



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:51 PM UTC

PDB ID : 7R3K / pdb_00007r3k
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:

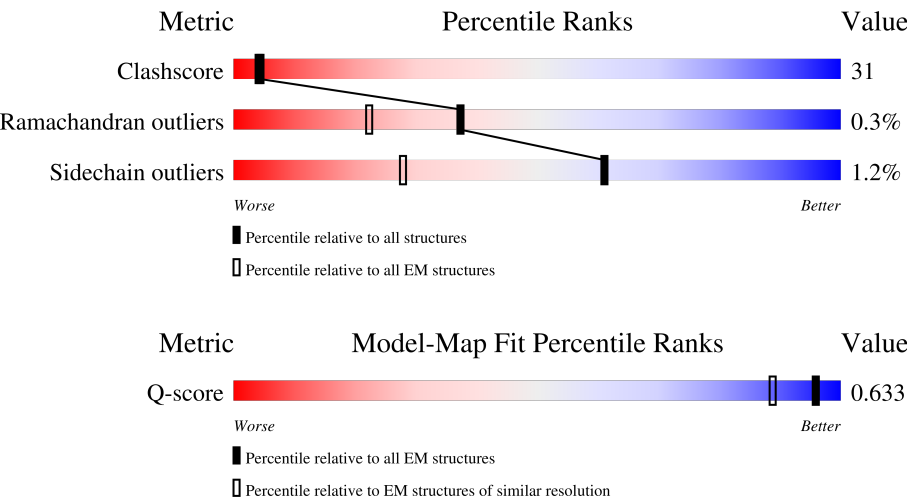
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7226 (2.02 - 3.02)

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	72%26%
2	B	735	68%32%
3	C	81	68%31%
4	D	196	54%19%27%

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Mol	Chain	Length	Quality of chain
5	E	97	
6	F	227	
7	G	126	
8	I	106	
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	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	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
19	CLA	B	821	X	-	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-
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

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
1	A	740	Total	C	N	O	S	0	0
			5811	3799	991	999	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5824	3825	977	1004	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			601	369	103	117	12		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

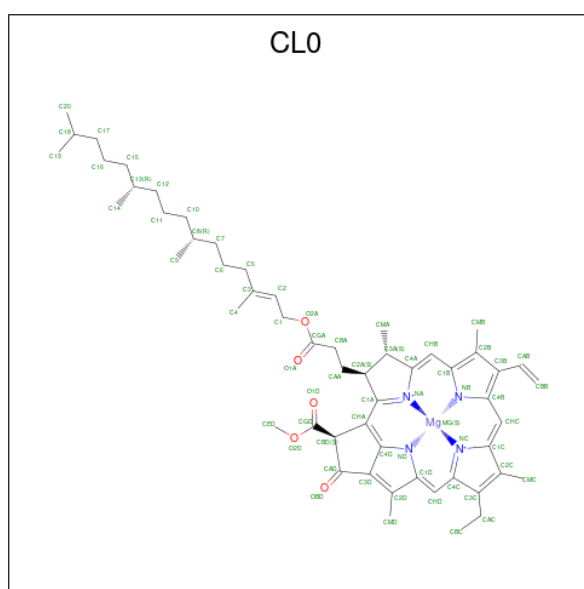
- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

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

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

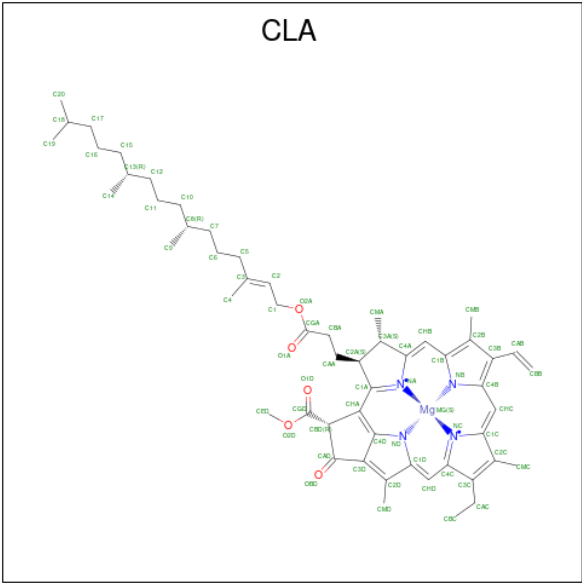
Mol	Chain	Residues	Atoms					AltConf	Trace
17	6	229	Total	C	N	O	S	0	0
			1766	1164	292	304	6		

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



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

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	1	1	Total 48	C 38	Mg 1	N 4	O 5	0
19	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	1	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	Z	1	Total 57	C 47	Mg 1	N 4	O 5	0
19	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	3	1	Total 46	C 36	Mg 1	N 4	O 5	0

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

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

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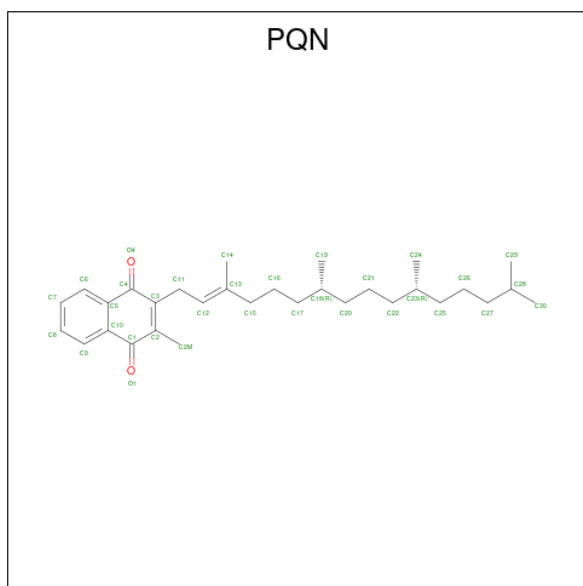
Mol	Chain	Residues	Atoms					AltConf
19	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
19	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	5	1	Total	C	Mg	N	O	0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

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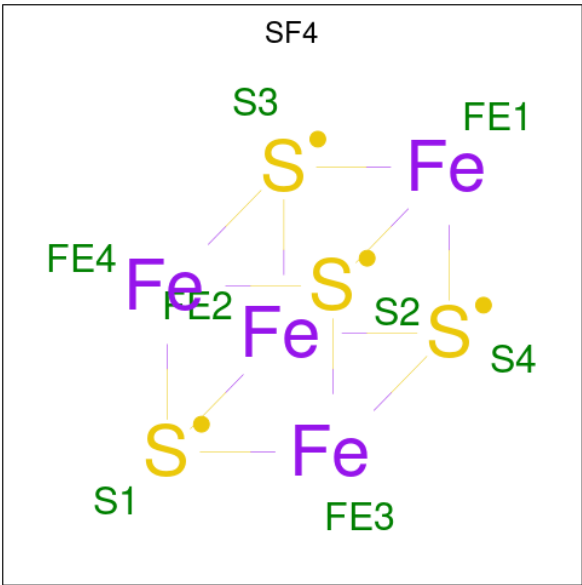
Mol	Chain	Residues	Atoms					AltConf
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	6	1	Total	C	Mg	N	O	0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

- Molecule 20 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



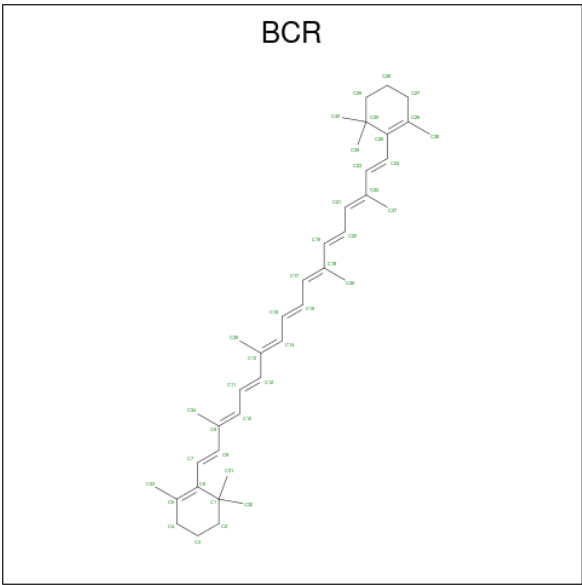
Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			33	31	2	
20	B	1	Total	C	O	0
			33	31	2	

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: 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 (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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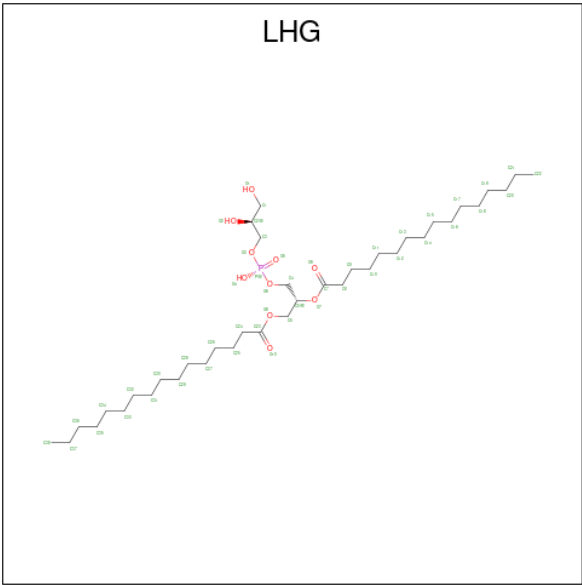
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	A	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 40 40	0
22	B	1	Total C 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 (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



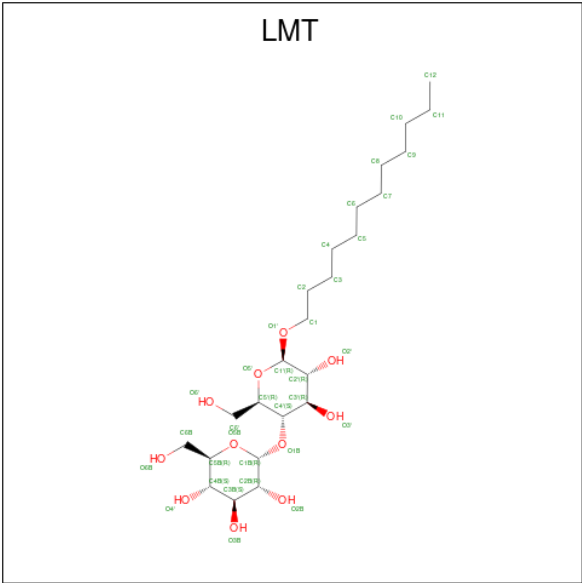
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C O P 35 24 10 1	0
23	A	1	Total C O P 49 38 10 1	0
23	1	1	Total C O P 23 12 10 1	0
23	1	1	Total C O P 43 32 10 1	0
23	Z	1	Total C O P 43 32 10 1	0

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

- Molecule 24 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



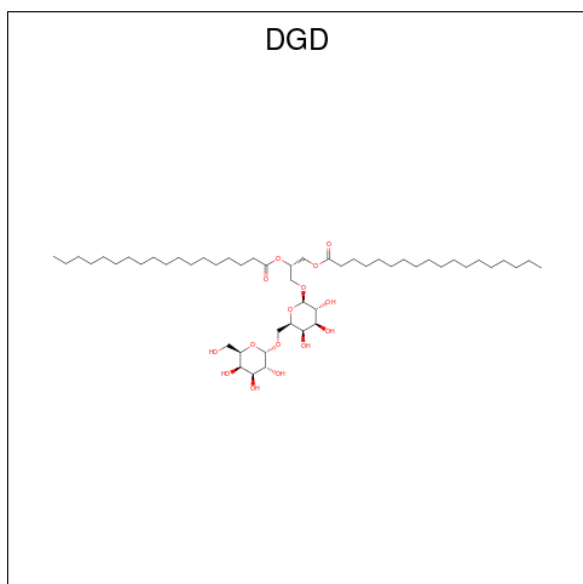
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			35	24	11	
24	A	1	Total	C	O	0
			35	24	11	
24	A	1	Total	C	O	0
			35	24	11	
24	A	1	Total	C	O	0
			35	24	11	

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

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

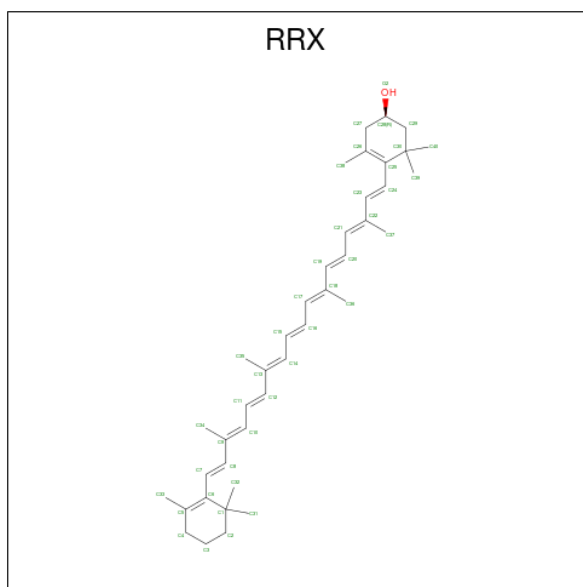


Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	C	O	0
			66	51	15	

- Molecule 26 is CALCIUM ION (CCD ID: CA) (formula: Ca).

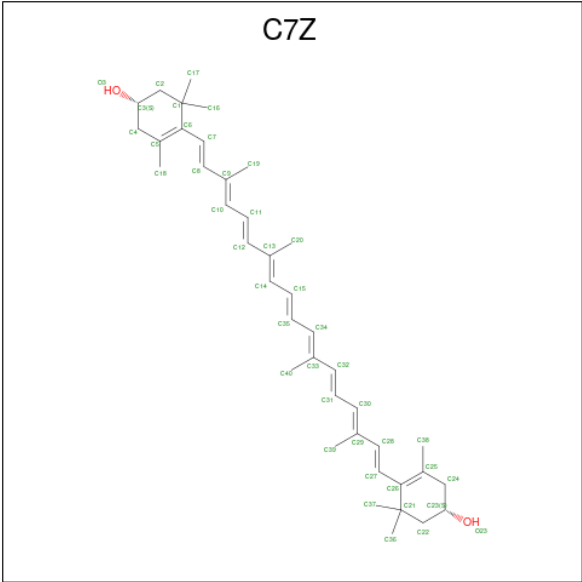
Mol	Chain	Residues	Atoms			AltConf
26	B	1	Total	Ca		0
			1	1		

- Molecule 27 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).



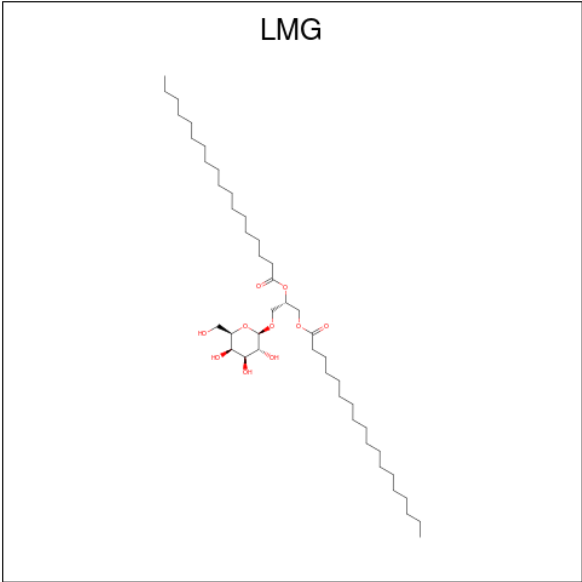
Mol	Chain	Residues	Atoms			AltConf
27	F	1	Total	C	O	0
			41	40	1	
27	4	1	Total	C	O	0
			41	40	1	
27	5	1	Total	C	O	0
			41	40	1	

- 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 (CCD ID: C7Z) (formula: C₄₀H₅₆O₂).



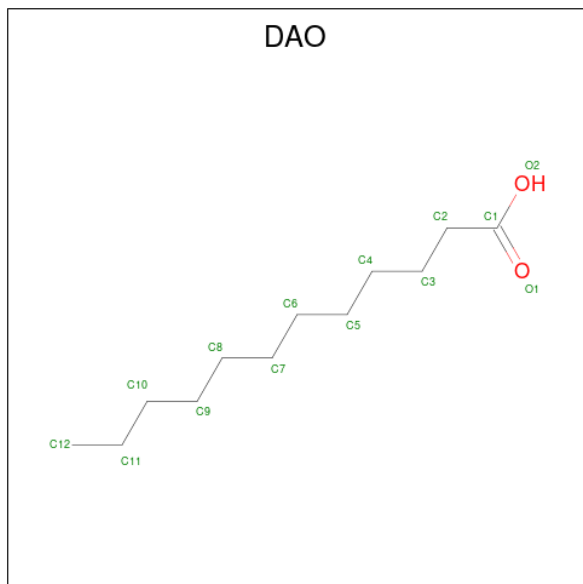
Mol	Chain	Residues	Atoms			AltConf
28	J	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	6	1	Total	C	O	0
			42	40	2	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



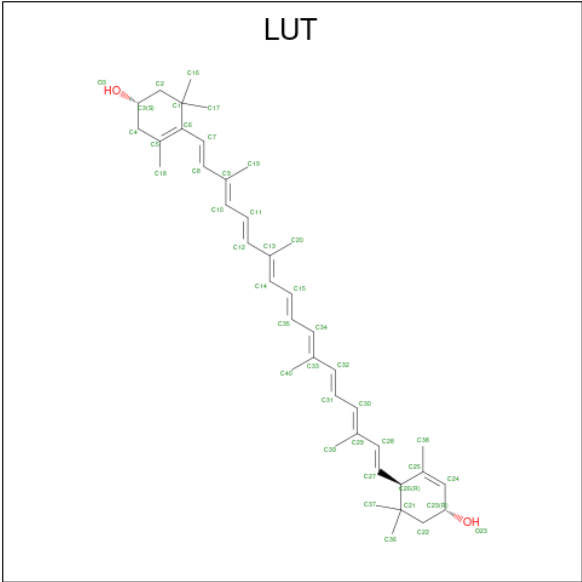
Mol	Chain	Residues	Atoms			AltConf
29	J	1	Total	C	O	0
			35	25	10	
29	J	1	Total	C	O	0
			45	35	10	
29	7	1	Total	C	O	0
			29	19	10	

- Molecule 30 is LAURIC ACID (CCD ID: DAO) (formula: $C_{12}H_{24}O_2$).



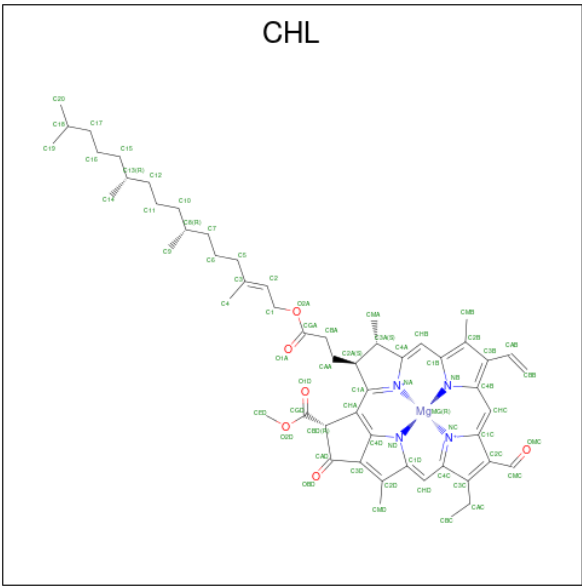
Mol	Chain	Residues	Atoms			AltConf
30	K	1	Total	C	O	0
			14	12	2	

- Molecule 31 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



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 (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



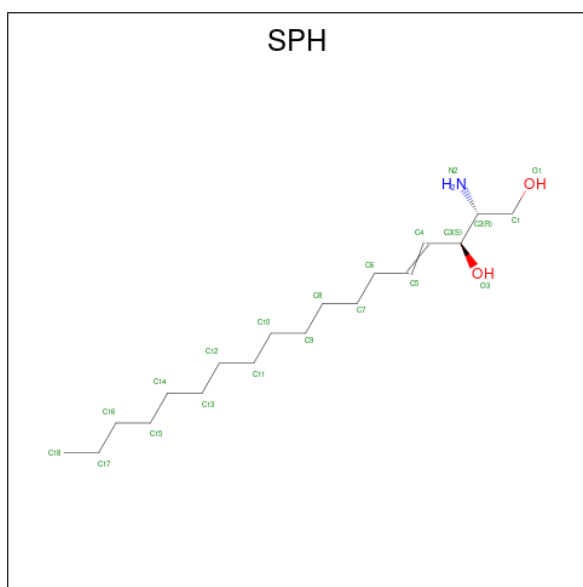
Mol	Chain	Residues	Atoms					AltConf
32	1	1	Total 61	C 50	Mg 1	N 4	O 6	0
32	1	1	Total 48	C 37	Mg 1	N 4	O 6	0
32	1	1	Total 48	C 37	Mg 1	N 4	O 6	0
32	Z	1	Total 57	C 46	Mg 1	N 4	O 6	0
32	Z	1	Total 63	C 52	Mg 1	N 4	O 6	0
32	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
32	Z	1	Total 46	C 35	Mg 1	N 4	O 6	0
32	3	1	Total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

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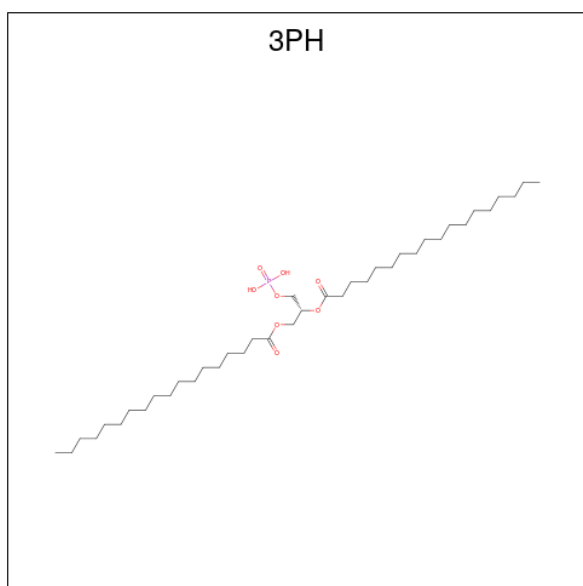
Mol	Chain	Residues	Atoms					AltConf
32	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
32	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
32	5	1	Total	C	Mg	N	O	0
			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 (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).



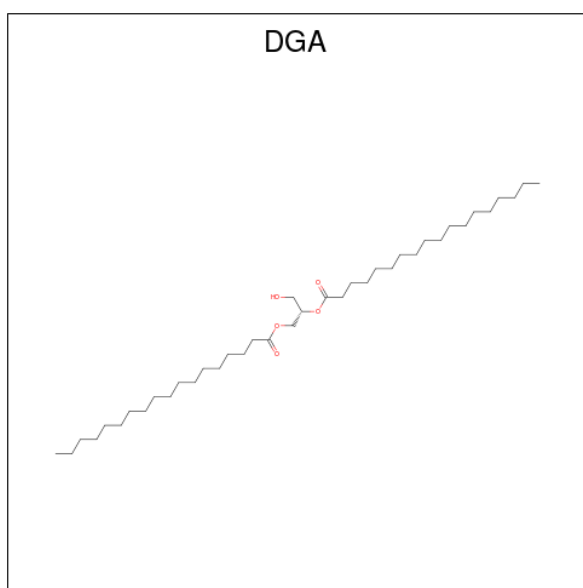
Mol	Chain	Residues	Atoms				AltConf
33	3	1	Total	C	N	O	0
			21	18	1	2	
33	7	1	Total	C	N	O	0
			21	18	1	2	
33	4	1	Total	C	N	O	0
			21	18	1	2	

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



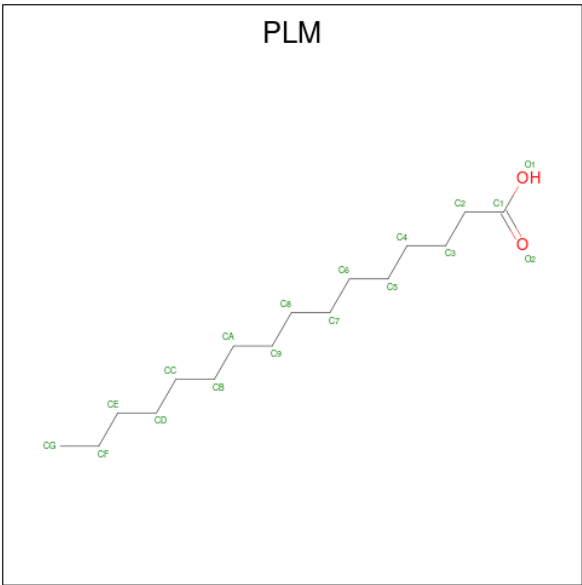
Mol	Chain	Residues	Atoms				AltConf
34	3	1	Total	C	O	P	0
			39	30	8	1	
34	8	1	Total	C	O	P	0
			30	21	8	1	
34	5	1	Total	C	O	P	0
			23	14	8	1	
34	6	1	Total	C	O	P	0
			29	20	8	1	

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



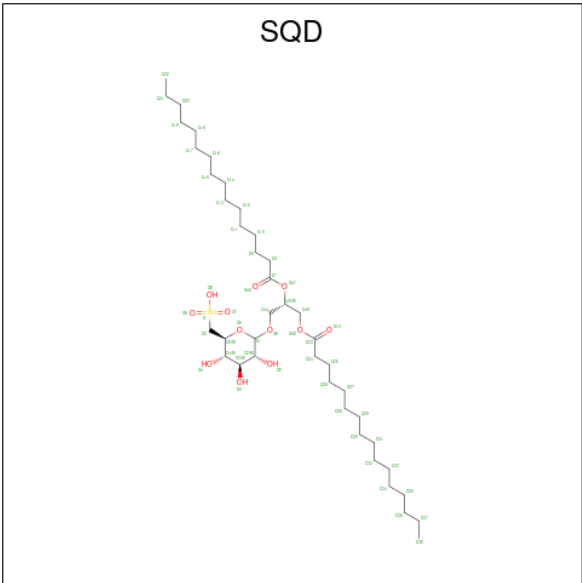
Mol	Chain	Residues	Atoms			AltConf
35	7	1	Total	C	O	0
			34	29	5	

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



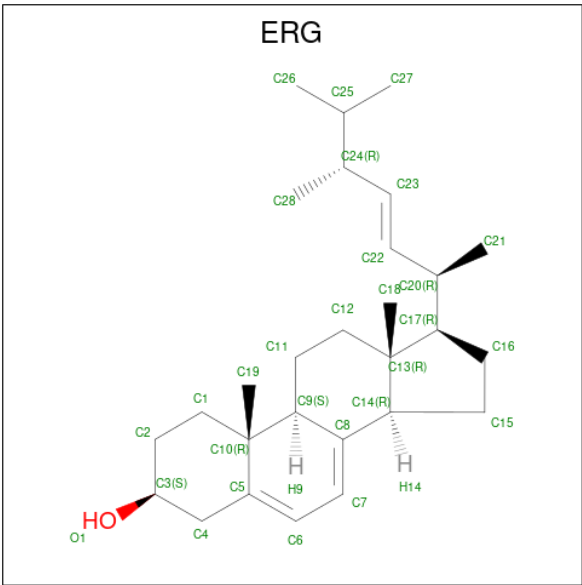
Mol	Chain	Residues	Atoms			AltConf
36	7	1	Total	C	O	0
			18	16	2	

- Molecule 37 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: 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 (CCD ID: 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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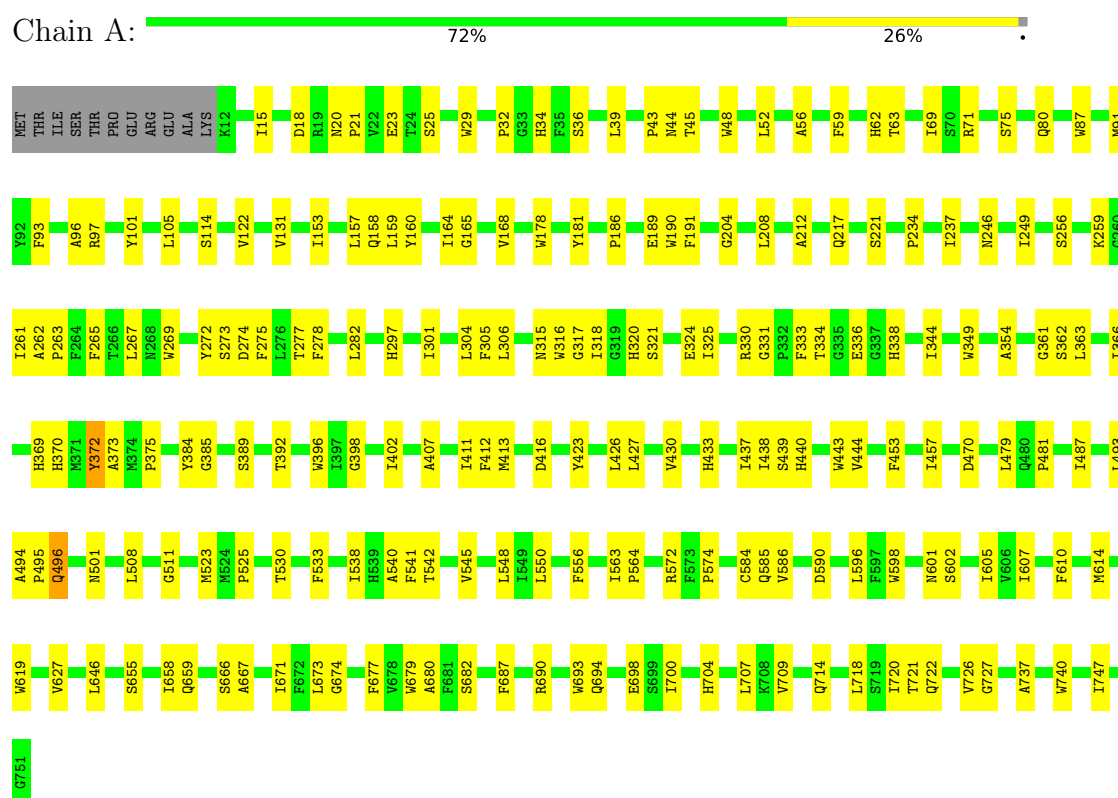
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Mol	Chain	Residues	Atoms		AltConf
39	Z	13	Total 13	O 13	0
39	3	31	Total 31	O 31	0
39	7	36	Total 36	O 36	0
39	8	31	Total 31	O 31	0
39	4	24	Total 24	O 24	0
39	5	18	Total 18	O 18	0
39	6	22	Total 22	O 22	0

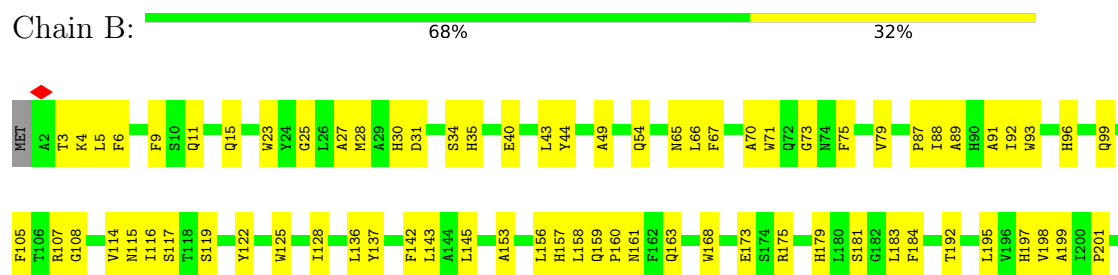
3 Residue-property plots

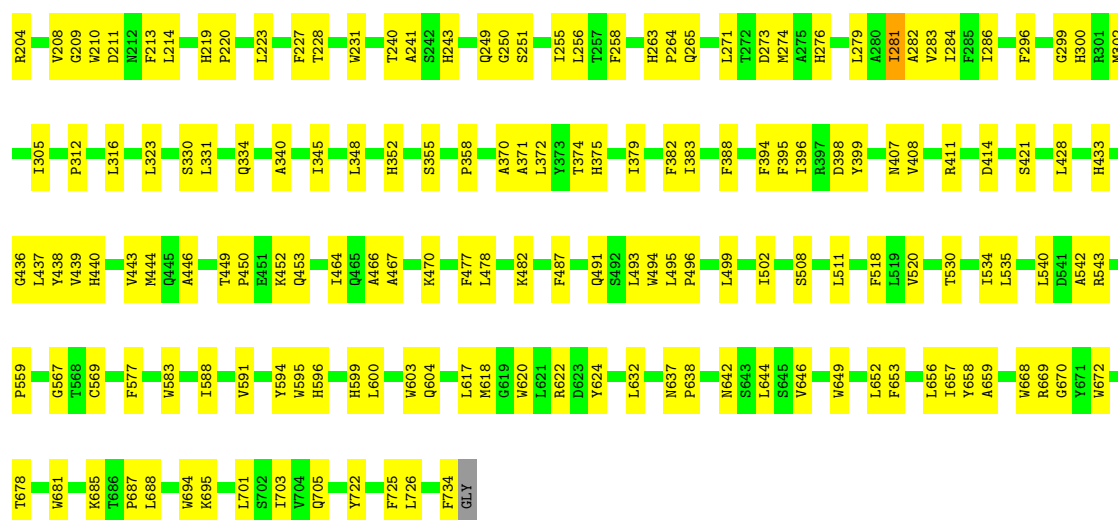
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





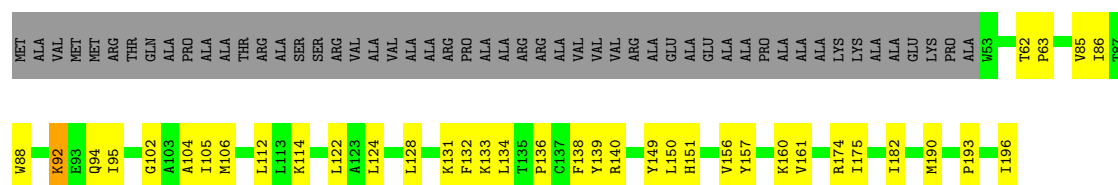
• Molecule 3: Photosystem I iron-sulfur center

Chain C: 68% 31%



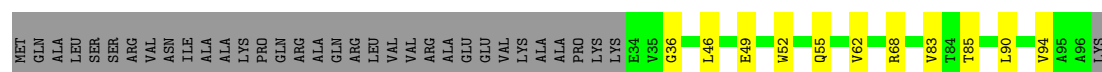
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D: 54% 19% 27%



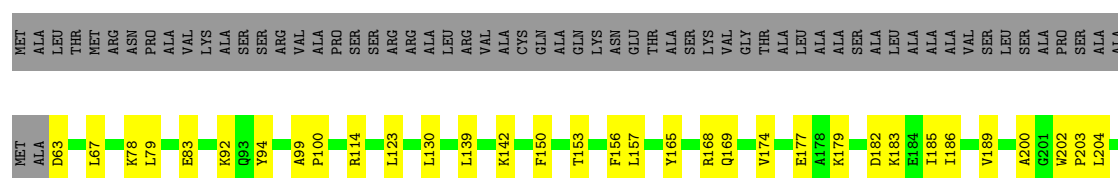
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

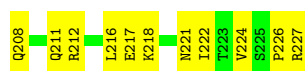
Chain E: 54% 11% 35%



• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

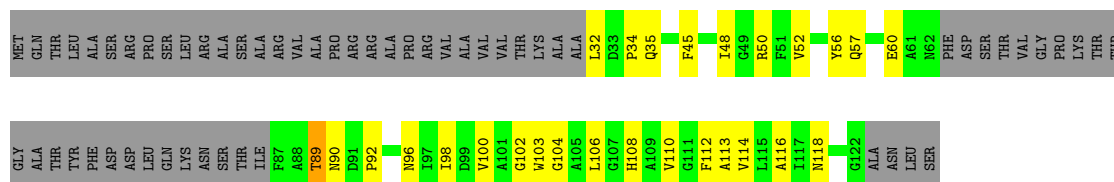
Chain F: 53% 19% 27%





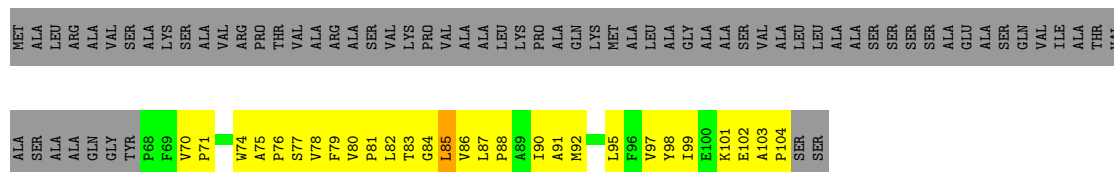
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain G: 32% 21% 47%



- Molecule 8: Photosystem I reaction center subunit VIII

Chain I: 8% 25% 65%



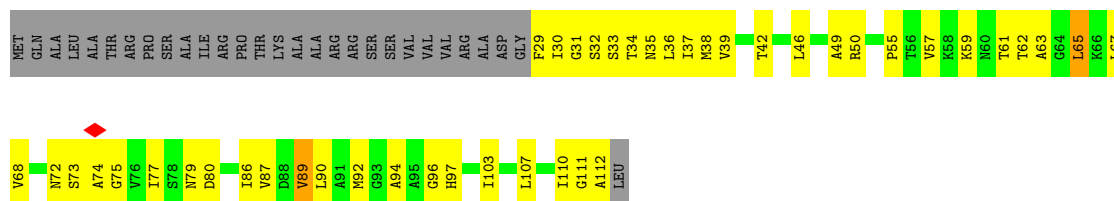
- Molecule 9: Photosystem I reaction center subunit IX

Chain J: 59% 37% 5%



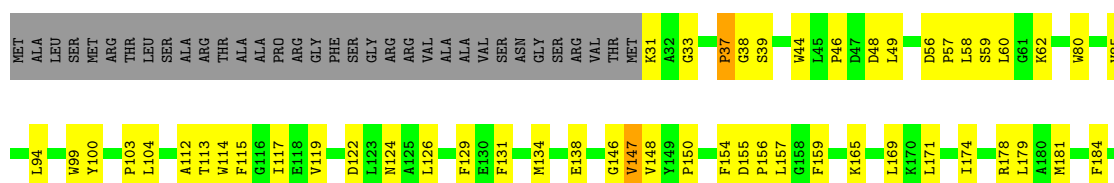
- Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic

Chain K: 35% 37% 26%



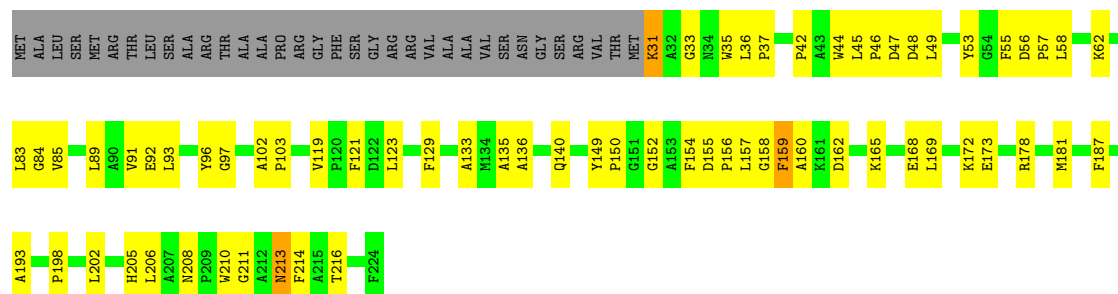
- Molecule 11: Chlorophyll a-b binding protein, chloroplastic

Chain 1: 57% 26% 15%

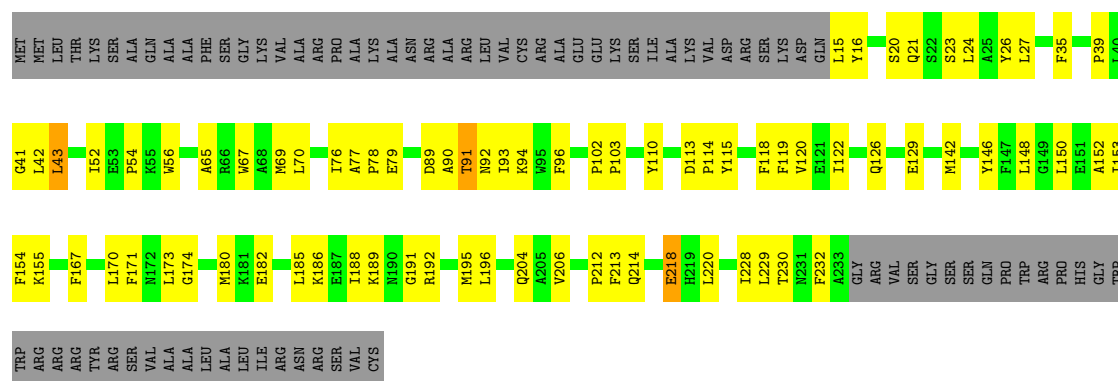




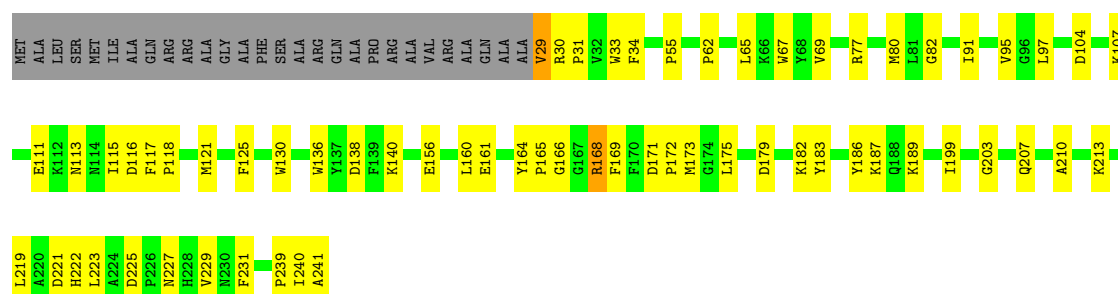
- Molecule 11: Chlorophyll a-b binding protein, chloroplastic



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

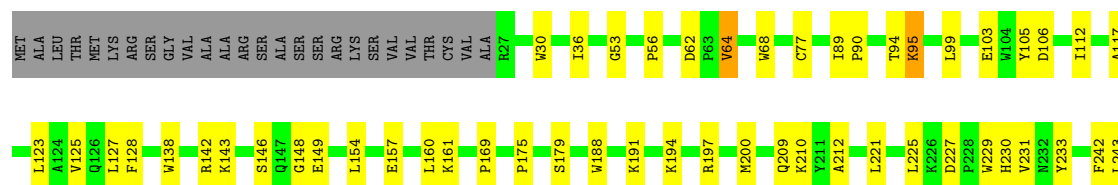


- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

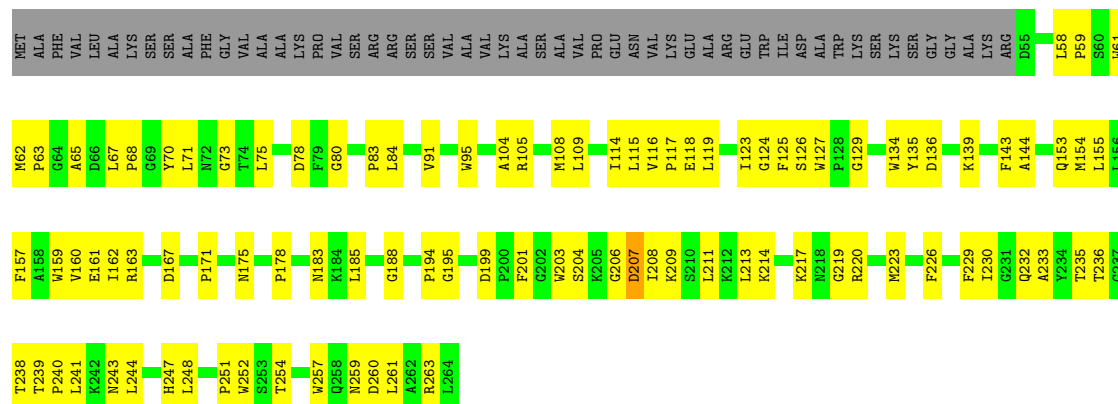


- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

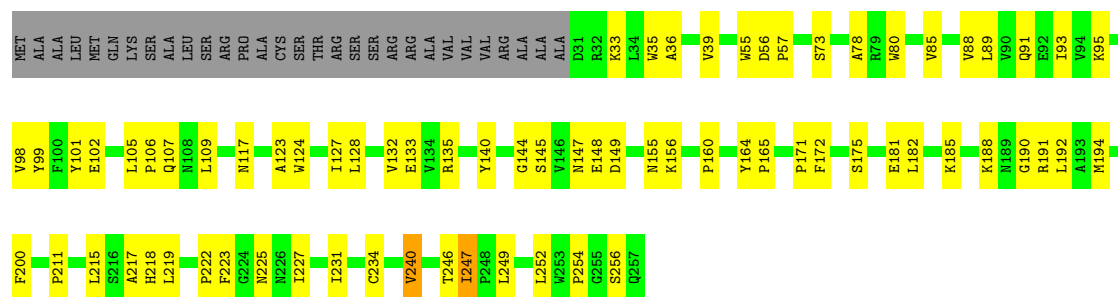




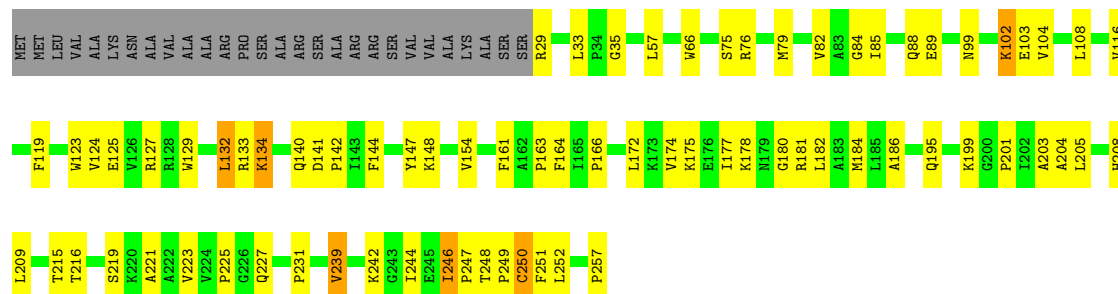
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic (Lhca4)



- Molecule 16: Chlorophyll a-b binding protein, chloroplastic



- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



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 ($\text{\AA}$)	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 ($\text{\AA}$)	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: LHG, SQD, SNC, CL0, C7Z, RRX, CA, CHL, SPH, PQN, CLA, DAO, SF4, ERG, DGA, PLM, LMT, 3PH, LUT, BCR, LMG, DGD

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	0.88	0/6007	1.07	1/8190 (0.0%)
2	B	0.90	0/6036	1.10	1/8242 (0.0%)
3	C	0.97	0/611	1.09	0/826
4	D	0.91	0/1154	1.08	1/1556 (0.1%)
5	E	0.98	0/506	1.06	0/689
6	F	0.87	0/1292	1.15	0/1747
7	G	0.93	0/505	1.19	0/685
8	I	0.97	0/293	1.11	0/406
9	J	0.90	0/331	1.16	0/454
10	K	1.00	0/575	1.25	0/779
11	1	0.90	0/1491	1.12	0/2028
11	Z	0.92	0/1491	1.17	1/2028 (0.0%)
12	3	0.89	0/1721	1.14	0/2336
13	7	0.89	0/1702	1.11	0/2310
14	8	0.89	0/1701	1.12	0/2315
15	4	0.90	0/1683	1.12	0/2296
16	5	0.90	0/1830	1.15	0/2492
17	6	0.93	0/1828	1.14	0/2497
All	All	0.90	0/30757	1.11	4/41876 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ASN	N-CA-C	-6.75	105.67	114.04
4	D	102	GLY	CA-C-O	-6.21	118.19	122.22
2	B	299	GLY	CA-C-O	-5.71	118.20	122.37
11	Z	154	PHE	N-CA-C	-5.02	107.15	113.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5811	0	5658	201	0
2	B	5824	0	5580	222	0
3	C	601	0	584	21	0
4	D	1135	0	1148	27	0
5	E	496	0	491	8	0
6	F	1266	0	1301	49	0
7	G	495	0	485	38	0
8	I	281	0	292	36	0
9	J	320	0	322	17	0
10	K	570	0	606	54	0
11	1	1445	0	1396	68	0
11	Z	1445	0	1396	67	0
12	3	1673	0	1631	81	0
13	7	1650	0	1589	69	0
14	8	1650	0	1629	81	0
15	4	1628	0	1576	107	0
16	5	1775	0	1746	85	0
17	6	1766	0	1765	111	0
18	A	65	0	72	9	0
19	1	554	0	504	80	0
19	3	692	0	669	110	0
19	4	553	0	507	100	0
19	5	855	0	809	159	0
19	6	704	0	687	143	0
19	7	720	0	670	93	0
19	8	579	0	560	95	0
19	A	2655	0	2744	390	0
19	B	2490	0	2539	396	0
19	F	110	0	104	15	0
19	G	96	0	71	16	0
19	I	55	0	49	5	0
19	J	42	0	30	4	0
19	K	195	0	150	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Z	564	0	532	73	0
20	A	33	0	46	4	0
20	B	33	0	46	4	0
21	A	8	0	0	5	0
21	C	16	0	0	5	0
22	3	160	0	224	42	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	70	0
22	B	240	0	336	77	0
22	F	40	0	56	9	0
22	G	40	0	56	12	0
22	K	40	0	56	14	0
23	1	66	0	72	10	0
23	3	20	0	12	4	0
23	4	49	0	74	15	0
23	5	37	0	44	7	0
23	6	81	0	108	21	0
23	7	37	0	44	3	0
23	8	38	0	46	7	0
23	A	84	0	114	11	0
23	Z	43	0	56	6	0
24	1	35	0	46	8	0
24	3	35	0	46	7	0
24	4	105	0	138	19	0
24	7	35	0	46	2	0
24	8	70	0	92	8	0
24	A	140	0	184	23	0
24	F	35	0	46	9	0
24	G	35	0	46	11	0
24	Z	70	0	91	13	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	3	0
28	J	42	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	7	29	0	28	1	0
29	J	80	0	103	14	0
30	K	14	0	23	4	0
31	1	84	0	112	15	0
31	3	84	0	112	13	0
31	4	42	0	56	11	0
31	5	42	0	56	9	0
31	6	84	0	112	14	0
31	7	84	0	112	16	0
31	8	84	0	112	13	0
31	Z	84	0	112	20	0
32	1	157	0	121	21	0
32	3	66	0	69	11	0
32	4	211	0	169	32	0
32	5	211	0	170	42	0
32	6	287	0	259	61	0
32	7	120	0	113	16	0
32	8	296	0	269	40	0
32	Z	232	0	209	50	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	2	0
34	6	29	0	31	4	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	3	0
39	C	35	0	0	0	0
39	D	28	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
39	K	4	0	0	1	0
39	Z	13	0	0	0	0
All	All	46504	0	45917	2886	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 31.

All (2886) 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: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
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:B:825:CLA:HBA1	19:B:826:CLA:HED2	1.38	1.02
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
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
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
19:8:313:CLA:H2	19:4:310:CLA:H71	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:4:308:CLA:HBA1	19:4:308:CLA:CBD	1.93	0.97
19:5:311:CLA:HMA1	32:5:318:CHL:HBC3	1.46	0.97
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
20:A:844:PQN:H142	22:F:302:BCR:H271	1.48	0.95
14:8:138:TRP:CD2	19:8:318:CLA:HMA2	2.01	0.95
19:B:835:CLA:H51	19:B:850:CLA:HMB2	1.47	0.93
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:A:802:CLA:HAB	2:B:583:TRP:CH2	2.04	0.92
19:4:311:CLA:HMB1	19:4:311:CLA:HBB1	1.52	0.92
19:A:807:CLA:HHC	19:A:807:CLA:HBB1	1.50	0.92
19:A:808:CLA:HHC	19:A:808:CLA:HBB1	1.51	0.91
19:A:832:CLA:HHC	19:A:832:CLA:HBB1	1.49	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
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
1:A:396:TRP:CD1	19:A:828:CLA:HAB	2.05	0.90
19:B:815:CLA:H112	22:B:842:BCR:H21C	1.51	0.89
19:6:309:CLA:HMB3	19:6:309:CLA:HBB1	1.52	0.89
19:B:812:CLA:HHC	19:B:812:CLA:HBB1	1.55	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
19:4:312:CLA:NC	23:4:320:LHG:HC42	1.88	0.88
1:A:389:SER:HB3	19:A:828:CLA:HMA1	1.53	0.88
19:5:306:CLA:HBB1	19:5:306:CLA:HMB3	1.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:8:318:CLA:HMC2	24:8:324:LMT:H123	1.57	0.87
19:G:1601:CLA:HHC	19:G:1601: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:829:CLA:HHC	19:A:829:CLA:HBB1	1.57	0.86
19:B:832:CLA:HMA2	29:J:1904:LMG:H151	1.56	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
19:5:313:CLA:HMB1	19:5:313:CLA:HBB1	1.58	0.85
19:A:814:CLA:H2	19:A:816:CLA:HMB2	1.57	0.85
12:3:43:LEU:HG	19:3:5011:CLA:HAA2	1.59	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: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
11:Z:57:PRO:HD2	31:Z:317:LUT:H23	1.57	0.84
19:3:5010:CLA:H11	19:3:5010:CLA:C4D	2.07	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
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
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
22:A:850:BCR:H23C	19:B:801:CLA:H101	1.62	0.82
11:1:58:LEU:HD12	31:1:5004:LUT:H221	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:3:76:ILE:HD13	12:3:212:PRO:HB2	1.62	0.81
14:8:142:ARG:HD2	37:8:302:SQD:H81	1.63	0.81
32:4:314:CHL:HHB	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
19:5:310:CLA:H72	19:5:314:CLA:H193	1.61	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
31:7:304:LUT:H371	31:7:304:LUT:H28	1.63	0.80
19:B:850:CLA:H122	19:B:850:CLA:HBA2	1.61	0.80
19:7:312:CLA:HHC	19:7:312:CLA:HBB1	1.62	0.80
19:A:841:CLA:HBA2	23:A:852:LHG:H161	1.64	0.80
19:B:833:CLA:HBA2	19:B:834:CLA:HMB3	1.63	0.80
22:3:5006:BCR:H21C	19:3:5012:CLA:C4C	2.11	0.80
16:5:191:ARG:HA	16:5:194:MET:HE3	1.63	0.80
22:6:307:BCR:H393	19:6:313:CLA:C7	2.11	0.80
4:D:95:ILE:HG12	4:D:105:ILE:HG12	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
1:A:679:TRP:CD2	18:A:801:CL0:H5	2.16	0.79
19:A:815:CLA:H101	22:3:5006:BCR:H14C	1.63	0.79
19:5:325:CLA:HHC	19:5:325:CLA:HBB1	1.64	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
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
19:1:5010:CLA:NB	19:1:5016:CLA:H13	1.96	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
11:1:169:LEU:HB3	19:1:5006:CLA:HMA2	1.64	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
19:4:306:CLA:HBB1	19:4:306:CLA:HMB3	1.65	0.78
19:4:312:CLA:C1C	23:4:320:LHG:HC42	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:827:CLA:HMA3	19:A:835:CLA:H51	1.63	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
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:826:CLA:H162	22:A:848:BCR:HC7	1.65	0.78
19:A:822:CLA:HMB1	19:A:823:CLA:H2	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
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:B:809:CLA:HBB1	19:B:809:CLA:HMB1	1.65	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
32:Z:313:CHL:HBB1	32:Z:313:CHL:HMB3	1.67	0.77
19:A:824:CLA:H161	19:A:839:CLA:HBA2	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
19:A:819:CLA:HMB1	19:A:819:CLA:HBB1	1.66	0.76
19:7:307:CLA:HMD2	19:7:312:CLA:H43	1.67	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
21:A:845:SF4:FE1	2:B:569:CYS:SG	1.77	0.76
19:A:816:CLA:HBB1	19:A:816:CLA:HMB1	1.68	0.75
19:3:5015:CLA:HMB1	19:3:5015:CLA:HBB1	1.67	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
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:A:827:CLA:HBB1	19:A:827:CLA:HMB3	1.67	0.75
15:4:211:LEU:HB3	19:4:306:CLA:HMA2	1.69	0.75
19:A:825:CLA:HBB1	19:A:825:CLA:HMB1	1.69	0.75
19:A:823:CLA:HBB1	19:A:823:CLA:HHC	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:311:CLA:H71	32:Z:313:CHL:HBA2	1.69	0.75
32:Z:309:CHL:HHD	32:Z:309:CHL:HBC3	1.67	0.75
19:B:818:CLA:HBB1	19:B:818:CLA:HMB1	1.69	0.74
19:1:5006:CLA:HMB3	19:1:5006:CLA:HBB1	1.67	0.74
19:Z:315:CLA:H141	19:Z:315:CLA:H171	1.68	0.74
13:7:136:TRP:CD2	19:7:317:CLA:HMA2	2.22	0.74
19:7:306:CLA:H71	19:7:307:CLA:HMA2	1.69	0.74
19:7:311:CLA:HMA2	19:7:318:CLA:HAC2	1.69	0.74
32:4:314:CHL:HMB3	32:4:314:CHL:HBB1	1.69	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
19:Z:303:CLA:HBB1	19:Z:303:CLA:HMB3	1.70	0.74
19:8:309:CLA:H122	32:8:315:CHL:H93	1.70	0.74
11:1:178:ARG:HA	11:1:181:MET:HE3	1.68	0.74
32:5:316:CHL:HMB1	32:5:316:CHL:HBB1	1.70	0.74
19:1:5007:CLA:HMB3	19:1:5007:CLA:HBB1	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
1:A:396:TRP:HD1	19:A:828:CLA:HAB	1.50	0.73
19:5:307:CLA:C4	19:5:307:CLA:H71	2.17	0.73
32:5:318:CHL:HMB1	32:5:318:CHL:HBB1	1.70	0.73
19:5:314:CLA:ND	23:5:323:LHG:H102	2.02	0.73
19:A:815:CLA:HBB1	19:A:815:CLA:HMB3	1.71	0.73
19:B:831:CLA:H151	19:B:836:CLA:H162	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:B:832:CLA:HBB1	19:B:832:CLA:HMB3	1.70	0.73
19:3:5008:CLA:HBB1	19:3:5008:CLA:HMB3	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:B:821:CLA:HMB1	19:B:821:CLA:HBB1	1.71	0.73
19:A:824:CLA:HMD3	19:A:825:CLA:HAB	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:B:850:CLA:HMC2	27:F:304:RRX:H17	1.71	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
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
19:B:831:CLA:HBC2	19:B:837:CLA:HMC2	1.69	0.72
27:5:302:RRX:H44	19:5:307:CLA:HMC2	1.71	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
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
21:A:845:SF4:FE1	2:B:569:CYS:HG	1.07	0.71
19:B:825:CLA:HMB1	19:B:825:CLA:HBB1	1.72	0.71
19:B:839:CLA:HBD	20:B:841:PQN:H302	1.73	0.71
22:3:5006:BCR:H393	19:3:5012:CLA:HMD2	1.72	0.71
19:8:310:CLA:HBB1	19:8:310:CLA:HMB3	1.73	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
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: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
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
19:3:5019: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:833:CLA:H112	19:A:857:CLA:HBC3	1.73	0.70
19:B:823:CLA:HAB	19:B:830:CLA:HMD2	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
19:4:307:CLA:HMA2	19:4:307:CLA:H62	1.73	0.70
22:6:308:BCR:HC8	22:6:308:BCR:C32	2.21	0.70
19:6:313:CLA:HMA1	32:6:319:CHL:HBC3	1.72	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
19:3:5013:CLA:HMB1	19:3:5013:CLA:HBB1	1.71	0.70
19:5:307:CLA:CAD	19:5:312:CLA:H2	2.22	0.70
2:B:54:GLN:HG2	19:B:806:CLA:HMA2	1.72	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
19:5:314:CLA:HMA3	23:5:323:LHG:H132	1.74	0.70
32:6:317:CHL:HBB1	32:6:317:CHL:HMB3	1.72	0.70
13:7:168:ARG:CZ	38:6:326:ERG:H12	2.22	0.70
1:A:707:LEU:HD23	6:F:216:LEU:HD23	1.73	0.70
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
11:Z:158:GLY:O	11:Z:159:PHE:HB2	1.91	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
19:B:840:CLA:HBB1	19:B:840:CLA:HMB3	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
19:Z:311:CLA:HMA2	32:Z:313:CHL:C3C	2.23	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: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
19:3:5013:CLA:HMA3	19:3:5019:CLA:C3C	2.22	0.69
2:B:241:ALA:HA	2:B:264:PRO:HG3	1.75	0.68
19:8:320:CLA:HHC	19:8:320:CLA:HBB1	1.73	0.68
19:A:820:CLA:H62	10:K:86:ILE:HG21	1.74	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
19:A:817:CLA:H102	19:A:817:CLA:HMC2	1.75	0.68
22:5:304:BCR:H321	22:5:304:BCR:HC8	1.75	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:823:CLA:H102	22:A:859:BCR:H292	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: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
32:8:317:CHL:HMB1	32:8:317:CHL:HBB1	1.76	0.68
19:6:301:CLA:HHC	19:6:301:CLA:HBB1	1.73	0.68
32:3:5017:CHL:HMB1	32:3:5017:CHL:HBB1	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:658:TYR:CE1	19:B:802:CLA:HMA3	2.30	0.67
19:B:833:CLA:H101	19:B:834:CLA:C1B	2.24	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
32:4:315:CHL:HMB1	32:4:315:CHL:HBB1	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
31:3:5003:LUT:H363	19:3:5011:CLA:H61	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
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
11:1:58:LEU:HB2	11:1:60:LEU:HG	1.76	0.67
19:B:821:CLA:HMD1	22:B:842:BCR:HC7	1.77	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
14:8:138:TRP:CE3	19:8:318:CLA:HMA2	2.29	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
11:1:210:TRP:CE2	19:1:5013:CLA:HMA3	2.29	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
11:1:85:VAL:HG11	31:1:5003:LUT:H12	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:584:CYS:HG	21:A:845:SF4:FE2	1.12	0.66
32:Z:313:CHL:HBA1	24:Z:319:LMT:O3'	1.95	0.66
32:7:315:CHL:HHC	32:7:315:CHL:HBB1	1.77	0.66
32:8:319:CHL:HMB3	32:8:319:CHL:HBB1	1.78	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:HHH	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
19:5:311:CLA:HMA3	32:5:318:CHL:HBC3	1.77	0.66
31:1:5004:LUT:H28	32:1:5009:CHL:H102	1.78	0.65
19:Z:308:CLA:HBB1	19:Z:308:CLA:HMB3	1.78	0.65
19:Z:314:CLA:C1	19:8:312:CLA:H143	2.25	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:A:837:CLA:HBB1	19:A:837:CLA:HMB3	1.77	0.65
19:5:325:CLA:HHC	19:5:325:CLA:CBB	2.25	0.65
19:B:805:CLA:HBB1	19:B:805:CLA:HMB1	1.78	0.65
19:Z:312:CLA:HMB1	19:Z:312:CLA:HBB1	1.77	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
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
19:B:819:CLA:HMB2	19:B:824:CLA:HED1	1.78	0.65
31:8:304:LUT:H391	31:8:304:LUT:C32	2.25	0.65
2:B:66:LEU:HD11	22:B:844:BCR:H271	1.79	0.65
2:B:371:ALA:HB1	19:B:827:CLA:HMA1	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
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
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
32:1:5017:CHL:HBB1	32:1:5017:CHL:HMB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:F:202:TRP:CD1	6:F:203:PRO:HD3	2.32	0.65
19:K:205:CLA:HHC	19:K:205:CLA:HBB1	1.79	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
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
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
15:4:105:ARG:HA	15:4:108:MET:HE3	1.80	0.64
19:6:323:CLA:HBB1	19:6:323:CLA:HMB1	1.78	0.64
19:A:805:CLA:H203	22:A:846:BCR:H10C	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
15:4:220:ARG:HA	15:4:223:MET:HE3	1.78	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
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
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)
19:B:819:CLA:HMB3	19:B:824:CLA:H2	1.79	0.63
8:I:88:PRO:O	8:I:92:MET:HG2	1.98	0.63
19:7:311:CLA:HMA2	19:7:318:CLA:CAC	2.28	0.63
19:8:309:CLA:HBA1	19:8:309:CLA:CBD	2.26	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:850:CLA:H71	19:B:850:CLA:ND	2.13	0.63
19:5:306:CLA:H62	19:5:307:CLA:HMA3	1.79	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
12:3:91:THR:O	12:3:92:ASN:C	2.41	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
19:K:204:CLA:HMB1	19:K:204:CLA:HBB1	1.78	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
19:5:310:CLA:HED1	39:5:411:HOH:O	1.98	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
16:5:227:ILE:HG13	19:5:308:CLA:HMD3	1.81	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
32:1:5014:CHL:HBB1	32:1:5014:CHL:HMB1	1.81	0.63
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:830:CLA:H122	19:A:841:CLA:HMA1	1.81	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
19:8:312:CLA:HMB1	19:8:312:CLA:HBB1	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
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
23:4:320:LHG:H181	19:6:322:CLA:HMA3	1.80	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
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
19:5:313:CLA:HBB1	19:5:313:CLA:CMB	2.29	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
11:Z:178:ARG:HA	11:Z:181:MET:HE3	1.82	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
19:B:822:CLA:HBB2	22:B:845:BCR:H343	1.82	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
14:8:138:TRP:CE3	19:8:318:CLA:CMA	2.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:317:CLA:H171	19:5:319:CLA:CBB	2.30	0.61
19:B:804:CLA:HMA3	19:B:804:CLA:C2	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
19:7:324:CLA:HBB1	19:7:324:CLA:HMB3	1.82	0.61
19:4:313:CLA:HBB1	19:4:313:CLA:HMB3	1.83	0.61
19:A:841:CLA:C4B	19:B:801:CLA:H172	2.31	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
13:7:55:PRO:HD2	31:7:304:LUT:H23	1.82	0.61
1:A:481:PRO:HG3	1:A:533:PHE:HB2	1.83	0.61
19:Z:308:CLA:HBB1	19:Z:308:CLA:CMB	2.30	0.61
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
1:A:178:TRP:HB2	19:A:811:CLA:HMC2	1.84	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
32:Z:309:CHL:HBB1	32:Z:309:CHL:HMB3	1.82	0.60
12:3:182:GLU:HG3	12:3:186:LYS:HE3	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
19:A:821:CLA:C4C	19:A:827:CLA:H161	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:G:108:HIS:ND1	22:G:1603:BCR:H12C	2.17	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
15:4:62:MET:HE2	15:4:65:ALA:HB2	1.83	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
19:8:307:CLA:HBB1	19:8:307:CLA:HMB1	1.83	0.60
1:A:320:HIS:HB3	1:A:325:ILE:HD11	1.83	0.59
19:A:814:CLA:HBA2	19:A:816:CLA:HMB3	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
19:7:310:CLA:OBD	19:7:317:CLA:H2	2.01	0.59
32:8:316:CHL:HBB1	32:8:316:CHL:HMB3	1.83	0.59
1:A:59:PHE:CD2	19:A:805:CLA:HMC2	2.37	0.59
2:B:65:ASN:OD1	19:B:808:CLA:HAA2	2.01	0.59
19:7:324:CLA:HBB1	19:7:324:CLA:CMB	2.33	0.59
15:4:201:PHE:HD2	27:4:303:RRX:H12	1.66	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: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
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:B:824:CLA:H92	19:B:824:CLA:HMA1	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
17:6:175:LYS:HZ1	19:6:310:CLA:HED1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:6:303:LHG:H142	19:6:322:CLA:ND	2.18	0.59
19:A:842:CLA:HHC	19:A:842:CLA:HBB1	1.83	0.59
19:B:814:CLA:HMA2	22:B:844:BCR:H282	1.85	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
19:A:827:CLA:C3B	19:A:835:CLA:HMA3	2.32	0.59
22:A:850:BCR:H23C	19:B:801:CLA:C10	2.32	0.59
19:B:839:CLA:C2C	22:B:847:BCR:H19C	2.33	0.59
19:4:307:CLA:H62	19:4:307:CLA:CMA	2.33	0.59
19:6:313:CLA:HBB1	19:6:313:CLA:HMB3	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
17:6:247:PRO:HG2	32:6:316:CHL:C4	2.32	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
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
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
19:3:5016:CLA:HBA1	19:3:5016:CLA:CHA	2.33	0.58
19:A:827:CLA:C4B	19:A:835:CLA:HMA3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:B:821:CLA:H93	7:G:45:PHE:HE2	1.69	0.58
19:B:835:CLA:C5	19:B:850:CLA:HMB2	2.27	0.58
14:8:64:VAL:HG23	38:8:325:ERG:H6	1.85	0.58
14:8:138:TRP:CG	19:8:318:CLA:HMA2	2.39	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
19:1:5007:CLA:HMC2	19:1:5012:CLA:H142	1.85	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
19:5:307: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
24:1:5002:LMT:H52	19:1:5016:CLA:H11	1.86	0.58
12:3:142:MET:HE2	12:3:142:MET:HA	1.85	0.58
19:3:5020:CLA:HBB1	19:3:5020:CLA:HMB1	1.86	0.58
18:A:801:CL0:H12	19:A:802:CLA:CAD	2.33	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
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
22:8:306:BCR:H291	19:8:312:CLA:O1A	2.04	0.58
19:5:308:CLA:HHC	19:5:308:CLA:CBB	2.28	0.58
19:5:309:CLA:H93	19:5:310:CLA:HMA1	1.85	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
19:B:823:CLA:CMD	19:B:824:CLA:HAB	2.34	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
15:4:161:GLU:HG3	19:4:316:CLA:C4B	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
10:K:107:LEU:HA	10:K:110:ILE:HG12	1.85	0.57
19:6:313:CLA:CMA	32:6:319:CHL:HBC3	2.33	0.57
12:3:79:GLU:CD	12:3:213:PHE:HB3	2.29	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
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: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
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
11:Z:123:LEU:HD11	32:Z:310:CHL:CBC	2.34	0.57
12:3:174:GLY:HA3	12:3:180:MET:HE2	1.86	0.57
17:6:172:LEU:HB2	19:6:309:CLA:HMA2	1.86	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:482:LYS:HG3	2:B:487:PHE:CZ	2.40	0.57
19:B:823:CLA:HMB2	19:B:823:CLA:H162	1.87	0.57
19:7:308:CLA:H151	19:7:308:CLA:H203	1.87	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
19:3:5014: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:1:224:PHE:CE1	14:8:123:LEU:HD23	2.38	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
1:A:679:TRP:CG	18:A:801:CL0:H5	2.40	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
19:A:821:CLA:H72	22:A:849:BCR:C12	2.31	0.56
19:B:822:CLA:CBB	22:B:845:BCR:H343	2.35	0.56
19:B:832:CLA:C1	29:J:1904:LMG:H112	2.35	0.56
19:B:835:CLA:H51	19:B:850:CLA:CMB	2.28	0.56
22:B:842:BCR:H343	7:G:102:GLY:HA2	1.87	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
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: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
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:A:813:CLA:HBB1	19:A:813:CLA:HMB1	1.86	0.56
19:B:814:CLA:H92	22:B:844:BCR:C17	2.36	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
19:7:307:CLA:HBB1	19:7:307:CLA:HMB3	1.87	0.56
14:8:30:TRP:HH2	34:8:322:3PH:H322	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
11:Z:155:ASP:HA	31:Z:318:LUT:H24	1.88	0.56
19:3:5009:CLA:HMD2	19:3:5014:CLA:H43	1.86	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
19:B:826:CLA:C3B	19:B:833:CLA:HMA2	2.34	0.56
10:K:30:ILE:HA	10:K:35:ASN:ND2	2.21	0.56
19:Z:314:CLA:HMA3	19:8:312:CLA:H101	1.86	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
11:1:154:PHE:C	11:1:156:PRO:HD3	2.31	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
19:6:310:CLA:HMD3	19:6:314:CLA:C4D	2.35	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
9:J:38:VAL:C	29:J:1904:LMG:H122	2.30	0.56
10:K:39:VAL:HA	19:K:202:CLA:O1A	2.05	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:839:CLA:HBB1	19:A:839:CLA:HMB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:4:211:LEU:CB	19:4:306:CLA:HMA2	2.35	0.56
19:5:310:CLA:CMB	19:5:310:CLA:HBB1	2.36	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
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: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
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
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: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
19:3:5013:CLA:H11	19:5:301:CLA:HMB2	1.88	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
17:6:108:LEU:N	17:6:108:LEU:HD12	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:B:825:CLA:HBB1	19:B:825:CLA:CMB	2.36	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: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
10:K:38:MET:HG3	19:K:202:CLA:HMD2	1.87	0.55
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
1:A:426:LEU:HB3	19:A:824:CLA:HMC2	1.88	0.55
19:A:827:CLA:HMA3	19:A:835:CLA:H71	1.88	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
19:8:308:CLA:HMD1	24:4:302:LMT:H82	1.89	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
19:3:5016: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:5:317:CLA:HMA1	19:5:321:CLA:HBC2	1.89	0.55
19:A:803:CLA:H192	19:A:841:CLA:H172	1.89	0.54
19:A:824:CLA:CMD	19:A:825:CLA:HAB	2.36	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
2:B:276:HIS:HB3	19:B:817:CLA:HMB2	1.88	0.54
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
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
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
19:4:313: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
11:Z:210:TRP:CE2	19:Z:307:CLA:HMA3	2.42	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
16:5:123:ALA:HB1	19:5:325:CLA:HAA1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:310:CLA:HBB1	19:5:310:CLA:HMB3	1.88	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
2:B:358:PRO:HG3	19:B:818:CLA:HBA1	1.90	0.54
2:B:355:SER:CB	19:B:826:CLA:HAC2	2.37	0.54
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
19:B:826:CLA:C4B	19:B:833:CLA:HMA2	2.37	0.54
19:4:308:CLA:CMB	19:4:308:CLA:HBB1	2.38	0.54
19:4:309:CLA:HMB1	19:4:309:CLA:HBB1	1.89	0.54
17:6:166:PRO:CG	19:6:309:CLA:H43	2.38	0.54
19:6:309:CLA:HMB3	19:6:309:CLA:CBB	2.34	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:840:CLA:H61	22:F:302:BCR:H17C	1.90	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
14:8:188:TRP:HB3	19:8:307:CLA:CMA	2.38	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
19:3:5009:CLA:C1C	19:3:5014:CLA:H121	2.37	0.54
19:4:308:CLA:HBB1	19:4:308:CLA:HMB1	1.90	0.54
19:5:310:CLA:C6	19:5:322:CLA:HAB	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:325:CLA:HBA1	19:5:325:CLA:CBD	2.38	0.54
19:6:309:CLA:HMD1	32:6:317:CHL:H11	1.90	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
10:K:77:ILE:HD11	12:3:21:GLN:HG2	1.89	0.53
12:3:94:LYS:HD2	12:3:96:PHE:CZ	2.42	0.53
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
19:5:311:CLA:H12	32:5:318:CHL:HMD3	1.89	0.53
2:B:518:PHE:HE2	19:B:836:CLA:C2D	2.21	0.53
19:B:832:CLA:CMA	29:J:1904:LMG:H151	2.35	0.53
19:B:833:CLA:HHC	19:B:833:CLA:CBB	2.33	0.53
11:1:31:LYS:HE3	11:1:33:GLY:O	2.08	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
19:8:307:CLA:HBB1	19:8:307:CLA:CMB	2.39	0.53
19:8:312:CLA:HBB1	19:8:312:CLA:CMB	2.39	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
2:B:173:GLU:HA	2:B:302:MET:HE3	1.90	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
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
2:B:168:TRP:CZ2	19:B:811:CLA:HMA1	2.44	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
22:3:5007:BCR:H311	19:3:5015:CLA:HMA2	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:812:CLA:HMB2	19:B:812:CLA:C14	2.38	0.53
19:B:825:CLA:H61	19:B:836:CLA:O1A	2.09	0.53
4:D:128:LEU:HA	4:D:132:PHE:HD2	1.74	0.53
32:1:5017:CHL:HAA2	32:1:5017:CHL:HBD	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:8:320:CLA:HHC	19:8:320:CLA:CBB	2.38	0.53
19:6:309:CLA:H71	19:6:310:CLA:HMA2	1.90	0.53
2:B:284:ILE:HG23	19:B:816:CLA:H192	1.90	0.53
4:D:94:GLN:H	4:D:106:MET:HG2	1.73	0.53
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
19:4:313:CLA:HBB1	19:4:313:CLA:CMB	2.38	0.53
19:6:301:CLA:H122	32:6:316:CHL:H71	1.91	0.53
19:6:309:CLA:CMD	32:6:317:CHL:H11	2.39	0.53
19:6:314:CLA:C1C	23:6:324:LHG:HC42	2.38	0.53
19:6:323:CLA:HBB1	19:6:323:CLA:CMB	2.39	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
24:Z:301:LMT:H4'	19:Z:315:CLA:HMA3	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
16:5:124:TRP:NE1	19:5:325:CLA:HMA2	2.24	0.53
19:A:821:CLA:HMB1	19:A:821:CLA:HBB1	1.91	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
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
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
19:4:306:CLA:CMB	19:4:307:CLA:HBA2	2.39	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:Z:304:CLA:HBB1	19:Z:304:CLA:HMB3	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
19:B:822:CLA:HAA2	24:1:5002:LMT:H1'	1.90	0.52
19:B:850:CLA:HBC2	19:B:850:CLA:HHH	1.90	0.52
22:3:5006:BCR:H21C	19:3:5012:CLA:CHD	2.39	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
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:814:CLA:HMA1	22:B:844:BCR:H402	1.92	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
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
19:5:309:CLA:H93	19:5:310:CLA:CMA	2.39	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
19:A:826:CLA:HBB1	19:A:826:CLA:HMB1	1.92	0.52
2:B:595:TRP:HB2	19:B:835:CLA:HMC1	1.90	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
2:B:156:LEU:C	2:B:158:LEU:H	2.16	0.52
2:B:520:VAL:HG21	2:B:594:TYR:HB2	1.92	0.52
10:K:97:HIS:ND1	22:K:206:BCR:H12C	2.25	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
1:A:700:ILE:HD13	19:A:840:CLA:HMD2	1.92	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
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: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
22:3:5007:BCR:H402	23:3:5021:LHG:HC41	1.92	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:803:CLA:CAC	19:B:804:CLA:HMC2	2.41	0.51
19:B:815:CLA:HMB1	19:B:815:CLA:HBB1	1.93	0.51
6:F:177:GLU:HG3	6:F:183:LYS:HD2	1.93	0.51
11:Z:44:TRP:CG	11:Z:62:LYS:HA	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HMA3	19:8:312:CLA:H112	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
14:8:188:TRP:HB3	19:8:307:CLA:HMA2	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
19:5:306:CLA:H62	19:5:307:CLA:CMA	2.40	0.51
19:5:311:CLA:HMB1	19:5:311:CLA:HBB1	1.91	0.51
19:6:312:CLA:CMB	19:6:312:CLA:HBB1	2.40	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: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:830:CLA:H112	23:A:852:LHG:H351	1.92	0.51
2:B:659:ALA:C	19:B:804:CLA:HAB	2.35	0.51
19:B:813:CLA:HMB1	19:B:813:CLA:HBB1	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
19:B:821:CLA:HMD3	22:B:842:BCR:H312	1.92	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
19:5:306:CLA:C6	19:5:307:CLA:HMA3	2.39	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
22:A:859:BCR:H291	19:K:204:CLA:HMB1	1.92	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
27:5:302:RRX:H44	19:5:307:CLA:CMC	2.40	0.51
19:6:313:CLA:H102	32:6:319:CHL:O1A	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:HG22	1:A:714:GLN:HB2	1.92	0.51
19:B:821:CLA:H8	19:B:822:CLA:H142	1.92	0.51
19:B:823:CLA:HMD3	19:B:824:CLA:HHC	1.91	0.51
19:B:829:CLA:H192	19:B:839:CLA:HMA2	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
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
19:4:306:CLA:HMB3	19:4:306:CLA:CBB	2.38	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
15:4:153:GLN:HG2	15:4:154:MET:HE2	1.93	0.51
15:4:206:GLY:O	15:4:207:ASP:C	2.53	0.51
16:5:217:ALA:HB1	16:5:225:ASN:HD22	1.74	0.51
19:A:821:CLA:HMB2	19:A:825:CLA:HMA2	1.93	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
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
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
19:A:814:CLA:H2	19:A:816:CLA:CMB	2.34	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:7:303:LUT:H26	19:7:306:CLA:O1A	2.11	0.50
14:8:138:TRP:CD2	19:8:318:CLA:CMA	2.86	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
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: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:78:VAL:C	8:I:81:PRO:HD2	2.36	0.50
8:I:83:THR:HB	19:I:201:CLA:C1	2.41	0.50
19:7:324:CLA:HMA1	19:6:312:CLA:H93	1.92	0.50
1:A:605:ILE:HG13	18:A:801:CL0:H66	1.93	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:695:LYS:HG2	19:B:838:CLA:HED3	1.93	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
19:7:316:CLA:HBB1	19:7:316:CLA:HMB3	1.92	0.50
19:8:309:CLA:C1C	19:8:309:CLA:H51	2.42	0.50
19:8:312:CLA:HMA2	32:8:319:CHL:CMC	2.41	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:672:TRP:HZ3	19:B:804:CLA:O1D	1.95	0.50
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
8:I:84:GLY:C	8:I:88:PRO:HG2	2.37	0.50
32:Z:309:CHL:CMD	15:4:178:PRO:HB3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:PHE:HE1	19:B:803:CLA:HMA1	1.76	0.50
1:A:709:VAL:HG12	6:F:168:ARG:HG3	1.93	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
19:1:5007:CLA:HMD2	19:1:5012:CLA:H12	1.92	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
16:5:101:TYR:CE2	32:5:315:CHL:HMA2	2.47	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:837:CLA:HBB1	19:A:837:CLA:CMB	2.41	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:439:VAL:HB	19:B:832:CLA:HMC2	1.93	0.50
19:B:814:CLA:H61	22:B:844:BCR:H362	1.93	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
2:B:271:LEU:HD23	2:B:274:MET:HE3	1.94	0.50
19:B:810:CLA:H2	19:B:810:CLA:O2D	2.11	0.50
19:B:840:CLA:HMC3	19:1:5010:CLA:H12	1.93	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
24:G:1604:LMT:H82	19:1:5010:CLA:HMD2	1.93	0.50
32:8:301:CHL:H2	37:8:302:SQD:H211	1.94	0.50
16:5:175:SER:OG	19:5:306:CLA:HAA2	2.12	0.50
16:5:223:PHE:CE2	19:5:313:CLA:HMA3	2.47	0.50
17:6:246:ILE:HG13	17:6:246:ILE:O	2.12	0.50
1:A:18:ASP:CG	1:A:71:ARG:HH22	2.19	0.49
2:B:23:TRP:CG	2:B:705:GLN:HE22	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:7:306:CLA:HBB1	19:7:306:CLA:HMB1	1.93	0.49
14:8:179:SER:HB3	19:8:307:CLA:HAA2	1.93	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
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
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
32:5:318:CHL:HBB1	32:5:318:CHL:CMB	2.41	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: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
24:G:1604:LMT:H4'	19:1:5016:CLA:HMA2	1.94	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
19:5:306:CLA:H72	19:5:307:CLA:HMA3	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
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:453:PHE:CE1	19:B:803:CLA:HMA1	2.47	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
19:B:807:CLA:H203	19:B:807:CLA:H152	1.94	0.49
19:B:833:CLA:H203	19:B:834:CLA:HMC1	1.94	0.49
19:B:850:CLA:H62	19:B:850:CLA:NC	2.26	0.49
17:6:247:PRO:HG2	32:6:316:CHL:H42	1.93	0.49
19:A:804:CLA:HBB1	19:A:804:CLA:HMB3	1.93	0.49
19:A:816:CLA:CHD	19:3:5016:CLA:HBB2	2.42	0.49
19:B:802:CLA:HMB3	19:B:803:CLA:OBD	2.12	0.49
19:B:838:CLA:HMB1	19:B:838:CLA:HBB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:3:5016: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
32:5:315:CHL:H203	19:6:320:CLA:HMC3	1.94	0.49
1:A:189:GLU:CD	1:A:189:GLU:H	2.19	0.49
1:A:330:ARG:HH21	1:A:336:GLU:HA	1.78	0.49
2:B:125:TRP:HA	2:B:128:ILE:HG12	1.95	0.49
19:B:819:CLA:HMB3	19:B:819:CLA:HBB1	1.94	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
32:6:315:CHL:HBB1	32:6:315:CHL:HHC	1.93	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: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
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
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
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
31:6:305:LUT:H11	19:6:310:CLA:HMC1	1.95	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: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:801:CLA:HMA3	19:B:801:CLA:C3	2.43	0.49
19:B:821:CLA:CAD	22:B:842:BCR:HC22	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:B:829:CLA:HBB1	19:B:829:CLA:HMB3	1.94	0.49
10:K:74:ALA:O	12:3:20:SER:HB2	2.12	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
19:4:306:CLA:HMB3	19:4:307:CLA:HBA2	1.95	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
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
19:7:307:CLA:HMB2	19:7:312:CLA:H151	1.94	0.48
32:8:315:CHL:HAA2	32:8:315:CHL:HBD	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
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
16:5:222:PRO:HG2	19:5:313:CLA:CMB	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:413:MET:HE1	1:A:427:LEU:HD11	1.95	0.48
1:A:677:PHE:CG	22:A:850:BCR:H363	2.48	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
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
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
2:B:348:LEU:HD13	19:B:826:CLA:HAA2	1.96	0.48
19:7:307:CLA:C4D	19:7:312:CLA:H61	2.42	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
19:5:322:CLA:CMD	28:6:304:C7Z:C38	2.91	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
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
19:1:5007:CLA:HBB1	19:1:5007:CLA:CMB	2.40	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
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
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
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
19:A:814:CLA:H93	35:7:302:DGA:HB32	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:100:VAL:HG21	19:G:1602:CLA:CMA	2.44	0.48
19:1:5010:CLA:O2D	19:1:5016:CLA:H62	2.14	0.48
23:1:5019:LHG:C20	37:8:302:SQD:H182	2.44	0.48
19:Z:314:CLA:HMA3	19:8:312:CLA:C10	2.43	0.48
22:8:303:BCR:H10C	22:8:303:BCR:C35	2.41	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
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
2:B:658:TYR:CD1	19:B:802:CLA:HMA3	2.49	0.48
19:B:822:CLA:HMC1	22:B:845:BCR:H10C	1.96	0.48
10:K:46:LEU:HB3	19:K:205:CLA:HBC1	1.96	0.48
19:3:5013:CLA:HMA3	19:3:5019:CLA:C2C	2.44	0.48
13:7:213:LYS:HE2	13:7:221:ASP:OD2	2.14	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: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
12:3:192:ARG:HA	12:3:195:MET:HE3	1.95	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:807:CLA:HMA2	19:B:829:CLA:C4B	2.44	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
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
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
17:6:181:ARG:HA	17:6:184:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:Z:156:PRO:O	11:Z:157:LEU:C	2.57	0.47
15:4:67:LEU:HD13	15:4:80:GLY:HA3	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
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
11:1:146:GLY:O	11:1:147:VAL:C	2.57	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
19:7:307: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
19:5:325:CLA:HMC2	17:6:209:LEU:HD21	1.96	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: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
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
16:5:85:VAL:HG11	27:5:302:RRX:H39	1.95	0.47
19:6:312:CLA:H71	19:6:312:CLA:H112	1.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:7:311: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
15:4:260:ASP:CG	15:4:263:ARG:HH21	2.22	0.47
32:4:314:CHL:HMA2	24:4:322:LMT:H51	1.96	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
19:B:823:CLA:HMD3	19:B:824:CLA:HAB	1.97	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
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
19:A:830:CLA:HMB3	19:A:830:CLA:HBB1	1.97	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
19:B:813:CLA:H11	22:B:843:BCR:C20	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:114:ARG:HD3	9:J:35:ASP:CG	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:218:LYS:HE3	6:F:221:ASN:HD21	1.79	0.47
7:G:100:VAL:HG21	19:G:1602:CLA:HMA1	1.97	0.47
10:K:111:GLY:O	10:K:112:ALA:C	2.57	0.47
11:Z:135:ALA:HA	19:Z:315:CLA:HAB	1.97	0.47
19:Z:303:CLA:HMD2	19:Z:312:CLA:H2	1.97	0.47
19:Z:314:CLA:HMA3	19:8:312:CLA:C11	2.45	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
14:8:62:ASP:CG	14:8:64:VAL:HG13	2.40	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:815:CLA:HMA2	24:A:853:LMT:H21	1.95	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
19:K:202:CLA:HMC3	22:K:206:BCR:H332	1.95	0.47
11:1:157:LEU:N	11:1:157:LEU:HD12	2.30	0.47
19:Z:312:CLA:HBB1	19:Z:312:CLA:CMB	2.44	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
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
19:5:311:CLA:HBB1	19:5:311:CLA:CMB	2.44	0.47
32:5:315:CHL:H172	19:6:323:CLA:C1D	2.45	0.47
1:A:540:ALA:HB1	19:A:838:CLA:HMB3	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:HAB	19:B:830:CLA:CMD	2.43	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
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
19:B:814:CLA:HMB3	19:B:828:CLA:H111	1.96	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:H403	23:3:5021:LHG:HC41	1.96	0.46
13:7:121:MET:HE3	13:7:125:PHE:CE1	2.50	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: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
3:C:22:PRO:C	4:D:122:LEU:HD23	2.40	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
11:1:94:LEU:HD12	19:1:5011:CLA:HMD2	1.98	0.46
24:3:5023:LMT:H101	19:7:307:CLA:HMD1	1.96	0.46
13:7:179:ASP:CG	13:7:182:LYS:HB2	2.41	0.46
15:4:248:LEU:HD21	19:4:313:CLA:HMC3	1.96	0.46
17:6:132:LEU:HD22	38:6:326:ERG:C21	2.44	0.46
19:A:806:CLA:H93	19:A:806:CLA:H61	1.69	0.46
19:A:806:CLA:H203	19:A:806:CLA:H152	1.96	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: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
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
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
19:5:306:CLA:HMB3	19:5:306:CLA:CBB	2.37	0.46
17:6:257:PRO:HG3	19:6:320:CLA:C3D	2.45	0.46
19:6:313:CLA:HBB1	19:6:313:CLA:CMB	2.44	0.46
19:A:818:CLA:C4A	19:A:818:CLA:H2	2.45	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:TRP:HZ3	19:A:802:CLA:HMD3	1.80	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:832:CLA:HBC2	19:A:839:CLA:HMC2	1.97	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
19:3:5020:CLA:HBB1	19:3:5020:CLA:CMB	2.46	0.46
15:4:109:LEU:HD11	19:4:306:CLA:HBC1	1.98	0.46
17:6:75:SER:OG	17:6:79:MET:HE2	2.15	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
19:A:803:CLA:HMA2	19:A:808:CLA:H192	1.96	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
19:B:833:CLA:HBA2	19:B:834:CLA:CMB	2.39	0.46
19:B:835:CLA:HMB3	19:B:835:CLA:HBB1	1.97	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
13:7:239:PRO:HG2	19:7:319:CLA:HMB2	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:826:CLA:HMB2	19:A:839:CLA:HBA1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:308:CLA:HMB3	19:Z:308:CLA:CBB	2.44	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
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
19:8:312:CLA:HMA2	32:8:319:CHL:C2C	2.46	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
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
17:6:75:SER:OG	17:6:180:GLY:HA3	2.16	0.46
19:6:312:CLA:HBB1	19:6:312:CLA:HMB1	1.98	0.46
19:A:804:CLA:H51	19:A:804:CLA:H8	1.38	0.46
19:A:821:CLA:H92	19:A:825:CLA:HMB2	1.98	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
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
1:A:389:SER:HB3	19:A:828:CLA:CMA	2.36	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:478:LEU:HD13	19:B:833:CLA:HMD1	1.98	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
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
19:7:324:CLA:HMB3	19:7:324:CLA:CBB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:5:307:CLA:H142	19:5:312:CLA:H101	1.98	0.46
19:5:314:CLA:CMA	23:5:323:LHG:H132	2.44	0.46
17:6:76:ARG:HA	17:6:79:MET:HE3	1.97	0.46
23:6:303:LHG:H132	23:6:303:LHG:C24	2.30	0.46
1:A:80:GLN:HG2	19:A:805:CLA:HMA2	1.98	0.46
1:A:190:TRP:CZ2	19:A:810:CLA:HMA1	2.51	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:812:CLA:O1D	19:B:813:CLA:HMC1	2.16	0.46
19:B:815:CLA:H11	19:B:815:CLA:H51	1.57	0.46
19:Z:308:CLA:HMD1	19:Z:315:CLA:C1D	2.46	0.46
19:Z:311:CLA:H41	19:Z:311:CLA:H61	1.61	0.46
19:8:311:CLA:CMB	19:8:311:CLA:HBB1	2.46	0.46
32:4:314:CHL:HBB1	32:4:314:CHL:CMB	2.42	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: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: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
11:1:115:PHE:CZ	19:1:5011:CLA:HMD1	2.51	0.45
11:1:138:GLU:HG3	19:1:5016:CLA:C4B	2.47	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
15:4:62:MET:CE	15:4:65:ALA:HB2	2.46	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:198:VAL:C	2:B:201:PRO:HD2	2.41	0.45
2:B:467:ALA:HB1	2:B:478:LEU:HD12	1.98	0.45
2:B:669:ARG:O	2:B:670:GLY:C	2.59	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
14:8:231:VAL:HG12	19:8:309:CLA:HED1	1.99	0.45
15:4:154:MET:HE1	19:4:316:CLA:HMC2	1.98	0.45
19:6:309:CLA:HBB1	19:6:309:CLA:CMB	2.37	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:819:CLA:HMB3	19:B:824:CLA:H62	1.98	0.45
19:B:825:CLA:H41	19:B:825:CLA:H62	1.43	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
14:8:197:ARG:HA	14:8:200:MET:HE3	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:4:317:CHL:HBB1	32:4:317:CHL:HHC	1.98	0.45
19:6:314:CLA:H61	19:6:314:CLA:H92	1.57	0.45
32:6:317:CHL:HBB1	32:6:317:CHL:CMB	2.44	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
19:B:807:CLA:H3A	19:B:807:CLA:HBA1	1.59	0.45
19:B:825:CLA:H142	19:B:835:CLA:H141	1.97	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
14:8:95:LYS:HB2	14:8:95:LYS:HZ3	1.81	0.45
15:4:123:ILE:HD12	15:4:125:PHE:HE1	1.82	0.45
19:4:311:CLA:HMA3	32:4:317:CHL:C1C	2.46	0.45
22:5:304:BCR:C4	23:6:324:LHG:HC82	2.12	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
19:A:836:CLA:HMB1	22:A:849:BCR:H282	1.98	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
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: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:806:CLA:HMA2	19:A:830:CLA:C4B	2.45	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:842:CLA:H92	19:F:303:CLA:HMD1	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:599:HIS:HB3	2:B:603:TRP:CZ2	2.52	0.45
13:7:186:TYR:CG	19:7:306:CLA:H12	2.52	0.45
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
19:8:318:CLA:HMC2	24:8:324:LMT:C12	2.39	0.45
19:4:311:CLA:HMA3	32:4:317:CHL:C2C	2.47	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
32:5:318:CHL:HMB1	32:5:318:CHL:CBB	2.44	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
19:A:802:CLA:HMA1	2:B:617:LEU:HD13	1.99	0.45
19:A:814:CLA:HBB1	19:A:814:CLA:HMB3	1.98	0.45
19:A:822:CLA:HMD2	22:A:859:BCR:H23C	1.99	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:Z:305:CLA:H102	19:Z:308:CLA:HMA1	1.98	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
16:5:222:PRO:HB3	19:5:313:CLA:CHB	2.46	0.45
31:5:303:LUT:H31	19:5:309:CLA:HMC2	1.99	0.45
19:6:301:CLA:H91	19:6:301:CLA:H111	1.67	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: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
19:1:5007:CLA:HMD3	19:1:5012:CLA:C4D	2.47	0.45
34:3:5022:3PH:H372	34:3:5022:3PH:H3A1	1.59	0.45
31:8:304:LUT:H32	19:8:307:CLA:HMC2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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:819:CLA:HBB1	19:A:819:CLA:CMB	2.42	0.45
19:A:833:CLA:H111	19:B:838:CLA:H42	1.99	0.45
19:B:818:CLA:HBB1	19:B:818:CLA:CMB	2.44	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
19:B:833:CLA:HMD3	39:B:921:HOH:O	2.17	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
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
19:3:5008:CLA:H62	19:3:5009:CLA:HMA3	1.98	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
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: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
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
19:3:5013:CLA:H141	19:3:5013:CLA:H161	1.87	0.44
33:4:301:SPH:H171	33:4:301:SPH:H141	1.72	0.44
19:4:308:CLA:H93	19:4:308:CLA:H112	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:819:CLA:H161	19:B:819:CLA:H122	1.68	0.44
19:B:819:CLA:HMA3	19:B:824:CLA:NB	2.32	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
19:Z:311:CLA:HMB1	19:Z:311:CLA:HBB1	1.98	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
19:8:313:CLA:HMA2	24:4:302:LMT:H5'	1.99	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:B:816:CLA:CGA	19:B:816:CLA:C1A	2.96	0.44
19:B:821:CLA:CMD	22:B:842:BCR:HC7	2.45	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
19:8:309: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:HBD	19:6:301:CLA:HAA1	1.99	0.44
19:6:301:CLA:H143	32:6:316:CHL:H62	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:4:134:TRP:CH2	24:4:322:LMT:H41	2.51	0.44
16:5:222:PRO:HG2	19:5:313:CLA:HMB3	1.98	0.44
19:6:301:CLA:H42	19:6:301:CLA:C1D	2.46	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
1:A:23:GLU:H	1:A:23:GLU:CD	2.26	0.44
19:A:821:CLA:HMA3	19:A:825:CLA:NB	2.32	0.44
19:A:826:CLA:C3B	19:A:839:CLA:HMA3	2.47	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
2:B:374:THR:HB	19:B:827:CLA:HMB2	1.99	0.44
19:B:808:CLA:H42	19:B:808:CLA:C1D	2.48	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
32:Z:313:CHL:HMB3	32:Z:313:CHL:CBB	2.42	0.44
22:3:5005:BCR:H15C	22:3:5005:BCR:H351	1.88	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
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
2:B:156:LEU:C	2:B:158:LEU:N	2.76	0.44
19:B:804:CLA:H93	19:B:804:CLA:H62	1.80	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
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
19:Z:305:CLA:HMC2	31:Z:317:LUT:C32	2.47	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
13:7:116:ASP:CG	13:7:118:PRO:HD2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:7:221:ASP:HB3	13:7:229:VAL:HG11	1.98	0.44
14:8:77:CYS:SG	14:8:200:MET:HE2	2.57	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
19:5:306:CLA:HMD1	32:5:316:CHL:O1A	2.18	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
32:6:317:CHL:HMB3	32:6:317:CHL:CBB	2.45	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
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
22:F:302:BCR:H352	19:F:303:CLA:CHC	2.48	0.44
11:1:134:MET:HG3	19:1:5016:CLA:HMC3	2.00	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
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
18:A:801:CL0:H12	19:A:802:CLA:OBD	2.18	0.44
19:A:834:CLA:H162	19:A:834:CLA:H141	1.81	0.44
19:A:843:CLA:HMB1	19:A:843:CLA:HBB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:TRP:HA	2:B:213:PHE:CD1	2.52	0.44
6:F:92:LYS:C	6:F:94:TYR:H	2.26	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
24:3:5023:LMT:H102	19:7:312:CLA:C1C	2.47	0.44
19:7:306:CLA:HMB2	19:7:307:CLA:HBA2	2.00	0.44
19:7:310:CLA:HBA1	19:7:310:CLA:H12	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
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:822:CLA:HMB2	19:B:840:CLA:C1D	2.47	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
19:7:306:CLA:H62	19:7:306:CLA:H41	1.67	0.43
19:5:313:CLA:HMB1	19:5:313:CLA:CBB	2.38	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
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
19:A:813:CLA:HBB1	19:A:813:CLA:CMB	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:817:CLA:HBC1	19:B:819:CLA:H172	2.00	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
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
11:Z:155:ASP:C	11:Z:156:PRO:O	2.59	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
32:5:318:CHL:HAA2	32:5:318:CHL:CBD	2.46	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
19:A:804:CLA:HBB1	19:A:804:CLA:CMB	2.48	0.43
2:B:87:PRO:HB3	2:B:122:TYR:CG	2.53	0.43
19:B:819:CLA:HBB1	19:B:819:CLA:CMB	2.48	0.43
19:B:821:CLA:HBB1	19:B:821:CLA:CMB	2.44	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
32:Z:309:CHL:HMD1	15:4:178:PRO:HB3	2.00	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
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:821:CLA:HBB1	19:A:821:CLA:CMB	2.48	0.43
19:A:832:CLA:HMC1	19:A:838:CLA:H172	2.00	0.43
24:A:855:LMT:H11	24:A:855:LMT:H2'	1.24	0.43
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
2:B:494:TRP:O	2:B:495:LEU:C	2.61	0.43
19:B:823:CLA:HMB2	19:B:823:CLA:C16	2.48	0.43
8:I:87:LEU:HB2	8:I:88:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:4:127:TRP:CD1	15:4:129:GLY:H	2.37	0.43
15:4:251:PRO:HG2	19:4:313:CLA:HMB2	1.99	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
19:A:802:CLA:O1D	19:B:802:CLA:H52	2.18	0.43
2:B:209:GLY:C	2:B:211:ASP:N	2.76	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
8:I:74:TRP:O	8:I:75:ALA:C	2.61	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
19:7:306:CLA:H71	19:7:307:CLA:CMA	2.42	0.43
15:4:115:LEU:HD21	15:4:229:PHE:CZ	2.53	0.43
15:4:154:MET:HE2	15:4:154:MET:HA	1.99	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
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: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
22:B:844:BCR:H15C	22:B:844:BCR:H351	1.92	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3:170:LEU:HG	16:5:35:TRP:HH2	1.84	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
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
19:A:836:CLA:CMB	22:A:849:BCR:H282	2.49	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:H3A	19:B:827:CLA:HBA2	1.54	0.43
19:B:827:CLA:H111	19:B:827:CLA:H71	1.55	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
19:J:1901:CLA:HBB1	19:J:1901:CLA:HMB1	1.99	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
19:5:317:CLA:CMA	19:5:321:CLA:HBC2	2.48	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
19:A:839:CLA:HBB1	19:A:839:CLA:CMB	2.48	0.43
2:B:66:LEU:CD1	22:B:844:BCR:H271	2.48	0.43
2:B:96:HIS:CE1	19:B:809:CLA:HMB3	2.54	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
11:Z:157:LEU:O	11:Z:158:GLY:C	2.60	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:CBD	19:8:312:CLA:HAA1	2.49	0.43
19:8:313:CLA:HMA2	24:4:302:LMT:H3'	2.00	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)
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
5:E:52:TRP:HA	5:E:55:GLN:CD	2.43	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
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
32:4:314:CHL:HMB3	32:4:314:CHL:CBB	2.42	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
19:5:310:CLA:HMB3	19:5:310:CLA:CBB	2.49	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
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:822:CLA:HMB3	19:1:5010:CLA:H42	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
11:1:210:TRP:CE2	19:1:5013:CLA:CMA	3.00	0.43
19:1:5007:CLA:C1D	19:1:5012:CLA:H62	2.48	0.43
11:Z:31:LYS:C	11:Z:33:GLY:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:Z:303:CLA:HMD3	19:Z:312:CLA:C4D	2.49	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
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
17:6:247:PRO:O	32:6:316:CHL:H42	2.19	0.43
1:A:370:HIS:CE1	19:A:827:CLA:NB	2.87	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
15:4:153:GLN:HG2	15:4:154:MET:CE	2.48	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:91:MET:HE1	19:A:808:CLA:HMA2	2.01	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:530:THR:O	2:B:534:ILE:HG13	2.20	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
8:I:85:LEU:C	8:I:88:PRO:HD2	2.44	0.42
10:K:110:ILE:HG23	19:K:203:CLA:HMA1	2.01	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
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
32:5:316:CHL:HMB1	32:5:316:CHL:CBB	2.44	0.42
31:6:305:LUT:H15	31:6:305:LUT:H201	1.94	0.42
19:A:826:CLA:HBB1	19:A:826:CLA:CMB	2.49	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
4:D:112:LEU:HD23	4:D:112:LEU:C	2.44	0.42
8:I:75:ALA:O	8:I:79:PHE:HD1	2.00	0.42
19:Z:305:CLA:H122	19:Z:305:CLA:H8	1.56	0.42
12:3:220:LEU:HD21	19:3:5015:CLA:HMC2	2.02	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
13:7:173:MET:HE3	19:7:324:CLA:H51	2.00	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
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:656:LEU:HA	19:B:803:CLA:HAA1	2.01	0.42
19:B:829:CLA:HBB1	19:B:829:CLA:CMB	2.50	0.42
19:B:836:CLA:C2C	29:J:1904:LMG:H261	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:1:156:PRO:HD2	31:1:5003:LUT:C23	2.49	0.42
19:1:5011:CLA:HMA3	32:1:5017:CHL:C3C	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
19:4:310:CLA:HMD1	19:4:316:CLA:C1D	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: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: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
19:8:312:CLA:H3A	19:8:312:CLA:HBA2	1.63	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: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:168:TRP:CE2	19:B:811:CLA:HMA1	2.54	0.42
2:B:273:ASP:HB3	19:B:817:CLA:HMA1	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:7:317:CLA:HBB1	19:7:317:CLA:HMB3	2.02	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:810:CLA:HMB2	8:I:81:PRO:HA	2.02	0.42
19:B:829:CLA:C19	19:B:839:CLA:HMA2	2.49	0.42
19:1:5013:CLA:HAA2	14:8:125:VAL:CG2	2.49	0.42
11:Z:31:LYS:C	11:Z:33:GLY:H	2.27	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
19:8:312:CLA:C4D	39:8:401:HOH:O	2.66	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
16:5:182:LEU:CB	19:5:306:CLA:HMA2	2.50	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
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:813:CLA:HBB1	19:B:813:CLA:CMB	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:J:1901:CLA:HBB1	19:J:1901:CLA:CMB	2.50	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
13:7:77:ARG:HA	13:7:80:MET:HE3	2.01	0.42
15:4:220:ARG:HA	15:4:223:MET:CE	2.48	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
19:B:835:CLA:HBB1	19:B:835:CLA:CMB	2.49	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
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:830:CLA:HBB1	19:A:830:CLA:CMB	2.50	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
3:C:62:PHE:CG	3:C:63:LEU:N	2.88	0.42
11:Z:35:TRP:CD2	11:Z:55:PHE:HD1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:8:307: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
1:A:372:TYR:CD1	1:A:372:TYR:C	2.97	0.41
19:A:803:CLA:H93	19:A:803:CLA:H62	1.77	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
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
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
19:4:311:CLA:HBB1	19:4:311:CLA:CMB	2.35	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
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
19:1:5012:CLA:CBB	22:8:306:BCR:H332	2.50	0.41
11:Z:140:GLN:HB3	19:Z:306:CLA:HMC2	2.02	0.41
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
19:4:313:CLA:HMB3	19:4:313:CLA:CBB	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
19:7:307:CLA:HBB1	19:7:307:CLA:CMB	2.50	0.41
19:8:307:CLA:HMB1	19:8:307:CLA:CBB	2.49	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
19:A:830:CLA:CMD	23:A:852:LHG:H282	2.51	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
19:Z:304:CLA:HBB1	19:Z:304:CLA:CMB	2.50	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
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: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
24:A:853:LMT:H12	24:A:853:LMT:H42	1.87	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
31:5:303:LUT:H34	19:5:309:CLA:HBB2	2.01	0.41
19:5:306:CLA:HBB1	19:5:306:CLA:CMB	2.37	0.41
1:A:584:CYS:SG	21:A:845:SF4:S1	3.16	0.41
19:A:822:CLA:O1A	19:K:204:CLA:HMB3	2.21	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
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:48:ASP:O	11:Z:49:LEU:C	2.63	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
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:HG12	22:6:308:BCR:HC7	2.03	0.41
17:6:244:ILE:HD11	22:6:308:BCR:H331	2.01	0.41
1:A:305:PHE:HZ	19:A:819:CLA:H142	1.85	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:K:204:CLA:HMB1	19:K:204:CLA:CBB	2.47	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
19:7:316:CLA:HBB1	19:7:316:CLA:CMB	2.50	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
19:6:302:CLA:HMA1	19:6:322:CLA:OBD	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
19:5:317:CLA:CMA	19:5:321:CLA:CBC	2.99	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
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
2:B:657:ILE:HG12	19:B:839:CLA:HMB3	2.02	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:815:CLA:HBB1	19:B:815:CLA:CMB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:Z:31:LYS:HE2	11:Z:33:GLY:O	2.21	0.41
19:Z:303:CLA:HMC3	31:Z:318:LUT:C19	2.51	0.41
12:3:94:LYS:HD3	39:3:5106:HOH:O	2.21	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
32:8:319:CHL:HMB3	32:8:319:CHL:CBB	2.50	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
19:4:308:CLA:HMB1	19:4:308:CLA:CBB	2.50	0.41
16:5:182:LEU:HB2	19:5:306:CLA:HMA2	2.02	0.41
19:5:306:CLA:C7	19:5:307:CLA:HMA3	2.50	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:815:CLA:HBB1	19:A:815:CLA:CMB	2.45	0.41
2:B:620:TRP:O	2:B:624:TYR:HB3	2.21	0.41
19:B:803:CLA:O1A	19:B:803:CLA:H3A	2.21	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
11:Z:169:LEU:C	32:Z:302:CHL:HMA1	2.46	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:831:CLA:HMA2	19:A:832:CLA:OBD	2.21	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
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
11:1:210:TRP:NE1	19:1:5013:CLA:HMA3	2.35	0.40
31:1:5003:LUT:H11	31:1:5003:LUT:H191	1.99	0.40
19:1:5007:CLA:HMD3	19:1:5012:CLA:CHA	2.50	0.40
19:1:5008:CLA:H143	24:Z:301:LMT:H122	2.03	0.40
19:1:5011:CLA:HMA3	32:1:5017:CHL:C2C	2.51	0.40
19:Z:306:CLA:HMA3	24:Z:319:LMT:H12	2.03	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
22:8:303:BCR:C34	33:4:301:SPH:H152	2.51	0.40
31:8:304:LUT:H193	19:8:308:CLA:HMC3	2.02	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
1:A:349:TRP:CB	19:A:805:CLA:HAC1	2.50	0.40
19:A:815:CLA:HMB1	24:A:853:LMT:H92	2.02	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
11:1:94:LEU:HD12	19:1:5011:CLA:CMD	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:7:306:CLA:HBB1	19:7:306:CLA:CMB	2.51	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
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: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
12:3:89:ASP:O	12:3:90:ALA:C	2.63	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
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
19:B:830:CLA:HBB2	19:B:837:CLA:CMC	2.51	0.40
7:G:102:GLY:O	7:G:106:LEU:HG	2.21	0.40
10:K:63:ALA:C	10:K:65:LEU:H	2.30	0.40
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
19:3:5009:CLA:HMD3	19:3:5014:CLA:C4D	2.51	0.40
14:8:194:LYS:HD3	19:8:313:CLA:O1D	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
22:A:859:BCR:H291	19:K:204:CLA:CMB	2.51	0.40
2:B:478:LEU:HD13	19:B:833:CLA:CMD	2.52	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:K:202:CLA:HMB2	22:K:206:BCR:H352	2.03	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
32:Z:302:CHL:H51	19:Z:303:CLA:HMA2	2.04	0.40
19:Z:308:CLA:CMB	19:Z:308:CLA:CBB	2.98	0.40
31:3:5003:LUT:H31	31:3:5003:LUT:H391	1.69	0.40
13:7:136:TRP:CG	19:7:317:CLA:HMA2	2.56	0.40
32:8:315:CHL:H12	32:8:315:CHL:H52	1.91	0.40
16:5:200:PHE:CE1	27:5:302:RRX:H57	2.56	0.40
17:6:204:ALA:O	17:6:205:LEU:C	2.63	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%)	48	67
2	B	731/735 (100%)	702 (96%)	28 (4%)	1 (0%)	48	67
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%)	24	41
11	Z	192/228 (84%)	178 (93%)	11 (6%)	3 (2%)	7	13
12	3	217/298 (73%)	206 (95%)	10 (5%)	1 (0%)	24	41
13	7	211/241 (88%)	200 (95%)	10 (5%)	1 (0%)	24	41
14	8	215/243 (88%)	210 (98%)	5 (2%)	0	100	100
15	4	208/264 (79%)	196 (94%)	10 (5%)	2 (1%)	12	23
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%)	37	53

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 ⓘ

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%)	596 (99%)	4 (1%)	76	89
2	B	596/597 (100%)	593 (100%)	3 (0%)	81	91
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	120/151 (80%)	119 (99%)	1 (1%)	73	88
5	E	54/81 (67%)	54 (100%)	0	100	100
6	F	127/169 (75%)	127 (100%)	0	100	100
7	G	47/94 (50%)	46 (98%)	1 (2%)	47	72
8	I	31/76 (41%)	30 (97%)	1 (3%)	34	60
9	J	35/37 (95%)	35 (100%)	0	100	100
10	K	58/80 (72%)	56 (97%)	2 (3%)	32	57
11	1	137/162 (85%)	135 (98%)	2 (2%)	57	79
11	Z	137/162 (85%)	135 (98%)	2 (2%)	57	79
12	3	167/230 (73%)	164 (98%)	3 (2%)	51	75
13	7	164/181 (91%)	162 (99%)	2 (1%)	63	82
14	8	163/183 (89%)	160 (98%)	3 (2%)	51	75
15	4	164/205 (80%)	161 (98%)	3 (2%)	51	75
16	5	184/206 (89%)	181 (98%)	3 (2%)	55	78
17	6	183/203 (90%)	176 (96%)	7 (4%)	29	53
All	All	3036/3497 (87%)	2999 (99%)	37 (1%)	61	82

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	PHE
1	A	372	TYR
1	A	496	GLN
1	A	627	VAL
2	B	99	GLN
2	B	145	LEU

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Mol	Chain	Res	Type
2	B	281	ILE
4	D	92	LYS
7	G	89	THR
8	I	85	LEU
10	K	65	LEU
10	K	89	VAL
11	1	37	PRO
11	1	224	PHE
11	Z	31	LYS
11	Z	213	ASN
12	3	43	LEU
12	3	126	GLN
12	3	218	GLU
13	7	29	VAL
13	7	168	ARG
14	8	64	VAL
14	8	95	LYS
14	8	112	ILE
15	4	91	VAL
15	4	209	LYS
15	4	236	THR
16	5	181	GLU
16	5	240	VAL
16	5	247	ILE
17	6	29	ARG
17	6	102	LYS
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 (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	94	HIS
1	A	116	GLN
1	A	182	HIS
1	A	217	GLN
1	A	225	ASN
1	A	338	HIS

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Mol	Chain	Res	Type
1	A	369	HIS
1	A	496	GLN
2	B	11	GLN
2	B	90	HIS
2	B	157	HIS
2	B	159	GLN
2	B	163	GLN
2	B	197	HIS
2	B	236	GLN
2	B	295	ASN
2	B	328	ASN
2	B	332	HIS
2	B	376	HIS
2	B	604	GLN
2	B	655	HIS
3	C	38	GLN
5	E	87	ASN
6	F	221	ASN
7	G	118	ASN
10	K	60	ASN
10	K	79	ASN
11	1	124	ASN
11	1	176	ASN
11	1	217	ASN
11	Z	213	ASN
12	3	21	GLN
12	3	204	GLN
12	3	215	ASN
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	147	ASN
16	5	159	ASN
16	5	189	ASN
16	5	203	GLN
16	5	221	ASN

