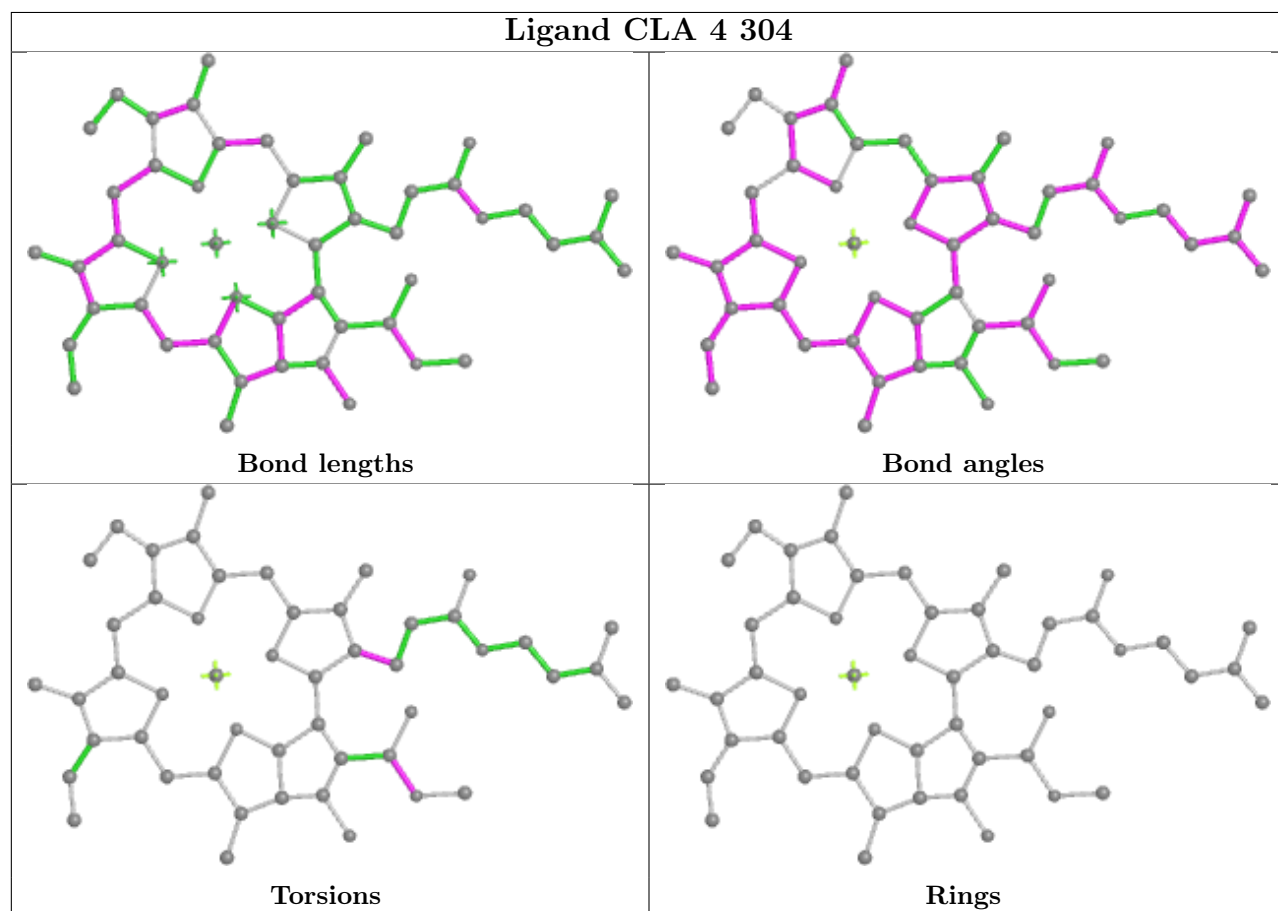
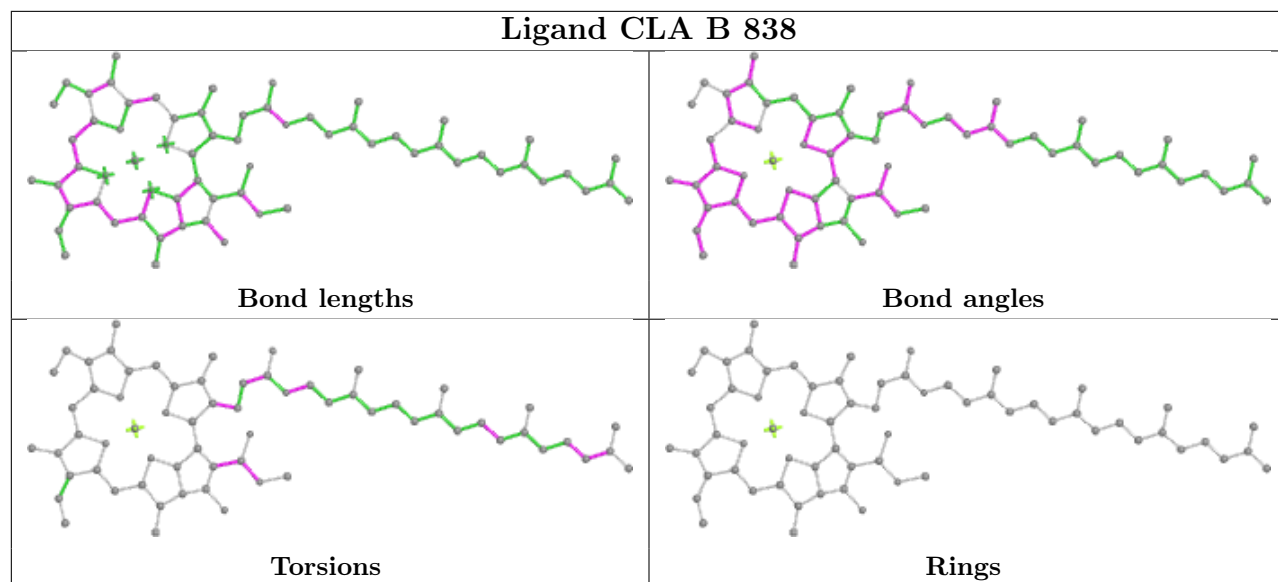


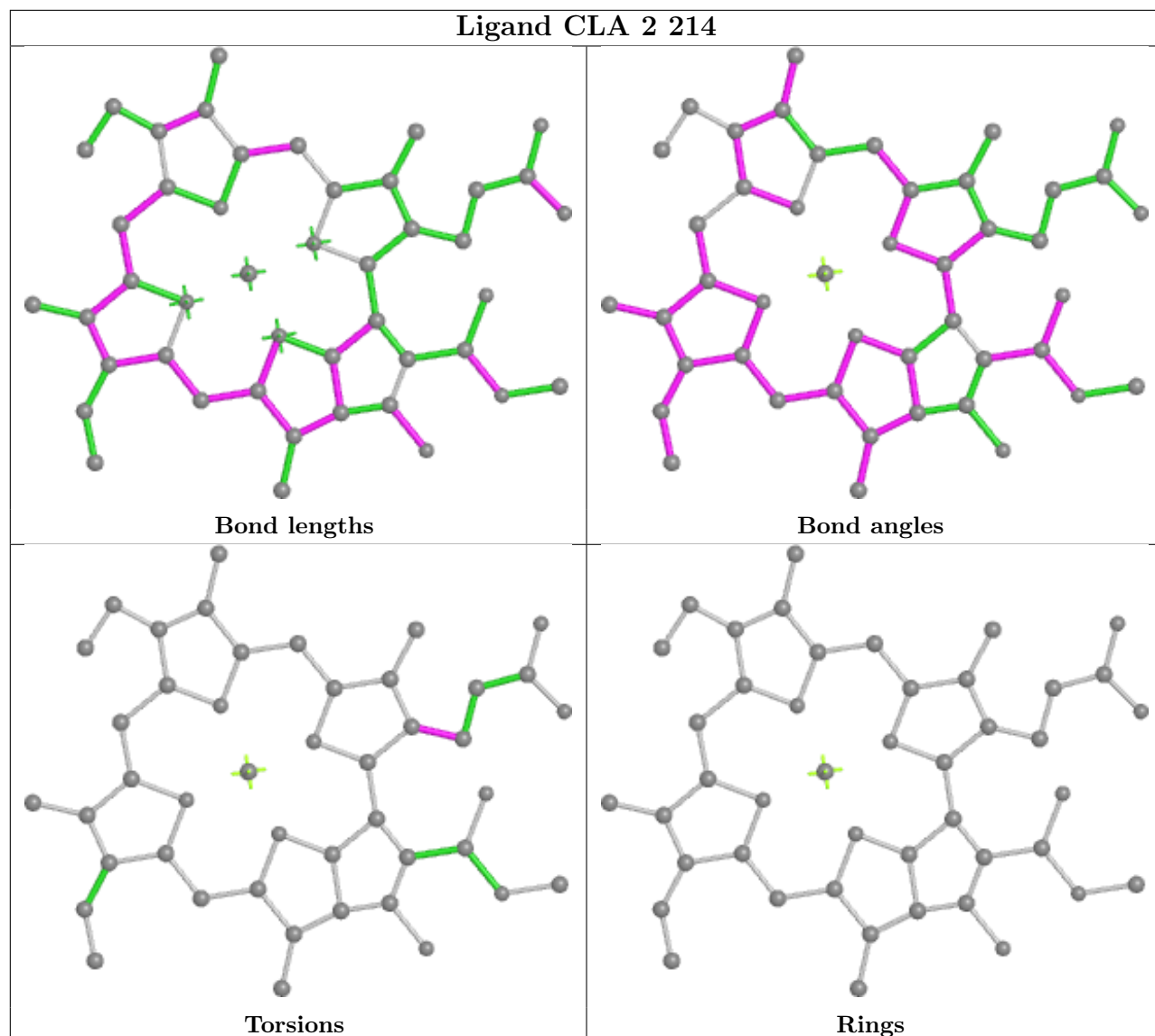


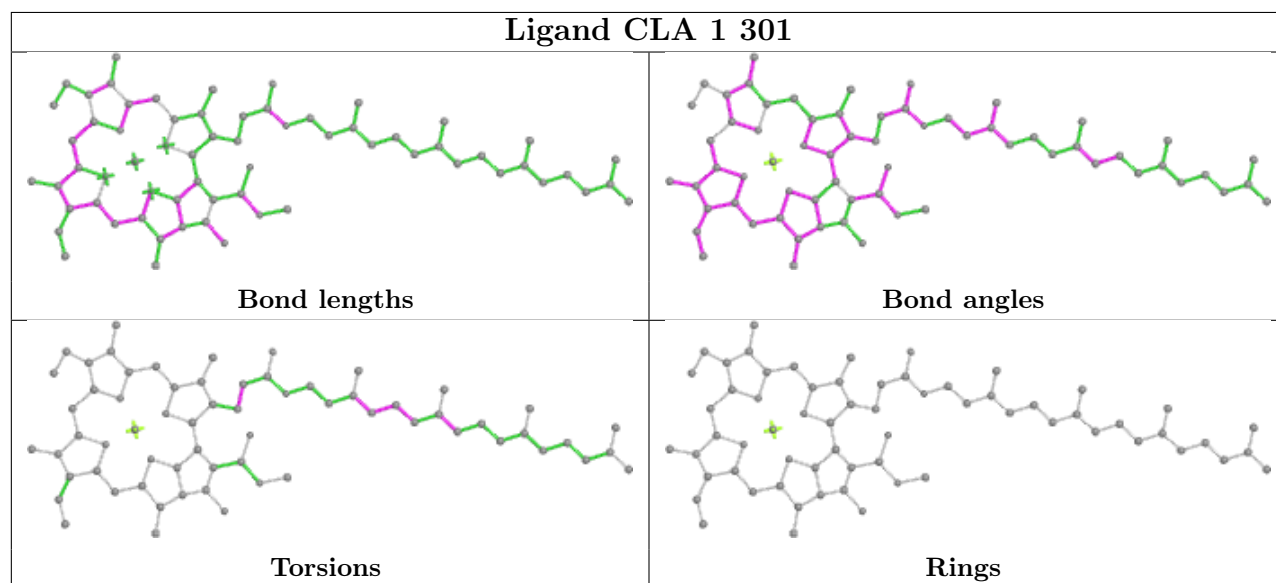
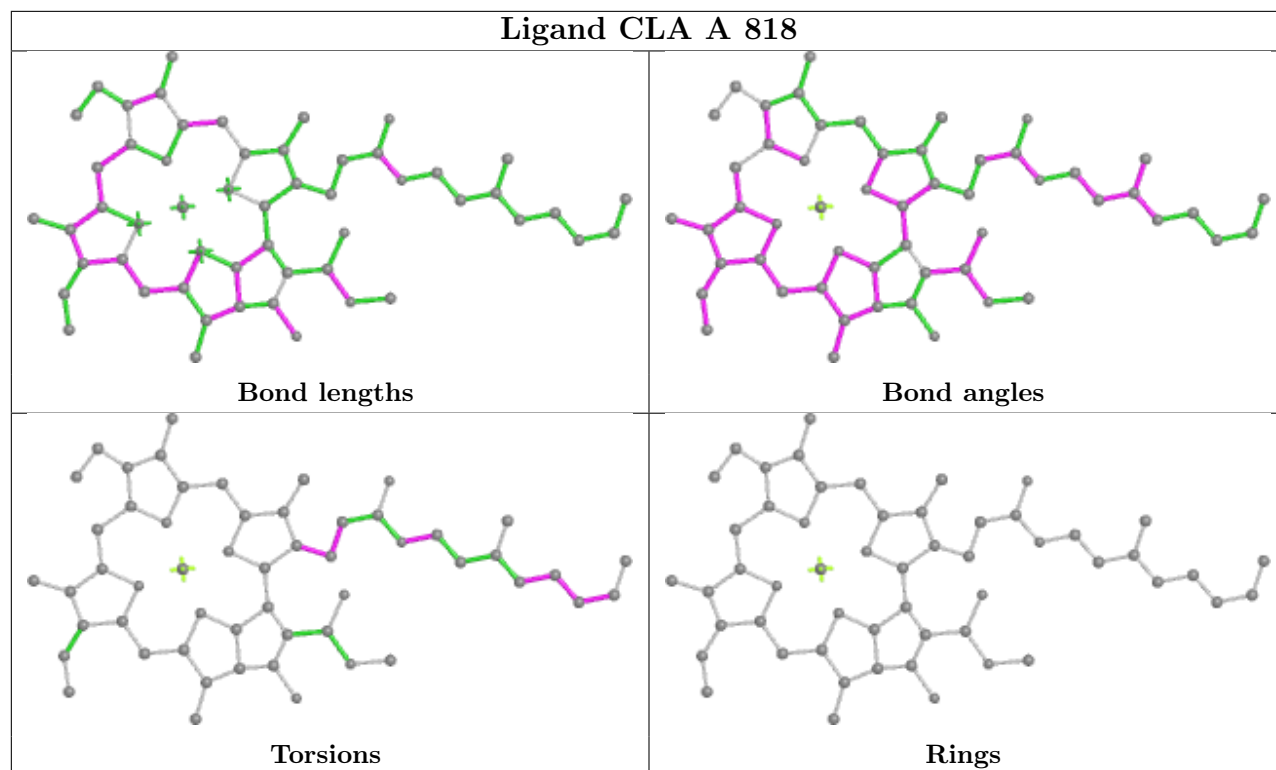


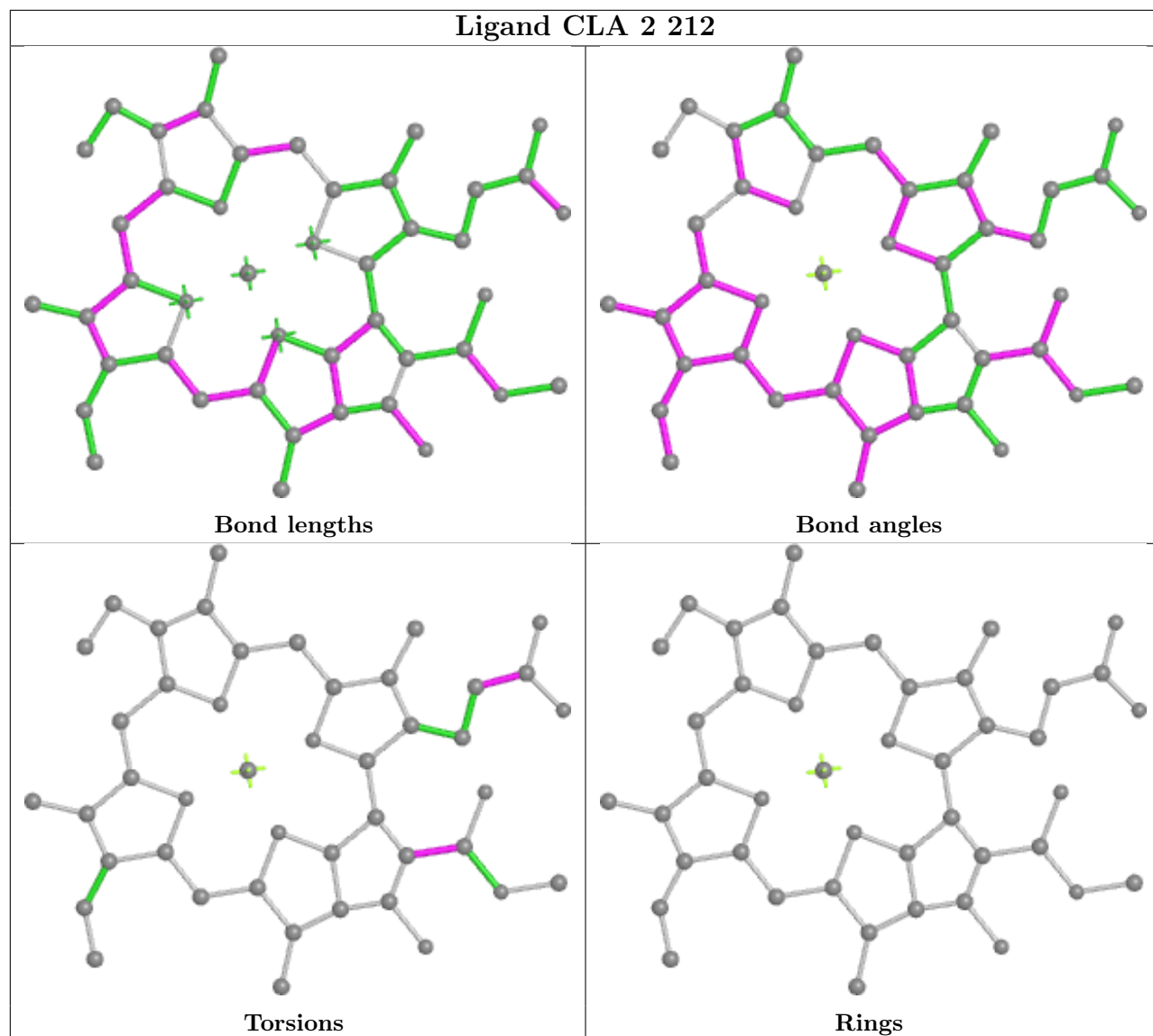


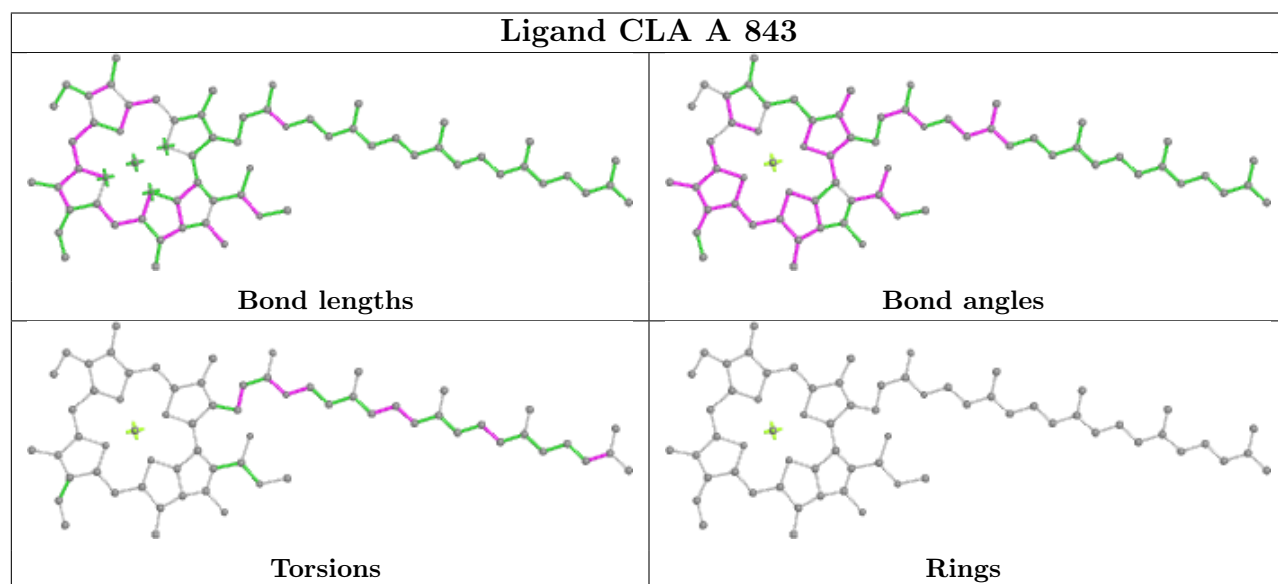
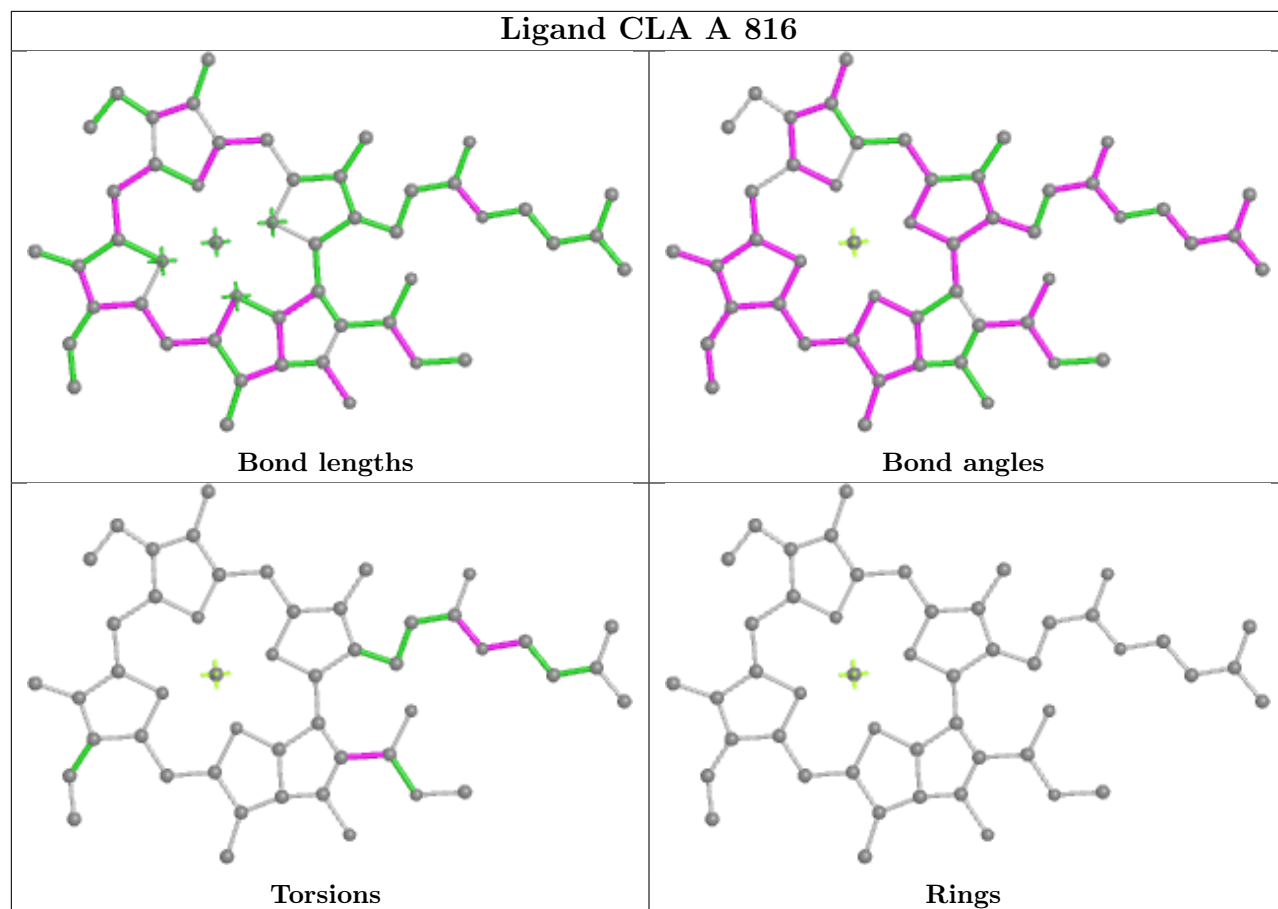


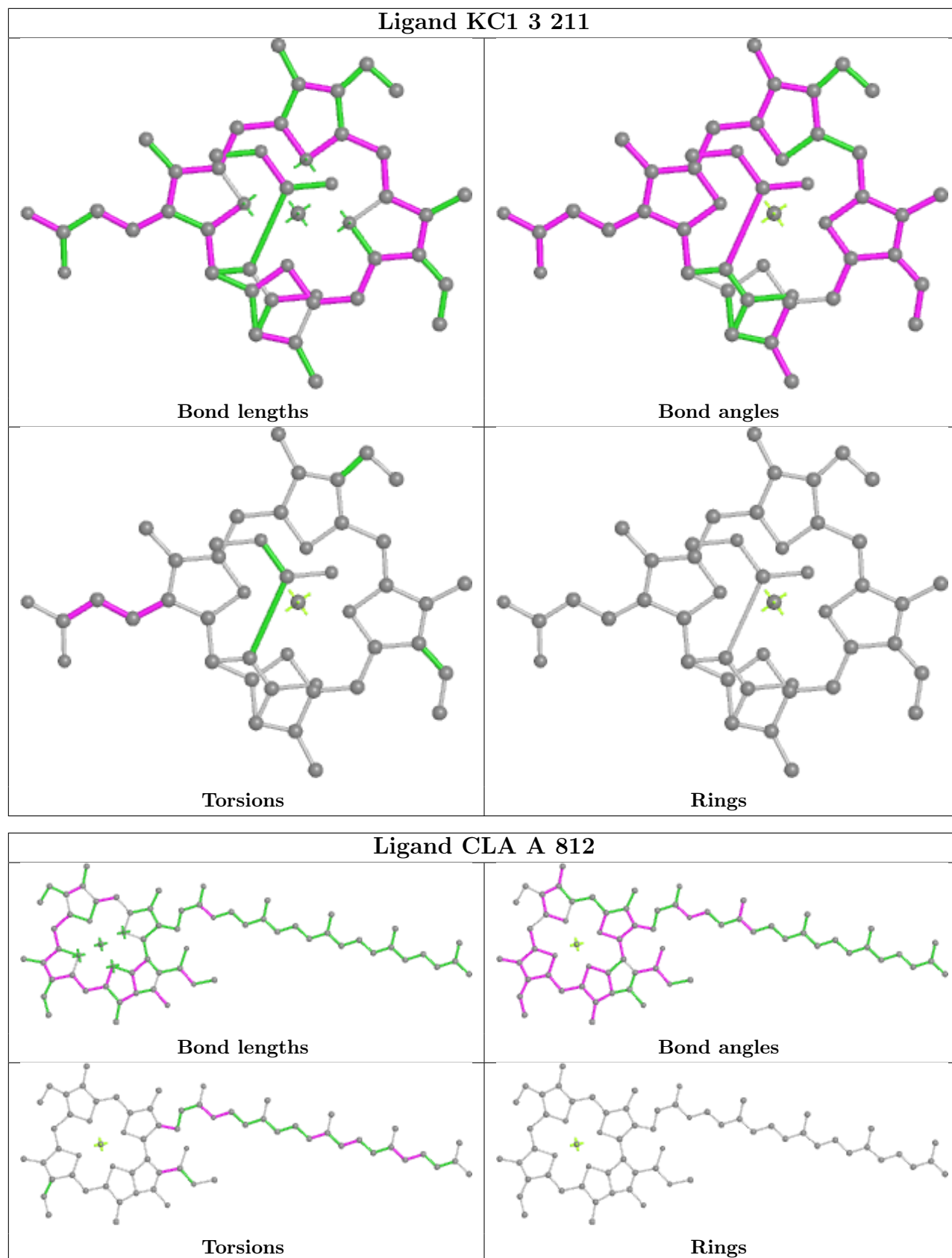


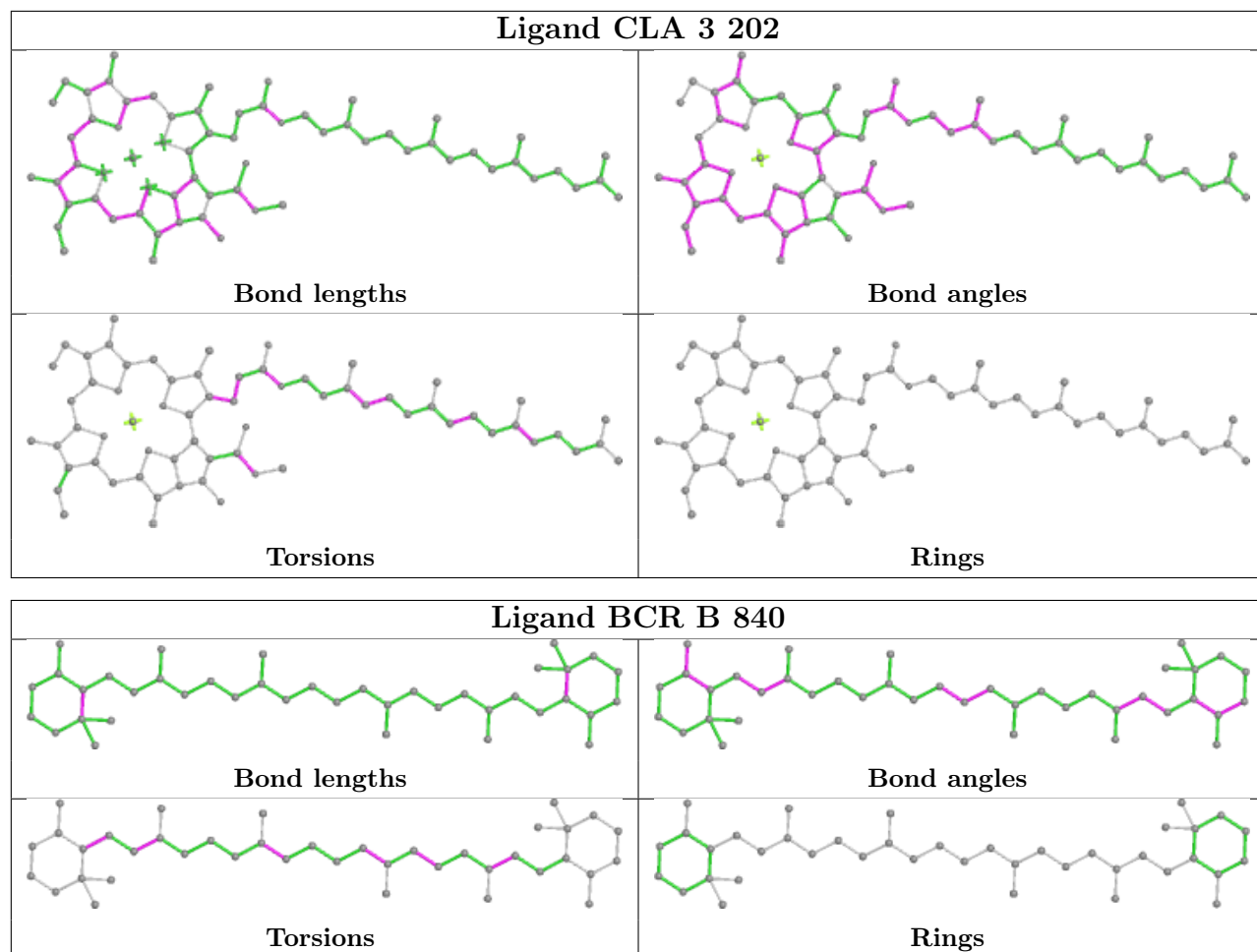


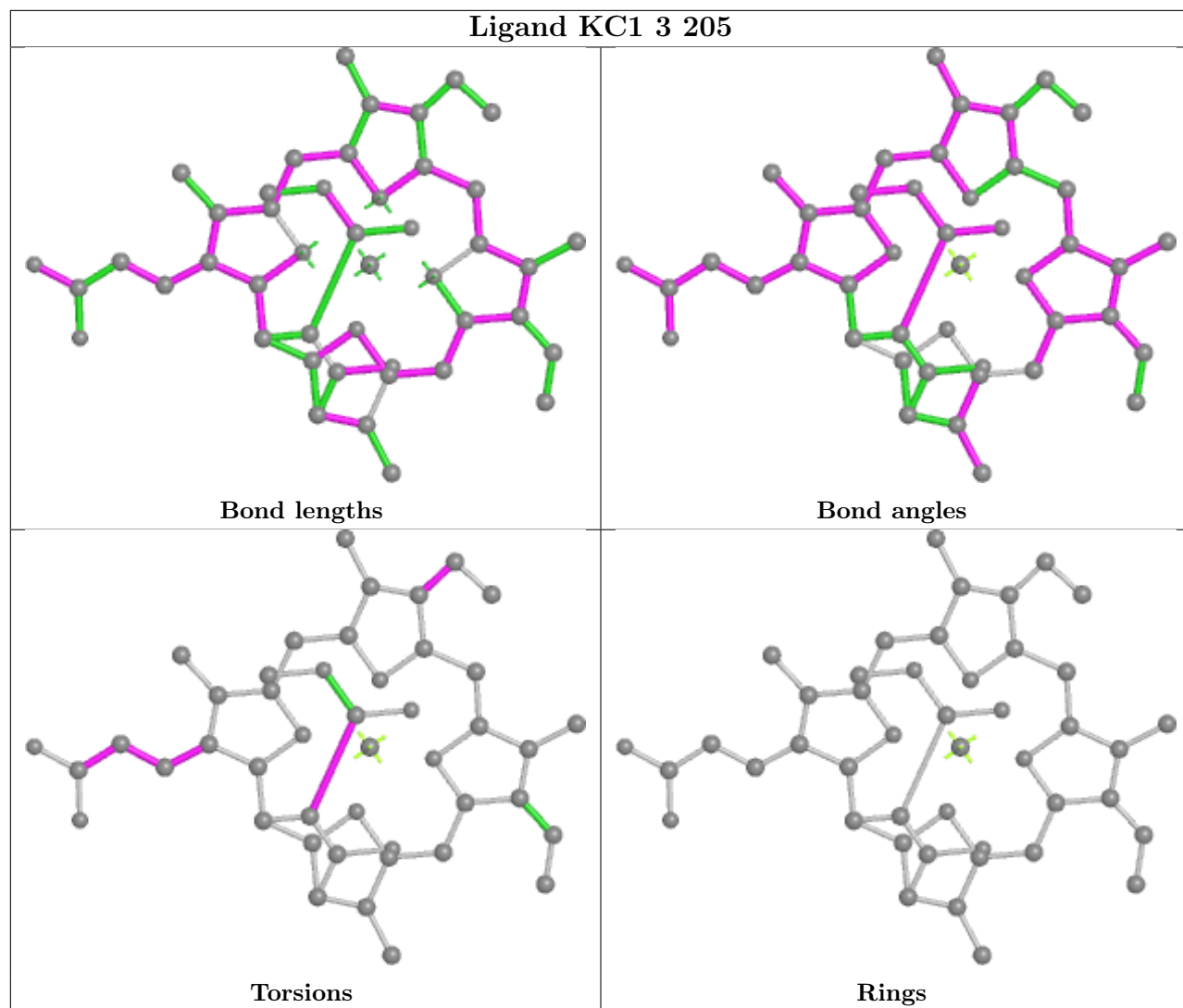


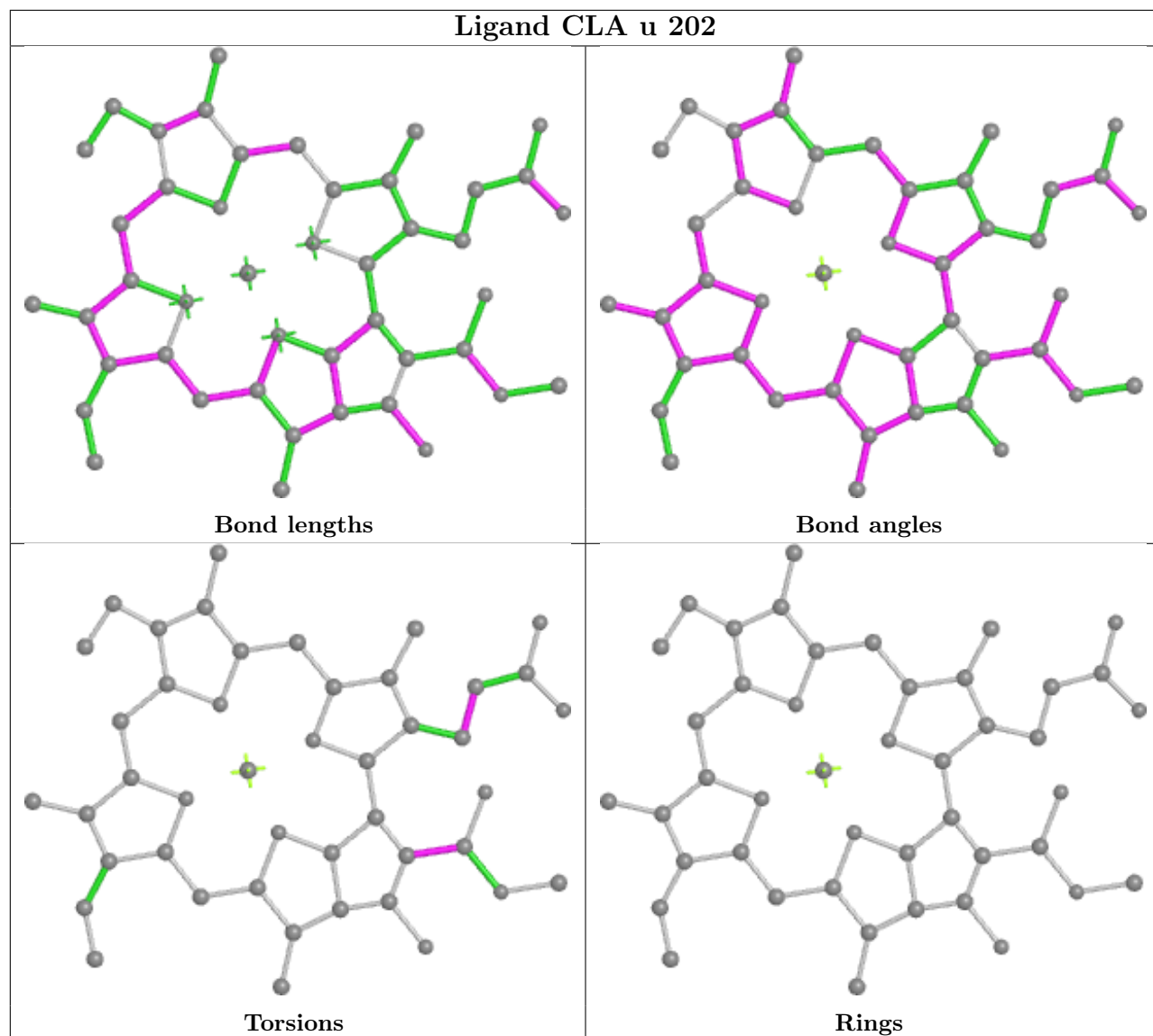


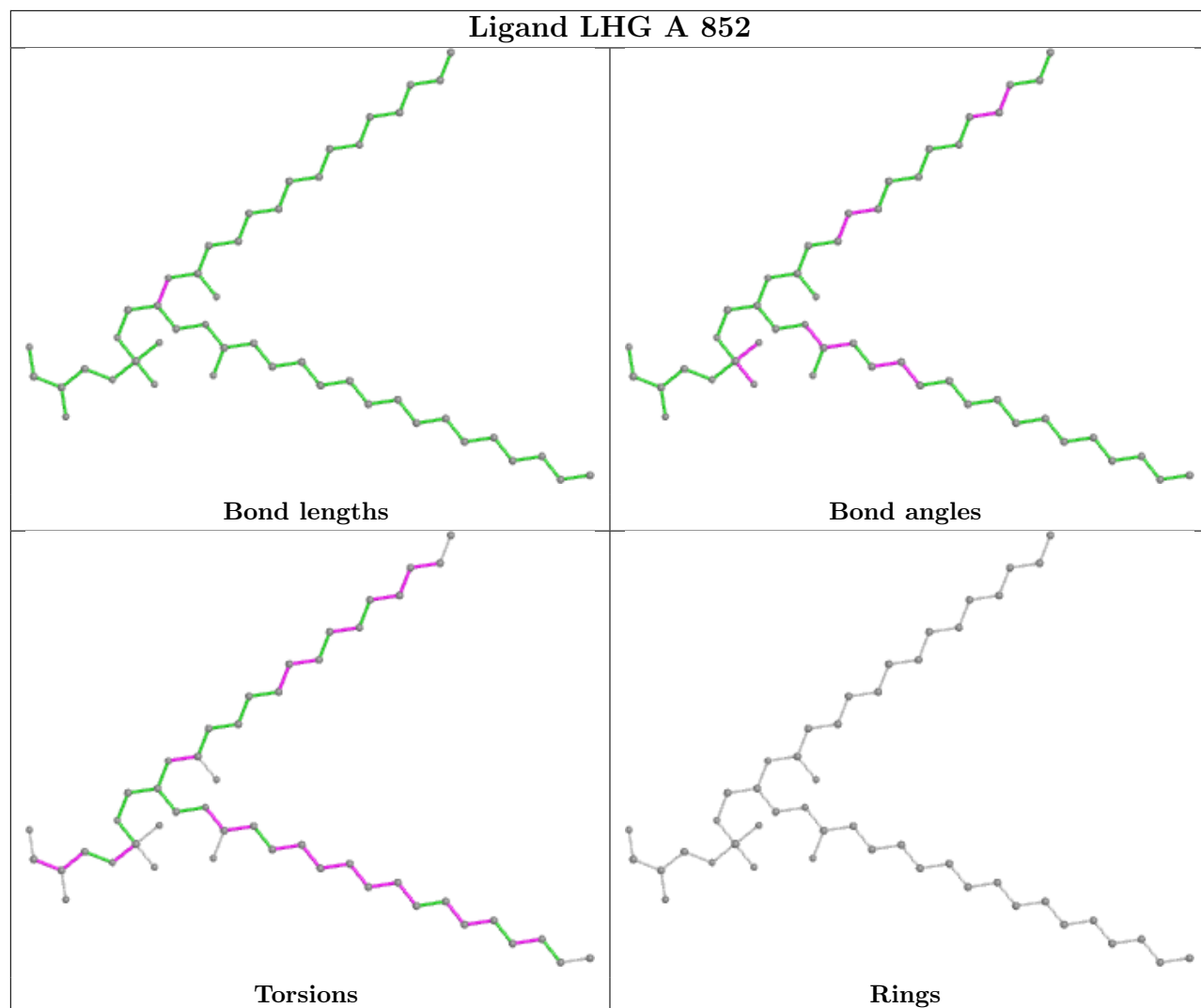


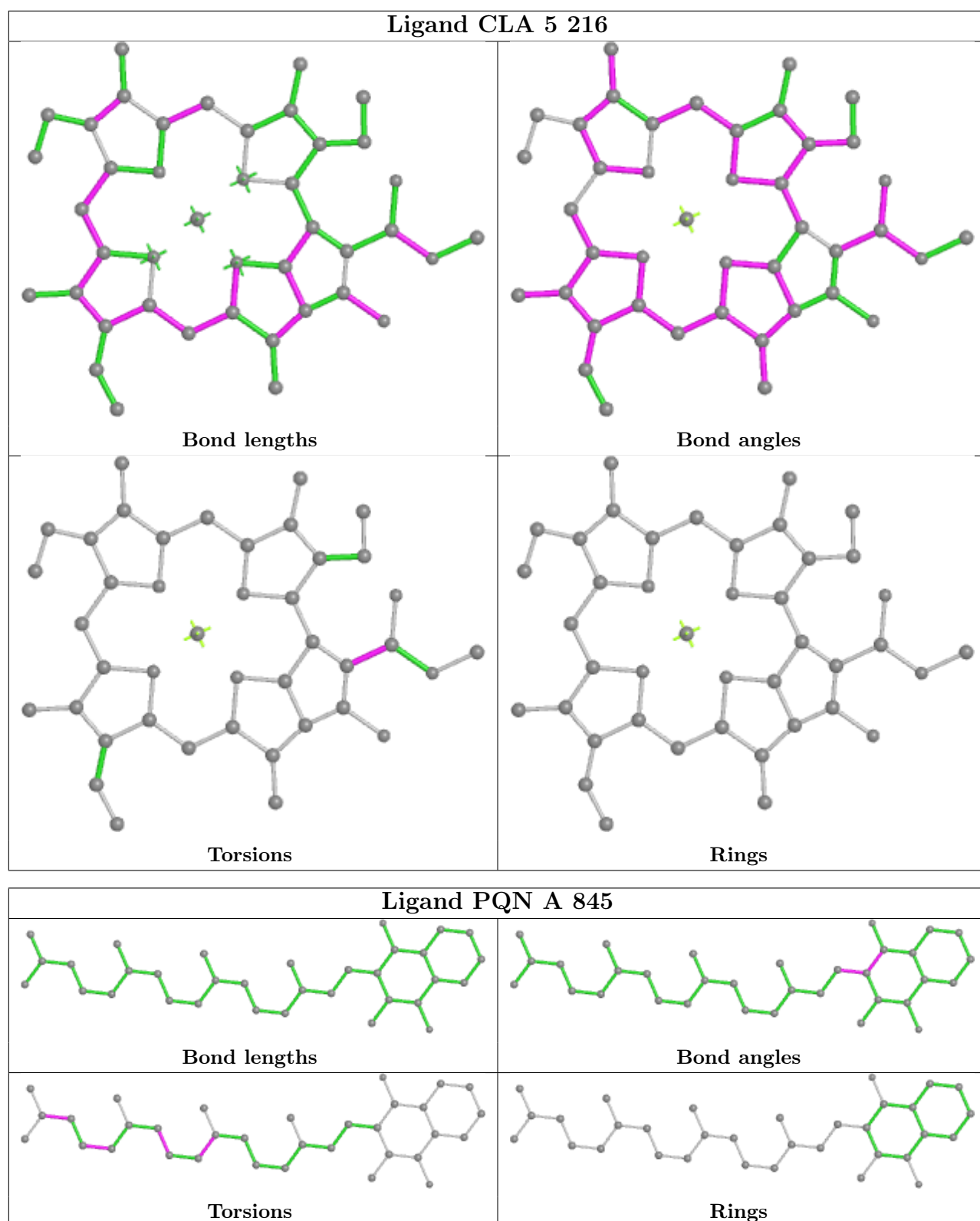


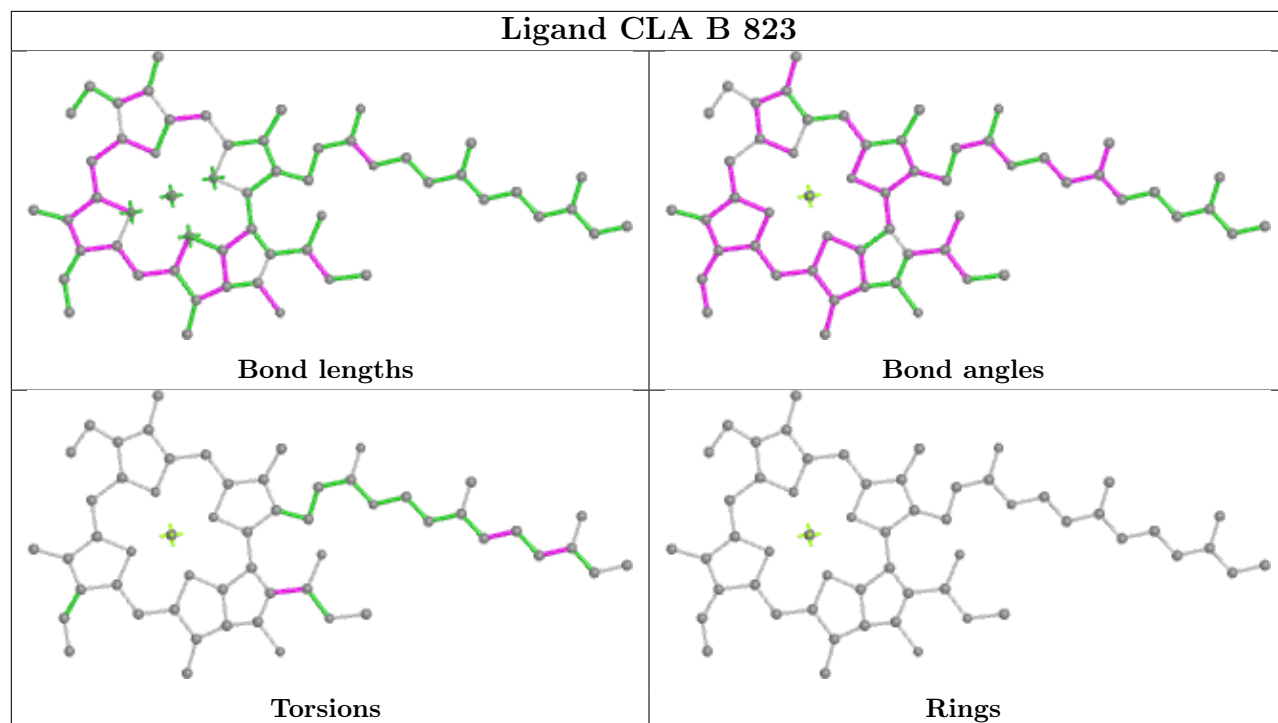


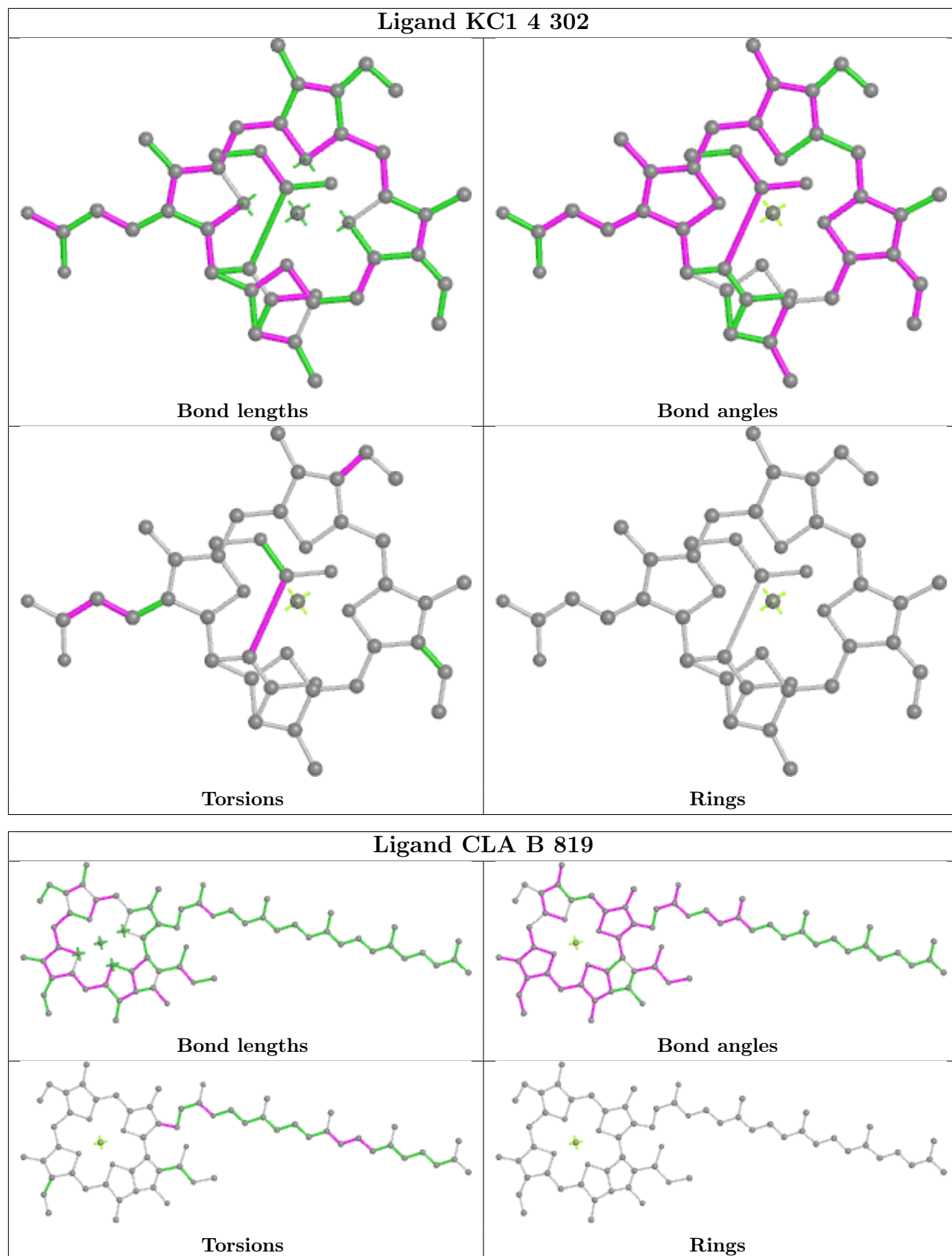


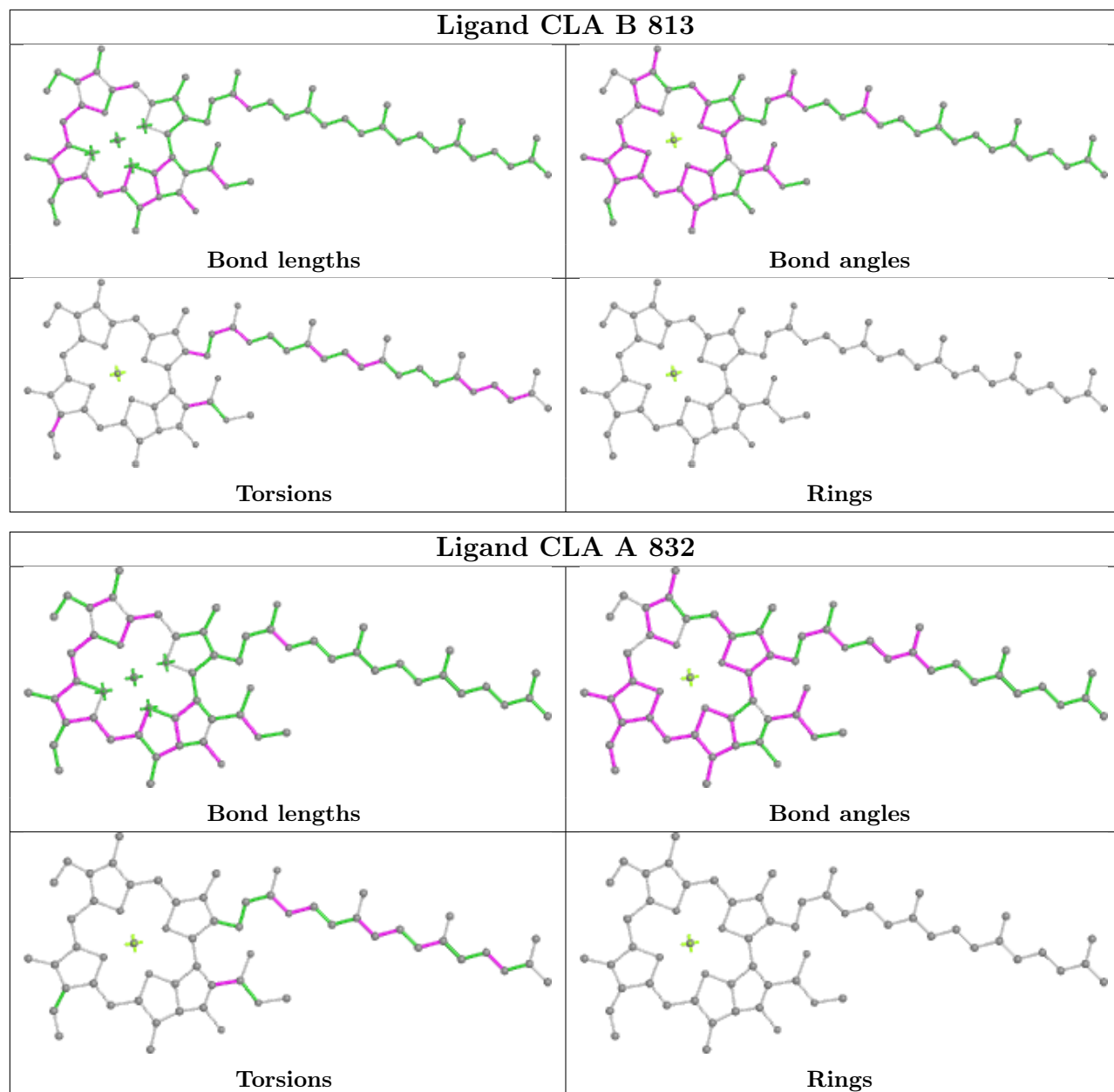


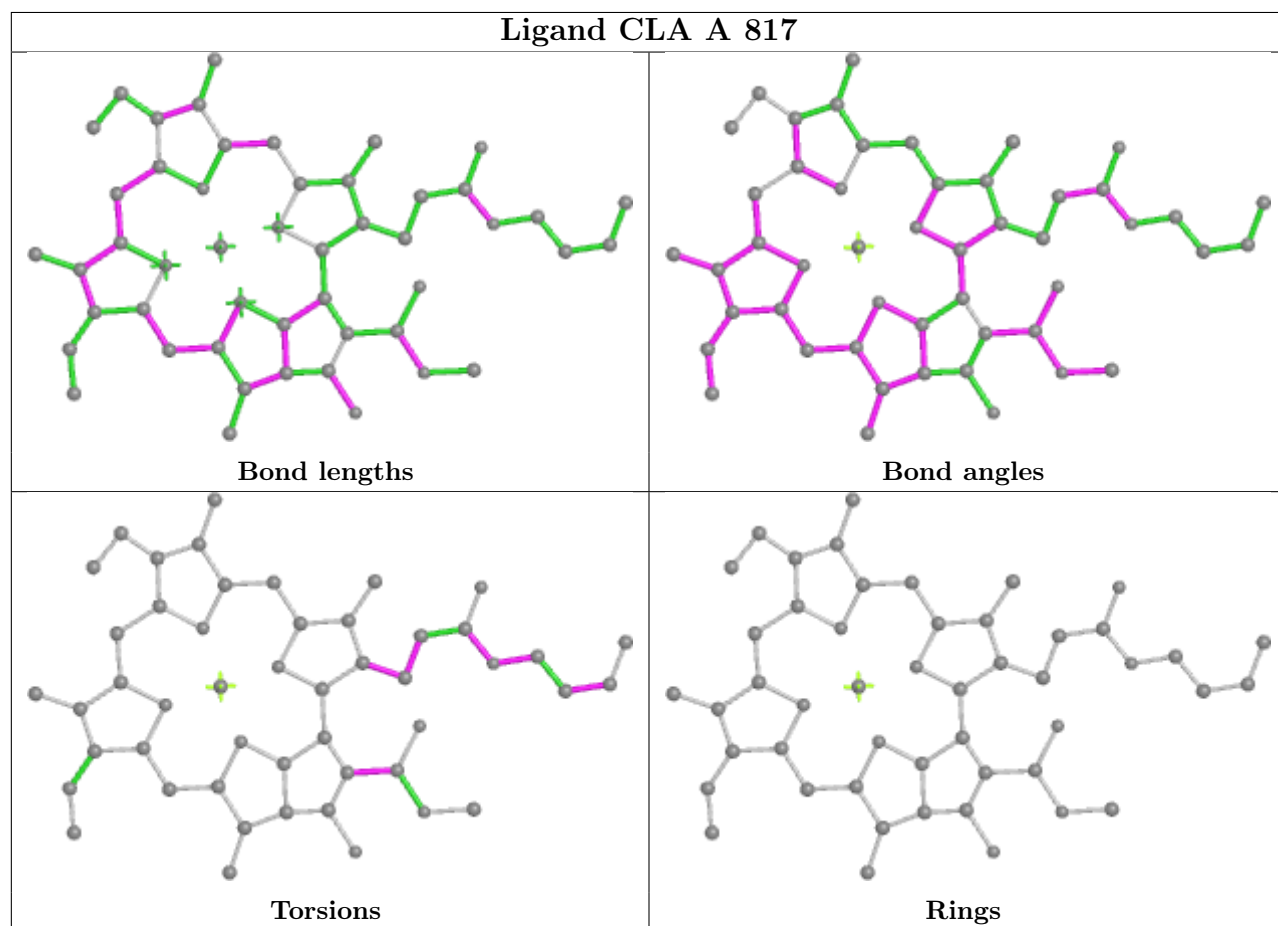
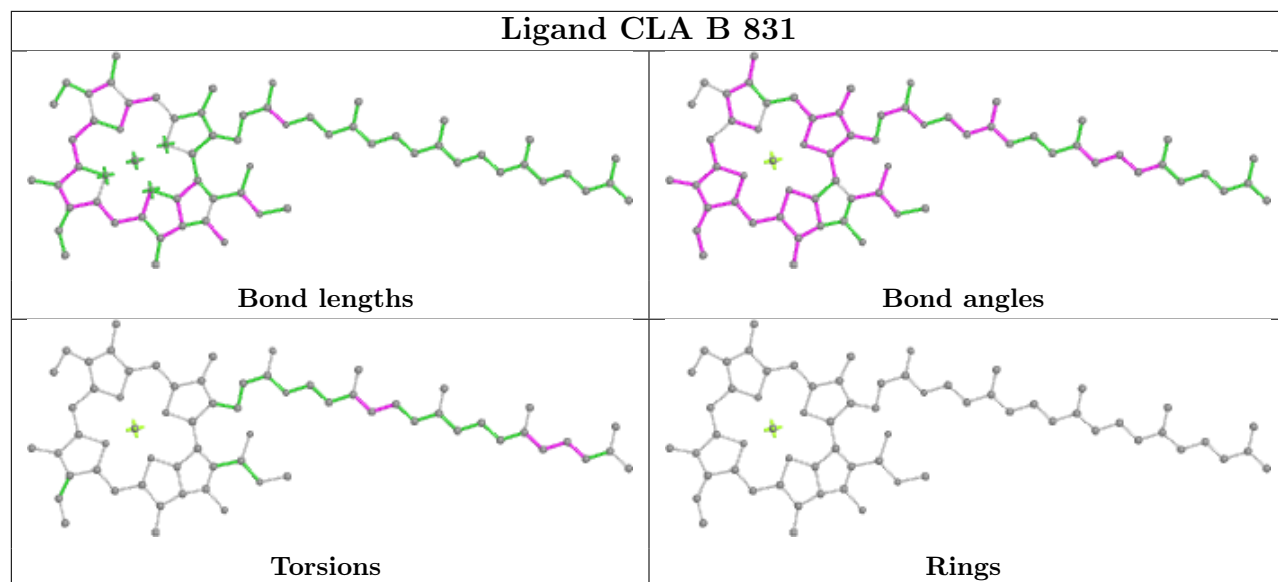


