



Full wwPDB EM Validation Report ⓘ

Apr 1, 2023 – 09:13 am BST

PDB ID : 7R3K
EMDB ID : EMD-14248
Title : Chlamydomonas reinhardtii TSP9 mutant small Photosystem I complex
Authors : Klaiman, D.; Schwartz, T.; Nelson, N.
Deposited on : 2022-02-07
Resolution : 2.52 Å(reported)
Based on initial model : 6JO5

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:

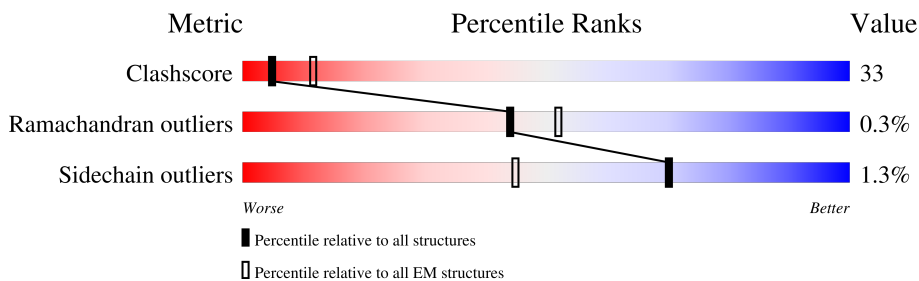
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.52 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	751	
2	B	735	
3	C	81	
4	D	196	
5	E	97	
6	F	227	
7	G	126	
8	I	106	

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Mol	Chain	Length	Quality of chain
9	J	41	
10	K	113	
11	1	228	
11	Z	228	
12	3	298	
13	7	241	
14	8	243	
15	4	264	
16	5	257	
17	6	257	

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	5006	X	-	-	-
19	CLA	1	5007	X	-	-	-
19	CLA	1	5008	X	-	-	-
19	CLA	1	5010	X	-	-	-
19	CLA	1	5011	X	-	-	-
19	CLA	1	5012	X	-	-	-
19	CLA	1	5013	X	-	-	-
19	CLA	1	5015	X	-	-	-
19	CLA	1	5016	X	-	X	-
19	CLA	1	5018	X	-	-	-
19	CLA	3	5008	X	-	-	-
19	CLA	3	5009	X	-	-	-
19	CLA	3	5010	X	-	-	-
19	CLA	3	5011	X	-	-	-
19	CLA	3	5012	X	-	-	-
19	CLA	3	5013	X	-	-	-
19	CLA	3	5014	X	-	-	-
19	CLA	3	5015	X	-	-	-
19	CLA	3	5016	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	3	5018	X	-	-	-
19	CLA	3	5019	X	-	-	-
19	CLA	3	5020	X	-	-	-
19	CLA	4	306	X	-	X	-
19	CLA	4	307	X	-	-	-
19	CLA	4	308	X	-	-	-
19	CLA	4	309	X	-	-	-
19	CLA	4	310	X	-	-	-
19	CLA	4	311	X	-	-	-
19	CLA	4	312	X	-	-	-
19	CLA	4	313	X	-	-	-
19	CLA	4	316	X	-	-	-
19	CLA	4	318	X	-	-	-
19	CLA	5	301	X	-	-	-
19	CLA	5	306	X	-	-	-
19	CLA	5	307	X	-	-	-
19	CLA	5	308	X	-	-	-
19	CLA	5	309	X	-	-	-
19	CLA	5	310	X	-	-	-
19	CLA	5	311	X	-	-	-
19	CLA	5	312	X	-	-	-
19	CLA	5	313	X	-	-	-
19	CLA	5	314	X	-	-	-
19	CLA	5	317	X	-	-	-
19	CLA	5	319	X	-	-	-
19	CLA	5	321	X	-	-	-
19	CLA	5	322	X	-	-	-
19	CLA	5	325	X	-	-	-
19	CLA	6	301	X	-	-	-
19	CLA	6	302	X	-	-	-
19	CLA	6	309	X	-	-	-
19	CLA	6	310	X	-	X	-
19	CLA	6	311	X	-	-	-
19	CLA	6	312	X	-	-	-
19	CLA	6	313	X	-	X	-
19	CLA	6	314	X	-	-	-
19	CLA	6	318	X	-	-	-
19	CLA	6	320	X	-	-	-
19	CLA	6	322	X	-	-	-
19	CLA	6	323	X	-	-	-
19	CLA	7	306	X	-	-	-
19	CLA	7	307	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	7	308	X	-	-	-
19	CLA	7	309	X	-	-	-
19	CLA	7	310	X	-	-	-
19	CLA	7	311	X	-	-	-
19	CLA	7	312	X	-	-	-
19	CLA	7	313	X	-	-	-
19	CLA	7	316	X	-	-	-
19	CLA	7	317	X	-	-	-
19	CLA	7	318	X	-	-	-
19	CLA	7	319	X	-	-	-
19	CLA	7	324	X	-	-	-
19	CLA	8	307	X	-	-	-
19	CLA	8	308	X	-	-	-
19	CLA	8	309	X	-	-	-
19	CLA	8	310	X	-	-	-
19	CLA	8	311	X	-	-	-
19	CLA	8	312	X	-	-	-
19	CLA	8	313	X	-	-	-
19	CLA	8	314	X	-	-	-
19	CLA	8	318	X	-	-	-
19	CLA	8	320	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	817	X	-	-	-
19	CLA	A	818	X	-	-	-
19	CLA	A	819	X	-	-	-
19	CLA	A	820	X	-	-	-
19	CLA	A	821	X	-	-	-
19	CLA	A	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	823	X	-	-	-
19	CLA	A	824	X	-	-	-
19	CLA	A	825	X	-	-	-
19	CLA	A	826	X	-	-	-
19	CLA	A	827	X	-	-	-
19	CLA	A	828	X	-	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	857	X	-	-	-
19	CLA	B	801	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	820	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	821	X	-	-	-
19	CLA	B	822	X	-	-	-
19	CLA	B	823	X	-	X	-
19	CLA	B	824	X	-	-	-
19	CLA	B	825	X	-	-	-
19	CLA	B	826	X	-	-	-
19	CLA	B	827	X	-	-	-
19	CLA	B	828	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	839	X	-	-	-
19	CLA	B	840	X	-	-	-
19	CLA	B	850	X	-	X	-
19	CLA	F	301	X	-	-	-
19	CLA	F	303	X	-	-	-
19	CLA	G	1601	X	-	-	-
19	CLA	G	1602	X	-	-	-
19	CLA	I	201	X	-	-	-
19	CLA	J	1901	X	-	-	-
19	CLA	K	202	X	-	-	-
19	CLA	K	203	X	-	-	-
19	CLA	K	204	X	-	-	-
19	CLA	K	205	X	-	-	-
19	CLA	Z	303	X	-	-	-
19	CLA	Z	304	X	-	-	-
19	CLA	Z	305	X	-	-	-
19	CLA	Z	306	X	-	-	-
19	CLA	Z	307	X	-	-	-
19	CLA	Z	308	X	-	-	-
19	CLA	Z	311	X	-	-	-
19	CLA	Z	312	X	-	-	-
19	CLA	Z	314	X	-	-	-
19	CLA	Z	315	X	-	-	-
21	SF4	A	845	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	SF4	C	102	-	-	X	-
22	BCR	3	5006	-	-	X	-
22	BCR	6	307	-	-	X	-
32	CHL	1	5009	X	-	-	-
32	CHL	1	5014	X	-	-	-
32	CHL	1	5017	X	-	-	-
32	CHL	3	5017	X	-	-	-
32	CHL	4	314	X	-	-	-
32	CHL	4	315	X	-	-	-
32	CHL	4	317	X	-	-	-
32	CHL	4	319	X	-	-	-
32	CHL	5	315	X	-	-	-
32	CHL	5	316	X	-	-	-
32	CHL	5	318	X	-	-	-
32	CHL	5	320	X	-	-	-
32	CHL	6	315	X	-	-	-
32	CHL	6	316	X	-	-	-
32	CHL	6	317	X	-	-	-
32	CHL	6	319	X	-	-	-
32	CHL	6	321	X	-	-	-
32	CHL	7	314	X	-	-	-
32	CHL	7	315	X	-	-	-
32	CHL	8	301	X	-	-	-
32	CHL	8	315	X	-	-	-
32	CHL	8	316	X	-	-	-
32	CHL	8	317	X	-	-	-
32	CHL	8	319	X	-	-	-
32	CHL	Z	302	X	-	-	-
32	CHL	Z	309	X	-	-	-
32	CHL	Z	310	X	-	-	-
32	CHL	Z	313	X	-	-	-
33	SPH	3	5001	-	-	X	-
38	ERG	6	326	-	-	X	-

2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 46504 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	740	5811	3799	991	999	22	0	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	733	5824	3825	977	1004	18	0	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	601	369	103	117	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	144	1135	725	201	202	7	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	63	496	316	87	93	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	165	1266	817	213	233	3	0	0

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	G	67	495	321	86	88	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	37	281	195	39	46	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	39	320	219	45	55	1	0	0

- Molecule 10 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	K	84	570	362	98	108	2	0	0

- Molecule 11 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	1	194	1445	941	240	261	3	0	0
11	Z	194	1445	941	240	261	3	0	0

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	3	219	1673	1092	270	303	8	0	0

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	7	213	1650	1072	274	298	6	0	0

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	8	217	1650	1073	280	293	4	0	0

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic (Lhca4).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	4	210	1628	1068	262	293	5	0	0

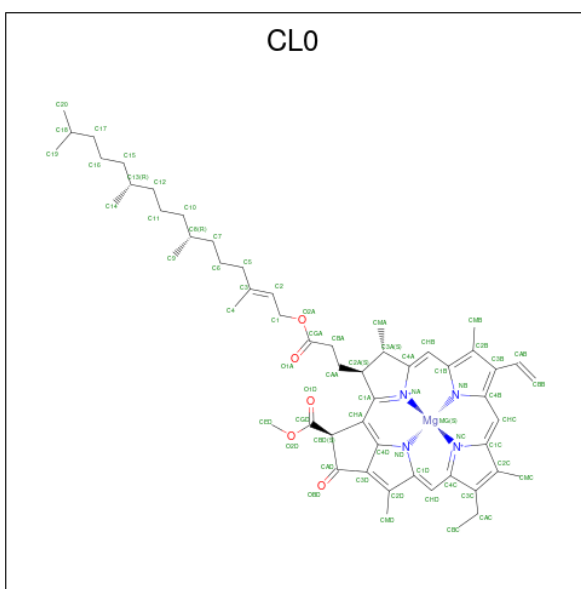
- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	5	227	1775	1154	297	316	8	0	0

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

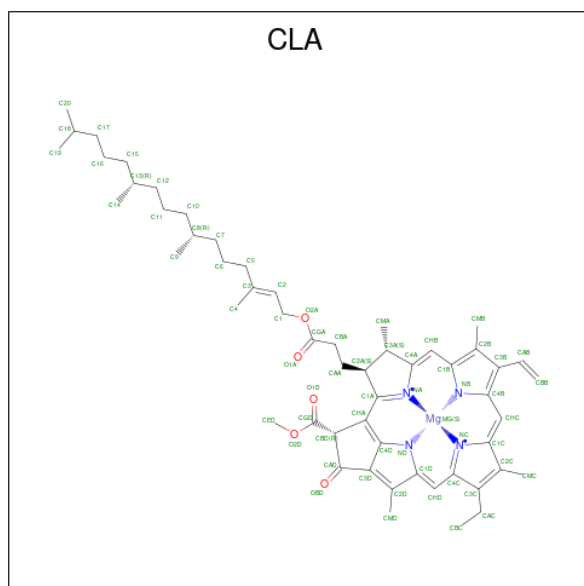
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	6	229	1766	1164	292	304	6	0	0

- 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
			Total	C	Mg	N	O	
19	A	1	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	55	45	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	51	41	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	56	46	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	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	61	51	1	4	5	0
19	A	1	60	50	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	60	50	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	55	45	1	4	5	0
19	A	1	57	47	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	A	1	50	40	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	65	55	1	4	5	0
19	A	1	65	55	1	4	5	0
19	A	1	55	45	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	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	52	42	1	4	5	0
19	A	1	52	42	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	65	55	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	55	45	1	4	5	0
19	B	1	52	42	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
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	60	50	1	4	5	0
19	B	1	57	47	1	4	5	0
19	B	1	65	55	1	4	5	0
19	B	1	59	49	1	4	5	0
19	B	1	60	50	1	4	5	0
19	B	1	65	55	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	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	65	55	1	4	5	0
19	B	1	60	50	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	50	40	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	58	48	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	60	50	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	52	42	1	4	5	0
19	B	1	46	36	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	65	55	1	4	5	0
19	F	1	45	35	1	4	5	0
19	G	1	50	40	1	4	5	0
19	G	1	46	36	1	4	5	0
19	I	1	55	45	1	4	5	0
19	J	1	42	34	1	4	3	0
19	K	1	46	36	1	4	5	0
19	K	1	55	45	1	4	5	0
19	K	1	49	39	1	4	5	0
19	K	1	45	35	1	4	5	0
19	1	1	65	55	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	55	45	1	4	5	0
19	1	1	55	45	1	4	5	0
19	1	1	60	50	1	4	5	0
19	1	1	48	38	1	4	5	0
19	1	1	50	40	1	4	5	0
19	1	1	60	50	1	4	5	0
19	1	1	51	41	1	4	5	0
19	Z	1	46	36	1	4	5	0
19	Z	1	50	40	1	4	5	0
19	Z	1	65	55	1	4	5	0
19	Z	1	50	40	1	4	5	0
19	Z	1	57	47	1	4	5	0
19	Z	1	65	55	1	4	5	0
19	Z	1	55	45	1	4	5	0
19	Z	1	65	55	1	4	5	0
19	Z	1	46	36	1	4	5	0
19	Z	1	65	55	1	4	5	0
19	3	1	65	55	1	4	5	0
19	3	1	46	36	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	3	1	65	55	1	4	5	0
19	3	1	60	50	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	60	50	1	4	5	0
19	3	1	45	35	1	4	5	0
19	3	1	60	50	1	4	5	0
19	3	1	60	50	1	4	5	0
19	3	1	55	45	1	4	5	0
19	3	1	46	36	1	4	5	0
19	7	1	60	50	1	4	5	0
19	7	1	50	40	1	4	5	0
19	7	1	65	55	1	4	5	0
19	7	1	65	55	1	4	5	0
19	7	1	61	51	1	4	5	0
19	7	1	56	46	1	4	5	0
19	7	1	65	55	1	4	5	0
19	7	1	43	35	1	4	3	0
19	7	1	50	40	1	4	5	0
19	7	1	50	40	1	4	5	0
19	7	1	42	34	1	4	3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	7	1	58	48	1	4	5	0
19	7	1	55	45	1	4	5	0
19	8	1	60	50	1	4	5	0
19	8	1	65	55	1	4	5	0
19	8	1	65	55	1	4	5	0
19	8	1	62	52	1	4	5	0
19	8	1	65	55	1	4	5	0
19	8	1	60	50	1	4	5	0
19	8	1	55	45	1	4	5	0
19	8	1	55	45	1	4	5	0
19	8	1	46	36	1	4	5	0
19	8	1	46	36	1	4	5	0
19	4	1	60	50	1	4	5	0
19	4	1	52	42	1	4	5	0
19	4	1	65	55	1	4	5	0
19	4	1	60	50	1	4	5	0
19	4	1	65	55	1	4	5	0
19	4	1	50	40	1	4	5	0
19	4	1	55	45	1	4	5	0
19	4	1	55	45	1	4	5	0
19	4	1	50	40	1	4	5	0

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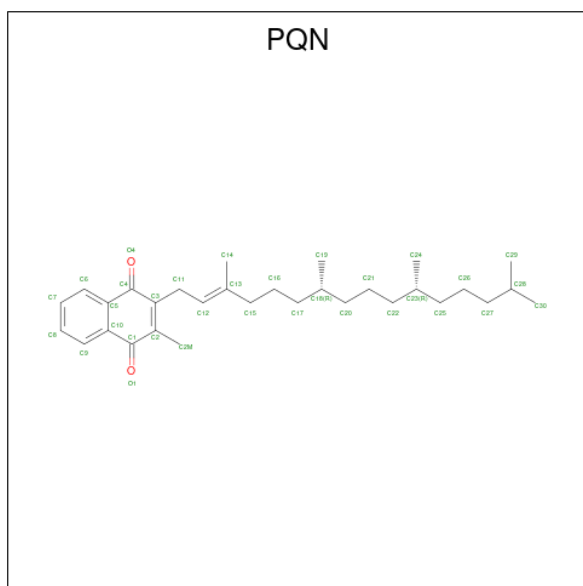
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
19	4	1	41	33	1	4	3	0
19	5	1	56	46	1	4	5	0
19	5	1	60	50	1	4	5	0
19	5	1	61	51	1	4	5	0
19	5	1	56	46	1	4	5	0
19	5	1	65	55	1	4	5	0
19	5	1	55	45	1	4	5	0
19	5	1	50	40	1	4	5	0
19	5	1	61	51	1	4	5	0
19	5	1	45	35	1	4	5	0
19	5	1	65	55	1	4	5	0
19	5	1	65	55	1	4	5	0
19	5	1	50	40	1	4	5	0
19	5	1	65	55	1	4	5	0
19	5	1	46	36	1	4	5	0
19	5	1	55	45	1	4	5	0
19	6	1	60	50	1	4	5	0
19	6	1	60	50	1	4	5	0
19	6	1	60	50	1	4	5	0
19	6	1	52	42	1	4	5	0
19	6	1	65	55	1	4	5	0

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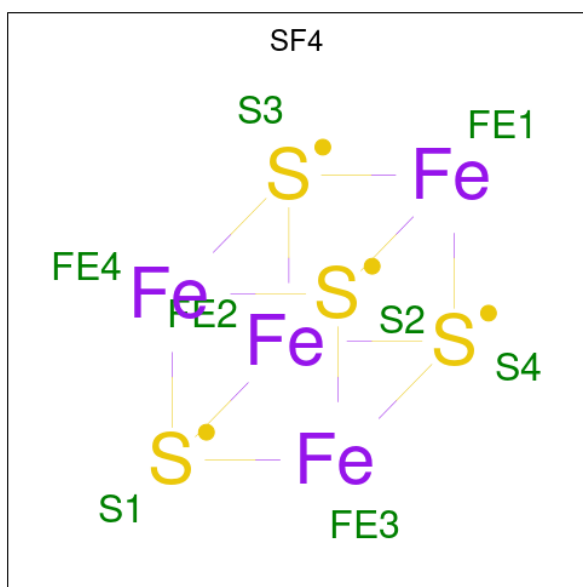
Mol	Chain	Residues	Atoms					AltConf
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 20 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



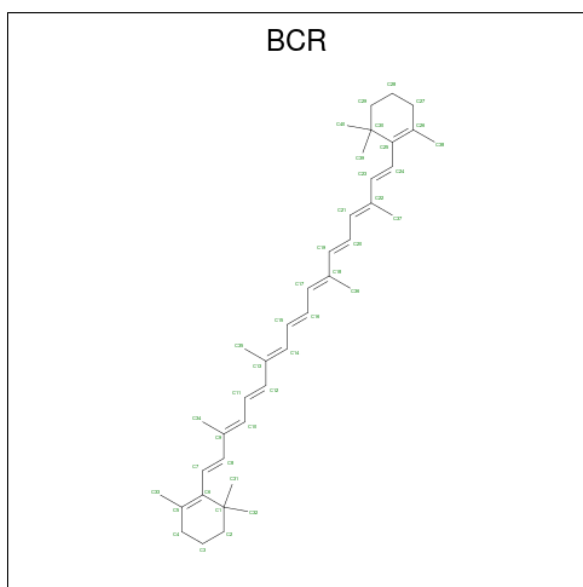
Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			33	31	2	
20	B	1	Total	C	O	0
			33	31	2	

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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	
21	C	1	Total	Fe S	0
			8	4 4	

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



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

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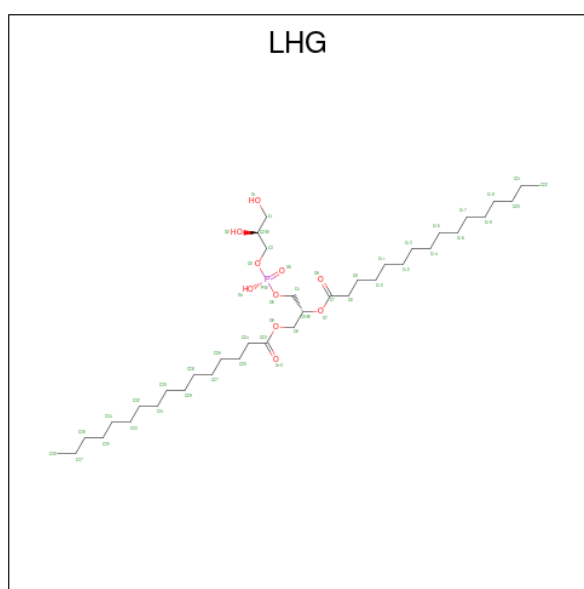
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	G	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	7	1	Total C 40 40	0
22	8	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
22	8	1	Total C 40 40	0
22	4	1	Total C 40 40	0
22	5	1	Total C 40 40	0
22	5	1	Total C 40 40	0
22	6	1	Total C 40 40	0
22	6	1	Total C 40 40	0

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



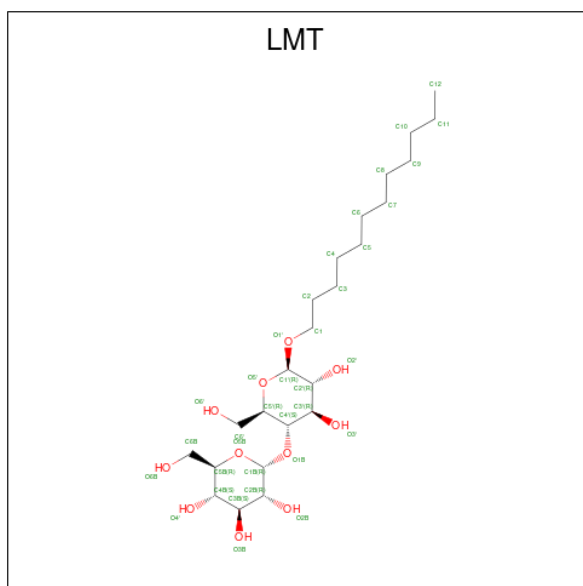
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C O P 35 24 10 1	0
23	A	1	Total C O P 49 38 10 1	0
23	1	1	Total C O P 23 12 10 1	0
23	1	1	Total C O P 43 32 10 1	0
23	Z	1	Total C O P 43 32 10 1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
23	3	1	Total 20	C 9	O 10	P 1	0
23	7	1	Total 37	C 26	O 10	P 1	0
23	8	1	Total 38	C 27	O 10	P 1	0
23	4	1	Total 49	C 38	O 10	P 1	0
23	5	1	Total 37	C 26	O 10	P 1	0
23	6	1	Total 32	C 21	O 10	P 1	0
23	6	1	Total 49	C 38	O 10	P 1	0

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



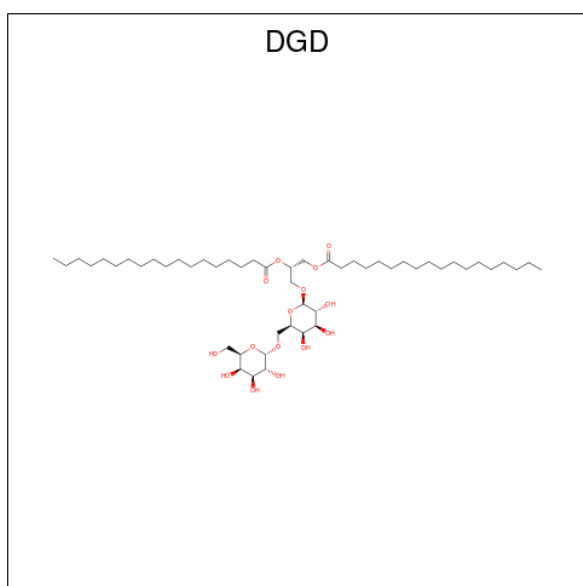
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	A	1	Total 35	C 24	O 11	0
24	A	1	Total 35	C 24	O 11	0
24	A	1	Total 35	C 24	O 11	0
24	A	1	Total 35	C 24	O 11	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
24	F	1	Total 35	C 24	O 11	0
24	G	1	Total 35	C 24	O 11	0
24	1	1	Total 35	C 24	O 11	0
24	Z	1	Total 35	C 24	O 11	0
24	Z	1	Total 35	C 24	O 11	0
24	3	1	Total 35	C 24	O 11	0
24	7	1	Total 35	C 24	O 11	0
24	8	1	Total 35	C 24	O 11	0
24	8	1	Total 35	C 24	O 11	0
24	4	1	Total 35	C 24	O 11	0
24	4	1	Total 35	C 24	O 11	0
24	4	1	Total 35	C 24	O 11	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

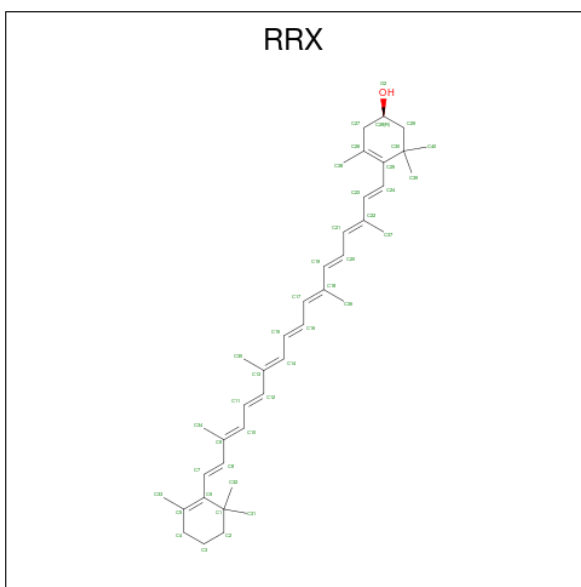


Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	C	O	0
			66	51	15	

- Molecule 26 is CALCIUM ION (three-letter code: CA) (formula: Ca).

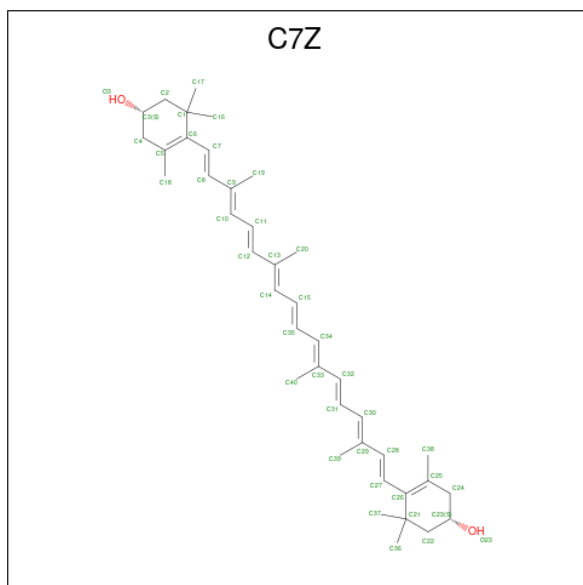
Mol	Chain	Residues	Atoms		AltConf
26	B	1	Total	Ca	0
			1	1	

- Molecule 27 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C₄₀H₅₆O).



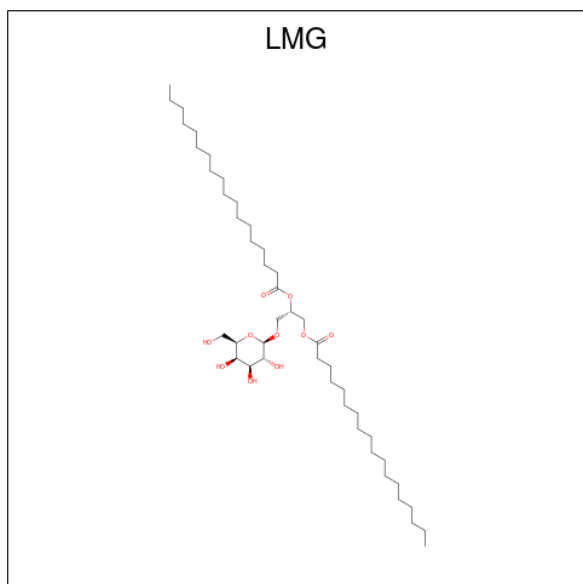
Mol	Chain	Residues	Atoms			AltConf
27	F	1	Total	C	O	0
			41	40	1	
27	4	1	Total	C	O	0
			41	40	1	
27	5	1	Total	C	O	0
			41	40	1	

- Molecule 28 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: C₄₀H₅₆O₂).



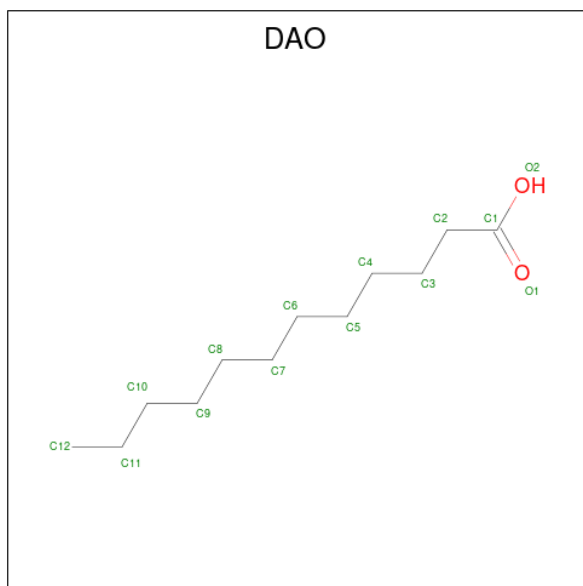
Mol	Chain	Residues	Atoms			AltConf
28	J	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	6	1	Total	C	O	0
			42	40	2	

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



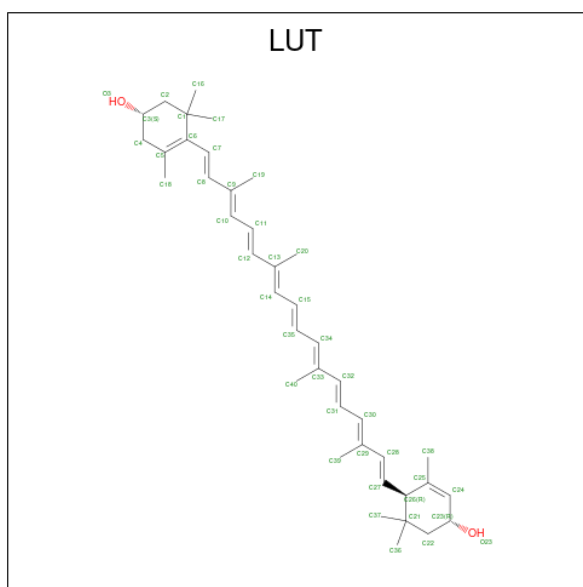
Mol	Chain	Residues	Atoms			AltConf
29	J	1	Total	C	O	0
			35	25	10	
29	J	1	Total	C	O	0
			45	35	10	
29	7	1	Total	C	O	0
			29	19	10	

- Molecule 30 is LAURIC ACID (three-letter code: DAO) (formula: C₁₂H₂₄O₂).



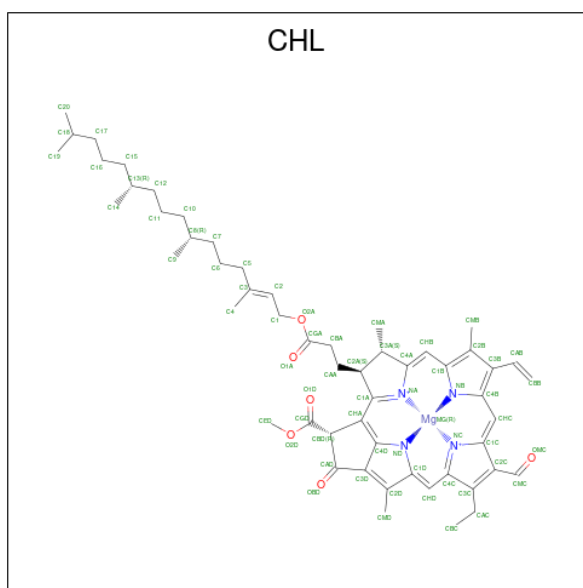
Mol	Chain	Residues	Atoms			AltConf
30	K	1	Total	C	O	0
			14	12	2	

- Molecule 31 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
31	1	1	Total	C	O	0
			42	40	2	
31	1	1	Total	C	O	0
			42	40	2	
31	Z	1	Total	C	O	0
			42	40	2	
31	Z	1	Total	C	O	0
			42	40	2	
31	3	1	Total	C	O	0
			42	40	2	
31	3	1	Total	C	O	0
			42	40	2	
31	7	1	Total	C	O	0
			42	40	2	
31	7	1	Total	C	O	0
			42	40	2	
31	8	1	Total	C	O	0
			42	40	2	
31	8	1	Total	C	O	0
			42	40	2	
31	4	1	Total	C	O	0
			42	40	2	
31	5	1	Total	C	O	0
			42	40	2	
31	6	1	Total	C	O	0
			42	40	2	
31	6	1	Total	C	O	0
			42	40	2	

- Molecule 32 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



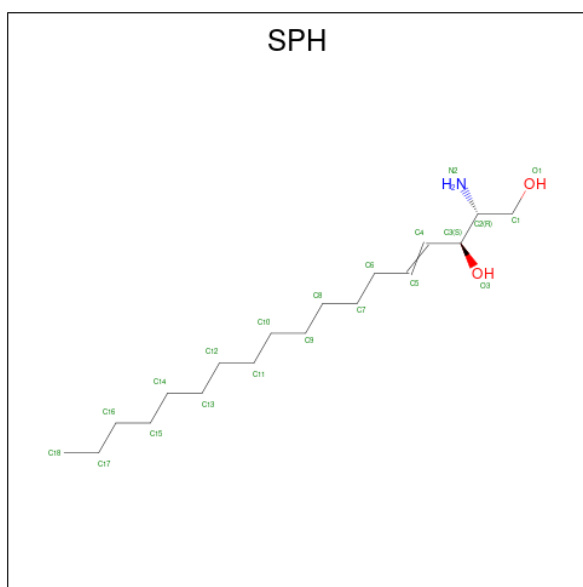
Mol	Chain	Residues	Atoms				AltConf	
32	1	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
32	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
32	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
32	Z	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
32	Z	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
32	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	Z	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
32	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	7	1	Total	C	Mg	N	O	0
			54	43	1	4	6	
32	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
32	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	8	1	Total	C	Mg	N	O	0
			57	46	1	4	6	

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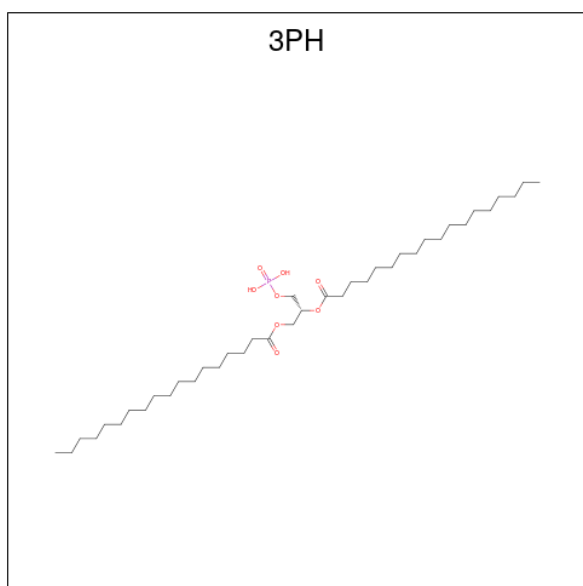
Mol	Chain	Residues	Atoms				AltConf	
32	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
32	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
32	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
32	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 33 is SPHINGOSINE (three-letter code: SPH) (formula: C₁₈H₃₇NO₂).



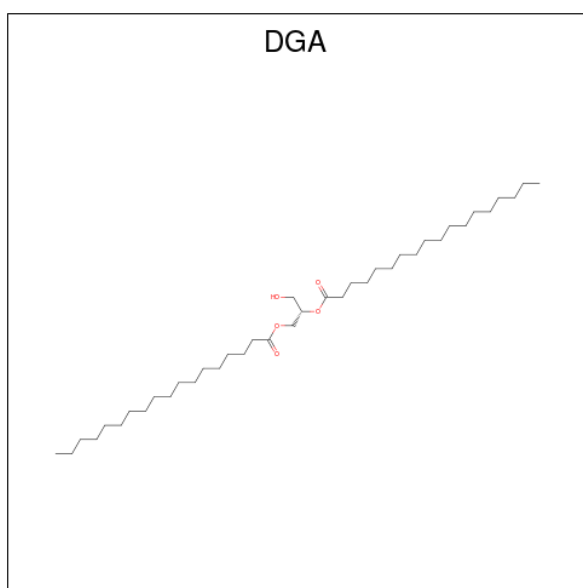
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
33	3	1	21	18	1	2	0
33	7	1	21	18	1	2	0
33	4	1	21	18	1	2	0

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



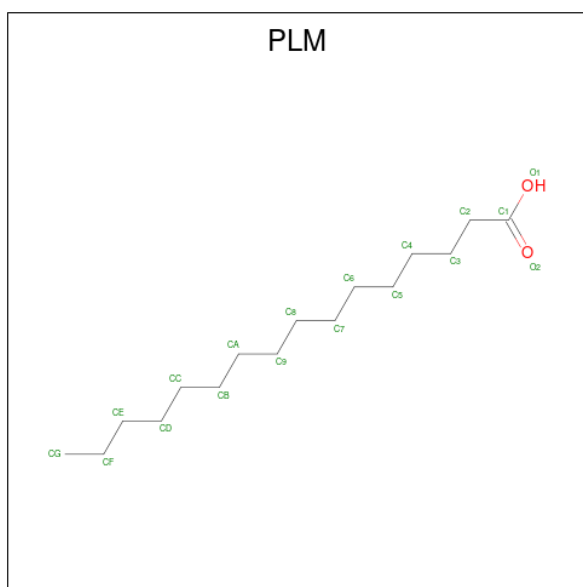
Mol	Chain	Residues	Atoms				AltConf
34	3	1	Total	C	O	P	0
			39	30	8	1	
34	8	1	Total	C	O	P	0
			30	21	8	1	
34	5	1	Total	C	O	P	0
			23	14	8	1	
34	6	1	Total	C	O	P	0
			29	20	8	1	

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



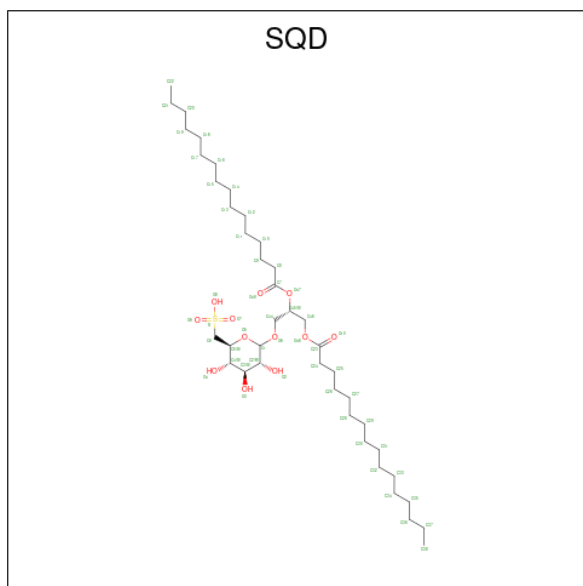
Mol	Chain	Residues	Atoms			AltConf
35	7	1	Total	C	O	0
			34	29	5	

- Molecule 36 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



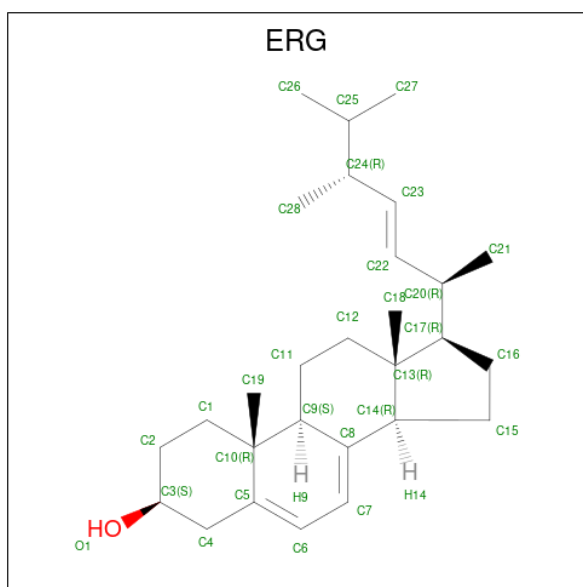
Mol	Chain	Residues	Atoms			AltConf
36	7	1	Total	C	O	0
			18	16	2	

- Molecule 37 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
37	8	1	Total	C	O	S	0
			48	35	12	1	

- Molecule 38 is ERGOSTEROL (three-letter code: ERG) (formula: $C_{28}H_{44}O$).



Mol	Chain	Residues	Atoms		AltConf
38	8	1	Total	C O	0
			29	28 1	
38	6	1	Total	C O	0
			29	28 1	

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	A	130	Total	O	0
			130	130	
39	B	113	Total	O	0
			113	113	
39	C	35	Total	O	0
			35	35	
39	D	28	Total	O	0
			28	28	
39	E	18	Total	O	0
			18	18	
39	F	29	Total	O	0
			29	29	
39	G	3	Total	O	0
			3	3	
39	J	8	Total	O	0
			8	8	
39	K	4	Total	O	0
			4	4	
39	1	27	Total	O	0
			27	27	

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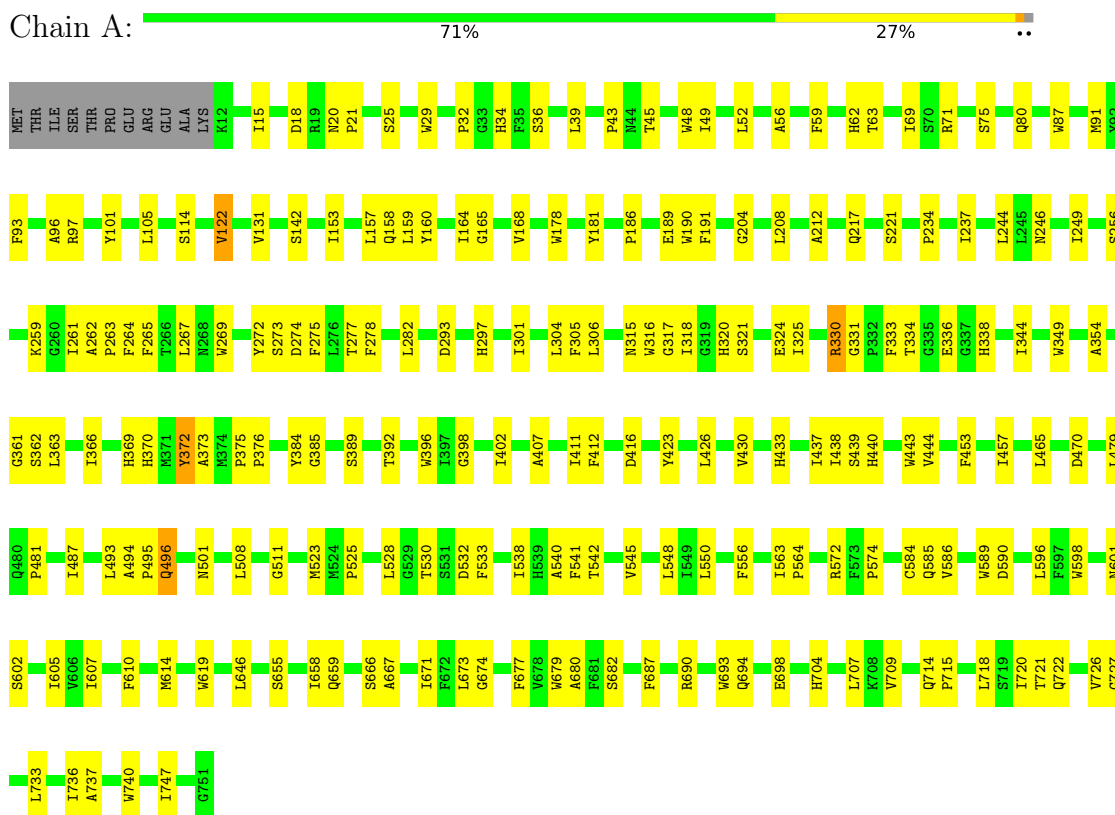
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Mol	Chain	Residues	Atoms		AltConf
39	Z	13	Total 13	O 13	0
39	3	31	Total 31	O 31	0
39	7	36	Total 36	O 36	0
39	8	31	Total 31	O 31	0
39	4	24	Total 24	O 24	0
39	5	18	Total 18	O 18	0
39	6	22	Total 22	O 22	0

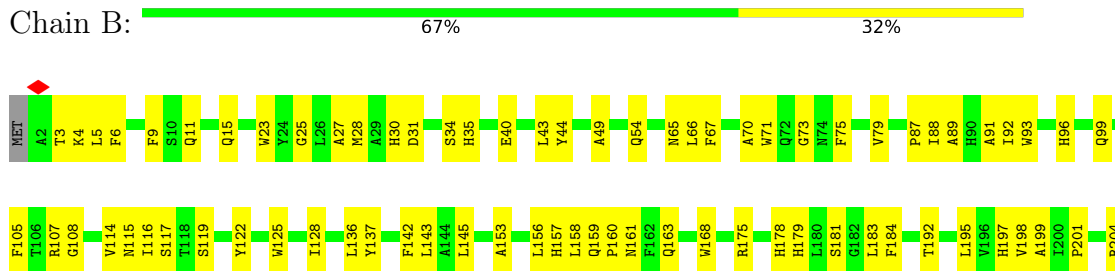
3 Residue-property plots [i](#)

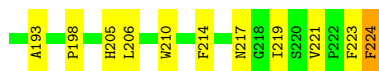
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



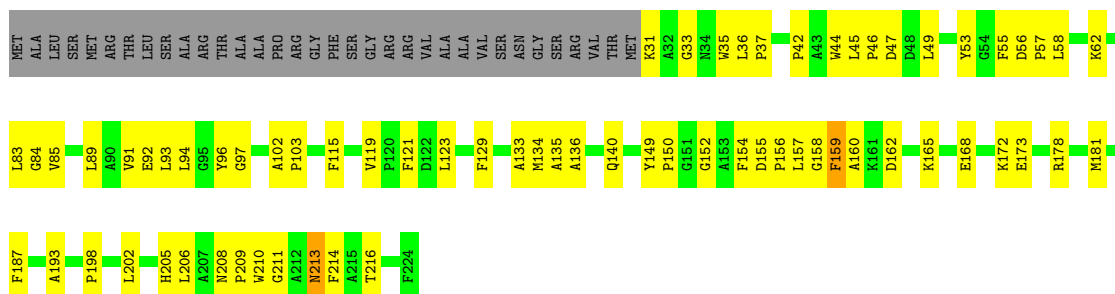
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





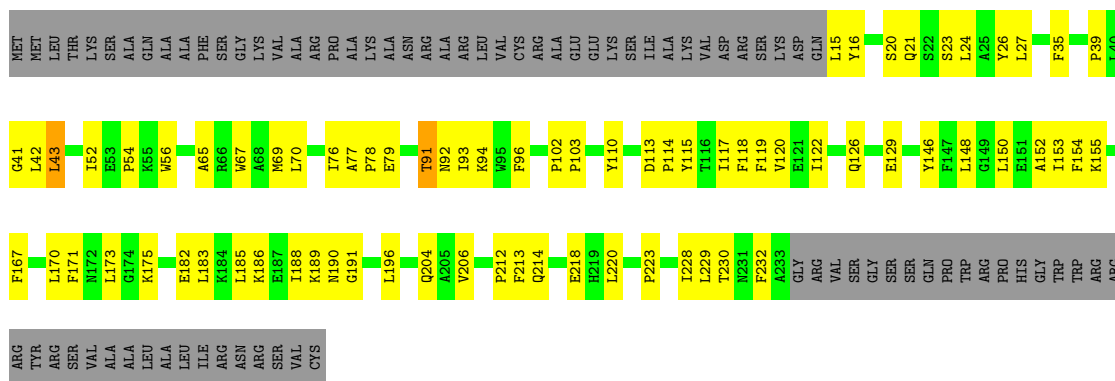
- Molecule 11: Chlorophyll a-b binding protein, chloroplastic

Chain Z: 55% 29% 15%



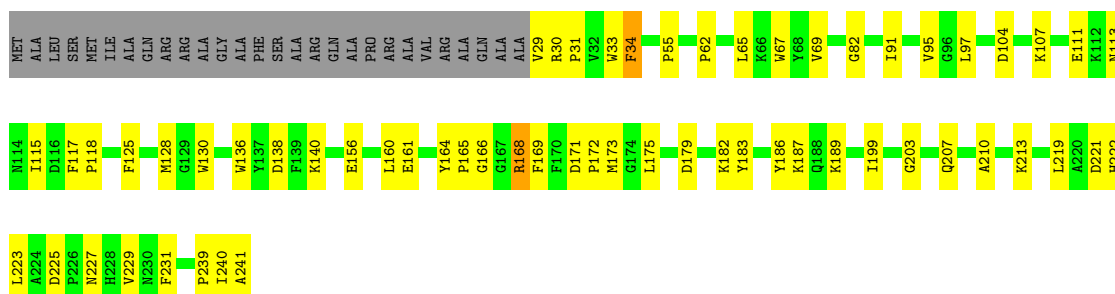
- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain 3: 48% 24% 27%



- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 7: 63% 24% 12%



- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 8: 68% 21% 11%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	173187	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	57.74	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	9000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (\AA)	327.59998, 327.59998, 327.59998	wwPDB
Map dimensions	390, 390, 390	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8399999, 0.8399999, 0.8399999	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: SF4, 3PH, DAO, LMT, SNC, RRX, ERG, PLM, CA, SQD, LMG, LUT, DGD, DGA, SPH, BCR, CL0, CHL, PQN, C7Z, LHG, CLA

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	0.58	0/6007	0.57	0/8190
2	B	0.59	0/6036	0.57	0/8242
3	C	0.63	0/611	0.58	0/826
4	D	0.59	0/1154	0.60	0/1556
5	E	0.63	0/506	0.57	0/689
6	F	0.57	0/1292	0.63	0/1747
7	G	0.64	0/505	0.58	0/685
8	I	0.61	0/293	0.56	0/406
9	J	0.58	0/331	0.54	0/454
10	K	0.67	0/575	0.61	0/779
11	1	0.60	0/1491	0.60	0/2028
11	Z	0.61	0/1491	0.62	0/2028
12	3	0.58	0/1721	0.63	0/2336
13	7	0.58	0/1702	0.61	0/2310
14	8	0.58	0/1701	0.61	0/2315
15	4	0.59	0/1683	0.60	0/2296
16	5	0.59	0/1830	0.62	0/2492
17	6	0.59	0/1828	0.62	0/2497
All	All	0.59	0/30757	0.59	0/41876

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	5811	0	5658	210	0
2	B	5824	0	5580	226	0
3	C	601	0	584	21	0
4	D	1135	0	1148	26	0
5	E	496	0	491	7	0
6	F	1266	0	1301	48	0
7	G	495	0	485	40	0
8	I	281	0	292	34	0
9	J	320	0	322	19	0
10	K	570	0	606	54	0
11	1	1445	0	1396	72	0
11	Z	1445	0	1396	66	0
12	3	1673	0	1631	81	0
13	7	1650	0	1589	69	0
14	8	1650	0	1629	83	0
15	4	1628	0	1576	103	0
16	5	1775	0	1746	90	0
17	6	1766	0	1765	116	0
18	A	65	0	72	12	0
19	1	554	0	504	89	0
19	3	692	0	669	125	0
19	4	553	0	507	107	0
19	5	855	0	809	171	0
19	6	704	0	687	161	0
19	7	720	0	670	109	0
19	8	579	0	560	104	0
19	A	2655	0	2744	441	0
19	B	2490	0	2539	439	0
19	F	110	0	104	18	0
19	G	96	0	71	18	0
19	I	55	0	49	12	0
19	J	42	0	30	4	0
19	K	195	0	150	41	0
19	Z	564	0	532	76	0
20	A	33	0	46	4	0
20	B	33	0	46	5	0
21	A	8	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	C	16	0	0	5	0
22	3	160	0	224	43	0
22	4	40	0	56	14	0
22	5	80	0	112	17	0
22	6	80	0	112	39	0
22	7	40	0	56	5	0
22	8	80	0	112	17	0
22	A	280	0	392	71	0
22	B	240	0	336	76	0
22	F	40	0	56	9	0
22	G	40	0	56	12	0
22	K	40	0	56	12	0
23	1	66	0	72	10	0
23	3	20	0	12	4	0
23	4	49	0	74	14	0
23	5	37	0	44	7	0
23	6	81	0	108	22	0
23	7	37	0	44	3	0
23	8	38	0	46	7	0
23	A	84	0	114	12	0
23	Z	43	0	56	6	0
24	1	35	0	46	9	0
24	3	35	0	46	7	0
24	4	105	0	138	20	0
24	7	35	0	46	2	0
24	8	70	0	92	8	0
24	A	140	0	184	22	0
24	F	35	0	46	9	0
24	G	35	0	46	11	0
24	Z	70	0	91	11	0
25	B	66	0	96	5	0
26	B	1	0	0	0	0
27	4	41	0	56	6	0
27	5	41	0	56	11	0
27	F	41	0	56	9	0
28	1	42	0	0	1	0
28	6	42	0	0	4	0
28	J	42	0	0	1	0
29	7	29	0	28	1	0
29	J	80	0	103	16	0
30	K	14	0	23	4	0
31	1	84	0	112	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	3	84	0	112	14	0
31	4	42	0	56	13	0
31	5	42	0	56	10	0
31	6	84	0	112	16	0
31	7	84	0	112	17	0
31	8	84	0	112	16	0
31	Z	84	0	112	22	0
32	1	157	0	121	23	0
32	3	66	0	69	13	0
32	4	211	0	169	32	0
32	5	211	0	170	44	0
32	6	287	0	259	63	0
32	7	120	0	113	18	0
32	8	296	0	269	45	0
32	Z	232	0	209	49	0
33	3	21	0	37	12	0
33	4	21	0	37	7	0
33	7	21	0	37	7	0
34	3	39	0	51	4	0
34	5	23	0	19	3	0
34	6	29	0	31	5	0
34	8	30	0	33	6	0
35	7	34	0	53	14	0
36	7	18	0	31	2	0
37	8	48	0	62	11	0
38	6	29	0	44	24	0
38	8	29	0	44	14	0
39	1	27	0	0	2	0
39	3	31	0	0	1	0
39	4	24	0	0	0	0
39	5	18	0	0	2	0
39	6	22	0	0	0	0
39	7	36	0	0	0	0
39	8	31	0	0	1	0
39	A	130	0	0	0	0
39	B	113	0	0	2	0
39	C	35	0	0	0	0
39	D	28	0	0	1	0
39	E	18	0	0	0	0
39	F	29	0	0	1	0
39	G	3	0	0	0	0
39	J	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	K	4	0	0	1	0
39	Z	13	0	0	0	0
All	All	46504	0	45917	3054	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 33.

All (3054) 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)
19:3:5010:CLA:O1A	19:3:5010:CLA:H2	1.36	1.13
23:4:320:LHG:HC92	23:4:320:LHG:H282	1.28	1.12
19:4:311:CLA:HBC2	19:4:311:CLA:HHD	1.33	1.10
19:5:307:CLA:HBB1	19:5:307:CLA:HHC	1.35	1.09
22:6:308:BCR:H21C	22:6:308:BCR:H361	1.32	1.09
23:Z:316:LHG:HC82	22:4:305:BCR:HC42	1.27	1.09
19:4:308:CLA:HBA1	19:4:308:CLA:HBD	1.21	1.08
19:A:815:CLA:H193	19:3:5016:CLA:HBC3	1.13	1.08
22:5:304:BCR:HC42	23:6:324:LHG:HC82	1.16	1.07
23:1:5019:LHG:H161	32:8:301:CHL:H62	1.34	1.05
19:A:814:CLA:H2	19:A:816:CLA:HMB2	1.37	1.05
19:5:311:CLA:HMA2	32:5:318:CHL:HBC3	1.05	1.04
19:B:850:CLA:HBB1	19:B:850:CLA:HHC	1.39	1.03
19:B:850:CLA:H72	19:B:850:CLA:C2	1.81	1.03
1:A:389:SER:HB3	19:A:828:CLA:HMA1	1.41	1.03
19:B:850:CLA:H2	19:B:850:CLA:C7	1.86	1.03
19:5:311:CLA:CMA	32:5:318:CHL:HBC3	1.89	1.03
22:5:305:BCR:H21C	22:5:305:BCR:H361	1.05	1.03
19:6:310:CLA:HBB1	19:6:310:CLA:HHC	1.37	1.02
19:6:313:CLA:HMA2	32:6:319:CHL:HBC3	1.41	1.02
19:4:307:CLA:H62	19:4:307:CLA:HMA3	1.40	1.02
19:B:825:CLA:HBA1	19:B:826:CLA:HED2	1.38	1.02
19:B:835:CLA:H51	19:B:850:CLA:HMB2	1.39	1.01
11:Z:159:PHE:HB3	32:Z:302:CHL:HBA1	1.40	1.01
3:C:14:CYS:SG	21:C:102:SF4:FE3	1.52	1.01
23:6:303:LHG:H241	23:6:303:LHG:H132	1.42	1.01
19:B:836:CLA:H152	27:F:304:RRX:H25	1.41	1.01
19:5:313:CLA:HMB1	19:5:313:CLA:HBB1	1.39	1.01
11:Z:210:TRP:HE1	19:Z:307:CLA:H71	1.23	1.00
19:B:823:CLA:HBA2	22:B:845:BCR:H14C	1.44	1.00
22:6:307:BCR:H291	19:6:313:CLA:H2	1.44	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:6:308:BCR:H341	22:6:308:BCR:H12C	1.44	0.98
19:3:5010:CLA:O1A	19:3:5010:CLA:C2	2.05	0.97
19:Z:308:CLA:HMB1	19:Z:308:CLA:HBB1	1.45	0.97
19:8:313:CLA:H2	19:4:310:CLA:H71	1.45	0.97
19:4:308:CLA:HBA1	19:4:308:CLA:CBD	1.93	0.97
19:B:825:CLA:HMB1	19:B:825:CLA:HBB1	1.47	0.96
2:B:4:LYS:HA	8:I:102:GLU:HA	1.46	0.96
22:5:305:BCR:H361	22:5:305:BCR:C21	1.94	0.96
19:5:308:CLA:HHC	19:5:308:CLA:HBB1	1.46	0.96
19:A:812:CLA:H202	19:A:820:CLA:H121	1.45	0.95
19:A:815:CLA:H193	19:3:5016:CLA:CBC	1.95	0.95
17:6:129:TRP:CE2	17:6:133:ARG:HD3	2.00	0.95
32:5:318:CHL:HMB1	32:5:318:CHL:HBB1	1.48	0.95
20:A:844:PQN:H142	22:F:302:BCR:H271	1.48	0.95
19:5:306:CLA:HBB1	19:5:306:CLA:HMB1	1.49	0.95
19:7:324:CLA:HMB1	19:7:324:CLA:HBB1	1.48	0.95
19:5:314:CLA:HMA3	23:5:323:LHG:H132	1.50	0.94
22:5:305:BCR:H21C	22:5:305:BCR:C36	1.98	0.93
19:5:314:CLA:HHC	19:5:314:CLA:HBB1	1.46	0.93
11:Z:160:ALA:HB2	32:Z:302:CHL:HAA2	1.48	0.93
19:B:850:CLA:H72	19:B:850:CLA:H2	0.94	0.92
19:1:5007:CLA:HMB1	19:1:5007:CLA:HBB1	1.50	0.92
19:A:802:CLA:HAB	2:B:583:TRP:CH2	2.04	0.92
19:4:311:CLA:HMB1	19:4:311:CLA:HBB1	1.51	0.92
19:A:807:CLA:HHC	19:A:807:CLA:HBB1	1.50	0.92
32:4:314:CHL:HMB1	32:4:314:CHL:HBB1	1.49	0.92
19:A:808:CLA:HHC	19:A:808:CLA:HBB1	1.51	0.91
32:Z:313:CHL:HMB1	32:Z:313:CHL:HBB1	1.53	0.91
19:A:832:CLA:HHC	19:A:832:CLA:HBB1	1.49	0.91
19:8:307:CLA:HBB1	19:8:307:CLA:HMB1	1.52	0.91
19:4:313:CLA:HBB1	19:4:313:CLA:HMB1	1.52	0.91
19:5:309:CLA:HHC	19:5:309:CLA:HBB1	1.51	0.91
6:F:211:GLN:HE22	38:8:325:ERG:H181	1.36	0.91
24:8:323:LMT:H1B	24:8:323:LMT:H6D	1.48	0.91
19:B:823:CLA:HAB	19:B:830:CLA:HMD2	1.51	0.91
19:6:323:CLA:HBB1	19:6:323:CLA:HMB1	1.51	0.90
22:6:307:BCR:C29	19:6:313:CLA:H2	2.00	0.90
19:4:310:CLA:HHC	19:4:310:CLA:HBB1	1.54	0.90
3:C:14:CYS:HG	21:C:102:SF4:FE3	0.73	0.90
19:4:307:CLA:HHC	19:4:307:CLA:HBB1	1.52	0.90
19:A:812:CLA:HBB1	19:A:812:CLA:HHC	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:6:317:CHL:HBB1	32:6:317:CHL:HMB1	1.52	0.90
1:A:396:TRP:CD1	19:A:828:CLA:HAB	2.05	0.90
19:A:819:CLA:HMB1	19:A:819:CLA:HBB1	1.53	0.90
19:B:818:CLA:HBB1	19:B:818:CLA:HMB1	1.54	0.89
19:A:837:CLA:HBB1	19:A:837:CLA:HMB1	1.52	0.89
19:B:815:CLA:H112	22:B:842:BCR:H21C	1.51	0.89
19:B:812:CLA:HHC	19:B:812:CLA:HBB1	1.55	0.89
32:5:316:CHL:HMB1	32:5:316:CHL:HBB1	1.54	0.89
17:6:164:PHE:CZ	17:6:166:PRO:HB3	2.08	0.89
19:B:833:CLA:HHC	19:B:833:CLA:HBB1	1.55	0.88
19:8:312:CLA:HMB1	19:8:312:CLA:HBB1	1.52	0.88
19:4:312:CLA:NC	23:4:320:LHG:HC42	1.88	0.88
19:B:809:CLA:HBB1	19:B:809:CLA:HMB1	1.56	0.88
19:A:816:CLA:HBB1	19:A:816:CLA:HMB1	1.54	0.88
19:B:821:CLA:HMD2	22:B:842:BCR:HC7	1.56	0.88
19:6:309:CLA:HMB1	19:6:309:CLA:HBB1	1.54	0.88
16:5:55:TRP:CH2	19:5:314:CLA:HED2	2.08	0.87
19:5:310:CLA:H61	19:5:322:CLA:HAB	1.55	0.87
19:5:310:CLA:HMB1	19:5:310:CLA:HBB1	1.54	0.87
19:B:821:CLA:HMB1	19:B:821:CLA:HBB1	1.55	0.87
19:F:301:CLA:H152	19:F:301:CLA:H192	1.56	0.87
19:7:308:CLA:HBA1	19:7:308:CLA:HBD	1.54	0.87
14:8:191:LYS:HG3	19:8:313:CLA:HED2	1.56	0.87
19:F:301:CLA:HBB1	22:F:302:BCR:H323	1.55	0.87
19:3:5013:CLA:HMB1	19:3:5013:CLA:HBB1	1.57	0.87
19:A:815:CLA:HBB1	19:A:815:CLA:HMB1	1.56	0.87
19:G:1601:CLA:HHC	19:G:1601:CLA:HBB1	1.55	0.86
19:Z:312:CLA:HMB1	19:Z:312:CLA:HBB1	1.55	0.86
19:8:309:CLA:HBD	19:8:309:CLA:HBA1	1.55	0.86
32:6:316:CHL:HMC	32:6:316:CHL:HBC2	1.57	0.86
19:5:321:CLA:HED1	23:6:324:LHG:H311	1.57	0.86
22:6:308:BCR:H321	22:6:308:BCR:HC8	1.56	0.86
1:A:443:TRP:HH2	19:A:838:CLA:H161	1.41	0.86
19:A:827:CLA:HBB1	19:A:827:CLA:HMB1	1.55	0.86
19:A:829:CLA:HHC	19:A:829:CLA:HBB1	1.57	0.86
19:4:308:CLA:H121	23:4:320:LHG:H151	1.56	0.86
19:B:819:CLA:H51	19:B:826:CLA:H142	1.55	0.86
32:Z:310:CHL:CBB	32:Z:313:CHL:HBB2	2.06	0.86
19:5:301:CLA:HHC	19:5:301:CLA:HBB1	1.56	0.86
19:4:308:CLA:HMB1	19:4:308:CLA:HBB1	1.56	0.85
12:3:43:LEU:HG	19:3:5011:CLA:HAA2	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:5020:CLA:HBB1	19:3:5020:CLA:HMB1	1.59	0.85
32:4:315:CHL:HMB1	32:4:315:CHL:HBB1	1.58	0.85
19:A:826:CLA:H171	19:A:839:CLA:H71	1.58	0.85
19:F:303:CLA:HHC	19:F:303:CLA:HBB1	1.58	0.85
19:3:5008:CLA:HBB1	19:3:5008:CLA:HMB1	1.56	0.85
19:6:313:CLA:HBB1	19:6:313:CLA:HMB1	1.56	0.85
19:5:317:CLA:HMA1	19:5:321:CLA:HBC2	1.57	0.84
19:B:831:CLA:HBA1	6:F:216:LEU:HD21	1.59	0.84
19:B:825:CLA:H51	19:B:840:CLA:H191	1.58	0.84
7:G:100:VAL:HG21	19:G:1602:CLA:HMA1	1.59	0.84
11:Z:57:PRO:HD2	31:Z:317:LUT:H23	1.57	0.84
32:8:317:CHL:HMB1	32:8:317:CHL:HBB1	1.59	0.84
19:A:813:CLA:HBB1	19:A:813:CLA:HMB1	1.60	0.84
15:4:211:LEU:HB3	19:4:306:CLA:HMA1	1.60	0.84
19:3:5010:CLA:H11	19:3:5010:CLA:C4D	2.07	0.84
19:5:311:CLA:HMA2	32:5:318:CHL:CBC	2.01	0.84
17:6:104:VAL:HB	32:6:319:CHL:HBC1	1.59	0.84
19:A:857:CLA:HBB1	19:A:857:CLA:HHC	1.60	0.84
19:Z:303:CLA:HBB1	19:Z:303:CLA:HMB1	1.58	0.84
32:8:301:CHL:H2	37:8:302:SQD:H191	1.56	0.84
19:4:310:CLA:HAC2	32:4:314:CHL:HBB2	1.60	0.84
31:6:306:LUT:H28	31:6:306:LUT:H371	1.59	0.84
22:3:5007:BCR:HC8	19:3:5015:CLA:CHB	2.08	0.83
2:B:284:ILE:HA	19:B:816:CLA:H172	1.60	0.83
4:D:85:VAL:HG22	4:D:114:LYS:HG2	1.59	0.83
19:6:301:CLA:H91	32:6:316:CHL:H43	1.60	0.83
19:B:826:CLA:H13	22:B:846:BCR:H17C	1.60	0.83
19:B:840:CLA:HBB1	19:B:840:CLA:HMB1	1.58	0.83
16:5:172:PHE:HD2	27:5:302:RRX:H13	1.41	0.83
19:A:821:CLA:H72	22:A:849:BCR:H12C	1.59	0.82
14:8:138:TRP:CE3	19:8:318:CLA:HMA1	2.14	0.82
22:A:850:BCR:H23C	19:B:801:CLA:H101	1.62	0.82
19:A:839:CLA:HBB1	19:A:839:CLA:HMB1	1.61	0.82
11:1:58:LEU:HD12	31:1:5004:LUT:H221	1.61	0.82
19:A:827:CLA:HMA1	19:A:835:CLA:H51	1.61	0.82
11:1:46:PRO:HG2	11:1:49:LEU:HB2	1.61	0.82
13:7:91:ILE:HG23	34:6:325:3PH:H262	1.62	0.82
19:A:818:CLA:H102	19:K:203:CLA:H92	1.62	0.82
19:A:821:CLA:HMB1	19:A:821:CLA:HBB1	1.61	0.82
11:1:112:ALA:HB3	11:1:119:VAL:HB	1.62	0.82
19:6:301:CLA:H42	19:6:301:CLA:CHD	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:826:CLA:HBB1	19:A:826:CLA:HMB1	1.62	0.81
12:3:76:ILE:HD13	12:3:212:PRO:HB2	1.62	0.81
19:B:819:CLA:HBB1	19:B:819:CLA:HMB1	1.63	0.81
14:8:142:ARG:HD2	37:8:302:SQD:H81	1.63	0.81
32:4:314:CHL:HBB1	24:4:322:LMT:H72	1.62	0.81
22:A:846:BCR:H281	33:3:5001:SPH:H142	1.63	0.81
1:A:439:SER:HB3	2:B:678:THR:HG22	1.62	0.81
19:A:804:CLA:HBB1	19:A:804:CLA:HMB1	1.63	0.81
19:5:310:CLA:H72	19:5:314:CLA:H193	1.61	0.81
19:6:312:CLA:HBB1	19:6:312:CLA:HMB1	1.62	0.81
2:B:371:ALA:HB1	19:B:827:CLA:HMA1	1.61	0.81
19:7:307:CLA:HBB1	19:7:307:CLA:HMB1	1.62	0.81
19:5:311:CLA:HMB1	19:5:311:CLA:HBB1	1.59	0.81
22:6:307:BCR:H393	19:6:313:CLA:H72	1.63	0.81
1:A:29:TRP:HE1	19:A:811:CLA:CHB	1.93	0.80
19:B:831:CLA:H2	27:F:304:RRX:H44	1.62	0.80
19:3:5012:CLA:HHC	19:3:5012:CLA:HBB1	1.63	0.80
32:3:5017:CHL:HMB1	32:3:5017:CHL:HBB1	1.62	0.80
31:7:304:LUT:H371	31:7:304:LUT:H28	1.63	0.80
19:B:813:CLA:HMB1	19:B:813:CLA:HBB1	1.62	0.80
19:B:850:CLA:H122	19:B:850:CLA:HBA2	1.61	0.80
19:3:5015:CLA:HMB1	19:3:5015:CLA:HBB1	1.63	0.80
32:1:5017:CHL:HBB1	32:1:5017:CHL:HMB1	1.61	0.80
19:7:312:CLA:HHC	19:7:312:CLA:HBB1	1.62	0.80
32:8:319:CHL:HMB1	32:8:319:CHL:HBB1	1.61	0.80
19:1:5007:CLA:HMC3	19:1:5012:CLA:H142	1.63	0.80
19:A:841:CLA:HBA2	23:A:852:LHG:H161	1.64	0.80
22:3:5006:BCR:H21C	19:3:5012:CLA:C4C	2.11	0.80
32:8:316:CHL:HMB1	32:8:316:CHL:HBB1	1.63	0.80
22:6:307:BCR:H393	19:6:313:CLA:C7	2.11	0.80
19:B:815:CLA:HMB1	19:B:815:CLA:HBB1	1.63	0.80
4:D:95:ILE:HG12	4:D:105:ILE:HG12	1.63	0.80
32:1:5014:CHL:HBB1	32:1:5014:CHL:HMB1	1.62	0.80
19:Z:304:CLA:HBB1	19:Z:304:CLA:HMB1	1.63	0.80
17:6:132:LEU:HG	17:6:154:VAL:HG11	1.64	0.80
19:B:828:CLA:HBB1	19:B:828:CLA:HHC	1.64	0.80
14:8:142:ARG:HD2	37:8:302:SQD:C8	2.12	0.80
19:8:308:CLA:HBB1	19:8:308:CLA:HHC	1.64	0.80
19:A:815:CLA:H101	22:3:5006:BCR:H14C	1.63	0.79
19:4:309:CLA:HMB1	19:4:309:CLA:HBB1	1.63	0.79
19:5:325:CLA:HHC	19:5:325:CLA:HBB1	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:6:309:CLA:HMD2	32:6:317:CHL:H11	1.63	0.79
19:A:803:CLA:HHC	19:A:803:CLA:HBB1	1.63	0.79
19:B:830:CLA:H12	19:B:840:CLA:H62	1.63	0.79
19:7:316:CLA:HBB1	19:7:316:CLA:HMB1	1.63	0.79
15:4:136:ASP:HB3	15:4:139:LYS:HE3	1.64	0.79
19:6:301:CLA:H42	19:6:301:CLA:C4C	2.12	0.79
19:B:829:CLA:HBB1	19:B:829:CLA:HMB1	1.64	0.79
19:1:5010:CLA:NB	19:1:5016:CLA:H13	1.96	0.79
19:A:830:CLA:HMB1	19:A:830:CLA:HBB1	1.65	0.79
32:Z:309:CHL:HBB1	32:Z:309:CHL:HMB1	1.64	0.79
14:8:148:GLY:HA3	14:8:161:LYS:HG3	1.64	0.79
19:5:325:CLA:HBA1	19:5:325:CLA:CHA	2.10	0.79
19:A:806:CLA:H2	19:A:806:CLA:HED2	1.64	0.78
8:I:75:ALA:HB3	8:I:76:PRO:HD3	1.63	0.78
11:1:155:ASP:HA	31:1:5003:LUT:H24	1.65	0.78
19:4:312:CLA:C1C	23:4:320:LHG:HC42	2.12	0.78
4:D:157:TYR:HB2	4:D:160:LYS:HE2	1.63	0.78
19:1:5010:CLA:C4B	19:1:5016:CLA:H13	2.13	0.78
19:8:312:CLA:H102	19:8:312:CLA:C15	2.14	0.78
15:4:95:TRP:CZ2	19:4:316:CLA:HAA2	2.18	0.78
17:6:82:VAL:HG11	31:6:305:LUT:H12	1.64	0.78
19:B:808:CLA:HMA1	19:I:201:CLA:HMB3	1.64	0.78
31:8:304:LUT:H32	31:8:304:LUT:H391	1.66	0.78
19:A:839:CLA:H162	22:A:849:BCR:H371	1.64	0.78
19:A:821:CLA:HMB2	19:A:825:CLA:HMA3	1.66	0.78
19:A:826:CLA:H162	22:A:848:BCR:HC7	1.65	0.78
19:7:306:CLA:HBB1	19:7:306:CLA:HMB1	1.65	0.77
19:J:1901:CLA:HBB1	19:J:1901:CLA:HMB1	1.66	0.77
1:A:584:CYS:SG	21:A:845:SF4:FE2	1.77	0.77
19:B:809:CLA:H2	19:B:809:CLA:HBA2	1.65	0.77
16:5:222:PRO:HG2	19:5:313:CLA:HMB3	1.64	0.77
19:1:5006:CLA:HMB1	19:1:5006:CLA:HBB1	1.66	0.77
1:A:265:PHE:HA	19:K:202:CLA:HAC2	1.67	0.77
17:6:129:TRP:CZ2	17:6:133:ARG:HD3	2.19	0.77
32:5:315:CHL:CBB	32:5:318:CHL:HBB2	2.15	0.77
19:3:5009:CLA:O1D	19:3:5014:CLA:H71	1.85	0.77
19:4:310:CLA:HMD2	19:4:316:CLA:C1D	2.15	0.77
1:A:453:PHE:HE1	19:B:803:CLA:HMA1	1.50	0.77
14:8:64:VAL:CG2	38:8:325:ERG:H6	2.15	0.77
17:6:221:ALA:HB2	17:6:231:PRO:HD3	1.66	0.77
19:B:835:CLA:HMB1	19:B:835:CLA:HBB1	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:824:CLA:H161	19:A:839:CLA:HBA2	1.65	0.76
2:B:54:GLN:HG2	19:B:806:CLA:HMA1	1.65	0.76
19:5:319:CLA:HHC	19:5:319:CLA:HBB1	1.67	0.76
1:A:550:LEU:HB3	22:A:849:BCR:H322	1.67	0.76
8:I:98:TYR:HA	8:I:101:LYS:HD3	1.68	0.76
1:A:305:PHE:HE1	19:A:821:CLA:HAB	1.50	0.76
22:6:308:BCR:H361	22:6:308:BCR:C21	2.14	0.76
6:F:211:GLN:HE22	38:8:325:ERG:C18	1.99	0.76
32:6:321:CHL:HHC	32:6:321:CHL:HBB1	1.67	0.76
1:A:453:PHE:CE1	19:B:803:CLA:HMA1	2.20	0.76
21:A:845:SF4:FE1	2:B:569:CYS:SG	1.77	0.76
19:8:311:CLA:HMB1	19:8:311:CLA:HBB1	1.67	0.76
19:A:843:CLA:HMB1	19:A:843:CLA:HBB1	1.68	0.75
22:4:305:BCR:H321	22:4:305:BCR:HC8	1.68	0.75
19:5:321:CLA:H193	19:6:320:CLA:H8	1.68	0.75
19:A:814:CLA:HBB1	19:A:814:CLA:HMB1	1.67	0.75
17:6:166:PRO:HB2	19:6:310:CLA:H62	1.68	0.75
19:A:834:CLA:HED2	19:A:834:CLA:H2A	1.68	0.75
19:5:317:CLA:HMA1	19:5:321:CLA:CBC	2.16	0.75
19:A:823:CLA:HBB1	19:A:823:CLA:HHC	1.67	0.75
19:Z:311:CLA:H71	32:Z:313:CHL:HBA2	1.69	0.75
19:B:819:CLA:HMB2	19:B:824:CLA:HMA3	1.68	0.75
32:Z:309:CHL:HHD	32:Z:309:CHL:HBC3	1.67	0.75
19:A:825:CLA:HBB1	19:A:825:CLA:HMB1	1.69	0.74
19:Z:315:CLA:H141	19:Z:315:CLA:H171	1.68	0.74
19:Z:306:CLA:HBB2	24:Z:319:LMT:H111	1.69	0.74
13:7:173:MET:HG2	19:7:324:CLA:H42	1.70	0.74
22:3:5006:BCR:H17C	19:3:5012:CLA:HBB1	1.69	0.74
19:A:836:CLA:HBB1	19:A:836:CLA:HHC	1.67	0.74
15:4:203:TRP:HB2	19:4:306:CLA:HBA1	1.68	0.74
32:5:320:CHL:HBB1	32:5:320:CHL:HHC	1.69	0.74
19:A:804:CLA:HBD	19:A:811:CLA:H2	1.68	0.74
19:B:828:CLA:H202	22:B:843:BCR:H11C	1.69	0.74
10:K:50:ARG:HG2	19:K:205:CLA:HMC3	1.68	0.74
19:8:309:CLA:H122	32:8:315:CHL:H93	1.70	0.74
16:5:127:ILE:HG13	19:5:325:CLA:HBA2	1.69	0.74
11:Z:210:TRP:NE1	19:Z:307:CLA:H71	2.01	0.74
32:Z:313:CHL:HAA2	32:Z:313:CHL:HBD	1.69	0.74
19:B:815:CLA:H62	22:B:842:BCR:H402	1.70	0.73
11:1:57:PRO:HD2	31:1:5004:LUT:H23	1.69	0.73
19:Z:305:CLA:HBB1	19:Z:305:CLA:HMB1	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:TRP:HD1	19:A:828:CLA:HAB	1.50	0.73
19:7:324:CLA:HMA1	19:6:312:CLA:H93	1.69	0.73
19:5:307:CLA:C4	19:5:307:CLA:H71	2.17	0.73
19:A:830:CLA:H122	19:A:841:CLA:HMA2	1.69	0.73
19:4:306:CLA:HMB2	19:4:307:CLA:HBA2	1.70	0.73
19:5:314:CLA:ND	23:5:323:LHG:H102	2.02	0.73
19:B:831:CLA:H151	19:B:836:CLA:H162	1.71	0.73
2:B:657:ILE:HG12	19:B:839:CLA:HMB3	1.71	0.73
22:B:845:BCR:H402	22:B:846:BCR:H383	1.68	0.73
31:5:303:LUT:H181	31:5:303:LUT:H8	1.70	0.73
19:5:322:CLA:HMD3	28:6:304:C7Z:C38	2.18	0.73
14:8:188:TRP:HB3	19:8:307:CLA:HMA1	1.69	0.73
31:6:305:LUT:H11	19:6:310:CLA:HMC2	1.71	0.73
1:A:305:PHE:CE1	19:A:821:CLA:HAB	2.23	0.73
32:8:301:CHL:H52	37:8:302:SQD:H211	1.69	0.73
19:Z:311:CLA:HMB1	19:Z:311:CLA:HBB1	1.70	0.73
19:7:324:CLA:H11	38:6:326:ERG:H42	1.71	0.72
31:8:305:LUT:H24	19:8:310:CLA:O1A	1.89	0.72
14:8:68:TRP:HZ2	19:8:318:CLA:HAA2	1.55	0.72
15:4:139:LYS:HG2	32:4:314:CHL:HED2	1.72	0.72
23:4:320:LHG:H282	23:4:320:LHG:C9	2.15	0.72
16:5:124:TRP:HH2	32:6:315:CHL:H192	1.53	0.72
11:Z:36:LEU:HD13	32:Z:309:CHL:HMA3	1.71	0.72
22:7:305:BCR:H281	33:7:321:SPH:H101	1.71	0.72
19:A:835:CLA:H203	22:A:848:BCR:H12C	1.71	0.72
19:B:837:CLA:H12	22:B:846:BCR:H352	1.72	0.72
15:4:109:LEU:HB3	19:4:311:CLA:HAB	1.72	0.72
19:4:311:CLA:HHD	19:4:311:CLA:CBC	2.18	0.72
19:A:807:CLA:HMA1	19:A:808:CLA:HMB3	1.69	0.72
22:A:846:BCR:H321	22:A:846:BCR:HC8	1.72	0.72
24:A:853:LMT:H21	24:A:853:LMT:H62	1.72	0.72
22:6:308:BCR:H341	22:6:308:BCR:C12	2.16	0.72
19:B:826:CLA:H162	22:B:846:BCR:H17C	1.72	0.72
14:8:68:TRP:CZ2	19:8:318:CLA:HAA2	2.25	0.72
1:A:598:TRP:HE1	19:B:804:CLA:C1D	2.03	0.71
19:B:821:CLA:H92	7:G:106:LEU:HD13	1.70	0.71
19:B:833:CLA:HBA2	19:B:834:CLA:HMB3	1.72	0.71
19:8:313:CLA:HMA1	24:4:302:LMT:H5'	1.72	0.71
32:4:314:CHL:HAB	32:4:317:CHL:HBB2	1.72	0.71
19:B:825:CLA:H92	19:B:835:CLA:H41	1.73	0.71
19:3:5012:CLA:HBC1	19:3:5018:CLA:HAC1	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:839:CLA:HBD	20:B:841:PQN:H302	1.73	0.71
19:7:309:CLA:HMB1	19:7:309:CLA:HBB1	1.72	0.71
17:6:248:THR:HA	32:6:316:CHL:O1A	1.91	0.71
22:6:308:BCR:H321	22:6:308:BCR:C8	2.20	0.71
19:A:806:CLA:HBB2	22:A:847:BCR:HC41	1.72	0.71
19:B:823:CLA:HMD2	19:B:824:CLA:HAB	1.72	0.71
11:1:169:LEU:HB3	19:1:5006:CLA:HMA1	1.72	0.71
32:4:319:CHL:HHC	32:4:319:CHL:HBB1	1.73	0.71
27:5:302:RRX:H7	19:5:306:CLA:H92	1.72	0.71
19:A:826:CLA:HMB2	19:A:839:CLA:HBA1	1.73	0.71
19:B:837:CLA:H18	19:B:837:CLA:H13	1.71	0.71
22:B:845:BCR:H403	22:B:846:BCR:H20C	1.73	0.71
19:5:306:CLA:HMD2	32:5:316:CHL:O1A	1.90	0.71
19:5:309:CLA:H93	19:5:310:CLA:HMA1	1.73	0.71
17:6:33:LEU:HD12	32:6:315:CHL:O1D	1.91	0.71
19:B:850:CLA:H141	19:B:850:CLA:H172	1.73	0.71
19:Z:308:CLA:HMD2	19:Z:315:CLA:C1D	2.19	0.71
19:3:5019:CLA:C9	19:5:314:CLA:H93	2.21	0.71
1:A:306:LEU:HB3	22:A:859:BCR:H15C	1.72	0.70
19:A:838:CLA:HBB1	19:A:838:CLA:HMB1	1.72	0.70
2:B:168:TRP:CE2	19:B:811:CLA:HMA1	2.26	0.70
19:B:814:CLA:HMB1	19:B:814:CLA:HBB1	1.73	0.70
19:A:833:CLA:H112	19:A:857:CLA:HBC3	1.73	0.70
19:F:301:CLA:H152	19:F:301:CLA:C19	2.20	0.70
15:4:230:ILE:HG23	24:4:322:LMT:H42	1.71	0.70
22:6:308:BCR:HC8	22:6:308:BCR:C32	2.21	0.70
19:B:823:CLA:H102	19:B:837:CLA:H193	1.73	0.70
15:4:61:TRP:HH2	23:6:303:LHG:HC62	1.55	0.70
16:5:155:ASN:HB3	32:5:320:CHL:C3D	2.21	0.70
19:B:801:CLA:H202	19:B:801:CLA:H151	1.72	0.70
22:3:5005:BCR:H362	19:3:5008:CLA:H142	1.74	0.70
19:8:310:CLA:HBB1	19:8:310:CLA:HMB1	1.71	0.70
19:5:307:CLA:CAD	19:5:312:CLA:H2	2.22	0.70
32:Z:309:CHL:HMD1	15:4:178:PRO:HB3	1.73	0.70
19:5:306:CLA:H2	19:5:306:CLA:C1B	2.21	0.70
19:B:831:CLA:H112	19:F:301:CLA:H172	1.74	0.70
15:4:195:GLY:CA	19:4:306:CLA:HED2	2.22	0.70
12:3:220:LEU:HD21	19:3:5015:CLA:HMC3	1.74	0.70
13:7:168:ARG:CZ	38:6:326:ERG:H12	2.22	0.70
16:5:182:LEU:HB3	19:5:306:CLA:HMA1	1.74	0.70
1:A:707:LEU:HD23	6:F:216:LEU:HD23	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:6:310:CLA:HHC	19:6:310:CLA:CBB	2.20	0.70
6:F:211:GLN:NE2	38:8:325:ERG:H181	2.07	0.70
19:8:313:CLA:HBC3	23:8:321:LHG:HC82	1.74	0.70
19:B:832:CLA:HMB1	19:B:832:CLA:HBB1	1.73	0.70
11:Z:158:GLY:O	11:Z:159:PHE:HB2	1.91	0.70
19:4:316:CLA:HMB2	24:4:321:LMT:H51	1.74	0.70
16:5:240:VAL:HG12	16:5:249:LEU:HD11	1.73	0.70
19:6:313:CLA:CHA	19:6:313:CLA:HBA1	2.20	0.70
3:C:14:CYS:SG	21:C:102:SF4:S4	2.89	0.69
19:3:5008:CLA:H18	32:3:5017:CHL:H92	1.73	0.69
1:A:97:ARG:HB2	24:A:856:LMT:H6D	1.74	0.69
32:7:315:CHL:H11	24:7:323:LMT:H42	1.73	0.69
19:4:307:CLA:C2D	19:4:312:CLA:H52	2.21	0.69
19:5:314:CLA:H2A	23:5:323:LHG:H141	1.74	0.69
19:F:301:CLA:H61	27:F:304:RRX:H49	1.74	0.69
19:1:5011:CLA:H52	32:1:5017:CHL:HAA2	1.73	0.69
11:Z:193:ALA:HB2	19:Z:314:CLA:HED3	1.74	0.69
14:8:191:LYS:HD3	19:8:308:CLA:CBA	2.22	0.69
19:5:325:CLA:HMC3	17:6:209:LEU:HD21	1.73	0.69
2:B:255:ILE:HG13	2:B:256:LEU:HG	1.75	0.69
2:B:659:ALA:HB3	19:B:804:CLA:HBB2	1.74	0.69
14:8:229:TRP:CH2	22:8:303:BCR:H24C	2.27	0.69
32:8:301:CHL:HBD	32:8:301:CHL:HAA1	1.73	0.69
15:4:114:ILE:CG1	31:4:304:LUT:H173	2.22	0.69
17:6:123:TRP:HH2	22:6:307:BCR:H323	1.57	0.69
2:B:204:ARG:HG2	2:B:251:SER:HB2	1.75	0.69
19:3:5013:CLA:H11	19:5:301:CLA:HMB2	1.74	0.69
1:A:584:CYS:HB3	2:B:668:TRP:HE3	1.56	0.69
19:B:820:CLA:HHC	19:B:820:CLA:HBB1	1.74	0.69
13:7:175:LEU:HD21	17:6:57:LEU:HD23	1.74	0.69
32:8:315:CHL:C4A	23:8:321:LHG:H281	2.22	0.69
2:B:54:GLN:HG2	19:B:806:CLA:CMA	2.23	0.69
19:B:825:CLA:C2B	22:B:846:BCR:H363	2.23	0.69
19:B:831:CLA:HBA1	6:F:216:LEU:CD2	2.22	0.69
11:Z:85:VAL:HG11	31:Z:318:LUT:H12	1.75	0.69
13:7:160:LEU:HG	13:7:161:GLU:HG3	1.73	0.69
15:4:233:ALA:HB3	24:4:322:LMT:H21	1.74	0.69
17:6:252:LEU:H	19:6:301:CLA:H11	1.58	0.69
19:B:802:CLA:HMB3	19:B:803:CLA:OBD	1.93	0.69
19:B:819:CLA:H12	19:B:824:CLA:HBB1	1.74	0.69
22:B:846:BCR:H361	22:B:846:BCR:H21C	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:ALA:HA	2:B:264:PRO:HG3	1.75	0.68
19:B:814:CLA:HMA1	22:B:844:BCR:H402	1.74	0.68
19:8:320:CLA:HHC	19:8:320:CLA:HBB1	1.73	0.68
19:Z:308:CLA:HMB1	19:Z:308:CLA:CBB	2.22	0.68
19:6:302:CLA:HMA1	19:6:322:CLA:CAD	2.23	0.68
19:A:820:CLA:H62	10:K:86:ILE:HG21	1.74	0.68
2:B:463:TRP:CG	19:B:850:CLA:HMA2	2.27	0.68
11:1:224:PHE:HE1	14:8:123:LEU:HD23	1.58	0.68
17:6:133:ARG:HD2	38:6:326:ERG:H24	1.75	0.68
22:5:304:BCR:H321	22:5:304:BCR:HC8	1.75	0.68
2:B:273:ASP:HB3	19:B:817:CLA:HMA1	1.74	0.68
24:G:1604:LMT:H82	19:1:5010:CLA:HMD3	1.74	0.68
11:1:58:LEU:CD1	31:1:5004:LUT:H221	2.23	0.68
23:Z:316:LHG:C8	22:4:305:BCR:HC42	2.14	0.68
15:4:211:LEU:HB3	19:4:306:CLA:CMA	2.23	0.68
19:A:817:CLA:HMC1	19:A:817:CLA:H13	1.76	0.68
19:A:823:CLA:H102	22:A:859:BCR:H292	1.76	0.68
11:1:94:LEU:HD12	19:1:5011:CLA:HMD3	1.74	0.68
19:7:318:CLA:HBB1	19:7:318:CLA:HMB1	1.76	0.68
22:A:846:BCR:H20C	22:A:847:BCR:H23C	1.74	0.68
11:Z:133:ALA:HB1	24:Z:319:LMT:H41	1.76	0.68
19:6:302:CLA:HHC	19:6:302:CLA:HBB1	1.76	0.68
19:1:5008:CLA:HMB1	19:1:5008:CLA:HBB1	1.75	0.68
19:Z:308:CLA:H43	14:8:154:LEU:HB2	1.76	0.68
13:7:125:PHE:HB3	36:7:322:PLM:HC2	1.74	0.68
19:6:301:CLA:HHC	19:6:301:CLA:HBB1	1.73	0.68
19:B:806:CLA:HBB1	19:B:806:CLA:HMB1	1.74	0.68
19:7:308:CLA:H141	19:7:308:CLA:H172	1.74	0.68
19:A:819:CLA:H12	19:A:819:CLA:CHB	2.24	0.67
19:B:833:CLA:H101	19:B:834:CLA:C1B	2.24	0.67
15:4:248:LEU:HD21	19:4:313:CLA:HMC3	1.76	0.67
17:6:164:PHE:HZ	17:6:166:PRO:HB3	1.59	0.67
22:B:845:BCR:H313	19:1:5010:CLA:HED1	1.75	0.67
22:6:307:BCR:H21C	19:6:313:CLA:H122	1.74	0.67
14:8:56:PRO:HD2	31:8:305:LUT:H23	1.75	0.67
31:8:304:LUT:H30	19:8:307:CLA:H52	1.77	0.67
15:4:201:PHE:CD2	27:4:303:RRX:H12	2.30	0.67
19:A:836:CLA:HMB1	22:A:849:BCR:H282	1.76	0.67
2:B:168:TRP:CZ2	19:B:811:CLA:HMA1	2.30	0.67
31:3:5003:LUT:H363	19:3:5011:CLA:H61	1.76	0.67
22:A:850:BCR:H24C	19:B:832:CLA:HMC2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:321:CLA:HMB1	19:5:321:CLA:HBB1	1.75	0.67
19:A:810:CLA:HMB1	19:A:810:CLA:HBB1	1.76	0.67
19:A:835:CLA:H101	22:A:849:BCR:H19C	1.76	0.67
19:B:821:CLA:C1B	19:B:822:CLA:H8	2.25	0.67
19:B:833:CLA:H203	19:B:834:CLA:HMC2	1.75	0.67
13:7:168:ARG:NH2	38:6:326:ERG:H12	2.10	0.67
19:4:311:CLA:HBC2	19:4:311:CLA:CHD	2.16	0.67
19:5:325:CLA:H92	32:6:315:CHL:H143	1.76	0.67
19:B:830:CLA:HBB2	19:B:837:CLA:HMC2	1.75	0.67
11:1:58:LEU:HB2	11:1:60:LEU:HG	1.76	0.67
24:G:1604:LMT:H112	19:1:5016:CLA:HAC2	1.76	0.67
24:8:323:LMT:H1B	24:8:323:LMT:C6'	2.24	0.67
19:A:831:CLA:HBA2	23:A:851:LHG:HC92	1.76	0.67
12:3:119:PHE:HE2	32:7:314:CHL:H91	1.57	0.67
19:A:810:CLA:HBA1	19:A:810:CLA:CHA	2.24	0.67
7:G:108:HIS:CG	22:G:1603:BCR:H12C	2.29	0.67
19:1:5016:CLA:HHC	19:1:5016:CLA:HBB1	1.77	0.67
22:6:307:BCR:H292	19:6:313:CLA:O1A	1.95	0.67
19:B:850:CLA:HHC	19:B:850:CLA:CBB	2.22	0.66
17:6:239:VAL:HG21	32:6:316:CHL:HED2	1.76	0.66
22:B:842:BCR:H372	22:G:1603:BCR:HC42	1.77	0.66
32:Z:309:CHL:C9	15:4:155:LEU:HD13	2.25	0.66
13:7:165:PRO:HB3	19:7:316:CLA:HBC2	1.76	0.66
15:4:114:ILE:HG13	31:4:304:LUT:H173	1.77	0.66
19:4:313:CLA:H52	19:4:313:CLA:H92	1.78	0.66
17:6:84:GLY:O	17:6:88:GLN:HG3	1.95	0.66
32:6:319:CHL:HHC	32:6:319:CHL:HBB1	1.76	0.66
10:K:97:HIS:CE1	22:K:206:BCR:H12C	2.30	0.66
19:7:308:CLA:HBA1	19:7:308:CLA:CBD	2.25	0.66
14:8:142:ARG:CD	37:8:302:SQD:H81	2.26	0.66
16:5:57:PRO:HD2	31:5:303:LUT:H23	1.76	0.66
22:A:859:BCR:H291	19:K:204:CLA:HMB1	1.75	0.66
11:1:85:VAL:HG11	31:1:5003:LUT:H12	1.76	0.66
11:1:193:ALA:HB2	19:1:5018:CLA:HED3	1.78	0.66
14:8:212:ALA:HB2	19:8:320:CLA:HED3	1.77	0.66
19:5:307:CLA:HHC	19:5:307:CLA:CBB	2.18	0.66
19:A:822:CLA:HMD2	22:A:859:BCR:H23C	1.78	0.66
32:Z:313:CHL:HBA1	24:Z:319:LMT:O3'	1.95	0.66
19:5:310:CLA:HMB1	19:5:310:CLA:CBB	2.26	0.66
19:B:813:CLA:H152	19:B:828:CLA:HMD2	1.76	0.66
32:7:315:CHL:HHC	32:7:315:CHL:HBB1	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:306:CLA:HMB1	19:4:306:CLA:HBB1	1.77	0.66
6:F:224:VAL:HB	6:F:227:ARG:HH12	1.61	0.66
32:Z:310:CHL:CBC	32:Z:310:CHL:HHD	2.26	0.66
19:7:324:CLA:H43	38:6:326:ERG:H41	1.76	0.66
19:5:311:CLA:H12	32:5:318:CHL:CMD	2.26	0.66
32:1:5014:CHL:HAB	32:1:5017:CHL:HBB2	1.77	0.66
1:A:36:SER:HB3	1:A:39:LEU:HB2	1.78	0.66
19:F:301:CLA:CBB	22:F:302:BCR:H323	2.26	0.66
19:B:830:CLA:HBB1	19:B:830:CLA:HMB1	1.76	0.65
31:1:5004:LUT:H28	32:1:5009:CHL:H102	1.78	0.65
19:Z:314:CLA:C1	19:8:312:CLA:H143	2.25	0.65
19:3:5009:CLA:HMD3	19:3:5014:CLA:H43	1.78	0.65
32:8:316:CHL:HMD1	24:8:324:LMT:O2'	1.95	0.65
1:A:508:LEU:HB2	1:A:523:MET:HG3	1.78	0.65
19:A:802:CLA:HAB	2:B:583:TRP:HH2	1.60	0.65
19:5:325:CLA:HHC	19:5:325:CLA:CBB	2.25	0.65
14:8:68:TRP:CE2	38:8:325:ERG:H14	2.31	0.65
17:6:244:ILE:HG13	22:6:308:BCR:H342	1.78	0.65
19:6:310:CLA:HMD2	19:6:314:CLA:ND	2.10	0.65
3:C:73:SER:H	3:C:76:SER:HB2	1.62	0.65
15:4:123:ILE:HG22	15:4:124:GLY:H	1.61	0.65
12:3:223:PRO:HG2	19:3:5015:CLA:HMB3	1.79	0.65
31:8:304:LUT:H391	31:8:304:LUT:C32	2.25	0.65
19:4:310:CLA:HMA2	19:4:310:CLA:H11	1.78	0.65
2:B:66:LEU:HD11	22:B:844:BCR:H271	1.79	0.65
19:B:825:CLA:C6	19:B:835:CLA:H42	2.26	0.65
5:E:90:LEU:HD22	5:E:90:LEU:H	1.61	0.65
11:1:104:LEU:HD21	32:1:5014:CHL:HED3	1.79	0.65
19:A:857:CLA:HMC3	19:B:838:CLA:ND	2.12	0.65
2:B:27:ALA:HB1	25:B:848:DGD:HB21	1.78	0.65
19:3:5020:CLA:O1A	19:7:319:CLA:H101	1.97	0.65
22:8:303:BCR:H352	22:8:303:BCR:H10C	1.79	0.65
19:4:311:CLA:HMB1	19:4:311:CLA:CBB	2.26	0.65
23:4:320:LHG:H112	23:4:320:LHG:C30	2.26	0.65
17:6:133:ARG:NH2	17:6:134:LYS:HE3	2.10	0.65
19:A:822:CLA:H43	19:K:204:CLA:C3	2.27	0.65
19:B:823:CLA:H12	22:B:845:BCR:H12C	1.79	0.65
19:Z:305:CLA:O1A	31:Z:317:LUT:H24	1.97	0.65
19:5:313:CLA:HMB1	19:5:313:CLA:CBB	2.22	0.65
19:A:805:CLA:HBB1	19:A:805:CLA:HMB1	1.79	0.65
6:F:202:TRP:CD1	6:F:203:PRO:HD3	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:K:205:CLA:HHC	19:K:205:CLA:HBB1	1.79	0.65
19:7:311:CLA:HMB1	19:7:311:CLA:HBB1	1.77	0.65
32:5:315:CHL:H141	19:6:323:CLA:H161	1.79	0.65
17:6:249:PRO:HB2	19:6:301:CLA:O1A	1.96	0.65
19:A:815:CLA:H142	19:3:5012:CLA:CBB	2.27	0.64
19:B:825:CLA:H142	19:B:835:CLA:C14	2.27	0.64
19:4:312:CLA:HBB1	19:4:312:CLA:HHC	1.78	0.64
1:A:550:LEU:CB	22:A:849:BCR:H322	2.28	0.64
19:Z:314:CLA:HMA2	19:8:312:CLA:H101	1.79	0.64
17:6:242:LYS:O	22:6:308:BCR:H311	1.98	0.64
1:A:680:ALA:HB3	19:B:801:CLA:HBB2	1.79	0.64
19:A:808:CLA:H102	19:A:830:CLA:H171	1.78	0.64
32:Z:309:CHL:HBA1	15:4:159:TRP:HA	1.79	0.64
32:5:315:CHL:HBB2	32:5:318:CHL:HBB2	1.78	0.64
19:A:819:CLA:CAB	19:A:819:CLA:H72	2.27	0.64
2:B:467:ALA:HB2	2:B:477:PHE:CZ	2.32	0.64
11:Z:58:LEU:HD21	14:8:175:PRO:HA	1.79	0.64
14:8:138:TRP:CD2	19:8:318:CLA:HMA2	2.33	0.64
23:4:320:LHG:H112	23:4:320:LHG:H302	1.78	0.64
19:A:832:CLA:H51	19:A:832:CLA:HBD	1.78	0.64
19:K:205:CLA:NB	22:K:206:BCR:H271	2.13	0.64
19:6:309:CLA:HMB1	19:6:309:CLA:CBB	2.26	0.64
19:A:805:CLA:H203	22:A:846:BCR:H10C	1.79	0.64
19:A:817:CLA:HBB1	19:A:817:CLA:HMB1	1.79	0.64
19:A:828:CLA:H191	22:A:858:BCR:H19C	1.78	0.64
14:8:68:TRP:CH2	38:8:325:ERG:H122	2.32	0.64
14:8:191:LYS:HD3	19:8:308:CLA:HBA1	1.80	0.64
6:F:202:TRP:CG	6:F:203:PRO:HD3	2.32	0.64
32:7:314:CHL:H52	32:7:314:CHL:H92	1.80	0.64
19:8:318:CLA:CMC	24:8:324:LMT:H123	2.28	0.64
19:A:809:CLA:HMA1	9:J:27:ILE:HD13	1.80	0.64
3:C:22:PRO:HG2	3:C:23:LEU:HD12	1.80	0.64
1:A:443:TRP:CH2	19:A:838:CLA:H161	2.28	0.64
19:A:833:CLA:HAB	19:A:834:CLA:HHB	1.79	0.64
19:B:801:CLA:HMB1	19:B:801:CLA:HBB1	1.79	0.64
10:K:89:VAL:HG13	22:K:206:BCR:H17C	1.80	0.64
1:A:598:TRP:CH2	19:B:803:CLA:HAB	2.33	0.64
19:A:806:CLA:HHC	19:A:806:CLA:HBB1	1.78	0.64
19:A:812:CLA:H171	19:A:820:CLA:H122	1.80	0.64
19:B:831:CLA:H152	27:F:304:RRX:H27	1.80	0.64
19:B:850:CLA:H172	19:B:850:CLA:C14	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:VAL:HB	19:B:832:CLA:HMD1	1.81	0.63
8:I:88:PRO:O	8:I:92:MET:HG2	1.98	0.63
19:8:309:CLA:HBA1	19:8:309:CLA:CBD	2.26	0.63
19:A:802:CLA:HMA2	2:B:617:LEU:HD13	1.78	0.63
4:D:140:ARG:HB2	4:D:150:LEU:HD11	1.80	0.63
9:J:28:GLU:HG3	19:J:1901:CLA:C1B	2.28	0.63
11:1:169:LEU:HB3	19:1:5006:CLA:CMA	2.27	0.63
15:4:194:PRO:HD2	19:4:306:CLA:OBD	1.98	0.63
17:6:102:LYS:NZ	17:6:102:LYS:HB3	2.13	0.63
1:A:75:SER:OG	1:A:181:TYR:HB2	1.98	0.63
1:A:315:ASN:HA	10:K:73:SER:HB2	1.80	0.63
19:B:823:CLA:HMA1	19:B:840:CLA:HED2	1.79	0.63
19:B:850:CLA:H71	19:B:850:CLA:ND	2.13	0.63
13:7:186:TYR:HB3	19:7:306:CLA:HMA1	1.80	0.63
19:5:309:CLA:H3A	19:5:309:CLA:CGA	2.26	0.63
19:B:815:CLA:C1B	22:B:842:BCR:H271	2.28	0.63
27:5:302:RRX:H17	27:5:302:RRX:H21	1.79	0.63
1:A:217:GLN:HA	1:A:221:SER:HB2	1.80	0.63
2:B:398:ASP:HA	4:D:182:ILE:HD13	1.81	0.63
2:B:646:VAL:HG21	19:B:808:CLA:HAC1	1.81	0.63
12:3:77:ALA:HB3	12:3:78:PRO:HD3	1.78	0.63
1:A:501:ASN:HB2	19:A:836:CLA:HED2	1.79	0.63
32:8:301:CHL:HHD	32:8:301:CHL:HBC3	1.79	0.63
19:4:308:CLA:HMB1	19:4:308:CLA:CBB	2.27	0.63
19:5:310:CLA:HED1	39:5:411:HOH:O	1.98	0.63
1:A:293:ASP:HB3	19:A:818:CLA:HMA1	1.79	0.63
19:B:830:CLA:H12	19:B:840:CLA:C6	2.28	0.63
12:3:65:ALA:HB1	12:3:191:GLY:HA3	1.79	0.63
32:5:318:CHL:HBD	32:5:318:CHL:HAA2	1.80	0.63
19:A:833:CLA:H102	19:B:838:CLA:H62	1.79	0.63
2:B:407:ASN:O	2:B:411:ARG:HG2	1.99	0.63
17:6:225:PRO:HA	34:6:325:3PH:H342	1.81	0.63
32:6:321:CHL:HBD	32:6:321:CHL:HAA2	1.80	0.63
19:7:324:CLA:HMB1	19:7:324:CLA:CBB	2.23	0.63
1:A:178:TRP:HB2	19:A:811:CLA:HMC3	1.80	0.62
19:A:820:CLA:H102	10:K:90:LEU:HD21	1.81	0.62
19:A:836:CLA:C4D	19:K:203:CLA:H12	2.29	0.62
22:4:305:BCR:H17C	32:4:317:CHL:H62	1.80	0.62
19:6:312:CLA:HMB1	19:6:312:CLA:CBB	2.29	0.62
2:B:5:LEU:CD2	8:I:103:ALA:HA	2.29	0.62
2:B:153:ALA:HB2	19:B:811:CLA:HBC2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:840:CLA:HMC3	19:1:5010:CLA:H12	1.80	0.62
11:1:159:PHE:HB2	19:1:5006:CLA:HBA1	1.81	0.62
19:4:313:CLA:HBA2	19:6:302:CLA:C15	2.29	0.62
2:B:3:THR:HG21	2:B:11:GLN:HE22	1.65	0.62
6:F:189:VAL:HG11	29:J:1903:LMG:H132	1.80	0.62
12:3:43:LEU:HD22	12:3:54:PRO:HA	1.81	0.62
19:B:825:CLA:H142	19:B:835:CLA:H143	1.81	0.62
19:A:842:CLA:C4B	20:A:844:PQN:H212	2.29	0.62
23:4:320:LHG:H111	19:6:302:CLA:NB	2.15	0.62
19:5:321:CLA:H193	19:6:320:CLA:C8	2.29	0.62
19:A:840:CLA:HAB	19:A:840:CLA:H121	1.81	0.62
31:8:304:LUT:H32	19:8:307:CLA:HMC2	1.80	0.62
19:4:309:CLA:H71	19:4:310:CLA:HMA1	1.81	0.62
17:6:175:LYS:NZ	19:6:310:CLA:HED1	2.14	0.62
2:B:345:ILE:HD11	19:B:818:CLA:H122	1.81	0.62
15:4:238:THR:HG23	15:4:243:ASN:OD1	1.99	0.62
19:5:311:CLA:H12	32:5:318:CHL:C2D	2.29	0.62
19:5:317:CLA:H171	19:5:319:CLA:HBB2	1.81	0.62
1:A:160:TYR:CD1	24:A:856:LMT:H5'	2.34	0.62
2:B:453:GLN:HE21	6:F:130:LEU:HD13	1.65	0.62
19:B:806:CLA:H2	19:B:806:CLA:HBA2	1.81	0.62
11:1:179:LEU:HD21	19:1:5007:CLA:HBC3	1.82	0.62
23:Z:316:LHG:H102	22:4:305:BCR:C33	2.30	0.62
17:6:66:TRP:CE3	38:6:326:ERG:H183	2.34	0.62
17:6:166:PRO:HG3	19:6:309:CLA:H43	1.81	0.62
18:A:801:CL0:H13	19:A:802:CLA:OBD	2.00	0.62
19:1:5007:CLA:ND	19:1:5012:CLA:H71	2.15	0.62
32:Z:302:CHL:CBB	31:Z:318:LUT:H34	2.30	0.62
19:5:306:CLA:H12	19:5:306:CLA:CHB	2.30	0.62
24:G:1604:LMT:H2'	19:1:5016:CLA:HMA1	1.80	0.62
19:7:307:CLA:HMD3	19:7:312:CLA:H43	1.81	0.62
11:1:219:ILE:HG21	19:1:5018:CLA:H52	1.82	0.61
32:Z:310:CHL:HBB2	32:Z:313:CHL:HBB2	1.82	0.61
2:B:487:PHE:O	2:B:491:GLN:HG2	2.00	0.61
2:B:540:LEU:HD21	22:B:845:BCR:H282	1.82	0.61
14:8:229:TRP:CZ2	22:8:303:BCR:H402	2.34	0.61
19:6:313:CLA:H12	32:6:319:CHL:C3D	2.30	0.61
19:5:306:CLA:HMB1	19:5:306:CLA:CBB	2.26	0.61
19:A:816:CLA:HBA2	35:7:302:DGA:HB21	1.81	0.61
2:B:210:TRP:HH2	22:B:844:BCR:H16C	1.65	0.61
19:B:822:CLA:CHA	19:B:822:CLA:HBA1	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:822:CLA:HBB2	22:B:845:BCR:H343	1.82	0.61
19:B:827:CLA:O1D	19:B:828:CLA:HMA1	2.01	0.61
19:B:850:CLA:HBC1	24:F:305:LMT:H52	1.81	0.61
19:3:5019:CLA:H92	19:5:314:CLA:H93	1.80	0.61
19:5:317:CLA:H171	19:5:319:CLA:CBB	2.30	0.61
3:C:9:ASP:HB2	5:E:68:ARG:NE	2.14	0.61
1:A:384:TYR:HB3	1:A:747:ILE:HD11	1.82	0.61
7:G:112:PHE:CZ	19:G:1601:CLA:HBC2	2.36	0.61
11:1:80:TRP:CE2	19:1:5015:CLA:HED3	2.35	0.61
32:Z:302:CHL:HBB2	31:Z:318:LUT:H34	1.83	0.61
31:3:5003:LUT:H28	31:3:5003:LUT:H371	1.81	0.61
38:6:326:ERG:H121	38:6:326:ERG:H283	1.82	0.61
12:3:146:TYR:CD1	24:3:5023:LMT:H5B	2.36	0.61
19:A:815:CLA:HMB2	24:A:853:LMT:H92	1.83	0.61
19:A:841:CLA:C4B	19:B:801:CLA:H172	2.31	0.61
15:4:252:TRP:CE3	19:4:313:CLA:HMA1	2.36	0.61
22:6:307:BCR:H19C	32:6:319:CHL:O2A	2.01	0.61
32:6:319:CHL:HAA2	32:6:319:CHL:HBD	1.83	0.61
1:A:265:PHE:HD1	33:3:5001:SPH:H111	1.66	0.61
11:Z:140:GLN:HB3	19:Z:306:CLA:HMC3	1.81	0.61
13:7:55:PRO:HD2	31:7:304:LUT:H23	1.82	0.61
14:8:138:TRP:CE3	19:8:318:CLA:CMA	2.83	0.61
32:5:316:CHL:HMB1	32:5:316:CHL:CBB	2.30	0.61
1:A:481:PRO:HG3	1:A:533:PHE:HB2	1.83	0.61
1:A:540:ALA:HB1	19:A:838:CLA:HMB3	1.82	0.60
19:A:815:CLA:C10	22:3:5006:BCR:H14C	2.29	0.60
19:I:201:CLA:C1B	19:I:201:CLA:H71	2.31	0.60
16:5:246:THR:H	17:6:227:GLN:NE2	1.99	0.60
23:6:303:LHG:H141	23:6:303:LHG:C26	2.31	0.60
19:A:822:CLA:C1D	22:A:859:BCR:H402	2.32	0.60
19:A:837:CLA:HAA1	19:A:838:CLA:HAA2	1.83	0.60
22:A:846:BCR:H362	22:A:847:BCR:H21C	1.83	0.60
19:B:823:CLA:H202	19:B:837:CLA:H192	1.82	0.60
19:B:828:CLA:H61	22:B:843:BCR:H23C	1.83	0.60
11:1:100:TYR:O	32:1:5014:CHL:HED1	2.01	0.60
19:5:310:CLA:HBA1	39:5:413:HOH:O	2.01	0.60
19:6:323:CLA:HMB1	19:6:323:CLA:CBB	2.29	0.60
1:A:190:TRP:CZ2	19:A:810:CLA:HMA1	2.37	0.60
19:A:808:CLA:C1C	19:A:828:CLA:H51	2.31	0.60
19:A:822:CLA:H62	19:A:823:CLA:H93	1.82	0.60
19:5:313:CLA:HBD	19:5:313:CLA:HBA2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:182:GLU:HG3	12:3:186:LYS:HE3	1.83	0.60
13:7:223:LEU:HD21	19:7:313:CLA:HMC3	1.83	0.60
15:4:134:TRP:HH2	24:4:322:LMT:H41	1.67	0.60
1:A:541:PHE:HZ	19:B:803:CLA:HBB2	1.67	0.60
19:A:821:CLA:H102	22:A:849:BCR:H12C	1.83	0.60
24:F:305:LMT:H5'	11:1:223:PHE:HB3	1.83	0.60
1:A:679:TRP:CE3	18:A:801:CL0:H4	2.36	0.60
19:A:821:CLA:C4C	19:A:827:CLA:H161	2.31	0.60
2:B:105:PHE:HA	2:B:107:ARG:NH1	2.17	0.60
23:1:5019:LHG:H192	37:8:302:SQD:H292	1.82	0.60
13:7:130:TRP:CZ2	22:7:305:BCR:HC8	2.37	0.60
15:4:83:PRO:HD2	31:4:304:LUT:H23	1.84	0.60
1:A:153:ILE:HA	19:A:814:CLA:HED1	1.83	0.60
19:A:833:CLA:NC	19:A:834:CLA:H93	2.16	0.60
2:B:96:HIS:CE1	19:B:809:CLA:HMB3	2.36	0.60
7:G:108:HIS:ND1	22:G:1603:BCR:H12C	2.17	0.60
1:A:59:PHE:CD2	19:A:805:CLA:HMC2	2.37	0.60
1:A:667:ALA:O	1:A:671:ILE:HG13	2.02	0.60
19:B:850:CLA:CBC	24:F:305:LMT:H52	2.32	0.60
19:A:823:CLA:C1B	30:K:201:DAO:H82	2.32	0.60
2:B:705:GLN:HG3	25:B:848:DGD:HA32	1.84	0.60
19:B:836:CLA:H152	27:F:304:RRX:C21	2.27	0.60
10:K:30:ILE:HA	10:K:35:ASN:HD22	1.67	0.60
19:1:5010:CLA:C1D	19:1:5016:CLA:H102	2.32	0.60
32:Z:309:CHL:H91	15:4:155:LEU:HD13	1.82	0.60
22:3:5004:BCR:H19C	19:3:5019:CLA:HBA1	1.84	0.60
1:A:49:ILE:HD12	19:A:842:CLA:HMB3	1.83	0.59
1:A:320:HIS:HB3	1:A:325:ILE:HD11	1.83	0.59
11:1:46:PRO:HB2	11:1:48:ASP:OD1	2.01	0.59
15:4:61:TRP:CH2	23:6:303:LHG:HC62	2.36	0.59
19:Z:305:CLA:H102	19:Z:308:CLA:HMA1	1.83	0.59
19:7:310:CLA:OBD	19:7:317:CLA:H2	2.01	0.59
2:B:65:ASN:OD1	19:B:808:CLA:HAA2	2.01	0.59
15:4:201:PHE:HD2	27:4:303:RRX:H12	1.66	0.59
32:5:318:CHL:HMB1	32:5:318:CHL:CBB	2.26	0.59
1:A:204:GLY:O	1:A:208:LEU:HB2	2.03	0.59
1:A:317:GLY:H	10:K:57:VAL:HG13	1.67	0.59
1:A:494:ALA:N	1:A:495:PRO:HD2	2.17	0.59
19:A:824:CLA:HMA1	19:A:843:CLA:HAB	1.84	0.59
19:B:827:CLA:C1D	19:B:827:CLA:H8	2.33	0.59
19:Z:308:CLA:H43	14:8:154:LEU:HD12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:317:CLA:C4A	19:5:317:CLA:HBA2	2.30	0.59
1:A:297:HIS:HB2	19:A:818:CLA:C1B	2.33	0.59
19:B:812:CLA:H203	19:B:820:CLA:CGA	2.33	0.59
19:B:819:CLA:H41	19:B:823:CLA:H92	1.83	0.59
19:Z:314:CLA:CMA	19:8:312:CLA:H101	2.32	0.59
19:5:308:CLA:H43	19:5:313:CLA:OBD	2.02	0.59
23:6:303:LHG:H142	19:6:322:CLA:ND	2.18	0.59
1:A:80:GLN:HG2	19:A:805:CLA:HMA1	1.84	0.59
19:A:842:CLA:HHC	19:A:842:CLA:HBB1	1.83	0.59
19:B:832:CLA:HMB2	19:F:301:CLA:CAB	2.33	0.59
14:8:138:TRP:CD2	19:8:318:CLA:CMA	2.86	0.59
19:8:309:CLA:HHC	19:8:309:CLA:HBB1	1.84	0.59
19:4:307:CLA:HHC	19:4:307:CLA:CBB	2.30	0.59
19:4:308:CLA:H121	23:4:320:LHG:C15	2.30	0.59
16:5:188:LYS:HD3	19:5:312:CLA:O1D	2.03	0.59
32:5:315:CHL:H141	19:6:323:CLA:H122	1.84	0.59
22:A:850:BCR:H23C	19:B:801:CLA:C10	2.32	0.59
19:B:823:CLA:HMA1	19:B:840:CLA:CED	2.33	0.59
19:B:839:CLA:C2C	22:B:847:BCR:H19C	2.33	0.59
18:A:801:CL0:H15	18:A:801:CL0:H11	1.83	0.59
17:6:205:LEU:O	17:6:209:LEU:HG	2.03	0.59
19:A:857:CLA:HHD	22:B:847:BCR:H383	1.84	0.59
6:F:150:PHE:HZ	24:F:305:LMT:H71	1.68	0.59
14:8:68:TRP:CE3	38:8:325:ERG:H9	2.38	0.59
19:8:307:CLA:HMB1	19:8:307:CLA:CBB	2.28	0.59
17:6:247:PRO:HG2	32:6:316:CHL:C4	2.32	0.59
19:A:830:CLA:HMD2	23:A:852:LHG:H282	1.85	0.59
19:A:832:CLA:HAC2	19:A:832:CLA:H203	1.84	0.59
31:1:5004:LUT:H181	31:1:5004:LUT:H8	1.85	0.59
11:Z:209:PRO:HG2	19:Z:307:CLA:HMB3	1.84	0.59
22:3:5007:BCR:C40	23:3:5021:LHG:HC41	2.32	0.59
14:8:191:LYS:CG	19:8:313:CLA:HED2	2.32	0.59
19:8:312:CLA:HBC3	19:8:312:CLA:HHD	1.85	0.59
16:5:105:LEU:HB3	16:5:107:GLN:NE2	2.18	0.59
16:5:144:GLY:HA2	16:5:147:ASN:ND2	2.17	0.59
32:5:315:CHL:H152	19:6:323:CLA:H193	1.83	0.59
23:6:303:LHG:H142	19:6:322:CLA:C1D	2.33	0.59
22:6:307:BCR:H292	19:6:313:CLA:H2	1.82	0.59
19:A:811:CLA:HBA1	19:A:811:CLA:CHA	2.31	0.58
19:A:832:CLA:C1D	19:A:832:CLA:H121	2.32	0.58
2:B:588:ILE:HA	2:B:591:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:118:PHE:CZ	12:3:122:ILE:HD11	2.37	0.58
32:8:301:CHL:HHC	32:8:301:CHL:HBB1	1.84	0.58
17:6:85:ILE:HG12	31:6:306:LUT:H41	1.85	0.58
19:A:814:CLA:H51	19:A:816:CLA:H112	1.84	0.58
19:B:826:CLA:H152	22:B:845:BCR:H373	1.84	0.58
22:B:844:BCR:HC8	22:B:844:BCR:H331	1.86	0.58
12:3:91:THR:O	12:3:92:ASN:C	2.41	0.58
19:3:5016:CLA:HBA1	19:3:5016:CLA:CHA	2.33	0.58
19:A:833:CLA:HAB	19:A:834:CLA:CHB	2.33	0.58
19:A:857:CLA:HHC	19:A:857:CLA:CBB	2.33	0.58
2:B:6:PHE:HB2	8:I:98:TYR:CE2	2.38	0.58
19:B:828:CLA:ND	22:B:843:BCR:H282	2.18	0.58
19:Z:308:CLA:H91	22:8:306:BCR:H353	1.86	0.58
19:4:306:CLA:H12	19:4:306:CLA:CHB	2.33	0.58
19:5:310:CLA:H61	19:5:322:CLA:CAB	2.31	0.58
17:6:149:LEU:HD12	32:6:321:CHL:HMD3	1.84	0.58
19:B:821:CLA:H93	7:G:45:PHE:HE2	1.69	0.58
13:7:128:MET:HG3	19:7:317:CLA:HMC3	1.85	0.58
14:8:64:VAL:HG23	38:8:325:ERG:H6	1.85	0.58
15:4:95:TRP:CH2	19:4:316:CLA:HAA2	2.38	0.58
19:A:820:CLA:HHC	19:A:820:CLA:HBB1	1.85	0.58
19:B:804:CLA:H141	19:B:810:CLA:HBC1	1.86	0.58
11:Z:213:ASN:HD21	11:Z:216:THR:HG23	1.67	0.58
13:7:227:ASN:HD21	34:5:324:3PH:H222	1.69	0.58
19:4:313:CLA:HMB1	19:4:313:CLA:CBB	2.27	0.58
19:5:307:CLA:NA	19:5:312:CLA:H91	2.18	0.58
19:5:309:CLA:HHC	19:5:309:CLA:CBB	2.31	0.58
19:6:311:CLA:H93	23:6:324:LHG:H322	1.86	0.58
1:A:208:LEU:HB3	22:A:847:BCR:C19	2.33	0.58
19:A:807:CLA:H2	19:A:809:CLA:H2	1.85	0.58
2:B:300:HIS:HB3	2:B:305:ILE:HD11	1.86	0.58
19:B:821:CLA:HMD2	22:B:842:BCR:C7	2.31	0.58
24:1:5002:LMT:H52	19:1:5016:CLA:H11	1.86	0.58
19:3:5016:CLA:O1D	19:3:5019:CLA:HMC3	2.03	0.58
19:A:813:CLA:HMA2	19:A:813:CLA:C2	2.34	0.58
2:B:375:HIS:HB2	19:B:827:CLA:C1B	2.34	0.58
19:K:205:CLA:C4B	22:K:206:BCR:H271	2.33	0.58
14:8:89:ILE:HB	14:8:90:PRO:HD3	1.86	0.58
32:4:314:CHL:HMB1	32:4:314:CHL:CBB	2.26	0.58
2:B:263:HIS:HE1	2:B:265:GLN:HB3	1.67	0.58
19:7:307:CLA:C5	19:7:312:CLA:H201	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:8:306:BCR:H291	19:8:312:CLA:O1A	2.04	0.58
31:5:303:LUT:C31	19:5:309:CLA:HMC2	2.33	0.58
19:5:308:CLA:HHC	19:5:308:CLA:CBB	2.28	0.58
17:6:242:LYS:HB2	22:6:308:BCR:H343	1.85	0.58
19:6:301:CLA:HHC	19:6:301:CLA:CBB	2.33	0.58
14:8:229:TRP:CG	22:8:303:BCR:H292	2.38	0.58
19:5:307:CLA:C1C	19:5:312:CLA:H122	2.33	0.58
1:A:282:LEU:HD21	1:A:375:PRO:HD2	1.85	0.58
2:B:395:PHE:CE2	22:B:846:BCR:H272	2.39	0.58
2:B:460:PHE:CG	19:B:850:CLA:HMB3	2.39	0.58
19:8:312:CLA:HMB1	19:8:312:CLA:CBB	2.32	0.58
15:4:161:GLU:HG3	19:4:316:CLA:C4B	2.34	0.58
19:5:311:CLA:HMB1	19:5:311:CLA:CBB	2.33	0.58
19:6:301:CLA:C1A	19:6:301:CLA:CGA	2.81	0.58
19:6:320:CLA:H121	19:6:320:CLA:H91	1.86	0.58
19:A:840:CLA:HMC3	19:A:842:CLA:C4D	2.33	0.57
2:B:175:ARG:HB2	19:B:813:CLA:HBC2	1.85	0.57
19:B:816:CLA:O1A	7:G:116:ALA:HB1	2.03	0.57
19:B:823:CLA:CMD	19:B:824:CLA:HAB	2.34	0.57
10:K:107:LEU:HA	10:K:110:ILE:HG12	1.85	0.57
19:7:310:CLA:HMD2	19:7:317:CLA:C1D	2.34	0.57
11:1:115:PHE:CZ	19:1:5011:CLA:HMD2	2.39	0.57
12:3:91:THR:O	12:3:93:ILE:HG23	2.02	0.57
22:3:5006:BCR:H17C	19:3:5012:CLA:CBB	2.32	0.57
19:8:311:CLA:HMB1	19:8:311:CLA:CBB	2.34	0.57
22:6:307:BCR:C21	19:6:313:CLA:H122	2.33	0.57
19:6:309:CLA:HBA1	19:6:309:CLA:CHA	2.34	0.57
19:A:804:CLA:HAB	19:A:806:CLA:CAD	2.33	0.57
19:A:811:CLA:HBB1	19:A:811:CLA:HMB1	1.86	0.57
19:A:824:CLA:H52	22:A:849:BCR:H363	1.86	0.57
7:G:103:TRP:HA	7:G:106:LEU:HD12	1.86	0.57
19:7:313:CLA:HBB1	19:7:313:CLA:HHC	1.85	0.57
1:A:265:PHE:CD1	33:3:5001:SPH:H111	2.39	0.57
19:B:815:CLA:H8	22:B:842:BCR:H23C	1.86	0.57
22:B:847:BCR:H321	22:B:847:BCR:HC8	1.85	0.57
17:6:125:GLU:HG3	19:6:318:CLA:C4B	2.34	0.57
38:6:326:ERG:H183	38:6:326:ERG:H213	1.86	0.57
5:E:36:GLY:HA3	5:E:62:VAL:HG11	1.85	0.57
6:F:208:GLN:O	6:F:212:ARG:HG2	2.04	0.57
11:Z:119:VAL:HG12	11:Z:121:PHE:HD2	1.69	0.57
19:7:309:CLA:H111	19:7:310:CLA:H151	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:8:148:GLY:HA3	14:8:161:LYS:CG	2.35	0.57
1:A:673:LEU:O	19:A:802:CLA:HBA1	2.05	0.57
19:A:843:CLA:CAD	19:A:843:CLA:H52	2.35	0.57
19:B:810:CLA:C2	19:B:810:CLA:H2A	2.35	0.57
19:I:201:CLA:H93	19:I:201:CLA:HMB2	1.87	0.57
11:Z:123:LEU:HD11	32:Z:310:CHL:CBC	2.34	0.57
1:A:20:ASN:N	1:A:21:PRO:HD3	2.19	0.57
2:B:450:PRO:O	2:B:453:GLN:HG2	2.04	0.57
2:B:478:LEU:HD13	19:B:833:CLA:HMD3	1.87	0.57
2:B:482:LYS:HG3	2:B:487:PHE:CZ	2.40	0.57
11:1:119:VAL:HG11	32:1:5017:CHL:HMD1	1.87	0.57
19:7:308:CLA:H151	19:7:308:CLA:H203	1.87	0.57
16:5:189:ASN:ND2	19:5:312:CLA:HMD1	2.19	0.57
38:6:326:ERG:H191	38:6:326:ERG:H182	1.85	0.57
19:A:836:CLA:H61	19:K:203:CLA:HBA2	1.87	0.57
19:B:806:CLA:H72	19:B:813:CLA:O1A	2.05	0.57
19:1:5008:CLA:H152	19:1:5012:CLA:HMC1	1.87	0.57
19:3:5014:CLA:C1C	23:3:5021:LHG:HC42	2.34	0.57
15:4:214:LYS:HG3	19:4:312:CLA:HED2	1.85	0.57
19:6:313:CLA:H12	32:6:319:CHL:C2D	2.34	0.57
23:6:324:LHG:H272	23:6:324:LHG:HC91	1.87	0.57
1:A:508:LEU:HD12	1:A:523:MET:HB3	1.87	0.57
19:B:832:CLA:CMA	29:J:1904:LMG:H151	2.35	0.57
11:1:224:PHE:CE1	14:8:123:LEU:HD23	2.38	0.57
19:Z:303:CLA:HMD2	19:Z:312:CLA:C1D	2.35	0.57
14:8:191:LYS:HD3	19:8:308:CLA:HBA2	1.87	0.57
31:4:304:LUT:H181	32:4:317:CHL:CBB	2.35	0.57
19:4:311:CLA:O1D	19:4:311:CLA:H2A	2.05	0.57
17:6:123:TRP:CH2	22:6:307:BCR:H323	2.38	0.57
17:6:178:LYS:HD3	19:6:314:CLA:O1D	2.05	0.57
19:A:815:CLA:H41	24:A:853:LMT:H82	1.86	0.57
19:A:821:CLA:H52	22:A:849:BCR:H16C	1.85	0.57
19:A:827:CLA:H193	19:A:827:CLA:H152	1.87	0.57
2:B:464:ILE:HD11	19:B:835:CLA:H2	1.86	0.57
2:B:694:TRP:HA	19:B:838:CLA:O1D	2.04	0.57
4:D:193:PRO:O	4:D:196:ILE:HG12	2.05	0.57
32:8:317:CHL:HMB1	32:8:317:CHL:CBB	2.34	0.57
32:5:315:CHL:H203	19:6:320:CLA:HMC1	1.86	0.57
19:A:821:CLA:H72	22:A:849:BCR:C12	2.31	0.56
19:B:816:CLA:HBB1	19:B:816:CLA:HMB1	1.87	0.56
19:B:822:CLA:CBB	22:B:845:BCR:H343	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:832:CLA:C1	29:J:1904:LMG:H112	2.35	0.56
22:B:842:BCR:H343	7:G:102:GLY:HA2	1.87	0.56
7:G:95:PHE:CE2	19:G:1602:CLA:HMB2	2.39	0.56
12:3:171:PHE:HE2	19:3:5008:CLA:H203	1.69	0.56
19:7:311:CLA:H42	33:7:321:SPH:H72	1.87	0.56
19:7:324:CLA:C1	38:6:326:ERG:H42	2.34	0.56
32:6:316:CHL:HHC	32:6:316:CHL:HBB1	1.87	0.56
1:A:733:LEU:HD22	19:A:841:CLA:HMA1	1.86	0.56
19:A:828:CLA:H191	22:A:858:BCR:C19	2.36	0.56
2:B:93:TRP:CZ2	8:I:77:SER:HA	2.40	0.56
19:B:808:CLA:H52	19:B:808:CLA:C1C	2.35	0.56
19:B:825:CLA:HMB1	19:B:825:CLA:CBB	2.29	0.56
19:B:826:CLA:H141	22:B:846:BCR:H15C	1.88	0.56
19:B:850:CLA:H12	19:B:850:CLA:C4A	2.35	0.56
31:7:304:LUT:H8	31:7:304:LUT:H181	1.87	0.56
19:4:306:CLA:HMB1	19:4:306:CLA:CBB	2.35	0.56
16:5:240:VAL:HG13	16:5:247:ILE:HG13	1.87	0.56
19:5:310:CLA:HBC1	32:5:315:CHL:CAB	2.34	0.56
19:5:321:CLA:HAC1	28:6:304:C7Z:C36	2.35	0.56
1:A:707:LEU:HD23	6:F:216:LEU:CD2	2.36	0.56
19:B:814:CLA:H92	22:B:844:BCR:C17	2.36	0.56
19:B:831:CLA:HBB1	19:B:831:CLA:HMB1	1.88	0.56
9:J:36:PRO:HA	29:J:1904:LMG:O2	2.04	0.56
32:Z:309:CHL:H41	32:Z:309:CHL:H71	1.86	0.56
14:8:30:TRP:HH2	34:8:322:3PH:H322	1.70	0.56
32:8:301:CHL:HAA1	32:8:301:CHL:CBD	2.36	0.56
16:5:91:GLN:HE22	16:5:98:VAL:HB	1.70	0.56
16:5:240:VAL:HG13	16:5:247:ILE:CG1	2.35	0.56
19:A:823:CLA:H11	10:K:65:LEU:HD23	1.87	0.56
2:B:646:VAL:HA	19:B:809:CLA:HAC1	1.87	0.56
19:B:812:CLA:HHC	19:B:812:CLA:CBB	2.34	0.56
19:F:303:CLA:HHC	19:F:303:CLA:CBB	2.32	0.56
11:1:39:SER:HB2	37:8:302:SQD:H61	1.88	0.56
14:8:233:TYR:CD1	19:8:309:CLA:H11	2.40	0.56
17:6:244:ILE:CG1	22:6:308:BCR:H342	2.35	0.56
1:A:677:PHE:HB2	19:A:802:CLA:O1A	2.05	0.56
19:A:817:CLA:H12	19:A:817:CLA:NA	2.20	0.56
19:A:843:CLA:HMC3	23:A:851:LHG:HC11	1.87	0.56
19:B:812:CLA:O1D	19:B:813:CLA:HMC1	2.05	0.56
9:J:33:PHE:HA	29:J:1904:LMG:O5	2.06	0.56
11:Z:58:LEU:CD2	14:8:175:PRO:HA	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Z:155:ASP:HA	31:Z:318:LUT:H24	1.88	0.56
19:Z:305:CLA:HMC2	31:Z:317:LUT:C32	2.35	0.56
13:7:95:VAL:HG23	13:7:97:LEU:HG	1.87	0.56
14:8:229:TRP:CE2	22:8:303:BCR:H402	2.41	0.56
15:4:135:TYR:CD1	24:4:322:LMT:H4'	2.41	0.56
19:4:308:CLA:HBA1	19:4:308:CLA:CHA	2.35	0.56
10:K:30:ILE:HA	10:K:35:ASN:ND2	2.21	0.56
11:1:134:MET:HG3	19:1:5016:CLA:HMC3	1.88	0.56
22:3:5006:BCR:H381	19:3:5018:CLA:C2C	2.36	0.56
22:5:304:BCR:C10	32:5:320:CHL:HBB2	2.36	0.56
1:A:610:PHE:HD1	19:A:837:CLA:HBC2	1.71	0.56
22:B:845:BCR:HC32	19:1:5016:CLA:H51	1.88	0.56
12:3:43:LEU:CD2	12:3:54:PRO:HA	2.35	0.56
17:6:99:ASN:O	17:6:103:GLU:HG3	2.06	0.56
19:A:828:CLA:O1D	19:A:829:CLA:HHB	2.06	0.56
2:B:340:ALA:HB2	22:B:846:BCR:H372	1.86	0.56
24:F:305:LMT:H1'	11:1:223:PHE:HB3	1.87	0.56
10:K:39:VAL:HA	19:K:202:CLA:O1A	2.05	0.56
19:7:311:CLA:HMA2	19:7:318:CLA:HAC2	1.87	0.56
15:4:63:PRO:HD2	19:6:302:CLA:O1D	2.06	0.56
16:5:165:PRO:HD2	19:5:306:CLA:OBD	2.05	0.56
17:6:66:TRP:HZ2	19:6:318:CLA:HAA2	1.70	0.56
1:A:262:ALA:HB3	1:A:263:PRO:HD3	1.88	0.56
19:A:841:CLA:H11	19:B:801:CLA:H192	1.87	0.56
19:B:825:CLA:HAA2	19:B:826:CLA:OBD	2.04	0.56
24:Z:301:LMT:H6E	19:Z:315:CLA:HAA2	1.88	0.56
12:3:152:ALA:HA	12:3:155:LYS:HE3	1.88	0.56
19:A:808:CLA:HHC	19:A:808:CLA:CBB	2.32	0.56
19:A:824:CLA:H11	22:A:848:BCR:H363	1.88	0.56
2:B:312:PRO:HG3	19:B:840:CLA:HBC2	1.88	0.56
13:7:239:PRO:HG2	19:7:319:CLA:HMB3	1.88	0.56
14:8:225:LEU:HD21	19:8:314:CLA:HMC3	1.88	0.56
32:8:317:CHL:HAA2	32:8:319:CHL:H112	1.87	0.56
19:A:822:CLA:C4D	22:A:859:BCR:H282	2.35	0.55
2:B:604:GLN:HG3	2:B:734:PHE:HZ	1.71	0.55
19:B:802:CLA:HMB3	19:B:803:CLA:CAD	2.35	0.55
19:B:809:CLA:HMB1	19:B:809:CLA:CBB	2.34	0.55
19:B:809:CLA:HBA2	19:B:809:CLA:C2	2.36	0.55
10:K:79:ASN:HB2	19:K:205:CLA:HBA2	1.88	0.55
19:A:820:CLA:HAA2	10:K:87:VAL:HG13	1.88	0.55
19:B:828:CLA:HHC	19:B:828:CLA:CBB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:7:311:CLA:C3C	33:7:321:SPH:H131	2.36	0.55
15:4:95:TRP:CD2	24:4:321:LMT:H1B	2.42	0.55
16:5:135:ARG:HD2	32:6:315:CHL:O2D	2.06	0.55
23:6:324:LHG:H291	23:6:324:LHG:H131	1.88	0.55
1:A:694:GLN:O	1:A:698:GLU:HG3	2.06	0.55
2:B:91:ALA:HA	2:B:114:VAL:HG12	1.89	0.55
2:B:271:LEU:HD23	2:B:274:MET:HE3	1.89	0.55
23:Z:316:LHG:H102	22:4:305:BCR:H333	1.88	0.55
34:3:5022:3PH:H242	13:7:33:TRP:HH2	1.71	0.55
13:7:136:TRP:CD1	13:7:140:LYS:HE3	2.41	0.55
19:A:824:CLA:CMD	19:A:825:CLA:HAB	2.36	0.55
19:A:833:CLA:C4D	19:A:834:CLA:H122	2.36	0.55
22:A:847:BCR:H272	24:A:853:LMT:H111	1.88	0.55
2:B:687:PRO:O	2:B:688:LEU:HB2	2.06	0.55
19:B:820:CLA:HBA1	7:G:98:ILE:HD12	1.89	0.55
13:7:67:TRP:HZ2	19:7:317:CLA:HAA2	1.71	0.55
22:7:305:BCR:H272	19:7:311:CLA:O1A	2.05	0.55
19:8:310:CLA:H93	19:8:311:CLA:HMA1	1.87	0.55
17:6:108:LEU:N	17:6:108:LEU:HD12	2.22	0.55
19:6:313:CLA:HMB1	19:6:313:CLA:CBB	2.34	0.55
1:A:15:ILE:HG21	19:A:810:CLA:HAA1	1.88	0.55
19:A:804:CLA:HED1	19:A:811:CLA:HBD	1.88	0.55
19:A:836:CLA:C1B	19:K:203:CLA:H52	2.36	0.55
19:B:810:CLA:H2	19:B:810:CLA:CGD	2.37	0.55
19:B:822:CLA:C1C	24:1:5002:LMT:H101	2.37	0.55
6:F:204:LEU:H	6:F:204:LEU:HD12	1.71	0.55
16:5:91:GLN:NE2	16:5:98:VAL:HB	2.21	0.55
16:5:172:PHE:CD2	27:5:302:RRX:H13	2.32	0.55
17:6:89:GLU:OE1	17:6:201:PRO:HG2	2.07	0.55
19:A:807:CLA:HHC	19:A:807:CLA:CBB	2.31	0.55
24:A:853:LMT:O6'	24:A:853:LMT:H5B	2.07	0.55
8:I:83:THR:HB	19:I:201:CLA:H12	1.89	0.55
19:1:5010:CLA:C1B	19:1:5016:CLA:H13	2.36	0.55
19:1:5018:CLA:HHC	19:1:5018:CLA:HBB1	1.88	0.55
11:Z:157:LEU:HD12	31:Z:318:LUT:H222	1.88	0.55
13:7:113:ASN:HB2	13:7:115:ILE:HG13	1.89	0.55
23:4:320:LHG:HC92	23:4:320:LHG:C28	2.19	0.55
19:6:318:CLA:HMA1	19:6:322:CLA:HBC2	1.89	0.55
19:B:803:CLA:H91	19:B:804:CLA:H8	1.89	0.55
19:B:831:CLA:H112	19:F:301:CLA:C17	2.36	0.55
32:1:5017:CHL:HMB1	32:1:5017:CHL:CBB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:82:GLY:HA2	31:7:304:LUT:H181	1.88	0.55
13:7:175:LEU:HD13	19:7:306:CLA:H11	1.88	0.55
13:7:199:ILE:HG22	19:7:308:CLA:CBB	2.37	0.55
19:5:314:CLA:HHC	19:5:314:CLA:CBB	2.28	0.55
19:5:321:CLA:H191	19:6:320:CLA:H92	1.88	0.55
17:6:172:LEU:CB	19:6:309:CLA:HMA1	2.36	0.55
19:A:828:CLA:H92	19:A:828:CLA:H41	1.87	0.55
19:B:817:CLA:C1C	19:B:817:CLA:H101	2.37	0.55
11:1:210:TRP:HB3	14:8:117:ALA:HB2	1.89	0.55
12:3:56:TRP:CH2	19:3:5018:CLA:HAA2	2.41	0.55
12:3:146:TYR:CZ	24:3:5023:LMT:H4'	2.41	0.55
13:7:225:ASP:HB3	13:7:229:VAL:HG23	1.87	0.55
32:4:314:CHL:HBD	32:4:314:CHL:HAA1	1.88	0.55
22:6:307:BCR:H291	19:6:313:CLA:C2	2.29	0.55
22:6:307:BCR:C21	19:6:313:CLA:H152	2.37	0.55
1:A:265:PHE:HB3	33:3:5001:SPH:H102	1.89	0.55
19:A:832:CLA:HHC	19:A:832:CLA:CBB	2.31	0.55
19:A:841:CLA:HBA1	19:A:841:CLA:CHA	2.36	0.55
22:A:850:BCR:C23	19:B:801:CLA:H101	2.36	0.55
19:B:805:CLA:HBB1	19:B:805:CLA:HMB1	1.88	0.55
19:3:5013:CLA:H172	19:5:319:CLA:HMB2	1.89	0.55
19:3:5016:CLA:C3D	35:7:302:DGA:HBN1	2.36	0.55
19:3:5020:CLA:HED1	23:7:320:LHG:H311	1.88	0.55
15:4:123:ILE:HB	15:4:125:PHE:HD1	1.71	0.55
16:5:217:ALA:HB1	16:5:225:ASN:ND2	2.22	0.55
19:6:318:CLA:HMA1	19:6:322:CLA:CBC	2.37	0.55
1:A:542:THR:HB	1:A:602:SER:HB2	1.89	0.55
19:A:822:CLA:NB	19:A:823:CLA:H8	2.22	0.55
19:A:843:CLA:H2	19:A:843:CLA:HBD	1.87	0.55
6:F:186:ILE:HD12	9:J:10:THR:HG22	1.89	0.55
7:G:45:PHE:CZ	7:G:110:VAL:HG21	2.42	0.55
14:8:229:TRP:CD2	22:8:303:BCR:H292	2.42	0.55
15:4:226:PHE:CE2	15:4:230:ILE:HD11	2.42	0.55
19:4:311:CLA:CBC	19:4:311:CLA:CHD	2.83	0.55
19:5:310:CLA:HMD2	19:5:317:CLA:C1D	2.37	0.55
17:6:169:LEU:HD12	19:6:309:CLA:HMA2	1.89	0.55
31:6:305:LUT:C11	19:6:310:CLA:HMC2	2.37	0.55
19:A:803:CLA:H192	19:A:841:CLA:H172	1.89	0.54
19:A:827:CLA:HMB1	19:A:827:CLA:CBB	2.35	0.54
19:A:836:CLA:HHC	19:A:836:CLA:CBB	2.35	0.54
2:B:192:THR:HG21	2:B:279:LEU:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:850:CLA:HBC1	24:F:305:LMT:H81	1.88	0.54
19:G:1601:CLA:HHC	19:G:1601:CLA:CBB	2.32	0.54
19:G:1602:CLA:HED2	19:G:1602:CLA:H2A	1.89	0.54
10:K:55:PRO:HG3	10:K:61:THR:CG2	2.37	0.54
11:Z:84:GLY:HA2	31:Z:317:LUT:H181	1.90	0.54
19:Z:305:CLA:H52	31:Z:317:LUT:H28	1.89	0.54
31:3:5003:LUT:H181	31:3:5003:LUT:H8	1.88	0.54
19:3:5009:CLA:C1A	19:3:5014:CLA:H8	2.38	0.54
24:3:5023:LMT:O2'	19:5:322:CLA:HMA3	2.07	0.54
16:5:99:TYR:HB3	16:5:102:GLU:HG2	1.88	0.54
19:A:824:CLA:HBB1	19:A:824:CLA:HHC	1.88	0.54
19:B:832:CLA:HAA2	9:J:36:PRO:HG2	1.89	0.54
13:7:173:MET:HG2	19:7:324:CLA:C4	2.36	0.54
19:7:324:CLA:H43	38:6:326:ERG:C4	2.37	0.54
16:5:242:VAL:HG21	32:5:315:CHL:HMD1	1.89	0.54
17:6:66:TRP:CE2	38:6:326:ERG:C19	2.90	0.54
19:A:823:CLA:HHC	19:A:823:CLA:CBB	2.36	0.54
19:B:834:CLA:HHC	19:B:834:CLA:HBB1	1.89	0.54
19:Z:308:CLA:HMD2	19:Z:315:CLA:ND	2.21	0.54
19:4:313:CLA:H71	22:6:307:BCR:H342	1.89	0.54
38:6:326:ERG:H121	38:6:326:ERG:C22	2.38	0.54
2:B:93:TRP:CE2	8:I:77:SER:HA	2.42	0.54
3:C:27:GLU:HB3	3:C:44:ARG:HH22	1.72	0.54
12:3:15:LEU:HD23	12:3:35:PHE:HD1	1.72	0.54
12:3:154:PHE:HZ	22:3:5005:BCR:HC41	1.72	0.54
19:8:313:CLA:O1A	24:4:302:LMT:H42	2.06	0.54
19:A:826:CLA:H171	19:A:839:CLA:C7	2.34	0.54
19:B:836:CLA:HBC2	29:J:1904:LMG:H252	1.87	0.54
13:7:67:TRP:CZ2	19:7:317:CLA:HAA2	2.43	0.54
19:8:311:CLA:HAC1	32:8:316:CHL:HBB2	1.90	0.54
15:4:135:TYR:CE1	24:4:322:LMT:H1B	2.42	0.54
19:4:307:CLA:HMA3	19:4:307:CLA:C6	2.26	0.54
16:5:123:ALA:HB1	19:5:325:CLA:HAA1	1.90	0.54
1:A:349:TRP:HB3	19:A:805:CLA:HAC1	1.90	0.54
19:A:808:CLA:HBB2	19:A:828:CLA:H202	1.89	0.54
19:A:817:CLA:H43	39:K:6002:HOH:O	2.08	0.54
19:A:822:CLA:HMB2	19:A:823:CLA:H2	1.88	0.54
2:B:358:PRO:HG3	19:B:818:CLA:HBA1	1.90	0.54
11:Z:134:MET:HG3	19:Z:315:CLA:HMC3	1.88	0.54
32:4:315:CHL:HMB1	32:4:315:CHL:CBB	2.34	0.54
2:B:355:SER:CB	19:B:826:CLA:HAC2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:530:THR:HG21	2:B:583:TRP:CE2	2.43	0.54
3:C:12:ILE:HG12	21:C:102:SF4:S2	2.48	0.54
31:1:5004:LUT:H32	32:1:5009:CHL:CBB	2.36	0.54
13:7:210:ALA:HB2	19:7:319:CLA:HED3	1.89	0.54
17:6:163:PRO:HD2	31:6:305:LUT:H23	1.90	0.54
19:6:310:CLA:NA	19:6:314:CLA:H91	2.23	0.54
1:A:338:HIS:HE1	23:A:851:LHG:HC12	1.71	0.54
19:A:804:CLA:HBA1	19:A:811:CLA:C1D	2.38	0.54
17:6:166:PRO:CG	19:6:309:CLA:H43	2.38	0.54
19:6:302:CLA:HMA1	19:6:322:CLA:OBD	2.07	0.54
19:6:312:CLA:H2	19:6:312:CLA:O1A	2.08	0.54
1:A:333:PHE:CD2	23:A:851:LHG:HC42	2.43	0.54
19:A:818:CLA:H8	19:A:836:CLA:HMA2	1.89	0.54
19:A:840:CLA:H61	22:F:302:BCR:H17C	1.90	0.54
32:Z:313:CHL:HMB1	32:Z:313:CHL:CBB	2.30	0.54
19:3:5016:CLA:H62	35:7:302:DGA:HBT1	1.90	0.54
36:7:322:PLM:H92	32:8:315:CHL:O1A	2.08	0.54
15:4:217:LYS:HD2	19:4:312:CLA:O1D	2.08	0.54
16:5:55:TRP:CZ2	19:5:314:CLA:HED2	2.42	0.54
22:5:304:BCR:H291	19:5:311:CLA:NB	2.22	0.54
19:5:308:CLA:C1A	19:5:308:CLA:CGA	2.85	0.54
32:5:320:CHL:HAA2	32:5:320:CHL:HBD	1.90	0.54
19:A:803:CLA:HHC	19:A:803:CLA:CBB	2.37	0.54
2:B:107:ARG:HE	2:B:116:ILE:HG12	1.73	0.54
2:B:649:TRP:CZ2	19:B:803:CLA:H61	2.43	0.54
19:B:837:CLA:HHC	19:B:837:CLA:HBB1	1.90	0.54
19:B:850:CLA:H143	19:B:850:CLA:C20	2.38	0.54
8:I:97:VAL:O	8:I:101:LYS:HG3	2.08	0.54
11:Z:89:LEU:HD21	11:Z:187:PHE:CZ	2.43	0.54
19:Z:308:CLA:OBD	19:Z:315:CLA:HBA2	2.08	0.54
12:3:183:LEU:HB3	19:3:5008:CLA:HMA1	1.88	0.54
19:3:5009:CLA:C1C	19:3:5014:CLA:H121	2.37	0.54
19:5:310:CLA:C6	19:5:322:CLA:HAB	2.35	0.54
19:5:325:CLA:HBA1	19:5:325:CLA:CBD	2.38	0.54
19:6:310:CLA:CAD	19:6:314:CLA:H2	2.38	0.54
19:A:815:CLA:H101	22:3:5006:BCR:C14	2.36	0.53
7:G:51:PHE:CE1	19:G:1602:CLA:HMC2	2.43	0.53
10:K:77:ILE:HD11	12:3:21:GLN:HG2	1.89	0.53
11:1:210:TRP:CD2	19:1:5013:CLA:HMA2	2.43	0.53
12:3:94:LYS:HD2	12:3:96:PHE:CZ	2.42	0.53
19:8:307:CLA:HMD2	32:8:317:CHL:CGA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:8:311:CLA:HAC1	32:8:316:CHL:CBB	2.38	0.53
19:A:818:CLA:HHC	19:A:818:CLA:HBB1	1.89	0.53
16:5:227:ILE:HB	19:5:308:CLA:H11	1.90	0.53
2:B:518:PHE:HE2	19:B:836:CLA:C2D	2.21	0.53
19:B:833:CLA:HHC	19:B:833:CLA:CBB	2.33	0.53
19:B:835:CLA:HMB1	19:B:835:CLA:CBB	2.38	0.53
11:1:31:LYS:HE3	11:1:33:GLY:O	2.08	0.53
11:Z:94:LEU:HD12	19:Z:311:CLA:HMD3	1.89	0.53
11:Z:173:GLU:HG3	32:Z:302:CHL:C4B	2.39	0.53
31:3:5002:LUT:H30	19:3:5008:CLA:H72	1.91	0.53
22:3:5006:BCR:H272	19:3:5018:CLA:CHC	2.38	0.53
19:7:324:CLA:HBB1	19:7:324:CLA:CMB	2.33	0.53
1:A:305:PHE:CZ	19:A:819:CLA:H142	2.44	0.53
1:A:690:ARG:HD3	2:B:567:GLY:HA3	1.90	0.53
19:A:839:CLA:HMB1	19:A:839:CLA:CBB	2.37	0.53
2:B:184:PHE:CE2	19:B:819:CLA:HBB2	2.44	0.53
11:1:57:PRO:HD2	31:1:5004:LUT:C23	2.38	0.53
19:8:311:CLA:HMD2	19:8:318:CLA:CHD	2.38	0.53
16:5:124:TRP:O	16:5:128:LEU:HG	2.08	0.53
1:A:674:GLY:HA2	22:A:850:BCR:H17C	1.90	0.53
19:A:808:CLA:C3D	19:A:828:CLA:HBA1	2.39	0.53
19:A:819:CLA:H171	19:A:835:CLA:H41	1.90	0.53
11:1:38:GLY:HA3	14:8:146:SER:HB2	1.90	0.53
12:3:23:SER:HB2	12:3:27:LEU:HD12	1.91	0.53
33:7:321:SPH:H91	19:6:301:CLA:HAC2	1.91	0.53
15:4:244:LEU:O	15:4:248:LEU:HG	2.08	0.53
1:A:412:PHE:CD1	1:A:416:ASP:HB2	2.44	0.53
1:A:658:ILE:HG13	1:A:659:GLN:HG3	1.90	0.53
19:B:808:CLA:H52	19:B:808:CLA:NC	2.24	0.53
19:B:825:CLA:H61	19:B:836:CLA:O1A	2.09	0.53
19:B:833:CLA:HBA2	19:B:834:CLA:CMB	2.39	0.53
4:D:128:LEU:HA	4:D:132:PHE:HD2	1.74	0.53
19:K:204:CLA:HMB1	19:K:204:CLA:HBB1	1.89	0.53
32:1:5017:CHL:HAA2	32:1:5017:CHL:HBD	1.91	0.53
12:3:118:PHE:CD1	19:3:5016:CLA:HBD	2.44	0.53
31:8:305:LUT:H361	19:8:310:CLA:H142	1.90	0.53
32:8:319:CHL:HMB1	32:8:319:CHL:CBB	2.36	0.53
19:8:320:CLA:HHC	19:8:320:CLA:CBB	2.38	0.53
2:B:284:ILE:HG23	19:B:816:CLA:H192	1.90	0.53
19:B:808:CLA:CMA	19:I:201:CLA:HMB3	2.35	0.53
4:D:94:GLN:H	4:D:106:MET:HG2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:3:5009:CLA:NC	19:3:5014:CLA:H121	2.24	0.53
13:7:189:LYS:HG3	19:7:312:CLA:HED2	1.89	0.53
32:8:316:CHL:HMB1	32:8:316:CHL:CBB	2.37	0.53
19:6:301:CLA:H122	32:6:316:CHL:H71	1.91	0.53
19:6:314:CLA:C1C	23:6:324:LHG:HC42	2.38	0.53
19:B:833:CLA:H112	19:B:833:CLA:H171	1.91	0.53
4:D:131:LYS:HD2	4:D:132:PHE:CZ	2.43	0.53
12:3:79:GLU:CD	12:3:213:PHE:HB3	2.29	0.53
19:7:307:CLA:HMB3	19:7:312:CLA:H151	1.90	0.53
23:8:321:LHG:H242	23:8:321:LHG:H131	1.90	0.53
24:8:323:LMT:H6D	24:8:323:LMT:C1B	2.31	0.53
19:A:832:CLA:H121	19:A:832:CLA:ND	2.24	0.53
19:A:838:CLA:H92	19:A:839:CLA:HHD	1.91	0.53
19:Z:307:CLA:H12	19:Z:307:CLA:H3A	1.91	0.53
14:8:103:GLU:HG2	14:8:105:TYR:CZ	2.43	0.53
16:5:128:LEU:HD12	32:5:318:CHL:HMA2	1.90	0.53
17:6:88:GLN:HG2	19:6:313:CLA:C4D	2.39	0.53
17:6:172:LEU:HD23	17:6:175:LYS:HD2	1.89	0.53
19:6:309:CLA:H2	19:6:309:CLA:CHB	2.39	0.53
19:A:824:CLA:H193	19:A:839:CLA:C3D	2.39	0.53
2:B:49:ALA:HB2	2:B:158:LEU:HG	1.91	0.53
2:B:70:ALA:HB2	2:B:136:LEU:HB2	1.91	0.53
19:B:830:CLA:HBC1	22:B:845:BCR:H19C	1.91	0.53
19:1:5007:CLA:HMB1	19:1:5007:CLA:CBB	2.32	0.53
32:Z:310:CHL:HHD	32:Z:310:CHL:HBC3	1.90	0.53
32:Z:310:CHL:H201	14:8:128:PHE:CD2	2.44	0.53
19:A:830:CLA:HMB1	19:A:830:CLA:CBB	2.37	0.52
19:A:840:CLA:HMC3	19:A:842:CLA:ND	2.24	0.52
2:B:71:TRP:CE2	8:I:71:PRO:HD2	2.44	0.52
19:B:829:CLA:H142	25:B:848:DGD:HAH1	1.90	0.52
19:A:829:CLA:C1C	22:A:847:BCR:HC42	2.39	0.52
2:B:440:HIS:O	2:B:444:MET:HG2	2.09	0.52
19:B:819:CLA:NB	19:B:824:CLA:H111	2.24	0.52
19:B:823:CLA:NA	22:B:845:BCR:H362	2.24	0.52
19:B:825:CLA:C3B	22:B:846:BCR:H363	2.39	0.52
24:1:5002:LMT:H31	19:1:5016:CLA:H11	1.91	0.52
32:1:5014:CHL:HBD	32:1:5014:CHL:HAA1	1.91	0.52
11:Z:91:VAL:HG13	11:Z:96:TYR:HB2	1.91	0.52
13:7:182:LYS:HD2	13:7:186:TYR:CE2	2.44	0.52
1:A:168:VAL:HG22	24:A:856:LMT:H112	1.90	0.52
1:A:316:TRP:CD1	10:K:87:VAL:HG21	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:822:CLA:HAA2	24:1:5002:LMT:H1'	1.90	0.52
19:B:850:CLA:HBC2	19:B:850:CLA:HHD	1.90	0.52
22:3:5006:BCR:H21C	19:3:5012:CLA:CHD	2.39	0.52
19:3:5011:CLA:HMB1	19:3:5011:CLA:HBB1	1.91	0.52
13:7:231:PHE:CD1	19:7:308:CLA:H11	2.44	0.52
16:5:132:VAL:HG11	22:5:304:BCR:H362	1.91	0.52
31:5:303:LUT:H31	19:5:309:CLA:HMC2	1.91	0.52
19:5:306:CLA:H62	19:5:307:CLA:CMA	2.40	0.52
19:5:314:CLA:C4D	23:5:323:LHG:H102	2.40	0.52
2:B:453:GLN:NE2	6:F:130:LEU:HD13	2.25	0.52
19:B:831:CLA:H171	27:F:304:RRX:H27	1.90	0.52
10:K:46:LEU:HD23	10:K:92:MET:HB2	1.90	0.52
19:Z:303:CLA:HMC2	31:Z:318:LUT:H11	1.91	0.52
12:3:15:LEU:HB3	12:3:35:PHE:O	2.09	0.52
19:3:5008:CLA:HBC2	32:3:5017:CHL:O1A	2.10	0.52
32:3:5017:CHL:H122	32:3:5017:CHL:H93	1.92	0.52
19:5:321:CLA:HBA1	23:6:324:LHG:H352	1.92	0.52
19:A:822:CLA:HBB1	30:K:201:DAO:H111	1.91	0.52
2:B:295:ASN:HD22	19:B:812:CLA:HMA2	1.73	0.52
19:B:836:CLA:HMB1	19:B:836:CLA:HBB1	1.91	0.52
7:G:92:PRO:HG3	19:G:1602:CLA:HBC2	1.91	0.52
15:4:68:PRO:HB3	15:4:70:TYR:CE2	2.44	0.52
19:4:307:CLA:H2A	19:4:307:CLA:H61	1.90	0.52
19:4:312:CLA:HHC	19:4:312:CLA:CBB	2.40	0.52
19:6:302:CLA:HHC	19:6:302:CLA:CBB	2.39	0.52
1:A:244:LEU:HD11	19:A:815:CLA:HMA3	1.92	0.52
18:A:801:CL0:H13	19:A:802:CLA:CAD	2.38	0.52
2:B:520:VAL:HG21	2:B:594:TYR:HB2	1.92	0.52
19:B:819:CLA:HMB1	19:B:819:CLA:CBB	2.37	0.52
19:B:832:CLA:HMA2	29:J:1904:LMG:H151	1.92	0.52
10:K:97:HIS:ND1	22:K:206:BCR:H12C	2.25	0.52
19:3:5019:CLA:HBB1	19:3:5019:CLA:HMB1	1.92	0.52
31:7:303:LUT:H28	19:7:306:CLA:H52	1.92	0.52
16:5:133:GLU:HG3	19:5:317:CLA:C4B	2.40	0.52
19:5:309:CLA:H93	19:5:310:CLA:CMA	2.39	0.52
19:A:826:CLA:HMB1	19:A:826:CLA:CBB	2.38	0.52
19:A:840:CLA:HED2	2:B:421:SER:HB2	1.90	0.52
9:J:36:PRO:HB2	29:J:1904:LMG:H111	1.91	0.52
10:K:32:SER:O	10:K:36:LEU:HG	2.10	0.52
19:K:205:CLA:HHC	19:K:205:CLA:CBB	2.39	0.52
22:3:5006:BCR:H17C	19:3:5012:CLA:CHC	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:168:ARG:NH1	38:6:326:ERG:H9	2.25	0.52
19:7:309:CLA:HMD2	32:7:314:CHL:CBB	2.40	0.52
15:4:95:TRP:HZ2	19:4:316:CLA:HAA2	1.68	0.52
15:4:109:LEU:CB	19:4:311:CLA:HAB	2.40	0.52
19:6:302:CLA:CHD	22:6:307:BCR:HC32	2.39	0.52
1:A:430:VAL:HA	1:A:433:HIS:CE1	2.45	0.52
19:A:825:CLA:HMB1	19:A:825:CLA:CBB	2.40	0.52
19:A:839:CLA:H101	22:A:848:BCR:H321	1.92	0.52
6:F:224:VAL:HB	6:F:227:ARG:NH1	2.24	0.52
9:J:5:THR:HB	29:J:1903:LMG:HC92	1.92	0.52
19:7:312:CLA:HHC	19:7:312:CLA:CBB	2.38	0.52
31:4:304:LUT:H182	32:4:317:CHL:OMC	2.09	0.52
22:4:305:BCR:H393	19:4:311:CLA:CHC	2.39	0.52
19:A:829:CLA:HHC	19:A:829:CLA:CBB	2.35	0.52
19:Z:307:CLA:HBA2	32:Z:309:CHL:H101	1.92	0.52
32:Z:309:CHL:HMA2	15:4:162:ILE:HG21	1.90	0.52
32:Z:313:CHL:HAA2	32:Z:313:CHL:CBD	2.38	0.52
12:3:117:ILE:HD13	19:3:5019:CLA:HMD3	1.91	0.52
22:3:5007:BCR:H402	23:3:5021:LHG:HC41	1.92	0.52
19:4:307:CLA:HMD2	19:4:312:CLA:C1D	2.40	0.52
31:5:303:LUT:H24	19:5:309:CLA:O1A	2.10	0.52
17:6:186:ALA:HA	19:6:311:CLA:HBB1	1.92	0.52
19:6:310:CLA:C2D	19:6:314:CLA:H52	2.39	0.52
1:A:373:ALA:CB	19:A:827:CLA:HAC2	2.40	0.52
1:A:385:GLY:HA2	1:A:747:ILE:HG21	1.91	0.52
19:A:818:CLA:H62	19:A:818:CLA:C1C	2.40	0.52
19:A:823:CLA:C10	22:A:859:BCR:H401	2.40	0.52
2:B:168:TRP:CD1	19:B:812:CLA:HED2	2.45	0.52
2:B:559:PRO:HG3	39:B:993:HOH:O	2.10	0.52
5:E:46:LEU:HD11	5:E:94:VAL:HG13	1.92	0.52
19:1:5016:CLA:HHC	19:1:5016:CLA:CBB	2.40	0.52
32:Z:310:CHL:HHD	32:Z:310:CHL:HBC2	1.92	0.52
31:7:304:LUT:H361	19:7:309:CLA:H121	1.90	0.52
14:8:36:ILE:HD12	14:8:53:GLY:HA3	1.91	0.52
14:8:148:GLY:HA2	14:8:157:GLU:O	2.10	0.52
15:4:239:THR:HB	15:4:240:PRO:HD2	1.92	0.52
17:6:66:TRP:CD2	38:6:326:ERG:H191	2.44	0.52
19:A:812:CLA:H2	19:A:812:CLA:ND	2.25	0.51
2:B:596:HIS:CE1	2:B:600:LEU:HD11	2.45	0.51
19:B:813:CLA:HMB1	19:B:813:CLA:CBB	2.38	0.51
6:F:177:GLU:HG3	6:F:183:LYS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Z:44:TRP:CG	11:Z:62:LYS:HA	2.46	0.51
16:5:182:LEU:CB	19:5:306:CLA:HMA1	2.38	0.51
17:6:223:VAL:HB	19:6:323:CLA:C1C	2.40	0.51
31:6:305:LUT:H28	19:6:309:CLA:H61	1.92	0.51
19:A:841:CLA:HBA1	19:A:841:CLA:HBD	1.92	0.51
2:B:142:PHE:CE1	19:B:814:CLA:H72	2.44	0.51
19:1:5013:CLA:HAA2	14:8:125:VAL:HG22	1.92	0.51
19:Z:314:CLA:HBB1	19:Z:314:CLA:HHC	1.90	0.51
32:7:315:CHL:HBD	32:7:315:CHL:HAA1	1.91	0.51
27:4:303:RRX:C21	19:4:306:CLA:H8	2.40	0.51
16:5:227:ILE:CG2	19:5:308:CLA:H11	2.39	0.51
19:A:809:CLA:H102	22:A:858:BCR:H332	1.92	0.51
19:A:812:CLA:H172	19:A:812:CLA:H121	1.92	0.51
19:A:816:CLA:HMB1	19:A:816:CLA:CBB	2.34	0.51
19:A:823:CLA:C1C	30:K:201:DAO:H123	2.40	0.51
2:B:214:LEU:HD21	22:B:844:BCR:H341	1.92	0.51
14:8:148:GLY:CA	14:8:161:LYS:HG3	2.35	0.51
19:5:319:CLA:HHC	19:5:319:CLA:CBB	2.39	0.51
17:6:195:GLN:HB3	17:6:250:CYS:SG	2.49	0.51
1:A:256:SER:HA	1:A:259:LYS:HE2	1.91	0.51
19:A:821:CLA:H121	22:A:849:BCR:H10C	1.93	0.51
19:A:827:CLA:HMA2	19:A:835:CLA:H71	1.92	0.51
19:A:830:CLA:H112	23:A:852:LHG:H351	1.92	0.51
19:B:820:CLA:HHC	19:B:820:CLA:CBB	2.39	0.51
19:B:821:CLA:HBD	7:G:57:GLN:HG2	1.92	0.51
11:1:154:PHE:C	11:1:156:PRO:HD3	2.31	0.51
19:Z:304:CLA:CGA	19:Z:304:CLA:C1A	2.88	0.51
31:7:304:LUT:H382	19:7:309:CLA:O1A	2.10	0.51
33:4:301:SPH:H181	31:4:304:LUT:H362	1.92	0.51
27:5:302:RRX:H44	19:5:307:CLA:CMC	2.40	0.51
19:5:307:CLA:H71	19:5:307:CLA:H42	1.90	0.51
1:A:501:ASN:HB3	19:A:817:CLA:HED2	1.92	0.51
19:B:830:CLA:HMB1	19:B:830:CLA:CBB	2.40	0.51
9:J:38:VAL:C	29:J:1904:LMG:H122	2.30	0.51
19:Z:305:CLA:HMB1	19:Z:305:CLA:CBB	2.40	0.51
22:3:5005:BCR:C20	32:3:5017:CHL:H193	2.41	0.51
14:8:30:TRP:HZ2	34:8:322:3PH:H221	1.76	0.51
14:8:194:LYS:HE3	23:8:321:LHG:HC42	1.93	0.51
19:8:309:CLA:CGA	19:8:309:CLA:C1A	2.89	0.51
19:4:307:CLA:NA	19:4:312:CLA:H92	2.24	0.51
17:6:179:ASN:ND2	19:6:314:CLA:HMD1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:6:313:CLA:H102	32:6:319:CHL:O1A	2.10	0.51
1:A:45:THR:HG22	1:A:714:GLN:HB2	1.92	0.51
19:A:804:CLA:HMB1	19:A:804:CLA:CBB	2.36	0.51
19:A:813:CLA:HMB1	19:A:813:CLA:CBB	2.38	0.51
19:B:806:CLA:HMB1	19:B:806:CLA:CBB	2.41	0.51
19:B:821:CLA:H8	19:B:822:CLA:H142	1.92	0.51
19:B:836:CLA:O1A	19:B:836:CLA:H2	2.10	0.51
19:1:5010:CLA:ND	19:1:5016:CLA:H102	2.24	0.51
16:5:218:HIS:CG	19:5:308:CLA:HAA2	2.46	0.51
19:A:822:CLA:HBA2	19:A:823:CLA:H92	1.93	0.51
19:A:837:CLA:HMB1	19:A:837:CLA:CBB	2.33	0.51
19:A:843:CLA:HMB1	19:A:843:CLA:CBB	2.41	0.51
2:B:30:HIS:HB2	19:B:829:CLA:O1A	2.11	0.51
2:B:87:PRO:HB2	2:B:117:SER:OG	2.10	0.51
19:B:837:CLA:H172	22:B:845:BCR:H352	1.93	0.51
7:G:90:ASN:HB3	19:G:1602:CLA:OBD	2.10	0.51
12:3:115:TYR:CE2	13:7:241:ALA:HA	2.46	0.51
14:8:188:TRP:CZ3	19:8:307:CLA:H43	2.46	0.51
16:5:140:TYR:OH	19:5:322:CLA:HBA2	2.11	0.51
19:A:842:CLA:H42	9:J:14:ILE:HG22	1.92	0.51
3:C:31:TRP:CZ2	3:C:33:GLY:HA3	2.46	0.51
19:1:5007:CLA:HMD1	19:1:5012:CLA:HBA2	1.92	0.51
16:5:217:ALA:HB1	16:5:225:ASN:HD22	1.74	0.51
19:A:838:CLA:H52	19:A:838:CLA:CHC	2.41	0.51
22:A:859:BCR:H372	10:K:94:ALA:HB3	1.92	0.51
22:A:859:BCR:C12	22:K:206:BCR:H333	2.40	0.51
19:B:811:CLA:HMB1	19:B:811:CLA:HBB1	1.93	0.51
19:B:829:CLA:HMB1	19:B:829:CLA:CBB	2.38	0.51
6:F:79:LEU:O	6:F:83:GLU:HG3	2.10	0.51
6:F:123:LEU:HD21	9:J:38:VAL:HG11	1.93	0.51
13:7:136:TRP:CE3	19:7:317:CLA:HMA1	2.45	0.51
19:7:324:CLA:O1A	19:7:324:CLA:HMA2	2.11	0.51
15:4:71:LEU:HB3	15:4:78:ASP:OD1	2.10	0.51
1:A:541:PHE:CZ	19:B:803:CLA:HBB2	2.44	0.51
32:Z:302:CHL:H12	32:Z:302:CHL:CHB	2.41	0.51
12:3:113:ASP:HB2	12:3:114:PRO:HD2	1.93	0.51
24:3:5023:LMT:H102	19:7:312:CLA:NC	2.25	0.51
13:7:171:ASP:HA	31:7:303:LUT:H24	1.92	0.51
13:7:189:LYS:HD3	19:7:307:CLA:HAA2	1.91	0.51
1:A:487:ILE:HG21	19:A:837:CLA:HED1	1.93	0.50
19:A:840:CLA:C4B	19:A:842:CLA:HMD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:857:CLA:HMB1	2:B:692:VAL:HG21	1.93	0.50
2:B:508:SER:HA	2:B:511:LEU:HD21	1.92	0.50
2:B:604:GLN:HG3	2:B:734:PHE:CZ	2.45	0.50
19:B:826:CLA:H162	22:B:846:BCR:C17	2.38	0.50
19:B:830:CLA:CMA	19:B:831:CLA:HED2	2.41	0.50
23:1:5019:LHG:HC81	22:8:306:BCR:HC21	1.92	0.50
31:7:303:LUT:H26	19:7:306:CLA:O1A	2.11	0.50
17:6:208:HIS:HA	17:6:215:THR:OG1	2.11	0.50
1:A:680:ALA:CB	19:B:801:CLA:HBB2	2.41	0.50
19:B:808:CLA:H112	19:B:808:CLA:H51	1.93	0.50
19:B:831:CLA:H71	19:B:831:CLA:H41	1.92	0.50
19:I:201:CLA:C1	19:I:201:CLA:HAA1	2.41	0.50
11:1:44:TRP:HB2	39:1:5126:HOH:O	2.11	0.50
32:Z:309:CHL:HMB1	32:Z:309:CHL:CBB	2.38	0.50
19:Z:311:CLA:C4A	19:Z:311:CLA:HBA2	2.42	0.50
12:3:129:GLU:HG3	19:3:5018:CLA:C4B	2.42	0.50
1:A:32:PRO:HB2	1:A:48:TRP:HH2	1.76	0.50
1:A:160:TYR:CZ	24:A:856:LMT:H3'	2.46	0.50
1:A:443:TRP:CZ2	19:A:832:CLA:HBB2	2.45	0.50
19:A:806:CLA:HHC	19:A:806:CLA:CBB	2.41	0.50
19:A:832:CLA:HMC2	19:A:838:CLA:H172	1.93	0.50
19:B:808:CLA:H102	19:B:809:CLA:H61	1.92	0.50
19:B:832:CLA:H43	22:F:302:BCR:HC22	1.92	0.50
8:I:83:THR:HB	19:I:201:CLA:C1	2.41	0.50
19:3:5013:CLA:HBA1	19:3:5019:CLA:HMD2	1.92	0.50
17:6:113:LEU:HD11	32:6:319:CHL:HMD3	1.93	0.50
1:A:605:ILE:HG13	18:A:801:CL0:H66	1.93	0.50
19:A:821:CLA:HMB1	19:A:821:CLA:CBB	2.37	0.50
19:A:828:CLA:C1C	22:A:850:BCR:HC22	2.42	0.50
19:A:842:CLA:HHC	19:A:842:CLA:CBB	2.41	0.50
2:B:295:ASN:ND2	19:B:812:CLA:HMA2	2.26	0.50
2:B:695:LYS:HG2	19:B:838:CLA:HED3	1.93	0.50
19:B:801:CLA:HMB1	19:B:801:CLA:CBB	2.40	0.50
19:F:301:CLA:H192	19:F:301:CLA:C15	2.35	0.50
10:K:42:THR:HA	10:K:96:GLY:HA3	1.92	0.50
19:8:309:CLA:C1C	19:8:309:CLA:H51	2.42	0.50
32:8:315:CHL:HHC	32:8:315:CHL:HBB1	1.93	0.50
17:6:129:TRP:HH2	23:6:303:LHG:C9	2.24	0.50
1:A:160:TYR:CE1	24:A:856:LMT:H5'	2.47	0.50
2:B:463:TRP:CD1	19:B:850:CLA:HMA2	2.47	0.50
2:B:672:TRP:HZ3	19:B:804:CLA:O1D	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:808:CLA:H51	19:B:808:CLA:C11	2.41	0.50
4:D:92:LYS:HE3	4:D:94:GLN:HG2	1.92	0.50
19:3:5013:CLA:HMB1	19:3:5013:CLA:CBB	2.37	0.50
19:3:5020:CLA:HMB1	19:3:5020:CLA:CBB	2.37	0.50
14:8:68:TRP:CD2	38:8:325:ERG:H14	2.47	0.50
15:4:114:ILE:HD11	31:4:304:LUT:C17	2.42	0.50
15:4:157:PHE:HZ	22:4:305:BCR:C37	2.25	0.50
17:6:102:LYS:HB3	17:6:102:LYS:HZ3	1.77	0.50
19:6:311:CLA:C1A	19:6:311:CLA:CGA	2.89	0.50
1:A:709:VAL:HG12	6:F:168:ARG:HG3	1.93	0.50
19:B:815:CLA:HMB1	19:B:815:CLA:CBB	2.38	0.50
19:B:821:CLA:H152	11:1:131:PHE:CZ	2.46	0.50
6:F:202:TRP:N	6:F:203:PRO:CD	2.75	0.50
7:G:108:HIS:CE1	22:G:1603:BCR:H14C	2.47	0.50
9:J:8:LEU:HB3	29:J:1903:LMG:H301	1.93	0.50
13:7:29:VAL:HG13	13:7:30:ARG:H	1.77	0.50
32:8:316:CHL:HAA1	32:8:316:CHL:HBD	1.93	0.50
17:6:124:VAL:HG11	22:6:307:BCR:H362	1.94	0.50
1:A:563:ILE:HD12	1:A:586:VAL:HG21	1.92	0.50
2:B:183:LEU:HD13	19:B:813:CLA:HHB	1.94	0.50
2:B:681:TRP:O	2:B:685:LYS:HG2	2.11	0.50
22:3:5004:BCR:C16	32:3:5017:CHL:HMB3	2.42	0.50
19:8:313:CLA:CMA	24:4:302:LMT:H5'	2.42	0.50
15:4:232:GLN:HE21	15:4:243:ASN:HD22	1.59	0.50
19:6:310:CLA:HBB1	19:6:310:CLA:CHC	2.25	0.50
32:6:316:CHL:CBB	32:6:319:CHL:HBB2	2.42	0.50
19:A:814:CLA:H93	35:7:302:DGA:HB22	1.92	0.50
19:A:838:CLA:HMB1	19:A:838:CLA:CBB	2.42	0.50
2:B:159:GLN:O	2:B:163:GLN:HG3	2.12	0.50
2:B:352:HIS:CE1	19:B:826:CLA:NB	2.80	0.50
2:B:465:GLN:NE2	19:B:835:CLA:HMD1	2.26	0.50
19:B:814:CLA:H61	22:B:844:BCR:H362	1.93	0.50
19:B:821:CLA:HMB1	19:B:821:CLA:CBB	2.36	0.50
32:Z:302:CHL:CBB	31:Z:318:LUT:H32	2.42	0.50
19:A:809:CLA:C4B	19:A:828:CLA:H192	2.42	0.50
19:B:810:CLA:H2	19:B:810:CLA:O2D	2.11	0.50
19:B:814:CLA:HMB1	19:B:814:CLA:CBB	2.41	0.50
7:G:45:PHE:HA	7:G:48:ILE:HG12	1.94	0.50
7:G:50:ARG:HG2	19:G:1602:CLA:CAB	2.42	0.50
32:Z:309:CHL:CMD	15:4:178:PRO:HB3	2.41	0.50
32:8:301:CHL:H2	37:8:302:SQD:H211	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:5:175:SER:OG	19:5:306:CLA:HAA2	2.12	0.50
17:6:246:ILE:HG13	17:6:246:ILE:O	2.12	0.50
19:A:814:CLA:HMB1	19:A:814:CLA:CBB	2.40	0.49
2:B:223:LEU:HB3	2:B:227:PHE:CE2	2.47	0.49
19:B:802:CLA:HHC	19:B:802:CLA:HBB1	1.94	0.49
19:B:805:CLA:HBA2	19:B:805:CLA:CHA	2.42	0.49
19:B:814:CLA:HMA2	22:B:844:BCR:H282	1.93	0.49
19:B:829:CLA:HBA1	19:B:829:CLA:CHA	2.37	0.49
24:G:1604:LMT:H71	19:1:5016:CLA:C1C	2.42	0.49
22:3:5005:BCR:H382	19:3:5009:CLA:HBB2	1.94	0.49
19:3:5012:CLA:HMD2	19:3:5018:CLA:C1D	2.41	0.49
32:3:5017:CHL:HMB1	32:3:5017:CHL:CBB	2.37	0.49
14:8:179:SER:HB3	19:8:307:CLA:HAA2	1.93	0.49
14:8:188:TRP:HB3	19:8:307:CLA:CMA	2.38	0.49
19:8:310:CLA:H121	19:8:311:CLA:H193	1.93	0.49
15:4:199:ASP:HA	27:4:303:RRX:H16	1.94	0.49
19:4:306:CLA:CMB	19:4:307:CLA:HBA2	2.39	0.49
17:6:133:ARG:CZ	17:6:134:LYS:HE3	2.42	0.49
17:6:247:PRO:HG2	32:6:316:CHL:H41	1.94	0.49
32:6:317:CHL:HBD	32:6:317:CHL:HAA1	1.94	0.49
19:B:822:CLA:HMA2	24:1:5002:LMT:H5'	1.93	0.49
22:B:842:BCR:H321	22:B:842:BCR:HC8	1.93	0.49
4:D:133:LYS:HD2	4:D:133:LYS:N	2.27	0.49
19:3:5016:CLA:H2	35:7:302:DGA:HBW2	1.93	0.49
14:8:30:TRP:CZ2	34:8:322:3PH:H221	2.47	0.49
17:6:108:LEU:N	17:6:108:LEU:CD1	2.76	0.49
17:6:140:GLN:NE2	17:6:148:LYS:HB2	2.28	0.49
17:6:244:ILE:CG1	22:6:308:BCR:HC7	2.41	0.49
18:A:801:CL0:CGD	18:A:801:CL0:H8	2.43	0.49
19:A:832:CLA:HMA1	2:B:686:THR:OG1	2.12	0.49
19:A:857:CLA:H52	19:A:857:CLA:NB	2.28	0.49
19:B:822:CLA:CAB	22:B:845:BCR:H343	2.42	0.49
19:F:301:CLA:HMC3	29:J:1904:LMG:H192	1.94	0.49
8:I:75:ALA:HB1	19:I:201:CLA:HMD1	1.93	0.49
11:1:115:PHE:CE2	19:1:5011:CLA:HMD2	2.47	0.49
11:1:210:TRP:CE2	19:1:5013:CLA:HMA2	2.47	0.49
14:8:138:TRP:CG	19:8:318:CLA:HMA2	2.47	0.49
15:4:206:GLY:O	15:4:208:ILE:N	2.46	0.49
31:4:304:LUT:H181	32:4:317:CHL:HBB1	1.94	0.49
19:6:310:CLA:O1A	19:6:310:CLA:H2A	2.12	0.49
32:6:315:CHL:H2	23:6:324:LHG:H161	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:PRO:HA	1:A:237:ILE:HD12	1.93	0.49
1:A:392:THR:HG22	19:A:828:CLA:CAB	2.43	0.49
1:A:646:LEU:HD22	2:B:652:LEU:HD21	1.93	0.49
19:A:820:CLA:HHC	19:A:820:CLA:CBB	2.42	0.49
2:B:34:SER:HB3	4:D:190:MET:SD	2.52	0.49
2:B:595:TRP:HB2	19:B:835:CLA:HMC1	1.93	0.49
19:B:807:CLA:H203	19:B:807:CLA:H152	1.94	0.49
19:B:850:CLA:H62	19:B:850:CLA:NC	2.26	0.49
14:8:169:PRO:HD3	32:8:317:CHL:HMD2	1.95	0.49
17:6:247:PRO:HG2	32:6:316:CHL:H42	1.93	0.49
32:6:317:CHL:HMB1	32:6:317:CHL:CBB	2.28	0.49
19:A:816:CLA:CHD	19:3:5016:CLA:HBB2	2.42	0.49
19:B:835:CLA:H51	19:B:850:CLA:CMB	2.28	0.49
28:1:5005:C7Z:C16	19:1:5011:CLA:H92	2.42	0.49
11:Z:168:GLU:O	11:Z:172:LYS:HG3	2.13	0.49
19:Z:312:CLA:HMB1	19:Z:312:CLA:CBB	2.35	0.49
19:3:5016:CLA:H12	13:7:240:ILE:HD11	1.95	0.49
15:4:260:ASP:HB3	19:4:318:CLA:CHB	2.43	0.49
19:6:311:CLA:HMC2	19:6:311:CLA:H92	1.95	0.49
1:A:330:ARG:HH21	1:A:336:GLU:HA	1.78	0.49
19:A:815:CLA:HMB1	19:A:815:CLA:CBB	2.37	0.49
19:A:840:CLA:HMB1	19:A:840:CLA:HBB1	1.95	0.49
2:B:125:TRP:HA	2:B:128:ILE:HG12	1.95	0.49
6:F:211:GLN:NE2	38:8:325:ERG:C18	2.69	0.49
32:5:315:CHL:H43	28:6:304:C7Z:C16	2.42	0.49
19:5:321:CLA:HMB1	19:5:321:CLA:CBB	2.42	0.49
32:6:315:CHL:HBB1	32:6:315:CHL:HHC	1.93	0.49
19:A:819:CLA:HMB1	19:A:819:CLA:CBB	2.33	0.49
19:A:826:CLA:H61	19:A:835:CLA:HAB	1.95	0.49
19:B:819:CLA:C1B	19:B:824:CLA:H111	2.42	0.49
19:B:820:CLA:H101	19:B:820:CLA:HMC2	1.93	0.49
19:G:1602:CLA:NC	22:G:1603:BCR:H292	2.28	0.49
11:1:104:LEU:CD2	32:1:5014:CHL:HED3	2.43	0.49
11:1:221:VAL:HB	11:1:224:PHE:HB2	1.93	0.49
19:1:5010:CLA:HMD2	19:1:5016:CLA:C1D	2.43	0.49
12:3:190:ASN:ND2	19:3:5014:CLA:HMD1	2.27	0.49
13:7:183:TYR:CZ	13:7:187:LYS:HD2	2.47	0.49
1:A:707:LEU:HD21	27:F:304:RRX:H43	1.95	0.49
1:A:709:VAL:CG1	6:F:168:ARG:HG3	2.42	0.49
19:A:806:CLA:H171	19:A:806:CLA:NC	2.27	0.49
2:B:263:HIS:CE1	2:B:265:GLN:HB3	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:825:CLA:CGA	19:B:835:CLA:HMA1	2.43	0.49
19:B:840:CLA:HMB1	19:B:840:CLA:CBB	2.39	0.49
12:3:189:LYS:HG3	19:3:5014:CLA:O1D	2.12	0.49
19:3:5010:CLA:H11	19:3:5010:CLA:CHA	2.41	0.49
19:7:324:CLA:HMD2	19:6:318:CLA:C1D	2.43	0.49
15:4:123:ILE:HB	15:4:125:PHE:CD1	2.48	0.49
22:5:304:BCR:H291	19:5:311:CLA:C4B	2.41	0.49
19:6:313:CLA:H202	19:6:313:CLA:H162	1.67	0.49
1:A:398:GLY:O	1:A:402:ILE:HG13	2.13	0.49
1:A:538:ILE:HG23	18:A:801:CL0:H70	1.94	0.49
19:A:817:CLA:HMB1	19:A:817:CLA:CBB	2.43	0.49
19:A:822:CLA:HAA2	10:K:61:THR:CG2	2.42	0.49
2:B:394:PHE:CD2	22:B:846:BCR:H281	2.48	0.49
19:B:821:CLA:CAD	22:B:842:BCR:HC22	2.42	0.49
19:B:824:CLA:HBB1	19:B:824:CLA:HMB1	1.93	0.49
19:B:829:CLA:H93	19:B:839:CLA:HED1	1.95	0.49
39:F:410:HOH:O	19:8:311:CLA:H42	2.12	0.49
23:1:5019:LHG:C19	37:8:302:SQD:H292	2.43	0.49
23:1:5019:LHG:H132	32:8:301:CHL:HBA1	1.95	0.49
12:3:118:PHE:CE2	19:3:5016:CLA:HBA2	2.47	0.49
19:7:316:CLA:HMB1	19:7:316:CLA:CBB	2.38	0.49
15:4:153:GLN:HG2	15:4:154:MET:HE3	1.95	0.49
19:4:316:CLA:HMA1	24:4:321:LMT:H41	1.94	0.49
16:5:240:VAL:CG1	16:5:249:LEU:HD11	2.40	0.49
19:5:307:CLA:OBD	19:5:312:CLA:H2	2.12	0.49
17:6:141:ASP:HB3	17:6:144:PHE:O	2.12	0.49
1:A:354:ALA:HB3	22:A:848:BCR:H272	1.95	0.49
19:A:814:CLA:H62	19:A:814:CLA:H41	1.58	0.49
2:B:559:PRO:HB3	2:B:703:ILE:HD12	1.94	0.49
19:B:814:CLA:H143	22:B:844:BCR:H21C	1.94	0.49
10:K:74:ALA:O	12:3:20:SER:HB2	2.12	0.49
32:1:5014:CHL:HMB1	32:1:5014:CHL:CBB	2.37	0.49
19:7:318:CLA:HMB1	19:7:318:CLA:CBB	2.41	0.49
14:8:106:ASP:HA	32:8:316:CHL:HED3	1.94	0.49
14:8:242:PHE:CE2	14:8:243:LEU:HG	2.47	0.49
19:5:325:CLA:HBA1	19:5:325:CLA:HBD	1.95	0.49
32:6:316:CHL:H72	32:6:316:CHL:C2	2.43	0.49
19:A:809:CLA:HBC3	19:A:828:CLA:H151	1.94	0.48
19:A:828:CLA:H111	19:A:828:CLA:H72	1.48	0.48
2:B:466:ALA:HA	2:B:470:LYS:O	2.13	0.48
2:B:577:PHE:CE2	19:B:829:CLA:HAC2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:G:1603:BCR:H321	22:G:1603:BCR:HC8	1.95	0.48
24:1:5002:LMT:H5B	24:1:5002:LMT:H6D	1.94	0.48
11:Z:37:PRO:HD2	32:Z:309:CHL:O2D	2.13	0.48
22:3:5004:BCR:H323	19:7:312:CLA:CBB	2.43	0.48
22:3:5006:BCR:H21C	19:3:5012:CLA:C3C	2.42	0.48
19:7:306:CLA:HMD2	19:7:316:CLA:O1A	2.13	0.48
19:7:306:CLA:H71	19:7:307:CLA:CMA	2.42	0.48
32:8:315:CHL:HAA2	32:8:315:CHL:HBD	1.95	0.48
19:5:325:CLA:HMB3	17:6:212:PRO:HG3	1.95	0.48
17:6:147:TYR:CE2	32:6:321:CHL:HAA1	2.47	0.48
19:A:838:CLA:H52	19:A:838:CLA:C1C	2.43	0.48
2:B:11:GLN:HE21	2:B:15:GLN:HE21	1.61	0.48
19:B:818:CLA:HMB1	19:B:818:CLA:CBB	2.35	0.48
22:B:845:BCR:H322	24:1:5002:LMT:H51	1.95	0.48
19:1:5008:CLA:H141	24:Z:301:LMT:H101	1.95	0.48
19:7:308:CLA:C1A	19:7:308:CLA:CGA	2.91	0.48
19:7:313:CLA:HHC	19:7:313:CLA:CBB	2.43	0.48
32:7:314:CHL:C2C	23:7:320:LHG:HC82	2.44	0.48
15:4:247:HIS:HA	15:4:254:THR:OG1	2.13	0.48
32:4:317:CHL:HAA2	32:4:317:CHL:HBD	1.95	0.48
16:5:33:LYS:HE3	19:5:314:CLA:HBC3	1.95	0.48
1:A:101:TYR:CE2	1:A:105:LEU:HD11	2.48	0.48
1:A:687:PHE:HB2	19:B:801:CLA:CBC	2.43	0.48
19:A:808:CLA:CAD	19:A:828:CLA:HAA2	2.42	0.48
19:A:823:CLA:H101	22:A:859:BCR:H401	1.95	0.48
19:B:825:CLA:C7	19:B:835:CLA:H42	2.43	0.48
12:3:150:LEU:O	12:3:153:ILE:HG12	2.13	0.48
19:3:5011:CLA:H111	19:3:5011:CLA:H72	1.66	0.48
22:7:305:BCR:C28	33:7:321:SPH:H101	2.42	0.48
1:A:677:PHE:CG	22:A:850:BCR:H363	2.48	0.48
19:A:804:CLA:HMA2	19:A:811:CLA:HMD2	1.96	0.48
19:A:805:CLA:HMB1	19:A:805:CLA:CBB	2.43	0.48
2:B:499:LEU:HA	2:B:502:ILE:HG22	1.96	0.48
8:I:80:VAL:HB	8:I:81:PRO:HD3	1.96	0.48
19:K:204:CLA:HMB1	19:K:204:CLA:CBB	2.44	0.48
12:3:102:PRO:HD2	19:3:5016:CLA:C2B	2.44	0.48
19:8:313:CLA:H3A	19:8:313:CLA:HBA2	1.39	0.48
19:5:314:CLA:CHD	23:5:323:LHG:HC82	2.44	0.48
19:A:803:CLA:HMA2	19:A:808:CLA:H192	1.96	0.48
2:B:5:LEU:HD23	8:I:103:ALA:HA	1.95	0.48
2:B:23:TRP:HE1	19:B:838:CLA:HBB1	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:348:LEU:HD13	19:B:826:CLA:HAA2	1.96	0.48
10:K:110:ILE:HG23	19:K:203:CLA:HMA1	1.95	0.48
19:7:307:CLA:C4D	19:7:312:CLA:H61	2.42	0.48
31:4:304:LUT:C31	19:4:309:CLA:HMC2	2.43	0.48
19:4:307:CLA:HBC3	19:4:307:CLA:HHD	1.95	0.48
22:5:305:BCR:H20C	19:6:323:CLA:H42	1.95	0.48
19:5:325:CLA:C2B	32:6:315:CHL:H193	2.43	0.48
18:A:801:CL0:H72	18:A:801:CL0:H10	1.53	0.48
19:B:832:CLA:HMB1	19:B:832:CLA:CBB	2.41	0.48
10:K:65:LEU:HD12	19:K:204:CLA:HAA2	1.95	0.48
11:1:148:VAL:O	11:1:150:PRO:HD3	2.13	0.48
22:5:304:BCR:H332	23:6:324:LHG:H121	1.95	0.48
32:5:315:CHL:CBB	32:5:318:CHL:CBB	2.90	0.48
17:6:208:HIS:CG	19:6:311:CLA:HAA2	2.49	0.48
1:A:261:ILE:HD12	1:A:265:PHE:HE2	1.79	0.48
1:A:679:TRP:CG	18:A:801:CL0:H5	2.48	0.48
19:A:815:CLA:H42	12:3:206:VAL:HG11	1.95	0.48
2:B:5:LEU:HD21	8:I:104:PRO:HD3	1.96	0.48
2:B:281:ILE:HG13	2:B:282:ALA:N	2.27	0.48
2:B:316:LEU:HD21	19:B:840:CLA:H12	1.96	0.48
3:C:58:CYS:HA	21:C:102:SF4:S4	2.54	0.48
19:3:5012:CLA:H151	19:3:5012:CLA:H18	1.51	0.48
13:7:164:TYR:CZ	13:7:187:LYS:HE3	2.49	0.48
19:7:311:CLA:HMB1	19:7:311:CLA:CBB	2.43	0.48
31:8:305:LUT:C31	19:8:310:CLA:HMC2	2.43	0.48
22:4:305:BCR:H403	32:4:317:CHL:H152	1.96	0.48
16:5:33:LYS:HE3	19:5:314:CLA:CBC	2.43	0.48
17:6:175:LYS:HZ1	19:6:310:CLA:HED1	1.78	0.48
31:6:305:LUT:H193	19:6:311:CLA:H202	1.94	0.48
31:6:306:LUT:H382	19:6:312:CLA:O1A	2.14	0.48
19:6:313:CLA:H121	32:6:319:CHL:H2	1.96	0.48
1:A:736:ILE:HG21	19:A:828:CLA:HMC2	1.96	0.48
19:A:805:CLA:HMC3	19:A:830:CLA:HMA1	1.96	0.48
19:A:814:CLA:H93	35:7:302:DGA:HB32	1.94	0.48
22:A:846:BCR:H292	19:K:202:CLA:HMC3	1.96	0.48
2:B:89:ALA:HB1	19:B:808:CLA:O1D	2.12	0.48
19:B:812:CLA:H111	19:B:812:CLA:CAB	2.44	0.48
24:F:305:LMT:H5'	11:1:223:PHE:CB	2.42	0.48
11:1:140:GLN:HB3	19:1:5015:CLA:HMC3	1.95	0.48
19:1:5006:CLA:HMB1	19:1:5006:CLA:CBB	2.40	0.48
19:1:5010:CLA:O2D	19:1:5016:CLA:H62	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1:5019:LHG:C20	37:8:302:SQD:H182	2.44	0.48
19:7:309:CLA:HMB1	19:7:309:CLA:CBB	2.43	0.48
22:8:303:BCR:H10C	22:8:303:BCR:C35	2.41	0.48
19:8:311:CLA:HMD2	19:8:318:CLA:C1D	2.44	0.48
15:4:175:ASN:HB3	15:4:185:LEU:HB2	1.96	0.48
32:4:314:CHL:H41	24:4:322:LMT:H112	1.94	0.48
16:5:117:ASN:ND2	17:6:219:SER:HB2	2.28	0.48
19:6:310:CLA:O1A	19:6:310:CLA:HMA2	2.14	0.48
1:A:586:VAL:HG13	2:B:670:GLY:HA3	1.96	0.48
19:A:806:CLA:C4D	19:A:806:CLA:H193	2.44	0.48
19:A:836:CLA:CHB	19:K:203:CLA:H93	2.44	0.48
2:B:195:LEU:HA	2:B:199:ALA:HB3	1.95	0.48
2:B:330:SER:O	2:B:334:GLN:HG3	2.13	0.48
19:J:1901:CLA:HMB1	19:J:1901:CLA:CBB	2.38	0.48
10:K:46:LEU:HB3	19:K:205:CLA:HBC1	1.96	0.48
13:7:213:LYS:HE2	13:7:221:ASP:OD2	2.14	0.48
14:8:242:PHE:CZ	19:8:320:CLA:HMC3	2.49	0.48
19:5:306:CLA:H91	19:5:306:CLA:H111	1.59	0.48
19:5:317:CLA:H41	19:5:317:CLA:H61	1.51	0.48
17:6:161:PHE:CE1	32:6:319:CHL:H121	2.49	0.48
19:A:827:CLA:H11	22:A:849:BCR:H351	1.95	0.48
2:B:197:HIS:O	2:B:208:VAL:HG11	2.13	0.48
19:K:203:CLA:H11	19:K:203:CLA:H51	1.64	0.48
11:1:56:ASP:N	11:1:57:PRO:HD3	2.29	0.48
19:Z:303:CLA:HMC2	31:Z:318:LUT:C11	2.43	0.48
19:Z:312:CLA:C1C	23:Z:316:LHG:HC41	2.43	0.48
19:Z:314:CLA:HHC	19:Z:314:CLA:CBB	2.44	0.48
19:5:310:CLA:HBC2	19:5:310:CLA:HMC1	1.95	0.48
19:5:312:CLA:HMB3	23:5:323:LHG:HC2	1.96	0.48
19:6:310:CLA:HMD2	19:6:314:CLA:C1D	2.43	0.48
1:A:511:GLY:HA2	1:A:525:PRO:HB3	1.96	0.47
19:A:814:CLA:H52	19:A:816:CLA:C1B	2.43	0.47
19:A:823:CLA:CHA	19:A:823:CLA:HBA2	2.44	0.47
19:A:830:CLA:H72	23:A:852:LHG:H172	1.96	0.47
19:B:820:CLA:C4A	19:B:820:CLA:H12	2.44	0.47
19:B:823:CLA:H192	19:B:840:CLA:HBA1	1.96	0.47
19:B:826:CLA:HBB1	19:B:833:CLA:HMA2	1.95	0.47
19:1:5007:CLA:HMD2	19:1:5012:CLA:C4D	2.43	0.47
12:3:119:PHE:CE2	32:7:314:CHL:H91	2.44	0.47
13:7:117:PHE:HB3	13:7:118:PRO:HD3	1.96	0.47
19:4:310:CLA:CAC	32:4:314:CHL:HBB2	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:5:303:LUT:H26	19:5:309:CLA:H61	1.95	0.47
22:5:304:BCR:H313	19:6:314:CLA:HAB	1.94	0.47
19:6:313:CLA:H93	19:6:313:CLA:H61	1.72	0.47
1:A:25:SER:HB3	29:7:301:LMG:HC61	1.95	0.47
1:A:453:PHE:CZ	1:A:457:ILE:HD11	2.49	0.47
1:A:596:LEU:HD21	19:A:830:CLA:HBC1	1.96	0.47
1:A:737:ALA:HA	22:A:850:BCR:HC42	1.95	0.47
19:A:808:CLA:C4D	19:A:828:CLA:H12	2.44	0.47
19:B:804:CLA:HMA2	19:B:804:CLA:C2	2.44	0.47
15:4:67:LEU:HD13	15:4:80:GLY:HA3	1.96	0.47
15:4:220:ARG:HA	15:4:223:MET:HE2	1.96	0.47
16:5:95:LYS:NZ	19:5:311:CLA:HED2	2.29	0.47
16:5:135:ARG:HD2	32:6:315:CHL:CED	2.43	0.47
19:6:301:CLA:H61	19:6:301:CLA:H41	1.35	0.47
19:6:309:CLA:CMD	32:6:317:CHL:H11	2.39	0.47
23:6:324:LHG:H362	23:6:324:LHG:H201	1.95	0.47
1:A:666:SER:HB2	2:B:446:ALA:HB1	1.96	0.47
19:A:802:CLA:CMA	2:B:617:LEU:HD13	2.45	0.47
19:A:821:CLA:HBC3	19:A:827:CLA:H202	1.95	0.47
20:A:844:PQN:H222	20:A:844:PQN:H18	1.66	0.47
19:A:857:CLA:H2	19:A:857:CLA:HBA2	1.96	0.47
19:B:822:CLA:HAB	22:B:845:BCR:H343	1.96	0.47
19:B:834:CLA:HHC	19:B:834:CLA:CBB	2.45	0.47
3:C:31:TRP:CE3	3:C:39:MET:HB2	2.49	0.47
19:G:1601:CLA:HBA2	19:G:1601:CLA:H3A	1.43	0.47
24:G:1604:LMT:H32	19:1:5016:CLA:CHB	2.43	0.47
32:Z:310:CHL:HHC	32:Z:310:CHL:HBB1	1.94	0.47
12:3:76:ILE:CD1	12:3:212:PRO:HB2	2.41	0.47
19:3:5015:CLA:HMB1	19:3:5015:CLA:CBB	2.38	0.47
19:7:307:CLA:C3B	19:7:312:CLA:H121	2.44	0.47
22:4:305:BCR:H21C	32:4:317:CHL:H91	1.96	0.47
16:5:227:ILE:HG13	19:5:308:CLA:CMD	2.45	0.47
19:5:307:CLA:HMD2	19:5:312:CLA:ND	2.29	0.47
19:6:311:CLA:H72	23:6:324:LHG:H182	1.95	0.47
1:A:80:GLN:HG2	19:A:805:CLA:CMA	2.44	0.47
19:A:807:CLA:C2	19:A:809:CLA:H2	2.42	0.47
19:A:812:CLA:H171	19:A:820:CLA:C12	2.44	0.47
2:B:156:LEU:C	2:B:158:LEU:H	2.16	0.47
2:B:428:LEU:HA	19:B:801:CLA:O2A	2.14	0.47
11:1:99:TRP:HE1	11:1:198:PRO:HD3	1.78	0.47
19:1:5011:CLA:HBA1	32:1:5017:CHL:C1D	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:5012:CLA:C1C	24:Z:301:LMT:H42	2.43	0.47
19:1:5013:CLA:H12	32:Z:310:CHL:H93	1.95	0.47
19:3:5012:CLA:CBC	19:3:5018:CLA:HAC1	2.40	0.47
19:4:318:CLA:HMB1	19:4:318:CLA:HBB1	1.94	0.47
16:5:85:VAL:HG11	27:5:302:RRX:H39	1.95	0.47
19:5:310:CLA:HBB1	19:5:310:CLA:CMB	2.36	0.47
19:6:312:CLA:H71	19:6:312:CLA:H112	1.69	0.47
19:A:817:CLA:C1A	19:A:817:CLA:CGA	2.92	0.47
19:A:819:CLA:H203	19:A:827:CLA:H3A	1.95	0.47
19:A:822:CLA:HBA1	10:K:65:LEU:CD2	2.45	0.47
2:B:3:THR:HG21	2:B:11:GLN:NE2	2.29	0.47
2:B:28:MET:O	2:B:35:HIS:HE1	1.97	0.47
22:B:847:BCR:H321	22:B:847:BCR:C8	2.43	0.47
11:Z:53:TYR:CE2	32:Z:309:CHL:HAC2	2.49	0.47
19:3:5008:CLA:HMB1	19:3:5008:CLA:CBB	2.36	0.47
19:7:311:CLA:H3A	19:7:311:CLA:HBA2	1.52	0.47
14:8:143:LYS:HG3	14:8:146:SER:HB3	1.97	0.47
19:5:310:CLA:HBC1	32:5:315:CHL:HAB	1.96	0.47
17:6:66:TRP:CE3	38:6:326:ERG:C18	2.97	0.47
17:6:161:PHE:HZ	32:6:317:CHL:C4B	2.28	0.47
19:6:323:CLA:HBA2	19:6:323:CLA:H3A	1.58	0.47
19:A:838:CLA:C9	19:A:839:CLA:HHD	2.45	0.47
2:B:128:ILE:HG22	19:B:818:CLA:HED2	1.96	0.47
2:B:137:TYR:OH	8:I:70:VAL:HG22	2.14	0.47
19:B:822:CLA:C3	24:G:1604:LMT:H11	2.45	0.47
22:B:846:BCR:H21C	22:B:846:BCR:C36	2.44	0.47
6:F:142:LYS:HG3	24:F:305:LMT:O3'	2.14	0.47
13:7:172:PRO:HB2	19:7:324:CLA:C4	2.44	0.47
15:4:58:LEU:HB2	15:4:59:PRO:HD2	1.95	0.47
15:4:235:THR:HG22	19:4:318:CLA:O1D	2.15	0.47
19:4:306:CLA:H61	19:4:306:CLA:H92	1.65	0.47
16:5:192:LEU:HG	27:5:302:RRX:H40	1.96	0.47
19:5:311:CLA:H12	32:5:318:CHL:HMD2	1.96	0.47
17:6:147:TYR:HB3	32:6:321:CHL:C3D	2.45	0.47
32:6:321:CHL:HHC	32:6:321:CHL:CBB	2.43	0.47
1:A:87:TRP:HA	19:A:807:CLA:HBB2	1.96	0.47
1:A:584:CYS:HB2	2:B:668:TRP:HB3	1.97	0.47
1:A:726:VAL:HA	19:A:841:CLA:O1D	2.15	0.47
19:A:814:CLA:H62	19:A:816:CLA:H11	1.96	0.47
2:B:637:ASN:HB2	2:B:638:PRO:HD2	1.96	0.47
19:B:806:CLA:H122	19:B:806:CLA:HBD	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:813:CLA:H11	22:B:843:BCR:C20	2.45	0.47
19:B:822:CLA:HMB3	19:B:840:CLA:C1D	2.45	0.47
19:B:833:CLA:H152	19:B:833:CLA:H111	1.47	0.47
19:B:837:CLA:HHC	19:B:837:CLA:CBB	2.44	0.47
4:D:92:LYS:HB2	4:D:92:LYS:NZ	2.29	0.47
6:F:218:LYS:HE3	6:F:221:ASN:HD21	1.79	0.47
11:Z:135:ALA:HA	19:Z:315:CLA:HAB	1.97	0.47
13:7:82:GLY:HA2	31:7:304:LUT:C18	2.45	0.47
13:7:156:GLU:HG2	13:7:169:PHE:CE1	2.50	0.47
19:7:308:CLA:H161	19:7:308:CLA:H192	1.78	0.47
14:8:105:TYR:CE2	14:8:210:LYS:HD3	2.49	0.47
14:8:123:LEU:O	14:8:127:LEU:HG	2.14	0.47
22:8:306:BCR:H391	19:8:312:CLA:H43	1.95	0.47
32:4:319:CHL:HAA2	32:4:319:CHL:HBD	1.96	0.47
16:5:148:GLU:HG3	16:5:156:LYS:HG3	1.96	0.47
19:5:321:CLA:C19	19:6:320:CLA:H92	2.44	0.47
17:6:66:TRP:CZ2	19:6:318:CLA:HAA2	2.50	0.47
32:6:319:CHL:HAA2	32:6:319:CHL:CBD	2.45	0.47
19:A:810:CLA:HMB1	19:A:810:CLA:CBB	2.41	0.47
2:B:219:HIS:CD2	2:B:220:PRO:HD2	2.49	0.47
2:B:436:GLY:HA3	19:B:832:CLA:HAB	1.97	0.47
8:I:95:LEU:O	8:I:99:ILE:HG12	2.14	0.47
11:1:157:LEU:N	11:1:157:LEU:HD12	2.30	0.47
11:Z:154:PHE:HB3	32:Z:302:CHL:HMD1	1.96	0.47
12:3:15:LEU:HD23	12:3:35:PHE:CD1	2.49	0.47
12:3:228:ILE:HB	19:3:5010:CLA:H12	1.96	0.47
19:3:5010:CLA:HHC	19:3:5010:CLA:HBB1	1.96	0.47
19:7:309:CLA:H71	19:7:310:CLA:HMA1	1.97	0.47
31:8:304:LUT:H32	31:8:304:LUT:C39	2.43	0.47
15:4:213:LEU:HD23	19:4:312:CLA:HED3	1.97	0.47
16:5:80:TRP:CE2	32:5:316:CHL:HED3	2.50	0.47
16:5:106:PRO:HA	16:5:109:LEU:HD12	1.97	0.47
32:5:315:CHL:H172	19:6:323:CLA:C1D	2.45	0.47
19:A:802:CLA:H201	19:A:808:CLA:H121	1.95	0.47
19:A:808:CLA:CAB	19:A:828:CLA:H93	2.45	0.47
19:A:824:CLA:HHC	19:A:824:CLA:CBB	2.44	0.47
19:A:827:CLA:H12	22:A:849:BCR:C17	2.45	0.47
20:B:841:PQN:H301	25:B:848:DGD:HAE2	1.97	0.47
32:1:5014:CHL:HAB	32:1:5017:CHL:CBB	2.43	0.47
19:1:5018:CLA:HHC	19:1:5018:CLA:CBB	2.44	0.47
11:Z:214:PHE:CE1	19:Z:307:CLA:HED2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:3:5023:LMT:H101	19:7:307:CLA:CMD	2.44	0.47
13:7:104:ASP:HA	32:7:315:CHL:HED3	1.97	0.47
31:7:304:LUT:H31	31:7:304:LUT:H391	1.66	0.47
19:7:324:CLA:H11	38:6:326:ERG:C4	2.43	0.47
14:8:56:PRO:HB3	34:8:322:3PH:H222	1.97	0.47
31:8:304:LUT:C32	19:8:307:CLA:HMC2	2.45	0.47
15:4:123:ILE:HG22	15:4:124:GLY:N	2.29	0.47
22:5:304:BCR:H321	22:5:304:BCR:C8	2.43	0.47
19:5:313:CLA:HBA2	19:5:313:CLA:CBD	2.45	0.47
32:6:319:CHL:H172	32:6:319:CHL:H13	1.77	0.47
1:A:93:PHE:CE1	24:A:856:LMT:H32	2.50	0.47
19:A:814:CLA:H91	19:A:816:CLA:ND	2.30	0.47
19:A:838:CLA:H51	19:A:839:CLA:CMD	2.45	0.47
22:A:848:BCR:H11C	22:A:848:BCR:H341	1.78	0.47
2:B:125:TRP:O	2:B:128:ILE:HG12	2.15	0.47
19:B:815:CLA:C1C	22:B:842:BCR:H393	2.44	0.47
19:B:821:CLA:H151	7:G:45:PHE:HZ	1.80	0.47
19:B:823:CLA:C17	19:B:840:CLA:H2	2.45	0.47
5:E:36:GLY:HA2	5:E:90:LEU:HD12	1.96	0.47
10:K:55:PRO:HA	10:K:67:LEU:HD11	1.97	0.47
12:3:119:PHE:HE2	32:7:314:CHL:C9	2.27	0.47
19:3:5012:CLA:HHC	19:3:5012:CLA:CBB	2.41	0.47
19:7:308:CLA:HHC	19:7:308:CLA:HBB1	1.96	0.47
31:4:304:LUT:C32	19:4:310:CLA:HMB2	2.45	0.47
19:4:312:CLA:H92	19:4:312:CLA:H61	1.58	0.47
19:5:311:CLA:HBA2	19:5:311:CLA:H3A	1.41	0.47
32:6:316:CHL:HBC2	32:6:316:CHL:CMC	2.36	0.47
19:A:812:CLA:HHC	19:A:812:CLA:CBB	2.36	0.46
19:A:817:CLA:H62	19:A:817:CLA:H41	1.44	0.46
2:B:659:ALA:C	19:B:804:CLA:HAB	2.35	0.46
19:B:819:CLA:HMB1	19:B:824:CLA:H2	1.95	0.46
9:J:4:PHE:O	9:J:8:LEU:HG	2.16	0.46
19:1:5013:CLA:CAD	32:Z:310:CHL:H18	2.45	0.46
11:Z:133:ALA:HB1	24:Z:319:LMT:C4	2.45	0.46
12:3:56:TRP:HH2	19:3:5018:CLA:HAA2	1.80	0.46
31:3:5003:LUT:C36	19:3:5011:CLA:H61	2.44	0.46
22:3:5007:BCR:H11C	22:3:5007:BCR:H341	1.36	0.46
22:3:5007:BCR:H311	19:3:5015:CLA:HMA1	1.96	0.46
22:3:5007:BCR:H403	23:3:5021:LHG:HC41	1.96	0.46
19:4:307:CLA:C3D	19:4:312:CLA:H52	2.45	0.46
19:5:325:CLA:HBB1	19:5:325:CLA:CHC	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:HD13	1:A:52:LEU:HA	1.97	0.46
1:A:465:LEU:HG	19:B:809:CLA:HMC3	1.97	0.46
1:A:470:ASP:HB3	19:A:834:CLA:CED	2.45	0.46
19:A:809:CLA:CHC	19:A:828:CLA:H192	2.45	0.46
2:B:653:PHE:CE2	2:B:657:ILE:HD11	2.50	0.46
19:B:802:CLA:H8	19:B:802:CLA:H51	1.53	0.46
19:B:817:CLA:O1D	19:B:818:CLA:HMA1	2.16	0.46
19:B:830:CLA:HMB2	19:B:831:CLA:C2D	2.45	0.46
19:F:301:CLA:H171	19:F:301:CLA:C14	2.45	0.46
10:K:55:PRO:HD3	19:K:204:CLA:CHB	2.45	0.46
19:5:321:CLA:HMA1	23:6:324:LHG:H222	1.96	0.46
17:6:132:LEU:HD22	38:6:326:ERG:C21	2.44	0.46
1:A:679:TRP:CD2	18:A:801:CL0:H5	2.50	0.46
19:A:806:CLA:H203	19:A:806:CLA:H152	1.96	0.46
19:A:806:CLA:H93	19:A:806:CLA:H61	1.69	0.46
19:A:835:CLA:HMD2	19:A:836:CLA:CAB	2.44	0.46
2:B:642:ASN:OD1	2:B:644:LEU:HB2	2.14	0.46
2:B:722:TYR:HB2	19:B:802:CLA:HED3	1.97	0.46
19:B:805:CLA:HMB1	19:B:805:CLA:CBB	2.45	0.46
19:B:819:CLA:C1D	19:B:824:CLA:H161	2.45	0.46
19:G:1602:CLA:C4C	22:G:1603:BCR:H292	2.45	0.46
11:Z:115:PHE:CZ	19:Z:311:CLA:HMD2	2.51	0.46
19:Z:305:CLA:C2B	19:Z:305:CLA:H51	2.45	0.46
12:3:230:THR:HA	33:3:5001:SPH:H11	1.96	0.46
19:3:5016:CLA:H61	19:3:5016:CLA:H101	1.43	0.46
13:7:130:TRP:CD1	22:7:305:BCR:H12C	2.51	0.46
19:8:308:CLA:HMD3	24:4:302:LMT:H82	1.97	0.46
23:8:321:LHG:H251	23:8:321:LHG:H142	1.98	0.46
19:5:301:CLA:HHC	19:5:301:CLA:CBB	2.34	0.46
17:6:257:PRO:HG3	19:6:320:CLA:C3D	2.45	0.46
1:A:293:ASP:CB	19:A:818:CLA:HMA1	2.44	0.46
19:A:818:CLA:C4A	19:A:818:CLA:H2	2.45	0.46
19:A:857:CLA:HMC2	19:B:838:CLA:H12	1.97	0.46
2:B:286:ILE:HB	22:B:842:BCR:H363	1.96	0.46
11:1:122:ASP:O	11:1:126:LEU:HG	2.15	0.46
23:1:5019:LHG:HC81	22:8:306:BCR:C2	2.45	0.46
11:Z:89:LEU:CD1	19:Z:312:CLA:H203	2.45	0.46
32:Z:309:CHL:H141	32:Z:309:CHL:H162	1.77	0.46
19:Z:314:CLA:CHA	19:Z:314:CLA:HBA2	2.45	0.46
12:3:21:GLN:HA	12:3:24:LEU:HD12	1.96	0.46
33:4:301:SPH:H142	33:4:301:SPH:H111	1.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:5:219:LEU:HD11	19:5:313:CLA:HMC3	1.98	0.46
17:6:123:TRP:HB2	19:6:302:CLA:H11	1.96	0.46
1:A:261:ILE:HG21	22:A:859:BCR:HC21	1.98	0.46
1:A:304:LEU:HB2	19:A:817:CLA:H141	1.97	0.46
1:A:385:GLY:HA2	1:A:747:ILE:CG2	2.46	0.46
19:A:816:CLA:HBD	24:A:854:LMT:C6'	2.46	0.46
19:A:821:CLA:H2	19:A:821:CLA:H62	1.58	0.46
19:A:822:CLA:H42	19:K:204:CLA:C1B	2.46	0.46
19:A:829:CLA:NB	22:A:847:BCR:HC22	2.30	0.46
19:A:833:CLA:H102	19:B:838:CLA:C6	2.45	0.46
19:A:838:CLA:H61	19:A:838:CLA:H102	1.53	0.46
2:B:231:TRP:CH2	19:B:816:CLA:H92	2.50	0.46
2:B:396:ILE:HD11	2:B:542:ALA:HB1	1.96	0.46
11:1:117:ILE:HD12	11:1:117:ILE:H	1.80	0.46
11:1:187:PHE:CE1	31:1:5003:LUT:H41	2.51	0.46
12:3:110:TYR:CE1	19:3:5013:CLA:HAA2	2.51	0.46
32:3:5017:CHL:HAA1	32:3:5017:CHL:HBD	1.98	0.46
15:4:109:LEU:HD11	19:4:306:CLA:HBC1	1.98	0.46
15:4:206:GLY:O	15:4:207:ASP:C	2.53	0.46
17:6:142:PRO:HB2	22:6:307:BCR:H322	1.96	0.46
38:6:326:ERG:H213	38:6:326:ERG:C18	2.46	0.46
1:A:160:TYR:CE1	24:A:856:LMT:H1'	2.51	0.46
2:B:296:PHE:CE1	19:B:820:CLA:HBD	2.51	0.46
2:B:681:TRP:CE2	2:B:685:LYS:HG3	2.50	0.46
10:K:42:THR:HB	19:K:202:CLA:O1A	2.16	0.46
19:Z:308:CLA:C4	14:8:154:LEU:HB2	2.44	0.46
22:3:5006:BCR:H321	22:3:5006:BCR:HC8	1.98	0.46
32:8:301:CHL:H2	37:8:302:SQD:C19	2.36	0.46
31:8:304:LUT:H401	31:8:304:LUT:H35	1.61	0.46
15:4:259:ASN:O	15:4:263:ARG:HG3	2.15	0.46
16:5:247:ILE:HD11	32:5:315:CHL:OBD	2.16	0.46
17:6:182:LEU:HD22	19:6:314:CLA:HAC1	1.97	0.46
31:6:305:LUT:H181	31:6:305:LUT:C8	2.45	0.46
1:A:267:LEU:HD12	10:K:34:THR:HG23	1.98	0.46
19:A:814:CLA:HBA2	19:A:816:CLA:HMB3	1.98	0.46
2:B:67:PHE:HZ	8:I:71:PRO:HG2	1.81	0.46
2:B:71:TRP:NE1	8:I:71:PRO:HD2	2.31	0.46
19:B:821:CLA:HAA2	7:G:56:TYR:CE2	2.51	0.46
23:1:5019:LHG:HC82	32:8:301:CHL:C2C	2.45	0.46
13:7:183:TYR:O	13:7:187:LYS:HG3	2.16	0.46
13:7:219:LEU:O	13:7:223:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:7:311:CLA:C1D	33:7:321:SPH:H102	2.45	0.46
14:8:128:PHE:CE1	32:8:301:CHL:H51	2.50	0.46
15:4:195:GLY:HA3	19:4:306:CLA:HED2	1.96	0.46
19:4:306:CLA:CGA	19:4:306:CLA:C3A	2.91	0.46
19:4:309:CLA:HMB1	19:4:309:CLA:CBB	2.40	0.46
32:4:315:CHL:HBD	32:4:315:CHL:HAA1	1.97	0.46
19:5:301:CLA:H72	19:5:319:CLA:HAA2	1.97	0.46
32:5:318:CHL:OMC	32:5:318:CHL:HAC1	2.15	0.46
19:5:322:CLA:CMD	28:6:304:C7Z:C38	2.91	0.46
17:6:75:SER:OG	17:6:180:GLY:HA3	2.16	0.46
19:A:804:CLA:H51	19:A:804:CLA:H8	1.38	0.46
2:B:466:ALA:HB3	2:B:477:PHE:HE1	1.81	0.46
2:B:543:ARG:HG3	39:B:919:HOH:O	2.16	0.46
19:B:801:CLA:CGA	19:B:801:CLA:H3A	2.46	0.46
19:B:807:CLA:H111	19:B:807:CLA:H71	1.36	0.46
19:B:834:CLA:HBA2	19:B:834:CLA:CHA	2.45	0.46
19:B:850:CLA:C14	19:B:850:CLA:C17	2.89	0.46
19:K:202:CLA:CHC	33:3:5001:SPH:H132	2.46	0.46
13:7:240:ILE:O	35:7:302:DGA:HG11	2.16	0.46
19:7:311:CLA:H92	19:7:311:CLA:H61	1.50	0.46
22:8:303:BCR:H343	33:4:301:SPH:H152	1.96	0.46
19:8:311:CLA:HMD2	19:8:318:CLA:C4C	2.45	0.46
15:4:157:PHE:HA	15:4:160:VAL:HG22	1.97	0.46
27:4:303:RRX:H25	19:4:306:CLA:H52	1.98	0.46
31:4:304:LUT:H28	19:4:309:CLA:H52	1.97	0.46
19:4:313:CLA:HBA1	17:6:116:VAL:HG22	1.98	0.46
16:5:149:ASP:HB2	16:5:155:ASN:HB2	1.97	0.46
19:A:812:CLA:CBB	19:A:812:CLA:H101	2.46	0.46
19:A:815:CLA:H141	19:A:815:CLA:H161	1.73	0.46
19:A:818:CLA:HHC	19:A:818:CLA:CBB	2.46	0.46
2:B:27:ALA:HB2	25:B:848:DGD:HA22	1.97	0.46
2:B:594:TYR:CZ	19:B:835:CLA:HBC2	2.51	0.46
4:D:174:ARG:HD2	5:E:49:GLU:OE2	2.16	0.46
7:G:51:PHE:CZ	19:G:1602:CLA:HMC2	2.50	0.46
10:K:50:ARG:HB2	19:K:205:CLA:HBC2	1.96	0.46
11:Z:149:TYR:HB3	32:Z:302:CHL:HED2	1.98	0.46
19:8:307:CLA:HMD2	32:8:317:CHL:O1A	2.16	0.46
19:8:307:CLA:HHD	32:8:317:CHL:O1A	2.16	0.46
19:8:312:CLA:HBC3	19:8:312:CLA:CHD	2.46	0.46
24:8:323:LMT:H1B	24:8:323:LMT:H6'2	1.70	0.46
15:4:109:LEU:HD11	19:4:306:CLA:CBC	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:307:CLA:H142	19:5:312:CLA:H101	1.98	0.46
23:6:303:LHG:H132	23:6:303:LHG:C24	2.30	0.46
19:6:309:CLA:HBB1	19:6:309:CLA:CMB	2.37	0.46
1:A:501:ASN:ND2	19:K:203:CLA:HED1	2.31	0.46
1:A:693:TRP:HZ3	19:B:801:CLA:O1D	1.99	0.46
19:A:806:CLA:HBB2	22:A:847:BCR:C4	2.43	0.46
19:A:840:CLA:HAB	19:A:840:CLA:C12	2.44	0.46
2:B:493:LEU:HD12	19:B:834:CLA:HED1	1.97	0.46
19:B:815:CLA:H11	19:B:815:CLA:H51	1.57	0.46
8:I:78:VAL:C	8:I:81:PRO:HD2	2.36	0.46
19:Z:311:CLA:H41	19:Z:311:CLA:H61	1.61	0.46
19:7:306:CLA:HMB1	19:7:306:CLA:CBB	2.41	0.46
19:8:318:CLA:HMC2	24:8:324:LMT:H123	1.96	0.46
24:4:322:LMT:H2'	24:4:322:LMT:H12	1.49	0.46
19:5:307:CLA:O1D	19:5:312:CLA:H92	2.16	0.46
17:6:249:PRO:HG3	19:6:301:CLA:H92	1.98	0.46
22:6:307:BCR:H291	19:6:313:CLA:H51	1.98	0.46
19:6:310:CLA:OBD	19:6:314:CLA:HBD	2.16	0.46
19:A:812:CLA:HMC3	19:A:820:CLA:CBC	2.46	0.45
19:A:832:CLA:H192	19:A:832:CLA:H162	1.62	0.45
19:A:841:CLA:HBA1	19:A:841:CLA:CBD	2.46	0.45
2:B:240:THR:HG22	2:B:250:GLY:O	2.15	0.45
19:B:816:CLA:HMB1	19:B:816:CLA:CBB	2.46	0.45
19:B:821:CLA:H2	19:B:821:CLA:H61	1.68	0.45
11:1:103:PRO:HB3	32:1:5017:CHL:HAC2	1.97	0.45
11:1:112:ALA:CB	11:1:119:VAL:HB	2.39	0.45
11:1:138:GLU:HG3	19:1:5016:CLA:C4B	2.47	0.45
15:4:62:MET:CE	15:4:65:ALA:HB2	2.46	0.45
23:4:320:LHG:H112	23:4:320:LHG:H301	1.98	0.45
1:A:59:PHE:HA	1:A:62:HIS:ND1	2.31	0.45
19:A:802:CLA:H62	19:A:802:CLA:H102	1.34	0.45
19:A:812:CLA:CGA	19:A:812:CLA:C1A	2.94	0.45
19:A:814:CLA:H51	19:A:816:CLA:H151	1.97	0.45
19:A:817:CLA:H121	19:K:203:CLA:HMD3	1.98	0.45
2:B:438:TYR:CD2	19:B:802:CLA:H203	2.51	0.45
19:B:806:CLA:H2	19:B:806:CLA:H61	1.56	0.45
19:B:837:CLA:HBA1	19:B:837:CLA:CHA	2.43	0.45
19:B:850:CLA:H92	19:B:850:CLA:H61	1.64	0.45
8:I:84:GLY:C	8:I:88:PRO:HG2	2.37	0.45
10:K:103:ILE:O	10:K:107:LEU:HG	2.17	0.45
11:1:205:HIS:CG	19:1:5008:CLA:HAA2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1:210:TRP:CE2	19:1:5013:CLA:CMA	3.00	0.45
19:Z:315:CLA:H111	19:Z:315:CLA:H143	1.45	0.45
19:3:5018:CLA:H62	19:3:5018:CLA:H2	1.71	0.45
33:7:321:SPH:H2	19:6:301:CLA:C3B	2.45	0.45
32:8:319:CHL:H143	32:8:319:CHL:H111	1.77	0.45
15:4:73:GLY:N	15:4:78:ASP:OD2	2.47	0.45
15:4:203:TRP:CB	19:4:306:CLA:HBA1	2.41	0.45
16:5:73:SER:N	19:5:317:CLA:HED2	2.30	0.45
17:6:129:TRP:HH2	23:6:303:LHG:HC91	1.80	0.45
1:A:740:TRP:CG	22:A:850:BCR:HC41	2.51	0.45
19:A:842:CLA:H152	19:A:842:CLA:H111	1.70	0.45
2:B:467:ALA:HB1	2:B:478:LEU:HD12	1.98	0.45
22:B:846:BCR:H15C	22:B:846:BCR:H351	1.79	0.45
6:F:150:PHE:CZ	24:F:305:LMT:H71	2.48	0.45
24:G:1604:LMT:H71	19:1:5016:CLA:CHC	2.47	0.45
12:3:232:PHE:HE1	22:3:5006:BCR:HC32	1.80	0.45
19:3:5011:CLA:HMB1	19:3:5011:CLA:CBB	2.46	0.45
14:8:231:VAL:HG12	19:8:309:CLA:HED1	1.99	0.45
19:8:310:CLA:HMB1	19:8:310:CLA:CBB	2.44	0.45
19:A:803:CLA:H193	22:A:858:BCR:H20C	1.98	0.45
19:A:815:CLA:H142	19:3:5012:CLA:HBB1	1.97	0.45
19:A:822:CLA:HHB	19:A:823:CLA:C2	2.47	0.45
19:B:810:CLA:HMA3	19:B:810:CLA:H61	1.98	0.45
19:B:825:CLA:H41	19:B:825:CLA:H62	1.43	0.45
19:B:835:CLA:HMB2	19:B:837:CLA:HED1	1.97	0.45
4:D:132:PHE:HB2	4:D:134:LEU:HG	1.99	0.45
10:K:72:ASN:ND2	10:K:75:GLY:HA2	2.31	0.45
10:K:97:HIS:CG	22:K:206:BCR:H12C	2.51	0.45
11:1:214:PHE:HA	11:1:217:ASN:OD1	2.17	0.45
19:Z:315:CLA:H11	19:Z:315:CLA:H52	1.74	0.45
12:3:69:MET:HG3	12:3:191:GLY:HA2	1.99	0.45
22:3:5005:BCR:H11C	22:3:5005:BCR:H341	1.64	0.45
19:7:306:CLA:H3A	19:7:306:CLA:O2A	2.16	0.45
14:8:209:GLN:HG2	19:8:309:CLA:C4D	2.46	0.45
15:4:116:VAL:HB	15:4:117:PRO:HD3	1.99	0.45
32:4:317:CHL:HBB1	32:4:317:CHL:HHC	1.98	0.45
17:6:172:LEU:HB3	19:6:309:CLA:HMA1	1.98	0.45
19:6:314:CLA:H61	19:6:314:CLA:H92	1.57	0.45
19:A:807:CLA:HMB3	19:A:808:CLA:HMA1	1.98	0.45
19:A:815:CLA:H121	22:3:5006:BCR:H14C	1.98	0.45
19:A:821:CLA:O1A	19:A:824:CLA:HBD	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:822:CLA:HBB1	19:A:822:CLA:HMB1	1.98	0.45
19:B:807:CLA:H3A	19:B:807:CLA:HBA1	1.59	0.45
19:B:822:CLA:HMB1	19:B:822:CLA:HBB1	1.97	0.45
19:B:825:CLA:H142	19:B:835:CLA:H141	1.97	0.45
19:Z:305:CLA:HMC2	31:Z:317:LUT:C31	2.46	0.45
19:Z:312:CLA:H111	19:Z:312:CLA:H93	1.57	0.45
22:3:5006:BCR:H17C	19:3:5012:CLA:HHC	1.99	0.45
13:7:97:LEU:HD13	19:6:301:CLA:HAA2	1.97	0.45
15:4:123:ILE:HD12	15:4:125:PHE:HE1	1.82	0.45
22:5:304:BCR:C4	23:6:324:LHG:HC82	2.12	0.45
19:5:317:CLA:CBB	19:5:317:CLA:HMB1	2.47	0.45
19:A:812:CLA:HAB	19:A:812:CLA:C19	2.46	0.45
19:A:818:CLA:H8	19:A:836:CLA:CMA	2.47	0.45
19:A:828:CLA:H61	22:A:850:BCR:H331	1.99	0.45
2:B:374:THR:HG22	19:B:827:CLA:CAB	2.47	0.45
2:B:495:LEU:HB2	2:B:496:PRO:HD3	1.97	0.45
2:B:653:PHE:CZ	2:B:657:ILE:HD11	2.51	0.45
19:B:823:CLA:H142	22:B:845:BCR:H17C	1.99	0.45
24:1:5002:LMT:H61	19:1:5016:CLA:H42	1.99	0.45
19:Z:304:CLA:HMB1	19:Z:304:CLA:CBB	2.39	0.45
13:7:31:PRO:HB2	32:7:314:CHL:HBC1	1.99	0.45
19:7:309:CLA:O1A	19:7:309:CLA:H2	2.17	0.45
32:7:314:CHL:HHC	32:7:314:CHL:HBB1	1.97	0.45
14:8:169:PRO:HG2	19:8:307:CLA:OBD	2.16	0.45
19:8:308:CLA:H112	19:8:308:CLA:H152	1.75	0.45
15:4:257:TRP:O	15:4:261:LEU:HG	2.16	0.45
1:A:18:ASP:CG	1:A:71:ARG:HH22	2.19	0.45
1:A:426:LEU:O	1:A:430:VAL:HG23	2.17	0.45
1:A:487:ILE:HD11	19:A:837:CLA:H2	1.99	0.45
1:A:572:ARG:HD2	1:A:721:THR:HG21	1.99	0.45
19:A:815:CLA:H142	19:3:5012:CLA:HBB2	1.98	0.45
19:A:816:CLA:H121	19:A:816:CLA:H91	1.99	0.45
19:A:824:CLA:H172	19:A:839:CLA:C4D	2.47	0.45
19:A:857:CLA:HBA2	19:A:857:CLA:C2	2.47	0.45
2:B:66:LEU:HD12	2:B:143:LEU:HD12	1.98	0.45
2:B:67:PHE:HZ	8:I:71:PRO:CG	2.30	0.45
2:B:433:HIS:O	2:B:437:LEU:HG	2.17	0.45
2:B:599:HIS:HB3	2:B:603:TRP:CZ2	2.52	0.45
19:B:831:CLA:HMB1	19:B:831:CLA:CBB	2.47	0.45
19:Z:311:CLA:HMB1	19:Z:311:CLA:CBB	2.45	0.45
13:7:186:TYR:CG	19:7:306:CLA:H12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:7:303:LUT:C8	31:7:303:LUT:H181	2.47	0.45
31:7:304:LUT:H181	31:7:304:LUT:C8	2.46	0.45
16:5:106:PRO:O	16:5:109:LEU:HB2	2.15	0.45
19:5:310:CLA:H62	19:5:310:CLA:H2	1.54	0.45
32:5:316:CHL:OMC	32:5:316:CHL:HAC1	2.15	0.45
19:6:322:CLA:H3A	19:6:322:CLA:HBA2	1.55	0.45
19:6:323:CLA:H121	19:6:323:CLA:H72	1.98	0.45
1:A:376:PRO:HB3	19:A:819:CLA:HMA2	1.98	0.45
19:A:823:CLA:H92	19:A:823:CLA:H61	1.70	0.45
2:B:284:ILE:HA	19:B:816:CLA:C17	2.38	0.45
2:B:370:ALA:HB1	2:B:726:LEU:HD11	1.98	0.45
19:B:833:CLA:H172	19:B:834:CLA:C1C	2.47	0.45
3:C:25:VAL:HG13	3:C:45:THR:HA	1.97	0.45
7:G:89:THR:OG1	19:G:1602:CLA:HAA1	2.16	0.45
19:K:202:CLA:ND	33:3:5001:SPH:H91	2.32	0.45
19:1:5008:CLA:C14	24:Z:301:LMT:H101	2.46	0.45
11:Z:155:ASP:N	11:Z:156:PRO:HD3	2.32	0.45
19:7:306:CLA:H71	19:7:307:CLA:HMA1	1.97	0.45
19:7:307:CLA:HMD2	19:7:312:CLA:C1D	2.46	0.45
15:4:159:TRP:O	15:4:163:ARG:HG2	2.16	0.45
15:4:183:ASN:HD21	32:4:319:CHL:HAA1	1.80	0.45
16:5:67:LEU:HD12	19:5:309:CLA:HMA2	1.98	0.45
16:5:222:PRO:HB3	19:5:313:CLA:CHB	2.46	0.45
19:5:306:CLA:HMB2	19:5:307:CLA:HBA2	1.99	0.45
19:6:301:CLA:H91	19:6:301:CLA:H111	1.67	0.45
31:6:306:LUT:C31	19:6:312:CLA:HMC2	2.46	0.45
19:6:318:CLA:HMB1	19:6:318:CLA:HBB1	1.99	0.45
1:A:718:LEU:HB3	1:A:722:GLN:HG2	1.97	0.45
19:A:821:CLA:H122	19:A:824:CLA:H93	1.98	0.45
19:A:833:CLA:C2	19:A:857:CLA:H43	2.47	0.45
19:A:841:CLA:NC	19:A:841:CLA:H52	2.32	0.45
19:A:857:CLA:HMC3	19:B:838:CLA:C4D	2.46	0.45
19:A:857:CLA:H52	19:A:857:CLA:C4B	2.46	0.45
2:B:9:PHE:HZ	2:B:25:GLY:O	2.00	0.45
2:B:228:THR:O	7:G:34:PRO:HG3	2.16	0.45
3:C:23:LEU:HD22	3:C:47:ASP:O	2.17	0.45
19:Z:308:CLA:HBB1	19:Z:308:CLA:CMB	2.30	0.45
34:3:5022:3PH:H372	34:3:5022:3PH:H3A1	1.59	0.45
34:8:322:3PH:H3D1	34:8:322:3PH:H3A1	1.45	0.45
15:4:167:ASP:OD1	15:4:171:PRO:HA	2.17	0.45
19:4:312:CLA:H41	19:4:312:CLA:H62	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:5:101:TYR:CD2	32:5:315:CHL:HMA2	2.52	0.45
16:5:215:LEU:HD12	16:5:219:LEU:HD13	1.98	0.45
32:5:316:CHL:HAA1	32:5:316:CHL:HBD	1.98	0.45
17:6:175:LYS:HZ3	19:6:310:CLA:HED1	1.80	0.45
31:6:305:LUT:H35	31:6:305:LUT:H401	1.87	0.45
22:6:308:BCR:H383	32:6:316:CHL:H12	1.98	0.45
1:A:679:TRP:CD2	18:A:801:CL0:CMA	3.00	0.45
19:A:805:CLA:H51	19:A:813:CLA:H12	1.98	0.45
19:A:818:CLA:H91	19:A:818:CLA:H111	1.75	0.45
19:A:833:CLA:H111	19:B:838:CLA:H42	1.99	0.45
19:B:826:CLA:H13	19:B:826:CLA:H102	1.70	0.45
19:B:831:CLA:H41	19:B:831:CLA:C7	2.47	0.45
19:B:833:CLA:H62	19:B:833:CLA:H102	1.48	0.45
8:I:86:VAL:O	8:I:90:ILE:HG12	2.16	0.45
11:1:184:PHE:CE1	31:1:5004:LUT:H10	2.52	0.45
19:1:5011:CLA:HMA2	32:1:5017:CHL:C3C	2.47	0.45
11:Z:42:PRO:HB3	11:Z:44:TRP:CZ2	2.52	0.45
11:Z:102:ALA:N	11:Z:103:PRO:HD2	2.31	0.45
32:Z:309:CHL:HED3	15:4:163:ARG:HD2	1.99	0.45
12:3:173:LEU:HD12	19:3:5008:CLA:H11	1.98	0.45
22:3:5006:BCR:C17	19:3:5012:CLA:CBB	2.95	0.45
14:8:103:GLU:HG2	14:8:105:TYR:CE2	2.52	0.45
19:8:310:CLA:H161	19:8:310:CLA:H122	1.80	0.45
19:4:307:CLA:H12	19:4:307:CLA:O2D	2.16	0.45
16:5:155:ASN:HB3	32:5:320:CHL:C4D	2.47	0.45
17:6:184:MET:HE3	19:6:312:CLA:HMC3	1.99	0.45
1:A:349:TRP:CZ2	19:A:825:CLA:H172	2.52	0.44
19:A:806:CLA:H93	19:A:806:CLA:H111	1.69	0.44
19:A:809:CLA:CBB	19:B:832:CLA:HBC2	2.47	0.44
19:A:826:CLA:C4B	19:A:839:CLA:HMA2	2.48	0.44
19:A:830:CLA:H62	19:A:830:CLA:H41	1.65	0.44
19:B:813:CLA:H203	22:B:843:BCR:H271	1.98	0.44
19:B:815:CLA:HED2	19:B:815:CLA:H2A	1.99	0.44
19:B:836:CLA:HMB1	19:B:836:CLA:CBB	2.47	0.44
7:G:56:TYR:O	7:G:60:GLU:HG2	2.17	0.44
11:1:103:PRO:HB3	32:1:5017:CHL:OMC	2.16	0.44
11:1:206:LEU:HD21	19:1:5013:CLA:HMC3	1.99	0.44
19:3:5013:CLA:H141	19:3:5013:CLA:H161	1.87	0.44
31:8:304:LUT:H172	19:8:309:CLA:HMB3	1.99	0.44
31:8:305:LUT:H3	19:8:312:CLA:HMA3	1.99	0.44
33:4:301:SPH:H171	33:4:301:SPH:H141	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:308:CLA:H93	19:4:308:CLA:H112	1.62	0.44
1:A:189:GLU:CD	1:A:189:GLU:H	2.19	0.44
19:A:821:CLA:C5	22:A:849:BCR:H16C	2.46	0.44
19:A:827:CLA:H152	19:A:827:CLA:H111	1.42	0.44
2:B:356:LEU:HG	19:B:826:CLA:HMC2	1.99	0.44
19:B:819:CLA:H161	19:B:819:CLA:H122	1.68	0.44
11:1:165:LYS:HG2	11:1:169:LEU:HD12	2.00	0.44
11:Z:56:ASP:N	11:Z:57:PRO:HD3	2.33	0.44
11:Z:115:PHE:CE2	19:Z:311:CLA:HMD2	2.53	0.44
12:3:146:TYR:CE1	24:3:5023:LMT:H4'	2.51	0.44
31:3:5002:LUT:H26	19:3:5008:CLA:O1A	2.17	0.44
13:7:222:HIS:HB2	19:7:308:CLA:HAA1	2.00	0.44
32:8:315:CHL:OMC	23:8:321:LHG:HC41	2.18	0.44
19:8:318:CLA:H3A	19:8:318:CLA:HBA2	1.31	0.44
1:A:574:PRO:HB3	1:A:720:ILE:HB	1.99	0.44
1:A:704:HIS:HA	1:A:709:VAL:HG23	2.00	0.44
19:A:811:CLA:HMB1	19:A:811:CLA:CBB	2.45	0.44
19:B:816:CLA:CGA	19:B:816:CLA:C1A	2.96	0.44
19:B:836:CLA:HAA1	19:B:836:CLA:HBD	1.99	0.44
10:K:33:SER:O	10:K:37:ILE:HG13	2.17	0.44
23:1:5019:LHG:H181	23:1:5019:LHG:H151	1.87	0.44
11:Z:205:HIS:CG	19:Z:304:CLA:HAA2	2.52	0.44
31:3:5002:LUT:H361	19:3:5008:CLA:H102	2.00	0.44
19:3:5012:CLA:H3A	19:3:5012:CLA:HBA1	1.68	0.44
13:7:65:LEU:O	13:7:69:VAL:HG23	2.16	0.44
19:7:306:CLA:H92	19:7:306:CLA:H61	1.61	0.44
19:7:310:CLA:H12	19:7:310:CLA:HMA2	1.99	0.44
19:8:309:CLA:HHC	19:8:309:CLA:CBB	2.46	0.44
19:8:314:CLA:CBA	32:8:315:CHL:H121	2.47	0.44
19:5:306:CLA:H12	19:5:306:CLA:C4A	2.47	0.44
19:6:301:CLA:H143	32:6:316:CHL:H62	1.99	0.44
19:6:301:CLA:HBD	19:6:301:CLA:HAA1	1.99	0.44
19:6:311:CLA:HBD	19:6:311:CLA:HAA1	1.99	0.44
1:A:263:PRO:HB2	1:A:272:TYR:CZ	2.53	0.44
18:A:801:CL0:CBB	19:B:802:CLA:HAA1	2.48	0.44
19:A:803:CLA:HMA1	19:A:808:CLA:H203	2.00	0.44
19:A:809:CLA:HBB2	19:B:832:CLA:CHD	2.48	0.44
19:A:824:CLA:H42	19:A:839:CLA:H92	1.99	0.44
19:A:828:CLA:O1D	19:A:829:CLA:HMA1	2.17	0.44
4:D:139:TYR:CE2	4:D:149:TYR:HD1	2.36	0.44
6:F:153:THR:O	6:F:157:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:311:CLA:H52	32:Z:313:CHL:HAA2	1.99	0.44
31:Z:317:LUT:H401	31:Z:317:LUT:H35	1.20	0.44
31:Z:318:LUT:H181	31:Z:318:LUT:C8	2.47	0.44
19:3:5008:CLA:H161	32:3:5017:CHL:H92	1.98	0.44
19:3:5010:CLA:HHC	19:3:5010:CLA:CBB	2.48	0.44
13:7:203:GLY:O	13:7:207:GLN:HG3	2.17	0.44
15:4:134:TRP:CH2	24:4:322:LMT:H41	2.51	0.44
19:6:301:CLA:H42	19:6:301:CLA:C1D	2.46	0.44
19:6:312:CLA:HBB1	19:6:312:CLA:CMB	2.40	0.44
19:6:318:CLA:HMB1	19:6:318:CLA:CBB	2.47	0.44
32:6:321:CHL:HAC2	32:6:321:CHL:OMC	2.17	0.44
38:6:326:ERG:H182	38:6:326:ERG:C19	2.46	0.44
2:B:5:LEU:HD21	8:I:103:ALA:HA	1.99	0.44
2:B:31:ASP:HB2	19:B:829:CLA:HAA1	1.99	0.44
2:B:243:HIS:HA	2:B:249:GLN:O	2.17	0.44
19:B:808:CLA:H42	19:B:808:CLA:C1D	2.48	0.44
19:B:824:CLA:HMB1	19:B:824:CLA:CBB	2.48	0.44
19:B:832:CLA:H8	19:F:303:CLA:HMA1	2.00	0.44
19:B:834:CLA:HMB1	22:B:846:BCR:HC32	1.99	0.44
19:B:839:CLA:HHC	19:B:839:CLA:CBB	2.47	0.44
4:D:156:VAL:HG13	4:D:160:LYS:HE3	1.98	0.44
6:F:99:ALA:HB3	6:F:100:PRO:HD3	2.00	0.44
7:G:32:LEU:HD11	11:1:124:ASN:HD22	1.82	0.44
7:G:100:VAL:CG1	22:G:1603:BCR:H17C	2.48	0.44
11:Z:57:PRO:HD2	31:Z:317:LUT:C23	2.39	0.44
22:3:5005:BCR:H15C	22:3:5005:BCR:H351	1.88	0.44
19:7:307:CLA:HMB1	19:7:307:CLA:CBB	2.40	0.44
15:4:118:GLU:HG2	15:4:241:LEU:HB2	1.98	0.44
33:4:301:SPH:H5	33:4:301:SPH:H82	1.74	0.44
16:5:101:TYR:CE2	32:5:315:CHL:HMA2	2.52	0.44
22:6:307:BCR:H331	22:6:307:BCR:C8	2.48	0.44
19:6:310:CLA:C3D	19:6:314:CLA:H52	2.47	0.44
1:A:272:TYR:HB3	1:A:275:PHE:CZ	2.53	0.44
19:A:805:CLA:H161	22:A:847:BCR:C14	2.47	0.44
19:A:819:CLA:C4D	19:A:829:CLA:H61	2.48	0.44
19:A:823:CLA:H71	19:A:823:CLA:H112	1.29	0.44
19:A:841:CLA:H102	19:A:841:CLA:H62	1.59	0.44
19:B:804:CLA:H93	19:B:804:CLA:H62	1.80	0.44
19:B:811:CLA:H2	19:B:812:CLA:HMD2	2.00	0.44
19:B:822:CLA:CHC	24:1:5002:LMT:H101	2.47	0.44
19:B:824:CLA:H141	19:B:824:CLA:H162	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:THR:HG23	4:D:63:PRO:HD2	2.00	0.44
19:F:301:CLA:H3A	22:F:302:BCR:C14	2.48	0.44
19:1:5011:CLA:HBA2	19:1:5011:CLA:H3A	1.54	0.44
31:Z:317:LUT:H11	31:Z:317:LUT:H191	1.82	0.44
12:3:229:LEU:HD22	33:3:5001:SPH:H61	2.00	0.44
13:7:136:TRP:CD2	19:7:317:CLA:HMA2	2.53	0.44
13:7:221:ASP:HB3	13:7:229:VAL:HG11	1.98	0.44
15:4:109:LEU:HG	19:4:306:CLA:HMC1	2.00	0.44
16:5:133:GLU:HG3	19:5:317:CLA:NB	2.33	0.44
16:5:135:ARG:NE	32:5:320:CHL:OMC	2.50	0.44
16:5:227:ILE:HG12	16:5:231:ILE:HB	2.00	0.44
17:6:98:TYR:CE2	32:6:316:CHL:HMA2	2.52	0.44
31:6:306:LUT:H391	31:6:306:LUT:H31	1.62	0.44
22:6:307:BCR:H15C	22:6:307:BCR:H351	1.81	0.44
1:A:142:SER:HB2	19:A:829:CLA:HMA2	2.00	0.44
1:A:246:ASN:ND2	1:A:249:ILE:HG13	2.33	0.44
19:A:815:CLA:H41	19:A:815:CLA:H62	1.83	0.44
2:B:388:PHE:HZ	19:B:825:CLA:HAB	1.82	0.44
4:D:138:PHE:CZ	4:D:151:HIS:HB3	2.53	0.44
6:F:174:VAL:HG12	6:F:183:LYS:HD3	2.00	0.44
7:G:89:THR:HB	7:G:96:ASN:HA	2.00	0.44
9:J:25:LEU:O	9:J:29:ILE:HG13	2.18	0.44
19:1:5008:CLA:H61	19:1:5008:CLA:H92	1.54	0.44
19:Z:303:CLA:HMB1	19:Z:303:CLA:CBB	2.37	0.44
13:7:186:TYR:CE1	19:7:306:CLA:H43	2.53	0.44
32:8:315:CHL:H112	32:8:315:CHL:H71	1.64	0.44
19:4:313:CLA:H41	19:4:313:CLA:H62	1.71	0.44
17:6:127:ARG:HD2	19:6:302:CLA:CED	2.47	0.44
17:6:144:PHE:HB2	17:6:147:TYR:HD2	1.82	0.44
17:6:175:LYS:HD3	19:6:310:CLA:HAA2	2.00	0.44
19:A:810:CLA:HBA2	12:3:52:ILE:HG13	2.00	0.44
19:A:835:CLA:H193	19:A:839:CLA:H151	2.00	0.44
2:B:160:PRO:O	2:B:161:ASN:HB2	2.18	0.44
2:B:258:PHE:HB2	19:B:816:CLA:O1D	2.18	0.44
19:B:815:CLA:C11	22:B:842:BCR:H21C	2.37	0.44
19:B:837:CLA:H93	19:B:837:CLA:H111	1.67	0.44
20:B:841:PQN:H111	20:B:841:PQN:H2M1	1.81	0.44
22:F:302:BCR:H352	19:F:303:CLA:CHC	2.48	0.44
19:I:201:CLA:HBB1	19:I:201:CLA:HMB1	1.99	0.44
19:1:5007:CLA:OBD	19:1:5012:CLA:HBD	2.18	0.44
11:Z:46:PRO:HD2	11:Z:49:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:305:CLA:H61	19:Z:305:CLA:H41	1.26	0.44
12:3:120:VAL:HG11	19:3:5019:CLA:HED3	1.99	0.44
16:5:78:ALA:HB1	16:5:190:GLY:HA3	1.99	0.44
16:5:252:LEU:HD21	22:5:305:BCR:H291	1.98	0.44
1:A:384:TYR:CE2	1:A:619:TRP:HB3	2.53	0.44
19:A:834:CLA:H162	19:A:834:CLA:H141	1.81	0.44
19:A:840:CLA:HMB1	19:A:840:CLA:CBB	2.48	0.44
2:B:210:TRP:HA	2:B:213:PHE:CD1	2.52	0.44
19:1:5007:CLA:O2D	19:1:5012:CLA:H2	2.18	0.44
11:Z:84:GLY:HA2	31:Z:317:LUT:C18	2.47	0.44
23:Z:316:LHG:H102	22:4:305:BCR:H332	1.98	0.44
19:3:5012:CLA:HMD2	19:3:5018:CLA:ND	2.33	0.44
24:3:5023:LMT:H102	19:7:312:CLA:C1C	2.47	0.44
19:7:310:CLA:H12	19:7:310:CLA:HBA1	1.79	0.44
19:8:308:CLA:H101	19:8:308:CLA:H161	1.99	0.44
16:5:155:ASN:HB3	32:5:320:CHL:C2D	2.47	0.44
16:5:160:PRO:HD2	16:5:164:TYR:O	2.18	0.44
17:6:147:TYR:HB3	32:6:321:CHL:C2D	2.47	0.44
19:A:826:CLA:H93	19:A:826:CLA:H112	1.72	0.43
24:A:854:LMT:H91	19:3:5016:CLA:C15	2.48	0.43
2:B:279:LEU:O	2:B:283:VAL:HG23	2.18	0.43
2:B:658:TYR:CE1	19:B:802:CLA:HMA1	2.53	0.43
19:B:802:CLA:HHC	19:B:802:CLA:CBB	2.48	0.43
19:B:821:CLA:H143	19:B:821:CLA:H111	1.62	0.43
19:B:821:CLA:H171	7:G:110:VAL:HG11	1.99	0.43
19:B:823:CLA:H102	19:B:823:CLA:H13	1.73	0.43
22:B:842:BCR:H20C	22:G:1603:BCR:HC42	1.99	0.43
22:B:847:BCR:HC8	22:B:847:BCR:C32	2.48	0.43
3:C:8:TYR:CZ	4:D:175:ILE:HG12	2.53	0.43
6:F:200:ALA:HB1	19:8:311:CLA:H203	2.00	0.43
10:K:29:PHE:CE2	33:3:5001:SPH:H71	2.53	0.43
12:3:148:LEU:HD12	22:3:5004:BCR:H342	1.99	0.43
19:3:5014:CLA:H101	19:3:5014:CLA:H62	1.49	0.43
19:3:5018:CLA:H3A	19:3:5018:CLA:HBA2	1.26	0.43
31:7:304:LUT:H15	31:7:304:LUT:H201	1.87	0.43
31:7:304:LUT:C31	19:7:309:CLA:HMC2	2.48	0.43
19:7:306:CLA:H62	19:7:306:CLA:H41	1.67	0.43
17:6:66:TRP:CE2	38:6:326:ERG:H192	2.53	0.43
1:A:97:ARG:HB2	24:A:856:LMT:C6'	2.46	0.43
1:A:334:THR:HB	1:A:426:LEU:CD2	2.48	0.43
1:A:373:ALA:HB2	19:A:827:CLA:HAC2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:SER:HA	1:A:658:ILE:HG12	1.99	0.43
19:A:805:CLA:H3A	19:A:805:CLA:HBA1	1.41	0.43
19:A:810:CLA:H121	19:A:812:CLA:HBC1	2.00	0.43
2:B:388:PHE:CD1	2:B:535:LEU:HD13	2.53	0.43
2:B:395:PHE:HE2	22:B:846:BCR:H272	1.81	0.43
19:B:817:CLA:HBC1	19:B:819:CLA:H172	2.00	0.43
19:B:822:CLA:CBB	19:B:822:CLA:HMB1	2.48	0.43
19:B:839:CLA:CHD	20:B:841:PQN:H212	2.48	0.43
22:B:846:BCR:H11C	22:B:846:BCR:H341	1.85	0.43
24:G:1604:LMT:H32	19:1:5016:CLA:C1B	2.48	0.43
11:1:150:PRO:CG	19:1:5015:CLA:HMD2	2.48	0.43
32:1:5009:CHL:HBA2	32:1:5009:CHL:H3A	1.69	0.43
11:Z:42:PRO:HB3	11:Z:44:TRP:CH2	2.53	0.43
31:3:5003:LUT:H181	31:3:5003:LUT:C8	2.47	0.43
13:7:130:TRP:HB2	32:8:315:CHL:H2	2.00	0.43
14:8:94:THR:HA	14:8:99:LEU:O	2.19	0.43
19:8:307:CLA:H62	19:8:307:CLA:H41	1.73	0.43
15:4:157:PHE:CZ	22:4:305:BCR:H373	2.53	0.43
19:4:318:CLA:HMB1	19:4:318:CLA:CBB	2.48	0.43
32:5:318:CHL:HAA2	32:5:318:CHL:CBD	2.46	0.43
19:6:312:CLA:HMD2	32:6:315:CHL:CBB	2.48	0.43
34:6:325:3PH:H242	34:6:325:3PH:H271	1.71	0.43
1:A:344:ILE:HG23	1:A:412:PHE:CE1	2.54	0.43
2:B:87:PRO:HB3	2:B:122:TYR:CG	2.53	0.43
19:B:811:CLA:HMB1	19:B:811:CLA:CBB	2.48	0.43
11:1:37:PRO:HA	14:8:149:GLU:OE2	2.18	0.43
32:1:5009:CHL:H61	32:1:5009:CHL:H41	1.81	0.43
19:Z:305:CLA:HBA2	19:Z:305:CLA:H3A	1.55	0.43
12:3:102:PRO:HB2	12:3:103:PRO:HD3	2.00	0.43
19:3:5020:CLA:CHA	19:3:5020:CLA:HBA1	2.45	0.43
19:3:5020:CLA:HED3	32:7:314:CHL:H12	1.99	0.43
19:7:308:CLA:H43	19:7:313:CLA:OBD	2.18	0.43
27:4:303:RRX:C23	27:4:303:RRX:H17	2.48	0.43
19:4:310:CLA:HHC	19:4:310:CLA:CBB	2.35	0.43
32:4:314:CHL:HMA1	24:4:322:LMT:C5	2.49	0.43
19:5:301:CLA:H61	19:5:319:CLA:O2D	2.17	0.43
1:A:114:SER:HB2	1:A:131:VAL:HG11	1.99	0.43
1:A:269:TRP:CH2	22:K:206:BCR:HC31	2.53	0.43
19:A:808:CLA:H191	19:A:841:CLA:O2A	2.17	0.43
19:A:819:CLA:CGA	19:A:829:CLA:HMD1	2.48	0.43
24:A:855:LMT:H11	24:A:855:LMT:H2'	1.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:LEU:HD23	2:B:158:LEU:HA	1.82	0.43
2:B:355:SER:HB3	19:B:826:CLA:HAC2	1.99	0.43
8:I:87:LEU:HB2	8:I:88:PRO:HD3	1.99	0.43
10:K:31:GLY:H	10:K:35:ASN:HD22	1.67	0.43
19:K:202:CLA:C3B	33:3:5001:SPH:H151	2.49	0.43
11:1:129:PHE:CD2	32:1:5017:CHL:HED2	2.54	0.43
19:1:5010:CLA:HHC	19:1:5010:CLA:HBB1	2.01	0.43
19:1:5012:CLA:H102	19:1:5012:CLA:H61	1.24	0.43
11:Z:91:VAL:HG12	11:Z:97:GLY:O	2.19	0.43
32:Z:302:CHL:H92	32:Z:302:CHL:H61	1.92	0.43
31:8:304:LUT:H361	19:8:307:CLA:H61	1.99	0.43
15:4:220:ARG:HA	15:4:223:MET:CE	2.48	0.43
23:4:320:LHG:H291	19:6:302:CLA:CBB	2.48	0.43
32:5:320:CHL:HHC	32:5:320:CHL:CBB	2.45	0.43
17:6:119:PHE:CE1	19:6:302:CLA:H92	2.54	0.43
19:6:312:CLA:O1A	19:6:312:CLA:C2	2.65	0.43
19:6:323:CLA:H161	19:6:323:CLA:H122	1.92	0.43
1:A:264:PHE:CZ	19:K:202:CLA:HMC1	2.54	0.43
19:A:802:CLA:O1D	19:B:802:CLA:H52	2.18	0.43
19:B:816:CLA:H8	7:G:113:ALA:HA	2.01	0.43
7:G:104:GLY:HA3	22:G:1603:BCR:C15	2.48	0.43
19:K:202:CLA:NC	33:3:5001:SPH:H112	2.33	0.43
19:1:5015:CLA:CHA	19:1:5015:CLA:HBA2	2.48	0.43
12:3:118:PHE:HE1	35:7:302:DGA:HBS2	1.84	0.43
12:3:229:LEU:HA	12:3:232:PHE:HD2	1.83	0.43
15:4:115:LEU:HD21	15:4:229:PHE:CZ	2.53	0.43
15:4:252:TRP:CD2	17:6:108:LEU:HG	2.54	0.43
23:4:320:LHG:H142	19:6:322:CLA:CED	2.49	0.43
27:5:302:RRX:H44	19:5:307:CLA:HMC1	1.98	0.43
19:5:314:CLA:C2D	23:5:323:LHG:HC91	2.48	0.43
17:6:104:VAL:HG21	19:6:313:CLA:HAA1	2.00	0.43
19:A:818:CLA:HAC1	19:A:835:CLA:H42	2.01	0.43
19:A:818:CLA:HBA2	19:A:818:CLA:H3A	1.57	0.43
19:A:823:CLA:HMA1	19:A:843:CLA:CBC	2.48	0.43
19:A:835:CLA:H152	22:A:849:BCR:H361	2.00	0.43
22:A:850:BCR:H15C	22:A:850:BCR:H351	1.91	0.43
2:B:414:ASP:HA	6:F:227:ARG:HE	1.83	0.43
2:B:632:LEU:HD22	2:B:725:PHE:HA	2.01	0.43
19:B:801:CLA:H143	19:B:801:CLA:H111	1.67	0.43
19:B:831:CLA:HBC2	19:B:837:CLA:CMC	2.47	0.43
22:B:844:BCR:H15C	22:B:844:BCR:H351	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:850:CLA:HED2	6:F:139:LEU:HD23	2.01	0.43
32:Z:310:CHL:H202	32:Z:310:CHL:H161	1.87	0.43
12:3:170:LEU:HG	16:5:35:TRP:HH2	1.84	0.43
13:7:136:TRP:CD2	19:7:317:CLA:CMA	3.02	0.43
13:7:229:VAL:HG12	19:7:308:CLA:HED1	2.01	0.43
14:8:62:ASP:OD2	14:8:64:VAL:HG13	2.19	0.43
14:8:64:VAL:HG23	38:8:325:ERG:H41	2.01	0.43
15:4:62:MET:HE2	15:4:65:ALA:HB2	2.01	0.43
31:6:305:LUT:H181	31:6:305:LUT:H8	2.01	0.43
32:6:316:CHL:HBD	32:6:316:CHL:HAA1	1.99	0.43
1:A:598:TRP:CH2	19:B:803:CLA:CAB	3.00	0.43
1:A:715:PRO:HB3	19:A:842:CLA:HMC3	1.99	0.43
19:A:818:CLA:HMD2	19:A:827:CLA:HMB2	1.99	0.43
19:A:839:CLA:CHC	23:A:851:LHG:H171	2.49	0.43
2:B:71:TRP:CD1	8:I:71:PRO:HD2	2.54	0.43
2:B:358:PRO:HG3	19:B:818:CLA:CBA	2.49	0.43
2:B:637:ASN:HB2	2:B:638:PRO:CD	2.49	0.43
19:B:827:CLA:H111	19:B:827:CLA:H71	1.55	0.43
19:B:827:CLA:H3A	19:B:827:CLA:HBA2	1.54	0.43
19:B:832:CLA:H11	29:J:1904:LMG:H112	2.01	0.43
19:B:839:CLA:HHC	19:B:839:CLA:HBB1	2.01	0.43
5:E:83:VAL:HG12	5:E:85:THR:H	1.84	0.43
11:1:59:SER:OG	11:1:62:LYS:HB2	2.17	0.43
19:Z:311:CLA:C2B	31:Z:317:LUT:H183	2.49	0.43
19:3:5013:CLA:HMA2	19:3:5019:CLA:CAC	2.49	0.43
19:5:325:CLA:HBD	19:5:325:CLA:CBA	2.48	0.43
17:6:66:TRP:CG	38:6:326:ERG:H191	2.54	0.43
1:A:43:PRO:HB3	1:A:48:TRP:CE3	2.53	0.43
1:A:208:LEU:HB3	22:A:847:BCR:H19C	2.01	0.43
19:A:824:CLA:H143	19:A:839:CLA:C2B	2.48	0.43
19:A:836:CLA:H42	19:K:203:CLA:C2D	2.48	0.43
2:B:66:LEU:CD1	22:B:844:BCR:H271	2.48	0.43
10:K:59:LYS:HA	10:K:68:VAL:O	2.19	0.43
10:K:67:LEU:HD12	10:K:67:LEU:HA	1.88	0.43
12:3:15:LEU:HG	12:3:16:TYR:CD1	2.53	0.43
12:3:35:PHE:CZ	12:3:189:LYS:HD3	2.54	0.43
19:7:307:CLA:C3D	19:7:312:CLA:H61	2.49	0.43
31:8:304:LUT:H11	31:8:304:LUT:H191	1.83	0.43
19:8:312:CLA:CBF	19:8:312:CLA:HAA1	2.49	0.43
19:4:306:CLA:H3A	19:4:306:CLA:HBA2	1.34	0.43
19:5:309:CLA:CGA	19:5:309:CLA:C3A	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:SER:O	19:A:811:CLA:HMA1	2.19	0.43
19:A:802:CLA:HMB3	19:B:802:CLA:C19	2.49	0.43
19:A:808:CLA:H111	19:A:808:CLA:H91	1.66	0.43
19:A:822:CLA:CBB	30:K:201:DAO:H111	2.49	0.43
19:A:824:CLA:H43	22:A:848:BCR:H352	2.00	0.43
2:B:379:ILE:O	2:B:383:ILE:HG13	2.19	0.43
19:B:803:CLA:H161	22:B:847:BCR:C8	2.49	0.43
19:B:825:CLA:HBA2	19:B:825:CLA:H3A	1.57	0.43
19:B:827:CLA:H143	19:B:827:CLA:H112	1.75	0.43
19:B:832:CLA:H61	19:B:832:CLA:H102	1.42	0.43
19:B:832:CLA:HMA1	29:J:1904:LMG:H151	2.00	0.43
6:F:156:PHE:HB2	22:F:302:BCR:H321	2.00	0.43
24:G:1604:LMT:H52	19:1:5016:CLA:C4B	2.49	0.43
11:Z:156:PRO:O	11:Z:157:LEU:C	2.57	0.43
19:Z:305:CLA:H143	19:Z:305:CLA:H161	1.64	0.43
12:3:167:PHE:CE2	32:3:5017:CHL:C1	3.02	0.43
19:3:5020:CLA:OBD	34:3:5022:3PH:H272	2.19	0.43
19:8:307:CLA:H3A	19:8:307:CLA:HBA2	1.23	0.43
19:8:312:CLA:C15	19:8:312:CLA:C10	2.86	0.43
19:8:314:CLA:C4D	32:8:315:CHL:H122	2.49	0.43
19:4:309:CLA:H3A	19:4:309:CLA:HBA2	1.50	0.43
16:5:36:ALA:HB3	16:5:39:VAL:CG1	2.49	0.43
16:5:185:LYS:HG3	19:5:312:CLA:HED2	2.01	0.43
19:5:307:CLA:NB	19:5:312:CLA:H112	2.34	0.43
32:5:315:CHL:HHC	32:5:315:CHL:HBB1	2.00	0.43
19:5:325:CLA:H92	32:6:315:CHL:H102	2.00	0.43
38:6:326:ERG:H121	38:6:326:ERG:C28	2.47	0.43
1:A:186:PRO:HB2	1:A:191:PHE:CE2	2.54	0.43
19:A:804:CLA:CBD	19:A:811:CLA:H2	2.42	0.43
19:A:805:CLA:H61	22:A:847:BCR:HC8	2.01	0.43
19:A:816:CLA:H12	35:7:302:DGA:HB32	2.01	0.43
19:A:840:CLA:CHC	19:A:842:CLA:HMD2	2.48	0.43
2:B:181:SER:HA	2:B:286:ILE:HA	2.01	0.43
2:B:443:VAL:HG21	19:B:832:CLA:HAC2	2.01	0.43
19:B:808:CLA:CMC	22:B:847:BCR:HC22	2.49	0.43
19:B:821:CLA:HED2	7:G:60:GLU:HB3	1.99	0.43
19:B:833:CLA:H101	19:B:834:CLA:NB	2.34	0.43
20:B:841:PQN:O4	20:B:841:PQN:H143	2.19	0.43
19:B:850:CLA:C2	19:B:850:CLA:C7	2.65	0.43
6:F:114:ARG:HD3	9:J:35:ASP:CG	2.39	0.43
11:1:146:GLY:O	11:1:147:VAL:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:5007:CLA:C1D	19:1:5012:CLA:H62	2.48	0.43
11:Z:92:GLU:OE1	11:Z:198:PRO:HD2	2.18	0.43
11:Z:210:TRP:HZ2	19:Z:307:CLA:H51	1.84	0.43
12:3:15:LEU:HG	12:3:16:TYR:HD1	1.83	0.43
12:3:42:LEU:HD13	19:3:5011:CLA:H42	2.01	0.43
12:3:110:TYR:HE1	19:3:5013:CLA:HAA2	1.83	0.43
12:3:214:GLN:HG2	12:3:218:GLU:OE1	2.19	0.43
31:3:5003:LUT:H15	31:3:5003:LUT:H201	1.91	0.43
22:3:5006:BCR:H393	19:3:5012:CLA:HMD3	2.01	0.43
19:3:5016:CLA:CAD	35:7:302:DGA:HBN1	2.49	0.43
13:7:222:HIS:CG	19:7:308:CLA:HAA1	2.54	0.43
19:7:319:CLA:H11	19:7:319:CLA:H52	1.66	0.43
32:8:315:CHL:H161	32:8:315:CHL:H141	1.63	0.43
15:4:183:ASN:HB3	32:4:319:CHL:C3D	2.49	0.43
19:4:307:CLA:H12	19:4:307:CLA:H52	1.63	0.43
31:5:303:LUT:H8	31:5:303:LUT:C18	2.44	0.43
32:5:315:CHL:CBB	19:6:323:CLA:H41	2.49	0.43
19:5:317:CLA:H192	19:5:319:CLA:HMC2	2.00	0.43
17:6:247:PRO:O	32:6:316:CHL:H42	2.19	0.43
19:6:323:CLA:HMD3	34:6:325:3PH:C35	2.49	0.43
1:A:370:HIS:CE1	19:A:827:CLA:NB	2.87	0.42
19:A:812:CLA:C3D	19:A:813:CLA:HMC3	2.48	0.42
19:A:818:CLA:O1A	19:A:827:CLA:HBB2	2.19	0.42
19:A:829:CLA:H8	19:A:829:CLA:H51	1.43	0.42
19:A:832:CLA:H62	19:A:832:CLA:H92	1.60	0.42
2:B:87:PRO:HB3	2:B:122:TYR:CD1	2.54	0.42
19:B:820:CLA:H12	19:B:820:CLA:CHB	2.49	0.42
19:B:820:CLA:H51	19:B:820:CLA:C4B	2.49	0.42
6:F:217:GLU:HB3	6:F:222:ILE:HD11	2.01	0.42
8:I:77:SER:O	8:I:81:PRO:HG2	2.19	0.42
19:K:202:CLA:C4C	33:3:5001:SPH:H112	2.49	0.42
11:1:113:THR:HG22	39:1:5101:HOH:O	2.18	0.42
11:1:179:LEU:CD2	19:1:5007:CLA:HBC3	2.48	0.42
19:1:5008:CLA:CGA	19:1:5008:CLA:C1A	2.97	0.42
19:3:5014:CLA:H51	19:3:5014:CLA:H11	1.81	0.42
19:7:319:CLA:H51	19:7:319:CLA:NA	2.35	0.42
16:5:91:GLN:HE21	16:5:95:LYS:HB2	1.83	0.42
1:A:34:HIS:CE1	19:A:811:CLA:HAA1	2.54	0.42
1:A:572:ARG:CG	1:A:721:THR:HG21	2.48	0.42
19:A:818:CLA:C15	19:A:836:CLA:H2	2.49	0.42
19:A:824:CLA:H152	19:A:839:CLA:NB	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:852:LHG:H122	23:A:852:LHG:H152	1.70	0.42
2:B:11:GLN:HE21	2:B:15:GLN:NE2	2.16	0.42
2:B:178:HIS:ND1	19:B:813:CLA:HMC2	2.35	0.42
2:B:530:THR:O	2:B:534:ILE:HG13	2.20	0.42
19:B:850:CLA:CMC	27:F:304:RRX:H17	2.49	0.42
6:F:150:PHE:O	6:F:153:THR:HB	2.19	0.42
6:F:179:LYS:HD3	6:F:182:ASP:OD2	2.18	0.42
7:G:90:ASN:HB3	19:G:1602:CLA:CAD	2.49	0.42
11:Z:89:LEU:O	11:Z:93:LEU:HG	2.19	0.42
11:Z:202:LEU:O	11:Z:206:LEU:HD13	2.20	0.42
32:7:315:CHL:H11	24:7:323:LMT:C4	2.45	0.42
32:8:301:CHL:HBC3	32:8:301:CHL:CHD	2.49	0.42
19:8:309:CLA:H51	19:8:309:CLA:NC	2.34	0.42
15:4:143:PHE:CE1	15:4:144:ALA:HB2	2.53	0.42
15:4:204:SER:HA	15:4:208:ILE:HD13	2.00	0.42
15:4:260:ASP:CG	15:4:263:ARG:HH21	2.22	0.42
19:5:301:CLA:H102	19:5:301:CLA:CAB	2.49	0.42
19:5:309:CLA:HBB1	19:5:309:CLA:CHC	2.37	0.42
19:5:309:CLA:H101	19:5:314:CLA:H102	2.01	0.42
31:6:305:LUT:H15	31:6:305:LUT:H201	1.94	0.42
19:B:807:CLA:HBB1	19:B:807:CLA:HMB1	2.00	0.42
19:B:821:CLA:C1C	19:B:822:CLA:H122	2.50	0.42
19:B:837:CLA:H2	19:B:840:CLA:H203	2.01	0.42
8:I:75:ALA:O	8:I:79:PHE:HD1	2.00	0.42
19:1:5008:CLA:HMB1	19:1:5008:CLA:CBB	2.44	0.42
19:Z:305:CLA:H122	19:Z:305:CLA:H8	1.56	0.42
12:3:229:LEU:HA	12:3:232:PHE:CD2	2.54	0.42
31:3:5002:LUT:H191	31:3:5002:LUT:H11	1.73	0.42
24:8:323:LMT:H6'2	24:8:323:LMT:O3B	2.19	0.42
15:4:84:LEU:HD11	33:4:301:SPH:H141	2.01	0.42
15:4:135:TYR:O	32:4:314:CHL:HED3	2.19	0.42
17:6:216:THR:HG22	19:6:311:CLA:HBA1	2.01	0.42
32:6:315:CHL:H52	32:6:315:CHL:H8	1.87	0.42
1:A:269:TRP:HH2	22:K:206:BCR:HC31	1.83	0.42
1:A:610:PHE:O	1:A:614:MET:HG2	2.18	0.42
19:A:827:CLA:CMA	19:A:835:CLA:H71	2.49	0.42
24:A:854:LMT:H5B	35:7:302:DGA:HA31	2.00	0.42
22:A:858:BCR:H15C	22:A:858:BCR:H351	1.88	0.42
2:B:40:GLU:O	2:B:43:LEU:HB3	2.19	0.42
2:B:373:TYR:OH	19:B:835:CLA:HMC3	2.19	0.42
2:B:656:LEU:HA	19:B:803:CLA:HAA1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:836:CLA:C2C	29:J:1904:LMG:H261	2.49	0.42
22:B:845:BCR:H341	22:B:845:BCR:H11C	1.77	0.42
7:G:32:LEU:HB2	7:G:118:ASN:ND2	2.33	0.42
9:J:23:ALA:O	9:J:27:ILE:HG13	2.19	0.42
10:K:55:PRO:HD2	19:K:204:CLA:HMB3	2.02	0.42
10:K:111:GLY:O	10:K:112:ALA:C	2.57	0.42
11:1:156:PRO:HD2	31:1:5003:LUT:C23	2.49	0.42
11:Z:83:LEU:HD11	32:Z:302:CHL:HBC1	2.02	0.42
19:Z:305:CLA:H161	19:Z:305:CLA:H202	1.75	0.42
12:3:39:PRO:HG2	31:3:5003:LUT:H23	2.01	0.42
12:3:67:TRP:CE2	32:3:5017:CHL:HED2	2.55	0.42
12:3:154:PHE:CZ	22:3:5005:BCR:HC41	2.54	0.42
19:3:5016:CLA:NB	35:7:302:DGA:HB81	2.34	0.42
31:8:304:LUT:H181	31:8:304:LUT:C8	2.50	0.42
16:5:145:SER:HB2	17:6:35:GLY:CA	2.49	0.42
19:5:306:CLA:H2	19:5:306:CLA:CHB	2.49	0.42
19:5:306:CLA:H62	19:5:307:CLA:H3A	2.02	0.42
19:5:312:CLA:H52	19:5:312:CLA:H8	1.78	0.42
19:6:320:CLA:HMD3	19:6:323:CLA:CBB	2.50	0.42
19:A:807:CLA:HMB1	22:A:858:BCR:HC7	2.00	0.42
19:A:832:CLA:H143	19:A:832:CLA:NC	2.35	0.42
2:B:71:TRP:CD1	8:I:70:VAL:HG13	2.54	0.42
2:B:223:LEU:HB3	2:B:227:PHE:HE2	1.84	0.42
19:B:819:CLA:C2B	19:B:824:CLA:H8	2.49	0.42
19:B:821:CLA:H93	7:G:45:PHE:CE2	2.52	0.42
19:B:827:CLA:H92	19:B:827:CLA:H62	1.67	0.42
19:B:836:CLA:HMB2	19:B:837:CLA:C2D	2.49	0.42
19:B:850:CLA:C2	19:B:850:CLA:HBA1	2.48	0.42
27:F:304:RRX:H28	27:F:304:RRX:H32	1.74	0.42
11:Z:31:LYS:N	11:Z:47:ASP:OD1	2.52	0.42
11:Z:49:LEU:HD21	19:Z:305:CLA:HED2	2.01	0.42
19:Z:312:CLA:HBA2	19:Z:312:CLA:H3A	1.50	0.42
19:7:317:CLA:HBA2	19:7:317:CLA:H3A	1.37	0.42
14:8:62:ASP:CG	14:8:64:VAL:HG13	2.40	0.42
19:8:312:CLA:H3A	19:8:312:CLA:HBA2	1.63	0.42
19:4:316:CLA:HMB1	19:4:316:CLA:CBB	2.50	0.42
17:6:127:ARG:HD2	19:6:302:CLA:HED2	2.01	0.42
17:6:199:LYS:HB3	17:6:203:ALA:HB3	2.00	0.42
1:A:440:HIS:O	1:A:444:VAL:HG23	2.19	0.42
19:A:811:CLA:H142	19:A:811:CLA:H112	1.88	0.42
19:A:818:CLA:O1D	19:A:819:CLA:HMA1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:834:CLA:H162	19:A:834:CLA:H192	1.81	0.42
2:B:119:SER:O	2:B:372:LEU:HD21	2.20	0.42
2:B:653:PHE:O	2:B:657:ILE:HG13	2.20	0.42
3:C:8:TYR:CE1	4:D:175:ILE:HG12	2.54	0.42
6:F:99:ALA:N	6:F:100:PRO:CD	2.82	0.42
6:F:186:ILE:CD1	9:J:10:THR:HG22	2.50	0.42
12:3:26:TYR:OH	12:3:41:GLY:HA2	2.20	0.42
12:3:185:LEU:O	12:3:188:ILE:HG22	2.20	0.42
22:3:5006:BCR:C18	19:3:5018:CLA:H142	2.50	0.42
31:7:304:LUT:H35	31:7:304:LUT:H401	1.81	0.42
19:8:313:CLA:C3C	24:4:302:LMT:H92	2.49	0.42
19:4:308:CLA:CHA	19:4:308:CLA:CBA	2.98	0.42
19:4:316:CLA:CHC	24:4:321:LMT:H121	2.50	0.42
27:5:302:RRX:H27	19:5:306:CLA:HAB	2.00	0.42
17:6:174:VAL:O	17:6:177:ILE:HG22	2.19	0.42
22:6:308:BCR:H15C	22:6:308:BCR:H351	1.76	0.42
1:A:318:ILE:HG13	19:A:820:CLA:HED1	2.02	0.42
1:A:331:GLY:HA3	23:A:851:LHG:P	2.59	0.42
2:B:530:THR:HG21	2:B:583:TRP:CZ2	2.54	0.42
19:B:804:CLA:CBB	19:B:804:CLA:HMB1	2.49	0.42
19:F:303:CLA:HMB3	9:J:26:LEU:HD21	2.01	0.42
11:1:80:TRP:CD1	19:1:5016:CLA:HMD3	2.54	0.42
19:1:5013:CLA:HAA2	14:8:125:VAL:CG2	2.49	0.42
11:Z:162:ASP:OD1	11:Z:165:LYS:HB2	2.19	0.42
19:3:5008:CLA:H161	32:3:5017:CHL:C9	2.50	0.42
35:7:302:DGA:HBV2	35:7:302:DGA:HBF1	1.68	0.42
14:8:185:TRP:CZ3	19:8:307:CLA:HMA2	2.53	0.42
19:8:312:CLA:C4D	39:8:401:HOH:O	2.66	0.42
15:4:153:GLN:HG2	15:4:154:MET:CE	2.48	0.42
15:4:161:GLU:HG3	19:4:316:CLA:NB	2.34	0.42
16:5:135:ARG:HD2	32:6:315:CHL:HED1	2.01	0.42
19:5:310:CLA:O2D	19:5:310:CLA:HBA2	2.20	0.42
32:5:315:CHL:H2	32:5:315:CHL:H61	1.80	0.42
19:5:321:CLA:H3A	19:5:321:CLA:HBA2	1.53	0.42
32:6:315:CHL:HBD	32:6:315:CHL:HAA1	2.01	0.42
32:6:317:CHL:CHB	32:6:319:CHL:H92	2.49	0.42
32:6:321:CHL:HAA2	32:6:321:CHL:CBD	2.48	0.42
1:A:160:TYR:O	1:A:164:ILE:HG12	2.19	0.42
1:A:274:ASP:N	1:A:274:ASP:OD1	2.53	0.42
1:A:423:TYR:HE1	4:D:104:ALA:HA	1.84	0.42
1:A:438:ILE:HG13	1:A:556:PHE:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:822:CLA:HMB1	19:A:822:CLA:CBB	2.50	0.42
19:A:824:CLA:H2	19:A:835:CLA:H171	2.02	0.42
23:A:851:LHG:H111	23:A:851:LHG:H142	1.65	0.42
19:B:824:CLA:H161	19:B:824:CLA:H192	1.84	0.42
3:C:38:GLN:NE2	4:D:161:VAL:HB	2.34	0.42
6:F:226:PRO:O	6:F:227:ARG:HB2	2.19	0.42
7:G:48:ILE:O	7:G:52:VAL:HB	2.19	0.42
8:I:80:VAL:HG22	19:I:201:CLA:HAA2	2.02	0.42
8:I:91:ALA:O	8:I:95:LEU:HG	2.20	0.42
29:J:1903:LMG:O9	29:J:1903:LMG:HC71	2.20	0.42
24:Z:301:LMT:H121	24:Z:301:LMT:H91	1.87	0.42
12:3:76:ILE:HD12	12:3:76:ILE:HA	1.89	0.42
22:3:5004:BCR:H402	19:3:5013:CLA:C1B	2.50	0.42
16:5:56:ASP:N	16:5:57:PRO:HD3	2.34	0.42
17:6:66:TRP:CD2	38:6:326:ERG:C19	3.02	0.42
17:6:82:VAL:CG1	31:6:305:LUT:H12	2.43	0.42
1:A:153:ILE:HG23	1:A:158:GLN:HB2	2.01	0.42
1:A:321:SER:HB3	1:A:324:GLU:HG3	2.01	0.42
1:A:392:THR:HG23	1:A:607:ILE:HG21	2.01	0.42
1:A:443:TRP:CD1	19:A:833:CLA:HED2	2.55	0.42
2:B:88:ILE:HD11	2:B:108:GLY:O	2.19	0.42
2:B:618:MET:HG3	2:B:622:ARG:NH1	2.34	0.42
19:B:802:CLA:HBA2	19:B:802:CLA:H3A	1.40	0.42
6:F:63:ASP:N	6:F:67:LEU:O	2.53	0.42
7:G:35:GLN:HB3	19:G:1601:CLA:HED2	2.02	0.42
11:1:187:PHE:HE1	31:1:5003:LUT:H41	1.85	0.42
19:1:5015:CLA:HMB1	19:1:5015:CLA:CBB	2.50	0.42
13:7:179:ASP:CG	13:7:182:LYS:HB2	2.41	0.42
32:8:315:CHL:CHB	23:8:321:LHG:H281	2.50	0.42
15:4:108:MET:SD	19:4:306:CLA:HAB	2.60	0.42
16:5:234:CYS:N	16:5:256:SER:O	2.49	0.42
1:A:501:ASN:HD21	19:K:203:CLA:HED1	1.85	0.42
19:A:822:CLA:HAA2	10:K:61:THR:HG21	2.02	0.42
19:A:823:CLA:C1	10:K:65:LEU:HD23	2.49	0.42
19:A:832:CLA:H71	19:A:832:CLA:H112	1.67	0.42
22:A:846:BCR:H291	22:3:5006:BCR:HC42	2.02	0.42
24:A:853:LMT:O1'	12:3:206:VAL:HG13	2.20	0.42
2:B:382:PHE:O	19:B:829:CLA:HAC1	2.20	0.42
2:B:701:LEU:HD22	2:B:705:GLN:NE2	2.35	0.42
19:B:826:CLA:C14	22:B:846:BCR:H15C	2.48	0.42
19:B:829:CLA:H93	19:B:829:CLA:H111	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:PHE:CG	3:C:63:LEU:N	2.88	0.42
19:1:5010:CLA:HMD2	19:1:5016:CLA:ND	2.35	0.42
11:Z:35:TRP:CD2	11:Z:55:PHE:HD1	2.38	0.42
11:Z:136:ALA:O	11:Z:140:GLN:HG2	2.19	0.42
11:Z:208:ASN:ND2	11:Z:211:GLY:HA3	2.35	0.42
22:3:5007:BCR:H311	19:3:5015:CLA:CMA	2.50	0.42
34:3:5022:3PH:H3E1	34:3:5022:3PH:H3B2	1.58	0.42
13:7:62:PRO:O	13:7:65:LEU:N	2.53	0.42
13:7:107:LYS:O	13:7:111:GLU:HG2	2.20	0.42
19:7:308:CLA:CBB	19:7:308:CLA:HHC	2.50	0.42
19:7:309:CLA:HMD2	32:7:314:CHL:HBB1	2.02	0.42
19:8:307:CLA:HBB1	19:8:308:CLA:HAA1	2.02	0.42
19:8:311:CLA:H141	19:8:311:CLA:H162	1.56	0.42
19:8:312:CLA:HAA1	19:8:312:CLA:HBD	2.02	0.42
38:8:325:ERG:H183	38:8:325:ERG:H20	1.70	0.42
15:4:119:LEU:O	15:4:123:ILE:HG13	2.20	0.42
19:6:310:CLA:OBD	19:6:314:CLA:H2	2.20	0.42
19:A:803:CLA:H93	19:A:803:CLA:H62	1.77	0.41
19:A:814:CLA:HBA2	19:A:816:CLA:CMB	2.50	0.41
22:A:847:BCR:H11C	22:A:847:BCR:H341	1.86	0.41
2:B:44:TYR:CE2	2:B:331:LEU:HD21	2.55	0.41
2:B:532:THR:HG21	19:B:837:CLA:HMB3	2.01	0.41
19:B:823:CLA:H61	19:B:837:CLA:H152	2.01	0.41
19:B:833:CLA:C19	19:B:834:CLA:HBC3	2.50	0.41
19:I:201:CLA:HMB1	19:I:201:CLA:CBB	2.50	0.41
11:1:171:LEU:HA	11:1:174:ILE:HG22	2.02	0.41
19:Z:311:CLA:C3B	31:Z:317:LUT:H183	2.50	0.41
14:8:157:GLU:HA	14:8:160:LEU:HD12	2.01	0.41
22:8:306:BCR:H24C	22:8:306:BCR:H371	1.83	0.41
38:8:325:ERG:H23	38:8:325:ERG:H263	1.81	0.41
16:5:222:PRO:HG2	19:5:313:CLA:CMB	2.43	0.41
34:5:324:3PH:H2	34:5:324:3PH:H221	1.45	0.41
17:6:123:TRP:CE3	19:6:302:CLA:HBA2	2.55	0.41
32:6:315:CHL:H91	32:6:315:CHL:H111	1.76	0.41
1:A:528:LEU:HD21	19:A:837:CLA:HMD2	2.02	0.41
19:A:827:CLA:H61	19:A:827:CLA:H2	1.65	0.41
19:A:836:CLA:H42	19:K:203:CLA:C1D	2.50	0.41
19:A:841:CLA:H11	19:A:841:CLA:H51	1.72	0.41
19:B:810:CLA:HHC	19:B:810:CLA:CBB	2.50	0.41
19:B:819:CLA:CMB	19:B:824:CLA:HMA3	2.45	0.41
19:1:5012:CLA:CBB	22:8:306:BCR:H332	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:8:311:CLA:H162	19:8:311:CLA:H192	1.76	0.41
15:4:126:SER:O	15:4:127:TRP:HB3	2.21	0.41
15:4:201:PHE:HB2	15:4:203:TRP:CD1	2.54	0.41
15:4:214:LYS:NZ	19:4:307:CLA:HED1	2.35	0.41
16:5:185:LYS:HD3	19:5:307:CLA:O1A	2.21	0.41
22:6:307:BCR:C23	22:6:307:BCR:H392	2.51	0.41
19:A:815:CLA:HED1	24:A:853:LMT:O3'	2.20	0.41
19:A:819:CLA:H2	19:A:819:CLA:H61	1.75	0.41
19:A:825:CLA:H102	19:A:825:CLA:H61	1.61	0.41
2:B:489:ASN:ND2	19:B:834:CLA:HMD1	2.35	0.41
19:B:819:CLA:CHD	19:B:824:CLA:H192	2.50	0.41
4:D:88:TRP:HB3	4:D:136:PRO:HB3	2.02	0.41
32:1:5009:CHL:HHC	32:1:5009:CHL:HBB1	2.03	0.41
19:1:5010:CLA:HBA1	19:1:5010:CLA:H3A	1.84	0.41
12:3:35:PHE:HZ	12:3:189:LYS:HD3	1.85	0.41
22:3:5006:BCR:H272	19:3:5018:CLA:C1C	2.50	0.41
13:7:138:ASP:CB	19:7:316:CLA:HAC1	2.50	0.41
35:7:302:DGA:HB41	35:7:302:DGA:HB72	1.66	0.41
15:4:75:LEU:HB2	19:4:309:CLA:HED1	2.03	0.41
16:5:80:TRP:CE2	19:5:317:CLA:HBC3	2.56	0.41
19:5:306:CLA:H41	19:5:306:CLA:H61	1.46	0.41
1:A:56:ALA:O	1:A:62:HIS:HE1	2.04	0.41
1:A:362:SER:O	1:A:366:ILE:HG13	2.20	0.41
1:A:585:GLN:HA	1:A:590:ASP:OD2	2.20	0.41
2:B:449:THR:HB	2:B:452:LYS:HG3	2.03	0.41
19:B:823:CLA:H171	19:B:840:CLA:H2	2.02	0.41
6:F:165:TYR:O	6:F:169:GLN:HG2	2.20	0.41
10:K:39:VAL:HA	19:K:202:CLA:CGA	2.51	0.41
19:K:203:CLA:HBA2	19:K:203:CLA:CHA	2.51	0.41
31:Z:317:LUT:H361	31:Z:317:LUT:H27	1.72	0.41
31:3:5003:LUT:H11	31:3:5003:LUT:H191	1.88	0.41
19:3:5019:CLA:HMB1	19:3:5019:CLA:CBB	2.50	0.41
32:8:301:CHL:HMC	32:8:301:CHL:HAC2	1.90	0.41
16:5:171:PRO:HD2	27:5:302:RRX:C27	2.50	0.41
19:5:301:CLA:H42	19:5:301:CLA:ND	2.35	0.41
1:A:426:LEU:HB3	19:A:824:CLA:HMC3	2.01	0.41
1:A:601:ASN:O	1:A:605:ILE:HG12	2.20	0.41
1:A:682:SER:HB2	1:A:727:GLY:O	2.20	0.41
19:A:810:CLA:H143	19:A:813:CLA:H111	2.03	0.41
19:A:827:CLA:C4B	19:A:835:CLA:HMA1	2.51	0.41
24:A:853:LMT:H12	24:A:853:LMT:H42	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:GLY:HA2	2:B:88:ILE:HB	2.02	0.41
2:B:282:ALA:O	2:B:286:ILE:HG13	2.21	0.41
19:B:803:CLA:H72	19:B:803:CLA:H111	1.39	0.41
19:B:821:CLA:C4D	22:B:842:BCR:HC42	2.51	0.41
19:B:823:CLA:H202	19:B:823:CLA:H161	1.82	0.41
19:J:1901:CLA:HBC2	28:J:1902:C7Z:C31	2.50	0.41
10:K:46:LEU:HA	10:K:92:MET:HG3	2.01	0.41
32:Z:302:CHL:HBB1	32:Z:302:CHL:HHC	2.03	0.41
19:7:307:CLA:C1B	19:7:312:CLA:H122	2.51	0.41
14:8:227:ASP:OD2	14:8:230:HIS:HB2	2.20	0.41
19:4:308:CLA:H92	19:4:308:CLA:H61	1.74	0.41
23:4:320:LHG:H111	19:6:302:CLA:C1B	2.49	0.41
16:5:82:MET:HE3	19:5:306:CLA:HMC3	2.02	0.41
31:5:303:LUT:H34	19:5:309:CLA:HBB2	2.01	0.41
1:A:584:CYS:SG	21:A:845:SF4:S1	3.16	0.41
19:A:821:CLA:HMA2	19:A:825:CLA:C1C	2.50	0.41
19:A:830:CLA:H92	19:A:830:CLA:H61	1.68	0.41
19:A:842:CLA:NB	20:A:844:PQN:H212	2.35	0.41
2:B:395:PHE:HA	2:B:399:TYR:HB2	2.02	0.41
19:B:804:CLA:H202	19:B:804:CLA:H162	1.75	0.41
19:B:823:CLA:H61	19:B:837:CLA:H122	2.03	0.41
19:B:823:CLA:H72	19:B:837:CLA:H101	2.02	0.41
3:C:22:PRO:C	4:D:122:LEU:HD23	2.40	0.41
6:F:185:ILE:HG13	6:F:186:ILE:HG12	2.03	0.41
10:K:62:THR:HG22	10:K:63:ALA:N	2.36	0.41
31:1:5003:LUT:H35	31:1:5003:LUT:H401	1.90	0.41
19:1:5008:CLA:H162	19:1:5008:CLA:H122	1.66	0.41
11:Z:42:PRO:HD2	11:Z:45:LEU:HD12	2.01	0.41
11:Z:173:GLU:HG3	32:Z:302:CHL:NB	2.35	0.41
12:3:148:LEU:CD1	22:3:5004:BCR:H342	2.50	0.41
12:3:167:PHE:CE2	32:3:5017:CHL:H12	2.56	0.41
19:3:5013:CLA:CHA	19:5:301:CLA:HMB3	2.51	0.41
32:7:314:CHL:H3A	32:7:314:CHL:HBA2	1.75	0.41
32:7:315:CHL:HBA2	32:7:315:CHL:H3A	1.65	0.41
15:4:157:PHE:CZ	22:4:305:BCR:C37	3.03	0.41
19:4:310:CLA:H142	19:4:310:CLA:H112	1.75	0.41
17:6:104:VAL:CB	32:6:319:CHL:HBC1	2.39	0.41
17:6:127:ARG:HA	19:6:302:CLA:HED1	2.02	0.41
17:6:244:ILE:HD11	22:6:308:BCR:H331	2.01	0.41
17:6:244:ILE:HG12	22:6:308:BCR:HC7	2.03	0.41
1:A:305:PHE:HZ	19:A:819:CLA:H142	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:GLY:HA2	1:A:398:GLY:HA2	2.02	0.41
1:A:433:HIS:CE1	1:A:437:ILE:HD11	2.56	0.41
19:A:819:CLA:H161	19:A:819:CLA:H122	1.73	0.41
2:B:198:VAL:HG11	19:B:814:CLA:O1D	2.20	0.41
2:B:323:LEU:HD11	2:B:408:VAL:CG2	2.51	0.41
19:B:811:CLA:HBA2	19:B:811:CLA:H3A	1.63	0.41
19:B:814:CLA:H92	19:B:814:CLA:H62	1.71	0.41
3:C:14:CYS:HB2	3:C:16:GLN:HG2	2.02	0.41
10:K:65:LEU:HD22	10:K:65:LEU:HA	1.88	0.41
22:K:206:BCR:H15C	22:K:206:BCR:H351	1.86	0.41
11:1:114:TRP:HA	19:1:5011:CLA:HBD	2.03	0.41
23:1:5019:LHG:H141	23:1:5019:LHG:H111	1.54	0.41
19:Z:303:CLA:HMD1	19:Z:312:CLA:H2	2.02	0.41
19:8:312:CLA:HMA1	32:8:319:CHL:CMC	2.51	0.41
15:4:114:ILE:HD11	31:4:304:LUT:H173	2.03	0.41
19:4:313:CLA:HBA1	19:4:313:CLA:H3A	1.88	0.41
16:5:132:VAL:HG11	22:5:304:BCR:H16C	2.03	0.41
19:5:319:CLA:HMD3	34:5:324:3PH:O22	2.20	0.41
1:A:493:LEU:O	1:A:496:GLN:HG2	2.21	0.41
19:A:802:CLA:CAB	2:B:583:TRP:CH2	2.92	0.41
19:A:814:CLA:H92	19:A:814:CLA:H61	1.77	0.41
2:B:75:PHE:O	2:B:79:VAL:HG13	2.21	0.41
6:F:78:LYS:HE3	6:F:78:LYS:HB2	1.82	0.41
6:F:211:GLN:OE1	38:8:325:ERG:H152	2.21	0.41
8:I:82:LEU:O	8:I:87:LEU:HG	2.21	0.41
9:J:8:LEU:HA	9:J:13:VAL:HG11	2.01	0.41
10:K:62:THR:HG22	10:K:63:ALA:H	1.86	0.41
10:K:79:ASN:HB2	19:K:205:CLA:H2A	2.02	0.41
12:3:70:LEU:HD11	19:3:5008:CLA:HBC1	2.03	0.41
12:3:196:LEU:HD13	22:3:5007:BCR:H371	2.03	0.41
19:3:5010:CLA:H61	19:3:5010:CLA:H41	1.78	0.41
19:7:319:CLA:H51	19:7:319:CLA:NB	2.36	0.41
15:4:114:ILE:CD1	31:4:304:LUT:H173	2.50	0.41
19:4:308:CLA:O1A	19:4:313:CLA:C3D	2.69	0.41
16:5:179:LEU:HD12	19:5:306:CLA:HMA2	2.02	0.41
19:6:320:CLA:HBA1	19:6:320:CLA:H3A	1.29	0.41
1:A:212:ALA:HA	19:A:815:CLA:HBB2	2.03	0.41
1:A:297:HIS:O	1:A:301:ILE:HG12	2.19	0.41
1:A:687:PHE:HB2	19:B:801:CLA:HBC1	2.03	0.41
19:A:807:CLA:HAA2	19:A:809:CLA:O2D	2.21	0.41
19:A:822:CLA:HBA1	10:K:65:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:825:CLA:H122	19:A:825:CLA:H8	1.75	0.41
2:B:179:HIS:O	2:B:184:PHE:HD1	2.04	0.41
19:B:807:CLA:HMB1	19:B:807:CLA:CBB	2.50	0.41
19:B:808:CLA:C10	19:B:809:CLA:H61	2.50	0.41
19:B:812:CLA:H141	19:B:812:CLA:H162	1.79	0.41
19:B:814:CLA:H8	19:B:814:CLA:H122	1.57	0.41
19:B:816:CLA:H2	7:G:116:ALA:HB1	2.02	0.41
19:B:835:CLA:H41	19:B:835:CLA:H61	1.76	0.41
24:G:1604:LMT:H112	19:1:5016:CLA:CAC	2.50	0.41
19:1:5006:CLA:HMB2	19:1:5007:CLA:HBA2	2.02	0.41
11:Z:31:LYS:HE2	11:Z:33:GLY:O	2.21	0.41
12:3:94:LYS:HD3	39:3:5106:HOH:O	2.21	0.41
31:3:5002:LUT:C11	19:3:5009:CLA:HMC2	2.51	0.41
13:7:34:PHE:CE1	32:7:314:CHL:HED2	2.56	0.41
14:8:56:PRO:CA	34:8:322:3PH:H222	2.51	0.41
19:8:307:CLA:H111	19:8:307:CLA:H91	1.74	0.41
22:4:305:BCR:H20C	32:4:315:CHL:CMA	2.51	0.41
19:4:306:CLA:H41	19:4:306:CLA:H62	1.80	0.41
16:5:191:ARG:HA	16:5:194:MET:CE	2.51	0.41
19:5:325:CLA:HMD3	19:6:311:CLA:CHB	2.51	0.41
17:6:133:ARG:HB2	17:6:134:LYS:HD2	2.03	0.41
17:6:175:LYS:NZ	19:6:310:CLA:CED	2.82	0.41
19:6:312:CLA:H3A	19:6:312:CLA:CGA	2.50	0.41
1:A:363:LEU:HD21	19:A:819:CLA:H93	2.02	0.41
1:A:407:ALA:O	1:A:411:ILE:HG13	2.20	0.41
1:A:658:ILE:HD12	2:B:622:ARG:HG3	2.03	0.41
19:A:810:CLA:O1A	19:A:812:CLA:HMD2	2.21	0.41
2:B:198:VAL:C	2:B:201:PRO:HD2	2.41	0.41
2:B:620:TRP:O	2:B:624:TYR:HB3	2.21	0.41
2:B:669:ARG:O	2:B:670:GLY:C	2.59	0.41
19:B:803:CLA:O1A	19:B:803:CLA:H3A	2.21	0.41
19:B:804:CLA:C2	19:B:804:CLA:CMA	2.99	0.41
19:B:823:CLA:H203	19:B:840:CLA:HMA2	2.03	0.41
22:B:842:BCR:C20	22:G:1603:BCR:H333	2.51	0.41
19:B:850:CLA:H143	19:B:850:CLA:H202	2.02	0.41
24:G:1604:LMT:H52	19:1:5016:CLA:NB	2.36	0.41
22:K:206:BCR:H11C	22:K:206:BCR:H341	1.95	0.41
11:Z:31:LYS:HG2	11:Z:33:GLY:O	2.20	0.41
19:Z:315:CLA:HBB1	19:Z:315:CLA:HHC	2.03	0.41
12:3:204:GLN:HG2	19:3:5010:CLA:C4D	2.51	0.41
19:3:5010:CLA:H72	19:3:5010:CLA:C1C	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:172:PRO:HB2	19:7:324:CLA:H41	2.02	0.41
19:7:319:CLA:H121	19:7:319:CLA:H8	1.65	0.41
14:8:221:LEU:O	14:8:225:LEU:HG	2.21	0.41
19:8:313:CLA:C2	19:4:310:CLA:H51	2.51	0.41
19:8:313:CLA:HMB1	19:8:313:CLA:CBB	2.51	0.41
16:5:88:VAL:HG22	31:5:303:LUT:H41	2.03	0.41
22:5:305:BCR:H342	22:5:305:BCR:HC7	1.93	0.41
19:5:310:CLA:HBA1	19:5:310:CLA:HBD	2.02	0.41
19:5:321:CLA:H92	19:5:321:CLA:H62	1.66	0.41
17:6:102:LYS:HD3	17:6:239:VAL:HG13	2.03	0.41
17:6:227:GLN:HA	34:6:325:3PH:H32	2.03	0.41
19:6:310:CLA:HBA1	19:6:310:CLA:H3A	1.89	0.41
1:A:157:LEU:HD21	24:A:854:LMT:H4'	2.03	0.40
19:A:815:CLA:H51	22:3:5006:BCR:HC8	2.03	0.40
19:A:833:CLA:C3D	19:A:834:CLA:H122	2.51	0.40
19:A:835:CLA:H162	19:A:835:CLA:H141	1.79	0.40
21:A:845:SF4:FE1	2:B:569:CYS:HG	1.31	0.40
22:A:846:BCR:H21C	22:A:847:BCR:H271	2.03	0.40
19:B:825:CLA:H62	19:B:835:CLA:H42	2.00	0.40
19:B:836:CLA:O1A	19:B:836:CLA:C2	2.66	0.40
19:B:850:CLA:HBA1	19:B:850:CLA:NA	2.25	0.40
3:C:77:MET:HB2	3:C:79:LEU:HG	2.03	0.40
6:F:156:PHE:CD2	22:F:302:BCR:H343	2.56	0.40
10:K:49:ALA:HB2	10:K:92:MET:SD	2.61	0.40
11:1:210:TRP:CZ3	14:8:125:VAL:HG21	2.56	0.40
31:1:5003:LUT:H11	31:1:5003:LUT:H191	1.99	0.40
19:1:5008:CLA:H143	24:Z:301:LMT:H122	2.03	0.40
11:Z:178:ARG:HA	11:Z:181:MET:CE	2.52	0.40
19:3:5013:CLA:H171	19:5:319:CLA:CHB	2.51	0.40
19:3:5014:CLA:H93	19:3:5014:CLA:H111	1.72	0.40
31:7:303:LUT:H15	31:7:303:LUT:H201	1.93	0.40
19:7:311:CLA:H12	19:7:318:CLA:HMD2	2.02	0.40
14:8:69:TYR:C	19:8:310:CLA:HMA1	2.42	0.40
22:8:303:BCR:C34	33:4:301:SPH:H152	2.51	0.40
16:5:89:LEU:O	16:5:93:ILE:HG13	2.21	0.40
16:5:91:GLN:NE2	16:5:95:LYS:HB2	2.36	0.40
16:5:105:LEU:HD13	16:5:107:GLN:NE2	2.36	0.40
31:5:303:LUT:H181	31:5:303:LUT:C8	2.44	0.40
22:6:307:BCR:H402	19:6:313:CLA:C1B	2.51	0.40
32:6:319:CHL:HMC	32:6:319:CHL:HAC1	1.83	0.40
1:A:87:TRP:O	1:A:91:MET:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:TRP:CB	19:A:805:CLA:HAC1	2.50	0.40
19:A:835:CLA:H93	22:A:849:BCR:C19	2.52	0.40
19:B:816:CLA:H162	19:B:816:CLA:H141	1.79	0.40
4:D:86:ILE:HG21	4:D:124:LEU:HD23	2.03	0.40
19:G:1601:CLA:CAB	22:G:1603:BCR:H352	2.52	0.40
22:3:5004:BCR:H392	19:3:5019:CLA:HAA1	2.02	0.40
19:3:5018:CLA:H93	19:3:5018:CLA:H61	1.81	0.40
13:7:183:TYR:CE2	13:7:187:LYS:HD2	2.56	0.40
19:7:311:CLA:H93	22:8:303:BCR:H372	2.02	0.40
19:4:309:CLA:H3A	19:4:309:CLA:CGA	2.45	0.40
32:4:319:CHL:HHC	32:4:319:CHL:CBB	2.48	0.40
16:5:200:PHE:CD1	16:5:211:PRO:HB3	2.57	0.40
19:6:310:CLA:C3D	19:6:314:CLA:H2	2.52	0.40
19:6:312:CLA:H162	19:6:312:CLA:H141	1.80	0.40
32:6:315:CHL:H142	32:6:315:CHL:H112	1.90	0.40
1:A:165:GLY:HA2	24:A:854:LMT:H102	2.04	0.40
1:A:589:TRP:NE1	19:A:830:CLA:HMD1	2.36	0.40
19:A:802:CLA:H91	19:B:832:CLA:HBC1	2.03	0.40
19:A:822:CLA:H62	19:A:822:CLA:H2	1.57	0.40
19:A:829:CLA:H111	19:A:829:CLA:H152	1.85	0.40
19:A:835:CLA:H93	22:A:849:BCR:H19C	2.04	0.40
22:A:859:BCR:H353	22:K:206:BCR:C5	2.51	0.40
2:B:6:PHE:HB2	8:I:98:TYR:CZ	2.56	0.40
2:B:92:ILE:HD11	2:B:115:ASN:OD1	2.21	0.40
19:B:808:CLA:HMA1	19:I:201:CLA:CMB	2.44	0.40
19:B:814:CLA:H61	19:B:814:CLA:H2	1.76	0.40
19:Z:311:CLA:HBA1	19:Z:311:CLA:H3A	1.90	0.40
19:3:5019:CLA:H52	19:3:5019:CLA:H12	1.66	0.40
23:7:320:LHG:H291	23:7:320:LHG:H322	1.42	0.40
32:4:314:CHL:CHB	24:4:322:LMT:H72	2.43	0.40
19:5:317:CLA:HBA1	19:5:317:CLA:H3A	1.71	0.40
19:6:310:CLA:NC	19:6:314:CLA:H8	2.37	0.40
1:A:63:THR:O	1:A:69:ILE:HD11	2.21	0.40
1:A:369:HIS:HA	1:A:372:TYR:CD2	2.56	0.40
1:A:545:VAL:O	1:A:548:LEU:HB3	2.22	0.40
19:A:814:CLA:O1A	19:A:816:CLA:HMA1	2.21	0.40
2:B:178:HIS:CG	19:B:813:CLA:HMC2	2.56	0.40
2:B:258:PHE:CZ	19:B:817:CLA:H61	2.56	0.40
2:B:411:ARG:HB3	19:B:830:CLA:O1D	2.21	0.40
19:B:819:CLA:HAA2	19:B:823:CLA:CAD	2.52	0.40
7:G:102:GLY:O	7:G:106:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Z:129:PHE:HE1	32:Z:313:CHL:O2A	2.04	0.40
11:Z:159:PHE:CB	32:Z:302:CHL:HBA1	2.28	0.40
19:Z:303:CLA:CMD	19:Z:312:CLA:H2	2.51	0.40
14:8:194:LYS:HD3	19:8:313:CLA:O1D	2.21	0.40
15:4:104:ALA:HB1	15:4:219:GLY:HA3	2.04	0.40
32:4:314:CHL:CAB	32:4:317:CHL:HBB2	2.48	0.40
32:4:317:CHL:HAB	32:4:317:CHL:HMB1	1.94	0.40
16:5:254:PRO:HD2	19:5:319:CLA:O1D	2.22	0.40
19:5:313:CLA:HBA2	19:5:313:CLA:CHA	2.51	0.40
19:6:320:CLA:H62	19:6:320:CLA:H102	1.60	0.40
1:A:96:ALA:HB2	1:A:159:LEU:HB2	2.03	0.40
1:A:212:ALA:HB1	19:A:814:CLA:HAB	2.03	0.40
1:A:273:SER:O	1:A:277:THR:HG22	2.22	0.40
1:A:479:LEU:HB2	1:A:530:THR:HG23	2.02	0.40
1:A:564:PRO:HD2	39:D:212:HOH:O	2.21	0.40
19:A:829:CLA:H92	19:A:829:CLA:HMD2	2.03	0.40
19:B:809:CLA:NC	22:B:847:BCR:HC21	2.36	0.40
19:B:826:CLA:H102	22:B:846:BCR:C17	2.51	0.40
3:C:15:THR:HG22	3:C:28:MET:HG3	2.02	0.40
19:F:301:CLA:H2	19:F:301:CLA:H62	1.85	0.40
7:G:110:VAL:O	7:G:114:VAL:HG23	2.22	0.40
10:K:50:ARG:NH1	10:K:80:ASP:OD1	2.55	0.40
19:1:5007:CLA:CAD	19:1:5012:CLA:HBD	2.52	0.40
19:1:5012:CLA:CHB	24:Z:301:LMT:H1'	2.52	0.40
31:3:5003:LUT:H31	31:3:5003:LUT:H391	1.69	0.40
32:8:315:CHL:H12	32:8:315:CHL:H52	1.91	0.40
19:4:306:CLA:HMD2	32:4:315:CHL:O1A	2.22	0.40
16:5:200:PHE:CE1	27:5:302:RRX:H57	2.56	0.40
17:6:251:PHE:CD2	19:6:320:CLA:H12	2.56	0.40
22:6:307:BCR:H393	19:6:313:CLA:C6	2.50	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	738/751 (98%)	713 (97%)	24 (3%)	1 (0%)	51	71
2	B	731/735 (100%)	702 (96%)	28 (4%)	1 (0%)	51	71
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	141/196 (72%)	133 (94%)	8 (6%)	0	100	100
5	E	61/97 (63%)	58 (95%)	3 (5%)	0	100	100
6	F	163/227 (72%)	159 (98%)	4 (2%)	0	100	100
7	G	63/126 (50%)	60 (95%)	3 (5%)	0	100	100
8	I	35/106 (33%)	33 (94%)	2 (6%)	0	100	100
9	J	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
10	K	82/113 (73%)	76 (93%)	6 (7%)	0	100	100
11	1	192/228 (84%)	185 (96%)	6 (3%)	1 (0%)	29	47
11	Z	192/228 (84%)	178 (93%)	11 (6%)	3 (2%)	9	16
12	3	217/298 (73%)	206 (95%)	10 (5%)	1 (0%)	29	47
13	7	211/241 (88%)	200 (95%)	10 (5%)	1 (0%)	29	47
14	8	215/243 (88%)	210 (98%)	5 (2%)	0	100	100
15	4	208/264 (79%)	196 (94%)	10 (5%)	2 (1%)	15	27
16	5	225/257 (88%)	217 (96%)	8 (4%)	0	100	100
17	6	227/257 (88%)	220 (97%)	7 (3%)	0	100	100
All	All	3816/4489 (85%)	3658 (96%)	148 (4%)	10 (0%)	44	59