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Mol	Chain	Res	Type
16	5	230	ASN
16	5	238	HIS
17	6	179	ASN
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	0.70	0	2,7,9	1.21	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 oligosaccharides 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$
19	CLA	B	807	2	69,73,73	1.36	7 (10%)	82,113,113	1.84	19 (23%)
19	CLA	B	828	-	69,73,73	1.34	6 (8%)	82,113,113	1.84	17 (20%)
19	CLA	B	837	-	69,73,73	1.34	6 (8%)	82,113,113	1.89	20 (24%)
19	CLA	A	820	-	64,68,73	1.40	6 (9%)	76,107,113	1.97	20 (26%)
19	CLA	Z	304	39	54,58,73	1.55	6 (11%)	64,95,113	2.09	18 (28%)
19	CLA	7	311	39	60,64,73	1.51	6 (10%)	71,102,113	2.06	18 (25%)
29	LMG	J	1903	-	35,35,55	0.46	0	43,43,63	1.13	2 (4%)
34	3PH	5	324	-	22,22,47	1.23	4 (18%)	25,27,52	1.27	3 (12%)
19	CLA	1	5015	39	54,58,73	1.57	6 (11%)	64,95,113	2.18	21 (32%)
19	CLA	5	311	39	54,58,73	1.56	6 (11%)	64,95,113	2.12	18 (28%)
28	C7Z	1	5005	-	43,43,43	5.44	27 (62%)	56,60,60	2.24	21 (37%)
19	CLA	K	203	39	59,63,73	1.46	7 (11%)	70,101,113	2.01	18 (25%)
18	CL0	A	801	-	58,73,73	3.19	17 (29%)	60,113,113	2.85	18 (30%)
32	CHL	6	317	39	45,59,74	1.72	7 (15%)	40,96,114	2.01	9 (22%)
19	CLA	5	313	-	49,53,73	1.62	6 (12%)	58,89,113	2.02	16 (27%)
32	CHL	6	319	39	60,74,74	1.56	9 (15%)	58,114,114	1.74	12 (20%)
19	CLA	A	835	-	69,73,73	1.34	6 (8%)	82,113,113	1.87	19 (23%)
19	CLA	1	5012	23	64,68,73	1.40	7 (10%)	76,107,113	1.92	19 (25%)
19	CLA	A	828	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	18 (21%)
22	BCR	3	5004	-	41,41,41	4.83	25 (60%)	56,56,56	2.43	21 (37%)
19	CLA	B	808	-	69,73,73	1.34	6 (8%)	82,113,113	1.89	16 (19%)
19	CLA	Z	307	-	61,65,73	1.49	6 (9%)	72,103,113	1.96	19 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	835	-	64,68,73	1.41	6 (9%)	76,107,113	1.98	19 (25%)
19	CLA	A	838	-	69,73,73	1.34	5 (7%)	82,113,113	1.89	17 (20%)
19	CLA	4	309	15	64,68,73	1.42	6 (9%)	76,107,113	2.14	20 (26%)
19	CLA	6	310	17	56,60,73	1.52	6 (10%)	65,97,113	2.02	19 (29%)
19	CLA	6	323	17	69,73,73	1.38	6 (8%)	82,113,113	1.87	18 (21%)
19	CLA	4	313	-	59,63,73	1.51	6 (10%)	70,101,113	2.02	18 (25%)
19	CLA	8	307	14	64,68,73	1.45	6 (9%)	76,107,113	2.05	19 (25%)
32	CHL	8	315	14	60,74,74	1.58	9 (15%)	58,114,114	1.71	12 (20%)
19	CLA	3	5020	12	50,54,73	1.64	6 (12%)	59,90,113	2.10	17 (28%)
35	DGA	7	302	-	33,33,43	1.24	3 (9%)	35,35,45	1.63	3 (8%)
32	CHL	6	315	17	60,74,74	1.67	8 (13%)	58,114,114	1.75	9 (15%)
19	CLA	A	822	-	59,63,73	1.45	6 (10%)	70,101,113	2.08	20 (28%)
19	CLA	F	303	39	49,53,73	1.59	6 (12%)	58,89,113	2.05	14 (24%)
19	CLA	1	5010	-	59,63,73	1.49	6 (10%)	70,101,113	2.02	17 (24%)
19	CLA	A	837	-	55,59,73	1.52	7 (12%)	64,96,113	2.11	19 (29%)
19	CLA	A	810	-	69,73,73	1.40	6 (8%)	82,113,113	1.93	19 (23%)
22	BCR	8	303	-	41,41,41	4.96	27 (65%)	56,56,56	2.53	21 (37%)
31	LUT	7	303	-	42,43,43	6.28	25 (59%)	51,60,60	2.11	19 (37%)
32	CHL	Z	302	11	51,65,74	1.77	8 (15%)	47,103,114	1.77	11 (23%)
19	CLA	A	827	-	69,73,73	1.35	6 (8%)	82,113,113	1.91	21 (25%)
19	CLA	7	307	13	54,58,73	1.59	6 (11%)	64,95,113	2.12	17 (26%)
19	CLA	B	811	-	60,64,73	1.45	7 (11%)	71,102,113	2.01	18 (25%)
32	CHL	5	320	16	37,51,74	1.68	8 (21%)	30,86,114	2.13	9 (30%)
19	CLA	B	820	-	60,64,73	1.44	6 (10%)	71,102,113	2.03	19 (26%)
19	CLA	A	814	-	64,68,73	1.40	6 (9%)	76,107,113	1.95	20 (26%)
19	CLA	3	5014	23	64,68,73	1.39	6 (9%)	76,107,113	1.93	18 (23%)
24	LMT	4	302	-	36,36,36	0.38	0	47,47,47	0.74	0
19	CLA	5	301	39	60,64,73	1.44	7 (11%)	71,102,113	1.99	20 (28%)
22	BCR	G	1603	-	41,41,41	4.91	27 (65%)	56,56,56	2.49	19 (33%)
19	CLA	6	313	17	69,73,73	1.39	6 (8%)	82,113,113	1.92	17 (20%)
30	DAO	K	201	-	13,13,13	0.61	0	13,13,13	0.56	0
19	CLA	A	804	19	59,63,73	1.45	6 (10%)	70,101,113	2.01	21 (30%)
19	CLA	1	5007	11	49,53,73	1.67	6 (12%)	58,89,113	2.06	16 (27%)
19	CLA	B	825	39	69,73,73	1.40	6 (8%)	82,113,113	1.87	18 (21%)
19	CLA	B	812	-	69,73,73	1.34	6 (8%)	82,113,113	1.86	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	G	1602	7	50,54,73	1.58	7 (14%)	59,90,113	2.07	18 (30%)
19	CLA	3	5010	12	69,73,73	1.39	6 (8%)	82,113,113	1.84	19 (23%)
32	CHL	8	301	11	50,64,74	1.55	9 (18%)	46,102,114	1.98	10 (21%)
38	ERG	8	325	-	32,32,32	4.04	13 (40%)	45,50,50	2.91	16 (35%)
19	CLA	A	811	19	69,73,73	1.34	7 (10%)	82,113,113	1.86	19 (23%)
32	CHL	5	315	39	60,74,74	1.53	8 (13%)	58,114,114	1.75	10 (17%)
23	LHG	6	324	19	48,48,48	0.45	1 (2%)	51,54,54	1.14	5 (9%)
19	CLA	3	5008	12	69,73,73	1.41	6 (8%)	82,113,113	1.93	20 (24%)
28	C7Z	6	304	-	43,43,43	5.43	27 (62%)	56,60,60	2.54	21 (37%)
19	CLA	3	5011	12	64,68,73	1.47	6 (9%)	76,107,113	2.10	21 (27%)
19	CLA	1	5008	39	69,73,73	1.39	6 (8%)	82,113,113	1.85	19 (23%)
19	CLA	A	809	1	60,64,73	1.44	6 (10%)	71,102,113	2.00	20 (28%)
19	CLA	A	833	-	69,73,73	1.34	6 (8%)	82,113,113	1.92	20 (24%)
31	LUT	3	5002	-	42,43,43	6.26	25 (59%)	51,60,60	2.15	19 (37%)
19	CLA	A	821	39	69,73,73	1.35	5 (7%)	82,113,113	1.85	19 (23%)
27	RRX	F	304	-	42,42,42	5.12	24 (57%)	56,58,58	2.40	19 (33%)
28	C7Z	J	1902	-	43,43,43	5.43	27 (62%)	56,60,60	2.26	18 (32%)
32	CHL	5	318	39	45,59,74	1.60	7 (15%)	40,96,114	2.02	10 (25%)
19	CLA	B	806	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	19 (23%)
22	BCR	5	304	-	41,41,41	4.92	25 (60%)	56,56,56	2.32	22 (39%)
21	SF4	A	845	2,1	0,12,12	-	-	-	-	-
36	PLM	7	322	-	17,17,17	0.59	0	17,17,17	1.08	0
31	LUT	5	303	-	42,43,43	6.21	25 (59%)	51,60,60	2.23	20 (39%)
19	CLA	1	5006	11	69,73,73	1.38	6 (8%)	82,113,113	1.91	21 (25%)
19	CLA	B	818	-	64,68,73	1.40	6 (9%)	76,107,113	1.91	19 (25%)
23	LHG	3	5021	19	19,19,48	0.83	1 (5%)	20,24,54	1.42	1 (5%)
19	CLA	B	803	39	69,73,73	1.36	6 (8%)	82,113,113	1.87	20 (24%)
19	CLA	B	816	-	69,73,73	1.35	6 (8%)	82,113,113	1.90	21 (25%)
19	CLA	Z	303	-	50,54,73	1.63	6 (12%)	59,90,113	2.07	16 (27%)
19	CLA	7	308	13	69,73,73	1.38	6 (8%)	82,113,113	1.99	18 (21%)
19	CLA	Z	314	11	50,54,73	1.58	7 (14%)	59,90,113	2.03	16 (27%)
19	CLA	A	842	39	69,73,73	1.34	6 (8%)	82,113,113	1.87	19 (23%)
32	CHL	6	316	39	55,69,74	1.68	9 (16%)	52,108,114	1.79	11 (21%)
19	CLA	5	308	16	60,64,73	1.48	6 (10%)	71,102,113	1.95	19 (26%)
31	LUT	4	304	-	42,43,43	6.27	24 (57%)	51,60,60	2.50	18 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	K	204	10	53,57,73	1.54	6 (11%)	61,93,113	2.14	18 (29%)
19	CLA	5	317	16	69,73,73	1.37	6 (8%)	82,113,113	1.94	19 (23%)
19	CLA	6	302	15	64,68,73	1.39	6 (9%)	76,107,113	1.93	19 (25%)
19	CLA	5	319	16	54,58,73	1.56	6 (11%)	64,95,113	2.11	20 (31%)
22	BCR	A	848	-	41,41,41	4.92	27 (65%)	56,56,56	2.67	20 (35%)
33	SPH	3	5001	-	19,20,20	0.63	0	18,21,21	1.12	1 (5%)
19	CLA	3	5018	12	64,68,73	1.43	6 (9%)	76,107,113	1.98	17 (22%)
19	CLA	4	318	15	45,49,73	1.66	7 (15%)	54,84,113	2.12	17 (31%)
19	CLA	G	1601	-	54,58,73	1.52	5 (9%)	64,95,113	2.07	19 (29%)
23	LHG	Z	316	19	42,42,48	0.45	0	45,48,54	1.20	3 (6%)
19	CLA	4	310	15	69,73,73	1.40	6 (8%)	82,113,113	1.95	23 (28%)
32	CHL	4	319	15	37,51,74	1.70	8 (21%)	30,86,114	2.15	10 (33%)
32	CHL	4	315	39	45,59,74	1.51	8 (17%)	40,96,114	2.11	11 (27%)
21	SF4	C	101	3	0,12,12	-	-	-	-	-
23	LHG	7	320	19	36,36,48	0.60	1 (2%)	39,42,54	1.45	5 (12%)
19	CLA	A	813	-	69,73,73	1.36	6 (8%)	82,113,113	1.96	20 (24%)
19	CLA	B	826	-	69,73,73	1.35	5 (7%)	82,113,113	1.90	20 (24%)
19	CLA	B	827	-	64,68,73	1.41	7 (10%)	76,107,113	1.97	21 (27%)
19	CLA	B	832	-	62,66,73	1.41	5 (8%)	73,104,113	2.02	19 (26%)
22	BCR	B	847	-	41,41,41	4.91	28 (68%)	56,56,56	2.28	20 (35%)
24	LMT	3	5023	-	36,36,36	0.36	0	47,47,47	0.80	1 (2%)
24	LMT	1	5002	-	36,36,36	0.40	0	47,47,47	0.72	1 (2%)
19	CLA	A	807	-	55,59,73	1.50	6 (10%)	64,96,113	2.11	19 (29%)
19	CLA	B	809	2	59,63,73	1.45	5 (8%)	70,101,113	1.96	18 (25%)
19	CLA	7	324	-	59,63,73	1.51	6 (10%)	70,101,113	2.01	18 (25%)
19	CLA	8	308	14	69,73,73	1.37	6 (8%)	82,113,113	1.90	19 (23%)
19	CLA	A	806	1	69,73,73	1.35	6 (8%)	82,113,113	1.91	21 (25%)
24	LMT	Z	319	19	36,36,36	0.44	0	47,47,47	0.76	1 (2%)
19	CLA	Z	305	11	69,73,73	1.38	6 (8%)	82,113,113	1.94	20 (24%)
22	BCR	4	305	-	41,41,41	4.90	26 (63%)	56,56,56	2.43	18 (32%)
19	CLA	B	834	39	49,53,73	1.59	6 (12%)	58,89,113	2.06	17 (29%)
22	BCR	A	859	-	41,41,41	4.93	27 (65%)	56,56,56	2.41	19 (33%)
19	CLA	5	307	16	65,69,73	1.41	6 (9%)	77,108,113	1.89	21 (27%)
22	BCR	A	849	-	41,41,41	4.89	27 (65%)	56,56,56	2.60	22 (39%)
22	BCR	A	846	-	41,41,41	4.94	27 (65%)	56,56,56	2.27	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LHG	1	5019	19	42,42,48	0.46	0	45,48,54	1.23	4 (8%)
19	CLA	A	831	-	54,58,73	1.52	6 (11%)	64,95,113	2.08	18 (28%)
23	LHG	8	321	19	37,37,48	0.43	0	40,43,54	1.13	3 (7%)
19	CLA	A	840	-	69,73,73	1.40	6 (8%)	82,113,113	1.81	17 (20%)
19	CLA	A	832	-	69,73,73	1.35	6 (8%)	82,113,113	1.94	21 (25%)
19	CLA	7	313	-	47,51,73	1.68	6 (12%)	55,86,113	2.08	15 (27%)
19	CLA	A	819	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	21 (25%)
19	CLA	5	321	-	69,73,73	1.39	6 (8%)	82,113,113	1.92	19 (23%)
33	SPH	7	321	-	19,20,20	0.66	0	18,21,21	1.17	2 (11%)
20	PQN	B	841	-	34,34,34	0.40	0	43,45,45	1.19	4 (9%)
20	PQN	A	844	-	34,34,34	0.41	0	43,45,45	1.21	5 (11%)
19	CLA	A	836	1	59,63,73	1.45	7 (11%)	70,101,113	2.01	19 (27%)
22	BCR	3	5007	-	41,41,41	4.89	26 (63%)	56,56,56	3.55	25 (44%)
19	CLA	B	817	-	63,67,73	1.40	6 (9%)	74,105,113	1.98	19 (25%)
19	CLA	A	829	-	69,73,73	1.35	6 (8%)	82,113,113	1.85	17 (20%)
29	LMG	J	1904	-	45,45,55	1.04	3 (6%)	53,53,63	1.08	2 (3%)
19	CLA	B	804	-	69,73,73	1.35	6 (8%)	82,113,113	1.84	18 (21%)
19	CLA	6	311	39	69,73,73	1.38	6 (8%)	82,113,113	2.06	21 (25%)
19	CLA	J	1901	9	46,50,73	1.65	6 (13%)	53,85,113	2.13	17 (32%)
19	CLA	5	312	23	65,69,73	1.39	6 (9%)	77,108,113	1.96	18 (23%)
29	LMG	7	301	-	29,29,55	0.54	0	37,37,63	1.24	4 (10%)
19	CLA	B	815	-	61,65,73	1.43	5 (8%)	72,103,113	2.02	20 (27%)
31	LUT	8	304	-	42,43,43	6.37	26 (61%)	51,60,60	2.03	15 (29%)
19	CLA	3	5013	39	69,73,73	1.40	6 (8%)	82,113,113	1.91	16 (19%)
19	CLA	1	5013	-	52,56,73	1.58	6 (11%)	61,92,113	2.11	17 (27%)
19	CLA	B	801	-	69,73,73	1.34	6 (8%)	82,113,113	1.81	18 (21%)
25	DGD	B	848	-	67,67,67	1.29	7 (10%)	81,81,81	1.01	3 (3%)
19	CLA	6	301	39	64,68,73	1.40	6 (9%)	76,107,113	1.99	19 (25%)
24	LMT	A	854	-	36,36,36	0.41	0	47,47,47	0.78	1 (2%)
19	CLA	B	819	39	69,73,73	1.34	5 (7%)	82,113,113	1.89	18 (21%)
19	CLA	A	857	39	56,60,73	1.50	7 (12%)	65,97,113	2.03	18 (27%)
31	LUT	6	306	-	42,43,43	6.27	26 (61%)	51,60,60	2.08	16 (31%)
19	CLA	A	823	-	61,65,73	1.43	7 (11%)	72,103,113	2.03	20 (27%)
19	CLA	5	306	16	64,68,73	1.44	6 (9%)	76,107,113	2.01	21 (27%)
19	CLA	A	841	-	69,73,73	1.35	6 (8%)	82,113,113	1.91	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LMT	A	853	-	36,36,36	0.38	0	47,47,47	0.83	1 (2%)
19	CLA	8	320	14	50,54,73	1.58	6 (12%)	59,90,113	2.05	16 (27%)
23	LHG	A	852	-	48,48,48	0.39	0	51,54,54	1.09	4 (7%)
19	CLA	3	5016	12	64,68,73	1.39	6 (9%)	76,107,113	1.98	19 (25%)
19	CLA	1	5016	11	64,68,73	1.40	6 (9%)	76,107,113	1.97	19 (25%)
19	CLA	B	821	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	18 (21%)
24	LMT	Z	301	-	36,36,36	0.32	0	47,47,47	0.99	2 (4%)
19	CLA	A	839	-	69,73,73	1.34	6 (8%)	82,113,113	1.89	20 (24%)
19	CLA	B	850	6	69,73,73	1.40	6 (8%)	82,113,113	1.90	20 (24%)
31	LUT	1	5003	-	42,43,43	6.32	25 (59%)	51,60,60	2.05	18 (35%)
19	CLA	4	306	15	64,68,73	1.43	6 (9%)	76,107,113	1.98	20 (26%)
19	CLA	B	840	23	69,73,73	1.41	6 (8%)	82,113,113	2.01	20 (24%)
19	CLA	7	312	23	69,73,73	1.34	7 (10%)	82,113,113	1.85	19 (23%)
19	CLA	8	311	-	69,73,73	1.40	6 (8%)	82,113,113	1.84	19 (23%)
19	CLA	B	830	-	54,58,73	1.52	6 (11%)	64,95,113	2.10	20 (31%)
34	3PH	8	322	-	29,29,47	1.06	4 (13%)	32,34,52	1.09	2 (6%)
19	CLA	6	318	17	54,58,73	1.56	6 (11%)	64,95,113	2.07	21 (32%)
22	BCR	5	305	-	41,41,41	4.89	24 (58%)	56,56,56	2.74	23 (41%)
32	CHL	5	316	39	45,59,74	2.03	7 (15%)	40,96,114	2.04	10 (25%)
19	CLA	A	818	-	64,68,73	1.39	6 (9%)	76,107,113	1.94	20 (26%)
19	CLA	A	825	39	69,73,73	1.36	7 (10%)	82,113,113	1.88	19 (23%)
19	CLA	7	306	13	64,68,73	1.45	6 (9%)	76,107,113	1.99	20 (26%)
19	CLA	A	816	39	65,69,73	1.40	6 (9%)	77,108,113	1.97	21 (27%)
33	SPH	4	301	-	19,20,20	0.67	0	18,21,21	0.96	0
19	CLA	B	813	-	69,73,73	1.35	6 (8%)	82,113,113	1.94	19 (23%)
22	BCR	B	844	-	41,41,41	4.97	27 (65%)	56,56,56	2.26	19 (33%)
32	CHL	7	314	13	60,74,74	1.61	10 (16%)	58,114,114	1.71	9 (15%)
22	BCR	3	5005	-	41,41,41	4.84	25 (60%)	56,56,56	2.78	20 (35%)
19	CLA	4	312	23	59,63,73	1.45	6 (10%)	70,101,113	2.00	17 (24%)
19	CLA	A	805	-	69,73,73	1.34	7 (10%)	82,113,113	1.87	17 (20%)
24	LMT	4	321	-	36,36,36	0.36	0	47,47,47	0.72	1 (2%)
19	CLA	F	301	-	69,73,73	1.39	7 (10%)	82,113,113	1.94	20 (24%)
19	CLA	A	815	-	69,73,73	1.39	6 (8%)	82,113,113	2.00	22 (26%)
31	LUT	8	305	-	42,43,43	6.20	26 (61%)	51,60,60	2.44	20 (39%)
23	LHG	5	323	19	36,36,48	0.44	0	39,42,54	1.18	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	7	310	-	65,69,73	1.43	6 (9%)	77,108,113	2.02	21 (27%)
22	BCR	B	846	-	41,41,41	4.93	28 (68%)	56,56,56	2.43	20 (35%)
31	LUT	3	5003	-	42,43,43	6.34	26 (61%)	51,60,60	2.17	15 (29%)
19	CLA	B	831	-	69,73,73	1.40	6 (8%)	82,113,113	2.01	20 (24%)
19	CLA	A	826	39	69,73,73	1.35	7 (10%)	82,113,113	1.92	18 (21%)
31	LUT	7	304	-	42,43,43	6.28	26 (61%)	51,60,60	2.35	17 (33%)
32	CHL	8	316	39	51,65,74	1.61	7 (13%)	47,103,114	1.89	11 (23%)
24	LMT	F	305	-	36,36,36	0.36	0	47,47,47	0.80	2 (4%)
19	CLA	Z	308	-	69,73,73	1.38	6 (8%)	82,113,113	1.94	22 (26%)
19	CLA	5	310	-	59,63,73	1.50	6 (10%)	70,101,113	2.07	23 (32%)
19	CLA	Z	315	11	69,73,73	1.38	6 (8%)	82,113,113	1.93	22 (26%)
19	CLA	Z	312	23	69,73,73	1.36	6 (8%)	82,113,113	1.90	19 (23%)
19	CLA	B	836	-	69,73,73	1.40	6 (8%)	82,113,113	1.94	17 (20%)
19	CLA	A	834	-	69,73,73	1.35	6 (8%)	82,113,113	1.89	18 (21%)
32	CHL	1	5009	11	55,69,74	1.57	10 (18%)	52,108,114	1.81	12 (23%)
32	CHL	1	5014	39	42,56,74	1.57	9 (21%)	36,92,114	2.02	12 (33%)
19	CLA	A	803	-	69,73,73	1.34	7 (10%)	82,113,113	1.90	20 (24%)
19	CLA	B	823	-	69,73,73	1.35	5 (7%)	82,113,113	1.88	20 (24%)
22	BCR	7	305	-	41,41,41	4.91	28 (68%)	56,56,56	2.41	21 (37%)
31	LUT	1	5004	-	42,43,43	6.19	25 (59%)	51,60,60	2.39	18 (35%)
19	CLA	8	312	39	64,68,73	1.60	8 (12%)	76,107,113	2.07	19 (25%)
19	CLA	B	810	-	56,60,73	1.49	6 (10%)	65,97,113	2.11	20 (30%)
19	CLA	A	830	-	69,73,73	1.35	5 (7%)	82,113,113	1.88	18 (21%)
19	CLA	5	314	16	69,73,73	1.37	6 (8%)	82,113,113	1.82	18 (21%)
19	CLA	6	309	17	64,68,73	1.43	6 (9%)	76,107,113	1.96	19 (25%)
27	RRX	5	302	-	42,42,42	5.08	24 (57%)	56,58,58	2.29	23 (41%)
23	LHG	1	5001	19	22,22,48	0.57	0	25,28,54	1.31	3 (12%)
19	CLA	8	309	14	69,73,73	1.38	6 (8%)	82,113,113	2.04	21 (25%)
19	CLA	7	309	13	69,73,73	1.40	6 (8%)	82,113,113	1.98	20 (24%)
19	CLA	4	308	15	69,73,73	1.39	6 (8%)	82,113,113	2.01	21 (25%)
22	BCR	A	858	-	41,41,41	4.94	27 (65%)	56,56,56	2.25	22 (39%)
32	CHL	8	317	39	45,59,74	1.71	8 (17%)	40,96,114	2.07	12 (30%)
22	BCR	6	308	-	41,41,41	4.89	25 (60%)	56,56,56	2.52	21 (37%)
19	CLA	7	317	13	54,58,73	1.51	6 (11%)	64,95,113	2.08	17 (26%)
23	LHG	6	303	-	31,31,48	0.50	0	34,37,54	1.22	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	A	850	-	41,41,41	4.93	27 (65%)	56,56,56	2.51	19 (33%)
19	CLA	3	5012	-	69,73,73	1.38	6 (8%)	82,113,113	1.93	22 (26%)
22	BCR	B	842	-	41,41,41	4.96	27 (65%)	56,56,56	2.27	19 (33%)
19	CLA	A	817	-	64,68,73	1.40	6 (9%)	76,107,113	1.97	17 (22%)
19	CLA	8	314	-	59,63,73	1.50	6 (10%)	70,101,113	2.08	20 (28%)
22	BCR	A	847	-	41,41,41	4.92	27 (65%)	56,56,56	2.51	20 (35%)
19	CLA	5	322	39	50,54,73	1.58	6 (12%)	59,90,113	2.13	16 (27%)
19	CLA	3	5015	-	49,53,73	1.62	6 (12%)	58,89,113	2.11	17 (29%)
19	CLA	3	5009	12	50,54,73	1.60	6 (12%)	59,90,113	2.03	17 (28%)
22	BCR	B	843	-	41,41,41	4.94	26 (63%)	56,56,56	2.54	22 (39%)
22	BCR	K	206	-	41,41,41	4.93	27 (65%)	56,56,56	2.37	21 (37%)
24	LMT	A	855	-	36,36,36	0.39	0	47,47,47	0.71	1 (2%)
19	CLA	4	316	15	54,58,73	1.56	6 (11%)	64,95,113	2.07	18 (28%)
32	CHL	4	314	39	45,59,74	1.77	7 (15%)	40,96,114	2.04	12 (30%)
24	LMT	4	322	-	36,36,36	0.42	0	47,47,47	0.78	1 (2%)
19	CLA	4	307	15	56,60,73	1.57	6 (10%)	65,97,113	2.05	17 (26%)
19	CLA	A	802	39	69,73,73	1.35	6 (8%)	82,113,113	1.87	20 (24%)
19	CLA	B	829	-	69,73,73	1.35	5 (7%)	82,113,113	1.91	19 (23%)
32	CHL	Z	310	39	60,74,74	1.78	9 (15%)	58,114,114	1.77	13 (22%)
19	CLA	1	5011	39	59,63,73	1.46	6 (10%)	70,101,113	2.07	18 (25%)
19	CLA	4	311	39	54,58,73	1.69	8 (14%)	64,95,113	2.10	18 (28%)
32	CHL	3	5017	39	60,74,74	1.68	7 (11%)	58,114,114	1.64	11 (18%)
19	CLA	7	316	39	54,58,73	1.57	6 (11%)	64,95,113	2.17	19 (29%)
19	CLA	B	833	-	69,73,73	1.34	7 (10%)	82,113,113	1.88	19 (23%)
22	BCR	6	307	-	41,41,41	4.91	26 (63%)	56,56,56	2.31	20 (35%)
19	CLA	B	805	-	49,53,73	1.60	7 (14%)	58,89,113	2.09	17 (29%)
31	LUT	Z	318	-	42,43,43	6.34	25 (59%)	51,60,60	2.20	15 (29%)
38	ERG	6	326	-	32,32,32	4.14	14 (43%)	45,50,50	2.73	15 (33%)
22	BCR	3	5006	-	41,41,41	4.91	28 (68%)	56,56,56	2.40	20 (35%)
27	RRX	4	303	-	42,42,42	5.10	24 (57%)	56,58,58	2.37	23 (41%)
19	CLA	Z	306	-	54,58,73	1.54	6 (11%)	64,95,113	2.06	17 (26%)
19	CLA	I	201	-	59,63,73	1.46	6 (10%)	70,101,113	2.01	21 (30%)
19	CLA	B	824	39	69,73,73	1.35	6 (8%)	82,113,113	1.88	19 (23%)
19	CLA	8	313	23	59,63,73	1.51	6 (10%)	70,101,113	2.05	19 (27%)
24	LMT	A	856	-	36,36,36	0.39	0	47,47,47	0.85	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	SQD	8	302	-	46,48,54	0.81	0	56,59,65	0.89	2 (3%)
19	CLA	K	202	-	50,54,73	1.59	6 (12%)	59,90,113	2.12	19 (32%)
19	CLA	1	5018	11	55,59,73	1.51	6 (10%)	64,96,113	2.04	19 (29%)
19	CLA	A	808	1	69,73,73	1.34	6 (8%)	82,113,113	1.89	19 (23%)
19	CLA	Z	311	24	59,63,73	1.52	6 (10%)	70,101,113	2.13	19 (27%)
19	CLA	6	320	39	65,69,73	1.43	6 (9%)	77,108,113	2.02	20 (25%)
23	LHG	A	851	19	34,34,48	0.45	0	37,40,54	1.27	3 (8%)
31	LUT	Z	317	-	42,43,43	6.26	26 (61%)	51,60,60	3.91	21 (41%)
19	CLA	6	312	17	69,73,73	1.38	6 (8%)	82,113,113	1.88	19 (23%)
19	CLA	B	802	-	69,73,73	1.34	5 (7%)	82,113,113	1.93	20 (24%)
19	CLA	B	839	-	50,54,73	1.58	6 (12%)	59,90,113	2.04	16 (27%)
19	CLA	6	322	-	50,54,73	1.62	6 (12%)	59,90,113	2.06	15 (25%)
19	CLA	7	319	13	62,66,73	1.43	6 (9%)	73,104,113	2.03	19 (26%)
19	CLA	B	814	-	64,68,73	1.40	6 (9%)	76,107,113	1.95	19 (25%)
19	CLA	6	314	23	59,63,73	1.45	6 (10%)	70,101,113	1.98	16 (22%)
24	LMT	G	1604	-	36,36,36	0.38	0	47,47,47	0.73	1 (2%)
19	CLA	B	838	39	56,60,73	1.50	7 (12%)	65,97,113	2.03	17 (26%)
21	SF4	C	102	3	0,12,12	-	-	-	-	-
22	BCR	8	306	-	41,41,41	4.86	25 (60%)	56,56,56	2.34	23 (41%)
19	CLA	A	824	-	69,73,73	1.35	6 (8%)	82,113,113	1.89	18 (21%)
23	LHG	4	320	19	48,48,48	0.40	0	51,54,54	1.14	4 (7%)
32	CHL	6	321	17	37,51,74	2.07	8 (21%)	30,86,114	2.25	12 (40%)
34	3PH	6	325	-	28,28,47	1.10	4 (14%)	31,33,52	1.19	2 (6%)
19	CLA	A	843	23	56,60,73	1.49	7 (12%)	65,97,113	2.10	19 (29%)
34	3PH	3	5022	-	38,38,47	0.96	4 (10%)	41,43,52	1.22	2 (4%)
32	CHL	1	5017	39	42,56,74	1.60	7 (16%)	36,92,114	2.00	11 (30%)
19	CLA	K	205	10	49,53,73	1.59	5 (10%)	58,89,113	2.10	16 (27%)
32	CHL	4	317	39	60,74,74	1.80	10 (16%)	58,114,114	1.66	12 (20%)
22	BCR	B	845	-	41,41,41	4.90	27 (65%)	56,56,56	2.52	20 (35%)
24	LMT	8	324	-	36,36,36	0.39	0	47,47,47	1.03	2 (4%)
24	LMT	8	323	-	36,36,36	0.34	0	47,47,47	1.04	3 (6%)
24	LMT	7	323	-	36,36,36	0.35	0	47,47,47	0.75	1 (2%)
31	LUT	6	305	-	42,43,43	6.25	25 (59%)	51,60,60	2.37	17 (33%)
19	CLA	8	310	14	66,70,73	1.43	6 (9%)	78,109,113	1.95	20 (25%)
19	CLA	5	325	-	59,63,73	1.50	6 (10%)	70,101,113	2.02	20 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	F	302	-	41,41,41	4.94	27 (65%)	56,56,56	2.45	19 (33%)
19	CLA	8	318	14	50,54,73	1.65	6 (12%)	59,90,113	2.10	16 (27%)
19	CLA	7	318	39	46,50,73	1.73	6 (13%)	53,85,113	2.09	15 (28%)
19	CLA	3	5019	39	59,63,73	1.50	6 (10%)	70,101,113	2.10	19 (27%)
32	CHL	8	319	39	60,74,74	1.79	9 (15%)	58,114,114	1.90	14 (24%)
19	CLA	5	309	16	69,73,73	1.36	6 (8%)	82,113,113	1.96	21 (25%)
32	CHL	7	315	39	48,62,74	1.54	8 (16%)	43,99,114	1.93	11 (25%)
32	CHL	Z	309	11	57,71,74	1.39	7 (12%)	54,110,114	1.63	9 (16%)
32	CHL	Z	313	39	40,54,74	1.90	8 (20%)	34,90,114	2.10	11 (32%)
19	CLA	A	812	-	69,73,73	1.37	6 (8%)	82,113,113	1.85	16 (19%)
19	CLA	B	822	-	63,67,73	1.41	6 (9%)	74,105,113	2.02	20 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	807	2	1/1/15/20	20/39/115/115	-
19	CLA	B	828	-	1/1/15/20	10/39/115/115	-
19	CLA	B	837	-	1/1/15/20	17/39/115/115	-
19	CLA	A	820	-	1/1/14/20	9/33/109/115	-
19	CLA	Z	304	39	1/1/12/20	0/21/97/115	-
19	CLA	7	311	39	1/1/13/20	9/29/105/115	-
29	LMG	J	1903	-	-	8/30/50/70	0/1/1/1
34	3PH	5	324	-	-	8/24/24/49	-
19	CLA	1	5015	39	1/1/12/20	6/21/97/115	-
19	CLA	5	311	39	1/1/12/20	10/21/97/115	-
28	C7Z	1	5005	-	-	9/29/67/67	0/2/2/2
19	CLA	K	203	39	1/1/13/20	7/27/103/115	-
18	CL0	A	801	-	3/3/20/25	12/37/135/135	-
32	CHL	6	317	39	3/3/17/26	7/21/119/137	-
19	CLA	5	313	-	1/1/11/20	6/15/91/115	-
32	CHL	6	319	39	3/3/20/26	13/39/137/137	-
19	CLA	A	835	-	1/1/15/20	10/39/115/115	-
19	CLA	1	5012	23	1/1/14/20	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	828	-	1/1/15/20	17/39/115/115	-
22	BCR	3	5004	-	-	13/29/63/63	0/2/2/2
19	CLA	B	808	-	1/1/15/20	18/39/115/115	-
19	CLA	Z	307	-	1/1/13/20	15/30/106/115	-
19	CLA	B	835	-	1/1/14/20	11/33/109/115	-
19	CLA	A	838	-	1/1/15/20	16/39/115/115	-
19	CLA	4	309	15	1/1/14/20	10/33/109/115	-
19	CLA	6	310	17	1/1/12/20	6/24/100/115	-
19	CLA	6	323	17	1/1/15/20	9/39/115/115	-
19	CLA	4	313	-	1/1/13/20	12/27/103/115	-
19	CLA	8	307	14	1/1/14/20	15/33/109/115	-
32	CHL	8	315	14	3/3/20/26	12/39/137/137	-
19	CLA	3	5020	12	1/1/11/20	8/17/93/115	-
35	DGA	7	302	-	-	22/35/35/45	-
32	CHL	6	315	17	3/3/20/26	12/39/137/137	-
19	CLA	A	822	-	1/1/13/20	10/27/103/115	-
19	CLA	F	303	39	1/1/11/20	4/15/91/115	-
19	CLA	1	5010	-	1/1/13/20	7/27/103/115	-
19	CLA	A	837	-	1/1/12/20	5/23/99/115	-
19	CLA	A	810	-	1/1/15/20	10/39/115/115	-
22	BCR	8	303	-	-	16/29/63/63	0/2/2/2
32	CHL	Z	302	11	3/3/18/26	6/29/127/137	-
31	LUT	7	303	-	-	5/29/67/67	0/2/2/2
19	CLA	A	827	-	1/1/15/20	19/39/115/115	-
19	CLA	7	307	13	1/1/12/20	3/21/97/115	-
19	CLA	B	811	-	1/1/13/20	11/29/105/115	-
32	CHL	5	320	16	3/3/15/26	2/12/110/137	-
19	CLA	B	820	-	1/1/13/20	13/29/105/115	-
19	CLA	A	814	-	1/1/14/20	10/33/109/115	-
19	CLA	3	5014	23	1/1/14/20	22/33/109/115	-
24	LMT	4	302	-	-	5/21/61/61	0/2/2/2
19	CLA	5	301	39	1/1/13/20	14/29/105/115	-
22	BCR	G	1603	-	-	8/29/63/63	0/2/2/2
19	CLA	6	313	17	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DAO	K	201	-	-	2/11/11/11	-
19	CLA	A	804	19	1/1/13/20	11/27/103/115	-
19	CLA	1	5007	11	1/1/11/20	4/15/91/115	-
19	CLA	B	825	39	1/1/15/20	12/39/115/115	-
19	CLA	B	812	-	1/1/15/20	12/39/115/115	-
19	CLA	G	1602	7	1/1/11/20	9/17/93/115	-
19	CLA	3	5010	12	1/1/15/20	11/39/115/115	-
32	CHL	8	301	11	3/3/18/26	7/27/125/137	-
38	ERG	8	325	-	-	10/13/71/71	0/4/4/4
19	CLA	A	811	19	1/1/15/20	11/39/115/115	-
32	CHL	5	315	39	3/3/20/26	17/39/137/137	-
23	LHG	6	324	19	-	31/53/53/53	-
19	CLA	3	5008	12	1/1/15/20	8/39/115/115	-
28	C7Z	6	304	-	-	13/29/67/67	0/2/2/2
19	CLA	3	5011	12	1/1/14/20	4/33/109/115	-
19	CLA	1	5008	39	1/1/15/20	11/39/115/115	-
19	CLA	A	809	1	1/1/13/20	9/29/105/115	-
19	CLA	A	833	-	1/1/15/20	16/39/115/115	-
31	LUT	3	5002	-	-	4/29/67/67	0/2/2/2
19	CLA	A	821	39	1/1/15/20	9/39/115/115	-
27	RRX	F	304	-	-	14/29/65/65	0/2/2/2
28	C7Z	J	1902	-	-	13/29/67/67	0/2/2/2
32	CHL	5	318	39	3/3/17/26	4/21/119/137	-
19	CLA	B	806	-	1/1/15/20	8/39/115/115	-
22	BCR	5	304	-	-	13/29/63/63	0/2/2/2
21	SF4	A	845	2,1	-	-	0/6/5/5
36	PLM	7	322	-	-	4/15/15/15	-
31	LUT	5	303	-	-	9/29/67/67	0/2/2/2
19	CLA	1	5006	11	1/1/15/20	16/39/115/115	-
19	CLA	B	818	-	1/1/14/20	15/33/109/115	-
23	LHG	3	5021	19	-	16/22/22/53	-
19	CLA	B	803	39	1/1/15/20	13/39/115/115	-
19	CLA	B	816	-	1/1/15/20	13/39/115/115	-
19	CLA	Z	303	-	1/1/11/20	7/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	7	308	13	1/1/15/20	11/39/115/115	-
19	CLA	Z	314	11	1/1/11/20	5/17/93/115	-
19	CLA	A	842	39	1/1/15/20	10/39/115/115	-
32	CHL	6	316	39	3/3/19/26	9/33/131/137	-
19	CLA	5	308	16	1/1/13/20	7/29/105/115	-
31	LUT	4	304	-	-	7/29/67/67	0/2/2/2
19	CLA	K	204	10	1/1/11/20	6/20/96/115	-
19	CLA	5	317	16	1/1/15/20	13/39/115/115	-
19	CLA	6	302	15	1/1/14/20	15/33/109/115	-
19	CLA	5	319	16	1/1/12/20	9/21/97/115	-
22	BCR	A	848	-	-	12/29/63/63	0/2/2/2
33	SPH	3	5001	-	-	14/21/21/21	-
19	CLA	3	5018	12	1/1/14/20	11/33/109/115	-
19	CLA	4	318	15	1/1/10/20	2/10/86/115	-
19	CLA	G	1601	-	1/1/12/20	7/21/97/115	-
23	LHG	Z	316	19	-	27/47/47/53	-
19	CLA	4	310	15	1/1/15/20	9/39/115/115	-
32	CHL	4	319	15	3/3/15/26	0/12/110/137	-
32	CHL	4	315	39	3/3/17/26	7/21/119/137	-
23	LHG	7	320	19	-	26/41/41/53	-
21	SF4	C	101	3	-	-	0/6/5/5
19	CLA	A	813	-	1/1/15/20	15/39/115/115	-
19	CLA	B	826	-	1/1/15/20	16/39/115/115	-
19	CLA	B	827	-	1/1/14/20	19/33/109/115	-
19	CLA	B	832	-	1/1/13/20	16/31/107/115	-
22	BCR	B	847	-	-	12/29/63/63	0/2/2/2
24	LMT	3	5023	-	-	6/21/61/61	0/2/2/2
24	LMT	1	5002	-	-	4/21/61/61	0/2/2/2
19	CLA	A	807	-	1/1/12/20	8/23/99/115	-
19	CLA	B	809	2	1/1/13/20	14/27/103/115	-
19	CLA	7	324	-	1/1/13/20	9/27/103/115	-
19	CLA	8	308	14	1/1/15/20	13/39/115/115	-
19	CLA	A	806	1	1/1/15/20	16/39/115/115	-
24	LMT	Z	319	19	-	8/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	Z	305	11	1/1/15/20	17/39/115/115	-
22	BCR	4	305	-	-	15/29/63/63	0/2/2/2
19	CLA	B	834	39	1/1/11/20	3/15/91/115	-
22	BCR	A	859	-	-	15/29/63/63	0/2/2/2
19	CLA	5	307	16	1/1/14/20	12/35/111/115	-
22	BCR	A	849	-	-	15/29/63/63	0/2/2/2
22	BCR	A	846	-	-	14/29/63/63	0/2/2/2
23	LHG	1	5019	19	-	31/47/47/53	-
19	CLA	A	831	-	1/1/12/20	2/21/97/115	-
23	LHG	8	321	19	-	23/42/42/53	-
19	CLA	A	840	-	1/1/15/20	12/39/115/115	-
19	CLA	A	832	-	1/1/15/20	19/39/115/115	-
19	CLA	7	313	-	1/1/10/20	1/13/89/115	-
19	CLA	A	819	-	1/1/15/20	11/39/115/115	-
19	CLA	5	321	-	1/1/15/20	14/39/115/115	-
33	SPH	7	321	-	-	11/21/21/21	-
20	PQN	B	841	-	-	10/23/43/43	0/2/2/2
20	PQN	A	844	-	-	6/23/43/43	0/2/2/2
19	CLA	A	836	1	1/1/13/20	11/27/103/115	-
22	BCR	3	5007	-	-	13/29/63/63	0/2/2/2
19	CLA	B	817	-	1/1/13/20	17/32/108/115	-
19	CLA	A	829	-	1/1/15/20	11/39/115/115	-
29	LMG	J	1904	-	-	8/40/60/70	0/1/1/1
19	CLA	B	804	-	1/1/15/20	10/39/115/115	-
19	CLA	6	311	39	1/1/15/20	10/39/115/115	-
19	CLA	J	1901	9	1/1/10/20	4/12/88/115	-
19	CLA	5	312	23	1/1/14/20	12/35/111/115	-
29	LMG	7	301	-	-	5/24/44/70	0/1/1/1
19	CLA	B	815	-	1/1/13/20	16/30/106/115	-
31	LUT	8	304	-	-	11/29/67/67	0/2/2/2
19	CLA	3	5013	39	1/1/15/20	13/39/115/115	-
19	CLA	1	5013	-	1/1/11/20	5/19/95/115	-
19	CLA	B	801	-	1/1/15/20	11/39/115/115	-
25	DGD	B	848	-	-	15/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	6	301	39	1/1/14/20	16/33/109/115	-
24	LMT	A	854	-	-	2/21/61/61	0/2/2/2
19	CLA	B	819	39	1/1/15/20	19/39/115/115	-
19	CLA	A	857	39	1/1/12/20	9/24/100/115	-
31	LUT	6	306	-	-	8/29/67/67	0/2/2/2
19	CLA	A	823	-	1/1/13/20	17/30/106/115	-
19	CLA	5	306	16	1/1/14/20	17/33/109/115	-
19	CLA	A	841	-	1/1/15/20	11/39/115/115	-
24	LMT	A	853	-	-	4/21/61/61	0/2/2/2
19	CLA	8	320	14	1/1/11/20	5/17/93/115	-
23	LHG	A	852	-	-	35/53/53/53	-
19	CLA	3	5016	12	1/1/14/20	13/33/109/115	-
19	CLA	1	5016	11	1/1/14/20	11/33/109/115	-
19	CLA	B	821	-	1/1/15/20	16/39/115/115	-
24	LMT	Z	301	-	-	8/21/61/61	0/2/2/2
19	CLA	A	839	-	1/1/15/20	13/39/115/115	-
19	CLA	B	850	6	1/1/15/20	19/39/115/115	-
31	LUT	1	5003	-	-	6/29/67/67	0/2/2/2
19	CLA	4	306	15	1/1/14/20	11/33/109/115	-
19	CLA	B	840	23	1/1/15/20	12/39/115/115	-
19	CLA	7	312	23	1/1/15/20	13/39/115/115	-
19	CLA	8	311	-	1/1/15/20	14/39/115/115	-
19	CLA	B	830	-	1/1/12/20	7/21/97/115	-
34	3PH	8	322	-	-	15/31/31/49	-
19	CLA	6	318	17	1/1/12/20	3/21/97/115	-
22	BCR	5	305	-	-	7/29/63/63	0/2/2/2
32	CHL	5	316	39	3/3/17/26	4/21/119/137	-
19	CLA	A	818	-	1/1/14/20	15/33/109/115	-
19	CLA	A	825	39	1/1/15/20	15/39/115/115	-
19	CLA	7	306	13	1/1/14/20	12/33/109/115	-
19	CLA	A	816	39	1/1/14/20	13/35/111/115	-
33	SPH	4	301	-	-	12/21/21/21	-
19	CLA	B	813	-	1/1/15/20	16/39/115/115	-
22	BCR	B	844	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CHL	7	314	13	3/3/20/26	14/39/137/137	-
22	BCR	3	5005	-	-	7/29/63/63	0/2/2/2
19	CLA	4	312	23	1/1/13/20	8/27/103/115	-
19	CLA	A	805	-	1/1/15/20	10/39/115/115	-
24	LMT	4	321	-	-	2/21/61/61	0/2/2/2
19	CLA	F	301	-	1/1/15/20	10/39/115/115	-
19	CLA	A	815	-	1/1/15/20	6/39/115/115	-
31	LUT	8	305	-	-	3/29/67/67	0/2/2/2
23	LHG	5	323	19	-	27/41/41/53	-
19	CLA	7	310	-	1/1/14/20	12/35/111/115	-
22	BCR	B	846	-	-	12/29/63/63	0/2/2/2
31	LUT	3	5003	-	-	6/29/67/67	0/2/2/2
19	CLA	B	831	-	1/1/15/20	15/39/115/115	-
19	CLA	A	826	39	1/1/15/20	11/39/115/115	-
31	LUT	7	304	-	-	5/29/67/67	0/2/2/2
32	CHL	8	316	39	3/3/18/26	11/29/127/137	-
24	LMT	F	305	-	-	4/21/61/61	0/2/2/2
19	CLA	Z	308	-	1/1/15/20	12/39/115/115	-
19	CLA	5	310	-	1/1/13/20	16/27/103/115	-
19	CLA	Z	315	11	1/1/15/20	13/39/115/115	-
19	CLA	Z	312	23	1/1/15/20	15/39/115/115	-
19	CLA	B	836	-	1/1/15/20	15/39/115/115	-
19	CLA	A	834	-	1/1/15/20	18/39/115/115	-
32	CHL	1	5009	11	3/3/19/26	12/33/131/137	-
32	CHL	1	5014	39	3/3/16/26	2/18/116/137	-
19	CLA	A	803	-	1/1/15/20	12/39/115/115	-
19	CLA	B	823	-	1/1/15/20	17/39/115/115	-
22	BCR	7	305	-	-	15/29/63/63	0/2/2/2
31	LUT	1	5004	-	-	4/29/67/67	0/2/2/2
19	CLA	8	312	39	1/1/14/20	12/33/109/115	-
19	CLA	B	810	-	1/1/12/20	9/24/100/115	-
19	CLA	A	830	-	1/1/15/20	11/39/115/115	-
19	CLA	5	314	16	1/1/15/20	17/39/115/115	-
19	CLA	6	309	17	1/1/14/20	8/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	RRX	5	302	-	-	7/29/65/65	0/2/2/2
23	LHG	1	5001	19	-	15/26/26/53	-
19	CLA	8	309	14	1/1/15/20	6/39/115/115	-
19	CLA	7	309	13	1/1/15/20	9/39/115/115	-
19	CLA	4	308	15	1/1/15/20	12/39/115/115	-
22	BCR	A	858	-	-	13/29/63/63	0/2/2/2
32	CHL	8	317	39	3/3/17/26	4/21/119/137	-
22	BCR	6	308	-	-	10/29/63/63	0/2/2/2
19	CLA	7	317	13	1/1/12/20	6/21/97/115	-
23	LHG	6	303	-	-	26/36/36/53	-
22	BCR	A	850	-	-	15/29/63/63	0/2/2/2
19	CLA	3	5012	-	1/1/15/20	7/39/115/115	-
22	BCR	B	842	-	-	13/29/63/63	0/2/2/2
19	CLA	A	817	-	1/1/14/20	12/33/109/115	-
19	CLA	8	314	-	1/1/13/20	12/27/103/115	-
22	BCR	A	847	-	-	12/29/63/63	0/2/2/2
19	CLA	5	322	39	1/1/11/20	8/17/93/115	-
19	CLA	3	5015	-	1/1/11/20	6/15/91/115	-
19	CLA	3	5009	12	1/1/11/20	4/17/93/115	-
22	BCR	B	843	-	-	14/29/63/63	0/2/2/2
22	BCR	K	206	-	-	10/29/63/63	0/2/2/2
24	LMT	A	855	-	-	3/21/61/61	0/2/2/2
19	CLA	4	316	15	1/1/12/20	5/21/97/115	-
32	CHL	4	314	39	3/3/17/26	5/21/119/137	-
24	LMT	4	322	-	-	4/21/61/61	0/2/2/2
19	CLA	4	307	15	1/1/12/20	8/24/100/115	-
19	CLA	A	802	39	1/1/15/20	12/39/115/115	-
19	CLA	B	829	-	1/1/15/20	14/39/115/115	-
32	CHL	Z	310	39	3/3/20/26	10/39/137/137	-
19	CLA	1	5011	39	1/1/13/20	11/27/103/115	-
19	CLA	4	311	39	1/1/12/20	6/21/97/115	-
32	CHL	3	5017	39	3/3/20/26	10/39/137/137	-
19	CLA	7	316	39	1/1/12/20	2/21/97/115	-
19	CLA	B	833	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	6	307	-	-	10/29/63/63	0/2/2/2
19	CLA	B	805	-	1/1/11/20	6/15/91/115	-
31	LUT	Z	318	-	-	6/29/67/67	0/2/2/2
38	ERG	6	326	-	-	8/13/71/71	0/4/4/4
22	BCR	3	5006	-	-	16/29/63/63	0/2/2/2
27	RRX	4	303	-	-	7/29/65/65	0/2/2/2
19	CLA	Z	306	-	1/1/12/20	11/21/97/115	-
19	CLA	I	201	-	1/1/13/20	13/27/103/115	-
19	CLA	B	824	39	1/1/15/20	13/39/115/115	-
19	CLA	8	313	23	1/1/13/20	12/27/103/115	-
24	LMT	A	856	-	-	8/21/61/61	0/2/2/2
37	SQD	8	302	-	-	10/43/63/69	0/1/1/1
19	CLA	K	202	-	1/1/11/20	6/17/93/115	-
19	CLA	1	5018	11	1/1/12/20	3/23/99/115	-
19	CLA	A	808	1	1/1/15/20	17/39/115/115	-
19	CLA	Z	311	24	1/1/13/20	11/27/103/115	-
19	CLA	6	320	39	1/1/14/20	13/35/111/115	-
23	LHG	A	851	19	-	22/39/39/53	-
31	LUT	Z	317	-	-	6/29/67/67	0/2/2/2
19	CLA	6	312	17	1/1/15/20	7/39/115/115	-
19	CLA	B	802	-	1/1/15/20	15/39/115/115	-
19	CLA	B	839	-	1/1/11/20	5/17/93/115	-
19	CLA	6	322	-	1/1/11/20	4/17/93/115	-
19	CLA	7	319	13	1/1/13/20	14/31/107/115	-
19	CLA	B	814	-	1/1/14/20	11/33/109/115	-
19	CLA	6	314	23	1/1/13/20	8/27/103/115	-
24	LMT	G	1604	-	-	2/21/61/61	0/2/2/2
19	CLA	B	838	39	1/1/12/20	6/24/100/115	-
21	SF4	C	102	3	-	-	0/6/5/5
22	BCR	8	306	-	-	9/29/63/63	0/2/2/2
19	CLA	A	824	-	1/1/15/20	13/39/115/115	-
23	LHG	4	320	19	-	34/53/53/53	-
32	CHL	6	321	17	3/3/15/26	4/12/110/137	-
34	3PH	6	325	-	-	15/30/30/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	843	23	1/1/12/20	10/24/100/115	-
34	3PH	3	5022	-	-	20/40/40/49	-
32	CHL	1	5017	39	3/3/16/26	0/18/116/137	-
19	CLA	K	205	10	1/1/11/20	7/15/91/115	-
32	CHL	4	317	39	3/3/20/26	7/39/137/137	-
22	BCR	B	845	-	-	14/29/63/63	0/2/2/2
24	LMT	8	324	-	-	3/21/61/61	0/2/2/2
24	LMT	8	323	-	-	4/21/61/61	0/2/2/2
24	LMT	7	323	-	-	3/21/61/61	0/2/2/2
31	LUT	6	305	-	-	5/29/67/67	0/2/2/2
19	CLA	8	310	14	1/1/14/20	8/36/112/115	-
19	CLA	5	325	-	1/1/13/20	11/27/103/115	-
22	BCR	F	302	-	-	12/29/63/63	0/2/2/2
19	CLA	8	318	14	1/1/11/20	5/17/93/115	-
19	CLA	7	318	39	1/1/10/20	4/12/88/115	-
19	CLA	3	5019	39	1/1/13/20	8/27/103/115	-
32	CHL	8	319	39	3/3/20/26	15/39/137/137	-
19	CLA	5	309	16	1/1/15/20	9/39/115/115	-
32	CHL	7	315	39	3/3/17/26	5/25/123/137	-
32	CHL	Z	309	11	3/3/19/26	16/36/134/137	-
32	CHL	Z	313	39	3/3/16/26	6/15/113/137	-
19	CLA	A	812	-	1/1/15/20	11/39/115/115	-
19	CLA	B	822	-	1/1/13/20	12/32/108/115	-