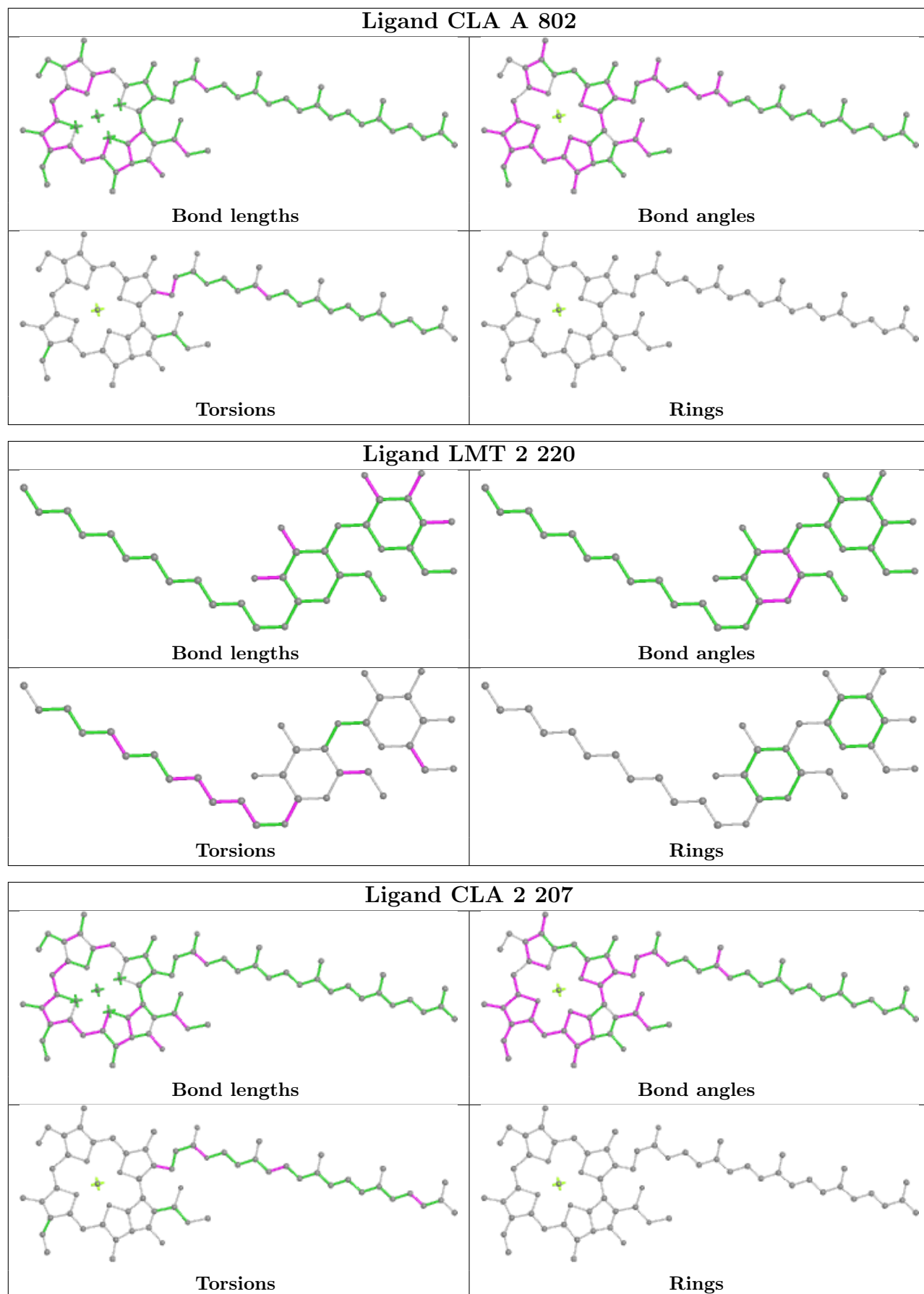


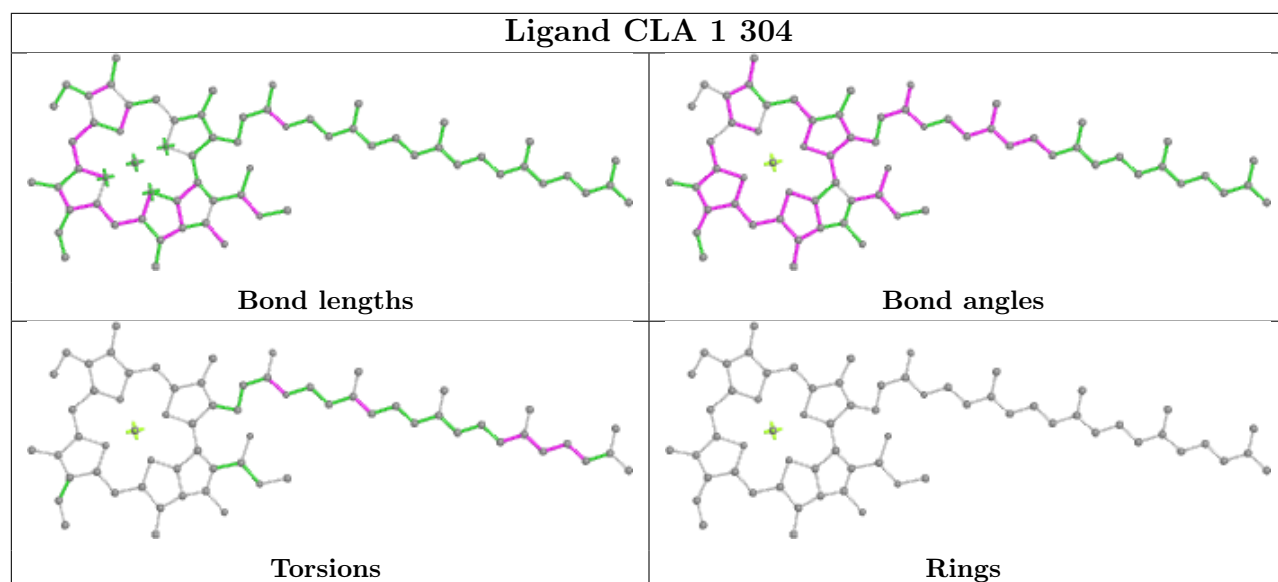
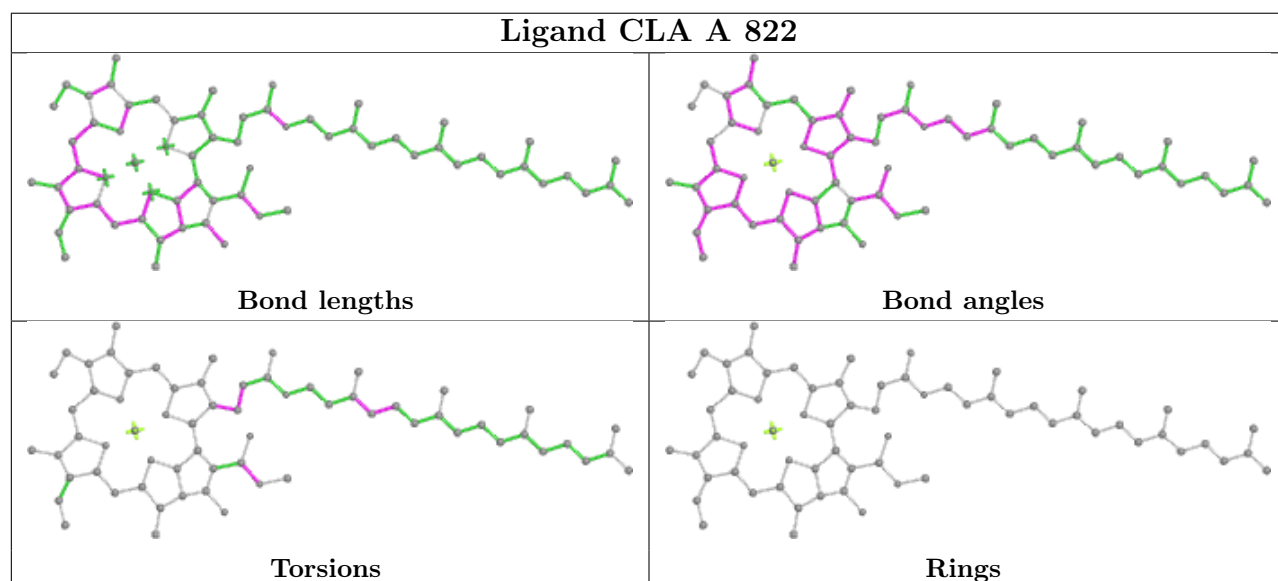
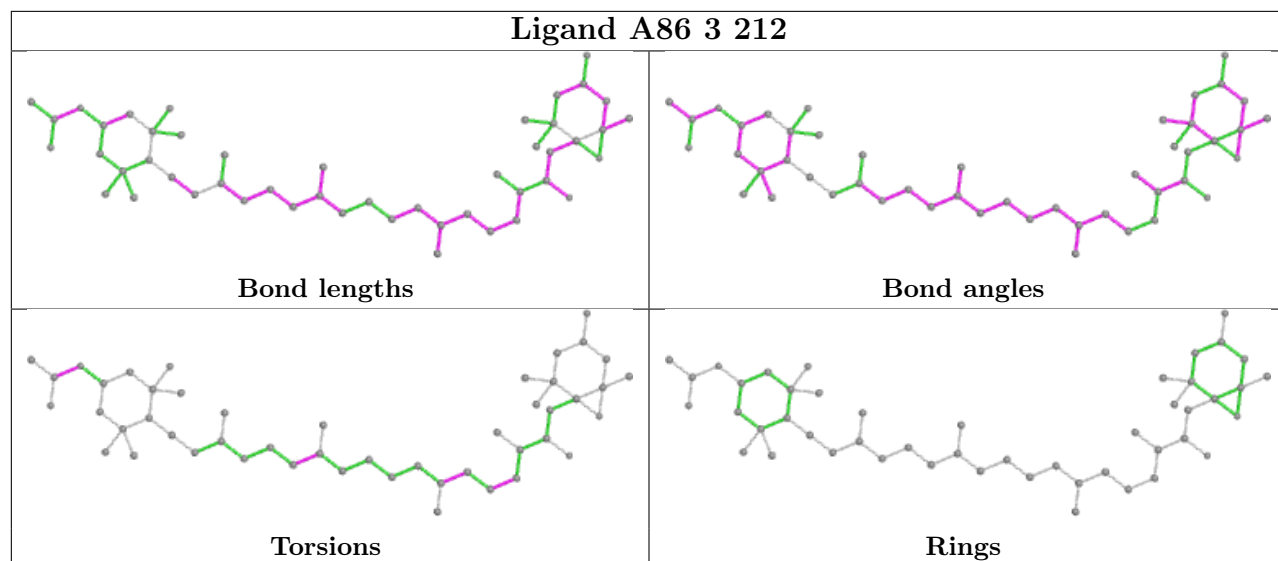


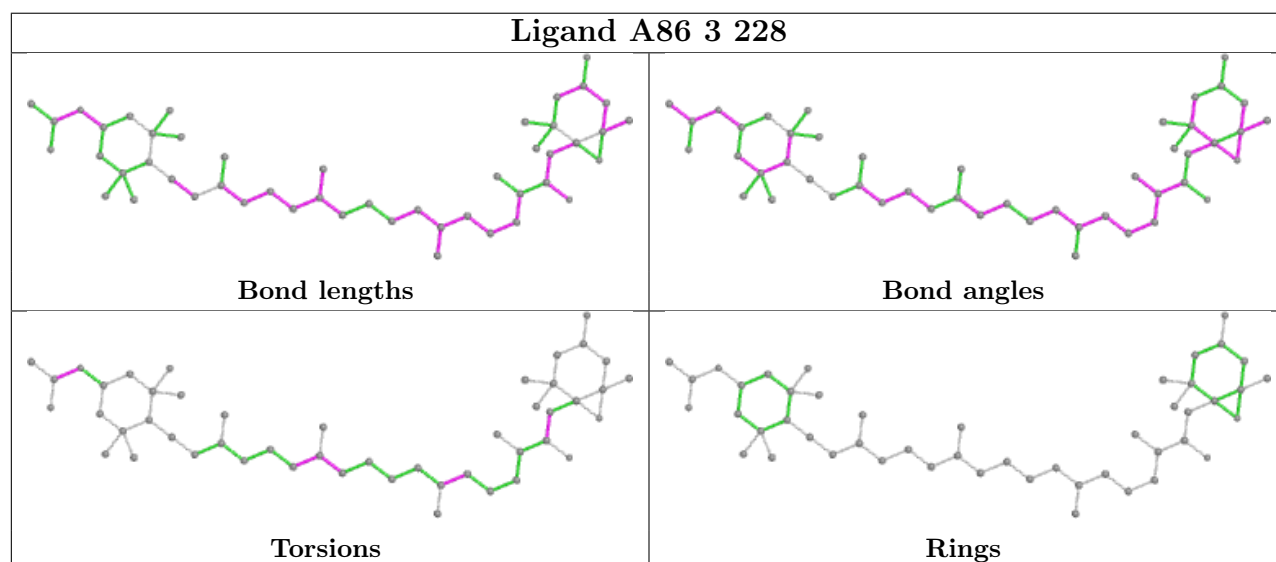
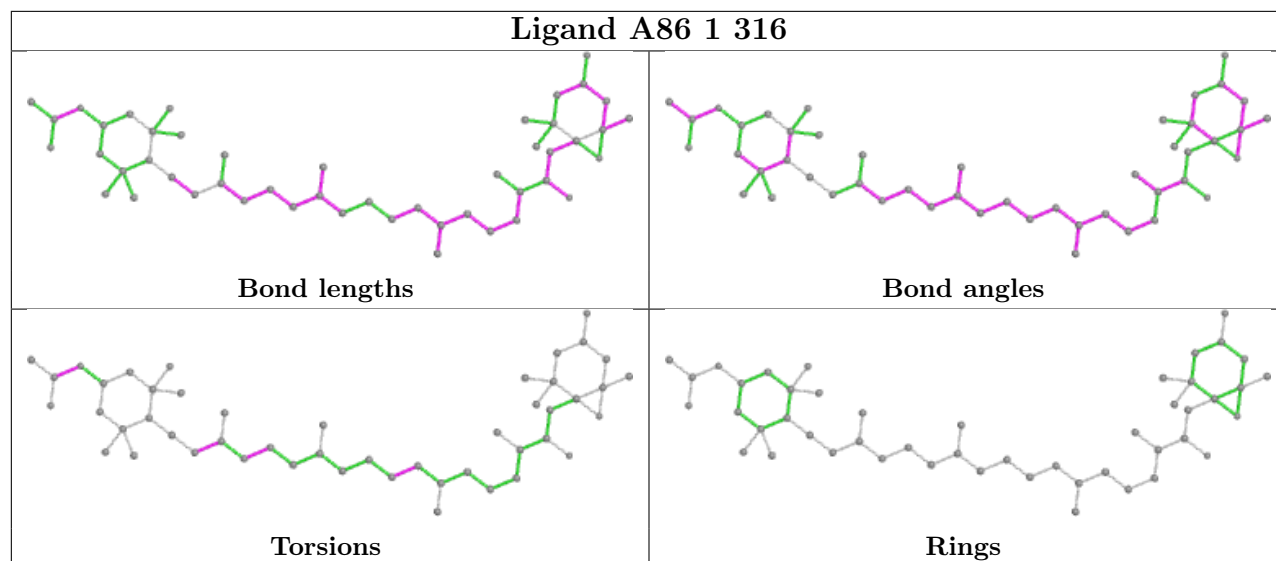


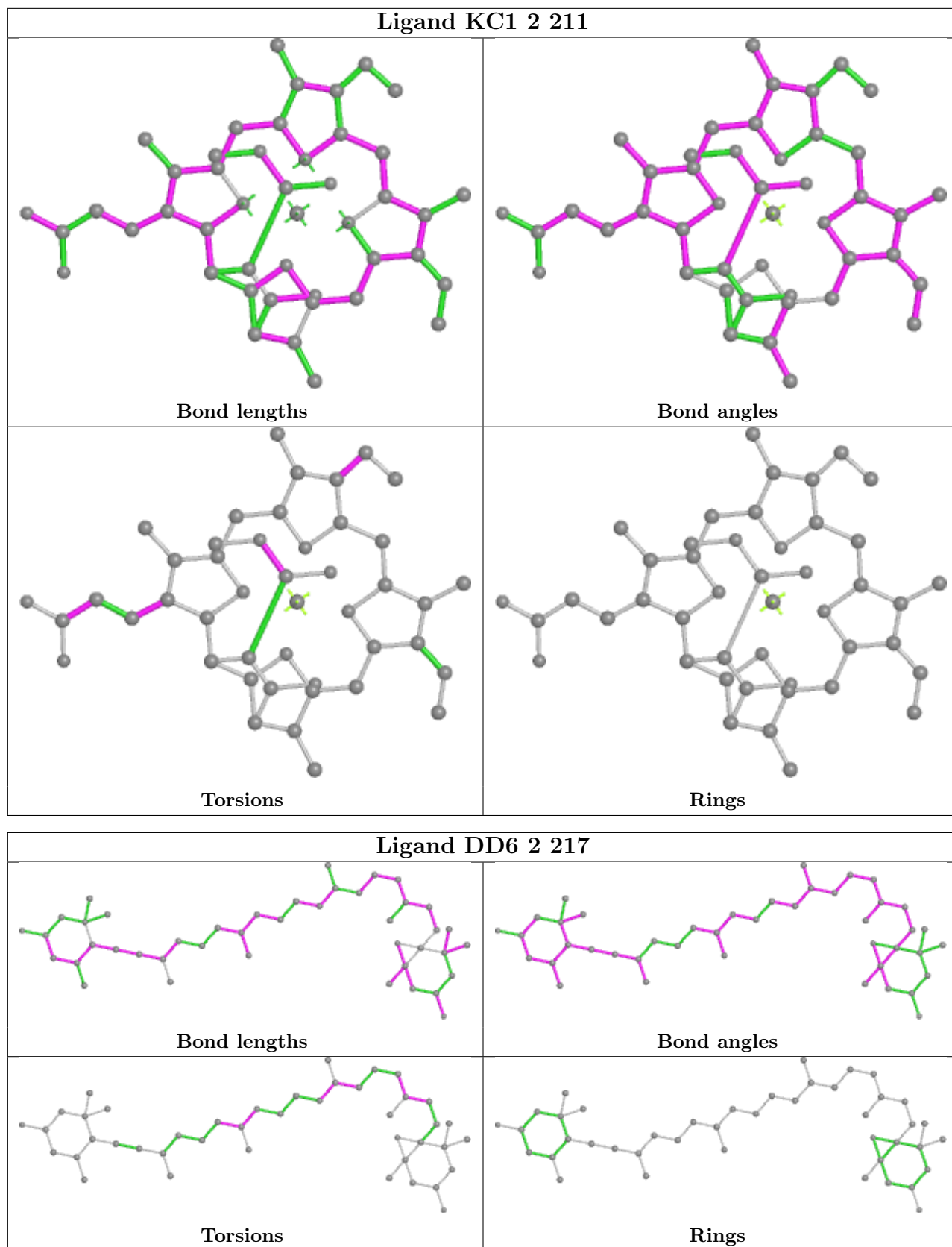


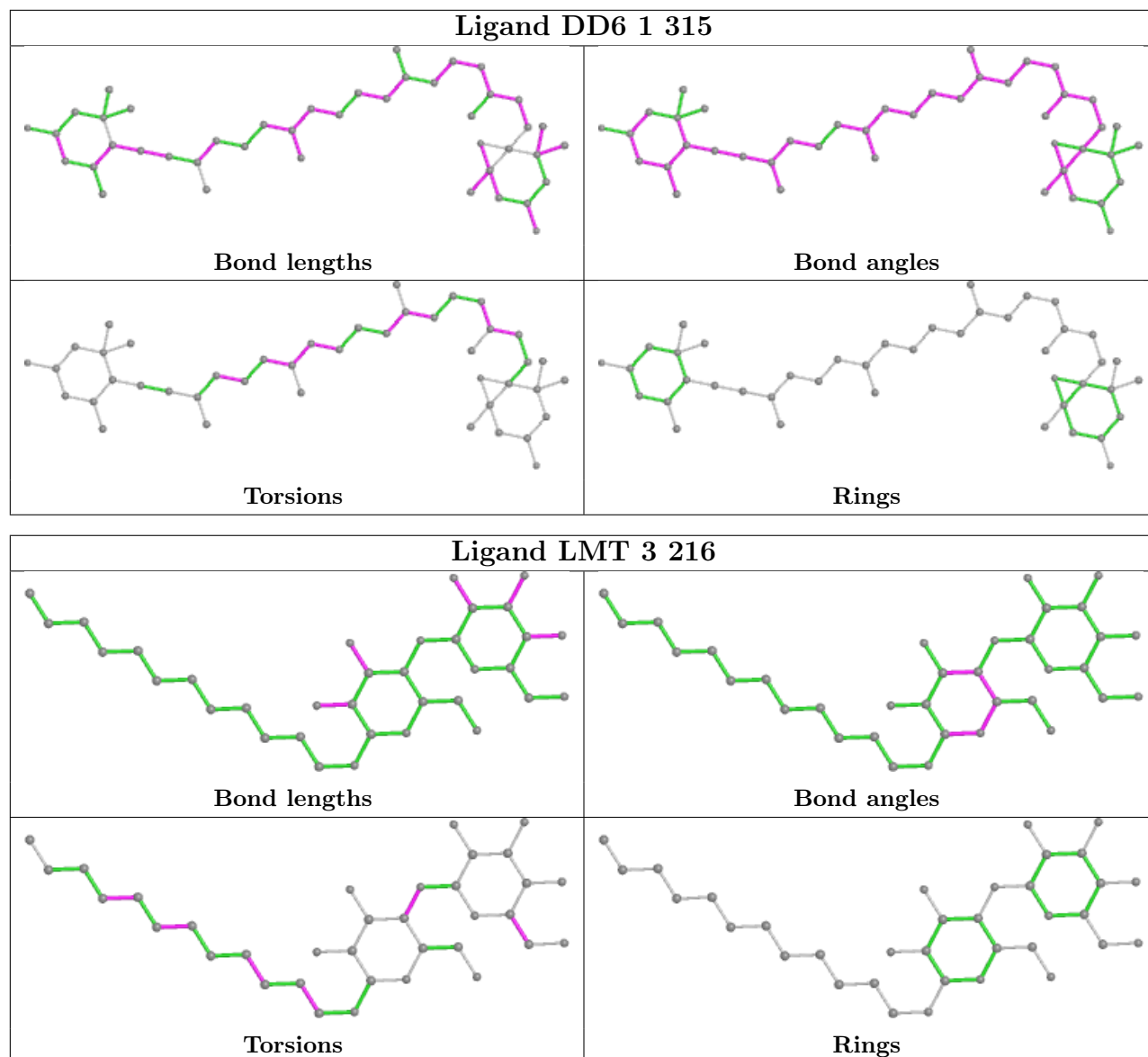


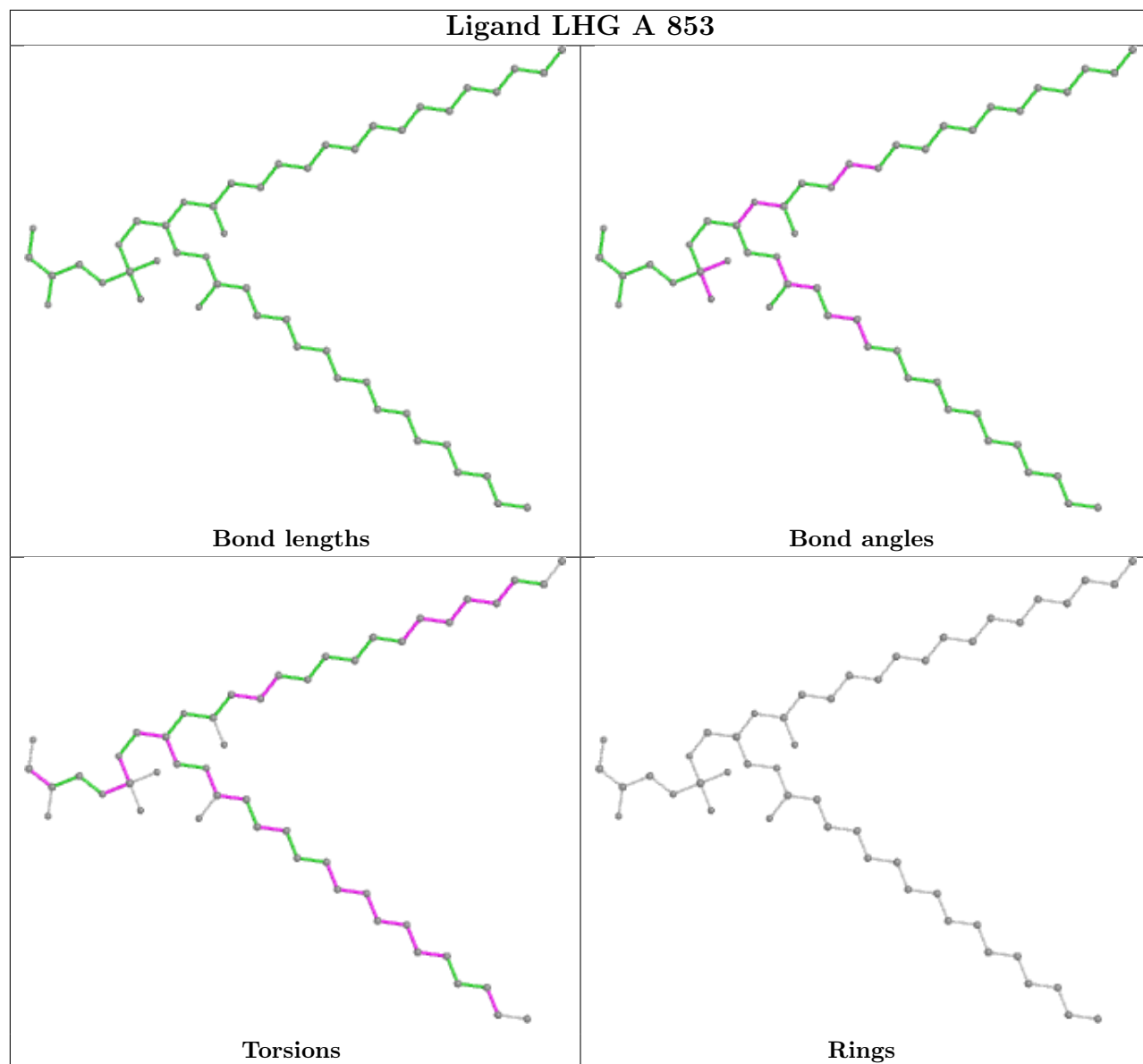


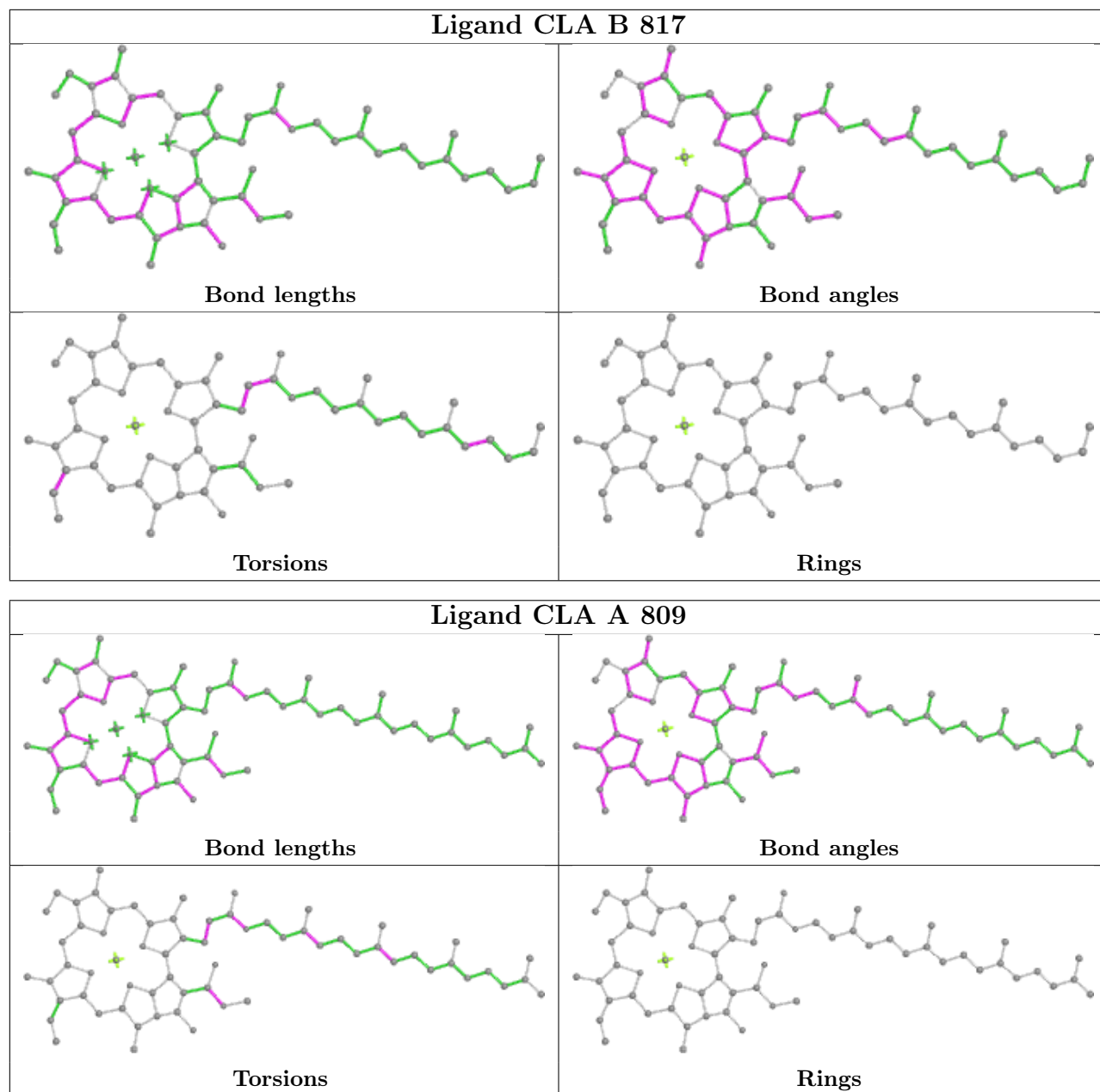


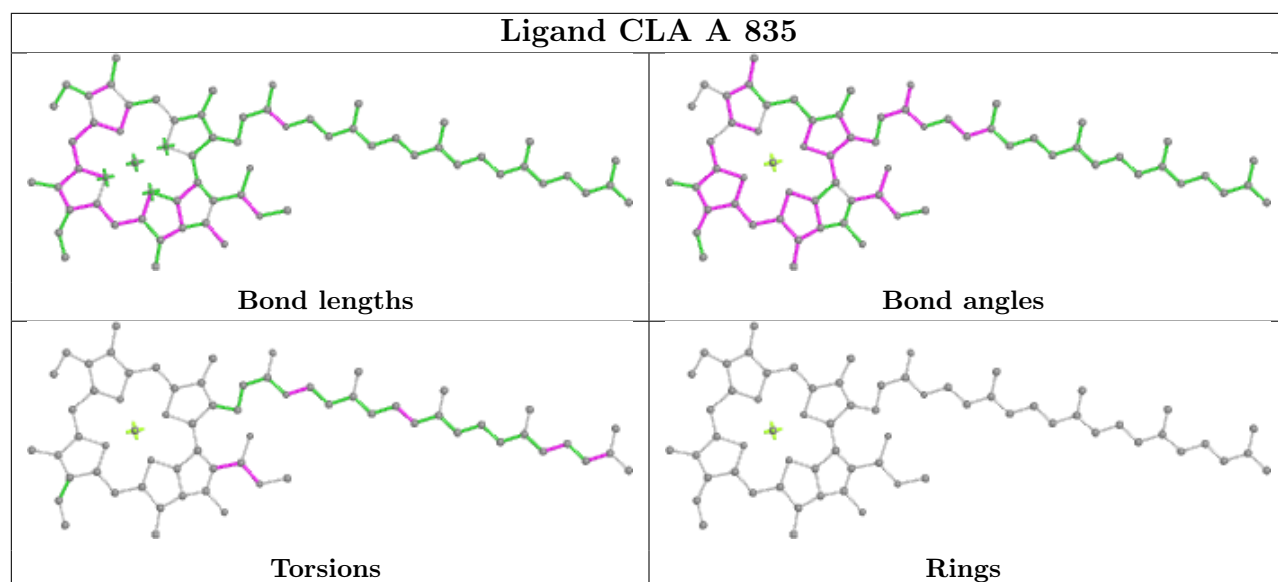
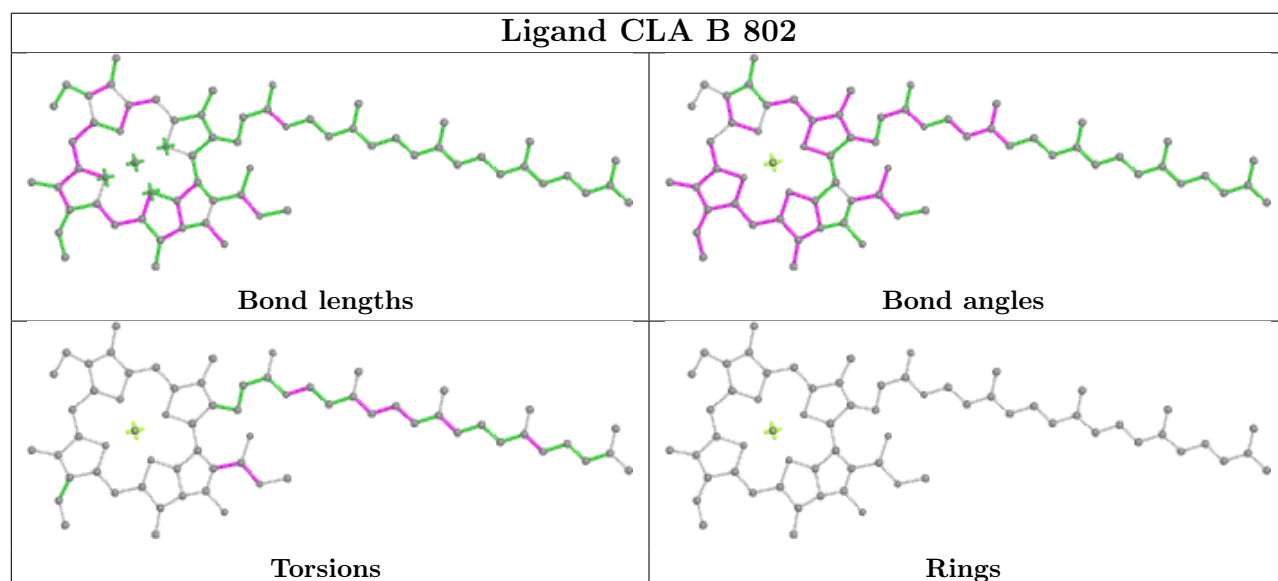
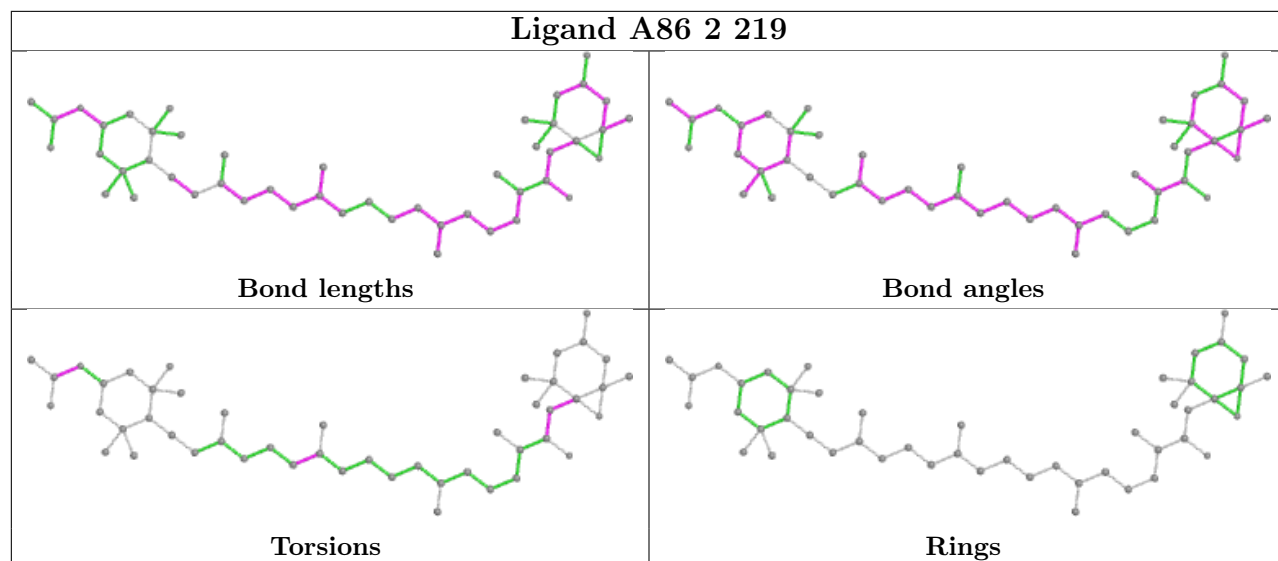




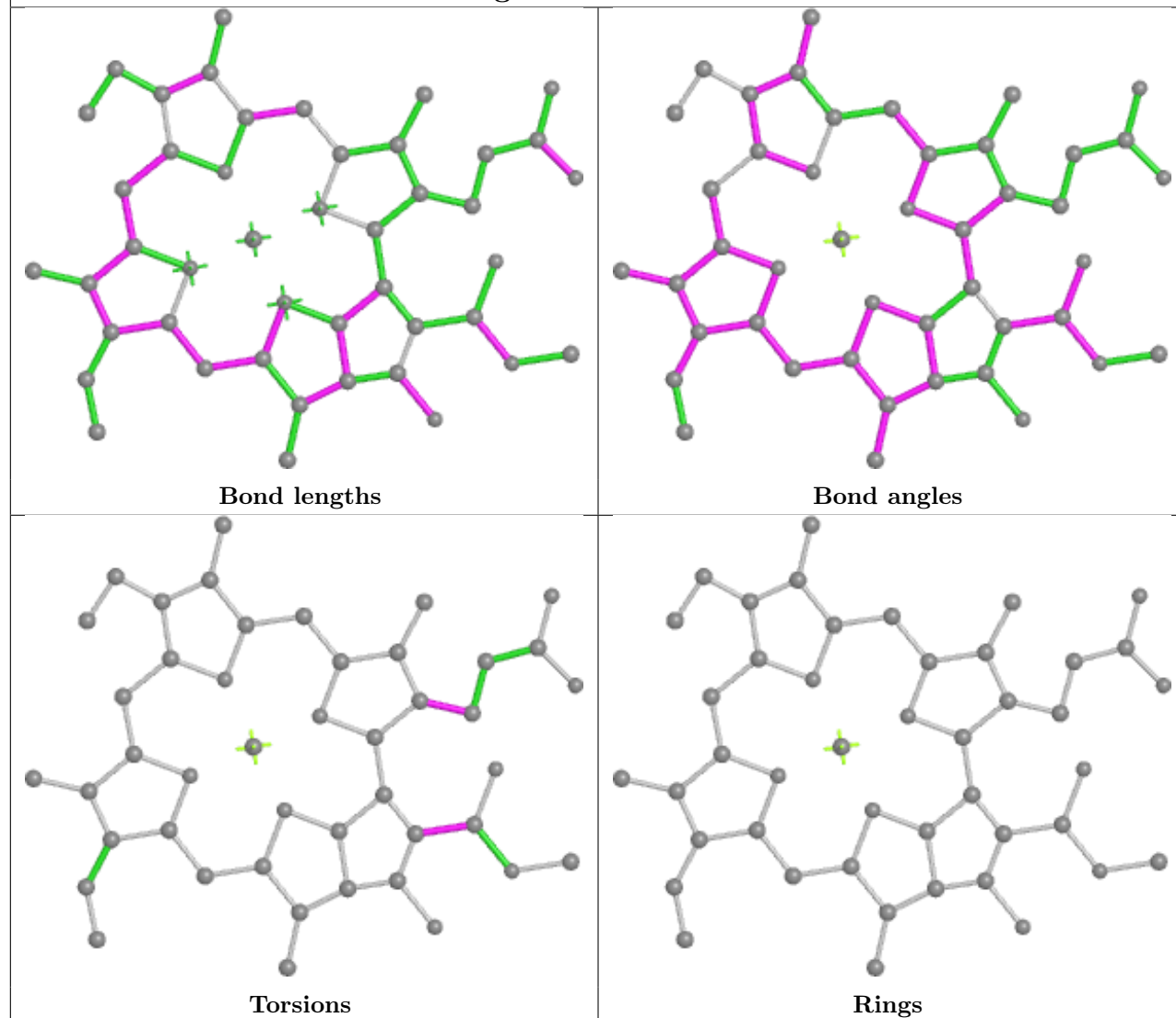




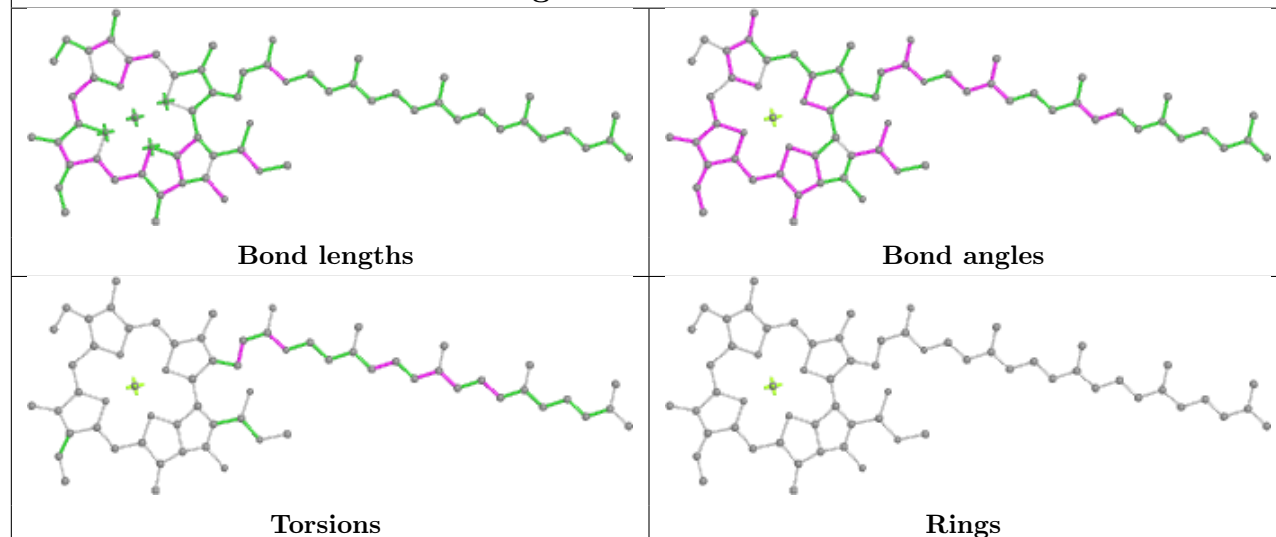


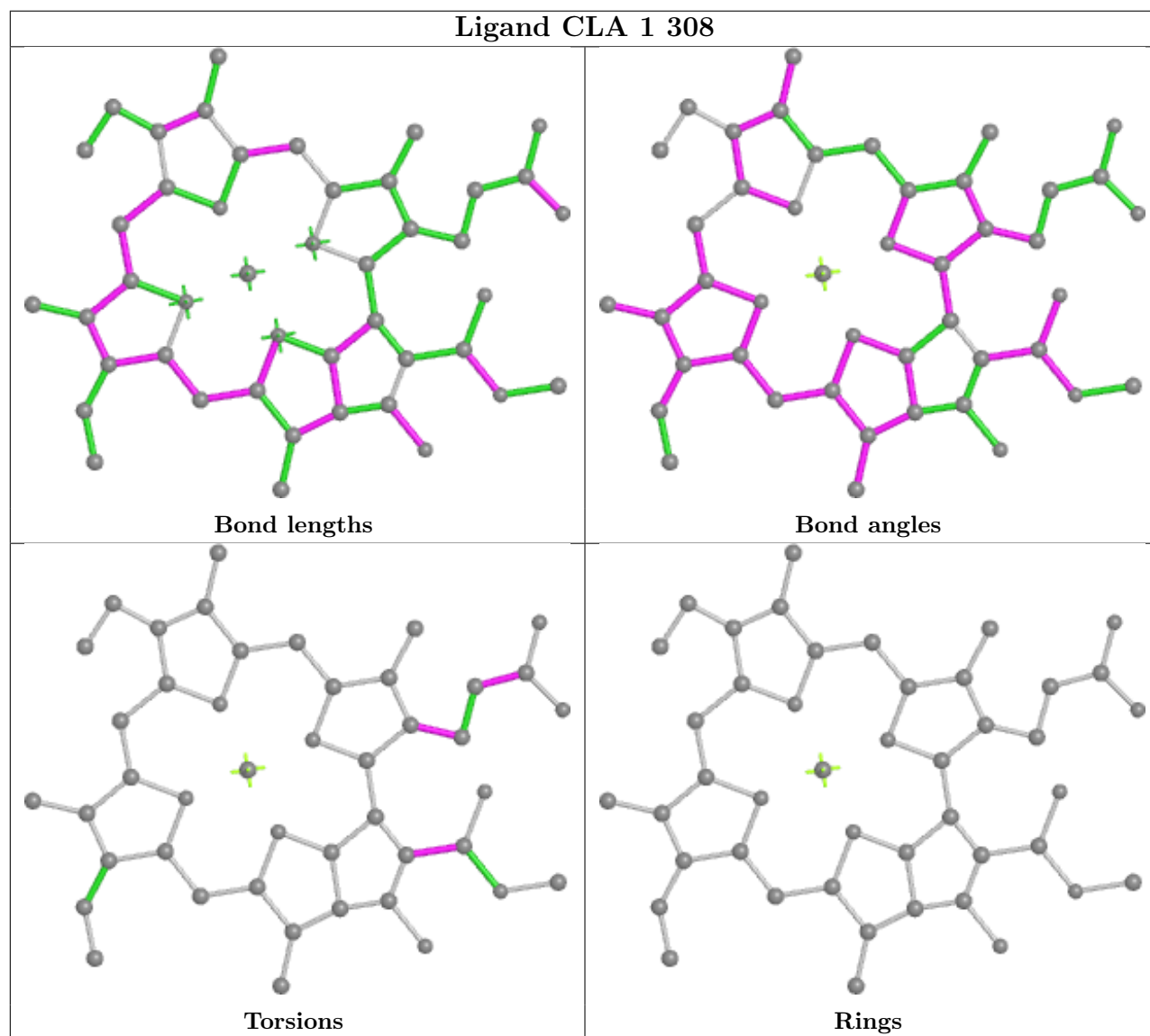
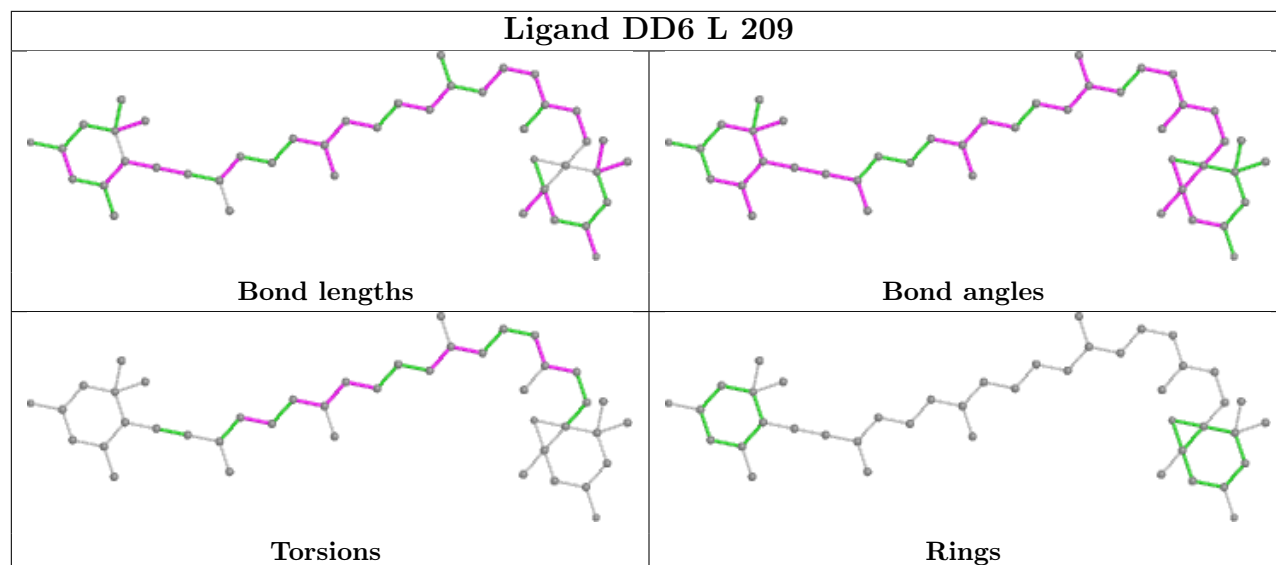


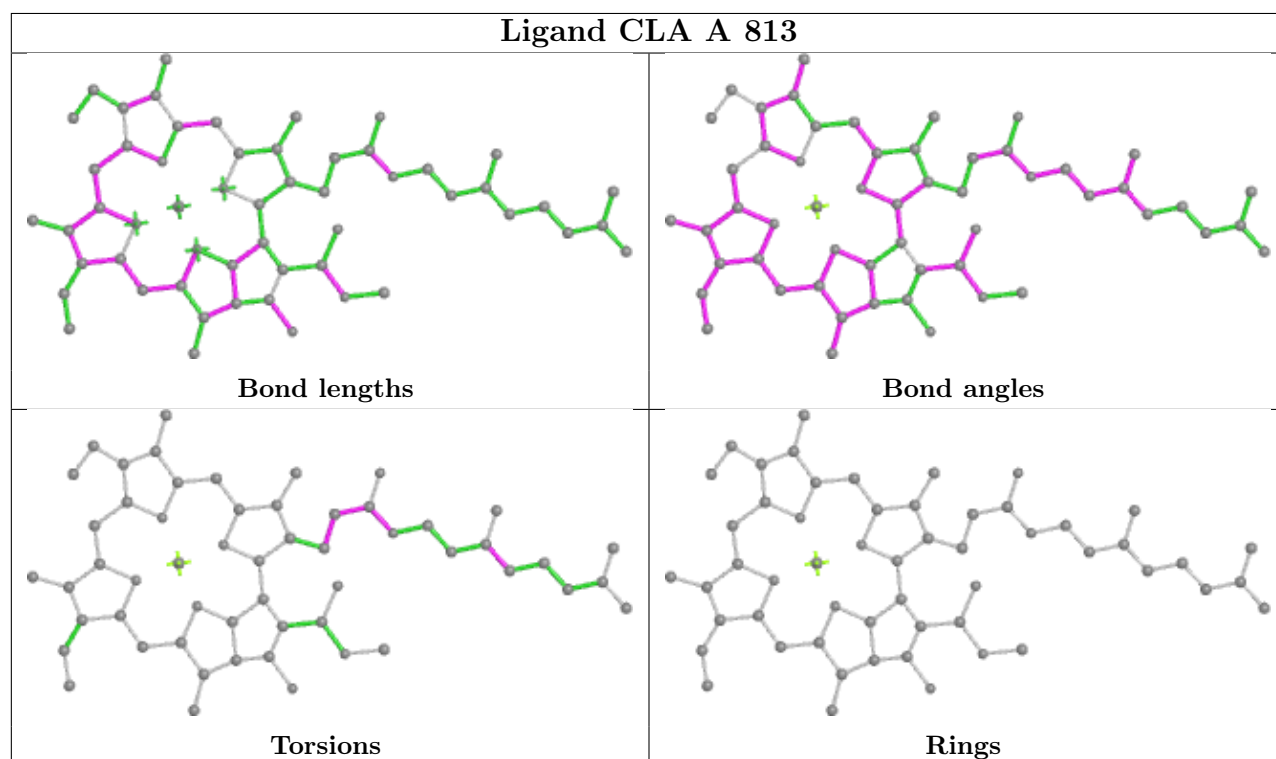
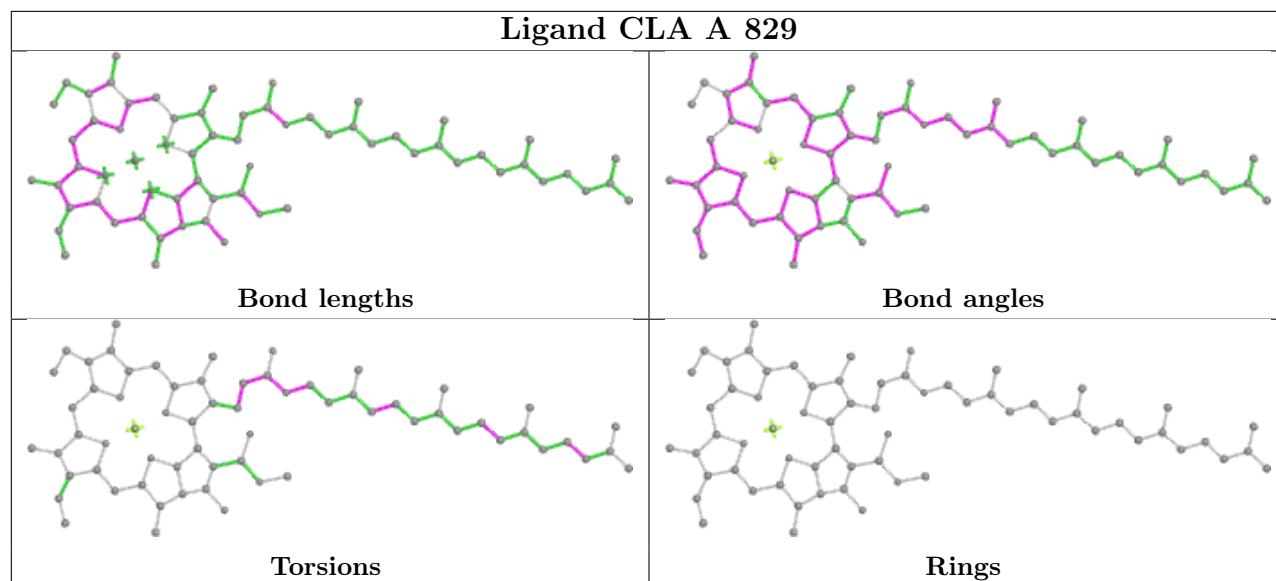
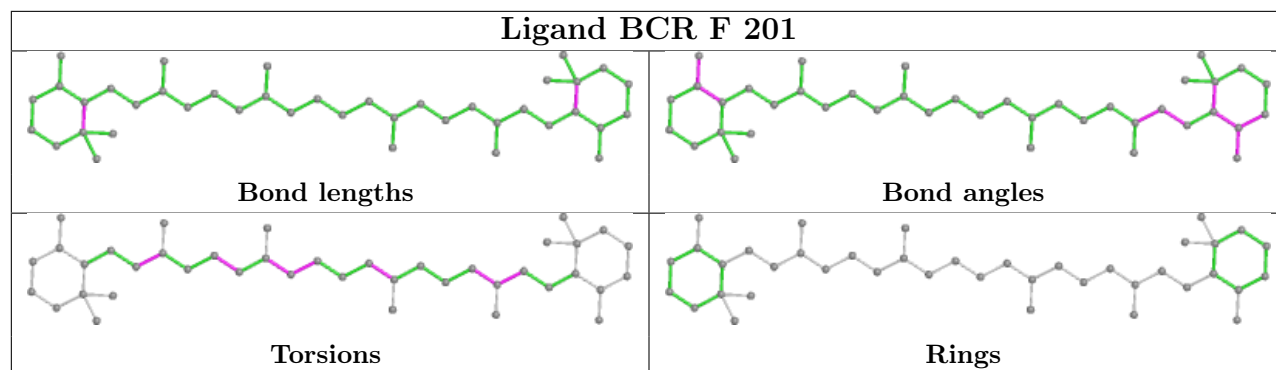
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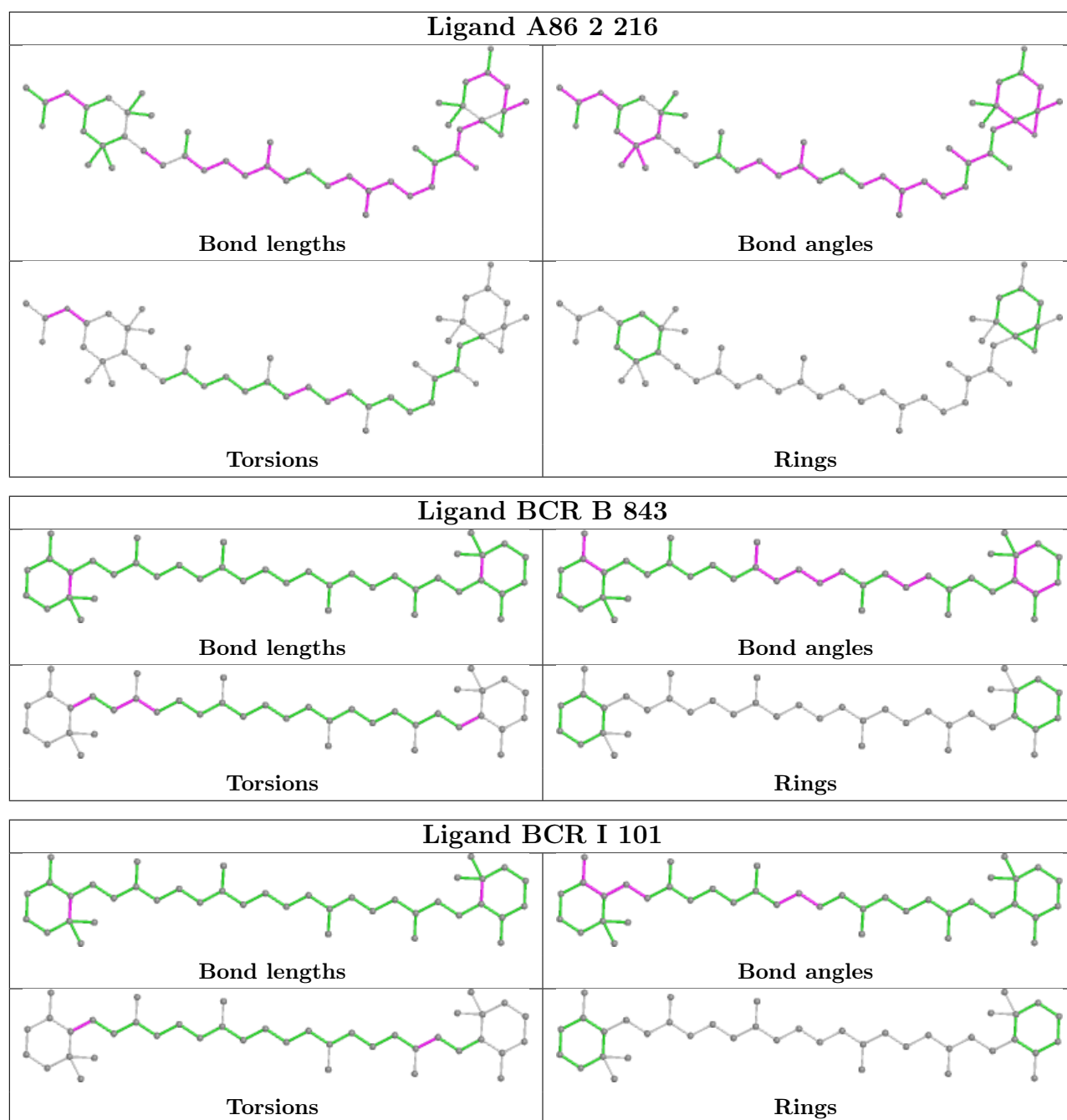