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	Z	150	PRO
12	3	91	THR
15	4	207	ASP
11	1	147	VAL
13	7	166	GLY
2	B	157	HIS
11	Z	152	GLY
11	Z	159	PHE
15	4	188	GLY
1	A	122	VAL

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	600/610 (98%)	595 (99%)	5 (1%)	81	92
2	B	596/597 (100%)	591 (99%)	5 (1%)	81	92
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	120/151 (80%)	118 (98%)	2 (2%)	60	81
5	E	54/81 (67%)	54 (100%)	0	100	100
6	F	127/169 (75%)	125 (98%)	2 (2%)	62	82
7	G	47/94 (50%)	46 (98%)	1 (2%)	53	76
8	I	31/76 (41%)	30 (97%)	1 (3%)	39	63
9	J	35/37 (95%)	35 (100%)	0	100	100
10	K	58/80 (72%)	57 (98%)	1 (2%)	60	81
11	1	137/162 (85%)	135 (98%)	2 (2%)	65	83
11	Z	137/162 (85%)	136 (99%)	1 (1%)	84	93
12	3	167/230 (73%)	164 (98%)	3 (2%)	59	80
13	7	164/181 (91%)	162 (99%)	2 (1%)	71	87
14	8	163/183 (89%)	160 (98%)	3 (2%)	59	80
15	4	164/205 (80%)	161 (98%)	3 (2%)	59	80
16	5	184/206 (89%)	181 (98%)	3 (2%)	62	82
17	6	183/203 (90%)	177 (97%)	6 (3%)	38	62
All	All	3036/3497 (87%)	2996 (99%)	40 (1%)	70	86

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	PHE
1	A	330	ARG
1	A	372	TYR
1	A	496	GLN
1	A	532	ASP
2	B	99	GLN

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Mol	Chain	Res	Type
2	B	145	LEU
2	B	258	PHE
2	B	354	TYR
2	B	578	TYR
4	D	92	LYS
4	D	189	ARG
6	F	162	TYR
6	F	175	LYS
7	G	89	THR
8	I	85	LEU
10	K	65	LEU
11	1	37	PRO
11	1	224	PHE
11	Z	213	ASN
12	3	43	LEU
12	3	126	GLN
12	3	175	LYS
13	7	34	PHE
13	7	168	ARG
14	8	64	VAL
14	8	95	LYS
14	8	153	PHE
15	4	91	VAL
15	4	135	TYR
15	4	139	LYS
16	5	181	GLU
16	5	221	ASN
16	5	240	VAL
17	6	29	ARG
17	6	132	LEU
17	6	134	LYS
17	6	239	VAL
17	6	246	ILE
17	6	250	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	217	GLN
1	A	225	ASN
1	A	369	HIS

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Mol	Chain	Res	Type
2	B	11	GLN
2	B	163	GLN
2	B	197	HIS
2	B	604	GLN
3	C	38	GLN
5	E	87	ASN
7	G	118	ASN
10	K	79	ASN
11	1	124	ASN
11	1	217	ASN
11	Z	176	ASN
11	Z	213	ASN
12	3	21	GLN
12	3	231	ASN
13	7	113	ASN
13	7	218	ASN
14	8	100	ASN
15	4	153	GLN
15	4	183	ASN
15	4	232	GLN
16	5	91	GLN
16	5	115	ASN
16	5	221	ASN
16	5	230	ASN
16	5	238	HIS
17	6	227	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SNC	D	137	4	4,7,8	0.67	0	1,7,9	1.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SNC	D	137	4	-	0/0/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 314 ligands modelled in this entry, 1 is monoatomic - leaving 313 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
24	LMT	A	856	-	36,36,36	0.38	0	47,47,47	0.83	2 (4%)
32	CHL	8	317	39	51,59,74	1.12	6 (11%)	55,96,114	1.44	11 (20%)
19	CLA	B	832	-	58,66,73	1.40	6 (10%)	67,104,113	2.12	17 (25%)
24	LMT	1	5002	-	36,36,36	0.39	0	47,47,47	0.70	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LUT	Z	318	-	42,43,43	6.02	27 (64%)	51,60,60	2.13	16 (31%)
19	CLA	8	308	14	65,73,73	1.36	8 (12%)	76,113,113	1.96	16 (21%)
19	CLA	4	310	15	65,73,73	1.39	7 (10%)	76,113,113	2.02	20 (26%)
19	CLA	5	317	16	65,73,73	1.36	7 (10%)	76,113,113	2.01	17 (22%)
32	CHL	3	5017	39	66,74,74	1.06	8 (12%)	73,114,114	1.51	11 (15%)
24	LMT	4	302	-	36,36,36	0.37	0	47,47,47	0.74	0
22	BCR	8	306	-	41,41,41	4.72	25 (60%)	56,56,56	2.29	22 (39%)
19	CLA	1	5010	-	55,63,73	1.48	7 (12%)	64,101,113	2.11	17 (26%)
19	CLA	K	204	10	49,57,73	1.54	7 (14%)	55,93,113	2.23	15 (27%)
19	CLA	B	834	39	45,53,73	1.61	7 (15%)	52,89,113	2.15	14 (26%)
19	CLA	B	833	-	65,73,73	1.34	7 (10%)	76,113,113	1.94	16 (21%)
31	LUT	6	305	-	42,43,43	5.96	28 (66%)	51,60,60	2.22	17 (33%)
19	CLA	8	318	14	46,54,73	1.64	8 (17%)	53,90,113	2.17	15 (28%)
19	CLA	7	309	13	65,73,73	1.37	7 (10%)	76,113,113	2.11	18 (23%)
19	CLA	5	301	39	56,64,73	1.44	7 (12%)	65,102,113	2.09	17 (26%)
19	CLA	A	819	-	65,73,73	1.33	8 (12%)	76,113,113	2.00	20 (26%)
32	CHL	4	314	39	51,59,74	1.09	4 (7%)	55,96,114	1.51	10 (18%)
19	CLA	B	838	39	52,60,73	1.50	8 (15%)	60,97,113	2.15	16 (26%)
33	SPH	7	321	-	19,20,20	0.64	0	18,21,21	1.15	2 (11%)
19	CLA	B	802	-	65,73,73	1.34	7 (10%)	76,113,113	2.00	16 (21%)
19	CLA	7	307	13	50,58,73	1.57	8 (16%)	58,95,113	2.28	16 (27%)
19	CLA	8	310	14	62,70,73	1.39	8 (12%)	72,109,113	2.08	20 (27%)
19	CLA	A	842	39	65,73,73	1.34	8 (12%)	76,113,113	1.94	16 (21%)
19	CLA	8	309	14	65,73,73	1.37	7 (10%)	76,113,113	2.14	19 (25%)
31	LUT	1	5004	-	42,43,43	5.90	28 (66%)	51,60,60	2.20	19 (37%)
19	CLA	B	817	-	59,67,73	1.40	8 (13%)	68,105,113	2.08	17 (25%)
19	CLA	7	313	-	43,51,73	1.69	7 (16%)	49,86,113	2.15	13 (26%)
22	BCR	3	5004	-	41,41,41	4.69	25 (60%)	56,56,56	2.38	21 (37%)
32	CHL	1	5014	39	48,56,74	0.96	2 (4%)	51,92,114	1.40	11 (21%)
19	CLA	A	816	39	61,69,73	1.38	8 (13%)	71,108,113	2.07	17 (23%)
19	CLA	1	5018	11	51,59,73	1.51	7 (13%)	59,96,113	2.13	17 (28%)
19	CLA	G	1601	-	50,58,73	1.52	7 (14%)	58,95,113	2.17	17 (29%)
19	CLA	B	811	-	56,64,73	1.44	9 (16%)	65,102,113	2.11	16 (24%)
19	CLA	I	201	-	55,63,73	1.45	8 (14%)	64,101,113	2.11	18 (28%)
19	CLA	6	314	23	55,63,73	1.46	7 (12%)	64,101,113	2.06	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	833	-	65,73,73	1.33	7 (10%)	76,113,113	2.01	18 (23%)
19	CLA	Z	304	39	50,58,73	1.54	8 (16%)	58,95,113	2.20	16 (27%)
19	CLA	7	319	13	58,66,73	1.42	7 (12%)	67,104,113	2.13	17 (25%)
19	CLA	3	5008	12	65,73,73	1.38	8 (12%)	76,113,113	2.05	18 (23%)
32	CHL	8	316	39	57,65,74	1.06	5 (8%)	62,103,114	1.44	12 (19%)
31	LUT	3	5002	-	42,43,43	5.96	27 (64%)	51,60,60	2.03	19 (37%)
22	BCR	6	308	-	41,41,41	4.75	25 (60%)	56,56,56	2.50	20 (35%)
19	CLA	B	801	-	65,73,73	1.33	7 (10%)	76,113,113	1.90	17 (22%)
24	LMT	A	855	-	36,36,36	0.39	0	47,47,47	0.70	1 (2%)
33	SPH	4	301	-	19,20,20	0.66	0	18,21,21	0.95	0
23	LHG	A	852	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
19	CLA	A	823	-	57,65,73	1.43	7 (12%)	66,103,113	2.12	18 (27%)
19	CLA	K	202	-	46,54,73	1.59	6 (13%)	53,90,113	2.22	15 (28%)
31	LUT	4	304	-	42,43,43	5.97	26 (61%)	51,60,60	2.35	20 (39%)
18	CL0	A	801	-	65,73,73	2.36	20 (30%)	76,113,113	2.51	21 (27%)
32	CHL	4	315	39	51,59,74	1.03	2 (3%)	55,96,114	1.48	11 (20%)
19	CLA	A	820	-	60,68,73	1.39	7 (11%)	70,107,113	2.06	18 (25%)
32	CHL	Z	302	11	57,65,74	1.10	6 (10%)	62,103,114	1.29	8 (12%)
19	CLA	3	5011	12	60,68,73	1.44	8 (13%)	70,107,113	2.24	20 (28%)
19	CLA	3	5019	39	55,63,73	1.48	8 (14%)	64,101,113	2.22	17 (26%)
19	CLA	6	323	17	65,73,73	1.35	7 (10%)	76,113,113	1.95	17 (22%)
19	CLA	B	825	39	65,73,73	1.38	8 (12%)	76,113,113	1.94	15 (19%)
28	C7Z	6	304	-	43,43,43	5.33	27 (62%)	58,60,60	2.52	25 (43%)
23	LHG	6	303	-	31,31,48	0.49	0	34,37,54	1.20	4 (11%)
24	LMT	F	305	-	36,36,36	0.36	0	47,47,47	0.79	2 (4%)
27	RRX	4	303	-	42,42,42	5.01	26 (61%)	57,58,58	2.30	23 (40%)
34	3PH	5	324	-	22,22,47	1.21	4 (18%)	26,27,52	1.22	3 (11%)
27	RRX	5	302	-	42,42,42	4.98	26 (61%)	57,58,58	2.24	23 (40%)
19	CLA	7	306	13	60,68,73	1.42	7 (11%)	70,107,113	2.11	20 (28%)
32	CHL	5	318	39	51,59,74	1.09	5 (9%)	55,96,114	1.59	9 (16%)
22	BCR	A	849	-	41,41,41	4.75	27 (65%)	56,56,56	2.56	20 (35%)
19	CLA	5	325	-	55,63,73	1.50	8 (14%)	64,101,113	2.08	18 (28%)
32	CHL	6	319	39	66,74,74	1.02	4 (6%)	73,114,114	1.39	11 (15%)
32	CHL	Z	310	39	66,74,74	1.02	6 (9%)	73,114,114	1.52	12 (16%)
19	CLA	B	813	-	65,73,73	1.34	5 (7%)	76,113,113	2.04	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	4	308	15	65,73,73	1.37	8 (12%)	76,113,113	2.10	18 (23%)
19	CLA	1	5016	11	60,68,73	1.40	7 (11%)	70,107,113	2.06	17 (24%)
19	CLA	B	835	-	60,68,73	1.39	6 (10%)	70,107,113	2.08	17 (24%)
19	CLA	A	809	1	56,64,73	1.44	7 (12%)	65,102,113	2.09	17 (26%)
19	CLA	Z	308	-	65,73,73	1.36	8 (12%)	76,113,113	2.01	20 (26%)
19	CLA	A	804	19	55,63,73	1.44	6 (10%)	64,101,113	2.12	20 (31%)
19	CLA	A	837	-	51,59,73	1.51	8 (15%)	59,96,113	2.23	17 (28%)
31	LUT	8	304	-	42,43,43	6.06	26 (61%)	51,60,60	2.05	16 (31%)
19	CLA	A	831	-	50,58,73	1.52	7 (14%)	58,95,113	2.22	16 (27%)
19	CLA	A	841	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	17 (22%)
19	CLA	8	314	-	55,63,73	1.50	8 (14%)	64,101,113	2.19	18 (28%)
19	CLA	4	318	15	41,49,73	1.66	8 (19%)	47,84,113	2.24	15 (31%)
31	LUT	Z	317	-	42,43,43	5.94	27 (64%)	51,60,60	3.86	21 (41%)
32	CHL	Z	309	11	63,71,74	0.86	2 (3%)	69,110,114	1.31	10 (14%)
19	CLA	3	5016	12	60,68,73	1.38	7 (11%)	70,107,113	2.07	17 (24%)
32	CHL	Z	313	39	46,54,74	1.15	6 (13%)	49,90,114	1.67	8 (16%)
19	CLA	3	5013	39	65,73,73	1.38	8 (12%)	76,113,113	2.02	16 (21%)
24	LMT	3	5023	-	36,36,36	0.36	0	47,47,47	0.79	1 (2%)
19	CLA	A	826	39	65,73,73	1.33	6 (9%)	76,113,113	2.01	16 (21%)
19	CLA	5	314	16	65,73,73	1.37	7 (10%)	76,113,113	1.88	16 (21%)
19	CLA	1	5007	11	45,53,73	1.66	8 (17%)	52,89,113	2.17	15 (28%)
32	CHL	7	315	39	54,62,74	1.10	3 (5%)	58,99,114	1.47	11 (18%)
19	CLA	3	5015	-	45,53,73	1.61	8 (17%)	52,89,113	2.22	16 (30%)
28	C7Z	J	1902	-	43,43,43	5.33	27 (62%)	58,60,60	2.23	19 (32%)
19	CLA	4	307	15	52,60,73	1.56	7 (13%)	60,97,113	2.15	16 (26%)
24	LMT	G	1604	-	36,36,36	0.37	0	47,47,47	0.72	1 (2%)
19	CLA	K	203	39	55,63,73	1.45	7 (12%)	64,101,113	2.10	16 (25%)
19	CLA	A	818	-	60,68,73	1.39	7 (11%)	70,107,113	2.02	18 (25%)
19	CLA	F	303	39	45,53,73	1.60	8 (17%)	52,89,113	2.12	12 (23%)
20	PQN	B	841	-	34,34,34	0.39	0	42,45,45	1.15	3 (7%)
19	CLA	Z	314	11	46,54,73	1.60	8 (17%)	53,90,113	2.10	14 (26%)
20	PQN	A	844	-	34,34,34	0.39	0	42,45,45	1.16	3 (7%)
23	LHG	1	5019	19	42,42,48	0.45	0	45,48,54	1.21	3 (6%)
19	CLA	B	807	2	65,73,73	1.35	9 (13%)	76,113,113	1.92	17 (22%)
19	CLA	A	822	-	55,63,73	1.45	7 (12%)	64,101,113	2.19	18 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMG	J	1904	-	45,45,55	0.93	3 (6%)	53,53,63	1.07	2 (3%)
19	CLA	7	317	13	50,58,73	1.50	8 (16%)	58,95,113	2.21	15 (25%)
31	LUT	8	305	-	42,43,43	5.92	29 (69%)	51,60,60	2.23	18 (35%)
19	CLA	3	5010	12	65,73,73	1.37	7 (10%)	76,113,113	1.88	17 (22%)
23	LHG	A	851	19	34,34,48	0.45	0	37,40,54	1.25	3 (8%)
19	CLA	A	813	-	65,73,73	1.33	6 (9%)	76,113,113	2.06	19 (25%)
23	LHG	6	324	19	48,48,48	0.44	0	51,54,54	1.12	3 (5%)
32	CHL	6	315	17	66,74,74	1.04	6 (9%)	73,114,114	1.34	11 (15%)
19	CLA	5	311	39	50,58,73	1.55	8 (16%)	58,95,113	2.25	16 (27%)
19	CLA	5	309	16	65,73,73	1.36	7 (10%)	76,113,113	2.04	19 (25%)
19	CLA	5	319	16	50,58,73	1.56	7 (14%)	58,95,113	2.22	18 (31%)
19	CLA	Z	305	11	65,73,73	1.34	7 (10%)	76,113,113	2.04	20 (26%)
19	CLA	B	810	-	52,60,73	1.50	7 (13%)	60,97,113	2.23	19 (31%)
19	CLA	4	313	-	55,63,73	1.50	7 (12%)	64,101,113	2.11	16 (25%)
38	ERG	6	326	-	31,32,32	3.42	13 (41%)	47,50,50	2.57	14 (29%)
24	LMT	7	323	-	36,36,36	0.35	0	47,47,47	0.74	0
29	LMG	7	301	-	29,29,55	0.52	0	37,37,63	1.22	4 (10%)
22	BCR	B	843	-	41,41,41	4.79	26 (63%)	56,56,56	2.50	21 (37%)
19	CLA	5	306	16	60,68,73	1.41	8 (13%)	70,107,113	2.10	18 (25%)
19	CLA	1	5008	39	65,73,73	1.36	8 (12%)	76,113,113	1.92	19 (25%)
22	BCR	8	303	-	41,41,41	4.82	27 (65%)	56,56,56	2.51	21 (37%)
38	ERG	8	325	-	31,32,32	3.33	12 (38%)	47,50,50	2.70	17 (36%)
19	CLA	B	820	-	56,64,73	1.44	7 (12%)	65,102,113	2.12	17 (26%)
19	CLA	A	828	-	65,73,73	1.34	8 (12%)	76,113,113	1.95	15 (19%)
33	SPH	3	5001	-	19,20,20	0.61	0	18,21,21	1.10	1 (5%)
19	CLA	Z	315	11	65,73,73	1.37	8 (12%)	76,113,113	1.98	20 (26%)
32	CHL	5	316	39	51,59,74	1.14	5 (9%)	55,96,114	1.49	9 (16%)
19	CLA	3	5014	23	60,68,73	1.39	7 (11%)	70,107,113	2.02	16 (22%)
22	BCR	K	206	-	41,41,41	4.78	27 (65%)	56,56,56	2.33	19 (33%)
19	CLA	Z	306	-	50,58,73	1.53	7 (14%)	58,95,113	2.16	14 (24%)
22	BCR	G	1603	-	41,41,41	4.77	27 (65%)	56,56,56	2.46	21 (37%)
19	CLA	A	806	1	65,73,73	1.35	8 (12%)	76,113,113	1.98	18 (23%)
29	LMG	J	1903	-	35,35,55	0.45	0	43,43,63	1.13	3 (6%)
19	CLA	8	311	-	65,73,73	1.39	7 (10%)	76,113,113	1.92	19 (25%)
28	C7Z	1	5005	-	43,43,43	5.33	27 (62%)	58,60,60	2.19	20 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	CHL	5	320	16	43,51,74	1.02	3 (6%)	45,86,114	1.56	11 (24%)
22	BCR	B	847	-	41,41,41	4.77	27 (65%)	56,56,56	2.23	20 (35%)
24	LMT	Z	301	-	36,36,36	0.32	0	47,47,47	0.98	3 (6%)
22	BCR	F	302	-	41,41,41	4.80	27 (65%)	56,56,56	2.41	19 (33%)
31	LUT	5	303	-	42,43,43	5.91	28 (66%)	51,60,60	2.06	18 (35%)
19	CLA	A	810	-	65,73,73	1.37	8 (12%)	76,113,113	2.01	18 (23%)
19	CLA	B	822	-	59,67,73	1.40	7 (11%)	68,105,113	2.13	18 (26%)
19	CLA	Z	303	-	46,54,73	1.61	8 (17%)	53,90,113	2.17	13 (24%)
22	BCR	B	844	-	41,41,41	4.82	27 (65%)	56,56,56	2.25	18 (32%)
22	BCR	4	305	-	41,41,41	4.75	25 (60%)	56,56,56	2.40	19 (33%)
22	BCR	7	305	-	41,41,41	4.77	26 (63%)	56,56,56	2.38	19 (33%)
19	CLA	Z	311	24	55,63,73	1.49	8 (14%)	64,101,113	2.25	17 (26%)
22	BCR	A	846	-	41,41,41	4.80	27 (65%)	56,56,56	2.24	18 (32%)
19	CLA	1	5011	39	55,63,73	1.45	8 (14%)	64,101,113	2.16	16 (25%)
23	LHG	5	323	19	36,36,48	0.43	0	39,42,54	1.16	3 (7%)
19	CLA	B	818	-	60,68,73	1.38	7 (11%)	70,107,113	2.03	17 (24%)
22	BCR	6	307	-	41,41,41	4.77	26 (63%)	56,56,56	2.29	20 (35%)
24	LMT	Z	319	19	36,36,36	0.44	0	47,47,47	0.75	1 (2%)
32	CHL	6	321	17	43,51,74	1.22	6 (13%)	45,86,114	1.82	12 (26%)
19	CLA	4	311	39	50,58,73	1.66	8 (16%)	58,95,113	2.19	17 (29%)
19	CLA	B	830	-	50,58,73	1.52	7 (14%)	58,95,113	2.23	17 (29%)
32	CHL	5	315	39	66,74,74	1.06	7 (10%)	73,114,114	1.27	9 (12%)
19	CLA	6	318	17	50,58,73	1.55	8 (16%)	58,95,113	2.19	18 (31%)
30	DAO	K	201	-	13,13,13	0.59	0	13,13,13	0.55	0
24	LMT	8	323	-	36,36,36	0.34	0	47,47,47	1.04	3 (6%)
19	CLA	A	821	39	65,73,73	1.33	7 (10%)	76,113,113	1.94	17 (22%)
19	CLA	A	839	-	65,73,73	1.32	6 (9%)	76,113,113	1.98	18 (23%)
19	CLA	B	831	-	65,73,73	1.38	8 (12%)	76,113,113	2.10	17 (22%)
19	CLA	6	309	17	60,68,73	1.43	8 (13%)	70,107,113	2.04	18 (25%)
19	CLA	A	812	-	65,73,73	1.36	7 (10%)	76,113,113	1.93	15 (19%)
32	CHL	8	301	11	56,64,74	1.10	4 (7%)	61,102,114	1.41	8 (13%)
22	BCR	3	5006	-	41,41,41	4.77	28 (68%)	56,56,56	2.37	20 (35%)
32	CHL	1	5017	39	48,56,74	0.95	2 (4%)	51,92,114	1.45	12 (23%)
19	CLA	3	5020	12	46,54,73	1.62	8 (17%)	53,90,113	2.20	16 (30%)
19	CLA	A	836	1	55,63,73	1.45	8 (14%)	64,101,113	2.11	14 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LUT	1	5003	-	42,43,43	6.04	27 (64%)	51,60,60	1.91	17 (33%)
19	CLA	B	850	6	65,73,73	1.38	7 (10%)	76,113,113	1.97	19 (25%)
24	LMT	A	853	-	36,36,36	0.38	0	47,47,47	0.82	1 (2%)
19	CLA	3	5018	12	60,68,73	1.41	8 (13%)	70,107,113	2.06	15 (21%)
19	CLA	B	819	39	65,73,73	1.33	7 (10%)	76,113,113	1.98	17 (22%)
19	CLA	A	843	23	52,60,73	1.48	8 (15%)	60,97,113	2.25	17 (28%)
19	CLA	6	320	39	61,69,73	1.42	8 (13%)	71,108,113	2.10	18 (25%)
32	CHL	6	316	39	61,69,74	1.06	5 (8%)	67,108,114	1.20	8 (11%)
23	LHG	Z	316	19	42,42,48	0.44	0	45,48,54	1.18	3 (6%)
31	LUT	6	306	-	42,43,43	5.96	27 (64%)	51,60,60	2.06	15 (29%)
34	3PH	6	325	-	28,28,47	1.08	4 (14%)	32,33,52	1.16	2 (6%)
31	LUT	3	5003	-	42,43,43	6.03	28 (66%)	51,60,60	2.20	18 (35%)
19	CLA	5	308	16	56,64,73	1.47	7 (12%)	65,102,113	2.04	17 (26%)
25	DGD	B	848	-	67,67,67	1.17	7 (10%)	81,81,81	1.00	2 (2%)
19	CLA	5	321	-	65,73,73	1.36	8 (12%)	76,113,113	2.02	16 (21%)
19	CLA	B	816	-	65,73,73	1.33	7 (10%)	76,113,113	2.00	18 (23%)
19	CLA	B	823	-	65,73,73	1.34	7 (10%)	76,113,113	1.96	18 (23%)
19	CLA	A	857	39	52,60,73	1.49	7 (13%)	60,97,113	2.17	17 (28%)
19	CLA	A	814	-	60,68,73	1.38	7 (11%)	70,107,113	2.05	19 (27%)
19	CLA	A	830	-	65,73,73	1.34	7 (10%)	76,113,113	1.97	16 (21%)
19	CLA	B	805	-	45,53,73	1.59	8 (17%)	52,89,113	2.19	14 (26%)
19	CLA	1	5015	39	50,58,73	1.55	7 (14%)	58,95,113	2.29	18 (31%)
19	CLA	7	310	-	61,69,73	1.41	8 (13%)	71,108,113	2.11	19 (26%)
19	CLA	B	815	-	57,65,73	1.41	6 (10%)	66,103,113	2.13	16 (24%)
19	CLA	B	840	23	65,73,73	1.38	8 (12%)	76,113,113	2.10	19 (25%)
22	BCR	A	858	-	41,41,41	4.80	27 (65%)	56,56,56	2.21	21 (37%)
22	BCR	A	848	-	41,41,41	4.77	27 (65%)	56,56,56	2.64	22 (39%)
23	LHG	7	320	19	36,36,48	0.59	1 (2%)	39,42,54	1.42	5 (12%)
19	CLA	B	804	-	65,73,73	1.34	8 (12%)	76,113,113	1.93	15 (19%)
32	CHL	8	315	14	66,74,74	1.03	5 (7%)	73,114,114	1.29	11 (15%)
19	CLA	G	1602	7	46,54,73	1.59	9 (19%)	53,90,113	2.13	15 (28%)
19	CLA	B	829	-	65,73,73	1.33	7 (10%)	76,113,113	2.01	18 (23%)
32	CHL	4	317	39	66,74,74	1.06	5 (7%)	73,114,114	1.33	9 (12%)
19	CLA	4	316	15	50,58,73	1.56	7 (14%)	58,95,113	2.16	17 (29%)
19	CLA	K	205	10	45,53,73	1.60	7 (15%)	52,89,113	2.18	14 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	7	316	39	50,58,73	1.55	8 (16%)	58,95,113	2.30	17 (29%)
19	CLA	B	808	-	65,73,73	1.33	7 (10%)	76,113,113	1.97	14 (18%)
22	BCR	3	5007	-	41,41,41	4.75	25 (60%)	56,56,56	3.51	25 (44%)
19	CLA	6	312	17	65,73,73	1.36	8 (12%)	76,113,113	1.97	18 (23%)
19	CLA	A	805	-	65,73,73	1.33	8 (12%)	76,113,113	1.96	16 (21%)
19	CLA	A	835	-	65,73,73	1.33	7 (10%)	76,113,113	1.95	16 (21%)
27	RRX	F	304	-	42,42,42	5.02	25 (59%)	57,58,58	2.38	21 (36%)
19	CLA	B	806	-	65,73,73	1.33	7 (10%)	76,113,113	1.98	18 (23%)
19	CLA	7	312	23	65,73,73	1.34	8 (12%)	76,113,113	1.92	15 (19%)
21	SF4	C	101	3	0,12,12	-	-	-	-	-
19	CLA	A	825	39	65,73,73	1.34	8 (12%)	76,113,113	1.97	18 (23%)
19	CLA	A	840	-	65,73,73	1.37	8 (12%)	76,113,113	1.89	16 (21%)
34	3PH	3	5022	-	38,38,47	0.95	4 (10%)	42,43,52	1.19	2 (4%)
22	BCR	3	5005	-	41,41,41	4.70	26 (63%)	56,56,56	2.73	20 (35%)
19	CLA	B	824	39	65,73,73	1.33	7 (10%)	76,113,113	1.97	17 (22%)
19	CLA	8	320	14	46,54,73	1.60	7 (15%)	53,90,113	2.13	14 (26%)
19	CLA	7	311	39	56,64,73	1.49	8 (14%)	65,102,113	2.16	17 (26%)
22	BCR	B	845	-	41,41,41	4.76	27 (65%)	56,56,56	2.48	21 (37%)
19	CLA	B	803	39	65,73,73	1.36	8 (12%)	76,113,113	1.94	17 (22%)
19	CLA	6	313	17	65,73,73	1.35	8 (12%)	76,113,113	2.00	16 (21%)
23	LHG	1	5001	19	22,22,48	0.56	0	25,28,54	1.29	2 (8%)
31	LUT	7	304	-	42,43,43	5.97	28 (66%)	51,60,60	2.38	18 (35%)
19	CLA	A	834	-	65,73,73	1.34	8 (12%)	76,113,113	1.96	16 (21%)
21	SF4	C	102	3	0,12,12	-	-	-	-	-
19	CLA	Z	312	23	65,73,73	1.33	7 (10%)	76,113,113	1.99	18 (23%)
22	BCR	A	859	-	41,41,41	4.79	27 (65%)	56,56,56	2.38	19 (33%)
36	PLM	7	322	-	17,17,17	0.58	0	17,17,17	1.09	0
19	CLA	B	809	2	55,63,73	1.44	7 (12%)	64,101,113	2.08	16 (25%)
31	LUT	7	303	-	42,43,43	6.00	28 (66%)	51,60,60	1.95	18 (35%)
19	CLA	A	829	-	65,73,73	1.34	7 (10%)	76,113,113	1.93	15 (19%)
37	SQD	8	302	-	47,48,54	0.83	0	56,59,65	0.95	3 (5%)
19	CLA	B	812	-	65,73,73	1.34	7 (10%)	76,113,113	1.93	16 (21%)
19	CLA	Z	307	-	57,65,73	1.48	7 (12%)	66,103,113	2.04	17 (25%)
19	CLA	A	832	-	65,73,73	1.34	8 (12%)	76,113,113	2.01	18 (23%)
22	BCR	5	304	-	41,41,41	4.77	25 (60%)	56,56,56	2.29	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	6	311	39	65,73,73	1.37	8 (12%)	76,113,113	2.15	19 (25%)
19	CLA	A	827	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	17 (22%)
19	CLA	B	839	-	46,54,73	1.59	7 (15%)	53,90,113	2.12	14 (26%)
24	LMT	4	322	-	36,36,36	0.41	0	47,47,47	0.76	1 (2%)
19	CLA	B	836	-	65,73,73	1.37	8 (12%)	76,113,113	2.05	15 (19%)
32	CHL	8	319	39	66,74,74	1.01	5 (7%)	73,114,114	1.49	12 (16%)
19	CLA	A	807	-	51,59,73	1.50	7 (13%)	59,96,113	2.19	16 (27%)
19	CLA	4	309	15	60,68,73	1.39	8 (13%)	70,107,113	2.27	19 (27%)
19	CLA	7	308	13	65,73,73	1.37	7 (10%)	76,113,113	2.06	18 (23%)
19	CLA	A	838	-	65,73,73	1.32	5 (7%)	76,113,113	1.99	15 (19%)
19	CLA	A	824	-	65,73,73	1.34	7 (10%)	76,113,113	1.97	16 (21%)
19	CLA	5	307	16	61,69,73	1.40	7 (11%)	71,108,113	1.97	19 (26%)
24	LMT	8	324	-	36,36,36	0.39	0	47,47,47	1.02	2 (4%)
19	CLA	5	312	23	61,69,73	1.38	7 (11%)	71,108,113	2.04	16 (22%)
19	CLA	6	322	-	46,54,73	1.63	8 (17%)	53,90,113	2.11	12 (22%)
19	CLA	6	302	15	60,68,73	1.39	7 (11%)	70,107,113	2.01	16 (22%)
19	CLA	A	802	39	65,73,73	1.35	7 (10%)	76,113,113	1.95	18 (23%)
19	CLA	7	318	39	42,50,73	1.72	8 (19%)	48,85,113	2.21	15 (31%)
19	CLA	B	814	-	60,68,73	1.39	7 (11%)	70,107,113	2.05	18 (25%)
22	BCR	A	847	-	41,41,41	4.78	27 (65%)	56,56,56	2.48	19 (33%)
19	CLA	J	1901	9	42,50,73	1.65	7 (16%)	48,85,113	2.25	17 (35%)
19	CLA	1	5012	23	60,68,73	1.39	8 (13%)	70,107,113	2.00	17 (24%)
19	CLA	1	5006	11	65,73,73	1.35	8 (12%)	76,113,113	2.01	20 (26%)
19	CLA	5	310	-	55,63,73	1.49	8 (14%)	64,101,113	2.16	21 (32%)
24	LMT	A	854	-	36,36,36	0.41	0	47,47,47	0.77	1 (2%)
32	CHL	6	317	39	51,59,74	1.11	4 (7%)	55,96,114	1.42	9 (16%)
19	CLA	A	811	19	65,73,73	1.33	8 (12%)	76,113,113	1.95	18 (23%)
19	CLA	8	313	23	55,63,73	1.49	8 (14%)	64,101,113	2.13	17 (26%)
19	CLA	3	5009	12	46,54,73	1.61	7 (15%)	53,90,113	2.10	13 (24%)
19	CLA	1	5013	-	48,56,73	1.58	8 (16%)	55,92,113	2.17	15 (27%)
23	LHG	8	321	19	37,37,48	0.43	0	40,43,54	1.11	3 (7%)
19	CLA	B	821	-	65,73,73	1.34	6 (9%)	76,113,113	1.98	17 (22%)
23	LHG	4	320	19	48,48,48	0.40	0	51,54,54	1.12	4 (7%)
19	CLA	3	5012	-	65,73,73	1.38	7 (10%)	76,113,113	1.99	20 (26%)
22	BCR	5	305	-	41,41,41	4.75	24 (58%)	56,56,56	2.73	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	8	307	14	60,68,73	1.43	8 (13%)	70,107,113	2.17	17 (24%)
19	CLA	8	312	39	60,68,73	1.56	7 (11%)	70,107,113	2.15	19 (27%)
22	BCR	A	850	-	41,41,41	4.79	27 (65%)	56,56,56	2.48	20 (35%)
19	CLA	A	815	-	65,73,73	1.36	8 (12%)	76,113,113	2.09	21 (27%)
19	CLA	F	301	-	65,73,73	1.39	8 (12%)	76,113,113	1.99	17 (22%)
19	CLA	B	826	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	17 (22%)
19	CLA	A	817	-	60,68,73	1.38	7 (11%)	70,107,113	2.07	15 (21%)
21	SF4	A	845	2,1	0,12,12	-	-	-	-	-
34	3PH	8	322	-	29,29,47	1.04	4 (13%)	33,34,52	1.11	2 (6%)
19	CLA	6	310	17	52,60,73	1.52	7 (13%)	60,97,113	2.13	17 (28%)
22	BCR	B	842	-	41,41,41	4.81	27 (65%)	56,56,56	2.25	19 (33%)
19	CLA	6	301	39	60,68,73	1.38	7 (11%)	70,107,113	2.07	16 (22%)
24	LMT	4	321	-	36,36,36	0.35	0	47,47,47	0.71	1 (2%)
19	CLA	A	803	-	65,73,73	1.33	7 (10%)	76,113,113	1.98	18 (23%)
19	CLA	5	322	39	46,54,73	1.58	7 (15%)	53,90,113	2.21	14 (26%)
32	CHL	1	5009	11	61,69,74	1.10	7 (11%)	67,108,114	1.30	12 (17%)
19	CLA	A	808	1	65,73,73	1.33	7 (10%)	76,113,113	1.96	17 (22%)
19	CLA	B	827	-	60,68,73	1.40	8 (13%)	70,107,113	2.05	18 (25%)
19	CLA	B	837	-	65,73,73	1.34	7 (10%)	76,113,113	1.96	17 (22%)
22	BCR	B	846	-	41,41,41	4.79	26 (63%)	56,56,56	2.40	21 (37%)
32	CHL	7	314	13	66,74,74	1.07	6 (9%)	73,114,114	1.13	7 (9%)
23	LHG	3	5021	19	19,19,48	0.93	1 (5%)	20,24,54	1.40	1 (5%)
19	CLA	4	306	15	60,68,73	1.42	7 (11%)	70,107,113	2.07	18 (25%)
19	CLA	4	312	23	55,63,73	1.46	7 (12%)	64,101,113	2.09	15 (23%)
19	CLA	5	313	-	45,53,73	1.62	7 (15%)	52,89,113	2.11	14 (26%)
19	CLA	B	828	-	65,73,73	1.34	7 (10%)	76,113,113	1.92	15 (19%)
35	DGA	7	302	-	33,33,43	1.22	3 (9%)	35,35,45	1.62	3 (8%)
32	CHL	4	319	15	43,51,74	1.04	3 (6%)	45,86,114	1.52	11 (24%)
19	CLA	7	324	-	55,63,73	1.49	8 (14%)	64,101,113	2.13	15 (23%)

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
24	LMT	A	856	-	-	8/21/61/61	0/2/2/2
32	CHL	8	317	39	3/3/17/26	3/21/119/137	-
19	CLA	B	832	-	1/1/13/20	16/29/107/115	-
24	LMT	1	5002	-	-	4/21/61/61	0/2/2/2
31	LUT	Z	318	-	-	6/29/67/67	0/2/2/2
19	CLA	8	308	14	1/1/15/20	13/37/115/115	-
19	CLA	4	310	15	1/1/15/20	12/37/115/115	-
19	CLA	5	317	16	1/1/15/20	14/37/115/115	-
32	CHL	3	5017	39	3/3/20/26	9/39/137/137	-
24	LMT	4	302	-	-	4/21/61/61	0/2/2/2
22	BCR	8	306	-	-	9/29/63/63	0/2/2/2
19	CLA	1	5010	-	1/1/13/20	7/25/103/115	-
19	CLA	K	204	10	1/1/11/20	9/18/96/115	-
19	CLA	B	834	39	1/1/11/20	5/13/91/115	-
19	CLA	B	833	-	1/1/15/20	13/37/115/115	-
31	LUT	6	305	-	-	5/29/67/67	0/2/2/2
19	CLA	8	318	14	1/1/11/20	3/15/93/115	-
19	CLA	7	309	13	1/1/15/20	10/37/115/115	-
19	CLA	5	301	39	1/1/13/20	16/27/105/115	-
19	CLA	A	819	-	1/1/15/20	13/37/115/115	-
32	CHL	4	314	39	3/3/17/26	6/21/119/137	-
19	CLA	B	838	39	1/1/12/20	6/22/100/115	-
33	SPH	7	321	-	-	12/21/21/21	-
19	CLA	B	802	-	1/1/15/20	17/37/115/115	-
19	CLA	7	307	13	1/1/12/20	4/19/97/115	-
19	CLA	8	310	14	1/1/14/20	8/34/112/115	-
19	CLA	A	842	39	1/1/15/20	12/37/115/115	-
19	CLA	8	309	14	1/1/15/20	8/37/115/115	-
31	LUT	1	5004	-	-	4/29/67/67	0/2/2/2
19	CLA	B	817	-	1/1/13/20	17/30/108/115	-
19	CLA	7	313	-	1/1/10/20	1/11/89/115	-
22	BCR	3	5004	-	-	13/29/63/63	0/2/2/2
32	CHL	1	5014	39	3/3/16/26	4/18/116/137	-
19	CLA	A	816	39	1/1/14/20	13/33/111/115	-
19	CLA	1	5018	11	1/1/12/20	5/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	G	1601	-	1/1/12/20	10/19/97/115	-
19	CLA	B	811	-	1/1/13/20	12/27/105/115	-
19	CLA	I	201	-	1/1/13/20	15/25/103/115	-
19	CLA	6	314	23	1/1/13/20	9/25/103/115	-
19	CLA	A	833	-	1/1/15/20	16/37/115/115	-
19	CLA	Z	304	39	1/1/12/20	2/19/97/115	-
19	CLA	7	319	13	1/1/13/20	17/29/107/115	-
19	CLA	3	5008	12	1/1/15/20	8/37/115/115	-
32	CHL	8	316	39	3/3/18/26	10/29/127/137	-
31	LUT	3	5002	-	-	4/29/67/67	0/2/2/2
22	BCR	6	308	-	-	10/29/63/63	0/2/2/2
19	CLA	B	801	-	1/1/15/20	12/37/115/115	-
24	LMT	A	855	-	-	3/21/61/61	0/2/2/2
33	SPH	4	301	-	-	12/21/21/21	-
23	LHG	A	852	-	-	35/53/53/53	-
19	CLA	A	823	-	1/1/13/20	17/28/106/115	-
19	CLA	K	202	-	1/1/11/20	8/15/93/115	-
32	CHL	4	315	39	3/3/17/26	8/21/119/137	-
18	CLO	A	801	-	3/3/20/25	12/37/135/135	-
31	LUT	4	304	-	-	7/29/67/67	0/2/2/2
19	CLA	A	820	-	1/1/14/20	11/31/109/115	-
32	CHL	Z	302	11	3/3/18/26	5/29/127/137	-
19	CLA	3	5011	12	1/1/14/20	4/31/109/115	-
19	CLA	3	5019	39	1/1/13/20	8/25/103/115	-
19	CLA	6	323	17	1/1/15/20	11/37/115/115	-
19	CLA	B	825	39	1/1/15/20	14/37/115/115	-
28	C7Z	6	304	-	-	13/29/67/67	0/2/2/2
23	LHG	6	303	-	-	26/36/36/53	-
24	LMT	F	305	-	-	4/21/61/61	0/2/2/2
27	RRX	4	303	-	-	7/29/65/65	0/2/2/2
34	3PH	5	324	-	-	8/24/24/49	-
27	RRX	5	302	-	-	7/29/65/65	0/2/2/2
19	CLA	7	306	13	1/1/14/20	12/31/109/115	-
32	CHL	5	318	39	3/3/17/26	2/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	A	849	-	-	15/29/63/63	0/2/2/2
19	CLA	5	325	-	1/1/13/20	12/25/103/115	-
32	CHL	6	319	39	3/3/20/26	13/39/137/137	-
32	CHL	Z	310	39	3/3/20/26	11/39/137/137	-
19	CLA	B	813	-	1/1/15/20	18/37/115/115	-
19	CLA	4	308	15	1/1/15/20	15/37/115/115	-
19	CLA	1	5016	11	1/1/14/20	14/31/109/115	-
19	CLA	B	835	-	1/1/14/20	12/31/109/115	-
19	CLA	A	809	1	1/1/13/20	9/27/105/115	-
19	CLA	Z	308	-	1/1/15/20	15/37/115/115	-
19	CLA	A	804	19	1/1/13/20	13/25/103/115	-
19	CLA	A	837	-	1/1/12/20	7/21/99/115	-
31	LUT	8	304	-	-	11/29/67/67	0/2/2/2
19	CLA	A	831	-	1/1/12/20	4/19/97/115	-
19	CLA	A	841	-	1/1/15/20	11/37/115/115	-
19	CLA	8	314	-	1/1/13/20	14/25/103/115	-
19	CLA	4	318	15	1/1/10/20	4/8/86/115	-
31	LUT	Z	317	-	-	6/29/67/67	0/2/2/2
32	CHL	Z	309	11	3/3/19/26	17/36/134/137	-
19	CLA	3	5016	12	1/1/14/20	15/31/109/115	-
32	CHL	Z	313	39	3/3/16/26	4/15/113/137	-
19	CLA	3	5013	39	1/1/15/20	15/37/115/115	-
24	LMT	3	5023	-	-	6/21/61/61	0/2/2/2
19	CLA	A	826	39	1/1/15/20	11/37/115/115	-
19	CLA	5	314	16	1/1/15/20	19/37/115/115	-
19	CLA	1	5007	11	1/1/11/20	5/13/91/115	-
32	CHL	7	315	39	3/3/17/26	6/25/123/137	-
19	CLA	3	5015	-	1/1/11/20	6/13/91/115	-
28	C7Z	J	1902	-	-	14/29/67/67	0/2/2/2
19	CLA	4	307	15	1/1/12/20	8/22/100/115	-
24	LMT	G	1604	-	-	1/21/61/61	0/2/2/2
19	CLA	K	203	39	1/1/13/20	10/25/103/115	-
19	CLA	A	818	-	1/1/14/20	15/31/109/115	-
19	CLA	F	303	39	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PQN	B	841	-	-	10/23/43/43	0/2/2/2
19	CLA	Z	314	11	1/1/11/20	7/15/93/115	-
20	PQN	A	844	-	-	6/23/43/43	0/2/2/2
23	LHG	1	5019	19	-	32/47/47/53	-
19	CLA	B	807	2	1/1/15/20	24/37/115/115	-
19	CLA	A	822	-	1/1/13/20	12/25/103/115	-
29	LMG	J	1904	-	-	8/40/60/70	0/1/1/1
19	CLA	7	317	13	1/1/12/20	8/19/97/115	-
31	LUT	8	305	-	-	3/29/67/67	0/2/2/2
19	CLA	3	5010	12	1/1/15/20	15/37/115/115	-
23	LHG	A	851	19	-	24/39/39/53	-
19	CLA	A	813	-	1/1/15/20	13/37/115/115	-
23	LHG	6	324	19	-	30/53/53/53	-
32	CHL	6	315	17	3/3/20/26	13/39/137/137	-
19	CLA	5	311	39	1/1/12/20	10/19/97/115	-
19	CLA	5	309	16	1/1/15/20	11/37/115/115	-
19	CLA	5	319	16	1/1/12/20	9/19/97/115	-
19	CLA	Z	305	11	1/1/15/20	16/37/115/115	-
19	CLA	B	810	-	1/1/12/20	10/22/100/115	-
19	CLA	4	313	-	1/1/13/20	12/25/103/115	-
38	ERG	6	326	-	-	8/13/71/71	0/4/4/4
24	LMT	7	323	-	-	4/21/61/61	0/2/2/2
29	LMG	7	301	-	-	5/24/44/70	0/1/1/1
22	BCR	B	843	-	-	14/29/63/63	0/2/2/2
19	CLA	5	306	16	1/1/14/20	17/31/109/115	-
19	CLA	1	5008	39	1/1/15/20	14/37/115/115	-
22	BCR	8	303	-	-	16/29/63/63	0/2/2/2
38	ERG	8	325	-	-	11/13/71/71	0/4/4/4
19	CLA	B	820	-	1/1/13/20	15/27/105/115	-
19	CLA	A	828	-	1/1/15/20	17/37/115/115	-
33	SPH	3	5001	-	-	14/21/21/21	-
19	CLA	Z	315	11	1/1/15/20	13/37/115/115	-
32	CHL	5	316	39	3/3/17/26	2/21/119/137	-
19	CLA	3	5014	23	1/1/14/20	22/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	K	206	-	-	10/29/63/63	0/2/2/2
19	CLA	Z	306	-	1/1/12/20	11/19/97/115	-
22	BCR	G	1603	-	-	9/29/63/63	0/2/2/2
19	CLA	A	806	1	1/1/15/20	17/37/115/115	-
29	LMG	J	1903	-	-	8/30/50/70	0/1/1/1
19	CLA	8	311	-	1/1/15/20	17/37/115/115	-
28	C7Z	1	5005	-	-	9/29/67/67	0/2/2/2
32	CHL	5	320	16	3/3/15/26	0/12/110/137	-
22	BCR	B	847	-	-	12/29/63/63	0/2/2/2
24	LMT	Z	301	-	-	6/21/61/61	0/2/2/2
22	BCR	F	302	-	-	12/29/63/63	0/2/2/2
31	LUT	5	303	-	-	9/29/67/67	0/2/2/2
19	CLA	A	810	-	1/1/15/20	16/37/115/115	-
19	CLA	B	822	-	1/1/13/20	15/30/108/115	-
19	CLA	Z	303	-	1/1/11/20	7/15/93/115	-
22	BCR	B	844	-	-	10/29/63/63	0/2/2/2
22	BCR	4	305	-	-	16/29/63/63	0/2/2/2
22	BCR	7	305	-	-	16/29/63/63	0/2/2/2
19	CLA	Z	311	24	1/1/13/20	11/25/103/115	-
22	BCR	A	846	-	-	14/29/63/63	0/2/2/2
19	CLA	1	5011	39	1/1/13/20	11/25/103/115	-
23	LHG	5	323	19	-	27/41/41/53	-
19	CLA	B	818	-	1/1/14/20	15/31/109/115	-
22	BCR	6	307	-	-	10/29/63/63	0/2/2/2
24	LMT	Z	319	19	-	8/21/61/61	0/2/2/2
32	CHL	6	321	17	3/3/15/26	2/12/110/137	-
19	CLA	4	311	39	1/1/12/20	7/19/97/115	-
19	CLA	B	830	-	1/1/12/20	9/19/97/115	-
32	CHL	5	315	39	3/3/20/26	15/39/137/137	-
19	CLA	6	318	17	1/1/12/20	3/19/97/115	-
30	DAO	K	201	-	-	2/11/11/11	-
24	LMT	8	323	-	-	4/21/61/61	0/2/2/2
19	CLA	A	821	39	1/1/15/20	11/37/115/115	-
19	CLA	A	839	-	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	831	-	1/1/15/20	16/37/115/115	-
19	CLA	6	309	17	1/1/14/20	7/31/109/115	-
19	CLA	A	812	-	1/1/15/20	12/37/115/115	-
32	CHL	8	301	11	3/3/18/26	10/27/125/137	-
22	BCR	3	5006	-	-	16/29/63/63	0/2/2/2
32	CHL	1	5017	39	3/3/16/26	1/18/116/137	-
19	CLA	3	5020	12	1/1/11/20	9/15/93/115	-
19	CLA	A	836	1	1/1/13/20	13/25/103/115	-
31	LUT	1	5003	-	-	6/29/67/67	0/2/2/2
19	CLA	B	850	6	1/1/15/20	22/37/115/115	-
24	LMT	A	853	-	-	4/21/61/61	0/2/2/2
19	CLA	3	5018	12	1/1/14/20	11/31/109/115	-
19	CLA	B	819	39	1/1/15/20	21/37/115/115	-
19	CLA	A	843	23	1/1/12/20	12/22/100/115	-
19	CLA	6	320	39	1/1/14/20	10/33/111/115	-
32	CHL	6	316	39	3/3/19/26	13/33/131/137	-
23	LHG	Z	316	19	-	27/47/47/53	-
31	LUT	6	306	-	-	8/29/67/67	0/2/2/2
34	3PH	6	325	-	-	15/30/30/49	-
31	LUT	3	5003	-	-	6/29/67/67	0/2/2/2
19	CLA	5	308	16	1/1/13/20	7/27/105/115	-
25	DGD	B	848	-	-	14/55/95/95	0/2/2/2
19	CLA	5	321	-	1/1/15/20	16/37/115/115	-
19	CLA	B	816	-	1/1/15/20	14/37/115/115	-
19	CLA	B	823	-	1/1/15/20	19/37/115/115	-
19	CLA	A	857	39	1/1/12/20	11/22/100/115	-
19	CLA	A	814	-	1/1/14/20	11/31/109/115	-
19	CLA	A	830	-	1/1/15/20	12/37/115/115	-
19	CLA	B	805	-	1/1/11/20	5/13/91/115	-
19	CLA	1	5015	39	1/1/12/20	6/19/97/115	-
19	CLA	7	310	-	1/1/14/20	14/33/111/115	-
19	CLA	B	815	-	1/1/13/20	16/28/106/115	-
19	CLA	B	840	23	1/1/15/20	14/37/115/115	-
22	BCR	A	858	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	A	848	-	-	12/29/63/63	0/2/2/2
23	LHG	7	320	19	-	26/41/41/53	-
19	CLA	B	804	-	1/1/15/20	12/37/115/115	-
32	CHL	8	315	14	3/3/20/26	14/39/137/137	-
19	CLA	G	1602	7	1/1/11/20	8/15/93/115	-
19	CLA	B	829	-	1/1/15/20	16/37/115/115	-
32	CHL	4	317	39	3/3/20/26	7/39/137/137	-
19	CLA	4	316	15	1/1/12/20	5/19/97/115	-
19	CLA	K	205	10	1/1/11/20	7/13/91/115	-
19	CLA	7	316	39	1/1/12/20	2/19/97/115	-
19	CLA	B	808	-	1/1/15/20	18/37/115/115	-
22	BCR	3	5007	-	-	13/29/63/63	0/2/2/2
19	CLA	6	312	17	1/1/15/20	8/37/115/115	-
19	CLA	A	805	-	1/1/15/20	13/37/115/115	-
19	CLA	A	835	-	1/1/15/20	10/37/115/115	-
27	RRX	F	304	-	-	14/29/65/65	0/2/2/2
19	CLA	B	806	-	1/1/15/20	11/37/115/115	-
19	CLA	7	312	23	1/1/15/20	15/37/115/115	-
21	SF4	C	101	3	-	-	0/6/5/5
19	CLA	A	825	39	1/1/15/20	16/37/115/115	-
19	CLA	A	840	-	1/1/15/20	14/37/115/115	-
34	3PH	3	5022	-	-	20/40/40/49	-
22	BCR	3	5005	-	-	7/29/63/63	0/2/2/2
19	CLA	B	824	39	1/1/15/20	13/37/115/115	-
19	CLA	8	320	14	1/1/11/20	7/15/93/115	-
19	CLA	7	311	39	1/1/13/20	9/27/105/115	-
22	BCR	B	845	-	-	14/29/63/63	0/2/2/2
19	CLA	B	803	39	1/1/15/20	13/37/115/115	-
19	CLA	6	313	17	1/1/15/20	18/37/115/115	-
23	LHG	1	5001	19	-	15/26/26/53	-
31	LUT	7	304	-	-	5/29/67/67	0/2/2/2
19	CLA	A	834	-	1/1/15/20	16/37/115/115	-
21	SF4	C	102	3	-	-	0/6/5/5
19	CLA	Z	312	23	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	A	859	-	-	16/29/63/63	0/2/2/2
36	PLM	7	322	-	-	4/15/15/15	-
19	CLA	B	809	2	1/1/13/20	14/25/103/115	-
31	LUT	7	303	-	-	5/29/67/67	0/2/2/2
19	CLA	A	829	-	1/1/15/20	12/37/115/115	-
37	SQD	8	302	-	-	10/43/63/69	0/1/1/1
19	CLA	B	812	-	1/1/15/20	12/37/115/115	-
19	CLA	Z	307	-	1/1/13/20	15/28/106/115	-
19	CLA	A	832	-	1/1/15/20	20/37/115/115	-
22	BCR	5	304	-	-	13/29/63/63	0/2/2/2
19	CLA	6	311	39	1/1/15/20	9/37/115/115	-
19	CLA	A	827	-	1/1/15/20	23/37/115/115	-
19	CLA	B	839	-	1/1/11/20	6/15/93/115	-
24	LMT	4	322	-	-	4/21/61/61	0/2/2/2
19	CLA	B	836	-	1/1/15/20	16/37/115/115	-
32	CHL	8	319	39	3/3/20/26	13/39/137/137	-
19	CLA	A	807	-	1/1/12/20	9/21/99/115	-
19	CLA	4	309	15	1/1/14/20	11/31/109/115	-
19	CLA	7	308	13	1/1/15/20	13/37/115/115	-
19	CLA	A	838	-	1/1/15/20	18/37/115/115	-
19	CLA	A	824	-	1/1/15/20	15/37/115/115	-
19	CLA	5	307	16	1/1/14/20	12/33/111/115	-
24	LMT	8	324	-	-	4/21/61/61	0/2/2/2
19	CLA	5	312	23	1/1/14/20	15/33/111/115	-
19	CLA	6	322	-	1/1/11/20	6/15/93/115	-
19	CLA	6	302	15	1/1/14/20	15/31/109/115	-
19	CLA	A	802	39	1/1/15/20	15/37/115/115	-
19	CLA	7	318	39	1/1/10/20	4/10/88/115	-
19	CLA	B	814	-	1/1/14/20	15/31/109/115	-
22	BCR	A	847	-	-	13/29/63/63	0/2/2/2
19	CLA	J	1901	9	1/1/10/20	6/10/88/115	-
19	CLA	1	5012	23	1/1/14/20	12/31/109/115	-
19	CLA	1	5006	11	1/1/15/20	16/37/115/115	-
19	CLA	5	310	-	1/1/13/20	15/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMT	A	854	-	-	2/21/61/61	0/2/2/2
32	CHL	6	317	39	3/3/17/26	8/21/119/137	-
19	CLA	A	811	19	1/1/15/20	12/37/115/115	-
19	CLA	8	313	23	1/1/13/20	14/25/103/115	-
19	CLA	3	5009	12	1/1/11/20	4/15/93/115	-
19	CLA	1	5013	-	1/1/11/20	3/17/95/115	-
23	LHG	8	321	19	-	22/42/42/53	-
19	CLA	B	821	-	1/1/15/20	16/37/115/115	-
23	LHG	4	320	19	-	34/53/53/53	-
19	CLA	3	5012	-	1/1/15/20	7/37/115/115	-
22	BCR	5	305	-	-	7/29/63/63	0/2/2/2
19	CLA	8	307	14	1/1/14/20	15/31/109/115	-
19	CLA	8	312	39	1/1/14/20	12/31/109/115	-
22	BCR	A	850	-	-	15/29/63/63	0/2/2/2
19	CLA	A	815	-	1/1/15/20	6/37/115/115	-
19	CLA	F	301	-	1/1/15/20	11/37/115/115	-
19	CLA	B	826	-	1/1/15/20	18/37/115/115	-
19	CLA	A	817	-	1/1/14/20	13/31/109/115	-
21	SF4	A	845	2,1	-	-	0/6/5/5
34	3PH	8	322	-	-	15/31/31/49	-
19	CLA	6	310	17	1/1/12/20	8/22/100/115	-
22	BCR	B	842	-	-	13/29/63/63	0/2/2/2
19	CLA	6	301	39	1/1/14/20	17/31/109/115	-
24	LMT	4	321	-	-	2/21/61/61	0/2/2/2
19	CLA	A	803	-	1/1/15/20	14/37/115/115	-
19	CLA	5	322	39	1/1/11/20	7/15/93/115	-
32	CHL	1	5009	11	3/3/19/26	14/33/131/137	-
19	CLA	A	808	1	1/1/15/20	17/37/115/115	-
19	CLA	B	827	-	1/1/14/20	19/31/109/115	-
19	CLA	B	837	-	1/1/15/20	19/37/115/115	-
22	BCR	B	846	-	-	13/29/63/63	0/2/2/2
32	CHL	7	314	13	3/3/20/26	15/39/137/137	-
23	LHG	3	5021	19	-	17/22/22/53	-
19	CLA	4	306	15	1/1/14/20	12/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	4	312	23	1/1/13/20	12/25/103/115	-
19	CLA	5	313	-	1/1/11/20	5/13/91/115	-
19	CLA	B	828	-	1/1/15/20	12/37/115/115	-
35	DGA	7	302	-	-	23/35/35/45	-
32	CHL	4	319	15	3/3/15/26	1/12/110/137	-
19	CLA	7	324	-	1/1/13/20	9/25/103/115	-