All (2691) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	5003	LUT	C24-C25	24.20	1.61	1.33
31	Z	318	LUT	C24-C25	24.10	1.61	1.33
31	8	304	LUT	C24-C25	24.03	1.61	1.33
31	3	5003	LUT	C24-C25	23.70	1.61	1.33
31	6	305	LUT	C24-C25	23.55	1.61	1.33
31	4	304	LUT	C24-C25	23.47	1.61	1.33
31	7	304	LUT	C24-C25	23.47	1.61	1.33
31	3	5002	LUT	C24-C25	23.46	1.61	1.33
31	7	303	LUT	C24-C25	23.42	1.61	1.33
31	6	306	LUT	C24-C25	23.26	1.60	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	305	LUT	C24-C25	22.94	1.60	1.33
31	Z	317	LUT	C24-C25	22.85	1.60	1.33
31	5	303	LUT	C24-C25	22.72	1.60	1.33
31	1	5004	LUT	C24-C25	22.70	1.60	1.33
28	J	1902	C7Z	C25-C26	16.38	1.62	1.34
28	1	5005	C7Z	C25-C26	16.33	1.61	1.34
28	6	304	C7Z	C25-C26	16.29	1.61	1.34
22	7	305	BCR	C26-C25	16.13	1.61	1.34
22	B	846	BCR	C26-C25	15.98	1.61	1.34
22	B	844	BCR	C26-C25	15.98	1.61	1.34
27	F	304	RRX	C26-C25	15.98	1.61	1.34
27	4	303	RRX	C26-C25	15.94	1.61	1.34
22	F	302	BCR	C26-C25	15.90	1.61	1.34
22	B	842	BCR	C26-C25	15.90	1.61	1.34
22	A	846	BCR	C26-C25	15.89	1.61	1.34
22	A	858	BCR	C26-C25	15.88	1.61	1.34
22	K	206	BCR	C26-C25	15.84	1.61	1.34
22	A	859	BCR	C26-C25	15.80	1.61	1.34
22	6	307	BCR	C26-C25	15.77	1.60	1.34
22	A	848	BCR	C26-C25	15.76	1.60	1.34
22	5	305	BCR	C26-C25	15.74	1.60	1.34
22	A	847	BCR	C26-C25	15.70	1.60	1.34
22	G	1603	BCR	C26-C25	15.70	1.60	1.34
22	5	304	BCR	C26-C25	15.69	1.60	1.34
22	A	850	BCR	C26-C25	15.64	1.60	1.34
22	B	845	BCR	C26-C25	15.63	1.60	1.34
22	3	5007	BCR	C26-C25	15.62	1.60	1.34
22	B	843	BCR	C26-C25	15.62	1.60	1.34
27	5	302	RRX	C26-C25	15.61	1.60	1.34
22	6	308	BCR	C26-C25	15.59	1.60	1.34
22	B	847	BCR	C26-C25	15.56	1.60	1.34
28	J	1902	C7Z	C5-C6	15.55	1.60	1.34
22	8	303	BCR	C26-C25	15.53	1.60	1.34
22	3	5004	BCR	C26-C25	15.48	1.60	1.34
28	1	5005	C7Z	C5-C6	15.47	1.60	1.34
22	A	849	BCR	C26-C25	15.41	1.60	1.34
22	3	5006	BCR	C26-C25	15.40	1.60	1.34
31	7	303	LUT	C5-C6	15.34	1.60	1.34
28	6	304	C7Z	C5-C6	15.32	1.60	1.34
31	5	303	LUT	C5-C6	15.28	1.60	1.34
22	4	305	BCR	C26-C25	15.27	1.60	1.34
31	Z	318	LUT	C5-C6	15.23	1.60	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	5005	BCR	C26-C25	15.22	1.60	1.34
31	1	5003	LUT	C5-C6	15.22	1.60	1.34
22	8	306	BCR	C26-C25	15.16	1.59	1.34
31	Z	317	LUT	C5-C6	15.16	1.59	1.34
31	1	5004	LUT	C5-C6	15.12	1.59	1.34
31	8	305	LUT	C5-C6	15.12	1.59	1.34
31	3	5003	LUT	C5-C6	15.11	1.59	1.34
31	8	304	LUT	C5-C6	15.09	1.59	1.34
31	6	305	LUT	C5-C6	15.02	1.59	1.34
31	3	5002	LUT	C5-C6	15.01	1.59	1.34
31	6	306	LUT	C5-C6	14.99	1.59	1.34
31	7	304	LUT	C5-C6	14.95	1.59	1.34
31	4	304	LUT	C5-C6	14.92	1.59	1.34
27	F	304	RRX	C5-C6	14.84	1.59	1.34
22	B	846	BCR	C5-C6	14.56	1.58	1.34
22	F	302	BCR	C5-C6	14.54	1.58	1.34
22	A	846	BCR	C5-C6	14.53	1.58	1.34
22	B	847	BCR	C5-C6	14.53	1.58	1.34
22	B	844	BCR	C5-C6	14.52	1.58	1.34
22	A	847	BCR	C5-C6	14.49	1.58	1.34
22	3	5006	BCR	C5-C6	14.41	1.58	1.34
22	6	307	BCR	C5-C6	14.36	1.58	1.34
27	5	302	RRX	C5-C6	14.34	1.58	1.34
22	B	842	BCR	C5-C6	14.34	1.58	1.34
22	A	849	BCR	C5-C6	14.33	1.58	1.34
22	G	1603	BCR	C5-C6	14.32	1.58	1.34
22	K	206	BCR	C5-C6	14.30	1.58	1.34
22	A	859	BCR	C5-C6	14.29	1.58	1.34
22	8	306	BCR	C5-C6	14.29	1.58	1.34
22	B	843	BCR	C5-C6	14.25	1.58	1.34
22	5	305	BCR	C5-C6	14.25	1.58	1.34
22	A	858	BCR	C5-C6	14.24	1.58	1.34
22	B	845	BCR	C5-C6	14.22	1.58	1.34
22	A	850	BCR	C5-C6	14.20	1.58	1.34
22	8	303	BCR	C5-C6	14.20	1.58	1.34
22	7	305	BCR	C5-C6	14.18	1.58	1.34
22	A	848	BCR	C5-C6	14.16	1.58	1.34
22	6	308	BCR	C5-C6	14.16	1.58	1.34
22	5	304	BCR	C5-C6	14.15	1.58	1.34
27	4	303	RRX	C5-C6	14.13	1.58	1.34
22	4	305	BCR	C5-C6	14.12	1.58	1.34
22	3	5007	BCR	C5-C6	14.01	1.58	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	304	LUT	C22-C21	-13.95	1.37	1.54
22	3	5004	BCR	C5-C6	13.94	1.57	1.34
31	1	5003	LUT	C22-C21	-13.93	1.37	1.54
31	7	303	LUT	C22-C21	-13.80	1.37	1.54
22	3	5005	BCR	C5-C6	13.80	1.57	1.34
31	1	5004	LUT	C22-C21	-13.63	1.38	1.54
31	Z	318	LUT	C22-C21	-13.62	1.38	1.54
31	8	305	LUT	C22-C21	-13.60	1.38	1.54
31	3	5002	LUT	C22-C21	-13.59	1.38	1.54
31	6	305	LUT	C22-C21	-13.56	1.38	1.54
31	4	304	LUT	C22-C21	-13.52	1.38	1.54
31	3	5003	LUT	C22-C21	-13.42	1.38	1.54
31	6	306	LUT	C22-C21	-13.20	1.38	1.54
31	7	304	LUT	C22-C21	-13.19	1.38	1.54
31	Z	317	LUT	C22-C21	-13.10	1.38	1.54
31	5	303	LUT	C22-C21	-13.07	1.38	1.54
38	6	326	ERG	C7-C8	12.76	1.63	1.34
38	8	325	ERG	C7-C8	12.52	1.63	1.34
31	7	303	LUT	C2-C3	-12.21	1.35	1.52
31	Z	317	LUT	C22-C23	12.15	1.66	1.52
31	5	303	LUT	C2-C3	-12.09	1.35	1.52
31	5	303	LUT	C22-C23	11.98	1.66	1.52
31	7	304	LUT	C22-C23	11.94	1.66	1.52
31	1	5003	LUT	C2-C3	-11.92	1.35	1.52
31	8	305	LUT	C2-C3	-11.91	1.35	1.52
31	6	306	LUT	C22-C23	11.90	1.66	1.52
27	4	303	RRX	C29-C28	-11.85	1.35	1.52
31	Z	318	LUT	C22-C23	11.79	1.66	1.52
31	3	5003	LUT	C22-C23	11.79	1.66	1.52
31	6	305	LUT	C2-C3	-11.78	1.35	1.52
31	6	306	LUT	C2-C3	-11.74	1.35	1.52
31	1	5004	LUT	C2-C3	-11.73	1.35	1.52
31	3	5003	LUT	C2-C3	-11.66	1.35	1.52
28	1	5005	C7Z	C24-C23	11.66	1.72	1.52
28	J	1902	C7Z	C24-C23	11.61	1.72	1.52
31	8	304	LUT	C2-C3	-11.58	1.35	1.52
31	4	304	LUT	C2-C3	-11.58	1.35	1.52
28	6	304	C7Z	C24-C23	11.51	1.72	1.52
31	3	5002	LUT	C2-C3	-11.49	1.36	1.52
27	5	302	RRX	C29-C28	-11.44	1.36	1.52
31	8	304	LUT	C22-C23	11.42	1.65	1.52
31	Z	317	LUT	C2-C3	-11.39	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	5004	LUT	C22-C23	11.38	1.65	1.52
31	Z	318	LUT	C2-C3	-11.38	1.36	1.52
31	3	5002	LUT	C22-C23	11.36	1.65	1.52
31	7	303	LUT	C22-C23	11.36	1.65	1.52
31	6	305	LUT	C22-C23	11.32	1.65	1.52
28	1	5005	C7Z	C22-C23	-11.27	1.36	1.52
31	4	304	LUT	C22-C23	11.26	1.65	1.52
31	8	305	LUT	C22-C23	11.24	1.65	1.52
28	J	1902	C7Z	C22-C23	-11.14	1.36	1.52
28	6	304	C7Z	C22-C23	-11.09	1.36	1.52
31	1	5003	LUT	C22-C23	10.99	1.65	1.52
31	7	304	LUT	C2-C3	-10.99	1.36	1.52
28	1	5005	C7Z	C2-C3	-10.57	1.37	1.52
27	F	304	RRX	C29-C28	-10.44	1.37	1.52
38	8	325	ERG	C13-C14	-10.27	1.39	1.56
32	8	319	CHL	C3A-C2A	-10.10	1.46	1.54
32	5	316	CHL	C3A-C2A	-9.99	1.46	1.54
28	J	1902	C7Z	C2-C3	-9.97	1.38	1.52
28	6	304	C7Z	C2-C3	-9.96	1.38	1.52
38	6	326	ERG	C13-C14	-9.95	1.39	1.56
32	3	5017	CHL	C3A-C2A	-9.15	1.46	1.54
18	A	801	CL0	C1D-C2D	9.09	1.49	1.39
18	A	801	CL0	C1B-C2B	9.07	1.49	1.39
18	A	801	CL0	C1A-CHA	9.06	1.50	1.40
32	Z	310	CHL	C3A-C2A	-8.76	1.47	1.54
32	4	317	CHL	C3A-C2A	-8.61	1.47	1.54
28	6	304	C7Z	C4-C3	8.46	1.67	1.52
22	3	5005	BCR	C30-C25	-8.26	1.43	1.53
28	J	1902	C7Z	C4-C3	8.24	1.66	1.52
32	4	314	CHL	C3A-C2A	-8.15	1.47	1.54
31	4	304	LUT	C1-C6	-8.15	1.43	1.53
22	8	306	BCR	C30-C25	-8.10	1.43	1.53
22	6	308	BCR	C30-C25	-8.10	1.43	1.53
27	F	304	RRX	C27-C28	8.09	1.66	1.52
22	3	5005	BCR	C1-C6	-8.09	1.43	1.53
28	1	5005	C7Z	C4-C3	7.91	1.66	1.52
22	3	5004	BCR	C30-C25	-7.89	1.43	1.53
27	4	303	RRX	C27-C28	7.87	1.66	1.52
22	8	303	BCR	C30-C25	-7.86	1.43	1.53
19	8	312	CLA	MG-NA	7.83	2.24	2.06
22	4	305	BCR	C1-C6	-7.78	1.43	1.53
22	5	304	BCR	C30-C25	-7.77	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	849	BCR	C30-C25	-7.76	1.43	1.53
27	5	302	RRX	C27-C28	7.74	1.65	1.52
31	7	304	LUT	C4-C3	7.74	1.65	1.52
31	3	5003	LUT	C4-C3	7.74	1.65	1.52
32	6	321	CHL	C3A-C2A	-7.73	1.48	1.54
32	8	317	CHL	C3A-C2A	-7.73	1.48	1.54
22	8	306	BCR	C1-C6	-7.72	1.43	1.53
22	5	305	BCR	C30-C25	-7.71	1.43	1.53
31	Z	318	LUT	C4-C3	7.68	1.65	1.52
31	4	304	LUT	C4-C3	7.67	1.65	1.52
22	3	5006	BCR	C30-C25	-7.60	1.44	1.53
22	4	305	BCR	C30-C25	-7.60	1.44	1.53
31	Z	318	LUT	C1-C6	-7.60	1.44	1.53
31	Z	317	LUT	C4-C3	7.57	1.65	1.52
22	G	1603	BCR	C30-C25	-7.56	1.44	1.53
22	5	304	BCR	C1-C6	-7.56	1.44	1.53
31	6	306	LUT	C32-C33	7.56	1.62	1.46
27	4	303	RRX	C30-C25	-7.55	1.44	1.53
31	6	305	LUT	C1-C6	-7.54	1.44	1.53
31	3	5003	LUT	C32-C33	7.53	1.62	1.46
31	8	305	LUT	C1-C6	-7.53	1.44	1.53
19	4	311	CLA	MG-NA	7.53	2.24	2.06
32	8	315	CHL	C3A-C2A	-7.53	1.48	1.54
31	8	304	LUT	C32-C33	7.53	1.62	1.46
22	6	307	BCR	C30-C25	-7.52	1.44	1.53
31	7	304	LUT	C32-C33	7.52	1.62	1.46
32	6	315	CHL	C3A-C2A	-7.51	1.48	1.54
31	3	5003	LUT	C1-C6	-7.50	1.44	1.53
22	K	206	BCR	C30-C25	-7.48	1.44	1.53
32	Z	313	CHL	C3A-C2A	-7.48	1.48	1.54
31	7	303	LUT	C1-C6	-7.47	1.44	1.53
22	A	850	BCR	C30-C25	-7.46	1.44	1.53
22	A	849	BCR	C1-C6	-7.46	1.44	1.53
31	3	5002	LUT	C1-C6	-7.45	1.44	1.53
22	A	858	BCR	C30-C25	-7.45	1.44	1.53
31	Z	317	LUT	C32-C33	7.43	1.61	1.46
22	B	842	BCR	C30-C25	-7.43	1.44	1.53
22	B	843	BCR	C30-C25	-7.42	1.44	1.53
31	1	5004	LUT	C4-C3	7.40	1.65	1.52
31	5	303	LUT	C1-C6	-7.39	1.44	1.53
31	6	305	LUT	C4-C3	7.39	1.65	1.52
22	6	307	BCR	C1-C6	-7.36	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	5007	BCR	C30-C25	-7.36	1.44	1.53
22	A	847	BCR	C30-C25	-7.35	1.44	1.53
22	5	305	BCR	C1-C6	-7.35	1.44	1.53
22	A	848	BCR	C30-C25	-7.33	1.44	1.53
22	B	845	BCR	C30-C25	-7.33	1.44	1.53
31	7	303	LUT	C4-C3	7.32	1.65	1.52
27	5	302	RRX	C30-C25	-7.32	1.44	1.53
22	B	846	BCR	C30-C25	-7.31	1.44	1.53
31	8	304	LUT	C1-C6	-7.30	1.44	1.53
22	B	847	BCR	C30-C25	-7.30	1.44	1.53
22	3	5004	BCR	C1-C6	-7.30	1.44	1.53
22	8	306	BCR	C2-C3	-7.29	1.35	1.52
22	A	848	BCR	C1-C6	-7.28	1.44	1.53
22	6	308	BCR	C1-C6	-7.26	1.44	1.53
32	8	316	CHL	C3A-C2A	-7.25	1.48	1.54
22	F	302	BCR	C30-C25	-7.25	1.44	1.53
31	3	5002	LUT	C4-C3	7.24	1.64	1.52
31	8	304	LUT	C4-C3	7.24	1.64	1.52
22	A	859	BCR	C30-C25	-7.22	1.44	1.53
31	3	5002	LUT	C32-C33	7.22	1.61	1.46
31	7	304	LUT	C1-C6	-7.22	1.44	1.53
31	1	5004	LUT	C1-C6	-7.21	1.44	1.53
22	5	304	BCR	C2-C3	-7.19	1.35	1.52
31	8	305	LUT	C4-C3	7.18	1.64	1.52
22	A	846	BCR	C30-C25	-7.18	1.44	1.53
31	Z	318	LUT	C32-C33	7.17	1.61	1.46
22	A	859	BCR	C1-C6	-7.14	1.44	1.53
22	6	308	BCR	C2-C3	-7.14	1.35	1.52
27	5	302	RRX	C2-C3	-7.13	1.35	1.52
31	6	306	LUT	C1-C6	-7.13	1.44	1.53
22	A	850	BCR	C1-C6	-7.12	1.44	1.53
22	5	305	BCR	C2-C3	-7.12	1.35	1.52
22	3	5004	BCR	C2-C3	-7.12	1.35	1.52
18	A	801	CL0	C3B-C4B	7.11	1.48	1.41
31	1	5003	LUT	C4-C3	7.10	1.64	1.52
27	4	303	RRX	C2-C3	-7.08	1.35	1.52
31	1	5003	LUT	C1-C6	-7.08	1.44	1.53
31	6	306	LUT	C4-C3	7.08	1.64	1.52
22	4	305	BCR	C2-C3	-7.08	1.35	1.52
31	5	303	LUT	C4-C3	7.07	1.64	1.52
22	6	307	BCR	C2-C3	-7.06	1.35	1.52
22	A	847	BCR	C2-C3	-7.04	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	6	316	CHL	C3A-C2A	-7.04	1.48	1.54
38	6	326	ERG	C16-C17	-7.04	1.40	1.54
22	8	303	BCR	C1-C6	-7.04	1.44	1.53
31	Z	317	LUT	C1-C6	-7.04	1.44	1.53
22	3	5005	BCR	C2-C3	-7.03	1.35	1.52
22	B	844	BCR	C2-C3	-7.03	1.35	1.52
22	B	844	BCR	C30-C25	-7.00	1.44	1.53
22	7	305	BCR	C30-C25	-6.98	1.44	1.53
22	F	302	BCR	C2-C3	-6.98	1.36	1.52
32	6	317	CHL	C3A-C2A	-6.97	1.48	1.54
31	4	304	LUT	C32-C33	6.95	1.60	1.46
31	1	5003	LUT	C32-C33	6.94	1.60	1.46
27	F	304	RRX	C30-C25	-6.94	1.44	1.53
22	B	843	BCR	C1-C6	-6.93	1.44	1.53
22	K	206	BCR	C1-C6	-6.93	1.44	1.53
22	B	844	BCR	C1-C6	-6.92	1.44	1.53
22	B	842	BCR	C2-C3	-6.92	1.36	1.52
22	G	1603	BCR	C2-C3	-6.92	1.36	1.52
22	3	5007	BCR	C1-C6	-6.91	1.44	1.53
22	3	5006	BCR	C1-C6	-6.90	1.45	1.53
22	3	5007	BCR	C29-C28	-6.89	1.36	1.52
22	7	305	BCR	C1-C6	-6.88	1.45	1.53
22	A	846	BCR	C2-C3	-6.88	1.36	1.52
31	6	305	LUT	C32-C33	6.87	1.60	1.46
22	A	858	BCR	C1-C6	-6.87	1.45	1.53
31	1	5004	LUT	C32-C33	6.86	1.60	1.46
22	5	305	BCR	C29-C28	-6.85	1.36	1.52
22	G	1603	BCR	C1-C6	-6.84	1.45	1.53
22	B	845	BCR	C1-C6	-6.83	1.45	1.53
27	F	304	RRX	C2-C3	-6.83	1.36	1.52
22	6	308	BCR	C29-C28	-6.82	1.36	1.52
22	A	849	BCR	C2-C3	-6.82	1.36	1.52
22	B	843	BCR	C2-C3	-6.82	1.36	1.52
22	B	847	BCR	C2-C3	-6.82	1.36	1.52
22	B	846	BCR	C2-C3	-6.81	1.36	1.52
38	8	325	ERG	C16-C17	-6.80	1.40	1.54
22	K	206	BCR	C2-C3	-6.80	1.36	1.52
22	5	304	BCR	C29-C28	-6.79	1.36	1.52
22	3	5004	BCR	C29-C28	-6.79	1.36	1.52
31	5	303	LUT	C32-C33	6.79	1.60	1.46
22	A	859	BCR	C2-C3	-6.78	1.36	1.52
31	7	303	LUT	C32-C33	6.77	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	303	BCR	C2-C3	-6.77	1.36	1.52
22	A	858	BCR	C2-C3	-6.76	1.36	1.52
22	6	307	BCR	C29-C28	-6.75	1.36	1.52
22	B	842	BCR	C1-C6	-6.74	1.45	1.53
22	F	302	BCR	C1-C6	-6.74	1.45	1.53
22	A	848	BCR	C2-C3	-6.72	1.36	1.52
22	3	5006	BCR	C2-C3	-6.71	1.36	1.52
22	4	305	BCR	C29-C28	-6.69	1.36	1.52
22	B	845	BCR	C2-C3	-6.68	1.36	1.52
32	Z	302	CHL	C3A-C2A	-6.67	1.48	1.54
22	A	846	BCR	C1-C6	-6.67	1.45	1.53
22	A	850	BCR	C2-C3	-6.67	1.36	1.52
31	8	305	LUT	C32-C33	6.66	1.60	1.46
27	4	303	RRX	C1-C6	-6.66	1.45	1.53
19	4	307	CLA	MG-NA	6.66	2.22	2.06
22	B	844	BCR	C29-C28	-6.65	1.36	1.52
22	A	849	BCR	C29-C28	-6.63	1.36	1.52
22	B	846	BCR	C29-C28	-6.62	1.36	1.52
22	3	5007	BCR	C2-C3	-6.62	1.36	1.52
22	3	5005	BCR	C29-C28	-6.61	1.36	1.52
22	A	846	BCR	C29-C28	-6.60	1.36	1.52
22	7	305	BCR	C2-C3	-6.60	1.36	1.52
22	A	847	BCR	C1-C6	-6.60	1.45	1.53
22	K	206	BCR	C29-C28	-6.59	1.37	1.52
22	A	859	BCR	C29-C28	-6.59	1.37	1.52
22	7	305	BCR	C29-C28	-6.57	1.37	1.52
22	F	302	BCR	C29-C28	-6.55	1.37	1.52
22	B	842	BCR	C29-C28	-6.54	1.37	1.52
22	8	306	BCR	C29-C28	-6.54	1.37	1.52
22	A	848	BCR	C29-C28	-6.52	1.37	1.52
38	6	326	ERG	C12-C11	-6.51	1.40	1.53
22	G	1603	BCR	C29-C28	-6.50	1.37	1.52
22	A	858	BCR	C29-C28	-6.48	1.37	1.52
22	A	847	BCR	C29-C28	-6.47	1.37	1.52
38	6	326	ERG	C7-C6	6.45	1.58	1.41
22	8	303	BCR	C29-C28	-6.42	1.37	1.52
22	B	845	BCR	C29-C28	-6.42	1.37	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	846	BCR	C1-C6	-6.37	1.45	1.53
22	A	850	BCR	C29-C28	-6.34	1.37	1.52
19	A	832	CLA	MG-NA	6.34	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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
19	B	807	CLA	MG-NA	6.31	2.21	2.06
19	A	820	CLA	MG-NA	6.31	2.21	2.06
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
19	1	5018	CLA	MG-NA	6.30	2.21	2.06
19	A	834	CLA	MG-NA	6.30	2.21	2.06
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
19	A	809	CLA	MG-NA	6.29	2.21	2.06
19	G	1601	CLA	MG-NA	6.29	2.21	2.06
32	7	314	CHL	C3A-C2A	-6.29	1.49	1.54
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
22	3	5006	BCR	C29-C28	-6.29	1.37	1.52
19	K	204	CLA	MG-NA	6.29	2.21	2.06
19	A	826	CLA	MG-NA	6.29	2.21	2.06
22	B	843	BCR	C29-C28	-6.29	1.37	1.52
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
19	6	314	CLA	MG-NA	6.27	2.21	2.06
19	A	833	CLA	MG-NA	6.27	2.21	2.06
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
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
38	8	325	ERG	C7-C6	6.26	1.58	1.41
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
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
22	B	847	BCR	C29-C28	-6.23	1.37	1.52
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	B	847	BCR	C1-C6	-6.22	1.45	1.53
38	8	325	ERG	C12-C11	-6.22	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
19	A	843	CLA	MG-NA	6.21	2.21	2.06
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
19	1	5011	CLA	MG-NA	6.20	2.21	2.06
19	A	839	CLA	MG-NA	6.20	2.21	2.06
19	A	830	CLA	MG-NA	6.20	2.21	2.06
27	5	302	RRX	C1-C6	-6.20	1.45	1.53
19	B	815	CLA	MG-NA	6.20	2.21	2.06
19	A	838	CLA	MG-NA	6.19	2.21	2.06
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
22	8	303	BCR	C12-C13	6.18	1.59	1.46
19	A	835	CLA	MG-NA	6.18	2.21	2.06
19	B	808	CLA	MG-NA	6.18	2.20	2.06
19	8	313	CLA	MG-NA	6.16	2.20	2.06
19	4	308	CLA	MG-NA	6.16	2.20	2.06
19	6	309	CLA	MG-NA	6.15	2.20	2.06
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	840	CLA	MG-NA	6.09	2.20	2.06
19	1	5008	CLA	MG-NA	6.08	2.20	2.06
32	6	319	CHL	C3A-C2A	-6.08	1.49	1.54
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
19	5	314	CLA	MG-NA	6.07	2.20	2.06
19	Z	304	CLA	MG-NA	6.06	2.20	2.06
19	Z	303	CLA	MG-NA	6.05	2.20	2.06
28	6	304	C7Z	C12-C13	6.05	1.58	1.46
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
19	6	313	CLA	MG-NA	6.03	2.20	2.06
19	A	810	CLA	MG-NA	6.02	2.20	2.06
19	5	308	CLA	MG-NA	6.02	2.20	2.06
19	5	313	CLA	MG-NA	6.02	2.20	2.06
19	8	309	CLA	MG-NA	6.02	2.20	2.06
38	8	325	ERG	C6-C5	6.01	1.48	1.34
19	6	311	CLA	MG-NA	6.01	2.20	2.06
28	6	304	C7Z	C1-C6	-6.01	1.46	1.53
28	J	1902	C7Z	C12-C13	6.00	1.58	1.46
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
19	6	322	CLA	MG-NA	5.98	2.20	2.06
19	B	850	CLA	MG-NA	5.98	2.20	2.06
27	F	304	RRX	C19-C18	5.98	1.58	1.46
19	1	5015	CLA	MG-NA	5.97	2.20	2.06
19	7	316	CLA	MG-NA	5.97	2.20	2.06
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
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
19	3	5015	CLA	MG-NA	5.92	2.20	2.06
19	Z	305	CLA	MG-NA	5.92	2.20	2.06
38	6	326	ERG	C6-C5	5.92	1.48	1.34
19	8	307	CLA	MG-NA	5.92	2.20	2.06
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
22	3	5006	BCR	C12-C13	5.91	1.58	1.46
19	Z	311	CLA	MG-NA	5.90	2.20	2.06
19	6	301	CLA	MG-NA	5.89	2.20	2.06
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
22	A	850	BCR	C12-C13	5.87	1.58	1.46
19	1	5013	CLA	MG-NA	5.87	2.20	2.06
19	A	815	CLA	MG-NA	5.87	2.20	2.06
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	5.85	1.58	1.46
22	B	843	BCR	C12-C13	5.84	1.58	1.46
27	F	304	RRX	C1-C6	-5.82	1.46	1.53
22	4	305	BCR	C12-C13	5.81	1.58	1.46
19	Z	308	CLA	MG-NA	5.81	2.20	2.06
22	B	847	BCR	C12-C13	5.80	1.58	1.46
19	1	5007	CLA	MG-NA	5.80	2.20	2.06
22	A	859	BCR	C12-C13	5.80	1.58	1.46
28	1	5005	C7Z	C12-C13	5.80	1.58	1.46
19	B	836	CLA	MG-NA	5.80	2.20	2.06
22	B	842	BCR	C12-C13	5.78	1.58	1.46
19	5	317	CLA	MG-NA	5.77	2.20	2.06
22	A	858	BCR	C12-C13	5.77	1.58	1.46
22	B	845	BCR	C12-C13	5.77	1.58	1.46
19	B	831	CLA	MG-NA	5.75	2.19	2.06
19	4	309	CLA	MG-NA	5.75	2.19	2.06
22	A	847	BCR	C12-C13	5.75	1.58	1.46
28	1	5005	C7Z	C1-C6	-5.75	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	846	BCR	C12-C13	5.71	1.58	1.46
22	F	302	BCR	C12-C13	5.70	1.58	1.46
22	A	848	BCR	C12-C13	5.70	1.58	1.46
22	3	5007	BCR	C12-C13	5.66	1.58	1.46
32	4	315	CHL	C3A-C2A	-5.66	1.49	1.54
22	B	844	BCR	C8-C9	5.64	1.58	1.46
22	6	308	BCR	C12-C13	5.63	1.58	1.46
22	G	1603	BCR	C12-C13	5.62	1.58	1.46
22	8	303	BCR	C8-C9	5.62	1.58	1.46
27	5	302	RRX	C19-C18	5.61	1.58	1.46
22	K	206	BCR	C12-C13	5.61	1.58	1.46
22	5	305	BCR	C12-C13	5.59	1.57	1.46
22	B	843	BCR	C8-C9	5.56	1.57	1.46
22	B	846	BCR	C12-C13	5.55	1.57	1.46
22	8	306	BCR	C12-C13	5.54	1.57	1.46
22	6	307	BCR	C12-C13	5.54	1.57	1.46
22	A	850	BCR	C8-C9	5.54	1.57	1.46
22	B	845	BCR	C8-C9	5.53	1.57	1.46
22	A	858	BCR	C8-C9	5.52	1.57	1.46
22	5	304	BCR	C12-C13	5.52	1.57	1.46
22	B	843	BCR	C23-C22	5.52	1.57	1.46
22	A	849	BCR	C12-C13	5.51	1.57	1.46
22	B	847	BCR	C8-C9	5.51	1.57	1.46
32	5	318	CHL	C3A-C2A	-5.51	1.50	1.54
22	3	5006	BCR	C8-C9	5.51	1.57	1.46
22	B	842	BCR	C8-C9	5.50	1.57	1.46
38	6	326	ERG	C12-C13	5.49	1.63	1.54
27	4	303	RRX	C19-C18	5.48	1.57	1.46
32	1	5009	CHL	C3B-C4B	5.48	1.46	1.41
22	7	305	BCR	C12-C13	5.47	1.57	1.46
22	F	302	BCR	C8-C9	5.46	1.57	1.46
22	A	848	BCR	C8-C9	5.45	1.57	1.46
22	A	859	BCR	C8-C9	5.45	1.57	1.46
28	J	1902	C7Z	C1-C6	-5.45	1.46	1.53
22	B	842	BCR	C23-C22	5.45	1.57	1.46
22	3	5004	BCR	C12-C13	5.45	1.57	1.46
22	A	846	BCR	C8-C9	5.44	1.57	1.46
22	B	843	BCR	C29-C30	5.40	1.66	1.54
22	4	305	BCR	C8-C9	5.39	1.57	1.46
22	B	847	BCR	C29-C30	5.39	1.66	1.54
22	5	304	BCR	C8-C9	5.39	1.57	1.46
22	A	847	BCR	C8-C9	5.39	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	850	BCR	C29-C30	5.38	1.66	1.54
22	K	206	BCR	C8-C9	5.38	1.57	1.46
18	A	801	CL0	CHC-C4B	5.37	1.48	1.39
22	3	5007	BCR	C23-C22	5.37	1.57	1.46
22	B	847	BCR	C23-C22	5.36	1.57	1.46
18	A	801	CL0	CHB-C1B	5.36	1.48	1.39
22	3	5006	BCR	C29-C30	5.35	1.66	1.54
22	G	1603	BCR	C8-C9	5.35	1.57	1.46
22	8	303	BCR	C23-C22	5.35	1.57	1.46
22	6	307	BCR	C8-C9	5.34	1.57	1.46
18	A	801	CL0	O2A-C1	5.34	1.60	1.46
22	A	858	BCR	C29-C30	5.34	1.66	1.54
22	A	859	BCR	C29-C30	5.32	1.66	1.54
32	1	5017	CHL	C3A-C2A	-5.32	1.50	1.54
22	F	302	BCR	C23-C22	5.32	1.57	1.46
22	3	5007	BCR	C8-C9	5.32	1.57	1.46
22	B	844	BCR	C23-C22	5.31	1.57	1.46
22	A	858	BCR	C23-C22	5.31	1.57	1.46
22	B	844	BCR	C29-C30	5.31	1.66	1.54
22	A	847	BCR	C29-C30	5.30	1.66	1.54
22	B	845	BCR	C29-C30	5.30	1.66	1.54
22	6	308	BCR	C8-C9	5.30	1.57	1.46
22	A	850	BCR	C23-C22	5.30	1.57	1.46
32	Z	309	CHL	C3A-C2A	-5.30	1.50	1.54
22	A	846	BCR	C29-C30	5.29	1.66	1.54
22	A	859	BCR	C23-C22	5.28	1.57	1.46
22	B	846	BCR	C23-C22	5.28	1.57	1.46
22	A	846	BCR	C23-C22	5.27	1.57	1.46
22	7	305	BCR	C29-C30	5.27	1.66	1.54
22	7	305	BCR	C8-C9	5.27	1.57	1.46
22	A	848	BCR	C29-C30	5.27	1.66	1.54
22	B	846	BCR	C8-C9	5.27	1.57	1.46
22	G	1603	BCR	C23-C22	5.26	1.57	1.46
22	7	305	BCR	C23-C22	5.26	1.57	1.46
22	F	302	BCR	C29-C30	5.26	1.66	1.54
22	4	305	BCR	C29-C30	5.25	1.66	1.54
22	3	5006	BCR	C23-C22	5.25	1.57	1.46
22	3	5005	BCR	C12-C13	5.24	1.57	1.46
22	A	849	BCR	C8-C9	5.23	1.57	1.46
32	Z	302	CHL	C3B-C4B	5.23	1.46	1.41
22	K	206	BCR	C29-C30	5.23	1.66	1.54
22	B	845	BCR	C23-C22	5.22	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	848	BCR	C23-C22	5.22	1.57	1.46
22	A	847	BCR	C23-C22	5.22	1.57	1.46
22	8	303	BCR	C29-C30	5.21	1.66	1.54
31	3	5002	LUT	C4-C5	-5.21	1.42	1.51
22	G	1603	BCR	C29-C30	5.21	1.66	1.54
32	6	315	CHL	C1A-CHA	-5.20	1.34	1.40
22	8	306	BCR	C8-C9	5.20	1.57	1.46
22	B	846	BCR	C29-C30	5.20	1.66	1.54
31	8	304	LUT	C4-C5	-5.18	1.43	1.51
22	K	206	BCR	C23-C22	5.18	1.57	1.46
22	A	849	BCR	C29-C30	5.17	1.65	1.54
31	8	305	LUT	C4-C5	-5.17	1.43	1.51
31	5	303	LUT	C4-C5	-5.16	1.43	1.51
22	B	842	BCR	C29-C30	5.15	1.65	1.54
22	3	5005	BCR	C29-C30	5.13	1.65	1.54
38	8	325	ERG	C12-C13	5.13	1.63	1.54
31	7	304	LUT	C4-C5	-5.11	1.43	1.51
32	7	315	CHL	C3A-C2A	-5.09	1.50	1.54
18	A	801	CL0	O2D-CGD	5.09	1.45	1.33
22	6	307	BCR	C29-C30	5.08	1.65	1.54
32	5	315	CHL	C1A-CHA	-5.08	1.34	1.40
22	3	5007	BCR	C29-C30	5.07	1.65	1.54
31	1	5003	LUT	C4-C5	-5.05	1.43	1.51
32	4	317	CHL	C3B-C4B	5.04	1.46	1.41
22	6	308	BCR	C29-C30	5.04	1.65	1.54
31	1	5004	LUT	C4-C5	-5.03	1.43	1.51
22	3	5004	BCR	C8-C9	5.03	1.56	1.46
22	3	5004	BCR	C29-C30	5.03	1.65	1.54
22	8	306	BCR	C29-C30	5.02	1.65	1.54
22	5	305	BCR	C8-C9	5.02	1.56	1.46
22	5	304	BCR	C23-C22	5.01	1.56	1.46
22	8	303	BCR	C15-C14	5.01	1.58	1.43
31	6	305	LUT	C4-C5	-5.00	1.43	1.51
22	A	849	BCR	C23-C22	5.00	1.56	1.46
32	5	316	CHL	C1A-CHA	-5.00	1.34	1.40
27	F	304	RRX	C8-C9	4.99	1.56	1.46
31	Z	317	LUT	C4-C5	-4.99	1.43	1.51
31	6	306	LUT	C4-C5	-4.99	1.43	1.51
27	F	304	RRX	C2-C1	4.98	1.65	1.54
22	5	305	BCR	C23-C22	4.98	1.56	1.46
22	5	305	BCR	C29-C30	4.98	1.65	1.54
32	7	314	CHL	C1A-CHA	-4.97	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	847	BCR	C15-C14	4.97	1.58	1.43
22	6	307	BCR	C23-C22	4.96	1.56	1.46
28	6	304	C7Z	C24-C25	-4.95	1.43	1.51
31	7	303	LUT	C4-C5	-4.95	1.43	1.51
27	5	302	RRX	C2-C1	4.95	1.65	1.54
32	1	5009	CHL	C1A-CHA	-4.93	1.34	1.40
22	B	842	BCR	C15-C14	4.93	1.58	1.43
31	Z	317	LUT	C8-C9	4.93	1.56	1.46
31	3	5003	LUT	C4-C5	-4.92	1.43	1.51
32	4	319	CHL	C3A-C2A	-4.91	1.50	1.54
22	B	843	BCR	C15-C14	4.91	1.58	1.43
22	8	303	BCR	C19-C18	4.90	1.56	1.46
32	Z	310	CHL	C1A-CHA	-4.90	1.34	1.40
22	A	850	BCR	C15-C14	4.90	1.58	1.43
32	5	315	CHL	C3B-C4B	4.89	1.46	1.41
22	B	846	BCR	C19-C18	4.88	1.56	1.46
22	B	844	BCR	C15-C14	4.88	1.58	1.43
27	F	304	RRX	C23-C22	4.87	1.56	1.46
22	A	859	BCR	C15-C14	4.86	1.58	1.43
31	4	304	LUT	C4-C5	-4.86	1.43	1.51
22	A	846	BCR	C15-C14	4.86	1.58	1.43
22	3	5007	BCR	C2-C1	4.85	1.65	1.54
31	Z	317	LUT	C12-C13	4.85	1.56	1.46
22	A	858	BCR	C15-C14	4.85	1.58	1.43
18	A	801	CL0	CHD-C1D	4.84	1.47	1.39
22	5	304	BCR	C15-C14	4.84	1.58	1.43
22	5	304	BCR	C29-C30	4.84	1.65	1.54
22	4	305	BCR	C15-C14	4.84	1.58	1.43
28	1	5005	C7Z	C24-C25	-4.83	1.43	1.51
22	4	305	BCR	C23-C22	4.83	1.56	1.46
18	A	801	CL0	OBD-CAD	4.82	1.28	1.22
22	3	5006	BCR	C15-C14	4.82	1.58	1.43
28	J	1902	C7Z	C24-C25	-4.82	1.43	1.51
22	6	308	BCR	C15-C14	4.81	1.58	1.43
22	F	302	BCR	C15-C14	4.81	1.58	1.43
32	1	5014	CHL	C3A-C2A	-4.80	1.50	1.54
22	A	848	BCR	C15-C14	4.80	1.58	1.43
22	3	5005	BCR	C8-C9	4.79	1.56	1.46
22	B	845	BCR	C15-C14	4.79	1.58	1.43
22	K	206	BCR	C15-C14	4.79	1.58	1.43
22	6	308	BCR	C23-C22	4.78	1.56	1.46
18	A	801	CL0	C3B-C2B	4.78	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	307	BCR	C15-C14	4.78	1.58	1.43
22	B	842	BCR	C19-C18	4.77	1.56	1.46
22	A	849	BCR	C15-C14	4.77	1.58	1.43
22	A	847	BCR	C15-C14	4.77	1.58	1.43
32	6	321	CHL	C1A-CHA	-4.76	1.34	1.40
32	5	318	CHL	C1A-CHA	-4.76	1.34	1.40
22	G	1603	BCR	C15-C14	4.76	1.57	1.43
27	F	304	RRX	C24-C25	4.75	1.61	1.45
22	3	5005	BCR	C23-C22	4.75	1.56	1.46
22	B	846	BCR	C15-C14	4.75	1.57	1.43
22	B	846	BCR	C2-C1	4.75	1.65	1.54
32	Z	313	CHL	C1A-CHA	-4.74	1.34	1.40
27	5	302	RRX	C8-C9	4.74	1.56	1.46
31	8	304	LUT	C31-C30	4.74	1.57	1.43
22	3	5007	BCR	C15-C14	4.74	1.57	1.43
22	A	850	BCR	C2-C1	4.74	1.64	1.54
22	A	858	BCR	C2-C1	4.72	1.64	1.54
22	B	843	BCR	C19-C18	4.72	1.56	1.46
22	7	305	BCR	C15-C14	4.72	1.57	1.43
22	A	848	BCR	C2-C1	4.71	1.64	1.54
28	6	304	C7Z	C28-C29	4.71	1.56	1.46
22	B	844	BCR	C19-C18	4.69	1.56	1.46
18	A	801	CL0	C3D-C4D	-4.69	1.34	1.41
22	8	303	BCR	C2-C1	4.69	1.64	1.54
22	B	845	BCR	C2-C1	4.69	1.64	1.54
18	A	801	CL0	CHD-C4C	4.68	1.48	1.39
22	A	850	BCR	C19-C18	4.67	1.56	1.46
27	F	304	RRX	C12-C13	4.67	1.56	1.46
32	3	5017	CHL	C1A-CHA	-4.67	1.34	1.40
22	3	5006	BCR	C2-C1	4.67	1.64	1.54
31	7	304	LUT	C12-C13	4.66	1.55	1.46
31	8	304	LUT	C8-C9	4.66	1.55	1.46
22	A	849	BCR	C2-C1	4.66	1.64	1.54
31	7	304	LUT	C8-C9	4.65	1.55	1.46
22	A	846	BCR	C19-C18	4.65	1.55	1.46
22	7	305	BCR	C2-C1	4.64	1.64	1.54
28	1	5005	C7Z	C28-C29	4.64	1.55	1.46
22	8	306	BCR	C15-C14	4.64	1.57	1.43
31	6	306	LUT	C8-C9	4.63	1.55	1.46
32	Z	302	CHL	C1A-CHA	-4.63	1.34	1.40
38	6	326	ERG	C13-C17	4.63	1.63	1.55
22	B	843	BCR	C2-C1	4.63	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Z	317	LUT	C15-C14	4.63	1.57	1.43
31	8	304	LUT	C12-C13	4.62	1.55	1.46
31	3	5003	LUT	C8-C9	4.61	1.55	1.46
31	Z	317	LUT	C35-C34	4.61	1.57	1.43
22	3	5006	BCR	C19-C18	4.61	1.55	1.46
27	4	303	RRX	C8-C9	4.61	1.55	1.46
31	Z	318	LUT	C4-C5	-4.61	1.43	1.51
22	K	206	BCR	C19-C18	4.61	1.55	1.46
22	5	305	BCR	C19-C18	4.60	1.55	1.46
22	G	1603	BCR	C19-C18	4.60	1.55	1.46
28	J	1902	C7Z	C28-C29	4.60	1.55	1.46
22	6	308	BCR	C19-C18	4.60	1.55	1.46
22	K	206	BCR	C2-C1	4.60	1.64	1.54
18	A	801	CL0	C3D-C2D	4.60	1.47	1.39
22	A	858	BCR	C19-C18	4.59	1.55	1.46
22	A	847	BCR	C19-C18	4.59	1.55	1.46
27	4	303	RRX	C2-C1	4.59	1.64	1.54
18	A	801	CL0	CHC-C1C	4.59	1.48	1.39
22	B	845	BCR	C19-C18	4.59	1.55	1.46
22	B	847	BCR	C19-C18	4.58	1.55	1.46
22	A	846	BCR	C2-C1	4.58	1.64	1.54
22	F	302	BCR	C19-C18	4.58	1.55	1.46
31	3	5003	LUT	C12-C13	4.58	1.55	1.46
22	3	5004	BCR	C15-C14	4.58	1.57	1.43
22	7	305	BCR	C19-C18	4.58	1.55	1.46
31	8	304	LUT	C15-C14	4.57	1.57	1.43
27	5	302	RRX	C24-C25	4.57	1.60	1.45
22	A	859	BCR	C19-C18	4.57	1.55	1.46
22	G	1603	BCR	C2-C1	4.56	1.64	1.54
22	4	305	BCR	C19-C18	4.56	1.55	1.46
22	5	305	BCR	C15-C14	4.56	1.57	1.43
22	B	842	BCR	C2-C1	4.56	1.64	1.54
22	F	302	BCR	C2-C1	4.56	1.64	1.54
22	A	859	BCR	C2-C1	4.56	1.64	1.54
22	8	306	BCR	C23-C22	4.56	1.55	1.46
22	5	304	BCR	C19-C18	4.54	1.55	1.46
28	1	5005	C7Z	C31-C30	4.54	1.57	1.43
28	6	304	C7Z	C31-C30	4.54	1.57	1.43
22	B	847	BCR	C2-C1	4.54	1.64	1.54
28	J	1902	C7Z	C31-C30	4.54	1.57	1.43
22	3	5005	BCR	C15-C14	4.54	1.57	1.43
22	B	844	BCR	C2-C1	4.53	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	5004	BCR	C2-C1	4.53	1.64	1.54
31	3	5003	LUT	C31-C30	4.52	1.57	1.43
31	3	5002	LUT	C8-C9	4.51	1.55	1.46
22	A	848	BCR	C19-C18	4.51	1.55	1.46
22	A	847	BCR	C2-C1	4.51	1.64	1.54
27	5	302	RRX	C23-C22	4.50	1.55	1.46
22	3	5004	BCR	C23-C22	4.49	1.55	1.46
27	4	303	RRX	C24-C25	4.49	1.60	1.45
22	3	5007	BCR	C19-C18	4.49	1.55	1.46
31	7	304	LUT	C31-C30	4.47	1.57	1.43
32	6	319	CHL	C1A-CHA	-4.47	1.34	1.40
32	7	314	CHL	C3B-C4B	4.47	1.45	1.41
31	4	304	LUT	C8-C9	4.47	1.55	1.46
31	6	306	LUT	C31-C30	4.46	1.57	1.43
31	8	304	LUT	C35-C34	4.46	1.57	1.43
32	5	320	CHL	C3A-C2A	-4.45	1.50	1.54
31	1	5003	LUT	C8-C9	4.45	1.55	1.46
27	4	303	RRX	C23-C22	4.45	1.55	1.46
22	3	5007	BCR	C20-C21	4.44	1.57	1.43
22	8	303	BCR	C20-C21	4.44	1.57	1.43
31	6	306	LUT	C12-C13	4.44	1.55	1.46
31	6	306	LUT	C15-C14	4.43	1.56	1.43
22	B	842	BCR	C20-C21	4.42	1.56	1.43
19	B	839	CLA	CBB-CAB	4.42	1.51	1.30
19	A	830	CLA	CBB-CAB	4.42	1.51	1.30
19	B	822	CLA	CBB-CAB	4.42	1.51	1.30
22	8	303	BCR	C28-C27	4.42	1.66	1.52
19	B	806	CLA	CBB-CAB	4.42	1.51	1.30
31	5	303	LUT	C8-C9	4.41	1.55	1.46
19	A	841	CLA	CBB-CAB	4.41	1.51	1.30
22	5	304	BCR	C20-C21	4.41	1.56	1.43
19	A	820	CLA	CBB-CAB	4.41	1.51	1.30
19	A	807	CLA	CBB-CAB	4.41	1.51	1.30
19	B	837	CLA	CBB-CAB	4.40	1.51	1.30
19	A	827	CLA	CBB-CAB	4.40	1.51	1.30
19	A	842	CLA	CBB-CAB	4.40	1.51	1.30
19	G	1601	CLA	CBB-CAB	4.40	1.51	1.30
19	A	835	CLA	CBB-CAB	4.40	1.51	1.30
19	B	824	CLA	CBB-CAB	4.40	1.51	1.30
19	5	301	CLA	CBB-CAB	4.40	1.51	1.30
19	A	857	CLA	CBB-CAB	4.40	1.51	1.30
19	B	834	CLA	CBB-CAB	4.40	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	303	CLA	CBB-CAB	4.40	1.51	1.30
19	B	813	CLA	CBB-CAB	4.40	1.51	1.30
19	B	832	CLA	CBB-CAB	4.40	1.51	1.30
19	A	805	CLA	CBB-CAB	4.40	1.51	1.30
19	A	834	CLA	CBB-CAB	4.39	1.51	1.30
19	A	828	CLA	CBB-CAB	4.39	1.51	1.30
19	J	1901	CLA	CBB-CAB	4.39	1.51	1.30
19	A	808	CLA	CBB-CAB	4.39	1.51	1.30
19	K	205	CLA	CBB-CAB	4.39	1.51	1.30
19	B	805	CLA	CBB-CAB	4.39	1.51	1.30
19	6	314	CLA	CBB-CAB	4.39	1.51	1.30
19	A	804	CLA	CBB-CAB	4.39	1.51	1.30
19	B	828	CLA	CBB-CAB	4.39	1.51	1.30
19	K	202	CLA	CBB-CAB	4.39	1.51	1.30
19	A	817	CLA	CBB-CAB	4.39	1.51	1.30
19	1	5015	CLA	CBB-CAB	4.39	1.51	1.30
19	A	802	CLA	CBB-CAB	4.39	1.51	1.30
19	B	826	CLA	CBB-CAB	4.39	1.51	1.30
22	B	844	BCR	C20-C21	4.39	1.56	1.43
19	A	821	CLA	CBB-CAB	4.39	1.51	1.30
19	B	807	CLA	CBB-CAB	4.39	1.51	1.30
19	B	821	CLA	CBB-CAB	4.39	1.51	1.30
19	B	819	CLA	CBB-CAB	4.39	1.51	1.30
19	B	804	CLA	CBB-CAB	4.39	1.51	1.30
19	B	820	CLA	CBB-CAB	4.39	1.51	1.30
19	A	836	CLA	CBB-CAB	4.39	1.51	1.30
19	B	815	CLA	CBB-CAB	4.39	1.51	1.30
27	F	304	RRX	C29-C30	4.39	1.68	1.54
31	6	306	LUT	C35-C34	4.39	1.56	1.43
19	B	838	CLA	CBB-CAB	4.39	1.51	1.30
19	6	302	CLA	CBB-CAB	4.39	1.51	1.30
19	B	809	CLA	CBB-CAB	4.39	1.51	1.30
19	B	814	CLA	CBB-CAB	4.39	1.51	1.30
19	8	320	CLA	CBB-CAB	4.39	1.51	1.30
19	4	312	CLA	CBB-CAB	4.39	1.51	1.30
19	B	818	CLA	CBB-CAB	4.39	1.51	1.30
19	1	5011	CLA	CBB-CAB	4.38	1.51	1.30
19	B	810	CLA	CBB-CAB	4.38	1.51	1.30
19	K	204	CLA	CBB-CAB	4.38	1.51	1.30
19	A	826	CLA	CBB-CAB	4.38	1.51	1.30
19	K	203	CLA	CBB-CAB	4.38	1.51	1.30
22	B	843	BCR	C20-C21	4.38	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	322	CLA	CBB-CAB	4.38	1.51	1.30
19	B	829	CLA	CBB-CAB	4.38	1.51	1.30
19	4	318	CLA	CBB-CAB	4.38	1.51	1.30
19	B	808	CLA	CBB-CAB	4.38	1.51	1.30
32	5	320	CHL	C3B-C4B	4.38	1.45	1.41
19	B	801	CLA	CBB-CAB	4.38	1.51	1.30
19	7	319	CLA	CBB-CAB	4.38	1.51	1.30
19	B	823	CLA	CBB-CAB	4.38	1.51	1.30
19	B	827	CLA	CBB-CAB	4.38	1.51	1.30
19	1	5018	CLA	CBB-CAB	4.38	1.51	1.30
22	A	850	BCR	C20-C21	4.38	1.56	1.43
19	7	317	CLA	CBB-CAB	4.38	1.51	1.30
31	3	5003	LUT	C15-C14	4.38	1.56	1.43
19	A	839	CLA	CBB-CAB	4.38	1.51	1.30
19	A	803	CLA	CBB-CAB	4.38	1.51	1.30
19	B	833	CLA	CBB-CAB	4.37	1.51	1.30
19	A	811	CLA	CBB-CAB	4.37	1.51	1.30
19	A	822	CLA	CBB-CAB	4.37	1.51	1.30
19	B	830	CLA	CBB-CAB	4.37	1.51	1.30
19	A	823	CLA	CBB-CAB	4.37	1.51	1.30
19	A	824	CLA	CBB-CAB	4.37	1.51	1.30
19	Z	314	CLA	CBB-CAB	4.37	1.51	1.30
19	A	816	CLA	CBB-CAB	4.37	1.51	1.30
19	1	5016	CLA	CBB-CAB	4.37	1.51	1.30
19	8	312	CLA	C1C-NC	-4.37	1.31	1.37
19	3	5016	CLA	CBB-CAB	4.37	1.51	1.30
19	A	813	CLA	CBB-CAB	4.37	1.51	1.30
19	B	816	CLA	CBB-CAB	4.37	1.51	1.30
19	7	312	CLA	CBB-CAB	4.37	1.51	1.30
22	B	847	BCR	C20-C21	4.36	1.56	1.43
19	A	818	CLA	CBB-CAB	4.36	1.51	1.30
19	A	819	CLA	CBB-CAB	4.36	1.51	1.30
19	3	5014	CLA	CBB-CAB	4.36	1.51	1.30
19	A	809	CLA	CBB-CAB	4.36	1.51	1.30
22	7	305	BCR	C20-C21	4.36	1.56	1.43
19	B	811	CLA	CBB-CAB	4.36	1.51	1.30
22	A	858	BCR	C20-C21	4.36	1.56	1.43
19	A	833	CLA	CBB-CAB	4.36	1.51	1.30
22	F	302	BCR	C20-C21	4.36	1.56	1.43
22	A	859	BCR	C20-C21	4.36	1.56	1.43
31	3	5002	LUT	C12-C13	4.36	1.55	1.46
19	A	814	CLA	CBB-CAB	4.36	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	831	CLA	CBB-CAB	4.36	1.51	1.30
22	A	846	BCR	C20-C21	4.36	1.56	1.43
32	6	317	CHL	C1A-CHA	-4.36	1.35	1.40
32	4	319	CHL	C3B-C4B	4.36	1.45	1.41
19	A	825	CLA	CBB-CAB	4.36	1.51	1.30
19	I	201	CLA	CBB-CAB	4.35	1.51	1.30
22	6	307	BCR	C2-C1	4.35	1.64	1.54
19	1	5012	CLA	CBB-CAB	4.35	1.51	1.30
32	6	316	CHL	C1A-CHA	-4.35	1.35	1.40
19	B	817	CLA	CBB-CAB	4.35	1.51	1.30
22	A	849	BCR	C19-C18	4.35	1.55	1.46
19	A	838	CLA	CBB-CAB	4.35	1.51	1.30
19	A	843	CLA	CBB-CAB	4.35	1.51	1.30
19	A	832	CLA	CBB-CAB	4.35	1.51	1.30
19	A	837	CLA	CBB-CAB	4.35	1.51	1.30
31	1	5004	LUT	C8-C9	4.35	1.55	1.46
19	G	1602	CLA	CBB-CAB	4.35	1.51	1.30
22	B	845	BCR	C20-C21	4.34	1.56	1.43
19	B	812	CLA	CBB-CAB	4.34	1.51	1.30
19	Z	307	CLA	CBB-CAB	4.34	1.51	1.30
19	5	312	CLA	CBB-CAB	4.34	1.51	1.30
22	8	306	BCR	C2-C1	4.34	1.64	1.54
19	A	829	CLA	CBB-CAB	4.34	1.51	1.30
32	Z	310	CHL	C3B-C4B	4.34	1.45	1.41
22	G	1603	BCR	C20-C21	4.34	1.56	1.43
19	B	802	CLA	CBB-CAB	4.34	1.51	1.30
31	Z	318	LUT	C8-C9	4.34	1.55	1.46
19	B	835	CLA	CBB-CAB	4.33	1.51	1.30
31	7	304	LUT	C35-C34	4.33	1.56	1.43
22	B	845	BCR	C28-C27	4.33	1.66	1.52
19	B	803	CLA	CBB-CAB	4.33	1.51	1.30
19	3	5010	CLA	CBB-CAB	4.33	1.51	1.30
19	4	313	CLA	CBB-CAB	4.33	1.51	1.30
19	Z	303	CLA	CBB-CAB	4.33	1.51	1.30
31	7	303	LUT	C8-C9	4.33	1.55	1.46
19	3	5015	CLA	CBB-CAB	4.32	1.51	1.30
22	3	5006	BCR	C28-C27	4.32	1.66	1.52
22	B	842	BCR	C28-C27	4.32	1.66	1.52
19	Z	315	CLA	CBB-CAB	4.32	1.51	1.30
28	6	304	C7Z	C32-C33	4.32	1.55	1.46
22	B	846	BCR	C20-C21	4.32	1.56	1.43
27	F	304	RRX	C11-C10	4.32	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Z	318	LUT	C12-C13	4.31	1.55	1.46
22	A	850	BCR	C28-C27	4.31	1.66	1.52
31	6	305	LUT	C8-C9	4.31	1.55	1.46
19	5	313	CLA	CBB-CAB	4.31	1.51	1.30
19	A	806	CLA	CBB-CAB	4.31	1.51	1.30
31	8	305	LUT	C23-C24	-4.31	1.44	1.50
19	6	320	CLA	CBB-CAB	4.31	1.51	1.30
27	F	304	RRX	C3-C4	4.31	1.66	1.52
19	4	308	CLA	CBB-CAB	4.31	1.51	1.30
22	K	206	BCR	C20-C21	4.31	1.56	1.43
27	5	302	RRX	C12-C13	4.30	1.55	1.46
22	G	1603	BCR	C28-C27	4.30	1.65	1.52
19	7	316	CLA	CBB-CAB	4.30	1.51	1.30
31	3	5003	LUT	C35-C34	4.30	1.56	1.43
19	7	313	CLA	CBB-CAB	4.30	1.51	1.30
31	1	5004	LUT	C12-C13	4.30	1.55	1.46
22	5	304	BCR	C2-C1	4.30	1.63	1.54
32	5	315	CHL	C3A-C2A	-4.30	1.51	1.54
31	7	304	LUT	C15-C14	4.30	1.56	1.43
19	Z	311	CLA	CBB-CAB	4.30	1.51	1.30
19	8	318	CLA	CBB-CAB	4.30	1.51	1.30
22	A	847	BCR	C20-C21	4.30	1.56	1.43
22	3	5006	BCR	C20-C21	4.30	1.56	1.43
19	4	306	CLA	CBB-CAB	4.30	1.51	1.30
19	6	318	CLA	CBB-CAB	4.29	1.51	1.30
22	A	858	BCR	C28-C27	4.29	1.65	1.52
19	5	307	CLA	CBB-CAB	4.29	1.51	1.30
19	5	306	CLA	CBB-CAB	4.29	1.51	1.30
22	A	849	BCR	C28-C27	4.29	1.65	1.52
19	6	313	CLA	CBB-CAB	4.29	1.51	1.30
19	1	5007	CLA	CBB-CAB	4.29	1.51	1.30
19	5	325	CLA	CBB-CAB	4.28	1.51	1.30
22	B	847	BCR	C28-C27	4.28	1.65	1.52
19	5	317	CLA	CBB-CAB	4.28	1.50	1.30
19	Z	306	CLA	CBB-CAB	4.28	1.50	1.30
19	1	5010	CLA	CBB-CAB	4.28	1.50	1.30
19	4	309	CLA	CBB-CAB	4.28	1.50	1.30
22	B	843	BCR	C28-C27	4.28	1.65	1.52
19	7	324	CLA	CBB-CAB	4.28	1.50	1.30
19	5	311	CLA	CBB-CAB	4.27	1.50	1.30
19	Z	304	CLA	CBB-CAB	4.27	1.50	1.30
19	3	5009	CLA	CBB-CAB	4.27	1.50	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	4	307	CLA	CBB-CAB	4.27	1.50	1.30
19	4	311	CLA	CBB-CAB	4.27	1.50	1.30
22	4	305	BCR	C20-C21	4.27	1.56	1.43
19	8	313	CLA	CBB-CAB	4.27	1.50	1.30
19	5	308	CLA	CBB-CAB	4.27	1.50	1.30
27	4	303	RRX	C12-C13	4.27	1.55	1.46
19	8	310	CLA	CBB-CAB	4.27	1.50	1.30
19	Z	308	CLA	CBB-CAB	4.26	1.50	1.30
19	8	309	CLA	CBB-CAB	4.26	1.50	1.30
19	7	307	CLA	CBB-CAB	4.26	1.50	1.30
19	7	309	CLA	CBB-CAB	4.26	1.50	1.30
22	3	5005	BCR	C19-C18	4.26	1.55	1.46
28	1	5005	C7Z	C32-C33	4.26	1.55	1.46
19	5	314	CLA	CBB-CAB	4.26	1.50	1.30
27	4	303	RRX	C3-C4	4.26	1.65	1.52
19	3	5020	CLA	CBB-CAB	4.26	1.50	1.30
22	6	307	BCR	C19-C18	4.26	1.55	1.46
19	1	5006	CLA	CBB-CAB	4.26	1.50	1.30
19	Z	305	CLA	CBB-CAB	4.26	1.50	1.30
31	5	303	LUT	C23-C24	-4.26	1.44	1.50
19	6	301	CLA	CBB-CAB	4.26	1.50	1.30
19	5	321	CLA	CBB-CAB	4.26	1.50	1.30
19	B	840	CLA	CBB-CAB	4.25	1.50	1.30
22	6	308	BCR	C2-C1	4.25	1.63	1.54
31	Z	318	LUT	C15-C14	4.25	1.56	1.43
19	8	307	CLA	CBB-CAB	4.25	1.50	1.30
19	7	306	CLA	CBB-CAB	4.25	1.50	1.30
19	1	5013	CLA	CBB-CAB	4.25	1.50	1.30
22	3	5005	BCR	C2-C1	4.25	1.63	1.54
19	6	323	CLA	CBB-CAB	4.25	1.50	1.30
32	1	5014	CHL	C3B-C4B	4.25	1.45	1.41
31	4	304	LUT	C15-C14	4.25	1.56	1.43
31	8	305	LUT	C8-C9	4.25	1.55	1.46
19	Z	312	CLA	CBB-CAB	4.25	1.50	1.30
31	5	303	LUT	C12-C13	4.25	1.55	1.46
19	3	5011	CLA	CBB-CAB	4.25	1.50	1.30
19	6	311	CLA	CBB-CAB	4.25	1.50	1.30
19	8	311	CLA	CBB-CAB	4.24	1.50	1.30
19	5	310	CLA	CBB-CAB	4.24	1.50	1.30
19	6	322	CLA	CBB-CAB	4.24	1.50	1.30
19	8	312	CLA	C4B-NB	-4.24	1.32	1.37
19	4	316	CLA	CBB-CAB	4.24	1.50	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	840	CLA	CBB-CAB	4.24	1.50	1.30
19	3	5008	CLA	CBB-CAB	4.24	1.50	1.30
19	8	312	CLA	CBB-CAB	4.24	1.50	1.30
31	1	5004	LUT	C23-C24	-4.24	1.44	1.50
19	8	314	CLA	CBB-CAB	4.24	1.50	1.30
19	6	310	CLA	CBB-CAB	4.24	1.50	1.30
19	3	5018	CLA	CBB-CAB	4.24	1.50	1.30
22	F	302	BCR	C28-C27	4.23	1.65	1.52
19	5	319	CLA	CBB-CAB	4.23	1.50	1.30
22	A	847	BCR	C28-C27	4.23	1.65	1.52
19	B	850	CLA	CBB-CAB	4.23	1.50	1.30
28	J	1902	C7Z	C32-C33	4.23	1.55	1.46
22	A	848	BCR	C20-C21	4.23	1.56	1.43
19	7	318	CLA	CBB-CAB	4.23	1.50	1.30
19	A	812	CLA	CBB-CAB	4.23	1.50	1.30
31	Z	318	LUT	C35-C34	4.23	1.56	1.43
19	7	310	CLA	CBB-CAB	4.23	1.50	1.30
31	4	304	LUT	C12-C13	4.23	1.55	1.46
22	K	206	BCR	C28-C27	4.23	1.65	1.52
19	7	311	CLA	CBB-CAB	4.23	1.50	1.30
31	3	5002	LUT	C31-C30	4.23	1.56	1.43
25	B	848	DGD	O1G-C1A	4.22	1.45	1.33
22	4	305	BCR	C2-C1	4.22	1.63	1.54
19	B	831	CLA	CBB-CAB	4.22	1.50	1.30
19	4	310	CLA	CBB-CAB	4.22	1.50	1.30
19	B	836	CLA	CBB-CAB	4.21	1.50	1.30
19	1	5008	CLA	CBB-CAB	4.21	1.50	1.30
32	4	317	CHL	C1A-CHA	-4.21	1.35	1.40
22	3	5005	BCR	C20-C21	4.21	1.56	1.43
19	6	309	CLA	CBB-CAB	4.21	1.50	1.30
19	3	5013	CLA	CBB-CAB	4.20	1.50	1.30
22	A	848	BCR	C28-C27	4.20	1.65	1.52
27	5	302	RRX	C27-C26	-4.20	1.44	1.51
19	A	810	CLA	CBB-CAB	4.20	1.50	1.30
31	Z	318	LUT	C31-C30	4.19	1.56	1.43
31	3	5002	LUT	C15-C14	4.19	1.56	1.43
19	3	5012	CLA	CBB-CAB	4.19	1.50	1.30
19	8	308	CLA	CBB-CAB	4.19	1.50	1.30
22	A	849	BCR	C20-C21	4.19	1.56	1.43
22	B	846	BCR	C28-C27	4.18	1.65	1.52
22	8	306	BCR	C28-C27	4.18	1.65	1.52
19	6	312	CLA	CBB-CAB	4.18	1.50	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	815	CLA	CBB-CAB	4.18	1.50	1.30
32	8	301	CHL	C1A-CHA	-4.17	1.35	1.40
19	5	309	CLA	CBB-CAB	4.17	1.50	1.30
32	1	5017	CHL	C3B-C4B	4.17	1.45	1.41
22	5	305	BCR	C2-C1	4.17	1.63	1.54
19	7	308	CLA	CBB-CAB	4.17	1.50	1.30
31	3	5002	LUT	C35-C34	4.17	1.56	1.43
22	5	304	BCR	C28-C27	4.17	1.65	1.52
19	3	5019	CLA	CBB-CAB	4.17	1.50	1.30
27	5	302	RRX	C11-C10	4.17	1.56	1.43
22	6	307	BCR	C20-C21	4.16	1.56	1.43
31	Z	317	LUT	C7-C6	4.16	1.59	1.45
22	A	846	BCR	C28-C27	4.16	1.65	1.52
22	B	844	BCR	C28-C27	4.16	1.65	1.52
22	7	305	BCR	C28-C27	4.16	1.65	1.52
22	A	859	BCR	C28-C27	4.16	1.65	1.52
32	8	315	CHL	C1A-CHA	-4.15	1.35	1.40
19	B	825	CLA	CBB-CAB	4.15	1.50	1.30
31	4	304	LUT	C35-C34	4.14	1.56	1.43
19	F	301	CLA	CBB-CAB	4.12	1.50	1.30
19	7	307	CLA	MG-ND	-4.12	1.97	2.05
31	4	304	LUT	C31-C30	4.12	1.56	1.43
28	1	5005	C7Z	C4-C5	-4.11	1.44	1.51
31	7	304	LUT	C7-C6	4.11	1.59	1.45
32	Z	309	CHL	C1A-CHA	-4.11	1.35	1.40
27	4	303	RRX	C11-C10	4.11	1.55	1.43
22	3	5004	BCR	C4-C5	-4.10	1.43	1.51
22	3	5005	BCR	C28-C27	4.10	1.65	1.52
22	5	305	BCR	C20-C21	4.10	1.55	1.43
32	8	316	CHL	C1A-CHA	-4.09	1.35	1.40
31	1	5003	LUT	C35-C34	4.09	1.55	1.43
27	5	302	RRX	C29-C30	4.09	1.67	1.54
31	6	305	LUT	C15-C14	4.08	1.55	1.43
32	6	315	CHL	C3B-C4B	4.08	1.45	1.41
19	4	311	CLA	C1C-NC	-4.08	1.31	1.37
19	Z	307	CLA	MG-ND	-4.07	1.97	2.05
22	4	305	BCR	C28-C27	4.07	1.65	1.52
38	8	325	ERG	C13-C17	4.07	1.62	1.55
22	6	308	BCR	C28-C27	4.07	1.65	1.52
27	5	302	RRX	C3-C4	4.07	1.65	1.52
31	Z	317	LUT	C31-C30	4.07	1.55	1.43
31	6	305	LUT	C12-C13	4.06	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	303	LUT	C15-C14	4.06	1.55	1.43
27	F	304	RRX	C15-C14	4.06	1.55	1.43
31	1	5003	LUT	C31-C30	4.06	1.55	1.43
19	Z	311	CLA	MG-ND	-4.05	1.97	2.05
31	1	5003	LUT	C15-C14	4.05	1.55	1.43
31	8	304	LUT	C7-C6	4.05	1.58	1.45
22	8	303	BCR	C16-C17	4.04	1.55	1.43
22	8	306	BCR	C19-C18	4.04	1.54	1.46
22	A	859	BCR	C3-C4	4.04	1.65	1.52
31	1	5004	LUT	C15-C14	4.04	1.55	1.43
32	6	316	CHL	C3B-C4B	4.04	1.45	1.41
28	J	1902	C7Z	C22-C21	4.03	1.66	1.54
19	B	840	CLA	MG-ND	-4.03	1.97	2.05
31	6	305	LUT	C31-C30	4.02	1.55	1.43
28	6	304	C7Z	C22-C21	4.02	1.66	1.54
22	5	305	BCR	C28-C27	4.02	1.65	1.52
31	Z	318	LUT	C7-C6	4.02	1.58	1.45
38	6	326	ERG	C16-C15	4.02	1.65	1.54
19	3	5020	CLA	MG-ND	-4.02	1.97	2.05
31	8	304	LUT	C28-C29	4.02	1.54	1.46
31	7	304	LUT	C28-C29	4.02	1.54	1.46
31	1	5004	LUT	C35-C34	4.02	1.55	1.43
31	5	303	LUT	C31-C30	4.02	1.55	1.43
22	3	5007	BCR	C28-C27	4.00	1.65	1.52
31	8	305	LUT	C12-C13	4.00	1.54	1.46
28	1	5005	C7Z	C22-C21	4.00	1.66	1.54
31	Z	317	LUT	C11-C10	4.00	1.55	1.43
32	4	317	CHL	C3B-C2B	-4.00	1.35	1.40
22	B	842	BCR	C16-C17	3.99	1.55	1.43
31	3	5002	LUT	C23-C24	-3.99	1.44	1.50
22	K	206	BCR	C3-C4	3.99	1.64	1.52
31	5	303	LUT	C35-C34	3.99	1.55	1.43
22	7	305	BCR	C3-C4	3.99	1.64	1.52
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	3	5003	LUT	C28-C29	3.98	1.54	1.46
31	1	5003	LUT	C12-C13	3.97	1.54	1.46
22	3	5005	BCR	C4-C5	-3.97	1.43	1.51
28	J	1902	C7Z	C11-C10	3.97	1.55	1.43
31	6	305	LUT	C35-C34	3.97	1.55	1.43
22	A	848	BCR	C3-C4	3.96	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Z	309	CHL	C3B-C4B	3.96	1.45	1.41
19	1	5007	CLA	MG-ND	-3.96	1.97	2.05
19	5	313	CLA	MG-ND	-3.96	1.97	2.05
22	A	850	BCR	C3-C4	3.96	1.64	1.52
22	6	307	BCR	C28-C27	3.96	1.64	1.52
31	7	303	LUT	C15-C14	3.96	1.55	1.43
31	1	5004	LUT	C31-C30	3.96	1.55	1.43
22	3	5004	BCR	C19-C18	3.96	1.54	1.46
22	A	858	BCR	C3-C4	3.95	1.64	1.52
31	6	306	LUT	C7-C6	3.95	1.58	1.45
28	6	304	C7Z	C11-C10	3.95	1.55	1.43
22	3	5004	BCR	C28-C27	3.95	1.64	1.52
19	7	318	CLA	MG-ND	-3.94	1.98	2.05
22	B	845	BCR	C3-C4	3.94	1.64	1.52
28	6	304	C7Z	C15-C14	3.94	1.55	1.43
31	7	303	LUT	C31-C30	3.94	1.55	1.43
19	4	310	CLA	MG-ND	-3.94	1.98	2.05
27	F	304	RRX	C16-C17	3.94	1.55	1.43
22	8	303	BCR	C3-C4	3.93	1.64	1.52
19	5	325	CLA	MG-ND	-3.93	1.98	2.05
31	3	5003	LUT	C7-C6	3.93	1.58	1.45
31	7	304	LUT	C21-C26	3.93	1.67	1.56
31	3	5002	LUT	C7-C6	3.93	1.58	1.45
22	3	5004	BCR	C20-C21	3.93	1.55	1.43
19	Z	303	CLA	MG-ND	-3.93	1.98	2.05
19	3	5008	CLA	MG-ND	-3.93	1.98	2.05
22	A	846	BCR	C3-C4	3.92	1.64	1.52
22	A	859	BCR	C16-C17	3.92	1.55	1.43
22	B	847	BCR	C16-C17	3.92	1.55	1.43
19	4	311	CLA	C4B-NB	-3.92	1.32	1.37
27	F	304	RRX	C27-C26	-3.92	1.44	1.51
22	A	849	BCR	C3-C4	3.91	1.64	1.52
22	B	843	BCR	C3-C4	3.91	1.64	1.52
19	6	313	CLA	MG-ND	-3.91	1.98	2.05
28	J	1902	C7Z	C15-C14	3.91	1.55	1.43
22	8	306	BCR	C27-C26	-3.91	1.43	1.51
31	6	305	LUT	C7-C6	3.90	1.58	1.45
19	A	815	CLA	MG-ND	-3.90	1.98	2.05
19	3	5011	CLA	MG-ND	-3.90	1.98	2.05
22	G	1603	BCR	C3-C4	3.90	1.64	1.52
31	1	5004	LUT	C7-C6	3.90	1.58	1.45
31	1	5003	LUT	C7-C6	3.89	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	1	5007	CLA	C1C-NC	-3.89	1.31	1.37
31	8	305	LUT	C15-C14	3.89	1.55	1.43
22	5	305	BCR	C4-C5	-3.89	1.43	1.51
31	4	304	LUT	C23-C24	-3.89	1.44	1.50
31	8	305	LUT	C31-C30	3.89	1.55	1.43
31	7	303	LUT	C23-C24	-3.89	1.44	1.50
19	3	5015	CLA	MG-ND	-3.89	1.98	2.05
31	5	303	LUT	C7-C6	3.89	1.58	1.45
22	B	843	BCR	C16-C17	3.89	1.55	1.43
31	7	303	LUT	C12-C13	3.88	1.54	1.46
22	3	5006	BCR	C16-C17	3.88	1.55	1.43
31	Z	317	LUT	C21-C26	3.88	1.67	1.56
19	8	314	CLA	MG-ND	-3.88	1.98	2.05
28	6	304	C7Z	C27-C26	3.88	1.58	1.45
31	7	303	LUT	C35-C34	3.88	1.55	1.43
32	8	301	CHL	C3A-C2A	-3.88	1.51	1.54
19	1	5015	CLA	MG-ND	-3.88	1.98	2.05
22	8	306	BCR	C20-C21	3.88	1.55	1.43
22	3	5007	BCR	C3-C4	3.88	1.64	1.52
22	B	844	BCR	C16-C17	3.88	1.55	1.43
19	3	5019	CLA	MG-ND	-3.87	1.98	2.05
31	6	306	LUT	C28-C29	3.87	1.54	1.46
22	B	844	BCR	C11-C10	3.87	1.55	1.43
22	B	842	BCR	C3-C4	3.87	1.64	1.52
22	6	307	BCR	C27-C26	-3.87	1.43	1.51
19	B	831	CLA	MG-ND	-3.87	1.98	2.05
28	6	304	C7Z	C4-C5	-3.87	1.45	1.51
22	4	305	BCR	C3-C4	3.86	1.64	1.52
28	1	5005	C7Z	C27-C26	3.86	1.58	1.45
22	A	858	BCR	C16-C17	3.86	1.55	1.43
31	8	304	LUT	C11-C10	3.86	1.55	1.43
31	1	5003	LUT	C23-C24	-3.86	1.45	1.50
22	5	304	BCR	C16-C17	3.86	1.55	1.43
22	3	5005	BCR	C27-C26	-3.86	1.43	1.51
22	8	303	BCR	C11-C10	3.86	1.55	1.43
22	6	308	BCR	C20-C21	3.86	1.55	1.43
22	A	850	BCR	C16-C17	3.86	1.55	1.43
22	3	5004	BCR	C27-C26	-3.86	1.43	1.51
22	3	5005	BCR	C3-C4	3.86	1.64	1.52
22	3	5006	BCR	C3-C4	3.86	1.64	1.52
22	B	842	BCR	C11-C10	3.85	1.55	1.43
32	8	319	CHL	C1A-CHA	-3.85	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	5010	CLA	MG-ND	-3.85	1.98	2.05
28	J	1902	C7Z	C27-C26	3.85	1.58	1.45
19	8	311	CLA	MG-ND	-3.84	1.98	2.05
22	A	850	BCR	C11-C10	3.84	1.55	1.43
22	A	846	BCR	C16-C17	3.84	1.55	1.43
22	B	844	BCR	C3-C4	3.84	1.64	1.52
32	7	314	CHL	C3B-C2B	-3.84	1.35	1.40
19	8	310	CLA	MG-ND	-3.84	1.98	2.05
19	4	313	CLA	MG-ND	-3.83	1.98	2.05
22	F	302	BCR	C3-C4	3.83	1.64	1.52
27	F	304	RRX	C20-C21	3.83	1.55	1.43
31	7	303	LUT	C7-C6	3.83	1.58	1.45
31	4	304	LUT	C7-C6	3.83	1.58	1.45
31	Z	317	LUT	C23-C24	-3.83	1.45	1.50
22	B	847	BCR	C3-C4	3.83	1.64	1.52
32	5	315	CHL	C3B-C2B	-3.83	1.35	1.40
31	Z	317	LUT	C28-C29	3.83	1.54	1.46
22	5	305	BCR	C3-C4	3.82	1.64	1.52
19	4	308	CLA	MG-ND	-3.82	1.98	2.05
22	B	842	BCR	C24-C25	3.82	1.58	1.45
28	1	5005	C7Z	C11-C10	3.82	1.55	1.43
32	Z	302	CHL	C3B-C2B	-3.82	1.35	1.40
19	1	5006	CLA	MG-ND	-3.82	1.98	2.05
28	1	5005	C7Z	C15-C14	3.82	1.55	1.43
31	7	304	LUT	C11-C10	3.82	1.55	1.43
32	8	301	CHL	C3B-C4B	3.82	1.45	1.41
22	A	847	BCR	C16-C17	3.82	1.55	1.43
31	6	306	LUT	C11-C10	3.82	1.55	1.43
22	K	206	BCR	C16-C17	3.81	1.55	1.43
19	A	840	CLA	MG-ND	-3.81	1.98	2.05
19	B	831	CLA	C1C-NC	-3.81	1.31	1.37
22	4	305	BCR	C27-C26	-3.81	1.43	1.51
22	B	845	BCR	C16-C17	3.81	1.55	1.43
22	4	305	BCR	C16-C17	3.81	1.55	1.43
19	7	307	CLA	C1C-NC	-3.81	1.31	1.37
22	A	859	BCR	C11-C10	3.80	1.55	1.43
19	5	307	CLA	MG-ND	-3.80	1.98	2.05
19	7	309	CLA	MG-ND	-3.80	1.98	2.05
22	A	848	BCR	C16-C17	3.80	1.55	1.43
19	B	836	CLA	C4B-NB	-3.80	1.32	1.37
22	6	308	BCR	C11-C10	3.80	1.55	1.43
22	A	847	BCR	C3-C4	3.80	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	305	BCR	C16-C17	3.80	1.55	1.43
19	5	314	CLA	MG-ND	-3.80	1.98	2.05
31	8	305	LUT	C35-C34	3.80	1.55	1.43
32	6	315	CHL	C3B-C2B	-3.80	1.35	1.40
31	3	5003	LUT	C11-C10	3.80	1.55	1.43
22	6	307	BCR	C16-C17	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	B	846	BCR	C16-C17	3.79	1.54	1.43
19	A	810	CLA	MG-ND	-3.79	1.98	2.05
28	J	1902	C7Z	C4-C5	-3.79	1.45	1.51
22	A	858	BCR	C11-C10	3.79	1.54	1.43
19	8	308	CLA	MG-ND	-3.79	1.98	2.05
22	B	846	BCR	C3-C4	3.79	1.64	1.52
19	Z	312	CLA	MG-ND	-3.79	1.98	2.05
22	B	845	BCR	C11-C10	3.78	1.54	1.43
22	A	846	BCR	C11-C10	3.78	1.54	1.43
28	6	304	C7Z	C35-C34	3.78	1.54	1.43
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
27	5	302	RRX	C4-C5	-3.78	1.44	1.51
22	3	5007	BCR	C27-C26	-3.78	1.44	1.51
22	F	302	BCR	C16-C17	3.78	1.54	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
19	8	313	CLA	MG-ND	-3.77	1.98	2.05
19	7	306	CLA	MG-ND	-3.77	1.98	2.05
31	Z	318	LUT	C28-C29	3.77	1.54	1.46
19	3	5013	CLA	C1C-NC	-3.76	1.31	1.37
19	8	318	CLA	MG-ND	-3.76	1.98	2.05
38	8	325	ERG	C16-C15	3.76	1.64	1.54
22	B	847	BCR	C11-C10	3.76	1.54	1.43
22	4	305	BCR	C11-C10	3.76	1.54	1.43
19	7	316	CLA	MG-ND	-3.76	1.98	2.05
32	6	319	CHL	C2C-C3C	-3.76	1.32	1.36
31	5	303	LUT	C21-C26	3.76	1.66	1.56
22	G	1603	BCR	C16-C17	3.76	1.54	1.43
19	1	5013	CLA	MG-ND	-3.75	1.98	2.05
22	A	858	BCR	C24-C25	3.75	1.57	1.45
22	F	302	BCR	C11-C10	3.75	1.54	1.43
22	A	847	BCR	C11-C10	3.75	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	8	307	CLA	MG-ND	-3.75	1.98	2.05
19	5	319	CLA	MG-ND	-3.75	1.98	2.05
19	6	312	CLA	MG-ND	-3.75	1.98	2.05
22	3	5006	BCR	C11-C10	3.75	1.54	1.43
19	7	308	CLA	MG-ND	-3.75	1.98	2.05
22	6	307	BCR	C3-C4	3.75	1.64	1.52
22	3	5007	BCR	C16-C17	3.75	1.54	1.43
19	5	308	CLA	MG-ND	-3.75	1.98	2.05
19	B	825	CLA	C4B-NB	-3.75	1.32	1.37
22	G	1603	BCR	C11-C10	3.74	1.54	1.43
27	4	303	RRX	C15-C14	3.74	1.54	1.43
19	Z	306	CLA	MG-ND	-3.74	1.98	2.05
27	4	303	RRX	C29-C30	3.74	1.66	1.54
22	B	843	BCR	C11-C10	3.74	1.54	1.43
19	5	321	CLA	MG-ND	-3.74	1.98	2.05
22	7	305	BCR	C11-C10	3.73	1.54	1.43
31	6	305	LUT	C23-C24	-3.73	1.45	1.50
19	B	831	CLA	C4B-NB	-3.73	1.33	1.37
19	7	311	CLA	MG-ND	-3.73	1.98	2.05
22	3	5007	BCR	C4-C5	-3.73	1.44	1.51
19	6	320	CLA	MG-ND	-3.73	1.98	2.05
19	6	323	CLA	MG-ND	-3.73	1.98	2.05
22	8	303	BCR	C24-C25	3.73	1.57	1.45
19	5	309	CLA	MG-ND	-3.73	1.98	2.05
22	3	5007	BCR	C11-C10	3.72	1.54	1.43
19	7	311	CLA	C1C-NC	-3.72	1.32	1.37
22	B	847	BCR	C24-C25	3.72	1.57	1.45
19	7	310	CLA	MG-ND	-3.72	1.98	2.05
22	A	849	BCR	C16-C17	3.72	1.54	1.43
27	5	302	RRX	C15-C14	3.72	1.54	1.43
22	A	850	BCR	C24-C25	3.72	1.57	1.45
22	F	302	BCR	C24-C25	3.72	1.57	1.45
19	8	309	CLA	MG-ND	-3.72	1.98	2.05
25	B	848	DGD	CAA-C9A	-3.71	1.33	1.51
19	5	306	CLA	MG-ND	-3.71	1.98	2.05
25	B	848	DGD	CGB-CFB	-3.71	1.33	1.51
22	B	845	BCR	C24-C25	3.71	1.57	1.45
32	7	315	CHL	C1A-CHA	-3.71	1.35	1.40
28	J	1902	C7Z	C35-C34	3.71	1.54	1.43
22	7	305	BCR	C4-C5	-3.71	1.44	1.51
32	Z	310	CHL	C3B-C2B	-3.71	1.35	1.40
19	4	306	CLA	MG-ND	-3.71	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	206	BCR	C11-C10	3.71	1.54	1.43
25	B	848	DGD	CDB-CCB	-3.70	1.33	1.51
32	7	315	CHL	C3B-C2B	-3.70	1.35	1.40
19	6	310	CLA	MG-ND	-3.70	1.98	2.05
22	5	304	BCR	C3-C4	3.70	1.64	1.52
29	J	1904	LMG	C25-C24	-3.70	1.33	1.51
29	J	1904	LMG	C22-C21	-3.70	1.33	1.51
28	J	1902	C7Z	C2-C1	3.70	1.65	1.54
22	A	848	BCR	C11-C10	3.70	1.54	1.43
19	8	313	CLA	C1C-NC	-3.70	1.32	1.37
22	3	5007	BCR	C24-C25	3.69	1.57	1.45
22	6	308	BCR	C3-C4	3.69	1.64	1.52
27	5	302	RRX	C16-C17	3.69	1.54	1.43
25	B	848	DGD	CGA-CFA	-3.69	1.33	1.51
19	Z	304	CLA	MG-ND	-3.69	1.98	2.05
31	6	306	LUT	C23-C24	-3.69	1.45	1.50
22	A	859	BCR	C24-C25	3.69	1.57	1.45
19	1	5008	CLA	MG-ND	-3.69	1.98	2.05
19	6	309	CLA	C4B-NB	-3.69	1.33	1.37
27	5	302	RRX	C20-C21	3.69	1.54	1.43
19	5	310	CLA	MG-ND	-3.69	1.98	2.05
19	7	311	CLA	C4B-NB	-3.69	1.33	1.37
25	B	848	DGD	CAB-C9B	-3.69	1.33	1.51
22	B	844	BCR	C24-C25	3.69	1.57	1.45
22	8	306	BCR	C4-C5	-3.68	1.44	1.51
22	5	305	BCR	C11-C10	3.68	1.54	1.43
22	B	846	BCR	C24-C25	3.68	1.57	1.45
32	8	301	CHL	C3B-C2B	-3.68	1.35	1.40
19	B	850	CLA	MG-ND	-3.68	1.98	2.05
22	A	846	BCR	C24-C25	3.68	1.57	1.45
31	4	304	LUT	C28-C29	3.68	1.53	1.46
31	1	5003	LUT	C28-C29	3.68	1.53	1.46
22	A	847	BCR	C24-C25	3.68	1.57	1.45
19	A	812	CLA	MG-ND	-3.68	1.98	2.05
29	J	1904	LMG	C19-C18	-3.68	1.33	1.51
19	3	5020	CLA	C4B-NB	-3.68	1.33	1.37
22	7	305	BCR	C24-C25	3.67	1.57	1.45
27	4	303	RRX	C27-C26	-3.67	1.45	1.51
19	6	318	CLA	MG-ND	-3.67	1.98	2.05
19	1	5010	CLA	MG-ND	-3.67	1.98	2.05
22	B	843	BCR	C24-C25	3.67	1.57	1.45
19	4	309	CLA	MG-ND	-3.67	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	5018	CLA	MG-ND	-3.67	1.98	2.05
22	B	843	BCR	C27-C26	-3.67	1.44	1.51
32	1	5009	CHL	C3B-C2B	-3.66	1.35	1.40
19	B	803	CLA	MG-ND	-3.66	1.98	2.05
19	8	307	CLA	C4B-NB	-3.66	1.33	1.37
19	K	204	CLA	MG-ND	-3.66	1.98	2.05
19	4	316	CLA	MG-ND	-3.66	1.98	2.05
32	6	321	CHL	C3B-C4B	3.66	1.45	1.41
27	4	303	RRX	C16-C17	3.66	1.54	1.43
22	K	206	BCR	C24-C25	3.66	1.57	1.45
19	7	307	CLA	C4B-NB	-3.66	1.33	1.37
22	3	5006	BCR	C24-C25	3.66	1.57	1.45
19	B	804	CLA	MG-ND	-3.66	1.98	2.05
31	8	305	LUT	C21-C26	3.66	1.66	1.56
28	6	304	C7Z	C2-C1	3.66	1.65	1.54
22	8	306	BCR	C16-C17	3.65	1.54	1.43
19	Z	315	CLA	MG-ND	-3.65	1.98	2.05
19	6	313	CLA	C1C-NC	-3.65	1.32	1.37
22	G	1603	BCR	C24-C25	3.65	1.57	1.45
25	B	848	DGD	CDA-CCA	-3.65	1.33	1.51
19	A	832	CLA	MG-ND	-3.65	1.98	2.05
19	3	5020	CLA	C1C-NC	-3.65	1.32	1.37
31	3	5002	LUT	C11-C10	3.65	1.54	1.43
22	6	307	BCR	C4-C5	-3.65	1.44	1.51
22	6	308	BCR	C16-C17	3.65	1.54	1.43
28	1	5005	C7Z	C35-C34	3.65	1.54	1.43
31	8	305	LUT	C7-C6	3.65	1.57	1.45
19	Z	311	CLA	C4B-NB	-3.64	1.33	1.37
22	A	847	BCR	C4-C5	-3.64	1.44	1.51
19	7	319	CLA	MG-ND	-3.64	1.98	2.05
22	A	849	BCR	C24-C25	3.64	1.57	1.45
19	6	322	CLA	MG-ND	-3.64	1.98	2.05
19	B	836	CLA	MG-ND	-3.64	1.98	2.05
19	4	308	CLA	C4B-NB	-3.64	1.33	1.37
22	5	304	BCR	C24-C25	3.64	1.57	1.45
27	4	303	RRX	C20-C21	3.64	1.54	1.43
22	8	303	BCR	C4-C5	-3.64	1.44	1.51
22	A	848	BCR	C24-C25	3.64	1.57	1.45
19	A	802	CLA	MG-ND	-3.64	1.98	2.05
22	8	306	BCR	C3-C4	3.64	1.63	1.52
31	1	5003	LUT	C21-C26	3.63	1.66	1.56
31	8	304	LUT	C21-C26	3.63	1.66	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	815	CLA	C1C-NC	-3.63	1.32	1.37
19	A	816	CLA	MG-ND	-3.63	1.98	2.05
19	K	203	CLA	MG-ND	-3.63	1.98	2.05
28	1	5005	C7Z	C21-C26	-3.63	1.49	1.53
19	3	5019	CLA	C1C-NC	-3.63	1.32	1.37
22	B	845	BCR	C4-C5	-3.63	1.44	1.51
19	8	318	CLA	C4B-NB	-3.63	1.33	1.37
22	6	307	BCR	C11-C10	3.63	1.54	1.43
19	3	5012	CLA	MG-ND	-3.62	1.98	2.05
19	B	840	CLA	C1C-NC	-3.62	1.32	1.37
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
19	B	840	CLA	C4B-NB	-3.62	1.33	1.37
31	Z	318	LUT	C11-C10	3.62	1.54	1.43
19	7	324	CLA	C1C-NC	-3.62	1.32	1.37
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	A	813	CLA	MG-ND	-3.61	1.98	2.05
32	4	314	CHL	C1A-CHA	-3.61	1.35	1.40
22	5	305	BCR	C27-C26	-3.61	1.44	1.51
27	F	304	RRX	C7-C6	3.61	1.57	1.45
19	B	815	CLA	MG-ND	-3.61	1.98	2.05
19	B	835	CLA	MG-ND	-3.61	1.98	2.05
19	I	201	CLA	MG-ND	-3.61	1.98	2.05
19	8	320	CLA	MG-ND	-3.61	1.98	2.05
19	6	311	CLA	MG-ND	-3.61	1.98	2.05
27	4	303	RRX	C4-C5	-3.61	1.44	1.51
22	B	843	BCR	C4-C5	-3.61	1.44	1.51
22	B	847	BCR	C4-C5	-3.61	1.44	1.51
19	6	314	CLA	MG-ND	-3.61	1.98	2.05
19	7	310	CLA	C1C-NC	-3.60	1.32	1.37
31	5	303	LUT	C11-C10	3.60	1.54	1.43
22	8	306	BCR	C11-C10	3.60	1.54	1.43
19	7	318	CLA	C4B-NB	-3.60	1.33	1.37
28	6	304	C7Z	C21-C26	-3.60	1.49	1.53
19	1	5008	CLA	C4B-NB	-3.60	1.33	1.37
19	A	810	CLA	C4B-NB	-3.60	1.33	1.37
19	B	820	CLA	MG-ND	-3.60	1.98	2.05
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	836	CLA	C1C-NC	-3.60	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	830	CLA	MG-ND	-3.60	1.98	2.05
31	1	5004	LUT	C21-C26	3.60	1.66	1.56
19	7	309	CLA	C1C-NC	-3.60	1.32	1.37
19	5	306	CLA	C4B-NB	-3.60	1.33	1.37
22	A	850	BCR	C4-C5	-3.60	1.44	1.51
22	B	846	BCR	C11-C10	3.59	1.54	1.43
19	7	313	CLA	C1C-NC	-3.59	1.32	1.37
22	3	5004	BCR	C3-C4	3.59	1.63	1.52
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	3	5019	CLA	C4B-NB	-3.59	1.33	1.37
19	B	837	CLA	MG-ND	-3.59	1.98	2.05
22	5	304	BCR	C11-C10	3.59	1.54	1.43
19	1	5007	CLA	C4B-NB	-3.59	1.33	1.37
31	4	304	LUT	C11-C10	3.59	1.54	1.43
19	6	322	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
22	A	858	BCR	C4-C5	-3.59	1.44	1.51
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
22	A	849	BCR	C27-C26	-3.58	1.44	1.51
19	B	832	CLA	MG-ND	-3.58	1.98	2.05
19	K	205	CLA	MG-ND	-3.58	1.98	2.05
22	K	206	BCR	C4-C5	-3.58	1.44	1.51
19	7	310	CLA	C4B-NB	-3.58	1.33	1.37
19	4	308	CLA	C1C-NC	-3.58	1.32	1.37
19	B	807	CLA	MG-ND	-3.58	1.98	2.05
19	3	5018	CLA	C1C-NC	-3.58	1.32	1.37
22	5	304	BCR	C4-C5	-3.58	1.44	1.51
19	8	311	CLA	C1C-NC	-3.58	1.32	1.37
19	A	837	CLA	MG-ND	-3.58	1.98	2.05
22	A	848	BCR	C4-C5	-3.58	1.44	1.51
22	3	5005	BCR	C16-C17	3.58	1.54	1.43
19	A	815	CLA	C4B-NB	-3.58	1.33	1.37
19	Z	311	CLA	C1C-NC	-3.58	1.32	1.37
22	3	5006	BCR	C27-C26	-3.58	1.44	1.51
19	6	309	CLA	MG-ND	-3.58	1.98	2.05
19	5	321	CLA	C1C-NC	-3.58	1.32	1.37
22	A	859	BCR	C27-C26	-3.58	1.44	1.51
19	5	311	CLA	C4B-NB	-3.57	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	303	CLA	C1C-NC	-3.57	1.32	1.37
19	B	818	CLA	MG-ND	-3.57	1.98	2.05
19	3	5008	CLA	C4B-NB	-3.57	1.33	1.37
19	B	809	CLA	MG-ND	-3.57	1.98	2.05
22	3	5004	BCR	C11-C10	3.57	1.54	1.43
28	1	5005	C7Z	C2-C1	3.57	1.65	1.54
19	5	310	CLA	C4B-NB	-3.57	1.33	1.37
19	5	321	CLA	C4B-NB	-3.57	1.33	1.37
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
19	3	5013	CLA	C4B-NB	-3.57	1.33	1.37
19	A	831	CLA	MG-ND	-3.57	1.98	2.05
19	A	836	CLA	MG-ND	-3.57	1.98	2.05
19	8	307	CLA	C1C-NC	-3.57	1.32	1.37
19	Z	303	CLA	C4B-NB	-3.57	1.33	1.37
19	A	814	CLA	MG-ND	-3.56	1.98	2.05
19	A	839	CLA	MG-ND	-3.56	1.98	2.05
31	1	5004	LUT	C11-C10	3.56	1.54	1.43
19	4	318	CLA	MG-ND	-3.56	1.98	2.05
19	7	316	CLA	C1C-NC	-3.56	1.32	1.37
22	5	304	BCR	C27-C26	-3.56	1.44	1.51
19	A	835	CLA	MG-ND	-3.56	1.98	2.05
19	6	313	CLA	C4B-NB	-3.56	1.33	1.37
19	B	823	CLA	MG-ND	-3.56	1.98	2.05
32	1	5014	CHL	CBB-CAB	3.56	1.51	1.29
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
19	Z	314	CLA	MG-ND	-3.55	1.98	2.05
38	8	325	ERG	C4-C5	3.55	1.58	1.51
19	5	311	CLA	C1C-NC	-3.55	1.32	1.37
19	6	311	CLA	C1C-NC	-3.55	1.32	1.37
19	A	829	CLA	MG-ND	-3.55	1.98	2.05
19	8	314	CLA	C1C-NC	-3.55	1.32	1.37
19	A	804	CLA	MG-ND	-3.55	1.98	2.05
22	5	305	BCR	C24-C25	3.55	1.57	1.45
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	842	BCR	C4-C5	-3.54	1.44	1.51
19	4	309	CLA	C4B-NB	-3.54	1.33	1.37
19	B	813	CLA	MG-ND	-3.54	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	826	CLA	MG-ND	-3.54	1.98	2.05
19	B	824	CLA	MG-ND	-3.54	1.98	2.05
32	Z	309	CHL	CBB-CAB	3.54	1.51	1.29
19	A	821	CLA	MG-ND	-3.54	1.98	2.05
19	B	811	CLA	MG-ND	-3.54	1.98	2.05
22	B	847	BCR	C27-C26	-3.54	1.44	1.51
22	A	849	BCR	C11-C10	3.54	1.54	1.43
19	A	822	CLA	MG-ND	-3.54	1.98	2.05
19	5	317	CLA	MG-ND	-3.54	1.98	2.05
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	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
31	6	305	LUT	C11-C10	3.53	1.54	1.43
19	A	825	CLA	MG-ND	-3.53	1.98	2.05
19	6	320	CLA	C1C-NC	-3.53	1.32	1.37
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	825	CLA	C1C-NC	-3.53	1.32	1.37
19	3	5011	CLA	C1C-NC	-3.53	1.32	1.37
32	1	5017	CHL	CBB-CAB	3.53	1.51	1.29
19	B	839	CLA	MG-ND	-3.53	1.98	2.05
19	A	826	CLA	MG-ND	-3.53	1.98	2.05
22	6	308	BCR	C4-C5	-3.53	1.44	1.51
19	3	5014	CLA	MG-ND	-3.53	1.98	2.05
19	5	312	CLA	MG-ND	-3.53	1.98	2.05
19	3	5013	CLA	MG-ND	-3.53	1.98	2.05
19	B	828	CLA	MG-ND	-3.53	1.98	2.05
22	7	305	BCR	C27-C26	-3.53	1.44	1.51
19	B	838	CLA	MG-ND	-3.53	1.98	2.05
19	4	307	CLA	C1C-NC	-3.52	1.32	1.37
19	A	809	CLA	MG-ND	-3.52	1.98	2.05
31	3	5002	LUT	C28-C29	3.52	1.53	1.46
19	A	819	CLA	MG-ND	-3.52	1.98	2.05
19	8	313	CLA	C4B-NB	-3.52	1.33	1.37
19	1	5008	CLA	C1C-NC	-3.52	1.32	1.37
19	Z	304	CLA	C1C-NC	-3.52	1.32	1.37
19	A	842	CLA	MG-ND	-3.52	1.98	2.05
19	3	5011	CLA	C4B-NB	-3.52	1.33	1.37
32	8	315	CHL	C3B-C2B	-3.52	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	6	310	CLA	C1C-NC	-3.52	1.32	1.37
31	Z	317	LUT	C2-C1	3.52	1.65	1.54
19	A	840	CLA	C1C-NC	-3.52	1.32	1.37
19	6	323	CLA	C1C-NC	-3.52	1.32	1.37
19	B	819	CLA	MG-ND	-3.51	1.98	2.05
19	5	322	CLA	MG-ND	-3.51	1.98	2.05
19	A	830	CLA	MG-ND	-3.51	1.98	2.05
22	6	307	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
27	5	302	RRX	C7-C6	3.51	1.57	1.45
31	7	303	LUT	C28-C29	3.51	1.53	1.46
19	5	308	CLA	C1C-NC	-3.51	1.32	1.37
22	A	846	BCR	C27-C26	-3.51	1.44	1.51
31	6	306	LUT	C19-C9	3.51	1.57	1.50
19	4	310	CLA	C1C-NC	-3.51	1.32	1.37
19	A	857	CLA	MG-ND	-3.50	1.98	2.05
19	A	840	CLA	C4B-NB	-3.50	1.33	1.37
31	Z	318	LUT	C21-C26	3.50	1.66	1.56
19	A	820	CLA	MG-ND	-3.50	1.98	2.05
19	B	810	CLA	MG-ND	-3.50	1.98	2.05
19	5	310	CLA	C1C-NC	-3.50	1.32	1.37
31	8	305	LUT	C38-C25	3.50	1.57	1.50
19	A	838	CLA	MG-ND	-3.50	1.98	2.05
22	5	305	BCR	C16-C17	3.50	1.54	1.43
19	A	824	CLA	MG-ND	-3.50	1.98	2.05
19	3	5018	CLA	C4B-NB	-3.50	1.33	1.37
19	F	303	CLA	MG-ND	-3.50	1.98	2.05
19	A	810	CLA	C1C-NC	-3.50	1.32	1.37
19	1	5006	CLA	C1C-NC	-3.49	1.32	1.37
31	4	304	LUT	C38-C25	3.49	1.57	1.50
22	3	5006	BCR	C4-C5	-3.49	1.44	1.51
19	B	805	CLA	MG-ND	-3.49	1.98	2.05
19	1	5018	CLA	MG-ND	-3.49	1.98	2.05
19	3	5008	CLA	C1C-NC	-3.49	1.32	1.37
19	1	5006	CLA	C4B-NB	-3.49	1.33	1.37
22	A	848	BCR	C27-C26	-3.49	1.44	1.51
22	A	849	BCR	C4-C5	-3.49	1.44	1.51
19	A	834	CLA	MG-ND	-3.49	1.98	2.05
19	1	5015	CLA	C1C-NC	-3.48	1.32	1.37
19	A	811	CLA	MG-ND	-3.48	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	5005	BCR	C11-C10	3.48	1.54	1.43
19	5	301	CLA	MG-ND	-3.48	1.98	2.05
31	7	303	LUT	C19-C9	3.48	1.57	1.50
19	5	319	CLA	C1C-NC	-3.48	1.32	1.37
19	1	5016	CLA	MG-ND	-3.48	1.98	2.05
22	A	858	BCR	C27-C26	-3.48	1.44	1.51
22	G	1603	BCR	C27-C26	-3.48	1.44	1.51
19	A	803	CLA	MG-ND	-3.48	1.98	2.05
22	3	5004	BCR	C16-C17	3.48	1.54	1.43
19	5	307	CLA	C1C-NC	-3.48	1.32	1.37
22	B	845	BCR	C27-C26	-3.47	1.44	1.51
31	1	5003	LUT	C11-C10	3.47	1.53	1.43
28	J	1902	C7Z	C21-C26	-3.47	1.49	1.53
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	3	5005	BCR	C24-C25	3.47	1.56	1.45
22	4	305	BCR	C24-C25	3.46	1.56	1.45
19	6	318	CLA	C4B-NB	-3.46	1.33	1.37
31	5	303	LUT	C38-C25	3.46	1.56	1.50
31	6	305	LUT	C28-C29	3.46	1.53	1.46
19	4	309	CLA	C1C-NC	-3.46	1.32	1.37
22	4	305	BCR	C4-C5	-3.46	1.44	1.51
22	A	847	BCR	C27-C26	-3.46	1.44	1.51
19	B	806	CLA	MG-ND	-3.46	1.98	2.05
19	A	808	CLA	MG-ND	-3.46	1.98	2.05
19	8	309	CLA	C1C-NC	-3.46	1.32	1.37
22	A	850	BCR	C27-C26	-3.46	1.44	1.51
28	J	1902	C7Z	C7-C6	3.45	1.56	1.45
31	7	304	LUT	C2-C1	3.45	1.65	1.54
19	A	806	CLA	MG-ND	-3.45	1.98	2.05
31	6	306	LUT	C38-C25	3.45	1.56	1.50
19	7	306	CLA	C1C-NC	-3.45	1.32	1.37
19	6	309	CLA	C1C-NC	-3.45	1.32	1.37
31	3	5002	LUT	C2-C1	3.45	1.65	1.54
19	8	314	CLA	C4B-NB	-3.45	1.33	1.37
19	6	312	CLA	C4B-NB	-3.45	1.33	1.37
19	6	322	CLA	C4B-NB	-3.45	1.33	1.37
32	4	319	CHL	CBB-CAB	3.45	1.50	1.29
31	Z	317	LUT	C38-C25	3.44	1.56	1.50
19	5	317	CLA	C1C-NC	-3.44	1.32	1.37
19	4	306	CLA	C1C-NC	-3.44	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	7	316	CLA	C4B-NB	-3.44	1.33	1.37
19	1	5010	CLA	C1C-NC	-3.44	1.32	1.37
19	3	5012	CLA	C1C-NC	-3.44	1.32	1.37
31	Z	317	LUT	C19-C9	3.44	1.57	1.50
19	Z	304	CLA	C4B-NB	-3.44	1.33	1.37
19	8	318	CLA	C1C-NC	-3.44	1.32	1.37
19	4	316	CLA	C1C-NC	-3.44	1.32	1.37
31	6	306	LUT	C2-C1	3.43	1.65	1.54
19	7	324	CLA	C4B-NB	-3.43	1.33	1.37
22	6	308	BCR	C24-C25	3.43	1.56	1.45
19	Z	308	CLA	C4B-NB	-3.43	1.33	1.37
31	8	304	LUT	C2-C1	3.43	1.65	1.54
32	5	320	CHL	CBB-CAB	3.43	1.50	1.29
22	6	308	BCR	C27-C26	-3.43	1.44	1.51
31	1	5003	LUT	C2-C1	3.43	1.65	1.54
22	A	846	BCR	C4-C5	-3.43	1.44	1.51
31	Z	318	LUT	C19-C9	3.43	1.57	1.50
31	8	305	LUT	C11-C10	3.43	1.53	1.43
19	6	318	CLA	C1C-NC	-3.42	1.32	1.37
19	6	311	CLA	C4B-NB	-3.42	1.33	1.37
22	B	844	BCR	C27-C26	-3.42	1.44	1.51
19	6	320	CLA	C4B-NB	-3.42	1.33	1.37
31	3	5003	LUT	C23-C24	-3.42	1.45	1.50
31	7	304	LUT	C23-C24	-3.42	1.45	1.50
19	5	325	CLA	C4B-NB	-3.42	1.33	1.37
19	6	312	CLA	C1C-NC	-3.41	1.32	1.37
31	7	304	LUT	C19-C9	3.41	1.57	1.50
19	5	306	CLA	C1C-NC	-3.41	1.32	1.37
19	7	317	CLA	MG-ND	-3.41	1.99	2.05
19	1	5013	CLA	C4B-NB	-3.41	1.33	1.37
19	1	5012	CLA	MG-ND	-3.40	1.99	2.05
22	F	302	BCR	C4-C5	-3.40	1.44	1.51
31	5	303	LUT	C19-C9	3.40	1.57	1.50
28	J	1902	C7Z	C18-C5	3.40	1.56	1.50
22	B	846	BCR	C27-C26	-3.40	1.44	1.51
19	B	850	CLA	C1C-NC	-3.40	1.32	1.37
19	5	325	CLA	C1C-NC	-3.40	1.32	1.37
31	6	305	LUT	C38-C25	3.40	1.56	1.50
28	6	304	C7Z	C7-C6	3.40	1.56	1.45
31	Z	318	LUT	C38-C25	3.40	1.56	1.50
35	7	302	DGA	OG2-CB1	3.40	1.43	1.34
31	3	5002	LUT	C38-C25	3.40	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	5015	CLA	C1C-NC	-3.39	1.32	1.37
19	Z	306	CLA	C1C-NC	-3.39	1.32	1.37
19	8	310	CLA	C4B-NB	-3.39	1.33	1.37
31	4	304	LUT	C19-C9	3.39	1.57	1.50
19	8	310	CLA	C1C-NC	-3.39	1.32	1.37
19	3	5015	CLA	C4B-NB	-3.39	1.33	1.37
22	K	206	BCR	C27-C26	-3.39	1.44	1.51
31	7	303	LUT	C11-C10	3.39	1.53	1.43
19	4	313	CLA	C1C-NC	-3.39	1.32	1.37
22	B	846	BCR	C4-C5	-3.39	1.44	1.51
19	5	313	CLA	C1C-NC	-3.38	1.32	1.37
32	4	315	CHL	CBB-CAB	3.38	1.50	1.29
19	F	301	CLA	C1C-NC	-3.38	1.32	1.37
19	A	812	CLA	C1C-NC	-3.38	1.32	1.37
22	G	1603	BCR	C4-C5	-3.37	1.44	1.51
22	B	844	BCR	C4-C5	-3.37	1.44	1.51
32	8	317	CHL	CBB-CAB	3.37	1.50	1.29
31	1	5003	LUT	C38-C25	3.37	1.56	1.50
31	7	303	LUT	C38-C25	3.37	1.56	1.50
19	4	307	CLA	MG-ND	-3.37	1.99	2.05
31	1	5004	LUT	C2-C1	3.37	1.64	1.54
32	6	321	CHL	CBB-CAB	3.37	1.50	1.29
28	6	304	C7Z	C18-C5	3.37	1.56	1.50
32	6	317	CHL	CBB-CAB	3.36	1.50	1.29
32	6	316	CHL	CBB-CAB	3.36	1.50	1.29
31	7	304	LUT	C38-C25	3.36	1.56	1.50
27	4	303	RRX	C7-C6	3.36	1.56	1.45
19	Z	307	CLA	C1C-NC	-3.36	1.32	1.37
22	F	302	BCR	C27-C26	-3.36	1.44	1.51
19	7	306	CLA	C4B-NB	-3.36	1.33	1.37
19	8	311	CLA	C4B-NB	-3.36	1.33	1.37
32	6	319	CHL	CBB-CAB	3.35	1.50	1.29
19	7	312	CLA	MG-ND	-3.35	1.99	2.05
31	8	305	LUT	C19-C9	3.35	1.57	1.50
19	7	309	CLA	C4B-NB	-3.35	1.33	1.37
19	1	5013	CLA	C1C-NC	-3.35	1.32	1.37
19	Z	308	CLA	C1C-NC	-3.35	1.32	1.37
31	3	5003	LUT	C19-C9	3.35	1.57	1.50
28	6	304	C7Z	C8-C9	3.35	1.53	1.46
32	4	314	CHL	CBB-CAB	3.35	1.50	1.29
31	1	5004	LUT	C38-C25	3.34	1.56	1.50
31	8	305	LUT	C28-C29	3.34	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	7	318	CLA	C1C-NC	-3.34	1.32	1.37
19	Z	307	CLA	C4B-NB	-3.34	1.33	1.37
32	8	319	CHL	CBB-CAB	3.34	1.50	1.29
31	1	5003	LUT	C19-C9	3.34	1.57	1.50
32	Z	313	CHL	CBB-CAB	3.33	1.50	1.29
19	4	313	CLA	C4B-NB	-3.33	1.33	1.37
19	B	850	CLA	C4B-NB	-3.33	1.33	1.37
19	Z	315	CLA	C1C-NC	-3.33	1.32	1.37
31	1	5004	LUT	C19-C9	3.33	1.57	1.50
19	4	307	CLA	C4B-NB	-3.33	1.33	1.37
32	5	316	CHL	CBB-CAB	3.33	1.50	1.29
19	4	306	CLA	C4B-NB	-3.32	1.33	1.37
19	5	309	CLA	C1C-NC	-3.32	1.32	1.37
19	Z	305	CLA	C4B-NB	-3.32	1.33	1.37
28	1	5005	C7Z	C18-C5	3.32	1.56	1.50
19	7	308	CLA	C1C-NC	-3.31	1.32	1.37
32	5	318	CHL	CBB-CAB	3.31	1.50	1.29
32	6	321	CHL	C3B-C2B	-3.31	1.35	1.40
27	F	304	RRX	C4-C5	-3.31	1.44	1.51
19	Z	305	CLA	C1C-NC	-3.31	1.32	1.37
31	4	304	LUT	C2-C1	3.31	1.64	1.54
32	4	315	CHL	C1A-CHA	-3.30	1.36	1.40
31	5	303	LUT	C28-C29	3.30	1.53	1.46
19	8	308	CLA	C1C-NC	-3.30	1.32	1.37
19	5	307	CLA	C4B-NB	-3.30	1.33	1.37
28	1	5005	C7Z	C7-C6	3.30	1.56	1.45
35	7	302	DGA	OG1-CA1	3.30	1.43	1.33
31	8	304	LUT	C38-C25	3.30	1.56	1.50
32	8	316	CHL	CBB-CAB	3.30	1.50	1.29
19	5	314	CLA	C1C-NC	-3.30	1.32	1.37
28	J	1902	C7Z	C8-C9	3.30	1.53	1.46
19	Z	312	CLA	C1C-NC	-3.29	1.32	1.37
31	3	5002	LUT	C19-C9	3.29	1.57	1.50
19	5	313	CLA	C4B-NB	-3.29	1.33	1.37
19	3	5009	CLA	C1C-NC	-3.29	1.32	1.37
19	Z	312	CLA	C4B-NB	-3.29	1.33	1.37
19	5	308	CLA	C4B-NB	-3.28	1.33	1.37
19	4	316	CLA	C4B-NB	-3.28	1.33	1.37
19	1	5015	CLA	C4B-NB	-3.28	1.33	1.37
22	8	306	BCR	C24-C25	3.28	1.56	1.45
31	Z	318	LUT	C2-C1	3.28	1.64	1.54
22	A	859	BCR	C4-C5	-3.27	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	3	5010	CLA	C1C-NC	-3.27	1.32	1.37
31	8	305	LUT	C2-C1	3.27	1.64	1.54
31	6	305	LUT	C2-C1	3.26	1.64	1.54
31	3	5003	LUT	C38-C25	3.26	1.56	1.50
31	3	5002	LUT	C40-C33	3.26	1.57	1.50
32	3	5017	CHL	CBB-CAB	3.26	1.49	1.29
32	6	319	CHL	C3B-C2B	-3.26	1.36	1.40
19	7	313	CLA	C4B-NB	-3.26	1.33	1.37
31	7	303	LUT	C40-C33	3.25	1.57	1.50
31	6	305	LUT	C19-C9	3.25	1.57	1.50
32	6	315	CHL	CBB-CAB	3.24	1.49	1.29
19	6	301	CLA	C1C-NC	-3.24	1.32	1.37
32	8	315	CHL	CBB-CAB	3.24	1.49	1.29
32	7	315	CHL	CBB-CAB	3.24	1.49	1.29
32	6	316	CHL	C3B-C2B	-3.24	1.36	1.40
19	5	319	CLA	C4B-NB	-3.23	1.33	1.37
32	1	5009	CHL	CHB-C4A	-3.23	1.34	1.38
32	5	315	CHL	CHB-C4A	-3.23	1.34	1.38
31	8	304	LUT	C23-C24	-3.22	1.45	1.50
31	7	303	LUT	C2-C1	3.22	1.64	1.54
19	4	310	CLA	C4B-NB	-3.22	1.33	1.37
19	6	310	CLA	C4B-NB	-3.22	1.33	1.37
31	5	303	LUT	C2-C1	3.22	1.64	1.54
22	3	5004	BCR	C24-C25	3.21	1.56	1.45
31	3	5003	LUT	C2-C1	3.21	1.64	1.54
19	6	323	CLA	C4B-NB	-3.21	1.33	1.37
22	B	842	BCR	C27-C26	-3.21	1.45	1.51
19	8	309	CLA	C4B-NB	-3.21	1.33	1.37
31	5	303	LUT	O23-C23	-3.21	1.38	1.43
19	F	301	CLA	C4B-NB	-3.21	1.33	1.37
31	3	5003	LUT	C40-C33	3.20	1.57	1.50
32	4	317	CHL	CBB-CAB	3.20	1.49	1.29
32	8	301	CHL	CBB-CAB	3.19	1.49	1.29
31	1	5003	LUT	C40-C33	3.19	1.57	1.50
19	3	5010	CLA	C4B-NB	-3.18	1.33	1.37
32	Z	310	CHL	CBB-CAB	3.17	1.49	1.29
31	6	305	LUT	C40-C33	3.17	1.57	1.50
19	8	320	CLA	C1C-NC	-3.17	1.32	1.37
22	8	303	BCR	C27-C26	-3.16	1.45	1.51
32	8	315	CHL	C3B-C4B	3.16	1.44	1.41
31	1	5004	LUT	O23-C23	-3.16	1.38	1.43
32	7	314	CHL	CBB-CAB	3.16	1.49	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	8	304	LUT	C19-C9	3.16	1.57	1.50
31	1	5004	LUT	C28-C29	3.16	1.52	1.46
19	5	317	CLA	C4B-NB	-3.16	1.33	1.37
31	3	5002	LUT	O23-C23	-3.16	1.38	1.43
31	6	306	LUT	C40-C33	3.16	1.57	1.50
19	6	301	CLA	C4B-NB	-3.15	1.33	1.37
19	A	813	CLA	C1C-NC	-3.15	1.32	1.37
31	7	304	LUT	C40-C33	3.15	1.57	1.50
19	7	317	CLA	C1C-NC	-3.14	1.32	1.37
19	G	1601	CLA	C1C-NC	-3.14	1.32	1.37
31	4	304	LUT	O23-C23	-3.14	1.38	1.43
31	Z	318	LUT	C40-C33	3.14	1.57	1.50
19	B	835	CLA	C1C-NC	-3.14	1.32	1.37
32	Z	302	CHL	CBB-CAB	3.13	1.48	1.29
19	8	308	CLA	C4B-NB	-3.13	1.33	1.37
32	Z	302	CHL	CHB-C4A	-3.13	1.34	1.38
19	Z	314	CLA	C1C-NC	-3.13	1.33	1.37
19	A	816	CLA	C1C-NC	-3.13	1.33	1.37
31	6	306	LUT	O23-C23	-3.13	1.38	1.43
32	1	5009	CHL	CBB-CAB	3.12	1.48	1.29
28	1	5005	C7Z	C8-C9	3.12	1.52	1.46
19	7	308	CLA	C4B-NB	-3.12	1.33	1.37
19	5	309	CLA	C4B-NB	-3.12	1.33	1.37
19	F	303	CLA	C1C-NC	-3.11	1.33	1.37
31	8	305	LUT	O23-C23	-3.11	1.38	1.43
19	5	301	CLA	C1C-NC	-3.11	1.33	1.37
38	6	326	ERG	C4-C5	3.11	1.57	1.51
19	A	824	CLA	C1C-NC	-3.10	1.33	1.37
32	1	5014	CHL	C1A-CHA	-3.10	1.36	1.40
19	1	5018	CLA	C1C-NC	-3.10	1.33	1.37
19	B	839	CLA	C1C-NC	-3.10	1.33	1.37
19	Z	306	CLA	C4B-NB	-3.10	1.33	1.37
19	1	5016	CLA	C1C-NC	-3.10	1.33	1.37
31	8	305	LUT	C40-C33	3.10	1.57	1.50
19	B	838	CLA	C1C-NC	-3.10	1.33	1.37
19	A	830	CLA	C1C-NC	-3.10	1.33	1.37
19	A	857	CLA	C1C-NC	-3.09	1.33	1.37
19	B	808	CLA	C1C-NC	-3.09	1.33	1.37
19	B	817	CLA	C1C-NC	-3.09	1.33	1.37
19	7	319	CLA	C1C-NC	-3.09	1.33	1.37
31	7	303	LUT	O23-C23	-3.09	1.38	1.43
19	7	312	CLA	C1C-NC	-3.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	823	CLA	C1C-NC	-3.09	1.33	1.37
19	A	805	CLA	C1C-NC	-3.09	1.33	1.37
19	K	205	CLA	C1C-NC	-3.08	1.33	1.37
19	A	808	CLA	C1C-NC	-3.08	1.33	1.37
19	B	827	CLA	C1C-NC	-3.08	1.33	1.37
19	A	832	CLA	C1C-NC	-3.08	1.33	1.37
19	A	821	CLA	C1C-NC	-3.08	1.33	1.37
32	6	321	CHL	CHB-C4A	-3.08	1.34	1.38
19	B	829	CLA	C1C-NC	-3.08	1.33	1.37
19	A	843	CLA	C1C-NC	-3.08	1.33	1.37
31	Z	318	LUT	C23-C24	-3.08	1.46	1.50
19	B	823	CLA	C1C-NC	-3.07	1.33	1.37
31	Z	317	LUT	C40-C33	3.07	1.57	1.50
19	K	202	CLA	C1C-NC	-3.07	1.33	1.37
19	A	820	CLA	C1C-NC	-3.07	1.33	1.37
32	5	315	CHL	CBB-CAB	3.07	1.48	1.29
19	B	832	CLA	C1C-NC	-3.07	1.33	1.37
31	4	304	LUT	C40-C33	3.07	1.57	1.50
19	A	827	CLA	C1C-NC	-3.06	1.33	1.37
19	A	841	CLA	C1C-NC	-3.06	1.33	1.37
19	A	812	CLA	C4B-NB	-3.06	1.33	1.37
32	7	315	CHL	CHB-C4A	-3.06	1.34	1.38
19	B	830	CLA	C1C-NC	-3.06	1.33	1.37
19	B	834	CLA	C1C-NC	-3.06	1.33	1.37
19	G	1602	CLA	C1C-NC	-3.06	1.33	1.37
19	B	828	CLA	C1C-NC	-3.06	1.33	1.37
19	A	814	CLA	C1C-NC	-3.06	1.33	1.37
19	A	829	CLA	C1C-NC	-3.06	1.33	1.37
19	A	836	CLA	C1C-NC	-3.05	1.33	1.37
19	I	201	CLA	C1C-NC	-3.05	1.33	1.37
19	3	5012	CLA	C4B-NB	-3.05	1.33	1.37
19	3	5014	CLA	C1C-NC	-3.05	1.33	1.37
31	1	5004	LUT	C40-C33	3.04	1.57	1.50
32	Z	310	CHL	CHB-C4A	-3.04	1.35	1.38
19	A	807	CLA	C1C-NC	-3.04	1.33	1.37
19	B	820	CLA	C1C-NC	-3.04	1.33	1.37
19	6	314	CLA	C1C-NC	-3.04	1.33	1.37
19	A	811	CLA	C1C-NC	-3.04	1.33	1.37
19	K	203	CLA	C1C-NC	-3.04	1.33	1.37
22	B	847	BCR	C34-C9	3.04	1.57	1.50
31	7	304	LUT	O23-C23	-3.04	1.38	1.43
19	A	834	CLA	C1C-NC	-3.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	837	CLA	C1C-NC	-3.04	1.33	1.37
19	B	837	CLA	C1C-NC	-3.04	1.33	1.37
19	A	838	CLA	C1C-NC	-3.03	1.33	1.37
19	5	314	CLA	C4B-NB	-3.03	1.33	1.37
19	B	816	CLA	C1C-NC	-3.03	1.33	1.37
19	5	322	CLA	C1C-NC	-3.03	1.33	1.37
31	5	303	LUT	C40-C33	3.03	1.57	1.50
19	B	821	CLA	C1C-NC	-3.03	1.33	1.37
19	B	807	CLA	C1C-NC	-3.03	1.33	1.37
19	K	204	CLA	C1C-NC	-3.03	1.33	1.37
19	4	318	CLA	C1C-NC	-3.03	1.33	1.37
19	4	312	CLA	C1C-NC	-3.03	1.33	1.37
19	J	1901	CLA	C1C-NC	-3.03	1.33	1.37
19	A	818	CLA	C1C-NC	-3.03	1.33	1.37
19	A	831	CLA	C1C-NC	-3.03	1.33	1.37
19	B	802	CLA	C1C-NC	-3.03	1.33	1.37
19	B	809	CLA	C1C-NC	-3.02	1.33	1.37
19	B	805	CLA	C1C-NC	-3.02	1.33	1.37
31	8	304	LUT	C40-C33	3.02	1.57	1.50
19	A	817	CLA	C1C-NC	-3.02	1.33	1.37
19	A	839	CLA	C1C-NC	-3.02	1.33	1.37
19	3	5016	CLA	C1C-NC	-3.02	1.33	1.37
19	5	312	CLA	C1C-NC	-3.02	1.33	1.37
19	B	810	CLA	C1C-NC	-3.02	1.33	1.37
19	B	822	CLA	C1C-NC	-3.01	1.33	1.37
19	B	815	CLA	C1C-NC	-3.01	1.33	1.37
19	A	822	CLA	C1C-NC	-3.01	1.33	1.37
19	A	819	CLA	C1C-NC	-3.01	1.33	1.37
19	A	825	CLA	C1C-NC	-3.01	1.33	1.37
32	5	320	CHL	C1A-CHA	-3.01	1.36	1.40
19	Z	315	CLA	C4B-NB	-3.00	1.33	1.37
19	B	826	CLA	C1C-NC	-3.00	1.33	1.37
19	B	833	CLA	C1C-NC	-3.00	1.33	1.37
19	6	302	CLA	C1C-NC	-3.00	1.33	1.37
32	8	301	CHL	CHB-C4A	-3.00	1.35	1.38
19	A	842	CLA	C1C-NC	-2.99	1.33	1.37
19	B	814	CLA	C1C-NC	-2.99	1.33	1.37
19	A	809	CLA	C1C-NC	-2.99	1.33	1.37
19	1	5011	CLA	C1C-NC	-2.99	1.33	1.37
19	A	828	CLA	C1C-NC	-2.98	1.33	1.37
19	B	813	CLA	C1C-NC	-2.98	1.33	1.37
19	A	835	CLA	C1C-NC	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	804	CLA	C1C-NC	-2.98	1.33	1.37
19	3	5009	CLA	C4B-NB	-2.98	1.33	1.37
19	K	202	CLA	C4B-NB	-2.98	1.33	1.37
32	6	316	CHL	CHB-C4A	-2.98	1.35	1.38
32	4	317	CHL	CHB-C4A	-2.98	1.35	1.38
19	B	829	CLA	C4B-NB	-2.98	1.34	1.37
31	1	5003	LUT	O23-C23	-2.98	1.38	1.43
19	A	813	CLA	C4B-NB	-2.98	1.34	1.37
19	A	833	CLA	C1C-NC	-2.98	1.33	1.37
32	8	319	CHL	C3B-C4B	2.97	1.44	1.41
19	1	5012	CLA	C1C-NC	-2.97	1.33	1.37
19	B	819	CLA	C1C-NC	-2.97	1.33	1.37
31	3	5003	LUT	O23-C23	-2.97	1.38	1.43
19	A	803	CLA	C1C-NC	-2.97	1.33	1.37
19	B	801	CLA	C1C-NC	-2.97	1.33	1.37
19	B	818	CLA	C1C-NC	-2.97	1.33	1.37
19	A	806	CLA	C1C-NC	-2.97	1.33	1.37
22	B	843	BCR	C34-C9	2.97	1.56	1.50
22	8	303	BCR	C34-C9	2.97	1.56	1.50
22	B	846	BCR	C34-C9	2.96	1.56	1.50
19	B	835	CLA	C4B-NB	-2.96	1.34	1.37
32	1	5017	CHL	C1A-CHA	-2.96	1.36	1.40
32	4	319	CHL	C1A-CHA	-2.96	1.36	1.40
19	A	802	CLA	C1C-NC	-2.96	1.33	1.37
19	B	806	CLA	C1C-NC	-2.96	1.33	1.37
19	B	818	CLA	C4B-NB	-2.96	1.34	1.37
31	8	304	LUT	O23-C23	-2.95	1.38	1.43
19	B	803	CLA	C1C-NC	-2.95	1.33	1.37
19	A	843	CLA	C4B-NB	-2.95	1.34	1.37
19	A	816	CLA	C4B-NB	-2.95	1.34	1.37
19	B	811	CLA	C1C-NC	-2.95	1.33	1.37
19	A	826	CLA	C1C-NC	-2.94	1.33	1.37
23	3	5021	LHG	O7-C5	-2.94	1.42	1.46
19	A	837	CLA	C4B-NB	-2.94	1.34	1.37
19	1	5010	CLA	C4B-NB	-2.93	1.34	1.37
22	K	206	BCR	C34-C9	2.93	1.56	1.50
19	A	811	CLA	C4B-NB	-2.93	1.34	1.37
22	A	849	BCR	C34-C9	2.93	1.56	1.50
19	B	824	CLA	C1C-NC	-2.93	1.33	1.37
19	A	838	CLA	C4B-NB	-2.93	1.34	1.37
22	B	842	BCR	C34-C9	2.92	1.56	1.50
19	B	812	CLA	C1C-NC	-2.92	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	848	BCR	C34-C9	2.92	1.56	1.50
22	A	858	BCR	C34-C9	2.92	1.56	1.50
19	A	804	CLA	C1C-NC	-2.92	1.33	1.37
22	A	847	BCR	C34-C9	2.91	1.56	1.50
19	I	201	CLA	C4B-NB	-2.91	1.34	1.37
18	A	801	CL0	CHB-C4A	-2.91	1.35	1.38
32	7	314	CHL	CHB-C4A	-2.91	1.35	1.38
19	A	814	CLA	C4B-NB	-2.91	1.34	1.37
19	B	827	CLA	C4B-NB	-2.91	1.34	1.37
32	3	5017	CHL	CHB-C4A	-2.91	1.35	1.38
22	B	844	BCR	C34-C9	2.90	1.56	1.50
32	8	317	CHL	C1A-CHA	-2.90	1.36	1.40
31	6	305	LUT	O23-C23	-2.90	1.38	1.43
32	6	315	CHL	CHB-C4A	-2.90	1.35	1.38
22	G	1603	BCR	C34-C9	2.90	1.56	1.50
22	A	859	BCR	C34-C9	2.89	1.56	1.50
32	8	319	CHL	CHB-C4A	-2.89	1.35	1.38
19	4	318	CLA	C4B-NB	-2.89	1.34	1.37
31	Z	317	LUT	O23-C23	-2.89	1.38	1.43
32	8	315	CHL	CHB-C4A	-2.89	1.35	1.38
19	B	803	CLA	C4B-NB	-2.89	1.34	1.37
19	A	819	CLA	C4B-NB	-2.89	1.34	1.37
22	B	844	BCR	C7-C6	2.88	1.54	1.45
19	5	312	CLA	C4B-NB	-2.88	1.34	1.37
19	A	839	CLA	C4B-NB	-2.88	1.34	1.37
19	B	819	CLA	C4B-NB	-2.88	1.34	1.37
22	3	5006	BCR	C34-C9	2.88	1.56	1.50
19	B	830	CLA	C4B-NB	-2.88	1.34	1.37
19	A	821	CLA	C4B-NB	-2.87	1.34	1.37
22	A	850	BCR	C34-C9	2.87	1.56	1.50
22	F	302	BCR	C34-C9	2.87	1.56	1.50
19	A	827	CLA	C4B-NB	-2.87	1.34	1.37
19	A	831	CLA	C4B-NB	-2.87	1.34	1.37
22	A	846	BCR	C34-C9	2.87	1.56	1.50
19	7	319	CLA	C4B-NB	-2.87	1.34	1.37
19	B	813	CLA	C4B-NB	-2.86	1.34	1.37
19	B	838	CLA	C4B-NB	-2.86	1.34	1.37
19	B	815	CLA	C4B-NB	-2.86	1.34	1.37
22	A	846	BCR	C7-C6	2.86	1.54	1.45
19	A	822	CLA	C4B-NB	-2.85	1.34	1.37
22	B	845	BCR	C34-C9	2.85	1.56	1.50
22	A	858	BCR	C7-C6	2.85	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	842	BCR	C7-C6	2.85	1.54	1.45
22	3	5007	BCR	C34-C9	2.85	1.56	1.50
19	B	816	CLA	C4B-NB	-2.85	1.34	1.37
19	J	1901	CLA	C4B-NB	-2.84	1.34	1.37
22	8	303	BCR	C7-C6	2.84	1.54	1.45
32	6	319	CHL	CHB-C4A	-2.84	1.35	1.38
32	4	314	CHL	C3B-C2B	-2.84	1.36	1.40
22	B	845	BCR	C7-C6	2.84	1.54	1.45
19	3	5016	CLA	C4B-NB	-2.84	1.34	1.37
19	A	825	CLA	C4B-NB	-2.83	1.34	1.37
19	A	830	CLA	C4B-NB	-2.83	1.34	1.37
19	B	821	CLA	C4B-NB	-2.83	1.34	1.37
19	A	817	CLA	C4B-NB	-2.83	1.34	1.37
19	7	317	CLA	C4B-NB	-2.83	1.34	1.37
19	8	320	CLA	C4B-NB	-2.83	1.34	1.37
32	Z	313	CHL	C3B-C4B	2.83	1.44	1.41
32	Z	313	CHL	CHB-C4A	-2.83	1.35	1.38
19	B	809	CLA	C4B-NB	-2.83	1.34	1.37
19	A	826	CLA	C4B-NB	-2.82	1.34	1.37
32	Z	309	CHL	C1D-C2D	2.82	1.42	1.39
22	F	302	BCR	C7-C6	2.82	1.54	1.45
22	6	307	BCR	C34-C9	2.82	1.56	1.50
19	B	832	CLA	C4B-NB	-2.81	1.34	1.37
32	5	320	CHL	C1D-C2D	2.81	1.42	1.39
19	B	814	CLA	C4B-NB	-2.81	1.34	1.37
22	B	847	BCR	C7-C6	2.81	1.54	1.45
31	Z	318	LUT	O23-C23	-2.81	1.38	1.43
19	A	835	CLA	C4B-NB	-2.81	1.34	1.37
19	3	5014	CLA	C4B-NB	-2.80	1.34	1.37
32	1	5009	CHL	C3A-C2A	-2.80	1.52	1.54
32	1	5017	CHL	C1D-C2D	2.80	1.42	1.39
19	K	204	CLA	C4B-NB	-2.80	1.34	1.37
22	3	5006	BCR	C7-C6	2.80	1.54	1.45
19	A	834	CLA	C4B-NB	-2.80	1.34	1.37
19	1	5011	CLA	C4B-NB	-2.80	1.34	1.37
32	8	316	CHL	CHB-C4A	-2.80	1.35	1.38
19	1	5012	CLA	C4B-NB	-2.79	1.34	1.37
22	A	859	BCR	C7-C6	2.79	1.54	1.45
19	5	322	CLA	C4B-NB	-2.79	1.34	1.37
22	3	5007	BCR	C39-C30	-2.79	1.48	1.53
19	B	817	CLA	C4B-NB	-2.79	1.34	1.37
19	A	802	CLA	C4B-NB	-2.79	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	5	320	CHL	CHB-C4A	-2.79	1.35	1.38
22	A	850	BCR	C7-C6	2.79	1.54	1.45
22	3	5007	BCR	C7-C6	2.79	1.54	1.45
19	A	828	CLA	C4B-NB	-2.79	1.34	1.37
19	B	823	CLA	C4B-NB	-2.78	1.34	1.37
22	4	305	BCR	C7-C6	2.78	1.54	1.45
22	7	305	BCR	C34-C9	2.78	1.56	1.50
19	A	805	CLA	C4B-NB	-2.78	1.34	1.37
19	K	203	CLA	C4B-NB	-2.78	1.34	1.37
19	B	801	CLA	C4B-NB	-2.77	1.34	1.37
19	B	807	CLA	C4B-NB	-2.77	1.34	1.37
32	4	314	CHL	CHB-C4A	-2.77	1.35	1.38
19	K	205	CLA	C4B-NB	-2.77	1.34	1.37
19	B	804	CLA	C4B-NB	-2.77	1.34	1.37
22	A	847	BCR	C7-C6	2.76	1.54	1.45
19	B	805	CLA	C4B-NB	-2.76	1.34	1.37
19	8	312	CLA	MG-NB	-2.76	2.00	2.05
32	1	5014	CHL	C1B-C2B	2.76	1.42	1.39
22	G	1603	BCR	C7-C6	2.75	1.54	1.45
32	Z	310	CHL	C1D-C2D	2.75	1.42	1.39
32	1	5017	CHL	CHB-C4A	-2.75	1.35	1.38
32	Z	309	CHL	C1B-C2B	2.74	1.42	1.39
22	K	206	BCR	C7-C6	2.74	1.54	1.45
22	6	308	BCR	C34-C9	2.74	1.56	1.50
22	B	843	BCR	C7-C6	2.73	1.54	1.45
19	Z	314	CLA	C4B-NB	-2.73	1.34	1.37
19	B	806	CLA	C4B-NB	-2.73	1.34	1.37
32	1	5017	CHL	C1B-C2B	2.73	1.42	1.39
22	7	305	BCR	C7-C6	2.73	1.54	1.45
34	5	324	3PH	O21-C2	-2.73	1.40	1.46
38	6	326	ERG	C1-C10	2.73	1.59	1.54
32	6	321	CHL	C1D-C2D	2.72	1.42	1.39
19	A	804	CLA	C4B-NB	-2.72	1.34	1.37
19	B	811	CLA	C4B-NB	-2.72	1.34	1.37
32	5	320	CHL	C1B-C2B	2.72	1.42	1.39
32	4	315	CHL	C1B-C2B	2.71	1.42	1.39
32	4	319	CHL	CHB-C4A	-2.71	1.35	1.38
19	A	832	CLA	C4B-NB	-2.71	1.34	1.37
22	B	846	BCR	C7-C6	2.71	1.54	1.45
22	8	306	BCR	C34-C9	2.71	1.56	1.50
32	6	317	CHL	C3B-C2B	-2.70	1.36	1.40
32	4	319	CHL	C1D-C2D	2.70	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	5	301	CLA	C4B-NB	-2.70	1.34	1.37
19	B	822	CLA	C4B-NB	-2.70	1.34	1.37
22	A	848	BCR	C7-C6	2.69	1.54	1.45
34	8	322	3PH	O21-C2	-2.69	1.40	1.46
22	6	308	BCR	C7-C6	2.69	1.54	1.45
32	1	5014	CHL	C1D-C2D	2.69	1.42	1.39
22	4	305	BCR	C34-C9	2.69	1.56	1.50
22	5	304	BCR	C7-C6	2.69	1.54	1.45
19	A	833	CLA	C4B-NB	-2.69	1.34	1.37
19	B	834	CLA	C4B-NB	-2.69	1.34	1.37
32	5	316	CHL	C1D-C2D	2.69	1.42	1.39
38	6	326	ERG	C1-C2	-2.69	1.48	1.53
19	B	824	CLA	C4B-NB	-2.68	1.34	1.37
19	B	839	CLA	C4B-NB	-2.68	1.34	1.37
32	4	319	CHL	C1B-C2B	2.68	1.42	1.39
19	B	826	CLA	C4B-NB	-2.68	1.34	1.37
19	6	314	CLA	C4B-NB	-2.68	1.34	1.37
22	5	305	BCR	C34-C9	2.67	1.56	1.50
22	5	304	BCR	C34-C9	2.67	1.56	1.50
32	6	319	CHL	C1D-C2D	2.67	1.42	1.39
19	Z	308	CLA	C3D-C4D	-2.67	1.38	1.44
19	B	808	CLA	C4B-NB	-2.67	1.34	1.37
32	6	319	CHL	C3B-C4B	2.67	1.44	1.41
19	A	836	CLA	C4B-NB	-2.66	1.34	1.37
19	G	1602	CLA	C4B-NB	-2.66	1.34	1.37
19	1	5018	CLA	C4B-NB	-2.66	1.34	1.37
32	6	317	CHL	C1B-C2B	2.65	1.42	1.39
32	7	315	CHL	C3B-C4B	2.65	1.44	1.41
19	B	810	CLA	C4B-NB	-2.65	1.34	1.37
19	1	5007	CLA	C3D-C4D	-2.65	1.38	1.44
19	A	823	CLA	C4B-NB	-2.64	1.34	1.37
19	A	841	CLA	C4B-NB	-2.64	1.34	1.37
32	4	314	CHL	C1D-C2D	2.64	1.42	1.39
22	6	307	BCR	C7-C6	2.64	1.54	1.45
19	B	833	CLA	C4B-NB	-2.63	1.34	1.37
19	A	842	CLA	C4B-NB	-2.63	1.34	1.37
19	B	837	CLA	C4B-NB	-2.63	1.34	1.37
32	8	317	CHL	C1B-C2B	2.63	1.42	1.39
22	B	843	BCR	C36-C18	2.63	1.56	1.50
32	5	316	CHL	CHB-C4A	-2.63	1.35	1.38
19	4	312	CLA	C4B-NB	-2.62	1.34	1.37
19	A	820	CLA	C4B-NB	-2.62	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	820	CLA	C4B-NB	-2.62	1.34	1.37
32	8	317	CHL	C3B-C2B	-2.62	1.36	1.40
19	6	302	CLA	C4B-NB	-2.62	1.34	1.37
32	8	301	CHL	C1D-C2D	2.61	1.42	1.39
32	8	317	CHL	CHB-C4A	-2.61	1.35	1.38
19	6	311	CLA	C3D-C4D	-2.61	1.38	1.44
19	A	809	CLA	C4B-NB	-2.61	1.34	1.37
32	5	318	CHL	C1D-C2D	2.60	1.42	1.39
22	A	849	BCR	C7-C6	2.60	1.54	1.45
32	6	316	CHL	C1D-C2D	2.60	1.42	1.39
19	1	5010	CLA	C3D-C4D	-2.60	1.38	1.44
32	5	316	CHL	C1B-C2B	2.60	1.42	1.39
19	1	5016	CLA	C4B-NB	-2.60	1.34	1.37
32	Z	302	CHL	C1D-C2D	2.59	1.42	1.39
19	4	310	CLA	C3D-C4D	-2.59	1.38	1.44
19	F	303	CLA	C4B-NB	-2.59	1.34	1.37
38	6	326	ERG	C19-C10	-2.59	1.50	1.54
22	8	306	BCR	C39-C30	-2.59	1.48	1.53
32	1	5014	CHL	CHB-C4A	-2.59	1.35	1.38
19	B	836	CLA	C3D-C4D	-2.59	1.38	1.44
19	A	824	CLA	C4B-NB	-2.59	1.34	1.37
19	8	311	CLA	C3D-C4D	-2.58	1.38	1.44
19	A	807	CLA	C4B-NB	-2.58	1.34	1.37
19	B	802	CLA	C4B-NB	-2.58	1.34	1.37
19	B	828	CLA	C4B-NB	-2.58	1.34	1.37
19	G	1601	CLA	C4B-NB	-2.58	1.34	1.37
32	6	315	CHL	C1D-C2D	2.58	1.42	1.39
19	4	311	CLA	MG-ND	-2.57	2.00	2.05
32	Z	313	CHL	C1D-C2D	2.57	1.42	1.39
32	Z	309	CHL	CHB-C4A	-2.57	1.35	1.38
19	A	808	CLA	C4B-NB	-2.57	1.34	1.37
19	A	806	CLA	C4B-NB	-2.57	1.34	1.37
19	A	829	CLA	C4B-NB	-2.57	1.34	1.37
28	J	1902	C7Z	C20-C13	2.56	1.56	1.50
19	8	318	CLA	C3D-C4D	-2.56	1.38	1.44
32	6	317	CHL	CHB-C4A	-2.56	1.35	1.38
32	4	314	CHL	C1B-C2B	2.55	1.42	1.39
22	6	307	BCR	C39-C30	-2.55	1.48	1.53
32	5	315	CHL	C1D-C2D	2.55	1.42	1.39
19	3	5013	CLA	C3D-C4D	-2.55	1.38	1.44
19	A	857	CLA	C4B-NB	-2.55	1.34	1.37
19	A	840	CLA	C3D-C4D	-2.55	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	6	317	CHL	C1D-C2D	2.55	1.42	1.39
32	5	318	CHL	C1B-C2B	2.54	1.42	1.39
32	5	318	CHL	CHB-C4A	-2.54	1.35	1.38
19	B	840	CLA	C3D-C4D	-2.54	1.38	1.44
19	7	310	CLA	C3D-C4D	-2.54	1.38	1.44
31	3	5003	LUT	C26-C27	2.54	1.54	1.50
28	1	5005	C7Z	C38-C25	2.54	1.55	1.50
19	B	812	CLA	C4B-NB	-2.53	1.34	1.37
19	B	831	CLA	C3D-C4D	-2.53	1.38	1.44
19	A	818	CLA	C4B-NB	-2.53	1.34	1.37
22	5	305	BCR	C7-C6	2.53	1.53	1.45
22	F	302	BCR	C36-C18	2.53	1.56	1.50
19	5	325	CLA	C3D-C4D	-2.53	1.38	1.44
22	5	304	BCR	C39-C30	-2.53	1.49	1.53
22	3	5004	BCR	C7-C6	2.52	1.53	1.45
19	7	307	CLA	C3D-C4D	-2.52	1.38	1.44
22	B	846	BCR	C36-C18	2.52	1.55	1.50
19	A	803	CLA	C4B-NB	-2.52	1.34	1.37
32	3	5017	CHL	C1D-C2D	2.52	1.42	1.39
28	6	304	C7Z	C20-C13	2.52	1.55	1.50
19	7	306	CLA	C3D-C4D	-2.52	1.38	1.44
32	8	315	CHL	C1D-C2D	2.52	1.42	1.39
19	7	312	CLA	C4B-NB	-2.51	1.34	1.37
22	A	846	BCR	C36-C18	2.51	1.55	1.50
32	Z	310	CHL	C2C-C3C	-2.51	1.33	1.36
22	K	206	BCR	C36-C18	2.51	1.55	1.50
32	7	315	CHL	C1D-C2D	2.50	1.42	1.39
22	8	306	BCR	C7-C6	2.50	1.53	1.45
22	8	303	BCR	C36-C18	2.50	1.55	1.50
22	B	847	BCR	C36-C18	2.50	1.55	1.50
19	Z	305	CLA	C3D-C4D	-2.50	1.38	1.44
32	8	316	CHL	C3B-C2B	-2.50	1.37	1.40
19	3	5012	CLA	C3D-C4D	-2.50	1.38	1.44
32	3	5017	CHL	C1B-C2B	2.50	1.42	1.39
32	8	316	CHL	C1B-C2B	2.50	1.42	1.39
22	3	5004	BCR	C34-C9	2.49	1.55	1.50
32	4	317	CHL	C1D-C2D	2.49	1.42	1.39
19	7	311	CLA	C3D-C4D	-2.49	1.38	1.44
22	A	847	BCR	C36-C18	2.48	1.55	1.50
31	1	5003	LUT	C18-C5	2.48	1.54	1.50
32	4	315	CHL	CHB-C4A	-2.48	1.35	1.38
32	6	319	CHL	C1B-C2B	2.48	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	842	BCR	C36-C18	2.48	1.55	1.50
19	5	310	CLA	C3D-C4D	-2.48	1.38	1.44
19	B	850	CLA	C3D-C4D	-2.48	1.38	1.44
19	B	825	CLA	C3D-C4D	-2.48	1.38	1.44
19	F	301	CLA	C3D-C4D	-2.48	1.38	1.44
19	7	308	CLA	C3D-C4D	-2.48	1.38	1.44
22	6	308	BCR	C39-C30	-2.47	1.49	1.53
19	7	324	CLA	C3D-C4D	-2.47	1.38	1.44
28	J	1902	C7Z	C38-C25	2.47	1.54	1.50
22	3	5005	BCR	C39-C30	-2.47	1.49	1.53
19	3	5008	CLA	C3D-C4D	-2.47	1.38	1.44
19	1	5013	CLA	C3D-C4D	-2.47	1.38	1.44
19	A	815	CLA	C3D-C4D	-2.47	1.38	1.44
22	A	858	BCR	C36-C18	2.47	1.55	1.50
19	7	313	CLA	C3D-C4D	-2.46	1.38	1.44
19	7	309	CLA	C3D-C4D	-2.46	1.38	1.44
19	5	308	CLA	C3D-C4D	-2.46	1.38	1.44
19	8	312	CLA	CHC-C1C	2.46	1.43	1.38
18	A	801	CL0	C3A-C2A	-2.46	1.52	1.54
22	B	844	BCR	C36-C18	2.46	1.55	1.50
27	F	304	RRX	C34-C9	2.46	1.55	1.50
32	8	319	CHL	C1B-C2B	2.46	1.42	1.39
19	3	5020	CLA	C3D-C4D	-2.46	1.38	1.44
19	A	812	CLA	C3D-C4D	-2.46	1.38	1.44
31	8	305	LUT	C18-C5	2.46	1.54	1.50
22	3	5005	BCR	C34-C9	2.46	1.55	1.50
19	1	5008	CLA	C3D-C4D	-2.46	1.38	1.44
19	Z	306	CLA	C3D-C4D	-2.45	1.38	1.44
19	6	320	CLA	C3D-C4D	-2.45	1.38	1.44
22	5	305	BCR	C39-C30	-2.45	1.49	1.53
22	3	5006	BCR	C36-C18	2.45	1.55	1.50
19	3	5018	CLA	C3D-C4D	-2.45	1.38	1.44
19	5	321	CLA	C3D-C4D	-2.45	1.38	1.44
32	Z	313	CHL	C1B-C2B	2.45	1.42	1.39
38	8	325	ERG	C1-C2	-2.45	1.48	1.53
22	7	305	BCR	C36-C18	2.45	1.55	1.50
19	5	307	CLA	C3D-C4D	-2.44	1.38	1.44
19	8	309	CLA	C3D-C4D	-2.44	1.38	1.44
19	7	316	CLA	C3D-C4D	-2.44	1.38	1.44
19	8	307	CLA	C3D-C4D	-2.44	1.38	1.44
19	5	317	CLA	C3D-C4D	-2.44	1.38	1.44
32	4	315	CHL	C1D-C2D	2.43	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	6	312	CLA	C3D-C4D	-2.43	1.38	1.44
19	5	306	CLA	C3D-C4D	-2.43	1.38	1.44
22	3	5004	BCR	C39-C30	-2.43	1.49	1.53
22	7	305	BCR	C38-C26	2.43	1.54	1.50
31	7	303	LUT	C18-C5	2.43	1.54	1.50
32	5	316	CHL	C3B-C2B	-2.43	1.37	1.40
32	5	318	CHL	C3B-C2B	-2.43	1.37	1.40
28	J	1902	C7Z	C40-C33	2.43	1.55	1.50
22	A	859	BCR	C36-C18	2.43	1.55	1.50
19	6	322	CLA	C3D-C4D	-2.43	1.38	1.44
34	3	5022	3PH	O21-C2	-2.43	1.40	1.46
19	6	318	CLA	C3D-C4D	-2.43	1.38	1.44
22	A	850	BCR	C36-C18	2.42	1.55	1.50
19	3	5011	CLA	C3D-C4D	-2.42	1.38	1.44
19	3	5019	CLA	C3D-C4D	-2.42	1.38	1.44
19	4	316	CLA	C3D-C4D	-2.42	1.38	1.44
38	8	325	ERG	C1-C10	2.41	1.58	1.54
32	8	315	CHL	C1B-C2B	2.41	1.42	1.39
28	6	304	C7Z	C38-C25	2.41	1.54	1.50
31	6	305	LUT	C18-C5	2.41	1.54	1.50
22	3	5005	BCR	C7-C6	2.41	1.53	1.45
32	Z	310	CHL	C1B-C2B	2.41	1.42	1.39
19	4	306	CLA	C3D-C4D	-2.41	1.38	1.44
32	8	316	CHL	C1D-C2D	2.41	1.42	1.39
32	3	5017	CHL	C3B-C2B	-2.41	1.37	1.40
19	7	318	CLA	C3D-C4D	-2.40	1.38	1.44
22	B	843	BCR	C39-C30	-2.40	1.49	1.53
22	G	1603	BCR	C36-C18	2.40	1.55	1.50
31	8	304	LUT	C18-C5	2.40	1.54	1.50
32	6	315	CHL	C1B-C2B	2.40	1.42	1.39
34	3	5022	3PH	O31-C31	2.40	1.40	1.33
22	B	843	BCR	C37-C22	2.39	1.55	1.50
32	1	5009	CHL	C1D-C2D	2.39	1.42	1.39
19	8	313	CLA	C3D-C4D	-2.39	1.38	1.44
19	5	309	CLA	C3D-C4D	-2.39	1.38	1.44
32	8	319	CHL	C1D-C2D	2.39	1.42	1.39
19	Z	315	CLA	C3D-C4D	-2.39	1.38	1.44
32	7	315	CHL	C1B-C2B	2.39	1.42	1.39
28	6	304	C7Z	C40-C33	2.39	1.55	1.50
19	A	810	CLA	C3D-C4D	-2.39	1.38	1.44
19	8	314	CLA	C3D-C4D	-2.39	1.38	1.44
19	4	311	CLA	MG-NB	-2.39	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	307	CLA	C3D-C4D	-2.39	1.38	1.44
31	1	5004	LUT	C18-C5	2.39	1.54	1.50
32	6	321	CHL	C1B-C2B	2.39	1.42	1.39
31	Z	318	LUT	C18-C5	2.38	1.54	1.50
28	1	5005	C7Z	C20-C13	2.38	1.55	1.50
19	1	5015	CLA	C3D-C4D	-2.38	1.38	1.44
32	7	314	CHL	C1B-C2B	2.38	1.42	1.39
32	8	301	CHL	C1B-C2B	2.38	1.42	1.39
19	3	5010	CLA	C3D-C4D	-2.38	1.38	1.44
19	1	5006	CLA	C3D-C4D	-2.38	1.38	1.44
19	3	5009	CLA	C3D-C4D	-2.38	1.38	1.44
19	6	323	CLA	C3D-C4D	-2.38	1.38	1.44
19	8	310	CLA	C3D-C4D	-2.38	1.38	1.44
22	4	305	BCR	C36-C18	2.38	1.55	1.50
22	B	845	BCR	C36-C18	2.38	1.55	1.50
19	4	309	CLA	C3D-C4D	-2.38	1.38	1.44
19	6	301	CLA	C3D-C4D	-2.37	1.38	1.44
19	5	313	CLA	C3D-C4D	-2.37	1.38	1.44
19	Z	311	CLA	C3D-C4D	-2.37	1.38	1.44
22	4	305	BCR	C39-C30	-2.37	1.49	1.53
23	7	320	LHG	O7-C5	-2.37	1.41	1.46
19	5	311	CLA	C3D-C4D	-2.37	1.38	1.44
19	4	307	CLA	C3D-C4D	-2.37	1.38	1.44
32	6	316	CHL	C1B-C2B	2.36	1.42	1.39
35	7	302	DGA	OG2-CG2	-2.36	1.41	1.46
31	8	304	LUT	C26-C27	2.36	1.53	1.50
34	5	324	3PH	O31-C31	2.36	1.40	1.33
32	Z	302	CHL	C1B-C2B	2.36	1.42	1.39
19	Z	304	CLA	C3D-C4D	-2.36	1.38	1.44
31	3	5003	LUT	C18-C5	2.36	1.54	1.50
19	4	313	CLA	C3D-C4D	-2.36	1.38	1.44
19	Z	303	CLA	C3D-C4D	-2.35	1.38	1.44
19	5	314	CLA	C3D-C4D	-2.35	1.38	1.44
19	6	309	CLA	C3D-C4D	-2.35	1.38	1.44
19	6	310	CLA	C3D-C4D	-2.35	1.38	1.44
19	8	308	CLA	C3D-C4D	-2.34	1.38	1.44
19	5	319	CLA	C3D-C4D	-2.34	1.38	1.44
34	6	325	3PH	O21-C2	-2.34	1.41	1.46
32	8	317	CHL	C1D-C2D	2.34	1.42	1.39
31	5	303	LUT	C18-C5	2.32	1.54	1.50
32	1	5009	CHL	C1B-C2B	2.32	1.42	1.39
19	8	312	CLA	C3D-C4D	-2.32	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	307	BCR	C36-C18	2.32	1.55	1.50
32	8	301	CHL	C2C-C3C	-2.32	1.34	1.36
32	7	314	CHL	C1D-C2D	2.32	1.42	1.39
22	B	842	BCR	C39-C30	-2.31	1.49	1.53
19	Z	312	CLA	C3D-C4D	-2.31	1.39	1.44
28	1	5005	C7Z	C40-C33	2.31	1.55	1.50
22	3	5007	BCR	C36-C18	2.31	1.55	1.50
31	3	5002	LUT	C18-C5	2.31	1.54	1.50
32	4	317	CHL	C1B-C2B	2.30	1.42	1.39
22	A	848	BCR	C36-C18	2.30	1.55	1.50
34	8	322	3PH	O31-C3	-2.30	1.40	1.45
34	6	325	3PH	O21-C21	2.30	1.40	1.34
27	4	303	RRX	C34-C9	2.30	1.55	1.50
22	G	1603	BCR	C39-C30	-2.30	1.49	1.53
34	6	325	3PH	O31-C31	2.29	1.40	1.33
19	6	313	CLA	C3D-C4D	-2.29	1.39	1.44
22	8	303	BCR	C39-C30	-2.29	1.49	1.53
22	A	846	BCR	C39-C30	-2.28	1.49	1.53
22	A	858	BCR	C39-C30	-2.27	1.49	1.53
32	5	315	CHL	C1B-C2B	2.27	1.42	1.39
32	5	320	CHL	C3B-C2B	-2.27	1.37	1.40
32	8	319	CHL	C2C-C3C	-2.27	1.34	1.36
38	6	326	ERG	C14-C8	2.27	1.57	1.51
28	1	5005	C7Z	C19-C9	2.26	1.55	1.50
28	6	304	C7Z	C19-C9	2.26	1.55	1.50
31	Z	317	LUT	C18-C5	2.26	1.54	1.50
22	8	303	BCR	C38-C26	2.25	1.54	1.50
22	B	844	BCR	C39-C30	-2.25	1.49	1.53
34	6	325	3PH	O31-C3	-2.25	1.40	1.45
22	B	847	BCR	C37-C22	2.25	1.55	1.50
22	A	859	BCR	C39-C30	-2.25	1.49	1.53
22	A	848	BCR	C38-C26	2.25	1.54	1.50
22	3	5006	BCR	C39-C30	-2.25	1.49	1.53
34	5	324	3PH	O31-C3	-2.24	1.40	1.45
22	A	850	BCR	C39-C30	-2.24	1.49	1.53
32	6	316	CHL	C2C-C3C	2.24	1.38	1.36
22	A	849	BCR	C36-C18	2.23	1.55	1.50
28	J	1902	C7Z	C19-C9	2.23	1.55	1.50
27	F	304	RRX	C33-C5	2.23	1.54	1.50
22	A	848	BCR	C39-C30	-2.23	1.49	1.53
31	6	306	LUT	C26-C27	2.23	1.53	1.50
22	B	847	BCR	C39-C30	-2.22	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	F	302	BCR	C39-C30	-2.22	1.49	1.53
19	4	308	CLA	C3D-C4D	-2.22	1.39	1.44
19	3	5015	CLA	C3D-C4D	-2.22	1.39	1.44
22	B	845	BCR	C39-C30	-2.22	1.49	1.53
22	A	847	BCR	C39-C30	-2.21	1.49	1.53
22	K	206	BCR	C39-C30	-2.21	1.49	1.53
22	A	847	BCR	C37-C22	2.21	1.55	1.50
22	A	859	BCR	C38-C26	2.21	1.54	1.50
31	6	306	LUT	C18-C5	2.20	1.54	1.50
34	8	322	3PH	O31-C31	2.20	1.39	1.33
31	7	304	LUT	C18-C5	2.20	1.54	1.50
22	F	302	BCR	C37-C22	2.20	1.55	1.50
32	4	319	CHL	C3B-C2B	-2.20	1.37	1.40
22	A	858	BCR	C38-C26	2.19	1.54	1.50
22	K	206	BCR	C37-C22	2.19	1.55	1.50
22	B	844	BCR	C38-C26	2.19	1.54	1.50
19	B	805	CLA	C1C-C2C	2.18	1.49	1.44
22	B	842	BCR	C38-C26	2.18	1.54	1.50
22	5	304	BCR	C36-C18	2.18	1.55	1.50
22	B	846	BCR	C39-C30	-2.18	1.49	1.53
22	8	306	BCR	C36-C18	2.18	1.55	1.50
22	A	846	BCR	C38-C26	2.18	1.54	1.50
22	6	308	BCR	C36-C18	2.18	1.55	1.50
22	B	842	BCR	C37-C22	2.18	1.55	1.50
34	3	5022	3PH	O21-C21	2.18	1.40	1.34
19	4	311	CLA	C3D-C4D	-2.18	1.39	1.44
22	A	850	BCR	C38-C26	2.17	1.54	1.50
22	A	859	BCR	C37-C22	2.17	1.55	1.50
22	A	858	BCR	C37-C22	2.17	1.55	1.50
22	A	847	BCR	C38-C26	2.17	1.54	1.50
27	5	302	RRX	C34-C9	2.17	1.55	1.50
32	8	319	CHL	C3B-C2B	-2.17	1.37	1.40
22	3	5005	BCR	C36-C18	2.17	1.55	1.50
22	B	845	BCR	C38-C26	2.16	1.54	1.50
22	F	302	BCR	C38-C26	2.16	1.54	1.50
22	3	5004	BCR	C36-C18	2.16	1.55	1.50
22	B	846	BCR	C38-C26	2.16	1.54	1.50
19	G	1602	CLA	C1C-C2C	2.16	1.48	1.44
22	A	846	BCR	C37-C22	2.15	1.55	1.50
22	K	206	BCR	C38-C26	2.15	1.54	1.50
22	A	850	BCR	C37-C22	2.15	1.55	1.50
22	B	844	BCR	C37-C22	2.15	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	8	325	ERG	C18-C13	-2.15	1.50	1.54
22	3	5006	BCR	C38-C26	2.15	1.54	1.50
22	3	5006	BCR	C37-C22	2.15	1.55	1.50
19	B	811	CLA	C1C-C2C	2.14	1.48	1.44
19	A	806	CLA	C1C-C2C	2.14	1.48	1.44
22	G	1603	BCR	C38-C26	2.14	1.54	1.50
19	A	818	CLA	C1C-C2C	2.14	1.48	1.44
34	3	5022	3PH	O31-C3	-2.14	1.40	1.45
19	J	1901	CLA	C1C-C2C	2.14	1.48	1.44
19	8	312	CLA	C1C-C2C	2.13	1.48	1.44
22	A	848	BCR	C37-C22	2.13	1.55	1.50
32	4	317	CHL	C3D-C2D	-2.13	1.36	1.39
22	B	845	BCR	C37-C22	2.13	1.55	1.50
22	B	847	BCR	C38-C26	2.13	1.54	1.50
19	B	812	CLA	C1C-C2C	2.13	1.48	1.44
22	8	303	BCR	C37-C22	2.12	1.55	1.50
19	4	312	CLA	C1C-C2C	2.11	1.48	1.44
19	A	841	CLA	C1C-C2C	2.11	1.48	1.44
32	4	317	CHL	C2C-C3C	-2.11	1.34	1.36
19	A	804	CLA	C1C-C2C	2.11	1.48	1.44
22	G	1603	BCR	C37-C22	2.11	1.55	1.50
19	F	303	CLA	C1C-C2C	2.11	1.48	1.44
32	Z	313	CHL	C3B-C2B	-2.10	1.37	1.40
22	A	849	BCR	C38-C26	2.10	1.54	1.50
22	A	849	BCR	C39-C30	-2.10	1.49	1.53
32	1	5014	CHL	CHA-CBD	2.10	1.54	1.51
19	G	1602	CLA	C3D-C4D	-2.09	1.39	1.44
19	B	806	CLA	C1C-C2C	2.09	1.48	1.44
19	A	829	CLA	C1C-C2C	2.09	1.48	1.44
19	5	301	CLA	C1C-C2C	2.09	1.48	1.44
19	I	201	CLA	C3D-C4D	-2.09	1.39	1.44
19	7	317	CLA	C3D-C4D	-2.09	1.39	1.44
19	B	821	CLA	C1C-C2C	2.09	1.48	1.44
19	A	802	CLA	C1C-C2C	2.09	1.48	1.44
19	5	312	CLA	C1C-C2C	2.09	1.48	1.44
22	6	307	BCR	C38-C26	2.09	1.54	1.50
19	B	803	CLA	C1C-C2C	2.09	1.48	1.44
19	1	5011	CLA	C3D-C4D	-2.09	1.39	1.44
19	A	809	CLA	C1C-C2C	2.09	1.48	1.44
19	B	822	CLA	C1C-C2C	2.09	1.48	1.44
19	1	5016	CLA	C1C-C2C	2.08	1.48	1.44
19	B	838	CLA	C1C-C2C	2.08	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	807	CLA	C1C-C2C	2.08	1.48	1.44
19	A	803	CLA	C1C-C2C	2.08	1.48	1.44
19	A	837	CLA	C1C-C2C	2.08	1.48	1.44
34	8	322	3PH	O21-C21	2.08	1.40	1.34
22	7	305	BCR	C37-C22	2.08	1.55	1.50
32	7	314	CHL	CHA-CBD	2.08	1.54	1.51
19	3	5014	CLA	C1C-C2C	2.08	1.48	1.44
31	8	305	LUT	C35-C15	-2.07	1.30	1.36
19	A	805	CLA	C3D-C4D	-2.07	1.39	1.44
19	A	826	CLA	C1C-C2C	2.07	1.48	1.44
19	B	818	CLA	C1C-C2C	2.07	1.48	1.44
19	6	314	CLA	C1C-C2C	2.07	1.48	1.44
19	A	857	CLA	C1C-C2C	2.07	1.48	1.44
19	A	837	CLA	C3D-C4D	-2.07	1.39	1.44
22	3	5006	BCR	C33-C5	2.07	1.54	1.50
31	Z	317	LUT	C28-C27	2.07	1.37	1.32
19	A	811	CLA	C1C-C2C	2.07	1.48	1.44
19	B	820	CLA	C1C-C2C	2.07	1.48	1.44
19	B	817	CLA	C3D-C4D	-2.07	1.39	1.44
32	1	5009	CHL	CHD-C1D	-2.07	1.36	1.39
19	A	822	CLA	C1C-C2C	2.07	1.48	1.44
19	B	801	CLA	C1C-C2C	2.07	1.48	1.44
19	A	834	CLA	C3D-C4D	-2.07	1.39	1.44
19	6	302	CLA	C1C-C2C	2.07	1.48	1.44
22	A	849	BCR	C37-C22	2.07	1.55	1.50
19	B	816	CLA	C1C-C2C	2.07	1.48	1.44
19	A	828	CLA	C1C-C2C	2.07	1.48	1.44
19	B	814	CLA	C1C-C2C	2.07	1.48	1.44
32	1	5009	CHL	C3D-C2D	-2.06	1.36	1.39
23	6	324	LHG	O7-C5	-2.06	1.41	1.46
19	B	824	CLA	C1C-C2C	2.06	1.48	1.44
19	B	833	CLA	C1C-C2C	2.06	1.48	1.44
19	4	311	CLA	CHC-C1C	2.06	1.42	1.38
19	A	820	CLA	C1C-C2C	2.06	1.48	1.44
19	A	824	CLA	C1C-C2C	2.06	1.48	1.44
22	7	305	BCR	C33-C5	2.06	1.54	1.50
22	3	5007	BCR	C37-C22	2.06	1.55	1.50
19	B	807	CLA	C3D-C4D	-2.06	1.39	1.44
19	B	804	CLA	C1A-CHA	2.06	1.51	1.43
19	A	827	CLA	C1C-C2C	2.06	1.48	1.44
19	B	839	CLA	C1C-C2C	2.06	1.48	1.44
19	A	842	CLA	C1C-C2C	2.06	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	827	CLA	C1C-C2C	2.05	1.48	1.44
19	B	807	CLA	C1C-C2C	2.05	1.48	1.44
19	7	312	CLA	C1C-C2C	2.05	1.48	1.44
19	Z	314	CLA	C1C-C2C	2.05	1.48	1.44
19	B	834	CLA	C1C-C2C	2.05	1.48	1.44
19	A	816	CLA	C3D-C4D	-2.05	1.39	1.44
19	1	5018	CLA	C1C-C2C	2.05	1.48	1.44
19	B	810	CLA	C1C-C2C	2.05	1.48	1.44
19	A	819	CLA	C1C-C2C	2.05	1.48	1.44
19	K	204	CLA	C3D-C4D	-2.05	1.39	1.44
19	5	322	CLA	C1C-C2C	2.04	1.48	1.44
19	A	825	CLA	C1C-C2C	2.04	1.48	1.44
19	3	5016	CLA	C1C-C2C	2.04	1.48	1.44
19	A	814	CLA	C3D-C4D	-2.04	1.39	1.44
19	A	819	CLA	C3D-C4D	-2.04	1.39	1.44
31	7	304	LUT	C26-C27	2.04	1.53	1.50
22	7	305	BCR	C39-C30	-2.04	1.49	1.53
19	B	830	CLA	C1C-C2C	2.04	1.48	1.44
19	A	808	CLA	C1C-C2C	2.04	1.48	1.44
19	A	811	CLA	C3D-C4D	-2.03	1.39	1.44
19	Z	314	CLA	C3D-C4D	-2.03	1.39	1.44
19	B	828	CLA	C1C-C2C	2.03	1.48	1.44
19	B	827	CLA	C3D-C4D	-2.03	1.39	1.44
19	A	833	CLA	C1C-C2C	2.03	1.48	1.44
19	7	312	CLA	C1A-CHA	2.03	1.51	1.43
19	A	823	CLA	C1C-C2C	2.03	1.48	1.44
32	8	317	CHL	CHC-C4B	-2.03	1.36	1.39
32	1	5014	CHL	C2C-C3C	2.03	1.38	1.36
32	8	315	CHL	CHA-CBD	2.03	1.54	1.51
34	5	324	3PH	O21-C21	2.02	1.40	1.34
22	B	846	BCR	C37-C22	2.02	1.54	1.50
19	A	836	CLA	C3D-C4D	-2.02	1.39	1.44
19	B	805	CLA	C3D-C4D	-2.02	1.39	1.44
19	A	843	CLA	C1C-C2C	2.02	1.48	1.44
19	4	318	CLA	C3D-C4D	-2.02	1.39	1.44
19	A	817	CLA	C1C-C2C	2.02	1.48	1.44
19	8	320	CLA	C1C-C2C	2.02	1.48	1.44
19	A	832	CLA	C3D-C4D	-2.02	1.39	1.44
19	A	835	CLA	C1C-C2C	2.02	1.48	1.44
22	B	846	BCR	C33-C5	2.02	1.54	1.50
19	A	836	CLA	C1C-C2C	2.02	1.48	1.44
19	A	843	CLA	C3D-C4D	-2.02	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	831	CLA	C1C-C2C	2.02	1.48	1.44
19	B	806	CLA	C3D-C4D	-2.02	1.39	1.44
19	B	811	CLA	C3D-C4D	-2.02	1.39	1.44
19	1	5012	CLA	C1A-CHA	2.02	1.51	1.43
19	K	202	CLA	C1A-CHA	2.01	1.51	1.43
19	A	826	CLA	C1A-CHA	2.01	1.51	1.43
32	4	315	CHL	CHA-CBD	2.01	1.54	1.51
19	1	5012	CLA	C1C-C2C	2.01	1.48	1.44
22	B	847	BCR	C33-C5	2.01	1.54	1.50
19	B	837	CLA	C3D-C4D	-2.01	1.39	1.44
27	4	303	RRX	C33-C5	2.01	1.54	1.50
19	A	803	CLA	C3D-C4D	-2.01	1.39	1.44
19	A	828	CLA	C3D-C4D	-2.01	1.39	1.44
19	A	825	CLA	MG-NC	2.01	2.11	2.06
19	B	808	CLA	C1C-C2C	2.01	1.48	1.44
19	K	203	CLA	C1C-C2C	2.01	1.48	1.44
19	4	318	CLA	C1C-C2C	2.01	1.48	1.44
19	7	319	CLA	C3D-C4D	-2.01	1.39	1.44
19	B	821	CLA	C1A-CHA	2.01	1.51	1.43
19	F	301	CLA	CHC-C1C	2.01	1.42	1.38
19	5	301	CLA	C3D-C4D	-2.01	1.39	1.44
19	B	833	CLA	C3D-C4D	-2.00	1.39	1.44
19	A	823	CLA	C3D-C4D	-2.00	1.39	1.44
22	4	305	BCR	C37-C22	2.00	1.54	1.50
27	5	302	RRX	C33-C5	2.00	1.54	1.50
19	A	857	CLA	C3D-C4D	-2.00	1.39	1.44
19	B	835	CLA	C3D-C4D	-2.00	1.39	1.44
19	A	805	CLA	C1C-C2C	2.00	1.48	1.44
19	B	813	CLA	C1A-CHA	2.00	1.51	1.43
32	4	315	CHL	C3B-C2B	-2.00	1.37	1.40
19	A	813	CLA	C3D-C4D	-2.00	1.39	1.44
19	B	838	CLA	C3D-C4D	-2.00	1.39	1.44
19	A	839	CLA	C1C-C2C	2.00	1.48	1.44
32	7	314	CHL	CHD-C1D	-2.00	1.36	1.39
19	K	203	CLA	C3D-C4D	-2.00	1.39	1.44