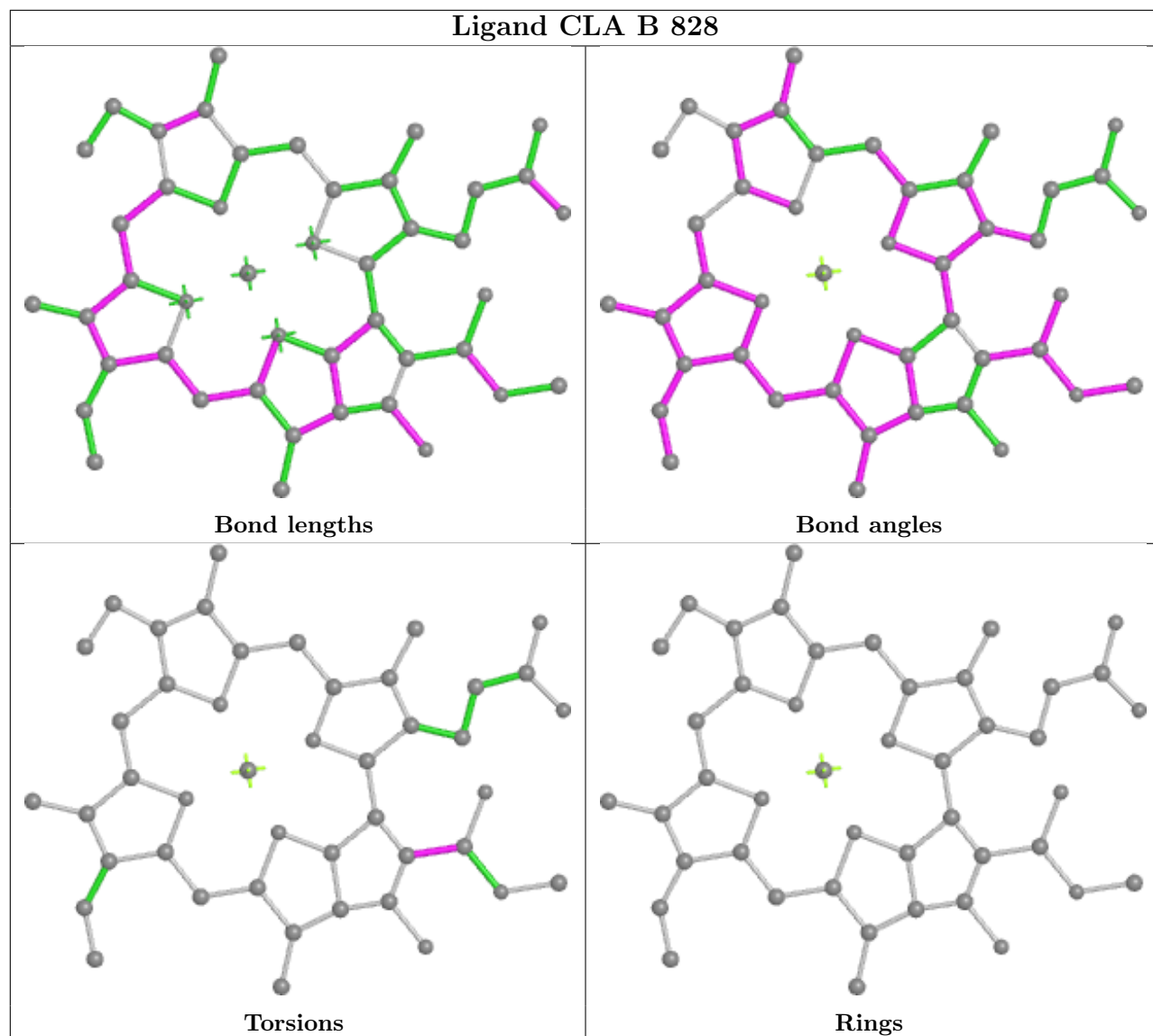
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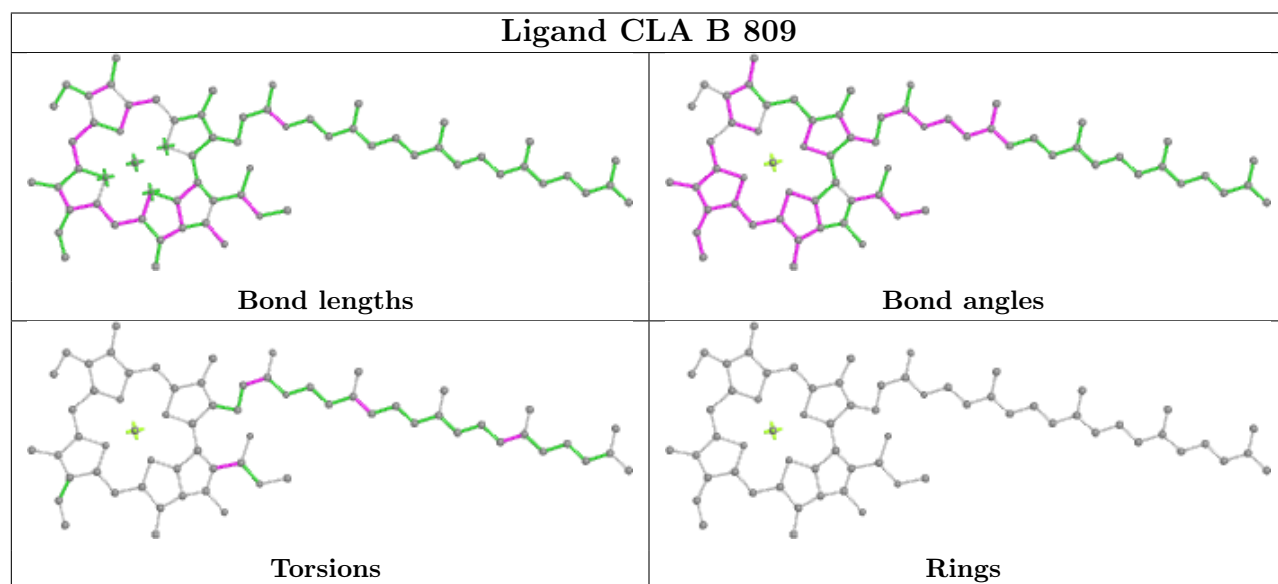
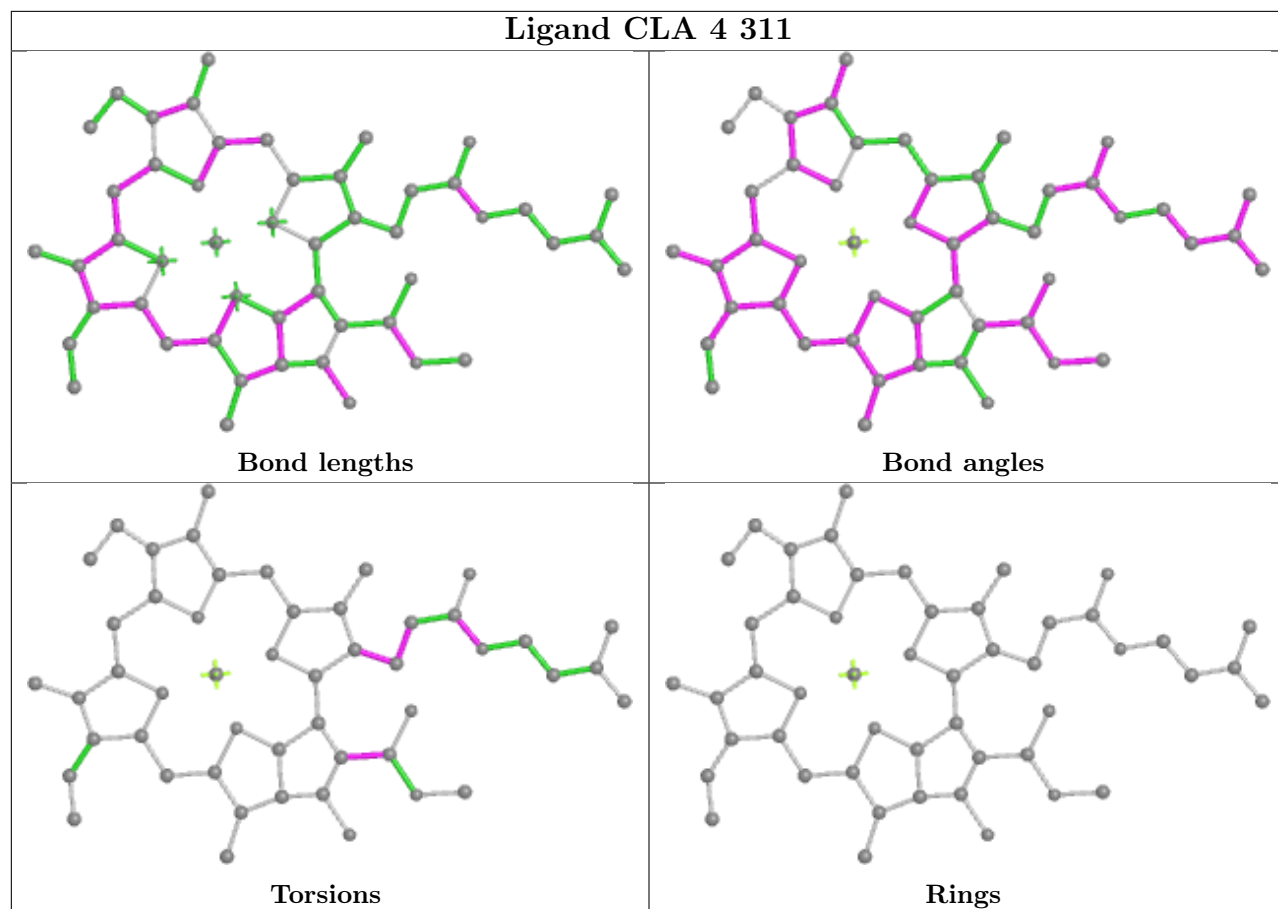


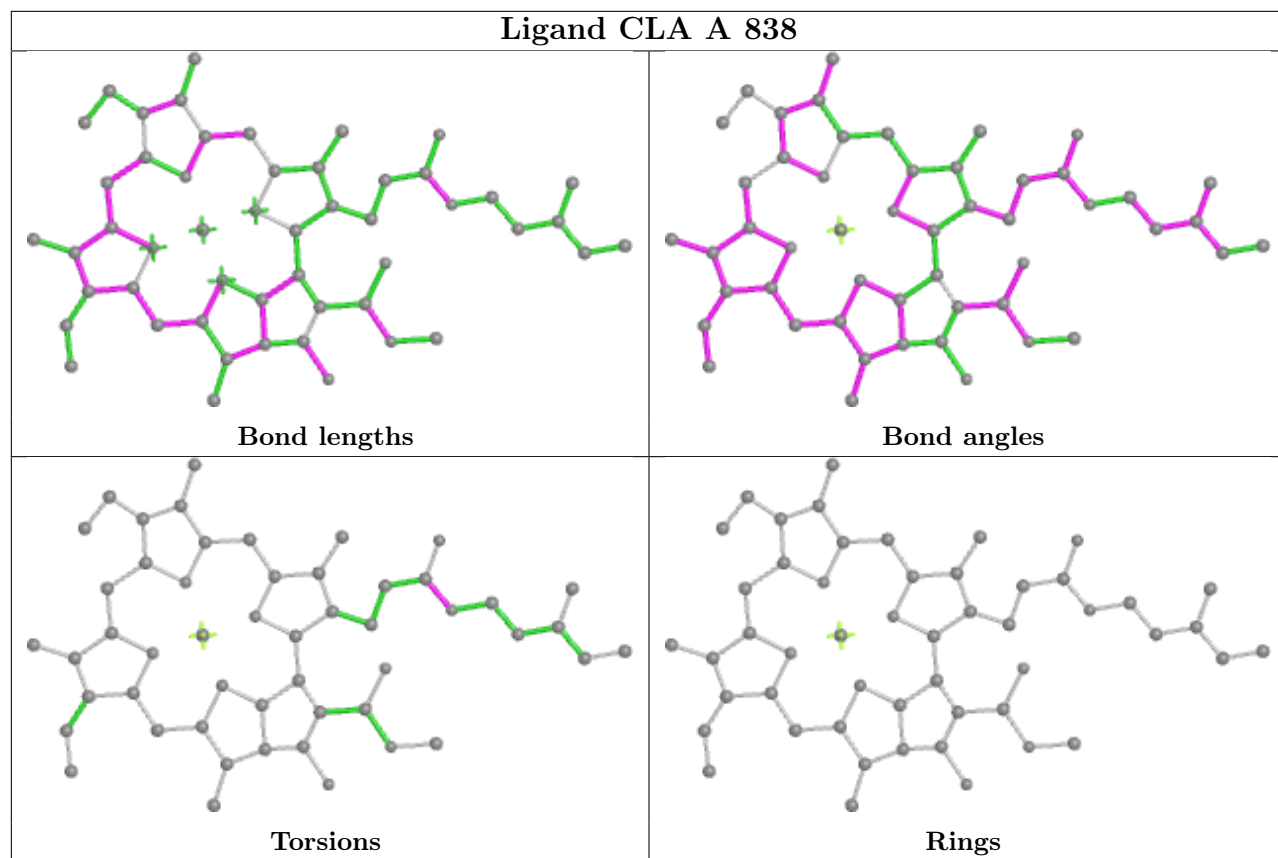


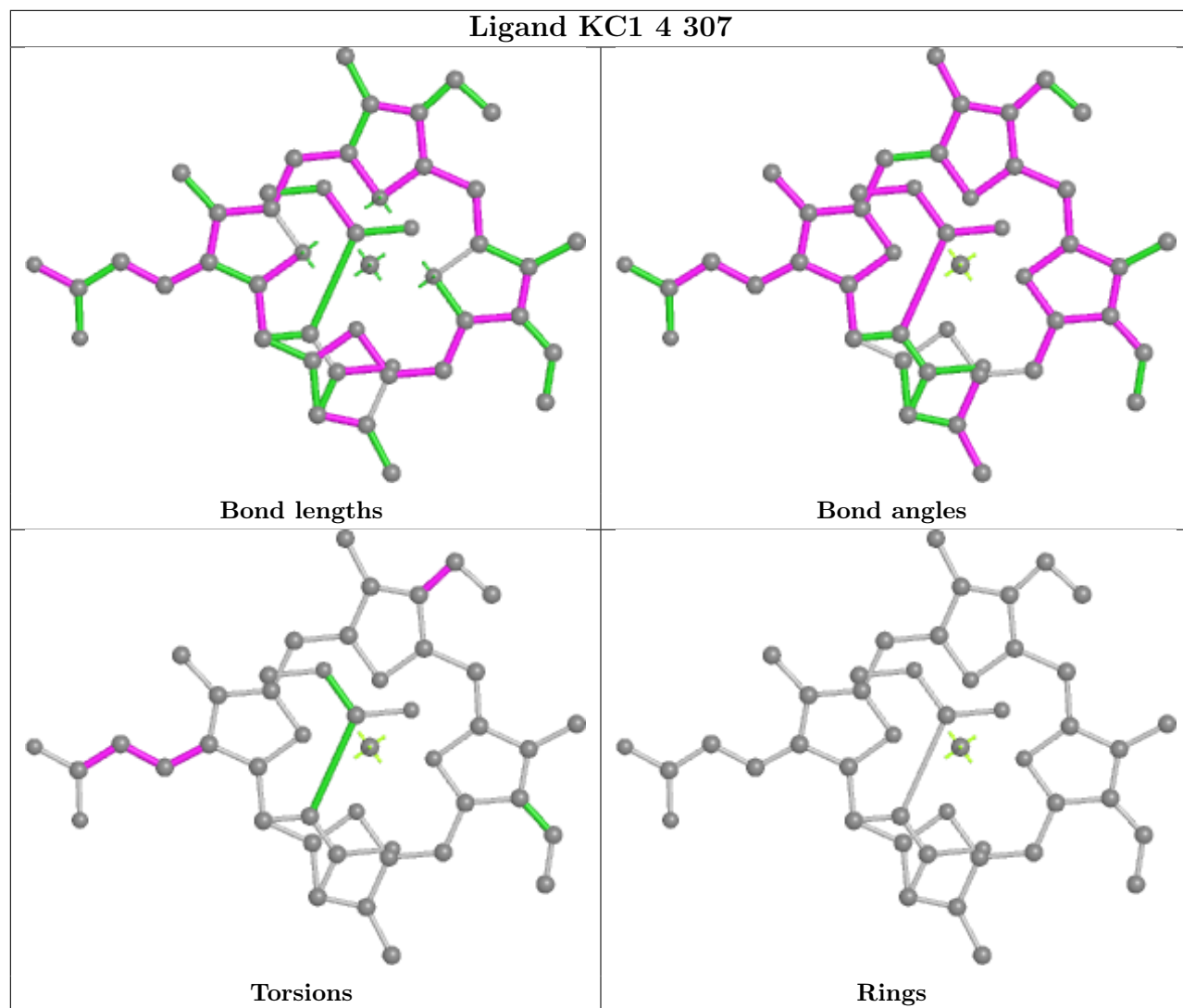


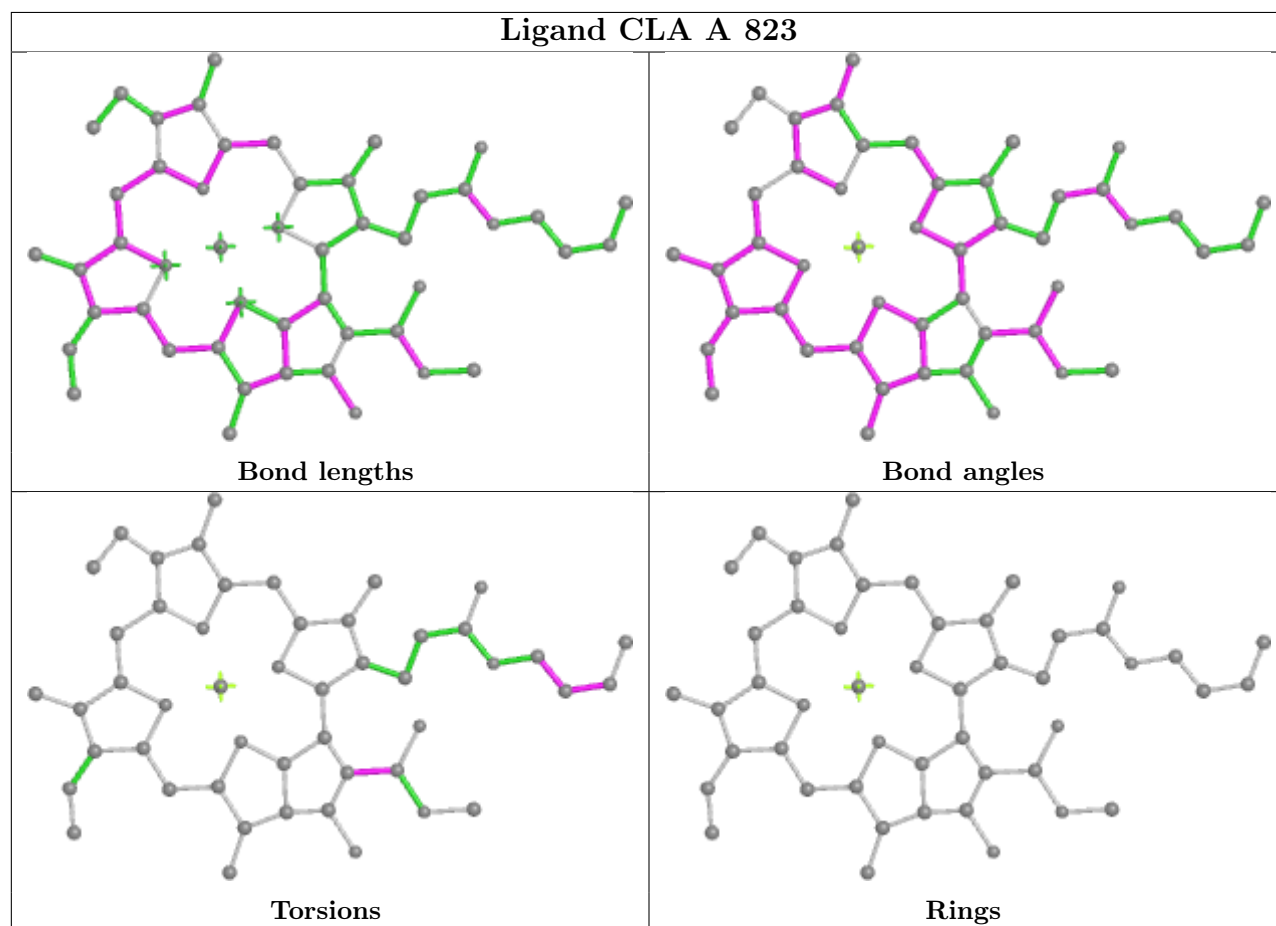
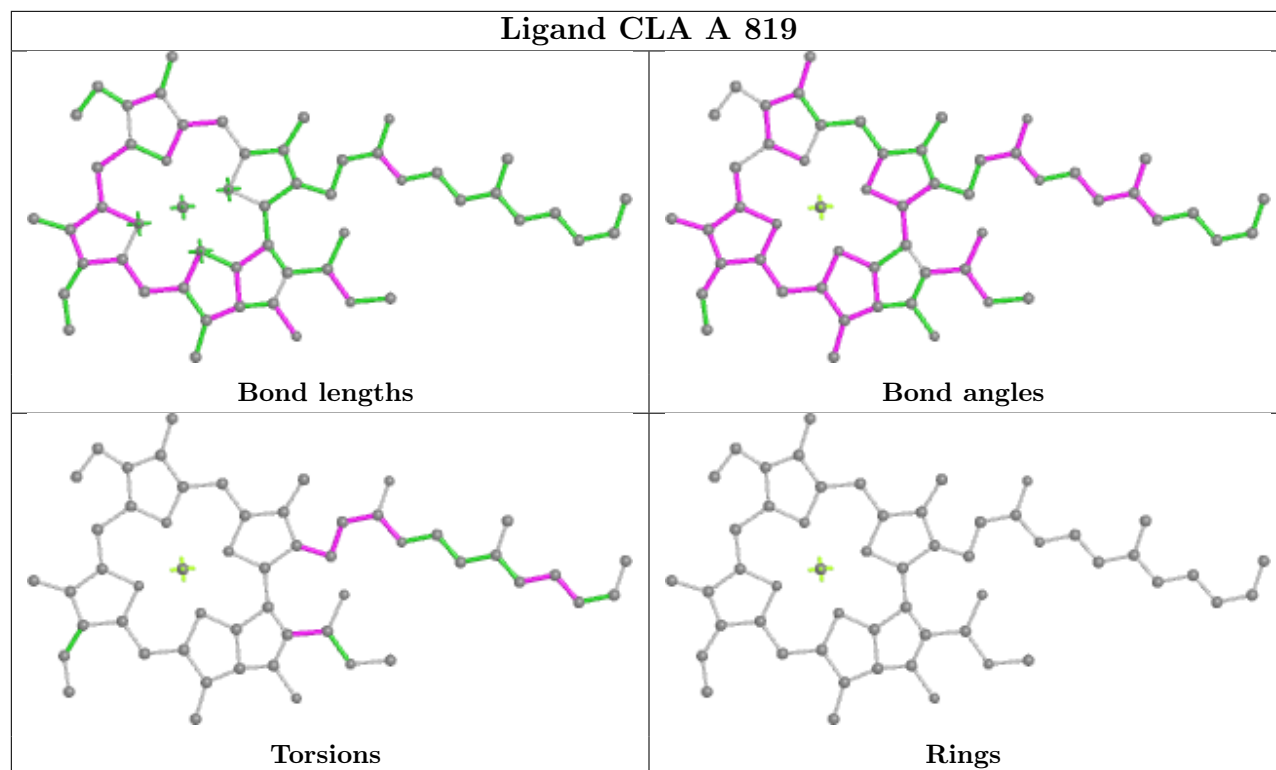


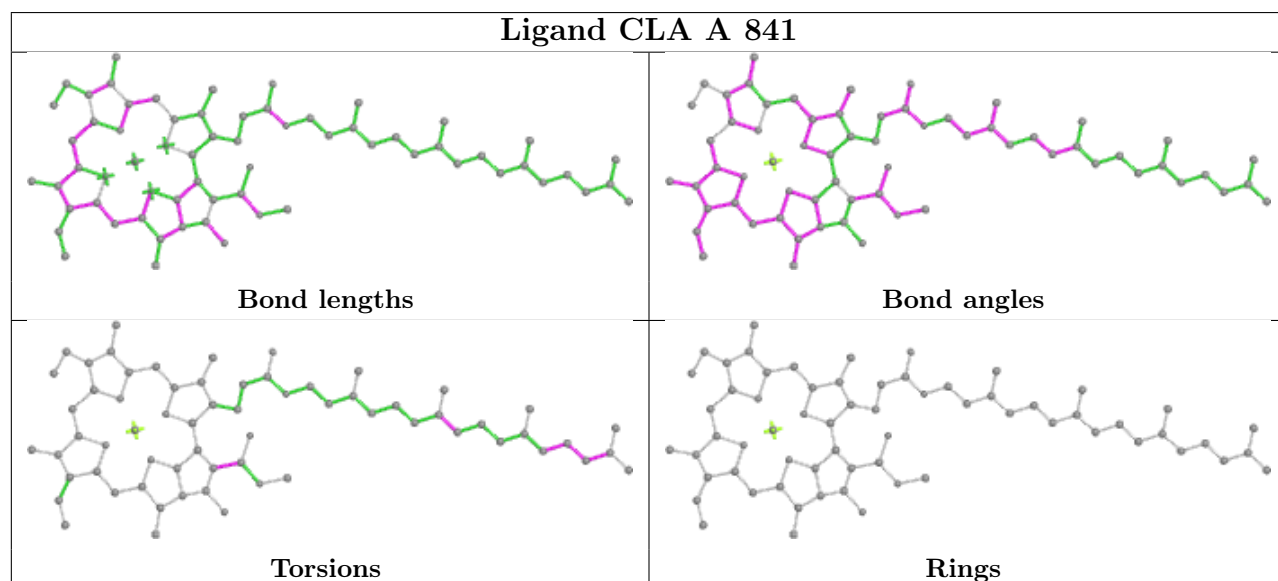
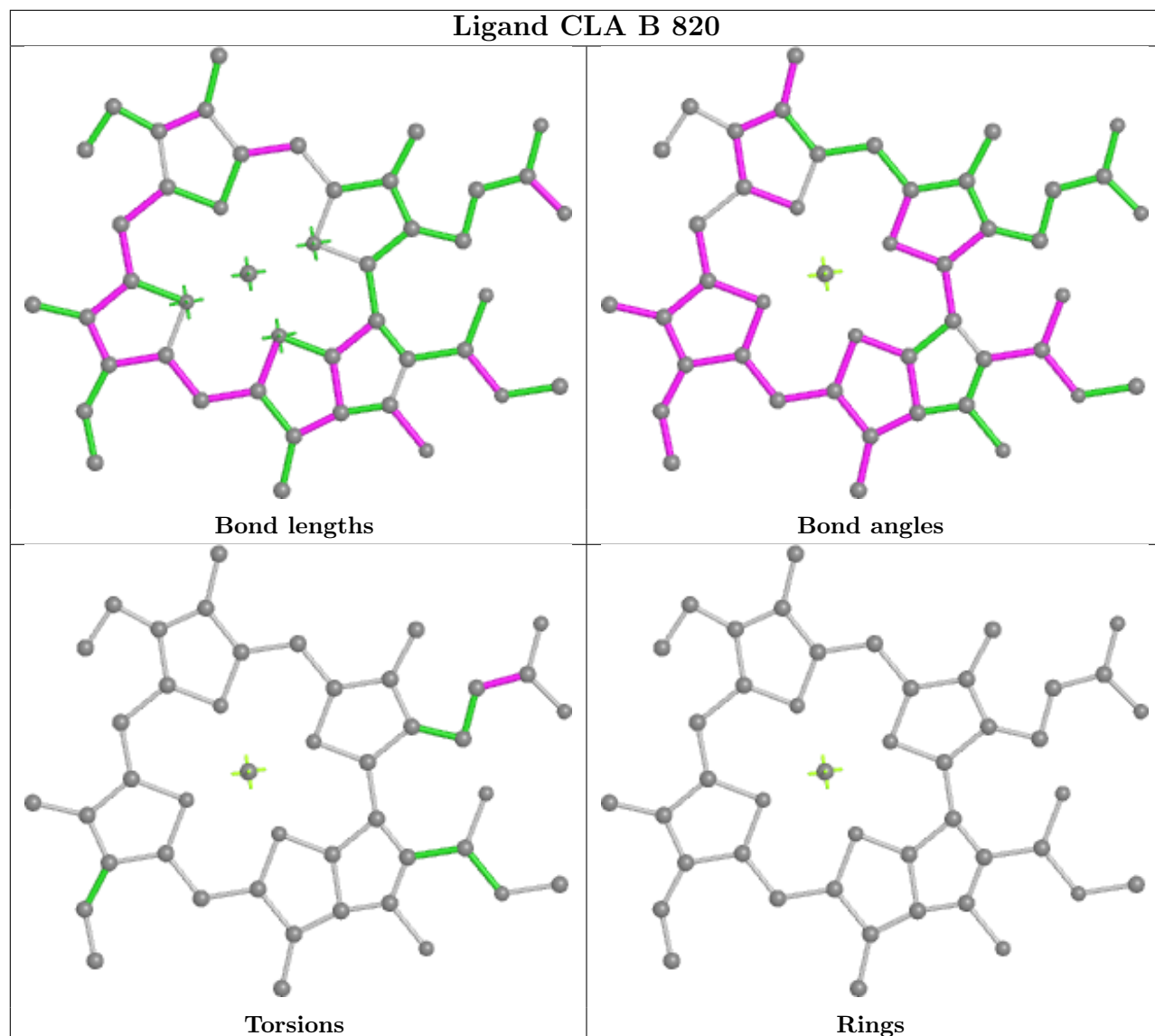


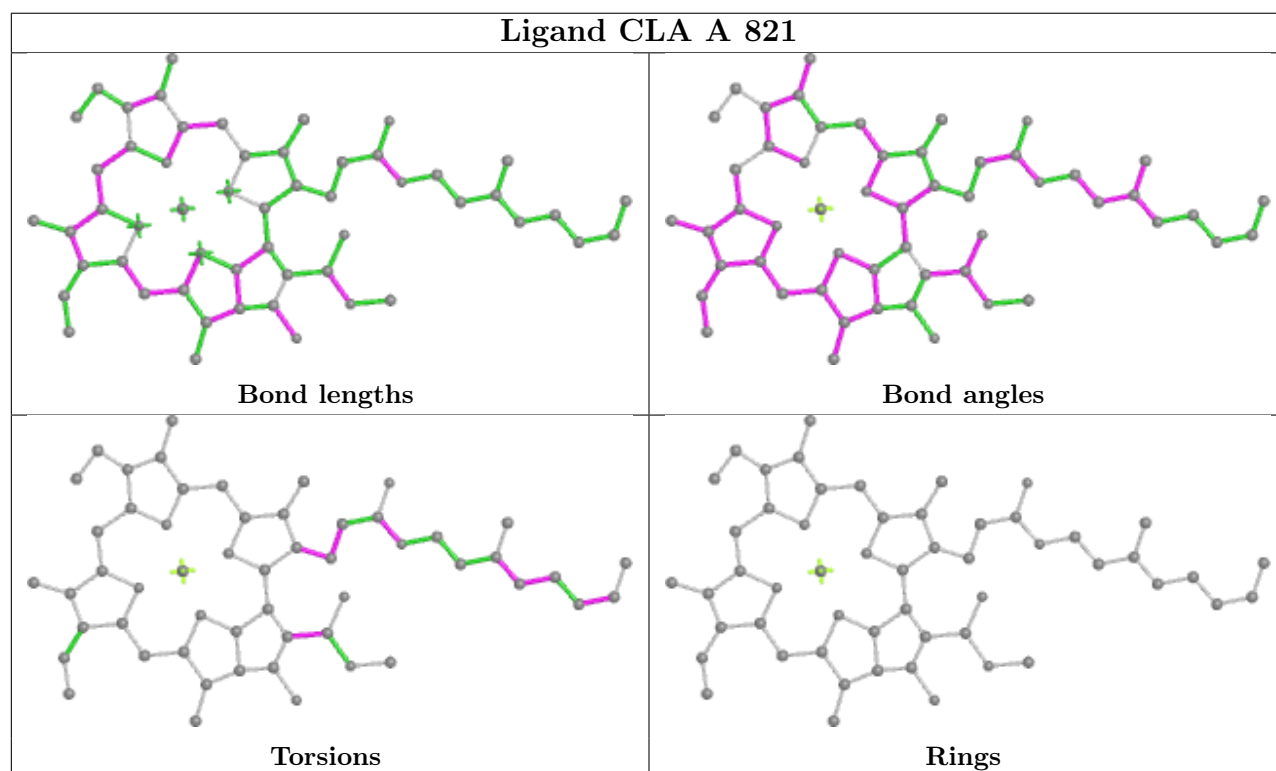
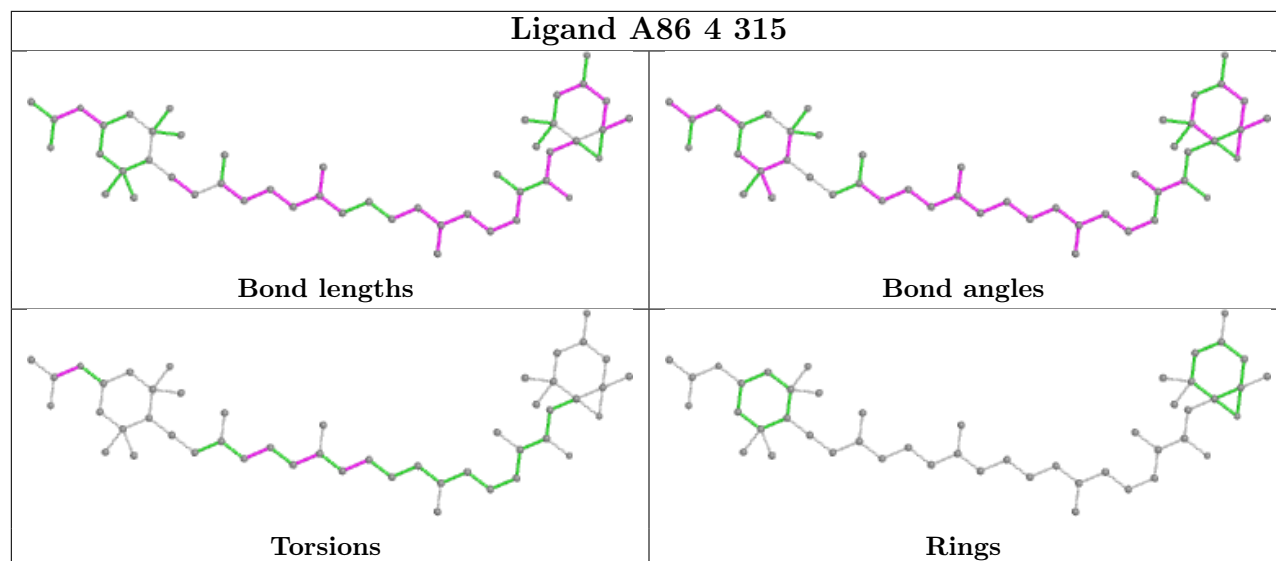


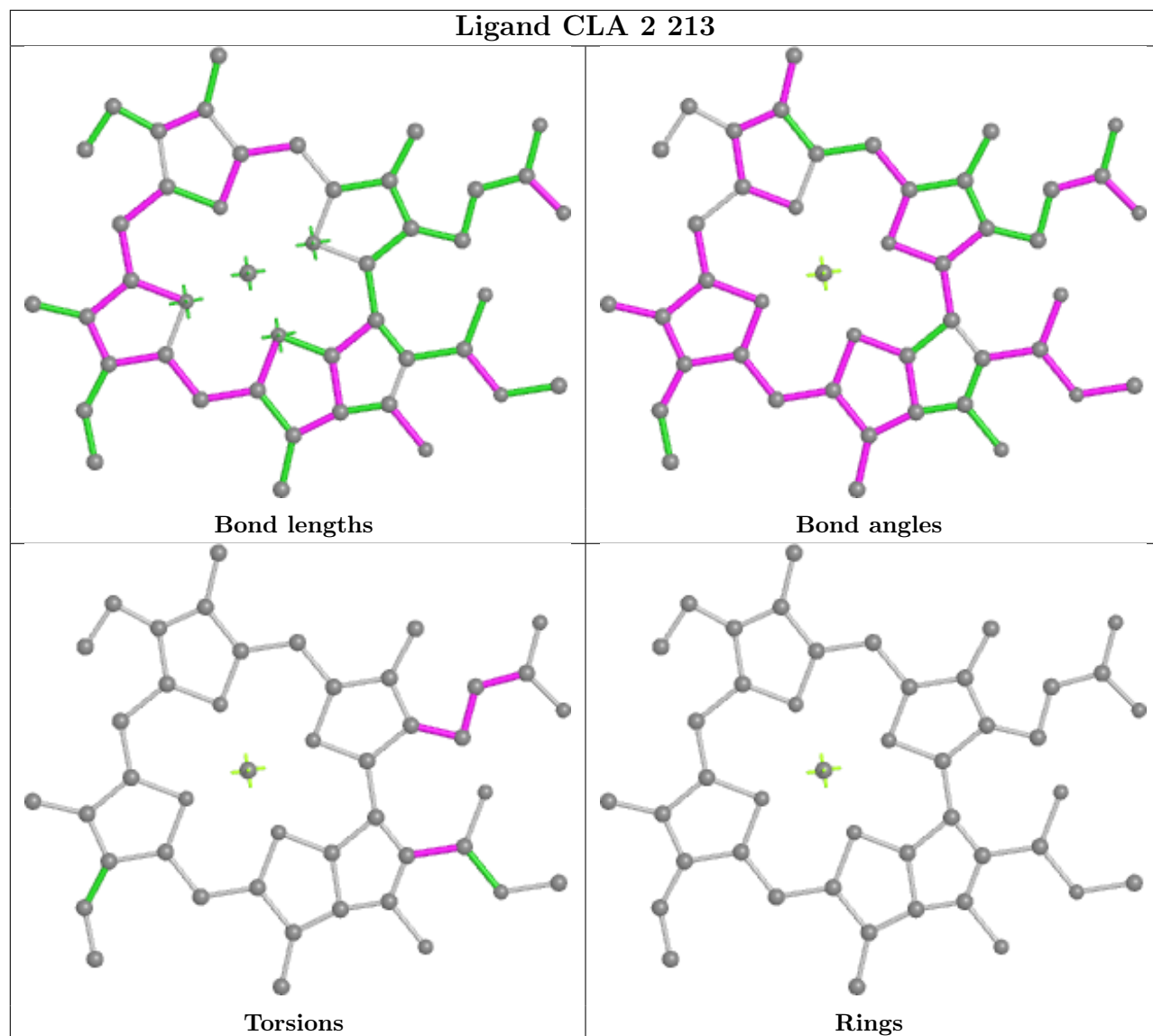


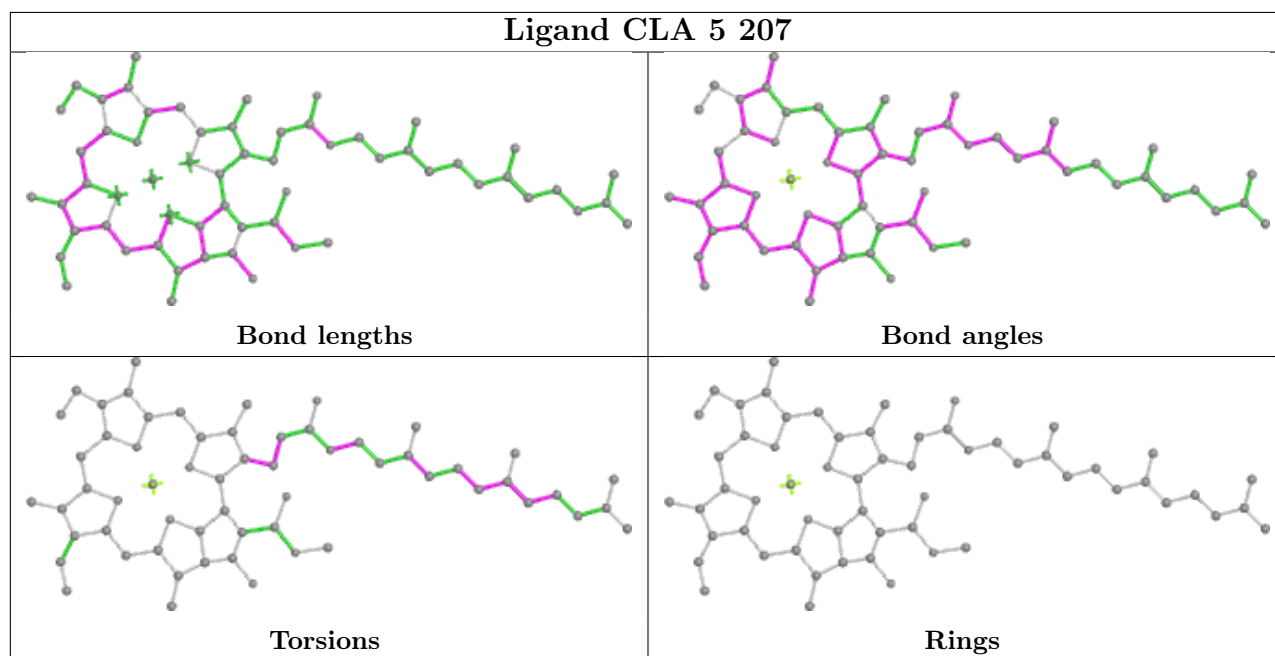
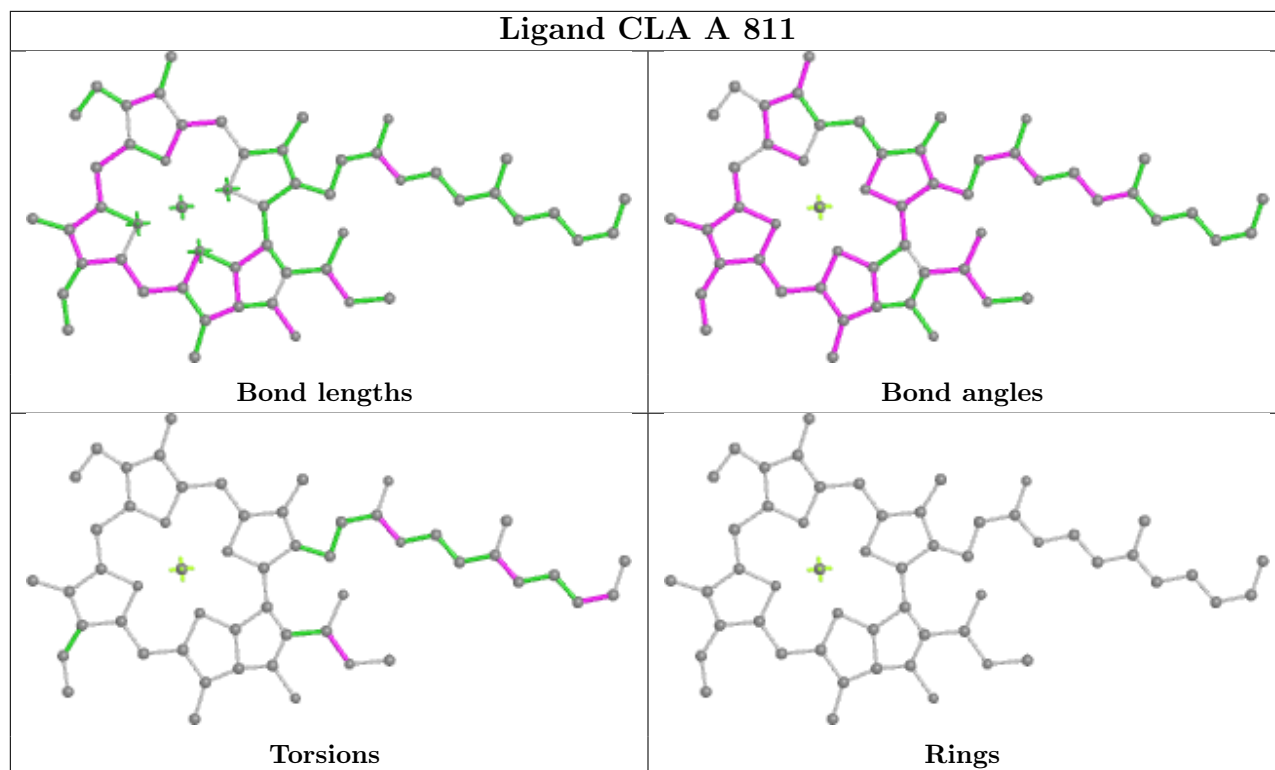


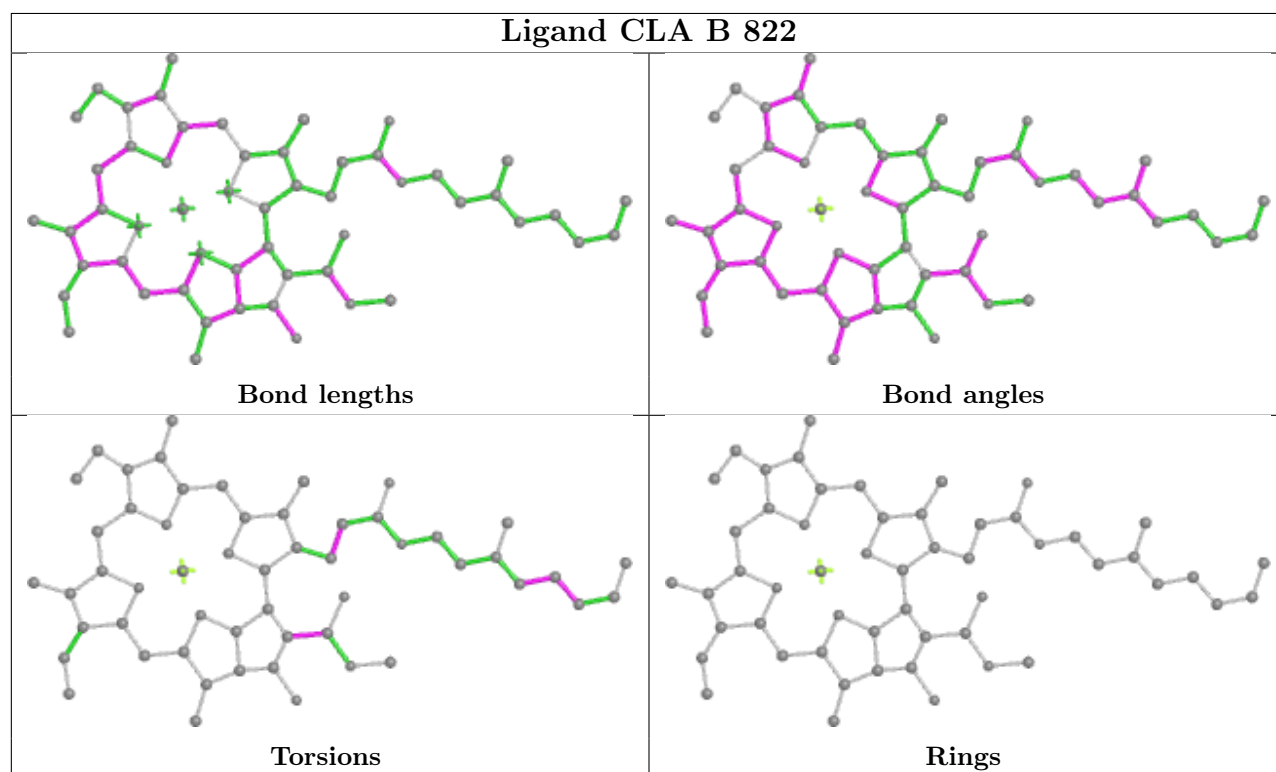
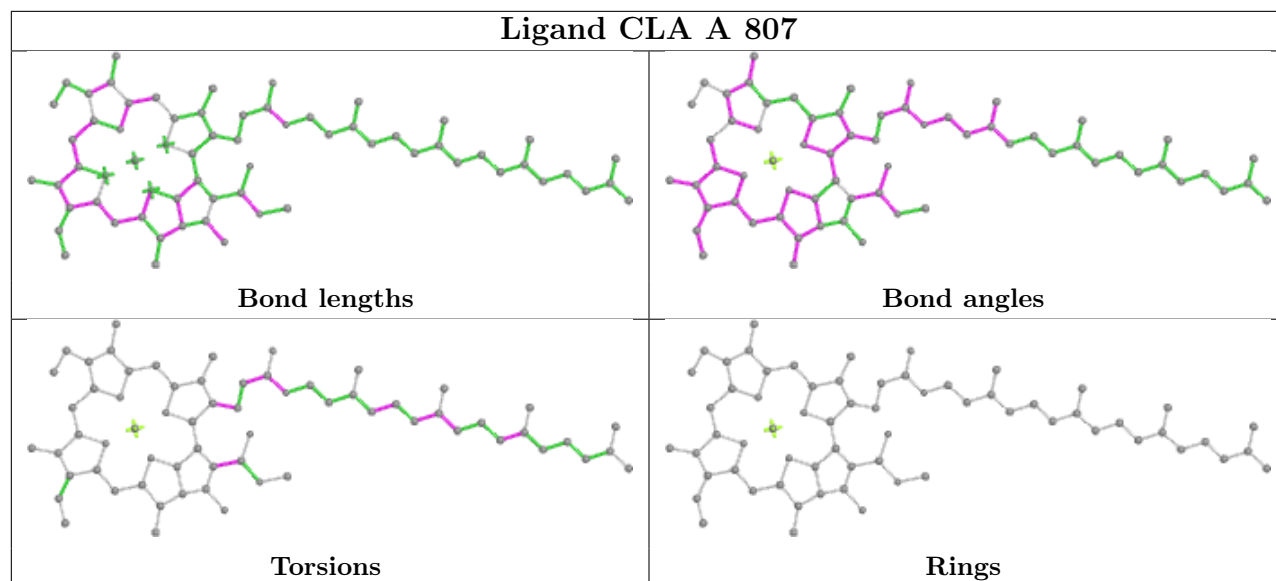
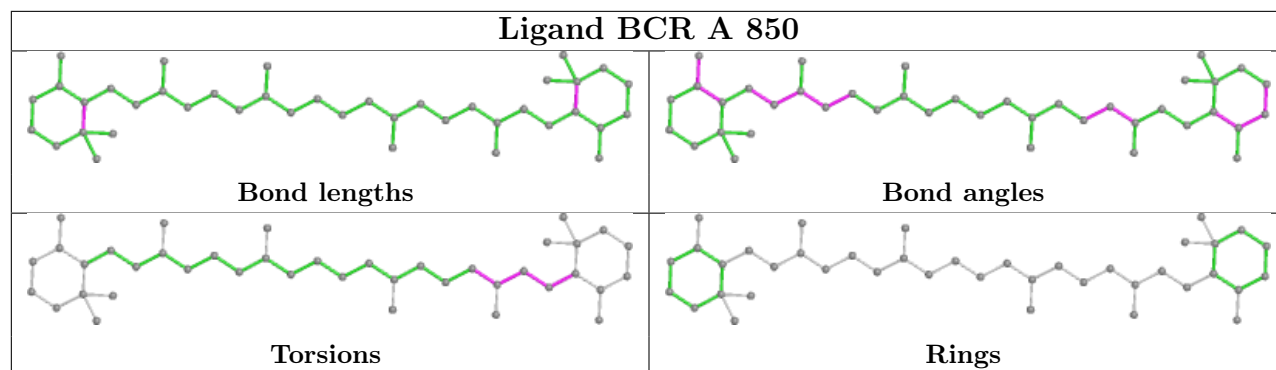


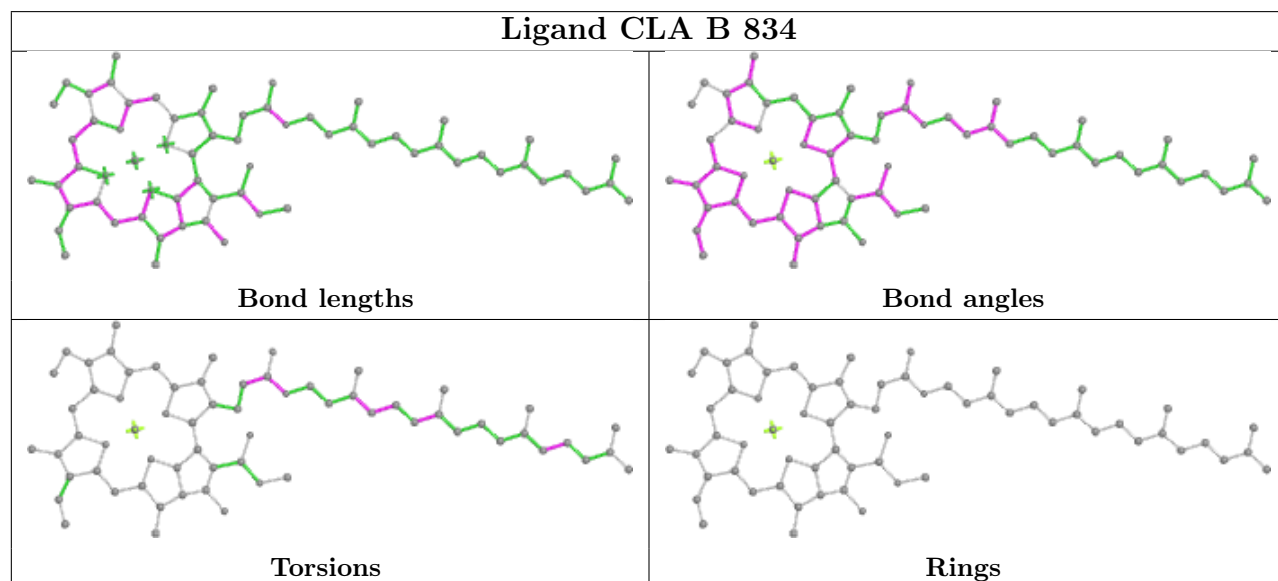
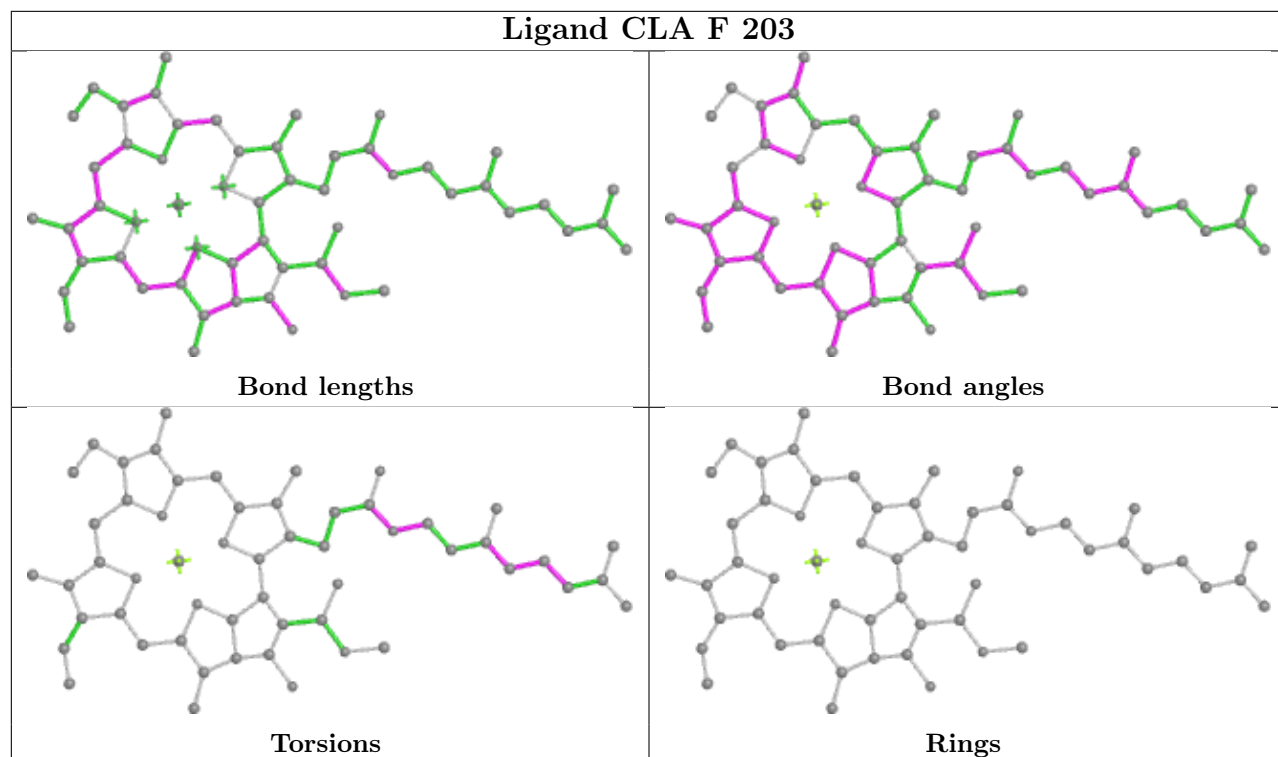
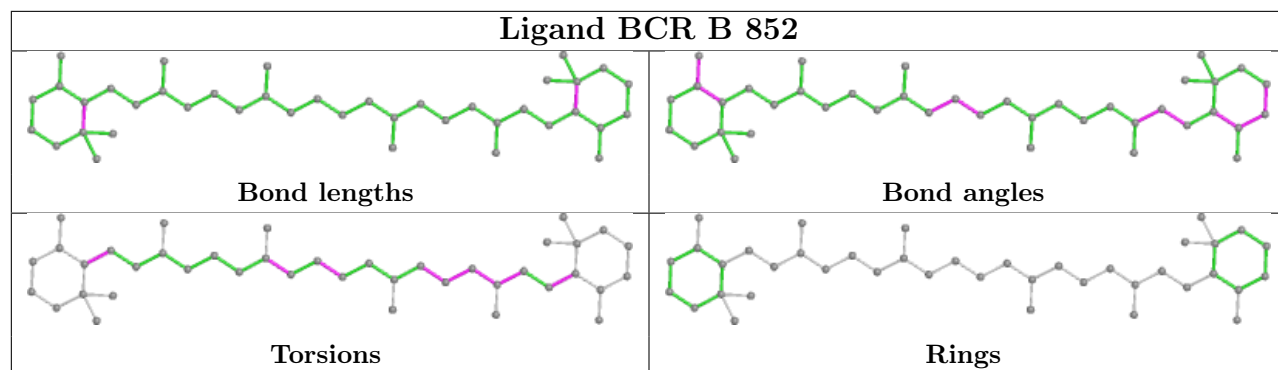