All (2860) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	5003	LUT	C24-C25	23.05	1.61	1.33
31	Z	318	LUT	C24-C25	22.96	1.61	1.33
31	8	304	LUT	C24-C25	22.89	1.61	1.33
31	3	5003	LUT	C24-C25	22.58	1.61	1.33
31	6	305	LUT	C24-C25	22.44	1.61	1.33
31	4	304	LUT	C24-C25	22.37	1.61	1.33
31	7	304	LUT	C24-C25	22.36	1.61	1.33
31	3	5002	LUT	C24-C25	22.35	1.61	1.33
31	7	303	LUT	C24-C25	22.32	1.61	1.33
31	6	306	LUT	C24-C25	22.16	1.60	1.33
31	8	305	LUT	C24-C25	21.86	1.60	1.33
31	Z	317	LUT	C24-C25	21.77	1.60	1.33
31	5	303	LUT	C24-C25	21.65	1.60	1.33
31	1	5004	LUT	C24-C25	21.63	1.60	1.33
28	J	1902	C7Z	C25-C26	15.89	1.62	1.34
28	1	5005	C7Z	C25-C26	15.84	1.61	1.34
28	6	304	C7Z	C25-C26	15.81	1.61	1.34
22	7	305	BCR	C26-C25	15.66	1.61	1.34
22	B	846	BCR	C26-C25	15.51	1.61	1.34
22	B	844	BCR	C26-C25	15.51	1.61	1.34
27	F	304	RRX	C26-C25	15.51	1.61	1.34
27	4	303	RRX	C26-C25	15.47	1.61	1.34
22	F	302	BCR	C26-C25	15.43	1.61	1.34
22	B	842	BCR	C26-C25	15.43	1.61	1.34
22	A	846	BCR	C26-C25	15.42	1.61	1.34
22	A	858	BCR	C26-C25	15.41	1.61	1.34
22	K	206	BCR	C26-C25	15.37	1.61	1.34
22	A	859	BCR	C26-C25	15.33	1.61	1.34
22	6	307	BCR	C26-C25	15.30	1.60	1.34
22	A	848	BCR	C26-C25	15.29	1.60	1.34
22	5	305	BCR	C26-C25	15.27	1.60	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	847	BCR	C26-C25	15.24	1.60	1.34
22	G	1603	BCR	C26-C25	15.24	1.60	1.34
22	5	304	BCR	C26-C25	15.22	1.60	1.34
22	A	850	BCR	C26-C25	15.18	1.60	1.34
22	B	845	BCR	C26-C25	15.17	1.60	1.34
22	3	5007	BCR	C26-C25	15.16	1.60	1.34
22	B	843	BCR	C26-C25	15.16	1.60	1.34
27	5	302	RRX	C26-C25	15.15	1.60	1.34
22	6	308	BCR	C26-C25	15.13	1.60	1.34
22	B	847	BCR	C26-C25	15.10	1.60	1.34
28	J	1902	C7Z	C5-C6	15.09	1.60	1.34
22	8	303	BCR	C26-C25	15.07	1.60	1.34
22	3	5004	BCR	C26-C25	15.03	1.60	1.34
28	1	5005	C7Z	C5-C6	15.02	1.60	1.34
22	A	849	BCR	C26-C25	14.95	1.60	1.34
22	3	5006	BCR	C26-C25	14.95	1.60	1.34
31	7	303	LUT	C5-C6	14.89	1.60	1.34
28	6	304	C7Z	C5-C6	14.87	1.60	1.34
31	5	303	LUT	C5-C6	14.83	1.60	1.34
22	4	305	BCR	C26-C25	14.82	1.60	1.34
31	Z	318	LUT	C5-C6	14.78	1.60	1.34
22	3	5005	BCR	C26-C25	14.78	1.60	1.34
31	1	5003	LUT	C5-C6	14.77	1.60	1.34
22	8	306	BCR	C26-C25	14.71	1.59	1.34
31	Z	317	LUT	C5-C6	14.71	1.59	1.34
31	1	5004	LUT	C5-C6	14.67	1.59	1.34
31	8	305	LUT	C5-C6	14.67	1.59	1.34
31	3	5003	LUT	C5-C6	14.67	1.59	1.34
31	8	304	LUT	C5-C6	14.65	1.59	1.34
31	6	305	LUT	C5-C6	14.58	1.59	1.34
31	3	5002	LUT	C5-C6	14.57	1.59	1.34
31	6	306	LUT	C5-C6	14.55	1.59	1.34
31	7	304	LUT	C5-C6	14.51	1.59	1.34
31	4	304	LUT	C5-C6	14.48	1.59	1.34
27	F	304	RRX	C5-C6	14.40	1.59	1.34
22	B	846	BCR	C5-C6	14.14	1.58	1.34
22	F	302	BCR	C5-C6	14.12	1.58	1.34
22	A	846	BCR	C5-C6	14.11	1.58	1.34
22	B	847	BCR	C5-C6	14.10	1.58	1.34
22	B	844	BCR	C5-C6	14.10	1.58	1.34
22	A	847	BCR	C5-C6	14.07	1.58	1.34
22	3	5006	BCR	C5-C6	13.99	1.58	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	307	BCR	C5-C6	13.94	1.58	1.34
27	5	302	RRX	C5-C6	13.92	1.58	1.34
22	B	842	BCR	C5-C6	13.92	1.58	1.34
22	A	849	BCR	C5-C6	13.91	1.58	1.34
22	G	1603	BCR	C5-C6	13.90	1.58	1.34
22	K	206	BCR	C5-C6	13.88	1.58	1.34
22	A	859	BCR	C5-C6	13.88	1.58	1.34
22	8	306	BCR	C5-C6	13.88	1.58	1.34
22	B	843	BCR	C5-C6	13.83	1.58	1.34
22	5	305	BCR	C5-C6	13.83	1.58	1.34
22	A	858	BCR	C5-C6	13.82	1.58	1.34
22	B	845	BCR	C5-C6	13.81	1.58	1.34
22	A	850	BCR	C5-C6	13.78	1.58	1.34
22	8	303	BCR	C5-C6	13.78	1.58	1.34
22	7	305	BCR	C5-C6	13.77	1.58	1.34
22	A	848	BCR	C5-C6	13.75	1.58	1.34
22	6	308	BCR	C5-C6	13.75	1.58	1.34
22	5	304	BCR	C5-C6	13.74	1.58	1.34
27	4	303	RRX	C5-C6	13.71	1.58	1.34
22	4	305	BCR	C5-C6	13.71	1.58	1.34
22	3	5007	BCR	C5-C6	13.61	1.58	1.34
31	8	304	LUT	C22-C21	-13.59	1.37	1.54
31	1	5003	LUT	C22-C21	-13.57	1.37	1.54
22	3	5004	BCR	C5-C6	13.53	1.57	1.34
31	7	303	LUT	C22-C21	-13.45	1.37	1.54
22	3	5005	BCR	C5-C6	13.40	1.57	1.34
31	1	5004	LUT	C22-C21	-13.28	1.38	1.54
31	Z	318	LUT	C22-C21	-13.27	1.38	1.54
31	8	305	LUT	C22-C21	-13.25	1.38	1.54
31	3	5002	LUT	C22-C21	-13.24	1.38	1.54
31	6	305	LUT	C22-C21	-13.21	1.38	1.54
31	4	304	LUT	C22-C21	-13.16	1.38	1.54
31	3	5003	LUT	C22-C21	-13.07	1.38	1.54
31	6	306	LUT	C22-C21	-12.85	1.38	1.54
31	7	304	LUT	C22-C21	-12.84	1.38	1.54
31	Z	317	LUT	C22-C21	-12.76	1.38	1.54
31	5	303	LUT	C22-C21	-12.72	1.38	1.54
31	7	303	LUT	C2-C3	-12.03	1.35	1.52
31	5	303	LUT	C2-C3	-11.91	1.35	1.52
28	1	5005	C7Z	C24-C23	11.75	1.72	1.52
31	1	5003	LUT	C2-C3	-11.74	1.35	1.52
31	8	305	LUT	C2-C3	-11.73	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	J	1902	C7Z	C24-C23	11.70	1.72	1.52
27	4	303	RRX	C29-C28	-11.67	1.35	1.52
31	6	305	LUT	C2-C3	-11.60	1.35	1.52
28	6	304	C7Z	C24-C23	11.60	1.72	1.52
31	6	306	LUT	C2-C3	-11.56	1.35	1.52
31	1	5004	LUT	C2-C3	-11.55	1.35	1.52
31	3	5003	LUT	C2-C3	-11.49	1.35	1.52
31	8	304	LUT	C2-C3	-11.40	1.35	1.52
31	4	304	LUT	C2-C3	-11.40	1.35	1.52
31	3	5002	LUT	C2-C3	-11.32	1.36	1.52
27	5	302	RRX	C29-C28	-11.27	1.36	1.52
31	Z	317	LUT	C2-C3	-11.22	1.36	1.52
31	Z	318	LUT	C2-C3	-11.20	1.36	1.52
28	1	5005	C7Z	C22-C23	-11.10	1.36	1.52
28	J	1902	C7Z	C22-C23	-10.97	1.36	1.52
28	6	304	C7Z	C22-C23	-10.92	1.36	1.52
31	7	304	LUT	C2-C3	-10.82	1.36	1.52
28	1	5005	C7Z	C2-C3	-10.41	1.37	1.52
27	F	304	RRX	C29-C28	-10.29	1.37	1.52
38	8	325	ERG	C13-C14	-10.05	1.39	1.56
28	J	1902	C7Z	C2-C3	-9.82	1.38	1.52
28	6	304	C7Z	C2-C3	-9.81	1.38	1.52
38	6	326	ERG	C13-C14	-9.74	1.39	1.56
18	A	801	CL0	MG-NA	9.06	2.27	2.06
28	6	304	C7Z	C4-C3	8.53	1.67	1.52
28	J	1902	C7Z	C4-C3	8.31	1.66	1.52
31	Z	317	LUT	C22-C23	8.19	1.66	1.53
27	F	304	RRX	C27-C28	8.16	1.66	1.52
31	5	303	LUT	C22-C23	8.08	1.66	1.53
31	7	304	LUT	C22-C23	8.05	1.66	1.53
31	6	306	LUT	C22-C23	8.02	1.66	1.53
28	1	5005	C7Z	C4-C3	7.98	1.66	1.52
31	Z	318	LUT	C22-C23	7.94	1.66	1.53
31	3	5003	LUT	C22-C23	7.94	1.66	1.53
27	4	303	RRX	C27-C28	7.94	1.66	1.52
19	8	312	CLA	MG-NA	7.83	2.24	2.06
27	5	302	RRX	C27-C28	7.81	1.65	1.52
31	7	304	LUT	C4-C3	7.81	1.65	1.52
31	3	5003	LUT	C4-C3	7.80	1.65	1.52
31	Z	318	LUT	C4-C3	7.74	1.65	1.52
31	4	304	LUT	C4-C3	7.74	1.65	1.52
31	8	304	LUT	C22-C23	7.69	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	5005	BCR	C30-C25	-7.69	1.43	1.53
31	1	5004	LUT	C22-C23	7.67	1.65	1.53
31	3	5002	LUT	C22-C23	7.65	1.65	1.53
31	7	303	LUT	C22-C23	7.65	1.65	1.53
31	Z	317	LUT	C4-C3	7.63	1.65	1.52
31	6	305	LUT	C22-C23	7.62	1.65	1.53
31	4	304	LUT	C22-C23	7.58	1.65	1.53
31	4	304	LUT	C1-C6	-7.58	1.43	1.53
31	8	305	LUT	C22-C23	7.57	1.65	1.53
22	8	306	BCR	C30-C25	-7.54	1.43	1.53
22	6	308	BCR	C30-C25	-7.54	1.43	1.53
31	6	306	LUT	C32-C33	7.53	1.62	1.45
19	4	311	CLA	MG-NA	7.53	2.24	2.06
22	3	5005	BCR	C1-C6	-7.53	1.43	1.53
31	3	5003	LUT	C32-C33	7.51	1.62	1.45
31	8	304	LUT	C32-C33	7.50	1.62	1.45
31	7	304	LUT	C32-C33	7.49	1.62	1.45
31	1	5004	LUT	C4-C3	7.47	1.65	1.52
31	6	305	LUT	C4-C3	7.46	1.65	1.52
31	Z	317	LUT	C32-C33	7.41	1.61	1.45
31	1	5003	LUT	C22-C23	7.39	1.65	1.53
31	7	303	LUT	C4-C3	7.39	1.65	1.52
22	3	5004	BCR	C30-C25	-7.34	1.43	1.53
22	8	303	BCR	C30-C25	-7.31	1.43	1.53
31	3	5002	LUT	C4-C3	7.30	1.64	1.52
31	8	304	LUT	C4-C3	7.30	1.64	1.52
31	8	305	LUT	C4-C3	7.24	1.64	1.52
22	4	305	BCR	C1-C6	-7.24	1.43	1.53
22	5	304	BCR	C30-C25	-7.24	1.43	1.53
22	A	849	BCR	C30-C25	-7.22	1.43	1.53
31	3	5002	LUT	C32-C33	7.19	1.61	1.45
22	8	306	BCR	C1-C6	-7.19	1.43	1.53
22	5	305	BCR	C30-C25	-7.17	1.43	1.53
31	1	5003	LUT	C4-C3	7.16	1.64	1.52
31	Z	318	LUT	C32-C33	7.15	1.61	1.45
31	6	306	LUT	C4-C3	7.14	1.64	1.52
31	5	303	LUT	C4-C3	7.13	1.64	1.52
22	3	5006	BCR	C30-C25	-7.08	1.44	1.53
22	4	305	BCR	C30-C25	-7.07	1.44	1.53
31	Z	318	LUT	C1-C6	-7.07	1.44	1.53
22	G	1603	BCR	C30-C25	-7.04	1.44	1.53
22	5	304	BCR	C1-C6	-7.03	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	4	303	RRX	C30-C25	-7.03	1.44	1.53
31	6	305	LUT	C1-C6	-7.02	1.44	1.53
31	8	305	LUT	C1-C6	-7.01	1.44	1.53
22	6	307	BCR	C30-C25	-7.00	1.44	1.53
22	8	306	BCR	C2-C3	-6.98	1.35	1.52
31	3	5003	LUT	C1-C6	-6.98	1.44	1.53
22	K	206	BCR	C30-C25	-6.96	1.44	1.53
31	7	303	LUT	C1-C6	-6.95	1.44	1.53
22	A	850	BCR	C30-C25	-6.95	1.44	1.53
22	A	849	BCR	C1-C6	-6.94	1.44	1.53
31	3	5002	LUT	C1-C6	-6.94	1.44	1.53
22	A	858	BCR	C30-C25	-6.93	1.44	1.53
31	4	304	LUT	C32-C33	6.93	1.60	1.45
31	1	5003	LUT	C32-C33	6.92	1.60	1.45
38	6	326	ERG	C16-C17	-6.92	1.40	1.54
22	B	842	BCR	C30-C25	-6.91	1.44	1.53
22	B	843	BCR	C30-C25	-6.91	1.44	1.53
22	5	304	BCR	C2-C3	-6.89	1.35	1.52
31	5	303	LUT	C1-C6	-6.88	1.44	1.53
31	6	305	LUT	C32-C33	6.85	1.60	1.45
22	6	307	BCR	C1-C6	-6.85	1.44	1.53
22	3	5007	BCR	C30-C25	-6.84	1.44	1.53
31	1	5004	LUT	C32-C33	6.84	1.60	1.45
22	6	308	BCR	C2-C3	-6.84	1.35	1.52
22	A	847	BCR	C30-C25	-6.84	1.44	1.53
27	5	302	RRX	C2-C3	-6.84	1.35	1.52
22	5	305	BCR	C1-C6	-6.84	1.44	1.53
22	5	305	BCR	C2-C3	-6.82	1.35	1.52
22	A	848	BCR	C30-C25	-6.82	1.44	1.53
22	3	5004	BCR	C2-C3	-6.82	1.35	1.52
22	B	845	BCR	C30-C25	-6.82	1.44	1.53
27	5	302	RRX	C30-C25	-6.81	1.44	1.53
22	B	846	BCR	C30-C25	-6.80	1.44	1.53
31	8	304	LUT	C1-C6	-6.79	1.44	1.53
22	B	847	BCR	C30-C25	-6.79	1.44	1.53
22	3	5004	BCR	C1-C6	-6.79	1.44	1.53
27	4	303	RRX	C2-C3	-6.79	1.35	1.52
22	4	305	BCR	C2-C3	-6.78	1.35	1.52
22	A	848	BCR	C1-C6	-6.77	1.44	1.53
22	6	307	BCR	C2-C3	-6.77	1.35	1.52
31	5	303	LUT	C32-C33	6.76	1.60	1.45
22	6	308	BCR	C1-C6	-6.75	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	303	LUT	C32-C33	6.75	1.60	1.45
22	A	847	BCR	C2-C3	-6.75	1.35	1.52
22	F	302	BCR	C30-C25	-6.74	1.44	1.53
22	3	5005	BCR	C2-C3	-6.74	1.35	1.52
22	B	844	BCR	C2-C3	-6.74	1.35	1.52
22	A	859	BCR	C30-C25	-6.72	1.44	1.53
31	7	304	LUT	C1-C6	-6.71	1.44	1.53
31	1	5004	LUT	C1-C6	-6.71	1.44	1.53
22	F	302	BCR	C2-C3	-6.69	1.36	1.52
38	8	325	ERG	C16-C17	-6.68	1.40	1.54
22	A	846	BCR	C30-C25	-6.68	1.44	1.53
19	4	307	CLA	MG-NA	6.66	2.22	2.06
22	A	859	BCR	C1-C6	-6.64	1.44	1.53
31	8	305	LUT	C32-C33	6.64	1.60	1.45
31	6	306	LUT	C1-C6	-6.63	1.44	1.53
22	B	842	BCR	C2-C3	-6.63	1.36	1.52
22	G	1603	BCR	C2-C3	-6.63	1.36	1.52
22	A	850	BCR	C1-C6	-6.63	1.44	1.53
22	3	5007	BCR	C29-C28	-6.60	1.36	1.52
22	A	846	BCR	C2-C3	-6.59	1.36	1.52
31	1	5003	LUT	C1-C6	-6.59	1.44	1.53
22	5	305	BCR	C29-C28	-6.56	1.36	1.52
22	8	303	BCR	C1-C6	-6.55	1.44	1.53
31	Z	317	LUT	C1-C6	-6.55	1.44	1.53
27	F	304	RRX	C2-C3	-6.54	1.36	1.52
22	6	308	BCR	C29-C28	-6.54	1.36	1.52
22	A	849	BCR	C2-C3	-6.54	1.36	1.52
22	B	843	BCR	C2-C3	-6.54	1.36	1.52
22	B	847	BCR	C2-C3	-6.53	1.36	1.52
22	B	846	BCR	C2-C3	-6.52	1.36	1.52
22	K	206	BCR	C2-C3	-6.51	1.36	1.52
22	B	844	BCR	C30-C25	-6.51	1.44	1.53
22	5	304	BCR	C29-C28	-6.51	1.36	1.52
22	3	5004	BCR	C29-C28	-6.51	1.36	1.52
22	A	859	BCR	C2-C3	-6.50	1.36	1.52
22	7	305	BCR	C30-C25	-6.49	1.44	1.53
22	8	303	BCR	C2-C3	-6.49	1.36	1.52
22	A	858	BCR	C2-C3	-6.48	1.36	1.52
22	6	307	BCR	C29-C28	-6.47	1.36	1.52
27	F	304	RRX	C30-C25	-6.46	1.44	1.53
22	B	843	BCR	C1-C6	-6.45	1.44	1.53
22	K	206	BCR	C1-C6	-6.45	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	844	BCR	C1-C6	-6.44	1.44	1.53
22	A	848	BCR	C2-C3	-6.44	1.36	1.52
22	3	5007	BCR	C1-C6	-6.43	1.44	1.53
22	3	5006	BCR	C2-C3	-6.43	1.36	1.52
22	3	5006	BCR	C1-C6	-6.42	1.45	1.53
22	4	305	BCR	C29-C28	-6.41	1.36	1.52
22	7	305	BCR	C1-C6	-6.40	1.45	1.53
22	B	845	BCR	C2-C3	-6.40	1.36	1.52
22	A	858	BCR	C1-C6	-6.39	1.45	1.53
22	A	850	BCR	C2-C3	-6.39	1.36	1.52
19	A	825	CLA	MG-NA	6.39	2.21	2.06
19	B	803	CLA	MG-NA	6.38	2.21	2.06
22	B	844	BCR	C29-C28	-6.37	1.36	1.52
22	G	1603	BCR	C1-C6	-6.36	1.45	1.53
22	B	845	BCR	C1-C6	-6.35	1.45	1.53
22	A	849	BCR	C29-C28	-6.35	1.36	1.52
22	B	846	BCR	C29-C28	-6.34	1.36	1.52
22	3	5007	BCR	C2-C3	-6.34	1.36	1.52
19	A	832	CLA	MG-NA	6.34	2.21	2.06
22	3	5005	BCR	C29-C28	-6.33	1.36	1.52
19	B	812	CLA	MG-NA	6.33	2.21	2.06
19	A	829	CLA	MG-NA	6.33	2.21	2.06
19	B	820	CLA	MG-NA	6.33	2.21	2.06
22	A	846	BCR	C29-C28	-6.33	1.36	1.52
22	7	305	BCR	C2-C3	-6.33	1.36	1.52
19	B	810	CLA	MG-NA	6.32	2.21	2.06
19	A	841	CLA	MG-NA	6.32	2.21	2.06
19	A	814	CLA	MG-NA	6.32	2.21	2.06
19	A	842	CLA	MG-NA	6.32	2.21	2.06
22	K	206	BCR	C29-C28	-6.32	1.37	1.52
19	B	807	CLA	MG-NA	6.31	2.21	2.06
19	A	820	CLA	MG-NA	6.31	2.21	2.06
22	A	859	BCR	C29-C28	-6.31	1.37	1.52
19	B	813	CLA	MG-NA	6.31	2.21	2.06
19	B	826	CLA	MG-NA	6.31	2.21	2.06
19	B	824	CLA	MG-NA	6.31	2.21	2.06
19	B	839	CLA	MG-NA	6.31	2.21	2.06
19	1	5016	CLA	MG-NA	6.31	2.21	2.06
19	A	802	CLA	MG-NA	6.31	2.21	2.06
19	B	811	CLA	MG-NA	6.30	2.21	2.06
19	B	804	CLA	MG-NA	6.30	2.21	2.06
19	B	827	CLA	MG-NA	6.30	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	5018	CLA	MG-NA	6.30	2.21	2.06
19	A	834	CLA	MG-NA	6.30	2.21	2.06
38	8	325	ERG	C6-C5	6.30	1.48	1.33
19	A	824	CLA	MG-NA	6.30	2.21	2.06
19	B	823	CLA	MG-NA	6.30	2.21	2.06
19	4	318	CLA	MG-NA	6.30	2.21	2.06
22	7	305	BCR	C29-C28	-6.30	1.37	1.52
19	A	809	CLA	MG-NA	6.29	2.21	2.06
19	G	1601	CLA	MG-NA	6.29	2.21	2.06
19	A	816	CLA	MG-NA	6.29	2.21	2.06
19	B	828	CLA	MG-NA	6.29	2.21	2.06
19	1	5012	CLA	MG-NA	6.29	2.21	2.06
19	K	204	CLA	MG-NA	6.29	2.21	2.06
19	A	826	CLA	MG-NA	6.29	2.21	2.06
19	B	822	CLA	MG-NA	6.28	2.21	2.06
19	G	1602	CLA	MG-NA	6.28	2.21	2.06
19	K	203	CLA	MG-NA	6.28	2.21	2.06
19	B	821	CLA	MG-NA	6.28	2.21	2.06
19	B	829	CLA	MG-NA	6.28	2.21	2.06
19	B	837	CLA	MG-NA	6.28	2.21	2.06
22	F	302	BCR	C29-C28	-6.28	1.37	1.52
19	A	817	CLA	MG-NA	6.28	2.21	2.06
19	5	312	CLA	MG-NA	6.28	2.21	2.06
19	B	805	CLA	MG-NA	6.28	2.21	2.06
19	A	803	CLA	MG-NA	6.28	2.21	2.06
19	A	806	CLA	MG-NA	6.27	2.21	2.06
19	3	5010	CLA	MG-NA	6.27	2.21	2.06
22	B	842	BCR	C1-C6	-6.27	1.45	1.53
19	6	314	CLA	MG-NA	6.27	2.21	2.06
22	F	302	BCR	C1-C6	-6.27	1.45	1.53
19	A	833	CLA	MG-NA	6.27	2.21	2.06
22	B	842	BCR	C29-C28	-6.27	1.37	1.52
19	B	816	CLA	MG-NA	6.27	2.21	2.06
19	6	302	CLA	MG-NA	6.27	2.21	2.06
19	A	818	CLA	MG-NA	6.27	2.21	2.06
22	8	306	BCR	C29-C28	-6.27	1.37	1.52
19	A	807	CLA	MG-NA	6.27	2.21	2.06
19	A	857	CLA	MG-NA	6.26	2.21	2.06
19	K	205	CLA	MG-NA	6.26	2.21	2.06
19	F	303	CLA	MG-NA	6.26	2.21	2.06
19	A	827	CLA	MG-NA	6.26	2.21	2.06
19	7	312	CLA	MG-NA	6.26	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	202	CLA	MG-NA	6.26	2.21	2.06
19	5	322	CLA	MG-NA	6.26	2.21	2.06
19	A	813	CLA	MG-NA	6.26	2.21	2.06
19	B	819	CLA	MG-NA	6.26	2.21	2.06
19	B	835	CLA	MG-NA	6.25	2.21	2.06
19	A	831	CLA	MG-NA	6.25	2.21	2.06
19	4	312	CLA	MG-NA	6.25	2.21	2.06
19	B	834	CLA	MG-NA	6.25	2.21	2.06
19	B	833	CLA	MG-NA	6.25	2.21	2.06
19	B	830	CLA	MG-NA	6.25	2.21	2.06
22	A	848	BCR	C29-C28	-6.25	1.37	1.52
19	B	814	CLA	MG-NA	6.24	2.21	2.06
19	J	1901	CLA	MG-NA	6.24	2.21	2.06
19	B	809	CLA	MG-NA	6.24	2.21	2.06
19	7	319	CLA	MG-NA	6.24	2.21	2.06
19	Z	314	CLA	MG-NA	6.24	2.21	2.06
19	A	804	CLA	MG-NA	6.24	2.21	2.06
19	A	837	CLA	MG-NA	6.24	2.21	2.06
19	A	808	CLA	MG-NA	6.24	2.21	2.06
19	B	806	CLA	MG-NA	6.24	2.21	2.06
19	5	301	CLA	MG-NA	6.24	2.21	2.06
19	7	318	CLA	MG-NA	6.24	2.21	2.06
19	8	320	CLA	MG-NA	6.23	2.21	2.06
19	A	811	CLA	MG-NA	6.23	2.21	2.06
19	A	823	CLA	MG-NA	6.23	2.21	2.06
22	G	1603	BCR	C29-C28	-6.22	1.37	1.52
19	B	802	CLA	MG-NA	6.22	2.21	2.06
19	3	5016	CLA	MG-NA	6.22	2.21	2.06
19	6	323	CLA	MG-NA	6.22	2.21	2.06
19	B	801	CLA	MG-NA	6.22	2.21	2.06
19	3	5014	CLA	MG-NA	6.22	2.21	2.06
19	A	828	CLA	MG-NA	6.21	2.21	2.06
19	7	309	CLA	MG-NA	6.21	2.21	2.06
22	A	858	BCR	C29-C28	-6.21	1.37	1.52
38	6	326	ERG	C6-C5	6.21	1.48	1.33
19	A	843	CLA	MG-NA	6.21	2.21	2.06
22	A	846	BCR	C1-C6	-6.21	1.45	1.53
19	B	818	CLA	MG-NA	6.21	2.21	2.06
19	A	819	CLA	MG-NA	6.20	2.21	2.06
19	I	201	CLA	MG-NA	6.20	2.21	2.06
19	B	838	CLA	MG-NA	6.20	2.21	2.06
19	4	316	CLA	MG-NA	6.20	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	5011	CLA	MG-NA	6.20	2.21	2.06
19	A	839	CLA	MG-NA	6.20	2.21	2.06
22	A	847	BCR	C29-C28	-6.20	1.37	1.52
19	A	830	CLA	MG-NA	6.20	2.21	2.06
19	B	815	CLA	MG-NA	6.20	2.21	2.06
19	A	838	CLA	MG-NA	6.19	2.21	2.06
27	4	303	RRX	C1-C6	-6.19	1.45	1.53
19	A	822	CLA	MG-NA	6.19	2.21	2.06
19	B	817	CLA	MG-NA	6.19	2.21	2.06
19	B	832	CLA	MG-NA	6.19	2.21	2.06
19	A	836	CLA	MG-NA	6.18	2.21	2.06
19	A	835	CLA	MG-NA	6.18	2.21	2.06
19	B	808	CLA	MG-NA	6.18	2.20	2.06
22	8	303	BCR	C12-C13	6.16	1.59	1.45
19	8	313	CLA	MG-NA	6.16	2.20	2.06
19	4	308	CLA	MG-NA	6.16	2.20	2.06
22	8	303	BCR	C29-C28	-6.15	1.37	1.52
19	6	309	CLA	MG-NA	6.15	2.20	2.06
22	B	845	BCR	C29-C28	-6.15	1.37	1.52
19	8	310	CLA	MG-NA	6.15	2.20	2.06
19	A	805	CLA	MG-NA	6.14	2.20	2.06
19	Z	307	CLA	MG-NA	6.14	2.20	2.06
22	A	847	BCR	C1-C6	-6.14	1.45	1.53
19	3	5009	CLA	MG-NA	6.13	2.20	2.06
19	7	311	CLA	MG-NA	6.13	2.20	2.06
19	Z	312	CLA	MG-NA	6.13	2.20	2.06
19	3	5008	CLA	MG-NA	6.12	2.20	2.06
19	7	308	CLA	MG-NA	6.12	2.20	2.06
19	6	312	CLA	MG-NA	6.12	2.20	2.06
19	A	821	CLA	MG-NA	6.11	2.20	2.06
19	4	313	CLA	MG-NA	6.10	2.20	2.06
19	4	310	CLA	MG-NA	6.09	2.20	2.06
19	F	301	CLA	MG-NA	6.09	2.20	2.06
38	6	326	ERG	C12-C11	-6.09	1.40	1.53
19	A	840	CLA	MG-NA	6.09	2.20	2.06
19	1	5008	CLA	MG-NA	6.08	2.20	2.06
19	6	320	CLA	MG-NA	6.08	2.20	2.06
19	5	325	CLA	MG-NA	6.08	2.20	2.06
19	6	318	CLA	MG-NA	6.08	2.20	2.06
22	A	850	BCR	C29-C28	-6.08	1.37	1.52
19	5	314	CLA	MG-NA	6.07	2.20	2.06
19	Z	304	CLA	MG-NA	6.06	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	303	CLA	MG-NA	6.05	2.20	2.06
19	6	310	CLA	MG-NA	6.05	2.20	2.06
19	1	5010	CLA	MG-NA	6.05	2.20	2.06
19	3	5020	CLA	MG-NA	6.04	2.20	2.06
19	8	311	CLA	MG-NA	6.03	2.20	2.06
28	6	304	C7Z	C12-C13	6.03	1.58	1.45
19	6	313	CLA	MG-NA	6.03	2.20	2.06
19	A	810	CLA	MG-NA	6.02	2.20	2.06
22	3	5006	BCR	C29-C28	-6.02	1.37	1.52
19	5	308	CLA	MG-NA	6.02	2.20	2.06
22	B	843	BCR	C29-C28	-6.02	1.37	1.52
19	5	313	CLA	MG-NA	6.02	2.20	2.06
19	8	309	CLA	MG-NA	6.02	2.20	2.06
19	6	311	CLA	MG-NA	6.01	2.20	2.06
19	4	306	CLA	MG-NA	6.00	2.20	2.06
19	7	317	CLA	MG-NA	5.99	2.20	2.06
19	5	311	CLA	MG-NA	5.99	2.20	2.06
28	J	1902	C7Z	C12-C13	5.98	1.58	1.45
19	6	322	CLA	MG-NA	5.98	2.20	2.06
19	B	850	CLA	MG-NA	5.98	2.20	2.06
19	1	5015	CLA	MG-NA	5.97	2.20	2.06
19	7	316	CLA	MG-NA	5.97	2.20	2.06
22	B	847	BCR	C29-C28	-5.97	1.37	1.52
19	Z	315	CLA	MG-NA	5.97	2.20	2.06
19	3	5012	CLA	MG-NA	5.97	2.20	2.06
19	7	306	CLA	MG-NA	5.96	2.20	2.06
19	A	812	CLA	MG-NA	5.96	2.20	2.06
19	7	313	CLA	MG-NA	5.96	2.20	2.06
27	F	304	RRX	C19-C18	5.96	1.58	1.45
19	B	825	CLA	MG-NA	5.96	2.20	2.06
19	Z	306	CLA	MG-NA	5.95	2.20	2.06
19	8	308	CLA	MG-NA	5.95	2.20	2.06
19	8	314	CLA	MG-NA	5.94	2.20	2.06
19	5	309	CLA	MG-NA	5.94	2.20	2.06
19	5	306	CLA	MG-NA	5.93	2.20	2.06
19	5	321	CLA	MG-NA	5.93	2.20	2.06
19	B	840	CLA	MG-NA	5.93	2.20	2.06
19	3	5019	CLA	MG-NA	5.93	2.20	2.06
22	B	846	BCR	C1-C6	-5.93	1.45	1.53
19	3	5015	CLA	MG-NA	5.92	2.20	2.06
19	Z	305	CLA	MG-NA	5.92	2.20	2.06
19	8	307	CLA	MG-NA	5.92	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	7	307	CLA	MG-NA	5.91	2.20	2.06
19	1	5006	CLA	MG-NA	5.91	2.20	2.06
19	8	318	CLA	MG-NA	5.91	2.20	2.06
19	5	319	CLA	MG-NA	5.91	2.20	2.06
19	3	5013	CLA	MG-NA	5.91	2.20	2.06
19	Z	311	CLA	MG-NA	5.90	2.20	2.06
38	6	326	ERG	C7-C6	5.90	1.58	1.41
19	6	301	CLA	MG-NA	5.89	2.20	2.06
22	3	5006	BCR	C12-C13	5.89	1.58	1.45
19	3	5018	CLA	MG-NA	5.88	2.20	2.06
19	7	324	CLA	MG-NA	5.88	2.20	2.06
19	7	310	CLA	MG-NA	5.88	2.20	2.06
19	3	5011	CLA	MG-NA	5.87	2.20	2.06
19	1	5013	CLA	MG-NA	5.87	2.20	2.06
19	A	815	CLA	MG-NA	5.87	2.20	2.06
22	A	850	BCR	C12-C13	5.86	1.58	1.45
19	5	307	CLA	MG-NA	5.85	2.20	2.06
19	5	310	CLA	MG-NA	5.85	2.20	2.06
22	B	844	BCR	C12-C13	5.83	1.58	1.45
22	B	843	BCR	C12-C13	5.82	1.58	1.45
38	8	325	ERG	C12-C11	-5.82	1.41	1.53
19	Z	308	CLA	MG-NA	5.81	2.20	2.06
19	1	5007	CLA	MG-NA	5.80	2.20	2.06
19	B	836	CLA	MG-NA	5.80	2.20	2.06
22	4	305	BCR	C12-C13	5.79	1.58	1.45
22	B	847	BCR	C1-C6	-5.79	1.45	1.53
22	B	847	BCR	C12-C13	5.79	1.58	1.45
22	A	859	BCR	C12-C13	5.78	1.58	1.45
28	1	5005	C7Z	C12-C13	5.78	1.58	1.45
19	5	317	CLA	MG-NA	5.77	2.20	2.06
27	5	302	RRX	C1-C6	-5.77	1.45	1.53
22	B	842	BCR	C12-C13	5.76	1.58	1.45
22	A	858	BCR	C12-C13	5.76	1.58	1.45
19	B	831	CLA	MG-NA	5.75	2.19	2.06
22	B	845	BCR	C12-C13	5.75	1.58	1.45
19	4	309	CLA	MG-NA	5.75	2.19	2.06
22	A	847	BCR	C12-C13	5.73	1.58	1.45
38	8	325	ERG	C7-C6	5.72	1.58	1.41
22	A	846	BCR	C12-C13	5.69	1.58	1.45
22	F	302	BCR	C12-C13	5.69	1.58	1.45
22	A	848	BCR	C12-C13	5.68	1.58	1.45
22	3	5007	BCR	C12-C13	5.65	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	844	BCR	C8-C9	5.62	1.58	1.45
22	6	308	BCR	C12-C13	5.62	1.58	1.45
22	G	1603	BCR	C12-C13	5.60	1.58	1.45
22	8	303	BCR	C8-C9	5.60	1.58	1.45
27	5	302	RRX	C19-C18	5.59	1.58	1.45
22	K	206	BCR	C12-C13	5.59	1.58	1.45
28	6	304	C7Z	C1-C6	-5.59	1.46	1.53
22	5	305	BCR	C12-C13	5.57	1.57	1.45
22	B	843	BCR	C8-C9	5.55	1.57	1.45
22	B	846	BCR	C12-C13	5.53	1.57	1.45
22	8	306	BCR	C12-C13	5.53	1.57	1.45
22	6	307	BCR	C12-C13	5.52	1.57	1.45
22	A	850	BCR	C8-C9	5.52	1.57	1.45
22	B	845	BCR	C8-C9	5.51	1.57	1.45
22	A	858	BCR	C8-C9	5.51	1.57	1.45
22	5	304	BCR	C12-C13	5.51	1.57	1.45
22	B	843	BCR	C23-C22	5.50	1.57	1.45
22	A	849	BCR	C12-C13	5.50	1.57	1.45
22	B	847	BCR	C8-C9	5.50	1.57	1.45
22	3	5006	BCR	C8-C9	5.49	1.57	1.45
22	B	842	BCR	C8-C9	5.48	1.57	1.45
27	4	303	RRX	C19-C18	5.47	1.57	1.45
22	7	305	BCR	C12-C13	5.46	1.57	1.45
22	F	302	BCR	C8-C9	5.44	1.57	1.45
22	A	848	BCR	C8-C9	5.44	1.57	1.45
22	A	859	BCR	C8-C9	5.44	1.57	1.45
22	B	842	BCR	C23-C22	5.43	1.57	1.45
22	3	5004	BCR	C12-C13	5.43	1.57	1.45
22	A	846	BCR	C8-C9	5.43	1.57	1.45
27	F	304	RRX	C1-C6	-5.41	1.46	1.53
22	4	305	BCR	C8-C9	5.38	1.57	1.45
22	5	304	BCR	C8-C9	5.37	1.57	1.45
22	A	847	BCR	C8-C9	5.37	1.57	1.45
22	K	206	BCR	C8-C9	5.36	1.57	1.45
22	3	5007	BCR	C23-C22	5.35	1.57	1.45
22	B	847	BCR	C23-C22	5.35	1.57	1.45
28	1	5005	C7Z	C1-C6	-5.35	1.46	1.53
22	B	843	BCR	C29-C30	5.34	1.66	1.54
22	B	847	BCR	C29-C30	5.34	1.66	1.54
22	G	1603	BCR	C8-C9	5.33	1.57	1.45
22	8	303	BCR	C23-C22	5.33	1.57	1.45
22	A	850	BCR	C29-C30	5.33	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	307	BCR	C8-C9	5.33	1.57	1.45
38	6	326	ERG	C12-C13	5.33	1.63	1.54
22	F	302	BCR	C23-C22	5.30	1.57	1.45
22	3	5007	BCR	C8-C9	5.30	1.57	1.45
22	3	5006	BCR	C29-C30	5.30	1.66	1.54
22	B	844	BCR	C23-C22	5.30	1.57	1.45
22	A	858	BCR	C23-C22	5.29	1.57	1.45
22	A	858	BCR	C29-C30	5.29	1.66	1.54
22	6	308	BCR	C8-C9	5.29	1.57	1.45
22	A	850	BCR	C23-C22	5.28	1.57	1.45
22	A	859	BCR	C29-C30	5.27	1.66	1.54
22	A	859	BCR	C23-C22	5.27	1.57	1.45
22	B	846	BCR	C23-C22	5.26	1.57	1.45
22	A	846	BCR	C23-C22	5.26	1.57	1.45
22	B	844	BCR	C29-C30	5.25	1.66	1.54
22	7	305	BCR	C8-C9	5.25	1.57	1.45
22	B	846	BCR	C8-C9	5.25	1.57	1.45
22	A	847	BCR	C29-C30	5.25	1.66	1.54
22	B	845	BCR	C29-C30	5.25	1.66	1.54
22	G	1603	BCR	C23-C22	5.25	1.57	1.45
22	7	305	BCR	C23-C22	5.25	1.57	1.45
22	A	846	BCR	C29-C30	5.24	1.66	1.54
31	3	5002	LUT	C4-C5	-5.24	1.42	1.51
22	3	5006	BCR	C23-C22	5.23	1.57	1.45
22	3	5005	BCR	C12-C13	5.23	1.57	1.45
22	7	305	BCR	C29-C30	5.22	1.66	1.54
22	A	849	BCR	C8-C9	5.22	1.57	1.45
22	A	848	BCR	C29-C30	5.22	1.66	1.54
31	8	304	LUT	C4-C5	-5.21	1.43	1.51
22	B	845	BCR	C23-C22	5.21	1.57	1.45
22	F	302	BCR	C29-C30	5.21	1.66	1.54
22	A	848	BCR	C23-C22	5.21	1.57	1.45
22	4	305	BCR	C29-C30	5.20	1.66	1.54
22	A	847	BCR	C23-C22	5.20	1.57	1.45
31	8	305	LUT	C4-C5	-5.20	1.43	1.51
31	5	303	LUT	C4-C5	-5.19	1.43	1.51
22	8	306	BCR	C8-C9	5.18	1.57	1.45
22	K	206	BCR	C29-C30	5.18	1.66	1.54
22	K	206	BCR	C23-C22	5.17	1.57	1.45
22	8	303	BCR	C29-C30	5.16	1.66	1.54
22	G	1603	BCR	C29-C30	5.16	1.66	1.54
18	A	801	CL0	CHC-C1C	5.15	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	846	BCR	C29-C30	5.15	1.66	1.54
31	7	304	LUT	C4-C5	-5.14	1.43	1.51
18	A	801	CL0	O2D-CGD	5.14	1.45	1.33
22	A	849	BCR	C29-C30	5.12	1.65	1.54
22	B	842	BCR	C29-C30	5.10	1.65	1.54
18	A	801	CL0	O2A-C1	5.10	1.60	1.46
22	3	5005	BCR	C29-C30	5.08	1.65	1.54
31	1	5003	LUT	C4-C5	-5.08	1.43	1.51
28	J	1902	C7Z	C1-C6	-5.06	1.46	1.53
31	1	5004	LUT	C4-C5	-5.06	1.43	1.51
31	6	305	LUT	C4-C5	-5.04	1.43	1.51
22	6	307	BCR	C29-C30	5.03	1.65	1.54
31	Z	317	LUT	C4-C5	-5.02	1.43	1.51
31	6	306	LUT	C4-C5	-5.02	1.43	1.51
22	3	5007	BCR	C29-C30	5.02	1.65	1.54
22	3	5004	BCR	C8-C9	5.01	1.56	1.45
22	5	305	BCR	C8-C9	5.00	1.56	1.45
22	5	304	BCR	C23-C22	5.00	1.56	1.45
22	6	308	BCR	C29-C30	4.99	1.65	1.54
22	A	849	BCR	C23-C22	4.98	1.56	1.45
28	6	304	C7Z	C24-C25	-4.98	1.43	1.51
27	F	304	RRX	C8-C9	4.98	1.56	1.45
31	7	303	LUT	C4-C5	-4.98	1.43	1.51
38	8	325	ERG	C12-C13	4.98	1.63	1.54
22	3	5004	BCR	C29-C30	4.98	1.65	1.54
22	8	306	BCR	C29-C30	4.97	1.65	1.54
22	5	305	BCR	C23-C22	4.96	1.56	1.45
31	3	5003	LUT	C4-C5	-4.95	1.43	1.51
22	6	307	BCR	C23-C22	4.94	1.56	1.45
22	8	303	BCR	C15-C14	4.93	1.58	1.43
27	F	304	RRX	C2-C1	4.93	1.65	1.54
22	5	305	BCR	C29-C30	4.93	1.65	1.54
31	Z	317	LUT	C8-C9	4.91	1.56	1.45
27	5	302	RRX	C2-C1	4.90	1.65	1.54
31	4	304	LUT	C4-C5	-4.89	1.43	1.51
22	8	303	BCR	C19-C18	4.89	1.56	1.45
22	B	847	BCR	C15-C14	4.88	1.58	1.43
22	B	846	BCR	C19-C18	4.86	1.56	1.45
28	1	5005	C7Z	C24-C25	-4.86	1.43	1.51
27	F	304	RRX	C23-C22	4.86	1.56	1.45
28	J	1902	C7Z	C24-C25	-4.85	1.43	1.51
22	B	842	BCR	C15-C14	4.85	1.58	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Z	317	LUT	C12-C13	4.83	1.56	1.45
22	B	843	BCR	C15-C14	4.83	1.58	1.43
22	A	850	BCR	C15-C14	4.82	1.58	1.43
22	4	305	BCR	C23-C22	4.81	1.56	1.45
22	3	5007	BCR	C2-C1	4.80	1.65	1.54
22	B	844	BCR	C15-C14	4.80	1.58	1.43
22	5	304	BCR	C29-C30	4.79	1.65	1.54
22	A	859	BCR	C15-C14	4.78	1.58	1.43
22	3	5005	BCR	C8-C9	4.78	1.56	1.45
22	A	846	BCR	C15-C14	4.78	1.58	1.43
22	6	308	BCR	C23-C22	4.77	1.56	1.45
22	A	858	BCR	C15-C14	4.77	1.58	1.43
22	5	304	BCR	C15-C14	4.76	1.58	1.43
22	4	305	BCR	C15-C14	4.76	1.58	1.43
22	B	842	BCR	C19-C18	4.76	1.56	1.45
22	3	5005	BCR	C23-C22	4.74	1.56	1.45
22	3	5006	BCR	C15-C14	4.74	1.58	1.43
27	5	302	RRX	C8-C9	4.73	1.56	1.45
22	6	308	BCR	C15-C14	4.73	1.58	1.43
22	F	302	BCR	C15-C14	4.73	1.58	1.43
22	A	848	BCR	C15-C14	4.71	1.58	1.43
22	B	845	BCR	C15-C14	4.71	1.58	1.43
22	K	206	BCR	C15-C14	4.71	1.58	1.43
22	B	843	BCR	C19-C18	4.71	1.56	1.45
28	6	304	C7Z	C28-C29	4.70	1.56	1.45
22	B	846	BCR	C2-C1	4.70	1.65	1.54
22	6	307	BCR	C15-C14	4.70	1.58	1.43
22	A	850	BCR	C2-C1	4.69	1.64	1.54
22	A	849	BCR	C15-C14	4.69	1.58	1.43
22	A	847	BCR	C15-C14	4.69	1.58	1.43
22	B	844	BCR	C19-C18	4.68	1.56	1.45
22	G	1603	BCR	C15-C14	4.67	1.57	1.43
18	A	801	CL0	CHD-C1D	4.67	1.47	1.38
22	A	858	BCR	C2-C1	4.67	1.64	1.54
22	B	846	BCR	C15-C14	4.67	1.57	1.43
18	A	801	CL0	C3B-C2B	4.67	1.46	1.40
22	A	848	BCR	C2-C1	4.67	1.64	1.54
31	8	304	LUT	C31-C30	4.66	1.57	1.43
22	A	850	BCR	C19-C18	4.66	1.56	1.45
27	F	304	RRX	C12-C13	4.66	1.56	1.45
22	3	5007	BCR	C15-C14	4.66	1.57	1.43
31	7	304	LUT	C12-C13	4.64	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	304	LUT	C8-C9	4.64	1.55	1.45
31	7	304	LUT	C8-C9	4.64	1.55	1.45
22	8	303	BCR	C2-C1	4.64	1.64	1.54
31	Z	318	LUT	C4-C5	-4.64	1.43	1.51
22	B	845	BCR	C2-C1	4.64	1.64	1.54
22	7	305	BCR	C15-C14	4.64	1.57	1.43
22	A	846	BCR	C19-C18	4.64	1.55	1.45
28	1	5005	C7Z	C28-C29	4.63	1.55	1.45
22	3	5006	BCR	C2-C1	4.62	1.64	1.54
31	6	306	LUT	C8-C9	4.62	1.55	1.45
31	8	304	LUT	C12-C13	4.61	1.55	1.45
22	A	849	BCR	C2-C1	4.61	1.64	1.54
18	A	801	CL0	C3C-C2C	4.60	1.46	1.36
31	3	5003	LUT	C8-C9	4.60	1.55	1.45
22	3	5006	BCR	C19-C18	4.60	1.55	1.45
27	4	303	RRX	C8-C9	4.60	1.55	1.45
22	7	305	BCR	C2-C1	4.59	1.64	1.54
22	K	206	BCR	C19-C18	4.59	1.55	1.45
22	5	305	BCR	C19-C18	4.59	1.55	1.45
22	G	1603	BCR	C19-C18	4.59	1.55	1.45
28	J	1902	C7Z	C28-C29	4.59	1.55	1.45
22	6	308	BCR	C19-C18	4.59	1.55	1.45
22	B	843	BCR	C2-C1	4.58	1.64	1.54
22	A	858	BCR	C19-C18	4.58	1.55	1.45
22	A	847	BCR	C19-C18	4.58	1.55	1.45
27	F	304	RRX	C24-C25	4.57	1.61	1.45
22	B	845	BCR	C19-C18	4.57	1.55	1.45
22	B	847	BCR	C19-C18	4.57	1.55	1.45
19	8	312	CLA	C1C-NC	-4.57	1.31	1.37
22	F	302	BCR	C19-C18	4.57	1.55	1.45
31	3	5003	LUT	C12-C13	4.57	1.55	1.45
22	7	305	BCR	C19-C18	4.56	1.55	1.45
22	8	306	BCR	C15-C14	4.56	1.57	1.43
22	A	859	BCR	C19-C18	4.55	1.55	1.45
22	K	206	BCR	C2-C1	4.55	1.64	1.54
22	4	305	BCR	C19-C18	4.55	1.55	1.45
31	Z	317	LUT	C15-C14	4.55	1.57	1.43
22	8	306	BCR	C23-C22	4.54	1.55	1.45
27	4	303	RRX	C2-C1	4.54	1.64	1.54
22	A	846	BCR	C2-C1	4.54	1.64	1.54
22	5	304	BCR	C19-C18	4.53	1.55	1.45
31	Z	317	LUT	C35-C34	4.53	1.57	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	1603	BCR	C2-C1	4.52	1.64	1.54
22	B	842	BCR	C2-C1	4.51	1.64	1.54
22	F	302	BCR	C2-C1	4.51	1.64	1.54
22	A	859	BCR	C2-C1	4.51	1.64	1.54
31	3	5002	LUT	C8-C9	4.50	1.55	1.45
22	A	848	BCR	C19-C18	4.50	1.55	1.45
22	3	5004	BCR	C15-C14	4.50	1.57	1.43
22	B	847	BCR	C2-C1	4.49	1.64	1.54
31	8	304	LUT	C15-C14	4.49	1.57	1.43
27	5	302	RRX	C23-C22	4.48	1.55	1.45
22	B	844	BCR	C2-C1	4.48	1.64	1.54
22	3	5004	BCR	C23-C22	4.48	1.55	1.45
22	5	305	BCR	C15-C14	4.48	1.57	1.43
22	3	5004	BCR	C2-C1	4.48	1.64	1.54
22	3	5007	BCR	C19-C18	4.48	1.55	1.45
38	6	326	ERG	C13-C17	4.47	1.63	1.55
28	1	5005	C7Z	C31-C30	4.46	1.57	1.43
28	6	304	C7Z	C31-C30	4.46	1.57	1.43
28	J	1902	C7Z	C31-C30	4.46	1.57	1.43
22	A	847	BCR	C2-C1	4.46	1.64	1.54
31	4	304	LUT	C8-C9	4.46	1.55	1.45
22	3	5005	BCR	C15-C14	4.45	1.57	1.43
31	1	5003	LUT	C8-C9	4.44	1.55	1.45
31	3	5003	LUT	C31-C30	4.44	1.57	1.43
27	4	303	RRX	C23-C22	4.43	1.55	1.45
31	6	306	LUT	C12-C13	4.43	1.55	1.45
31	5	303	LUT	C8-C9	4.40	1.55	1.45
22	8	303	BCR	C28-C27	4.40	1.66	1.52
27	5	302	RRX	C24-C25	4.40	1.60	1.45
31	7	304	LUT	C31-C30	4.39	1.57	1.43
31	6	306	LUT	C31-C30	4.38	1.57	1.43
31	8	304	LUT	C35-C34	4.38	1.57	1.43
22	3	5007	BCR	C20-C21	4.36	1.57	1.43
22	8	303	BCR	C20-C21	4.36	1.57	1.43
31	3	5002	LUT	C12-C13	4.35	1.55	1.45
31	6	306	LUT	C15-C14	4.35	1.56	1.43
18	A	801	CL0	C3D-C4D	-4.34	1.34	1.44
22	B	842	BCR	C20-C21	4.34	1.56	1.43
22	A	849	BCR	C19-C18	4.34	1.55	1.45
31	1	5004	LUT	C8-C9	4.34	1.55	1.45
22	5	304	BCR	C20-C21	4.33	1.56	1.43
31	Z	318	LUT	C8-C9	4.32	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	4	303	RRX	C24-C25	4.32	1.60	1.45
31	7	303	LUT	C8-C9	4.31	1.55	1.45
22	B	845	BCR	C28-C27	4.31	1.66	1.52
22	B	844	BCR	C20-C21	4.31	1.56	1.43
22	6	307	BCR	C2-C1	4.31	1.64	1.54
31	6	306	LUT	C35-C34	4.31	1.56	1.43
28	6	304	C7Z	C32-C33	4.31	1.55	1.45
31	Z	318	LUT	C12-C13	4.30	1.55	1.45
22	3	5006	BCR	C28-C27	4.30	1.66	1.52
22	B	843	BCR	C20-C21	4.30	1.56	1.43
22	B	842	BCR	C28-C27	4.30	1.66	1.52
31	6	305	LUT	C8-C9	4.30	1.55	1.45
22	A	850	BCR	C20-C21	4.30	1.56	1.43
31	3	5003	LUT	C15-C14	4.30	1.56	1.43
22	A	850	BCR	C28-C27	4.29	1.66	1.52
22	8	306	BCR	C2-C1	4.29	1.64	1.54
27	5	302	RRX	C12-C13	4.29	1.55	1.45
27	F	304	RRX	C3-C4	4.29	1.66	1.52
31	1	5004	LUT	C12-C13	4.29	1.55	1.45
22	G	1603	BCR	C28-C27	4.28	1.65	1.52
22	B	847	BCR	C20-C21	4.28	1.56	1.43
22	7	305	BCR	C20-C21	4.28	1.56	1.43
22	A	858	BCR	C20-C21	4.28	1.56	1.43
22	F	302	BCR	C20-C21	4.28	1.56	1.43
22	A	859	BCR	C20-C21	4.28	1.56	1.43
22	A	846	BCR	C20-C21	4.28	1.56	1.43
22	A	858	BCR	C28-C27	4.27	1.65	1.52
22	A	849	BCR	C28-C27	4.27	1.65	1.52
22	B	847	BCR	C28-C27	4.26	1.65	1.52
22	B	845	BCR	C20-C21	4.26	1.56	1.43
22	B	843	BCR	C28-C27	4.26	1.65	1.52
19	4	311	CLA	C1C-NC	-4.26	1.31	1.37
22	G	1603	BCR	C20-C21	4.26	1.56	1.43
27	4	303	RRX	C12-C13	4.25	1.55	1.45
22	5	304	BCR	C2-C1	4.25	1.63	1.54
31	7	304	LUT	C35-C34	4.25	1.56	1.43
22	3	5005	BCR	C19-C18	4.25	1.55	1.45
28	1	5005	C7Z	C32-C33	4.25	1.55	1.45
22	6	307	BCR	C19-C18	4.25	1.55	1.45
27	4	303	RRX	C3-C4	4.24	1.65	1.52
31	8	305	LUT	C8-C9	4.24	1.55	1.45
22	B	846	BCR	C20-C21	4.24	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	F	304	RRX	C11-C10	4.24	1.56	1.43
31	5	303	LUT	C12-C13	4.24	1.55	1.45
27	5	302	RRX	C27-C26	-4.23	1.44	1.51
22	K	206	BCR	C20-C21	4.22	1.56	1.43
28	J	1902	C7Z	C32-C33	4.22	1.55	1.45
31	3	5003	LUT	C35-C34	4.22	1.56	1.43
22	F	302	BCR	C28-C27	4.22	1.65	1.52
31	7	304	LUT	C15-C14	4.22	1.56	1.43
31	4	304	LUT	C12-C13	4.22	1.55	1.45
22	A	847	BCR	C28-C27	4.22	1.65	1.52
22	A	847	BCR	C20-C21	4.21	1.56	1.43
22	3	5006	BCR	C20-C21	4.21	1.56	1.43
25	B	848	DGD	O1G-C1A	4.21	1.45	1.33
22	K	206	BCR	C28-C27	4.21	1.65	1.52
22	6	308	BCR	C2-C1	4.21	1.63	1.54
22	3	5005	BCR	C2-C1	4.20	1.63	1.54
27	F	304	RRX	C29-C30	4.20	1.68	1.54
22	4	305	BCR	C20-C21	4.19	1.56	1.43
22	A	848	BCR	C28-C27	4.18	1.65	1.52
22	4	305	BCR	C2-C1	4.17	1.63	1.54
31	Z	318	LUT	C15-C14	4.17	1.56	1.43
31	4	304	LUT	C15-C14	4.17	1.56	1.43
22	B	846	BCR	C28-C27	4.17	1.65	1.52
22	8	306	BCR	C28-C27	4.16	1.65	1.52
22	A	848	BCR	C20-C21	4.15	1.56	1.43
22	5	304	BCR	C28-C27	4.15	1.65	1.52
31	Z	318	LUT	C35-C34	4.15	1.56	1.43
22	A	846	BCR	C28-C27	4.14	1.65	1.52
28	1	5005	C7Z	C4-C5	-4.14	1.44	1.51
31	3	5002	LUT	C31-C30	4.14	1.56	1.43
22	B	844	BCR	C28-C27	4.14	1.65	1.52
22	7	305	BCR	C28-C27	4.14	1.65	1.52
22	A	859	BCR	C28-C27	4.14	1.65	1.52
22	5	305	BCR	C2-C1	4.13	1.63	1.54
22	3	5005	BCR	C20-C21	4.13	1.56	1.43
19	7	307	CLA	MG-ND	-4.12	1.97	2.05
31	Z	318	LUT	C31-C30	4.11	1.56	1.43
31	3	5002	LUT	C15-C14	4.11	1.56	1.43
31	8	305	LUT	C23-C24	-4.11	1.44	1.50
22	A	849	BCR	C20-C21	4.10	1.56	1.43
31	3	5002	LUT	C35-C34	4.09	1.56	1.43
27	5	302	RRX	C11-C10	4.08	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	307	BCR	C20-C21	4.08	1.56	1.43
22	3	5005	BCR	C28-C27	4.08	1.65	1.52
19	Z	307	CLA	MG-ND	-4.07	1.97	2.05
19	1	5007	CLA	C1C-NC	-4.06	1.31	1.37
31	5	303	LUT	C23-C24	-4.06	1.44	1.50
22	4	305	BCR	C28-C27	4.06	1.65	1.52
31	4	304	LUT	C35-C34	4.06	1.56	1.43
31	6	305	LUT	C12-C13	4.05	1.54	1.45
22	6	308	BCR	C28-C27	4.05	1.65	1.52
27	5	302	RRX	C3-C4	4.05	1.65	1.52
19	Z	311	CLA	MG-ND	-4.05	1.97	2.05
31	1	5004	LUT	C23-C24	-4.04	1.44	1.50
31	4	304	LUT	C31-C30	4.04	1.56	1.43
22	8	306	BCR	C19-C18	4.03	1.54	1.45
19	B	840	CLA	MG-ND	-4.03	1.97	2.05
27	4	303	RRX	C11-C10	4.03	1.55	1.43
22	A	859	BCR	C3-C4	4.03	1.65	1.52
19	3	5020	CLA	MG-ND	-4.02	1.97	2.05
22	5	305	BCR	C20-C21	4.01	1.55	1.43
38	6	326	ERG	C16-C15	4.01	1.65	1.54
31	8	304	LUT	C28-C29	4.01	1.54	1.45
31	7	304	LUT	C28-C29	4.01	1.54	1.45
31	1	5003	LUT	C35-C34	4.01	1.55	1.43
22	5	305	BCR	C28-C27	4.00	1.65	1.52
31	Z	317	LUT	C7-C6	4.00	1.59	1.45
31	6	305	LUT	C15-C14	4.00	1.55	1.43
18	A	801	CL0	CHD-C4C	4.00	1.48	1.39
31	8	305	LUT	C12-C13	3.99	1.54	1.45
22	3	5007	BCR	C28-C27	3.99	1.65	1.52
31	Z	317	LUT	C31-C30	3.99	1.55	1.43
19	7	313	CLA	MG-ND	-3.99	1.97	2.05
19	7	324	CLA	MG-ND	-3.99	1.97	2.05
31	6	306	LUT	C21-C26	3.98	1.67	1.56
31	5	303	LUT	C15-C14	3.97	1.55	1.43
19	B	831	CLA	C1C-NC	-3.97	1.31	1.37
27	F	304	RRX	C15-C14	3.97	1.55	1.43
31	1	5003	LUT	C31-C30	3.97	1.55	1.43
22	K	206	BCR	C3-C4	3.97	1.64	1.52
19	7	307	CLA	C1C-NC	-3.97	1.31	1.37
22	7	305	BCR	C3-C4	3.97	1.64	1.52
31	3	5003	LUT	C28-C29	3.97	1.54	1.45
31	1	5003	LUT	C15-C14	3.97	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	303	BCR	C16-C17	3.96	1.55	1.43
19	1	5007	CLA	MG-ND	-3.96	1.97	2.05
31	1	5003	LUT	C12-C13	3.96	1.54	1.45
19	5	313	CLA	MG-ND	-3.96	1.97	2.05
31	1	5004	LUT	C15-C14	3.96	1.55	1.43
31	7	304	LUT	C7-C6	3.95	1.59	1.45
27	F	304	RRX	C27-C26	-3.95	1.44	1.51
22	A	848	BCR	C3-C4	3.95	1.64	1.52
22	3	5004	BCR	C19-C18	3.95	1.54	1.45
22	A	850	BCR	C3-C4	3.94	1.64	1.52
19	7	318	CLA	MG-ND	-3.94	1.98	2.05
22	6	307	BCR	C28-C27	3.94	1.64	1.52
31	6	305	LUT	C31-C30	3.94	1.55	1.43
22	A	858	BCR	C3-C4	3.94	1.64	1.52
19	4	310	CLA	MG-ND	-3.94	1.98	2.05
19	5	325	CLA	MG-ND	-3.93	1.98	2.05
31	1	5004	LUT	C35-C34	3.93	1.55	1.43
31	5	303	LUT	C31-C30	3.93	1.55	1.43
22	3	5004	BCR	C28-C27	3.93	1.64	1.52
31	7	304	LUT	C21-C26	3.93	1.67	1.56
38	8	325	ERG	C13-C17	3.93	1.62	1.55
22	B	845	BCR	C3-C4	3.93	1.64	1.52
19	Z	303	CLA	MG-ND	-3.93	1.98	2.05
19	3	5008	CLA	MG-ND	-3.93	1.98	2.05
19	3	5013	CLA	C1C-NC	-3.92	1.31	1.37
22	8	303	BCR	C3-C4	3.92	1.64	1.52
31	Z	317	LUT	C11-C10	3.92	1.55	1.43
22	B	842	BCR	C16-C17	3.91	1.55	1.43
19	6	313	CLA	MG-ND	-3.91	1.98	2.05
22	A	846	BCR	C3-C4	3.91	1.64	1.52
31	5	303	LUT	C35-C34	3.90	1.55	1.43
27	5	302	RRX	C29-C30	3.90	1.67	1.54
19	A	815	CLA	MG-ND	-3.90	1.98	2.05
22	A	849	BCR	C3-C4	3.90	1.64	1.52
28	6	304	C7Z	C4-C5	-3.90	1.45	1.51
19	3	5011	CLA	MG-ND	-3.90	1.98	2.05
32	4	317	CHL	C3B-C2B	-3.90	1.35	1.40
22	B	843	BCR	C3-C4	3.90	1.64	1.52
31	8	304	LUT	C7-C6	3.89	1.58	1.45
19	3	5015	CLA	MG-ND	-3.89	1.98	2.05
28	J	1902	C7Z	C11-C10	3.89	1.55	1.43
31	6	305	LUT	C35-C34	3.88	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	7	311	CLA	C1C-NC	-3.88	1.32	1.37
22	G	1603	BCR	C3-C4	3.88	1.64	1.52
31	Z	317	LUT	C21-C26	3.88	1.67	1.56
19	8	314	CLA	MG-ND	-3.88	1.98	2.05
19	1	5015	CLA	MG-ND	-3.88	1.98	2.05
31	7	303	LUT	C15-C14	3.88	1.55	1.43
31	1	5004	LUT	C31-C30	3.87	1.55	1.43
19	3	5019	CLA	MG-ND	-3.87	1.98	2.05
31	7	303	LUT	C12-C13	3.87	1.54	1.45
22	3	5004	BCR	C4-C5	-3.87	1.43	1.51
28	6	304	C7Z	C11-C10	3.87	1.55	1.43
19	B	831	CLA	MG-ND	-3.87	1.98	2.05
31	Z	318	LUT	C7-C6	3.87	1.58	1.45
31	6	306	LUT	C28-C29	3.86	1.54	1.45
22	3	5007	BCR	C3-C4	3.86	1.64	1.52
28	6	304	C7Z	C15-C14	3.86	1.55	1.43
31	7	303	LUT	C31-C30	3.86	1.55	1.43
22	B	842	BCR	C3-C4	3.86	1.64	1.52
27	F	304	RRX	C16-C17	3.85	1.55	1.43
19	8	313	CLA	C1C-NC	-3.85	1.32	1.37
19	3	5010	CLA	MG-ND	-3.85	1.98	2.05
28	J	1902	C7Z	C22-C21	3.85	1.66	1.54
22	4	305	BCR	C3-C4	3.85	1.64	1.52
22	3	5004	BCR	C20-C21	3.85	1.55	1.43
28	6	304	C7Z	C22-C21	3.84	1.66	1.54
19	8	311	CLA	MG-ND	-3.84	1.98	2.05
22	3	5005	BCR	C3-C4	3.84	1.64	1.52
22	3	5006	BCR	C3-C4	3.84	1.64	1.52
22	A	859	BCR	C16-C17	3.84	1.55	1.43
22	B	847	BCR	C16-C17	3.84	1.55	1.43
19	8	310	CLA	MG-ND	-3.84	1.98	2.05
19	4	313	CLA	MG-ND	-3.83	1.98	2.05
28	J	1902	C7Z	C15-C14	3.83	1.55	1.43
22	B	844	BCR	C3-C4	3.82	1.64	1.52
28	J	1902	C7Z	C4-C5	-3.82	1.45	1.51
28	1	5005	C7Z	C22-C21	3.82	1.66	1.54
19	4	308	CLA	MG-ND	-3.82	1.98	2.05
22	F	302	BCR	C3-C4	3.82	1.64	1.52
19	1	5006	CLA	MG-ND	-3.82	1.98	2.05
31	Z	317	LUT	C28-C29	3.82	1.54	1.45
22	B	847	BCR	C3-C4	3.82	1.64	1.52
19	A	840	CLA	MG-ND	-3.81	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	305	LUT	C15-C14	3.81	1.55	1.43
31	8	305	LUT	C31-C30	3.81	1.55	1.43
22	5	305	BCR	C3-C4	3.81	1.64	1.52
19	6	313	CLA	C1C-NC	-3.81	1.32	1.37
19	5	307	CLA	MG-ND	-3.80	1.98	2.05
22	B	843	BCR	C16-C17	3.80	1.55	1.43
19	7	309	CLA	MG-ND	-3.80	1.98	2.05
19	3	5020	CLA	C1C-NC	-3.80	1.32	1.37
31	6	306	LUT	C7-C6	3.80	1.58	1.45
22	3	5006	BCR	C16-C17	3.80	1.55	1.43
31	3	5002	LUT	C23-C24	-3.80	1.44	1.50
19	5	314	CLA	MG-ND	-3.80	1.98	2.05
31	7	303	LUT	C35-C34	3.80	1.55	1.43
31	4	304	LUT	C21-C26	3.80	1.67	1.56
19	Z	308	CLA	MG-ND	-3.80	1.98	2.05
22	8	306	BCR	C20-C21	3.79	1.55	1.43
22	B	844	BCR	C16-C17	3.79	1.55	1.43
19	A	810	CLA	MG-ND	-3.79	1.98	2.05
22	B	844	BCR	C11-C10	3.79	1.55	1.43
19	8	308	CLA	MG-ND	-3.79	1.98	2.05
19	Z	312	CLA	MG-ND	-3.79	1.98	2.05
22	A	847	BCR	C3-C4	3.79	1.64	1.52
19	A	815	CLA	C1C-NC	-3.79	1.32	1.37
31	3	5003	LUT	C7-C6	3.78	1.58	1.45
19	3	5009	CLA	MG-ND	-3.78	1.98	2.05
31	3	5003	LUT	C21-C26	3.78	1.66	1.56
31	6	305	LUT	C21-C26	3.78	1.66	1.56
22	A	858	BCR	C16-C17	3.78	1.55	1.43
19	3	5019	CLA	C1C-NC	-3.78	1.32	1.37
31	8	304	LUT	C11-C10	3.78	1.55	1.43
31	3	5002	LUT	C7-C6	3.78	1.58	1.45
22	5	304	BCR	C16-C17	3.78	1.55	1.43
19	Z	305	CLA	MG-ND	-3.78	1.98	2.05
19	5	311	CLA	MG-ND	-3.78	1.98	2.05
22	8	303	BCR	C11-C10	3.78	1.55	1.43
22	6	308	BCR	C20-C21	3.78	1.55	1.43
19	B	840	CLA	C1C-NC	-3.78	1.32	1.37
22	A	850	BCR	C16-C17	3.78	1.55	1.43
19	8	313	CLA	MG-ND	-3.77	1.98	2.05
19	7	324	CLA	C1C-NC	-3.77	1.32	1.37
22	B	842	BCR	C11-C10	3.77	1.55	1.43
22	B	846	BCR	C3-C4	3.77	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	7	306	CLA	MG-ND	-3.77	1.98	2.05
19	8	318	CLA	MG-ND	-3.76	1.98	2.05
19	7	316	CLA	MG-ND	-3.76	1.98	2.05
31	Z	318	LUT	C28-C29	3.76	1.54	1.45
22	A	850	BCR	C11-C10	3.76	1.55	1.43
22	A	846	BCR	C16-C17	3.76	1.55	1.43
31	5	303	LUT	C21-C26	3.76	1.66	1.56
19	7	310	CLA	C1C-NC	-3.75	1.32	1.37
19	1	5013	CLA	MG-ND	-3.75	1.98	2.05
38	8	325	ERG	C16-C15	3.75	1.64	1.54
19	8	307	CLA	MG-ND	-3.75	1.98	2.05
31	6	305	LUT	C7-C6	3.75	1.58	1.45
27	F	304	RRX	C20-C21	3.75	1.55	1.43
19	5	319	CLA	MG-ND	-3.75	1.98	2.05
19	6	312	CLA	MG-ND	-3.75	1.98	2.05
19	7	308	CLA	MG-ND	-3.75	1.98	2.05
22	3	5005	BCR	C4-C5	-3.75	1.43	1.51
19	5	308	CLA	MG-ND	-3.75	1.98	2.05
31	1	5004	LUT	C7-C6	3.75	1.58	1.45
19	B	836	CLA	C1C-NC	-3.75	1.32	1.37
19	7	309	CLA	C1C-NC	-3.75	1.32	1.37
31	1	5003	LUT	C7-C6	3.74	1.58	1.45
19	Z	306	CLA	MG-ND	-3.74	1.98	2.05
32	7	314	CHL	C3B-C2B	-3.74	1.35	1.40
19	7	313	CLA	C1C-NC	-3.74	1.32	1.37
19	5	321	CLA	MG-ND	-3.74	1.98	2.05
19	6	322	CLA	C1C-NC	-3.74	1.32	1.37
31	5	303	LUT	C7-C6	3.74	1.58	1.45
28	1	5005	C7Z	C11-C10	3.74	1.55	1.43
28	1	5005	C7Z	C15-C14	3.74	1.55	1.43
22	6	307	BCR	C3-C4	3.73	1.64	1.52
31	7	304	LUT	C11-C10	3.73	1.55	1.43
32	5	315	CHL	C3B-C2B	-3.73	1.35	1.40
22	A	847	BCR	C16-C17	3.73	1.55	1.43
31	6	306	LUT	C11-C10	3.73	1.55	1.43
19	7	311	CLA	MG-ND	-3.73	1.98	2.05
22	K	206	BCR	C16-C17	3.73	1.55	1.43
28	6	304	C7Z	C27-C26	3.73	1.58	1.45
19	4	308	CLA	C1C-NC	-3.73	1.32	1.37
19	6	320	CLA	MG-ND	-3.73	1.98	2.05
19	3	5018	CLA	C1C-NC	-3.73	1.32	1.37
19	6	323	CLA	MG-ND	-3.73	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	8	311	CLA	C1C-NC	-3.73	1.32	1.37
19	5	309	CLA	MG-ND	-3.73	1.98	2.05
32	Z	302	CHL	C3B-C2B	-3.73	1.35	1.40
22	B	845	BCR	C16-C17	3.72	1.55	1.43
22	4	305	BCR	C16-C17	3.72	1.55	1.43
19	Z	311	CLA	C1C-NC	-3.72	1.32	1.37
19	5	321	CLA	C1C-NC	-3.72	1.32	1.37
22	A	859	BCR	C11-C10	3.72	1.55	1.43
19	Z	303	CLA	C1C-NC	-3.72	1.32	1.37
19	7	310	CLA	MG-ND	-3.72	1.98	2.05
22	A	848	BCR	C16-C17	3.72	1.55	1.43
22	6	308	BCR	C11-C10	3.72	1.55	1.43
22	7	305	BCR	C16-C17	3.72	1.55	1.43
31	8	305	LUT	C35-C34	3.72	1.55	1.43
31	3	5003	LUT	C11-C10	3.72	1.55	1.43
19	8	309	CLA	MG-ND	-3.72	1.98	2.05
22	6	307	BCR	C16-C17	3.71	1.55	1.43
19	8	307	CLA	C1C-NC	-3.71	1.32	1.37
28	1	5005	C7Z	C27-C26	3.71	1.58	1.45
22	B	846	BCR	C16-C17	3.71	1.54	1.43
19	7	316	CLA	C1C-NC	-3.71	1.32	1.37
19	5	306	CLA	MG-ND	-3.71	1.98	2.05
22	A	858	BCR	C11-C10	3.71	1.54	1.43
19	4	306	CLA	MG-ND	-3.71	1.98	2.05
32	6	315	CHL	C3B-C2B	-3.71	1.35	1.40
27	4	303	RRX	C27-C26	-3.70	1.45	1.51
22	B	845	BCR	C11-C10	3.70	1.54	1.43
31	4	304	LUT	C23-C24	-3.70	1.44	1.50
19	6	310	CLA	MG-ND	-3.70	1.98	2.05
22	A	846	BCR	C11-C10	3.70	1.54	1.43
28	6	304	C7Z	C35-C34	3.70	1.54	1.43
28	J	1902	C7Z	C27-C26	3.70	1.58	1.45
19	5	311	CLA	C1C-NC	-3.70	1.32	1.37
19	6	311	CLA	C1C-NC	-3.70	1.32	1.37
31	7	303	LUT	C23-C24	-3.70	1.44	1.50
22	F	302	BCR	C16-C17	3.70	1.54	1.43
19	8	314	CLA	C1C-NC	-3.69	1.32	1.37
19	Z	304	CLA	MG-ND	-3.69	1.98	2.05
22	8	306	BCR	C27-C26	-3.69	1.43	1.51
19	1	5008	CLA	MG-ND	-3.69	1.98	2.05
19	5	310	CLA	MG-ND	-3.69	1.98	2.05
22	5	304	BCR	C3-C4	3.69	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	303	LUT	C7-C6	3.68	1.58	1.45
31	4	304	LUT	C7-C6	3.68	1.58	1.45
19	B	850	CLA	MG-ND	-3.68	1.98	2.05
22	B	847	BCR	C11-C10	3.68	1.54	1.43
19	A	812	CLA	MG-ND	-3.68	1.98	2.05
22	6	308	BCR	C3-C4	3.68	1.64	1.52
22	4	305	BCR	C11-C10	3.68	1.54	1.43
19	6	320	CLA	C1C-NC	-3.68	1.32	1.37
19	B	825	CLA	C1C-NC	-3.68	1.32	1.37
19	3	5011	CLA	C1C-NC	-3.68	1.32	1.37
22	5	305	BCR	C4-C5	-3.67	1.43	1.51
22	G	1603	BCR	C16-C17	3.67	1.54	1.43
19	6	318	CLA	MG-ND	-3.67	1.98	2.05
31	4	304	LUT	C28-C29	3.67	1.53	1.45
31	1	5003	LUT	C28-C29	3.67	1.53	1.45
22	B	842	BCR	C24-C25	3.67	1.58	1.45
22	F	302	BCR	C11-C10	3.67	1.54	1.43
22	A	847	BCR	C11-C10	3.67	1.54	1.43
31	1	5003	LUT	C23-C24	-3.67	1.45	1.50
19	1	5010	CLA	MG-ND	-3.67	1.98	2.05
19	4	307	CLA	C1C-NC	-3.67	1.32	1.37
22	3	5006	BCR	C11-C10	3.67	1.54	1.43
19	4	309	CLA	MG-ND	-3.67	1.98	2.05
19	3	5018	CLA	MG-ND	-3.67	1.98	2.05
22	3	5007	BCR	C16-C17	3.67	1.54	1.43
19	1	5008	CLA	C1C-NC	-3.66	1.32	1.37
19	Z	304	CLA	C1C-NC	-3.66	1.32	1.37
22	G	1603	BCR	C11-C10	3.66	1.54	1.43
27	4	303	RRX	C15-C14	3.66	1.54	1.43
19	B	803	CLA	MG-ND	-3.66	1.98	2.05
19	K	204	CLA	MG-ND	-3.66	1.98	2.05
19	4	316	CLA	MG-ND	-3.66	1.98	2.05
19	6	310	CLA	C1C-NC	-3.66	1.32	1.37
22	B	843	BCR	C11-C10	3.66	1.54	1.43
19	A	840	CLA	C1C-NC	-3.66	1.32	1.37
19	6	323	CLA	C1C-NC	-3.66	1.32	1.37
19	B	804	CLA	MG-ND	-3.66	1.98	2.05
31	8	305	LUT	C21-C26	3.66	1.66	1.56
19	Z	315	CLA	MG-ND	-3.65	1.98	2.05
22	6	307	BCR	C27-C26	-3.65	1.43	1.51
19	5	308	CLA	C1C-NC	-3.65	1.32	1.37
22	7	305	BCR	C11-C10	3.65	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	832	CLA	MG-ND	-3.65	1.98	2.05
19	4	310	CLA	C1C-NC	-3.65	1.32	1.37
19	5	310	CLA	C1C-NC	-3.65	1.32	1.37
22	3	5005	BCR	C27-C26	-3.64	1.43	1.51
19	7	319	CLA	MG-ND	-3.64	1.98	2.05
19	6	322	CLA	MG-ND	-3.64	1.98	2.05
22	3	5007	BCR	C11-C10	3.64	1.54	1.43
19	B	836	CLA	MG-ND	-3.64	1.98	2.05
22	3	5004	BCR	C27-C26	-3.64	1.43	1.51
31	Z	317	LUT	C23-C24	-3.64	1.45	1.50
19	A	810	CLA	C1C-NC	-3.64	1.32	1.37
22	A	849	BCR	C16-C17	3.64	1.54	1.43
19	1	5006	CLA	C1C-NC	-3.64	1.32	1.37
27	5	302	RRX	C15-C14	3.64	1.54	1.43
19	A	802	CLA	MG-ND	-3.64	1.98	2.05
31	1	5003	LUT	C21-C26	3.63	1.66	1.56
19	3	5008	CLA	C1C-NC	-3.63	1.32	1.37
31	8	304	LUT	C21-C26	3.63	1.66	1.56
19	A	816	CLA	MG-ND	-3.63	1.98	2.05
19	K	203	CLA	MG-ND	-3.63	1.98	2.05
19	1	5015	CLA	C1C-NC	-3.63	1.32	1.37
19	3	5012	CLA	MG-ND	-3.62	1.98	2.05
28	J	1902	C7Z	C35-C34	3.62	1.54	1.43
31	7	303	LUT	C21-C26	3.62	1.66	1.56
19	B	827	CLA	MG-ND	-3.62	1.98	2.05
19	B	825	CLA	MG-ND	-3.62	1.98	2.05
22	K	206	BCR	C11-C10	3.62	1.54	1.43
19	5	319	CLA	C1C-NC	-3.62	1.32	1.37
22	8	306	BCR	C3-C4	3.62	1.63	1.52
19	6	301	CLA	MG-ND	-3.62	1.98	2.05
19	6	302	CLA	MG-ND	-3.62	1.98	2.05
19	5	307	CLA	C1C-NC	-3.62	1.32	1.37
32	Z	310	CHL	C3B-C2B	-3.62	1.35	1.40
19	A	813	CLA	MG-ND	-3.61	1.98	2.05
22	A	848	BCR	C11-C10	3.61	1.54	1.43
27	5	302	RRX	C16-C17	3.61	1.54	1.43
19	B	815	CLA	MG-ND	-3.61	1.98	2.05
32	7	315	CHL	C3B-C2B	-3.61	1.35	1.40
19	B	835	CLA	MG-ND	-3.61	1.98	2.05
19	I	201	CLA	MG-ND	-3.61	1.98	2.05
22	A	858	BCR	C24-C25	3.61	1.57	1.45
19	8	320	CLA	MG-ND	-3.61	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	6	311	CLA	MG-ND	-3.61	1.98	2.05
27	5	302	RRX	C20-C21	3.61	1.54	1.43
19	6	314	CLA	MG-ND	-3.61	1.98	2.05
22	5	305	BCR	C11-C10	3.60	1.54	1.43
19	4	309	CLA	C1C-NC	-3.60	1.32	1.37
19	B	820	CLA	MG-ND	-3.60	1.98	2.05
19	8	309	CLA	C1C-NC	-3.60	1.32	1.37
22	4	305	BCR	C27-C26	-3.60	1.43	1.51
19	B	816	CLA	MG-ND	-3.60	1.98	2.05
19	K	202	CLA	MG-ND	-3.60	1.98	2.05
19	B	830	CLA	MG-ND	-3.60	1.98	2.05
31	1	5004	LUT	C21-C26	3.60	1.66	1.56
32	8	301	CHL	C3B-C2B	-3.59	1.35	1.40
19	A	828	CLA	MG-ND	-3.59	1.98	2.05
19	G	1602	CLA	MG-ND	-3.59	1.98	2.05
19	B	837	CLA	MG-ND	-3.59	1.98	2.05
19	7	306	CLA	C1C-NC	-3.59	1.32	1.37
19	6	309	CLA	C1C-NC	-3.59	1.32	1.37
19	B	821	CLA	MG-ND	-3.59	1.98	2.05
19	1	5011	CLA	MG-ND	-3.59	1.98	2.05
19	G	1601	CLA	MG-ND	-3.59	1.98	2.05
19	B	814	CLA	MG-ND	-3.59	1.98	2.05
19	J	1901	CLA	MG-ND	-3.59	1.98	2.05
19	B	832	CLA	MG-ND	-3.58	1.98	2.05
19	K	205	CLA	MG-ND	-3.58	1.98	2.05
19	5	317	CLA	C1C-NC	-3.58	1.32	1.37
22	8	303	BCR	C24-C25	3.58	1.57	1.45
22	3	5004	BCR	C3-C4	3.58	1.63	1.52
19	B	807	CLA	MG-ND	-3.58	1.98	2.05
22	B	847	BCR	C24-C25	3.58	1.57	1.45
19	4	306	CLA	C1C-NC	-3.58	1.32	1.37
19	A	837	CLA	MG-ND	-3.58	1.98	2.05
19	1	5010	CLA	C1C-NC	-3.58	1.32	1.37
27	4	303	RRX	C16-C17	3.58	1.54	1.43
19	6	309	CLA	MG-ND	-3.58	1.98	2.05
19	3	5012	CLA	C1C-NC	-3.58	1.32	1.37
32	1	5009	CHL	C3B-C2B	-3.57	1.35	1.40
19	8	318	CLA	C1C-NC	-3.57	1.32	1.37
22	A	850	BCR	C24-C25	3.57	1.57	1.45
22	F	302	BCR	C24-C25	3.57	1.57	1.45
19	4	316	CLA	C1C-NC	-3.57	1.32	1.37
19	B	818	CLA	MG-ND	-3.57	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	4	303	RRX	C29-C30	3.57	1.66	1.54
22	8	306	BCR	C16-C17	3.57	1.54	1.43
19	B	809	CLA	MG-ND	-3.57	1.98	2.05
19	4	312	CLA	MG-ND	-3.57	1.98	2.05
19	A	823	CLA	MG-ND	-3.57	1.98	2.05
19	B	822	CLA	MG-ND	-3.57	1.98	2.05
27	5	302	RRX	C4-C5	-3.57	1.44	1.51
19	A	831	CLA	MG-ND	-3.57	1.98	2.05
19	A	836	CLA	MG-ND	-3.57	1.98	2.05
22	3	5007	BCR	C27-C26	-3.57	1.44	1.51
18	A	801	CL0	OBD-CAD	3.57	1.28	1.22
31	3	5002	LUT	C11-C10	3.57	1.54	1.43
22	B	845	BCR	C24-C25	3.57	1.57	1.45
19	A	814	CLA	MG-ND	-3.56	1.98	2.05
19	A	839	CLA	MG-ND	-3.56	1.98	2.05
22	6	308	BCR	C16-C17	3.56	1.54	1.43
28	1	5005	C7Z	C35-C34	3.56	1.54	1.43
19	4	318	CLA	MG-ND	-3.56	1.98	2.05
19	A	835	CLA	MG-ND	-3.56	1.98	2.05
19	B	823	CLA	MG-ND	-3.56	1.98	2.05
19	6	318	CLA	C1C-NC	-3.56	1.32	1.37
19	B	801	CLA	MG-ND	-3.56	1.98	2.05
31	3	5002	LUT	C21-C26	3.56	1.66	1.56
19	A	843	CLA	MG-ND	-3.55	1.98	2.05
27	4	303	RRX	C20-C21	3.55	1.54	1.43
19	Z	314	CLA	MG-ND	-3.55	1.98	2.05
18	A	801	CL0	MG-NC	3.55	2.14	2.06
19	A	829	CLA	MG-ND	-3.55	1.98	2.05
22	3	5007	BCR	C24-C25	3.55	1.57	1.45
19	6	312	CLA	C1C-NC	-3.55	1.32	1.37
19	5	306	CLA	C1C-NC	-3.55	1.32	1.37
22	A	859	BCR	C24-C25	3.55	1.57	1.45
19	A	804	CLA	MG-ND	-3.55	1.98	2.05
31	6	305	LUT	C23-C24	-3.55	1.45	1.50
19	B	802	CLA	MG-ND	-3.55	1.98	2.05
19	A	805	CLA	MG-ND	-3.55	1.98	2.05
22	B	844	BCR	C24-C25	3.54	1.57	1.45
22	6	307	BCR	C11-C10	3.54	1.54	1.43
19	B	813	CLA	MG-ND	-3.54	1.98	2.05
22	B	846	BCR	C24-C25	3.54	1.57	1.45
19	B	826	CLA	MG-ND	-3.54	1.98	2.05
19	B	824	CLA	MG-ND	-3.54	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Z	318	LUT	C11-C10	3.54	1.54	1.43
22	A	846	BCR	C24-C25	3.54	1.57	1.45
19	A	821	CLA	MG-ND	-3.54	1.98	2.05
19	B	811	CLA	MG-ND	-3.54	1.98	2.05
19	A	822	CLA	MG-ND	-3.54	1.98	2.05
19	5	317	CLA	MG-ND	-3.54	1.98	2.05
22	A	847	BCR	C24-C25	3.54	1.57	1.45
19	3	5016	CLA	MG-ND	-3.54	1.98	2.05
19	B	833	CLA	MG-ND	-3.54	1.98	2.05
19	A	833	CLA	MG-ND	-3.54	1.98	2.05
19	B	850	CLA	C1C-NC	-3.54	1.32	1.37
19	5	325	CLA	C1C-NC	-3.54	1.32	1.37
19	A	841	CLA	MG-ND	-3.54	1.98	2.05
19	A	827	CLA	MG-ND	-3.53	1.98	2.05
19	B	834	CLA	MG-ND	-3.53	1.98	2.05
22	7	305	BCR	C24-C25	3.53	1.57	1.45
19	A	825	CLA	MG-ND	-3.53	1.98	2.05
19	A	817	CLA	MG-ND	-3.53	1.98	2.05
19	B	817	CLA	MG-ND	-3.53	1.98	2.05
19	B	839	CLA	MG-ND	-3.53	1.98	2.05
19	3	5015	CLA	C1C-NC	-3.53	1.32	1.37
19	A	826	CLA	MG-ND	-3.53	1.98	2.05
19	3	5014	CLA	MG-ND	-3.53	1.98	2.05
28	J	1902	C7Z	C2-C1	3.53	1.65	1.54
19	5	312	CLA	MG-ND	-3.53	1.98	2.05
19	Z	306	CLA	C1C-NC	-3.53	1.32	1.37
19	3	5013	CLA	MG-ND	-3.53	1.98	2.05
22	B	843	BCR	C24-C25	3.53	1.57	1.45
19	B	828	CLA	MG-ND	-3.53	1.98	2.05
19	B	838	CLA	MG-ND	-3.53	1.98	2.05
19	8	310	CLA	C1C-NC	-3.52	1.32	1.37
31	5	303	LUT	C11-C10	3.52	1.54	1.43
19	4	313	CLA	C1C-NC	-3.52	1.32	1.37
19	A	809	CLA	MG-ND	-3.52	1.98	2.05
22	8	306	BCR	C11-C10	3.52	1.54	1.43
19	A	819	CLA	MG-ND	-3.52	1.98	2.05
22	3	5007	BCR	C4-C5	-3.52	1.44	1.51
19	A	842	CLA	MG-ND	-3.52	1.98	2.05
19	5	313	CLA	C1C-NC	-3.52	1.32	1.37
22	K	206	BCR	C24-C25	3.52	1.57	1.45
22	3	5006	BCR	C24-C25	3.52	1.57	1.45
19	B	819	CLA	MG-ND	-3.51	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	301	CLA	C1C-NC	-3.51	1.32	1.37
19	5	322	CLA	MG-ND	-3.51	1.98	2.05
19	A	830	CLA	MG-ND	-3.51	1.98	2.05
31	3	5002	LUT	C28-C29	3.51	1.53	1.45
22	G	1603	BCR	C24-C25	3.51	1.57	1.45
19	A	818	CLA	MG-ND	-3.51	1.98	2.05
19	B	808	CLA	MG-ND	-3.51	1.98	2.05
19	B	812	CLA	MG-ND	-3.51	1.98	2.05
19	A	812	CLA	C1C-NC	-3.51	1.32	1.37
22	B	846	BCR	C11-C10	3.51	1.54	1.43
22	5	304	BCR	C11-C10	3.51	1.54	1.43
31	4	304	LUT	C11-C10	3.51	1.54	1.43
19	A	857	CLA	MG-ND	-3.50	1.98	2.05
31	8	305	LUT	C7-C6	3.50	1.57	1.45
31	Z	318	LUT	C21-C26	3.50	1.66	1.56
31	6	306	LUT	C23-C24	-3.50	1.45	1.50
19	A	820	CLA	MG-ND	-3.50	1.98	2.05
19	B	810	CLA	MG-ND	-3.50	1.98	2.05
22	A	849	BCR	C24-C25	3.50	1.57	1.45
19	A	838	CLA	MG-ND	-3.50	1.98	2.05
31	7	303	LUT	C28-C29	3.50	1.53	1.45
22	7	305	BCR	C4-C5	-3.50	1.44	1.51
19	A	824	CLA	MG-ND	-3.50	1.98	2.05
19	F	303	CLA	MG-ND	-3.50	1.98	2.05
22	5	304	BCR	C24-C25	3.50	1.57	1.45
22	A	848	BCR	C24-C25	3.49	1.57	1.45
22	3	5005	BCR	C16-C17	3.49	1.54	1.43
19	Z	307	CLA	C1C-NC	-3.49	1.32	1.37
19	B	805	CLA	MG-ND	-3.49	1.98	2.05
19	1	5018	CLA	MG-ND	-3.49	1.98	2.05
22	3	5004	BCR	C11-C10	3.49	1.54	1.43
28	6	304	C7Z	C2-C1	3.49	1.65	1.54
19	A	834	CLA	MG-ND	-3.49	1.98	2.05
19	A	811	CLA	MG-ND	-3.48	1.98	2.05
19	1	5013	CLA	C1C-NC	-3.48	1.32	1.37
19	5	301	CLA	MG-ND	-3.48	1.98	2.05
19	Z	308	CLA	C1C-NC	-3.48	1.32	1.37
31	1	5004	LUT	C11-C10	3.48	1.54	1.43
19	1	5016	CLA	MG-ND	-3.48	1.98	2.05
22	8	306	BCR	C4-C5	-3.48	1.44	1.51
19	A	803	CLA	MG-ND	-3.48	1.98	2.05
27	F	304	RRX	C7-C6	3.47	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	7	318	CLA	C1C-NC	-3.47	1.32	1.37
19	A	807	CLA	MG-ND	-3.47	1.98	2.05
19	B	829	CLA	MG-ND	-3.47	1.98	2.05
19	F	301	CLA	MG-ND	-3.47	1.98	2.05
22	B	843	BCR	C27-C26	-3.46	1.44	1.51
19	Z	315	CLA	C1C-NC	-3.46	1.32	1.37
23	3	5021	LHG	O7-C5	-3.46	1.42	1.46
19	B	806	CLA	MG-ND	-3.46	1.98	2.05
19	A	808	CLA	MG-ND	-3.46	1.98	2.05
31	8	305	LUT	C38-C25	3.46	1.57	1.50
22	A	849	BCR	C11-C10	3.46	1.54	1.43
31	6	305	LUT	C28-C29	3.45	1.53	1.45
19	A	806	CLA	MG-ND	-3.45	1.98	2.05
31	6	305	LUT	C11-C10	3.45	1.54	1.43
19	5	309	CLA	C1C-NC	-3.45	1.32	1.37
31	4	304	LUT	C38-C25	3.45	1.57	1.50
19	7	308	CLA	C1C-NC	-3.44	1.32	1.37
22	6	307	BCR	C4-C5	-3.44	1.44	1.51
22	A	847	BCR	C4-C5	-3.44	1.44	1.51
19	Z	305	CLA	C1C-NC	-3.44	1.32	1.37
22	8	303	BCR	C4-C5	-3.43	1.44	1.51
19	8	308	CLA	C1C-NC	-3.43	1.32	1.37
32	8	315	CHL	C3B-C2B	-3.43	1.35	1.40
19	5	314	CLA	C1C-NC	-3.43	1.32	1.37
22	B	845	BCR	C4-C5	-3.43	1.44	1.51
19	Z	312	CLA	C1C-NC	-3.42	1.32	1.37
22	5	305	BCR	C16-C17	3.42	1.54	1.43
19	3	5009	CLA	C1C-NC	-3.42	1.32	1.37
31	5	303	LUT	C38-C25	3.42	1.56	1.50
31	8	305	LUT	C30-C29	-3.42	1.31	1.35
31	6	306	LUT	C19-C9	3.41	1.57	1.50
22	5	305	BCR	C27-C26	-3.41	1.44	1.51
19	7	317	CLA	MG-ND	-3.41	1.99	2.05
22	5	305	BCR	C24-C25	3.41	1.57	1.45
28	1	5005	C7Z	C2-C1	3.41	1.65	1.54
27	4	303	RRX	C4-C5	-3.41	1.44	1.51
31	6	306	LUT	C38-C25	3.41	1.56	1.50
22	B	843	BCR	C4-C5	-3.41	1.44	1.51
19	1	5012	CLA	MG-ND	-3.40	1.99	2.05
22	B	847	BCR	C4-C5	-3.40	1.44	1.51
22	3	5005	BCR	C11-C10	3.40	1.54	1.43
19	3	5010	CLA	C1C-NC	-3.40	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Z	317	LUT	C38-C25	3.40	1.56	1.50
22	A	850	BCR	C4-C5	-3.39	1.44	1.51
22	3	5004	BCR	C16-C17	3.39	1.54	1.43
35	7	302	DGA	OG2-CB1	3.39	1.43	1.34
31	1	5003	LUT	C11-C10	3.39	1.53	1.43
31	7	303	LUT	C19-C9	3.39	1.57	1.50
22	A	858	BCR	C4-C5	-3.39	1.44	1.51
27	4	303	RRX	C17-C18	-3.39	1.31	1.35
22	A	849	BCR	C27-C26	-3.38	1.44	1.51
22	K	206	BCR	C4-C5	-3.38	1.44	1.51
22	5	304	BCR	C4-C5	-3.38	1.44	1.51
31	7	303	LUT	C30-C29	-3.38	1.31	1.35
22	A	848	BCR	C4-C5	-3.38	1.44	1.51
22	3	5006	BCR	C27-C26	-3.38	1.44	1.51
22	A	859	BCR	C27-C26	-3.38	1.44	1.51
22	6	307	BCR	C24-C25	3.38	1.57	1.45
27	5	302	RRX	C7-C6	3.37	1.57	1.45
19	4	307	CLA	MG-ND	-3.37	1.99	2.05
28	1	5005	C7Z	C21-C26	-3.37	1.49	1.53
18	A	801	CL0	C1D-ND	-3.37	1.33	1.37
19	B	839	CLA	CBB-CAB	3.37	1.51	1.29
19	A	830	CLA	CBB-CAB	3.37	1.51	1.29
19	B	822	CLA	CBB-CAB	3.37	1.51	1.29
19	B	806	CLA	CBB-CAB	3.37	1.51	1.29
19	6	301	CLA	C1C-NC	-3.37	1.32	1.37
32	1	5014	CHL	CBB-CAB	3.37	1.51	1.29
22	5	304	BCR	C27-C26	-3.36	1.44	1.51
19	A	841	CLA	CBB-CAB	3.36	1.51	1.29
19	A	820	CLA	CBB-CAB	3.36	1.51	1.29
19	A	807	CLA	CBB-CAB	3.36	1.51	1.29
19	B	837	CLA	CBB-CAB	3.36	1.51	1.29
19	A	827	CLA	CBB-CAB	3.35	1.51	1.29
31	6	305	LUT	C38-C25	3.35	1.56	1.50
19	A	842	CLA	CBB-CAB	3.35	1.51	1.29
19	G	1601	CLA	CBB-CAB	3.35	1.51	1.29
19	A	835	CLA	CBB-CAB	3.35	1.51	1.29
19	B	824	CLA	CBB-CAB	3.35	1.51	1.29
19	5	301	CLA	CBB-CAB	3.35	1.51	1.29
31	Z	317	LUT	C2-C1	3.35	1.65	1.54
19	7	312	CLA	MG-ND	-3.35	1.99	2.05
31	Z	318	LUT	C38-C25	3.35	1.56	1.50
31	3	5002	LUT	C38-C25	3.35	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	857	CLA	CBB-CAB	3.35	1.51	1.29
19	B	834	CLA	CBB-CAB	3.35	1.51	1.29
19	F	303	CLA	CBB-CAB	3.35	1.51	1.29
19	B	813	CLA	CBB-CAB	3.35	1.51	1.29
19	B	832	CLA	CBB-CAB	3.35	1.51	1.29
19	A	805	CLA	CBB-CAB	3.35	1.51	1.29
19	A	834	CLA	CBB-CAB	3.35	1.51	1.29
19	A	828	CLA	CBB-CAB	3.35	1.51	1.29
19	J	1901	CLA	CBB-CAB	3.35	1.51	1.29
19	A	808	CLA	CBB-CAB	3.35	1.51	1.29
32	Z	309	CHL	CBB-CAB	3.35	1.51	1.29
19	K	205	CLA	CBB-CAB	3.35	1.51	1.29
19	B	805	CLA	CBB-CAB	3.35	1.51	1.29
19	6	314	CLA	CBB-CAB	3.35	1.51	1.29
19	A	804	CLA	CBB-CAB	3.35	1.51	1.29
22	B	842	BCR	C4-C5	-3.35	1.44	1.51
19	B	828	CLA	CBB-CAB	3.35	1.51	1.29
19	K	202	CLA	CBB-CAB	3.35	1.51	1.29
19	A	817	CLA	CBB-CAB	3.35	1.51	1.29
19	1	5015	CLA	CBB-CAB	3.35	1.51	1.29
31	Z	317	LUT	C19-C9	3.35	1.57	1.50
19	A	802	CLA	CBB-CAB	3.35	1.51	1.29
19	B	826	CLA	CBB-CAB	3.35	1.51	1.29
19	A	821	CLA	CBB-CAB	3.35	1.51	1.29
19	B	807	CLA	CBB-CAB	3.35	1.51	1.29
19	B	821	CLA	CBB-CAB	3.35	1.51	1.29
19	B	819	CLA	CBB-CAB	3.35	1.51	1.29
19	B	804	CLA	CBB-CAB	3.34	1.51	1.29
19	B	820	CLA	CBB-CAB	3.34	1.51	1.29
19	A	836	CLA	CBB-CAB	3.34	1.51	1.29
31	1	5004	LUT	C30-C29	-3.34	1.31	1.35
19	B	815	CLA	CBB-CAB	3.34	1.51	1.29
19	B	838	CLA	CBB-CAB	3.34	1.51	1.29
19	6	302	CLA	CBB-CAB	3.34	1.51	1.29
19	B	809	CLA	CBB-CAB	3.34	1.51	1.29
31	8	305	LUT	C11-C10	3.34	1.53	1.43
19	B	814	CLA	CBB-CAB	3.34	1.51	1.29
19	8	320	CLA	CBB-CAB	3.34	1.51	1.29
19	4	312	CLA	CBB-CAB	3.34	1.51	1.29
28	6	304	C7Z	C21-C26	-3.34	1.49	1.53
22	B	847	BCR	C27-C26	-3.34	1.44	1.51
19	B	818	CLA	CBB-CAB	3.34	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	5011	CLA	CBB-CAB	3.34	1.51	1.29
19	B	810	CLA	CBB-CAB	3.34	1.51	1.29
19	K	204	CLA	CBB-CAB	3.34	1.51	1.29
19	A	826	CLA	CBB-CAB	3.34	1.51	1.29
19	K	203	CLA	CBB-CAB	3.34	1.51	1.29
19	5	322	CLA	CBB-CAB	3.34	1.51	1.29
19	B	829	CLA	CBB-CAB	3.34	1.51	1.29
28	6	304	C7Z	C8-C9	3.34	1.53	1.45
32	1	5017	CHL	CBB-CAB	3.34	1.51	1.29
19	4	318	CLA	CBB-CAB	3.34	1.51	1.29
19	B	808	CLA	CBB-CAB	3.34	1.51	1.29
19	B	801	CLA	CBB-CAB	3.34	1.51	1.29
19	7	319	CLA	CBB-CAB	3.34	1.51	1.29
19	B	823	CLA	CBB-CAB	3.34	1.51	1.29
19	B	827	CLA	CBB-CAB	3.34	1.51	1.29
19	1	5018	CLA	CBB-CAB	3.34	1.51	1.29
31	Z	318	LUT	C19-C9	3.34	1.57	1.50
19	7	317	CLA	CBB-CAB	3.34	1.51	1.29
19	A	839	CLA	CBB-CAB	3.34	1.51	1.29
19	A	803	CLA	CBB-CAB	3.33	1.51	1.29
31	8	305	LUT	C28-C29	3.33	1.53	1.45
19	B	833	CLA	CBB-CAB	3.33	1.51	1.29
19	A	811	CLA	CBB-CAB	3.33	1.51	1.29
19	A	822	CLA	CBB-CAB	3.33	1.51	1.29
19	B	830	CLA	CBB-CAB	3.33	1.51	1.29
22	6	308	BCR	C4-C5	-3.33	1.44	1.51
22	3	5005	BCR	C24-C25	3.33	1.56	1.45
19	A	823	CLA	CBB-CAB	3.33	1.51	1.29
19	A	824	CLA	CBB-CAB	3.33	1.51	1.29
19	Z	314	CLA	CBB-CAB	3.33	1.51	1.29
19	A	816	CLA	CBB-CAB	3.33	1.51	1.29
19	1	5016	CLA	CBB-CAB	3.33	1.51	1.29
19	3	5016	CLA	CBB-CAB	3.33	1.51	1.29
19	A	813	CLA	CBB-CAB	3.33	1.51	1.29
22	4	305	BCR	C24-C25	3.33	1.56	1.45
19	B	816	CLA	CBB-CAB	3.33	1.51	1.29
22	7	305	BCR	C27-C26	-3.33	1.44	1.51
31	1	5003	LUT	C38-C25	3.33	1.56	1.50
19	7	312	CLA	CBB-CAB	3.33	1.51	1.29
31	7	303	LUT	C38-C25	3.33	1.56	1.50
19	A	818	CLA	CBB-CAB	3.33	1.51	1.29
19	A	819	CLA	CBB-CAB	3.33	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	5014	CLA	CBB-CAB	3.33	1.51	1.29
19	A	809	CLA	CBB-CAB	3.33	1.51	1.29
19	B	811	CLA	CBB-CAB	3.32	1.51	1.29
19	A	833	CLA	CBB-CAB	3.32	1.51	1.29
19	A	814	CLA	CBB-CAB	3.32	1.51	1.29
31	7	304	LUT	C19-C9	3.32	1.57	1.50
19	A	831	CLA	CBB-CAB	3.32	1.51	1.29
19	A	825	CLA	CBB-CAB	3.32	1.51	1.29
19	I	201	CLA	CBB-CAB	3.32	1.51	1.29
19	1	5012	CLA	CBB-CAB	3.32	1.51	1.29
31	7	304	LUT	C38-C25	3.32	1.56	1.50
28	J	1902	C7Z	C7-C6	3.32	1.56	1.45
19	B	817	CLA	CBB-CAB	3.32	1.51	1.29
19	A	838	CLA	CBB-CAB	3.32	1.51	1.29
19	A	843	CLA	CBB-CAB	3.32	1.51	1.29
19	A	832	CLA	CBB-CAB	3.32	1.51	1.29
19	A	837	CLA	CBB-CAB	3.32	1.51	1.29
31	5	303	LUT	C19-C9	3.31	1.57	1.50
22	A	846	BCR	C27-C26	-3.31	1.44	1.51
19	G	1602	CLA	CBB-CAB	3.31	1.51	1.29
19	B	812	CLA	CBB-CAB	3.31	1.51	1.29
19	Z	307	CLA	CBB-CAB	3.31	1.51	1.29
19	5	312	CLA	CBB-CAB	3.31	1.51	1.29
19	A	829	CLA	CBB-CAB	3.31	1.51	1.29
19	B	802	CLA	CBB-CAB	3.31	1.51	1.29
19	B	835	CLA	CBB-CAB	3.31	1.51	1.29
31	7	303	LUT	C11-C10	3.30	1.53	1.43
19	B	803	CLA	CBB-CAB	3.30	1.51	1.29
19	3	5010	CLA	CBB-CAB	3.30	1.51	1.29
19	4	313	CLA	CBB-CAB	3.30	1.51	1.29
28	J	1902	C7Z	C18-C5	3.30	1.56	1.50
19	Z	303	CLA	CBB-CAB	3.30	1.51	1.29
31	1	5004	LUT	C38-C25	3.30	1.56	1.50
22	6	308	BCR	C24-C25	3.30	1.56	1.45
31	4	304	LUT	C19-C9	3.30	1.57	1.50
22	3	5006	BCR	C4-C5	-3.30	1.44	1.51
19	8	312	CLA	CHC-C1C	3.30	1.43	1.35
19	3	5015	CLA	CBB-CAB	3.30	1.51	1.29
35	7	302	DGA	OG1-CA1	3.30	1.43	1.33
31	5	303	LUT	C28-C29	3.30	1.53	1.45
22	A	848	BCR	C27-C26	-3.29	1.44	1.51
19	Z	315	CLA	CBB-CAB	3.29	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	849	BCR	C4-C5	-3.29	1.44	1.51
31	7	304	LUT	C2-C1	3.29	1.65	1.54
31	3	5002	LUT	C2-C1	3.29	1.65	1.54
28	J	1902	C7Z	C8-C9	3.29	1.53	1.45
19	8	320	CLA	C1C-NC	-3.29	1.32	1.37
19	5	313	CLA	CBB-CAB	3.29	1.51	1.29
19	A	806	CLA	CBB-CAB	3.29	1.51	1.29
19	6	320	CLA	CBB-CAB	3.29	1.51	1.29
19	4	308	CLA	CBB-CAB	3.28	1.51	1.29
22	A	858	BCR	C27-C26	-3.28	1.44	1.51
22	G	1603	BCR	C27-C26	-3.28	1.44	1.51
38	8	325	ERG	C4-C5	3.28	1.58	1.51
19	7	316	CLA	CBB-CAB	3.28	1.51	1.29
19	7	313	CLA	CBB-CAB	3.28	1.51	1.29
22	B	845	BCR	C27-C26	-3.28	1.44	1.51
19	Z	311	CLA	CBB-CAB	3.28	1.51	1.29
19	8	318	CLA	CBB-CAB	3.28	1.51	1.29
19	4	306	CLA	CBB-CAB	3.28	1.51	1.29
31	6	306	LUT	C2-C1	3.28	1.65	1.54
19	6	318	CLA	CBB-CAB	3.27	1.51	1.29
19	5	307	CLA	CBB-CAB	3.27	1.51	1.29
19	5	306	CLA	CBB-CAB	3.27	1.51	1.29
31	8	304	LUT	C2-C1	3.27	1.65	1.54
19	6	313	CLA	CBB-CAB	3.27	1.51	1.29
31	1	5003	LUT	C2-C1	3.27	1.65	1.54
19	1	5007	CLA	CBB-CAB	3.27	1.51	1.29
19	8	312	CLA	C4B-NB	-3.27	1.32	1.35
19	5	325	CLA	CBB-CAB	3.27	1.51	1.29
22	4	305	BCR	C4-C5	-3.27	1.44	1.51
19	A	813	CLA	C1C-NC	-3.27	1.32	1.37
28	6	304	C7Z	C18-C5	3.27	1.56	1.50
28	6	304	C7Z	C7-C6	3.27	1.56	1.45
22	A	847	BCR	C27-C26	-3.27	1.44	1.51
19	5	317	CLA	CBB-CAB	3.27	1.50	1.29
19	Z	306	CLA	CBB-CAB	3.27	1.50	1.29
19	1	5010	CLA	CBB-CAB	3.27	1.50	1.29
19	4	309	CLA	CBB-CAB	3.26	1.50	1.29
22	A	850	BCR	C27-C26	-3.26	1.44	1.51
19	7	324	CLA	CBB-CAB	3.26	1.50	1.29
19	7	317	CLA	C1C-NC	-3.26	1.32	1.37
19	F	301	CLA	C3B-C2B	-3.26	1.35	1.40
19	G	1601	CLA	C1C-NC	-3.26	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	311	CLA	CBB-CAB	3.26	1.50	1.29
19	Z	304	CLA	CBB-CAB	3.26	1.50	1.29
31	8	305	LUT	C19-C9	3.26	1.57	1.50
32	4	319	CHL	CBB-CAB	3.26	1.50	1.29
19	3	5009	CLA	CBB-CAB	3.26	1.50	1.29
19	4	307	CLA	CBB-CAB	3.26	1.50	1.29
19	4	311	CLA	CBB-CAB	3.26	1.50	1.29
31	3	5003	LUT	C19-C9	3.26	1.57	1.50
19	8	313	CLA	CBB-CAB	3.26	1.50	1.29
19	5	308	CLA	CBB-CAB	3.26	1.50	1.29
31	8	304	LUT	C38-C25	3.26	1.56	1.50
19	8	310	CLA	CBB-CAB	3.26	1.50	1.29
19	B	835	CLA	C1C-NC	-3.26	1.32	1.37
19	Z	308	CLA	CBB-CAB	3.25	1.50	1.29
25	B	848	DGD	CAA-C9A	-3.25	1.33	1.51
19	8	308	CLA	C3B-C2B	-3.25	1.35	1.40
19	8	309	CLA	CBB-CAB	3.25	1.50	1.29
19	7	307	CLA	CBB-CAB	3.25	1.50	1.29
19	7	309	CLA	CBB-CAB	3.25	1.50	1.29
19	5	314	CLA	CBB-CAB	3.25	1.50	1.29
19	3	5020	CLA	CBB-CAB	3.25	1.50	1.29
25	B	848	DGD	CGB-CFB	-3.25	1.33	1.51
19	Z	314	CLA	C1C-NC	-3.25	1.33	1.37
19	1	5006	CLA	CBB-CAB	3.25	1.50	1.29
19	Z	305	CLA	CBB-CAB	3.25	1.50	1.29
19	6	301	CLA	CBB-CAB	3.25	1.50	1.29
19	A	816	CLA	C1C-NC	-3.25	1.33	1.37
19	5	321	CLA	CBB-CAB	3.25	1.50	1.29
19	B	840	CLA	CBB-CAB	3.25	1.50	1.29
31	1	5003	LUT	C19-C9	3.25	1.57	1.50
19	8	307	CLA	CBB-CAB	3.25	1.50	1.29
25	B	848	DGD	CDB-CCB	-3.25	1.33	1.51
19	7	306	CLA	CBB-CAB	3.25	1.50	1.29
32	5	320	CHL	CBB-CAB	3.24	1.50	1.29
19	1	5013	CLA	CBB-CAB	3.24	1.50	1.29
19	6	323	CLA	CBB-CAB	3.24	1.50	1.29
29	J	1904	LMG	C25-C24	-3.24	1.33	1.51
19	Z	312	CLA	CBB-CAB	3.24	1.50	1.29
19	3	5011	CLA	CBB-CAB	3.24	1.50	1.29
19	6	311	CLA	CBB-CAB	3.24	1.50	1.29
29	J	1904	LMG	C22-C21	-3.24	1.33	1.51
19	8	311	CLA	CBB-CAB	3.24	1.50	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	5004	LUT	C19-C9	3.24	1.57	1.50
19	5	310	CLA	CBB-CAB	3.24	1.50	1.29
22	6	308	BCR	C27-C26	-3.24	1.44	1.51
19	6	322	CLA	CBB-CAB	3.24	1.50	1.29
25	B	848	DGD	CGA-CFA	-3.24	1.33	1.51
22	A	846	BCR	C4-C5	-3.24	1.44	1.51
19	4	316	CLA	CBB-CAB	3.24	1.50	1.29
19	A	840	CLA	CBB-CAB	3.24	1.50	1.29
19	3	5008	CLA	CBB-CAB	3.24	1.50	1.29
19	8	312	CLA	CBB-CAB	3.24	1.50	1.29
19	8	314	CLA	CBB-CAB	3.23	1.50	1.29
19	6	310	CLA	CBB-CAB	3.23	1.50	1.29
19	3	5018	CLA	CBB-CAB	3.23	1.50	1.29
31	3	5003	LUT	C23-C24	-3.23	1.45	1.50
31	7	304	LUT	C23-C24	-3.23	1.45	1.50
19	5	319	CLA	CBB-CAB	3.23	1.50	1.29
19	B	850	CLA	CBB-CAB	3.23	1.50	1.29
25	B	848	DGD	CAB-C9B	-3.23	1.33	1.51
32	6	321	CHL	C3B-C2B	-3.23	1.35	1.40
27	4	303	RRX	C7-C6	3.23	1.56	1.45
19	F	303	CLA	C1C-NC	-3.23	1.33	1.37
19	7	318	CLA	CBB-CAB	3.23	1.50	1.29
22	B	844	BCR	C27-C26	-3.23	1.44	1.51
19	A	812	CLA	CBB-CAB	3.23	1.50	1.29
19	7	310	CLA	CBB-CAB	3.23	1.50	1.29
19	7	311	CLA	CBB-CAB	3.23	1.50	1.29
31	5	303	LUT	C30-C29	-3.23	1.31	1.35
29	J	1904	LMG	C19-C18	-3.23	1.33	1.51
19	5	301	CLA	C1C-NC	-3.22	1.33	1.37
19	A	824	CLA	C1C-NC	-3.22	1.33	1.37
28	J	1902	C7Z	C21-C26	-3.22	1.49	1.53
19	B	831	CLA	CBB-CAB	3.22	1.50	1.29
19	4	310	CLA	CBB-CAB	3.22	1.50	1.29
31	3	5003	LUT	C38-C25	3.22	1.56	1.50
19	B	836	CLA	CBB-CAB	3.22	1.50	1.29
19	1	5008	CLA	CBB-CAB	3.22	1.50	1.29
19	1	5018	CLA	C1C-NC	-3.22	1.33	1.37
28	1	5005	C7Z	C18-C5	3.22	1.56	1.50
19	B	839	CLA	C1C-NC	-3.22	1.33	1.37
22	F	302	BCR	C4-C5	-3.21	1.44	1.51
19	1	5016	CLA	C1C-NC	-3.21	1.33	1.37
19	B	838	CLA	C1C-NC	-3.21	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	5004	LUT	C2-C1	3.21	1.64	1.54
19	6	309	CLA	CBB-CAB	3.21	1.50	1.29
22	B	846	BCR	C27-C26	-3.21	1.44	1.51
19	7	313	CLA	C3B-C2B	-3.21	1.35	1.40
27	5	302	RRX	C17-C18	-3.21	1.31	1.35
19	A	830	CLA	C1C-NC	-3.21	1.33	1.37
19	3	5013	CLA	CBB-CAB	3.21	1.50	1.29
19	A	857	CLA	C1C-NC	-3.21	1.33	1.37
19	B	808	CLA	C1C-NC	-3.21	1.33	1.37
19	7	308	CLA	C3B-C2B	-3.21	1.35	1.40
19	A	810	CLA	CBB-CAB	3.21	1.50	1.29
31	3	5002	LUT	C19-C9	3.21	1.57	1.50
19	B	817	CLA	C1C-NC	-3.20	1.33	1.37
19	7	319	CLA	C1C-NC	-3.20	1.33	1.37
19	7	312	CLA	C1C-NC	-3.20	1.33	1.37
25	B	848	DGD	CDA-CCA	-3.20	1.33	1.51
19	3	5012	CLA	CBB-CAB	3.20	1.50	1.29
19	A	823	CLA	C1C-NC	-3.20	1.33	1.37
19	8	308	CLA	CBB-CAB	3.20	1.50	1.29
19	A	805	CLA	C1C-NC	-3.20	1.33	1.37
19	K	205	CLA	C1C-NC	-3.20	1.33	1.37
19	A	808	CLA	C1C-NC	-3.20	1.33	1.37
19	B	827	CLA	C1C-NC	-3.20	1.33	1.37
22	K	206	BCR	C27-C26	-3.20	1.44	1.51
19	A	832	CLA	C1C-NC	-3.20	1.33	1.37
22	B	846	BCR	C4-C5	-3.20	1.44	1.51
32	4	315	CHL	CBB-CAB	3.20	1.50	1.29
19	A	821	CLA	C1C-NC	-3.19	1.33	1.37
19	6	312	CLA	CBB-CAB	3.19	1.50	1.29
19	B	829	CLA	C1C-NC	-3.19	1.33	1.37
19	A	815	CLA	CBB-CAB	3.19	1.50	1.29
32	8	317	CHL	CBB-CAB	3.19	1.50	1.29
19	A	843	CLA	C1C-NC	-3.19	1.33	1.37
19	5	309	CLA	CBB-CAB	3.19	1.50	1.29
19	B	823	CLA	C1C-NC	-3.19	1.33	1.37
32	6	321	CHL	CBB-CAB	3.19	1.50	1.29
19	7	308	CLA	CBB-CAB	3.19	1.50	1.29
22	G	1603	BCR	C4-C5	-3.19	1.44	1.51
19	K	202	CLA	C1C-NC	-3.19	1.33	1.37
22	B	844	BCR	C4-C5	-3.19	1.44	1.51
19	3	5019	CLA	CBB-CAB	3.18	1.50	1.29
19	A	820	CLA	C1C-NC	-3.18	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	6	317	CHL	CBB-CAB	3.18	1.50	1.29
32	6	316	CHL	CBB-CAB	3.18	1.50	1.29
19	B	832	CLA	C1C-NC	-3.18	1.33	1.37
32	6	319	CHL	C3B-C2B	-3.18	1.36	1.40
19	A	827	CLA	C1C-NC	-3.18	1.33	1.37
19	A	841	CLA	C1C-NC	-3.17	1.33	1.37
19	B	830	CLA	C1C-NC	-3.17	1.33	1.37
19	B	825	CLA	CBB-CAB	3.17	1.50	1.29
32	6	319	CHL	CBB-CAB	3.17	1.50	1.29
31	3	5002	LUT	C40-C33	3.17	1.57	1.50
19	B	834	CLA	C1C-NC	-3.17	1.33	1.37
19	G	1602	CLA	C1C-NC	-3.17	1.33	1.37
19	B	828	CLA	C1C-NC	-3.17	1.33	1.37
28	1	5005	C7Z	C7-C6	3.17	1.56	1.45
22	F	302	BCR	C27-C26	-3.17	1.44	1.51
19	A	814	CLA	C1C-NC	-3.17	1.33	1.37
19	A	829	CLA	C1C-NC	-3.17	1.33	1.37
31	6	305	LUT	C30-C29	-3.17	1.31	1.35
19	A	836	CLA	C1C-NC	-3.17	1.33	1.37
19	I	201	CLA	C1C-NC	-3.17	1.33	1.37
32	4	314	CHL	CBB-CAB	3.17	1.50	1.29
31	7	303	LUT	C40-C33	3.16	1.57	1.50
19	3	5014	CLA	C1C-NC	-3.16	1.33	1.37
19	A	812	CLA	C3B-C2B	-3.16	1.36	1.40
31	6	305	LUT	C19-C9	3.16	1.57	1.50
32	8	319	CHL	CBB-CAB	3.16	1.50	1.29
32	6	316	CHL	C3B-C2B	-3.16	1.36	1.40
19	A	807	CLA	C1C-NC	-3.16	1.33	1.37
19	B	820	CLA	C1C-NC	-3.16	1.33	1.37
19	F	301	CLA	CBB-CAB	3.15	1.50	1.29
19	6	314	CLA	C1C-NC	-3.15	1.33	1.37
31	4	304	LUT	C2-C1	3.15	1.64	1.54
19	A	811	CLA	C1C-NC	-3.15	1.33	1.37
32	Z	313	CHL	CBB-CAB	3.15	1.50	1.29
19	K	203	CLA	C1C-NC	-3.15	1.33	1.37
31	1	5004	LUT	C28-C29	3.15	1.52	1.45
19	A	834	CLA	C1C-NC	-3.15	1.33	1.37
22	8	306	BCR	C24-C25	3.15	1.56	1.45
19	A	837	CLA	C1C-NC	-3.15	1.33	1.37
19	B	837	CLA	C1C-NC	-3.15	1.33	1.37
32	5	316	CHL	CBB-CAB	3.15	1.50	1.29
19	A	838	CLA	C1C-NC	-3.15	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	4	319	CHL	C4B-NB	3.15	1.38	1.35
19	B	816	CLA	C1C-NC	-3.15	1.33	1.37
19	5	322	CLA	C1C-NC	-3.15	1.33	1.37
19	B	821	CLA	C1C-NC	-3.14	1.33	1.37
19	5	314	CLA	C3B-C2B	-3.14	1.36	1.40
19	B	807	CLA	C1C-NC	-3.14	1.33	1.37
19	K	204	CLA	C1C-NC	-3.14	1.33	1.37
19	4	318	CLA	C1C-NC	-3.14	1.33	1.37
19	4	312	CLA	C1C-NC	-3.14	1.33	1.37
19	J	1901	CLA	C1C-NC	-3.14	1.33	1.37
19	A	818	CLA	C1C-NC	-3.14	1.33	1.37
19	A	831	CLA	C1C-NC	-3.14	1.33	1.37
19	B	802	CLA	C1C-NC	-3.14	1.33	1.37
19	B	850	CLA	C3B-C2B	-3.14	1.36	1.40
19	B	809	CLA	C1C-NC	-3.14	1.33	1.37
19	B	805	CLA	C1C-NC	-3.13	1.33	1.37
32	5	318	CHL	CBB-CAB	3.13	1.50	1.29
19	A	817	CLA	C1C-NC	-3.13	1.33	1.37
19	A	839	CLA	C1C-NC	-3.13	1.33	1.37
19	3	5016	CLA	C1C-NC	-3.13	1.33	1.37
32	1	5014	CHL	C4B-NB	3.13	1.38	1.35
19	5	312	CLA	C1C-NC	-3.13	1.33	1.37
19	B	810	CLA	C1C-NC	-3.13	1.33	1.37
27	F	304	RRX	C4-C5	-3.13	1.44	1.51
19	5	319	CLA	C3B-C2B	-3.13	1.36	1.40
19	B	822	CLA	C1C-NC	-3.12	1.33	1.37
19	B	815	CLA	C1C-NC	-3.12	1.33	1.37
19	A	822	CLA	C1C-NC	-3.12	1.33	1.37
31	Z	318	LUT	C2-C1	3.12	1.64	1.54
19	A	819	CLA	C1C-NC	-3.12	1.33	1.37
32	8	316	CHL	CBB-CAB	3.12	1.50	1.29
19	A	825	CLA	C1C-NC	-3.12	1.33	1.37
31	3	5003	LUT	C40-C33	3.12	1.57	1.50
19	5	309	CLA	C3B-C2B	-3.12	1.36	1.40
28	1	5005	C7Z	C8-C9	3.11	1.52	1.45
31	8	305	LUT	C2-C1	3.11	1.64	1.54
19	B	826	CLA	C1C-NC	-3.11	1.33	1.37
31	6	305	LUT	C2-C1	3.11	1.64	1.54
19	B	833	CLA	C1C-NC	-3.11	1.33	1.37
19	6	302	CLA	C1C-NC	-3.11	1.33	1.37
31	1	5003	LUT	C40-C33	3.11	1.57	1.50
19	A	842	CLA	C1C-NC	-3.10	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	814	CLA	C1C-NC	-3.10	1.33	1.37
19	5	307	CLA	C3B-C2B	-3.10	1.36	1.40
19	A	809	CLA	C1C-NC	-3.10	1.33	1.37
19	1	5011	CLA	C1C-NC	-3.09	1.33	1.37
19	A	828	CLA	C1C-NC	-3.09	1.33	1.37
19	B	813	CLA	C1C-NC	-3.09	1.33	1.37
19	A	835	CLA	C1C-NC	-3.09	1.33	1.37
19	B	804	CLA	C1C-NC	-3.09	1.33	1.37
22	A	859	BCR	C4-C5	-3.09	1.44	1.51
32	Z	309	CHL	C4B-NB	3.09	1.38	1.35
22	3	5004	BCR	C24-C25	3.09	1.56	1.45
32	3	5017	CHL	CBB-CAB	3.08	1.49	1.29
19	A	833	CLA	C1C-NC	-3.08	1.33	1.37
19	8	309	CLA	C3B-C2B	-3.08	1.36	1.40
31	6	305	LUT	C40-C33	3.08	1.57	1.50
19	1	5012	CLA	C1C-NC	-3.08	1.33	1.37
19	B	819	CLA	C1C-NC	-3.08	1.33	1.37
19	A	803	CLA	C1C-NC	-3.08	1.33	1.37
19	B	801	CLA	C1C-NC	-3.08	1.33	1.37
19	B	818	CLA	C1C-NC	-3.08	1.33	1.37
19	A	806	CLA	C1C-NC	-3.07	1.33	1.37
31	8	304	LUT	C19-C9	3.07	1.57	1.50
31	6	306	LUT	C40-C33	3.07	1.57	1.50
32	6	315	CHL	CBB-CAB	3.07	1.49	1.29
31	7	303	LUT	C2-C1	3.07	1.64	1.54
31	5	303	LUT	C2-C1	3.07	1.64	1.54
18	A	801	CL0	C3D-C2D	3.06	1.47	1.39
19	A	802	CLA	C1C-NC	-3.06	1.33	1.37
19	B	806	CLA	C1C-NC	-3.06	1.33	1.37
32	8	315	CHL	CBB-CAB	3.06	1.49	1.29
32	7	315	CHL	CBB-CAB	3.06	1.49	1.29
31	3	5003	LUT	C2-C1	3.06	1.64	1.54
31	7	304	LUT	C40-C33	3.06	1.57	1.50
19	B	803	CLA	C1C-NC	-3.06	1.33	1.37
31	Z	318	LUT	C40-C33	3.05	1.57	1.50
19	B	811	CLA	C1C-NC	-3.05	1.33	1.37
19	A	826	CLA	C1C-NC	-3.05	1.33	1.37
19	3	5012	CLA	C3B-C2B	-3.05	1.36	1.40
31	8	304	LUT	C23-C24	-3.04	1.45	1.50
32	8	319	CHL	C3A-C2A	-3.04	1.46	1.54
19	B	824	CLA	C1C-NC	-3.04	1.33	1.37
22	B	842	BCR	C27-C26	-3.03	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	310	CLA	C3B-C2B	-3.03	1.36	1.40
31	5	303	LUT	O23-C23	-3.03	1.38	1.43
32	4	317	CHL	CBB-CAB	3.02	1.49	1.29
32	8	301	CHL	CBB-CAB	3.02	1.49	1.29
19	B	812	CLA	C1C-NC	-3.02	1.33	1.37
19	A	804	CLA	C1C-NC	-3.02	1.33	1.37
31	8	305	LUT	C40-C33	3.01	1.57	1.50
32	5	316	CHL	C3A-C2A	-3.01	1.46	1.54
32	Z	310	CHL	CBB-CAB	3.00	1.49	1.29
32	5	320	CHL	C4B-NB	3.00	1.37	1.35
32	1	5017	CHL	C4B-NB	3.00	1.37	1.35
19	Z	315	CLA	C3B-C2B	-2.99	1.36	1.40
31	Z	317	LUT	C40-C33	2.99	1.57	1.50
22	8	303	BCR	C27-C26	-2.99	1.45	1.51
32	7	314	CHL	CBB-CAB	2.99	1.49	1.29
19	4	311	CLA	CHC-C1C	2.98	1.42	1.35
31	4	304	LUT	C40-C33	2.98	1.57	1.50
32	Z	302	CHL	C4B-NB	2.98	1.37	1.35
19	6	322	CLA	C3B-C2B	-2.98	1.36	1.40
19	5	325	CLA	C3B-C2B	-2.98	1.36	1.40
31	1	5004	LUT	O23-C23	-2.98	1.38	1.43
19	6	320	CLA	C3B-C2B	-2.98	1.36	1.40
31	3	5002	LUT	O23-C23	-2.98	1.38	1.43
32	4	317	CHL	C4B-NB	2.97	1.37	1.35
32	Z	302	CHL	CBB-CAB	2.97	1.48	1.29
19	1	5010	CLA	C3B-C2B	-2.96	1.36	1.40
31	1	5004	LUT	C40-C33	2.96	1.57	1.50
31	4	304	LUT	O23-C23	-2.96	1.38	1.43
31	1	5003	LUT	C30-C29	-2.96	1.31	1.35
31	8	305	LUT	C34-C33	-2.96	1.31	1.35
32	1	5009	CHL	CBB-CAB	2.95	1.48	1.29
22	B	847	BCR	C34-C9	2.95	1.57	1.50
31	5	303	LUT	C40-C33	2.95	1.57	1.50
31	6	306	LUT	O23-C23	-2.95	1.38	1.43
19	3	5009	CLA	C3B-C2B	-2.95	1.36	1.40
32	8	301	CHL	C4B-NB	2.94	1.37	1.35
19	6	311	CLA	C3B-C2B	-2.94	1.36	1.40
19	F	301	CLA	CHC-C1C	2.94	1.42	1.35
31	8	304	LUT	C40-C33	2.94	1.57	1.50
32	5	318	CHL	C4B-NB	2.94	1.37	1.35
31	8	305	LUT	O23-C23	-2.93	1.38	1.43
19	5	308	CLA	C3B-C2B	-2.92	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	303	LUT	O23-C23	-2.91	1.38	1.43
19	6	310	CLA	C3B-C2B	-2.91	1.36	1.40
32	5	315	CHL	CBB-CAB	2.90	1.48	1.29
31	Z	318	LUT	C23-C24	-2.90	1.46	1.50
19	1	5013	CLA	C3B-C2B	-2.89	1.36	1.40
19	3	5010	CLA	C3B-C2B	-2.89	1.36	1.40
19	8	307	CLA	C3B-C2B	-2.89	1.36	1.40
31	1	5004	LUT	C34-C33	-2.89	1.32	1.35
22	B	843	BCR	C34-C9	2.88	1.56	1.50
22	8	303	BCR	C34-C9	2.88	1.56	1.50
19	5	317	CLA	C3B-C2B	-2.88	1.36	1.40
32	1	5009	CHL	C4B-NB	2.88	1.37	1.35
22	B	846	BCR	C34-C9	2.88	1.56	1.50
38	6	326	ERG	C4-C5	2.87	1.57	1.51
31	7	304	LUT	O23-C23	-2.86	1.38	1.43
27	F	304	RRX	C17-C18	-2.86	1.32	1.35
19	8	308	CLA	CHC-C1C	2.85	1.42	1.35
22	K	206	BCR	C34-C9	2.85	1.56	1.50
31	3	5002	LUT	C30-C29	-2.85	1.32	1.35
22	A	849	BCR	C34-C9	2.85	1.56	1.50
19	8	314	CLA	C3B-C2B	-2.85	1.36	1.40
22	B	842	BCR	C34-C9	2.84	1.56	1.50
32	Z	310	CHL	C4B-NB	2.84	1.37	1.35
22	A	848	BCR	C34-C9	2.84	1.56	1.50
22	A	858	BCR	C34-C9	2.84	1.56	1.50
19	4	307	CLA	CHC-C1C	2.84	1.42	1.35
22	A	847	BCR	C34-C9	2.83	1.56	1.50
32	6	316	CHL	C4B-NB	2.83	1.37	1.35
31	7	303	LUT	C34-C33	-2.83	1.32	1.35
22	B	844	BCR	C34-C9	2.82	1.56	1.50
32	1	5009	CHL	C1D-ND	-2.82	1.34	1.37
22	G	1603	BCR	C34-C9	2.82	1.56	1.50
32	4	315	CHL	C4B-NB	2.82	1.37	1.35
32	7	314	CHL	C4B-NB	2.81	1.37	1.35
22	A	859	BCR	C34-C9	2.81	1.56	1.50
19	A	818	CLA	CHC-C1C	2.81	1.42	1.35
19	A	806	CLA	CHC-C1C	2.81	1.42	1.35
19	A	809	CLA	CHC-C1C	2.81	1.42	1.35
32	7	314	CHL	C1D-ND	-2.81	1.34	1.37
19	B	812	CLA	CHC-C1C	2.81	1.42	1.35
31	1	5003	LUT	O23-C23	-2.81	1.38	1.43
19	6	301	CLA	C3B-C2B	-2.80	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	5003	LUT	O23-C23	-2.80	1.38	1.43
32	5	315	CHL	C4B-NB	2.80	1.37	1.35
22	3	5006	BCR	C34-C9	2.80	1.56	1.50
19	A	804	CLA	CHC-C1C	2.80	1.42	1.35
19	Z	315	CLA	CHC-C1C	2.80	1.42	1.35
19	4	311	CLA	C4B-NB	-2.80	1.32	1.35
32	6	321	CHL	C4B-NB	2.80	1.37	1.35
22	A	850	BCR	C34-C9	2.79	1.56	1.50
22	F	302	BCR	C34-C9	2.79	1.56	1.50
22	A	846	BCR	C34-C9	2.79	1.56	1.50
32	8	315	CHL	C4B-NB	2.79	1.37	1.35
19	5	309	CLA	CHC-C1C	2.79	1.42	1.35
19	B	805	CLA	CHC-C1C	2.79	1.42	1.35
19	Z	308	CLA	C3B-C2B	-2.79	1.36	1.40
31	8	304	LUT	O23-C23	-2.79	1.38	1.43
19	B	822	CLA	CHC-C1C	2.78	1.42	1.35
19	A	811	CLA	CHC-C1C	2.78	1.42	1.35
19	A	805	CLA	CHC-C1C	2.78	1.42	1.35
19	1	5012	CLA	CHC-C1C	2.78	1.42	1.35
19	4	307	CLA	C3B-C2B	-2.78	1.36	1.40
19	B	835	CLA	CHC-C1C	2.78	1.42	1.35
32	8	316	CHL	C1D-ND	-2.78	1.34	1.37
19	B	806	CLA	CHC-C1C	2.77	1.42	1.35
19	A	819	CLA	CHC-C1C	2.77	1.42	1.35
32	4	314	CHL	C3B-C2B	-2.77	1.36	1.40
22	B	845	BCR	C34-C9	2.77	1.56	1.50
19	A	829	CLA	CHC-C1C	2.77	1.42	1.35
22	B	844	BCR	C7-C6	2.77	1.54	1.45
18	A	801	CL0	C4D-CHA	2.77	1.48	1.38
19	J	1901	CLA	CHC-C1C	2.77	1.42	1.35
22	3	5007	BCR	C34-C9	2.77	1.56	1.50
19	B	838	CLA	CHC-C1C	2.77	1.42	1.35
32	4	314	CHL	C4B-NB	2.77	1.37	1.35
31	5	303	LUT	C34-C33	-2.77	1.32	1.35
19	G	1602	CLA	CHC-C1C	2.77	1.42	1.35
19	1	5018	CLA	CHC-C1C	2.77	1.42	1.35
19	Z	307	CLA	C3B-C2B	-2.77	1.36	1.40
19	B	801	CLA	CHC-C1C	2.76	1.42	1.35
19	3	5018	CLA	C3B-C2B	-2.76	1.36	1.40
19	4	308	CLA	C3B-C2B	-2.76	1.36	1.40
19	B	821	CLA	CHC-C1C	2.76	1.42	1.35
19	A	837	CLA	CHC-C1C	2.76	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Z	313	CHL	C4B-NB	2.76	1.37	1.35
19	A	826	CLA	CHC-C1C	2.76	1.42	1.35
32	5	315	CHL	C1D-ND	-2.76	1.34	1.37
19	B	818	CLA	CHC-C1C	2.76	1.42	1.35
19	A	812	CLA	CHC-C1C	2.75	1.42	1.35
19	A	841	CLA	CHC-C1C	2.75	1.42	1.35
19	Z	314	CLA	CHC-C1C	2.75	1.42	1.35
19	A	820	CLA	CHC-C1C	2.75	1.42	1.35
19	A	823	CLA	CHC-C1C	2.75	1.42	1.35
19	B	808	CLA	CHC-C1C	2.75	1.42	1.35
19	B	833	CLA	CHC-C1C	2.75	1.42	1.35
19	6	312	CLA	C3B-C2B	-2.75	1.36	1.40
19	6	309	CLA	C3B-C2B	-2.75	1.36	1.40
19	A	825	CLA	CHC-C1C	2.75	1.42	1.35
19	B	814	CLA	CHC-C1C	2.75	1.42	1.35
32	3	5017	CHL	C3A-C2A	-2.75	1.46	1.54
22	A	846	BCR	C7-C6	2.75	1.54	1.45
19	A	824	CLA	CHC-C1C	2.74	1.42	1.35
19	B	816	CLA	CHC-C1C	2.74	1.42	1.35
19	B	824	CLA	CHC-C1C	2.74	1.42	1.35
19	A	822	CLA	CHC-C1C	2.74	1.42	1.35
32	6	315	CHL	C4B-NB	2.74	1.37	1.35
19	A	833	CLA	CHC-C1C	2.74	1.42	1.35
19	A	831	CLA	CHC-C1C	2.74	1.42	1.35
19	4	306	CLA	C3B-C2B	-2.74	1.36	1.40
22	6	307	BCR	C34-C9	2.74	1.56	1.50
19	1	5016	CLA	CHC-C1C	2.74	1.42	1.35
19	A	835	CLA	CHC-C1C	2.74	1.42	1.35
19	5	314	CLA	CHC-C1C	2.74	1.42	1.35
31	6	305	LUT	O23-C23	-2.74	1.38	1.43
19	B	802	CLA	CHC-C1C	2.74	1.42	1.35
19	5	310	CLA	C3B-C2B	-2.74	1.36	1.40
22	A	858	BCR	C7-C6	2.74	1.54	1.45
19	B	834	CLA	CHC-C1C	2.73	1.42	1.35
19	A	842	CLA	CHC-C1C	2.73	1.42	1.35
19	B	817	CLA	CHC-C1C	2.73	1.42	1.35
19	A	830	CLA	CHC-C1C	2.73	1.42	1.35
22	B	842	BCR	C7-C6	2.73	1.54	1.45
32	Z	313	CHL	C1D-ND	-2.73	1.34	1.37
19	B	829	CLA	CHC-C1C	2.73	1.42	1.35
19	A	802	CLA	CHC-C1C	2.73	1.42	1.35
22	8	303	BCR	C7-C6	2.73	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	803	CLA	CHC-C1C	2.73	1.42	1.35
19	A	817	CLA	CHC-C1C	2.73	1.42	1.35
19	B	828	CLA	CHC-C1C	2.73	1.42	1.35
19	1	5011	CLA	CHC-C1C	2.73	1.42	1.35
19	3	5012	CLA	CHC-C1C	2.73	1.42	1.35
31	Z	317	LUT	O23-C23	-2.73	1.38	1.43
22	B	845	BCR	C7-C6	2.72	1.54	1.45
19	4	312	CLA	CHC-C1C	2.72	1.41	1.35
19	5	308	CLA	CHC-C1C	2.72	1.41	1.35
19	B	811	CLA	CHC-C1C	2.72	1.41	1.35
19	6	302	CLA	CHC-C1C	2.72	1.41	1.35
19	5	312	CLA	CHC-C1C	2.72	1.41	1.35
19	7	312	CLA	CHC-C1C	2.72	1.41	1.35
19	A	807	CLA	CHC-C1C	2.72	1.41	1.35
19	4	316	CLA	C3B-C2B	-2.72	1.36	1.40
19	A	828	CLA	CHC-C1C	2.72	1.41	1.35
19	8	311	CLA	C3B-C2B	-2.72	1.36	1.40
19	B	826	CLA	CHC-C1C	2.71	1.41	1.35
19	A	821	CLA	CHC-C1C	2.71	1.41	1.35
19	5	301	CLA	CHC-C1C	2.71	1.41	1.35
19	3	5014	CLA	CHC-C1C	2.71	1.41	1.35
31	4	304	LUT	C30-C29	-2.71	1.32	1.35
19	A	857	CLA	CHC-C1C	2.71	1.41	1.35
22	F	302	BCR	C7-C6	2.71	1.54	1.45
32	6	319	CHL	C4B-NB	2.71	1.37	1.35
19	A	827	CLA	CHC-C1C	2.71	1.41	1.35
19	B	807	CLA	CHC-C1C	2.70	1.41	1.35
19	6	314	CLA	CHC-C1C	2.70	1.41	1.35
19	B	823	CLA	CHC-C1C	2.70	1.41	1.35
19	B	820	CLA	CHC-C1C	2.70	1.41	1.35
19	A	836	CLA	CHC-C1C	2.70	1.41	1.35
19	7	317	CLA	CHC-C1C	2.70	1.41	1.35
22	7	305	BCR	C34-C9	2.70	1.56	1.50
19	A	808	CLA	CHC-C1C	2.70	1.41	1.35
19	A	832	CLA	CHC-C1C	2.70	1.41	1.35
22	B	847	BCR	C7-C6	2.70	1.54	1.45
32	8	301	CHL	C1D-ND	-2.70	1.34	1.37
19	B	815	CLA	CHC-C1C	2.70	1.41	1.35
19	7	306	CLA	CHC-C1C	2.70	1.41	1.35
19	4	318	CLA	CHC-C1C	2.70	1.41	1.35
19	B	803	CLA	CHC-C1C	2.70	1.41	1.35
19	B	813	CLA	CHC-C1C	2.70	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	303	CLA	CHC-C1C	2.70	1.41	1.35
19	B	830	CLA	CHC-C1C	2.69	1.41	1.35
19	6	311	CLA	CHC-C1C	2.69	1.41	1.35
19	B	839	CLA	CHC-C1C	2.69	1.41	1.35
19	A	834	CLA	CHC-C1C	2.69	1.41	1.35
19	B	832	CLA	CHC-C1C	2.69	1.41	1.35
19	B	819	CLA	CHC-C1C	2.69	1.41	1.35
22	3	5006	BCR	C7-C6	2.69	1.54	1.45
19	7	319	CLA	CHC-C1C	2.69	1.41	1.35
19	5	322	CLA	CHC-C1C	2.69	1.41	1.35
19	B	810	CLA	CHC-C1C	2.69	1.41	1.35
19	B	827	CLA	CHC-C1C	2.69	1.41	1.35
19	8	320	CLA	CHC-C1C	2.68	1.41	1.35
22	3	5007	BCR	C39-C30	-2.68	1.48	1.53
19	B	825	CLA	CHC-C1C	2.68	1.41	1.35
22	A	859	BCR	C7-C6	2.68	1.54	1.45
32	5	316	CHL	C4B-NB	2.68	1.37	1.35
19	A	816	CLA	CHC-C1C	2.68	1.41	1.35
19	6	322	CLA	CHC-C1C	2.68	1.41	1.35
19	K	205	CLA	CHC-C1C	2.68	1.41	1.35
22	A	850	BCR	C7-C6	2.68	1.54	1.45
19	5	310	CLA	CHC-C1C	2.68	1.41	1.35
22	3	5007	BCR	C7-C6	2.68	1.54	1.45
19	7	310	CLA	C3B-C2B	-2.68	1.36	1.40
19	A	839	CLA	CHC-C1C	2.67	1.41	1.35
19	6	312	CLA	CHC-C1C	2.67	1.41	1.35
19	K	203	CLA	CHC-C1C	2.67	1.41	1.35
19	4	310	CLA	CHC-C1C	2.67	1.41	1.35
19	B	809	CLA	CHC-C1C	2.67	1.41	1.35
19	Z	305	CLA	CHC-C1C	2.67	1.41	1.35
22	4	305	BCR	C7-C6	2.67	1.54	1.45
31	Z	318	LUT	C30-C29	-2.67	1.32	1.35
19	B	804	CLA	CHC-C1C	2.67	1.41	1.35
19	3	5011	CLA	C3B-C2B	-2.67	1.36	1.40
19	B	837	CLA	CHC-C1C	2.67	1.41	1.35
19	6	310	CLA	CHC-C1C	2.66	1.41	1.35
19	3	5016	CLA	CHC-C1C	2.66	1.41	1.35
22	6	308	BCR	C34-C9	2.66	1.56	1.50
19	G	1601	CLA	CHC-C1C	2.66	1.41	1.35
19	1	5010	CLA	CHC-C1C	2.66	1.41	1.35
19	Z	308	CLA	C3D-C4D	-2.66	1.38	1.44
19	3	5010	CLA	CHC-C1C	2.66	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	202	CLA	CHC-C1C	2.65	1.41	1.35
22	A	847	BCR	C7-C6	2.65	1.54	1.45
31	Z	318	LUT	O23-C23	-2.65	1.38	1.43
19	A	838	CLA	CHC-C1C	2.65	1.41	1.35
19	A	814	CLA	CHC-C1C	2.65	1.41	1.35
31	1	5003	LUT	C34-C33	-2.65	1.32	1.35
19	I	201	CLA	CHC-C1C	2.64	1.41	1.35
31	3	5003	LUT	C26-C27	2.64	1.54	1.50
19	B	831	CLA	C3B-C2B	-2.64	1.36	1.40
19	8	318	CLA	C3B-C2B	-2.64	1.36	1.40
19	K	204	CLA	CHC-C1C	2.64	1.41	1.35
19	8	311	CLA	CHC-C1C	2.64	1.41	1.35
22	G	1603	BCR	C7-C6	2.64	1.54	1.45
32	6	317	CHL	C3B-C2B	-2.64	1.36	1.40
19	1	5015	CLA	C3B-C2B	-2.64	1.36	1.40
18	A	801	CL0	C4B-CHC	2.64	1.48	1.41
19	3	5009	CLA	CHC-C1C	2.63	1.41	1.35
19	Z	306	CLA	CHC-C1C	2.63	1.41	1.35
22	K	206	BCR	C7-C6	2.63	1.54	1.45
19	1	5007	CLA	C3D-C4D	-2.63	1.38	1.44
22	8	306	BCR	C34-C9	2.63	1.56	1.50
19	B	802	CLA	C3B-C2B	-2.63	1.36	1.40
18	A	801	CL0	C1B-CHB	2.63	1.48	1.41
19	3	5013	CLA	C3B-C2B	-2.63	1.36	1.40
19	A	813	CLA	CHC-C1C	2.63	1.41	1.35
38	6	326	ERG	C1-C10	2.63	1.59	1.54
32	7	315	CHL	C4B-NB	2.63	1.37	1.35
32	Z	310	CHL	C3A-C2A	-2.62	1.47	1.54
22	B	843	BCR	C7-C6	2.62	1.54	1.45
19	B	836	CLA	C4B-NB	-2.62	1.32	1.35
19	4	313	CLA	C3B-C2B	-2.62	1.36	1.40
22	7	305	BCR	C7-C6	2.62	1.54	1.45
19	7	318	CLA	CHC-C1C	2.62	1.41	1.35
19	3	5011	CLA	CHC-C1C	2.62	1.41	1.35
19	5	317	CLA	CHC-C1C	2.62	1.41	1.35
19	5	311	CLA	CHC-C1C	2.61	1.41	1.35
19	8	309	CLA	CHC-C1C	2.61	1.41	1.35
22	4	305	BCR	C34-C9	2.61	1.56	1.50
19	A	843	CLA	CHC-C1C	2.61	1.41	1.35
19	1	5013	CLA	CHC-C1C	2.61	1.41	1.35
19	7	316	CLA	C3B-C2B	-2.61	1.36	1.40
19	5	319	CLA	CHC-C1C	2.60	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	306	CLA	C3B-C2B	-2.60	1.36	1.40
22	5	305	BCR	C34-C9	2.60	1.56	1.50
22	5	304	BCR	C34-C9	2.60	1.56	1.50
22	B	846	BCR	C7-C6	2.60	1.54	1.45
19	5	313	CLA	C3B-C2B	-2.60	1.36	1.40
19	4	306	CLA	CHC-C1C	2.59	1.41	1.35
19	6	301	CLA	CHC-C1C	2.59	1.41	1.35
19	3	5015	CLA	CHC-C1C	2.59	1.41	1.35
19	6	311	CLA	C3D-C4D	-2.59	1.38	1.44
22	A	848	BCR	C7-C6	2.59	1.54	1.45
19	B	834	CLA	C3B-C2B	-2.59	1.36	1.40
19	Z	307	CLA	CHC-C1C	2.58	1.41	1.35
19	1	5010	CLA	C3D-C4D	-2.58	1.38	1.44
22	6	308	BCR	C7-C6	2.58	1.54	1.45
22	5	304	BCR	C7-C6	2.58	1.54	1.45
19	7	318	CLA	C3B-C2B	-2.58	1.36	1.40
19	4	310	CLA	C3D-C4D	-2.58	1.38	1.44
19	A	810	CLA	C3B-C2B	-2.58	1.36	1.40
19	Z	306	CLA	C3B-C2B	-2.58	1.36	1.40
19	5	313	CLA	CHC-C1C	2.58	1.41	1.35
32	4	317	CHL	C3A-C2A	-2.58	1.47	1.54
19	Z	308	CLA	CHC-C1C	2.58	1.41	1.35
19	4	311	CLA	MG-ND	-2.57	2.00	2.05
19	B	836	CLA	C3D-C4D	-2.57	1.38	1.44
32	8	317	CHL	C4B-NB	2.57	1.37	1.35
19	7	313	CLA	CHC-C1C	2.57	1.41	1.35
19	A	810	CLA	CHC-C1C	2.57	1.41	1.35
19	8	311	CLA	C3D-C4D	-2.57	1.38	1.44
19	B	836	CLA	C3B-C2B	-2.57	1.36	1.40
19	4	316	CLA	CHC-C1C	2.57	1.41	1.35
32	6	317	CHL	C4B-NB	2.56	1.37	1.35
34	5	324	3PH	O21-C2	-2.56	1.40	1.46
19	3	5008	CLA	C3B-C2B	-2.56	1.36	1.40
19	7	324	CLA	C3B-C2B	-2.56	1.36	1.40
19	A	840	CLA	CHC-C1C	2.56	1.41	1.35
19	4	313	CLA	CHC-C1C	2.56	1.41	1.35
19	5	325	CLA	CHC-C1C	2.55	1.41	1.35
19	6	309	CLA	CHC-C1C	2.55	1.41	1.35
32	8	317	CHL	C3B-C2B	-2.55	1.36	1.40
22	B	843	BCR	C36-C18	2.55	1.56	1.50
19	A	806	CLA	C3B-C2B	-2.55	1.36	1.40
19	7	310	CLA	CHC-C1C	2.55	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	311	CLA	C3B-C2B	-2.55	1.36	1.40
19	8	318	CLA	C3D-C4D	-2.55	1.38	1.44
19	B	850	CLA	CHC-C1C	2.54	1.41	1.35
19	1	5007	CLA	C3B-C2B	-2.54	1.36	1.40
19	5	312	CLA	C3B-C2B	-2.54	1.36	1.40
19	B	825	CLA	C4B-NB	-2.54	1.32	1.35
19	5	306	CLA	CHC-C1C	2.54	1.41	1.35
19	8	313	CLA	C3B-C2B	-2.54	1.36	1.40
19	Z	312	CLA	CHC-C1C	2.54	1.41	1.35
19	3	5013	CLA	C3D-C4D	-2.54	1.38	1.44
18	A	801	CL0	C1C-NC	-2.54	1.34	1.37
19	6	323	CLA	CHC-C1C	2.53	1.41	1.35
19	A	840	CLA	C3D-C4D	-2.53	1.38	1.44
19	7	308	CLA	CHC-C1C	2.53	1.41	1.35
22	6	307	BCR	C7-C6	2.53	1.54	1.45
19	8	313	CLA	CHC-C1C	2.53	1.41	1.35
19	A	836	CLA	C3B-C2B	-2.53	1.36	1.40
19	6	318	CLA	CHC-C1C	2.53	1.41	1.35
34	8	322	3PH	O21-C2	-2.53	1.40	1.46
19	B	840	CLA	C3D-C4D	-2.53	1.38	1.44
19	5	307	CLA	CHC-C1C	2.53	1.41	1.35
19	7	310	CLA	C3D-C4D	-2.53	1.38	1.44
31	6	305	LUT	C34-C33	-2.52	1.32	1.35
19	B	831	CLA	C4B-NB	-2.52	1.33	1.35
19	5	321	CLA	CHC-C1C	2.52	1.41	1.35
19	B	836	CLA	CHC-C1C	2.52	1.41	1.35
19	3	5018	CLA	CHC-C1C	2.52	1.41	1.35
19	6	318	CLA	C3B-C2B	-2.52	1.36	1.40
19	8	314	CLA	CHC-C1C	2.52	1.41	1.35
19	B	831	CLA	C3D-C4D	-2.52	1.38	1.44
19	5	321	CLA	C3B-C2B	-2.52	1.36	1.40
32	1	5009	CHL	CHC-C1C	2.51	1.41	1.35
19	5	325	CLA	C3D-C4D	-2.51	1.38	1.44
19	1	5008	CLA	CHC-C1C	2.51	1.41	1.35
38	6	326	ERG	C1-C2	-2.51	1.48	1.53
19	8	310	CLA	CHC-C1C	2.51	1.41	1.35
19	7	307	CLA	C3D-C4D	-2.51	1.38	1.44
19	A	832	CLA	C3B-C2B	-2.51	1.36	1.40
19	8	320	CLA	C3B-C2B	-2.51	1.36	1.40
19	6	320	CLA	CHC-C1C	2.50	1.41	1.35
19	4	309	CLA	C3B-C2B	-2.50	1.36	1.40
19	7	306	CLA	C3D-C4D	-2.50	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	818	CLA	C3B-C2B	-2.50	1.36	1.40
19	8	318	CLA	CHC-C1C	2.50	1.41	1.35
19	B	803	CLA	C3B-C2B	-2.50	1.36	1.40
19	3	5019	CLA	C3B-C2B	-2.50	1.36	1.40
22	A	849	BCR	C7-C6	2.49	1.54	1.45
32	8	319	CHL	C4B-NB	2.49	1.37	1.35
32	3	5017	CHL	C1D-ND	-2.49	1.34	1.37
22	8	306	BCR	C39-C30	-2.49	1.48	1.53
32	Z	302	CHL	C1D-ND	-2.49	1.34	1.37
28	J	1902	C7Z	C20-C13	2.49	1.56	1.50
31	4	304	LUT	C34-C33	-2.49	1.32	1.35
19	Z	305	CLA	C3D-C4D	-2.49	1.38	1.44
19	3	5012	CLA	C3D-C4D	-2.48	1.38	1.44
19	7	311	CLA	C3B-C2B	-2.48	1.36	1.40
19	A	815	CLA	C3B-C2B	-2.48	1.36	1.40
19	3	5008	CLA	CHC-C1C	2.48	1.41	1.35
19	7	309	CLA	CHC-C1C	2.48	1.41	1.35
19	7	311	CLA	C3D-C4D	-2.47	1.38	1.44
19	A	815	CLA	CHC-C1C	2.47	1.41	1.35
38	6	326	ERG	C19-C10	-2.47	1.50	1.54
32	3	5017	CHL	C4B-NB	2.47	1.37	1.35
31	8	304	LUT	C26-C27	2.47	1.53	1.50
19	6	302	CLA	C3B-C2B	-2.47	1.36	1.40
19	1	5006	CLA	CHC-C1C	2.47	1.41	1.35
19	1	5015	CLA	CHC-C1C	2.47	1.41	1.35
19	4	308	CLA	CHC-C1C	2.47	1.41	1.35
19	5	310	CLA	C3D-C4D	-2.47	1.38	1.44
19	4	309	CLA	CHC-C1C	2.46	1.41	1.35
19	B	812	CLA	C3B-C2B	-2.46	1.36	1.40
19	B	825	CLA	C3B-C2B	-2.46	1.36	1.40
19	B	850	CLA	C3D-C4D	-2.46	1.38	1.44
19	B	825	CLA	C3D-C4D	-2.46	1.38	1.44
19	F	301	CLA	C3D-C4D	-2.46	1.38	1.44
19	7	308	CLA	C3D-C4D	-2.46	1.38	1.44
28	1	5005	C7Z	C38-C25	2.46	1.55	1.50
19	7	324	CLA	C3D-C4D	-2.46	1.38	1.44
19	B	810	CLA	C3B-C2B	-2.46	1.37	1.40
19	B	817	CLA	C3B-C2B	-2.46	1.37	1.40
19	6	309	CLA	C4B-NB	-2.46	1.33	1.35
22	F	302	BCR	C36-C18	2.46	1.56	1.50
22	6	307	BCR	C39-C30	-2.46	1.48	1.53
19	7	311	CLA	C4B-NB	-2.46	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	8	316	CHL	C4B-NB	2.46	1.37	1.35
19	Z	303	CLA	C3B-C2B	-2.45	1.37	1.40
19	3	5008	CLA	C3D-C4D	-2.45	1.38	1.44
19	Z	311	CLA	CHC-C1C	2.45	1.41	1.35
19	3	5019	CLA	CHC-C1C	2.45	1.41	1.35
19	4	312	CLA	C3B-C2B	-2.45	1.37	1.40
19	1	5013	CLA	C3D-C4D	-2.45	1.38	1.44
19	A	815	CLA	C3D-C4D	-2.45	1.38	1.44
22	B	846	BCR	C36-C18	2.45	1.55	1.50
19	7	313	CLA	C3D-C4D	-2.45	1.38	1.44
19	B	826	CLA	C3B-C2B	-2.45	1.37	1.40
19	7	309	CLA	C3D-C4D	-2.45	1.38	1.44
32	5	318	CHL	C1D-ND	-2.45	1.34	1.37
19	5	308	CLA	C3D-C4D	-2.45	1.38	1.44
28	6	304	C7Z	C20-C13	2.45	1.55	1.50
19	3	5020	CLA	C3D-C4D	-2.44	1.38	1.44
19	Z	304	CLA	CHC-C1C	2.44	1.41	1.35
19	A	812	CLA	C3D-C4D	-2.44	1.38	1.44
22	A	846	BCR	C36-C18	2.44	1.55	1.50
19	3	5020	CLA	C4B-NB	-2.44	1.33	1.35
19	1	5008	CLA	C3D-C4D	-2.44	1.38	1.44
19	Z	306	CLA	C3D-C4D	-2.44	1.38	1.44
19	6	320	CLA	C3D-C4D	-2.44	1.38	1.44
22	K	206	BCR	C36-C18	2.44	1.55	1.50
19	Z	304	CLA	C3B-C2B	-2.44	1.37	1.40
32	8	316	CHL	C3B-C2B	-2.44	1.37	1.40
19	3	5018	CLA	C3D-C4D	-2.44	1.38	1.44
19	A	840	CLA	C3B-C2B	-2.44	1.37	1.40
19	5	321	CLA	C3D-C4D	-2.43	1.38	1.44
19	A	833	CLA	C3B-C2B	-2.43	1.37	1.40
27	4	303	RRX	C14-C13	-2.43	1.32	1.35
32	4	314	CHL	C3A-C2A	-2.43	1.47	1.54
22	8	303	BCR	C36-C18	2.43	1.55	1.50
22	5	304	BCR	C39-C30	-2.43	1.49	1.53
19	Z	314	CLA	C3B-C2B	-2.43	1.37	1.40
22	B	847	BCR	C36-C18	2.43	1.55	1.50
19	5	307	CLA	C3D-C4D	-2.43	1.38	1.44
19	8	309	CLA	C3D-C4D	-2.43	1.38	1.44
19	7	316	CLA	C3D-C4D	-2.43	1.38	1.44
22	5	305	BCR	C7-C6	2.43	1.53	1.45
19	7	309	CLA	C3B-C2B	-2.43	1.37	1.40
19	8	307	CLA	C3D-C4D	-2.43	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	G	1602	CLA	C3B-C2B	-2.42	1.37	1.40
19	5	317	CLA	C3D-C4D	-2.42	1.38	1.44
22	3	5004	BCR	C34-C9	2.42	1.55	1.50
19	7	324	CLA	CHC-C1C	2.42	1.41	1.35
19	1	5006	CLA	C3B-C2B	-2.42	1.37	1.40
27	5	302	RRX	C14-C13	-2.42	1.32	1.35
32	6	315	CHL	C1D-ND	-2.42	1.34	1.37
22	3	5004	BCR	C7-C6	2.42	1.53	1.45
19	6	312	CLA	C3D-C4D	-2.42	1.38	1.44
19	7	316	CLA	CHC-C1C	2.42	1.41	1.35
19	5	306	CLA	C3D-C4D	-2.42	1.38	1.44
19	8	307	CLA	C4B-NB	-2.42	1.33	1.35
19	7	311	CLA	CHC-C1C	2.42	1.41	1.35
19	5	322	CLA	C3B-C2B	-2.42	1.37	1.40
19	6	322	CLA	C3D-C4D	-2.41	1.38	1.44
22	A	847	BCR	C36-C18	2.41	1.55	1.50
19	6	318	CLA	C3D-C4D	-2.41	1.38	1.44
19	K	205	CLA	C3B-C2B	-2.41	1.37	1.40
19	A	803	CLA	C3B-C2B	-2.41	1.37	1.40
19	1	5008	CLA	C3B-C2B	-2.41	1.37	1.40
19	8	307	CLA	CHC-C1C	2.41	1.41	1.35
22	B	842	BCR	C36-C18	2.41	1.55	1.50
19	7	307	CLA	C4B-NB	-2.41	1.33	1.35
19	5	301	CLA	C3B-C2B	-2.41	1.37	1.40
31	1	5003	LUT	C18-C5	2.41	1.54	1.50
31	7	304	LUT	C34-C33	-2.41	1.32	1.35
19	3	5020	CLA	C3B-C2B	-2.41	1.37	1.40
19	A	824	CLA	C3B-C2B	-2.41	1.37	1.40
19	A	802	CLA	C3B-C2B	-2.41	1.37	1.40
32	6	316	CHL	C1D-ND	-2.41	1.34	1.37
19	A	809	CLA	C3B-C2B	-2.41	1.37	1.40
19	3	5011	CLA	C3D-C4D	-2.40	1.38	1.44
19	3	5019	CLA	C3D-C4D	-2.40	1.38	1.44
19	7	306	CLA	C3B-C2B	-2.40	1.37	1.40
19	4	316	CLA	C3D-C4D	-2.40	1.38	1.44
22	8	306	BCR	C7-C6	2.40	1.53	1.45
19	A	841	CLA	C3B-C2B	-2.40	1.37	1.40
28	J	1902	C7Z	C38-C25	2.40	1.54	1.50
34	3	5022	3PH	O31-C31	2.40	1.40	1.33
19	A	829	CLA	C3B-C2B	-2.40	1.37	1.40
22	A	858	BCR	C36-C18	2.39	1.55	1.50
19	B	804	CLA	C3B-C2B	-2.39	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	306	CLA	C3D-C4D	-2.39	1.38	1.44
19	1	5018	CLA	C3B-C2B	-2.39	1.37	1.40
19	Z	311	CLA	C4B-NB	-2.39	1.33	1.35
19	7	318	CLA	C3D-C4D	-2.39	1.38	1.44
22	B	844	BCR	C36-C18	2.39	1.55	1.50
27	F	304	RRX	C34-C9	2.39	1.55	1.50
19	7	312	CLA	C3B-C2B	-2.39	1.37	1.40
19	3	5020	CLA	CHC-C1C	2.39	1.41	1.35
19	B	831	CLA	CHC-C1C	2.39	1.41	1.35
22	3	5005	BCR	C34-C9	2.39	1.55	1.50
31	8	305	LUT	C18-C5	2.38	1.54	1.50
19	4	308	CLA	C4B-NB	-2.38	1.33	1.35
19	B	833	CLA	C3B-C2B	-2.38	1.37	1.40
22	3	5006	BCR	C36-C18	2.38	1.55	1.50
22	6	308	BCR	C39-C30	-2.38	1.49	1.53
19	8	313	CLA	C3D-C4D	-2.38	1.38	1.44
19	5	309	CLA	C3D-C4D	-2.38	1.38	1.44
19	3	5014	CLA	C3B-C2B	-2.38	1.37	1.40
19	Z	315	CLA	C3D-C4D	-2.38	1.38	1.44
22	7	305	BCR	C36-C18	2.38	1.55	1.50
19	A	842	CLA	C3B-C2B	-2.38	1.37	1.40
22	3	5005	BCR	C39-C30	-2.38	1.49	1.53
19	A	810	CLA	C3D-C4D	-2.38	1.38	1.44
19	8	314	CLA	C3D-C4D	-2.37	1.38	1.44
19	1	5007	CLA	CHC-C1C	2.37	1.41	1.35
19	Z	307	CLA	C3D-C4D	-2.37	1.38	1.44
19	B	828	CLA	C3B-C2B	-2.37	1.37	1.40
19	Z	305	CLA	C3B-C2B	-2.37	1.37	1.40
19	6	313	CLA	C3B-C2B	-2.37	1.37	1.40
32	5	316	CHL	C3B-C2B	-2.37	1.37	1.40
32	5	318	CHL	C3B-C2B	-2.37	1.37	1.40
32	5	315	CHL	CHC-C1C	2.37	1.41	1.35
19	1	5015	CLA	C3D-C4D	-2.37	1.38	1.44
19	8	318	CLA	C4B-NB	-2.37	1.33	1.35
19	3	5010	CLA	C3D-C4D	-2.37	1.38	1.44
19	A	823	CLA	C3B-C2B	-2.37	1.37	1.40
19	1	5006	CLA	C3D-C4D	-2.37	1.38	1.44
19	3	5009	CLA	C3D-C4D	-2.37	1.38	1.44
19	6	323	CLA	C3D-C4D	-2.37	1.38	1.44
32	Z	310	CHL	C1D-ND	-2.37	1.34	1.37
19	8	310	CLA	C3D-C4D	-2.37	1.38	1.44
27	4	303	RRX	C10-C9	-2.36	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	309	CLA	C3D-C4D	-2.36	1.38	1.44
19	6	314	CLA	C3B-C2B	-2.36	1.37	1.40
34	5	324	3PH	O31-C31	2.36	1.40	1.33
19	B	840	CLA	C4B-NB	-2.36	1.33	1.35
19	6	301	CLA	C3D-C4D	-2.36	1.38	1.44
28	J	1902	C7Z	C40-C33	2.36	1.55	1.50
19	B	820	CLA	C3B-C2B	-2.36	1.37	1.40
19	5	313	CLA	C3D-C4D	-2.36	1.38	1.44
22	7	305	BCR	C38-C26	2.36	1.54	1.50
31	7	303	LUT	C18-C5	2.36	1.54	1.50
22	A	859	BCR	C36-C18	2.36	1.55	1.50
19	Z	311	CLA	C3D-C4D	-2.36	1.38	1.44
22	5	305	BCR	C39-C30	-2.36	1.49	1.53
19	A	807	CLA	C3B-C2B	-2.36	1.37	1.40
19	5	311	CLA	C3D-C4D	-2.36	1.38	1.44
19	G	1601	CLA	C3B-C2B	-2.36	1.37	1.40
22	A	850	BCR	C36-C18	2.36	1.55	1.50
19	4	307	CLA	C3D-C4D	-2.36	1.38	1.44
19	1	5016	CLA	C3B-C2B	-2.36	1.37	1.40
19	6	323	CLA	C3B-C2B	-2.35	1.37	1.40
31	7	303	LUT	C14-C13	-2.35	1.32	1.35
32	6	319	CHL	C1D-ND	-2.35	1.34	1.37
19	B	808	CLA	C3B-C2B	-2.35	1.37	1.40
19	B	839	CLA	C3B-C2B	-2.35	1.37	1.40
32	3	5017	CHL	C3B-C2B	-2.35	1.37	1.40
19	A	834	CLA	C3B-C2B	-2.34	1.37	1.40
19	Z	304	CLA	C3D-C4D	-2.34	1.38	1.44
19	4	313	CLA	C3D-C4D	-2.34	1.38	1.44
31	6	306	LUT	C26-C27	2.34	1.53	1.50
19	A	808	CLA	C3B-C2B	-2.34	1.37	1.40
22	3	5004	BCR	C39-C30	-2.34	1.49	1.53
19	Z	303	CLA	C3D-C4D	-2.34	1.38	1.44
28	6	304	C7Z	C38-C25	2.34	1.54	1.50
31	6	305	LUT	C18-C5	2.34	1.54	1.50
19	5	314	CLA	C3D-C4D	-2.33	1.38	1.44
19	6	309	CLA	C3D-C4D	-2.33	1.38	1.44
19	6	310	CLA	C3D-C4D	-2.33	1.38	1.44
22	G	1603	BCR	C36-C18	2.33	1.55	1.50
19	6	313	CLA	CHC-C1C	2.33	1.40	1.35
19	7	318	CLA	C4B-NB	-2.33	1.33	1.35
19	B	840	CLA	C3B-C2B	-2.33	1.37	1.40
19	3	5013	CLA	CHC-C1C	2.33	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	8	308	CLA	C3D-C4D	-2.33	1.38	1.44
31	8	304	LUT	C18-C5	2.33	1.54	1.50
38	8	325	ERG	C1-C10	2.33	1.58	1.54
19	5	319	CLA	C3D-C4D	-2.33	1.38	1.44
19	Z	303	CLA	CHC-C1C	2.33	1.40	1.35
22	B	843	BCR	C37-C22	2.33	1.55	1.50
19	1	5008	CLA	C4B-NB	-2.33	1.33	1.35
19	K	204	CLA	C3B-C2B	-2.33	1.37	1.40
19	A	810	CLA	C4B-NB	-2.33	1.33	1.35
32	3	5017	CHL	C1B-NB	-2.32	1.33	1.35
19	B	837	CLA	C3B-C2B	-2.32	1.37	1.40
19	A	820	CLA	C3B-C2B	-2.32	1.37	1.40
28	6	304	C7Z	C40-C33	2.32	1.55	1.50
19	5	306	CLA	C4B-NB	-2.32	1.33	1.35
18	A	801	CL0	C1D-C2D	2.32	1.49	1.45
31	1	5004	LUT	C18-C5	2.32	1.54	1.50
28	1	5005	C7Z	C20-C13	2.31	1.55	1.50
32	4	317	CHL	CHC-C1C	2.31	1.40	1.35
19	3	5019	CLA	C4B-NB	-2.31	1.33	1.35
31	Z	318	LUT	C18-C5	2.31	1.54	1.50
19	1	5007	CLA	C4B-NB	-2.31	1.33	1.35
22	3	5005	BCR	C7-C6	2.31	1.53	1.45
22	B	843	BCR	C39-C30	-2.31	1.49	1.53
31	3	5002	LUT	C34-C33	-2.31	1.32	1.35
22	4	305	BCR	C36-C18	2.31	1.55	1.50
22	B	845	BCR	C36-C18	2.31	1.55	1.50
19	8	312	CLA	C3D-C4D	-2.31	1.39	1.44
19	B	827	CLA	C3B-C2B	-2.30	1.37	1.40
32	6	321	CHL	C3A-C2A	-2.30	1.48	1.54
32	8	317	CHL	C3A-C2A	-2.30	1.48	1.54
19	F	303	CLA	C3B-C2B	-2.30	1.37	1.40
19	7	310	CLA	C4B-NB	-2.30	1.33	1.35
31	6	305	LUT	C14-C13	-2.30	1.32	1.35
19	Z	312	CLA	C3D-C4D	-2.29	1.39	1.44
34	6	325	3PH	O31-C31	2.29	1.40	1.33
19	A	815	CLA	C4B-NB	-2.29	1.33	1.35
27	5	302	RRX	C10-C9	-2.29	1.32	1.35
19	5	311	CLA	C4B-NB	-2.29	1.33	1.35
32	Z	302	CHL	CHC-C1C	2.29	1.40	1.35
38	8	325	ERG	C1-C2	-2.29	1.48	1.53
34	6	325	3PH	O21-C21	2.29	1.40	1.34
19	K	203	CLA	C3B-C2B	-2.29	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	5003	LUT	C18-C5	2.29	1.54	1.50
19	3	5008	CLA	C4B-NB	-2.29	1.33	1.35
19	5	310	CLA	C4B-NB	-2.28	1.33	1.35
19	5	321	CLA	C4B-NB	-2.28	1.33	1.35
22	4	305	BCR	C39-C30	-2.28	1.49	1.53
19	3	5013	CLA	C4B-NB	-2.28	1.33	1.35
34	3	5022	3PH	O21-C2	-2.28	1.40	1.46
19	7	307	CLA	C3B-C2B	-2.28	1.37	1.40
19	4	311	CLA	C3B-C2B	-2.28	1.37	1.40
19	6	313	CLA	C3D-C4D	-2.28	1.39	1.44
19	Z	303	CLA	C4B-NB	-2.28	1.33	1.35
19	7	307	CLA	CHC-C1C	2.27	1.40	1.35
19	6	313	CLA	C4B-NB	-2.27	1.33	1.35
19	B	805	CLA	C1C-C2C	2.27	1.49	1.44
19	Z	312	CLA	C3B-C2B	-2.27	1.37	1.40
32	8	319	CHL	C1D-ND	-2.26	1.35	1.37
31	5	303	LUT	C18-C5	2.26	1.54	1.50
22	6	307	BCR	C36-C18	2.25	1.55	1.50
19	3	5015	CLA	C3B-C2B	-2.25	1.37	1.40
34	8	322	3PH	O31-C3	-2.25	1.40	1.45
19	Z	311	CLA	C3B-C2B	-2.24	1.37	1.40
19	4	309	CLA	C4B-NB	-2.24	1.33	1.35
28	1	5005	C7Z	C40-C33	2.24	1.55	1.50
31	8	305	LUT	C14-C13	-2.24	1.32	1.35
22	3	5007	BCR	C36-C18	2.24	1.55	1.50
32	8	315	CHL	C3A-C2A	-2.24	1.48	1.54
19	A	857	CLA	C3B-C2B	-2.24	1.37	1.40
31	3	5002	LUT	C18-C5	2.24	1.54	1.50
19	G	1602	CLA	C1C-C2C	2.24	1.48	1.44
19	B	824	CLA	C3B-C2B	-2.24	1.37	1.40
22	A	848	BCR	C36-C18	2.24	1.55	1.50
32	6	315	CHL	C3A-C2A	-2.23	1.48	1.54
19	7	319	CLA	C3B-C2B	-2.23	1.37	1.40
27	4	303	RRX	C34-C9	2.23	1.55	1.50
23	7	320	LHG	O7-C5	-2.23	1.41	1.46
31	Z	318	LUT	C34-C33	-2.23	1.32	1.35
22	B	842	BCR	C39-C30	-2.23	1.49	1.53
19	3	5016	CLA	C3B-C2B	-2.23	1.37	1.40
32	Z	313	CHL	C3A-C2A	-2.22	1.48	1.54
19	B	840	CLA	CHC-C1C	2.22	1.40	1.35
19	B	811	CLA	C1C-C2C	2.22	1.48	1.44
19	A	806	CLA	C1C-C2C	2.22	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	818	CLA	C1C-C2C	2.22	1.48	1.44
31	1	5004	LUT	C14-C13	-2.22	1.32	1.35
35	7	302	DGA	OG2-CG2	-2.22	1.41	1.46
19	J	1901	CLA	C1C-C2C	2.22	1.48	1.44
19	8	312	CLA	C1C-C2C	2.21	1.48	1.44
19	A	816	CLA	C3B-C2B	-2.21	1.37	1.40
32	5	320	CHL	C3B-C2B	-2.21	1.37	1.40
22	G	1603	BCR	C39-C30	-2.21	1.49	1.53
19	8	313	CLA	C4B-NB	-2.21	1.33	1.35
19	4	308	CLA	C3D-C4D	-2.21	1.39	1.44
19	3	5011	CLA	C4B-NB	-2.21	1.33	1.35
34	8	322	3PH	O31-C31	2.21	1.39	1.33
19	B	812	CLA	C1C-C2C	2.21	1.48	1.44
19	A	828	CLA	C3B-C2B	-2.21	1.37	1.40
19	3	5015	CLA	C3D-C4D	-2.20	1.39	1.44
22	8	303	BCR	C39-C30	-2.20	1.49	1.53
34	6	325	3PH	O21-C2	-2.20	1.41	1.46
34	6	325	3PH	O31-C3	-2.20	1.40	1.45
28	1	5005	C7Z	C19-C9	2.20	1.55	1.50
31	6	306	LUT	C30-C29	-2.19	1.32	1.35
19	4	312	CLA	C1C-C2C	2.19	1.48	1.44
28	6	304	C7Z	C19-C9	2.19	1.55	1.50
19	A	841	CLA	C1C-C2C	2.19	1.48	1.44
19	A	831	CLA	C3B-C2B	-2.19	1.37	1.40
22	A	846	BCR	C39-C30	-2.19	1.49	1.53
34	5	324	3PH	O31-C3	-2.19	1.40	1.45
31	Z	317	LUT	C18-C5	2.19	1.54	1.50
19	A	804	CLA	C1C-C2C	2.19	1.48	1.44
22	A	858	BCR	C39-C30	-2.19	1.49	1.53
19	A	840	CLA	C4B-NB	-2.19	1.33	1.35
22	8	303	BCR	C38-C26	2.19	1.54	1.50
19	F	303	CLA	C1C-C2C	2.18	1.48	1.44
19	K	202	CLA	C3B-C2B	-2.18	1.37	1.40
22	B	847	BCR	C37-C22	2.18	1.55	1.50
32	8	317	CHL	C1D-ND	-2.18	1.35	1.37
22	A	848	BCR	C38-C26	2.18	1.54	1.50
19	3	5018	CLA	C4B-NB	-2.18	1.33	1.35
32	6	315	CHL	C1A-CHA	-2.18	1.34	1.43
19	B	838	CLA	C3B-C2B	-2.17	1.37	1.40
19	B	806	CLA	C1C-C2C	2.17	1.48	1.44
19	B	801	CLA	C3B-C2B	-2.17	1.37	1.40
22	A	849	BCR	C36-C18	2.17	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	829	CLA	C1C-C2C	2.17	1.48	1.44
19	5	301	CLA	C1C-C2C	2.17	1.48	1.44
19	1	5006	CLA	C4B-NB	-2.17	1.33	1.35
34	3	5022	3PH	O21-C21	2.17	1.40	1.34
28	J	1902	C7Z	C19-C9	2.17	1.55	1.50
19	B	821	CLA	C1C-C2C	2.17	1.48	1.44
22	B	844	BCR	C39-C30	-2.17	1.49	1.53
19	A	802	CLA	C1C-C2C	2.16	1.48	1.44
19	5	312	CLA	C1C-C2C	2.16	1.48	1.44
19	B	803	CLA	C1C-C2C	2.16	1.48	1.44
19	8	310	CLA	C3B-C2B	-2.16	1.37	1.40
19	A	809	CLA	C1C-C2C	2.16	1.48	1.44
19	B	822	CLA	C1C-C2C	2.16	1.48	1.44
22	A	859	BCR	C39-C30	-2.16	1.49	1.53
27	F	304	RRX	C33-C5	2.16	1.54	1.50
19	1	5016	CLA	C1C-C2C	2.16	1.48	1.44
19	4	311	CLA	C3D-C4D	-2.16	1.39	1.44
22	3	5005	BCR	C10-C9	-2.16	1.32	1.35
22	3	5006	BCR	C39-C30	-2.16	1.49	1.53
31	7	304	LUT	C26-C27	2.16	1.53	1.50
19	1	5012	CLA	C3B-C2B	-2.16	1.37	1.40
19	B	838	CLA	C1C-C2C	2.16	1.48	1.44
22	A	850	BCR	C39-C30	-2.16	1.49	1.53
19	A	807	CLA	C1C-C2C	2.16	1.48	1.44
19	A	803	CLA	C1C-C2C	2.16	1.48	1.44
19	A	837	CLA	C1C-C2C	2.16	1.48	1.44
31	3	5003	LUT	C34-C33	-2.16	1.32	1.35
32	8	316	CHL	C3A-C2A	-2.16	1.48	1.54
19	3	5014	CLA	C1C-C2C	2.15	1.48	1.44
31	7	304	LUT	C30-C29	-2.15	1.32	1.35
19	4	318	CLA	C3B-C2B	-2.15	1.37	1.40
19	A	826	CLA	C1C-C2C	2.15	1.48	1.44
19	B	818	CLA	C1C-C2C	2.15	1.48	1.44
19	6	314	CLA	C1C-C2C	2.15	1.48	1.44
19	A	857	CLA	C1C-C2C	2.15	1.48	1.44
31	Z	317	LUT	C34-C33	-2.15	1.32	1.35
19	A	811	CLA	C1C-C2C	2.15	1.48	1.44
22	A	847	BCR	C37-C22	2.15	1.55	1.50
19	B	820	CLA	C1C-C2C	2.15	1.48	1.44
19	A	822	CLA	C1C-C2C	2.15	1.48	1.44
19	B	801	CLA	C1C-C2C	2.15	1.48	1.44
22	A	859	BCR	C38-C26	2.15	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	6	302	CLA	C1C-C2C	2.14	1.48	1.44
19	B	816	CLA	C1C-C2C	2.14	1.48	1.44
19	A	828	CLA	C1C-C2C	2.14	1.48	1.44
19	B	814	CLA	C1C-C2C	2.14	1.48	1.44
22	A	848	BCR	C39-C30	-2.14	1.49	1.53
32	4	319	CHL	C3B-C2B	-2.14	1.37	1.40
32	5	315	CHL	C1A-CHA	-2.14	1.34	1.43
22	B	847	BCR	C39-C30	-2.14	1.49	1.53
22	F	302	BCR	C39-C30	-2.14	1.49	1.53
31	6	306	LUT	C18-C5	2.14	1.54	1.50
19	B	824	CLA	C1C-C2C	2.14	1.48	1.44
19	B	833	CLA	C1C-C2C	2.14	1.48	1.44
31	7	304	LUT	C18-C5	2.14	1.54	1.50
32	3	5017	CHL	C1C-NC	-2.14	1.34	1.37
19	A	820	CLA	C1C-C2C	2.14	1.48	1.44
22	F	302	BCR	C37-C22	2.14	1.55	1.50
19	A	824	CLA	C1C-C2C	2.14	1.48	1.44
19	A	827	CLA	C1C-C2C	2.13	1.48	1.44
19	B	839	CLA	C1C-C2C	2.13	1.48	1.44
22	B	845	BCR	C39-C30	-2.13	1.49	1.53
19	A	842	CLA	C1C-C2C	2.13	1.48	1.44
19	7	317	CLA	C3B-C2B	-2.13	1.37	1.40
19	B	827	CLA	C1C-C2C	2.13	1.48	1.44
19	B	807	CLA	C1C-C2C	2.13	1.48	1.44
19	7	312	CLA	C1C-C2C	2.13	1.48	1.44
19	Z	314	CLA	C1C-C2C	2.13	1.48	1.44
22	A	858	BCR	C38-C26	2.13	1.54	1.50
22	A	847	BCR	C39-C30	-2.13	1.49	1.53
19	B	809	CLA	C3B-C2B	-2.13	1.37	1.40
19	B	834	CLA	C1C-C2C	2.13	1.48	1.44
22	K	206	BCR	C37-C22	2.13	1.55	1.50
19	B	823	CLA	C3B-C2B	-2.13	1.37	1.40
22	K	206	BCR	C39-C30	-2.13	1.49	1.53
38	6	326	ERG	C14-C8	2.13	1.57	1.51
22	B	844	BCR	C38-C26	2.13	1.54	1.50
19	6	318	CLA	C4B-NB	-2.13	1.33	1.35
19	1	5018	CLA	C1C-C2C	2.13	1.48	1.44
19	B	810	CLA	C1C-C2C	2.12	1.48	1.44
19	A	819	CLA	C1C-C2C	2.12	1.48	1.44
19	5	322	CLA	C1C-C2C	2.12	1.48	1.44
19	A	825	CLA	C1C-C2C	2.12	1.48	1.44
19	1	5011	CLA	C3B-C2B	-2.12	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	842	BCR	C38-C26	2.12	1.54	1.50
32	5	316	CHL	C1A-CHA	-2.12	1.34	1.43
22	5	304	BCR	C36-C18	2.12	1.55	1.50
19	3	5016	CLA	C1C-C2C	2.12	1.48	1.44
22	8	306	BCR	C36-C18	2.12	1.55	1.50
22	A	846	BCR	C38-C26	2.12	1.54	1.50
22	6	308	BCR	C36-C18	2.12	1.55	1.50
32	8	319	CHL	C3B-C2B	-2.11	1.37	1.40
22	B	842	BCR	C37-C22	2.11	1.55	1.50
19	B	830	CLA	C1C-C2C	2.11	1.48	1.44
19	A	808	CLA	C1C-C2C	2.11	1.48	1.44
22	A	850	BCR	C38-C26	2.11	1.54	1.50
32	7	314	CHL	C1A-CHA	-2.11	1.34	1.43
22	A	859	BCR	C37-C22	2.11	1.55	1.50
19	B	828	CLA	C1C-C2C	2.11	1.48	1.44
19	A	835	CLA	C3B-C2B	-2.11	1.37	1.40
19	A	833	CLA	C1C-C2C	2.11	1.48	1.44
22	A	847	BCR	C38-C26	2.11	1.54	1.50
22	A	858	BCR	C37-C22	2.11	1.55	1.50
19	A	823	CLA	C1C-C2C	2.11	1.48	1.44
27	5	302	RRX	C34-C9	2.11	1.55	1.50
19	8	314	CLA	C4B-NB	-2.11	1.33	1.35
19	A	822	CLA	C3B-C2B	-2.10	1.37	1.40
19	B	807	CLA	C1B-NB	2.10	1.37	1.35
19	6	312	CLA	C4B-NB	-2.10	1.33	1.35
19	6	322	CLA	C4B-NB	-2.10	1.33	1.35
22	3	5005	BCR	C36-C18	2.10	1.55	1.50
19	B	819	CLA	C3B-C2B	-2.10	1.37	1.40
32	1	5009	CHL	C1A-CHA	-2.10	1.34	1.43
22	B	845	BCR	C38-C26	2.10	1.54	1.50
22	F	302	BCR	C38-C26	2.10	1.54	1.50
19	A	843	CLA	C1C-C2C	2.10	1.48	1.44
22	B	846	BCR	C39-C30	-2.10	1.49	1.53
31	8	305	LUT	C35-C15	-2.10	1.30	1.36
22	3	5004	BCR	C36-C18	2.10	1.55	1.50
19	A	817	CLA	C1C-C2C	2.10	1.48	1.44
19	8	320	CLA	C1C-C2C	2.10	1.48	1.44
19	B	829	CLA	C3B-C2B	-2.10	1.37	1.40
19	I	201	CLA	C3B-C2B	-2.10	1.37	1.40
19	B	822	CLA	C3B-C2B	-2.10	1.37	1.40
22	B	846	BCR	C38-C26	2.10	1.54	1.50
19	A	835	CLA	C1C-C2C	2.09	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	5003	LUT	C30-C29	-2.09	1.33	1.35
32	Z	310	CHL	C1A-CHA	-2.09	1.34	1.43
19	A	836	CLA	C1C-C2C	2.09	1.48	1.44
22	A	846	BCR	C37-C22	2.09	1.55	1.50
19	A	831	CLA	C1C-C2C	2.09	1.48	1.44
22	K	206	BCR	C38-C26	2.09	1.54	1.50
22	A	850	BCR	C37-C22	2.09	1.55	1.50
19	7	316	CLA	C4B-NB	-2.09	1.33	1.35
32	6	316	CHL	C3A-C2A	-2.09	1.48	1.54
19	B	818	CLA	C3B-C2B	-2.09	1.37	1.40
19	A	819	CLA	C3B-C2B	-2.09	1.37	1.40
19	1	5012	CLA	C1C-C2C	2.09	1.48	1.44
34	3	5022	3PH	O31-C3	-2.09	1.40	1.45
32	6	321	CHL	C1D-ND	-2.09	1.35	1.37
19	Z	304	CLA	C4B-NB	-2.09	1.33	1.35
22	B	844	BCR	C37-C22	2.09	1.55	1.50
22	3	5006	BCR	C38-C26	2.08	1.54	1.50
22	3	5006	BCR	C37-C22	2.08	1.55	1.50
19	B	808	CLA	C1C-C2C	2.08	1.48	1.44
19	7	324	CLA	C4B-NB	-2.08	1.33	1.35
19	K	203	CLA	C1C-C2C	2.08	1.48	1.44
19	4	318	CLA	C1C-C2C	2.08	1.48	1.44
19	G	1602	CLA	C3D-C4D	-2.08	1.39	1.44
19	Z	308	CLA	C4B-NB	-2.08	1.33	1.35
19	A	805	CLA	C1C-C2C	2.08	1.48	1.44
19	A	839	CLA	C1C-C2C	2.08	1.48	1.44
19	I	201	CLA	C3D-C4D	-2.08	1.39	1.44
32	7	314	CHL	CHC-C1C	2.08	1.40	1.35
22	G	1603	BCR	C38-C26	2.08	1.54	1.50
19	B	805	CLA	C3B-C2B	-2.08	1.37	1.40
19	7	317	CLA	C3D-C4D	-2.08	1.39	1.44
19	B	829	CLA	C1C-C2C	2.07	1.48	1.44
19	1	5011	CLA	C1C-C2C	2.07	1.48	1.44
19	1	5011	CLA	C3D-C4D	-2.07	1.39	1.44
19	7	319	CLA	C1C-C2C	2.07	1.48	1.44
19	A	821	CLA	C3B-C2B	-2.07	1.37	1.40
19	B	830	CLA	C3B-C2B	-2.07	1.37	1.40
19	B	802	CLA	C1C-C2C	2.07	1.48	1.44
22	A	848	BCR	C37-C22	2.07	1.55	1.50
19	B	823	CLA	C1C-C2C	2.07	1.48	1.44
32	6	317	CHL	C3A-C2A	-2.07	1.48	1.54
34	8	322	3PH	O21-C21	2.07	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	811	CLA	C3B-C2B	-2.07	1.37	1.40
19	6	311	CLA	C4B-NB	-2.06	1.33	1.35
22	B	845	BCR	C37-C22	2.06	1.55	1.50
22	B	847	BCR	C38-C26	2.06	1.54	1.50
19	A	830	CLA	C1C-C2C	2.06	1.48	1.44
19	B	815	CLA	C1C-C2C	2.06	1.48	1.44
19	6	320	CLA	C4B-NB	-2.06	1.33	1.35
19	A	805	CLA	C3D-C4D	-2.06	1.39	1.44
22	8	303	BCR	C37-C22	2.06	1.55	1.50
19	A	830	CLA	C3B-C2B	-2.06	1.37	1.40
19	A	837	CLA	C3D-C4D	-2.06	1.39	1.44
19	B	835	CLA	C1C-C2C	2.06	1.48	1.44
19	B	837	CLA	C1C-C2C	2.06	1.48	1.44
19	A	837	CLA	C3B-C2B	-2.06	1.37	1.40
19	B	817	CLA	C3D-C4D	-2.06	1.39	1.44
19	A	805	CLA	C3B-C2B	-2.06	1.37	1.40
19	5	325	CLA	C4B-NB	-2.06	1.33	1.35
32	6	321	CHL	C1A-CHA	-2.06	1.34	1.43
19	A	834	CLA	C3D-C4D	-2.05	1.39	1.44
19	A	825	CLA	C3B-C2B	-2.05	1.37	1.40
32	5	318	CHL	C1A-CHA	-2.05	1.34	1.43
19	B	809	CLA	C1C-C2C	2.05	1.48	1.44
19	B	807	CLA	C3B-C2B	-2.05	1.37	1.40
19	1	5012	CLA	C1B-NB	2.05	1.37	1.35
19	1	5013	CLA	C4B-NB	-2.05	1.33	1.35
32	Z	313	CHL	C1A-CHA	-2.05	1.34	1.43
19	B	826	CLA	C1C-C2C	2.05	1.48	1.44
32	8	315	CHL	C1D-ND	-2.05	1.35	1.37
32	Z	313	CHL	C3B-C2B	-2.05	1.37	1.40
38	8	325	ERG	C18-C13	-2.05	1.50	1.54
19	F	301	CLA	C1C-C2C	2.05	1.48	1.44
31	5	303	LUT	C14-C13	-2.05	1.33	1.35
18	A	801	CL0	C4C-C3C	2.05	1.48	1.45
19	A	816	CLA	C1C-C2C	2.05	1.48	1.44
19	B	804	CLA	C1C-C2C	2.04	1.48	1.44
22	G	1603	BCR	C37-C22	2.04	1.55	1.50
19	B	807	CLA	C3D-C4D	-2.04	1.39	1.44
19	7	317	CLA	C1C-C2C	2.04	1.48	1.44
19	B	811	CLA	C3B-C2B	-2.04	1.37	1.40
19	A	814	CLA	C1C-C2C	2.04	1.48	1.44
19	B	819	CLA	C1C-C2C	2.04	1.48	1.44
19	A	821	CLA	C1C-C2C	2.04	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	J	1901	CLA	C3B-C2B	-2.04	1.37	1.40
19	B	804	CLA	C1A-CHA	2.04	1.51	1.43
22	A	849	BCR	C38-C26	2.04	1.54	1.50
19	A	816	CLA	C3D-C4D	-2.04	1.39	1.44
32	5	315	CHL	C3D-C4D	-2.04	1.39	1.44
19	K	204	CLA	C3D-C4D	-2.03	1.39	1.44
19	A	842	CLA	C1B-NB	2.03	1.37	1.35
32	1	5009	CHL	C3D-C4D	-2.03	1.39	1.44
19	B	811	CLA	C1B-NB	2.03	1.37	1.35
19	Z	315	CLA	C1C-C2C	2.03	1.48	1.44
32	3	5017	CHL	C1A-CHA	-2.03	1.34	1.43
19	8	308	CLA	C1C-C2C	2.03	1.48	1.44
19	B	814	CLA	C3B-C2B	-2.03	1.37	1.40
19	A	814	CLA	C3D-C4D	-2.03	1.39	1.44
19	A	819	CLA	C3D-C4D	-2.03	1.39	1.44
19	A	834	CLA	C1C-C2C	2.03	1.48	1.44
19	A	806	CLA	C1B-NB	2.03	1.37	1.35
19	A	832	CLA	C1C-C2C	2.03	1.48	1.44
22	6	307	BCR	C38-C26	2.02	1.54	1.50
19	A	811	CLA	C3D-C4D	-2.02	1.39	1.44
19	Z	314	CLA	C3D-C4D	-2.02	1.39	1.44
32	8	317	CHL	C3D-C4D	-2.02	1.39	1.44
19	B	827	CLA	C3D-C4D	-2.02	1.39	1.44
19	8	310	CLA	C4B-NB	-2.02	1.33	1.35
32	Z	302	CHL	C1A-CHA	-2.02	1.34	1.43
22	A	849	BCR	C39-C30	-2.02	1.49	1.53
19	B	838	CLA	C1B-NB	2.02	1.37	1.35
18	A	801	CL0	C1C-C2C	2.02	1.48	1.44
19	I	201	CLA	C1C-C2C	2.02	1.48	1.44
22	7	305	BCR	C37-C22	2.01	1.55	1.50
19	G	1601	CLA	C1C-C2C	2.01	1.48	1.44
34	5	324	3PH	O21-C21	2.01	1.40	1.34
19	3	5015	CLA	C4B-NB	-2.01	1.33	1.35
19	B	832	CLA	C1C-C2C	2.01	1.48	1.44
19	7	312	CLA	C1A-CHA	2.01	1.51	1.43
19	A	813	CLA	C3B-C2B	-2.01	1.37	1.40
19	B	817	CLA	C1C-C2C	2.01	1.48	1.44
19	A	836	CLA	C3D-C4D	-2.01	1.39	1.44
19	B	805	CLA	C3D-C4D	-2.01	1.39	1.44
31	Z	317	LUT	C28-C27	2.01	1.37	1.32
22	3	5006	BCR	C33-C5	2.01	1.54	1.50
19	4	318	CLA	C3D-C4D	-2.01	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	817	CLA	C3B-C2B	-2.01	1.37	1.40
19	B	816	CLA	C3B-C2B	-2.01	1.37	1.40
19	F	303	CLA	C1B-NB	2.01	1.37	1.35
19	G	1602	CLA	C1B-NB	2.01	1.37	1.35
19	B	803	CLA	C1B-NB	2.01	1.37	1.35
19	A	825	CLA	MG-NC	2.01	2.11	2.06
19	K	205	CLA	C1C-C2C	2.01	1.48	1.44
19	A	843	CLA	C3B-C2B	-2.01	1.37	1.40
19	A	832	CLA	C3D-C4D	-2.01	1.39	1.44
19	A	827	CLA	C3B-C2B	-2.01	1.37	1.40
22	A	849	BCR	C37-C22	2.01	1.55	1.50
19	A	843	CLA	C3D-C4D	-2.00	1.39	1.44
19	B	806	CLA	C3D-C4D	-2.00	1.39	1.44
19	B	811	CLA	C3D-C4D	-2.00	1.39	1.44
19	A	828	CLA	C1B-NB	2.00	1.37	1.35