All (4900) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Z	317	LUT	C35-C34-C33	-14.21	107.35	127.28
18	A	801	CL0	C1B-CHB-C4A	14.18	130.44	121.32
31	Z	317	LUT	C31-C30-C29	-13.65	108.13	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	5007	BCR	C11-C10-C9	-11.46	111.21	127.28
22	3	5007	BCR	C20-C21-C22	-10.67	112.31	127.28
19	B	831	CLA	C4A-NA-C1A	9.91	111.20	106.68
19	8	307	CLA	C4A-NA-C1A	9.61	111.06	106.68
19	B	836	CLA	C4A-NA-C1A	9.59	111.05	106.68
19	4	309	CLA	C4A-NA-C1A	9.58	111.05	106.68
38	8	325	ERG	C15-C14-C8	-9.54	107.47	120.42
19	7	307	CLA	C4A-NA-C1A	9.53	111.03	106.68
19	5	317	CLA	C4A-NA-C1A	9.53	111.03	106.68
19	7	311	CLA	C4A-NA-C1A	9.48	111.00	106.68
19	3	5013	CLA	C4A-NA-C1A	9.47	111.00	106.68
38	6	326	ERG	C15-C14-C8	-9.46	107.58	120.42
19	7	316	CLA	C4A-NA-C1A	9.42	110.98	106.68
19	3	5018	CLA	C4A-NA-C1A	9.40	110.97	106.68
19	B	840	CLA	C4A-NA-C1A	9.37	110.95	106.68
19	5	321	CLA	C4A-NA-C1A	9.32	110.93	106.68
19	6	313	CLA	C4A-NA-C1A	9.26	110.90	106.68
19	1	5006	CLA	C4A-NA-C1A	9.25	110.90	106.68
19	8	309	CLA	C4A-NA-C1A	9.24	110.89	106.68
19	A	815	CLA	C4A-NA-C1A	9.20	110.88	106.68
19	A	838	CLA	C4A-NA-C1A	9.17	110.86	106.68
19	A	843	CLA	C4A-NA-C1A	9.17	110.86	106.68
19	A	810	CLA	C4A-NA-C1A	9.16	110.86	106.68
19	3	5020	CLA	C4A-NA-C1A	9.16	110.86	106.68
19	5	306	CLA	C4A-NA-C1A	9.14	110.85	106.68
19	A	822	CLA	C4A-NA-C1A	9.13	110.84	106.68
19	Z	304	CLA	C4A-NA-C1A	9.12	110.84	106.68
19	7	310	CLA	C4A-NA-C1A	9.09	110.83	106.68
19	B	810	CLA	C4A-NA-C1A	9.07	110.82	106.68
19	7	306	CLA	C4A-NA-C1A	9.05	110.81	106.68
19	1	5007	CLA	C4A-NA-C1A	9.04	110.81	106.68
19	5	322	CLA	C4A-NA-C1A	9.04	110.80	106.68
19	4	308	CLA	C4A-NA-C1A	9.02	110.80	106.68
19	K	202	CLA	C4A-NA-C1A	9.01	110.79	106.68
19	B	802	CLA	C4A-NA-C1A	9.00	110.78	106.68
19	7	308	CLA	C4A-NA-C1A	8.99	110.78	106.68
19	7	319	CLA	C4A-NA-C1A	8.98	110.78	106.68
19	1	5015	CLA	C4A-NA-C1A	8.98	110.78	106.68
31	Z	317	LUT	C32-C33-C34	8.97	133.12	119.01
19	Z	312	CLA	C4A-NA-C1A	8.96	110.77	106.68
19	3	5014	CLA	C4A-NA-C1A	8.95	110.76	106.68
19	3	5011	CLA	C4A-NA-C1A	8.94	110.76	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	301	CLA	C4A-NA-C1A	8.94	110.76	106.68
19	A	817	CLA	C4A-NA-C1A	8.93	110.75	106.68
38	8	325	ERG	C13-C17-C20	-8.93	108.68	119.38
19	Z	311	CLA	C4A-NA-C1A	8.93	110.75	106.68
19	I	201	CLA	C4A-NA-C1A	8.92	110.75	106.68
22	5	305	BCR	C7-C8-C9	-8.92	113.04	126.23
19	A	826	CLA	C4A-NA-C1A	8.90	110.74	106.68
19	5	311	CLA	C4A-NA-C1A	8.90	110.74	106.68
19	A	839	CLA	C4A-NA-C1A	8.88	110.73	106.68
19	B	827	CLA	C4A-NA-C1A	8.86	110.72	106.68
19	3	5019	CLA	C4A-NA-C1A	8.86	110.72	106.68
19	3	5008	CLA	C4A-NA-C1A	8.84	110.71	106.68
19	A	816	CLA	C4A-NA-C1A	8.83	110.71	106.68
19	7	317	CLA	C4A-NA-C1A	8.83	110.71	106.68
19	4	306	CLA	C4A-NA-C1A	8.83	110.71	106.68
19	3	5015	CLA	C4A-NA-C1A	8.81	110.70	106.68
19	3	5016	CLA	C4A-NA-C1A	8.81	110.70	106.68
18	A	801	CL0	O2D-CGD-CBD	8.81	120.63	110.95
19	G	1601	CLA	C4A-NA-C1A	8.81	110.70	106.68
19	B	832	CLA	C4A-NA-C1A	8.79	110.69	106.68
19	K	204	CLA	C4A-NA-C1A	8.79	110.69	106.68
19	A	813	CLA	C4A-NA-C1A	8.78	110.69	106.68
19	Z	303	CLA	C4A-NA-C1A	8.77	110.68	106.68
19	A	808	CLA	C4A-NA-C1A	8.75	110.67	106.68
19	7	309	CLA	C4A-NA-C1A	8.75	110.67	106.68
19	8	318	CLA	C4A-NA-C1A	8.74	110.67	106.68
19	A	827	CLA	C4A-NA-C1A	8.73	110.66	106.68
19	A	841	CLA	C4A-NA-C1A	8.73	110.66	106.68
19	B	826	CLA	C4A-NA-C1A	8.73	110.66	106.68
19	4	312	CLA	C4A-NA-C1A	8.72	110.66	106.68
19	B	819	CLA	C4A-NA-C1A	8.72	110.66	106.68
19	B	808	CLA	C4A-NA-C1A	8.71	110.65	106.68
19	B	815	CLA	C4A-NA-C1A	8.70	110.65	106.68
19	5	310	CLA	C4A-NA-C1A	8.70	110.65	106.68
19	7	312	CLA	C4A-NA-C1A	8.68	110.64	106.68
19	5	325	CLA	C4A-NA-C1A	8.68	110.64	106.68
19	B	813	CLA	C4A-NA-C1A	8.68	110.64	106.68
19	6	311	CLA	C4A-NA-C1A	8.67	110.63	106.68
19	B	806	CLA	C4A-NA-C1A	8.66	110.63	106.68
19	K	205	CLA	C4A-NA-C1A	8.65	110.62	106.68
19	B	822	CLA	C4A-NA-C1A	8.64	110.62	106.68
19	5	319	CLA	C4A-NA-C1A	8.63	110.62	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	836	CLA	C4A-NA-C1A	8.63	110.62	106.68
19	6	314	CLA	C4A-NA-C1A	8.63	110.61	106.68
19	A	831	CLA	C4A-NA-C1A	8.63	110.61	106.68
19	B	805	CLA	C4A-NA-C1A	8.62	110.61	106.68
19	B	829	CLA	C4A-NA-C1A	8.62	110.61	106.68
19	B	821	CLA	C4A-NA-C1A	8.61	110.61	106.68
19	B	850	CLA	C4A-NA-C1A	8.61	110.61	106.68
19	Z	308	CLA	C4A-NA-C1A	8.60	110.60	106.68
19	A	833	CLA	C4A-NA-C1A	8.59	110.60	106.68
19	B	816	CLA	C4A-NA-C1A	8.59	110.60	106.68
19	B	817	CLA	C4A-NA-C1A	8.59	110.60	106.68
19	A	828	CLA	C4A-NA-C1A	8.59	110.60	106.68
19	B	814	CLA	C4A-NA-C1A	8.58	110.59	106.68
19	8	320	CLA	C4A-NA-C1A	8.58	110.59	106.68
19	A	825	CLA	C4A-NA-C1A	8.58	110.59	106.68
19	A	818	CLA	C4A-NA-C1A	8.57	110.59	106.68
19	A	805	CLA	C4A-NA-C1A	8.55	110.58	106.68
19	A	814	CLA	C4A-NA-C1A	8.55	110.58	106.68
19	A	807	CLA	C4A-NA-C1A	8.55	110.58	106.68
19	B	828	CLA	C4A-NA-C1A	8.55	110.58	106.68
19	A	811	CLA	C4A-NA-C1A	8.54	110.58	106.68
19	5	301	CLA	C4A-NA-C1A	8.53	110.57	106.68
19	7	313	CLA	C4A-NA-C1A	8.53	110.57	106.68
19	B	830	CLA	C4A-NA-C1A	8.53	110.57	106.68
19	1	5011	CLA	C4A-NA-C1A	8.52	110.57	106.68
19	A	824	CLA	C4A-NA-C1A	8.51	110.56	106.68
19	B	804	CLA	C4A-NA-C1A	8.50	110.56	106.68
19	B	839	CLA	C4A-NA-C1A	8.50	110.56	106.68
19	4	313	CLA	C4A-NA-C1A	8.49	110.55	106.68
19	5	309	CLA	C4A-NA-C1A	8.49	110.55	106.68
19	A	834	CLA	C4A-NA-C1A	8.49	110.55	106.68
19	A	804	CLA	C4A-NA-C1A	8.48	110.55	106.68
19	B	820	CLA	C4A-NA-C1A	8.48	110.55	106.68
19	1	5016	CLA	C4A-NA-C1A	8.48	110.55	106.68
19	1	5008	CLA	C4A-NA-C1A	8.48	110.55	106.68
19	J	1901	CLA	C4A-NA-C1A	8.48	110.55	106.68
19	6	302	CLA	C4A-NA-C1A	8.47	110.55	106.68
19	Z	305	CLA	C4A-NA-C1A	8.47	110.54	106.68
19	B	811	CLA	C4A-NA-C1A	8.46	110.54	106.68
19	B	823	CLA	C4A-NA-C1A	8.46	110.54	106.68
19	4	318	CLA	C4A-NA-C1A	8.46	110.54	106.68
19	A	835	CLA	C4A-NA-C1A	8.45	110.54	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	824	CLA	C4A-NA-C1A	8.42	110.52	106.68
19	B	837	CLA	C4A-NA-C1A	8.41	110.52	106.68
19	B	838	CLA	C4A-NA-C1A	8.41	110.52	106.68
19	K	203	CLA	C4A-NA-C1A	8.40	110.51	106.68
19	1	5012	CLA	C4A-NA-C1A	8.40	110.51	106.68
19	A	837	CLA	C4A-NA-C1A	8.40	110.51	106.68
19	5	312	CLA	C4A-NA-C1A	8.39	110.51	106.68
19	5	314	CLA	C4A-NA-C1A	8.39	110.51	106.68
19	6	318	CLA	C4A-NA-C1A	8.39	110.51	106.68
19	3	5012	CLA	C4A-NA-C1A	8.38	110.50	106.68
19	6	309	CLA	C4A-NA-C1A	8.38	110.50	106.68
19	F	303	CLA	C4A-NA-C1A	8.38	110.50	106.68
19	8	313	CLA	C4A-NA-C1A	8.38	110.50	106.68
19	A	819	CLA	C4A-NA-C1A	8.37	110.50	106.68
19	A	829	CLA	C4A-NA-C1A	8.36	110.49	106.68
19	8	310	CLA	C4A-NA-C1A	8.35	110.49	106.68
19	7	324	CLA	C4A-NA-C1A	8.35	110.49	106.68
19	8	314	CLA	C4A-NA-C1A	8.34	110.48	106.68
19	1	5018	CLA	C4A-NA-C1A	8.33	110.48	106.68
19	A	803	CLA	C4A-NA-C1A	8.32	110.48	106.68
19	A	840	CLA	C4A-NA-C1A	8.32	110.48	106.68
19	B	801	CLA	C4A-NA-C1A	8.32	110.48	106.68
19	B	825	CLA	C4A-NA-C1A	8.32	110.48	106.68
19	B	834	CLA	C4A-NA-C1A	8.32	110.47	106.68
19	Z	306	CLA	C4A-NA-C1A	8.31	110.47	106.68
19	Z	315	CLA	C4A-NA-C1A	8.31	110.47	106.68
19	1	5013	CLA	C4A-NA-C1A	8.31	110.47	106.68
19	A	802	CLA	C4A-NA-C1A	8.30	110.46	106.68
19	B	818	CLA	C4A-NA-C1A	8.30	110.46	106.68
19	5	313	CLA	C4A-NA-C1A	8.29	110.46	106.68
19	A	830	CLA	C4A-NA-C1A	8.28	110.46	106.68
19	B	809	CLA	C4A-NA-C1A	8.28	110.45	106.68
19	B	835	CLA	C4A-NA-C1A	8.27	110.45	106.68
19	A	823	CLA	C4A-NA-C1A	8.26	110.45	106.68
19	B	833	CLA	C4A-NA-C1A	8.25	110.44	106.68
19	G	1602	CLA	C4A-NA-C1A	8.25	110.44	106.68
19	A	842	CLA	C4A-NA-C1A	8.23	110.43	106.68
19	8	308	CLA	C4A-NA-C1A	8.22	110.43	106.68
19	A	820	CLA	C4A-NA-C1A	8.20	110.42	106.68
19	Z	314	CLA	C4A-NA-C1A	8.20	110.42	106.68
19	A	821	CLA	C4A-NA-C1A	8.18	110.41	106.68
19	F	301	CLA	C4A-NA-C1A	8.16	110.40	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	5010	CLA	C4A-NA-C1A	8.16	110.40	106.68
19	B	803	CLA	C4A-NA-C1A	8.13	110.39	106.68
19	B	812	CLA	C4A-NA-C1A	8.09	110.37	106.68
19	A	832	CLA	C4A-NA-C1A	8.08	110.37	106.68
19	A	806	CLA	C4A-NA-C1A	8.07	110.36	106.68
22	3	5007	BCR	C24-C23-C22	-8.06	114.32	126.23
19	6	322	CLA	C4A-NA-C1A	8.04	110.35	106.68
22	3	5005	BCR	C11-C10-C9	-8.04	116.01	127.28
19	6	323	CLA	C4A-NA-C1A	8.03	110.34	106.68
19	6	320	CLA	C4A-NA-C1A	8.02	110.34	106.68
19	4	316	CLA	C4A-NA-C1A	8.02	110.34	106.68
19	A	809	CLA	C4A-NA-C1A	8.01	110.33	106.68
19	3	5009	CLA	C4A-NA-C1A	8.00	110.33	106.68
19	6	310	CLA	C4A-NA-C1A	7.98	110.32	106.68
22	6	308	BCR	C15-C14-C13	-7.96	116.12	127.28
19	A	857	CLA	C4A-NA-C1A	7.95	110.31	106.68
19	7	318	CLA	C4A-NA-C1A	7.95	110.31	106.68
19	5	307	CLA	C4A-NA-C1A	7.93	110.30	106.68
19	A	812	CLA	C4A-NA-C1A	7.91	110.29	106.68
19	1	5010	CLA	C4A-NA-C1A	7.87	110.27	106.68
19	6	312	CLA	C4A-NA-C1A	7.87	110.27	106.68
19	B	807	CLA	C4A-NA-C1A	7.84	110.25	106.68
19	Z	307	CLA	C4A-NA-C1A	7.81	110.24	106.68
19	4	310	CLA	C4A-NA-C1A	7.68	110.18	106.68
32	7	314	CHL	C1B-CHB-C4A	7.61	126.22	121.32
19	5	308	CLA	C4A-NA-C1A	7.59	110.14	106.68
28	6	304	C7Z	C11-C10-C9	-7.46	116.81	127.28
19	8	311	CLA	C4A-NA-C1A	7.45	110.08	106.68
32	8	301	CHL	C1B-CHB-C4A	7.43	126.10	121.32
22	A	848	BCR	C15-C14-C13	-7.31	117.03	127.28
32	5	315	CHL	C1B-CHB-C4A	7.30	126.02	121.32
32	6	315	CHL	C1B-CHB-C4A	7.28	126.01	121.32
32	4	315	CHL	C1B-CHB-C4A	7.27	126.00	121.32
32	6	316	CHL	C1B-CHB-C4A	7.26	126.00	121.32
22	5	305	BCR	C11-C10-C9	-7.10	117.32	127.28
22	A	847	BCR	C16-C17-C18	-7.06	117.38	127.28
31	8	304	LUT	C35-C34-C33	-7.06	117.38	127.28
22	8	303	BCR	C38-C26-C25	-7.02	116.82	124.48
27	4	303	RRX	C33-C5-C6	-7.02	116.82	124.48
32	8	315	CHL	C1B-CHB-C4A	6.99	125.82	121.32
32	6	317	CHL	C1B-CHB-C4A	6.92	125.78	121.32
31	8	305	LUT	C7-C8-C9	-6.92	116.00	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	5	316	CHL	C1B-CHB-C4A	6.88	125.75	121.32
22	4	305	BCR	C20-C21-C22	-6.85	117.67	127.28
22	8	303	BCR	C16-C17-C18	-6.85	117.68	127.28
35	7	302	DGA	CDB-CCB-CBB	-6.82	79.90	114.37
31	1	5004	LUT	C7-C8-C9	-6.81	116.17	126.23
32	1	5009	CHL	C1B-CHB-C4A	6.79	125.69	121.32
31	6	306	LUT	C31-C30-C29	-6.79	117.76	127.28
22	B	846	BCR	C15-C14-C13	-6.76	117.80	127.28
32	8	317	CHL	C1B-CHB-C4A	6.75	125.66	121.32
27	4	303	RRX	C24-C23-C22	-6.66	116.38	126.23
31	5	303	LUT	C26-C27-C28	-6.60	114.31	124.58
22	3	5007	BCR	C7-C8-C9	-6.57	116.52	126.23
22	5	304	BCR	C16-C17-C18	-6.54	118.10	127.28
22	3	5005	BCR	C20-C21-C22	-6.54	118.11	127.28
19	4	309	CLA	O2D-CGD-CBD	6.52	122.62	111.23
19	8	312	CLA	CMD-C2D-C1D	6.51	136.19	124.73
22	A	849	BCR	C16-C17-C18	-6.49	118.18	127.28
19	8	312	CLA	C1D-ND-C4D	-6.47	101.77	106.31
31	3	5002	LUT	C11-C10-C9	-6.46	118.21	127.28
22	5	304	BCR	C33-C5-C6	-6.46	117.43	124.48
31	8	305	LUT	C26-C27-C28	-6.44	114.55	124.58
22	F	302	BCR	C24-C23-C22	-6.43	116.73	126.23
31	6	305	LUT	C11-C10-C9	-6.40	118.30	127.28
19	6	320	CLA	O2D-CGD-CBD	6.37	122.37	111.23
22	6	308	BCR	C38-C26-C25	-6.36	117.54	124.48
31	4	304	LUT	C11-C10-C9	-6.35	118.37	127.28
28	6	304	C7Z	C1-C6-C5	-6.31	114.01	122.64
31	7	304	LUT	C31-C30-C29	-6.31	118.43	127.28
27	F	304	RRX	C11-C10-C9	-6.29	118.45	127.28
31	4	304	LUT	C1-C6-C5	-6.29	114.04	122.64
28	1	5005	C7Z	C35-C34-C33	-6.27	118.48	127.28
31	1	5004	LUT	C26-C27-C28	-6.27	114.82	124.58
22	6	308	BCR	C20-C21-C22	-6.26	118.50	127.28
27	5	302	RRX	C24-C23-C22	-6.26	116.97	126.23
19	A	813	CLA	O2D-CGD-CBD	6.26	122.17	111.23
22	G	1603	BCR	C38-C26-C25	-6.24	117.67	124.48
31	5	303	LUT	C7-C8-C9	-6.24	117.00	126.23
32	6	319	CHL	C1B-CHB-C4A	6.24	125.34	121.32
22	B	842	BCR	C15-C14-C13	-6.23	118.55	127.28
22	A	849	BCR	C24-C23-C22	-6.22	117.03	126.23
31	3	5003	LUT	C31-C30-C29	-6.22	118.55	127.28
32	Z	302	CHL	C1B-CHB-C4A	6.20	125.31	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	5007	BCR	C4-C5-C6	-6.20	114.32	122.70
22	B	844	BCR	C24-C23-C22	-6.18	117.09	126.23
31	3	5003	LUT	C7-C8-C9	-6.17	117.10	126.23
32	Z	310	CHL	C1B-CHB-C4A	6.16	125.29	121.32
22	B	843	BCR	C11-C10-C9	-6.15	118.65	127.28
22	7	305	BCR	C20-C21-C22	-6.14	118.67	127.28
19	4	311	CLA	CMD-C2D-C1D	6.10	135.48	124.73
22	3	5006	BCR	C16-C17-C18	-6.05	118.80	127.28
22	3	5005	BCR	C4-C5-C6	-6.04	114.54	122.70
19	B	840	CLA	O2D-CGD-CBD	6.03	121.78	111.23
19	1	5011	CLA	CMD-C2D-C1D	6.01	135.31	124.73
22	6	307	BCR	C11-C10-C9	-6.01	118.85	127.28
32	7	315	CHL	C1B-CHB-C4A	6.01	125.19	121.32
38	6	326	ERG	C15-C14-C13	-6.00	98.84	104.21
19	4	307	CLA	CMD-C2D-C1D	5.98	135.25	124.73
22	3	5006	BCR	C27-C26-C25	-5.93	114.69	122.70
27	F	304	RRX	C15-C14-C13	-5.93	118.96	127.28
19	4	308	CLA	O2D-CGD-CBD	5.92	121.57	111.23
22	B	847	BCR	C27-C26-C25	-5.90	114.73	122.70
22	A	848	BCR	C16-C17-C18	-5.89	119.01	127.28
19	5	309	CLA	O2D-CGD-CBD	5.88	121.52	111.23
19	4	307	CLA	C4A-NA-C1A	5.88	109.36	106.68
19	1	5010	CLA	CMD-C2D-C1D	5.88	135.08	124.73
22	4	305	BCR	C38-C26-C25	-5.87	118.08	124.48
19	7	310	CLA	CMD-C2D-C1D	5.86	135.04	124.73
31	1	5004	LUT	C11-C10-C9	-5.86	119.06	127.28
32	4	317	CHL	C1B-CHB-C4A	5.84	125.08	121.32
19	Z	311	CLA	CMD-C2D-C1D	5.82	134.98	124.73
22	A	850	BCR	C4-C5-C6	-5.82	114.84	122.70
32	1	5014	CHL	C1B-CHB-C4A	5.80	125.05	121.32
38	8	325	ERG	C18-C13-C12	-5.79	102.07	110.61
22	B	843	BCR	C1-C6-C5	-5.78	114.73	122.64
31	Z	317	LUT	C31-C32-C33	5.78	142.22	126.36
19	A	832	CLA	O2D-CGD-CBD	5.77	121.31	111.23
22	A	847	BCR	C15-C14-C13	-5.77	119.19	127.28
19	1	5006	CLA	CMD-C2D-C1D	5.76	134.88	124.73
22	G	1603	BCR	C20-C21-C22	-5.76	119.19	127.28
27	F	304	RRX	C16-C17-C18	-5.76	119.20	127.28
22	3	5007	BCR	C1-C6-C5	-5.75	114.77	122.64
31	7	304	LUT	C1-C6-C5	-5.75	114.78	122.64
31	4	304	LUT	C18-C5-C6	-5.75	118.21	124.48
22	3	5004	BCR	C24-C23-C22	-5.75	117.73	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	6	304	C7Z	C15-C14-C13	-5.75	119.22	127.28
19	K	205	CLA	CMD-C2D-C1D	5.75	134.85	124.73
19	7	306	CLA	CMD-C2D-C1D	5.74	134.84	124.73
22	B	846	BCR	C20-C21-C22	-5.74	119.23	127.28
19	3	5012	CLA	CMD-C2D-C1D	5.73	134.81	124.73
22	3	5005	BCR	C27-C26-C25	-5.72	114.97	122.70
31	Z	318	LUT	C7-C8-C9	-5.72	117.78	126.23
19	6	310	CLA	CMD-C2D-C1D	5.71	134.79	124.73
28	6	304	C7Z	C31-C30-C29	-5.70	119.29	127.28
19	F	301	CLA	CMD-C2D-C1D	5.70	134.76	124.73
19	B	824	CLA	O2D-CGD-CBD	5.69	121.17	111.23
32	8	319	CHL	C1B-CHB-C4A	5.68	124.98	121.32
19	4	310	CLA	O2D-CGD-CBD	5.68	121.16	111.23
19	5	308	CLA	CMD-C2D-C1D	5.68	134.73	124.73
19	8	308	CLA	O2D-CGD-CBD	5.68	121.15	111.23
31	4	304	LUT	C26-C27-C28	-5.67	115.75	124.58
19	7	309	CLA	O2D-CGD-CBD	5.67	121.14	111.23
19	A	814	CLA	O2D-CGD-CBD	5.67	121.13	111.23
22	8	306	BCR	C27-C26-C25	-5.66	115.05	122.70
22	B	843	BCR	C38-C26-C25	-5.66	118.31	124.48
19	A	839	CLA	CMD-C2D-C1D	5.65	134.68	124.73
19	B	822	CLA	CMD-C2D-C1D	5.65	134.68	124.73
19	8	308	CLA	CMD-C2D-C1D	5.65	134.67	124.73
22	3	5007	BCR	C38-C26-C25	-5.65	118.32	124.48
19	A	823	CLA	CMD-C2D-C1D	5.65	134.67	124.73
19	5	325	CLA	CMD-C2D-C1D	5.64	134.66	124.73
19	6	322	CLA	CMD-C2D-C1D	5.64	134.66	124.73
19	B	813	CLA	O2D-CGD-CBD	5.64	121.09	111.23
19	B	831	CLA	O2D-CGD-CBD	5.64	121.09	111.23
22	7	305	BCR	C4-C5-C6	-5.64	115.09	122.70
19	5	306	CLA	CMD-C2D-C1D	5.63	134.63	124.73
19	8	314	CLA	CMD-C2D-C1D	5.62	134.63	124.73
28	1	5005	C7Z	C31-C30-C29	-5.62	119.40	127.28
19	5	311	CLA	CMD-C2D-C1D	5.61	134.61	124.73
22	F	302	BCR	C16-C17-C18	-5.61	119.41	127.28
19	B	829	CLA	CMD-C2D-C1D	5.61	134.60	124.73
19	A	815	CLA	CMD-C2D-C1D	5.61	134.60	124.73
31	7	304	LUT	C11-C10-C9	-5.60	119.42	127.28
19	A	811	CLA	CMD-C2D-C1D	5.60	134.59	124.73
22	K	206	BCR	C11-C10-C9	-5.59	119.43	127.28
22	7	305	BCR	C16-C17-C18	-5.59	119.44	127.28
19	3	5011	CLA	O2D-CGD-CBD	5.59	121.00	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	812	CLA	CMD-C2D-C1D	5.59	134.56	124.73
19	Z	314	CLA	CMD-C2D-C1D	5.58	134.56	124.73
19	B	833	CLA	CMD-C2D-C1D	5.58	134.55	124.73
19	6	309	CLA	CMD-C2D-C1D	5.58	134.55	124.73
19	1	5013	CLA	CMD-C2D-C1D	5.57	134.54	124.73
38	6	326	ERG	C11-C9-C10	-5.57	100.27	113.65
19	G	1602	CLA	CMD-C2D-C1D	5.57	134.54	124.73
19	A	807	CLA	CMD-C2D-C1D	5.57	134.53	124.73
19	B	811	CLA	CMD-C2D-C1D	5.57	134.53	124.73
19	Z	305	CLA	CMD-C2D-C1D	5.57	134.53	124.73
19	7	318	CLA	O2D-CGD-CBD	5.56	120.96	111.23
22	F	302	BCR	C38-C26-C25	-5.56	118.41	124.48
19	B	838	CLA	CMD-C2D-C1D	5.56	134.52	124.73
19	4	308	CLA	CMD-C2D-C1D	5.56	134.52	124.73
32	4	314	CHL	C1B-CHB-C4A	5.56	124.90	121.32
19	1	5015	CLA	O2D-CGD-CBD	5.56	120.95	111.23
19	A	814	CLA	CMD-C2D-C1D	5.56	134.52	124.73
19	4	309	CLA	CMD-C2D-C1D	5.56	134.51	124.73
19	5	307	CLA	CMD-C2D-C1D	5.56	134.51	124.73
19	6	311	CLA	C1-C2-C3	-5.56	117.09	126.20
22	A	859	BCR	C1-C6-C5	-5.55	115.05	122.64
19	B	806	CLA	CMD-C2D-C1D	5.55	134.50	124.73
19	K	204	CLA	CMD-C2D-C1D	5.55	134.50	124.73
19	6	311	CLA	CMD-C2D-C1D	5.55	134.50	124.73
19	B	813	CLA	CMD-C2D-C1D	5.55	134.50	124.73
19	A	833	CLA	CMD-C2D-C1D	5.54	134.49	124.73
19	5	319	CLA	CMD-C2D-C1D	5.54	134.49	124.73
19	Z	308	CLA	O2D-CGD-CBD	5.54	120.92	111.23
19	B	814	CLA	CMD-C2D-C1D	5.54	134.48	124.73
19	A	820	CLA	O2D-CGD-CBD	5.54	120.91	111.23
19	B	826	CLA	CMD-C2D-C1D	5.54	134.48	124.73
22	8	306	BCR	C24-C23-C22	-5.54	118.05	126.23
19	F	301	CLA	O2D-CGD-CBD	5.53	120.91	111.23
31	6	305	LUT	C7-C8-C9	-5.53	118.05	126.23
19	A	808	CLA	CMD-C2D-C1D	5.53	134.47	124.73
19	B	824	CLA	CMD-C2D-C1D	5.53	134.47	124.73
19	3	5016	CLA	CMD-C2D-C1D	5.53	134.46	124.73
19	A	803	CLA	CMD-C2D-C1D	5.53	134.46	124.73
19	A	813	CLA	CMD-C2D-C1D	5.53	134.46	124.73
19	B	810	CLA	CMD-C2D-C1D	5.53	134.46	124.73
19	A	817	CLA	CMD-C2D-C1D	5.53	134.46	124.73
19	A	822	CLA	CMD-C2D-C1D	5.53	134.46	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	311	CLA	O2D-CGD-CBD	5.52	120.89	111.23
19	8	307	CLA	CMD-C2D-C1D	5.52	134.45	124.73
19	7	319	CLA	CMD-C2D-C1D	5.52	134.44	124.73
28	J	1902	C7Z	C31-C30-C29	-5.52	119.54	127.28
22	G	1603	BCR	C16-C17-C18	-5.51	119.54	127.28
19	A	806	CLA	CMD-C2D-C1D	5.51	134.44	124.73
19	B	817	CLA	CMD-C2D-C1D	5.51	134.44	124.73
19	A	834	CLA	CMD-C2D-C1D	5.51	134.44	124.73
19	A	827	CLA	CMD-C2D-C1D	5.51	134.44	124.73
19	B	819	CLA	CMD-C2D-C1D	5.51	134.43	124.73
19	5	322	CLA	CMD-C2D-C1D	5.51	134.43	124.73
19	I	201	CLA	CMD-C2D-C1D	5.51	134.43	124.73
19	Z	311	CLA	O2D-CGD-CBD	5.51	120.86	111.23
19	A	841	CLA	CMD-C2D-C1D	5.50	134.42	124.73
19	3	5010	CLA	CMD-C2D-C1D	5.50	134.42	124.73
22	B	846	BCR	C33-C5-C6	-5.50	118.48	124.48
19	3	5013	CLA	CMD-C2D-C1D	5.50	134.42	124.73
19	4	306	CLA	CMD-C2D-C1D	5.50	134.41	124.73
19	B	850	CLA	CMD-C2D-C1D	5.49	134.40	124.73
19	B	827	CLA	CMD-C2D-C1D	5.49	134.40	124.73
19	J	1901	CLA	CMD-C2D-C1D	5.49	134.40	124.73
38	8	325	ERG	C12-C13-C17	5.49	124.69	116.60
19	B	816	CLA	CMD-C2D-C1D	5.49	134.40	124.73
19	B	837	CLA	O2D-CGD-CBD	5.49	120.83	111.23
19	4	318	CLA	CMD-C2D-C1D	5.49	134.40	124.73
19	6	301	CLA	CMD-C2D-C1D	5.49	134.39	124.73
19	A	821	CLA	CMD-C2D-C1D	5.49	134.39	124.73
19	A	809	CLA	CMD-C2D-C1D	5.49	134.39	124.73
19	A	820	CLA	CMD-C2D-C1D	5.48	134.38	124.73
28	J	1902	C7Z	C11-C10-C9	-5.48	119.59	127.28
19	A	805	CLA	CMD-C2D-C1D	5.48	134.38	124.73
22	3	5007	BCR	C33-C5-C6	-5.48	118.51	124.48
19	B	818	CLA	CMD-C2D-C1D	5.48	134.37	124.73
19	A	828	CLA	CMD-C2D-C1D	5.48	134.37	124.73
22	5	305	BCR	C38-C26-C25	-5.48	118.51	124.48
19	A	818	CLA	CMD-C2D-C1D	5.47	134.37	124.73
19	8	312	CLA	O2D-CGD-CBD	5.47	120.80	111.23
22	A	859	BCR	C24-C23-C22	-5.47	118.14	126.23
19	A	838	CLA	CMD-C2D-C1D	5.47	134.36	124.73
19	A	843	CLA	CMD-C2D-C1D	5.47	134.35	124.73
19	5	310	CLA	CMD-C2D-C1D	5.47	134.35	124.73
19	A	826	CLA	O2D-CGD-CBD	5.46	120.78	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	805	CLA	CMD-C2D-C1D	5.46	134.35	124.73
19	Z	303	CLA	CMD-C2D-C1D	5.46	134.35	124.73
19	B	830	CLA	CMD-C2D-C1D	5.46	134.35	124.73
31	1	5003	LUT	C26-C27-C28	-5.46	116.08	124.58
19	B	807	CLA	CMD-C2D-C1D	5.46	134.35	124.73
22	B	844	BCR	C33-C5-C6	-5.46	118.53	124.48
19	B	821	CLA	CMD-C2D-C1D	5.46	134.34	124.73
19	K	203	CLA	CMD-C2D-C1D	5.46	134.34	124.73
19	A	812	CLA	O2D-CGD-CBD	5.46	120.77	111.23
19	A	816	CLA	CMD-C2D-C1D	5.46	134.34	124.73
19	Z	303	CLA	O2D-CGD-CBD	5.46	120.77	111.23
19	B	834	CLA	CMD-C2D-C1D	5.46	134.34	124.73
19	A	857	CLA	CMD-C2D-C1D	5.45	134.33	124.73
19	B	832	CLA	O2D-CGD-CBD	5.45	120.76	111.23
19	A	836	CLA	CMD-C2D-C1D	5.45	134.33	124.73
19	A	830	CLA	CMD-C2D-C1D	5.45	134.33	124.73
22	A	848	BCR	C11-C10-C9	-5.45	119.64	127.28
19	5	301	CLA	CMD-C2D-C1D	5.45	134.32	124.73
31	Z	317	LUT	C30-C31-C32	5.45	138.98	123.20
19	A	831	CLA	CMD-C2D-C1D	5.45	134.32	124.73
19	K	202	CLA	CMD-C2D-C1D	5.44	134.31	124.73
19	A	837	CLA	CMD-C2D-C1D	5.44	134.31	124.73
19	B	808	CLA	CMD-C2D-C1D	5.44	134.31	124.73
19	5	321	CLA	CMD-C2D-C1D	5.44	134.30	124.73
19	1	5018	CLA	CMD-C2D-C1D	5.44	134.30	124.73
19	A	832	CLA	CMD-C2D-C1D	5.44	134.30	124.73
19	A	825	CLA	CMD-C2D-C1D	5.43	134.30	124.73
19	6	302	CLA	O2D-CGD-CBD	5.43	120.73	111.23
19	A	822	CLA	O2D-CGD-CBD	5.43	120.73	111.23
19	B	805	CLA	O2D-CGD-CBD	5.43	120.72	111.23
19	1	5015	CLA	CMD-C2D-C1D	5.43	134.29	124.73
19	F	303	CLA	CMD-C2D-C1D	5.43	134.28	124.73
19	B	837	CLA	CMD-C2D-C1D	5.43	134.28	124.73
23	3	5021	LHG	O7-C7-O9	-5.42	118.74	125.70
19	Z	315	CLA	CMD-C2D-C1D	5.42	134.28	124.73
19	A	803	CLA	O2D-CGD-CBD	5.42	120.70	111.23
19	A	804	CLA	CMD-C2D-C1D	5.42	134.27	124.73
19	7	316	CLA	CMD-C2D-C1D	5.42	134.27	124.73
19	8	311	CLA	O2D-CGD-CBD	5.42	120.70	111.23
19	A	824	CLA	CMD-C2D-C1D	5.41	134.26	124.73
19	B	839	CLA	CMD-C2D-C1D	5.41	134.25	124.73
31	8	305	LUT	C21-C26-C27	-5.41	106.61	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	312	CLA	CMD-C2D-C1D	5.41	134.25	124.73
19	1	5016	CLA	CMD-C2D-C1D	5.41	134.25	124.73
19	A	837	CLA	O2D-CGD-CBD	5.41	120.68	111.23
19	Z	308	CLA	CMD-C2D-C1D	5.40	134.23	124.73
19	A	819	CLA	CMD-C2D-C1D	5.39	134.23	124.73
19	5	319	CLA	O2D-CGD-CBD	5.39	120.66	111.23
19	B	823	CLA	CMD-C2D-C1D	5.39	134.22	124.73
22	A	850	BCR	C20-C21-C22	-5.39	119.72	127.28
19	3	5009	CLA	CMD-C2D-C1D	5.38	134.21	124.73
19	4	310	CLA	CMD-C2D-C1D	5.38	134.21	124.73
19	8	320	CLA	CMD-C2D-C1D	5.38	134.21	124.73
19	B	831	CLA	CMD-C2D-C1D	5.38	134.20	124.73
22	B	845	BCR	C1-C6-C5	-5.38	115.29	122.64
19	B	840	CLA	CMD-C2D-C1D	5.37	134.19	124.73
19	A	809	CLA	O2D-CGD-CBD	5.37	120.62	111.23
19	A	825	CLA	O2D-CGD-CBD	5.37	120.62	111.23
19	A	823	CLA	O2D-CGD-CBD	5.37	120.62	111.23
19	1	5011	CLA	O2D-CGD-CBD	5.37	120.62	111.23
19	8	311	CLA	CMD-C2D-C1D	5.36	134.17	124.73
22	5	304	BCR	C38-C26-C25	-5.36	118.64	124.48
19	B	815	CLA	CMD-C2D-C1D	5.36	134.16	124.73
22	B	845	BCR	C11-C10-C9	-5.35	119.77	127.28
19	3	5011	CLA	CMD-C2D-C1D	5.35	134.16	124.73
19	A	812	CLA	CMD-C2D-C1D	5.35	134.15	124.73
19	7	309	CLA	CMD-C2D-C1D	5.34	134.14	124.73
19	1	5012	CLA	CMD-C2D-C1D	5.34	134.13	124.73
19	1	5010	CLA	O2D-CGD-CBD	5.34	120.57	111.23
19	B	818	CLA	O2D-CGD-CBD	5.34	120.56	111.23
19	8	318	CLA	CMD-C2D-C1D	5.34	134.13	124.73
19	B	820	CLA	CMD-C2D-C1D	5.34	134.12	124.73
19	A	835	CLA	CMD-C2D-C1D	5.33	134.12	124.73
19	A	842	CLA	CMD-C2D-C1D	5.33	134.11	124.73
19	A	810	CLA	O2D-CGD-CBD	5.33	120.54	111.23
19	7	311	CLA	CMD-C2D-C1D	5.33	134.11	124.73
19	B	809	CLA	CMD-C2D-C1D	5.32	134.10	124.73
19	B	832	CLA	CMD-C2D-C1D	5.32	134.10	124.73
19	B	815	CLA	O2D-CGD-CBD	5.32	120.53	111.23
19	B	803	CLA	CMD-C2D-C1D	5.32	134.10	124.73
19	6	313	CLA	CMD-C2D-C1D	5.32	134.09	124.73
19	6	302	CLA	CMD-C2D-C1D	5.31	134.09	124.73
22	A	850	BCR	C7-C8-C9	-5.31	118.38	126.23
19	Z	307	CLA	CMD-C2D-C1D	5.31	134.08	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	802	CLA	O2D-CGD-CBD	5.31	120.52	111.23
19	B	836	CLA	CMD-C2D-C1D	5.31	134.08	124.73
22	5	305	BCR	C1-C6-C5	-5.31	115.38	122.64
19	B	822	CLA	O2D-CGD-CBD	5.31	120.51	111.23
19	1	5013	CLA	O2D-CGD-CBD	5.31	120.50	111.23
19	7	310	CLA	O2D-CGD-CBD	5.30	120.50	111.23
19	4	307	CLA	O2D-CGD-CBD	5.30	120.50	111.23
19	3	5020	CLA	CMD-C2D-C1D	5.30	134.06	124.73
19	A	802	CLA	O2D-CGD-CBD	5.30	120.49	111.23
19	B	836	CLA	O2D-CGD-CBD	5.30	120.49	111.23
19	3	5020	CLA	O2D-CGD-CBD	5.30	120.49	111.23
19	A	808	CLA	O2D-CGD-CBD	5.29	120.49	111.23
19	A	826	CLA	CMD-C2D-C1D	5.29	134.05	124.73
19	K	202	CLA	O2D-CGD-CBD	5.29	120.48	111.23
19	A	802	CLA	CMD-C2D-C1D	5.29	134.04	124.73
19	J	1901	CLA	O2D-CGD-CBD	5.29	120.47	111.23
19	7	316	CLA	C1-C2-C3	-5.28	118.21	126.76
19	7	312	CLA	CMD-C2D-C1D	5.28	134.03	124.73
19	8	309	CLA	CMD-C2D-C1D	5.28	134.03	124.73
22	F	302	BCR	C20-C21-C22	-5.28	119.87	127.28
19	G	1601	CLA	CMD-C2D-C1D	5.28	134.02	124.73
19	6	318	CLA	CMD-C2D-C1D	5.28	134.02	124.73
19	B	835	CLA	CMD-C2D-C1D	5.28	134.02	124.73
19	3	5019	CLA	CMD-C2D-C1D	5.27	134.02	124.73
19	B	814	CLA	O2D-CGD-CBD	5.27	120.45	111.23
19	Z	304	CLA	CMD-C2D-C1D	5.27	134.02	124.73
22	8	303	BCR	C1-C6-C5	-5.27	115.44	122.64
19	3	5014	CLA	CMD-C2D-C1D	5.27	134.01	124.73
19	B	812	CLA	O2D-CGD-CBD	5.27	120.44	111.23
19	3	5008	CLA	CMD-C2D-C1D	5.26	134.00	124.73
19	B	801	CLA	CMD-C2D-C1D	5.26	133.99	124.73
22	B	845	BCR	C15-C14-C13	-5.26	119.91	127.28
19	3	5015	CLA	O2D-CGD-CBD	5.26	120.42	111.23
19	8	313	CLA	O2D-CGD-CBD	5.25	120.41	111.23
19	A	834	CLA	O2D-CGD-CBD	5.25	120.41	111.23
22	B	845	BCR	C27-C26-C25	-5.25	115.62	122.70
19	7	308	CLA	CMD-C2D-C1D	5.24	133.95	124.73
19	4	313	CLA	CMD-C2D-C1D	5.24	133.95	124.73
19	B	828	CLA	CMD-C2D-C1D	5.23	133.94	124.73
19	5	322	CLA	O2D-CGD-CBD	5.23	120.38	111.23
19	A	830	CLA	O2D-CGD-CBD	5.23	120.38	111.23
32	8	319	CHL	C1-O2A-CGA	5.23	129.31	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	311	CLA	C1-C2-C3	-5.22	117.64	126.20
22	A	850	BCR	C27-C26-C25	-5.22	115.65	122.70
19	7	313	CLA	O2D-CGD-CBD	5.22	120.36	111.23
19	4	311	CLA	C4A-NA-C1A	5.22	109.06	106.68
19	8	318	CLA	O2D-CGD-CBD	5.21	120.34	111.23
22	A	848	BCR	C1-C6-C5	-5.21	115.52	122.64
19	A	841	CLA	O2D-CGD-CBD	5.21	120.34	111.23
31	6	306	LUT	C7-C8-C9	-5.20	118.53	126.23
19	G	1602	CLA	O2D-CGD-CBD	5.20	120.33	111.23
31	Z	318	LUT	C11-C10-C9	-5.20	119.99	127.28
19	7	324	CLA	CMD-C2D-C1D	5.19	133.88	124.73
19	B	811	CLA	O2D-CGD-CBD	5.19	120.31	111.23
19	6	301	CLA	O2D-CGD-CBD	5.19	120.30	111.23
19	A	827	CLA	O2D-CGD-CBD	5.19	120.30	111.23
19	B	816	CLA	O2D-CGD-CBD	5.19	120.30	111.23
19	B	806	CLA	O2D-CGD-CBD	5.19	120.30	111.23
19	7	307	CLA	CMD-C2D-C1D	5.18	133.86	124.73
19	B	829	CLA	O2D-CGD-CBD	5.18	120.29	111.23
19	A	807	CLA	O2D-CGD-CBD	5.18	120.28	111.23
19	3	5015	CLA	CMD-C2D-C1D	5.18	133.84	124.73
32	5	318	CHL	C1B-CHB-C4A	5.17	124.65	121.32
19	A	815	CLA	O2D-CGD-CBD	5.17	120.27	111.23
19	3	5019	CLA	O2D-CGD-CBD	5.17	120.27	111.23
19	A	833	CLA	O2D-CGD-CBD	5.17	120.26	111.23
19	3	5016	CLA	O2D-CGD-CBD	5.17	120.26	111.23
19	7	317	CLA	CMD-C2D-C1D	5.17	133.83	124.73
19	8	309	CLA	C1-C2-C3	-5.16	117.73	126.20
31	7	304	LUT	C7-C8-C9	-5.16	118.59	126.23
19	6	310	CLA	O2D-CGD-CBD	5.16	120.26	111.23
22	G	1603	BCR	C33-C5-C6	-5.16	118.85	124.48
19	6	313	CLA	O2D-CGD-CBD	5.16	120.25	111.23
19	B	804	CLA	CMD-C2D-C1D	5.15	133.81	124.73
19	4	313	CLA	O2D-CGD-CBD	5.15	120.24	111.23
19	6	323	CLA	O2D-CGD-CBD	5.15	120.24	111.23
19	B	802	CLA	CMD-C2D-C1D	5.15	133.80	124.73
32	4	319	CHL	C1B-CHB-C4A	5.15	124.63	121.32
19	B	838	CLA	O2D-CGD-CBD	5.14	120.22	111.23
19	B	834	CLA	O2D-CGD-CBD	5.14	120.22	111.23
19	5	313	CLA	O2D-CGD-CBD	5.14	120.22	111.23
32	6	321	CHL	C1C-CHC-C4B	5.14	134.47	116.07
19	A	806	CLA	O2D-CGD-CBD	5.14	120.22	111.23
22	A	846	BCR	C33-C5-C6	-5.13	118.88	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	306	CLA	O2D-CGD-CBD	5.13	120.20	111.23
19	5	317	CLA	O2D-CGD-CBD	5.13	120.20	111.23
19	B	833	CLA	O2D-CGD-CBD	5.13	120.20	111.23
19	K	205	CLA	O2D-CGD-CBD	5.13	120.20	111.23
19	I	201	CLA	O2D-CGD-CBD	5.13	120.19	111.23
22	3	5005	BCR	C30-C25-C26	-5.13	115.63	122.64
19	4	316	CLA	CMD-C2D-C1D	5.12	133.75	124.73
19	B	803	CLA	O2D-CGD-CBD	5.12	120.18	111.23
19	3	5019	CLA	C1-C2-C3	-5.12	117.81	126.20
19	Z	306	CLA	CMD-C2D-C1D	5.12	133.74	124.73
19	A	816	CLA	O2D-CGD-CBD	5.12	120.18	111.23
22	6	308	BCR	C33-C5-C6	-5.11	118.90	124.48
19	5	313	CLA	CMD-C2D-C1D	5.11	133.73	124.73
19	1	5007	CLA	CMD-C2D-C1D	5.11	133.73	124.73
19	5	308	CLA	O2D-CGD-CBD	5.11	120.17	111.23
22	B	843	BCR	C4-C5-C6	-5.11	115.80	122.70
19	B	826	CLA	O2D-CGD-CBD	5.11	120.16	111.23
19	B	830	CLA	O2D-CGD-CBD	5.11	120.16	111.23
22	A	848	BCR	C4-C5-C6	-5.11	115.81	122.70
19	K	204	CLA	O2A-C1-C2	5.10	121.14	108.99
31	6	305	LUT	C21-C26-C27	-5.10	106.96	112.83
22	3	5007	BCR	C16-C17-C18	-5.10	120.12	127.28
19	8	307	CLA	O2D-CGD-CBD	5.10	120.15	111.23
19	8	310	CLA	CMD-C2D-C1D	5.10	133.71	124.73
19	5	309	CLA	CMD-C2D-C1D	5.10	133.71	124.73
22	B	847	BCR	C16-C17-C18	-5.10	120.13	127.28
22	A	858	BCR	C33-C5-C6	-5.10	118.92	124.48
19	5	314	CLA	CMD-C2D-C1D	5.10	133.70	124.73
19	8	314	CLA	O2D-CGD-CBD	5.09	120.13	111.23
19	B	817	CLA	O2D-CGD-CBD	5.09	120.12	111.23
19	B	804	CLA	O2D-CGD-CBD	5.09	120.12	111.23
19	A	804	CLA	O2D-CGD-CBD	5.09	120.12	111.23
22	A	859	BCR	C15-C14-C13	-5.08	120.15	127.28
22	B	843	BCR	C33-C5-C6	-5.08	118.94	124.48
19	3	5009	CLA	O2D-CGD-CBD	5.08	120.11	111.23
19	K	204	CLA	O2D-CGD-CBD	5.08	120.11	111.23
19	B	827	CLA	O2D-CGD-CBD	5.08	120.11	111.23
31	Z	318	LUT	C26-C27-C28	-5.07	116.68	124.58
19	Z	307	CLA	O2D-CGD-CBD	5.07	120.10	111.23
31	6	305	LUT	C35-C34-C33	-5.07	120.17	127.28
32	6	321	CHL	C1A-CHA-C4D	5.07	127.44	118.98
19	F	303	CLA	O2D-CGD-CBD	5.07	120.09	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	843	BCR	C15-C14-C13	-5.07	120.17	127.28
19	B	835	CLA	O2D-CGD-CBD	5.05	120.06	111.23
19	6	323	CLA	CMD-C2D-C1D	5.05	133.62	124.73
19	A	817	CLA	O2D-CGD-CBD	5.05	120.06	111.23
19	5	312	CLA	O2D-CGD-CBD	5.05	120.06	111.23
31	6	305	LUT	C26-C27-C28	-5.05	116.72	124.58
22	A	850	BCR	C1-C6-C5	-5.05	115.74	122.64
18	A	801	CL0	O2A-CGA-O1A	-5.05	111.01	123.63
38	6	326	ERG	C12-C13-C17	5.04	124.03	116.60
31	8	304	LUT	C11-C10-C9	-5.04	120.21	127.28
19	1	5016	CLA	O2D-CGD-CBD	5.04	120.03	111.23
19	5	312	CLA	CMD-C2D-C1D	5.04	133.60	124.73
19	8	312	CLA	C3B-C4B-NB	-5.03	106.04	110.53
32	1	5017	CHL	C1B-CHB-C4A	5.03	124.56	121.32
22	K	206	BCR	C1-C6-C5	-5.03	115.76	122.64
19	B	825	CLA	CMD-C2D-C1D	5.03	133.59	124.73
19	3	5018	CLA	CMD-C2D-C1D	5.03	133.59	124.73
19	5	301	CLA	O2D-CGD-CBD	5.03	120.03	111.23
19	A	829	CLA	CMD-C2D-C1D	5.03	133.58	124.73
19	1	5008	CLA	CMD-C2D-C1D	5.03	133.58	124.73
19	5	317	CLA	CMD-C2D-C1D	5.02	133.58	124.73
19	A	818	CLA	O2D-CGD-CBD	5.02	120.01	111.23
19	7	312	CLA	O2D-CGD-CBD	5.02	120.01	111.23
19	5	321	CLA	O2D-CGD-CBD	5.02	120.01	111.23
22	4	305	BCR	C1-C6-C5	-5.02	115.77	122.64
19	7	308	CLA	O2D-CGD-CBD	5.02	120.00	111.23
19	A	836	CLA	O2D-CGD-CBD	5.02	120.00	111.23
19	6	320	CLA	CMD-C2D-C1D	5.01	133.56	124.73
22	A	849	BCR	C30-C25-C26	-5.01	115.79	122.64
22	B	845	BCR	C16-C17-C18	-5.01	120.25	127.28
32	3	5017	CHL	C1C-CHC-C4B	5.01	133.98	116.07
28	J	1902	C7Z	C27-C28-C29	-5.00	118.83	126.23
19	4	316	CLA	O2D-CGD-CBD	5.00	119.98	111.23
19	A	821	CLA	O2D-CGD-CBD	5.00	119.97	111.23
22	F	302	BCR	C33-C5-C6	-5.00	119.03	124.48
19	6	314	CLA	O2D-CGD-CBD	4.99	119.96	111.23
22	A	846	BCR	C15-C14-C13	-4.99	120.28	127.28
19	Z	312	CLA	O2D-CGD-CBD	4.99	119.95	111.23
19	B	839	CLA	O2D-CGD-CBD	4.99	119.95	111.23
31	Z	317	LUT	C21-C26-C27	-4.98	107.10	112.83
19	B	820	CLA	O2D-CGD-CBD	4.98	119.93	111.23
32	Z	313	CHL	C1C-CHC-C4B	4.97	133.86	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	5013	CLA	O2D-CGD-CBD	4.97	119.92	111.23
19	4	311	CLA	C1D-ND-C4D	-4.97	102.83	106.31
27	5	302	RRX	C33-C5-C6	-4.96	119.07	124.48
19	G	1601	CLA	O2D-CGD-CBD	4.96	119.90	111.23
22	7	305	BCR	C1-C6-C5	-4.96	115.86	122.64
22	K	206	BCR	C4-C5-C6	-4.96	116.00	122.70
19	A	828	CLA	O2D-CGD-CBD	4.96	119.89	111.23
19	A	840	CLA	CMD-C2D-C1D	4.96	133.46	124.73
19	B	809	CLA	O2D-CGD-CBD	4.95	119.89	111.23
22	6	307	BCR	C15-C14-C13	-4.94	120.35	127.28
19	A	835	CLA	O2D-CGD-CBD	4.94	119.87	111.23
19	4	312	CLA	CMD-C2D-C1D	4.94	133.42	124.73
28	6	304	C7Z	C7-C8-C9	-4.93	118.94	126.23
31	3	5002	LUT	C7-C8-C9	-4.93	118.94	126.23
22	A	847	BCR	C20-C21-C22	-4.93	120.36	127.28
19	8	313	CLA	CMD-C2D-C1D	4.93	133.41	124.73
19	A	819	CLA	O2D-CGD-CBD	4.93	119.85	111.23
19	A	857	CLA	O2D-CGD-CBD	4.92	119.84	111.23
22	A	859	BCR	C33-C5-C6	-4.92	119.11	124.48
19	5	325	CLA	O2D-CGD-CBD	4.92	119.83	111.23
19	8	320	CLA	O2D-CGD-CBD	4.92	119.83	111.23
19	B	807	CLA	O2D-CGD-CBD	4.92	119.83	111.23
27	F	304	RRX	C33-C5-C6	-4.91	119.12	124.48
19	7	318	CLA	CMD-C2D-C1D	4.91	133.37	124.73
22	B	842	BCR	C38-C26-C25	-4.91	119.13	124.48
19	6	318	CLA	O2D-CGD-CBD	4.91	119.81	111.23
22	B	844	BCR	C7-C8-C9	-4.90	118.98	126.23
19	A	805	CLA	O2D-CGD-CBD	4.90	119.79	111.23
19	6	314	CLA	CMD-C2D-C1D	4.90	133.35	124.73
19	6	322	CLA	O2D-CGD-CBD	4.90	119.79	111.23
19	Z	312	CLA	CMD-C2D-C1D	4.89	133.35	124.73
19	B	808	CLA	O2D-CGD-CBD	4.89	119.79	111.23
31	Z	317	LUT	C40-C33-C34	-4.89	114.89	122.82
19	Z	314	CLA	O2D-CGD-CBD	4.89	119.78	111.23
32	5	320	CHL	C1C-CHC-C4B	4.89	133.57	116.07
19	A	839	CLA	O2D-CGD-CBD	4.89	119.77	111.23
19	Z	315	CLA	O2D-CGD-CBD	4.88	119.76	111.23
19	B	819	CLA	O2D-CGD-CBD	4.88	119.76	111.23
22	G	1603	BCR	C27-C26-C25	-4.87	116.12	122.70
19	K	203	CLA	O2D-CGD-CBD	4.87	119.75	111.23
22	B	842	BCR	C11-C12-C13	-4.87	113.02	126.36
19	Z	304	CLA	O2D-CGD-CBD	4.86	119.73	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	307	CLA	O2D-CGD-CBD	4.86	119.73	111.23
22	B	847	BCR	C30-C25-C26	-4.86	116.00	122.64
19	A	838	CLA	O2D-CGD-CBD	4.86	119.72	111.23
19	8	309	CLA	O2D-CGD-CBD	4.86	119.72	111.23
22	B	845	BCR	C4-C5-C6	-4.86	116.14	122.70
32	8	316	CHL	C1C-CHC-C4B	4.85	133.44	116.07
19	3	5010	CLA	O2D-CGD-CBD	4.85	119.71	111.23
19	3	5018	CLA	O2D-CGD-CBD	4.85	119.71	111.23
32	1	5017	CHL	C1C-CHC-C4B	4.85	133.43	116.07
19	7	319	CLA	O2D-CGD-CBD	4.85	119.70	111.23
19	5	306	CLA	O2D-CGD-CBD	4.85	119.70	111.23
32	8	319	CHL	C1C-CHC-C4B	4.84	133.41	116.07
19	B	801	CLA	O2D-CGD-CBD	4.84	119.70	111.23
22	A	848	BCR	C20-C21-C22	-4.84	120.49	127.28
19	4	311	CLA	O2D-CGD-CBD	4.84	119.69	111.23
19	7	306	CLA	O2D-CGD-CBD	4.83	119.68	111.23
22	A	858	BCR	C1-C6-C5	-4.83	116.03	122.64
19	4	306	CLA	O2D-CGD-CBD	4.83	119.68	111.23
32	Z	309	CHL	C1C-CHC-C4B	4.83	133.36	116.07
19	4	318	CLA	O2D-CGD-CBD	4.82	119.66	111.23
32	4	319	CHL	C1C-CHC-C4B	4.82	133.32	116.07
28	6	304	C7Z	C35-C34-C33	-4.82	120.52	127.28
19	7	317	CLA	O2D-CGD-CBD	4.82	119.66	111.23
19	A	831	CLA	O2D-CGD-CBD	4.82	119.66	111.23
22	A	850	BCR	C15-C14-C13	-4.82	120.52	127.28
22	5	304	BCR	C20-C21-C22	-4.82	120.53	127.28
19	5	310	CLA	O2D-CGD-CBD	4.81	119.64	111.23
19	4	312	CLA	O2D-CGD-CBD	4.81	119.64	111.23
19	3	5011	CLA	O2A-C1-C2	4.81	126.61	108.11
19	A	810	CLA	CMD-C2D-C1D	4.80	133.18	124.73
22	K	206	BCR	C7-C8-C9	-4.79	119.14	126.23
19	B	835	CLA	C1-C2-C3	-4.79	118.34	126.20
19	A	842	CLA	O2D-CGD-CBD	4.79	119.61	111.23
19	A	843	CLA	O2D-CGD-CBD	4.79	119.61	111.23
19	B	823	CLA	O2D-CGD-CBD	4.79	119.60	111.23
19	B	828	CLA	O2D-CGD-CBD	4.78	119.59	111.23
19	3	5012	CLA	O2D-CGD-CBD	4.78	119.59	111.23
23	7	320	LHG	C5-O7-C7	-4.77	106.37	117.80
19	A	824	CLA	O2D-CGD-CBD	4.77	119.57	111.23
19	1	5008	CLA	O2D-CGD-CBD	4.77	119.57	111.23
22	3	5006	BCR	C20-C21-C22	-4.77	120.58	127.28
22	A	847	BCR	C11-C10-C9	-4.77	120.59	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	8	316	CHL	C1B-CHB-C4A	4.76	124.39	121.32
22	A	846	BCR	C20-C21-C22	-4.76	120.60	127.28
19	6	309	CLA	O2D-CGD-CBD	4.76	119.56	111.23
32	3	5017	CHL	C1A-CHA-C4D	4.76	126.93	118.98
22	B	847	BCR	C20-C21-C22	-4.76	120.60	127.28
19	B	821	CLA	O2D-CGD-CBD	4.75	119.54	111.23
31	Z	317	LUT	C27-C28-C29	-4.75	116.10	126.32
19	1	5012	CLA	O2D-CGD-CBD	4.75	119.53	111.23
19	B	810	CLA	O2D-CGD-CBD	4.74	119.52	111.23
31	7	303	LUT	C26-C27-C28	-4.74	117.20	124.58
22	A	847	BCR	C33-C5-C6	-4.74	119.31	124.48
32	7	315	CHL	C1C-CHC-C4B	4.74	133.02	116.07
19	7	313	CLA	CMD-C2D-C1D	4.73	133.06	124.73
22	3	5005	BCR	C24-C23-C22	-4.72	119.25	126.23
22	A	848	BCR	C7-C8-C9	-4.72	119.25	126.23
31	3	5002	LUT	C26-C27-C28	-4.72	117.23	124.58
22	3	5005	BCR	C7-C8-C9	-4.71	119.27	126.23
31	3	5003	LUT	C11-C10-C9	-4.71	120.67	127.28
22	K	206	BCR	C15-C14-C13	-4.71	120.67	127.28
22	A	849	BCR	C4-C5-C6	-4.71	116.35	122.70
19	5	311	CLA	O2D-CGD-CBD	4.70	119.45	111.23
22	3	5005	BCR	C38-C26-C25	-4.70	119.36	124.48
32	Z	309	CHL	C1B-CHB-C4A	4.69	124.34	121.32
19	1	5018	CLA	O2D-CGD-CBD	4.69	119.43	111.23
22	B	845	BCR	C38-C26-C25	-4.69	119.36	124.48
32	1	5014	CHL	C1C-CHC-C4B	4.68	132.83	116.07
28	J	1902	C7Z	C35-C34-C33	-4.68	120.72	127.28
19	Z	305	CLA	C1-C2-C3	-4.68	118.53	126.20
32	4	314	CHL	C1C-CHC-C4B	4.67	132.78	116.07
22	4	305	BCR	C11-C10-C9	-4.67	120.73	127.28
19	B	820	CLA	C1-C2-C3	-4.67	118.55	126.20
19	7	324	CLA	O2D-CGD-CBD	4.66	119.38	111.23
32	5	318	CHL	C1C-CHC-C4B	4.66	132.74	116.07
22	A	849	BCR	C11-C10-C9	-4.66	120.75	127.28
19	A	829	CLA	O2D-CGD-CBD	4.65	119.37	111.23
31	4	304	LUT	C7-C8-C9	-4.65	119.35	126.23
32	Z	313	CHL	CHA-C1A-C2A	-4.65	122.39	133.31
32	4	317	CHL	C1C-CHC-C4B	4.64	132.68	116.07
22	B	846	BCR	C11-C10-C9	-4.64	120.77	127.28
31	7	304	LUT	C21-C26-C27	4.64	118.16	112.83
19	A	811	CLA	O2D-CGD-CBD	4.63	119.33	111.23
22	A	859	BCR	C16-C17-C18	-4.63	120.78	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	843	BCR	C7-C8-C9	-4.63	119.39	126.23
32	5	320	CHL	C1B-CHB-C4A	4.63	124.30	121.32
19	7	316	CLA	O2D-CGD-CBD	4.63	119.32	111.23
22	A	849	BCR	C33-C5-C6	-4.62	119.44	124.48
22	8	303	BCR	C11-C10-C9	-4.62	120.79	127.28
22	6	308	BCR	C15-C16-C17	-4.62	114.06	123.52
19	1	5007	CLA	O2D-CGD-CBD	4.62	119.30	111.23
32	6	317	CHL	C1C-CHC-C4B	4.61	132.57	116.07
22	B	842	BCR	C30-C25-C26	-4.61	116.34	122.64
27	5	302	RRX	C38-C26-C25	-4.60	119.46	124.48
28	J	1902	C7Z	C7-C8-C9	-4.59	119.44	126.23
27	4	303	RRX	C38-C26-C25	-4.59	119.47	124.48
22	B	847	BCR	C38-C26-C25	-4.59	119.48	124.48
22	3	5006	BCR	C38-C26-C25	-4.59	119.48	124.48
22	A	850	BCR	C16-C17-C18	-4.59	120.85	127.28
22	3	5007	BCR	C29-C30-C25	4.58	117.10	110.44
32	Z	310	CHL	C1C-CHC-C4B	4.58	132.47	116.07
22	A	849	BCR	C15-C14-C13	-4.58	120.85	127.28
19	6	311	CLA	O2A-C1-C2	4.58	125.74	108.11
32	1	5009	CHL	C1C-CHC-C4B	4.58	132.44	116.07
19	A	832	CLA	C1-C2-C3	-4.58	118.70	126.20
28	1	5005	C7Z	C27-C28-C29	-4.57	119.47	126.23
22	8	303	BCR	C4-C5-C6	-4.57	116.52	122.70
19	6	312	CLA	O2D-CGD-CBD	4.57	119.22	111.23
22	B	846	BCR	C38-C26-C25	-4.56	119.50	124.48
22	4	305	BCR	C33-C5-C6	-4.56	119.50	124.48
22	A	858	BCR	C4-C5-C6	-4.56	116.54	122.70
32	6	319	CHL	C1C-CHC-C4B	4.56	132.38	116.07
22	B	846	BCR	C24-C23-C22	-4.55	119.50	126.23
19	1	5016	CLA	C1-C2-C3	-4.55	118.74	126.20
32	Z	302	CHL	C1C-CHC-C4B	4.55	132.36	116.07
31	Z	317	LUT	C11-C10-C9	-4.55	120.90	127.28
22	3	5005	BCR	C15-C14-C13	-4.55	120.90	127.28
22	5	305	BCR	C33-C5-C6	-4.54	119.53	124.48
32	8	317	CHL	C1C-CHC-C4B	4.54	132.32	116.07
19	A	815	CLA	C1-C2-C3	-4.54	118.76	126.20
22	8	306	BCR	C20-C21-C22	-4.53	120.92	127.28
22	3	5004	BCR	C4-C5-C6	-4.53	116.58	122.70
32	5	316	CHL	C1C-CHC-C4B	4.52	132.25	116.07
19	B	825	CLA	O2D-CGD-CBD	4.52	119.13	111.23
22	B	846	BCR	C7-C8-C9	-4.51	119.56	126.23
19	7	308	CLA	C1-C2-C3	-4.51	118.81	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	815	CLA	C1-C2-C3	-4.51	118.81	126.20
32	4	315	CHL	C1C-CHC-C4B	4.50	132.18	116.07
22	8	303	BCR	C7-C8-C9	-4.50	119.58	126.23
22	B	844	BCR	C15-C14-C13	-4.50	120.97	127.28
19	3	5014	CLA	O2D-CGD-CBD	4.49	119.08	111.23
32	Z	313	CHL	C1A-CHA-C4D	4.48	126.47	118.98
22	A	846	BCR	C16-C17-C18	-4.48	120.99	127.28
19	Z	305	CLA	O2D-CGD-CBD	4.47	119.05	111.23
22	3	5006	BCR	C30-C25-C26	-4.47	116.53	122.64
32	6	316	CHL	C1C-CHC-C4B	4.47	132.05	116.07
19	B	850	CLA	O2D-CGD-CBD	4.46	119.03	111.23
19	4	307	CLA	C1-C2-C3	-4.46	118.89	126.20
19	1	5011	CLA	C1-C2-C3	-4.45	118.90	126.20
19	B	822	CLA	C1-C2-C3	-4.45	118.90	126.20
22	G	1603	BCR	C24-C23-C22	-4.45	119.65	126.23
32	8	315	CHL	C1C-CHC-C4B	4.45	132.00	116.07
31	Z	317	LUT	C1-C6-C5	-4.45	116.56	122.64
32	5	315	CHL	C1C-CHC-C4B	4.44	131.97	116.07
22	7	305	BCR	C24-C23-C22	-4.44	119.66	126.23
31	Z	318	LUT	C18-C5-C6	-4.44	119.64	124.48
18	A	801	CL0	CHA-C1A-C2A	-4.44	122.88	133.31
32	5	318	CHL	C1-C2-C3	-4.44	119.58	126.76
32	6	315	CHL	C1C-CHC-C4B	4.44	131.95	116.07
22	A	847	BCR	C38-C26-C25	-4.43	119.65	124.48
38	8	325	ERG	C9-C10-C5	4.43	116.72	109.66
22	4	305	BCR	C15-C14-C13	-4.43	121.07	127.28
22	A	847	BCR	C27-C26-C25	-4.42	116.73	122.70
22	8	306	BCR	C38-C26-C25	-4.42	119.66	124.48
22	A	859	BCR	C20-C21-C22	-4.42	121.08	127.28
32	8	301	CHL	C1C-CHC-C4B	4.42	131.87	116.07
28	1	5005	C7Z	C18-C5-C6	-4.42	119.67	124.48
22	5	305	BCR	C11-C12-C13	-4.41	114.27	126.36
22	3	5004	BCR	C16-C17-C18	-4.41	121.09	127.28
22	3	5004	BCR	C33-C5-C6	-4.41	119.67	124.48
19	7	307	CLA	O2D-CGD-CBD	4.40	118.93	111.23
22	A	849	BCR	C20-C21-C22	-4.40	121.10	127.28
31	4	304	LUT	C21-C26-C27	-4.40	107.76	112.83
19	8	307	CLA	O2A-C1-C2	4.40	125.03	108.11
22	B	843	BCR	C27-C26-C25	-4.40	116.76	122.70
22	7	305	BCR	C15-C14-C13	-4.40	121.11	127.28
32	6	321	CHL	CHA-C1A-C2A	-4.39	123.00	133.31
32	7	314	CHL	C1C-CHC-C4B	4.39	131.77	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	846	BCR	C38-C26-C25	-4.39	119.70	124.48
19	8	314	CLA	C1-C2-C3	-4.39	119.01	126.20
19	A	831	CLA	C1-C2-C3	-4.38	119.67	126.76
19	A	840	CLA	O2D-CGD-CBD	4.38	118.89	111.23
23	A	852	LHG	O7-C7-C8	4.38	120.96	111.48
32	5	318	CHL	CHA-C1A-C2A	-4.38	123.03	133.31
28	J	1902	C7Z	C15-C14-C13	-4.38	121.14	127.28
22	A	850	BCR	C38-C26-C25	-4.37	119.71	124.48
22	6	307	BCR	C16-C17-C18	-4.37	121.14	127.28
22	B	845	BCR	C30-C25-C26	-4.37	116.66	122.64
19	A	804	CLA	C1-C2-C3	-4.36	119.05	126.20
31	1	5004	LUT	C21-C26-C27	-4.36	107.82	112.83
22	B	844	BCR	C38-C26-C25	-4.35	119.74	124.48
22	3	5004	BCR	C27-C26-C25	-4.34	116.84	122.70
19	1	5006	CLA	O2D-CGD-CBD	4.34	118.82	111.23
31	3	5003	LUT	C18-C5-C6	-4.34	119.75	124.48
22	6	308	BCR	C11-C12-C13	-4.34	114.47	126.36
22	A	849	BCR	C27-C26-C25	-4.34	116.84	122.70
19	5	314	CLA	O2D-CGD-CBD	4.33	118.81	111.23
22	3	5007	BCR	C16-C15-C14	-4.33	114.66	123.52
22	3	5006	BCR	C11-C10-C9	-4.33	121.21	127.28
31	5	303	LUT	C35-C34-C33	-4.33	121.21	127.28
19	7	309	CLA	O2A-C1-C2	4.32	124.75	108.11
32	8	319	CHL	C1-C2-C3	-4.32	119.11	126.20
23	4	320	LHG	O7-C7-C8	4.31	120.81	111.48
19	8	310	CLA	O2A-C1-C2	4.31	124.71	108.11
19	7	317	CLA	C1-C2-C3	-4.31	119.79	126.76
22	B	845	BCR	C20-C21-C22	-4.31	121.24	127.28
32	3	5017	CHL	CHA-C1A-C2A	-4.31	123.20	133.31
19	6	312	CLA	O2A-C1-C2	4.31	124.68	108.11
19	4	311	CLA	C3B-C4B-NB	-4.30	106.69	110.53
19	A	829	CLA	C1-C2-C3	-4.30	119.14	126.20
19	8	309	CLA	O2A-C1-C2	4.30	124.67	108.11
31	7	304	LUT	C35-C34-C33	-4.30	121.24	127.28
31	8	305	LUT	C35-C34-C33	-4.30	121.24	127.28
29	J	1903	LMG	O7-C10-C11	4.30	120.78	111.48
19	B	821	CLA	C1-C2-C3	-4.30	119.16	126.20
23	6	324	LHG	O7-C7-C8	4.29	120.77	111.48
18	A	801	CL0	O2A-CGA-CBA	4.29	124.91	111.83
19	3	5008	CLA	O2D-CGD-CBD	4.29	118.72	111.23
19	7	307	CLA	C1-C2-C3	-4.28	119.83	126.76
38	6	326	ERG	C13-C17-C20	-4.28	114.26	119.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	302	BCR	C30-C25-C26	-4.27	116.80	122.64
19	5	309	CLA	O2A-C1-C2	4.27	124.55	108.11
19	3	5008	CLA	O2A-C1-C2	4.27	124.54	108.11
22	K	206	BCR	C24-C23-C22	-4.26	119.93	126.23
23	A	851	LHG	O7-C7-C8	4.25	120.68	111.48
32	5	316	CHL	CHA-C1A-C2A	-4.25	123.33	133.31
19	F	301	CLA	C3B-C4B-NB	-4.25	106.74	110.53
19	7	311	CLA	O2D-CGD-CBD	4.24	118.65	111.23
22	K	206	BCR	C38-C26-C25	-4.24	119.85	124.48
22	G	1603	BCR	C15-C14-C13	-4.24	121.34	127.28
29	7	301	LMG	O7-C10-C11	4.24	120.64	111.48
22	A	848	BCR	C33-C5-C6	-4.23	119.87	124.48
22	B	842	BCR	C33-C5-C6	-4.23	119.87	124.48
22	6	307	BCR	C33-C5-C6	-4.22	119.88	124.48
27	F	304	RRX	C20-C21-C22	-4.22	121.36	127.28
22	A	858	BCR	C30-C25-C26	-4.21	116.88	122.64
22	A	858	BCR	C15-C14-C13	-4.21	121.37	127.28
22	8	303	BCR	C20-C21-C22	-4.21	121.37	127.28
28	J	1902	C7Z	C18-C5-C6	-4.21	119.89	124.48
23	Z	316	LHG	O7-C7-C8	4.21	120.58	111.48
19	A	807	CLA	C1-C2-C3	-4.20	119.31	126.20
31	1	5004	LUT	C35-C34-C33	-4.20	121.38	127.28
19	8	310	CLA	O2D-CGD-CBD	4.20	118.58	111.23
22	A	848	BCR	C27-C26-C25	-4.20	117.03	122.70
22	A	859	BCR	C27-C26-C25	-4.20	117.03	122.70
31	7	303	LUT	C31-C30-C29	-4.19	121.40	127.28
38	6	326	ERG	C19-C10-C1	-4.18	103.07	109.43
19	8	313	CLA	C1-C2-C3	-4.18	119.35	126.20
19	B	832	CLA	C1-C2-C3	-4.18	119.35	126.20
31	Z	318	LUT	C1-C6-C5	-4.18	116.93	122.64
31	7	303	LUT	C7-C8-C9	-4.17	120.06	126.23
22	A	858	BCR	C27-C26-C25	-4.17	117.07	122.70
23	7	320	LHG	O7-C7-C8	4.17	120.50	111.48
23	1	5001	LHG	O7-C7-C8	4.17	120.50	111.48
31	4	304	LUT	C17-C1-C6	-4.17	103.71	110.24
19	6	320	CLA	C1-C2-C3	-4.17	119.37	126.20
22	A	850	BCR	C30-C25-C26	-4.16	116.95	122.64
22	B	847	BCR	C1-C6-C5	-4.16	116.95	122.64
22	A	848	BCR	C38-C26-C25	-4.16	119.94	124.48
22	A	850	BCR	C33-C5-C6	-4.16	119.94	124.48
19	A	823	CLA	C1-C2-C3	-4.16	119.38	126.20
22	3	5004	BCR	C2-C1-C6	4.16	116.48	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	812	CLA	O2A-C1-C2	4.16	124.10	108.11
19	A	837	CLA	C1-C2-C3	-4.16	119.39	126.20
19	4	316	CLA	C1-C2-C3	-4.14	120.06	126.76
22	8	303	BCR	C33-C5-C6	-4.14	119.97	124.48
22	G	1603	BCR	C11-C10-C9	-4.14	121.47	127.28
22	A	849	BCR	C7-C8-C9	-4.13	120.13	126.23
32	6	317	CHL	CHA-C1A-C2A	-4.12	123.63	133.31
19	3	5016	CLA	C1-C2-C3	-4.12	119.45	126.20
19	B	811	CLA	C1-C2-C3	-4.11	119.46	126.20
22	F	302	BCR	C11-C10-C9	-4.11	121.51	127.28
25	B	848	DGD	O2G-C1B-C2B	4.11	120.38	111.48
28	J	1902	C7Z	C38-C25-C26	-4.11	120.00	124.48
32	5	315	CHL	C1-O2A-CGA	4.11	126.60	116.65
19	A	843	CLA	C1-C2-C3	-4.11	119.47	126.20
19	A	816	CLA	C1-C2-C3	-4.10	119.47	126.20
22	K	206	BCR	C30-C25-C26	-4.10	117.04	122.64
19	5	312	CLA	C1-C2-C3	-4.09	119.50	126.20
23	5	323	LHG	O7-C7-C8	4.09	120.33	111.48
19	4	309	CLA	O2A-C1-C2	4.08	123.81	108.11
32	4	314	CHL	CHA-C1A-C2A	-4.08	123.73	133.31
22	3	5006	BCR	C33-C5-C6	-4.08	120.03	124.48
32	1	5017	CHL	CHA-C1A-C2A	-4.08	123.74	133.31
27	F	304	RRX	C24-C23-C22	-4.07	120.21	126.23
32	1	5014	CHL	CHA-C1A-C2A	-4.07	123.75	133.31
19	A	833	CLA	C1-C2-C3	-4.07	119.53	126.20
23	1	5019	LHG	O7-C7-C8	4.07	120.28	111.48
22	6	308	BCR	C23-C24-C25	-4.07	116.13	127.00
19	7	324	CLA	O2A-C1-C2	4.06	123.74	108.11
32	8	316	CHL	CHA-C1A-C2A	-4.06	123.77	133.31
32	6	319	CHL	CHA-C1A-C2A	-4.06	123.77	133.31
19	7	311	CLA	C1-C2-C3	-4.06	119.55	126.20
19	B	836	CLA	O2A-C1-C2	4.05	123.70	108.11
32	7	314	CHL	C3D-C4D-CHA	4.04	114.68	108.54
31	5	303	LUT	C15-C14-C13	-4.04	121.62	127.28
32	8	301	CHL	C3D-C4D-CHA	4.04	114.67	108.54
31	1	5003	LUT	C35-C34-C33	-4.03	121.62	127.28
19	6	320	CLA	O2A-C1-C2	4.03	123.62	108.11
22	G	1603	BCR	C1-C6-C5	-4.03	117.13	122.64
19	A	810	CLA	C1-C2-C3	-4.03	119.60	126.20
32	Z	309	CHL	CHA-C1A-C2A	-4.02	123.86	133.31
31	Z	317	LUT	C40-C33-C32	-4.02	111.94	118.09
32	5	320	CHL	CHA-C1A-C2A	-4.02	123.86	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	5005	BCR	C1-C6-C5	-4.02	117.14	122.64
27	F	304	RRX	C30-C25-C26	-4.02	117.14	122.64
19	A	820	CLA	C1-C2-C3	-4.02	119.61	126.20
19	B	819	CLA	C1-C2-C3	-4.02	119.61	126.20
27	5	302	RRX	C2-C1-C6	4.02	116.27	110.44
32	1	5009	CHL	CHA-C1A-C2A	-4.01	123.89	133.31
22	K	206	BCR	C33-C5-C6	-4.01	120.11	124.48
22	6	307	BCR	C11-C12-C13	-4.01	115.38	126.36
31	Z	317	LUT	C28-C29-C30	4.00	125.31	119.01
22	A	859	BCR	C38-C26-C25	-4.00	120.12	124.48
19	B	830	CLA	C1-C2-C3	-4.00	120.29	126.76
19	7	319	CLA	C1-C2-C3	-4.00	119.65	126.20
22	3	5004	BCR	C8-C7-C6	-4.00	116.32	127.00
31	1	5004	LUT	C31-C30-C29	-3.99	121.68	127.28
19	A	821	CLA	C1-C2-C3	-3.99	119.65	126.20
18	A	801	CL0	C1C-CHC-C4B	3.99	130.36	116.07
22	3	5004	BCR	C11-C10-C9	-3.99	121.68	127.28
38	6	326	ERG	C1-C10-C5	3.99	115.62	108.74
19	5	309	CLA	C1-C2-C3	-3.99	119.66	126.20
28	6	304	C7Z	C38-C25-C26	-3.99	120.13	124.48
22	A	859	BCR	C11-C10-C9	-3.98	121.69	127.28
19	7	324	CLA	C1-C2-C3	-3.98	119.67	126.20
19	A	812	CLA	C3B-C4B-NB	-3.98	106.98	110.53
22	3	5005	BCR	C33-C5-C6	-3.97	120.15	124.48
31	8	304	LUT	C32-C33-C34	3.97	125.26	119.01
27	4	303	RRX	C20-C21-C22	-3.97	121.70	127.28
19	A	819	CLA	C1-C2-C3	-3.97	119.69	126.20
19	B	802	CLA	C1-C2-C3	-3.97	119.69	126.20
19	8	307	CLA	C1-O2A-CGA	3.97	126.26	116.65
19	A	817	CLA	C1-C2-C3	-3.97	119.70	126.20
28	6	304	C7Z	C27-C28-C29	-3.97	120.37	126.23
19	8	314	CLA	O2A-C1-C2	3.96	123.36	108.11
32	7	314	CHL	CHA-C1A-C2A	-3.96	124.00	133.31
32	8	317	CHL	C3D-C4D-CHA	3.96	114.56	108.54
22	A	848	BCR	C30-C25-C26	-3.96	117.23	122.64
23	8	321	LHG	O7-C7-C8	3.96	120.04	111.48
32	4	319	CHL	CHA-C1A-C2A	-3.95	124.02	133.31
19	4	309	CLA	C1-C2-C3	-3.95	119.72	126.20
32	5	320	CHL	C1A-CHA-C4D	3.95	125.57	118.98
22	8	306	BCR	C15-C14-C13	-3.95	121.74	127.28
31	6	306	LUT	C21-C26-C27	3.95	117.36	112.83
32	Z	310	CHL	C3C-C4C-NC	-3.94	105.02	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	5004	BCR	C38-C26-C25	-3.94	120.19	124.48
19	B	808	CLA	C1-C2-C3	-3.94	119.75	126.20
22	3	5004	BCR	C15-C14-C13	-3.93	121.76	127.28
32	Z	310	CHL	CHA-C1A-C2A	-3.93	124.08	133.31
32	6	315	CHL	CHA-C1A-C2A	-3.93	124.08	133.31
32	6	321	CHL	C3D-C4D-CHA	3.93	114.51	108.54
22	5	305	BCR	C16-C17-C18	-3.92	121.78	127.28
19	1	5015	CLA	C1-C2-C3	-3.92	120.42	126.76
22	8	306	BCR	C21-C20-C19	-3.92	111.85	123.20
31	6	305	LUT	C18-C5-C6	-3.92	120.21	124.48
29	J	1904	LMG	O7-C10-C11	3.92	119.95	111.48
22	6	307	BCR	C20-C21-C22	-3.91	121.79	127.28
19	3	5019	CLA	O2A-C1-C2	3.91	123.15	108.11
19	A	842	CLA	C1-C2-C3	-3.91	119.80	126.20
19	B	833	CLA	C1-C2-C3	-3.90	119.80	126.20
22	B	842	BCR	C1-C6-C5	-3.89	117.32	122.64
22	A	858	BCR	C38-C26-C25	-3.89	120.24	124.48
27	5	302	RRX	C10-C11-C12	-3.89	111.94	123.20
38	6	326	ERG	C16-C17-C13	-3.88	99.27	103.84
23	6	303	LHG	O7-C7-C8	3.88	119.88	111.48
32	4	315	CHL	C3D-C4D-CHA	3.88	114.44	108.54
32	4	314	CHL	C3D-C4D-CHA	3.87	114.42	108.54
19	K	203	CLA	C1-C2-C3	-3.87	119.85	126.20
22	A	846	BCR	C11-C10-C9	-3.87	121.85	127.28
32	8	316	CHL	C1A-CHA-C4D	3.87	125.44	118.98
22	5	305	BCR	C23-C24-C25	-3.86	116.67	127.00
31	6	306	LUT	C11-C10-C9	-3.86	121.86	127.28
28	1	5005	C7Z	C15-C14-C13	-3.86	121.87	127.28
32	8	315	CHL	CHA-C1A-C2A	-3.86	124.25	133.31
19	4	308	CLA	C1-C2-C3	-3.85	119.89	126.20
19	4	310	CLA	C1-C2-C3	-3.85	119.90	126.20
32	Z	309	CHL	C1-C2-C3	-3.84	119.90	126.20
22	3	5006	BCR	C24-C23-C22	-3.84	120.55	126.23
22	5	305	BCR	C16-C15-C14	-3.84	115.66	123.52
19	A	841	CLA	C1-C2-C3	-3.84	119.91	126.20
22	B	842	BCR	C20-C21-C22	-3.83	121.90	127.28
19	4	307	CLA	C3B-C4B-NB	-3.83	107.11	110.53
19	A	827	CLA	O2A-C1-C2	3.83	122.83	108.11
19	B	814	CLA	C1-C2-C3	-3.82	119.93	126.20
32	Z	309	CHL	C3D-C4D-CHA	3.82	114.35	108.54
31	3	5002	LUT	C18-C5-C6	-3.82	120.31	124.48
32	1	5014	CHL	C3D-C4D-CHA	3.81	114.34	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	8	315	CHL	C3D-C4D-CHA	3.81	114.33	108.54
22	G	1603	BCR	C30-C25-C26	-3.81	117.43	122.64
19	A	819	CLA	O2A-C1-C2	3.80	122.74	108.11
22	A	859	BCR	C29-C30-C25	3.80	115.96	110.44
22	3	5005	BCR	C16-C17-C18	-3.80	121.95	127.28
28	1	5005	C7Z	C38-C25-C26	-3.80	120.34	124.48
22	5	305	BCR	C4-C5-C6	-3.80	117.58	122.70
19	Z	315	CLA	C3B-C4B-NB	-3.79	107.14	110.53
22	8	303	BCR	C24-C23-C22	-3.79	120.62	126.23
22	5	304	BCR	C30-C25-C26	-3.79	117.45	122.64
32	8	316	CHL	C3D-C4D-CHA	3.79	114.30	108.54
19	A	828	CLA	C1-C2-C3	-3.78	120.00	126.20
19	3	5011	CLA	O2A-CGA-CBA	3.78	123.36	111.83
19	Z	315	CLA	C1-C2-C3	-3.78	120.00	126.20
22	3	5007	BCR	C23-C22-C21	3.78	124.95	119.01
19	6	322	CLA	C3B-C4B-NB	-3.78	107.16	110.53
22	A	846	BCR	C24-C23-C22	-3.78	120.65	126.23
22	B	847	BCR	C33-C5-C6	-3.78	120.36	124.48
22	7	305	BCR	C38-C26-C25	-3.77	120.36	124.48
32	8	316	CHL	C1-C2-C3	-3.77	120.02	126.20
32	4	315	CHL	C1-C2-C3	-3.77	120.66	126.76
19	A	835	CLA	C1-C2-C3	-3.77	120.03	126.20
32	6	316	CHL	C3D-C4D-CHA	3.77	114.26	108.54
32	7	315	CHL	C3D-C4D-CHA	3.76	114.26	108.54
22	B	844	BCR	C4-C5-C6	-3.76	117.62	122.70
27	5	302	RRX	C30-C25-C26	-3.76	117.50	122.64
27	4	303	RRX	C10-C11-C12	-3.76	112.31	123.20
35	7	302	DGA	OG2-CB1-CB2	3.76	119.61	111.48
32	4	315	CHL	CHA-C1A-C2A	-3.75	124.49	133.31
19	3	5013	CLA	O2A-C1-C2	3.75	122.55	108.11
28	1	5005	C7Z	C7-C8-C9	-3.75	120.69	126.23
22	A	847	BCR	C7-C8-C9	-3.75	120.69	126.23
32	8	301	CHL	CHA-C1A-C2A	-3.75	124.51	133.31
28	1	5005	C7Z	C21-C26-C25	-3.74	117.52	122.64
19	B	840	CLA	O2D-CGD-O1D	-3.74	116.57	123.85
19	6	309	CLA	O2A-C1-C2	3.74	122.49	108.11
31	8	305	LUT	C18-C5-C6	-3.73	120.41	124.48
38	8	325	ERG	C12-C13-C14	3.73	112.82	107.19
19	A	826	CLA	C1-C2-C3	-3.73	120.09	126.20
32	4	317	CHL	CHA-C1A-C2A	-3.73	124.56	133.31
22	4	305	BCR	C24-C23-C22	-3.72	120.73	126.23
31	8	305	LUT	C15-C14-C13	-3.72	122.06	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	308	CLA	O2A-C1-C2	3.72	122.43	108.11
19	A	833	CLA	O2A-C1-C2	3.72	122.43	108.11
34	6	325	3PH	O21-C21-C22	3.72	119.53	111.48
32	4	319	CHL	C1A-CHA-C4D	3.72	125.18	118.98
22	A	849	BCR	C1-C6-C5	-3.72	117.56	122.64
22	A	847	BCR	C30-C25-C26	-3.71	117.56	122.64
19	3	5010	CLA	O2A-CGA-CBA	3.71	123.16	111.83
19	8	308	CLA	C3B-C4B-NB	-3.71	107.22	110.53
19	A	824	CLA	C1-C2-C3	-3.71	120.11	126.20
22	A	848	BCR	C24-C23-C22	-3.71	120.74	126.23
32	6	316	CHL	CHA-C1A-C2A	-3.71	124.59	133.31
32	Z	302	CHL	CHA-C1A-C2A	-3.71	124.59	133.31
27	4	303	RRX	C4-C5-C6	-3.71	117.69	122.70
32	4	314	CHL	C1A-CHA-C4D	3.71	125.17	118.98
27	F	304	RRX	C7-C8-C9	-3.71	120.75	126.23
19	7	309	CLA	O2A-CGA-CBA	3.71	123.14	111.83
32	1	5009	CHL	C3D-C4D-CHA	3.71	114.18	108.54
32	Z	302	CHL	C3D-C4D-CHA	3.71	114.18	108.54
19	A	806	CLA	C1-C2-C3	-3.71	120.12	126.20
19	7	309	CLA	O2D-CGD-O1D	-3.70	116.64	123.85
32	1	5017	CHL	C3D-C4D-CHA	3.70	114.17	108.54
19	4	313	CLA	C1-C2-C3	-3.70	120.14	126.20
19	4	310	CLA	O2A-C1-C2	3.70	122.34	108.11
19	B	817	CLA	O2A-C1-C2	3.70	122.34	108.11
19	A	809	CLA	C1-C2-C3	-3.70	120.14	126.20
22	8	306	BCR	C30-C25-C26	-3.69	117.59	122.64
18	A	801	CL0	C1-C2-C3	-3.69	120.15	126.20
22	3	5007	BCR	C37-C22-C21	-3.69	116.84	122.82
34	3	5022	3PH	O21-C21-C22	3.69	119.47	111.48
31	7	303	LUT	C18-C5-C6	-3.69	120.46	124.48
32	Z	310	CHL	C3D-C4D-CHA	3.69	114.15	108.54
27	5	302	RRX	C4-C5-C6	-3.68	117.73	122.70
19	B	829	CLA	O2A-C1-C2	3.68	122.28	108.11
19	6	323	CLA	O2A-C1-C2	3.68	122.27	108.11
22	6	307	BCR	C38-C26-C25	-3.68	120.47	124.48
19	B	807	CLA	C1-C2-C3	-3.68	120.17	126.20
32	5	318	CHL	C3D-C4D-CHA	3.68	114.13	108.54
19	5	319	CLA	O2A-C1-C2	3.68	122.26	108.11
32	5	318	CHL	C1A-CHA-C4D	3.68	125.12	118.98
19	5	312	CLA	O2A-C1-C2	3.68	122.25	108.11
19	A	830	CLA	C1-C2-C3	-3.67	120.18	126.20
22	6	307	BCR	C24-C23-C22	-3.67	120.80	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	304	CLA	C1-C2-C3	-3.67	120.82	126.76
32	6	317	CHL	C3D-C4D-CHA	3.67	114.12	108.54
19	5	311	CLA	O2A-C1-C2	3.67	122.23	108.11
38	8	325	ERG	C16-C15-C14	-3.67	99.27	105.25
32	5	316	CHL	C3D-C4D-CHA	3.66	114.11	108.54
19	A	823	CLA	O2A-C1-C2	3.66	122.20	108.11
32	4	319	CHL	C3D-C4D-CHA	3.66	114.10	108.54
19	A	805	CLA	C1-C2-C3	-3.66	120.20	126.20
32	6	319	CHL	C3C-C4C-NC	-3.66	105.71	114.65
22	7	305	BCR	C33-C5-C6	-3.65	120.50	124.48
19	A	824	CLA	O2A-C1-C2	3.65	122.15	108.11
22	B	843	BCR	C30-C25-C26	-3.65	117.65	122.64
19	7	306	CLA	O2A-C1-C2	3.65	122.14	108.11
32	6	315	CHL	C3D-C4D-CHA	3.65	114.08	108.54
19	5	308	CLA	O2A-C1-C2	3.65	122.14	108.11
22	A	846	BCR	C27-C26-C25	-3.64	117.78	122.70
32	3	5017	CHL	C3D-C4D-CHA	3.64	114.07	108.54
32	5	315	CHL	CHA-C1A-C2A	-3.64	124.77	133.31
22	F	302	BCR	C16-C15-C14	-3.64	116.08	123.52
28	6	304	C7Z	C21-C26-C25	-3.63	117.67	122.64
19	Z	312	CLA	C1-C2-C3	-3.63	120.24	126.20
22	A	849	BCR	C38-C26-C25	-3.63	120.52	124.48
32	8	319	CHL	C3D-C4D-CHA	3.63	114.06	108.54
19	7	311	CLA	O2A-C1-C2	3.63	122.08	108.11
31	8	304	LUT	C1-C6-C5	-3.63	117.68	122.64
19	B	816	CLA	O2A-C1-C2	3.63	122.08	108.11
19	4	313	CLA	O2A-C1-C2	3.63	122.07	108.11
32	3	5017	CHL	C3C-C4C-NC	-3.63	105.78	114.65
32	7	315	CHL	CHA-C1A-C2A	-3.63	124.79	133.31
19	A	839	CLA	C1-C2-C3	-3.63	120.26	126.20
19	1	5018	CLA	C1-C2-C3	-3.63	120.26	126.20
19	4	307	CLA	C1D-ND-C4D	-3.62	103.77	106.31
22	B	846	BCR	C27-C26-C25	-3.62	117.81	122.70
32	8	319	CHL	CHA-C1A-C2A	-3.62	124.81	133.31
32	7	315	CHL	C1A-CHA-C4D	3.62	125.02	118.98
32	6	319	CHL	C1C-C2C-CMC	3.62	133.32	126.80
19	A	840	CLA	O2A-C1-C2	3.61	122.01	108.11
19	A	817	CLA	O2A-C1-C2	3.61	122.01	108.11
32	5	320	CHL	C3D-C4D-CHA	3.61	114.03	108.54
38	6	326	ERG	C18-C13-C14	-3.60	104.37	110.35
19	3	5012	CLA	C3B-C4B-NB	-3.60	107.32	110.53
19	7	308	CLA	O2A-C1-C2	3.60	121.96	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	813	CLA	C1-C2-C3	-3.60	120.31	126.20
22	B	845	BCR	C33-C5-C6	-3.60	120.56	124.48
19	A	803	CLA	C1-C2-C3	-3.59	120.31	126.20
22	8	306	BCR	C33-C5-C6	-3.59	120.56	124.48
22	8	306	BCR	C7-C8-C9	-3.59	120.92	126.23
19	B	808	CLA	O2A-C1-C2	3.59	121.93	108.11
31	1	5003	LUT	C7-C8-C9	-3.59	120.93	126.23
19	8	313	CLA	O2A-C1-C2	3.59	121.92	108.11
18	A	801	CL0	CBC-CAC-C3C	-3.59	107.73	112.87
32	1	5017	CHL	C1A-CHA-C4D	3.59	124.97	118.98
20	B	841	PQN	C11-C12-C13	-3.58	120.66	126.83
19	3	5014	CLA	O2A-C1-C2	3.58	121.89	108.11
31	3	5003	LUT	C35-C34-C33	-3.58	122.26	127.28
32	6	315	CHL	C3C-C4C-NC	-3.58	105.90	114.65
19	3	5018	CLA	C1-C2-C3	-3.58	120.33	126.20
22	4	305	BCR	C16-C17-C18	-3.57	122.27	127.28
19	B	825	CLA	O2A-C1-C2	3.57	121.86	108.11
19	1	5016	CLA	O2A-C1-C2	3.57	121.85	108.11
19	B	823	CLA	C1-C2-C3	-3.57	120.35	126.20
22	A	849	BCR	C38-C26-C27	3.56	121.19	113.60
34	5	324	3PH	O21-C21-C22	3.56	119.18	111.48
22	8	306	BCR	C23-C24-C25	-3.56	117.49	127.00
19	6	323	CLA	O2A-CGA-CBA	3.56	122.68	111.83
19	B	831	CLA	O2A-C1-C2	3.56	121.80	108.11
27	F	304	RRX	C38-C26-C25	-3.56	120.60	124.48
19	7	319	CLA	O2A-C1-C2	3.56	121.79	108.11
22	A	846	BCR	C1-C6-C5	-3.55	117.78	122.64
19	3	5011	CLA	CAA-C2A-C3A	-3.55	103.41	113.00
32	5	316	CHL	C3C-C4C-NC	-3.55	105.98	114.65
19	1	5010	CLA	C3B-C4B-NB	-3.55	107.36	110.53
32	8	317	CHL	CHA-C1A-C2A	-3.55	124.98	133.31
31	7	304	LUT	C15-C14-C13	-3.55	122.30	127.28
22	B	846	BCR	C15-C16-C17	-3.54	116.27	123.52
22	5	305	BCR	C36-C18-C17	-3.54	117.08	122.82
19	6	311	CLA	C3B-C4B-NB	-3.54	107.37	110.53
19	A	857	CLA	O2A-C1-C2	3.54	121.73	108.11
32	8	301	CHL	C3C-C4C-NC	-3.54	106.00	114.65
19	B	809	CLA	O2A-C1-C2	3.54	121.73	108.11
19	4	311	CLA	C1-C2-C3	-3.54	121.04	126.76
19	7	307	CLA	O2A-C1-C2	3.54	121.72	108.11
22	B	842	BCR	C11-C10-C9	-3.54	122.32	127.28
19	A	818	CLA	O2A-C1-C2	3.54	121.72	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	830	CLA	O2A-C1-C2	3.54	121.71	108.11
31	4	304	LUT	C35-C34-C33	-3.53	122.32	127.28
19	A	813	CLA	O2A-C1-C2	3.53	121.71	108.11
19	B	813	CLA	O2A-C1-C2	3.53	121.71	108.11
19	5	310	CLA	C3B-C4B-NB	-3.53	107.38	110.53
19	A	830	CLA	O2A-C1-C2	3.53	121.68	108.11
19	B	822	CLA	O2A-C1-C2	3.53	121.68	108.11
22	K	206	BCR	C20-C21-C22	-3.53	122.33	127.28
22	A	847	BCR	C24-C23-C22	-3.52	121.02	126.23
19	A	843	CLA	O2A-C1-C2	3.52	121.67	108.11
32	6	319	CHL	C3D-C4D-CHA	3.52	113.89	108.54
22	A	858	BCR	C24-C23-C22	-3.52	121.02	126.23
19	1	5010	CLA	O2A-C1-C2	3.52	121.66	108.11
22	3	5004	BCR	C20-C21-C22	-3.52	122.34	127.28
19	B	829	CLA	C1-C2-C3	-3.52	120.43	126.20
19	1	5015	CLA	O2A-C1-C2	3.52	121.64	108.11
19	A	829	CLA	O2A-C1-C2	3.52	121.64	108.11
32	5	315	CHL	C3D-C4D-CHA	3.51	113.88	108.54
19	6	301	CLA	O2A-C1-C2	3.51	121.62	108.11
19	4	306	CLA	O2A-C1-C2	3.51	121.62	108.11
22	B	844	BCR	C16-C17-C18	-3.50	122.36	127.28
31	5	303	LUT	C21-C26-C27	-3.50	108.80	112.83
31	7	303	LUT	C15-C14-C13	-3.50	122.37	127.28
19	4	307	CLA	O2A-C1-C2	3.50	121.58	108.11
38	6	326	ERG	C9-C10-C5	3.50	115.23	109.66
22	B	842	BCR	C4-C5-C6	-3.50	117.98	122.70
22	A	858	BCR	C16-C17-C18	-3.49	122.38	127.28
19	5	319	CLA	C3B-C4B-NB	-3.49	107.41	110.53
22	6	307	BCR	C23-C24-C25	-3.49	117.67	127.00
19	5	311	CLA	C1-C2-C3	-3.49	121.11	126.76
19	6	318	CLA	O2A-C1-C2	3.49	121.54	108.11
22	F	302	BCR	C20-C19-C18	-3.49	116.80	126.36
31	3	5002	LUT	C35-C34-C33	-3.49	122.39	127.28
19	6	313	CLA	O2A-C1-C2	3.49	121.52	108.11
19	8	312	CLA	C2D-C1D-ND	3.49	113.58	110.13
19	7	313	CLA	C3B-C4B-NB	-3.48	107.42	110.53
22	3	5004	BCR	C21-C20-C19	-3.48	113.11	123.20
32	4	317	CHL	C3D-C4D-CHA	3.48	113.83	108.54
32	Z	313	CHL	C3D-C4D-CHA	3.48	113.83	108.54
32	8	315	CHL	C3C-C4C-NC	-3.48	106.15	114.65
19	A	842	CLA	O2A-C1-C2	3.48	121.49	108.11
31	7	303	LUT	C30-C31-C32	-3.48	113.13	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	816	CLA	C1-C2-C3	-3.47	120.50	126.20
19	5	321	CLA	O2A-C1-C2	3.47	121.47	108.11
19	5	308	CLA	C3B-C4B-NB	-3.47	107.43	110.53
19	B	820	CLA	O2A-C1-C2	3.47	121.45	108.11
19	B	825	CLA	C3B-C4B-NB	-3.47	107.43	110.53
19	B	810	CLA	O2A-C1-C2	3.47	121.45	108.11
19	5	309	CLA	C3B-C4B-NB	-3.47	107.44	110.53
19	A	812	CLA	O2A-CGA-CBA	3.47	122.41	111.83
34	3	5022	3PH	O31-C31-C32	3.46	122.40	111.83
19	B	804	CLA	O2A-C1-C2	3.46	121.43	108.11
19	5	317	CLA	C3B-C4B-NB	-3.46	107.44	110.53
19	Z	311	CLA	O2A-C1-C2	3.46	121.42	108.11
22	4	305	BCR	C29-C30-C25	3.46	115.46	110.44
19	4	310	CLA	C3B-C4B-NB	-3.46	107.44	110.53
22	8	306	BCR	C16-C17-C18	-3.46	122.43	127.28
19	B	818	CLA	O2A-C1-C2	3.46	121.40	108.11
19	4	316	CLA	O2A-C1-C2	3.46	121.40	108.11
19	Z	306	CLA	C1-C2-C3	-3.45	121.17	126.76
19	4	312	CLA	C1-C2-C3	-3.45	120.54	126.20
31	1	5003	LUT	C21-C26-C27	-3.45	108.86	112.83
19	7	317	CLA	O2A-C1-C2	3.45	121.39	108.11
19	A	834	CLA	C1-C2-C3	-3.45	120.54	126.20
19	B	837	CLA	C1-C2-C3	-3.45	120.54	126.20
19	B	813	CLA	C1-C2-C3	-3.45	120.55	126.20
19	B	803	CLA	O2A-C1-C2	3.44	121.36	108.11
31	4	304	LUT	C15-C14-C13	-3.44	122.45	127.28
32	7	315	CHL	C3C-C4C-NC	-3.44	106.24	114.65
19	1	5013	CLA	C3B-C4B-NB	-3.44	107.46	110.53
19	B	835	CLA	O2A-C1-C2	3.44	121.34	108.11
19	8	310	CLA	O2A-CGA-CBA	3.44	122.32	111.83
19	4	311	CLA	CMA-C3A-C4A	3.43	121.00	111.77
19	G	1601	CLA	C1-C2-C3	-3.43	121.21	126.76
22	3	5006	BCR	C7-C8-C9	-3.43	121.16	126.23
31	1	5003	LUT	C18-C5-C6	-3.43	120.74	124.48
22	3	5007	BCR	C8-C9-C10	3.43	124.40	119.01
31	6	305	LUT	C15-C14-C13	-3.43	122.47	127.28
19	1	5018	CLA	O2A-C1-C2	3.43	121.30	108.11
22	B	844	BCR	C29-C30-C25	3.42	115.41	110.44
19	4	316	CLA	C3B-C4B-NB	-3.42	107.47	110.53
19	6	310	CLA	C3B-C4B-NB	-3.42	107.47	110.53
22	B	845	BCR	C24-C23-C22	-3.42	121.17	126.23
22	4	305	BCR	C27-C26-C25	-3.42	118.08	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	838	CLA	O2A-C1-C2	3.42	121.27	108.11
19	B	824	CLA	O2A-C1-C2	3.42	121.27	108.11
32	8	319	CHL	C1A-CHA-C4D	3.42	124.69	118.98
38	8	325	ERG	C11-C9-C10	-3.42	105.45	113.65
19	A	806	CLA	O2A-C1-C2	3.42	121.26	108.11
22	8	303	BCR	C33-C5-C4	3.41	120.88	113.60
19	A	803	CLA	O2A-C1-C2	3.41	121.24	108.11
31	6	306	LUT	C35-C34-C33	-3.41	122.49	127.28
31	Z	317	LUT	C7-C8-C9	-3.41	121.19	126.23
22	F	302	BCR	C27-C26-C25	-3.41	118.10	122.70
19	B	806	CLA	O2A-C1-C2	3.41	121.23	108.11
32	8	301	CHL	C1A-CHA-C4D	3.41	124.67	118.98
19	K	203	CLA	O2A-C1-C2	3.41	121.22	108.11
19	5	317	CLA	O2A-C1-C2	3.41	121.22	108.11
22	8	303	BCR	C30-C25-C26	-3.41	117.98	122.64
19	1	5013	CLA	O2A-C1-C2	3.41	120.85	109.44
19	Z	307	CLA	O2A-C1-C2	3.41	121.22	108.11
22	B	842	BCR	C23-C24-C25	-3.41	117.90	127.00
19	5	301	CLA	O2A-C1-C2	3.40	121.21	108.11
32	1	5009	CHL	C1-C2-C3	-3.40	120.62	126.20
19	A	836	CLA	C1-C2-C3	-3.40	120.62	126.20
19	A	820	CLA	O2A-C1-C2	3.40	121.20	108.11
22	5	305	BCR	C35-C13-C14	-3.40	117.31	122.82
22	4	305	BCR	C23-C24-C25	-3.40	117.92	127.00
19	B	825	CLA	O2A-CGA-CBA	3.40	122.20	111.83
19	A	808	CLA	C1-C2-C3	-3.40	120.63	126.20
19	B	807	CLA	O2A-C1-C2	3.40	121.18	108.11
19	5	307	CLA	C1-C2-C3	-3.40	120.63	126.20
19	B	825	CLA	O2D-CGD-O1D	-3.39	117.24	123.85
19	3	5016	CLA	O2A-C1-C2	3.39	121.17	108.11
19	6	312	CLA	O2A-CGA-CBA	3.39	122.18	111.83
22	B	843	BCR	C16-C17-C18	-3.39	122.53	127.28
19	3	5008	CLA	C1-C2-C3	-3.39	120.65	126.20
19	5	314	CLA	O2A-C1-C2	3.39	121.14	108.11
19	B	827	CLA	O2A-C1-C2	3.39	121.14	108.11
22	6	307	BCR	C21-C20-C19	-3.39	113.39	123.20
32	Z	310	CHL	C1-O2A-CGA	3.38	124.84	116.65
19	A	815	CLA	O2A-C1-C2	3.38	121.13	108.11
19	Z	305	CLA	O2A-C1-C2	3.38	121.13	108.11
27	4	303	RRX	C16-C17-C18	-3.38	122.53	127.28
19	7	308	CLA	CAA-C2A-C3A	-3.38	103.86	113.00
32	6	321	CHL	C3C-C4C-NC	-3.38	106.39	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	6	315	CHL	C1A-CHA-C4D	3.38	124.62	118.98
19	A	809	CLA	O2A-C1-C2	3.38	121.11	108.11
19	F	301	CLA	O2A-C1-C2	3.38	121.11	108.11
19	A	837	CLA	O2A-C1-C2	3.38	121.10	108.11
24	8	323	LMT	C1B-O1B-C4'	-3.38	109.98	117.98
22	A	846	BCR	C30-C25-C26	-3.37	118.03	122.64
32	1	5014	CHL	C1A-CHA-C4D	3.37	124.61	118.98
19	B	812	CLA	O2A-C1-C2	3.37	121.08	108.11
19	7	306	CLA	O2A-CGA-CBA	3.37	122.11	111.83
19	B	814	CLA	O2A-C1-C2	3.37	121.08	108.11
19	B	840	CLA	C1-C2-C3	-3.37	120.68	126.20
19	3	5009	CLA	C3B-C4B-NB	-3.37	107.52	110.53
27	5	302	RRX	C16-C15-C14	-3.37	116.63	123.52
19	B	850	CLA	C3B-C4B-NB	-3.37	107.52	110.53
22	3	5006	BCR	C15-C14-C13	-3.37	122.55	127.28
32	Z	302	CHL	C3C-C4C-NC	-3.36	106.43	114.65
19	A	835	CLA	O2A-C1-C2	3.36	121.05	108.11
19	Z	306	CLA	C3B-C4B-NB	-3.36	107.53	110.53
22	B	847	BCR	C8-C7-C6	-3.36	118.02	127.00
19	B	821	CLA	O2A-C1-C2	3.36	121.04	108.11
19	Z	308	CLA	C3B-C4B-NB	-3.36	107.53	110.53
19	5	310	CLA	O2A-C1-C2	3.35	121.01	108.11
19	8	313	CLA	C3B-C4B-NB	-3.35	107.54	110.53
19	B	850	CLA	O2A-C1-C2	3.35	121.01	108.11
19	A	802	CLA	O2A-C1-C2	3.35	121.01	108.11
22	F	302	BCR	C8-C7-C6	-3.35	118.05	127.00
32	4	317	CHL	C3C-C4C-NC	-3.35	106.47	114.65
19	6	312	CLA	C3B-C4B-NB	-3.35	107.54	110.53
19	8	312	CLA	C4B-CHC-C1C	3.35	134.12	126.25
19	8	309	CLA	C3B-C4B-NB	-3.35	107.54	110.53
31	1	5004	LUT	C15-C14-C13	-3.34	122.59	127.28
22	F	302	BCR	C1-C6-C5	-3.34	118.07	122.64
19	Z	312	CLA	O2A-C1-C2	3.34	120.97	108.11
22	3	5007	BCR	C2-C1-C6	3.34	115.29	110.44
19	A	831	CLA	O2A-C1-C2	3.34	120.97	108.11
22	3	5004	BCR	C23-C24-C25	-3.34	118.08	127.00
32	8	317	CHL	C3C-C4C-NC	-3.34	106.49	114.65
22	A	858	BCR	C20-C21-C22	-3.34	122.59	127.28
19	3	5010	CLA	C3B-C4B-NB	-3.34	107.55	110.53
32	8	319	CHL	C3C-C4C-NC	-3.34	106.50	114.65
22	A	859	BCR	C4-C5-C6	-3.33	118.20	122.70
22	3	5006	BCR	C4-C5-C6	-3.33	118.20	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	841	CLA	O2A-C1-C2	3.33	120.94	108.11
19	B	802	CLA	O2A-C1-C2	3.33	120.94	108.11
19	8	312	CLA	O2A-C1-C2	3.33	120.93	108.11
28	6	304	C7Z	C18-C5-C6	-3.33	120.85	124.48
22	5	305	BCR	C12-C13-C14	3.33	124.25	119.01
19	A	816	CLA	O2A-C1-C2	3.33	120.93	108.11
22	B	845	BCR	C7-C8-C9	-3.33	121.31	126.23
19	6	301	CLA	C3B-C4B-NB	-3.33	107.56	110.53
22	3	5004	BCR	C29-C30-C25	3.33	115.27	110.44
19	A	826	CLA	O2A-C1-C2	3.33	120.91	108.11
32	Z	309	CHL	C3C-C4C-NC	-3.32	106.53	114.65
19	B	828	CLA	O2A-C1-C2	3.32	120.89	108.11
31	8	305	LUT	C11-C10-C9	-3.32	122.62	127.28
32	4	314	CHL	C3C-C4C-NC	-3.32	106.54	114.65
19	A	810	CLA	O2A-C1-C2	3.32	120.88	108.11
32	6	315	CHL	C1-C2-C3	-3.32	120.76	126.20
27	5	302	RRX	C8-C7-C6	-3.31	118.15	127.00
27	F	304	RRX	C4-C5-C6	-3.31	118.23	122.70
31	Z	318	LUT	C22-C23-C24	3.31	116.10	111.18
19	4	312	CLA	O2A-C1-C2	3.31	120.84	108.11
19	7	310	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
19	5	307	CLA	O2A-C1-C2	3.31	120.83	108.11
19	B	832	CLA	O2A-C1-C2	3.31	120.83	108.11
19	1	5011	CLA	O2A-C1-C2	3.30	120.82	108.11
19	A	840	CLA	C1-C2-C3	-3.30	120.79	126.20
32	6	317	CHL	C3C-C4C-NC	-3.30	106.59	114.65
19	4	311	CLA	C2D-C1D-ND	3.30	113.39	110.13
22	A	846	BCR	C4-C5-C6	-3.30	118.25	122.70
22	3	5007	BCR	C30-C25-C26	-3.29	118.13	122.64
24	A	853	LMT	C1B-O1B-C4'	-3.29	110.17	117.98
27	4	303	RRX	C8-C7-C6	-3.29	118.21	127.00
19	Z	308	CLA	O2A-C1-C2	3.29	120.77	108.11
22	B	847	BCR	C23-C24-C25	-3.29	118.21	127.00
19	B	831	CLA	C1-C2-C3	-3.29	120.81	126.20
19	B	826	CLA	O2A-C1-C2	3.29	120.76	108.11
19	A	840	CLA	C3B-C4B-NB	-3.29	107.60	110.53
19	B	815	CLA	O2A-C1-C2	3.28	120.75	108.11
19	5	325	CLA	C3B-C4B-NB	-3.28	107.60	110.53
18	A	801	CL0	O2A-C1-C2	3.28	120.74	108.11
19	A	822	CLA	O2A-C1-C2	3.28	120.74	108.11
22	3	5007	BCR	C27-C26-C25	-3.28	118.27	122.70
19	A	805	CLA	O2A-C1-C2	3.28	120.73	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	312	CLA	C3B-C4B-NB	-3.28	107.61	110.53
19	B	828	CLA	C1-C2-C3	-3.28	120.83	126.20
22	6	307	BCR	C29-C30-C25	3.27	115.19	110.44
31	7	303	LUT	C35-C34-C33	-3.27	122.69	127.28
19	7	318	CLA	C3B-C4B-NB	-3.27	107.61	110.53
22	K	206	BCR	C38-C26-C27	3.27	120.56	113.60
19	3	5019	CLA	C3B-C4B-NB	-3.27	107.61	110.53
24	8	323	LMT	C1-O1'-C1'	-3.27	108.10	113.68
32	3	5017	CHL	C1B-CHB-C4A	3.26	123.42	121.32
32	5	315	CHL	C3C-C4C-NC	-3.26	106.67	114.65
19	3	5014	CLA	C1-C2-C3	-3.26	120.85	126.20
19	6	314	CLA	O2A-C1-C2	3.26	120.65	108.11
22	7	305	BCR	C7-C8-C9	-3.26	121.41	126.23
19	8	312	CLA	CHD-C1D-ND	-3.26	120.22	124.80
22	3	5005	BCR	C8-C7-C6	-3.26	118.30	127.00
32	8	315	CHL	C1-O2A-CGA	3.26	124.54	116.65
19	A	811	CLA	O2A-C1-C2	3.26	120.64	108.11
32	4	317	CHL	C1A-CHA-C4D	3.25	124.41	118.98
19	A	806	CLA	C3B-C4B-NB	-3.25	107.63	110.53
19	B	803	CLA	C3B-C4B-NB	-3.25	107.63	110.53
19	6	323	CLA	C1-C2-C3	-3.25	120.87	126.20
22	K	206	BCR	C16-C17-C18	-3.25	122.72	127.28
19	A	809	CLA	C3B-C4B-NB	-3.25	107.63	110.53
19	A	818	CLA	C3B-C4B-NB	-3.25	107.63	110.53
19	A	832	CLA	O2A-C1-C2	3.25	120.61	108.11
19	B	836	CLA	O2A-CGA-CBA	3.25	121.74	111.83
19	3	5018	CLA	O2A-C1-C2	3.24	120.58	108.11
22	8	303	BCR	C27-C26-C25	-3.24	118.33	122.70
22	B	847	BCR	C4-C5-C6	-3.24	118.33	122.70
19	B	819	CLA	O2A-C1-C2	3.24	120.56	108.11
22	B	843	BCR	C24-C23-C22	-3.23	121.45	126.23
19	A	834	CLA	O2A-C1-C2	3.23	120.55	108.11
31	1	5003	LUT	C8-C7-C6	-3.23	118.38	127.00
19	3	5011	CLA	C3B-C4B-NB	-3.22	107.65	110.53
22	7	305	BCR	C33-C5-C4	3.22	120.47	113.60
19	6	302	CLA	O2A-C1-C2	3.22	120.51	108.11
19	3	5008	CLA	O2A-CGA-CBA	3.22	121.66	111.83
31	Z	318	LUT	C15-C14-C13	-3.22	122.77	127.28
32	8	315	CHL	C1A-CHA-C4D	3.21	124.34	118.98
19	B	840	CLA	C2C-C1C-NC	3.21	113.36	109.98
31	6	306	LUT	C18-C5-C6	-3.21	120.98	124.48
22	A	849	BCR	C8-C7-C6	-3.21	118.42	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	303	RRX	C7-C8-C9	-3.21	121.49	126.23
22	A	847	BCR	C4-C5-C6	-3.21	118.37	122.70
32	Z	313	CHL	C3C-C4C-NC	-3.20	106.82	114.65
32	8	316	CHL	C3C-C4C-NC	-3.20	106.82	114.65
32	8	317	CHL	C1A-CHA-C4D	3.20	124.33	118.98
22	G	1603	BCR	C7-C8-C9	-3.20	121.50	126.23
19	A	808	CLA	O2A-C1-C2	3.20	120.42	108.11
19	A	832	CLA	C3B-C4B-NB	-3.20	107.67	110.53
19	A	821	CLA	O2A-C1-C2	3.20	120.42	108.11
31	3	5002	LUT	C15-C14-C13	-3.20	122.80	127.28
32	4	315	CHL	C3C-C4C-NC	-3.19	106.85	114.65
19	5	306	CLA	O2A-C1-C2	3.19	120.39	108.11
19	6	313	CLA	C1-C2-C3	-3.19	120.97	126.20
32	6	319	CHL	C1A-CHA-C4D	3.18	124.30	118.98
19	F	301	CLA	C1-C2-C3	-3.18	120.98	126.20
38	6	326	ERG	C19-C10-C9	-3.18	105.69	110.98
27	5	302	RRX	C20-C21-C22	-3.18	122.81	127.28
22	B	846	BCR	C36-C18-C19	3.18	122.95	118.09
32	7	314	CHL	C3C-C4C-NC	-3.18	106.88	114.65
19	8	311	CLA	C3B-C4B-NB	-3.18	107.69	110.53
31	8	305	LUT	C30-C31-C32	-3.18	113.99	123.20
23	6	324	LHG	O8-C23-C24	3.18	121.53	111.83
19	8	311	CLA	C1-C2-C3	-3.18	120.99	126.20
19	A	836	CLA	O2A-C1-C2	3.18	120.33	108.11
24	Z	301	LMT	C1B-O1B-C4'	-3.18	110.45	117.98
22	A	848	BCR	C23-C24-C25	-3.18	118.52	127.00
32	1	5009	CHL	C3C-C4C-NC	-3.17	106.89	114.65
19	8	311	CLA	O2A-C1-C2	3.17	120.32	108.11
19	8	310	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
19	Z	308	CLA	C1-C2-C3	-3.17	121.00	126.20
19	5	314	CLA	C3B-C4B-NB	-3.17	107.70	110.53
19	B	811	CLA	O2A-C1-C2	3.17	120.31	108.11
31	7	303	LUT	C21-C26-C27	-3.17	109.18	112.83
19	B	823	CLA	O2A-C1-C2	3.17	120.30	108.11
32	5	318	CHL	C3C-C4C-NC	-3.17	106.91	114.65
19	8	308	CLA	C1D-ND-C4D	-3.17	104.09	106.31
19	6	322	CLA	C1D-ND-C4D	-3.17	104.09	106.31
19	4	311	CLA	C4B-CHC-C1C	3.17	133.69	126.25
22	5	304	BCR	C23-C24-C25	-3.17	118.54	127.00
22	A	849	BCR	C20-C19-C18	-3.17	117.68	126.36
22	3	5004	BCR	C38-C26-C27	3.17	120.34	113.60
19	1	5010	CLA	C1-C2-C3	-3.17	121.01	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	807	CLA	O2A-C1-C2	3.16	120.28	108.11
19	8	312	CLA	CMD-C2D-C3D	-3.16	120.44	127.69
31	Z	317	LUT	C35-C15-C14	-3.16	117.05	123.52
31	7	303	LUT	C8-C7-C6	-3.16	118.55	127.00
19	A	829	CLA	C3B-C4B-NB	-3.16	107.71	110.53
19	B	813	CLA	CMA-C3A-C4A	3.16	120.26	111.77
19	4	306	CLA	C3B-C4B-NB	-3.16	107.71	110.53
19	6	323	CLA	C3B-C4B-NB	-3.16	107.71	110.53
32	1	5009	CHL	C1A-CHA-C4D	3.15	124.25	118.98
31	Z	317	LUT	C39-C29-C30	-3.15	117.71	122.82
27	5	302	RRX	C16-C17-C18	-3.15	122.86	127.28
19	B	812	CLA	C3B-C4B-NB	-3.15	107.72	110.53
19	F	301	CLA	C1D-ND-C4D	-3.15	104.10	106.31
19	8	312	CLA	C4A-NA-C1A	3.15	108.12	106.68
19	A	822	CLA	C1-C2-C3	-3.15	121.04	126.20
19	B	837	CLA	O2A-C1-C2	3.15	120.22	108.11
22	A	859	BCR	C8-C7-C6	-3.15	118.59	127.00
22	6	307	BCR	C38-C26-C27	3.15	120.31	113.60
32	7	314	CHL	C1A-CHA-C4D	3.15	124.23	118.98
19	Z	306	CLA	O2A-C1-C2	3.14	120.21	108.11
19	A	840	CLA	O2A-CGA-CBA	3.14	121.42	111.83
22	B	842	BCR	C8-C7-C6	-3.14	118.60	127.00
19	B	801	CLA	O2A-C1-C2	3.14	120.20	108.11
19	Z	307	CLA	C3B-C4B-NB	-3.14	107.73	110.53
22	5	304	BCR	C27-C26-C25	-3.14	118.46	122.70
19	B	806	CLA	C1-C2-C3	-3.14	121.06	126.20
22	3	5006	BCR	C38-C26-C27	3.14	120.29	113.60
19	G	1602	CLA	C3B-C4B-NB	-3.14	107.73	110.53
19	A	825	CLA	CMA-C3A-C4A	3.14	120.20	111.77
19	A	857	CLA	C1-C2-C3	-3.14	121.06	126.20
31	1	5003	LUT	C30-C31-C32	-3.14	114.12	123.20
19	3	5012	CLA	C1-C2-C3	-3.13	121.06	126.20
19	A	857	CLA	C3B-C4B-NB	-3.13	107.73	110.53
19	B	811	CLA	CMA-C3A-C4A	3.13	120.19	111.77
19	A	836	CLA	C3B-C4B-NB	-3.13	107.74	110.53
19	Z	315	CLA	C1D-ND-C4D	-3.13	104.12	106.31
19	5	322	CLA	C1D-ND-C4D	-3.13	104.12	106.31
19	4	311	CLA	O2A-C1-C2	3.13	120.14	108.11
22	5	304	BCR	C15-C14-C13	-3.13	122.89	127.28
19	8	308	CLA	O2A-C1-C2	3.13	120.13	108.11
19	B	826	CLA	C1-C2-C3	-3.13	121.08	126.20
22	6	307	BCR	C7-C8-C9	-3.12	121.61	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	827	CLA	C1-C2-C3	-3.12	121.08	126.20
19	A	804	CLA	O2A-C1-C2	3.12	120.12	108.11
19	A	828	CLA	CMA-C3A-C4A	3.12	120.16	111.77
19	8	312	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
19	4	312	CLA	C3B-C4B-NB	-3.12	107.75	110.53
22	3	5007	BCR	C34-C9-C10	-3.12	117.76	122.82
19	4	313	CLA	C3B-C4B-NB	-3.12	107.75	110.53
19	A	825	CLA	C1-C2-C3	-3.12	121.09	126.20
22	7	305	BCR	C27-C26-C25	-3.12	118.49	122.70
19	B	828	CLA	CMA-C3A-C4A	3.12	120.15	111.77
19	B	802	CLA	C3B-C4B-NB	-3.12	107.75	110.53
22	8	306	BCR	C8-C7-C6	-3.12	118.68	127.00
22	A	850	BCR	C24-C23-C22	-3.11	121.63	126.23
22	6	307	BCR	C27-C26-C25	-3.11	118.50	122.70
19	6	311	CLA	O2A-CGA-CBA	3.11	121.33	111.83
22	A	850	BCR	C11-C10-C9	-3.11	122.91	127.28
31	5	303	LUT	C11-C10-C9	-3.11	122.91	127.28
31	6	305	LUT	C30-C31-C32	-3.11	114.18	123.20
19	7	307	CLA	C2C-C1C-NC	3.11	113.25	109.98
22	3	5005	BCR	C11-C12-C13	-3.11	117.84	126.36
19	A	812	CLA	C1D-ND-C4D	-3.11	104.13	106.31
31	8	305	LUT	C31-C30-C29	-3.10	122.92	127.28
19	4	309	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
19	B	840	CLA	O2A-C1-C2	3.10	120.05	108.11
19	A	815	CLA	O2A-CGA-CBA	3.10	121.30	111.83
31	6	305	LUT	C35-C15-C14	-3.10	117.17	123.52
22	6	308	BCR	C24-C23-C22	-3.10	121.65	126.23
19	5	322	CLA	CMA-C3A-C4A	3.10	120.10	111.77
19	B	818	CLA	C1-C2-C3	-3.10	121.12	126.20
32	5	315	CHL	C1A-CHA-C4D	3.10	124.15	118.98
19	6	309	CLA	C3B-C4B-NB	-3.10	107.77	110.53
32	Z	310	CHL	C1A-CHA-C4D	3.09	124.14	118.98
19	8	310	CLA	C1-C2-C3	-3.09	121.13	126.20
19	7	312	CLA	C1-C2-C3	-3.09	121.13	126.20
19	7	310	CLA	C3B-C4B-NB	-3.09	107.77	110.53
32	7	315	CHL	C1-C2-C3	-3.09	121.14	126.20
19	7	312	CLA	O2A-C1-C2	3.09	119.99	108.11
19	6	312	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
22	7	305	BCR	C38-C26-C27	3.09	120.17	113.60
19	1	5015	CLA	C3B-C4B-NB	-3.09	107.78	110.53
19	A	822	CLA	C1D-ND-C4D	-3.08	104.15	106.31
28	1	5005	C7Z	C8-C7-C6	-3.08	118.76	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	7	316	CLA	C1C-C2C-C3C	-3.08	103.74	106.98
20	A	844	PQN	C14-C13-C15	3.08	120.58	115.23
31	7	303	LUT	C35-C15-C14	-3.08	117.22	123.52
19	5	306	CLA	C1D-ND-C4D	-3.08	104.15	106.31
22	3	5005	BCR	C23-C24-C25	-3.08	118.77	127.00
19	B	834	CLA	C3B-C4B-NB	-3.08	107.78	110.53
19	Z	312	CLA	C3B-C4B-NB	-3.08	107.78	110.53
22	4	305	BCR	C4-C5-C6	-3.08	118.54	122.70
19	3	5009	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
19	A	839	CLA	O2A-C1-C2	3.08	119.95	108.11
19	A	824	CLA	C3B-C4B-NB	-3.08	107.78	110.53
31	5	303	LUT	C30-C31-C32	-3.08	114.29	123.20
19	1	5008	CLA	C6-C5-C3	-3.07	105.98	113.47
22	6	308	BCR	C27-C26-C25	-3.07	118.55	122.70
19	A	807	CLA	CMA-C3A-C4A	3.07	120.03	111.77
19	7	312	CLA	C3B-C4B-NB	-3.07	107.79	110.53
31	8	304	LUT	C8-C7-C6	-3.07	118.80	127.00
19	6	310	CLA	O2A-C1-C2	3.07	119.92	108.11
19	A	823	CLA	C3B-C4B-NB	-3.07	107.79	110.53
19	4	309	CLA	C1C-C2C-C3C	-3.07	103.75	106.98
19	3	5011	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
19	4	310	CLA	C11-C12-C13	-3.07	105.77	115.97
19	8	314	CLA	C3B-C4B-NB	-3.07	107.79	110.53
22	5	305	BCR	C27-C26-C25	-3.07	118.56	122.70
19	Z	303	CLA	C2C-C1C-NC	3.07	113.20	109.98
19	7	317	CLA	C1D-ND-C4D	-3.07	104.16	106.31
19	8	312	CLA	CMA-C3A-C4A	3.06	120.01	111.77
19	7	310	CLA	O2A-C1-C2	3.06	119.89	108.11
22	3	5004	BCR	C33-C5-C4	3.06	120.12	113.60
19	5	306	CLA	C3B-C4B-NB	-3.06	107.80	110.53
19	5	307	CLA	C3B-C4B-NB	-3.06	107.80	110.53
23	6	303	LHG	O8-C23-C24	3.06	121.15	111.83
27	5	302	RRX	C35-C13-C12	3.05	122.75	118.09
19	6	302	CLA	C1-C2-C3	-3.05	121.20	126.20
19	B	836	CLA	C3B-C4B-NB	-3.05	107.81	110.53
19	7	308	CLA	C3B-C4B-NB	-3.05	107.81	110.53
31	Z	318	LUT	C21-C26-C27	-3.05	109.32	112.83
19	8	309	CLA	C6-C5-C3	-3.05	106.04	113.47
19	4	310	CLA	O2A-CGA-CBA	3.05	121.13	111.83
19	6	311	CLA	C1D-ND-C4D	-3.05	104.17	106.31
19	8	318	CLA	CAA-CBA-CGA	-3.05	104.55	113.21
22	6	307	BCR	C33-C5-C4	3.05	120.09	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	841	CLA	C3B-C4B-NB	-3.05	107.81	110.53
19	B	803	CLA	CMA-C3A-C4A	3.05	119.96	111.77
19	5	309	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
19	A	842	CLA	CMA-C3A-C4A	3.04	119.96	111.77
19	A	829	CLA	CMA-C3A-C4A	3.04	119.95	111.77
19	B	823	CLA	CMA-C3A-C4A	3.04	119.95	111.77
19	F	301	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
19	Z	311	CLA	C1C-C2C-C3C	-3.04	103.78	106.98
32	5	320	CHL	C3C-C4C-NC	-3.04	107.22	114.65
22	A	859	BCR	C20-C19-C18	-3.04	118.02	126.36
19	B	801	CLA	C1-C2-C3	-3.04	121.22	126.20
32	Z	309	CHL	C1A-CHA-C4D	3.04	124.05	118.98
19	B	822	CLA	C1D-ND-C4D	-3.04	104.18	106.31
31	8	305	LUT	C10-C11-C12	-3.04	114.41	123.20
19	A	842	CLA	C3B-C4B-NB	-3.03	107.82	110.53
19	Z	314	CLA	C3B-C4B-NB	-3.03	107.82	110.53
32	Z	313	CHL	C1B-CHB-C4A	3.03	123.27	121.32
28	J	1902	C7Z	C38-C25-C24	3.03	120.00	114.42
19	A	802	CLA	C3B-C4B-NB	-3.03	107.82	110.53
22	6	308	BCR	C7-C8-C9	-3.03	121.75	126.23
32	4	319	CHL	C3C-C4C-NC	-3.03	107.25	114.65
19	A	825	CLA	O2A-C1-C2	3.03	119.77	108.11
22	5	304	BCR	C7-C8-C9	-3.03	121.75	126.23
19	8	307	CLA	O2A-CGA-CBA	3.03	121.07	111.83
22	A	846	BCR	C38-C26-C27	3.03	120.05	113.60
27	5	302	RRX	C33-C5-C4	3.03	120.05	113.60
19	A	803	CLA	C3B-C4B-NB	-3.03	107.83	110.53
19	A	820	CLA	C3B-C4B-NB	-3.03	107.83	110.53
19	7	318	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
19	Z	306	CLA	C1D-ND-C4D	-3.03	104.19	106.31
19	5	314	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
22	G	1603	BCR	C4-C5-C6	-3.03	118.62	122.70
19	5	310	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
19	A	812	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
19	5	312	CLA	CMA-C3A-C4A	3.02	119.90	111.77
28	J	1902	C7Z	C1-C6-C5	-3.02	118.50	122.64
19	8	313	CLA	C1D-ND-C4D	-3.02	104.19	106.31
22	B	842	BCR	C33-C5-C4	3.02	120.04	113.60
32	1	5017	CHL	C3C-C4C-NC	-3.02	107.27	114.65
31	3	5003	LUT	C15-C14-C13	-3.02	123.05	127.28
19	Z	305	CLA	C1D-ND-C4D	-3.02	104.20	106.31
19	1	5018	CLA	C3B-C4B-NB	-3.02	107.84	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	835	CLA	CMA-C3A-C4A	3.01	119.87	111.77
19	B	833	CLA	C3B-C4B-NB	-3.01	107.84	110.53
22	A	847	BCR	C38-C26-C27	3.01	120.02	113.60
22	B	844	BCR	C1-C6-C5	-3.01	118.52	122.64
19	B	838	CLA	CMA-C3A-C4A	3.01	119.86	111.77
19	A	805	CLA	C1D-ND-C4D	-3.01	104.20	106.31
19	A	857	CLA	CMA-C3A-C4A	3.01	119.86	111.77
19	A	833	CLA	CMA-C3A-C4A	3.01	119.85	111.77
19	B	817	CLA	C3B-C4B-NB	-3.01	107.85	110.53
19	B	808	CLA	C1D-ND-C4D	-3.00	104.20	106.31
19	B	831	CLA	C1D-ND-C4D	-3.00	104.20	106.31
19	5	301	CLA	C1-C2-C3	-3.00	121.28	126.20
19	A	811	CLA	CMA-C3A-C4A	3.00	119.85	111.77
19	8	318	CLA	C3B-C4B-NB	-3.00	107.85	110.53
19	B	824	CLA	C1-C2-C3	-3.00	121.28	126.20
19	5	322	CLA	C3B-C4B-NB	-3.00	107.85	110.53
32	Z	313	CHL	CMA-C3A-C4A	3.00	121.08	114.61
19	A	818	CLA	C1-C2-C3	-3.00	121.28	126.20
19	B	828	CLA	C3B-C4B-NB	-3.00	107.85	110.53
19	B	803	CLA	C2C-C1C-NC	3.00	113.13	109.98
32	Z	302	CHL	C1A-CHA-C4D	3.00	123.99	118.98
28	J	1902	C7Z	C31-C32-C33	-3.00	118.14	126.36
19	6	320	CLA	C3B-C4B-NB	-3.00	107.85	110.53
19	7	324	CLA	C3B-C4B-NB	-3.00	107.85	110.53
19	B	840	CLA	C1C-C2C-C3C	-3.00	103.83	106.98
19	6	320	CLA	O2A-CGA-CBA	3.00	120.97	111.83
22	3	5005	BCR	C15-C16-C17	-3.00	117.39	123.52
23	A	851	LHG	O8-C23-C24	2.99	120.97	111.83
32	8	317	CHL	C4D-CHA-CBD	-2.99	105.95	108.97
19	B	803	CLA	C1-C2-C3	-2.99	121.29	126.20
31	1	5003	LUT	C11-C10-C9	-2.99	123.08	127.28
19	A	817	CLA	CMA-C3A-C4A	2.99	119.82	111.77
22	A	859	BCR	C38-C26-C27	2.99	119.98	113.60
19	A	807	CLA	C3B-C4B-NB	-2.99	107.86	110.53
19	Z	305	CLA	C3B-C4B-NB	-2.99	107.86	110.53
19	A	811	CLA	C1-C2-C3	-2.99	121.30	126.20
19	5	310	CLA	CMA-C3A-C4A	2.99	119.81	111.77
19	1	5016	CLA	C3B-C4B-NB	-2.99	107.86	110.53
32	Z	310	CHL	C1C-C2C-CMC	2.99	132.19	126.80
19	K	202	CLA	CMA-C3A-C4A	2.99	119.81	111.77
19	B	826	CLA	C3B-C4B-NB	-2.99	107.86	110.53
32	5	316	CHL	CMA-C3A-C4A	2.99	121.05	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	308	CLA	C3B-C4B-NB	-2.99	107.86	110.53
19	3	5008	CLA	CAA-C2A-C3A	-2.99	104.93	113.00
19	A	811	CLA	C1D-ND-C4D	-2.99	104.22	106.31
31	1	5004	LUT	C18-C5-C6	-2.99	121.23	124.48
31	6	305	LUT	C31-C30-C29	-2.98	123.09	127.28
19	B	826	CLA	CMA-C3A-C4A	2.98	119.79	111.77
19	5	308	CLA	C1D-ND-C4D	-2.98	104.22	106.31
19	B	805	CLA	CMA-C3A-C4A	2.98	119.79	111.77
19	G	1601	CLA	O2A-C1-C2	2.98	119.58	108.11
19	5	317	CLA	C1D-ND-C4D	-2.98	104.22	106.31
22	5	305	BCR	C30-C25-C26	-2.98	118.56	122.64
22	7	305	BCR	C15-C16-C17	-2.98	117.42	123.52
19	B	805	CLA	C3B-C4B-NB	-2.98	107.87	110.53
22	B	845	BCR	C33-C5-C4	2.98	119.95	113.60
19	7	316	CLA	O2A-C1-C2	2.98	119.57	108.11
32	1	5014	CHL	C3C-C4C-NC	-2.98	107.37	114.65
22	A	848	BCR	C38-C26-C27	2.98	119.94	113.60
19	B	838	CLA	O2A-C1-C2	2.97	119.55	108.11
19	B	810	CLA	C1-C2-C3	-2.97	121.33	126.20
19	A	833	CLA	C3B-C4B-NB	-2.97	107.88	110.53
19	B	820	CLA	CMA-C3A-C4A	2.97	119.76	111.77
19	6	311	CLA	CMA-C3A-C4A	2.97	119.76	111.77
19	5	309	CLA	O2A-CGA-CBA	2.97	120.89	111.83
22	4	305	BCR	C8-C7-C6	-2.97	119.06	127.00
19	A	818	CLA	CMA-C3A-C4A	2.97	119.75	111.77
22	G	1603	BCR	C8-C7-C6	-2.97	119.06	127.00
28	6	304	C7Z	C11-C12-C13	-2.97	118.22	126.36
19	5	308	CLA	O2A-CGA-CBA	2.97	120.89	111.83
19	F	303	CLA	C3B-C4B-NB	-2.97	107.88	110.53
32	4	314	CHL	C1-O2A-CGA	2.97	123.83	116.65
22	A	847	BCR	C23-C24-C25	-2.97	119.08	127.00
19	F	303	CLA	C1D-ND-C4D	-2.97	104.23	106.31
19	5	325	CLA	O2A-C1-C2	2.97	119.52	108.11
22	6	308	BCR	C36-C18-C19	2.96	122.62	118.09
19	B	824	CLA	O2A-CGA-CBA	2.96	120.87	111.83
19	B	820	CLA	C3B-C4B-NB	-2.96	107.89	110.53
19	6	318	CLA	C1-C2-C3	-2.96	121.97	126.76
19	B	805	CLA	C1D-ND-C4D	-2.96	104.23	106.31
19	F	301	CLA	CAA-CBA-CGA	-2.96	104.80	113.21
22	3	5006	BCR	C23-C24-C25	-2.96	119.09	127.00
19	A	824	CLA	CMA-C3A-C4A	2.96	119.73	111.77
19	1	5012	CLA	O2A-C1-C2	2.96	119.50	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	301	CLA	CMA-C3A-C4A	2.96	119.73	111.77
19	6	310	CLA	C1D-ND-C4D	-2.96	104.24	106.31
19	6	314	CLA	C3B-C4B-NB	-2.96	107.89	110.53
19	B	839	CLA	C2C-C1C-NC	2.96	113.09	109.98
19	5	301	CLA	C3B-C4B-NB	-2.96	107.89	110.53
32	6	317	CHL	C1A-CHA-C4D	2.96	123.92	118.98
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
31	3	5003	LUT	C1-C6-C5	-2.96	118.60	122.64
31	3	5002	LUT	C30-C31-C32	-2.96	114.64	123.20
22	6	307	BCR	C8-C7-C6	-2.96	119.10	127.00
19	Z	315	CLA	O2A-C1-C2	2.96	119.48	108.11
19	I	201	CLA	CMA-C3A-C4A	2.95	119.72	111.77
38	6	326	ERG	C13-C14-C8	-2.95	108.38	113.59
22	4	305	BCR	C38-C26-C27	2.95	119.89	113.60
22	6	308	BCR	C1-C6-C5	-2.95	118.60	122.64
19	6	301	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
19	A	813	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
31	4	304	LUT	C8-C7-C6	-2.95	119.11	127.00
19	7	311	CLA	C6-C5-C3	-2.95	106.28	113.47
19	K	204	CLA	CMA-C3A-C4A	2.95	119.70	111.77
19	3	5020	CLA	C1C-C2C-C3C	-2.95	103.88	106.98
19	6	309	CLA	O2A-CGA-CBA	2.95	120.83	111.83
19	A	807	CLA	C1D-ND-C4D	-2.95	104.24	106.31
19	A	838	CLA	C1D-ND-C4D	-2.95	104.24	106.31
19	B	817	CLA	C1D-ND-C4D	-2.95	104.24	106.31
19	B	810	CLA	C3B-C4B-NB	-2.95	107.90	110.53
29	7	301	LMG	O8-C28-C29	2.95	120.82	111.83
19	B	825	CLA	C1D-ND-C4D	-2.95	104.24	106.31
19	A	832	CLA	CMA-C3A-C4A	2.95	119.69	111.77
19	B	809	CLA	C1-C2-C3	-2.95	121.37	126.20
19	A	820	CLA	CMA-C3A-C4A	2.95	119.69	111.77
22	4	305	BCR	C7-C8-C9	-2.95	121.88	126.23
19	J	1901	CLA	CMA-C3A-C4A	2.94	119.69	111.77
19	A	809	CLA	CMA-C3A-C4A	2.94	119.69	111.77
28	6	304	C7Z	C18-C5-C4	2.94	119.83	114.42
19	K	204	CLA	C2C-C1C-NC	2.94	113.07	109.98
31	1	5004	LUT	C18-C5-C4	2.94	119.83	114.42
19	A	819	CLA	CMA-C3A-C4A	2.94	119.67	111.77
19	5	301	CLA	C1D-ND-C4D	-2.94	104.25	106.31
19	6	302	CLA	C3B-C4B-NB	-2.94	107.91	110.53
19	A	835	CLA	C1D-ND-C4D	-2.94	104.25	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	8	305	LUT	C35-C15-C14	-2.94	117.51	123.52
19	3	5012	CLA	O2A-C1-C2	2.94	119.41	108.11
19	A	806	CLA	C1D-ND-C4D	-2.94	104.25	106.31
19	B	804	CLA	C3B-C4B-NB	-2.93	107.91	110.53
19	B	836	CLA	C1D-ND-C4D	-2.93	104.25	106.31
19	F	303	CLA	CMA-C3A-C4A	2.93	119.66	111.77
19	K	203	CLA	CMA-C3A-C4A	2.93	119.66	111.77
19	G	1601	CLA	C3B-C4B-NB	-2.93	107.91	110.53
19	A	837	CLA	CMA-C3A-C4A	2.93	119.66	111.77
19	A	810	CLA	C3B-C4B-NB	-2.93	107.91	110.53
19	1	5012	CLA	CMA-C3A-C4A	2.93	119.65	111.77
19	3	5012	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
19	I	201	CLA	C1-C2-C3	-2.93	121.40	126.20
19	B	827	CLA	C3B-C4B-NB	-2.93	107.92	110.53
19	B	822	CLA	CMA-C3A-C4A	2.93	119.64	111.77
19	A	836	CLA	C1D-ND-C4D	-2.93	104.26	106.31
19	B	816	CLA	C1D-ND-C4D	-2.93	104.26	106.31
19	B	818	CLA	CMA-C3A-C4A	2.93	119.64	111.77
19	1	5008	CLA	C3B-C4B-NB	-2.93	107.92	110.53
19	8	320	CLA	C3B-C4B-NB	-2.93	107.92	110.53
19	A	803	CLA	CMA-C3A-C4A	2.93	119.64	111.77
19	K	205	CLA	CMA-C3A-C4A	2.93	119.64	111.77
19	B	834	CLA	CMA-C3A-C4A	2.93	119.64	111.77
19	A	814	CLA	CMA-C3A-C4A	2.92	119.63	111.77
31	7	303	LUT	C27-C28-C29	-2.92	120.04	126.32
19	8	313	CLA	CMA-C3A-C4A	2.92	119.63	111.77
19	B	811	CLA	C1D-ND-C4D	-2.92	104.26	106.31
20	A	844	PQN	C11-C12-C13	-2.92	121.80	126.83
32	4	317	CHL	C1C-C2C-CMC	2.92	132.07	126.80
31	Z	318	LUT	C35-C34-C33	-2.92	123.18	127.28
28	1	5005	C7Z	C38-C25-C24	2.92	119.79	114.42
31	8	304	LUT	C18-C5-C6	-2.92	121.30	124.48
19	B	828	CLA	C1D-ND-C4D	-2.92	104.26	106.31
22	A	848	BCR	C33-C5-C4	2.92	119.82	113.60
19	A	833	CLA	C1D-ND-C4D	-2.92	104.27	106.31
19	4	312	CLA	C1D-ND-C4D	-2.92	104.27	106.31
19	3	5015	CLA	C3B-C4B-NB	-2.92	107.93	110.53
19	7	312	CLA	CMA-C3A-C4A	2.91	119.61	111.77
19	7	310	CLA	C1-C2-C3	-2.91	121.42	126.20
19	5	306	CLA	C1C-C2C-C3C	-2.91	103.92	106.98
19	4	309	CLA	C1D-ND-C4D	-2.91	104.27	106.31
22	6	307	BCR	C2-C1-C6	2.91	114.67	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	303	CLA	C1C-C2C-C3C	-2.91	103.92	106.98
19	F	301	CLA	O2A-CGA-CBA	2.91	120.71	111.83
19	6	314	CLA	CMA-C3A-C4A	2.91	119.60	111.77
19	B	806	CLA	C1D-ND-C4D	-2.91	104.27	106.31
19	B	816	CLA	CMA-C3A-C4A	2.91	119.59	111.77
19	A	811	CLA	C3B-C4B-NB	-2.91	107.93	110.53
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	A	826	CLA	CMA-C3A-C4A	2.91	119.59	111.77
32	Z	313	CHL	C4D-CHA-CBD	-2.91	106.03	108.97
19	8	311	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
19	B	829	CLA	CMA-C3A-C4A	2.91	119.59	111.77
19	5	319	CLA	C1D-ND-C4D	-2.91	104.27	106.31
19	A	808	CLA	C1D-ND-C4D	-2.91	104.27	106.31
19	A	834	CLA	CMA-C3A-C4A	2.91	119.58	111.77
19	8	310	CLA	C3B-C4B-NB	-2.90	107.94	110.53
19	I	201	CLA	C1D-ND-C4D	-2.90	104.27	106.31
22	B	843	BCR	C23-C24-C25	-2.90	119.24	127.00
19	8	314	CLA	O2A-CGA-CBA	2.90	120.69	111.83
22	B	842	BCR	C27-C26-C25	-2.90	118.78	122.70
19	6	313	CLA	C2C-C1C-NC	2.90	113.03	109.98
19	7	310	CLA	O2A-CGA-CBA	2.90	120.68	111.83
22	B	845	BCR	C23-C24-C25	-2.90	119.25	127.00
19	A	827	CLA	CMA-C3A-C4A	2.90	119.57	111.77
31	7	304	LUT	C27-C28-C29	-2.90	120.09	126.32
19	B	817	CLA	CMA-C3A-C4A	2.90	119.57	111.77
19	K	205	CLA	C3B-C4B-NB	-2.90	107.94	110.53
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
23	Z	316	LHG	O8-C23-C24	2.90	120.67	111.83
19	A	838	CLA	C1-C2-C3	-2.90	121.45	126.20
19	A	818	CLA	C1D-ND-C4D	-2.90	104.28	106.31
22	B	846	BCR	C11-C12-C13	-2.90	118.42	126.36
19	8	310	CLA	C1C-C2C-C3C	-2.90	103.93	106.98
19	6	320	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
19	A	828	CLA	O2A-C1-C2	2.90	119.25	108.11
19	6	318	CLA	C3B-C4B-NB	-2.90	107.94	110.53
22	A	850	BCR	C38-C26-C27	2.90	119.77	113.60
19	3	5018	CLA	C1D-ND-C4D	-2.89	104.28	106.31
19	4	312	CLA	CMA-C3A-C4A	2.89	119.55	111.77
23	A	852	LHG	O8-C23-C24	2.89	120.66	111.83
22	A	847	BCR	C2-C1-C6	2.89	114.64	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	301	CLA	C1D-ND-C4D	-2.89	104.28	106.31
19	4	308	CLA	C1C-C2C-C3C	-2.89	103.94	106.98
19	B	837	CLA	C1D-ND-C4D	-2.89	104.28	106.31
19	J	1901	CLA	C1D-ND-C4D	-2.89	104.29	106.31
22	B	847	BCR	C21-C20-C19	-2.89	114.83	123.20
19	Z	305	CLA	C6-C5-C3	-2.88	106.44	113.47
31	1	5003	LUT	C10-C11-C12	-2.88	114.84	123.20
19	5	325	CLA	C1-C2-C3	-2.88	121.47	126.20
25	B	848	DGD	O1G-C1A-C2A	2.88	120.62	111.83
19	5	313	CLA	C3B-C4B-NB	-2.88	107.96	110.53
19	A	827	CLA	C1D-ND-C4D	-2.88	104.29	106.31
19	G	1602	CLA	C1D-ND-C4D	-2.88	104.29	106.31
22	5	305	BCR	C2-C1-C6	2.88	114.62	110.44
19	3	5018	CLA	C3B-C4B-NB	-2.88	107.96	110.53
19	A	804	CLA	C1D-ND-C4D	-2.88	104.29	106.31
22	6	308	BCR	C35-C13-C14	-2.88	118.15	122.82
19	B	807	CLA	C2C-C1C-NC	2.88	113.01	109.98
19	8	308	CLA	C1-C2-C3	-2.88	121.48	126.20
19	A	840	CLA	C1C-C2C-C3C	-2.88	103.95	106.98
19	8	313	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
19	A	830	CLA	CMA-C3A-C4A	2.88	119.51	111.77
19	B	808	CLA	C3B-C4B-NB	-2.88	107.96	110.53
19	8	320	CLA	C1D-ND-C4D	-2.88	104.29	106.31
19	4	318	CLA	CMA-C3A-C4A	2.88	119.51	111.77
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	6	323	CLA	C1C-C2C-C3C	-2.88	103.95	106.98
19	B	832	CLA	C1D-ND-C4D	-2.88	104.29	106.31
19	7	318	CLA	C1C-C2C-C3C	-2.88	103.95	106.98
31	6	306	LUT	C15-C14-C13	-2.88	123.25	127.28
19	1	5006	CLA	C1D-ND-C4D	-2.87	104.30	106.31
19	7	306	CLA	C3B-C4B-NB	-2.87	107.96	110.53
32	6	316	CHL	C3C-C4C-NC	-2.87	107.62	114.65
19	3	5016	CLA	CMA-C3A-C4A	2.87	119.50	111.77
19	A	803	CLA	C1D-ND-C4D	-2.87	104.30	106.31
31	5	303	LUT	C15-C35-C34	-2.87	117.64	123.52
28	6	304	C7Z	C38-C25-C24	2.87	119.70	114.42
22	8	306	BCR	C4-C5-C6	-2.87	118.82	122.70
19	A	822	CLA	CMA-C3A-C4A	2.87	119.49	111.77
19	A	839	CLA	C1D-ND-C4D	-2.87	104.30	106.31
19	7	312	CLA	C1D-ND-C4D	-2.87	104.30	106.31
19	B	837	CLA	C3B-C4B-NB	-2.87	107.97	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	828	CLA	C3B-C4B-NB	-2.87	107.97	110.53
22	A	850	BCR	C23-C24-C25	-2.87	119.34	127.00
38	8	325	ERG	C14-C13-C17	2.87	102.72	99.72
19	B	804	CLA	C1-C2-C3	-2.87	121.50	126.20
19	4	318	CLA	CAA-C2A-C3A	-2.87	109.66	116.23
19	3	5011	CLA	CMA-C3A-C4A	2.87	119.48	111.77
19	A	808	CLA	C3B-C4B-NB	-2.87	107.97	110.53
19	4	310	CLA	C6-C5-C3	-2.86	106.49	113.47
19	B	831	CLA	C2C-C1C-NC	2.86	112.99	109.98
19	3	5020	CLA	C2C-C1C-NC	2.86	112.99	109.98
19	6	314	CLA	C1-C2-C3	-2.86	121.51	126.20
19	B	802	CLA	C1D-ND-C4D	-2.86	104.30	106.31
19	1	5018	CLA	C1D-ND-C4D	-2.86	104.31	106.31
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	A	814	CLA	O2A-C1-C2	2.86	119.11	108.11
31	6	305	LUT	C27-C28-C29	-2.86	120.17	126.32
19	A	815	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
19	B	824	CLA	C3B-C4B-NB	-2.86	107.98	110.53
19	8	309	CLA	CAA-C2A-C3A	-2.86	105.27	113.00
19	B	815	CLA	C1D-ND-C4D	-2.86	104.31	106.31
19	A	841	CLA	CMA-C3A-C4A	2.86	119.46	111.77
19	6	302	CLA	CMA-C3A-C4A	2.86	119.45	111.77
19	B	826	CLA	C1D-ND-C4D	-2.86	104.31	106.31
19	B	830	CLA	C1D-ND-C4D	-2.86	104.31	106.31
19	5	314	CLA	C1-C2-C3	-2.85	121.52	126.20
19	B	817	CLA	C1-C2-C3	-2.85	121.52	126.20
28	1	5005	C7Z	C35-C15-C14	-2.85	117.68	123.52
32	8	301	CHL	C4D-CHA-CBD	-2.85	106.09	108.97
19	5	321	CLA	C1C-C2C-C3C	-2.85	103.98	106.98
19	Z	311	CLA	C2C-C1C-NC	2.85	112.98	109.98
19	I	201	CLA	O2A-C1-C2	2.85	119.08	108.11
19	6	318	CLA	C1D-ND-C4D	-2.85	104.31	106.31
19	5	311	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
31	8	304	LUT	C40-C33-C34	-2.85	118.20	122.82
19	Z	304	CLA	C1C-C2C-C3C	-2.85	103.98	106.98
19	B	850	CLA	C1D-ND-C4D	-2.85	104.31	106.31
19	3	5008	CLA	C1C-C2C-C3C	-2.85	103.98	106.98
19	8	312	CLA	C6-C5-C3	-2.85	106.53	113.47
28	J	1902	C7Z	C18-C5-C4	2.85	119.66	114.42
19	7	307	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
19	8	312	CLA	O2A-CGA-CBA	2.85	120.52	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	5016	CLA	C1D-ND-C4D	-2.85	104.31	106.31
19	I	201	CLA	C2C-C1C-NC	2.85	112.97	109.98
19	8	320	CLA	CMA-C3A-C4A	2.85	119.42	111.77
19	7	311	CLA	C3B-C4B-NB	-2.85	107.99	110.53
19	A	841	CLA	C1D-ND-C4D	-2.85	104.31	106.31
19	7	310	CLA	C1D-ND-C4D	-2.85	104.31	106.31
19	8	308	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
19	8	307	CLA	C1C-C2C-C3C	-2.85	103.99	106.98
19	B	833	CLA	O2A-C1-C2	2.84	119.06	108.11
19	B	829	CLA	C1D-ND-C4D	-2.84	104.32	106.31
27	F	304	RRX	C11-C12-C13	-2.84	118.57	126.36
22	G	1603	BCR	C33-C5-C4	2.84	119.66	113.60
22	8	306	BCR	C38-C26-C27	2.84	119.66	113.60
19	A	817	CLA	C1D-ND-C4D	-2.84	104.32	106.31
23	A	851	LHG	C5-O7-C7	-2.84	111.00	117.80
19	A	808	CLA	CMA-C3A-C4A	2.84	119.41	111.77
19	B	803	CLA	C1C-C2C-C3C	-2.84	103.99	106.98
19	B	809	CLA	C2C-C1C-NC	2.84	112.96	109.98
19	B	833	CLA	C1D-ND-C4D	-2.84	104.32	106.31
19	3	5012	CLA	C1D-ND-C4D	-2.84	104.32	106.31
19	A	813	CLA	C2C-C1C-NC	2.84	112.96	109.98
31	1	5003	LUT	C15-C14-C13	-2.84	123.30	127.28
24	A	854	LMT	C1B-O1B-C4'	-2.84	111.26	117.98
19	G	1601	CLA	C2C-C1C-NC	2.84	112.96	109.98
19	6	301	CLA	C1-C2-C3	-2.84	121.55	126.20
19	1	5015	CLA	CMA-C3A-C4A	2.83	119.39	111.77
19	K	202	CLA	C2C-C1C-NC	2.83	112.96	109.98
19	B	831	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
19	B	830	CLA	C3B-C4B-NB	-2.83	108.00	110.53
19	8	307	CLA	C3B-C4B-NB	-2.83	108.00	110.53
32	8	319	CHL	C4D-CHA-CBD	-2.83	106.11	108.97
19	7	308	CLA	O2A-CGA-CBA	2.83	120.47	111.83
22	B	846	BCR	C8-C7-C6	-2.83	119.43	127.00
31	8	305	LUT	C20-C13-C12	2.83	122.42	118.09
19	A	823	CLA	C1D-ND-C4D	-2.83	104.33	106.31
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	B	806	CLA	CMA-C3A-C4A	2.83	119.38	111.77
19	B	836	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
19	1	5013	CLA	C1D-ND-C4D	-2.83	104.33	106.31
19	B	807	CLA	CMA-C3A-C4A	2.83	119.38	111.77
19	B	831	CLA	O2D-CGD-O1D	-2.83	118.34	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	847	BCR	C8-C7-C6	-2.83	119.44	127.00
19	A	809	CLA	C1D-ND-C4D	-2.83	104.33	106.31
19	3	5014	CLA	C1D-ND-C4D	-2.83	104.33	106.31
19	5	321	CLA	C3B-C4B-NB	-2.83	108.01	110.53
19	B	812	CLA	CMA-C3A-C4A	2.83	119.37	111.77
19	A	836	CLA	CMA-C3A-C4A	2.83	119.37	111.77
19	A	857	CLA	C1D-ND-C4D	-2.83	104.33	106.31
19	4	310	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
19	5	310	CLA	C6-C5-C3	-2.83	106.58	113.47
19	B	812	CLA	C1-C2-C3	-2.83	121.57	126.20
19	B	807	CLA	C3B-C4B-NB	-2.83	108.01	110.53
19	5	311	CLA	C3B-C4B-NB	-2.83	108.01	110.53
27	4	303	RRX	C15-C16-C17	-2.82	117.74	123.52
19	A	837	CLA	C1D-ND-C4D	-2.82	104.33	106.31
32	4	317	CHL	C4D-CHA-CBD	-2.82	106.12	108.97
19	5	321	CLA	C1-C2-C3	-2.82	121.57	126.20
19	B	836	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
19	A	804	CLA	C3B-C4B-NB	-2.82	108.01	110.53
19	Z	306	CLA	CMA-C3A-C4A	2.82	119.36	111.77
19	3	5016	CLA	C1D-ND-C4D	-2.82	104.33	106.31
19	A	843	CLA	C2C-C1C-NC	2.82	112.95	109.98
27	5	302	RRX	C15-C14-C13	-2.82	123.32	127.28
27	4	303	RRX	C1-C6-C5	-2.82	118.78	122.64
32	4	314	CHL	C1-C2-C3	-2.82	122.20	126.76
19	3	5014	CLA	C3B-C4B-NB	-2.82	108.01	110.53
19	A	816	CLA	C2C-C1C-NC	2.82	112.94	109.98
32	8	319	CHL	C1C-C2C-CMC	2.82	131.88	126.80
22	B	844	BCR	C27-C26-C25	-2.82	118.90	122.70
19	B	801	CLA	C3B-C4B-NB	-2.82	108.02	110.53
19	1	5012	CLA	O2A-CGA-CBA	2.82	120.42	111.83
19	6	309	CLA	C1-C2-C3	-2.82	121.58	126.20
19	B	839	CLA	C1C-C2C-C3C	-2.81	104.02	106.98
19	7	311	CLA	C1C-C2C-C3C	-2.81	104.02	106.98
19	6	309	CLA	C1C-C2C-C3C	-2.81	104.02	106.98
19	7	308	CLA	C6-C5-C3	-2.81	106.61	113.47
19	4	311	CLA	CAA-CBA-CGA	-2.81	105.22	113.21
19	B	822	CLA	C3B-C4B-NB	-2.81	108.02	110.53
19	7	311	CLA	C2C-C1C-NC	2.81	112.94	109.98
19	B	839	CLA	CMA-C3A-C4A	2.81	119.33	111.77
19	A	831	CLA	C1D-ND-C4D	-2.81	104.34	106.31
19	B	832	CLA	CMA-C3A-C4A	2.81	119.33	111.77
19	B	813	CLA	C2C-C1C-NC	2.81	112.93	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	843	CLA	C1C-C2C-C3C	-2.81	104.03	106.98
19	K	204	CLA	C1C-C2C-C3C	-2.81	104.03	106.98
19	3	5012	CLA	C4B-CHC-C1C	2.81	132.85	126.25
19	A	832	CLA	C2C-C1C-NC	2.81	112.93	109.98
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
19	7	310	CLA	C1C-C2C-C3C	-2.81	104.03	106.98
19	A	810	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
19	A	820	CLA	C1D-ND-C4D	-2.81	104.34	106.31
19	7	319	CLA	C3B-C4B-NB	-2.81	108.03	110.53
19	B	809	CLA	C1C-C2C-C3C	-2.81	104.03	106.98
19	6	318	CLA	C1C-C2C-C3C	-2.81	104.03	106.98
19	A	802	CLA	C1C-C2C-C3C	-2.80	104.03	106.98
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	Z	304	CLA	O2A-C1-C2	2.80	118.90	108.11
19	8	318	CLA	C2C-C1C-NC	2.80	112.93	109.98
19	4	307	CLA	C4B-CHC-C1C	2.80	132.84	126.25
22	A	858	BCR	C33-C5-C4	2.80	119.57	113.60
19	A	819	CLA	C3B-C4B-NB	-2.80	108.03	110.53
19	1	5007	CLA	C2C-C1C-NC	2.80	112.92	109.98
19	7	319	CLA	C1D-ND-C4D	-2.80	104.35	106.31
22	A	849	BCR	C16-C15-C14	-2.80	117.79	123.52
19	7	313	CLA	CMA-C3A-C4A	2.80	119.30	111.77
19	A	823	CLA	C2C-C1C-NC	2.80	112.92	109.98
19	B	827	CLA	C2C-C1C-NC	2.80	112.92	109.98
19	7	307	CLA	C1C-C2C-C3C	-2.80	104.04	106.98
22	6	308	BCR	C12-C13-C14	2.80	123.41	119.01
19	A	824	CLA	C1D-ND-C4D	-2.80	104.35	106.31
19	B	812	CLA	C1D-ND-C4D	-2.80	104.35	106.31
19	B	835	CLA	C3B-C4B-NB	-2.80	108.03	110.53
32	4	315	CHL	C1-O2A-CGA	2.80	123.42	116.65
19	Z	312	CLA	C6-C5-C3	-2.80	106.66	113.47
22	5	304	BCR	C24-C23-C22	-2.80	122.10	126.23
19	F	303	CLA	C4B-CHC-C1C	2.80	132.82	126.25
19	A	823	CLA	CMA-C3A-C4A	2.79	119.28	111.77
19	Z	314	CLA	C1D-ND-C4D	-2.79	104.35	106.31
31	7	304	LUT	C18-C5-C4	2.79	119.56	114.42
19	B	821	CLA	CMA-C3A-C4A	2.79	119.28	111.77
22	A	846	BCR	C8-C7-C6	-2.79	119.53	127.00
19	A	828	CLA	C1D-ND-C4D	-2.79	104.35	106.31
19	B	837	CLA	C2C-C1C-NC	2.79	112.92	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	5012	CLA	O2A-CGA-CBA	2.79	120.35	111.83
32	7	315	CHL	C4D-CHA-CBD	-2.79	106.15	108.97
19	A	830	CLA	C1D-ND-C4D	-2.79	104.35	106.31
19	B	804	CLA	C2C-C1C-NC	2.79	112.91	109.98
19	6	302	CLA	C1C-C2C-C3C	-2.79	104.04	106.98
22	8	306	BCR	C11-C10-C9	-2.79	123.36	127.28
19	8	318	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
19	Z	307	CLA	C1-C2-C3	-2.79	121.62	126.20
19	1	5012	CLA	C3B-C4B-NB	-2.79	108.04	110.53
19	B	810	CLA	O2A-CGA-CBA	2.79	120.34	111.83
19	3	5013	CLA	C1C-C2C-C3C	-2.79	104.05	106.98
19	7	319	CLA	CMA-C3A-C4A	2.79	119.27	111.77
19	K	203	CLA	C2C-C1C-NC	2.79	112.91	109.98
19	5	301	CLA	C4B-CHC-C1C	2.79	132.80	126.25
19	1	5011	CLA	CMD-C2D-C3D	-2.79	121.30	127.69
19	7	324	CLA	C2C-C1C-NC	2.79	112.91	109.98
32	6	321	CHL	C4D-CHA-CBD	-2.79	106.16	108.97
22	8	306	BCR	C33-C5-C4	2.79	119.54	113.60
24	G	1604	LMT	C1B-O1B-C4'	-2.79	111.37	117.98
22	A	846	BCR	C23-C24-C25	-2.79	119.56	127.00
19	B	814	CLA	C1D-ND-C4D	-2.78	104.36	106.31
19	4	307	CLA	C1C-C2C-C3C	-2.78	104.05	106.98
19	3	5020	CLA	C3B-C4B-NB	-2.78	108.05	110.53
22	3	5006	BCR	C1-C6-C5	-2.78	118.83	122.64
19	7	319	CLA	C2C-C1C-NC	2.78	112.91	109.98
19	1	5016	CLA	C1C-C2C-C3C	-2.78	104.05	106.98
19	K	203	CLA	C3B-C4B-NB	-2.78	108.05	110.53
31	3	5002	LUT	C18-C5-C4	2.78	119.54	114.42
19	8	307	CLA	C2C-C1C-NC	2.78	112.90	109.98
19	B	827	CLA	CMA-C3A-C4A	2.78	119.25	111.77
19	B	802	CLA	O2A-CGA-CBA	2.78	120.31	111.83
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
19	A	822	CLA	O2A-CGA-CBA	2.78	120.30	111.83
22	B	845	BCR	C38-C26-C27	2.78	119.52	113.60
19	B	821	CLA	C1D-ND-C4D	-2.78	104.36	106.31
19	5	306	CLA	CMA-C3A-C4A	2.78	119.23	111.77
19	B	829	CLA	C3B-C4B-NB	-2.78	108.05	110.53
19	B	838	CLA	C3B-C4B-NB	-2.78	108.05	110.53
24	4	322	LMT	C1B-O1B-C4'	-2.78	111.40	117.98
19	5	307	CLA	C1D-ND-C4D	-2.77	104.36	106.31
19	A	823	CLA	C4B-CHC-C1C	2.77	132.77	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	837	CLA	C1C-C2C-C3C	-2.77	104.06	106.98
19	8	309	CLA	C1C-C2C-C3C	-2.77	104.06	106.98
19	7	312	CLA	C4B-CHC-C1C	2.77	132.77	126.25
22	6	308	BCR	C8-C7-C6	-2.77	119.59	127.00
19	B	827	CLA	C1-C2-C3	-2.77	121.65	126.20
19	6	312	CLA	C1-C2-C3	-2.77	121.66	126.20
19	1	5015	CLA	C1D-ND-C4D	-2.77	104.37	106.31
19	A	832	CLA	C1C-C2C-C3C	-2.77	104.06	106.98
19	B	809	CLA	CMA-C3A-C4A	2.77	119.22	111.77
19	B	816	CLA	C3B-C4B-NB	-2.77	108.06	110.53
22	5	304	BCR	C8-C7-C6	-2.77	119.60	127.00
19	1	5012	CLA	C2C-C1C-NC	2.77	112.89	109.98
19	B	810	CLA	C1D-ND-C4D	-2.77	104.37	106.31
29	J	1903	LMG	O8-C28-C29	2.77	120.27	111.83
19	6	322	CLA	C4B-CHC-C1C	2.77	132.75	126.25
19	A	834	CLA	C3B-C4B-NB	-2.77	108.06	110.53
19	1	5006	CLA	C3B-C4B-NB	-2.77	108.06	110.53
19	A	807	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
19	5	325	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
19	1	5012	CLA	C1D-ND-C4D	-2.76	104.37	106.31
19	6	323	CLA	C1D-ND-C4D	-2.76	104.37	106.31
19	A	807	CLA	C2C-C1C-NC	2.76	112.89	109.98
19	A	814	CLA	C1C-C2C-C3C	-2.76	104.07	106.98
19	A	843	CLA	CMA-C3A-C4A	2.76	119.20	111.77
19	B	832	CLA	C2C-C1C-NC	2.76	112.89	109.98
19	3	5018	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
19	7	316	CLA	C2C-C1C-NC	2.76	112.88	109.98
23	7	320	LHG	O8-C23-C24	2.76	120.26	111.83
19	7	324	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
22	8	303	BCR	C35-C13-C12	2.76	122.31	118.09
23	1	5001	LHG	C5-O7-C7	-2.76	111.19	117.80
19	A	805	CLA	CMA-C3A-C4A	2.76	119.19	111.77
19	B	824	CLA	C2C-C1C-NC	2.76	112.88	109.98
19	4	309	CLA	C2C-C1C-NC	2.76	112.88	109.98
19	A	822	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
23	1	5019	LHG	O8-C23-C24	2.76	120.25	111.83
19	B	831	CLA	C3B-C4B-NB	-2.76	108.07	110.53
19	8	312	CLA	CAA-CBA-CGA	-2.76	105.37	113.21
19	B	838	CLA	C1D-ND-C4D	-2.76	104.38	106.31
19	3	5019	CLA	O2A-CGA-CBA	2.76	120.25	111.83
19	3	5016	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
19	B	830	CLA	C2C-C1C-NC	2.76	112.88	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	846	BCR	C30-C25-C26	-2.76	118.87	122.64
32	5	316	CHL	C1A-CHA-C4D	2.76	123.58	118.98
19	6	310	CLA	O2A-CGA-CBA	2.76	120.24	111.83
19	4	318	CLA	C3B-C4B-NB	-2.76	108.07	110.53
19	4	306	CLA	C1-O2A-CGA	2.76	123.32	116.65
19	4	306	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
19	A	805	CLA	C3B-C4B-NB	-2.76	108.07	110.53
19	A	825	CLA	C3B-C4B-NB	-2.75	108.07	110.53
19	3	5008	CLA	CMA-C3A-C4A	2.75	119.17	111.77
19	F	303	CLA	C2C-C1C-NC	2.75	112.87	109.98
19	K	205	CLA	C2C-C1C-NC	2.75	112.87	109.98
19	B	820	CLA	C2C-C1C-NC	2.75	112.87	109.98
19	6	314	CLA	C2C-C1C-NC	2.75	112.87	109.98
19	B	811	CLA	C3B-C4B-NB	-2.75	108.07	110.53
38	8	325	ERG	C4-C5-C10	-2.75	112.90	116.42
19	Z	308	CLA	C1D-ND-C4D	-2.75	104.38	106.31
31	8	305	LUT	C15-C35-C34	-2.75	117.89	123.52
32	8	316	CHL	C1-O2A-CGA	2.75	123.31	116.65
19	A	839	CLA	C2C-C1C-NC	2.75	112.87	109.98
19	4	310	CLA	C4B-CHC-C1C	2.75	132.71	126.25
19	A	842	CLA	C2C-C1C-NC	2.75	112.87	109.98
19	4	318	CLA	C2C-C1C-NC	2.75	112.87	109.98
19	4	307	CLA	CHD-C1D-ND	-2.75	120.93	124.80
19	5	312	CLA	C1D-ND-C4D	-2.75	104.38	106.31
31	8	305	LUT	C39-C29-C28	2.75	122.29	118.09
19	3	5013	CLA	O2A-CGA-CBA	2.75	120.22	111.83
19	6	313	CLA	C1C-C2C-C3C	-2.75	104.09	106.98
19	A	802	CLA	C2C-C1C-NC	2.75	112.87	109.98
24	1	5002	LMT	C1B-O1B-C4'	-2.75	111.46	117.98
19	A	819	CLA	C1D-ND-C4D	-2.75	104.38	106.31
19	B	839	CLA	C1D-ND-C4D	-2.75	104.38	106.31
19	A	838	CLA	C1C-C2C-C3C	-2.75	104.09	106.98
19	7	316	CLA	O2A-CGA-CBA	2.75	120.21	111.83
19	A	814	CLA	C2C-C1C-NC	2.75	112.87	109.98
22	B	845	BCR	C15-C16-C17	-2.75	117.90	123.52
19	J	1901	CLA	C3B-C4B-NB	-2.75	108.08	110.53
31	5	303	LUT	C31-C30-C29	-2.75	123.43	127.28
19	4	313	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
19	A	829	CLA	C1D-ND-C4D	-2.74	104.39	106.31
27	4	303	RRX	C15-C14-C13	-2.74	123.43	127.28
19	3	5019	CLA	C1C-C2C-C3C	-2.74	104.09	106.98
19	G	1601	CLA	C4B-CHC-C1C	2.74	132.70	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	801	CL0	O1D-CGD-CBD	-2.74	120.56	124.72
19	6	320	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
19	6	302	CLA	C2C-C1C-NC	2.74	112.86	109.98
19	B	812	CLA	C4B-CHC-C1C	2.74	132.69	126.25
19	B	834	CLA	C1D-ND-C4D	-2.74	104.39	106.31
19	7	308	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
19	4	307	CLA	CMA-C3A-C4A	2.74	119.14	111.77
22	A	848	BCR	C15-C16-C17	-2.74	117.91	123.52
20	A	844	PQN	C11-C3-C2	-2.74	120.19	124.89
27	F	304	RRX	C38-C26-C27	2.74	119.46	114.42
19	B	838	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
19	3	5016	CLA	C2C-C1C-NC	2.74	112.86	109.98
19	3	5010	CLA	CMA-C3A-C4A	2.74	119.13	111.77
19	B	820	CLA	C1D-ND-C4D	-2.74	104.39	106.31
19	G	1601	CLA	C1D-ND-C4D	-2.74	104.39	106.31
31	5	303	LUT	C22-C23-C24	2.74	115.25	111.18
19	7	319	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
19	6	320	CLA	C2C-C1C-NC	2.74	112.86	109.98
19	1	5015	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
19	A	808	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
19	A	808	CLA	C2C-C1C-NC	2.74	112.86	109.98
19	Z	304	CLA	C2C-C1C-NC	2.74	112.86	109.98
28	1	5005	C7Z	C31-C32-C33	-2.73	118.86	126.36
19	A	808	CLA	C4B-CHC-C1C	2.73	132.68	126.25
19	5	317	CLA	C1-C2-C3	-2.73	121.72	126.20
19	1	5010	CLA	C1D-ND-C4D	-2.73	104.39	106.31
19	A	824	CLA	C2C-C1C-NC	2.73	112.85	109.98
19	B	818	CLA	C3B-C4B-NB	-2.73	108.09	110.53
19	G	1602	CLA	CMA-C3A-C4A	2.73	119.12	111.77
19	4	307	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
22	3	5007	BCR	C35-C13-C12	2.73	122.26	118.09
31	Z	317	LUT	C18-C5-C4	2.73	119.44	114.42
19	B	823	CLA	C1D-ND-C4D	-2.73	104.39	106.31
19	K	203	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
19	Z	308	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
19	B	823	CLA	C2C-C1C-NC	2.73	112.85	109.98
19	Z	312	CLA	CMA-C3A-C4A	2.73	119.11	111.77
22	A	858	BCR	C7-C8-C9	-2.73	122.19	126.23
20	B	841	PQN	C2M-C2-C3	-2.73	119.96	124.45
19	A	857	CLA	C4B-CHC-C1C	2.73	132.66	126.25
19	4	306	CLA	CMA-C3A-C4A	2.73	119.11	111.77
19	A	807	CLA	C4B-CHC-C1C	2.73	132.66	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	858	BCR	C38-C26-C27	2.73	119.41	113.60
19	A	802	CLA	C1-C2-C3	-2.73	121.73	126.20
22	8	306	BCR	C2-C1-C6	2.73	114.40	110.44
19	B	807	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
31	1	5003	LUT	C35-C15-C14	-2.73	117.94	123.52
19	B	808	CLA	C2C-C1C-NC	2.73	112.84	109.98
19	3	5013	CLA	C2C-C1C-NC	2.72	112.84	109.98
31	1	5004	LUT	C30-C31-C32	-2.72	115.31	123.20
19	B	819	CLA	C2C-C1C-NC	2.72	112.84	109.98
19	B	802	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
19	B	827	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
22	B	843	BCR	C33-C5-C4	2.72	119.40	113.60
19	B	833	CLA	C4B-CHC-C1C	2.72	132.65	126.25
19	B	813	CLA	C1D-ND-C4D	-2.72	104.40	106.31
19	3	5015	CLA	CMA-C3A-C4A	2.72	119.08	111.77
32	6	321	CHL	CAA-C2A-C1A	-2.72	107.96	113.35
19	B	807	CLA	C1D-ND-C4D	-2.72	104.40	106.31
19	A	836	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
19	5	319	CLA	C1-O2A-CGA	2.72	123.23	116.65
19	B	837	CLA	CMA-C3A-C4A	2.72	119.08	111.77
19	8	314	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
19	5	313	CLA	C2C-C1C-NC	2.72	112.84	109.98
19	6	323	CLA	C2C-C1C-NC	2.72	112.84	109.98
19	5	309	CLA	C4B-CHC-C1C	2.72	132.64	126.25
19	A	826	CLA	C1D-ND-C4D	-2.72	104.41	106.31
19	K	205	CLA	C1D-ND-C4D	-2.72	104.41	106.31
19	A	838	CLA	C2C-C1C-NC	2.72	112.83	109.98
27	4	303	RRX	C11-C10-C9	-2.72	123.47	127.28
19	5	319	CLA	C4B-CHC-C1C	2.72	132.63	126.25
19	A	837	CLA	C3B-C4B-NB	-2.72	108.11	110.53
19	A	822	CLA	C2C-C1C-NC	2.71	112.83	109.98
22	G	1603	BCR	C23-C24-C25	-2.71	119.75	127.00
38	8	325	ERG	C15-C14-C13	-2.71	101.78	104.21
19	1	5011	CLA	C1D-ND-C4D	-2.71	104.41	106.31
19	6	301	CLA	O2A-CGA-CBA	2.71	120.11	111.83
32	6	315	CHL	C4D-CHA-CBD	-2.71	106.23	108.97
19	7	316	CLA	CMA-C3A-C4A	2.71	119.06	111.77
19	5	325	CLA	C4B-CHC-C1C	2.71	132.62	126.25
32	4	315	CHL	C1A-CHA-C4D	2.71	123.51	118.98
19	7	317	CLA	C3B-C4B-NB	-2.71	108.11	110.53
19	A	839	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
19	A	857	CLA	C2C-C1C-NC	2.71	112.83	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	816	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
19	A	815	CLA	C1-O2A-CGA	2.71	123.21	116.65
19	B	828	CLA	C4B-CHC-C1C	2.71	132.62	126.25
19	F	303	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
19	A	828	CLA	C2C-C1C-NC	2.71	112.83	109.98
22	A	858	BCR	C8-C7-C6	-2.71	119.76	127.00
31	4	304	LUT	C7-C6-C5	-2.71	115.32	121.56
19	A	820	CLA	C2C-C1C-NC	2.71	112.83	109.98
22	B	847	BCR	C33-C5-C4	2.71	119.37	113.60
19	6	309	CLA	C2C-C1C-NC	2.71	112.82	109.98
19	A	802	CLA	C1D-ND-C4D	-2.71	104.41	106.31
19	B	808	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
19	I	201	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
19	3	5014	CLA	C2C-C1C-NC	2.70	112.82	109.98
32	8	316	CHL	C4D-CHA-CBD	-2.70	106.24	108.97
22	A	848	BCR	C8-C7-C6	-2.70	119.77	127.00
19	7	311	CLA	C4B-CHC-C1C	2.70	132.61	126.25
19	B	839	CLA	C3B-C4B-NB	-2.70	108.12	110.53
19	A	814	CLA	O2A-CGA-CBA	2.70	120.08	111.83
19	A	834	CLA	C1D-ND-C4D	-2.70	104.42	106.31
19	A	840	CLA	C1D-ND-C4D	-2.70	104.42	106.31
19	Z	306	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
22	3	5004	BCR	C15-C16-C17	-2.70	117.99	123.52
19	K	204	CLA	C1D-ND-C4D	-2.70	104.42	106.31
19	1	5006	CLA	C4B-CHC-C1C	2.70	132.60	126.25
22	A	849	BCR	C33-C5-C4	2.70	119.35	113.60
19	B	814	CLA	C3B-C4B-NB	-2.70	108.12	110.53
29	J	1904	LMG	O8-C28-C29	2.70	120.06	111.83
19	8	308	CLA	C4B-CHC-C1C	2.70	132.59	126.25
24	A	855	LMT	C1B-O1B-C4'	-2.70	111.58	117.98
19	A	842	CLA	C1D-ND-C4D	-2.70	104.42	106.31
19	1	5018	CLA	CMA-C3A-C4A	2.70	119.02	111.77
19	A	826	CLA	C2C-C1C-NC	2.70	112.81	109.98
19	B	826	CLA	C2C-C1C-NC	2.70	112.81	109.98
19	3	5019	CLA	C1D-ND-C4D	-2.70	104.42	106.31
19	5	321	CLA	C1D-ND-C4D	-2.70	104.42	106.31
19	7	313	CLA	C4B-CHC-C1C	2.69	132.58	126.25
19	7	308	CLA	CHA-C4D-ND	2.69	138.11	132.55
22	7	305	BCR	C1-C6-C7	2.69	122.96	115.65
19	A	823	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
19	B	824	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
19	Z	315	CLA	C4B-CHC-C1C	2.69	132.58	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	322	CLA	CMA-C3A-C4A	2.69	119.01	111.77
19	A	857	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
19	A	833	CLA	C2C-C1C-NC	2.69	112.81	109.98
19	1	5018	CLA	C4B-CHC-C1C	2.69	132.58	126.25
19	A	822	CLA	C3B-C4B-NB	-2.69	108.13	110.53
22	3	5006	BCR	C33-C5-C4	2.69	119.33	113.60
19	A	834	CLA	C2C-C1C-NC	2.69	112.81	109.98
19	4	312	CLA	C2C-C1C-NC	2.69	112.81	109.98
19	5	325	CLA	CMA-C3A-C4A	2.69	119.01	111.77
19	1	5006	CLA	CMA-C3A-C4A	2.69	119.01	111.77
19	3	5018	CLA	O2A-CGA-CBA	2.69	120.04	111.83
23	4	320	LHG	O8-C23-C24	2.69	120.04	111.83
22	B	844	BCR	C38-C26-C27	2.69	119.33	113.60
19	5	310	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
19	Z	303	CLA	CMA-C3A-C4A	2.69	119.00	111.77
19	B	823	CLA	C3B-C4B-NB	-2.69	108.13	110.53
19	3	5008	CLA	C3B-C4B-NB	-2.69	108.13	110.53
19	1	5008	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
19	5	314	CLA	C4B-CHC-C1C	2.69	132.57	126.25
19	A	833	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
19	B	801	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
19	1	5016	CLA	C2C-C1C-NC	2.69	112.81	109.98
22	A	858	BCR	C23-C24-C25	-2.69	119.82	127.00
19	A	825	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
19	1	5012	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
19	B	838	CLA	C2C-C1C-NC	2.69	112.81	109.98
19	8	314	CLA	C2C-C1C-NC	2.69	112.81	109.98
19	5	319	CLA	CMA-C3A-C4A	2.69	119.00	111.77
19	3	5016	CLA	C3B-C4B-NB	-2.69	108.13	110.53
19	8	320	CLA	C4B-CHC-C1C	2.69	132.57	126.25
19	4	311	CLA	CHD-C1D-ND	-2.69	121.02	124.80
27	F	304	RRX	C33-C5-C4	2.69	119.32	113.60
19	B	806	CLA	C3B-C4B-NB	-2.69	108.13	110.53
19	K	205	CLA	C1C-C2C-C3C	-2.69	104.16	106.98
19	Z	307	CLA	C1C-C2C-C3C	-2.69	104.16	106.98
22	3	5007	BCR	C39-C30-C25	-2.69	106.03	110.24
19	B	835	CLA	C2C-C1C-NC	2.68	112.80	109.98
19	A	821	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
19	B	819	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
19	B	829	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
19	6	318	CLA	C2C-C1C-NC	2.68	112.80	109.98
23	8	321	LHG	O8-C23-C24	2.68	120.02	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	814	CLA	C2C-C1C-NC	2.68	112.80	109.98
19	7	312	CLA	C2C-C1C-NC	2.68	112.80	109.98
19	8	313	CLA	C4B-CHC-C1C	2.68	132.55	126.25
19	A	815	CLA	CMA-C3A-C4A	2.68	118.98	111.77
27	F	304	RRX	C8-C7-C6	-2.68	119.84	127.00
22	B	842	BCR	C16-C17-C18	-2.68	123.52	127.28
19	6	314	CLA	C1D-ND-C4D	-2.68	104.43	106.31
19	B	820	CLA	C4B-CHC-C1C	2.68	132.55	126.25
19	B	804	CLA	O2A-CGA-CBA	2.68	120.01	111.83
22	A	850	BCR	C33-C5-C4	2.68	119.31	113.60
19	5	307	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
19	5	311	CLA	O2A-CGA-CBA	2.68	120.01	111.83
19	B	831	CLA	CMA-C3A-C4A	2.68	118.98	111.77
19	4	309	CLA	O2A-CGA-CBA	2.68	120.00	111.83
19	A	828	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
19	8	311	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
19	4	312	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
27	4	303	RRX	C16-C15-C14	-2.68	118.04	123.52
19	A	831	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
19	4	310	CLA	CHA-C4D-ND	2.68	138.07	132.55
19	Z	307	CLA	C2C-C1C-NC	2.68	112.79	109.98
19	7	313	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
19	B	837	CLA	C1C-C2C-C3C	-2.68	104.17	106.98
19	Z	311	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
19	A	803	CLA	C4B-CHC-C1C	2.68	132.54	126.25
19	1	5010	CLA	CMD-C2D-C3D	-2.67	121.56	127.69
29	7	301	LMG	C8-O7-C10	-2.67	111.39	117.80
19	4	316	CLA	CMA-C3A-C4A	2.67	118.96	111.77
19	A	831	CLA	C3B-C4B-NB	-2.67	108.14	110.53
19	A	843	CLA	C1D-ND-C4D	-2.67	104.44	106.31
19	A	842	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
19	B	818	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
19	7	317	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
19	Z	306	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
19	5	308	CLA	C1-C2-C3	-2.67	121.82	126.20
31	6	305	LUT	C8-C7-C6	-2.67	119.86	127.00
19	A	820	CLA	C4B-CHC-C1C	2.67	132.53	126.25
19	A	835	CLA	C3B-C4B-NB	-2.67	108.15	110.53
19	B	832	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
19	3	5018	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
22	6	308	BCR	C33-C5-C4	2.67	119.29	113.60
19	Z	315	CLA	C6-C5-C3	-2.67	106.97	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	824	CLA	C4B-CHC-C1C	2.67	132.52	126.25
19	6	314	CLA	O2A-CGA-CBA	2.67	119.97	111.83
19	4	316	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
19	A	818	CLA	C4B-CHC-C1C	2.67	132.52	126.25
19	A	824	CLA	C1C-C2C-C3C	-2.67	104.18	106.98
19	5	308	CLA	C4B-CHC-C1C	2.67	132.52	126.25
22	5	304	BCR	C33-C5-C4	2.67	119.28	113.60
19	A	829	CLA	C4B-CHC-C1C	2.67	132.51	126.25
19	7	318	CLA	CMA-C3A-C4A	2.67	118.94	111.77
19	A	825	CLA	C2C-C1C-NC	2.66	112.78	109.98
19	4	309	CLA	C4B-CHC-C1C	2.66	132.51	126.25
38	8	325	ERG	C11-C12-C13	-2.66	108.24	112.74
31	1	5003	LUT	C39-C29-C28	2.66	122.16	118.09
19	6	301	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
19	A	814	CLA	C1D-ND-C4D	-2.66	104.44	106.31
19	8	308	CLA	C2D-C1D-ND	2.66	112.76	110.13
19	B	833	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
19	A	821	CLA	C2C-C1C-NC	2.66	112.78	109.98
19	4	311	CLA	CMD-C2D-C3D	-2.66	121.58	127.69
19	A	806	CLA	C4B-CHC-C1C	2.66	132.51	126.25
19	5	314	CLA	CMA-C3A-C4A	2.66	118.93	111.77
19	6	302	CLA	C1D-ND-C4D	-2.66	104.44	106.31
19	A	826	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
19	3	5011	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
19	1	5012	CLA	C1-C2-C3	-2.66	121.84	126.20
31	6	305	LUT	C11-C12-C13	-2.66	119.06	126.36
19	B	827	CLA	C1D-ND-C4D	-2.66	104.44	106.31
19	A	826	CLA	C3B-C4B-NB	-2.66	108.16	110.53
19	4	318	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
19	K	205	CLA	C4B-CHC-C1C	2.66	132.50	126.25
19	Z	314	CLA	C4B-CHC-C1C	2.66	132.50	126.25
19	8	312	CLA	CHA-C4D-ND	2.66	138.04	132.55
19	Z	312	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
19	1	5011	CLA	C3B-C4B-NB	-2.66	108.16	110.53
19	3	5011	CLA	C1D-ND-C4D	-2.66	104.45	106.31
19	6	322	CLA	CHD-C1D-ND	-2.66	121.06	124.80
19	4	307	CLA	CMD-C2D-C3D	-2.66	121.59	127.69
19	A	830	CLA	C2C-C1C-NC	2.66	112.77	109.98
23	1	5019	LHG	C5-O7-C7	-2.66	111.44	117.80
19	A	842	CLA	C4B-CHC-C1C	2.66	132.50	126.25
28	1	5005	C7Z	C11-C10-C9	-2.66	123.55	127.28