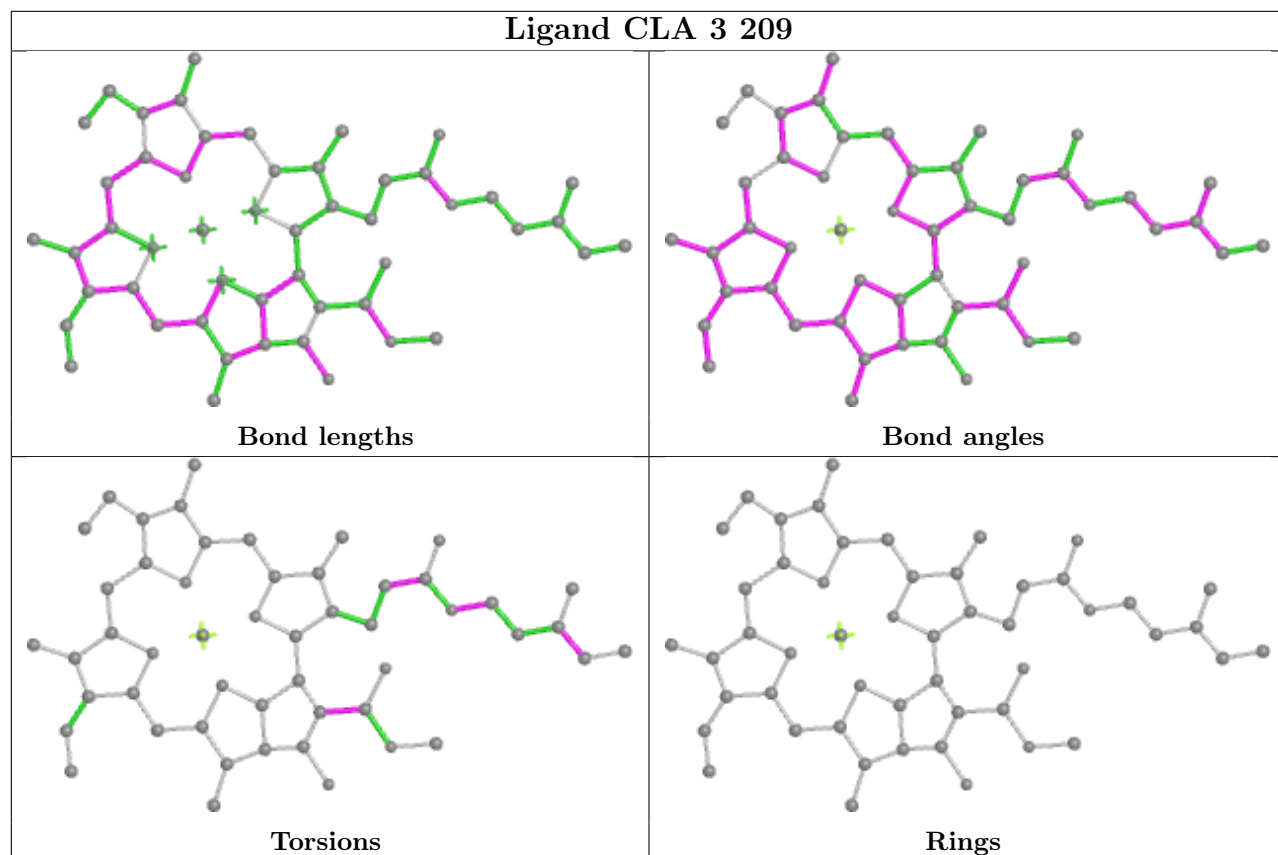
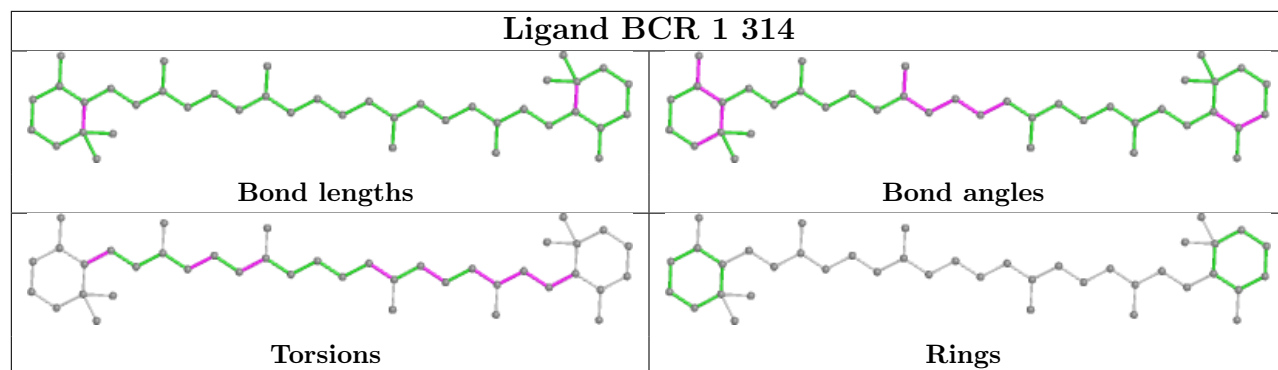


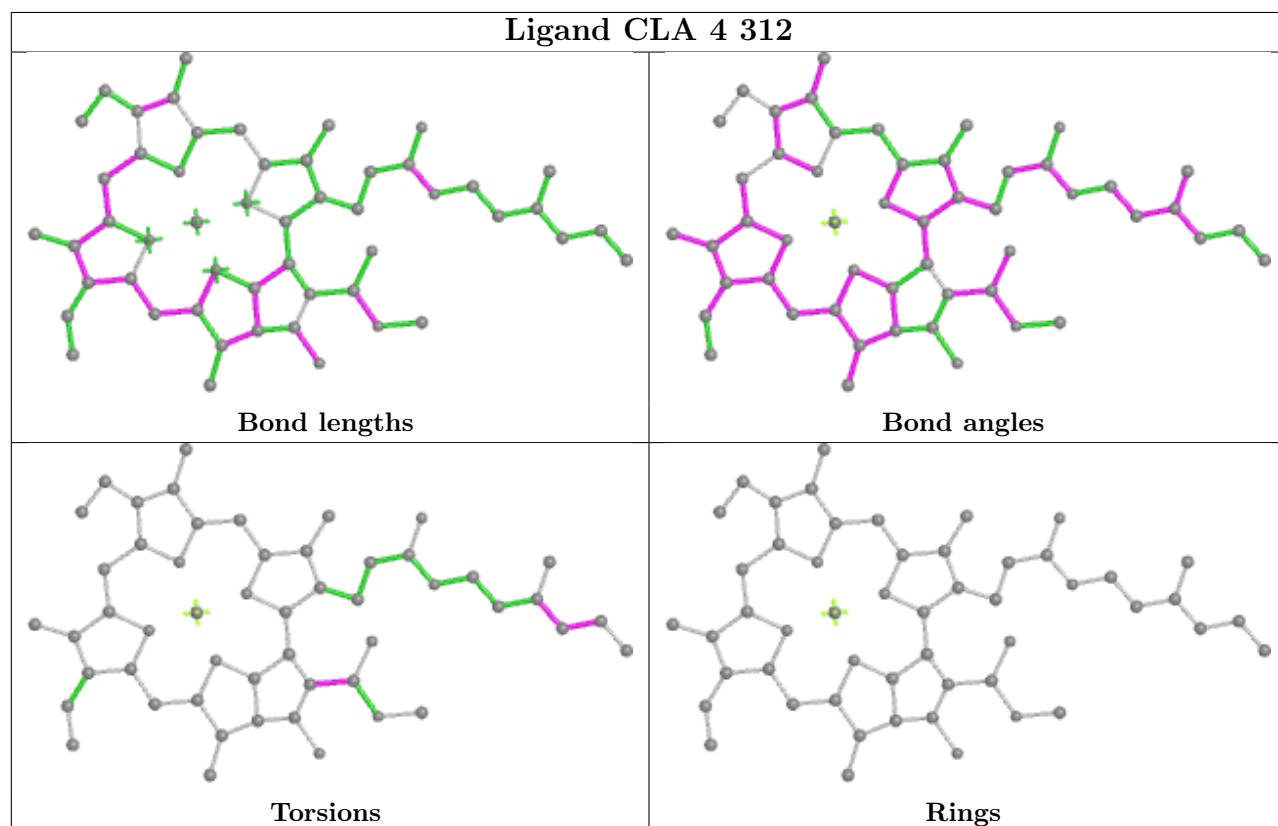
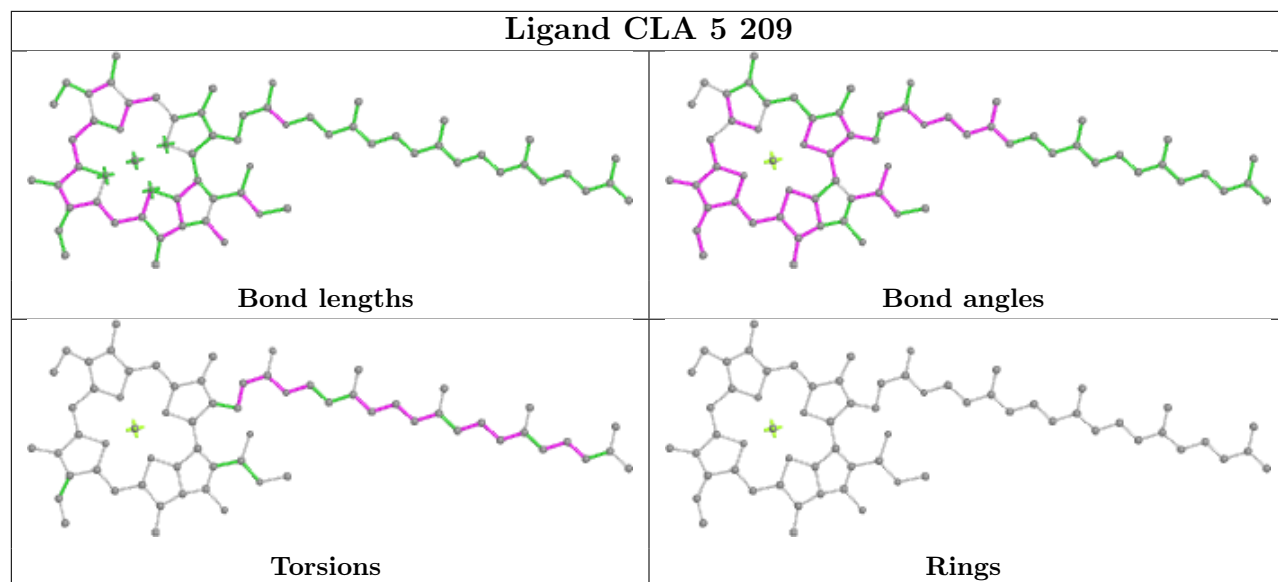


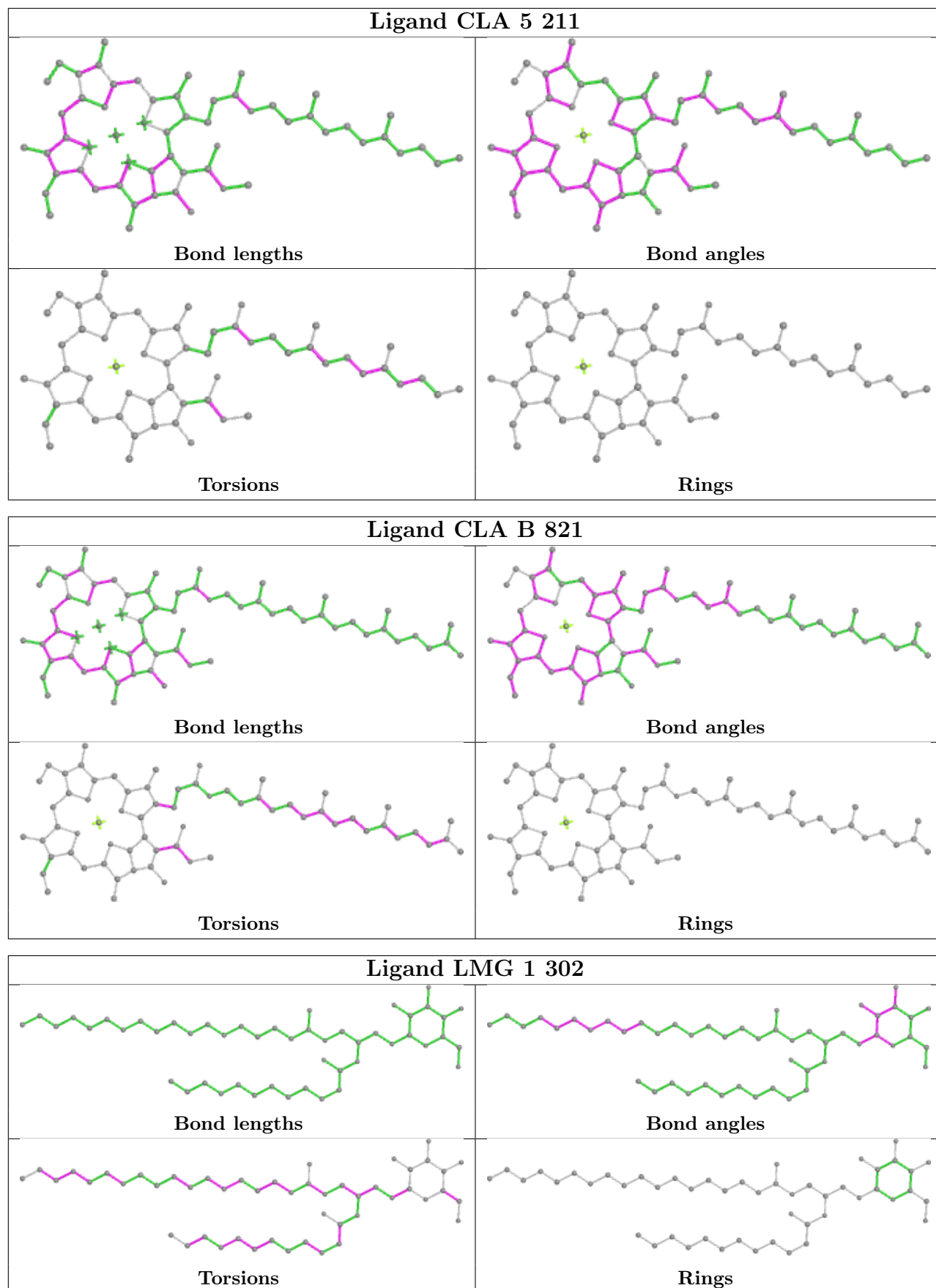


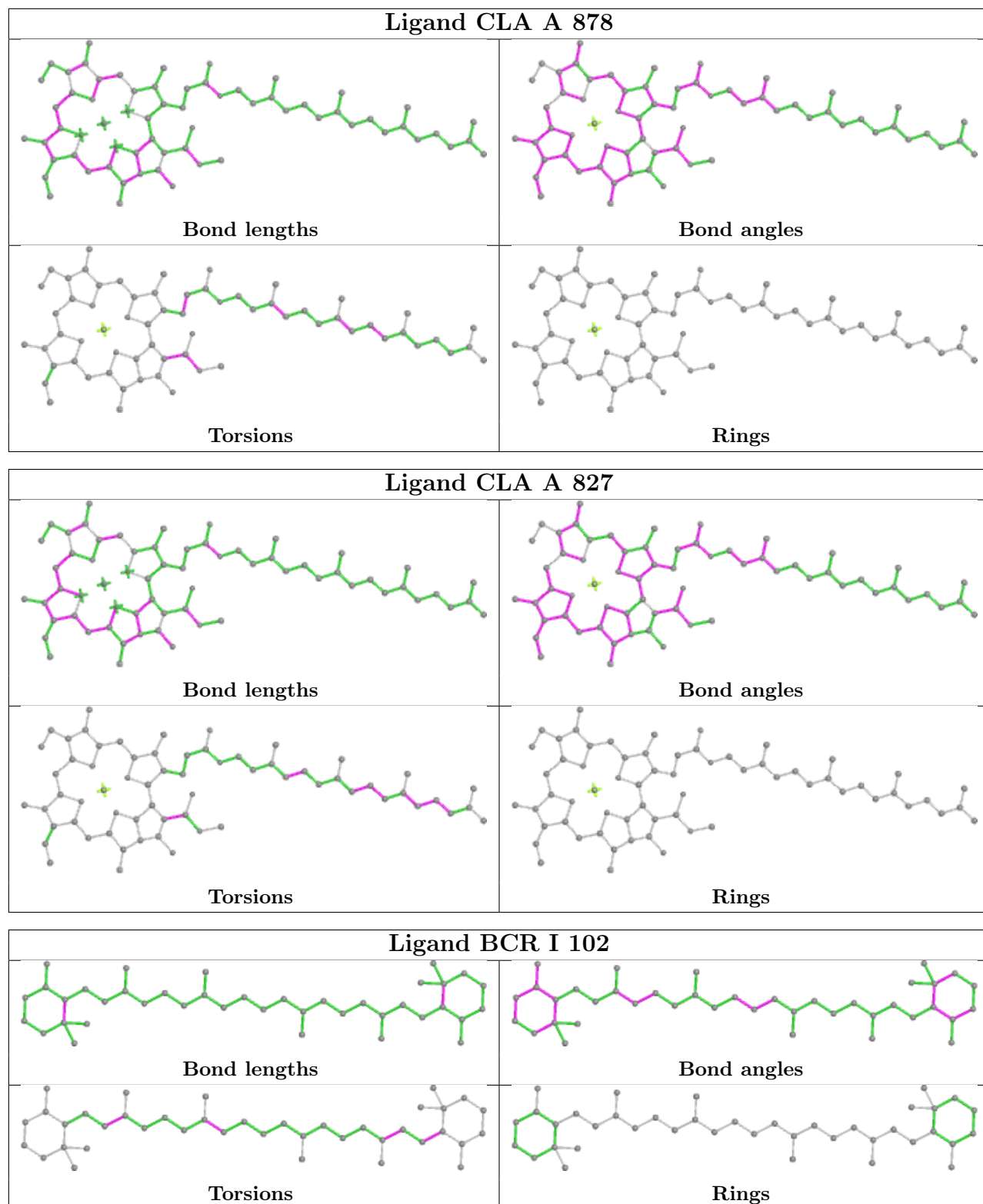


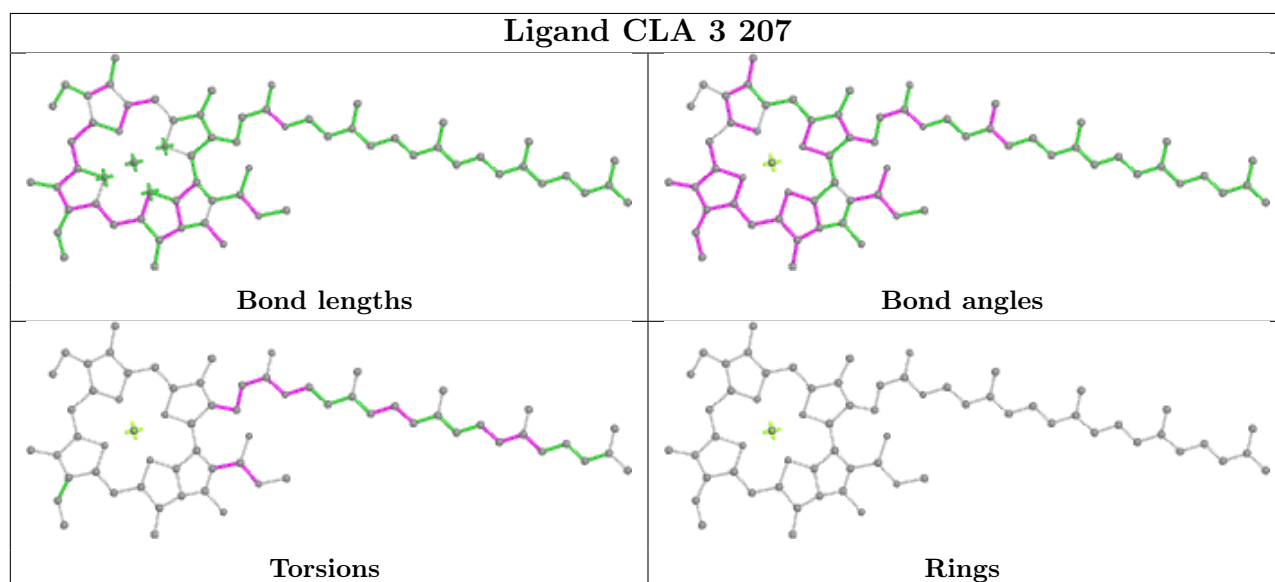
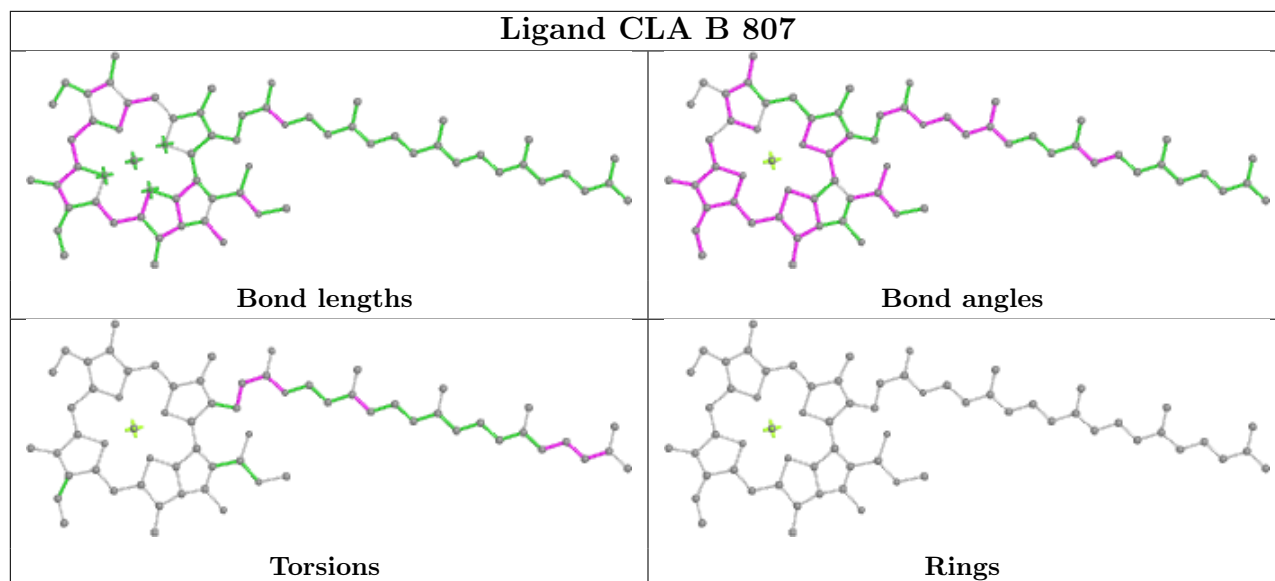
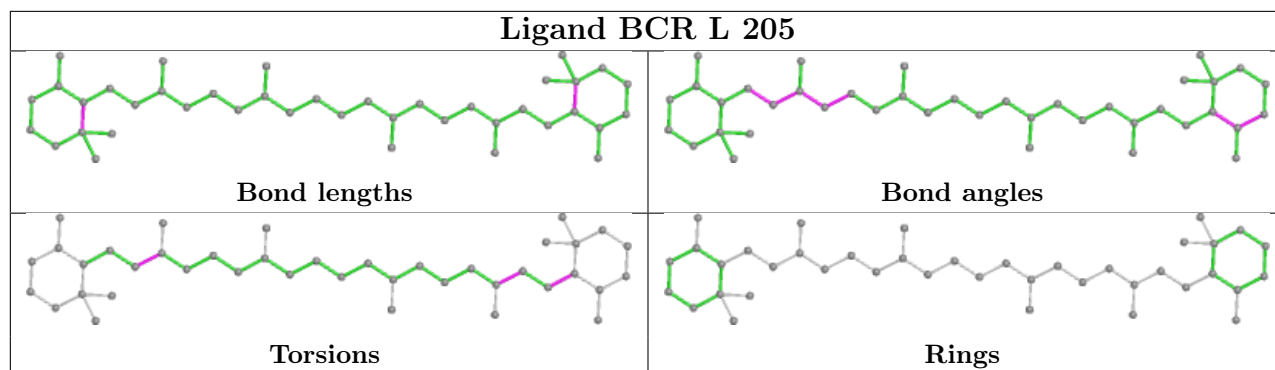


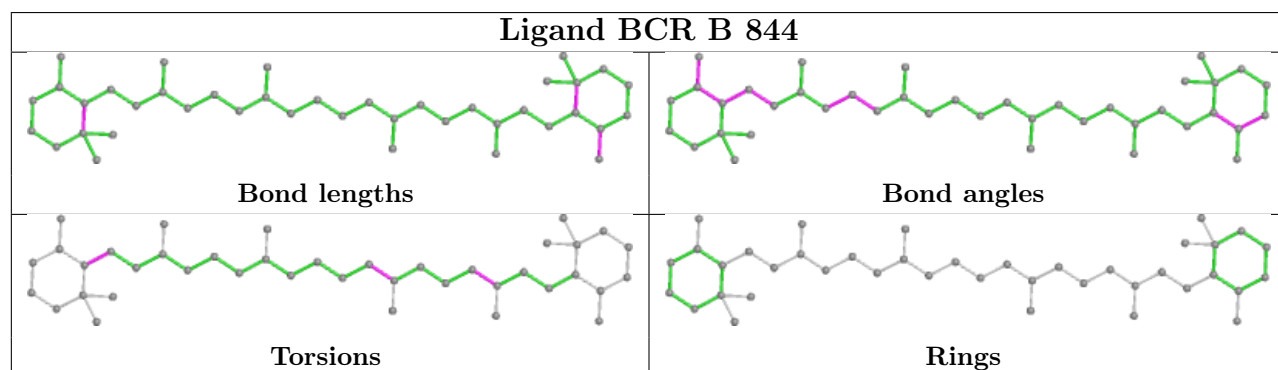
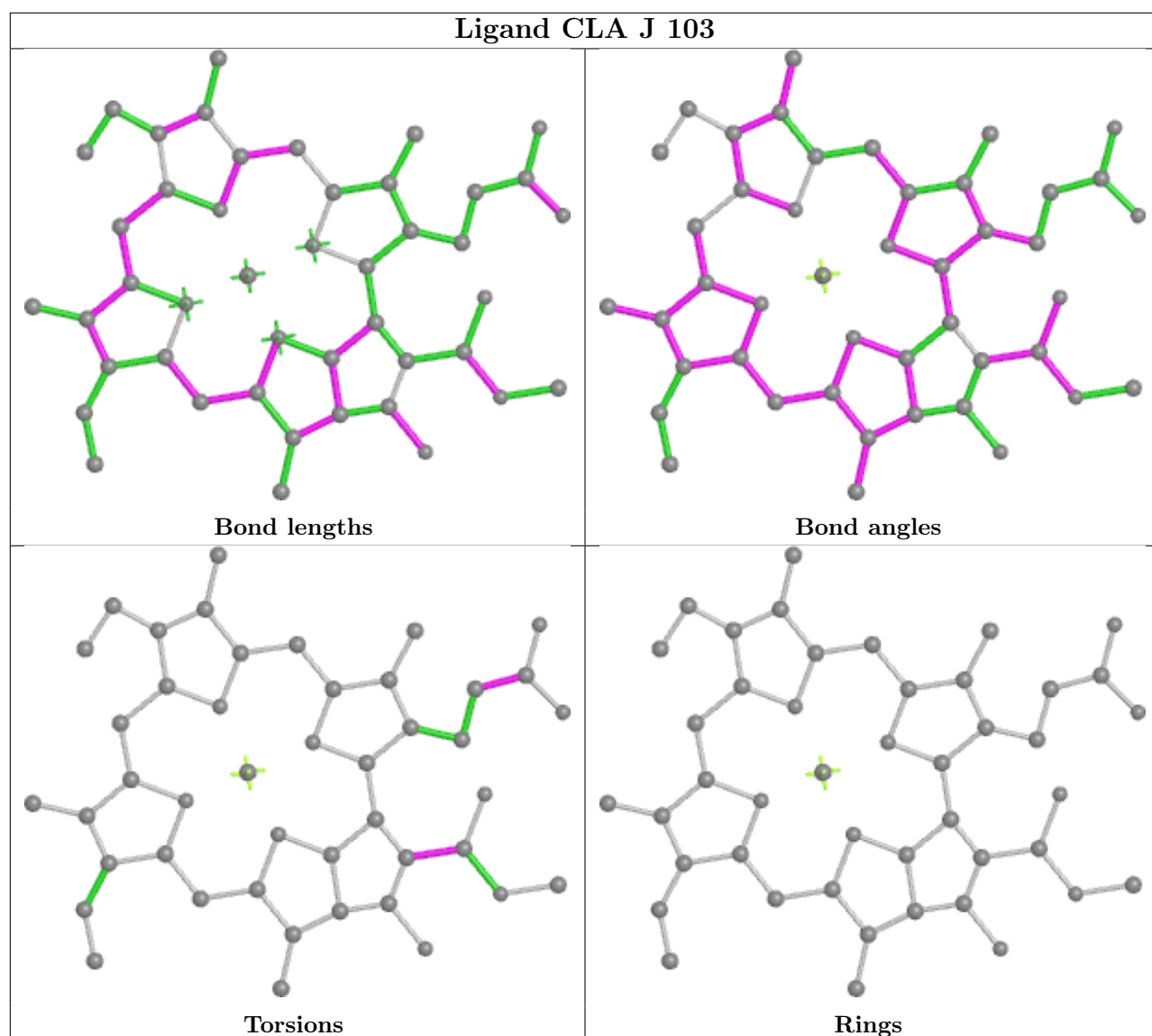


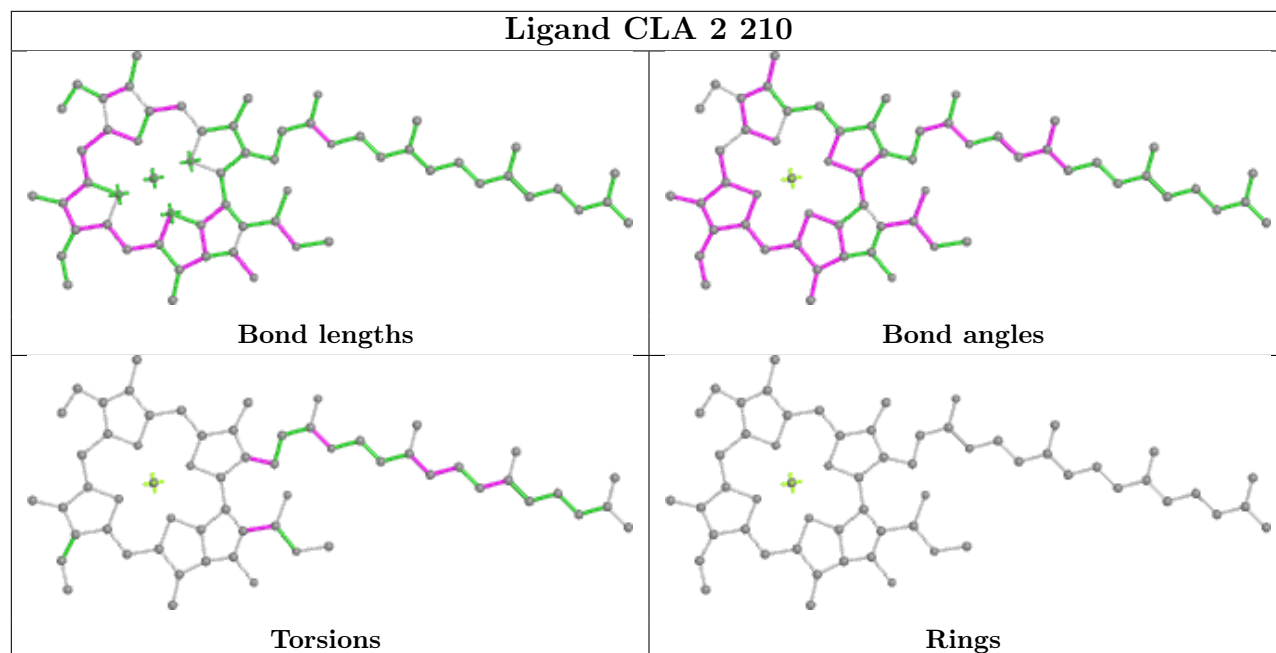
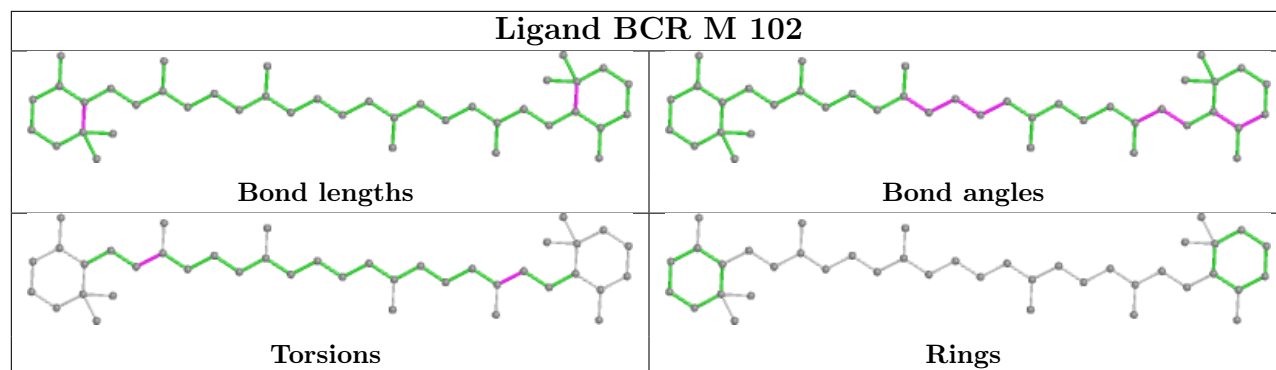


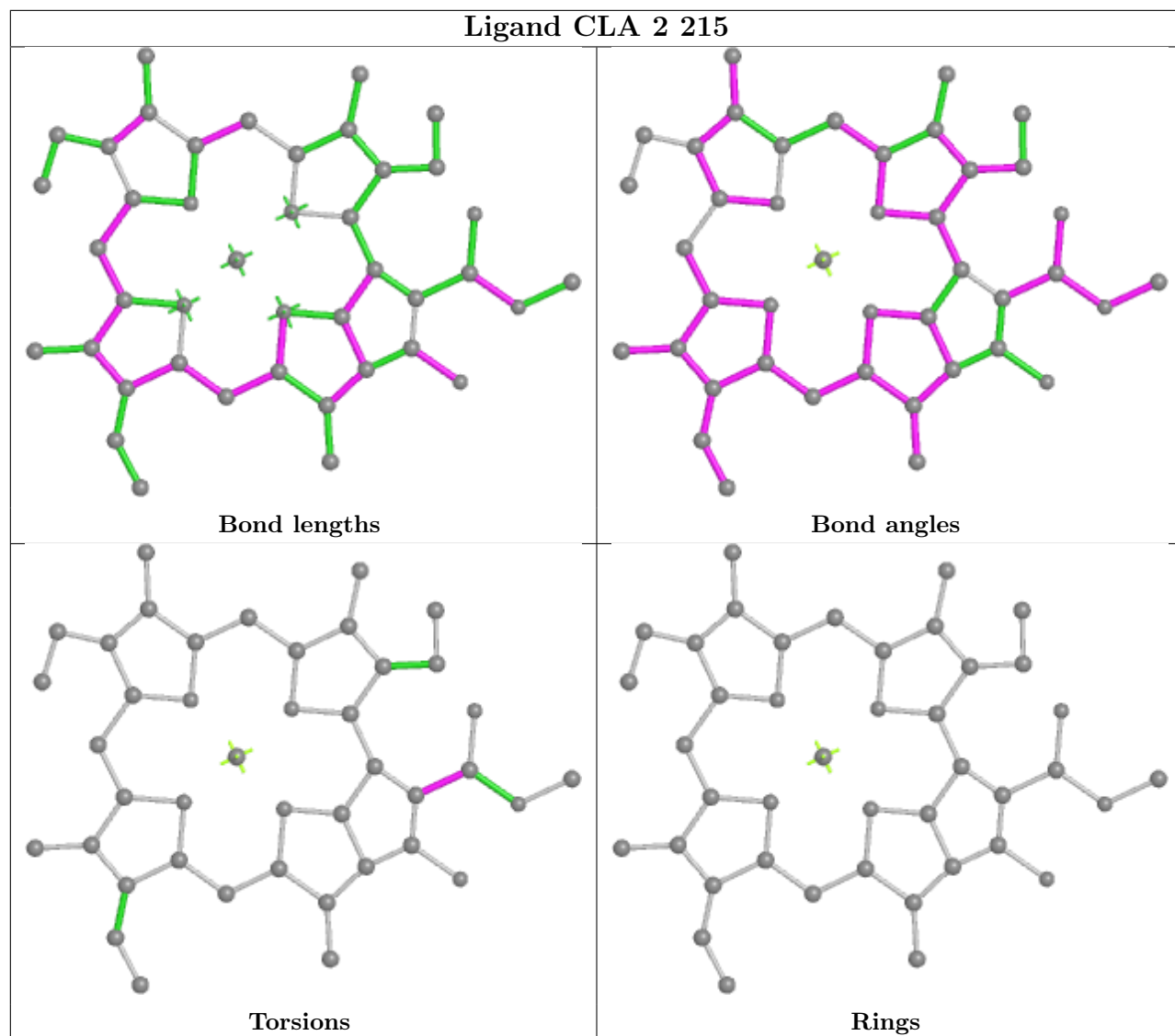


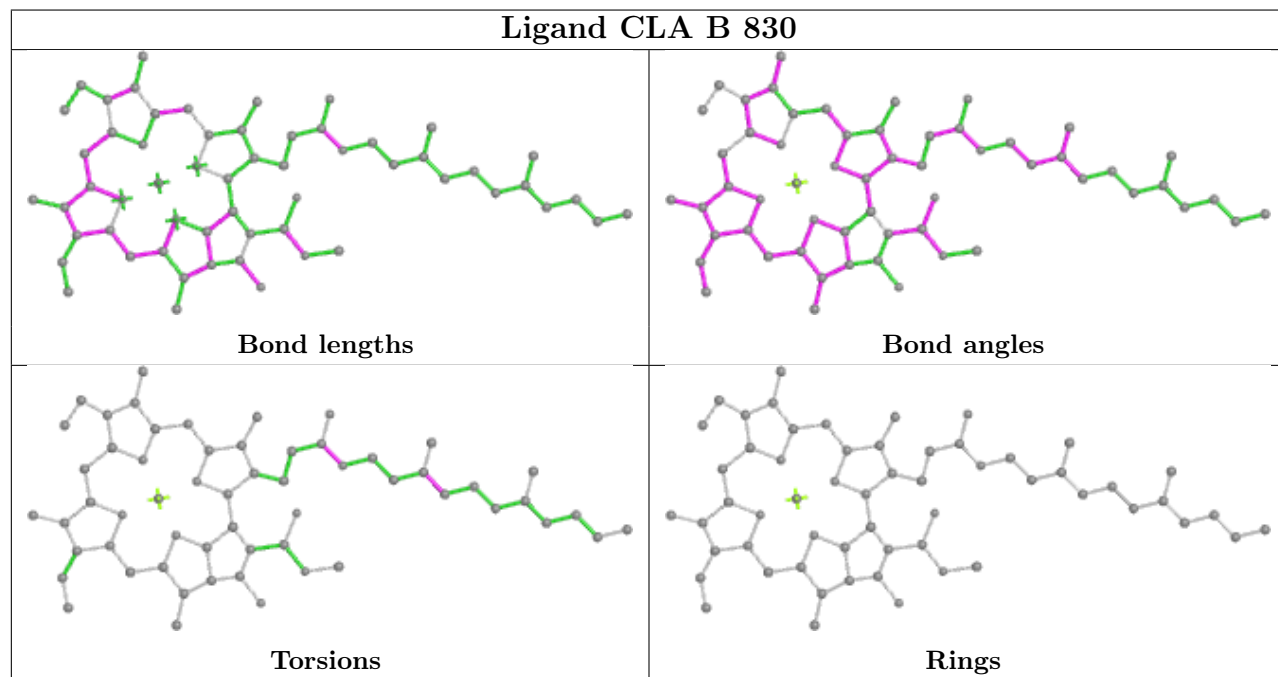
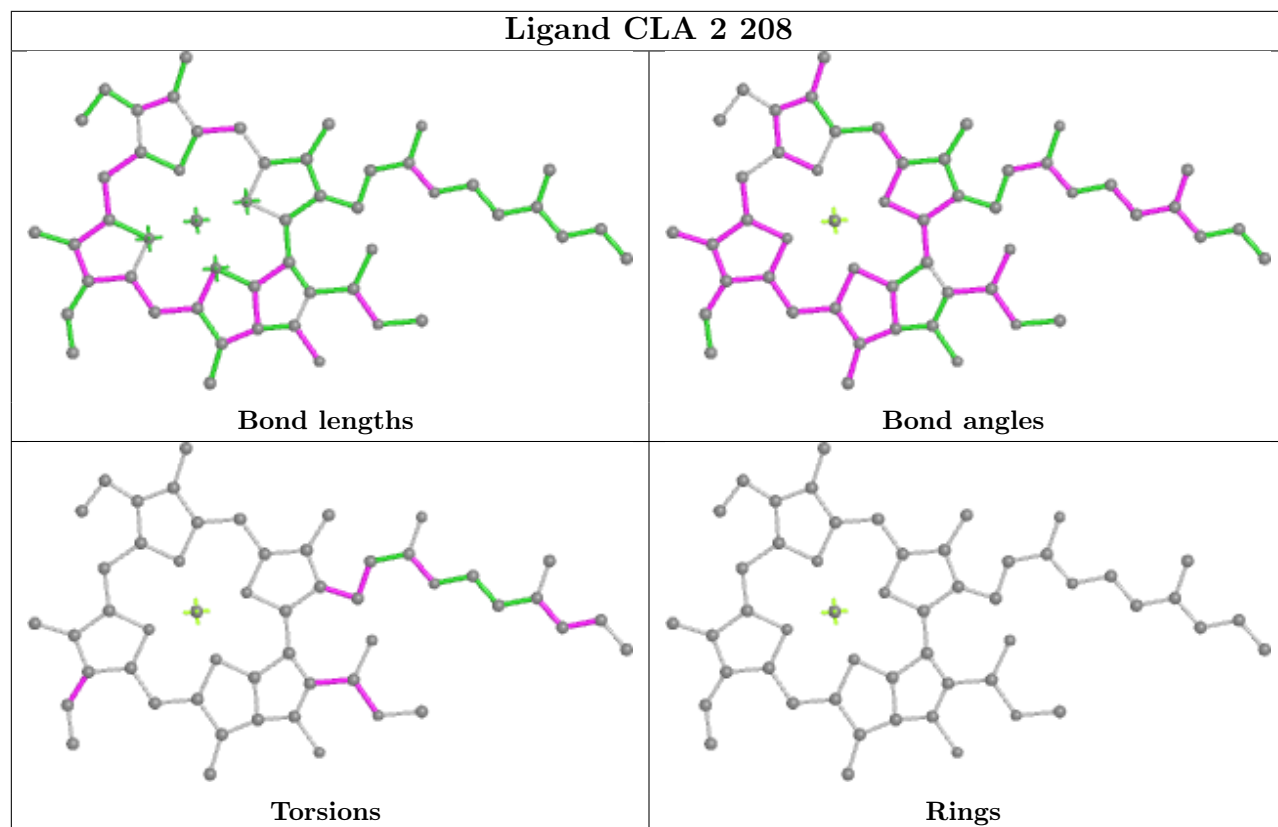


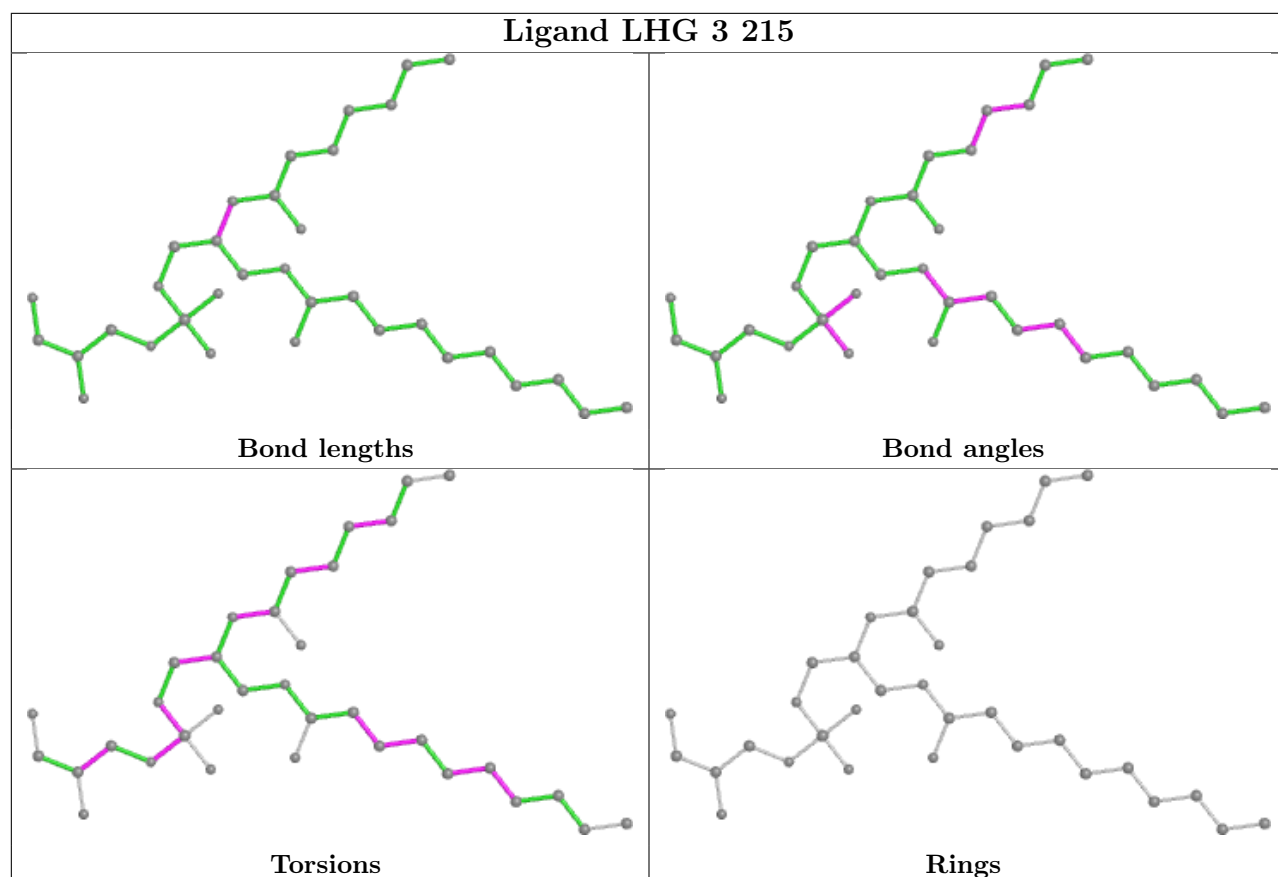
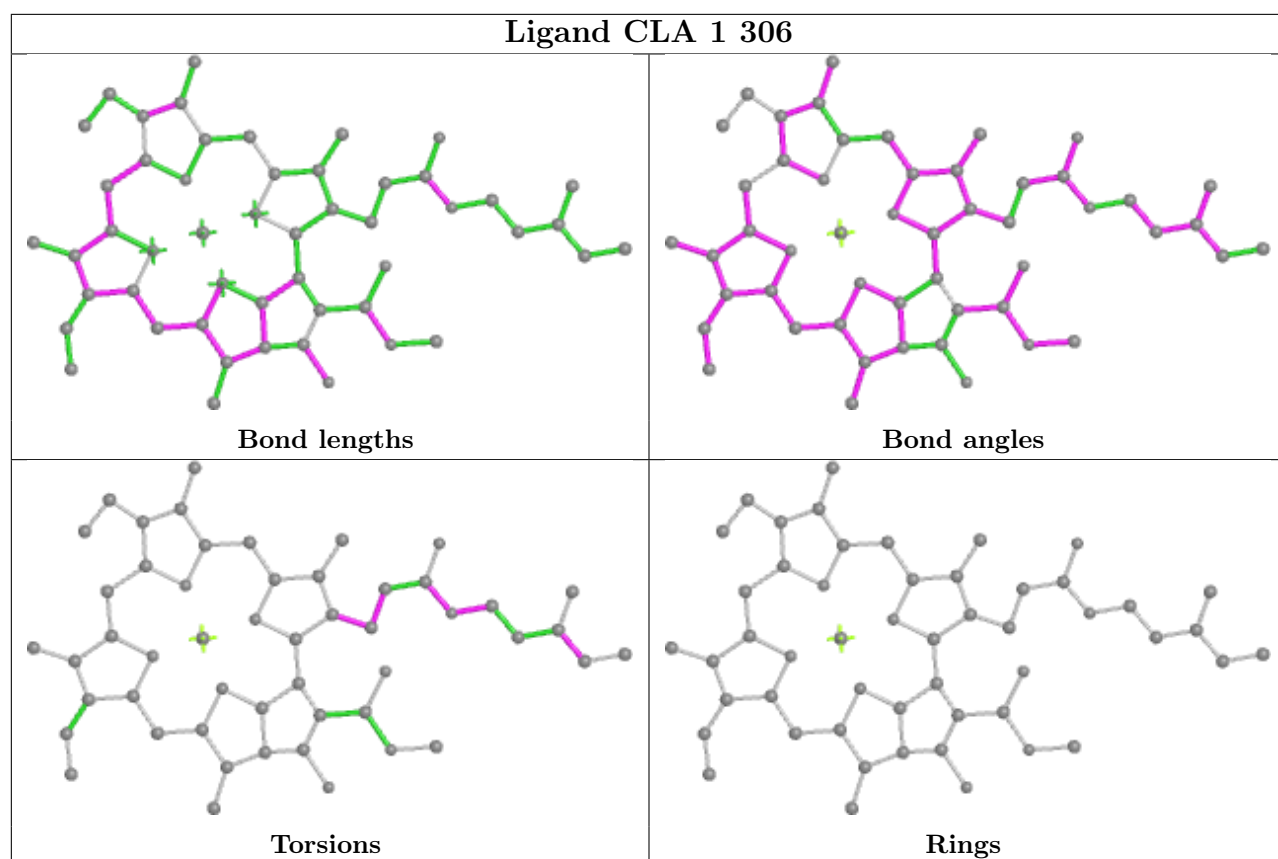


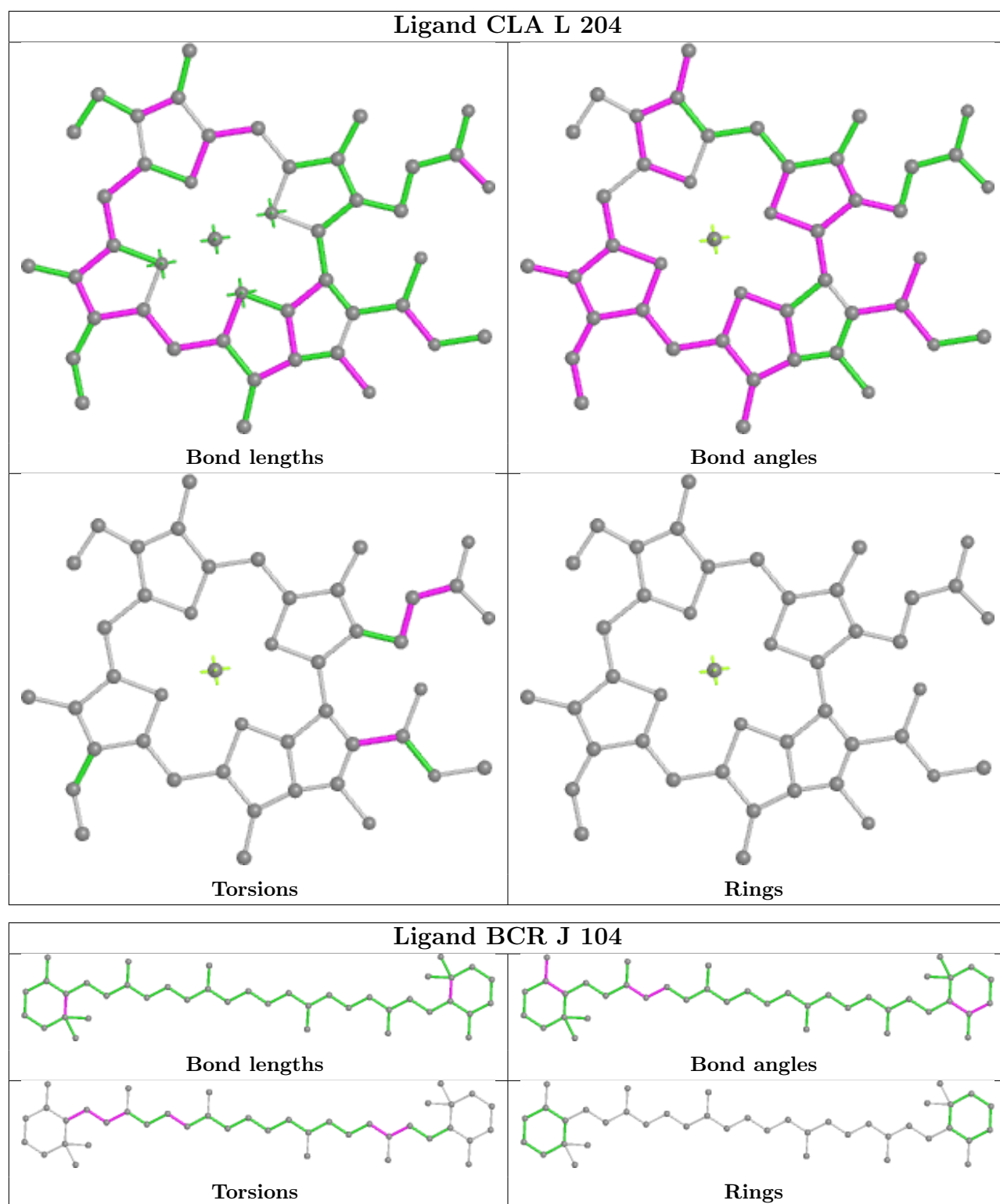


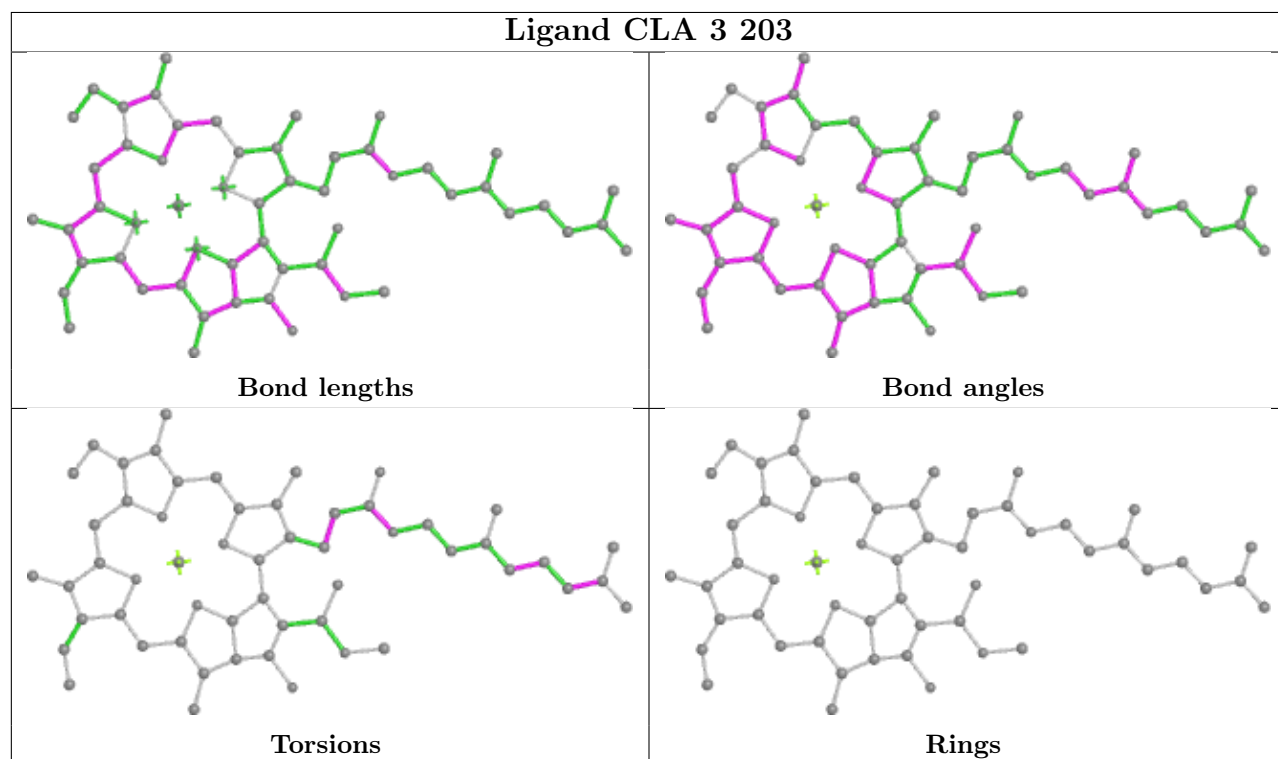
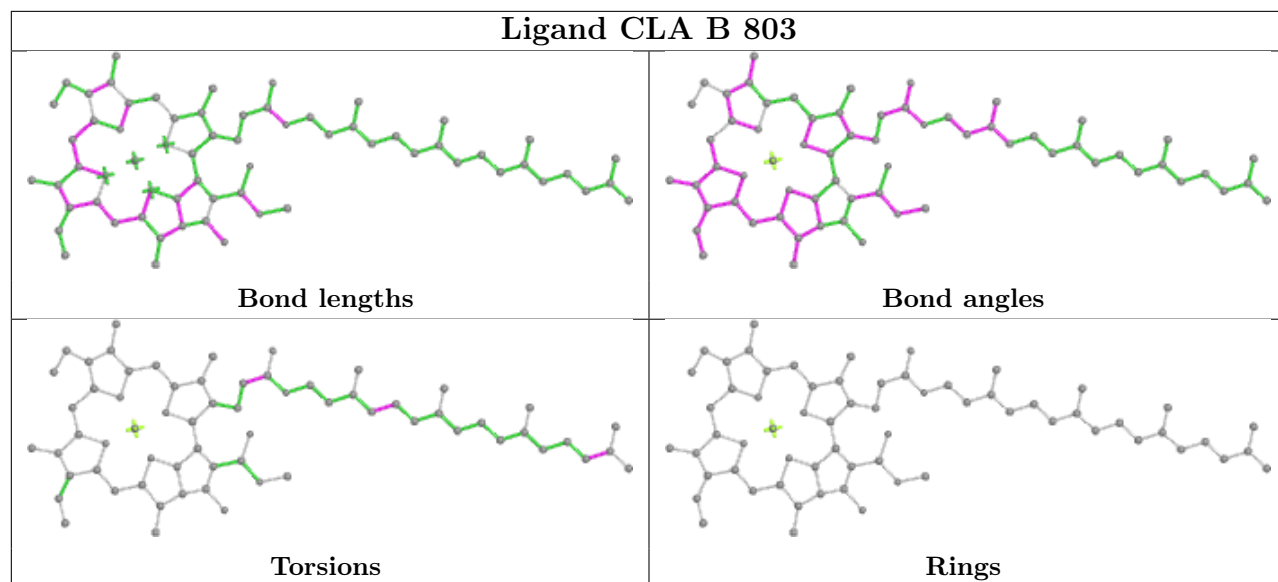