All (4512) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Z	317	LUT	C35-C34-C33	-13.98	107.35	127.31
31	Z	317	LUT	C31-C30-C29	-13.44	108.13	127.31
22	3	5007	BCR	C11-C10-C9	-11.28	111.21	127.31
22	3	5007	BCR	C20-C21-C22	-10.51	112.31	127.31
19	B	831	CLA	C4A-NA-C1A	9.99	111.20	106.71
19	8	307	CLA	C4A-NA-C1A	9.70	111.06	106.71
19	B	836	CLA	C4A-NA-C1A	9.67	111.05	106.71
19	4	309	CLA	C4A-NA-C1A	9.66	111.05	106.71
19	7	307	CLA	C4A-NA-C1A	9.61	111.03	106.71
19	5	317	CLA	C4A-NA-C1A	9.61	111.03	106.71
19	7	311	CLA	C4A-NA-C1A	9.56	111.00	106.71
19	3	5013	CLA	C4A-NA-C1A	9.55	111.00	106.71
19	7	316	CLA	C4A-NA-C1A	9.50	110.98	106.71
19	3	5018	CLA	C4A-NA-C1A	9.48	110.97	106.71
19	B	840	CLA	C4A-NA-C1A	9.44	110.95	106.71
19	5	321	CLA	C4A-NA-C1A	9.40	110.93	106.71
19	6	313	CLA	C4A-NA-C1A	9.34	110.90	106.71
19	1	5006	CLA	C4A-NA-C1A	9.33	110.90	106.71
19	8	309	CLA	C4A-NA-C1A	9.31	110.89	106.71
19	A	815	CLA	C4A-NA-C1A	9.28	110.88	106.71
19	A	838	CLA	C4A-NA-C1A	9.25	110.86	106.71
19	A	843	CLA	C4A-NA-C1A	9.24	110.86	106.71
31	Z	317	LUT	C32-C33-C34	9.24	133.12	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	810	CLA	C4A-NA-C1A	9.23	110.86	106.71
19	3	5020	CLA	C4A-NA-C1A	9.23	110.86	106.71
19	5	306	CLA	C4A-NA-C1A	9.22	110.85	106.71
19	A	822	CLA	C4A-NA-C1A	9.20	110.84	106.71
19	Z	304	CLA	C4A-NA-C1A	9.20	110.84	106.71
19	7	310	CLA	C4A-NA-C1A	9.16	110.83	106.71
19	B	810	CLA	C4A-NA-C1A	9.14	110.82	106.71
19	7	306	CLA	C4A-NA-C1A	9.13	110.81	106.71
19	1	5007	CLA	C4A-NA-C1A	9.12	110.81	106.71
19	5	322	CLA	C4A-NA-C1A	9.11	110.80	106.71
19	4	308	CLA	C4A-NA-C1A	9.10	110.80	106.71
19	K	202	CLA	C4A-NA-C1A	9.08	110.79	106.71
19	B	802	CLA	C4A-NA-C1A	9.07	110.78	106.71
19	7	308	CLA	C4A-NA-C1A	9.06	110.78	106.71
19	7	319	CLA	C4A-NA-C1A	9.06	110.78	106.71
19	1	5015	CLA	C4A-NA-C1A	9.05	110.78	106.71
19	Z	312	CLA	C4A-NA-C1A	9.04	110.77	106.71
19	3	5014	CLA	C4A-NA-C1A	9.02	110.76	106.71
19	3	5011	CLA	C4A-NA-C1A	9.01	110.76	106.71
19	6	301	CLA	C4A-NA-C1A	9.01	110.76	106.71
19	A	817	CLA	C4A-NA-C1A	9.01	110.75	106.71
19	Z	311	CLA	C4A-NA-C1A	9.00	110.75	106.71
19	I	201	CLA	C4A-NA-C1A	8.99	110.75	106.71
19	A	826	CLA	C4A-NA-C1A	8.97	110.74	106.71
19	5	311	CLA	C4A-NA-C1A	8.97	110.74	106.71
19	A	839	CLA	C4A-NA-C1A	8.95	110.73	106.71
19	B	827	CLA	C4A-NA-C1A	8.93	110.72	106.71
19	3	5019	CLA	C4A-NA-C1A	8.93	110.72	106.71
19	3	5008	CLA	C4A-NA-C1A	8.91	110.71	106.71
19	A	816	CLA	C4A-NA-C1A	8.90	110.71	106.71
19	7	317	CLA	C4A-NA-C1A	8.90	110.71	106.71
19	4	306	CLA	C4A-NA-C1A	8.90	110.71	106.71
19	3	5015	CLA	C4A-NA-C1A	8.88	110.70	106.71
19	3	5016	CLA	C4A-NA-C1A	8.88	110.70	106.71
19	G	1601	CLA	C4A-NA-C1A	8.88	110.70	106.71
19	B	832	CLA	C4A-NA-C1A	8.86	110.69	106.71
19	K	204	CLA	C4A-NA-C1A	8.86	110.69	106.71
19	A	813	CLA	C4A-NA-C1A	8.85	110.69	106.71
19	Z	303	CLA	C4A-NA-C1A	8.84	110.68	106.71
19	A	808	CLA	C4A-NA-C1A	8.82	110.67	106.71
19	7	309	CLA	C4A-NA-C1A	8.81	110.67	106.71
19	8	318	CLA	C4A-NA-C1A	8.81	110.67	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	827	CLA	C4A-NA-C1A	8.80	110.66	106.71
19	A	841	CLA	C4A-NA-C1A	8.80	110.66	106.71
19	B	826	CLA	C4A-NA-C1A	8.80	110.66	106.71
19	4	312	CLA	C4A-NA-C1A	8.79	110.66	106.71
19	B	819	CLA	C4A-NA-C1A	8.79	110.66	106.71
19	B	808	CLA	C4A-NA-C1A	8.78	110.65	106.71
19	B	815	CLA	C4A-NA-C1A	8.77	110.65	106.71
19	5	310	CLA	C4A-NA-C1A	8.77	110.65	106.71
19	7	312	CLA	C4A-NA-C1A	8.75	110.64	106.71
19	5	325	CLA	C4A-NA-C1A	8.75	110.64	106.71
19	B	813	CLA	C4A-NA-C1A	8.75	110.64	106.71
19	6	311	CLA	C4A-NA-C1A	8.73	110.63	106.71
19	B	806	CLA	C4A-NA-C1A	8.73	110.63	106.71
22	5	305	BCR	C7-C8-C9	-8.73	113.04	126.23
19	K	205	CLA	C4A-NA-C1A	8.72	110.62	106.71
19	B	822	CLA	C4A-NA-C1A	8.71	110.62	106.71
19	5	319	CLA	C4A-NA-C1A	8.70	110.62	106.71
19	A	836	CLA	C4A-NA-C1A	8.70	110.62	106.71
19	6	314	CLA	C4A-NA-C1A	8.69	110.61	106.71
19	A	831	CLA	C4A-NA-C1A	8.69	110.61	106.71
19	B	805	CLA	C4A-NA-C1A	8.69	110.61	106.71
19	B	829	CLA	C4A-NA-C1A	8.68	110.61	106.71
19	B	821	CLA	C4A-NA-C1A	8.68	110.61	106.71
19	B	850	CLA	C4A-NA-C1A	8.68	110.61	106.71
19	Z	308	CLA	C4A-NA-C1A	8.67	110.60	106.71
19	A	833	CLA	C4A-NA-C1A	8.66	110.60	106.71
19	B	816	CLA	C4A-NA-C1A	8.66	110.60	106.71
19	B	817	CLA	C4A-NA-C1A	8.66	110.60	106.71
19	A	828	CLA	C4A-NA-C1A	8.66	110.60	106.71
19	B	814	CLA	C4A-NA-C1A	8.65	110.59	106.71
19	8	320	CLA	C4A-NA-C1A	8.65	110.59	106.71
19	A	825	CLA	C4A-NA-C1A	8.65	110.59	106.71
19	A	818	CLA	C4A-NA-C1A	8.64	110.59	106.71
19	A	805	CLA	C4A-NA-C1A	8.62	110.58	106.71
19	A	814	CLA	C4A-NA-C1A	8.62	110.58	106.71
19	A	807	CLA	C4A-NA-C1A	8.62	110.58	106.71
19	B	828	CLA	C4A-NA-C1A	8.61	110.58	106.71
19	A	811	CLA	C4A-NA-C1A	8.61	110.58	106.71
19	5	301	CLA	C4A-NA-C1A	8.60	110.57	106.71
19	7	313	CLA	C4A-NA-C1A	8.59	110.57	106.71
19	B	830	CLA	C4A-NA-C1A	8.59	110.57	106.71
19	1	5011	CLA	C4A-NA-C1A	8.59	110.57	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	824	CLA	C4A-NA-C1A	8.57	110.56	106.71
19	B	804	CLA	C4A-NA-C1A	8.57	110.56	106.71
19	B	839	CLA	C4A-NA-C1A	8.56	110.56	106.71
19	4	313	CLA	C4A-NA-C1A	8.56	110.55	106.71
38	8	325	ERG	C15-C14-C8	-8.56	107.47	120.44
19	5	309	CLA	C4A-NA-C1A	8.55	110.55	106.71
19	A	834	CLA	C4A-NA-C1A	8.55	110.55	106.71
19	A	804	CLA	C4A-NA-C1A	8.55	110.55	106.71
19	B	820	CLA	C4A-NA-C1A	8.55	110.55	106.71
19	1	5016	CLA	C4A-NA-C1A	8.55	110.55	106.71
19	1	5008	CLA	C4A-NA-C1A	8.55	110.55	106.71
19	J	1901	CLA	C4A-NA-C1A	8.54	110.55	106.71
19	6	302	CLA	C4A-NA-C1A	8.54	110.55	106.71
19	Z	305	CLA	C4A-NA-C1A	8.53	110.54	106.71
19	B	811	CLA	C4A-NA-C1A	8.53	110.54	106.71
19	B	823	CLA	C4A-NA-C1A	8.52	110.54	106.71
19	4	318	CLA	C4A-NA-C1A	8.52	110.54	106.71
19	A	835	CLA	C4A-NA-C1A	8.52	110.54	106.71
19	B	824	CLA	C4A-NA-C1A	8.49	110.52	106.71
38	6	326	ERG	C15-C14-C8	-8.48	107.58	120.44
19	B	837	CLA	C4A-NA-C1A	8.48	110.52	106.71
19	B	838	CLA	C4A-NA-C1A	8.47	110.52	106.71
19	K	203	CLA	C4A-NA-C1A	8.47	110.51	106.71
19	1	5012	CLA	C4A-NA-C1A	8.46	110.51	106.71
19	A	837	CLA	C4A-NA-C1A	8.46	110.51	106.71
19	5	312	CLA	C4A-NA-C1A	8.46	110.51	106.71
19	5	314	CLA	C4A-NA-C1A	8.46	110.51	106.71
19	6	318	CLA	C4A-NA-C1A	8.45	110.51	106.71
19	3	5012	CLA	C4A-NA-C1A	8.45	110.50	106.71
19	6	309	CLA	C4A-NA-C1A	8.45	110.50	106.71
19	F	303	CLA	C4A-NA-C1A	8.44	110.50	106.71
19	8	313	CLA	C4A-NA-C1A	8.44	110.50	106.71
19	A	819	CLA	C4A-NA-C1A	8.43	110.50	106.71
19	A	829	CLA	C4A-NA-C1A	8.42	110.49	106.71
19	8	310	CLA	C4A-NA-C1A	8.41	110.49	106.71
19	7	324	CLA	C4A-NA-C1A	8.41	110.49	106.71
19	8	314	CLA	C4A-NA-C1A	8.40	110.48	106.71
19	1	5018	CLA	C4A-NA-C1A	8.39	110.48	106.71
19	A	803	CLA	C4A-NA-C1A	8.39	110.48	106.71
19	A	840	CLA	C4A-NA-C1A	8.39	110.48	106.71
19	B	801	CLA	C4A-NA-C1A	8.39	110.48	106.71
19	B	825	CLA	C4A-NA-C1A	8.39	110.48	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	834	CLA	C4A-NA-C1A	8.38	110.47	106.71
19	Z	306	CLA	C4A-NA-C1A	8.38	110.47	106.71
19	Z	315	CLA	C4A-NA-C1A	8.37	110.47	106.71
19	1	5013	CLA	C4A-NA-C1A	8.37	110.47	106.71
19	A	802	CLA	C4A-NA-C1A	8.36	110.46	106.71
19	B	818	CLA	C4A-NA-C1A	8.36	110.46	106.71
19	5	313	CLA	C4A-NA-C1A	8.36	110.46	106.71
19	A	830	CLA	C4A-NA-C1A	8.34	110.46	106.71
19	B	809	CLA	C4A-NA-C1A	8.34	110.45	106.71
19	B	835	CLA	C4A-NA-C1A	8.34	110.45	106.71
38	8	325	ERG	C13-C17-C20	-8.33	108.68	119.43
19	A	823	CLA	C4A-NA-C1A	8.32	110.45	106.71
19	B	833	CLA	C4A-NA-C1A	8.32	110.44	106.71
19	G	1602	CLA	C4A-NA-C1A	8.32	110.44	106.71
19	A	842	CLA	C4A-NA-C1A	8.29	110.43	106.71
19	8	308	CLA	C4A-NA-C1A	8.29	110.43	106.71
19	A	820	CLA	C4A-NA-C1A	8.27	110.42	106.71
19	Z	314	CLA	C4A-NA-C1A	8.26	110.42	106.71
19	A	821	CLA	C4A-NA-C1A	8.24	110.41	106.71
19	F	301	CLA	C4A-NA-C1A	8.23	110.40	106.71
19	3	5010	CLA	C4A-NA-C1A	8.22	110.40	106.71
19	B	803	CLA	C4A-NA-C1A	8.19	110.39	106.71
19	B	812	CLA	C4A-NA-C1A	8.15	110.37	106.71
19	A	832	CLA	C4A-NA-C1A	8.14	110.37	106.71
19	A	806	CLA	C4A-NA-C1A	8.13	110.36	106.71
19	6	322	CLA	C4A-NA-C1A	8.10	110.35	106.71
19	6	323	CLA	C4A-NA-C1A	8.09	110.34	106.71
19	6	320	CLA	C4A-NA-C1A	8.08	110.34	106.71
19	4	316	CLA	C4A-NA-C1A	8.08	110.34	106.71
19	A	809	CLA	C4A-NA-C1A	8.07	110.33	106.71
19	3	5009	CLA	C4A-NA-C1A	8.06	110.33	106.71
19	6	310	CLA	C4A-NA-C1A	8.04	110.32	106.71
19	A	857	CLA	C4A-NA-C1A	8.01	110.31	106.71
19	7	318	CLA	C4A-NA-C1A	8.01	110.31	106.71
19	5	307	CLA	C4A-NA-C1A	7.98	110.30	106.71
19	A	812	CLA	C4A-NA-C1A	7.97	110.29	106.71
19	1	5010	CLA	C4A-NA-C1A	7.93	110.27	106.71
19	6	312	CLA	C4A-NA-C1A	7.92	110.27	106.71
22	3	5005	BCR	C11-C10-C9	-7.92	116.01	127.31
19	B	807	CLA	C4A-NA-C1A	7.89	110.25	106.71
22	3	5007	BCR	C24-C23-C22	-7.89	114.32	126.23
19	Z	307	CLA	C4A-NA-C1A	7.86	110.24	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	308	BCR	C15-C14-C13	-7.84	116.12	127.31
19	4	310	CLA	C4A-NA-C1A	7.73	110.18	106.71
19	5	308	CLA	C4A-NA-C1A	7.65	110.14	106.71
18	A	801	CL0	CMD-C2D-C1D	7.58	138.08	124.71
19	8	311	CLA	C4A-NA-C1A	7.50	110.08	106.71
28	6	304	C7Z	C11-C10-C9	-7.36	116.81	127.31
22	A	848	BCR	C15-C14-C13	-7.20	117.03	127.31
22	5	305	BCR	C11-C10-C9	-7.00	117.32	127.31
22	A	847	BCR	C16-C17-C18	-6.96	117.38	127.31
31	8	304	LUT	C35-C34-C33	-6.96	117.38	127.31
22	8	303	BCR	C38-C26-C25	-6.86	116.82	124.53
27	4	303	RRX	C33-C5-C6	-6.86	116.82	124.53
19	3	5011	CLA	O2A-C1-C2	6.84	126.61	108.64
35	7	302	DGA	CDB-CCB-CBB	-6.80	79.90	114.42
31	8	305	LUT	C7-C8-C9	-6.77	116.00	126.23
22	4	305	BCR	C20-C21-C22	-6.76	117.67	127.31
22	8	303	BCR	C16-C17-C18	-6.75	117.68	127.31
31	6	306	LUT	C31-C30-C29	-6.69	117.76	127.31
22	B	846	BCR	C15-C14-C13	-6.67	117.80	127.31
31	1	5004	LUT	C7-C8-C9	-6.66	116.17	126.23
18	A	801	CL0	C4A-NA-C1A	6.65	109.70	106.71
27	4	303	RRX	C24-C23-C22	-6.52	116.38	126.23
19	8	312	CLA	CMD-C2D-C1D	6.51	136.19	124.71
19	6	311	CLA	O2A-C1-C2	6.51	125.74	108.64
22	5	304	BCR	C16-C17-C18	-6.45	118.10	127.31
22	3	5005	BCR	C20-C21-C22	-6.45	118.11	127.31
22	3	5007	BCR	C7-C8-C9	-6.43	116.52	126.23
19	8	312	CLA	C1D-ND-C4D	-6.42	101.77	106.33
22	A	849	BCR	C16-C17-C18	-6.40	118.18	127.31
19	4	309	CLA	O2D-CGD-CBD	6.39	122.62	111.27
31	3	5002	LUT	C11-C10-C9	-6.37	118.21	127.31
22	5	304	BCR	C33-C5-C6	-6.32	117.43	124.53
31	6	305	LUT	C11-C10-C9	-6.31	118.30	127.31
22	F	302	BCR	C24-C23-C22	-6.29	116.73	126.23
31	4	304	LUT	C11-C10-C9	-6.26	118.37	127.31
19	6	320	CLA	O2D-CGD-CBD	6.25	122.37	111.27
19	8	307	CLA	O2A-C1-C2	6.24	125.03	108.64
22	6	308	BCR	C38-C26-C25	-6.22	117.54	124.53
31	7	304	LUT	C31-C30-C29	-6.22	118.43	127.31
27	F	304	RRX	C11-C10-C9	-6.21	118.45	127.31
28	1	5005	C7Z	C35-C34-C33	-6.19	118.48	127.31
22	6	308	BCR	C20-C21-C22	-6.18	118.50	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	842	BCR	C15-C14-C13	-6.14	118.55	127.31
19	A	813	CLA	O2D-CGD-CBD	6.14	122.17	111.27
31	3	5003	LUT	C31-C30-C29	-6.14	118.55	127.31
19	7	309	CLA	O2A-C1-C2	6.13	124.75	108.64
27	5	302	RRX	C24-C23-C22	-6.13	116.97	126.23
19	8	310	CLA	O2A-C1-C2	6.12	124.71	108.64
31	5	303	LUT	C7-C8-C9	-6.11	117.00	126.23
19	4	311	CLA	CMD-C2D-C1D	6.11	135.48	124.71
22	G	1603	BCR	C38-C26-C25	-6.11	117.67	124.53
28	6	304	C7Z	C1-C6-C5	-6.10	114.01	122.61
19	6	312	CLA	O2A-C1-C2	6.10	124.68	108.64
19	8	309	CLA	O2A-C1-C2	6.10	124.67	108.64
18	A	801	CL0	C2D-C1D-ND	6.10	114.60	110.10
22	A	849	BCR	C24-C23-C22	-6.09	117.03	126.23
18	A	801	CL0	C2C-C1C-NC	6.09	115.67	109.97
31	4	304	LUT	C1-C6-C5	-6.08	114.04	122.61
22	B	843	BCR	C11-C10-C9	-6.07	118.65	127.31
22	7	305	BCR	C20-C21-C22	-6.06	118.67	127.31
19	5	309	CLA	O2A-C1-C2	6.06	124.55	108.64
22	B	844	BCR	C24-C23-C22	-6.05	117.09	126.23
19	3	5008	CLA	O2A-C1-C2	6.05	124.54	108.64
31	3	5003	LUT	C7-C8-C9	-6.04	117.10	126.23
38	6	326	ERG	C15-C14-C13	-6.02	98.84	104.21
19	1	5011	CLA	CMD-C2D-C1D	6.01	135.31	124.71
19	4	307	CLA	CMD-C2D-C1D	5.98	135.25	124.71
22	3	5006	BCR	C16-C17-C18	-5.96	118.80	127.31
22	6	307	BCR	C11-C10-C9	-5.93	118.85	127.31
19	B	840	CLA	O2D-CGD-CBD	5.91	121.78	111.27
19	4	307	CLA	C4A-NA-C1A	5.91	109.36	106.71
19	A	812	CLA	O2A-C1-C2	5.88	124.10	108.64
19	1	5010	CLA	CMD-C2D-C1D	5.88	135.08	124.71
19	7	310	CLA	CMD-C2D-C1D	5.86	135.04	124.71
27	F	304	RRX	C15-C14-C13	-5.85	118.96	127.31
19	Z	311	CLA	CMD-C2D-C1D	5.83	134.98	124.71
22	A	848	BCR	C16-C17-C18	-5.81	119.01	127.31
19	4	308	CLA	O2D-CGD-CBD	5.80	121.57	111.27
22	3	5007	BCR	C4-C5-C6	-5.79	114.32	122.73
31	1	5004	LUT	C11-C10-C9	-5.78	119.06	127.31
19	4	309	CLA	O2A-C1-C2	5.77	123.81	108.64
19	1	5006	CLA	CMD-C2D-C1D	5.77	134.88	124.71
19	5	309	CLA	O2D-CGD-CBD	5.77	121.52	111.27
19	K	205	CLA	CMD-C2D-C1D	5.75	134.85	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	7	324	CLA	O2A-C1-C2	5.75	123.74	108.64
19	7	306	CLA	CMD-C2D-C1D	5.75	134.84	124.71
22	4	305	BCR	C38-C26-C25	-5.74	118.08	124.53
31	Z	317	LUT	C40-C33-C34	-5.74	114.89	122.92
19	B	836	CLA	O2A-C1-C2	5.73	123.70	108.64
19	3	5012	CLA	CMD-C2D-C1D	5.73	134.81	124.71
19	6	310	CLA	CMD-C2D-C1D	5.72	134.79	124.71
19	F	301	CLA	CMD-C2D-C1D	5.70	134.76	124.71
19	6	320	CLA	O2A-C1-C2	5.70	123.62	108.64
22	A	847	BCR	C15-C14-C13	-5.69	119.19	127.31
22	G	1603	BCR	C20-C21-C22	-5.69	119.19	127.31
27	F	304	RRX	C16-C17-C18	-5.68	119.20	127.31
19	5	308	CLA	CMD-C2D-C1D	5.68	134.73	124.71
28	6	304	C7Z	C15-C14-C13	-5.67	119.22	127.31
22	B	846	BCR	C20-C21-C22	-5.66	119.23	127.31
19	A	839	CLA	CMD-C2D-C1D	5.66	134.68	124.71
19	A	832	CLA	O2D-CGD-CBD	5.65	121.31	111.27
19	B	822	CLA	CMD-C2D-C1D	5.65	134.68	124.71
19	8	308	CLA	CMD-C2D-C1D	5.65	134.67	124.71
19	A	823	CLA	CMD-C2D-C1D	5.65	134.67	124.71
19	5	325	CLA	CMD-C2D-C1D	5.65	134.66	124.71
19	6	322	CLA	CMD-C2D-C1D	5.64	134.66	124.71
22	3	5005	BCR	C4-C5-C6	-5.64	114.54	122.73
19	5	306	CLA	CMD-C2D-C1D	5.63	134.63	124.71
22	3	5004	BCR	C24-C23-C22	-5.63	117.73	126.23
19	8	314	CLA	CMD-C2D-C1D	5.63	134.63	124.71
31	4	304	LUT	C18-C5-C6	-5.63	118.21	124.53
31	Z	317	LUT	C31-C32-C33	5.62	142.22	126.42
28	6	304	C7Z	C31-C30-C29	-5.62	119.29	127.31
19	5	311	CLA	CMD-C2D-C1D	5.62	134.61	124.71
19	B	829	CLA	CMD-C2D-C1D	5.61	134.60	124.71
19	A	815	CLA	CMD-C2D-C1D	5.61	134.60	124.71
19	A	811	CLA	CMD-C2D-C1D	5.61	134.59	124.71
19	8	314	CLA	O2A-C1-C2	5.60	123.36	108.64
31	Z	318	LUT	C7-C8-C9	-5.60	117.78	126.23
22	B	843	BCR	C1-C6-C5	-5.59	114.73	122.61
19	B	812	CLA	CMD-C2D-C1D	5.59	134.56	124.71
19	Z	314	CLA	CMD-C2D-C1D	5.59	134.56	124.71
19	B	833	CLA	CMD-C2D-C1D	5.58	134.55	124.71
19	6	309	CLA	CMD-C2D-C1D	5.58	134.55	124.71
19	1	5013	CLA	CMD-C2D-C1D	5.58	134.54	124.71
19	B	824	CLA	O2D-CGD-CBD	5.58	121.17	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	1602	CLA	CMD-C2D-C1D	5.57	134.54	124.71
19	A	807	CLA	CMD-C2D-C1D	5.57	134.53	124.71
19	B	811	CLA	CMD-C2D-C1D	5.57	134.53	124.71
19	Z	305	CLA	CMD-C2D-C1D	5.57	134.53	124.71
19	B	838	CLA	CMD-C2D-C1D	5.57	134.52	124.71
19	4	308	CLA	CMD-C2D-C1D	5.57	134.52	124.71
19	4	310	CLA	O2D-CGD-CBD	5.57	121.16	111.27
22	3	5007	BCR	C1-C6-C5	-5.57	114.77	122.61
19	A	814	CLA	CMD-C2D-C1D	5.56	134.52	124.71
19	8	308	CLA	O2D-CGD-CBD	5.56	121.15	111.27
31	7	304	LUT	C1-C6-C5	-5.56	114.78	122.61
19	4	309	CLA	CMD-C2D-C1D	5.56	134.51	124.71
19	5	307	CLA	CMD-C2D-C1D	5.56	134.51	124.71
19	7	309	CLA	O2D-CGD-CBD	5.56	121.14	111.27
19	A	814	CLA	O2D-CGD-CBD	5.55	121.13	111.27
19	B	806	CLA	CMD-C2D-C1D	5.55	134.50	124.71
19	K	204	CLA	CMD-C2D-C1D	5.55	134.50	124.71
19	6	311	CLA	CMD-C2D-C1D	5.55	134.50	124.71
19	B	813	CLA	CMD-C2D-C1D	5.55	134.50	124.71
19	A	833	CLA	CMD-C2D-C1D	5.55	134.49	124.71
19	5	319	CLA	CMD-C2D-C1D	5.55	134.49	124.71
19	B	814	CLA	CMD-C2D-C1D	5.54	134.48	124.71
28	1	5005	C7Z	C31-C30-C29	-5.54	119.40	127.31
19	B	826	CLA	CMD-C2D-C1D	5.54	134.48	124.71
22	B	843	BCR	C38-C26-C25	-5.54	118.31	124.53
22	F	302	BCR	C16-C17-C18	-5.54	119.41	127.31
22	3	5006	BCR	C27-C26-C25	-5.54	114.69	122.73
19	A	808	CLA	CMD-C2D-C1D	5.53	134.47	124.71
19	B	824	CLA	CMD-C2D-C1D	5.53	134.47	124.71
19	3	5016	CLA	CMD-C2D-C1D	5.53	134.46	124.71
19	A	803	CLA	CMD-C2D-C1D	5.53	134.46	124.71
19	A	813	CLA	CMD-C2D-C1D	5.53	134.46	124.71
19	B	810	CLA	CMD-C2D-C1D	5.53	134.46	124.71
19	A	817	CLA	CMD-C2D-C1D	5.53	134.46	124.71
19	A	822	CLA	CMD-C2D-C1D	5.53	134.46	124.71
31	7	304	LUT	C11-C10-C9	-5.53	119.42	127.31
22	3	5007	BCR	C38-C26-C25	-5.53	118.32	124.53
19	B	813	CLA	O2D-CGD-CBD	5.53	121.09	111.27
19	8	307	CLA	CMD-C2D-C1D	5.53	134.45	124.71
19	B	831	CLA	O2D-CGD-CBD	5.53	121.09	111.27
19	3	5019	CLA	O2A-C1-C2	5.52	123.15	108.64
19	7	319	CLA	CMD-C2D-C1D	5.52	134.44	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	206	BCR	C11-C10-C9	-5.52	119.43	127.31
19	A	806	CLA	CMD-C2D-C1D	5.52	134.44	124.71
19	B	817	CLA	CMD-C2D-C1D	5.52	134.44	124.71
19	A	834	CLA	CMD-C2D-C1D	5.52	134.44	124.71
19	A	827	CLA	CMD-C2D-C1D	5.52	134.44	124.71
19	B	819	CLA	CMD-C2D-C1D	5.52	134.43	124.71
19	5	322	CLA	CMD-C2D-C1D	5.51	134.43	124.71
22	7	305	BCR	C16-C17-C18	-5.51	119.44	127.31
19	I	201	CLA	CMD-C2D-C1D	5.51	134.43	124.71
19	A	841	CLA	CMD-C2D-C1D	5.51	134.42	124.71
19	3	5010	CLA	CMD-C2D-C1D	5.51	134.42	124.71
22	B	847	BCR	C27-C26-C25	-5.51	114.73	122.73
19	3	5013	CLA	CMD-C2D-C1D	5.51	134.42	124.71
19	4	306	CLA	CMD-C2D-C1D	5.50	134.41	124.71
19	B	850	CLA	CMD-C2D-C1D	5.50	134.40	124.71
19	B	827	CLA	CMD-C2D-C1D	5.50	134.40	124.71
19	J	1901	CLA	CMD-C2D-C1D	5.50	134.40	124.71
19	B	816	CLA	CMD-C2D-C1D	5.50	134.40	124.71
19	4	318	CLA	CMD-C2D-C1D	5.49	134.40	124.71
19	6	301	CLA	CMD-C2D-C1D	5.49	134.39	124.71
19	A	821	CLA	CMD-C2D-C1D	5.49	134.39	124.71
19	A	809	CLA	CMD-C2D-C1D	5.49	134.39	124.71
18	A	801	CL0	C1C-C2C-C3C	-5.49	101.18	106.96
19	A	820	CLA	CMD-C2D-C1D	5.49	134.38	124.71
19	A	805	CLA	CMD-C2D-C1D	5.49	134.38	124.71
19	B	818	CLA	CMD-C2D-C1D	5.48	134.37	124.71
19	A	828	CLA	CMD-C2D-C1D	5.48	134.37	124.71
19	A	818	CLA	CMD-C2D-C1D	5.48	134.37	124.71
19	3	5011	CLA	O2D-CGD-CBD	5.48	121.00	111.27
19	A	838	CLA	CMD-C2D-C1D	5.47	134.36	124.71
19	A	843	CLA	CMD-C2D-C1D	5.47	134.35	124.71
19	5	310	CLA	CMD-C2D-C1D	5.47	134.35	124.71
19	B	805	CLA	CMD-C2D-C1D	5.47	134.35	124.71
19	Z	303	CLA	CMD-C2D-C1D	5.47	134.35	124.71
19	B	830	CLA	CMD-C2D-C1D	5.47	134.35	124.71
19	B	807	CLA	CMD-C2D-C1D	5.47	134.35	124.71
19	B	821	CLA	CMD-C2D-C1D	5.46	134.34	124.71
19	K	203	CLA	CMD-C2D-C1D	5.46	134.34	124.71
19	A	816	CLA	CMD-C2D-C1D	5.46	134.34	124.71
19	B	834	CLA	CMD-C2D-C1D	5.46	134.34	124.71
19	A	857	CLA	CMD-C2D-C1D	5.46	134.33	124.71
19	A	836	CLA	CMD-C2D-C1D	5.46	134.33	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	830	CLA	CMD-C2D-C1D	5.45	134.33	124.71
19	7	318	CLA	O2D-CGD-CBD	5.45	120.96	111.27
19	5	301	CLA	CMD-C2D-C1D	5.45	134.32	124.71
19	A	831	CLA	CMD-C2D-C1D	5.45	134.32	124.71
19	1	5015	CLA	O2D-CGD-CBD	5.45	120.95	111.27
19	K	202	CLA	CMD-C2D-C1D	5.45	134.31	124.71
22	F	302	BCR	C38-C26-C25	-5.45	118.41	124.53
19	A	837	CLA	CMD-C2D-C1D	5.44	134.31	124.71
28	J	1902	C7Z	C31-C30-C29	-5.44	119.54	127.31
19	B	808	CLA	CMD-C2D-C1D	5.44	134.31	124.71
19	5	321	CLA	CMD-C2D-C1D	5.44	134.30	124.71
22	G	1603	BCR	C16-C17-C18	-5.44	119.54	127.31
19	1	5018	CLA	CMD-C2D-C1D	5.44	134.30	124.71
19	A	832	CLA	CMD-C2D-C1D	5.44	134.30	124.71
19	A	825	CLA	CMD-C2D-C1D	5.44	134.30	124.71
19	1	5015	CLA	CMD-C2D-C1D	5.43	134.29	124.71
22	A	850	BCR	C4-C5-C6	-5.43	114.84	122.73
19	F	303	CLA	CMD-C2D-C1D	5.43	134.28	124.71
19	B	837	CLA	CMD-C2D-C1D	5.43	134.28	124.71
19	Z	308	CLA	O2D-CGD-CBD	5.43	120.92	111.27
19	Z	315	CLA	CMD-C2D-C1D	5.43	134.28	124.71
19	A	820	CLA	O2D-CGD-CBD	5.43	120.91	111.27
38	8	325	ERG	C12-C13-C17	5.43	124.69	116.57
19	F	301	CLA	O2D-CGD-CBD	5.42	120.91	111.27
19	A	804	CLA	CMD-C2D-C1D	5.42	134.27	124.71
19	7	316	CLA	CMD-C2D-C1D	5.42	134.27	124.71
22	8	306	BCR	C24-C23-C22	-5.42	118.05	126.23
19	A	824	CLA	CMD-C2D-C1D	5.42	134.26	124.71
31	6	305	LUT	C7-C8-C9	-5.41	118.05	126.23
19	B	839	CLA	CMD-C2D-C1D	5.41	134.25	124.71
19	6	311	CLA	O2D-CGD-CBD	5.41	120.89	111.27
19	6	312	CLA	CMD-C2D-C1D	5.41	134.25	124.71
19	1	5016	CLA	CMD-C2D-C1D	5.41	134.25	124.71
28	J	1902	C7Z	C11-C10-C9	-5.41	119.59	127.31
19	A	827	CLA	O2A-C1-C2	5.40	122.83	108.64
19	Z	308	CLA	CMD-C2D-C1D	5.40	134.23	124.71
19	A	819	CLA	CMD-C2D-C1D	5.40	134.23	124.71
19	Z	311	CLA	O2D-CGD-CBD	5.40	120.86	111.27
38	8	325	ERG	C18-C13-C12	-5.39	102.07	110.59
19	B	823	CLA	CMD-C2D-C1D	5.39	134.22	124.71
19	3	5009	CLA	CMD-C2D-C1D	5.39	134.21	124.71
19	4	310	CLA	CMD-C2D-C1D	5.39	134.21	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	8	320	CLA	CMD-C2D-C1D	5.39	134.21	124.71
22	B	846	BCR	C33-C5-C6	-5.39	118.48	124.53
19	B	831	CLA	CMD-C2D-C1D	5.38	134.20	124.71
19	B	837	CLA	O2D-CGD-CBD	5.38	120.83	111.27
22	A	848	BCR	C11-C10-C9	-5.38	119.64	127.31
19	B	840	CLA	CMD-C2D-C1D	5.38	134.19	124.71
22	A	859	BCR	C1-C6-C5	-5.37	115.05	122.61
38	6	326	ERG	C11-C9-C10	-5.37	100.27	113.58
19	A	819	CLA	O2A-C1-C2	5.37	122.74	108.64
19	8	311	CLA	CMD-C2D-C1D	5.36	134.17	124.71
23	3	5021	LHG	O7-C7-O9	-5.36	118.74	125.57
22	3	5007	BCR	C33-C5-C6	-5.36	118.51	124.53
19	B	815	CLA	CMD-C2D-C1D	5.36	134.16	124.71
19	8	312	CLA	O2D-CGD-CBD	5.36	120.80	111.27
22	5	305	BCR	C38-C26-C25	-5.36	118.51	124.53
19	3	5011	CLA	CMD-C2D-C1D	5.36	134.16	124.71
22	A	859	BCR	C24-C23-C22	-5.36	118.14	126.23
19	A	826	CLA	O2D-CGD-CBD	5.35	120.78	111.27
19	A	812	CLA	CMD-C2D-C1D	5.35	134.15	124.71
19	A	812	CLA	O2D-CGD-CBD	5.35	120.77	111.27
19	7	309	CLA	CMD-C2D-C1D	5.35	134.14	124.71
19	Z	303	CLA	O2D-CGD-CBD	5.35	120.77	111.27
19	1	5012	CLA	CMD-C2D-C1D	5.35	134.13	124.71
22	B	844	BCR	C33-C5-C6	-5.34	118.53	124.53
19	B	832	CLA	O2D-CGD-CBD	5.34	120.76	111.27
22	3	5005	BCR	C27-C26-C25	-5.34	114.97	122.73
19	8	318	CLA	CMD-C2D-C1D	5.34	134.13	124.71
19	B	820	CLA	CMD-C2D-C1D	5.34	134.12	124.71
19	A	835	CLA	CMD-C2D-C1D	5.34	134.12	124.71
19	A	842	CLA	CMD-C2D-C1D	5.33	134.11	124.71
19	7	311	CLA	CMD-C2D-C1D	5.33	134.11	124.71
19	B	809	CLA	CMD-C2D-C1D	5.33	134.10	124.71
19	B	832	CLA	CMD-C2D-C1D	5.33	134.10	124.71
19	B	803	CLA	CMD-C2D-C1D	5.33	134.10	124.71
19	6	302	CLA	O2D-CGD-CBD	5.32	120.73	111.27
19	A	822	CLA	O2D-CGD-CBD	5.32	120.73	111.27
19	B	805	CLA	O2D-CGD-CBD	5.32	120.72	111.27
19	6	313	CLA	CMD-C2D-C1D	5.32	134.09	124.71
19	6	302	CLA	CMD-C2D-C1D	5.32	134.09	124.71
22	A	850	BCR	C20-C21-C22	-5.32	119.72	127.31
19	Z	307	CLA	CMD-C2D-C1D	5.32	134.08	124.71
19	B	836	CLA	CMD-C2D-C1D	5.32	134.08	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	803	CLA	O2D-CGD-CBD	5.31	120.70	111.27
19	8	311	CLA	O2D-CGD-CBD	5.31	120.70	111.27
19	3	5020	CLA	CMD-C2D-C1D	5.30	134.06	124.71
19	A	826	CLA	CMD-C2D-C1D	5.30	134.05	124.71
19	A	837	CLA	O2D-CGD-CBD	5.30	120.68	111.27
19	3	5013	CLA	O2A-C1-C2	5.30	122.55	108.64
19	A	802	CLA	CMD-C2D-C1D	5.29	134.04	124.71
22	8	306	BCR	C27-C26-C25	-5.29	115.05	122.73
19	7	312	CLA	CMD-C2D-C1D	5.29	134.03	124.71
19	8	309	CLA	CMD-C2D-C1D	5.29	134.03	124.71
19	5	319	CLA	O2D-CGD-CBD	5.28	120.66	111.27
22	B	845	BCR	C11-C10-C9	-5.28	119.77	127.31
19	G	1601	CLA	CMD-C2D-C1D	5.28	134.02	124.71
19	6	318	CLA	CMD-C2D-C1D	5.28	134.02	124.71
19	B	835	CLA	CMD-C2D-C1D	5.28	134.02	124.71
19	3	5019	CLA	CMD-C2D-C1D	5.28	134.02	124.71
19	Z	304	CLA	CMD-C2D-C1D	5.28	134.02	124.71
19	7	316	CLA	C1-C2-C3	-5.28	118.21	126.75
19	3	5014	CLA	CMD-C2D-C1D	5.27	134.01	124.71
19	6	309	CLA	O2A-C1-C2	5.27	122.49	108.64
18	A	801	CL0	O2D-CGD-CBD	5.27	120.63	111.27
19	3	5008	CLA	CMD-C2D-C1D	5.27	134.00	124.71
19	B	801	CLA	CMD-C2D-C1D	5.27	133.99	124.71
22	7	305	BCR	C4-C5-C6	-5.27	115.09	122.73
19	A	809	CLA	O2D-CGD-CBD	5.26	120.62	111.27
19	A	825	CLA	O2D-CGD-CBD	5.26	120.62	111.27
19	A	823	CLA	O2D-CGD-CBD	5.26	120.62	111.27
19	1	5011	CLA	O2D-CGD-CBD	5.26	120.62	111.27
19	4	308	CLA	O2A-C1-C2	5.25	122.43	108.64
19	A	833	CLA	O2A-C1-C2	5.25	122.43	108.64
22	5	304	BCR	C38-C26-C25	-5.25	118.64	124.53
19	7	308	CLA	CMD-C2D-C1D	5.24	133.95	124.71
19	4	313	CLA	CMD-C2D-C1D	5.24	133.95	124.71
19	B	828	CLA	CMD-C2D-C1D	5.24	133.94	124.71
19	4	311	CLA	C4A-NA-C1A	5.23	109.06	106.71
19	1	5010	CLA	O2D-CGD-CBD	5.23	120.57	111.27
19	B	818	CLA	O2D-CGD-CBD	5.23	120.56	111.27
19	A	810	CLA	O2D-CGD-CBD	5.22	120.54	111.27
19	4	310	CLA	O2A-C1-C2	5.21	122.34	108.64
19	B	817	CLA	O2A-C1-C2	5.21	122.34	108.64
19	B	815	CLA	O2D-CGD-CBD	5.21	120.53	111.27
22	F	302	BCR	C20-C21-C22	-5.21	119.87	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	802	CLA	O2D-CGD-CBD	5.20	120.52	111.27
19	K	204	CLA	O2A-C1-C2	5.20	121.14	108.97
22	A	850	BCR	C7-C8-C9	-5.20	118.38	126.23
19	B	822	CLA	O2D-CGD-CBD	5.20	120.51	111.27
22	B	845	BCR	C1-C6-C5	-5.20	115.29	122.61
19	7	324	CLA	CMD-C2D-C1D	5.20	133.88	124.71
19	1	5013	CLA	O2D-CGD-CBD	5.20	120.50	111.27
19	7	310	CLA	O2D-CGD-CBD	5.20	120.50	111.27
19	4	307	CLA	O2D-CGD-CBD	5.19	120.50	111.27
19	A	802	CLA	O2D-CGD-CBD	5.19	120.49	111.27
19	B	829	CLA	O2A-C1-C2	5.19	122.28	108.64
19	B	836	CLA	O2D-CGD-CBD	5.19	120.49	111.27
19	3	5020	CLA	O2D-CGD-CBD	5.19	120.49	111.27
19	6	323	CLA	O2A-C1-C2	5.19	122.27	108.64
22	B	845	BCR	C15-C14-C13	-5.19	119.91	127.31
19	7	307	CLA	CMD-C2D-C1D	5.19	133.86	124.71
19	A	808	CLA	O2D-CGD-CBD	5.19	120.49	111.27
19	K	202	CLA	O2D-CGD-CBD	5.19	120.48	111.27
19	5	319	CLA	O2A-C1-C2	5.18	122.26	108.64
19	5	312	CLA	O2A-C1-C2	5.18	122.25	108.64
19	3	5015	CLA	CMD-C2D-C1D	5.18	133.84	124.71
19	J	1901	CLA	O2D-CGD-CBD	5.18	120.47	111.27
19	6	311	CLA	C1-C2-C3	-5.17	117.09	126.04
19	5	311	CLA	O2A-C1-C2	5.17	122.23	108.64
19	7	317	CLA	CMD-C2D-C1D	5.17	133.83	124.71
19	B	814	CLA	O2D-CGD-CBD	5.17	120.45	111.27
19	A	823	CLA	O2A-C1-C2	5.16	122.20	108.64
19	B	812	CLA	O2D-CGD-CBD	5.16	120.44	111.27
19	B	804	CLA	CMD-C2D-C1D	5.16	133.81	124.71
19	B	802	CLA	CMD-C2D-C1D	5.15	133.80	124.71
19	3	5015	CLA	O2D-CGD-CBD	5.15	120.42	111.27
19	8	313	CLA	O2D-CGD-CBD	5.15	120.41	111.27
19	A	834	CLA	O2D-CGD-CBD	5.15	120.41	111.27
19	A	824	CLA	O2A-C1-C2	5.14	122.15	108.64
19	7	306	CLA	O2A-C1-C2	5.14	122.14	108.64
19	5	308	CLA	O2A-C1-C2	5.14	122.14	108.64
22	5	305	BCR	C1-C6-C5	-5.14	115.38	122.61
31	Z	318	LUT	C11-C10-C9	-5.13	119.99	127.31
19	4	316	CLA	CMD-C2D-C1D	5.13	133.75	124.71
19	5	322	CLA	O2D-CGD-CBD	5.13	120.38	111.27
19	A	830	CLA	O2D-CGD-CBD	5.13	120.38	111.27
19	Z	306	CLA	CMD-C2D-C1D	5.12	133.74	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	313	CLA	CMD-C2D-C1D	5.12	133.73	124.71
19	1	5007	CLA	CMD-C2D-C1D	5.12	133.73	124.71
19	7	311	CLA	O2A-C1-C2	5.11	122.08	108.64
19	B	816	CLA	O2A-C1-C2	5.11	122.08	108.64
19	7	313	CLA	O2D-CGD-CBD	5.11	120.36	111.27
19	4	313	CLA	O2A-C1-C2	5.11	122.07	108.64
19	8	318	CLA	O2D-CGD-CBD	5.11	120.34	111.27
19	8	310	CLA	CMD-C2D-C1D	5.10	133.71	124.71
19	A	841	CLA	O2D-CGD-CBD	5.10	120.34	111.27
19	5	309	CLA	CMD-C2D-C1D	5.10	133.71	124.71
19	5	314	CLA	CMD-C2D-C1D	5.10	133.70	124.71
32	6	321	CHL	CHD-C1D-ND	-5.10	119.77	124.45
19	G	1602	CLA	O2D-CGD-CBD	5.10	120.33	111.27
31	6	306	LUT	C7-C8-C9	-5.10	118.53	126.23
22	8	303	BCR	C1-C6-C5	-5.10	115.44	122.61
19	A	840	CLA	O2A-C1-C2	5.09	122.01	108.64
19	A	817	CLA	O2A-C1-C2	5.09	122.01	108.64
32	6	321	CHL	C4D-CHA-C1A	5.09	127.44	121.25
19	B	811	CLA	O2D-CGD-CBD	5.09	120.31	111.27
19	6	301	CLA	O2D-CGD-CBD	5.09	120.30	111.27
19	A	827	CLA	O2D-CGD-CBD	5.08	120.30	111.27
19	B	816	CLA	O2D-CGD-CBD	5.08	120.30	111.27
19	B	806	CLA	O2D-CGD-CBD	5.08	120.30	111.27
19	B	829	CLA	O2D-CGD-CBD	5.08	120.29	111.27
19	A	807	CLA	O2D-CGD-CBD	5.07	120.28	111.27
19	7	308	CLA	O2A-C1-C2	5.07	121.96	108.64
19	A	815	CLA	O2D-CGD-CBD	5.07	120.27	111.27
19	3	5019	CLA	O2D-CGD-CBD	5.06	120.27	111.27
19	A	833	CLA	O2D-CGD-CBD	5.06	120.26	111.27
19	3	5016	CLA	O2D-CGD-CBD	5.06	120.26	111.27
19	6	310	CLA	O2D-CGD-CBD	5.06	120.26	111.27
19	B	808	CLA	O2A-C1-C2	5.06	121.93	108.64
19	6	323	CLA	CMD-C2D-C1D	5.06	133.62	124.71
31	7	304	LUT	C7-C8-C9	-5.06	118.59	126.23
19	8	313	CLA	O2A-C1-C2	5.05	121.92	108.64
19	6	313	CLA	O2D-CGD-CBD	5.05	120.25	111.27
22	G	1603	BCR	C33-C5-C6	-5.05	118.85	124.53
31	Z	317	LUT	C30-C31-C32	5.05	138.98	123.22
19	4	313	CLA	O2D-CGD-CBD	5.05	120.24	111.27
19	6	323	CLA	O2D-CGD-CBD	5.05	120.24	111.27
19	3	5014	CLA	O2A-C1-C2	5.04	121.89	108.64
19	5	312	CLA	CMD-C2D-C1D	5.04	133.60	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	838	CLA	O2D-CGD-CBD	5.04	120.22	111.27
19	B	834	CLA	O2D-CGD-CBD	5.04	120.22	111.27
22	A	848	BCR	C1-C6-C5	-5.04	115.52	122.61
19	5	313	CLA	O2D-CGD-CBD	5.04	120.22	111.27
19	B	825	CLA	CMD-C2D-C1D	5.04	133.59	124.71
22	3	5007	BCR	C16-C17-C18	-5.04	120.12	127.31
19	3	5018	CLA	CMD-C2D-C1D	5.04	133.59	124.71
19	A	806	CLA	O2D-CGD-CBD	5.04	120.22	111.27
19	A	829	CLA	CMD-C2D-C1D	5.03	133.58	124.71
19	1	5008	CLA	CMD-C2D-C1D	5.03	133.58	124.71
22	B	847	BCR	C16-C17-C18	-5.03	120.13	127.31
19	B	825	CLA	O2A-C1-C2	5.03	121.86	108.64
19	5	317	CLA	CMD-C2D-C1D	5.03	133.58	124.71
19	Z	306	CLA	O2D-CGD-CBD	5.03	120.20	111.27
19	5	317	CLA	O2D-CGD-CBD	5.03	120.20	111.27
19	1	5016	CLA	O2A-C1-C2	5.03	121.85	108.64
22	A	846	BCR	C33-C5-C6	-5.03	118.88	124.53
19	B	833	CLA	O2D-CGD-CBD	5.03	120.20	111.27
19	K	205	CLA	O2D-CGD-CBD	5.02	120.20	111.27
19	I	201	CLA	O2D-CGD-CBD	5.02	120.19	111.27
19	6	320	CLA	CMD-C2D-C1D	5.02	133.56	124.71
22	A	859	BCR	C15-C14-C13	-5.02	120.15	127.31
19	B	803	CLA	O2D-CGD-CBD	5.02	120.18	111.27
19	A	816	CLA	O2D-CGD-CBD	5.01	120.18	111.27
19	B	831	CLA	O2A-C1-C2	5.01	121.80	108.64
22	6	308	BCR	C33-C5-C6	-5.01	118.90	124.53
19	5	308	CLA	O2D-CGD-CBD	5.01	120.17	111.27
19	7	319	CLA	O2A-C1-C2	5.01	121.79	108.64
31	6	305	LUT	C35-C34-C33	-5.01	120.17	127.31
19	B	826	CLA	O2D-CGD-CBD	5.01	120.16	111.27
19	B	830	CLA	O2D-CGD-CBD	5.01	120.16	111.27
22	B	843	BCR	C15-C14-C13	-5.00	120.17	127.31
19	8	307	CLA	O2D-CGD-CBD	5.00	120.15	111.27
22	A	858	BCR	C33-C5-C6	-4.99	118.92	124.53
19	8	314	CLA	O2D-CGD-CBD	4.99	120.13	111.27
18	A	801	CL0	O2A-CGA-O1A	-4.99	111.01	123.59
18	A	801	CL0	CHD-C1D-ND	-4.98	119.87	124.45
19	A	857	CLA	O2A-C1-C2	4.98	121.73	108.64
19	B	817	CLA	O2D-CGD-CBD	4.98	120.12	111.27
38	6	326	ERG	C12-C13-C17	4.98	124.03	116.57
19	B	809	CLA	O2A-C1-C2	4.98	121.73	108.64
19	B	804	CLA	O2D-CGD-CBD	4.98	120.12	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	804	CLA	O2D-CGD-CBD	4.98	120.12	111.27
19	7	307	CLA	O2A-C1-C2	4.98	121.72	108.64
19	A	818	CLA	O2A-C1-C2	4.98	121.72	108.64
22	B	843	BCR	C33-C5-C6	-4.98	118.94	124.53
19	3	5009	CLA	O2D-CGD-CBD	4.98	120.11	111.27
19	K	204	CLA	O2D-CGD-CBD	4.98	120.11	111.27
19	B	830	CLA	O2A-C1-C2	4.98	121.71	108.64
19	B	827	CLA	O2D-CGD-CBD	4.97	120.11	111.27
19	A	813	CLA	O2A-C1-C2	4.97	121.71	108.64
31	8	304	LUT	C11-C10-C9	-4.97	120.21	127.31
19	B	813	CLA	O2A-C1-C2	4.97	121.71	108.64
19	Z	307	CLA	O2D-CGD-CBD	4.97	120.10	111.27
19	F	303	CLA	O2D-CGD-CBD	4.97	120.09	111.27
19	A	830	CLA	O2A-C1-C2	4.96	121.68	108.64
32	3	5017	CHL	CHD-C1D-ND	-4.96	119.89	124.45
19	B	822	CLA	O2A-C1-C2	4.96	121.68	108.64
19	A	840	CLA	CMD-C2D-C1D	4.96	133.46	124.71
32	Z	313	CHL	CHD-C1D-ND	-4.96	119.90	124.45
19	A	843	CLA	O2A-C1-C2	4.96	121.67	108.64
22	3	5005	BCR	C30-C25-C26	-4.96	115.63	122.61
19	1	5010	CLA	O2A-C1-C2	4.95	121.66	108.64
19	1	5015	CLA	O2A-C1-C2	4.95	121.64	108.64
19	B	835	CLA	O2D-CGD-CBD	4.95	120.06	111.27
19	A	829	CLA	O2A-C1-C2	4.95	121.64	108.64
19	A	817	CLA	O2D-CGD-CBD	4.95	120.06	111.27
32	Z	310	CHL	C3C-C4C-NC	-4.95	105.02	110.57
19	5	312	CLA	O2D-CGD-CBD	4.95	120.06	111.27
32	Z	310	CHL	C2C-C3C-C4C	4.95	110.01	106.49
22	B	845	BCR	C16-C17-C18	-4.94	120.25	127.31
19	6	301	CLA	O2A-C1-C2	4.94	121.62	108.64
19	4	312	CLA	CMD-C2D-C1D	4.94	133.42	124.71
19	4	306	CLA	O2A-C1-C2	4.94	121.62	108.64
18	A	801	CL0	C3D-C2D-C1D	-4.94	99.09	105.83
19	4	311	CLA	C1D-ND-C4D	-4.94	102.83	106.33
19	8	313	CLA	CMD-C2D-C1D	4.94	133.41	124.71
19	1	5016	CLA	O2D-CGD-CBD	4.93	120.03	111.27
19	5	301	CLA	O2D-CGD-CBD	4.93	120.03	111.27
22	A	846	BCR	C15-C14-C13	-4.93	120.28	127.31
19	4	307	CLA	O2A-C1-C2	4.92	121.58	108.64
19	A	818	CLA	O2D-CGD-CBD	4.92	120.01	111.27
19	7	312	CLA	O2D-CGD-CBD	4.92	120.01	111.27
19	5	321	CLA	O2D-CGD-CBD	4.92	120.01	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	7	308	CLA	O2D-CGD-CBD	4.91	120.00	111.27
19	A	836	CLA	O2D-CGD-CBD	4.91	120.00	111.27
19	7	318	CLA	CMD-C2D-C1D	4.91	133.37	124.71
19	6	318	CLA	O2A-C1-C2	4.91	121.54	108.64
19	6	313	CLA	O2A-C1-C2	4.90	121.52	108.64
32	8	319	CHL	C1-O2A-CGA	4.90	129.31	116.44
19	6	314	CLA	CMD-C2D-C1D	4.90	133.35	124.71
32	6	319	CHL	C2C-C3C-C4C	4.90	109.98	106.49
22	B	845	BCR	C27-C26-C25	-4.90	115.62	122.73
19	4	316	CLA	O2D-CGD-CBD	4.90	119.98	111.27
19	Z	312	CLA	CMD-C2D-C1D	4.90	133.35	124.71
19	A	821	CLA	O2D-CGD-CBD	4.90	119.97	111.27
28	J	1902	C7Z	C27-C28-C29	-4.90	118.83	126.23
22	F	302	BCR	C33-C5-C6	-4.90	119.03	124.53
19	6	314	CLA	O2D-CGD-CBD	4.89	119.96	111.27
19	A	842	CLA	O2A-C1-C2	4.89	121.49	108.64
19	Z	312	CLA	O2D-CGD-CBD	4.89	119.95	111.27
19	B	839	CLA	O2D-CGD-CBD	4.88	119.95	111.27
19	5	321	CLA	O2A-C1-C2	4.88	121.47	108.64
22	A	850	BCR	C1-C6-C5	-4.88	115.74	122.61
22	6	307	BCR	C15-C14-C13	-4.88	120.35	127.31
19	B	820	CLA	O2A-C1-C2	4.88	121.45	108.64
22	A	850	BCR	C27-C26-C25	-4.88	115.65	122.73
19	B	810	CLA	O2A-C1-C2	4.88	121.45	108.64
19	B	820	CLA	O2D-CGD-CBD	4.88	119.93	111.27
19	B	804	CLA	O2A-C1-C2	4.87	121.43	108.64
22	A	847	BCR	C20-C21-C22	-4.87	120.36	127.31
19	3	5013	CLA	O2D-CGD-CBD	4.87	119.92	111.27
22	K	206	BCR	C1-C6-C5	-4.87	115.76	122.61
19	Z	311	CLA	O2A-C1-C2	4.87	121.42	108.64
27	5	302	RRX	C33-C5-C6	-4.86	119.07	124.53
19	B	818	CLA	O2A-C1-C2	4.86	121.40	108.64
19	4	316	CLA	O2A-C1-C2	4.86	121.40	108.64
19	G	1601	CLA	O2D-CGD-CBD	4.86	119.90	111.27
22	4	305	BCR	C1-C6-C5	-4.86	115.77	122.61
19	Z	311	CLA	C1-C2-C3	-4.86	117.64	126.04
19	A	828	CLA	O2D-CGD-CBD	4.85	119.89	111.27
19	B	809	CLA	O2D-CGD-CBD	4.85	119.89	111.27
19	7	317	CLA	O2A-C1-C2	4.85	121.39	108.64
22	A	849	BCR	C30-C25-C26	-4.84	115.79	122.61
19	B	803	CLA	O2A-C1-C2	4.84	121.36	108.64
19	A	835	CLA	O2D-CGD-CBD	4.84	119.87	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	835	CLA	O2A-C1-C2	4.83	121.34	108.64
28	6	304	C7Z	C7-C8-C9	-4.83	118.94	126.23
31	3	5002	LUT	C7-C8-C9	-4.83	118.94	126.23
19	A	819	CLA	O2D-CGD-CBD	4.83	119.85	111.27
19	A	857	CLA	O2D-CGD-CBD	4.82	119.84	111.27
31	8	305	LUT	C21-C26-C27	-4.82	106.61	112.70
22	A	859	BCR	C33-C5-C6	-4.82	119.11	124.53
19	5	325	CLA	O2D-CGD-CBD	4.82	119.83	111.27
19	8	320	CLA	O2D-CGD-CBD	4.82	119.83	111.27
19	1	5018	CLA	O2A-C1-C2	4.82	121.30	108.64
19	B	807	CLA	O2D-CGD-CBD	4.82	119.83	111.27
27	F	304	RRX	C33-C5-C6	-4.81	119.12	124.53
22	B	842	BCR	C38-C26-C25	-4.81	119.13	124.53
19	A	838	CLA	O2A-C1-C2	4.81	121.27	108.64
19	B	824	CLA	O2A-C1-C2	4.81	121.27	108.64
19	A	810	CLA	CMD-C2D-C1D	4.81	133.18	124.71
19	6	318	CLA	O2D-CGD-CBD	4.80	119.81	111.27
19	A	806	CLA	O2A-C1-C2	4.80	121.26	108.64
19	8	309	CLA	C1-C2-C3	-4.80	117.73	126.04
22	B	844	BCR	C7-C8-C9	-4.80	118.98	126.23
19	A	805	CLA	O2D-CGD-CBD	4.80	119.79	111.27
19	A	803	CLA	O2A-C1-C2	4.80	121.24	108.64
19	6	322	CLA	O2D-CGD-CBD	4.79	119.79	111.27
22	7	305	BCR	C1-C6-C5	-4.79	115.86	122.61
19	B	808	CLA	O2D-CGD-CBD	4.79	119.79	111.27
19	Z	314	CLA	O2D-CGD-CBD	4.79	119.78	111.27
19	B	806	CLA	O2A-C1-C2	4.79	121.23	108.64
19	K	203	CLA	O2A-C1-C2	4.79	121.22	108.64
19	5	317	CLA	O2A-C1-C2	4.79	121.22	108.64
19	Z	307	CLA	O2A-C1-C2	4.79	121.22	108.64
19	A	839	CLA	O2D-CGD-CBD	4.78	119.77	111.27
19	5	301	CLA	O2A-C1-C2	4.78	121.21	108.64
19	Z	315	CLA	O2D-CGD-CBD	4.78	119.76	111.27
19	A	820	CLA	O2A-C1-C2	4.78	121.20	108.64
22	A	848	BCR	C20-C21-C22	-4.78	120.49	127.31
19	B	819	CLA	O2D-CGD-CBD	4.78	119.76	111.27
22	B	843	BCR	C4-C5-C6	-4.78	115.80	122.73
19	B	807	CLA	O2A-C1-C2	4.77	121.18	108.64
19	K	203	CLA	O2D-CGD-CBD	4.77	119.75	111.27
22	A	848	BCR	C4-C5-C6	-4.77	115.81	122.73
22	B	842	BCR	C11-C12-C13	-4.77	113.02	126.42
19	3	5016	CLA	O2A-C1-C2	4.77	121.17	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	304	CLA	O2D-CGD-CBD	4.76	119.73	111.27
19	5	307	CLA	O2D-CGD-CBD	4.76	119.73	111.27
19	3	5019	CLA	C1-C2-C3	-4.76	117.81	126.04
28	6	304	C7Z	C35-C34-C33	-4.76	120.52	127.31
19	5	314	CLA	O2A-C1-C2	4.76	121.14	108.64
19	A	838	CLA	O2D-CGD-CBD	4.76	119.72	111.27
19	8	309	CLA	O2D-CGD-CBD	4.76	119.72	111.27
19	B	827	CLA	O2A-C1-C2	4.76	121.14	108.64
22	A	850	BCR	C15-C14-C13	-4.76	120.52	127.31
19	A	815	CLA	O2A-C1-C2	4.75	121.13	108.64
22	5	304	BCR	C20-C21-C22	-4.75	120.53	127.31
19	Z	305	CLA	O2A-C1-C2	4.75	121.13	108.64
19	3	5010	CLA	O2D-CGD-CBD	4.75	119.71	111.27
19	3	5018	CLA	O2D-CGD-CBD	4.75	119.71	111.27
19	A	809	CLA	O2A-C1-C2	4.75	121.11	108.64
19	F	301	CLA	O2A-C1-C2	4.75	121.11	108.64
19	7	319	CLA	O2D-CGD-CBD	4.75	119.70	111.27
19	5	306	CLA	O2D-CGD-CBD	4.75	119.70	111.27
19	B	801	CLA	O2D-CGD-CBD	4.74	119.70	111.27
19	A	837	CLA	O2A-C1-C2	4.74	121.10	108.64
19	4	311	CLA	O2D-CGD-CBD	4.74	119.69	111.27
19	B	812	CLA	O2A-C1-C2	4.74	121.08	108.64
19	B	814	CLA	O2A-C1-C2	4.74	121.08	108.64
19	7	306	CLA	O2D-CGD-CBD	4.73	119.68	111.27
19	7	313	CLA	CMD-C2D-C1D	4.73	133.06	124.71
19	4	306	CLA	O2D-CGD-CBD	4.73	119.68	111.27
19	4	318	CLA	O2D-CGD-CBD	4.72	119.66	111.27
19	A	835	CLA	O2A-C1-C2	4.72	121.05	108.64
19	7	317	CLA	O2D-CGD-CBD	4.72	119.66	111.27
19	A	831	CLA	O2D-CGD-CBD	4.72	119.66	111.27
19	B	821	CLA	O2A-C1-C2	4.72	121.04	108.64
22	3	5006	BCR	C20-C21-C22	-4.71	120.58	127.31
19	8	312	CLA	C2D-C1D-ND	4.71	113.58	110.10
19	5	310	CLA	O2D-CGD-CBD	4.71	119.64	111.27
19	5	310	CLA	O2A-C1-C2	4.71	121.01	108.64
22	A	847	BCR	C11-C10-C9	-4.71	120.59	127.31
19	4	312	CLA	O2D-CGD-CBD	4.71	119.64	111.27
19	B	850	CLA	O2A-C1-C2	4.71	121.01	108.64
19	A	802	CLA	O2A-C1-C2	4.71	121.01	108.64
22	A	846	BCR	C20-C21-C22	-4.70	120.60	127.31
22	B	847	BCR	C20-C21-C22	-4.70	120.60	127.31
22	B	847	BCR	C30-C25-C26	-4.70	116.00	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	312	CLA	O2A-C1-C2	4.69	120.97	108.64
22	K	206	BCR	C7-C8-C9	-4.69	119.14	126.23
19	A	842	CLA	O2D-CGD-CBD	4.69	119.61	111.27
19	A	843	CLA	O2D-CGD-CBD	4.69	119.61	111.27
19	A	831	CLA	O2A-C1-C2	4.69	120.97	108.64
19	B	823	CLA	O2D-CGD-CBD	4.69	119.60	111.27
19	B	828	CLA	O2D-CGD-CBD	4.69	119.59	111.27
19	3	5012	CLA	O2D-CGD-CBD	4.68	119.59	111.27
19	A	841	CLA	O2A-C1-C2	4.68	120.94	108.64
19	B	802	CLA	O2A-C1-C2	4.68	120.94	108.64
19	8	312	CLA	O2A-C1-C2	4.68	120.93	108.64
19	A	816	CLA	O2A-C1-C2	4.68	120.93	108.64
19	A	824	CLA	O2D-CGD-CBD	4.67	119.57	111.27
19	1	5008	CLA	O2D-CGD-CBD	4.67	119.57	111.27
22	A	858	BCR	C1-C6-C5	-4.67	116.03	122.61
19	A	826	CLA	O2A-C1-C2	4.67	120.91	108.64
32	3	5017	CHL	C4D-CHA-C1A	4.67	126.93	121.25
19	6	309	CLA	O2D-CGD-CBD	4.67	119.56	111.27
19	B	828	CLA	O2A-C1-C2	4.66	120.89	108.64
19	A	810	CLA	O2A-C1-C2	4.66	120.88	108.64
19	B	821	CLA	O2D-CGD-CBD	4.66	119.54	111.27
19	1	5012	CLA	O2D-CGD-CBD	4.65	119.53	111.27
31	3	5003	LUT	C11-C10-C9	-4.65	120.67	127.31
22	K	206	BCR	C15-C14-C13	-4.65	120.67	127.31
22	A	847	BCR	C33-C5-C6	-4.65	119.31	124.53
32	6	315	CHL	CHD-C1D-ND	-4.65	120.18	124.45
19	B	810	CLA	O2D-CGD-CBD	4.65	119.52	111.27
19	4	312	CLA	O2A-C1-C2	4.65	120.84	108.64
19	5	307	CLA	O2A-C1-C2	4.64	120.83	108.64
19	B	832	CLA	O2A-C1-C2	4.64	120.83	108.64
23	7	320	LHG	C5-O7-C7	-4.64	106.37	117.79
19	1	5011	CLA	O2A-C1-C2	4.64	120.82	108.64
22	K	206	BCR	C4-C5-C6	-4.63	116.00	122.73
22	3	5005	BCR	C24-C23-C22	-4.63	119.25	126.23
22	A	848	BCR	C7-C8-C9	-4.62	119.25	126.23
32	5	318	CHL	CHD-C1D-ND	-4.62	120.21	124.45
28	J	1902	C7Z	C35-C34-C33	-4.62	120.72	127.31
19	Z	308	CLA	O2A-C1-C2	4.62	120.77	108.64
19	B	826	CLA	O2A-C1-C2	4.61	120.76	108.64
22	3	5005	BCR	C7-C8-C9	-4.61	119.27	126.23
19	8	312	CLA	CHD-C1D-ND	-4.61	120.22	124.45
32	4	317	CHL	CHD-C1D-ND	-4.61	120.22	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	815	CLA	O2A-C1-C2	4.61	120.75	108.64
22	4	305	BCR	C11-C10-C9	-4.61	120.73	127.31
22	3	5005	BCR	C38-C26-C25	-4.61	119.36	124.53
19	5	311	CLA	O2D-CGD-CBD	4.61	119.45	111.27
18	A	801	CL0	O2A-C1-C2	4.61	120.74	108.64
19	A	822	CLA	O2A-C1-C2	4.61	120.74	108.64
19	A	805	CLA	O2A-C1-C2	4.60	120.73	108.64
22	B	845	BCR	C38-C26-C25	-4.60	119.36	124.53
22	A	849	BCR	C11-C10-C9	-4.60	120.75	127.31
22	6	308	BCR	C15-C16-C17	-4.60	114.06	123.47
19	1	5018	CLA	O2D-CGD-CBD	4.59	119.43	111.27
22	B	846	BCR	C11-C10-C9	-4.58	120.77	127.31
22	A	859	BCR	C16-C17-C18	-4.57	120.78	127.31
19	6	314	CLA	O2A-C1-C2	4.57	120.65	108.64
19	7	324	CLA	O2D-CGD-CBD	4.57	119.38	111.27
19	A	811	CLA	O2A-C1-C2	4.57	120.64	108.64
22	8	303	BCR	C11-C10-C9	-4.57	120.79	127.31
19	A	829	CLA	O2D-CGD-CBD	4.56	119.37	111.27
31	4	304	LUT	C7-C8-C9	-4.56	119.35	126.23
19	A	832	CLA	O2A-C1-C2	4.56	120.61	108.64
22	G	1603	BCR	C27-C26-C25	-4.55	116.12	122.73
32	6	319	CHL	CHD-C1D-ND	-4.55	120.27	124.45
19	3	5018	CLA	O2A-C1-C2	4.55	120.58	108.64
31	6	305	LUT	C21-C26-C27	-4.54	106.96	112.70
22	B	845	BCR	C4-C5-C6	-4.54	116.14	122.73
19	B	819	CLA	O2A-C1-C2	4.54	120.56	108.64
19	A	811	CLA	O2D-CGD-CBD	4.54	119.33	111.27
19	A	834	CLA	O2A-C1-C2	4.53	120.55	108.64
22	A	849	BCR	C33-C5-C6	-4.53	119.44	124.53
22	B	843	BCR	C7-C8-C9	-4.53	119.39	126.23
19	7	316	CLA	O2D-CGD-CBD	4.53	119.32	111.27
22	A	850	BCR	C16-C17-C18	-4.53	120.85	127.31
22	A	849	BCR	C15-C14-C13	-4.53	120.85	127.31
19	1	5007	CLA	O2D-CGD-CBD	4.52	119.30	111.27
19	6	302	CLA	O2A-C1-C2	4.52	120.51	108.64
27	5	302	RRX	C38-C26-C25	-4.51	119.46	124.53
27	4	303	RRX	C38-C26-C25	-4.50	119.47	124.53
22	B	847	BCR	C38-C26-C25	-4.50	119.48	124.53
22	3	5006	BCR	C38-C26-C25	-4.50	119.48	124.53
28	J	1902	C7Z	C7-C8-C9	-4.50	119.44	126.23
31	Z	317	LUT	C11-C10-C9	-4.49	120.90	127.31
32	5	315	CHL	CHD-C1D-ND	-4.49	120.32	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Z	302	CHL	CHD-C1D-ND	-4.49	120.33	124.45
22	3	5005	BCR	C15-C14-C13	-4.49	120.90	127.31
19	A	808	CLA	O2A-C1-C2	4.48	120.42	108.64
19	A	821	CLA	O2A-C1-C2	4.48	120.42	108.64
28	1	5005	C7Z	C27-C28-C29	-4.48	119.47	126.23
22	8	306	BCR	C20-C21-C22	-4.48	120.92	127.31
19	6	312	CLA	O2D-CGD-CBD	4.48	119.22	111.27
22	B	846	BCR	C38-C26-C25	-4.47	119.50	124.53
22	4	305	BCR	C33-C5-C6	-4.47	119.50	124.53
19	5	306	CLA	O2A-C1-C2	4.47	120.39	108.64
22	B	846	BCR	C24-C23-C22	-4.46	119.50	126.23
19	4	311	CLA	C2D-C1D-ND	4.46	113.39	110.10
22	5	305	BCR	C33-C5-C6	-4.45	119.53	124.53
22	B	842	BCR	C30-C25-C26	-4.45	116.34	122.61
19	A	836	CLA	O2A-C1-C2	4.45	120.33	108.64
19	B	835	CLA	C1-C2-C3	-4.45	118.34	126.04
19	8	311	CLA	O2A-C1-C2	4.45	120.32	108.64
19	B	811	CLA	O2A-C1-C2	4.44	120.31	108.64
22	B	844	BCR	C15-C14-C13	-4.44	120.97	127.31
19	B	823	CLA	O2A-C1-C2	4.44	120.30	108.64
31	Z	317	LUT	C21-C26-C27	-4.43	107.10	112.70
32	5	318	CHL	C1-C2-C3	-4.43	119.58	126.75
19	A	807	CLA	O2A-C1-C2	4.43	120.28	108.64
22	A	846	BCR	C16-C17-C18	-4.43	120.99	127.31
19	B	825	CLA	O2D-CGD-CBD	4.43	119.13	111.27
22	B	846	BCR	C7-C8-C9	-4.42	119.56	126.23
19	B	837	CLA	O2A-C1-C2	4.41	120.22	108.64
19	Z	306	CLA	O2A-C1-C2	4.40	120.21	108.64
22	8	303	BCR	C7-C8-C9	-4.40	119.58	126.23
19	B	801	CLA	O2A-C1-C2	4.40	120.20	108.64
22	A	849	BCR	C4-C5-C6	-4.40	116.35	122.73
19	3	5014	CLA	O2D-CGD-CBD	4.39	119.08	111.27
23	A	852	LHG	O7-C7-C8	4.39	120.96	111.50
19	A	831	CLA	C1-C2-C3	-4.38	119.67	126.75
19	4	311	CLA	O2A-C1-C2	4.38	120.14	108.64
19	Z	305	CLA	O2D-CGD-CBD	4.38	119.05	111.27
19	8	308	CLA	O2A-C1-C2	4.38	120.13	108.64
22	4	305	BCR	C15-C14-C13	-4.37	121.07	127.31
19	A	804	CLA	O2A-C1-C2	4.37	120.12	108.64
32	Z	310	CHL	CHD-C1D-ND	-4.37	120.44	124.45
19	B	850	CLA	O2D-CGD-CBD	4.37	119.03	111.27
22	A	859	BCR	C20-C21-C22	-4.37	121.08	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	1603	BCR	C24-C23-C22	-4.36	119.65	126.23
22	3	5004	BCR	C16-C17-C18	-4.36	121.09	127.31
31	Z	318	LUT	C18-C5-C6	-4.36	119.64	124.53
22	A	849	BCR	C20-C21-C22	-4.35	121.10	127.31
22	7	305	BCR	C24-C23-C22	-4.35	119.66	126.23
22	3	5007	BCR	C37-C22-C21	-4.35	116.84	122.92
19	B	840	CLA	O2A-C1-C2	4.34	120.05	108.64
22	A	847	BCR	C38-C26-C25	-4.34	119.65	124.53
22	7	305	BCR	C15-C14-C13	-4.34	121.11	127.31
19	Z	305	CLA	C1-C2-C3	-4.34	118.53	126.04
22	8	306	BCR	C38-C26-C25	-4.34	119.66	124.53
32	6	319	CHL	C3C-C4C-NC	-4.33	105.71	110.57
19	B	820	CLA	C1-C2-C3	-4.33	118.55	126.04
28	1	5005	C7Z	C18-C5-C6	-4.33	119.67	124.53
32	5	320	CHL	CHD-C1D-ND	-4.33	120.48	124.45
22	5	305	BCR	C11-C12-C13	-4.32	114.27	126.42
22	3	5004	BCR	C33-C5-C6	-4.32	119.67	124.53
28	J	1902	C7Z	C15-C14-C13	-4.32	121.14	127.31
23	4	320	LHG	O7-C7-C8	4.32	120.81	111.50
22	3	5006	BCR	C30-C25-C26	-4.32	116.53	122.61
22	6	307	BCR	C16-C17-C18	-4.32	121.14	127.31
19	7	312	CLA	O2A-C1-C2	4.32	119.99	108.64
31	7	304	LUT	C21-C26-C27	4.31	118.16	112.70
19	7	307	CLA	O2D-CGD-CBD	4.31	118.93	111.27
19	A	839	CLA	O2A-C1-C2	4.30	119.95	108.64
22	3	5007	BCR	C16-C15-C14	-4.30	114.66	123.47
19	7	317	CLA	C1-C2-C3	-4.30	119.79	126.75
29	J	1903	LMG	O7-C10-C11	4.30	120.78	111.50
22	A	846	BCR	C38-C26-C25	-4.30	119.70	124.53
31	Z	317	LUT	C1-C6-C5	-4.30	116.56	122.61
23	6	324	LHG	O7-C7-C8	4.30	120.77	111.50
22	3	5007	BCR	C29-C30-C25	4.30	117.10	110.48
32	4	319	CHL	CHD-C1D-ND	-4.30	120.50	124.45
19	6	310	CLA	O2A-C1-C2	4.29	119.92	108.64
32	8	301	CHL	CHD-C1D-ND	-4.29	120.51	124.45
19	A	840	CLA	O2D-CGD-CBD	4.29	118.89	111.27
22	A	850	BCR	C38-C26-C25	-4.29	119.71	124.53
32	Z	313	CHL	C4D-CHA-C1A	4.29	126.47	121.25
19	7	310	CLA	O2A-C1-C2	4.28	119.89	108.64
19	7	307	CLA	C1-C2-C3	-4.28	119.83	126.75
22	3	5006	BCR	C11-C10-C9	-4.28	121.21	127.31
22	8	303	BCR	C4-C5-C6	-4.28	116.52	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	5	303	LUT	C35-C34-C33	-4.28	121.21	127.31
32	1	5009	CHL	CHD-C1D-ND	-4.27	120.53	124.45
32	3	5017	CHL	C3C-C4C-NC	-4.27	105.78	110.57
22	B	844	BCR	C38-C26-C25	-4.27	119.74	124.53
22	A	858	BCR	C4-C5-C6	-4.27	116.54	122.73
32	Z	309	CHL	CHD-C1D-ND	-4.26	120.54	124.45
23	A	851	LHG	O7-C7-C8	4.26	120.68	111.50
31	3	5003	LUT	C18-C5-C6	-4.26	119.75	124.53
22	B	845	BCR	C20-C21-C22	-4.26	121.24	127.31
22	6	308	BCR	C11-C12-C13	-4.25	114.47	126.42
31	7	304	LUT	C35-C34-C33	-4.25	121.24	127.31
31	8	305	LUT	C35-C34-C33	-4.25	121.24	127.31
19	1	5006	CLA	O2D-CGD-CBD	4.25	118.82	111.27
19	A	832	CLA	C1-C2-C3	-4.25	118.70	126.04
29	7	301	LMG	O7-C10-C11	4.24	120.64	111.50
19	5	314	CLA	O2D-CGD-CBD	4.24	118.81	111.27
19	A	825	CLA	O2A-C1-C2	4.24	119.77	108.64
22	3	5004	BCR	C4-C5-C6	-4.23	116.58	122.73
22	B	845	BCR	C30-C25-C26	-4.23	116.66	122.61
32	6	317	CHL	CHD-C1D-ND	-4.22	120.57	124.45
19	1	5016	CLA	C1-C2-C3	-4.22	118.74	126.04
38	8	325	ERG	C6-C7-C8	-4.22	113.77	122.07
23	Z	316	LHG	O7-C7-C8	4.21	120.58	111.50
32	8	315	CHL	CHD-C1D-ND	-4.21	120.58	124.45
19	A	815	CLA	C1-C2-C3	-4.21	118.76	126.04
19	3	5008	CLA	O2D-CGD-CBD	4.20	118.72	111.27
32	4	314	CHL	CHD-C1D-ND	-4.19	120.61	124.45
22	G	1603	BCR	C15-C14-C13	-4.19	121.34	127.31
19	7	308	CLA	C1-C2-C3	-4.18	118.81	126.04
19	B	815	CLA	C1-C2-C3	-4.18	118.81	126.04
23	7	320	LHG	O7-C7-C8	4.18	120.50	111.50
23	1	5001	LHG	O7-C7-C8	4.17	120.50	111.50
22	K	206	BCR	C24-C23-C22	-4.17	119.93	126.23
22	5	305	BCR	C36-C18-C17	-4.17	117.08	122.92
27	F	304	RRX	C20-C21-C22	-4.17	121.36	127.31
19	G	1601	CLA	O2A-C1-C2	4.17	119.58	108.64
32	6	315	CHL	C3C-C4C-NC	-4.16	105.90	110.57
22	K	206	BCR	C38-C26-C25	-4.16	119.85	124.53
19	7	316	CLA	O2A-C1-C2	4.16	119.57	108.64
22	A	858	BCR	C15-C14-C13	-4.16	121.37	127.31
22	8	303	BCR	C20-C21-C22	-4.16	121.37	127.31
19	7	311	CLA	O2D-CGD-CBD	4.15	118.65	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	838	CLA	O2A-C1-C2	4.15	119.55	108.64
31	1	5004	LUT	C35-C34-C33	-4.15	121.38	127.31
22	A	848	BCR	C33-C5-C6	-4.15	119.87	124.53
22	B	842	BCR	C33-C5-C6	-4.15	119.87	124.53
31	Z	317	LUT	C28-C29-C30	4.15	125.31	118.94
18	A	801	CL0	O2A-CGA-CBA	4.14	124.91	111.91
31	7	303	LUT	C31-C30-C29	-4.14	121.40	127.31
19	5	325	CLA	O2A-C1-C2	4.14	119.52	108.64
22	6	307	BCR	C33-C5-C6	-4.14	119.88	124.53
19	4	316	CLA	C1-C2-C3	-4.14	120.06	126.75
22	A	847	BCR	C27-C26-C25	-4.14	116.73	122.73
19	4	307	CLA	C1-C2-C3	-4.14	118.89	126.04
19	1	5012	CLA	O2A-C1-C2	4.13	119.50	108.64
19	1	5011	CLA	C1-C2-C3	-4.13	118.90	126.04
28	J	1902	C7Z	C18-C5-C6	-4.13	119.89	124.53
19	B	822	CLA	C1-C2-C3	-4.13	118.90	126.04
22	F	302	BCR	C30-C25-C26	-4.13	116.80	122.61
19	Z	315	CLA	O2A-C1-C2	4.13	119.48	108.64
31	8	304	LUT	C32-C33-C34	4.12	125.26	118.94
25	B	848	DGD	O2G-C1B-C2B	4.12	120.38	111.50
19	8	310	CLA	O2D-CGD-CBD	4.11	118.58	111.27
32	Z	310	CHL	CHD-C4C-C3C	4.11	130.88	124.84
22	B	843	BCR	C27-C26-C25	-4.11	116.76	122.73
32	6	316	CHL	CHD-C1D-ND	-4.10	120.69	124.45
19	3	5012	CLA	O2A-C1-C2	4.10	119.41	108.64
32	5	316	CHL	C3C-C4C-NC	-4.10	105.98	110.57
23	5	323	LHG	O7-C7-C8	4.10	120.33	111.50
32	5	316	CHL	CHD-C1D-ND	-4.09	120.69	124.45
22	G	1603	BCR	C11-C10-C9	-4.09	121.47	127.31
31	7	303	LUT	C7-C8-C9	-4.08	120.06	126.23
22	A	848	BCR	C38-C26-C25	-4.08	119.94	124.53
32	1	5017	CHL	CHD-C1D-ND	-4.08	120.70	124.45
22	A	850	BCR	C33-C5-C6	-4.08	119.94	124.53
32	8	301	CHL	C3C-C4C-NC	-4.08	106.00	110.57
23	1	5019	LHG	O7-C7-C8	4.07	120.28	111.50
32	8	301	CHL	C2C-C3C-C4C	4.07	109.39	106.49
22	A	858	BCR	C30-C25-C26	-4.07	116.88	122.61
19	8	314	CLA	C1-C2-C3	-4.07	119.01	126.04
22	F	302	BCR	C11-C10-C9	-4.06	121.51	127.31
31	4	304	LUT	C17-C1-C6	-4.06	103.71	110.30
22	8	303	BCR	C33-C5-C6	-4.06	119.97	124.53
22	3	5004	BCR	C27-C26-C25	-4.06	116.84	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	849	BCR	C27-C26-C25	-4.05	116.84	122.73
19	A	804	CLA	C1-C2-C3	-4.04	119.05	126.04
19	A	828	CLA	O2A-C1-C2	4.04	119.25	108.64
22	A	849	BCR	C7-C8-C9	-4.04	120.13	126.23
31	Z	318	LUT	C1-C6-C5	-4.04	116.93	122.61
28	J	1902	C7Z	C38-C25-C26	-4.03	120.00	124.53
38	6	326	ERG	C19-C10-C1	-4.02	103.07	109.43
22	A	850	BCR	C30-C25-C26	-4.02	116.95	122.61
22	B	847	BCR	C1-C6-C5	-4.02	116.95	122.61
22	5	305	BCR	C35-C13-C14	-4.01	117.31	122.92
38	6	326	ERG	C13-C17-C20	-4.01	114.26	119.43
32	1	5014	CHL	CHD-C1D-ND	-4.01	120.77	124.45
32	8	319	CHL	C1-C2-C3	-4.01	119.11	126.04
22	3	5006	BCR	C33-C5-C6	-4.00	120.03	124.53
19	B	830	CLA	C1-C2-C3	-4.00	120.29	126.75
31	5	303	LUT	C15-C14-C13	-3.99	121.62	127.31
19	A	829	CLA	C1-C2-C3	-3.99	119.14	126.04
27	F	304	RRX	C24-C23-C22	-3.99	120.21	126.23
19	A	814	CLA	O2A-C1-C2	3.99	119.11	108.64
31	1	5003	LUT	C35-C34-C33	-3.98	121.62	127.31
19	B	821	CLA	C1-C2-C3	-3.98	119.16	126.04
19	I	201	CLA	O2A-C1-C2	3.98	119.08	108.64
19	B	833	CLA	O2A-C1-C2	3.97	119.06	108.64
23	8	321	LHG	O7-C7-C8	3.96	120.04	111.50
22	K	206	BCR	C30-C25-C26	-3.96	117.04	122.61
31	1	5004	LUT	C31-C30-C29	-3.95	121.68	127.31
22	3	5004	BCR	C11-C10-C9	-3.95	121.68	127.31
22	A	849	BCR	C38-C26-C27	3.94	121.19	113.62
32	8	315	CHL	C3C-C4C-NC	-3.94	106.15	110.57
22	6	308	BCR	C23-C24-C25	-3.94	116.13	127.20
22	A	859	BCR	C11-C10-C9	-3.94	121.69	127.31
22	K	206	BCR	C33-C5-C6	-3.93	120.11	124.53
22	6	307	BCR	C11-C12-C13	-3.93	115.38	126.42
22	A	859	BCR	C38-C26-C25	-3.93	120.12	124.53
27	4	303	RRX	C20-C21-C22	-3.93	121.70	127.31
22	A	848	BCR	C27-C26-C25	-3.93	117.03	122.73
22	A	859	BCR	C27-C26-C25	-3.92	117.03	122.73
29	J	1904	LMG	O7-C10-C11	3.92	119.95	111.50
32	8	319	CHL	CHD-C1D-ND	-3.92	120.85	124.45
22	3	5007	BCR	C23-C22-C21	3.92	124.95	118.94
19	1	5015	CLA	C1-C2-C3	-3.92	120.42	126.75
28	6	304	C7Z	C38-C25-C26	-3.91	120.13	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	7	314	CHL	CHD-C1D-ND	-3.91	120.86	124.45
31	4	304	LUT	C21-C26-C27	-3.91	107.76	112.70
19	Z	304	CLA	O2A-C1-C2	3.91	118.90	108.64
22	8	306	BCR	C15-C14-C13	-3.90	121.74	127.31
22	3	5005	BCR	C33-C5-C6	-3.90	120.15	124.53
22	A	858	BCR	C27-C26-C25	-3.90	117.07	122.73
22	3	5004	BCR	C2-C1-C6	3.90	116.48	110.48
31	Z	317	LUT	C40-C33-C32	-3.89	111.94	118.08
19	A	807	CLA	C1-C2-C3	-3.89	119.31	126.04
22	G	1603	BCR	C1-C6-C5	-3.89	117.13	122.61
22	3	5004	BCR	C15-C14-C13	-3.89	121.76	127.31
23	6	303	LHG	O7-C7-C8	3.89	119.88	111.50
22	3	5005	BCR	C1-C6-C5	-3.88	117.14	122.61
27	F	304	RRX	C30-C25-C26	-3.88	117.14	122.61
28	6	304	C7Z	C27-C28-C29	-3.88	120.37	126.23
32	7	315	CHL	CHD-C1D-ND	-3.88	120.89	124.45
22	5	305	BCR	C16-C17-C18	-3.88	121.78	127.31
18	A	801	CL0	C1D-ND-C4D	-3.88	103.58	106.33
22	3	5004	BCR	C8-C7-C6	-3.87	116.32	127.20
32	5	315	CHL	C1-O2A-CGA	3.87	126.60	116.44
19	8	313	CLA	C1-C2-C3	-3.87	119.35	126.04
19	B	832	CLA	C1-C2-C3	-3.87	119.35	126.04
22	6	307	BCR	C20-C21-C22	-3.87	121.79	127.31
22	3	5004	BCR	C38-C26-C25	-3.87	120.19	124.53
31	1	5004	LUT	C21-C26-C27	-3.86	107.82	112.70
32	7	315	CHL	C3C-C4C-NC	-3.86	106.24	110.57
19	6	320	CLA	C1-C2-C3	-3.86	119.37	126.04
19	A	823	CLA	C1-C2-C3	-3.85	119.38	126.04
19	A	837	CLA	C1-C2-C3	-3.85	119.39	126.04
31	6	305	LUT	C18-C5-C6	-3.85	120.21	124.53
19	4	307	CLA	CHD-C1D-ND	-3.83	120.93	124.45
31	Z	318	LUT	C22-C23-C24	3.83	116.10	111.74
22	A	846	BCR	C11-C10-C9	-3.83	121.85	127.31
22	A	848	BCR	C30-C25-C26	-3.82	117.23	122.61
22	A	858	BCR	C38-C26-C25	-3.82	120.24	124.53
22	5	305	BCR	C16-C15-C14	-3.82	115.66	123.47
31	6	306	LUT	C11-C10-C9	-3.82	121.86	127.31
28	1	5005	C7Z	C15-C14-C13	-3.81	121.87	127.31
19	3	5016	CLA	C1-C2-C3	-3.81	119.45	126.04
19	B	811	CLA	C1-C2-C3	-3.81	119.46	126.04
31	7	304	LUT	C2-C3-C4	3.81	115.52	110.30
19	A	843	CLA	C1-C2-C3	-3.80	119.47	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	816	CLA	C1-C2-C3	-3.80	119.47	126.04
38	6	326	ERG	C16-C17-C13	-3.79	99.27	103.84
22	B	842	BCR	C20-C21-C22	-3.79	121.90	127.31
32	6	321	CHL	C1B-CHB-C4A	-3.79	122.62	130.12
19	5	312	CLA	C1-C2-C3	-3.79	119.50	126.04
22	8	303	BCR	C33-C5-C4	3.78	120.88	113.62
19	A	833	CLA	C1-C2-C3	-3.77	119.53	126.04
32	4	315	CHL	C1-C2-C3	-3.76	120.66	126.75
27	5	302	RRX	C2-C1-C6	3.76	116.27	110.48
35	7	302	DGA	OG2-CB1-CB2	3.76	119.61	111.50
22	3	5006	BCR	C24-C23-C22	-3.76	120.55	126.23
22	B	842	BCR	C1-C6-C5	-3.76	117.32	122.61
22	3	5005	BCR	C16-C17-C18	-3.76	121.95	127.31
19	7	311	CLA	C1-C2-C3	-3.76	119.55	126.04
38	6	326	ERG	C1-C10-C5	3.75	115.62	108.75
31	3	5002	LUT	C18-C5-C6	-3.75	120.31	124.53
22	5	305	BCR	C23-C24-C25	-3.75	116.67	127.20
19	8	307	CLA	C1-O2A-CGA	3.74	126.26	116.44
19	4	311	CLA	CHD-C1D-ND	-3.74	121.02	124.45
32	6	321	CHL	C3C-C4C-NC	-3.73	106.39	110.57
28	1	5005	C7Z	C38-C25-C26	-3.73	120.34	124.53
19	A	810	CLA	C1-C2-C3	-3.72	119.60	126.04
34	6	325	3PH	O21-C21-C22	3.72	119.53	111.50
31	Z	317	LUT	C39-C29-C30	-3.72	117.71	122.92
19	B	840	CLA	O2D-CGD-O1D	-3.72	116.57	123.84
19	A	820	CLA	C1-C2-C3	-3.72	119.61	126.04
19	B	819	CLA	C1-C2-C3	-3.72	119.61	126.04
22	8	303	BCR	C24-C23-C22	-3.71	120.62	126.23
22	B	847	BCR	C33-C5-C6	-3.71	120.36	124.53
22	7	305	BCR	C38-C26-C25	-3.71	120.36	124.53
22	A	846	BCR	C24-C23-C22	-3.70	120.65	126.23
19	7	319	CLA	C1-C2-C3	-3.70	119.65	126.04
34	3	5022	3PH	O21-C21-C22	3.70	119.47	111.50
32	Z	302	CHL	C3C-C4C-NC	-3.69	106.43	110.57
19	A	821	CLA	C1-C2-C3	-3.69	119.65	126.04
19	6	322	CLA	CHD-C1D-ND	-3.69	121.06	124.45
19	5	309	CLA	C1-C2-C3	-3.69	119.66	126.04
31	6	306	LUT	C21-C26-C27	3.69	117.36	112.70
20	B	841	PQN	C11-C12-C13	-3.68	120.66	126.79
19	7	324	CLA	C1-C2-C3	-3.68	119.67	126.04
22	3	5007	BCR	C34-C9-C10	-3.68	117.76	122.92
19	7	309	CLA	O2D-CGD-O1D	-3.68	116.64	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	8	305	LUT	C15-C14-C13	-3.68	122.06	127.31
22	G	1603	BCR	C30-C25-C26	-3.68	117.43	122.61
19	A	819	CLA	C1-C2-C3	-3.67	119.69	126.04
19	B	802	CLA	C1-C2-C3	-3.67	119.69	126.04
28	1	5005	C7Z	C7-C8-C9	-3.67	120.69	126.23
22	A	847	BCR	C7-C8-C9	-3.67	120.69	126.23
19	A	817	CLA	C1-C2-C3	-3.67	119.70	126.04
19	Z	304	CLA	C1-C2-C3	-3.67	120.82	126.75
31	8	305	LUT	C18-C5-C6	-3.67	120.41	124.53
32	8	316	CHL	CHD-C1D-ND	-3.66	121.09	124.45
22	5	304	BCR	C30-C25-C26	-3.66	117.45	122.61
38	8	325	ERG	C16-C15-C14	-3.66	99.27	105.30
32	4	317	CHL	C3C-C4C-NC	-3.66	106.47	110.57
19	4	309	CLA	C1-C2-C3	-3.65	119.72	126.04
19	1	5006	CLA	CHD-C1D-ND	-3.65	121.10	124.45
19	3	5011	CLA	O2A-CGA-CBA	3.65	123.36	111.91
31	3	5003	LUT	C2-C3-C4	3.65	115.30	110.30
22	4	305	BCR	C24-C23-C22	-3.64	120.73	126.23
22	8	306	BCR	C21-C20-C19	-3.64	111.85	123.22
32	8	317	CHL	C3C-C4C-NC	-3.64	106.49	110.57
19	B	808	CLA	C1-C2-C3	-3.64	119.75	126.04
22	A	848	BCR	C24-C23-C22	-3.64	120.74	126.23
32	6	315	CHL	C2C-C3C-C4C	3.63	109.08	106.49
27	5	302	RRX	C30-C25-C26	-3.63	117.50	122.61
32	8	319	CHL	C3C-C4C-NC	-3.63	106.50	110.57
27	F	304	RRX	C7-C8-C9	-3.63	120.75	126.23
31	7	303	LUT	C18-C5-C6	-3.63	120.46	124.53
38	6	326	ERG	C18-C13-C14	-3.62	104.37	110.24
28	1	5005	C7Z	C21-C26-C25	-3.62	117.52	122.61
22	K	206	BCR	C38-C26-C27	3.62	120.56	113.62
22	6	307	BCR	C38-C26-C25	-3.61	120.47	124.53
27	5	302	RRX	C10-C11-C12	-3.61	111.94	123.22
19	B	840	CLA	C2C-C1C-NC	3.61	113.36	109.97
19	A	842	CLA	C1-C2-C3	-3.61	119.80	126.04
19	4	307	CLA	C1D-ND-C4D	-3.61	103.77	106.33
19	B	833	CLA	C1-C2-C3	-3.61	119.80	126.04
22	F	302	BCR	C16-C15-C14	-3.61	116.08	123.47
19	8	308	CLA	C2D-C1D-ND	3.61	112.76	110.10
32	Z	309	CHL	C3C-C4C-NC	-3.60	106.53	110.57
22	6	307	BCR	C24-C23-C22	-3.60	120.80	126.23
32	4	314	CHL	C3C-C4C-NC	-3.59	106.54	110.57
22	A	849	BCR	C1-C6-C5	-3.59	117.56	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	305	BCR	C33-C5-C6	-3.59	120.50	124.53
22	A	847	BCR	C30-C25-C26	-3.59	117.56	122.61
19	3	5010	CLA	O2A-CGA-CBA	3.59	123.16	111.91
19	7	309	CLA	O2A-CGA-CBA	3.58	123.14	111.91
19	5	308	CLA	CHD-C1D-ND	-3.58	121.17	124.45
19	K	203	CLA	C1-C2-C3	-3.58	119.85	126.04
32	3	5017	CHL	CHC-C1C-NC	3.57	129.63	124.20
22	A	849	BCR	C38-C26-C25	-3.57	120.52	124.53
19	6	310	CLA	CHD-C1D-ND	-3.57	121.17	124.45
22	8	306	BCR	C30-C25-C26	-3.57	117.59	122.61
22	7	305	BCR	C33-C5-C4	3.57	120.47	113.62
34	5	324	3PH	O21-C21-C22	3.56	119.18	111.50
38	6	326	ERG	C6-C7-C8	-3.56	115.06	122.07
22	A	859	BCR	C29-C30-C25	3.56	115.96	110.48
22	3	5007	BCR	C8-C9-C10	3.56	124.40	118.94
19	4	308	CLA	C1-C2-C3	-3.56	119.89	126.04
19	4	310	CLA	C1-C2-C3	-3.55	119.90	126.04
32	5	320	CHL	C4D-CHA-C1A	3.55	125.57	121.25
32	Z	309	CHL	C1-C2-C3	-3.55	119.90	126.04
32	6	317	CHL	C3C-C4C-NC	-3.55	106.59	110.57
22	5	305	BCR	C4-C5-C6	-3.55	117.58	122.73
19	A	841	CLA	C1-C2-C3	-3.55	119.91	126.04
19	7	306	CLA	CHD-C1D-ND	-3.54	121.20	124.45
31	3	5003	LUT	C35-C34-C33	-3.54	122.26	127.31
19	1	5010	CLA	CHD-C1D-ND	-3.54	121.20	124.45
22	4	305	BCR	C16-C17-C18	-3.53	122.27	127.31
19	B	814	CLA	C1-C2-C3	-3.53	119.93	126.04
22	B	845	BCR	C33-C5-C6	-3.53	120.56	124.53
19	4	311	CLA	C1-C2-C3	-3.53	121.04	126.75
19	3	5012	CLA	CHD-C1D-ND	-3.53	121.21	124.45
22	8	306	BCR	C33-C5-C6	-3.53	120.56	124.53
19	F	301	CLA	C2D-C1D-ND	3.53	112.70	110.10
31	5	303	LUT	C21-C26-C25	3.52	117.73	111.42
22	B	843	BCR	C30-C25-C26	-3.52	117.65	122.61
22	B	844	BCR	C4-C5-C6	-3.52	117.62	122.73
22	B	846	BCR	C15-C16-C17	-3.52	116.27	123.47
22	8	306	BCR	C7-C8-C9	-3.52	120.92	126.23
19	Z	305	CLA	CHD-C1D-ND	-3.51	121.22	124.45
31	1	5003	LUT	C7-C8-C9	-3.51	120.93	126.23
28	6	304	C7Z	C21-C26-C25	-3.51	117.67	122.61
31	7	304	LUT	C15-C14-C13	-3.51	122.30	127.31
31	8	304	LUT	C1-C6-C5	-3.51	117.68	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	5004	BCR	C38-C26-C27	3.50	120.34	113.62
38	8	325	ERG	C12-C13-C14	3.50	112.82	107.27
22	B	842	BCR	C11-C10-C9	-3.50	122.32	127.31
19	7	307	CLA	C2C-C1C-NC	3.50	113.25	109.97
27	F	304	RRX	C38-C26-C25	-3.50	120.60	124.53
27	4	303	RRX	C10-C11-C12	-3.50	112.31	123.22
31	4	304	LUT	C35-C34-C33	-3.50	122.32	127.31
31	Z	318	LUT	C2-C3-C4	3.50	115.09	110.30
19	A	828	CLA	C1-C2-C3	-3.49	120.00	126.04
19	Z	315	CLA	C1-C2-C3	-3.49	120.00	126.04
22	K	206	BCR	C20-C21-C22	-3.49	122.33	127.31
32	8	316	CHL	C1-C2-C3	-3.49	120.02	126.04
19	5	311	CLA	C1-C2-C3	-3.48	121.11	126.75
22	6	307	BCR	C38-C26-C27	3.48	120.31	113.62
22	3	5004	BCR	C20-C21-C22	-3.48	122.34	127.31
19	A	835	CLA	C1-C2-C3	-3.48	120.03	126.04
19	5	317	CLA	C2D-C1D-ND	3.48	112.67	110.10
32	5	315	CHL	C3C-C4C-NC	-3.48	106.67	110.57
19	1	5006	CLA	O2A-C1-C2	3.48	117.77	108.64
32	3	5017	CHL	CHD-C4C-C3C	3.47	129.94	124.84
22	3	5006	BCR	C38-C26-C27	3.47	120.29	113.62
27	4	303	RRX	C4-C5-C6	-3.47	117.69	122.73
22	B	844	BCR	C16-C17-C18	-3.46	122.36	127.31
31	7	303	LUT	C15-C14-C13	-3.46	122.37	127.31
32	Z	313	CHL	CMA-C3A-C4A	3.46	121.08	111.77
24	8	323	LMT	C1-O1'-C1'	-3.46	108.10	113.84
22	5	305	BCR	C12-C13-C14	3.46	124.25	118.94
22	8	306	BCR	C23-C24-C25	-3.46	117.49	127.20
22	A	858	BCR	C16-C17-C18	-3.46	122.38	127.31
32	Z	313	CHL	C1B-CHB-C4A	-3.46	123.27	130.12
32	4	317	CHL	C2C-C3C-C4C	3.45	108.95	106.49
22	A	847	BCR	C24-C23-C22	-3.45	121.02	126.23
19	8	311	CLA	CHD-C1D-ND	-3.45	121.28	124.45
32	5	316	CHL	CMA-C3A-C4A	3.45	121.05	111.77
22	A	858	BCR	C24-C23-C22	-3.45	121.02	126.23
31	3	5002	LUT	C35-C34-C33	-3.45	122.39	127.31
19	Z	306	CLA	C1-C2-C3	-3.45	121.17	126.75
19	Z	303	CLA	C2C-C1C-NC	3.45	113.20	109.97
27	5	302	RRX	C4-C5-C6	-3.45	117.73	122.73
19	A	826	CLA	C1-C2-C3	-3.44	120.09	126.04
37	8	302	SQD	O7-S-C6	-3.44	102.85	106.94
32	8	316	CHL	C4D-CHA-C1A	3.44	125.44	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	307	CLA	CHD-C1D-ND	-3.44	121.30	124.45
19	4	311	CLA	CMA-C3A-C4A	3.43	121.00	111.77
19	1	5015	CLA	C2D-C1D-ND	3.43	112.64	110.10
19	6	323	CLA	O2A-CGA-CBA	3.43	122.68	111.91
19	3	5013	CLA	CHD-C1D-ND	-3.43	121.30	124.45
19	A	824	CLA	C1-C2-C3	-3.43	120.11	126.04
22	A	846	BCR	C1-C6-C5	-3.43	117.78	122.61
19	G	1601	CLA	C1-C2-C3	-3.43	121.21	126.75
22	F	302	BCR	C20-C19-C18	-3.42	116.80	126.42
19	3	5018	CLA	CHD-C1D-ND	-3.42	121.31	124.45
19	5	306	CLA	CHD-C1D-ND	-3.42	121.31	124.45
19	A	806	CLA	C1-C2-C3	-3.42	120.12	126.04
32	8	319	CHL	C2C-C3C-C4C	3.42	108.93	106.49
19	3	5011	CLA	CAA-C2A-C3A	-3.42	103.41	112.78
19	F	301	CLA	CHD-C1D-ND	-3.42	121.31	124.45
22	8	306	BCR	C16-C17-C18	-3.42	122.43	127.31
19	4	313	CLA	C1-C2-C3	-3.41	120.14	126.04
22	7	305	BCR	C38-C26-C27	3.41	120.17	113.62
19	Z	315	CLA	C2D-C1D-ND	3.41	112.62	110.10
19	A	809	CLA	C1-C2-C3	-3.41	120.14	126.04
22	A	846	BCR	C27-C26-C25	-3.41	117.78	122.73
18	A	801	CL0	C1-C2-C3	-3.41	120.15	126.04
22	6	308	BCR	C35-C13-C14	-3.41	118.15	122.92
31	4	304	LUT	C15-C14-C13	-3.40	122.45	127.31
19	8	313	CLA	C2D-C1D-ND	3.40	112.61	110.10
19	1	5013	CLA	CHD-C1D-ND	-3.40	121.33	124.45
19	B	807	CLA	C1-C2-C3	-3.40	120.17	126.04
22	6	307	BCR	C23-C24-C25	-3.39	117.67	127.20
19	A	830	CLA	C1-C2-C3	-3.39	120.18	126.04
31	6	305	LUT	C15-C14-C13	-3.39	122.47	127.31
19	A	822	CLA	C2D-C1D-ND	3.39	112.60	110.10
22	B	846	BCR	C27-C26-C25	-3.39	117.81	122.73
19	3	5015	CLA	C2D-C1D-ND	3.39	112.60	110.10
22	3	5004	BCR	C33-C5-C4	3.39	120.12	113.62
19	7	313	CLA	C2D-C1D-ND	3.38	112.60	110.10
32	3	5017	CHL	C1B-CHB-C4A	-3.38	123.42	130.12
19	7	310	CLA	CHD-C1D-ND	-3.38	121.35	124.45
19	5	322	CLA	C2D-C1D-ND	3.38	112.59	110.10
19	A	805	CLA	C1-C2-C3	-3.38	120.20	126.04
19	B	803	CLA	C2C-C1C-NC	3.38	113.13	109.97
19	B	825	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
31	6	306	LUT	C35-C34-C33	-3.37	122.49	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	8	304	LUT	C40-C33-C34	-3.37	118.20	122.92
31	1	5003	LUT	C18-C5-C6	-3.37	120.74	124.53
32	5	318	CHL	C4A-NA-C1A	3.37	108.22	106.71
22	6	307	BCR	C33-C5-C4	3.37	120.09	113.62
19	A	857	CLA	C6-C5-C3	-3.37	109.11	114.62
22	3	5006	BCR	C7-C8-C9	-3.36	121.16	126.23
19	1	5013	CLA	O2A-C1-C2	3.36	120.85	109.49
19	8	314	CLA	CHD-C1D-ND	-3.35	121.37	124.45
19	Z	312	CLA	C1-C2-C3	-3.35	120.24	126.04
22	B	843	BCR	C16-C17-C18	-3.35	122.53	127.31
19	A	805	CLA	CHD-C1D-ND	-3.35	121.37	124.45
19	7	324	CLA	CHD-C1D-ND	-3.35	121.37	124.45
22	A	846	BCR	C38-C26-C27	3.35	120.05	113.62
32	4	315	CHL	CHD-C1D-ND	-3.35	121.38	124.45
22	B	845	BCR	C24-C23-C22	-3.35	121.17	126.23
27	5	302	RRX	C33-C5-C4	3.35	120.05	113.62
27	4	303	RRX	C16-C17-C18	-3.35	122.53	127.31
32	Z	313	CHL	C3C-C4C-NC	-3.35	106.82	110.57
19	A	839	CLA	C1-C2-C3	-3.35	120.26	126.04
19	1	5018	CLA	C1-C2-C3	-3.35	120.26	126.04
19	A	812	CLA	O2A-CGA-CBA	3.34	122.41	111.91
27	5	302	RRX	C16-C15-C14	-3.34	116.63	123.47
32	8	316	CHL	C3C-C4C-NC	-3.34	106.82	110.57
22	B	842	BCR	C33-C5-C4	3.34	120.04	113.62
34	3	5022	3PH	O31-C31-C32	3.34	122.40	111.91
19	5	319	CLA	C2D-C1D-ND	3.34	112.57	110.10
31	Z	317	LUT	C7-C8-C9	-3.34	121.19	126.23
22	3	5006	BCR	C15-C14-C13	-3.33	122.55	127.31
22	A	847	BCR	C38-C26-C27	3.33	120.02	113.62
19	4	306	CLA	CHD-C1D-ND	-3.33	121.39	124.45
19	B	839	CLA	C2C-C1C-NC	3.33	113.09	109.97
19	4	309	CLA	CHD-C1D-ND	-3.33	121.40	124.45
19	Z	308	CLA	CHD-C1D-ND	-3.32	121.40	124.45
32	4	315	CHL	C3C-C4C-NC	-3.32	106.85	110.57
19	A	813	CLA	C1-C2-C3	-3.32	120.31	126.04
19	8	310	CLA	O2A-CGA-CBA	3.32	122.32	111.91
19	A	803	CLA	C1-C2-C3	-3.32	120.31	126.04
19	1	5008	CLA	O2A-C1-C2	3.31	117.35	108.64
19	3	5019	CLA	CHD-C1D-ND	-3.31	121.41	124.45
22	B	842	BCR	C23-C24-C25	-3.31	117.90	127.20
22	A	859	BCR	C38-C26-C27	3.31	119.98	113.62
19	K	204	CLA	C2C-C1C-NC	3.31	113.07	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	1	5004	LUT	C15-C14-C13	-3.31	122.59	127.31
22	4	305	BCR	C23-C24-C25	-3.31	117.92	127.20
22	A	858	BCR	C20-C21-C22	-3.30	122.59	127.31
19	3	5018	CLA	C1-C2-C3	-3.30	120.33	126.04
19	3	5009	CLA	CHD-C1D-ND	-3.30	121.42	124.45
22	B	845	BCR	C33-C5-C4	3.30	119.95	113.62
19	8	318	CLA	CHD-C1D-ND	-3.29	121.43	124.45
32	7	314	CHL	C3C-C4C-NC	-3.29	106.88	110.57
19	B	823	CLA	C1-C2-C3	-3.29	120.35	126.04
22	A	848	BCR	C38-C26-C27	3.29	119.94	113.62
19	A	812	CLA	CHD-C1D-ND	-3.29	121.43	124.45
22	8	303	BCR	C30-C25-C26	-3.29	117.98	122.61
19	A	822	CLA	CHD-C1D-ND	-3.29	121.43	124.45
19	7	317	CLA	CHD-C1D-ND	-3.29	121.43	124.45
19	7	310	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
31	8	305	LUT	C11-C10-C9	-3.28	122.62	127.31
38	8	325	ERG	C11-C9-C10	-3.28	105.45	113.58
32	1	5009	CHL	C3C-C4C-NC	-3.28	106.89	110.57
19	A	814	CLA	CHD-C1D-ND	-3.28	121.44	124.45
19	B	825	CLA	O2A-CGA-CBA	3.28	122.20	111.91
19	6	310	CLA	C6-C5-C3	-3.28	109.26	114.62
28	6	304	C7Z	C18-C5-C6	-3.28	120.85	124.53
19	7	307	CLA	C2D-C1D-ND	3.28	112.52	110.10
19	6	312	CLA	O2A-CGA-CBA	3.27	122.18	111.91
22	B	842	BCR	C4-C5-C6	-3.27	117.98	122.73
22	B	847	BCR	C8-C7-C6	-3.27	118.02	127.20
19	B	826	CLA	C2D-C1D-ND	3.27	112.51	110.10
22	4	305	BCR	C38-C26-C27	3.27	119.89	113.62
19	6	313	CLA	C2C-C1C-NC	3.27	113.03	109.97
19	A	818	CLA	C2D-C1D-ND	3.27	112.51	110.10
32	5	318	CHL	C3C-C4C-NC	-3.27	106.91	110.57
22	B	845	BCR	C7-C8-C9	-3.26	121.31	126.23
19	5	312	CLA	C2D-C1D-ND	3.26	112.50	110.10
22	F	302	BCR	C8-C7-C6	-3.26	118.05	127.20
19	7	308	CLA	CAA-C2A-C3A	-3.26	103.86	112.78
22	A	846	BCR	C30-C25-C26	-3.26	118.03	122.61
19	B	822	CLA	CHD-C1D-ND	-3.26	121.46	124.45
19	B	822	CLA	C2D-C1D-ND	3.26	112.50	110.10
19	5	311	CLA	CHD-C1D-ND	-3.25	121.46	124.45
19	7	306	CLA	O2A-CGA-CBA	3.25	122.11	111.91
22	3	5004	BCR	C23-C24-C25	-3.25	118.08	127.20
19	B	836	CLA	CHD-C1D-ND	-3.25	121.47	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	839	CLA	CHD-C1D-ND	-3.25	121.47	124.45
19	B	829	CLA	C1-C2-C3	-3.24	120.43	126.04
19	5	310	CLA	CHD-C1D-ND	-3.24	121.47	124.45
19	5	317	CLA	CHD-C1D-ND	-3.24	121.48	124.45
22	3	5004	BCR	C21-C20-C19	-3.24	113.11	123.22
19	B	805	CLA	C2D-C1D-ND	3.24	112.49	110.10
19	B	807	CLA	C2C-C1C-NC	3.24	113.01	109.97
22	4	305	BCR	C29-C30-C25	3.24	115.46	110.48
19	B	802	CLA	C2D-C1D-ND	3.24	112.49	110.10
19	8	320	CLA	C2D-C1D-ND	3.23	112.49	110.10
31	7	303	LUT	C35-C34-C33	-3.23	122.69	127.31
19	A	815	CLA	CHD-C1D-ND	-3.23	121.48	124.45
19	B	834	CLA	CHD-C1D-ND	-3.23	121.48	124.45
19	3	5011	CLA	C2D-C1D-ND	3.23	112.49	110.10
32	4	319	CHL	C4D-CHA-C1A	3.23	125.18	121.25
19	A	837	CLA	CHD-C1D-ND	-3.23	121.48	124.45
31	7	303	LUT	C30-C31-C32	-3.23	113.13	123.22
19	B	819	CLA	CHD-C1D-ND	-3.23	121.49	124.45
19	I	201	CLA	C2D-C1D-ND	3.23	112.48	110.10
19	4	312	CLA	C2D-C1D-ND	3.23	112.48	110.10
22	A	848	BCR	C33-C5-C4	3.23	119.82	113.62
22	F	302	BCR	C1-C6-C5	-3.23	118.07	122.61
19	3	5011	CLA	CHD-C1D-ND	-3.23	121.49	124.45
24	8	323	LMT	C1B-O1B-C4'	-3.23	109.98	117.96
27	5	302	RRX	C8-C7-C6	-3.22	118.15	127.20
32	4	314	CHL	C4D-CHA-C1A	3.22	125.17	121.25
19	A	831	CLA	CHD-C1D-ND	-3.22	121.49	124.45
19	B	831	CLA	C2C-C1C-NC	3.22	112.99	109.97
19	4	308	CLA	C2D-C1D-ND	3.22	112.48	110.10
19	Z	306	CLA	CHD-C1D-ND	-3.22	121.49	124.45
19	3	5010	CLA	O2A-C1-C2	3.22	117.10	108.64
19	3	5020	CLA	C2C-C1C-NC	3.22	112.99	109.97
19	A	811	CLA	CHD-C1D-ND	-3.22	121.50	124.45
19	A	806	CLA	CHD-C1D-ND	-3.22	121.50	124.45
22	K	206	BCR	C16-C17-C18	-3.22	122.72	127.31
19	B	837	CLA	C2D-C1D-ND	3.21	112.47	110.10
19	Z	311	CLA	C2C-C1C-NC	3.21	112.98	109.97
19	A	819	CLA	CHD-C1D-ND	-3.21	121.51	124.45
22	B	844	BCR	C29-C30-C25	3.20	115.41	110.48
19	3	5019	CLA	C2D-C1D-ND	3.20	112.47	110.10
19	A	803	CLA	CHD-C1D-ND	-3.20	121.51	124.45
22	A	850	BCR	C38-C26-C27	3.20	119.77	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	816	CLA	C1-C2-C3	-3.20	120.50	126.04
19	A	811	CLA	C2D-C1D-ND	3.20	112.46	110.10
19	B	825	CLA	C2D-C1D-ND	3.20	112.46	110.10
27	4	303	RRX	C8-C7-C6	-3.20	118.21	127.20
19	I	201	CLA	C2C-C1C-NC	3.20	112.97	109.97
22	4	305	BCR	C27-C26-C25	-3.20	118.08	122.73
32	Z	310	CHL	C1-O2A-CGA	3.20	124.84	116.44
22	B	847	BCR	C23-C24-C25	-3.20	118.21	127.20
32	4	315	CHL	C4A-NA-C1A	3.20	108.14	106.71
19	A	841	CLA	C2D-C1D-ND	3.19	112.46	110.10
19	B	809	CLA	C2C-C1C-NC	3.19	112.96	109.97
22	F	302	BCR	C27-C26-C25	-3.19	118.10	122.73
19	A	813	CLA	C2C-C1C-NC	3.19	112.96	109.97
19	B	839	CLA	C2D-C1D-ND	3.19	112.46	110.10
22	7	305	BCR	C7-C8-C9	-3.19	121.41	126.23
19	G	1601	CLA	C2C-C1C-NC	3.19	112.96	109.97
19	5	322	CLA	CHD-C1D-ND	-3.19	121.52	124.45
19	K	202	CLA	C2C-C1C-NC	3.19	112.96	109.97
19	A	829	CLA	C2D-C1D-ND	3.19	112.45	110.10
19	B	806	CLA	CHD-C1D-ND	-3.19	121.53	124.45
19	5	321	CLA	CHD-C1D-ND	-3.18	121.53	124.45
31	Z	318	LUT	C15-C14-C13	-3.18	122.77	127.31
19	A	827	CLA	C2D-C1D-ND	3.18	112.45	110.10
19	4	312	CLA	C1-C2-C3	-3.18	120.54	126.04
19	A	833	CLA	C2D-C1D-ND	3.18	112.45	110.10
22	3	5007	BCR	C30-C25-C26	-3.18	118.13	122.61
19	A	834	CLA	C1-C2-C3	-3.18	120.54	126.04
19	B	837	CLA	C1-C2-C3	-3.18	120.54	126.04
19	A	804	CLA	C2D-C1D-ND	3.18	112.45	110.10
19	5	301	CLA	C2D-C1D-ND	3.18	112.45	110.10
32	5	318	CHL	C4D-CHA-C1A	3.18	125.12	121.25
19	B	813	CLA	CHD-C1D-ND	-3.18	121.53	124.45
19	A	843	CLA	C2C-C1C-NC	3.18	112.95	109.97
19	B	813	CLA	C1-C2-C3	-3.18	120.55	126.04
38	6	326	ERG	C19-C10-C9	-3.17	105.69	111.03
19	G	1601	CLA	C2D-C1D-ND	3.17	112.44	110.10
19	3	5014	CLA	C2D-C1D-ND	3.17	112.44	110.10
19	3	5008	CLA	CHD-C1D-ND	-3.17	121.54	124.45
19	A	816	CLA	C2C-C1C-NC	3.17	112.94	109.97
19	A	820	CLA	C2D-C1D-ND	3.17	112.44	110.10
22	3	5005	BCR	C8-C7-C6	-3.17	118.30	127.20
19	7	319	CLA	CHD-C1D-ND	-3.17	121.54	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	843	BCR	C24-C23-C22	-3.17	121.45	126.23
19	A	803	CLA	C2D-C1D-ND	3.16	112.44	110.10
19	B	818	CLA	CHD-C1D-ND	-3.16	121.55	124.45
19	7	311	CLA	C2C-C1C-NC	3.16	112.94	109.97
19	G	1602	CLA	C2D-C1D-ND	3.16	112.44	110.10
31	3	5002	LUT	C15-C14-C13	-3.16	122.80	127.31
31	6	306	LUT	C18-C5-C6	-3.16	120.98	124.53
19	B	813	CLA	C2C-C1C-NC	3.16	112.93	109.97
19	4	307	CLA	C2D-C1D-ND	3.16	112.43	110.10
19	8	308	CLA	C1D-ND-C4D	-3.16	104.09	106.33
19	6	322	CLA	C1D-ND-C4D	-3.16	104.09	106.33
19	A	832	CLA	C2C-C1C-NC	3.16	112.93	109.97
19	A	836	CLA	C2D-C1D-ND	3.16	112.43	110.10
19	B	817	CLA	C2D-C1D-ND	3.16	112.43	110.10
19	B	834	CLA	C2D-C1D-ND	3.16	112.43	110.10
19	B	813	CLA	CMA-C3A-C4A	3.16	120.26	111.77
19	A	838	CLA	CHD-C1D-ND	-3.16	121.55	124.45
19	B	801	CLA	CHD-C1D-ND	-3.16	121.55	124.45
19	8	310	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
20	A	844	PQN	C14-C13-C15	3.15	120.58	115.27
19	B	831	CLA	CHD-C1D-ND	-3.15	121.56	124.45
19	8	318	CLA	C2C-C1C-NC	3.15	112.93	109.97
19	1	5007	CLA	C2C-C1C-NC	3.15	112.92	109.97
27	5	302	RRX	C20-C21-C22	-3.15	122.81	127.31
19	7	316	CLA	CHD-C1D-ND	-3.15	121.56	124.45
22	6	307	BCR	C21-C20-C19	-3.15	113.39	123.22
19	B	814	CLA	CHD-C1D-ND	-3.15	121.56	124.45
19	A	823	CLA	C2C-C1C-NC	3.15	112.92	109.97
19	B	827	CLA	C2C-C1C-NC	3.15	112.92	109.97
24	A	853	LMT	C1B-O1B-C4'	-3.15	110.17	117.96
19	A	834	CLA	CHD-C1D-ND	-3.14	121.56	124.45
22	G	1603	BCR	C33-C5-C4	3.14	119.66	113.62
22	8	306	BCR	C38-C26-C27	3.14	119.66	113.62
19	F	301	CLA	C1D-ND-C4D	-3.14	104.10	106.33
31	1	5003	LUT	C8-C7-C6	-3.14	118.38	127.20
19	B	837	CLA	C2C-C1C-NC	3.14	112.92	109.97
32	Z	302	CHL	C2C-C3C-C4C	3.14	108.73	106.49
27	4	303	RRX	C7-C8-C9	-3.14	121.49	126.23
19	B	804	CLA	C2C-C1C-NC	3.14	112.91	109.97
19	B	816	CLA	C2D-C1D-ND	3.14	112.42	110.10
19	4	310	CLA	C11-C12-C13	-3.14	105.77	115.92
19	B	837	CLA	CHD-C1D-ND	-3.14	121.57	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Z	317	LUT	C35-C15-C14	-3.14	117.05	123.47
19	K	203	CLA	C2C-C1C-NC	3.14	112.91	109.97
19	A	823	CLA	CHD-C1D-ND	-3.14	121.57	124.45
19	B	839	CLA	CHD-C1D-ND	-3.14	121.57	124.45
19	8	312	CLA	C4A-NA-C1A	3.14	108.12	106.71
19	7	324	CLA	C2C-C1C-NC	3.14	112.91	109.97
19	A	825	CLA	CMA-C3A-C4A	3.14	120.20	111.77
19	B	803	CLA	CHD-C1D-ND	-3.13	121.57	124.45
19	5	313	CLA	CHD-C1D-ND	-3.13	121.57	124.45
32	1	5009	CHL	C1-C2-C3	-3.13	120.62	126.04
22	G	1603	BCR	C7-C8-C9	-3.13	121.50	126.23
19	A	836	CLA	C1-C2-C3	-3.13	120.62	126.04
19	B	815	CLA	C2D-C1D-ND	3.13	112.41	110.10
19	B	836	CLA	O2A-CGA-CBA	3.13	121.74	111.91
19	B	811	CLA	CMA-C3A-C4A	3.13	120.19	111.77
19	7	319	CLA	C2C-C1C-NC	3.13	112.91	109.97
32	Z	309	CHL	C2C-C3C-C4C	3.13	108.72	106.49
19	8	307	CLA	C2C-C1C-NC	3.13	112.90	109.97
19	A	843	CLA	C6-C5-C3	-3.13	109.50	114.62
19	A	808	CLA	C1-C2-C3	-3.13	120.63	126.04
19	5	307	CLA	C1-C2-C3	-3.13	120.63	126.04
19	A	831	CLA	C2D-C1D-ND	3.13	112.41	110.10
22	A	849	BCR	C8-C7-C6	-3.13	118.42	127.20
22	3	5007	BCR	C2-C1-C6	3.13	115.29	110.48
32	7	315	CHL	CHC-C1C-NC	3.12	128.94	124.20
19	A	836	CLA	CHD-C1D-ND	-3.12	121.58	124.45
19	B	830	CLA	C2D-C1D-ND	3.12	112.41	110.10
19	J	1901	CLA	C2D-C1D-ND	3.12	112.41	110.10
19	Z	315	CLA	C1D-ND-C4D	-3.12	104.12	106.33
19	6	301	CLA	C2D-C1D-ND	3.12	112.41	110.10
19	5	322	CLA	C1D-ND-C4D	-3.12	104.12	106.33
22	A	859	BCR	C4-C5-C6	-3.12	118.20	122.73
22	3	5006	BCR	C4-C5-C6	-3.12	118.20	122.73
19	6	318	CLA	CHD-C1D-ND	-3.12	121.59	124.45
19	8	312	CLA	CMD-C2D-C3D	-3.12	120.44	127.61
19	3	5008	CLA	C1-C2-C3	-3.12	120.65	126.04
19	A	828	CLA	CMA-C3A-C4A	3.12	120.16	111.77
19	1	5008	CLA	CHD-C1D-ND	-3.12	121.59	124.45
19	B	827	CLA	C2D-C1D-ND	3.12	112.40	110.10
19	1	5018	CLA	C2D-C1D-ND	3.12	112.40	110.10
19	3	5018	CLA	C2D-C1D-ND	3.12	112.40	110.10
19	7	317	CLA	C2D-C1D-ND	3.12	112.40	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	302	RRX	C16-C17-C18	-3.12	122.86	127.31
19	4	308	CLA	CHD-C1D-ND	-3.12	121.59	124.45
19	A	808	CLA	C2D-C1D-ND	3.12	112.40	110.10
19	5	321	CLA	C2D-C1D-ND	3.12	112.40	110.10
19	B	828	CLA	CMA-C3A-C4A	3.12	120.15	111.77
19	B	808	CLA	C2D-C1D-ND	3.12	112.40	110.10
19	1	5012	CLA	C2D-C1D-ND	3.12	112.40	110.10
19	1	5012	CLA	C2C-C1C-NC	3.11	112.89	109.97
19	Z	314	CLA	CHD-C1D-ND	-3.11	121.59	124.45
22	3	5004	BCR	C29-C30-C25	3.11	115.27	110.48
19	A	804	CLA	CHD-C1D-ND	-3.11	121.59	124.45
19	A	807	CLA	C2C-C1C-NC	3.11	112.89	109.97
19	5	319	CLA	CHD-C1D-ND	-3.11	121.60	124.45
19	B	832	CLA	C2C-C1C-NC	3.11	112.89	109.97
22	A	849	BCR	C20-C19-C18	-3.11	117.68	126.42
19	7	316	CLA	C2C-C1C-NC	3.11	112.88	109.97
19	B	838	CLA	CHD-C1D-ND	-3.11	121.60	124.45
19	Z	315	CLA	CHD-C1D-ND	-3.11	121.60	124.45
19	B	824	CLA	C2C-C1C-NC	3.11	112.88	109.97
19	4	309	CLA	C2C-C1C-NC	3.11	112.88	109.97
19	3	5012	CLA	C2D-C1D-ND	3.11	112.39	110.10
19	3	5008	CLA	O2A-CGA-CBA	3.11	121.66	111.91
19	B	817	CLA	CHD-C1D-ND	-3.11	121.60	124.45
19	1	5016	CLA	CHD-C1D-ND	-3.11	121.60	124.45
19	A	826	CLA	C2D-C1D-ND	3.10	112.39	110.10
19	B	828	CLA	C2D-C1D-ND	3.10	112.39	110.10
19	F	303	CLA	C2D-C1D-ND	3.10	112.39	110.10
19	B	840	CLA	C1-C2-C3	-3.10	120.68	126.04
19	B	830	CLA	C2C-C1C-NC	3.10	112.88	109.97
19	Z	304	CLA	CHD-C1D-ND	-3.10	121.60	124.45
19	6	323	CLA	CHD-C1D-ND	-3.10	121.60	124.45
19	B	810	CLA	C2D-C1D-ND	3.10	112.39	110.10
19	8	312	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
27	F	304	RRX	C4-C5-C6	-3.10	118.23	122.73
19	A	828	CLA	CHD-C1D-ND	-3.10	121.61	124.45
22	A	858	BCR	C33-C5-C4	3.10	119.57	113.62
19	A	812	CLA	C1D-ND-C4D	-3.10	104.13	106.33
32	7	315	CHL	C4D-CHA-C1A	3.10	125.02	121.25
19	A	817	CLA	CHD-C1D-ND	-3.10	121.61	124.45
19	B	805	CLA	CHD-C1D-ND	-3.10	121.61	124.45
19	5	322	CLA	CMA-C3A-C4A	3.10	120.10	111.77
19	A	821	CLA	CHD-C1D-ND	-3.10	121.61	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	303	CLA	C2C-C1C-NC	3.10	112.87	109.97
19	K	205	CLA	C2C-C1C-NC	3.10	112.87	109.97
19	B	820	CLA	C2C-C1C-NC	3.10	112.87	109.97
19	6	314	CLA	C2C-C1C-NC	3.10	112.87	109.97
19	6	302	CLA	C2D-C1D-ND	3.10	112.39	110.10
19	A	802	CLA	CHD-C1D-ND	-3.10	121.61	124.45
19	A	838	CLA	C2D-C1D-ND	3.10	112.39	110.10
19	A	839	CLA	C2C-C1C-NC	3.09	112.87	109.97
32	8	319	CHL	CMA-C3A-C4A	3.09	120.09	111.77
22	5	304	BCR	C15-C14-C13	-3.09	122.89	127.31
19	A	842	CLA	C2C-C1C-NC	3.09	112.87	109.97
19	4	318	CLA	C2C-C1C-NC	3.09	112.87	109.97
22	A	848	BCR	C23-C24-C25	-3.09	118.52	127.20
19	A	802	CLA	C2C-C1C-NC	3.09	112.87	109.97
19	B	806	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	B	846	BCR	C36-C18-C19	3.09	122.95	118.08
19	8	307	CLA	CHD-C1D-ND	-3.09	121.61	124.45
19	A	817	CLA	C2D-C1D-ND	3.09	112.38	110.10
19	A	814	CLA	C2C-C1C-NC	3.09	112.87	109.97
22	B	844	BCR	C34-C9-C10	-3.09	118.60	122.92
31	5	303	LUT	C21-C26-C27	-3.09	108.80	112.70
19	B	821	CLA	CHD-C1D-ND	-3.09	121.62	124.45
19	B	833	CLA	CHD-C1D-ND	-3.09	121.62	124.45
19	1	5016	CLA	C2D-C1D-ND	3.09	112.38	110.10
19	6	318	CLA	C2D-C1D-ND	3.09	112.38	110.10
22	A	846	BCR	C4-C5-C6	-3.09	118.25	122.73
19	4	309	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
19	6	302	CLA	C2C-C1C-NC	3.08	112.86	109.97
32	8	315	CHL	C1-O2A-CGA	3.08	124.54	116.44
22	5	304	BCR	C23-C24-C25	-3.08	118.54	127.20
19	8	309	CLA	C2D-C1D-ND	3.08	112.38	110.10
22	8	306	BCR	C33-C5-C4	3.08	119.54	113.62
19	3	5016	CLA	C2C-C1C-NC	3.08	112.86	109.97
19	3	5016	CLA	CHD-C1D-ND	-3.08	121.62	124.45
31	5	303	LUT	C22-C23-C24	3.08	115.25	111.74
22	A	850	BCR	C11-C10-C9	-3.08	122.91	127.31
31	5	303	LUT	C11-C10-C9	-3.08	122.91	127.31
31	7	303	LUT	C8-C7-C6	-3.08	118.55	127.20
19	7	309	CLA	CHD-C1D-ND	-3.08	121.62	124.45
19	B	823	CLA	CHD-C1D-ND	-3.08	121.62	124.45
19	A	822	CLA	C1D-ND-C4D	-3.08	104.15	106.33
19	6	320	CLA	C2C-C1C-NC	3.08	112.86	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	808	CLA	C2C-C1C-NC	3.08	112.86	109.97
19	Z	304	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	6	305	LUT	C35-C15-C14	-3.08	117.17	123.47
19	A	824	CLA	C2C-C1C-NC	3.08	112.85	109.97
19	5	306	CLA	C1D-ND-C4D	-3.07	104.15	106.33
19	1	5011	CLA	CHD-C1D-ND	-3.07	121.63	124.45
31	8	305	LUT	C31-C30-C29	-3.07	122.92	127.31
19	B	823	CLA	C2C-C1C-NC	3.07	112.85	109.97
22	B	845	BCR	C38-C26-C27	3.07	119.52	113.62
22	3	5007	BCR	C27-C26-C25	-3.07	118.27	122.73
19	B	811	CLA	C2D-C1D-ND	3.07	112.37	110.10
19	A	807	CLA	CMA-C3A-C4A	3.07	120.03	111.77
19	4	307	CLA	C6-C5-C3	-3.07	109.60	114.62
19	A	805	CLA	C2D-C1D-ND	3.07	112.36	110.10
19	A	832	CLA	C2D-C1D-ND	3.07	112.36	110.10
19	B	832	CLA	C2D-C1D-ND	3.07	112.36	110.10
19	6	312	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
19	B	808	CLA	C2C-C1C-NC	3.07	112.84	109.97
19	3	5016	CLA	C2D-C1D-ND	3.07	112.36	110.10
23	6	324	LHG	O8-C23-C24	3.07	121.53	111.91
19	3	5013	CLA	C2C-C1C-NC	3.07	112.84	109.97
22	A	859	BCR	C8-C7-C6	-3.07	118.59	127.20
19	B	819	CLA	C2C-C1C-NC	3.06	112.84	109.97
32	8	315	CHL	CHC-C1C-NC	3.06	128.85	124.20
19	8	312	CLA	CMA-C3A-C4A	3.06	120.01	111.77
19	A	809	CLA	C2D-C1D-ND	3.06	112.36	110.10
22	B	842	BCR	C8-C7-C6	-3.06	118.60	127.20
22	6	307	BCR	C29-C30-C25	3.06	115.19	110.48
19	A	816	CLA	C2D-C1D-ND	3.06	112.36	110.10
19	7	316	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
19	K	202	CLA	CHD-C1D-ND	-3.06	121.64	124.45
19	7	317	CLA	C1D-ND-C4D	-3.06	104.16	106.33
19	A	835	CLA	C2D-C1D-ND	3.06	112.36	110.10
19	B	829	CLA	C2D-C1D-ND	3.06	112.36	110.10
19	3	5009	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
19	5	313	CLA	C2C-C1C-NC	3.06	112.84	109.97
19	6	323	CLA	C2C-C1C-NC	3.06	112.84	109.97
19	6	312	CLA	CHD-C1D-ND	-3.06	121.64	124.45
22	6	307	BCR	C7-C8-C9	-3.06	121.61	126.23
19	A	838	CLA	C2C-C1C-NC	3.06	112.83	109.97
19	A	819	CLA	C2D-C1D-ND	3.06	112.36	110.10
19	5	306	CLA	C2D-C1D-ND	3.06	112.36	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	802	CLA	C2D-C1D-ND	3.05	112.36	110.10
31	7	303	LUT	C35-C15-C14	-3.05	117.22	123.47
32	1	5017	CHL	C4D-CHA-C1A	3.05	124.97	121.25
19	A	822	CLA	C2C-C1C-NC	3.05	112.83	109.97
22	3	5005	BCR	C11-C12-C13	-3.05	117.84	126.42
32	6	315	CHL	C1-C2-C3	-3.05	120.76	126.04
19	B	811	CLA	CHD-C1D-ND	-3.05	121.65	124.45
19	B	801	CLA	C2D-C1D-ND	3.05	112.35	110.10
19	7	319	CLA	C2D-C1D-ND	3.05	112.35	110.10
19	A	857	CLA	C2C-C1C-NC	3.05	112.83	109.97
22	A	850	BCR	C24-C23-C22	-3.05	121.63	126.23
19	4	318	CLA	CHD-C1D-ND	-3.05	121.65	124.45
19	3	5011	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
19	A	828	CLA	C2C-C1C-NC	3.05	112.83	109.97
32	4	317	CHL	CMA-C3A-C4A	3.05	119.96	111.77
19	4	309	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
19	A	820	CLA	C2C-C1C-NC	3.05	112.83	109.97
28	J	1902	C7Z	C38-C25-C24	3.05	120.00	114.36
19	7	311	CLA	CHD-C1D-ND	-3.05	121.66	124.45
19	8	308	CLA	CHD-C1D-ND	-3.05	121.66	124.45
19	B	803	CLA	CMA-C3A-C4A	3.05	119.96	111.77
19	A	824	CLA	C2D-C1D-ND	3.05	112.35	110.10
19	A	842	CLA	CMA-C3A-C4A	3.04	119.96	111.77
32	Z	309	CHL	CHD-C4C-C3C	3.04	129.31	124.84
19	6	309	CLA	C2C-C1C-NC	3.04	112.82	109.97
19	A	829	CLA	CMA-C3A-C4A	3.04	119.95	111.77
19	B	821	CLA	C2D-C1D-ND	3.04	112.35	110.10
19	B	823	CLA	CMA-C3A-C4A	3.04	119.95	111.77
19	6	311	CLA	C1D-ND-C4D	-3.04	104.17	106.33
19	3	5014	CLA	C2C-C1C-NC	3.04	112.82	109.97
19	A	830	CLA	CHD-C1D-ND	-3.04	121.66	124.45
31	1	5003	LUT	C21-C26-C27	-3.04	108.86	112.70
19	J	1901	CLA	CHD-C1D-ND	-3.04	121.66	124.45
19	A	825	CLA	CHD-C1D-ND	-3.04	121.66	124.45
19	6	309	CLA	CHD-C1D-ND	-3.04	121.66	124.45
19	A	840	CLA	C1-C2-C3	-3.04	120.79	126.04
19	A	833	CLA	CHD-C1D-ND	-3.04	121.66	124.45
19	A	807	CLA	C2D-C1D-ND	3.04	112.34	110.10
19	1	5006	CLA	C2D-C1D-ND	3.04	112.34	110.10
24	Z	301	LMT	C1B-O1B-C4'	-3.04	110.45	117.96
32	8	317	CHL	CHD-C1D-ND	-3.04	121.66	124.45
22	8	306	BCR	C8-C7-C6	-3.04	118.68	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	843	CLA	C2D-C1D-ND	3.04	112.34	110.10
19	B	820	CLA	C2D-C1D-ND	3.04	112.34	110.10
19	B	826	CLA	CHD-C1D-ND	-3.03	121.67	124.45
19	A	835	CLA	CHD-C1D-ND	-3.03	121.67	124.45
22	6	308	BCR	C24-C23-C22	-3.03	121.65	126.23
19	A	826	CLA	C2C-C1C-NC	3.03	112.81	109.97
19	B	826	CLA	C2C-C1C-NC	3.03	112.81	109.97
19	B	822	CLA	C1D-ND-C4D	-3.03	104.18	106.33
22	8	303	BCR	C27-C26-C25	-3.03	118.33	122.73
19	A	809	CLA	CHD-C1D-ND	-3.03	121.67	124.45
19	A	830	CLA	C2D-C1D-ND	3.03	112.34	110.10
22	B	847	BCR	C4-C5-C6	-3.03	118.33	122.73
19	A	840	CLA	O2A-CGA-CBA	3.03	121.42	111.91
19	B	816	CLA	CHD-C1D-ND	-3.03	121.67	124.45
19	B	840	CLA	CHD-C1D-ND	-3.03	121.67	124.45
19	A	833	CLA	C2C-C1C-NC	3.03	112.81	109.97
19	A	823	CLA	C2D-C1D-ND	3.03	112.34	110.10
19	A	807	CLA	CHD-C1D-ND	-3.03	121.67	124.45
19	1	5018	CLA	CHD-C1D-ND	-3.03	121.67	124.45
19	A	834	CLA	C2C-C1C-NC	3.03	112.81	109.97
19	4	312	CLA	C2C-C1C-NC	3.03	112.81	109.97
19	B	812	CLA	C2D-C1D-ND	3.03	112.33	110.10
19	5	309	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
19	B	831	CLA	C1-C2-C3	-3.03	120.81	126.04
19	B	829	CLA	CHD-C1D-ND	-3.03	121.67	124.45
19	1	5016	CLA	C2C-C1C-NC	3.03	112.81	109.97
19	F	301	CLA	O2D-CGD-O1D	-3.02	117.92	123.84
19	B	838	CLA	C2C-C1C-NC	3.02	112.81	109.97
19	8	314	CLA	C2C-C1C-NC	3.02	112.81	109.97
19	5	312	CLA	CMA-C3A-C4A	3.02	119.90	111.77
32	Z	310	CHL	CMA-C3A-C4A	3.02	119.90	111.77
19	Z	311	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
19	Z	306	CLA	C1D-ND-C4D	-3.02	104.19	106.33
19	B	835	CLA	C2C-C1C-NC	3.02	112.80	109.97
19	5	301	CLA	CHD-C1D-ND	-3.02	121.68	124.45
19	A	828	CLA	C2D-C1D-ND	3.02	112.33	110.10
19	6	318	CLA	C2C-C1C-NC	3.02	112.80	109.97
19	A	857	CLA	C2D-C1D-ND	3.02	112.33	110.10
19	Z	312	CLA	C2D-C1D-ND	3.02	112.33	110.10
19	B	814	CLA	C2C-C1C-NC	3.02	112.80	109.97
19	7	312	CLA	C2C-C1C-NC	3.02	112.80	109.97
22	A	858	BCR	C38-C26-C27	3.02	119.41	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	8	313	CLA	C1D-ND-C4D	-3.02	104.19	106.33
19	K	205	CLA	CHD-C1D-ND	-3.02	121.68	124.45
19	5	309	CLA	C2D-C1D-ND	3.02	112.33	110.10
19	B	828	CLA	C1-C2-C3	-3.01	120.83	126.04
19	B	835	CLA	CMA-C3A-C4A	3.01	119.87	111.77
19	Z	307	CLA	C2C-C1C-NC	3.01	112.79	109.97
19	Z	305	CLA	C1D-ND-C4D	-3.01	104.20	106.33
22	B	843	BCR	C33-C5-C4	3.01	119.40	113.62
19	B	804	CLA	C2D-C1D-ND	3.01	112.32	110.10
19	6	310	CLA	C2D-C1D-ND	3.01	112.32	110.10
19	B	838	CLA	CMA-C3A-C4A	3.01	119.86	111.77
28	6	304	C7Z	C2-C3-C4	3.01	114.42	110.30
19	A	857	CLA	CMA-C3A-C4A	3.01	119.86	111.77
19	7	318	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
19	8	320	CLA	CHD-C1D-ND	-3.01	121.69	124.45
19	6	320	CLA	CHD-C1D-ND	-3.01	121.69	124.45
19	5	314	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
19	A	833	CLA	CMA-C3A-C4A	3.01	119.85	111.77
19	5	310	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
28	1	5005	C7Z	C8-C7-C6	-3.01	118.76	127.20
19	A	812	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
19	A	820	CLA	CHD-C1D-ND	-3.00	121.69	124.45
19	A	811	CLA	CMA-C3A-C4A	3.00	119.85	111.77
19	A	805	CLA	C1D-ND-C4D	-3.00	104.20	106.33
34	8	322	3PH	O21-C21-C22	3.00	119.18	110.80
22	A	847	BCR	C4-C5-C6	-3.00	118.37	122.73
19	A	806	CLA	C2D-C1D-ND	3.00	112.32	110.10
19	A	837	CLA	C2D-C1D-ND	3.00	112.32	110.10
19	B	833	CLA	C2D-C1D-ND	3.00	112.32	110.10
19	B	824	CLA	CHD-C1D-ND	-3.00	121.69	124.45
19	3	5010	CLA	CHD-C1D-ND	-3.00	121.69	124.45
22	3	5005	BCR	C23-C24-C25	-3.00	118.77	127.20
32	4	314	CHL	CMA-C3A-C4A	3.00	119.84	111.77
19	6	311	CLA	O2A-CGA-CBA	3.00	121.33	111.91
19	3	5014	CLA	C1-C2-C3	-3.00	120.85	126.04
20	A	844	PQN	C11-C12-C13	-3.00	121.80	126.79
19	7	312	CLA	C2D-C1D-ND	3.00	112.31	110.10
19	B	808	CLA	C1D-ND-C4D	-3.00	104.20	106.33
19	B	831	CLA	C1D-ND-C4D	-3.00	104.20	106.33
32	1	5014	CHL	CMA-C3A-C4A	3.00	119.83	111.77
19	B	830	CLA	CHD-C1D-ND	-3.00	121.70	124.45
19	6	314	CLA	C2D-C1D-ND	3.00	112.31	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	825	CLA	C2C-C1C-NC	3.00	112.78	109.97
19	B	832	CLA	CHD-C1D-ND	-3.00	121.70	124.45
19	A	841	CLA	CHD-C1D-ND	-3.00	121.70	124.45
19	A	857	CLA	CHD-C1D-ND	-3.00	121.70	124.45
19	A	821	CLA	C2C-C1C-NC	3.00	112.78	109.97
22	B	847	BCR	C33-C5-C4	2.99	119.37	113.62
19	B	814	CLA	C2D-C1D-ND	2.99	112.31	110.10
19	Z	314	CLA	C2D-C1D-ND	2.99	112.31	110.10
19	A	817	CLA	CMA-C3A-C4A	2.99	119.82	111.77
32	5	320	CHL	C3C-C4C-NC	-2.99	107.22	110.57
19	K	202	CLA	C2D-C1D-ND	2.99	112.31	110.10
19	6	311	CLA	C2D-C1D-ND	2.99	112.31	110.10
31	8	304	LUT	C8-C7-C6	-2.99	118.80	127.20
19	A	815	CLA	O2A-CGA-CBA	2.99	121.30	111.91
19	7	306	CLA	C2D-C1D-ND	2.99	112.31	110.10
31	6	306	LUT	C39-C29-C30	-2.99	118.73	122.92
19	5	310	CLA	CMA-C3A-C4A	2.99	119.81	111.77
19	A	830	CLA	C2C-C1C-NC	2.99	112.77	109.97
19	6	323	CLA	C1-C2-C3	-2.99	120.87	126.04
19	A	825	CLA	C2D-C1D-ND	2.99	112.31	110.10
19	8	320	CLA	C2C-C1C-NC	2.99	112.77	109.97
19	K	202	CLA	CMA-C3A-C4A	2.99	119.81	111.77
19	A	827	CLA	CHD-C1D-ND	-2.99	121.71	124.45
19	B	807	CLA	CHD-C1D-ND	-2.99	121.71	124.45
22	A	859	BCR	C20-C19-C18	-2.99	118.02	126.42
31	3	5003	LUT	C15-C14-C13	-2.99	123.05	127.31
19	J	1901	CLA	C2C-C1C-NC	2.99	112.77	109.97
22	A	849	BCR	C33-C5-C4	2.99	119.35	113.62
19	6	302	CLA	CHD-C1D-ND	-2.98	121.71	124.45
19	B	826	CLA	CMA-C3A-C4A	2.98	119.79	111.77
19	B	835	CLA	CHD-C1D-ND	-2.98	121.71	124.45
19	B	805	CLA	CMA-C3A-C4A	2.98	119.79	111.77
19	5	325	CLA	C2C-C1C-NC	2.98	112.77	109.97
19	A	808	CLA	CHD-C1D-ND	-2.98	121.71	124.45
19	A	811	CLA	C1D-ND-C4D	-2.98	104.22	106.33
19	3	5019	CLA	C2C-C1C-NC	2.98	112.77	109.97
19	A	813	CLA	CHD-C1D-ND	-2.98	121.72	124.45
19	F	303	CLA	CHD-C1D-ND	-2.98	121.72	124.45
19	Z	303	CLA	CHD-C1D-ND	-2.98	121.72	124.45
19	G	1602	CLA	CHD-C1D-ND	-2.98	121.72	124.45
19	A	827	CLA	C2C-C1C-NC	2.98	112.76	109.97
19	5	308	CLA	C1D-ND-C4D	-2.98	104.22	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	8	314	CLA	C2D-C1D-ND	2.98	112.30	110.10
19	8	318	CLA	CAA-CBA-CGA	-2.98	104.55	113.25
19	5	317	CLA	C1D-ND-C4D	-2.98	104.22	106.33
22	3	5006	BCR	C33-C5-C4	2.98	119.33	113.62
19	B	840	CLA	C1C-C2C-C3C	-2.98	103.83	106.96
19	B	838	CLA	C6-C5-C3	-2.98	109.75	114.62
19	A	818	CLA	CHD-C1D-ND	-2.98	121.72	124.45
19	I	201	CLA	CHD-C1D-ND	-2.98	121.72	124.45
19	3	5014	CLA	CHD-C1D-ND	-2.98	121.72	124.45
19	8	310	CLA	CHD-C1D-ND	-2.98	121.72	124.45
19	B	828	CLA	C2C-C1C-NC	2.98	112.76	109.97
19	4	308	CLA	C2C-C1C-NC	2.98	112.76	109.97
19	5	321	CLA	C2C-C1C-NC	2.98	112.76	109.97
19	B	836	CLA	C2D-C1D-ND	2.98	112.30	110.10
22	B	844	BCR	C38-C26-C27	2.98	119.33	113.62
19	Z	314	CLA	C2C-C1C-NC	2.97	112.76	109.97
19	A	839	CLA	C2D-C1D-ND	2.97	112.30	110.10
19	A	841	CLA	C2C-C1C-NC	2.97	112.76	109.97
19	4	318	CLA	C2D-C1D-ND	2.97	112.30	110.10
19	B	820	CLA	CMA-C3A-C4A	2.97	119.76	111.77
19	K	204	CLA	CHD-C1D-ND	-2.97	121.72	124.45
31	Z	317	LUT	C2-C3-C4	2.97	114.37	110.30
19	5	310	CLA	C2D-C1D-ND	2.97	112.29	110.10
27	F	304	RRX	C33-C5-C4	2.97	119.32	113.62
19	6	311	CLA	CMA-C3A-C4A	2.97	119.76	111.77
19	4	316	CLA	CHD-C1D-ND	-2.97	121.72	124.45
22	3	5005	BCR	C15-C16-C17	-2.97	117.39	123.47
19	A	818	CLA	CMA-C3A-C4A	2.97	119.75	111.77
19	A	832	CLA	CHD-C1D-ND	-2.97	121.73	124.45
19	B	850	CLA	C2D-C1D-ND	2.97	112.29	110.10
19	7	310	CLA	C2D-C1D-ND	2.97	112.29	110.10
22	6	308	BCR	C7-C8-C9	-2.97	121.75	126.23
19	6	311	CLA	CHD-C1D-ND	-2.97	121.73	124.45
27	5	302	RRX	C35-C13-C12	2.97	122.75	118.08
22	5	304	BCR	C7-C8-C9	-2.97	121.75	126.23
32	4	319	CHL	C3C-C4C-NC	-2.97	107.25	110.57
19	B	809	CLA	CHD-C1D-ND	-2.97	121.73	124.45
22	A	850	BCR	C33-C5-C4	2.96	119.31	113.62
31	1	5003	LUT	C11-C10-C9	-2.96	123.08	127.31
19	5	309	CLA	CHD-C1D-ND	-2.96	121.73	124.45
19	F	303	CLA	C1D-ND-C4D	-2.96	104.23	106.33
19	B	823	CLA	C2D-C1D-ND	2.96	112.29	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	8	310	CLA	C2D-C1D-ND	2.96	112.29	110.10
19	A	824	CLA	CMA-C3A-C4A	2.96	119.73	111.77
19	A	836	CLA	C2C-C1C-NC	2.96	112.75	109.97
19	5	301	CLA	CMA-C3A-C4A	2.96	119.73	111.77
19	B	810	CLA	CHD-C1D-ND	-2.96	121.73	124.45
19	B	824	CLA	C2D-C1D-ND	2.96	112.28	110.10
19	B	831	CLA	C2D-C1D-ND	2.96	112.28	110.10
31	8	305	LUT	C30-C31-C32	-2.96	113.99	123.22
19	K	203	CLA	CHD-C1D-ND	-2.96	121.74	124.45
19	B	805	CLA	C1D-ND-C4D	-2.96	104.23	106.33
31	Z	317	LUT	C22-C23-C24	2.96	115.11	111.74
19	3	5014	CLA	CMA-C3A-C4A	2.96	119.72	111.77
19	A	816	CLA	CMA-C3A-C4A	2.96	119.72	111.77
19	5	322	CLA	C2C-C1C-NC	2.96	112.74	109.97
28	6	304	C7Z	C18-C5-C4	2.96	119.83	114.36
19	B	838	CLA	C2D-C1D-ND	2.96	112.28	110.10
19	6	318	CLA	C1-C2-C3	-2.96	121.97	126.75
31	1	5004	LUT	C18-C5-C4	2.96	119.83	114.36
19	I	201	CLA	CMA-C3A-C4A	2.95	119.72	111.77
31	6	305	LUT	C31-C30-C29	-2.95	123.09	127.31
19	6	310	CLA	C1D-ND-C4D	-2.95	104.24	106.33
19	A	817	CLA	C2C-C1C-NC	2.95	112.74	109.97
22	7	305	BCR	C15-C16-C17	-2.95	117.42	123.47
32	7	315	CHL	CHD-C4C-C3C	2.95	129.18	124.84
19	3	5008	CLA	C2D-C1D-ND	2.95	112.28	110.10
22	6	308	BCR	C33-C5-C4	2.95	119.29	113.62
19	3	5020	CLA	CHD-C1D-ND	-2.95	121.74	124.45
19	A	815	CLA	C2C-C1C-NC	2.95	112.74	109.97
19	A	837	CLA	C2C-C1C-NC	2.95	112.74	109.97
19	7	316	CLA	C2D-C1D-ND	2.95	112.28	110.10
19	K	204	CLA	CMA-C3A-C4A	2.95	119.70	111.77
19	A	813	CLA	C2D-C1D-ND	2.95	112.28	110.10
19	1	5012	CLA	CHD-C1D-ND	-2.95	121.74	124.45
22	5	304	BCR	C33-C5-C4	2.95	119.28	113.62
19	A	832	CLA	CMA-C3A-C4A	2.95	119.69	111.77
28	J	1902	C7Z	C31-C32-C33	-2.95	118.14	126.42
19	B	808	CLA	CHD-C1D-ND	-2.95	121.75	124.45
19	A	820	CLA	CMA-C3A-C4A	2.95	119.69	111.77
19	B	815	CLA	C2C-C1C-NC	2.95	112.73	109.97
23	6	303	LHG	O8-C23-C24	2.95	121.15	111.91
19	J	1901	CLA	CMA-C3A-C4A	2.94	119.69	111.77
19	A	807	CLA	C1D-ND-C4D	-2.94	104.24	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	838	CLA	C1D-ND-C4D	-2.94	104.24	106.33
19	B	817	CLA	C1D-ND-C4D	-2.94	104.24	106.33
19	6	322	CLA	C2D-C1D-ND	2.94	112.27	110.10
19	B	812	CLA	CHD-C1D-ND	-2.94	121.75	124.45
19	A	809	CLA	CMA-C3A-C4A	2.94	119.69	111.77
19	B	825	CLA	C1D-ND-C4D	-2.94	104.24	106.33
19	B	833	CLA	C2C-C1C-NC	2.94	112.73	109.97
32	1	5017	CHL	C3C-C4C-NC	-2.94	107.27	110.57
19	A	814	CLA	C2D-C1D-ND	2.94	112.27	110.10
19	5	312	CLA	C2C-C1C-NC	2.94	112.73	109.97
19	A	831	CLA	C2C-C1C-NC	2.94	112.73	109.97
19	B	834	CLA	C2C-C1C-NC	2.94	112.73	109.97
31	1	5004	LUT	C18-C5-C6	-2.94	121.23	124.53
19	7	318	CLA	CAA-C2A-C3A	-2.94	106.91	114.26
22	5	304	BCR	C27-C26-C25	-2.94	118.46	122.73
19	A	819	CLA	CMA-C3A-C4A	2.94	119.67	111.77
19	4	310	CLA	O2A-CGA-CBA	2.94	121.13	111.91
19	4	306	CLA	C2D-C1D-ND	2.94	112.27	110.10
19	1	5011	CLA	C2C-C1C-NC	2.94	112.72	109.97
32	5	320	CHL	C1B-CHB-C4A	-2.94	124.30	130.12
19	A	835	CLA	C2C-C1C-NC	2.94	112.72	109.97
19	B	822	CLA	C2C-C1C-NC	2.94	112.72	109.97
19	B	818	CLA	C2D-C1D-ND	2.94	112.27	110.10
19	3	5020	CLA	C2D-C1D-ND	2.94	112.27	110.10
19	1	5007	CLA	C2D-C1D-ND	2.94	112.27	110.10
19	5	313	CLA	C2D-C1D-ND	2.94	112.27	110.10
19	5	301	CLA	C1D-ND-C4D	-2.94	104.25	106.33
19	6	301	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
19	A	813	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
19	F	303	CLA	CMA-C3A-C4A	2.93	119.66	111.77
19	A	835	CLA	C1D-ND-C4D	-2.93	104.25	106.33
28	1	5005	C7Z	C38-C25-C24	2.93	119.79	114.36
19	K	203	CLA	CMA-C3A-C4A	2.93	119.66	111.77
19	A	837	CLA	CMA-C3A-C4A	2.93	119.66	111.77
19	A	824	CLA	CHD-C1D-ND	-2.93	121.76	124.45
19	B	815	CLA	CHD-C1D-ND	-2.93	121.76	124.45
19	B	811	CLA	C2C-C1C-NC	2.93	112.72	109.97
19	A	806	CLA	C1D-ND-C4D	-2.93	104.25	106.33
22	A	847	BCR	C33-C5-C4	2.93	119.25	113.62
19	1	5012	CLA	CMA-C3A-C4A	2.93	119.65	111.77
19	K	204	CLA	C2D-C1D-ND	2.93	112.26	110.10
19	B	836	CLA	C1D-ND-C4D	-2.93	104.25	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	313	CLA	C1-C2-C3	-2.93	120.97	126.04
19	A	829	CLA	C2C-C1C-NC	2.93	112.72	109.97
19	A	843	CLA	CHD-C1D-ND	-2.93	121.76	124.45
19	3	5020	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
19	B	822	CLA	CMA-C3A-C4A	2.93	119.64	111.77
19	B	818	CLA	CMA-C3A-C4A	2.93	119.64	111.77
19	4	306	CLA	C2C-C1C-NC	2.93	112.72	109.97
19	A	803	CLA	CMA-C3A-C4A	2.93	119.64	111.77
19	F	301	CLA	C1-C2-C3	-2.93	120.98	126.04
19	1	5013	CLA	C2D-C1D-ND	2.93	112.26	110.10
19	Z	306	CLA	C2D-C1D-ND	2.93	112.26	110.10
19	A	806	CLA	C2C-C1C-NC	2.93	112.71	109.97
19	K	205	CLA	CMA-C3A-C4A	2.93	119.64	111.77
19	5	312	CLA	CHD-C1D-ND	-2.93	121.77	124.45
22	B	843	BCR	C38-C26-C27	2.93	119.24	113.62
19	B	834	CLA	CMA-C3A-C4A	2.93	119.64	111.77
19	A	836	CLA	C1D-ND-C4D	-2.93	104.26	106.33
19	B	816	CLA	C1D-ND-C4D	-2.93	104.26	106.33
19	8	309	CLA	CHD-C1D-ND	-2.92	121.77	124.45
19	A	814	CLA	CMA-C3A-C4A	2.92	119.63	111.77
19	8	313	CLA	CMA-C3A-C4A	2.92	119.63	111.77
19	Z	303	CLA	C2D-C1D-ND	2.92	112.26	110.10
19	B	810	CLA	C2C-C1C-NC	2.92	112.71	109.97
19	8	311	CLA	C1-C2-C3	-2.92	120.99	126.04
19	A	842	CLA	CHD-C1D-ND	-2.92	121.77	124.45
19	A	803	CLA	C2C-C1C-NC	2.92	112.71	109.97
19	5	307	CLA	C2D-C1D-ND	2.92	112.26	110.10
19	8	307	CLA	O2A-CGA-CBA	2.92	121.07	111.91
22	7	305	BCR	C27-C26-C25	-2.92	118.49	122.73
19	B	811	CLA	C1D-ND-C4D	-2.92	104.26	106.33
19	3	5009	CLA	C2D-C1D-ND	2.92	112.25	110.10
22	6	307	BCR	C27-C26-C25	-2.92	118.50	122.73
28	J	1902	C7Z	C1-C6-C5	-2.92	118.50	122.61
28	6	304	C7Z	C11-C12-C13	-2.92	118.22	126.42
19	Z	308	CLA	C1-C2-C3	-2.92	121.00	126.04
31	1	5003	LUT	C30-C31-C32	-2.92	114.12	123.22
32	Z	309	CHL	C1B-CHB-C4A	-2.92	124.34	130.12
19	B	828	CLA	C1D-ND-C4D	-2.92	104.26	106.33
19	7	312	CLA	CMA-C3A-C4A	2.91	119.61	111.77
19	B	813	CLA	C2D-C1D-ND	2.91	112.25	110.10
19	Z	307	CLA	CHD-C1D-ND	-2.91	121.78	124.45
22	A	859	BCR	C33-C5-C4	2.91	119.21	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	833	CLA	C1D-ND-C4D	-2.91	104.27	106.33
19	4	312	CLA	C1D-ND-C4D	-2.91	104.27	106.33
22	6	308	BCR	C12-C13-C14	2.91	123.41	118.94
19	3	5012	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
19	B	816	CLA	C2C-C1C-NC	2.91	112.70	109.97
31	8	305	LUT	C35-C15-C14	-2.91	117.51	123.47
19	B	804	CLA	CHD-C1D-ND	-2.91	121.78	124.45
19	6	314	CLA	CMA-C3A-C4A	2.91	119.60	111.77
19	Z	312	CLA	CHD-C1D-ND	-2.91	121.78	124.45
19	B	816	CLA	CMA-C3A-C4A	2.91	119.59	111.77
19	1	5016	CLA	CMA-C3A-C4A	2.91	119.59	111.77
19	B	808	CLA	CMA-C3A-C4A	2.91	119.59	111.77
19	1	5010	CLA	C1-C2-C3	-2.91	121.01	126.04
19	Z	305	CLA	C2D-C1D-ND	2.91	112.25	110.10
19	A	826	CLA	CMA-C3A-C4A	2.91	119.59	111.77
19	1	5018	CLA	C2C-C1C-NC	2.91	112.70	109.97
19	4	309	CLA	C1D-ND-C4D	-2.91	104.27	106.33
19	3	5008	CLA	C2C-C1C-NC	2.91	112.70	109.97
19	B	829	CLA	CMA-C3A-C4A	2.91	119.59	111.77
19	7	318	CLA	CHD-C1D-ND	-2.91	121.78	124.45
19	B	806	CLA	C1D-ND-C4D	-2.91	104.27	106.33
19	B	802	CLA	CHD-C1D-ND	-2.91	121.78	124.45
19	B	828	CLA	CHD-C1D-ND	-2.91	121.78	124.45
19	A	834	CLA	CMA-C3A-C4A	2.91	119.58	111.77
22	B	844	BCR	C1-C6-C5	-2.90	118.52	122.61
19	B	827	CLA	CHD-C1D-ND	-2.90	121.78	124.45
19	5	319	CLA	C1D-ND-C4D	-2.90	104.27	106.33
19	A	808	CLA	C1D-ND-C4D	-2.90	104.27	106.33
19	6	301	CLA	C2C-C1C-NC	2.90	112.69	109.97
19	A	827	CLA	CMA-C3A-C4A	2.90	119.57	111.77
19	I	201	CLA	C1D-ND-C4D	-2.90	104.27	106.33
31	1	5003	LUT	C21-C26-C25	2.90	116.61	111.42
19	B	840	CLA	C2D-C1D-ND	2.90	112.24	110.10
19	B	817	CLA	CMA-C3A-C4A	2.90	119.57	111.77
19	7	317	CLA	C2C-C1C-NC	2.90	112.69	109.97
19	5	321	CLA	CMA-C3A-C4A	2.90	119.56	111.77
19	B	830	CLA	CMA-C3A-C4A	2.90	119.56	111.77
19	5	301	CLA	C2C-C1C-NC	2.90	112.69	109.97
22	4	305	BCR	C8-C7-C6	-2.90	119.06	127.20
22	G	1603	BCR	C8-C7-C6	-2.90	119.06	127.20
19	B	801	CLA	C2C-C1C-NC	2.90	112.69	109.97
32	1	5017	CHL	CMA-C3A-C4A	2.90	119.56	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	821	CLA	C2C-C1C-NC	2.90	112.69	109.97
31	6	305	LUT	C30-C31-C32	-2.89	114.18	123.22
19	4	312	CLA	CMA-C3A-C4A	2.89	119.55	111.77
19	A	818	CLA	C1D-ND-C4D	-2.89	104.28	106.33
28	6	304	C7Z	C19-C9-C10	-2.89	118.87	122.92
22	A	847	BCR	C23-C24-C25	-2.89	119.08	127.20
19	A	840	CLA	CHD-C1D-ND	-2.89	121.80	124.45
19	A	822	CLA	C1-C2-C3	-2.89	121.04	126.04
32	8	316	CHL	C1B-CHB-C4A	-2.89	124.39	130.12
19	F	301	CLA	CAA-CBA-CGA	-2.89	104.80	113.25
31	Z	318	LUT	C35-C34-C33	-2.89	123.18	127.31
19	B	829	CLA	C2C-C1C-NC	2.89	112.68	109.97
19	7	309	CLA	C2C-C1C-NC	2.89	112.68	109.97
19	7	318	CLA	C2D-C1D-ND	2.89	112.23	110.10
19	3	5018	CLA	C1D-ND-C4D	-2.89	104.28	106.33
19	5	325	CLA	CHD-C1D-ND	-2.89	121.80	124.45
19	5	306	CLA	C1C-C2C-C3C	-2.89	103.92	106.96
19	Z	303	CLA	C1C-C2C-C3C	-2.89	103.92	106.96
19	8	311	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
19	B	835	CLA	C2D-C1D-ND	2.89	112.23	110.10
22	3	5006	BCR	C23-C24-C25	-2.89	119.09	127.20
19	6	320	CLA	O2A-CGA-CBA	2.89	120.97	111.91
19	K	203	CLA	C2D-C1D-ND	2.89	112.23	110.10
19	6	301	CLA	C1D-ND-C4D	-2.89	104.28	106.33
19	8	313	CLA	CHD-C1D-ND	-2.89	121.80	124.45
28	6	304	C7Z	C38-C25-C24	2.89	119.70	114.36
23	A	851	LHG	O8-C23-C24	2.89	120.97	111.91
19	A	826	CLA	CHD-C1D-ND	-2.89	121.80	124.45
19	B	837	CLA	C1D-ND-C4D	-2.89	104.28	106.33
19	4	309	CLA	C2D-C1D-ND	2.88	112.23	110.10
18	A	801	CL0	CMC-C2C-C1C	2.88	129.43	125.04
22	4	305	BCR	C4-C5-C6	-2.88	118.54	122.73
19	J	1901	CLA	C1D-ND-C4D	-2.88	104.29	106.33
22	4	305	BCR	C7-C8-C9	-2.88	121.88	126.23
22	6	307	BCR	C8-C7-C6	-2.88	119.10	127.20
19	B	806	CLA	C1-C2-C3	-2.88	121.06	126.04
19	B	809	CLA	C2D-C1D-ND	2.88	112.23	110.10
32	Z	313	CHL	C2C-C3C-C4C	2.88	108.54	106.49
19	A	857	CLA	C1-C2-C3	-2.88	121.06	126.04
19	5	311	CLA	C2C-C1C-NC	2.88	112.67	109.97
22	6	308	BCR	C36-C18-C19	2.88	122.62	118.08
31	4	304	LUT	C8-C7-C6	-2.88	119.11	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	1601	CLA	CHD-C1D-ND	-2.88	121.81	124.45
19	B	850	CLA	CHD-C1D-ND	-2.88	121.81	124.45
19	A	827	CLA	C1D-ND-C4D	-2.88	104.29	106.33
19	G	1602	CLA	C1D-ND-C4D	-2.88	104.29	106.33
19	6	320	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	6	308	BCR	C27-C26-C25	-2.88	118.55	122.73
19	3	5012	CLA	C1-C2-C3	-2.88	121.06	126.04
19	4	313	CLA	C2D-C1D-ND	2.88	112.22	110.10
19	A	830	CLA	CMA-C3A-C4A	2.88	119.51	111.77
19	B	802	CLA	C2C-C1C-NC	2.88	112.67	109.97
19	4	318	CLA	CMA-C3A-C4A	2.88	119.51	111.77
19	A	804	CLA	C1D-ND-C4D	-2.88	104.29	106.33
19	A	806	CLA	CMA-C3A-C4A	2.88	119.51	111.77
19	A	838	CLA	CMA-C3A-C4A	2.88	119.51	111.77
19	8	310	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
31	8	304	LUT	C18-C5-C6	-2.88	121.30	124.53
19	A	834	CLA	C2D-C1D-ND	2.88	112.22	110.10
19	7	309	CLA	C2D-C1D-ND	2.88	112.22	110.10
22	5	305	BCR	C30-C25-C26	-2.87	118.56	122.61
19	3	5015	CLA	C2C-C1C-NC	2.87	112.67	109.97
19	8	320	CLA	C1D-ND-C4D	-2.87	104.29	106.33
19	5	325	CLA	C2D-C1D-ND	2.87	112.22	110.10
19	3	5016	CLA	CMA-C3A-C4A	2.87	119.50	111.77
19	B	832	CLA	C1D-ND-C4D	-2.87	104.29	106.33
19	A	812	CLA	C2D-C1D-ND	2.87	112.22	110.10
19	B	803	CLA	C2D-C1D-ND	2.87	112.22	110.10
22	5	305	BCR	C27-C26-C25	-2.87	118.56	122.73
19	1	5006	CLA	C1D-ND-C4D	-2.87	104.30	106.33
19	B	826	CLA	C1-C2-C3	-2.87	121.08	126.04
19	A	822	CLA	CMA-C3A-C4A	2.87	119.49	111.77
19	Z	311	CLA	CHD-C1D-ND	-2.87	121.82	124.45
19	A	803	CLA	C1D-ND-C4D	-2.87	104.30	106.33
19	A	827	CLA	C1-C2-C3	-2.87	121.08	126.04
19	B	820	CLA	CHD-C1D-ND	-2.87	121.82	124.45
19	4	308	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
19	A	839	CLA	C1D-ND-C4D	-2.87	104.30	106.33
19	7	312	CLA	C1D-ND-C4D	-2.87	104.30	106.33
19	K	205	CLA	C2D-C1D-ND	2.87	112.22	110.10
19	3	5011	CLA	CMA-C3A-C4A	2.87	119.48	111.77
19	3	5008	CLA	CAA-C2A-C3A	-2.87	104.93	112.78
19	3	5009	CLA	C2C-C1C-NC	2.87	112.66	109.97
19	A	825	CLA	C1-C2-C3	-2.86	121.09	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	J	1902	C7Z	C18-C5-C4	2.86	119.66	114.36
19	8	310	CLA	C2C-C1C-NC	2.86	112.66	109.97
19	5	309	CLA	O2A-CGA-CBA	2.86	120.89	111.91
19	B	806	CLA	C2C-C1C-NC	2.86	112.65	109.97
19	5	308	CLA	O2A-CGA-CBA	2.86	120.89	111.91
19	B	810	CLA	C6-C5-C3	-2.86	109.94	114.62
31	5	303	LUT	C30-C31-C32	-2.86	114.29	123.22
22	8	303	BCR	C36-C18-C17	-2.86	118.92	122.92
19	B	810	CLA	CMA-C3A-C4A	2.86	119.46	111.77
19	Z	304	CLA	CMA-C3A-C4A	2.86	119.46	111.77
19	8	313	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
19	A	842	CLA	C2D-C1D-ND	2.86	112.21	110.10
19	3	5010	CLA	C2D-C1D-ND	2.86	112.21	110.10
19	B	802	CLA	C1D-ND-C4D	-2.86	104.30	106.33
19	A	841	CLA	CMA-C3A-C4A	2.86	119.46	111.77
19	A	840	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
19	1	5018	CLA	C1D-ND-C4D	-2.86	104.31	106.33
19	6	302	CLA	CMA-C3A-C4A	2.86	119.45	111.77
19	A	804	CLA	C2C-C1C-NC	2.86	112.65	109.97
19	A	809	CLA	C2C-C1C-NC	2.86	112.65	109.97
19	B	824	CLA	O2A-CGA-CBA	2.86	120.87	111.91
19	B	815	CLA	C1D-ND-C4D	-2.86	104.31	106.33
32	8	315	CHL	CMA-C3A-C4A	2.86	119.45	111.77
19	6	323	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
19	7	318	CLA	C1C-C2C-C3C	-2.85	103.95	106.96
19	Z	312	CLA	C2C-C1C-NC	2.85	112.65	109.97
19	B	826	CLA	C1D-ND-C4D	-2.85	104.31	106.33
19	B	830	CLA	C1D-ND-C4D	-2.85	104.31	106.33
32	1	5014	CHL	C3C-C4C-NC	-2.85	107.37	110.57
19	B	819	CLA	C2D-C1D-ND	2.85	112.21	110.10
31	3	5003	LUT	C1-C6-C5	-2.85	118.60	122.61
31	8	304	LUT	C2-C3-C4	2.85	114.21	110.30
19	1	5008	CLA	C6-C5-C3	-2.85	105.98	113.45
22	6	308	BCR	C1-C6-C5	-2.85	118.60	122.61
19	6	318	CLA	C1D-ND-C4D	-2.85	104.31	106.33
19	A	840	CLA	C2C-C1C-NC	2.85	112.64	109.97
31	6	306	LUT	C15-C14-C13	-2.85	123.25	127.31
19	B	850	CLA	C1D-ND-C4D	-2.85	104.31	106.33
31	5	303	LUT	C15-C35-C34	-2.85	117.64	123.47
19	5	314	CLA	C2D-C1D-ND	2.85	112.20	110.10
22	B	846	BCR	C11-C12-C13	-2.85	118.42	126.42
19	8	320	CLA	CMA-C3A-C4A	2.85	119.42	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	818	CLA	C1-C2-C3	-2.85	121.12	126.04
19	B	836	CLA	C2C-C1C-NC	2.85	112.64	109.97
19	1	5016	CLA	C1D-ND-C4D	-2.84	104.31	106.33
19	A	821	CLA	C2D-C1D-ND	2.84	112.20	110.10
19	B	818	CLA	C2C-C1C-NC	2.84	112.64	109.97
19	A	841	CLA	C1D-ND-C4D	-2.84	104.31	106.33
19	7	310	CLA	C1D-ND-C4D	-2.84	104.31	106.33
19	B	812	CLA	C2C-C1C-NC	2.84	112.64	109.97
19	6	309	CLA	O2A-CGA-CBA	2.84	120.83	111.91
19	A	815	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	7	313	CLA	C2C-C1C-NC	2.84	112.63	109.97
29	7	301	LMG	O8-C28-C29	2.84	120.82	111.91
19	B	829	CLA	C1D-ND-C4D	-2.84	104.32	106.33
19	7	310	CLA	C2C-C1C-NC	2.84	112.63	109.97
19	A	808	CLA	CMA-C3A-C4A	2.84	119.41	111.77
19	8	310	CLA	C1-C2-C3	-2.84	121.13	126.04
19	7	312	CLA	C1-C2-C3	-2.84	121.13	126.04
19	A	817	CLA	C1D-ND-C4D	-2.84	104.32	106.33
32	7	315	CHL	C1-C2-C3	-2.84	121.14	126.04
22	B	843	BCR	C23-C24-C25	-2.84	119.24	127.20
19	B	833	CLA	C1D-ND-C4D	-2.84	104.32	106.33
19	3	5012	CLA	C1D-ND-C4D	-2.84	104.32	106.33
19	1	5015	CLA	CMA-C3A-C4A	2.83	119.39	111.77
32	5	318	CHL	CMA-C3A-C4A	2.83	119.39	111.77
19	A	816	CLA	CHD-C1D-ND	-2.83	121.85	124.45
22	G	1603	BCR	C4-C5-C6	-2.83	118.62	122.73
19	5	311	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
19	7	318	CLA	C2C-C1C-NC	2.83	112.63	109.97
22	B	845	BCR	C23-C24-C25	-2.83	119.25	127.20
19	5	321	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
19	1	5008	CLA	CMA-C3A-C4A	2.83	119.38	111.77
19	8	310	CLA	CMA-C3A-C4A	2.83	119.38	111.77
19	7	307	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
19	B	806	CLA	CMA-C3A-C4A	2.83	119.38	111.77
19	Z	304	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
19	A	823	CLA	C1D-ND-C4D	-2.83	104.33	106.33
19	A	810	CLA	CHD-C1D-ND	-2.83	121.85	124.45
19	3	5008	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
19	B	807	CLA	CMA-C3A-C4A	2.83	119.38	111.77
28	1	5005	C7Z	C35-C15-C14	-2.83	117.68	123.47
19	8	308	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
32	5	316	CHL	C2C-C3C-C4C	2.83	108.50	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	8	309	CLA	C6-C5-C3	-2.83	106.04	113.45
19	B	812	CLA	CMA-C3A-C4A	2.83	119.37	111.77
19	1	5013	CLA	C1D-ND-C4D	-2.83	104.33	106.33
19	Z	306	CLA	C2C-C1C-NC	2.83	112.62	109.97
19	A	836	CLA	CMA-C3A-C4A	2.83	119.37	111.77
22	B	842	BCR	C38-C26-C27	2.83	119.04	113.62
22	B	847	BCR	C38-C26-C27	2.83	119.04	113.62
19	A	809	CLA	C1D-ND-C4D	-2.83	104.33	106.33
19	3	5014	CLA	C1D-ND-C4D	-2.83	104.33	106.33
19	A	810	CLA	C2D-C1D-ND	2.83	112.19	110.10
19	8	307	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
32	8	319	CHL	C4D-CHA-C1A	2.82	124.69	121.25
19	A	857	CLA	C1D-ND-C4D	-2.82	104.33	106.33
31	8	305	LUT	C10-C11-C12	-2.82	114.41	123.22
19	Z	306	CLA	CMA-C3A-C4A	2.82	119.36	111.77
19	A	837	CLA	C1D-ND-C4D	-2.82	104.33	106.33
19	Z	311	CLA	C2D-C1D-ND	2.82	112.18	110.10
19	3	5016	CLA	C1D-ND-C4D	-2.82	104.33	106.33
19	B	803	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
19	B	825	CLA	CHD-C1D-ND	-2.82	121.86	124.45
19	B	850	CLA	C2C-C1C-NC	2.82	112.61	109.97
32	4	314	CHL	C1-O2A-CGA	2.82	123.83	116.44
32	4	314	CHL	C1-C2-C3	-2.81	122.20	126.75
19	B	831	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
19	B	839	CLA	CMA-C3A-C4A	2.81	119.33	111.77
19	B	831	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
32	8	301	CHL	C4D-CHA-C1A	2.81	124.67	121.25
19	7	312	CLA	CHD-C1D-ND	-2.81	121.87	124.45
38	8	325	ERG	C14-C13-C17	2.81	102.72	99.72
19	B	832	CLA	CMA-C3A-C4A	2.81	119.33	111.77
31	1	5003	LUT	C15-C14-C13	-2.81	123.30	127.31
19	B	807	CLA	C2D-C1D-ND	2.81	112.17	110.10
31	7	304	LUT	C18-C5-C4	2.81	119.56	114.36
19	4	310	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
19	A	831	CLA	C1D-ND-C4D	-2.81	104.34	106.33
19	B	836	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
19	Z	314	CLA	CMA-C3A-C4A	2.81	119.32	111.77
19	4	308	CLA	CMA-C3A-C4A	2.81	119.32	111.77
22	A	846	BCR	C33-C5-C4	2.81	119.01	113.62
19	4	316	CLA	C2C-C1C-NC	2.81	112.60	109.97
32	8	317	CHL	C4A-NA-C1A	2.81	107.97	106.71
19	B	836	CLA	O2D-CGD-O1D	-2.81	118.35	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1	5017	CHL	C1B-CHB-C4A	-2.81	124.56	130.12
19	F	301	CLA	O2A-CGA-CBA	2.81	120.71	111.91
19	B	814	CLA	CMA-C3A-C4A	2.80	119.31	111.77
19	B	815	CLA	CMA-C3A-C4A	2.80	119.31	111.77
19	1	5015	CLA	CHD-C1D-ND	-2.80	121.88	124.45
19	A	820	CLA	C1D-ND-C4D	-2.80	104.34	106.33
19	6	302	CLA	C1-C2-C3	-2.80	121.20	126.04
19	7	308	CLA	C2C-C1C-NC	2.80	112.60	109.97
31	7	304	LUT	C22-C23-C24	2.80	114.93	111.74
19	1	5008	CLA	C2C-C1C-NC	2.80	112.60	109.97
22	A	850	BCR	C23-C24-C25	-2.80	119.34	127.20
19	3	5015	CLA	CHD-C1D-ND	-2.80	121.88	124.45
27	4	303	RRX	C15-C16-C17	-2.80	117.74	123.47
19	6	312	CLA	C2C-C1C-NC	2.80	112.59	109.97
19	6	301	CLA	CHD-C1D-ND	-2.80	121.88	124.45
19	7	313	CLA	CMA-C3A-C4A	2.80	119.30	111.77
19	8	314	CLA	O2A-CGA-CBA	2.80	120.69	111.91
19	7	319	CLA	C1D-ND-C4D	-2.80	104.35	106.33
19	A	829	CLA	CHD-C1D-ND	-2.80	121.88	124.45
31	3	5002	LUT	C18-C5-C4	2.80	119.54	114.36
19	7	310	CLA	O2A-CGA-CBA	2.80	120.68	111.91
27	5	302	RRX	C15-C14-C13	-2.80	123.32	127.31
19	A	824	CLA	C1D-ND-C4D	-2.80	104.35	106.33
19	B	812	CLA	C1D-ND-C4D	-2.80	104.35	106.33
19	A	823	CLA	CMA-C3A-C4A	2.79	119.28	111.77
19	B	821	CLA	CMA-C3A-C4A	2.79	119.28	111.77
27	F	304	RRX	C11-C12-C13	-2.79	118.57	126.42
19	B	839	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
19	7	311	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
19	6	309	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
19	Z	314	CLA	C1D-ND-C4D	-2.79	104.35	106.33
23	Z	316	LHG	O8-C23-C24	2.79	120.67	111.91
19	B	801	CLA	C1-C2-C3	-2.79	121.22	126.04
19	A	828	CLA	C1D-ND-C4D	-2.79	104.35	106.33
19	4	313	CLA	C2C-C1C-NC	2.79	112.59	109.97
19	A	830	CLA	C1D-ND-C4D	-2.79	104.35	106.33
19	7	319	CLA	CMA-C3A-C4A	2.79	119.27	111.77
19	A	810	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
23	A	852	LHG	O8-C23-C24	2.79	120.66	111.91
19	A	843	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
19	K	204	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
19	8	307	CLA	C2D-C1D-ND	2.79	112.16	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	819	CLA	C2C-C1C-NC	2.79	112.58	109.97
19	7	310	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
19	B	809	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
19	6	318	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
31	7	303	LUT	C21-C26-C27	-2.78	109.18	112.70
19	A	802	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
19	B	814	CLA	C1D-ND-C4D	-2.78	104.36	106.33
19	7	324	CLA	C2D-C1D-ND	2.78	112.15	110.10
19	B	827	CLA	CMA-C3A-C4A	2.78	119.25	111.77
19	6	311	CLA	C5-C3-C2	2.78	126.74	121.12
19	8	309	CLA	CMA-C3A-C4A	2.78	119.24	111.77
19	7	308	CLA	CMA-C3A-C4A	2.78	119.24	111.77
25	B	848	DGD	O1G-C1A-C2A	2.78	120.62	111.91
19	1	5007	CLA	CHD-C1D-ND	-2.78	121.90	124.45
19	7	307	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
19	5	306	CLA	CMA-C3A-C4A	2.78	119.23	111.77
22	B	844	BCR	C37-C22-C21	-2.78	119.03	122.92
19	Z	308	CLA	C2D-C1D-ND	2.77	112.15	110.10
22	A	849	BCR	C16-C15-C14	-2.77	117.79	123.47
19	B	821	CLA	C1D-ND-C4D	-2.77	104.36	106.33
19	A	805	CLA	C2C-C1C-NC	2.77	112.57	109.97
19	8	313	CLA	C2C-C1C-NC	2.77	112.57	109.97
19	5	307	CLA	C1D-ND-C4D	-2.77	104.36	106.33
19	Z	308	CLA	C2C-C1C-NC	2.77	112.57	109.97
19	5	306	CLA	C2C-C1C-NC	2.77	112.57	109.97
19	B	809	CLA	CMA-C3A-C4A	2.77	119.22	111.77
19	4	312	CLA	CHD-C1D-ND	-2.77	121.91	124.45
19	1	5015	CLA	C1D-ND-C4D	-2.77	104.37	106.33
19	6	302	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
32	6	315	CHL	C4D-CHA-C1A	2.77	124.62	121.25
19	A	815	CLA	C2D-C1D-ND	2.77	112.14	110.10
38	6	326	ERG	C7-C6-C5	-2.77	118.34	123.20
19	8	318	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
32	4	319	CHL	C1B-CHB-C4A	-2.77	124.63	130.12
19	3	5013	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
22	B	846	BCR	C8-C7-C6	-2.77	119.43	127.20
19	B	810	CLA	C1D-ND-C4D	-2.77	104.37	106.33
22	8	303	BCR	C38-C26-C27	2.77	118.93	113.62
22	4	305	BCR	C33-C5-C4	2.77	118.93	113.62
22	8	306	BCR	C11-C10-C9	-2.76	123.36	127.31
19	5	314	CLA	C2C-C1C-NC	2.76	112.56	109.97
32	6	316	CHL	CHB-C4A-NA	2.76	128.34	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	843	CLA	CMA-C3A-C4A	2.76	119.20	111.77
19	1	5012	CLA	C1D-ND-C4D	-2.76	104.37	106.33
19	6	323	CLA	C1D-ND-C4D	-2.76	104.37	106.33
22	K	206	BCR	C33-C5-C4	2.76	118.92	113.62
22	A	847	BCR	C8-C7-C6	-2.76	119.44	127.20
19	4	310	CLA	CHD-C1D-ND	-2.76	121.92	124.45
19	4	307	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
32	1	5014	CHL	C4D-CHA-C1A	2.76	124.61	121.25
19	1	5016	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
19	A	805	CLA	CMA-C3A-C4A	2.76	119.19	111.77
32	4	315	CHL	CHB-C4A-NA	2.76	128.33	124.51
19	4	318	CLA	CAA-C2A-C3A	-2.76	109.66	116.10
32	5	318	CHL	C1B-CHB-C4A	-2.76	124.65	130.12
23	A	851	LHG	C5-O7-C7	-2.76	111.00	117.79
19	B	805	CLA	C2C-C1C-NC	2.76	112.56	109.97
19	B	838	CLA	C1D-ND-C4D	-2.76	104.38	106.33
19	1	5015	CLA	C2C-C1C-NC	2.76	112.56	109.97
19	5	301	CLA	C1-C2-C3	-2.76	121.28	126.04
19	8	311	CLA	C2C-C1C-NC	2.76	112.55	109.97
19	B	824	CLA	C1-C2-C3	-2.76	121.28	126.04
19	A	811	CLA	C2C-C1C-NC	2.76	112.55	109.97
27	F	304	RRX	C38-C26-C27	2.75	119.46	114.36
19	5	307	CLA	C2C-C1C-NC	2.75	112.55	109.97
19	A	818	CLA	C1-C2-C3	-2.75	121.28	126.04
19	3	5008	CLA	CMA-C3A-C4A	2.75	119.17	111.77
31	8	305	LUT	C20-C13-C12	2.75	122.42	118.08
19	A	837	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
19	8	309	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
19	G	1602	CLA	C2C-C1C-NC	2.75	112.55	109.97
19	Z	308	CLA	C1D-ND-C4D	-2.75	104.38	106.33
19	A	832	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
31	3	5002	LUT	C30-C31-C32	-2.75	114.64	123.22
19	4	311	CLA	CAA-CBA-CGA	-2.75	105.22	113.25
19	5	312	CLA	C1D-ND-C4D	-2.75	104.38	106.33
19	B	803	CLA	C1-C2-C3	-2.75	121.29	126.04
31	Z	317	LUT	C18-C5-C4	2.75	119.44	114.36
19	1	5011	CLA	CMD-C2D-C3D	-2.75	121.30	127.61
19	A	819	CLA	C1D-ND-C4D	-2.75	104.38	106.33
19	B	839	CLA	C1D-ND-C4D	-2.75	104.38	106.33
19	3	5018	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
19	A	807	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
19	5	325	CLA	C1C-C2C-C3C	-2.74	104.07	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	811	CLA	C1-C2-C3	-2.74	121.30	126.04
19	8	312	CLA	O2A-CGA-CBA	2.74	120.52	111.91
19	A	814	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
19	A	829	CLA	C1D-ND-C4D	-2.74	104.39	106.33
19	8	309	CLA	CAA-C2A-C3A	-2.74	105.27	112.78
19	5	314	CLA	CHD-C1D-ND	-2.74	121.94	124.45
19	5	311	CLA	C2D-C1D-ND	2.74	112.12	110.10
19	7	324	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
19	4	307	CLA	CMA-C3A-C4A	2.74	119.14	111.77
19	A	822	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
19	B	834	CLA	C1D-ND-C4D	-2.74	104.39	106.33
22	A	850	BCR	C34-C9-C10	-2.74	119.09	122.92
19	3	5010	CLA	CMA-C3A-C4A	2.74	119.13	111.77
22	5	304	BCR	C24-C23-C22	-2.74	122.10	126.23
19	7	311	CLA	C6-C5-C3	-2.74	106.28	113.45
19	6	320	CLA	C2D-C1D-ND	2.74	112.12	110.10
19	3	5016	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
19	B	820	CLA	C1D-ND-C4D	-2.74	104.39	106.33
19	G	1601	CLA	C1D-ND-C4D	-2.74	104.39	106.33
19	4	306	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
19	G	1602	CLA	CMA-C3A-C4A	2.73	119.12	111.77
19	1	5010	CLA	C1D-ND-C4D	-2.73	104.39	106.33
19	7	307	CLA	CHD-C1D-ND	-2.73	121.94	124.45
19	Z	312	CLA	CMA-C3A-C4A	2.73	119.11	111.77
19	B	823	CLA	C1D-ND-C4D	-2.73	104.39	106.33
19	5	308	CLA	C2D-C1D-ND	2.73	112.12	110.10
22	A	846	BCR	C8-C7-C6	-2.73	119.53	127.20
19	7	308	CLA	O2A-CGA-CBA	2.73	120.47	111.91
19	4	306	CLA	CMA-C3A-C4A	2.73	119.11	111.77
19	B	810	CLA	C1-C2-C3	-2.73	121.33	126.04
19	6	313	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
32	6	321	CHL	CMA-C3A-C4A	2.73	119.10	111.77
19	4	313	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
19	A	838	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
19	A	840	CLA	C2D-C1D-ND	2.73	112.11	110.10
19	Z	304	CLA	C2D-C1D-ND	2.73	112.11	110.10
31	8	305	LUT	C15-C35-C34	-2.73	117.89	123.47
38	8	325	ERG	C15-C14-C13	-2.72	101.78	104.21
27	4	303	RRX	C1-C6-C5	-2.72	118.78	122.61
22	A	846	BCR	C23-C24-C25	-2.72	119.56	127.20
19	3	5019	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
22	B	842	BCR	C27-C26-C25	-2.72	118.78	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	320	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
22	B	845	BCR	C15-C16-C17	-2.72	117.90	123.47
19	3	5015	CLA	CMA-C3A-C4A	2.72	119.08	111.77
31	5	303	LUT	C31-C30-C29	-2.72	123.43	127.31
22	6	307	BCR	C2-C1-C6	2.72	114.67	110.48
19	B	813	CLA	C1D-ND-C4D	-2.72	104.40	106.33
20	B	841	PQN	C2M-C2-C3	-2.72	119.96	124.40
19	7	308	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
19	1	5015	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
19	B	837	CLA	CMA-C3A-C4A	2.72	119.08	111.77
19	B	807	CLA	C1D-ND-C4D	-2.72	104.40	106.33
27	4	303	RRX	C15-C14-C13	-2.72	123.43	127.31
19	B	838	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
19	A	826	CLA	C1D-ND-C4D	-2.72	104.41	106.33
19	K	205	CLA	C1D-ND-C4D	-2.72	104.41	106.33
19	4	307	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
19	7	319	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
22	A	848	BCR	C15-C16-C17	-2.71	117.91	123.47
19	1	5012	CLA	O2A-CGA-CBA	2.71	120.42	111.91
19	A	808	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
19	1	5011	CLA	C1D-ND-C4D	-2.71	104.41	106.33
19	7	316	CLA	CMA-C3A-C4A	2.71	119.06	111.77
32	8	317	CHL	CMA-C3A-C4A	2.71	119.06	111.77
19	6	323	CLA	C2D-C1D-ND	2.71	112.10	110.10
22	6	308	BCR	C8-C7-C6	-2.71	119.59	127.20
24	A	854	LMT	C1B-O1B-C4'	-2.71	111.26	117.96
19	K	203	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
19	Z	308	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
32	5	316	CHL	CHD-C4C-C3C	2.71	128.82	124.84
22	5	304	BCR	C8-C7-C6	-2.71	119.60	127.20
19	B	807	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
19	A	802	CLA	C1D-ND-C4D	-2.70	104.41	106.33
19	B	809	CLA	C1-C2-C3	-2.70	121.37	126.04
32	8	316	CHL	CMA-C3A-C4A	2.70	119.03	111.77
19	A	834	CLA	C1D-ND-C4D	-2.70	104.42	106.33
19	A	840	CLA	C1D-ND-C4D	-2.70	104.42	106.33
31	1	5003	LUT	C35-C15-C14	-2.70	117.94	123.47
22	A	847	BCR	C2-C1-C6	2.70	114.64	110.48
19	B	802	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
19	B	827	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
19	K	204	CLA	C1D-ND-C4D	-2.70	104.42	106.33
19	A	836	CLA	C1C-C2C-C3C	-2.70	104.12	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	846	BCR	C33-C5-C4	2.70	118.80	113.62
19	8	314	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
19	8	312	CLA	CAA-CBA-CGA	-2.70	105.37	113.25
19	A	842	CLA	C1D-ND-C4D	-2.70	104.42	106.33
19	1	5018	CLA	CMA-C3A-C4A	2.70	119.02	111.77
31	3	5003	LUT	C28-C29-C30	2.69	123.08	118.94
19	3	5019	CLA	C1D-ND-C4D	-2.69	104.42	106.33
19	5	321	CLA	C1D-ND-C4D	-2.69	104.42	106.33
19	6	322	CLA	CMA-C3A-C4A	2.69	119.01	111.77
19	4	310	CLA	C2C-C1C-NC	2.69	112.49	109.97
19	5	319	CLA	C2C-C1C-NC	2.69	112.49	109.97
22	5	305	BCR	C2-C1-C6	2.69	114.62	110.48
19	5	325	CLA	CMA-C3A-C4A	2.69	119.01	111.77
27	4	303	RRX	C11-C10-C9	-2.69	123.47	127.31
19	1	5006	CLA	CMA-C3A-C4A	2.69	119.01	111.77
19	6	313	CLA	CHD-C1D-ND	-2.69	121.98	124.45
22	8	306	BCR	C4-C5-C6	-2.69	118.82	122.73
19	3	5012	CLA	O2A-CGA-CBA	2.69	120.35	111.91
19	Z	303	CLA	CMA-C3A-C4A	2.69	119.00	111.77
19	A	839	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
28	1	5005	C7Z	C31-C32-C33	-2.69	118.86	126.42
19	A	816	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
19	5	319	CLA	CMA-C3A-C4A	2.69	119.00	111.77
19	F	303	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
19	B	810	CLA	O2A-CGA-CBA	2.69	120.34	111.91
19	I	201	CLA	C1-C2-C3	-2.69	121.40	126.04
22	B	847	BCR	C21-C20-C19	-2.69	114.83	123.22
22	3	5006	BCR	C1-C6-C5	-2.68	118.83	122.61
22	8	303	BCR	C35-C13-C12	2.68	122.31	118.08
31	1	5003	LUT	C10-C11-C12	-2.68	114.84	123.22
19	B	808	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
19	I	201	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
22	5	304	BCR	C36-C18-C17	-2.68	119.17	122.92
23	1	5001	LHG	C5-O7-C7	-2.68	111.19	117.79
31	1	5004	LUT	C21-C26-C25	2.68	116.22	111.42
19	6	311	CLA	C2C-C1C-NC	2.68	112.48	109.97
19	7	308	CLA	CHA-C4D-ND	2.68	138.11	132.50
19	A	815	CLA	CMA-C3A-C4A	2.68	118.98	111.77
19	Z	306	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
19	A	810	CLA	C2C-C1C-NC	2.68	112.48	109.97
19	6	314	CLA	C1D-ND-C4D	-2.68	104.43	106.33
19	B	831	CLA	CMA-C3A-C4A	2.68	118.98	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	7	308	CLA	CHD-C1D-ND	-2.68	121.99	124.45
19	B	802	CLA	O2A-CGA-CBA	2.68	120.31	111.91
32	5	320	CHL	CHC-C1C-NC	2.68	128.27	124.20
19	3	5018	CLA	C2C-C1C-NC	2.68	112.48	109.97
31	Z	318	LUT	C21-C26-C27	-2.68	109.32	112.70
22	3	5004	BCR	C15-C16-C17	-2.68	117.99	123.47
19	A	822	CLA	O2A-CGA-CBA	2.68	120.30	111.91
19	Z	305	CLA	C6-C5-C3	-2.67	106.44	113.45
32	8	317	CHL	CHC-C1C-NC	2.67	128.26	124.20
19	4	316	CLA	CMA-C3A-C4A	2.67	118.96	111.77
19	B	825	CLA	C2C-C1C-NC	2.67	112.48	109.97
22	A	858	BCR	C7-C8-C9	-2.67	122.19	126.23
19	A	843	CLA	C1D-ND-C4D	-2.67	104.44	106.33
19	1	5008	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
19	A	823	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
19	B	824	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	8	305	LUT	C39-C29-C28	2.67	122.29	118.08
19	7	310	CLA	C1-C2-C3	-2.67	121.42	126.04
19	A	825	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
19	A	857	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
20	B	841	PQN	C14-C13-C15	2.67	119.76	115.27
22	5	305	BCR	C33-C5-C4	2.67	118.75	113.62
19	3	5010	CLA	C2C-C1C-NC	2.67	112.47	109.97
19	5	310	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
19	A	833	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
19	B	801	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
19	1	5012	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
29	J	1903	LMG	O8-C28-C29	2.67	120.27	111.91
19	7	318	CLA	CMA-C3A-C4A	2.67	118.94	111.77
19	4	310	CLA	CHA-C4D-ND	2.66	138.07	132.50
19	K	205	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
19	Z	307	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
24	G	1604	LMT	C1B-O1B-C4'	-2.66	111.37	117.96
19	A	814	CLA	C1D-ND-C4D	-2.66	104.44	106.33
19	5	307	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
19	A	821	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
19	B	819	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
19	B	829	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
19	5	314	CLA	CMA-C3A-C4A	2.66	118.93	111.77
19	6	302	CLA	C1D-ND-C4D	-2.66	104.44	106.33
32	4	319	CHL	CMA-C3A-C4A	2.66	118.92	111.77
23	7	320	LHG	O8-C23-C24	2.66	120.26	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	827	CLA	C1D-ND-C4D	-2.66	104.44	106.33
19	7	313	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	B	846	BCR	C30-C25-C26	-2.66	118.87	122.61
23	1	5019	LHG	O8-C23-C24	2.66	120.25	111.91
32	4	315	CHL	C1-O2A-CGA	2.66	123.42	116.44
19	Z	311	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
19	3	5011	CLA	C1D-ND-C4D	-2.66	104.45	106.33
19	3	5019	CLA	O2A-CGA-CBA	2.66	120.25	111.91
22	B	842	BCR	C16-C17-C18	-2.66	123.52	127.31
19	A	828	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
19	8	311	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
19	4	312	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
19	5	310	CLA	C1D-ND-C4D	-2.66	104.45	106.33
19	A	838	CLA	C1-C2-C3	-2.66	121.45	126.04
19	4	310	CLA	C6-C5-C3	-2.66	106.49	113.45
22	3	5007	BCR	C35-C13-C12	2.66	122.26	118.08
19	A	831	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
19	Z	306	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
19	6	310	CLA	O2A-CGA-CBA	2.66	120.24	111.91
19	6	309	CLA	CMA-C3A-C4A	2.66	118.91	111.77
19	B	837	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
19	4	318	CLA	C1D-ND-C4D	-2.65	104.45	106.33
19	5	311	CLA	C1D-ND-C4D	-2.65	104.45	106.33
19	4	316	CLA	C2D-C1D-ND	2.65	112.06	110.10
22	G	1603	BCR	C23-C24-C25	-2.65	119.75	127.20
19	B	824	CLA	CMA-C3A-C4A	2.65	118.91	111.77
27	4	303	RRX	C16-C15-C14	-2.65	118.04	123.47
24	4	322	LMT	C1B-O1B-C4'	-2.65	111.40	117.96
19	A	842	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
19	B	818	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
19	B	818	CLA	C1D-ND-C4D	-2.65	104.45	106.33
19	5	309	CLA	C1D-ND-C4D	-2.65	104.45	106.33
19	7	317	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
19	B	801	CLA	C1D-ND-C4D	-2.65	104.45	106.33
19	Z	303	CLA	C1D-ND-C4D	-2.65	104.45	106.33
38	8	325	ERG	C4-C5-C10	-2.65	112.90	116.42
19	8	309	CLA	C1D-ND-C4D	-2.65	104.45	106.33
22	A	858	BCR	C8-C7-C6	-2.65	119.76	127.20
19	B	832	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
19	3	5018	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
19	3	5013	CLA	O2A-CGA-CBA	2.65	120.22	111.91
19	A	810	CLA	CMA-C3A-C4A	2.65	118.89	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	8	312	CLA	CHA-C4D-ND	2.65	138.04	132.50
19	5	309	CLA	CMA-C3A-C4A	2.65	118.89	111.77
19	4	313	CLA	CHD-C1D-ND	-2.65	122.02	124.45
38	8	325	ERG	C11-C12-C13	-2.65	108.24	112.78
19	4	316	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
22	B	846	BCR	C38-C26-C27	2.65	118.70	113.62
22	A	848	BCR	C8-C7-C6	-2.65	119.77	127.20
19	A	818	CLA	C2C-C1C-NC	2.65	112.45	109.97
19	7	316	CLA	O2A-CGA-CBA	2.64	120.21	111.91
22	3	5005	BCR	C38-C26-C27	2.64	118.70	113.62
19	A	824	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
19	6	314	CLA	CHD-C1D-ND	-2.64	122.02	124.45
19	8	310	CLA	CMB-C2B-C3B	2.64	129.62	124.68
19	5	325	CLA	C1-C2-C3	-2.64	121.47	126.04
19	8	312	CLA	C6-C5-C3	-2.64	106.53	113.45
19	A	804	CLA	CMA-C3A-C4A	2.64	118.88	111.77
19	6	301	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
19	B	835	CLA	C1D-ND-C4D	-2.64	104.46	106.33
19	7	306	CLA	CHA-C4D-ND	2.64	138.03	132.50
19	8	311	CLA	C2D-C1D-ND	2.64	112.05	110.10
19	B	833	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
32	3	5017	CHL	CMA-C3A-C4A	2.64	118.87	111.77
19	B	804	CLA	CMA-C3A-C4A	2.64	118.87	111.77
19	A	826	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
19	3	5011	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
22	B	844	BCR	C27-C26-C25	-2.64	118.90	122.73
32	4	315	CHL	CHC-C1C-NC	2.64	128.21	124.20
19	4	318	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
19	8	308	CLA	C1-C2-C3	-2.64	121.48	126.04
19	Z	312	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
38	6	326	ERG	C13-C14-C8	-2.64	108.38	113.48
24	8	324	LMT	O2'-C2'-C3'	-2.64	104.26	110.35
19	1	5010	CLA	CMD-C2D-C3D	-2.63	121.56	127.61
19	6	301	CLA	CMA-C3A-C4A	2.63	118.85	111.77
32	4	314	CHL	C1B-CHB-C4A	-2.63	124.90	130.12
19	A	832	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
28	1	5005	C7Z	C11-C10-C9	-2.63	123.55	127.31
19	1	5010	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
22	B	846	BCR	C16-C17-C18	-2.63	123.55	127.31
22	3	5007	BCR	C39-C30-C25	-2.63	106.03	110.30
22	7	305	BCR	C11-C10-C9	-2.63	123.56	127.31
19	1	5008	CLA	C11-C12-C13	-2.63	107.42	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	858	BCR	C23-C24-C25	-2.63	119.82	127.20
19	A	827	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
19	5	311	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
19	1	5010	CLA	CMA-C3A-C4A	2.63	118.84	111.77
19	4	311	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
19	6	313	CLA	C2D-C1D-ND	2.63	112.04	110.10
19	K	203	CLA	C1D-ND-C4D	-2.63	104.47	106.33
24	1	5002	LMT	C1B-O1B-C4'	-2.63	111.46	117.96
32	6	316	CHL	C3C-C4C-NC	-2.63	107.62	110.57
19	B	804	CLA	C1-C2-C3	-2.63	121.50	126.04
19	A	835	CLA	CMA-C3A-C4A	2.63	118.83	111.77
19	B	819	CLA	CMA-C3A-C4A	2.63	118.83	111.77
22	A	858	BCR	C11-C10-C9	-2.63	123.56	127.31
19	A	831	CLA	CMA-C3A-C4A	2.63	118.83	111.77
19	1	5006	CLA	CMB-C2B-C3B	2.62	129.59	124.68
19	A	804	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
32	7	314	CHL	C2C-C3C-C4C	2.62	108.36	106.49
27	F	304	RRX	C8-C7-C6	-2.62	119.84	127.20
19	6	314	CLA	C1-C2-C3	-2.62	121.51	126.04
32	6	317	CHL	CHC-C1C-NC	2.62	128.18	124.20
19	A	806	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
19	G	1601	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
19	6	314	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
19	4	306	CLA	C1-O2A-CGA	2.62	123.32	116.44
19	4	311	CLA	CMD-C2D-C3D	-2.62	121.58	127.61
19	7	309	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
19	7	312	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
19	3	5015	CLA	C1D-ND-C4D	-2.62	104.47	106.33
19	7	316	CLA	C1D-ND-C4D	-2.62	104.47	106.33
19	A	835	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
19	A	841	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
19	3	5012	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
22	A	848	BCR	C35-C13-C14	-2.62	119.25	122.92
19	5	310	CLA	C6-C5-C3	-2.62	106.58	113.45
19	8	309	CLA	C2C-C1C-NC	2.62	112.42	109.97
19	A	821	CLA	C1D-ND-C4D	-2.62	104.47	106.33
19	7	306	CLA	C1D-ND-C4D	-2.62	104.47	106.33
19	B	823	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
32	8	301	CHL	CHD-C4C-C3C	2.62	128.69	124.84
19	4	310	CLA	C2D-C1D-ND	2.62	112.03	110.10
19	3	5018	CLA	CMA-C3A-C4A	2.62	118.81	111.77
19	A	820	CLA	C1C-C2C-C3C	-2.62	104.20	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	307	CLA	CMD-C2D-C3D	-2.62	121.59	127.61
19	4	306	CLA	C1D-ND-C4D	-2.62	104.48	106.33
31	6	305	LUT	C11-C12-C13	-2.62	119.06	126.42
32	8	316	CHL	C1-O2A-CGA	2.62	123.31	116.44
19	8	312	CLA	CMB-C2B-C3B	2.62	129.57	124.68
19	3	5020	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
19	5	314	CLA	C1-C2-C3	-2.62	121.52	126.04
19	B	817	CLA	C1-C2-C3	-2.61	121.52	126.04
31	6	305	LUT	C8-C7-C6	-2.61	119.86	127.20
19	6	301	CLA	O2A-CGA-CBA	2.61	120.11	111.91
22	A	859	BCR	C16-C15-C14	-2.61	118.12	123.47
19	B	834	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
19	B	829	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
19	5	325	CLA	CHA-C4D-ND	2.61	137.96	132.50
19	Z	305	CLA	CMA-C3A-C4A	2.61	118.79	111.77
19	B	820	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	3	5003	LUT	C39-C29-C30	-2.61	119.26	122.92
19	B	809	CLA	C1D-ND-C4D	-2.61	104.48	106.33
19	A	825	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
19	1	5011	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
22	A	847	BCR	C36-C18-C17	-2.61	119.27	122.92
28	J	1902	C7Z	C11-C12-C13	-2.61	119.08	126.42
19	3	5014	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
32	5	320	CHL	CMA-C3A-C4A	2.61	118.79	111.77
19	6	318	CLA	CMA-C3A-C4A	2.61	118.79	111.77
19	7	308	CLA	C6-C5-C3	-2.61	106.61	113.45
19	5	317	CLA	C2C-C1C-NC	2.61	112.42	109.97
19	1	5008	CLA	C2D-C1D-ND	2.61	112.03	110.10
19	B	817	CLA	C2C-C1C-NC	2.61	112.41	109.97
19	B	814	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
19	1	5007	CLA	C1D-ND-C4D	-2.61	104.48	106.33
19	7	313	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
22	F	302	BCR	C33-C5-C4	2.61	118.62	113.62
19	A	832	CLA	C1D-ND-C4D	-2.60	104.48	106.33
19	Z	311	CLA	C1D-ND-C4D	-2.60	104.48	106.33
19	5	317	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
19	A	814	CLA	O2A-CGA-CBA	2.60	120.08	111.91
27	4	303	RRX	C33-C5-C4	2.60	118.62	113.62
19	Z	314	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
19	7	308	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
32	4	314	CHL	CHD-C4C-C3C	2.60	128.66	124.84
19	B	826	CLA	C1C-C2C-C3C	-2.60	104.22	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	5013	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
19	7	306	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
19	G	1601	CLA	CMA-C3A-C4A	2.60	118.76	111.77
19	B	850	CLA	CHA-C4D-ND	2.60	137.94	132.50
19	5	307	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
29	J	1904	LMG	O8-C28-C29	2.60	120.06	111.91
29	7	301	LMG	C8-O7-C10	-2.60	111.39	117.79
19	7	316	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
19	Z	307	CLA	CHA-C4D-ND	2.60	137.93	132.50
19	6	301	CLA	C1-C2-C3	-2.60	121.55	126.04
32	4	317	CHL	C4D-CHA-C1A	2.60	124.41	121.25
19	4	308	CLA	C1D-ND-C4D	-2.60	104.49	106.33
19	3	5015	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
19	J	1901	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
19	5	319	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
32	8	319	CHL	C1B-CHB-C4A	-2.59	124.98	130.12
19	B	824	CLA	C1D-ND-C4D	-2.59	104.49	106.33
22	A	848	BCR	C11-C12-C13	-2.59	119.13	126.42
38	8	325	ERG	C18-C13-C17	-2.59	106.88	111.71
19	Z	312	CLA	C6-C5-C3	-2.59	106.66	113.45
19	3	5010	CLA	C1D-ND-C4D	-2.59	104.49	106.33
19	4	310	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
19	3	5018	CLA	O2A-CGA-CBA	2.59	120.04	111.91
22	A	846	BCR	C7-C8-C9	-2.59	122.32	126.23
23	4	320	LHG	O8-C23-C24	2.59	120.04	111.91
19	6	301	CLA	CHA-C4D-ND	2.59	137.92	132.50
19	1	5011	CLA	C2D-C1D-ND	2.59	112.01	110.10
22	B	844	BCR	C15-C16-C17	-2.59	118.17	123.47
31	1	5003	LUT	C39-C29-C28	2.59	122.16	118.08
19	Z	312	CLA	C1D-ND-C4D	-2.59	104.50	106.33
31	Z	317	LUT	C15-C35-C34	2.59	128.78	123.47
27	F	304	RRX	C23-C24-C25	-2.59	119.93	127.20
19	A	837	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
19	5	308	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
19	1	5006	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
19	B	812	CLA	C1-C2-C3	-2.59	121.57	126.04
22	7	305	BCR	C8-C7-C6	-2.59	119.94	127.20
19	5	321	CLA	C1-C2-C3	-2.59	121.57	126.04
19	5	319	CLA	C1-O2A-CGA	2.59	123.23	116.44
19	A	803	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
19	Z	305	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
19	8	308	CLA	CMA-C3A-C4A	2.59	118.72	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	312	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	8	304	LUT	C38-C25-C24	-2.58	118.03	123.56
19	A	817	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
23	8	321	LHG	O8-C23-C24	2.58	120.02	111.91
38	6	326	ERG	C18-C13-C17	-2.58	106.90	111.71
19	B	803	CLA	C1D-ND-C4D	-2.58	104.50	106.33
19	B	804	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
19	1	5015	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	8	304	LUT	C7-C8-C9	-2.58	122.33	126.23
19	7	306	CLA	CMA-C3A-C4A	2.58	118.71	111.77
31	Z	318	LUT	C31-C30-C29	-2.58	123.62	127.31
19	5	312	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
19	Z	311	CLA	CHA-C4D-ND	2.58	137.90	132.50
19	B	804	CLA	O2A-CGA-CBA	2.58	120.01	111.91
31	6	306	LUT	C18-C5-C4	2.58	119.14	114.36
19	5	311	CLA	O2A-CGA-CBA	2.58	120.01	111.91
23	1	5019	LHG	C5-O7-C7	-2.58	111.44	117.79
19	A	826	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
19	A	815	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
19	A	830	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
19	4	308	CLA	CHA-C4D-ND	2.58	137.90	132.50
19	6	309	CLA	C1-C2-C3	-2.58	121.58	126.04
19	4	309	CLA	O2A-CGA-CBA	2.58	120.00	111.91
19	K	202	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
19	4	313	CLA	CMA-C3A-C4A	2.58	118.70	111.77
19	A	815	CLA	C1-O2A-CGA	2.58	123.21	116.44
24	A	855	LMT	C1B-O1B-C4'	-2.58	111.58	117.96
19	1	5008	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
31	6	306	LUT	C22-C23-C24	2.58	114.67	111.74
19	A	815	CLA	C1D-ND-C4D	-2.58	104.50	106.33
19	K	202	CLA	C1D-ND-C4D	-2.58	104.50	106.33
32	8	316	CHL	C2C-C3C-C4C	2.58	108.33	106.49
19	5	313	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
19	B	806	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
19	3	5015	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
19	B	822	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
22	F	302	BCR	C15-C14-C13	-2.57	123.64	127.31
31	7	304	LUT	C39-C29-C30	-2.57	119.32	122.92
32	7	315	CHL	C4A-NA-C1A	2.57	107.86	106.71
19	3	5009	CLA	C1D-ND-C4D	-2.57	104.51	106.33
19	B	816	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
18	A	801	CL0	O2D-CGD-O1D	-2.57	118.81	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	320	CLA	C1D-ND-C4D	-2.57	104.51	106.33
19	6	323	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
19	B	812	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
19	6	314	CLA	O2A-CGA-CBA	2.57	119.97	111.91
19	5	322	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
19	Z	315	CLA	CMA-C3A-C4A	2.57	118.67	111.77
23	5	323	LHG	C5-O7-C7	-2.57	111.47	117.79
19	A	834	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
19	B	819	CLA	C1D-ND-C4D	-2.56	104.51	106.33
19	B	830	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
19	8	313	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
19	A	839	CLA	CMA-C3A-C4A	2.56	118.66	111.77
19	B	828	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
19	A	813	CLA	CHA-C4D-ND	2.56	137.86	132.50
31	1	5003	LUT	C18-C5-C4	2.56	119.10	114.36
27	4	303	RRX	C30-C29-C28	-2.56	107.86	113.64
19	8	320	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
23	A	852	LHG	C5-O7-C7	-2.56	111.48	117.79
19	6	302	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
19	A	819	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
27	F	304	RRX	C34-C9-C10	-2.56	119.34	122.92
22	5	305	BCR	C36-C18-C19	2.56	122.11	118.08
19	F	301	CLA	CHA-C4D-ND	2.56	137.85	132.50
19	7	313	CLA	CHD-C1D-ND	-2.56	122.10	124.45
22	7	305	BCR	C37-C22-C21	-2.56	119.34	122.92
19	B	811	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
32	1	5014	CHL	C1B-CHB-C4A	-2.56	125.05	130.12
19	7	324	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
19	Z	307	CLA	C1-C2-C3	-2.55	121.62	126.04
19	5	301	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
19	5	313	CLA	CMA-C3A-C4A	2.55	118.64	111.77
19	A	825	CLA	C1D-ND-C4D	-2.55	104.52	106.33
19	1	5006	CLA	C2C-C1C-NC	2.55	112.36	109.97
19	A	811	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
19	6	311	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
19	1	5011	CLA	CHA-C4D-ND	2.55	137.84	132.50
19	6	313	CLA	CHA-C4D-ND	2.55	137.84	132.50
19	5	313	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
19	4	310	CLA	C1D-ND-C4D	-2.55	104.52	106.33
19	B	804	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
19	7	312	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
19	8	311	CLA	C1D-ND-C4D	-2.55	104.52	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	850	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
19	3	5009	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
19	4	311	CLA	O2A-CGA-CBA	2.55	119.91	111.91
19	4	311	CLA	CHA-C4D-ND	2.55	137.83	132.50
19	3	5008	CLA	CHA-C4D-ND	2.55	137.83	132.50
22	B	843	BCR	C34-C9-C10	-2.55	119.35	122.92
19	8	307	CLA	CMA-C3A-C4A	2.55	118.62	111.77
19	1	5018	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
19	7	318	CLA	CHA-C4D-ND	2.55	137.83	132.50
32	6	317	CHL	CMA-C3A-C4A	2.55	118.62	111.77
19	B	812	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
22	8	306	BCR	C2-C1-C6	2.55	114.40	110.48
19	F	301	CLA	CMA-C3A-C4A	2.55	118.61	111.77
19	B	810	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
19	3	5020	CLA	CMA-C3A-C4A	2.54	118.61	111.77
19	5	322	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
32	8	315	CHL	C4D-CHA-C1A	2.54	124.34	121.25
23	8	321	LHG	C5-O7-C7	-2.54	111.53	117.79
19	Z	308	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
32	4	317	CHL	C1B-CHB-C4A	-2.54	125.08	130.12
19	B	805	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
19	Z	305	CLA	C2C-C1C-NC	2.54	112.35	109.97
19	A	814	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
19	A	829	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
19	A	811	CLA	O2A-CGA-CBA	2.54	119.88	111.91
20	A	844	PQN	C2M-C2-C3	-2.54	120.25	124.40
19	3	5011	CLA	C2C-C1C-NC	2.54	112.35	109.97
19	B	833	CLA	CMA-C3A-C4A	2.54	118.60	111.77
22	B	842	BCR	C35-C13-C14	-2.54	119.36	122.92
19	A	805	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
32	6	321	CHL	CHD-C4C-C3C	2.54	128.57	124.84
19	5	321	CLA	O2A-CGA-CBA	2.54	119.88	111.91
19	1	5013	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
19	6	309	CLA	C2D-C1D-ND	2.54	111.97	110.10
19	1	5015	CLA	CHA-C4D-ND	2.54	137.81	132.50
19	6	309	CLA	CHA-C4D-ND	2.54	137.81	132.50
19	B	827	CLA	C1-C2-C3	-2.54	121.65	126.04
22	7	305	BCR	C1-C6-C7	2.54	122.96	115.78
19	6	312	CLA	C1-C2-C3	-2.54	121.66	126.04
32	6	317	CHL	CHB-C4A-NA	2.54	128.02	124.51
31	4	304	LUT	C7-C6-C5	-2.54	115.32	121.46
19	A	806	CLA	O2A-CGA-CBA	2.54	119.86	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	813	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
19	B	805	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
31	1	5004	LUT	C30-C31-C32	-2.53	115.31	123.22
31	1	5003	LUT	C38-C25-C24	-2.53	118.14	123.56
19	B	824	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
22	3	5006	BCR	C20-C19-C18	-2.53	119.31	126.42
19	1	5006	CLA	O2A-CGA-CBA	2.53	119.85	111.91
34	6	325	3PH	O31-C31-C32	2.53	119.84	111.91
22	G	1603	BCR	C20-C19-C18	-2.53	119.31	126.42
32	3	5017	CHL	C4A-NA-C1A	2.53	107.84	106.71
32	8	317	CHL	C4D-CHA-C1A	2.53	124.33	121.25
19	6	322	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
19	A	802	CLA	CMA-C3A-C4A	2.53	118.56	111.77
19	8	314	CLA	CAA-C2A-C3A	-2.53	105.86	112.78
19	5	310	CLA	CBA-CAA-C2A	-2.53	106.41	113.86
22	B	845	BCR	C8-C7-C6	-2.53	120.11	127.20
19	B	818	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
22	B	847	BCR	C15-C16-C17	-2.52	118.30	123.47
19	6	312	CLA	C2D-C1D-ND	2.52	111.96	110.10
19	B	825	CLA	C1-O2A-CGA	2.52	123.06	116.44
22	3	5005	BCR	C34-C9-C10	-2.52	119.39	122.92
19	B	825	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
31	6	305	LUT	C18-C5-C4	2.52	119.02	114.36
19	7	311	CLA	CMA-C3A-C4A	2.52	118.54	111.77
19	3	5009	CLA	CHA-C4D-ND	2.52	137.77	132.50
32	1	5009	CHL	C1-O2A-CGA	2.52	123.05	116.44
23	7	320	LHG	O7-C7-O9	-2.52	117.62	123.70
19	1	5010	CLA	CHA-C4D-ND	2.52	137.76	132.50
19	A	809	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
19	4	313	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
28	6	304	C7Z	C28-C27-C26	-2.51	120.14	127.20
19	Z	315	CLA	CAA-C2A-C3A	-2.51	105.89	112.78
19	7	311	CLA	C2D-C1D-ND	2.51	111.96	110.10
22	5	305	BCR	C8-C9-C10	2.51	122.80	118.94
19	A	830	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
19	Z	306	CLA	O2A-CGA-CBA	2.51	119.79	111.91
19	5	317	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
19	Z	304	CLA	CHA-C4D-ND	2.51	137.75	132.50
19	B	835	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
19	6	310	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
22	K	206	BCR	C20-C19-C18	-2.51	119.36	126.42
19	B	821	CLA	C1C-C2C-C3C	-2.51	104.32	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	824	CLA	CHA-C4D-ND	2.51	137.75	132.50
32	8	317	CHL	CHD-C4C-C3C	2.51	128.53	124.84
19	8	307	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
19	Z	307	CLA	CMA-C3A-C4A	2.51	118.51	111.77
24	8	323	LMT	C1B-O5B-C5B	-2.51	108.77	113.69
19	6	312	CLA	CMA-C3A-C4A	2.51	118.51	111.77
28	1	5005	C7Z	C1-C6-C5	-2.51	119.08	122.61
19	8	314	CLA	C1D-ND-C4D	-2.51	104.55	106.33
19	7	306	CLA	CAA-C2A-C3A	-2.51	105.92	112.78
19	A	838	CLA	O2A-CGA-CBA	2.51	119.77	111.91
28	1	5005	C7Z	C18-C5-C4	2.51	119.00	114.36
32	6	319	CHL	C4D-CHA-C1A	2.50	124.30	121.25
32	8	319	CHL	CHB-C4A-NA	2.50	127.97	124.51
19	A	802	CLA	CHA-C4D-ND	2.50	137.74	132.50
31	1	5003	LUT	C15-C35-C34	-2.50	118.35	123.47
22	8	303	BCR	C23-C24-C25	-2.50	120.18	127.20
18	A	801	CL0	C3D-C4D-ND	2.50	114.28	110.24
19	5	317	CLA	C1-C2-C3	-2.50	121.72	126.04
19	Z	305	CLA	CAA-CBA-CGA	-2.50	105.95	113.25
19	4	312	CLA	O2A-CGA-CBA	2.50	119.75	111.91
19	6	310	CLA	C2C-C1C-NC	2.50	112.31	109.97
19	8	310	CLA	CHA-C1A-NA	-2.50	120.67	126.40
19	5	313	CLA	CAA-CBA-CGA	-2.50	105.87	112.51
19	A	843	CLA	CHA-C4D-ND	2.50	137.73	132.50
19	Z	311	CLA	CMA-C3A-C4A	2.50	118.49	111.77
19	B	832	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
22	8	306	BCR	C15-C16-C17	-2.50	118.36	123.47
19	3	5010	CLA	CHA-C4D-ND	2.50	137.73	132.50
19	8	307	CLA	CHA-C4D-ND	2.50	137.73	132.50
32	4	319	CHL	CHC-C1C-NC	2.50	127.99	124.20
19	4	308	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
19	5	308	CLA	CHA-C4D-ND	2.50	137.72	132.50
34	8	322	3PH	O31-C31-C32	2.50	119.74	111.91
19	B	802	CLA	CHA-C4D-ND	2.50	137.72	132.50
32	4	315	CHL	CMA-C3A-C4A	2.50	118.48	111.77
19	8	309	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
19	8	310	CLA	CHA-C4D-ND	2.49	137.72	132.50
19	5	311	CLA	CAA-CBA-CGA	-2.49	105.96	113.25
22	B	844	BCR	C11-C10-C9	-2.49	123.75	127.31
19	A	802	CLA	C1-C2-C3	-2.49	121.73	126.04
19	1	5007	CLA	CMA-C3A-C4A	2.49	118.48	111.77
22	B	846	BCR	C23-C24-C25	-2.49	120.20	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	815	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
32	8	317	CHL	CHB-C4A-NA	2.49	127.96	124.51
19	3	5010	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
19	7	324	CLA	C1D-ND-C4D	-2.49	104.56	106.33
19	4	316	CLA	C1D-ND-C4D	-2.49	104.56	106.33
33	7	321	SPH	C3-C4-C5	-2.49	119.23	124.79
19	6	302	CLA	CHA-C4D-ND	2.49	137.71	132.50
19	7	307	CLA	C1D-ND-C4D	-2.49	104.57	106.33
22	8	303	BCR	C34-C9-C10	-2.49	119.44	122.92
32	7	315	CHL	C1B-CHB-C4A	-2.49	125.19	130.12
38	8	325	ERG	C24-C23-C22	-2.49	117.94	125.67
22	3	5006	BCR	C16-C15-C14	-2.49	118.38	123.47
19	A	803	CLA	O2A-CGA-CBA	2.49	119.71	111.91
19	B	803	CLA	CHA-C4D-ND	2.49	137.70	132.50
19	4	308	CLA	O2A-CGA-CBA	2.49	119.71	111.91
19	5	306	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
31	1	5004	LUT	C15-C35-C34	-2.48	118.38	123.47
19	5	325	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
19	5	314	CLA	C1C-C2C-C3C	-2.48	104.34	106.96
19	A	810	CLA	C1D-ND-C4D	-2.48	104.57	106.33
19	4	313	CLA	O2A-CGA-CBA	2.48	119.70	111.91
19	5	312	CLA	O2A-CGA-CBA	2.48	119.70	111.91
19	3	5015	CLA	CMB-C2B-C3B	2.48	129.32	124.68
19	8	309	CLA	CHA-C4D-ND	2.48	137.69	132.50
19	Z	311	CLA	CMD-C2D-C3D	-2.48	121.91	127.61
19	Z	312	CLA	CAA-CBA-CGA	-2.48	106.00	113.25
19	B	826	CLA	CHA-C4D-ND	2.48	137.69	132.50
19	B	813	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
22	K	206	BCR	C23-C24-C25	-2.48	120.24	127.20
19	5	317	CLA	CMA-C3A-C4A	2.48	118.44	111.77
19	6	318	CLA	O2A-CGA-CBA	2.48	119.69	111.91
19	3	5010	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
18	A	801	CL0	CMB-C2B-C3B	2.48	129.31	124.68
19	6	320	CLA	O1D-CGD-CBD	-2.48	119.41	124.48
19	B	829	CLA	CHA-C4D-ND	2.48	137.68	132.50
19	K	205	CLA	CHA-C4D-ND	2.48	137.68	132.50
18	A	801	CL0	CAA-C2A-C3A	-2.48	105.99	112.78
31	Z	318	LUT	C8-C7-C6	-2.48	120.25	127.20
19	5	314	CLA	O2A-CGA-CBA	2.48	119.68	111.91
27	4	303	RRX	C38-C26-C27	2.48	118.94	114.36
19	Z	315	CLA	C6-C5-C3	-2.48	106.97	113.45
31	1	5003	LUT	C19-C9-C8	2.47	121.98	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	301	LMT	C4B-C3B-C2B	-2.47	106.50	110.82
19	B	827	CLA	CHA-C4D-ND	2.47	137.67	132.50
27	F	304	RRX	C1-C6-C5	-2.47	119.13	122.61
19	A	834	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
19	B	811	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
19	B	815	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
19	B	807	CLA	O2A-CGA-CBA	2.47	119.67	111.91
19	1	5013	CLA	O2A-CGA-CBA	2.47	119.67	111.91
31	4	304	LUT	C30-C31-C32	-2.47	115.50	123.22
23	5	323	LHG	O8-C23-C24	2.47	119.66	111.91
27	5	302	RRX	C21-C20-C19	-2.47	115.51	123.22
32	4	314	CHL	CHC-C1C-NC	2.47	127.95	124.20
19	1	5010	CLA	C2D-C1D-ND	2.47	111.92	110.10
19	7	310	CLA	CMA-C3A-C4A	2.47	118.41	111.77
35	7	302	DGA	OG1-CA1-CA2	2.47	119.66	111.91
19	1	5011	CLA	CMA-C3A-C4A	2.47	118.41	111.77
19	7	310	CLA	CHA-C4D-ND	2.47	137.66	132.50
19	8	318	CLA	C2D-C1D-ND	2.47	111.92	110.10
19	Z	315	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
19	A	816	CLA	C1D-ND-C4D	-2.47	104.58	106.33
19	B	804	CLA	C1D-ND-C4D	-2.47	104.58	106.33
22	3	5005	BCR	C20-C19-C18	-2.47	119.49	126.42
19	8	311	CLA	CMA-C3A-C4A	2.47	118.40	111.77
19	7	316	CLA	CHA-C4D-ND	2.46	137.65	132.50
19	G	1602	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
19	3	5012	CLA	CMA-C3A-C4A	2.46	118.39	111.77
19	G	1602	CLA	CHA-C4D-ND	2.46	137.65	132.50
32	5	316	CHL	CHC-C1C-NC	2.46	127.94	124.20
32	1	5009	CHL	C4D-CHA-C1A	2.46	124.25	121.25
19	6	310	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
19	B	808	CLA	CHA-C4D-ND	2.46	137.65	132.50
32	6	315	CHL	CMA-C3A-C4A	2.46	118.39	111.77
19	A	821	CLA	CHA-C4D-ND	2.46	137.65	132.50
19	8	314	CLA	CHA-C4D-ND	2.46	137.65	132.50
19	8	318	CLA	CHA-C4D-ND	2.46	137.65	132.50
19	5	308	CLA	CMD-C2D-C3D	-2.46	121.95	127.61
19	Z	305	CLA	CMB-C2B-C3B	2.46	129.28	124.68
19	7	310	CLA	CMD-C2D-C3D	-2.46	121.96	127.61
19	3	5012	CLA	CHA-C4D-ND	2.46	137.64	132.50
19	4	313	CLA	CHA-C4D-ND	2.46	137.64	132.50
31	8	304	LUT	C18-C5-C4	2.46	118.91	114.36
19	A	841	CLA	CHA-C4D-ND	2.46	137.64	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	313	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
19	6	318	CLA	CHA-C4D-ND	2.46	137.64	132.50
19	A	818	CLA	CHA-C4D-ND	2.46	137.64	132.50
19	A	818	CLA	O2A-CGA-CBA	2.46	119.61	111.91
19	8	312	CLA	C3B-C4B-NB	-2.46	106.04	109.21
19	A	839	CLA	CHA-C4D-ND	2.45	137.63	132.50
19	B	840	CLA	CHA-C4D-ND	2.45	137.63	132.50
19	A	826	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	Z	317	LUT	C19-C9-C10	-2.45	119.49	122.92
19	4	311	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
19	4	307	CLA	O2A-CGA-CBA	2.45	119.60	111.91
19	B	802	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
19	B	812	CLA	CHA-C4D-ND	2.45	137.63	132.50
19	B	835	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
19	B	838	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
19	5	308	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
32	7	314	CHL	C4D-CHA-C1A	2.45	124.23	121.25
27	4	303	RRX	C35-C13-C12	2.45	121.94	118.08
19	4	308	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
19	B	836	CLA	CHA-C4D-ND	2.45	137.62	132.50
19	A	810	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
19	A	808	CLA	CHA-C4D-ND	2.45	137.62	132.50
19	K	203	CLA	CHA-C4D-ND	2.45	137.62	132.50
19	5	306	CLA	O2A-CGA-CBA	2.45	119.59	111.91
19	Z	307	CLA	C2D-C1D-ND	2.45	111.91	110.10
31	7	304	LUT	C40-C33-C34	-2.45	119.49	122.92
19	A	835	CLA	O2A-CGA-CBA	2.45	119.59	111.91
31	7	303	LUT	C20-C13-C12	2.45	121.93	118.08
19	6	320	CLA	CMA-C3A-C4A	2.45	118.35	111.77
32	6	316	CHL	CMA-C3A-C4A	2.45	118.35	111.77
31	Z	318	LUT	C30-C31-C32	-2.45	115.58	123.22
19	1	5011	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
19	A	832	CLA	CHA-C4D-ND	2.45	137.61	132.50
24	8	324	LMT	C1B-O1B-C4'	-2.45	111.91	117.96
19	A	857	CLA	CHA-C4D-ND	2.44	137.61	132.50
19	5	312	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
19	7	309	CLA	CHA-C4D-ND	2.44	137.61	132.50
24	4	321	LMT	C1B-O1B-C4'	-2.44	111.92	117.96
19	7	317	CLA	CMA-C3A-C4A	2.44	118.34	111.77
23	6	324	LHG	O8-C23-O10	-2.44	117.43	123.59
19	5	308	CLA	C1-C2-C3	-2.44	121.82	126.04
19	1	5013	CLA	CHA-C4D-ND	2.44	137.61	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	8	309	CLA	O2A-CGA-CBA	2.44	119.57	111.91
19	7	324	CLA	CMA-C3A-C4A	2.44	118.34	111.77
31	3	5002	LUT	C8-C7-C6	-2.44	120.34	127.20
24	Z	319	LMT	C1B-O1B-C4'	-2.44	111.92	117.96
19	I	201	CLA	CHA-C4D-ND	2.44	137.61	132.50
19	A	813	CLA	O2A-CGA-CBA	2.44	119.57	111.91
19	7	307	CLA	CHA-C4D-ND	2.44	137.60	132.50
19	6	312	CLA	CHA-C4D-ND	2.44	137.60	132.50
19	A	816	CLA	CHA-C4D-ND	2.44	137.60	132.50
19	A	813	CLA	C1D-ND-C4D	-2.44	104.60	106.33
32	Z	310	CHL	C1B-CHB-C4A	-2.44	125.29	130.12
19	6	322	CLA	C2C-C1C-NC	2.44	112.26	109.97
19	G	1601	CLA	CHA-C4D-ND	2.44	137.60	132.50
19	5	310	CLA	C2C-C1C-NC	2.44	112.26	109.97
19	A	827	CLA	CHA-C4D-ND	2.44	137.60	132.50
19	K	202	CLA	CHA-C4D-ND	2.44	137.60	132.50
19	5	322	CLA	CHA-C4D-ND	2.44	137.60	132.50
19	A	806	CLA	CHA-C4D-ND	2.44	137.60	132.50
19	4	318	CLA	CHA-C4D-ND	2.44	137.60	132.50
22	6	307	BCR	C1-C6-C5	-2.44	119.18	122.61
19	7	311	CLA	C1D-ND-C4D	-2.44	104.60	106.33
19	Z	303	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	8	305	LUT	C18-C5-C4	2.44	118.87	114.36
19	B	822	CLA	CHA-C4D-ND	2.44	137.59	132.50
31	8	304	LUT	C8-C9-C10	2.44	122.68	118.94
19	A	823	CLA	CHA-C4D-ND	2.44	137.59	132.50
32	6	321	CHL	C2C-C3C-C4C	2.44	108.22	106.49
19	1	5008	CLA	CHA-C4D-ND	2.43	137.59	132.50
19	B	833	CLA	CHA-C4D-ND	2.43	137.59	132.50
32	5	315	CHL	C2C-C3C-C4C	2.43	108.22	106.49
19	1	5012	CLA	C1-C2-C3	-2.43	121.84	126.04
19	5	314	CLA	C1D-ND-C4D	-2.43	104.61	106.33
19	A	830	CLA	CHA-C4D-ND	2.43	137.59	132.50
19	Z	315	CLA	CHA-C4D-ND	2.43	137.59	132.50
19	4	307	CLA	CHA-C4D-ND	2.43	137.59	132.50
19	A	833	CLA	CHA-C4D-ND	2.43	137.59	132.50
19	B	814	CLA	CHA-C4D-ND	2.43	137.59	132.50
32	6	321	CHL	CMA-C3A-C2A	2.43	123.64	113.83
19	B	810	CLA	CHA-C4D-ND	2.43	137.58	132.50
19	A	810	CLA	CHA-C4D-ND	2.43	137.58	132.50
19	A	820	CLA	CHA-C4D-ND	2.43	137.58	132.50
19	6	311	CLA	CHA-C4D-ND	2.43	137.58	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	307	BCR	C15-C16-C17	-2.43	118.50	123.47
19	B	821	CLA	CHA-C4D-ND	2.43	137.58	132.50
19	7	313	CLA	C1D-ND-C4D	-2.43	104.61	106.33
19	A	812	CLA	CHA-C4D-ND	2.43	137.58	132.50
19	B	805	CLA	CHA-C4D-ND	2.43	137.58	132.50
19	B	801	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
19	7	306	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
19	6	314	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
19	8	311	CLA	C16-C15-C13	-2.43	108.07	115.92
19	8	308	CLA	CHA-C4D-ND	2.43	137.58	132.50
19	5	313	CLA	C1D-ND-C4D	-2.43	104.61	106.33
19	B	801	CLA	CHA-C4D-ND	2.43	137.57	132.50
32	6	319	CHL	CMA-C3A-C4A	2.43	118.29	111.77
19	3	5016	CLA	CHA-C4D-ND	2.43	137.57	132.50
19	5	306	CLA	CHA-C4D-ND	2.43	137.57	132.50
32	Z	302	CHL	C1B-CHB-C4A	-2.42	125.31	130.12
28	1	5005	C7Z	C10-C11-C12	-2.42	115.65	123.22
19	K	205	CLA	CMD-C2D-C3D	-2.42	122.04	127.61
19	7	313	CLA	CHA-C4D-ND	2.42	137.57	132.50
19	1	5008	CLA	C11-C10-C8	-2.42	108.08	115.92
19	K	204	CLA	CHA-C4D-ND	2.42	137.57	132.50
19	7	312	CLA	CHA-C4D-ND	2.42	137.57	132.50
19	5	308	CLA	C2C-C1C-NC	2.42	112.24	109.97
28	1	5005	C7Z	C40-C33-C34	-2.42	119.53	122.92
19	1	5010	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
19	A	805	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
19	Z	303	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
22	A	847	BCR	C1-C6-C5	-2.42	119.20	122.61
19	5	310	CLA	CHA-C4D-ND	2.42	137.57	132.50
19	B	820	CLA	CHA-C4D-ND	2.42	137.56	132.50
19	J	1901	CLA	CHA-C4D-ND	2.42	137.56	132.50
19	Z	312	CLA	CHA-C4D-ND	2.42	137.56	132.50
19	1	5013	CLA	C2C-C1C-NC	2.42	112.24	109.97
19	B	817	CLA	CHA-C4D-ND	2.42	137.56	132.50
19	A	825	CLA	CHA-C4D-ND	2.42	137.56	132.50
22	A	858	BCR	C1-C6-C7	2.42	122.62	115.78
19	5	309	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
19	Z	314	CLA	CHA-C4D-ND	2.42	137.56	132.50
19	7	306	CLA	C2C-C1C-NC	2.42	112.24	109.97
22	B	847	BCR	C34-C9-C8	2.42	121.89	118.08
19	K	202	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
19	A	807	CLA	CHA-C4D-ND	2.42	137.56	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	6	321	CHL	CHC-C1C-NC	2.42	127.87	124.20
19	A	804	CLA	CHA-C4D-ND	2.42	137.55	132.50
32	8	315	CHL	CHB-C4A-NA	2.42	127.85	124.51
22	B	846	BCR	C1-C6-C7	2.42	122.61	115.78
19	4	316	CLA	CHA-C4D-ND	2.42	137.55	132.50
19	B	818	CLA	CHA-C4D-ND	2.41	137.55	132.50
19	B	835	CLA	CHA-C4D-ND	2.41	137.55	132.50
19	3	5015	CLA	CHA-C4D-ND	2.41	137.55	132.50
32	6	319	CHL	C1B-CHB-C4A	-2.41	125.34	130.12
19	A	803	CLA	CHA-C4D-ND	2.41	137.55	132.50
19	B	815	CLA	CHA-C4D-ND	2.41	137.55	132.50
19	8	320	CLA	CHA-C4D-ND	2.41	137.55	132.50
19	3	5011	CLA	CHA-C4D-ND	2.41	137.55	132.50
23	7	320	LHG	O8-C23-O10	-2.41	117.50	123.59
19	A	820	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
19	A	838	CLA	CHA-C4D-ND	2.41	137.54	132.50
19	3	5020	CLA	CHA-C4D-ND	2.41	137.54	132.50
19	1	5006	CLA	C1-O2A-CGA	2.41	122.77	116.44
19	Z	305	CLA	C16-C15-C13	-2.41	108.13	115.92
19	A	828	CLA	CHA-C4D-ND	2.41	137.54	132.50
19	1	5015	CLA	O2A-CGA-CBA	2.41	119.47	111.91
19	A	811	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
31	4	304	LUT	C31-C30-C29	-2.41	123.87	127.31
19	4	309	CLA	O1D-CGD-CBD	-2.41	119.56	124.48
28	1	5005	C7Z	C28-C27-C26	-2.41	120.44	127.20
19	1	5008	CLA	O2A-CGA-CBA	2.41	119.47	111.91
19	B	822	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
19	Z	315	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
19	7	318	CLA	CMB-C2B-C3B	2.41	129.18	124.68
22	G	1603	BCR	C16-C15-C14	-2.41	118.55	123.47
19	A	824	CLA	CHA-C4D-ND	2.41	137.53	132.50
19	B	804	CLA	CHA-C4D-ND	2.41	137.53	132.50
19	B	813	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
19	5	319	CLA	CHA-C4D-ND	2.41	137.53	132.50
19	5	301	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
19	B	819	CLA	CHA-C4D-ND	2.40	137.53	132.50
28	J	1902	C7Z	C19-C9-C10	-2.40	119.56	122.92
19	B	816	CLA	CHA-C4D-ND	2.40	137.53	132.50
19	1	5012	CLA	CHA-C4D-ND	2.40	137.53	132.50
19	A	831	CLA	CHA-C4D-ND	2.40	137.52	132.50
19	B	825	CLA	CMA-C3A-C4A	2.40	118.23	111.77
22	A	850	BCR	C20-C19-C18	-2.40	119.67	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	814	CLA	CHA-C4D-ND	2.40	137.52	132.50
19	8	314	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
19	4	306	CLA	CHA-C4D-ND	2.40	137.52	132.50
31	6	306	LUT	C1-C6-C5	-2.40	119.23	122.61
19	6	311	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
19	A	818	CLA	C1C-C2C-C3C	-2.40	104.43	106.96
19	6	309	CLA	CHA-C1A-NA	-2.40	120.90	126.40
19	F	303	CLA	CHA-C4D-ND	2.40	137.52	132.50
19	A	823	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
19	6	322	CLA	CMD-C2D-C3D	-2.40	122.10	127.61
19	6	323	CLA	CHA-C4D-ND	2.40	137.52	132.50
31	6	305	LUT	C1-C6-C5	-2.40	119.24	122.61
19	3	5019	CLA	CHA-C4D-ND	2.40	137.51	132.50
19	B	832	CLA	CHA-C4D-ND	2.40	137.51	132.50
19	A	809	CLA	O2A-CGA-CBA	2.40	119.43	111.91
19	7	309	CLA	CMA-C3A-C4A	2.40	118.22	111.77
19	A	836	CLA	CHA-C4D-ND	2.40	137.51	132.50
19	5	307	CLA	O2A-CGA-CBA	2.40	119.43	111.91
19	5	321	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
19	4	312	CLA	CHA-C4D-ND	2.39	137.51	132.50
19	A	840	CLA	CHA-C4D-ND	2.39	137.51	132.50
32	4	317	CHL	CHB-C4A-NA	2.39	127.82	124.51
19	8	314	CLA	CMA-C3A-C4A	2.39	118.21	111.77
19	A	837	CLA	CHA-C4D-ND	2.39	137.51	132.50
19	A	842	CLA	CHA-C4D-ND	2.39	137.51	132.50
19	1	5007	CLA	C1C-C2C-C3C	-2.39	104.44	106.96
19	5	309	CLA	C1-O2A-CGA	2.39	122.72	116.44
19	A	809	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
19	B	807	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
22	3	5006	BCR	C8-C7-C6	-2.39	120.48	127.20
22	8	303	BCR	C1-C6-C7	2.39	122.55	115.78
19	A	829	CLA	CHA-C4D-ND	2.39	137.50	132.50
19	5	307	CLA	CHA-C4D-ND	2.39	137.50	132.50
19	7	311	CLA	O2A-CGA-CBA	2.39	119.41	111.91
19	A	839	CLA	CMD-C2D-C3D	-2.39	122.11	127.61
19	B	813	CLA	CHA-C4D-ND	2.39	137.50	132.50
22	B	845	BCR	C34-C9-C10	-2.39	119.57	122.92
19	6	312	CLA	CHA-C1A-NA	-2.39	120.92	126.40
19	A	809	CLA	CHA-C4D-ND	2.39	137.50	132.50
19	A	819	CLA	CMB-C2B-C3B	2.39	129.15	124.68
19	A	803	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
31	7	304	LUT	C37-C21-C26	2.39	113.17	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	818	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
19	Z	314	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
19	B	840	CLA	C1D-ND-C4D	-2.39	104.64	106.33
19	B	809	CLA	CHA-C4D-ND	2.39	137.50	132.50
19	Z	304	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
19	3	5012	CLA	CAA-CBA-CGA	-2.39	106.28	113.25
19	8	313	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	3	5002	LUT	C35-C15-C14	-2.39	118.58	123.47
19	5	321	CLA	CHA-C4D-ND	2.39	137.49	132.50
19	8	308	CLA	O2A-CGA-CBA	2.39	119.40	111.91
19	B	808	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
19	F	303	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
22	6	307	BCR	C34-C9-C10	-2.39	119.58	122.92
19	B	834	CLA	CHA-C4D-ND	2.39	137.49	132.50
19	6	320	CLA	CHA-C4D-ND	2.39	137.49	132.50
19	5	306	CLA	C1-O2A-CGA	2.38	122.70	116.44
19	A	819	CLA	CHA-C4D-ND	2.38	137.49	132.50
19	B	809	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
22	B	843	BCR	C15-C16-C17	-2.38	118.59	123.47
19	5	308	CLA	CMA-C3A-C4A	2.38	118.18	111.77
19	B	837	CLA	CHA-C4D-ND	2.38	137.48	132.50
19	8	311	CLA	CHA-C4D-ND	2.38	137.48	132.50
32	5	315	CHL	C4D-CHA-C1A	2.38	124.15	121.25
19	B	811	CLA	CHA-C4D-ND	2.38	137.48	132.50
32	5	316	CHL	CHB-C4A-NA	2.38	127.81	124.51
23	Z	316	LHG	C6-C5-C4	-2.38	106.15	111.79
19	5	325	CLA	C1D-ND-C4D	-2.38	104.64	106.33
19	1	5018	CLA	CHA-C4D-ND	2.38	137.48	132.50
19	7	309	CLA	CHA-C1A-NA	-2.38	120.94	126.40
19	G	1602	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
32	6	316	CHL	CMA-C3A-C2A	2.38	123.43	113.83
22	3	5006	BCR	C36-C18-C17	-2.38	119.59	122.92
22	B	844	BCR	C8-C9-C10	2.38	122.59	118.94
19	5	309	CLA	CHA-C4D-ND	2.38	137.48	132.50
32	Z	310	CHL	C4D-CHA-C1A	2.38	124.14	121.25
19	6	310	CLA	CHA-C4D-ND	2.38	137.48	132.50
19	5	314	CLA	CHA-C4D-ND	2.38	137.47	132.50
22	B	843	BCR	C11-C12-C13	-2.38	119.73	126.42
19	A	813	CLA	CMA-C3A-C4A	2.38	118.17	111.77
22	5	304	BCR	C38-C26-C27	2.38	118.18	113.62
32	Z	310	CHL	CHC-C1C-NC	2.38	127.81	124.20
27	5	302	RRX	C34-C9-C8	2.38	121.82	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	817	CLA	CHA-C4D-ND	2.38	137.47	132.50
22	B	845	BCR	C35-C13-C14	-2.38	119.59	122.92
19	B	806	CLA	CHA-C4D-ND	2.38	137.47	132.50
19	B	807	CLA	CHA-C4D-ND	2.38	137.47	132.50
19	5	311	CLA	CHA-C4D-ND	2.38	137.47	132.50
32	8	319	CHL	CMA-C3A-C2A	2.38	123.41	113.83
32	8	316	CHL	CHD-C4C-C3C	2.38	128.33	124.84
19	3	5019	CLA	O2D-CGD-O1D	-2.37	119.19	123.84
31	1	5003	LUT	C31-C30-C29	-2.37	123.92	127.31
19	1	5007	CLA	CHA-C4D-ND	2.37	137.47	132.50
19	B	813	CLA	O2A-CGA-CBA	2.37	119.36	111.91
19	3	5020	CLA	CMB-C2B-C3B	2.37	129.12	124.68
19	3	5008	CLA	C1D-ND-C4D	-2.37	104.65	106.33
19	8	318	CLA	C1D-ND-C4D	-2.37	104.65	106.33
19	A	834	CLA	CHA-C4D-ND	2.37	137.46	132.50
22	8	303	BCR	C20-C19-C18	-2.37	119.75	126.42
19	1	5016	CLA	CHA-C4D-ND	2.37	137.46	132.50
19	A	811	CLA	CHA-C4D-ND	2.37	137.46	132.50
19	B	828	CLA	CHA-C4D-ND	2.37	137.46	132.50
19	B	839	CLA	CHA-C4D-ND	2.37	137.46	132.50
19	5	301	CLA	CHA-C4D-ND	2.37	137.46	132.50
19	6	314	CLA	CHA-C4D-ND	2.37	137.46	132.50
22	5	304	BCR	C21-C20-C19	-2.37	115.82	123.22
19	3	5013	CLA	C2D-C1D-ND	2.37	111.85	110.10
19	Z	308	CLA	CMA-C3A-C4A	2.37	118.14	111.77
19	4	309	CLA	CMA-C3A-C4A	2.37	118.14	111.77
19	7	319	CLA	CHA-C4D-ND	2.37	137.46	132.50
19	6	313	CLA	CMA-C3A-C4A	2.37	118.14	111.77
19	4	312	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
19	A	802	CLA	O2A-CGA-CBA	2.37	119.34	111.91
19	6	310	CLA	CMD-C2D-C3D	-2.37	122.17	127.61
19	4	308	CLA	CHA-C1A-NA	-2.37	120.98	126.40
22	B	845	BCR	C11-C12-C13	-2.37	119.77	126.42
19	B	830	CLA	O2A-CGA-CBA	2.37	119.33	111.91
19	3	5010	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
31	8	304	LUT	C22-C23-C24	2.37	114.43	111.74
19	Z	305	CLA	CHA-C4D-ND	2.37	137.45	132.50
19	B	818	CLA	CMB-C2B-C3B	2.37	129.10	124.68
31	7	303	LUT	C10-C11-C12	-2.36	115.84	123.22
32	1	5017	CHL	C1-O2A-CGA	2.36	123.60	116.73
19	5	319	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
19	5	310	CLA	C1-O2A-CGA	2.36	122.64	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	6	319	CHL	C1-O2A-CGA	2.36	122.64	116.44
19	A	842	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
19	B	834	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
19	1	5006	CLA	CMD-C2D-C3D	-2.36	122.18	127.61
19	B	850	CLA	CBA-CAA-C2A	-2.36	106.89	113.86
31	7	304	LUT	C8-C9-C10	2.36	122.56	118.94
27	4	303	RRX	C34-C9-C8	2.36	121.80	118.08
19	B	838	CLA	CHA-C4D-ND	2.36	137.44	132.50
19	B	817	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
19	3	5013	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
31	5	303	LUT	C20-C13-C12	2.36	121.80	118.08
19	A	817	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
27	5	302	RRX	C12-C13-C14	-2.36	115.32	118.94
22	5	305	BCR	C20-C21-C22	-2.36	123.94	127.31
19	7	306	CLA	CMB-C2B-C3B	2.36	129.09	124.68
19	B	814	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
19	4	310	CLA	CMA-C3A-C4A	2.36	118.11	111.77
34	5	324	3PH	O31-C31-C32	2.36	119.31	111.91
31	6	306	LUT	C28-C29-C30	2.36	122.56	118.94
19	3	5013	CLA	CHA-C4D-ND	2.36	137.43	132.50
19	6	313	CLA	CHA-C1A-NA	-2.36	121.00	126.40
19	5	312	CLA	CHA-C4D-ND	2.36	137.43	132.50
27	F	304	RRX	C29-C28-C27	2.36	113.53	110.30
31	3	5002	LUT	C19-C9-C10	-2.36	119.62	122.92
22	B	846	BCR	C4-C5-C6	-2.36	119.31	122.73
19	4	316	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
19	A	835	CLA	CHA-C4D-ND	2.35	137.42	132.50
38	8	325	ERG	C18-C13-C14	-2.35	106.43	110.24
19	8	311	CLA	O2A-CGA-CBA	2.35	119.29	111.91
19	4	318	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
19	B	817	CLA	C1C-C2C-C3C	-2.35	104.48	106.96
19	Z	307	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
19	B	840	CLA	O2A-CGA-CBA	2.35	119.28	111.91
19	B	830	CLA	CHA-C4D-ND	2.35	137.42	132.50
19	A	808	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
19	8	309	CLA	CHA-C1A-NA	-2.35	121.02	126.40
19	A	841	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
19	5	317	CLA	CHA-C4D-ND	2.35	137.41	132.50
19	5	313	CLA	CHA-C4D-ND	2.35	137.41	132.50
19	7	306	CLA	CMD-C2D-C3D	-2.35	122.21	127.61
19	8	320	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
31	Z	318	LUT	C39-C29-C28	2.35	121.78	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	836	CLA	CMA-C3A-C4A	2.35	118.08	111.77
19	A	805	CLA	CHA-C4D-ND	2.35	137.41	132.50
19	4	306	CLA	O2A-CGA-CBA	2.35	119.27	111.91
19	3	5013	CLA	CMD-C2D-C3D	-2.35	122.22	127.61
19	A	812	CLA	CMA-C3A-C4A	2.35	118.08	111.77
19	Z	312	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
22	B	844	BCR	C20-C21-C22	-2.35	123.96	127.31
19	4	306	CLA	C1-C2-C3	-2.35	121.99	126.04
19	5	317	CLA	CBA-CAA-C2A	-2.34	106.94	113.86
19	7	308	CLA	CHA-C1A-NA	-2.34	121.03	126.40
19	6	323	CLA	CMA-C3A-C4A	2.34	118.07	111.77
22	5	304	BCR	C1-C6-C5	-2.34	119.31	122.61
19	3	5013	CLA	C1D-ND-C4D	-2.34	104.67	106.33
19	1	5006	CLA	CHA-C4D-ND	2.34	137.40	132.50
19	7	324	CLA	O2A-CGA-CBA	2.34	119.26	111.91
19	B	806	CLA	O2A-CGA-CBA	2.34	119.26	111.91
19	Z	306	CLA	CHA-C4D-ND	2.34	137.40	132.50
19	4	313	CLA	C1D-ND-C4D	-2.34	104.67	106.33
31	7	303	LUT	C19-C9-C8	2.34	121.77	118.08
19	B	817	CLA	O2A-CGA-CBA	2.34	119.25	111.91
19	Z	305	CLA	O2A-CGA-CBA	2.34	119.25	111.91
19	A	802	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
19	B	820	CLA	O2A-CGA-CBA	2.34	119.25	111.91
19	6	302	CLA	O2A-CGA-CBA	2.34	119.25	111.91
19	B	835	CLA	CMB-C2B-C3B	2.34	129.06	124.68
19	5	311	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
19	7	309	CLA	C1D-ND-C4D	-2.34	104.67	106.33
19	A	827	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
31	7	303	LUT	C15-C35-C34	-2.34	118.69	123.47
22	3	5005	BCR	C33-C5-C4	2.34	118.11	113.62
32	Z	313	CHL	CMA-C3A-C2A	2.34	123.25	113.83
31	8	304	LUT	C35-C15-C14	-2.34	118.69	123.47
19	1	5016	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
19	A	823	CLA	CMD-C2D-C3D	-2.34	122.24	127.61
19	A	816	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
19	3	5020	CLA	C1D-ND-C4D	-2.34	104.68	106.33
31	Z	318	LUT	C15-C35-C34	-2.33	118.69	123.47
19	B	823	CLA	CHA-C4D-ND	2.33	137.38	132.50
19	6	309	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
19	7	319	CLA	O2A-CGA-CBA	2.33	119.23	111.91
28	J	1902	C7Z	C28-C27-C26	-2.33	120.65	127.20
19	7	311	CLA	CHA-C4D-ND	2.33	137.38	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	850	CLA	CMA-C3A-C4A	2.33	118.04	111.77
32	7	314	CHL	CAA-C2A-C1A	-2.33	104.34	111.97
18	A	801	CL0	C4-C3-C5	2.33	119.19	115.27
19	8	313	CLA	O2A-CGA-CBA	2.33	119.22	111.91
19	A	834	CLA	O2A-CGA-CBA	2.33	119.22	111.91
19	5	301	CLA	O2A-CGA-CBA	2.33	119.22	111.91
19	J	1901	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
19	B	827	CLA	C6-C5-C3	-2.33	107.35	113.45
19	Z	305	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
19	3	5014	CLA	CHA-C4D-ND	2.33	137.37	132.50
22	3	5007	BCR	C33-C5-C4	2.33	118.09	113.62
31	5	303	LUT	C36-C21-C26	-2.33	106.02	109.55
19	6	309	CLA	C1D-ND-C4D	-2.33	104.68	106.33
19	5	306	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
19	6	322	CLA	CHA-C4D-ND	2.33	137.37	132.50
19	A	812	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
19	A	815	CLA	CHA-C4D-ND	2.33	137.36	132.50
31	7	304	LUT	C19-C9-C10	-2.33	119.67	122.92
19	A	813	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
22	3	5004	BCR	C30-C25-C26	-2.32	119.34	122.61
19	A	815	CLA	CAA-CBA-CGA	-2.32	106.46	113.25
19	Z	308	CLA	CHA-C4D-ND	2.32	137.36	132.50
19	B	833	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
19	A	807	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
19	A	822	CLA	CHA-C4D-ND	2.32	137.35	132.50
22	A	850	BCR	C36-C18-C17	-2.32	119.67	122.92
19	3	5018	CLA	CHA-C4D-ND	2.32	137.35	132.50
22	F	302	BCR	C29-C30-C25	2.32	114.05	110.48
22	F	302	BCR	C38-C26-C27	2.32	118.07	113.62
19	B	833	CLA	CMD-C2D-C3D	-2.32	122.28	127.61
32	8	315	CHL	CHD-C4C-C3C	2.32	128.25	124.84
19	Z	315	CLA	OBD-CAD-C3D	-2.32	122.94	128.52
19	B	801	CLA	CMA-C3A-C4A	2.32	118.00	111.77
31	3	5003	LUT	C22-C23-C24	2.32	114.38	111.74
32	Z	310	CHL	CHB-C4A-NA	2.32	127.71	124.51
19	B	839	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
19	B	850	CLA	C1-C2-C3	-2.32	122.04	126.04
19	A	819	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
19	3	5012	CLA	C2C-C1C-NC	2.31	112.14	109.97
22	K	206	BCR	C8-C7-C6	-2.31	120.70	127.20
19	3	5012	CLA	CMD-C2D-C3D	-2.31	122.29	127.61
31	5	303	LUT	C39-C29-C28	2.31	121.72	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	807	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
27	4	303	RRX	C2-C1-C6	2.31	114.04	110.48
19	5	311	CLA	CMA-C3A-C4A	2.31	117.99	111.77
22	5	304	BCR	C1-C6-C7	2.31	122.32	115.78
19	B	822	CLA	CMD-C2D-C3D	-2.31	122.29	127.61
19	4	309	CLA	CMD-C2D-C3D	-2.31	122.29	127.61
19	B	826	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
22	B	842	BCR	C20-C19-C18	-2.31	119.92	126.42
19	A	804	CLA	O2A-CGA-CBA	2.31	119.16	111.91
19	B	812	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
19	8	307	CLA	C1D-ND-C4D	-2.31	104.69	106.33
22	3	5007	BCR	C36-C18-C19	2.31	121.72	118.08
19	A	827	CLA	O2A-CGA-CBA	2.31	119.15	111.91
32	1	5017	CHL	C2C-C3C-C4C	2.31	108.13	106.49
32	1	5009	CHL	CHB-C4A-NA	2.31	127.70	124.51
19	5	307	CLA	CMA-C3A-C4A	2.31	117.97	111.77
31	1	5004	LUT	C17-C1-C6	-2.31	106.56	110.30
19	B	829	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
19	4	316	CLA	O2A-CGA-CBA	2.30	119.14	111.91
19	6	323	CLA	C6-C5-C3	-2.30	107.41	113.45
31	3	5003	LUT	C4-C5-C6	-2.30	115.71	120.85
19	A	821	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
19	1	5008	CLA	CMB-C2B-C3B	2.30	128.99	124.68
32	Z	309	CHL	C4D-CHA-C1A	2.30	124.05	121.25
19	A	806	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
19	B	813	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
22	B	843	BCR	C8-C7-C6	-2.30	120.74	127.20
19	B	823	CLA	O2A-CGA-CBA	2.30	119.13	111.91
19	7	308	CLA	C6-C7-C8	-2.30	108.49	115.92
28	6	304	C7Z	C8-C9-C10	2.30	122.47	118.94
32	6	317	CHL	CHD-C4C-C3C	2.30	128.22	124.84
19	A	822	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
19	A	831	CLA	O2A-CGA-CBA	2.30	119.12	111.91
27	4	303	RRX	C21-C20-C19	-2.30	116.05	123.22
19	B	823	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
19	5	314	CLA	CHA-C1A-NA	-2.30	121.14	126.40
19	A	833	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
19	3	5016	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
19	7	310	CLA	C1-O2A-CGA	2.29	122.47	116.44
19	7	317	CLA	CHA-C4D-ND	2.29	137.30	132.50
31	4	304	LUT	C35-C15-C14	-2.29	118.78	123.47
19	7	307	CLA	O2A-CGA-CBA	2.29	119.11	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	8	308	CLA	C3D-C2D-C1D	-2.29	102.70	105.83
32	8	317	CHL	C1-C2-C3	-2.29	123.04	126.75
19	B	826	CLA	O2A-CGA-CBA	2.29	119.10	111.91
19	1	5013	CLA	CMD-C2D-C3D	-2.29	122.34	127.61
19	6	309	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
19	A	831	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
19	B	825	CLA	CMB-C2B-C3B	2.29	128.96	124.68
19	K	204	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
31	3	5002	LUT	C4-C5-C6	-2.29	115.74	120.85
31	3	5002	LUT	C16-C1-C6	-2.29	106.58	110.30
19	Z	312	CLA	CMB-C2B-C3B	2.29	128.96	124.68
32	5	318	CHL	C2C-C3C-C4C	2.29	108.12	106.49
19	B	837	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
28	J	1902	C7Z	C8-C7-C6	-2.29	120.78	127.20
19	1	5007	CLA	CAA-CBA-CGA	-2.29	106.44	112.51
19	B	825	CLA	CHA-C4D-ND	2.29	137.28	132.50
19	5	309	CLA	C2C-C1C-NC	2.29	112.11	109.97
19	A	810	CLA	O2A-CGA-CBA	2.29	119.08	111.91
19	Z	315	CLA	C2C-C1C-NC	2.29	112.11	109.97
19	B	837	CLA	O1D-CGD-CBD	-2.29	119.81	124.48
19	3	5011	CLA	CMB-C2B-C3B	2.29	128.96	124.68
27	5	302	RRX	C38-C26-C27	2.29	118.59	114.36
22	8	306	BCR	C10-C11-C12	-2.29	116.08	123.22
19	A	815	CLA	CMD-C2D-C3D	-2.29	122.36	127.61
22	B	847	BCR	C15-C14-C13	-2.28	124.05	127.31
19	B	814	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
19	B	803	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
19	B	838	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
32	8	315	CHL	CMA-C3A-C2A	2.28	123.04	113.83
19	4	310	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
19	B	811	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
19	F	301	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
22	3	5004	BCR	C3-C4-C5	-2.28	110.00	114.08
19	Z	314	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
19	Z	307	CLA	O2A-CGA-CBA	2.28	119.07	111.91
31	8	305	LUT	C28-C29-C30	-2.28	115.44	118.94
19	6	312	CLA	C1D-ND-C4D	-2.28	104.72	106.33
24	A	856	LMT	O1'-C1'-C2'	2.28	111.86	108.30
22	A	847	BCR	C35-C13-C14	-2.28	119.73	122.92
22	3	5007	BCR	C10-C11-C12	2.28	130.33	123.22
19	K	204	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
19	B	832	CLA	O2A-CGA-CBA	2.28	119.06	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	6	304	C7Z	C20-C13-C14	-2.28	119.73	122.92
19	B	803	CLA	O2A-CGA-CBA	2.28	119.06	111.91
19	A	832	CLA	CHA-C1A-NA	-2.28	121.18	126.40
19	5	319	CLA	O2A-CGA-CBA	2.28	119.05	111.91
31	1	5004	LUT	C20-C13-C12	2.28	121.67	118.08
32	3	5017	CHL	CHD-C1D-C2D	2.28	130.26	125.48
19	B	820	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
19	B	850	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
28	J	1902	C7Z	C21-C26-C25	-2.28	119.41	122.61
22	6	308	BCR	C4-C5-C6	-2.28	119.43	122.73
31	4	304	LUT	C18-C5-C4	2.28	118.57	114.36
32	1	5009	CHL	C4A-NA-C1A	2.28	107.73	106.71
19	B	809	CLA	O2A-CGA-CBA	2.28	119.05	111.91
22	5	304	BCR	C34-C9-C8	2.28	121.66	118.08
19	B	813	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
22	B	843	BCR	C30-C25-C24	2.27	122.21	115.78
19	A	840	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
32	5	320	CHL	CHD-C4C-C3C	2.27	128.18	124.84
19	7	308	CLA	C2D-C1D-ND	2.27	111.78	110.10
19	B	821	CLA	CMB-C2B-C3B	2.27	128.93	124.68
19	A	839	CLA	O2A-CGA-CBA	2.27	119.04	111.91
19	1	5015	CLA	C3D-C2D-C1D	-2.27	102.73	105.83
19	A	821	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
22	8	303	BCR	C35-C13-C14	-2.27	119.74	122.92
31	7	304	LUT	C4-C5-C6	-2.27	115.78	120.85
22	B	847	BCR	C7-C6-C5	-2.27	115.96	121.46
31	1	5004	LUT	C35-C15-C14	-2.27	118.82	123.47
19	B	830	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
19	5	308	CLA	C6-C5-C3	-2.27	107.50	113.45
19	5	307	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
19	A	819	CLA	C1-O2A-CGA	2.27	122.40	116.44
19	3	5015	CLA	C3D-C2D-C1D	-2.27	102.73	105.83
28	6	304	C7Z	C39-C29-C30	-2.27	119.74	122.92
22	A	849	BCR	C32-C1-C6	-2.27	106.62	110.30
19	I	201	CLA	O2A-CGA-CBA	2.27	119.03	111.91
19	B	819	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
22	G	1603	BCR	C10-C11-C12	-2.26	116.15	123.22
32	1	5017	CHL	CHC-C1C-NC	2.26	127.64	124.20
33	3	5001	SPH	C3-C4-C5	-2.26	119.74	124.79
19	B	824	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
19	A	830	CLA	O2A-CGA-CBA	2.26	119.01	111.91
19	Z	307	CLA	CAA-C2A-C3A	-2.26	106.58	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	310	CLA	CMA-C3A-C4A	2.26	117.85	111.77
19	A	838	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
19	3	5008	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
31	8	304	LUT	C4-C5-C6	-2.26	115.81	120.85
19	1	5018	CLA	O2A-CGA-CBA	2.26	119.00	111.91
19	Z	305	CLA	C11-C12-C13	-2.26	108.61	115.92
22	8	306	BCR	C29-C28-C27	2.26	116.43	111.38
34	5	324	3PH	C2-O21-C21	-2.26	112.23	117.79
24	A	856	LMT	C1B-O1B-C4'	-2.26	112.37	117.96
22	4	305	BCR	C15-C16-C17	-2.26	118.85	123.47
22	A	849	BCR	C23-C24-C25	-2.26	120.86	127.20
19	A	811	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
32	4	317	CHL	CMA-C3A-C2A	2.26	122.94	113.83
27	F	304	RRX	C35-C13-C14	-2.26	119.76	122.92
19	A	812	CLA	C1-C2-C3	-2.26	122.14	126.04
19	6	312	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
19	A	815	CLA	CMB-C2B-C3B	2.26	128.90	124.68
19	7	318	CLA	C1D-ND-C4D	-2.26	104.73	106.33
19	1	5012	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
19	7	318	CLA	CHA-C1A-NA	-2.25	121.24	126.40
19	A	802	CLA	CHA-C1A-NA	-2.25	121.24	126.40
31	3	5002	LUT	C1-C6-C5	-2.25	119.44	122.61
19	A	817	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
19	A	813	CLA	CHA-C1A-NA	-2.25	121.24	126.40
19	B	821	CLA	O2A-CGA-CBA	2.25	118.98	111.91
19	6	313	CLA	C1D-ND-C4D	-2.25	104.73	106.33
19	3	5016	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
32	Z	302	CHL	C4D-CHA-C1A	2.25	123.99	121.25
22	F	302	BCR	C35-C13-C12	2.25	121.62	118.08
19	7	324	CLA	CHA-C4D-ND	2.25	137.21	132.50
31	5	303	LUT	C35-C15-C14	-2.25	118.86	123.47
19	1	5007	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
19	A	833	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
19	5	325	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
19	B	808	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
32	8	317	CHL	C1B-CHB-C4A	-2.25	125.66	130.12
19	A	857	CLA	O2A-CGA-CBA	2.25	118.96	111.91
19	B	811	CLA	O2A-CGA-CBA	2.25	118.96	111.91
19	A	810	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
31	5	303	LUT	C18-C5-C4	2.25	118.52	114.36
19	B	807	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
19	1	5006	CLA	CMB-C2B-C1B	-2.25	125.01	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	827	CLA	O1D-CGD-CBD	-2.25	119.89	124.48
19	B	806	CLA	CMD-C2D-C3D	-2.25	122.45	127.61
32	6	315	CHL	CHD-C4C-C3C	2.25	128.14	124.84
19	K	203	CLA	CHA-C1A-NA	-2.25	121.25	126.40
19	A	838	CLA	CMD-C2D-C3D	-2.25	122.45	127.61
19	A	814	CLA	CMD-C2D-C3D	-2.25	122.45	127.61
19	G	1602	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
19	3	5020	CLA	CHA-C1A-NA	-2.24	121.26	126.40
19	4	309	CLA	C1-O2A-CGA	2.24	122.33	116.44
19	A	834	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
32	1	5014	CHL	CHC-C1C-NC	2.24	127.61	124.20
31	6	305	LUT	C19-C9-C10	-2.24	119.78	122.92
19	Z	303	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
19	3	5015	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
32	6	315	CHL	CHC-C1C-NC	2.24	127.60	124.20
19	B	831	CLA	CHA-C4D-ND	2.24	137.19	132.50
19	A	837	CLA	CMB-C2B-C3B	2.24	128.87	124.68
19	A	817	CLA	O2A-CGA-CBA	2.24	118.94	111.91
19	1	5010	CLA	C2C-C1C-NC	2.24	112.07	109.97
31	6	306	LUT	C11-C12-C13	-2.24	120.13	126.42
19	A	808	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
19	G	1601	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
19	A	805	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
19	B	810	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
19	A	843	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
19	B	816	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
19	K	205	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
19	A	857	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
19	7	307	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
32	6	315	CHL	CHB-C4A-NA	2.24	127.60	124.51
32	6	316	CHL	C1-C2-C3	-2.24	122.18	126.04
32	1	5009	CHL	C1B-CHB-C4A	-2.24	125.69	130.12
19	7	312	CLA	CAA-C2A-C3A	-2.24	106.66	112.78
31	1	5004	LUT	C39-C29-C28	2.23	121.60	118.08
19	B	806	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
19	B	817	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
19	A	809	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
19	4	309	CLA	CHA-C4D-ND	2.23	137.17	132.50
19	3	5013	CLA	C1-C2-C3	-2.23	122.18	126.04
19	8	307	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
19	B	804	CLA	CHA-C1A-NA	-2.23	121.29	126.40
22	F	302	BCR	C4-C5-C6	-2.23	119.49	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	4	320	LHG	C6-C5-C4	-2.23	106.51	111.79
19	B	802	CLA	CHA-C1A-NA	-2.23	121.29	126.40
19	8	308	CLA	CHA-C1A-NA	-2.23	121.29	126.40
19	7	307	CLA	CHA-C1A-NA	-2.23	121.29	126.40
19	A	841	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
31	6	305	LUT	C21-C26-C25	2.23	115.41	111.42
32	6	319	CHL	CHD-C4C-C3C	2.23	128.12	124.84
19	K	203	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
19	1	5018	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
19	A	812	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
19	A	822	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
19	A	832	CLA	O2A-CGA-CBA	2.23	118.90	111.91
19	7	311	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
19	A	830	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
19	B	818	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
19	8	318	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
19	Z	304	CLA	C1D-ND-C4D	-2.23	104.75	106.33
19	A	803	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
19	7	319	CLA	O2D-CGD-O1D	-2.23	119.49	123.84
19	4	310	CLA	CHA-C1A-NA	-2.23	121.30	126.40
19	A	828	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
19	3	5008	CLA	CMB-C2B-C3B	2.22	128.84	124.68
27	F	304	RRX	C2-C1-C6	2.22	113.91	110.48
19	B	824	CLA	O1D-CGD-CBD	-2.22	119.93	124.48
19	7	319	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
19	B	816	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
19	8	314	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
19	A	804	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
19	B	801	CLA	O2A-CGA-CBA	2.22	118.88	111.91
19	3	5008	CLA	CHA-C1A-NA	-2.22	121.31	126.40
19	A	806	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
19	7	311	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
27	5	302	RRX	C15-C16-C17	-2.22	118.93	123.47
19	A	828	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
19	7	317	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
19	J	1901	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
19	B	827	CLA	O2A-CGA-CBA	2.22	118.87	111.91
19	A	837	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
19	1	5006	CLA	CHA-C1A-NA	-2.22	121.32	126.40
19	A	820	CLA	O2A-CGA-CBA	2.22	118.87	111.91
32	Z	313	CHL	CMB-C2B-C1B	-2.22	125.05	128.46
31	7	304	LUT	C28-C29-C30	2.22	122.34	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	311	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
19	A	841	CLA	O2A-CGA-CBA	2.22	118.87	111.91
31	7	303	LUT	C18-C5-C4	2.22	118.46	114.36
31	3	5002	LUT	C31-C30-C29	-2.22	124.15	127.31
19	A	840	CLA	CMA-C3A-C4A	2.22	117.73	111.77
19	A	819	CLA	O2A-CGA-CBA	2.22	118.86	111.91
19	5	306	CLA	C1-C2-C3	-2.22	122.21	126.04
19	A	813	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
32	1	5014	CHL	CMA-C3A-C2A	2.21	122.76	113.83
19	A	821	CLA	CMA-C3A-C4A	2.21	117.72	111.77
19	3	5009	CLA	CMA-C3A-C4A	2.21	117.72	111.77
19	Z	315	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
19	3	5010	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
19	8	318	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
19	8	312	CLA	CMB-C2B-C1B	-2.21	125.07	128.46
19	7	324	CLA	CAA-C2A-C1A	-2.21	104.73	111.97
19	A	857	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
19	6	311	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
19	Z	311	CLA	CMB-C2B-C3B	2.21	128.81	124.68
19	A	820	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
31	3	5003	LUT	C38-C25-C24	-2.21	118.83	123.56
32	1	5017	CHL	CMA-C3A-C2A	2.21	122.73	113.83
19	B	801	CLA	CHA-C1A-NA	-2.21	121.34	126.40
19	F	301	CLA	C1C-C2C-C3C	-2.21	104.64	106.96
19	B	820	CLA	C6-C5-C3	-2.21	107.67	113.45
32	5	316	CHL	C1B-CHB-C4A	-2.21	125.75	130.12
32	1	5014	CHL	CMB-C2B-C1B	-2.21	125.07	128.46
19	8	313	CLA	CAA-CBA-CGA	-2.21	106.81	113.25
19	5	319	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
19	A	816	CLA	CHA-C1A-NA	-2.21	121.35	126.40
32	1	5017	CHL	CHD-C4C-C3C	2.20	128.08	124.84
31	5	303	LUT	C18-C5-C6	-2.20	122.05	124.53
31	Z	317	LUT	C8-C9-C10	2.20	122.32	118.94
32	6	321	CHL	CHD-C1D-C2D	2.20	130.10	125.48
19	5	310	CLA	O2A-CGA-CBA	2.20	118.83	111.91
19	K	204	CLA	O2A-CGA-CBA	2.20	118.83	111.91
19	3	5009	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
31	3	5003	LUT	C11-C12-C13	-2.20	120.22	126.42
19	A	814	CLA	C1-C2-C3	-2.20	122.23	126.04
32	8	319	CHL	CMB-C2B-C1B	-2.20	125.08	128.46
19	8	308	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
19	Z	311	CLA	O2A-CGA-CBA	2.20	118.82	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	315	CLA	CHA-C1A-NA	-2.20	121.36	126.40
19	A	805	CLA	O2A-CGA-CBA	2.20	118.82	111.91
19	B	821	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
19	8	312	CLA	C6-C7-C8	-2.20	108.80	115.92
31	7	303	LUT	C21-C26-C25	2.20	115.36	111.42
19	A	839	CLA	CAA-CBA-CGA	-2.20	106.82	113.25
19	3	5010	CLA	CHA-C1A-NA	-2.20	121.36	126.40
31	3	5002	LUT	C38-C25-C24	-2.20	118.85	123.56
19	4	318	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
22	A	859	BCR	C7-C8-C9	-2.20	122.91	126.23
19	A	814	CLA	CHA-C1A-NA	-2.20	121.36	126.40
31	3	5002	LUT	C2-C3-C4	2.20	113.31	110.30
19	5	310	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
19	K	203	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
19	3	5009	CLA	CHA-C1A-NA	-2.20	121.36	126.40
19	I	201	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
19	A	818	CLA	C6-C5-C3	-2.20	107.69	113.45
22	F	302	BCR	C7-C8-C9	-2.20	122.92	126.23
19	7	313	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
19	B	850	CLA	O2A-CGA-CBA	2.20	118.80	111.91
31	6	305	LUT	C2-C3-C4	2.20	113.31	110.30
32	1	5009	CHL	C2C-C3C-C4C	2.20	108.05	106.49
19	A	836	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
19	I	201	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
19	A	832	CLA	O1D-CGD-CBD	-2.19	119.99	124.48
19	B	840	CLA	C1-O2A-CGA	2.19	122.20	116.44
22	5	304	BCR	C11-C12-C13	-2.19	120.25	126.42
19	B	819	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
28	6	304	C7Z	C24-C25-C26	-2.19	115.96	120.85
19	B	829	CLA	O2A-CGA-CBA	2.19	118.79	111.91
19	A	814	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
19	B	812	CLA	CHA-C1A-NA	-2.19	121.38	126.40
19	5	325	CLA	C6-C5-C3	-2.19	107.70	113.45
19	A	831	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
32	6	317	CHL	C1B-CHB-C4A	-2.19	125.78	130.12
19	B	821	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
32	Z	309	CHL	CHC-C1C-NC	2.19	127.53	124.20
32	6	317	CHL	C4D-CHA-C1A	2.19	123.92	121.25
19	6	320	CLA	CAA-CBA-CGA	-2.19	106.85	113.25
19	A	841	CLA	CHA-C1A-NA	-2.19	121.38	126.40
19	A	827	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
19	A	824	CLA	CMD-C2D-C3D	-2.19	122.58	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	8	304	LUT	C19-C9-C10	-2.19	119.86	122.92
19	A	825	CLA	CHA-C1A-NA	-2.19	121.39	126.40
19	A	843	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
19	B	819	CLA	CMB-C2B-C3B	2.19	128.77	124.68
19	F	303	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
31	1	5004	LUT	C11-C12-C13	-2.19	120.27	126.42
22	B	845	BCR	C30-C25-C24	2.19	121.97	115.78
19	A	823	CLA	CHA-C1A-NA	-2.19	121.39	126.40
19	B	833	CLA	CHA-C1A-NA	-2.19	121.39	126.40
19	A	835	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
19	B	822	CLA	CHA-C1A-NA	-2.18	121.40	126.40
22	A	849	BCR	C10-C11-C12	-2.18	116.40	123.22
22	7	305	BCR	C23-C24-C25	-2.18	121.07	127.20
19	A	842	CLA	O2A-CGA-CBA	2.18	118.76	111.91
19	B	816	CLA	O2A-CGA-CBA	2.18	118.76	111.91
19	B	831	CLA	C6-C5-C3	-2.18	107.73	113.45
31	8	305	LUT	C12-C13-C14	-2.18	115.59	118.94
32	1	5017	CHL	CMB-C2B-C1B	-2.18	125.11	128.46
32	3	5017	CHL	CMB-C2B-C1B	-2.18	125.11	128.46
19	B	826	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
19	B	823	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
19	1	5018	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
19	5	322	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
22	3	5007	BCR	C21-C20-C19	2.18	130.02	123.22
19	7	308	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
19	B	838	CLA	C1-C2-C3	-2.18	122.27	126.04
19	B	803	CLA	OBD-CAD-C3D	-2.18	123.27	128.52
32	8	316	CHL	CMB-C2B-C1B	-2.18	125.11	128.46
19	4	308	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
19	3	5011	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
31	3	5002	LUT	C15-C35-C34	-2.18	119.01	123.47
19	A	835	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
19	8	310	CLA	CMB-C2B-C1B	-2.18	125.12	128.46
19	B	814	CLA	O2A-CGA-CBA	2.18	118.74	111.91
31	4	304	LUT	C11-C12-C13	-2.18	120.30	126.42
19	7	306	CLA	CHA-C1A-NA	-2.17	121.42	126.40
19	5	317	CLA	O2A-CGA-CBA	2.17	118.73	111.91
19	G	1602	CLA	OBD-CAD-C3D	-2.17	123.29	128.52
22	B	844	BCR	C23-C22-C21	2.17	122.28	118.94
32	7	315	CHL	CHB-C4A-NA	2.17	127.52	124.51
19	B	803	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
19	8	314	CLA	C3D-C2D-C1D	-2.17	102.86	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	8	310	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
19	K	202	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
19	B	827	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
32	6	319	CHL	CHB-C4A-NA	2.17	127.51	124.51
19	7	306	CLA	OBD-CAD-C3D	-2.17	123.30	128.52
19	A	836	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
19	8	311	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
19	4	306	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
19	1	5016	CLA	O2A-CGA-CBA	2.17	118.72	111.91
19	B	830	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
19	8	308	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
19	5	301	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
19	7	309	CLA	CMB-C2B-C3B	2.17	128.74	124.68
32	8	315	CHL	C1B-CHB-C4A	-2.17	125.82	130.12
19	B	803	CLA	CHA-C1A-NA	-2.17	121.43	126.40
19	A	825	CLA	CMB-C2B-C3B	2.17	128.74	124.68
19	A	822	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
19	7	312	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
19	A	818	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
31	3	5003	LUT	C21-C26-C27	2.17	115.44	112.70
22	K	206	BCR	C27-C26-C25	-2.17	119.58	122.73
19	4	308	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
19	A	802	CLA	OBD-CAD-C3D	-2.17	123.31	128.52
19	F	301	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
19	6	323	CLA	CHA-C1A-NA	-2.16	121.44	126.40
37	8	302	SQD	O3-C3-C2	-2.16	105.34	110.35
19	7	316	CLA	CMD-C2D-C3D	-2.16	122.63	127.61
19	A	825	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
19	A	810	CLA	CMB-C2B-C3B	2.16	128.73	124.68
32	4	314	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
19	3	5019	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
22	4	305	BCR	C24-C25-C26	-2.16	116.22	121.46
19	A	820	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
19	B	835	CLA	O2A-CGA-CBA	2.16	118.69	111.91
22	K	206	BCR	C10-C11-C12	-2.16	116.47	123.22
19	A	832	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
22	A	846	BCR	C29-C30-C25	2.16	113.81	110.48
19	B	813	CLA	CHA-C1A-NA	-2.16	121.45	126.40
19	B	839	CLA	CHA-C1A-NA	-2.16	121.45	126.40
19	8	310	CLA	C1D-ND-C4D	-2.16	104.80	106.33
19	6	320	CLA	CAA-C2A-C1A	-2.16	104.90	111.97
19	G	1601	CLA	CHA-C1A-NA	-2.16	121.46	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	805	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
19	1	5010	CLA	C1-O2A-CGA	2.16	122.10	116.44
27	5	302	RRX	C1-C6-C5	-2.16	119.58	122.61
19	6	313	CLA	CMD-C2D-C3D	-2.16	122.66	127.61
19	Z	308	CLA	C1-O2A-CGA	2.15	122.10	116.44
32	5	315	CHL	CMB-C2B-C1B	-2.15	125.15	128.46
19	B	834	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
22	G	1603	BCR	C38-C26-C27	2.15	117.75	113.62
19	8	307	CLA	CHA-C1A-NA	-2.15	121.46	126.40
19	Z	307	CLA	CHA-C1A-NA	-2.15	121.47	126.40
19	8	314	CLA	CHA-C1A-NA	-2.15	121.47	126.40
19	B	823	CLA	C6-C5-C3	-2.15	107.81	113.45
22	G	1603	BCR	C36-C18-C17	-2.15	119.91	122.92
32	Z	309	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
19	B	810	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
19	A	810	CLA	CHA-C1A-NA	-2.15	121.47	126.40
31	7	303	LUT	C39-C29-C28	2.15	121.47	118.08
19	3	5012	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
32	Z	302	CHL	C3B-C4B-NB	-2.15	106.43	109.21
19	B	829	CLA	CHA-C1A-NA	-2.15	121.47	126.40
19	1	5016	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
19	B	836	CLA	CMB-C2B-C3B	2.15	128.70	124.68
28	6	304	C7Z	C4-C5-C6	-2.15	116.05	120.85
19	A	842	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
32	8	316	CHL	C4A-NA-C1A	2.15	107.67	106.71
19	1	5008	CLA	C1-C2-C3	-2.15	122.32	126.04
19	5	325	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
19	B	831	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
19	Z	308	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
19	5	314	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
19	A	820	CLA	CHA-C1A-NA	-2.15	121.48	126.40
19	A	821	CLA	CHA-C1A-NA	-2.15	121.48	126.40
32	7	314	CHL	CMB-C2B-C1B	-2.15	125.17	128.46
32	4	319	CHL	CHB-C4A-NA	2.15	127.48	124.51
38	8	325	ERG	C19-C10-C9	-2.15	107.42	111.03
23	6	303	LHG	C5-O7-C7	-2.15	112.51	117.79
19	4	306	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
38	8	325	ERG	C7-C6-C5	-2.14	119.44	123.20
32	Z	310	CHL	CMA-C3A-C2A	2.14	122.48	113.83
19	A	806	CLA	C11-C12-C13	-2.14	108.99	115.92
19	B	840	CLA	CMA-C3A-C4A	2.14	117.54	111.77
19	1	5007	CLA	CBA-CAA-C2A	-2.14	107.53	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	6	316	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
31	8	305	LUT	C21-C26-C25	2.14	115.26	111.42
28	1	5005	C7Z	C4-C5-C6	-2.14	116.07	120.85
19	A	826	CLA	CMB-C2B-C3B	2.14	128.69	124.68
19	J	1901	CLA	CHA-C1A-NA	-2.14	121.49	126.40
19	B	840	CLA	CMB-C2B-C3B	2.14	128.69	124.68
19	A	829	CLA	O2A-CGA-CBA	2.14	118.63	111.91
32	5	316	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
24	F	305	LMT	O5B-C5B-C6B	2.14	111.76	106.44
19	3	5019	CLA	CMB-C2B-C3B	2.14	128.68	124.68
19	B	809	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
19	6	301	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
32	4	319	CHL	CHD-C4C-C3C	2.14	127.99	124.84
32	1	5009	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
19	5	319	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
19	B	826	CLA	CHA-C1A-NA	-2.14	121.50	126.40
19	A	814	CLA	CMB-C2B-C3B	2.14	128.68	124.68
19	B	815	CLA	CMB-C2B-C3B	2.14	128.68	124.68
19	6	301	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
19	B	832	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
19	5	321	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
19	B	837	CLA	CHA-C1A-NA	-2.14	121.50	126.40
22	4	305	BCR	C37-C22-C21	-2.14	119.93	122.92
19	7	318	CLA	CMC-C2C-C1C	2.14	128.29	125.04
19	6	322	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
22	5	305	BCR	C29-C30-C25	2.14	113.77	110.48
19	A	819	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
22	6	308	BCR	C38-C26-C27	2.14	117.72	113.62
31	4	304	LUT	C2-C3-C4	2.14	113.23	110.30
19	A	822	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
19	A	831	CLA	CHA-C1A-NA	-2.14	121.50	126.40
19	Z	304	CLA	O2A-CGA-CBA	2.14	118.61	111.91
31	Z	317	LUT	C15-C14-C13	-2.14	124.26	127.31
27	4	303	RRX	C12-C13-C14	-2.14	115.66	118.94
27	5	302	RRX	C29-C28-C27	2.14	113.23	110.30
32	8	301	CHL	CHB-C4A-NA	2.13	127.46	124.51
19	5	325	CLA	CHA-C1A-NA	-2.13	121.51	126.40
19	Z	307	CLA	C1D-ND-C4D	-2.13	104.82	106.33
22	G	1603	BCR	C37-C22-C21	-2.13	119.93	122.92
31	1	5004	LUT	C37-C21-C26	-2.13	106.31	109.55
19	1	5012	CLA	C1-O2A-CGA	2.13	122.04	116.44
27	F	304	RRX	C36-C18-C17	-2.13	119.94	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	313	CLA	CHA-C1A-NA	-2.13	121.51	126.40
32	Z	302	CHL	C1-O2A-CGA	2.13	122.04	116.44
22	A	859	BCR	C23-C24-C25	-2.13	121.21	127.20
32	5	318	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
22	A	848	BCR	C20-C19-C18	-2.13	120.42	126.42
19	K	205	CLA	CHA-C1A-NA	-2.13	121.51	126.40
19	3	5012	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
32	Z	309	CHL	CAA-C2A-C1A	-2.13	104.99	111.97
19	7	311	CLA	CAA-CBA-CGA	-2.13	107.03	113.25
32	5	315	CHL	CHB-C4A-NA	2.13	127.46	124.51
19	A	816	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
19	B	820	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
19	5	310	CLA	CMB-C2B-C3B	2.13	128.66	124.68
19	5	319	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
19	B	828	CLA	O2A-CGA-CBA	2.13	118.59	111.91
19	B	837	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
19	Z	307	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
19	B	827	CLA	CHA-C1A-NA	-2.13	121.52	126.40
22	3	5007	BCR	C3-C4-C5	-2.13	110.27	114.08
19	B	826	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
19	7	313	CLA	CHA-C1A-NA	-2.13	121.52	126.40
19	Z	303	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
19	A	837	CLA	CHA-C1A-NA	-2.13	121.52	126.40
19	B	815	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
19	1	5012	CLA	CHA-C1A-NA	-2.13	121.53	126.40
22	B	842	BCR	C36-C18-C19	2.13	121.43	118.08
19	1	5012	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
22	A	848	BCR	C36-C18-C17	-2.13	119.94	122.92
31	3	5003	LUT	C18-C5-C4	2.13	118.30	114.36
19	A	803	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
19	B	822	CLA	O2A-CGA-CBA	2.13	118.58	111.91
32	6	317	CHL	CMB-C2B-C1B	-2.13	125.20	128.46
19	B	810	CLA	CHA-C1A-NA	-2.13	121.53	126.40
19	A	809	CLA	CHA-C1A-NA	-2.12	121.53	126.40
19	6	312	CLA	C16-C15-C13	-2.12	109.05	115.92
19	B	839	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
19	6	302	CLA	CHA-C1A-NA	-2.12	121.53	126.40
19	A	804	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
19	8	318	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
32	Z	302	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
19	8	309	CLA	C11-C10-C8	-2.12	109.06	115.92
32	Z	310	CHL	CMB-C2B-C1B	-2.12	125.20	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	803	CLA	CHA-C1A-NA	-2.12	121.54	126.40
19	I	201	CLA	C6-C5-C3	-2.12	107.89	113.45
19	A	804	CLA	C6-C5-C3	-2.12	107.89	113.45
32	1	5014	CHL	C1-O2A-CGA	2.12	122.89	116.73
32	1	5009	CHL	CMA-C3A-C4A	2.12	117.47	111.77
22	5	304	BCR	C11-C10-C9	-2.12	124.28	127.31
19	8	310	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
19	1	5006	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
19	4	311	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
19	3	5011	CLA	C1-O2A-CGA	2.12	122.00	116.44
19	F	301	CLA	CHA-C1A-NA	-2.12	121.55	126.40
31	8	305	LUT	C19-C9-C8	2.12	121.41	118.08
22	B	842	BCR	C7-C8-C9	-2.12	123.04	126.23
32	8	317	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
32	5	320	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
19	B	835	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
19	6	302	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
19	1	5008	CLA	C1D-ND-C4D	-2.11	104.83	106.33
19	A	821	CLA	CMB-C2B-C3B	2.11	128.63	124.68
19	B	824	CLA	CHA-C1A-NA	-2.11	121.56	126.40
28	6	304	C7Z	C40-C33-C34	-2.11	119.96	122.92
32	4	315	CHL	CHD-C4C-C3C	2.11	127.95	124.84
19	B	850	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
22	B	847	BCR	C8-C9-C10	-2.11	115.70	118.94
22	6	308	BCR	C19-C18-C17	-2.11	115.70	118.94
19	7	307	CLA	CMB-C2B-C3B	2.11	128.63	124.68
19	A	816	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
31	6	306	LUT	C8-C7-C6	-2.11	121.27	127.20
31	1	5004	LUT	C22-C23-C24	2.11	114.14	111.74
19	4	310	CLA	C6-C7-C8	-2.11	109.09	115.92
28	1	5005	C7Z	C39-C29-C30	-2.11	119.97	122.92
19	5	309	CLA	CHA-C1A-NA	-2.11	121.56	126.40
19	7	306	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
22	6	308	BCR	C34-C9-C8	2.11	121.40	118.08
19	8	320	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
22	K	206	BCR	C16-C15-C14	-2.11	119.15	123.47
19	A	805	CLA	CMB-C2B-C3B	2.11	128.63	124.68
27	5	302	RRX	C27-C26-C25	-2.11	116.14	120.85
32	1	5014	CHL	CHB-C4A-NA	2.11	127.43	124.51
31	3	5002	LUT	C11-C12-C13	-2.11	120.49	126.42
19	3	5012	CLA	CMC-C2C-C1C	2.11	128.25	125.04
22	B	843	BCR	C20-C21-C22	-2.11	124.30	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	5007	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
19	3	5008	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
19	B	834	CLA	CHA-C1A-NA	-2.11	121.57	126.40
19	G	1601	CLA	O2A-CGA-CBA	2.11	118.52	111.91
19	A	829	CLA	CHA-C1A-NA	-2.11	121.57	126.40
19	B	821	CLA	CHA-C1A-NA	-2.11	121.57	126.40
19	B	812	CLA	O2A-CGA-CBA	2.11	118.52	111.91
32	4	317	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
19	A	826	CLA	CHA-C1A-NA	-2.11	121.57	126.40
19	3	5020	CLA	CAA-CBA-CGA	-2.11	107.09	113.25
19	A	816	CLA	O2A-CGA-CBA	2.11	118.52	111.91
32	4	315	CHL	CMB-C2B-C1B	-2.11	125.23	128.46
19	B	809	CLA	CHA-C1A-NA	-2.10	121.58	126.40
22	B	846	BCR	C35-C13-C14	-2.10	119.98	122.92
19	4	316	CLA	CHA-C1A-NA	-2.10	121.58	126.40
19	A	815	CLA	C16-C15-C13	-2.10	109.12	115.92
19	3	5014	CLA	C1-O2A-CGA	2.10	121.96	116.44
19	A	802	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
32	8	301	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
19	A	833	CLA	CHA-C1A-NA	-2.10	121.58	126.40
19	5	312	CLA	CHA-C1A-NA	-2.10	121.58	126.40
19	1	5006	CLA	CAA-CBA-CGA	-2.10	107.11	113.25
32	1	5009	CHL	C3B-C4B-NB	-2.10	106.49	109.21
19	1	5010	CLA	O2A-CGA-CBA	2.10	118.50	111.91
19	3	5011	CLA	CMC-C2C-C1C	2.10	128.24	125.04
19	5	306	CLA	C6-C7-C8	-2.10	109.12	115.92
19	3	5020	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
19	5	313	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
19	6	314	CLA	CHA-C1A-NA	-2.10	121.58	126.40
32	1	5014	CHL	C2C-C3C-C4C	2.10	107.99	106.49
22	5	305	BCR	C24-C23-C22	-2.10	123.06	126.23
19	8	310	CLA	CMC-C2C-C1C	2.10	128.24	125.04
19	A	808	CLA	O2A-CGA-CBA	2.10	118.50	111.91
32	8	319	CHL	CHD-C4C-C3C	2.10	127.93	124.84
19	A	815	CLA	CHA-C1A-NA	-2.10	121.59	126.40
19	4	306	CLA	CHA-C1A-NA	-2.10	121.59	126.40
19	4	311	CLA	CMB-C2B-C3B	2.10	128.60	124.68
32	6	321	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
19	A	824	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
31	7	303	LUT	C8-C9-C10	-2.10	115.72	118.94
19	4	306	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
19	5	322	CLA	C3D-C2D-C1D	-2.10	102.97	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	828	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
19	7	309	CLA	C6-C5-C3	-2.10	107.95	113.45
19	B	814	CLA	CHA-C1A-NA	-2.10	121.59	126.40
19	B	840	CLA	CHA-C1A-NA	-2.10	121.59	126.40
19	Z	305	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
19	6	312	CLA	CAA-C2A-C3A	-2.10	107.04	112.78
22	B	847	BCR	C10-C11-C12	-2.10	116.67	123.22
32	4	319	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
19	4	309	CLA	CMB-C2B-C3B	2.10	128.60	124.68
19	A	811	CLA	CHA-C1A-NA	-2.10	121.60	126.40
32	5	315	CHL	CMA-C3A-C4A	2.10	117.41	111.77
23	4	320	LHG	O7-C7-O9	-2.10	118.64	123.70
19	4	318	CLA	CHA-C1A-NA	-2.10	121.60	126.40
19	B	819	CLA	O2A-CGA-CBA	2.09	118.48	111.91
19	A	813	CLA	CMB-C2B-C3B	2.09	128.60	124.68
19	A	842	CLA	CHA-C1A-NA	-2.09	121.60	126.40
19	B	805	CLA	CHA-C1A-NA	-2.09	121.60	126.40
19	A	811	CLA	CMB-C2B-C3B	2.09	128.60	124.68
19	1	5015	CLA	OBD-CAD-C3D	-2.09	123.48	128.52
19	A	825	CLA	O2A-CGA-CBA	2.09	118.48	111.91
19	B	818	CLA	O2A-CGA-CBA	2.09	118.47	111.91
32	6	319	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
19	A	820	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
22	B	843	BCR	C35-C13-C14	-2.09	119.99	122.92
19	4	316	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
19	J	1901	CLA	CAA-C2A-C3A	-2.09	109.03	114.26
19	B	827	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
19	A	804	CLA	CMB-C2B-C3B	2.09	128.59	124.68
19	B	831	CLA	CMB-C2B-C3B	2.09	128.59	124.68
19	3	5011	CLA	CHA-C1A-NA	-2.09	121.61	126.40
19	B	836	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
32	8	315	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
19	6	309	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
19	Z	304	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
32	6	315	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
19	Z	315	CLA	C11-C12-C13	-2.09	109.17	115.92
19	3	5014	CLA	O2D-CGD-O1D	-2.09	119.76	123.84
19	6	311	CLA	C7-C6-C5	-2.09	107.69	113.36
28	J	1902	C7Z	C2-C3-C4	2.09	113.16	110.30
19	5	307	CLA	C6-C7-C8	-2.09	109.17	115.92
32	1	5017	CHL	CHB-C4A-NA	2.09	127.40	124.51
19	6	309	CLA	C11-C10-C8	-2.09	109.18	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	308	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
19	1	5013	CLA	CMA-C3A-C4A	2.09	117.38	111.77
19	A	812	CLA	C2C-C1C-NC	2.09	111.93	109.97
32	8	316	CHL	CHB-C4A-NA	2.09	127.40	124.51
19	8	320	CLA	CHA-C1A-NA	-2.09	121.62	126.40
19	4	307	CLA	CHA-C1A-NA	-2.08	121.62	126.40
19	8	312	CLA	C1C-C2C-C3C	-2.08	104.77	106.96
19	B	810	CLA	C1-O2A-CGA	2.08	121.91	116.44
19	A	811	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
19	B	840	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
19	A	809	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
31	3	5003	LUT	O3-C3-C2	-2.08	105.66	109.80
19	B	840	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
19	Z	314	CLA	CHA-C1A-NA	-2.08	121.63	126.40
22	A	858	BCR	C10-C11-C12	-2.08	116.72	123.22
19	A	827	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
28	6	304	C7Z	C31-C32-C33	-2.08	120.57	126.42
19	B	830	CLA	CHA-C1A-NA	-2.08	121.63	126.40
19	B	806	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
32	6	316	CHL	C1B-CHB-C4A	-2.08	126.00	130.12
19	B	801	CLA	CMB-C2B-C3B	2.08	128.57	124.68
19	3	5015	CLA	CAA-CBA-CGA	-2.08	106.99	112.51
19	A	819	CLA	C16-C15-C13	-2.08	109.20	115.92
19	6	311	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
19	4	309	CLA	CBC-CAC-C3C	-2.08	106.70	112.43
19	8	311	CLA	CMB-C2B-C3B	2.08	128.57	124.68
19	4	310	CLA	C11-C10-C8	-2.08	109.20	115.92
32	4	315	CHL	C1B-CHB-C4A	-2.08	126.00	130.12
19	A	802	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
19	1	5016	CLA	CHA-C1A-NA	-2.08	121.64	126.40
19	3	5019	CLA	CMA-C3A-C4A	2.08	117.36	111.77
19	6	318	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
18	A	801	CL0	CMD-C2D-C3D	-2.08	122.83	127.61
19	7	309	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
19	8	309	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
31	Z	318	LUT	C11-C12-C13	-2.08	120.58	126.42
19	5	306	CLA	CHA-C1A-NA	-2.08	121.64	126.40
19	B	816	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
19	1	5006	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
19	A	823	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
19	J	1901	CLA	CMB-C2B-C3B	2.08	128.56	124.68
19	3	5013	CLA	CMB-C2B-C3B	2.08	128.56	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	4	304	LUT	C38-C25-C24	-2.08	119.12	123.56
19	B	828	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
32	7	315	CHL	CMB-C2B-C1B	-2.08	125.27	128.46
19	A	804	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
19	B	805	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
19	B	802	CLA	C6-C5-C3	-2.07	108.01	113.45
19	A	804	CLA	CHA-C1A-NA	-2.07	121.65	126.40
19	5	319	CLA	CHA-C1A-NA	-2.07	121.65	126.40
32	6	315	CHL	C1B-CHB-C4A	-2.07	126.01	130.12
19	7	310	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
19	Z	311	CLA	CBA-CAA-C2A	-2.07	107.74	113.86
19	B	835	CLA	CHA-C1A-NA	-2.07	121.65	126.40
19	A	826	CLA	CMD-C2D-C3D	-2.07	122.84	127.61
32	5	320	CHL	C2C-C3C-C4C	2.07	107.97	106.49
19	J	1901	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
19	5	321	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
19	5	322	CLA	CHA-C1A-NA	-2.07	121.65	126.40
22	8	303	BCR	C15-C14-C13	-2.07	124.35	127.31
19	A	834	CLA	CHA-C1A-NA	-2.07	121.65	126.40
19	7	310	CLA	CAA-CBA-CGA	-2.07	107.20	113.25
19	A	818	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
19	B	837	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
19	A	827	CLA	CHA-C1A-NA	-2.07	121.65	126.40
27	5	302	RRX	C11-C10-C9	-2.07	124.35	127.31
24	F	305	LMT	C1B-O5B-C5B	-2.07	109.62	113.69
19	I	201	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
32	5	315	CHL	C1B-CHB-C4A	-2.07	126.02	130.12
27	4	303	RRX	C30-C25-C26	-2.07	119.70	122.61
22	8	306	BCR	C16-C15-C14	-2.07	119.23	123.47
19	B	823	CLA	C6-C7-C8	-2.07	109.23	115.92
31	3	5003	LUT	C16-C1-C6	-2.07	106.94	110.30
19	B	834	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
19	3	5018	CLA	CAA-CBA-CGA	-2.07	107.21	113.25
19	5	307	CLA	CAA-CBA-CGA	-2.07	107.21	113.25
19	B	801	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
19	A	843	CLA	CHA-C1A-NA	-2.07	121.67	126.40
19	1	5015	CLA	CHA-C1A-NA	-2.07	121.67	126.40
19	G	1602	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
19	5	317	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
24	3	5023	LMT	O1B-C4'-C3'	2.07	112.78	107.28
19	5	309	CLA	C6-C7-C8	-2.07	109.24	115.92
19	5	301	CLA	CHA-C1A-NA	-2.06	121.67	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	819	CLA	CHA-C1A-NA	-2.06	121.67	126.40
19	G	1602	CLA	CHA-C1A-NA	-2.06	121.67	126.40
19	B	839	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
19	A	829	CLA	O2D-CGD-O1D	-2.06	119.80	123.84
19	A	857	CLA	CHA-C1A-NA	-2.06	121.67	126.40
19	K	202	CLA	CHA-C1A-NA	-2.06	121.67	126.40
19	I	201	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
19	3	5014	CLA	CHA-C1A-NA	-2.06	121.68	126.40
19	B	807	CLA	C6-C5-C3	-2.06	108.05	113.45
19	3	5014	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
19	Z	308	CLA	CAA-CBA-CGA	-2.06	107.23	113.25
19	A	808	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
19	A	813	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
29	J	1903	LMG	C7-O1-C1	-2.06	109.72	113.74
19	K	204	CLA	CHA-C1A-NA	-2.06	121.68	126.40
19	3	5019	CLA	CHA-C1A-NA	-2.06	121.68	126.40
19	Z	308	CLA	O2A-CGA-CBA	2.06	118.37	111.91
19	3	5013	CLA	C1-O2A-CGA	2.06	121.84	116.44
22	B	846	BCR	C36-C18-C17	-2.06	120.04	122.92
19	B	833	CLA	O2A-CGA-CBA	2.06	118.36	111.91
32	6	321	CHL	CHB-C4A-NA	2.06	127.36	124.51
19	B	820	CLA	CHA-C1A-NA	-2.06	121.69	126.40
32	5	320	CHL	CMA-C3A-C2A	2.06	122.12	113.83
19	1	5011	CLA	CHA-C1A-NA	-2.06	121.69	126.40
22	A	858	BCR	C29-C30-C25	2.06	113.64	110.48
32	4	319	CHL	C2C-C3C-C4C	2.06	107.95	106.49
19	A	840	CLA	CHA-C1A-NA	-2.05	121.69	126.40
19	B	838	CLA	O2A-CGA-CBA	2.05	118.36	111.91
18	A	801	CL0	C3C-C4C-NC	2.05	112.88	110.57
19	A	837	CLA	O2A-CGA-CBA	2.05	118.35	111.91
19	4	316	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
19	A	839	CLA	O2D-CGD-O1D	-2.05	119.82	123.84
19	B	817	CLA	CHA-C1A-NA	-2.05	121.69	126.40
19	1	5007	CLA	CMB-C2B-C3B	2.05	128.52	124.68
19	7	309	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
19	A	824	CLA	CHA-C1A-NA	-2.05	121.70	126.40
19	A	823	CLA	O2A-CGA-CBA	2.05	118.35	111.91
19	B	830	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
19	3	5016	CLA	CHA-C1A-NA	-2.05	121.70	126.40
19	A	806	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
19	B	832	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
32	3	5017	CHL	C1-C2-C3	-2.05	122.49	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	318	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
19	B	822	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
19	A	810	CLA	C11-C12-C13	-2.05	109.29	115.92
32	6	319	CHL	C1-C2-C3	-2.05	122.50	126.04
19	7	316	CLA	CHA-C1A-NA	-2.05	121.70	126.40
19	B	813	CLA	CMB-C2B-C3B	2.05	128.51	124.68
19	A	814	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
19	8	320	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
19	A	833	CLA	O2A-CGA-CBA	2.05	118.34	111.91
19	K	203	CLA	O2A-CGA-CBA	2.05	118.33	111.91
19	B	814	CLA	CMB-C2B-C3B	2.05	128.51	124.68
19	1	5018	CLA	CHA-C1A-NA	-2.05	121.71	126.40
19	B	802	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
19	6	310	CLA	C1-C2-C3	-2.05	122.50	126.04
19	Z	312	CLA	O2A-CGA-CBA	2.05	118.33	111.91
19	Z	315	CLA	CMD-C2D-C3D	-2.05	122.91	127.61
19	3	5012	CLA	CAA-C2A-C1A	-2.05	105.27	111.97
19	A	821	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
19	8	311	CLA	CHA-C1A-NA	-2.05	121.71	126.40
31	1	5004	LUT	C19-C9-C10	-2.04	120.06	122.92
19	B	816	CLA	CHA-C1A-NA	-2.04	121.72	126.40
19	7	319	CLA	CHA-C1A-NA	-2.04	121.72	126.40
19	8	313	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
19	A	806	CLA	C11-C10-C8	-2.04	109.32	115.92
37	8	302	SQD	O8-S-C6	-2.04	102.48	105.74
22	8	306	BCR	C34-C9-C8	2.04	121.30	118.08
19	A	815	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
22	A	850	BCR	C37-C22-C21	-2.04	120.06	122.92
19	G	1601	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
19	A	839	CLA	CHA-C1A-NA	-2.04	121.72	126.40
19	B	807	CLA	CHA-C1A-NA	-2.04	121.72	126.40
19	6	320	CLA	CHA-C1A-NA	-2.04	121.72	126.40
19	6	310	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
19	1	5013	CLA	CHA-C1A-NA	-2.04	121.72	126.40
19	A	803	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
19	4	312	CLA	CHA-C1A-NA	-2.04	121.73	126.40
31	4	304	LUT	C39-C29-C28	2.04	121.29	118.08
19	B	832	CLA	CAA-CBA-CGA	-2.04	107.29	113.25
19	7	317	CLA	O2A-CGA-CBA	2.04	118.31	111.91
19	4	318	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
32	7	315	CHL	CMA-C3A-C4A	2.04	117.25	111.77
19	5	307	CLA	CHA-C1A-NA	-2.04	121.73	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	831	CLA	O2A-CGA-CBA	2.04	118.30	111.91
19	B	811	CLA	CHA-C1A-NA	-2.04	121.73	126.40
31	4	304	LUT	C15-C35-C34	-2.04	119.30	123.47
22	A	859	BCR	C10-C11-C12	-2.04	116.86	123.22
19	5	309	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
19	A	835	CLA	CHA-C1A-NA	-2.04	121.73	126.40
22	A	848	BCR	C34-C9-C10	-2.04	120.07	122.92
19	3	5010	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	5	303	LUT	C10-C11-C12	-2.04	116.86	123.22
19	B	815	CLA	CHA-C1A-NA	-2.04	121.74	126.40
19	A	832	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
19	B	814	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
19	A	807	CLA	CHA-C1A-NA	-2.03	121.74	126.40
22	A	850	BCR	C8-C7-C6	-2.03	121.49	127.20
19	G	1601	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
19	7	319	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
19	5	301	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
19	B	823	CLA	CHA-C1A-NA	-2.03	121.74	126.40
19	3	5016	CLA	O2A-CGA-CBA	2.03	118.29	111.91
19	A	818	CLA	CHA-C1A-NA	-2.03	121.74	126.40
19	1	5011	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
19	B	806	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
19	4	313	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
33	7	321	SPH	C1-C2-C3	-2.03	108.65	113.03
22	5	304	BCR	C4-C5-C6	-2.03	119.78	122.73
19	3	5015	CLA	CHA-C1A-NA	-2.03	121.75	126.40
19	A	819	CLA	CHA-C1A-NA	-2.03	121.75	126.40
19	Z	308	CLA	C6-C5-C3	-2.03	108.14	113.45
19	B	850	CLA	CHA-C1A-NA	-2.03	121.75	126.40
19	8	318	CLA	O2A-CGA-CBA	2.03	120.24	112.23
28	6	304	C7Z	C8-C7-C6	-2.03	121.51	127.20
23	6	303	LHG	O8-C23-O10	-2.03	118.48	123.59
19	K	205	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
22	B	847	BCR	C30-C25-C24	2.03	121.51	115.78
22	7	305	BCR	C30-C25-C24	2.03	121.51	115.78
32	8	301	CHL	C1B-CHB-C4A	-2.03	126.10	130.12
19	7	310	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
22	A	858	BCR	C15-C16-C17	-2.03	119.32	123.47
31	3	5002	LUT	C21-C26-C27	-2.03	110.14	112.70
19	A	840	CLA	CMB-C2B-C3B	2.03	128.47	124.68
28	6	304	C7Z	C15-C35-C34	-2.03	119.33	123.47
19	A	843	CLA	C3D-C2D-C1D	-2.03	103.07	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	830	CLA	CHA-C1A-NA	-2.03	121.76	126.40
19	A	825	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
19	A	833	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
19	K	202	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
19	K	202	CLA	CAA-C2A-C3A	-2.02	107.23	112.78
19	A	828	CLA	CHA-C1A-NA	-2.02	121.76	126.40
19	A	808	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
19	8	307	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
19	1	5008	CLA	CHA-C1A-NA	-2.02	121.76	126.40
19	5	325	CLA	O2A-CGA-CBA	2.02	118.26	111.91
19	B	806	CLA	CMB-C2B-C3B	2.02	128.46	124.68
19	6	313	CLA	O2A-CGA-CBA	2.02	118.26	111.91
19	7	317	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
19	B	829	CLA	CMB-C2B-C3B	2.02	128.46	124.68
19	5	308	CLA	CHA-C1A-NA	-2.02	121.77	126.40
19	5	309	CLA	CMC-C2C-C1C	2.02	128.12	125.04
19	A	822	CLA	CAA-CBA-CGA	-2.02	107.35	113.25
31	Z	318	LUT	C3-C4-C5	2.02	115.88	111.85
19	5	312	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
19	B	810	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
19	A	824	CLA	O2A-CGA-CBA	2.02	118.25	111.91
22	3	5004	BCR	C28-C27-C26	-2.02	110.47	114.08
19	A	819	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
19	Z	314	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
19	B	818	CLA	CHA-C1A-NA	-2.02	121.78	126.40
19	5	310	CLA	CAA-CBA-CGA	-2.02	107.36	113.25
19	7	306	CLA	C11-C10-C8	-2.02	109.40	115.92
22	3	5006	BCR	C37-C22-C21	-2.02	120.10	122.92
28	J	1902	C7Z	C39-C29-C30	-2.02	120.10	122.92
19	3	5020	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
31	6	306	LUT	C31-C32-C33	-2.02	120.75	126.42
31	5	303	LUT	C28-C29-C30	-2.02	115.85	118.94
19	B	822	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
19	A	839	CLA	CMB-C2B-C3B	2.01	128.45	124.68
31	4	304	LUT	C19-C9-C10	-2.01	120.10	122.92
31	6	305	LUT	C4-C5-C6	-2.01	116.36	120.85
19	B	850	CLA	C5-C3-C2	2.01	125.19	121.12
22	A	846	BCR	C15-C16-C17	-2.01	119.35	123.47
19	6	318	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
19	1	5015	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
29	7	301	LMG	O7-C10-O9	-2.01	118.84	123.70
19	5	317	CLA	CAA-C2A-C1A	-2.01	105.38	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	5011	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
24	Z	301	LMT	C1B-C2B-C3B	-2.01	105.81	110.00
19	A	807	CLA	O2A-CGA-CBA	2.01	118.22	111.91
19	1	5016	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
19	A	823	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
19	B	817	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
19	B	829	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
19	6	318	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
31	7	303	LUT	C12-C13-C14	-2.01	115.86	118.94
19	4	313	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
19	Z	312	CLA	CHA-C1A-NA	-2.01	121.80	126.40
19	J	1901	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
19	B	850	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
19	5	310	CLA	OBD-CAD-C3D	-2.01	123.69	128.52
19	6	323	CLA	CMD-C2D-C3D	-2.01	123.00	127.61
19	5	310	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
19	8	311	CLA	C1-O2A-CGA	2.01	121.71	116.44
22	A	858	BCR	C20-C19-C18	-2.01	120.78	126.42
31	7	304	LUT	C20-C13-C12	2.01	121.24	118.08
32	7	314	CHL	CHB-C4A-NA	2.01	127.29	124.51
19	Z	308	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
19	A	841	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
32	5	320	CHL	CHB-C4A-NA	2.00	127.28	124.51
19	A	833	CLA	O1D-CGD-CBD	-2.00	120.38	124.48
19	5	307	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
19	8	313	CLA	CHA-C1A-NA	-2.00	121.81	126.40
19	A	804	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
19	B	816	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
19	7	316	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
19	1	5010	CLA	CAA-CBA-CGA	-2.00	107.40	113.25
19	8	318	CLA	CHA-C1A-NA	-2.00	121.81	126.40
19	3	5016	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
32	4	319	CHL	CMA-C3A-C2A	2.00	121.90	113.83
19	6	318	CLA	CHA-C1A-NA	-2.00	121.81	126.40
19	Z	304	CLA	C1-O2A-CGA	2.00	121.69	116.44
22	3	5004	BCR	C36-C18-C19	2.00	121.23	118.08
19	1	5018	CLA	C3D-C2D-C1D	-2.00	103.10	105.83

All (273) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	801	CL0	NA

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Mol	Chain	Res	Type	Atom
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	817	CLA	ND
19	A	818	CLA	ND
19	A	819	CLA	ND
19	A	820	CLA	ND
19	A	821	CLA	ND
19	A	822	CLA	ND
19	A	823	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

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Mol	Chain	Res	Type	Atom
19	A	842	CLA	ND
19	A	843	CLA	ND
19	A	857	CLA	ND
19	B	801	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
19	B	818	CLA	ND
19	B	819	CLA	ND
19	B	820	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	828	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	839	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	840	CLA	ND
19	B	850	CLA	ND
19	F	301	CLA	ND
19	F	303	CLA	ND
19	G	1601	CLA	ND
19	G	1602	CLA	ND
19	I	201	CLA	ND
19	J	1901	CLA	ND
19	K	202	CLA	ND
19	K	203	CLA	ND
19	K	204	CLA	ND
19	K	205	CLA	ND
19	1	5006	CLA	ND
19	1	5007	CLA	ND
19	1	5008	CLA	ND
19	1	5010	CLA	ND
19	1	5011	CLA	ND
19	1	5012	CLA	ND
19	1	5013	CLA	ND
19	1	5015	CLA	ND
19	1	5016	CLA	ND
19	1	5018	CLA	ND
19	Z	303	CLA	ND
19	Z	304	CLA	ND
19	Z	305	CLA	ND
19	Z	306	CLA	ND
19	Z	307	CLA	ND
19	Z	308	CLA	ND
19	Z	311	CLA	ND
19	Z	312	CLA	ND
19	Z	314	CLA	ND
19	Z	315	CLA	ND
19	3	5008	CLA	ND
19	3	5009	CLA	ND
19	3	5010	CLA	ND
19	3	5011	CLA	ND
19	3	5012	CLA	ND
19	3	5013	CLA	ND
19	3	5014	CLA	ND
19	3	5015	CLA	ND
19	3	5016	CLA	ND
19	3	5018	CLA	ND

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Mol	Chain	Res	Type	Atom
19	3	5019	CLA	ND
19	3	5020	CLA	ND
19	7	306	CLA	ND
19	7	307	CLA	ND
19	7	308	CLA	ND
19	7	309	CLA	ND
19	7	310	CLA	ND
19	7	311	CLA	ND
19	7	312	CLA	ND
19	7	313	CLA	ND
19	7	316	CLA	ND
19	7	317	CLA	ND
19	7	318	CLA	ND
19	7	319	CLA	ND
19	7	324	CLA	ND
19	8	307	CLA	ND
19	8	308	CLA	ND
19	8	309	CLA	ND
19	8	310	CLA	ND
19	8	311	CLA	ND
19	8	312	CLA	ND
19	8	313	CLA	ND
19	8	314	CLA	ND
19	8	318	CLA	ND
19	8	320	CLA	ND
19	4	306	CLA	ND
19	4	307	CLA	ND
19	4	308	CLA	ND
19	4	309	CLA	ND
19	4	310	CLA	ND
19	4	311	CLA	ND
19	4	312	CLA	ND
19	4	313	CLA	ND
19	4	316	CLA	ND
19	4	318	CLA	ND
19	5	301	CLA	ND
19	5	306	CLA	ND
19	5	307	CLA	ND
19	5	308	CLA	ND
19	5	309	CLA	ND
19	5	310	CLA	ND
19	5	311	CLA	ND

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Mol	Chain	Res	Type	Atom
19	5	312	CLA	ND
19	5	313	CLA	ND
19	5	314	CLA	ND
19	5	317	CLA	ND
19	5	319	CLA	ND
19	5	321	CLA	ND
19	5	322	CLA	ND
19	5	325	CLA	ND
19	6	301	CLA	ND
19	6	302	CLA	ND
19	6	309	CLA	ND
19	6	310	CLA	ND
19	6	311	CLA	ND
19	6	312	CLA	ND
19	6	313	CLA	ND
19	6	314	CLA	ND
19	6	318	CLA	ND
19	6	320	CLA	ND
19	6	322	CLA	ND
19	6	323	CLA	ND
32	1	5009	CHL	NA
32	1	5009	CHL	ND
32	1	5009	CHL	NC
32	1	5014	CHL	NA
32	1	5014	CHL	ND
32	1	5014	CHL	NC
32	1	5017	CHL	NA
32	1	5017	CHL	ND
32	1	5017	CHL	NC
32	Z	302	CHL	NA
32	Z	302	CHL	ND
32	Z	302	CHL	NC
32	Z	309	CHL	NA
32	Z	309	CHL	ND
32	Z	309	CHL	NC
32	Z	310	CHL	NA
32	Z	310	CHL	ND
32	Z	310	CHL	NC
32	Z	313	CHL	NA
32	Z	313	CHL	ND
32	Z	313	CHL	NC
32	3	5017	CHL	NA

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Mol	Chain	Res	Type	Atom
32	3	5017	CHL	ND
32	3	5017	CHL	NC
32	7	314	CHL	NA
32	7	314	CHL	ND
32	7	314	CHL	NC
32	7	315	CHL	NA
32	7	315	CHL	ND
32	7	315	CHL	NC
32	8	301	CHL	NA
32	8	301	CHL	ND
32	8	301	CHL	NC
32	8	315	CHL	NA
32	8	315	CHL	ND
32	8	315	CHL	NC
32	8	316	CHL	NA
32	8	316	CHL	ND
32	8	316	CHL	NC
32	8	317	CHL	NA
32	8	317	CHL	ND
32	8	317	CHL	NC
32	8	319	CHL	NA
32	8	319	CHL	ND
32	8	319	CHL	NC
32	4	314	CHL	NA
32	4	314	CHL	ND
32	4	314	CHL	NC
32	4	315	CHL	NA
32	4	315	CHL	ND
32	4	315	CHL	NC
32	4	317	CHL	NA
32	4	317	CHL	ND
32	4	317	CHL	NC
32	4	319	CHL	NA
32	4	319	CHL	ND
32	4	319	CHL	NC
32	5	315	CHL	NA
32	5	315	CHL	ND
32	5	315	CHL	NC
32	5	316	CHL	NA
32	5	316	CHL	ND
32	5	316	CHL	NC
32	5	318	CHL	NA

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Mol	Chain	Res	Type	Atom
32	5	318	CHL	ND
32	5	318	CHL	NC
32	5	320	CHL	NA
32	5	320	CHL	ND
32	5	320	CHL	NC
32	6	315	CHL	NA
32	6	315	CHL	ND
32	6	315	CHL	NC
32	6	316	CHL	NA
32	6	316	CHL	ND
32	6	316	CHL	NC
32	6	317	CHL	NA
32	6	317	CHL	ND
32	6	317	CHL	NC
32	6	319	CHL	NA
32	6	319	CHL	ND
32	6	319	CHL	NC
32	6	321	CHL	NA
32	6	321	CHL	ND
32	6	321	CHL	NC