19	5	310	CLA	C1D-ND-C4D	-2.66	104.45	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	832	CLA	C4B-CHC-C1C	2.66	132.49	126.25
31	4	304	LUT	C30-C31-C32	-2.66	115.50	123.20
19	8	320	CLA	C2C-C1C-NC	2.66	112.77	109.98
19	Z	304	CLA	C3B-C4B-NB	-2.66	108.16	110.53
22	B	846	BCR	C16-C17-C18	-2.66	123.55	127.28
19	4	318	CLA	C1D-ND-C4D	-2.66	104.45	106.31
19	5	311	CLA	C1D-ND-C4D	-2.66	104.45	106.31
19	6	309	CLA	CMA-C3A-C4A	2.66	118.91	111.77
28	J	1902	C7Z	C11-C12-C13	-2.66	119.08	126.36
27	5	302	RRX	C21-C20-C19	-2.65	115.51	123.20
19	7	306	CLA	CHA-C4D-ND	2.65	138.03	132.55
22	7	305	BCR	C11-C10-C9	-2.65	123.56	127.28
20	B	841	PQN	C11-C3-C2	-2.65	120.34	124.89
19	B	830	CLA	C4B-CHC-C1C	2.65	132.49	126.25
19	B	824	CLA	CMA-C3A-C4A	2.65	118.91	111.77
19	J	1901	CLA	C2C-C1C-NC	2.65	112.77	109.98
19	B	818	CLA	C1D-ND-C4D	-2.65	104.45	106.31
19	5	309	CLA	C1D-ND-C4D	-2.65	104.45	106.31
19	B	801	CLA	C1D-ND-C4D	-2.65	104.45	106.31
19	Z	303	CLA	C1D-ND-C4D	-2.65	104.45	106.31
22	A	847	BCR	C33-C5-C4	2.65	119.25	113.60
19	A	827	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
19	5	311	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
19	5	325	CLA	C2C-C1C-NC	2.65	112.77	109.98
19	A	812	CLA	C4B-CHC-C1C	2.65	132.48	126.25
19	A	832	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
19	A	817	CLA	C3B-C4B-NB	-2.65	108.16	110.53
19	3	5019	CLA	C2C-C1C-NC	2.65	112.77	109.98
19	8	309	CLA	C1D-ND-C4D	-2.65	104.45	106.31
19	B	825	CLA	C1-O2A-CGA	2.65	123.06	116.65
22	A	858	BCR	C11-C10-C9	-2.65	123.56	127.28
19	4	312	CLA	C4B-CHC-C1C	2.65	132.48	126.25
19	1	5010	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
19	4	311	CLA	O2A-CGA-CBA	2.65	119.91	111.83
19	A	827	CLA	C2C-C1C-NC	2.65	112.76	109.98
19	7	316	CLA	C3B-C4B-NB	-2.65	108.17	110.53
19	A	810	CLA	CMA-C3A-C4A	2.65	118.89	111.77
19	3	5011	CLA	C4B-CHC-C1C	2.65	132.47	126.25
19	5	309	CLA	CMA-C3A-C4A	2.65	118.89	111.77
22	A	846	BCR	C7-C8-C9	-2.65	122.32	126.23
27	F	304	RRX	C23-C24-C25	-2.65	119.93	127.00
22	B	843	BCR	C38-C26-C27	2.65	119.24	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	8	325	ERG	C18-C13-C17	-2.65	106.88	111.68
19	4	311	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
19	A	804	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
19	B	828	CLA	C2C-C1C-NC	2.64	112.76	109.98
19	4	308	CLA	C2C-C1C-NC	2.64	112.76	109.98
19	5	321	CLA	C2C-C1C-NC	2.64	112.76	109.98
19	4	316	CLA	C4B-CHC-C1C	2.64	132.47	126.25
19	A	806	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
19	G	1601	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
19	6	314	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
32	1	5009	CHL	C1-O2A-CGA	2.64	123.05	116.65
19	Z	314	CLA	C2C-C1C-NC	2.64	112.76	109.98
22	7	305	BCR	C8-C7-C6	-2.64	119.94	127.00
19	7	309	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
19	7	312	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
19	A	841	CLA	C2C-C1C-NC	2.64	112.76	109.98
19	A	804	CLA	CMA-C3A-C4A	2.64	118.88	111.77
19	B	835	CLA	C1D-ND-C4D	-2.64	104.46	106.31
19	A	835	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
19	A	841	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
19	3	5012	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
19	8	314	CLA	CAA-C2A-C3A	-2.64	105.86	113.00
23	5	323	LHG	C5-O7-C7	-2.64	111.47	117.80
31	Z	317	LUT	C22-C23-C24	2.64	115.11	111.18
19	B	804	CLA	CMA-C3A-C4A	2.64	118.87	111.77
19	B	825	CLA	C4B-CHC-C1C	2.64	132.46	126.25
19	6	313	CLA	C4B-CHC-C1C	2.64	132.46	126.25
19	B	823	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
19	A	811	CLA	O2A-CGA-CBA	2.64	119.88	111.83
32	8	301	CHL	C1C-C2C-CMC	2.64	131.56	126.80
19	A	820	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
22	A	859	BCR	C16-C15-C14	-2.64	118.12	123.52
31	8	304	LUT	C7-C8-C9	-2.64	122.33	126.23
19	5	321	CLA	O2A-CGA-CBA	2.64	119.88	111.83
22	A	848	BCR	C11-C12-C13	-2.64	119.13	126.36
23	A	852	LHG	C5-O7-C7	-2.64	111.48	117.80
38	6	326	ERG	C18-C13-C17	-2.64	106.90	111.68
19	1	5016	CLA	C4B-CHC-C1C	2.64	132.44	126.25
19	B	834	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
19	A	836	CLA	C4B-CHC-C1C	2.63	132.44	126.25
19	6	301	CLA	CMA-C3A-C4A	2.63	118.85	111.77
19	B	820	CLA	C1C-C2C-C3C	-2.63	104.21	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	806	CLA	O2A-CGA-CBA	2.63	119.86	111.83
19	B	815	CLA	C3B-C4B-NB	-2.63	108.18	110.53
22	A	859	BCR	C33-C5-C4	2.63	119.21	113.60
32	5	320	CHL	C4D-CHA-CBD	-2.63	106.31	108.97
33	7	321	SPH	C3-C4-C5	-2.63	119.23	124.69
19	1	5006	CLA	CHD-C1D-ND	-2.63	121.10	124.80
22	5	305	BCR	C36-C18-C19	2.63	122.11	118.09
19	A	825	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
19	1	5011	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
19	3	5020	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
19	3	5014	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
19	A	836	CLA	C2C-C1C-NC	2.63	112.75	109.98
19	A	815	CLA	C3B-C4B-NB	-2.63	108.18	110.53
19	B	829	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
19	1	5010	CLA	CMA-C3A-C4A	2.63	118.84	111.77
19	Z	315	CLA	CAA-C2A-C3A	-2.63	105.89	113.00
19	K	203	CLA	C1D-ND-C4D	-2.63	104.47	106.31
31	Z	318	LUT	C30-C31-C32	-2.63	115.58	123.20
19	1	5006	CLA	O2A-CGA-CBA	2.63	119.85	111.83
19	B	814	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
34	6	325	3PH	O31-C31-C32	2.63	119.84	111.83
19	7	313	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
19	5	322	CLA	C2C-C1C-NC	2.63	112.74	109.98
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
19	1	5007	CLA	C4B-CHC-C1C	2.63	132.42	126.25
19	A	817	CLA	C2C-C1C-NC	2.63	112.74	109.98
19	A	831	CLA	CMA-C3A-C4A	2.63	118.83	111.77
19	5	317	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
19	5	325	CLA	CHA-C4D-ND	2.62	137.96	132.55
19	Z	314	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
19	A	815	CLA	C2C-C1C-NC	2.62	112.74	109.98
19	A	837	CLA	C2C-C1C-NC	2.62	112.74	109.98
19	B	826	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
19	1	5013	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
19	7	306	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
19	7	306	CLA	CAA-C2A-C3A	-2.62	105.92	113.00
32	3	5017	CHL	C4D-CHA-CBD	-2.62	106.32	108.97
19	A	809	CLA	C4B-CHC-C1C	2.62	132.41	126.25
19	3	5015	CLA	C1D-ND-C4D	-2.62	104.47	106.31
19	7	316	CLA	C1D-ND-C4D	-2.62	104.47	106.31
32	5	318	CHL	C4D-CHA-CBD	-2.62	106.33	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	307	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
19	5	306	CLA	C4B-CHC-C1C	2.62	132.41	126.25
23	8	321	LHG	C5-O7-C7	-2.62	111.53	117.80
19	B	815	CLA	C2C-C1C-NC	2.62	112.73	109.98
19	A	821	CLA	C1D-ND-C4D	-2.62	104.47	106.31
19	7	306	CLA	C1D-ND-C4D	-2.62	104.47	106.31
37	8	302	SQD	O7-S-C6	-2.62	102.85	106.76
19	7	308	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
19	3	5018	CLA	CMA-C3A-C4A	2.62	118.81	111.77
19	4	306	CLA	C1D-ND-C4D	-2.62	104.48	106.31
27	4	303	RRX	C30-C29-C28	-2.62	107.86	113.59
19	J	1901	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
19	5	319	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
19	B	833	CLA	C2C-C1C-NC	2.62	112.73	109.98
22	B	844	BCR	C15-C16-C17	-2.62	118.17	123.52
19	K	204	CLA	C3B-C4B-NB	-2.61	108.20	110.53
19	7	316	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
19	5	312	CLA	C2C-C1C-NC	2.61	112.73	109.98
19	B	817	CLA	C4B-CHC-C1C	2.61	132.39	126.25
19	A	831	CLA	C2C-C1C-NC	2.61	112.73	109.98
19	B	834	CLA	C2C-C1C-NC	2.61	112.73	109.98
20	B	841	PQN	C14-C13-C15	2.61	119.76	115.23
19	4	310	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
19	B	821	CLA	C3B-C4B-NB	-2.61	108.20	110.53
19	Z	305	CLA	CMA-C3A-C4A	2.61	118.79	111.77
19	6	320	CLA	C4B-CHC-C1C	2.61	132.39	126.25
19	3	5015	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
19	B	809	CLA	C1D-ND-C4D	-2.61	104.48	106.31
19	B	850	CLA	CHA-C4D-ND	2.61	137.94	132.55
18	A	801	CL0	CMC-C2C-C1C	2.61	129.43	124.73
19	1	5011	CLA	C2C-C1C-NC	2.61	112.72	109.98
19	1	5006	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
19	6	310	CLA	C4B-CHC-C1C	2.61	132.38	126.25
19	A	835	CLA	C2C-C1C-NC	2.61	112.72	109.98
19	B	822	CLA	C2C-C1C-NC	2.61	112.72	109.98
19	B	839	CLA	C4B-CHC-C1C	2.61	132.38	126.25
19	6	318	CLA	CMA-C3A-C4A	2.61	118.79	111.77
19	Z	307	CLA	CHA-C4D-ND	2.61	137.93	132.55
19	Z	306	CLA	O2A-CGA-CBA	2.61	119.79	111.83
19	A	827	CLA	C3B-C4B-NB	-2.61	108.20	110.53
19	A	803	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
19	Z	305	CLA	C1C-C2C-C3C	-2.61	104.24	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	312	CLA	C4B-CHC-C1C	2.61	132.38	126.25
19	6	312	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
19	B	811	CLA	C2C-C1C-NC	2.61	112.72	109.98
28	1	5005	C7Z	C10-C11-C12	-2.61	115.65	123.20
19	B	840	CLA	C3B-C4B-NB	-2.61	108.20	110.53
19	1	5007	CLA	C1D-ND-C4D	-2.61	104.48	106.31
19	A	837	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
19	5	308	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
19	A	817	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
22	B	844	BCR	C34-C9-C10	-2.60	118.60	122.82
31	Z	318	LUT	C31-C30-C29	-2.60	123.62	127.28
19	1	5015	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
19	A	829	CLA	C2C-C1C-NC	2.60	112.72	109.98
19	A	832	CLA	C1D-ND-C4D	-2.60	104.48	106.31
19	Z	311	CLA	C1D-ND-C4D	-2.60	104.48	106.31
19	F	301	CLA	C2D-C1D-ND	2.60	112.70	110.13
23	7	320	LHG	O7-C7-O9	-2.60	117.62	123.70
19	5	312	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
19	A	838	CLA	O2A-CGA-CBA	2.60	119.77	111.83
19	B	810	CLA	C4B-CHC-C1C	2.60	132.37	126.25
19	A	815	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
19	A	830	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
19	6	301	CLA	CHA-C4D-ND	2.60	137.92	132.55
19	4	306	CLA	C2C-C1C-NC	2.60	112.72	109.98
19	A	806	CLA	C2C-C1C-NC	2.60	112.71	109.98
19	3	5013	CLA	C3B-C4B-NB	-2.60	108.21	110.53
19	B	811	CLA	C4B-CHC-C1C	2.60	132.36	126.25
28	1	5005	C7Z	C1-C6-C5	-2.60	119.08	122.64
32	4	315	CHL	C4D-CHA-CBD	-2.60	106.34	108.97
19	K	202	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
19	7	309	CLA	C3B-C4B-NB	-2.60	108.21	110.53
19	G	1601	CLA	CMA-C3A-C4A	2.60	118.76	111.77
38	8	325	ERG	C24-C23-C22	-2.60	117.94	125.81
19	B	808	CLA	C4B-CHC-C1C	2.60	132.36	126.25
19	B	804	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
19	1	5008	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
19	5	322	CLA	C4B-CHC-C1C	2.60	132.36	126.25
19	B	837	CLA	C4B-CHC-C1C	2.60	132.36	126.25
19	B	806	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
19	3	5015	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
19	A	826	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
19	Z	311	CLA	C4B-CHC-C1C	2.60	132.35	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	810	CLA	C2C-C1C-NC	2.60	112.71	109.98
19	B	813	CLA	C4B-CHC-C1C	2.60	132.35	126.25
19	4	312	CLA	O2A-CGA-CBA	2.60	119.75	111.83
19	A	803	CLA	C2C-C1C-NC	2.60	112.71	109.98
24	8	324	LMT	O2'-C2'-C3'	-2.60	104.26	110.38
22	F	302	BCR	C15-C14-C13	-2.60	123.64	127.28
19	B	822	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
19	4	308	CLA	C1D-ND-C4D	-2.60	104.49	106.31
19	B	816	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
32	6	319	CHL	C4D-CHA-CBD	-2.59	106.35	108.97
34	8	322	3PH	O31-C31-C32	2.59	119.74	111.83
19	Z	311	CLA	CHA-C4D-ND	2.59	137.90	132.55
19	5	313	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
19	A	827	CLA	C4B-CHC-C1C	2.59	132.34	126.25
19	B	824	CLA	C1D-ND-C4D	-2.59	104.49	106.31
18	A	801	CL0	CAA-C2A-C3A	-2.59	105.99	113.00
19	4	308	CLA	CHA-C4D-ND	2.59	137.90	132.55
19	3	5010	CLA	C1D-ND-C4D	-2.59	104.49	106.31
19	B	812	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
32	4	314	CHL	C4D-CHA-CBD	-2.59	106.36	108.97
19	5	322	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
19	Z	312	CLA	C1D-ND-C4D	-2.59	104.50	106.31
32	6	316	CHL	C4D-CHA-CBD	-2.59	106.36	108.97
18	A	801	CL0	O2D-CGD-O1D	-2.59	118.81	123.85
19	B	816	CLA	C2C-C1C-NC	2.59	112.70	109.98
19	6	320	CLA	O1D-CGD-CBD	-2.59	119.41	124.52
19	A	830	CLA	C3B-C4B-NB	-2.59	108.22	110.53
19	A	834	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
19	6	323	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
19	B	830	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
19	8	313	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
19	A	841	CLA	C4B-CHC-C1C	2.59	132.33	126.25
31	3	5003	LUT	C28-C29-C30	2.59	123.08	119.01
19	8	308	CLA	CMA-C3A-C4A	2.59	118.72	111.77
19	B	828	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
19	1	5018	CLA	C2C-C1C-NC	2.58	112.70	109.98
19	5	308	CLA	CHD-C1D-ND	-2.58	121.17	124.80
19	3	5015	CLA	C4B-CHC-C1C	2.58	132.32	126.25
19	8	310	CLA	C4B-CHC-C1C	2.58	132.32	126.25
19	6	314	CLA	C4B-CHC-C1C	2.58	132.32	126.25
19	8	320	CLA	C1C-C2C-C3C	-2.58	104.26	106.98
19	3	5008	CLA	C2C-C1C-NC	2.58	112.70	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	302	CLA	C4B-CHC-C1C	2.58	132.32	126.25
19	A	803	CLA	O2A-CGA-CBA	2.58	119.71	111.83
19	6	301	CLA	C4B-CHC-C1C	2.58	132.32	126.25
19	B	803	CLA	C1D-ND-C4D	-2.58	104.50	106.31
19	A	819	CLA	C1C-C2C-C3C	-2.58	104.26	106.98
19	7	306	CLA	CMA-C3A-C4A	2.58	118.71	111.77
19	A	821	CLA	C3B-C4B-NB	-2.58	108.22	110.53
19	4	308	CLA	O2A-CGA-CBA	2.58	119.71	111.83
19	8	314	CLA	C4B-CHC-C1C	2.58	132.32	126.25
19	4	306	CLA	C4B-CHC-C1C	2.58	132.31	126.25
19	4	313	CLA	O2A-CGA-CBA	2.58	119.70	111.83
19	5	312	CLA	O2A-CGA-CBA	2.58	119.70	111.83
19	B	811	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
19	6	301	CLA	C2C-C1C-NC	2.58	112.69	109.98
22	B	845	BCR	C8-C7-C6	-2.58	120.11	127.00
19	4	313	CLA	CMA-C3A-C4A	2.58	118.70	111.77
19	6	310	CLA	CHD-C1D-ND	-2.58	121.17	124.80
19	6	302	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
19	A	815	CLA	C1D-ND-C4D	-2.58	104.50	106.31
19	K	202	CLA	C1D-ND-C4D	-2.58	104.50	106.31
19	B	834	CLA	C4B-CHC-C1C	2.58	132.31	126.25
19	7	317	CLA	C2C-C1C-NC	2.58	112.69	109.98
19	5	301	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
19	6	318	CLA	O2A-CGA-CBA	2.58	119.69	111.83
19	5	301	CLA	C2C-C1C-NC	2.58	112.69	109.98
19	A	811	CLA	C1C-C2C-C3C	-2.57	104.27	106.98
19	6	311	CLA	C1C-C2C-C3C	-2.57	104.27	106.98
19	A	813	CLA	CHA-C4D-ND	2.57	137.86	132.55
19	B	818	CLA	C4B-CHC-C1C	2.57	132.30	126.25
19	B	801	CLA	C2C-C1C-NC	2.57	112.69	109.98
19	5	313	CLA	C1C-C2C-C3C	-2.57	104.27	106.98
19	B	821	CLA	C2C-C1C-NC	2.57	112.69	109.98
19	5	310	CLA	C4B-CHC-C1C	2.57	132.30	126.25
22	3	5006	BCR	C20-C19-C18	-2.57	119.31	126.36
19	5	314	CLA	O2A-CGA-CBA	2.57	119.68	111.83
19	B	804	CLA	C1C-C2C-C3C	-2.57	104.27	106.98
19	3	5009	CLA	C1D-ND-C4D	-2.57	104.51	106.31
19	7	324	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
22	G	1603	BCR	C20-C19-C18	-2.57	119.31	126.36
19	B	850	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
19	3	5009	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
19	1	5008	CLA	C11-C12-C13	-2.57	107.42	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	858	BCR	C1-C6-C7	2.57	122.62	115.65
19	F	301	CLA	CHA-C4D-ND	2.57	137.85	132.55
31	Z	317	LUT	C15-C35-C34	2.57	128.78	123.52
19	4	306	CLA	C1-C2-C3	-2.57	121.99	126.20
19	6	320	CLA	C1D-ND-C4D	-2.57	104.51	106.31
19	B	829	CLA	C2C-C1C-NC	2.57	112.68	109.98
19	7	309	CLA	C2C-C1C-NC	2.57	112.68	109.98
19	1	5018	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
19	B	831	CLA	C4B-CHC-C1C	2.57	132.29	126.25
19	B	805	CLA	C4B-CHC-C1C	2.57	132.29	126.25
19	B	807	CLA	O2A-CGA-CBA	2.57	119.67	111.83
19	1	5013	CLA	O2A-CGA-CBA	2.57	119.67	111.83
19	7	312	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
19	A	830	CLA	C4B-CHC-C1C	2.57	132.28	126.25
19	6	311	CLA	C4B-CHC-C1C	2.57	132.28	126.25
19	5	317	CLA	C2D-C1D-ND	2.57	112.67	110.13
23	5	323	LHG	O8-C23-C24	2.57	119.66	111.83
19	A	833	CLA	C4B-CHC-C1C	2.57	132.28	126.25
19	B	810	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
28	6	304	C7Z	C28-C27-C26	-2.57	120.14	127.00
19	Z	315	CLA	CMA-C3A-C4A	2.57	118.67	111.77
22	B	846	BCR	C1-C6-C7	2.57	122.61	115.65
19	B	806	CLA	C4B-CHC-C1C	2.57	132.28	126.25
19	6	309	CLA	C4B-CHC-C1C	2.57	132.28	126.25
35	7	302	DGA	OG1-CA1-CA2	2.57	119.66	111.83
27	F	304	RRX	C1-C6-C5	-2.56	119.13	122.64
31	6	306	LUT	C18-C5-C4	2.56	119.14	114.42
19	1	5011	CLA	CHA-C4D-ND	2.56	137.84	132.55
19	6	313	CLA	CHA-C4D-ND	2.56	137.84	132.55
19	B	809	CLA	C3B-C4B-NB	-2.56	108.24	110.53
19	B	819	CLA	C1D-ND-C4D	-2.56	104.51	106.31
19	A	839	CLA	CMA-C3A-C4A	2.56	118.66	111.77
19	B	812	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
19	B	802	CLA	C4B-CHC-C1C	2.56	132.27	126.25
19	A	829	CLA	C1C-C2C-C3C	-2.56	104.28	106.98
19	7	306	CLA	C4B-CHC-C1C	2.56	132.27	126.25
19	A	805	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
19	4	311	CLA	CHA-C4D-ND	2.56	137.83	132.55
19	3	5008	CLA	CHA-C4D-ND	2.56	137.83	132.55
19	5	322	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
19	5	311	CLA	C2C-C1C-NC	2.56	112.67	109.98
19	7	306	CLA	CHD-C1D-ND	-2.56	121.20	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	826	CLA	C4B-CHC-C1C	2.56	132.27	126.25
19	Z	308	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
19	7	309	CLA	C4B-CHC-C1C	2.56	132.26	126.25
19	7	318	CLA	CHA-C4D-ND	2.56	137.83	132.55
24	8	324	LMT	C1B-O1B-C4'	-2.56	111.91	117.98
19	B	805	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
19	A	814	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
19	4	308	CLA	O1D-CGD-CBD	-2.56	119.47	124.52
19	Z	305	CLA	CAA-CBA-CGA	-2.56	105.95	113.21
19	B	802	CLA	C2C-C1C-NC	2.56	112.67	109.98
19	A	813	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
19	B	805	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
24	4	321	LMT	C1B-O1B-C4'	-2.56	111.92	117.98
19	1	5010	CLA	CHD-C1D-ND	-2.56	121.20	124.80
19	1	5013	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
22	B	842	BCR	C38-C26-C27	2.56	119.04	113.60
22	B	847	BCR	C38-C26-C27	2.56	119.04	113.60
24	Z	319	LMT	C1B-O1B-C4'	-2.56	111.92	117.98
19	Z	312	CLA	C4B-CHC-C1C	2.55	132.25	126.25
19	3	5015	CLA	C2C-C1C-NC	2.55	112.67	109.98
19	B	840	CLA	C4B-CHC-C1C	2.55	132.25	126.25
19	5	313	CLA	CMA-C3A-C4A	2.55	118.64	111.77
22	8	303	BCR	C23-C24-C25	-2.55	120.18	127.00
19	3	5012	CLA	CHD-C1D-ND	-2.55	121.21	124.80
19	A	825	CLA	C1D-ND-C4D	-2.55	104.52	106.31
20	A	844	PQN	C2M-C2-C3	-2.55	120.25	124.45
22	K	206	BCR	C20-C19-C18	-2.55	119.36	126.36
19	5	311	CLA	CAA-CBA-CGA	-2.55	105.96	113.21
19	B	807	CLA	C4B-CHC-C1C	2.55	132.25	126.25
19	7	317	CLA	C4B-CHC-C1C	2.55	132.25	126.25
19	A	818	CLA	O2A-CGA-CBA	2.55	119.61	111.83
19	4	310	CLA	C1D-ND-C4D	-2.55	104.52	106.31
19	8	311	CLA	C1D-ND-C4D	-2.55	104.52	106.31
19	1	5015	CLA	CHA-C4D-ND	2.55	137.81	132.55
19	6	309	CLA	CHA-C4D-ND	2.55	137.81	132.55
22	B	847	BCR	C15-C16-C17	-2.55	118.30	123.52
19	6	322	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
19	F	301	CLA	C4B-CHC-C1C	2.55	132.24	126.25
19	3	5010	CLA	C4B-CHC-C1C	2.55	132.24	126.25
19	A	843	CLA	C3B-C4B-NB	-2.55	108.25	110.53
19	8	307	CLA	CMA-C3A-C4A	2.55	118.62	111.77
19	4	307	CLA	O2A-CGA-CBA	2.55	119.60	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	835	CLA	C4B-CHC-C1C	2.55	132.24	126.25
19	J	1901	CLA	C4B-CHC-C1C	2.55	132.24	126.25
22	5	304	BCR	C21-C20-C19	-2.55	115.82	123.20
19	B	824	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
31	1	5003	LUT	C18-C5-C4	2.55	119.10	114.42
19	3	5009	CLA	C2C-C1C-NC	2.55	112.66	109.98
19	F	301	CLA	CMA-C3A-C4A	2.55	118.61	111.77
31	1	5003	LUT	C19-C9-C8	2.55	121.98	118.09
19	8	310	CLA	C2C-C1C-NC	2.54	112.66	109.98
19	3	5020	CLA	CMA-C3A-C4A	2.54	118.61	111.77
32	6	316	CHL	C1A-CHA-C4D	2.54	123.23	118.98
22	B	846	BCR	C23-C24-C25	-2.54	120.20	127.00
19	5	306	CLA	O2A-CGA-CBA	2.54	119.59	111.83
19	B	825	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
19	B	806	CLA	C2C-C1C-NC	2.54	112.65	109.98
19	A	813	CLA	C4B-CHC-C1C	2.54	132.23	126.25
19	Z	305	CLA	CHD-C1D-ND	-2.54	121.22	124.80
19	A	835	CLA	O2A-CGA-CBA	2.54	119.59	111.83
19	B	821	CLA	C4B-CHC-C1C	2.54	132.23	126.25
19	1	5015	CLA	C4B-CHC-C1C	2.54	132.23	126.25
32	8	319	CHL	CMA-C3A-C4A	2.54	120.09	114.61
22	8	303	BCR	C1-C6-C7	2.54	122.55	115.65
19	A	814	CLA	C3B-C4B-NB	-2.54	108.26	110.53
19	B	818	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
31	7	303	LUT	C10-C11-C12	-2.54	115.84	123.20
19	B	833	CLA	CMA-C3A-C4A	2.54	118.60	111.77
22	A	846	BCR	C33-C5-C4	2.54	119.01	113.60
19	A	819	CLA	C4B-CHC-C1C	2.54	132.22	126.25
19	A	809	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
19	A	815	CLA	C4B-CHC-C1C	2.54	132.22	126.25
19	5	321	CLA	C4B-CHC-C1C	2.54	132.22	126.25
19	A	804	CLA	C2C-C1C-NC	2.54	112.65	109.98
19	A	809	CLA	C2C-C1C-NC	2.54	112.65	109.98
19	B	850	CLA	C1-C2-C3	-2.54	122.04	126.20
19	Z	312	CLA	CAA-CBA-CGA	-2.54	106.00	113.21
19	8	309	CLA	O2A-CGA-CBA	2.54	119.57	111.83
24	8	323	LMT	C1B-O5B-C5B	-2.54	108.77	113.72
19	4	313	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
19	Z	312	CLA	C2C-C1C-NC	2.54	112.65	109.98
19	A	813	CLA	O2A-CGA-CBA	2.54	119.57	111.83
19	B	829	CLA	C4B-CHC-C1C	2.54	132.21	126.25
19	7	310	CLA	C4B-CHC-C1C	2.54	132.21	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	5015	CLA	C2D-C1D-ND	2.54	112.64	110.13
19	A	811	CLA	C4B-CHC-C1C	2.53	132.21	126.25
19	8	309	CLA	C4B-CHC-C1C	2.53	132.21	126.25
19	4	313	CLA	C4B-CHC-C1C	2.53	132.21	126.25
19	4	318	CLA	C4B-CHC-C1C	2.53	132.21	126.25
19	B	835	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
19	6	310	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
19	A	840	CLA	C2C-C1C-NC	2.53	112.64	109.98
19	A	826	CLA	C4B-CHC-C1C	2.53	132.20	126.25
19	B	821	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
22	K	206	BCR	C23-C24-C25	-2.53	120.24	127.00
32	Z	310	CHL	C4C-CHD-C1D	2.53	125.12	116.07
19	3	5009	CLA	CHA-C4D-ND	2.53	137.77	132.55
19	B	836	CLA	C2C-C1C-NC	2.53	112.64	109.98
19	3	5010	CLA	O2A-CGA-O1A	-2.53	117.30	123.63
22	6	307	BCR	C1-C6-C5	-2.53	119.18	122.64
19	A	830	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
19	1	5010	CLA	CHA-C4D-ND	2.53	137.76	132.55
19	1	5006	CLA	C1-O2A-CGA	2.53	122.77	116.65
31	Z	318	LUT	C8-C7-C6	-2.53	120.25	127.00
19	B	819	CLA	C3B-C4B-NB	-2.53	108.27	110.53
19	5	317	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
19	B	818	CLA	C2C-C1C-NC	2.53	112.64	109.98
31	1	5003	LUT	C15-C35-C34	-2.53	118.35	123.52
19	A	802	CLA	CMA-C3A-C4A	2.53	118.56	111.77
19	B	812	CLA	C2C-C1C-NC	2.53	112.64	109.98
19	8	310	CLA	CHA-C1A-NA	-2.53	120.67	126.39
19	7	313	CLA	C2C-C1C-NC	2.52	112.63	109.98
19	8	307	CLA	O2D-CGD-O1D	-2.52	118.93	123.85
31	6	306	LUT	C27-C28-C29	-2.52	120.89	126.32
19	7	310	CLA	C2C-C1C-NC	2.52	112.63	109.98
22	8	306	BCR	C15-C16-C17	-2.52	118.36	123.52
19	7	308	CLA	C4B-CHC-C1C	2.52	132.18	126.25
19	8	318	CLA	C4B-CHC-C1C	2.52	132.18	126.25
31	7	304	LUT	C22-C23-C24	2.52	114.93	111.18
32	8	317	CHL	C4D-ND-C1D	2.52	107.13	105.22
19	Z	311	CLA	CMD-C2D-C3D	-2.52	121.91	127.69
19	Z	304	CLA	CHA-C4D-ND	2.52	137.75	132.55
19	B	824	CLA	CHA-C4D-ND	2.52	137.75	132.55
27	4	303	RRX	C35-C13-C12	2.52	121.94	118.09
31	6	306	LUT	C39-C29-C30	-2.52	118.73	122.82
19	A	840	CLA	C4B-CHC-C1C	2.52	132.17	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	7	311	CLA	CMA-C3A-C4A	2.52	118.54	111.77
19	I	201	CLA	C3B-C4B-NB	-2.52	108.28	110.53
19	1	5010	CLA	C4B-CHC-C1C	2.52	132.17	126.25
19	Z	315	CLA	C2D-C1D-ND	2.52	112.62	110.13
19	7	318	CLA	C2C-C1C-NC	2.52	112.63	109.98
31	7	303	LUT	C20-C13-C12	2.52	121.93	118.09
19	4	309	CLA	O1D-CGD-CBD	-2.52	119.56	124.52
22	B	844	BCR	C11-C10-C9	-2.52	123.75	127.28
19	B	815	CLA	C4B-CHC-C1C	2.52	132.16	126.25
19	3	5020	CLA	C4B-CHC-C1C	2.52	132.16	126.25
19	B	832	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
19	G	1602	CLA	C4B-CHC-C1C	2.51	132.16	126.25
19	4	308	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
19	B	815	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
19	4	309	CLA	C3B-C4B-NB	-2.51	108.29	110.53
19	A	802	CLA	CHA-C4D-ND	2.51	137.74	132.55
22	A	847	BCR	C1-C6-C5	-2.51	119.20	122.64
19	A	805	CLA	C4B-CHC-C1C	2.51	132.16	126.25
19	Z	305	CLA	C4B-CHC-C1C	2.51	132.16	126.25
19	B	836	CLA	C4B-CHC-C1C	2.51	132.16	126.25
19	5	313	CLA	C4B-CHC-C1C	2.51	132.16	126.25
19	B	827	CLA	C6-C5-C3	-2.51	107.35	113.47
22	3	5006	BCR	C16-C15-C14	-2.51	118.38	123.52
19	Z	306	CLA	C2C-C1C-NC	2.51	112.62	109.98
19	8	309	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
22	B	846	BCR	C4-C5-C6	-2.51	119.31	122.70
19	B	809	CLA	C4B-CHC-C1C	2.51	132.15	126.25
19	Z	307	CLA	C4B-CHC-C1C	2.51	132.15	126.25
19	1	5006	CLA	O2A-C1-C2	2.51	117.77	108.11
19	8	313	CLA	C2D-C1D-ND	2.51	112.61	110.13
19	A	843	CLA	CHA-C4D-ND	2.51	137.73	132.55
31	1	5004	LUT	C15-C35-C34	-2.51	118.38	123.52
19	3	5010	CLA	CHA-C4D-ND	2.51	137.73	132.55
19	8	307	CLA	CHA-C4D-ND	2.51	137.73	132.55
19	B	832	CLA	C4B-CHC-C1C	2.51	132.15	126.25
19	5	309	CLA	C1-O2A-CGA	2.51	122.72	116.65
19	Z	307	CLA	CMA-C3A-C4A	2.51	118.51	111.77
19	5	308	CLA	CHA-C4D-ND	2.51	137.72	132.55
19	6	312	CLA	CMA-C3A-C4A	2.51	118.51	111.77
19	B	838	CLA	C4B-CHC-C1C	2.51	132.14	126.25
22	3	5005	BCR	C20-C19-C18	-2.51	119.49	126.36
19	B	802	CLA	CHA-C4D-ND	2.51	137.72	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	314	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
19	A	843	CLA	C4B-CHC-C1C	2.51	132.14	126.25
19	1	5007	CLA	C3B-C4B-NB	-2.51	108.29	110.53
19	8	314	CLA	C1D-ND-C4D	-2.51	104.55	106.31
19	8	310	CLA	CHA-C4D-ND	2.51	137.72	132.55
19	A	810	CLA	C4B-CHC-C1C	2.51	132.14	126.25
19	3	5008	CLA	C4B-CHC-C1C	2.51	132.14	126.25
19	1	5015	CLA	O2A-CGA-CBA	2.50	119.47	111.83
19	A	825	CLA	C4B-CHC-C1C	2.50	132.13	126.25
19	3	5019	CLA	C4B-CHC-C1C	2.50	132.13	126.25
19	A	822	CLA	C4B-CHC-C1C	2.50	132.13	126.25
19	1	5008	CLA	O2A-CGA-CBA	2.50	119.47	111.83
19	A	835	CLA	C4B-CHC-C1C	2.50	132.13	126.25
19	B	850	CLA	C2C-C1C-NC	2.50	112.61	109.98
32	6	316	CHL	C4C-CHD-C1D	2.50	125.02	116.07
19	A	822	CLA	C2D-C1D-ND	2.50	112.60	110.13
31	6	305	LUT	C18-C5-C4	2.50	119.02	114.42
19	B	813	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
19	5	306	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
32	4	319	CHL	C4D-CHA-CBD	-2.50	106.44	108.97
22	8	303	BCR	C38-C26-C27	2.50	118.93	113.60
19	6	302	CLA	CHA-C4D-ND	2.50	137.71	132.55
19	5	325	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
19	8	311	CLA	CHD-C1D-ND	-2.50	121.28	124.80
22	4	305	BCR	C33-C5-C4	2.50	118.93	113.60
19	3	5010	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
19	5	308	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
19	7	310	CLA	CMD-C2D-C3D	-2.50	121.96	127.69
19	B	819	CLA	C4B-CHC-C1C	2.50	132.12	126.25
19	A	837	CLA	C4B-CHC-C1C	2.50	132.12	126.25
19	A	816	CLA	C3B-C4B-NB	-2.50	108.30	110.53
19	Z	311	CLA	CMA-C3A-C4A	2.50	118.49	111.77
19	5	306	CLA	C1-O2A-CGA	2.50	122.70	116.65
22	K	206	BCR	C33-C5-C4	2.50	118.92	113.60
19	B	814	CLA	C4B-CHC-C1C	2.50	132.12	126.25
19	3	5015	CLA	C2D-C1D-ND	2.50	112.60	110.13
19	7	313	CLA	C2D-C1D-ND	2.50	112.60	110.13
19	5	311	CLA	C4B-CHC-C1C	2.50	132.12	126.25
19	B	803	CLA	CHA-C4D-ND	2.50	137.70	132.55
19	3	5013	CLA	C4B-CHC-C1C	2.50	132.12	126.25
19	7	318	CLA	C4B-CHC-C1C	2.50	132.12	126.25
19	4	316	CLA	C2C-C1C-NC	2.49	112.60	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	5007	CLA	CMA-C3A-C4A	2.49	118.48	111.77
19	B	832	CLA	C3B-C4B-NB	-2.49	108.30	110.53
19	A	817	CLA	C4B-CHC-C1C	2.49	132.11	126.25
19	5	322	CLA	C2D-C1D-ND	2.49	112.59	110.13
19	Z	311	CLA	C3B-C4B-NB	-2.49	108.31	110.53
19	8	309	CLA	CHA-C4D-ND	2.49	137.69	132.55
19	A	809	CLA	O2A-CGA-CBA	2.49	119.43	111.83
19	A	831	CLA	C4B-CHC-C1C	2.49	132.10	126.25
19	5	307	CLA	CHD-C1D-ND	-2.49	121.30	124.80
31	3	5002	LUT	C8-C7-C6	-2.49	120.34	127.00
19	7	319	CLA	C4B-CHC-C1C	2.49	132.10	126.25
19	B	826	CLA	CHA-C4D-ND	2.49	137.69	132.55
19	5	307	CLA	O2A-CGA-CBA	2.49	119.43	111.83
19	A	804	CLA	C4B-CHC-C1C	2.49	132.10	126.25
19	7	324	CLA	C1D-ND-C4D	-2.49	104.56	106.31
19	4	316	CLA	C1D-ND-C4D	-2.49	104.56	106.31
19	8	307	CLA	C4B-CHC-C1C	2.49	132.10	126.25
19	6	312	CLA	C4B-CHC-C1C	2.49	132.10	126.25
19	7	308	CLA	C2C-C1C-NC	2.49	112.60	109.98
31	6	306	LUT	C1-C6-C5	-2.49	119.23	122.64
19	1	5008	CLA	C2C-C1C-NC	2.49	112.60	109.98
19	A	834	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
19	7	307	CLA	C1D-ND-C4D	-2.49	104.57	106.31
19	Z	315	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
19	3	5013	CLA	CHD-C1D-ND	-2.49	121.30	124.80
19	B	811	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
19	B	815	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
28	1	5005	C7Z	C18-C5-C4	2.49	119.00	114.42
31	6	305	LUT	C1-C6-C5	-2.49	119.24	122.64
19	B	829	CLA	CHA-C4D-ND	2.49	137.68	132.55
19	K	205	CLA	CHA-C4D-ND	2.49	137.68	132.55
22	B	847	BCR	C34-C9-C8	2.49	121.89	118.09
22	F	302	BCR	C29-C30-C25	2.49	114.05	110.44
19	6	312	CLA	C2C-C1C-NC	2.49	112.59	109.98
32	5	315	CHL	C4D-CHA-CBD	-2.49	106.46	108.97
31	8	304	LUT	C27-C28-C29	-2.49	120.98	126.32
19	6	323	CLA	C6-C5-C3	-2.49	107.41	113.47
19	6	323	CLA	C4B-CHC-C1C	2.49	132.09	126.25
19	7	311	CLA	O2A-CGA-CBA	2.49	119.41	111.83
19	G	1602	CLA	C1C-C2C-C3C	-2.49	104.37	106.98
19	6	318	CLA	C4B-CHC-C1C	2.49	132.09	126.25
32	6	317	CHL	C4D-CHA-CBD	-2.48	106.46	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	4	317	CHL	CMA-C3A-C4A	2.48	119.96	114.61
19	6	311	CLA	C5-C3-C2	2.48	126.74	121.17
19	3	5018	CLA	CHD-C1D-ND	-2.48	121.31	124.80
19	5	306	CLA	CHD-C1D-ND	-2.48	121.31	124.80
19	B	827	CLA	CHA-C4D-ND	2.48	137.67	132.55
19	A	810	CLA	C1D-ND-C4D	-2.48	104.57	106.31
19	8	311	CLA	C4B-CHC-C1C	2.48	132.09	126.25
19	4	308	CLA	C4B-CHC-C1C	2.48	132.08	126.25
19	5	310	CLA	CBA-CAA-C2A	-2.48	106.41	113.79
19	A	839	CLA	C4B-CHC-C1C	2.48	132.08	126.25
19	A	816	CLA	C4B-CHC-C1C	2.48	132.08	126.25
19	I	201	CLA	C4B-CHC-C1C	2.48	132.08	126.25
19	F	301	CLA	CHD-C1D-ND	-2.48	121.31	124.80
19	5	313	CLA	CAA-CBA-CGA	-2.48	105.87	112.49
19	8	308	CLA	O2A-CGA-CBA	2.48	119.40	111.83
27	4	303	RRX	C2-C1-C6	2.48	114.04	110.44
19	4	313	CLA	C2C-C1C-NC	2.48	112.59	109.98
19	5	317	CLA	CMA-C3A-C4A	2.48	118.44	111.77
23	6	324	LHG	O8-C23-O10	-2.48	117.43	123.63
19	6	310	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
19	B	816	CLA	C4B-CHC-C1C	2.48	132.07	126.25
19	A	812	CLA	C1-C2-C3	-2.48	122.14	126.20
19	7	310	CLA	CHA-C4D-ND	2.48	137.66	132.55
19	A	819	CLA	C2C-C1C-NC	2.48	112.58	109.98
19	5	310	CLA	C1-O2A-CGA	2.48	122.64	116.65
32	6	319	CHL	C1-O2A-CGA	2.48	122.64	116.65
19	B	850	CLA	C4B-CHC-C1C	2.48	132.07	126.25
19	4	311	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
19	7	316	CLA	CHA-C4D-ND	2.47	137.65	132.55
19	6	313	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
19	G	1602	CLA	CHA-C4D-ND	2.47	137.65	132.55
19	B	827	CLA	C4B-CHC-C1C	2.47	132.06	126.25
19	5	308	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
19	A	838	CLA	C4B-CHC-C1C	2.47	132.06	126.25
19	Z	304	CLA	C4B-CHC-C1C	2.47	132.06	126.25
19	1	5012	CLA	C4B-CHC-C1C	2.47	132.06	126.25
19	B	808	CLA	CHA-C4D-ND	2.47	137.65	132.55
19	A	821	CLA	CHA-C4D-ND	2.47	137.65	132.55
19	8	314	CLA	CHA-C4D-ND	2.47	137.65	132.55
19	8	318	CLA	CHA-C4D-ND	2.47	137.65	132.55
19	A	810	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
19	3	5012	CLA	CHA-C4D-ND	2.47	137.64	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	313	CLA	CHA-C4D-ND	2.47	137.64	132.55
19	7	310	CLA	CMA-C3A-C4A	2.47	118.41	111.77
19	B	822	CLA	C4B-CHC-C1C	2.47	132.05	126.25
27	4	303	RRX	C21-C20-C19	-2.47	116.05	123.20
19	1	5011	CLA	CMA-C3A-C4A	2.47	118.41	111.77
19	A	841	CLA	CHA-C4D-ND	2.47	137.64	132.55
19	B	802	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
19	B	813	CLA	O2A-CGA-CBA	2.47	119.36	111.83
19	B	835	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
19	B	838	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
19	6	318	CLA	CHA-C4D-ND	2.47	137.64	132.55
19	5	319	CLA	C2D-C1D-ND	2.47	112.57	110.13
19	A	818	CLA	CHA-C4D-ND	2.47	137.64	132.55
19	1	5013	CLA	CHD-C1D-ND	-2.47	121.33	124.80
19	A	821	CLA	C4B-CHC-C1C	2.47	132.04	126.25
19	8	311	CLA	CMA-C3A-C4A	2.47	118.40	111.77
19	A	805	CLA	C2C-C1C-NC	2.46	112.57	109.98
19	A	839	CLA	CHA-C4D-ND	2.46	137.63	132.55
19	K	205	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
19	A	816	CLA	C1D-ND-C4D	-2.46	104.58	106.31
19	B	804	CLA	C1D-ND-C4D	-2.46	104.58	106.31
19	B	840	CLA	CHA-C4D-ND	2.46	137.63	132.55
19	8	313	CLA	C2C-C1C-NC	2.46	112.57	109.98
19	A	834	CLA	C4B-CHC-C1C	2.46	132.04	126.25
24	Z	301	LMT	C4B-C3B-C2B	-2.46	106.50	110.83
19	A	826	CLA	CHA-C4D-ND	2.46	137.63	132.55
19	3	5012	CLA	CMA-C3A-C4A	2.46	118.39	111.77
19	Z	308	CLA	C2C-C1C-NC	2.46	112.57	109.98
19	1	5008	CLA	C4B-CHC-C1C	2.46	132.04	126.25
19	A	814	CLA	C4B-CHC-C1C	2.46	132.04	126.25
19	5	306	CLA	C2C-C1C-NC	2.46	112.57	109.98
19	A	802	CLA	O2A-CGA-CBA	2.46	119.34	111.83
19	1	5011	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
32	6	321	CHL	CMA-C3A-C2A	2.46	123.64	114.13
19	B	812	CLA	CHA-C4D-ND	2.46	137.63	132.55
19	K	202	CLA	C3B-C4B-NB	-2.46	108.33	110.53
22	3	5007	BCR	C10-C11-C12	2.46	130.33	123.20
32	7	315	CHL	C4D-ND-C1D	2.46	107.09	105.22
19	5	312	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
22	5	304	BCR	C1-C6-C7	2.46	122.32	115.65
19	B	830	CLA	O2A-CGA-CBA	2.46	119.33	111.83
19	B	836	CLA	CHA-C4D-ND	2.46	137.62	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	303	RRX	C38-C26-C27	2.46	118.94	114.42
19	A	808	CLA	CHA-C4D-ND	2.46	137.62	132.55
19	K	203	CLA	CHA-C4D-ND	2.46	137.62	132.55
19	B	824	CLA	C4B-CHC-C1C	2.46	132.02	126.25
19	5	314	CLA	C2C-C1C-NC	2.46	112.56	109.98
22	8	306	BCR	C10-C11-C12	-2.46	116.08	123.20
31	3	5003	LUT	C4-C5-C6	-2.46	115.71	120.76
19	Z	306	CLA	C4B-CHC-C1C	2.46	132.02	126.25
28	1	5005	C7Z	C28-C27-C26	-2.46	120.44	127.00
19	A	832	CLA	CHA-C4D-ND	2.45	137.61	132.55
32	6	316	CHL	C1-C2-C3	-2.45	122.18	126.20
19	A	857	CLA	CHA-C4D-ND	2.45	137.61	132.55
22	6	307	BCR	C15-C16-C17	-2.45	118.50	123.52
32	Z	310	CHL	CMA-C3A-C4A	2.45	119.90	114.61
19	7	310	CLA	CHD-C1D-ND	-2.45	121.35	124.80
19	7	309	CLA	CHA-C4D-ND	2.45	137.61	132.55
19	1	5013	CLA	CHA-C4D-ND	2.45	137.61	132.55
32	8	301	CHL	C4C-CHD-C1D	2.45	124.84	116.07
19	I	201	CLA	CHA-C4D-ND	2.45	137.61	132.55
19	B	805	CLA	C2C-C1C-NC	2.45	112.56	109.98
34	5	324	3PH	O31-C31-C32	2.45	119.31	111.83
19	7	307	CLA	CHA-C4D-ND	2.45	137.60	132.55
19	6	312	CLA	CHA-C4D-ND	2.45	137.60	132.55
19	5	308	CLA	C6-C5-C3	-2.45	107.50	113.47
19	3	5013	CLA	C1-C2-C3	-2.45	122.18	126.20
19	7	324	CLA	C4B-CHC-C1C	2.45	132.01	126.25
19	1	5015	CLA	C2C-C1C-NC	2.45	112.56	109.98
19	A	816	CLA	CHA-C4D-ND	2.45	137.60	132.55
19	1	5011	CLA	C4B-CHC-C1C	2.45	132.01	126.25
19	8	311	CLA	C2C-C1C-NC	2.45	112.55	109.98
23	7	320	LHG	O8-C23-O10	-2.45	117.50	123.63
19	G	1601	CLA	CHA-C4D-ND	2.45	137.60	132.55
19	A	811	CLA	C2C-C1C-NC	2.45	112.55	109.98
19	A	827	CLA	CHA-C4D-ND	2.45	137.60	132.55
19	K	202	CLA	CHA-C4D-ND	2.45	137.60	132.55
19	5	322	CLA	CHA-C4D-ND	2.45	137.60	132.55
19	6	320	CLA	CMA-C3A-C4A	2.45	118.35	111.77
19	K	204	CLA	C4B-CHC-C1C	2.45	132.00	126.25
19	5	307	CLA	C2C-C1C-NC	2.45	112.55	109.98
19	A	806	CLA	CHA-C4D-ND	2.45	137.60	132.55
19	4	318	CLA	CHA-C4D-ND	2.45	137.60	132.55
19	Z	303	CLA	CHA-C4D-ND	2.45	137.60	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	1602	CLA	C2C-C1C-NC	2.45	112.55	109.98
19	B	822	CLA	CHA-C4D-ND	2.45	137.59	132.55
19	A	838	CLA	C3B-C4B-NB	-2.45	108.35	110.53
19	A	839	CLA	C3B-C4B-NB	-2.45	108.35	110.53
19	A	823	CLA	CHA-C4D-ND	2.45	137.59	132.55
19	3	5016	CLA	C4B-CHC-C1C	2.45	132.00	126.25
19	8	311	CLA	O2A-CGA-CBA	2.45	119.29	111.83
19	1	5010	CLA	C1C-C2C-C3C	-2.44	104.41	106.98
27	5	302	RRX	C34-C9-C8	2.44	121.82	118.09
19	B	801	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
19	1	5008	CLA	CHA-C4D-ND	2.44	137.59	132.55
19	B	823	CLA	C4B-CHC-C1C	2.44	131.99	126.25
19	B	840	CLA	O2A-CGA-CBA	2.44	119.28	111.83
19	7	306	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
19	6	314	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
19	B	833	CLA	CHA-C4D-ND	2.44	137.59	132.55
19	7	317	CLA	CMA-C3A-C4A	2.44	118.34	111.77
19	7	324	CLA	CMA-C3A-C4A	2.44	118.34	111.77
19	A	830	CLA	CHA-C4D-ND	2.44	137.59	132.55
19	5	309	CLA	C1C-C2C-C3C	-2.44	104.41	106.98
19	Z	315	CLA	CHA-C4D-ND	2.44	137.59	132.55
19	4	307	CLA	CHA-C4D-ND	2.44	137.59	132.55
19	3	5012	CLA	CAA-CBA-CGA	-2.44	106.28	113.21
22	A	850	BCR	C20-C19-C18	-2.44	119.67	126.36
19	A	833	CLA	CHA-C4D-ND	2.44	137.59	132.55
19	B	814	CLA	CHA-C4D-ND	2.44	137.59	132.55
31	8	304	LUT	C18-C5-C4	2.44	118.91	114.42
19	B	810	CLA	CHA-C4D-ND	2.44	137.58	132.55
31	3	5002	LUT	C4-C5-C6	-2.44	115.74	120.76
19	A	810	CLA	CHA-C4D-ND	2.44	137.58	132.55
22	B	846	BCR	C33-C5-C4	2.44	118.80	113.60
19	4	306	CLA	O2A-CGA-CBA	2.44	119.27	111.83
19	A	820	CLA	CHA-C4D-ND	2.44	137.58	132.55
19	6	311	CLA	CHA-C4D-ND	2.44	137.58	132.55
19	6	322	CLA	CMD-C2D-C3D	-2.44	122.10	127.69
19	A	805	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
19	Z	303	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
22	3	5006	BCR	C8-C7-C6	-2.44	120.48	127.00
19	B	821	CLA	CHA-C4D-ND	2.44	137.58	132.55
32	1	5017	CHL	C1-O2A-CGA	2.44	123.60	116.67
19	8	314	CLA	CHD-C1D-ND	-2.44	121.37	124.80
19	A	812	CLA	CHA-C4D-ND	2.44	137.58	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	805	CLA	CHA-C4D-ND	2.44	137.58	132.55
19	A	813	CLA	C1D-ND-C4D	-2.44	104.60	106.31
19	3	5014	CLA	C4B-CHC-C1C	2.44	131.98	126.25
19	8	308	CLA	CHA-C4D-ND	2.44	137.58	132.55
28	6	304	C7Z	C19-C9-C10	-2.44	118.87	122.82
19	A	805	CLA	CHD-C1D-ND	-2.44	121.37	124.80
19	7	324	CLA	CHD-C1D-ND	-2.44	121.37	124.80
19	7	307	CLA	C4B-CHC-C1C	2.44	131.97	126.25
19	B	801	CLA	CHA-C4D-ND	2.44	137.57	132.55
19	7	324	CLA	O2A-CGA-CBA	2.44	119.26	111.83
19	B	806	CLA	O2A-CGA-CBA	2.44	119.26	111.83
19	K	202	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
19	3	5016	CLA	CHA-C4D-ND	2.43	137.57	132.55
19	5	306	CLA	CHA-C4D-ND	2.43	137.57	132.55
19	7	311	CLA	C1D-ND-C4D	-2.43	104.60	106.31
19	7	313	CLA	CHA-C4D-ND	2.43	137.57	132.55
22	G	1603	BCR	C10-C11-C12	-2.43	116.15	123.20
19	1	5013	CLA	C4B-CHC-C1C	2.43	131.97	126.25
19	5	307	CLA	C4B-CHC-C1C	2.43	131.97	126.25
19	B	817	CLA	O2A-CGA-CBA	2.43	119.25	111.83
19	Z	305	CLA	O2A-CGA-CBA	2.43	119.25	111.83
19	K	204	CLA	CHA-C4D-ND	2.43	137.57	132.55
19	7	312	CLA	CHA-C4D-ND	2.43	137.57	132.55
19	B	820	CLA	O2A-CGA-CBA	2.43	119.25	111.83
19	6	302	CLA	O2A-CGA-CBA	2.43	119.25	111.83
22	5	304	BCR	C1-C6-C5	-2.43	119.31	122.64
19	5	306	CLA	C1-C2-C3	-2.43	122.21	126.20
19	5	310	CLA	CHA-C4D-ND	2.43	137.57	132.55
19	A	839	CLA	CMD-C2D-C3D	-2.43	122.11	127.69
22	G	1603	BCR	C16-C15-C14	-2.43	118.55	123.52
19	B	820	CLA	CHA-C4D-ND	2.43	137.56	132.55
19	J	1901	CLA	CHA-C4D-ND	2.43	137.56	132.55
19	Z	312	CLA	CHA-C4D-ND	2.43	137.56	132.55
22	B	847	BCR	C7-C6-C5	-2.43	115.96	121.56
19	B	817	CLA	CHA-C4D-ND	2.43	137.56	132.55
19	5	314	CLA	C1D-ND-C4D	-2.43	104.61	106.31
19	A	825	CLA	CHA-C4D-ND	2.43	137.56	132.55
19	A	813	CLA	O1D-CGD-CBD	-2.43	119.73	124.52
19	K	203	CLA	C4B-CHC-C1C	2.43	131.96	126.25
19	Z	314	CLA	CHA-C4D-ND	2.43	137.56	132.55
31	4	304	LUT	C31-C30-C29	-2.43	123.87	127.28
27	4	303	RRX	C34-C9-C8	2.43	121.80	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	828	CLA	C4B-CHC-C1C	2.43	131.96	126.25
19	A	807	CLA	CHA-C4D-ND	2.43	137.56	132.55
19	A	820	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
31	5	303	LUT	C20-C13-C12	2.43	121.80	118.09
32	4	314	CHL	CMA-C3A-C4A	2.43	119.84	114.61
22	6	308	BCR	C4-C5-C6	-2.43	119.43	122.70
19	7	313	CLA	C1D-ND-C4D	-2.43	104.61	106.31
19	A	811	CLA	O2D-CGD-O1D	-2.43	119.13	123.85
19	A	804	CLA	CHA-C4D-ND	2.43	137.55	132.55
19	7	319	CLA	O2A-CGA-CBA	2.42	119.23	111.83
19	4	316	CLA	CHA-C4D-ND	2.42	137.55	132.55
19	5	313	CLA	C1D-ND-C4D	-2.42	104.61	106.31
32	1	5014	CHL	CMA-C3A-C4A	2.42	119.83	114.61
19	B	818	CLA	CHA-C4D-ND	2.42	137.55	132.55
19	B	835	CLA	CHA-C4D-ND	2.42	137.55	132.55
19	3	5015	CLA	CHA-C4D-ND	2.42	137.55	132.55
19	B	822	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
19	4	306	CLA	CHD-C1D-ND	-2.42	121.39	124.80
19	Z	315	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
19	6	309	CLA	CHA-C1A-NA	-2.42	120.90	126.39
19	A	803	CLA	CHA-C4D-ND	2.42	137.55	132.55
19	B	815	CLA	CHA-C4D-ND	2.42	137.55	132.55
19	8	320	CLA	CHA-C4D-ND	2.42	137.55	132.55
19	3	5011	CLA	CHA-C4D-ND	2.42	137.55	132.55
19	8	313	CLA	O2A-CGA-CBA	2.42	119.22	111.83
19	A	834	CLA	O2A-CGA-CBA	2.42	119.22	111.83
19	5	301	CLA	O2A-CGA-CBA	2.42	119.22	111.83
31	7	304	LUT	C4-C5-C6	-2.42	115.78	120.76
19	B	813	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
19	B	801	CLA	C4B-CHC-C1C	2.42	131.94	126.25
19	7	316	CLA	C4B-CHC-C1C	2.42	131.94	126.25
19	5	301	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
19	A	818	CLA	C1C-C2C-C3C	-2.42	104.43	106.98
19	A	838	CLA	CHA-C4D-ND	2.42	137.54	132.55
19	3	5020	CLA	CHA-C4D-ND	2.42	137.54	132.55
19	A	802	CLA	C4B-CHC-C1C	2.42	131.94	126.25
19	A	828	CLA	CHA-C4D-ND	2.42	137.54	132.55
22	B	843	BCR	C30-C25-C24	2.42	122.21	115.65
19	4	309	CLA	CHD-C1D-ND	-2.42	121.40	124.80
31	8	305	LUT	C18-C5-C4	2.42	118.87	114.42
19	A	814	CLA	C1-C2-C3	-2.42	122.23	126.20
19	Z	308	CLA	CHD-C1D-ND	-2.42	121.40	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	843	BCR	C11-C12-C13	-2.42	119.73	126.36
19	7	307	CLA	C2D-C1D-ND	2.42	112.52	110.13
19	8	314	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
32	1	5017	CHL	C4D-CHA-CBD	-2.42	106.53	108.97
22	5	305	BCR	C33-C5-C4	2.42	118.75	113.60
19	A	824	CLA	CHA-C4D-ND	2.42	137.53	132.55
19	B	804	CLA	CHA-C4D-ND	2.42	137.53	132.55
19	6	311	CLA	O2D-CGD-O1D	-2.42	119.15	123.85
23	Z	316	LHG	C6-C5-C4	-2.42	106.15	111.78
19	1	5007	CLA	C1C-C2C-C3C	-2.41	104.44	106.98
19	6	312	CLA	CHA-C1A-NA	-2.41	120.92	126.39
19	A	823	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
19	5	319	CLA	CHA-C4D-ND	2.41	137.53	132.55
31	Z	318	LUT	C39-C29-C28	2.41	121.78	118.09
19	B	819	CLA	CHA-C4D-ND	2.41	137.53	132.55
22	3	5004	BCR	C30-C25-C26	-2.41	119.34	122.64
19	B	816	CLA	CHA-C4D-ND	2.41	137.53	132.55
19	1	5012	CLA	CHA-C4D-ND	2.41	137.53	132.55
19	5	321	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
31	3	5002	LUT	C35-C15-C14	-2.41	118.58	123.52
19	B	826	CLA	C2D-C1D-ND	2.41	112.51	110.13
22	8	303	BCR	C20-C19-C18	-2.41	119.75	126.36
19	A	831	CLA	CHA-C4D-ND	2.41	137.52	132.55
19	3	5019	CLA	CHD-C1D-ND	-2.41	121.41	124.80
19	A	814	CLA	CHA-C4D-ND	2.41	137.52	132.55
19	A	818	CLA	C2D-C1D-ND	2.41	112.51	110.13
19	4	306	CLA	CHA-C4D-ND	2.41	137.52	132.55
31	8	304	LUT	C4-C5-C6	-2.41	115.81	120.76
19	A	809	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
19	B	807	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
22	B	843	BCR	C15-C16-C17	-2.41	118.59	123.52
22	5	305	BCR	C8-C9-C10	2.41	122.80	119.01
32	6	316	CHL	CMA-C3A-C2A	2.41	123.43	114.13
19	F	303	CLA	CHA-C4D-ND	2.41	137.52	132.55
19	6	310	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
19	6	323	CLA	CHA-C4D-ND	2.41	137.52	132.55
22	8	303	BCR	C36-C18-C17	-2.41	118.92	122.82
31	7	303	LUT	C19-C9-C8	2.41	121.77	118.09
19	3	5019	CLA	CHA-C4D-ND	2.41	137.51	132.55
19	B	832	CLA	CHA-C4D-ND	2.41	137.51	132.55
19	A	836	CLA	CHA-C4D-ND	2.41	137.51	132.55
19	A	803	CLA	O2D-CGD-O1D	-2.41	119.17	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	5009	CLA	C4B-CHC-C1C	2.41	131.90	126.25
22	B	845	BCR	C11-C12-C13	-2.41	119.77	126.36
19	7	309	CLA	CHA-C1A-NA	-2.41	120.94	126.39
19	B	813	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
19	A	818	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
19	Z	314	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
19	Z	304	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
19	4	312	CLA	CHA-C4D-ND	2.40	137.51	132.55
19	5	312	CLA	C2D-C1D-ND	2.40	112.50	110.13
19	A	840	CLA	CHA-C4D-ND	2.40	137.51	132.55
32	8	319	CHL	CMA-C3A-C2A	2.40	123.41	114.13
19	A	837	CLA	CHA-C4D-ND	2.40	137.51	132.55
19	A	842	CLA	CHA-C4D-ND	2.40	137.51	132.55
19	A	804	CLA	O2A-CGA-CBA	2.40	119.16	111.83
19	B	813	CLA	C3B-C4B-NB	-2.40	108.39	110.53
19	1	5006	CLA	CMD-C2D-C3D	-2.40	122.18	127.69
19	B	808	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
19	F	303	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
19	B	825	CLA	CMA-C3A-C4A	2.40	118.23	111.77
19	7	310	CLA	C1-O2A-CGA	2.40	122.47	116.65
19	B	822	CLA	C2D-C1D-ND	2.40	112.50	110.13
19	1	5008	CLA	O2A-C1-C2	2.40	117.35	108.11
19	3	5009	CLA	CHD-C1D-ND	-2.40	121.42	124.80
19	A	829	CLA	CHA-C4D-ND	2.40	137.50	132.55
19	5	307	CLA	CHA-C4D-ND	2.40	137.50	132.55
19	B	813	CLA	CHA-C4D-ND	2.40	137.50	132.55
19	B	809	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
19	K	202	CLA	C4B-CHC-C1C	2.40	131.89	126.25
19	8	318	CLA	CHD-C1D-ND	-2.40	121.43	124.80
19	A	809	CLA	CHA-C4D-ND	2.40	137.50	132.55
32	3	5017	CHL	C4D-ND-C1D	2.40	107.04	105.22
19	A	827	CLA	O2A-CGA-CBA	2.40	119.15	111.83
19	B	809	CLA	CHA-C4D-ND	2.40	137.50	132.55
19	7	309	CLA	CMA-C3A-C4A	2.40	118.22	111.77
19	G	1602	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
19	A	812	CLA	CHD-C1D-ND	-2.40	121.43	124.80
19	8	313	CLA	CHA-C4D-ND	2.40	137.49	132.55
32	Z	302	CHL	C4D-CHA-CBD	-2.40	106.55	108.97
19	5	321	CLA	CHA-C4D-ND	2.40	137.49	132.55
19	4	316	CLA	O2A-CGA-CBA	2.40	119.14	111.83
19	A	822	CLA	CHD-C1D-ND	-2.40	121.43	124.80
19	7	317	CLA	CHD-C1D-ND	-2.40	121.43	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	838	CLA	C1-C2-C3	-2.40	122.27	126.20
19	B	834	CLA	CHA-C4D-ND	2.40	137.49	132.55
19	6	320	CLA	CHA-C4D-ND	2.40	137.49	132.55
19	8	314	CLA	CMA-C3A-C4A	2.39	118.21	111.77
31	1	5003	LUT	C31-C30-C29	-2.39	123.92	127.28
19	A	819	CLA	CHA-C4D-ND	2.39	137.49	132.55
22	B	846	BCR	C38-C26-C27	2.39	118.70	113.60
22	3	5005	BCR	C38-C26-C27	2.39	118.70	113.60
19	B	837	CLA	CHA-C4D-ND	2.39	137.48	132.55
19	8	311	CLA	CHA-C4D-ND	2.39	137.48	132.55
19	B	823	CLA	O2A-CGA-CBA	2.39	119.13	111.83
19	4	310	CLA	C2C-C1C-NC	2.39	112.49	109.98
19	5	319	CLA	C2C-C1C-NC	2.39	112.49	109.98
19	B	811	CLA	CHA-C4D-ND	2.39	137.48	132.55
19	4	308	CLA	CHA-C1A-NA	-2.39	120.98	126.39
19	1	5018	CLA	CHA-C4D-ND	2.39	137.48	132.55
19	3	5019	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
19	A	814	CLA	CHD-C1D-ND	-2.39	121.44	124.80
31	7	304	LUT	C37-C21-C26	2.39	113.17	109.55
19	B	805	CLA	C2D-C1D-ND	2.39	112.49	110.13
19	B	837	CLA	O1D-CGD-CBD	-2.39	119.81	124.52
33	3	5001	SPH	C3-C4-C5	-2.39	119.74	124.69
19	5	309	CLA	CHA-C4D-ND	2.39	137.48	132.55
19	7	306	CLA	CMD-C2D-C3D	-2.39	122.21	127.69
19	6	310	CLA	CHA-C4D-ND	2.39	137.48	132.55
19	A	831	CLA	O2A-CGA-CBA	2.39	119.12	111.83
19	5	314	CLA	CHA-C4D-ND	2.39	137.47	132.55
19	B	802	CLA	C2D-C1D-ND	2.39	112.49	110.13
19	3	5013	CLA	CMD-C2D-C3D	-2.39	122.22	127.69
19	8	320	CLA	C2D-C1D-ND	2.39	112.49	110.13
27	F	304	RRX	C2-C1-C6	2.39	113.91	110.44
19	B	840	CLA	C1D-ND-C4D	-2.39	104.64	106.31
19	A	817	CLA	CHA-C4D-ND	2.39	137.47	132.55
19	3	5011	CLA	C2D-C1D-ND	2.39	112.49	110.13
19	B	806	CLA	CHA-C4D-ND	2.39	137.47	132.55
19	B	807	CLA	CHA-C4D-ND	2.39	137.47	132.55
19	5	311	CLA	CHA-C4D-ND	2.38	137.47	132.55
19	7	307	CLA	O2A-CGA-CBA	2.38	119.11	111.83
19	Z	308	CLA	C4B-CHC-C1C	2.38	131.85	126.25
19	4	312	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
19	B	826	CLA	O2A-CGA-CBA	2.38	119.10	111.83
19	5	308	CLA	CMA-C3A-C4A	2.38	118.18	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	5007	CLA	CHA-C4D-ND	2.38	137.47	132.55
19	I	201	CLA	C2D-C1D-ND	2.38	112.48	110.13
19	6	311	CLA	C2C-C1C-NC	2.38	112.48	109.98
19	A	834	CLA	CHA-C4D-ND	2.38	137.46	132.55
19	3	5010	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
19	4	312	CLA	C2D-C1D-ND	2.38	112.48	110.13
19	1	5016	CLA	CHA-C4D-ND	2.38	137.46	132.55
19	A	810	CLA	C2C-C1C-NC	2.38	112.48	109.98
19	B	820	CLA	C6-C5-C3	-2.38	107.67	113.47
19	A	811	CLA	CHA-C4D-ND	2.38	137.46	132.55
19	6	313	CLA	CHA-C1A-NA	-2.38	121.00	126.39
19	B	828	CLA	CHA-C4D-ND	2.38	137.46	132.55
19	B	839	CLA	CHA-C4D-ND	2.38	137.46	132.55
19	5	301	CLA	CHA-C4D-ND	2.38	137.46	132.55
19	6	314	CLA	CHA-C4D-ND	2.38	137.46	132.55
19	5	319	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
19	7	319	CLA	CHA-C4D-ND	2.38	137.46	132.55
31	5	303	LUT	C39-C29-C28	2.38	121.72	118.09
19	5	325	CLA	C1D-ND-C4D	-2.38	104.64	106.31
19	5	311	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
19	A	842	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
19	B	834	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
19	3	5018	CLA	C2C-C1C-NC	2.38	112.48	109.98
19	A	813	CLA	CMA-C3A-C4A	2.38	118.17	111.77
22	5	305	BCR	C20-C21-C22	-2.38	123.94	127.28
22	F	302	BCR	C4-C5-C6	-2.38	119.49	122.70
19	A	810	CLA	O2A-CGA-CBA	2.38	119.08	111.83
19	B	817	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
19	4	308	CLA	C2D-C1D-ND	2.38	112.48	110.13
19	5	317	CLA	C4B-CHC-C1C	2.38	131.84	126.25
19	A	815	CLA	CAA-CBA-CGA	-2.38	106.46	113.21
19	3	5013	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
19	A	819	CLA	C1-O2A-CGA	2.38	122.40	116.65
19	A	823	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
28	J	1902	C7Z	C28-C27-C26	-2.38	120.65	127.00
19	A	817	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
19	B	825	CLA	C2C-C1C-NC	2.38	112.48	109.98
22	3	5007	BCR	C36-C18-C19	2.37	121.72	118.09
19	B	814	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
19	8	311	CLA	C16-C15-C13	-2.37	108.07	115.97
19	Z	307	CLA	CAA-C2A-C3A	-2.37	106.58	113.00
19	Z	305	CLA	CHA-C4D-ND	2.37	137.45	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	822	CLA	CHD-C1D-ND	-2.37	121.46	124.80
19	8	309	CLA	CHA-C1A-NA	-2.37	121.02	126.39
19	Z	307	CLA	O2A-CGA-CBA	2.37	119.07	111.83
19	6	309	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
19	B	817	CLA	C1C-C2C-C3C	-2.37	104.48	106.98
19	5	311	CLA	CHD-C1D-ND	-2.37	121.46	124.80
19	Z	303	CLA	C4B-CHC-C1C	2.37	131.82	126.25
19	3	5010	CLA	C2C-C1C-NC	2.37	112.47	109.98
19	1	5008	CLA	C11-C10-C8	-2.37	108.08	115.97
19	4	316	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
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	3	5008	CLA	C1D-ND-C4D	-2.37	104.65	106.31
19	8	318	CLA	C1D-ND-C4D	-2.37	104.65	106.31
19	B	838	CLA	CHA-C4D-ND	2.37	137.44	132.55
19	A	818	CLA	C6-C5-C3	-2.37	107.69	113.47
19	B	832	CLA	O2A-CGA-CBA	2.37	119.06	111.83
19	6	313	CLA	CMA-C3A-C4A	2.37	118.14	111.77
19	B	803	CLA	O2A-CGA-CBA	2.37	119.06	111.83
19	B	836	CLA	CHD-C1D-ND	-2.37	121.47	124.80
19	Z	305	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
19	3	5018	CLA	C4B-CHC-C1C	2.37	131.82	126.25
19	7	308	CLA	CHA-C1A-NA	-2.37	121.03	126.39
19	4	318	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
19	5	319	CLA	O2A-CGA-CBA	2.37	119.05	111.83
19	B	837	CLA	C2D-C1D-ND	2.37	112.47	110.13
19	5	306	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
19	A	839	CLA	CHD-C1D-ND	-2.37	121.47	124.80
19	Z	307	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
19	5	310	CLA	CHD-C1D-ND	-2.37	121.47	124.80
19	5	325	CLA	C6-C5-C3	-2.37	107.70	113.47
19	A	808	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
19	3	5013	CLA	CHA-C4D-ND	2.37	137.43	132.55
19	B	809	CLA	O2A-CGA-CBA	2.37	119.05	111.83
19	A	841	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
19	5	312	CLA	CHA-C4D-ND	2.36	137.43	132.55
22	B	844	BCR	C20-C21-C22	-2.36	123.96	127.28
19	A	839	CLA	O2A-CGA-CBA	2.36	119.04	111.83
24	A	856	LMT	C1B-O1B-C4'	-2.36	112.37	117.98
24	A	856	LMT	O1'-C1'-C2'	2.36	111.86	108.27
19	1	5008	CLA	C1-C2-C3	-2.36	122.32	126.20
19	5	317	CLA	CHD-C1D-ND	-2.36	121.48	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	8	320	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
19	3	5019	CLA	C2D-C1D-ND	2.36	112.47	110.13
19	A	807	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
28	J	1902	C7Z	C21-C26-C25	-2.36	119.41	122.64
32	Z	313	CHL	CMA-C3A-C2A	2.36	123.25	114.13
31	7	303	LUT	C15-C35-C34	-2.36	118.69	123.52
19	A	835	CLA	CHA-C4D-ND	2.36	137.42	132.55
19	A	811	CLA	C2D-C1D-ND	2.36	112.46	110.13
19	B	825	CLA	C2D-C1D-ND	2.36	112.46	110.13
19	Z	312	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
31	8	304	LUT	C35-C15-C14	-2.36	118.69	123.52
38	8	325	ERG	C18-C13-C14	-2.36	106.43	110.35
19	I	201	CLA	O2A-CGA-CBA	2.36	119.03	111.83
31	Z	318	LUT	C15-C35-C34	-2.36	118.69	123.52
19	A	815	CLA	CHD-C1D-ND	-2.36	121.48	124.80
19	B	834	CLA	CHD-C1D-ND	-2.36	121.48	124.80
19	A	810	CLA	CAA-C2A-C3A	-2.36	106.62	113.00
19	B	830	CLA	CHA-C4D-ND	2.36	137.42	132.55
19	4	310	CLA	CMA-C3A-C4A	2.36	118.11	111.77
19	A	837	CLA	CHD-C1D-ND	-2.36	121.48	124.80
19	Z	305	CLA	C16-C15-C13	-2.36	108.13	115.97
19	B	803	CLA	C4B-CHC-C1C	2.36	131.79	126.25
19	5	317	CLA	CHA-C4D-ND	2.36	137.41	132.55
19	B	833	CLA	CMD-C2D-C3D	-2.36	122.28	127.69
19	5	313	CLA	CHA-C4D-ND	2.36	137.41	132.55
22	F	302	BCR	C33-C5-C4	2.36	118.62	113.60
19	B	819	CLA	CHD-C1D-ND	-2.36	121.49	124.80
22	K	206	BCR	C8-C7-C6	-2.36	120.70	127.00
19	A	802	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
19	A	805	CLA	CHA-C4D-ND	2.36	137.41	132.55
19	A	841	CLA	C2D-C1D-ND	2.36	112.46	110.13
19	3	5011	CLA	CHD-C1D-ND	-2.36	121.49	124.80
19	B	831	CLA	C6-C5-C3	-2.35	107.73	113.47
27	4	303	RRX	C33-C5-C4	2.35	118.62	113.60
22	3	5007	BCR	C21-C20-C19	2.35	130.02	123.20
19	B	839	CLA	C2D-C1D-ND	2.35	112.46	110.13
19	3	5015	CLA	CAA-C2A-C3A	-2.35	106.64	113.00
19	A	827	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
19	3	5012	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
19	A	830	CLA	O2A-CGA-CBA	2.35	119.01	111.83
19	B	822	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
19	4	309	CLA	CMD-C2D-C3D	-2.35	122.29	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	5006	CLA	CHA-C4D-ND	2.35	137.40	132.55
19	A	831	CLA	CHD-C1D-ND	-2.35	121.49	124.80
19	1	5016	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
19	Z	306	CLA	CHD-C1D-ND	-2.35	121.49	124.80
19	A	816	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
19	1	5018	CLA	O2A-CGA-CBA	2.35	119.00	111.83
19	B	812	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
19	Z	306	CLA	CHA-C4D-ND	2.35	137.40	132.55
31	6	306	LUT	C22-C23-C24	2.35	114.67	111.18
19	A	829	CLA	C2D-C1D-ND	2.35	112.45	110.13
19	A	818	CLA	C2C-C1C-NC	2.35	112.45	109.98
31	1	5004	LUT	C17-C1-C6	-2.35	106.56	110.24
22	B	842	BCR	C20-C19-C18	-2.35	119.92	126.36
19	A	811	CLA	CHD-C1D-ND	-2.35	121.50	124.80
19	B	827	CLA	O1D-CGD-CBD	-2.35	119.89	124.52
19	A	827	CLA	C2D-C1D-ND	2.35	112.45	110.13
19	A	806	CLA	CHD-C1D-ND	-2.35	121.50	124.80
19	A	812	CLA	C1C-C2C-C3C	-2.35	104.51	106.98
19	B	836	CLA	CMA-C3A-C4A	2.35	118.08	111.77
19	7	312	CLA	CAA-C2A-C3A	-2.35	106.66	113.00
19	A	833	CLA	C2D-C1D-ND	2.35	112.45	110.13
19	A	812	CLA	CMA-C3A-C4A	2.35	118.08	111.77
19	B	829	CLA	CMD-C2D-C3D	-2.35	122.31	127.69
22	A	849	BCR	C10-C11-C12	-2.35	116.40	123.20
19	4	309	CLA	C1-O2A-CGA	2.35	122.33	116.65
27	5	302	RRX	C12-C13-C14	-2.35	115.32	119.01
19	J	1901	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
19	A	804	CLA	C2D-C1D-ND	2.35	112.45	110.13
19	5	301	CLA	C2D-C1D-ND	2.35	112.45	110.13
32	Z	313	CHL	C1C-C2C-CMC	2.35	131.03	126.80
19	6	323	CLA	CMA-C3A-C4A	2.34	118.07	111.77
32	1	5009	CHL	C4D-CHA-CBD	-2.34	106.60	108.97
19	A	813	CLA	C3B-C4B-NB	-2.34	108.44	110.53
22	B	843	BCR	C8-C7-C6	-2.34	120.74	127.00
19	A	806	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
19	B	823	CLA	CHA-C4D-ND	2.34	137.38	132.55
22	8	306	BCR	C29-C28-C27	2.34	116.43	111.28
19	B	821	CLA	O2A-CGA-CBA	2.34	118.98	111.83
31	1	5004	LUT	C20-C13-C12	2.34	121.67	118.09
19	Z	315	CLA	OBD-CAD-C3D	-2.34	122.94	128.42
19	A	819	CLA	CHD-C1D-ND	-2.34	121.51	124.80
19	3	5013	CLA	C1D-ND-C4D	-2.34	104.67	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	7	311	CLA	CHA-C4D-ND	2.34	137.38	132.55
19	G	1601	CLA	C2D-C1D-ND	2.34	112.44	110.13
19	3	5014	CLA	C2D-C1D-ND	2.34	112.44	110.13
19	A	803	CLA	CHD-C1D-ND	-2.34	121.51	124.80
22	5	304	BCR	C34-C9-C8	2.34	121.66	118.09
19	B	833	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
19	A	820	CLA	C2D-C1D-ND	2.34	112.44	110.13
19	4	313	CLA	C1D-ND-C4D	-2.34	104.67	106.31
31	3	5002	LUT	C1-C6-C5	-2.34	119.44	122.64
32	8	317	CHL	C3D-C4D-ND	-2.34	109.19	112.94
19	A	857	CLA	O2A-CGA-CBA	2.34	118.96	111.83
19	B	811	CLA	O2A-CGA-CBA	2.34	118.96	111.83
19	3	5014	CLA	CHA-C4D-ND	2.34	137.37	132.55
19	3	5010	CLA	O2A-C1-C2	2.34	117.10	108.11
28	6	304	C7Z	C24-C25-C26	-2.34	115.96	120.76
19	6	313	CLA	C3B-C4B-NB	-2.34	108.44	110.53
31	3	5002	LUT	C21-C26-C27	-2.34	110.14	112.83
19	6	322	CLA	CHA-C4D-ND	2.33	137.37	132.55
19	7	309	CLA	C1D-ND-C4D	-2.33	104.67	106.31
22	B	844	BCR	C37-C22-C21	-2.33	119.03	122.82
19	A	803	CLA	C2D-C1D-ND	2.33	112.44	110.13
19	A	815	CLA	CHA-C4D-ND	2.33	137.36	132.55
31	8	304	LUT	C8-C9-C10	2.33	122.68	119.01
19	G	1602	CLA	C2D-C1D-ND	2.33	112.44	110.13
19	1	5013	CLA	CMD-C2D-C3D	-2.33	122.34	127.69
31	3	5002	LUT	C16-C1-C6	-2.33	106.58	110.24
19	Z	308	CLA	CHA-C4D-ND	2.33	137.36	132.55
19	3	5020	CLA	C1D-ND-C4D	-2.33	104.68	106.31
19	B	850	CLA	CMA-C3A-C4A	2.33	118.04	111.77
19	4	307	CLA	C2D-C1D-ND	2.33	112.43	110.13
19	B	839	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
19	5	322	CLA	CHD-C1D-ND	-2.33	121.52	124.80
19	A	836	CLA	C2D-C1D-ND	2.33	112.43	110.13
19	A	819	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
19	A	817	CLA	O2A-CGA-CBA	2.33	118.94	111.83
28	J	1902	C7Z	C8-C7-C6	-2.33	120.78	127.00
19	B	817	CLA	C2D-C1D-ND	2.33	112.43	110.13
19	B	834	CLA	C2D-C1D-ND	2.33	112.43	110.13
19	A	822	CLA	CHA-C4D-ND	2.33	137.35	132.55
19	A	807	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
19	A	822	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
31	5	303	LUT	C36-C21-C26	-2.33	106.02	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	806	CLA	CHD-C1D-ND	-2.33	121.53	124.80
22	B	845	BCR	C30-C25-C24	2.33	121.97	115.65
19	3	5018	CLA	CHA-C4D-ND	2.33	137.35	132.55
19	B	826	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
32	6	321	CHL	C1A-CHA-CBD	-2.33	126.40	132.36
19	5	321	CLA	CHD-C1D-ND	-2.33	121.53	124.80
19	8	309	CLA	C2C-C1C-NC	2.33	112.42	109.98
34	5	324	3PH	C2-O21-C21	-2.33	112.23	117.80
19	A	815	CLA	CMD-C2D-C3D	-2.33	122.36	127.69
19	B	814	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
19	6	309	CLA	C1D-ND-C4D	-2.32	104.68	106.31
19	B	838	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
19	B	824	CLA	O1D-CGD-CBD	-2.32	119.93	124.52
19	B	823	CLA	C6-C5-C3	-2.32	107.81	113.47
19	4	310	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
19	B	811	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
19	F	301	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
32	5	315	CHL	C4C-CHD-C1D	2.32	124.38	116.07
19	Z	314	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
19	B	813	CLA	CHD-C1D-ND	-2.32	121.53	124.80
22	K	206	BCR	C10-C11-C12	-2.32	116.47	123.20
19	B	850	CLA	CBA-CAA-C2A	-2.32	106.89	113.79
19	A	821	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
19	K	204	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
19	3	5008	CLA	CHD-C1D-ND	-2.32	121.54	124.80
19	5	314	CLA	CHA-C1A-NA	-2.32	121.14	126.39
22	A	846	BCR	C29-C30-C25	2.32	113.81	110.44
31	4	304	LUT	C35-C15-C14	-2.32	118.78	123.52
18	A	801	CL0	CMB-C2B-C3B	2.32	129.31	124.68
18	A	801	CL0	C4C-CHD-C1D	2.32	124.36	116.07
19	7	319	CLA	CHD-C1D-ND	-2.32	121.54	124.80
19	5	317	CLA	C2C-C1C-NC	2.32	112.42	109.98
19	B	801	CLA	CMA-C3A-C4A	2.32	118.00	111.77
19	A	832	CLA	O2A-CGA-CBA	2.32	118.90	111.83
19	B	850	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
19	B	816	CLA	C2D-C1D-ND	2.32	112.42	110.13
19	B	817	CLA	C2C-C1C-NC	2.32	112.41	109.98
19	B	813	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
22	4	305	BCR	C24-C25-C26	-2.31	116.22	121.56
22	F	302	BCR	C35-C13-C12	2.31	121.62	118.09
31	3	5002	LUT	C27-C28-C29	-2.31	121.35	126.32
19	B	818	CLA	CHD-C1D-ND	-2.31	121.55	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	311	CLA	CMA-C3A-C4A	2.31	117.99	111.77
19	A	821	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
19	A	822	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
22	A	849	BCR	C32-C1-C6	-2.31	106.62	110.24
19	B	823	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
19	5	307	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
19	Z	303	CLA	C3B-C4B-NB	-2.31	108.47	110.53
19	B	815	CLA	C2D-C1D-ND	2.31	112.41	110.13
19	B	801	CLA	O2A-CGA-CBA	2.31	118.88	111.83
19	A	833	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
19	3	5016	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
19	6	311	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
19	A	820	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
19	A	838	CLA	CHD-C1D-ND	-2.31	121.55	124.80
19	B	801	CLA	CHD-C1D-ND	-2.31	121.55	124.80
19	6	309	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
19	B	827	CLA	O2A-CGA-CBA	2.31	118.87	111.83
22	K	206	BCR	C27-C26-C25	-2.31	119.58	122.70
32	8	315	CHL	CMA-C3A-C2A	2.31	123.04	114.13
19	A	831	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
19	B	819	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
19	A	820	CLA	O2A-CGA-CBA	2.31	118.87	111.83
19	B	831	CLA	CHD-C1D-ND	-2.31	121.56	124.80
19	A	831	CLA	C2D-C1D-ND	2.31	112.41	110.13
19	5	307	CLA	CMA-C3A-C4A	2.31	117.97	111.77
19	8	307	CLA	C1D-ND-C4D	-2.31	104.69	106.31
19	A	841	CLA	O2A-CGA-CBA	2.31	118.87	111.83
19	K	204	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
19	B	837	CLA	O2D-CGD-O1D	-2.30	119.36	123.85
19	7	316	CLA	CHD-C1D-ND	-2.30	121.56	124.80
19	B	830	CLA	C2D-C1D-ND	2.30	112.41	110.13
19	J	1901	CLA	C2D-C1D-ND	2.30	112.41	110.13
19	A	819	CLA	O2A-CGA-CBA	2.30	118.86	111.83
19	B	814	CLA	CHD-C1D-ND	-2.30	121.56	124.80
19	B	824	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
19	B	804	CLA	C4B-CHC-C1C	2.30	131.66	126.25
19	6	301	CLA	C2D-C1D-ND	2.30	112.41	110.13
19	5	317	CLA	CBA-CAA-C2A	-2.30	106.94	113.79
22	B	847	BCR	C15-C14-C13	-2.30	124.05	127.28
22	A	850	BCR	C34-C9-C10	-2.30	119.09	122.82
19	7	317	CLA	CHA-C4D-ND	2.30	137.30	132.55
19	B	827	CLA	C2D-C1D-ND	2.30	112.40	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	5018	CLA	C2D-C1D-ND	2.30	112.40	110.13
19	3	5018	CLA	C2D-C1D-ND	2.30	112.40	110.13
19	7	317	CLA	C2D-C1D-ND	2.30	112.40	110.13
19	A	834	CLA	CHD-C1D-ND	-2.30	121.56	124.80
19	A	832	CLA	CHA-C1A-NA	-2.30	121.18	126.39
19	B	803	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
32	8	317	CHL	C1-C2-C3	-2.30	123.04	126.76
19	A	808	CLA	C2D-C1D-ND	2.30	112.40	110.13
19	5	321	CLA	C2D-C1D-ND	2.30	112.40	110.13
22	A	849	BCR	C23-C24-C25	-2.30	120.86	127.00
19	A	811	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
31	1	5004	LUT	C39-C29-C28	2.30	121.60	118.09
19	B	808	CLA	C2D-C1D-ND	2.30	112.40	110.13
19	1	5012	CLA	C2D-C1D-ND	2.30	112.40	110.13
19	6	312	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
19	B	837	CLA	CHD-C1D-ND	-2.30	121.57	124.80
19	A	823	CLA	CHD-C1D-ND	-2.30	121.57	124.80
19	B	839	CLA	CHD-C1D-ND	-2.30	121.57	124.80
31	1	5004	LUT	C35-C15-C14	-2.30	118.82	123.52
32	1	5017	CHL	CMA-C3A-C4A	2.30	119.56	114.61
19	B	825	CLA	CHA-C4D-ND	2.30	137.28	132.55
19	B	803	CLA	CHD-C1D-ND	-2.29	121.57	124.80
19	5	313	CLA	CHD-C1D-ND	-2.29	121.57	124.80
32	6	315	CHL	C4C-CHD-C1D	2.29	124.28	116.07
22	5	305	BCR	C29-C30-C25	2.29	113.77	110.44
19	A	832	CLA	O1D-CGD-CBD	-2.29	119.99	124.52
19	8	308	CLA	C3D-C2D-C1D	-2.29	102.70	105.83
19	B	840	CLA	C1-O2A-CGA	2.29	122.20	116.65
19	5	310	CLA	O2A-CGA-CBA	2.29	118.83	111.83
19	A	817	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
19	A	814	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
19	K	204	CLA	O2A-CGA-CBA	2.29	118.83	111.83
19	B	820	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
19	3	5016	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
19	3	5012	CLA	C2D-C1D-ND	2.29	112.39	110.13
19	Z	311	CLA	O2A-CGA-CBA	2.29	118.82	111.83
19	A	840	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
19	A	805	CLA	O2A-CGA-CBA	2.29	118.82	111.83
28	6	304	C7Z	C4-C5-C6	-2.29	116.05	120.76
19	A	833	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
19	5	325	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
19	I	201	CLA	C6-C5-C3	-2.29	107.89	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	826	CLA	C2D-C1D-ND	2.29	112.39	110.13
19	B	828	CLA	C2D-C1D-ND	2.29	112.39	110.13
19	F	303	CLA	C2D-C1D-ND	2.29	112.39	110.13
19	B	808	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
19	A	804	CLA	C6-C5-C3	-2.29	107.89	113.47
19	A	836	CLA	CHD-C1D-ND	-2.29	121.58	124.80
19	B	810	CLA	C2D-C1D-ND	2.29	112.39	110.13
19	B	807	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
19	B	830	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
19	B	806	CLA	CMD-C2D-C3D	-2.29	122.45	127.69
19	6	318	CLA	CHD-C1D-ND	-2.29	121.59	124.80
19	A	838	CLA	CMD-C2D-C3D	-2.29	122.45	127.69
19	A	814	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
19	1	5008	CLA	CHD-C1D-ND	-2.28	121.59	124.80
19	G	1602	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
19	4	308	CLA	CHD-C1D-ND	-2.28	121.59	124.80
19	B	850	CLA	O2A-CGA-CBA	2.28	118.80	111.83
19	8	310	CLA	CAA-C2A-C3A	-2.28	106.83	113.00
18	A	801	CL0	C4-C3-C5	2.28	119.19	115.23
19	6	302	CLA	C2D-C1D-ND	2.28	112.39	110.13
22	4	305	BCR	C15-C16-C17	-2.28	118.85	123.52
19	A	838	CLA	C2D-C1D-ND	2.28	112.39	110.13
19	A	834	CLA	CMD-C2D-C3D	-2.28	122.45	127.69
32	7	314	CHL	C4D-CHA-CBD	-2.28	106.67	108.97
19	Z	303	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
28	1	5005	C7Z	C4-C5-C6	-2.28	116.07	120.76
19	B	829	CLA	O2A-CGA-CBA	2.28	118.79	111.83
19	Z	314	CLA	CHD-C1D-ND	-2.28	121.59	124.80
32	4	317	CHL	CMA-C3A-C2A	2.28	122.94	114.13
19	A	804	CLA	CHD-C1D-ND	-2.28	121.59	124.80
19	B	806	CLA	C2D-C1D-ND	2.28	112.38	110.13
22	B	844	BCR	C8-C9-C10	2.28	122.59	119.01
19	5	319	CLA	CHD-C1D-ND	-2.28	121.60	124.80
19	A	817	CLA	C2D-C1D-ND	2.28	112.38	110.13
19	A	808	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
19	A	805	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
19	B	810	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
19	B	838	CLA	CHD-C1D-ND	-2.28	121.60	124.80
19	A	838	CLA	O2D-CGD-O1D	-2.28	119.42	123.85
19	3	5008	CLA	O2D-CGD-O1D	-2.28	119.42	123.85
19	7	318	CLA	CHA-C1A-NA	-2.28	121.24	126.39
19	1	5016	CLA	C2D-C1D-ND	2.28	112.38	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	315	CLA	CHD-C1D-ND	-2.28	121.60	124.80
19	6	312	CLA	C1D-ND-C4D	-2.28	104.72	106.31
19	A	802	CLA	CHA-C1A-NA	-2.28	121.24	126.39
19	B	817	CLA	CHD-C1D-ND	-2.28	121.60	124.80
19	1	5016	CLA	CHD-C1D-ND	-2.28	121.60	124.80
31	3	5003	LUT	C21-C26-C27	2.28	115.44	112.83
19	6	318	CLA	C2D-C1D-ND	2.28	112.38	110.13
19	A	813	CLA	CHA-C1A-NA	-2.28	121.24	126.39
31	6	306	LUT	C11-C12-C13	-2.27	120.13	126.36
31	5	303	LUT	C35-C15-C14	-2.27	118.86	123.52
22	3	5004	BCR	C3-C4-C5	-2.27	110.00	114.06
19	B	817	CLA	CMD-C2D-C3D	-2.27	122.47	127.69
19	1	5015	CLA	C3D-C2D-C1D	-2.27	102.73	105.83
19	A	809	CLA	CMD-C2D-C3D	-2.27	122.47	127.69
19	Z	304	CLA	CHD-C1D-ND	-2.27	121.60	124.80
19	6	323	CLA	CHD-C1D-ND	-2.27	121.60	124.80
19	8	309	CLA	C2D-C1D-ND	2.27	112.38	110.13
19	A	828	CLA	CHD-C1D-ND	-2.27	121.61	124.80
19	8	307	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
19	A	817	CLA	CHD-C1D-ND	-2.27	121.61	124.80
19	B	805	CLA	CHD-C1D-ND	-2.27	121.61	124.80
19	3	5015	CLA	C3D-C2D-C1D	-2.27	102.73	105.83
19	A	821	CLA	CHD-C1D-ND	-2.27	121.61	124.80
19	1	5007	CLA	CAA-CBA-CGA	-2.27	106.44	112.49
19	A	842	CLA	O2A-CGA-CBA	2.27	118.76	111.83
19	B	816	CLA	O2A-CGA-CBA	2.27	118.76	111.83
19	1	5012	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
19	A	841	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
31	8	305	LUT	C28-C29-C30	-2.27	115.44	119.01
19	A	802	CLA	CHD-C1D-ND	-2.27	121.61	124.80
19	K	203	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
19	K	203	CLA	CHA-C1A-NA	-2.27	121.25	126.39
19	A	812	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
19	1	5006	CLA	C2C-C1C-NC	2.27	112.36	109.98
27	5	302	RRX	C38-C26-C27	2.27	118.59	114.42
19	7	311	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
19	3	5020	CLA	CHA-C1A-NA	-2.27	121.26	126.39
19	A	830	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
19	B	818	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
19	8	318	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
19	A	803	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
19	8	307	CLA	CHD-C1D-ND	-2.27	121.61	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	5007	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
19	B	811	CLA	C2D-C1D-ND	2.26	112.37	110.13
19	7	309	CLA	C6-C5-C3	-2.26	107.95	113.47
19	B	821	CLA	CHD-C1D-ND	-2.26	121.62	124.80
19	B	833	CLA	CHD-C1D-ND	-2.26	121.62	124.80
19	B	814	CLA	O2A-CGA-CBA	2.26	118.74	111.83
19	7	319	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
19	A	805	CLA	C2D-C1D-ND	2.26	112.36	110.13
19	A	832	CLA	C2D-C1D-ND	2.26	112.36	110.13
19	B	832	CLA	C2D-C1D-ND	2.26	112.36	110.13
19	B	816	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
19	6	310	CLA	CMA-C3A-C4A	2.26	117.85	111.77
23	4	320	LHG	C6-C5-C4	-2.26	106.51	111.78
19	8	314	CLA	CMD-C2D-C3D	-2.26	122.50	127.69
19	5	317	CLA	O2A-CGA-CBA	2.26	118.73	111.83
19	3	5016	CLA	C2D-C1D-ND	2.26	112.36	110.13
31	7	304	LUT	C8-C9-C10	2.26	122.56	119.01
32	3	5017	CHL	C1-C2-C3	-2.26	122.49	126.20
19	3	5016	CLA	CHD-C1D-ND	-2.26	121.62	124.80
19	A	828	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
32	6	319	CHL	C1-C2-C3	-2.26	122.50	126.20
19	7	309	CLA	CHD-C1D-ND	-2.26	121.62	124.80
19	J	1901	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
19	A	837	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
19	B	823	CLA	CHD-C1D-ND	-2.26	121.62	124.80
19	A	809	CLA	C2D-C1D-ND	2.26	112.36	110.13
19	6	311	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
19	7	324	CLA	CHA-C4D-ND	2.26	137.21	132.55
19	5	314	CLA	CAA-C2A-C3A	-2.26	106.90	113.00
19	1	5016	CLA	O2A-CGA-CBA	2.26	118.72	111.83
19	Z	305	CLA	C2C-C1C-NC	2.26	112.35	109.98
19	A	816	CLA	C2D-C1D-ND	2.26	112.36	110.13
31	6	306	LUT	C28-C29-C30	2.26	122.56	119.01
31	4	304	LUT	C18-C5-C4	2.26	118.57	114.42
19	3	5011	CLA	C2C-C1C-NC	2.26	112.35	109.98
19	A	835	CLA	C2D-C1D-ND	2.26	112.36	110.13
19	6	310	CLA	C1-C2-C3	-2.26	122.50	126.20
19	B	829	CLA	C2D-C1D-ND	2.26	112.36	110.13
19	1	5011	CLA	CHD-C1D-ND	-2.26	121.63	124.80
19	8	313	CLA	CAA-CBA-CGA	-2.25	106.81	113.21
19	A	813	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
19	B	804	CLA	CHA-C1A-NA	-2.25	121.29	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	304	BCR	C36-C18-C17	-2.25	119.17	122.82
19	G	1601	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
19	A	819	CLA	C2D-C1D-ND	2.25	112.36	110.13
19	5	306	CLA	C2D-C1D-ND	2.25	112.36	110.13
19	B	802	CLA	CHA-C1A-NA	-2.25	121.29	126.39
19	8	308	CLA	CHA-C1A-NA	-2.25	121.29	126.39
19	A	843	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
19	B	816	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
19	K	205	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
19	7	307	CLA	CHA-C1A-NA	-2.25	121.29	126.39
19	1	5010	CLA	C1-O2A-CGA	2.25	122.10	116.65
31	8	304	LUT	C38-C25-C24	-2.25	118.03	123.36
22	B	847	BCR	C10-C11-C12	-2.25	116.67	123.20
19	A	802	CLA	C2D-C1D-ND	2.25	112.36	110.13
19	7	318	CLA	C1D-ND-C4D	-2.25	104.73	106.31
19	A	857	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
19	B	801	CLA	C2D-C1D-ND	2.25	112.35	110.13
19	3	5010	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
19	Z	308	CLA	C1-O2A-CGA	2.25	122.10	116.65
19	7	319	CLA	C2D-C1D-ND	2.25	112.35	110.13
19	7	308	CLA	C6-C7-C8	-2.25	108.49	115.97
19	B	806	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
19	B	835	CLA	O2A-CGA-CBA	2.25	118.69	111.83
19	A	857	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
19	A	839	CLA	CAA-CBA-CGA	-2.25	106.82	113.21
19	4	310	CLA	CHA-C1A-NA	-2.25	121.30	126.39
19	6	313	CLA	C1D-ND-C4D	-2.25	104.73	106.31
19	B	831	CLA	CHA-C4D-ND	2.25	137.19	132.55
19	K	202	CLA	CHD-C1D-ND	-2.25	121.64	124.80
22	A	859	BCR	C7-C8-C9	-2.25	122.91	126.23
27	5	302	RRX	C27-C26-C25	-2.25	116.14	120.76
32	8	315	CHL	CMA-C3A-C4A	2.25	119.45	114.61
19	A	824	CLA	C2D-C1D-ND	2.25	112.35	110.13
34	8	322	3PH	O21-C21-C22	2.24	119.18	110.93
27	5	302	RRX	C15-C16-C17	-2.24	118.93	123.52
19	6	312	CLA	CHD-C1D-ND	-2.24	121.64	124.80
19	B	821	CLA	C2D-C1D-ND	2.24	112.35	110.13
19	1	5018	CLA	O2D-CGD-O1D	-2.24	119.48	123.85
22	F	302	BCR	C7-C8-C9	-2.24	122.92	126.23
19	3	5009	CLA	CMD-C2D-C3D	-2.24	122.54	127.69
19	3	5008	CLA	CHA-C1A-NA	-2.24	121.31	126.39
19	3	5012	CLA	CAA-C2A-C3A	-2.24	106.94	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	811	CLA	CHD-C1D-ND	-2.24	121.65	124.80
19	1	5006	CLA	CHA-C1A-NA	-2.24	121.32	126.39
19	7	319	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
32	8	316	CHL	CMD-C2D-C3D	2.24	129.16	124.68
19	B	821	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
19	4	309	CLA	CHA-C4D-ND	2.24	137.17	132.55
19	A	828	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
19	6	320	CLA	CAA-CBA-CGA	-2.24	106.85	113.21
27	5	302	RRX	C1-C6-C5	-2.24	119.58	122.64
19	A	807	CLA	C2D-C1D-ND	2.24	112.34	110.13
19	1	5006	CLA	C2D-C1D-ND	2.24	112.34	110.13
19	B	802	CLA	C6-C5-C3	-2.24	108.01	113.47
19	4	318	CLA	CHD-C1D-ND	-2.24	121.65	124.80
19	4	318	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
31	3	5003	LUT	C11-C12-C13	-2.24	120.22	126.36
19	5	310	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
19	A	843	CLA	C2D-C1D-ND	2.24	112.34	110.13
19	B	820	CLA	C2D-C1D-ND	2.24	112.34	110.13
19	A	804	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
19	7	311	CLA	CHD-C1D-ND	-2.24	121.66	124.80
19	8	308	CLA	CHD-C1D-ND	-2.24	121.66	124.80
19	7	307	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
22	A	858	BCR	C10-C11-C12	-2.24	116.72	123.20
38	6	326	ERG	C7-C6-C5	-2.24	118.34	122.95
19	A	806	CLA	O2D-CGD-O1D	-2.24	119.50	123.85
19	7	311	CLA	O2D-CGD-O1D	-2.24	119.50	123.85
19	A	830	CLA	C2D-C1D-ND	2.23	112.34	110.13
19	7	317	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
19	A	836	CLA	CMD-C2D-C3D	-2.23	122.56	127.69
19	I	201	CLA	CMD-C2D-C3D	-2.23	122.56	127.69
32	1	5014	CHL	CMA-C3A-C2A	2.23	122.76	114.13
19	A	830	CLA	CHD-C1D-ND	-2.23	121.66	124.80
19	J	1901	CLA	CHD-C1D-ND	-2.23	121.66	124.80
19	A	825	CLA	CHD-C1D-ND	-2.23	121.66	124.80
19	A	823	CLA	C2D-C1D-ND	2.23	112.34	110.13
31	3	5002	LUT	C31-C30-C29	-2.23	124.15	127.28
19	A	831	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
19	B	812	CLA	C2D-C1D-ND	2.23	112.33	110.13
19	6	309	CLA	CHD-C1D-ND	-2.23	121.66	124.80
19	A	833	CLA	CHD-C1D-ND	-2.23	121.66	124.80
19	A	827	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
19	B	826	CLA	CHD-C1D-ND	-2.23	121.67	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	801	CLA	CHA-C1A-NA	-2.23	121.34	126.39
19	A	824	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
31	5	303	LUT	C18-C5-C6	-2.23	122.05	124.48
19	A	835	CLA	CHD-C1D-ND	-2.23	121.67	124.80
19	F	301	CLA	C1C-C2C-C3C	-2.23	104.64	106.98
31	5	303	LUT	C18-C5-C4	2.23	118.52	114.42
22	5	304	BCR	C11-C12-C13	-2.23	120.25	126.36
19	A	843	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
19	F	303	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
32	1	5017	CHL	CMA-C3A-C2A	2.23	122.73	114.13
19	A	829	CLA	O2A-CGA-CBA	2.23	118.63	111.83
19	A	816	CLA	CHA-C1A-NA	-2.23	121.35	126.39
19	A	809	CLA	CHD-C1D-ND	-2.23	121.67	124.80
19	5	319	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
19	1	5012	CLA	C1-O2A-CGA	2.23	122.04	116.65
19	B	816	CLA	CHD-C1D-ND	-2.23	121.67	124.80
32	Z	302	CHL	C1-O2A-CGA	2.23	122.04	116.65
19	8	318	CLA	O2D-CGD-O1D	-2.23	119.52	123.85
19	B	840	CLA	CHD-C1D-ND	-2.23	121.67	124.80
19	A	828	CLA	C2D-C1D-ND	2.23	112.33	110.13
19	Z	303	CLA	O1D-CGD-CBD	-2.23	120.13	124.52
19	A	807	CLA	CHD-C1D-ND	-2.23	121.67	124.80
19	1	5018	CLA	CHD-C1D-ND	-2.23	121.67	124.80
19	A	857	CLA	C2D-C1D-ND	2.22	112.33	110.13
19	Z	312	CLA	C2D-C1D-ND	2.22	112.33	110.13
19	Z	315	CLA	CHA-C1A-NA	-2.22	121.36	126.39
19	8	308	CLA	C1C-C2C-C3C	-2.22	104.64	106.98
19	B	829	CLA	CHD-C1D-ND	-2.22	121.67	124.80
19	B	807	CLA	C6-C5-C3	-2.22	108.05	113.47
19	A	803	CLA	O1D-CGD-CBD	-2.22	120.13	124.52
19	5	309	CLA	C2D-C1D-ND	2.22	112.33	110.13
31	1	5004	LUT	C11-C12-C13	-2.22	120.27	126.36
32	7	314	CHL	C4C-CHD-C1D	2.22	124.02	116.07
19	Z	304	CLA	O2A-CGA-CBA	2.22	118.61	111.83
19	Z	304	CLA	C1D-ND-C4D	-2.22	104.75	106.31
19	3	5010	CLA	CHA-C1A-NA	-2.22	121.36	126.39
19	B	826	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
19	A	814	CLA	CHA-C1A-NA	-2.22	121.36	126.39
19	B	823	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
19	1	5018	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
19	5	322	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
19	6	310	CLA	C2C-C1C-NC	2.22	112.31	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	7	308	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
19	3	5009	CLA	CHA-C1A-NA	-2.22	121.36	126.39
19	8	318	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
19	5	301	CLA	CHD-C1D-ND	-2.22	121.68	124.80
32	5	318	CHL	CMA-C3A-C4A	2.22	119.39	114.61
19	B	804	CLA	C2D-C1D-ND	2.22	112.32	110.13
19	6	310	CLA	C2D-C1D-ND	2.22	112.32	110.13
22	7	305	BCR	C23-C24-C25	-2.22	121.07	127.00
19	4	308	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
19	K	205	CLA	CHD-C1D-ND	-2.22	121.68	124.80
19	A	835	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
19	B	828	CLA	O2A-CGA-CBA	2.22	118.59	111.83
19	A	840	CLA	CMA-C3A-C4A	2.22	117.73	111.77
19	B	812	CLA	CHA-C1A-NA	-2.21	121.38	126.39
19	A	821	CLA	CMA-C3A-C4A	2.21	117.72	111.77
19	A	806	CLA	C2D-C1D-ND	2.21	112.32	110.13
19	A	837	CLA	C2D-C1D-ND	2.21	112.32	110.13
19	B	833	CLA	C2D-C1D-ND	2.21	112.32	110.13
19	3	5009	CLA	CMA-C3A-C4A	2.21	117.72	111.77
19	K	203	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
19	B	803	CLA	CMD-C2D-C3D	-2.21	122.61	127.69
19	B	822	CLA	O2A-CGA-CBA	2.21	118.58	111.83
19	I	201	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
31	7	303	LUT	C39-C29-C28	2.21	121.47	118.09
19	A	841	CLA	CHA-C1A-NA	-2.21	121.38	126.39
19	Z	315	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
19	Z	305	CLA	C11-C12-C13	-2.21	108.61	115.97
19	7	312	CLA	C2D-C1D-ND	2.21	112.31	110.13
19	8	320	CLA	CHD-C1D-ND	-2.21	121.69	124.80
19	6	320	CLA	CHD-C1D-ND	-2.21	121.69	124.80
19	K	202	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
19	B	827	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
19	6	314	CLA	C2D-C1D-ND	2.21	112.31	110.13
19	A	825	CLA	CHA-C1A-NA	-2.21	121.39	126.39
19	3	5011	CLA	C1-O2A-CGA	2.21	122.00	116.65
19	7	324	CLA	CAA-C2A-C1A	-2.21	104.73	111.97
19	8	311	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
19	4	306	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
31	4	304	LUT	C11-C12-C13	-2.21	120.30	126.36
19	A	820	CLA	CHD-C1D-ND	-2.21	121.69	124.80
19	B	830	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
23	6	303	LHG	C5-O7-C7	-2.21	112.51	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	8	308	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
19	5	301	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
19	B	819	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
19	A	822	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
19	B	824	CLA	CHD-C1D-ND	-2.21	121.69	124.80
19	3	5010	CLA	CHD-C1D-ND	-2.21	121.69	124.80
19	A	823	CLA	CHA-C1A-NA	-2.21	121.39	126.39
19	7	312	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
19	A	818	CLA	CMD-C2D-C3D	-2.21	122.63	127.69
22	A	858	BCR	C29-C30-C25	2.21	113.64	110.44
19	B	814	CLA	C2D-C1D-ND	2.21	112.31	110.13
19	Z	314	CLA	C2D-C1D-ND	2.21	112.31	110.13
19	B	833	CLA	CHA-C1A-NA	-2.21	121.39	126.39
19	6	312	CLA	CAA-C2A-C3A	-2.21	107.04	113.00
19	B	821	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
19	B	830	CLA	CHD-C1D-ND	-2.21	121.70	124.80
19	B	822	CLA	CHA-C1A-NA	-2.21	121.40	126.39
19	K	202	CLA	C2D-C1D-ND	2.21	112.31	110.13
19	6	311	CLA	C2D-C1D-ND	2.21	112.31	110.13
19	5	319	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
19	B	832	CLA	CHD-C1D-ND	-2.21	121.70	124.80
19	7	306	CLA	C2D-C1D-ND	2.20	112.31	110.13
19	A	841	CLA	CHD-C1D-ND	-2.20	121.70	124.80
19	A	857	CLA	CHD-C1D-ND	-2.20	121.70	124.80
31	1	5003	LUT	C38-C25-C24	-2.20	118.14	123.36
19	7	316	CLA	CMD-C2D-C3D	-2.20	122.63	127.69
32	1	5009	CHL	C1C-C2C-CMC	2.20	130.78	126.80
19	A	825	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
19	A	825	CLA	C2D-C1D-ND	2.20	112.31	110.13
19	A	820	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
31	3	5002	LUT	C15-C35-C34	-2.20	119.01	123.52
19	B	803	CLA	OBD-CAD-C3D	-2.20	123.27	128.42
19	A	832	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
19	A	835	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
22	A	848	BCR	C35-C13-C14	-2.20	119.25	122.82
19	A	827	CLA	CHD-C1D-ND	-2.20	121.71	124.80
19	B	807	CLA	CHD-C1D-ND	-2.20	121.71	124.80
19	6	309	CLA	CAA-C2A-C3A	-2.20	107.06	113.00
28	6	304	C7Z	C8-C9-C10	2.20	122.47	119.01
31	7	303	LUT	C18-C5-C4	2.20	118.46	114.42
19	6	302	CLA	CHD-C1D-ND	-2.20	121.71	124.80
32	3	5017	CHL	C1A-CHA-CBD	-2.20	126.73	132.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	844	PQN	C12-C11-C3	-2.20	106.67	112.08
19	7	306	CLA	CHA-C1A-NA	-2.20	121.42	126.39
19	B	805	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
19	7	313	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
19	B	836	CLA	C1-C2-C3	-2.20	122.60	126.20
19	8	314	CLA	C2D-C1D-ND	2.20	112.30	110.13
19	B	835	CLA	CHD-C1D-ND	-2.20	121.71	124.80
19	6	313	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
19	A	808	CLA	CHD-C1D-ND	-2.19	121.71	124.80
19	3	5014	CLA	C1-O2A-CGA	2.19	121.96	116.65
19	B	834	CLA	CMD-C2D-C3D	-2.19	122.66	127.69
19	G	1602	CLA	OBD-CAD-C3D	-2.19	123.29	128.42
19	A	813	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	F	303	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	Z	303	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	G	1601	CLA	O2A-CGA-CBA	2.19	118.52	111.83
19	B	836	CLA	C2D-C1D-ND	2.19	112.30	110.13
19	B	812	CLA	O2A-CGA-CBA	2.19	118.52	111.83
19	G	1602	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	A	839	CLA	C2D-C1D-ND	2.19	112.30	110.13
31	3	5003	LUT	C39-C29-C30	-2.19	119.26	122.82
19	A	816	CLA	O2A-CGA-CBA	2.19	118.52	111.83
19	4	318	CLA	C2D-C1D-ND	2.19	112.30	110.13
22	A	847	BCR	C36-C18-C17	-2.19	119.27	122.82
19	A	818	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	I	201	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	3	5014	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	8	310	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	B	803	CLA	CHA-C1A-NA	-2.19	121.43	126.39
19	1	5016	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
19	5	310	CLA	C2D-C1D-ND	2.19	112.29	110.13
19	7	306	CLA	OBD-CAD-C3D	-2.19	123.30	128.42
19	A	842	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
32	1	5014	CHL	C1-O2A-CGA	2.19	122.89	116.67
22	A	859	BCR	C10-C11-C12	-2.19	116.86	123.20
32	5	316	CHL	C4C-CHD-C1D	2.19	123.90	116.07
19	B	831	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
31	8	304	LUT	C22-C23-C24	2.19	114.43	111.18
19	K	204	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	Z	308	CLA	C6-C5-C3	-2.19	108.14	113.47
31	5	303	LUT	C10-C11-C12	-2.19	116.86	123.20
19	1	5010	CLA	O2A-CGA-CBA	2.19	118.50	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	316	CLA	CHD-C1D-ND	-2.19	121.72	124.80
19	B	850	CLA	C2D-C1D-ND	2.19	112.29	110.13
19	7	310	CLA	C2D-C1D-ND	2.19	112.29	110.13
19	Z	308	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
22	B	842	BCR	C36-C18-C19	2.19	121.43	118.09
19	6	323	CLA	CHA-C1A-NA	-2.19	121.44	126.39
19	A	832	CLA	CHD-C1D-ND	-2.19	121.73	124.80
19	A	802	CLA	OBD-CAD-C3D	-2.19	123.31	128.42
19	A	836	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
19	6	311	CLA	CHD-C1D-ND	-2.19	121.73	124.80
19	A	808	CLA	O2A-CGA-CBA	2.18	118.50	111.83
19	B	809	CLA	CHD-C1D-ND	-2.18	121.73	124.80
19	B	823	CLA	C2D-C1D-ND	2.18	112.29	110.13
19	8	310	CLA	C2D-C1D-ND	2.18	112.29	110.13
19	5	309	CLA	CHD-C1D-ND	-2.18	121.73	124.80
24	3	5023	LMT	O1B-C4'-C3'	2.18	112.78	107.23
19	Z	308	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
19	B	813	CLA	CHA-C1A-NA	-2.18	121.45	126.39
19	B	839	CLA	CHA-C1A-NA	-2.18	121.45	126.39
19	B	824	CLA	C2D-C1D-ND	2.18	112.28	110.13
19	B	831	CLA	C2D-C1D-ND	2.18	112.28	110.13
19	B	819	CLA	O2A-CGA-CBA	2.18	118.48	111.83
19	B	809	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
19	B	810	CLA	CHD-C1D-ND	-2.18	121.73	124.80
19	K	203	CLA	CHD-C1D-ND	-2.18	121.74	124.80
19	5	319	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
19	A	809	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
32	Z	302	CHL	C4C-CHD-C1D	2.18	123.86	116.07
19	G	1601	CLA	CHA-C1A-NA	-2.18	121.46	126.39
19	B	838	CLA	C2D-C1D-ND	2.18	112.28	110.13
19	A	825	CLA	O2A-CGA-CBA	2.18	118.48	111.83
19	6	301	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
19	3	5011	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
19	B	832	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
19	5	321	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
19	7	311	CLA	CAA-CBA-CGA	-2.18	107.03	113.21
19	B	818	CLA	O2A-CGA-CBA	2.18	118.47	111.83
31	8	305	LUT	C19-C9-C8	2.18	121.41	118.09
19	3	5008	CLA	C2D-C1D-ND	2.18	112.28	110.13
19	A	819	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
19	8	307	CLA	CHA-C1A-NA	-2.18	121.46	126.39
19	B	806	CLA	O1D-CGD-CBD	-2.18	120.23	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	5020	CLA	CHD-C1D-ND	-2.18	121.74	124.80
19	7	316	CLA	C2D-C1D-ND	2.18	112.28	110.13
19	Z	307	CLA	CHA-C1A-NA	-2.18	121.47	126.39
19	8	314	CLA	CHA-C1A-NA	-2.18	121.47	126.39
19	A	813	CLA	C2D-C1D-ND	2.17	112.28	110.13
19	1	5012	CLA	CHD-C1D-ND	-2.17	121.74	124.80
32	7	314	CHL	CMD-C2D-C3D	2.17	129.03	124.68
19	A	810	CLA	CHA-C1A-NA	-2.17	121.47	126.39
19	B	810	CLA	C1-O2A-CGA	2.17	121.91	116.65
19	A	802	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
19	8	314	CLA	C3D-C2D-C1D	-2.17	102.86	105.83
19	B	829	CLA	CHA-C1A-NA	-2.17	121.47	126.39
31	8	305	LUT	C12-C13-C14	-2.17	115.59	119.01
32	Z	310	CHL	C1-C2-C3	-2.17	122.64	126.20
19	B	808	CLA	CHD-C1D-ND	-2.17	121.75	124.80
19	B	816	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
19	A	823	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
19	B	812	CLA	CHD-C1D-ND	-2.17	121.75	124.80
19	6	322	CLA	C2D-C1D-ND	2.17	112.27	110.13
19	A	816	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
19	B	820	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
22	6	308	BCR	C34-C9-C8	2.17	121.40	118.09
19	B	837	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
19	Z	307	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
19	A	814	CLA	C2D-C1D-ND	2.17	112.27	110.13
19	A	820	CLA	CHA-C1A-NA	-2.17	121.48	126.39
19	A	821	CLA	CHA-C1A-NA	-2.17	121.48	126.39
32	1	5014	CHL	C4D-CHA-CBD	-2.17	106.78	108.97
19	J	1901	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
32	1	5009	CHL	CMD-C2D-C3D	2.17	129.01	124.68
23	4	320	LHG	O7-C7-O9	-2.17	118.64	123.70
19	B	815	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
19	B	810	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
19	4	308	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
19	1	5012	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
19	6	322	CLA	C2C-C1C-NC	2.17	112.26	109.98
22	A	859	BCR	C23-C24-C25	-2.17	121.21	127.00
22	A	848	BCR	C20-C19-C18	-2.17	120.42	126.36
32	7	315	CHL	C3D-C4D-ND	-2.17	109.46	112.94
19	F	301	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
19	4	306	CLA	C2D-C1D-ND	2.17	112.27	110.13
19	5	310	CLA	C2C-C1C-NC	2.17	112.26	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J	1901	CLA	CHA-C1A-NA	-2.16	121.49	126.39
19	B	818	CLA	C2D-C1D-ND	2.16	112.27	110.13
19	3	5020	CLA	C2D-C1D-ND	2.16	112.27	110.13
19	1	5007	CLA	C2D-C1D-ND	2.16	112.27	110.13
19	5	313	CLA	C2D-C1D-ND	2.16	112.27	110.13
19	3	5019	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
19	B	839	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
19	A	824	CLA	CHD-C1D-ND	-2.16	121.76	124.80
19	B	815	CLA	CHD-C1D-ND	-2.16	121.76	124.80
19	A	804	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
22	B	842	BCR	C7-C8-C9	-2.16	123.04	126.23
22	5	304	BCR	C4-C5-C6	-2.16	119.78	122.70
32	Z	310	CHL	CMA-C3A-C2A	2.16	122.48	114.13
32	Z	302	CHL	CMD-C2D-C3D	2.16	129.00	124.68
19	B	826	CLA	CHA-C1A-NA	-2.16	121.50	126.39
19	A	843	CLA	CHD-C1D-ND	-2.16	121.76	124.80
22	B	847	BCR	C30-C25-C24	2.16	121.51	115.65
22	7	305	BCR	C30-C25-C24	2.16	121.51	115.65
19	K	204	CLA	C2D-C1D-ND	2.16	112.26	110.13
19	4	306	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
19	B	837	CLA	CHA-C1A-NA	-2.16	121.50	126.39
31	7	304	LUT	C39-C29-C30	-2.16	119.32	122.82
19	5	312	CLA	CHD-C1D-ND	-2.16	121.77	124.80
18	A	801	CL0	C4D-ND-C1D	-2.16	103.58	105.22
19	6	320	CLA	CAA-C2A-C1A	-2.16	104.90	111.97
19	8	309	CLA	CHD-C1D-ND	-2.16	121.77	124.80
19	A	831	CLA	CHA-C1A-NA	-2.16	121.50	126.39
19	1	5013	CLA	C2D-C1D-ND	2.16	112.26	110.13
19	Z	306	CLA	C2D-C1D-ND	2.16	112.26	110.13
19	B	802	CLA	CAA-C2A-C3A	-2.16	107.17	113.00
19	I	201	CLA	O1D-CGD-CBD	-2.16	120.27	124.52
32	8	317	CHL	CMD-C2D-C3D	2.16	128.99	124.68
19	A	842	CLA	CHD-C1D-ND	-2.16	121.77	124.80
19	5	325	CLA	CHA-C1A-NA	-2.16	121.51	126.39
19	A	821	CLA	CAA-C2A-C3A	-2.16	107.17	113.00
19	8	312	CLA	C6-C7-C8	-2.15	108.80	115.97
19	A	808	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
19	Z	303	CLA	C2D-C1D-ND	2.15	112.26	110.13
19	5	313	CLA	CHA-C1A-NA	-2.15	121.51	126.39
19	B	835	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
19	K	205	CLA	CHA-C1A-NA	-2.15	121.51	126.39
19	6	302	CLA	CMD-C2D-C3D	-2.15	122.75	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	307	CLA	C2D-C1D-ND	2.15	112.26	110.13
19	3	5020	CLA	CAA-CBA-CGA	-2.15	107.09	113.21
19	3	5012	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
19	8	310	CLA	C1D-ND-C4D	-2.15	104.80	106.31
19	6	322	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
22	5	304	BCR	C38-C26-C27	2.15	118.18	113.60
19	5	308	CLA	C2C-C1C-NC	2.15	112.24	109.98
19	3	5009	CLA	C2D-C1D-ND	2.15	112.25	110.13
19	B	827	CLA	CHA-C1A-NA	-2.15	121.52	126.39
31	Z	317	LUT	C15-C14-C13	-2.15	124.26	127.28
19	5	306	CLA	C6-C5-C3	-2.15	108.23	113.47
19	8	320	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
19	7	313	CLA	CHA-C1A-NA	-2.15	121.52	126.39
31	3	5003	LUT	C22-C23-C24	2.15	114.38	111.18
19	5	325	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
19	Z	307	CLA	CHD-C1D-ND	-2.15	121.78	124.80
19	1	5013	CLA	C2C-C1C-NC	2.15	112.24	109.98
27	4	303	RRX	C30-C25-C26	-2.15	119.70	122.64
19	A	837	CLA	CHA-C1A-NA	-2.15	121.52	126.39
19	B	804	CLA	CHD-C1D-ND	-2.15	121.78	124.80
19	1	5012	CLA	CHA-C1A-NA	-2.15	121.53	126.39
19	Z	312	CLA	CHD-C1D-ND	-2.15	121.78	124.80
19	A	806	CLA	C6-C5-C3	-2.15	108.23	113.47
27	F	304	RRX	C34-C9-C10	-2.15	119.34	122.82
19	1	5006	CLA	CAA-CBA-CGA	-2.15	107.11	113.21
19	7	306	CLA	C2C-C1C-NC	2.15	112.24	109.98
19	B	813	CLA	C2D-C1D-ND	2.15	112.25	110.13
19	B	810	CLA	CHA-C1A-NA	-2.15	121.53	126.39
32	5	315	CHL	CMD-C2D-C3D	2.15	128.97	124.68
24	F	305	LMT	O5B-C5B-C6B	2.15	111.76	106.44
19	7	318	CLA	CHD-C1D-ND	-2.15	121.78	124.80
22	7	305	BCR	C37-C22-C21	-2.15	119.34	122.82
19	A	806	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
19	B	832	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
32	Z	309	CHL	C4C-CHD-C1D	2.15	123.75	116.07
19	A	809	CLA	CHA-C1A-NA	-2.15	121.53	126.39
22	5	305	BCR	C24-C23-C22	-2.15	123.06	126.23
31	6	306	LUT	C8-C7-C6	-2.15	121.27	127.00
19	B	802	CLA	CHD-C1D-ND	-2.14	121.78	124.80
19	B	828	CLA	CHD-C1D-ND	-2.14	121.78	124.80
19	3	5013	CLA	C1-O2A-CGA	2.14	121.84	116.65
19	B	840	CLA	CMA-C3A-C4A	2.14	117.54	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	6	302	CLA	CHA-C1A-NA	-2.14	121.53	126.39
19	B	827	CLA	CHD-C1D-ND	-2.14	121.78	124.80
19	8	318	CLA	O2A-CGA-CBA	2.14	120.24	112.14
19	Z	305	CLA	C2D-C1D-ND	2.14	112.25	110.13
38	8	325	ERG	C19-C10-C9	-2.14	107.42	110.98
19	A	802	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
31	3	5002	LUT	C11-C12-C13	-2.14	120.49	126.36
19	A	803	CLA	CHA-C1A-NA	-2.14	121.54	126.39
19	Z	308	CLA	O2A-CGA-CBA	2.14	118.37	111.83
31	1	5004	LUT	C27-C28-C29	-2.14	121.72	126.32
31	6	305	LUT	C4-C5-C6	-2.14	116.36	120.76
18	A	801	CL0	C4C-C3C-C2C	-2.14	104.91	113.37
19	B	833	CLA	O2A-CGA-CBA	2.14	118.36	111.83
19	6	301	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
19	B	838	CLA	O2A-CGA-CBA	2.14	118.36	111.83
19	A	816	CLA	C6-C5-C3	-2.14	108.26	113.47
19	F	301	CLA	CHA-C1A-NA	-2.14	121.55	126.39
22	K	206	BCR	C2-C1-C6	2.14	113.55	110.44
19	A	837	CLA	O2A-CGA-CBA	2.14	118.35	111.83
22	B	843	BCR	C34-C9-C10	-2.14	119.35	122.82
19	A	840	CLA	CHD-C1D-ND	-2.14	121.80	124.80
19	B	828	CLA	CMD-C2D-C3D	-2.14	122.79	127.69
19	B	840	CLA	C2D-C1D-ND	2.14	112.24	110.13
19	A	822	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
19	A	823	CLA	O2A-CGA-CBA	2.14	118.35	111.83
19	4	316	CLA	CAA-CBA-CGA	-2.14	107.14	113.21
19	5	325	CLA	CHD-C1D-ND	-2.14	121.80	124.80
22	K	206	BCR	C16-C15-C14	-2.14	119.15	123.52
22	5	304	BCR	C11-C10-C9	-2.13	124.28	127.28
19	7	310	CLA	CAA-C2A-C3A	-2.13	107.23	113.00
19	B	824	CLA	CHA-C1A-NA	-2.13	121.56	126.39
37	8	302	SQD	O3-C3-C2	-2.13	105.34	110.38
19	4	308	CLA	C6-C5-C3	-2.13	108.27	113.47
31	1	5004	LUT	C37-C21-C26	-2.13	106.31	109.55
32	8	315	CHL	C4C-CHD-C1D	2.13	123.70	116.07
19	K	202	CLA	CAA-C2A-C3A	-2.13	107.23	113.00
19	Z	307	CLA	C6-C5-C3	-2.13	108.27	113.47
19	8	313	CLA	CHD-C1D-ND	-2.13	121.80	124.80
19	A	826	CLA	CHD-C1D-ND	-2.13	121.80	124.80
19	A	833	CLA	O2A-CGA-CBA	2.13	118.34	111.83
19	5	309	CLA	CHA-C1A-NA	-2.13	121.56	126.39
19	K	203	CLA	O2A-CGA-CBA	2.13	118.33	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	7	318	CLA	C2D-C1D-ND	2.13	112.23	110.13
19	B	825	CLA	C1-C2-C3	-2.13	122.71	126.20
19	Z	312	CLA	O2A-CGA-CBA	2.13	118.33	111.83
32	1	5009	CHL	C4C-CHD-C1D	2.13	123.69	116.07
22	B	842	BCR	C35-C13-C14	-2.13	119.36	122.82
19	B	826	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
19	B	834	CLA	CHA-C1A-NA	-2.13	121.57	126.39
22	B	843	BCR	C21-C20-C19	-2.13	117.03	123.20
19	A	829	CLA	CHA-C1A-NA	-2.13	121.57	126.39
19	B	821	CLA	CHA-C1A-NA	-2.13	121.57	126.39
19	B	835	CLA	C2D-C1D-ND	2.13	112.23	110.13
19	G	1601	CLA	CHD-C1D-ND	-2.13	121.81	124.80
19	A	826	CLA	CHA-C1A-NA	-2.13	121.57	126.39
19	B	836	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
19	Z	304	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
19	B	850	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
19	K	203	CLA	C2D-C1D-ND	2.13	112.23	110.13
19	Z	307	CLA	C1D-ND-C4D	-2.13	104.82	106.31
19	B	850	CLA	CHD-C1D-ND	-2.13	121.81	124.80
32	8	319	CHL	C3D-C4D-ND	-2.13	109.53	112.94
19	B	814	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
19	7	307	CLA	C3B-C4B-NB	-2.13	108.63	110.53
22	A	850	BCR	C30-C25-C24	2.13	121.42	115.65
27	4	303	RRX	C12-C13-C14	-2.13	115.66	119.01
19	4	309	CLA	C2D-C1D-ND	2.13	112.23	110.13
19	B	809	CLA	CHA-C1A-NA	-2.13	121.58	126.39
19	1	5011	CLA	O1D-CGD-CBD	-2.13	120.33	124.52
19	B	809	CLA	C2D-C1D-ND	2.12	112.23	110.13
19	4	316	CLA	CHA-C1A-NA	-2.12	121.58	126.39
22	B	843	BCR	C20-C21-C22	-2.12	124.30	127.28
19	A	833	CLA	CHA-C1A-NA	-2.12	121.58	126.39
27	F	304	RRX	C27-C26-C25	-2.12	116.39	120.76
19	5	312	CLA	CHA-C1A-NA	-2.12	121.58	126.39
19	7	317	CLA	O2A-CGA-CBA	2.12	118.31	111.83
19	6	314	CLA	CHA-C1A-NA	-2.12	121.58	126.39
19	B	840	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
19	Z	311	CLA	CHD-C1D-ND	-2.12	121.82	124.80
19	B	831	CLA	O2A-CGA-CBA	2.12	118.30	111.83
32	4	314	CHL	C4C-CHD-C1D	2.12	123.66	116.07
31	7	304	LUT	C28-C29-C30	2.12	122.34	119.01
31	8	305	LUT	O23-C23-C24	-2.12	106.06	110.39
19	4	313	CLA	C2D-C1D-ND	2.12	112.22	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	820	CLA	CHD-C1D-ND	-2.12	121.82	124.80
19	B	835	CLA	C6-C5-C3	-2.12	108.30	113.47
22	3	5007	BCR	C3-C4-C5	-2.12	110.27	114.06
19	A	815	CLA	CHA-C1A-NA	-2.12	121.59	126.39
19	8	310	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
19	4	306	CLA	CHA-C1A-NA	-2.12	121.59	126.39
32	8	319	CHL	CMD-C2D-C3D	2.12	128.92	124.68
19	K	205	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
19	A	834	CLA	C2D-C1D-ND	2.12	112.22	110.13
19	7	309	CLA	C2D-C1D-ND	2.12	112.22	110.13
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	B	814	CLA	CHA-C1A-NA	-2.12	121.59	126.39
19	B	840	CLA	CHA-C1A-NA	-2.12	121.59	126.39
19	5	325	CLA	C2D-C1D-ND	2.12	112.22	110.13
19	B	850	CLA	CAA-C2A-C3A	-2.12	107.28	113.00
19	7	309	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
19	8	309	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
19	A	812	CLA	C2D-C1D-ND	2.12	112.22	110.13
19	B	803	CLA	C2D-C1D-ND	2.12	112.22	110.13
19	A	811	CLA	CHA-C1A-NA	-2.12	121.60	126.39
19	7	310	CLA	CAA-CBA-CGA	-2.12	107.20	113.21
19	3	5016	CLA	O2A-CGA-CBA	2.12	118.29	111.83
19	4	318	CLA	CHA-C1A-NA	-2.12	121.60	126.39
19	A	842	CLA	CHA-C1A-NA	-2.12	121.60	126.39
19	B	805	CLA	CHA-C1A-NA	-2.12	121.60	126.39
22	3	5005	BCR	C33-C5-C4	2.11	118.11	113.60
22	3	5005	BCR	C34-C9-C10	-2.11	119.39	122.82
28	J	1902	C7Z	C1-C6-C7	2.11	121.39	115.65
22	B	846	BCR	C7-C6-C5	-2.11	116.69	121.56
19	A	816	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
19	A	824	CLA	O2D-CGD-O1D	-2.11	119.73	123.85
19	3	5018	CLA	CAA-CBA-CGA	-2.11	107.21	113.21
19	K	205	CLA	C2D-C1D-ND	2.11	112.22	110.13
28	6	304	C7Z	C31-C32-C33	-2.11	120.57	126.36
19	A	826	CLA	CMD-C2D-C3D	-2.11	122.84	127.69
19	5	307	CLA	CAA-CBA-CGA	-2.11	107.21	113.21
19	7	306	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
19	1	5015	CLA	OBD-CAD-C3D	-2.11	123.48	128.42
19	4	309	CLA	CBC-CAC-C3C	-2.11	106.70	112.42
19	3	5011	CLA	CHA-C1A-NA	-2.11	121.61	126.39
32	Z	313	CHL	CMD-C2D-C3D	2.11	128.90	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	6	319	CHL	C4C-CHD-C1D	2.11	123.62	116.07
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
32	5	318	CHL	CMD-C2D-C3D	2.11	128.90	124.68
31	Z	318	LUT	C11-C12-C13	-2.11	120.58	126.36
19	B	822	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
19	1	5008	CLA	C1D-ND-C4D	-2.11	104.83	106.31
31	Z	317	LUT	C8-C9-C10	2.11	122.32	119.01
31	3	5003	LUT	C18-C5-C4	2.11	118.30	114.42
22	3	5007	BCR	C33-C5-C4	2.11	118.09	113.60
19	A	842	CLA	C2D-C1D-ND	2.11	112.21	110.13
19	3	5010	CLA	C2D-C1D-ND	2.11	112.21	110.13
19	5	325	CLA	O2A-CGA-CBA	2.11	118.26	111.83
19	8	320	CLA	CHA-C1A-NA	-2.11	121.62	126.39
19	8	312	CLA	C1C-C2C-C3C	-2.11	104.77	106.98
19	6	313	CLA	O2A-CGA-CBA	2.11	118.26	111.83
19	B	801	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
19	4	307	CLA	CHA-C1A-NA	-2.11	121.62	126.39
22	B	847	BCR	C8-C9-C10	-2.10	115.70	119.01
22	6	308	BCR	C19-C18-C17	-2.10	115.70	119.01
19	Z	308	CLA	CAA-CBA-CGA	-2.10	107.23	113.21
31	3	5003	LUT	C16-C1-C6	-2.10	106.94	110.24
19	1	5007	CLA	CBA-CAA-C2A	-2.10	107.53	113.79
19	A	809	CLA	C6-C5-C3	-2.10	108.34	113.47
19	A	824	CLA	O2A-CGA-CBA	2.10	118.25	111.83
19	Z	314	CLA	CHA-C1A-NA	-2.10	121.63	126.39
33	7	321	SPH	C1-C2-C3	-2.10	108.65	113.00
19	3	5014	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
19	B	819	CLA	C2D-C1D-ND	2.10	112.21	110.13
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	B	830	CLA	CHA-C1A-NA	-2.10	121.63	126.39
22	6	308	BCR	C1-C6-C7	2.10	121.35	115.65
19	6	301	CLA	C6-C5-C3	-2.10	108.35	113.47
19	3	5014	CLA	CMD-C2D-C3D	-2.10	122.87	127.69
19	A	806	CLA	C11-C12-C13	-2.10	108.99	115.97
22	8	306	BCR	C34-C9-C8	2.10	121.30	118.09
22	F	302	BCR	C38-C26-C27	2.10	118.07	113.60
22	B	843	BCR	C7-C6-C5	-2.10	116.72	121.56
19	1	5016	CLA	CHA-C1A-NA	-2.10	121.64	126.39
32	4	315	CHL	CMD-C2D-C3D	2.10	128.88	124.68
19	A	816	CLA	CHD-C1D-ND	-2.10	121.85	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
24	F	305	LMT	C1B-O5B-C5B	-2.10	109.62	113.72
19	5	314	CLA	C2D-C1D-ND	2.10	112.20	110.13
19	5	306	CLA	CHA-C1A-NA	-2.10	121.64	126.39
31	4	304	LUT	C39-C29-C28	2.10	121.29	118.09
19	A	833	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
19	F	301	CLA	CAA-C2A-C3A	-2.10	107.34	113.00
19	A	821	CLA	C2D-C1D-ND	2.10	112.20	110.13
19	A	804	CLA	O1D-CGD-CBD	-2.10	120.39	124.52
19	A	804	CLA	CHA-C1A-NA	-2.10	121.65	126.39
19	5	319	CLA	CHA-C1A-NA	-2.10	121.65	126.39
19	A	810	CLA	CHD-C1D-ND	-2.10	121.85	124.80
19	3	5016	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
22	8	306	BCR	C16-C15-C14	-2.09	119.23	123.52
19	B	835	CLA	CHA-C1A-NA	-2.09	121.65	126.39
19	A	807	CLA	O2A-CGA-CBA	2.09	118.22	111.83
19	4	316	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
19	5	322	CLA	CHA-C1A-NA	-2.09	121.65	126.39
19	6	318	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
19	A	834	CLA	CHA-C1A-NA	-2.09	121.65	126.39
19	A	827	CLA	CHA-C1A-NA	-2.09	121.65	126.39
19	A	820	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
19	1	5006	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
19	6	318	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
19	6	311	CLA	C7-C6-C5	-2.09	107.69	113.26
19	B	827	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
19	8	311	CLA	C1-O2A-CGA	2.09	121.71	116.65
31	7	303	LUT	C8-C9-C10	-2.09	115.72	119.01
19	B	828	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
19	B	825	CLA	CHD-C1D-ND	-2.09	121.86	124.80
22	7	305	BCR	C29-C30-C25	2.09	113.47	110.44
32	1	5017	CHL	CMD-C2D-C3D	2.09	128.85	124.68
22	8	303	BCR	C34-C9-C10	-2.09	119.44	122.82
19	A	807	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
19	7	318	CLA	CMC-C2C-C1C	2.09	128.29	125.03
19	A	843	CLA	CHA-C1A-NA	-2.09	121.67	126.39
19	A	839	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
19	1	5015	CLA	CHA-C1A-NA	-2.09	121.67	126.39
19	1	5013	CLA	CMA-C3A-C4A	2.09	117.38	111.77
32	6	319	CHL	CMD-C2D-C3D	2.09	128.85	124.68
22	8	303	BCR	C15-C14-C13	-2.09	124.35	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	315	CLA	CMD-C2D-C3D	-2.09	122.91	127.69
27	5	302	RRX	C11-C10-C9	-2.08	124.35	127.28
19	5	301	CLA	CHA-C1A-NA	-2.08	121.67	126.39
32	6	321	CHL	CMA-C3A-C4A	2.08	119.10	114.61
19	A	836	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
19	K	202	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
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	B	819	CLA	CHA-C1A-NA	-2.08	121.67	126.39
19	G	1602	CLA	CHA-C1A-NA	-2.08	121.67	126.39
19	Z	304	CLA	C1-O2A-CGA	2.08	121.69	116.65
19	5	301	CLA	C6-C5-C3	-2.08	108.39	113.47
19	A	857	CLA	CHA-C1A-NA	-2.08	121.67	126.39
19	K	202	CLA	CHA-C1A-NA	-2.08	121.67	126.39
19	B	805	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
19	B	832	CLA	CAA-CBA-CGA	-2.08	107.29	113.21
19	7	312	CLA	CHD-C1D-ND	-2.08	121.87	124.80
19	A	826	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
32	4	315	CHL	C4C-CHD-C1D	2.08	123.52	116.07
19	A	827	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
29	7	301	LMG	O7-C10-O9	-2.08	118.84	123.70
32	8	315	CHL	C4D-CHA-CBD	-2.08	106.87	108.97
19	A	810	CLA	C2D-C1D-ND	2.08	112.19	110.13
19	3	5014	CLA	CHA-C1A-NA	-2.08	121.68	126.39
32	6	317	CHL	C4C-CHD-C1D	2.08	123.52	116.07
19	G	1601	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
19	A	841	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
19	B	827	CLA	C1-O2A-CGA	2.08	121.69	116.65
19	6	311	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
32	4	319	CHL	CMD-C2D-C3D	2.08	128.84	124.68
19	6	312	CLA	C16-C15-C13	-2.08	109.05	115.97
19	1	5015	CLA	CHD-C1D-ND	-2.08	121.88	124.80
19	B	837	CLA	O2A-CGA-CBA	2.08	118.17	111.83
19	K	204	CLA	CHA-C1A-NA	-2.08	121.68	126.39
19	3	5019	CLA	CHA-C1A-NA	-2.08	121.68	126.39
19	Z	311	CLA	C2D-C1D-ND	2.08	112.18	110.13
19	3	5019	CLA	CMA-C3A-C4A	2.08	117.36	111.77
19	8	309	CLA	C11-C10-C8	-2.08	109.06	115.97
19	6	318	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
22	B	844	BCR	C23-C22-C21	2.08	122.28	119.01
19	A	829	CLA	O2D-CGD-O1D	-2.08	119.80	123.85
19	B	820	CLA	CHA-C1A-NA	-2.08	121.69	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	304	BCR	C2-C1-C6	2.08	113.46	110.44
19	A	836	CLA	O2A-CGA-CBA	2.08	118.17	111.83
19	3	5015	CLA	CHD-C1D-ND	-2.08	121.88	124.80
19	1	5011	CLA	CHA-C1A-NA	-2.08	121.69	126.39
19	6	301	CLA	CHD-C1D-ND	-2.08	121.88	124.80
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	A	840	CLA	CHA-C1A-NA	-2.08	121.69	126.39
32	6	317	CHL	CMD-C2D-C3D	2.07	128.83	124.68
19	A	829	CLA	CHD-C1D-ND	-2.07	121.88	124.80
19	7	310	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
32	3	5017	CHL	C3D-C4D-ND	-2.07	109.61	112.94
19	A	842	CLA	C6-C5-C3	-2.07	108.42	113.47
19	B	817	CLA	CHA-C1A-NA	-2.07	121.69	126.39
32	6	321	CHL	CMD-C2D-C3D	2.07	128.83	124.68
19	A	824	CLA	CHA-C1A-NA	-2.07	121.70	126.39
19	5	321	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
19	3	5016	CLA	CHA-C1A-NA	-2.07	121.70	126.39
19	A	827	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
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	I	201	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
19	7	316	CLA	CHA-C1A-NA	-2.07	121.70	126.39
32	5	320	CHL	CMA-C3A-C2A	2.07	122.12	114.13
19	B	807	CLA	C2D-C1D-ND	2.07	112.17	110.13
31	5	303	LUT	C1-C6-C5	-2.07	119.81	122.64
19	A	843	CLA	O2A-CGA-CBA	2.07	118.14	111.83
19	B	834	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
19	B	830	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
23	A	852	LHG	O7-C7-O9	-2.07	118.87	123.70
19	B	802	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
19	6	302	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
19	1	5018	CLA	CHA-C1A-NA	-2.07	121.71	126.39
19	A	839	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
19	4	310	CLA	C6-C7-C8	-2.07	109.09	115.97
32	5	316	CHL	C4D-CHA-CBD	-2.07	106.88	108.97
32	4	317	CHL	CMD-C2D-C3D	2.07	128.81	124.68
32	Z	309	CHL	CMD-C2D-C3D	2.07	128.81	124.68
22	8	303	BCR	C29-C30-C25	2.07	113.44	110.44
28	1	5005	C7Z	C24-C25-C26	-2.07	116.51	120.76
19	8	311	CLA	CHA-C1A-NA	-2.07	121.71	126.39
19	G	1602	CLA	C3D-C2D-C1D	-2.07	103.01	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	5	317	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
32	8	317	CHL	CMA-C3A-C4A	2.07	119.06	114.61
19	A	822	CLA	CAA-CBA-CGA	-2.06	107.35	113.21
19	B	803	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
19	B	816	CLA	CHA-C1A-NA	-2.06	121.72	126.39
19	7	319	CLA	CHA-C1A-NA	-2.06	121.72	126.39
22	G	1603	BCR	C29-C30-C25	2.06	113.44	110.44
19	3	5015	CLA	CAA-CBA-CGA	-2.06	106.99	112.49
19	B	839	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
32	1	5014	CHL	CMD-C2D-C3D	2.06	128.81	124.68
31	7	304	LUT	C20-C13-C12	2.06	121.24	118.09
31	4	304	LUT	C15-C35-C34	-2.06	119.30	123.52
32	Z	302	CHL	C1C-C2C-CMC	2.06	130.52	126.80
22	3	5006	BCR	C30-C25-C24	2.06	121.24	115.65
19	7	317	CLA	CMD-C2D-C3D	-2.06	122.96	127.69
19	A	839	CLA	CHA-C1A-NA	-2.06	121.72	126.39
32	8	301	CHL	CMD-C2D-C3D	2.06	128.80	124.68
22	A	850	BCR	C8-C7-C6	-2.06	121.49	127.00
19	1	5007	CLA	CHD-C1D-ND	-2.06	121.90	124.80
19	5	310	CLA	CAA-CBA-CGA	-2.06	107.36	113.21
19	B	807	CLA	CHA-C1A-NA	-2.06	121.72	126.39
19	6	320	CLA	CHA-C1A-NA	-2.06	121.72	126.39
19	A	827	CLA	C1-O2A-CGA	2.06	121.64	116.65
32	1	5014	CHL	C4C-CHD-C1D	2.06	123.44	116.07
19	1	5013	CLA	CHA-C1A-NA	-2.06	121.72	126.39
19	4	312	CLA	CHA-C1A-NA	-2.06	121.73	126.39
19	1	5006	CLA	C6-C5-C3	-2.06	108.45	113.47
19	A	813	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
19	A	815	CLA	C16-C15-C13	-2.06	109.12	115.97
19	3	5012	CLA	CMC-C2C-C1C	2.06	128.25	125.03
19	A	821	CLA	O2A-CGA-CBA	2.06	118.11	111.83
23	6	303	LHG	O8-C23-O10	-2.06	118.48	123.63
19	5	307	CLA	CHA-C1A-NA	-2.06	121.73	126.39
19	5	310	CLA	C1-C2-C3	-2.06	122.82	126.20
19	B	811	CLA	CHA-C1A-NA	-2.06	121.73	126.39
19	A	835	CLA	CHA-C1A-NA	-2.06	121.73	126.39
19	5	306	CLA	C6-C7-C8	-2.06	109.12	115.97
22	B	844	BCR	C10-C11-C12	-2.06	117.24	123.20
19	4	312	CLA	CHD-C1D-ND	-2.06	121.91	124.80
32	5	320	CHL	CMD-C2D-C3D	2.06	128.79	124.68
22	3	5004	BCR	C36-C18-C19	2.06	121.23	118.09
19	B	815	CLA	O1D-CGD-CBD	-2.06	120.46	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	6	326	ERG	C20-C22-C23	-2.06	119.59	125.81
19	B	815	CLA	CHA-C1A-NA	-2.06	121.74	126.39
19	3	5020	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
31	Z	317	LUT	C19-C9-C10	-2.06	119.49	122.82
19	3	5012	CLA	C2C-C1C-NC	2.05	112.14	109.98
28	6	304	C7Z	C8-C7-C6	-2.05	121.51	127.00
19	A	832	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
19	A	807	CLA	CHA-C1A-NA	-2.05	121.74	126.39
19	B	816	CLA	C1-O2A-CGA	2.05	121.62	116.65
19	7	309	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
32	8	316	CHL	CMA-C3A-C4A	2.05	119.03	114.61
19	8	307	CLA	C2D-C1D-ND	2.05	112.16	110.13
19	3	5009	CLA	O2A-CGA-CBA	2.05	119.89	112.14
19	B	823	CLA	CHA-C1A-NA	-2.05	121.74	126.39
19	B	830	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
19	A	818	CLA	CHA-C1A-NA	-2.05	121.74	126.39
19	4	310	CLA	CHD-C1D-ND	-2.05	121.92	124.80
19	B	822	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
19	1	5015	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
19	3	5011	CLA	CMC-C2C-C1C	2.05	128.24	125.03
19	3	5011	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
31	7	304	LUT	C40-C33-C34	-2.05	119.49	122.82
22	A	858	BCR	C15-C16-C17	-2.05	119.32	123.52
19	3	5015	CLA	CHA-C1A-NA	-2.05	121.75	126.39
28	6	304	C7Z	C15-C35-C34	-2.05	119.33	123.52
19	8	310	CLA	CMC-C2C-C1C	2.05	128.24	125.03
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	7	324	CLA	C2D-C1D-ND	2.05	112.15	110.13
19	A	819	CLA	CHA-C1A-NA	-2.05	121.75	126.39
19	4	313	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
23	6	303	LHG	O7-C7-O9	-2.05	118.92	123.70
22	K	206	BCR	C36-C18-C19	2.05	121.22	118.09
19	B	850	CLA	CHA-C1A-NA	-2.05	121.75	126.39
19	4	310	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
19	1	5011	CLA	O2A-CGA-CBA	2.05	118.08	111.83
19	6	323	CLA	CMD-C2D-C3D	-2.05	123.00	127.69
31	6	306	LUT	C31-C32-C33	-2.05	120.75	126.36
19	3	5012	CLA	CAA-C2A-C1A	-2.05	105.27	111.97
19	1	5010	CLA	CAA-CBA-CGA	-2.05	107.40	113.21
19	B	831	CLA	C1-O2A-CGA	2.05	121.60	116.65
19	A	830	CLA	CHA-C1A-NA	-2.05	121.76	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	315	CLA	C11-C12-C13	-2.04	109.17	115.97
32	8	315	CHL	CMD-C2D-C3D	2.04	128.77	124.68
19	A	828	CLA	CHA-C1A-NA	-2.04	121.76	126.39
19	Z	308	CLA	C2D-C1D-ND	2.04	112.15	110.13
19	1	5008	CLA	CHA-C1A-NA	-2.04	121.76	126.39
22	A	849	BCR	C29-C30-C25	2.04	113.41	110.44
19	5	307	CLA	C6-C7-C8	-2.04	109.17	115.97
19	8	313	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
19	6	309	CLA	C11-C10-C8	-2.04	109.18	115.97
19	A	815	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
32	6	316	CHL	CMD-C2D-C3D	2.04	128.76	124.68
19	5	308	CLA	CHA-C1A-NA	-2.04	121.77	126.39
19	G	1602	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
19	6	310	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	1	5003	LUT	C20-C13-C12	2.04	121.20	118.09
19	6	318	CLA	CBC-CAC-C3C	-2.04	106.89	112.42
19	Z	311	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
19	A	803	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
19	A	815	CLA	C2D-C1D-ND	2.04	112.14	110.13
19	K	202	CLA	CAA-CBA-CGA	-2.04	107.42	113.21
19	4	318	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
22	7	305	BCR	C10-C11-C12	-2.04	117.29	123.20
23	1	5001	LHG	O7-C7-O9	-2.04	118.94	123.70
22	A	846	BCR	C15-C16-C17	-2.04	119.35	123.52
19	B	818	CLA	CHA-C1A-NA	-2.04	121.78	126.39
19	5	309	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
19	5	314	CLA	CHD-C1D-ND	-2.04	121.94	124.80
22	A	858	BCR	C20-C19-C18	-2.04	120.78	126.36
19	3	5010	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
19	B	802	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
19	A	819	CLA	C16-C15-C13	-2.04	109.20	115.97
19	A	828	CLA	O2A-CGA-CBA	2.04	118.04	111.83
19	B	833	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
19	4	310	CLA	C11-C10-C8	-2.04	109.20	115.97
19	Z	306	CLA	CMD-C2D-C3D	-2.04	123.02	127.69
19	4	310	CLA	C1-O2A-CGA	2.04	121.58	116.65
19	7	324	CLA	CMD-C2D-C3D	-2.03	123.02	127.69
19	3	5009	CLA	CAA-CBA-CGA	-2.03	107.43	113.21
19	A	832	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
19	Z	311	CLA	CBA-CAA-C2A	-2.03	107.74	113.79
32	4	317	CHL	C3D-C4D-ND	-2.03	109.68	112.94
23	6	324	LHG	O7-C7-O9	-2.03	118.95	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	7	315	CHL	CMD-C2D-C3D	2.03	128.75	124.68
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	806	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
19	4	313	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	3	5002	LUT	C40-C33-C32	2.03	121.19	118.09
19	7	307	CLA	CHD-C1D-ND	-2.03	121.94	124.80
19	5	309	CLA	C2C-C1C-NC	2.03	112.11	109.98
19	Z	315	CLA	C2C-C1C-NC	2.03	112.11	109.98
19	Z	312	CLA	CHA-C1A-NA	-2.03	121.80	126.39
28	1	5005	C7Z	C40-C33-C34	-2.03	119.53	122.82
19	B	826	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
28	1	5005	C7Z	C20-C13-C12	2.03	121.18	118.09
19	B	823	CLA	C6-C7-C8	-2.03	109.23	115.97
22	3	5006	BCR	C10-C11-C12	-2.03	117.33	123.20
19	A	843	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
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
22	6	308	BCR	C29-C30-C25	2.02	113.38	110.44
19	1	5015	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
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	K	204	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
19	5	310	CLA	OBD-CAD-C3D	-2.02	123.69	128.42
19	8	313	CLA	CHA-C1A-NA	-2.02	121.81	126.39
19	3	5008	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
19	3	5019	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
19	8	318	CLA	CHA-C1A-NA	-2.02	121.81	126.39
19	5	309	CLA	C6-C7-C8	-2.02	109.24	115.97
22	5	305	BCR	C7-C6-C5	-2.02	116.90	121.56
19	6	318	CLA	CHA-C1A-NA	-2.02	121.81	126.39
19	5	312	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
25	B	848	DGD	O2G-C1B-O1B	-2.02	118.98	123.70
19	B	818	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
19	B	810	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
19	8	308	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
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	5	311	CLA	C2D-C1D-ND	2.02	112.12	110.13
32	5	316	CHL	C1-O2A-CGA	2.02	121.54	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	1	5019	LHG	O4-P-O5	2.02	121.83	112.44
19	A	837	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
19	6	320	CLA	C2D-C1D-ND	2.02	112.12	110.13
22	A	849	BCR	C37-C22-C23	2.01	121.17	118.09
22	A	846	BCR	C21-C20-C19	-2.01	117.36	123.20
19	A	816	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
32	Z	310	CHL	C4D-CHA-CBD	-2.01	106.94	108.97
19	7	312	CLA	O2A-CGA-CBA	2.01	117.98	111.83
19	6	318	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
19	8	312	CLA	C2B-C1B-NB	-2.01	108.24	110.33
19	6	322	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
32	6	321	CHL	C1B-CHB-C4A	2.01	122.62	121.32
32	4	319	CHL	CMA-C3A-C2A	2.01	121.90	114.13
31	5	303	LUT	O23-C23-C24	-2.01	106.28	110.39
19	A	836	CLA	CHA-C1A-NA	-2.01	121.83	126.39
19	B	825	CLA	CHA-C1A-NA	-2.01	121.83	126.39
19	5	317	CLA	CAA-C2A-C1A	-2.01	105.38	111.97
28	J	1902	C7Z	C19-C9-C10	-2.01	119.56	122.82
23	6	324	LHG	C5-O7-C7	-2.01	112.98	117.80
31	8	305	LUT	C8-C7-C6	-2.01	121.62	127.00
19	1	5016	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
19	B	815	CLA	CAA-CBA-CGA	-2.01	107.50	113.21
19	B	804	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
19	4	313	CLA	CHA-C1A-NA	-2.01	121.84	126.39
19	6	310	CLA	CHA-C1A-NA	-2.01	121.84	126.39
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	5	308	CLA	C2D-C1D-ND	2.01	112.12	110.13
32	4	314	CHL	CMD-C2D-C3D	2.01	128.70	124.68
31	5	303	LUT	C28-C29-C30	-2.01	115.85	119.01
22	3	5004	BCR	C28-C27-C26	-2.01	110.47	114.06
19	J	1901	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
19	A	810	CLA	C11-C12-C13	-2.01	109.29	115.97
19	7	313	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
19	5	310	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
19	A	840	CLA	C2D-C1D-ND	2.01	112.11	110.13
19	Z	304	CLA	C2D-C1D-ND	2.01	112.11	110.13
19	B	834	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
19	5	309	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
22	8	306	BCR	C1-C6-C5	-2.01	119.89	122.64
22	6	307	BCR	C4-C5-C6	-2.01	119.99	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	847	BCR	C11-C12-C13	-2.01	120.86	126.36
19	7	309	CLA	O1A-CGA-CBA	-2.01	115.93	123.78
19	Z	308	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
19	Z	303	CLA	CHA-C1A-NA	-2.01	121.85	126.39
24	7	323	LMT	C1B-O1B-C4'	-2.01	113.22	117.98
22	A	858	BCR	C34-C9-C8	2.01	121.15	118.09
31	6	305	LUT	C20-C13-C12	2.01	121.15	118.09
19	A	835	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
19	A	841	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
19	6	313	CLA	CHD-C1D-ND	-2.00	121.98	124.80
31	7	303	LUT	C12-C13-C14	-2.00	115.86	119.01
19	5	307	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
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	I	201	CLA	CHA-C1A-NA	-2.00	121.86	126.39
19	B	815	CLA	O2A-CGA-CBA	2.00	117.94	111.83
27	5	302	RRX	C1-C6-C7	2.00	121.08	115.65
32	4	319	CHL	CMA-C3A-C4A	2.00	118.92	114.61
19	5	321	CLA	CBC-CAC-C3C	-2.00	107.00	112.42
19	B	831	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
22	B	845	BCR	C34-C9-C10	-2.00	119.57	122.82
22	A	847	BCR	C21-C20-C19	-2.00	117.40	123.20
19	1	5018	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
19	A	806	CLA	C11-C10-C8	-2.00	109.32	115.97
19	7	312	CLA	CHA-C1A-NA	-2.00	121.86	126.39