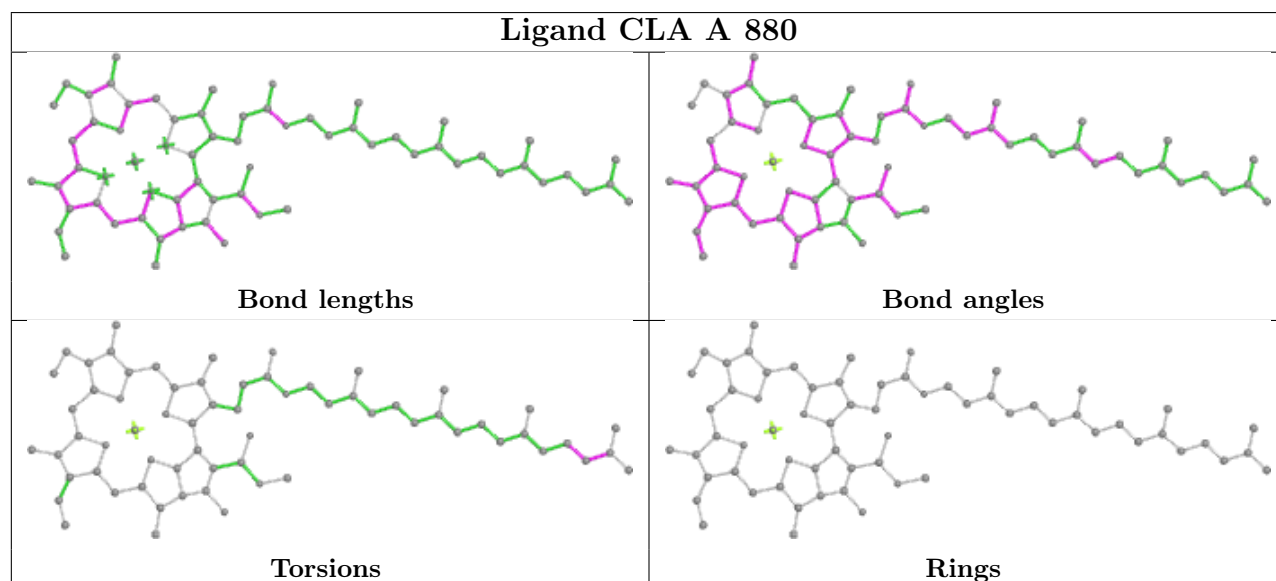
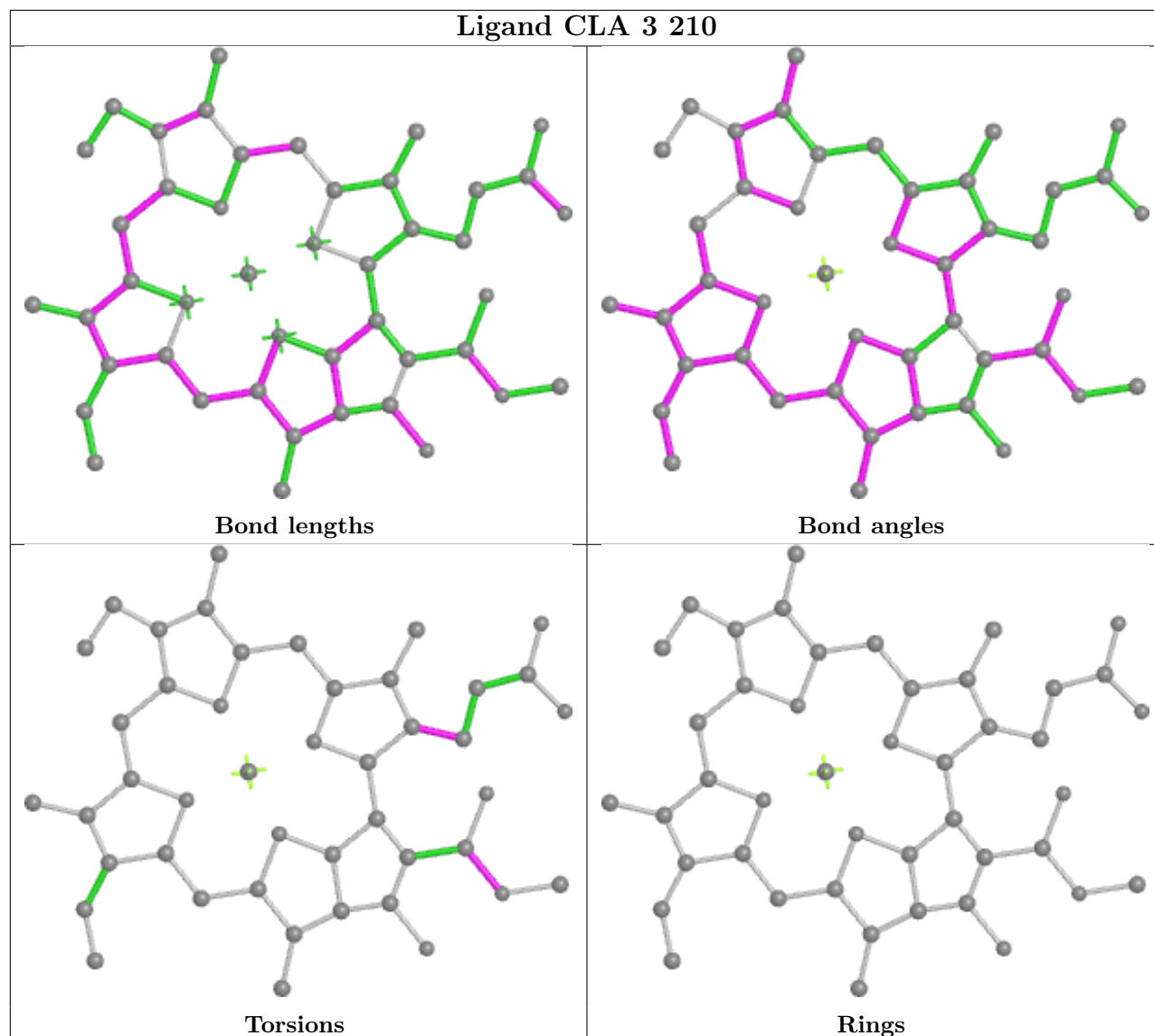


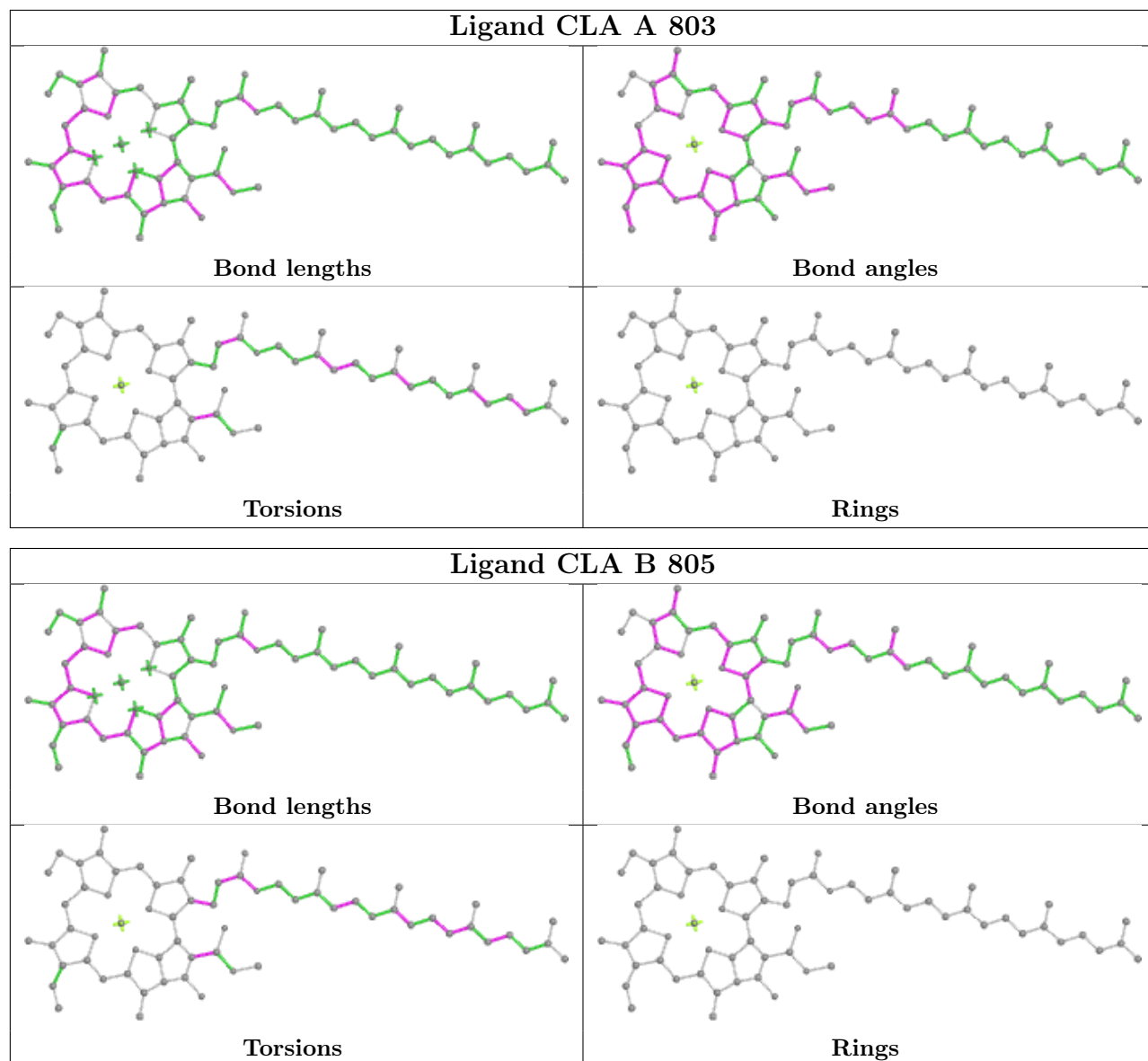


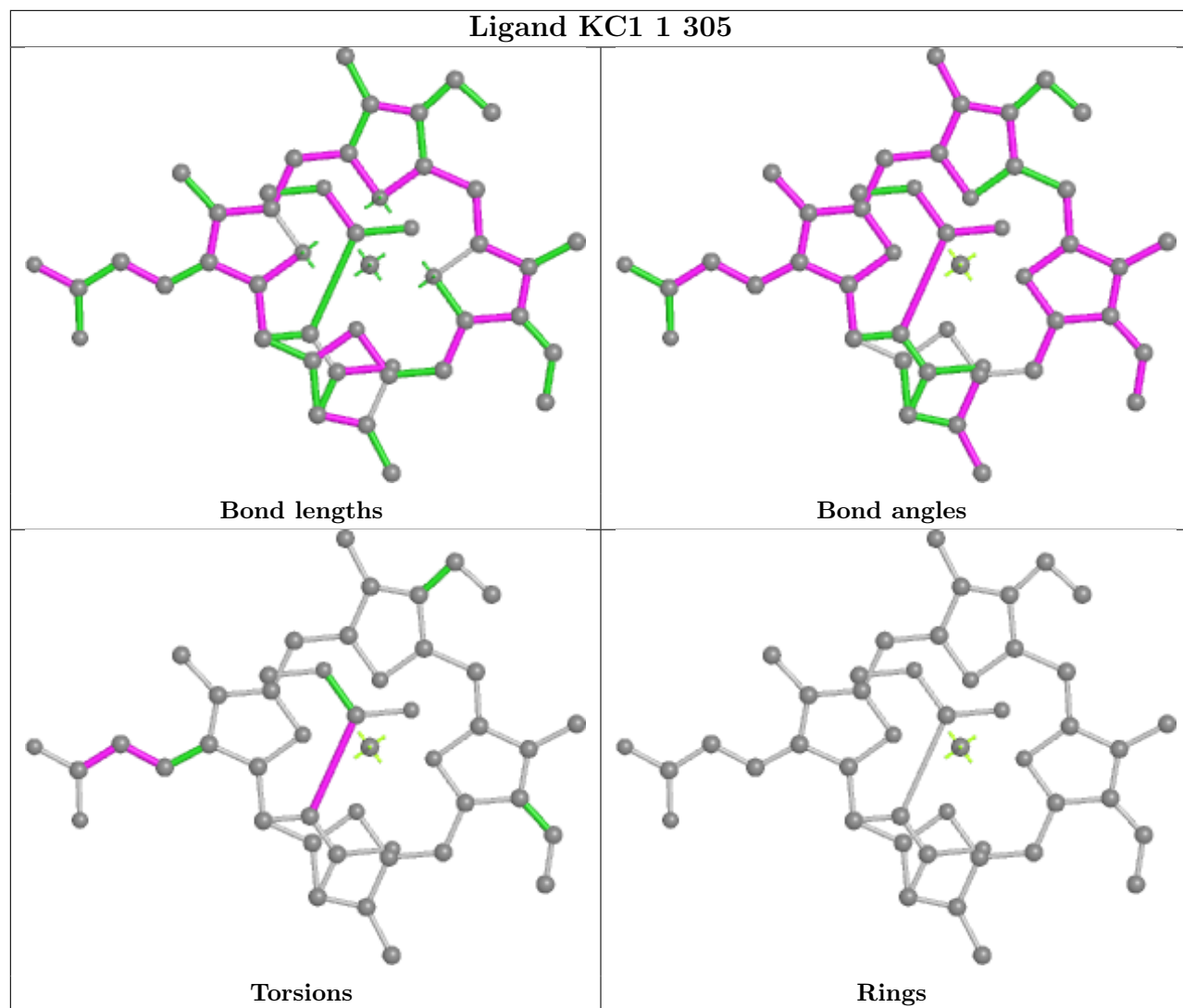


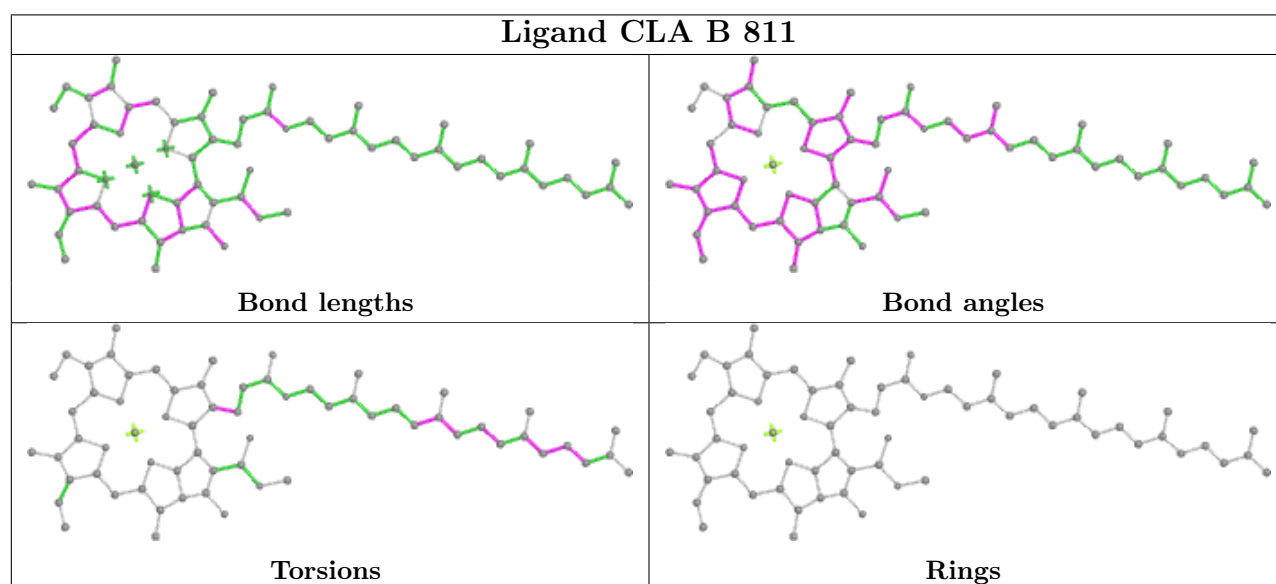
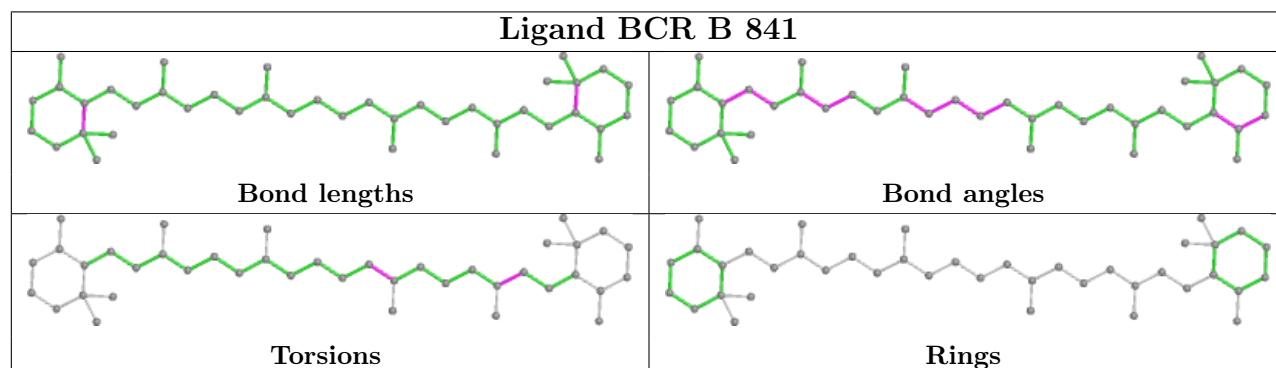
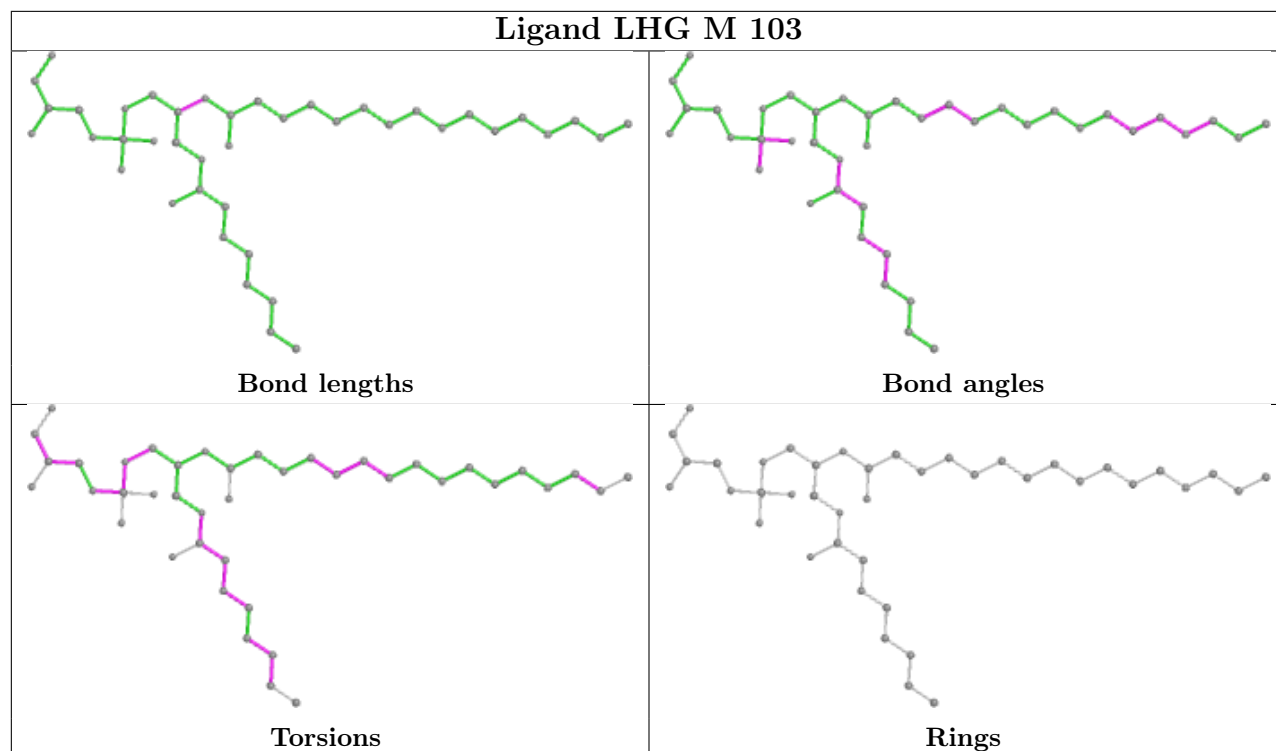


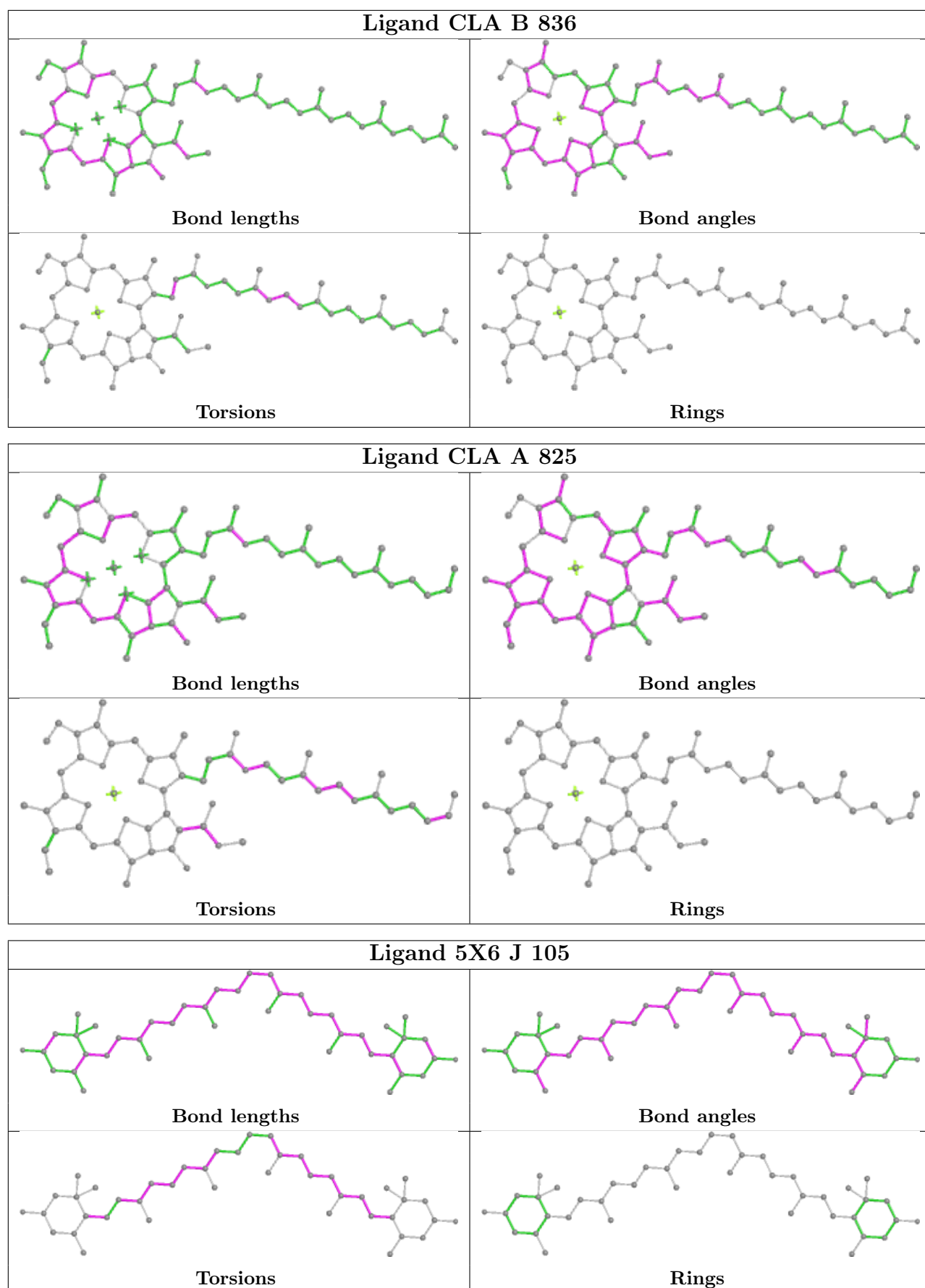


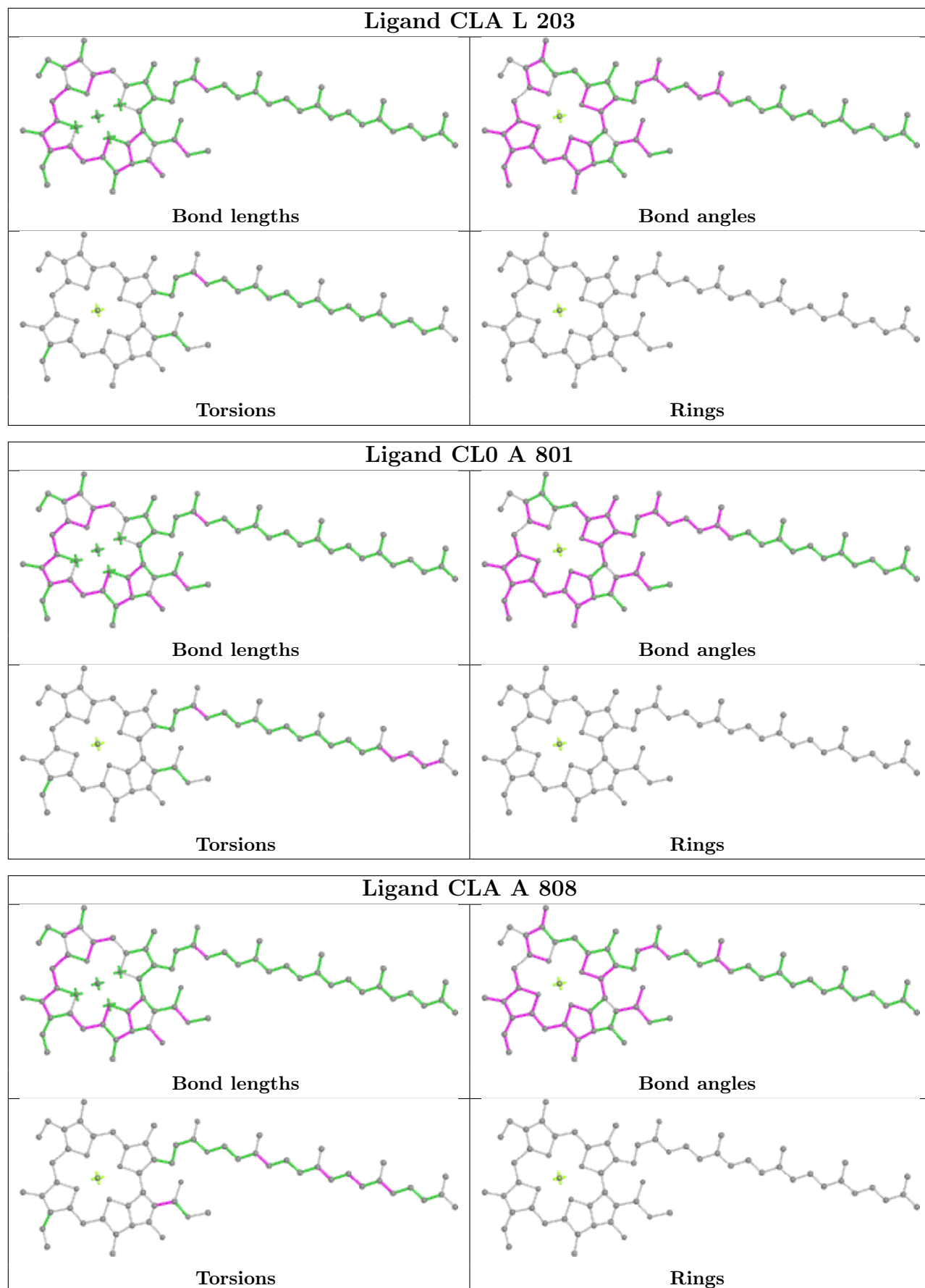


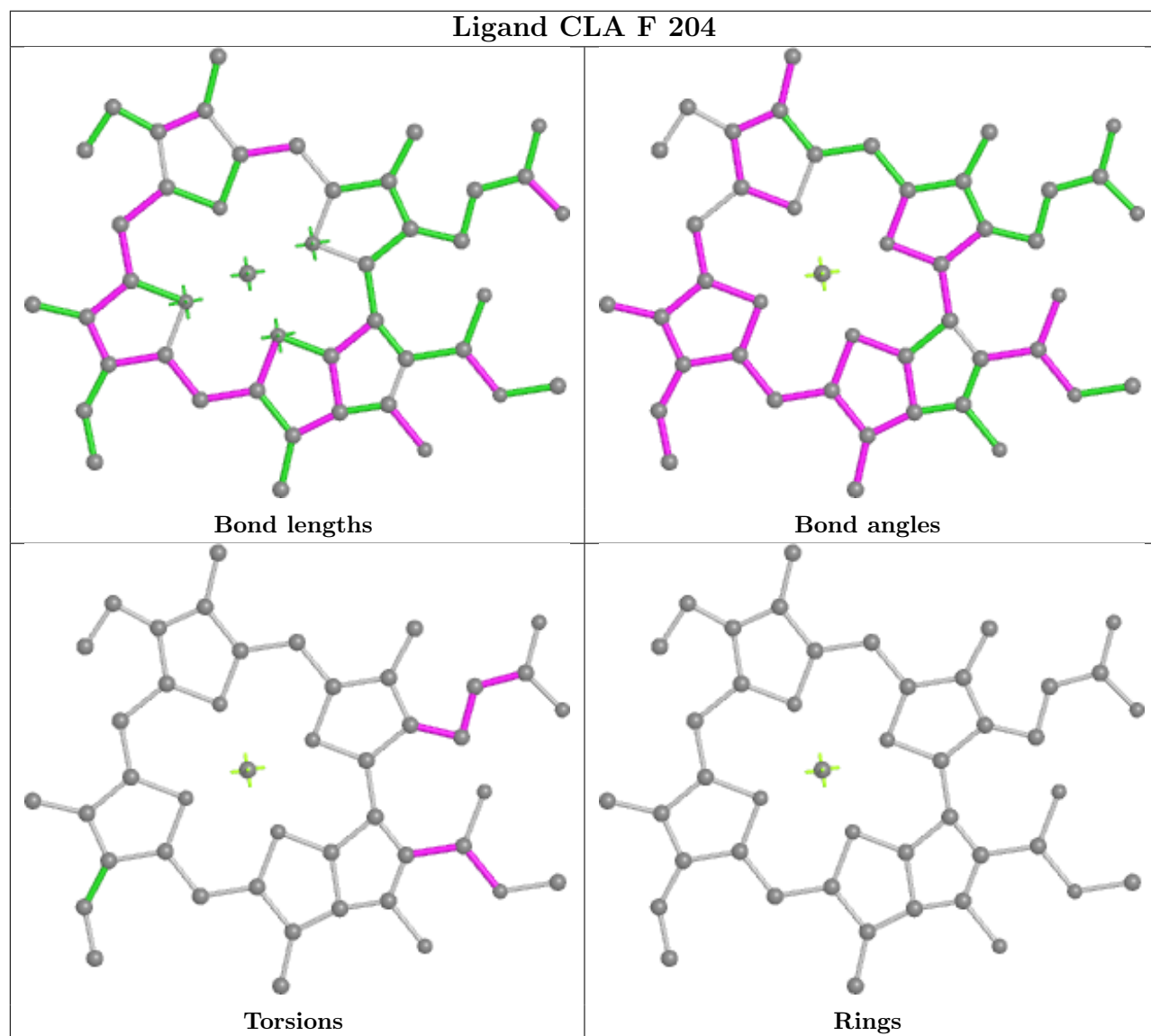
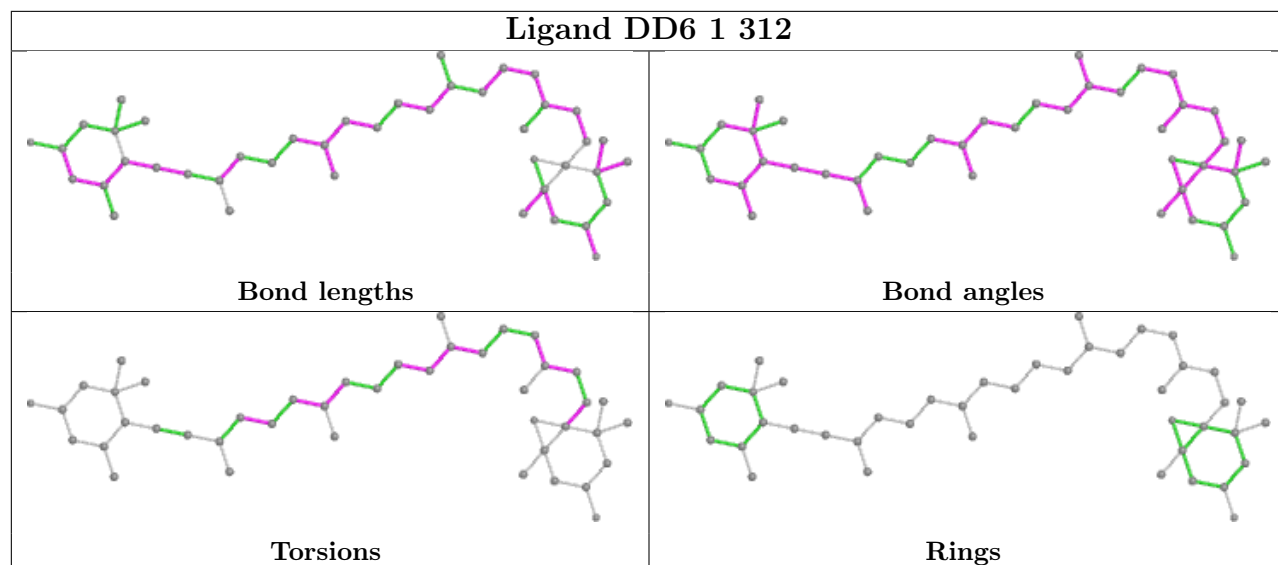


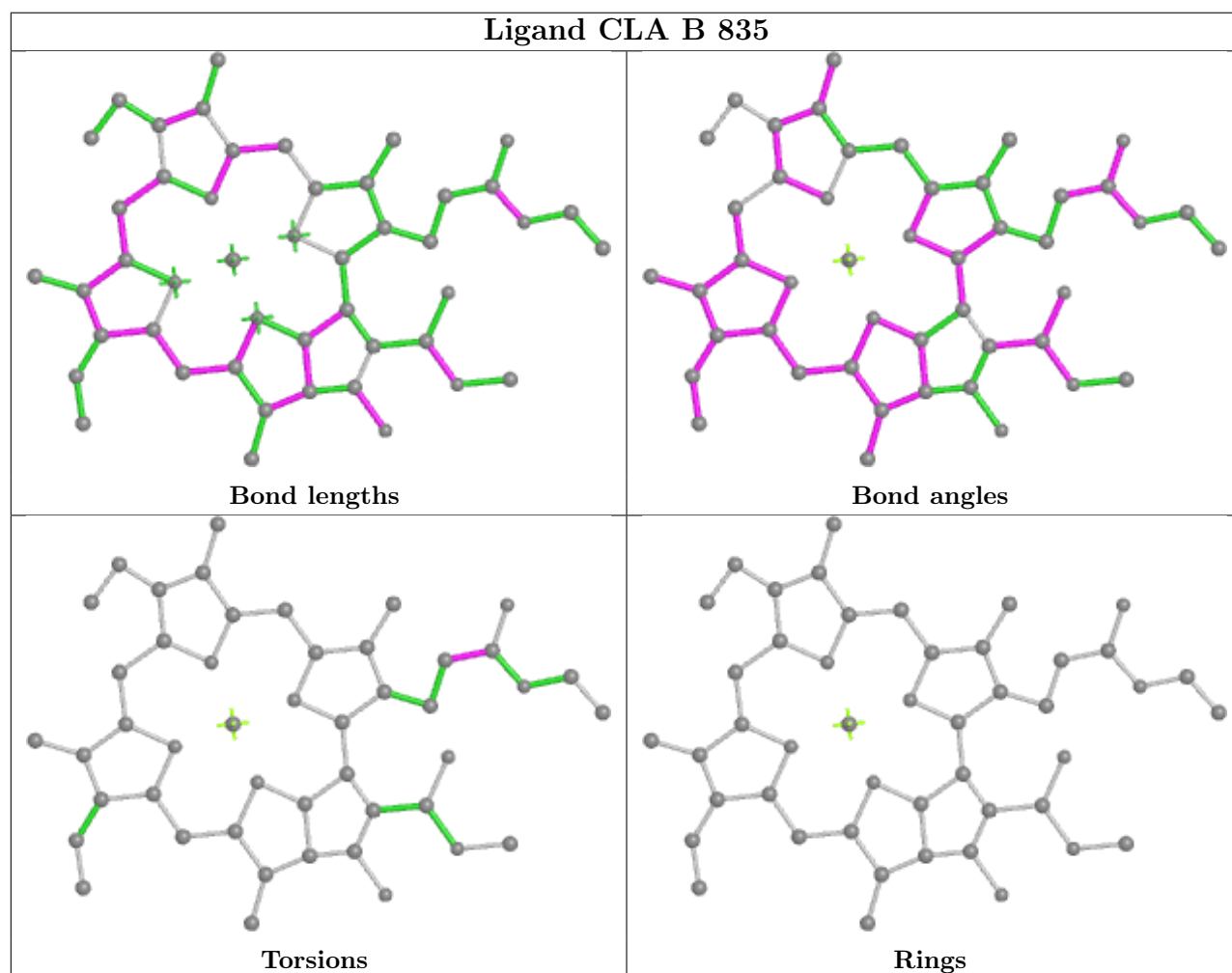
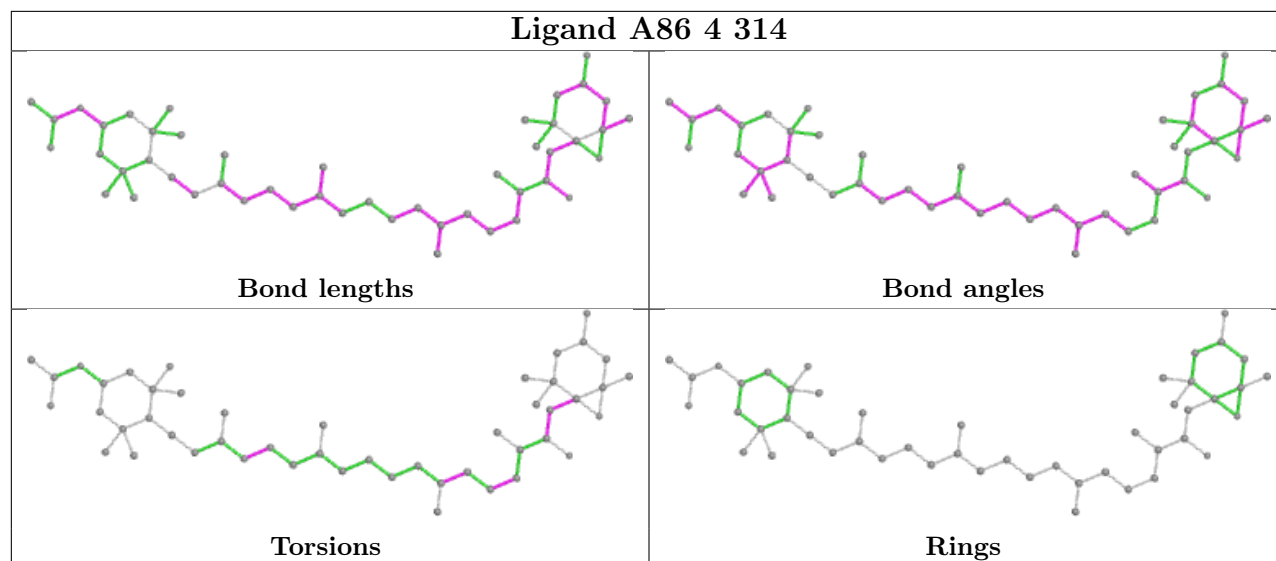


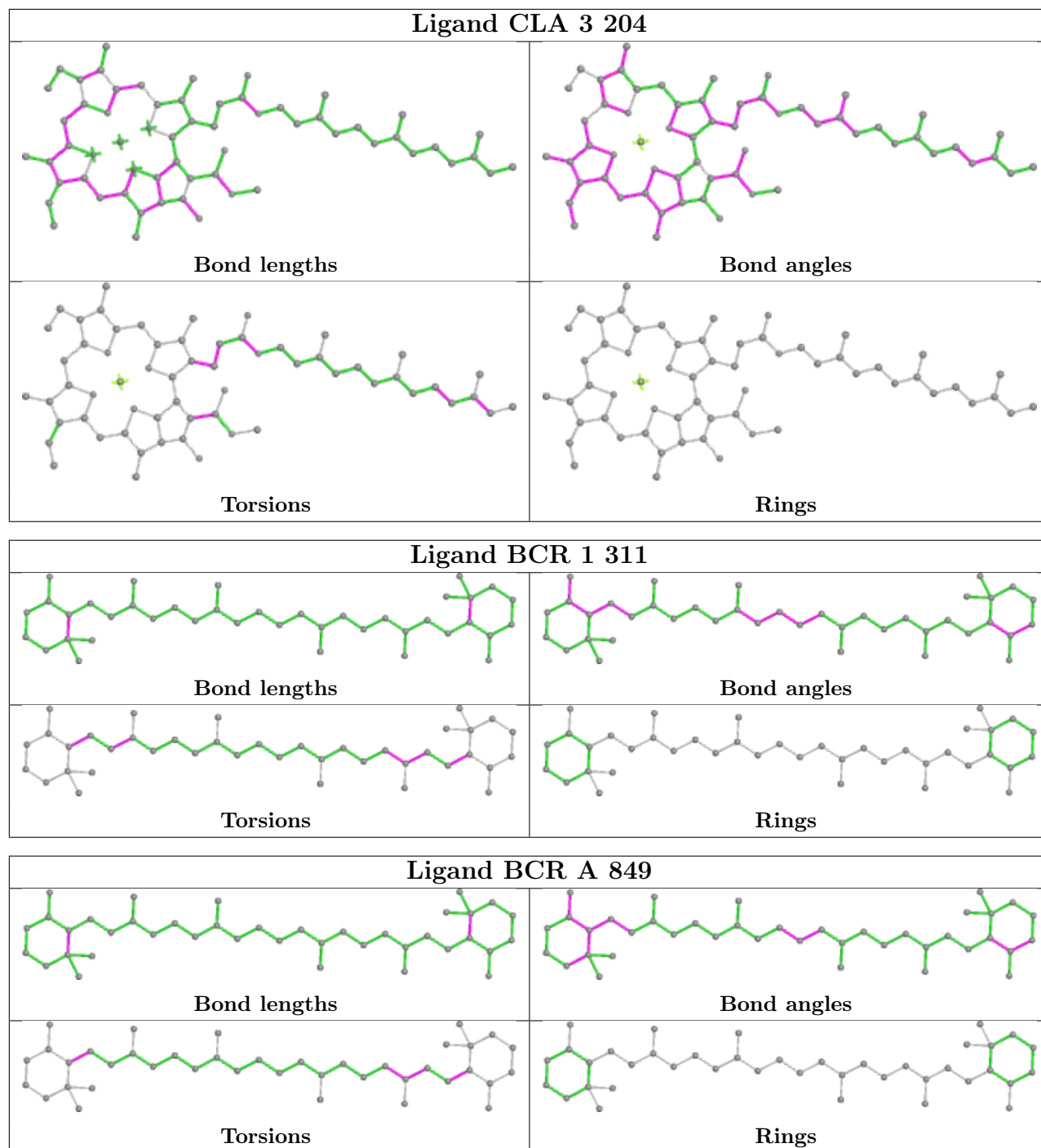


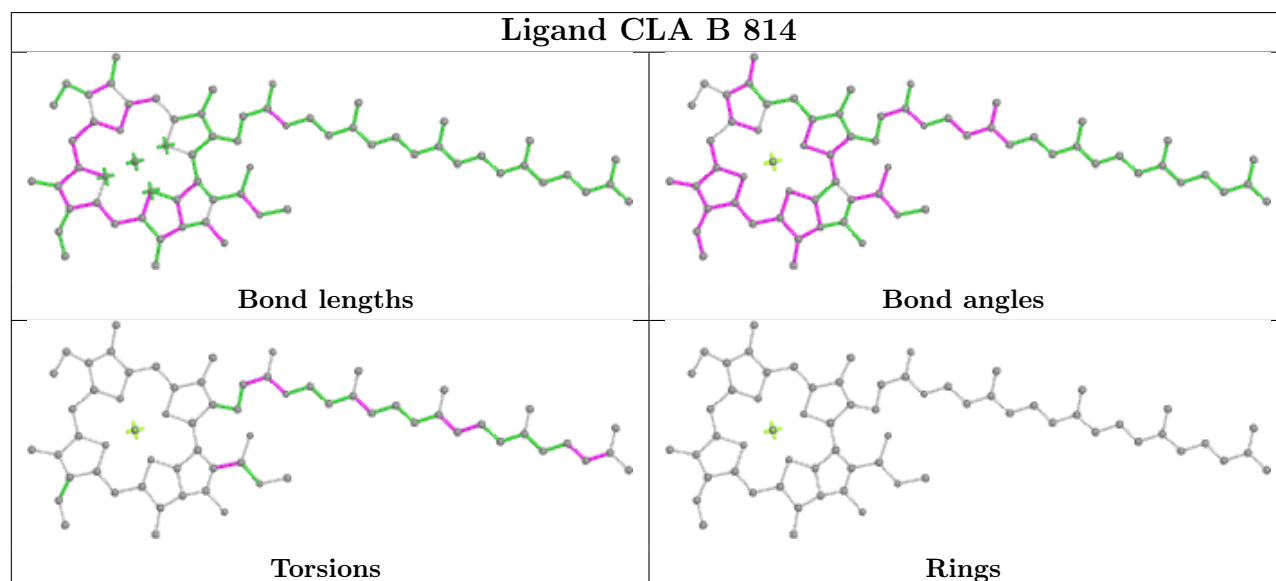
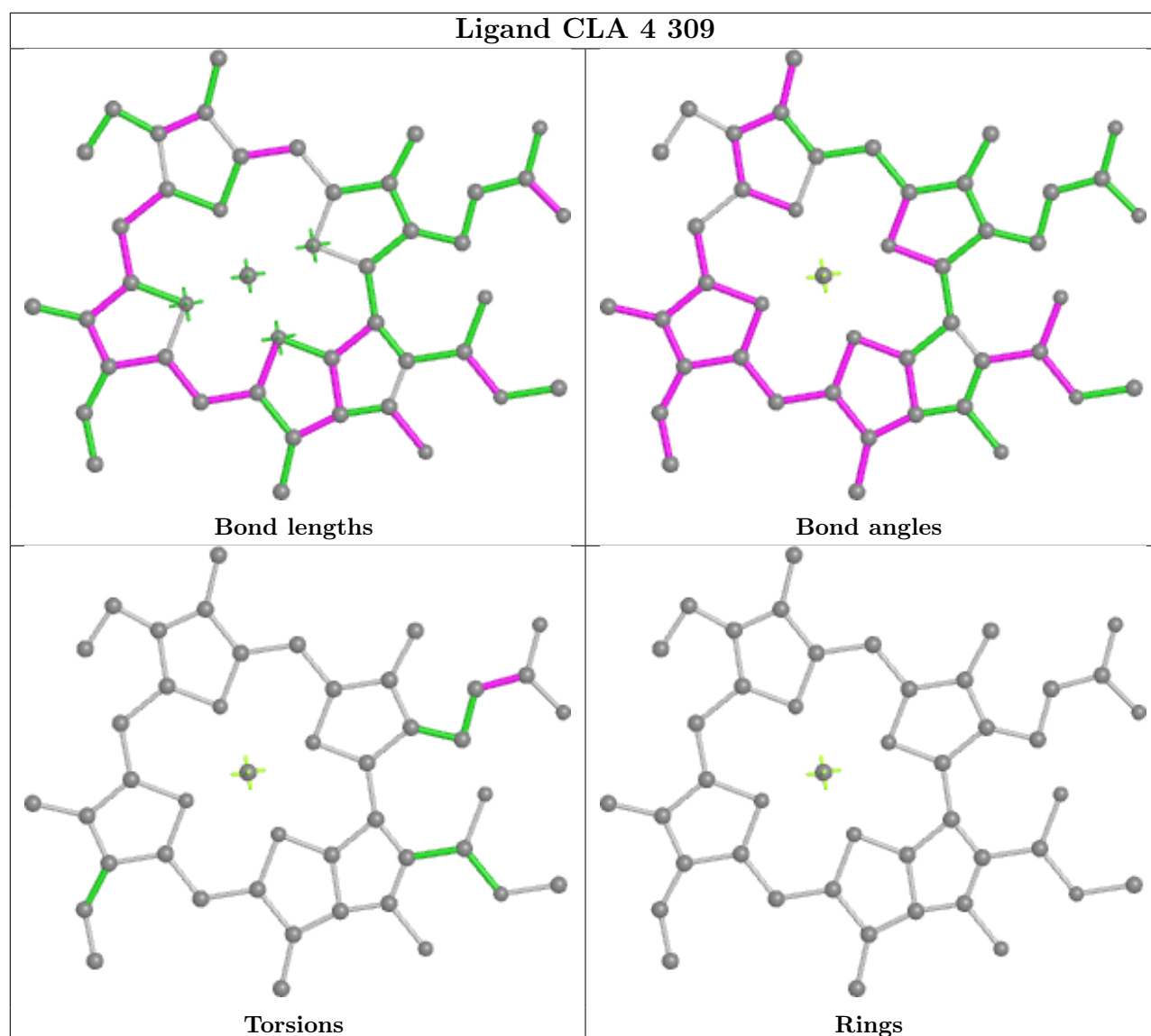


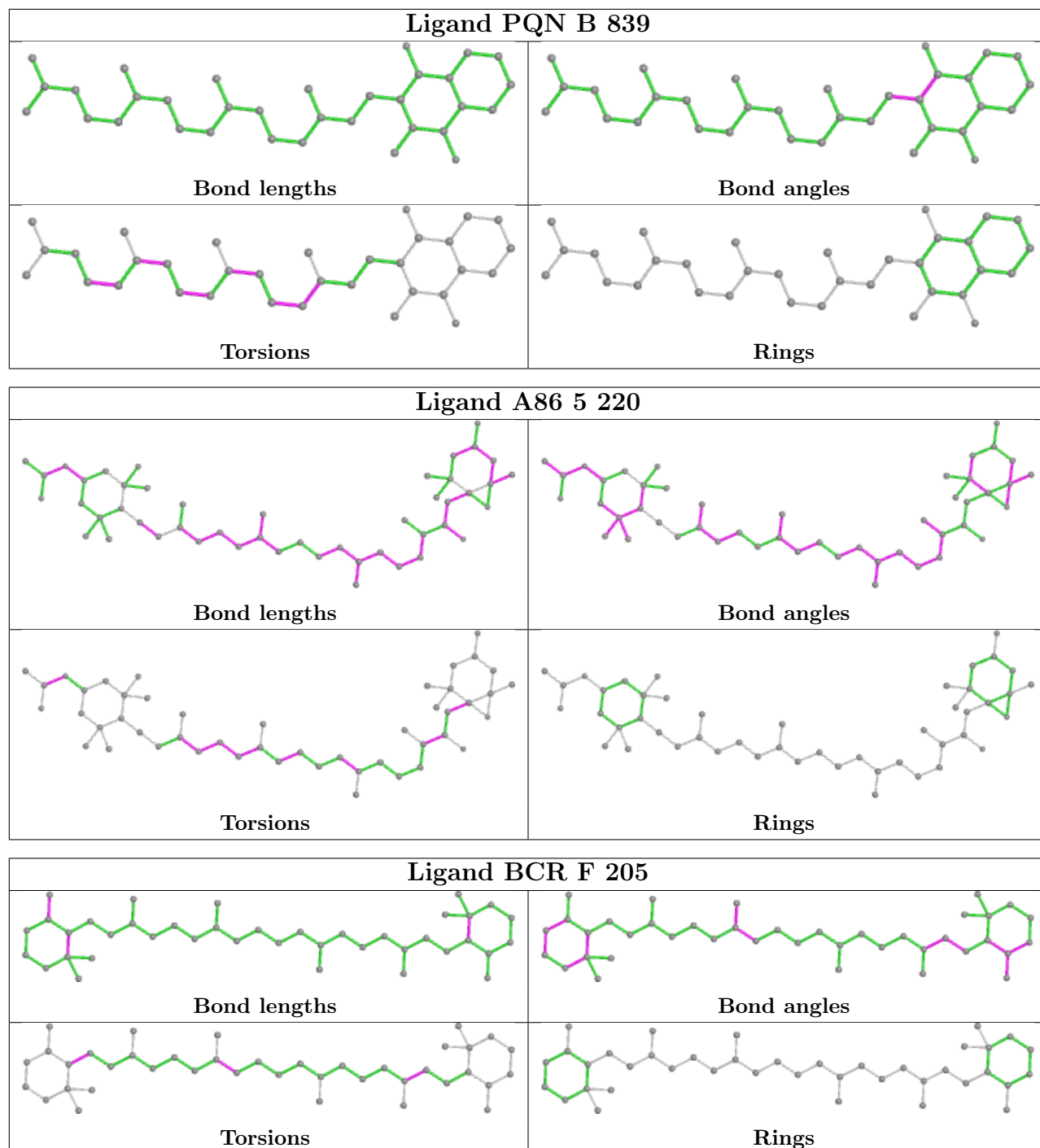


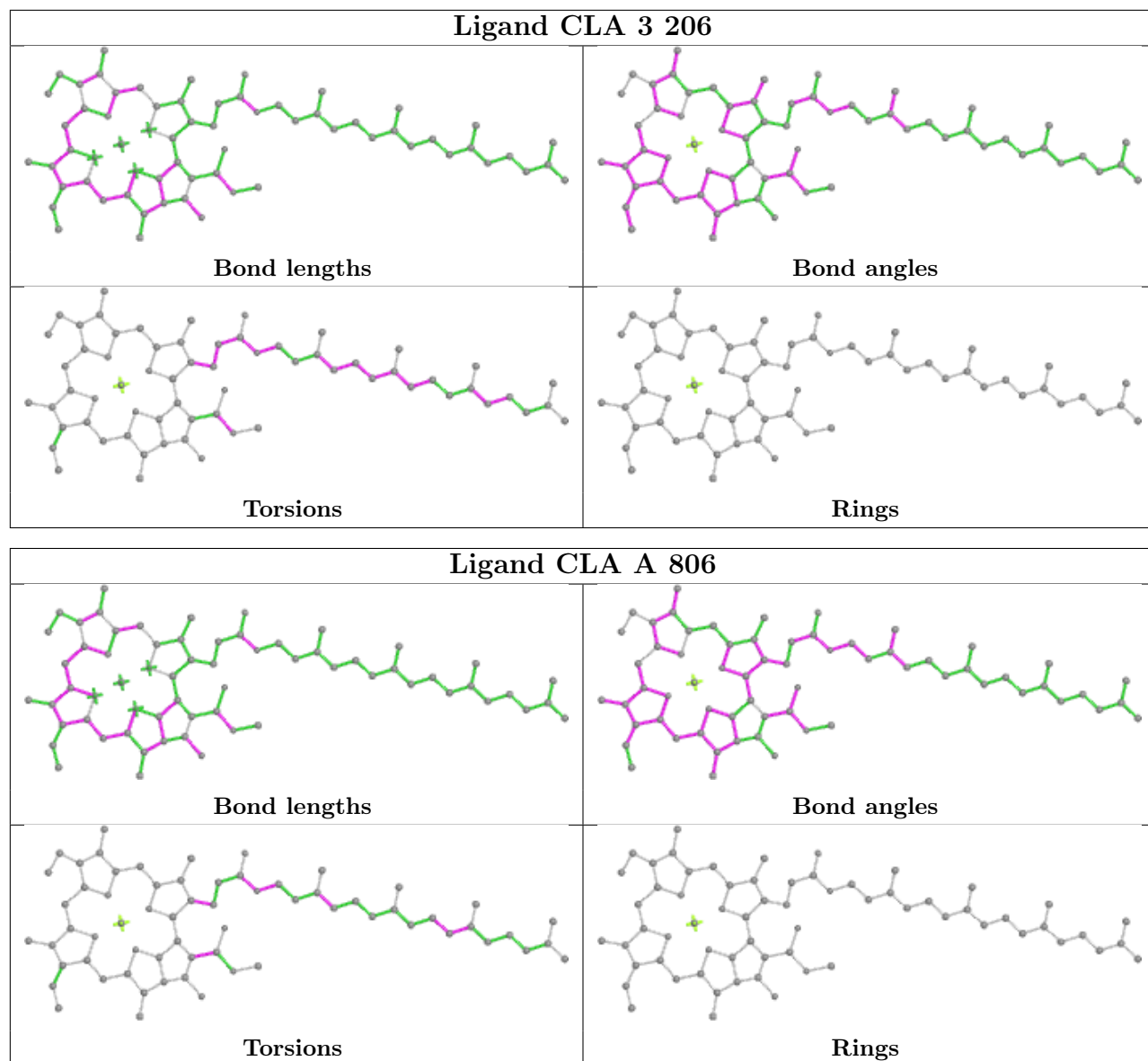


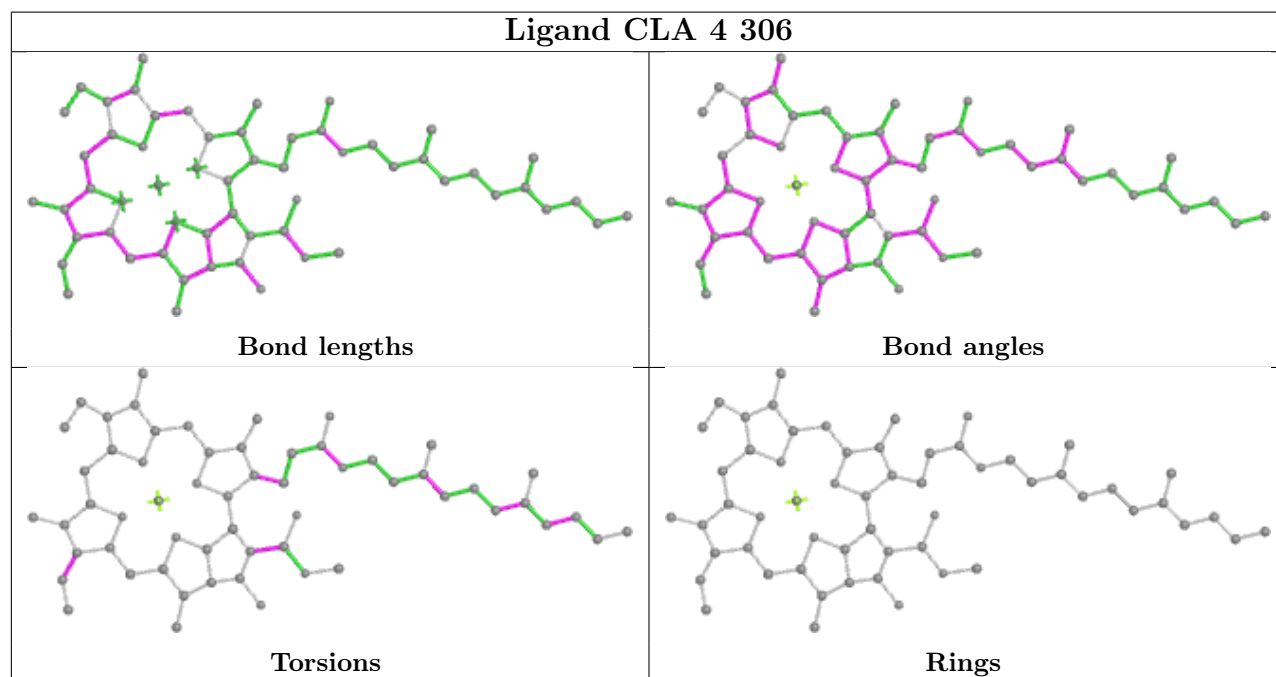
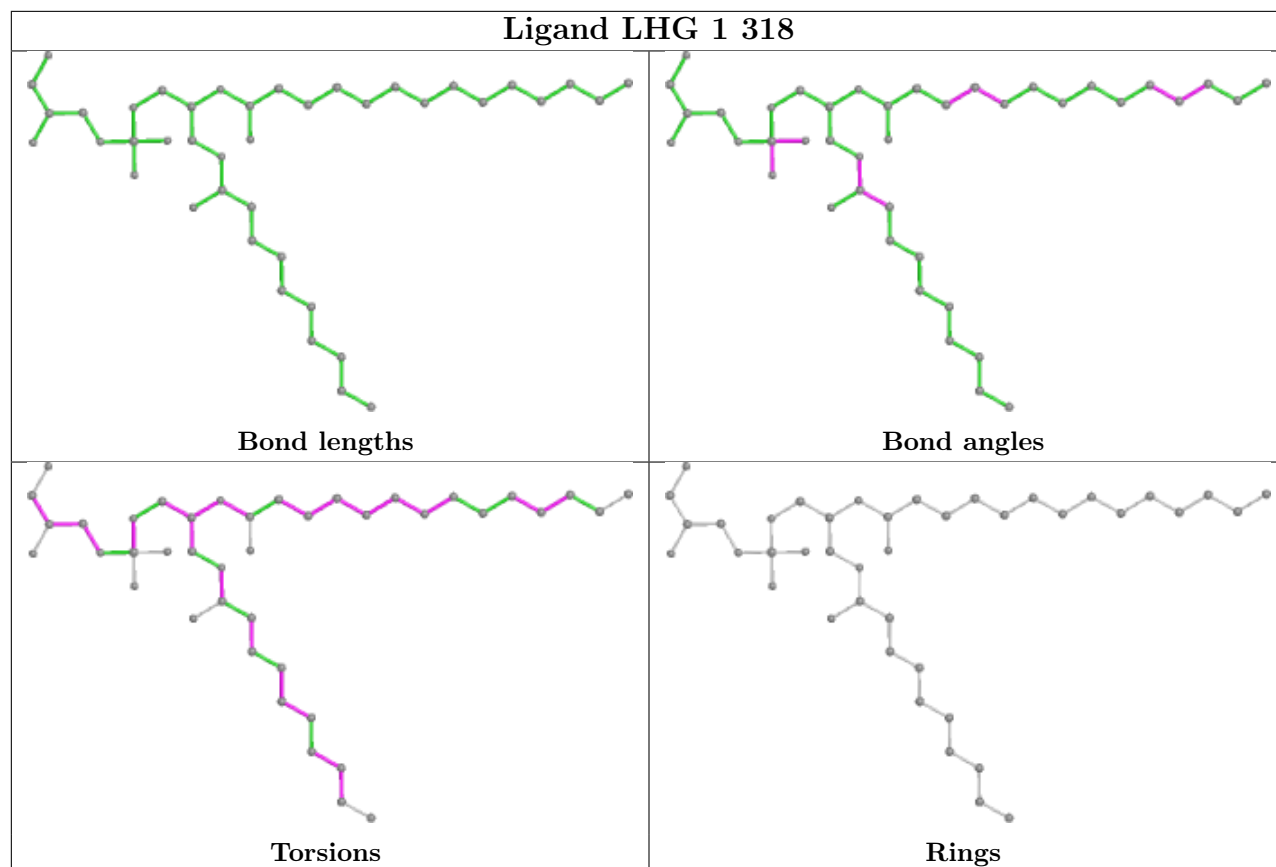