All (3534) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	802	CLA	C2-C1-O2A-CGA
19	A	802	CLA	CHA-CBD-CGD-O1D
19	A	803	CLA	C1A-C2A-CAA-CBA
19	A	803	CLA	CBA-CGA-O2A-C1
19	A	803	CLA	O1A-CGA-O2A-C1
19	A	804	CLA	C3A-C2A-CAA-CBA
19	A	805	CLA	C3A-C2A-CAA-CBA
19	A	805	CLA	CHA-CBD-CGD-O1D
19	A	805	CLA	CHA-CBD-CGD-O2D
19	A	806	CLA	C1A-C2A-CAA-CBA
19	A	806	CLA	C3A-C2A-CAA-CBA
19	A	806	CLA	CBA-CGA-O2A-C1
19	A	807	CLA	C1A-C2A-CAA-CBA
19	A	807	CLA	C3A-C2A-CAA-CBA
19	A	808	CLA	C3A-C2A-CAA-CBA
19	A	808	CLA	CHA-CBD-CGD-O1D
19	A	808	CLA	CHA-CBD-CGD-O2D
19	A	809	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	810	CLA	C1A-C2A-CAA-CBA
19	A	810	CLA	C3A-C2A-CAA-CBA
19	A	811	CLA	C1A-C2A-CAA-CBA
19	A	811	CLA	CBD-CGD-O2D-CED
19	A	813	CLA	C11-C10-C8-C9
19	A	814	CLA	C2-C1-O2A-CGA
19	A	817	CLA	C2-C3-C5-C6
19	A	817	CLA	C4-C3-C5-C6
19	A	818	CLA	C1A-C2A-CAA-CBA
19	A	818	CLA	C3A-C2A-CAA-CBA
19	A	818	CLA	C2-C1-O2A-CGA
19	A	818	CLA	CBD-CGD-O2D-CED
19	A	819	CLA	C1A-C2A-CAA-CBA
19	A	819	CLA	C3A-C2A-CAA-CBA
19	A	822	CLA	C1A-C2A-CAA-CBA
19	A	822	CLA	C3A-C2A-CAA-CBA
19	A	822	CLA	C2-C1-O2A-CGA
19	A	823	CLA	C1A-C2A-CAA-CBA
19	A	824	CLA	C1A-C2A-CAA-CBA
19	A	824	CLA	C3A-C2A-CAA-CBA
19	A	825	CLA	C2-C1-O2A-CGA
19	A	826	CLA	C1A-C2A-CAA-CBA
19	A	826	CLA	C3A-C2A-CAA-CBA
19	A	826	CLA	C11-C10-C8-C9
19	A	828	CLA	CBD-CGD-O2D-CED
19	A	830	CLA	CBD-CGD-O2D-CED
19	A	832	CLA	C1A-C2A-CAA-CBA
19	A	834	CLA	CBD-CGD-O2D-CED
19	A	836	CLA	C1A-C2A-CAA-CBA
19	A	836	CLA	C3A-C2A-CAA-CBA
19	A	838	CLA	C1A-C2A-CAA-CBA
19	A	838	CLA	C3A-C2A-CAA-CBA
19	A	838	CLA	C2-C1-O2A-CGA
19	A	839	CLA	C2-C1-O2A-CGA
19	A	839	CLA	CHA-CBD-CGD-O1D
19	A	840	CLA	C1A-C2A-CAA-CBA
19	A	841	CLA	C1A-C2A-CAA-CBA
19	A	841	CLA	C3A-C2A-CAA-CBA
19	A	841	CLA	CBD-CGD-O2D-CED
19	A	843	CLA	C2-C1-O2A-CGA
19	A	843	CLA	CHA-CBD-CGD-O1D
19	A	843	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	A	857	CLA	C2A-CAA-CBA-CGA
19	A	857	CLA	C2-C1-O2A-CGA
19	B	801	CLA	CHA-CBD-CGD-O1D
19	B	802	CLA	CHA-CBD-CGD-O1D
19	B	802	CLA	CHA-CBD-CGD-O2D
19	B	802	CLA	CBD-CGD-O2D-CED
19	B	803	CLA	C2-C1-O2A-CGA
19	B	804	CLA	CHA-CBD-CGD-O1D
19	B	804	CLA	CHA-CBD-CGD-O2D
19	B	804	CLA	CBD-CGD-O2D-CED
19	B	804	CLA	C6-C7-C8-C9
19	B	805	CLA	C1A-C2A-CAA-CBA
19	B	807	CLA	C6-C7-C8-C9
19	B	808	CLA	C1A-C2A-CAA-CBA
19	B	808	CLA	C3A-C2A-CAA-CBA
19	B	808	CLA	C2-C1-O2A-CGA
19	B	809	CLA	C3A-C2A-CAA-CBA
19	B	810	CLA	C1A-C2A-CAA-CBA
19	B	810	CLA	C3A-C2A-CAA-CBA
19	B	810	CLA	CBA-CGA-O2A-C1
19	B	810	CLA	O1A-CGA-O2A-C1
19	B	810	CLA	CBD-CGD-O2D-CED
19	B	812	CLA	C1A-C2A-CAA-CBA
19	B	812	CLA	C3A-C2A-CAA-CBA
19	B	812	CLA	C2-C1-O2A-CGA
19	B	812	CLA	C6-C7-C8-C9
19	B	813	CLA	CHA-CBD-CGD-O1D
19	B	813	CLA	CHA-CBD-CGD-O2D
19	B	813	CLA	C11-C12-C13-C14
19	B	815	CLA	C1A-C2A-CAA-CBA
19	B	815	CLA	C3A-C2A-CAA-CBA
19	B	815	CLA	CHA-CBD-CGD-O2D
19	B	816	CLA	CBD-CGD-O2D-CED
19	B	817	CLA	C1A-C2A-CAA-CBA
19	B	817	CLA	C3A-C2A-CAA-CBA
19	B	817	CLA	C2-C1-O2A-CGA
19	B	818	CLA	C1A-C2A-CAA-CBA
19	B	818	CLA	C3A-C2A-CAA-CBA
19	B	818	CLA	C6-C7-C8-C9
19	B	819	CLA	C1A-C2A-CAA-CBA
19	B	819	CLA	C3A-C2A-CAA-CBA
19	B	820	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	B	820	CLA	C3A-C2A-CAA-CBA
19	B	821	CLA	CBA-CGA-O2A-C1
19	B	821	CLA	O1A-CGA-O2A-C1
19	B	822	CLA	C1A-C2A-CAA-CBA
19	B	823	CLA	C3A-C2A-CAA-CBA
19	B	824	CLA	CHA-CBD-CGD-O1D
19	B	824	CLA	CHA-CBD-CGD-O2D
19	B	825	CLA	C3A-C2A-CAA-CBA
19	B	825	CLA	C2-C3-C5-C6
19	B	825	CLA	C4-C3-C5-C6
19	B	827	CLA	C1A-C2A-CAA-CBA
19	B	827	CLA	C3A-C2A-CAA-CBA
19	B	827	CLA	C2-C1-O2A-CGA
19	B	827	CLA	CBD-CGD-O2D-CED
19	B	828	CLA	C1A-C2A-CAA-CBA
19	B	828	CLA	C3A-C2A-CAA-CBA
19	B	828	CLA	C6-C7-C8-C9
19	B	829	CLA	C1A-C2A-CAA-CBA
19	B	831	CLA	C1A-C2A-CAA-CBA
19	B	831	CLA	C3A-C2A-CAA-CBA
19	B	832	CLA	C1A-C2A-CAA-CBA
19	B	832	CLA	C3A-C2A-CAA-CBA
19	B	833	CLA	C2-C1-O2A-CGA
19	B	833	CLA	CBD-CGD-O2D-CED
19	B	835	CLA	CBD-CGD-O2D-CED
19	B	836	CLA	C1A-C2A-CAA-CBA
19	B	836	CLA	C3A-C2A-CAA-CBA
19	B	836	CLA	C2-C1-O2A-CGA
19	B	836	CLA	C2-C3-C5-C6
19	B	836	CLA	C4-C3-C5-C6
19	B	837	CLA	C1A-C2A-CAA-CBA
19	B	837	CLA	C2-C1-O2A-CGA
19	B	839	CLA	CBD-CGD-O2D-CED
19	B	840	CLA	C3A-C2A-CAA-CBA
19	B	840	CLA	CHA-CBD-CGD-O1D
19	B	840	CLA	CHA-CBD-CGD-O2D
19	B	850	CLA	CBA-CGA-O2A-C1
19	B	850	CLA	O1A-CGA-O2A-C1
19	B	850	CLA	CAD-CBD-CGD-O1D
19	B	850	CLA	CAD-CBD-CGD-O2D
19	F	303	CLA	CBD-CGD-O2D-CED
19	G	1601	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	G	1601	CLA	C3A-C2A-CAA-CBA
19	G	1601	CLA	C2-C1-O2A-CGA
19	G	1602	CLA	CBA-CGA-O2A-C1
19	I	201	CLA	C1A-C2A-CAA-CBA
19	I	201	CLA	C3A-C2A-CAA-CBA
19	I	201	CLA	C2-C1-O2A-CGA
19	J	1901	CLA	C1A-C2A-CAA-CBA
19	J	1901	CLA	CHA-CBD-CGD-O1D
19	K	203	CLA	C1A-C2A-CAA-CBA
19	K	204	CLA	C2-C1-O2A-CGA
19	K	205	CLA	C3A-C2A-CAA-CBA
19	K	205	CLA	CBD-CGD-O2D-CED
19	1	5006	CLA	C1A-C2A-CAA-CBA
19	1	5006	CLA	C3A-C2A-CAA-CBA
19	1	5008	CLA	CHA-CBD-CGD-O1D
19	1	5008	CLA	CHA-CBD-CGD-O2D
19	1	5011	CLA	C1A-C2A-CAA-CBA
19	1	5011	CLA	C3A-C2A-CAA-CBA
19	1	5016	CLA	C3A-C2A-CAA-CBA
19	1	5016	CLA	CBD-CGD-O2D-CED
19	1	5018	CLA	CHA-CBD-CGD-O1D
19	1	5018	CLA	CHA-CBD-CGD-O2D
19	Z	305	CLA	C3A-C2A-CAA-CBA
19	Z	305	CLA	C6-C7-C8-C9
19	Z	306	CLA	C3A-C2A-CAA-CBA
19	Z	306	CLA	C2A-CAA-CBA-CGA
19	Z	306	CLA	C2-C1-O2A-CGA
19	Z	307	CLA	C4-C3-C5-C6
19	Z	311	CLA	CBD-CGD-O2D-CED
19	Z	312	CLA	C1A-C2A-CAA-CBA
19	Z	312	CLA	C3A-C2A-CAA-CBA
19	Z	314	CLA	CBD-CGD-O2D-CED
19	3	5008	CLA	C1A-C2A-CAA-CBA
19	3	5010	CLA	C2-C1-O2A-CGA
19	3	5011	CLA	C2-C1-O2A-CGA
19	3	5013	CLA	C1A-C2A-CAA-CBA
19	3	5013	CLA	C3A-C2A-CAA-CBA
19	3	5014	CLA	C1A-C2A-CAA-CBA
19	3	5014	CLA	C3A-C2A-CAA-CBA
19	3	5014	CLA	CHA-CBD-CGD-O1D
19	3	5016	CLA	C1A-C2A-CAA-CBA
19	3	5016	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	3	5018	CLA	C1A-C2A-CAA-CBA
19	3	5018	CLA	C3A-C2A-CAA-CBA
19	3	5020	CLA	C1A-C2A-CAA-CBA
19	3	5020	CLA	CBA-CGA-O2A-C1
19	3	5020	CLA	O1A-CGA-O2A-C1
19	7	306	CLA	C1A-C2A-CAA-CBA
19	7	306	CLA	C2-C1-O2A-CGA
19	7	308	CLA	C1A-C2A-CAA-CBA
19	7	309	CLA	C2-C1-O2A-CGA
19	7	310	CLA	CBA-CGA-O2A-C1
19	7	310	CLA	O1A-CGA-O2A-C1
19	7	311	CLA	C1A-C2A-CAA-CBA
19	7	311	CLA	C3A-C2A-CAA-CBA
19	7	317	CLA	C3A-C2A-CAA-CBA
19	7	318	CLA	C1A-C2A-CAA-CBA
19	7	319	CLA	CBA-CGA-O2A-C1
19	7	324	CLA	C2-C1-O2A-CGA
19	7	324	CLA	CBD-CGD-O2D-CED
19	8	307	CLA	C1A-C2A-CAA-CBA
19	8	307	CLA	C3A-C2A-CAA-CBA
19	8	307	CLA	C11-C10-C8-C9
19	8	309	CLA	C1A-C2A-CAA-CBA
19	8	310	CLA	C1A-C2A-CAA-CBA
19	8	310	CLA	C2-C1-O2A-CGA
19	8	312	CLA	C1A-C2A-CAA-CBA
19	8	312	CLA	C3A-C2A-CAA-CBA
19	8	313	CLA	C1A-C2A-CAA-CBA
19	8	313	CLA	C3A-C2A-CAA-CBA
19	8	314	CLA	C1A-C2A-CAA-CBA
19	8	318	CLA	C3A-C2A-CAA-CBA
19	4	306	CLA	C1A-C2A-CAA-CBA
19	4	306	CLA	C3A-C2A-CAA-CBA
19	4	306	CLA	CBD-CGD-O2D-CED
19	4	307	CLA	C2-C1-O2A-CGA
19	4	308	CLA	C1A-C2A-CAA-CBA
19	4	308	CLA	C3A-C2A-CAA-CBA
19	4	309	CLA	C3A-C2A-CAA-CBA
19	4	310	CLA	CBA-CGA-O2A-C1
19	4	310	CLA	O1A-CGA-O2A-C1
19	4	310	CLA	CBD-CGD-O2D-CED
19	4	312	CLA	CHA-CBD-CGD-O1D
19	4	312	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	4	313	CLA	C2-C1-O2A-CGA
19	4	313	CLA	CBD-CGD-O2D-CED
19	4	316	CLA	C1A-C2A-CAA-CBA
19	4	316	CLA	C3A-C2A-CAA-CBA
19	4	318	CLA	CHA-CBD-CGD-O1D
19	4	318	CLA	CHA-CBD-CGD-O2D
19	4	318	CLA	CBD-CGD-O2D-CED
19	5	301	CLA	C1A-C2A-CAA-CBA
19	5	301	CLA	C3A-C2A-CAA-CBA
19	5	301	CLA	C2-C1-O2A-CGA
19	5	301	CLA	CBD-CGD-O2D-CED
19	5	306	CLA	C1A-C2A-CAA-CBA
19	5	306	CLA	C3A-C2A-CAA-CBA
19	5	306	CLA	C2-C3-C5-C6
19	5	306	CLA	C4-C3-C5-C6
19	5	306	CLA	C11-C10-C8-C9
19	5	309	CLA	C3A-C2A-CAA-CBA
19	5	310	CLA	C1A-C2A-CAA-CBA
19	5	310	CLA	C2A-CAA-CBA-CGA
19	5	310	CLA	CBD-CGD-O2D-CED
19	5	311	CLA	C1A-C2A-CAA-CBA
19	5	311	CLA	C3A-C2A-CAA-CBA
19	5	311	CLA	C2-C1-O2A-CGA
19	5	311	CLA	CBD-CGD-O2D-CED
19	5	313	CLA	C1A-C2A-CAA-CBA
19	5	313	CLA	CBD-CGD-O2D-CED
19	5	314	CLA	CHA-CBD-CGD-O1D
19	5	314	CLA	CHA-CBD-CGD-O2D
19	5	314	CLA	CBD-CGD-O2D-CED
19	5	317	CLA	C1A-C2A-CAA-CBA
19	5	317	CLA	C3A-C2A-CAA-CBA
19	5	319	CLA	C1A-C2A-CAA-CBA
19	5	319	CLA	C3A-C2A-CAA-CBA
19	5	321	CLA	C1A-C2A-CAA-CBA
19	5	321	CLA	C3A-C2A-CAA-CBA
19	5	321	CLA	C11-C12-C13-C14
19	5	325	CLA	C1A-C2A-CAA-CBA
19	5	325	CLA	CBD-CGD-O2D-CED
19	6	309	CLA	C1A-C2A-CAA-CBA
19	6	310	CLA	C2-C1-O2A-CGA
19	6	311	CLA	C2-C1-O2A-CGA
19	6	312	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	6	313	CLA	C1A-C2A-CAA-CBA
19	6	313	CLA	C2-C1-O2A-CGA
19	6	313	CLA	C6-C7-C8-C9
19	6	318	CLA	C1A-C2A-CAA-CBA
19	6	318	CLA	C3A-C2A-CAA-CBA
19	6	320	CLA	C3A-C2A-CAA-CBA
19	6	322	CLA	C1A-C2A-CAA-CBA
19	6	322	CLA	CHA-CBD-CGD-O1D
19	6	322	CLA	CHA-CBD-CGD-O2D
20	B	841	PQN	C17-C18-C20-C21
22	A	846	BCR	C1-C6-C7-C8
22	A	846	BCR	C5-C6-C7-C8
22	A	846	BCR	C7-C8-C9-C10
22	A	846	BCR	C7-C8-C9-C34
22	A	846	BCR	C11-C12-C13-C14
22	A	846	BCR	C11-C12-C13-C35
22	A	846	BCR	C21-C22-C23-C24
22	A	846	BCR	C37-C22-C23-C24
22	A	847	BCR	C11-C12-C13-C14
22	A	847	BCR	C11-C12-C13-C35
22	A	847	BCR	C21-C22-C23-C24
22	A	847	BCR	C37-C22-C23-C24
22	A	848	BCR	C7-C8-C9-C10
22	A	848	BCR	C7-C8-C9-C34
22	A	848	BCR	C11-C12-C13-C14
22	A	848	BCR	C11-C12-C13-C35
22	A	849	BCR	C5-C6-C7-C8
22	A	849	BCR	C11-C12-C13-C14
22	A	849	BCR	C11-C12-C13-C35
22	A	849	BCR	C13-C14-C15-C16
22	A	849	BCR	C15-C16-C17-C18
22	A	849	BCR	C17-C18-C19-C20
22	A	849	BCR	C36-C18-C19-C20
22	A	849	BCR	C19-C20-C21-C22
22	A	849	BCR	C37-C22-C23-C24
22	A	850	BCR	C11-C12-C13-C14
22	A	850	BCR	C11-C12-C13-C35
22	A	858	BCR	C7-C8-C9-C10
22	A	858	BCR	C7-C8-C9-C34
22	A	858	BCR	C11-C12-C13-C14
22	A	858	BCR	C11-C12-C13-C35
22	A	858	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
22	A	858	BCR	C36-C18-C19-C20
22	A	858	BCR	C21-C22-C23-C24
22	A	858	BCR	C37-C22-C23-C24
22	A	859	BCR	C11-C12-C13-C14
22	A	859	BCR	C11-C12-C13-C35
22	B	842	BCR	C1-C6-C7-C8
22	B	842	BCR	C11-C12-C13-C14
22	B	842	BCR	C21-C22-C23-C24
22	B	842	BCR	C37-C22-C23-C24
22	B	843	BCR	C5-C6-C7-C8
22	B	843	BCR	C7-C8-C9-C10
22	B	843	BCR	C7-C8-C9-C34
22	B	843	BCR	C9-C10-C11-C12
22	B	843	BCR	C36-C18-C19-C20
22	B	844	BCR	C19-C20-C21-C22
22	B	845	BCR	C7-C8-C9-C10
22	B	845	BCR	C7-C8-C9-C34
22	B	845	BCR	C11-C12-C13-C14
22	B	845	BCR	C11-C12-C13-C35
22	B	845	BCR	C36-C18-C19-C20
22	B	845	BCR	C21-C22-C23-C24
22	B	845	BCR	C37-C22-C23-C24
22	B	846	BCR	C1-C6-C7-C8
22	B	846	BCR	C11-C12-C13-C14
22	B	846	BCR	C11-C12-C13-C35
22	B	846	BCR	C17-C18-C19-C20
22	B	846	BCR	C36-C18-C19-C20
22	B	847	BCR	C1-C6-C7-C8
22	B	847	BCR	C7-C8-C9-C10
22	B	847	BCR	C7-C8-C9-C34
22	B	847	BCR	C15-C16-C17-C18
22	B	847	BCR	C19-C20-C21-C22
22	B	847	BCR	C21-C22-C23-C24
22	B	847	BCR	C37-C22-C23-C24
22	F	302	BCR	C7-C8-C9-C10
22	F	302	BCR	C7-C8-C9-C34
22	F	302	BCR	C11-C12-C13-C14
22	F	302	BCR	C11-C12-C13-C35
22	F	302	BCR	C21-C22-C23-C24
22	F	302	BCR	C37-C22-C23-C24
22	G	1603	BCR	C1-C6-C7-C8
22	G	1603	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	G	1603	BCR	C37-C22-C23-C24
22	K	206	BCR	C15-C16-C17-C18
22	K	206	BCR	C21-C22-C23-C24
22	K	206	BCR	C37-C22-C23-C24
22	K	206	BCR	C23-C24-C25-C26
22	3	5004	BCR	C1-C6-C7-C8
22	3	5004	BCR	C21-C22-C23-C24
22	3	5004	BCR	C37-C22-C23-C24
22	3	5005	BCR	C7-C8-C9-C10
22	3	5005	BCR	C7-C8-C9-C34
22	3	5005	BCR	C11-C12-C13-C35
22	3	5006	BCR	C1-C6-C7-C8
22	3	5006	BCR	C23-C24-C25-C30
22	3	5007	BCR	C7-C8-C9-C10
22	3	5007	BCR	C7-C8-C9-C34
22	3	5007	BCR	C15-C16-C17-C18
22	3	5007	BCR	C17-C18-C19-C20
22	3	5007	BCR	C36-C18-C19-C20
22	3	5007	BCR	C21-C22-C23-C24
22	3	5007	BCR	C37-C22-C23-C24
22	7	305	BCR	C7-C8-C9-C10
22	7	305	BCR	C7-C8-C9-C34
22	7	305	BCR	C11-C12-C13-C14
22	7	305	BCR	C11-C12-C13-C35
22	7	305	BCR	C17-C18-C19-C20
22	7	305	BCR	C36-C18-C19-C20
22	7	305	BCR	C23-C24-C25-C26
22	8	303	BCR	C1-C6-C7-C8
22	8	303	BCR	C5-C6-C7-C8
22	8	303	BCR	C15-C16-C17-C18
22	8	303	BCR	C17-C18-C19-C20
22	8	303	BCR	C36-C18-C19-C20
22	8	303	BCR	C23-C24-C25-C26
22	8	306	BCR	C11-C12-C13-C14
22	8	306	BCR	C11-C12-C13-C35
22	8	306	BCR	C17-C18-C19-C20
22	8	306	BCR	C36-C18-C19-C20
22	8	306	BCR	C23-C24-C25-C30
22	4	305	BCR	C1-C6-C7-C8
22	4	305	BCR	C13-C14-C15-C16
22	4	305	BCR	C15-C16-C17-C18
22	4	305	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
22	4	305	BCR	C36-C18-C19-C20
22	5	304	BCR	C1-C6-C7-C8
22	5	304	BCR	C5-C6-C7-C8
22	5	304	BCR	C11-C12-C13-C35
22	6	307	BCR	C17-C18-C19-C20
22	6	307	BCR	C36-C18-C19-C20
22	6	308	BCR	C1-C6-C7-C8
22	6	308	BCR	C5-C6-C7-C8
22	6	308	BCR	C9-C10-C11-C12
22	6	308	BCR	C11-C12-C13-C14
22	6	308	BCR	C11-C12-C13-C35
23	A	851	LHG	C1-C2-C3-O3
23	A	851	LHG	C4-O6-P-O5
23	A	851	LHG	C8-C7-O7-C5
23	A	852	LHG	O1-C1-C2-C3
23	A	852	LHG	C1-C2-C3-O3
23	A	852	LHG	O2-C2-C3-O3
23	A	852	LHG	C3-O3-P-O5
23	A	852	LHG	C4-O6-P-O5
23	1	5001	LHG	O1-C1-C2-C3
23	1	5001	LHG	C1-C2-C3-O3
23	1	5001	LHG	C3-O3-P-O5
23	1	5001	LHG	C4-O6-P-O4
23	1	5001	LHG	O9-C7-O7-C5
23	1	5019	LHG	O1-C1-C2-C3
23	1	5019	LHG	C3-O3-P-O5
23	Z	316	LHG	C1-C2-C3-O3
23	3	5021	LHG	O1-C1-C2-O2
23	3	5021	LHG	C1-C2-C3-O3
23	3	5021	LHG	C3-O3-P-O4
23	3	5021	LHG	O9-C7-O7-C5
23	7	320	LHG	C3-O3-P-O4
23	8	321	LHG	O1-C1-C2-C3
23	8	321	LHG	C3-O3-P-O5
23	4	320	LHG	C6-C5-O7-C7
23	4	320	LHG	C8-C7-O7-C5
23	5	323	LHG	C1-C2-C3-O3
23	5	323	LHG	C3-O3-P-O5
23	5	323	LHG	C4-O6-P-O4
23	5	323	LHG	O9-C7-O7-C5
23	5	323	LHG	C8-C7-O7-C5
23	6	303	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
23	6	303	LHG	C3-O3-P-O4
23	6	303	LHG	C3-O3-P-O5
23	6	303	LHG	C4-O6-P-O5
23	6	303	LHG	O7-C5-C6-O8
23	6	324	LHG	O2-C2-C3-O3
23	6	324	LHG	C8-C7-O7-C5
24	A	853	LMT	C2-C1-O1'-C1'
24	A	855	LMT	C2'-C1'-O1'-C1
24	A	855	LMT	C2-C1-O1'-C1'
24	A	856	LMT	O5'-C1'-O1'-C1
24	A	856	LMT	C2-C1-O1'-C1'
24	1	5002	LMT	O5'-C1'-O1'-C1
24	Z	301	LMT	C2'-C1'-O1'-C1
24	Z	301	LMT	O5'-C1'-O1'-C1
24	Z	319	LMT	C2'-C1'-O1'-C1
24	Z	319	LMT	O5'-C1'-O1'-C1
24	7	323	LMT	O5'-C1'-O1'-C1
24	8	323	LMT	C2-C1-O1'-C1'
24	8	324	LMT	O5'-C1'-O1'-C1
24	4	321	LMT	O5'-C1'-O1'-C1
24	4	322	LMT	C2'-C1'-O1'-C1
24	4	322	LMT	C2-C1-O1'-C1'
25	B	848	DGD	O1B-C1B-O2G-C2G
27	F	304	RRX	C23-C24-C25-C26
27	F	304	RRX	C1-C6-C7-C8
27	F	304	RRX	C5-C6-C7-C8
27	4	303	RRX	C37-C22-C23-C24
27	4	303	RRX	C21-C22-C23-C24
27	4	303	RRX	C7-C8-C9-C10
27	4	303	RRX	C7-C8-C9-C34
27	4	303	RRX	C5-C6-C7-C8
28	J	1902	C7Z	C7-C8-C9-C19
28	J	1902	C7Z	C7-C8-C9-C10
28	J	1902	C7Z	C31-C32-C33-C34
28	J	1902	C7Z	C31-C32-C33-C40
28	1	5005	C7Z	C21-C26-C27-C28
28	1	5005	C7Z	C7-C8-C9-C19
28	1	5005	C7Z	C7-C8-C9-C10
28	1	5005	C7Z	C31-C32-C33-C34
28	1	5005	C7Z	C31-C32-C33-C40
28	1	5005	C7Z	C27-C28-C29-C30
28	6	304	C7Z	C21-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
28	6	304	C7Z	C11-C12-C13-C20
28	6	304	C7Z	C11-C12-C13-C14
28	6	304	C7Z	C31-C32-C33-C34
28	6	304	C7Z	C31-C32-C33-C40
29	J	1903	LMG	C11-C10-O7-C8
29	7	301	LMG	C11-C10-O7-C8
31	1	5003	LUT	C7-C8-C9-C10
31	1	5003	LUT	C7-C8-C9-C19
31	1	5003	LUT	C11-C12-C13-C14
31	1	5003	LUT	C11-C12-C13-C20
31	Z	318	LUT	C11-C12-C13-C14
31	Z	318	LUT	C11-C12-C13-C20
31	Z	318	LUT	C31-C32-C33-C34
31	Z	318	LUT	C31-C32-C33-C40
31	3	5002	LUT	C11-C12-C13-C14
31	3	5002	LUT	C11-C12-C13-C20
31	3	5003	LUT	C21-C26-C27-C28
31	7	303	LUT	C7-C8-C9-C10
31	7	303	LUT	C7-C8-C9-C19
31	7	303	LUT	C11-C12-C13-C14
31	7	303	LUT	C11-C12-C13-C20
31	7	304	LUT	C21-C26-C27-C28
31	8	304	LUT	C21-C26-C27-C28
31	8	304	LUT	C25-C26-C27-C28
31	8	305	LUT	C7-C8-C9-C19
31	4	304	LUT	C1-C6-C7-C8
31	4	304	LUT	C5-C6-C7-C8
31	4	304	LUT	C11-C12-C13-C14
31	4	304	LUT	C11-C12-C13-C20
31	5	303	LUT	C1-C6-C7-C8
31	5	303	LUT	C5-C6-C7-C8
31	5	303	LUT	C7-C8-C9-C10
31	5	303	LUT	C7-C8-C9-C19
31	5	303	LUT	C11-C12-C13-C14
31	5	303	LUT	C11-C12-C13-C20
31	5	303	LUT	C31-C32-C33-C34
31	5	303	LUT	C31-C32-C33-C40
31	6	305	LUT	C7-C8-C9-C10
31	6	305	LUT	C11-C12-C13-C14
31	6	305	LUT	C11-C12-C13-C20
31	6	306	LUT	C11-C12-C13-C14
31	6	306	LUT	C11-C12-C13-C20

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Mol	Chain	Res	Type	Atoms
31	6	306	LUT	C21-C26-C27-C28
31	6	306	LUT	C25-C26-C27-C28
32	1	5009	CHL	C1A-C2A-CAA-CBA
32	1	5009	CHL	C3A-C2A-CAA-CBA
32	Z	302	CHL	C1A-C2A-CAA-CBA
32	Z	302	CHL	C3A-C2A-CAA-CBA
32	Z	310	CHL	C2C-C3C-CAC-CBC
32	Z	310	CHL	C4C-C3C-CAC-CBC
32	7	314	CHL	C1A-C2A-CAA-CBA
32	7	314	CHL	C3A-C2A-CAA-CBA
32	7	315	CHL	C1A-C2A-CAA-CBA
32	7	315	CHL	C3A-C2A-CAA-CBA
32	8	316	CHL	C1A-C2A-CAA-CBA
32	8	319	CHL	C2-C1-O2A-CGA
32	4	317	CHL	C11-C12-C13-C14
32	6	316	CHL	C1A-C2A-CAA-CBA
32	6	316	CHL	C3A-C2A-CAA-CBA
32	6	316	CHL	CHA-CBD-CGD-O1D
32	6	316	CHL	CHA-CBD-CGD-O2D
32	6	317	CHL	C1A-C2A-CAA-CBA
32	6	317	CHL	C3A-C2A-CAA-CBA
33	3	5001	SPH	O1-C1-C2-N2
33	3	5001	SPH	O1-C1-C2-C3
33	3	5001	SPH	C1-C2-C3-O3
33	3	5001	SPH	C1-C2-C3-C4
33	3	5001	SPH	N2-C2-C3-C4
33	3	5001	SPH	C2-C3-C4-C5
33	3	5001	SPH	O3-C3-C4-C5
33	7	321	SPH	O1-C1-C2-N2
33	7	321	SPH	C1-C2-C3-O3
33	7	321	SPH	C1-C2-C3-C4
33	7	321	SPH	N2-C2-C3-C4
33	4	301	SPH	C2-C3-C4-C5
33	4	301	SPH	O3-C3-C4-C5
34	3	5022	3PH	C3-C2-O21-C21
34	8	322	3PH	C1-O11-P-O13
34	8	322	3PH	C1-O11-P-O14
34	8	322	3PH	C22-C21-O21-C2
34	5	324	3PH	O22-C21-O21-C2
34	5	324	3PH	C22-C21-O21-C2
35	7	302	DGA	CG1-CG2-CG3-OXT
35	7	302	DGA	OG2-CG2-CG3-OXT

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Mol	Chain	Res	Type	Atoms
37	8	302	SQD	C8-C7-O47-C45
38	8	325	ERG	C13-C17-C20-C21
38	8	325	ERG	C13-C17-C20-C22
38	8	325	ERG	C16-C17-C20-C21
38	8	325	ERG	C16-C17-C20-C22
38	6	326	ERG	C16-C17-C20-C21
38	6	326	ERG	C16-C17-C20-C22
19	4	311	CLA	C2C-C3C-CAC-CBC
19	A	828	CLA	O1D-CGD-O2D-CED
19	A	842	CLA	O1D-CGD-O2D-CED
19	B	834	CLA	O1D-CGD-O2D-CED
19	K	205	CLA	O1D-CGD-O2D-CED
19	5	307	CLA	O1D-CGD-O2D-CED
19	5	310	CLA	O1D-CGD-O2D-CED
19	A	817	CLA	O1D-CGD-O2D-CED
19	B	802	CLA	O1D-CGD-O2D-CED
19	B	804	CLA	O1D-CGD-O2D-CED
19	B	807	CLA	O1D-CGD-O2D-CED
19	B	809	CLA	O1D-CGD-O2D-CED
19	B	810	CLA	O1D-CGD-O2D-CED
19	G	1601	CLA	O1D-CGD-O2D-CED
19	J	1901	CLA	O1D-CGD-O2D-CED
19	1	5016	CLA	O1D-CGD-O2D-CED
19	3	5009	CLA	O1D-CGD-O2D-CED
19	7	307	CLA	O1D-CGD-O2D-CED
19	8	320	CLA	O1D-CGD-O2D-CED
19	4	318	CLA	O1D-CGD-O2D-CED
19	5	313	CLA	O1D-CGD-O2D-CED
19	5	314	CLA	O1D-CGD-O2D-CED
19	6	310	CLA	O1D-CGD-O2D-CED
19	A	802	CLA	CBD-CGD-O2D-CED
19	A	808	CLA	CBD-CGD-O2D-CED
19	A	816	CLA	CBD-CGD-O2D-CED
19	A	817	CLA	CBD-CGD-O2D-CED
19	A	821	CLA	CBD-CGD-O2D-CED
19	A	823	CLA	CBD-CGD-O2D-CED
19	A	825	CLA	CBD-CGD-O2D-CED
19	A	826	CLA	CBD-CGD-O2D-CED
19	A	827	CLA	CBD-CGD-O2D-CED
19	A	833	CLA	CBD-CGD-O2D-CED
19	A	835	CLA	CBD-CGD-O2D-CED
19	A	842	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	843	CLA	CBD-CGD-O2D-CED
19	B	801	CLA	CBD-CGD-O2D-CED
19	B	803	CLA	CBD-CGD-O2D-CED
19	B	805	CLA	CBD-CGD-O2D-CED
19	B	807	CLA	CBD-CGD-O2D-CED
19	B	809	CLA	CBD-CGD-O2D-CED
19	B	811	CLA	CBD-CGD-O2D-CED
19	B	817	CLA	CBD-CGD-O2D-CED
19	B	820	CLA	CBD-CGD-O2D-CED
19	B	822	CLA	CBD-CGD-O2D-CED
19	B	826	CLA	CBD-CGD-O2D-CED
19	B	829	CLA	CBD-CGD-O2D-CED
19	B	834	CLA	CBD-CGD-O2D-CED
19	B	838	CLA	CBD-CGD-O2D-CED
19	G	1601	CLA	CBD-CGD-O2D-CED
19	G	1602	CLA	CBD-CGD-O2D-CED
19	J	1901	CLA	CBD-CGD-O2D-CED
19	K	204	CLA	CBD-CGD-O2D-CED
19	1	5007	CLA	CBD-CGD-O2D-CED
19	1	5011	CLA	CBD-CGD-O2D-CED
19	1	5015	CLA	CBD-CGD-O2D-CED
19	Z	306	CLA	CBD-CGD-O2D-CED
19	3	5009	CLA	CBD-CGD-O2D-CED
19	3	5016	CLA	CBD-CGD-O2D-CED
19	7	307	CLA	CBD-CGD-O2D-CED
19	7	310	CLA	CBD-CGD-O2D-CED
19	7	318	CLA	CBD-CGD-O2D-CED
19	7	319	CLA	CBD-CGD-O2D-CED
19	8	309	CLA	CBD-CGD-O2D-CED
19	8	310	CLA	CBD-CGD-O2D-CED
19	8	320	CLA	CBD-CGD-O2D-CED
19	4	307	CLA	CBD-CGD-O2D-CED
19	5	306	CLA	CBD-CGD-O2D-CED
19	5	307	CLA	CBD-CGD-O2D-CED
19	5	319	CLA	CBD-CGD-O2D-CED
19	5	322	CLA	CBD-CGD-O2D-CED
19	6	310	CLA	CBD-CGD-O2D-CED
32	3	5017	CHL	CBD-CGD-O2D-CED
32	6	316	CHL	CBD-CGD-O2D-CED
19	A	804	CLA	O1A-CGA-O2A-C1
19	A	806	CLA	O1A-CGA-O2A-C1
19	A	807	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	813	CLA	O1A-CGA-O2A-C1
19	A	815	CLA	O1A-CGA-O2A-C1
19	A	816	CLA	O1A-CGA-O2A-C1
19	B	825	CLA	O1A-CGA-O2A-C1
19	1	5013	CLA	O1A-CGA-O2A-C1
19	7	312	CLA	O1A-CGA-O2A-C1
19	7	319	CLA	O1A-CGA-O2A-C1
19	4	311	CLA	O1A-CGA-O2A-C1
29	7	301	LMG	O10-C28-O8-C9
32	Z	310	CHL	O1A-CGA-O2A-C1
34	3	5022	3PH	O32-C31-O31-C3
19	Z	314	CLA	O1A-CGA-O2A-C1
19	4	311	CLA	C4C-C3C-CAC-CBC
24	3	5023	LMT	C3'-C4'-O1B-C1B
19	A	802	CLA	O1D-CGD-O2D-CED
19	A	811	CLA	O1D-CGD-O2D-CED
19	A	821	CLA	O1D-CGD-O2D-CED
19	A	843	CLA	O1D-CGD-O2D-CED
19	B	811	CLA	O1D-CGD-O2D-CED
19	B	820	CLA	O1D-CGD-O2D-CED
19	B	827	CLA	O1D-CGD-O2D-CED
19	B	829	CLA	O1D-CGD-O2D-CED
19	1	5011	CLA	O1D-CGD-O2D-CED
19	7	324	CLA	O1D-CGD-O2D-CED
19	5	319	CLA	O1D-CGD-O2D-CED
19	5	322	CLA	O1D-CGD-O2D-CED
19	3	5009	CLA	CBA-CGA-O2A-C1
32	6	316	CHL	C4C-C3C-CAC-CBC
25	B	848	DGD	C2G-C1G-O1G-C1A
19	A	830	CLA	O1D-CGD-O2D-CED
19	A	834	CLA	O1D-CGD-O2D-CED
19	A	841	CLA	O1D-CGD-O2D-CED
19	B	801	CLA	O1D-CGD-O2D-CED
19	B	803	CLA	O1D-CGD-O2D-CED
19	B	816	CLA	O1D-CGD-O2D-CED
19	B	817	CLA	O1D-CGD-O2D-CED
19	B	835	CLA	O1D-CGD-O2D-CED
19	F	303	CLA	O1D-CGD-O2D-CED
19	Z	311	CLA	O1D-CGD-O2D-CED
19	4	306	CLA	O1D-CGD-O2D-CED
19	4	307	CLA	O1D-CGD-O2D-CED
19	4	310	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	4	313	CLA	O1D-CGD-O2D-CED
19	5	301	CLA	O1D-CGD-O2D-CED
19	A	804	CLA	CBA-CGA-O2A-C1
19	A	807	CLA	CBA-CGA-O2A-C1
19	A	815	CLA	CBA-CGA-O2A-C1
19	B	825	CLA	CBA-CGA-O2A-C1
19	B	837	CLA	CBA-CGA-O2A-C1
19	Z	307	CLA	CBA-CGA-O2A-C1
19	4	311	CLA	CBA-CGA-O2A-C1
19	4	312	CLA	CBA-CGA-O2A-C1
19	5	306	CLA	CBA-CGA-O2A-C1
29	7	301	LMG	C29-C28-O8-C9
32	Z	310	CHL	CBA-CGA-O2A-C1
19	A	804	CLA	CBD-CGD-O2D-CED
19	A	812	CLA	CBD-CGD-O2D-CED
19	A	857	CLA	CBD-CGD-O2D-CED
19	B	808	CLA	CBD-CGD-O2D-CED
19	B	812	CLA	CBD-CGD-O2D-CED
19	B	815	CLA	CBD-CGD-O2D-CED
19	B	818	CLA	CBD-CGD-O2D-CED
19	B	819	CLA	CBD-CGD-O2D-CED
19	B	821	CLA	CBD-CGD-O2D-CED
19	B	831	CLA	CBD-CGD-O2D-CED
19	B	832	CLA	CBD-CGD-O2D-CED
19	B	837	CLA	CBD-CGD-O2D-CED
19	F	301	CLA	CBD-CGD-O2D-CED
19	K	202	CLA	CBD-CGD-O2D-CED
19	1	5018	CLA	CBD-CGD-O2D-CED
19	3	5015	CLA	CBD-CGD-O2D-CED
19	8	313	CLA	CBD-CGD-O2D-CED
19	4	308	CLA	CBD-CGD-O2D-CED
19	6	301	CLA	CBD-CGD-O2D-CED
32	6	321	CHL	CBD-CGD-O2D-CED
19	A	825	CLA	O1A-CGA-O2A-C1
19	A	828	CLA	O1A-CGA-O2A-C1
19	A	831	CLA	O1A-CGA-O2A-C1
19	A	832	CLA	O1A-CGA-O2A-C1
19	A	835	CLA	O1A-CGA-O2A-C1
19	A	857	CLA	O1A-CGA-O2A-C1
19	B	806	CLA	O1A-CGA-O2A-C1
19	B	809	CLA	O1A-CGA-O2A-C1
19	B	819	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	823	CLA	O1A-CGA-O2A-C1
19	B	830	CLA	O1A-CGA-O2A-C1
19	B	833	CLA	O1A-CGA-O2A-C1
19	B	837	CLA	O1A-CGA-O2A-C1
19	B	838	CLA	O1A-CGA-O2A-C1
19	K	204	CLA	O1A-CGA-O2A-C1
19	1	5006	CLA	O1A-CGA-O2A-C1
19	1	5012	CLA	O1A-CGA-O2A-C1
19	Z	307	CLA	O1A-CGA-O2A-C1
19	Z	315	CLA	O1A-CGA-O2A-C1
19	4	312	CLA	O1A-CGA-O2A-C1
19	5	306	CLA	O1A-CGA-O2A-C1
19	5	310	CLA	O1A-CGA-O2A-C1
19	5	312	CLA	O1A-CGA-O2A-C1
19	6	314	CLA	O1A-CGA-O2A-C1
29	J	1904	LMG	O10-C28-O8-C9
34	8	322	3PH	O32-C31-O31-C3
35	7	302	DGA	OA1-CA1-OG1-CG1
37	8	302	SQD	O10-C23-O48-C46
19	B	839	CLA	O1A-CGA-O2A-C1
19	8	320	CLA	O1A-CGA-O2A-C1
19	6	322	CLA	O1A-CGA-O2A-C1
19	A	818	CLA	O1D-CGD-O2D-CED
19	B	833	CLA	O1D-CGD-O2D-CED
19	Z	314	CLA	O1D-CGD-O2D-CED
19	5	311	CLA	O1D-CGD-O2D-CED
24	A	856	LMT	O5B-C1B-O1B-C4'
32	Z	309	CHL	C2C-C3C-CAC-CBC
19	A	809	CLA	O1D-CGD-O2D-CED
24	8	323	LMT	O5B-C1B-O1B-C4'
19	Z	315	CLA	CBD-CGD-O2D-CED
19	3	5012	CLA	CBD-CGD-O2D-CED
32	6	319	CHL	CBD-CGD-O2D-CED
19	A	802	CLA	C8-C10-C11-C12
19	B	839	CLA	O1D-CGD-O2D-CED
19	Z	306	CLA	O1D-CGD-O2D-CED
19	8	310	CLA	O1D-CGD-O2D-CED
19	5	325	CLA	O1D-CGD-O2D-CED
23	A	851	LHG	O9-C7-O7-C5
23	6	324	LHG	O9-C7-O7-C5
29	7	301	LMG	O9-C10-O7-C8
34	8	322	3PH	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
37	8	302	SQD	O49-C7-O47-C45
19	B	839	CLA	CBA-CGA-O2A-C1
19	Z	303	CLA	CBA-CGA-O2A-C1
19	Z	314	CLA	CBA-CGA-O2A-C1
19	8	320	CLA	CBA-CGA-O2A-C1
19	6	322	CLA	CBA-CGA-O2A-C1
32	Z	309	CHL	C4C-C3C-CAC-CBC
32	6	316	CHL	C2C-C3C-CAC-CBC
19	K	202	CLA	O1A-CGA-O2A-C1
19	Z	303	CLA	O1A-CGA-O2A-C1
19	1	5015	CLA	O1D-CGD-O2D-CED
19	A	802	CLA	C3-C5-C6-C7
19	A	818	CLA	C3-C5-C6-C7
19	A	819	CLA	C3-C5-C6-C7
19	A	821	CLA	C3-C5-C6-C7
19	A	827	CLA	C3-C5-C6-C7
19	A	828	CLA	C3-C5-C6-C7
19	A	838	CLA	C3-C5-C6-C7
19	A	841	CLA	C3-C5-C6-C7
19	B	801	CLA	C3-C5-C6-C7
19	B	807	CLA	C3-C5-C6-C7
19	B	808	CLA	C3-C5-C6-C7
19	B	812	CLA	C3-C5-C6-C7
19	B	815	CLA	C3-C5-C6-C7
19	B	817	CLA	C3-C5-C6-C7
19	B	818	CLA	C3-C5-C6-C7
19	B	820	CLA	C3-C5-C6-C7
19	B	823	CLA	C3-C5-C6-C7
19	B	825	CLA	C3-C5-C6-C7
19	I	201	CLA	C3-C5-C6-C7
19	1	5008	CLA	C3-C5-C6-C7
19	1	5010	CLA	C3-C5-C6-C7
19	Z	308	CLA	C3-C5-C6-C7
19	7	308	CLA	C3-C5-C6-C7
19	8	314	CLA	C3-C5-C6-C7
19	4	308	CLA	C3-C5-C6-C7
19	5	306	CLA	C3-C5-C6-C7
19	5	307	CLA	C3-C5-C6-C7
19	5	308	CLA	C3-C5-C6-C7
19	5	312	CLA	C3-C5-C6-C7
19	5	314	CLA	C3-C5-C6-C7
32	8	301	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
32	8	315	CHL	C3-C5-C6-C7
32	8	316	CHL	C3-C5-C6-C7
19	A	813	CLA	CBA-CGA-O2A-C1
19	A	814	CLA	CBA-CGA-O2A-C1
19	A	816	CLA	CBA-CGA-O2A-C1
19	A	831	CLA	CBA-CGA-O2A-C1
19	A	835	CLA	CBA-CGA-O2A-C1
19	A	857	CLA	CBA-CGA-O2A-C1
19	B	806	CLA	CBA-CGA-O2A-C1
19	B	809	CLA	CBA-CGA-O2A-C1
19	B	830	CLA	CBA-CGA-O2A-C1
19	B	832	CLA	CBA-CGA-O2A-C1
19	B	838	CLA	CBA-CGA-O2A-C1
19	G	1601	CLA	CBA-CGA-O2A-C1
19	1	5013	CLA	CBA-CGA-O2A-C1
19	7	312	CLA	CBA-CGA-O2A-C1
19	5	310	CLA	CBA-CGA-O2A-C1
19	5	312	CLA	CBA-CGA-O2A-C1
19	6	314	CLA	CBA-CGA-O2A-C1
29	J	1904	LMG	C29-C28-O8-C9
32	1	5009	CHL	CBA-CGA-O2A-C1
34	3	5022	3PH	C32-C31-O31-C3
37	8	302	SQD	C24-C23-O48-C46
23	1	5001	LHG	C8-C7-O7-C5
25	B	848	DGD	C2B-C1B-O2G-C2G
19	A	823	CLA	O1D-CGD-O2D-CED
19	A	826	CLA	O1D-CGD-O2D-CED
19	A	833	CLA	O1D-CGD-O2D-CED
19	B	805	CLA	O1D-CGD-O2D-CED
19	7	310	CLA	O1D-CGD-O2D-CED
19	8	309	CLA	O1D-CGD-O2D-CED
19	B	814	CLA	CBD-CGD-O2D-CED
19	B	840	CLA	CBD-CGD-O2D-CED
19	4	312	CLA	CBD-CGD-O2D-CED
19	B	820	CLA	O1A-CGA-O2A-C1
19	G	1602	CLA	O1A-CGA-O2A-C1
19	3	5009	CLA	O1A-CGA-O2A-C1
19	A	825	CLA	C8-C10-C11-C12
19	K	202	CLA	CBA-CGA-O2A-C1
19	B	810	CLA	C3-C5-C6-C7
19	4	307	CLA	C3-C5-C6-C7
19	A	814	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	3	5014	CLA	C4-C3-C5-C6
19	5	317	CLA	C4-C3-C5-C6
29	J	1904	LMG	C8-C9-O8-C28
19	7	312	CLA	CBD-CGD-O2D-CED
19	6	314	CLA	CBD-CGD-O2D-CED
19	B	817	CLA	C2A-CAA-CBA-CGA
19	B	829	CLA	C2A-CAA-CBA-CGA
19	5	311	CLA	C2A-CAA-CBA-CGA
19	5	319	CLA	C2A-CAA-CBA-CGA
19	8	307	CLA	O1A-CGA-O2A-C1
19	B	836	CLA	C8-C10-C11-C12
25	B	848	DGD	C8A-C9A-CAA-CBA
25	B	848	DGD	CBA-CCA-CDA-CEA
32	8	301	CHL	C2C-C3C-CAC-CBC
19	A	803	CLA	C3-C5-C6-C7
19	A	804	CLA	C3-C5-C6-C7
19	A	809	CLA	C3-C5-C6-C7
19	A	823	CLA	C3-C5-C6-C7
19	A	836	CLA	C3-C5-C6-C7
19	A	842	CLA	C3-C5-C6-C7
19	B	828	CLA	C3-C5-C6-C7
19	1	5012	CLA	C3-C5-C6-C7
19	Z	307	CLA	C3-C5-C6-C7
19	6	313	CLA	C3-C5-C6-C7
19	A	819	CLA	CBA-CGA-O2A-C1
19	A	822	CLA	CBA-CGA-O2A-C1
19	A	825	CLA	CBA-CGA-O2A-C1
19	A	828	CLA	CBA-CGA-O2A-C1
19	A	832	CLA	CBA-CGA-O2A-C1
19	A	839	CLA	CBA-CGA-O2A-C1
19	B	813	CLA	CBA-CGA-O2A-C1
19	B	817	CLA	CBA-CGA-O2A-C1
19	B	818	CLA	CBA-CGA-O2A-C1
19	B	819	CLA	CBA-CGA-O2A-C1
19	B	823	CLA	CBA-CGA-O2A-C1
19	B	833	CLA	CBA-CGA-O2A-C1
19	K	204	CLA	CBA-CGA-O2A-C1
19	1	5006	CLA	CBA-CGA-O2A-C1
19	1	5012	CLA	CBA-CGA-O2A-C1
19	Z	315	CLA	CBA-CGA-O2A-C1
19	7	311	CLA	CBA-CGA-O2A-C1
19	4	307	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	4	309	CLA	CBA-CGA-O2A-C1
34	8	322	3PH	C32-C31-O31-C3
35	7	302	DGA	CA2-CA1-OG1-CG1
23	4	320	LHG	C23-C24-C25-C26
24	8	323	LMT	C2B-C1B-O1B-C4'
19	B	822	CLA	O1D-CGD-O2D-CED
19	3	5016	CLA	O1D-CGD-O2D-CED
19	A	836	CLA	CBD-CGD-O2D-CED
23	1	5019	LHG	C11-C12-C13-C14
32	8	301	CHL	C4C-C3C-CAC-CBC
19	A	825	CLA	O1D-CGD-O2D-CED
19	B	826	CLA	O1D-CGD-O2D-CED
19	B	838	CLA	O1D-CGD-O2D-CED
19	G	1602	CLA	O1D-CGD-O2D-CED
19	K	204	CLA	O1D-CGD-O2D-CED
32	3	5017	CHL	O1D-CGD-O2D-CED
23	4	320	LHG	O9-C7-O7-C5
29	J	1903	LMG	O9-C10-O7-C8
19	A	814	CLA	O1A-CGA-O2A-C1
19	A	819	CLA	O1A-CGA-O2A-C1
19	A	822	CLA	O1A-CGA-O2A-C1
19	A	841	CLA	O1A-CGA-O2A-C1
19	B	814	CLA	O1A-CGA-O2A-C1
19	B	832	CLA	O1A-CGA-O2A-C1
19	G	1601	CLA	O1A-CGA-O2A-C1
19	I	201	CLA	O1A-CGA-O2A-C1
19	3	5016	CLA	O1A-CGA-O2A-C1
32	1	5009	CHL	O1A-CGA-O2A-C1
32	Z	302	CHL	O1A-CGA-O2A-C1
32	3	5017	CHL	O1A-CGA-O2A-C1
22	A	846	BCR	C19-C20-C21-C22
22	A	848	BCR	C15-C16-C17-C18
22	A	850	BCR	C19-C20-C21-C22
22	A	858	BCR	C19-C20-C21-C22
22	A	859	BCR	C15-C16-C17-C18
22	G	1603	BCR	C19-C20-C21-C22
22	3	5006	BCR	C19-C20-C21-C22
22	8	303	BCR	C13-C14-C15-C16
22	8	306	BCR	C19-C20-C21-C22
22	5	304	BCR	C19-C20-C21-C22
27	F	304	RRX	C19-C20-C21-C22
19	A	804	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	1	5019	LHG	C13-C14-C15-C16
19	A	803	CLA	CBD-CGD-O2D-CED
19	A	807	CLA	CBD-CGD-O2D-CED
19	A	838	CLA	CBD-CGD-O2D-CED
19	B	823	CLA	CBD-CGD-O2D-CED
19	1	5006	CLA	CBD-CGD-O2D-CED
19	3	5013	CLA	CBD-CGD-O2D-CED
19	7	317	CLA	CBD-CGD-O2D-CED
19	8	311	CLA	CBD-CGD-O2D-CED
19	4	316	CLA	CBD-CGD-O2D-CED
19	5	312	CLA	CBD-CGD-O2D-CED
19	6	302	CLA	CBD-CGD-O2D-CED
19	A	816	CLA	O1D-CGD-O2D-CED
19	1	5007	CLA	O1D-CGD-O2D-CED
23	A	851	LHG	O2-C2-C3-O3
23	1	5019	LHG	O2-C2-C3-O3
23	3	5021	LHG	O2-C2-C3-O3
23	4	320	LHG	O2-C2-C3-O3
19	A	805	CLA	C3-C5-C6-C7
19	A	822	CLA	C3-C5-C6-C7
19	A	832	CLA	C3-C5-C6-C7
19	A	833	CLA	C3-C5-C6-C7
19	B	804	CLA	C3-C5-C6-C7
19	B	824	CLA	C3-C5-C6-C7
19	B	829	CLA	C3-C5-C6-C7
19	B	835	CLA	C3-C5-C6-C7
19	B	837	CLA	C3-C5-C6-C7
19	B	850	CLA	C3-C5-C6-C7
19	3	5010	CLA	C3-C5-C6-C7
19	7	310	CLA	C3-C5-C6-C7
19	8	308	CLA	C3-C5-C6-C7
32	5	315	CHL	C3-C5-C6-C7
19	A	841	CLA	CBA-CGA-O2A-C1
19	B	807	CLA	CBA-CGA-O2A-C1
19	B	840	CLA	CBA-CGA-O2A-C1
19	Z	305	CLA	CBA-CGA-O2A-C1
19	3	5019	CLA	CBA-CGA-O2A-C1
19	8	307	CLA	CBA-CGA-O2A-C1
19	4	306	CLA	CBA-CGA-O2A-C1
19	5	309	CLA	CBA-CGA-O2A-C1
19	5	321	CLA	CBA-CGA-O2A-C1
32	5	315	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	817	CLA	O1A-CGA-O2A-C1
19	B	818	CLA	O1A-CGA-O2A-C1
19	Z	305	CLA	O1A-CGA-O2A-C1
19	7	311	CLA	O1A-CGA-O2A-C1
19	A	827	CLA	O1D-CGD-O2D-CED
19	A	835	CLA	O1D-CGD-O2D-CED
19	7	318	CLA	O1D-CGD-O2D-CED
19	A	810	CLA	C8-C10-C11-C12
23	Z	316	LHG	C8-C7-O7-C5
29	J	1904	LMG	C11-C10-O7-C8
34	3	5022	3PH	C22-C21-O21-C2
35	7	302	DGA	CB1-CB2-CB3-CB4
19	A	805	CLA	CBD-CGD-O2D-CED
19	B	830	CLA	CBD-CGD-O2D-CED
19	3	5014	CLA	CBD-CGD-O2D-CED
19	7	316	CLA	CBD-CGD-O2D-CED
32	8	317	CHL	CBD-CGD-O2D-CED
34	6	325	3PH	C24-C25-C26-C27
19	Z	305	CLA	C8-C10-C11-C12
19	B	840	CLA	O1A-CGA-O2A-C1
23	A	851	LHG	C11-C12-C13-C14
23	5	323	LHG	C11-C12-C13-C14
19	5	306	CLA	O1D-CGD-O2D-CED
23	5	323	LHG	C23-C24-C25-C26
19	A	829	CLA	C5-C6-C7-C8
19	B	819	CLA	C3-C5-C6-C7
19	B	831	CLA	C3-C5-C6-C7
19	7	312	CLA	C3-C5-C6-C7
19	B	814	CLA	CBA-CGA-O2A-C1
19	B	820	CLA	CBA-CGA-O2A-C1
19	I	201	CLA	CBA-CGA-O2A-C1
19	3	5016	CLA	CBA-CGA-O2A-C1
32	Z	302	CHL	CBA-CGA-O2A-C1
32	3	5017	CHL	CBA-CGA-O2A-C1
23	3	5021	LHG	C24-C23-O8-C6
23	Z	316	LHG	O9-C7-O7-C5
19	A	839	CLA	O1A-CGA-O2A-C1
19	B	813	CLA	O1A-CGA-O2A-C1
19	4	306	CLA	O1A-CGA-O2A-C1
19	4	307	CLA	O1A-CGA-O2A-C1
19	A	843	CLA	C3-C5-C6-C7
19	B	802	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	Z	305	CLA	C4-C3-C5-C6
19	7	306	CLA	C4-C3-C5-C6
19	6	301	CLA	C4-C3-C5-C6
19	Z	305	CLA	C2-C3-C5-C6
19	Z	307	CLA	C2-C3-C5-C6
19	7	306	CLA	C2-C3-C5-C6
19	6	301	CLA	C2-C3-C5-C6
32	1	5009	CHL	C2-C3-C5-C6
19	B	839	CLA	C2A-CAA-CBA-CGA
19	1	5016	CLA	C2A-CAA-CBA-CGA
19	3	5018	CLA	C2A-CAA-CBA-CGA
32	8	301	CHL	C2A-CAA-CBA-CGA
19	B	821	CLA	O1D-CGD-O2D-CED
19	7	319	CLA	O1D-CGD-O2D-CED
32	6	316	CHL	O1D-CGD-O2D-CED
19	B	807	CLA	O1A-CGA-O2A-C1
19	3	5019	CLA	O1A-CGA-O2A-C1
19	4	309	CLA	O1A-CGA-O2A-C1
19	5	309	CLA	O1A-CGA-O2A-C1
19	5	321	CLA	O1A-CGA-O2A-C1
32	5	315	CHL	O1A-CGA-O2A-C1
19	A	816	CLA	C3-C5-C6-C7
19	A	834	CLA	C3-C5-C6-C7
19	6	312	CLA	C3-C5-C6-C7
19	B	822	CLA	CBA-CGA-O2A-C1
19	5	325	CLA	CBA-CGA-O2A-C1
19	A	808	CLA	O1D-CGD-O2D-CED
23	7	320	LHG	C29-C30-C31-C32
19	B	815	CLA	O1D-CGD-O2D-CED
19	A	804	CLA	O1D-CGD-O2D-CED
19	A	857	CLA	O1D-CGD-O2D-CED
19	B	818	CLA	O1D-CGD-O2D-CED
19	B	819	CLA	O1D-CGD-O2D-CED
19	B	831	CLA	O1D-CGD-O2D-CED
19	B	832	CLA	O1D-CGD-O2D-CED
32	6	321	CHL	O1D-CGD-O2D-CED
19	1	5018	CLA	O1D-CGD-O2D-CED
23	7	320	LHG	C1-C2-C3-O3
23	4	320	LHG	C1-C2-C3-O3
23	6	303	LHG	C1-C2-C3-O3
34	3	5022	3PH	O22-C21-O21-C2
19	B	822	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	5	325	CLA	O1A-CGA-O2A-C1
32	8	316	CHL	O1A-CGA-O2A-C1
19	B	837	CLA	O1D-CGD-O2D-CED
19	A	823	CLA	CBA-CGA-O2A-C1
19	A	824	CLA	CBA-CGA-O2A-C1
19	A	833	CLA	CBA-CGA-O2A-C1
19	A	834	CLA	CBA-CGA-O2A-C1
19	8	313	CLA	CBA-CGA-O2A-C1
19	4	313	CLA	CBA-CGA-O2A-C1
19	5	311	CLA	CBA-CGA-O2A-C1
32	8	316	CHL	CBA-CGA-O2A-C1
32	8	319	CHL	CBA-CGA-O2A-C1
19	B	824	CLA	CBD-CGD-O2D-CED
22	B	842	BCR	C9-C10-C11-C12
22	3	5006	BCR	C15-C16-C17-C18
22	3	5007	BCR	C13-C14-C15-C16
22	6	307	BCR	C9-C10-C11-C12
23	5	323	LHG	C25-C26-C27-C28
35	7	302	DGA	CCB-CDB-CEB-CFB
19	8	313	CLA	O1A-CGA-O2A-C1
35	7	302	DGA	CBB-CAB-CB9-CB8
19	B	812	CLA	O1D-CGD-O2D-CED
19	K	202	CLA	O1D-CGD-O2D-CED
19	3	5015	CLA	O1D-CGD-O2D-CED
20	A	844	PQN	C18-C20-C21-C22
32	Z	310	CHL	C13-C15-C16-C17
23	Z	316	LHG	O2-C2-C3-O3
23	5	323	LHG	O2-C2-C3-O3
19	A	839	CLA	C3-C5-C6-C7
23	A	852	LHG	C7-C8-C9-C10
19	A	857	CLA	C3-C5-C6-C7
19	6	310	CLA	C3-C5-C6-C7
24	A	856	LMT	C2'-C1'-O1'-C1
32	8	316	CHL	C4-C3-C5-C6
19	A	814	CLA	C2-C3-C5-C6
19	5	317	CLA	C2-C3-C5-C6
32	7	314	CHL	C2-C3-C5-C6
32	8	316	CHL	C2-C3-C5-C6
19	A	802	CLA	C11-C12-C13-C14
19	A	803	CLA	C6-C7-C8-C9
19	A	806	CLA	C6-C7-C8-C9
19	A	808	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
19	A	809	CLA	C6-C7-C8-C9
19	A	812	CLA	C6-C7-C8-C9
19	A	818	CLA	C6-C7-C8-C9
19	A	818	CLA	C11-C10-C8-C9
19	A	819	CLA	C6-C7-C8-C9
19	A	820	CLA	C6-C7-C8-C9
19	A	823	CLA	C6-C7-C8-C9
19	A	826	CLA	C6-C7-C8-C9
19	A	829	CLA	C11-C10-C8-C9
19	A	830	CLA	C6-C7-C8-C9
19	A	832	CLA	C6-C7-C8-C9
19	A	840	CLA	C6-C7-C8-C9
19	B	801	CLA	C6-C7-C8-C9
19	B	816	CLA	C11-C10-C8-C9
19	B	819	CLA	C11-C10-C8-C9
19	B	821	CLA	C6-C7-C8-C9
19	B	821	CLA	C11-C10-C8-C9
19	B	822	CLA	C11-C10-C8-C9
19	B	823	CLA	C11-C10-C8-C9
19	B	825	CLA	C11-C10-C8-C9
19	B	840	CLA	C11-C10-C8-C9
19	B	850	CLA	C6-C7-C8-C9
19	1	5006	CLA	C6-C7-C8-C9
19	1	5008	CLA	C6-C7-C8-C9
19	Z	307	CLA	C6-C7-C8-C9
19	Z	308	CLA	C6-C7-C8-C9
19	Z	312	CLA	C11-C10-C8-C9
19	Z	315	CLA	C11-C12-C13-C14
19	3	5010	CLA	C14-C13-C15-C16
19	3	5014	CLA	C11-C10-C8-C9
19	3	5018	CLA	C6-C7-C8-C9
19	7	306	CLA	C6-C7-C8-C9
19	7	311	CLA	C6-C7-C8-C9
19	7	312	CLA	C6-C7-C8-C9
19	8	310	CLA	C6-C7-C8-C9
19	8	311	CLA	C11-C10-C8-C9
19	4	308	CLA	C6-C7-C8-C9
19	5	317	CLA	C6-C7-C8-C9
19	5	321	CLA	C6-C7-C8-C9
19	5	321	CLA	C11-C10-C8-C9
19	6	301	CLA	C11-C10-C8-C9
19	6	312	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
32	8	315	CHL	C14-C13-C15-C16
32	6	315	CHL	C11-C10-C8-C9
19	A	808	CLA	C2A-CAA-CBA-CGA
19	A	829	CLA	C2A-CAA-CBA-CGA
32	7	314	CHL	C2A-CAA-CBA-CGA
32	4	315	CHL	C2A-CAA-CBA-CGA
22	A	846	BCR	C36-C18-C19-C20
22	A	847	BCR	C7-C8-C9-C34
22	A	847	BCR	C36-C18-C19-C20
22	A	848	BCR	C37-C22-C23-C24
22	A	849	BCR	C7-C8-C9-C34
22	A	850	BCR	C36-C18-C19-C20
22	A	850	BCR	C37-C22-C23-C24
22	A	859	BCR	C7-C8-C9-C34
22	B	842	BCR	C11-C12-C13-C35
22	B	842	BCR	C36-C18-C19-C20
22	B	843	BCR	C37-C22-C23-C24
22	B	844	BCR	C7-C8-C9-C34
22	B	844	BCR	C36-C18-C19-C20
22	B	846	BCR	C7-C8-C9-C34
22	G	1603	BCR	C36-C18-C19-C20
22	K	206	BCR	C36-C18-C19-C20
22	3	5004	BCR	C7-C8-C9-C34
22	3	5005	BCR	C37-C22-C23-C24
22	3	5006	BCR	C11-C12-C13-C35
22	3	5006	BCR	C36-C18-C19-C20
22	3	5006	BCR	C37-C22-C23-C24
22	3	5007	BCR	C11-C12-C13-C35
22	4	305	BCR	C7-C8-C9-C34
22	4	305	BCR	C11-C12-C13-C35
22	4	305	BCR	C37-C22-C23-C24
22	5	304	BCR	C7-C8-C9-C34
22	6	307	BCR	C11-C12-C13-C35
22	6	308	BCR	C7-C8-C9-C34
27	F	304	RRX	C7-C8-C9-C34
28	J	1902	C7Z	C27-C28-C29-C39
28	1	5005	C7Z	C27-C28-C29-C39
31	Z	317	LUT	C7-C8-C9-C19
31	Z	317	LUT	C31-C32-C33-C40
31	3	5003	LUT	C27-C28-C29-C39
31	7	304	LUT	C27-C28-C29-C39
31	8	304	LUT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
31	8	304	LUT	C11-C12-C13-C20
31	8	304	LUT	C27-C28-C29-C39
31	6	306	LUT	C27-C28-C29-C39
22	A	846	BCR	C17-C18-C19-C20
22	A	847	BCR	C17-C18-C19-C20
22	A	848	BCR	C21-C22-C23-C24
22	A	849	BCR	C7-C8-C9-C10
22	A	850	BCR	C17-C18-C19-C20
22	A	850	BCR	C21-C22-C23-C24
22	A	859	BCR	C21-C22-C23-C24
22	B	843	BCR	C11-C12-C13-C14
22	B	843	BCR	C17-C18-C19-C20
22	B	843	BCR	C21-C22-C23-C24
22	B	844	BCR	C7-C8-C9-C10
22	B	846	BCR	C7-C8-C9-C10
22	F	302	BCR	C17-C18-C19-C20
22	G	1603	BCR	C17-C18-C19-C20
22	K	206	BCR	C17-C18-C19-C20
22	3	5005	BCR	C11-C12-C13-C14
22	3	5005	BCR	C21-C22-C23-C24
22	3	5006	BCR	C11-C12-C13-C14
22	3	5006	BCR	C17-C18-C19-C20
22	3	5007	BCR	C11-C12-C13-C14
22	4	305	BCR	C7-C8-C9-C10
22	4	305	BCR	C11-C12-C13-C14
22	4	305	BCR	C21-C22-C23-C24
22	5	304	BCR	C7-C8-C9-C10
22	5	304	BCR	C11-C12-C13-C14
22	6	307	BCR	C11-C12-C13-C14
27	F	304	RRX	C7-C8-C9-C10
27	5	302	RRX	C21-C22-C23-C24
28	J	1902	C7Z	C27-C28-C29-C30
31	Z	317	LUT	C7-C8-C9-C10
31	Z	317	LUT	C31-C32-C33-C34
31	3	5003	LUT	C27-C28-C29-C30
31	7	304	LUT	C27-C28-C29-C30
31	8	304	LUT	C7-C8-C9-C10
31	8	304	LUT	C27-C28-C29-C30
31	8	305	LUT	C7-C8-C9-C10
31	6	306	LUT	C27-C28-C29-C30
29	J	1904	LMG	O9-C10-O7-C8
23	7	320	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
23	8	321	LHG	C8-C7-O7-C5
23	A	852	LHG	C23-C24-C25-C26
23	6	324	LHG	C23-C24-C25-C26
35	7	302	DGA	CA1-CA2-CA3-CA4
19	4	313	CLA	O1A-CGA-O2A-C1
19	5	311	CLA	O1A-CGA-O2A-C1
32	8	319	CHL	O1A-CGA-O2A-C1
32	Z	310	CHL	C10-C11-C12-C13
32	4	317	CHL	C5-C6-C7-C8
19	A	812	CLA	O1D-CGD-O2D-CED
24	8	324	LMT	C3'-C4'-O1B-C1B
19	B	808	CLA	O1D-CGD-O2D-CED
19	B	836	CLA	C3-C5-C6-C7
19	Z	311	CLA	C3-C5-C6-C7
19	8	310	CLA	C3-C5-C6-C7
19	A	808	CLA	CBA-CGA-O2A-C1
19	A	827	CLA	CBA-CGA-O2A-C1
23	6	324	LHG	C24-C23-O8-C6
19	A	812	CLA	C8-C10-C11-C12
19	7	311	CLA	C5-C6-C7-C8
32	1	5009	CHL	C8-C10-C11-C12
32	8	319	CHL	C8-C10-C11-C12
19	A	833	CLA	O1A-CGA-O2A-C1
32	Z	313	CHL	CBD-CGD-O2D-CED
19	1	5008	CLA	C13-C15-C16-C17
19	3	5010	CLA	C5-C6-C7-C8
19	4	308	CLA	C8-C10-C11-C12
19	4	312	CLA	C5-C6-C7-C8
19	5	307	CLA	C5-C6-C7-C8
23	3	5021	LHG	O10-C23-O8-C6
23	7	320	LHG	C7-C8-C9-C10
23	8	321	LHG	C23-C24-C25-C26
19	A	832	CLA	C15-C16-C17-C18
19	B	825	CLA	C13-C15-C16-C17
19	8	307	CLA	C5-C6-C7-C8
19	A	808	CLA	C3-C5-C6-C7
29	J	1903	LMG	C8-C9-O8-C28
23	6	324	LHG	C9-C10-C11-C12
19	8	313	CLA	O1D-CGD-O2D-CED
19	A	812	CLA	C2-C1-O2A-CGA
19	A	827	CLA	C2-C1-O2A-CGA
19	A	828	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	B	813	CLA	C2-C1-O2A-CGA
19	B	814	CLA	C2-C1-O2A-CGA
19	B	829	CLA	C2-C1-O2A-CGA
19	B	830	CLA	C2-C1-O2A-CGA
19	1	5015	CLA	C2-C1-O2A-CGA
19	Z	308	CLA	C2-C1-O2A-CGA
19	7	319	CLA	C2-C1-O2A-CGA
19	5	308	CLA	C2-C1-O2A-CGA
19	6	302	CLA	C2-C1-O2A-CGA
34	3	5022	3PH	C3B-C3C-C3D-C3E
19	A	835	CLA	C8-C10-C11-C12
19	8	311	CLA	C8-C10-C11-C12
32	6	319	CHL	C10-C11-C12-C13
23	7	320	LHG	C23-C24-C25-C26
19	A	815	CLA	CBD-CGD-O2D-CED
19	8	307	CLA	CBD-CGD-O2D-CED
24	3	5023	LMT	C6-C7-C8-C9
19	Z	312	CLA	C8-C10-C11-C12
19	A	802	CLA	C6-C7-C8-C10
19	A	823	CLA	C11-C10-C8-C7
19	A	827	CLA	C6-C7-C8-C10
19	A	838	CLA	C6-C7-C8-C10
19	A	841	CLA	C6-C7-C8-C10
19	B	803	CLA	C11-C10-C8-C7
19	B	807	CLA	C11-C10-C8-C7
19	B	808	CLA	C11-C10-C8-C7
19	B	813	CLA	C6-C7-C8-C10
19	B	819	CLA	C11-C10-C8-C7
19	B	821	CLA	C11-C10-C8-C7
19	B	826	CLA	C6-C7-C8-C10
19	B	827	CLA	C11-C10-C8-C7
19	B	832	CLA	C6-C7-C8-C10
19	B	833	CLA	C6-C7-C8-C10
19	1	5012	CLA	C6-C7-C8-C10
19	3	5014	CLA	C6-C7-C8-C10
19	6	311	CLA	C6-C7-C8-C10
19	6	320	CLA	C6-C7-C8-C10
32	5	315	CHL	C12-C13-C15-C16
19	A	834	CLA	O1A-CGA-O2A-C1
22	A	847	BCR	C15-C16-C17-C18
22	A	848	BCR	C13-C14-C15-C16
22	A	859	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	A	859	BCR	C13-C14-C15-C16
22	B	845	BCR	C19-C20-C21-C22
22	F	302	BCR	C19-C20-C21-C22
22	3	5004	BCR	C9-C10-C11-C12
22	8	303	BCR	C19-C20-C21-C22
22	8	306	BCR	C9-C10-C11-C12
22	5	304	BCR	C9-C10-C11-C12
27	F	304	RRX	C9-C10-C11-C12
19	B	813	CLA	C2A-CAA-CBA-CGA
19	I	201	CLA	C2A-CAA-CBA-CGA
19	8	318	CLA	C2A-CAA-CBA-CGA
19	6	313	CLA	C2A-CAA-CBA-CGA
32	8	316	CHL	C2A-CAA-CBA-CGA
32	6	317	CHL	C2A-CAA-CBA-CGA
19	F	301	CLA	O1D-CGD-O2D-CED
19	Z	315	CLA	O1D-CGD-O2D-CED
19	4	308	CLA	O1D-CGD-O2D-CED
19	6	301	CLA	O1D-CGD-O2D-CED
19	A	817	CLA	C8-C10-C11-C12
19	B	821	CLA	C10-C11-C12-C13
19	1	5008	CLA	C5-C6-C7-C8
19	6	301	CLA	C5-C6-C7-C8
19	6	323	CLA	C8-C10-C11-C12
19	A	824	CLA	O1A-CGA-O2A-C1
24	A	853	LMT	O5'-C1'-O1'-C1
24	3	5023	LMT	O5'-C1'-O1'-C1
32	6	319	CHL	O1D-CGD-O2D-CED
34	8	322	3PH	C32-C33-C34-C35
23	1	5001	LHG	O2-C2-C3-O3
23	7	320	LHG	O2-C2-C3-O3
23	8	321	LHG	O2-C2-C3-O3
23	6	303	LHG	O2-C2-C3-O3
19	B	811	CLA	C3-C5-C6-C7
19	B	833	CLA	C3-C5-C6-C7
19	5	325	CLA	C3-C5-C6-C7
19	1	5006	CLA	C5-C6-C7-C8
19	Z	315	CLA	C10-C11-C12-C13
19	B	814	CLA	O1D-CGD-O2D-CED
19	A	823	CLA	O1A-CGA-O2A-C1
19	A	806	CLA	C5-C6-C7-C8
19	A	813	CLA	C8-C10-C11-C12
19	A	832	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	B	801	CLA	C5-C6-C7-C8
19	B	816	CLA	C8-C10-C11-C12
19	B	825	CLA	C5-C6-C7-C8
19	1	5012	CLA	C5-C6-C7-C8
19	1	5016	CLA	C8-C10-C11-C12
19	3	5018	CLA	C5-C6-C7-C8
19	8	307	CLA	C10-C11-C12-C13
19	8	312	CLA	C5-C6-C7-C8
19	6	314	CLA	C5-C6-C7-C8
32	6	315	CHL	C8-C10-C11-C12
19	4	312	CLA	O1D-CGD-O2D-CED
19	A	808	CLA	O1A-CGA-O2A-C1
19	A	827	CLA	O1A-CGA-O2A-C1
23	6	324	LHG	O10-C23-O8-C6
19	A	806	CLA	C8-C10-C11-C12
19	A	823	CLA	C5-C6-C7-C8
19	B	840	CLA	C10-C11-C12-C13
19	B	850	CLA	C8-C10-C11-C12
19	3	5013	CLA	C13-C15-C16-C17
19	4	308	CLA	C5-C6-C7-C8
23	A	852	LHG	C3-O3-P-O6
23	A	852	LHG	C4-O6-P-O3
23	1	5001	LHG	C3-O3-P-O6
23	1	5001	LHG	C4-O6-P-O3
23	1	5019	LHG	C3-O3-P-O6
23	3	5021	LHG	C3-O3-P-O6
23	7	320	LHG	C3-O3-P-O6
23	4	320	LHG	C3-O3-P-O6
23	5	323	LHG	C3-O3-P-O6
23	5	323	LHG	C4-O6-P-O3
23	6	303	LHG	C3-O3-P-O6
23	6	324	LHG	C4-O6-P-O3
19	A	811	CLA	C3-C5-C6-C7
19	A	826	CLA	C3-C5-C6-C7
19	B	827	CLA	C3-C5-C6-C7
19	B	829	CLA	CBA-CGA-O2A-C1
19	8	311	CLA	CBA-CGA-O2A-C1
19	5	314	CLA	CBA-CGA-O2A-C1
23	4	320	LHG	C24-C23-O8-C6
19	B	820	CLA	C5-C6-C7-C8
19	7	319	CLA	C8-C10-C11-C12
19	3	5012	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	4	320	LHG	C29-C30-C31-C32
23	A	851	LHG	C7-C8-C9-C10
23	1	5019	LHG	C1-C2-C3-O3
23	8	321	LHG	C1-C2-C3-O3
23	6	324	LHG	C1-C2-C3-O3
23	7	320	LHG	O9-C7-O7-C5
23	8	321	LHG	O9-C7-O7-C5
19	A	823	CLA	C4-C3-C5-C6
32	1	5009	CHL	C4-C3-C5-C6
32	7	314	CHL	C4-C3-C5-C6
19	3	5016	CLA	C8-C10-C11-C12
19	7	312	CLA	O1D-CGD-O2D-CED
19	A	813	CLA	C2A-CAA-CBA-CGA
19	B	814	CLA	C2A-CAA-CBA-CGA
19	B	830	CLA	C2A-CAA-CBA-CGA
19	B	831	CLA	C2A-CAA-CBA-CGA
19	3	5013	CLA	C2A-CAA-CBA-CGA
19	3	5020	CLA	C2A-CAA-CBA-CGA
19	8	312	CLA	C2A-CAA-CBA-CGA
19	5	301	CLA	C2A-CAA-CBA-CGA
19	6	320	CLA	C2A-CAA-CBA-CGA
19	8	314	CLA	C6-C7-C8-C9
19	B	803	CLA	C3-C5-C6-C7
19	Z	312	CLA	C3-C5-C6-C7
19	4	309	CLA	C3-C5-C6-C7
19	A	811	CLA	CBA-CGA-O2A-C1
19	A	830	CLA	CBA-CGA-O2A-C1
19	Z	306	CLA	CBA-CGA-O2A-C1
32	4	317	CHL	CBA-CGA-O2A-C1
38	6	326	ERG	C21-C20-C22-C23
19	A	815	CLA	C13-C15-C16-C17
32	Z	302	CHL	C5-C6-C7-C8
22	B	843	BCR	C15-C16-C17-C18
22	K	206	BCR	C19-C20-C21-C22
22	3	5006	BCR	C13-C14-C15-C16
22	7	305	BCR	C15-C16-C17-C18
22	4	305	BCR	C9-C10-C11-C12
23	Z	316	LHG	C23-C24-C25-C26
23	8	321	LHG	C7-C8-C9-C10
23	Z	316	LHG	C13-C14-C15-C16
23	A	852	LHG	C8-C7-O7-C5
23	1	5019	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
35	7	302	DGA	CB2-CB1-OG2-CG2
19	B	828	CLA	C8-C10-C11-C12
19	B	840	CLA	C5-C6-C7-C8
19	Z	315	CLA	C8-C10-C11-C12
19	B	806	CLA	C3-C5-C6-C7
19	6	302	CLA	C3-C5-C6-C7
23	7	320	LHG	C28-C29-C30-C31
23	6	324	LHG	C11-C12-C13-C14
33	7	321	SPH	C10-C11-C12-C13
19	6	314	CLA	O1D-CGD-O2D-CED
19	B	809	CLA	C6-C7-C8-C9
19	I	201	CLA	C6-C7-C8-C9
19	Z	311	CLA	C6-C7-C8-C9
19	8	307	CLA	C11-C12-C13-C14
19	8	313	CLA	C6-C7-C8-C10
19	4	313	CLA	C6-C7-C8-C10
19	5	325	CLA	C6-C7-C8-C9
18	A	801	CL0	CBA-CGA-O2A-C1
19	6	302	CLA	CBA-CGA-O2A-C1
23	1	5019	LHG	C14-C15-C16-C17
23	Z	316	LHG	C28-C29-C30-C31
33	7	321	SPH	C12-C13-C14-C15
19	3	5013	CLA	O1D-CGD-O2D-CED
23	A	852	LHG	O9-C7-O7-C5
23	1	5019	LHG	O9-C7-O7-C5
35	7	302	DGA	OB1-CB1-OG2-CG2
19	8	314	CLA	C5-C6-C7-C8
19	1	5008	CLA	CBD-CGD-O2D-CED
19	5	317	CLA	CBD-CGD-O2D-CED
23	7	320	LHG	C11-C12-C13-C14
19	A	836	CLA	O1D-CGD-O2D-CED
23	6	303	LHG	C13-C14-C15-C16
23	4	320	LHG	C7-C8-C9-C10
23	6	303	LHG	C7-C8-C9-C10
24	A	853	LMT	C2'-C1'-O1'-C1
24	A	854	LMT	C2'-C1'-O1'-C1
24	3	5023	LMT	C2'-C1'-O1'-C1
19	A	836	CLA	CBA-CGA-O2A-C1
19	B	827	CLA	CBA-CGA-O2A-C1
23	A	852	LHG	C13-C14-C15-C16
23	5	323	LHG	C28-C29-C30-C31
23	6	324	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	A	804	CLA	C6-C7-C8-C9
19	7	324	CLA	C6-C7-C8-C9
19	A	807	CLA	O1D-CGD-O2D-CED
19	A	838	CLA	O1D-CGD-O2D-CED
19	B	840	CLA	O1D-CGD-O2D-CED
19	5	312	CLA	O1D-CGD-O2D-CED
19	B	827	CLA	C4-C3-C5-C6
32	6	315	CHL	C4-C3-C5-C6
34	6	325	3PH	C25-C26-C27-C28
32	6	315	CHL	C2-C3-C5-C6
19	A	829	CLA	C6-C7-C8-C9
19	B	827	CLA	C11-C10-C8-C9
19	B	836	CLA	C6-C7-C8-C9
19	3	5008	CLA	C6-C7-C8-C9
19	5	312	CLA	C6-C7-C8-C9
20	A	844	PQN	C21-C22-C23-C24
32	6	315	CHL	C11-C12-C13-C14
19	8	311	CLA	O1D-CGD-O2D-CED
23	5	323	LHG	C7-C8-C9-C10
23	A	851	LHG	C13-C14-C15-C16
23	A	852	LHG	C12-C13-C14-C15
23	8	321	LHG	C28-C29-C30-C31
24	3	5023	LMT	C4-C5-C6-C7
19	B	814	CLA	C8-C10-C11-C12
19	B	823	CLA	C5-C6-C7-C8
19	7	306	CLA	C5-C6-C7-C8
19	6	312	CLA	C8-C10-C11-C12
20	A	844	PQN	C25-C26-C27-C28
19	1	5011	CLA	C2A-CAA-CBA-CGA
19	7	317	CLA	C2A-CAA-CBA-CGA
22	A	848	BCR	C36-C18-C19-C20
22	A	859	BCR	C36-C18-C19-C20
22	A	859	BCR	C37-C22-C23-C24
22	B	842	BCR	C7-C8-C9-C34
22	B	843	BCR	C11-C12-C13-C35
22	B	847	BCR	C36-C18-C19-C20
22	F	302	BCR	C36-C18-C19-C20
22	3	5006	BCR	C7-C8-C9-C34
22	8	303	BCR	C7-C8-C9-C34
22	8	306	BCR	C7-C8-C9-C34
22	5	304	BCR	C36-C18-C19-C20
27	F	304	RRX	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
27	F	304	RRX	C36-C18-C19-C20
27	5	302	RRX	C37-C22-C23-C24
28	J	1902	C7Z	C11-C12-C13-C20
28	6	304	C7Z	C7-C8-C9-C19
28	6	304	C7Z	C27-C28-C29-C39
31	Z	318	LUT	C7-C8-C9-C19
31	4	304	LUT	C7-C8-C9-C19
31	6	305	LUT	C7-C8-C9-C19
23	A	851	LHG	O1-C1-C2-C3
23	Z	316	LHG	O1-C1-C2-C3
23	3	5021	LHG	O1-C1-C2-C3
23	4	320	LHG	O1-C1-C2-C3
23	5	323	LHG	O1-C1-C2-C3
23	6	324	LHG	O1-C1-C2-C3
22	A	847	BCR	C7-C8-C9-C10
22	A	848	BCR	C17-C18-C19-C20
22	A	849	BCR	C21-C22-C23-C24
22	A	859	BCR	C7-C8-C9-C10
22	A	859	BCR	C17-C18-C19-C20
22	B	842	BCR	C7-C8-C9-C10
22	B	842	BCR	C17-C18-C19-C20
22	B	845	BCR	C17-C18-C19-C20
22	B	847	BCR	C17-C18-C19-C20
22	3	5004	BCR	C7-C8-C9-C10
22	3	5006	BCR	C7-C8-C9-C10
22	8	303	BCR	C7-C8-C9-C10
22	8	306	BCR	C7-C8-C9-C10
22	5	304	BCR	C17-C18-C19-C20
22	6	308	BCR	C7-C8-C9-C10
27	F	304	RRX	C21-C22-C23-C24
27	F	304	RRX	C17-C18-C19-C20
28	J	1902	C7Z	C11-C12-C13-C14
28	6	304	C7Z	C7-C8-C9-C10
28	6	304	C7Z	C27-C28-C29-C30
31	Z	318	LUT	C7-C8-C9-C10
31	3	5003	LUT	C7-C8-C9-C10
31	4	304	LUT	C7-C8-C9-C10
19	3	5019	CLA	C3-C5-C6-C7
19	B	826	CLA	C13-C15-C16-C17
23	A	851	LHG	C23-C24-C25-C26
19	1	5006	CLA	O1D-CGD-O2D-CED
23	A	852	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	7	320	LHG	C11-C10-C9-C8
23	4	320	LHG	C16-C17-C18-C19
23	4	320	LHG	C30-C31-C32-C33
23	6	303	LHG	C11-C12-C13-C14
19	A	836	CLA	C6-C7-C8-C9
19	A	836	CLA	C6-C7-C8-C10
19	I	201	CLA	C6-C7-C8-C10
19	8	307	CLA	C11-C12-C13-C15
24	A	854	LMT	O5'-C1'-O1'-C1
37	8	302	SQD	O5-C1-O6-C44
19	B	823	CLA	C8-C10-C11-C12
32	8	301	CHL	C5-C6-C7-C8
19	7	317	CLA	O1D-CGD-O2D-CED
24	8	324	LMT	C5'-C4'-O1B-C1B
34	3	5022	3PH	C22-C23-C24-C25
35	7	302	DGA	CB4-CB5-CB6-CB7
38	6	326	ERG	C13-C17-C20-C22
19	A	803	CLA	O1D-CGD-O2D-CED
23	4	320	LHG	C28-C29-C30-C31
24	4	322	LMT	C2-C3-C4-C5
23	1	5019	LHG	C7-C8-C9-C10
19	7	309	CLA	C8-C10-C11-C12
35	7	302	DGA	CA4-CA5-CA6-CA7
35	7	302	DGA	CB5-CB6-CB7-CB8
18	A	801	CL0	C3-C5-C6-C7
19	5	321	CLA	C3-C5-C6-C7
19	A	823	CLA	C8-C10-C11-C12
19	A	803	CLA	C3A-C2A-CAA-CBA
19	A	825	CLA	C3A-C2A-CAA-CBA
19	A	833	CLA	C3A-C2A-CAA-CBA
19	A	837	CLA	C3A-C2A-CAA-CBA
19	A	840	CLA	C3A-C2A-CAA-CBA
19	B	806	CLA	C3A-C2A-CAA-CBA
19	B	813	CLA	C3A-C2A-CAA-CBA
19	B	822	CLA	C3A-C2A-CAA-CBA
19	B	826	CLA	C3A-C2A-CAA-CBA
19	B	829	CLA	C3A-C2A-CAA-CBA
19	B	835	CLA	C3A-C2A-CAA-CBA
19	K	202	CLA	C3A-C2A-CAA-CBA
19	Z	311	CLA	C3A-C2A-CAA-CBA
19	3	5015	CLA	C3A-C2A-CAA-CBA
19	7	308	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	8	308	CLA	C3A-C2A-CAA-CBA
19	8	309	CLA	C3A-C2A-CAA-CBA
19	8	314	CLA	C3A-C2A-CAA-CBA
19	5	310	CLA	C3A-C2A-CAA-CBA
19	5	313	CLA	C3A-C2A-CAA-CBA
19	5	322	CLA	C3A-C2A-CAA-CBA
19	5	325	CLA	C3A-C2A-CAA-CBA
19	6	313	CLA	C3A-C2A-CAA-CBA
32	8	316	CHL	C3A-C2A-CAA-CBA
19	B	801	CLA	C8-C10-C11-C12
19	K	203	CLA	C5-C6-C7-C8
32	8	319	CHL	C15-C16-C17-C18
32	6	315	CHL	C10-C11-C12-C13
32	6	316	CHL	C5-C6-C7-C8
19	6	302	CLA	O1D-CGD-O2D-CED
19	A	830	CLA	O1A-CGA-O2A-C1
19	B	829	CLA	O1A-CGA-O2A-C1
19	Z	306	CLA	O1A-CGA-O2A-C1
23	4	320	LHG	O10-C23-O8-C6
19	4	313	CLA	C6-C7-C8-C9
19	5	306	CLA	C11-C12-C13-C15
32	1	5009	CHL	C11-C12-C13-C14
32	5	315	CHL	C16-C17-C18-C20
19	A	826	CLA	C8-C10-C11-C12
19	B	830	CLA	O1D-CGD-O2D-CED
19	4	309	CLA	CBD-CGD-O2D-CED
19	6	320	CLA	CBD-CGD-O2D-CED
38	8	325	ERG	C22-C23-C24-C25
38	6	326	ERG	C17-C20-C22-C23
19	A	813	CLA	C3-C5-C6-C7
19	B	821	CLA	C8-C10-C11-C12
19	7	324	CLA	C4-C3-C5-C6
32	6	319	CHL	CBA-CGA-O2A-C1
19	A	827	CLA	C2-C3-C5-C6
19	B	827	CLA	C2-C3-C5-C6
19	3	5014	CLA	C2-C3-C5-C6
19	7	324	CLA	C2-C3-C5-C6
19	8	314	CLA	C2-C3-C5-C6
32	5	315	CHL	C2-C3-C5-C6
38	8	325	ERG	C21-C20-C22-C23
38	8	325	ERG	C22-C23-C24-C28
38	6	326	ERG	C22-C23-C24-C28

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Mol	Chain	Res	Type	Atoms
23	A	852	LHG	C34-C35-C36-C37
23	A	851	LHG	O1-C1-C2-O2
23	8	321	LHG	O1-C1-C2-O2
23	4	320	LHG	O1-C1-C2-O2
23	5	323	LHG	O1-C1-C2-O2
23	1	5001	LHG	C7-C8-C9-C10
23	6	303	LHG	C23-C24-C25-C26
19	4	316	CLA	O1D-CGD-O2D-CED
19	8	311	CLA	O1A-CGA-O2A-C1
19	K	203	CLA	C6-C7-C8-C9
19	7	324	CLA	C6-C7-C8-C10
34	3	5022	3PH	C25-C26-C27-C28
19	B	821	CLA	C3-C5-C6-C7
19	7	319	CLA	C3-C5-C6-C7
32	Z	310	CHL	C3-C5-C6-C7
18	A	801	CL0	O1A-CGA-O2A-C1
19	A	811	CLA	O1A-CGA-O2A-C1
19	B	827	CLA	O1A-CGA-O2A-C1
19	5	314	CLA	O1A-CGA-O2A-C1
19	6	302	CLA	O1A-CGA-O2A-C1
19	A	824	CLA	C2-C1-O2A-CGA
19	A	834	CLA	C2-C1-O2A-CGA
19	B	809	CLA	C2-C1-O2A-CGA
19	B	816	CLA	C2-C1-O2A-CGA
19	B	823	CLA	C2-C1-O2A-CGA
19	B	832	CLA	C2-C1-O2A-CGA
19	1	5016	CLA	C2-C1-O2A-CGA
19	Z	305	CLA	C2-C1-O2A-CGA
19	Z	307	CLA	C2-C1-O2A-CGA
19	3	5008	CLA	C2-C1-O2A-CGA
19	3	5014	CLA	C2-C1-O2A-CGA
19	7	317	CLA	C2-C1-O2A-CGA
19	5	307	CLA	C2-C1-O2A-CGA
23	A	851	LHG	C9-C10-C11-C12
23	1	5019	LHG	C29-C30-C31-C32
23	6	303	LHG	C11-C10-C9-C8
33	7	321	SPH	C9-C10-C11-C12
19	A	836	CLA	O1A-CGA-O2A-C1
23	A	851	LHG	C11-C10-C9-C8
23	6	324	LHG	C34-C35-C36-C37
34	6	325	3PH	C22-C23-C24-C25
19	Z	315	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	8	313	CLA	C3-C5-C6-C7
22	A	846	BCR	C23-C24-C25-C26
22	A	847	BCR	C1-C6-C7-C8
22	A	847	BCR	C23-C24-C25-C26
22	A	848	BCR	C5-C6-C7-C8
22	A	849	BCR	C23-C24-C25-C26
22	A	850	BCR	C23-C24-C25-C26
22	A	858	BCR	C1-C6-C7-C8
22	A	859	BCR	C1-C6-C7-C8
22	B	842	BCR	C5-C6-C7-C8
22	B	842	BCR	C23-C24-C25-C30
22	B	843	BCR	C23-C24-C25-C26
22	B	845	BCR	C1-C6-C7-C8
22	B	845	BCR	C23-C24-C25-C26
22	B	845	BCR	C23-C24-C25-C30
22	B	847	BCR	C5-C6-C7-C8
22	B	847	BCR	C23-C24-C25-C30
22	F	302	BCR	C1-C6-C7-C8
22	K	206	BCR	C23-C24-C25-C30
22	3	5004	BCR	C5-C6-C7-C8
22	3	5005	BCR	C23-C24-C25-C26
22	3	5006	BCR	C5-C6-C7-C8
22	3	5006	BCR	C23-C24-C25-C26
22	3	5007	BCR	C5-C6-C7-C8
22	7	305	BCR	C1-C6-C7-C8
22	7	305	BCR	C23-C24-C25-C30
22	8	303	BCR	C23-C24-C25-C30
22	4	305	BCR	C5-C6-C7-C8
22	4	305	BCR	C23-C24-C25-C26
22	6	307	BCR	C23-C24-C25-C30
27	F	304	RRX	C23-C24-C25-C30
27	4	303	RRX	C1-C6-C7-C8
27	5	302	RRX	C23-C24-C25-C30
27	5	302	RRX	C1-C6-C7-C8
28	J	1902	C7Z	C1-C6-C7-C8
28	J	1902	C7Z	C5-C6-C7-C8
28	6	304	C7Z	C5-C6-C7-C8
31	8	305	LUT	C5-C6-C7-C8
19	A	821	CLA	CBA-CGA-O2A-C1
19	1	5015	CLA	CBA-CGA-O2A-C1
19	A	828	CLA	C5-C6-C7-C8
19	B	813	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	7	310	CLA	C5-C6-C7-C8
32	5	315	CHL	C10-C11-C12-C13
19	5	308	CLA	C11-C10-C8-C9
23	7	320	LHG	C10-C11-C12-C13
32	8	319	CHL	C10-C11-C12-C13
19	A	827	CLA	C4-C3-C5-C6
19	A	841	CLA	C4-C3-C5-C6
19	3	5008	CLA	C4-C3-C5-C6
19	8	312	CLA	C4-C3-C5-C6
19	8	314	CLA	C4-C3-C5-C6
32	5	315	CHL	C4-C3-C5-C6
19	B	823	CLA	O1D-CGD-O2D-CED
19	A	825	CLA	C6-C7-C8-C10
19	A	826	CLA	C11-C10-C8-C7
19	A	826	CLA	C11-C12-C13-C15
19	A	827	CLA	C11-C12-C13-C15
19	A	829	CLA	C6-C7-C8-C10
19	A	832	CLA	C11-C10-C8-C7
19	A	835	CLA	C6-C7-C8-C10
19	B	802	CLA	C6-C7-C8-C10
19	B	806	CLA	C6-C7-C8-C10
19	B	820	CLA	C6-C7-C8-C10
19	B	823	CLA	C6-C7-C8-C10
19	B	823	CLA	C11-C10-C8-C7
19	B	825	CLA	C11-C10-C8-C7
19	B	831	CLA	C6-C7-C8-C10
19	B	835	CLA	C6-C7-C8-C10
19	B	836	CLA	C6-C7-C8-C10
19	B	840	CLA	C11-C10-C8-C7
19	Z	308	CLA	C11-C10-C8-C7
19	Z	312	CLA	C11-C10-C8-C7
19	Z	315	CLA	C6-C7-C8-C10
19	Z	315	CLA	C11-C12-C13-C15
19	3	5008	CLA	C6-C7-C8-C10
19	3	5014	CLA	C11-C10-C8-C7
19	3	5016	CLA	C6-C7-C8-C10
19	7	308	CLA	C6-C7-C8-C10
19	7	319	CLA	C6-C7-C8-C10
19	8	308	CLA	C6-C7-C8-C10
19	8	312	CLA	C2-C3-C5-C6
19	5	301	CLA	C6-C7-C8-C10
19	5	307	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	5	312	CLA	C6-C7-C8-C10
19	5	321	CLA	C11-C10-C8-C7
19	6	301	CLA	C6-C7-C8-C10
19	6	312	CLA	C11-C10-C8-C7
19	6	313	CLA	C11-C10-C8-C7
19	6	323	CLA	C6-C7-C8-C10
20	A	844	PQN	C21-C22-C23-C25
32	8	319	CHL	C11-C12-C13-C15
19	A	840	CLA	C3-C5-C6-C7
19	B	813	CLA	C3-C5-C6-C7
32	4	317	CHL	O1A-CGA-O2A-C1
32	6	319	CHL	O1A-CGA-O2A-C1
23	1	5019	LHG	C28-C29-C30-C31
37	8	302	SQD	C9-C10-C11-C12
19	A	820	CLA	C8-C10-C11-C12
19	A	840	CLA	C8-C10-C11-C12
22	B	842	BCR	C15-C16-C17-C18
22	B	843	BCR	C13-C14-C15-C16
22	7	305	BCR	C19-C20-C21-C22
22	6	307	BCR	C19-C20-C21-C22
19	A	804	CLA	C6-C7-C8-C10
19	A	822	CLA	C6-C7-C8-C9
19	A	805	CLA	O1D-CGD-O2D-CED
19	3	5014	CLA	O1D-CGD-O2D-CED
32	8	317	CHL	O1D-CGD-O2D-CED
34	6	325	3PH	O22-C21-O21-C2
19	A	810	CLA	CBA-CGA-O2A-C1
19	8	312	CLA	CBA-CGA-O2A-C1
23	A	851	LHG	C24-C23-O8-C6
23	A	852	LHG	C11-C12-C13-C14
24	Z	301	LMT	O1'-C1-C2-C3
19	B	809	CLA	C2A-CAA-CBA-CGA
19	6	318	CLA	C2A-CAA-CBA-CGA
19	5	321	CLA	C8-C10-C11-C12
20	B	841	PQN	C15-C16-C17-C18
23	A	852	LHG	C33-C34-C35-C36
19	7	316	CLA	O1D-CGD-O2D-CED
36	7	322	PLM	C1-C2-C3-C4
19	6	313	CLA	C15-C16-C17-C18
23	A	852	LHG	C28-C29-C30-C31
34	8	322	3PH	C3A-C3B-C3C-C3D
19	A	817	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	824	CLA	CBA-CGA-O2A-C1
19	3	5016	CLA	C5-C6-C7-C8
23	8	321	LHG	C11-C12-C13-C14
34	6	325	3PH	C22-C21-O21-C2
23	A	851	LHG	O6-C4-C5-O7
34	3	5022	3PH	C24-C25-C26-C27
35	7	302	DGA	CB3-CB4-CB5-CB6
19	3	5010	CLA	C8-C10-C11-C12
19	5	306	CLA	C8-C10-C11-C12
19	3	5019	CLA	CBD-CGD-O2D-CED
19	7	306	CLA	CBD-CGD-O2D-CED
19	A	816	CLA	C5-C6-C7-C8
23	A	852	LHG	O7-C5-C6-O8
24	A	853	LMT	O5'-C5'-C6'-O6'
24	4	322	LMT	O5'-C5'-C6'-O6'
19	8	314	CLA	C6-C7-C8-C10
24	Z	319	LMT	C5'-C4'-O1B-C1B
35	7	302	DGA	CA3-CA4-CA5-CA6
19	A	834	CLA	C8-C10-C11-C12
19	B	807	CLA	C8-C10-C11-C12
19	Z	312	CLA	C5-C6-C7-C8
19	5	306	CLA	C5-C6-C7-C8
19	F	301	CLA	C4-C3-C5-C6
19	Z	311	CLA	C4-C3-C5-C6
19	A	823	CLA	C2-C3-C5-C6
19	A	805	CLA	C6-C7-C8-C9
19	A	808	CLA	C6-C7-C8-C9
19	A	823	CLA	C11-C10-C8-C9
19	A	824	CLA	C6-C7-C8-C9
19	A	827	CLA	C6-C7-C8-C9
19	A	835	CLA	C6-C7-C8-C9
19	B	802	CLA	C6-C7-C8-C9
19	B	803	CLA	C11-C10-C8-C9
19	B	806	CLA	C6-C7-C8-C9
19	B	808	CLA	C11-C10-C8-C9
19	B	808	CLA	C14-C13-C15-C16
19	B	813	CLA	C6-C7-C8-C9
19	B	814	CLA	C6-C7-C8-C9
19	B	815	CLA	C6-C7-C8-C9
19	B	820	CLA	C6-C7-C8-C9
19	B	823	CLA	C6-C7-C8-C9
19	B	826	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	B	837	CLA	C6-C7-C8-C9
19	Z	308	CLA	C11-C10-C8-C9
19	Z	312	CLA	C6-C7-C8-C9
19	Z	315	CLA	C6-C7-C8-C9
19	7	308	CLA	C6-C7-C8-C9
19	7	319	CLA	C6-C7-C8-C9
19	8	308	CLA	C6-C7-C8-C9
19	5	301	CLA	C6-C7-C8-C9
19	5	308	CLA	C6-C7-C8-C9
19	5	314	CLA	C11-C10-C8-C9
19	6	301	CLA	C6-C7-C8-C9
19	6	311	CLA	C6-C7-C8-C9
19	6	313	CLA	C11-C10-C8-C9
19	6	323	CLA	C6-C7-C8-C9
32	5	315	CHL	C6-C7-C8-C9
32	5	315	CHL	C14-C13-C15-C16
19	B	850	CLA	C2C-C3C-CAC-CBC
19	A	820	CLA	C2A-CAA-CBA-CGA
19	A	833	CLA	C2A-CAA-CBA-CGA
19	B	850	CLA	C2A-CAA-CBA-CGA
19	3	5014	CLA	C2A-CAA-CBA-CGA
19	4	316	CLA	C2A-CAA-CBA-CGA
19	5	319	CLA	CBA-CGA-O2A-C1
22	7	305	BCR	C37-C22-C23-C24
27	F	304	RRX	C11-C12-C13-C35
31	3	5003	LUT	C7-C8-C9-C19
19	A	833	CLA	C5-C6-C7-C8
22	B	844	BCR	C17-C18-C19-C20
22	7	305	BCR	C21-C22-C23-C24
19	A	821	CLA	O1A-CGA-O2A-C1
19	1	5015	CLA	O1A-CGA-O2A-C1
19	A	804	CLA	C1A-C2A-CAA-CBA
19	A	805	CLA	C1A-C2A-CAA-CBA
19	A	808	CLA	C1A-C2A-CAA-CBA
19	A	809	CLA	C1A-C2A-CAA-CBA
19	A	820	CLA	C1A-C2A-CAA-CBA
19	A	821	CLA	C1A-C2A-CAA-CBA
19	A	825	CLA	C1A-C2A-CAA-CBA
19	A	833	CLA	C1A-C2A-CAA-CBA
19	A	834	CLA	C1A-C2A-CAA-CBA
19	A	835	CLA	C1A-C2A-CAA-CBA
19	A	837	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	A	839	CLA	C1A-C2A-CAA-CBA
19	B	809	CLA	C1A-C2A-CAA-CBA
19	B	813	CLA	C1A-C2A-CAA-CBA
19	B	816	CLA	C1A-C2A-CAA-CBA
19	B	821	CLA	C1A-C2A-CAA-CBA
19	B	823	CLA	C1A-C2A-CAA-CBA
19	B	825	CLA	C1A-C2A-CAA-CBA
19	B	826	CLA	C1A-C2A-CAA-CBA
19	B	830	CLA	C1A-C2A-CAA-CBA
19	B	834	CLA	C1A-C2A-CAA-CBA
19	B	835	CLA	C1A-C2A-CAA-CBA
19	B	838	CLA	C1A-C2A-CAA-CBA
19	B	840	CLA	C1A-C2A-CAA-CBA
19	B	850	CLA	C1A-C2A-CAA-CBA
19	F	301	CLA	C1A-C2A-CAA-CBA
19	K	202	CLA	C1A-C2A-CAA-CBA
19	K	205	CLA	C1A-C2A-CAA-CBA
19	1	5015	CLA	C1A-C2A-CAA-CBA
19	1	5016	CLA	C1A-C2A-CAA-CBA
19	Z	305	CLA	C1A-C2A-CAA-CBA
19	Z	306	CLA	C1A-C2A-CAA-CBA
19	Z	307	CLA	C1A-C2A-CAA-CBA
19	Z	311	CLA	C1A-C2A-CAA-CBA
19	Z	314	CLA	C1A-C2A-CAA-CBA
19	3	5011	CLA	C1A-C2A-CAA-CBA
19	3	5015	CLA	C1A-C2A-CAA-CBA
19	7	309	CLA	C1A-C2A-CAA-CBA
19	7	312	CLA	C1A-C2A-CAA-CBA
19	7	313	CLA	C1A-C2A-CAA-CBA
19	7	317	CLA	C1A-C2A-CAA-CBA
19	8	308	CLA	C1A-C2A-CAA-CBA
19	8	318	CLA	C1A-C2A-CAA-CBA
19	8	320	CLA	C1A-C2A-CAA-CBA
19	4	309	CLA	C1A-C2A-CAA-CBA
19	4	311	CLA	C1A-C2A-CAA-CBA
19	5	309	CLA	C1A-C2A-CAA-CBA
19	5	322	CLA	C1A-C2A-CAA-CBA
19	6	302	CLA	C1A-C2A-CAA-CBA
19	6	312	CLA	C1A-C2A-CAA-CBA
19	6	320	CLA	C1A-C2A-CAA-CBA
19	6	323	CLA	C1A-C2A-CAA-CBA
32	4	315	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	1	5011	CLA	C6-C7-C8-C9
19	5	325	CLA	C6-C7-C8-C10
23	6	324	LHG	C16-C17-C18-C19
34	5	324	3PH	C22-C23-C24-C25
22	A	846	BCR	C15-C16-C17-C18
22	A	849	BCR	C9-C10-C11-C12
22	A	859	BCR	C19-C20-C21-C22
22	B	845	BCR	C15-C16-C17-C18
28	6	304	C7Z	C33-C34-C35-C15
19	A	818	CLA	C8-C10-C11-C12
19	A	820	CLA	C5-C6-C7-C8
19	B	807	CLA	C5-C6-C7-C8
19	B	817	CLA	C8-C10-C11-C12
19	Z	308	CLA	C8-C10-C11-C12
19	7	312	CLA	C5-C6-C7-C8
19	7	324	CLA	C5-C6-C7-C8
32	8	319	CHL	C13-C15-C16-C17
23	6	303	LHG	C4-O6-P-O3
23	A	852	LHG	C19-C20-C21-C22
23	1	5019	LHG	C23-C24-C25-C26
19	4	310	CLA	C3-C5-C6-C7
23	4	320	LHG	C19-C20-C21-C22
19	A	834	CLA	C5-C6-C7-C8
19	B	850	CLA	C5-C6-C7-C8
24	A	856	LMT	O5'-C5'-C6'-O6'
23	A	852	LHG	O6-C4-C5-C6
23	3	5021	LHG	O6-C4-C5-C6
23	6	303	LHG	O6-C4-C5-C6
34	5	324	3PH	O11-C1-C2-C3
19	5	310	CLA	C2C-C3C-CAC-CBC
23	6	324	LHG	C13-C14-C15-C16
19	A	830	CLA	C5-C6-C7-C8
37	8	302	SQD	C45-C46-O48-C23
19	B	809	CLA	C6-C7-C8-C10
19	Z	311	CLA	C6-C7-C8-C10
23	A	852	LHG	C30-C31-C32-C33
24	A	856	LMT	O5B-C5B-C6B-O6B
24	Z	319	LMT	C3'-C4'-O1B-C1B
19	1	5016	CLA	C3-C5-C6-C7
19	3	5014	CLA	C3-C5-C6-C7
19	A	838	CLA	C4-C3-C5-C6
19	J	1901	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	7	318	CLA	C3A-C2A-CAA-CBA
23	4	320	LHG	C11-C12-C13-C14
36	7	322	PLM	C2-C3-C4-C5
37	8	302	SQD	C10-C11-C12-C13
19	A	817	CLA	O1A-CGA-O2A-C1
23	4	320	LHG	C15-C16-C17-C18
19	1	5006	CLA	C2A-CAA-CBA-CGA
32	5	316	CHL	C2A-CAA-CBA-CGA
19	1	5010	CLA	C6-C7-C8-C9
19	Z	312	CLA	C16-C17-C18-C20
19	4	306	CLA	C11-C12-C13-C15
24	A	855	LMT	O5B-C5B-C6B-O6B
24	1	5002	LMT	O5B-C5B-C6B-O6B
24	4	302	LMT	O5'-C5'-C6'-O6'
23	A	851	LHG	C4-C5-C6-O8
23	Z	316	LHG	C4-C5-C6-O8
23	3	5021	LHG	C4-C5-C6-O8
23	5	323	LHG	C4-C5-C6-O8
23	6	324	LHG	C4-C5-C6-O8
25	B	848	DGD	O1G-C1G-C2G-C3G
32	1	5009	CHL	C5-C6-C7-C8
23	Z	316	LHG	C11-C12-C13-C14
23	5	323	LHG	C13-C14-C15-C16
38	6	326	ERG	C22-C23-C24-C25
34	3	5022	3PH	C31-C32-C33-C34
19	A	810	CLA	O1A-CGA-O2A-C1
19	8	312	CLA	O1A-CGA-O2A-C1
19	5	319	CLA	O1A-CGA-O2A-C1
23	8	321	LHG	C13-C14-C15-C16
19	B	824	CLA	O1D-CGD-O2D-CED
19	A	827	CLA	C8-C10-C11-C12
32	8	315	CHL	CAA-CBA-CGA-O2A
19	B	827	CLA	C5-C6-C7-C8
23	4	320	LHG	C25-C26-C27-C28
24	Z	319	LMT	O5'-C5'-C6'-O6'
23	1	5001	LHG	O1-C1-C2-O2
23	Z	316	LHG	O1-C1-C2-O2
23	6	303	LHG	O1-C1-C2-O2
33	4	301	SPH	C5-C6-C7-C8
19	A	814	CLA	C5-C6-C7-C8
23	6	324	LHG	C30-C31-C32-C33
19	A	825	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	I	201	CLA	C4-C3-C5-C6
19	6	311	CLA	C4-C3-C5-C6
23	Z	316	LHG	C24-C23-O8-C6
24	7	323	LMT	O5'-C5'-C6'-O6'
23	4	320	LHG	C35-C36-C37-C38
34	3	5022	3PH	C27-C28-C29-C2A
19	B	833	CLA	C15-C16-C17-C18
19	1	5008	CLA	C8-C10-C11-C12
23	6	324	LHG	C28-C29-C30-C31
24	Z	301	LMT	O5'-C5'-C6'-O6'
19	1	5013	CLA	C2A-CAA-CBA-CGA
19	8	309	CLA	C5-C6-C7-C8
19	A	810	CLA	C2-C1-O2A-CGA
19	B	818	CLA	C2-C1-O2A-CGA
19	B	826	CLA	C2-C1-O2A-CGA
19	B	831	CLA	C2-C1-O2A-CGA
19	K	203	CLA	C2-C1-O2A-CGA
19	1	5018	CLA	C2-C1-O2A-CGA
19	8	311	CLA	C2-C1-O2A-CGA
19	8	313	CLA	C2-C1-O2A-CGA
23	5	323	LHG	C26-C27-C28-C29
19	Z	305	CLA	C3-C5-C6-C7
19	7	309	CLA	C3-C5-C6-C7
19	A	815	CLA	O1D-CGD-O2D-CED
19	A	832	CLA	C5-C6-C7-C8
19	6	309	CLA	C8-C10-C11-C12
19	A	802	CLA	CBA-CGA-O2A-C1
23	4	320	LHG	O6-C4-C5-O7
23	5	323	LHG	O6-C4-C5-O7
19	4	306	CLA	C11-C12-C13-C14
32	5	315	CHL	C16-C17-C18-C19
19	B	824	CLA	O1A-CGA-O2A-C1
19	A	824	CLA	C3-C5-C6-C7
19	1	5006	CLA	C8-C10-C11-C12
23	6	324	LHG	C35-C36-C37-C38
23	7	320	LHG	O7-C5-C6-O8
23	5	323	LHG	O7-C5-C6-O8
19	A	822	CLA	C5-C6-C7-C8
23	A	851	LHG	O10-C23-O8-C6
24	F	305	LMT	C2-C3-C4-C5
18	A	801	CL0	C6-C7-C8-C10
19	A	802	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	A	803	CLA	C6-C7-C8-C10
19	A	805	CLA	C6-C7-C8-C10
19	A	806	CLA	C6-C7-C8-C10
19	A	806	CLA	C11-C12-C13-C15
19	A	808	CLA	C6-C7-C8-C10
19	A	811	CLA	C6-C7-C8-C10
19	A	812	CLA	C6-C7-C8-C10
19	A	813	CLA	C6-C7-C8-C10
19	A	813	CLA	C11-C12-C13-C15
19	A	816	CLA	C6-C7-C8-C10
19	A	818	CLA	C6-C7-C8-C10
19	A	821	CLA	C11-C12-C13-C15
19	A	823	CLA	C6-C7-C8-C10
19	A	824	CLA	C6-C7-C8-C10
19	A	826	CLA	C6-C7-C8-C10
19	A	829	CLA	C11-C10-C8-C7
19	A	833	CLA	C6-C7-C8-C10
19	A	834	CLA	C6-C7-C8-C10
19	A	839	CLA	C6-C7-C8-C10
19	B	803	CLA	C6-C7-C8-C10
19	B	804	CLA	C11-C10-C8-C7
19	B	807	CLA	C11-C12-C13-C15
19	B	808	CLA	C6-C7-C8-C10
19	B	814	CLA	C11-C10-C8-C7
19	B	815	CLA	C6-C7-C8-C10
19	B	815	CLA	C11-C10-C8-C7
19	B	816	CLA	C6-C7-C8-C10
19	B	816	CLA	C11-C10-C8-C7
19	B	817	CLA	C6-C7-C8-C10
19	B	817	CLA	C11-C10-C8-C7
19	B	818	CLA	C11-C10-C8-C7
19	B	819	CLA	C6-C7-C8-C10
19	B	822	CLA	C11-C10-C8-C7
19	B	825	CLA	C6-C7-C8-C10
19	B	826	CLA	C11-C10-C8-C7
19	B	831	CLA	C11-C10-C8-C7
19	B	835	CLA	C11-C10-C8-C7
19	B	836	CLA	C11-C12-C13-C15
19	B	836	CLA	C12-C13-C15-C16
19	B	837	CLA	C6-C7-C8-C10
19	B	850	CLA	C11-C10-C8-C7
19	I	201	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	1	5012	CLA	C11-C10-C8-C7
19	1	5016	CLA	C6-C7-C8-C10
19	Z	312	CLA	C6-C7-C8-C10
19	3	5010	CLA	C12-C13-C15-C16
19	3	5013	CLA	C6-C7-C8-C10
19	7	309	CLA	C11-C12-C13-C15
19	8	307	CLA	C11-C10-C8-C7
19	8	311	CLA	C11-C10-C8-C7
19	8	311	CLA	C11-C12-C13-C15
19	8	312	CLA	C6-C7-C8-C10
19	4	308	CLA	C6-C7-C8-C10
19	5	307	CLA	C11-C10-C8-C7
19	5	308	CLA	C6-C7-C8-C10
19	6	301	CLA	C11-C10-C8-C7
19	6	309	CLA	C6-C7-C8-C10
20	B	841	PQN	C21-C22-C23-C25
32	8	315	CHL	C11-C10-C8-C7
32	8	319	CHL	C11-C10-C8-C7
32	5	315	CHL	C6-C7-C8-C10
32	6	319	CHL	C6-C7-C8-C10
24	4	321	LMT	C3-C4-C5-C6
18	A	801	CL0	C6-C7-C8-C9
19	A	802	CLA	C6-C7-C8-C9
19	A	806	CLA	C11-C12-C13-C14
19	A	811	CLA	C6-C7-C8-C9
19	A	812	CLA	C14-C13-C15-C16
19	A	813	CLA	C6-C7-C8-C9
19	A	816	CLA	C6-C7-C8-C9
19	A	817	CLA	C6-C7-C8-C9
19	A	821	CLA	C6-C7-C8-C9
19	A	832	CLA	C14-C13-C15-C16
19	A	833	CLA	C6-C7-C8-C9
19	A	834	CLA	C6-C7-C8-C9
19	A	839	CLA	C6-C7-C8-C9
19	A	841	CLA	C6-C7-C8-C9
19	A	842	CLA	C6-C7-C8-C9
19	B	803	CLA	C6-C7-C8-C9
19	B	804	CLA	C11-C10-C8-C9
19	B	807	CLA	C11-C12-C13-C14
19	B	808	CLA	C6-C7-C8-C9
19	B	817	CLA	C6-C7-C8-C9
19	B	819	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	B	821	CLA	C11-C12-C13-C14
19	B	824	CLA	C6-C7-C8-C9
19	B	825	CLA	C6-C7-C8-C9
19	B	826	CLA	C11-C10-C8-C9
19	B	835	CLA	C6-C7-C8-C9
19	B	836	CLA	C14-C13-C15-C16
19	1	5012	CLA	C6-C7-C8-C9
19	1	5016	CLA	C6-C7-C8-C9
19	3	5013	CLA	C6-C7-C8-C9
19	3	5014	CLA	C6-C7-C8-C9
19	7	309	CLA	C6-C7-C8-C9
19	8	308	CLA	C14-C13-C15-C16
19	4	308	CLA	C11-C10-C8-C9
19	4	309	CLA	C6-C7-C8-C9
19	5	306	CLA	C6-C7-C8-C9
19	5	307	CLA	C6-C7-C8-C9
19	6	302	CLA	C6-C7-C8-C9
19	6	320	CLA	C6-C7-C8-C9
20	B	841	PQN	C16-C17-C18-C19
20	B	841	PQN	C21-C22-C23-C24
22	5	304	BCR	C15-C16-C17-C18
22	6	308	BCR	C13-C14-C15-C16
31	8	304	LUT	C29-C30-C31-C32
32	4	317	CHL	C8-C10-C11-C12
19	A	810	CLA	C2A-CAA-CBA-CGA
23	4	320	LHG	C13-C14-C15-C16
34	8	322	3PH	C3B-C3C-C3D-C3E
22	8	303	BCR	C37-C22-C23-C24
22	6	307	BCR	C7-C8-C9-C34
31	7	304	LUT	C7-C8-C9-C19
19	Z	312	CLA	C16-C17-C18-C19
23	1	5019	LHG	C31-C32-C33-C34
22	8	303	BCR	C21-C22-C23-C24
22	5	304	BCR	C21-C22-C23-C24
31	6	306	LUT	C7-C8-C9-C10
19	A	828	CLA	C10-C11-C12-C13
19	5	301	CLA	CBA-CGA-O2A-C1
19	5	307	CLA	CBA-CGA-O2A-C1
19	6	313	CLA	CBA-CGA-O2A-C1
19	F	301	CLA	C13-C15-C16-C17
19	1	5011	CLA	C5-C6-C7-C8
32	Z	309	CHL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
33	3	5001	SPH	C7-C8-C9-C10
33	4	301	SPH	C7-C8-C9-C10
32	6	315	CHL	C5-C6-C7-C8
23	1	5019	LHG	O6-C4-C5-C6
23	7	320	LHG	O6-C4-C5-C6
19	B	809	CLA	C3-C5-C6-C7
19	5	301	CLA	C3-C5-C6-C7
32	Z	309	CHL	CBA-CGA-O2A-C1
19	B	837	CLA	C8-C10-C11-C12
19	7	308	CLA	C15-C16-C17-C18
19	8	307	CLA	O1D-CGD-O2D-CED
19	A	830	CLA	C4-C3-C5-C6
29	J	1904	LMG	C28-C29-C30-C31
32	Z	313	CHL	O1D-CGD-O2D-CED
18	A	801	CL0	C5-C6-C7-C8
19	A	812	CLA	C15-C16-C17-C18
19	B	802	CLA	C8-C10-C11-C12
19	B	816	CLA	C5-C6-C7-C8
19	B	815	CLA	C2A-CAA-CBA-CGA
19	B	802	CLA	CBA-CGA-O2A-C1
19	B	803	CLA	CBA-CGA-O2A-C1
19	3	5012	CLA	CBA-CGA-O2A-C1
34	6	325	3PH	C32-C31-O31-C3
23	3	5021	LHG	C2-C3-O3-P
34	6	325	3PH	C2-C1-O11-P
19	A	828	CLA	C3A-C2A-CAA-CBA
19	A	835	CLA	C3A-C2A-CAA-CBA
19	A	839	CLA	C3A-C2A-CAA-CBA
19	B	802	CLA	C3A-C2A-CAA-CBA
19	B	807	CLA	C3A-C2A-CAA-CBA
19	B	816	CLA	C3A-C2A-CAA-CBA
19	7	319	CLA	C3A-C2A-CAA-CBA
19	6	301	CLA	C3A-C2A-CAA-CBA
19	6	322	CLA	C3A-C2A-CAA-CBA
19	6	323	CLA	C3A-C2A-CAA-CBA
32	4	315	CHL	C3A-C2A-CAA-CBA
22	4	305	BCR	C19-C20-C21-C22
28	J	1902	C7Z	C9-C10-C11-C12
24	1	5002	LMT	C2-C1-O1'-C1'
24	4	302	LMT	C2-C1-O1'-C1'
32	1	5009	CHL	C11-C12-C13-C15
19	A	843	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	8	301	CHL	CBA-CGA-O2A-C1
19	B	819	CLA	C8-C10-C11-C12
23	A	852	LHG	C4-C5-C6-O8
23	1	5001	LHG	C4-C5-C6-O8
23	7	320	LHG	C4-C5-C6-O8
23	6	303	LHG	C4-C5-C6-O8
34	3	5022	3PH	C1-C2-C3-O31
34	5	324	3PH	C1-C2-C3-O31
23	6	324	LHG	C19-C20-C21-C22
19	Z	307	CLA	C8-C10-C11-C12
19	B	831	CLA	C13-C15-C16-C17
23	6	324	LHG	C33-C34-C35-C36
33	3	5001	SPH	C11-C10-C9-C8
35	7	302	DGA	CB7-CB8-CB9-CAB
19	B	831	CLA	C4-C3-C5-C6
32	8	315	CHL	C4-C3-C5-C6
19	B	827	CLA	C11-C12-C13-C15
19	1	5010	CLA	C6-C7-C8-C10
19	F	301	CLA	C2-C3-C5-C6
23	7	320	LHG	C25-C26-C27-C28
33	3	5001	SPH	C10-C11-C12-C13
19	A	838	CLA	C8-C10-C11-C12
19	4	306	CLA	C10-C11-C12-C13
23	A	851	LHG	C4-O6-P-O3
23	1	5019	LHG	C4-O6-P-O3
19	A	835	CLA	C3-C5-C6-C7
19	A	843	CLA	C2A-CAA-CBA-CGA
32	Z	309	CHL	C2A-CAA-CBA-CGA
32	4	314	CHL	C2A-CAA-CBA-CGA
23	A	852	LHG	O1-C1-C2-O2
19	Z	305	CLA	C5-C6-C7-C8
19	4	308	CLA	C10-C11-C12-C13
23	1	5019	LHG	C15-C16-C17-C18
19	B	815	CLA	C8-C10-C11-C12
23	3	5021	LHG	O6-C4-C5-O7
23	7	320	LHG	O6-C4-C5-O7
34	8	322	3PH	O11-C1-C2-O21
19	B	811	CLA	CBA-CGA-O2A-C1
23	7	320	LHG	C9-C10-C11-C12
19	1	5008	CLA	O1D-CGD-O2D-CED
23	Z	316	LHG	O10-C23-O8-C6
19	A	822	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	1	5011	CLA	C6-C7-C8-C10
19	3	5019	CLA	C6-C7-C8-C9
19	A	805	CLA	CAA-CBA-CGA-O2A
19	6	313	CLA	C5-C6-C7-C8
19	A	802	CLA	O1A-CGA-O2A-C1
23	A	851	LHG	O7-C5-C6-O8
23	3	5021	LHG	O7-C5-C6-O8
34	3	5022	3PH	O21-C2-C3-O31
34	5	324	3PH	O21-C2-C3-O31
19	3	5012	CLA	C15-C16-C17-C18
19	B	827	CLA	C11-C12-C13-C14
19	K	203	CLA	C6-C7-C8-C10
19	7	309	CLA	C16-C17-C18-C19
19	6	314	CLA	C6-C7-C8-C9
19	A	832	CLA	C8-C10-C11-C12
19	B	832	CLA	C5-C6-C7-C8
19	4	306	CLA	C5-C6-C7-C8
19	5	314	CLA	C2-C1-O2A-CGA
19	5	321	CLA	C2-C1-O2A-CGA
19	A	833	CLA	C11-C10-C8-C9
19	A	839	CLA	C11-C12-C13-C14
19	A	839	CLA	C14-C13-C15-C16
19	B	816	CLA	C6-C7-C8-C9
19	B	822	CLA	C6-C7-C8-C9
19	B	827	CLA	C6-C7-C8-C9
19	B	833	CLA	C14-C13-C15-C16
19	Z	305	CLA	C11-C10-C8-C9
19	7	312	CLA	C11-C10-C8-C9
19	8	311	CLA	C6-C7-C8-C9
19	6	309	CLA	C6-C7-C8-C9
32	8	319	CHL	C11-C12-C13-C14
32	7	314	CHL	C8-C10-C11-C12
23	7	320	LHG	C2-C3-O3-P
23	7	320	LHG	C5-C4-O6-P
33	4	301	SPH	O1-C1-C2-C3
19	6	302	CLA	C2A-CAA-CBA-CGA
19	3	5012	CLA	C3-C5-C6-C7
22	A	849	BCR	C1-C6-C7-C8
22	A	850	BCR	C1-C6-C7-C8
22	A	850	BCR	C23-C24-C25-C30
22	A	858	BCR	C23-C24-C25-C30
22	A	859	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
22	A	859	BCR	C23-C24-C25-C30
22	B	846	BCR	C5-C6-C7-C8
22	F	302	BCR	C23-C24-C25-C26
22	K	206	BCR	C1-C6-C7-C8
22	5	305	BCR	C5-C6-C7-C8
22	6	307	BCR	C23-C24-C25-C26
27	5	302	RRX	C5-C6-C7-C8
28	J	1902	C7Z	C25-C26-C27-C28
32	Z	309	CHL	C5-C6-C7-C8
31	6	306	LUT	C7-C8-C9-C19
23	4	320	LHG	C31-C32-C33-C34
22	3	5006	BCR	C21-C22-C23-C24
31	8	304	LUT	C11-C12-C13-C14
19	5	321	CLA	C5-C6-C7-C8
19	6	313	CLA	C8-C10-C11-C12
29	J	1903	LMG	C10-C11-C12-C13
33	4	301	SPH	C10-C11-C12-C13
19	8	313	CLA	C6-C7-C8-C9
19	5	306	CLA	C11-C12-C13-C14
19	B	811	CLA	C11-C10-C8-C9
32	8	315	CHL	C8-C10-C11-C12
19	6	313	CLA	O1A-CGA-O2A-C1
25	B	848	DGD	CDA-CEA-CFA-CGA
19	B	827	CLA	C10-C11-C12-C13
23	A	851	LHG	O6-C4-C5-C6
23	8	321	LHG	O6-C4-C5-C6
34	3	5022	3PH	O11-C1-C2-C3
34	6	325	3PH	O11-C1-C2-C3
19	I	201	CLA	CAA-CBA-CGA-O2A
19	5	317	CLA	O1D-CGD-O2D-CED
19	A	808	CLA	C11-C10-C8-C7
19	A	813	CLA	C11-C10-C8-C7
19	A	817	CLA	C6-C7-C8-C10
19	A	818	CLA	C11-C10-C8-C7
19	A	819	CLA	C11-C12-C13-C15
19	A	821	CLA	C6-C7-C8-C10
19	A	828	CLA	C6-C7-C8-C10
19	A	833	CLA	C11-C10-C8-C7
19	A	840	CLA	C6-C7-C8-C10
19	A	840	CLA	C11-C10-C8-C7
19	A	842	CLA	C6-C7-C8-C10
19	A	842	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	B	801	CLA	C6-C7-C8-C10
19	B	804	CLA	C6-C7-C8-C10
19	B	807	CLA	C6-C7-C8-C10
19	B	813	CLA	C11-C12-C13-C15
19	B	824	CLA	C6-C7-C8-C10
19	B	828	CLA	C6-C7-C8-C10
19	B	833	CLA	C12-C13-C15-C16
19	B	840	CLA	C6-C7-C8-C10
19	B	850	CLA	C11-C12-C13-C15
19	1	5008	CLA	C6-C7-C8-C10
19	Z	305	CLA	C6-C7-C8-C10
19	Z	305	CLA	C11-C10-C8-C7
19	Z	307	CLA	C6-C7-C8-C10
19	Z	308	CLA	C6-C7-C8-C10
19	Z	308	CLA	C11-C12-C13-C15
19	7	308	CLA	C11-C10-C8-C7
19	7	309	CLA	C6-C7-C8-C10
19	7	310	CLA	C11-C10-C8-C7
19	7	312	CLA	C11-C10-C8-C7
19	8	307	CLA	C6-C7-C8-C10
19	8	308	CLA	C12-C13-C15-C16
19	4	309	CLA	C6-C7-C8-C10
19	5	306	CLA	C6-C7-C8-C10
19	5	306	CLA	C11-C10-C8-C7
19	5	312	CLA	C11-C12-C13-C15
19	5	314	CLA	C11-C12-C13-C15
19	5	321	CLA	C11-C12-C13-C15
19	6	302	CLA	C6-C7-C8-C10
19	6	302	CLA	C11-C10-C8-C7
19	6	313	CLA	C6-C7-C8-C10
19	6	323	CLA	C11-C12-C13-C15
20	B	841	PQN	C16-C17-C18-C20
32	4	317	CHL	C11-C12-C13-C15
32	3	5017	CHL	C3-C5-C6-C7
19	5	301	CLA	O1A-CGA-O2A-C1
19	A	810	CLA	C5-C6-C7-C8
22	A	847	BCR	C19-C20-C21-C22
22	B	847	BCR	C13-C14-C15-C16
22	G	1603	BCR	C9-C10-C11-C12
22	G	1603	BCR	C15-C16-C17-C18
22	K	206	BCR	C9-C10-C11-C12
22	7	305	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	5	302	RRX	C19-C20-C21-C22
19	A	829	CLA	CBA-CGA-O2A-C1
32	7	314	CHL	CBA-CGA-O2A-C1
19	B	822	CLA	C8-C10-C11-C12
19	B	828	CLA	C5-C6-C7-C8
19	6	311	CLA	C8-C10-C11-C12
32	Z	310	CHL	C15-C16-C17-C18
19	A	809	CLA	C2A-CAA-CBA-CGA
32	6	315	CHL	C2A-CAA-CBA-CGA
19	A	806	CLA	C3-C5-C6-C7
19	B	814	CLA	C3-C5-C6-C7
19	K	203	CLA	C3-C5-C6-C7
34	3	5022	3PH	C34-C35-C36-C37
33	4	301	SPH	C12-C13-C14-C15
23	1	5019	LHG	C17-C18-C19-C20
19	B	808	CLA	CAD-CBD-CGD-O2D
19	B	825	CLA	CAD-CBD-CGD-O2D
32	3	5017	CHL	CAD-CBD-CGD-O2D
32	8	301	CHL	CAD-CBD-CGD-O2D
33	7	321	SPH	O3-C3-C4-C5
34	6	325	3PH	C27-C28-C29-C2A
19	A	827	CLA	C10-C11-C12-C13
19	A	838	CLA	C5-C6-C7-C8
19	B	829	CLA	C5-C6-C7-C8
19	Z	311	CLA	C5-C6-C7-C8
23	8	321	LHG	C24-C23-O8-C6
20	B	841	PQN	C14-C13-C15-C16
19	B	818	CLA	C11-C12-C13-C14
24	G	1604	LMT	O5'-C1'-O1'-C1
19	6	311	CLA	C2-C3-C5-C6
23	8	321	LHG	C30-C31-C32-C33
19	B	803	CLA	O1A-CGA-O2A-C1
19	5	307	CLA	O1A-CGA-O2A-C1
23	A	852	LHG	O6-C4-C5-O7
23	1	5019	LHG	O6-C4-C5-O7
23	8	321	LHG	O6-C4-C5-O7
23	6	324	LHG	O6-C4-C5-O7
34	3	5022	3PH	O11-C1-C2-O21
34	5	324	3PH	O11-C1-C2-O21
34	6	325	3PH	O11-C1-C2-O21
23	4	320	LHG	C11-C10-C9-C8
19	8	313	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
32	5	318	CHL	C2A-CAA-CBA-CGA
34	8	322	3PH	C39-C3A-C3B-C3C
24	Z	319	LMT	O5B-C1B-O1B-C4'
19	A	806	CLA	C16-C17-C18-C19
19	A	815	CLA	C16-C17-C18-C20
19	3	5019	CLA	C6-C7-C8-C10
19	6	309	CLA	C11-C12-C13-C15
20	B	841	PQN	C26-C27-C28-C30
19	A	819	CLA	CHA-CBD-CGD-O1D
19	A	821	CLA	CHA-CBD-CGD-O1D
19	A	828	CLA	CHA-CBD-CGD-O1D
19	A	828	CLA	CHA-CBD-CGD-O2D
19	A	832	CLA	CHA-CBD-CGD-O1D
19	A	832	CLA	CHA-CBD-CGD-O2D
19	A	839	CLA	CHA-CBD-CGD-O2D
19	B	801	CLA	CHA-CBD-CGD-O2D
19	B	815	CLA	CHA-CBD-CGD-O1D
19	B	819	CLA	CHA-CBD-CGD-O1D
19	B	819	CLA	CHA-CBD-CGD-O2D
19	B	832	CLA	CHA-CBD-CGD-O1D
19	B	832	CLA	CHA-CBD-CGD-O2D
19	G	1602	CLA	CHA-CBD-CGD-O1D
19	G	1602	CLA	CHA-CBD-CGD-O2D
19	J	1901	CLA	CHA-CBD-CGD-O2D
19	Z	303	CLA	CHA-CBD-CGD-O1D
19	Z	303	CLA	CHA-CBD-CGD-O2D
19	Z	306	CLA	CHA-CBD-CGD-O2D
19	3	5014	CLA	CHA-CBD-CGD-O2D
19	7	310	CLA	CHA-CBD-CGD-O1D
19	7	310	CLA	CHA-CBD-CGD-O2D
19	8	314	CLA	CHA-CBD-CGD-O1D
19	8	314	CLA	CHA-CBD-CGD-O2D
31	4	304	LUT	C9-C10-C11-C12
32	Z	309	CHL	CHA-CBD-CGD-O1D
32	Z	310	CHL	CHA-CBD-CGD-O1D
32	7	314	CHL	CHA-CBD-CGD-O1D
32	7	314	CHL	CHA-CBD-CGD-O2D
32	8	315	CHL	CHA-CBD-CGD-O1D
32	8	315	CHL	CHA-CBD-CGD-O2D
32	5	318	CHL	C2C-C3C-CAC-CBC
35	7	302	DGA	CA5-CA6-CA7-CA8
19	7	324	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	3	5012	CLA	O1A-CGA-O2A-C1
32	Z	309	CHL	O1A-CGA-O2A-C1
32	8	301	CHL	O1A-CGA-O2A-C1
37	8	302	SQD	C2-C1-O6-C44
23	4	320	LHG	C33-C34-C35-C36
23	1	5001	LHG	O7-C5-C6-O8
19	4	310	CLA	C5-C6-C7-C8
19	B	802	CLA	O1A-CGA-O2A-C1
19	B	811	CLA	O1A-CGA-O2A-C1
33	3	5001	SPH	N2-C2-C3-O3
33	7	321	SPH	N2-C2-C3-O3
19	6	320	CLA	O1D-CGD-O2D-CED
34	8	322	3PH	C38-C39-C3A-C3B
19	A	843	CLA	O1A-CGA-O2A-C1
19	A	819	CLA	C11-C12-C13-C14
19	B	829	CLA	C6-C7-C8-C9
19	B	831	CLA	C6-C7-C8-C9
19	B	833	CLA	C6-C7-C8-C9
19	B	840	CLA	C6-C7-C8-C9
19	B	850	CLA	C14-C13-C15-C16
19	3	5013	CLA	C11-C10-C8-C9
19	7	310	CLA	C6-C7-C8-C9
19	7	310	CLA	C11-C10-C8-C9
19	8	307	CLA	C6-C7-C8-C9
19	8	308	CLA	C11-C10-C8-C9
19	5	312	CLA	C11-C12-C13-C14
19	5	314	CLA	C6-C7-C8-C9
19	5	314	CLA	C11-C12-C13-C14
20	B	841	PQN	C19-C18-C20-C21
33	3	5001	SPH	C13-C14-C15-C16
19	6	323	CLA	C3-C5-C6-C7
19	Z	305	CLA	C2A-CAA-CBA-CGA
19	4	307	CLA	C2A-CAA-CBA-CGA
23	8	321	LHG	O10-C23-O8-C6
32	7	314	CHL	O1A-CGA-O2A-C1
34	6	325	3PH	O32-C31-O31-C3
22	5	304	BCR	C37-C22-C23-C24
31	1	5004	LUT	C7-C8-C9-C19
31	1	5004	LUT	C11-C12-C13-C20
31	3	5002	LUT	C7-C8-C9-C19
31	8	304	LUT	C31-C32-C33-C40
33	3	5001	SPH	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	6	307	BCR	C7-C8-C9-C10
27	F	304	RRX	C11-C12-C13-C14
31	1	5004	LUT	C7-C8-C9-C10
31	1	5004	LUT	C11-C12-C13-C14
31	3	5002	LUT	C7-C8-C9-C10
31	7	304	LUT	C7-C8-C9-C10
31	8	304	LUT	C31-C32-C33-C34
33	4	301	SPH	C11-C10-C9-C8
19	A	816	CLA	C1A-C2A-CAA-CBA
19	B	802	CLA	C1A-C2A-CAA-CBA
19	B	806	CLA	C1A-C2A-CAA-CBA
19	B	807	CLA	C1A-C2A-CAA-CBA
19	7	319	CLA	C1A-C2A-CAA-CBA
19	8	311	CLA	C16-C17-C18-C19
20	A	844	PQN	C26-C27-C28-C30
19	A	839	CLA	C8-C10-C11-C12
19	B	809	CLA	C5-C6-C7-C8
32	5	315	CHL	C15-C16-C17-C18
19	A	840	CLA	C2-C1-O2A-CGA
19	A	842	CLA	C2-C1-O2A-CGA
19	B	806	CLA	C2-C1-O2A-CGA
19	3	5019	CLA	C2-C1-O2A-CGA
19	F	301	CLA	CBA-CGA-O2A-C1
32	6	315	CHL	CBA-CGA-O2A-C1
22	A	846	BCR	C9-C10-C11-C12
28	6	304	C7Z	C13-C14-C15-C35
24	3	5023	LMT	C11-C10-C9-C8
19	B	820	CLA	C4-C3-C5-C6
19	4	312	CLA	C3-C5-C6-C7
19	A	841	CLA	C2-C3-C5-C6
19	3	5008	CLA	C2-C3-C5-C6
19	A	829	CLA	O1A-CGA-O2A-C1
23	A	852	LHG	C3-O3-P-O4
23	A	852	LHG	C4-O6-P-O4
23	1	5001	LHG	C3-O3-P-O4
23	1	5019	LHG	C3-O3-P-O4
23	4	320	LHG	C3-O3-P-O5
23	5	323	LHG	C3-O3-P-O4
23	6	303	LHG	C4-O6-P-O4
23	6	324	LHG	C4-O6-P-O5
23	Z	316	LHG	O6-C4-C5-C6
23	4	320	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
23	5	323	LHG	O6-C4-C5-C6
34	8	322	3PH	O11-C1-C2-C3
19	B	808	CLA	C8-C10-C11-C12
32	6	316	CHL	C2A-CAA-CBA-CGA
19	A	814	CLA	C3-C5-C6-C7
19	6	301	CLA	C3-C5-C6-C7
19	4	309	CLA	O1D-CGD-O2D-CED
19	5	310	CLA	C4C-C3C-CAC-CBC
24	4	302	LMT	C3'-C4'-O1B-C1B
19	A	814	CLA	C11-C12-C13-C15
19	A	832	CLA	CAD-CBD-CGD-O1D
19	5	322	CLA	CAD-CBD-CGD-O1D
32	Z	309	CHL	CAD-CBD-CGD-O1D
32	Z	310	CHL	CAD-CBD-CGD-O1D
32	7	314	CHL	CAD-CBD-CGD-O1D
32	8	315	CHL	CAD-CBD-CGD-O1D
19	Z	312	CLA	C13-C15-C16-C17
19	7	306	CLA	O1D-CGD-O2D-CED
23	4	320	LHG	C9-C10-C11-C12
19	A	803	CLA	C11-C10-C8-C7
19	A	809	CLA	C6-C7-C8-C10
19	A	816	CLA	C11-C10-C8-C7
19	A	824	CLA	C11-C10-C8-C7
19	A	827	CLA	C11-C10-C8-C7
19	A	839	CLA	C11-C10-C8-C7
19	A	840	CLA	C12-C13-C15-C16
19	B	801	CLA	C11-C10-C8-C7
19	B	802	CLA	C11-C10-C8-C7
19	B	812	CLA	C11-C10-C8-C7
19	B	821	CLA	C6-C7-C8-C10
19	B	829	CLA	C6-C7-C8-C10
19	B	832	CLA	C11-C10-C8-C7
19	B	833	CLA	C11-C12-C13-C15
19	B	837	CLA	C11-C12-C13-C15
19	3	5013	CLA	C11-C10-C8-C7
19	3	5018	CLA	C6-C7-C8-C10
19	7	308	CLA	C12-C13-C15-C16
19	7	310	CLA	C6-C7-C8-C10
19	7	312	CLA	C6-C7-C8-C10
19	7	312	CLA	C11-C12-C13-C15
19	8	308	CLA	C11-C10-C8-C7
19	4	310	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	5	309	CLA	C6-C7-C8-C10
19	5	312	CLA	C11-C10-C8-C7
19	5	314	CLA	C6-C7-C8-C10
19	5	317	CLA	C6-C7-C8-C10
19	5	317	CLA	C11-C12-C13-C15
19	6	312	CLA	C6-C7-C8-C10
23	Z	316	LHG	O6-C4-C5-O7
31	3	5003	LUT	C25-C26-C27-C28
32	8	315	CHL	C12-C13-C15-C16
32	6	319	CHL	C11-C10-C8-C7
32	6	319	CHL	C12-C13-C15-C16
32	6	315	CHL	O1A-CGA-O2A-C1
19	Z	306	CLA	CAA-CBA-CGA-O2A
19	A	816	CLA	C8-C10-C11-C12
24	F	305	LMT	C3'-C4'-O1B-C1B
23	1	5019	LHG	C10-C11-C12-C13
19	A	808	CLA	C8-C10-C11-C12
19	B	815	CLA	C5-C6-C7-C8
32	1	5009	CHL	CBD-CGD-O2D-CED
19	A	824	CLA	C2A-CAA-CBA-CGA
19	A	825	CLA	C2A-CAA-CBA-CGA
19	B	820	CLA	C2A-CAA-CBA-CGA
19	A	832	CLA	C16-C17-C18-C19
19	7	306	CLA	C11-C12-C13-C15
33	4	301	SPH	O1-C1-C2-N2
25	B	848	DGD	O1G-C1G-C2G-O2G
36	7	322	PLM	C8-C9-CA-CB
38	8	325	ERG	C17-C20-C22-C23
23	8	321	LHG	C9-C10-C11-C12
29	J	1903	LMG	C8-C7-O1-C1
29	7	301	LMG	C8-C7-O1-C1
19	A	838	CLA	CAA-CBA-CGA-O2A
19	B	818	CLA	C11-C12-C13-C15
32	Z	309	CHL	C8-C10-C11-C12
32	Z	309	CHL	C13-C15-C16-C17
19	F	301	CLA	O1A-CGA-O2A-C1
19	7	311	CLA	C11-C10-C8-C9
32	8	316	CHL	C11-C10-C8-C9
20	B	841	PQN	C12-C13-C15-C16
19	B	808	CLA	CAA-CBA-CGA-O2A
19	B	804	CLA	C13-C15-C16-C17
19	A	824	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
19	A	838	CLA	C6-C7-C8-C9
19	A	840	CLA	C11-C10-C8-C9
19	B	815	CLA	C11-C10-C8-C9
19	B	831	CLA	C11-C10-C8-C9
19	B	836	CLA	C11-C12-C13-C14
19	B	837	CLA	C11-C10-C8-C9
19	B	850	CLA	C11-C10-C8-C9
19	B	850	CLA	C11-C12-C13-C14
19	Z	308	CLA	C11-C12-C13-C14
19	3	5010	CLA	C6-C7-C8-C9
19	7	308	CLA	C11-C10-C8-C9
19	8	312	CLA	C6-C7-C8-C9
19	4	306	CLA	C6-C7-C8-C9
19	6	302	CLA	C11-C10-C8-C9
32	6	316	CHL	C6-C7-C8-C9
32	6	319	CHL	C6-C7-C8-C9
19	3	5019	CLA	O1D-CGD-O2D-CED
19	8	312	CLA	C2C-C3C-CAC-CBC
24	F	305	LMT	C5'-C4'-O1B-C1B
19	A	829	CLA	C3-C5-C6-C7
32	8	319	CHL	C3-C5-C6-C7
19	A	806	CLA	C16-C17-C18-C20
24	4	302	LMT	C5'-C4'-O1B-C1B
36	7	322	PLM	C6-C7-C8-C9
19	A	818	CLA	O1A-CGA-O2A-C1
18	A	801	CL0	CAA-CBA-CGA-O2A
19	A	814	CLA	C8-C10-C11-C12
19	B	831	CLA	C8-C10-C11-C12
22	B	846	BCR	C18-C19-C20-C21
22	3	5007	BCR	C10-C11-C12-C13
22	3	5007	BCR	C18-C19-C20-C21
22	8	303	BCR	C10-C11-C12-C13
22	5	305	BCR	C18-C19-C20-C21
22	6	308	BCR	C18-C19-C20-C21
31	Z	317	LUT	C30-C31-C32-C33
22	7	305	BCR	C13-C14-C15-C16
27	4	303	RRX	C9-C10-C11-C12
22	3	5004	BCR	C36-C18-C19-C20
19	B	837	CLA	C15-C16-C17-C18
24	F	305	LMT	C5-C6-C7-C8
24	Z	319	LMT	C2B-C1B-O1B-C4'
23	6	303	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
32	7	315	CHL	C5-C6-C7-C8
23	A	851	LHG	C14-C15-C16-C17
19	Z	311	CLA	C2-C3-C5-C6
19	B	802	CLA	C16-C17-C18-C20
23	1	5019	LHG	C24-C25-C26-C27
19	8	313	CLA	C5-C6-C7-C8
33	7	321	SPH	C2-C3-C4-C5
19	6	323	CLA	CAA-CBA-CGA-O2A
35	7	302	DGA	CB9-CAB-CBB-CCB
29	J	1903	LMG	C7-C8-O7-C10
34	6	325	3PH	C3-C2-O21-C21
19	B	828	CLA	C2A-CAA-CBA-CGA
19	8	311	CLA	C2A-CAA-CBA-CGA
32	8	315	CHL	C2A-CAA-CBA-CGA
30	K	201	DAO	C5-C6-C7-C8
19	A	817	CLA	C2-C1-O2A-CGA
19	5	309	CLA	C2-C1-O2A-CGA
19	5	317	CLA	C2-C1-O2A-CGA
19	3	5011	CLA	C11-C12-C13-C15
25	B	848	DGD	O1G-C1A-C2A-C3A
23	A	852	LHG	C10-C11-C12-C13
19	B	803	CLA	C5-C6-C7-C8
34	8	322	3PH	C1-O11-P-O12
23	6	303	LHG	O6-C4-C5-O7
19	4	312	CLA	C6-C7-C8-C9
19	3	5010	CLA	C4-C3-C5-C6
22	G	1603	BCR	C5-C6-C7-C8
19	B	850	CLA	C13-C15-C16-C17
33	4	301	SPH	C11-C12-C13-C14
19	6	301	CLA	CBA-CGA-O2A-C1
23	Z	316	LHG	C31-C32-C33-C34
19	7	309	CLA	C16-C17-C18-C20
19	6	314	CLA	C6-C7-C8-C10
32	5	315	CHL	C5-C6-C7-C8
19	A	827	CLA	C2A-CAA-CBA-CGA
32	8	317	CHL	C2A-CAA-CBA-CGA
25	B	848	DGD	O1A-C1A-O1G-C1G
23	Z	316	LHG	O7-C5-C6-O8
23	6	324	LHG	O7-C5-C6-O8
19	A	818	CLA	CBA-CGA-O2A-C1
23	A	851	LHG	C3-O3-P-O6
23	3	5021	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
23	7	320	LHG	C4-O6-P-O3
23	8	321	LHG	C4-O6-P-O3
23	4	320	LHG	C4-O6-P-O3
23	A	852	LHG	C25-C26-C27-C28
19	B	807	CLA	C16-C17-C18-C19
19	1	5012	CLA	C11-C12-C13-C14
19	5	312	CLA	C5-C6-C7-C8
23	Z	316	LHG	C29-C30-C31-C32
19	6	310	CLA	CBA-CGA-O2A-C1
19	B	824	CLA	C15-C16-C17-C18
19	A	810	CLA	C6-C7-C8-C10
19	A	810	CLA	C11-C12-C13-C15
19	A	819	CLA	C6-C7-C8-C10
19	B	821	CLA	C11-C12-C13-C15
19	B	822	CLA	C6-C7-C8-C10
19	B	828	CLA	C11-C12-C13-C15
19	3	5008	CLA	C11-C12-C13-C15
19	3	5010	CLA	C6-C7-C8-C10
19	7	306	CLA	C6-C7-C8-C10
19	8	309	CLA	C11-C12-C13-C15
19	5	321	CLA	C6-C7-C8-C10
32	7	314	CHL	C11-C10-C8-C7
32	8	319	CHL	C12-C13-C15-C16
19	A	842	CLA	C11-C10-C8-C9
19	B	801	CLA	C11-C10-C8-C9
19	B	802	CLA	C11-C10-C8-C9
19	B	814	CLA	C11-C10-C8-C9
19	B	832	CLA	C6-C7-C8-C9
19	B	835	CLA	C11-C10-C8-C9
19	1	5012	CLA	C11-C10-C8-C9
19	5	307	CLA	C11-C10-C8-C9
19	5	309	CLA	C6-C7-C8-C9
19	5	312	CLA	C11-C10-C8-C9
19	5	317	CLA	C11-C12-C13-C14
32	6	319	CHL	C11-C10-C8-C9
19	3	5013	CLA	C8-C10-C11-C12
23	6	303	LHG	C8-C7-O7-C5
22	A	858	BCR	C9-C10-C11-C12
22	5	305	BCR	C9-C10-C11-C12
31	6	305	LUT	C9-C10-C11-C12
19	Z	315	CLA	C16-C17-C18-C19
19	B	804	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
19	3	5014	CLA	C8-C10-C11-C12
19	5	310	CLA	C5-C6-C7-C8
23	1	5019	LHG	C26-C27-C28-C29
19	B	802	CLA	CAA-CBA-CGA-O2A
19	Z	312	CLA	C2A-CAA-CBA-CGA
22	3	5004	BCR	C11-C12-C13-C35
19	8	311	CLA	C16-C17-C18-C20
34	3	5022	3PH	C3A-C3B-C3C-C3D
19	8	314	CLA	CBA-CGA-O2A-C1
23	3	5021	LHG	C5-C4-O6-P
23	5	323	LHG	C5-C4-O6-P
19	3	5014	CLA	O1A-CGA-O2A-C1
34	3	5022	3PH	C36-C37-C38-C39
19	A	809	CLA	C11-C10-C8-C7
19	B	811	CLA	C11-C10-C8-C7
19	5	308	CLA	C11-C10-C8-C7
19	A	838	CLA	C2-C3-C5-C6
19	6	310	CLA	O1A-CGA-O2A-C1
34	5	324	3PH	C21-C22-C23-C24
32	Z	309	CHL	CBD-CGD-O2D-CED
32	8	315	CHL	CAA-CBA-CGA-O1A
19	A	833	CLA	C8-C10-C11-C12
19	6	301	CLA	O1A-CGA-O2A-C1
19	3	5018	CLA	CBD-CGD-O2D-CED
25	B	848	DGD	C2A-C1A-O1G-C1G
22	F	302	BCR	C15-C16-C17-C18
28	1	5005	C7Z	C33-C34-C35-C15
19	B	821	CLA	C5-C6-C7-C8
19	7	306	CLA	C8-C10-C11-C12
19	5	314	CLA	C8-C10-C11-C12
19	8	308	CLA	O1A-CGA-O2A-C1
38	6	326	ERG	C13-C17-C20-C21
37	8	302	SQD	C23-C24-C25-C26
32	3	5017	CHL	C16-C17-C18-C19
19	4	313	CLA	C3-C5-C6-C7
19	1	5012	CLA	C8-C10-C11-C12
19	6	301	CLA	C8-C10-C11-C12
19	B	808	CLA	O1A-CGA-O2A-C1
33	4	301	SPH	C14-C15-C16-C17
34	3	5022	3PH	C37-C38-C39-C3A
32	1	5009	CHL	O1D-CGD-O2D-CED
19	A	805	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	5	310	CLA	C2-C1-O2A-CGA
32	5	316	CHL	C2-C1-O2A-CGA
23	6	324	LHG	C11-C10-C9-C8
19	5	307	CLA	C8-C10-C11-C12
32	7	314	CHL	C5-C6-C7-C8
19	3	5011	CLA	C11-C12-C13-C14
23	Z	316	LHG	C27-C28-C29-C30
19	B	819	CLA	C2A-CAA-CBA-CGA
19	7	310	CLA	C2A-CAA-CBA-CGA
19	7	311	CLA	C2A-CAA-CBA-CGA
19	5	325	CLA	C2A-CAA-CBA-CGA
32	5	315	CHL	C2A-CAA-CBA-CGA
19	1	5010	CLA	C5-C6-C7-C8
23	6	303	LHG	C2-C3-O3-P
19	A	811	CLA	C3A-C2A-CAA-CBA
19	B	811	CLA	C3A-C2A-CAA-CBA
19	3	5020	CLA	C3A-C2A-CAA-CBA
19	5	314	CLA	C3A-C2A-CAA-CBA
19	6	309	CLA	C3A-C2A-CAA-CBA
32	4	314	CHL	C3A-C2A-CAA-CBA
19	A	827	CLA	C16-C17-C18-C20
32	4	315	CHL	CBA-CGA-O2A-C1
19	A	817	CLA	C5-C6-C7-C8
19	A	817	CLA	C3-C5-C6-C7
33	3	5001	SPH	C9-C10-C11-C12
19	5	301	CLA	CAA-CBA-CGA-O2A
19	A	816	CLA	C11-C10-C8-C9
19	A	825	CLA	C6-C7-C8-C9
19	A	840	CLA	C11-C12-C13-C14
19	A	840	CLA	C14-C13-C15-C16
19	B	802	CLA	C11-C12-C13-C14
19	B	807	CLA	C11-C10-C8-C9
19	B	812	CLA	C11-C10-C8-C9
19	B	824	CLA	C14-C13-C15-C16
19	B	832	CLA	C11-C10-C8-C9
19	1	5006	CLA	C14-C13-C15-C16
19	1	5016	CLA	C11-C10-C8-C9
19	7	308	CLA	C14-C13-C15-C16
32	3	5017	CHL	C11-C12-C13-C14
19	B	818	CLA	C5-C6-C7-C8
19	4	313	CLA	C5-C6-C7-C8
32	7	314	CHL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	6	324	LHG	C25-C26-C27-C28
23	Z	316	LHG	C26-C27-C28-C29
19	A	819	CLA	C8-C10-C11-C12
19	B	836	CLA	C5-C6-C7-C8
22	A	850	BCR	C11-C10-C9-C34
22	A	850	BCR	C16-C17-C18-C36
22	B	844	BCR	C11-C10-C9-C34
22	B	844	BCR	C20-C21-C22-C37
22	B	846	BCR	C20-C21-C22-C37
22	8	303	BCR	C11-C10-C9-C34
22	5	305	BCR	C35-C13-C14-C15
22	5	305	BCR	C16-C17-C18-C36
19	B	826	CLA	C3-C5-C6-C7
19	B	838	CLA	C2A-CAA-CBA-CGA
19	Z	311	CLA	C2A-CAA-CBA-CGA
32	6	319	CHL	C2A-CAA-CBA-CGA
23	A	851	LHG	C15-C16-C17-C18
23	8	321	LHG	C12-C13-C14-C15
23	A	852	LHG	C27-C28-C29-C30
19	A	832	CLA	C16-C17-C18-C20
19	B	810	CLA	O2A-C1-C2-C3
19	B	817	CLA	O2A-C1-C2-C3
19	5	310	CLA	O2A-C1-C2-C3
25	B	848	DGD	CCA-CDA-CEA-CFA
35	7	302	DGA	CB6-CB7-CB8-CB9
19	4	311	CLA	CBD-CGD-O2D-CED
32	Z	309	CHL	O1D-CGD-O2D-CED
23	7	320	LHG	C4-C5-O7-C7
29	J	1904	LMG	C9-C8-O7-C10
19	4	313	CLA	C4-C3-C5-C6
19	A	828	CLA	C1A-C2A-CAA-CBA
19	F	303	CLA	C1A-C2A-CAA-CBA
19	Z	315	CLA	C1A-C2A-CAA-CBA
19	5	314	CLA	C1A-C2A-CAA-CBA
19	6	301	CLA	C1A-C2A-CAA-CBA
32	4	314	CHL	C1A-C2A-CAA-CBA
19	4	307	CLA	CAA-CBA-CGA-O2A
18	A	801	CL0	C11-C10-C8-C7
19	A	803	CLA	C11-C12-C13-C15
19	A	808	CLA	C11-C12-C13-C15
19	A	812	CLA	C11-C10-C8-C7
19	A	812	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	A	825	CLA	C11-C12-C13-C15
19	A	828	CLA	C11-C10-C8-C7
19	A	830	CLA	C6-C7-C8-C10
19	A	832	CLA	C6-C7-C8-C10
19	A	834	CLA	C11-C12-C13-C15
19	A	838	CLA	C11-C10-C8-C7
19	B	819	CLA	C11-C12-C13-C15
19	F	301	CLA	C11-C12-C13-C15
19	1	5006	CLA	C6-C7-C8-C10
19	Z	307	CLA	C11-C10-C8-C7
19	3	5010	CLA	C11-C10-C8-C7
19	3	5018	CLA	C11-C10-C8-C7
19	7	310	CLA	C11-C12-C13-C15
19	5	309	CLA	C11-C10-C8-C7
19	5	314	CLA	C11-C10-C8-C7
32	Z	309	CHL	C11-C10-C8-C7
32	6	315	CHL	C11-C10-C8-C7
19	B	812	CLA	C5-C6-C7-C8
19	5	317	CLA	C10-C11-C12-C13
19	6	320	CLA	C8-C10-C11-C12
22	3	5004	BCR	C19-C20-C21-C22
31	Z	317	LUT	C33-C34-C35-C15
19	5	314	CLA	C10-C11-C12-C13
19	8	314	CLA	O1A-CGA-O2A-C1
23	6	303	LHG	C9-C10-C11-C12
19	B	829	CLA	C8-C10-C11-C12
19	3	5014	CLA	C11-C12-C13-C15
19	A	837	CLA	C2A-CAA-CBA-CGA
19	B	807	CLA	C2A-CAA-CBA-CGA
23	Z	316	LHG	C30-C31-C32-C33
24	8	323	LMT	C11-C10-C9-C8
38	8	325	ERG	C23-C24-C25-C27
19	B	807	CLA	C15-C16-C17-C18
19	8	308	CLA	C8-C10-C11-C12
19	B	808	CLA	CBA-CGA-O2A-C1
23	A	852	LHG	C24-C23-O8-C6
23	5	323	LHG	C11-C10-C9-C8
23	1	5001	LHG	O6-C4-C5-C6
19	6	301	CLA	C11-C12-C13-C15
32	Z	313	CHL	CAA-CBA-CGA-O2A
19	B	812	CLA	CAA-CBA-CGA-O2A
24	1	5002	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
24	Z	319	LMT	C4-C5-C6-C7
19	B	805	CLA	CAA-CBA-CGA-O1A
19	A	813	CLA	C13-C15-C16-C17
19	A	818	CLA	C11-C12-C13-C15
24	A	856	LMT	C3'-C4'-O1B-C1B
22	A	850	BCR	C11-C10-C9-C8
22	A	850	BCR	C16-C17-C18-C19
22	B	844	BCR	C11-C10-C9-C8
22	B	844	BCR	C20-C21-C22-C23
22	B	846	BCR	C20-C21-C22-C23
22	8	303	BCR	C11-C10-C9-C8
22	5	305	BCR	C12-C13-C14-C15
22	5	305	BCR	C16-C17-C18-C19
32	Z	313	CHL	CAA-CBA-CGA-O1A
19	3	5014	CLA	CBA-CGA-O2A-C1
22	A	848	BCR	C19-C20-C21-C22
22	B	846	BCR	C13-C14-C15-C16
22	3	5006	BCR	C9-C10-C11-C12
22	6	308	BCR	C15-C16-C17-C18
27	5	302	RRX	C9-C10-C11-C12
19	B	805	CLA	CAA-CBA-CGA-O2A
19	Z	308	CLA	C16-C17-C18-C20
19	1	5011	CLA	C3-C5-C6-C7
19	A	804	CLA	C2-C1-O2A-CGA
19	B	801	CLA	C2-C1-O2A-CGA
19	B	850	CLA	C4C-C3C-CAC-CBC
19	A	810	CLA	C6-C7-C8-C9
19	1	5008	CLA	C11-C10-C8-C9
19	4	310	CLA	C6-C7-C8-C9
19	4	310	CLA	C11-C10-C8-C9
23	4	320	LHG	C17-C18-C19-C20
32	1	5009	CHL	C10-C11-C12-C13
33	7	321	SPH	O1-C1-C2-C3
19	B	807	CLA	CAA-CBA-CGA-O2A
19	A	822	CLA	C2C-C3C-CAC-CBC
23	A	852	LHG	O10-C23-O8-C6
22	A	847	BCR	C23-C24-C25-C30
22	A	859	BCR	C5-C6-C7-C8
22	7	305	BCR	C5-C6-C7-C8
22	4	305	BCR	C23-C24-C25-C30
28	J	1902	C7Z	C21-C26-C27-C28
19	A	829	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
34	3	5022	3PH	C23-C24-C25-C26
19	6	313	CLA	C13-C15-C16-C17
28	6	304	C7Z	C9-C10-C11-C12
31	5	303	LUT	C9-C10-C11-C12
18	A	801	CL0	C4-C3-C5-C6
19	A	810	CLA	C4-C3-C5-C6
19	B	807	CLA	C16-C17-C18-C20
32	6	315	CHL	C15-C16-C17-C18
18	A	801	CL0	C2-C3-C5-C6
23	6	303	LHG	C10-C11-C12-C13
25	B	848	DGD	O6D-C5D-C6D-O5D
19	4	308	CLA	C15-C16-C17-C18
19	B	836	CLA	CAA-CBA-CGA-O2A
19	6	302	CLA	C11-C12-C13-C15
19	B	807	CLA	C10-C11-C12-C13
19	B	822	CLA	C5-C6-C7-C8
19	5	301	CLA	C11-C10-C8-C9
19	3	5018	CLA	O1D-CGD-O2D-CED
19	Z	307	CLA	CAA-CBA-CGA-O2A
19	6	309	CLA	CAA-CBA-CGA-O2A
32	4	315	CHL	O1A-CGA-O2A-C1
19	Z	303	CLA	O1D-CGD-O2D-CED
19	B	817	CLA	C10-C11-C12-C13
19	A	819	CLA	C11-C10-C8-C7
19	A	830	CLA	C2-C3-C5-C6
19	A	832	CLA	C12-C13-C15-C16
19	A	842	CLA	C11-C12-C13-C15
19	B	812	CLA	C6-C7-C8-C10
19	8	310	CLA	C6-C7-C8-C10
19	4	308	CLA	C11-C10-C8-C7
19	4	310	CLA	C6-C7-C8-C10
23	1	5019	LHG	O1-C1-C2-O2
19	B	832	CLA	C3-C5-C6-C7
22	B	844	BCR	C13-C14-C15-C16
19	1	5007	CLA	CAA-CBA-CGA-O2A
24	7	323	LMT	C9-C10-C11-C12
19	B	826	CLA	C10-C11-C12-C13
19	8	308	CLA	CBA-CGA-O2A-C1
19	A	807	CLA	CAA-CBA-CGA-O2A
19	B	824	CLA	CAA-CBA-CGA-O2A
35	7	302	DGA	CEB-CFB-CGB-CHB
25	B	848	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
19	A	830	CLA	C3-C5-C6-C7
19	A	805	CLA	CAA-CBA-CGA-O1A
19	B	835	CLA	C4-C3-C5-C6
19	4	312	CLA	C4-C3-C5-C6
32	3	5017	CHL	C4-C3-C5-C6
32	8	319	CHL	C4-C3-C5-C6
19	B	831	CLA	C2-C3-C5-C6
19	3	5010	CLA	C2-C3-C5-C6
32	8	315	CHL	C2-C3-C5-C6
23	5	323	LHG	C29-C30-C31-C32
19	A	857	CLA	CAA-CBA-CGA-O2A
19	B	819	CLA	CAA-CBA-CGA-O2A
19	B	837	CLA	CAA-CBA-CGA-O2A
23	1	5019	LHG	O8-C23-C24-C25
23	8	321	LHG	C25-C26-C27-C28
19	7	311	CLA	C11-C10-C8-C7
19	5	301	CLA	C11-C10-C8-C7
32	8	316	CHL	C11-C10-C8-C7
18	A	801	CL0	C11-C10-C8-C9
19	A	803	CLA	C11-C10-C8-C9
19	A	808	CLA	C11-C12-C13-C14
19	A	812	CLA	C11-C10-C8-C9
19	A	825	CLA	C11-C12-C13-C14
19	A	827	CLA	C11-C10-C8-C9
19	A	834	CLA	C11-C12-C13-C14
19	A	839	CLA	C11-C10-C8-C9
19	B	819	CLA	C11-C12-C13-C14
19	B	828	CLA	C11-C12-C13-C14
19	B	837	CLA	C11-C12-C13-C14
19	F	301	CLA	C11-C12-C13-C14
19	Z	307	CLA	C11-C10-C8-C9
19	3	5008	CLA	C11-C12-C13-C14
19	3	5010	CLA	C11-C10-C8-C9
19	3	5012	CLA	C14-C13-C15-C16
19	3	5016	CLA	C6-C7-C8-C9
19	3	5018	CLA	C11-C10-C8-C9
19	7	312	CLA	C11-C12-C13-C14
19	6	313	CLA	C11-C12-C13-C14
19	6	323	CLA	C11-C12-C13-C14
32	7	314	CHL	C6-C7-C8-C9
35	7	302	DGA	CB2-CB3-CB4-CB5
19	3	5015	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
19	B	808	CLA	C13-C15-C16-C17
19	B	811	CLA	C5-C6-C7-C8
19	A	812	CLA	C3A-C2A-CAA-CBA
19	A	829	CLA	C3A-C2A-CAA-CBA
19	A	843	CLA	C3A-C2A-CAA-CBA
19	F	303	CLA	C3A-C2A-CAA-CBA
19	G	1602	CLA	C3A-C2A-CAA-CBA
19	3	5016	CLA	C3A-C2A-CAA-CBA
19	8	310	CLA	C3A-C2A-CAA-CBA
19	4	313	CLA	C3A-C2A-CAA-CBA
32	1	5014	CHL	C3A-C2A-CAA-CBA
19	B	815	CLA	CAA-CBA-CGA-O2A
19	7	306	CLA	CAA-CBA-CGA-O2A
23	5	323	LHG	O8-C23-C24-C25
33	4	301	SPH	C4-C5-C6-C7
34	6	325	3PH	C29-C2A-C2B-C2C
19	1	5007	CLA	CAD-CBD-CGD-O2D
19	Z	308	CLA	CAD-CBD-CGD-O2D
19	4	311	CLA	CAD-CBD-CGD-O2D
32	1	5009	CHL	CAD-CBD-CGD-O2D
32	1	5014	CHL	CAD-CBD-CGD-O2D
32	1	5017	CHL	CAD-CBD-CGD-O2D
32	4	319	CHL	CAD-CBD-CGD-O2D
32	6	315	CHL	CAD-CBD-CGD-O2D
19	1	5012	CLA	C11-C12-C13-C15
19	7	308	CLA	C5-C6-C7-C8
23	6	324	LHG	C31-C32-C33-C34
19	B	823	CLA	C15-C16-C17-C18
19	8	312	CLA	C10-C11-C12-C13
19	B	807	CLA	C2-C1-O2A-CGA
19	A	837	CLA	CAA-CBA-CGA-O2A
19	1	5006	CLA	CAA-CBA-CGA-O2A
19	3	5014	CLA	CAA-CBA-CGA-O2A
34	6	325	3PH	O21-C21-C22-C23
19	A	820	CLA	O1D-CGD-O2D-CED
19	B	817	CLA	C4-C3-C5-C6
20	A	844	PQN	C13-C15-C16-C17
19	A	832	CLA	CAA-CBA-CGA-O2A
19	B	809	CLA	CAA-CBA-CGA-O2A
19	5	322	CLA	CAA-CBA-CGA-O2A
23	4	320	LHG	O8-C23-C24-C25
22	3	5004	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	3	5004	BCR	C17-C18-C19-C20
19	A	809	CLA	C11-C10-C8-C9
19	1	5007	CLA	CAA-CBA-CGA-O1A
32	6	319	CHL	C13-C15-C16-C17
19	A	824	CLA	CAA-CBA-CGA-O2A
19	3	5010	CLA	CAA-CBA-CGA-O2A
19	5	319	CLA	CAA-CBA-CGA-O2A
19	6	302	CLA	CAA-CBA-CGA-O2A
19	K	205	CLA	CAA-CBA-CGA-O2A
24	A	856	LMT	C5'-C4'-O1B-C1B
19	A	803	CLA	O2A-C1-C2-C3
19	A	805	CLA	O2A-C1-C2-C3
19	A	806	CLA	O2A-C1-C2-C3
19	A	807	CLA	O2A-C1-C2-C3
19	A	827	CLA	O2A-C1-C2-C3
19	A	839	CLA	O2A-C1-C2-C3
19	B	814	CLA	O2A-C1-C2-C3
19	Z	308	CLA	O2A-C1-C2-C3
32	7	315	CHL	O2A-C1-C2-C3
32	8	301	CHL	O2A-C1-C2-C3
32	4	314	CHL	O2A-C1-C2-C3
32	4	315	CHL	O2A-C1-C2-C3
32	4	317	CHL	O2A-C1-C2-C3
32	6	317	CHL	O2A-C1-C2-C3
19	3	5020	CLA	C2C-C3C-CAC-CBC
23	A	851	LHG	C12-C13-C14-C15
19	B	808	CLA	C2A-CAA-CBA-CGA
19	A	823	CLA	CAA-CBA-CGA-O2A
19	B	811	CLA	CAA-CBA-CGA-O2A
23	1	5019	LHG	O7-C7-C8-C9
32	Z	309	CHL	CAA-CBA-CGA-O2A
19	3	5015	CLA	CAA-CBA-CGA-O1A
19	A	827	CLA	C16-C17-C18-C19
19	3	5014	CLA	C11-C12-C13-C14
30	K	201	DAO	C9-C10-C11-C12
19	A	802	CLA	CHA-CBD-CGD-O2D
19	A	804	CLA	CHA-CBD-CGD-O1D
19	A	804	CLA	CHA-CBD-CGD-O2D
19	A	806	CLA	CHA-CBD-CGD-O1D
19	A	810	CLA	CHA-CBD-CGD-O1D
19	A	810	CLA	CHA-CBD-CGD-O2D
19	A	819	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	A	821	CLA	CHA-CBD-CGD-O2D
19	A	822	CLA	CHA-CBD-CGD-O1D
19	A	822	CLA	CHA-CBD-CGD-O2D
19	A	824	CLA	CHA-CBD-CGD-O1D
19	A	824	CLA	CHA-CBD-CGD-O2D
19	A	827	CLA	CHA-CBD-CGD-O2D
19	A	831	CLA	CHA-CBD-CGD-O1D
19	A	831	CLA	CHA-CBD-CGD-O2D
19	A	834	CLA	CHA-CBD-CGD-O1D
19	A	834	CLA	CHA-CBD-CGD-O2D
19	A	836	CLA	CHA-CBD-CGD-O1D
19	A	836	CLA	CHA-CBD-CGD-O2D
19	A	837	CLA	CHA-CBD-CGD-O1D
19	A	837	CLA	CHA-CBD-CGD-O2D
19	A	838	CLA	CHA-CBD-CGD-O1D
19	A	838	CLA	CHA-CBD-CGD-O2D
19	A	840	CLA	CHA-CBD-CGD-O1D
19	A	840	CLA	CHA-CBD-CGD-O2D
19	A	842	CLA	CHA-CBD-CGD-O1D
19	A	842	CLA	CHA-CBD-CGD-O2D
19	A	857	CLA	CHA-CBD-CGD-O1D
19	A	857	CLA	CHA-CBD-CGD-O2D
19	B	803	CLA	CHA-CBD-CGD-O1D
19	B	803	CLA	CHA-CBD-CGD-O2D
19	B	806	CLA	CHA-CBD-CGD-O1D
19	B	806	CLA	CHA-CBD-CGD-O2D
19	B	807	CLA	CHA-CBD-CGD-O2D
19	B	814	CLA	CHA-CBD-CGD-O1D
19	B	814	CLA	CHA-CBD-CGD-O2D
19	B	820	CLA	CHA-CBD-CGD-O1D
19	B	820	CLA	CHA-CBD-CGD-O2D
19	B	821	CLA	CHA-CBD-CGD-O1D
19	B	823	CLA	CHA-CBD-CGD-O1D
19	B	823	CLA	CHA-CBD-CGD-O2D
19	B	826	CLA	CHA-CBD-CGD-O1D
19	B	826	CLA	CHA-CBD-CGD-O2D
19	B	827	CLA	CHA-CBD-CGD-O1D
19	B	827	CLA	CHA-CBD-CGD-O2D
19	B	828	CLA	CHA-CBD-CGD-O2D
19	B	830	CLA	CHA-CBD-CGD-O1D
19	B	830	CLA	CHA-CBD-CGD-O2D
19	B	834	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	B	834	CLA	CHA-CBD-CGD-O2D
19	B	836	CLA	CHA-CBD-CGD-O2D
19	B	837	CLA	CHA-CBD-CGD-O1D
19	B	837	CLA	CHA-CBD-CGD-O2D
19	B	850	CLA	CHA-CBD-CGD-O1D
19	B	850	CLA	CHA-CBD-CGD-O2D
19	I	201	CLA	CHA-CBD-CGD-O1D
19	I	201	CLA	CHA-CBD-CGD-O2D
19	K	202	CLA	CHA-CBD-CGD-O1D
19	K	202	CLA	CHA-CBD-CGD-O2D
19	K	203	CLA	CHA-CBD-CGD-O1D
19	K	203	CLA	CHA-CBD-CGD-O2D
19	K	204	CLA	CHA-CBD-CGD-O1D
19	K	204	CLA	CHA-CBD-CGD-O2D
19	1	5016	CLA	CHA-CBD-CGD-O1D
19	1	5016	CLA	CHA-CBD-CGD-O2D
19	Z	304	CLA	CHA-CBD-CGD-O1D
19	Z	304	CLA	CHA-CBD-CGD-O2D
19	Z	305	CLA	CHA-CBD-CGD-O1D
19	Z	306	CLA	CHA-CBD-CGD-O1D
19	Z	307	CLA	CHA-CBD-CGD-O1D
19	Z	307	CLA	CHA-CBD-CGD-O2D
19	Z	308	CLA	CHA-CBD-CGD-O1D
19	Z	308	CLA	CHA-CBD-CGD-O2D
19	Z	314	CLA	CHA-CBD-CGD-O1D
19	Z	314	CLA	CHA-CBD-CGD-O2D
19	3	5010	CLA	CHA-CBD-CGD-O1D
19	3	5010	CLA	CHA-CBD-CGD-O2D
19	3	5016	CLA	CHA-CBD-CGD-O1D
19	3	5016	CLA	CHA-CBD-CGD-O2D
19	7	308	CLA	CHA-CBD-CGD-O2D
19	7	312	CLA	CHA-CBD-CGD-O1D
19	7	312	CLA	CHA-CBD-CGD-O2D
19	7	317	CLA	CHA-CBD-CGD-O2D
19	7	319	CLA	CHA-CBD-CGD-O2D
19	8	309	CLA	CHA-CBD-CGD-O1D
19	8	309	CLA	CHA-CBD-CGD-O2D
19	8	311	CLA	CHA-CBD-CGD-O2D
19	8	313	CLA	CHA-CBD-CGD-O1D
19	8	313	CLA	CHA-CBD-CGD-O2D
19	8	320	CLA	CHA-CBD-CGD-O1D
19	8	320	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	4	308	CLA	CHA-CBD-CGD-O1D
19	4	308	CLA	CHA-CBD-CGD-O2D
19	4	309	CLA	CHA-CBD-CGD-O2D
19	5	301	CLA	CHA-CBD-CGD-O1D
19	5	301	CLA	CHA-CBD-CGD-O2D
19	5	309	CLA	CHA-CBD-CGD-O1D
19	5	309	CLA	CHA-CBD-CGD-O2D
19	5	312	CLA	CHA-CBD-CGD-O2D
19	5	321	CLA	CHA-CBD-CGD-O1D
19	5	321	CLA	CHA-CBD-CGD-O2D
19	6	323	CLA	CHA-CBD-CGD-O1D
19	6	323	CLA	CHA-CBD-CGD-O2D
22	B	845	BCR	C13-C14-C15-C16
28	1	5005	C7Z	C13-C14-C15-C35
31	7	303	LUT	C9-C10-C11-C12
32	Z	309	CHL	CHA-CBD-CGD-O2D
32	Z	310	CHL	CHA-CBD-CGD-O2D
19	A	813	CLA	CAA-CBA-CGA-O2A
19	A	833	CLA	CAA-CBA-CGA-O2A
19	1	5011	CLA	CAA-CBA-CGA-O2A
19	B	817	CLA	C2-C3-C5-C6
19	5	310	CLA	C3-C5-C6-C7
19	5	314	CLA	C5-C6-C7-C8
23	6	324	LHG	O6-C4-C5-C6
19	5	308	CLA	C5-C6-C7-C8
19	A	843	CLA	CAA-CBA-CGA-O2A
19	B	822	CLA	CAA-CBA-CGA-O2A
19	B	835	CLA	CAA-CBA-CGA-O2A
19	5	311	CLA	CAA-CBA-CGA-O2A
23	Z	316	LHG	O8-C23-C24-C25
23	6	303	LHG	O7-C7-C8-C9
23	1	5019	LHG	O7-C5-C6-O8
34	8	322	3PH	O21-C2-C3-O31
19	1	5010	CLA	O1D-CGD-O2D-CED
23	7	320	LHG	O8-C23-C24-C25
19	B	813	CLA	CAA-CBA-CGA-O2A
19	8	307	CLA	C4-C3-C5-C6
23	1	5019	LHG	C27-C28-C29-C30
19	A	825	CLA	C11-C10-C8-C7
19	A	839	CLA	C11-C12-C13-C15
19	B	818	CLA	C6-C7-C8-C10
19	B	823	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	Z	312	CLA	C11-C12-C13-C15
19	3	5013	CLA	C11-C12-C13-C15
19	7	319	CLA	C11-C10-C8-C7
19	6	320	CLA	C11-C10-C8-C7
19	A	836	CLA	CAA-CBA-CGA-O2A
19	1	5010	CLA	CAA-CBA-CGA-O2A
19	7	319	CLA	CAA-CBA-CGA-O2A
19	5	310	CLA	CAA-CBA-CGA-O2A
19	6	311	CLA	CAA-CBA-CGA-O2A
19	A	828	CLA	C6-C7-C8-C9
19	A	828	CLA	C11-C12-C13-C14
19	A	838	CLA	C11-C10-C8-C9
19	B	823	CLA	C11-C12-C13-C14
19	B	826	CLA	C11-C12-C13-C14
19	1	5006	CLA	C11-C12-C13-C14
19	6	312	CLA	C11-C10-C8-C9
22	B	843	BCR	C19-C20-C21-C22
28	J	1902	C7Z	C29-C30-C31-C32
19	A	857	CLA	CAA-CBA-CGA-O1A
19	A	818	CLA	C11-C12-C13-C14
19	K	204	CLA	C2A-CAA-CBA-CGA
19	A	820	CLA	CBD-CGD-O2D-CED
19	A	832	CLA	CAA-CBA-CGA-O1A
23	4	320	LHG	O10-C23-C24-C25
19	3	5016	CLA	CAA-CBA-CGA-O2A
31	1	5003	LUT	C31-C32-C33-C40
19	A	807	CLA	CAA-CBA-CGA-O1A
19	B	815	CLA	CAA-CBA-CGA-O1A
23	1	5019	LHG	O10-C23-C24-C25
19	8	308	CLA	C4-C3-C5-C6
19	B	820	CLA	C2-C3-C5-C6
23	6	324	LHG	C17-C18-C19-C20
31	1	5003	LUT	C31-C32-C33-C34
32	6	317	CHL	CBA-CGA-O2A-C1
19	B	819	CLA	C15-C16-C17-C18
18	A	801	CL0	C1A-C2A-CAA-CBA
19	A	829	CLA	C1A-C2A-CAA-CBA
19	A	842	CLA	C1A-C2A-CAA-CBA
19	B	811	CLA	C1A-C2A-CAA-CBA
19	B	824	CLA	C1A-C2A-CAA-CBA
19	G	1602	CLA	C1A-C2A-CAA-CBA
32	1	5014	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	8	301	CHL	C1A-C2A-CAA-CBA
23	A	852	LHG	C11-C10-C9-C8
19	B	819	CLA	CAA-CBA-CGA-O1A
19	B	832	CLA	C8-C10-C11-C12
19	K	205	CLA	CAA-CBA-CGA-O1A
19	4	312	CLA	C2-C1-O2A-CGA
19	A	824	CLA	CAA-CBA-CGA-O1A
19	B	837	CLA	CAA-CBA-CGA-O1A
19	5	322	CLA	CAA-CBA-CGA-O1A
19	6	302	CLA	CAA-CBA-CGA-O1A
35	7	302	DGA	OG1-CG1-CG2-CG3
23	Z	316	LHG	C11-C10-C9-C8
19	K	205	CLA	C2C-C3C-CAC-CBC
23	Z	316	LHG	C10-C11-C12-C13
19	A	820	CLA	C11-C12-C13-C15
19	B	809	CLA	CAA-CBA-CGA-O1A
19	5	310	CLA	CAA-CBA-CGA-O1A
19	A	806	CLA	C15-C16-C17-C18
29	J	1903	LMG	C12-C13-C14-C15
19	Z	303	CLA	CAA-CBA-CGA-O2A
19	Z	312	CLA	CAA-CBA-CGA-O2A
19	3	5020	CLA	CAA-CBA-CGA-O2A
23	Z	316	LHG	O7-C7-C8-C9
19	8	311	CLA	C3-C5-C6-C7
19	A	837	CLA	CAA-CBA-CGA-O1A
19	1	5006	CLA	CAA-CBA-CGA-O1A
19	3	5014	CLA	CAA-CBA-CGA-O1A
19	3	5016	CLA	CAA-CBA-CGA-O1A
19	5	319	CLA	CAA-CBA-CGA-O1A
23	Z	316	LHG	O10-C23-C24-C25
34	6	325	3PH	O22-C21-C22-C23
19	A	838	CLA	O1A-CGA-O2A-C1
23	1	5019	LHG	C4-O6-P-O5
23	3	5021	LHG	C4-O6-P-O5
23	8	321	LHG	C4-O6-P-O5
23	4	320	LHG	C4-O6-P-O5
38	8	325	ERG	C23-C24-C25-C26
38	8	325	ERG	C28-C24-C25-C27
19	A	813	CLA	CAA-CBA-CGA-O1A
19	A	836	CLA	CAA-CBA-CGA-O1A
19	A	843	CLA	CAA-CBA-CGA-O1A
19	1	5011	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
23	5	323	LHG	O10-C23-C24-C25
19	5	309	CLA	C3-C5-C6-C7
24	Z	301	LMT	C11-C10-C9-C8
19	A	823	CLA	CAA-CBA-CGA-O1A
19	B	811	CLA	CAA-CBA-CGA-O1A
19	B	822	CLA	CAA-CBA-CGA-O1A
19	1	5010	CLA	CAA-CBA-CGA-O1A
23	1	5019	LHG	O9-C7-C8-C9
19	3	5020	CLA	C4C-C3C-CAC-CBC
23	A	852	LHG	C16-C17-C18-C19
19	1	5012	CLA	CAA-CBA-CGA-O2A
19	6	313	CLA	CAA-CBA-CGA-O2A
19	B	837	CLA	C13-C15-C16-C17
23	A	852	LHG	C35-C36-C37-C38
23	6	324	LHG	C15-C16-C17-C18
19	A	833	CLA	CAA-CBA-CGA-O1A
19	6	311	CLA	CAA-CBA-CGA-O1A
19	B	826	CLA	CAA-CBA-CGA-O2A
19	6	314	CLA	CAA-CBA-CGA-O2A
29	J	1903	LMG	O7-C10-C11-C12
19	5	311	CLA	CAA-CBA-CGA-O1A
23	7	320	LHG	O10-C23-C24-C25
19	5	325	CLA	C4-C3-C5-C6
19	B	804	CLA	C16-C17-C18-C20
19	A	803	CLA	CAD-CBD-CGD-O1D
19	A	814	CLA	CAD-CBD-CGD-O1D
19	A	820	CLA	CAD-CBD-CGD-O1D
19	A	823	CLA	CAD-CBD-CGD-O1D
19	A	827	CLA	CAD-CBD-CGD-O1D
19	B	807	CLA	CAD-CBD-CGD-O1D
19	B	822	CLA	CAD-CBD-CGD-O1D
19	B	828	CLA	CAD-CBD-CGD-O1D
19	B	829	CLA	CAD-CBD-CGD-O1D
19	G	1601	CLA	CAD-CBD-CGD-O1D
19	7	308	CLA	CAD-CBD-CGD-O1D
19	7	317	CLA	CAD-CBD-CGD-O1D
19	7	319	CLA	CAD-CBD-CGD-O1D
19	4	306	CLA	CAD-CBD-CGD-O1D
19	5	312	CLA	CAD-CBD-CGD-O1D
19	6	301	CLA	CAD-CBD-CGD-O1D
19	6	311	CLA	CAD-CBD-CGD-O1D
23	7	320	LHG	C6-C5-O7-C7

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Mol	Chain	Res	Type	Atoms
19	B	816	CLA	O1A-CGA-O2A-C1
32	6	317	CHL	O1A-CGA-O2A-C1
19	B	813	CLA	CAA-CBA-CGA-O1A
32	Z	309	CHL	CAA-CBA-CGA-O1A
19	1	5008	CLA	CAA-CBA-CGA-O2A
19	7	307	CLA	CAA-CBA-CGA-O2A
19	3	5018	CLA	C8-C10-C11-C12
19	4	309	CLA	C5-C6-C7-C8
19	A	802	CLA	C11-C10-C8-C9
19	A	825	CLA	C11-C10-C8-C9
19	F	301	CLA	C11-C10-C8-C9
19	Z	312	CLA	C11-C12-C13-C14
19	3	5013	CLA	C11-C12-C13-C14
19	7	319	CLA	C11-C10-C8-C9
19	8	311	CLA	C14-C13-C15-C16
19	6	320	CLA	C11-C10-C8-C9
32	8	315	CHL	C11-C10-C8-C9
32	6	319	CHL	C14-C13-C15-C16
19	I	201	CLA	CAA-CBA-CGA-O1A
29	J	1904	LMG	C21-C22-C23-C24
19	A	810	CLA	CAA-CBA-CGA-O2A
19	B	810	CLA	CAA-CBA-CGA-O2A
19	B	829	CLA	CAA-CBA-CGA-O2A
19	B	850	CLA	CAA-CBA-CGA-O2A
19	K	203	CLA	CAA-CBA-CGA-O2A
19	3	5013	CLA	CAA-CBA-CGA-O2A
19	4	310	CLA	CAA-CBA-CGA-O2A
19	5	317	CLA	CAA-CBA-CGA-O2A
32	6	316	CHL	CAA-CBA-CGA-O2A
32	6	317	CHL	CAA-CBA-CGA-O2A
19	B	819	CLA	C10-C11-C12-C13
19	B	816	CLA	CBA-CGA-O2A-C1
19	A	806	CLA	CAA-CBA-CGA-O2A
19	A	811	CLA	CAA-CBA-CGA-O2A
19	A	820	CLA	CAA-CBA-CGA-O2A
19	8	314	CLA	CAA-CBA-CGA-O2A
19	6	310	CLA	CAA-CBA-CGA-O2A
32	7	315	CHL	CAA-CBA-CGA-O2A
32	4	314	CHL	CAA-CBA-CGA-O2A
19	5	313	CLA	CAA-CBA-CGA-O2A
19	B	835	CLA	CAA-CBA-CGA-O1A
23	6	303	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	B	818	CLA	C4-C3-C5-C6
19	A	802	CLA	C11-C10-C8-C7
19	A	811	CLA	C11-C10-C8-C7
19	A	814	CLA	C11-C10-C8-C7
19	A	816	CLA	C11-C12-C13-C15
19	A	817	CLA	C11-C10-C8-C7
19	A	820	CLA	C6-C7-C8-C10
19	A	828	CLA	C11-C12-C13-C15
19	A	830	CLA	C11-C12-C13-C15
19	A	834	CLA	C11-C10-C8-C7
19	A	839	CLA	C12-C13-C15-C16
19	B	813	CLA	C11-C10-C8-C7
19	B	826	CLA	C11-C12-C13-C15
19	1	5006	CLA	C11-C12-C13-C15
19	1	5008	CLA	C12-C13-C15-C16
19	4	313	CLA	C2-C3-C5-C6
19	6	313	CLA	C11-C12-C13-C15
19	B	829	CLA	CAA-CBA-CGA-O1A
19	7	307	CLA	CAA-CBA-CGA-O1A
19	7	319	CLA	CAA-CBA-CGA-O1A
19	5	317	CLA	CAA-CBA-CGA-O1A
23	Z	316	LHG	O9-C7-C8-C9
19	B	814	CLA	CAA-CBA-CGA-O2A
19	G	1601	CLA	CAA-CBA-CGA-O2A
19	K	204	CLA	CAA-CBA-CGA-O2A
19	8	311	CLA	CAA-CBA-CGA-O2A
19	4	312	CLA	CAA-CBA-CGA-O2A
19	5	325	CLA	CAA-CBA-CGA-O2A
32	4	315	CHL	CAA-CBA-CGA-O2A
19	7	309	CLA	CBA-CGA-O2A-C1
19	A	827	CLA	C15-C16-C17-C18
22	B	846	BCR	C21-C22-C23-C24
19	B	850	CLA	CAA-CBA-CGA-O1A
19	Z	303	CLA	CAA-CBA-CGA-O1A
19	8	314	CLA	CAA-CBA-CGA-O1A
19	6	310	CLA	CAA-CBA-CGA-O1A
32	6	316	CHL	CAA-CBA-CGA-O1A
22	A	850	BCR	C13-C14-C15-C16
22	3	5004	BCR	C13-C14-C15-C16
24	Z	301	LMT	C2-C3-C4-C5
24	7	323	LMT	C2-C1-O1'-C1'
24	8	324	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
19	A	827	CLA	CAA-CBA-CGA-O2A
19	5	312	CLA	CAA-CBA-CGA-O2A
35	7	302	DGA	OG1-CA1-CA2-CA3
19	4	310	CLA	C10-C11-C12-C13
19	A	810	CLA	CAA-CBA-CGA-O1A
19	A	811	CLA	CAA-CBA-CGA-O1A
19	B	810	CLA	CAA-CBA-CGA-O1A
19	1	5008	CLA	CAA-CBA-CGA-O1A
19	3	5013	CLA	CAA-CBA-CGA-O1A
32	4	314	CHL	CAA-CBA-CGA-O1A
32	4	315	CHL	CAA-CBA-CGA-O1A
32	6	317	CHL	CAA-CBA-CGA-O1A
33	7	321	SPH	C11-C10-C9-C8
19	B	833	CLA	C13-C15-C16-C17
19	A	830	CLA	CAA-CBA-CGA-O2A
19	B	806	CLA	CAA-CBA-CGA-O2A
19	B	831	CLA	CAA-CBA-CGA-O2A
19	1	5016	CLA	CAA-CBA-CGA-O2A
32	1	5014	CHL	CAA-CBA-CGA-O2A
19	G	1601	CLA	CAA-CBA-CGA-O1A
19	3	5020	CLA	CAA-CBA-CGA-O1A
32	7	315	CHL	CAA-CBA-CGA-O1A
19	B	813	CLA	C16-C17-C18-C19
19	B	816	CLA	C10-C11-C12-C13
19	B	826	CLA	CAA-CBA-CGA-O1A
19	K	203	CLA	CAA-CBA-CGA-O1A
19	Z	312	CLA	CAA-CBA-CGA-O1A
19	6	314	CLA	CAA-CBA-CGA-O1A
19	B	839	CLA	CAA-CBA-CGA-O2A
19	Z	308	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

311 monomers are involved in 2490 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	856	LMT	8	0
32	8	317	CHL	7	0
19	B	832	CLA	19	0
24	1	5002	LMT	9	0
31	Z	318	LUT	9	0
19	8	308	CLA	8	0
19	4	310	CLA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	5	317	CLA	14	0
32	3	5017	CHL	13	0
24	4	302	LMT	5	0
22	8	306	BCR	7	0
19	1	5010	CLA	13	0
19	K	204	CLA	8	0
19	B	834	CLA	13	0
19	B	833	CLA	14	0
31	6	305	LUT	11	0
19	8	318	CLA	13	0
19	7	309	CLA	10	0
19	5	301	CLA	8	0
19	A	819	CLA	15	0
32	4	314	CHL	13	0
19	B	838	CLA	9	0
33	7	321	SPH	7	0
19	B	802	CLA	12	0
19	7	307	CLA	14	0
19	8	310	CLA	9	0
19	A	842	CLA	12	0
19	8	309	CLA	12	0
31	1	5004	LUT	8	0
19	B	817	CLA	5	0
19	7	313	CLA	4	0
22	3	5004	BCR	7	0
32	1	5014	CHL	8	0
19	A	816	CLA	16	0
19	1	5018	CLA	4	0
19	G	1601	CLA	6	0
19	B	811	CLA	7	0
19	I	201	CLA	12	0
19	6	314	CLA	16	0
19	A	833	CLA	11	0
19	Z	304	CLA	4	0
19	7	319	CLA	7	0
19	3	5008	CLA	14	0
32	8	316	CHL	7	0
31	3	5002	LUT	5	0
22	6	308	BCR	16	0
19	B	801	CLA	16	0
24	A	855	LMT	1	0
33	4	301	SPH	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	852	LHG	5	0
19	A	823	CLA	18	0
19	K	202	CLA	11	0
31	4	304	LUT	13	0
18	A	801	CL0	12	0
32	4	315	CHL	5	0
19	A	820	CLA	10	0
32	Z	302	CHL	14	0
19	3	5011	CLA	7	0
19	3	5019	CLA	12	0
19	6	323	CLA	14	0
19	B	825	CLA	19	0
28	6	304	C7Z	4	0
23	6	303	LHG	9	0
24	F	305	LMT	9	0
27	4	303	RRX	6	0
34	5	324	3PH	3	0
27	5	302	RRX	11	0
19	7	306	CLA	14	0
32	5	318	CHL	15	0
22	A	849	BCR	17	0
19	5	325	CLA	15	0
32	6	319	CHL	17	0
32	Z	310	CHL	11	0
19	B	813	CLA	11	0
19	4	308	CLA	11	0
19	1	5016	CLA	26	0
19	B	835	CLA	19	0
19	A	809	CLA	10	0
19	Z	308	CLA	11	0
19	A	804	CLA	9	0
19	A	837	CLA	7	0
31	8	304	LUT	11	0
19	A	831	CLA	1	0
19	A	841	CLA	14	0
19	8	314	CLA	3	0
19	4	318	CLA	4	0
31	Z	317	LUT	13	0
32	Z	309	CHL	16	0
19	3	5016	CLA	16	0
32	Z	313	CHL	10	0
19	3	5013	CLA	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	3	5023	LMT	7	0
19	A	826	CLA	9	0
19	5	314	CLA	16	0
19	1	5007	CLA	13	0
32	7	315	CHL	6	0
19	3	5015	CLA	7	0
28	J	1902	C7Z	1	0
19	4	307	CLA	15	0
24	G	1604	LMT	11	0
19	K	203	CLA	13	0
19	A	818	CLA	17	0
19	F	303	CLA	5	0
20	B	841	PQN	5	0
19	Z	314	CLA	7	0
20	A	844	PQN	4	0
23	1	5019	LHG	10	0
19	B	807	CLA	5	0
19	A	822	CLA	19	0
29	J	1904	LMG	12	0
19	7	317	CLA	9	0
31	8	305	LUT	5	0
19	3	5010	CLA	10	0
23	A	851	LHG	7	0
19	A	813	CLA	6	0
23	6	324	LHG	13	0
32	6	315	CHL	15	0
19	5	311	CLA	12	0
19	5	309	CLA	14	0
19	5	319	CLA	11	0
19	Z	305	CLA	14	0
19	B	810	CLA	6	0
19	4	313	CLA	11	0
38	6	326	ERG	24	0
24	7	323	LMT	2	0
29	7	301	LMG	1	0
22	B	843	BCR	5	0
19	5	306	CLA	20	0
19	1	5008	CLA	10	0
22	8	303	BCR	10	0
38	8	325	ERG	14	0
19	B	820	CLA	9	0
19	A	828	CLA	22	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	3	5001	SPH	12	0
19	Z	315	CLA	10	0
32	5	316	CHL	6	0
19	3	5014	CLA	11	0
22	K	206	BCR	12	0
19	Z	306	CLA	2	0
22	G	1603	BCR	12	0
19	A	806	CLA	11	0
29	J	1903	LMG	4	0
19	8	311	CLA	13	0
28	1	5005	C7Z	1	0
32	5	320	CHL	8	0
22	B	847	BCR	8	0
24	Z	301	LMT	7	0
22	F	302	BCR	9	0
31	5	303	LUT	10	0
19	A	810	CLA	9	0
19	B	822	CLA	16	0
19	Z	303	CLA	7	0
22	B	844	BCR	11	0
22	4	305	BCR	14	0
22	7	305	BCR	5	0
19	Z	311	CLA	12	0
22	A	846	BCR	8	0
19	1	5011	CLA	9	0
23	5	323	LHG	7	0
19	B	818	CLA	7	0
22	6	307	BCR	23	0
24	Z	319	LMT	4	0
32	6	321	CHL	9	0
19	4	311	CLA	10	0
19	B	830	CLA	10	0
32	5	315	CHL	18	0
19	6	318	CLA	8	0
30	K	201	DAO	4	0
24	8	323	LMT	5	0
19	A	821	CLA	17	0
19	A	839	CLA	19	0
19	B	831	CLA	15	0
19	6	309	CLA	13	0
19	A	812	CLA	14	0
32	8	301	CHL	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	3	5006	BCR	21	0
32	1	5017	CHL	12	0
19	3	5020	CLA	7	0
19	A	836	CLA	14	0
31	1	5003	LUT	7	0
19	B	850	CLA	29	0
24	A	853	LMT	8	0
19	3	5018	CLA	14	0
19	B	819	CLA	17	0
19	A	843	CLA	7	0
19	6	320	CLA	11	0
32	6	316	CHL	17	0
23	Z	316	LHG	6	0
31	6	306	LUT	5	0
34	6	325	3PH	5	0
31	3	5003	LUT	9	0
19	5	308	CLA	8	0
25	B	848	DGD	5	0
19	5	321	CLA	14	0
19	B	816	CLA	12	0
19	B	823	CLA	22	0
19	A	857	CLA	13	0
19	A	814	CLA	17	0
19	A	830	CLA	12	0
19	B	805	CLA	3	0
19	1	5015	CLA	5	0
19	7	310	CLA	6	0
19	B	815	CLA	10	0
19	B	840	CLA	16	0
22	A	858	BCR	6	0
22	A	848	BCR	7	0
23	7	320	LHG	3	0
19	B	804	CLA	11	0
32	8	315	CHL	13	0
19	G	1602	CLA	12	0
19	B	829	CLA	10	0
32	4	317	CHL	11	0
19	4	316	CLA	10	0
19	K	205	CLA	9	0
19	7	316	CLA	5	0
19	B	808	CLA	14	0
22	3	5007	BCR	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	6	312	CLA	13	0
19	A	805	CLA	13	0
19	A	835	CLA	16	0
27	F	304	RRX	9	0
19	B	806	CLA	8	0
19	7	312	CLA	14	0
19	A	825	CLA	8	0
19	A	840	CLA	10	0
34	3	5022	3PH	4	0
22	3	5005	BCR	7	0
19	B	824	CLA	15	0
19	8	320	CLA	4	0
19	7	311	CLA	11	0
22	B	845	BCR	18	0
19	B	803	CLA	14	0
19	6	313	CLA	25	0
31	7	304	LUT	12	0
19	A	834	CLA	9	0
21	C	102	SF4	5	0
19	Z	312	CLA	9	0
22	A	859	BCR	12	0
36	7	322	PLM	2	0
19	B	809	CLA	10	0
31	7	303	LUT	5	0
19	A	829	CLA	12	0
37	8	302	SQD	11	0
19	B	812	CLA	10	0
19	Z	307	CLA	7	0
19	A	832	CLA	13	0
22	5	304	BCR	11	0
19	6	311	CLA	10	0
19	A	827	CLA	19	0
19	B	839	CLA	7	0
24	4	322	LMT	11	0
19	B	836	CLA	13	0
32	8	319	CHL	5	0
19	A	807	CLA	9	0
19	4	309	CLA	8	0
19	7	308	CLA	14	0
19	A	838	CLA	13	0
19	A	824	CLA	17	0
19	5	307	CLA	18	0

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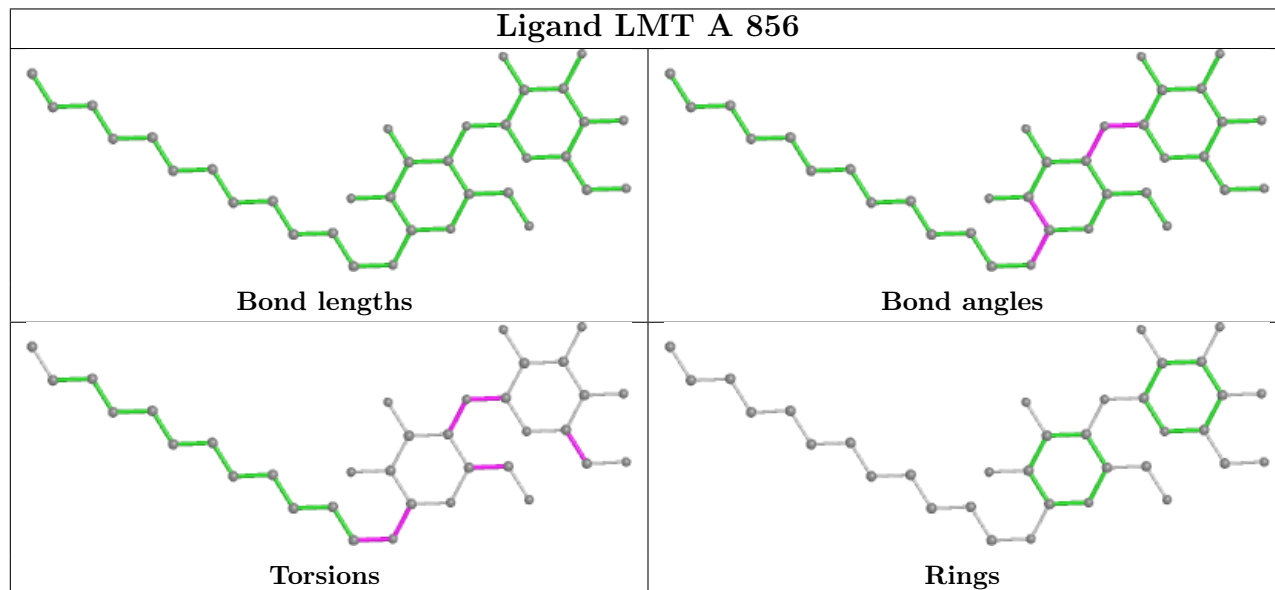
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24	8	324	LMT	3	0
19	5	312	CLA	13	0
19	6	322	CLA	8	0
19	6	302	CLA	16	0
19	A	802	CLA	14	0
19	7	318	CLA	4	0
19	B	814	CLA	12	0
22	A	847	BCR	13	0
19	J	1901	CLA	4	0
19	1	5012	CLA	13	0
19	1	5006	CLA	6	0
19	5	310	CLA	18	0
24	A	854	LMT	5	0
32	6	317	CHL	7	0
19	A	811	CLA	13	0
19	8	313	CLA	12	0
19	3	5009	CLA	7	0
19	1	5013	CLA	8	0
23	8	321	LHG	7	0
19	B	821	CLA	20	0
23	4	320	LHG	14	0
19	3	5012	CLA	20	0
22	5	305	BCR	6	0
19	8	307	CLA	19	0
19	8	312	CLA	17	0
22	A	850	BCR	11	0
19	A	815	CLA	20	0
19	F	301	CLA	13	0
19	B	826	CLA	17	0
19	A	817	CLA	10	0
21	A	845	SF4	4	0
34	8	322	3PH	6	0
19	6	310	CLA	24	0
22	B	842	BCR	16	0
19	6	301	CLA	18	0
24	4	321	LMT	4	0
19	A	803	CLA	7	0
19	5	322	CLA	7	0
32	1	5009	CHL	5	0
19	A	808	CLA	16	0
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19	B	837	CLA	18	0

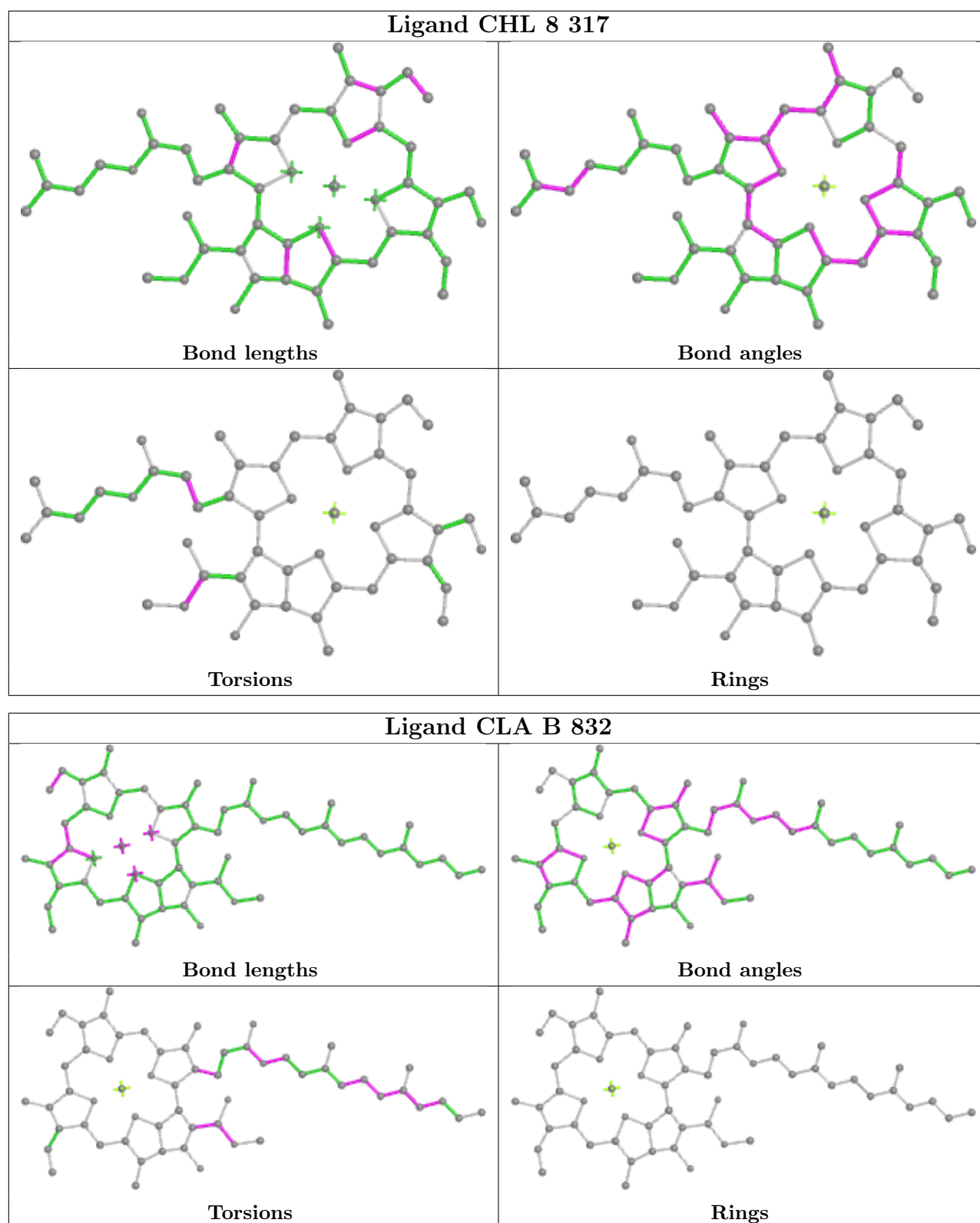
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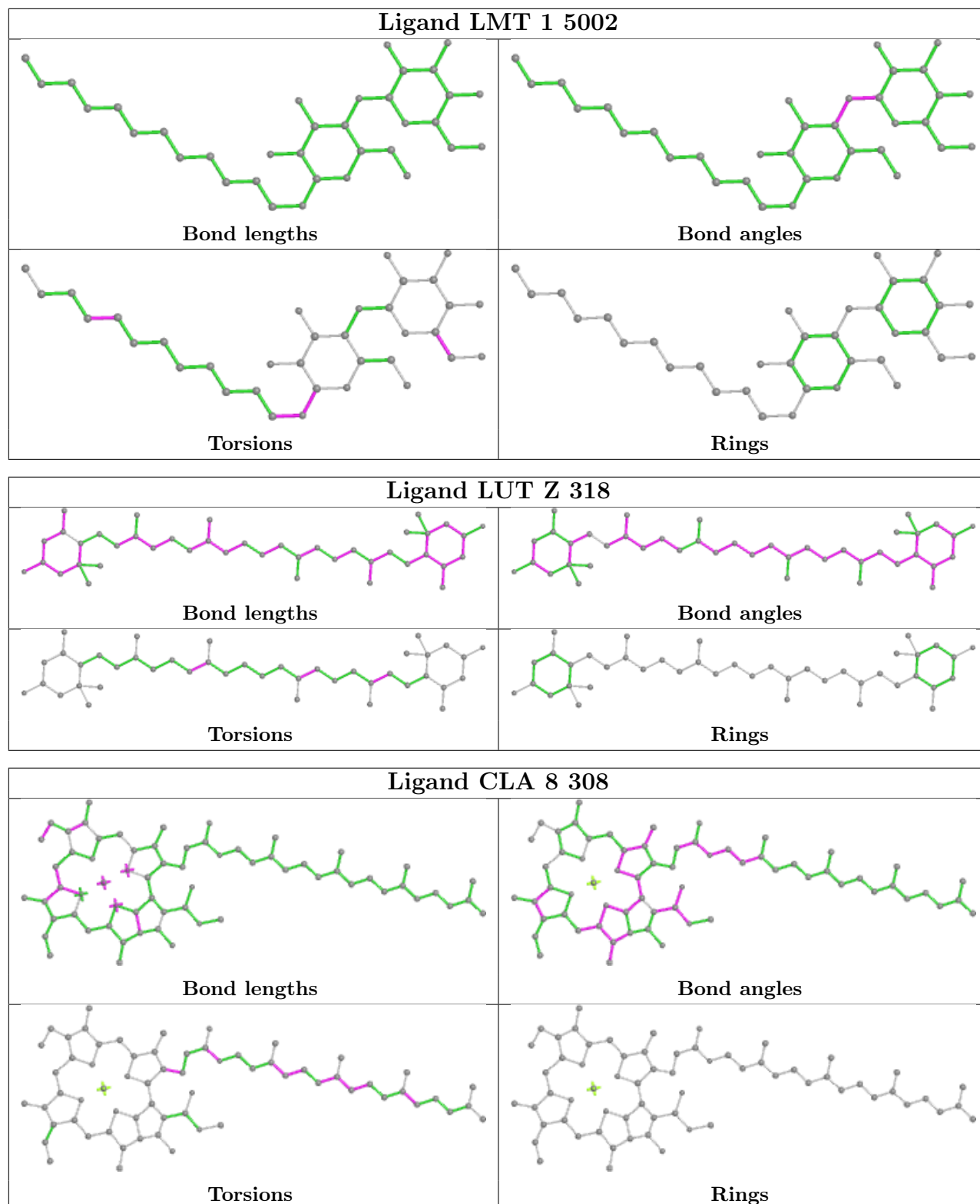
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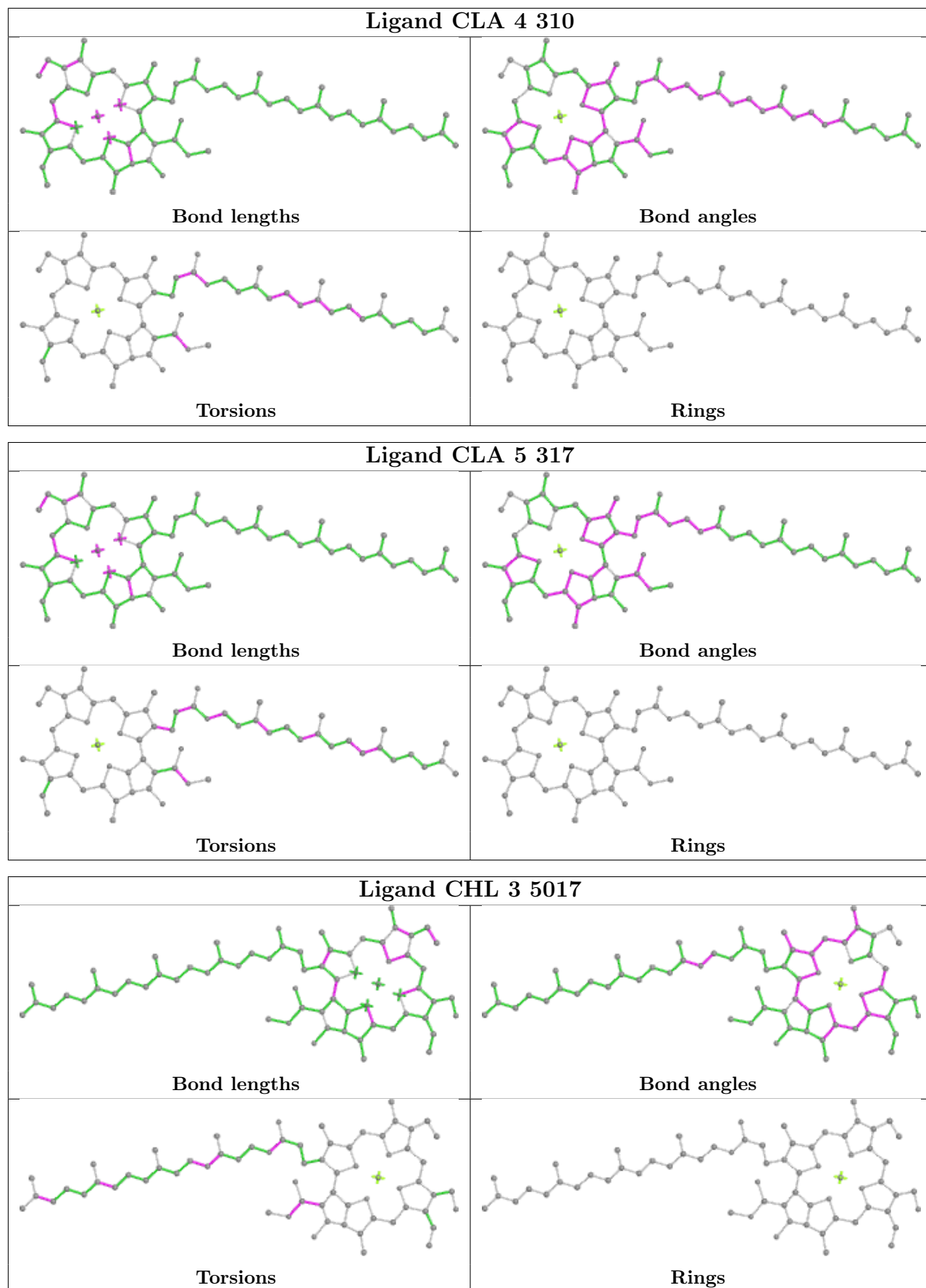
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	846	BCR	20	0
32	7	314	CHL	12	0
23	3	5021	LHG	4	0
19	4	306	CLA	23	0
19	4	312	CLA	13	0
19	5	313	CLA	10	0
19	B	828	CLA	7	0
35	7	302	DGA	14	0
32	4	319	CHL	5	0
19	7	324	CLA	15	0

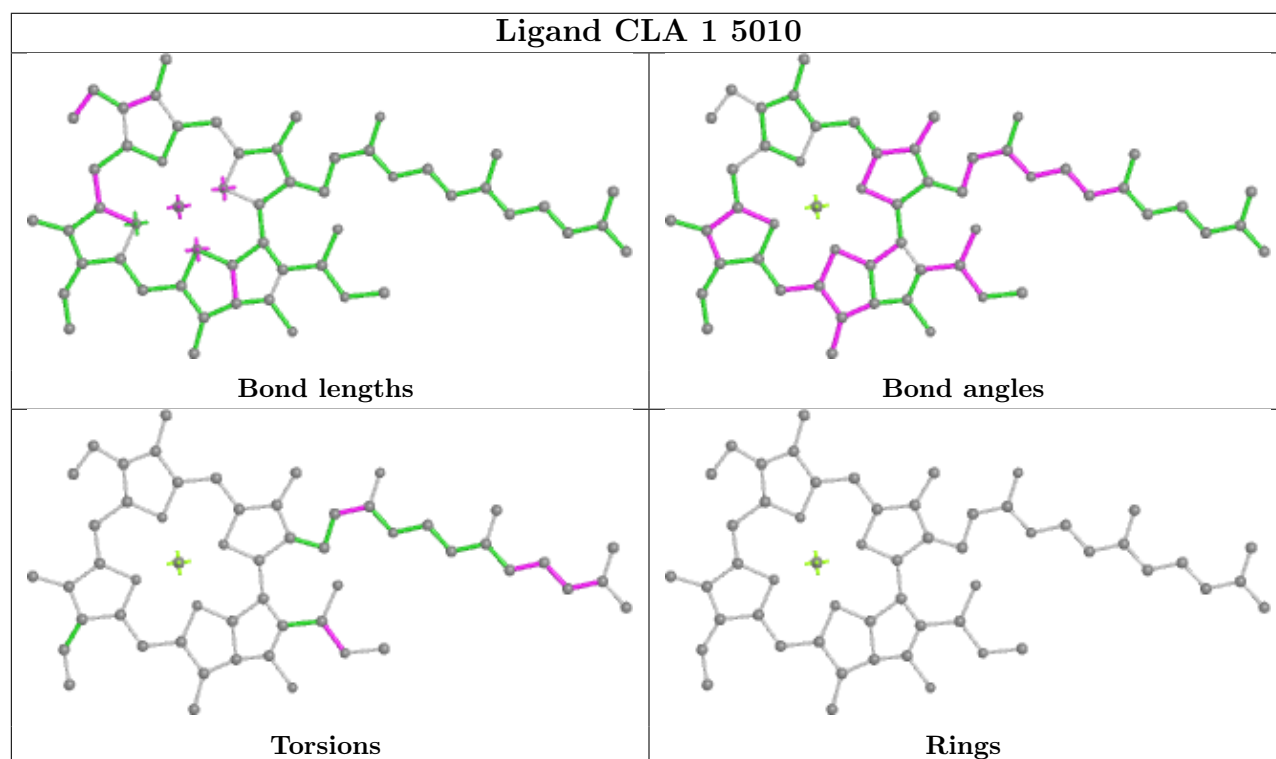
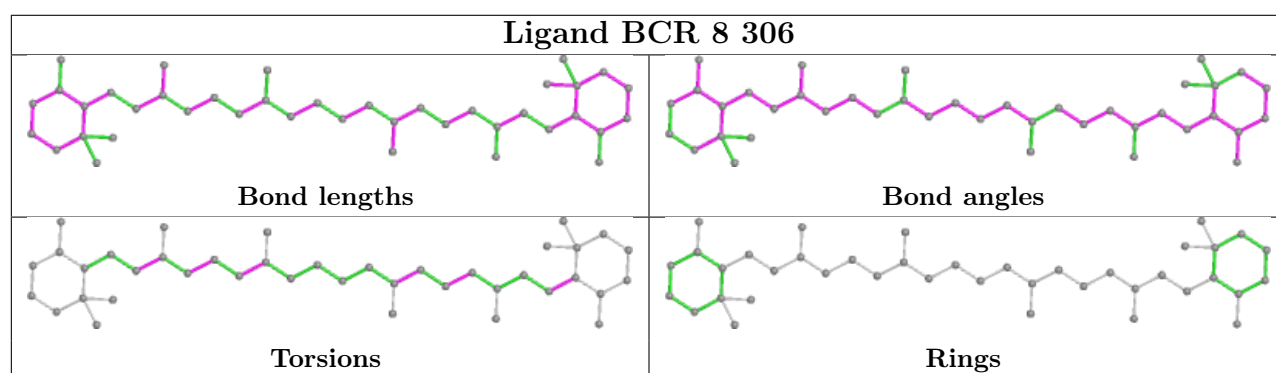
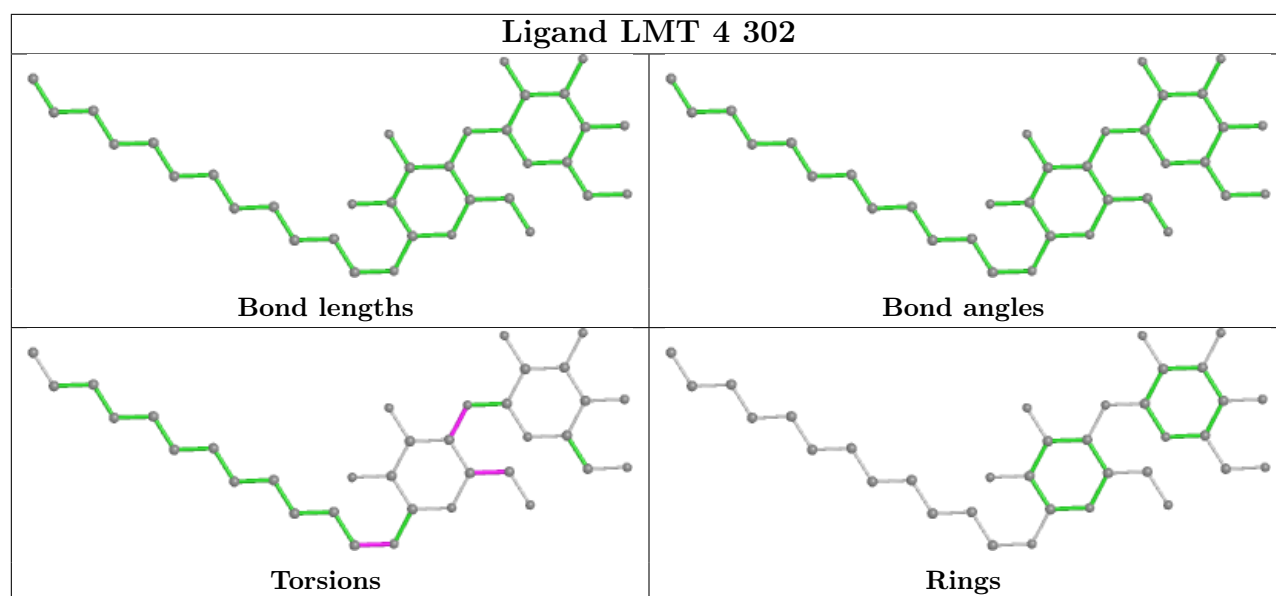
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

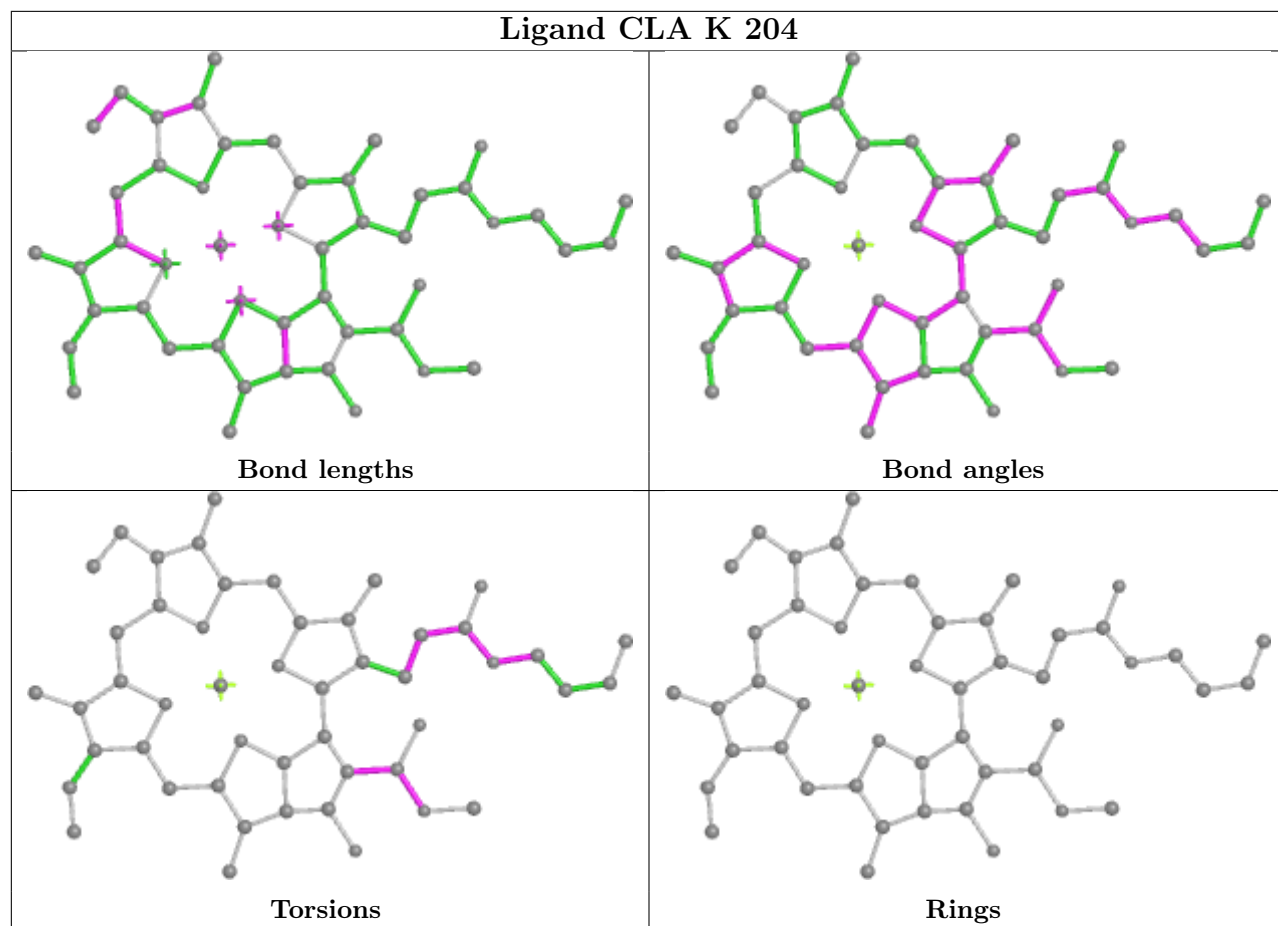


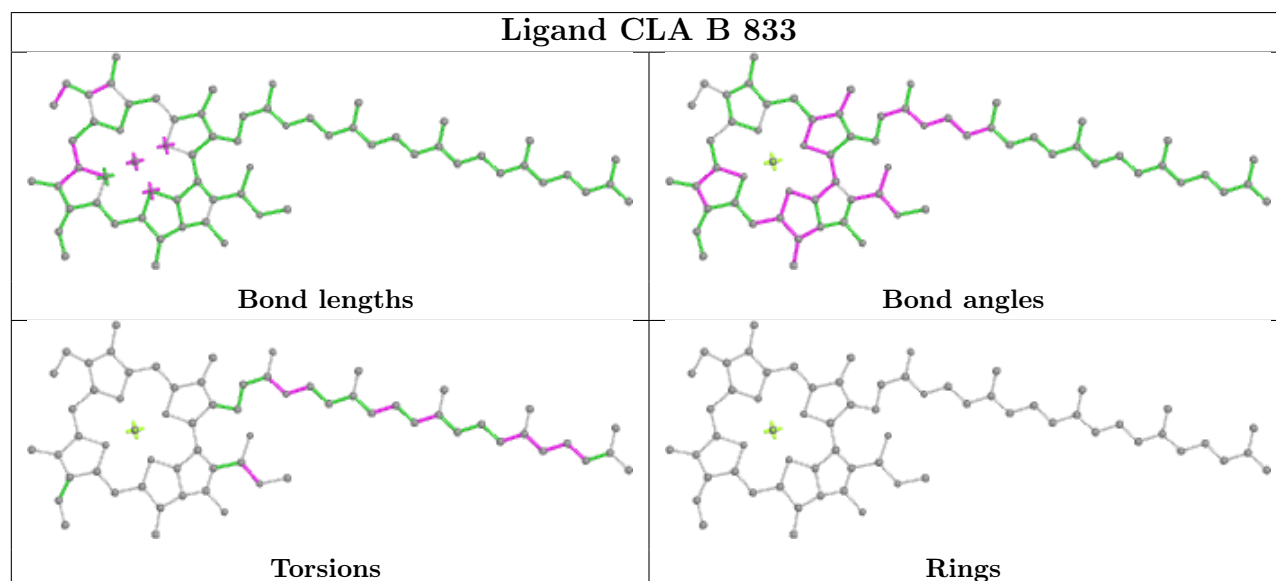
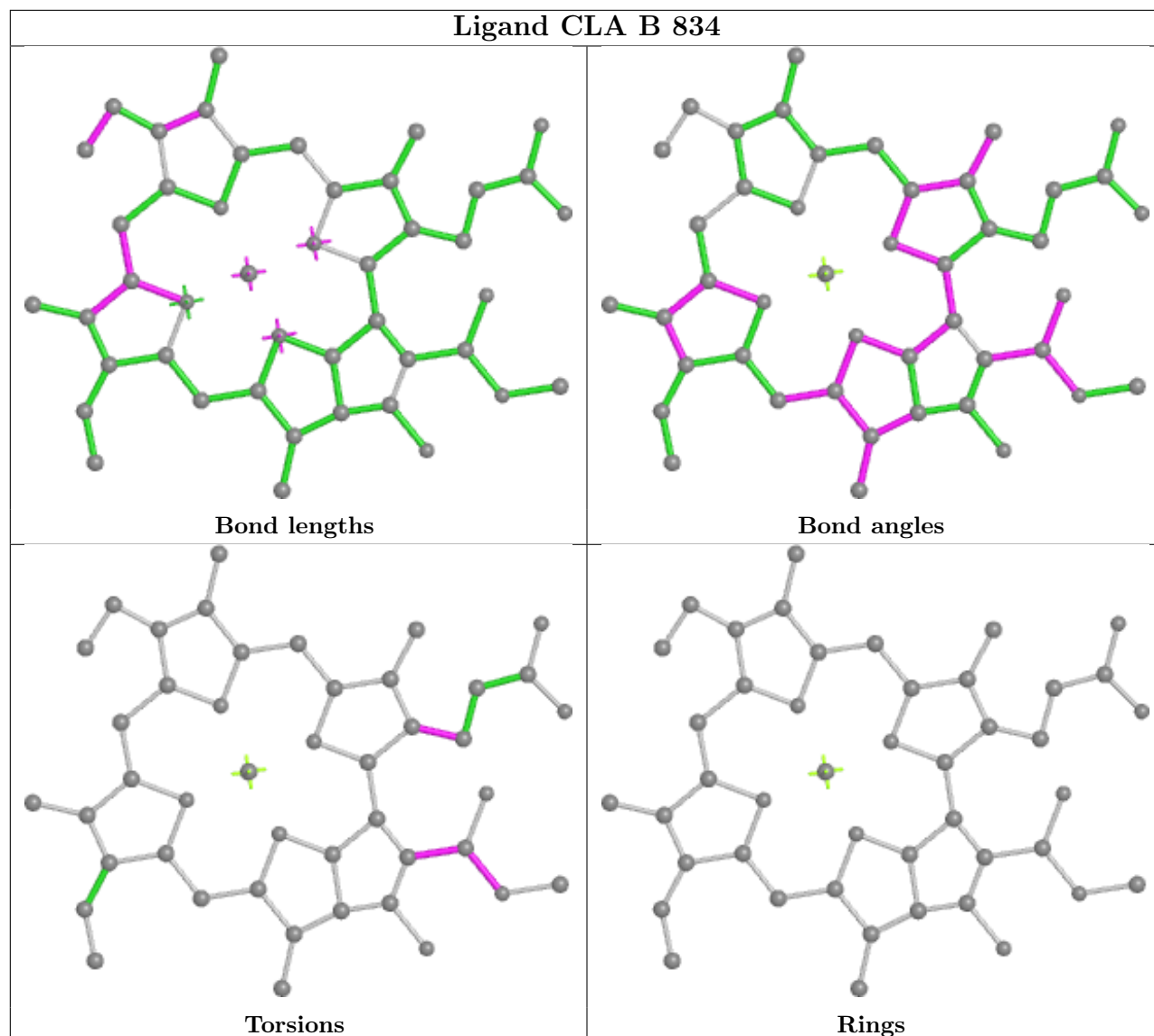