All (273) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	801	CL0	ND
18	A	801	CL0	NA
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

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
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
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

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Mol	Chain	Res	Type	Atom
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	ND
32	1	5009	CHL	NA
32	1	5009	CHL	NC
32	1	5014	CHL	ND
32	1	5014	CHL	NA
32	1	5014	CHL	NC
32	1	5017	CHL	ND
32	1	5017	CHL	NA
32	1	5017	CHL	NC
32	Z	302	CHL	ND
32	Z	302	CHL	NA
32	Z	302	CHL	NC
32	Z	309	CHL	ND
32	Z	309	CHL	NA
32	Z	309	CHL	NC
32	Z	310	CHL	ND
32	Z	310	CHL	NA
32	Z	310	CHL	NC
32	Z	313	CHL	ND
32	Z	313	CHL	NA
32	Z	313	CHL	NC
32	3	5017	CHL	ND
32	3	5017	CHL	NA
32	3	5017	CHL	NC
32	7	314	CHL	ND
32	7	314	CHL	NA
32	7	314	CHL	NC
32	7	315	CHL	ND
32	7	315	CHL	NA
32	7	315	CHL	NC
32	8	301	CHL	ND
32	8	301	CHL	NA
32	8	301	CHL	NC
32	8	315	CHL	ND

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Mol	Chain	Res	Type	Atom
32	8	315	CHL	NA
32	8	315	CHL	NC
32	8	316	CHL	ND
32	8	316	CHL	NA
32	8	316	CHL	NC
32	8	317	CHL	ND
32	8	317	CHL	NA
32	8	317	CHL	NC
32	8	319	CHL	ND
32	8	319	CHL	NA
32	8	319	CHL	NC
32	4	314	CHL	ND
32	4	314	CHL	NA
32	4	314	CHL	NC
32	4	315	CHL	ND
32	4	315	CHL	NA
32	4	315	CHL	NC
32	4	317	CHL	ND
32	4	317	CHL	NA
32	4	317	CHL	NC
32	4	319	CHL	ND
32	4	319	CHL	NA
32	4	319	CHL	NC
32	5	315	CHL	ND
32	5	315	CHL	NA
32	5	315	CHL	NC
32	5	316	CHL	ND
32	5	316	CHL	NA
32	5	316	CHL	NC
32	5	318	CHL	ND
32	5	318	CHL	NA
32	5	318	CHL	NC
32	5	320	CHL	ND
32	5	320	CHL	NA
32	5	320	CHL	NC
32	6	315	CHL	ND
32	6	315	CHL	NA
32	6	315	CHL	NC
32	6	316	CHL	ND
32	6	316	CHL	NA
32	6	316	CHL	NC
32	6	317	CHL	ND

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Mol	Chain	Res	Type	Atom
32	6	317	CHL	NA
32	6	317	CHL	NC
32	6	319	CHL	ND
32	6	319	CHL	NA
32	6	319	CHL	NC
32	6	321	CHL	ND
32	6	321	CHL	NA
32	6	321	CHL	NC

All (3322) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	802	CLA	C2-C1-O2A-CGA
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	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
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	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

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Mol	Chain	Res	Type	Atoms
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	CHA-CBD-CGD-O1D
19	A	834	CLA	CHA-CBD-CGD-O2D
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	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	857	CLA	C2-C1-O2A-CGA
19	B	802	CLA	CBD-CGD-O2D-CED
19	B	803	CLA	C2-C1-O2A-CGA
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

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Mol	Chain	Res	Type	Atoms
19	B	812	CLA	C2-C1-O2A-CGA
19	B	812	CLA	C6-C7-C8-C9
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-O1D
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
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	821	CLA	CHA-CBD-CGD-O2D
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	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	832	CLA	CHA-CBD-CGD-O1D
19	B	832	CLA	CHA-CBD-CGD-O2D
19	B	833	CLA	C2-C1-O2A-CGA
19	B	833	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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	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
19	G	1601	CLA	C3A-C2A-CAA-CBA
19	G	1601	CLA	C2-C1-O2A-CGA
19	G	1602	CLA	CHA-CBD-CGD-O1D
19	G	1602	CLA	CHA-CBD-CGD-O2D
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	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	5011	CLA	C1A-C2A-CAA-CBA
19	1	5011	CLA	C3A-C2A-CAA-CBA
19	1	5013	CLA	C2B-C3B-CAB-CBB
19	1	5013	CLA	C4B-C3B-CAB-CBB
19	1	5016	CLA	C3A-C2A-CAA-CBA
19	1	5016	CLA	CBD-CGD-O2D-CED
19	Z	303	CLA	CHA-CBD-CGD-O1D
19	Z	303	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	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
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	C2B-C3B-CAB-CBB
19	3	5014	CLA	C4B-C3B-CAB-CBB
19	3	5016	CLA	C1A-C2A-CAA-CBA
19	3	5016	CLA	C2-C1-O2A-CGA
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

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Mol	Chain	Res	Type	Atoms
19	8	313	CLA	C3A-C2A-CAA-CBA
19	8	314	CLA	C1A-C2A-CAA-CBA
19	8	314	CLA	C2B-C3B-CAB-CBB
19	8	314	CLA	C4B-C3B-CAB-CBB
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	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	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	C11-C10-C8-C9
19	5	309	CLA	C3A-C2A-CAA-CBA
19	5	310	CLA	C1A-C2A-CAA-CBA
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	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

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Mol	Chain	Res	Type	Atoms
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
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
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	C21-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	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	858	BCR	C7-C8-C9-C10
22	A	858	BCR	C7-C8-C9-C34
22	A	858	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	A	858	BCR	C17-C18-C19-C20
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	C21-C22-C23-C24
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	847	BCR	C1-C6-C7-C8
22	B	847	BCR	C7-C8-C9-C10
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	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
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	C23-C24-C25-C26
22	3	5004	BCR	C21-C22-C23-C24
22	3	5004	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
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	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	C11-C12-C13-C14
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	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	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
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

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Mol	Chain	Res	Type	Atoms
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	C3-O3-P-O6
23	A	852	LHG	C4-O6-P-O3
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	C3-O3-P-O6
23	1	5001	LHG	C4-O6-P-O3
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	1	5019	LHG	C3-O3-P-O6
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	C3-O3-P-O6
23	3	5021	LHG	O9-C7-O7-C5
23	7	320	LHG	C3-O3-P-O4
23	7	320	LHG	C3-O3-P-O6
23	8	321	LHG	O1-C1-C2-C3
23	8	321	LHG	C3-O3-P-O5
23	4	320	LHG	C3-O3-P-O6
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	C3-O3-P-O6
23	5	323	LHG	C4-O6-P-O3
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
23	6	303	LHG	C3-O3-P-O4
23	6	303	LHG	C3-O3-P-O5
23	6	303	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
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	C4-O6-P-O3
23	6	324	LHG	C8-C7-O7-C5
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	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
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	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	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	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	C11-C12-C13-C14
31	Z	318	LUT	C11-C12-C13-C14
31	Z	318	LUT	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
31	3	5002	LUT	C11-C12-C13-C14
31	3	5003	LUT	C21-C26-C27-C28
31	3	5003	LUT	C25-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	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	C31-C32-C33-C34
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	C21-C26-C27-C28
31	6	306	LUT	C25-C26-C27-C28
32	1	5009	CHL	C3A-C2A-CAA-CBA
32	Z	302	CHL	C3A-C2A-CAA-CBA
32	Z	309	CHL	C4C-C3C-CAC-CBC
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	C3A-C2A-CAA-CBA
32	8	301	CHL	C4C-C3C-CAC-CBC
32	8	319	CHL	C2-C1-O2A-CGA
32	4	317	CHL	C11-C12-C13-C14
32	6	316	CHL	C3A-C2A-CAA-CBA
32	6	316	CHL	C4C-C3C-CAC-CBC
32	6	317	CHL	C3A-C2A-CAA-CBA
33	3	5001	SPH	O1-C1-C2-N2
33	3	5001	SPH	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
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	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
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	6	326	ERG	C16-C17-C20-C21
38	6	326	ERG	C16-C17-C20-C22
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
24	3	5023	LMT	C3'-C4'-O1B-C1B
19	4	311	CLA	C2C-C3C-CAC-CBC
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

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Mol	Chain	Res	Type	Atoms
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	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
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

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Mol	Chain	Res	Type	Atoms
19	7	310	CLA	CBD-CGD-O2D-CED
19	7	318	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
19	A	804	CLA	O1A-CGA-O2A-C1
19	A	806	CLA	O1A-CGA-O2A-C1
19	A	807	CLA	O1A-CGA-O2A-C1
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	A	811	CLA	O1D-CGD-O2D-CED
19	A	821	CLA	O1D-CGD-O2D-CED
19	7	324	CLA	O1D-CGD-O2D-CED
19	G	1602	CLA	CBA-CGA-O2A-C1
25	B	848	DGD	C2G-C1G-O1G-C1A
19	4	311	CLA	C4C-C3C-CAC-CBC
19	A	802	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	829	CLA	O1D-CGD-O2D-CED
19	1	5011	CLA	O1D-CGD-O2D-CED
19	5	319	CLA	O1D-CGD-O2D-CED
19	5	322	CLA	O1D-CGD-O2D-CED
19	A	804	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
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
32	6	316	CHL	CBD-CGD-O2D-CED
24	A	856	LMT	O5B-C1B-O1B-C4'
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
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

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Mol	Chain	Res	Type	Atoms
19	6	322	CLA	O1A-CGA-O2A-C1
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	827	CLA	O1D-CGD-O2D-CED
19	B	835	CLA	O1D-CGD-O2D-CED
19	4	307	CLA	O1D-CGD-O2D-CED
24	8	323	LMT	O5B-C1B-O1B-C4'
32	Z	309	CHL	C2C-C3C-CAC-CBC
19	A	818	CLA	O1D-CGD-O2D-CED
19	A	830	CLA	O1D-CGD-O2D-CED
19	A	834	CLA	O1D-CGD-O2D-CED
19	F	303	CLA	O1D-CGD-O2D-CED
19	Z	311	CLA	O1D-CGD-O2D-CED
19	Z	314	CLA	O1D-CGD-O2D-CED
19	4	306	CLA	O1D-CGD-O2D-CED
19	4	310	CLA	O1D-CGD-O2D-CED
19	4	313	CLA	O1D-CGD-O2D-CED
19	5	301	CLA	O1D-CGD-O2D-CED
19	5	311	CLA	O1D-CGD-O2D-CED
19	A	802	CLA	C8-C10-C11-C12
19	A	808	CLA	CBD-CGD-O2D-CED
19	7	319	CLA	CBD-CGD-O2D-CED
32	6	316	CHL	C2C-C3C-CAC-CBC
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
37	8	302	SQD	O49-C7-O47-C45
19	B	839	CLA	CBA-CGA-O2A-C1
19	Z	314	CLA	CBA-CGA-O2A-C1
19	3	5009	CLA	CBA-CGA-O2A-C1
19	8	320	CLA	CBA-CGA-O2A-C1
19	6	322	CLA	CBA-CGA-O2A-C1
19	K	202	CLA	O1A-CGA-O2A-C1
19	Z	303	CLA	O1A-CGA-O2A-C1
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

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Mol	Chain	Res	Type	Atoms
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
32	8	315	CHL	C3-C5-C6-C7
32	8	316	CHL	C3-C5-C6-C7
19	B	833	CLA	O1D-CGD-O2D-CED
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

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Mol	Chain	Res	Type	Atoms
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
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	6	301	CLA	CBD-CGD-O2D-CED
32	6	321	CHL	CBD-CGD-O2D-CED
23	1	5001	LHG	C8-C7-O7-C5
25	B	848	DGD	C2B-C1B-O2G-C2G
19	A	809	CLA	O1D-CGD-O2D-CED
19	Z	306	CLA	O1D-CGD-O2D-CED
19	8	310	CLA	O1D-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	B	839	CLA	O1D-CGD-O2D-CED
19	1	5015	CLA	O1D-CGD-O2D-CED
19	5	325	CLA	O1D-CGD-O2D-CED
19	A	814	CLA	C4-C3-C5-C6
19	A	817	CLA	C4-C3-C5-C6
19	B	825	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	Z	307	CLA	C4-C3-C5-C6
19	5	306	CLA	C4-C3-C5-C6
19	5	317	CLA	C4-C3-C5-C6
19	A	817	CLA	C2-C3-C5-C6
19	B	825	CLA	C2-C3-C5-C6
19	5	306	CLA	C2-C3-C5-C6
19	Z	303	CLA	CBA-CGA-O2A-C1
19	4	308	CLA	CBD-CGD-O2D-CED
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	A	857	CLA	C2A-CAA-CBA-CGA
19	B	810	CLA	C3-C5-C6-C7
19	Z	306	CLA	C2A-CAA-CBA-CGA
19	4	307	CLA	C3-C5-C6-C7
19	5	310	CLA	C2A-CAA-CBA-CGA
19	8	307	CLA	O1A-CGA-O2A-C1
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
29	J	1904	LMG	C8-C9-O8-C28
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

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Mol	Chain	Res	Type	Atoms
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
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
32	8	301	CHL	C2C-C3C-CAC-CBC
24	8	323	LMT	C2B-C1B-O1B-C4'
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	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
23	4	320	LHG	O9-C7-O7-C5
29	J	1903	LMG	O9-C10-O7-C8
19	K	202	CLA	CBA-CGA-O2A-C1
25	B	848	DGD	C8A-C9A-CAA-CBA
25	B	848	DGD	CBA-CCA-CDA-CEA
19	B	822	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	3	5016	CLA	O1D-CGD-O2D-CED
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	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	825	CLA	C8-C10-C11-C12
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	825	CLA	O1D-CGD-O2D-CED
19	B	826	CLA	O1D-CGD-O2D-CED
19	G	1602	CLA	O1D-CGD-O2D-CED
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
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	B	838	CLA	O1D-CGD-O2D-CED
19	K	204	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	3	5017	CHL	O1D-CGD-O2D-CED
19	B	836	CLA	C8-C10-C11-C12
19	B	814	CLA	CBD-CGD-O2D-CED
19	B	840	CLA	CBD-CGD-O2D-CED
19	4	312	CLA	CBD-CGD-O2D-CED
23	Z	316	LHG	C8-C7-O7-C5
29	J	1904	LMG	C11-C10-O7-C8
34	3	5022	3PH	C22-C21-O21-C2
19	B	840	CLA	O1A-CGA-O2A-C1
23	1	5019	LHG	C11-C12-C13-C14
19	A	816	CLA	O1D-CGD-O2D-CED
19	1	5007	CLA	O1D-CGD-O2D-CED
19	B	819	CLA	C3-C5-C6-C7
19	B	831	CLA	C3-C5-C6-C7
19	7	312	CLA	C3-C5-C6-C7
23	5	323	LHG	C23-C24-C25-C26
19	7	312	CLA	CBD-CGD-O2D-CED
19	6	314	CLA	CBD-CGD-O2D-CED
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	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
19	Z	305	CLA	C4-C3-C5-C6
19	3	5014	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	7	306	CLA	C2-C3-C5-C6
19	6	301	CLA	C2-C3-C5-C6
32	1	5009	CHL	C2-C3-C5-C6
19	A	804	CLA	C5-C6-C7-C8
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
23	Z	316	LHG	O9-C7-O7-C5
23	1	5019	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
19	A	836	CLA	CBD-CGD-O2D-CED
19	A	810	CLA	C8-C10-C11-C12
19	A	843	CLA	C3-C5-C6-C7
19	B	817	CLA	C2A-CAA-CBA-CGA
19	5	306	CLA	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
24	Z	301	LMT	O5'-C1'-O1'-C1
19	Z	305	CLA	C8-C10-C11-C12
19	B	822	CLA	CBA-CGA-O2A-C1
19	5	325	CLA	CBA-CGA-O2A-C1
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
23	3	5021	LHG	C24-C23-O8-C6
19	A	829	CLA	C5-C6-C7-C8
23	5	323	LHG	C11-C12-C13-C14
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	830	CLA	CBD-CGD-O2D-CED
32	8	317	CHL	CBD-CGD-O2D-CED
35	7	302	DGA	CB1-CB2-CB3-CB4
19	B	802	CLA	C5-C6-C7-C8
22	B	842	BCR	C9-C10-C11-C12
22	3	5006	BCR	C15-C16-C17-C18
22	3	5007	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
22	6	307	BCR	C9-C10-C11-C12
19	B	822	CLA	O1A-CGA-O2A-C1
19	5	325	CLA	O1A-CGA-O2A-C1
32	8	316	CHL	O1A-CGA-O2A-C1
34	3	5022	3PH	O22-C21-O21-C2
23	7	320	LHG	C1-C2-C3-O3
23	4	320	LHG	C1-C2-C3-O3
23	6	303	LHG	C1-C2-C3-O3
19	A	808	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	A	805	CLA	CBD-CGD-O2D-CED
19	3	5014	CLA	CBD-CGD-O2D-CED
19	7	316	CLA	CBD-CGD-O2D-CED
23	A	851	LHG	C11-C12-C13-C14
34	6	325	3PH	C24-C25-C26-C27
19	B	815	CLA	O1D-CGD-O2D-CED
19	8	313	CLA	O1A-CGA-O2A-C1
19	A	814	CLA	C2-C3-C5-C6
19	Z	307	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
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

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Mol	Chain	Res	Type	Atoms
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
32	8	315	CHL	C14-C13-C15-C16
32	6	315	CHL	C11-C10-C8-C9
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
32	6	321	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	Z	301	LMT	C2'-C1'-O1'-C1
24	8	324	LMT	C3'-C4'-O1B-C1B
23	Z	316	LHG	O2-C2-C3-O3
23	5	323	LHG	O2-C2-C3-O3
19	B	832	CLA	O1D-CGD-O2D-CED
19	1	5018	CLA	O1D-CGD-O2D-CED
19	B	837	CLA	O1D-CGD-O2D-CED
22	A	846	BCR	C11-C12-C13-C35
22	A	846	BCR	C36-C18-C19-C20
22	A	846	BCR	C37-C22-C23-C24
22	A	847	BCR	C7-C8-C9-C34
22	A	847	BCR	C36-C18-C19-C20
22	A	847	BCR	C37-C22-C23-C24
22	A	848	BCR	C37-C22-C23-C24
22	A	849	BCR	C7-C8-C9-C34
22	A	850	BCR	C11-C12-C13-C35
22	A	850	BCR	C36-C18-C19-C20
22	A	850	BCR	C37-C22-C23-C24
22	A	858	BCR	C11-C12-C13-C35
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	845	BCR	C11-C12-C13-C35
22	B	845	BCR	C36-C18-C19-C20
22	B	845	BCR	C37-C22-C23-C24
22	B	846	BCR	C7-C8-C9-C34
22	B	846	BCR	C36-C18-C19-C20
22	B	847	BCR	C7-C8-C9-C34
22	F	302	BCR	C11-C12-C13-C35
22	G	1603	BCR	C36-C18-C19-C20
22	K	206	BCR	C36-C18-C19-C20
22	K	206	BCR	C37-C22-C23-C24
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	5007	BCR	C11-C12-C13-C35
22	7	305	BCR	C7-C8-C9-C34
22	7	305	BCR	C11-C12-C13-C35
22	4	305	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
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
27	4	303	RRX	C7-C8-C9-C34
28	J	1902	C7Z	C27-C28-C29-C39
31	1	5003	LUT	C7-C8-C9-C19
31	1	5003	LUT	C11-C12-C13-C20
31	Z	317	LUT	C7-C8-C9-C19
31	Z	318	LUT	C11-C12-C13-C20
31	Z	318	LUT	C31-C32-C33-C40
31	3	5002	LUT	C11-C12-C13-C20
31	3	5003	LUT	C27-C28-C29-C39
31	7	304	LUT	C27-C28-C29-C39
31	8	304	LUT	C7-C8-C9-C19
31	5	303	LUT	C11-C12-C13-C20
31	5	303	LUT	C31-C32-C33-C40
31	6	306	LUT	C11-C12-C13-C20
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	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

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Mol	Chain	Res	Type	Atoms
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
28	1	5005	C7Z	C27-C28-C29-C30
31	7	304	LUT	C27-C28-C29-C30
31	8	304	LUT	C7-C8-C9-C10
31	8	305	LUT	C7-C8-C9-C10
19	A	857	CLA	C3-C5-C6-C7
19	6	310	CLA	C3-C5-C6-C7
23	A	852	LHG	C7-C8-C9-C10
19	4	313	CLA	O1A-CGA-O2A-C1
19	5	311	CLA	O1A-CGA-O2A-C1
32	8	319	CHL	O1A-CGA-O2A-C1
19	A	839	CLA	C3-C5-C6-C7
19	Z	311	CLA	C3-C5-C6-C7
29	J	1904	LMG	O9-C10-O7-C8
23	7	320	LHG	C8-C7-O7-C5
23	8	321	LHG	C8-C7-O7-C5
23	7	320	LHG	C29-C30-C31-C32
19	B	812	CLA	O1D-CGD-O2D-CED
19	K	202	CLA	O1D-CGD-O2D-CED
19	3	5015	CLA	O1D-CGD-O2D-CED
19	A	808	CLA	CBA-CGA-O2A-C1
19	A	827	CLA	CBA-CGA-O2A-C1
23	6	324	LHG	C24-C23-O8-C6
23	6	324	LHG	C23-C24-C25-C26
19	A	812	CLA	C2-C1-O2A-CGA
19	A	827	CLA	C2-C1-O2A-CGA
19	A	828	CLA	C2-C1-O2A-CGA
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

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Mol	Chain	Res	Type	Atoms
19	A	833	CLA	O1A-CGA-O2A-C1
32	Z	310	CHL	C13-C15-C16-C17
19	B	836	CLA	C3-C5-C6-C7
19	8	310	CLA	C3-C5-C6-C7
19	A	812	CLA	O1D-CGD-O2D-CED
19	B	824	CLA	CBD-CGD-O2D-CED
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	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	320	CLA	C6-C7-C8-C10
32	5	315	CHL	C12-C13-C15-C16
23	5	323	LHG	C25-C26-C27-C28
32	8	316	CHL	C4-C3-C5-C6
19	7	311	CLA	C5-C6-C7-C8
32	Z	310	CHL	C10-C11-C12-C13
19	B	808	CLA	O1D-CGD-O2D-CED
22	A	847	BCR	C15-C16-C17-C18
22	A	848	BCR	C13-C14-C15-C16
22	A	859	BCR	C9-C10-C11-C12
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
35	7	302	DGA	CBB-CAB-CB9-CB8
35	7	302	DGA	CCB-CDB-CEB-CFB
19	A	808	CLA	C3-C5-C6-C7
20	A	844	PQN	C18-C20-C21-C22
29	J	1903	LMG	C8-C9-O8-C28

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Mol	Chain	Res	Type	Atoms
23	3	5021	LHG	O10-C23-O8-C6
23	A	852	LHG	C23-C24-C25-C26
35	7	302	DGA	CA1-CA2-CA3-CA4
19	A	834	CLA	O1A-CGA-O2A-C1
32	8	319	CHL	C8-C10-C11-C12
32	4	317	CHL	C5-C6-C7-C8
19	A	829	CLA	C2A-CAA-CBA-CGA
19	B	813	CLA	C2A-CAA-CBA-CGA
19	B	829	CLA	C2A-CAA-CBA-CGA
19	I	201	CLA	C2A-CAA-CBA-CGA
19	5	311	CLA	C2A-CAA-CBA-CGA
19	5	319	CLA	C2A-CAA-CBA-CGA
19	A	812	CLA	C8-C10-C11-C12
19	A	832	CLA	C15-C16-C17-C18
19	8	307	CLA	C5-C6-C7-C8
32	1	5009	CHL	C8-C10-C11-C12
23	7	320	LHG	C7-C8-C9-C10
23	8	321	LHG	C23-C24-C25-C26
19	8	313	CLA	O1D-CGD-O2D-CED
19	A	824	CLA	O1A-CGA-O2A-C1
19	B	833	CLA	C3-C5-C6-C7
24	A	853	LMT	O5'-C1'-O1'-C1
24	3	5023	LMT	O5'-C1'-O1'-C1
19	B	825	CLA	C13-C15-C16-C17
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	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
32	Z	313	CHL	CBD-CGD-O2D-CED
19	A	823	CLA	O1A-CGA-O2A-C1
23	7	320	LHG	C23-C24-C25-C26
19	A	835	CLA	C8-C10-C11-C12
19	8	311	CLA	C8-C10-C11-C12
32	6	319	CHL	C10-C11-C12-C13
19	B	811	CLA	C3-C5-C6-C7
19	5	325	CLA	C3-C5-C6-C7
19	F	301	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	Z	315	CLA	O1D-CGD-O2D-CED
19	4	308	CLA	O1D-CGD-O2D-CED
19	B	821	CLA	C10-C11-C12-C13
19	1	5008	CLA	C5-C6-C7-C8
19	Z	312	CLA	C8-C10-C11-C12
19	6	301	CLA	C5-C6-C7-C8
19	6	301	CLA	O1D-CGD-O2D-CED
19	A	817	CLA	C8-C10-C11-C12
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	A	815	CLA	CBD-CGD-O2D-CED
19	8	307	CLA	CBD-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
32	6	319	CHL	O1D-CGD-O2D-CED
19	6	323	CLA	C8-C10-C11-C12
19	A	811	CLA	C3-C5-C6-C7
19	A	826	CLA	C3-C5-C6-C7
19	B	827	CLA	C3-C5-C6-C7
38	6	326	ERG	C21-C20-C22-C23
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	6	324	LHG	C9-C10-C11-C12
23	7	320	LHG	O9-C7-O7-C5
23	8	321	LHG	O9-C7-O7-C5
23	1	5019	LHG	C1-C2-C3-O3
23	8	321	LHG	C1-C2-C3-O3
23	6	324	LHG	C1-C2-C3-O3
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	814	CLA	O1D-CGD-O2D-CED
19	A	811	CLA	CBA-CGA-O2A-C1
19	A	830	CLA	CBA-CGA-O2A-C1
19	Z	306	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	4	317	CHL	CBA-CGA-O2A-C1
34	3	5022	3PH	C3B-C3C-C3D-C3E
19	A	813	CLA	C8-C10-C11-C12
19	A	832	CLA	C13-C15-C16-C17
19	B	816	CLA	C8-C10-C11-C12
19	1	5006	CLA	C5-C6-C7-C8
19	Z	315	CLA	C10-C11-C12-C13
19	3	5018	CLA	C5-C6-C7-C8
19	8	312	CLA	C5-C6-C7-C8
19	6	314	CLA	C5-C6-C7-C8
19	B	806	CLA	C3-C5-C6-C7
24	3	5023	LMT	C6-C7-C8-C9
19	4	312	CLA	O1D-CGD-O2D-CED
19	A	806	CLA	C5-C6-C7-C8
19	B	801	CLA	C5-C6-C7-C8
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	8	307	CLA	C10-C11-C12-C13
32	6	315	CHL	C8-C10-C11-C12
19	A	823	CLA	C5-C6-C7-C8
19	B	840	CLA	C10-C11-C12-C13
19	3	5013	CLA	C13-C15-C16-C17
19	4	308	CLA	C5-C6-C7-C8
18	A	801	CL0	CBA-CGA-O2A-C1
19	6	302	CLA	CBA-CGA-O2A-C1
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	5012	CLA	O1D-CGD-O2D-CED
19	A	806	CLA	C8-C10-C11-C12
19	B	820	CLA	C5-C6-C7-C8
38	6	326	ERG	C13-C17-C20-C22
19	B	803	CLA	C3-C5-C6-C7
19	Z	312	CLA	C3-C5-C6-C7
19	4	309	CLA	C3-C5-C6-C7
23	A	852	LHG	C8-C7-O7-C5
23	1	5019	LHG	C8-C7-O7-C5
35	7	302	DGA	CB2-CB1-OG2-CG2
24	A	853	LMT	C2'-C1'-O1'-C1
24	A	854	LMT	C2'-C1'-O1'-C1
24	A	856	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
24	3	5023	LMT	C2'-C1'-O1'-C1
19	B	850	CLA	C8-C10-C11-C12
19	7	312	CLA	O1D-CGD-O2D-CED
19	A	836	CLA	CBA-CGA-O2A-C1
19	B	827	CLA	CBA-CGA-O2A-C1
19	8	314	CLA	C6-C7-C8-C9
38	8	325	ERG	C22-C23-C24-C25
38	6	326	ERG	C17-C20-C22-C23
34	8	322	3PH	C32-C33-C34-C35
19	7	319	CLA	C8-C10-C11-C12
24	8	324	LMT	C5'-C4'-O1B-C1B
19	6	302	CLA	C3-C5-C6-C7
19	A	815	CLA	C13-C15-C16-C17
19	3	5016	CLA	C8-C10-C11-C12
32	Z	302	CHL	C5-C6-C7-C8
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	844	BCR	C36-C18-C19-C20
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	3	5006	BCR	C37-C22-C23-C24
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
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	1	5005	C7Z	C27-C28-C29-C39
28	6	304	C7Z	C7-C8-C9-C19
28	6	304	C7Z	C27-C28-C29-C39
31	Z	317	LUT	C31-C32-C33-C40
31	Z	318	LUT	C7-C8-C9-C19
31	8	304	LUT	C27-C28-C29-C39
31	4	304	LUT	C7-C8-C9-C19
31	6	305	LUT	C7-C8-C9-C19
22	A	847	BCR	C7-C8-C9-C10
22	A	848	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
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	5005	BCR	C21-C22-C23-C24
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	317	LUT	C7-C8-C9-C10
31	Z	317	LUT	C31-C32-C33-C34
31	Z	318	LUT	C7-C8-C9-C10
31	3	5003	LUT	C7-C8-C9-C10
31	3	5003	LUT	C27-C28-C29-C30
31	8	304	LUT	C27-C28-C29-C30
31	4	304	LUT	C7-C8-C9-C10
31	6	306	LUT	C27-C28-C29-C30
19	A	808	CLA	C2A-CAA-CBA-CGA
19	B	831	CLA	C2A-CAA-CBA-CGA
19	1	5011	CLA	C2A-CAA-CBA-CGA
19	8	318	CLA	C2A-CAA-CBA-CGA
19	6	313	CLA	C2A-CAA-CBA-CGA
32	7	314	CHL	C2A-CAA-CBA-CGA
32	4	315	CHL	C2A-CAA-CBA-CGA
32	6	317	CHL	C2A-CAA-CBA-CGA
19	B	828	CLA	C8-C10-C11-C12
19	B	840	CLA	C5-C6-C7-C8
19	Z	315	CLA	C8-C10-C11-C12
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

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Mol	Chain	Res	Type	Atoms
23	5	323	LHG	O1-C1-C2-C3
23	6	324	LHG	O1-C1-C2-C3
23	A	851	LHG	C7-C8-C9-C10
19	I	201	CLA	C6-C7-C8-C9
19	8	307	CLA	C11-C12-C13-C14
19	4	313	CLA	C6-C7-C8-C10
19	5	325	CLA	C6-C7-C8-C9
19	6	314	CLA	O1D-CGD-O2D-CED
19	3	5019	CLA	C3-C5-C6-C7
23	A	852	LHG	O9-C7-O7-C5
23	1	5019	LHG	O9-C7-O7-C5
35	7	302	DGA	OB1-CB1-OG2-CG2
24	A	854	LMT	O5'-C1'-O1'-C1
37	8	302	SQD	O5-C1-O6-C44
23	4	320	LHG	C29-C30-C31-C32
19	3	5014	CLA	C2-C3-C5-C6
19	3	5013	CLA	O1D-CGD-O2D-CED
38	8	325	ERG	C21-C20-C22-C23
38	8	325	ERG	C22-C23-C24-C28
38	6	326	ERG	C22-C23-C24-C28
23	Z	316	LHG	C23-C24-C25-C26
23	8	321	LHG	C7-C8-C9-C10
19	5	321	CLA	C3-C5-C6-C7
19	A	836	CLA	O1D-CGD-O2D-CED
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
19	A	804	CLA	C6-C7-C8-C9
19	B	809	CLA	C6-C7-C8-C9
19	I	201	CLA	C6-C7-C8-C10
19	Z	311	CLA	C6-C7-C8-C9
19	7	324	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	8	307	CLA	C11-C12-C13-C15
19	8	313	CLA	C6-C7-C8-C10
19	7	306	CLA	C5-C6-C7-C8
19	8	314	CLA	C5-C6-C7-C8
19	6	312	CLA	C8-C10-C11-C12
23	1	5019	LHG	C14-C15-C16-C17
23	Z	316	LHG	C13-C14-C15-C16
23	Z	316	LHG	C28-C29-C30-C31
33	7	321	SPH	C10-C11-C12-C13
19	1	5008	CLA	CBD-CGD-O2D-CED
19	5	317	CLA	CBD-CGD-O2D-CED
23	7	320	LHG	C28-C29-C30-C31
23	6	324	LHG	C11-C12-C13-C14
19	B	826	CLA	C13-C15-C16-C17
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
32	6	319	CHL	CBA-CGA-O2A-C1
33	7	321	SPH	C12-C13-C14-C15
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
24	4	322	LMT	C2-C1-O1'-C1'
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
32	8	301	CHL	C5-C6-C7-C8
19	B	827	CLA	C4B-C3B-CAB-CBB
19	Z	306	CLA	C4B-C3B-CAB-CBB
19	6	320	CLA	C4B-C3B-CAB-CBB
23	4	320	LHG	C7-C8-C9-C10
23	6	303	LHG	C7-C8-C9-C10
19	A	836	CLA	C6-C7-C8-C9
19	A	836	CLA	C6-C7-C8-C10
19	7	324	CLA	C6-C7-C8-C10
19	5	306	CLA	C11-C12-C13-C15
32	1	5009	CHL	C11-C12-C13-C14
19	8	311	CLA	O1D-CGD-O2D-CED
19	A	813	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	5	301	CLA	C2A-CAA-CBA-CGA
19	6	320	CLA	C2A-CAA-CBA-CGA
32	8	316	CHL	C2A-CAA-CBA-CGA
19	B	814	CLA	C8-C10-C11-C12
19	B	823	CLA	C5-C6-C7-C8
20	A	844	PQN	C25-C26-C27-C28
23	6	324	LHG	C10-C11-C12-C13
19	A	825	CLA	C6-C7-C8-C10
19	A	826	CLA	C11-C12-C13-C15
19	A	827	CLA	C11-C12-C13-C15
19	A	832	CLA	C11-C10-C8-C7
19	B	823	CLA	C11-C10-C8-C7
19	B	835	CLA	C6-C7-C8-C10
19	3	5016	CLA	C6-C7-C8-C10
19	5	321	CLA	C11-C10-C8-C7
19	6	312	CLA	C11-C10-C8-C7
23	5	323	LHG	C28-C29-C30-C31
23	5	323	LHG	C7-C8-C9-C10
23	7	320	LHG	C11-C12-C13-C14
34	6	325	3PH	C25-C26-C27-C28
19	8	311	CLA	O1A-CGA-O2A-C1
19	A	813	CLA	C3-C5-C6-C7
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
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

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Mol	Chain	Res	Type	Atoms
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	1	5006	CLA	O1D-CGD-O2D-CED
19	7	317	CLA	O1D-CGD-O2D-CED
19	B	801	CLA	C8-C10-C11-C12
19	B	823	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
23	1	5001	LHG	C7-C8-C9-C10
23	6	303	LHG	C23-C24-C25-C26
19	A	803	CLA	O1D-CGD-O2D-CED
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	K	203	CLA	C6-C7-C8-C9
19	4	313	CLA	C6-C7-C8-C9
32	5	315	CHL	C16-C17-C18-C20
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
23	A	852	LHG	C9-C10-C11-C12
23	7	320	LHG	C11-C10-C9-C8
23	6	303	LHG	C13-C14-C15-C16
19	A	826	CLA	C8-C10-C11-C12
19	7	309	CLA	C8-C10-C11-C12
19	A	821	CLA	CBA-CGA-O2A-C1
19	1	5015	CLA	CBA-CGA-O2A-C1
18	A	801	CL0	C3-C5-C6-C7
19	B	821	CLA	C3-C5-C6-C7
19	7	319	CLA	C3-C5-C6-C7
32	Z	310	CHL	C3-C5-C6-C7
19	A	823	CLA	C8-C10-C11-C12
23	A	851	LHG	C23-C24-C25-C26
23	1	5019	LHG	C7-C8-C9-C10
19	B	821	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	A	852	LHG	C13-C14-C15-C16
24	3	5023	LMT	C4-C5-C6-C7
34	3	5022	3PH	C22-C23-C24-C25
19	A	836	CLA	O1A-CGA-O2A-C1
23	A	852	LHG	C12-C13-C14-C15
24	4	322	LMT	C2-C3-C4-C5
19	A	804	CLA	C6-C7-C8-C10
19	A	822	CLA	C6-C7-C8-C9
22	A	847	BCR	C1-C6-C7-C8
22	A	849	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	845	BCR	C23-C24-C25-C30
22	B	846	BCR	C1-C6-C7-C8
22	B	847	BCR	C23-C24-C25-C30
22	3	5004	BCR	C5-C6-C7-C8
22	3	5006	BCR	C5-C6-C7-C8
22	3	5006	BCR	C23-C24-C25-C26
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	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
23	4	320	LHG	C16-C17-C18-C19
35	7	302	DGA	CB4-CB5-CB6-CB7
19	4	309	CLA	CBD-CGD-O2D-CED
19	6	320	CLA	CBD-CGD-O2D-CED
19	6	302	CLA	O1D-CGD-O2D-CED
19	A	810	CLA	CBA-CGA-O2A-C1
19	Z	315	CLA	C3-C5-C6-C7
19	B	830	CLA	O1D-CGD-O2D-CED
19	B	814	CLA	C2A-CAA-CBA-CGA
19	B	830	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	3	5013	CLA	C2A-CAA-CBA-CGA
19	3	5020	CLA	C2A-CAA-CBA-CGA
19	7	317	CLA	C2A-CAA-CBA-CGA
19	8	312	CLA	C2A-CAA-CBA-CGA
32	4	317	CHL	O1A-CGA-O2A-C1
32	6	319	CHL	O1A-CGA-O2A-C1
23	A	851	LHG	C13-C14-C15-C16
19	A	841	CLA	C4-C3-C5-C6
19	3	5008	CLA	C4-C3-C5-C6
19	A	823	CLA	C2-C3-C5-C6
23	A	852	LHG	C34-C35-C36-C37
23	8	321	LHG	C28-C29-C30-C31
19	8	312	CLA	CBA-CGA-O2A-C1
23	A	851	LHG	C24-C23-O8-C6
19	B	813	CLA	C3-C5-C6-C7
32	6	315	CHL	C11-C12-C13-C14
34	3	5022	3PH	C25-C26-C27-C28
19	4	316	CLA	O1D-CGD-O2D-CED
19	B	813	CLA	C8-C10-C11-C12
23	4	320	LHG	C30-C31-C32-C33
23	6	303	LHG	C11-C12-C13-C14
24	Z	301	LMT	O1'-C1-C2-C3
19	8	313	CLA	C3-C5-C6-C7
19	A	817	CLA	CBA-CGA-O2A-C1
19	B	824	CLA	CBA-CGA-O2A-C1
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	8	314	CLA	C6-C7-C8-C10
38	6	326	ERG	C22-C23-C24-C25
34	6	325	3PH	C22-C21-O21-C2
24	Z	319	LMT	C5'-C4'-O1B-C1B
19	A	828	CLA	C5-C6-C7-C8
34	6	325	3PH	O22-C21-O21-C2
23	A	851	LHG	C9-C10-C11-C12
33	7	321	SPH	C9-C10-C11-C12
23	A	851	LHG	C11-C10-C9-C8
23	6	303	LHG	C11-C10-C9-C8
22	7	305	BCR	C37-C22-C23-C24
31	3	5003	LUT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
31	8	304	LUT	C11-C12-C13-C20
23	4	320	LHG	C28-C29-C30-C31
23	6	324	LHG	C34-C35-C36-C37
19	A	840	CLA	C3-C5-C6-C7
22	B	844	BCR	C17-C18-C19-C20
22	7	305	BCR	C21-C22-C23-C24
32	5	315	CHL	C10-C11-C12-C13
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	5	308	CLA	C11-C10-C8-C9
19	1	5011	CLA	C6-C7-C8-C9
19	5	325	CLA	C6-C7-C8-C10
19	B	827	CLA	C4-C3-C5-C6
19	Z	311	CLA	C4-C3-C5-C6
32	6	315	CHL	C4-C3-C5-C6
32	6	315	CHL	C2-C3-C5-C6
35	7	302	DGA	CA4-CA5-CA6-CA7
19	3	5016	CLA	C5-C6-C7-C8
19	7	310	CLA	C5-C6-C7-C8
35	7	302	DGA	CB5-CB6-CB7-CB8
19	A	821	CLA	O1A-CGA-O2A-C1
19	1	5015	CLA	O1A-CGA-O2A-C1
24	4	322	LMT	O5'-C5'-C6'-O6'
19	A	840	CLA	C8-C10-C11-C12
19	3	5010	CLA	C8-C10-C11-C12
32	8	319	CHL	C10-C11-C12-C13
24	Z	319	LMT	C3'-C4'-O1B-C1B
19	5	319	CLA	CBA-CGA-O2A-C1
23	1	5019	LHG	C28-C29-C30-C31
37	8	302	SQD	C9-C10-C11-C12
23	A	851	LHG	O6-C4-C5-O7
19	B	823	CLA	O1D-CGD-O2D-CED
23	7	320	LHG	C10-C11-C12-C13
19	A	816	CLA	C5-C6-C7-C8
19	A	820	CLA	C8-C10-C11-C12
19	5	321	CLA	C8-C10-C11-C12
20	B	841	PQN	C15-C16-C17-C18
19	B	809	CLA	C6-C7-C8-C10
19	Z	311	CLA	C6-C7-C8-C10
19	A	834	CLA	C8-C10-C11-C12
19	Z	312	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	6	313	CLA	C15-C16-C17-C18
19	3	5014	CLA	O1D-CGD-O2D-CED
32	8	317	CHL	O1D-CGD-O2D-CED
23	A	852	LHG	O7-C5-C6-O8
19	A	805	CLA	O1D-CGD-O2D-CED
24	A	853	LMT	O5'-C5'-C6'-O6'
19	B	826	CLA	C2-C1-O2A-CGA
19	B	831	CLA	C2-C1-O2A-CGA
19	1	5010	CLA	C6-C7-C8-C9
19	A	833	CLA	C5-C6-C7-C8
19	5	306	CLA	C5-C6-C7-C8
19	5	306	CLA	C8-C10-C11-C12
24	A	856	LMT	O5'-C5'-C6'-O6'
19	A	838	CLA	C4-C3-C5-C6
19	B	807	CLA	C5-C6-C7-C8
19	B	850	CLA	C2C-C3C-CAC-CBC
19	B	809	CLA	C2A-CAA-CBA-CGA
19	6	318	CLA	C2A-CAA-CBA-CGA
32	5	316	CHL	C2A-CAA-CBA-CGA
19	3	5019	CLA	CBD-CGD-O2D-CED
19	7	306	CLA	CBD-CGD-O2D-CED
19	7	316	CLA	O1D-CGD-O2D-CED
34	3	5022	3PH	C24-C25-C26-C27
34	8	322	3PH	C3A-C3B-C3C-C3D
23	4	320	LHG	C19-C20-C21-C22
37	8	302	SQD	C45-C46-O48-C23
19	Z	308	CLA	C8-C10-C11-C12
32	8	319	CHL	C13-C15-C16-C17
23	A	852	LHG	C19-C20-C21-C22
24	A	856	LMT	O5B-C5B-C6B-O6B
23	1	5019	LHG	C29-C30-C31-C32
35	7	302	DGA	CB3-CB4-CB5-CB6
23	1	5001	LHG	O1-C1-C2-O2
23	Z	316	LHG	O1-C1-C2-O2
23	6	303	LHG	O1-C1-C2-O2
19	A	817	CLA	O1A-CGA-O2A-C1
19	4	310	CLA	C3-C5-C6-C7
35	7	302	DGA	CA3-CA4-CA5-CA6
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
19	B	807	CLA	C8-C10-C11-C12
34	6	325	3PH	C22-C23-C24-C25
19	A	810	CLA	O1A-CGA-O2A-C1
19	8	312	CLA	O1A-CGA-O2A-C1
19	5	319	CLA	O1A-CGA-O2A-C1
19	5	310	CLA	C2C-C3C-CAC-CBC
19	A	820	CLA	C5-C6-C7-C8
19	A	830	CLA	C5-C6-C7-C8
19	B	850	CLA	C5-C6-C7-C8
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
24	A	855	LMT	O5B-C5B-C6B-O6B
24	1	5002	LMT	O5B-C5B-C6B-O6B
24	4	302	LMT	O5'-C5'-C6'-O6'
19	1	5016	CLA	C3-C5-C6-C7
19	3	5014	CLA	C3-C5-C6-C7
18	A	801	CL0	C6-C7-C8-C10
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	813	CLA	C11-C12-C13-C15
19	A	816	CLA	C6-C7-C8-C10
19	A	821	CLA	C11-C12-C13-C15
19	A	829	CLA	C11-C10-C8-C7
19	A	833	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	815	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
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	826	CLA	C11-C10-C8-C7
19	B	836	CLA	C12-C13-C15-C16
19	B	837	CLA	C6-C7-C8-C10
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	5	308	CLA	C6-C7-C8-C10
19	6	301	CLA	C11-C10-C8-C7
19	6	309	CLA	C6-C7-C8-C10
32	8	315	CHL	C11-C10-C8-C7
32	8	319	CHL	C11-C10-C8-C7
32	5	315	CHL	C6-C7-C8-C10
19	Z	312	CLA	C16-C17-C18-C20
19	4	306	CLA	C11-C12-C13-C15
19	J	1901	CLA	C3A-C2A-CAA-CBA
19	7	318	CLA	C3A-C2A-CAA-CBA
19	B	817	CLA	C8-C10-C11-C12
19	7	312	CLA	C5-C6-C7-C8
19	7	324	CLA	C5-C6-C7-C8
32	5	315	CHL	C4-C3-C5-C6
19	B	827	CLA	C2-C3-C5-C6
19	8	312	CLA	C2-C3-C5-C6
32	5	315	CHL	C2-C3-C5-C6
23	A	852	LHG	C11-C12-C13-C14
23	6	324	LHG	C16-C17-C18-C19
19	A	818	CLA	C8-C10-C11-C12
19	A	834	CLA	C5-C6-C7-C8
38	8	325	ERG	C16-C17-C20-C22
19	3	5014	CLA	C2A-CAA-CBA-CGA
19	4	316	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	A	802	CLA	C6-C7-C8-C9
19	A	805	CLA	C6-C7-C8-C9
19	A	806	CLA	C11-C12-C13-C14
19	A	808	CLA	C6-C7-C8-C9
19	A	821	CLA	C6-C7-C8-C9
19	A	827	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	804	CLA	C11-C10-C8-C9
19	B	807	CLA	C11-C12-C13-C14
19	B	808	CLA	C14-C13-C15-C16
19	B	814	CLA	C6-C7-C8-C9
19	B	815	CLA	C6-C7-C8-C9
19	B	824	CLA	C6-C7-C8-C9
19	B	826	CLA	C11-C10-C8-C9
19	1	5012	CLA	C6-C7-C8-C9
19	Z	312	CLA	C6-C7-C8-C9
19	7	309	CLA	C6-C7-C8-C9
19	8	308	CLA	C14-C13-C15-C16
19	5	308	CLA	C6-C7-C8-C9
19	5	314	CLA	C11-C10-C8-C9
19	6	320	CLA	C6-C7-C8-C9
20	B	841	PQN	C16-C17-C18-C19
32	5	315	CHL	C14-C13-C15-C16
36	7	322	PLM	C1-C2-C3-C4
22	5	304	BCR	C15-C16-C17-C18
22	6	308	BCR	C13-C14-C15-C16
31	8	304	LUT	C29-C30-C31-C32
23	A	852	LHG	C33-C34-C35-C36
23	Z	316	LHG	C24-C23-O8-C6
23	A	852	LHG	C30-C31-C32-C33
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
23	A	852	LHG	C28-C29-C30-C31
23	8	321	LHG	C11-C12-C13-C14
36	7	322	PLM	C2-C3-C4-C5
19	A	802	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	Z	319	LMT	O5'-C5'-C6'-O6'
19	4	306	CLA	C11-C12-C13-C14
32	5	315	CHL	C16-C17-C18-C19
19	A	827	CLA	C8-C10-C11-C12
32	Z	302	CHL	CHA-CBD-CGD-O1D
32	Z	313	CHL	CHA-CBD-CGD-O1D
32	4	314	CHL	CHA-CBD-CGD-O1D
32	6	321	CHL	CHA-CBD-CGD-O1D
32	6	321	CHL	CHA-CBD-CGD-O2D
19	A	814	CLA	C5-C6-C7-C8
32	1	5009	CHL	C5-C6-C7-C8
24	7	323	LMT	O5'-C5'-C6'-O6'
19	B	824	CLA	O1A-CGA-O2A-C1
22	8	303	BCR	C37-C22-C23-C24
22	6	307	BCR	C7-C8-C9-C34
31	7	304	LUT	C7-C8-C9-C19
24	Z	301	LMT	O5'-C5'-C6'-O6'
22	8	303	BCR	C21-C22-C23-C24
22	5	304	BCR	C21-C22-C23-C24
31	6	306	LUT	C7-C8-C9-C10
23	A	851	LHG	O10-C23-O8-C6
19	A	825	CLA	C5-C6-C7-C8
19	1	5006	CLA	C2A-CAA-CBA-CGA
19	1	5013	CLA	C2A-CAA-CBA-CGA
23	1	5019	LHG	C23-C24-C25-C26
37	8	302	SQD	C10-C11-C12-C13
34	5	324	3PH	C22-C23-C24-C25
19	B	827	CLA	C5-C6-C7-C8
22	4	305	BCR	C19-C20-C21-C22
28	J	1902	C7Z	C9-C10-C11-C12
19	Z	312	CLA	C16-C17-C18-C19
19	Z	305	CLA	C3-C5-C6-C7
19	7	309	CLA	C3-C5-C6-C7
23	4	320	LHG	O6-C4-C5-O7
23	5	323	LHG	O6-C4-C5-O7
19	A	822	CLA	C5-C6-C7-C8
23	6	324	LHG	C13-C14-C15-C16
19	B	824	CLA	O1D-CGD-O2D-CED
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	A	830	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	8	312	CLA	C4-C3-C5-C6
19	A	824	CLA	C3-C5-C6-C7
23	4	320	LHG	C15-C16-C17-C18
23	4	320	LHG	C11-C12-C13-C14
23	7	320	LHG	O7-C5-C6-O8
23	5	323	LHG	O7-C5-C6-O8
23	8	321	LHG	C13-C14-C15-C16
32	Z	309	CHL	CBA-CGA-O2A-C1
23	Z	316	LHG	C11-C12-C13-C14
23	1	5019	LHG	C31-C32-C33-C34
32	8	315	CHL	CAA-CBA-CGA-O2A
23	5	323	LHG	C13-C14-C15-C16
19	B	833	CLA	C15-C16-C17-C18
19	1	5008	CLA	C8-C10-C11-C12
33	4	301	SPH	C5-C6-C7-C8
23	4	320	LHG	C35-C36-C37-C38
19	F	301	CLA	C13-C15-C16-C17
19	8	309	CLA	C5-C6-C7-C8
23	4	320	LHG	C25-C26-C27-C28
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
19	A	828	CLA	C10-C11-C12-C13
32	Z	309	CHL	C10-C11-C12-C13
23	6	324	LHG	C30-C31-C32-C33
19	A	832	CLA	C5-C6-C7-C8
19	6	309	CLA	C8-C10-C11-C12
19	A	815	CLA	O1D-CGD-O2D-CED
19	B	811	CLA	C11-C10-C8-C9
19	B	831	CLA	C4-C3-C5-C6
19	I	201	CLA	C4-C3-C5-C6
32	8	315	CHL	C4-C3-C5-C6
24	F	305	LMT	C2-C3-C4-C5
19	A	843	CLA	CBA-CGA-O2A-C1
32	8	301	CHL	CBA-CGA-O2A-C1
23	6	324	LHG	C35-C36-C37-C38
34	3	5022	3PH	C31-C32-C33-C34
23	6	324	LHG	C28-C29-C30-C31
34	3	5022	3PH	C27-C28-C29-C2A
23	A	852	LHG	O1-C1-C2-O2
24	A	853	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
24	A	855	LMT	C2-C1-O1'-C1'
24	1	5002	LMT	C2-C1-O1'-C1'
18	A	801	CL0	C6-C7-C8-C9
19	A	811	CLA	C6-C7-C8-C9
19	A	812	CLA	C14-C13-C15-C16
19	A	816	CLA	C6-C7-C8-C9
19	A	832	CLA	C14-C13-C15-C16
19	A	833	CLA	C6-C7-C8-C9
19	A	833	CLA	C11-C10-C8-C9
19	B	803	CLA	C6-C7-C8-C9
19	B	808	CLA	C6-C7-C8-C9
19	B	816	CLA	C6-C7-C8-C9
19	B	817	CLA	C6-C7-C8-C9
19	B	819	CLA	C6-C7-C8-C9
19	B	821	CLA	C11-C12-C13-C14
19	B	833	CLA	C14-C13-C15-C16
19	B	835	CLA	C6-C7-C8-C9
19	B	836	CLA	C14-C13-C15-C16
19	1	5016	CLA	C6-C7-C8-C9
19	Z	305	CLA	C11-C10-C8-C9
19	3	5013	CLA	C6-C7-C8-C9
19	3	5014	CLA	C6-C7-C8-C9
19	7	312	CLA	C11-C10-C8-C9
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	6	302	CLA	C6-C7-C8-C9
19	6	309	CLA	C6-C7-C8-C9
23	5	323	LHG	C26-C27-C28-C29
19	1	5006	CLA	C8-C10-C11-C12
23	3	5021	LHG	C2-C3-O3-P
34	6	325	3PH	C2-C1-O11-P
19	A	828	CLA	C4B-C3B-CAB-CBB
34	8	322	3PH	C3B-C3C-C3D-C3E
19	7	308	CLA	C15-C16-C17-C18
19	B	827	CLA	C11-C12-C13-C15
19	A	810	CLA	C2A-CAA-CBA-CGA
19	B	815	CLA	C2A-CAA-CBA-CGA
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	809	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	5	301	CLA	C3-C5-C6-C7
23	1	5019	LHG	O6-C4-C5-C6
23	7	320	LHG	O6-C4-C5-C6
24	4	321	LMT	C3-C4-C5-C6
19	A	812	CLA	C6-C7-C8-C10
19	A	813	CLA	C11-C10-C8-C7
19	A	818	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	823	CLA	C6-C7-C8-C10
19	A	826	CLA	C6-C7-C8-C10
19	A	833	CLA	C11-C10-C8-C7
19	A	842	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	814	CLA	C11-C10-C8-C7
19	B	815	CLA	C11-C10-C8-C7
19	B	824	CLA	C6-C7-C8-C10
19	B	828	CLA	C6-C7-C8-C10
19	B	831	CLA	C11-C10-C8-C7
19	B	833	CLA	C12-C13-C15-C16
19	B	835	CLA	C11-C10-C8-C7
19	B	836	CLA	C11-C12-C13-C15
19	B	840	CLA	C6-C7-C8-C10
19	B	850	CLA	C11-C10-C8-C7
19	1	5012	CLA	C11-C10-C8-C7
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	7	309	CLA	C6-C7-C8-C10
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	8	312	CLA	C6-C7-C8-C10
19	4	308	CLA	C6-C7-C8-C10
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	307	CLA	C11-C10-C8-C7
19	5	312	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
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	313	CLA	C6-C7-C8-C10
20	B	841	PQN	C16-C17-C18-C20
32	4	317	CHL	C11-C12-C13-C15
32	6	319	CHL	C6-C7-C8-C10
19	B	816	CLA	C5-C6-C7-C8
32	4	317	CHL	C8-C10-C11-C12
32	6	315	CHL	C5-C6-C7-C8
33	3	5001	SPH	C7-C8-C9-C10
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
19	A	827	CLA	C2-C3-C5-C6
33	4	301	SPH	C7-C8-C9-C10
19	Z	307	CLA	C8-C10-C11-C12
23	Z	316	LHG	O10-C23-O8-C6
19	1	5011	CLA	C5-C6-C7-C8
19	B	811	CLA	CBA-CGA-O2A-C1
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
27	5	302	RRX	C19-C20-C21-C22
19	B	831	CLA	C13-C15-C16-C17
27	F	304	RRX	C11-C12-C13-C35
31	6	306	LUT	C7-C8-C9-C19
23	4	320	LHG	C13-C14-C15-C16
19	A	802	CLA	O1A-CGA-O2A-C1
32	Z	309	CHL	C2A-CAA-CBA-CGA
32	4	314	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	4	306	CLA	C10-C11-C12-C13
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
19	B	815	CLA	C8-C10-C11-C12
32	1	5009	CHL	C11-C12-C13-C15
19	A	838	CLA	C8-C10-C11-C12
19	B	837	CLA	C8-C10-C11-C12
19	Z	305	CLA	C5-C6-C7-C8
23	6	324	LHG	C19-C20-C21-C22
19	4	308	CLA	C10-C11-C12-C13
19	A	827	CLA	C4-C3-C5-C6
19	7	324	CLA	C4-C3-C5-C6
19	8	314	CLA	C4-C3-C5-C6
19	A	835	CLA	C3-C5-C6-C7
19	8	307	CLA	O1D-CGD-O2D-CED
32	Z	313	CHL	O1D-CGD-O2D-CED
19	6	313	CLA	C5-C6-C7-C8
23	3	5021	LHG	O6-C4-C5-O7
23	7	320	LHG	O6-C4-C5-O7
34	8	322	3PH	O11-C1-C2-O21
22	A	846	BCR	C23-C24-C25-C26
22	B	845	BCR	C1-C6-C7-C8
22	F	302	BCR	C1-C6-C7-C8
22	3	5004	BCR	C1-C6-C7-C8
22	3	5006	BCR	C23-C24-C25-C30
22	8	303	BCR	C1-C6-C7-C8
22	8	306	BCR	C23-C24-C25-C30
22	4	305	BCR	C23-C24-C25-C26
28	1	5005	C7Z	C21-C26-C27-C28
28	6	304	C7Z	C21-C26-C27-C28
31	8	305	LUT	C5-C6-C7-C8
31	4	304	LUT	C1-C6-C7-C8
23	7	320	LHG	C2-C3-O3-P
33	7	321	SPH	O1-C1-C2-N2
33	4	301	SPH	O1-C1-C2-N2
19	B	819	CLA	C8-C10-C11-C12
31	4	304	LUT	C9-C10-C11-C12
19	A	822	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	1	5010	CLA	C6-C7-C8-C10
19	A	843	CLA	C2A-CAA-CBA-CGA
19	6	302	CLA	C2A-CAA-CBA-CGA
19	A	832	CLA	C8-C10-C11-C12
19	B	832	CLA	C5-C6-C7-C8
19	4	306	CLA	C5-C6-C7-C8
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	6	313	CLA	O1A-CGA-O2A-C1
23	6	324	LHG	C33-C34-C35-C36
35	7	302	DGA	CB7-CB8-CB9-CAB
19	3	5012	CLA	C15-C16-C17-C18
19	I	201	CLA	C2-C3-C5-C6
19	7	324	CLA	C2-C3-C5-C6
19	8	314	CLA	C2-C3-C5-C6
33	3	5001	SPH	C11-C10-C9-C8
33	3	5001	SPH	C10-C11-C12-C13
33	7	321	SPH	O3-C3-C4-C5
19	K	203	CLA	C6-C7-C8-C10
23	7	320	LHG	C25-C26-C27-C28
29	J	1904	LMG	C28-C29-C30-C31
19	A	829	CLA	CBA-CGA-O2A-C1
32	7	314	CHL	CBA-CGA-O2A-C1
19	5	301	CLA	O1A-CGA-O2A-C1
19	3	5012	CLA	C3-C5-C6-C7
19	A	819	CLA	C11-C12-C13-C14
19	B	827	CLA	C6-C7-C8-C9
19	B	829	CLA	C6-C7-C8-C9
19	B	833	CLA	C6-C7-C8-C9
19	B	837	CLA	C6-C7-C8-C9
19	B	840	CLA	C6-C7-C8-C9
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