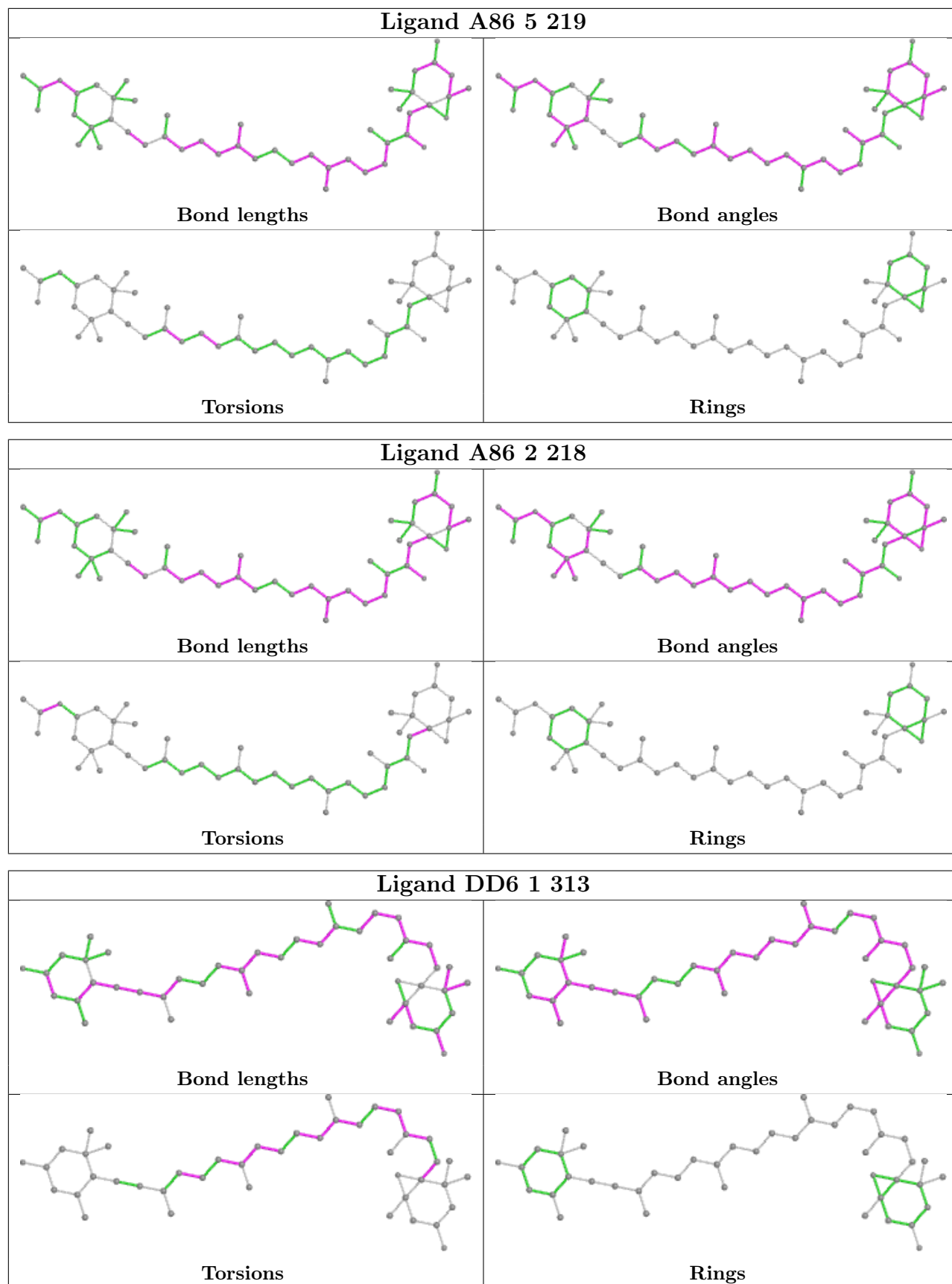


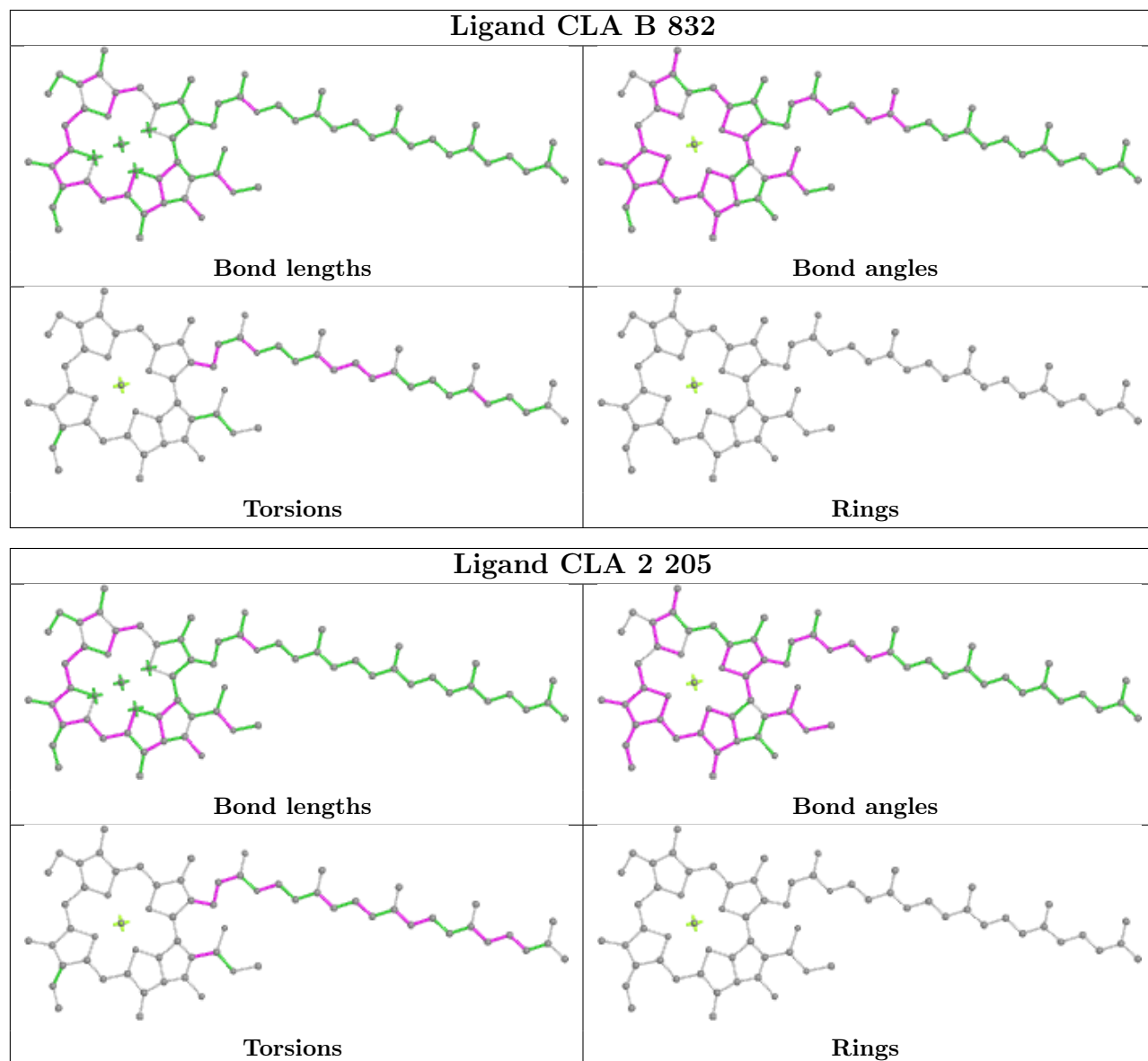


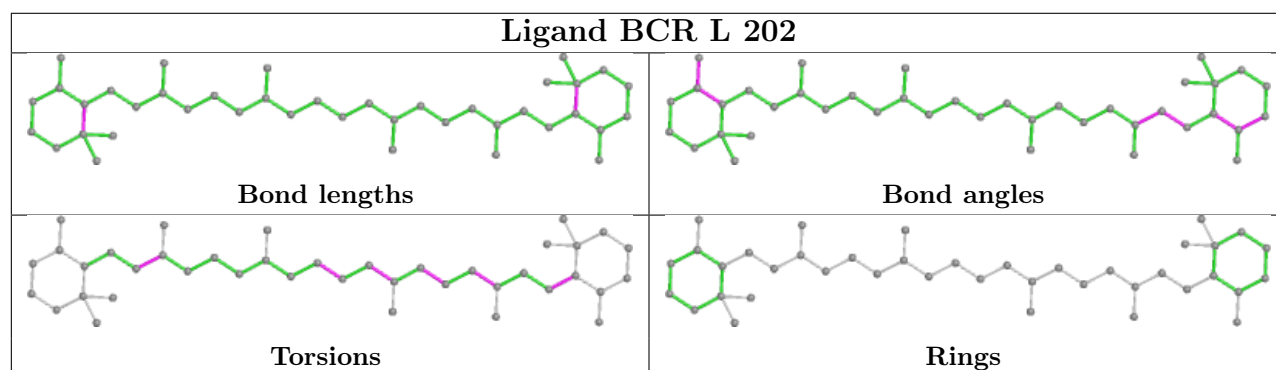
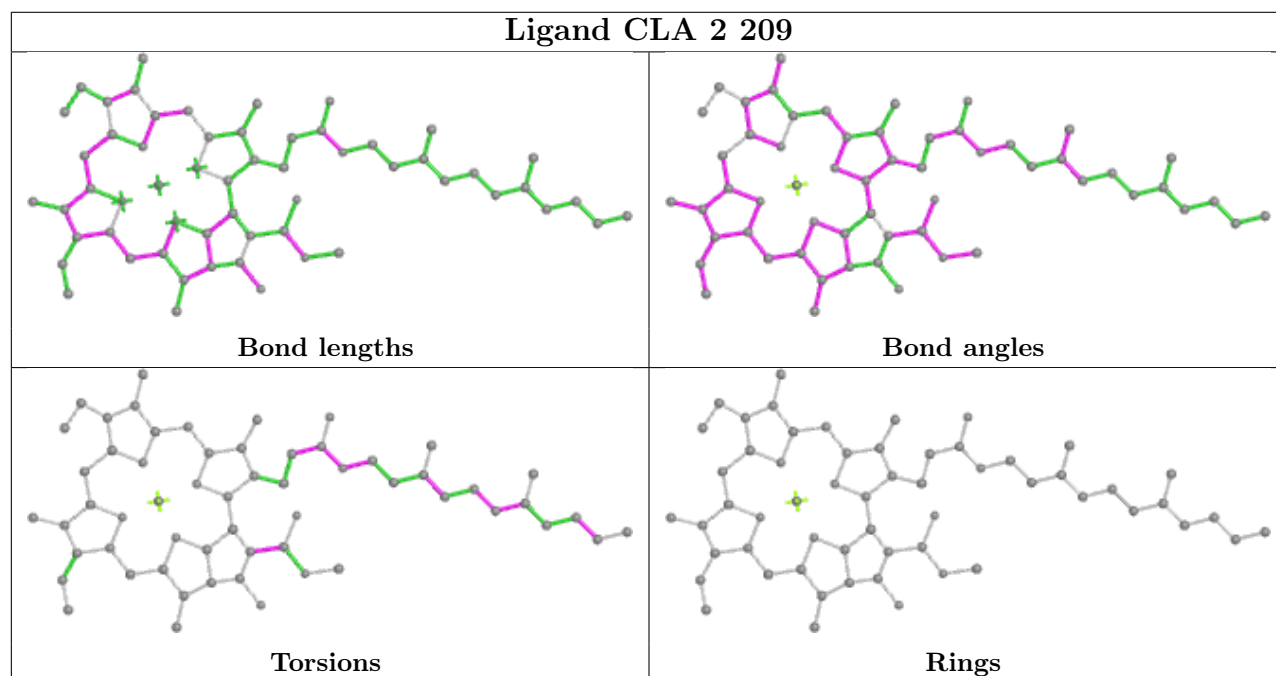
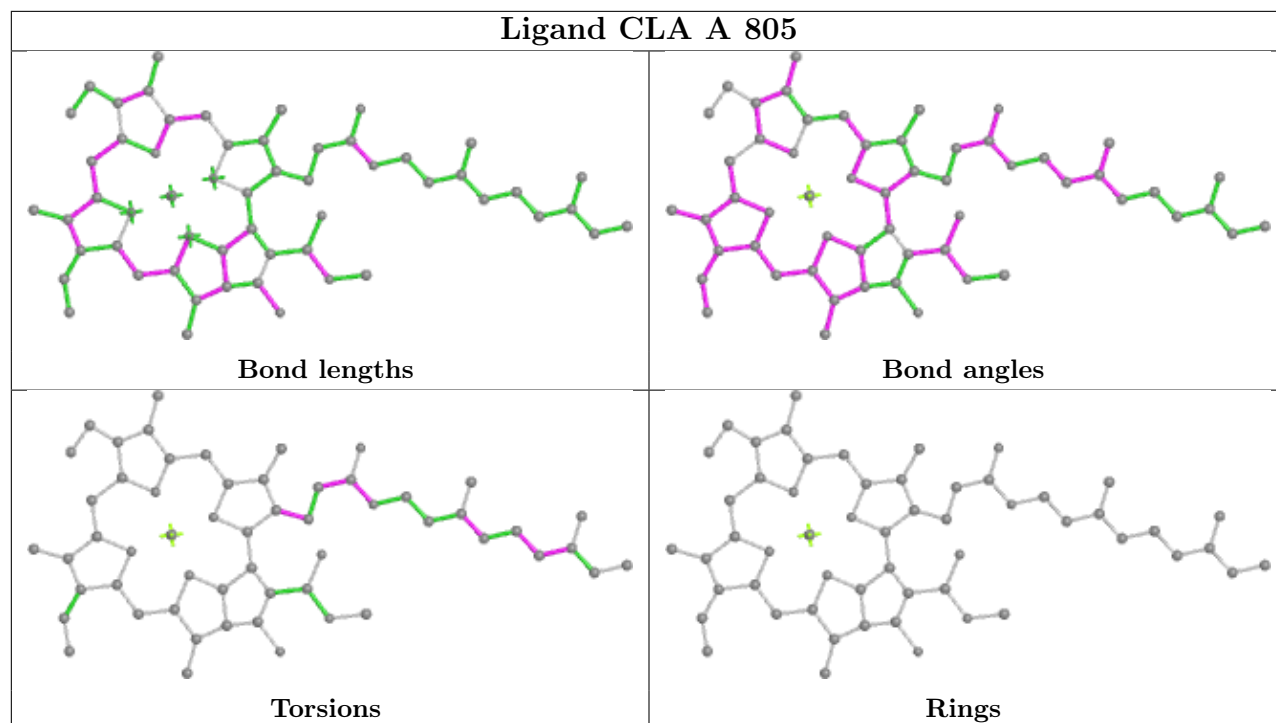


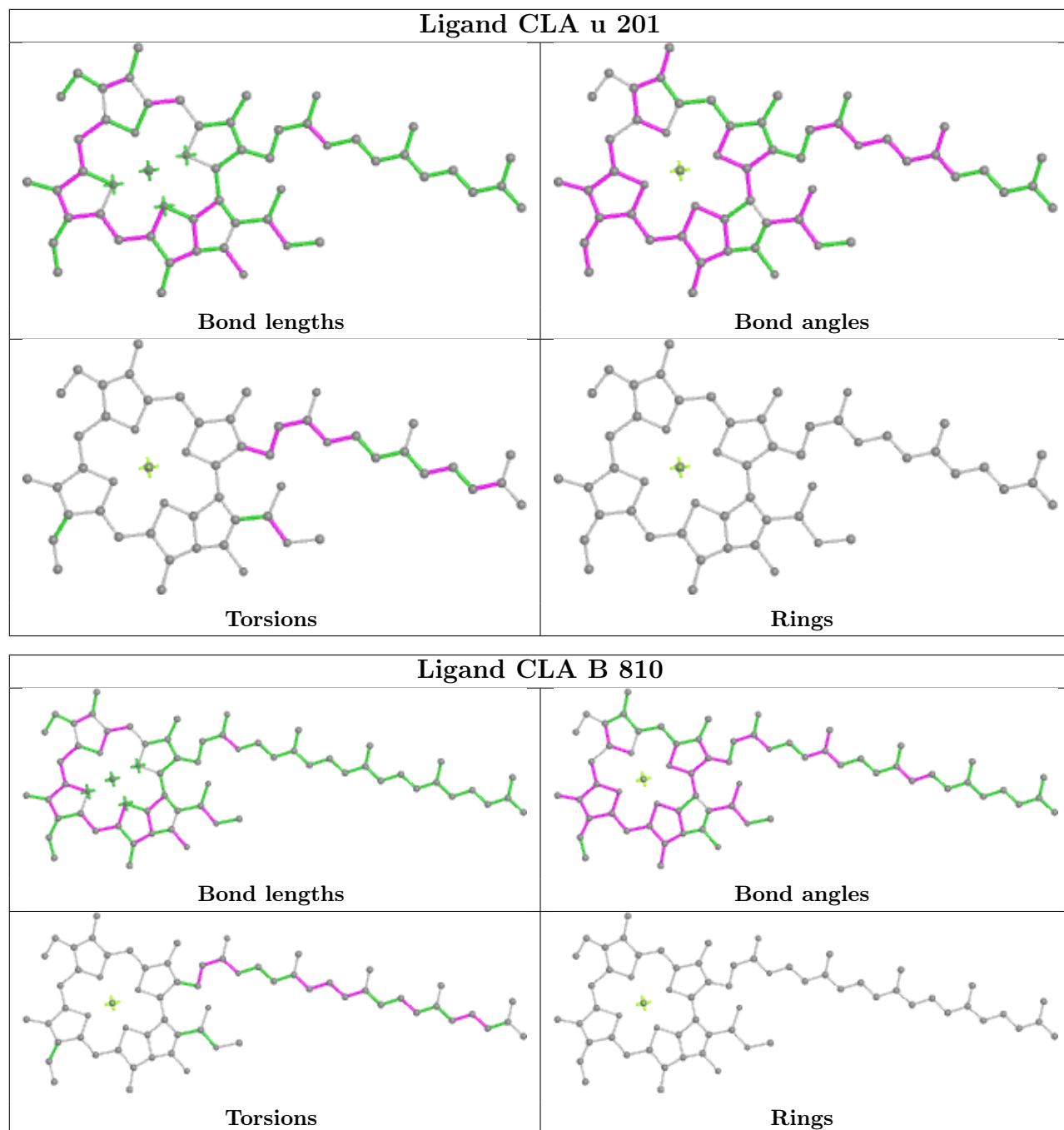


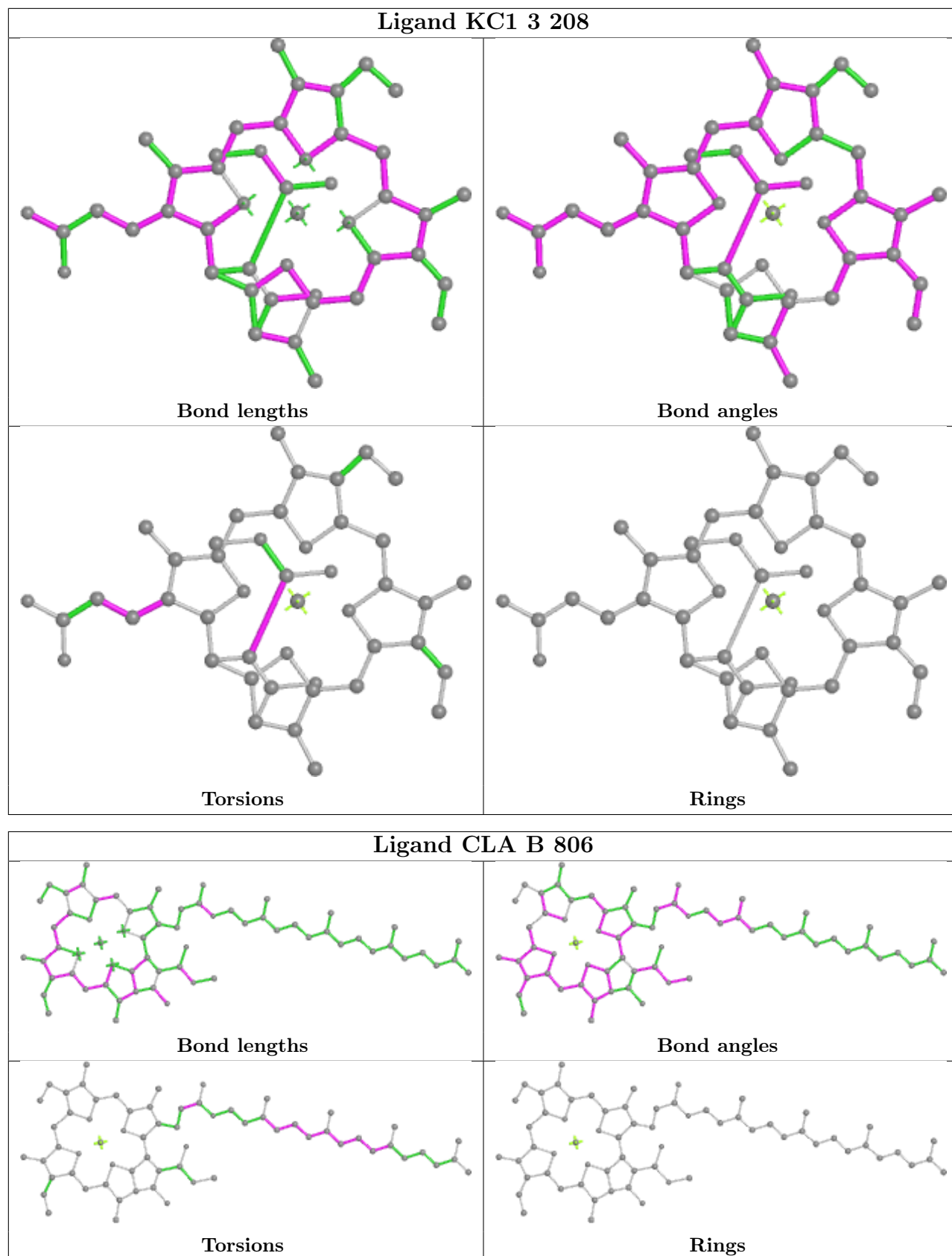


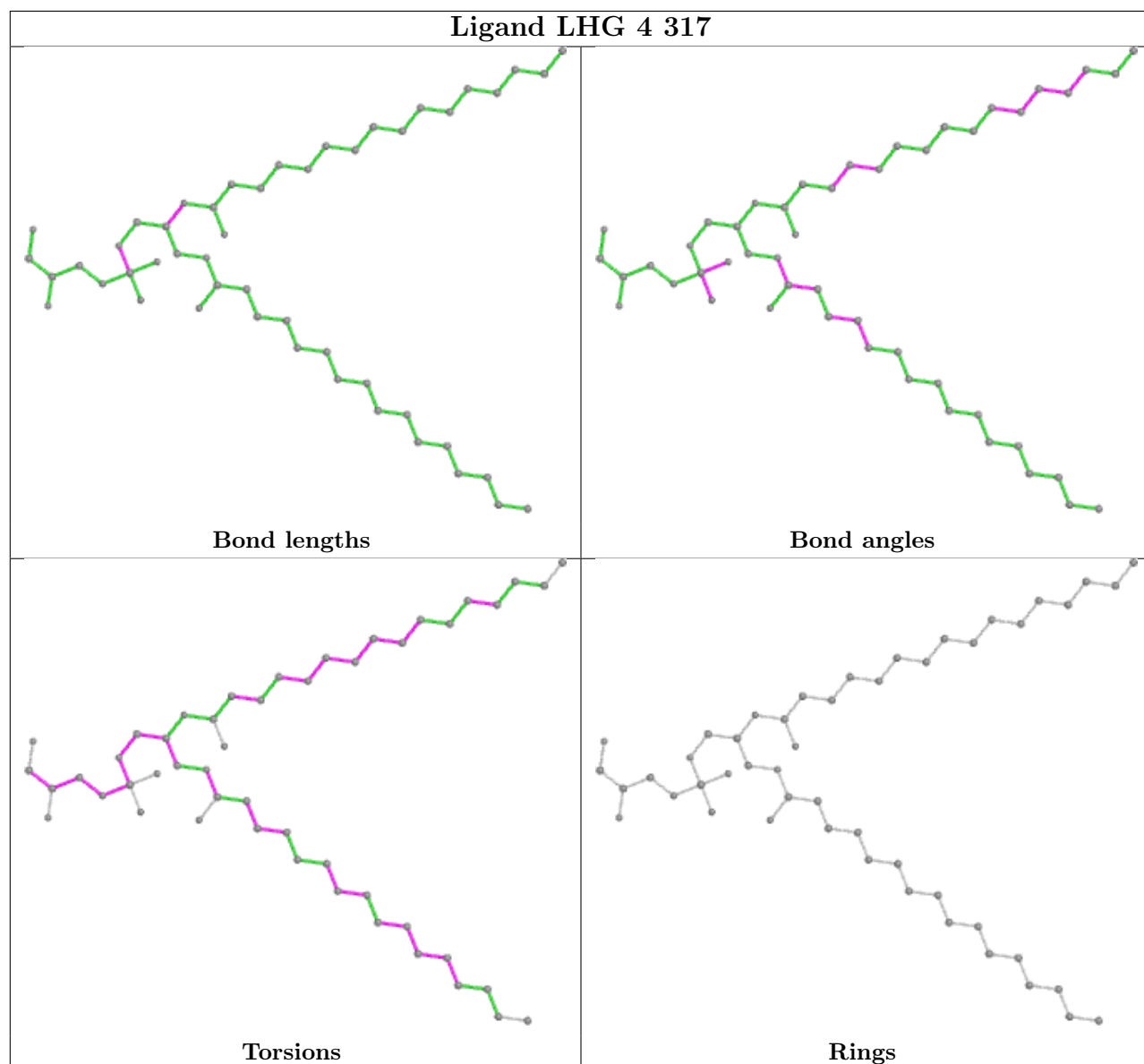
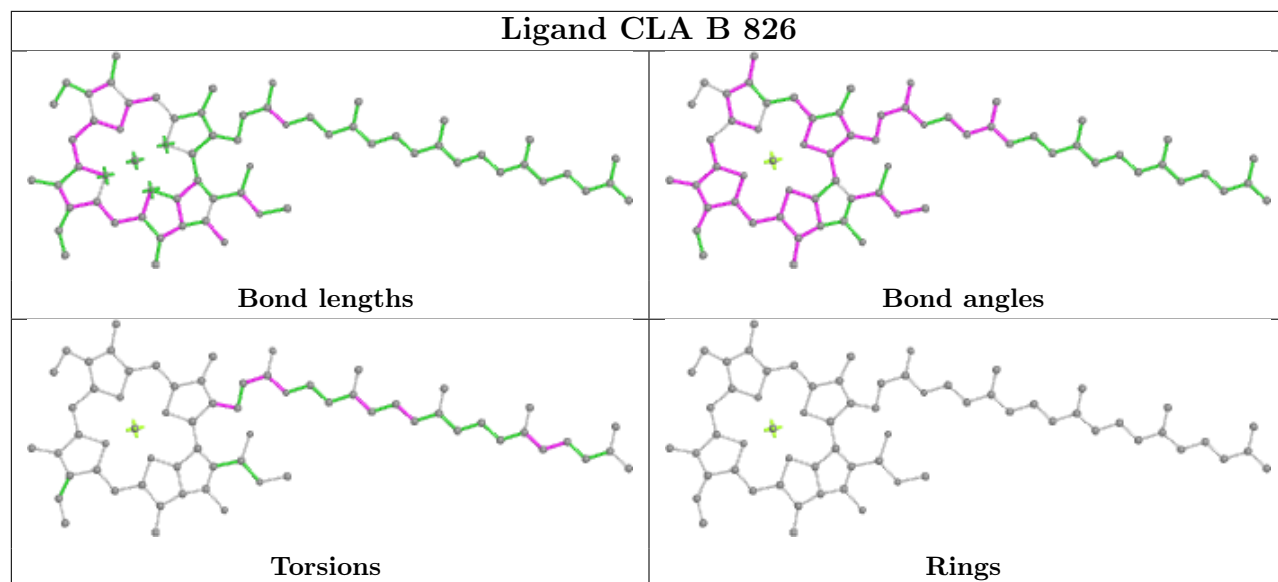


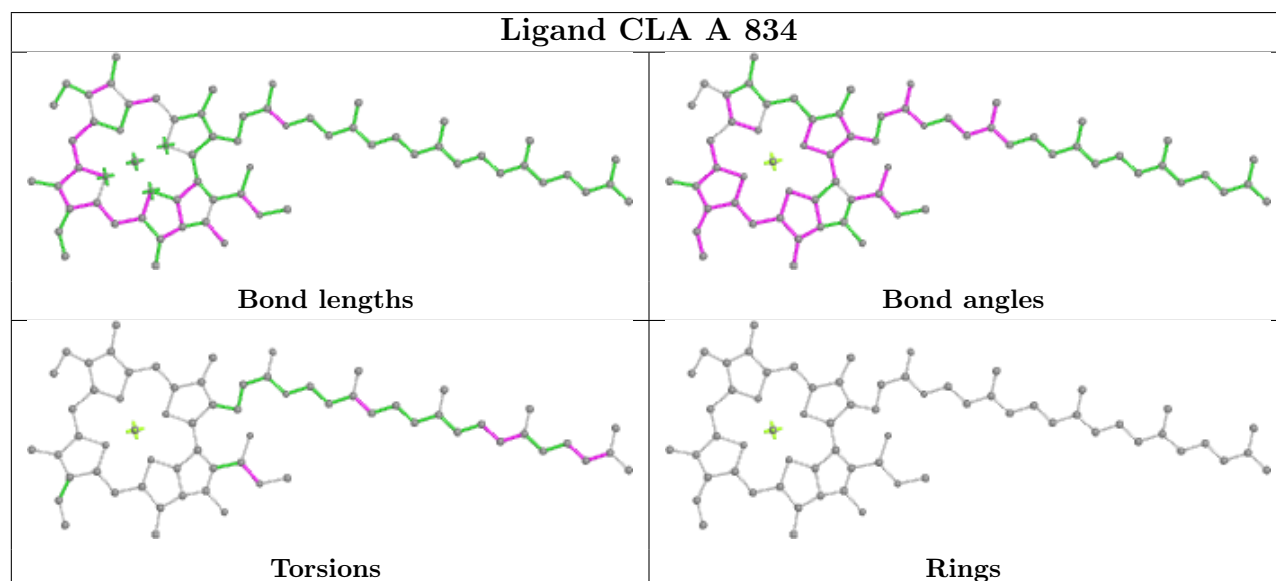
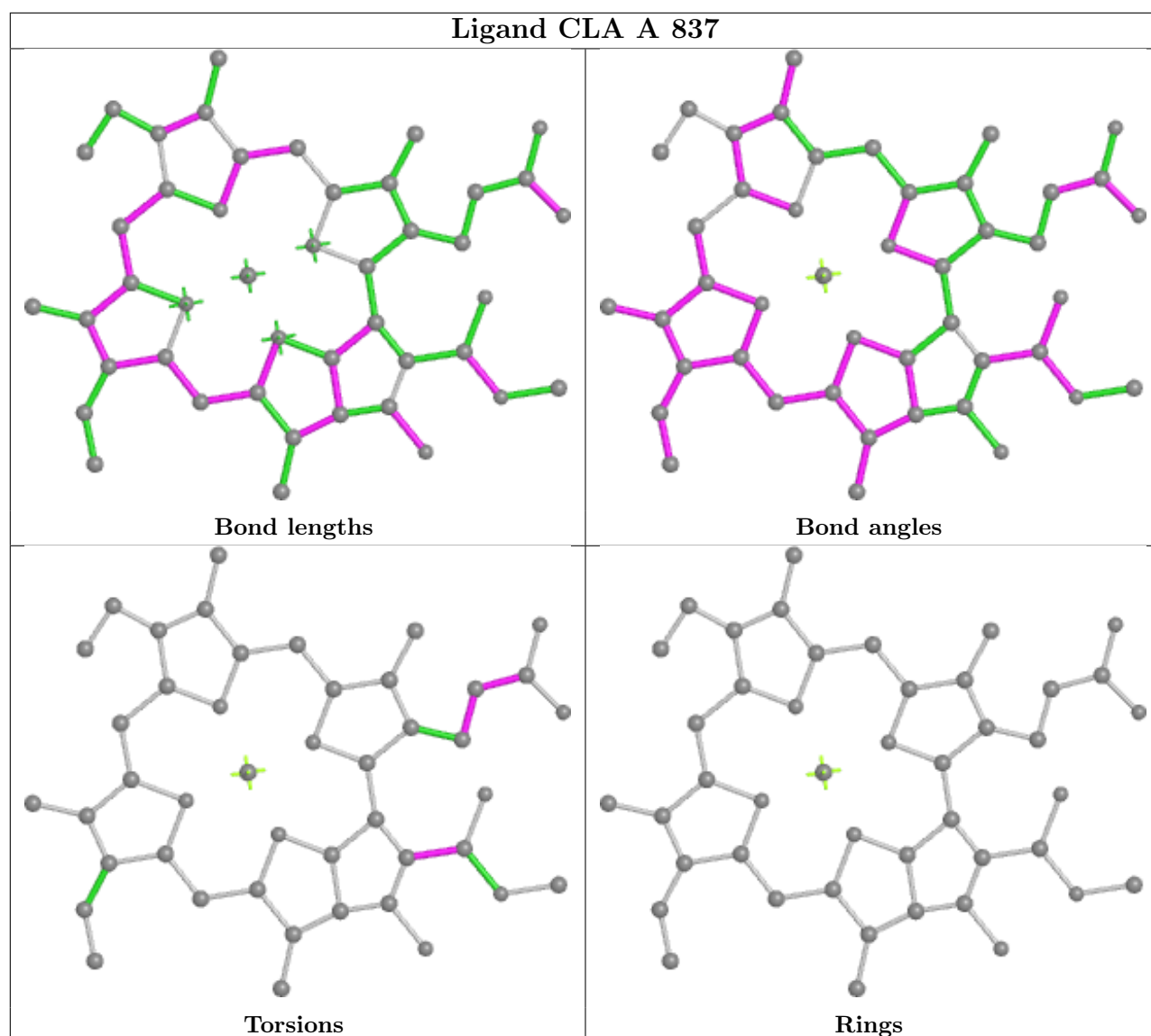


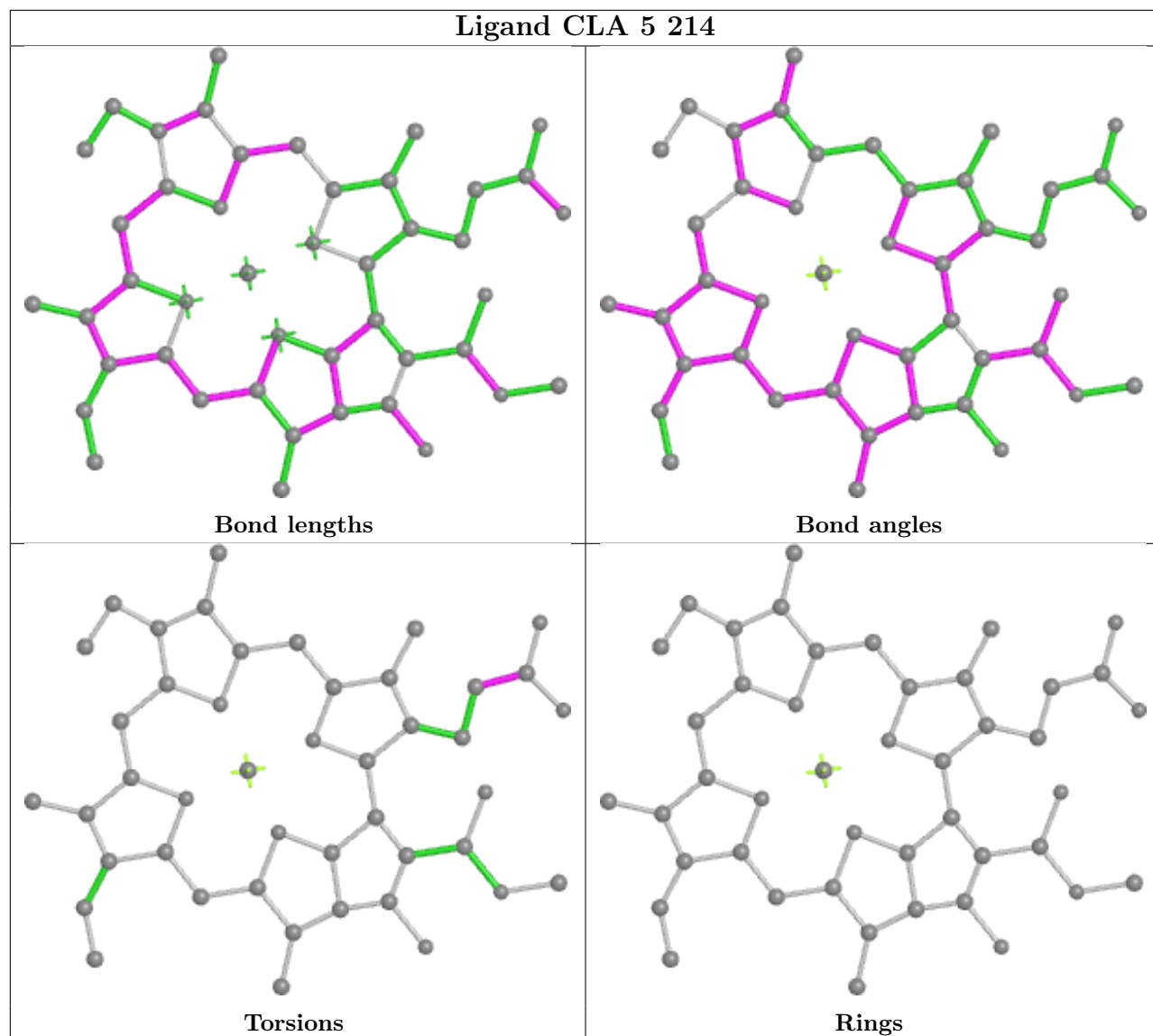


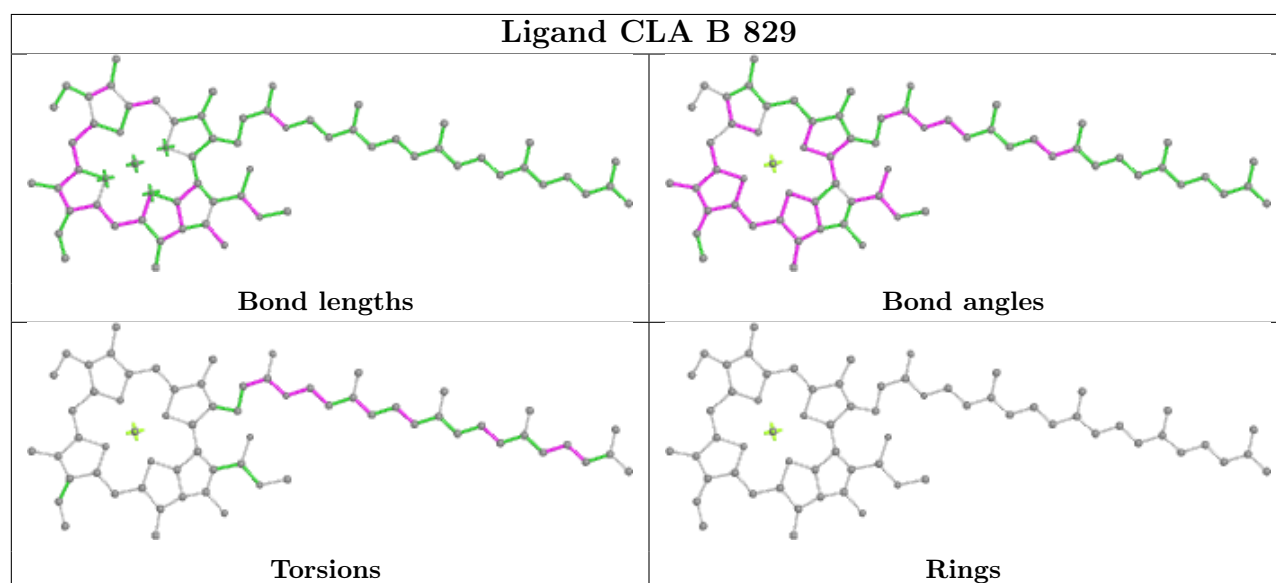
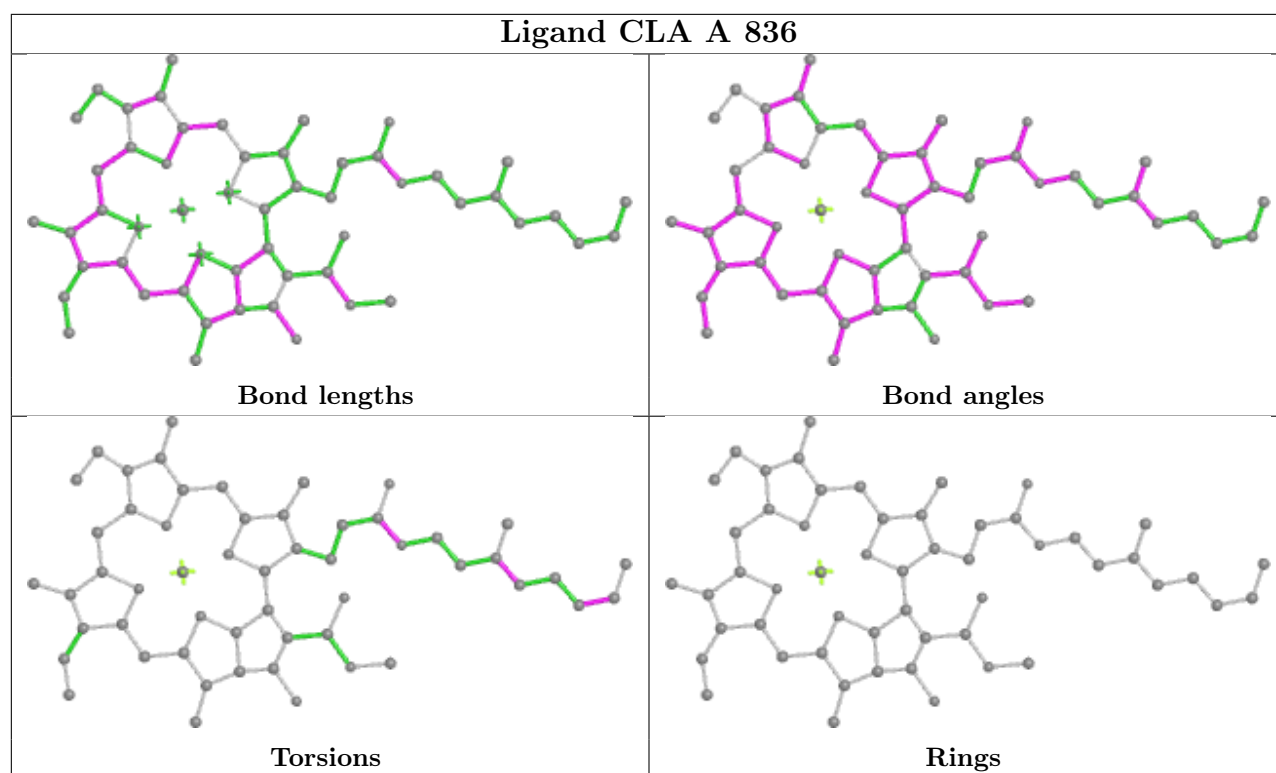


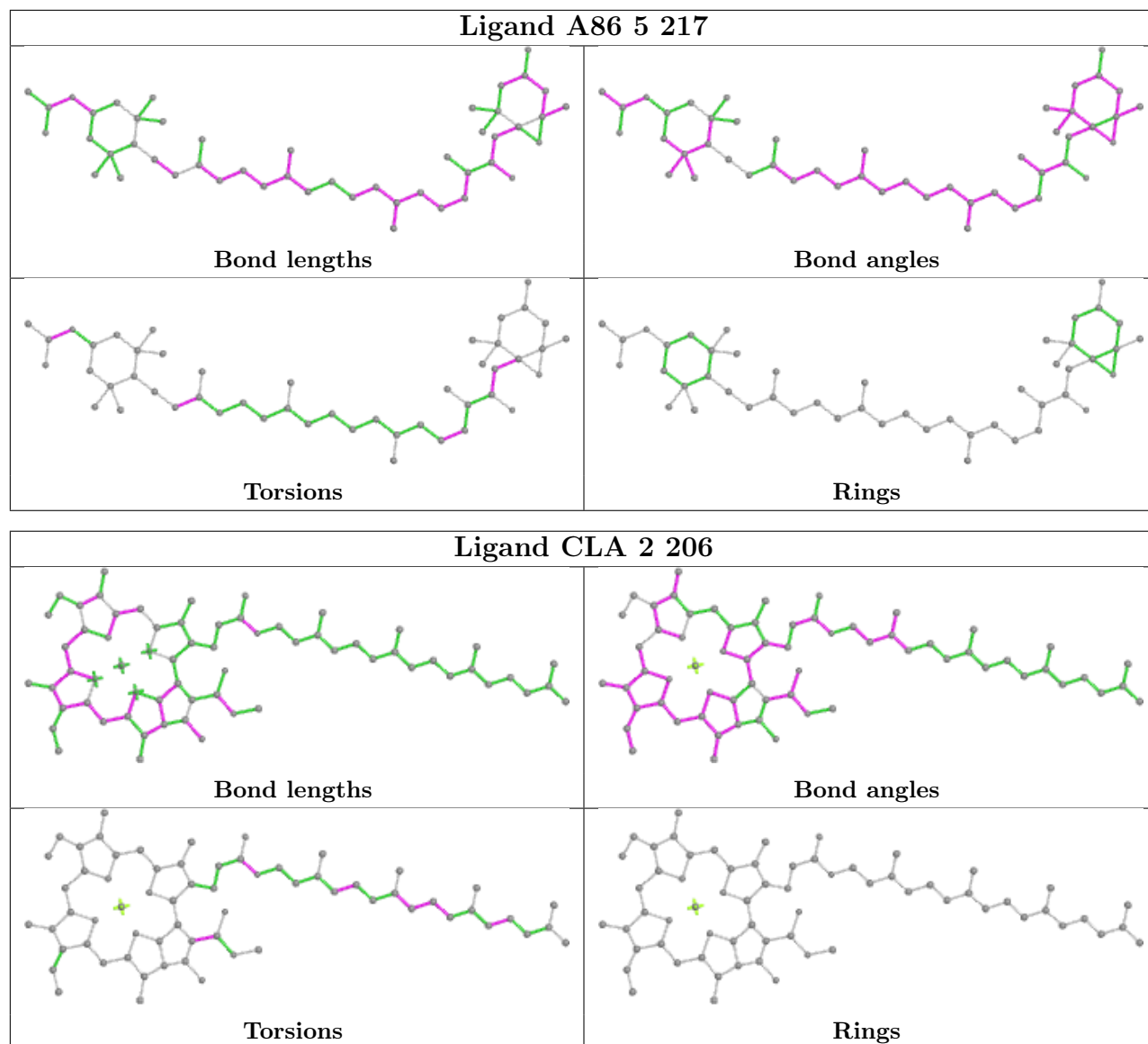


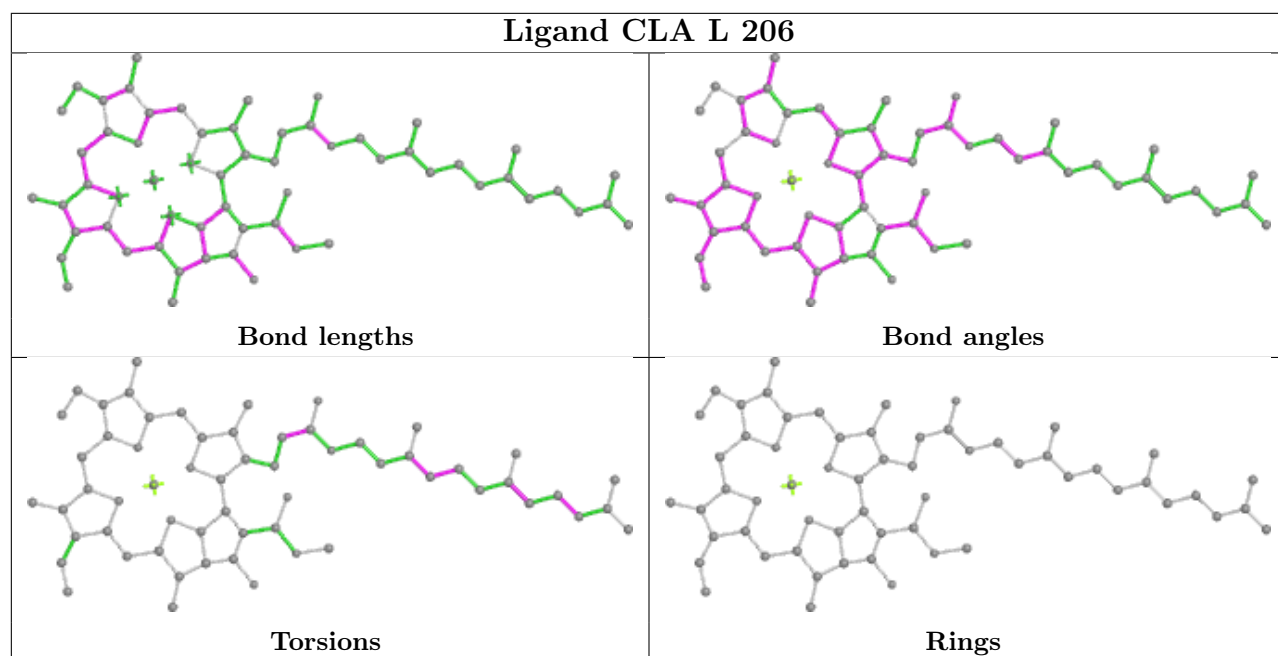
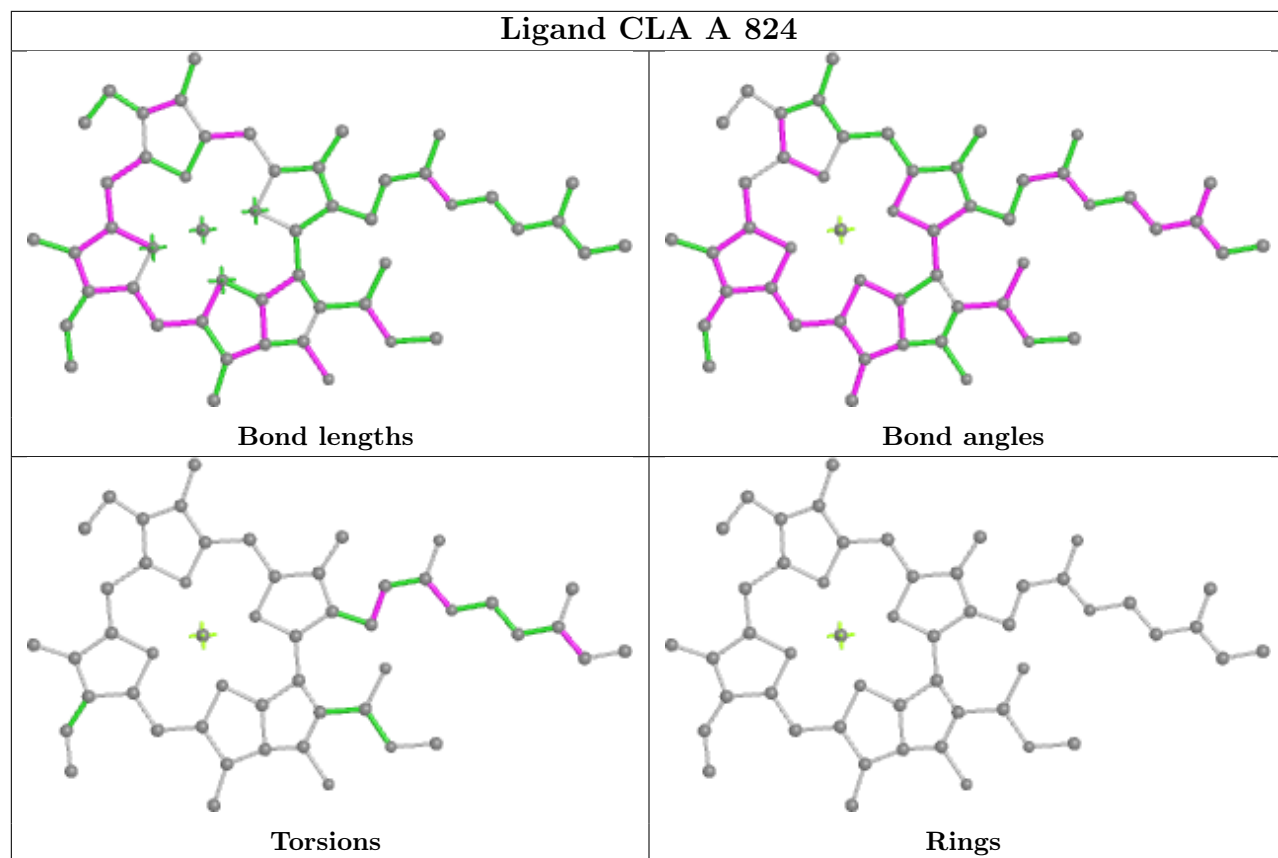