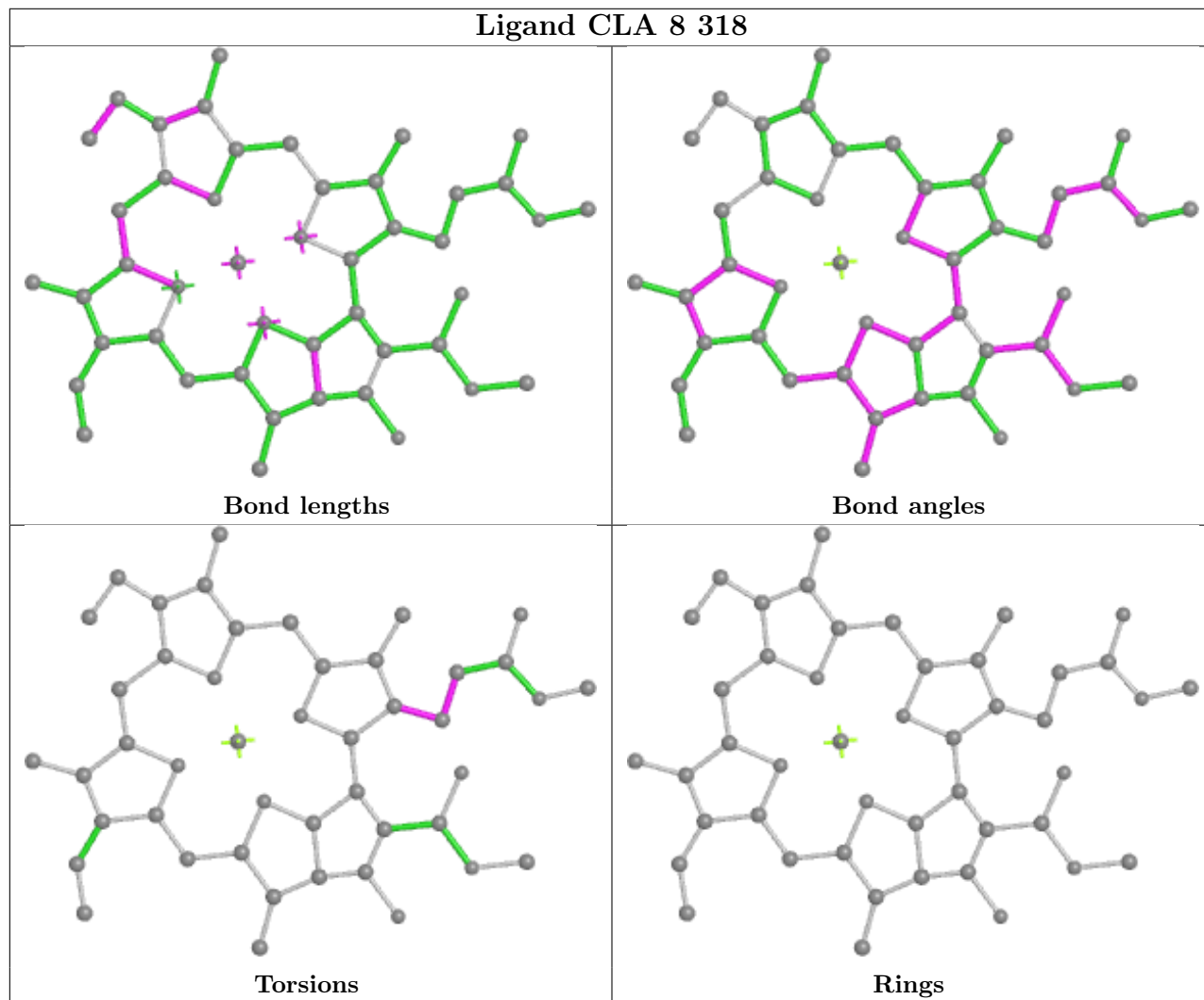
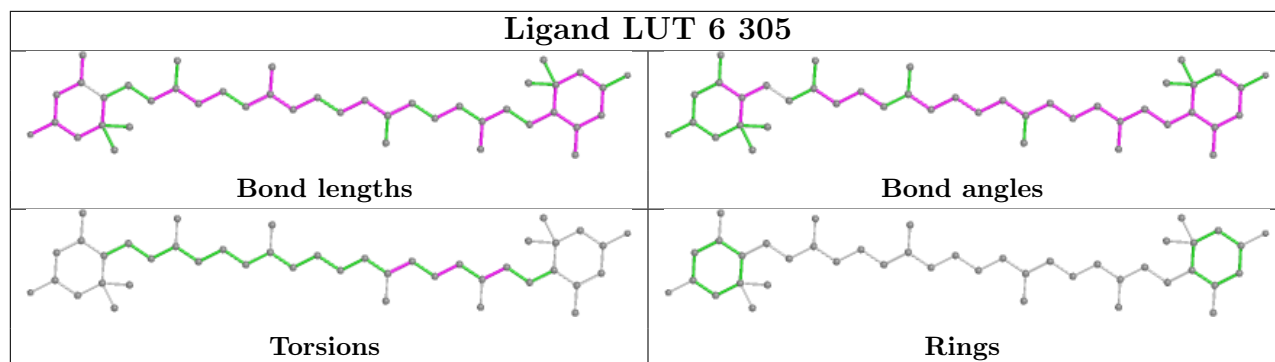


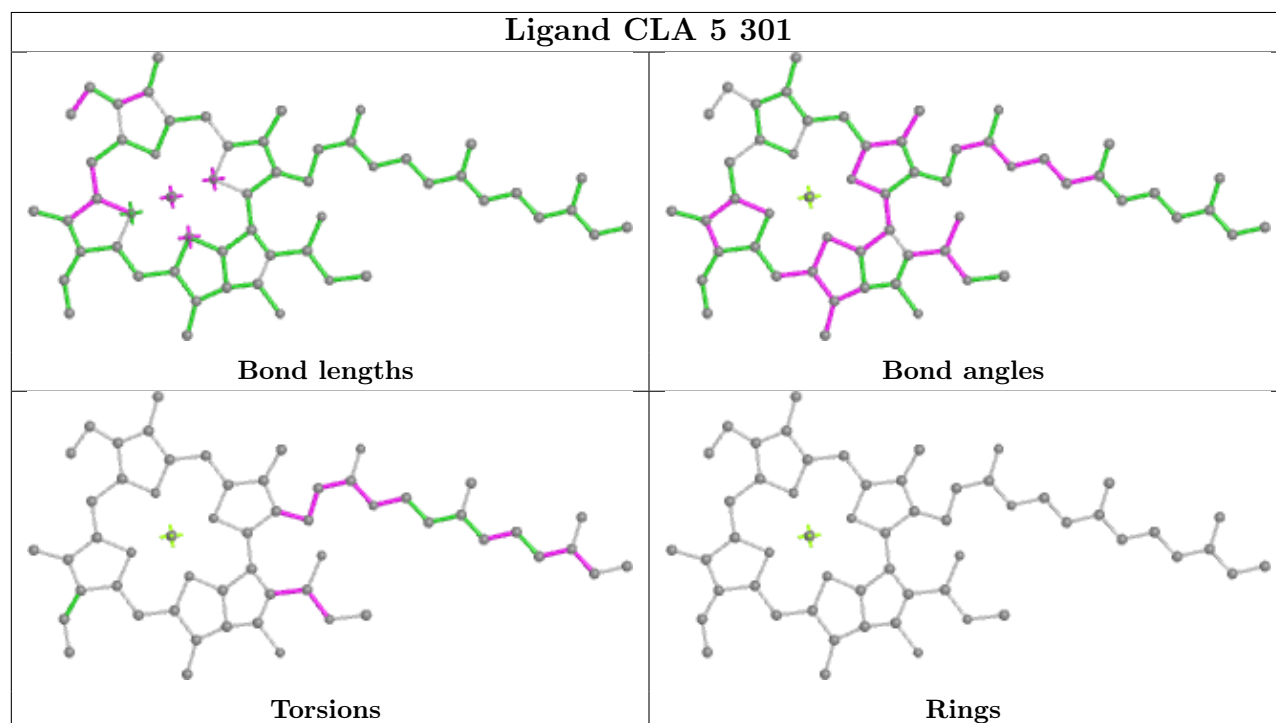
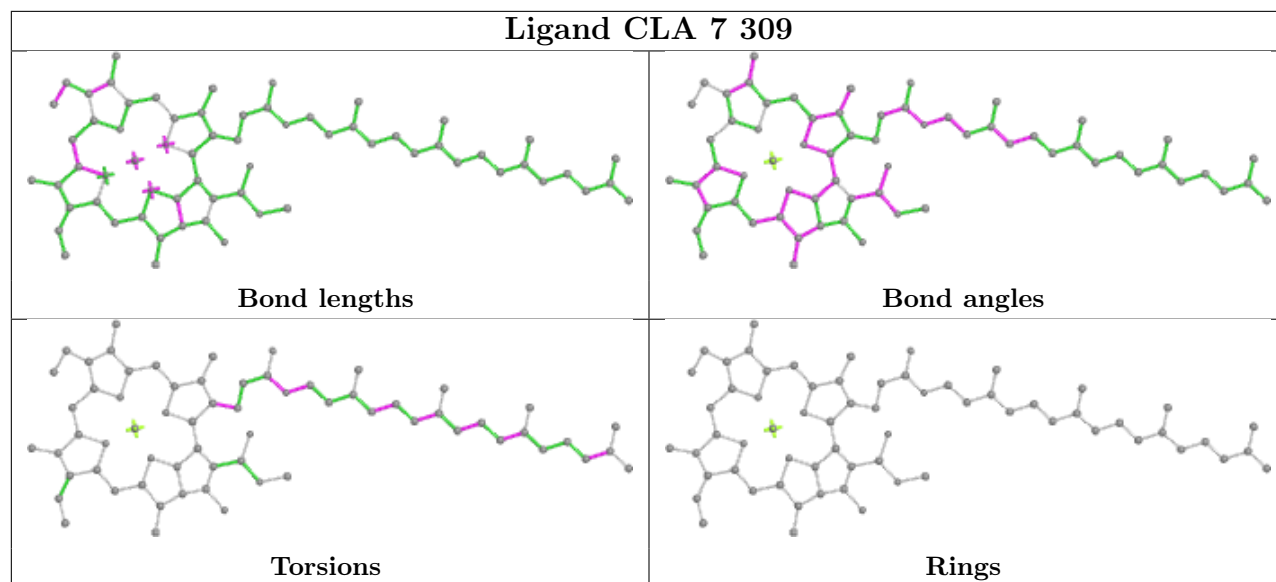


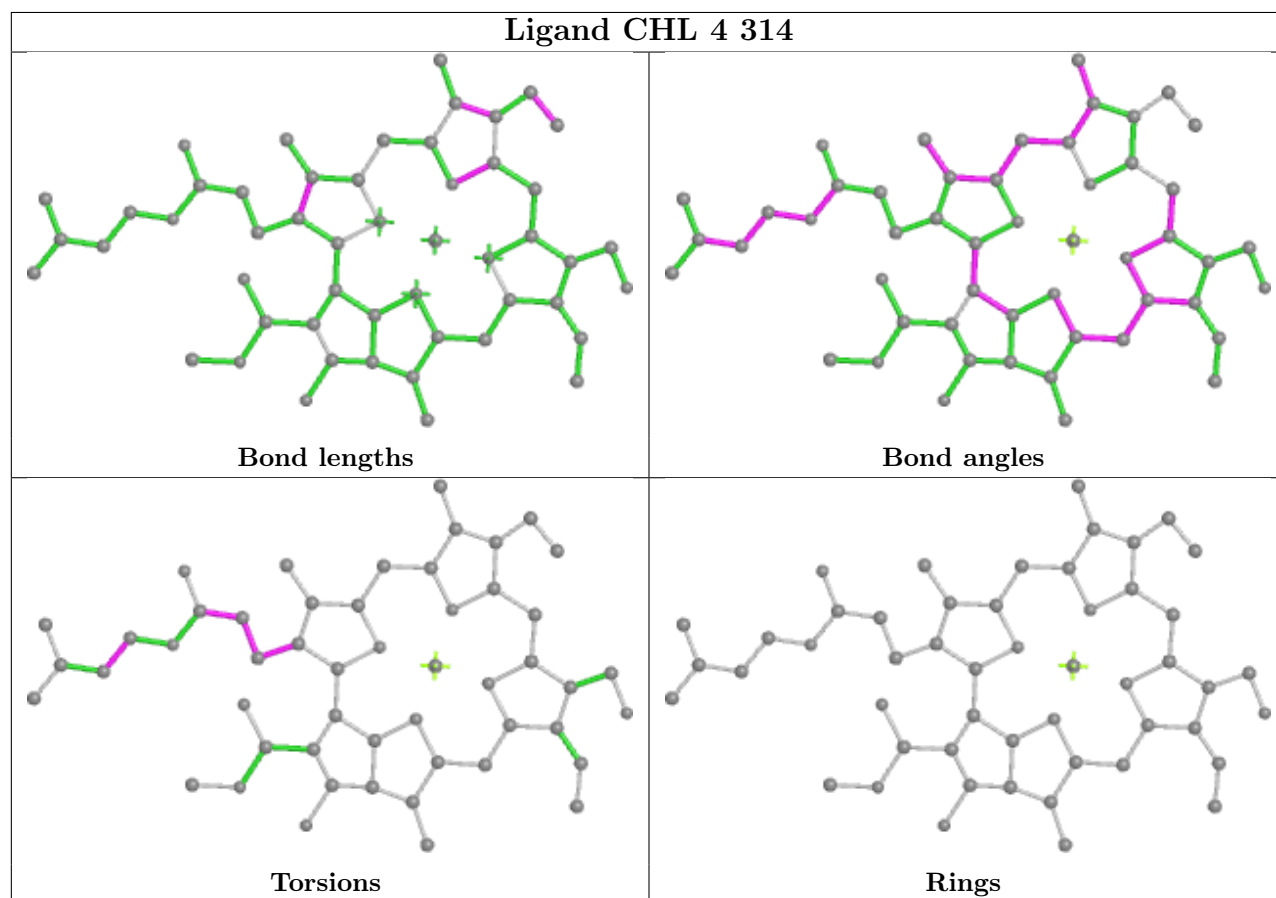
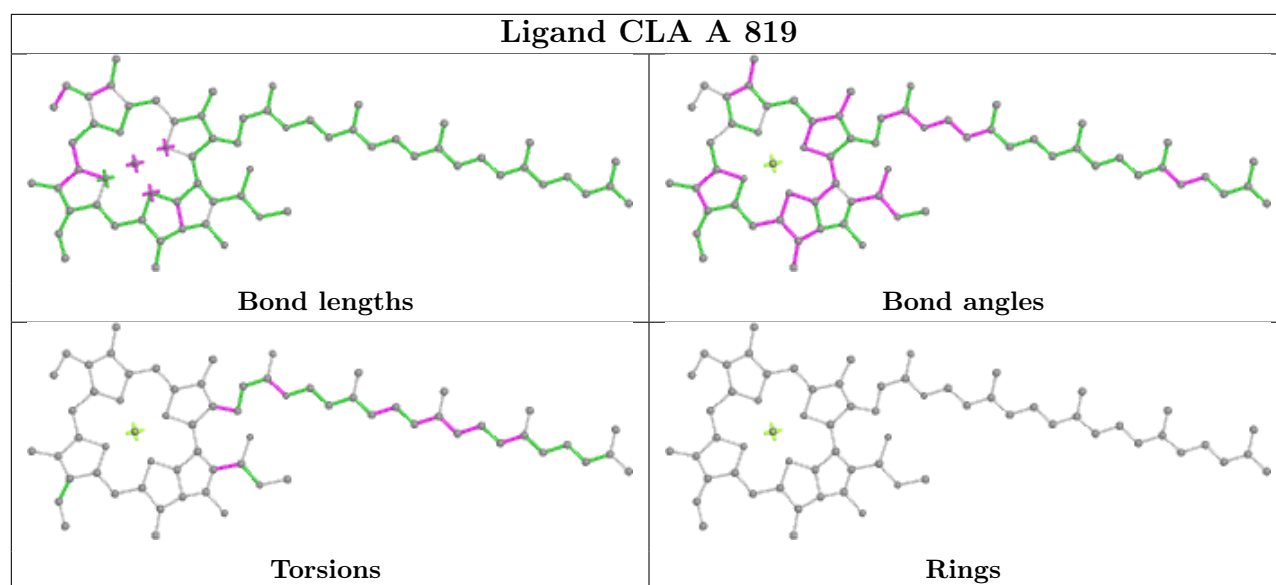


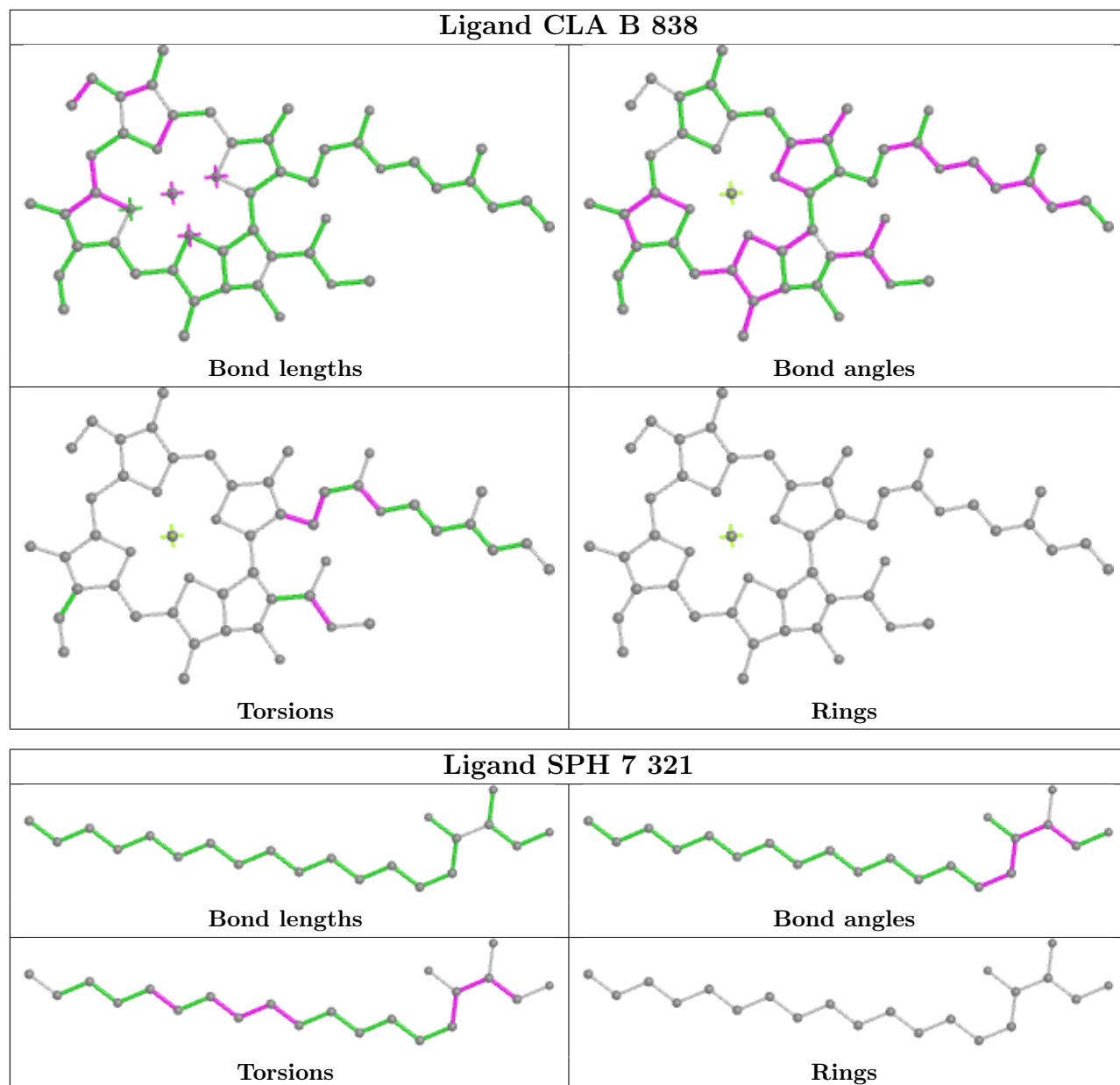


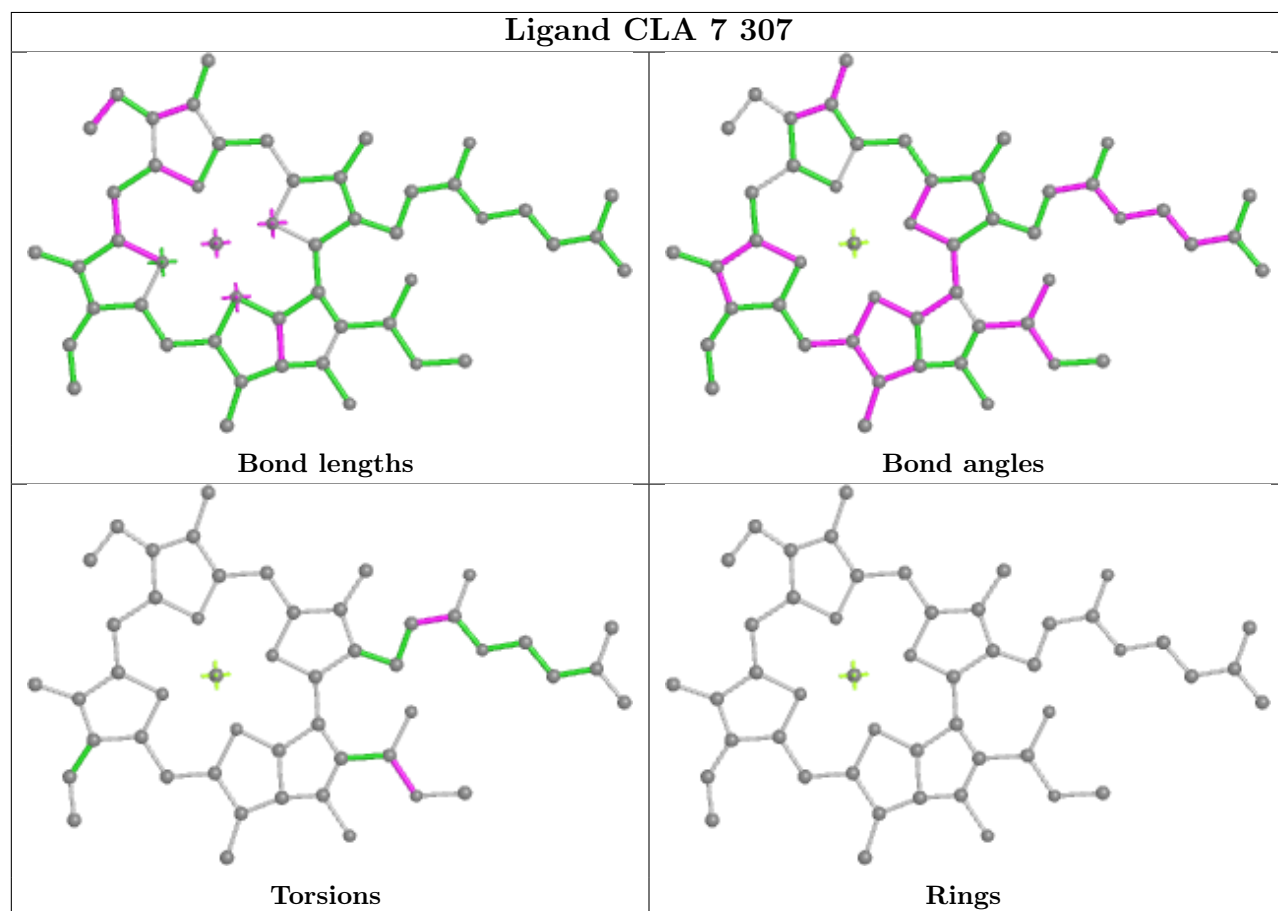
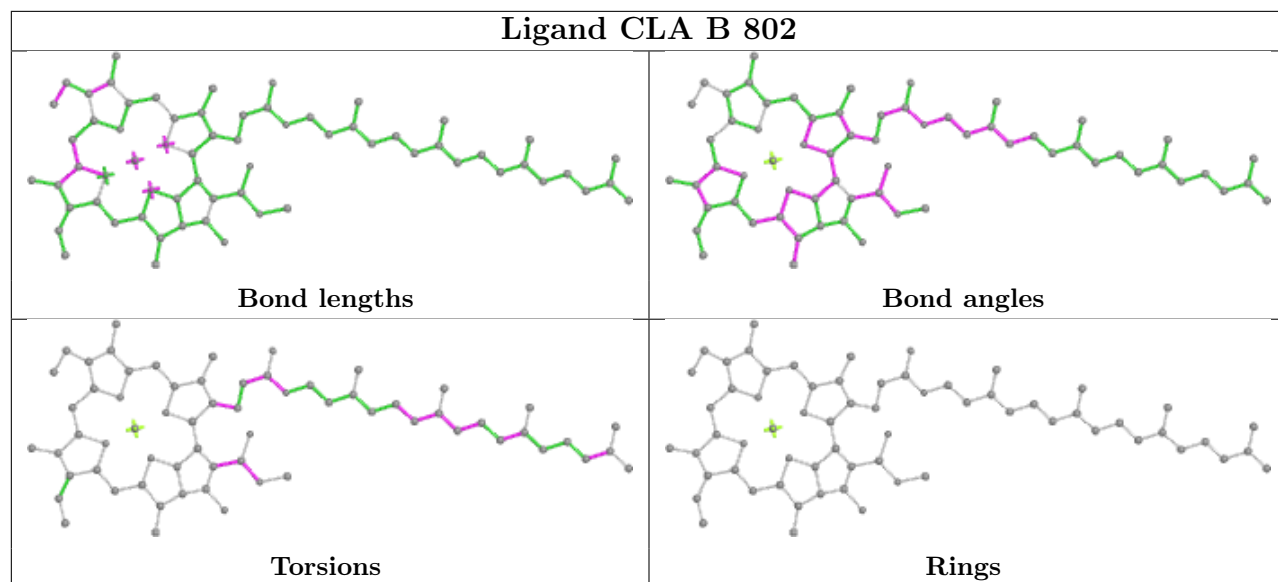


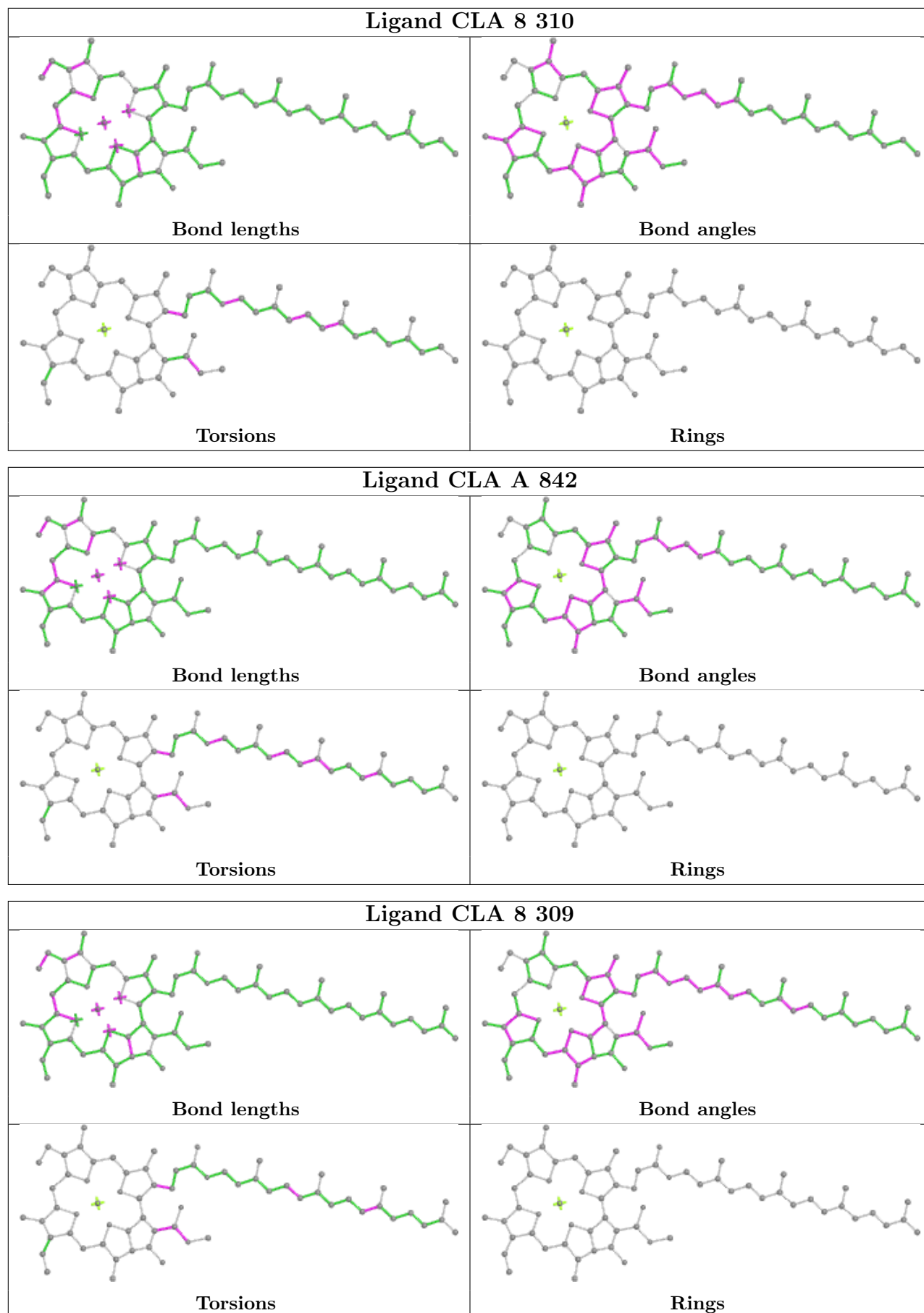


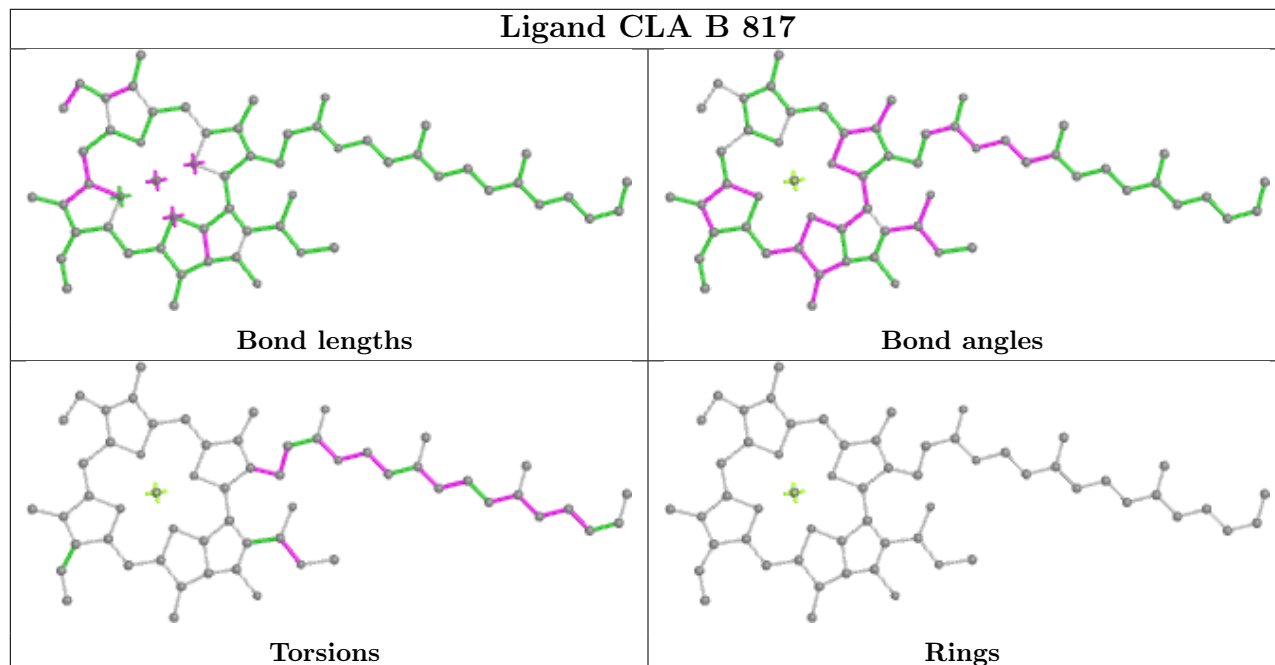
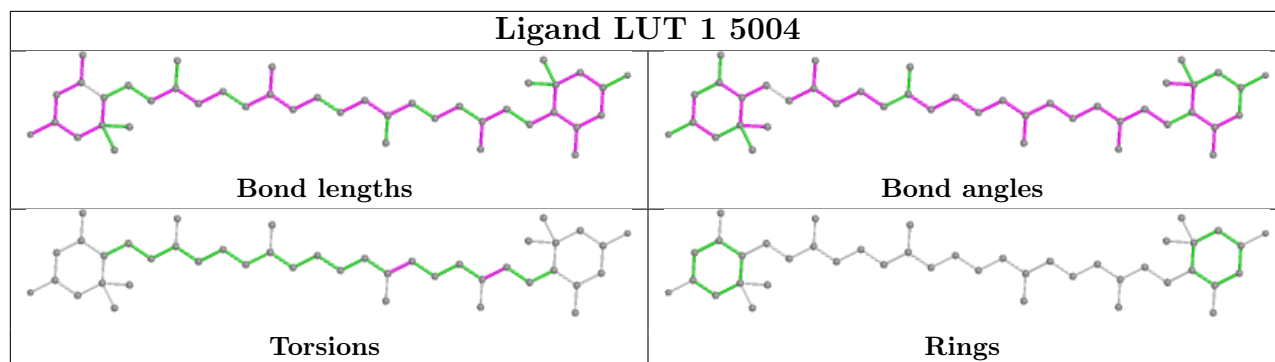


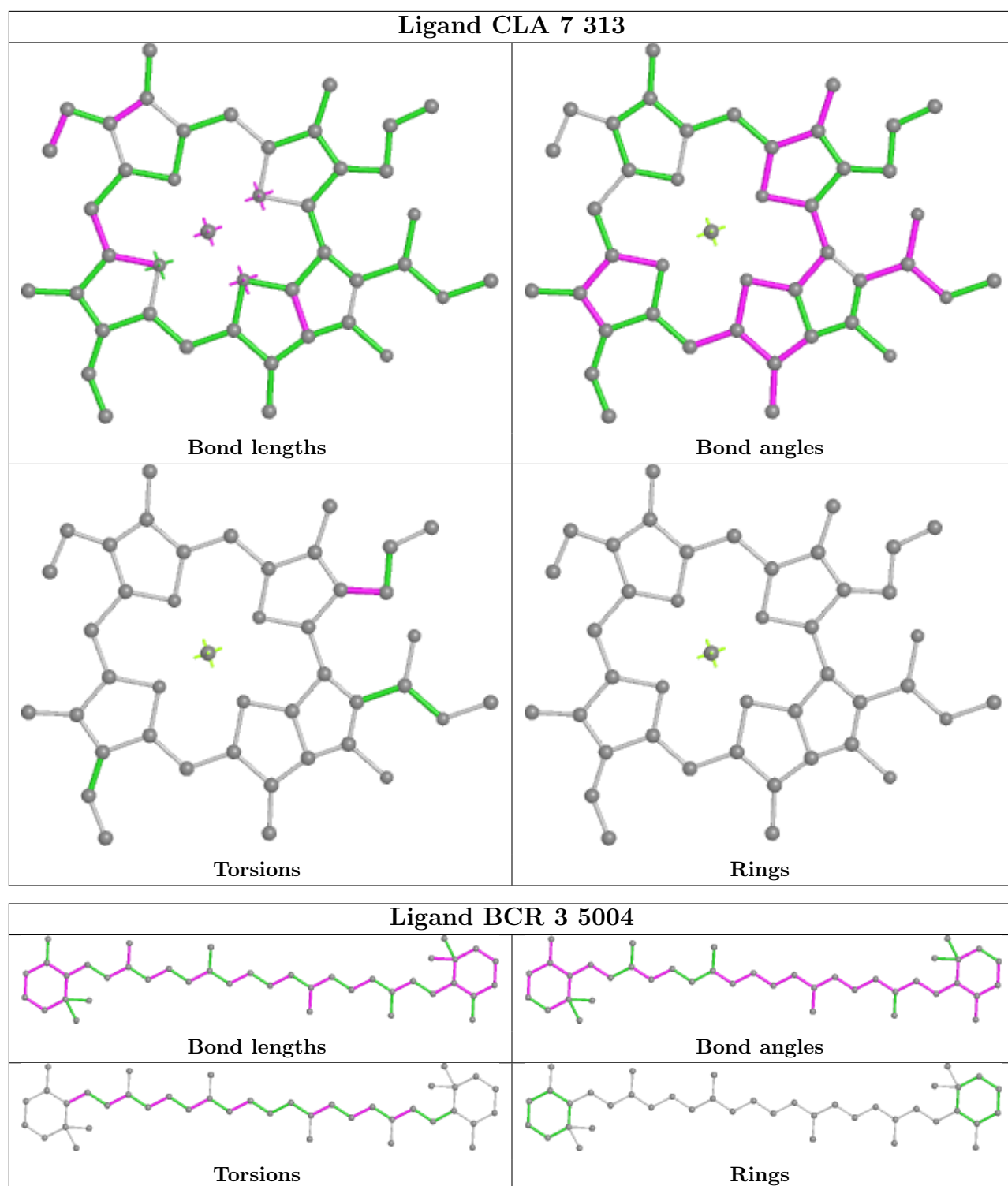


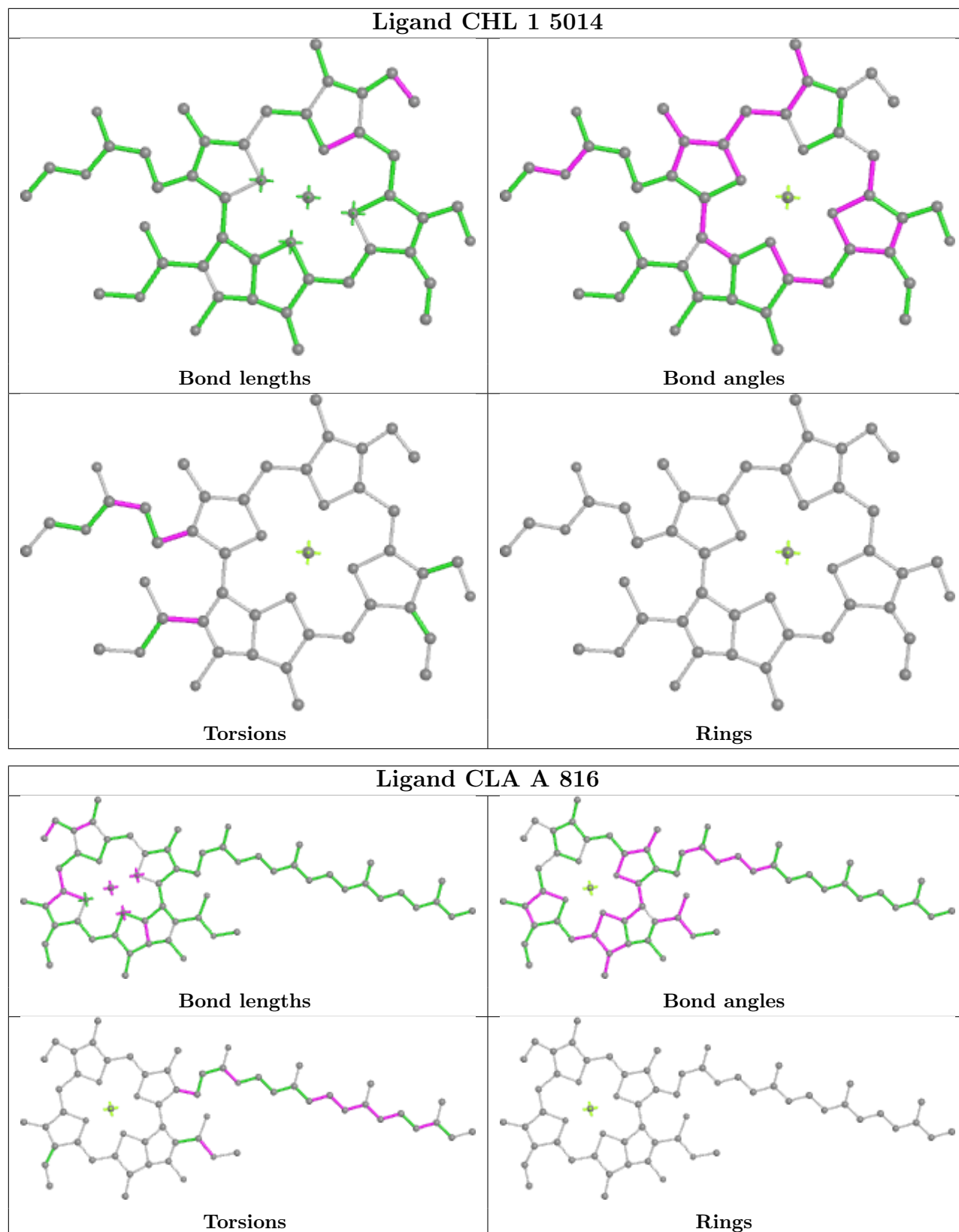


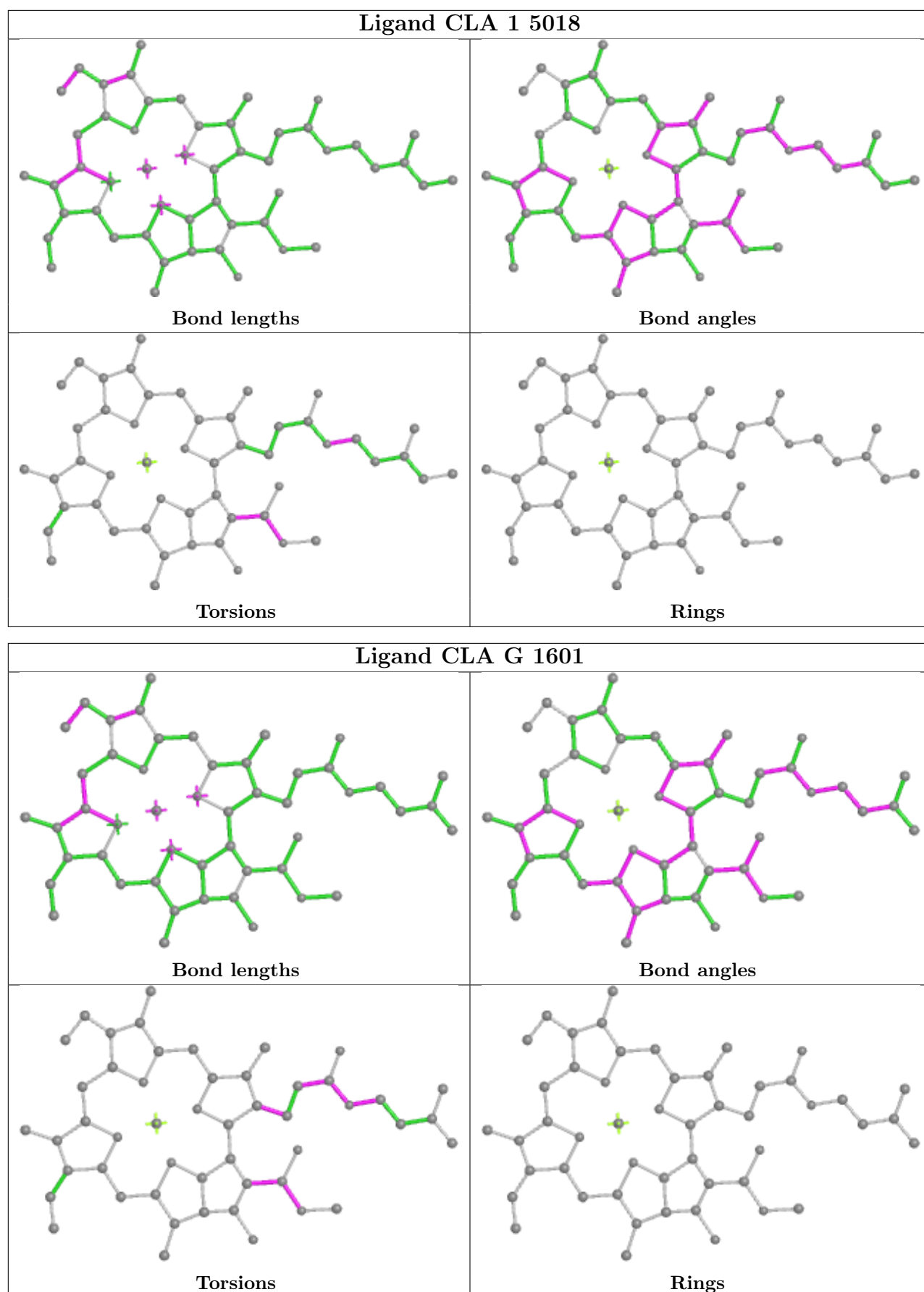


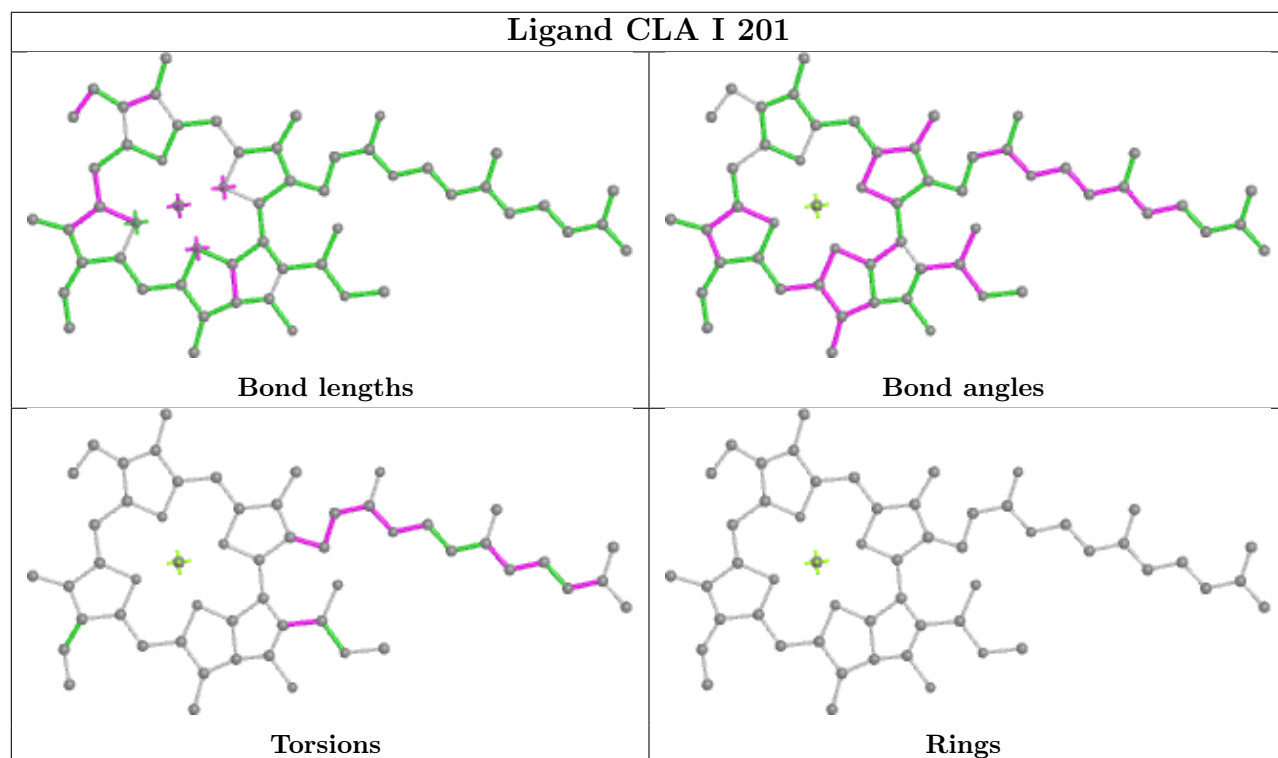
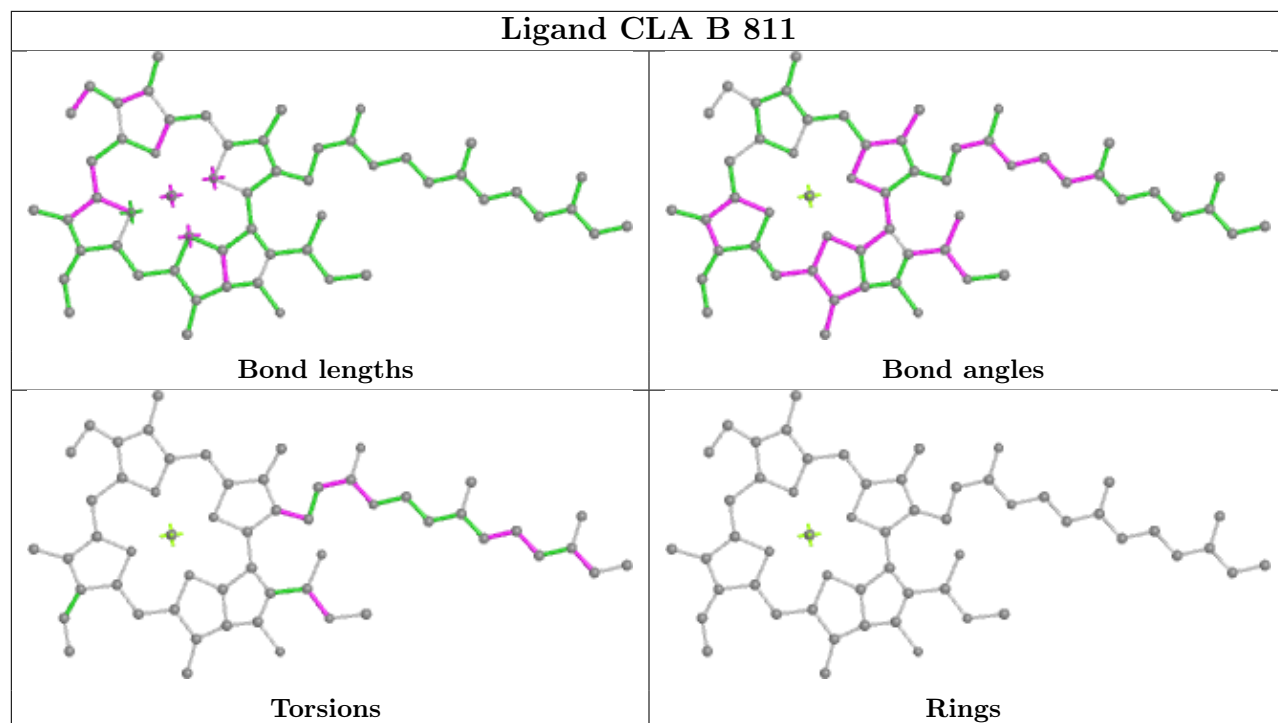


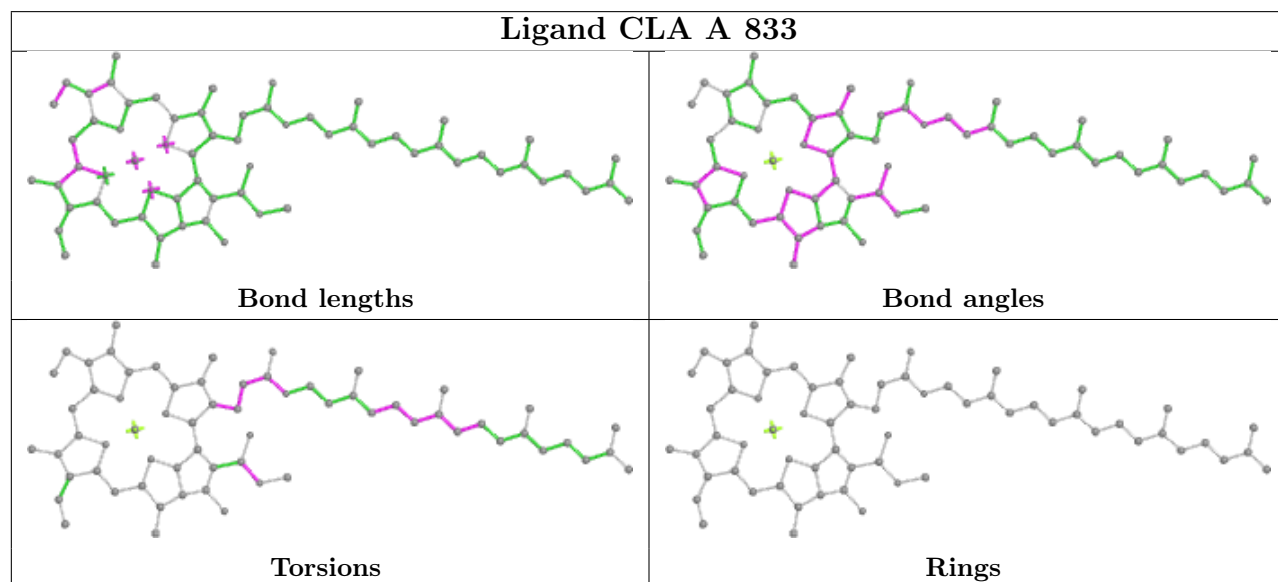
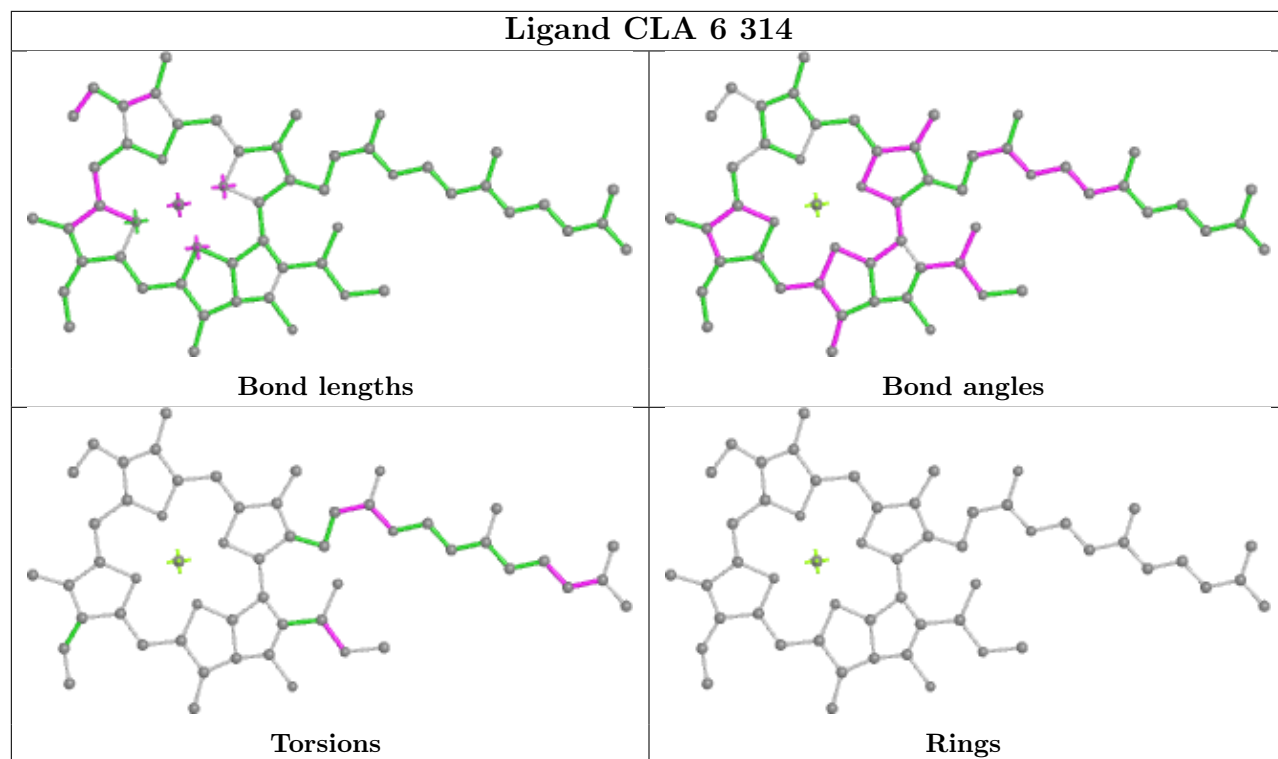


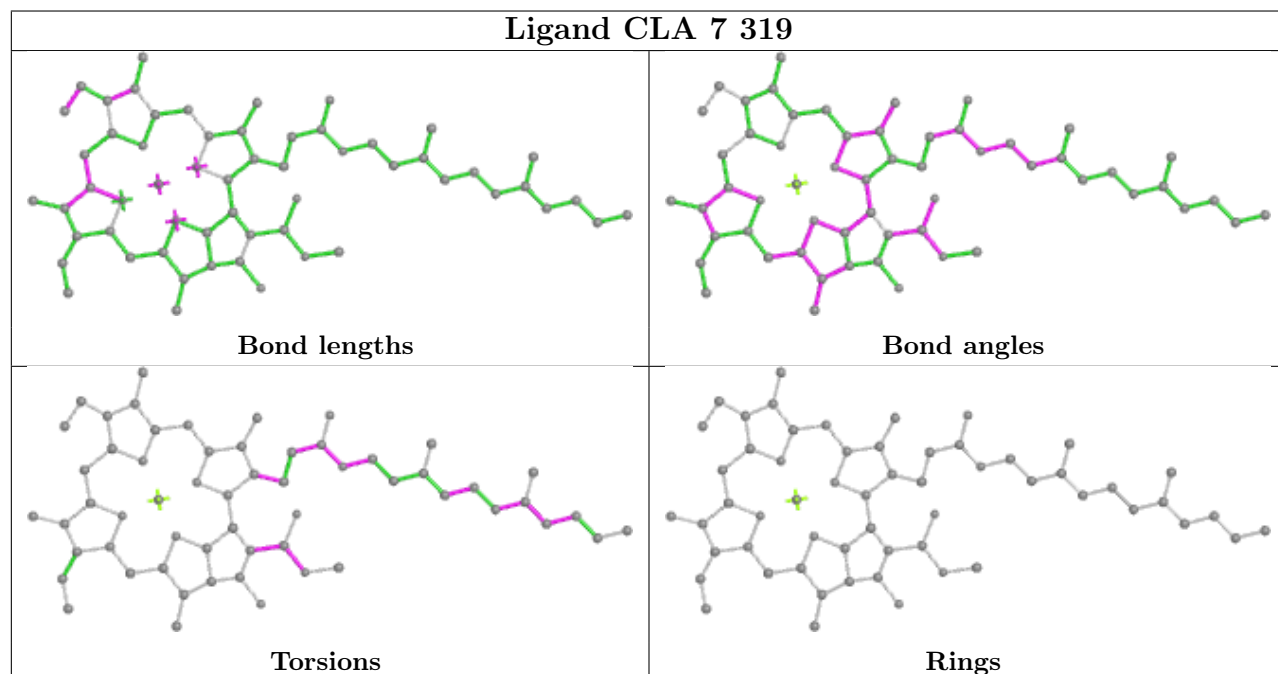
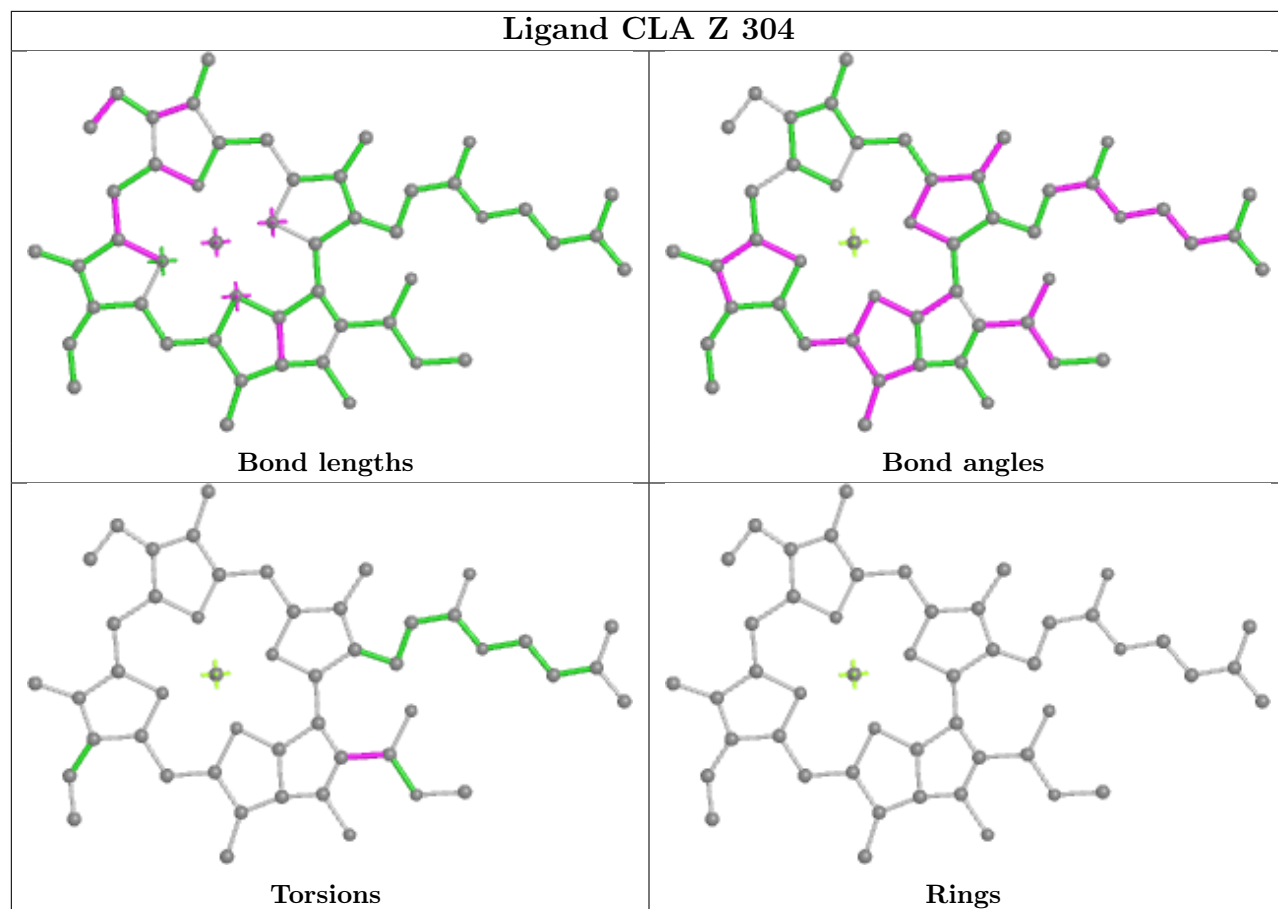


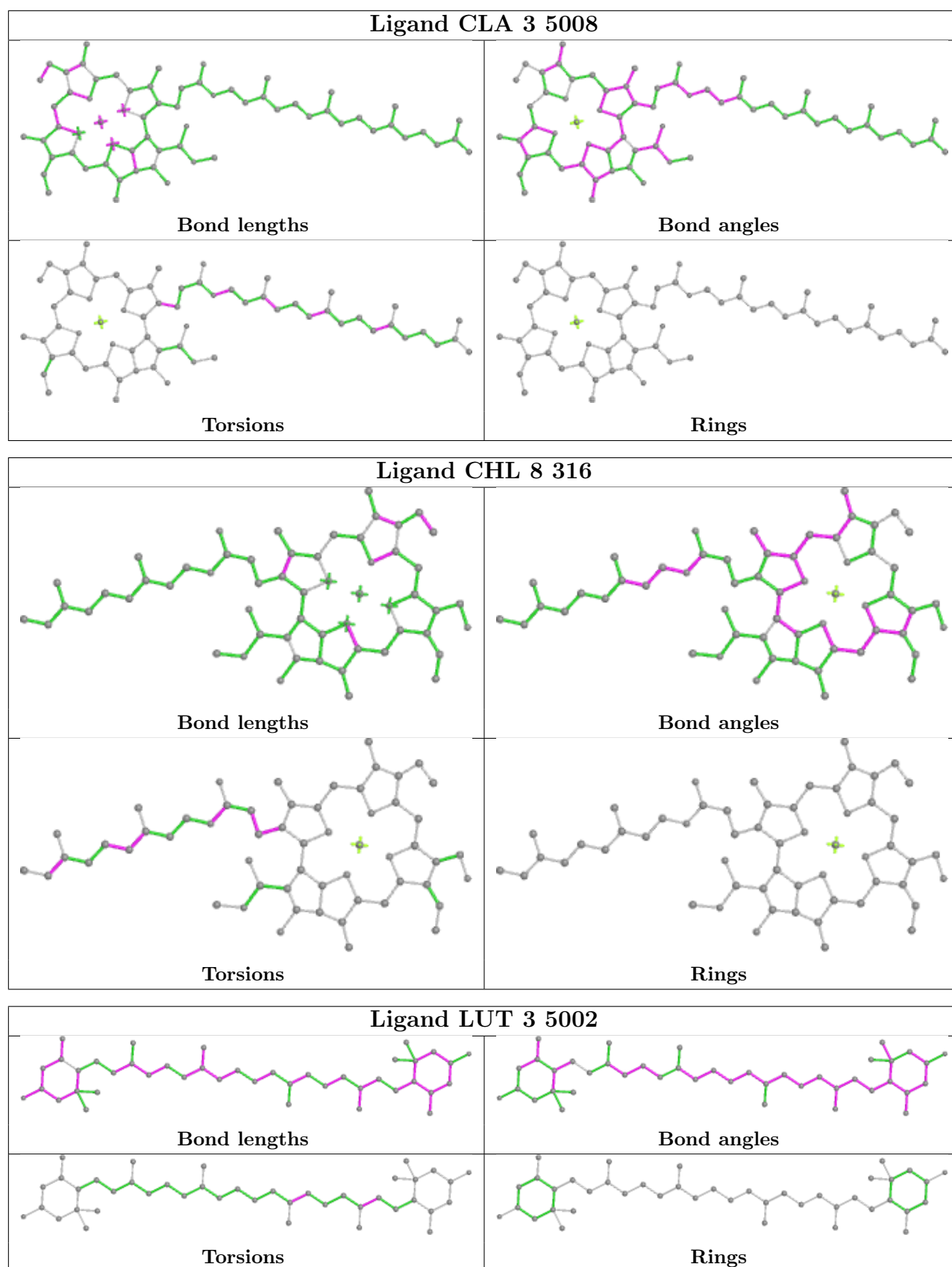


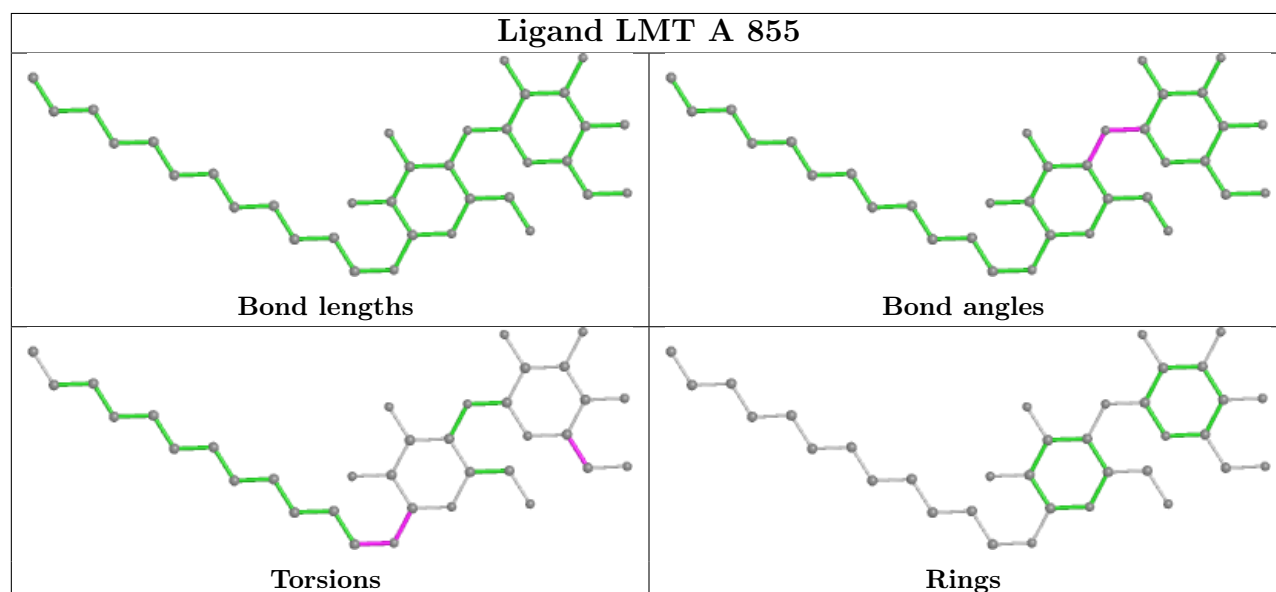
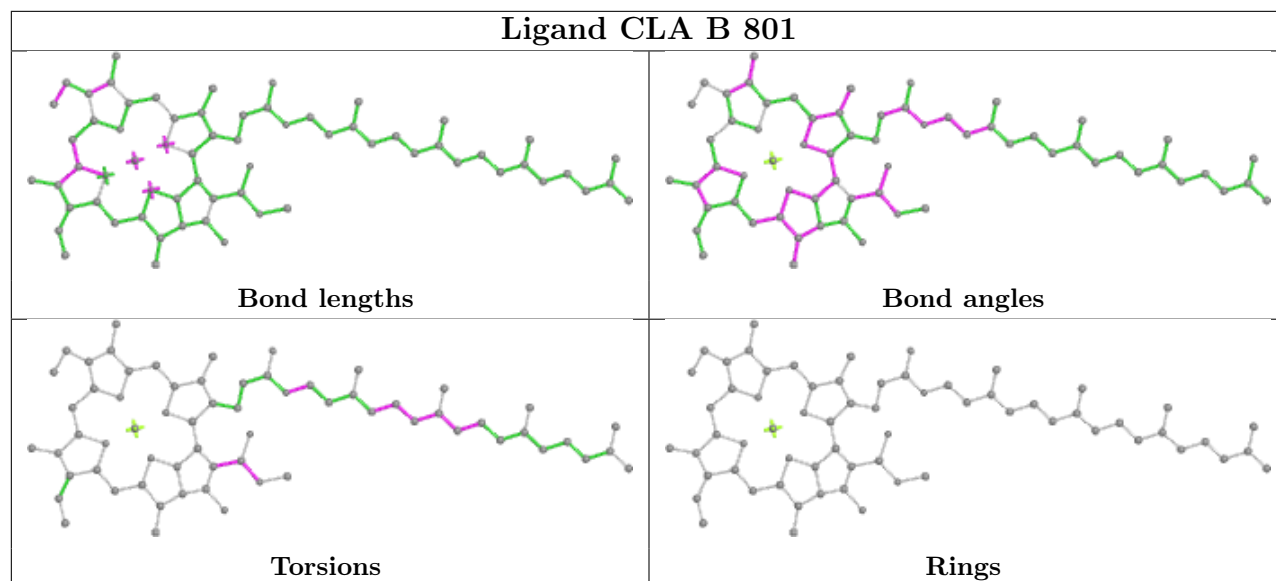
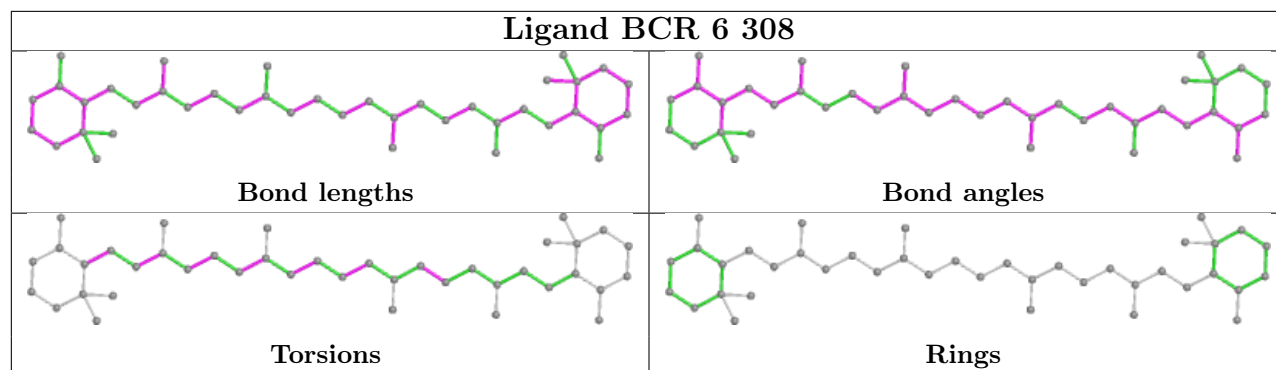


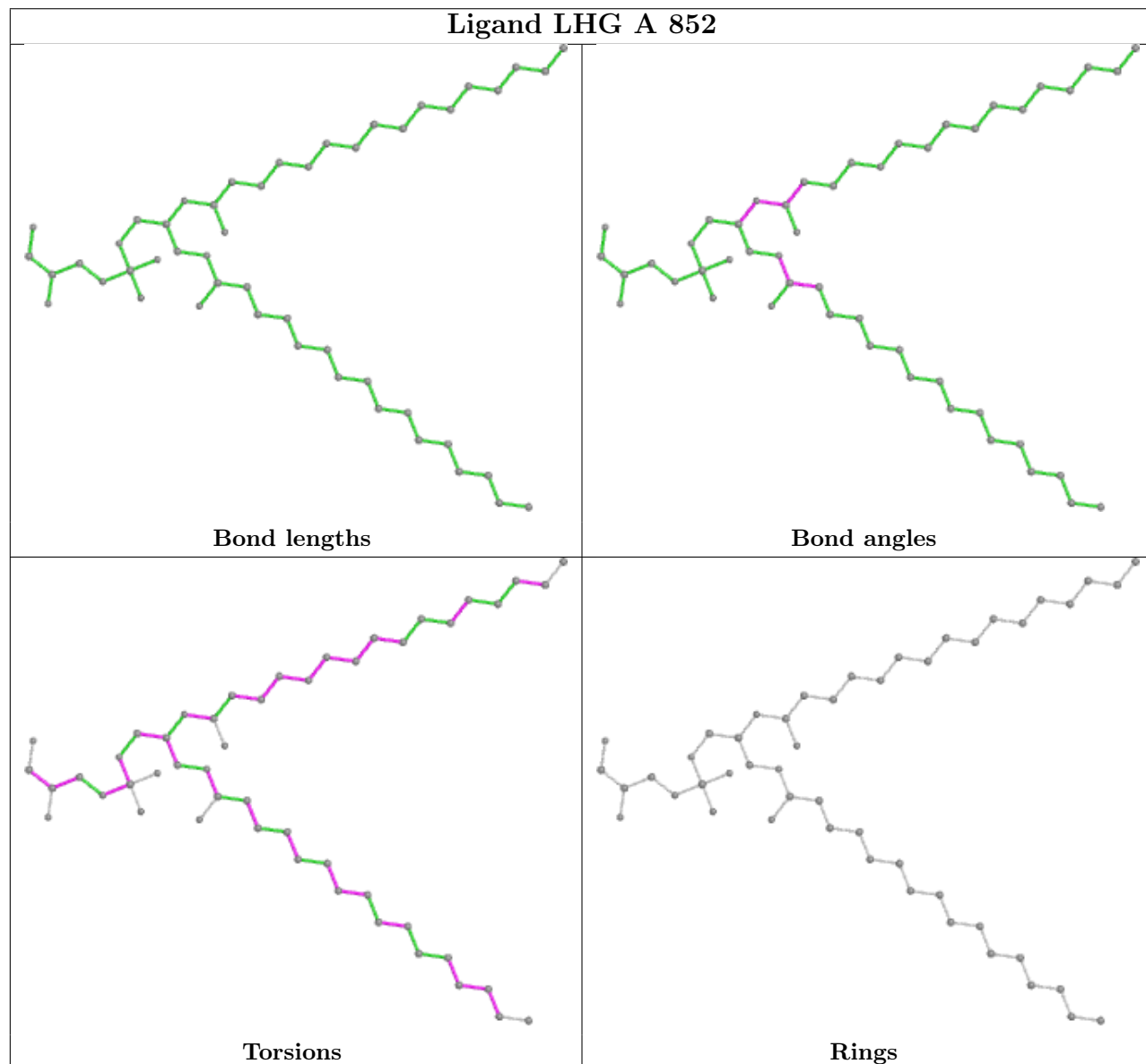
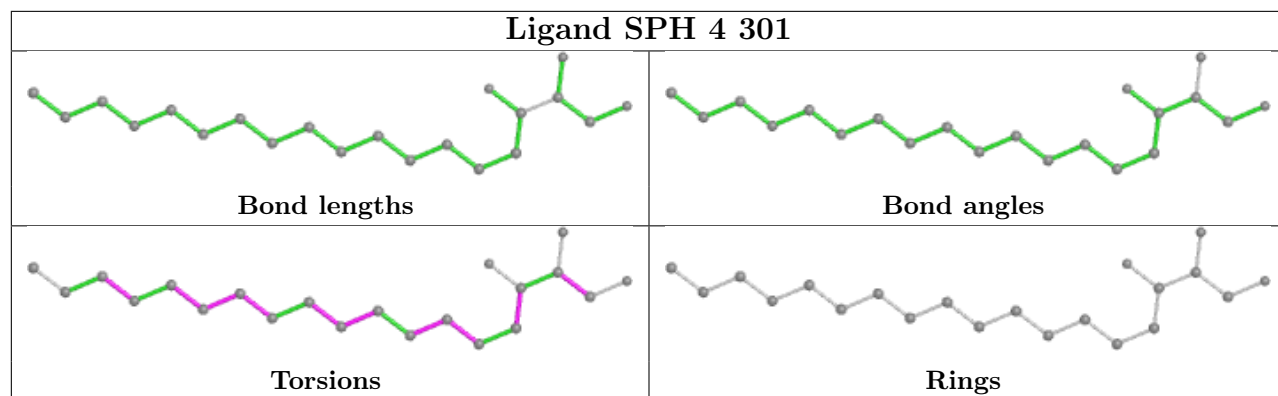


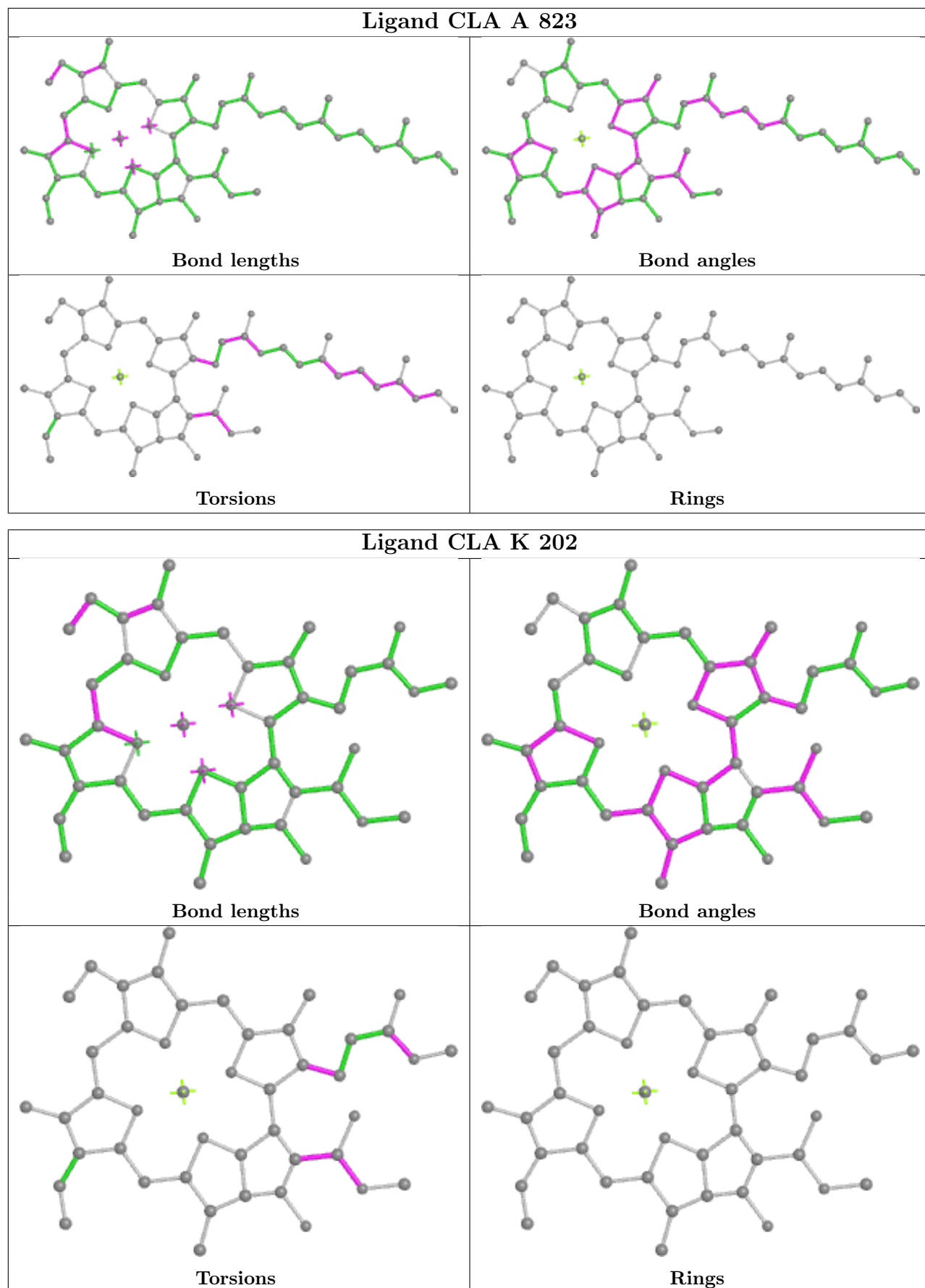


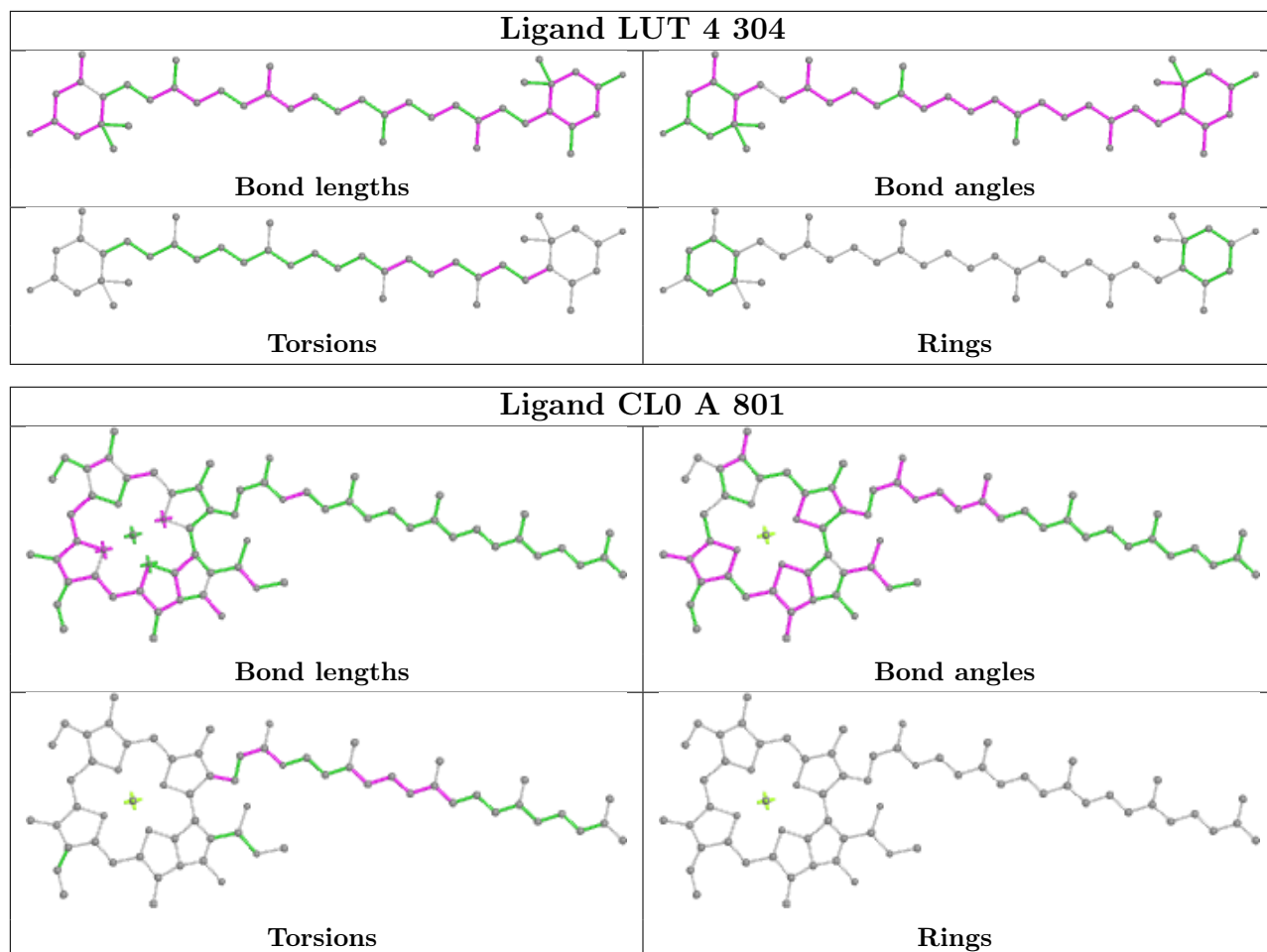


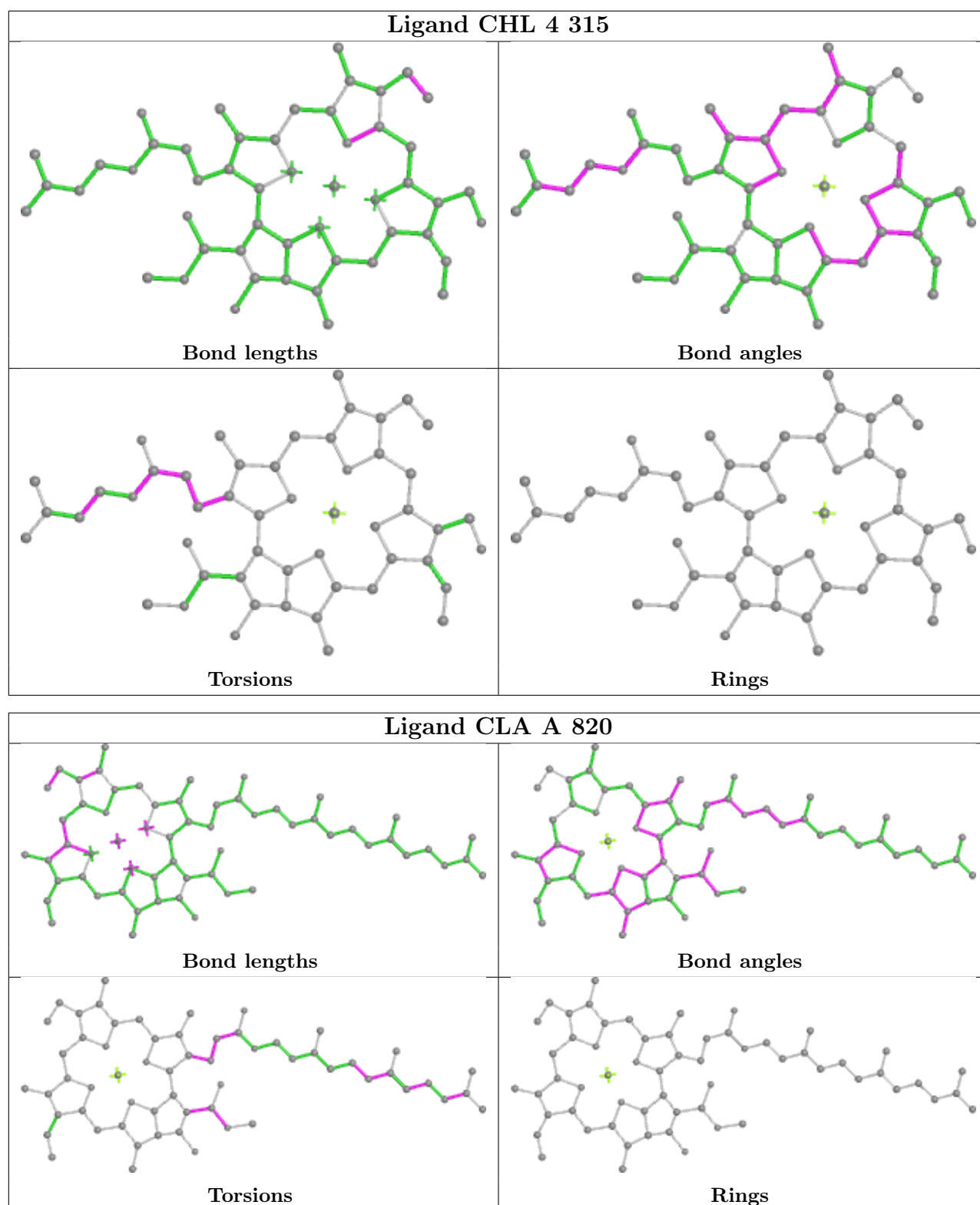


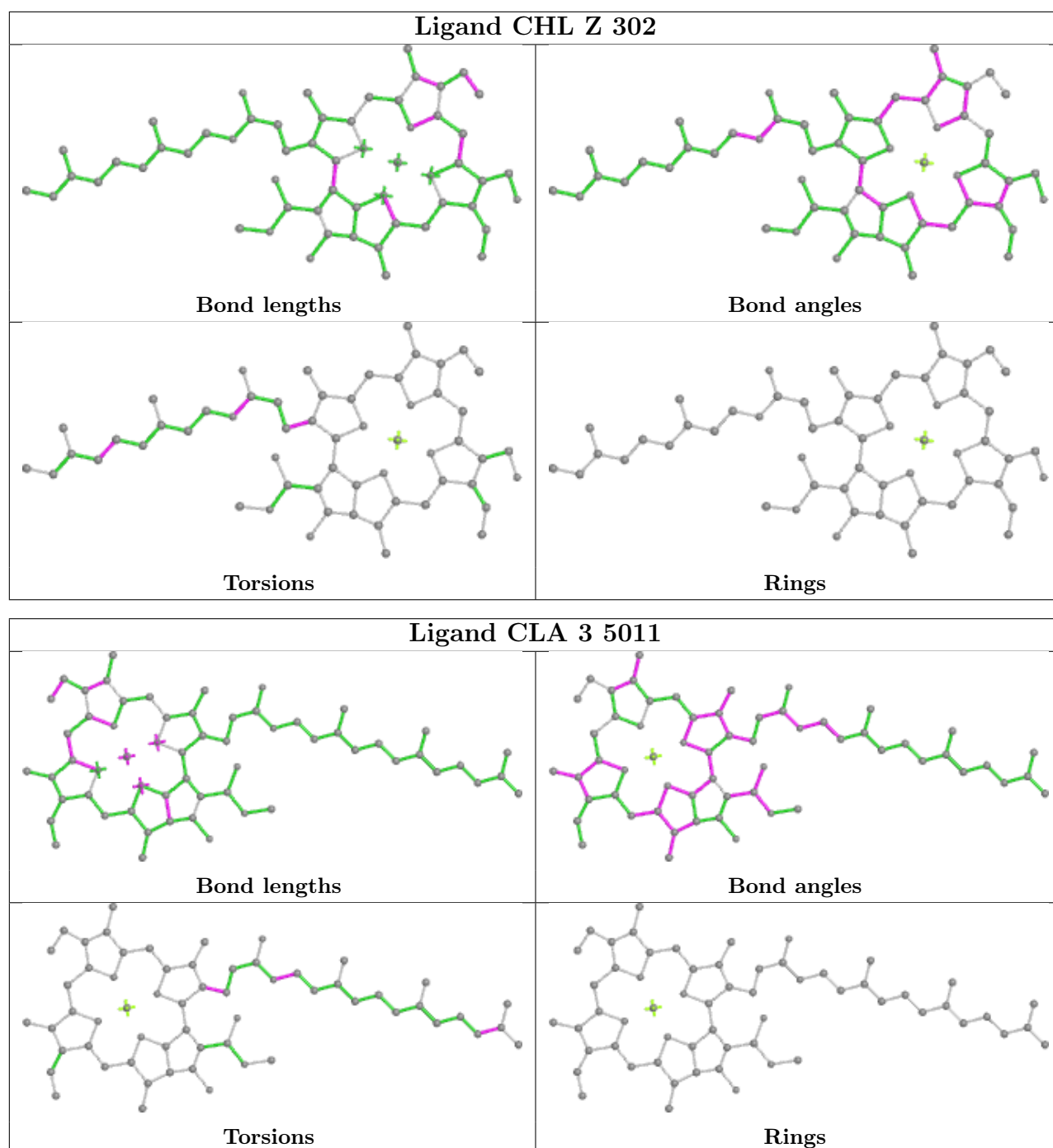


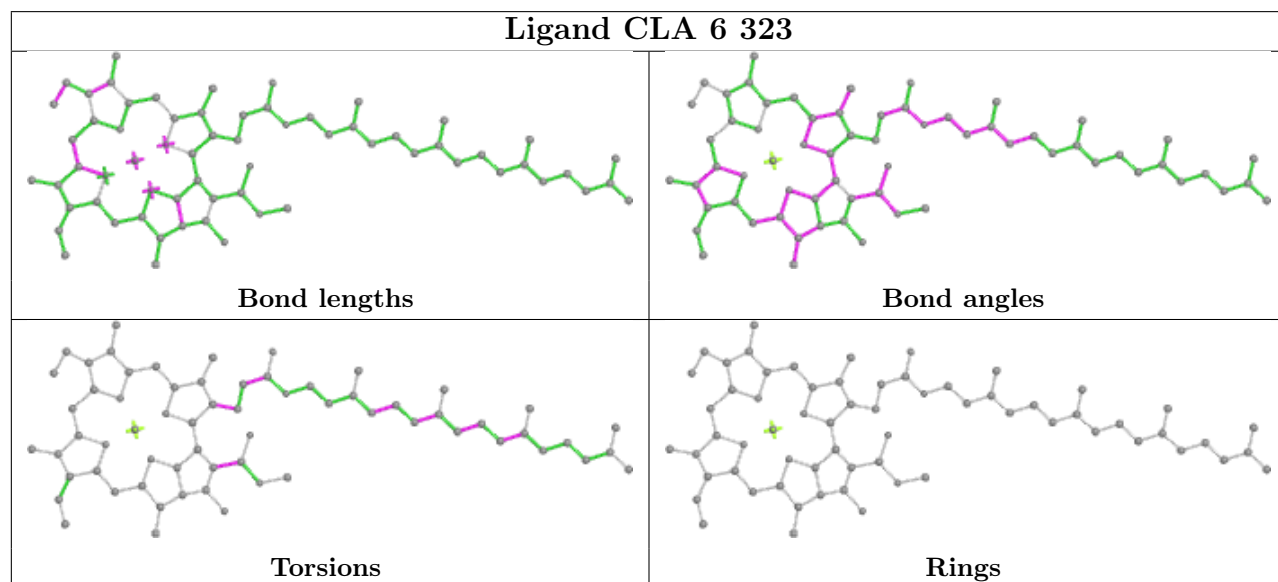
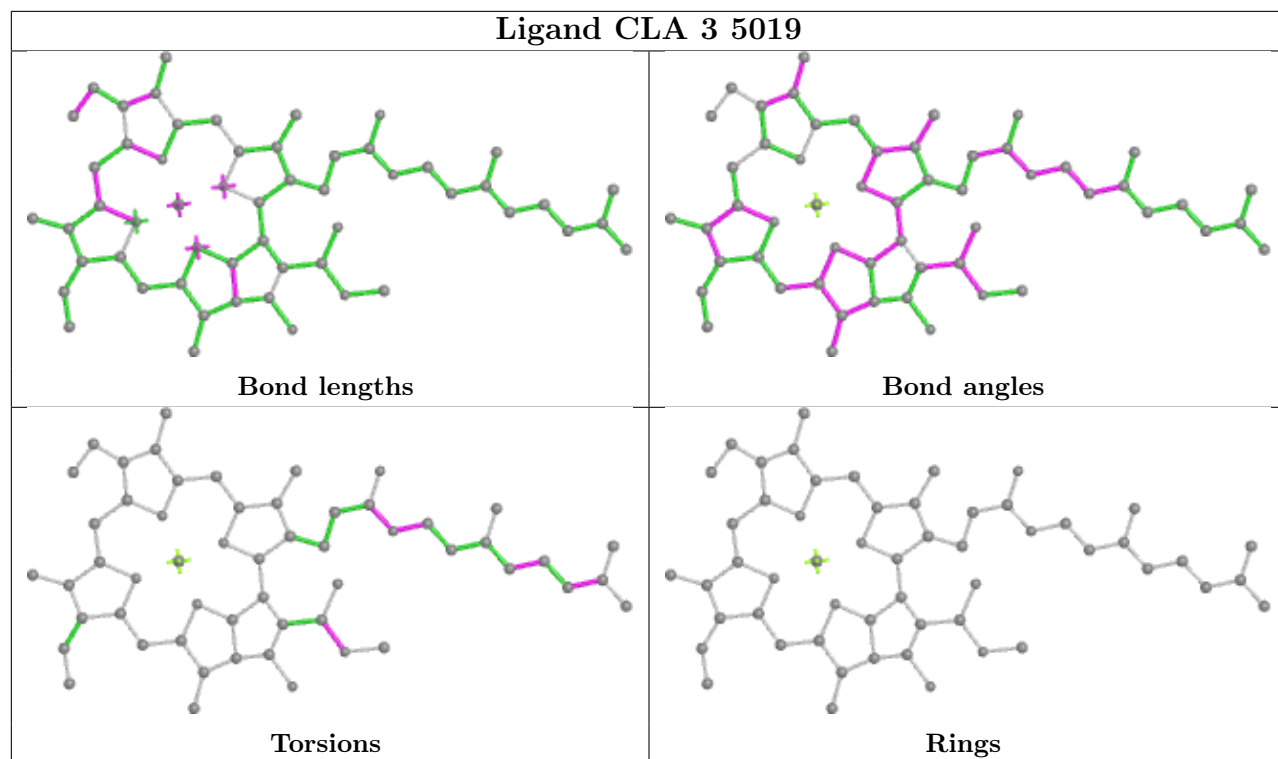


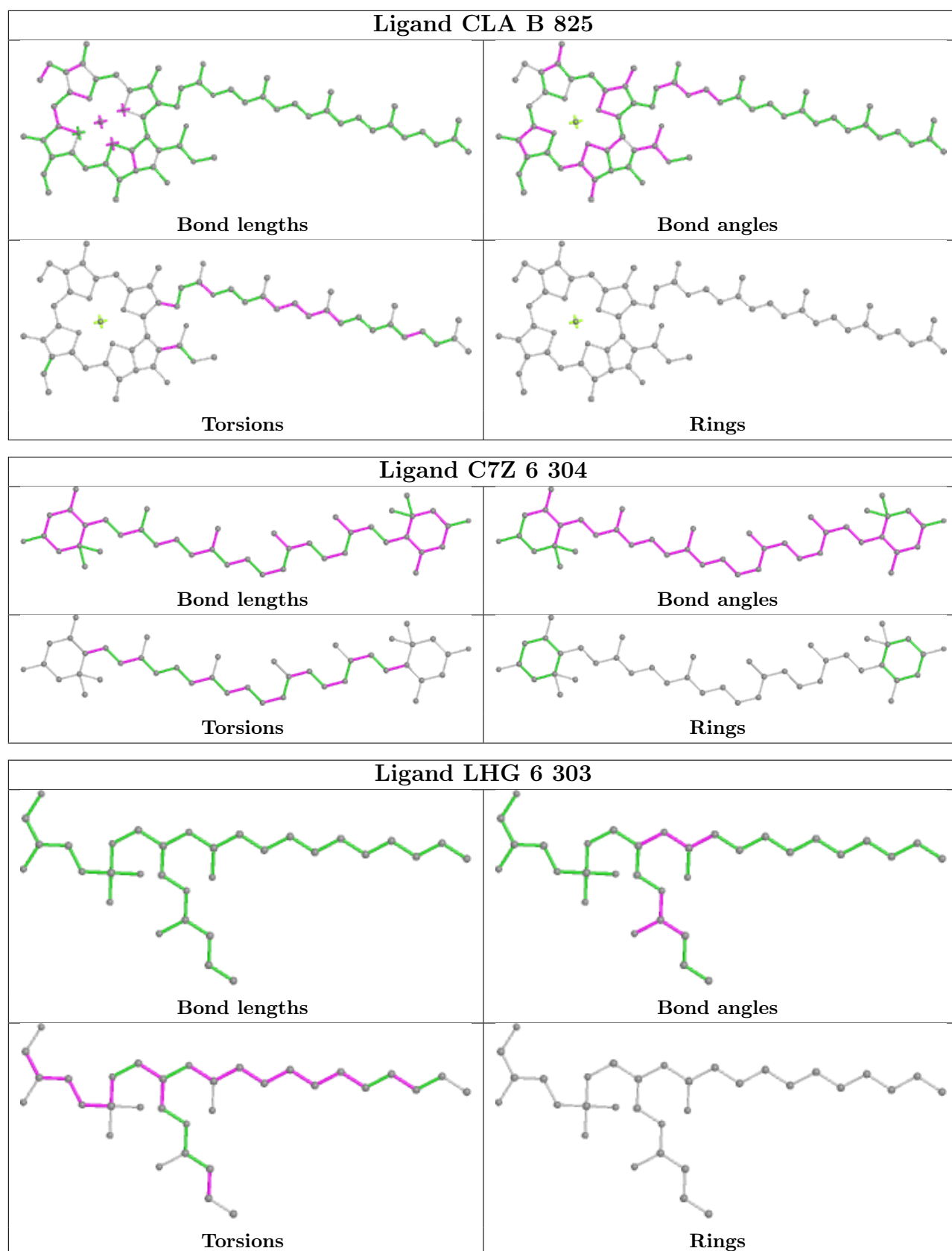


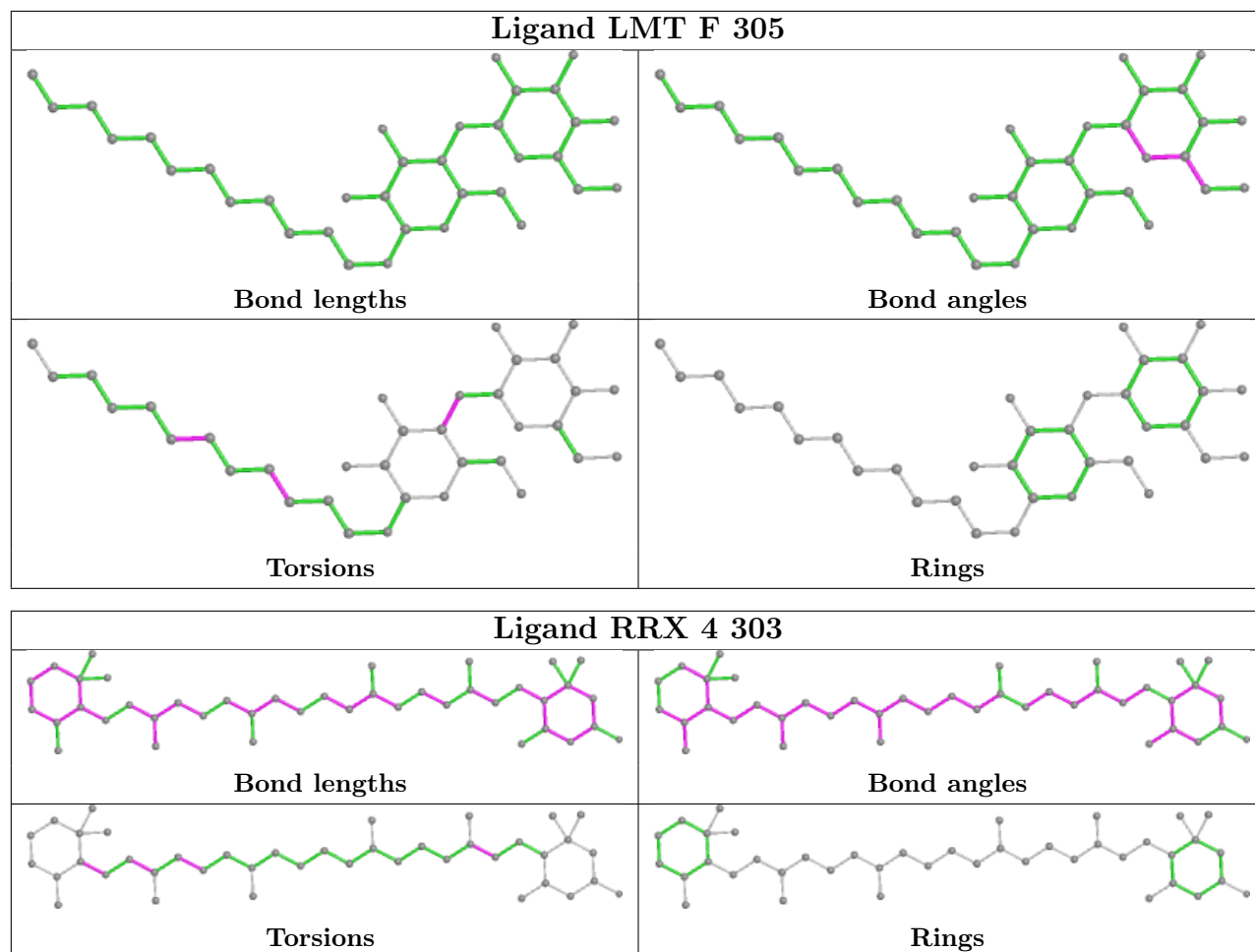


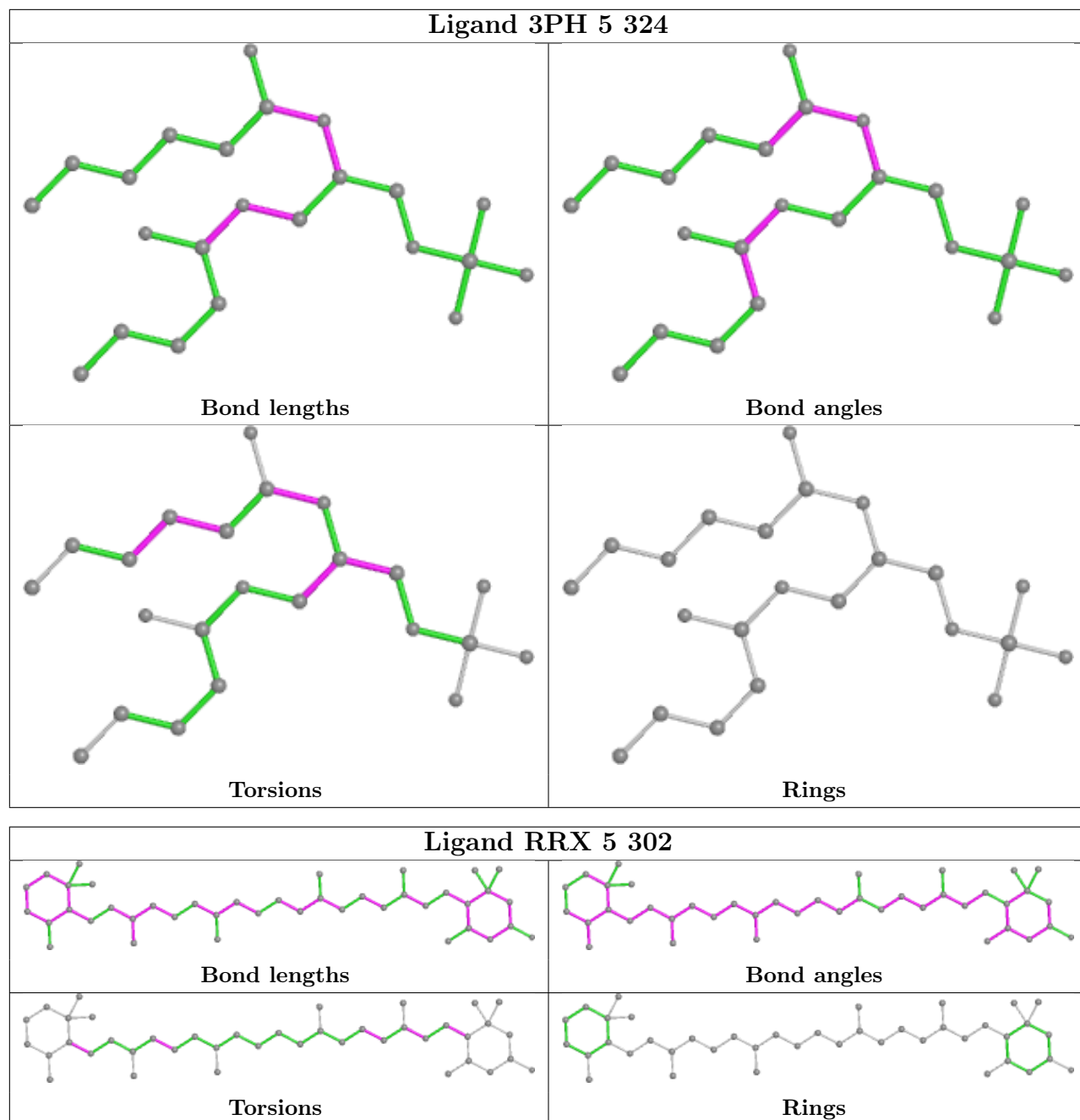


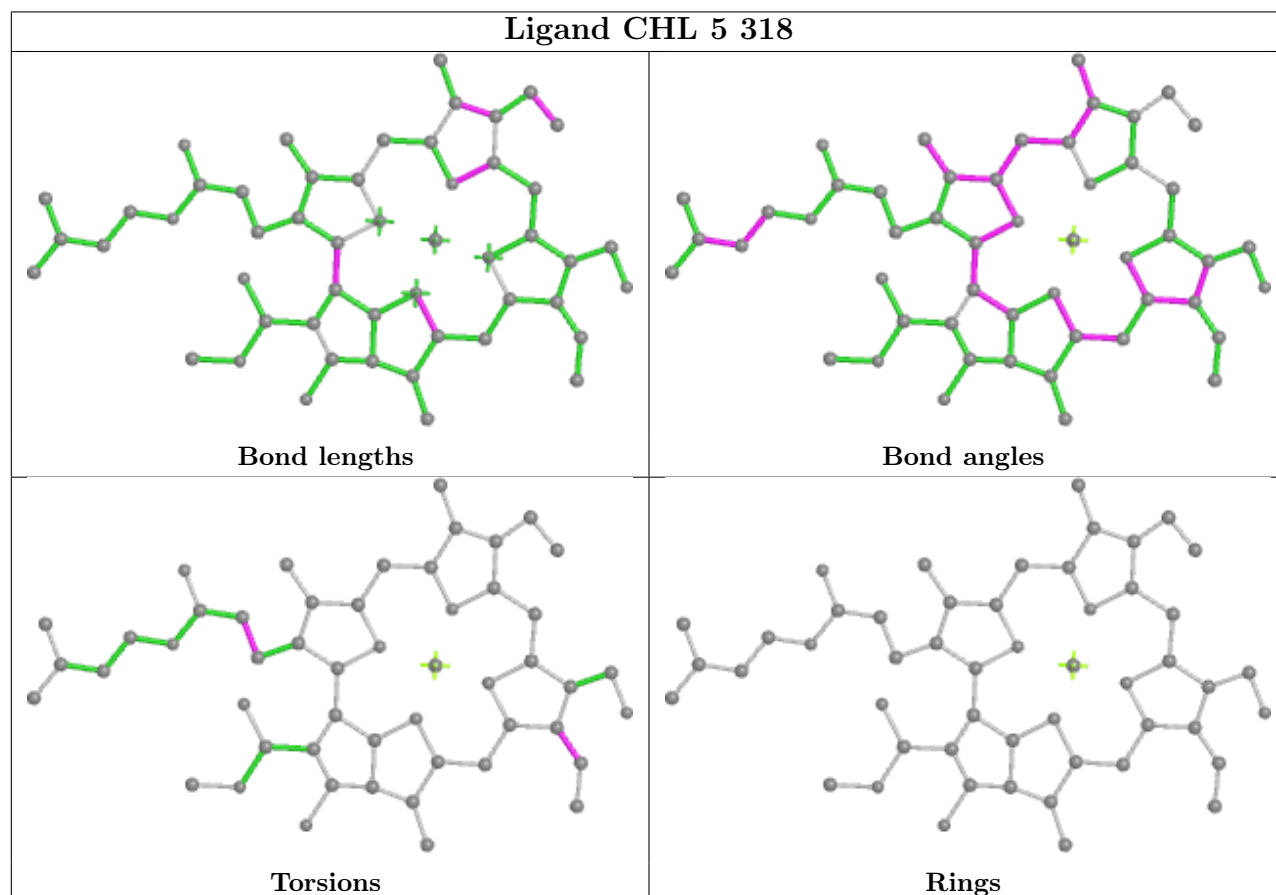
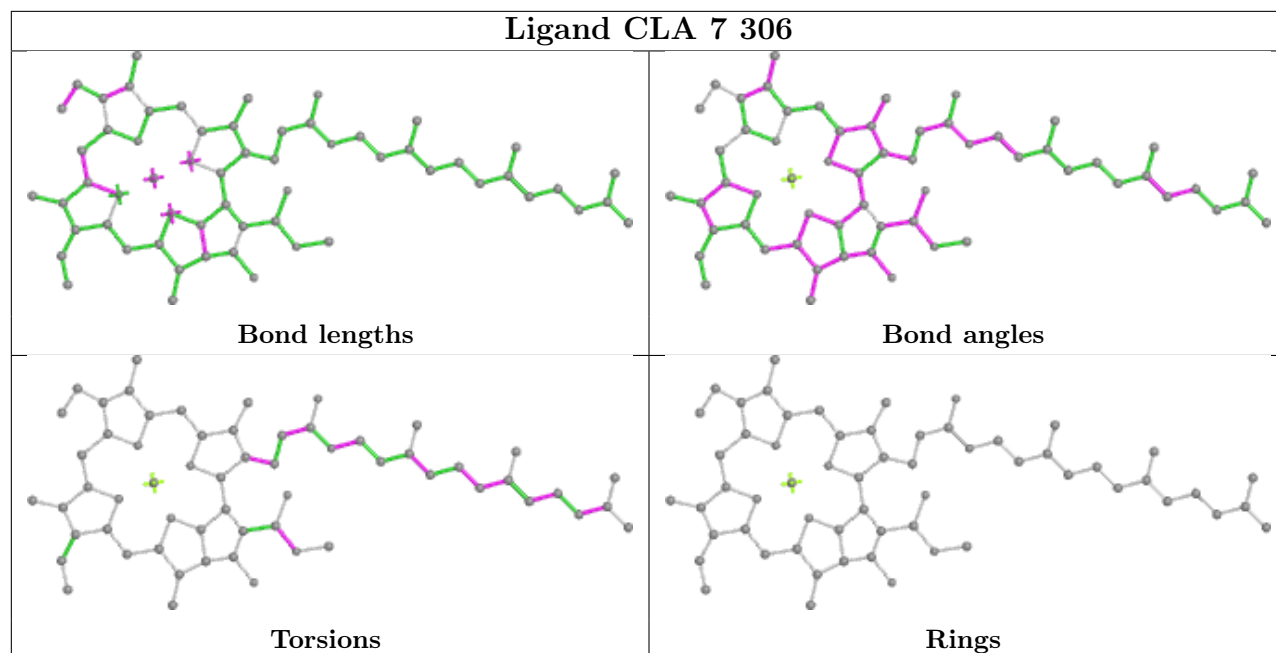


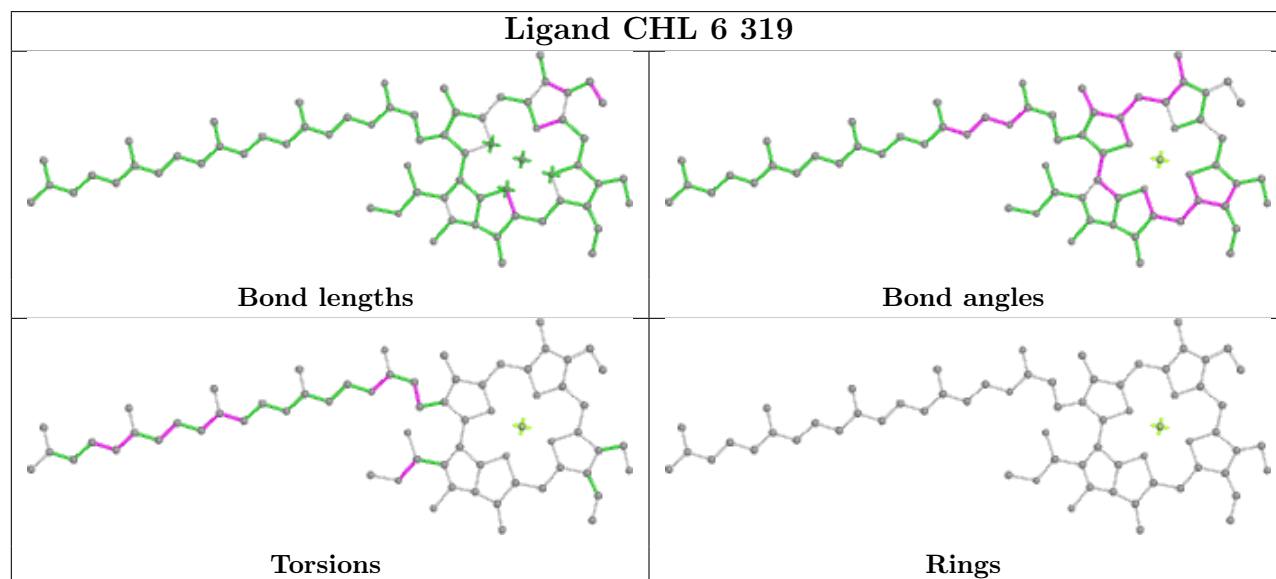
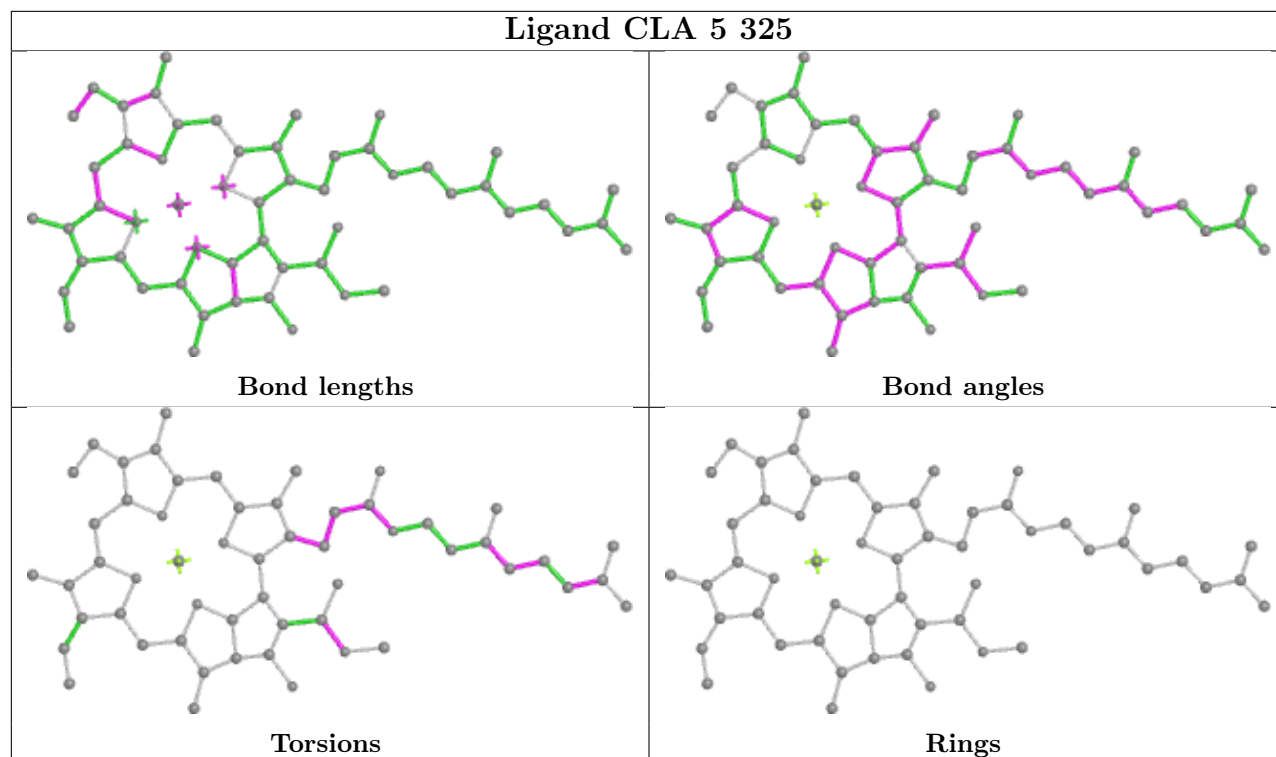
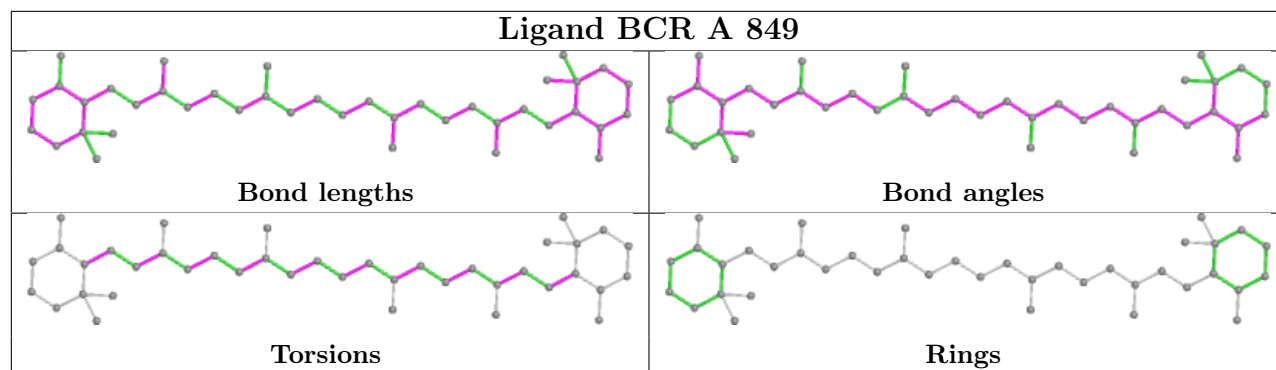


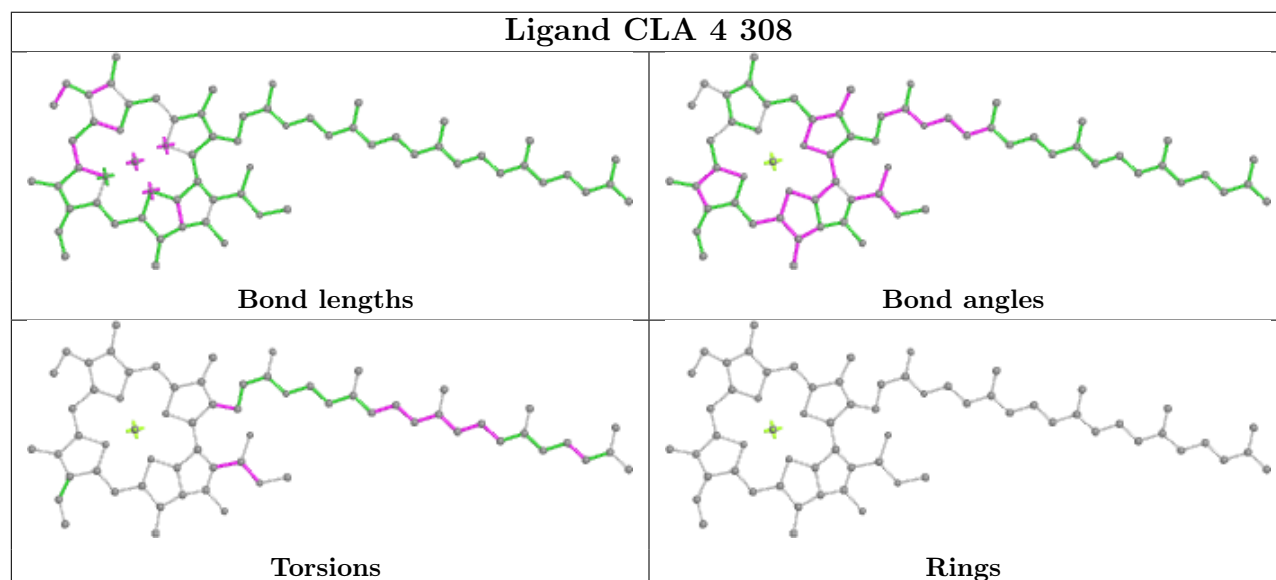
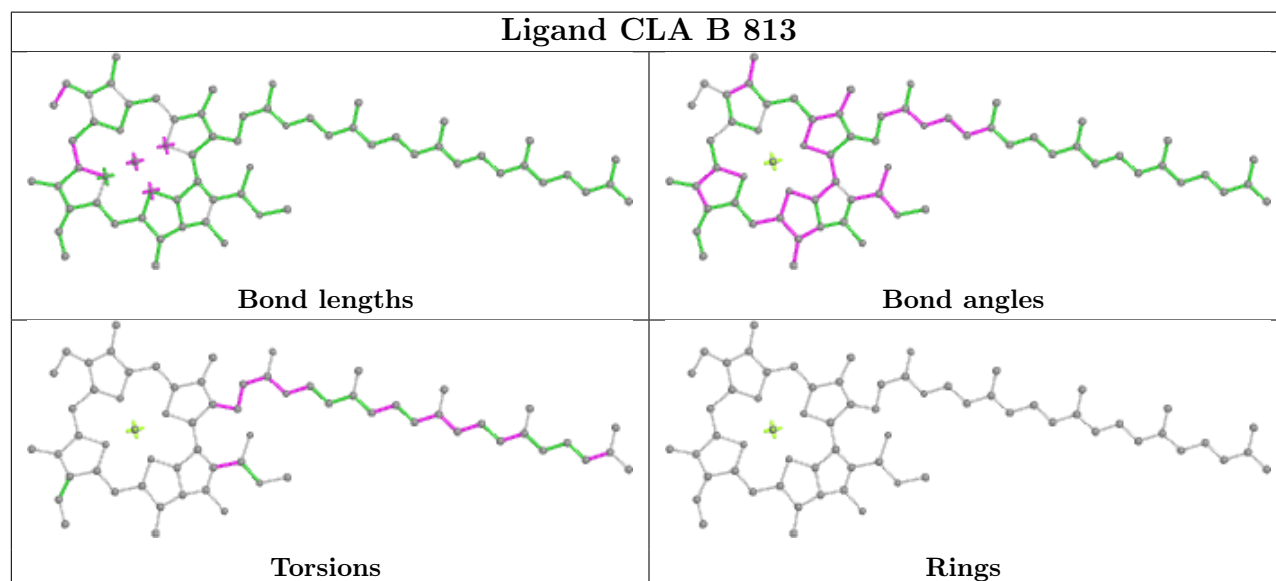
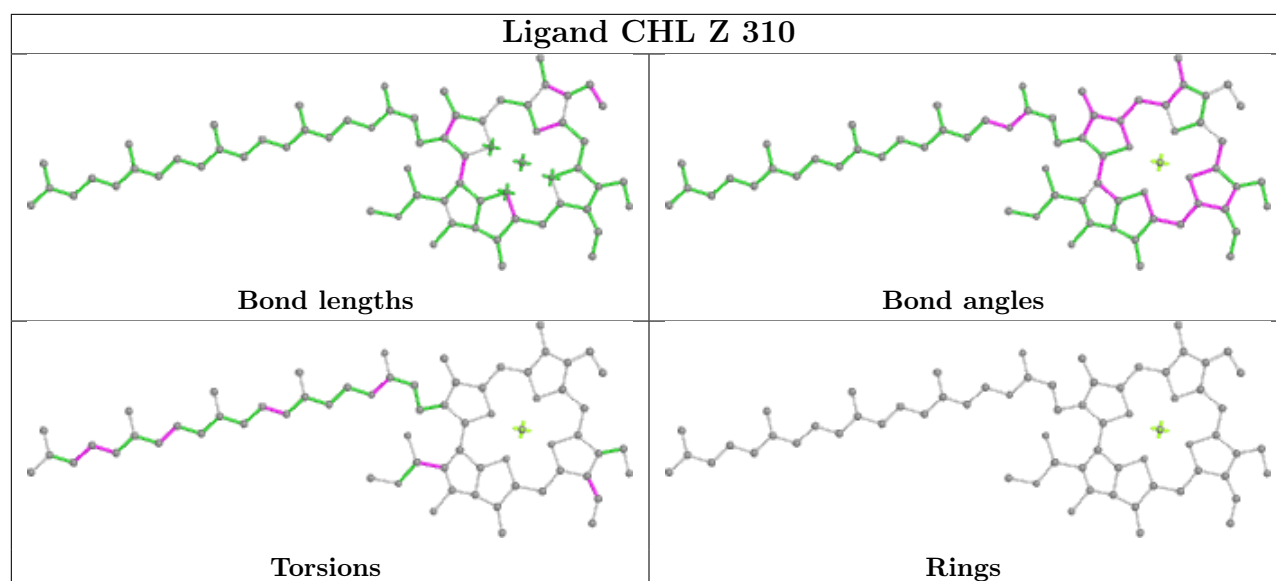


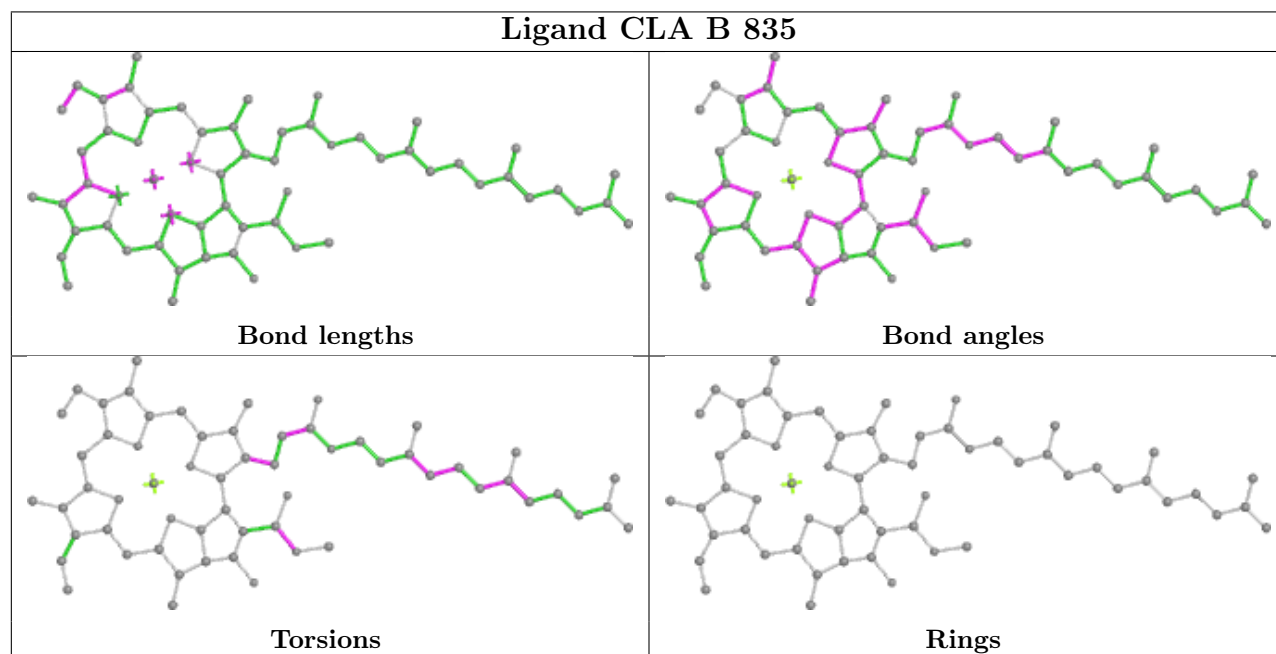
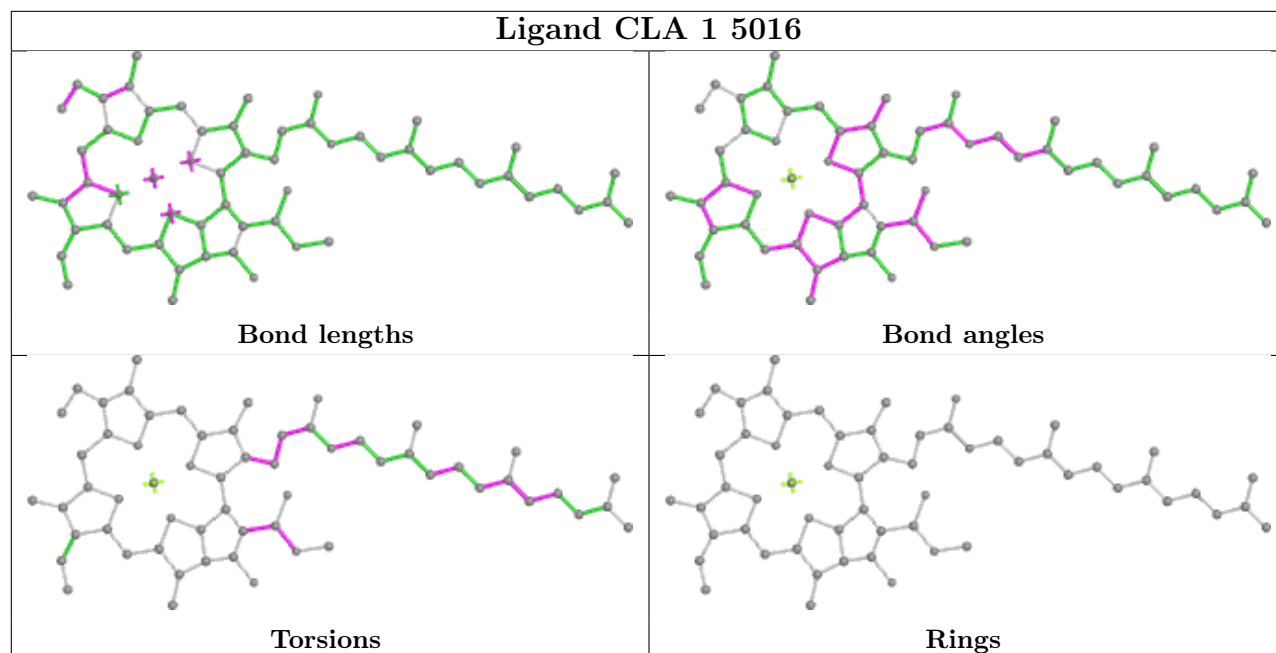


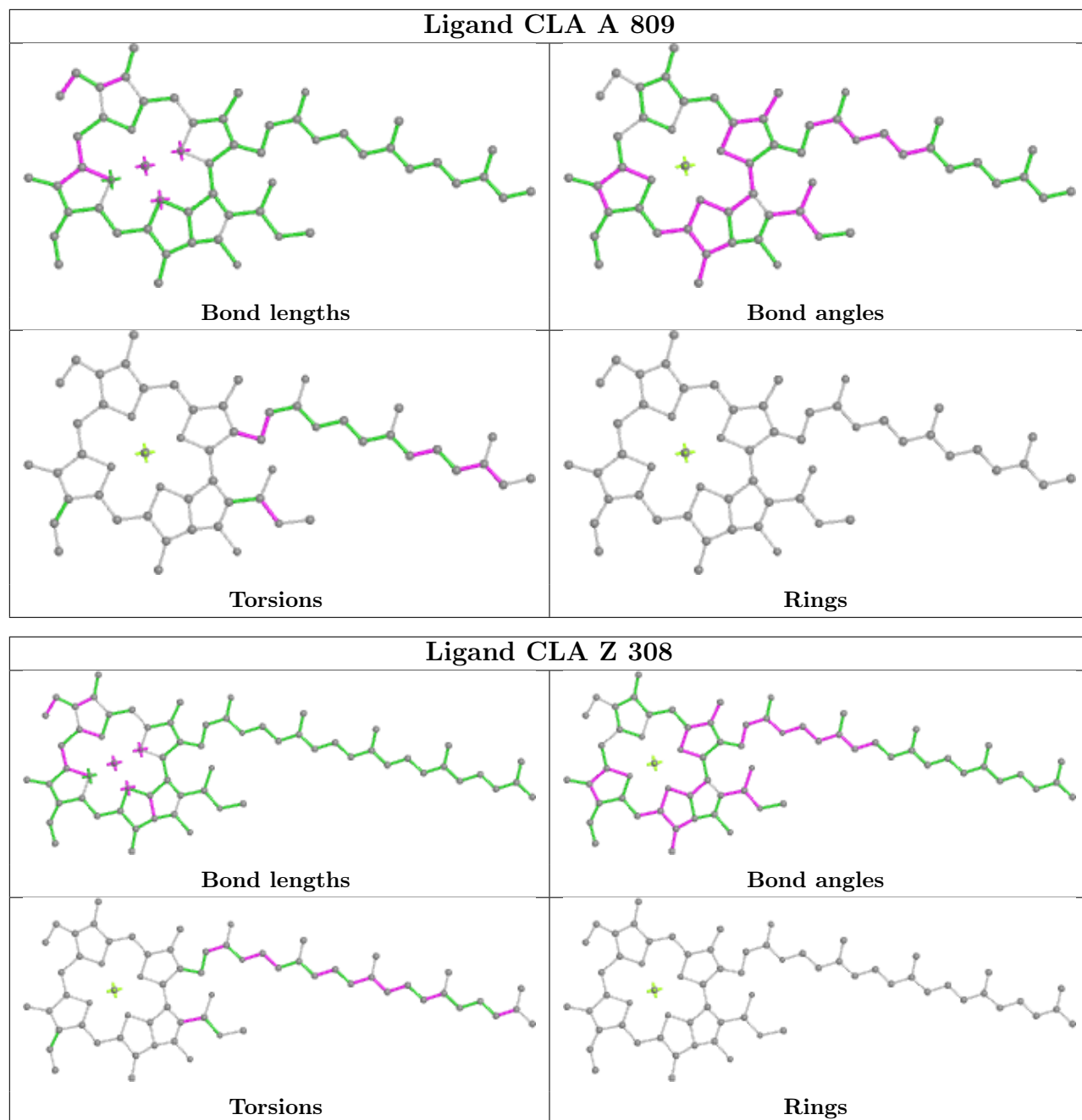


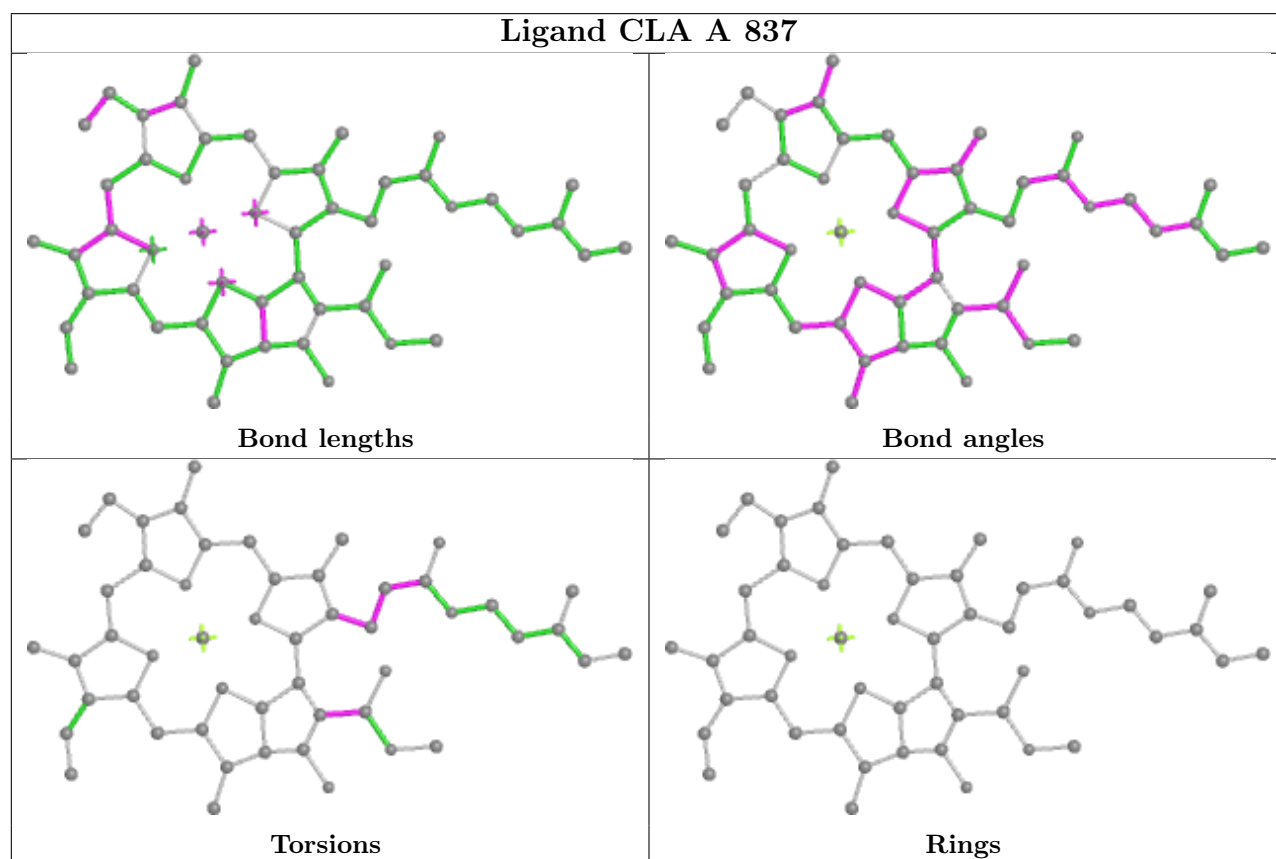
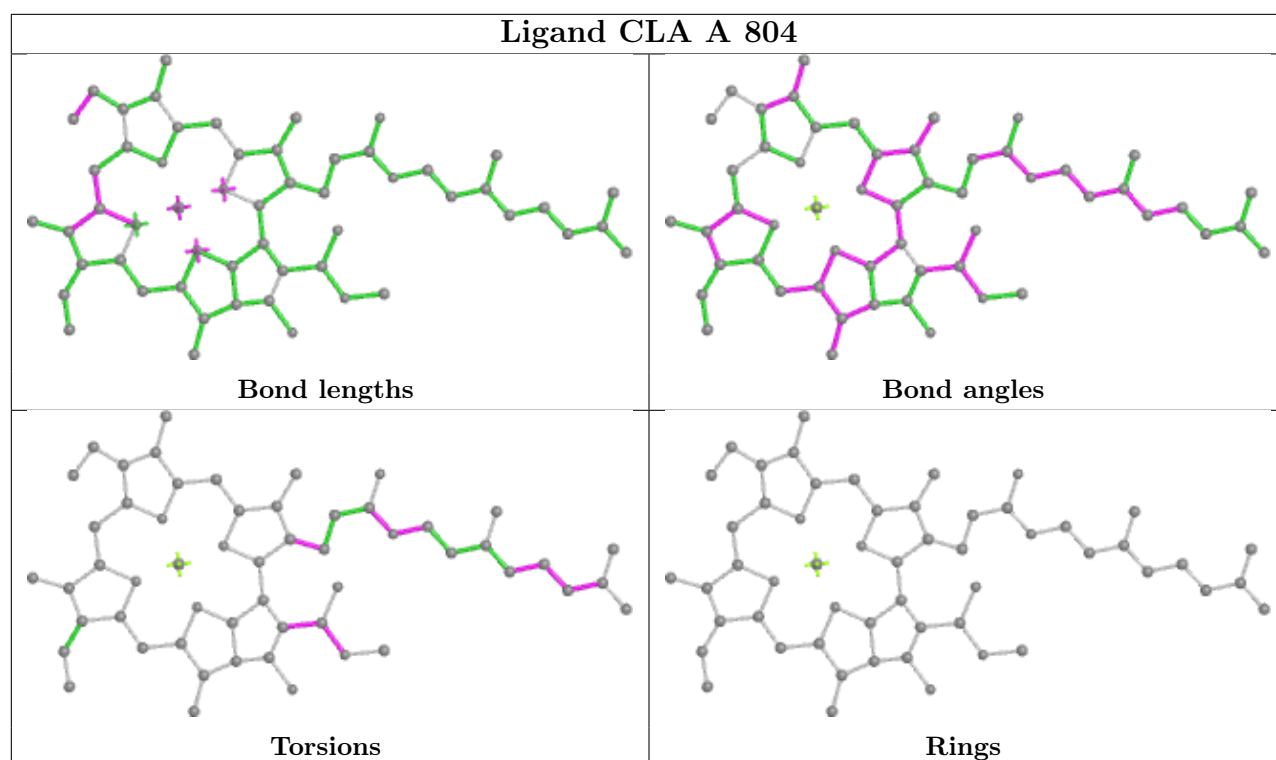


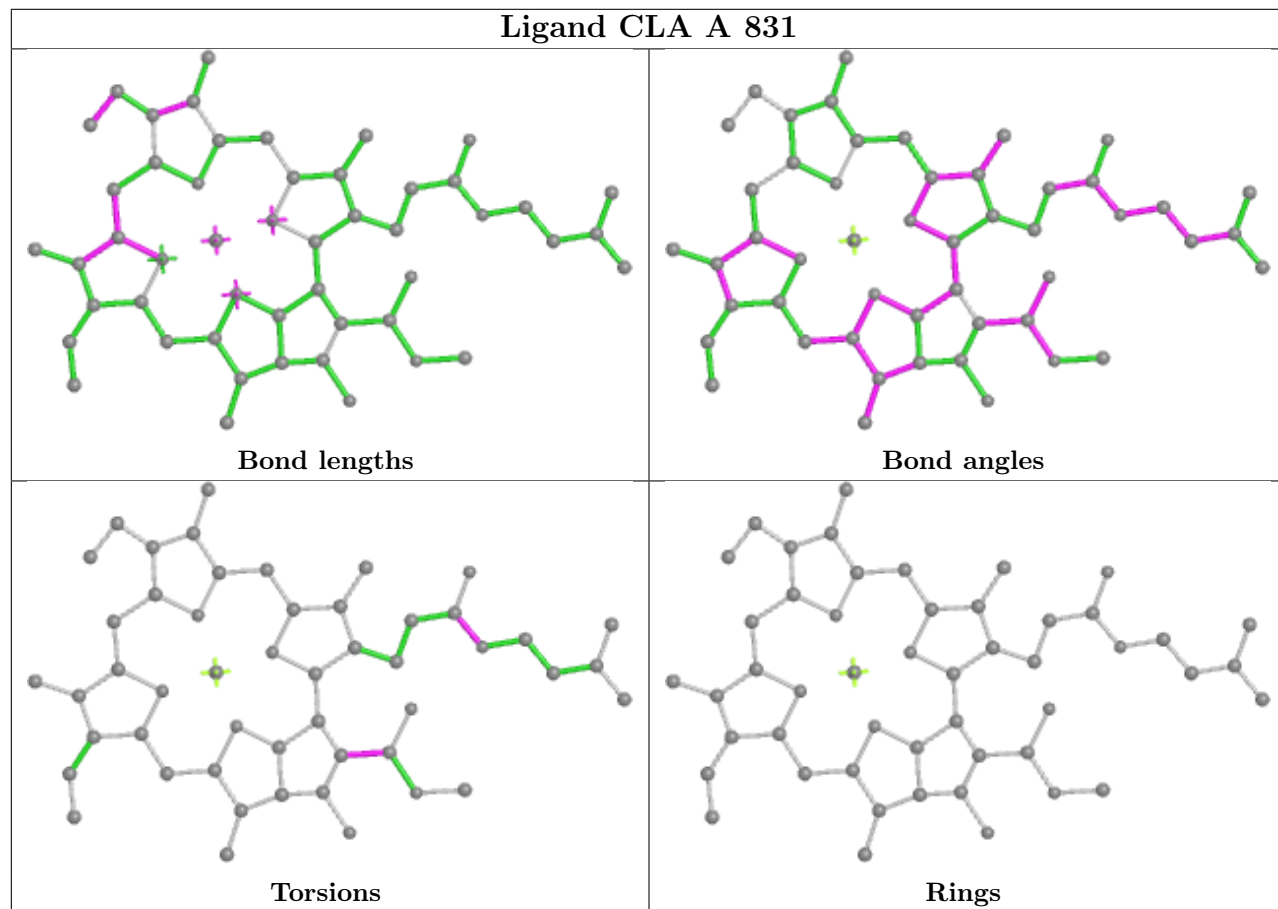
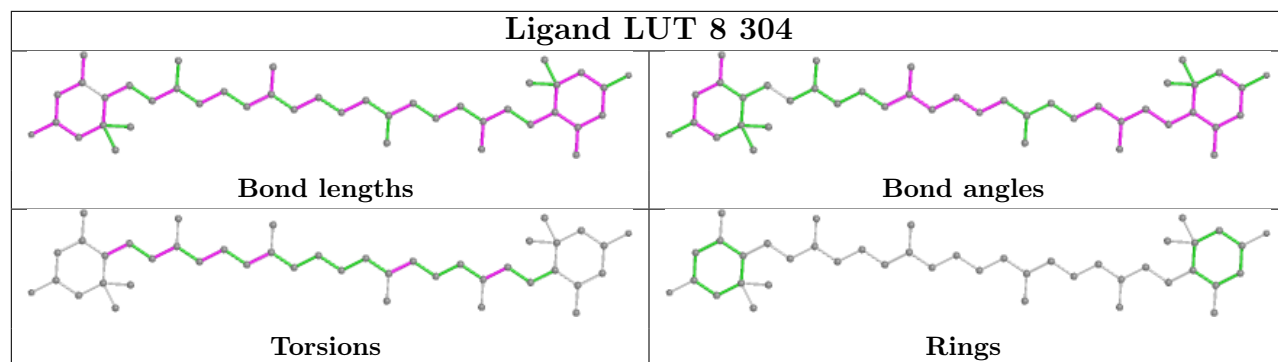


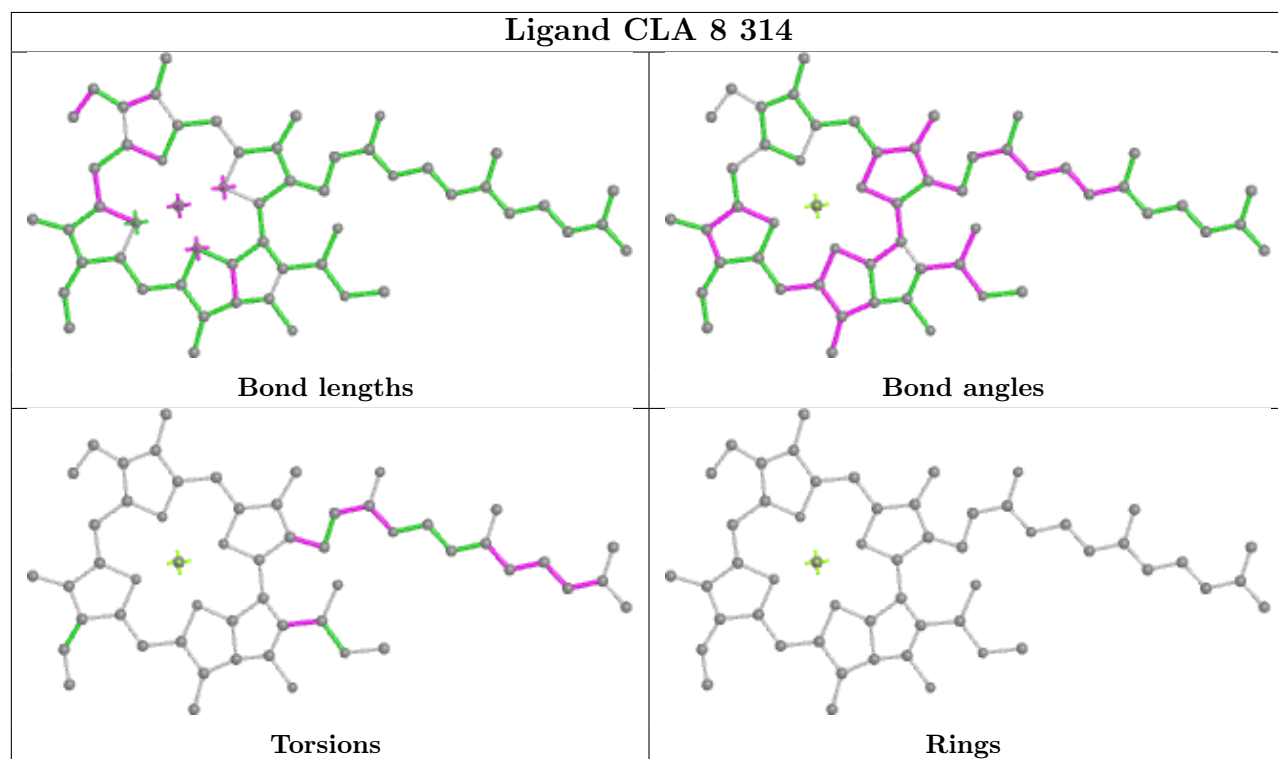
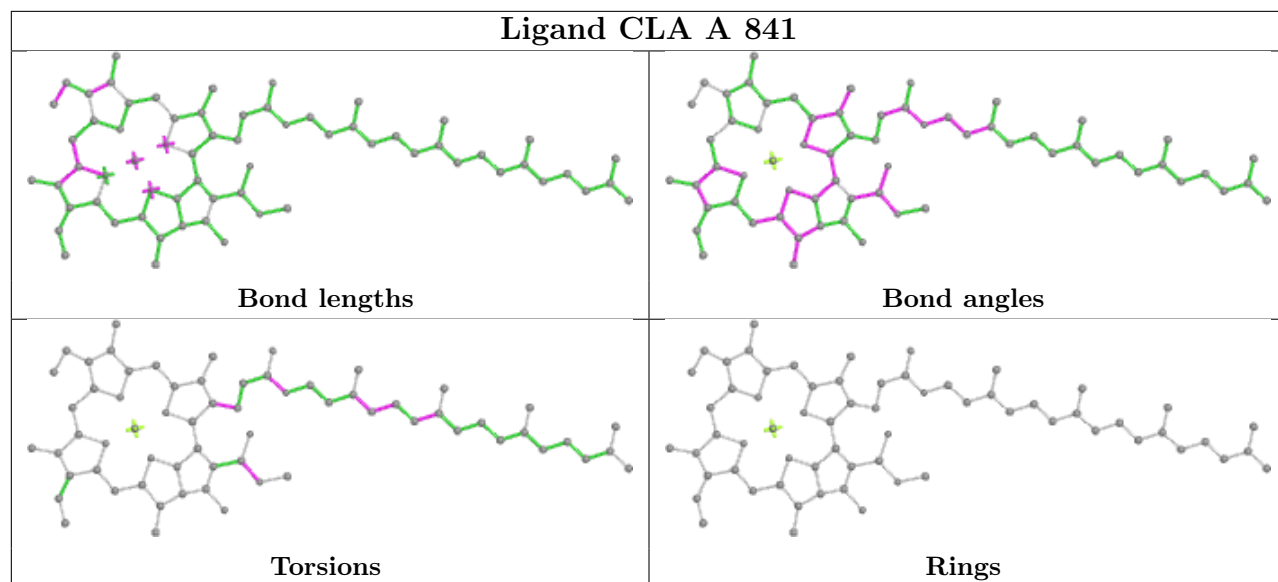


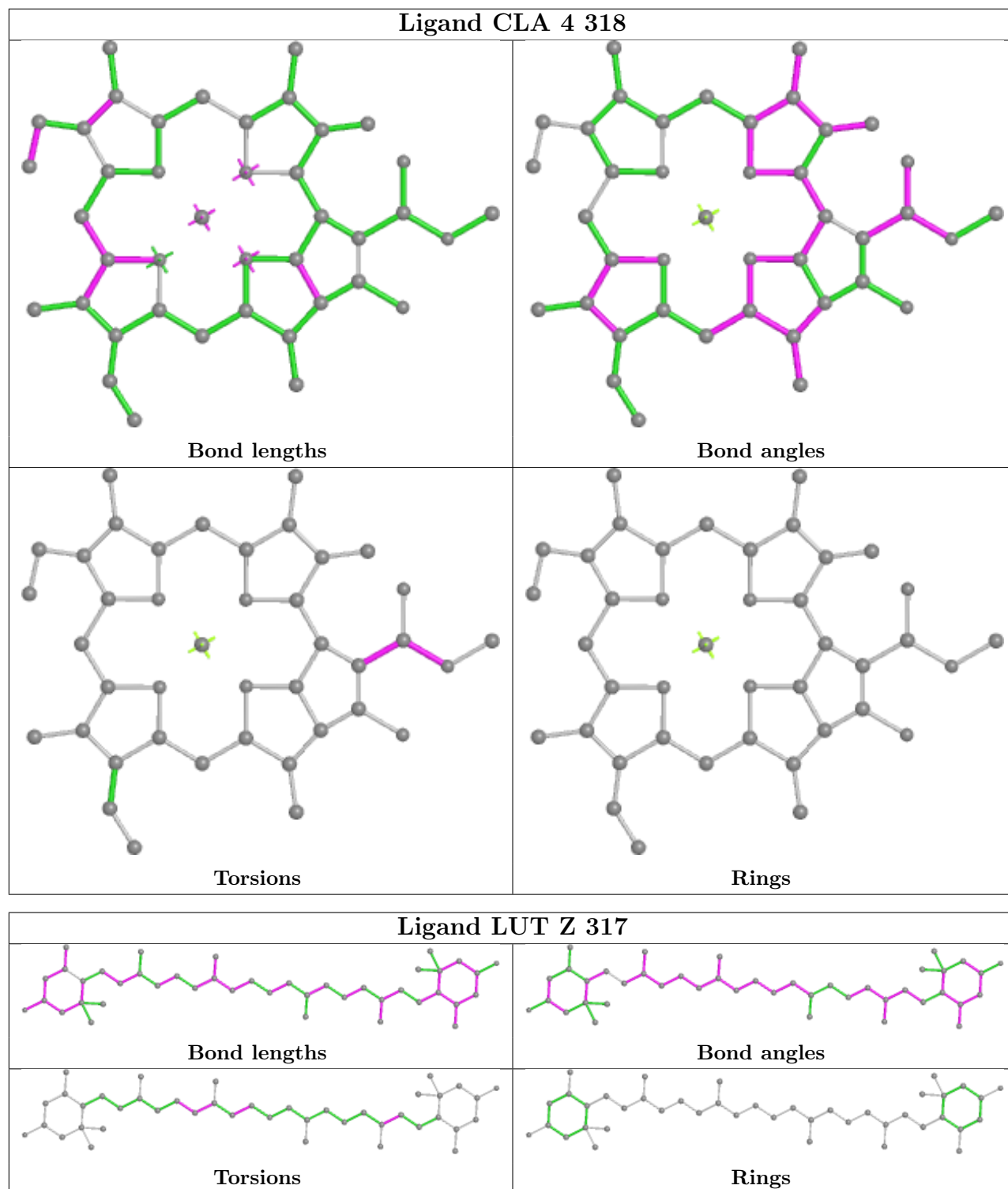


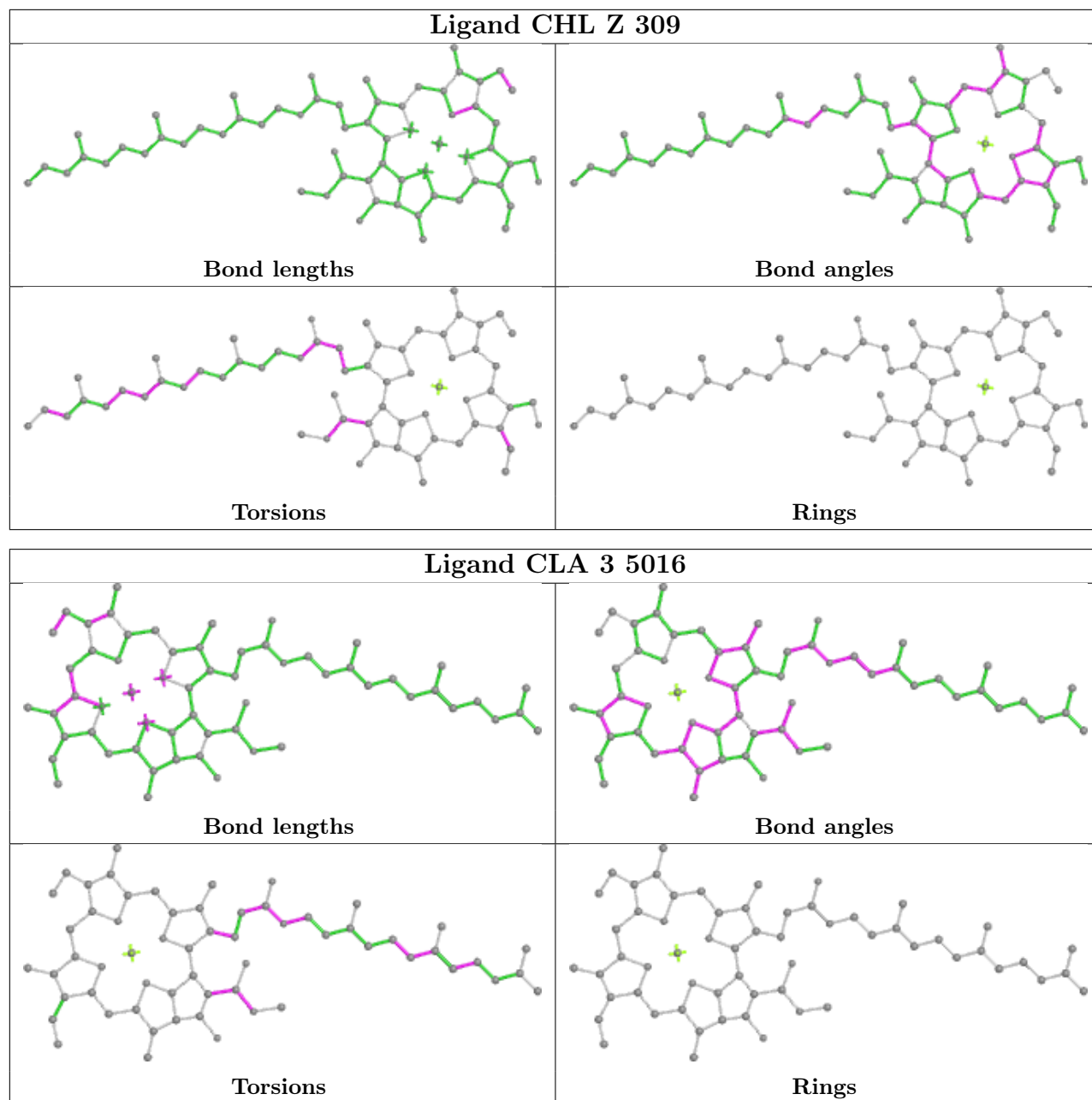


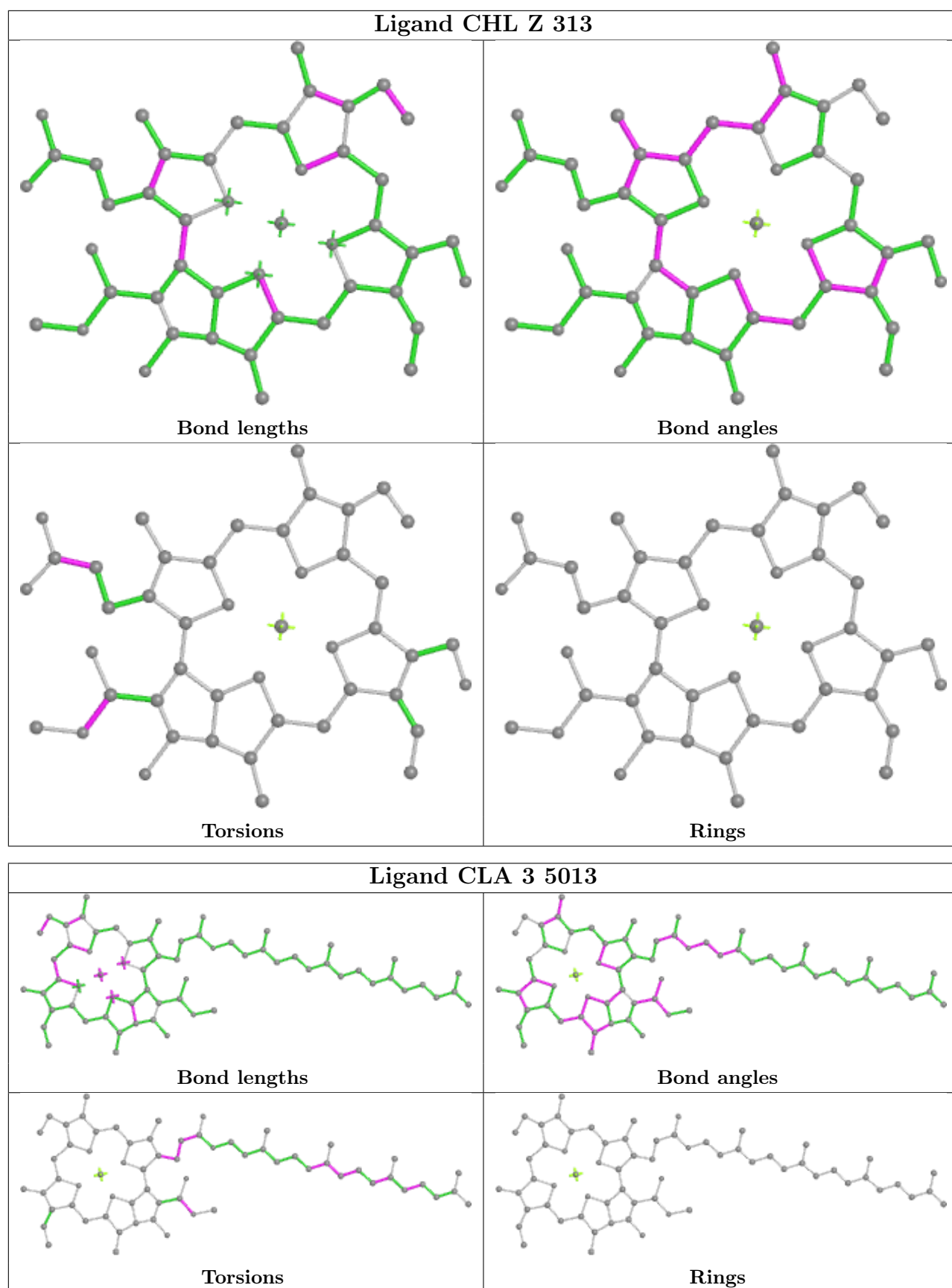


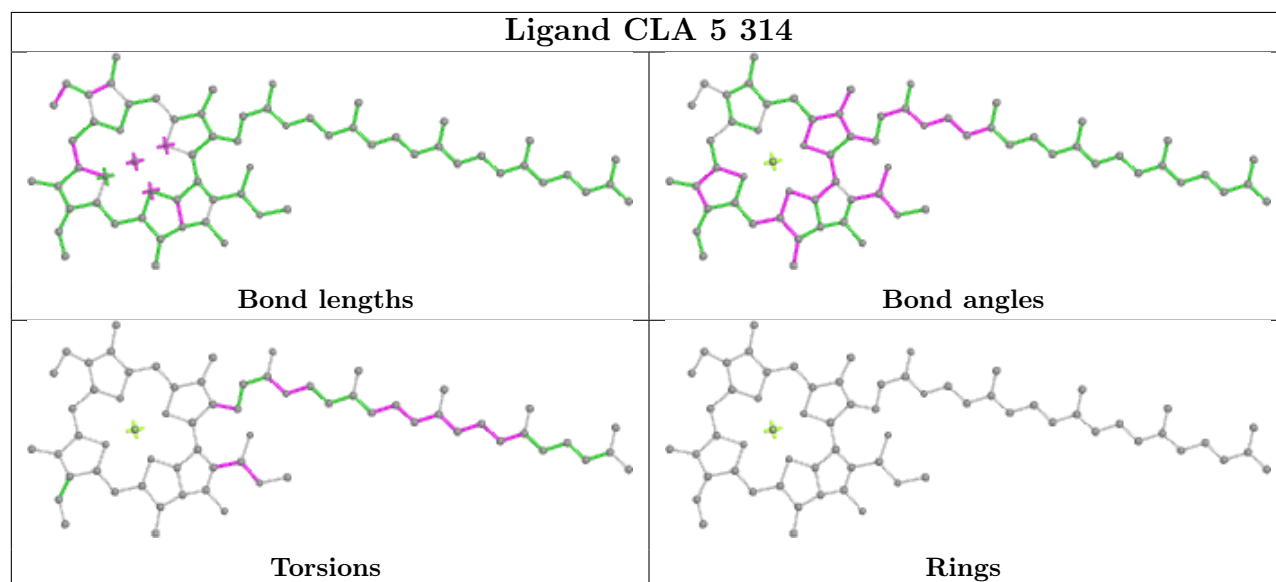
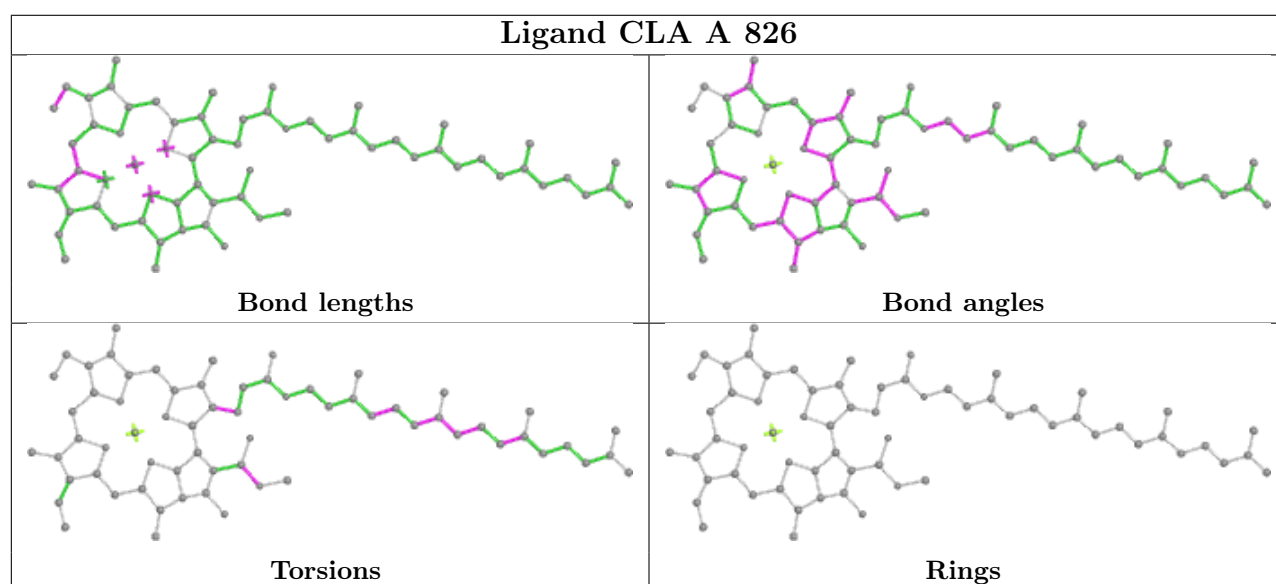
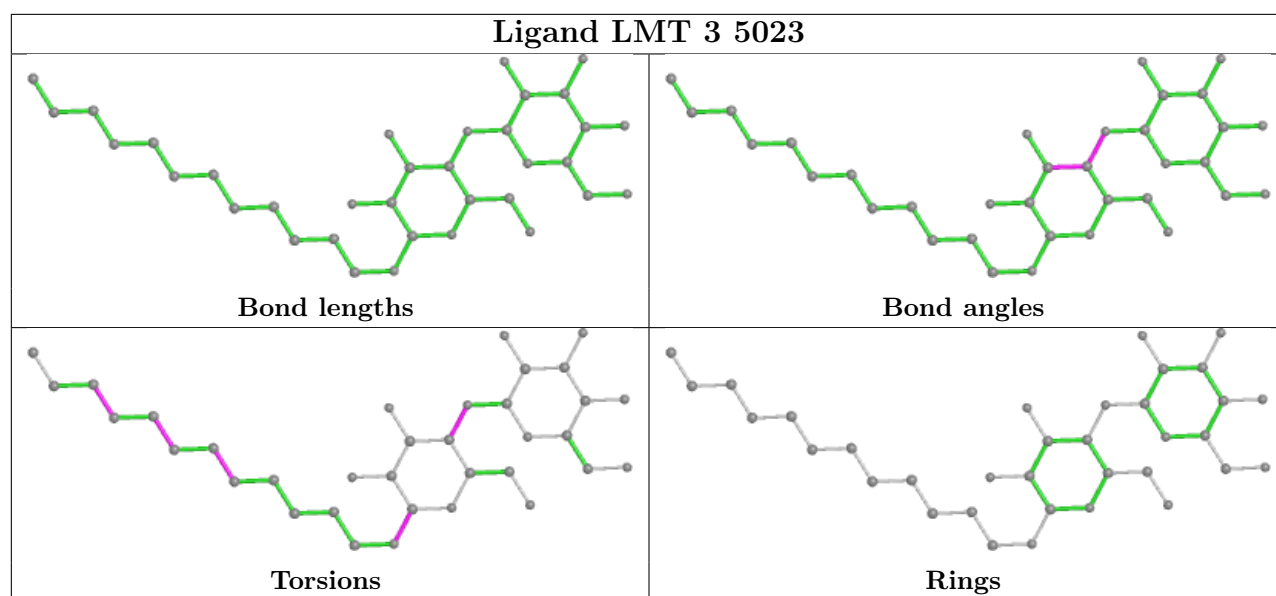


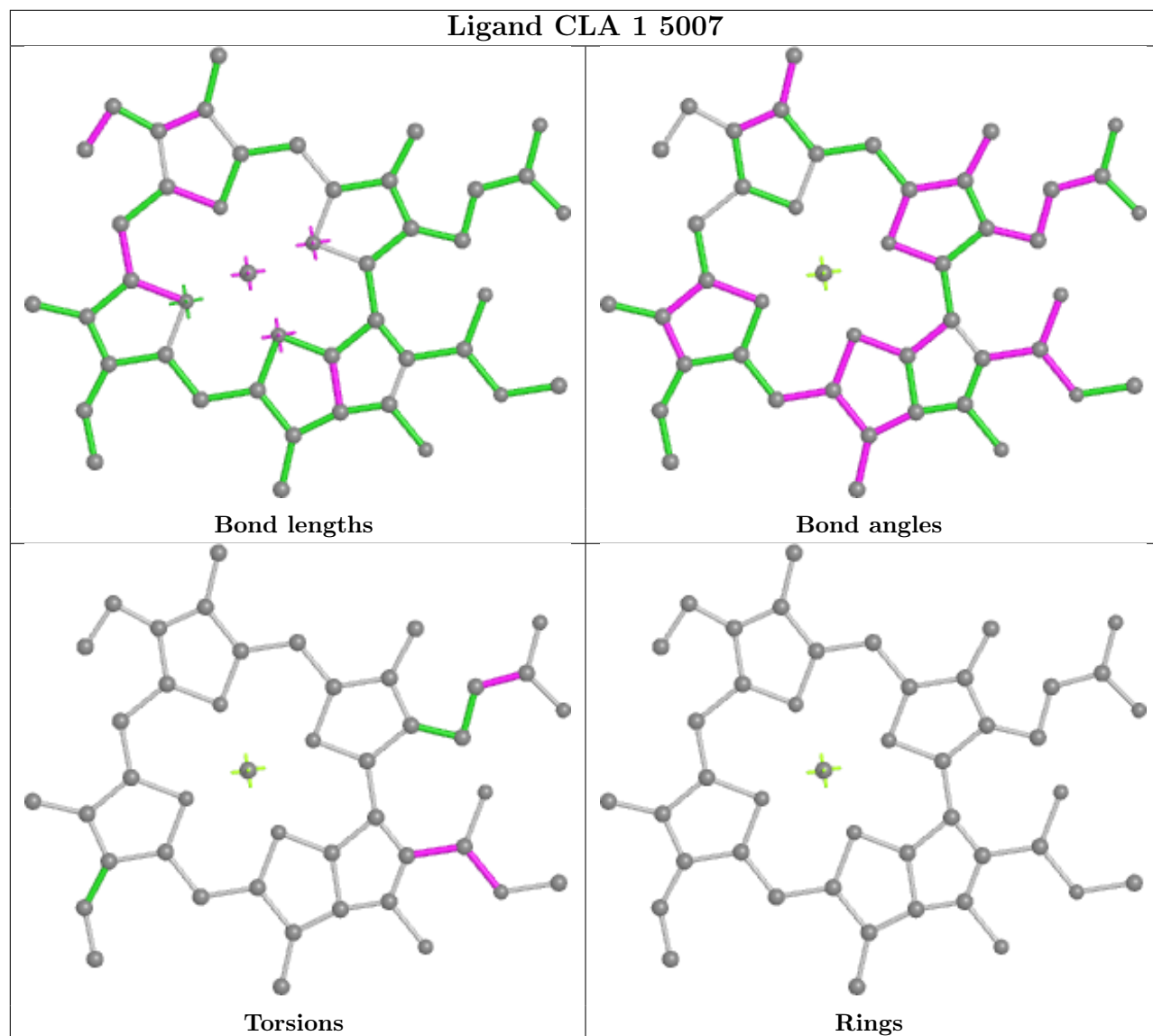


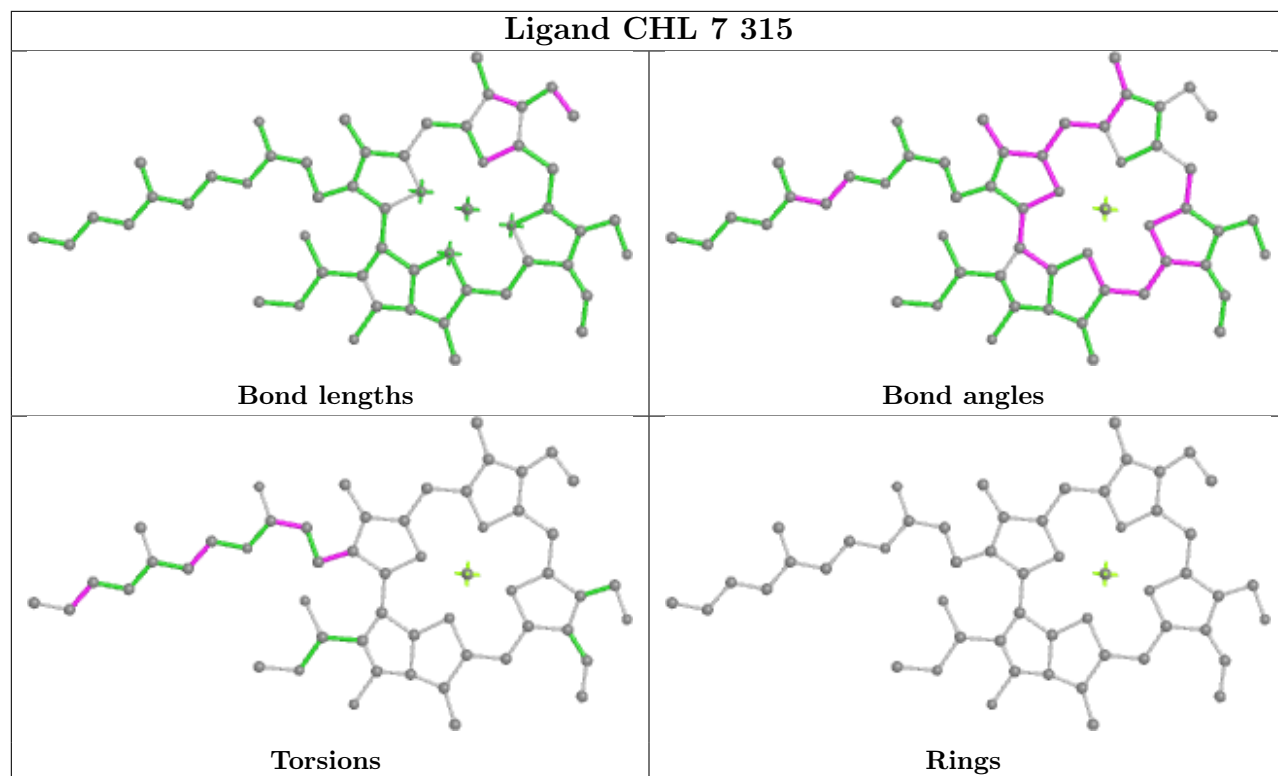


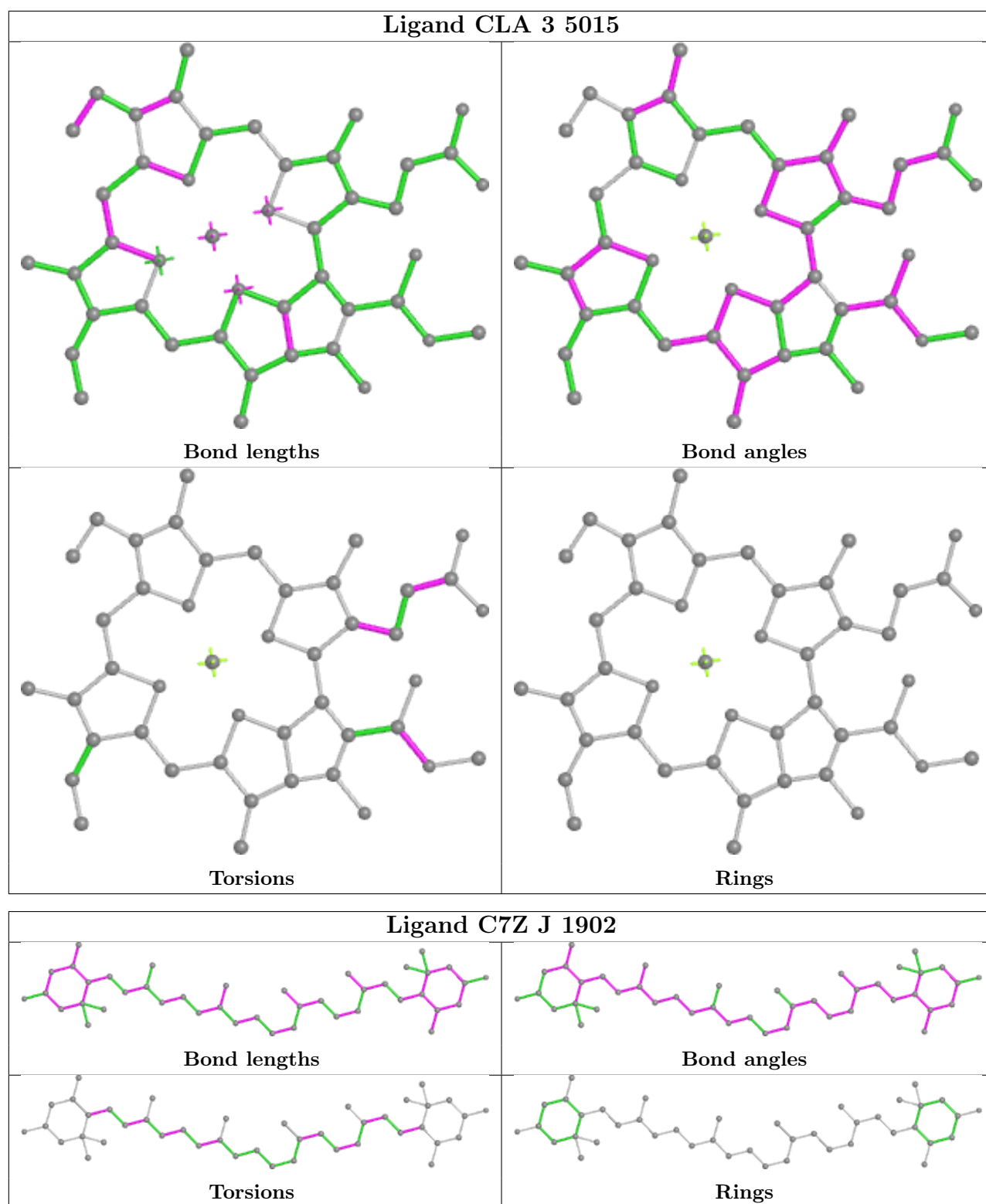


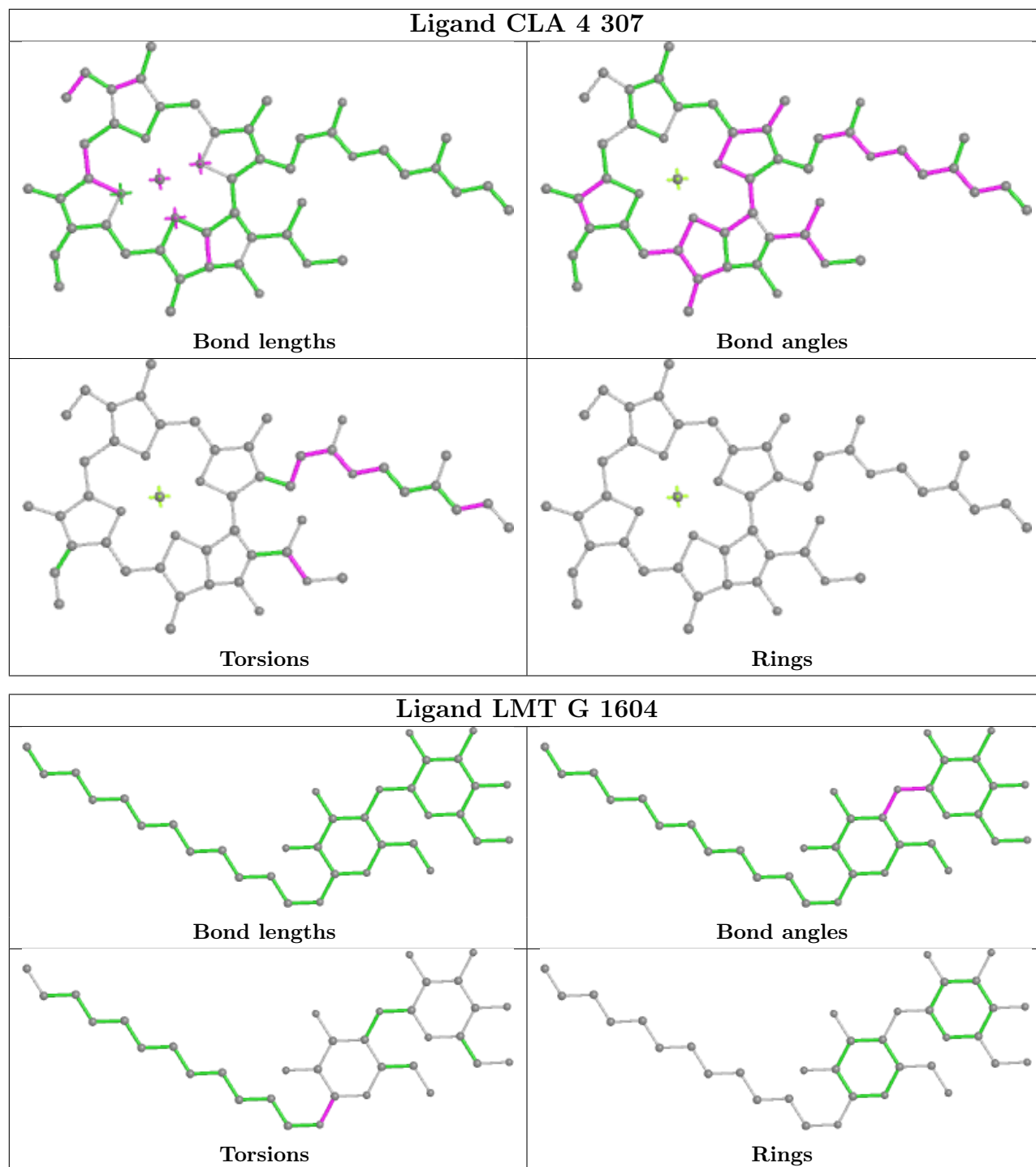


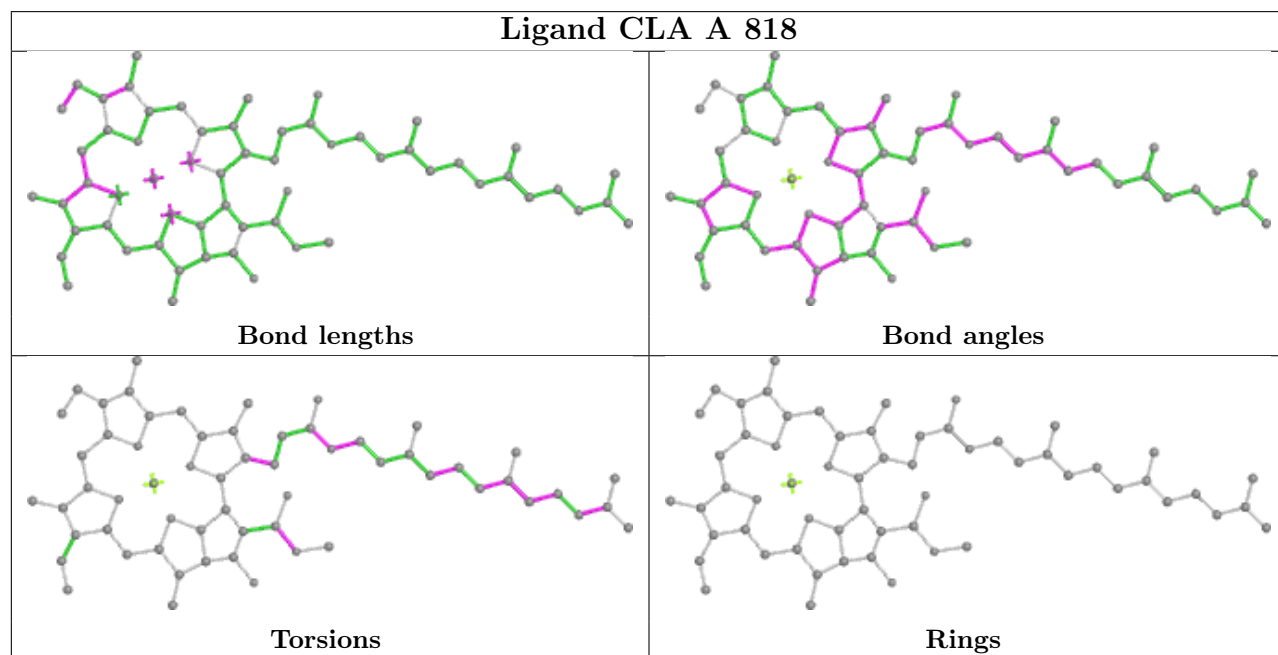
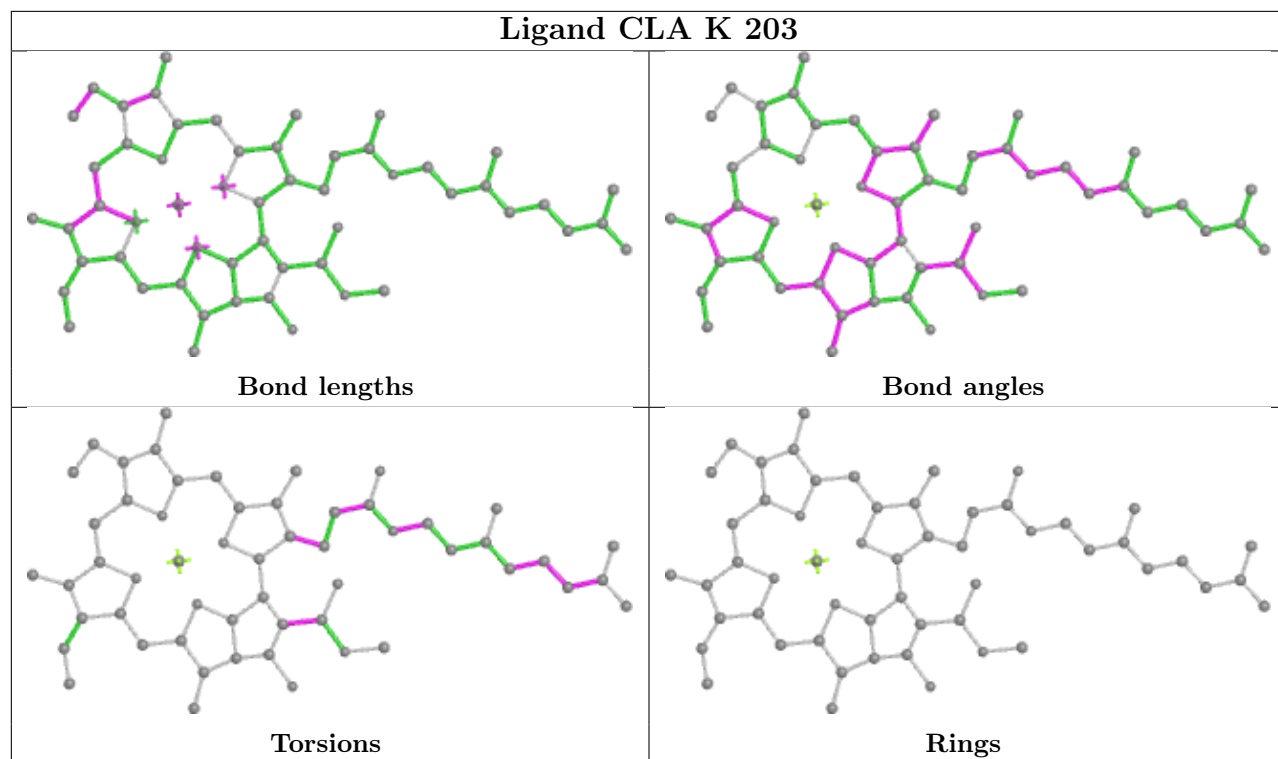


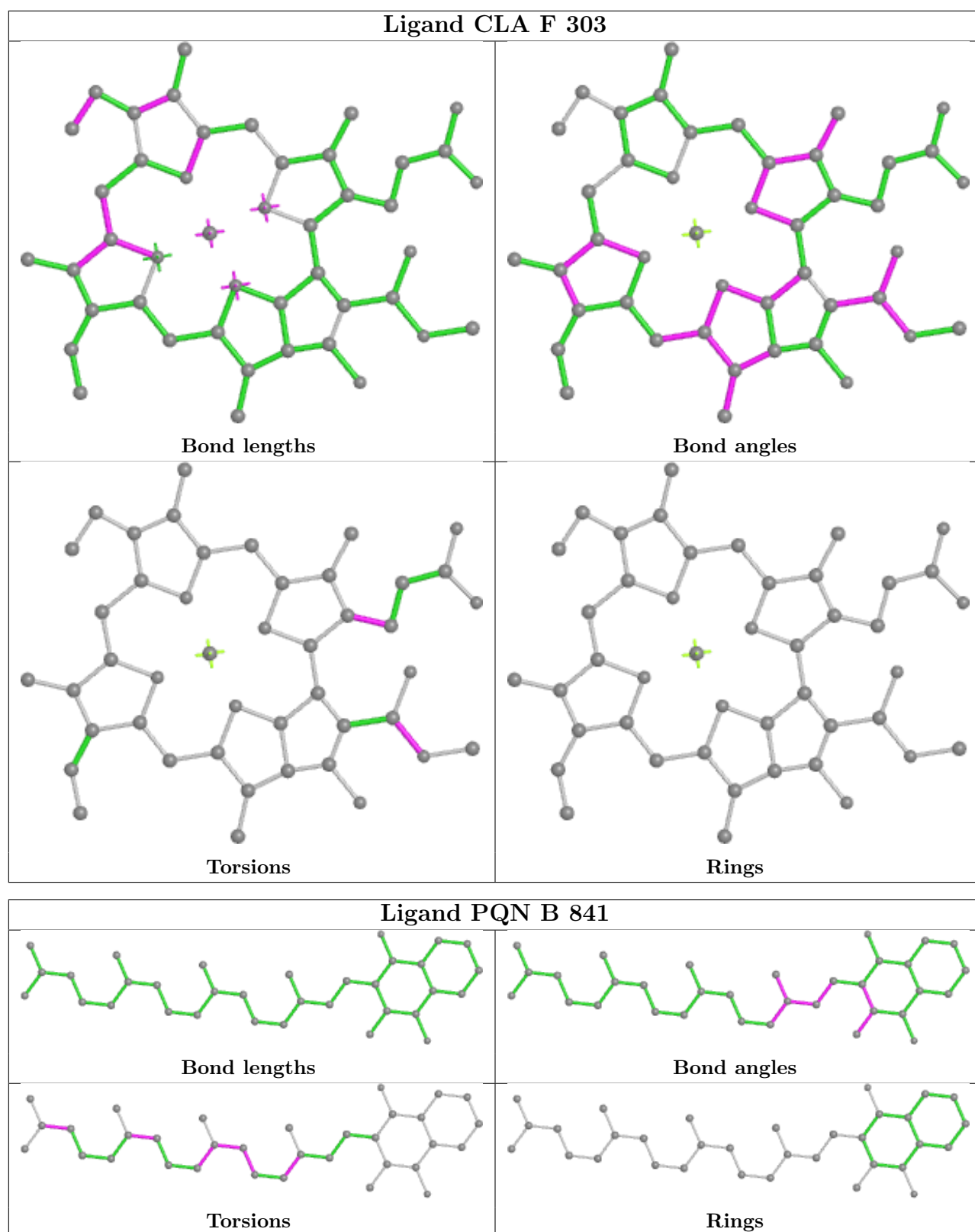


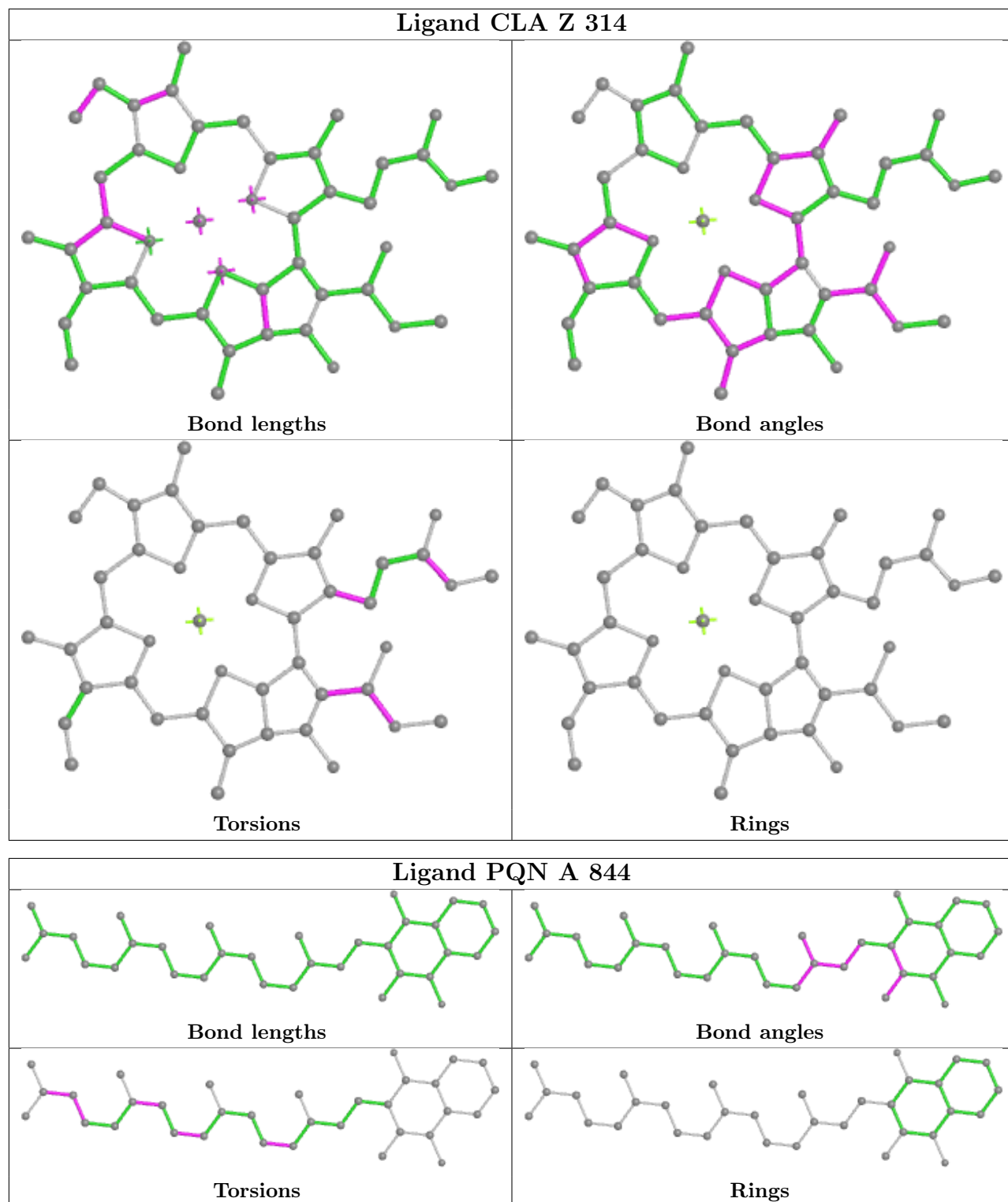


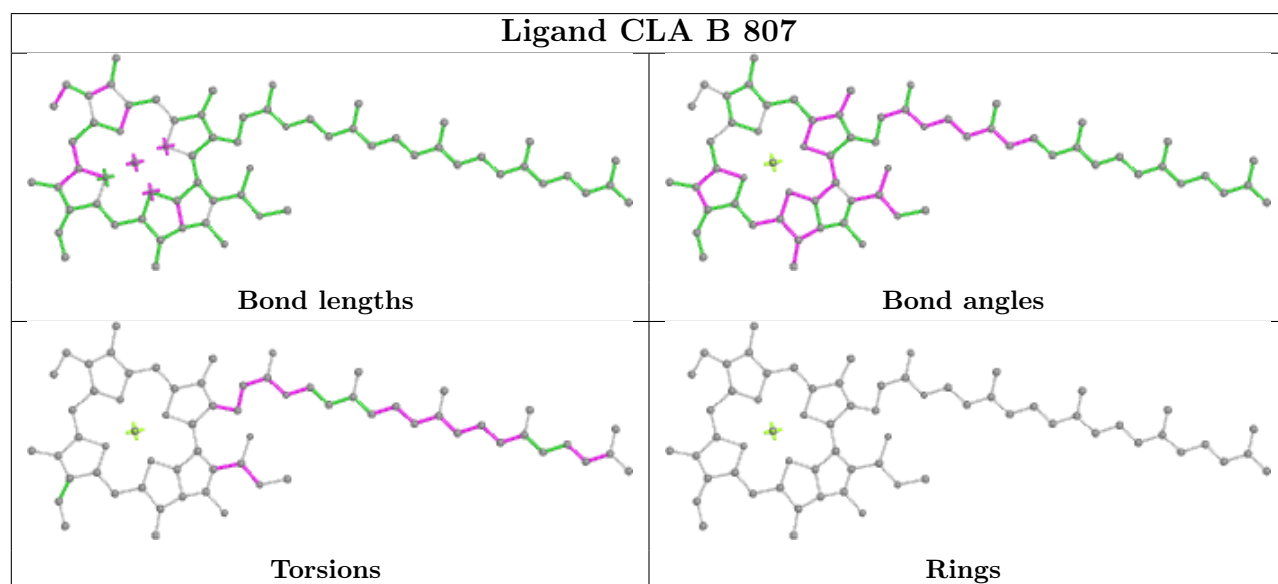
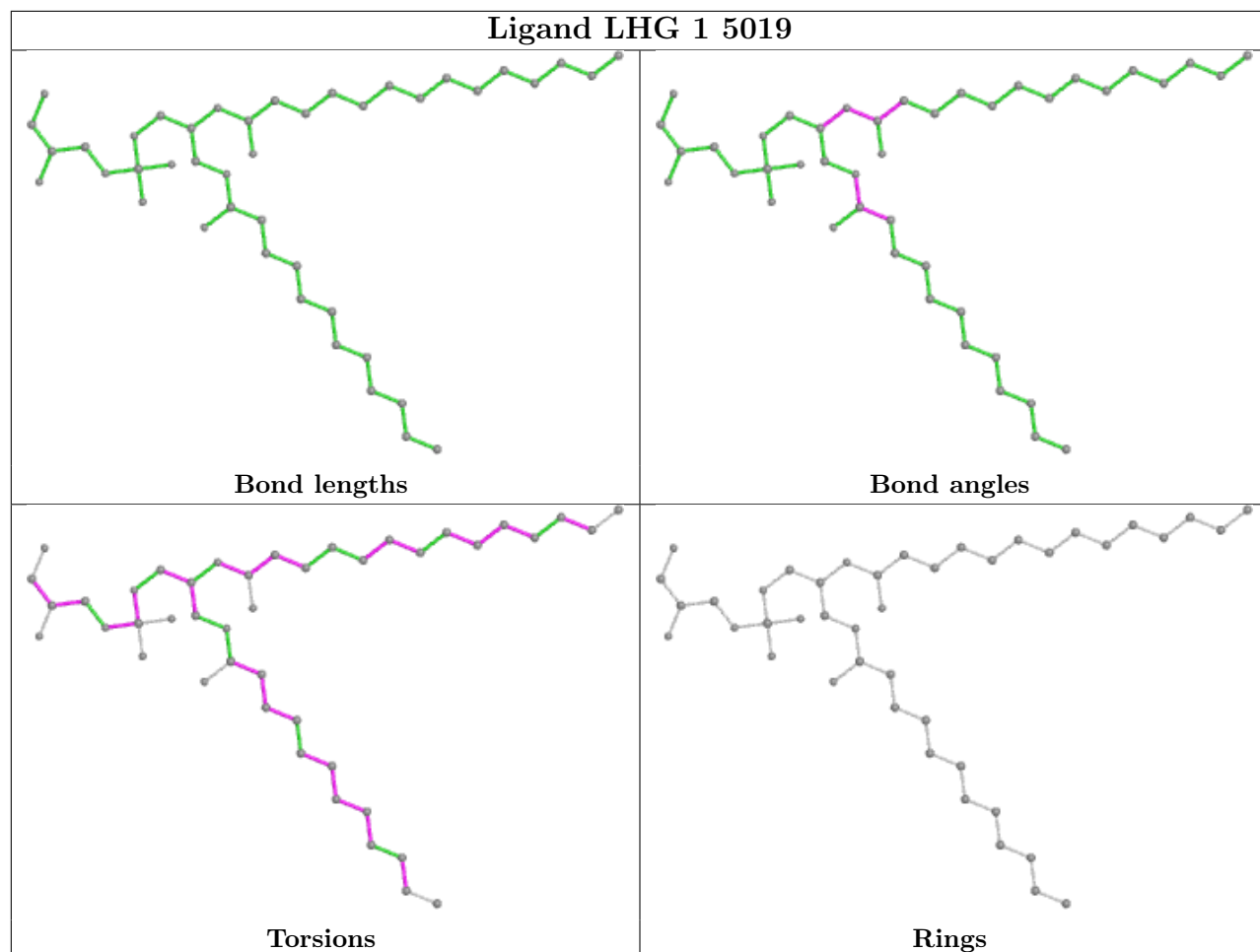


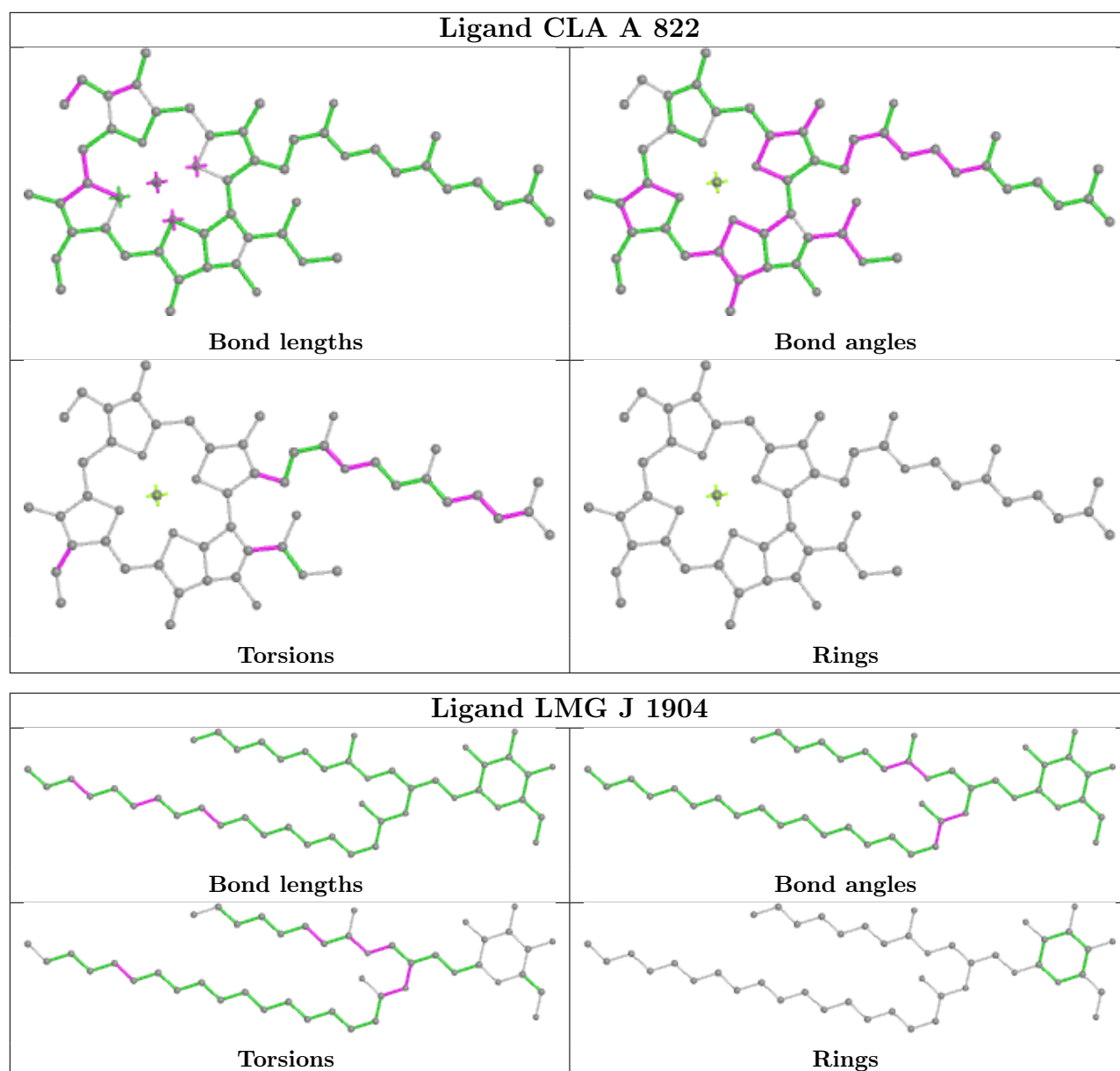


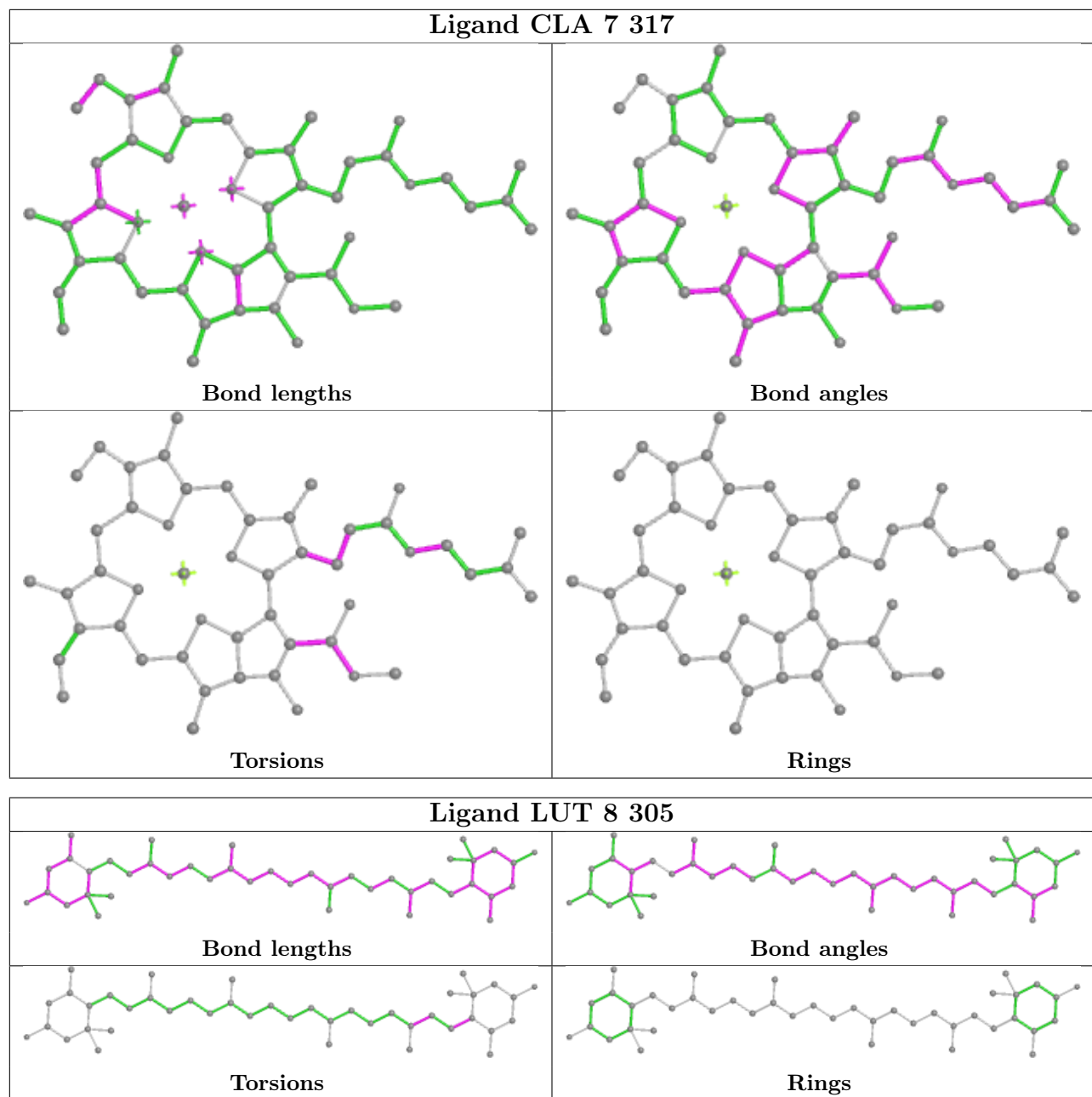


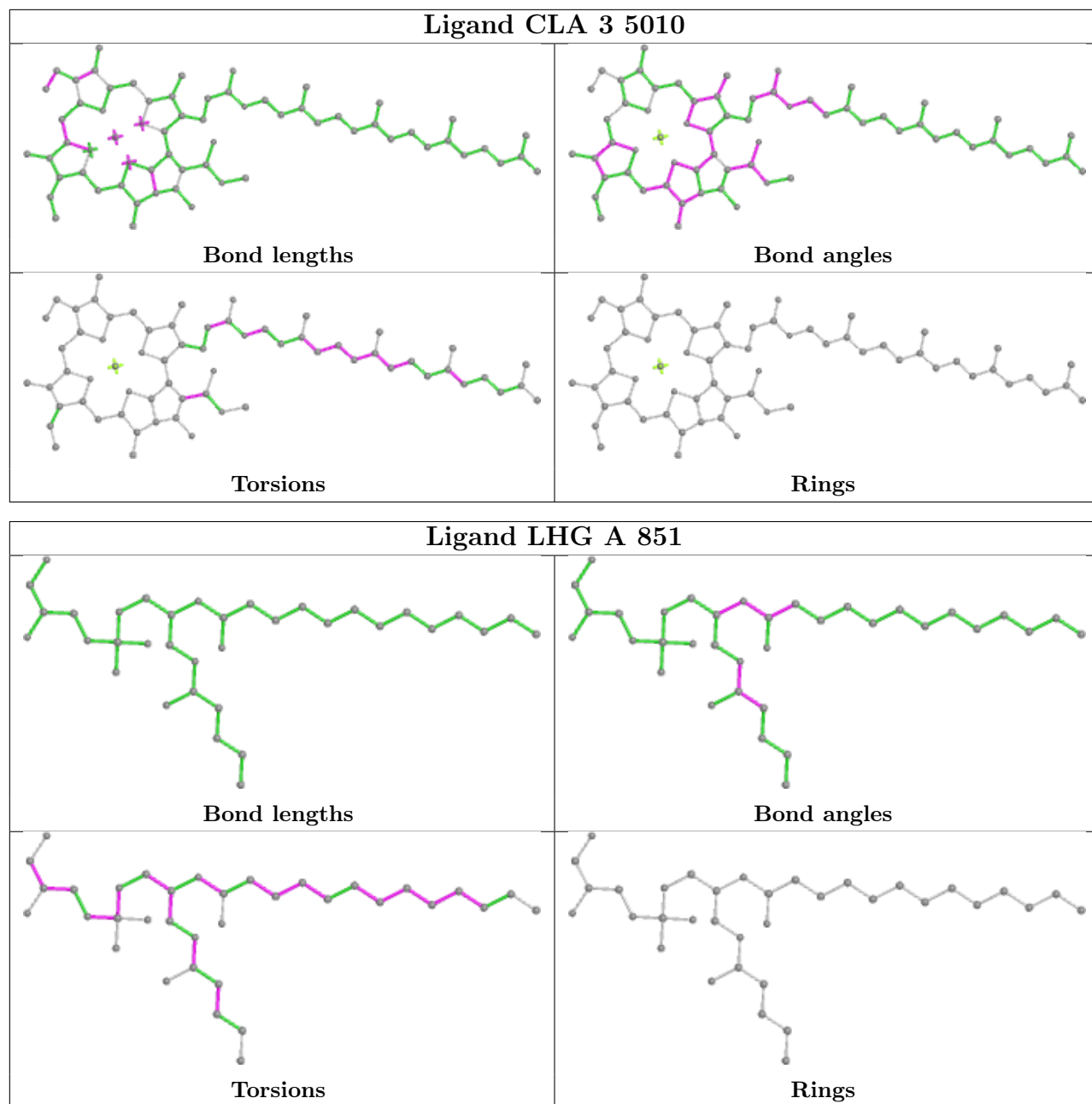


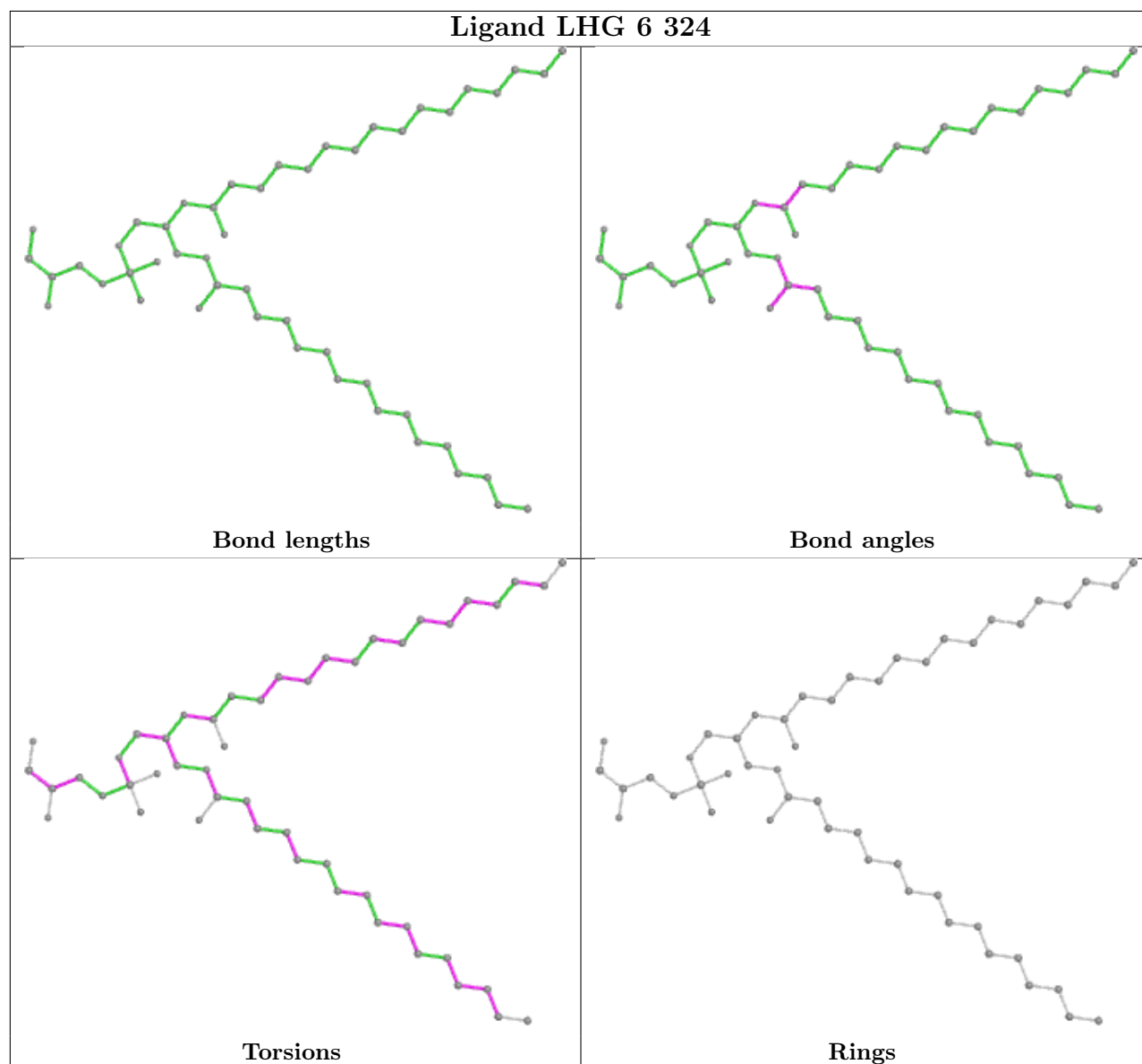
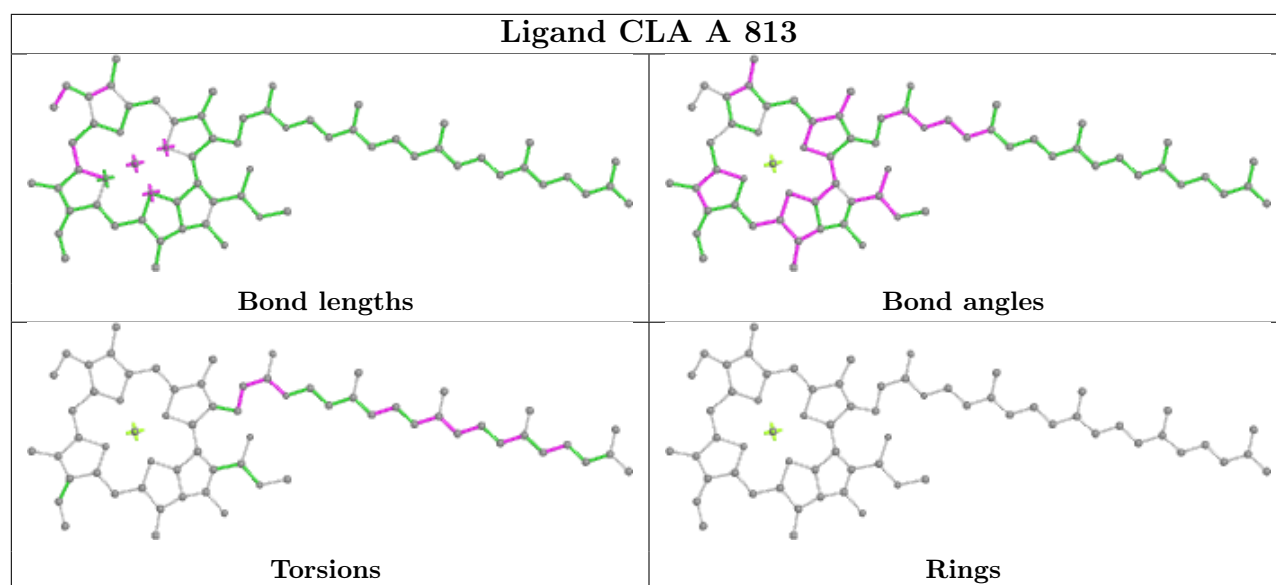


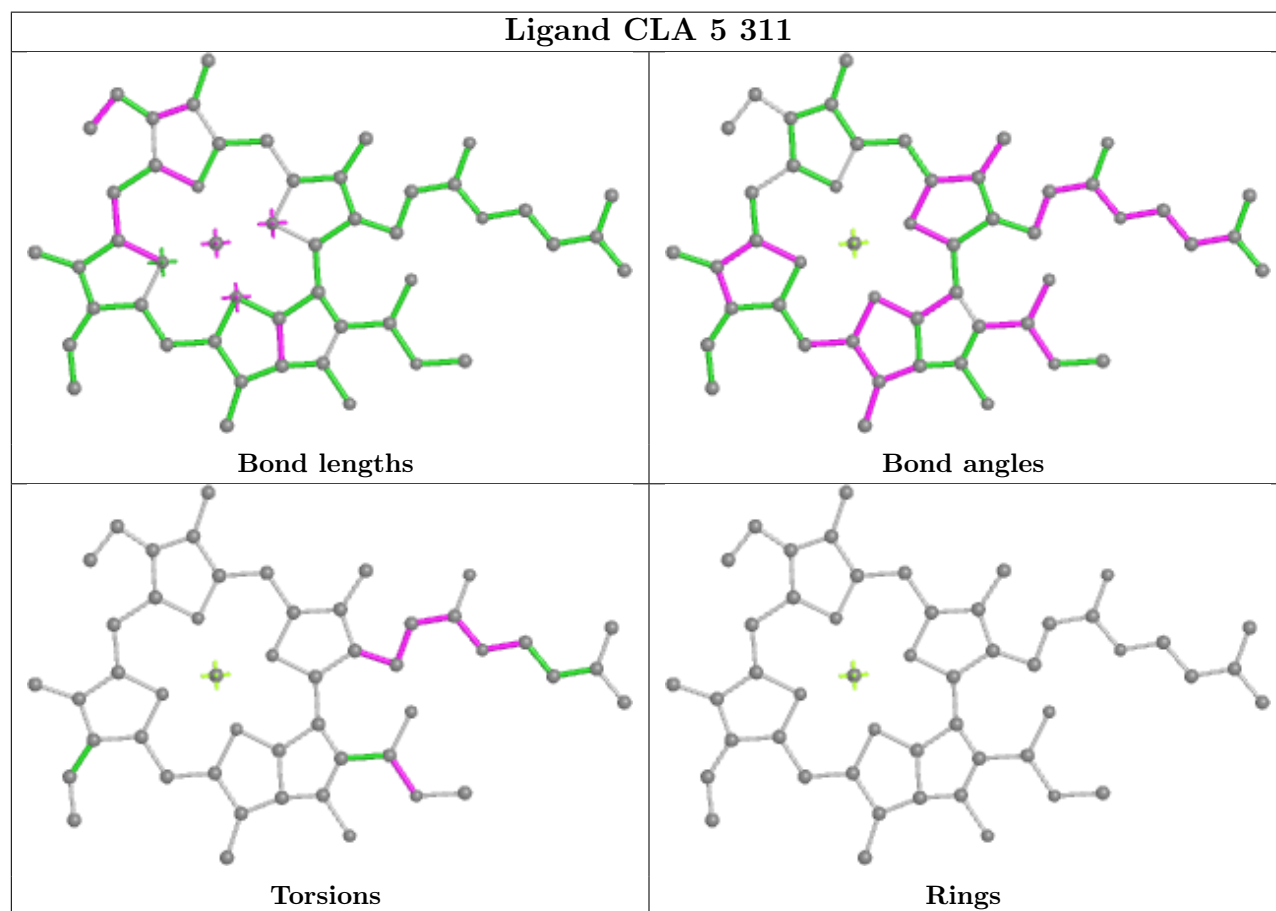
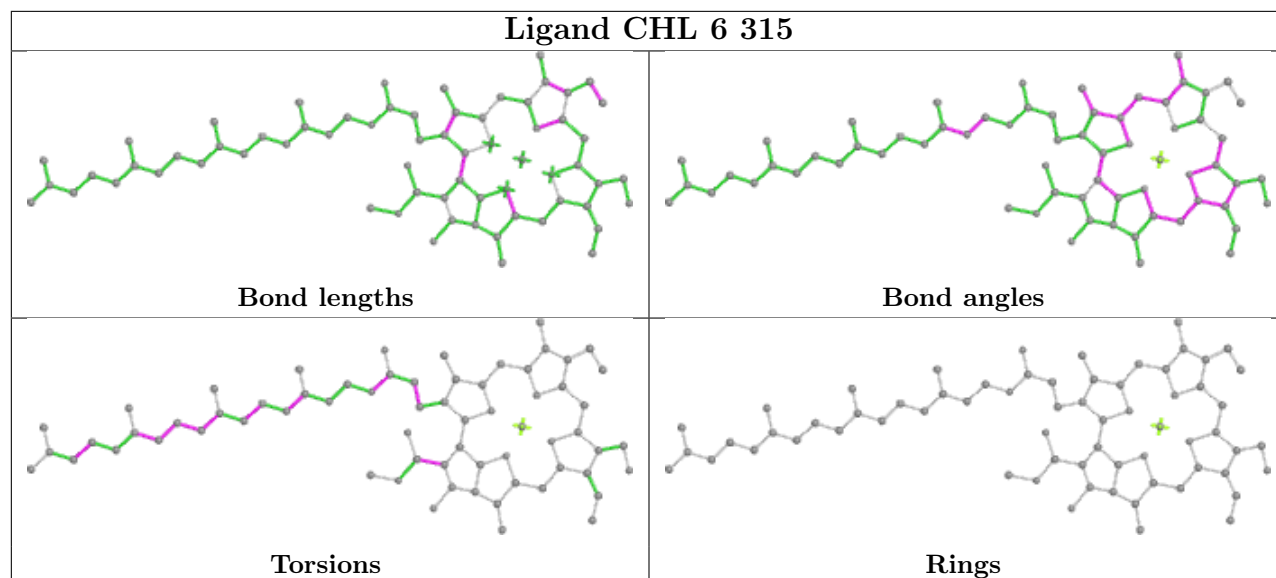