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Mol	Chain	Res	Type	Atoms
23	1	5019	LHG	C15-C16-C17-C18
33	4	301	SPH	O1-C1-C2-C3
23	7	320	LHG	C9-C10-C11-C12
19	1	5011	CLA	C6-C7-C8-C10
19	3	5019	CLA	C6-C7-C8-C9
19	8	313	CLA	C6-C7-C8-C9
32	3	5017	CHL	C3-C5-C6-C7
19	1	5008	CLA	O1D-CGD-O2D-CED
24	Z	319	LMT	O5B-C1B-O1B-C4'
19	B	827	CLA	C10-C11-C12-C13
19	B	814	CLA	C3-C5-C6-C7
22	A	846	BCR	C9-C10-C11-C12
28	6	304	C7Z	C13-C14-C15-C35
19	A	805	CLA	CAA-CBA-CGA-O2A
19	5	306	CLA	C11-C12-C13-C14
32	Z	310	CHL	C15-C16-C17-C18
32	7	314	CHL	C8-C10-C11-C12
19	5	307	CLA	O1A-CGA-O2A-C1
19	A	806	CLA	C3-C5-C6-C7
19	K	203	CLA	C3-C5-C6-C7
23	8	321	LHG	C24-C23-O8-C6
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	B	827	CLA	C11-C12-C13-C14
19	3	5019	CLA	C6-C7-C8-C10
19	7	309	CLA	C16-C17-C18-C19
19	6	314	CLA	C6-C7-C8-C9
19	B	803	CLA	O1A-CGA-O2A-C1
19	6	313	CLA	C8-C10-C11-C12
32	Z	309	CHL	C5-C6-C7-C8
22	5	304	BCR	C37-C22-C23-C24
31	1	5004	LUT	C7-C8-C9-C19
31	3	5002	LUT	C7-C8-C9-C19
31	8	304	LUT	C31-C32-C33-C40
19	A	808	CLA	C11-C10-C8-C7
19	A	809	CLA	C6-C7-C8-C10
19	A	828	CLA	C6-C7-C8-C10
19	A	840	CLA	C6-C7-C8-C10
19	A	840	CLA	C11-C10-C8-C7
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	820	CLA	C6-C7-C8-C10
19	B	829	CLA	C6-C7-C8-C10
19	B	833	CLA	C11-C12-C13-C15
19	B	850	CLA	C11-C12-C13-C15
19	1	5008	CLA	C6-C7-C8-C10
19	Z	308	CLA	C6-C7-C8-C10
19	Z	308	CLA	C11-C12-C13-C15
19	Z	315	CLA	C6-C7-C8-C10
19	3	5013	CLA	C11-C10-C8-C7
19	3	5018	CLA	C6-C7-C8-C10
19	7	308	CLA	C11-C10-C8-C7
19	7	310	CLA	C6-C7-C8-C10
19	7	310	CLA	C11-C10-C8-C7
19	8	308	CLA	C6-C7-C8-C10
19	8	308	CLA	C11-C10-C8-C7
19	5	307	CLA	C6-C7-C8-C10
19	5	314	CLA	C6-C7-C8-C10
19	6	302	CLA	C11-C10-C8-C7
19	6	323	CLA	C11-C12-C13-C15
20	B	841	PQN	C21-C22-C23-C25
19	A	838	CLA	C5-C6-C7-C8
19	B	829	CLA	C5-C6-C7-C8
19	5	321	CLA	C5-C6-C7-C8
22	3	5006	BCR	C21-C22-C23-C24
22	6	307	BCR	C7-C8-C9-C10
31	1	5004	LUT	C7-C8-C9-C10
31	3	5002	LUT	C7-C8-C9-C10
31	7	304	LUT	C7-C8-C9-C10
31	8	304	LUT	C11-C12-C13-C14
31	8	304	LUT	C31-C32-C33-C34
19	3	5012	CLA	O1A-CGA-O2A-C1
32	Z	309	CHL	O1A-CGA-O2A-C1
29	J	1903	LMG	C8-C7-O1-C1
29	7	301	LMG	C8-C7-O1-C1
23	4	320	LHG	C31-C32-C33-C34
19	A	809	CLA	C2A-CAA-CBA-CGA
32	6	315	CHL	C2A-CAA-CBA-CGA
20	B	841	PQN	C14-C13-C15-C16
32	8	301	CHL	O1A-CGA-O2A-C1
23	1	5019	LHG	C17-C18-C19-C20
33	4	301	SPH	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
32	8	315	CHL	C8-C10-C11-C12
19	B	802	CLA	O1A-CGA-O2A-C1
19	B	811	CLA	O1A-CGA-O2A-C1
25	B	848	DGD	CDA-CEA-CFA-CGA
19	A	843	CLA	O1A-CGA-O2A-C1
19	A	810	CLA	C5-C6-C7-C8
23	8	321	LHG	C30-C31-C32-C33
19	I	201	CLA	CAA-CBA-CGA-O2A
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
29	J	1903	LMG	C10-C11-C12-C13
19	B	822	CLA	C8-C10-C11-C12
19	B	828	CLA	C5-C6-C7-C8
19	6	311	CLA	C8-C10-C11-C12
19	5	317	CLA	O1D-CGD-O2D-CED
19	7	324	CLA	C3-C5-C6-C7
19	6	323	CLA	C3-C5-C6-C7
34	3	5022	3PH	C34-C35-C36-C37
19	F	301	CLA	C4-C3-C5-C6
32	5	318	CHL	C2A-CAA-CBA-CGA
24	4	302	LMT	C3'-C4'-O1B-C1B
19	A	841	CLA	C2-C3-C5-C6
19	3	5008	CLA	C2-C3-C5-C6
33	3	5001	SPH	N2-C2-C3-O3
33	7	321	SPH	N2-C2-C3-O3
23	1	5001	LHG	O7-C5-C6-O8
19	A	824	CLA	C6-C7-C8-C9
19	A	839	CLA	C11-C12-C13-C14
19	A	839	CLA	C14-C13-C15-C16
19	8	311	CLA	C6-C7-C8-C9
32	8	319	CHL	C11-C12-C13-C14
19	B	818	CLA	C11-C12-C13-C14
35	7	302	DGA	CA5-CA6-CA7-CA8
34	6	325	3PH	C27-C28-C29-C2A
32	5	318	CHL	C2C-C3C-CAC-CBC
33	4	301	SPH	C12-C13-C14-C15
23	4	320	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
19	A	827	CLA	C10-C11-C12-C13
19	Z	311	CLA	C5-C6-C7-C8
23	8	321	LHG	O10-C23-O8-C6
32	7	314	CHL	O1A-CGA-O2A-C1
34	6	325	3PH	O32-C31-O31-C3
34	8	322	3PH	C39-C3A-C3B-C3C
19	A	810	CLA	C2-C1-O2A-CGA
19	B	818	CLA	C2-C1-O2A-CGA
19	K	203	CLA	C2-C1-O2A-CGA
19	1	5018	CLA	C2-C1-O2A-CGA
22	7	305	BCR	C13-C14-C15-C16
27	4	303	RRX	C9-C10-C11-C12
37	8	302	SQD	C2-C1-O6-C44
19	F	301	CLA	CBA-CGA-O2A-C1
19	A	815	CLA	C16-C17-C18-C20
19	A	839	CLA	C8-C10-C11-C12
32	5	315	CHL	C15-C16-C17-C18
19	B	820	CLA	C4-C3-C5-C6
19	6	301	CLA	C3-C5-C6-C7
24	F	305	LMT	C3'-C4'-O1B-C1B
23	4	320	LHG	C33-C34-C35-C36
19	8	313	CLA	C2A-CAA-CBA-CGA
32	6	315	CHL	CBA-CGA-O2A-C1
19	A	806	CLA	C16-C17-C18-C19
19	6	309	CLA	C11-C12-C13-C15
20	B	841	PQN	C26-C27-C28-C30
38	8	325	ERG	C17-C20-C22-C23
19	A	829	CLA	O1A-CGA-O2A-C1
19	4	312	CLA	C3-C5-C6-C7
32	8	316	CHL	C11-C10-C8-C9
19	B	818	CLA	C11-C12-C13-C15
19	A	814	CLA	C3-C5-C6-C7
34	8	322	3PH	C38-C39-C3A-C3B
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	6	311	CLA	C4B-C3B-CAB-CBB
19	6	320	CLA	O1D-CGD-O2D-CED
19	4	310	CLA	C5-C6-C7-C8
27	F	304	RRX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	1	5004	LUT	C11-C12-C13-C14
33	3	5001	SPH	C13-C14-C15-C16
19	Z	305	CLA	C2A-CAA-CBA-CGA
19	4	307	CLA	C2A-CAA-CBA-CGA
23	Z	316	LHG	O6-C4-C5-C6
23	4	320	LHG	O6-C4-C5-C6
23	5	323	LHG	O6-C4-C5-C6
33	4	301	SPH	C11-C10-C9-C8
33	3	5001	SPH	C6-C7-C8-C9
19	A	816	CLA	C8-C10-C11-C12
19	A	803	CLA	C11-C10-C8-C7
19	A	813	CLA	C6-C7-C8-C10
19	A	816	CLA	C11-C10-C8-C7
19	A	824	CLA	C6-C7-C8-C10
19	A	824	CLA	C11-C10-C8-C7
19	A	827	CLA	C11-C10-C8-C7
19	A	834	CLA	C6-C7-C8-C10
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	832	CLA	C11-C10-C8-C7
19	B	837	CLA	C11-C12-C13-C15
19	7	308	CLA	C12-C13-C15-C16
19	7	312	CLA	C6-C7-C8-C10
19	7	312	CLA	C11-C12-C13-C15
19	4	310	CLA	C11-C10-C8-C7
19	5	309	CLA	C6-C7-C8-C10
19	5	312	CLA	C11-C10-C8-C7
19	5	317	CLA	C6-C7-C8-C10
19	5	317	CLA	C11-C12-C13-C15
19	6	312	CLA	C6-C7-C8-C10
32	8	315	CHL	C12-C13-C15-C16
32	6	319	CHL	C11-C10-C8-C7
32	6	319	CHL	C12-C13-C15-C16
19	A	806	CLA	C16-C17-C18-C20
19	8	311	CLA	C16-C17-C18-C19
20	A	844	PQN	C26-C27-C28-C30
24	F	305	LMT	C5'-C4'-O1B-C1B
32	6	315	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	4	302	LMT	C5'-C4'-O1B-C1B
24	3	5023	LMT	C11-C10-C9-C8
24	Z	319	LMT	C2B-C1B-O1B-C4'
19	B	809	CLA	C5-C6-C7-C8
38	6	326	ERG	C13-C17-C20-C21
20	B	841	PQN	C12-C13-C15-C16
23	Z	316	LHG	O6-C4-C5-O7
32	6	316	CHL	C2A-CAA-CBA-CGA
19	A	813	CLA	C6-C7-C8-C9
19	A	834	CLA	C6-C7-C8-C9
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	850	CLA	C11-C10-C8-C9
19	B	850	CLA	C11-C12-C13-C14
19	B	850	CLA	C14-C13-C15-C16
19	Z	308	CLA	C11-C12-C13-C14
19	7	308	CLA	C11-C10-C8-C9
19	8	312	CLA	C6-C7-C8-C9
19	5	307	CLA	C6-C7-C8-C9
19	6	302	CLA	C11-C10-C8-C9
20	B	841	PQN	C21-C22-C23-C24
32	6	319	CHL	C6-C7-C8-C9
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	B	804	CLA	C13-C15-C16-C17
19	B	808	CLA	C8-C10-C11-C12
19	F	301	CLA	O1A-CGA-O2A-C1
25	B	848	DGD	O1G-C1G-C2G-O2G
19	A	814	CLA	C8-C10-C11-C12
19	B	831	CLA	C8-C10-C11-C12
19	7	311	CLA	C11-C10-C8-C9
19	A	814	CLA	C11-C12-C13-C15
19	6	311	CLA	C4-C3-C5-C6
23	4	320	LHG	C9-C10-C11-C12
19	B	837	CLA	C15-C16-C17-C18
19	Z	311	CLA	C2-C3-C5-C6
32	Z	309	CHL	C13-C15-C16-C17
19	A	832	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	5	322	CLA	CAD-CBD-CGD-O2D
32	Z	309	CHL	CAD-CBD-CGD-O2D
32	Z	310	CHL	CAD-CBD-CGD-O2D
32	7	314	CHL	CAD-CBD-CGD-O2D
32	8	315	CHL	CAD-CBD-CGD-O2D
19	5	310	CLA	C4C-C3C-CAC-CBC
19	4	309	CLA	O1D-CGD-O2D-CED
19	Z	312	CLA	C13-C15-C16-C17
19	A	829	CLA	C3-C5-C6-C7
32	8	319	CHL	C3-C5-C6-C7
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	818	CLA	O1A-CGA-O2A-C1
18	A	801	CL0	CHA-CBD-CGD-O1D
18	A	801	CL0	CHA-CBD-CGD-O2D
19	A	806	CLA	CHA-CBD-CGD-O1D
19	A	806	CLA	CHA-CBD-CGD-O2D
19	A	813	CLA	CHA-CBD-CGD-O1D
19	A	813	CLA	CHA-CBD-CGD-O2D
19	A	832	CLA	CAD-CBD-CGD-O1D
19	B	821	CLA	CHA-CBD-CGD-O1D
19	Z	305	CLA	CHA-CBD-CGD-O1D
19	Z	305	CLA	CHA-CBD-CGD-O2D
19	Z	308	CLA	CHA-CBD-CGD-O1D
19	Z	308	CLA	CHA-CBD-CGD-O2D
19	5	322	CLA	CAD-CBD-CGD-O1D
19	6	320	CLA	CHA-CBD-CGD-O1D
19	6	320	CLA	CHA-CBD-CGD-O2D
22	F	302	BCR	C15-C16-C17-C18
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	1	5019	LHG	C4-O6-P-O3
23	3	5021	LHG	C4-O6-P-O5
23	8	321	LHG	C4-O6-P-O5
23	4	320	LHG	C3-O3-P-O5
23	4	320	LHG	C4-O6-P-O5
23	5	323	LHG	C3-O3-P-O4
23	6	303	LHG	C4-O6-P-O3
23	6	303	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
23	6	324	LHG	C4-O6-P-O5
28	1	5005	C7Z	C33-C34-C35-C15
32	Z	302	CHL	CHA-CBD-CGD-O2D
32	Z	309	CHL	CAD-CBD-CGD-O1D
32	Z	310	CHL	CAD-CBD-CGD-O1D
32	Z	313	CHL	CHA-CBD-CGD-O2D
32	7	314	CHL	CAD-CBD-CGD-O1D
32	7	315	CHL	CHA-CBD-CGD-O2D
32	8	315	CHL	CAD-CBD-CGD-O1D
32	8	316	CHL	CHA-CBD-CGD-O1D
32	8	316	CHL	CHA-CBD-CGD-O2D
32	8	317	CHL	CHA-CBD-CGD-O2D
32	8	319	CHL	CHA-CBD-CGD-O2D
32	4	314	CHL	CHA-CBD-CGD-O2D
32	4	315	CHL	CHA-CBD-CGD-O1D
32	4	315	CHL	CHA-CBD-CGD-O2D
32	4	317	CHL	CHA-CBD-CGD-O2D
32	5	315	CHL	CHA-CBD-CGD-O1D
32	5	315	CHL	CHA-CBD-CGD-O2D
32	5	316	CHL	CHA-CBD-CGD-O1D
32	5	316	CHL	CHA-CBD-CGD-O2D
32	5	318	CHL	CHA-CBD-CGD-O1D
32	5	318	CHL	CHA-CBD-CGD-O2D
32	5	320	CHL	CHA-CBD-CGD-O1D
32	5	320	CHL	CHA-CBD-CGD-O2D
32	6	317	CHL	CHA-CBD-CGD-O2D
32	6	319	CHL	CHA-CBD-CGD-O2D
23	1	5019	LHG	C10-C11-C12-C13
36	7	322	PLM	C8-C9-CA-CB
19	3	5010	CLA	C4-C3-C5-C6
19	B	827	CLA	C2B-C3B-CAB-CBB
19	Z	306	CLA	C2B-C3B-CAB-CBB
19	6	320	CLA	C2B-C3B-CAB-CBB
22	A	849	BCR	C1-C6-C7-C8
22	A	850	BCR	C1-C6-C7-C8
22	K	206	BCR	C23-C24-C25-C30
23	7	320	LHG	C5-C4-O6-P
31	1	5004	LUT	C11-C12-C13-C20
33	7	321	SPH	C2-C3-C4-C5
19	7	306	CLA	O1D-CGD-O2D-CED
19	A	808	CLA	C8-C10-C11-C12
19	B	815	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	A	832	CLA	C16-C17-C18-C19
19	3	5011	CLA	C11-C12-C13-C15
19	7	306	CLA	C11-C12-C13-C15
34	8	322	3PH	C1-O11-P-O12
23	8	321	LHG	C9-C10-C11-C12
19	8	312	CLA	C2C-C3C-CAC-CBC
32	Z	309	CHL	C8-C10-C11-C12
19	A	809	CLA	C11-C10-C8-C7
29	J	1903	LMG	C7-C8-O7-C10
34	6	325	3PH	C3-C2-O21-C21
36	7	322	PLM	C6-C7-C8-C9
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
19	Z	306	CLA	CAA-CBA-CGA-O2A
19	B	850	CLA	C13-C15-C16-C17
19	F	301	CLA	C2-C3-C5-C6
19	7	309	CLA	C16-C17-C18-C20
19	6	314	CLA	C6-C7-C8-C10
32	7	315	CHL	C5-C6-C7-C8
34	8	322	3PH	O11-C1-C2-C3
24	F	305	LMT	C5-C6-C7-C8
32	5	315	CHL	C5-C6-C7-C8
19	A	824	CLA	C11-C10-C8-C9
19	A	835	CLA	C6-C7-C8-C9
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	820	CLA	C6-C7-C8-C9
19	B	832	CLA	C6-C7-C8-C9
19	B	835	CLA	C11-C10-C8-C9
19	B	837	CLA	C11-C10-C8-C9
19	1	5012	CLA	C11-C10-C8-C9
19	Z	308	CLA	C11-C10-C8-C9
19	Z	315	CLA	C6-C7-C8-C9
19	7	319	CLA	C6-C7-C8-C9
19	8	308	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	4	306	CLA	C6-C7-C8-C9
19	5	307	CLA	C11-C10-C8-C9
19	5	317	CLA	C11-C12-C13-C14
32	5	315	CHL	C6-C7-C8-C9
32	6	316	CHL	C6-C7-C8-C9
19	A	810	CLA	C11-C12-C13-C15
19	A	819	CLA	C6-C7-C8-C10
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	828	CLA	C11-C12-C13-C15
19	Z	308	CLA	C11-C10-C8-C7
19	3	5008	CLA	C11-C12-C13-C15
19	7	306	CLA	C6-C7-C8-C10
19	8	309	CLA	C11-C12-C13-C15
19	5	321	CLA	C6-C7-C8-C10
19	6	301	CLA	C6-C7-C8-C10
32	7	314	CHL	C11-C10-C8-C7
32	8	319	CHL	C12-C13-C15-C16
23	6	303	LHG	O6-C4-C5-O7
24	G	1604	LMT	O5'-C1'-O1'-C1
32	8	315	CHL	C2A-CAA-CBA-CGA
19	8	311	CLA	C16-C17-C18-C20
19	A	838	CLA	CAA-CBA-CGA-O2A
30	K	201	DAO	C5-C6-C7-C8
32	1	5009	CHL	CBD-CGD-O2D-CED
19	B	824	CLA	C15-C16-C17-C18
19	3	5019	CLA	O1D-CGD-O2D-CED
19	A	838	CLA	C2-C3-C5-C6
23	1	5019	LHG	C24-C25-C26-C27
23	6	303	LHG	O9-C7-O7-C5
23	A	851	LHG	C14-C15-C16-C17
23	Z	316	LHG	O7-C5-C6-O8
23	6	324	LHG	O7-C5-C6-O8
19	B	808	CLA	CAA-CBA-CGA-O2A
19	6	301	CLA	CBA-CGA-O2A-C1
22	3	5004	BCR	C19-C20-C21-C22
31	Z	317	LUT	C33-C34-C35-C15
23	A	852	LHG	C10-C11-C12-C13
19	B	802	CLA	C16-C17-C18-C20
35	7	302	DGA	CB9-CAB-CBB-CCB
19	8	313	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	5	312	CLA	C5-C6-C7-C8
33	4	301	SPH	C11-C12-C13-C14
18	A	801	CL0	CAA-CBA-CGA-O2A
19	A	818	CLA	CBA-CGA-O2A-C1
25	B	848	DGD	O1A-C1A-O1G-C1G
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	6	323	CLA	CAA-CBA-CGA-O2A
19	B	803	CLA	C5-C6-C7-C8
19	6	310	CLA	CBA-CGA-O2A-C1
25	B	848	DGD	O1G-C1A-C2A-C3A
22	3	5004	BCR	C36-C18-C19-C20
19	4	312	CLA	C6-C7-C8-C9
23	6	303	LHG	C8-C7-O7-C5
23	Z	316	LHG	C31-C32-C33-C34
19	A	833	CLA	C8-C10-C11-C12
23	A	852	LHG	C25-C26-C27-C28
19	A	827	CLA	C2A-CAA-CBA-CGA
19	B	828	CLA	C2A-CAA-CBA-CGA
19	8	311	CLA	C2A-CAA-CBA-CGA
32	8	317	CHL	C2A-CAA-CBA-CGA
22	A	848	BCR	C19-C20-C21-C22
22	3	5006	BCR	C9-C10-C11-C12
22	6	308	BCR	C15-C16-C17-C18
19	3	5011	CLA	C11-C12-C13-C14
19	8	314	CLA	CBA-CGA-O2A-C1
24	4	302	LMT	C2-C1-O1'-C1'
19	B	807	CLA	C16-C17-C18-C19
19	1	5012	CLA	C11-C12-C13-C14
19	B	802	CLA	C6-C7-C8-C9
19	B	806	CLA	C6-C7-C8-C9
19	5	309	CLA	C6-C7-C8-C9
19	5	312	CLA	C11-C10-C8-C9
19	6	301	CLA	C6-C7-C8-C9
32	6	319	CHL	C11-C10-C8-C9
19	3	5014	CLA	O1A-CGA-O2A-C1
19	B	804	CLA	C2C-C3C-CAC-CBC
19	Z	307	CLA	C4B-C3B-CAB-CBB
19	3	5013	CLA	C8-C10-C11-C12
19	5	307	CLA	C8-C10-C11-C12
19	A	827	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
19	Z	315	CLA	C16-C17-C18-C19
19	3	5014	CLA	C8-C10-C11-C12
19	5	310	CLA	C5-C6-C7-C8
19	6	310	CLA	O1A-CGA-O2A-C1
19	B	802	CLA	CAA-CBA-CGA-O2A
23	Z	316	LHG	C29-C30-C31-C32
19	6	311	CLA	C2-C3-C5-C6
19	6	301	CLA	O1A-CGA-O2A-C1
22	B	846	BCR	C13-C14-C15-C16
27	5	302	RRX	C9-C10-C11-C12
32	8	315	CHL	CAA-CBA-CGA-O1A
19	A	803	CLA	C11-C12-C13-C15
19	A	828	CLA	C11-C10-C8-C7
19	B	819	CLA	C11-C10-C8-C7
19	B	821	CLA	C11-C10-C8-C7
19	7	310	CLA	C11-C12-C13-C15
19	7	319	CLA	C6-C7-C8-C10
19	5	309	CLA	C11-C10-C8-C7
19	6	311	CLA	C6-C7-C8-C10
32	Z	309	CHL	C11-C10-C8-C7
32	7	314	CHL	C5-C6-C7-C8
23	1	5019	LHG	C26-C27-C28-C29
19	8	308	CLA	O1A-CGA-O2A-C1
25	B	848	DGD	C2A-C1A-O1G-C1G
19	A	832	CLA	C16-C17-C18-C20
19	B	818	CLA	C5-C6-C7-C8
19	4	313	CLA	C5-C6-C7-C8
32	7	314	CHL	C10-C11-C12-C13
19	B	808	CLA	O1A-CGA-O2A-C1
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	4	313	CLA	C4-C3-C5-C6
19	5	314	CLA	C3A-C2A-CAA-CBA
19	6	309	CLA	C3A-C2A-CAA-CBA
32	4	314	CHL	C3A-C2A-CAA-CBA
34	3	5022	3PH	C3A-C3B-C3C-C3D
34	3	5022	3PH	C36-C37-C38-C39
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

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Mol	Chain	Res	Type	Atoms
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	4	313	CLA	C3-C5-C6-C7
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	3	5019	CLA	C2-C1-O2A-CGA
19	5	321	CLA	C2-C1-O2A-CGA
28	6	304	C7Z	C9-C10-C11-C12
31	5	303	LUT	C9-C10-C11-C12
33	4	301	SPH	C14-C15-C16-C17
32	3	5017	CHL	C16-C17-C18-C19
19	B	812	CLA	C5-C6-C7-C8
19	1	5012	CLA	C8-C10-C11-C12
19	5	317	CLA	C10-C11-C12-C13
19	6	301	CLA	C8-C10-C11-C12
19	6	320	CLA	C8-C10-C11-C12
22	3	5004	BCR	C11-C12-C13-C35
34	3	5022	3PH	C37-C38-C39-C3A
19	5	314	CLA	C10-C11-C12-C13
24	A	856	LMT	C3'-C4'-O1B-C1B
19	3	5014	CLA	C11-C12-C13-C15
23	Z	316	LHG	C27-C28-C29-C30
19	Z	312	CLA	C2A-CAA-CBA-CGA
32	5	315	CHL	C2A-CAA-CBA-CGA
32	Z	313	CHL	CAA-CBA-CGA-O2A
19	B	807	CLA	C15-C16-C17-C18
19	1	5011	CLA	C3-C5-C6-C7
19	A	816	CLA	C11-C10-C8-C9
19	A	823	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	803	CLA	C11-C10-C8-C9
19	B	808	CLA	C11-C10-C8-C9
19	B	812	CLA	C11-C10-C8-C9
19	B	823	CLA	C6-C7-C8-C9
19	B	824	CLA	C14-C13-C15-C16
19	B	832	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
19	1	5006	CLA	C14-C13-C15-C16
19	1	5016	CLA	C11-C10-C8-C9
19	7	308	CLA	C6-C7-C8-C9
19	7	308	CLA	C14-C13-C15-C16
19	6	313	CLA	C11-C10-C8-C9
19	6	323	CLA	C6-C7-C8-C9
32	3	5017	CHL	C11-C12-C13-C14
32	Z	309	CHL	CBD-CGD-O2D-CED
32	4	315	CHL	CBA-CGA-O2A-C1
23	6	324	LHG	C11-C10-C9-C8
23	7	320	LHG	C4-C5-O7-C7
29	J	1904	LMG	C9-C8-O7-C10
33	3	5001	SPH	C9-C10-C11-C12
19	A	817	CLA	C3-C5-C6-C7
32	3	5017	CHL	C1A-C2A-CAA-CBA
19	1	5010	CLA	C5-C6-C7-C8
19	3	5018	CLA	CBD-CGD-O2D-CED
19	5	301	CLA	CAA-CBA-CGA-O2A
23	A	851	LHG	C15-C16-C17-C18
23	1	5019	LHG	O1-C1-C2-O2
19	B	826	CLA	C3-C5-C6-C7
32	1	5009	CHL	O1D-CGD-O2D-CED
19	B	819	CLA	C2A-CAA-CBA-CGA
19	7	311	CLA	C2A-CAA-CBA-CGA
19	5	325	CLA	C2A-CAA-CBA-CGA
19	A	813	CLA	C13-C15-C16-C17
19	A	817	CLA	C5-C6-C7-C8
19	8	314	CLA	O1A-CGA-O2A-C1
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
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
23	A	852	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
23	8	321	LHG	C12-C13-C14-C15
19	A	818	CLA	C11-C12-C13-C15
19	B	805	CLA	CAA-CBA-CGA-O1A
34	5	324	3PH	C21-C22-C23-C24
35	7	302	DGA	CB6-CB7-CB8-CB9
19	A	828	CLA	C2B-C3B-CAB-CBB
19	Z	307	CLA	C2B-C3B-CAB-CBB
19	6	311	CLA	C2B-C3B-CAB-CBB
22	A	847	BCR	C23-C24-C25-C26
22	A	848	BCR	C5-C6-C7-C8
22	A	850	BCR	C23-C24-C25-C26
22	A	850	BCR	C23-C24-C25-C30
22	A	858	BCR	C23-C24-C25-C30
22	A	859	BCR	C23-C24-C25-C30
22	B	843	BCR	C23-C24-C25-C26
22	B	845	BCR	C23-C24-C25-C26
22	B	847	BCR	C5-C6-C7-C8
22	K	206	BCR	C1-C6-C7-C8
22	3	5005	BCR	C23-C24-C25-C26
22	3	5007	BCR	C5-C6-C7-C8
32	Z	313	CHL	CAA-CBA-CGA-O1A
19	A	819	CLA	C8-C10-C11-C12
19	B	836	CLA	C5-C6-C7-C8
23	3	5021	LHG	C5-C4-O6-P
23	5	323	LHG	C5-C4-O6-P
23	6	303	LHG	C2-C3-O3-P
19	5	301	CLA	C11-C10-C8-C9
19	A	810	CLA	C4-C3-C5-C6
23	6	324	LHG	C25-C26-C27-C28
23	Z	316	LHG	C26-C27-C28-C29
37	8	302	SQD	C23-C24-C25-C26
19	B	805	CLA	CAA-CBA-CGA-O2A
24	8	323	LMT	C11-C10-C9-C8
18	A	801	CL0	C11-C10-C8-C7
19	A	808	CLA	C11-C12-C13-C15
19	A	812	CLA	C11-C10-C8-C7
19	A	819	CLA	C11-C10-C8-C7
19	A	825	CLA	C11-C12-C13-C15
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

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Mol	Chain	Res	Type	Atoms
19	A	842	CLA	C11-C12-C13-C15
19	B	819	CLA	C11-C12-C13-C15
19	B	823	CLA	C6-C7-C8-C10
19	B	840	CLA	C11-C10-C8-C7
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	308	CLA	C6-C7-C8-C10
19	6	313	CLA	C11-C10-C8-C7
19	6	323	CLA	C6-C7-C8-C10
32	6	315	CHL	C11-C10-C8-C7
19	B	807	CLA	C16-C17-C18-C20
19	B	838	CLA	C2A-CAA-CBA-CGA
19	7	310	CLA	C2A-CAA-CBA-CGA
23	Z	316	LHG	C30-C31-C32-C33
25	B	848	DGD	CCA-CDA-CEA-CFA
19	4	307	CLA	CAA-CBA-CGA-O2A
19	6	301	CLA	C11-C12-C13-C15
19	B	811	CLA	C11-C10-C8-C7
19	5	301	CLA	C11-C10-C8-C7
19	5	308	CLA	C11-C10-C8-C7
19	B	829	CLA	C8-C10-C11-C12
32	8	319	CHL	C4-C3-C5-C6
23	A	852	LHG	C24-C23-O8-C6
24	1	5002	LMT	C7-C8-C9-C10
19	A	830	CLA	C2-C3-C5-C6
24	Z	319	LMT	C4-C5-C6-C7
19	8	311	CLA	C2-C1-O2A-CGA
19	B	812	CLA	CAA-CBA-CGA-O2A
19	B	808	CLA	CBA-CGA-O2A-C1
23	6	303	LHG	C9-C10-C11-C12
19	Z	311	CLA	C2A-CAA-CBA-CGA
32	6	319	CHL	C2A-CAA-CBA-CGA
19	B	813	CLA	C6-C7-C8-C9
19	4	310	CLA	C11-C10-C8-C9
19	6	311	CLA	C6-C7-C8-C9
19	8	308	CLA	C8-C10-C11-C12
32	Z	309	CHL	O1D-CGD-O2D-CED
22	B	844	BCR	C13-C14-C15-C16
19	6	313	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	Z	308	CLA	C16-C17-C18-C20
23	5	323	LHG	C11-C10-C9-C8
33	7	321	SPH	O1-C1-C2-C3
19	B	817	CLA	C4-C3-C5-C6
32	3	5017	CHL	C4-C3-C5-C6
19	4	308	CLA	C15-C16-C17-C18
19	B	817	CLA	C2-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
19	4	311	CLA	CBD-CGD-O2D-CED
19	3	5014	CLA	CBA-CGA-O2A-C1
19	B	807	CLA	C10-C11-C12-C13
25	B	848	DGD	O6D-C5D-C6D-O5D
19	A	809	CLA	C11-C10-C8-C9
19	B	807	CLA	C2A-CAA-CBA-CGA
23	4	320	LHG	C17-C18-C19-C20
19	B	807	CLA	CAA-CBA-CGA-O2A
19	B	835	CLA	C4-C3-C5-C6
19	4	312	CLA	C4-C3-C5-C6
19	A	834	CLA	C4B-C3B-CAB-CBB
19	B	803	CLA	C4B-C3B-CAB-CBB
19	8	318	CLA	C4B-C3B-CAB-CBB
23	A	852	LHG	O10-C23-O8-C6
19	A	829	CLA	CAA-CBA-CGA-O2A
24	A	856	LMT	C5'-C4'-O1B-C1B
34	3	5022	3PH	C23-C24-C25-C26
19	1	5007	CLA	CAA-CBA-CGA-O2A
19	1	5012	CLA	C11-C12-C13-C15
19	6	302	CLA	C11-C12-C13-C15
32	1	5009	CHL	C10-C11-C12-C13
32	7	315	CHL	CHA-CBD-CGD-O1D
32	6	317	CHL	CHA-CBD-CGD-O1D
19	B	836	CLA	CAA-CBA-CGA-O2A
19	A	822	CLA	C2C-C3C-CAC-CBC
19	B	826	CLA	C10-C11-C12-C13
23	1	5001	LHG	O6-C4-C5-C6
19	6	309	CLA	CAA-CBA-CGA-O2A
19	B	817	CLA	C10-C11-C12-C13
32	6	315	CHL	C15-C16-C17-C18
19	B	812	CLA	C6-C7-C8-C10
19	B	813	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	B	826	CLA	C6-C7-C8-C10
19	8	310	CLA	C6-C7-C8-C10
22	B	845	BCR	C13-C14-C15-C16
31	7	303	LUT	C9-C10-C11-C12
19	Z	307	CLA	CAA-CBA-CGA-O2A
23	6	303	LHG	C10-C11-C12-C13
19	A	803	CLA	C11-C10-C8-C9
19	A	829	CLA	C6-C7-C8-C9
19	B	826	CLA	C6-C7-C8-C9
19	B	827	CLA	C11-C10-C8-C9
19	B	836	CLA	C6-C7-C8-C9
19	1	5008	CLA	C11-C10-C8-C9
19	5	301	CLA	C6-C7-C8-C9
19	5	312	CLA	C6-C7-C8-C9
19	6	323	CLA	C11-C12-C13-C14
20	A	844	PQN	C21-C22-C23-C24
35	7	302	DGA	CEB-CFB-CGB-CHB
32	4	315	CHL	O1A-CGA-O2A-C1
19	B	808	CLA	C13-C15-C16-C17
19	B	811	CLA	C5-C6-C7-C8
25	B	848	DGD	C2A-C3A-C4A-C5A
19	3	5015	CLA	CAA-CBA-CGA-O2A
19	A	837	CLA	C2A-CAA-CBA-CGA
19	A	817	CLA	C2-C1-O2A-CGA
19	8	313	CLA	C2-C1-O2A-CGA
19	5	309	CLA	C2-C1-O2A-CGA
19	5	314	CLA	C2-C1-O2A-CGA
19	5	317	CLA	C2-C1-O2A-CGA
19	3	5014	CLA	C11-C12-C13-C14
19	B	822	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
38	8	325	ERG	C23-C24-C25-C27
19	B	824	CLA	CAA-CBA-CGA-O2A
19	B	823	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	8	312	CLA	C10-C11-C12-C13
19	7	306	CLA	CAA-CBA-CGA-O2A
19	B	810	CLA	O2A-C1-C2-C3
19	B	817	CLA	O2A-C1-C2-C3
19	5	310	CLA	O2A-C1-C2-C3
19	3	5010	CLA	CAA-CBA-CGA-O2A
28	1	5005	C7Z	C13-C14-C15-C35
19	A	805	CLA	CAA-CBA-CGA-O1A
19	A	827	CLA	C16-C17-C18-C19
19	1	5007	CLA	CAA-CBA-CGA-O1A
32	6	319	CHL	C13-C15-C16-C17
19	8	307	CLA	C4-C3-C5-C6
19	B	820	CLA	C2-C3-C5-C6
24	7	323	LMT	C9-C10-C11-C12
19	8	308	CLA	CBA-CGA-O2A-C1
33	4	301	SPH	C4-C5-C6-C7
19	B	832	CLA	C3-C5-C6-C7
23	8	321	LHG	C25-C26-C27-C28
19	3	5018	CLA	O1D-CGD-O2D-CED
23	5	323	LHG	C29-C30-C31-C32
19	K	205	CLA	CAA-CBA-CGA-O2A
35	7	302	DGA	CB2-CB3-CB4-CB5
19	Z	303	CLA	O1D-CGD-O2D-CED
19	8	308	CLA	C4-C3-C5-C6
22	B	843	BCR	C19-C20-C21-C22
28	J	1902	C7Z	C29-C30-C31-C32
19	A	830	CLA	C3-C5-C6-C7
23	6	324	LHG	C31-C32-C33-C34
19	7	308	CLA	C5-C6-C7-C8
19	3	5015	CLA	CAA-CBA-CGA-O1A
34	6	325	3PH	C29-C2A-C2B-C2C
19	A	807	CLA	CAA-CBA-CGA-O2A
19	3	5020	CLA	C2C-C3C-CAC-CBC
34	8	322	3PH	O21-C2-C3-O31
19	A	827	CLA	C11-C10-C8-C9
19	A	839	CLA	C11-C10-C8-C9
19	B	837	CLA	C11-C12-C13-C14
19	3	5008	CLA	C6-C7-C8-C9
19	3	5008	CLA	C11-C12-C13-C14
19	3	5012	CLA	C14-C13-C15-C16
19	3	5016	CLA	C6-C7-C8-C9
19	7	312	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	7	314	CHL	C6-C7-C8-C9
19	A	818	CLA	C11-C12-C13-C14
23	6	324	LHG	O6-C4-C5-C6
19	B	850	CLA	C4C-C3C-CAC-CBC
19	A	857	CLA	CAA-CBA-CGA-O2A
19	B	837	CLA	CAA-CBA-CGA-O2A
23	1	5019	LHG	O8-C23-C24-C25
19	A	814	CLA	C11-C10-C8-C7
19	A	816	CLA	C11-C12-C13-C15
19	A	825	CLA	C11-C10-C8-C7
19	A	826	CLA	C11-C10-C8-C7
19	A	829	CLA	C6-C7-C8-C10
19	B	818	CLA	C6-C7-C8-C10
19	B	823	CLA	C11-C12-C13-C15
19	B	825	CLA	C11-C10-C8-C7
19	B	836	CLA	C6-C7-C8-C10
19	1	5008	CLA	C12-C13-C15-C16
19	Z	312	CLA	C11-C12-C13-C15
19	Z	315	CLA	C11-C12-C13-C15
19	3	5008	CLA	C6-C7-C8-C10
19	3	5013	CLA	C11-C12-C13-C15
19	7	319	CLA	C11-C10-C8-C7
19	5	301	CLA	C6-C7-C8-C10
19	5	312	CLA	C6-C7-C8-C10
19	6	320	CLA	C11-C10-C8-C7
20	A	844	PQN	C21-C22-C23-C25
20	A	844	PQN	C13-C15-C16-C17
19	A	834	CLA	C2B-C3B-CAB-CBB
19	B	803	CLA	C2B-C3B-CAB-CBB
19	8	318	CLA	C2B-C3B-CAB-CBB
19	5	313	CLA	C2B-C3B-CAB-CBB
22	A	859	BCR	C23-C24-C25-C26
22	B	846	BCR	C5-C6-C7-C8
22	F	302	BCR	C23-C24-C25-C26
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
19	B	819	CLA	CAA-CBA-CGA-O2A
19	3	5014	CLA	CAA-CBA-CGA-O2A
23	A	851	LHG	C12-C13-C14-C15
19	B	815	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
23	5	323	LHG	O8-C23-C24-C25
19	5	314	CLA	C5-C6-C7-C8
19	5	325	CLA	C4-C3-C5-C6
19	5	322	CLA	CAA-CBA-CGA-O2A
19	5	308	CLA	C5-C6-C7-C8
19	B	808	CLA	C2A-CAA-CBA-CGA
19	B	819	CLA	C15-C16-C17-C18
19	A	832	CLA	CAA-CBA-CGA-O2A
19	5	310	CLA	C3-C5-C6-C7
23	1	5019	LHG	C27-C28-C29-C30
19	A	820	CLA	O1D-CGD-O2D-CED
19	A	824	CLA	CAA-CBA-CGA-O2A
19	6	302	CLA	CAA-CBA-CGA-O2A
23	4	320	LHG	O8-C23-C24-C25
34	6	325	3PH	O21-C21-C22-C23
30	K	201	DAO	C9-C10-C11-C12
19	7	311	CLA	C11-C10-C8-C7
32	8	316	CHL	C11-C10-C8-C7
19	B	818	CLA	C4-C3-C5-C6
19	A	837	CLA	CAA-CBA-CGA-O2A
19	B	809	CLA	CAA-CBA-CGA-O2A
19	1	5006	CLA	CAA-CBA-CGA-O2A
19	4	313	CLA	C2-C3-C5-C6
18	A	801	CL0	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	834	CLA	C11-C12-C13-C14
19	B	819	CLA	C11-C12-C13-C14
19	B	828	CLA	C11-C12-C13-C14
19	F	301	CLA	C11-C12-C13-C14
19	Z	307	CLA	C11-C10-C8-C9
19	3	5010	CLA	C11-C10-C8-C9
19	3	5018	CLA	C11-C10-C8-C9
19	6	313	CLA	C11-C12-C13-C14
19	A	806	CLA	C15-C16-C17-C18
31	1	5003	LUT	C31-C32-C33-C40
19	A	823	CLA	CAA-CBA-CGA-O2A
19	A	843	CLA	CAA-CBA-CGA-O2A
19	B	811	CLA	CAA-CBA-CGA-O2A
19	5	311	CLA	CAA-CBA-CGA-O2A
19	5	319	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
32	Z	309	CHL	CAA-CBA-CGA-O2A
35	7	302	DGA	OG1-CG1-CG2-CG3
19	A	842	CLA	C1A-C2A-CAA-CBA
19	B	824	CLA	C1A-C2A-CAA-CBA
19	B	826	CLA	C4B-C3B-CAB-CBB
19	G	1602	CLA	C1A-C2A-CAA-CBA
19	G	1602	CLA	C4B-C3B-CAB-CBB
19	K	205	CLA	CAA-CBA-CGA-O1A
19	A	813	CLA	CAA-CBA-CGA-O2A
19	A	833	CLA	CAA-CBA-CGA-O2A
19	B	835	CLA	CAA-CBA-CGA-O2A
19	1	5011	CLA	CAA-CBA-CGA-O2A
19	5	310	CLA	CAA-CBA-CGA-O2A
23	6	303	LHG	O7-C7-C8-C9
23	1	5019	LHG	O7-C5-C6-O8
22	3	5004	BCR	C11-C12-C13-C14
22	3	5004	BCR	C17-C18-C19-C20
19	K	205	CLA	C2C-C3C-CAC-CBC
22	A	850	BCR	C13-C14-C15-C16
22	3	5004	BCR	C13-C14-C15-C16
19	B	832	CLA	C8-C10-C11-C12
19	B	813	CLA	CAA-CBA-CGA-O2A
19	B	822	CLA	CAA-CBA-CGA-O2A
23	1	5019	LHG	O7-C7-C8-C9
23	7	320	LHG	O8-C23-C24-C25
19	K	204	CLA	C2A-CAA-CBA-CGA
23	6	324	LHG	C17-C18-C19-C20
19	B	837	CLA	C13-C15-C16-C17
29	J	1903	LMG	C12-C13-C14-C15
19	1	5010	CLA	O1D-CGD-O2D-CED
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	6	311	CLA	CAA-CBA-CGA-O2A
23	A	852	LHG	C11-C10-C9-C8
19	A	804	CLA	C2-C1-O2A-CGA
19	A	805	CLA	C2-C1-O2A-CGA
19	5	310	CLA	C2-C1-O2A-CGA
23	Z	316	LHG	O8-C23-C24-C25
19	A	802	CLA	C11-C10-C8-C7
19	A	811	CLA	C11-C10-C8-C7
19	A	817	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
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	B	813	CLA	C11-C10-C8-C7
19	B	826	CLA	C11-C12-C13-C15
19	B	831	CLA	C6-C7-C8-C10
19	1	5006	CLA	C11-C12-C13-C15
19	Z	312	CLA	C11-C10-C8-C7
19	3	5014	CLA	C11-C10-C8-C7
19	6	313	CLA	C11-C12-C13-C15
32	8	319	CHL	C11-C12-C13-C15
32	8	319	CHL	C2-C3-C5-C6
19	A	820	CLA	C11-C12-C13-C15
23	7	320	LHG	C6-C5-O7-C7
23	Z	316	LHG	C11-C10-C9-C8
19	3	5016	CLA	CAA-CBA-CGA-O2A
24	Z	301	LMT	C11-C10-C9-C8
23	Z	316	LHG	C10-C11-C12-C13
23	6	324	LHG	C15-C16-C17-C18
19	A	857	CLA	CAA-CBA-CGA-O1A
19	A	838	CLA	O1A-CGA-O2A-C1
19	B	819	CLA	C10-C11-C12-C13
19	A	823	CLA	C3A-C2A-CAA-CBA
19	A	832	CLA	C3A-C2A-CAA-CBA
19	B	805	CLA	C3A-C2A-CAA-CBA
19	A	820	CLA	CBD-CGD-O2D-CED
19	8	311	CLA	C3-C5-C6-C7
23	A	852	LHG	C16-C17-C18-C19
19	A	807	CLA	CAA-CBA-CGA-O1A
19	A	832	CLA	CAA-CBA-CGA-O1A
23	4	320	LHG	O10-C23-C24-C25
29	J	1904	LMG	C21-C22-C23-C24
19	4	309	CLA	C5-C6-C7-C8
23	A	852	LHG	C35-C36-C37-C38
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	B	815	CLA	CAA-CBA-CGA-O1A
19	6	302	CLA	CAA-CBA-CGA-O1A
19	B	804	CLA	C16-C17-C18-C20
19	3	5018	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	A	817	CLA	C6-C7-C8-C9
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	825	CLA	C6-C7-C8-C9
19	B	826	CLA	C11-C12-C13-C14
19	1	5006	CLA	C11-C12-C13-C14
19	I	201	CLA	CAA-CBA-CGA-O1A
23	1	5019	LHG	O10-C23-C24-C25
19	A	827	CLA	C15-C16-C17-C18
22	A	858	BCR	C15-C16-C17-C18
38	8	325	ERG	C23-C24-C25-C26
19	A	824	CLA	CAA-CBA-CGA-O1A
19	B	809	CLA	CAA-CBA-CGA-O1A
19	B	819	CLA	CAA-CBA-CGA-O1A
19	3	5014	CLA	CAA-CBA-CGA-O1A
32	6	317	CHL	CBA-CGA-O2A-C1
19	Z	303	CLA	CAA-CBA-CGA-O2A
19	B	816	CLA	O1A-CGA-O2A-C1
32	6	317	CHL	O1A-CGA-O2A-C1
19	B	837	CLA	CAA-CBA-CGA-O1A
34	6	325	3PH	O22-C21-C22-C23
19	5	309	CLA	C3-C5-C6-C7
19	B	826	CLA	CAA-CBA-CGA-O2A
19	6	314	CLA	CAA-CBA-CGA-O2A
31	1	5003	LUT	C31-C32-C33-C34
19	A	836	CLA	CAA-CBA-CGA-O1A
19	A	843	CLA	CAA-CBA-CGA-O1A
19	1	5006	CLA	CAA-CBA-CGA-O1A
19	3	5016	CLA	CAA-CBA-CGA-O1A
19	5	310	CLA	CAA-CBA-CGA-O1A
19	5	319	CLA	CAA-CBA-CGA-O1A
19	5	322	CLA	CAA-CBA-CGA-O1A
19	3	5020	CLA	C4C-C3C-CAC-CBC
19	B	833	CLA	C13-C15-C16-C17
24	Z	301	LMT	C2-C3-C4-C5
19	A	813	CLA	CAA-CBA-CGA-O1A
19	1	5010	CLA	CAA-CBA-CGA-O1A
19	1	5011	CLA	CAA-CBA-CGA-O1A
23	5	323	LHG	O10-C23-C24-C25
19	B	801	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
19	6	309	CLA	C11-C12-C13-C14
23	8	321	LHG	C4-C5-C6-O8
23	4	320	LHG	C4-C5-C6-O8
24	Z	301	LMT	C4-C5-C6-C7
19	B	813	CLA	CAA-CBA-CGA-O1A
19	5	311	CLA	CAA-CBA-CGA-O1A
23	Z	316	LHG	O10-C23-C24-C25
32	Z	309	CHL	CAA-CBA-CGA-O1A
19	4	310	CLA	C10-C11-C12-C13
19	3	5013	CLA	CAA-CBA-CGA-O2A
32	6	316	CHL	CAA-CBA-CGA-O2A
24	4	302	LMT	C7-C8-C9-C10
19	A	837	CLA	CAA-CBA-CGA-O1A
19	B	811	CLA	CAA-CBA-CGA-O1A
23	1	5019	LHG	O9-C7-C8-C9
19	B	808	CLA	CAD-CBD-CGD-O2D
32	3	5017	CHL	CAD-CBD-CGD-O2D
24	Z	301	LMT	C3-C4-C5-C6
19	K	203	CLA	CAA-CBA-CGA-O2A
19	5	317	CLA	CAA-CBA-CGA-O2A
19	A	823	CLA	CAA-CBA-CGA-O1A
19	A	833	CLA	CAA-CBA-CGA-O1A
19	B	822	CLA	CAA-CBA-CGA-O1A
19	6	311	CLA	CAA-CBA-CGA-O1A
23	7	320	LHG	O10-C23-C24-C25
23	7	320	LHG	C27-C28-C29-C30
19	B	816	CLA	C10-C11-C12-C13
19	B	801	CLA	C2-C1-O2A-CGA
32	5	316	CHL	C2-C1-O2A-CGA
19	B	829	CLA	CAA-CBA-CGA-O2A
19	1	5008	CLA	CAA-CBA-CGA-O2A
19	7	307	CLA	CAA-CBA-CGA-O2A
32	1	5014	CHL	CAA-CBA-CGA-O2A
32	4	314	CHL	CAA-CBA-CGA-O2A
18	A	801	CL0	C1A-C2A-CAA-CBA
19	B	813	CLA	C16-C17-C18-C19
19	5	310	CLA	C6-C7-C8-C9
19	5	314	CLA	C16-C17-C18-C20
24	G	1604	LMT	C7-C8-C9-C10
19	5	313	CLA	CAA-CBA-CGA-O2A
23	8	321	LHG	C11-C10-C9-C8
19	A	802	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	B	810	CLA	CAA-CBA-CGA-O2A
19	B	850	CLA	CAA-CBA-CGA-O2A
19	1	5012	CLA	CAA-CBA-CGA-O2A
29	J	1903	LMG	O7-C10-C11-C12
32	6	317	CHL	CAA-CBA-CGA-O2A
19	7	319	CLA	CAA-CBA-CGA-O1A
23	6	303	LHG	O9-C7-C8-C9
19	A	811	CLA	CAA-CBA-CGA-O2A
19	6	313	CLA	CAA-CBA-CGA-O2A
23	6	324	LHG	O8-C23-C24-C25
32	7	315	CHL	CAA-CBA-CGA-O2A
32	4	315	CHL	CAA-CBA-CGA-O2A
19	B	831	CLA	C15-C16-C17-C18
19	Z	303	CLA	CAA-CBA-CGA-O1A
23	Z	316	LHG	O9-C7-C8-C9
25	B	848	DGD	CDB-CEB-CFB-CGB

There are no ring outliers.

311 monomers are involved in 2285 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	807	CLA	4	0
19	B	828	CLA	6	0
19	B	837	CLA	15	0
19	A	820	CLA	9	0
19	Z	304	CLA	4	0
19	7	311	CLA	9	0
29	J	1903	LMG	4	0
34	5	324	3PH	2	0
19	1	5015	CLA	2	0
19	5	311	CLA	12	0
28	1	5005	C7Z	1	0
19	K	203	CLA	12	0
18	A	801	CL0	9	0
32	6	317	CHL	8	0
19	5	313	CLA	11	0
32	6	319	CHL	17	0
19	A	835	CLA	15	0
19	1	5012	CLA	13	0
19	A	828	CLA	21	0
22	3	5004	BCR	6	0
19	B	808	CLA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Z	307	CLA	7	0
19	B	835	CLA	16	0
19	A	838	CLA	11	0
19	4	309	CLA	5	0
19	6	310	CLA	21	0
19	6	323	CLA	12	0
19	4	313	CLA	12	0
19	8	307	CLA	16	0
32	8	315	CHL	13	0
19	3	5020	CLA	7	0
35	7	302	DGA	14	0
32	6	315	CHL	14	0
19	A	822	CLA	18	0
19	F	303	CLA	4	0
19	1	5010	CLA	12	0
19	A	837	CLA	6	0
19	A	810	CLA	6	0
22	8	303	BCR	10	0
31	7	303	LUT	5	0
32	Z	302	CHL	15	0
19	A	827	CLA	17	0
19	7	307	CLA	15	0
19	B	811	CLA	4	0
32	5	320	CHL	8	0
19	B	820	CLA	8	0
19	A	814	CLA	15	0
19	3	5014	CLA	11	0
24	4	302	LMT	6	0
19	5	301	CLA	7	0
22	G	1603	BCR	12	0
19	6	313	CLA	26	0
30	K	201	DAO	4	0
19	A	804	CLA	8	0
19	1	5007	CLA	13	0
19	B	825	CLA	18	0
19	B	812	CLA	8	0
19	G	1602	CLA	10	0
19	3	5010	CLA	10	0
32	8	301	CHL	14	0
38	8	325	ERG	14	0
19	A	811	CLA	9	0
32	5	315	CHL	16	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	6	324	LHG	12	0
19	3	5008	CLA	13	0
28	6	304	C7Z	3	0
19	3	5011	CLA	5	0
19	1	5008	CLA	7	0
19	A	809	CLA	9	0
19	A	833	CLA	11	0
31	3	5002	LUT	4	0
19	A	821	CLA	18	0
27	F	304	RRX	9	0
28	J	1902	C7Z	1	0
32	5	318	CHL	15	0
19	B	806	CLA	6	0
22	5	304	BCR	11	0
21	A	845	SF4	5	0
36	7	322	PLM	2	0
31	5	303	LUT	9	0
19	1	5006	CLA	4	0
19	B	818	CLA	6	0
23	3	5021	LHG	4	0
19	B	803	CLA	14	0
19	B	816	CLA	10	0
19	Z	303	CLA	6	0
19	7	308	CLA	14	0
19	Z	314	CLA	10	0
19	A	842	CLA	7	0
32	6	316	CHL	16	0
19	5	308	CLA	9	0
31	4	304	LUT	11	0
19	K	204	CLA	9	0
19	5	317	CLA	12	0
19	6	302	CLA	15	0
19	5	319	CLA	8	0
22	A	848	BCR	7	0
33	3	5001	SPH	12	0
19	3	5018	CLA	12	0
19	4	318	CLA	2	0
19	G	1601	CLA	6	0
23	Z	316	LHG	6	0
19	4	310	CLA	8	0
32	4	319	CHL	5	0
32	4	315	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	7	320	LHG	3	0
19	A	813	CLA	4	0
19	B	826	CLA	17	0
19	B	827	CLA	9	0
19	B	832	CLA	14	0
22	B	847	BCR	8	0
24	3	5023	LMT	7	0
24	1	5002	LMT	8	0
19	A	807	CLA	6	0
19	B	809	CLA	8	0
19	7	324	CLA	14	0
19	8	308	CLA	9	0
19	A	806	CLA	12	0
24	Z	319	LMT	5	0
19	Z	305	CLA	11	0
22	4	305	BCR	14	0
19	B	834	CLA	11	0
22	A	859	BCR	13	0
19	5	307	CLA	20	0
22	A	849	BCR	18	0
22	A	846	BCR	7	0
23	1	5019	LHG	10	0
19	A	831	CLA	2	0
23	8	321	LHG	7	0
19	A	840	CLA	5	0
19	A	832	CLA	14	0
19	7	313	CLA	3	0
19	A	819	CLA	12	0
19	5	321	CLA	12	0
33	7	321	SPH	7	0
20	B	841	PQN	4	0
20	A	844	PQN	4	0
19	A	836	CLA	13	0
22	3	5007	BCR	8	0
19	B	817	CLA	5	0
19	A	829	CLA	8	0
29	J	1904	LMG	10	0
19	B	804	CLA	10	0
19	6	311	CLA	8	0
19	J	1901	CLA	4	0
19	5	312	CLA	10	0
29	7	301	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	815	CLA	10	0
31	8	304	LUT	10	0
19	3	5013	CLA	9	0
19	1	5013	CLA	7	0
19	B	801	CLA	15	0
25	B	848	DGD	5	0
19	6	301	CLA	18	0
24	A	854	LMT	5	0
19	B	819	CLA	18	0
19	A	857	CLA	9	0
31	6	306	LUT	4	0
19	A	823	CLA	17	0
19	5	306	CLA	22	0
19	A	841	CLA	13	0
24	A	853	LMT	9	0
19	8	320	CLA	3	0
23	A	852	LHG	5	0
19	3	5016	CLA	15	0
19	1	5016	CLA	23	0
19	B	821	CLA	21	0
24	Z	301	LMT	8	0
19	A	839	CLA	20	0
19	B	850	CLA	27	0
31	1	5003	LUT	7	0
19	4	306	CLA	22	0
19	B	840	CLA	12	0
19	7	312	CLA	13	0
19	8	311	CLA	8	0
19	B	830	CLA	8	0
34	8	322	3PH	6	0
19	6	318	CLA	3	0
22	5	305	BCR	6	0
32	5	316	CHL	6	0
19	A	818	CLA	12	0
19	A	825	CLA	9	0
19	7	306	CLA	13	0
19	A	816	CLA	14	0
33	4	301	SPH	7	0
19	B	813	CLA	8	0
22	B	844	BCR	11	0
32	7	314	CHL	10	0
22	3	5005	BCR	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	4	312	CLA	12	0
19	A	805	CLA	10	0
24	4	321	LMT	2	0
19	F	301	CLA	11	0
19	A	815	CLA	20	0
31	8	305	LUT	3	0
23	5	323	LHG	7	0
19	7	310	CLA	3	0
22	B	846	BCR	19	0
31	3	5003	LUT	9	0
19	B	831	CLA	12	0
19	A	826	CLA	9	0
31	7	304	LUT	11	0
32	8	316	CHL	5	0
24	F	305	LMT	9	0
19	Z	308	CLA	11	0
19	5	310	CLA	16	0
19	Z	315	CLA	9	0
19	Z	312	CLA	9	0
19	B	836	CLA	10	0
19	A	834	CLA	9	0
32	1	5009	CHL	5	0
32	1	5014	CHL	7	0
19	A	803	CLA	6	0
19	B	823	CLA	23	0
22	7	305	BCR	5	0
31	1	5004	LUT	8	0
19	8	312	CLA	20	0
19	B	810	CLA	6	0
19	A	830	CLA	11	0
19	5	314	CLA	17	0
19	6	309	CLA	12	0
27	5	302	RRX	11	0
19	8	309	CLA	11	0
19	7	309	CLA	4	0
19	4	308	CLA	12	0
22	A	858	BCR	5	0
32	8	317	CHL	3	0
22	6	308	BCR	16	0
19	7	317	CLA	7	0
23	6	303	LHG	9	0
22	A	850	BCR	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	3	5012	CLA	18	0
22	B	842	BCR	17	0
19	A	817	CLA	7	0
19	8	314	CLA	2	0
22	A	847	BCR	13	0
19	5	322	CLA	5	0
19	3	5015	CLA	5	0
19	3	5009	CLA	8	0
22	B	843	BCR	5	0
22	K	206	BCR	14	0
24	A	855	LMT	1	0
19	4	316	CLA	8	0
32	4	314	CHL	14	0
24	4	322	LMT	11	0
19	4	307	CLA	14	0
19	A	802	CLA	14	0
19	B	829	CLA	13	0
32	Z	310	CHL	11	0
19	1	5011	CLA	10	0
19	4	311	CLA	12	0
32	3	5017	CHL	11	0
19	7	316	CLA	4	0
19	B	833	CLA	17	0
22	6	307	BCR	23	0
19	B	805	CLA	2	0
31	Z	318	LUT	8	0
38	6	326	ERG	24	0
22	3	5006	BCR	21	0
27	4	303	RRX	6	0
19	Z	306	CLA	3	0
19	I	201	CLA	5	0
19	B	824	CLA	16	0
19	8	313	CLA	12	0
24	A	856	LMT	8	0
37	8	302	SQD	11	0
19	K	202	CLA	12	0
19	1	5018	CLA	4	0
19	A	808	CLA	14	0
19	Z	311	CLA	9	0
19	6	320	CLA	10	0
23	A	851	LHG	6	0
31	Z	317	LUT	12	0

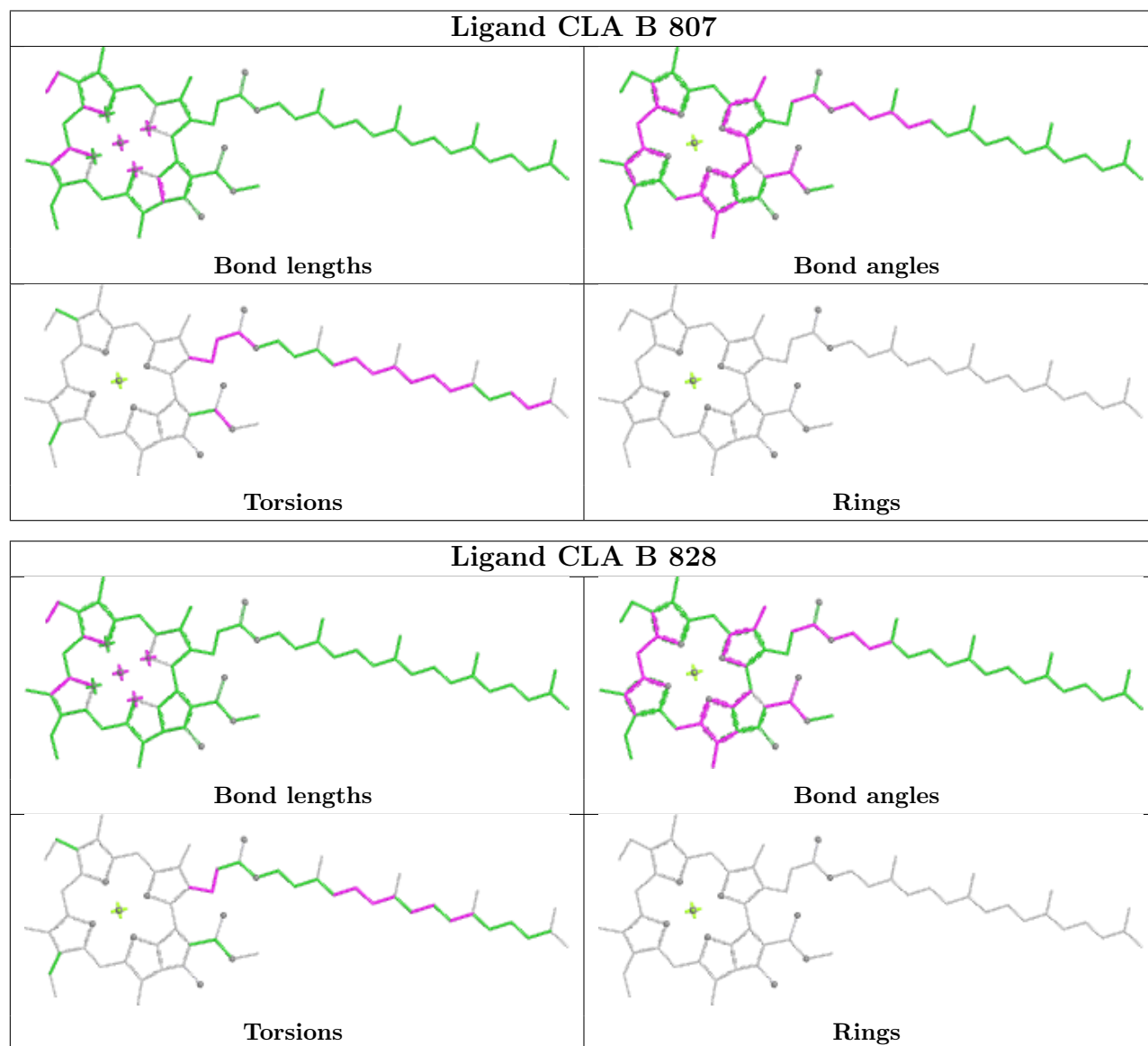
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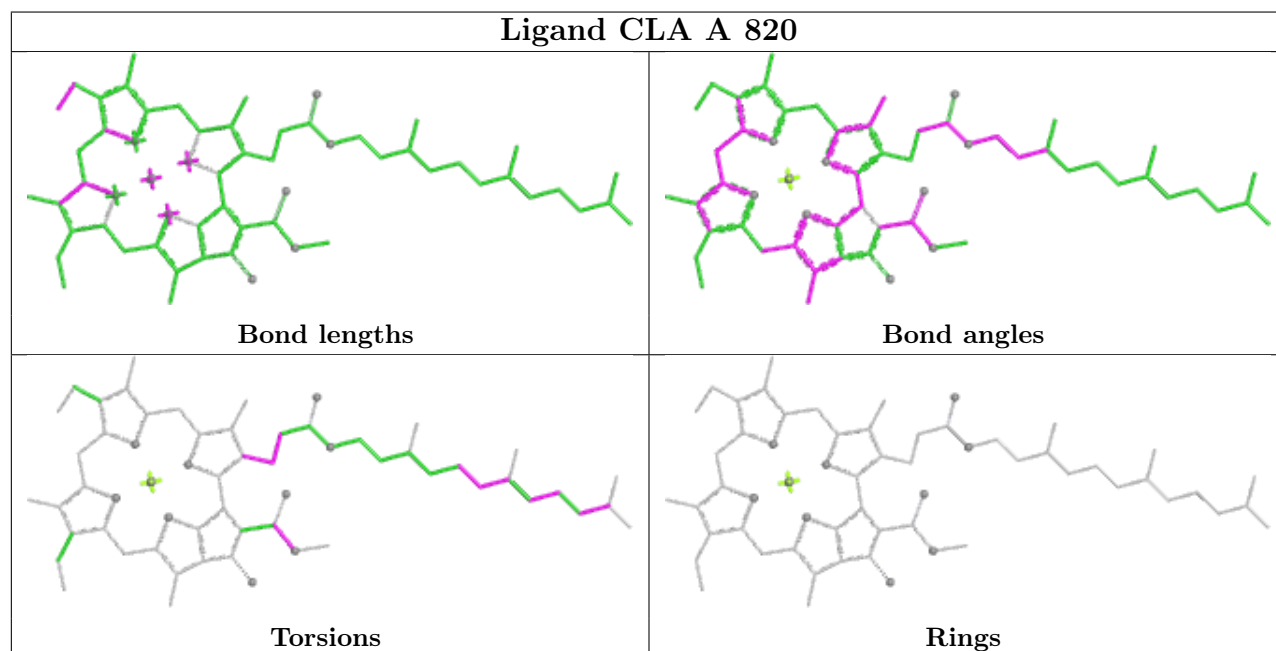
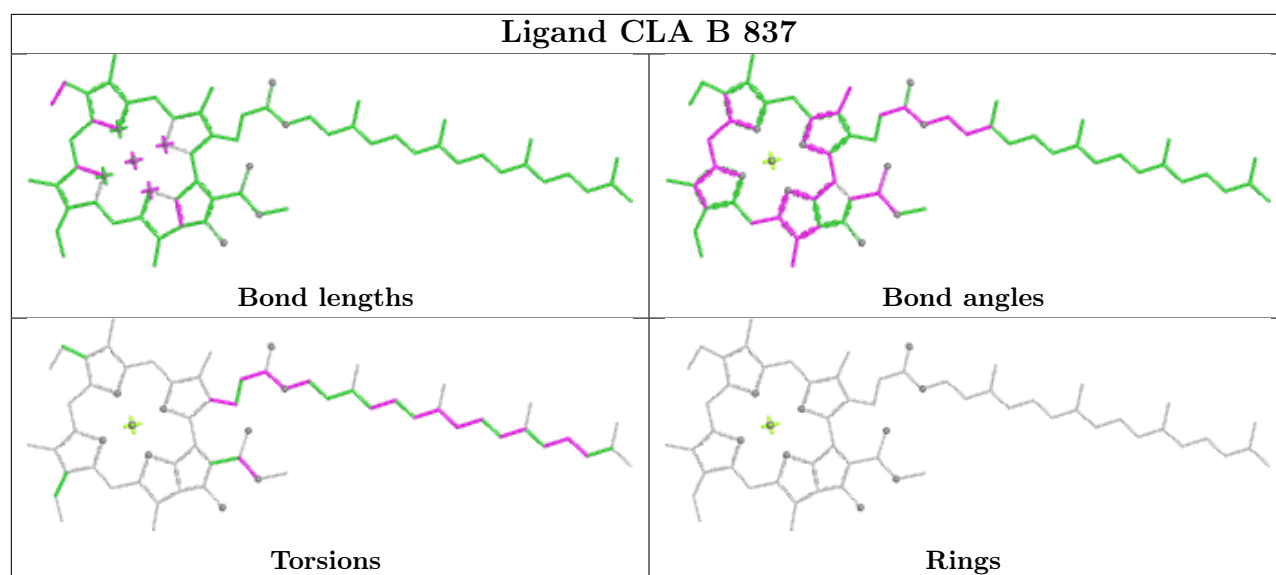
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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19	B	802	CLA	11	0
19	B	839	CLA	9	0
19	6	322	CLA	6	0
19	7	319	CLA	7	0
19	B	814	CLA	11	0
19	6	314	CLA	14	0
24	G	1604	LMT	11	0
19	B	838	CLA	7	0
21	C	102	SF4	5	0
22	8	306	BCR	7	0
19	A	824	CLA	17	0
23	4	320	LHG	15	0
32	6	321	CHL	8	0
34	6	325	3PH	4	0
19	A	843	CLA	3	0
34	3	5022	3PH	4	0
32	1	5017	CHL	11	0
19	K	205	CLA	8	0
32	4	317	CHL	12	0
22	B	845	BCR	19	0
24	8	324	LMT	3	0
24	8	323	LMT	5	0
24	7	323	LMT	2	0
31	6	305	LUT	10	0
19	8	310	CLA	5	0
19	5	325	CLA	14	0
22	F	302	BCR	9	0
19	8	318	CLA	11	0
19	7	318	CLA	2	0
19	3	5019	CLA	8	0
32	8	319	CHL	6	0
19	5	309	CLA	12	0
32	7	315	CHL	6	0
32	Z	309	CHL	15	0
32	Z	313	CHL	11	0
19	A	812	CLA	11	0
19	B	822	CLA	15	0

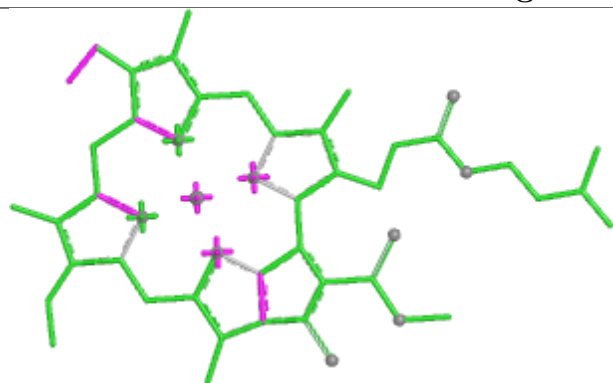
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

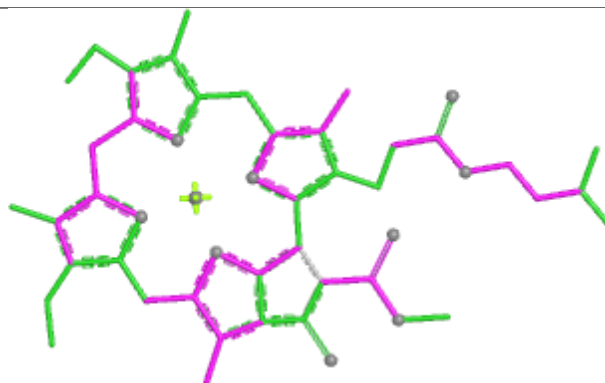




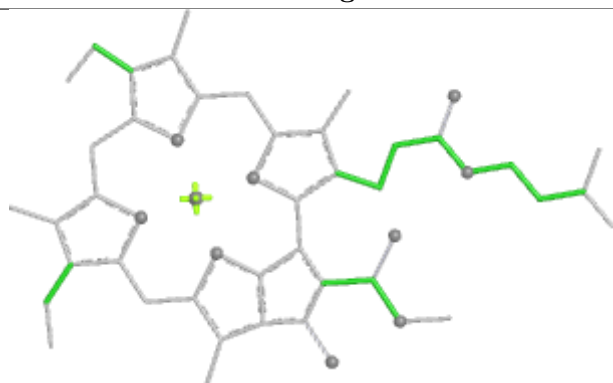
Ligand CLA Z 304



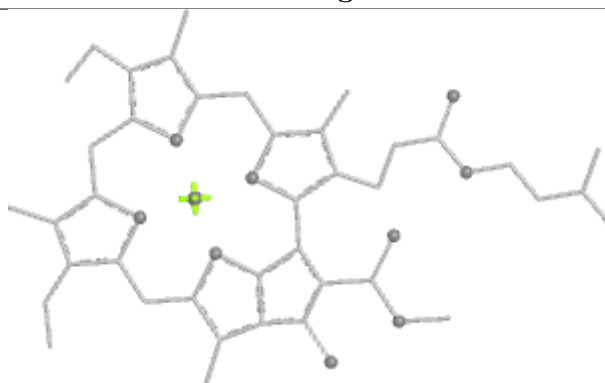
Bond lengths



Bond angles

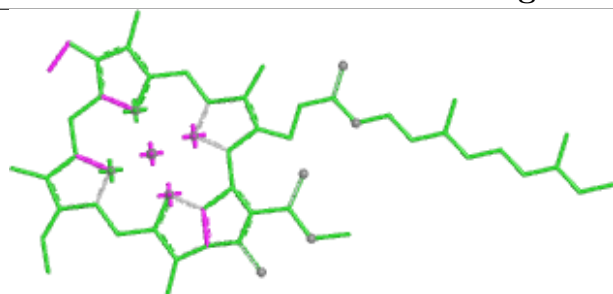


Torsions

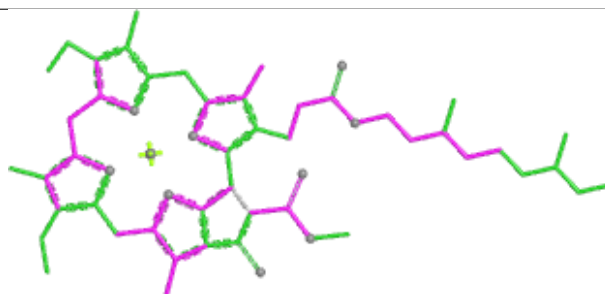


Rings

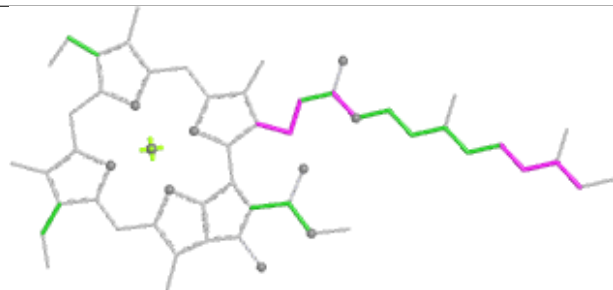
Ligand CLA 7 311



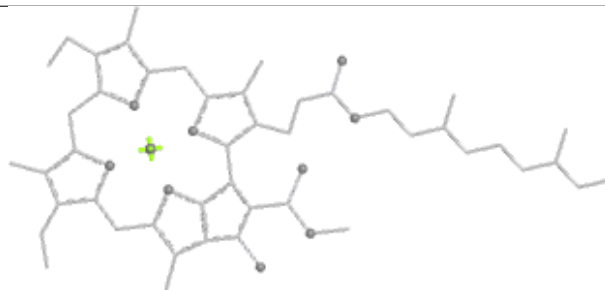
Bond lengths



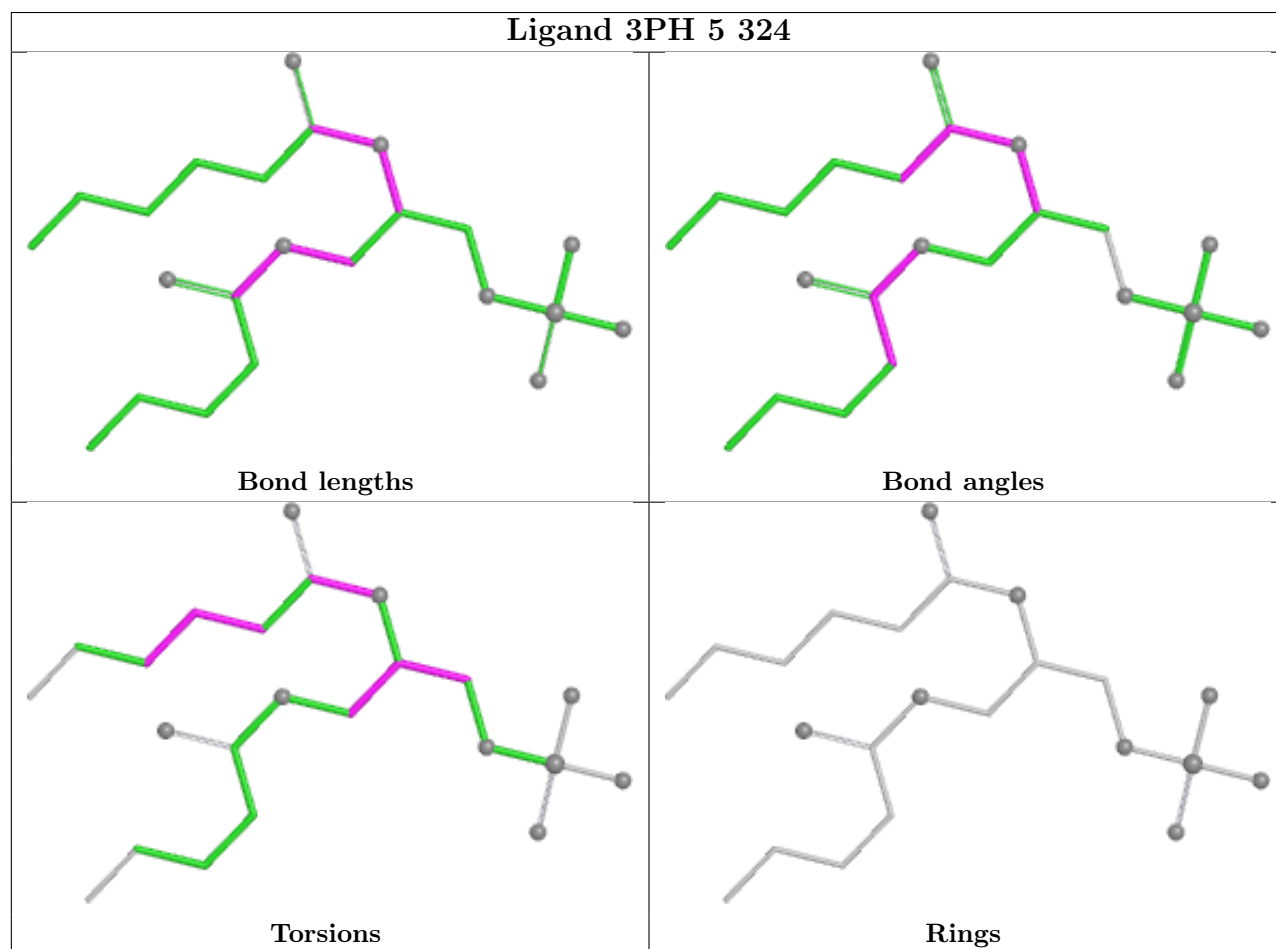
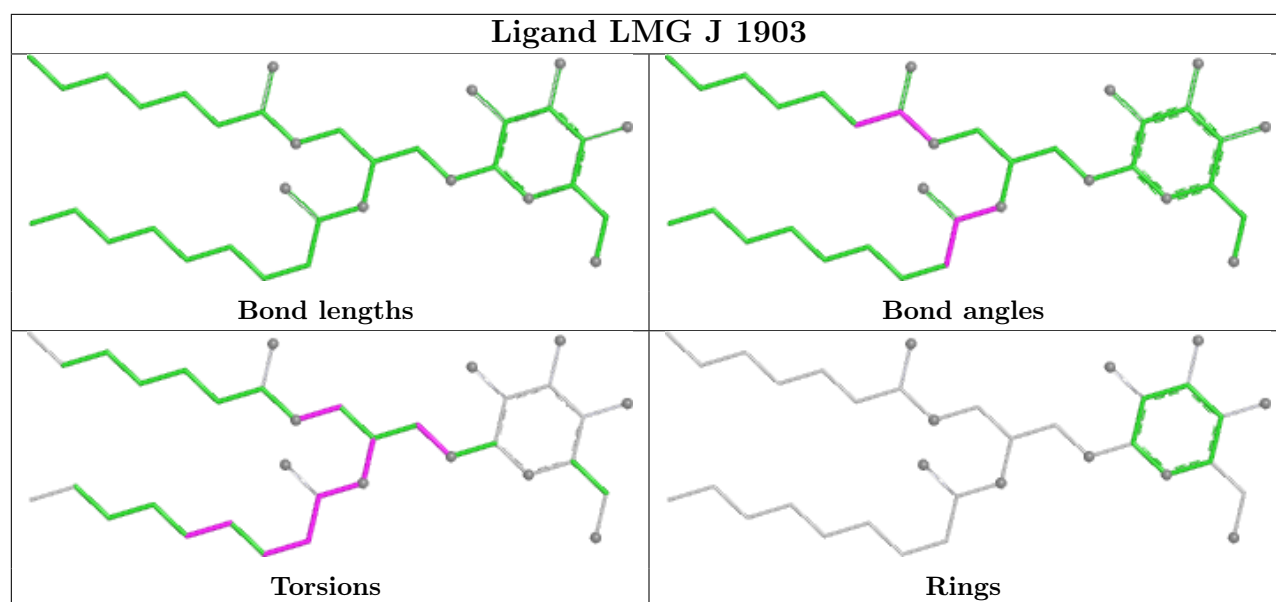
Bond angles

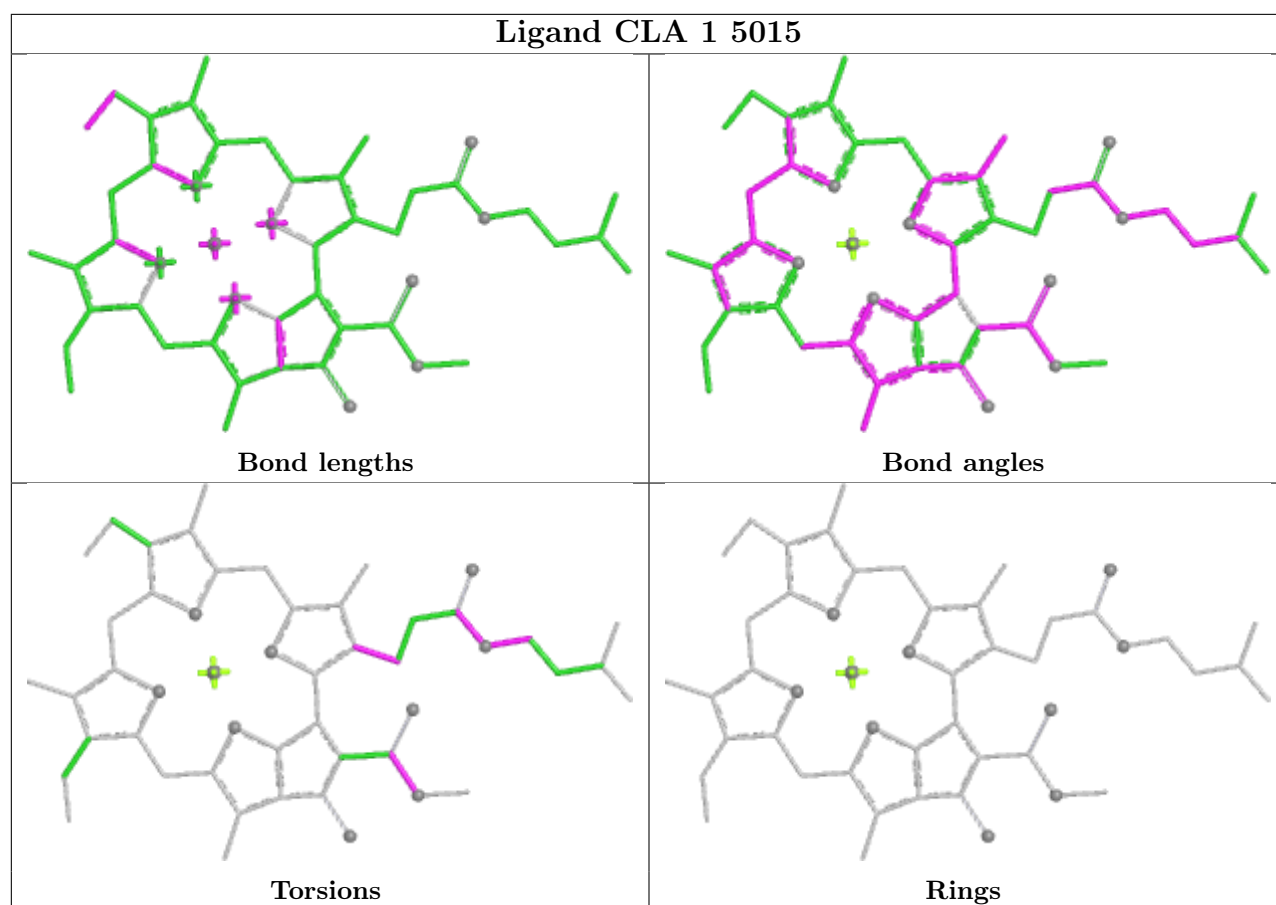


Torsions

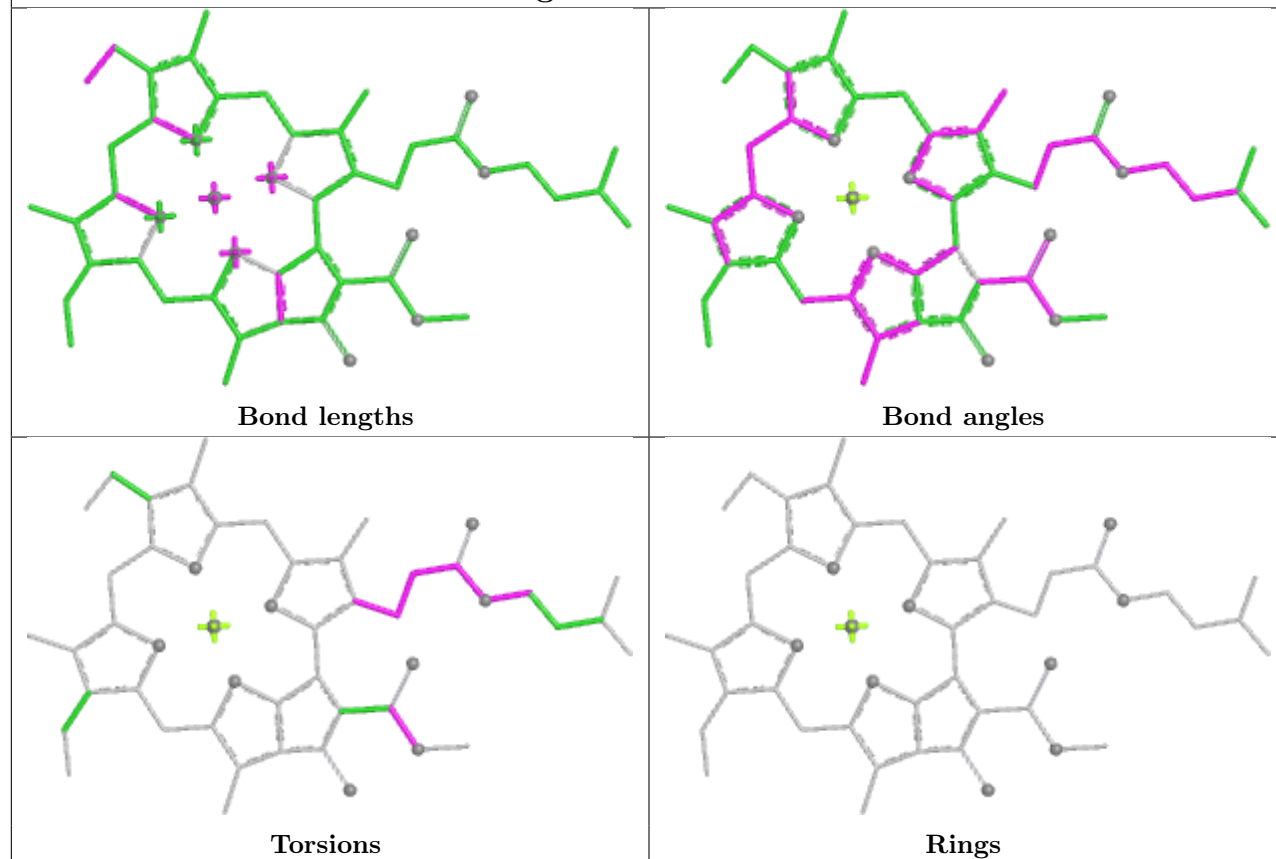


Rings

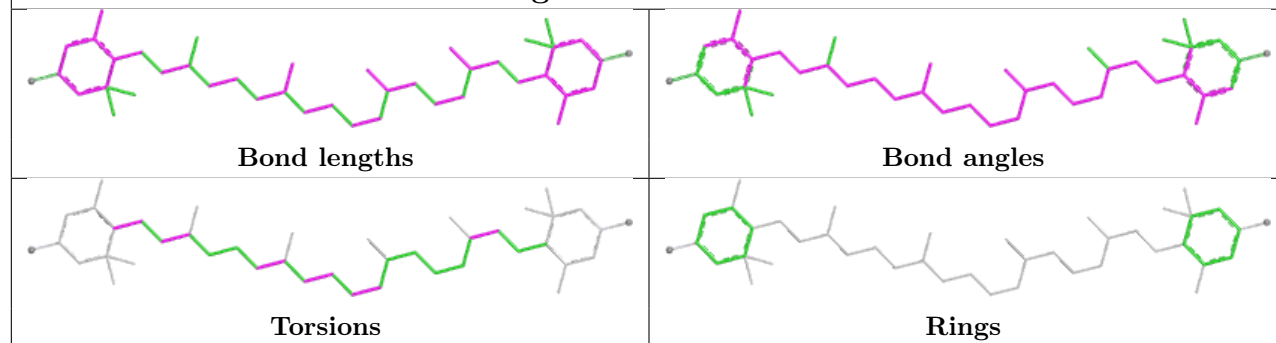




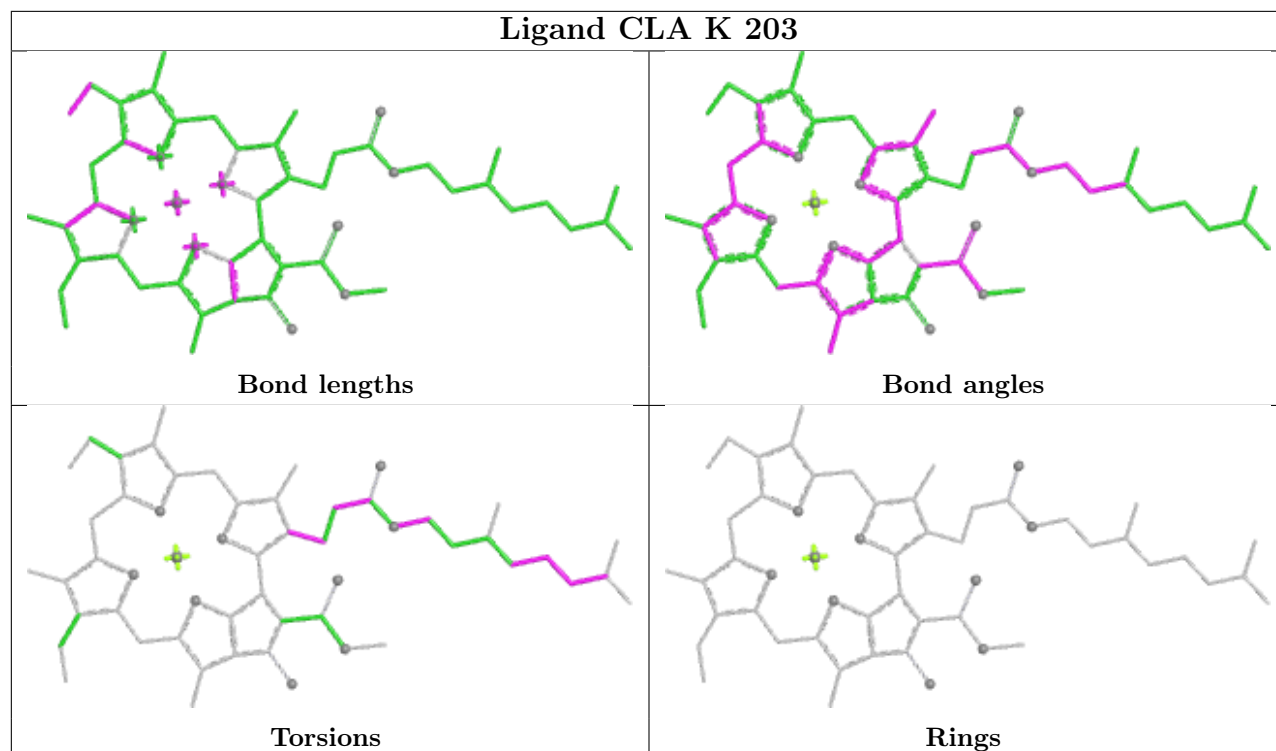
Ligand CLA 5 311



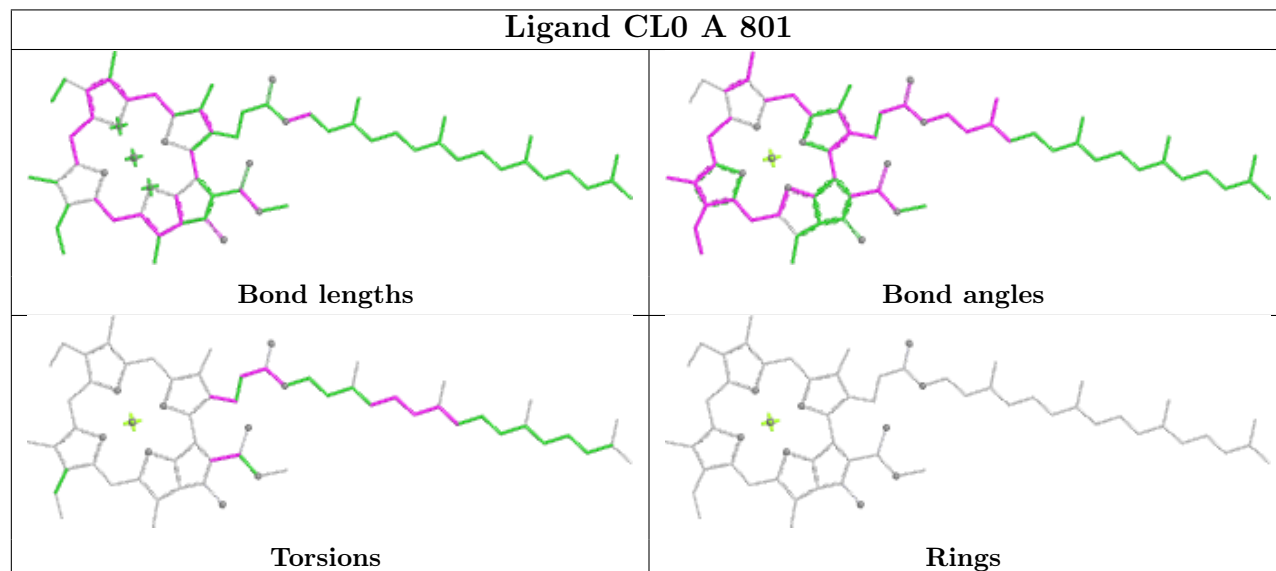
Ligand C7Z 1 5005

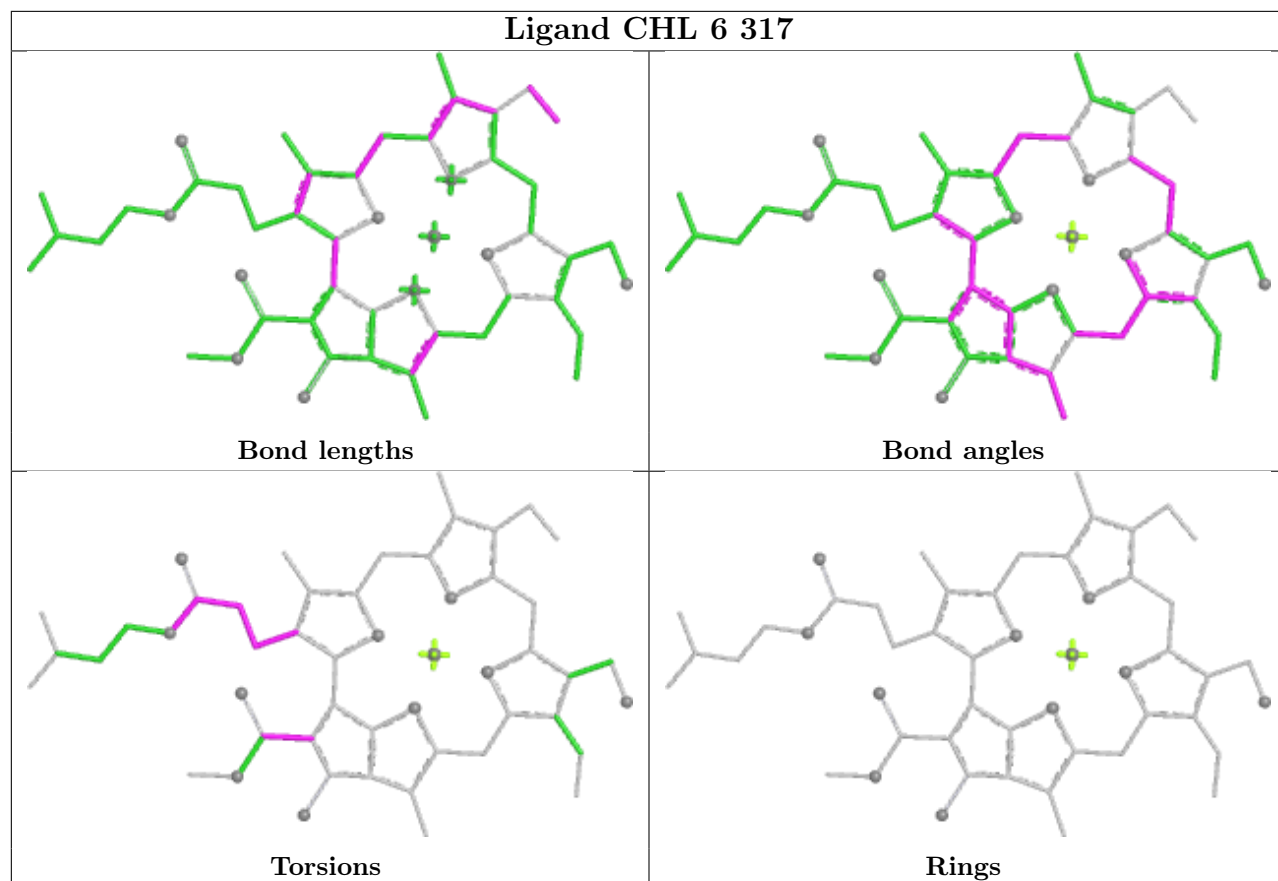


Ligand CLA K 203

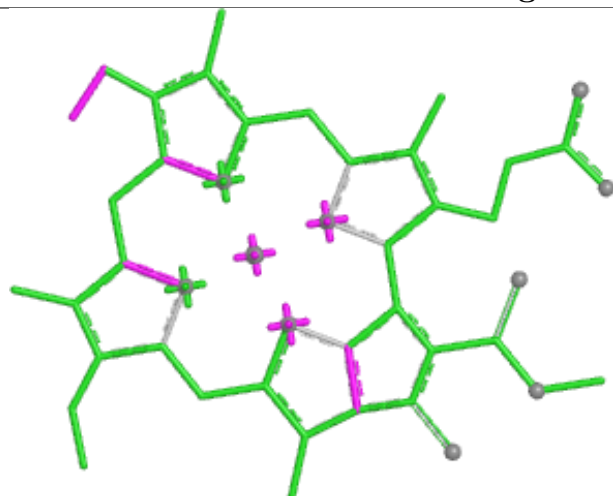


Ligand CL0 A 801

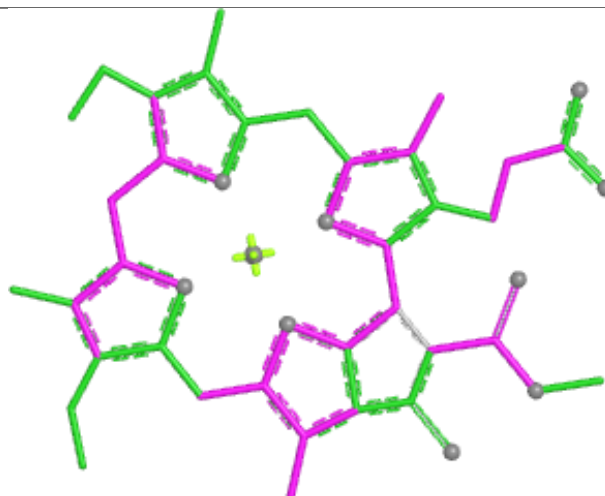




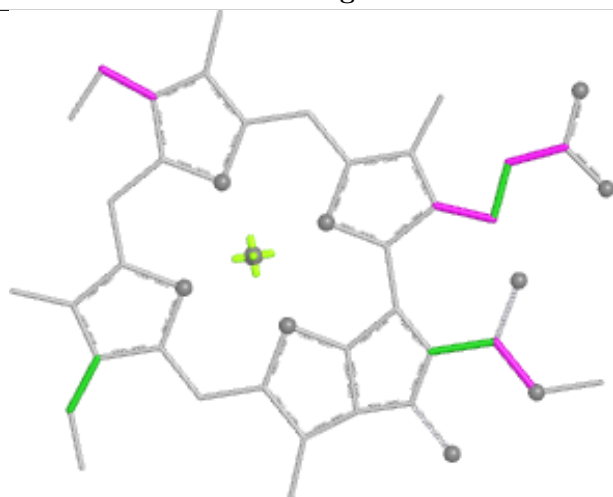
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Bond lengths



Bond angles

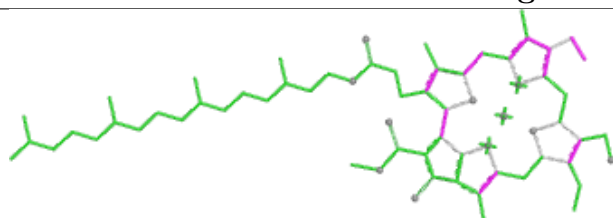


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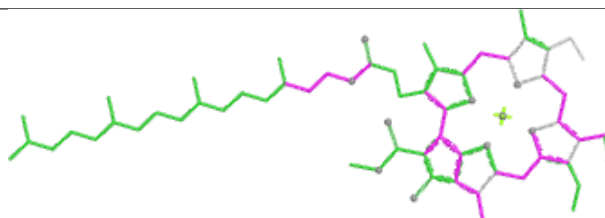


Rings

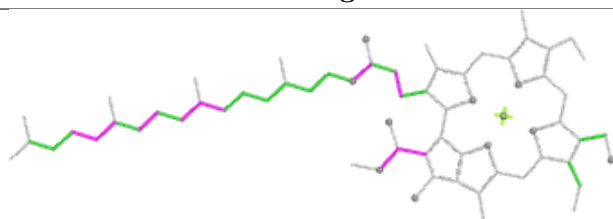
Ligand CHL 6 319



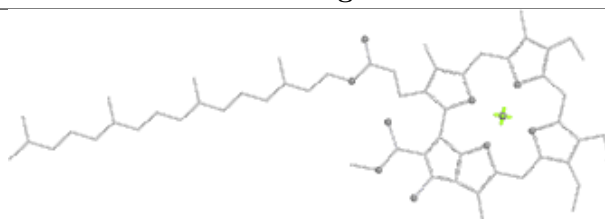
Bond lengths



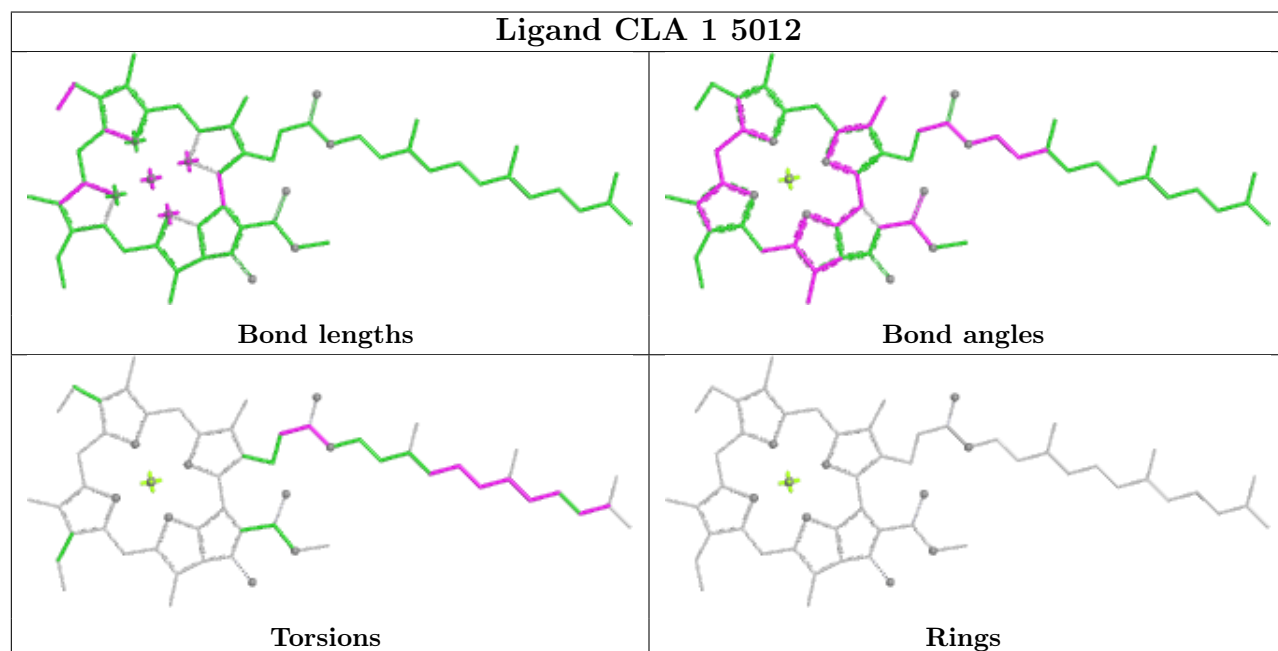
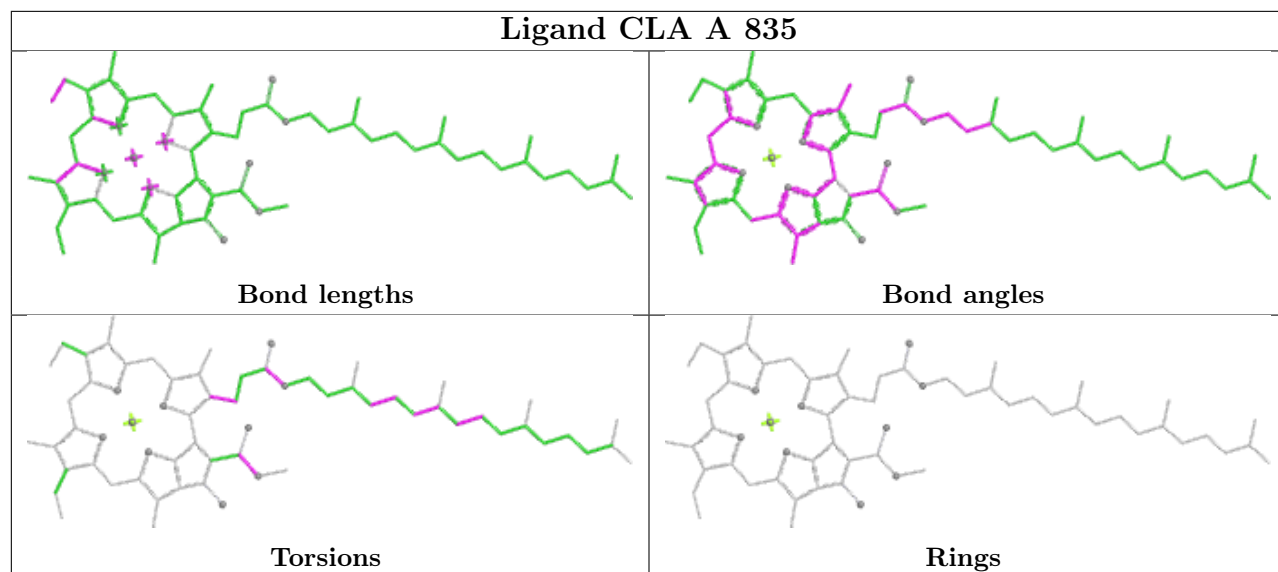
Bond angles

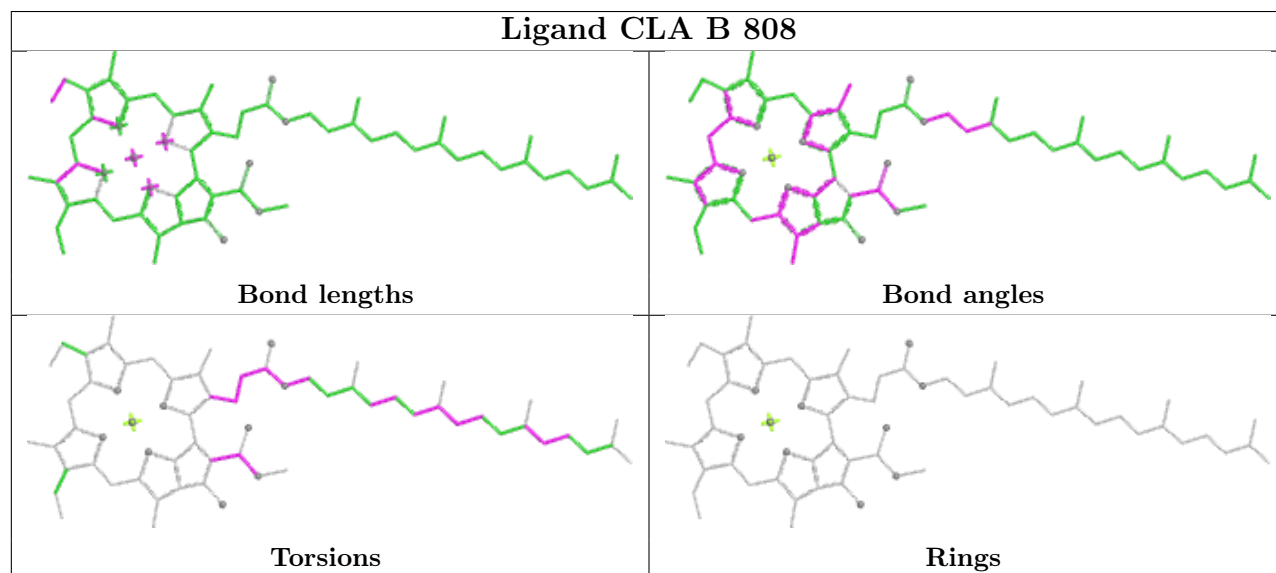
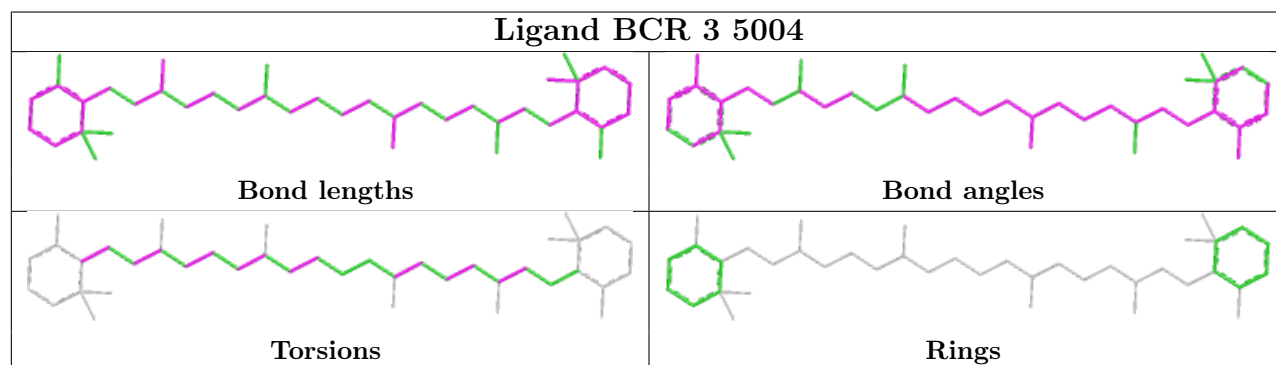
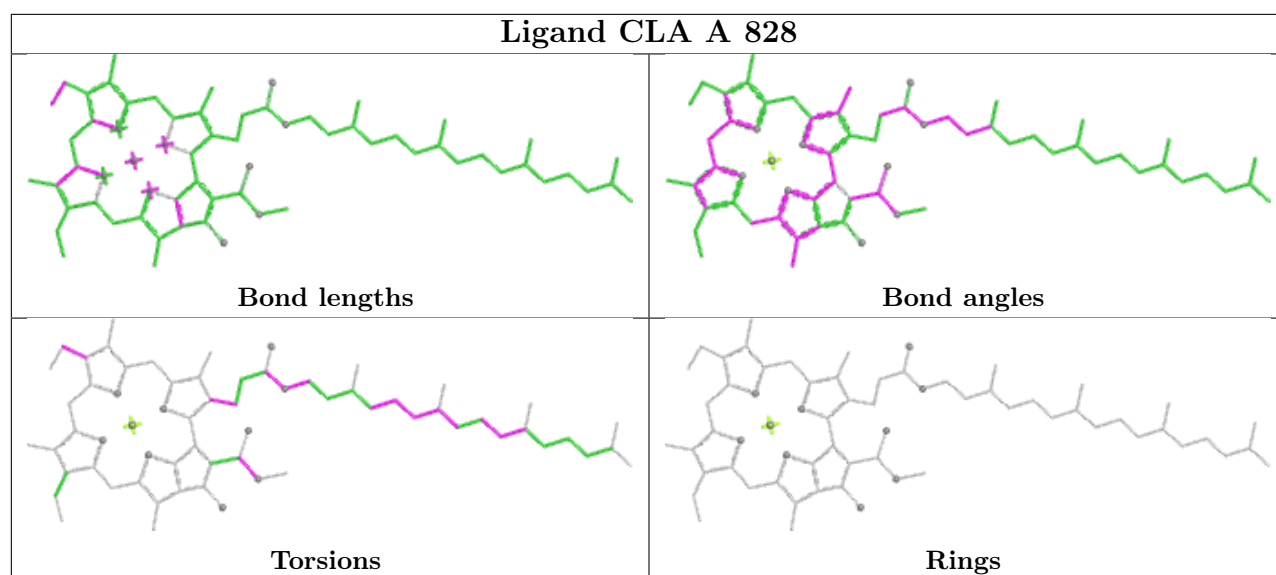