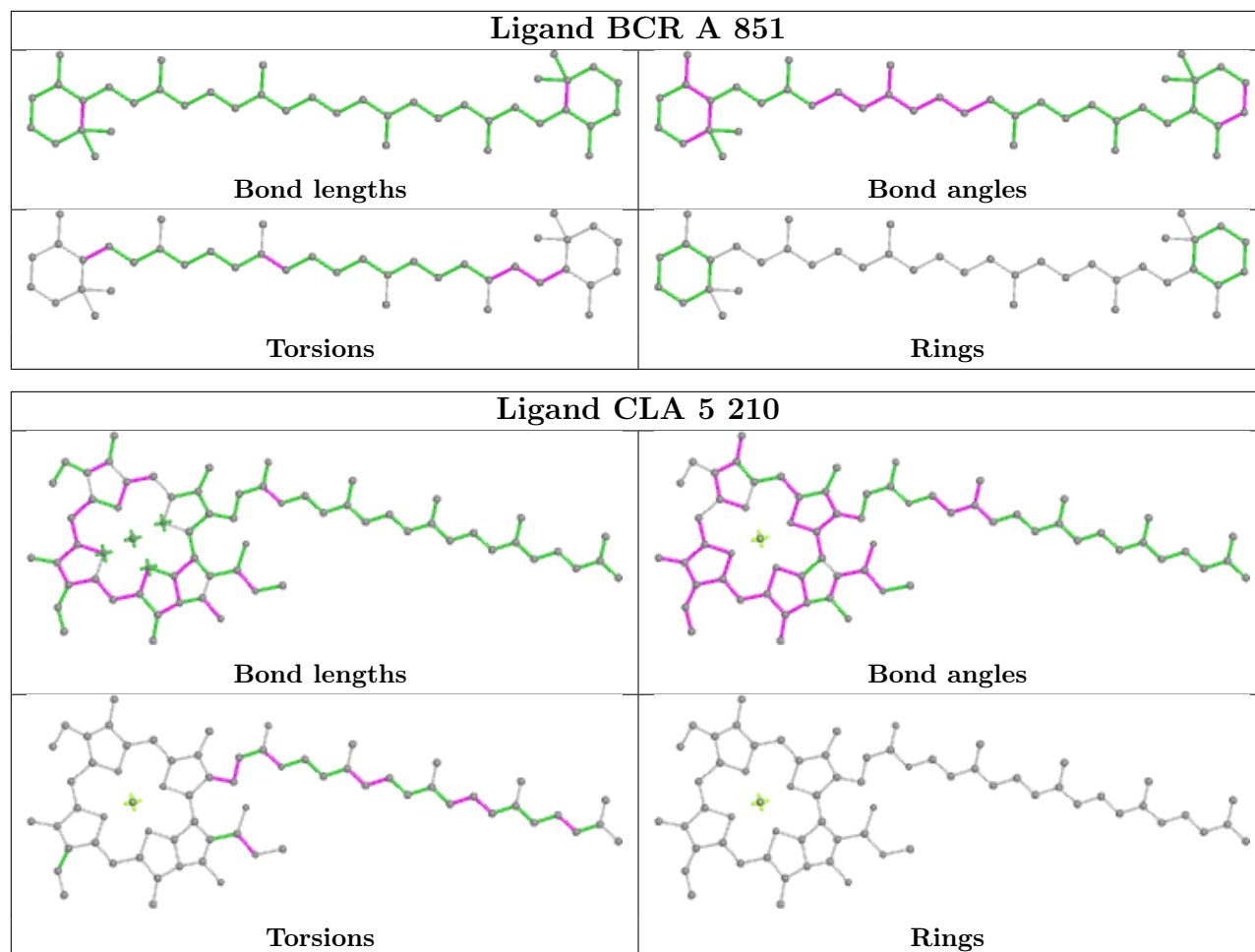


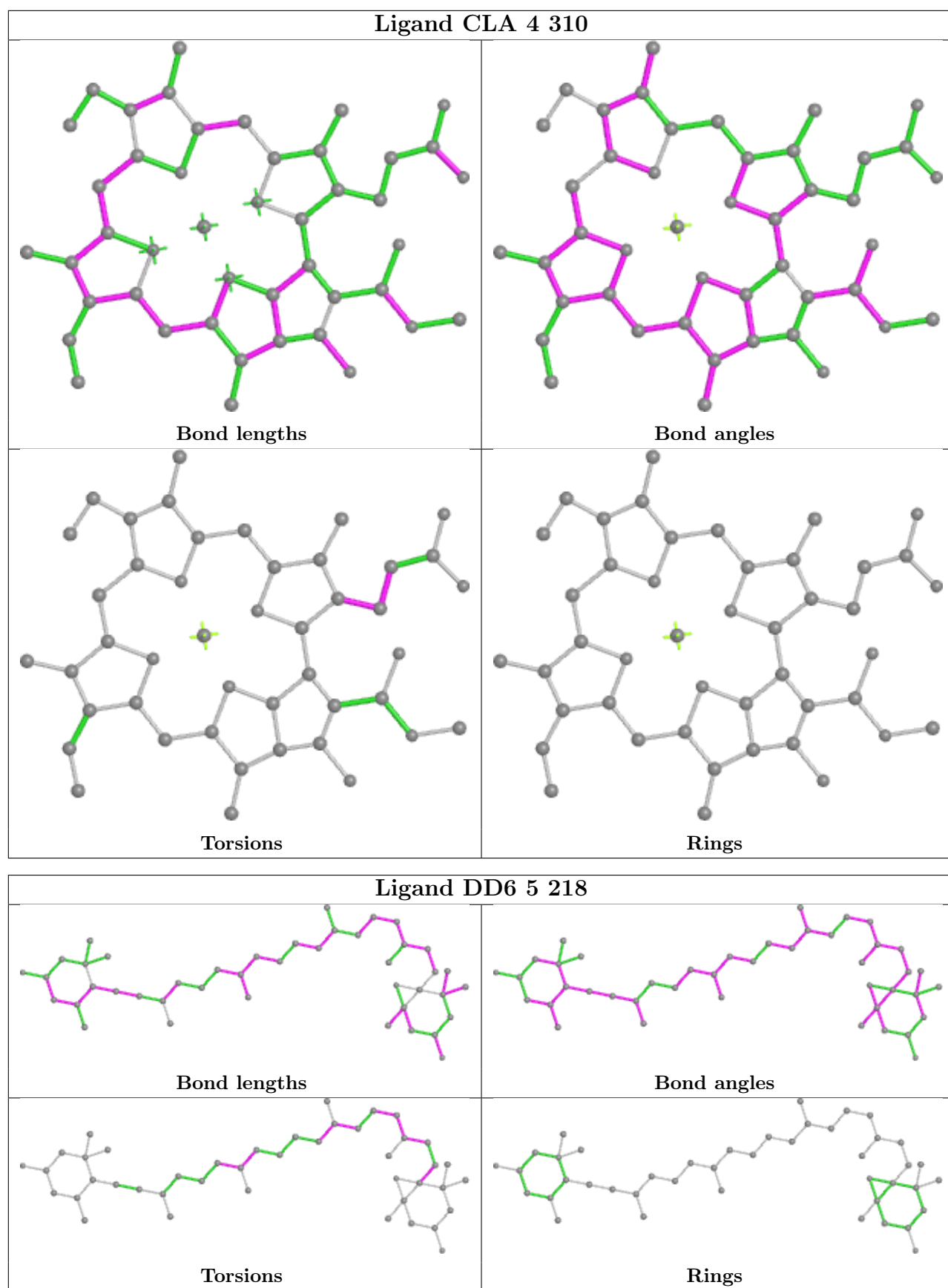


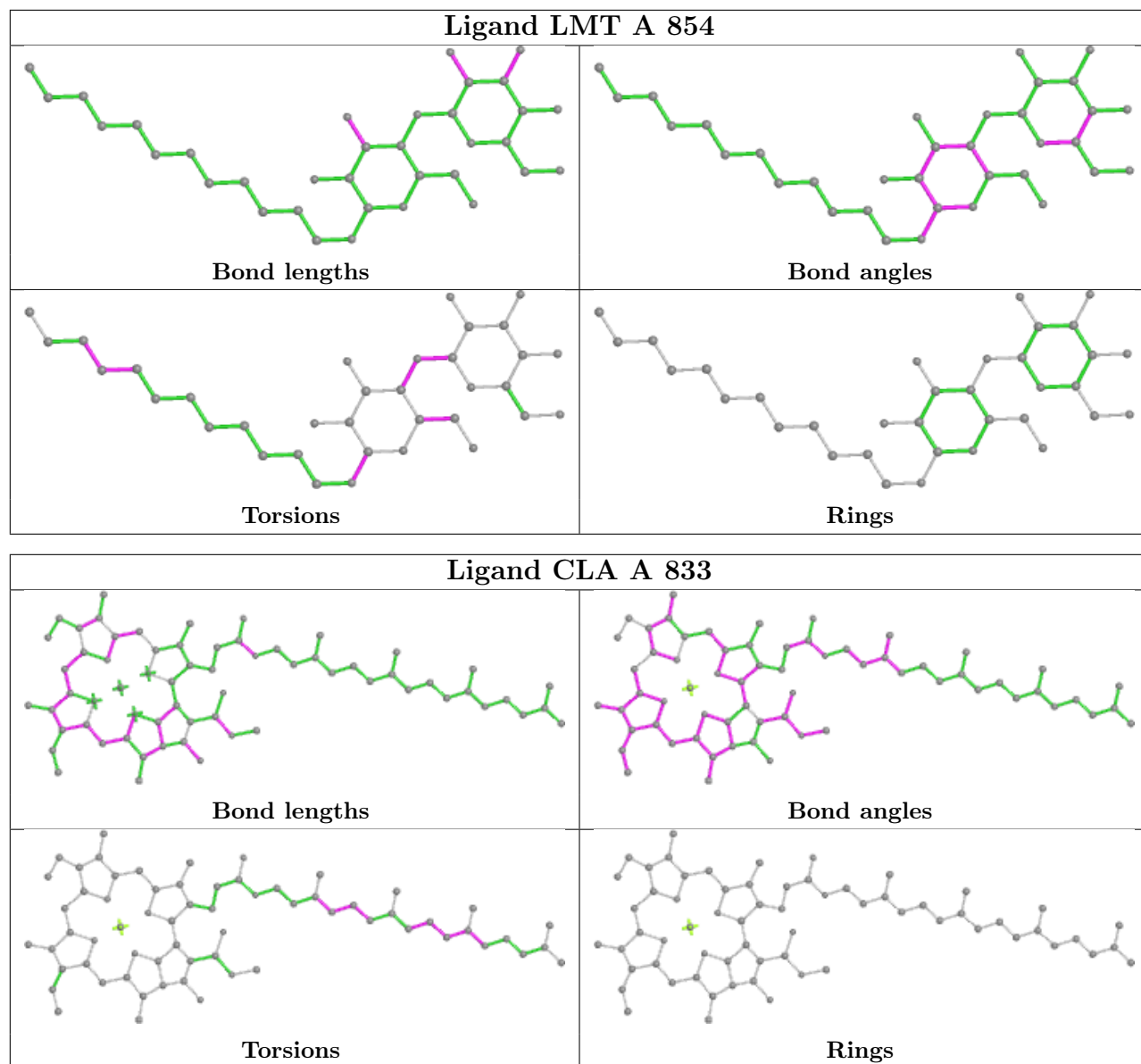


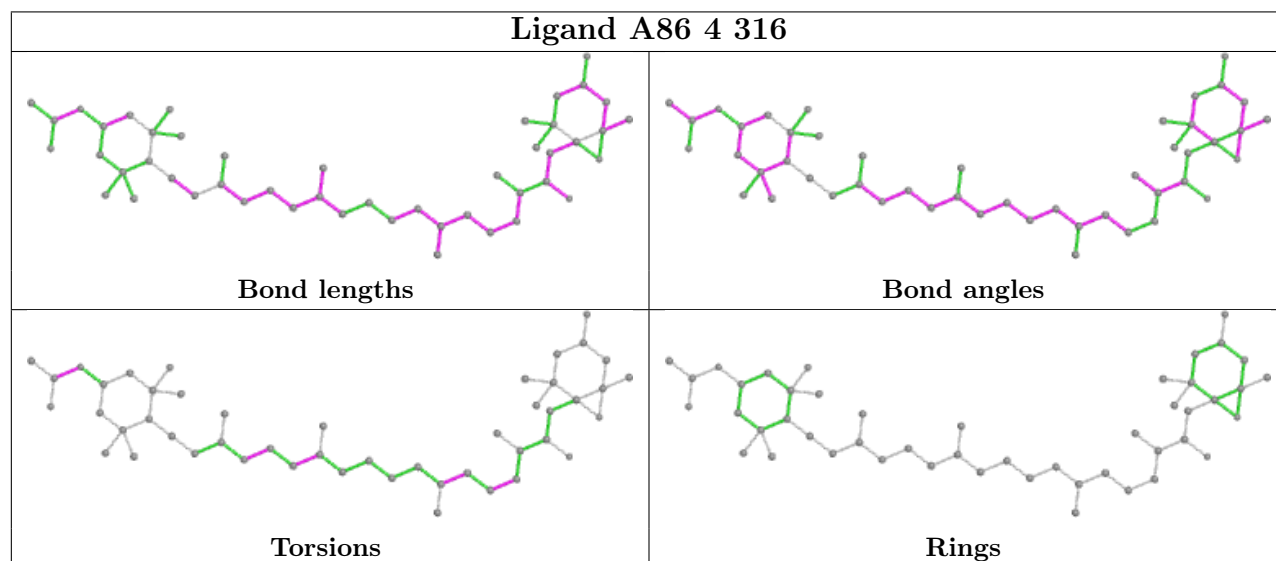
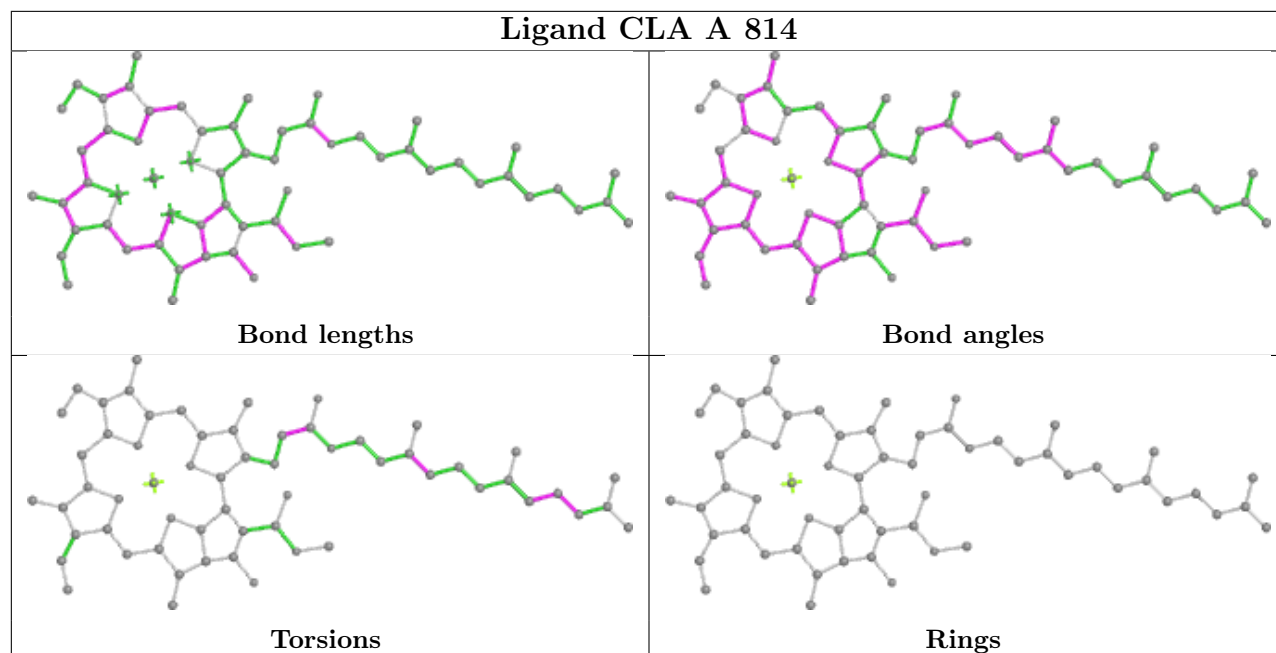


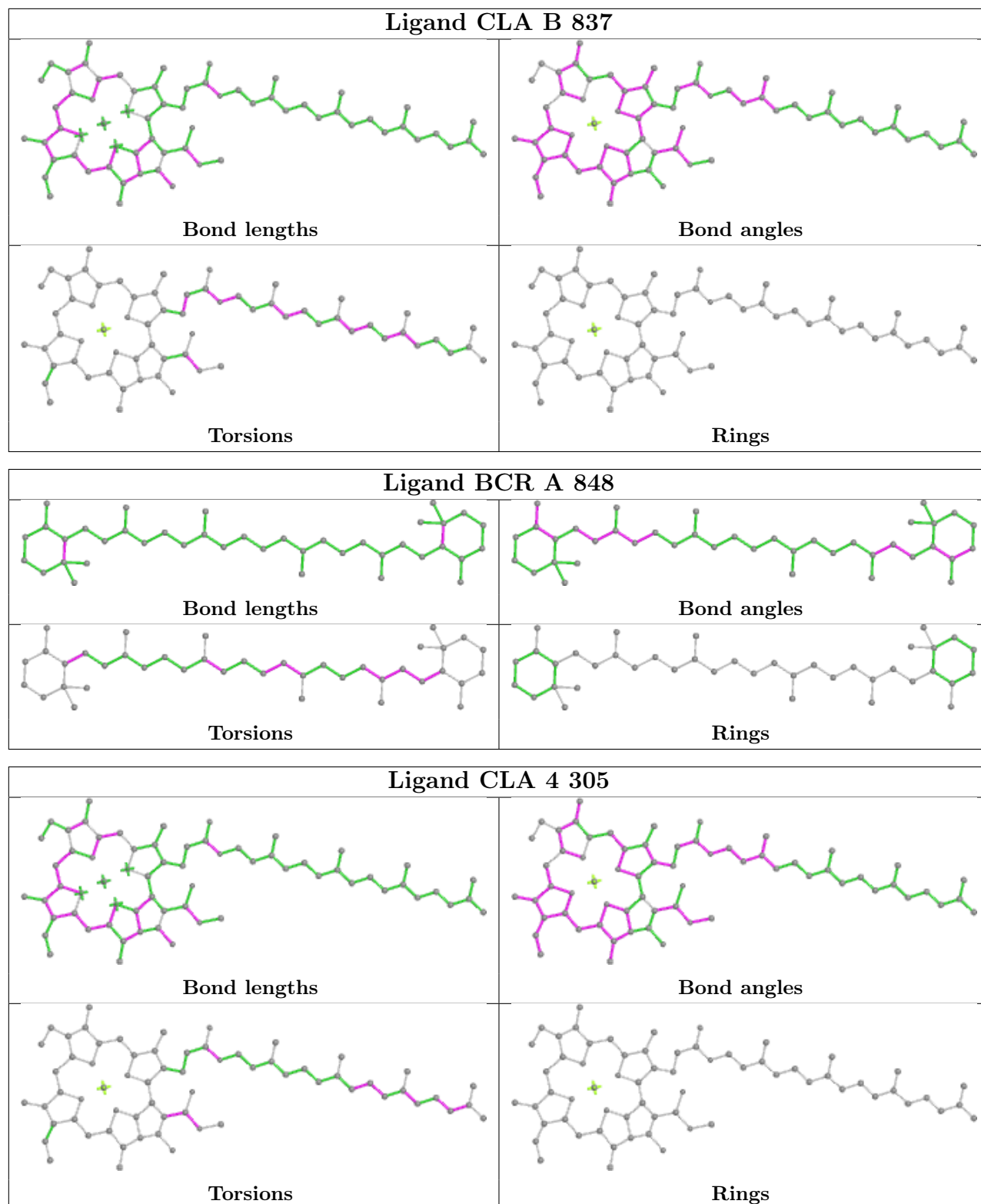


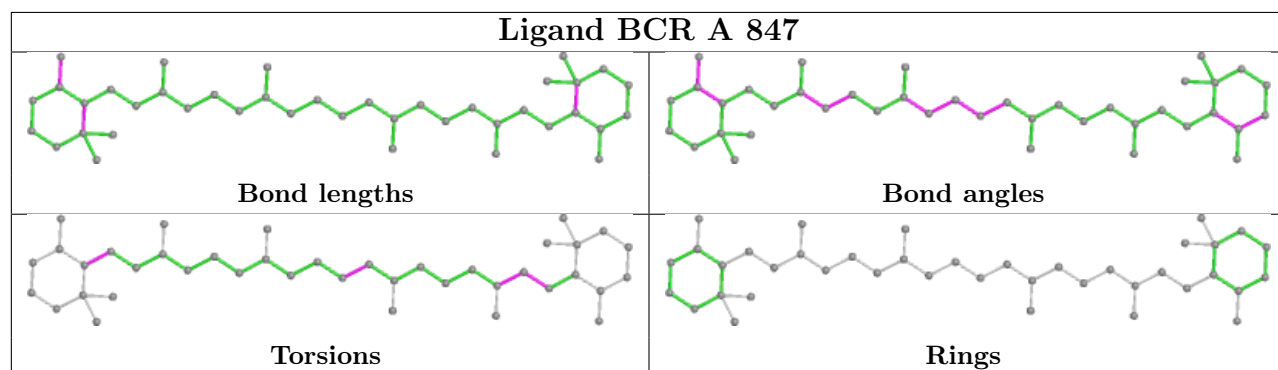
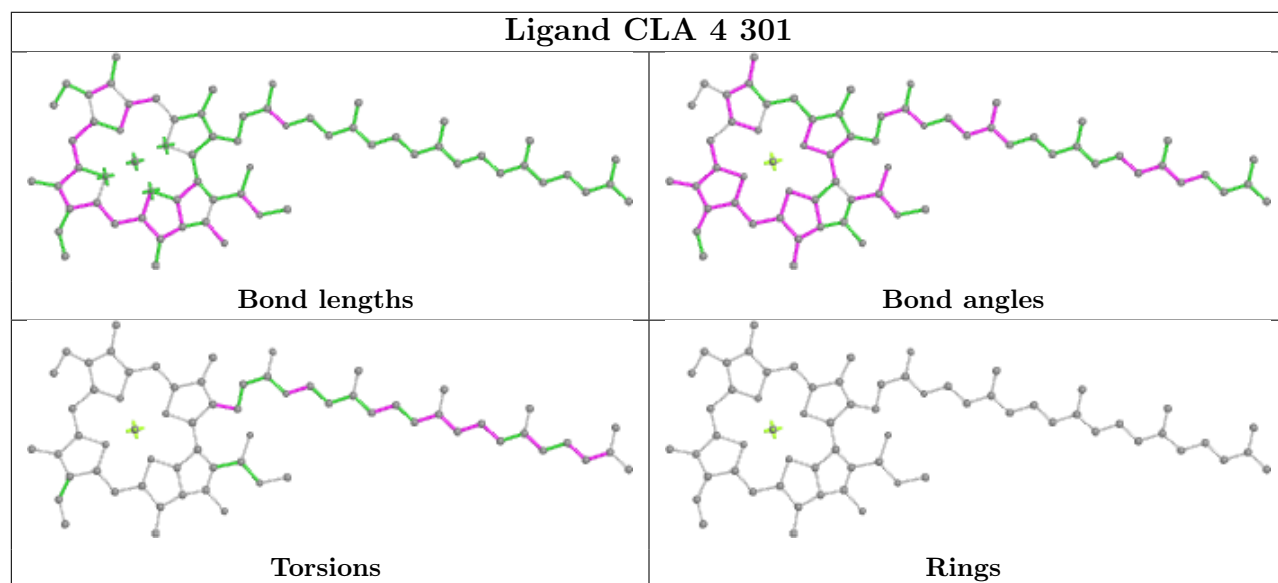
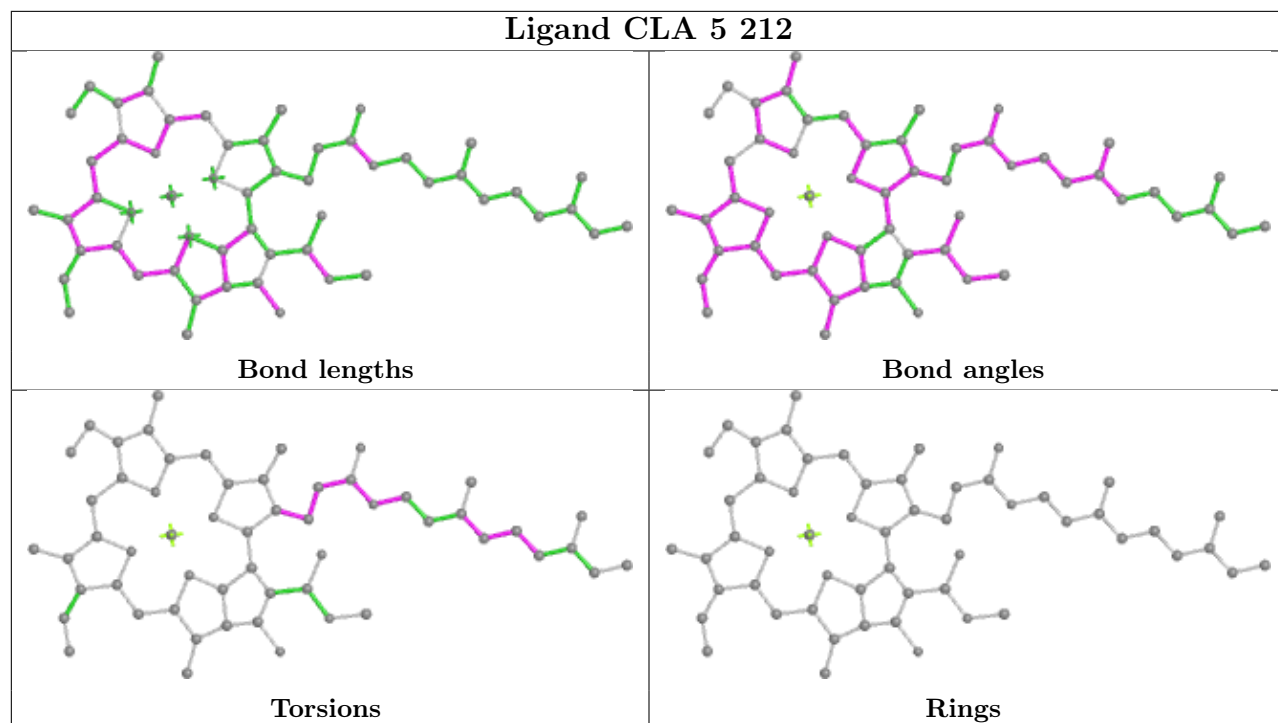


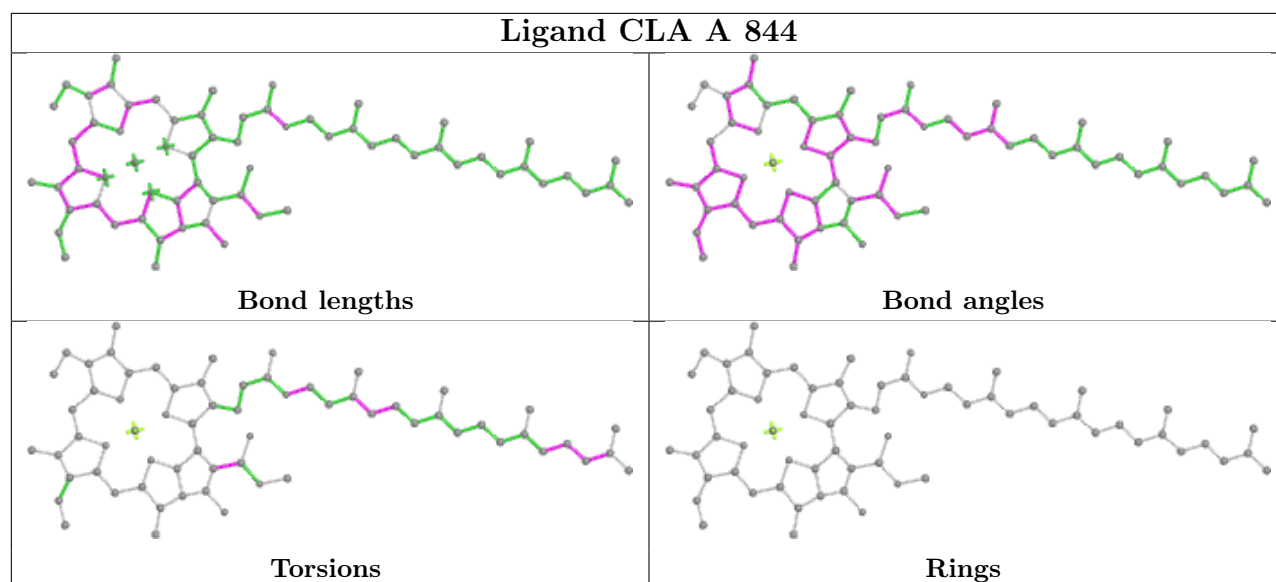
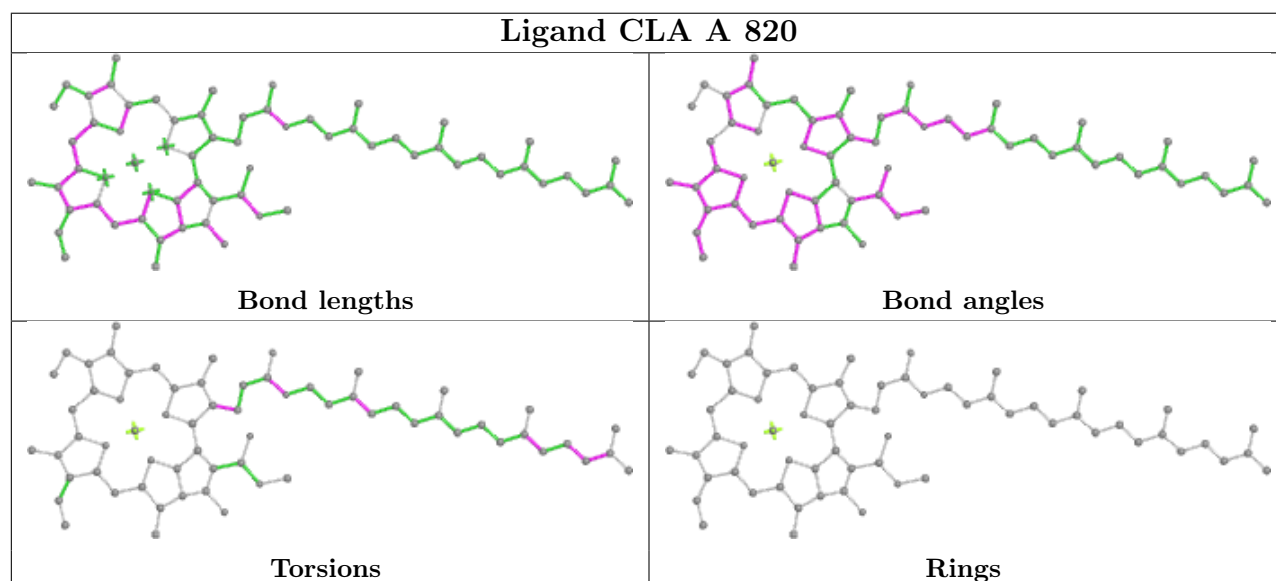
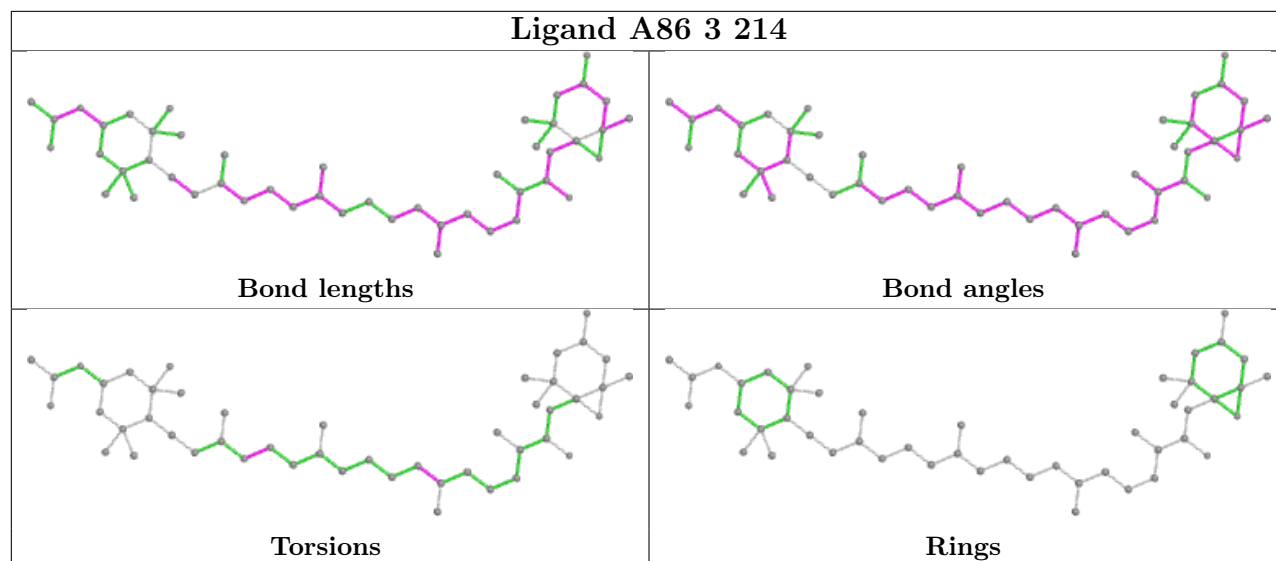


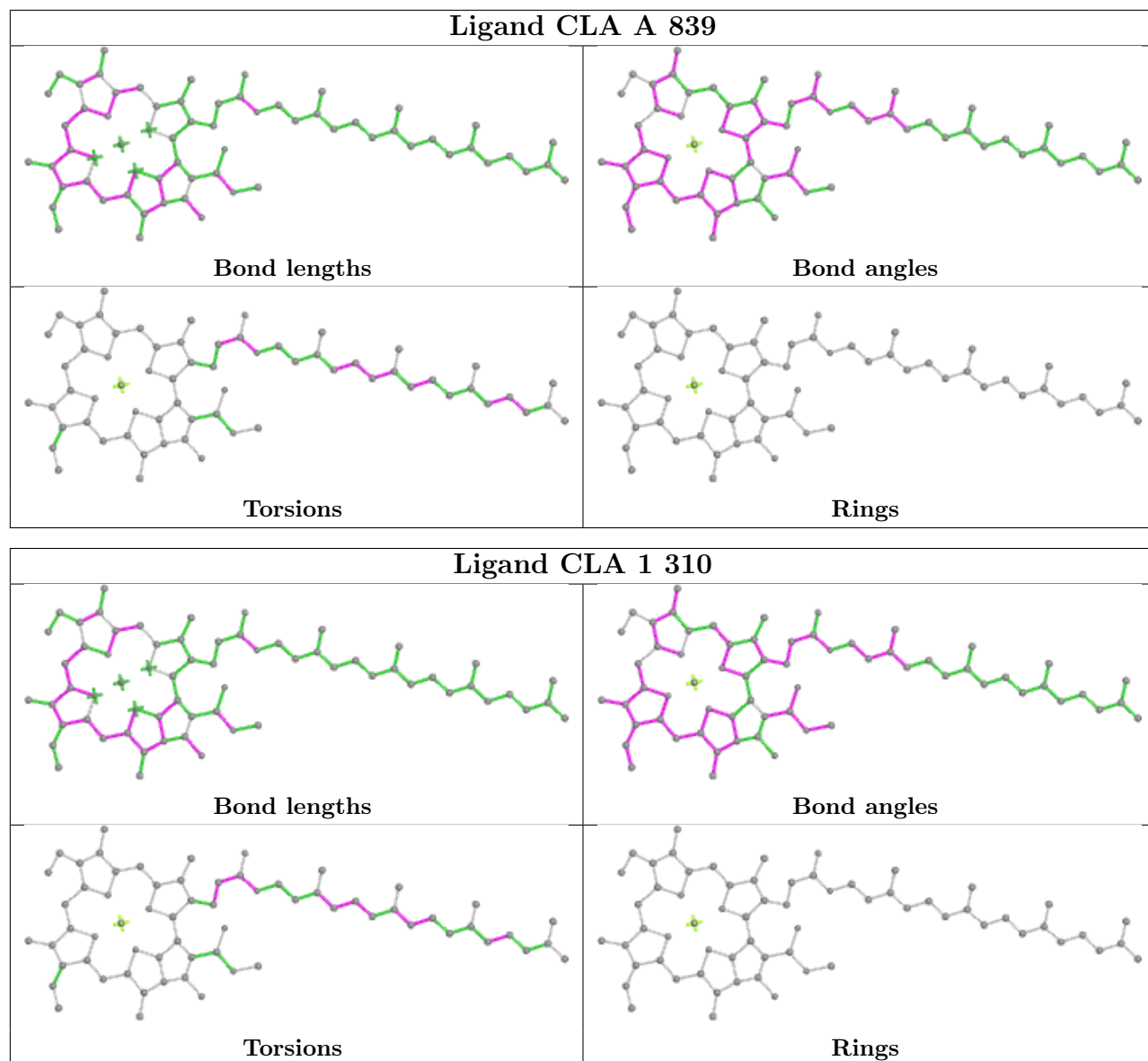


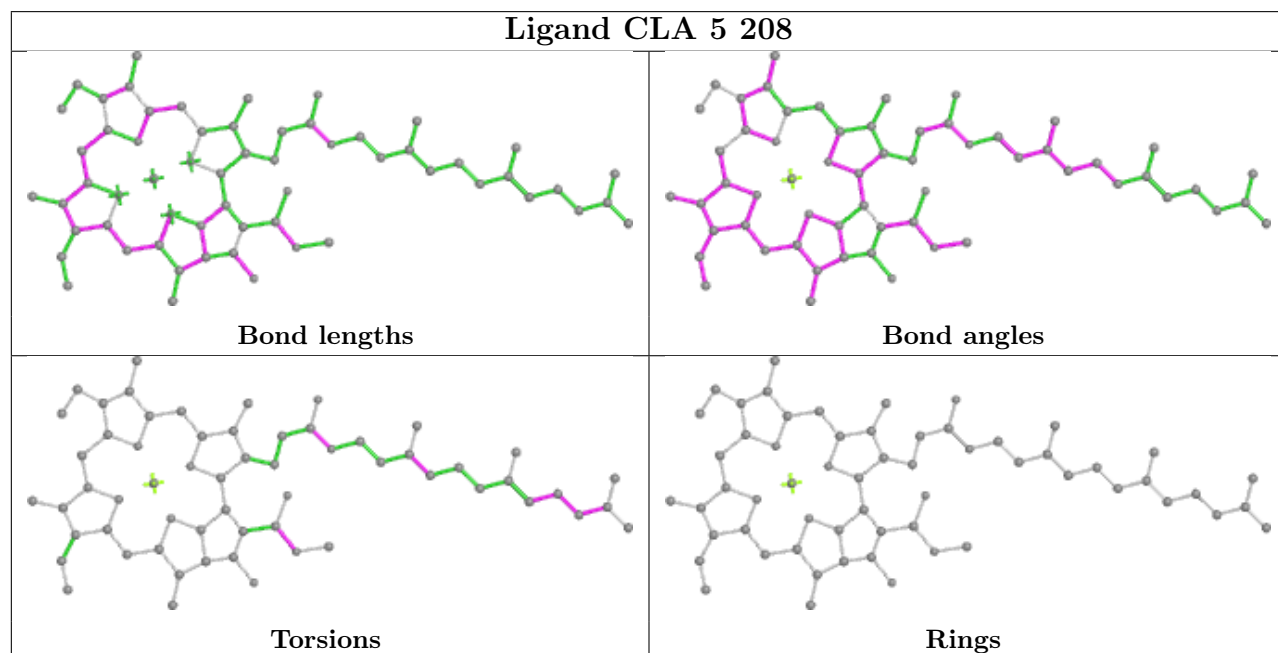
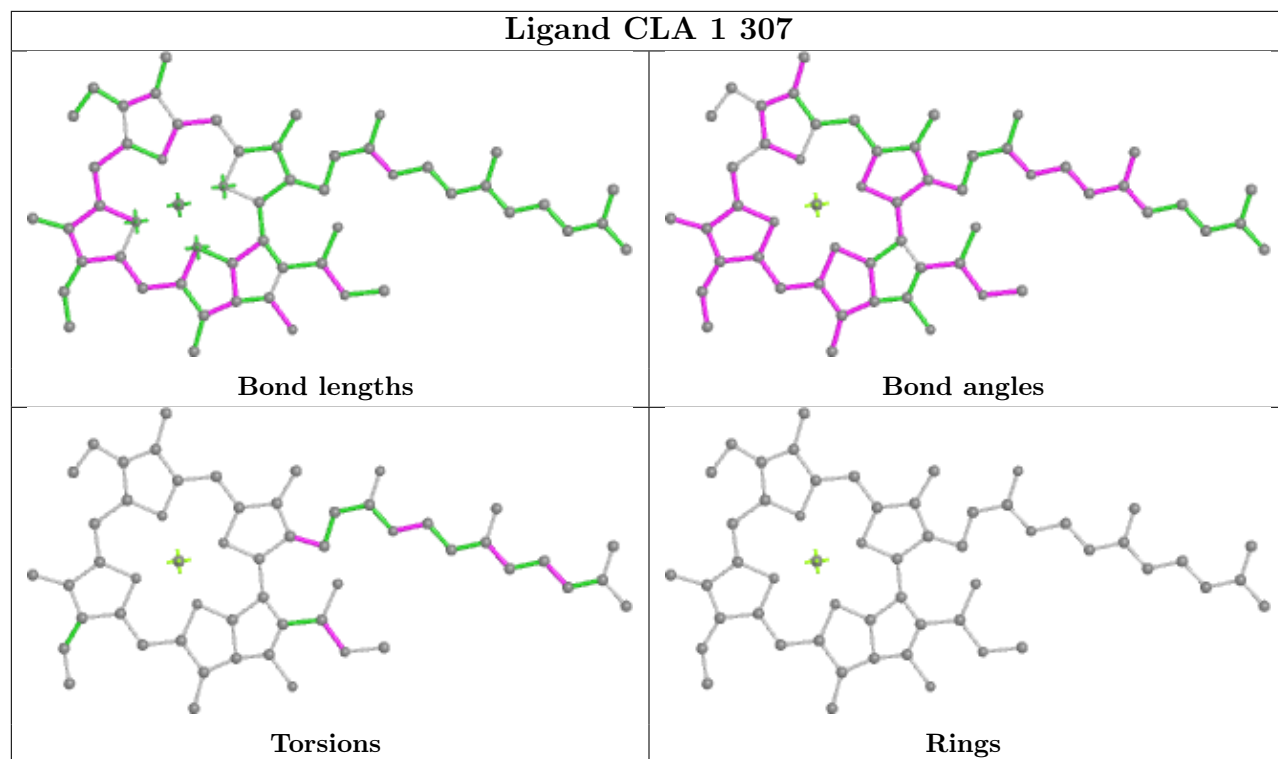


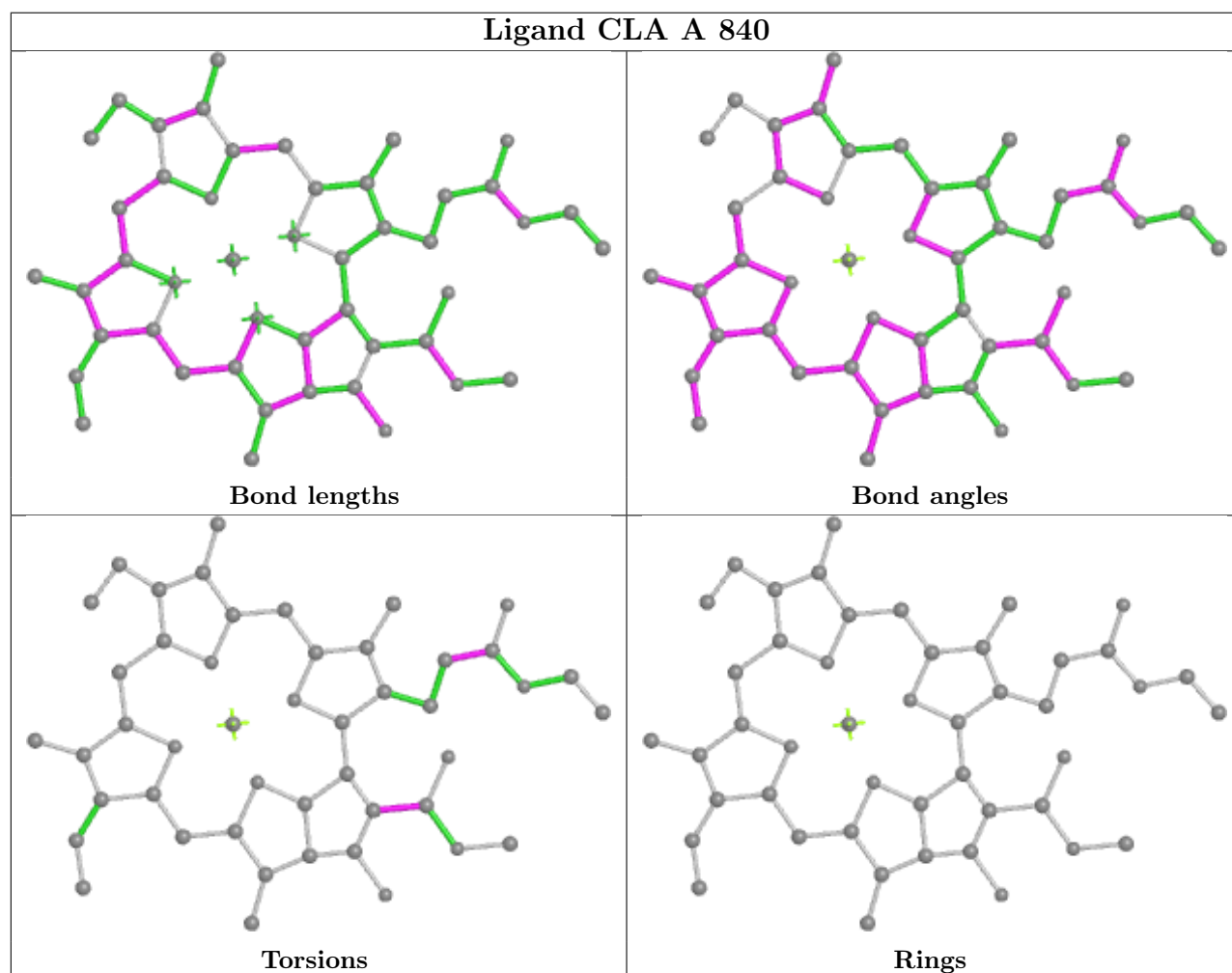
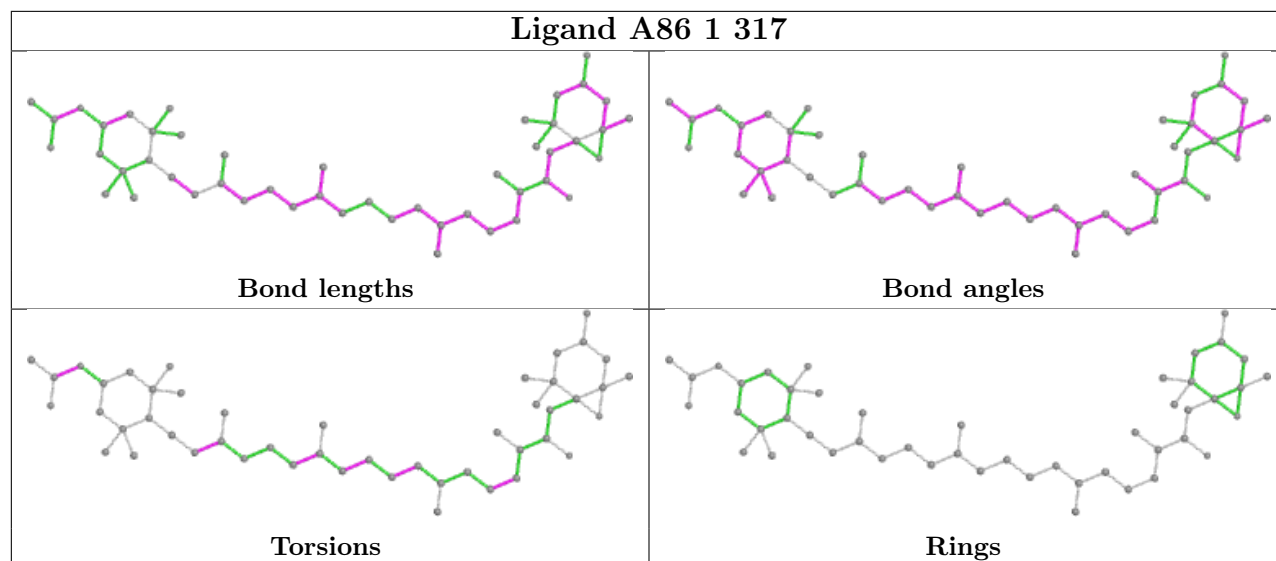


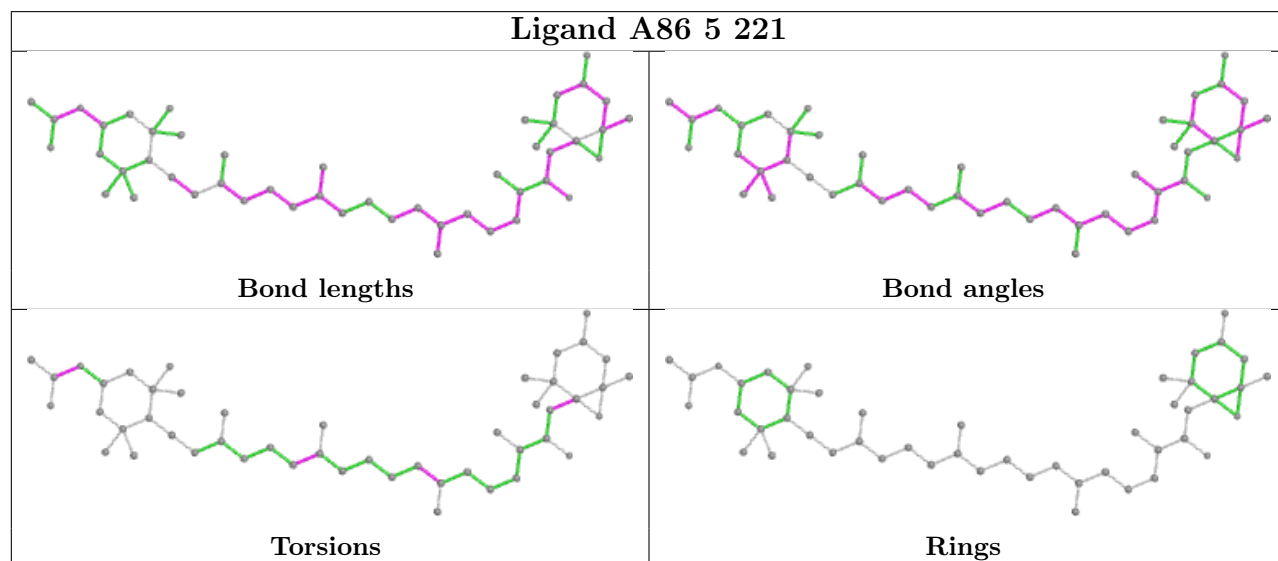
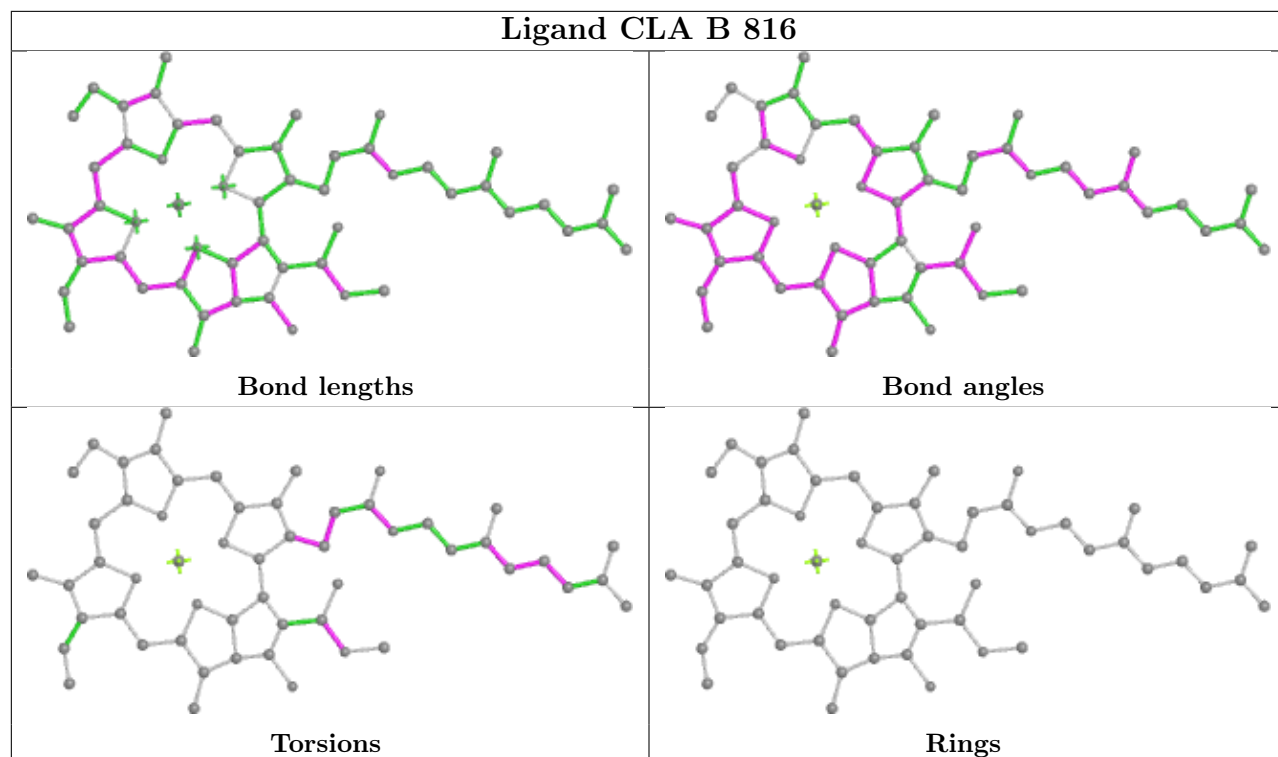


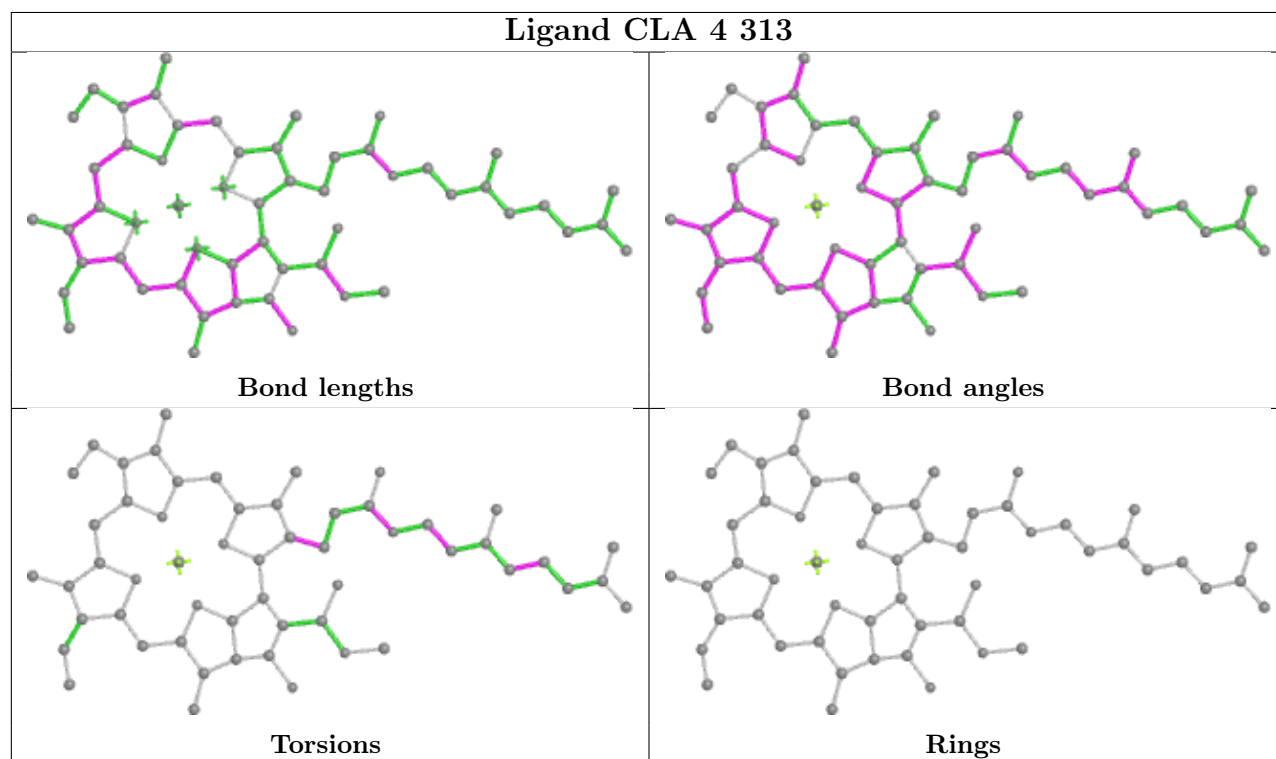
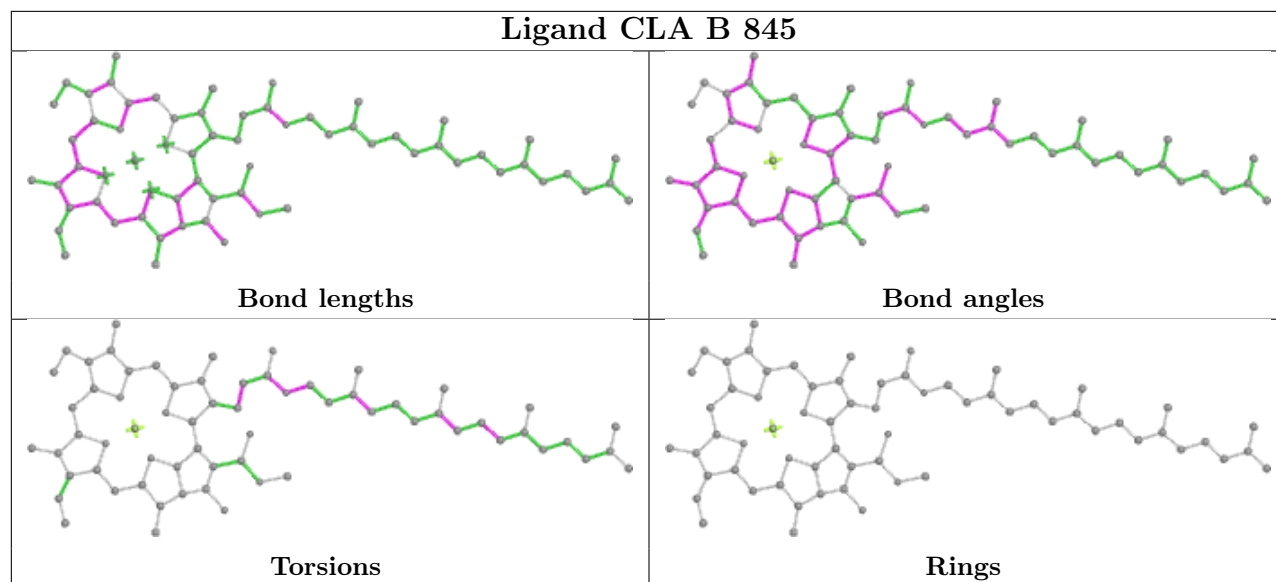