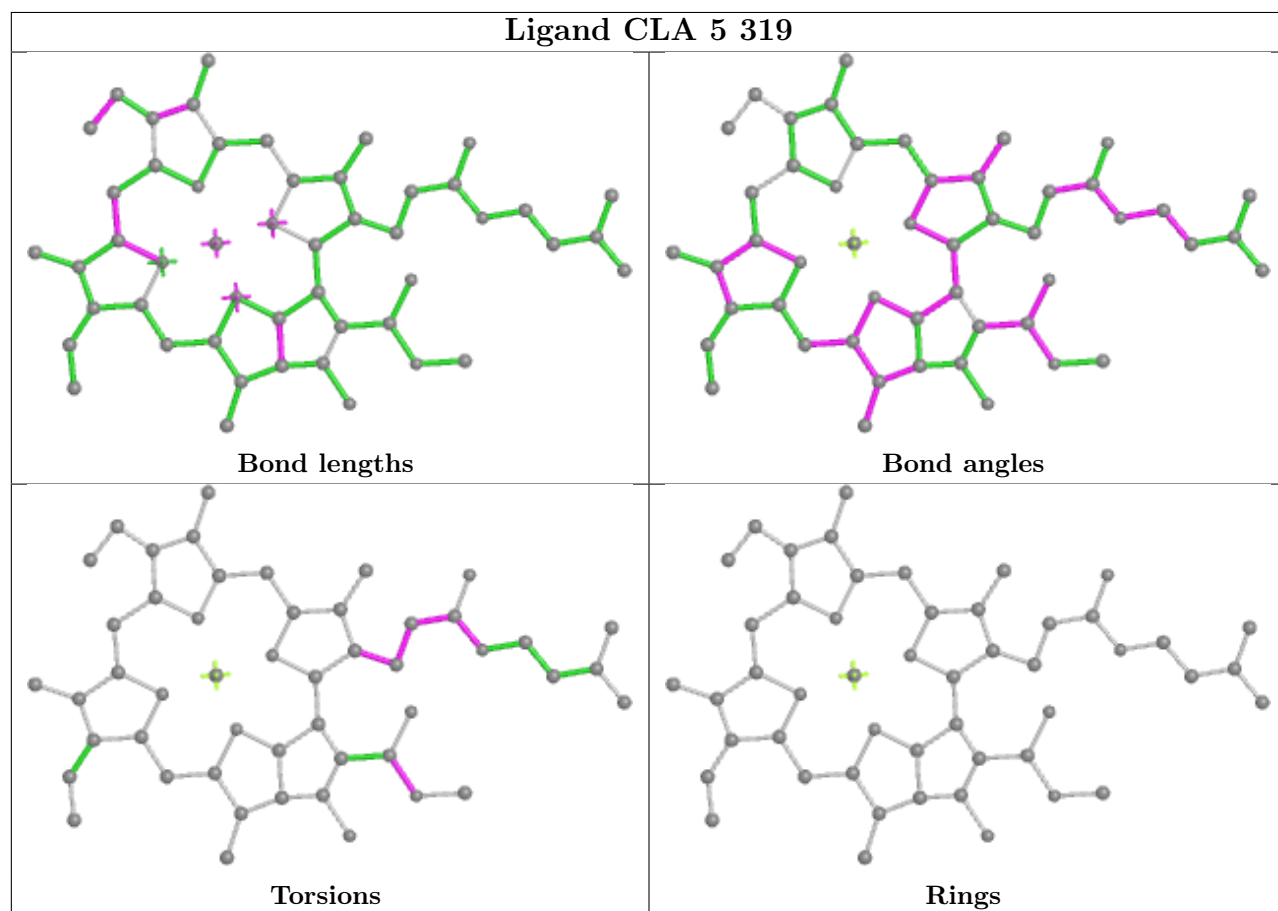
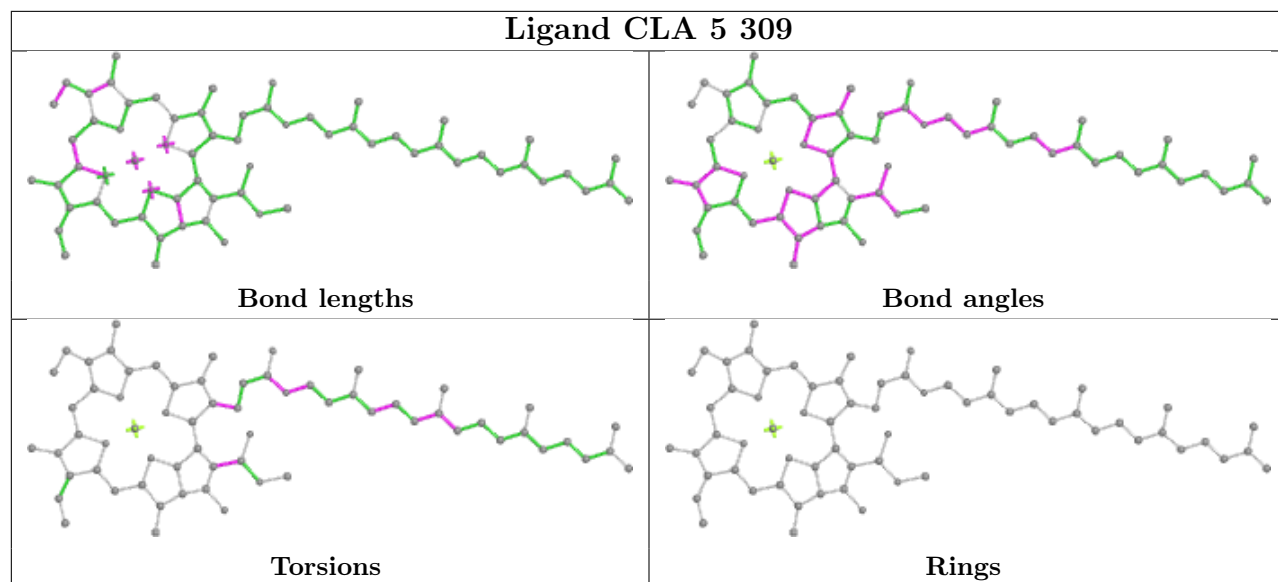


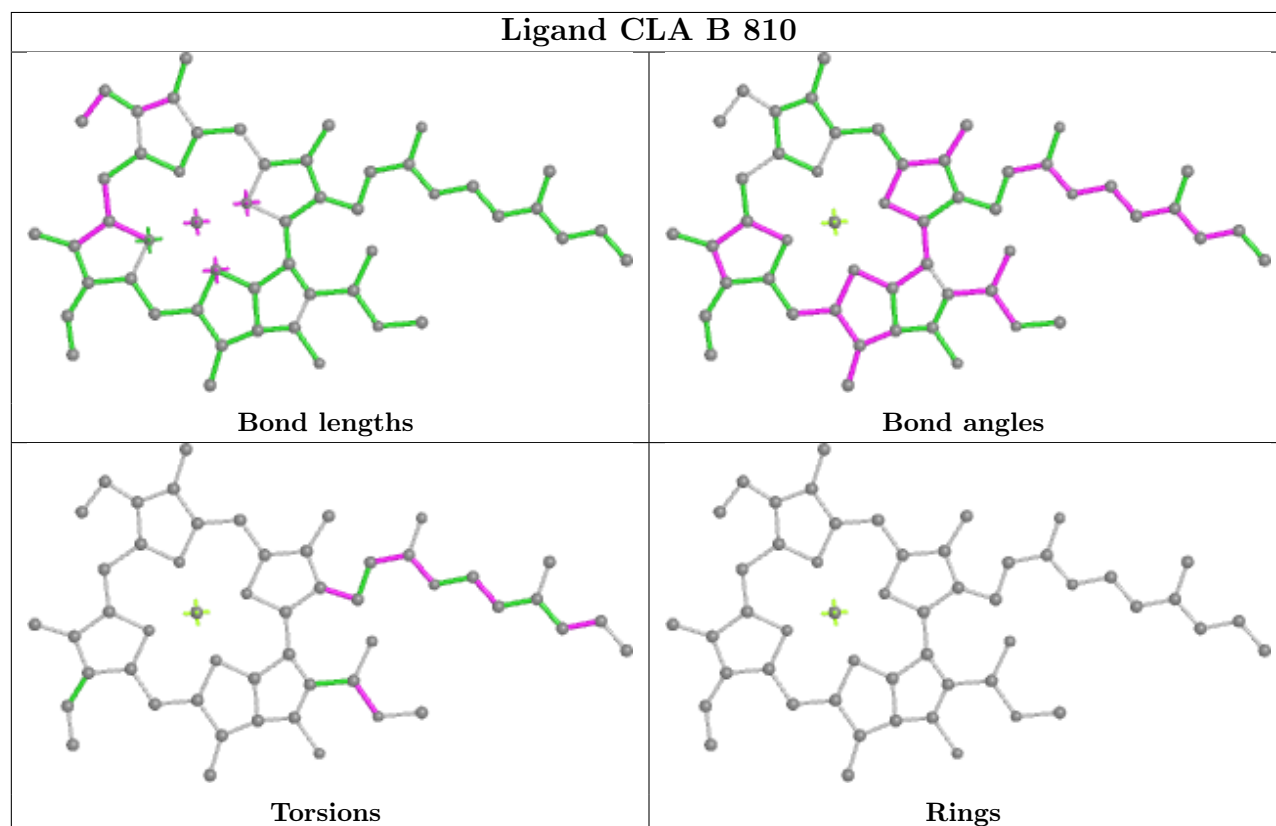
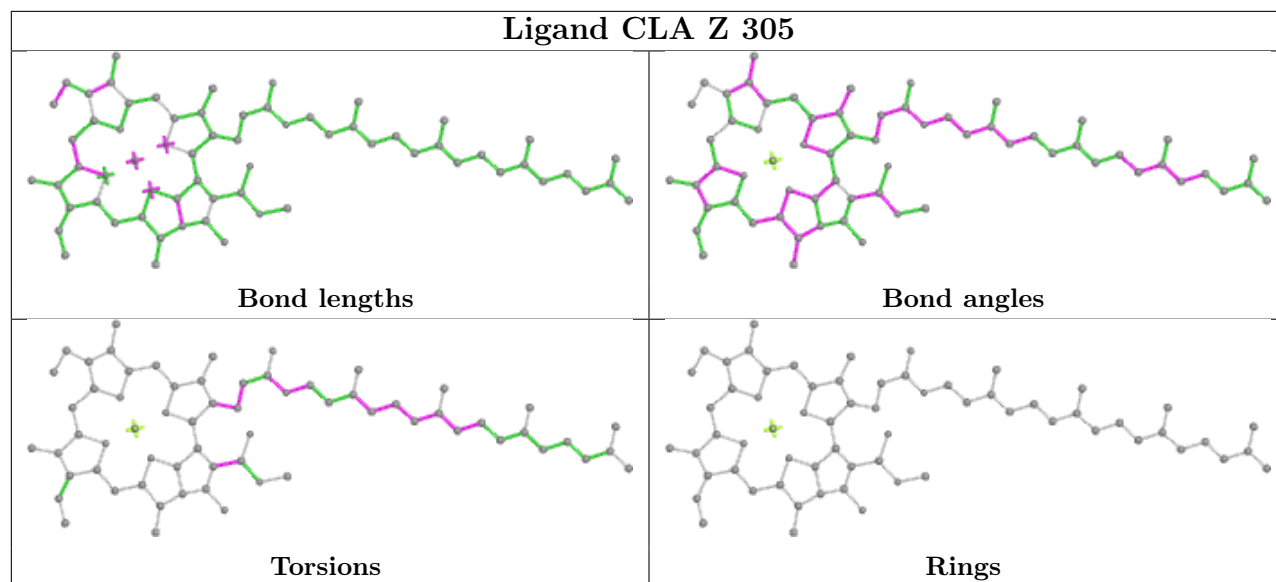


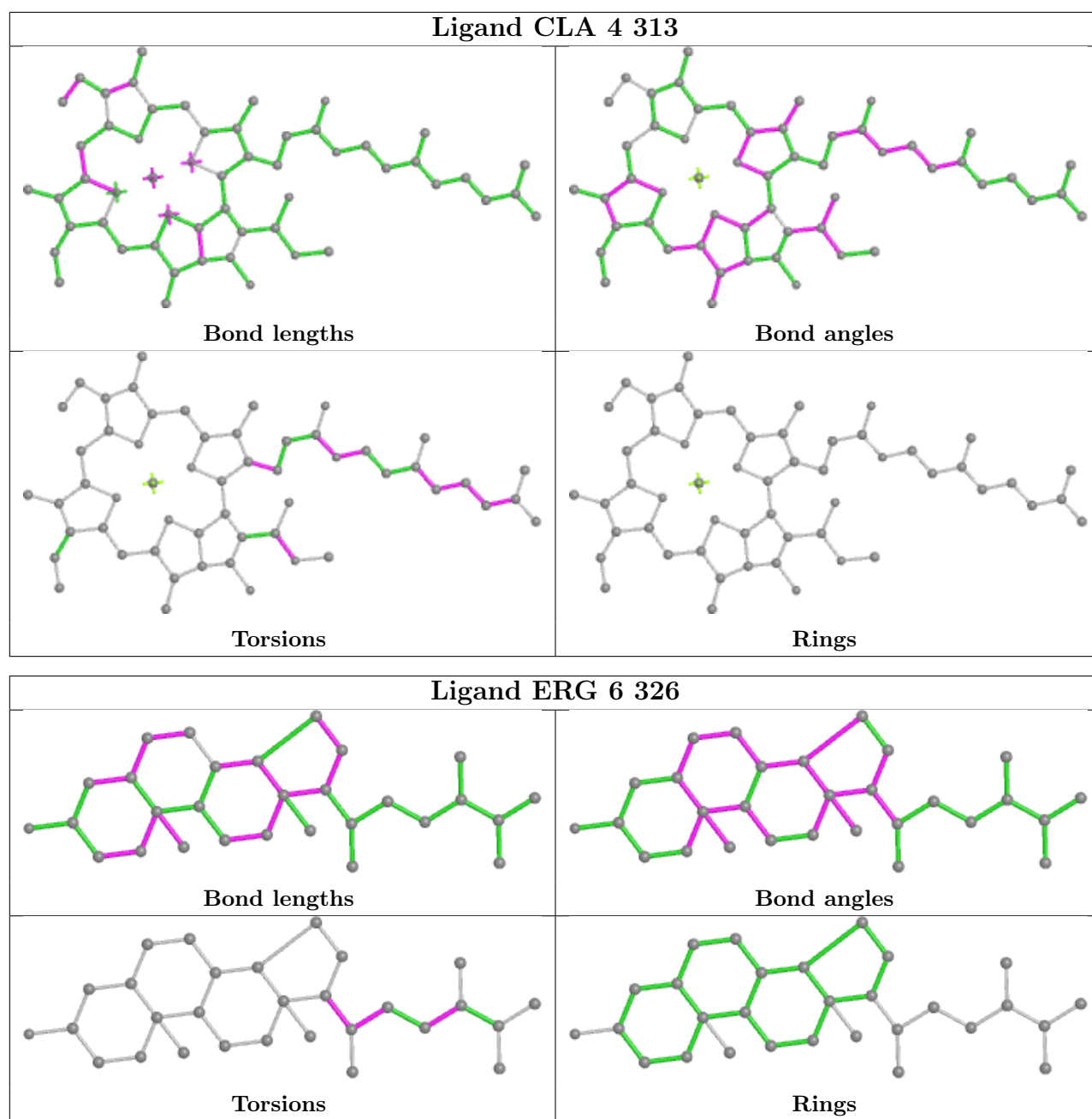


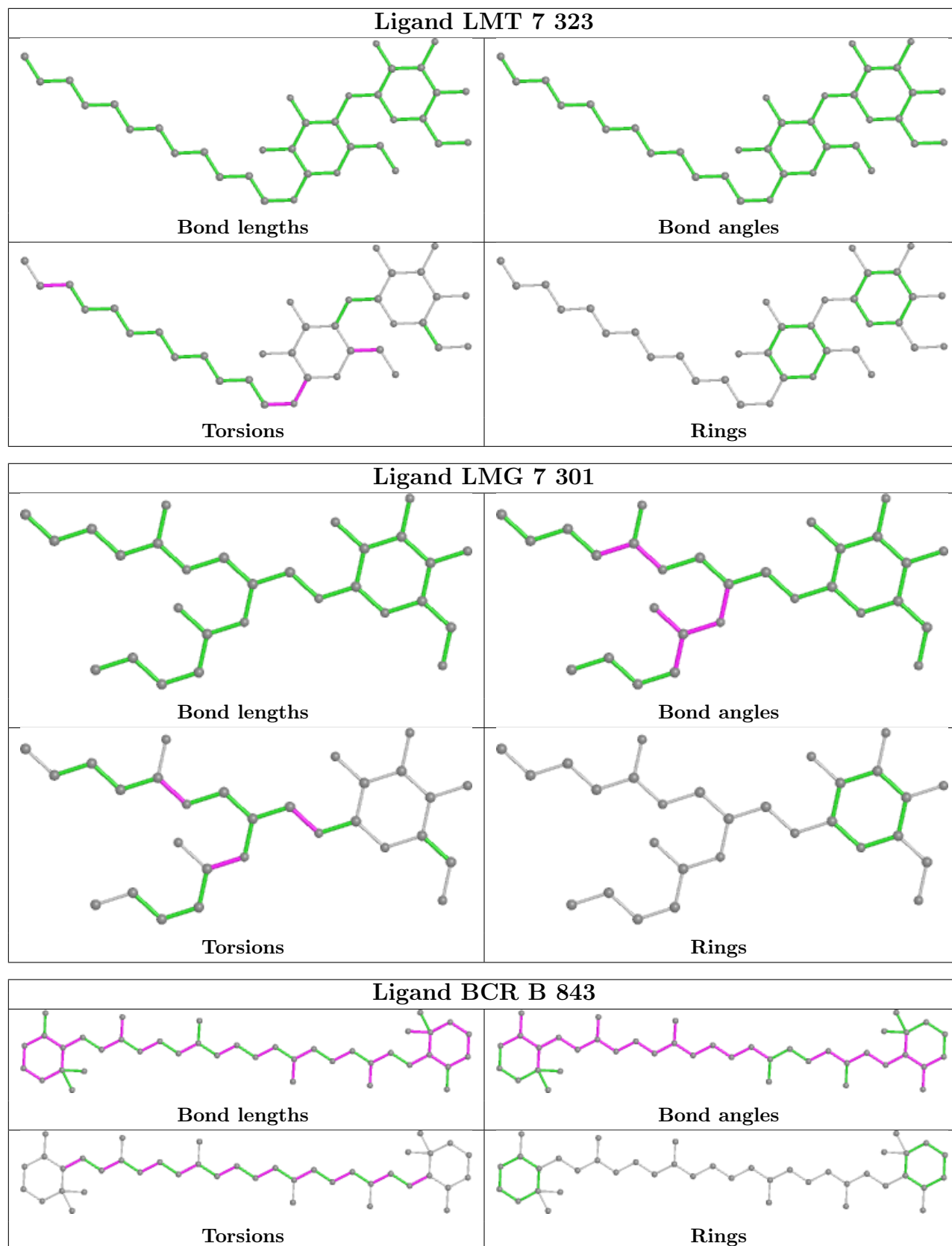


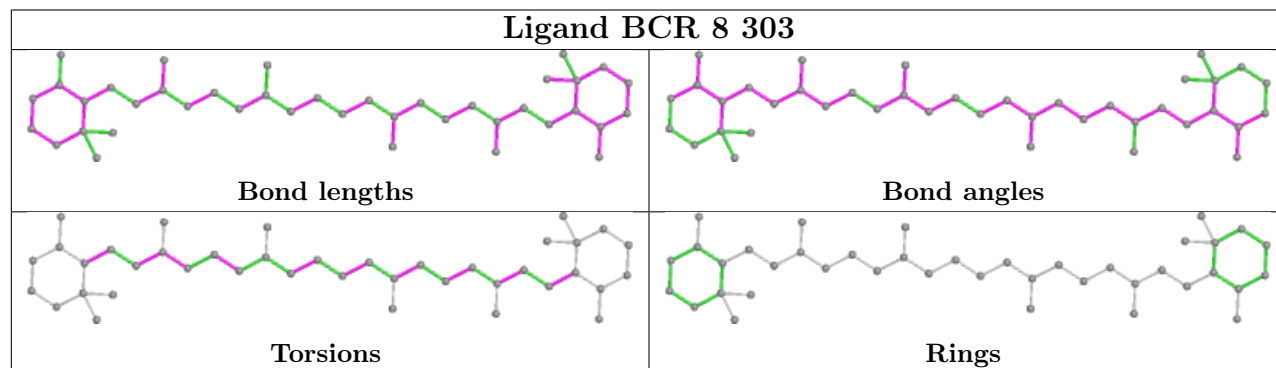
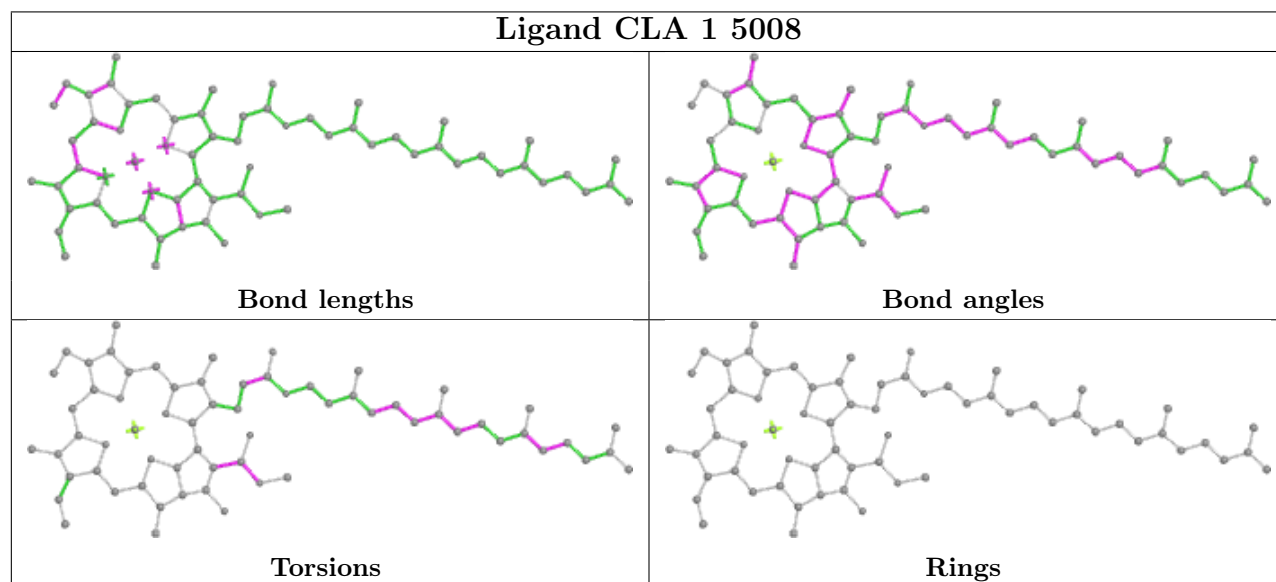
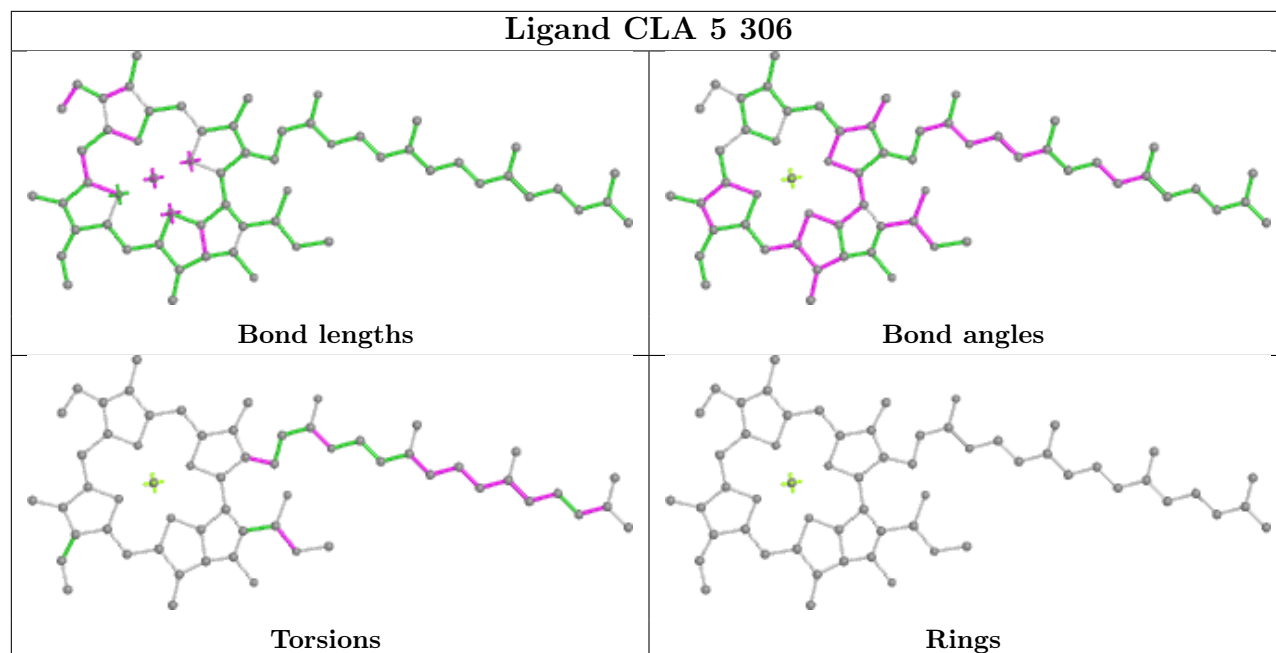


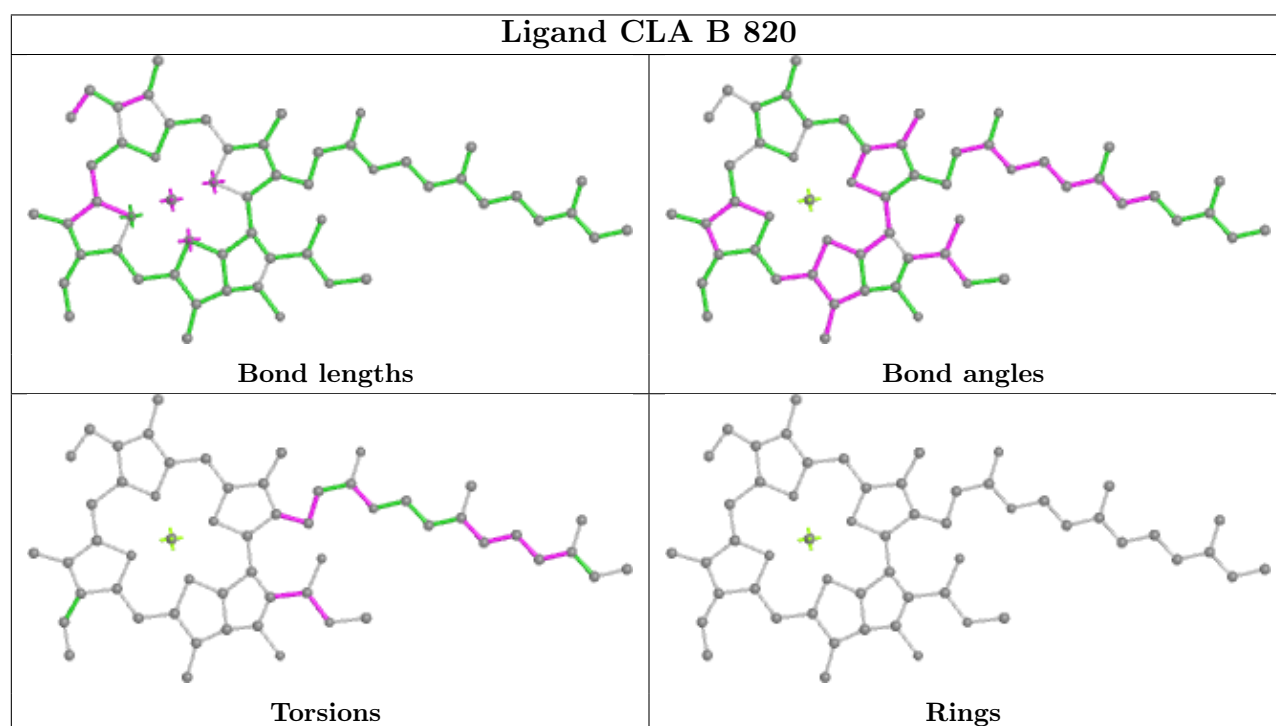
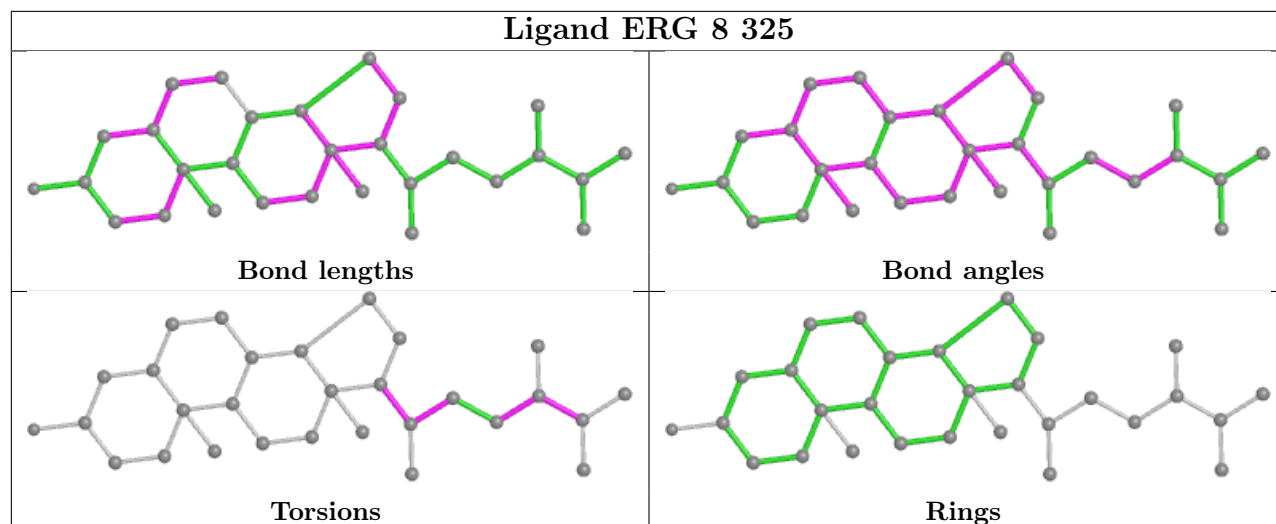


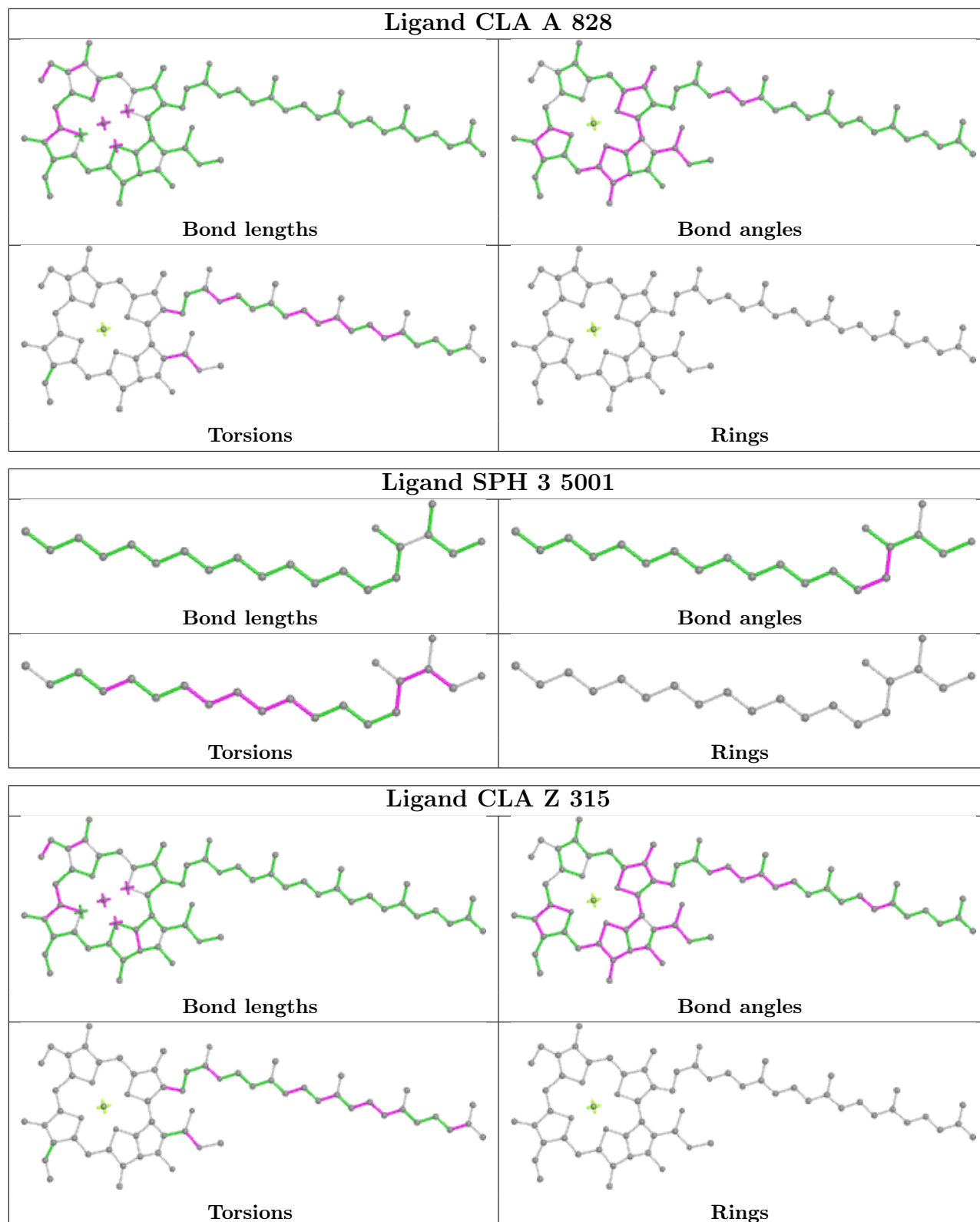


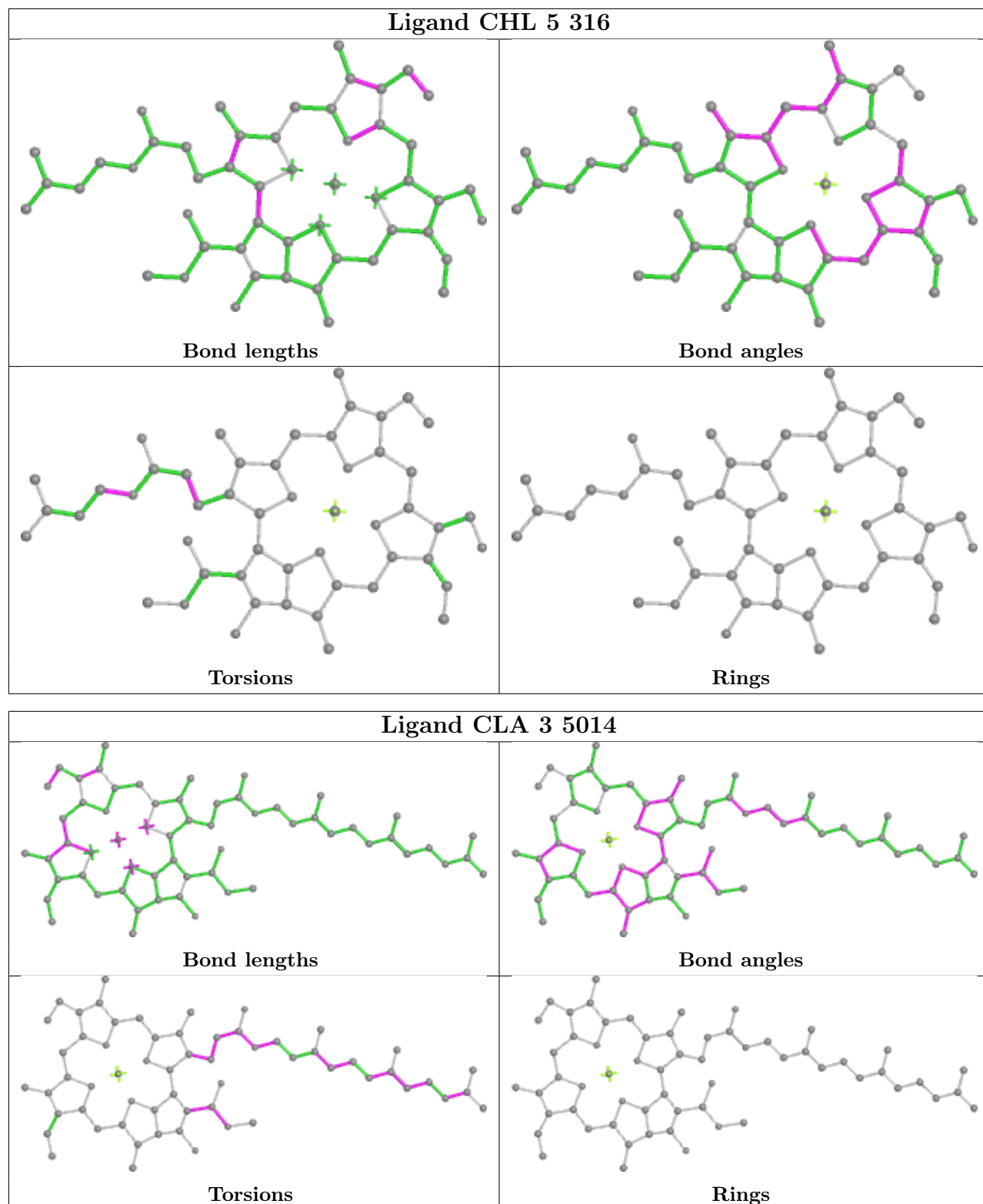


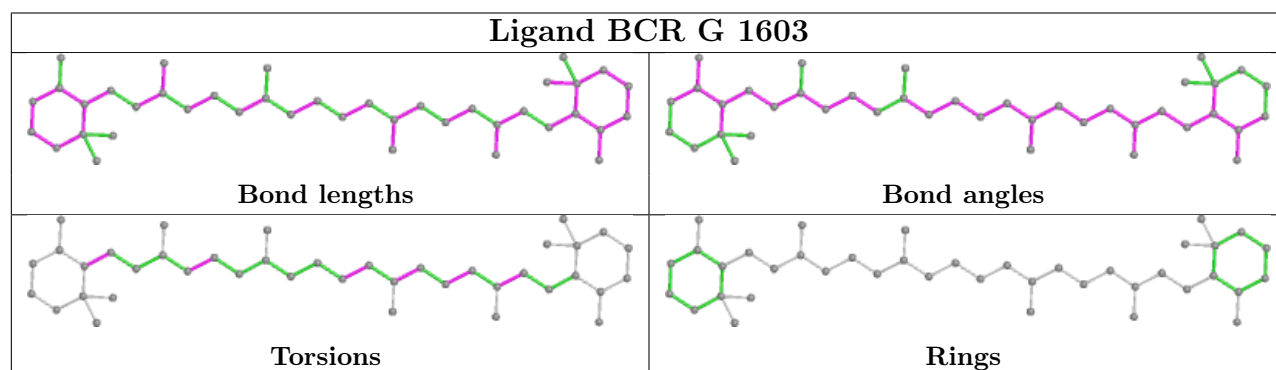
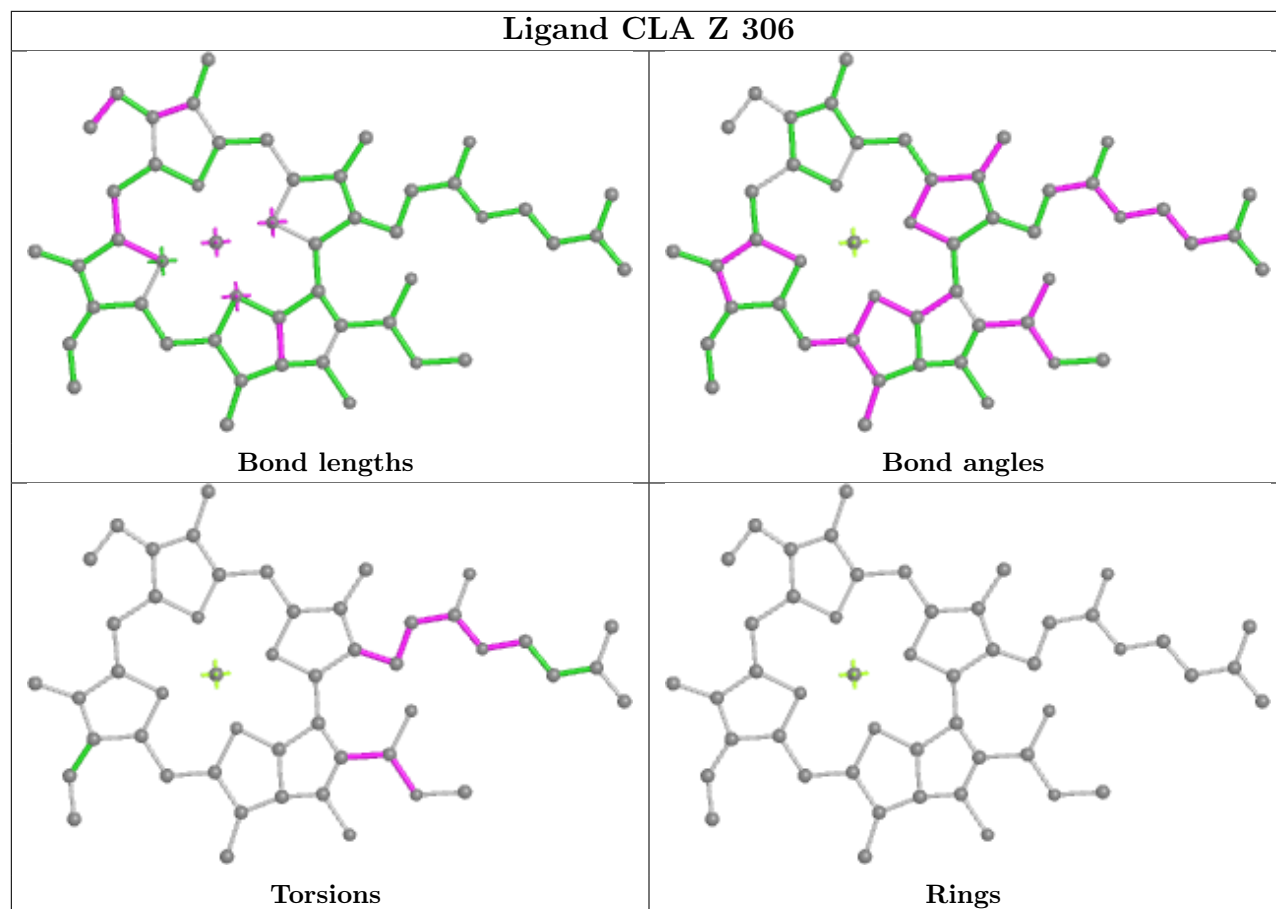
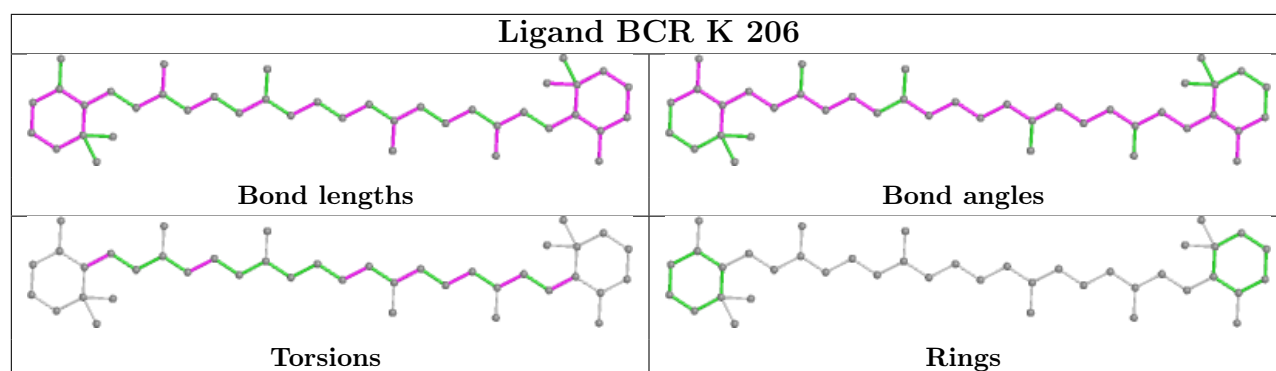


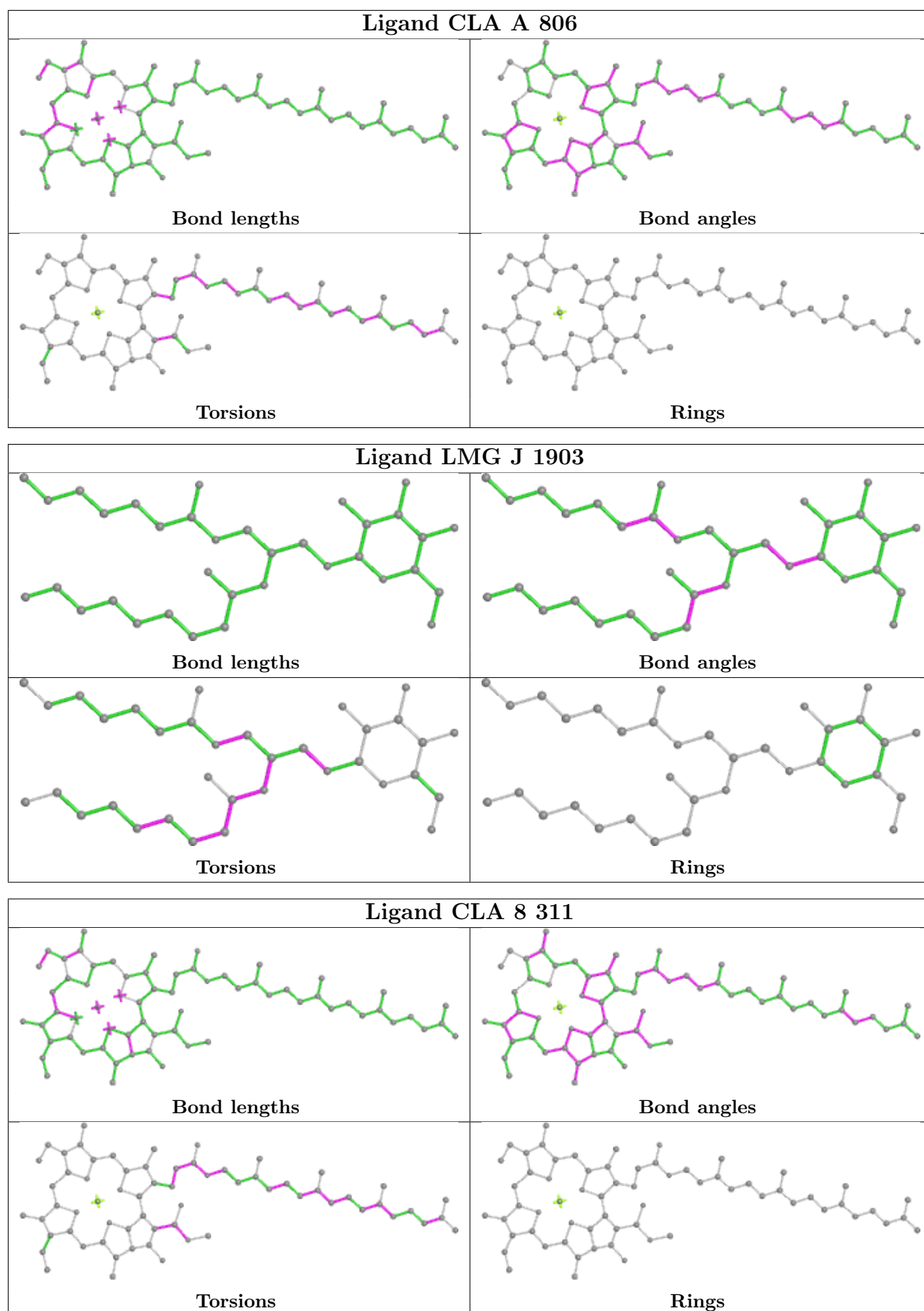


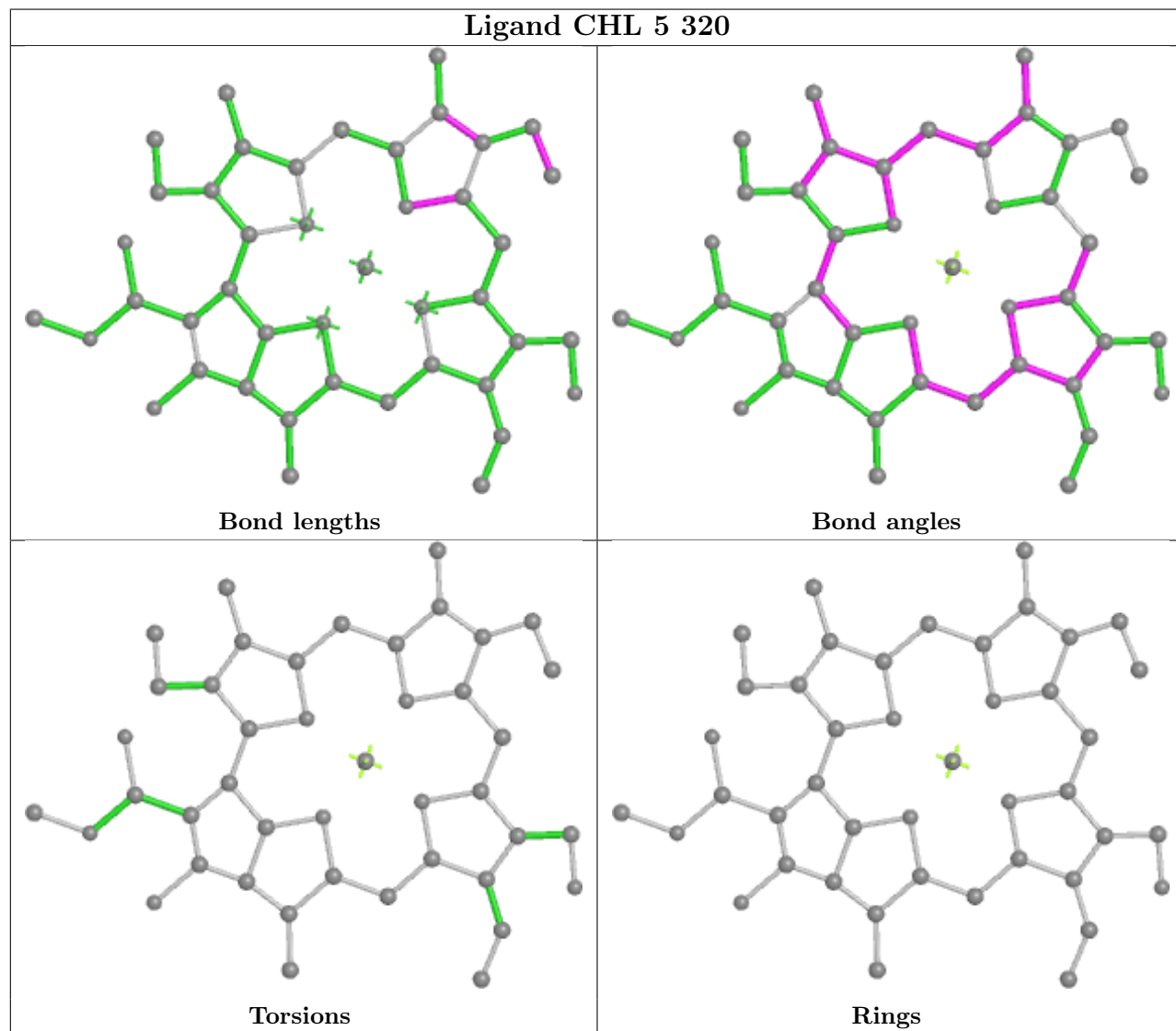
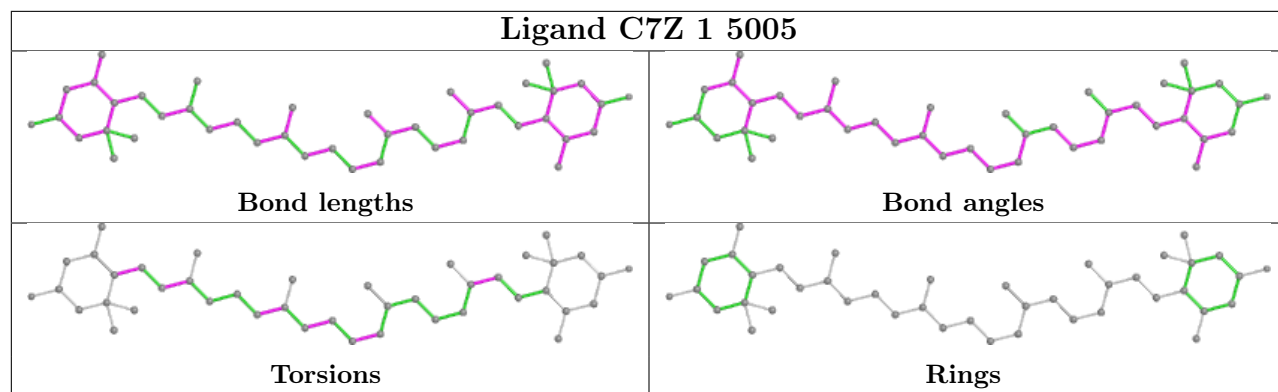


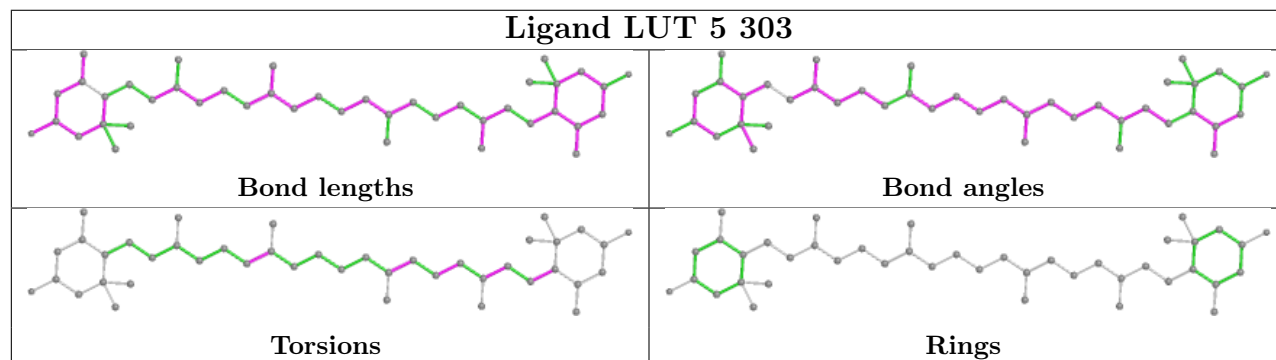
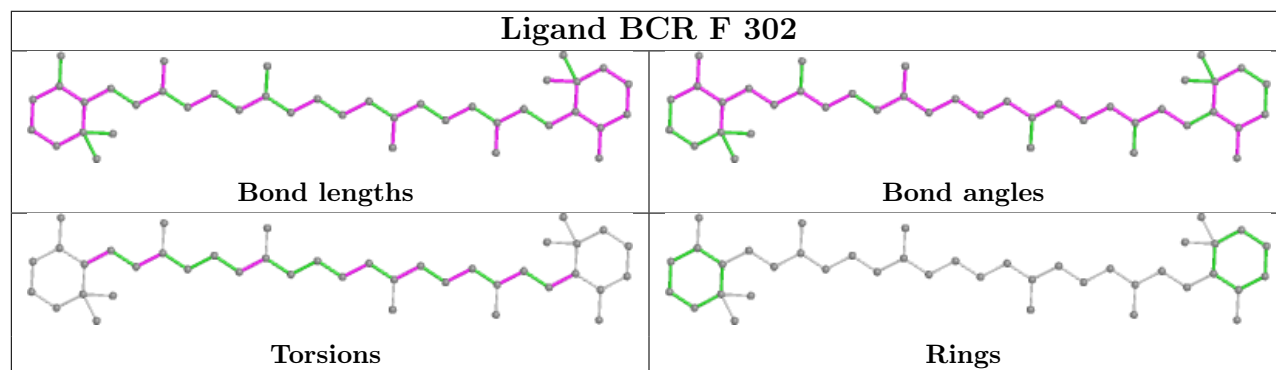
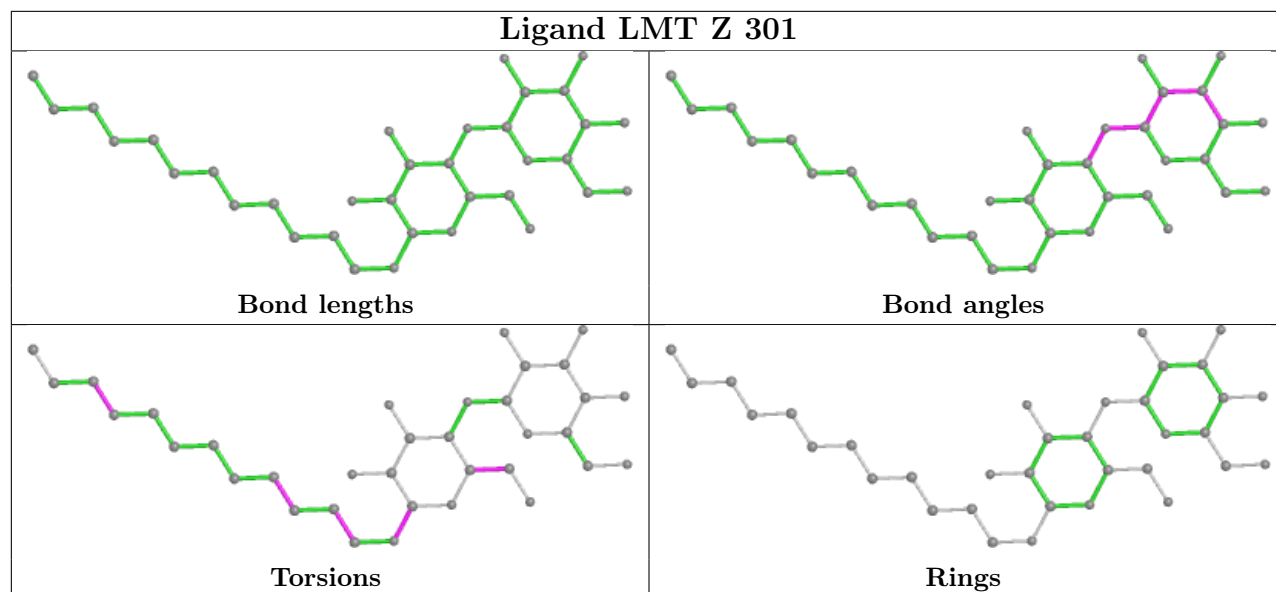
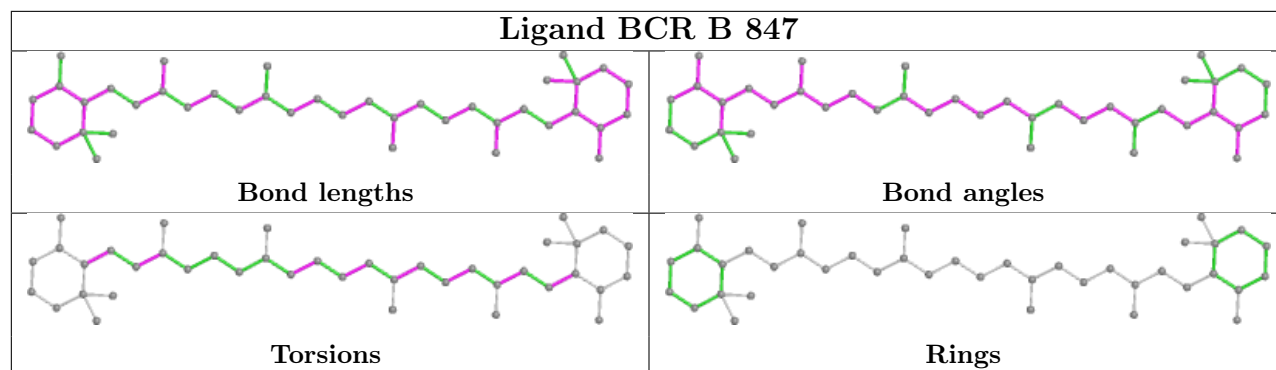


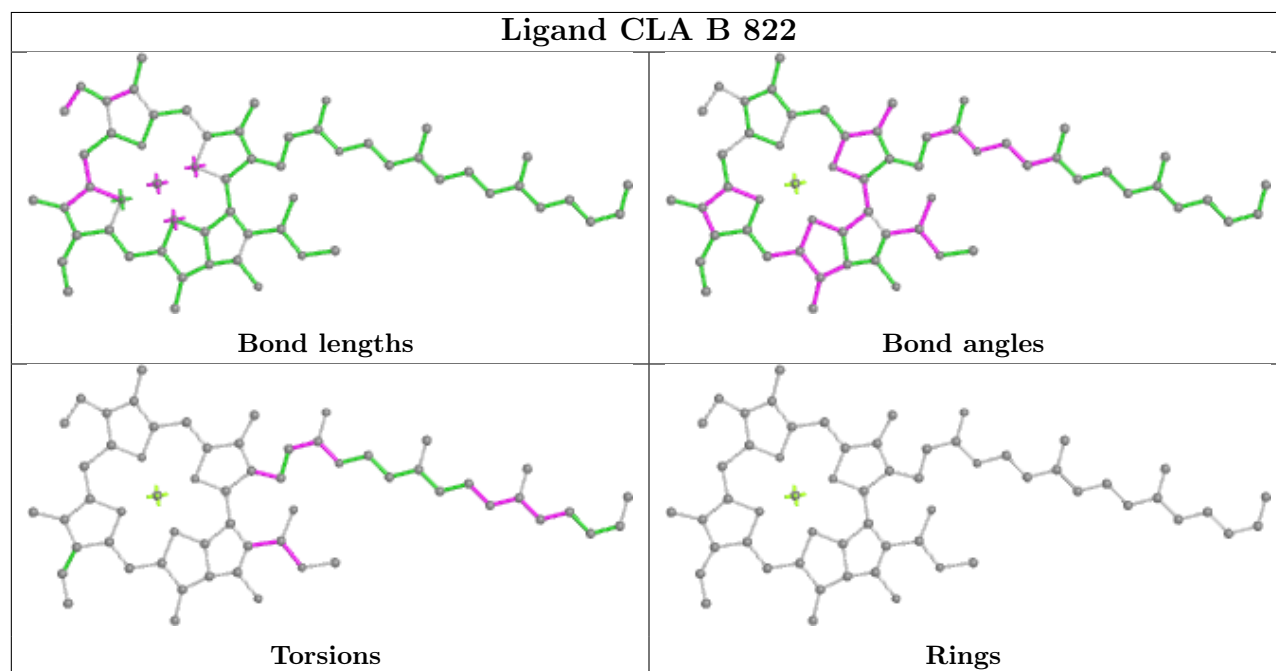
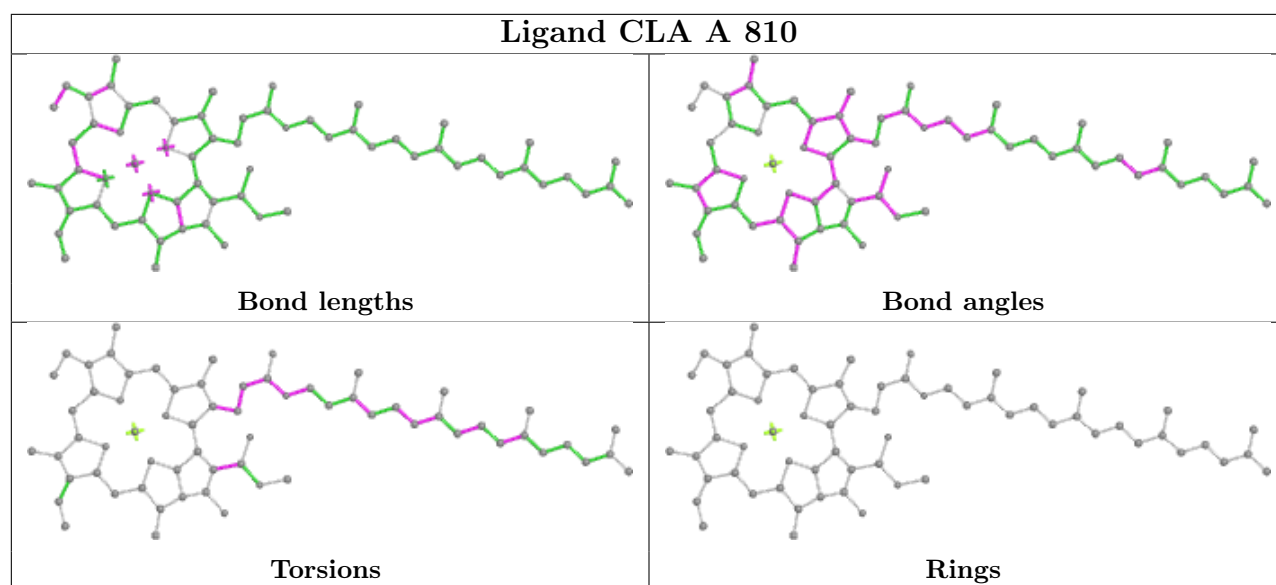


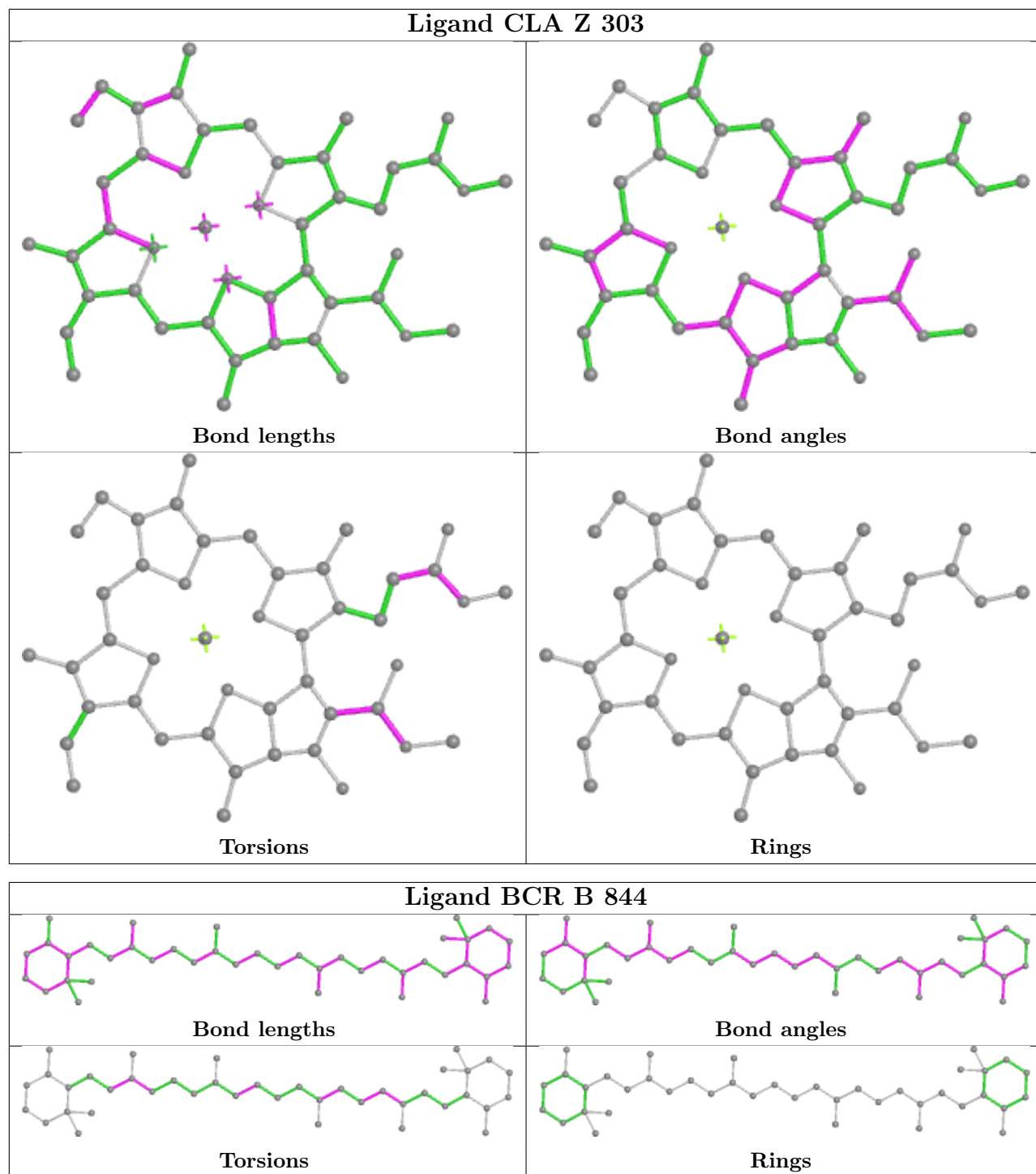


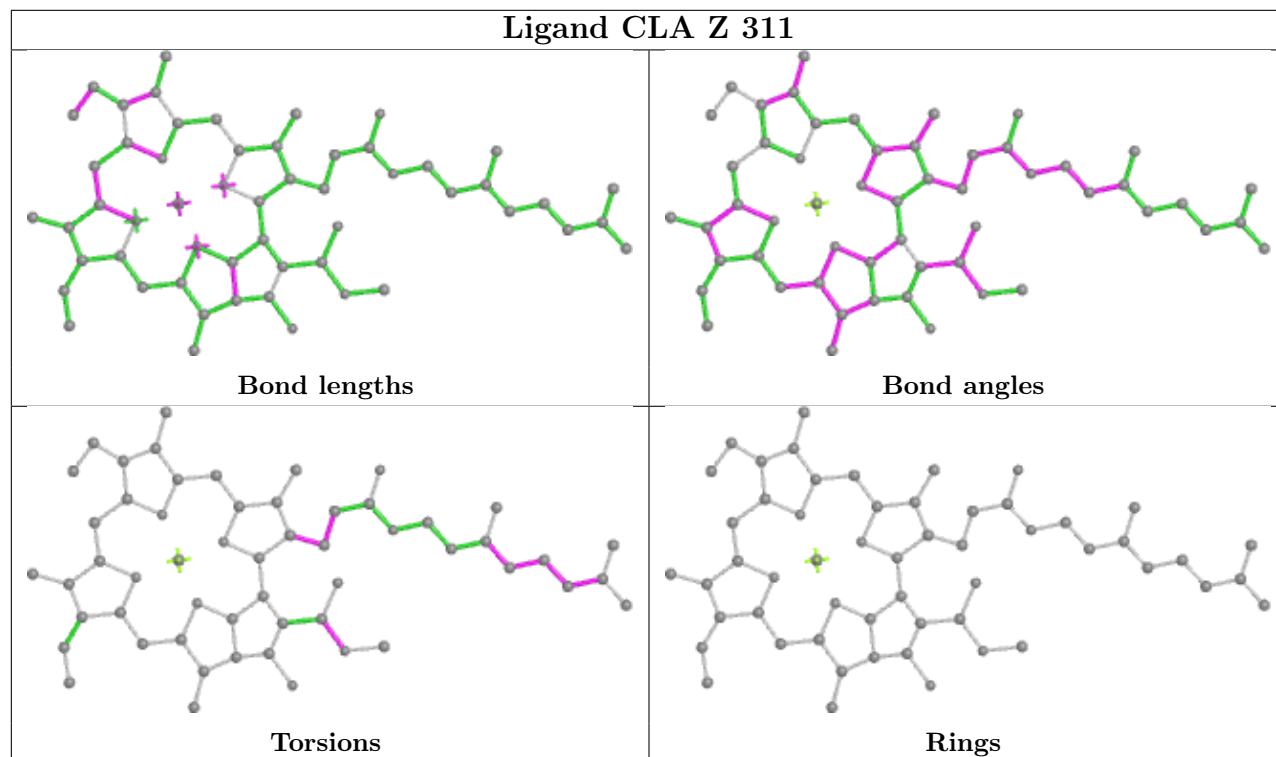
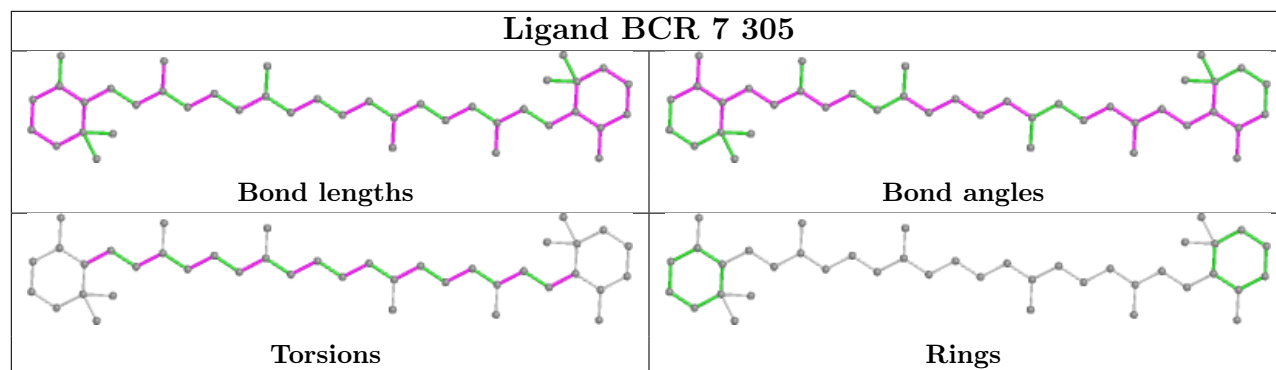
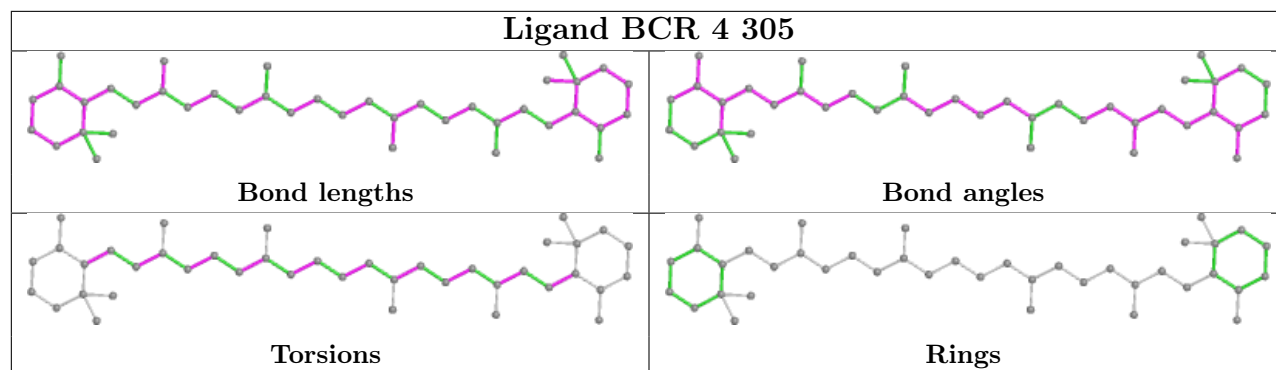


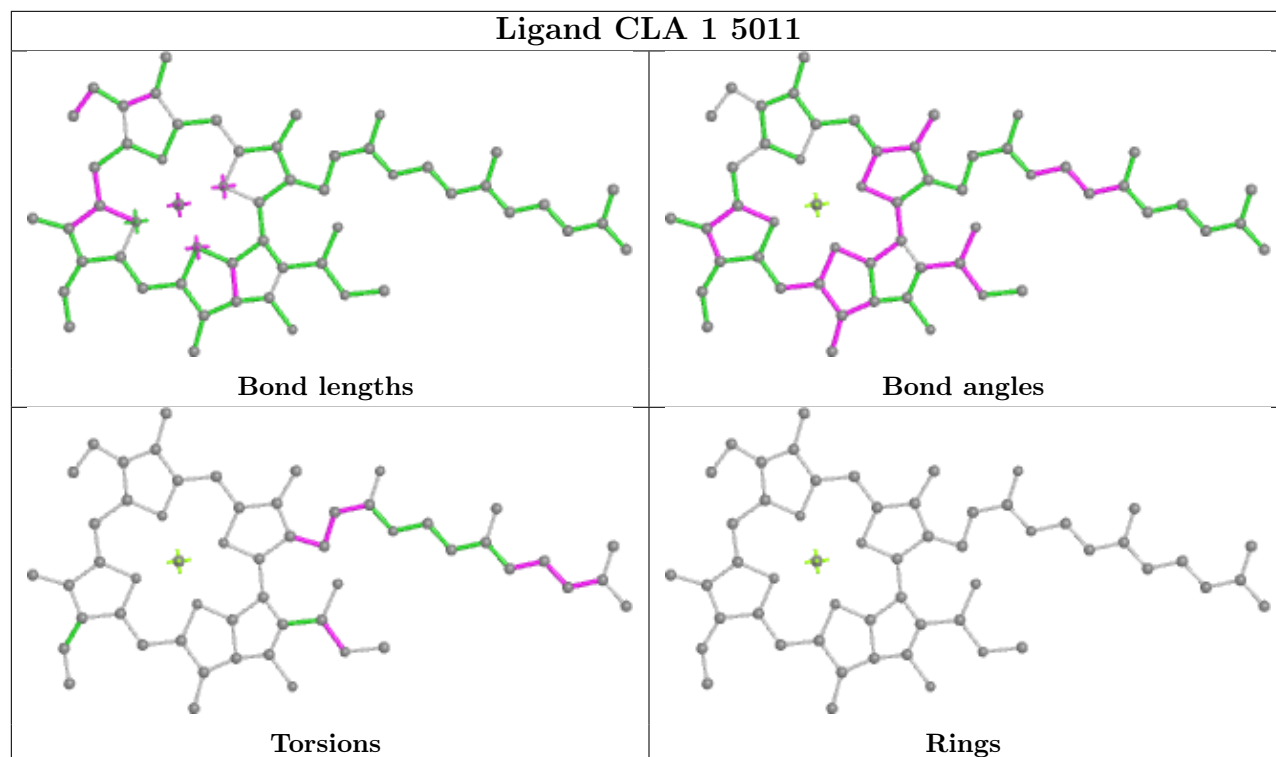
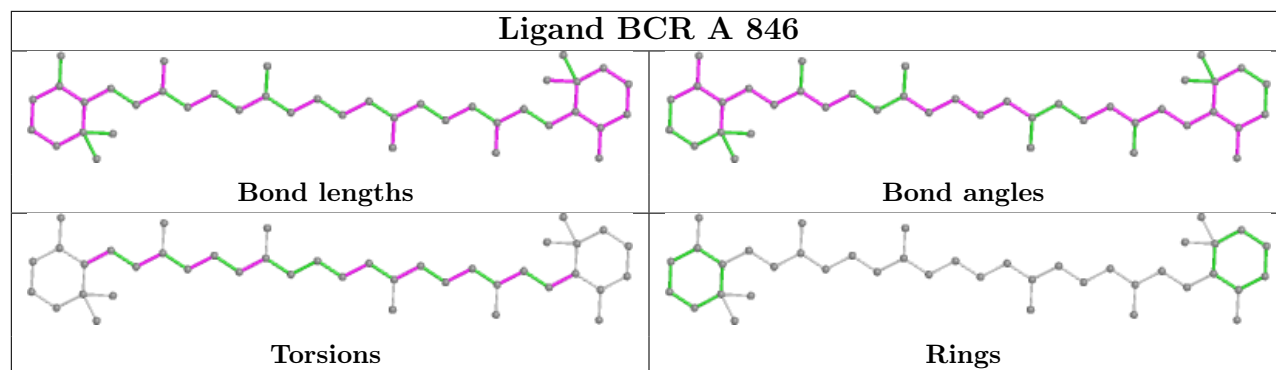


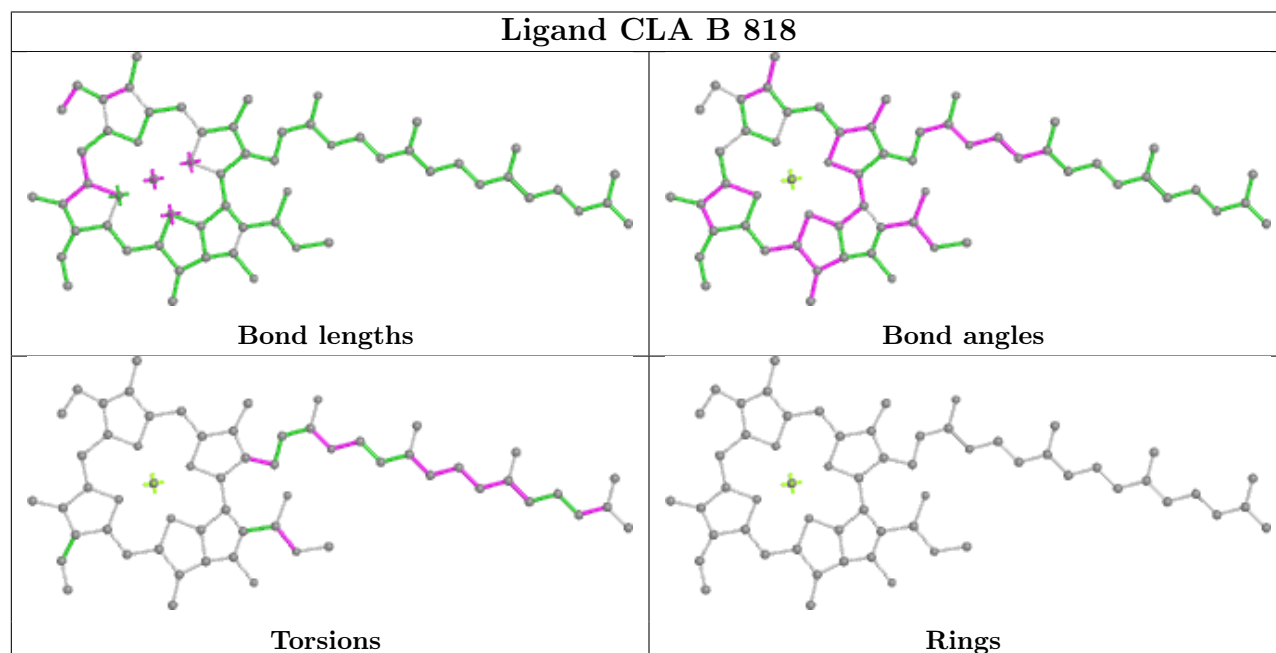
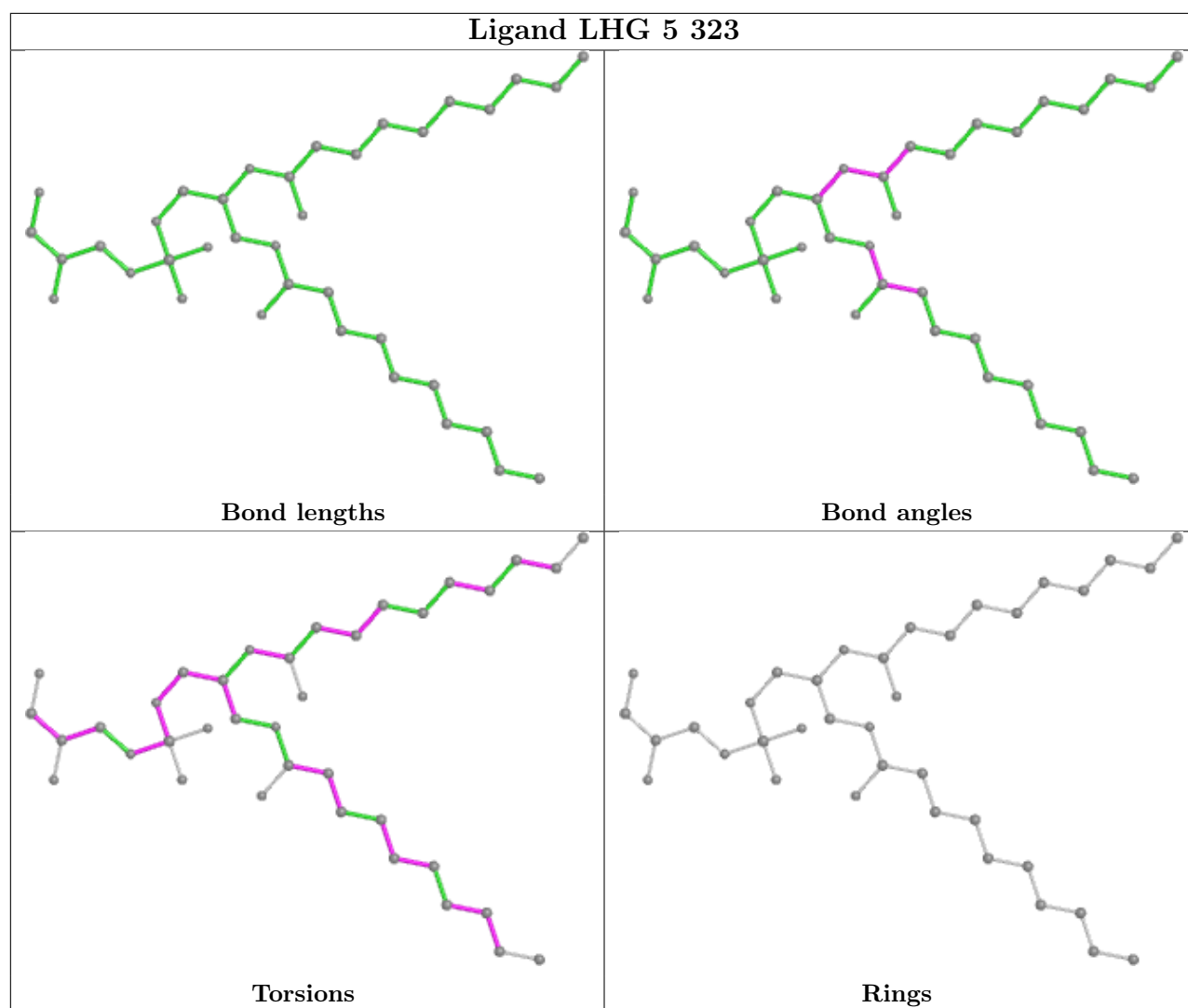


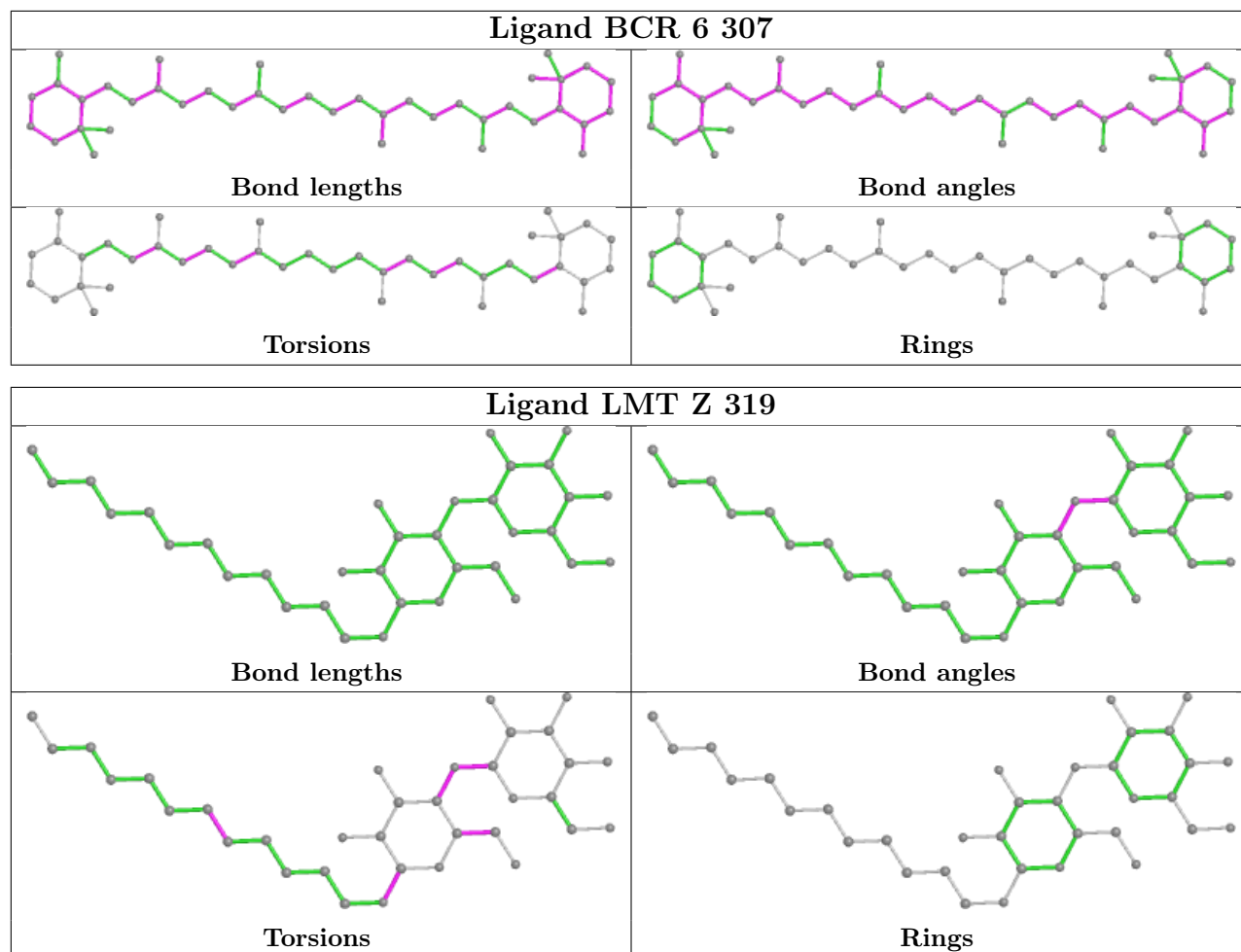


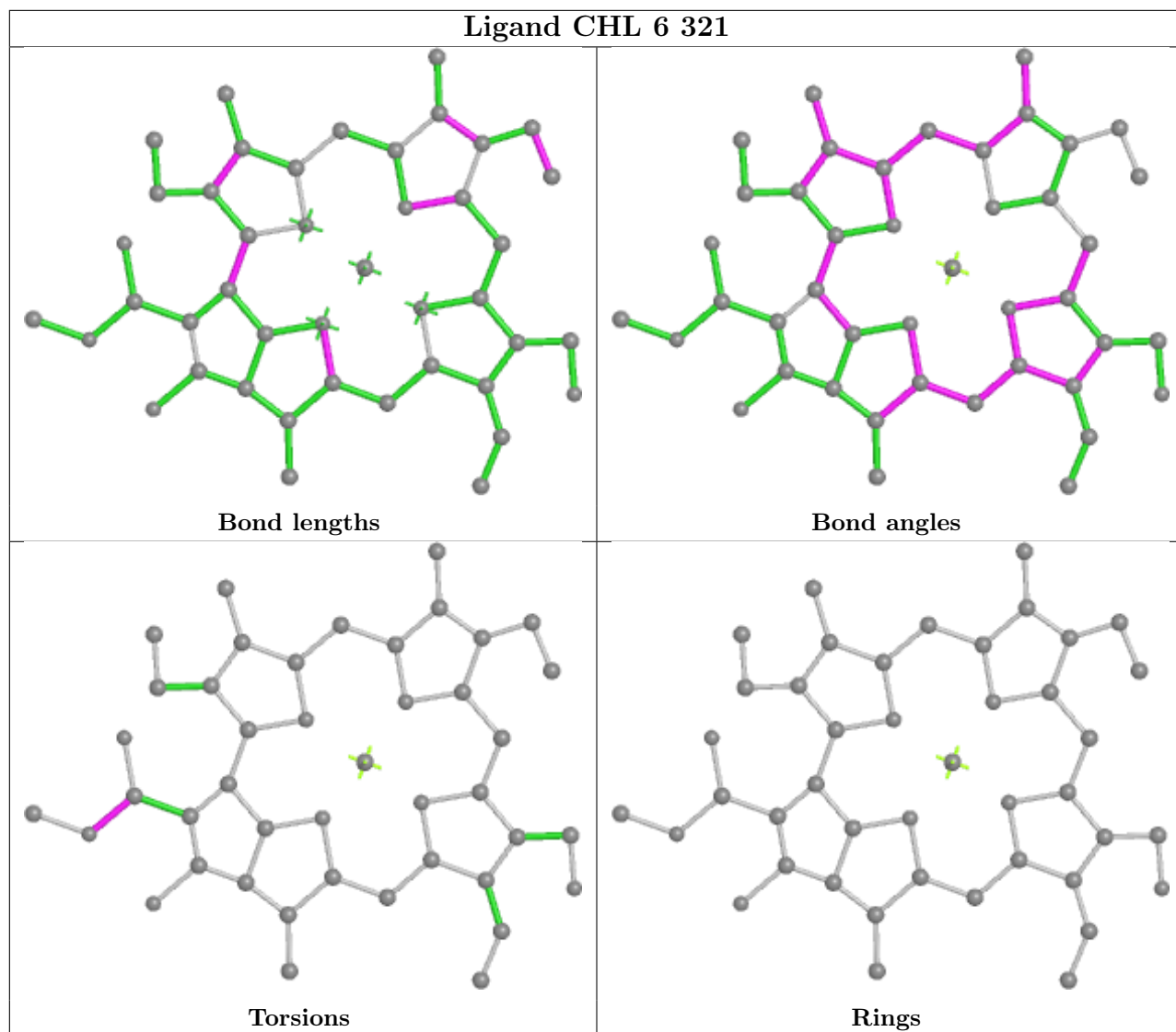


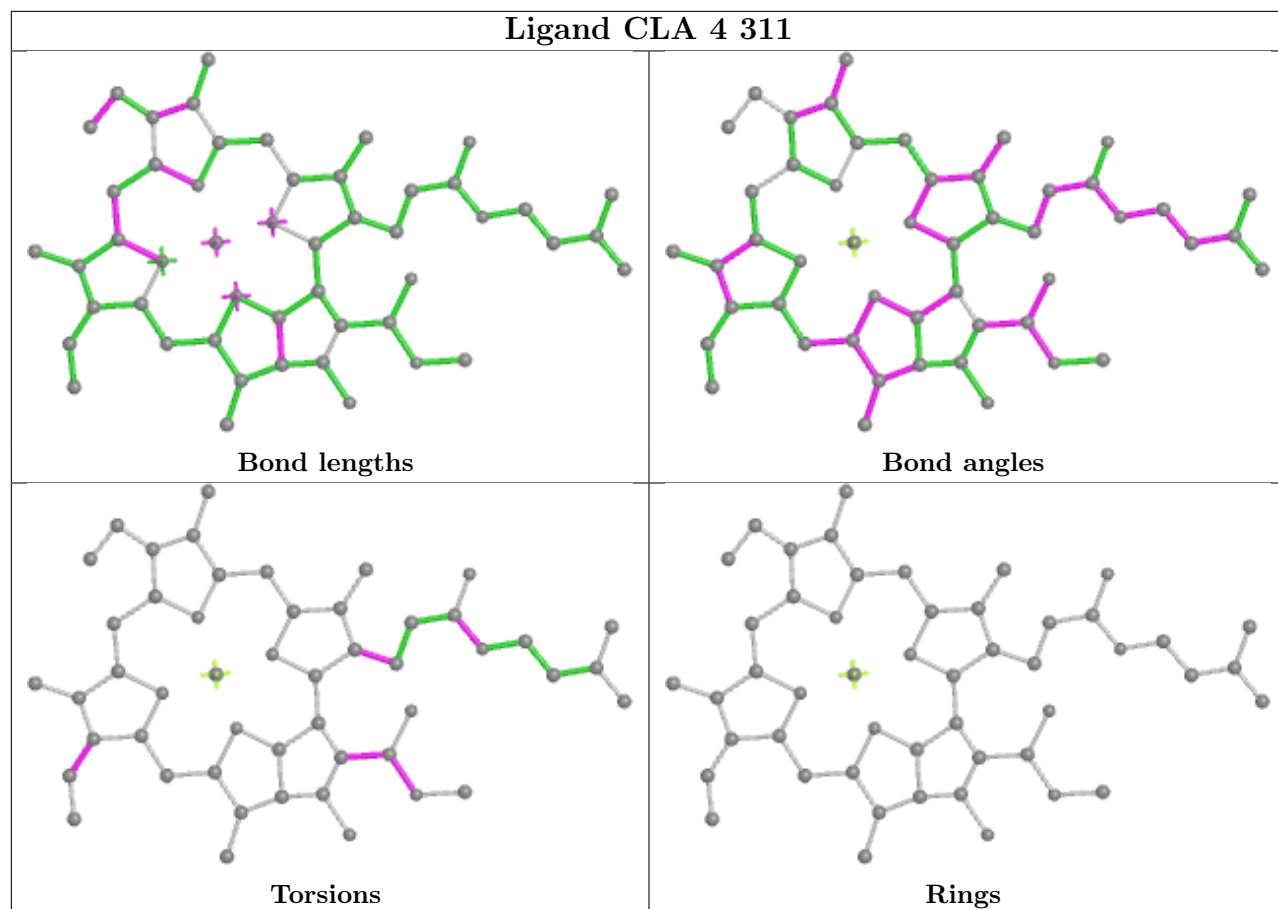


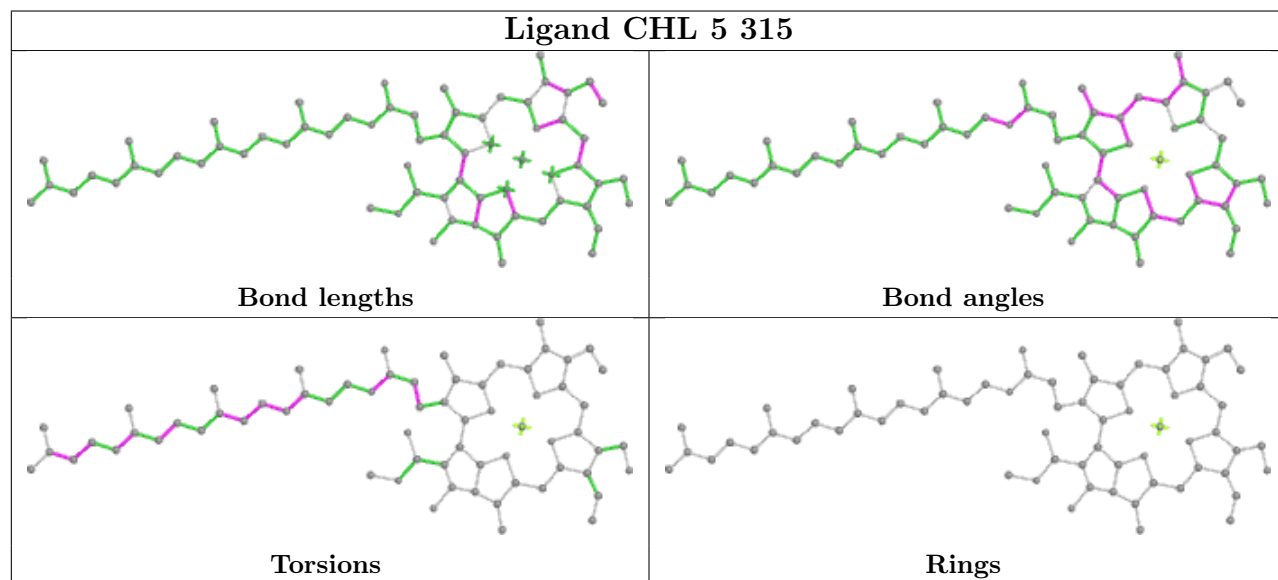
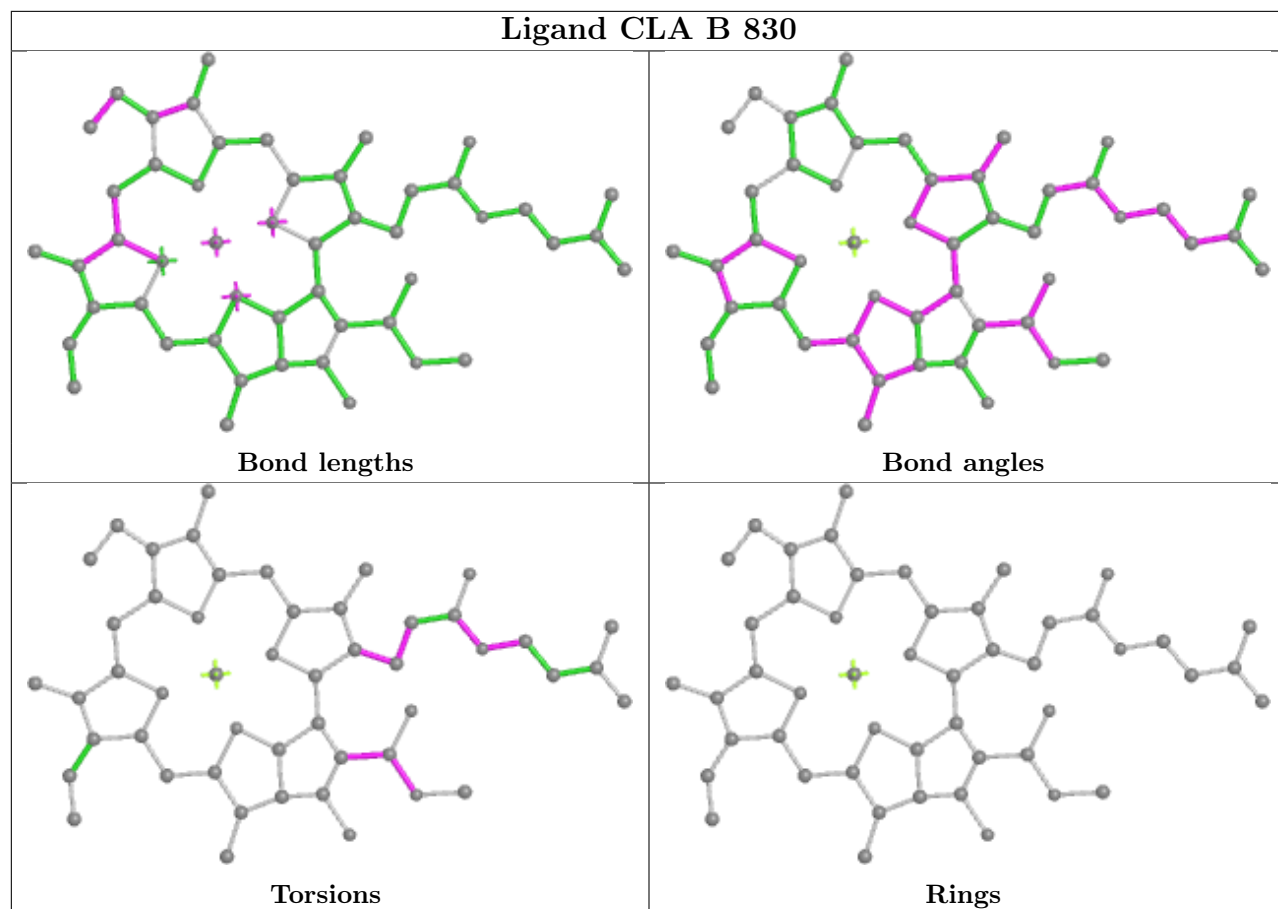


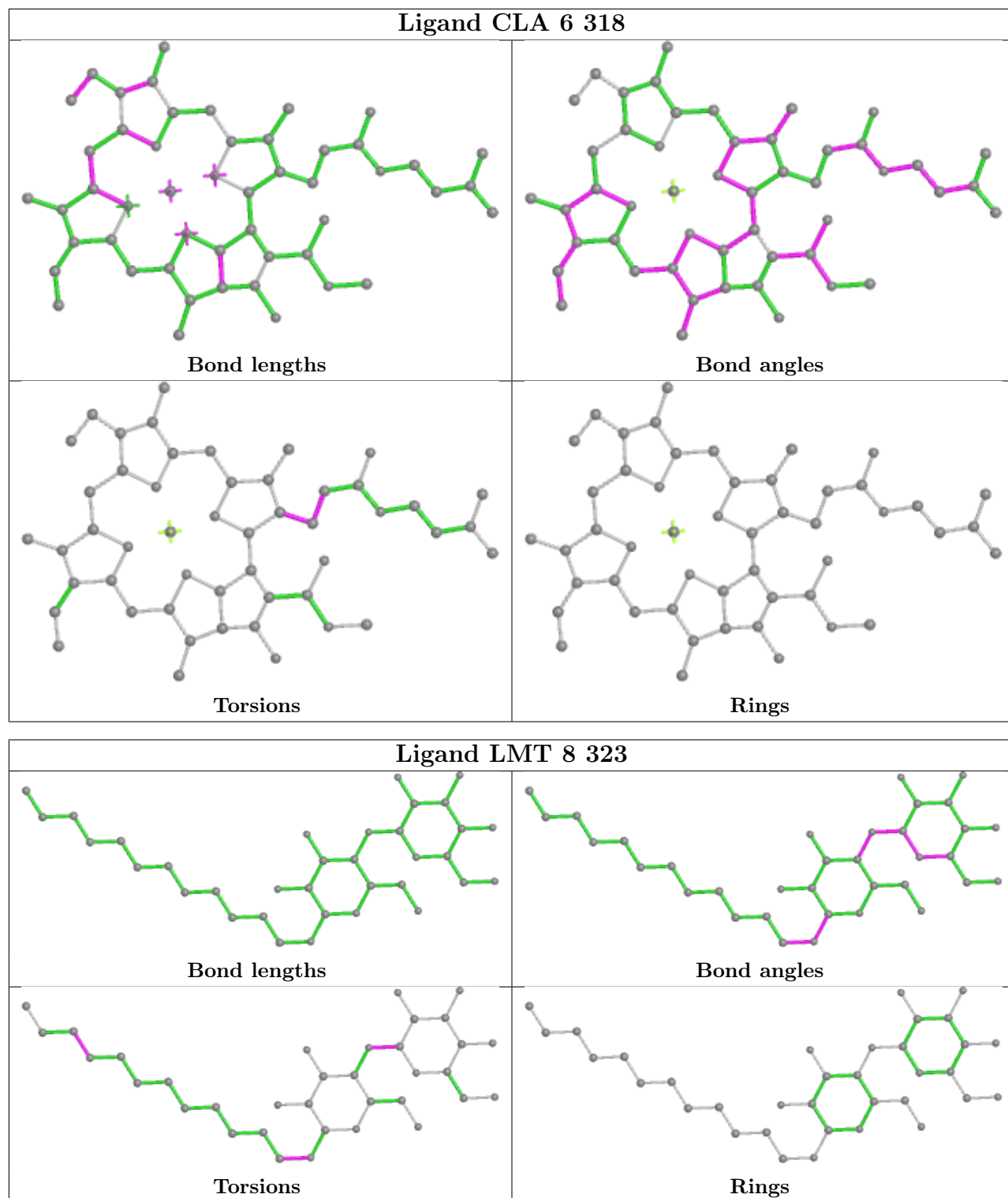


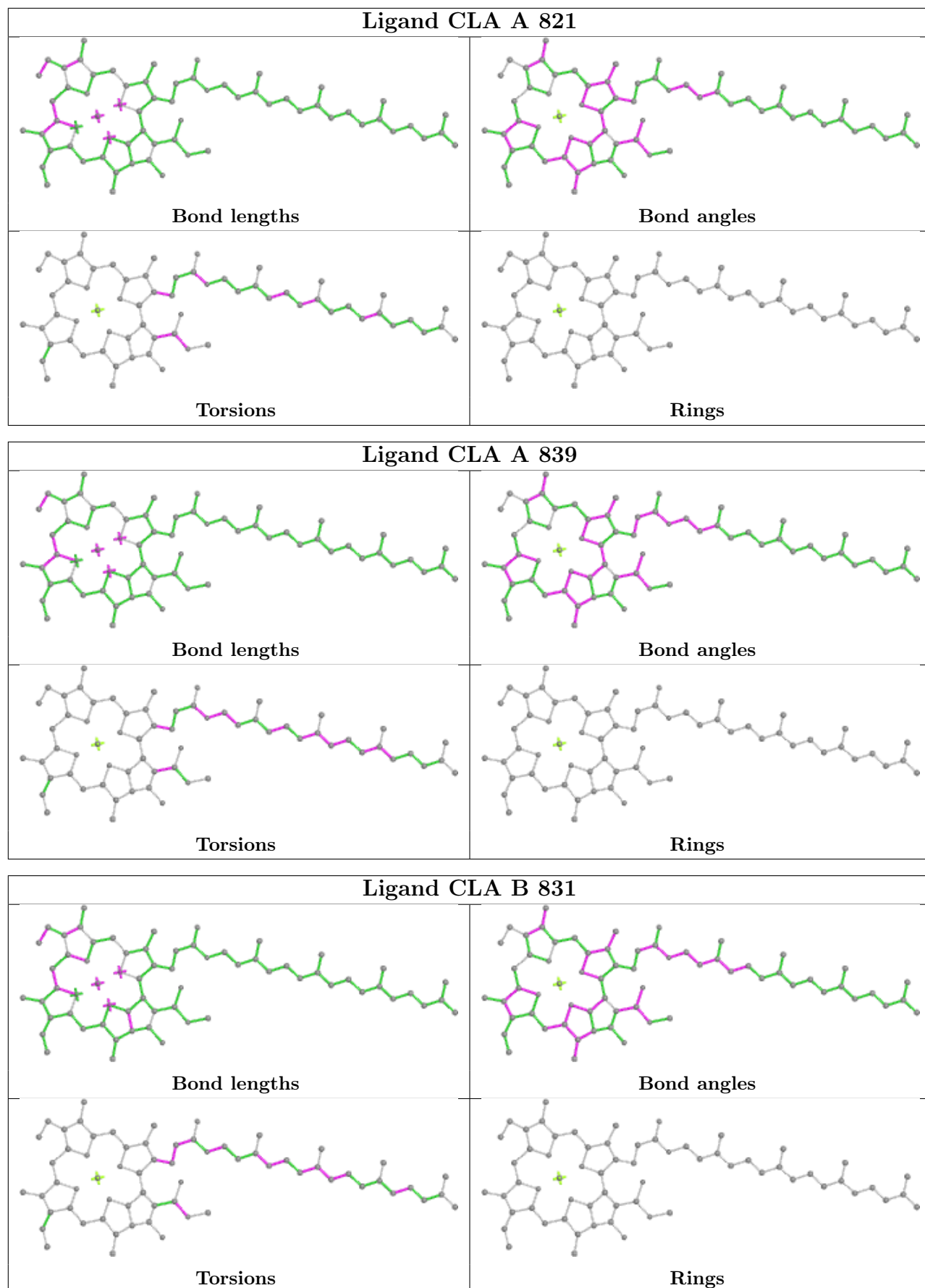


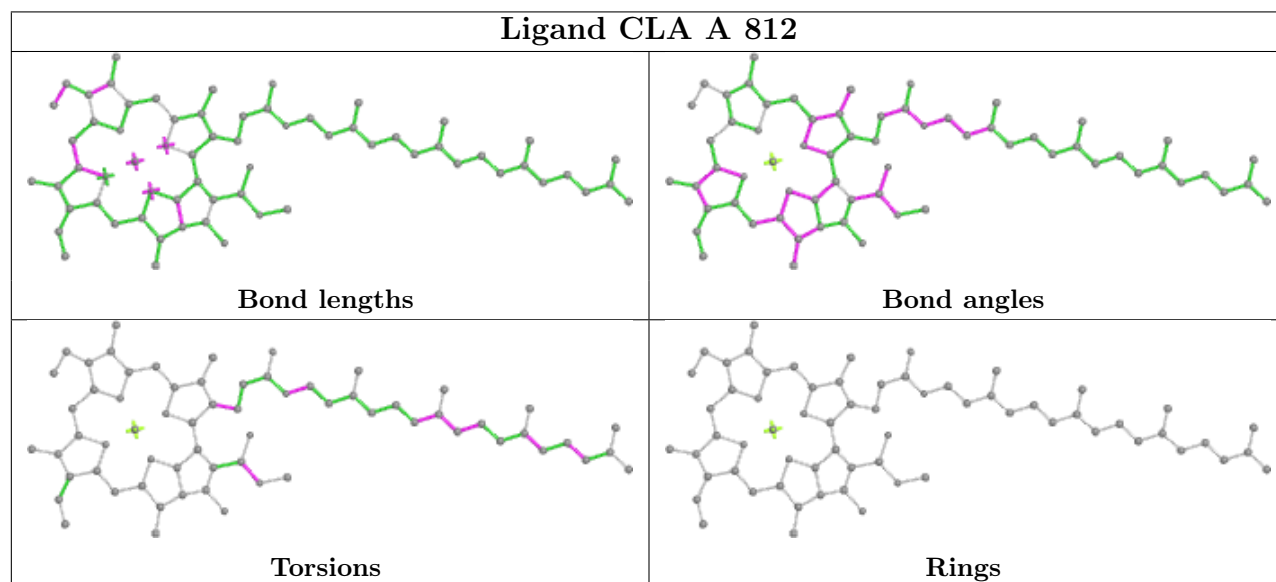
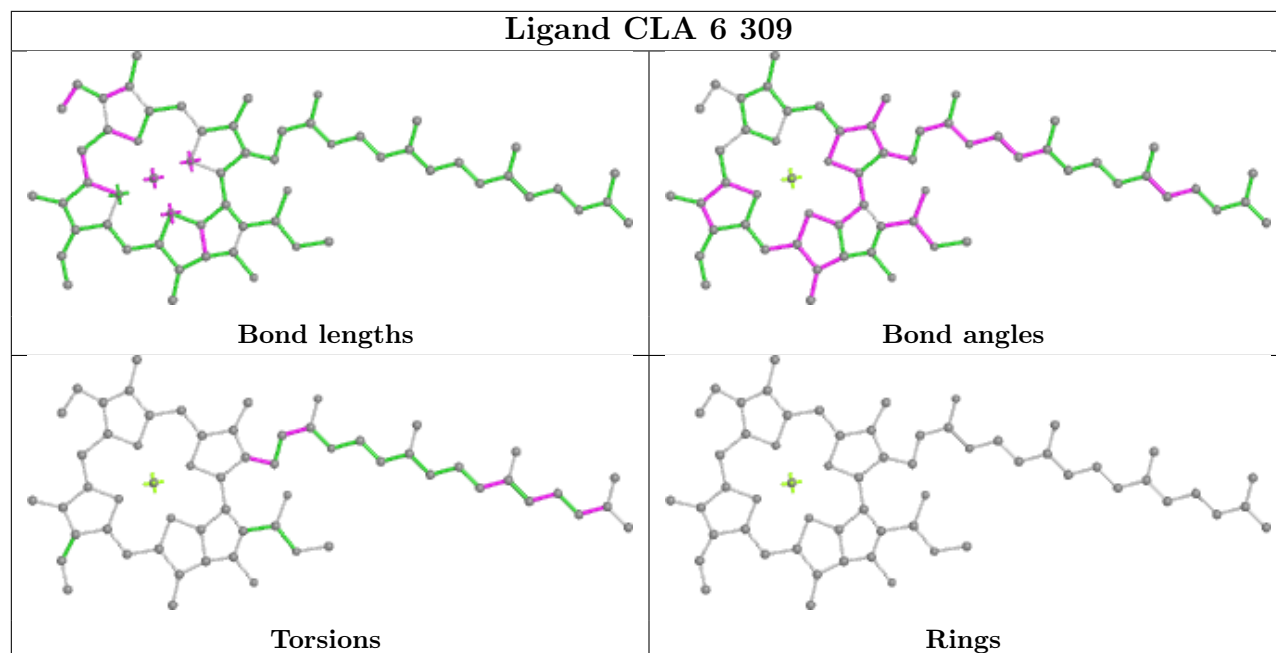


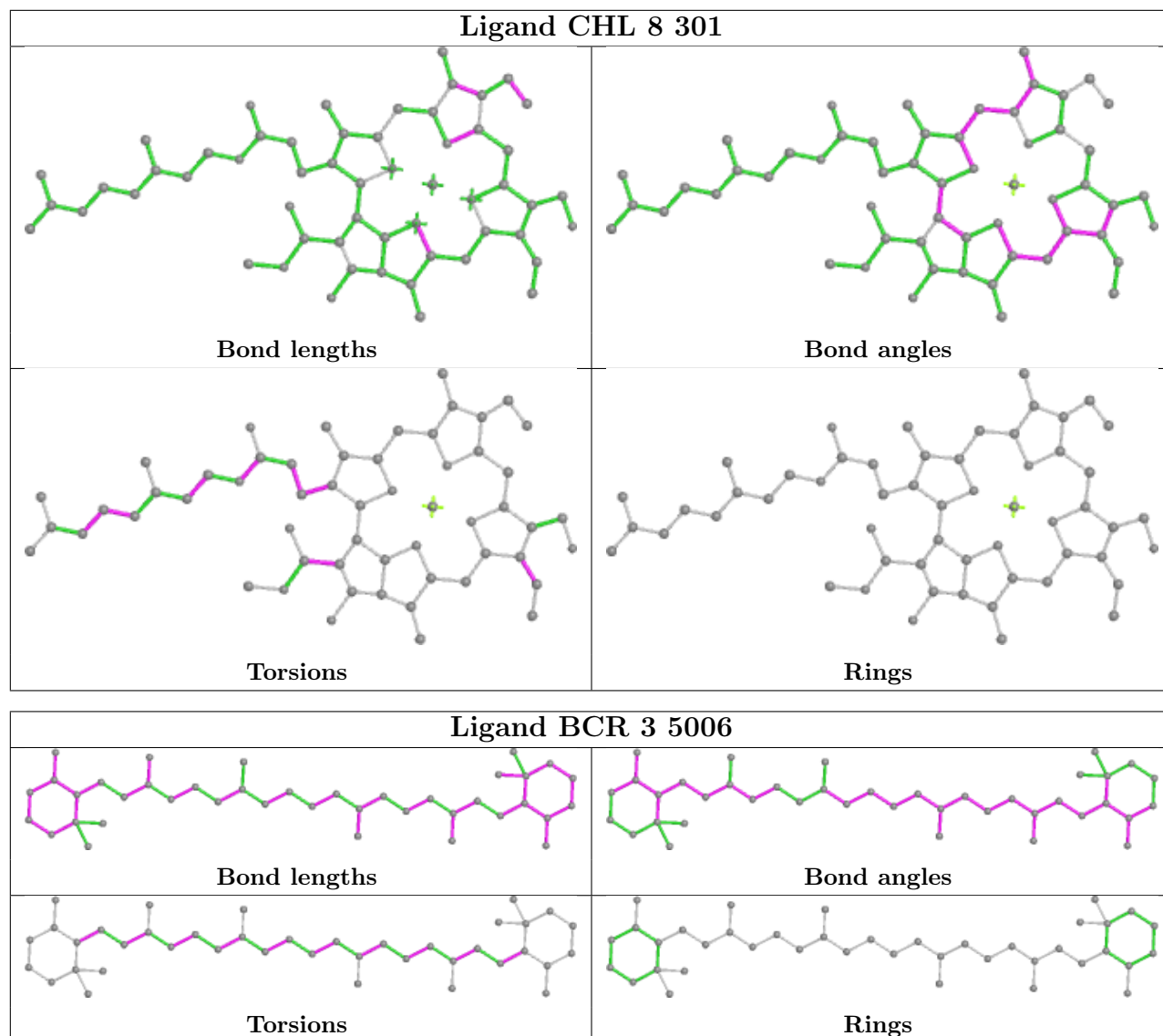


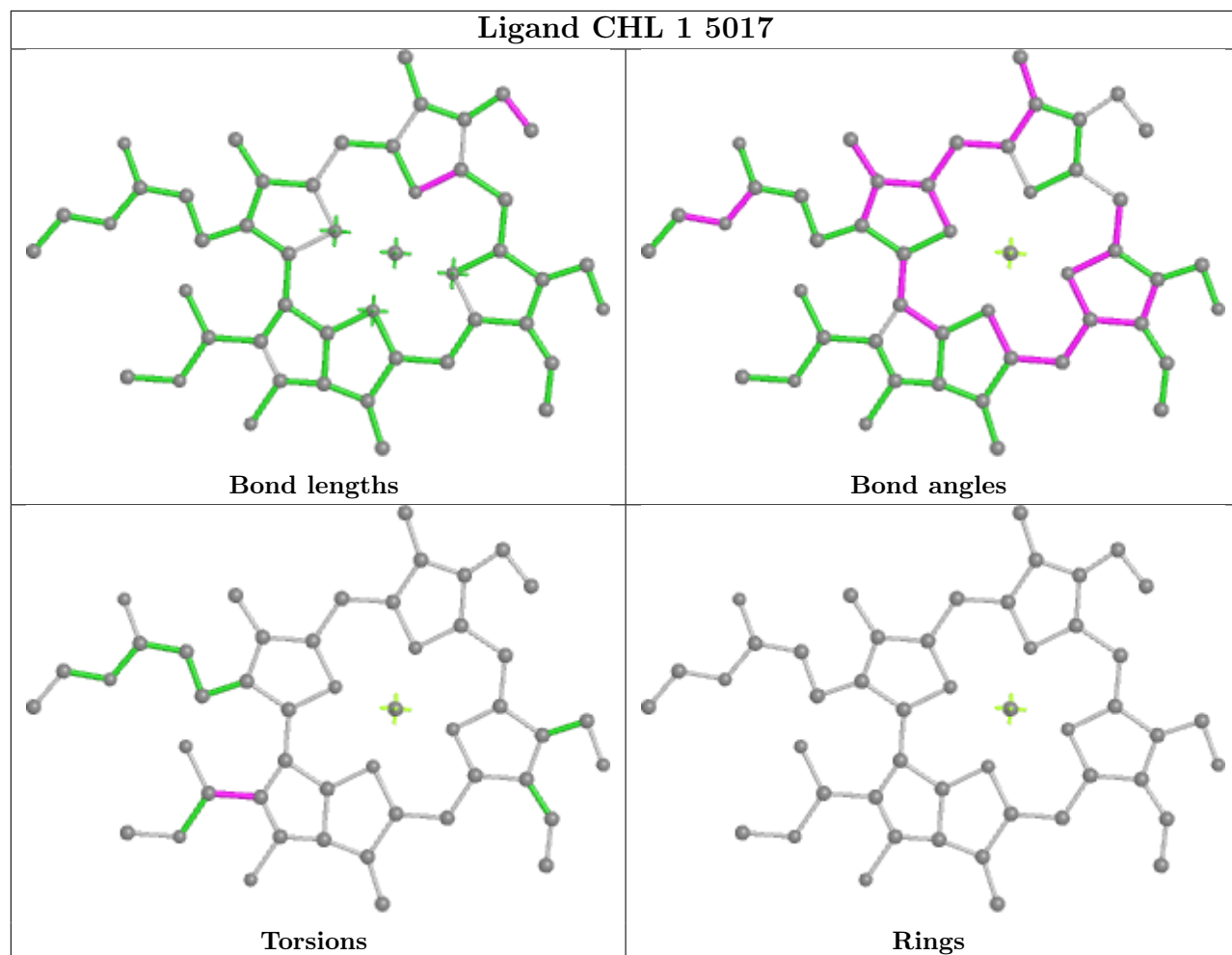


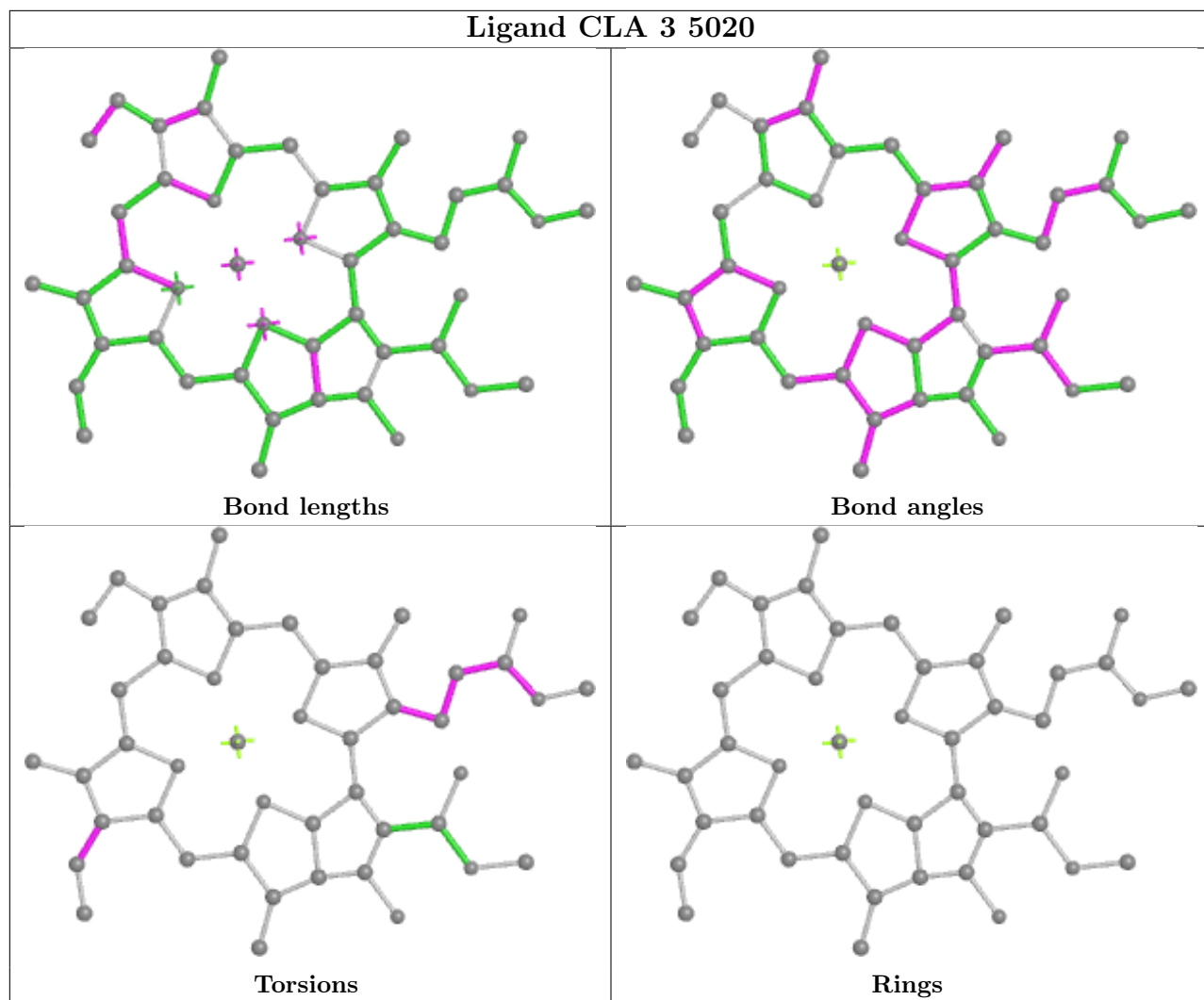


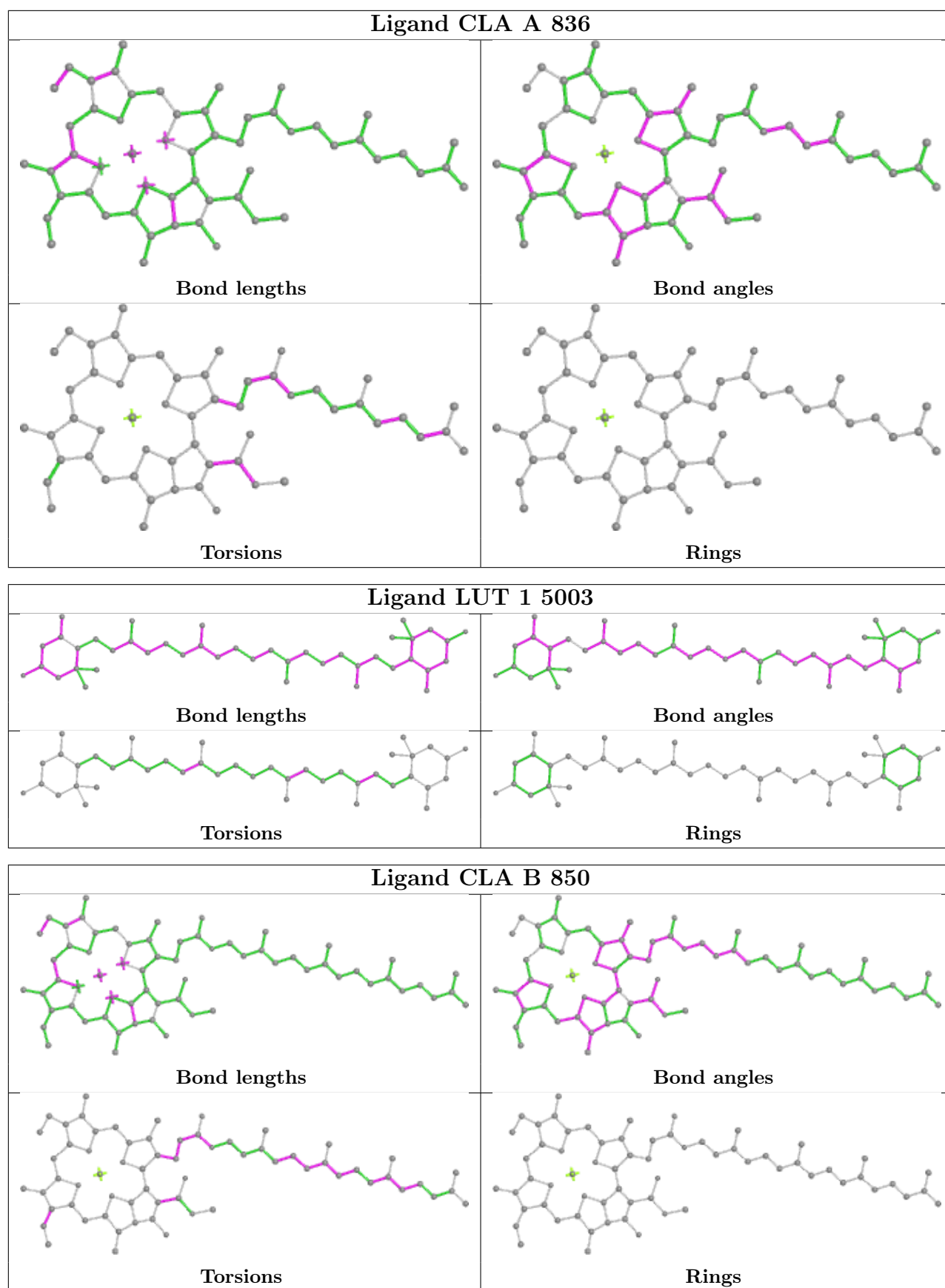


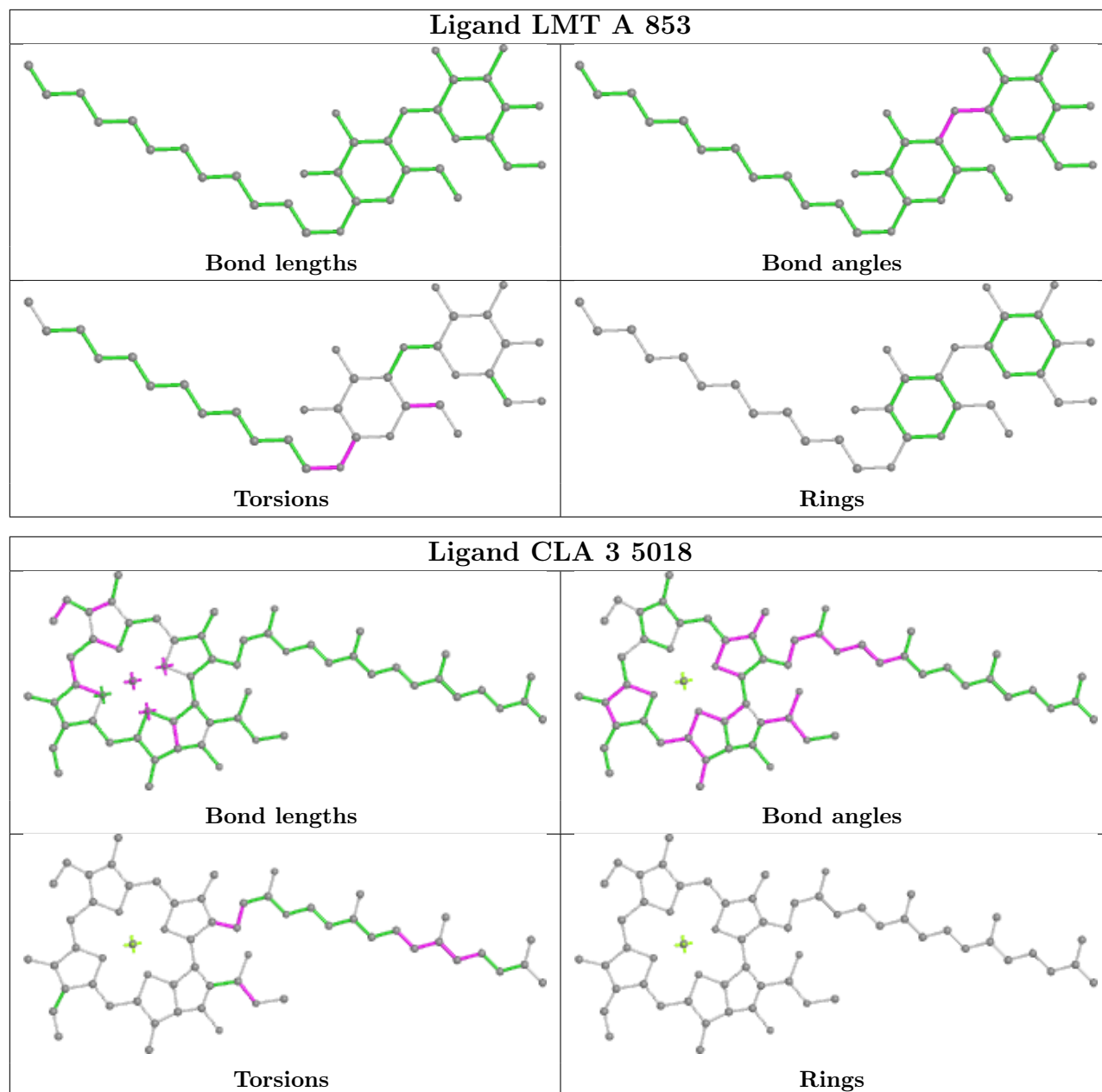


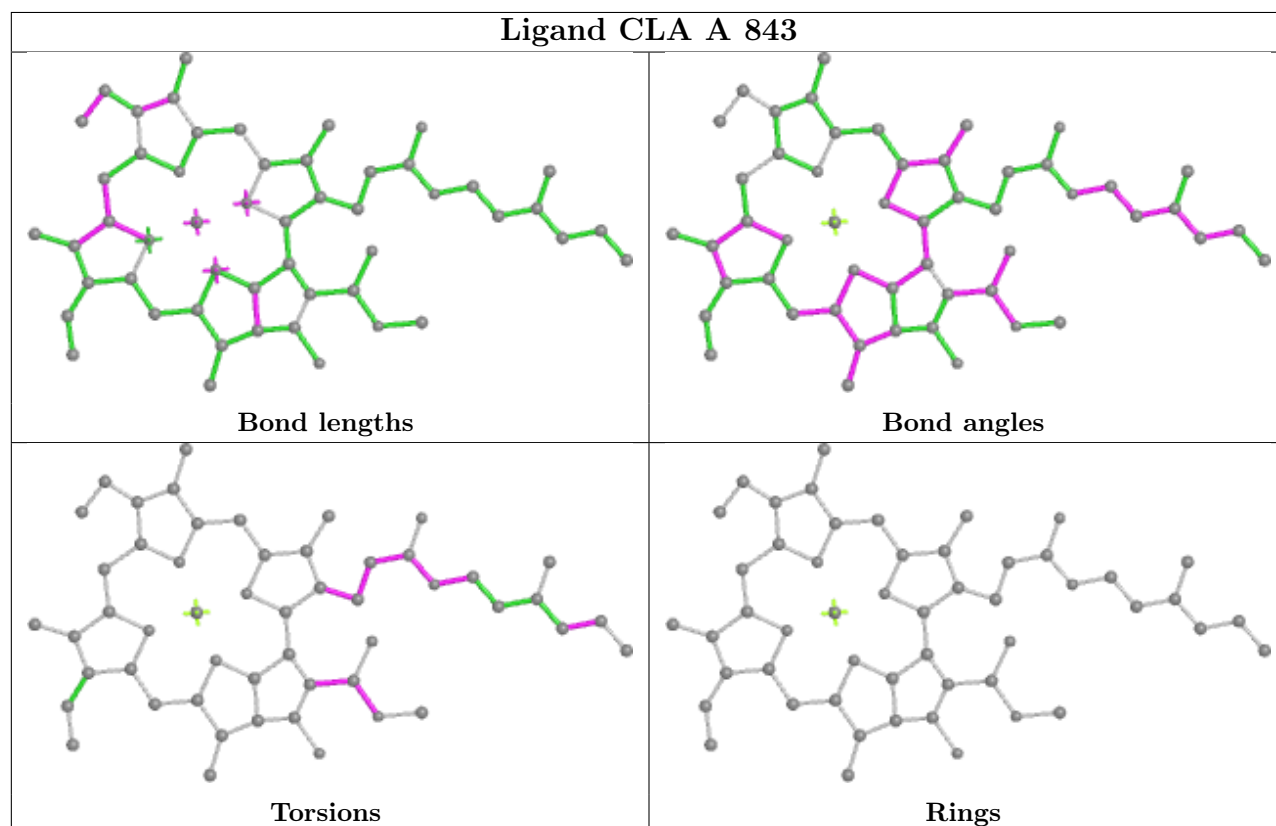
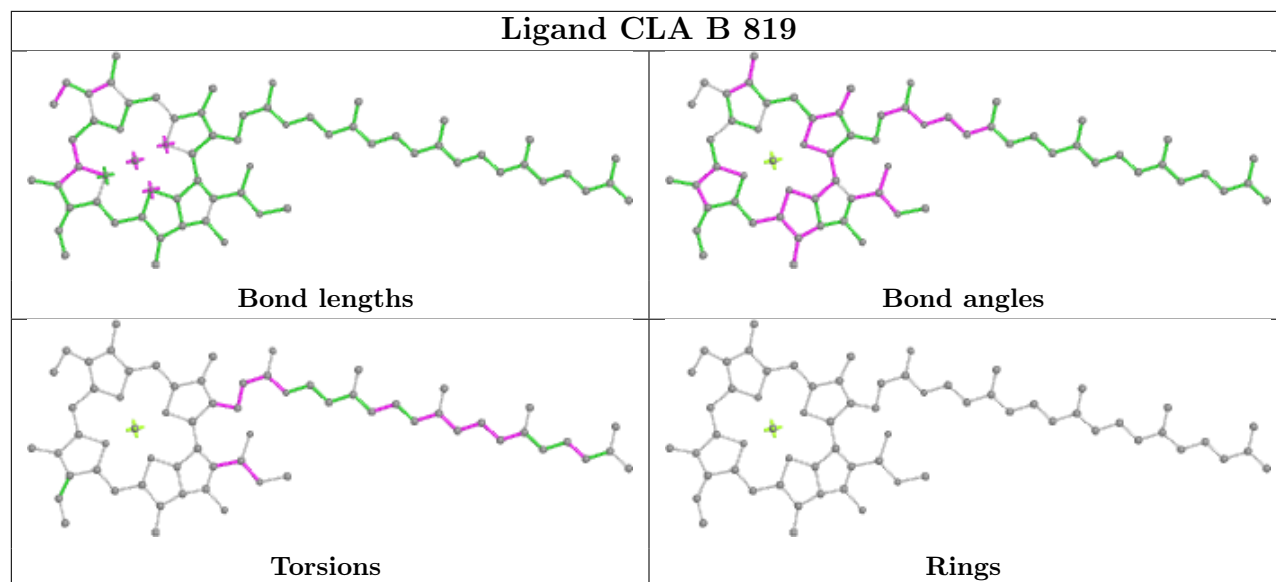


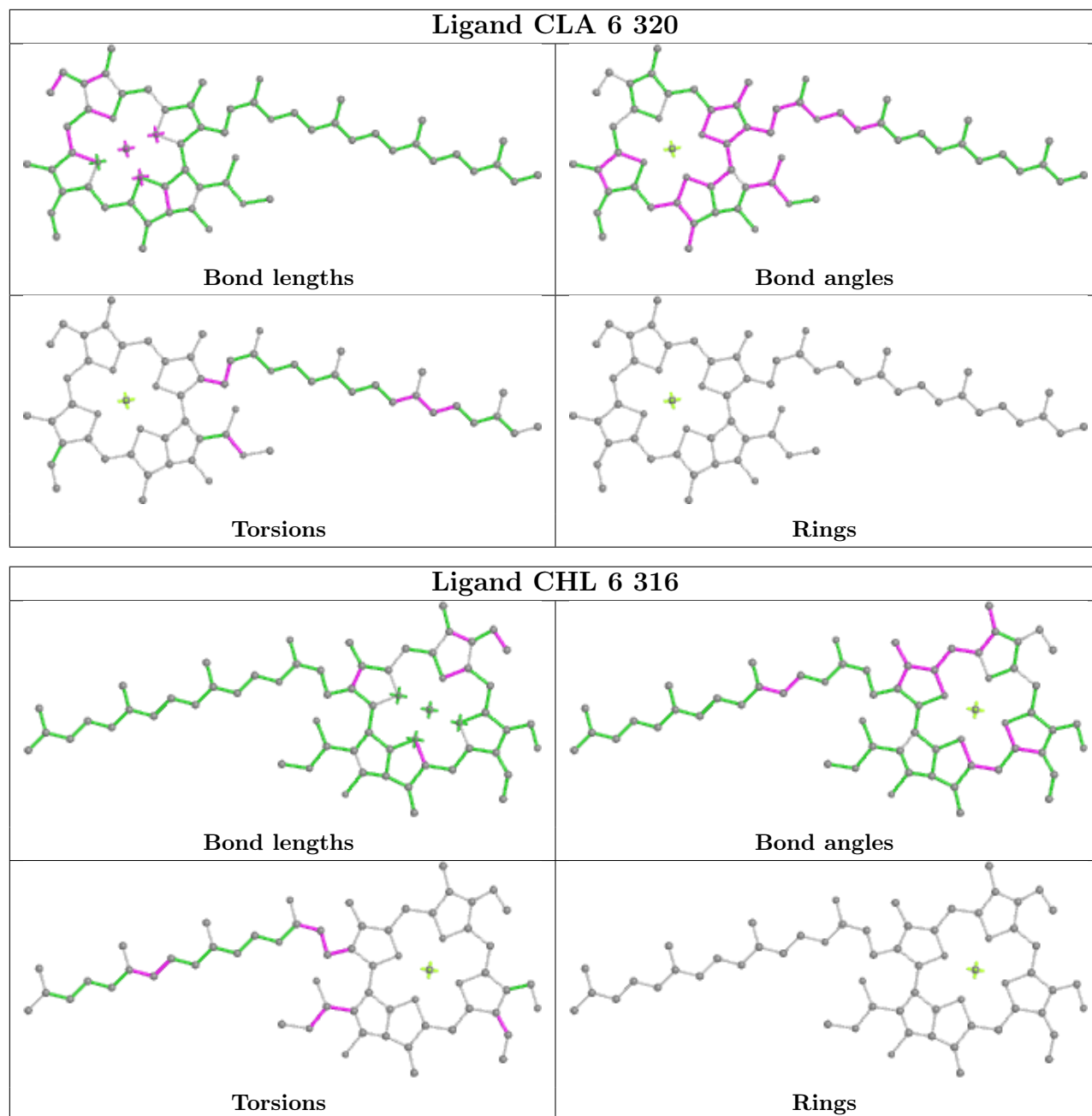


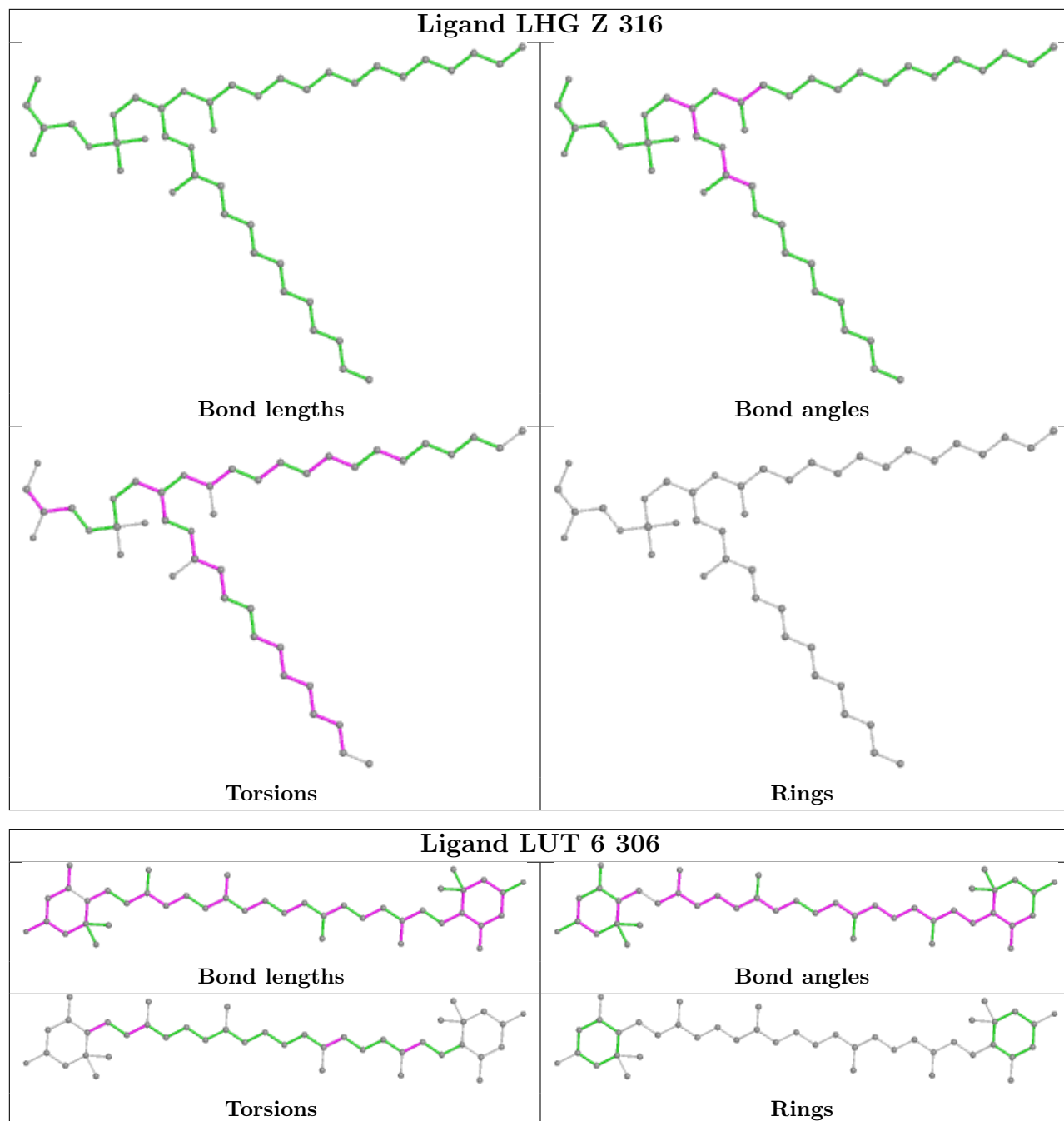


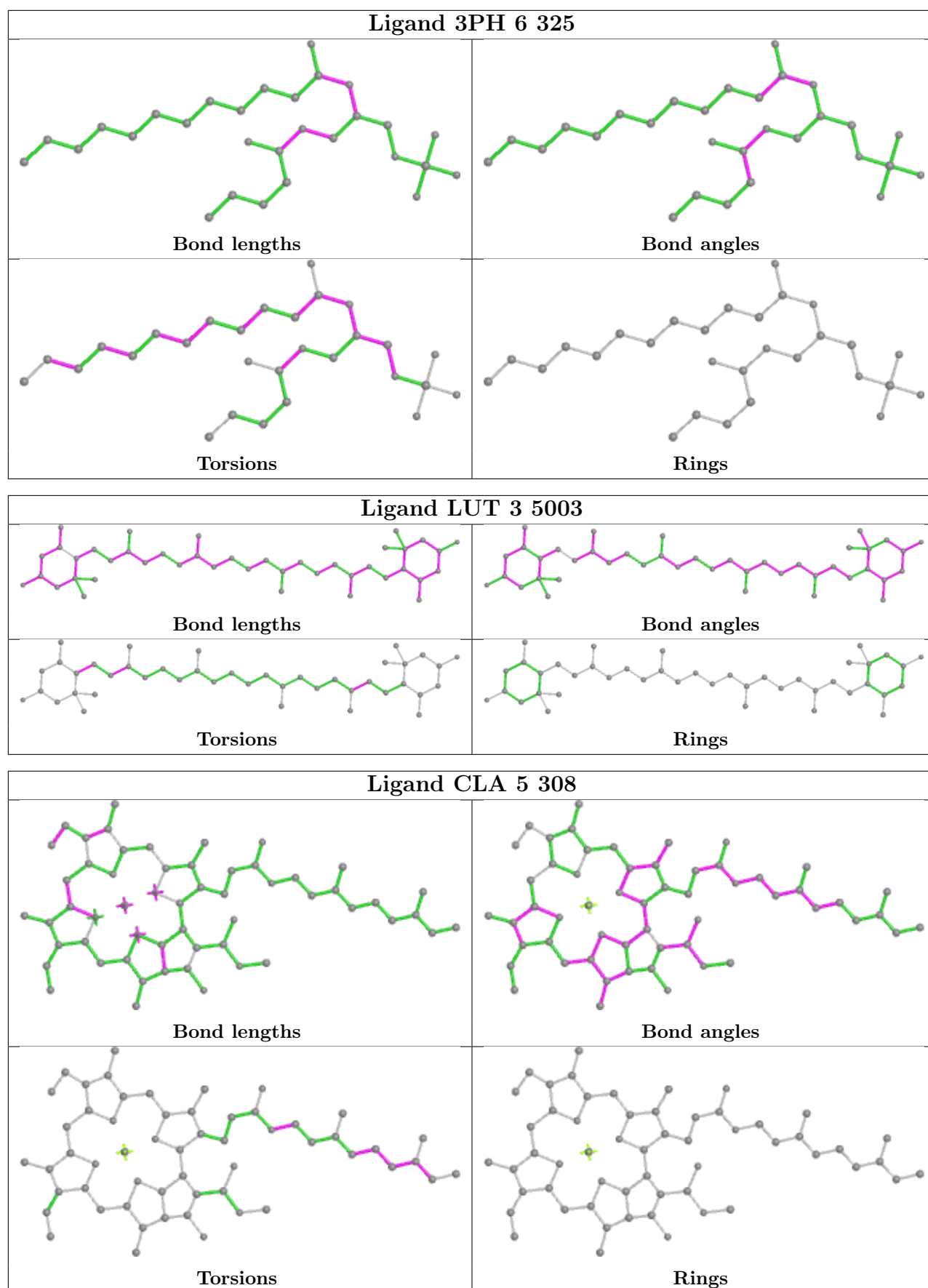


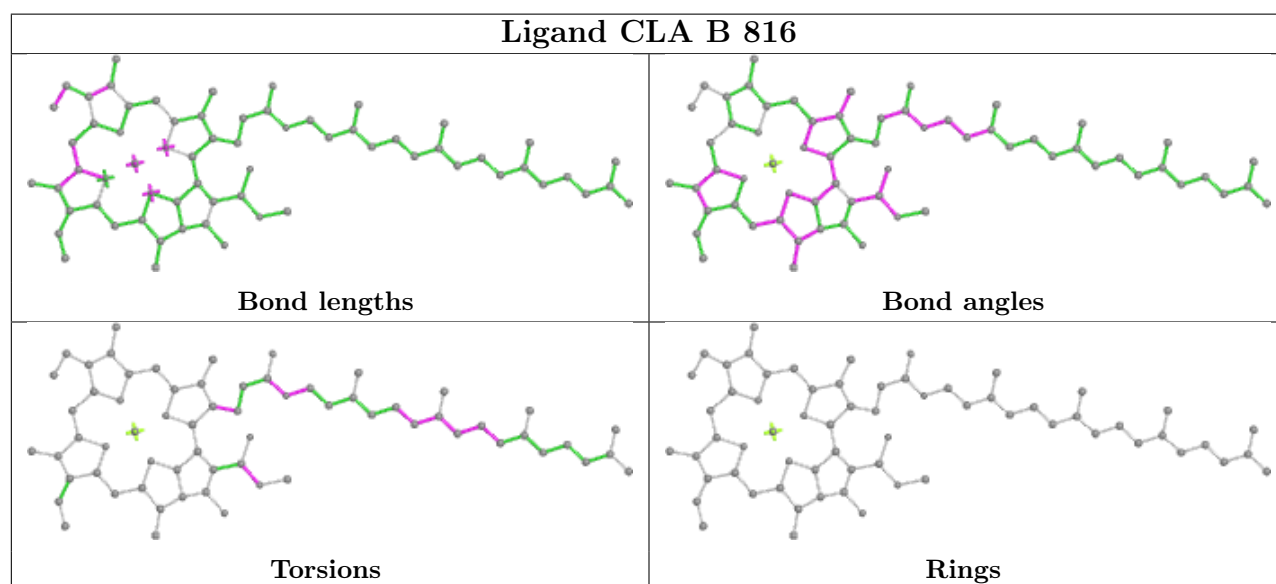
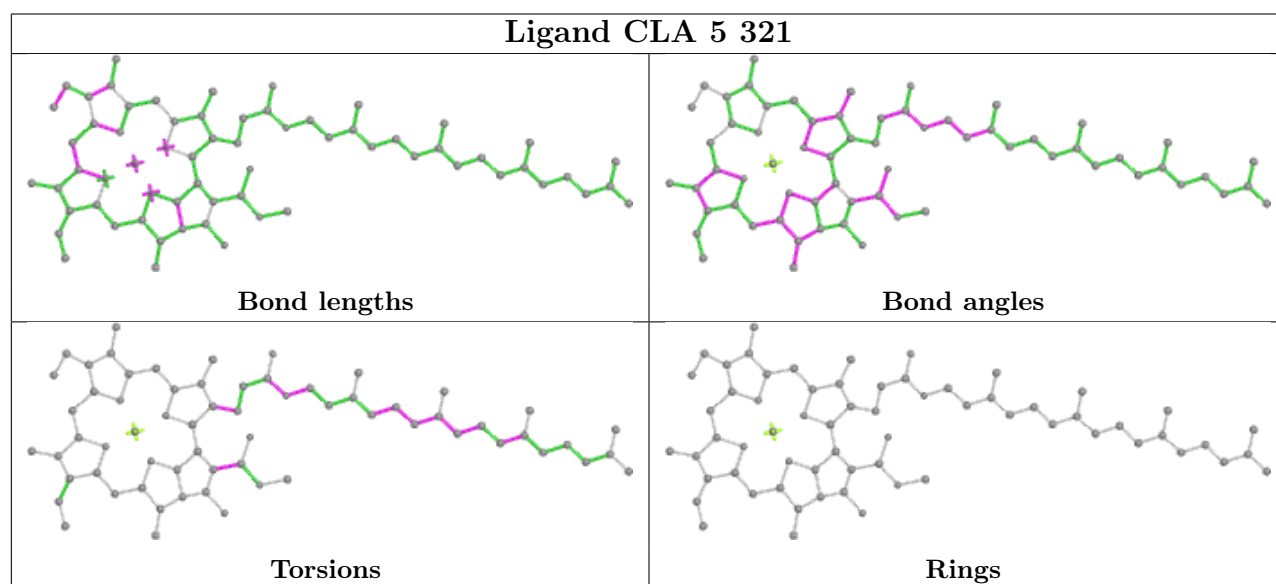
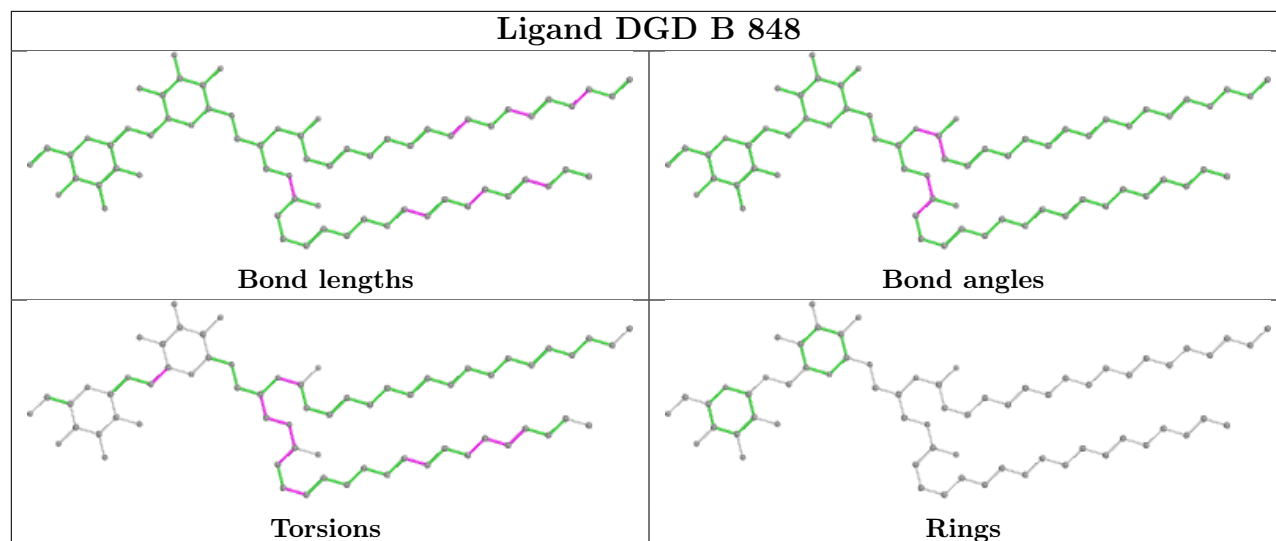


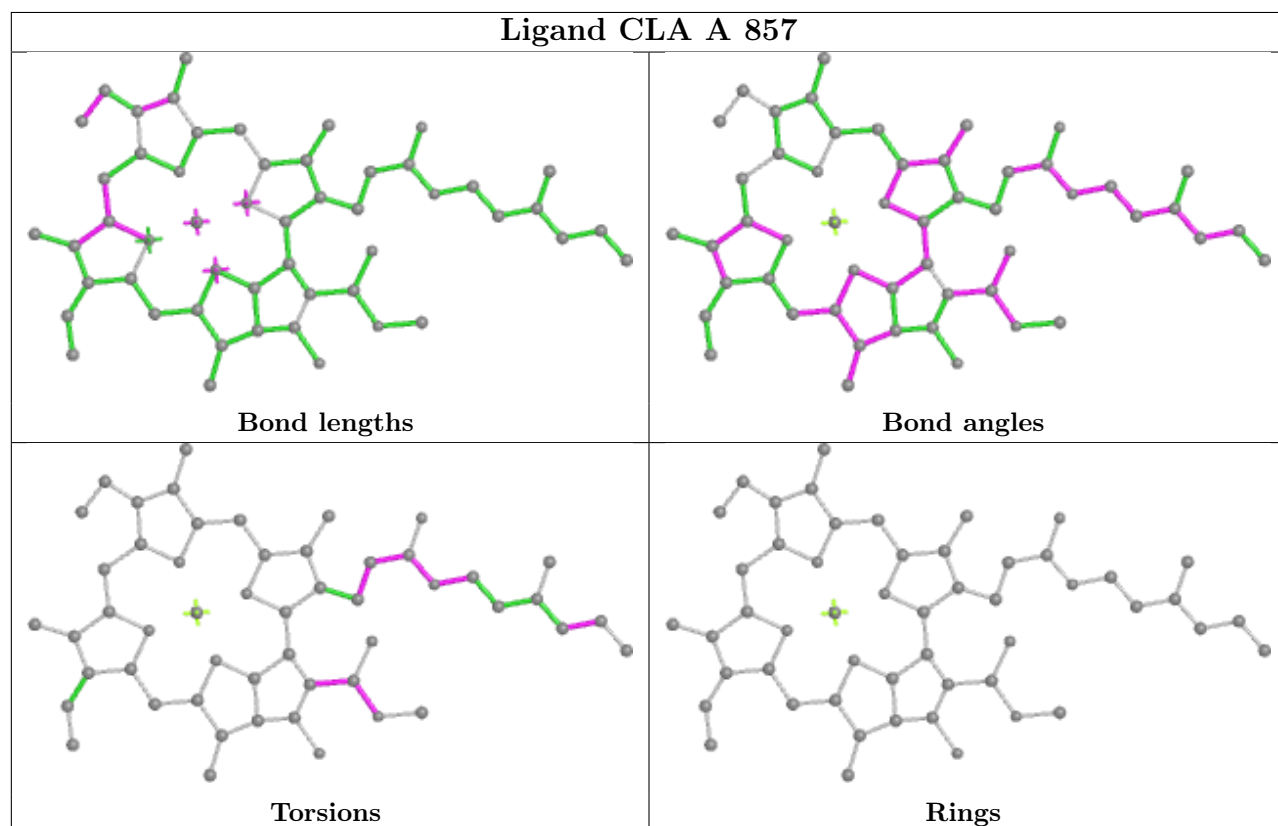
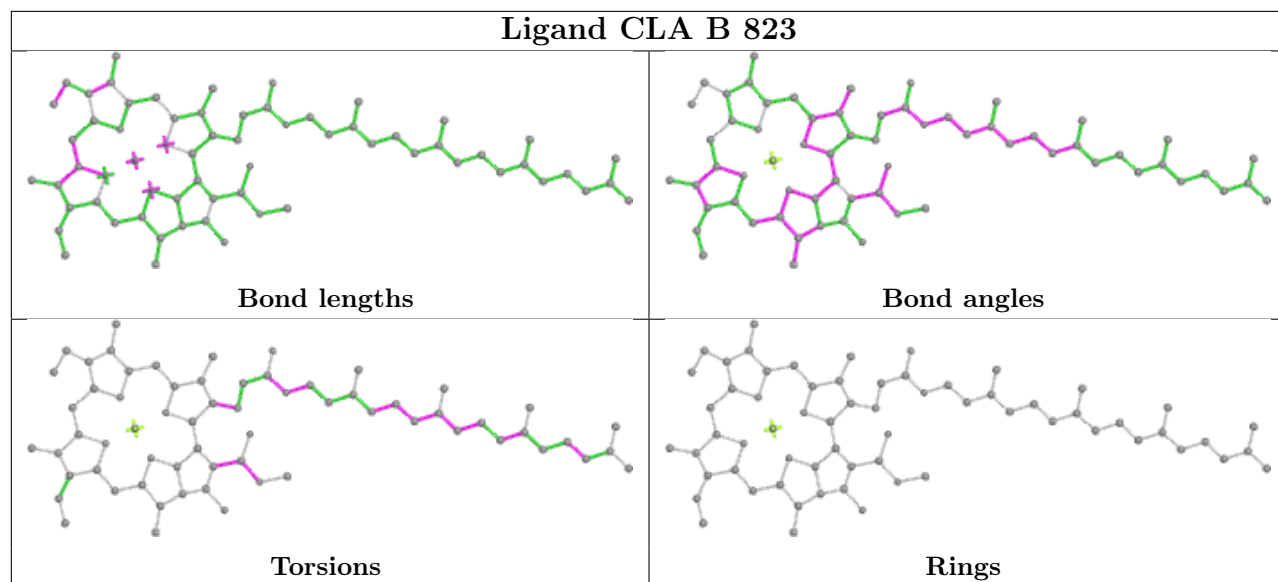


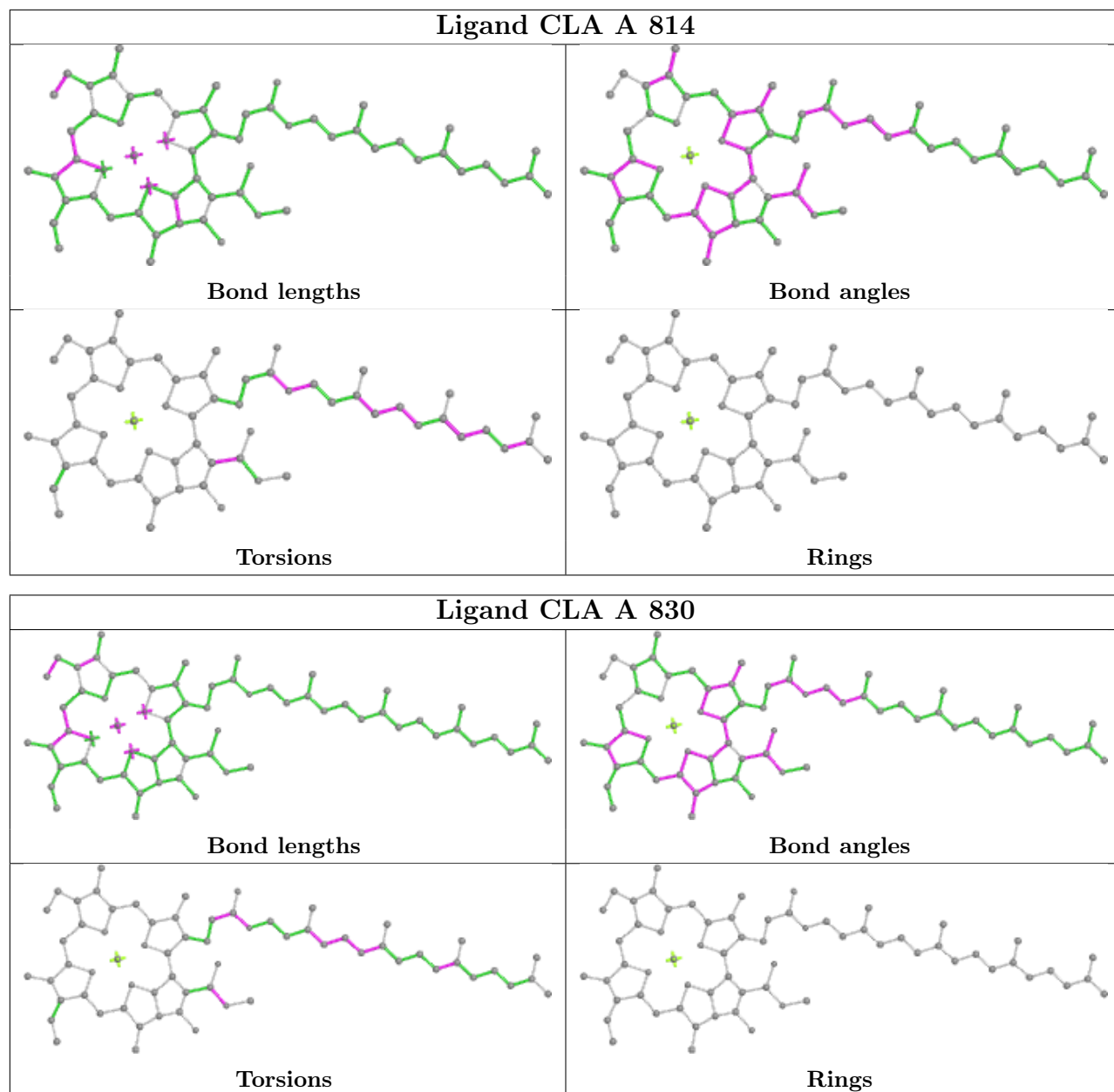


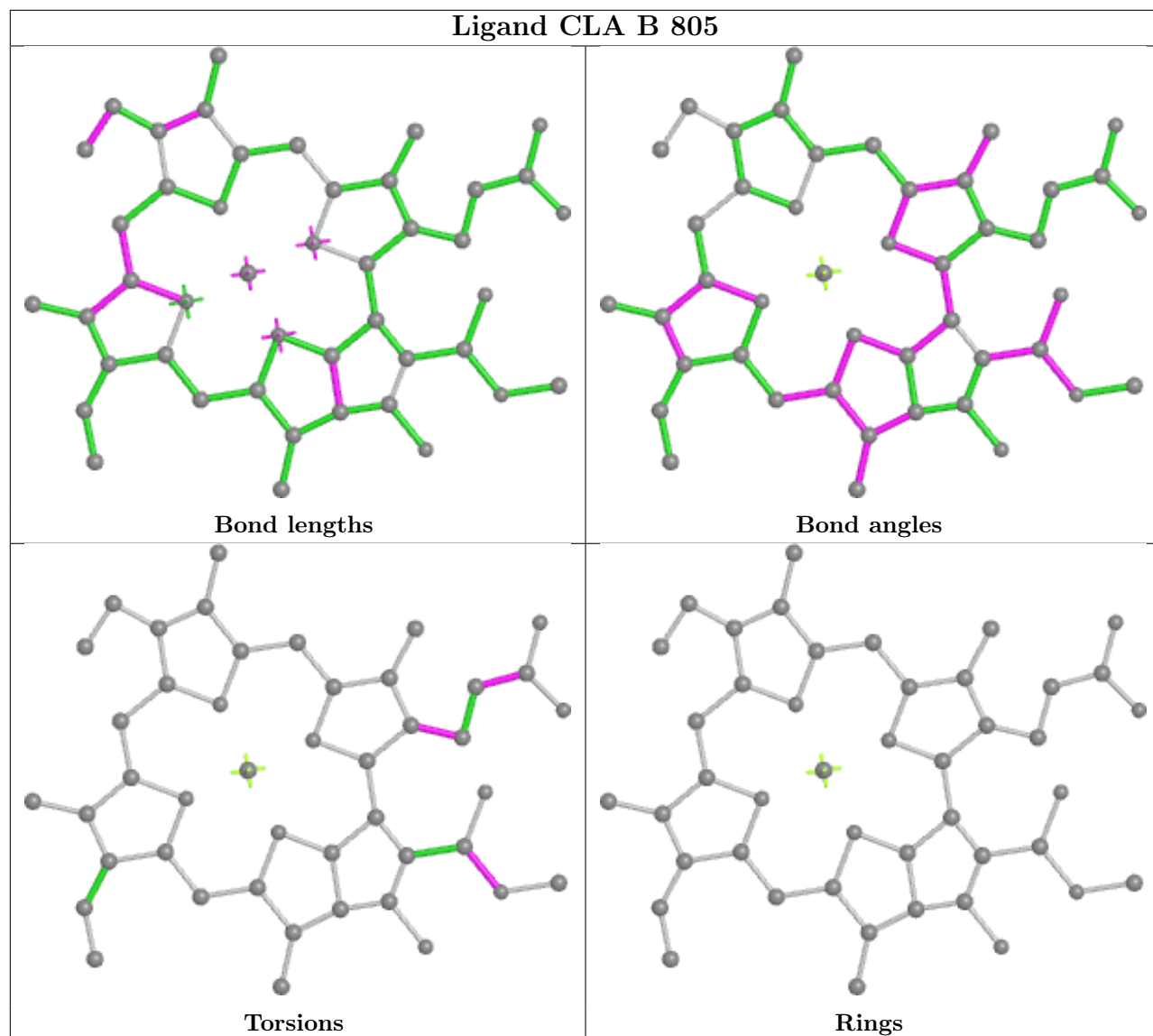


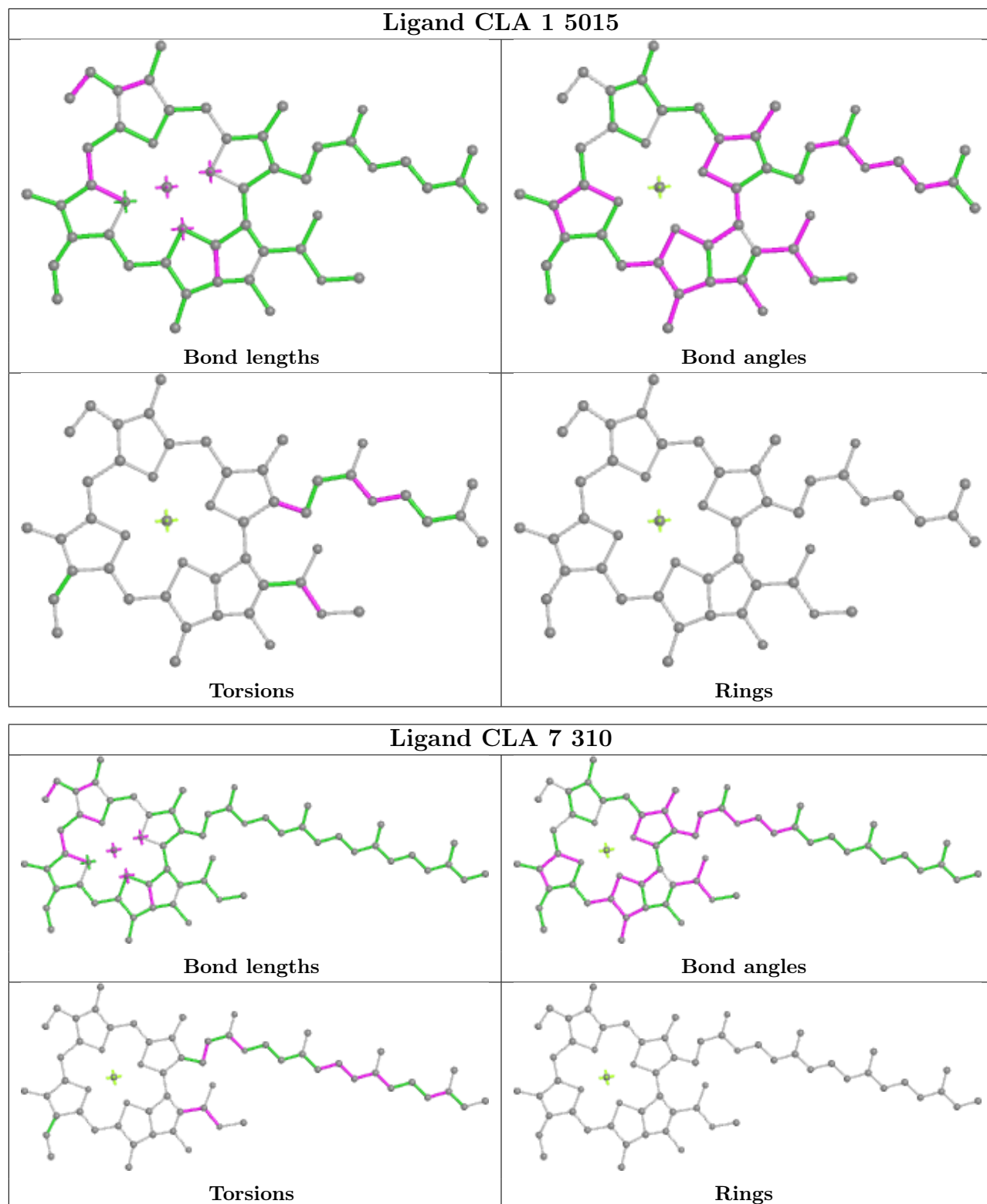


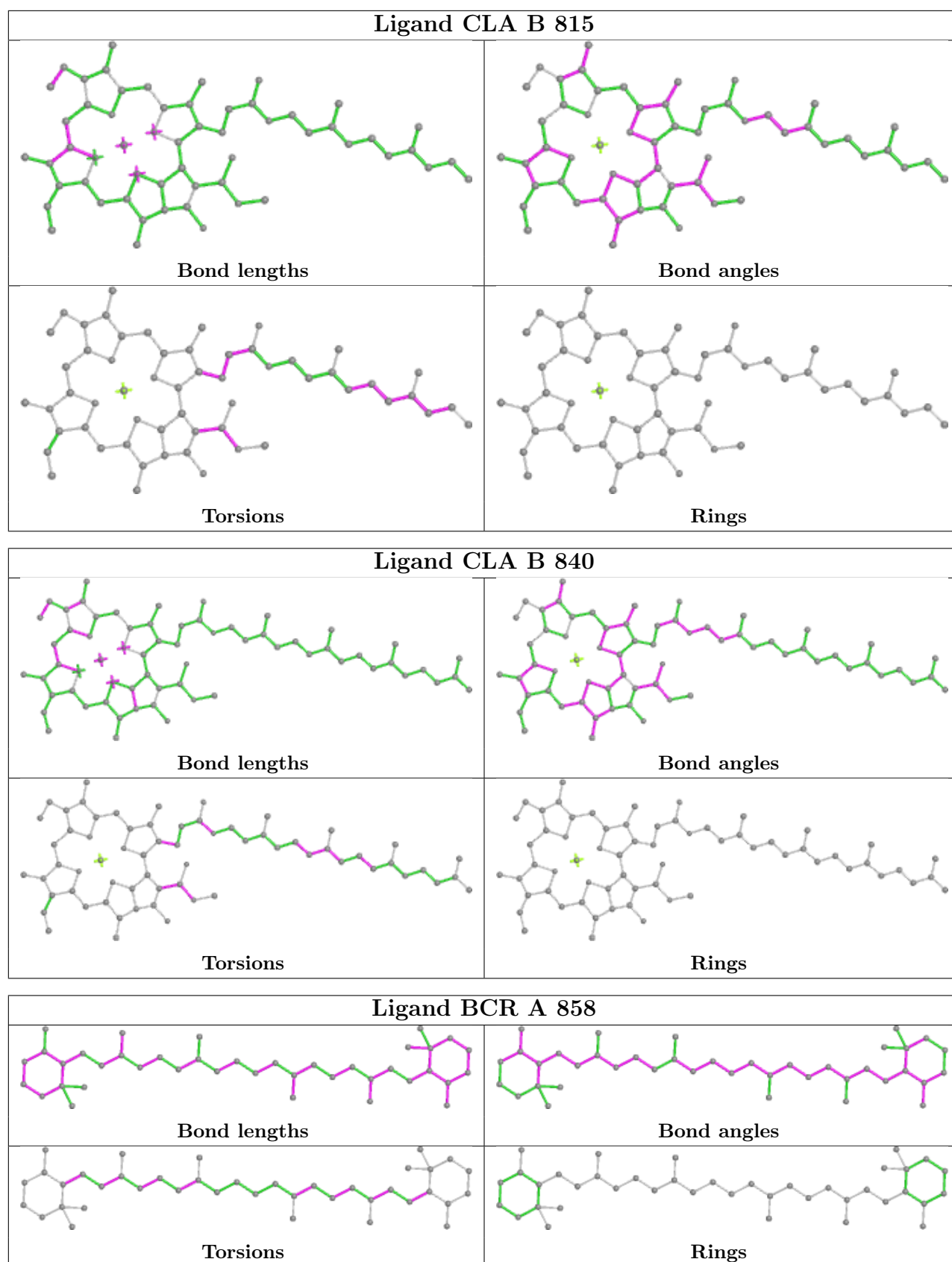


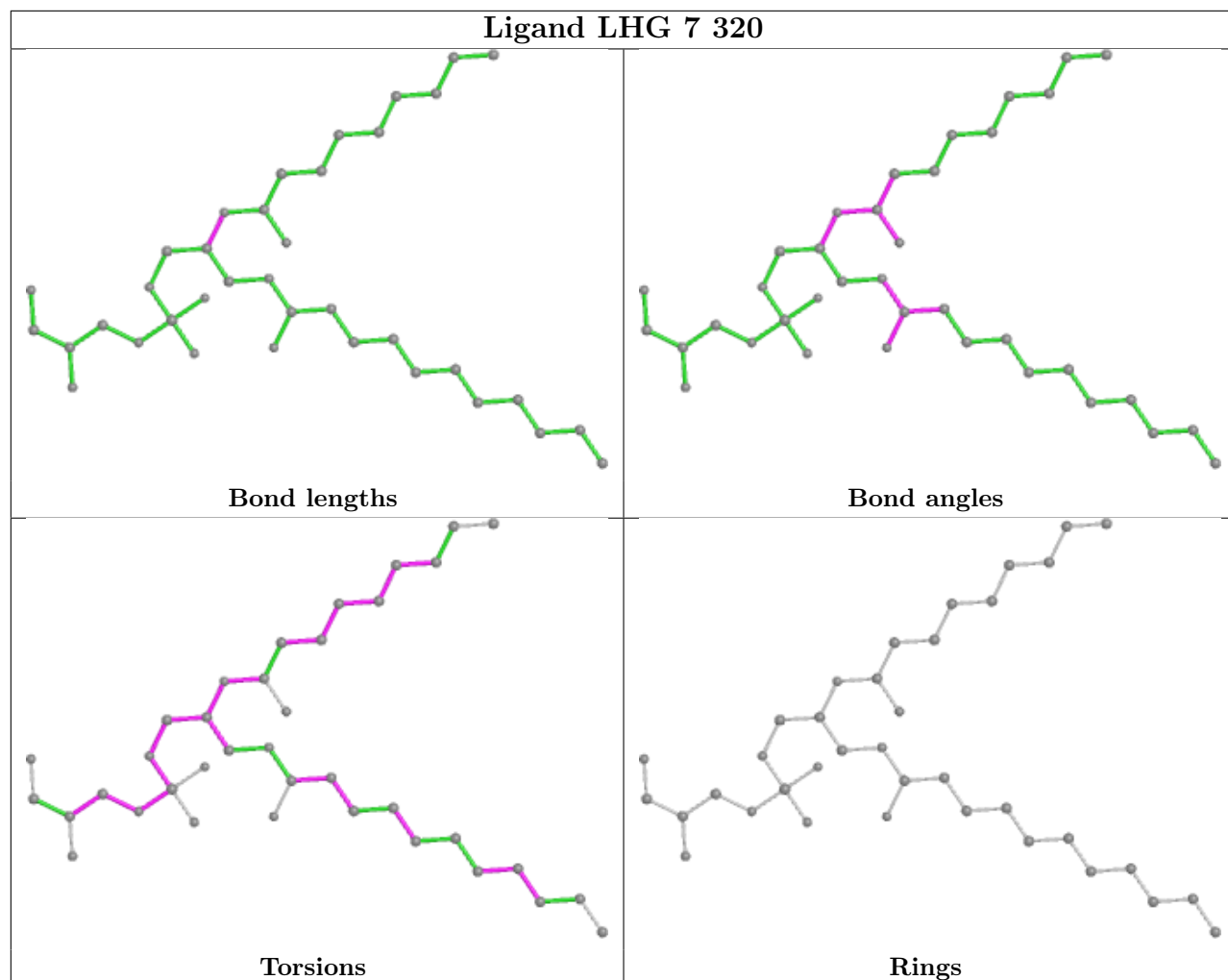
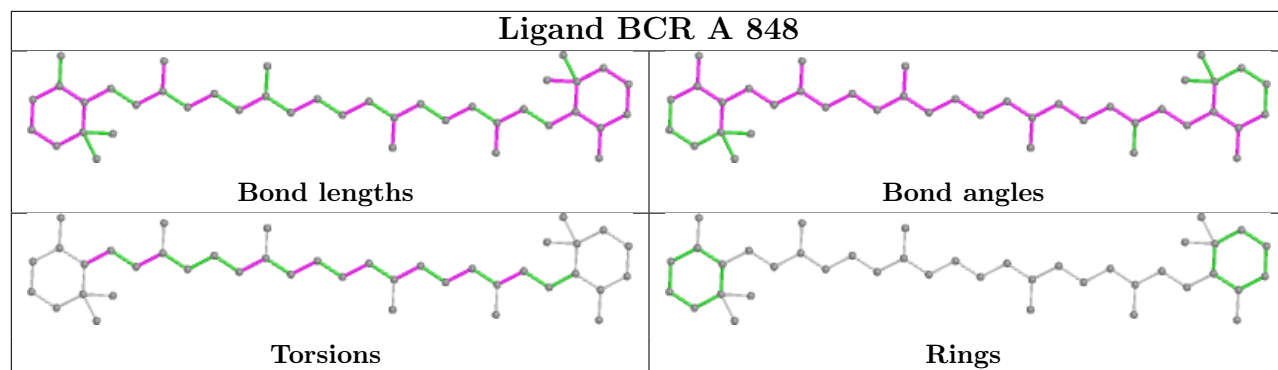


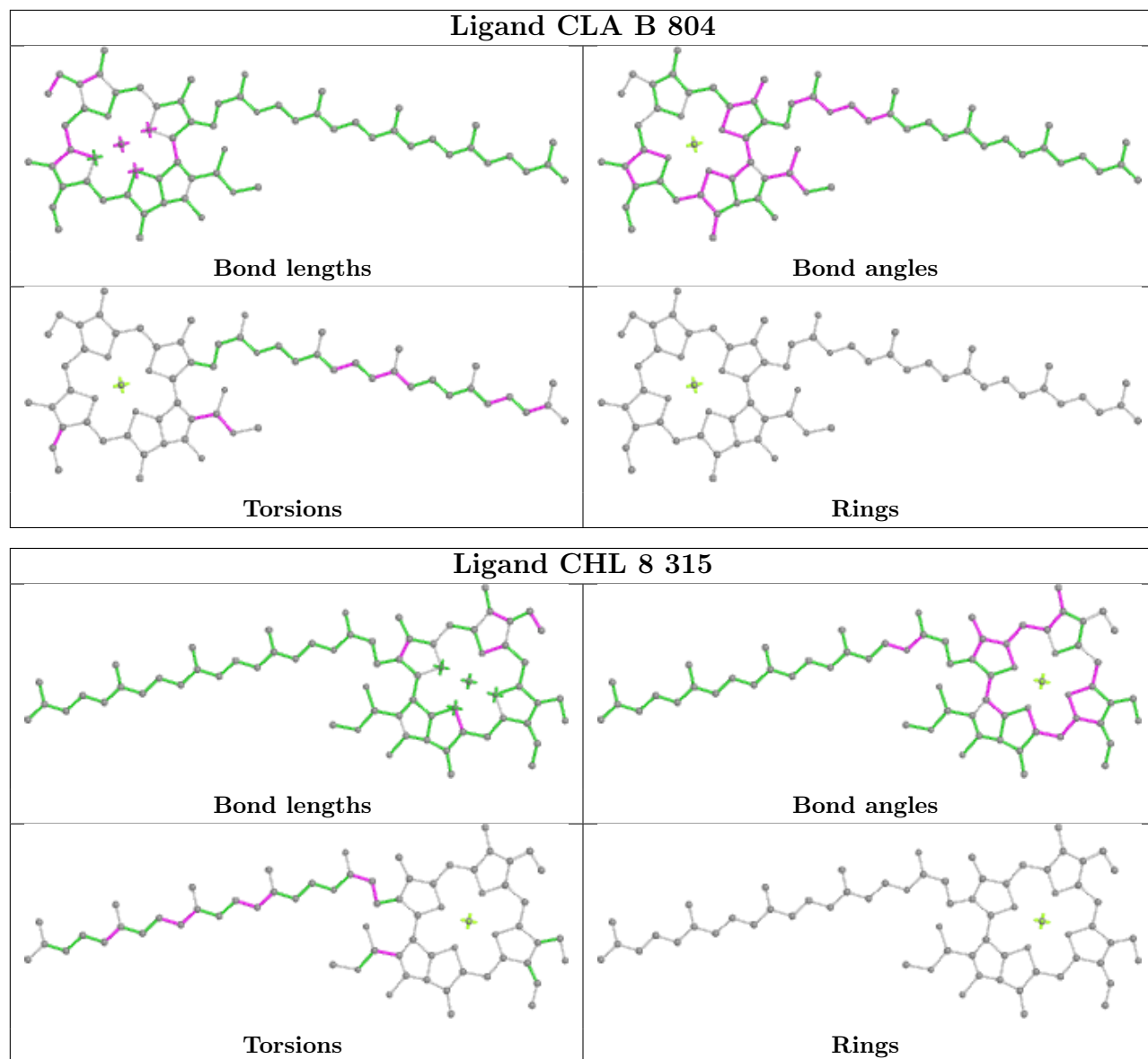


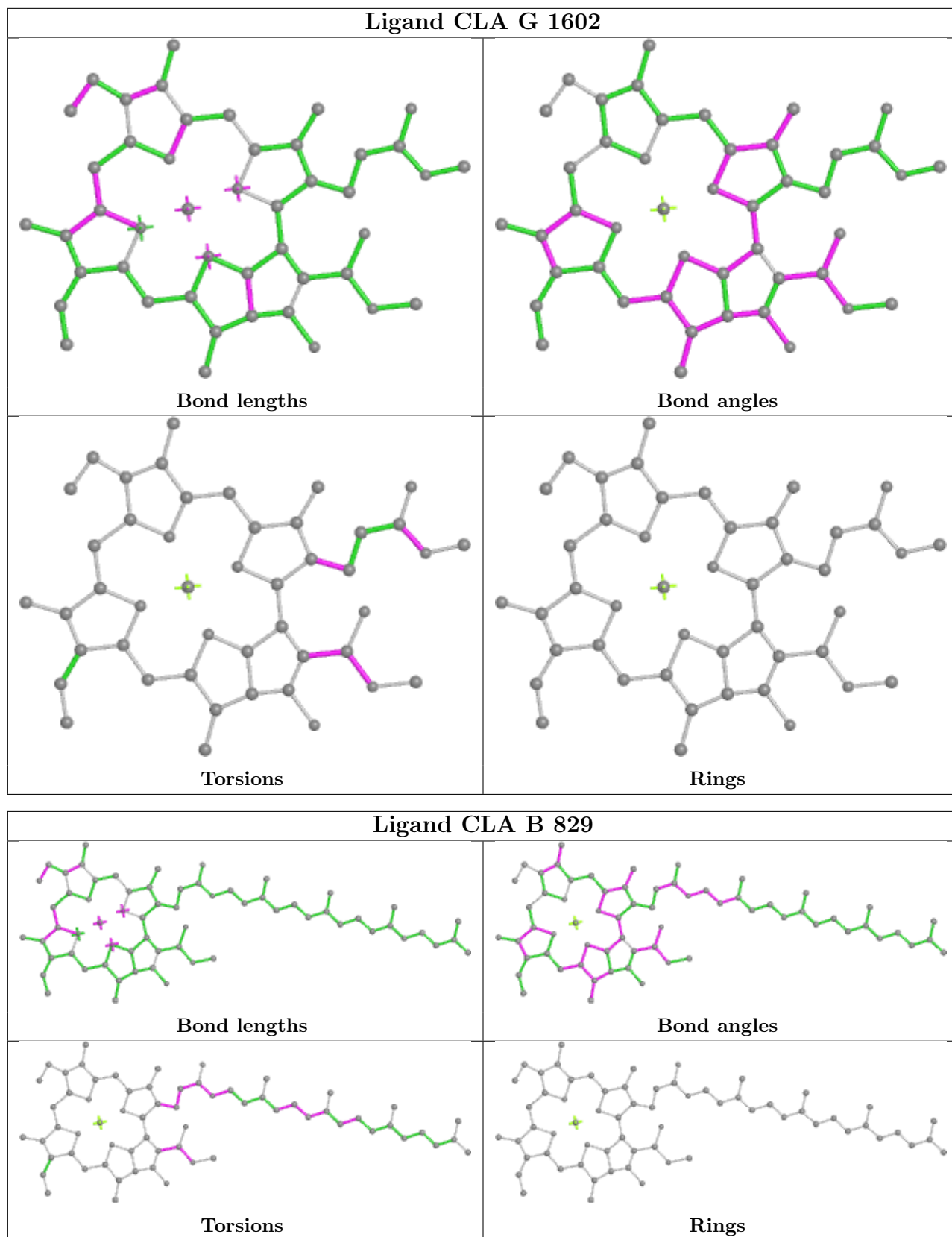


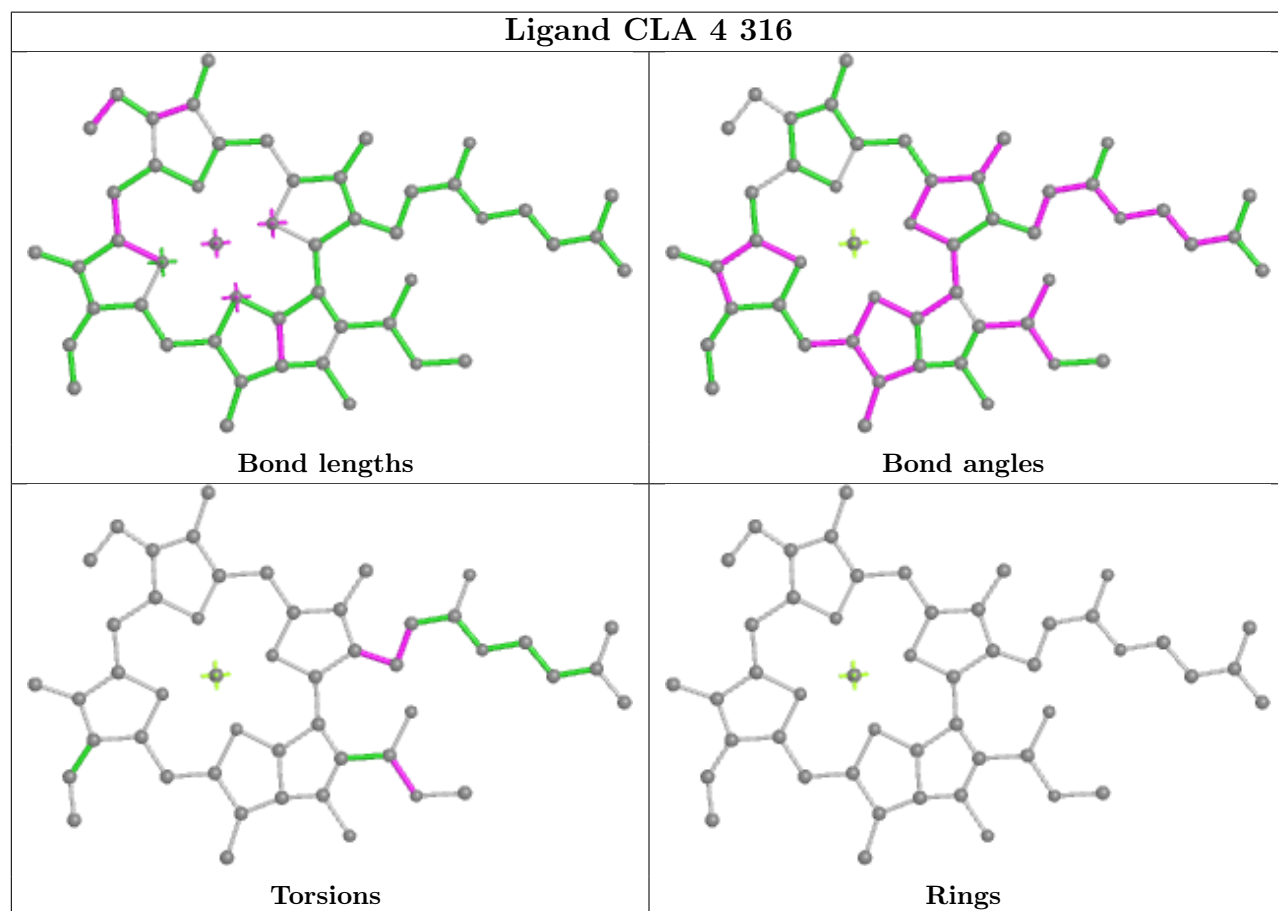
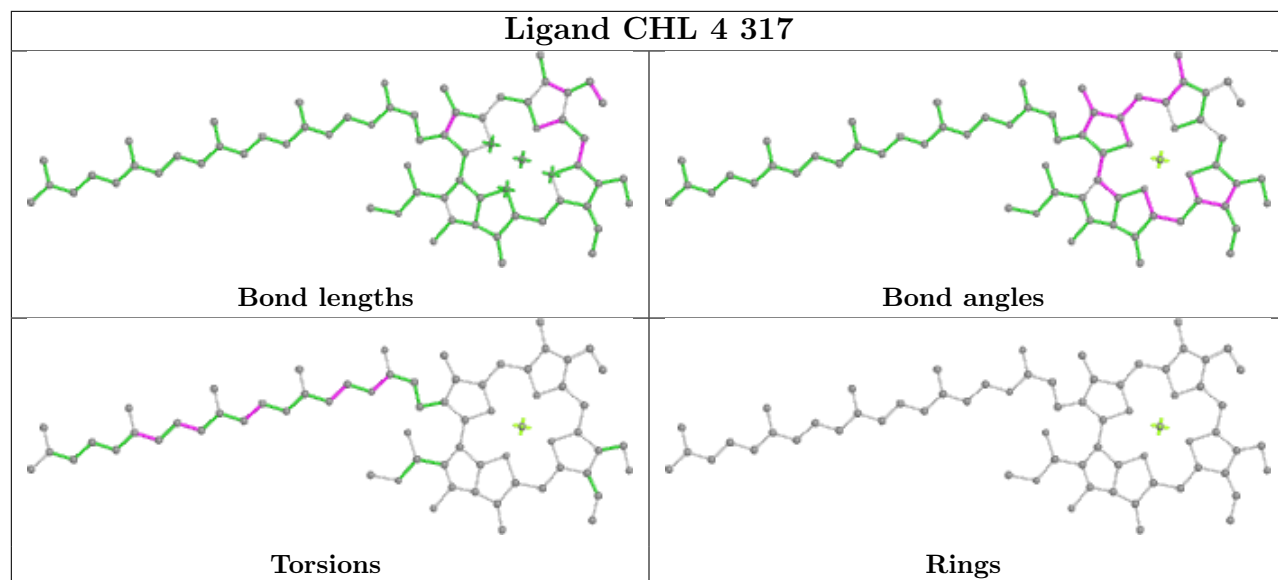


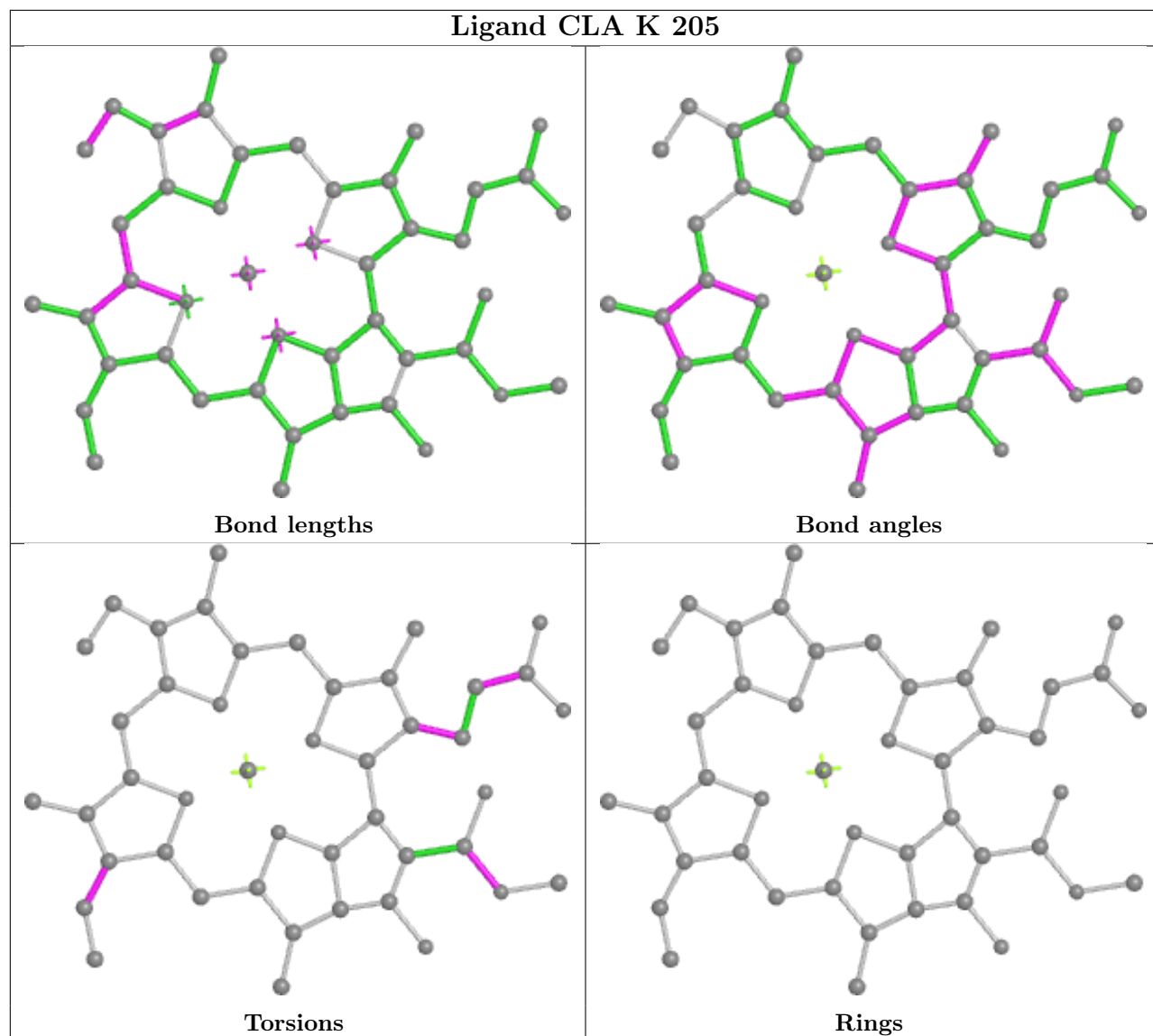


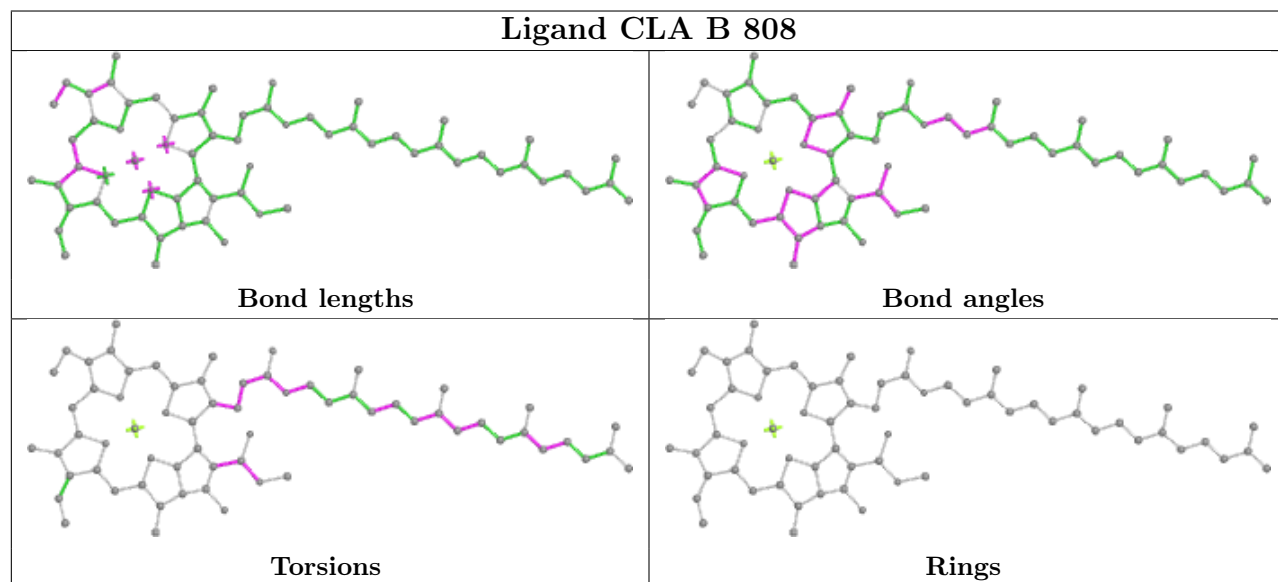
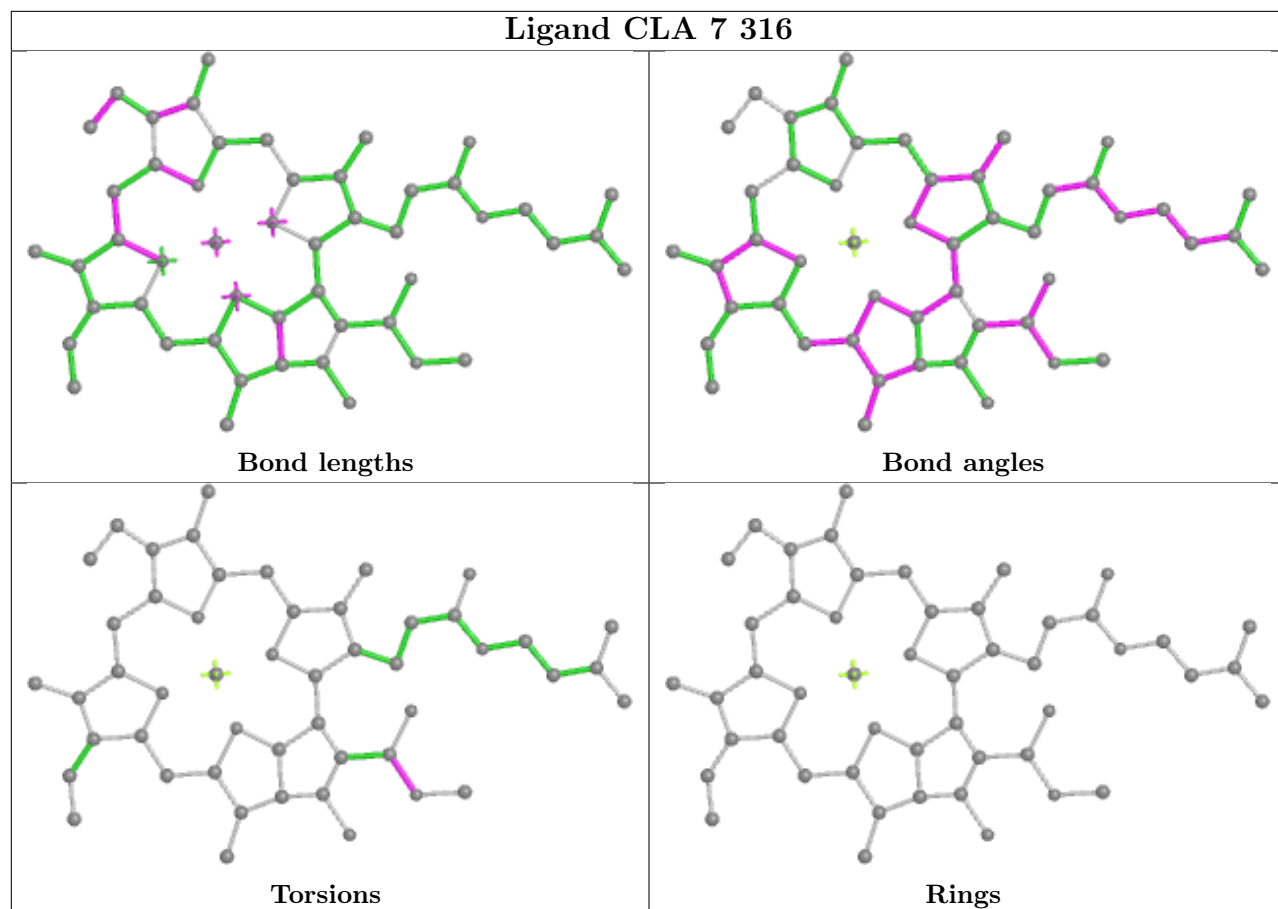


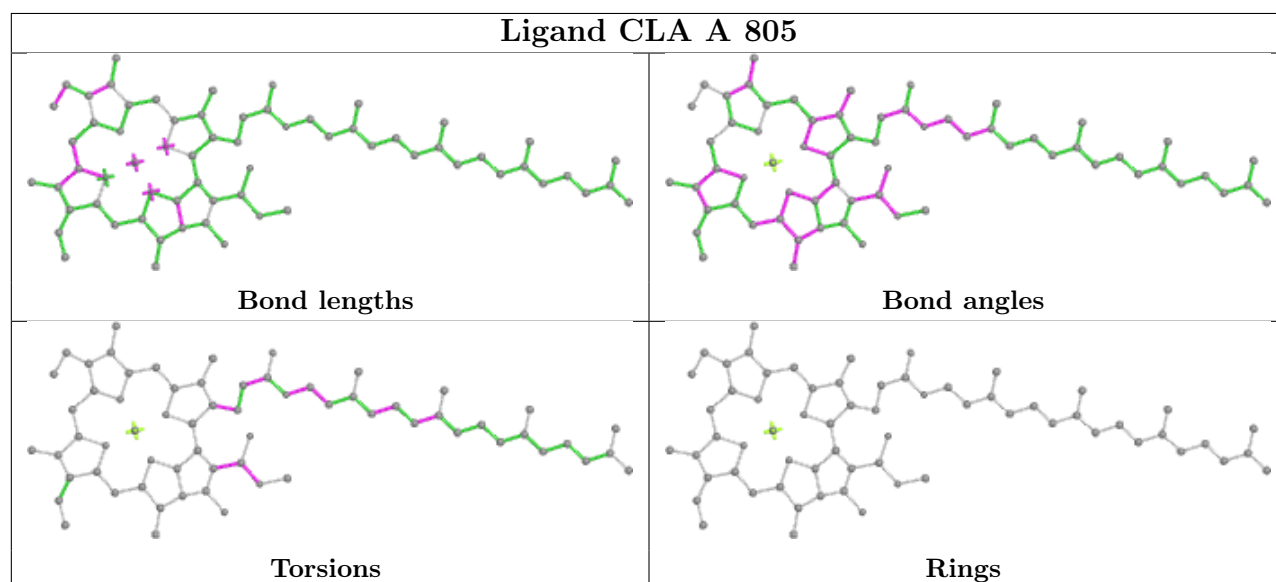
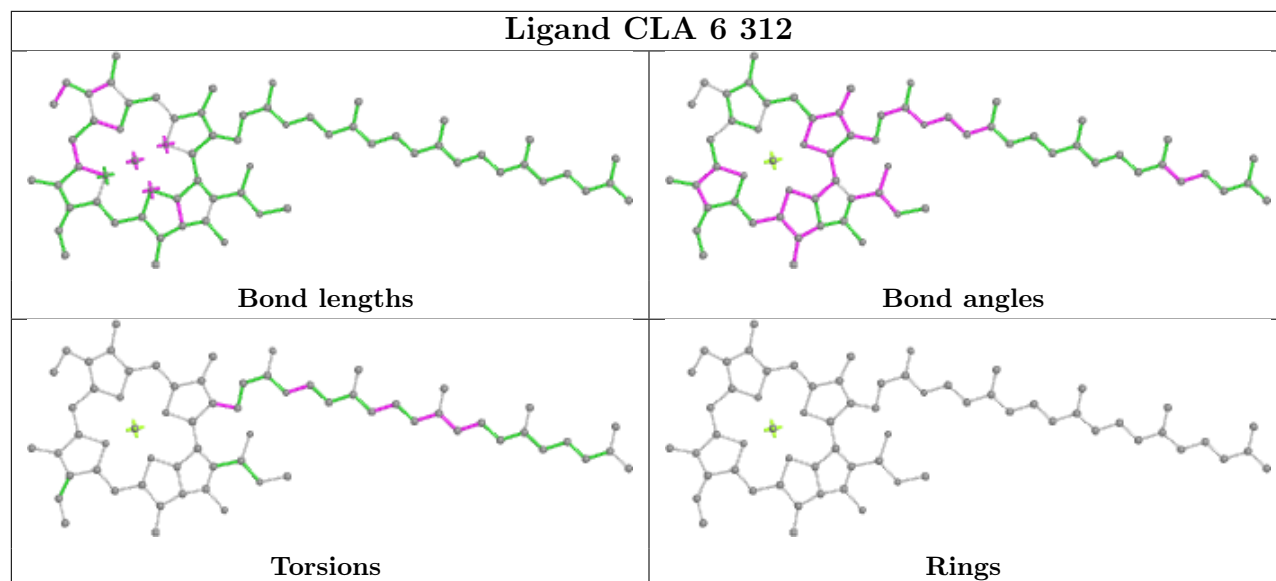
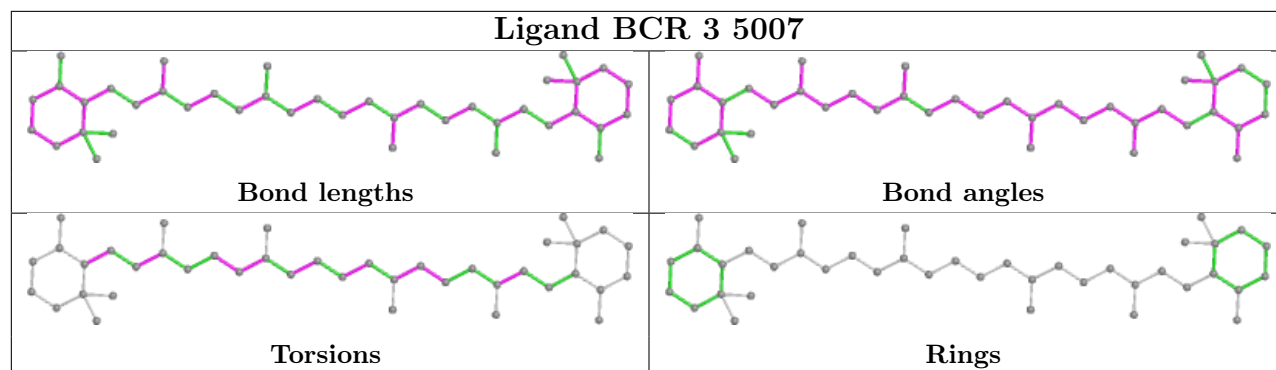


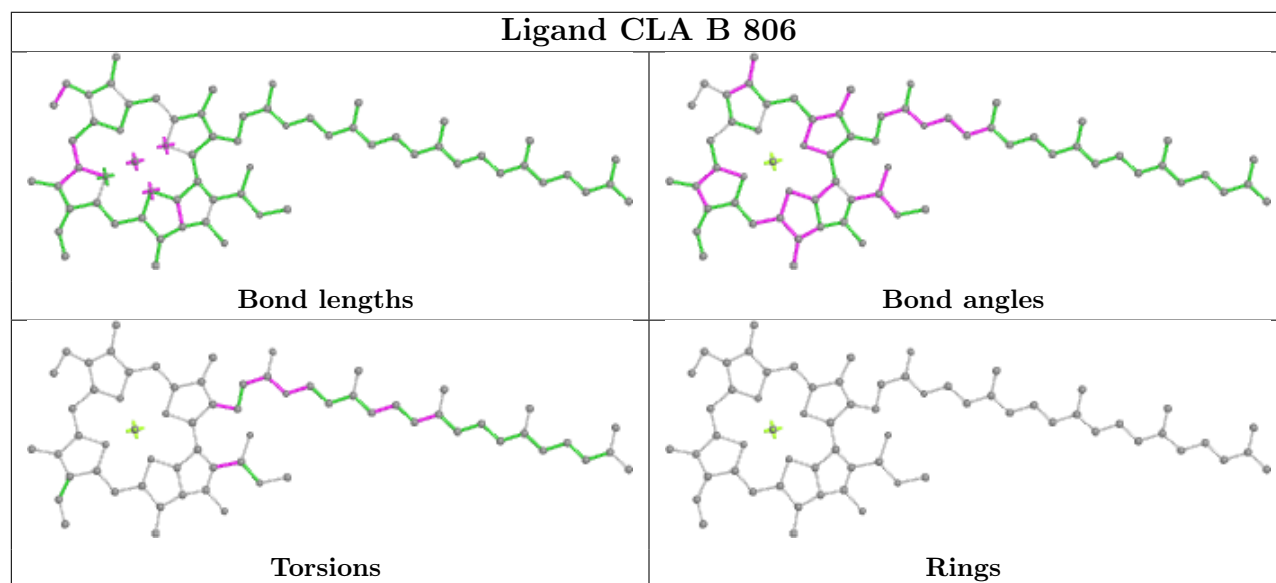
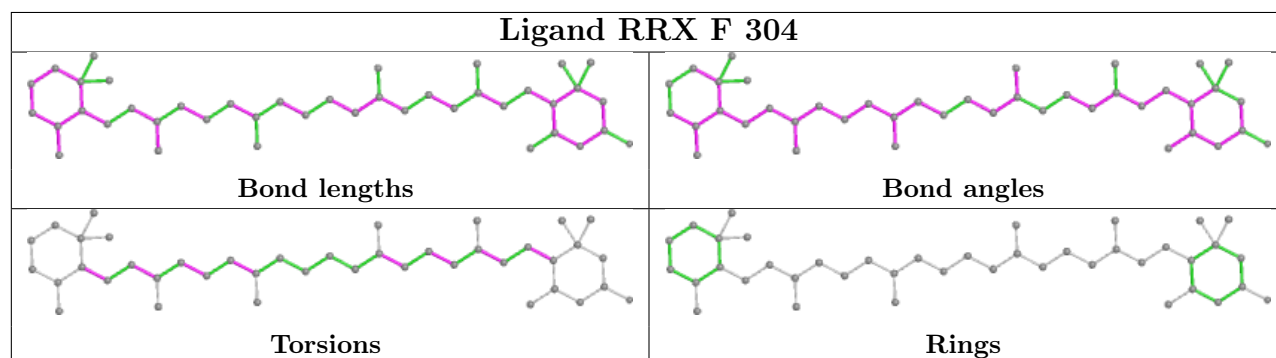
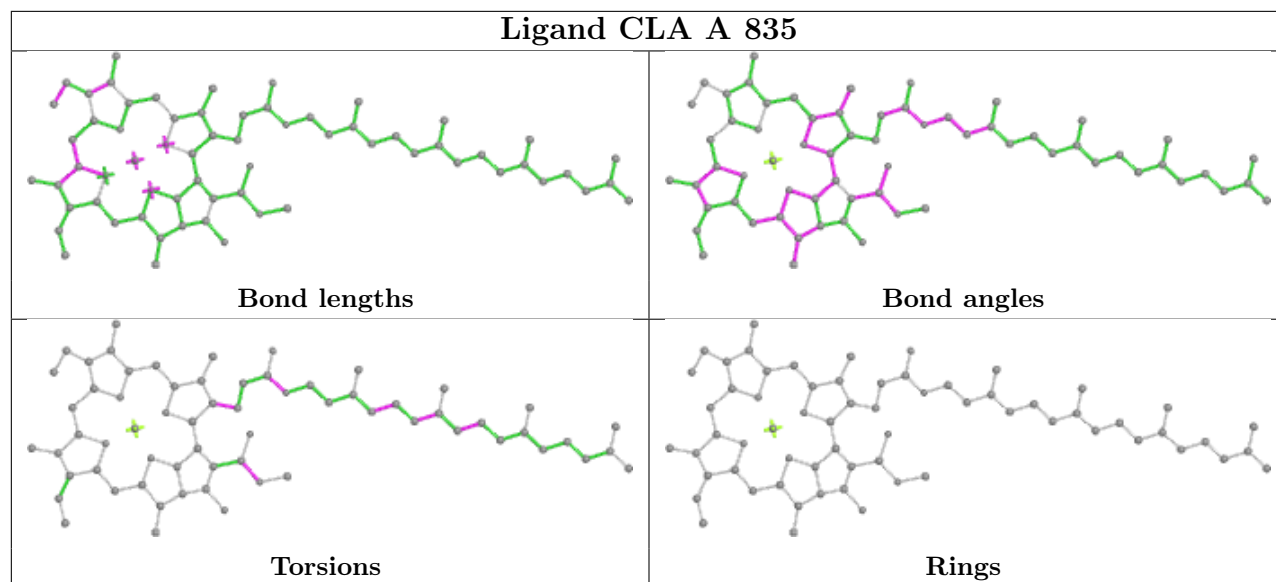


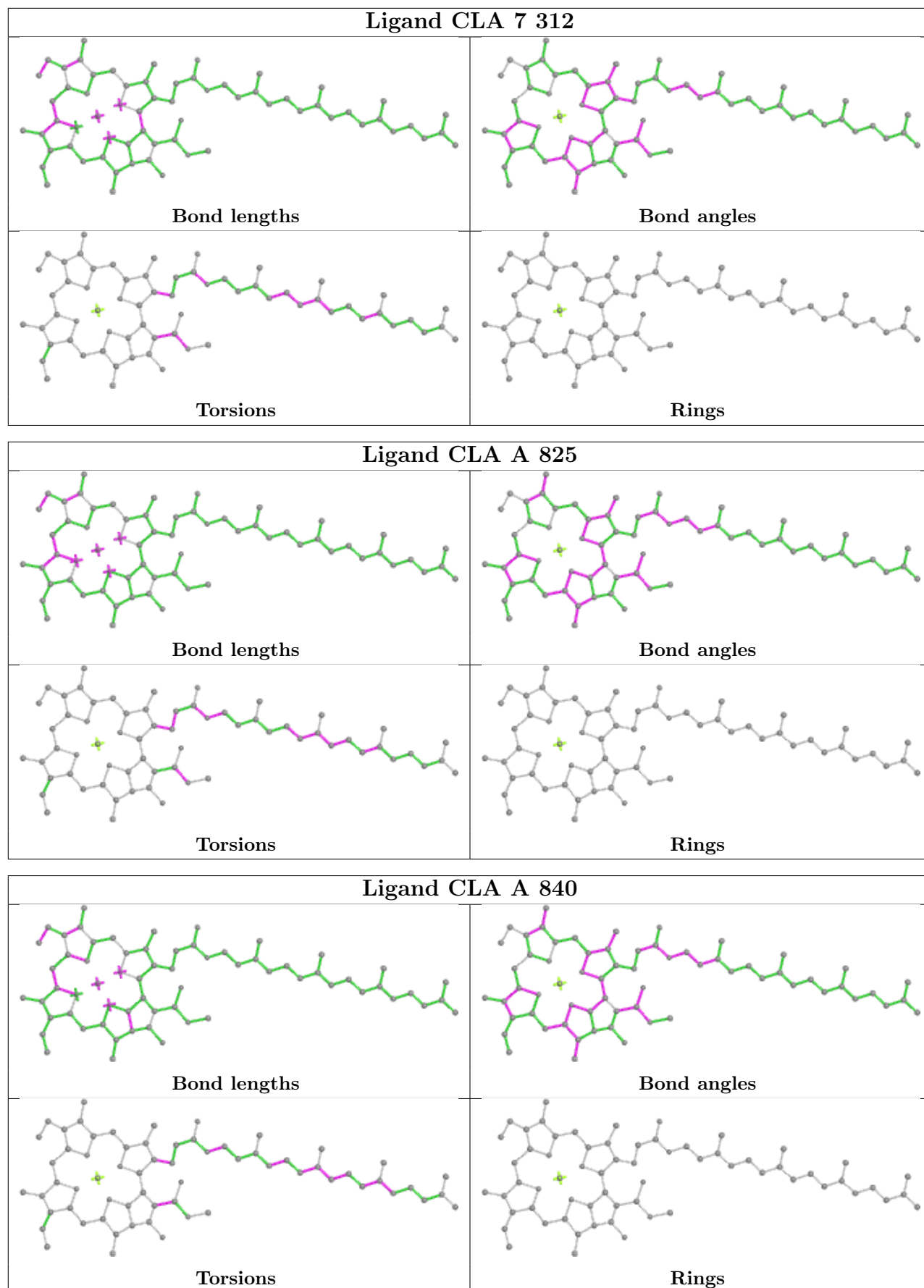


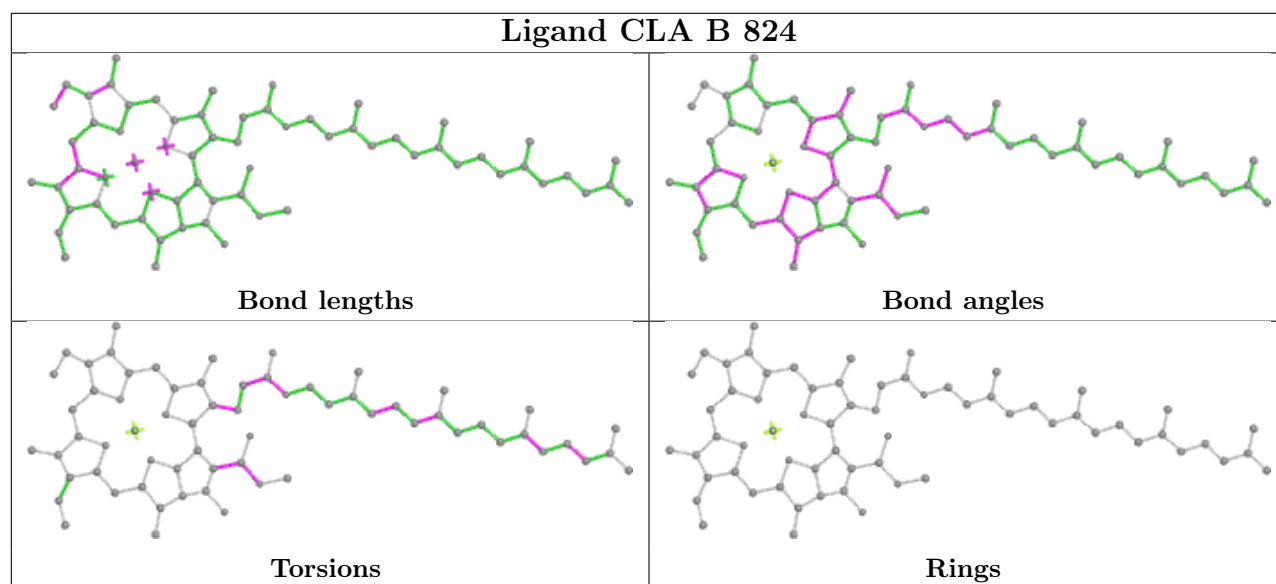
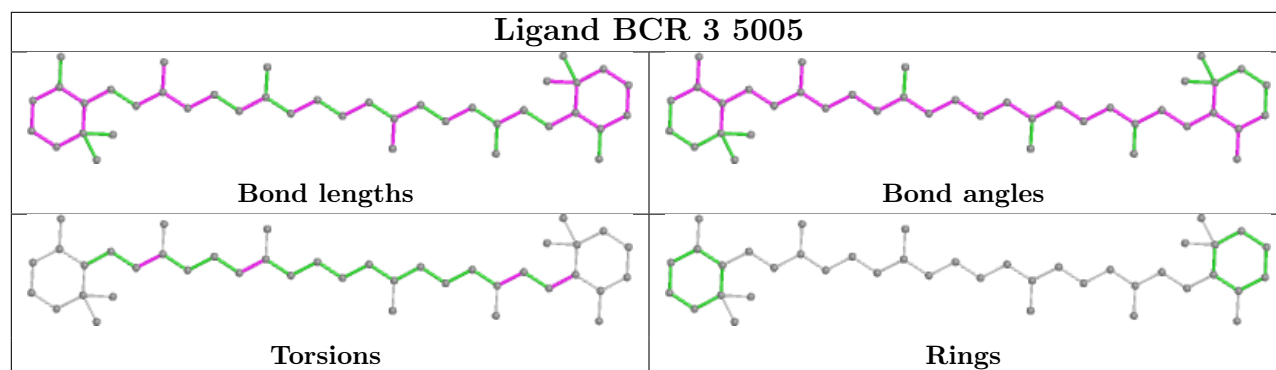
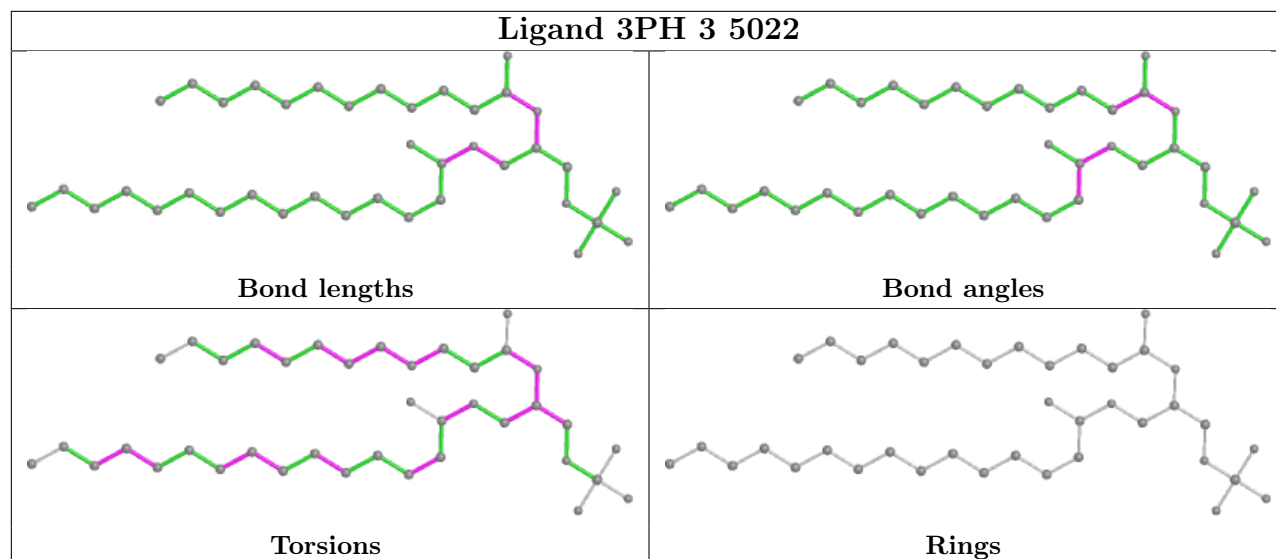


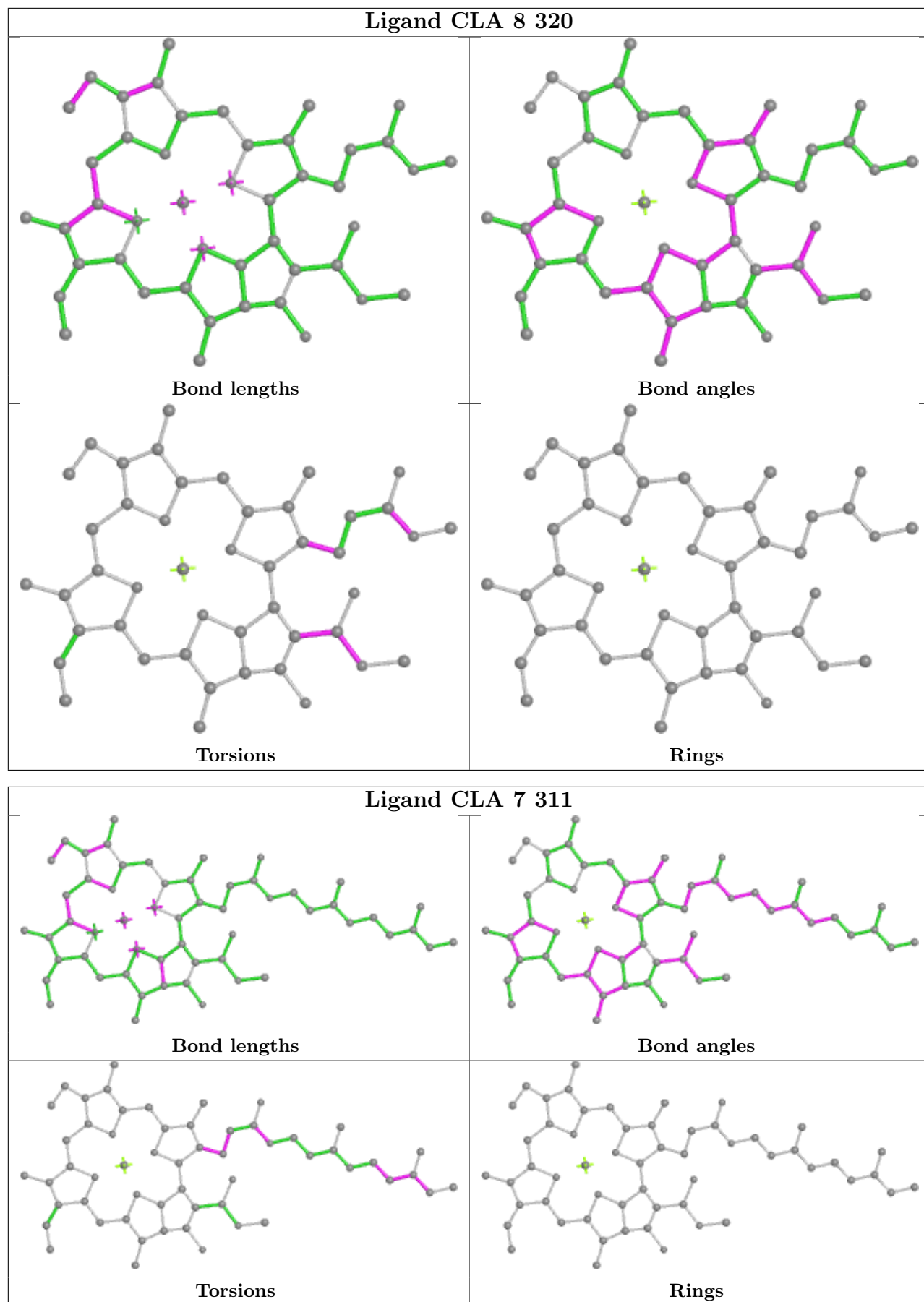


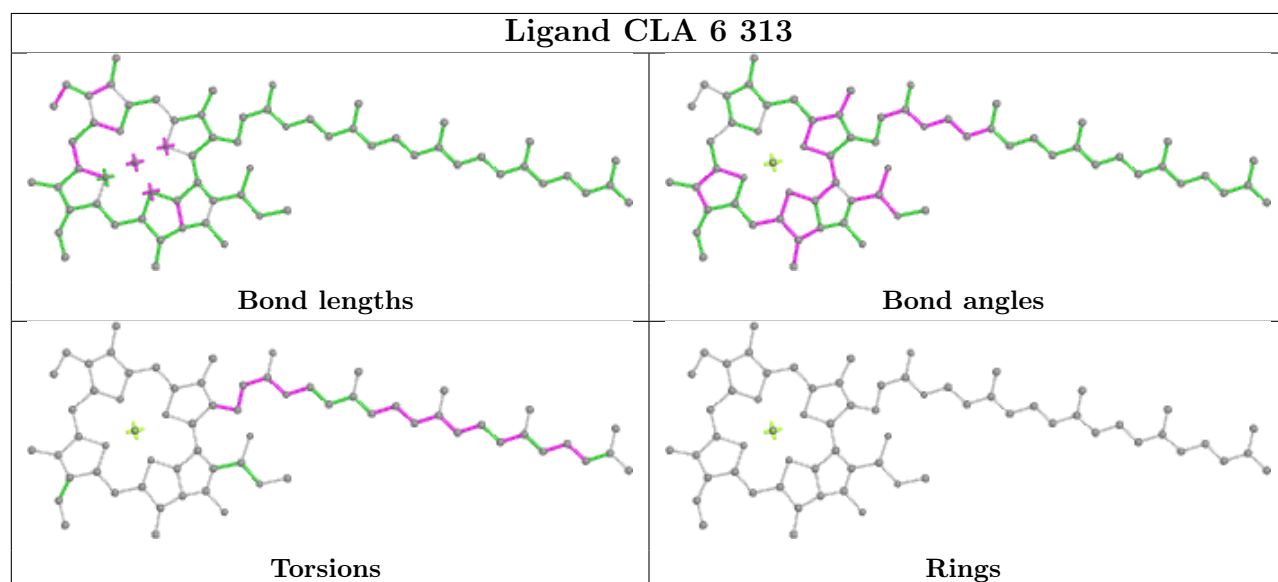
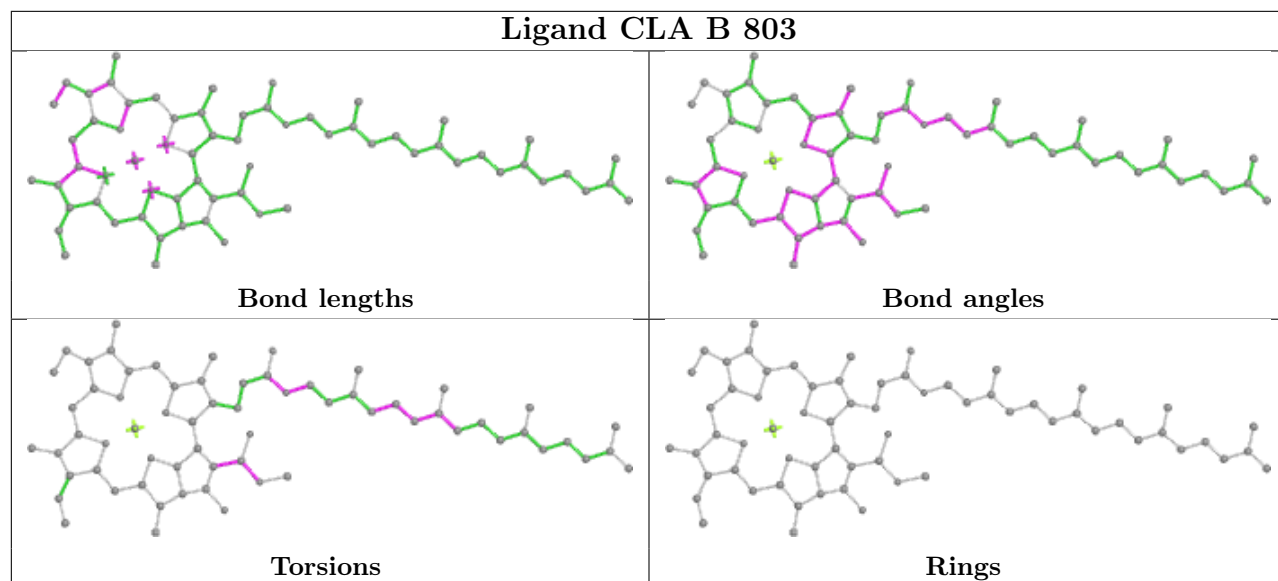
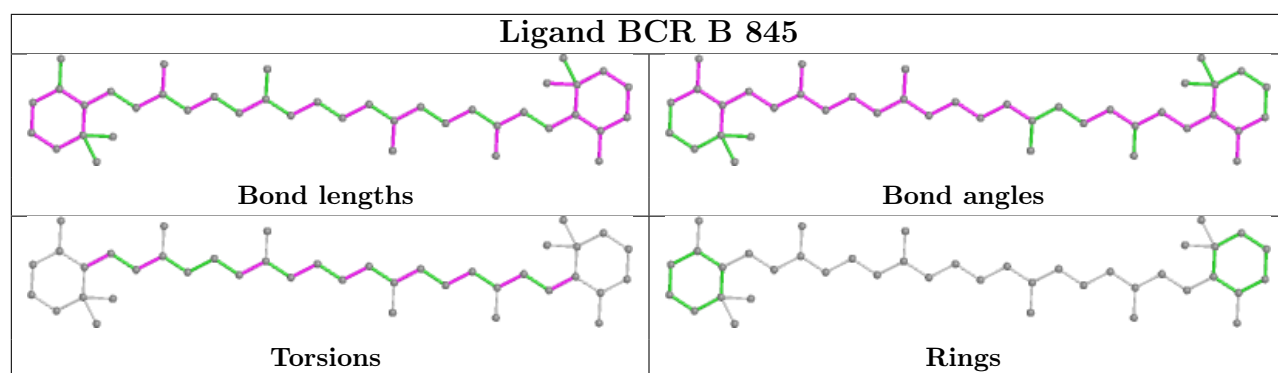


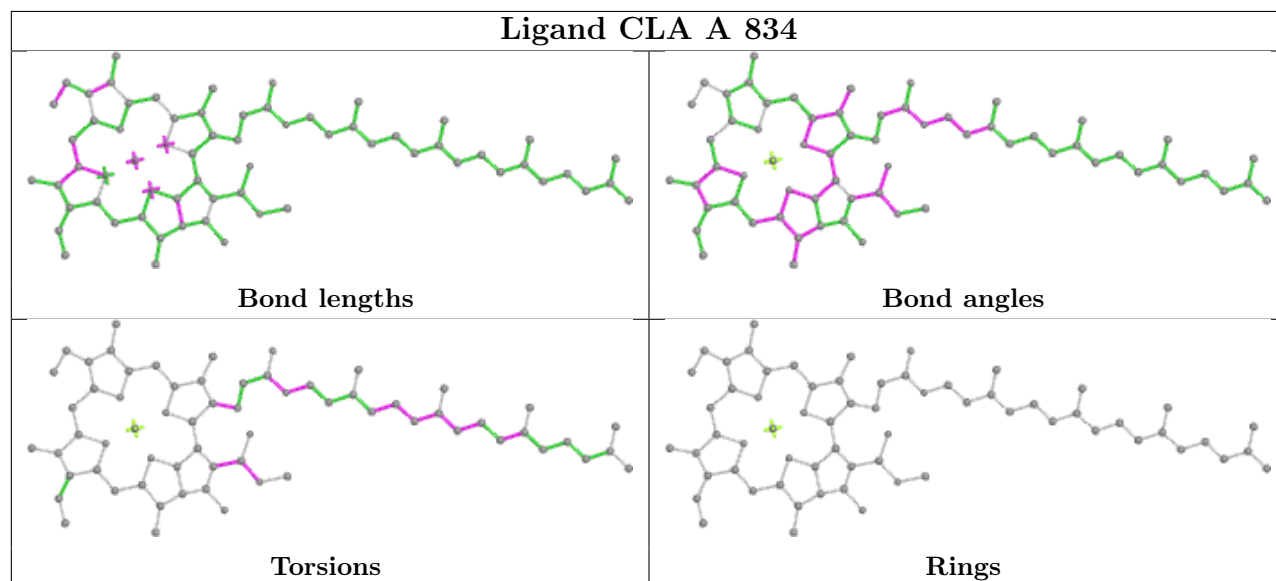
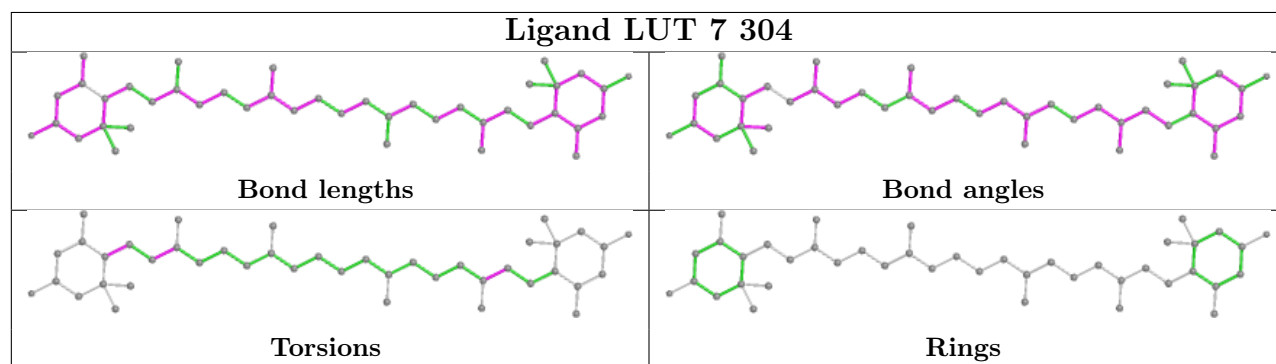
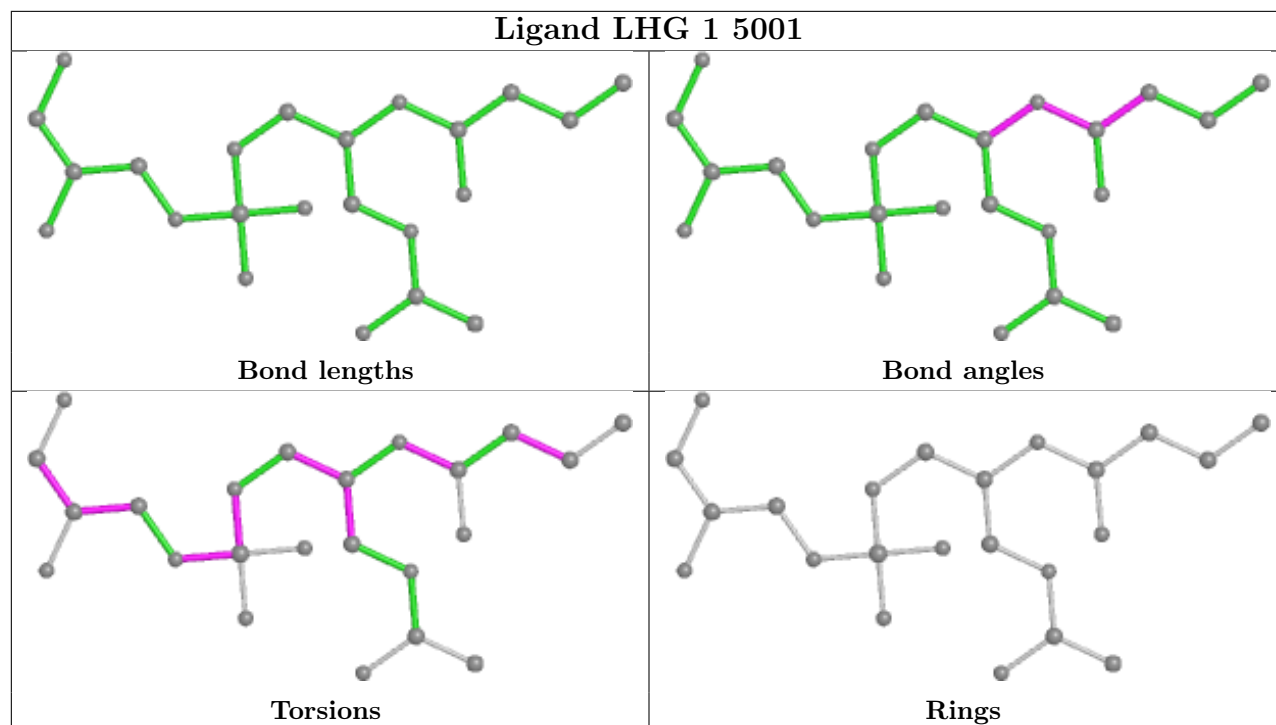


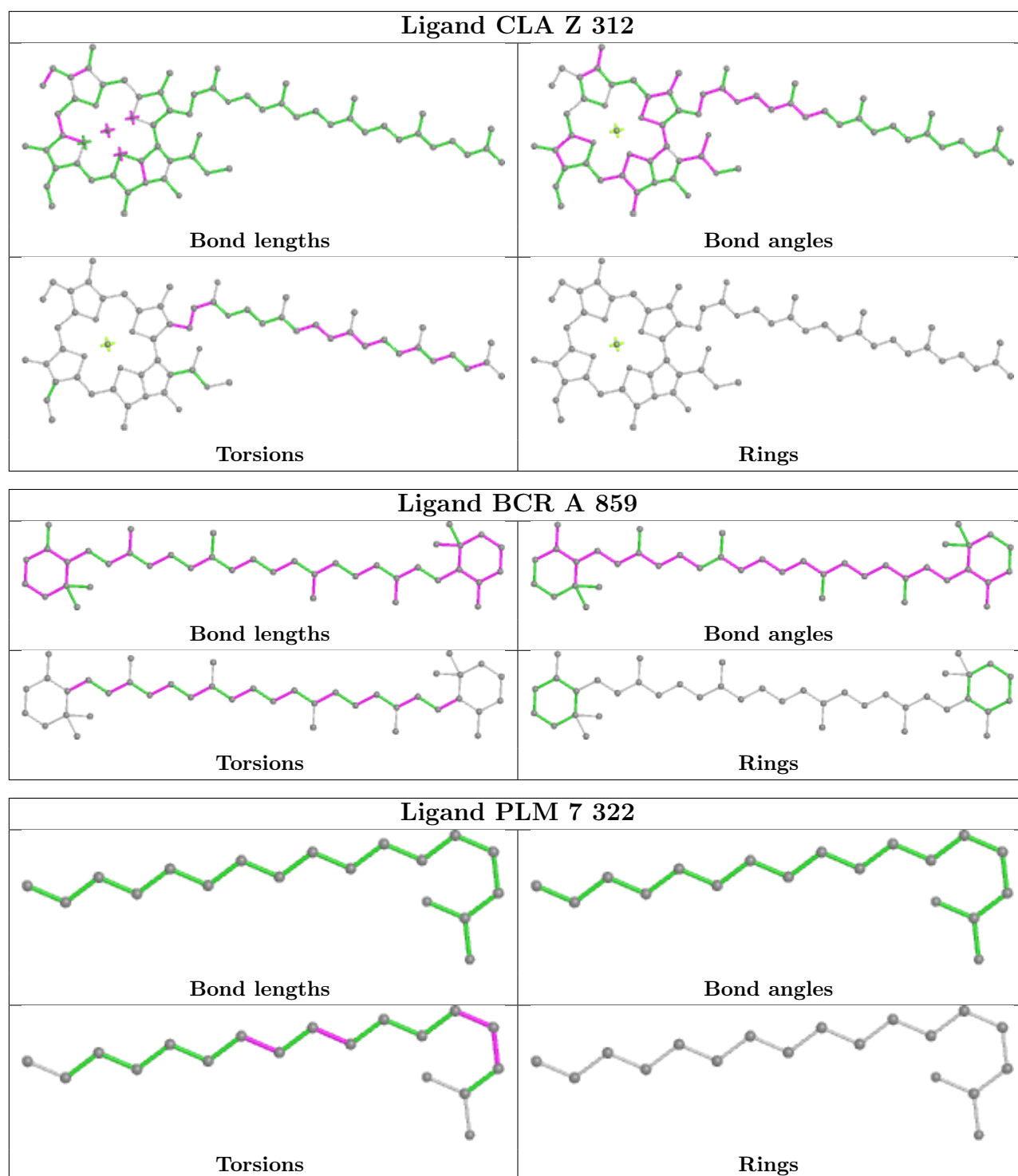


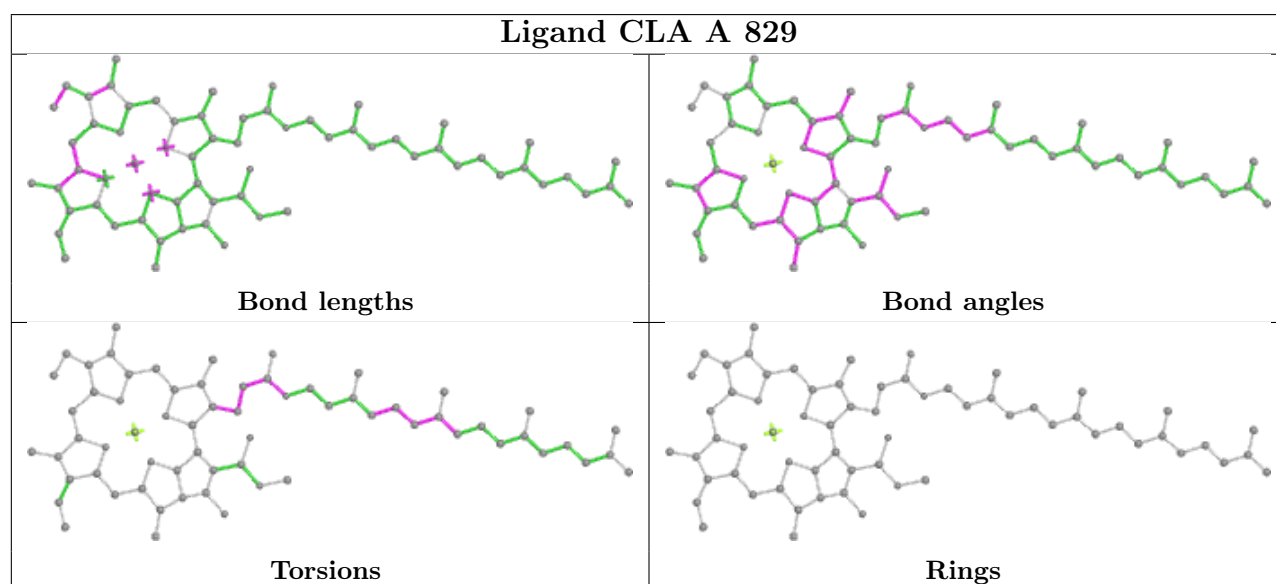
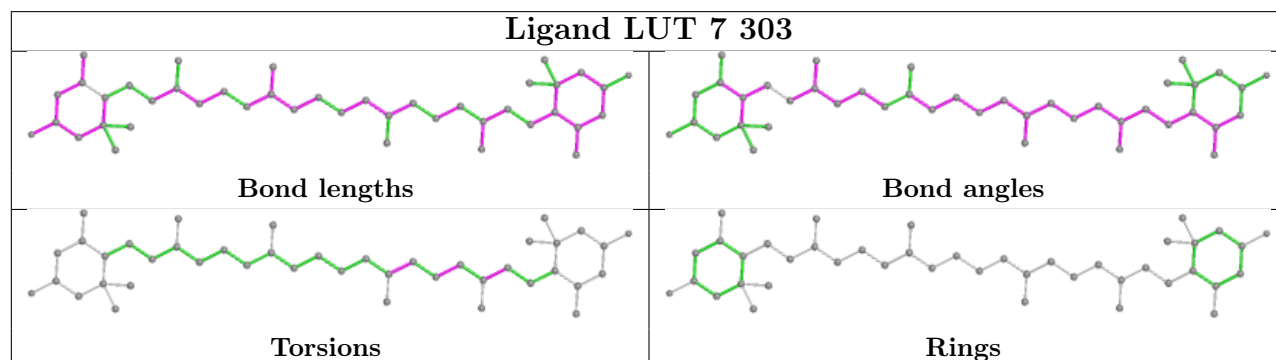
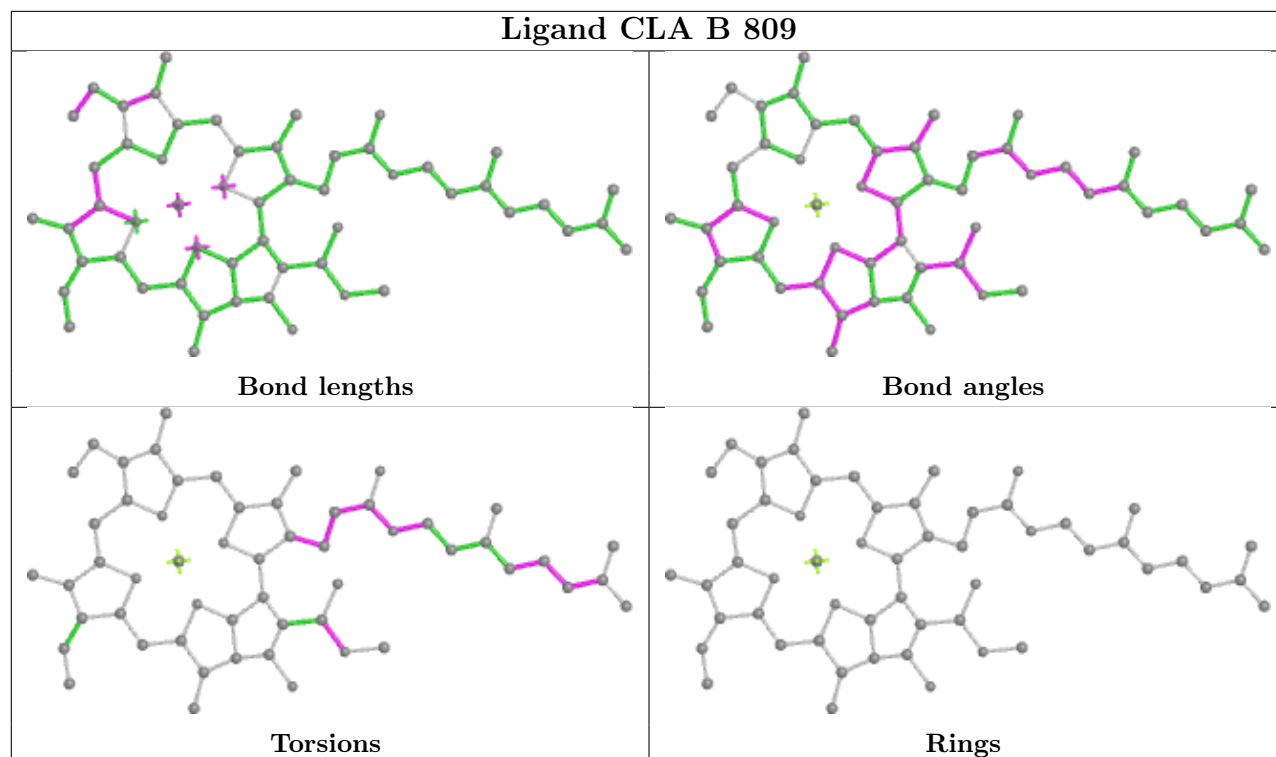


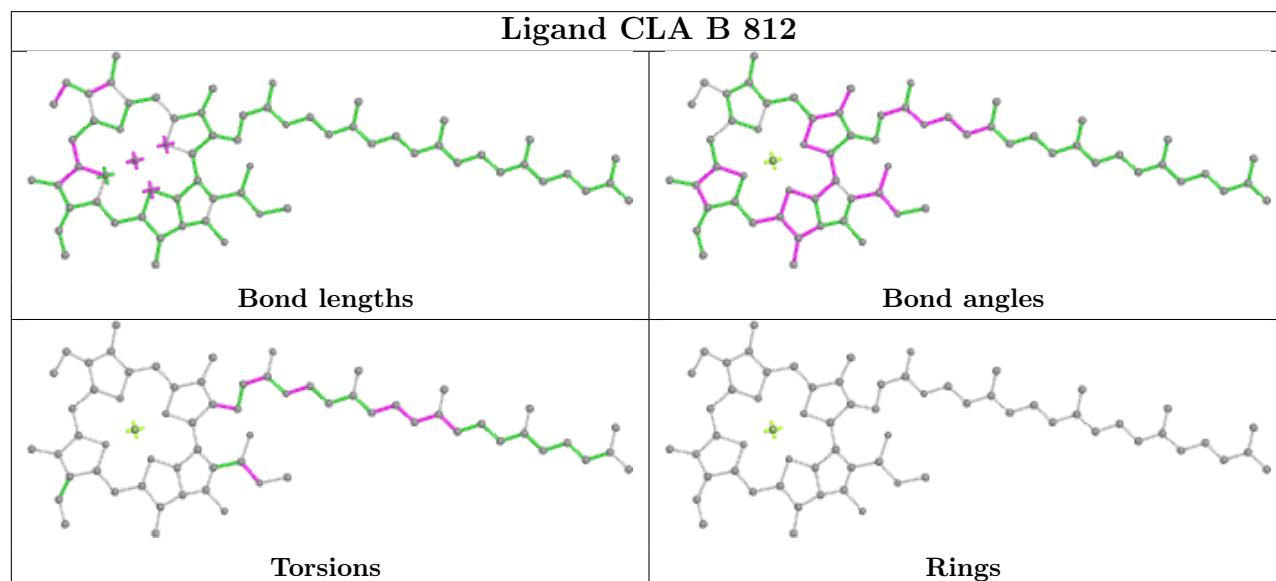
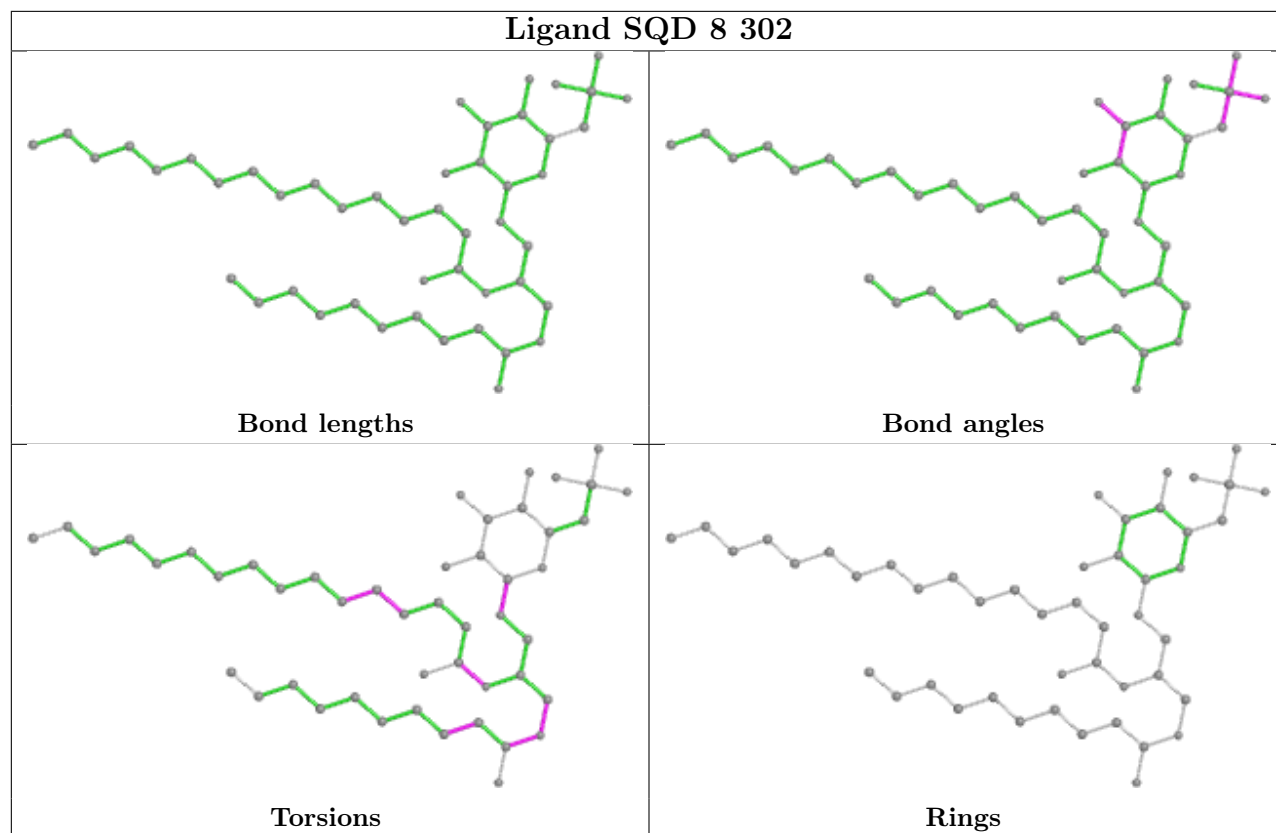


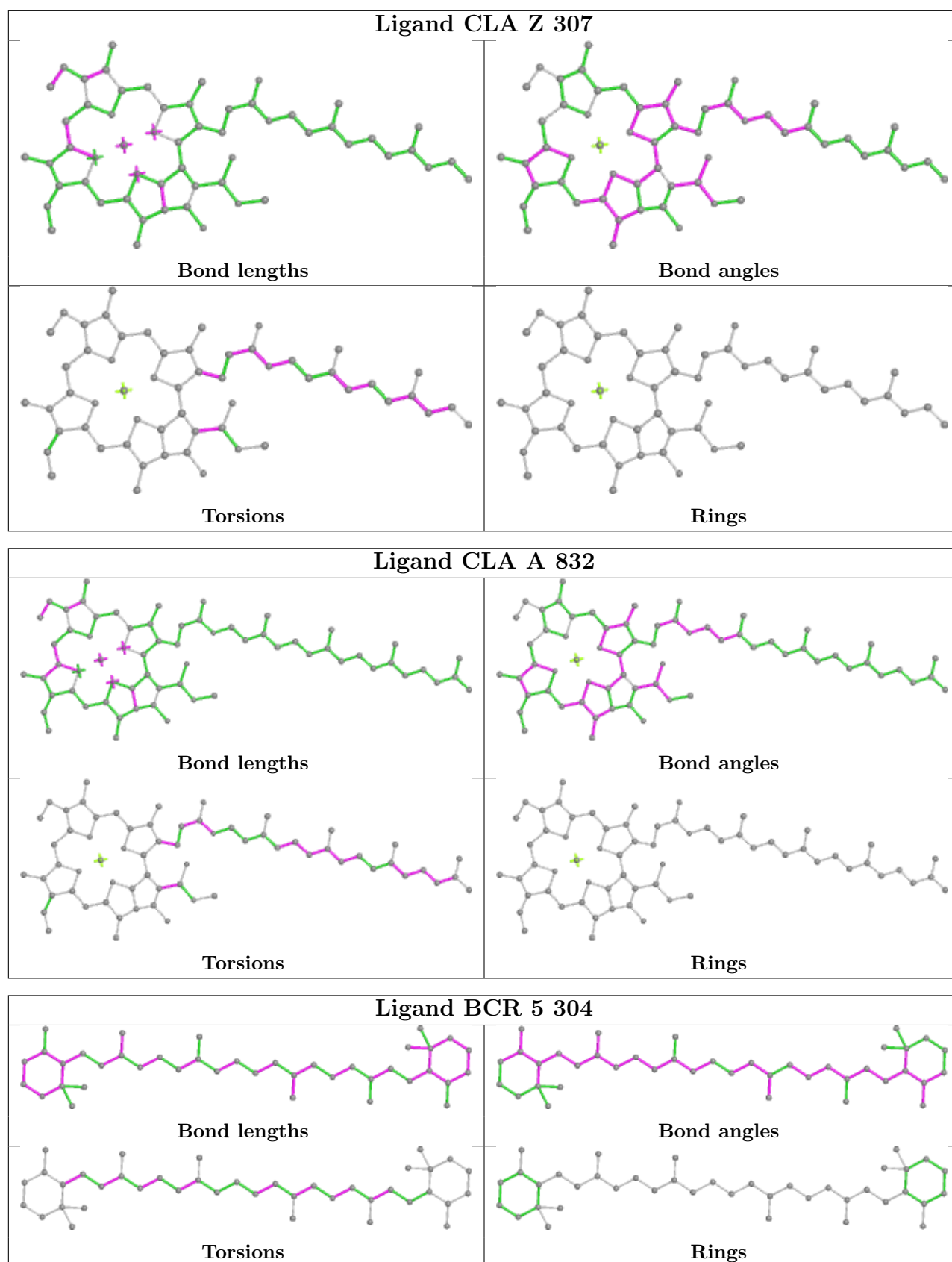


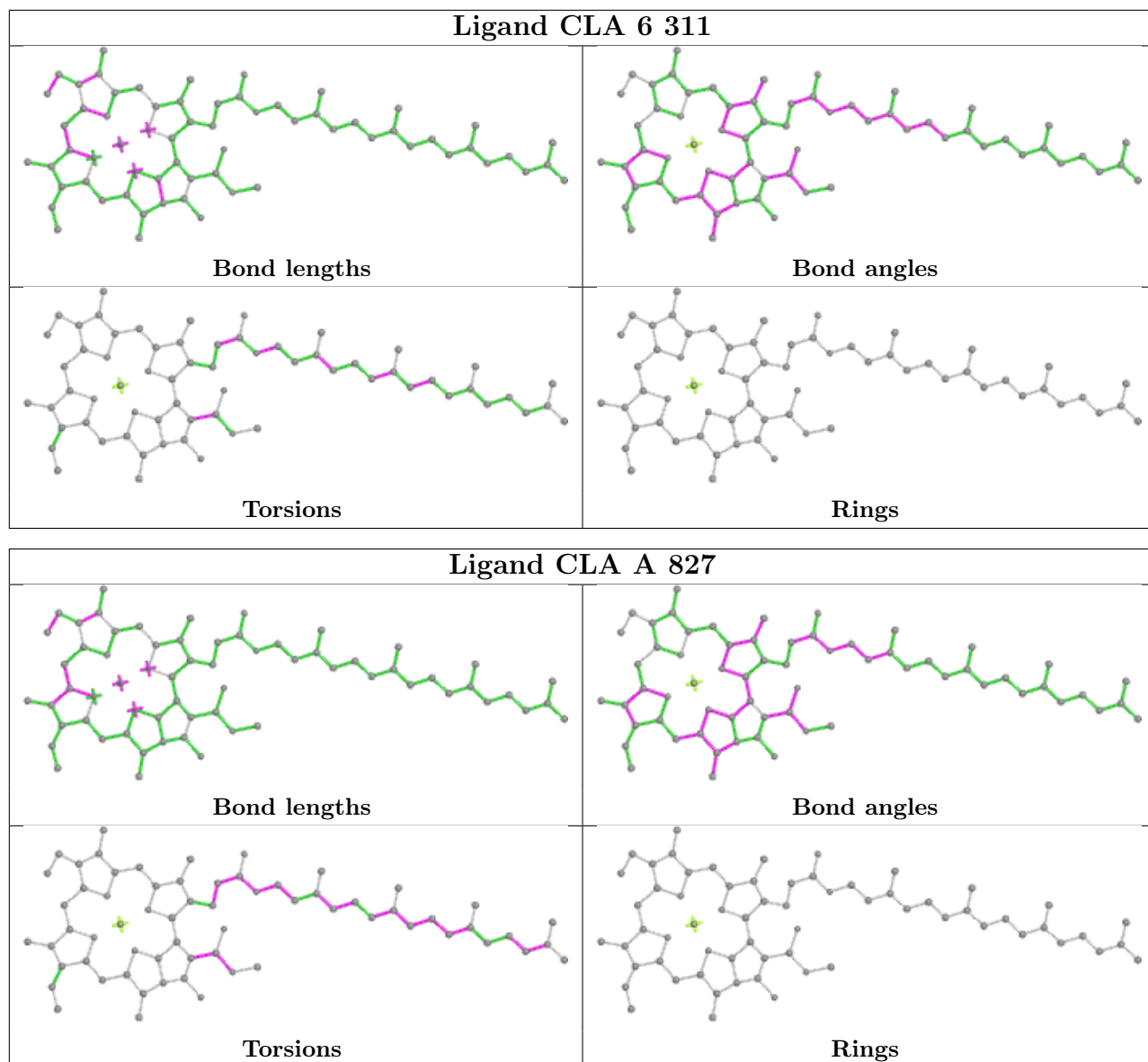


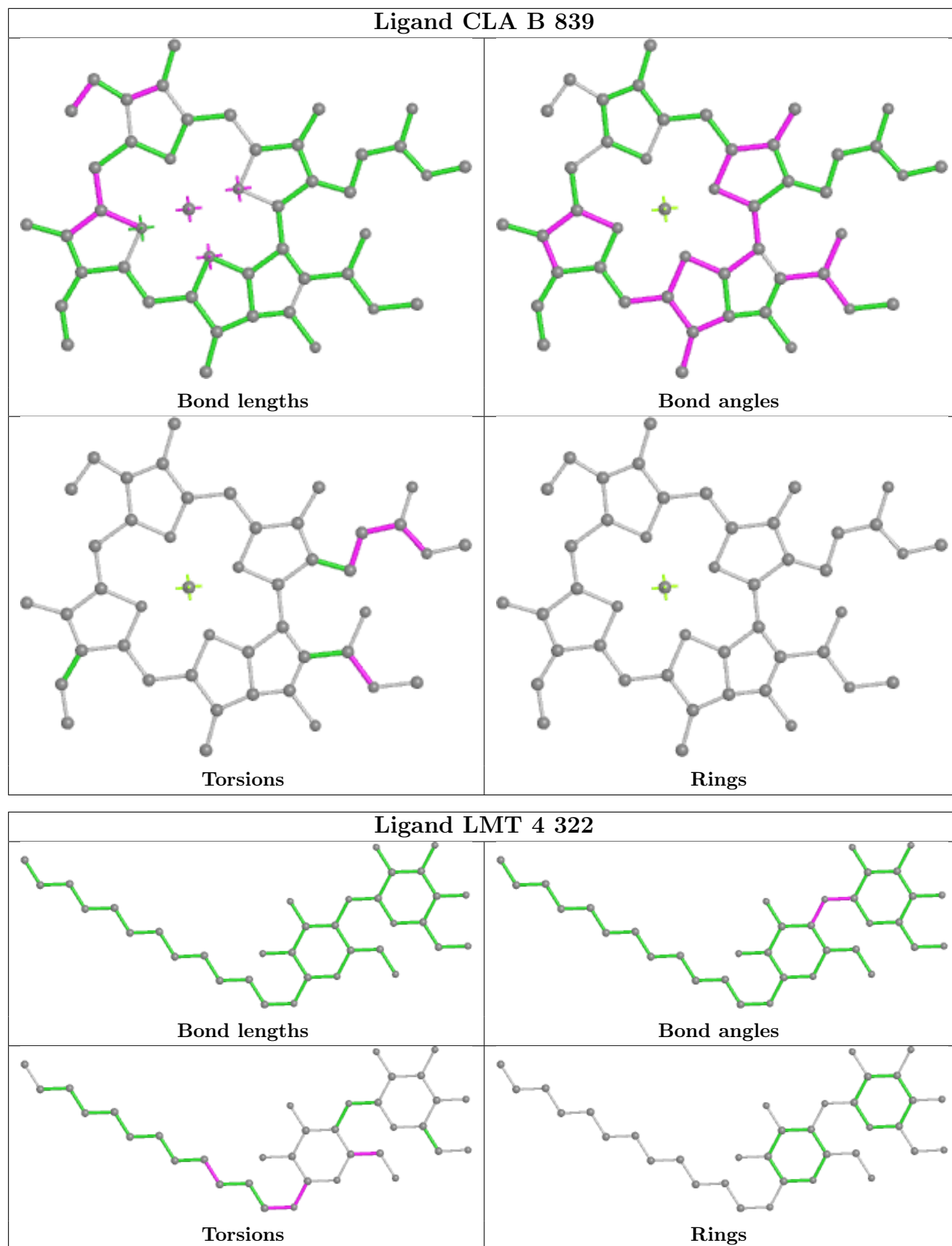


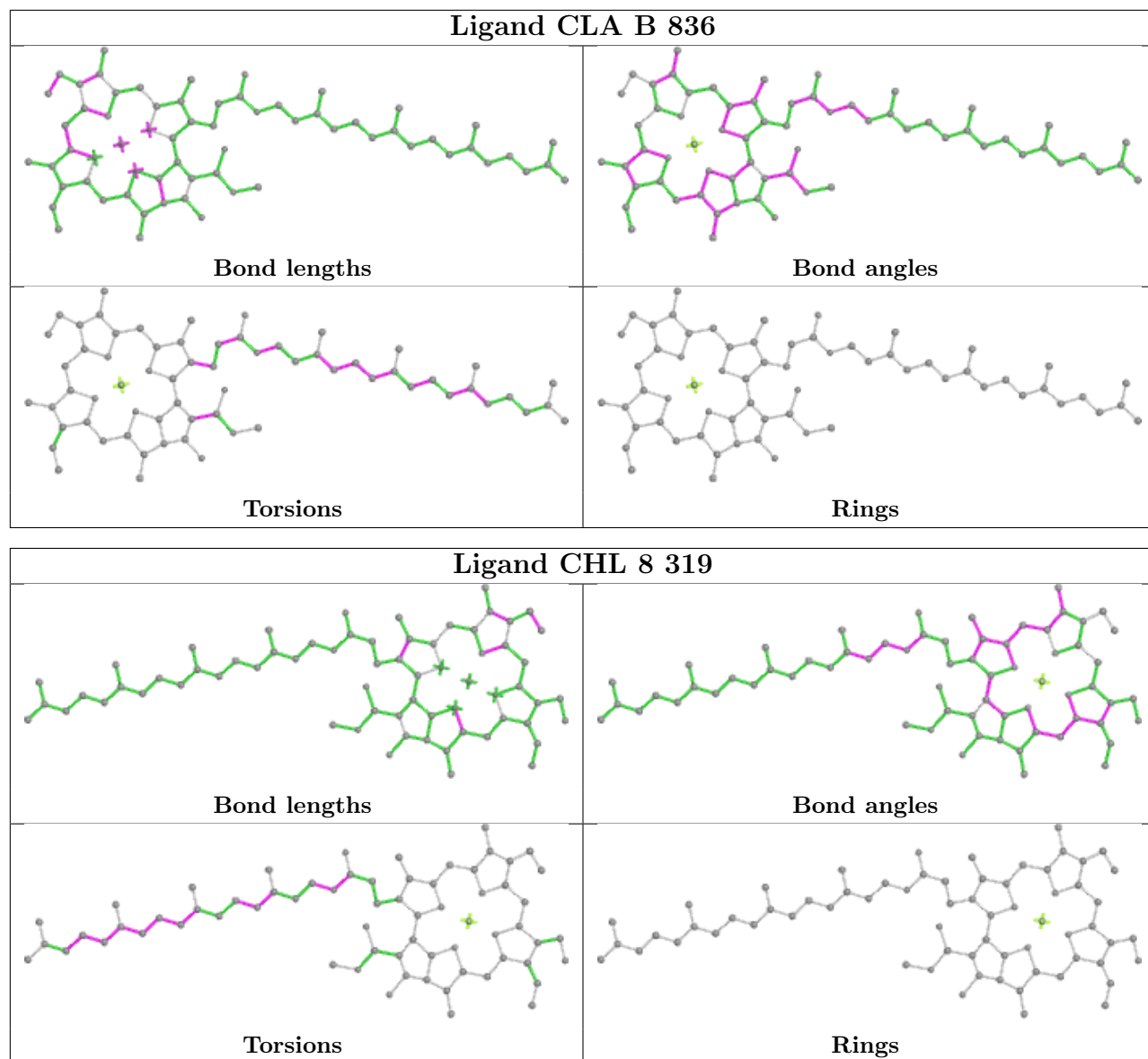


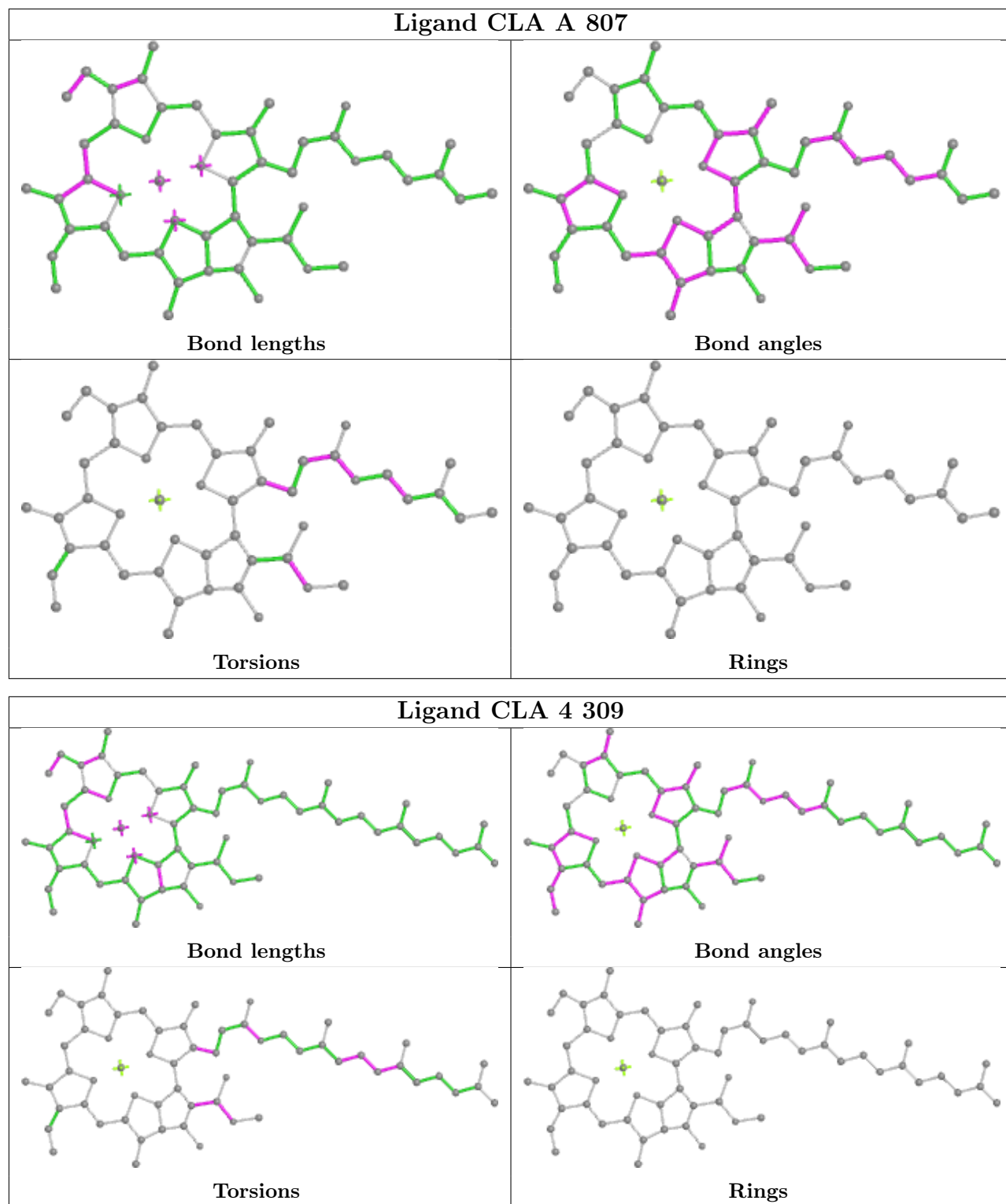


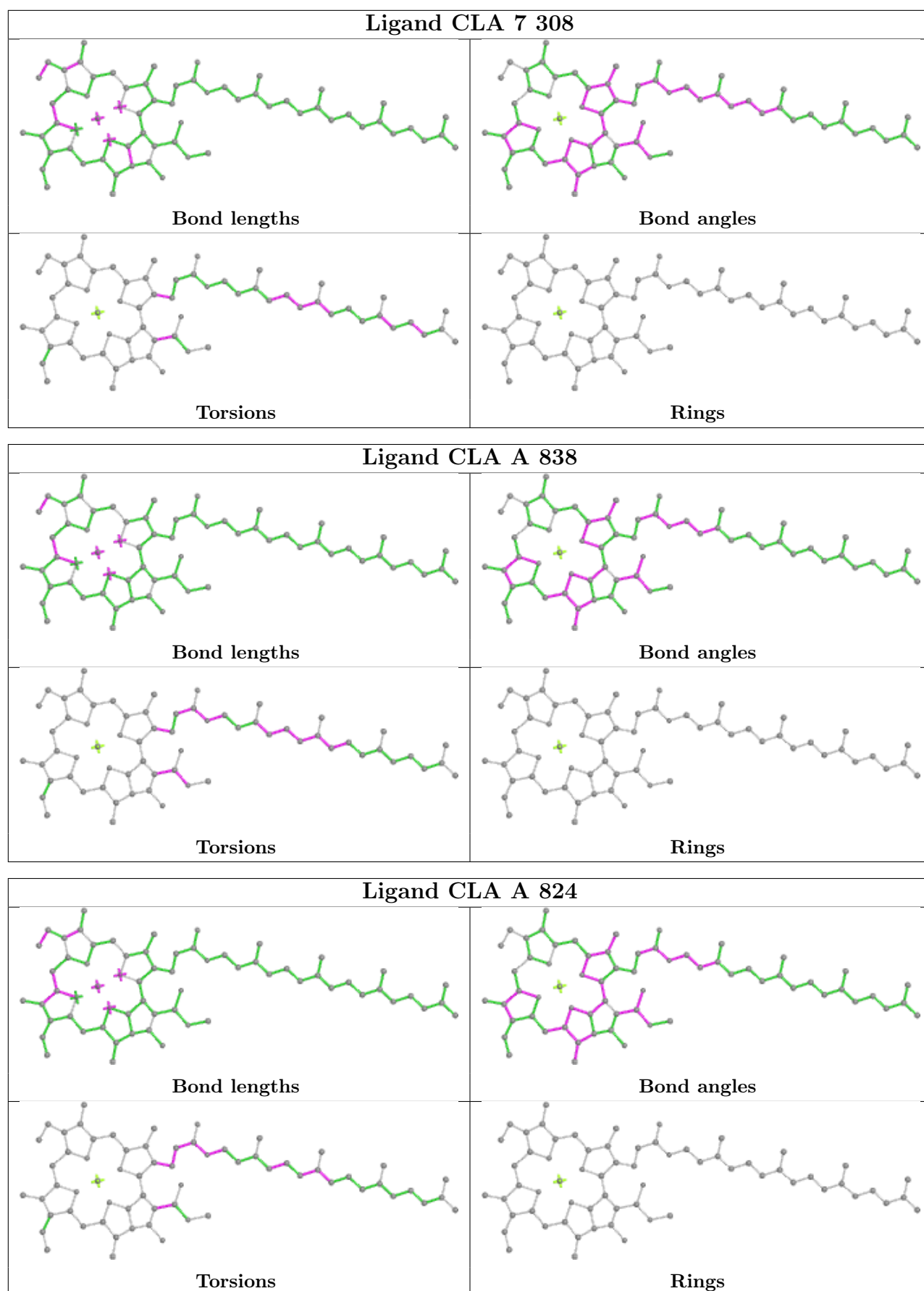


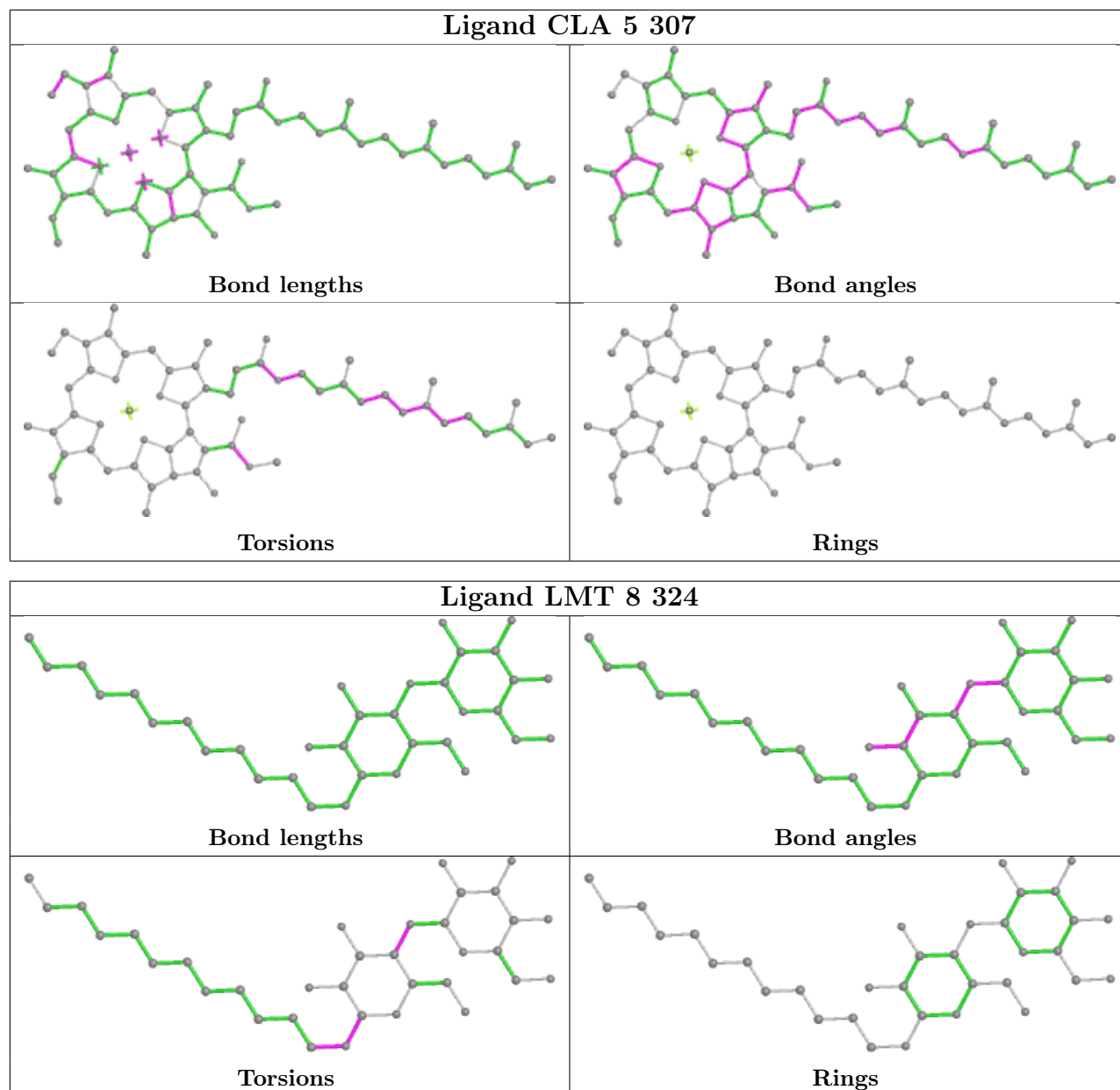


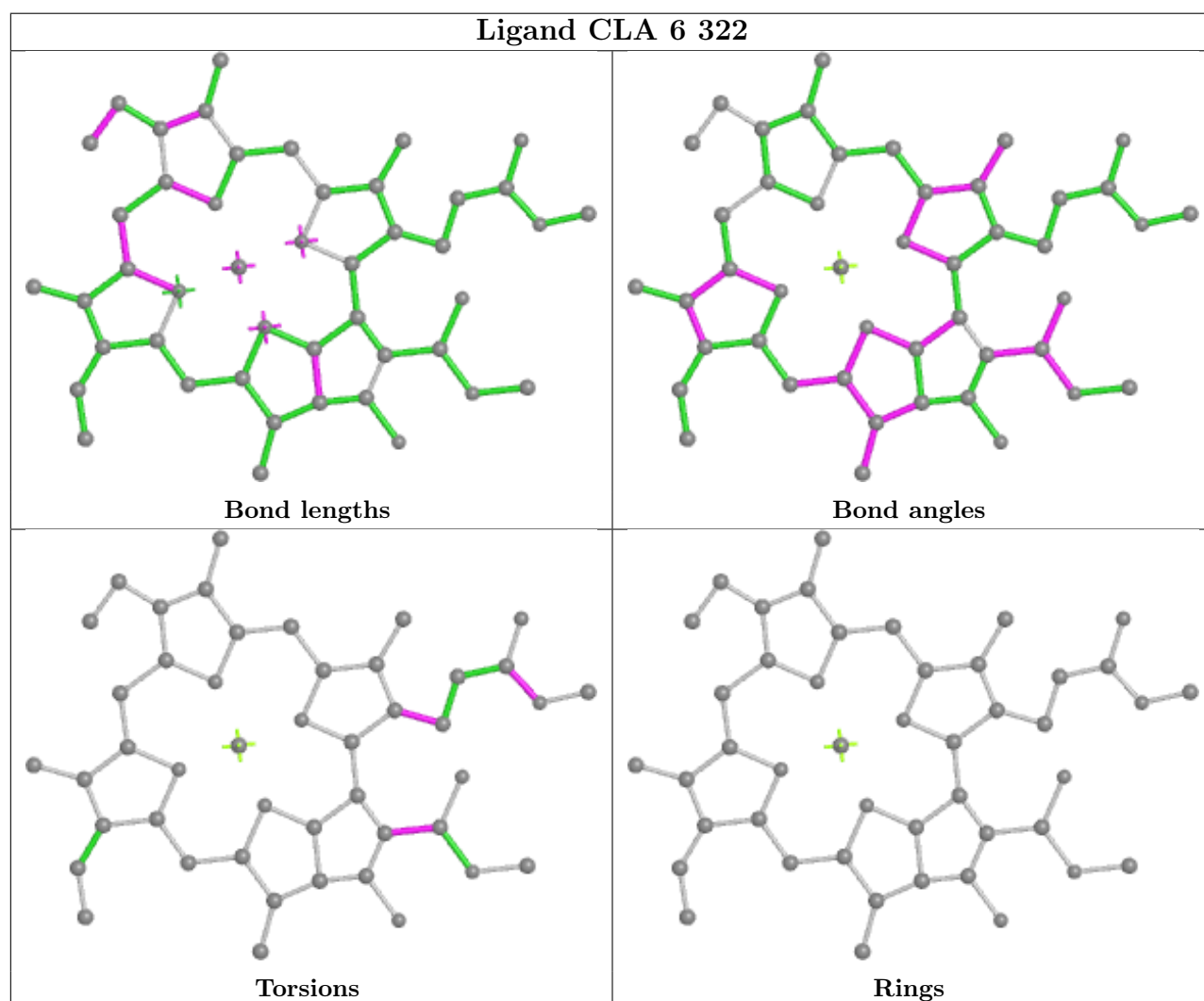
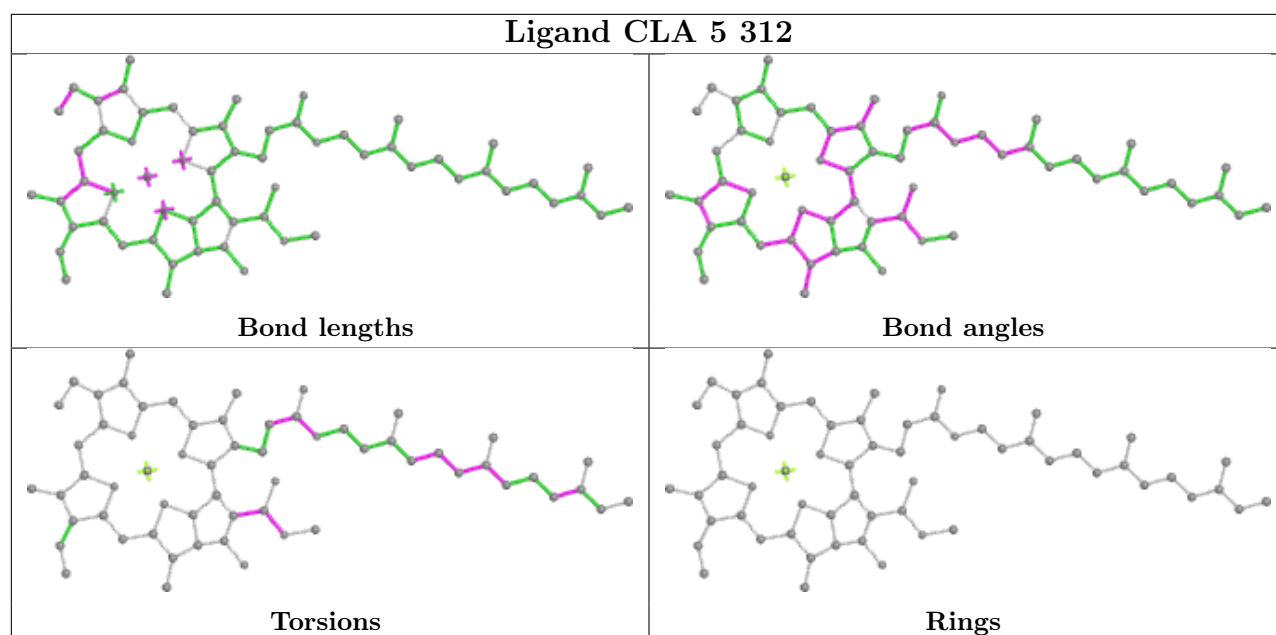


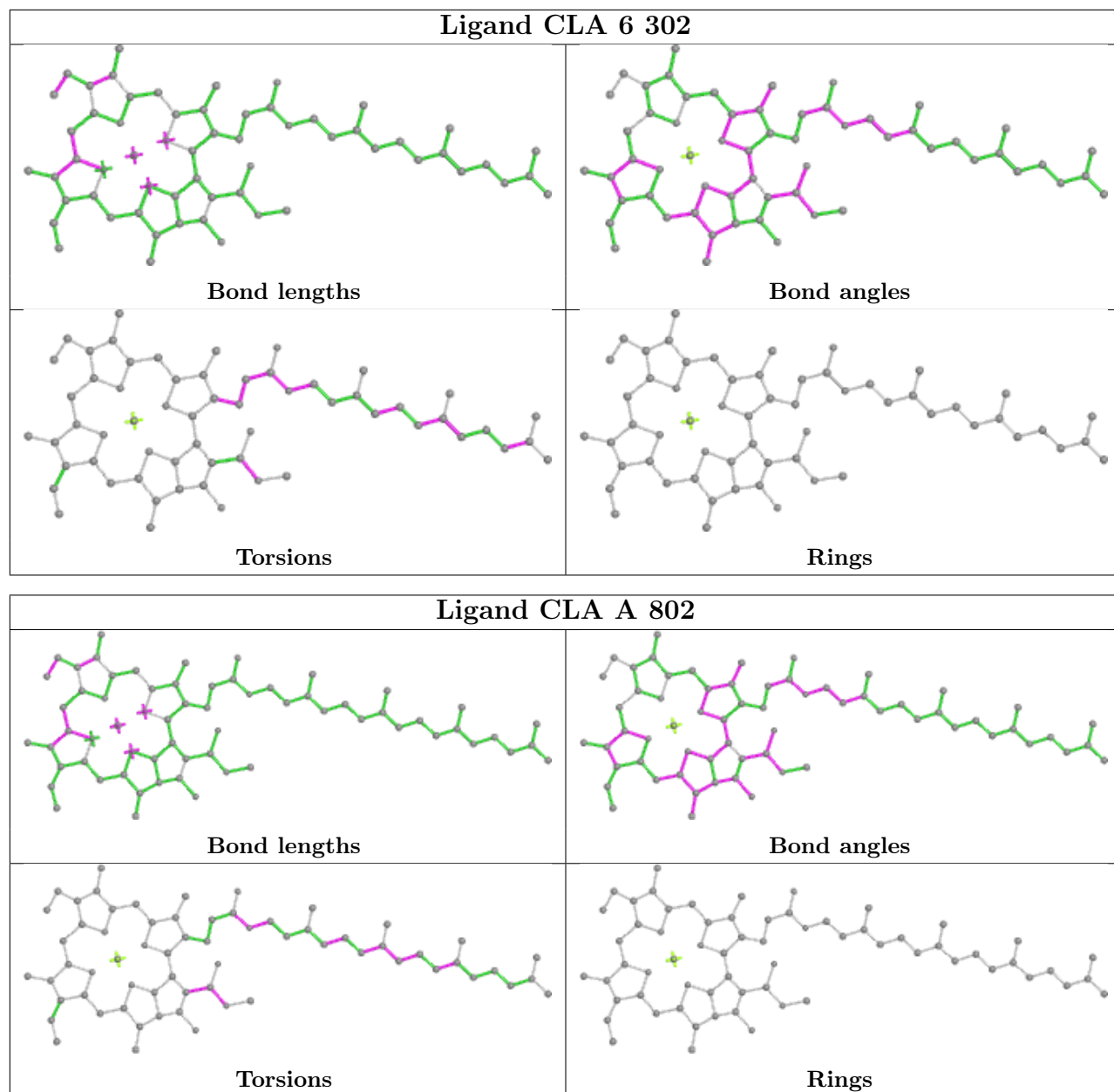


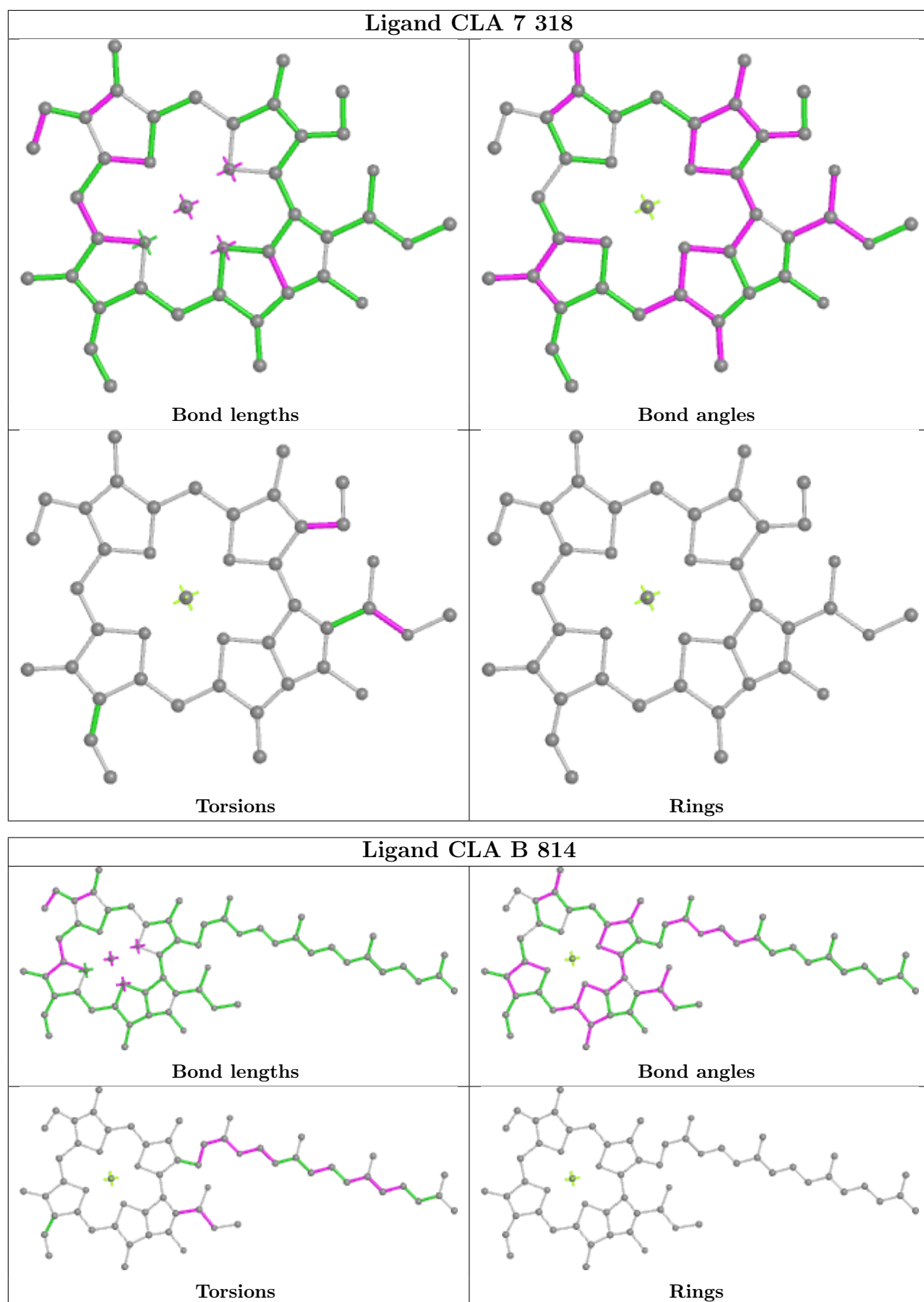


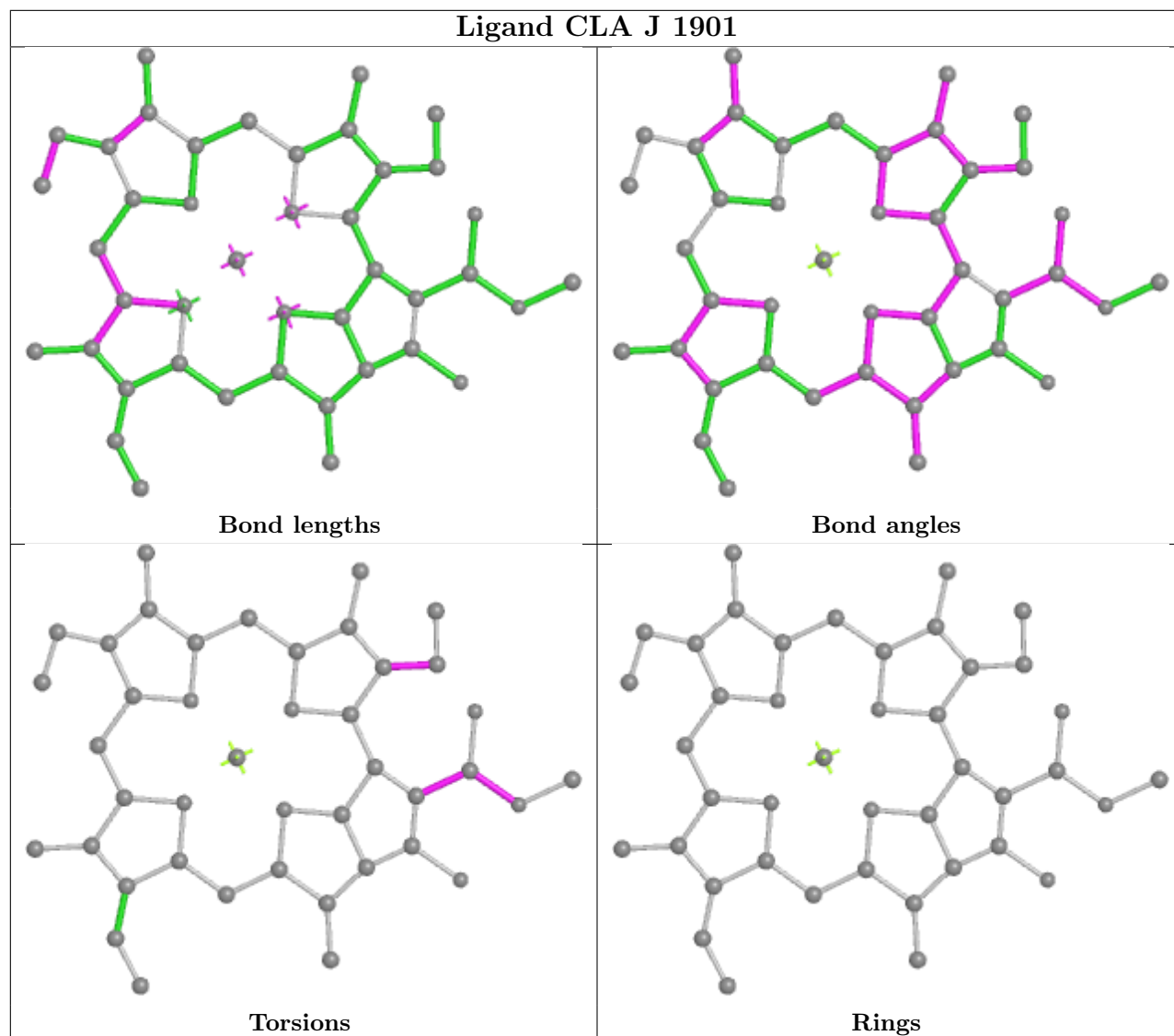
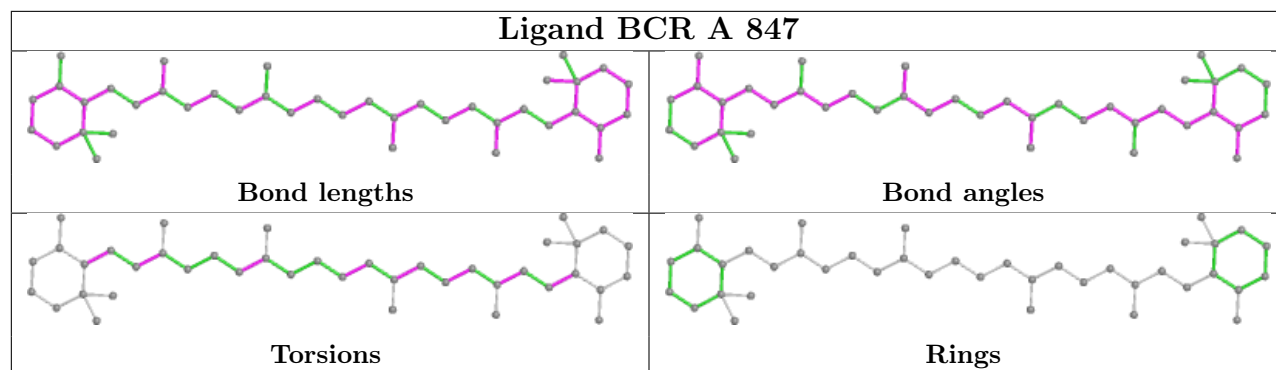


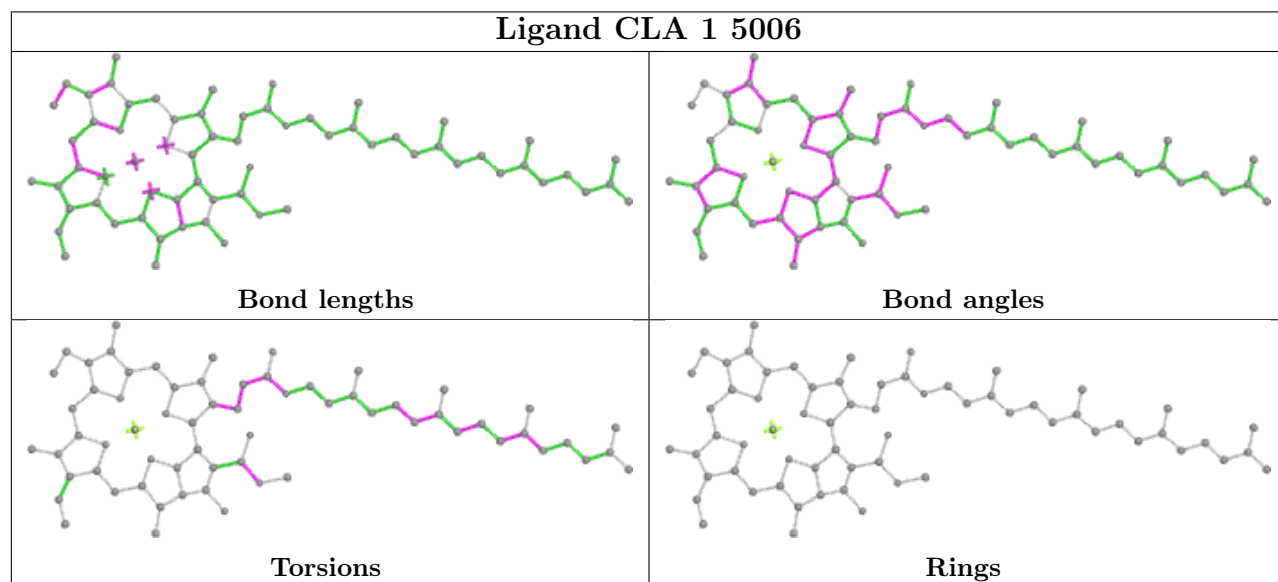
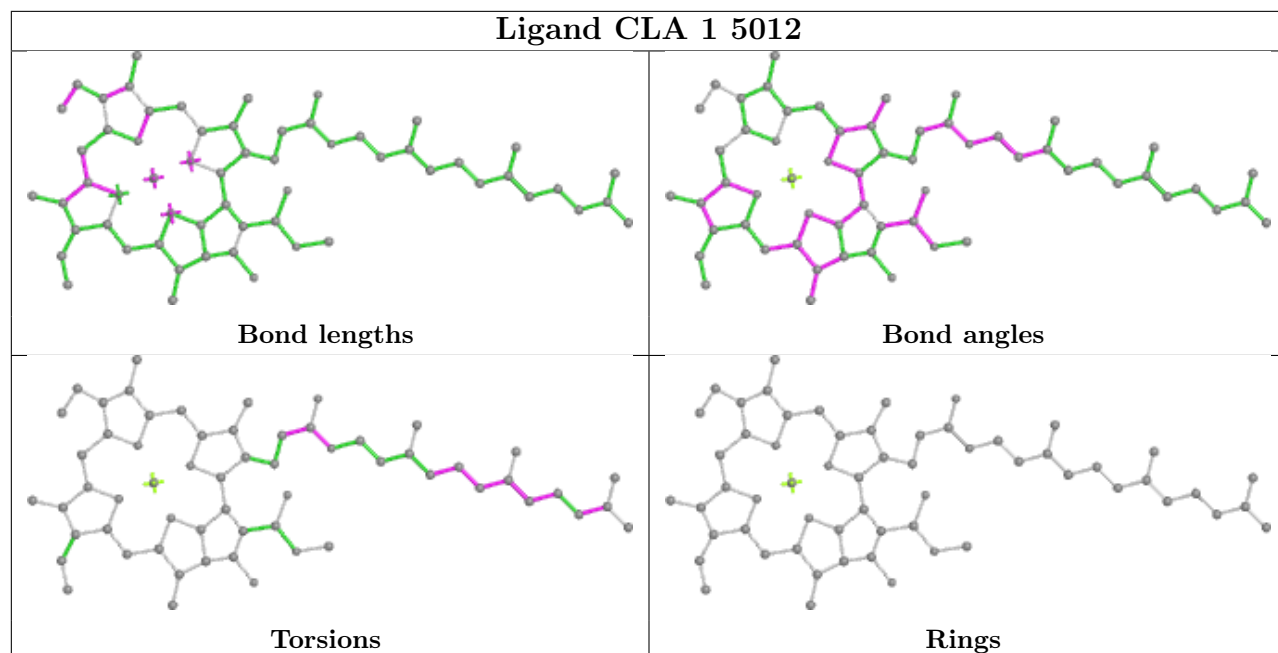


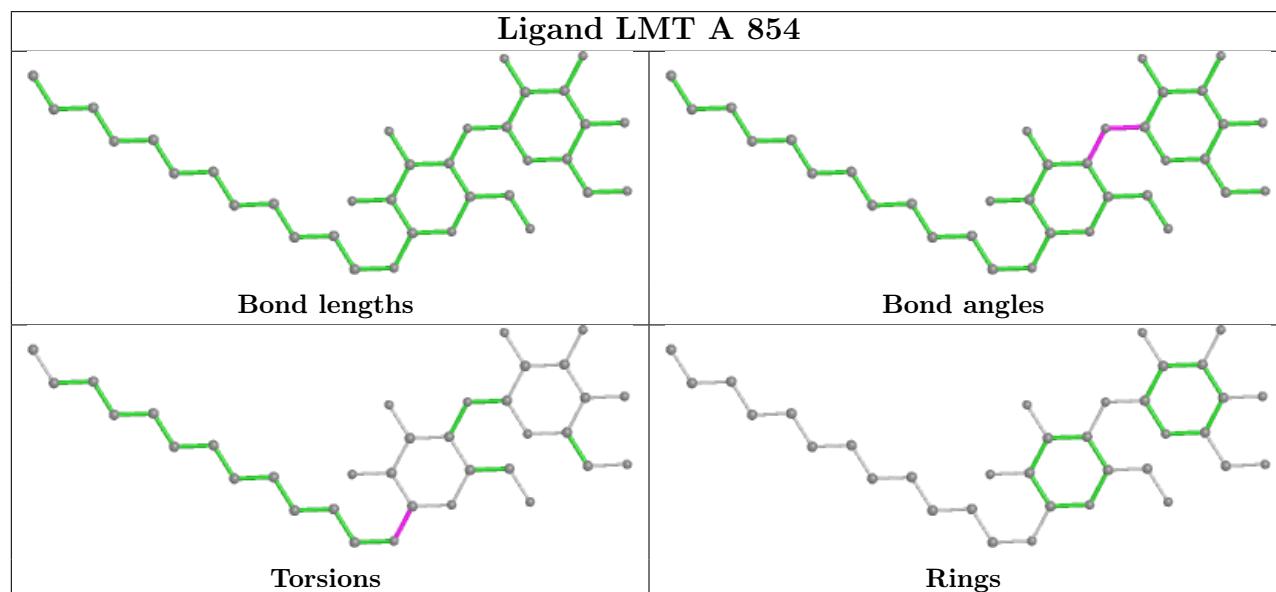
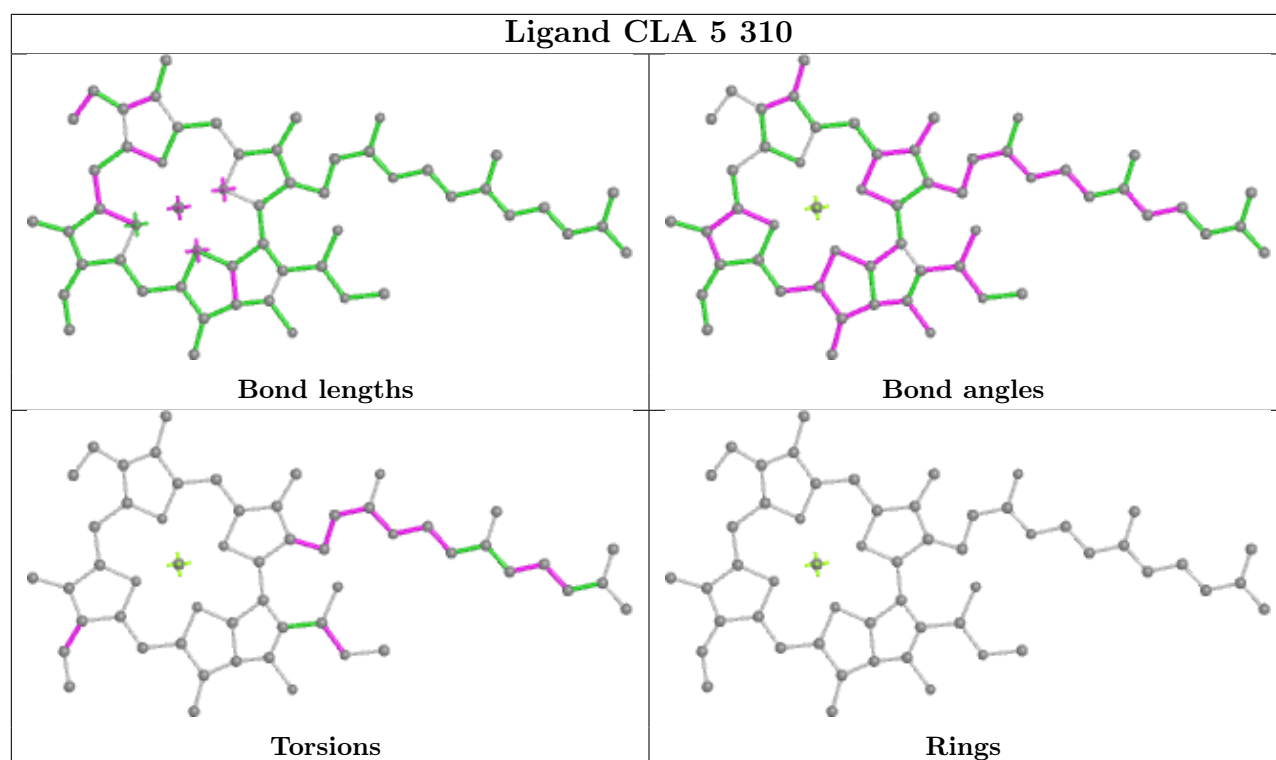


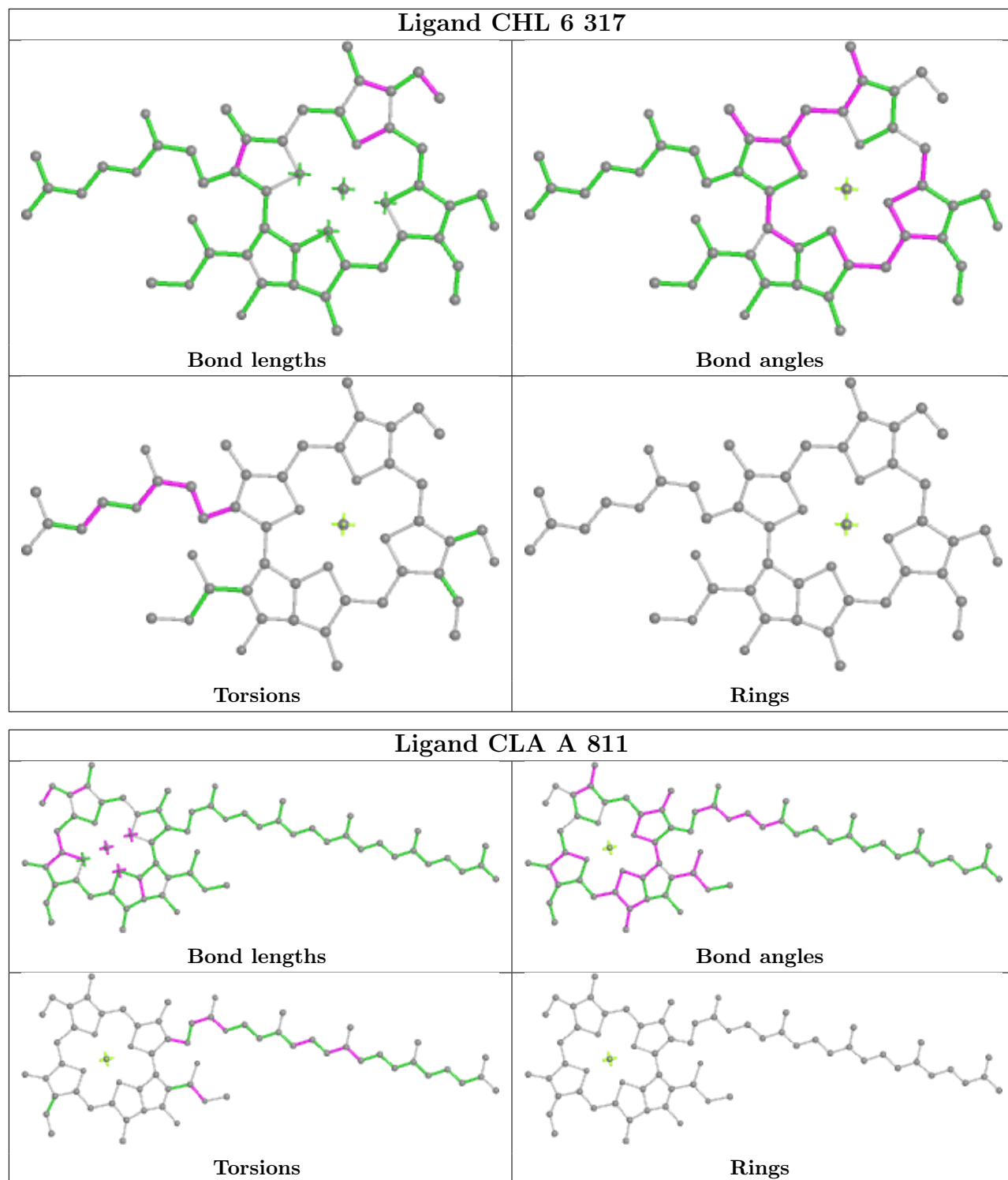


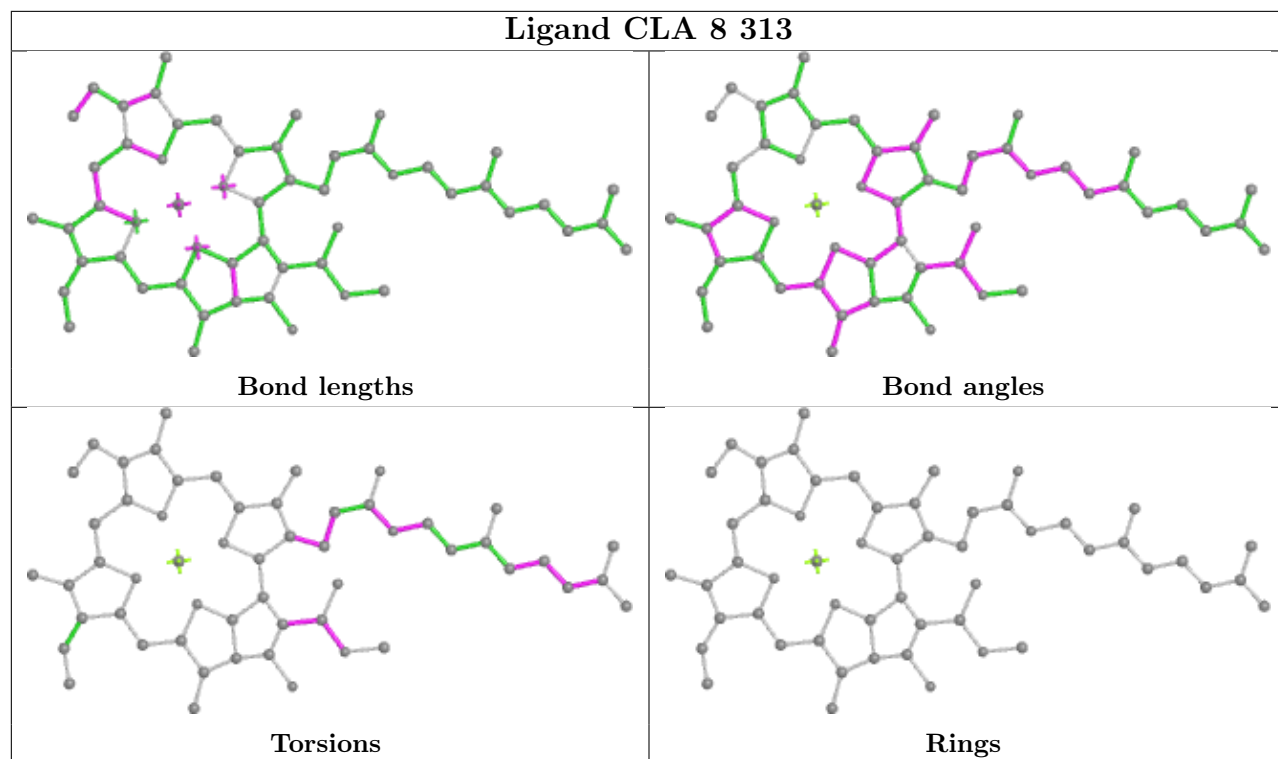


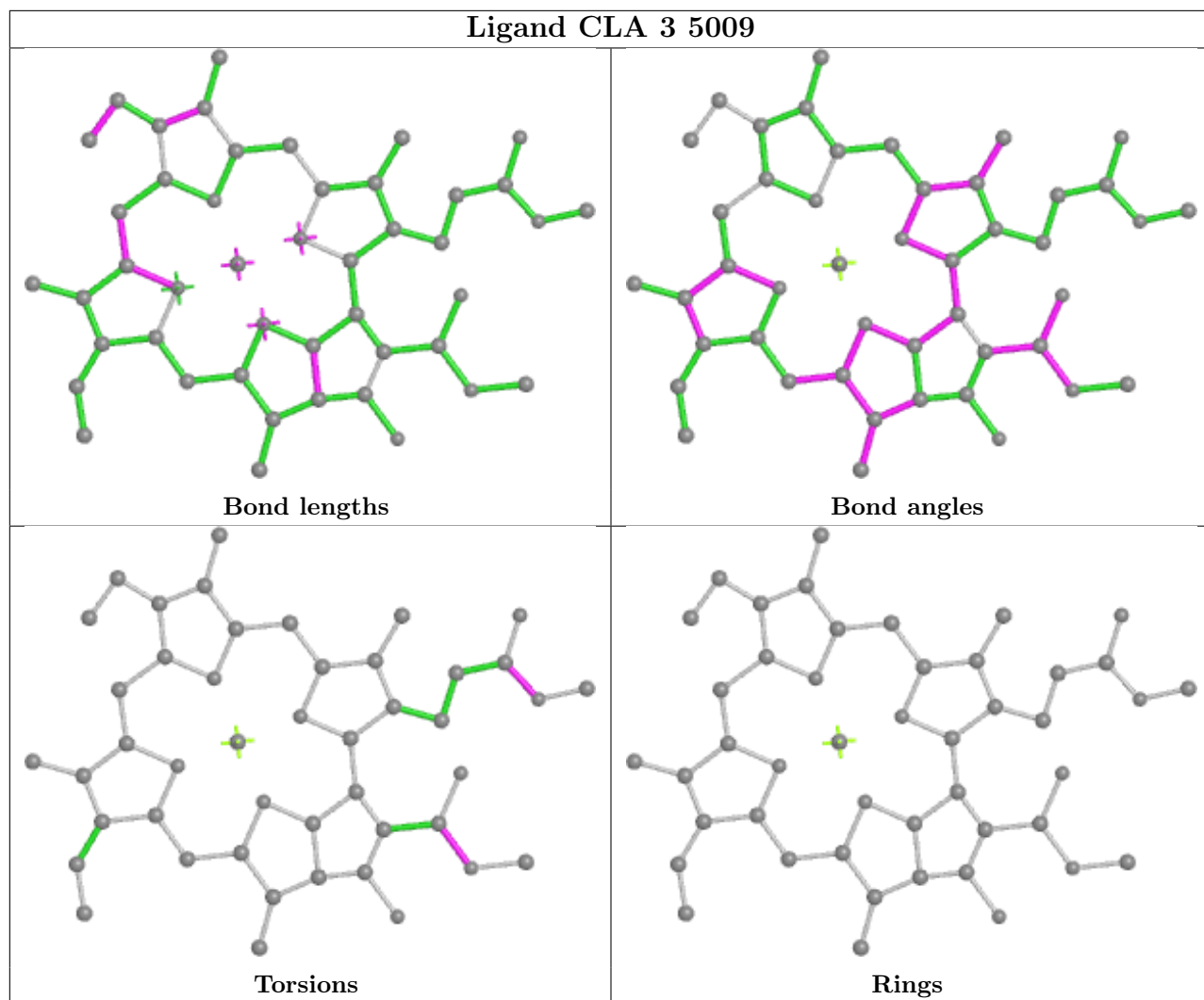


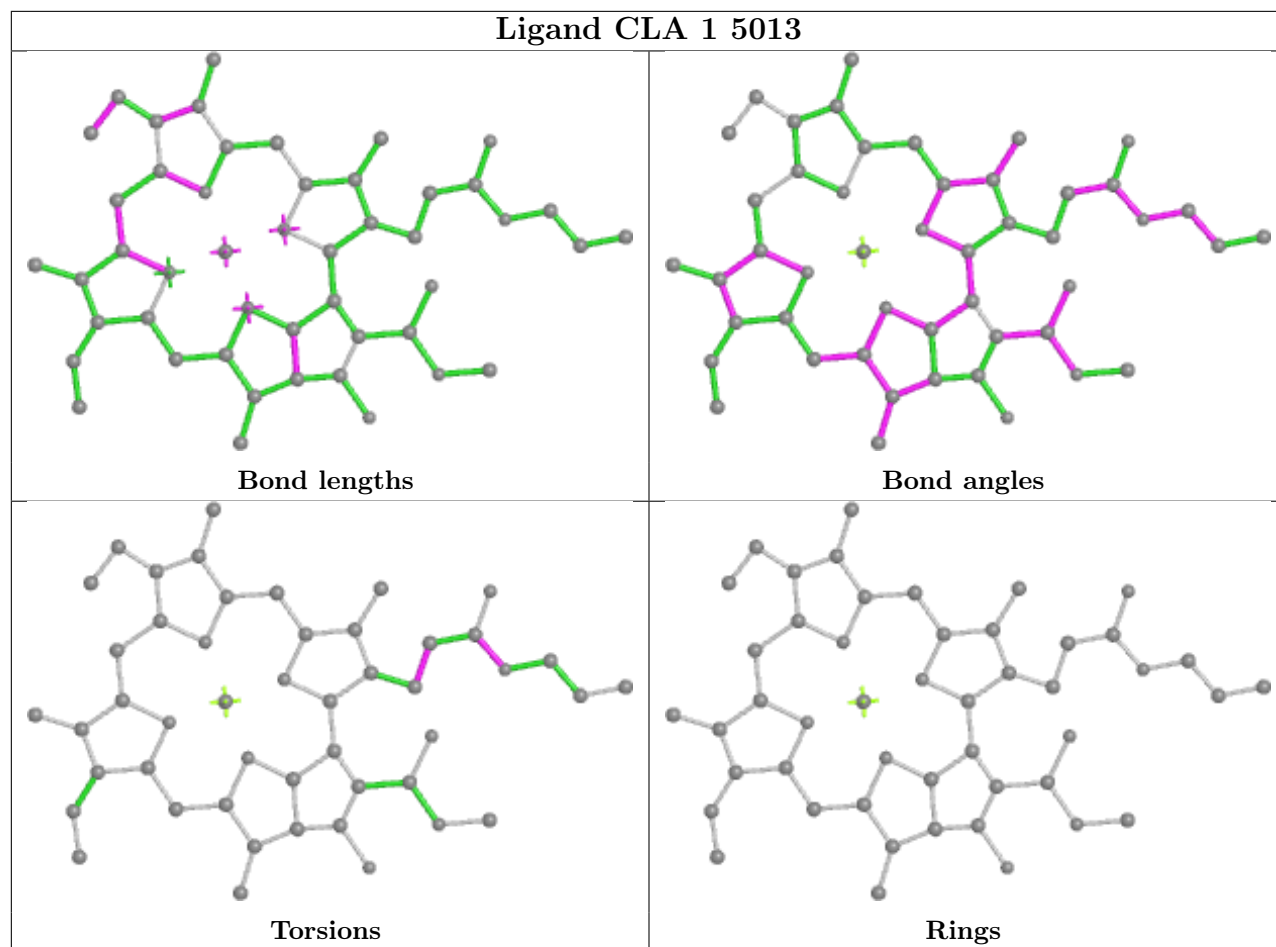


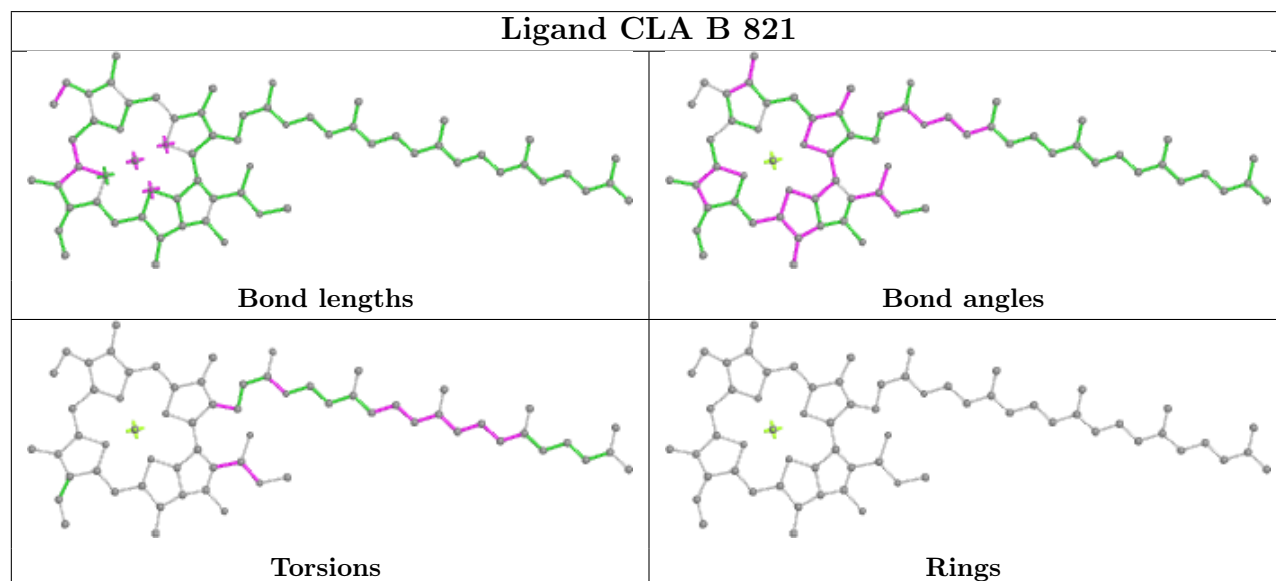
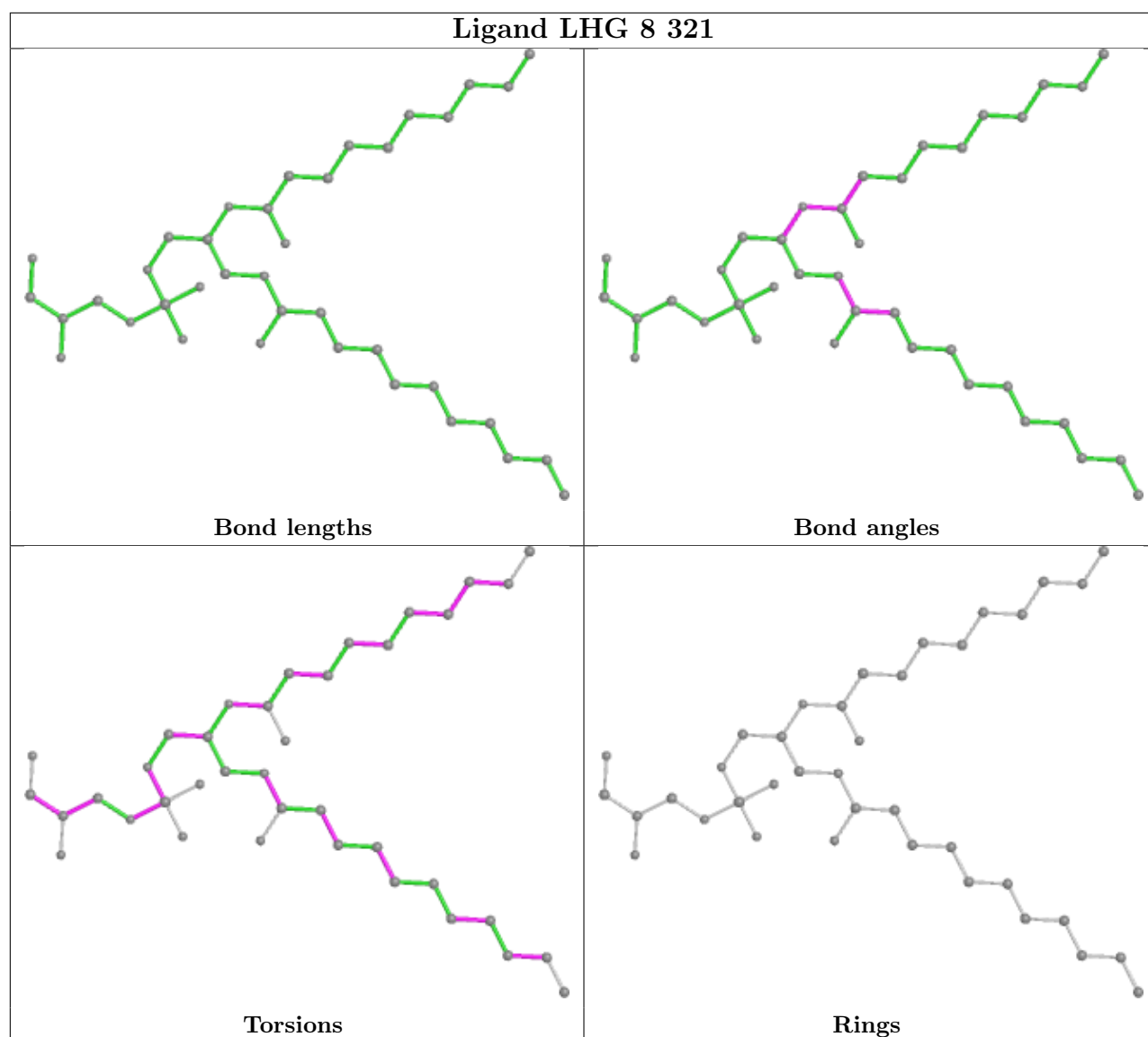


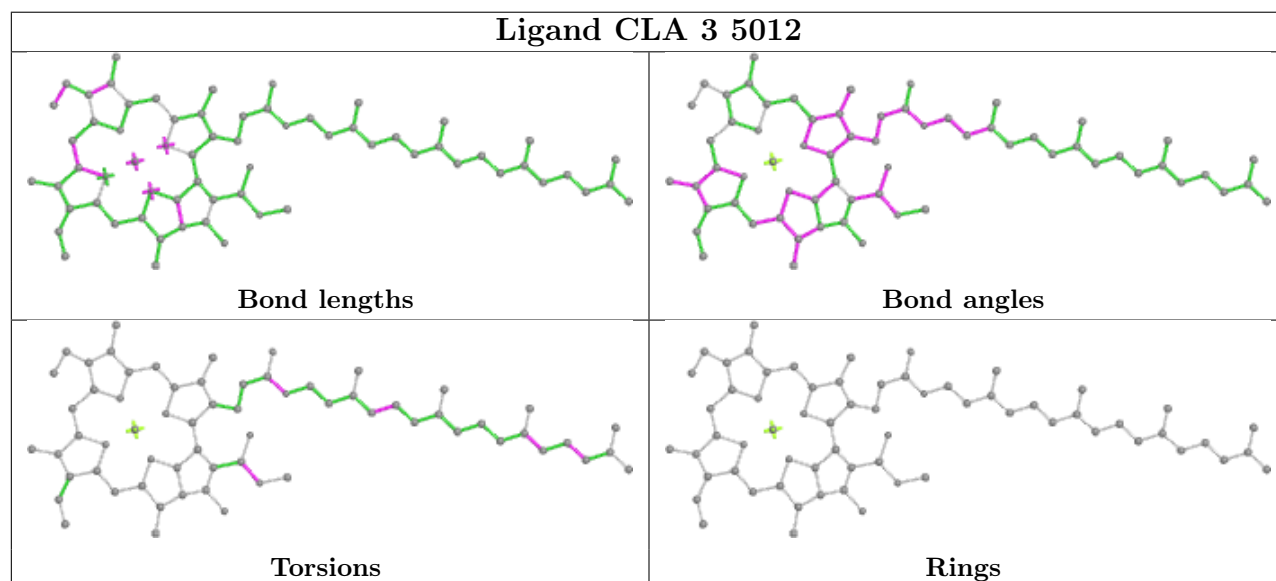
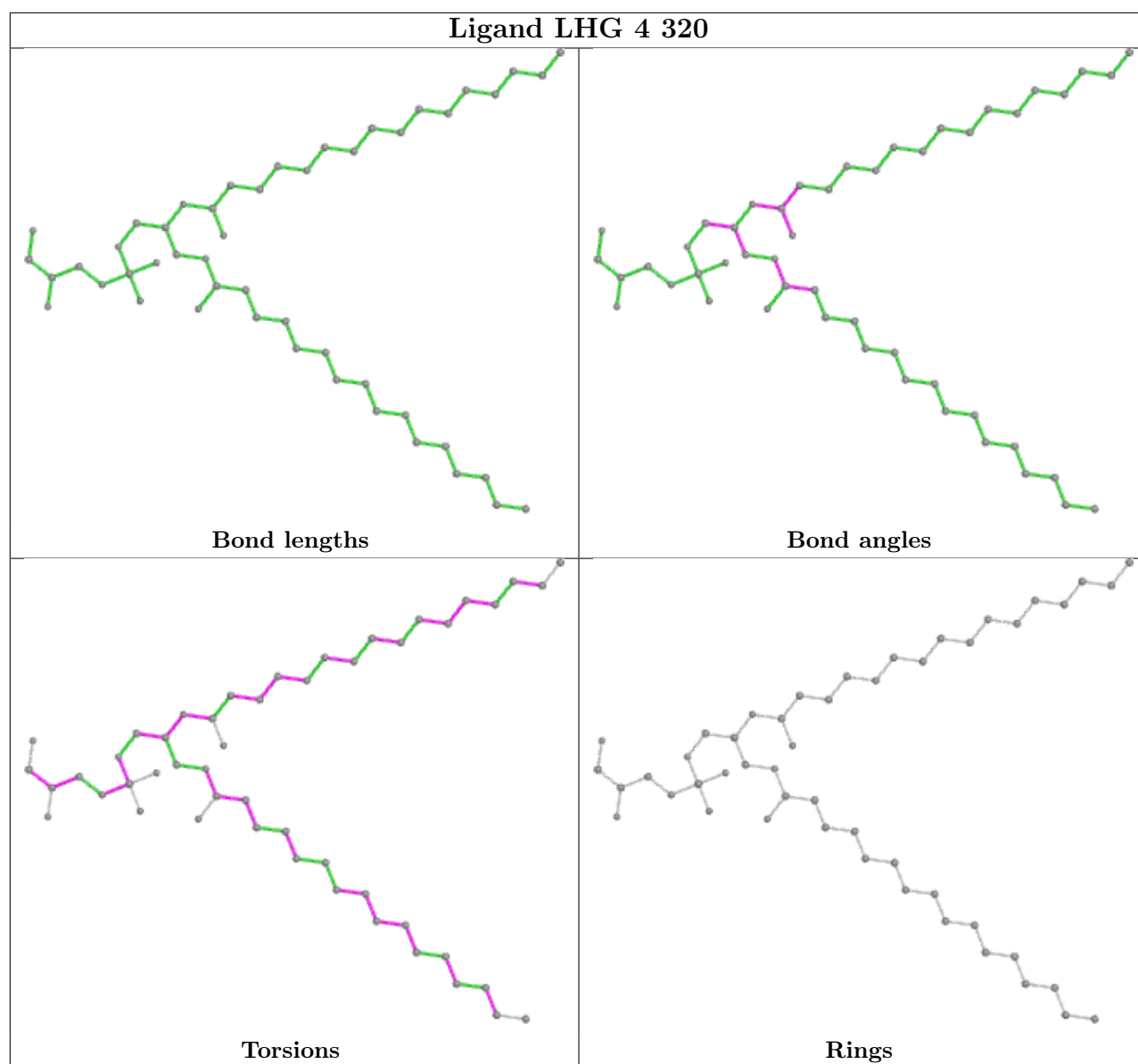


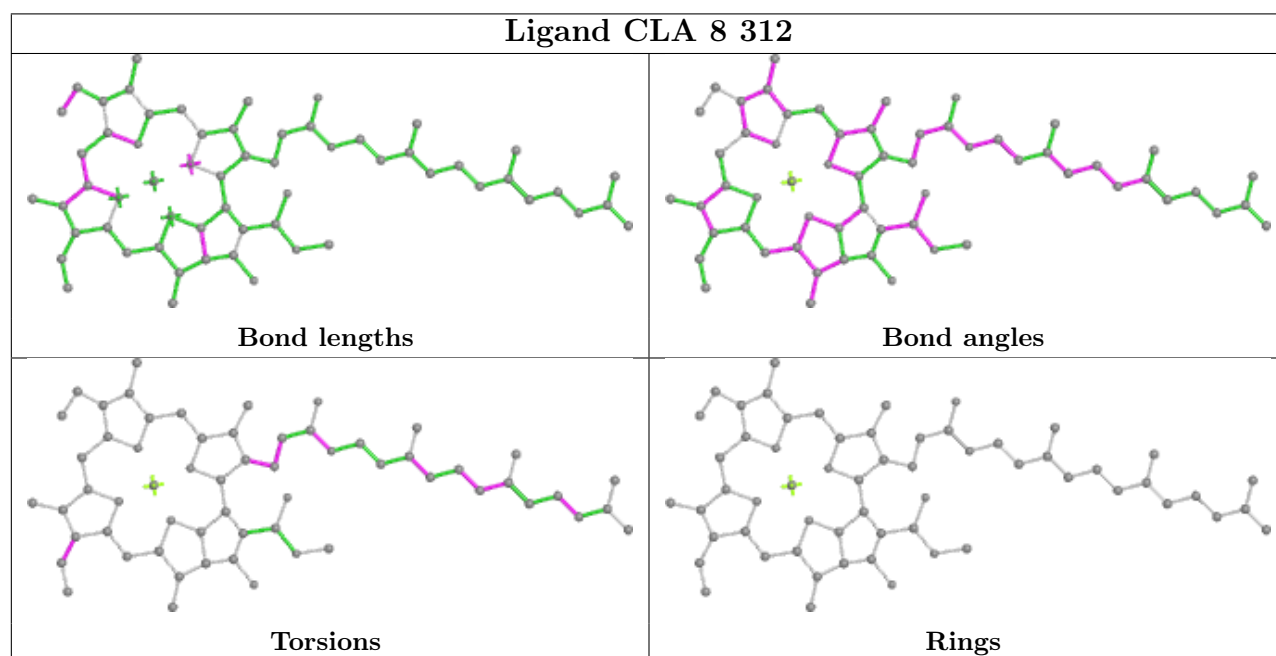
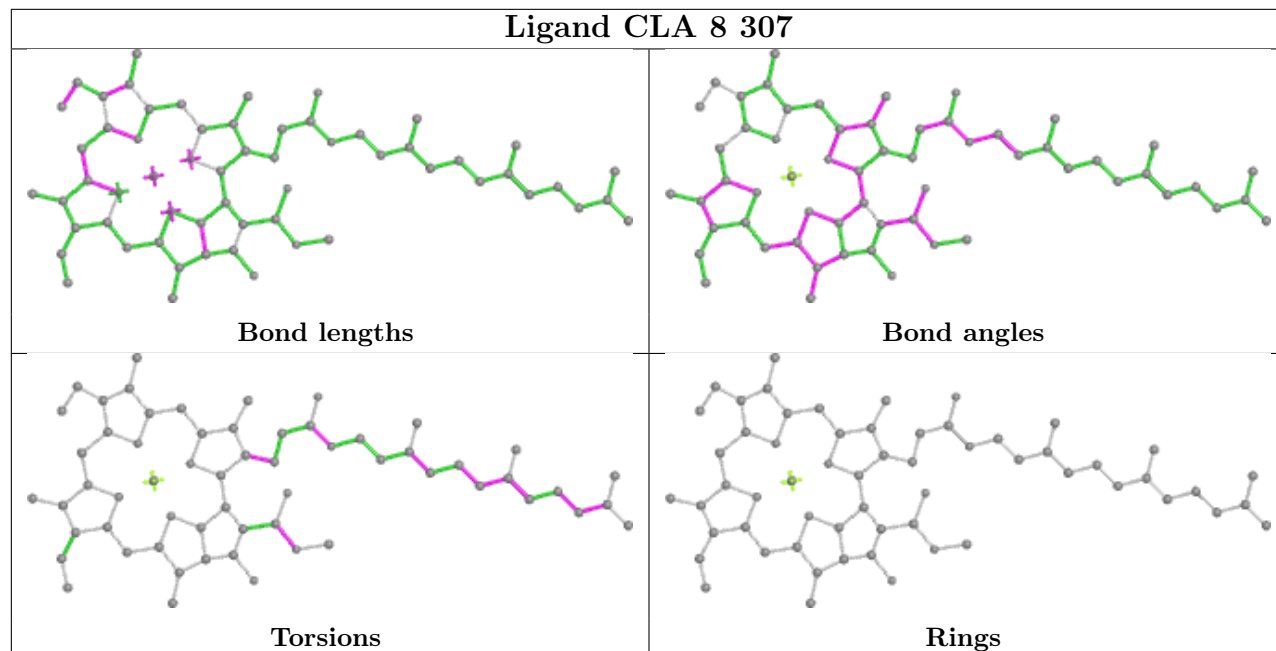
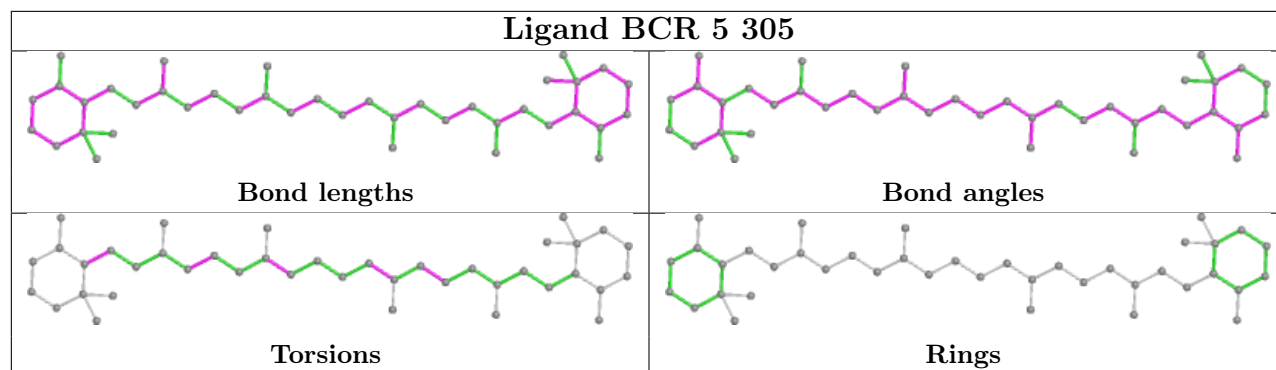


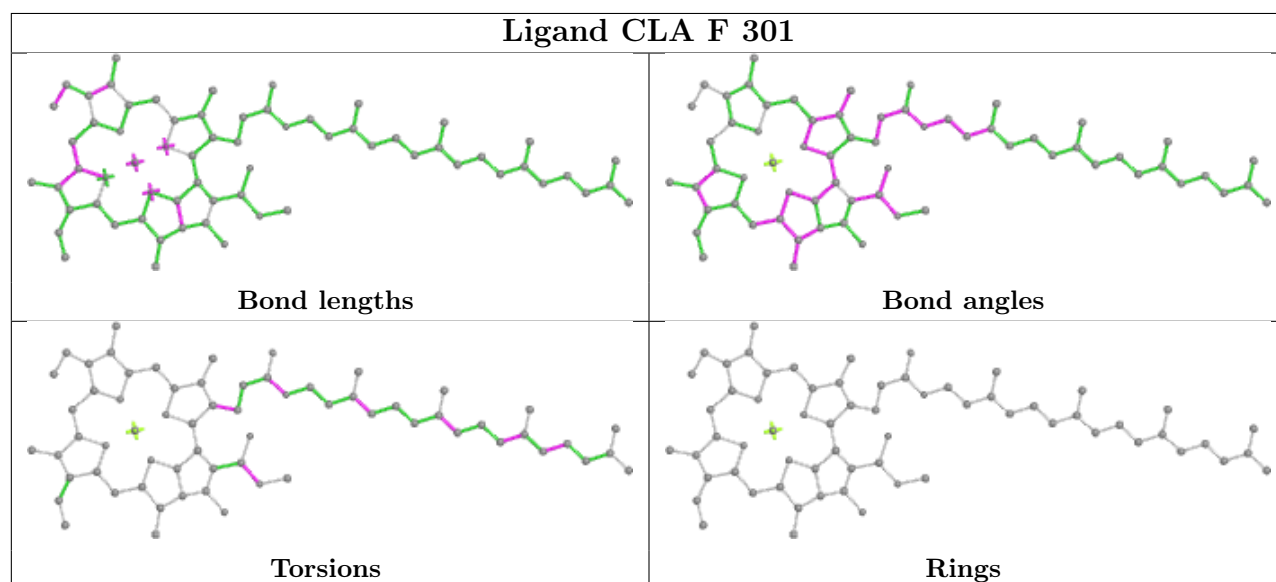
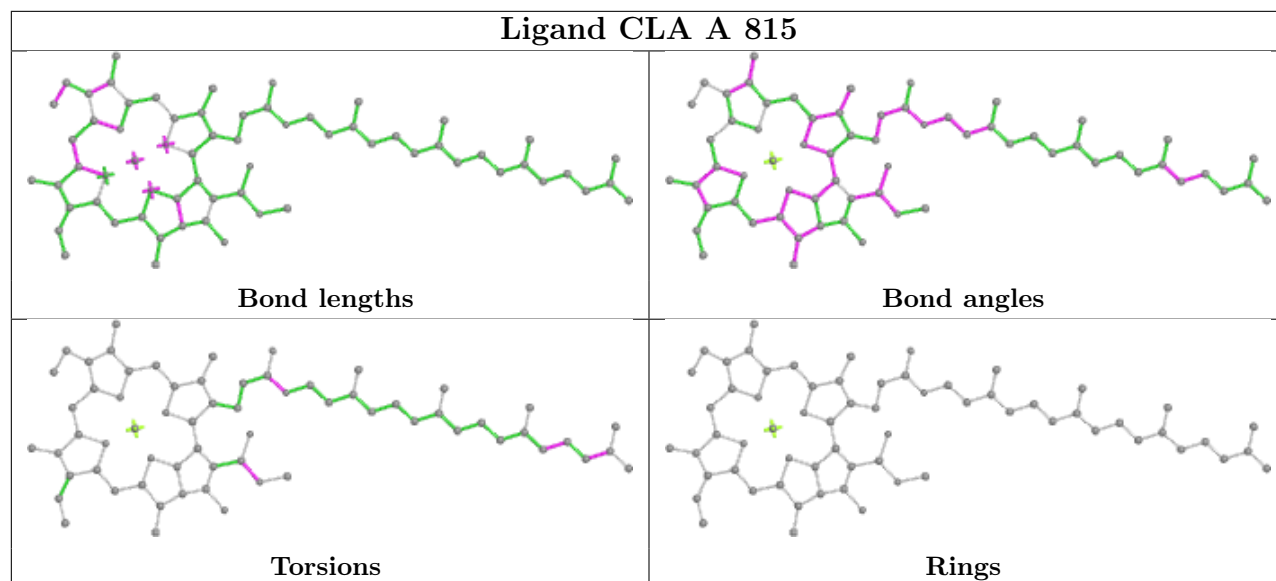
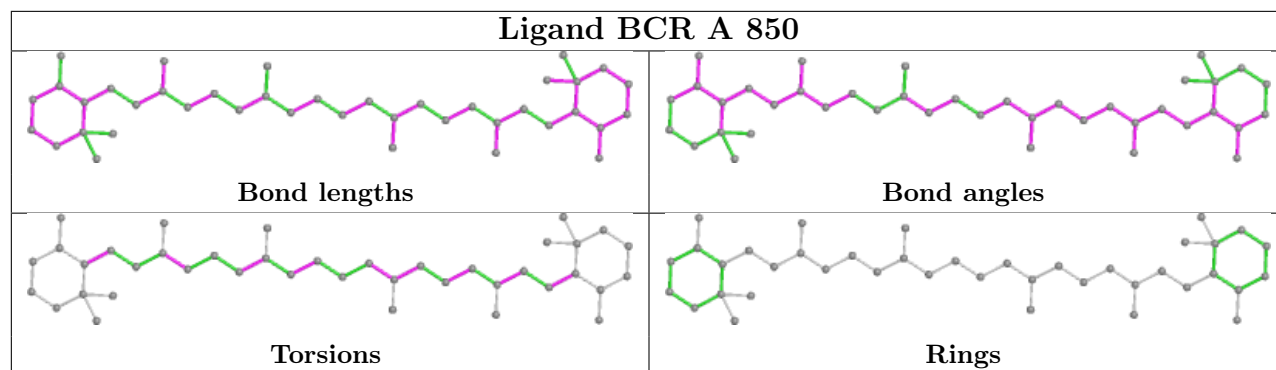


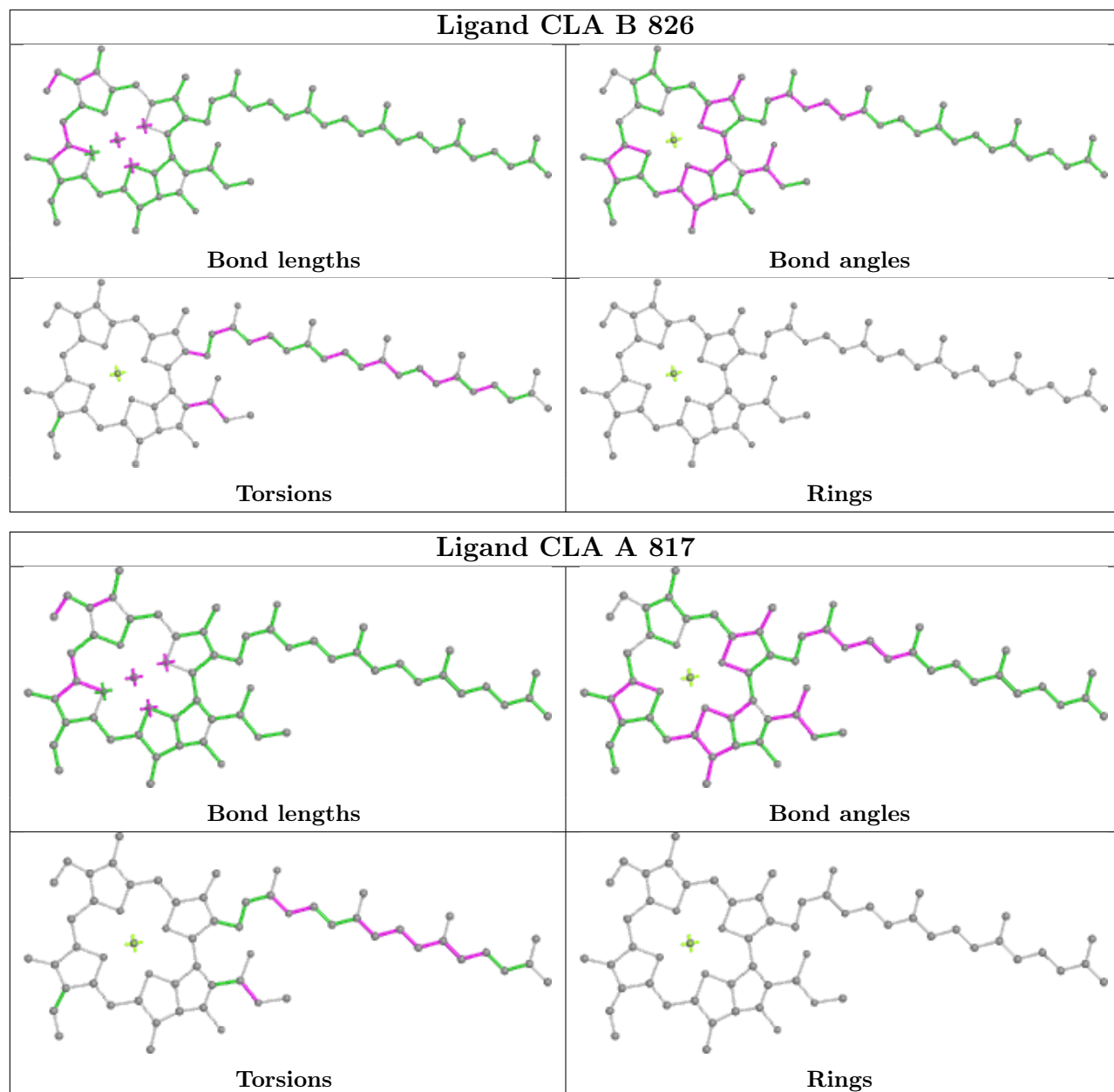


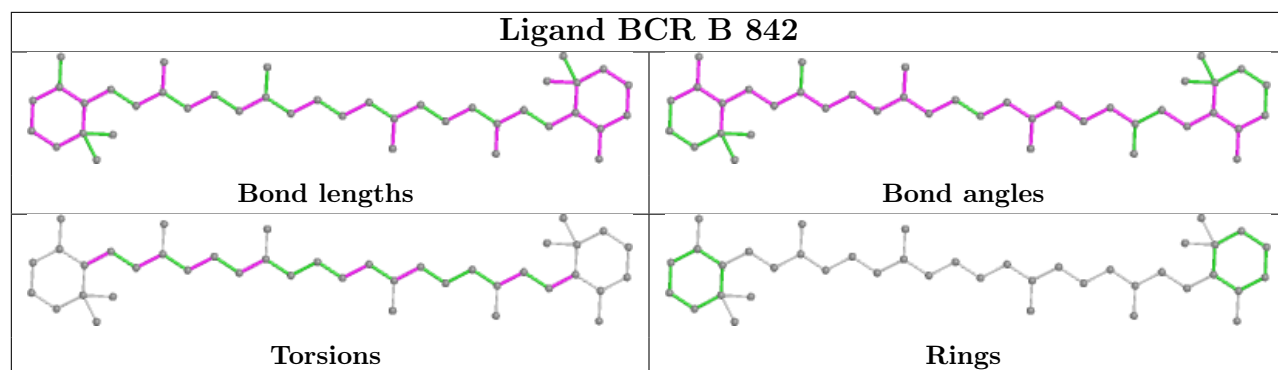
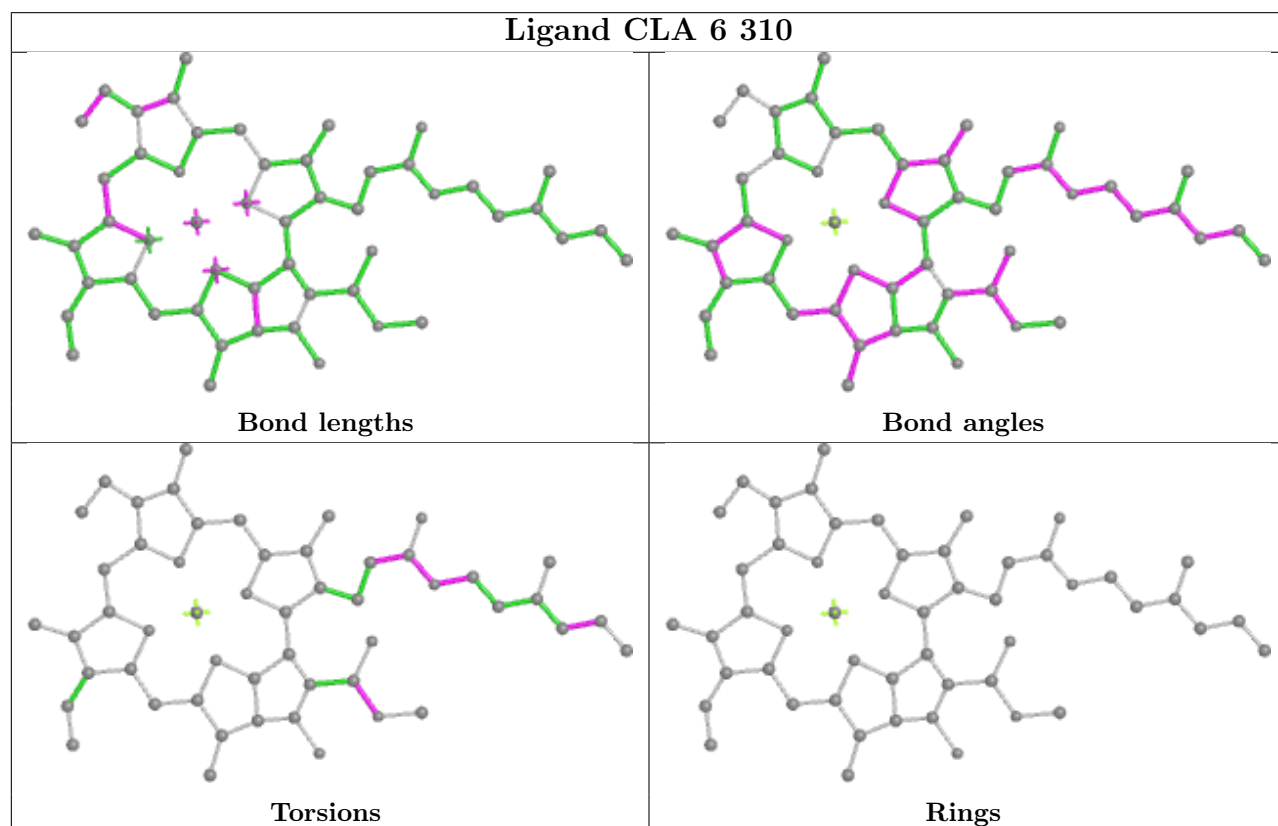
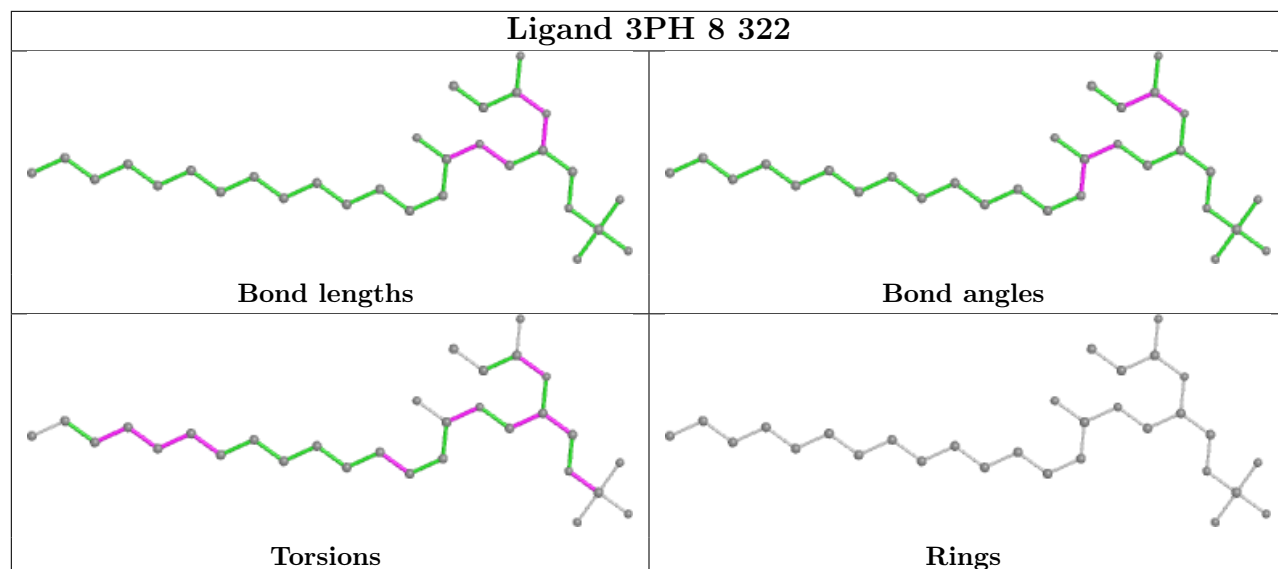


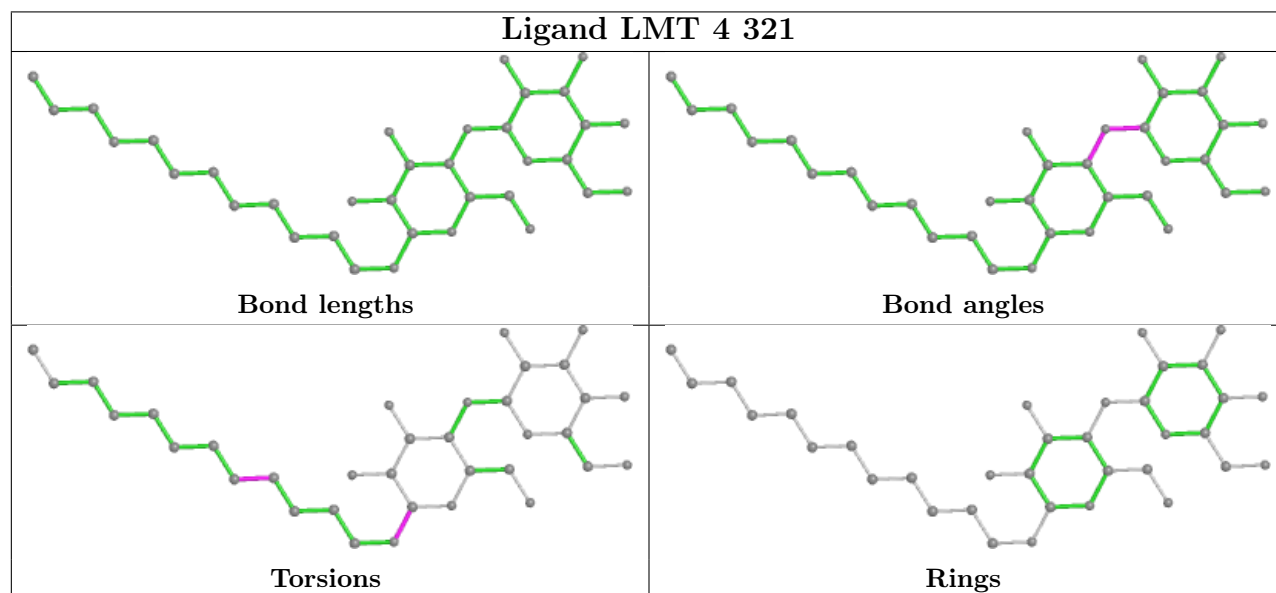
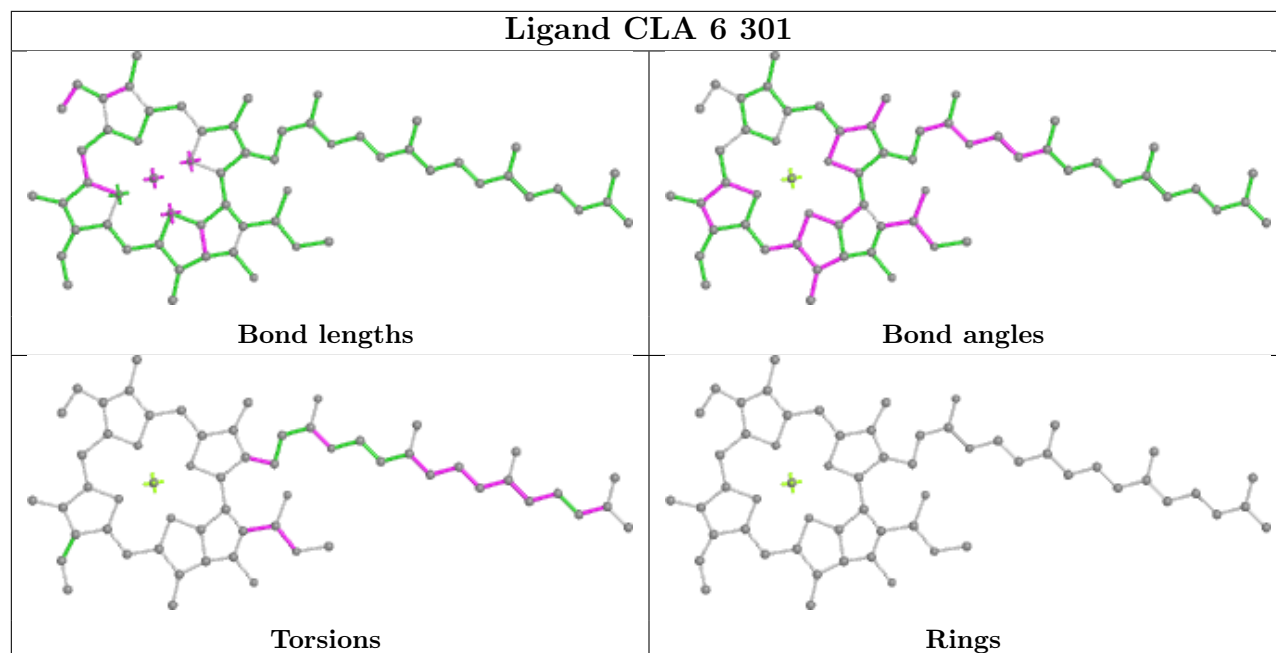


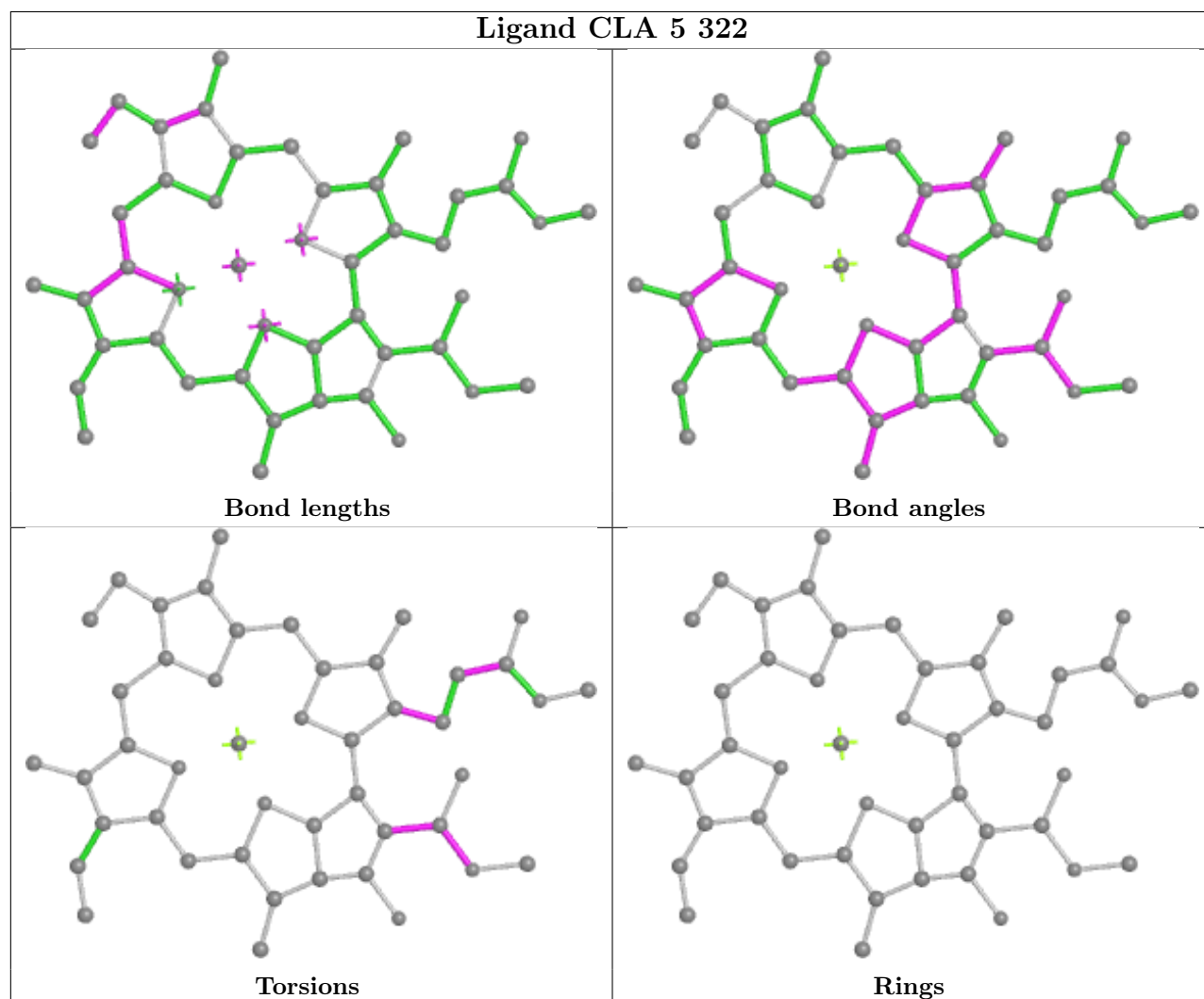
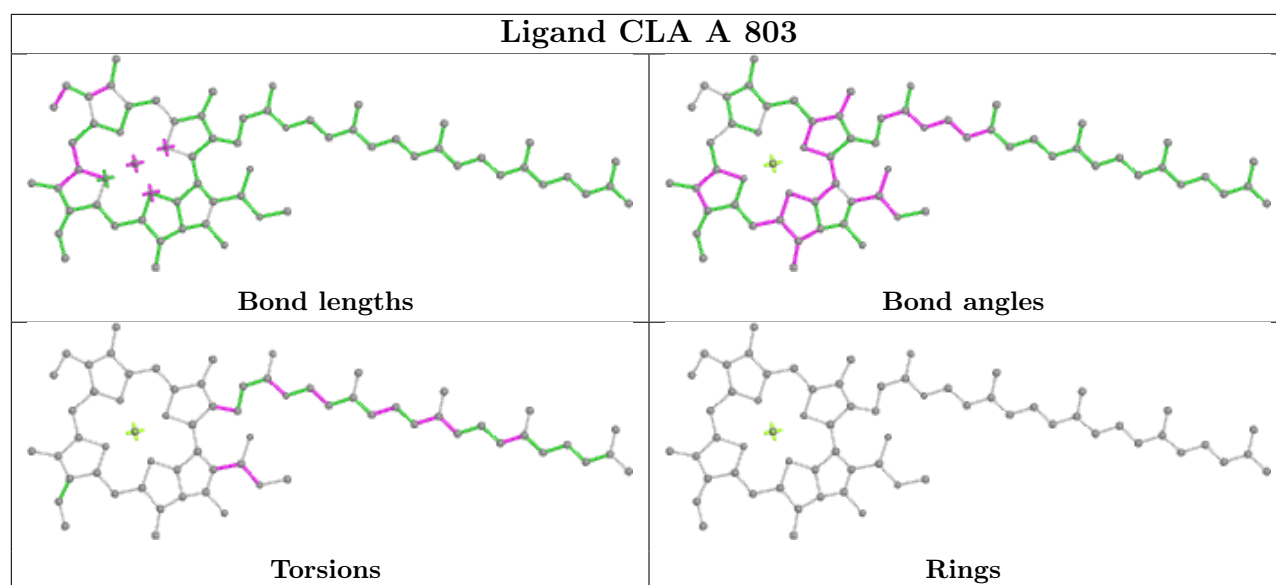


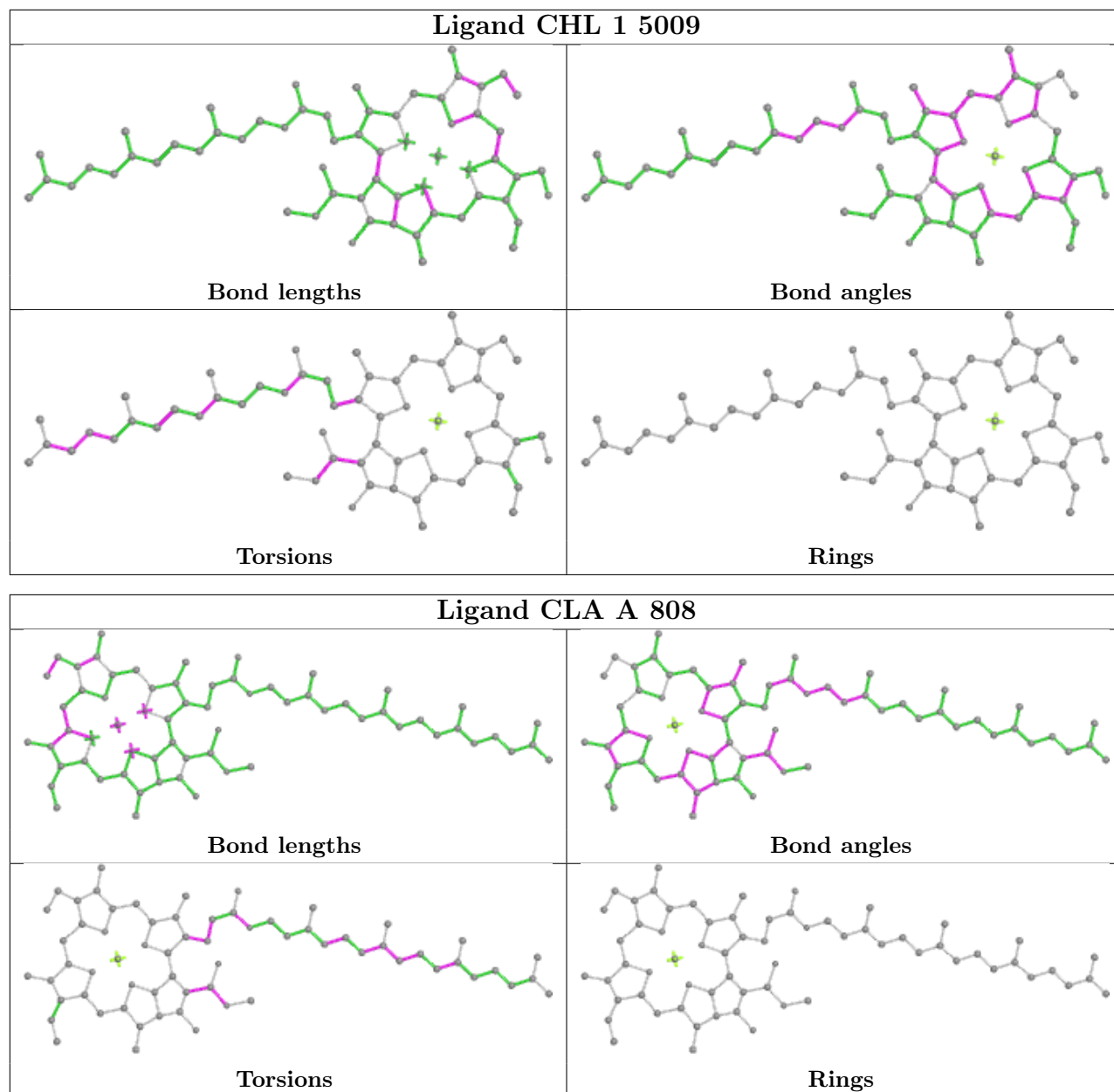


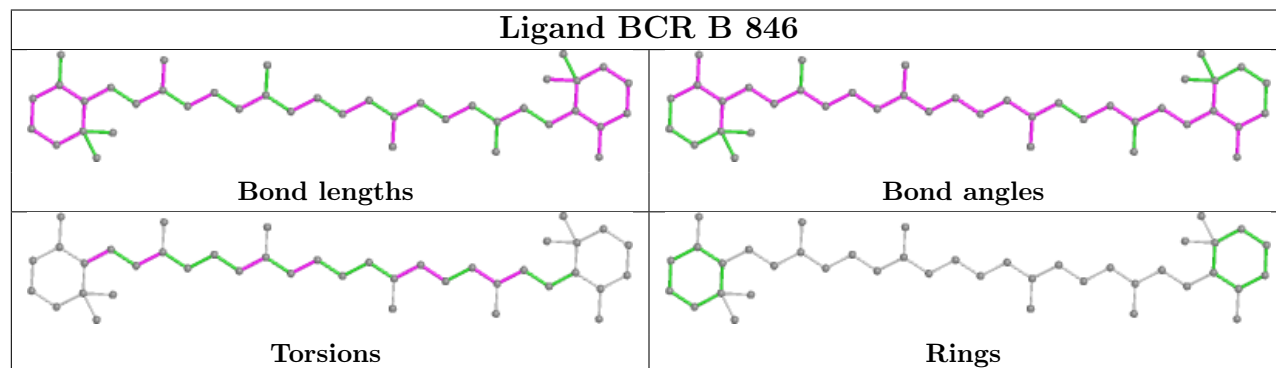
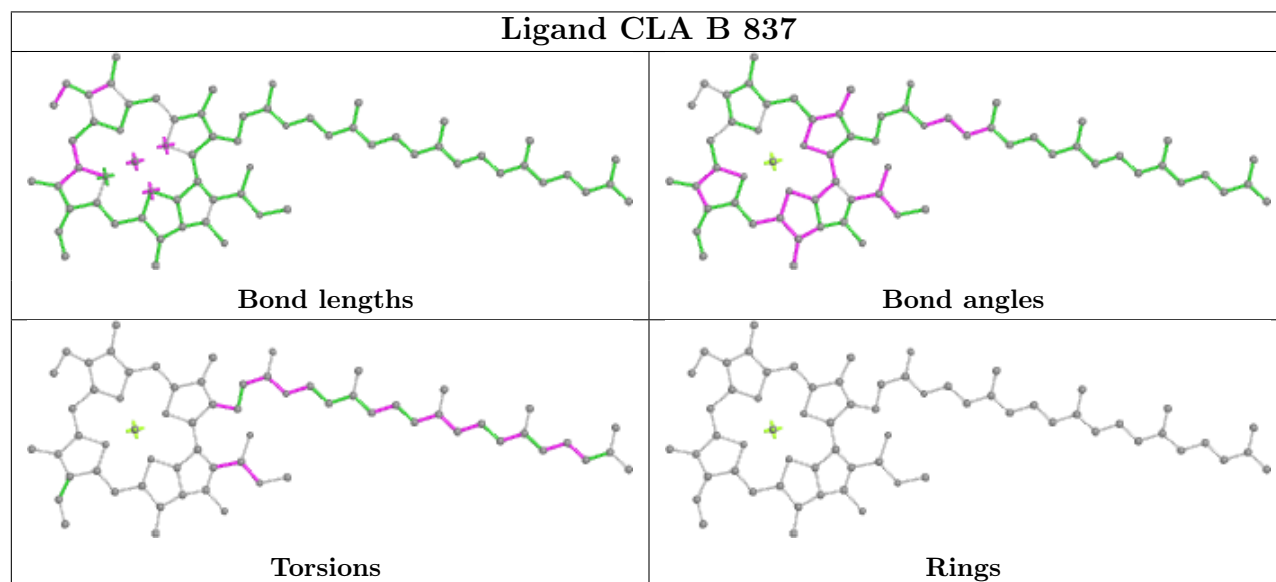
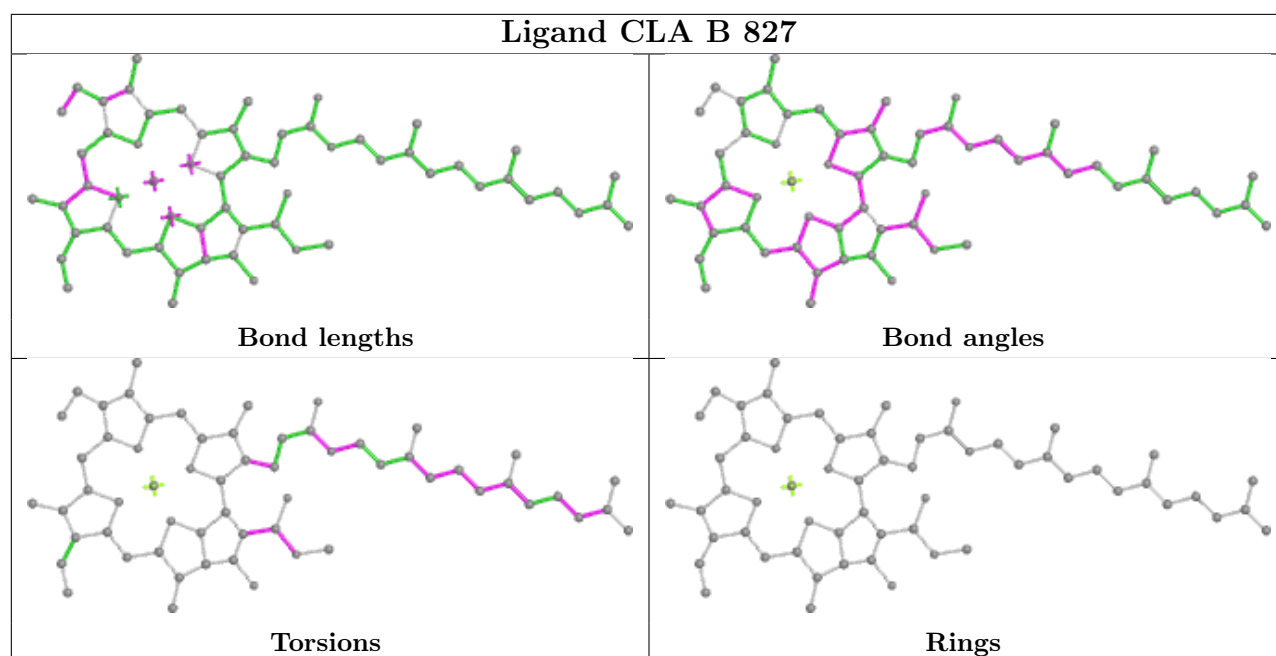


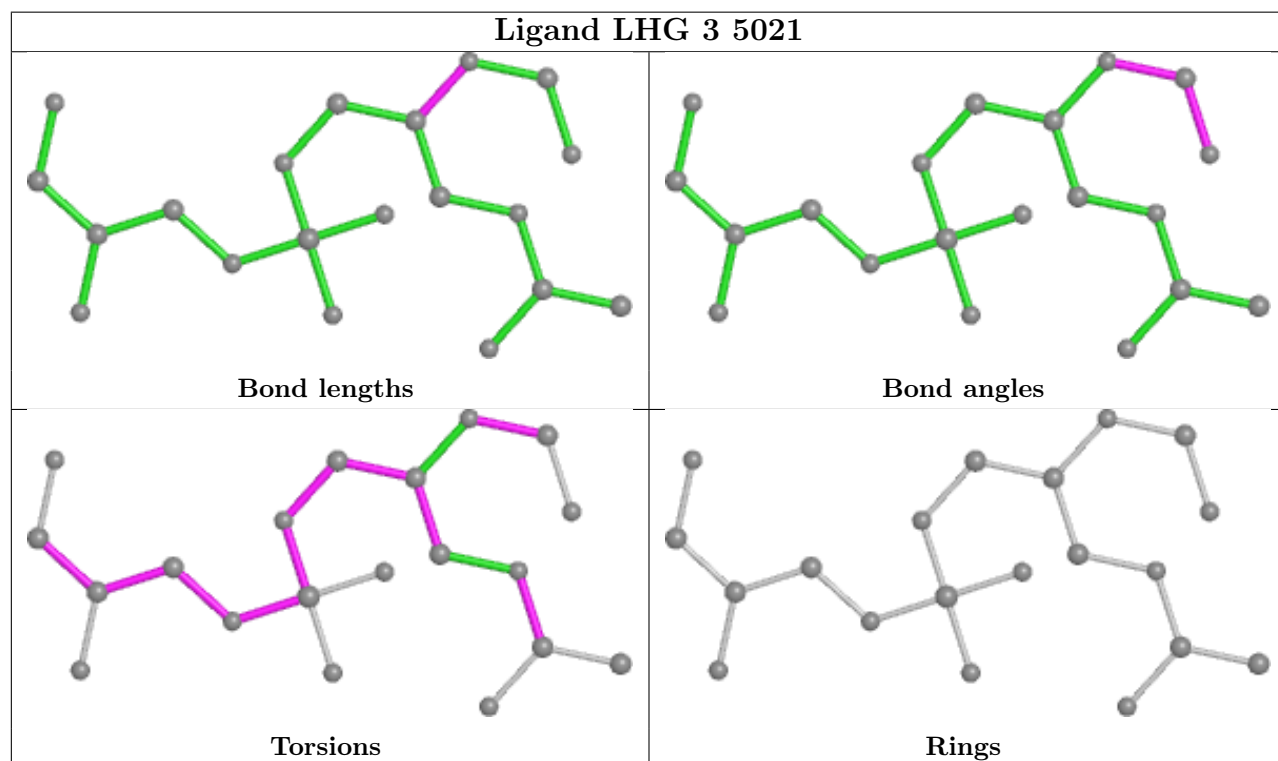
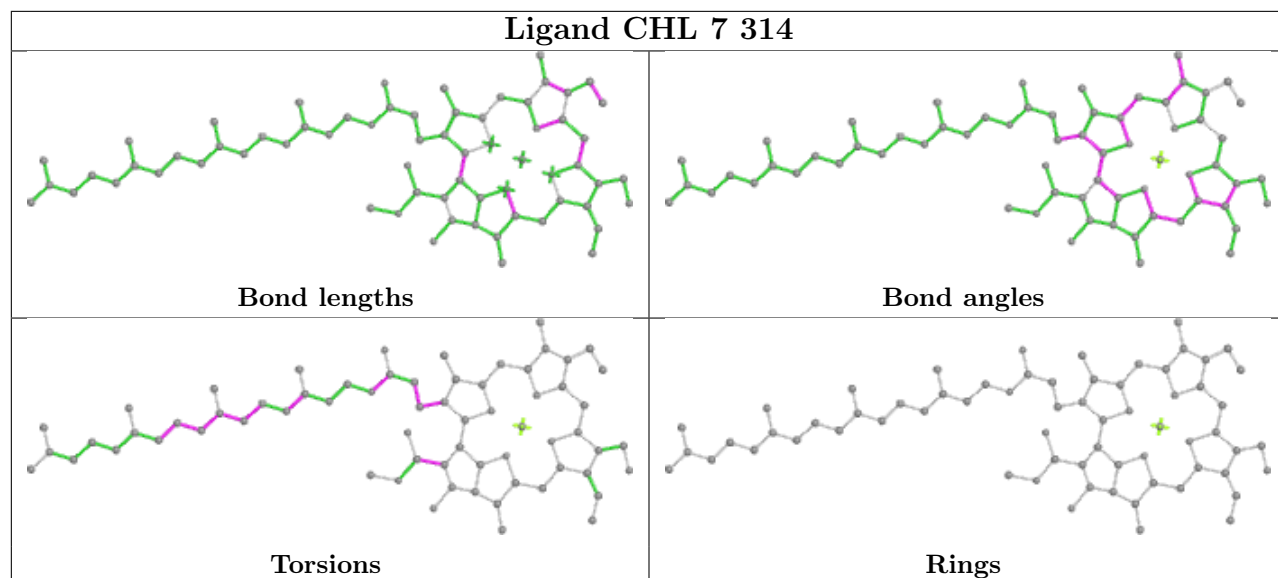


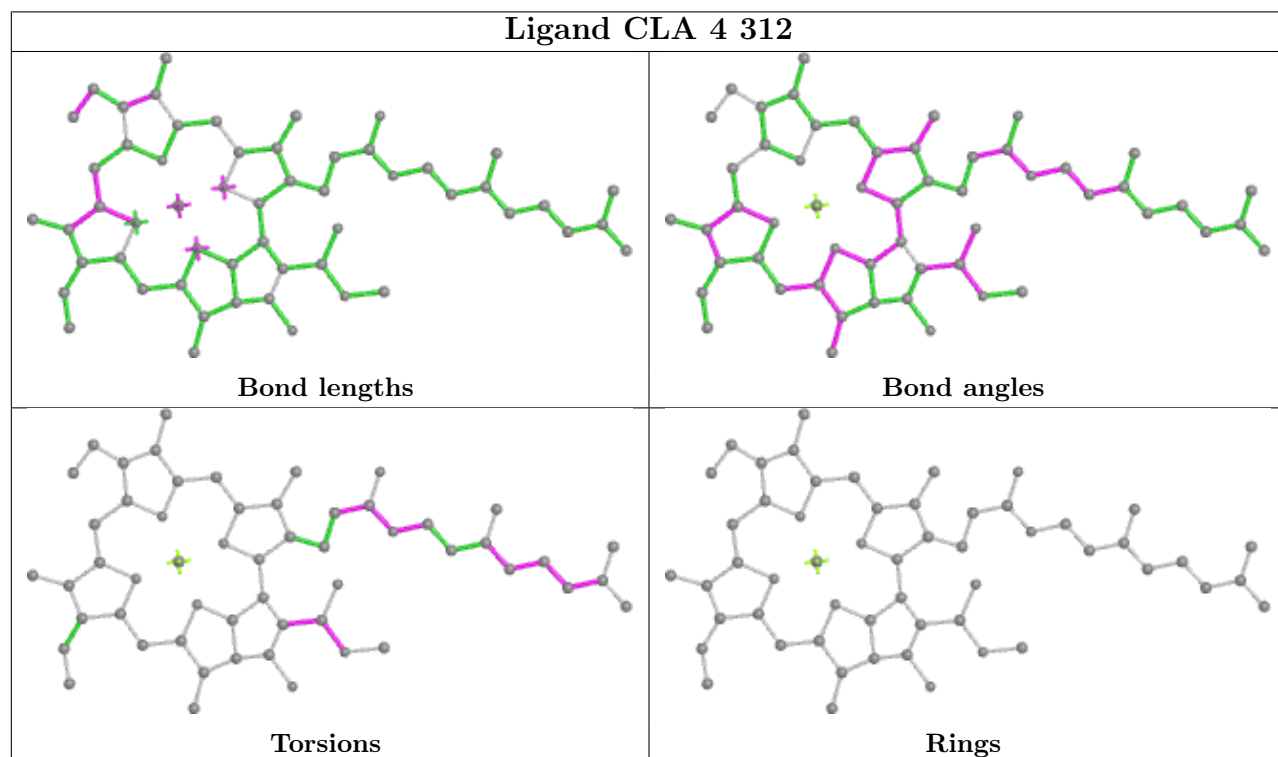
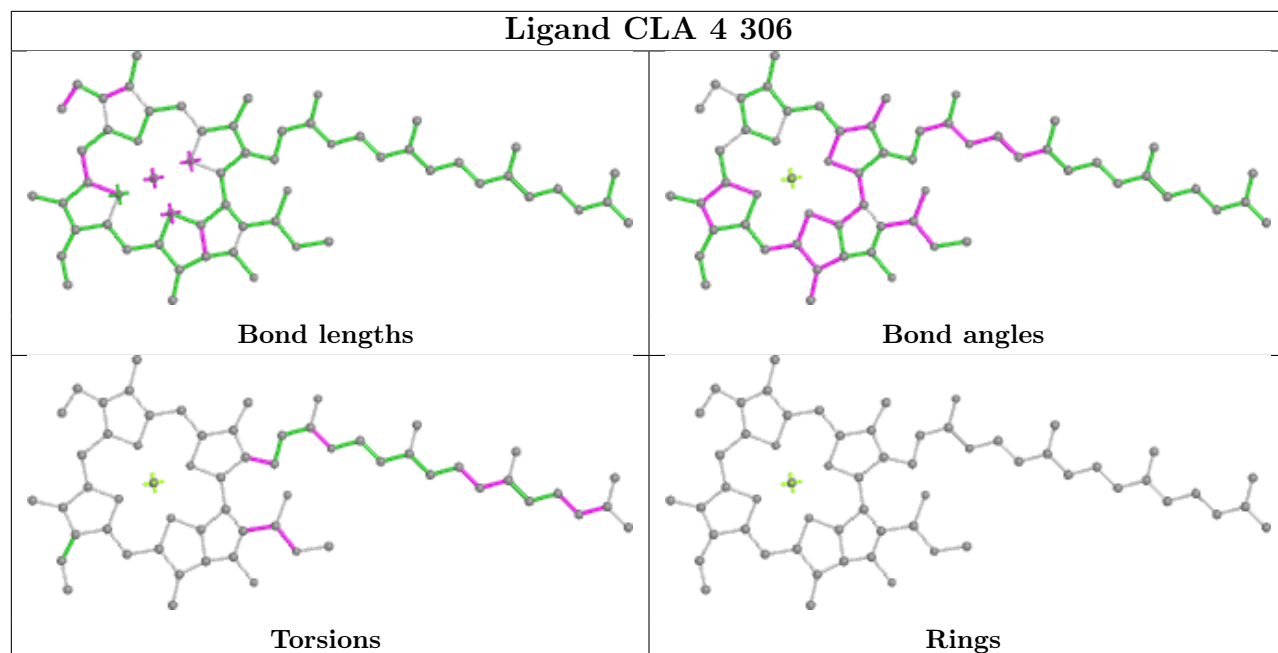


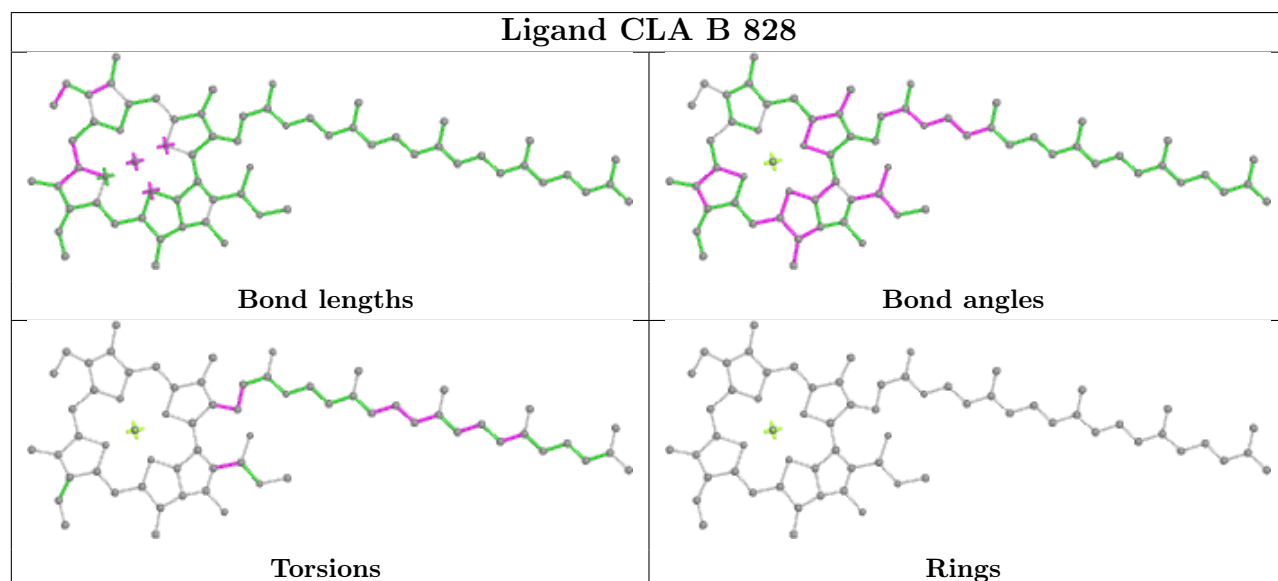
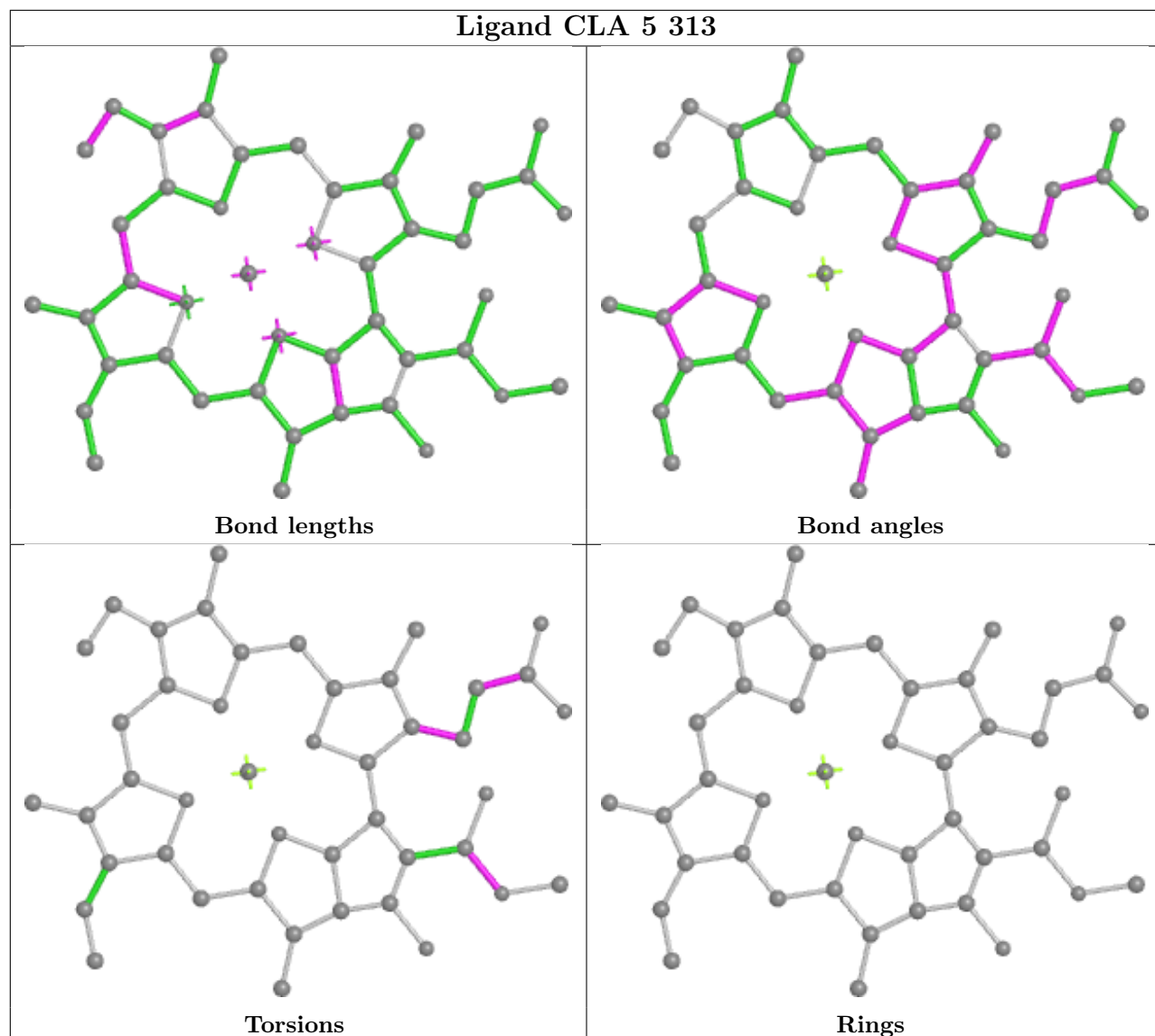


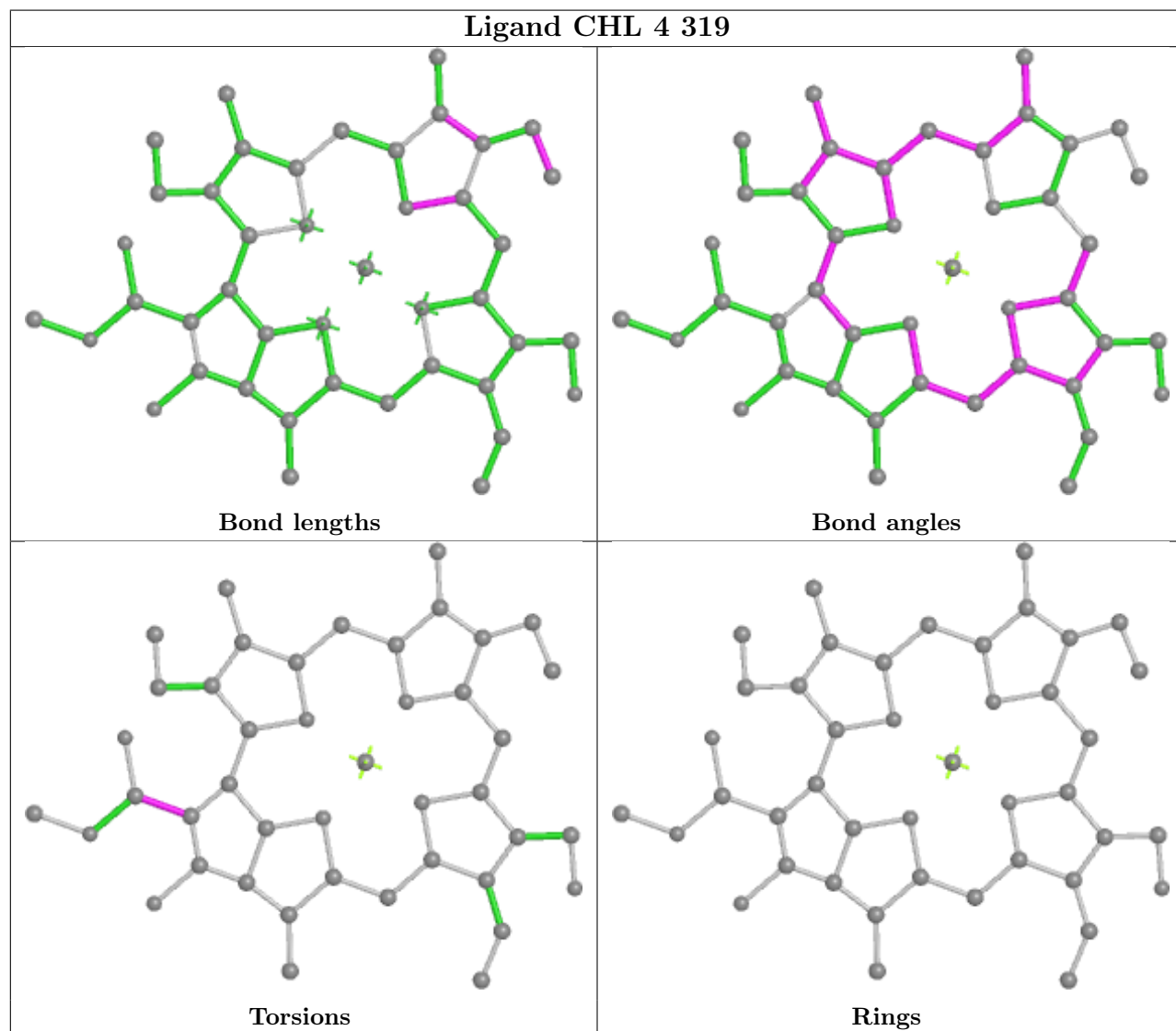
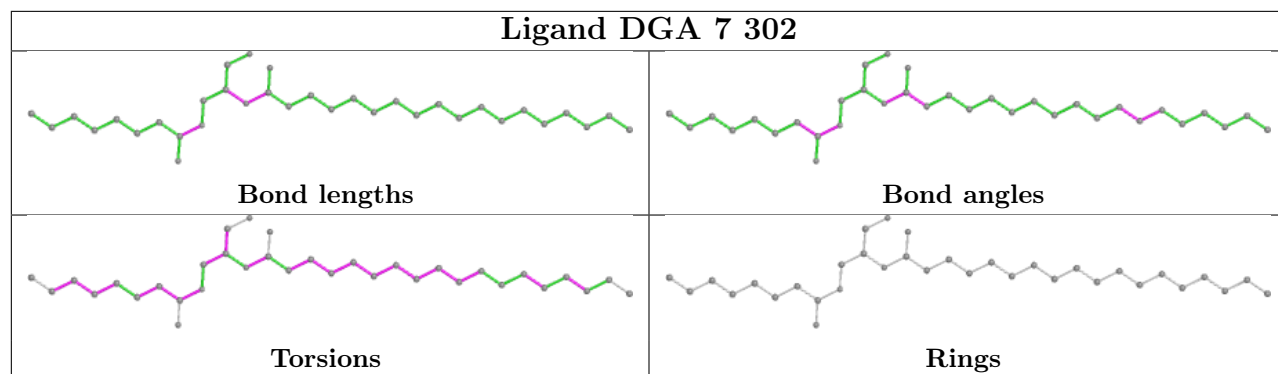


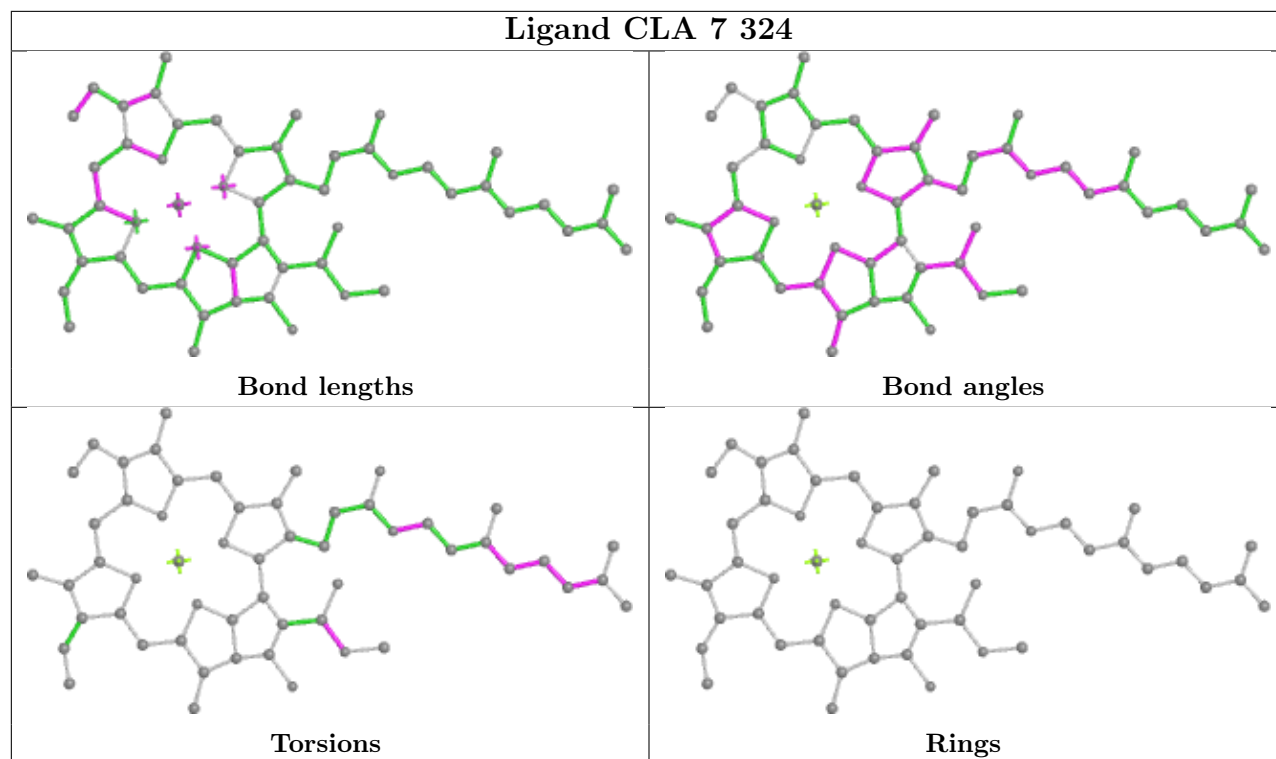












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

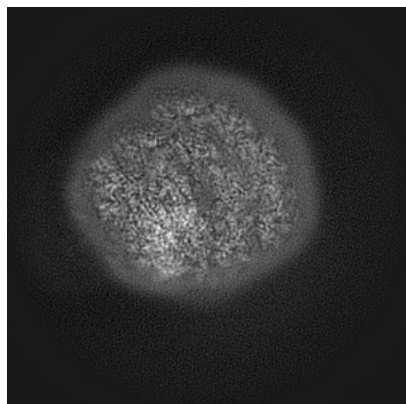
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14248. These allow visual inspection of the internal detail of the map and identification of artifacts.

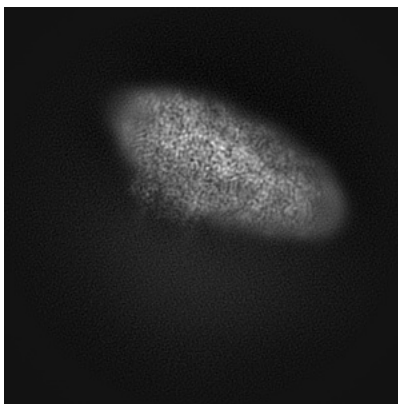
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

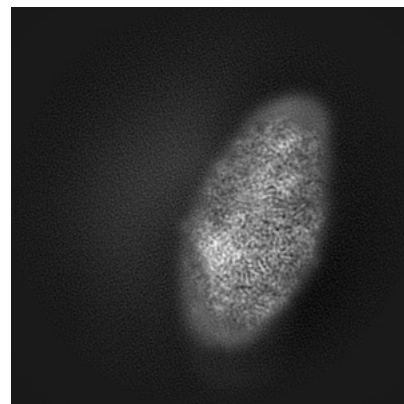
6.1.1 Primary map



X

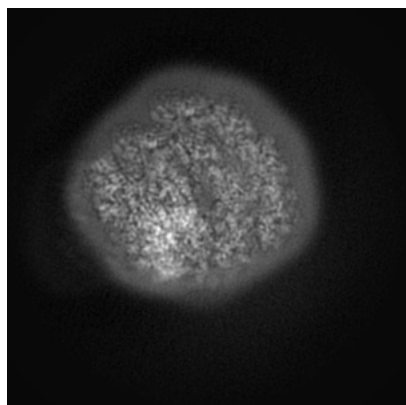


Y

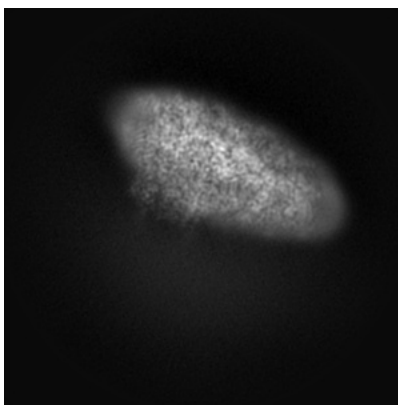


Z

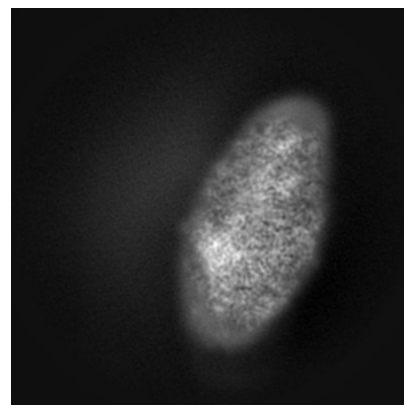
6.1.2 Raw map



X



Y

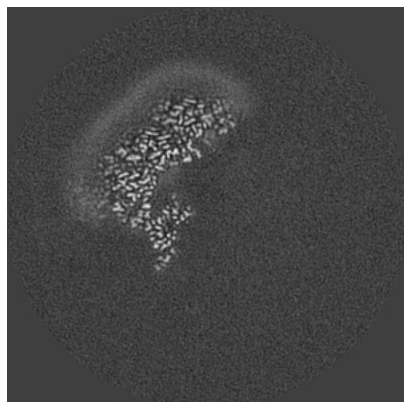


Z

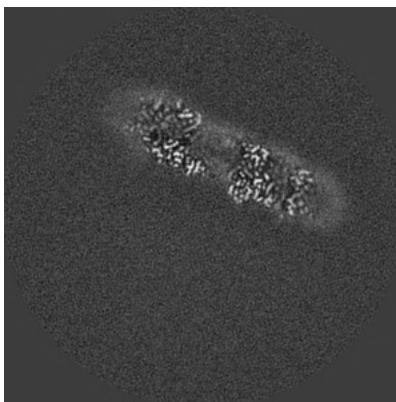
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

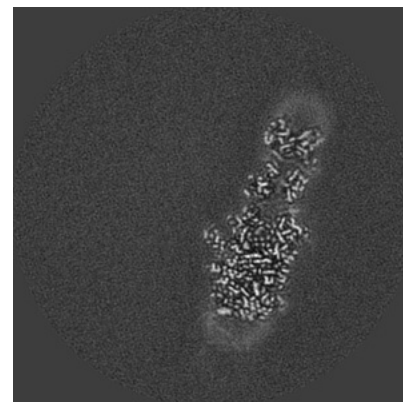
6.2.1 Primary map



X Index: 195

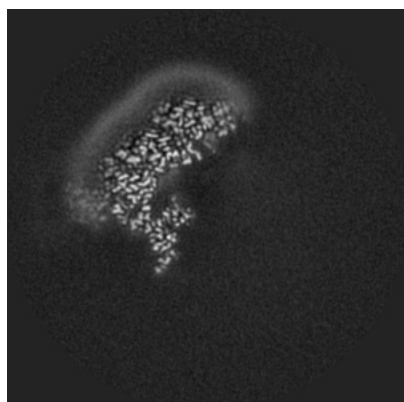


Y Index: 195

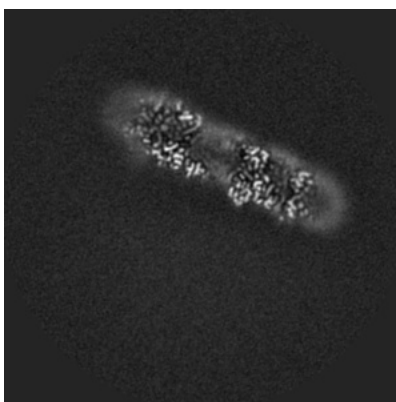


Z Index: 195

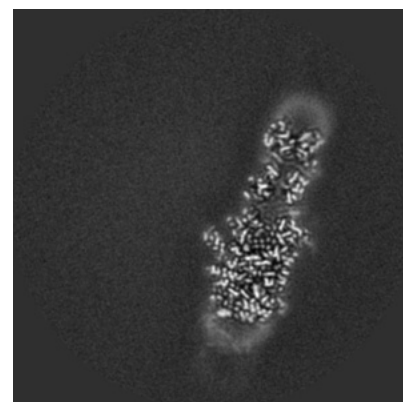
6.2.2 Raw map



X Index: 195



Y Index: 195

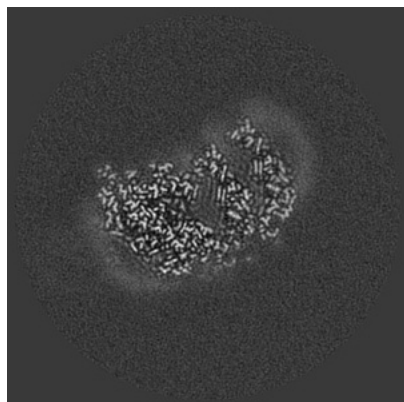


Z Index: 195

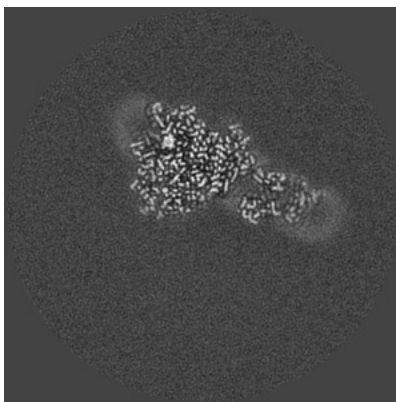
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

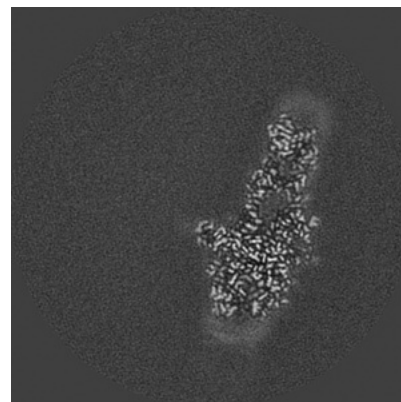
6.3.1 Primary map



X Index: 252

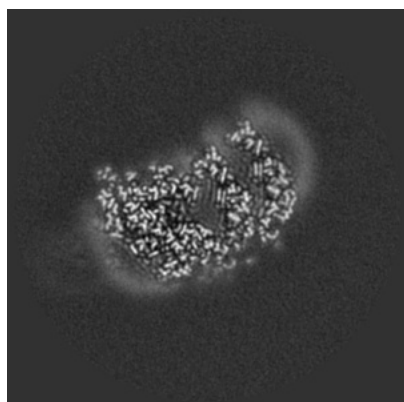


Y Index: 151

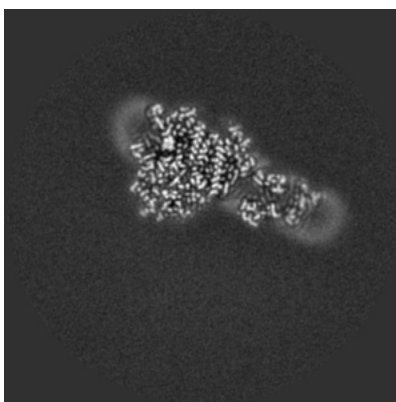


Z Index: 187

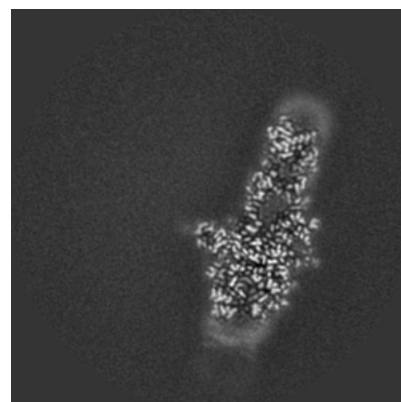
6.3.2 Raw map



X Index: 252



Y Index: 151

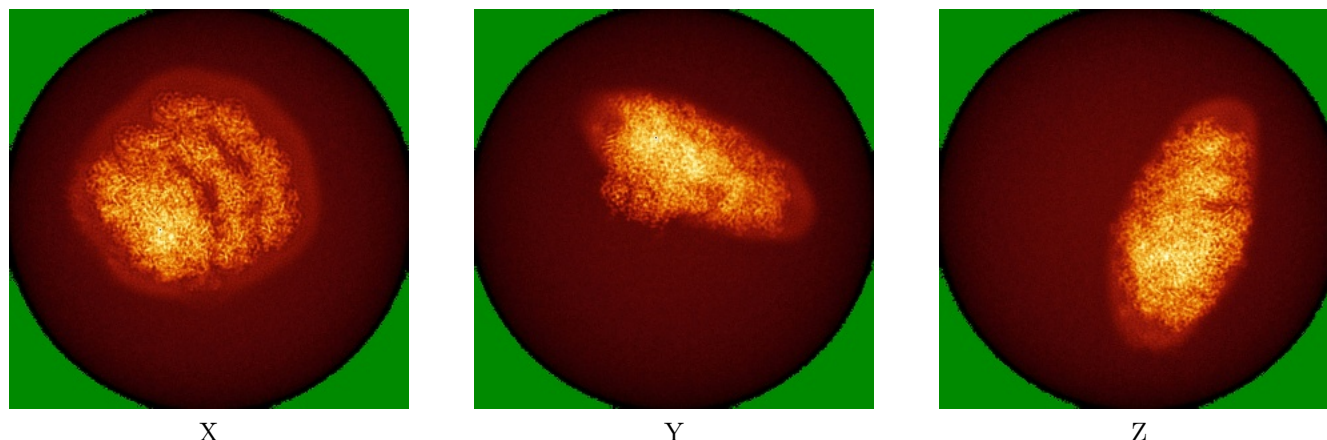


Z Index: 187

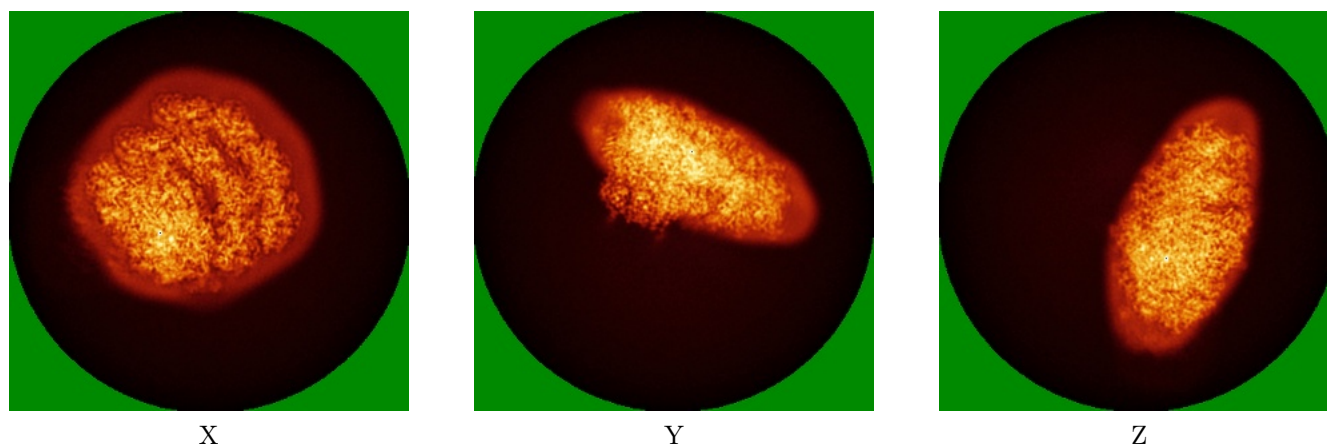
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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.

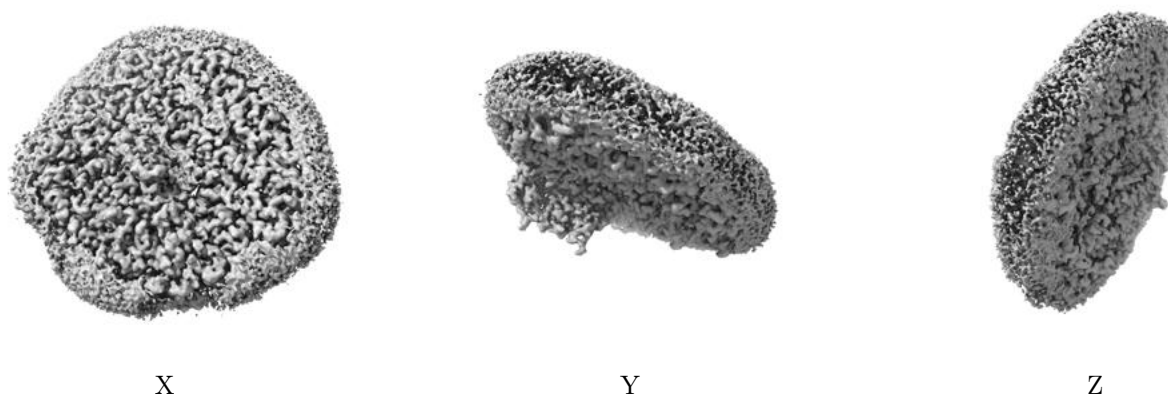
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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.

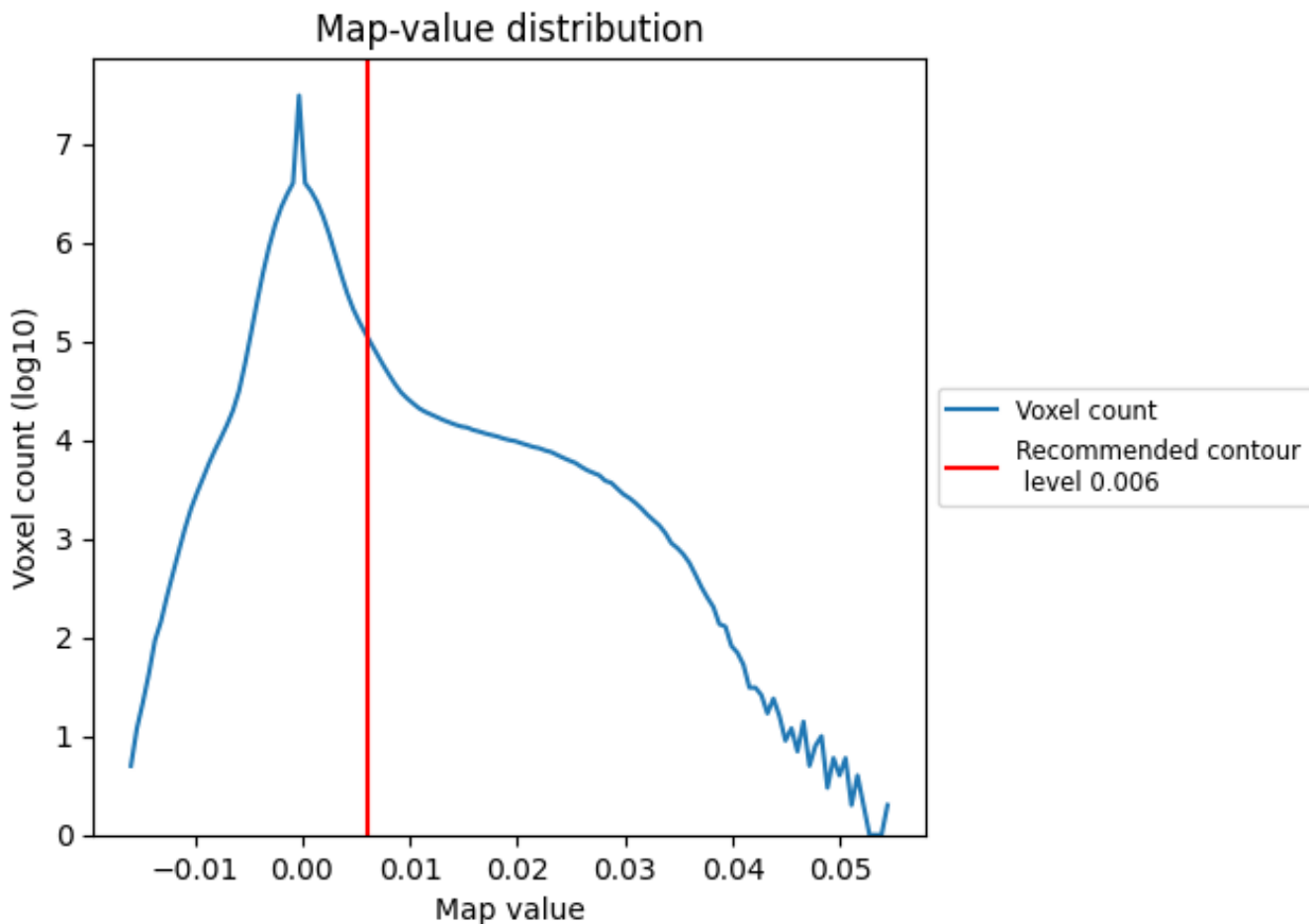
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

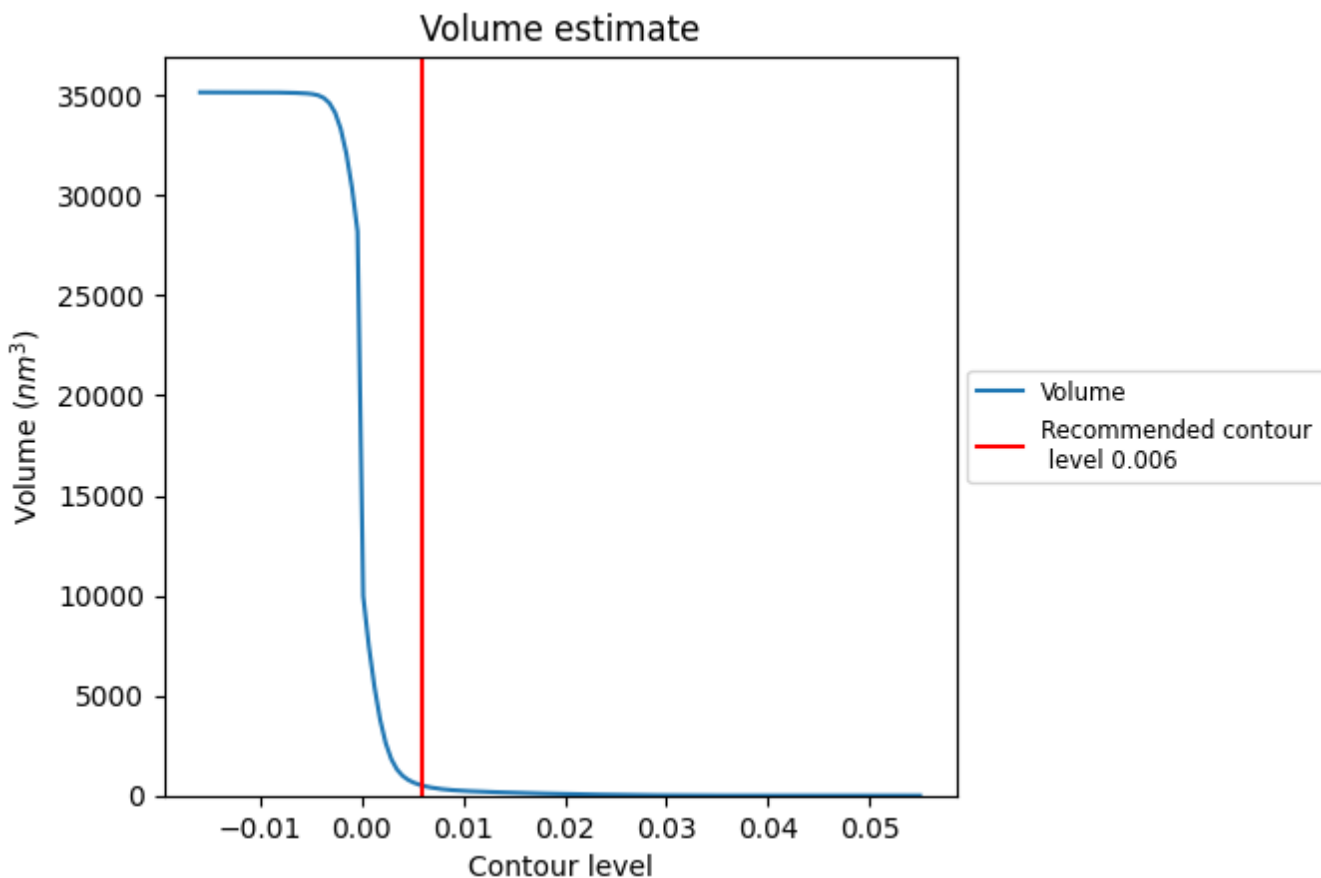
This section contains the results of statistical analysis of the map.

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.

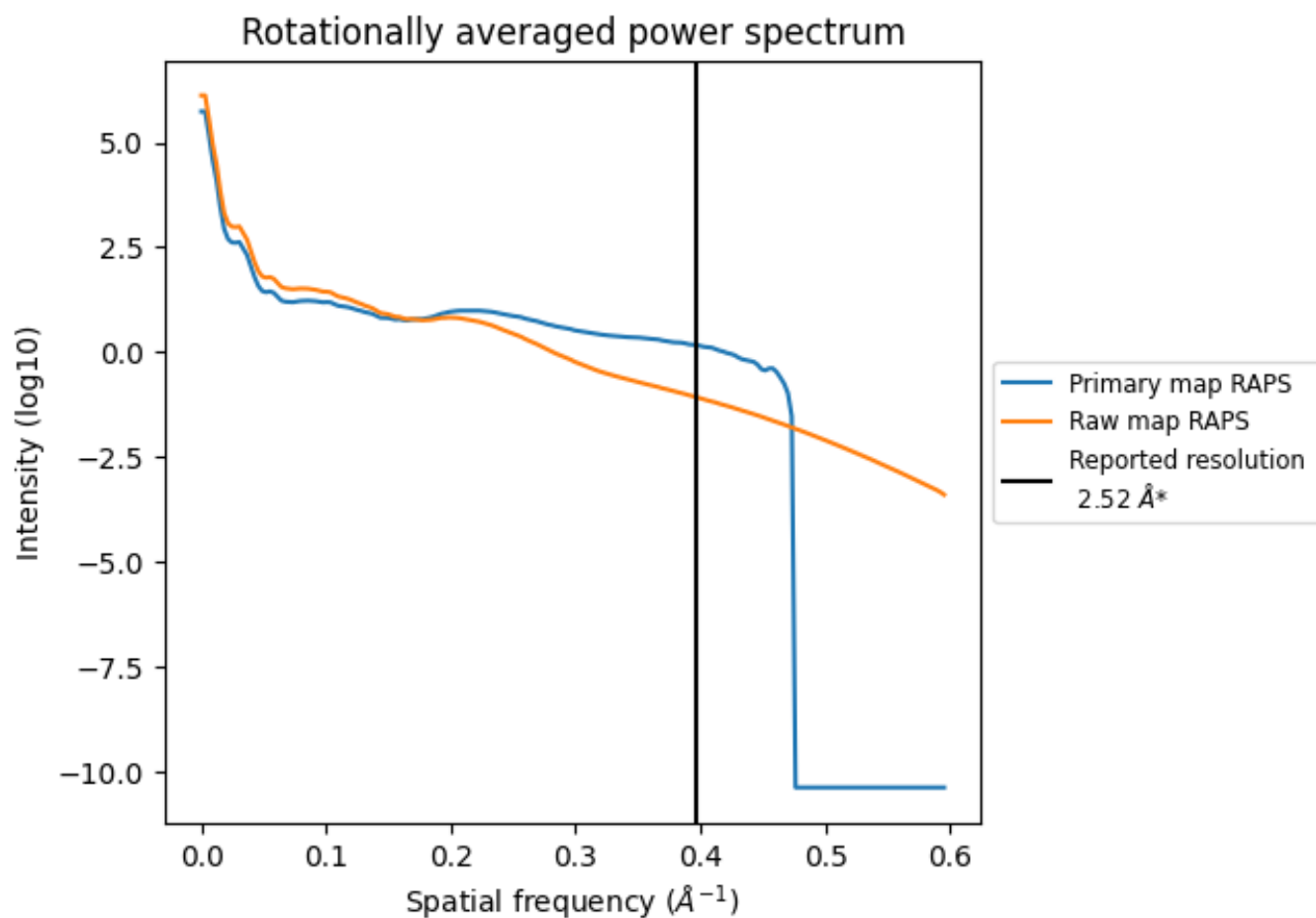
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 497 nm³; this corresponds to an approximate mass of 449 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](#)

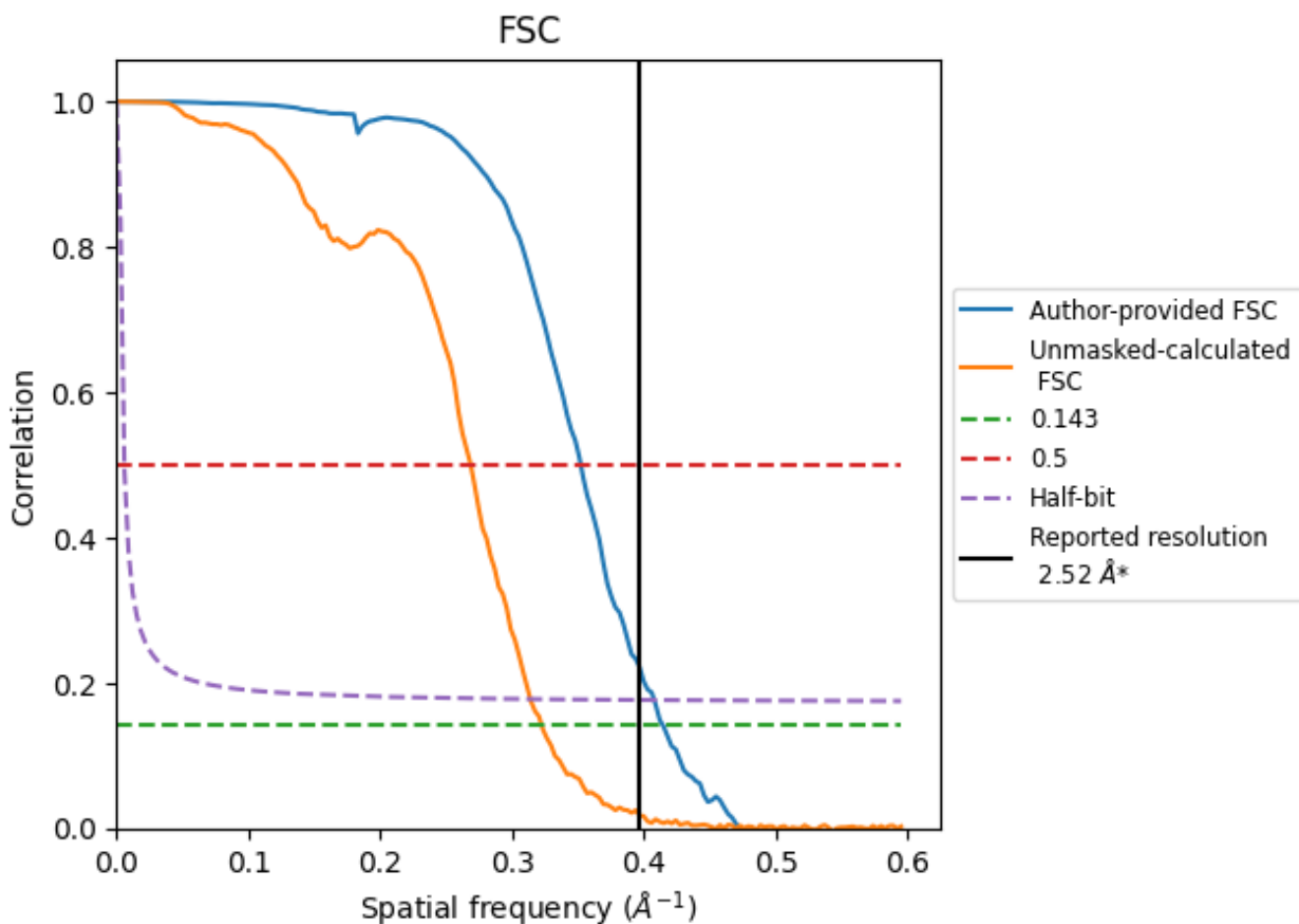


*Reported resolution corresponds to spatial frequency of 0.397 Å⁻¹

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 0.397 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	2.42	2.84	2.45
Unmasked-calculated*	3.10	3.72	3.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.10 differs from the reported value 2.52 by more than 10 %

9 Map-model fit [i](#)

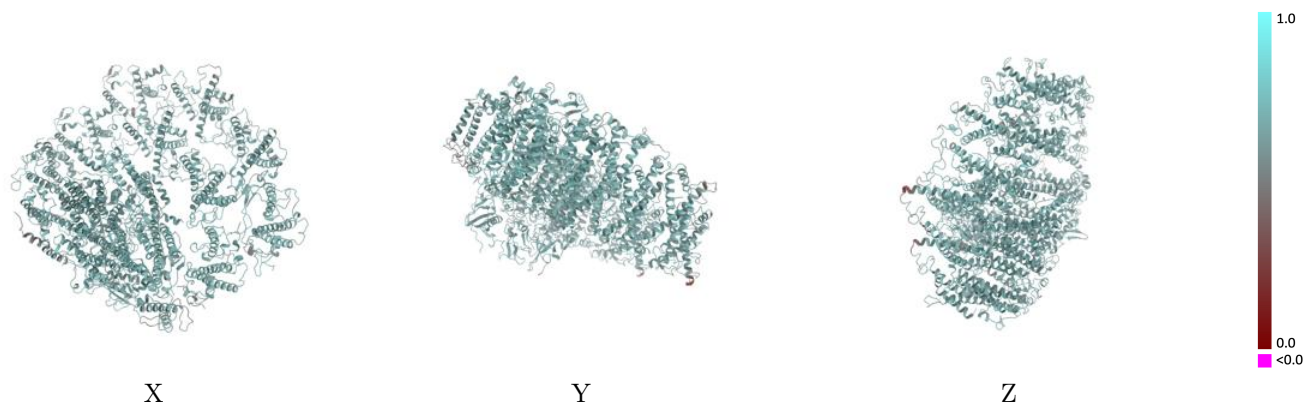
This section contains information regarding the fit between EMDB map EMD-14248 and PDB model 7R3K. Per-residue inclusion information can be found in section 3 on page 38.

9.1 Map-model overlay [i](#)



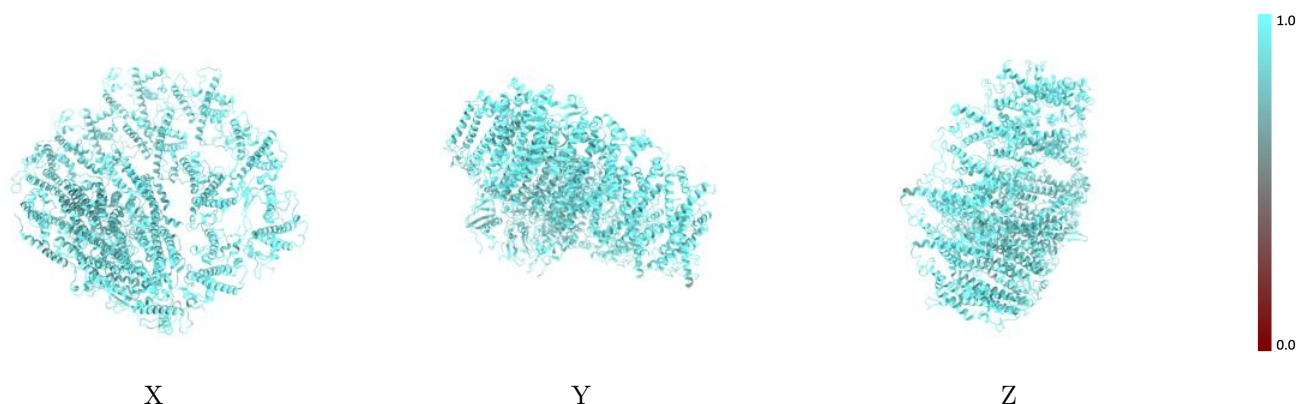
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



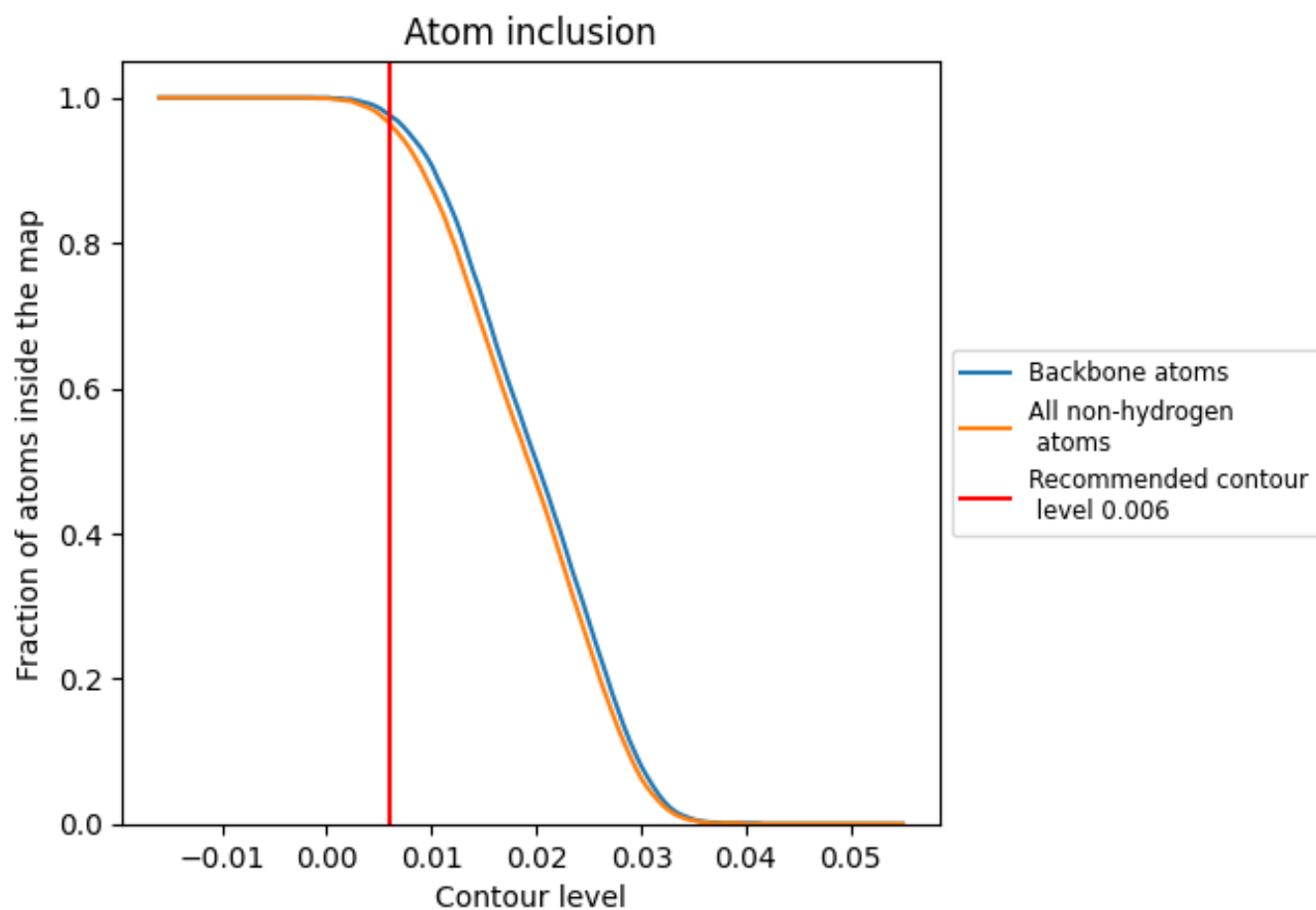
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.9650	 0.6330
1	 0.9590	 0.6210
3	 0.9620	 0.6300
4	 0.9570	 0.6120
5	 0.9600	 0.6220
6	 0.9680	 0.6260
7	 0.9720	 0.6480
8	 0.9770	 0.6500
A	 0.9710	 0.6480
B	 0.9690	 0.6450
C	 0.9870	 0.6580
D	 0.9740	 0.6410
E	 0.9690	 0.6340
F	 0.9690	 0.6490
G	 0.9520	 0.5770
I	 0.8390	 0.5170
J	 0.9600	 0.6270
K	 0.8880	 0.5350
Z	 0.9510	 0.6010