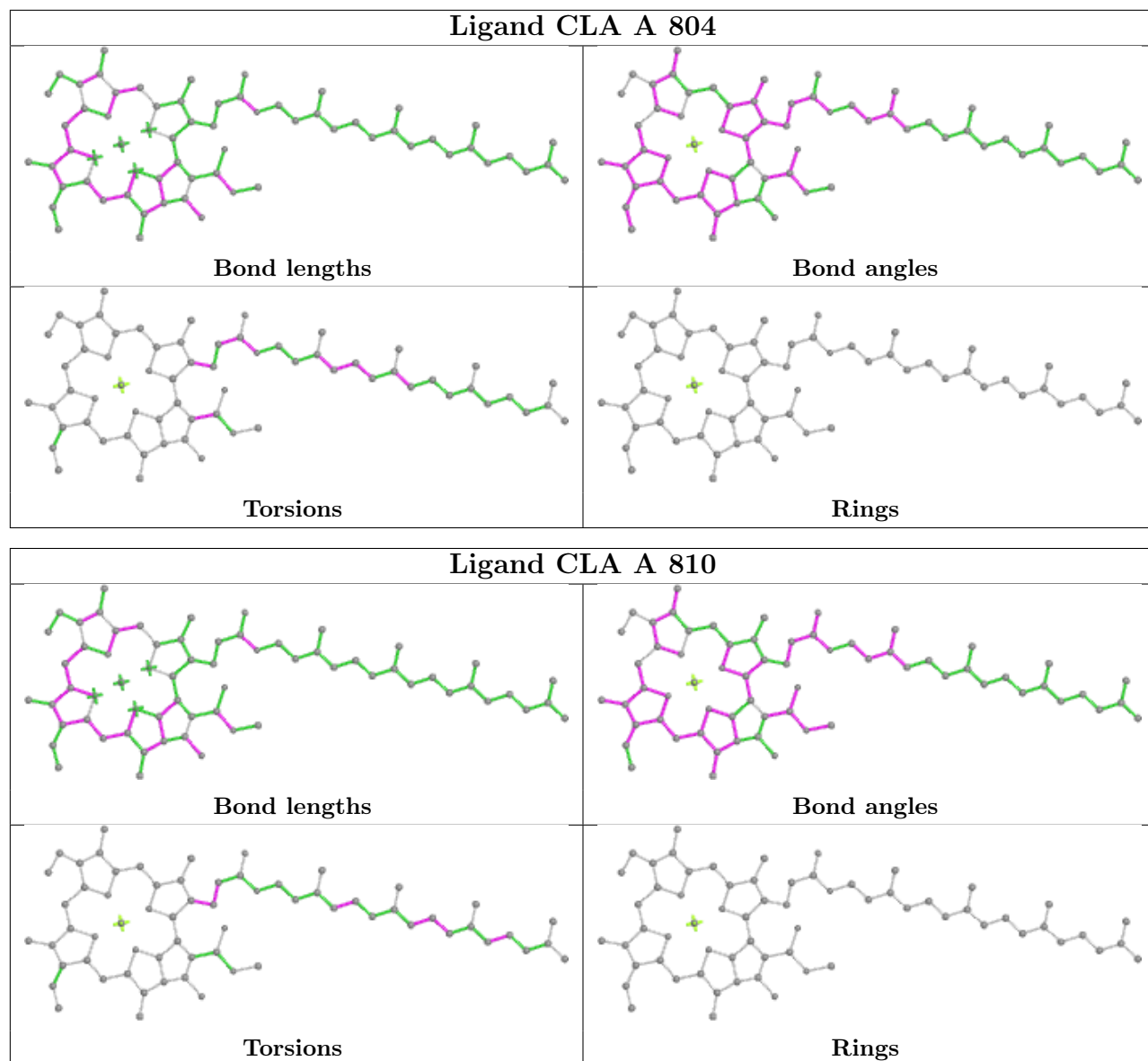


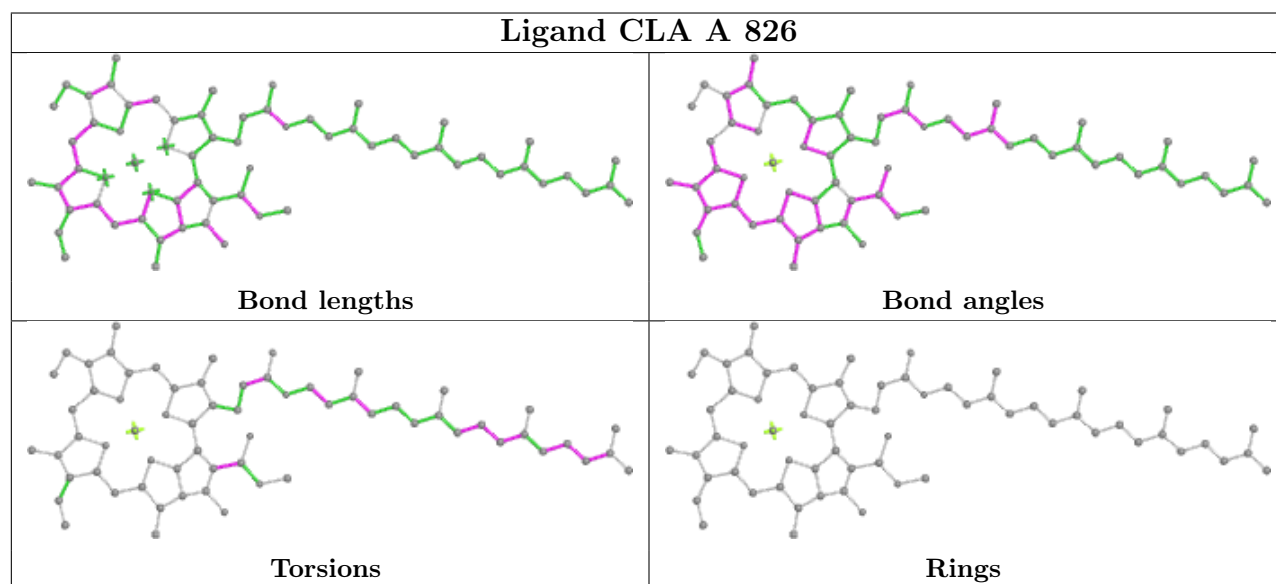
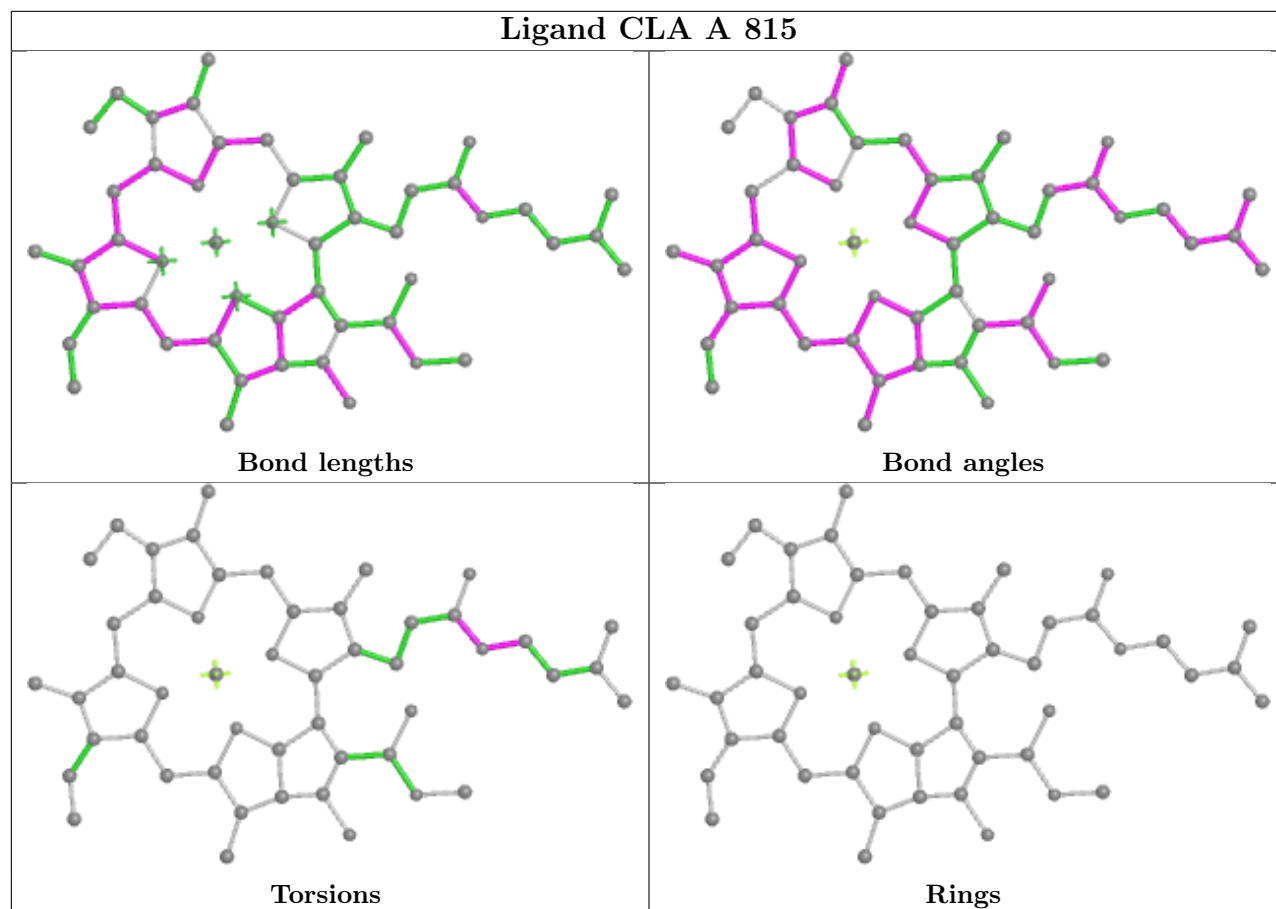


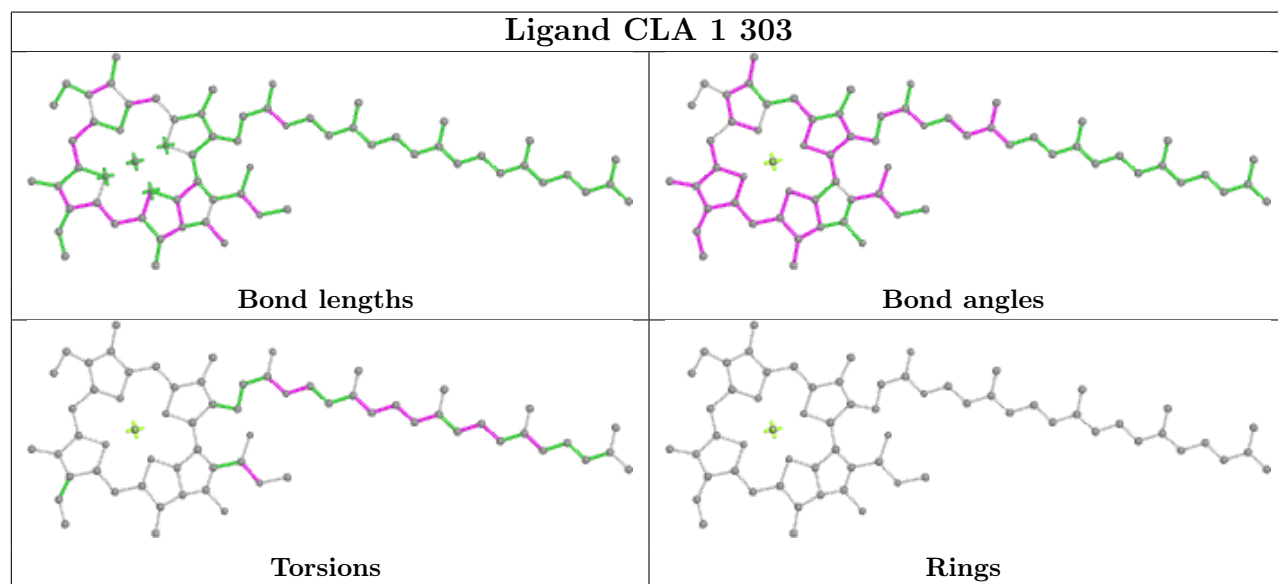
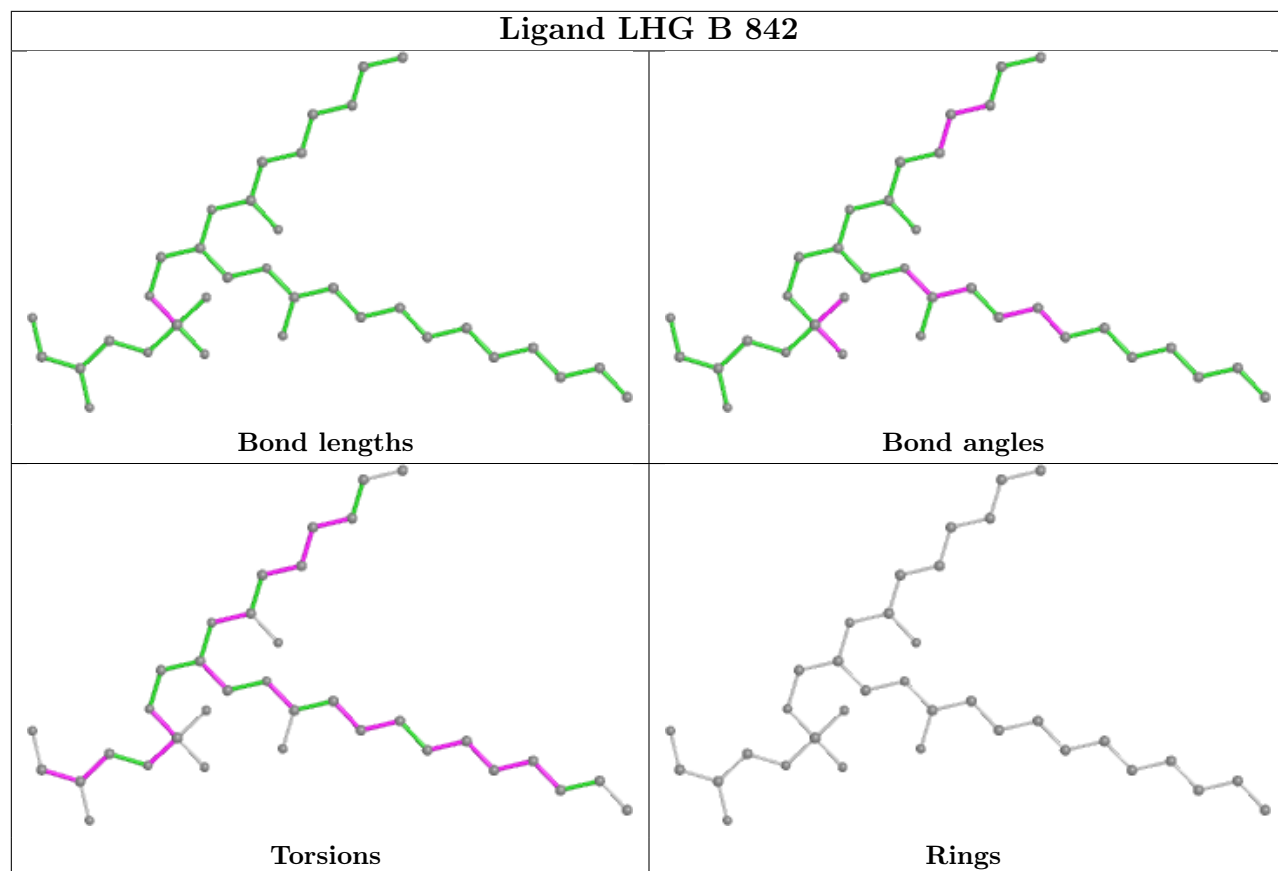


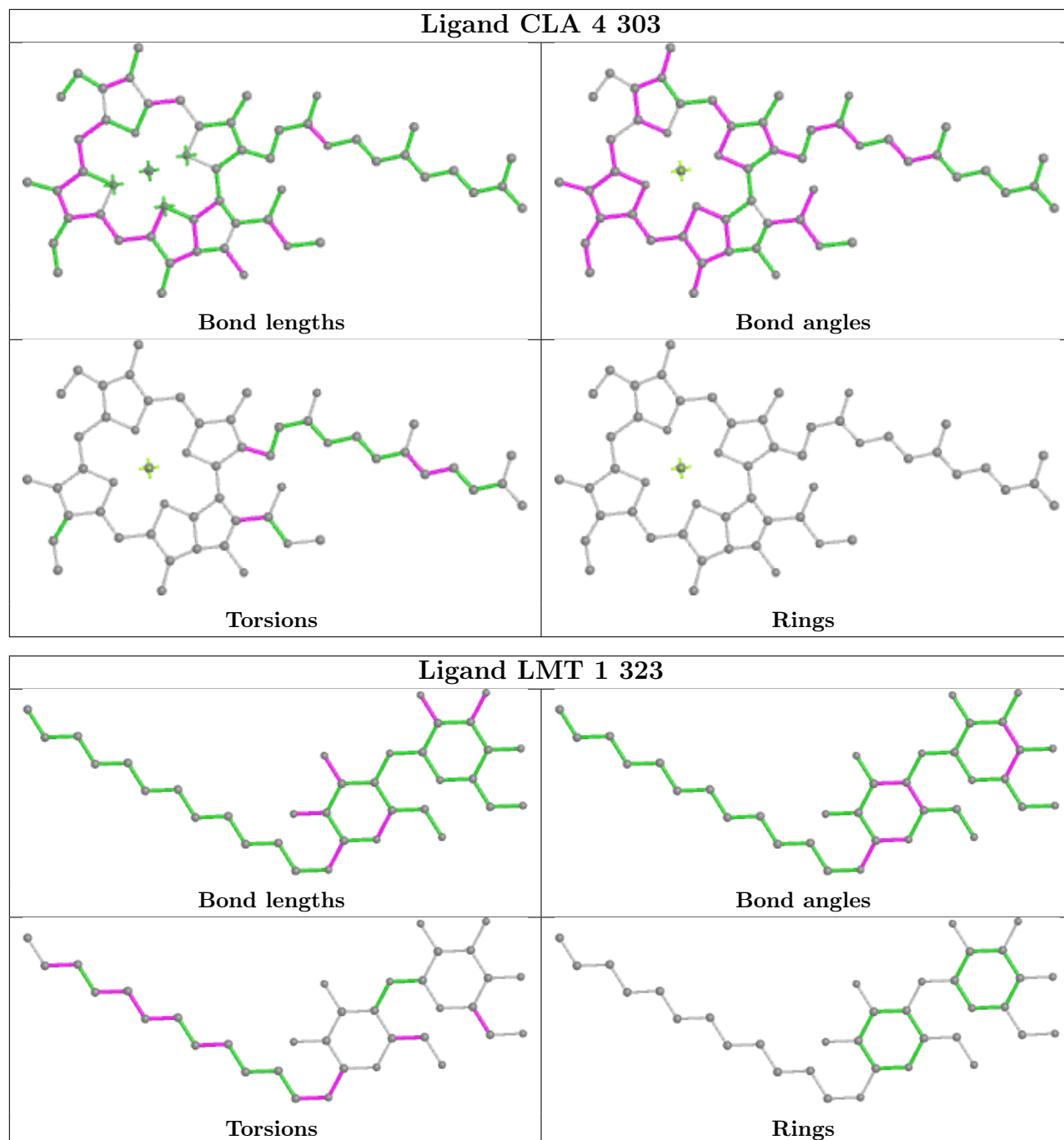


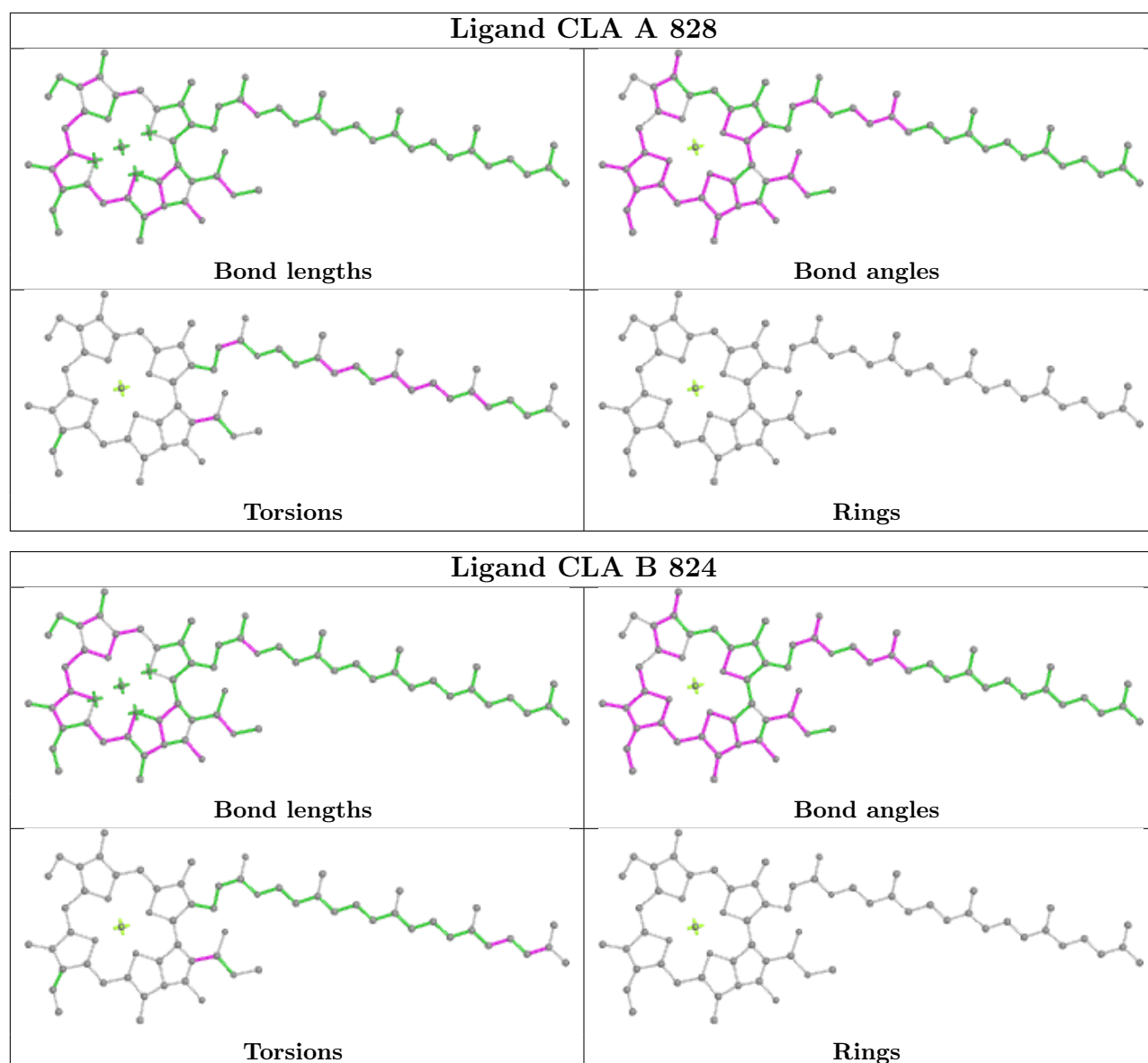












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

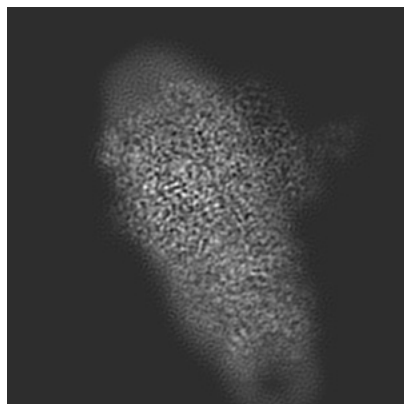
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38457. These allow visual inspection of the internal detail of the map and identification of artifacts.

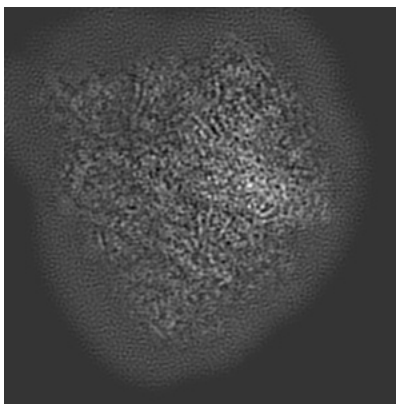
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

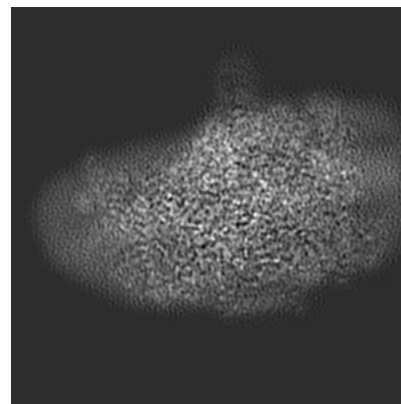
6.1.1 Primary map



X

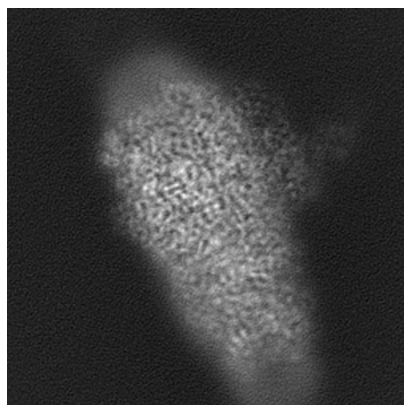


Y

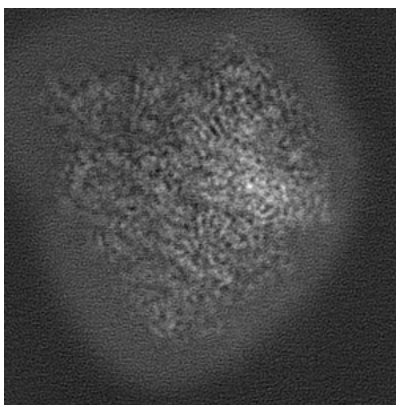


Z

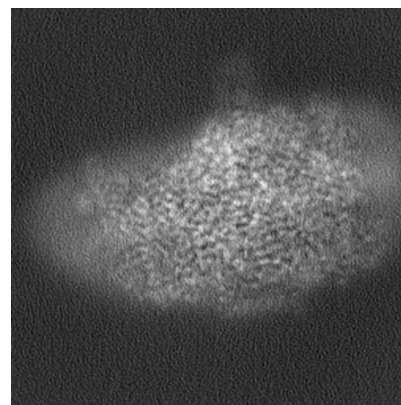
6.1.2 Raw map



X



Y

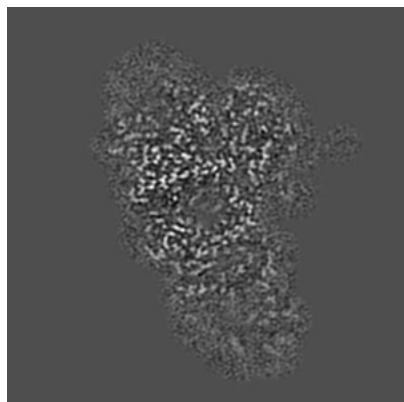


Z

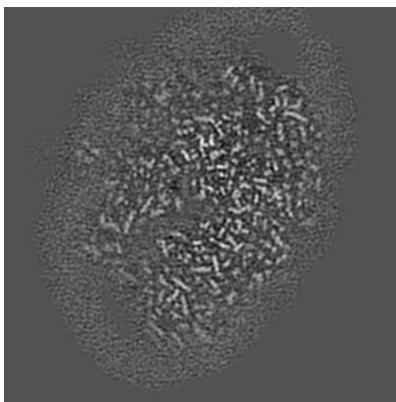
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

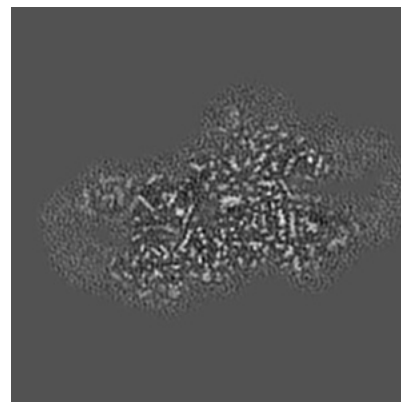
6.2.1 Primary map



X Index: 127

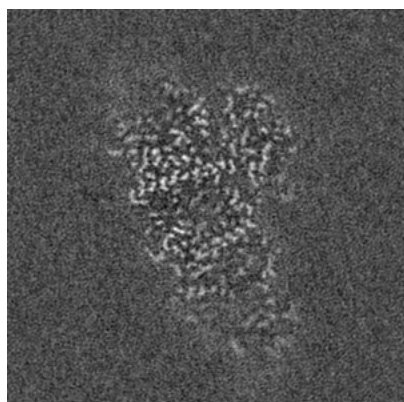


Y Index: 127

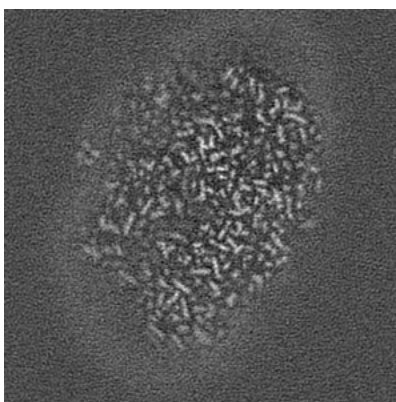


Z Index: 127

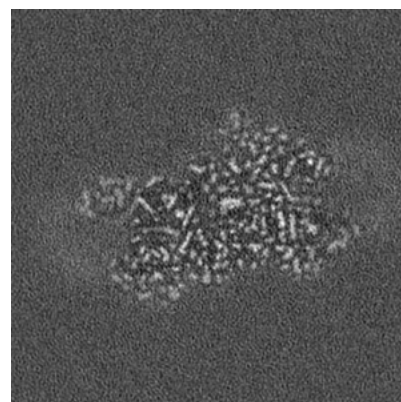
6.2.2 Raw map



X Index: 127



Y Index: 127

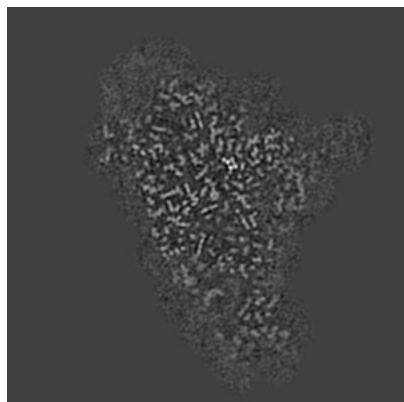


Z Index: 127

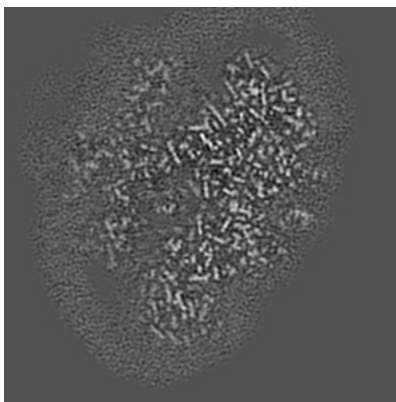
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

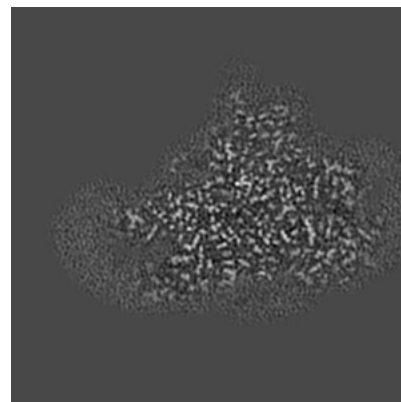
6.3.1 Primary map



X Index: 142

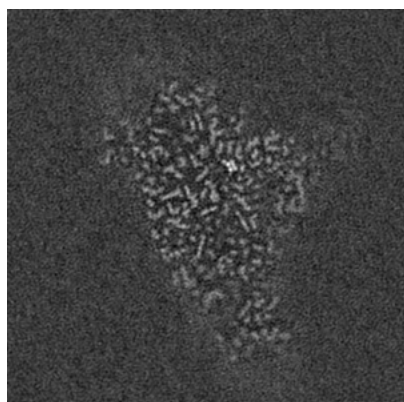


Y Index: 133

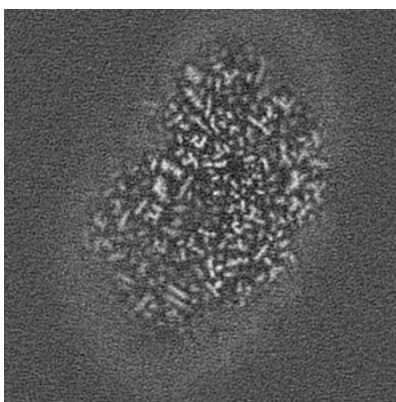


Z Index: 149

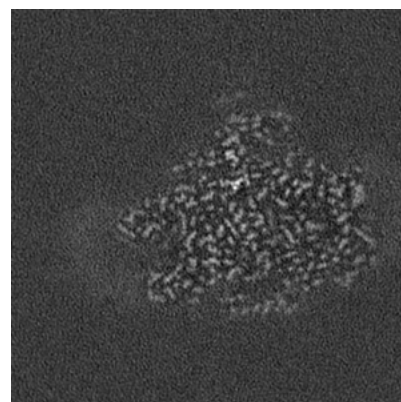
6.3.2 Raw map



X Index: 142



Y Index: 121

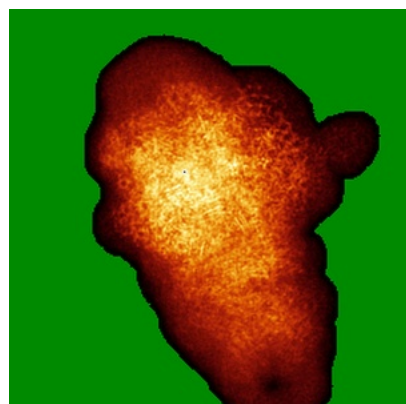


Z Index: 155

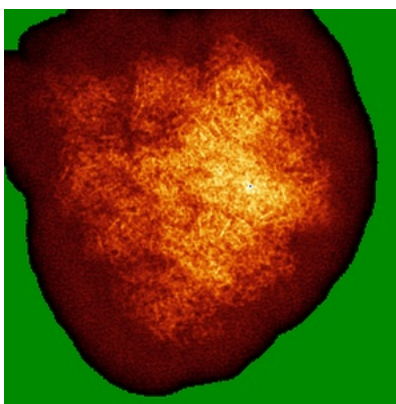
The images above show the largest variance slices of the map in three orthogonal directions.

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

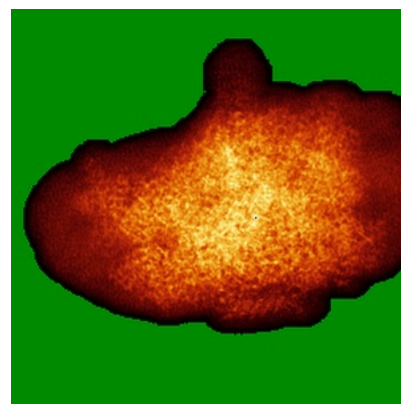
6.4.1 Primary map



X

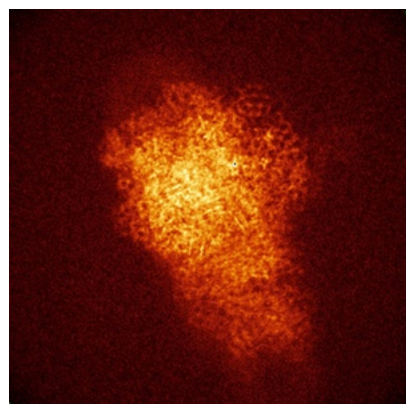


Y

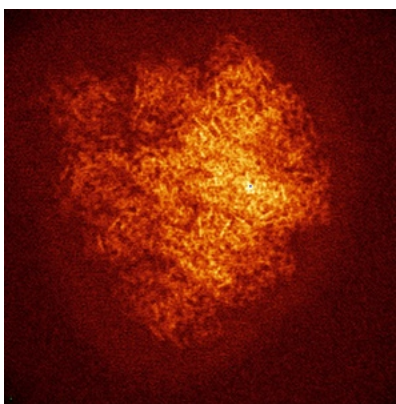


Z

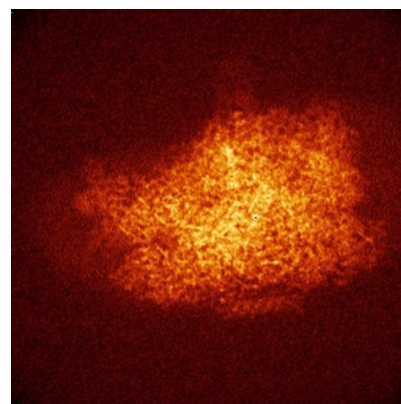
6.4.2 Raw map



X



Y

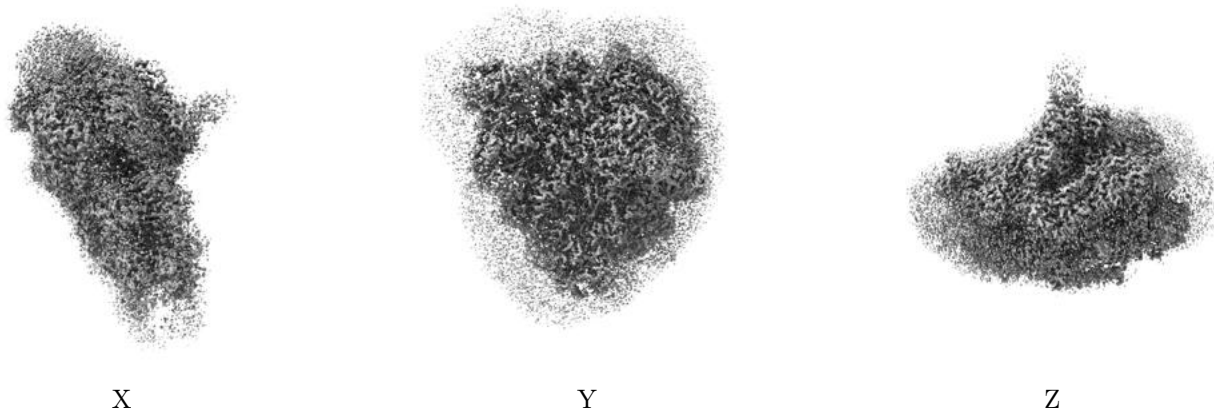


Z

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

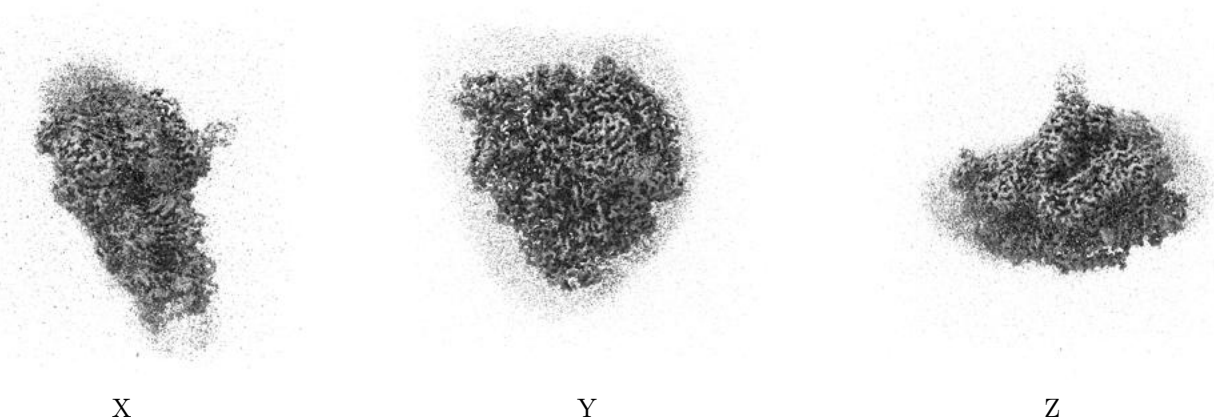
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

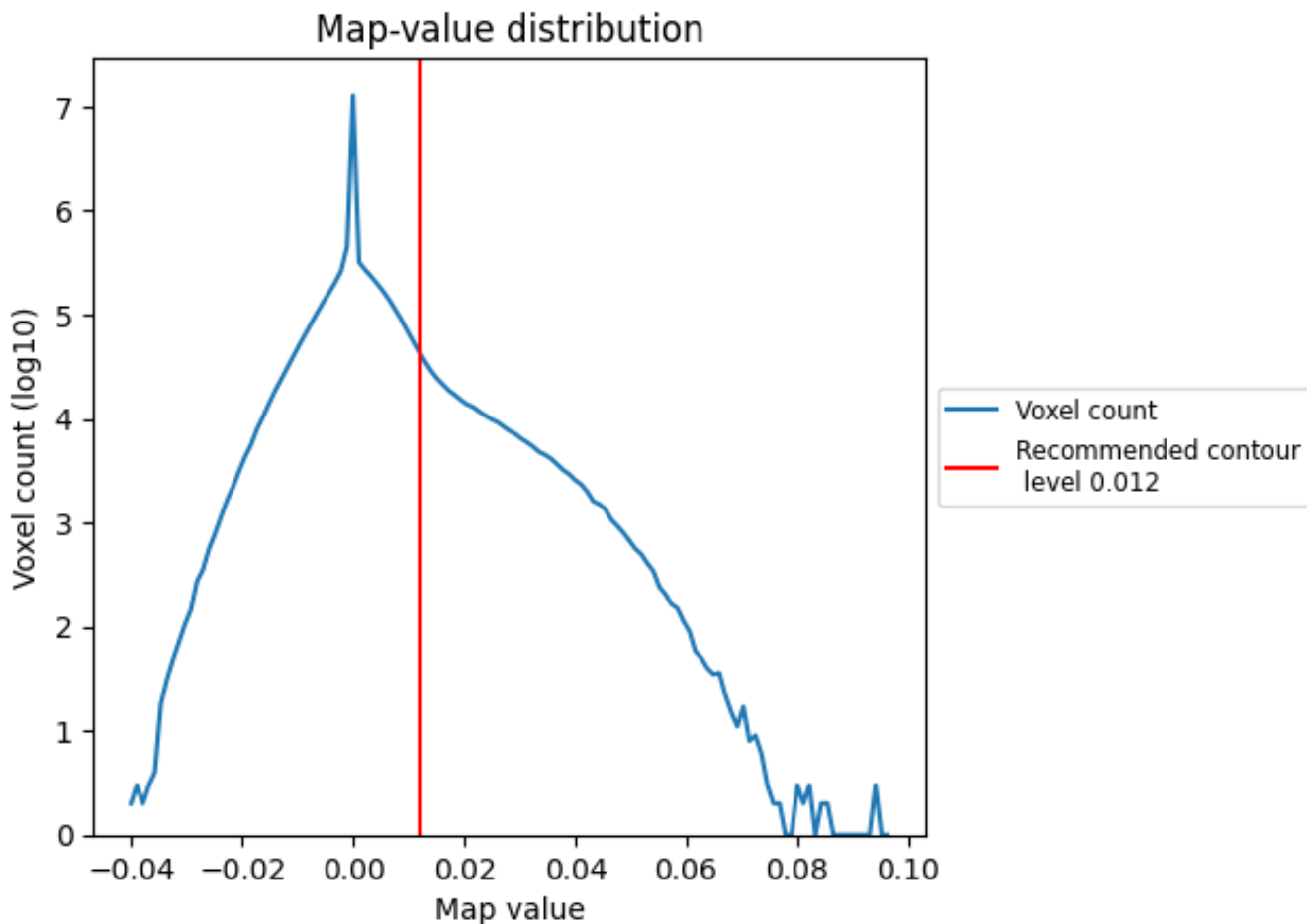
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

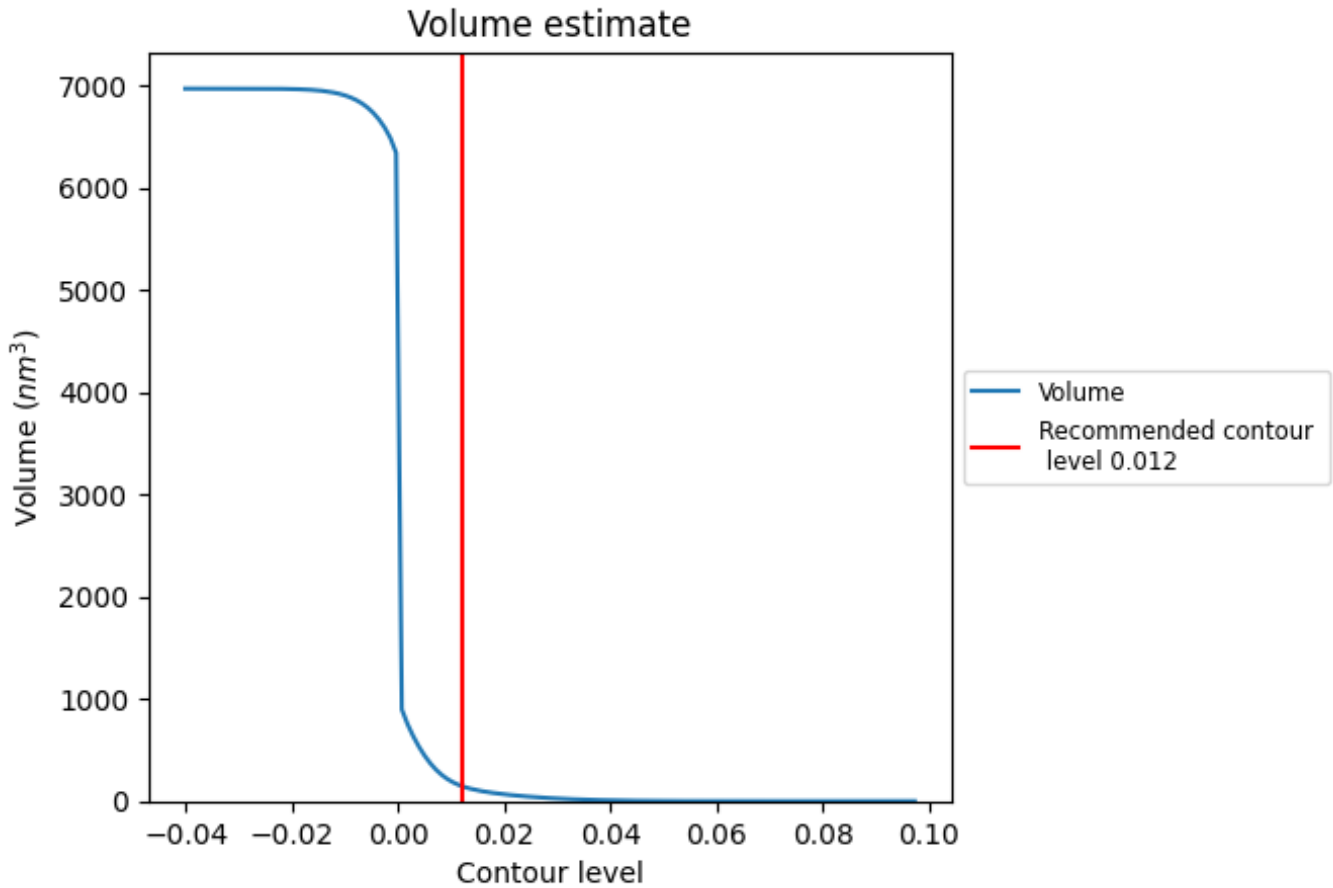
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

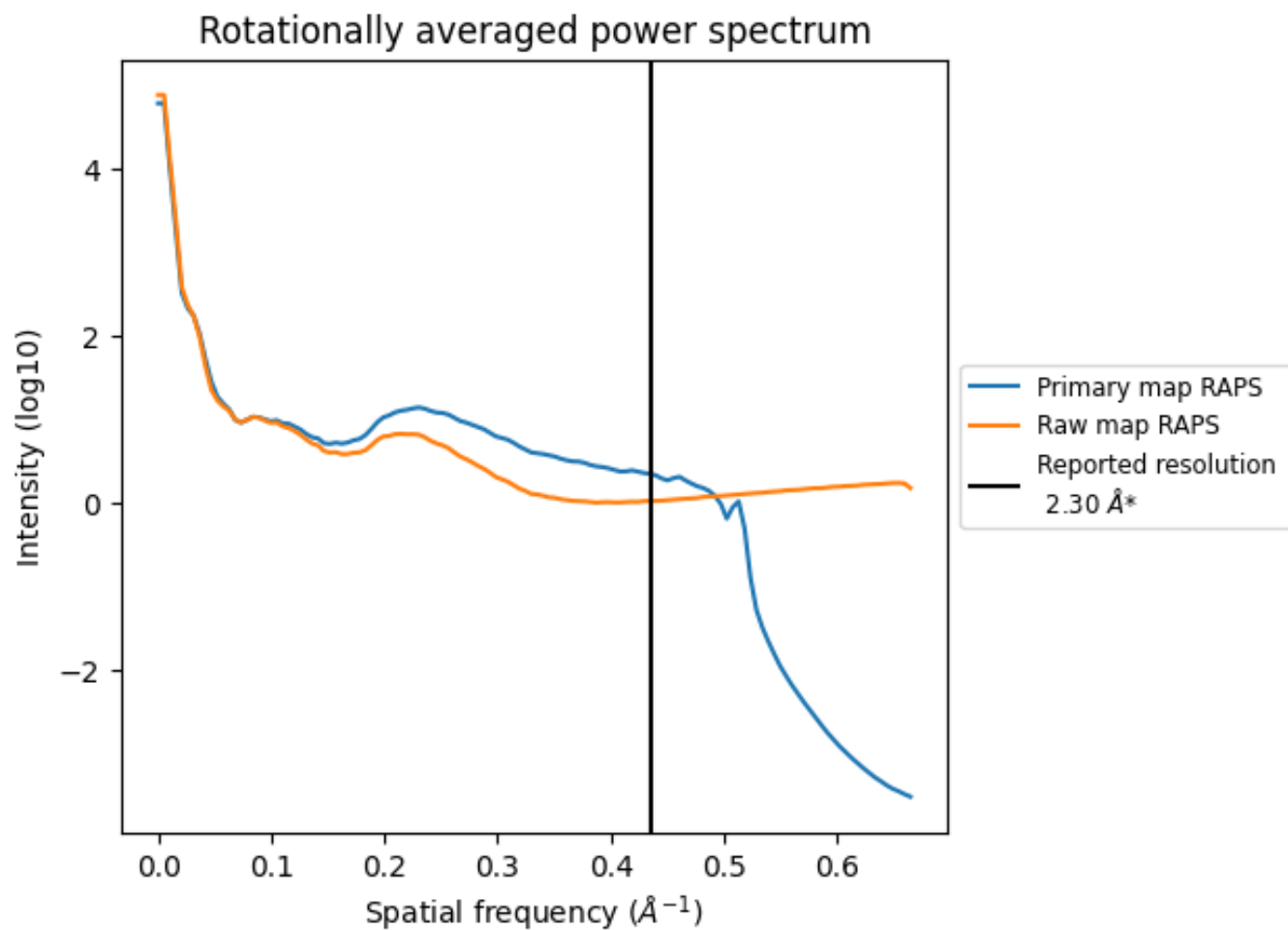
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 149 nm^3 ; this corresponds to an approximate mass of 134 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](#)

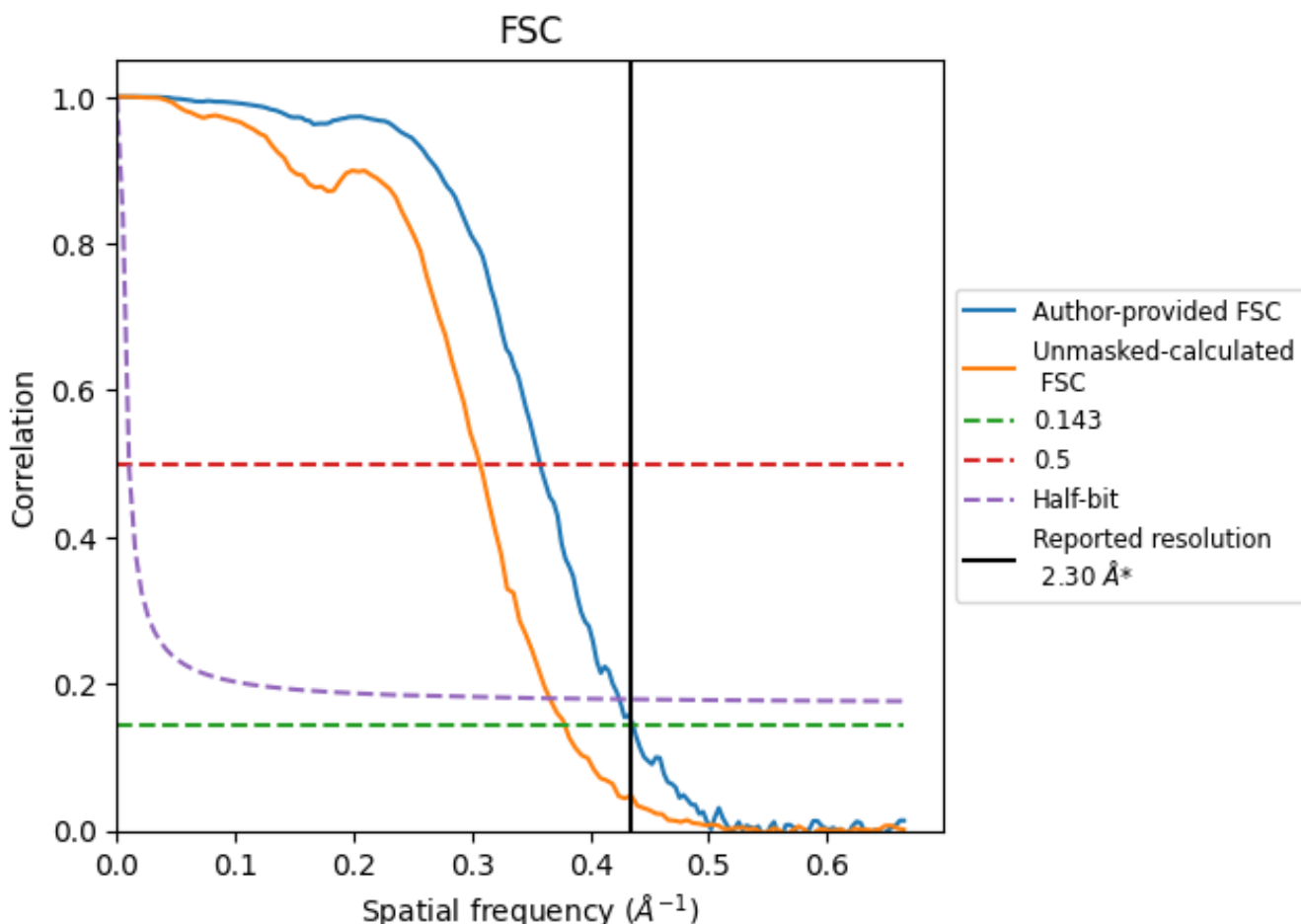


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.435 \AA^{-1}

8.2 Resolution estimates [i](#)

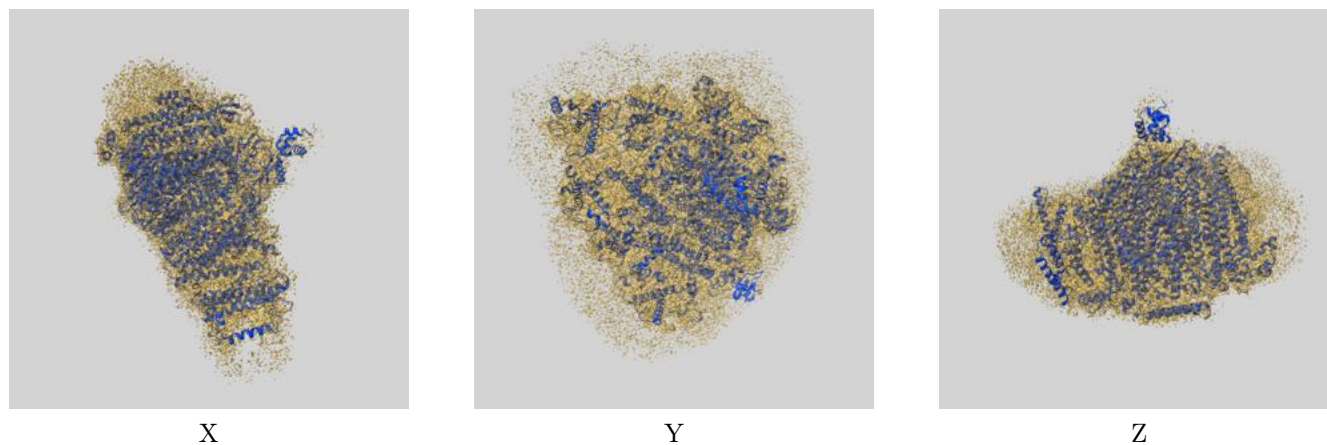
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.29	2.80	2.35
Unmasked-calculated*	2.64	3.26	2.73

*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 2.64 differs from the reported value 2.3 by more than 10 %

9 Map-model fit [i](#)

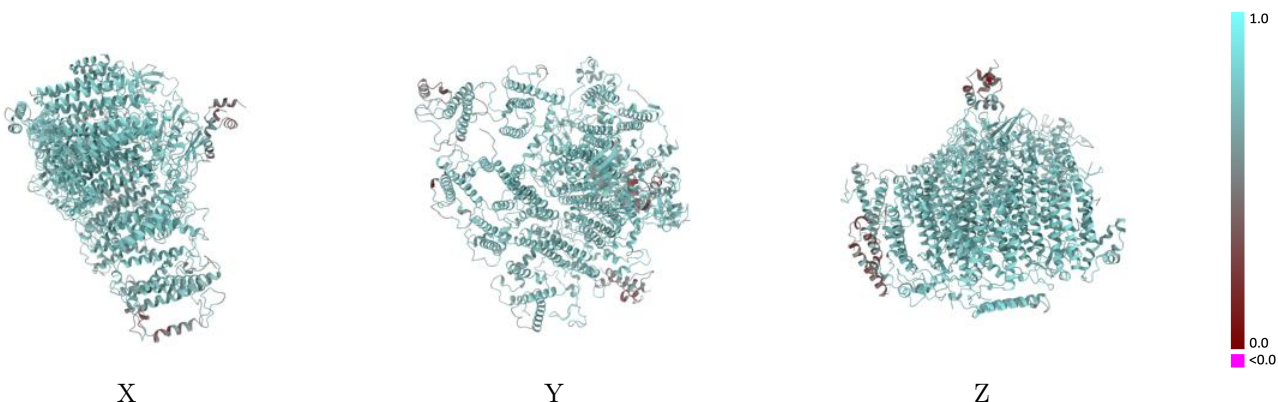
This section contains information regarding the fit between EMDB map EMD-38457 and PDB model 8XLS. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay [i](#)



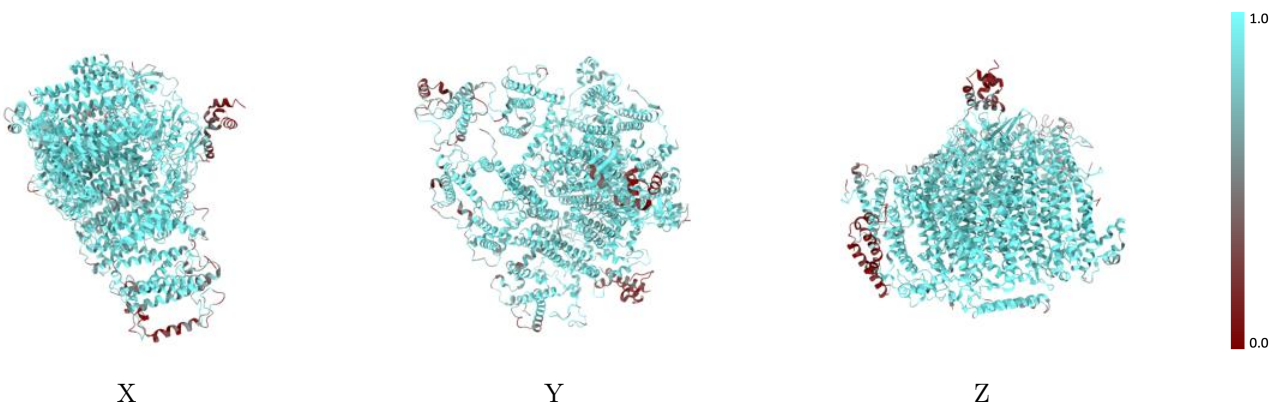
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



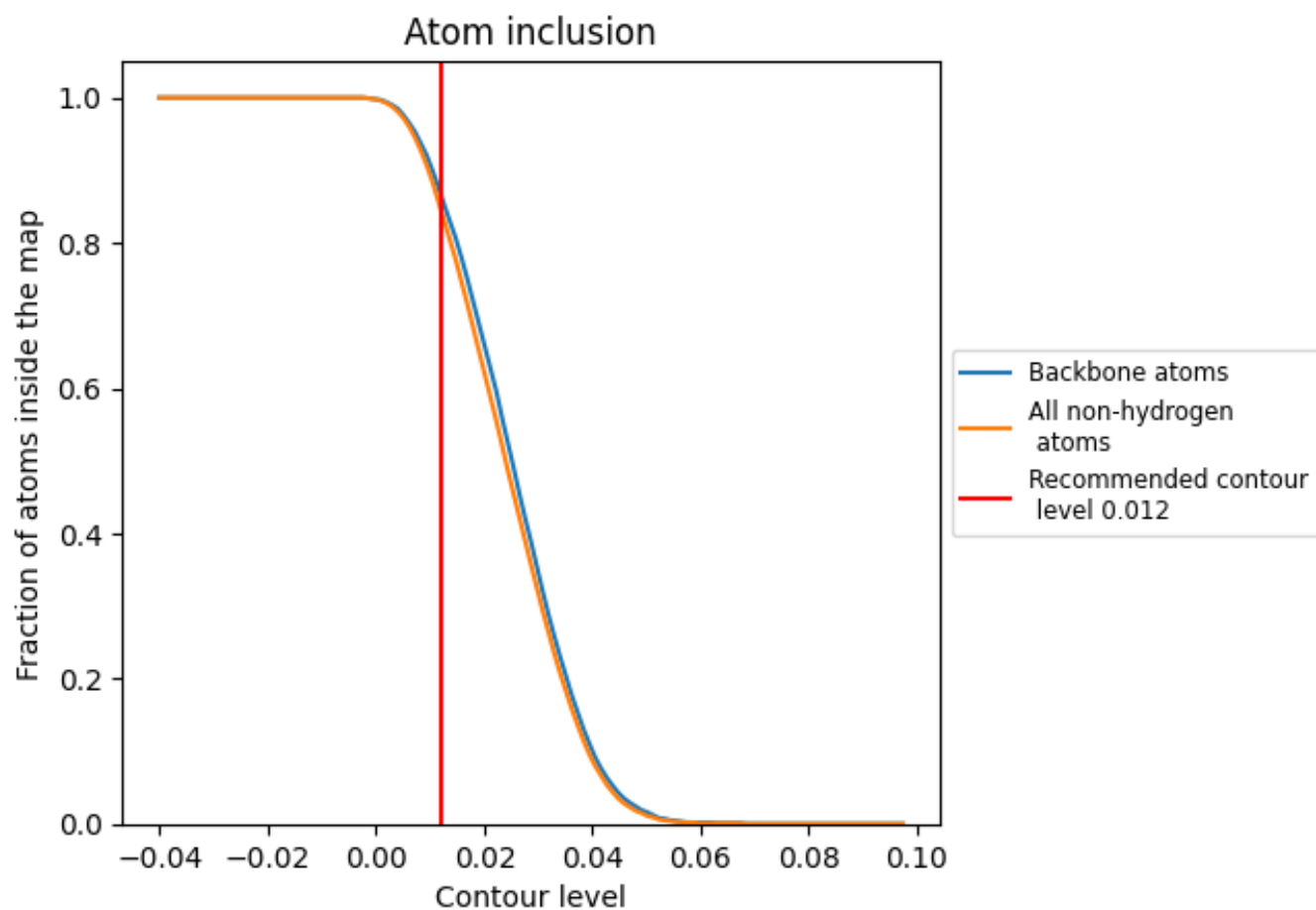
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 84% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8450	 0.7000
1	 0.7930	 0.6780
2	 0.7590	 0.6490
3	 0.7860	 0.6700
4	 0.5900	 0.5890
5	 0.7560	 0.6470
A	 0.9140	 0.7340
B	 0.9300	 0.7390
C	 0.9780	 0.7600
D	 0.9360	 0.7310
E	 0.8460	 0.7050
F	 0.8780	 0.7060
I	 0.9350	 0.7340
J	 0.9060	 0.7140
L	 0.9040	 0.7280
M	 0.8620	 0.7220
W	 0.5100	 0.5830
u	 0.2160	 0.4540