Torsions

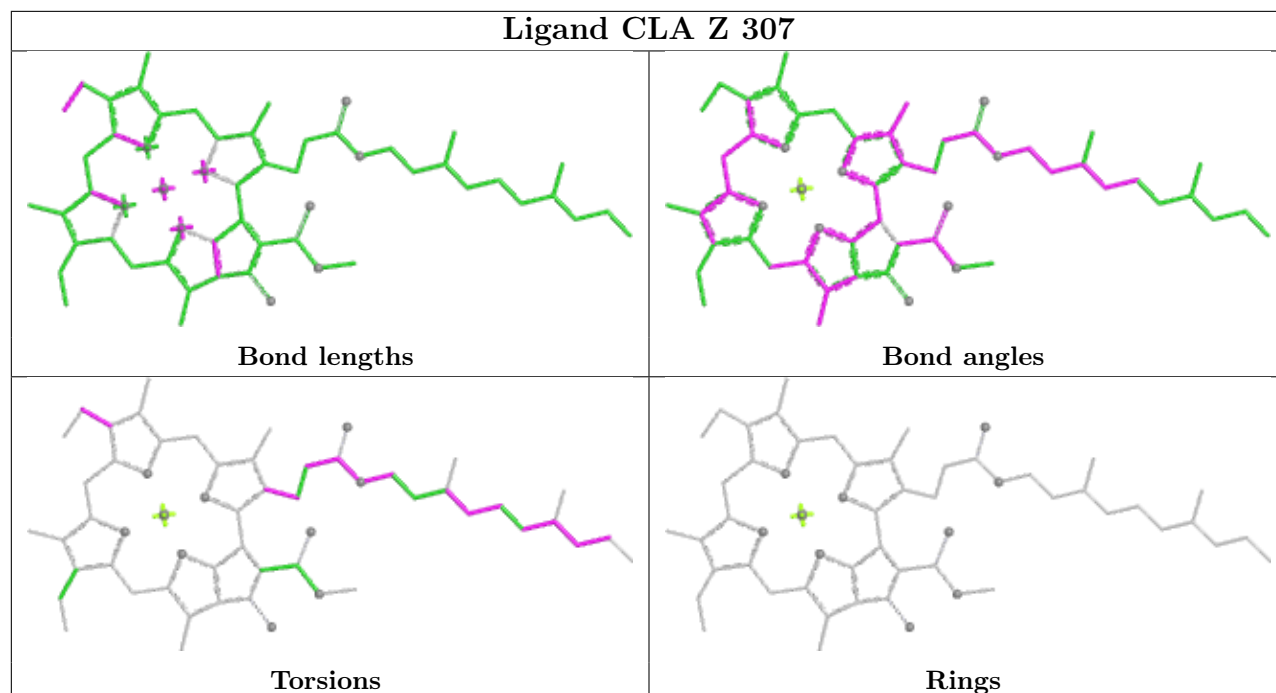


Rings

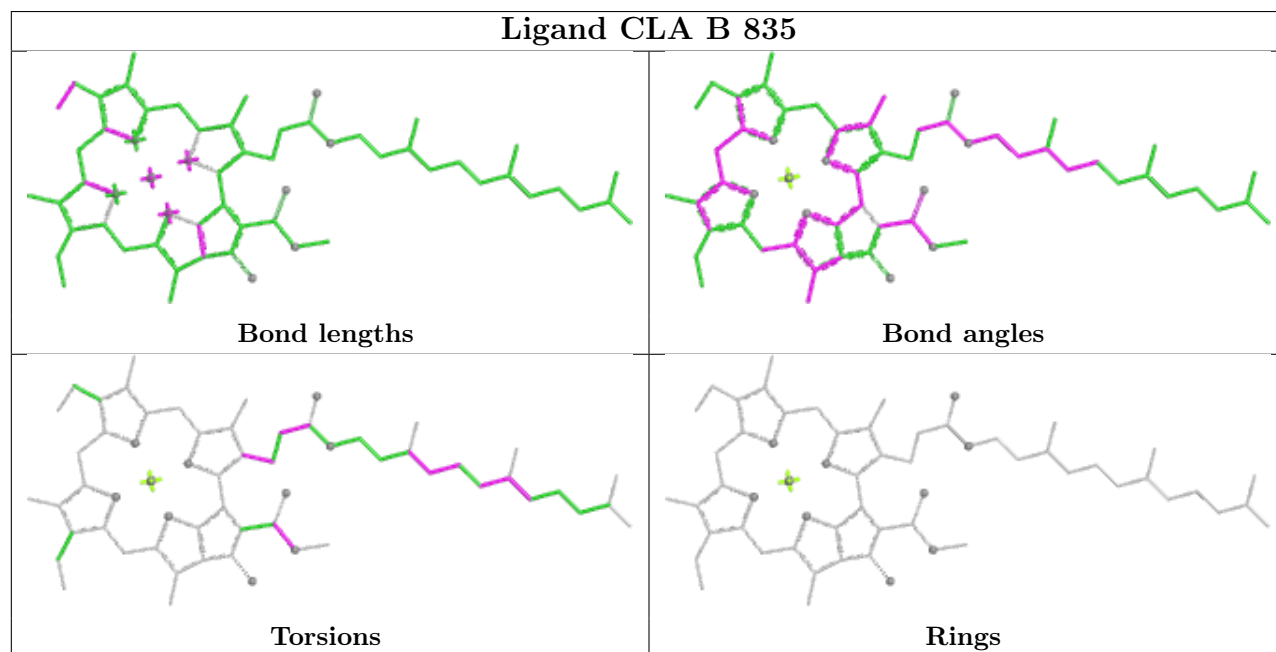


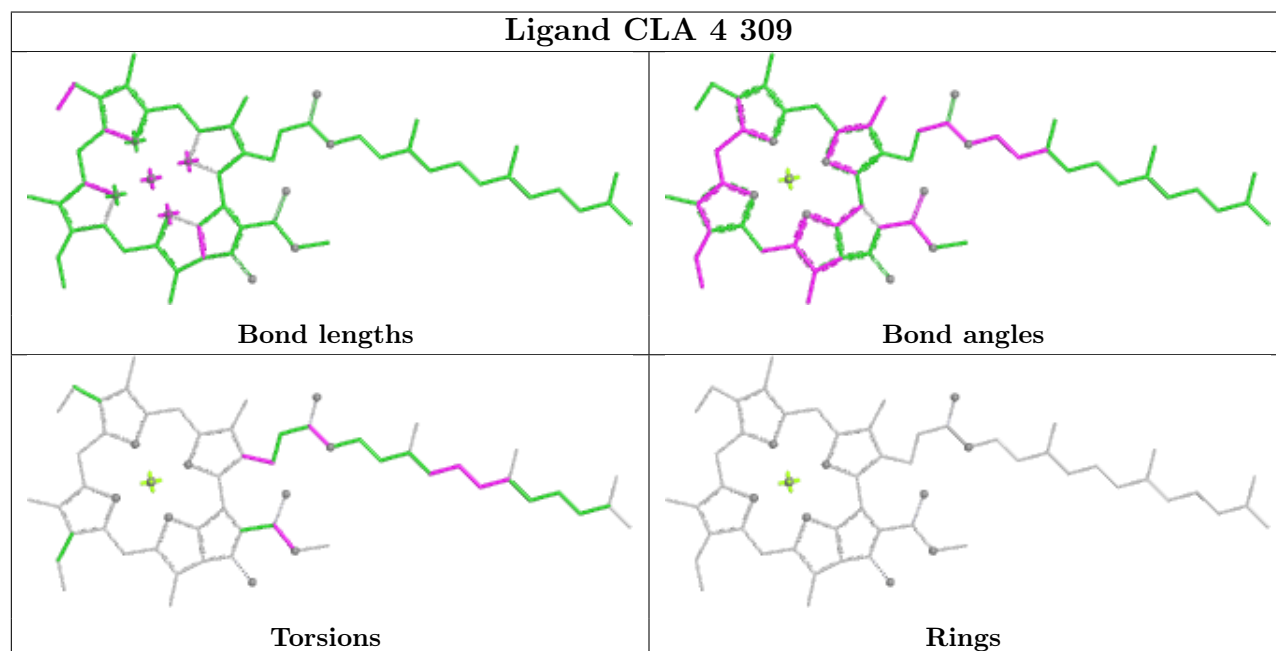
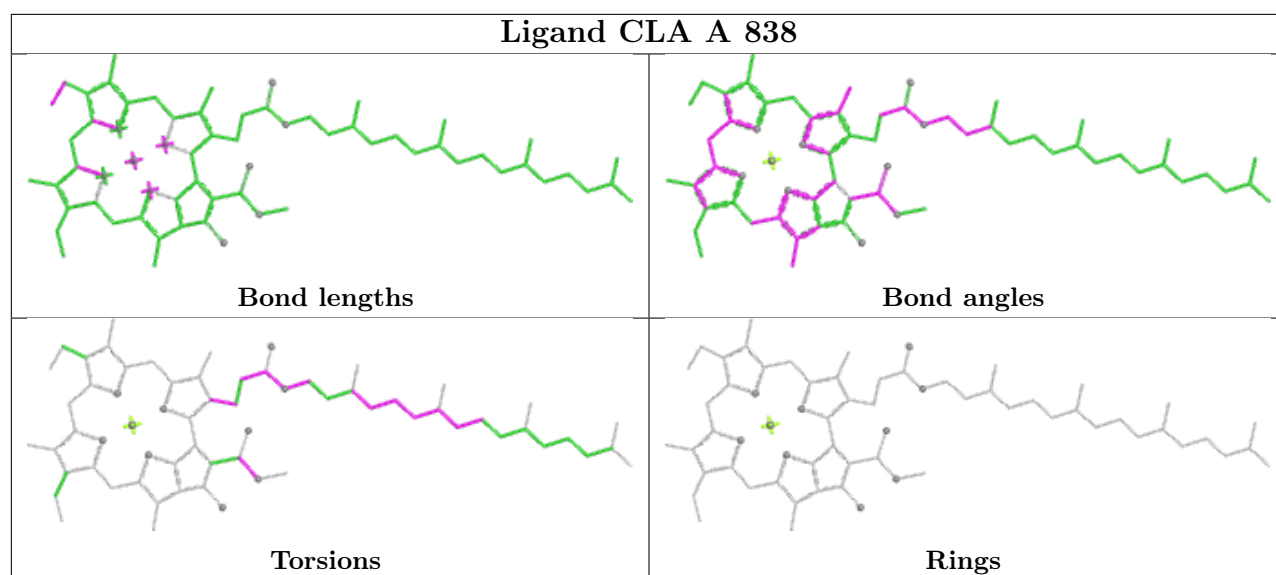


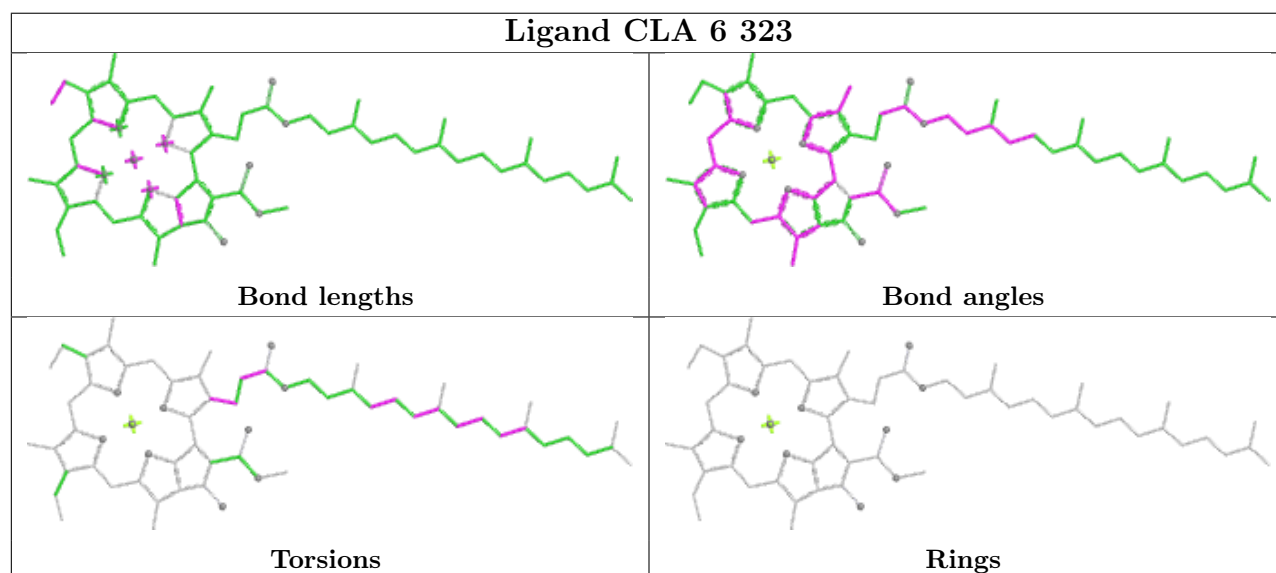
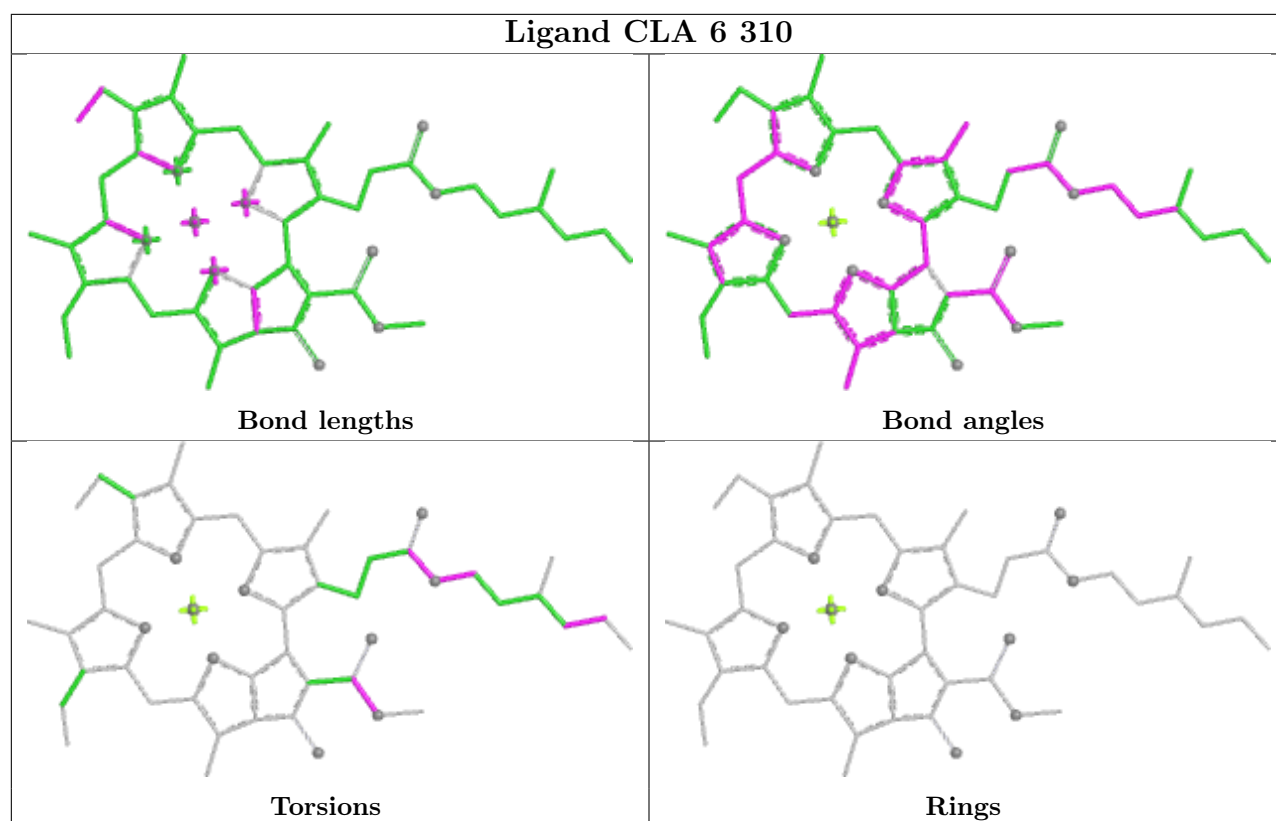
Ligand CLA Z 307

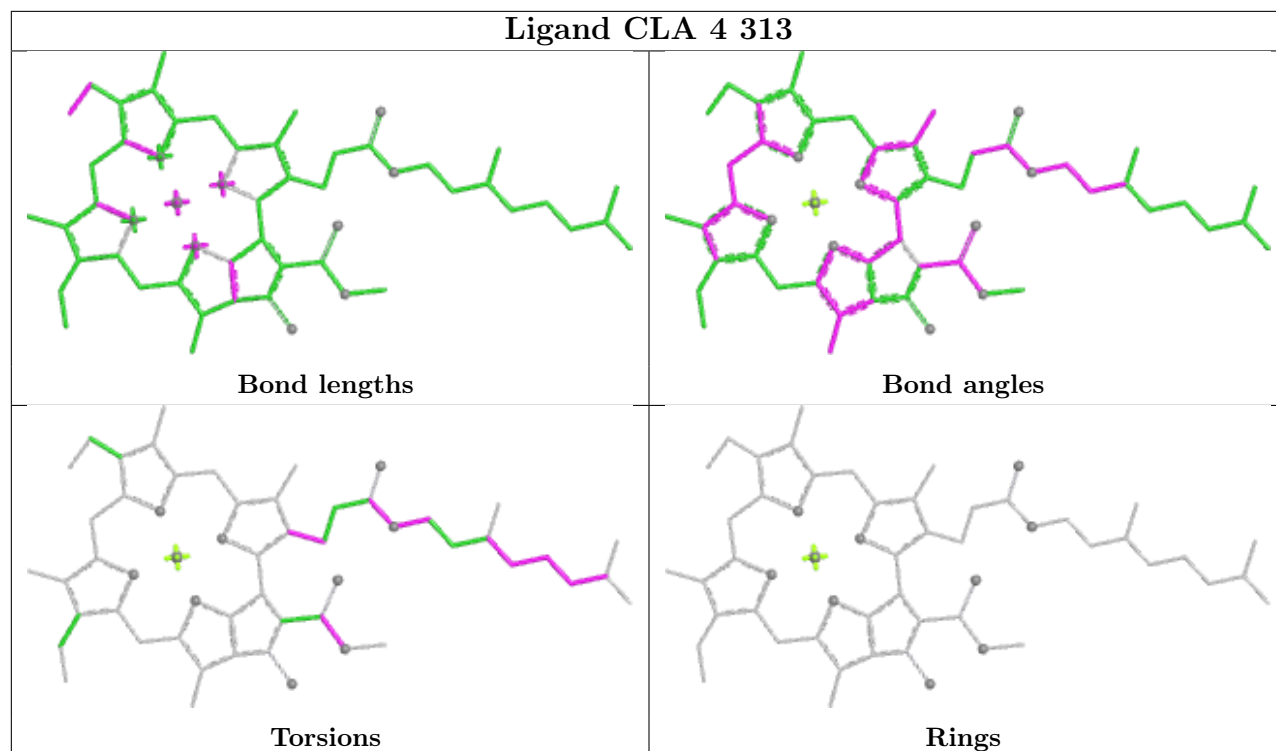
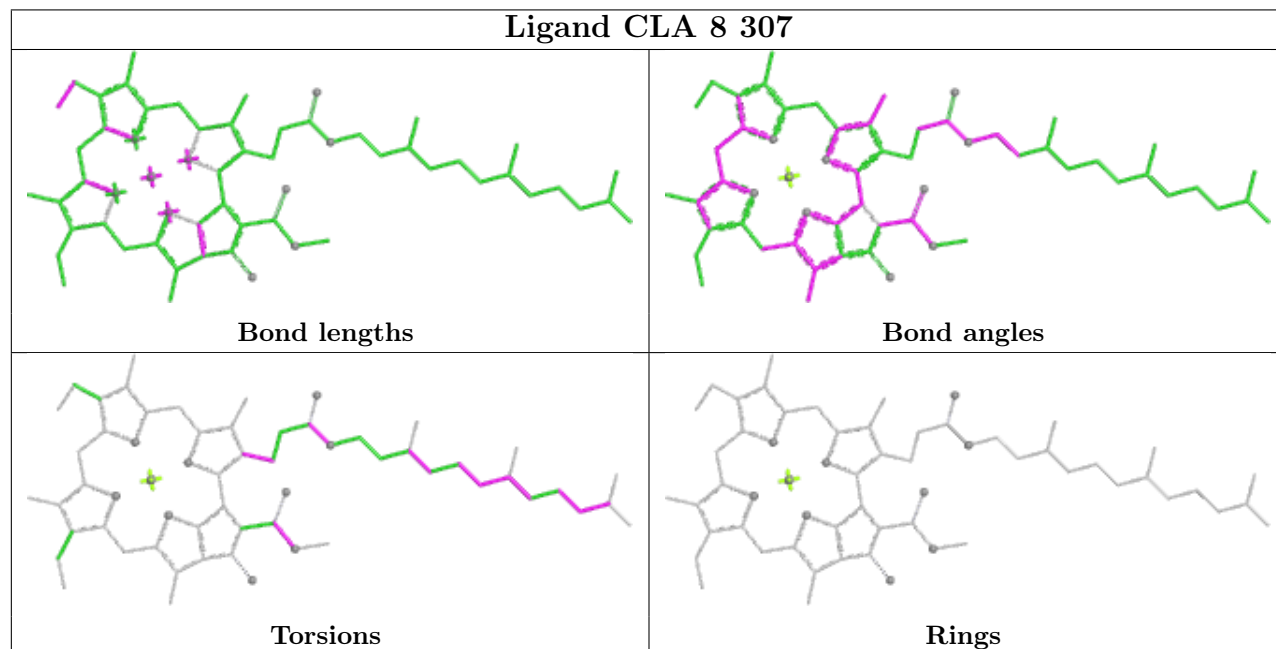


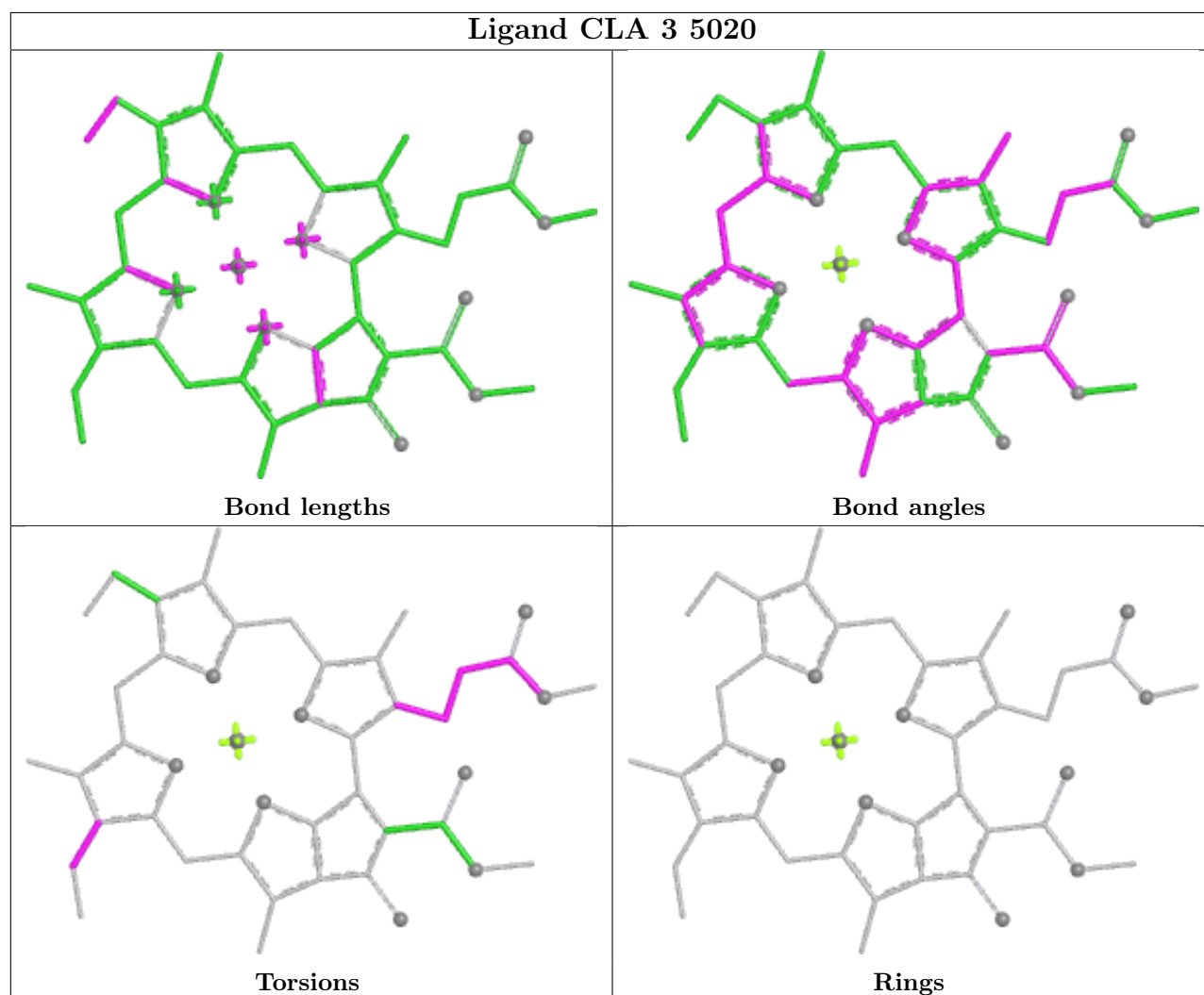
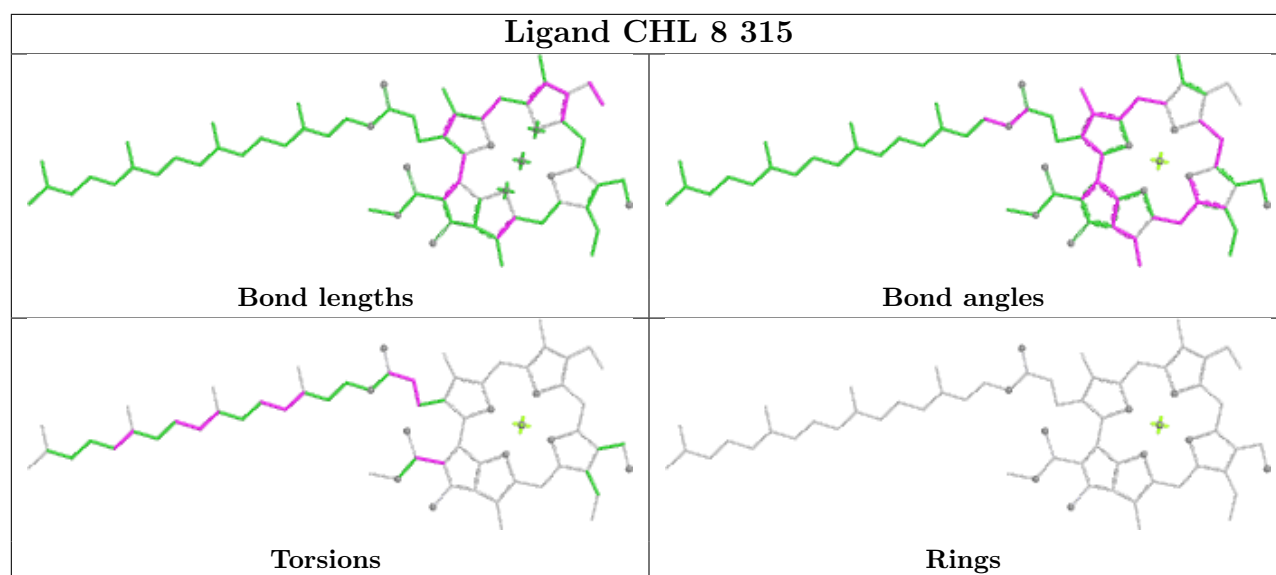
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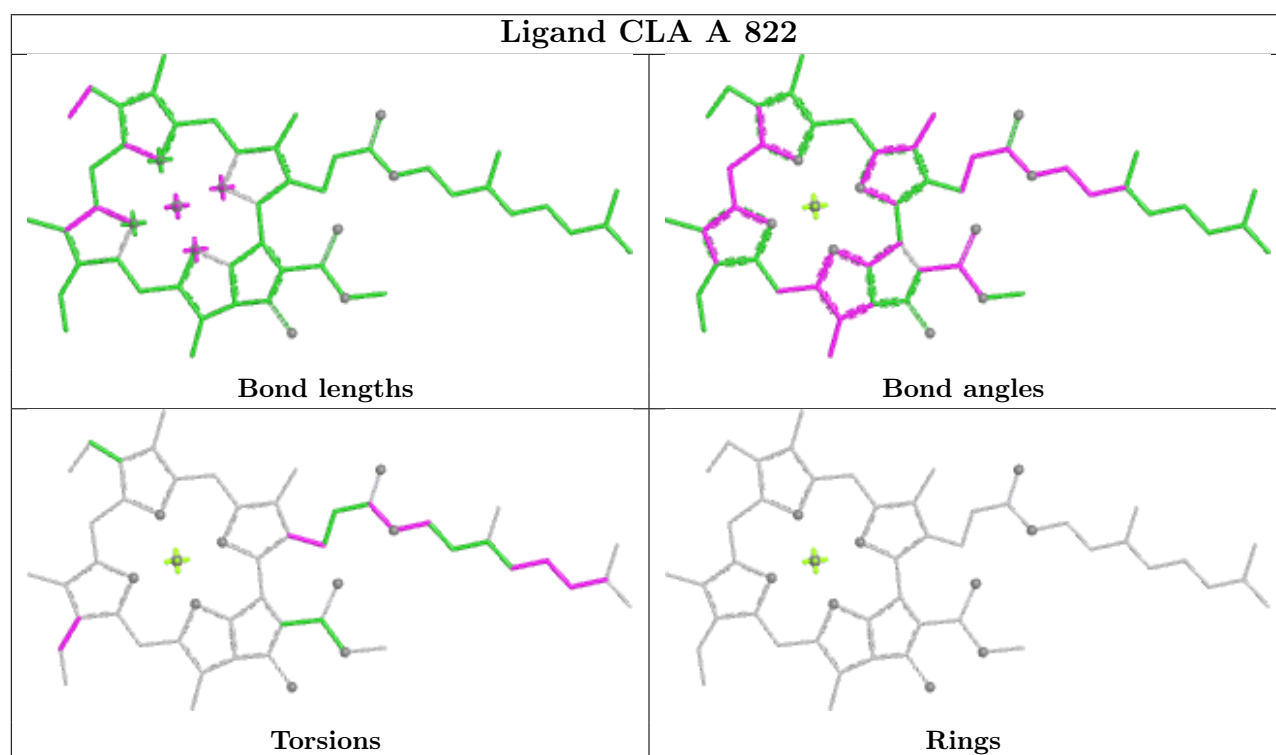
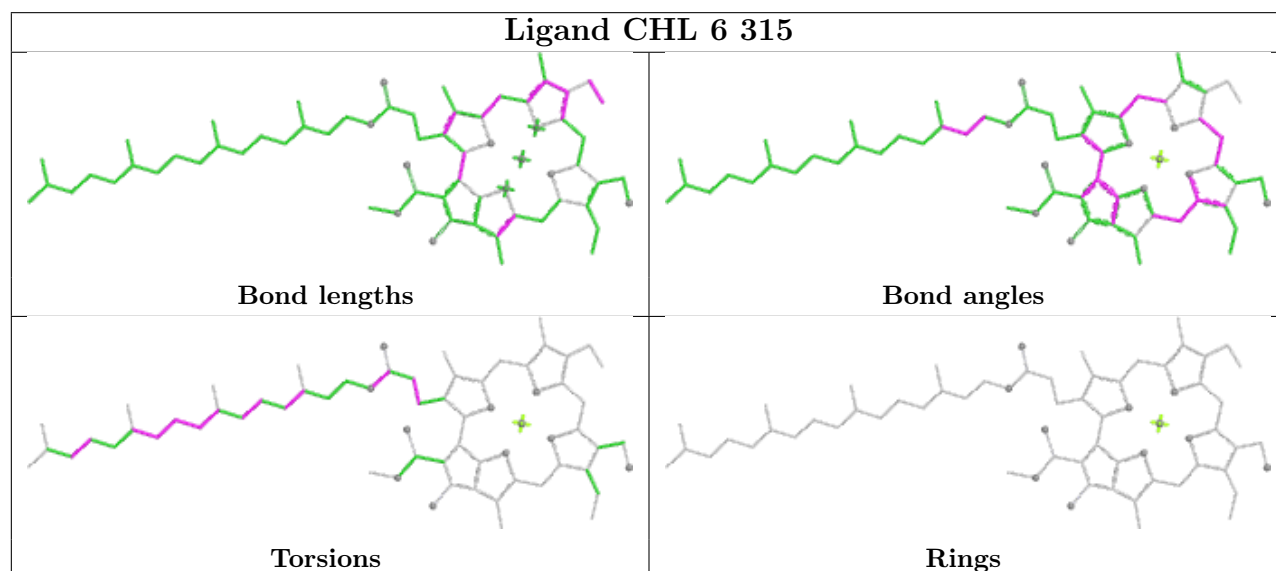
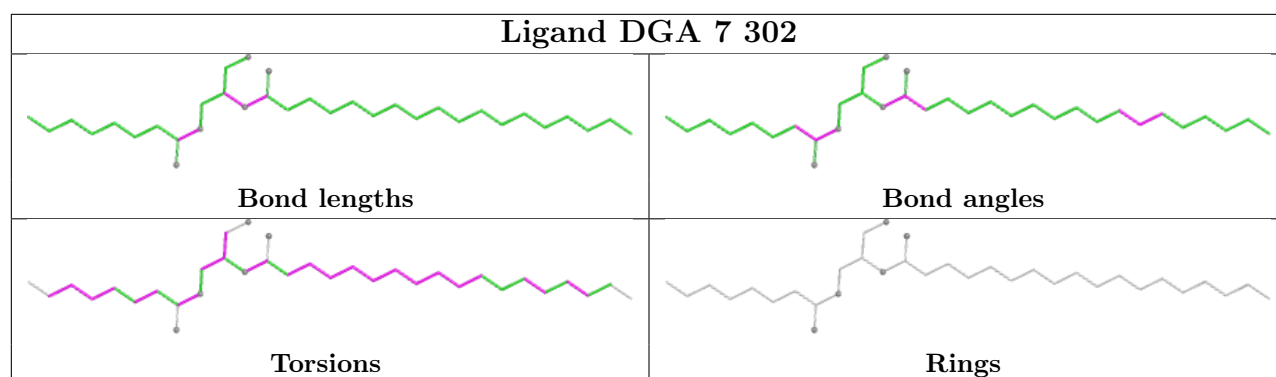




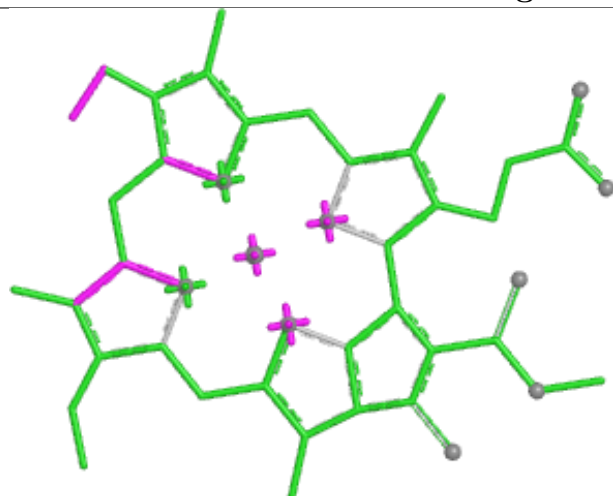


Ligand CLA 4 313**Ligand CLA 8 307**

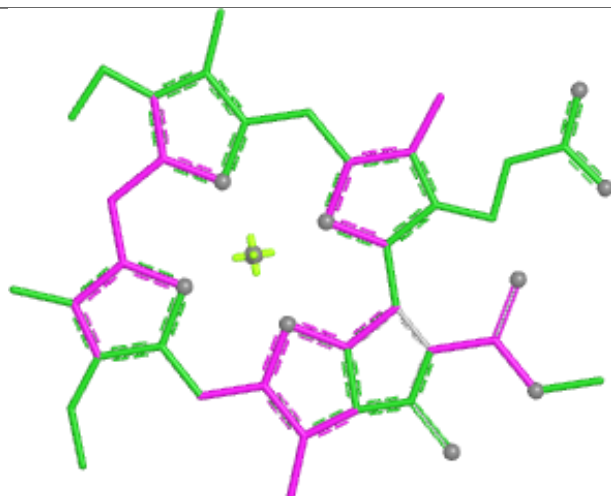




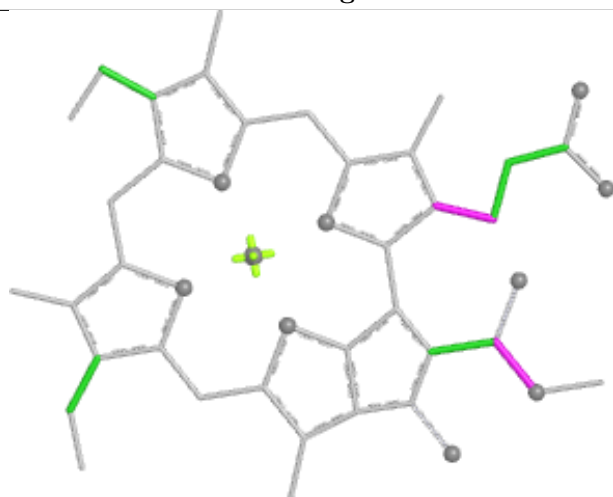
Ligand CLA F 303



Bond lengths



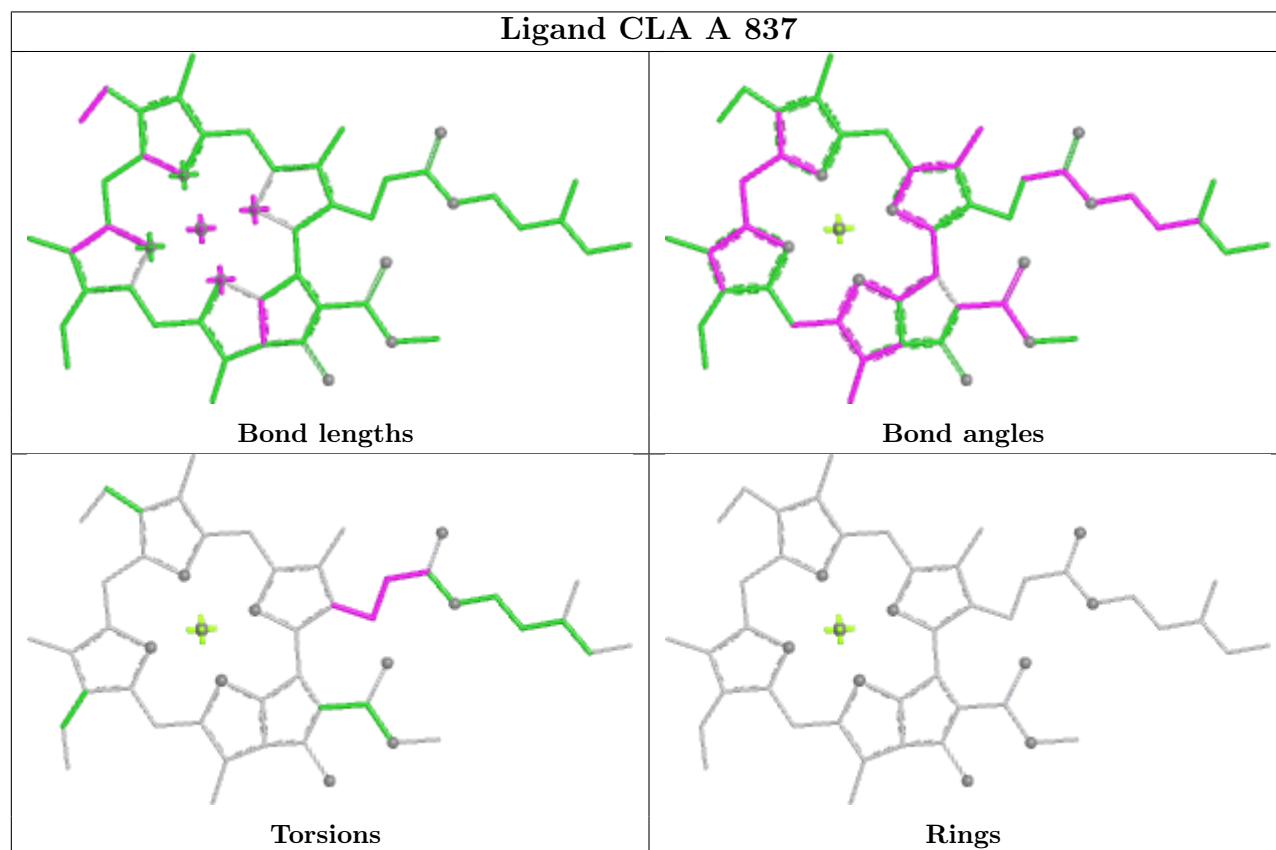
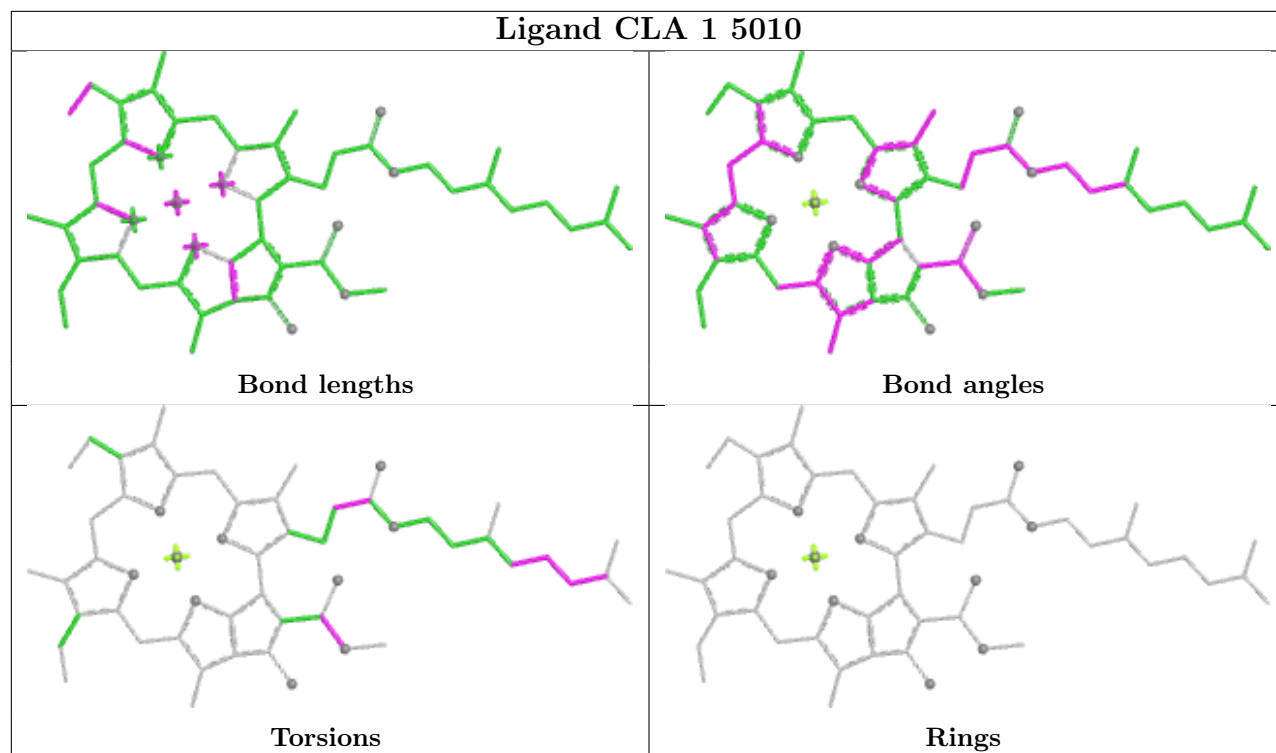
Bond angles

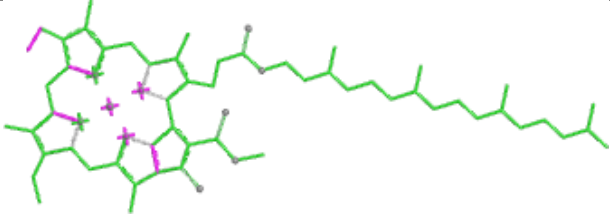
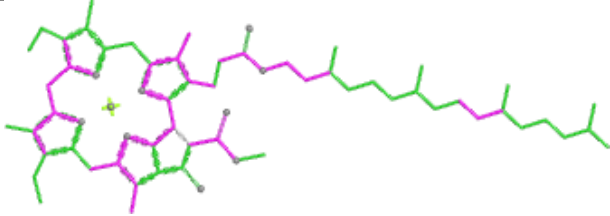
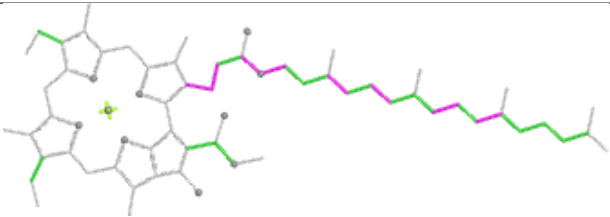
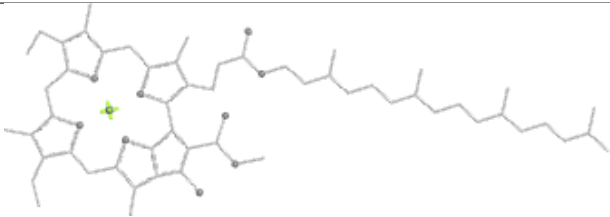
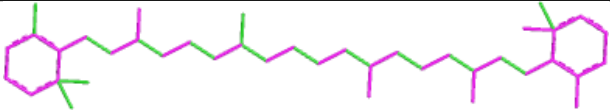
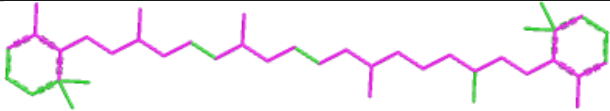
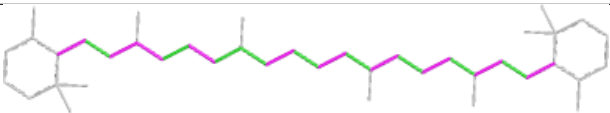
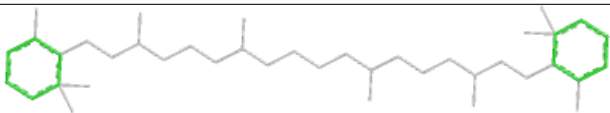
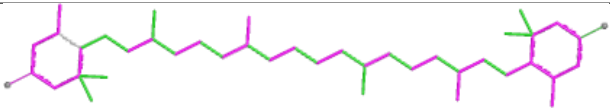
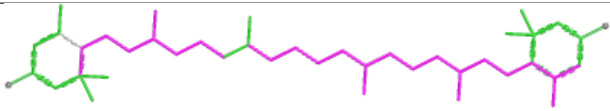
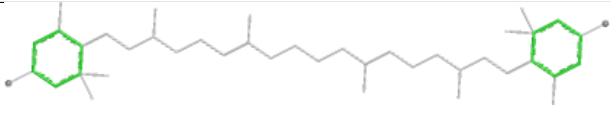


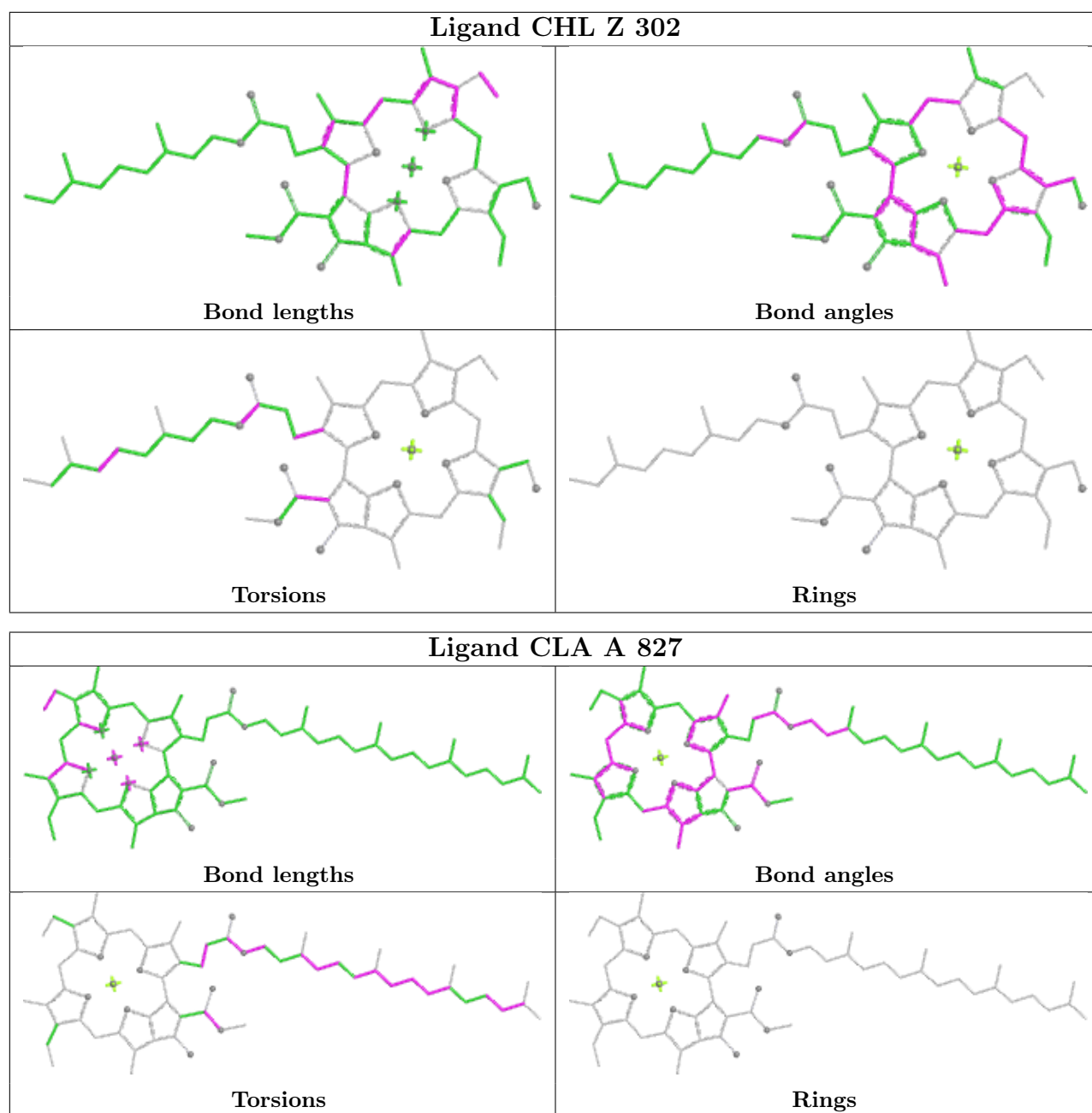
Torsions



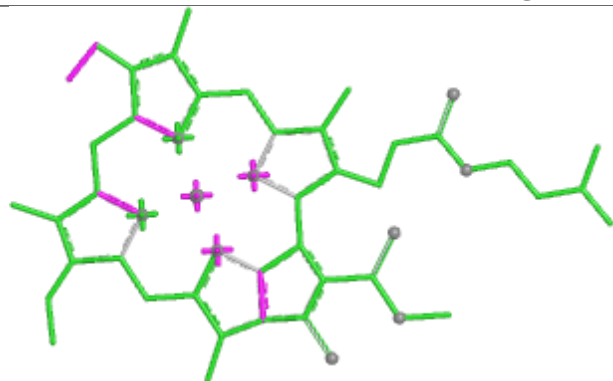
Rings



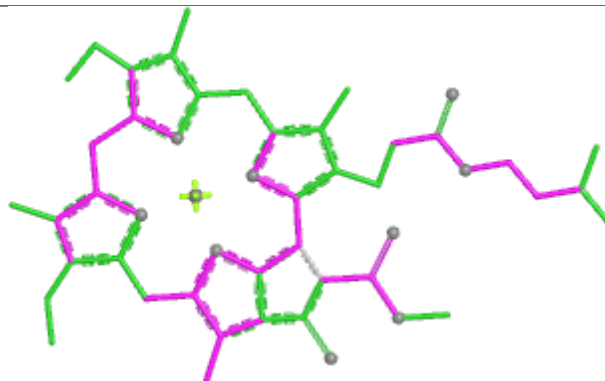
Ligand CLA A 810	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 8 303	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT 7 303	
 Bond lengths	 Bond angles
 Torsions	 Rings



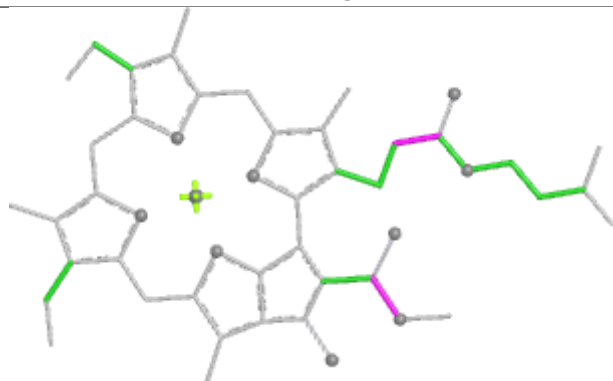
Ligand CLA 7 307



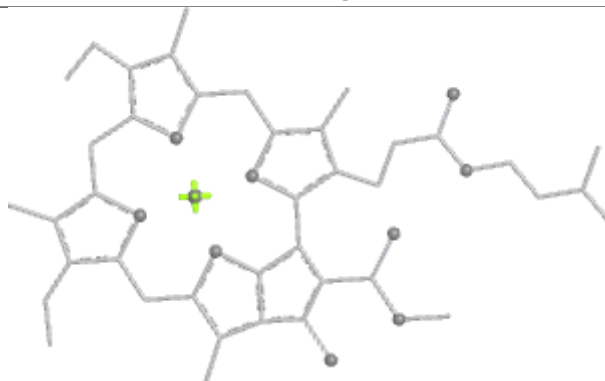
Bond lengths



Bond angles

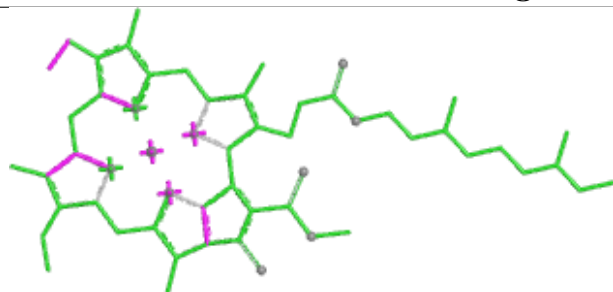


Torsions

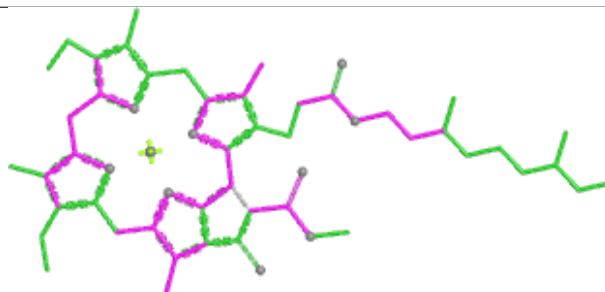


Rings

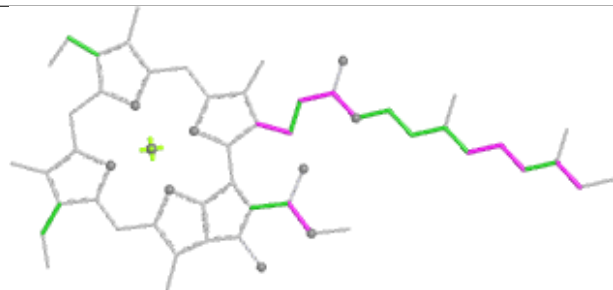
Ligand CLA B 811



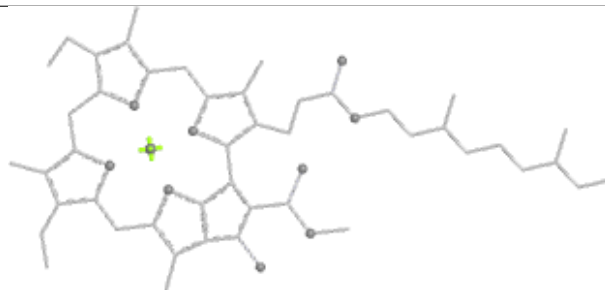
Bond lengths



Bond angles

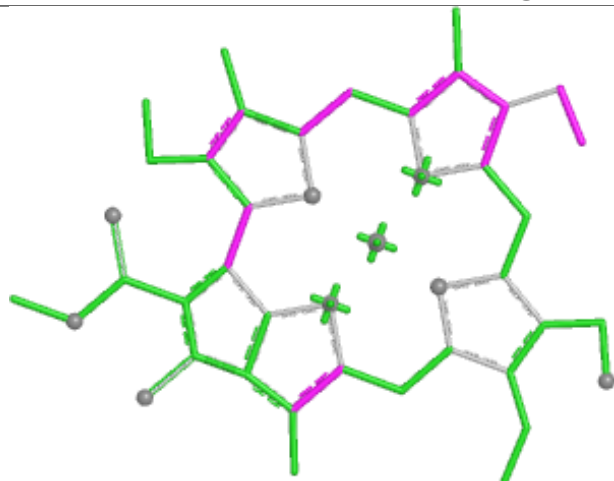


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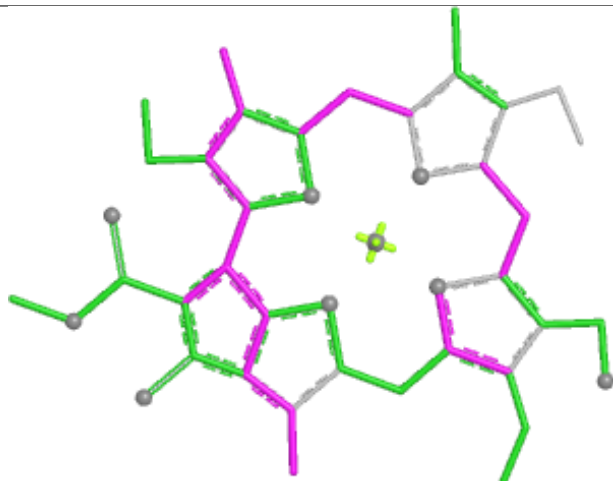


Rings

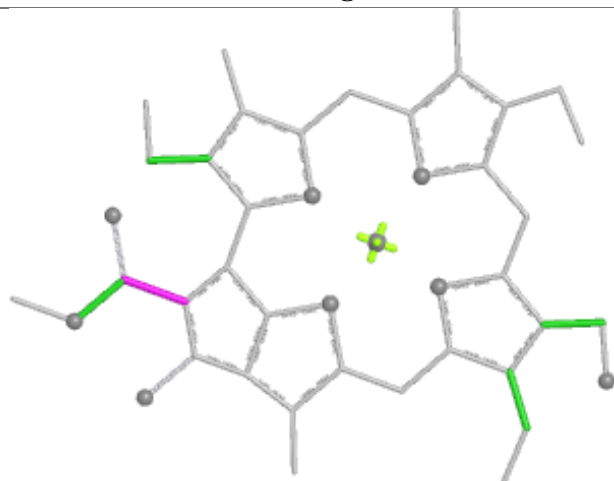
Ligand CHL 5 320



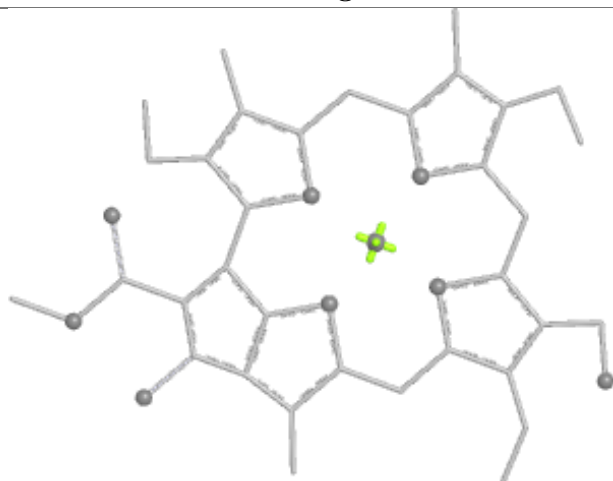
Bond lengths



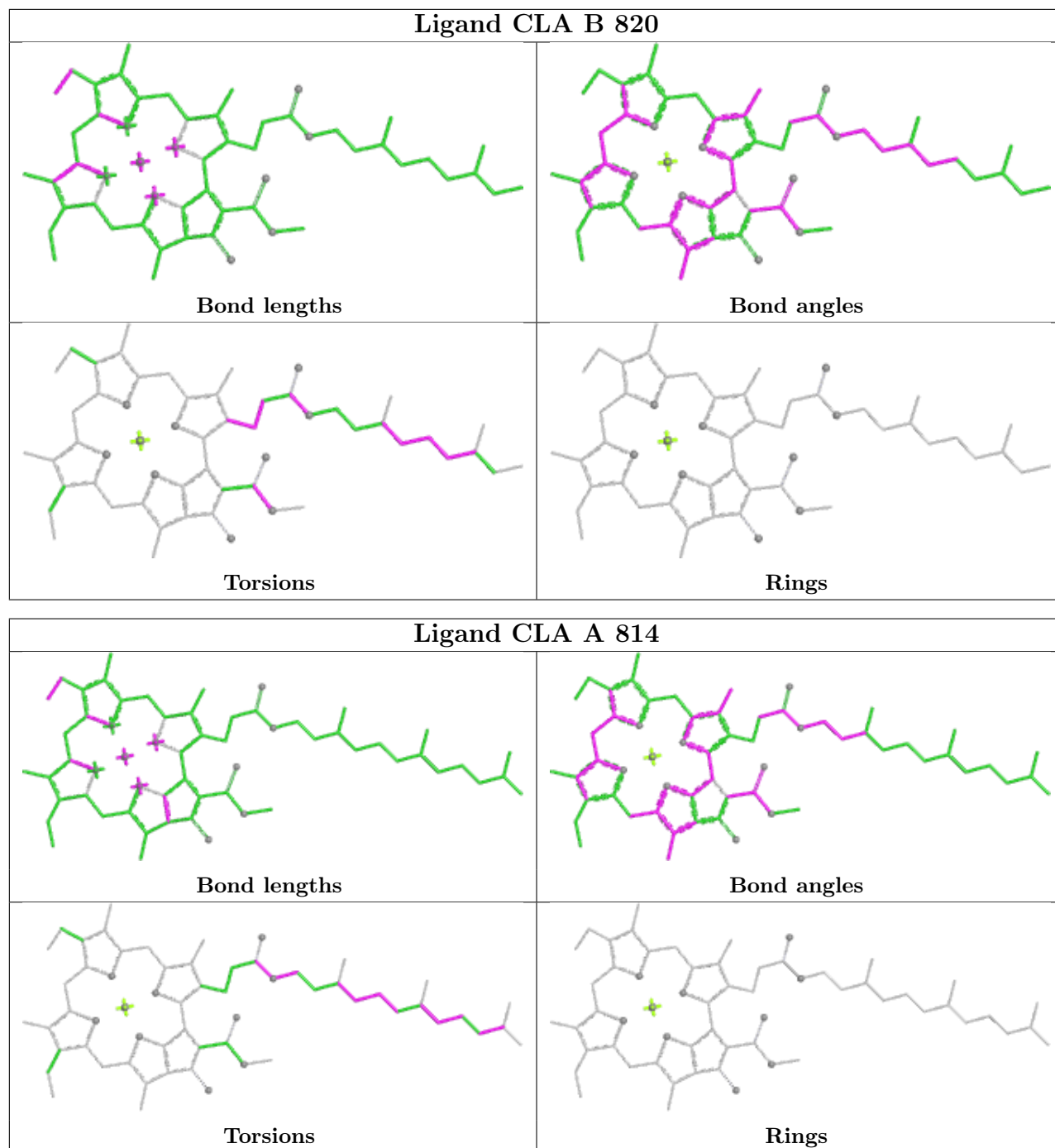
Bond angles

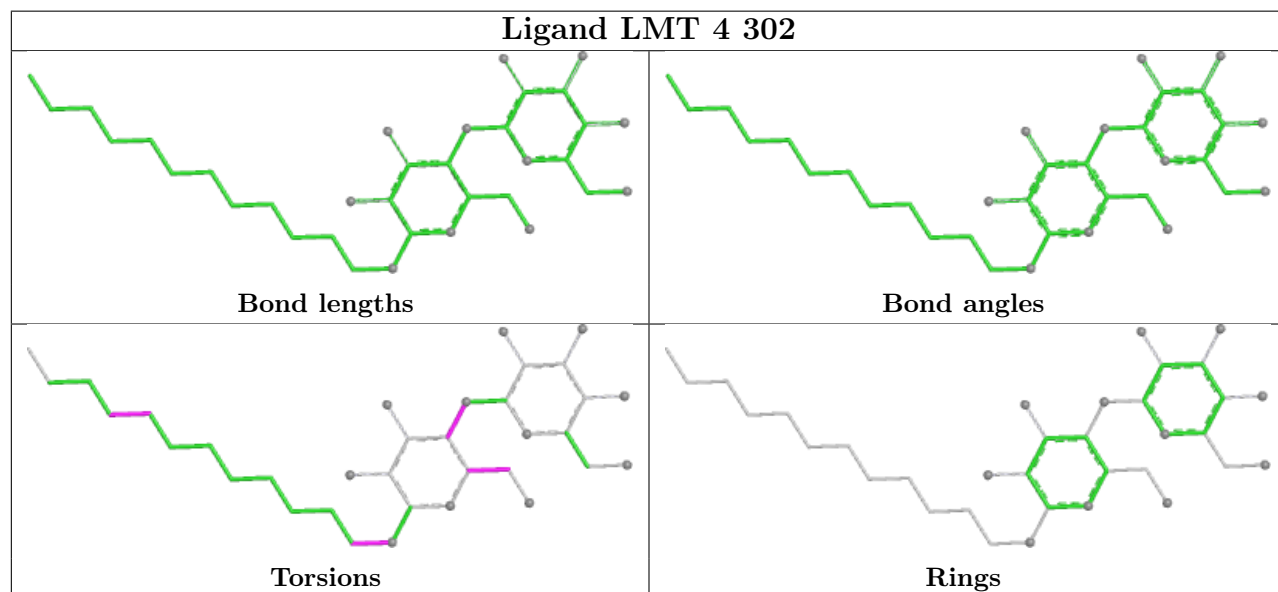
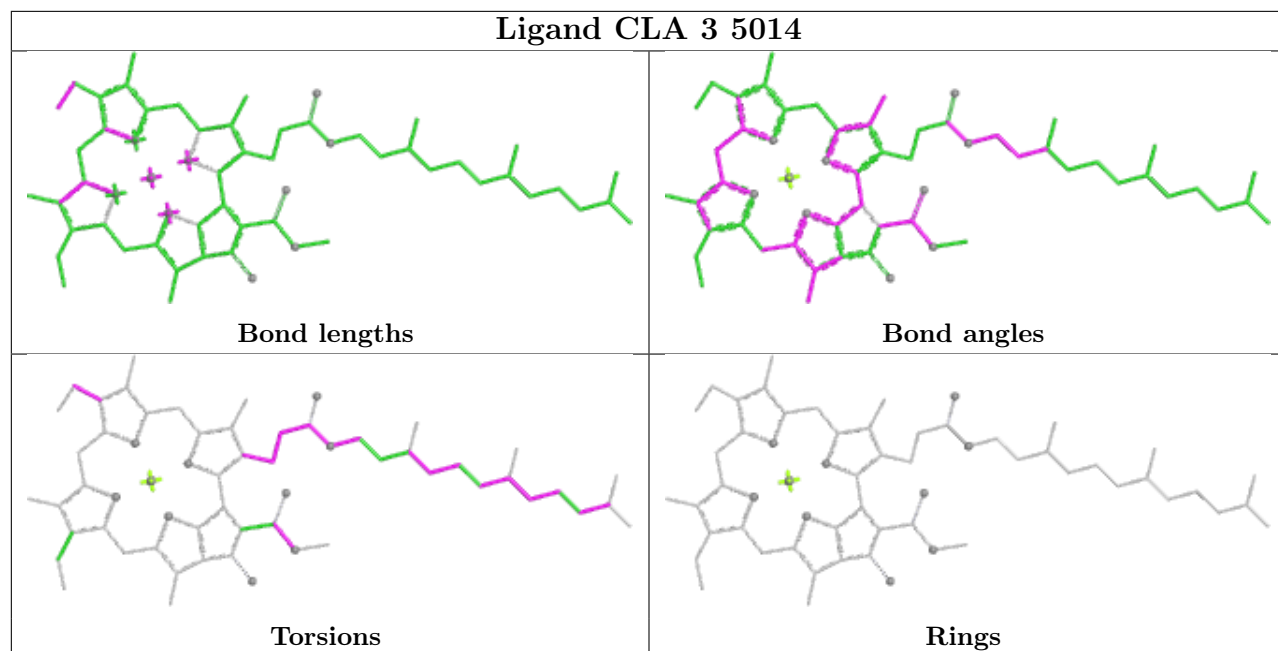


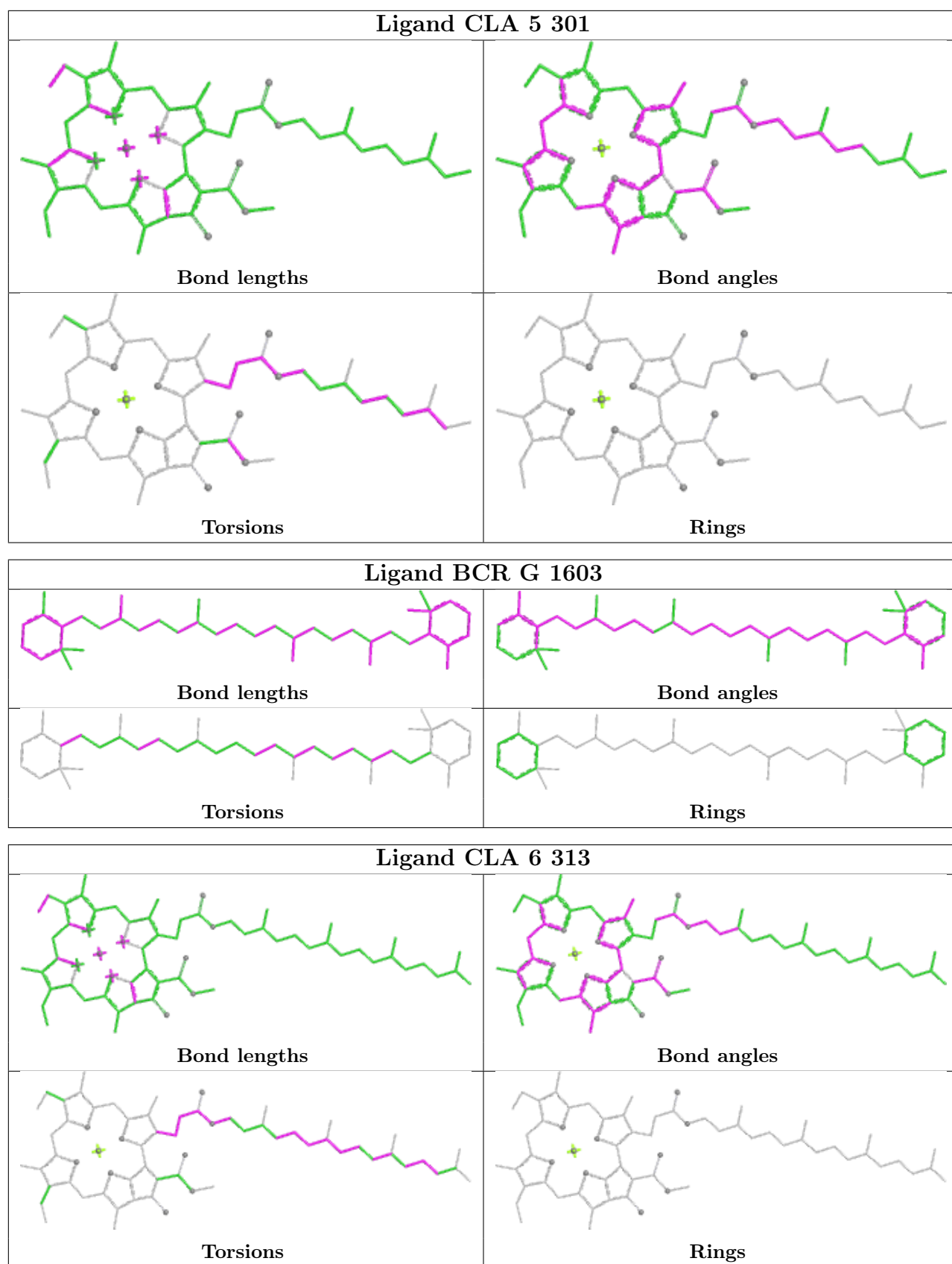
Torsions

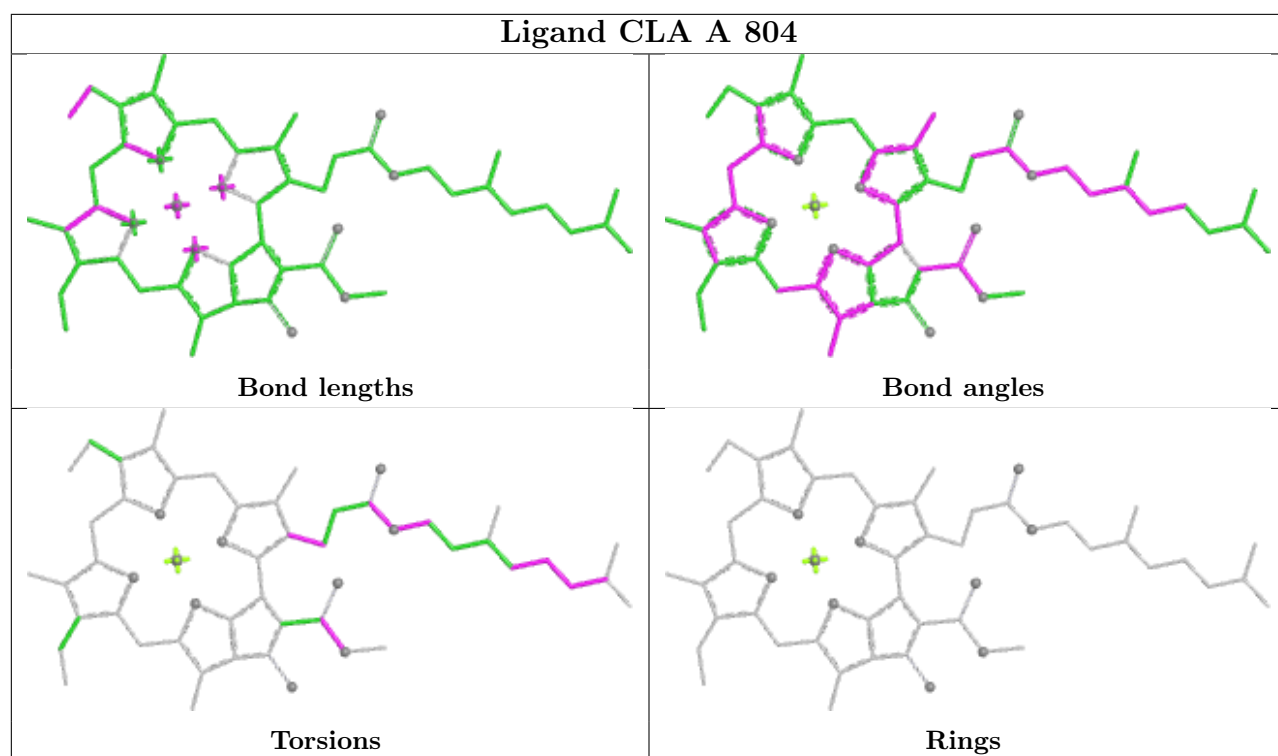


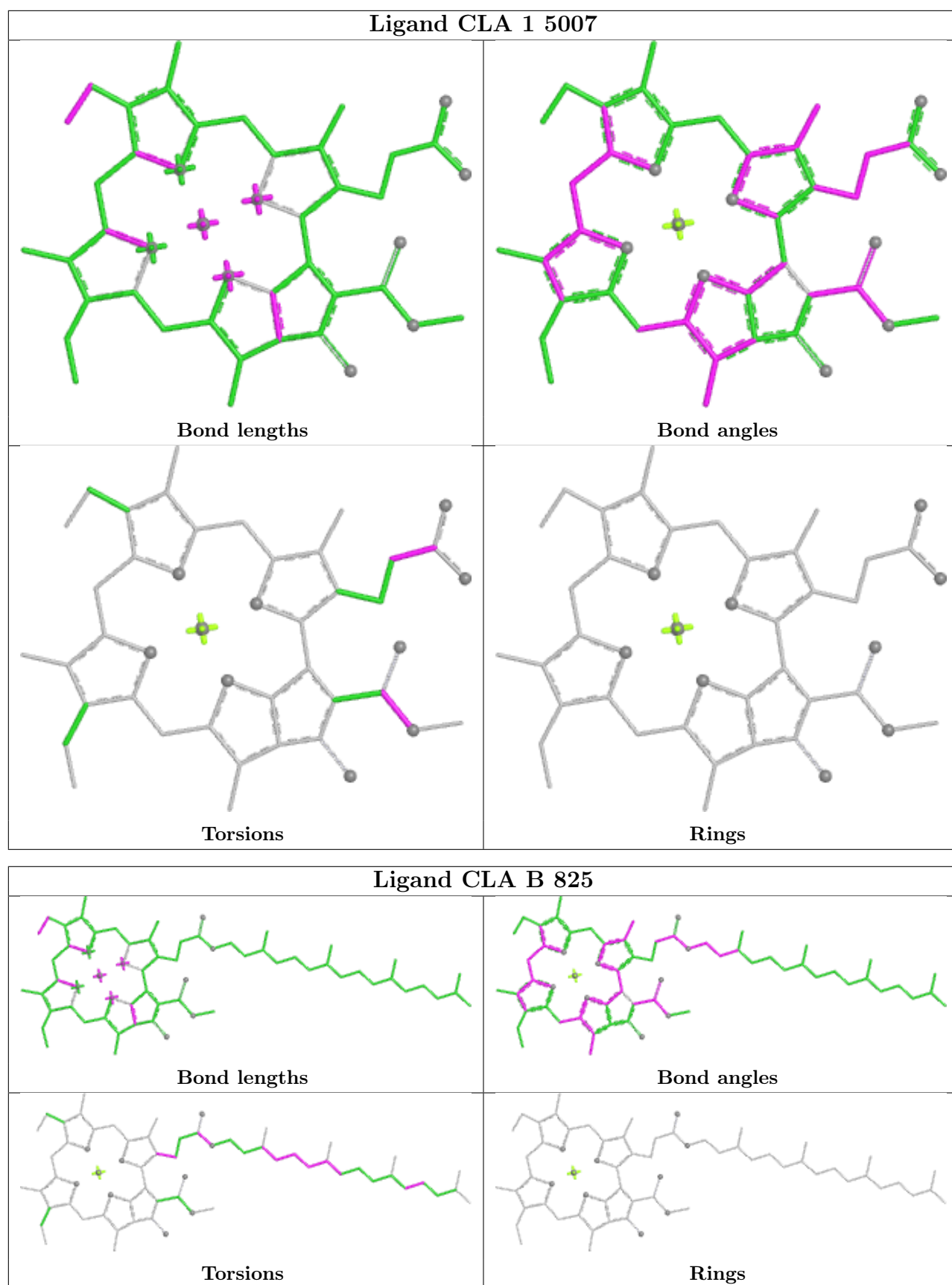
Rings

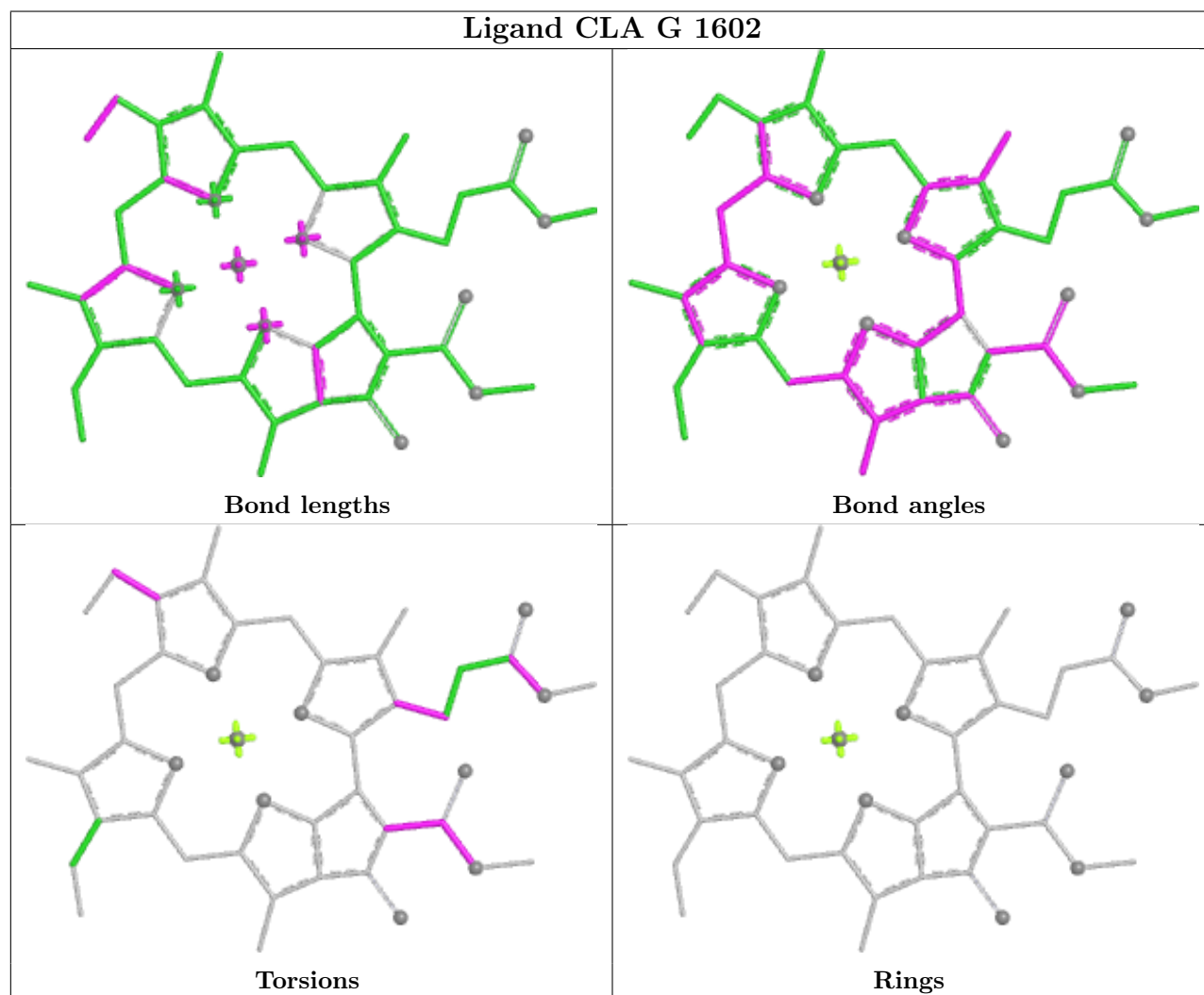
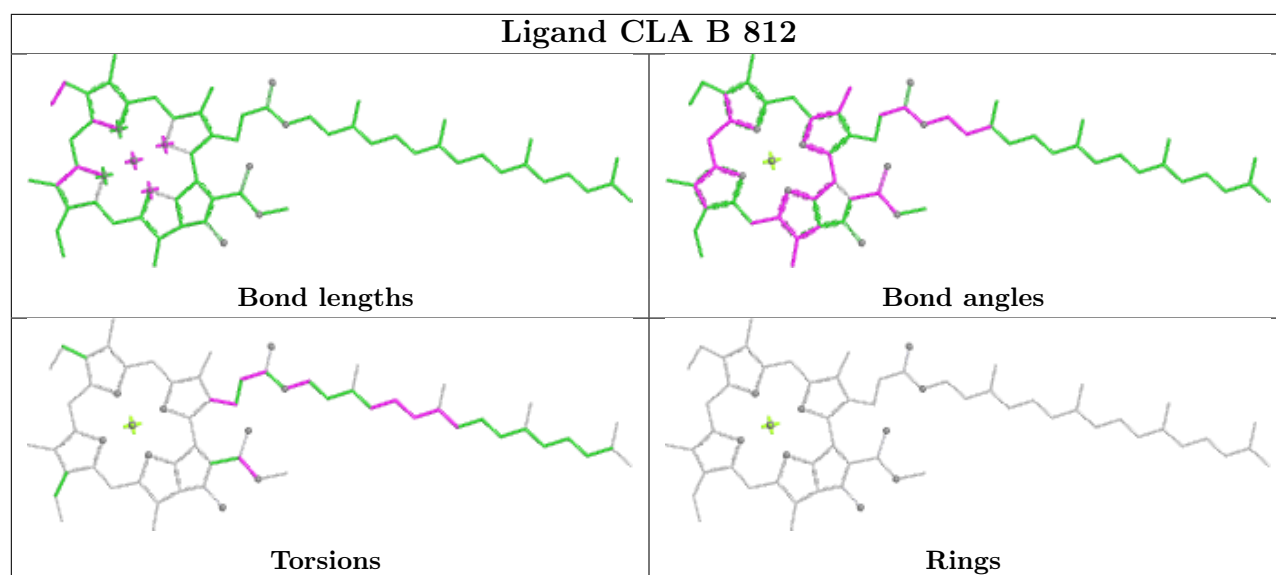


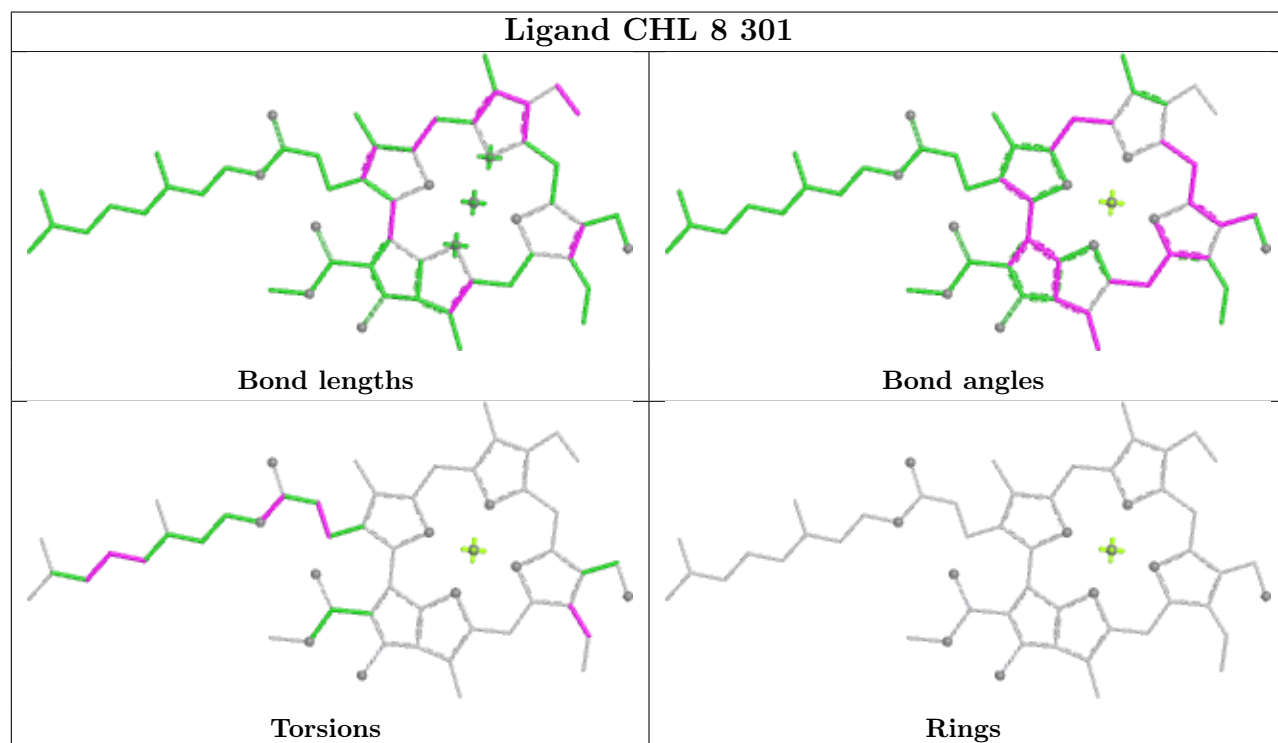
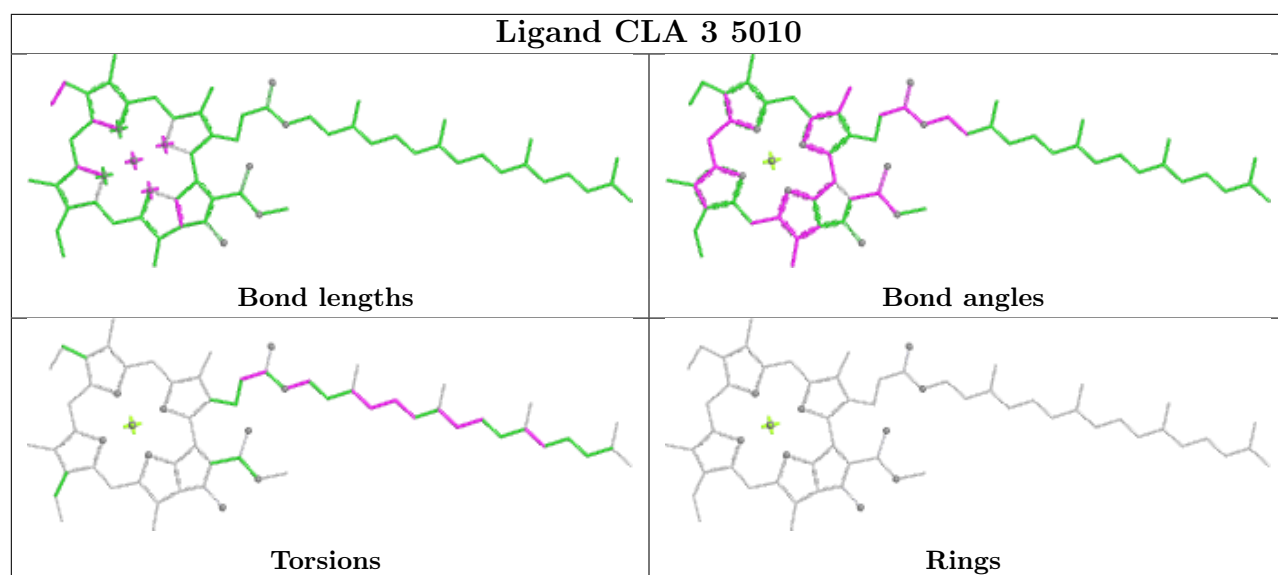


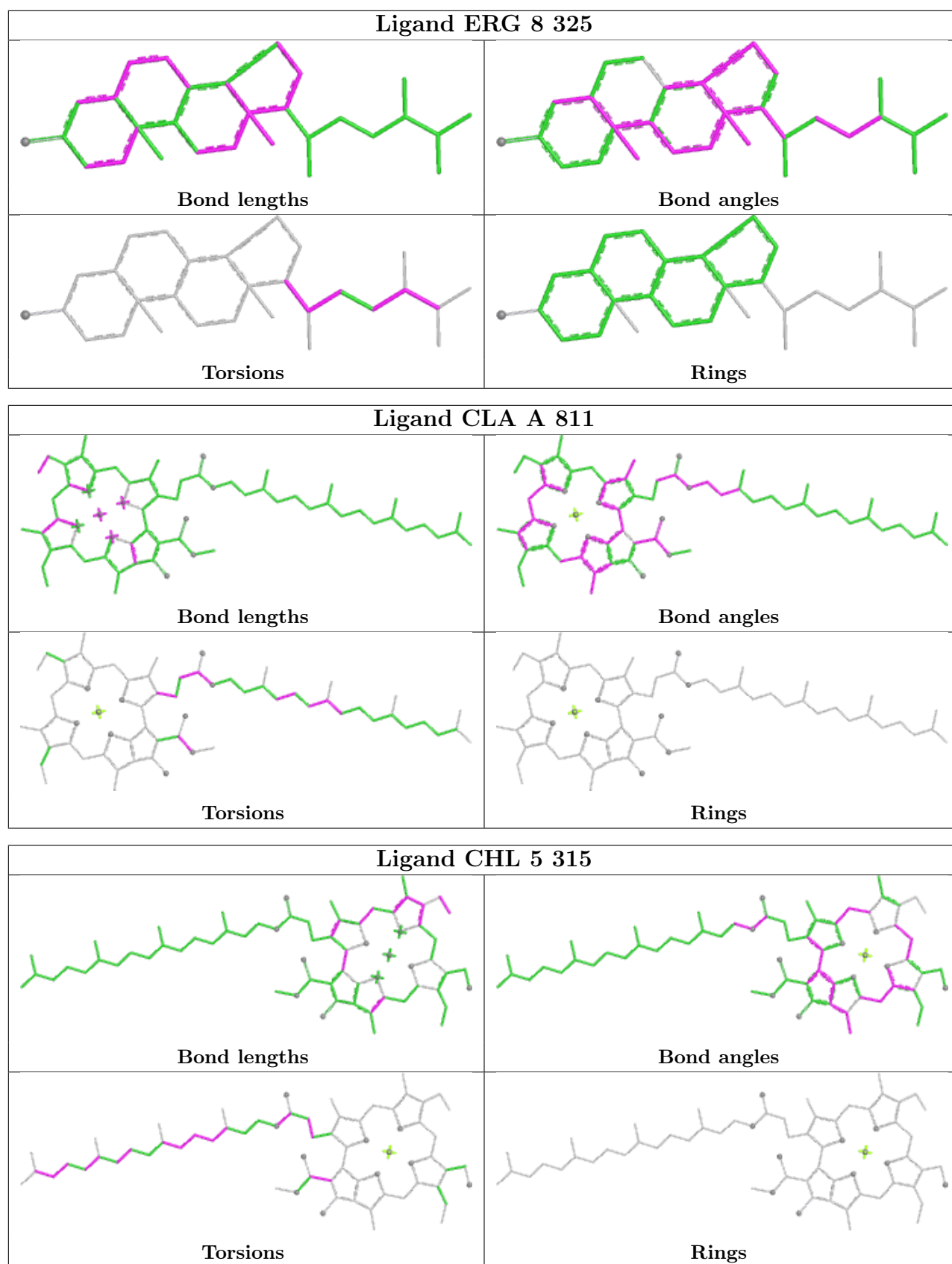


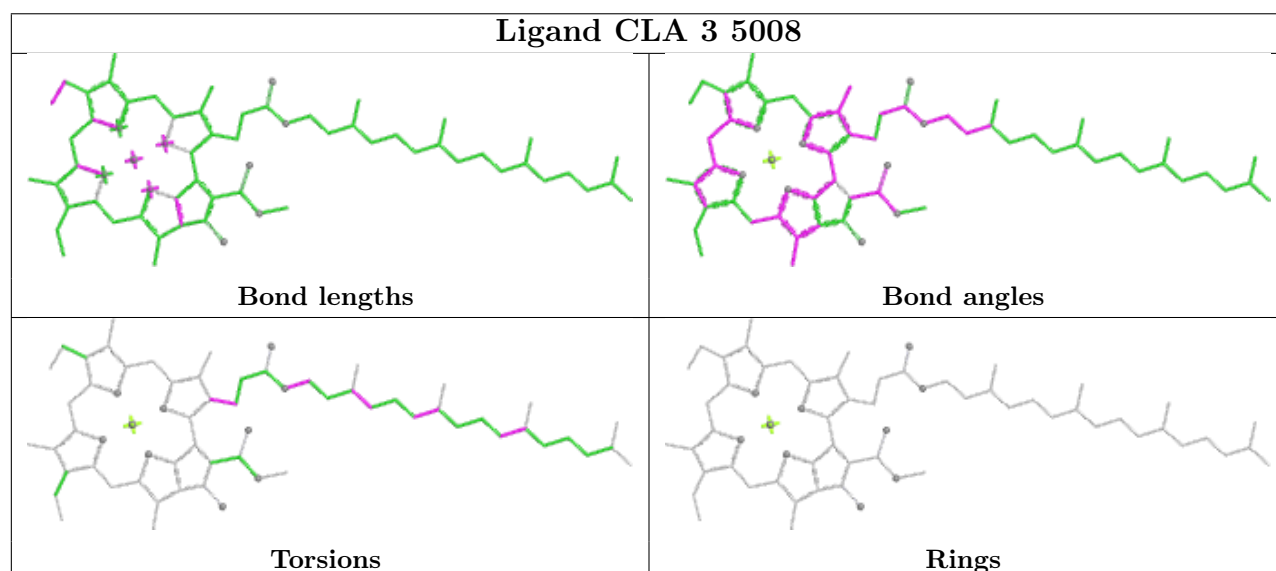
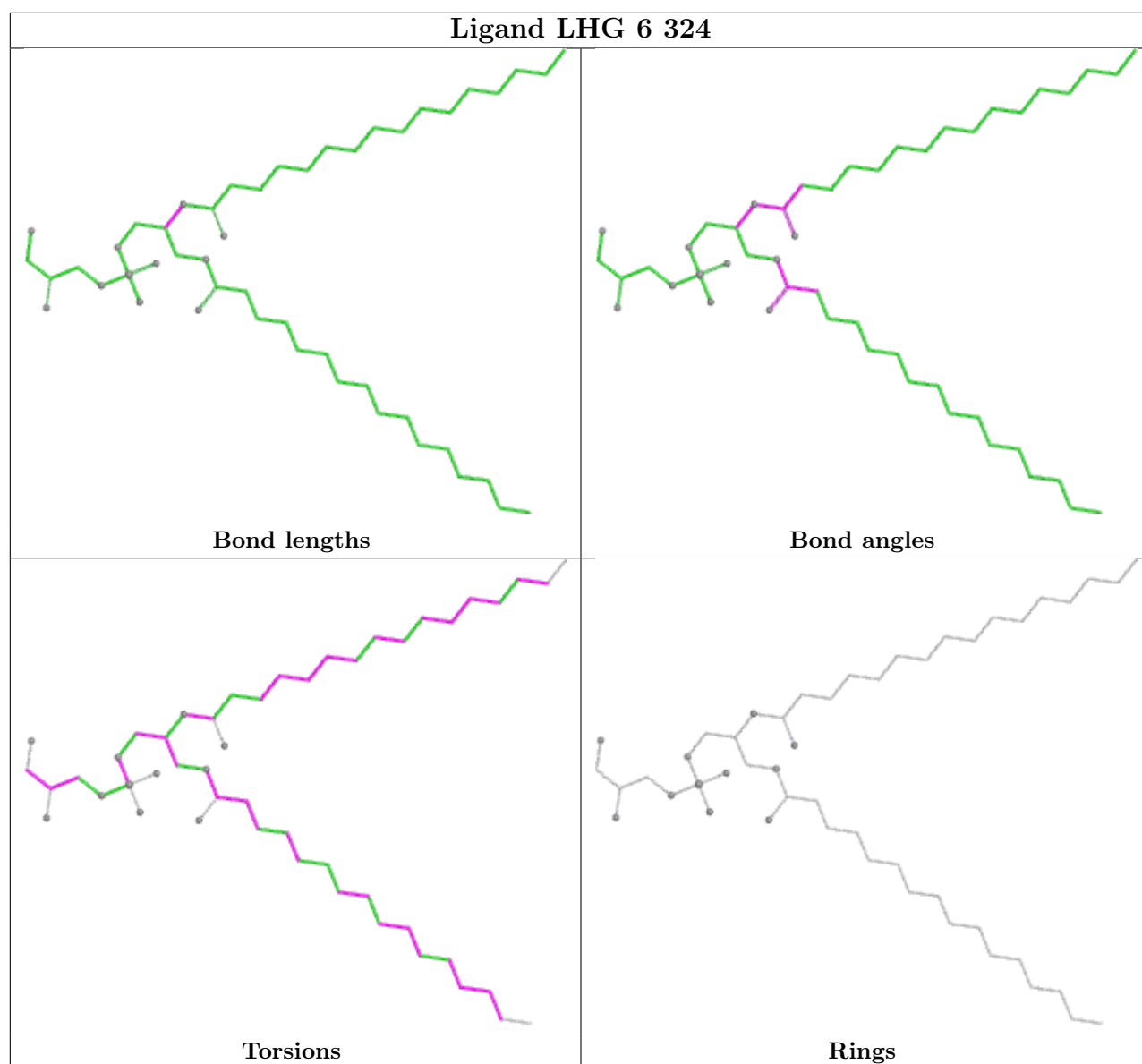


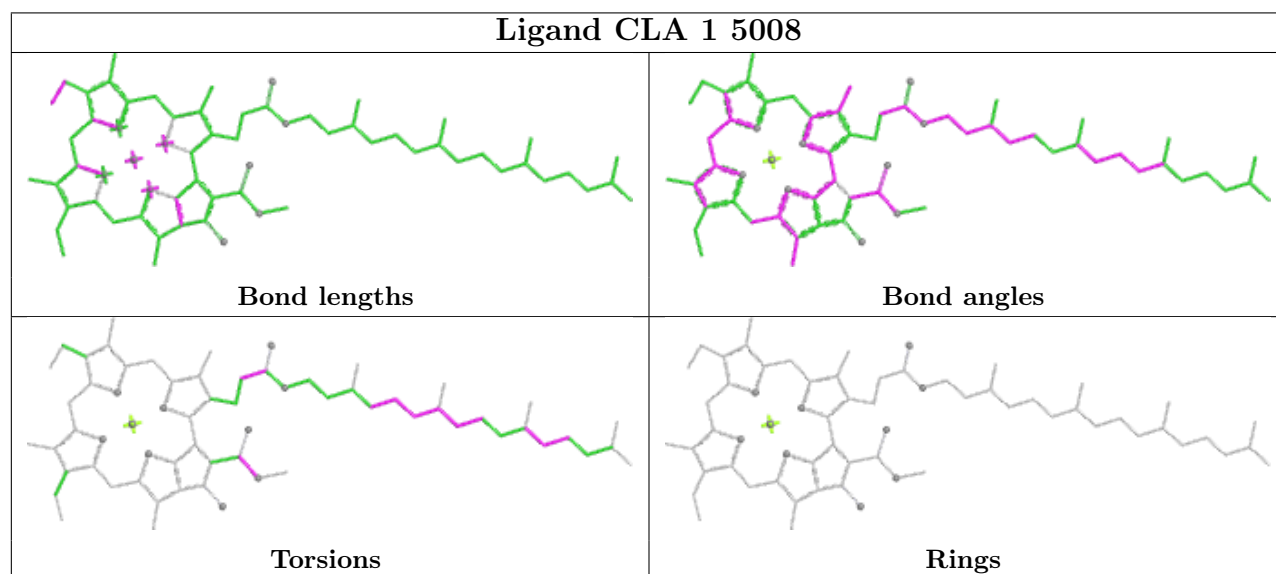
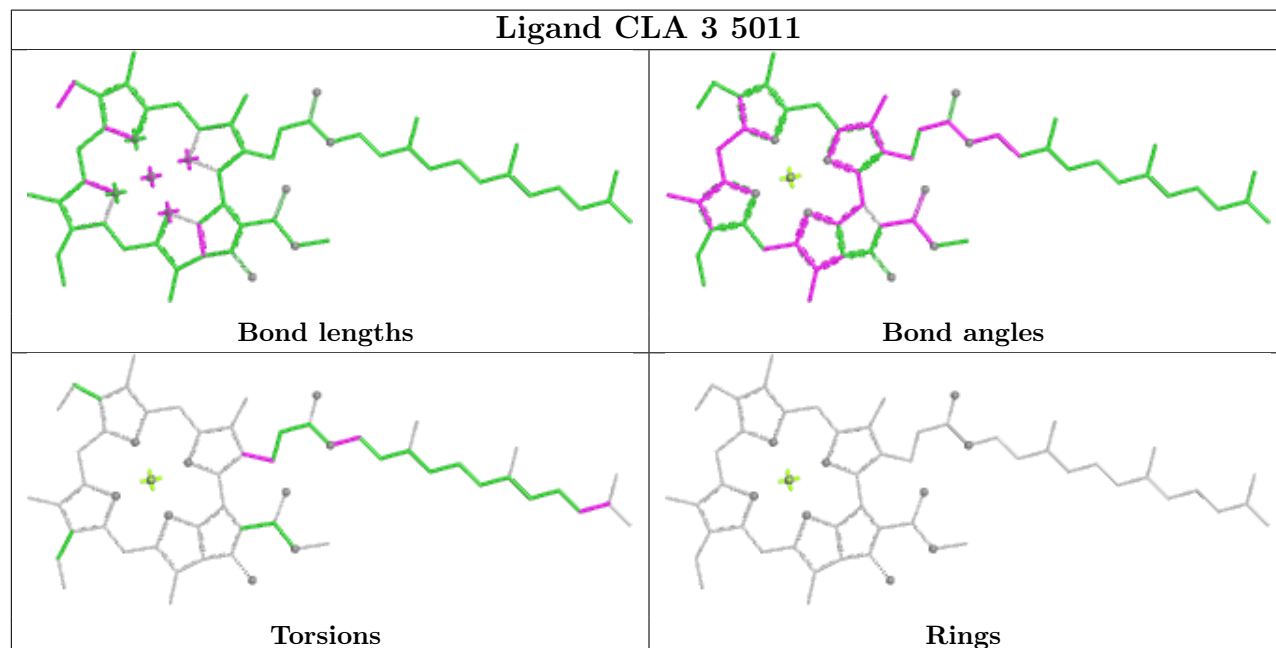
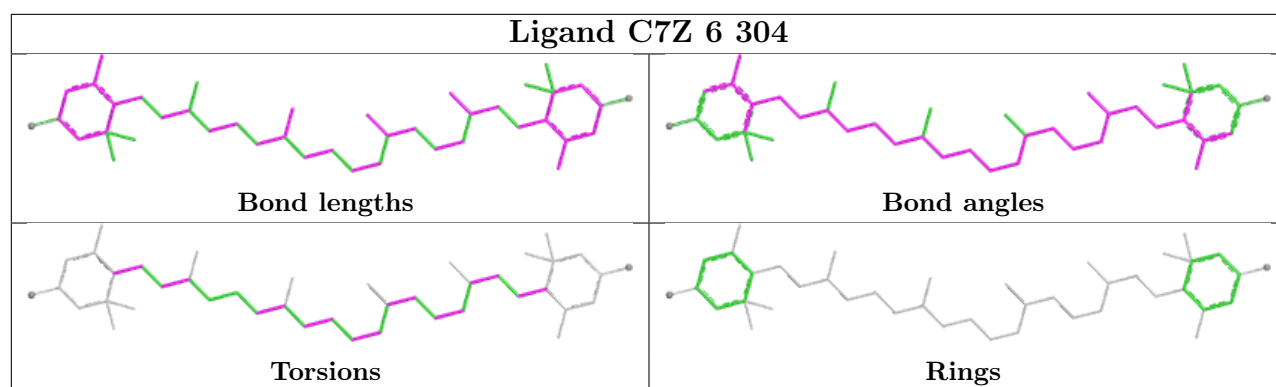


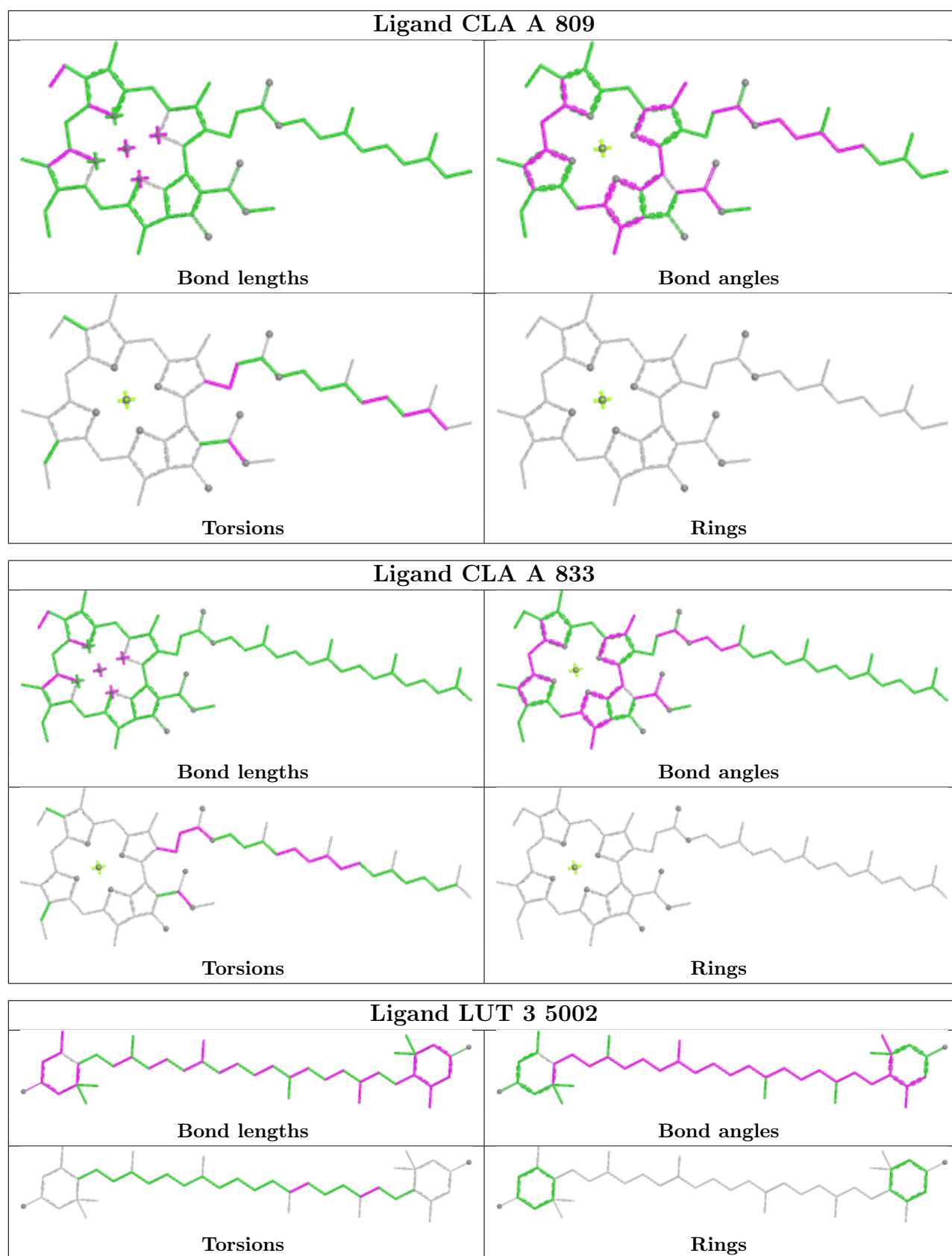


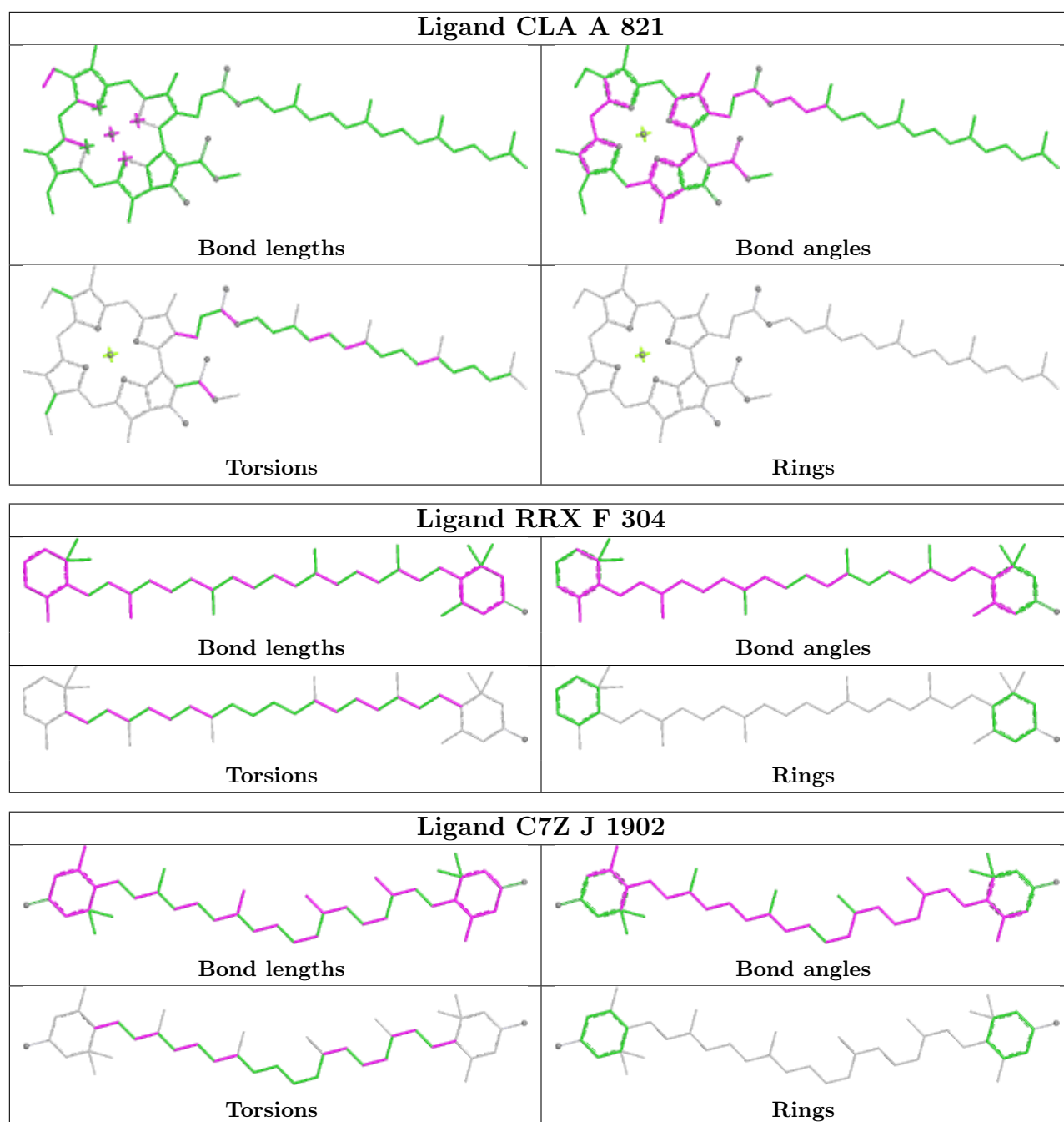




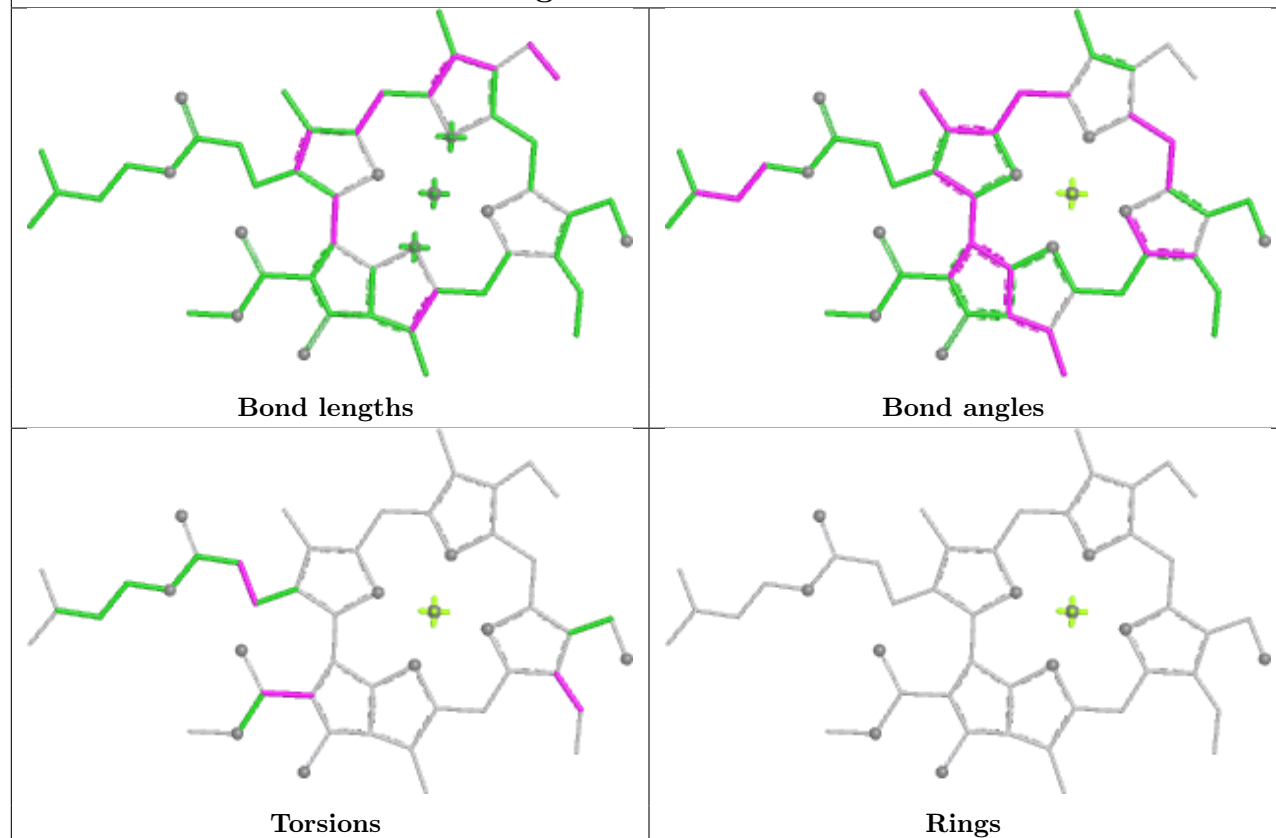




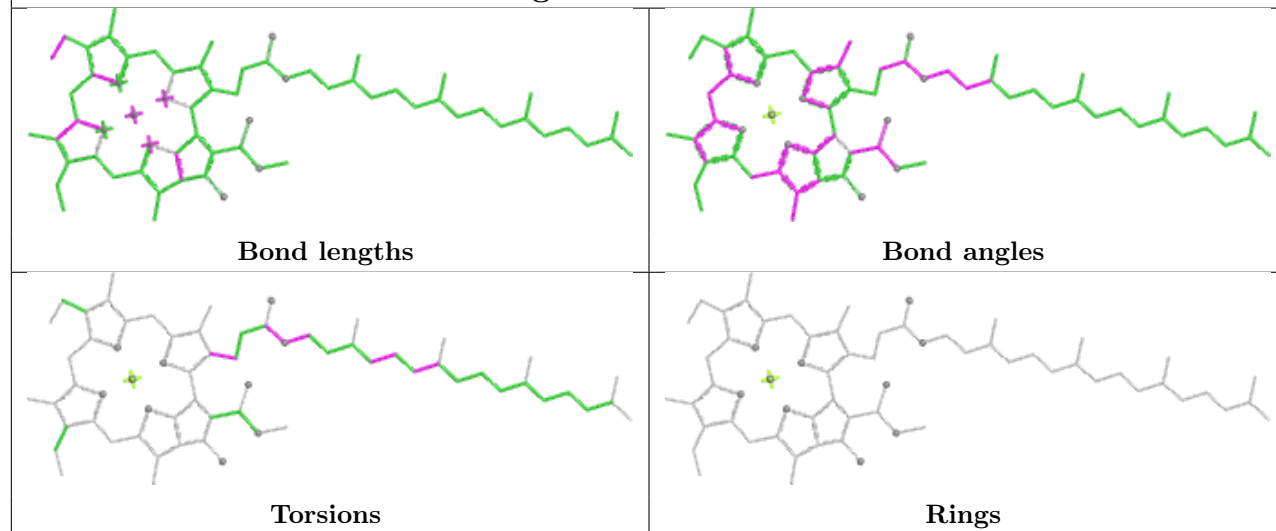


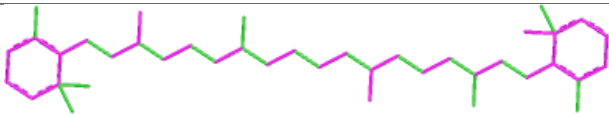
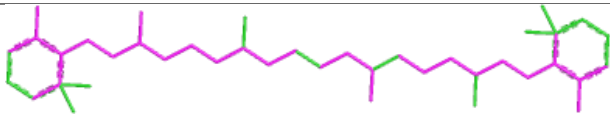
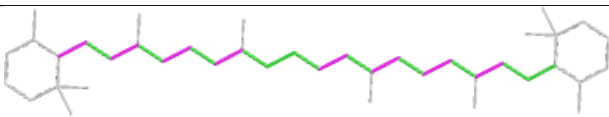
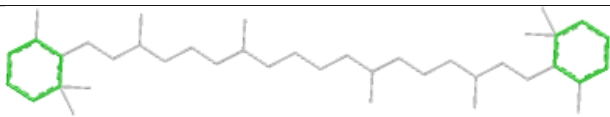


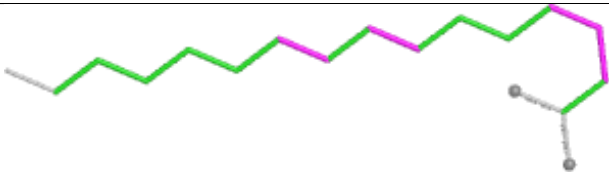
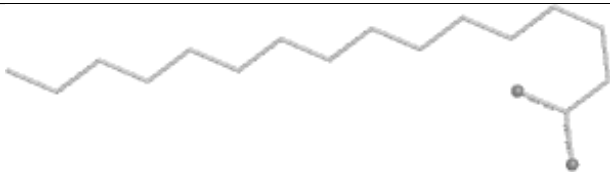
Ligand CHL 5 318

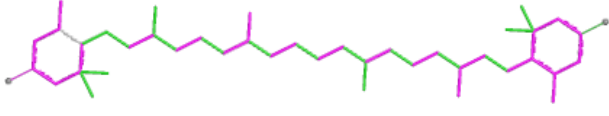
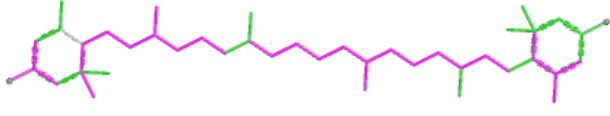
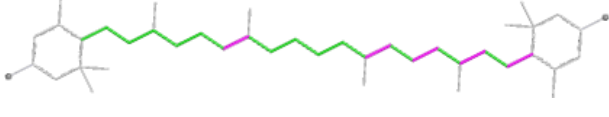
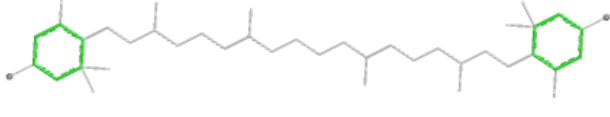


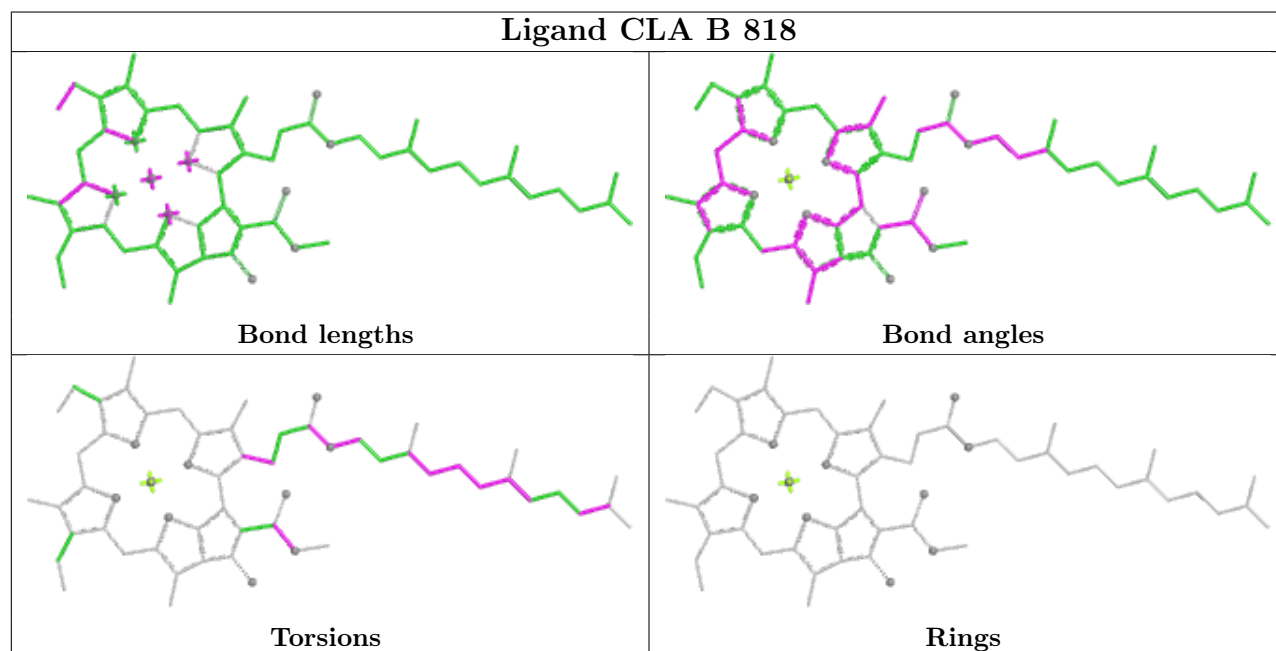
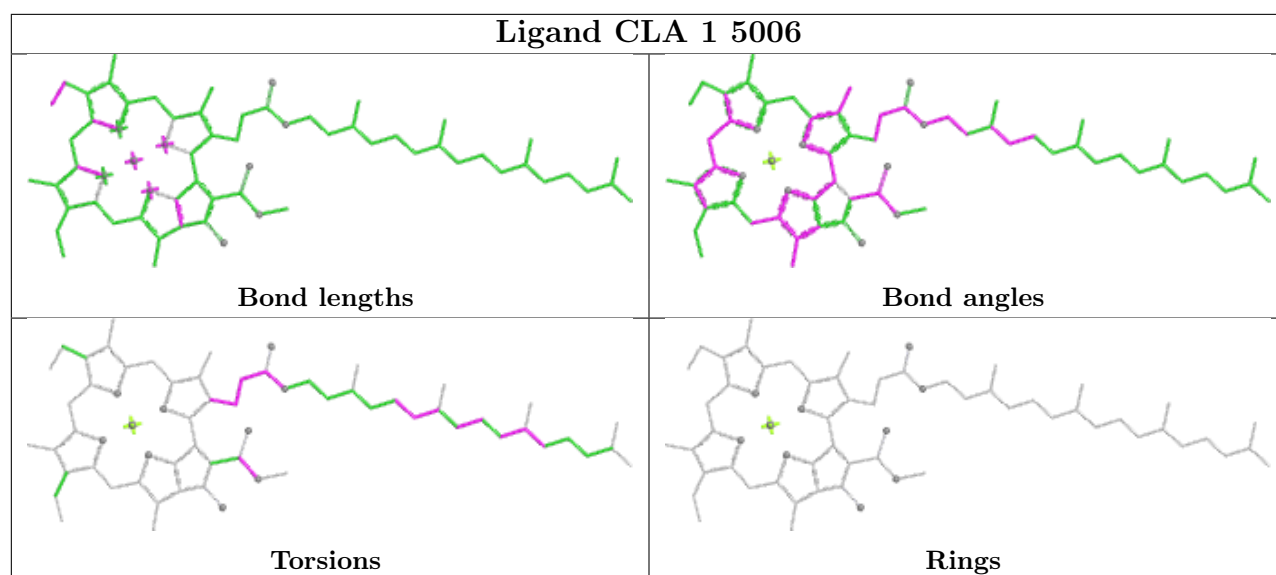
Ligand CLA B 806

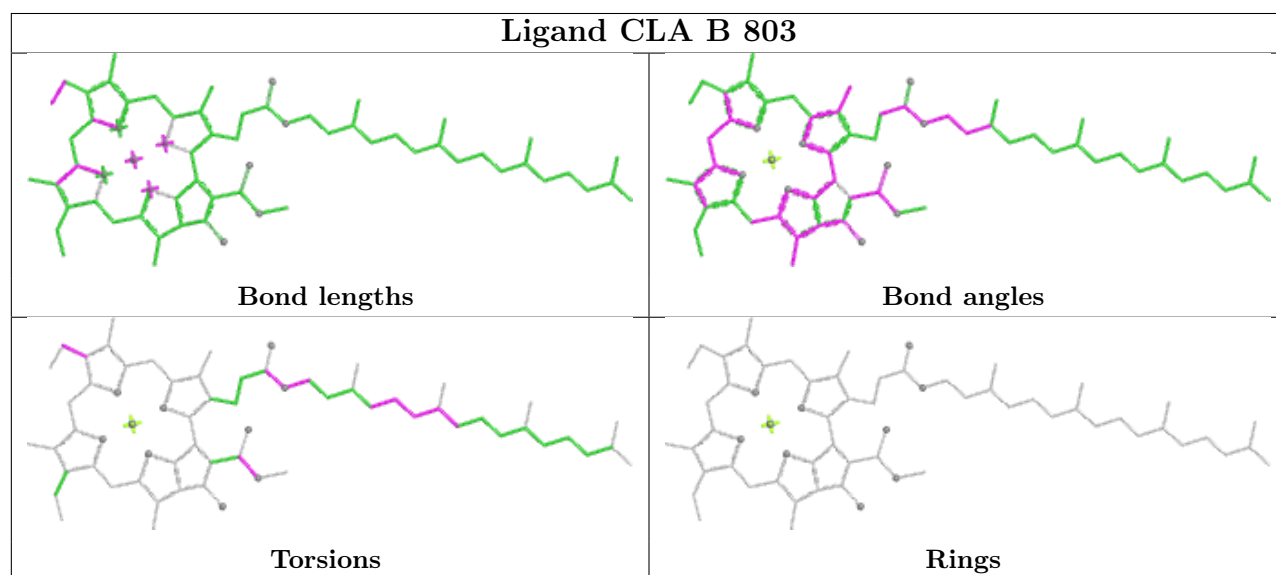
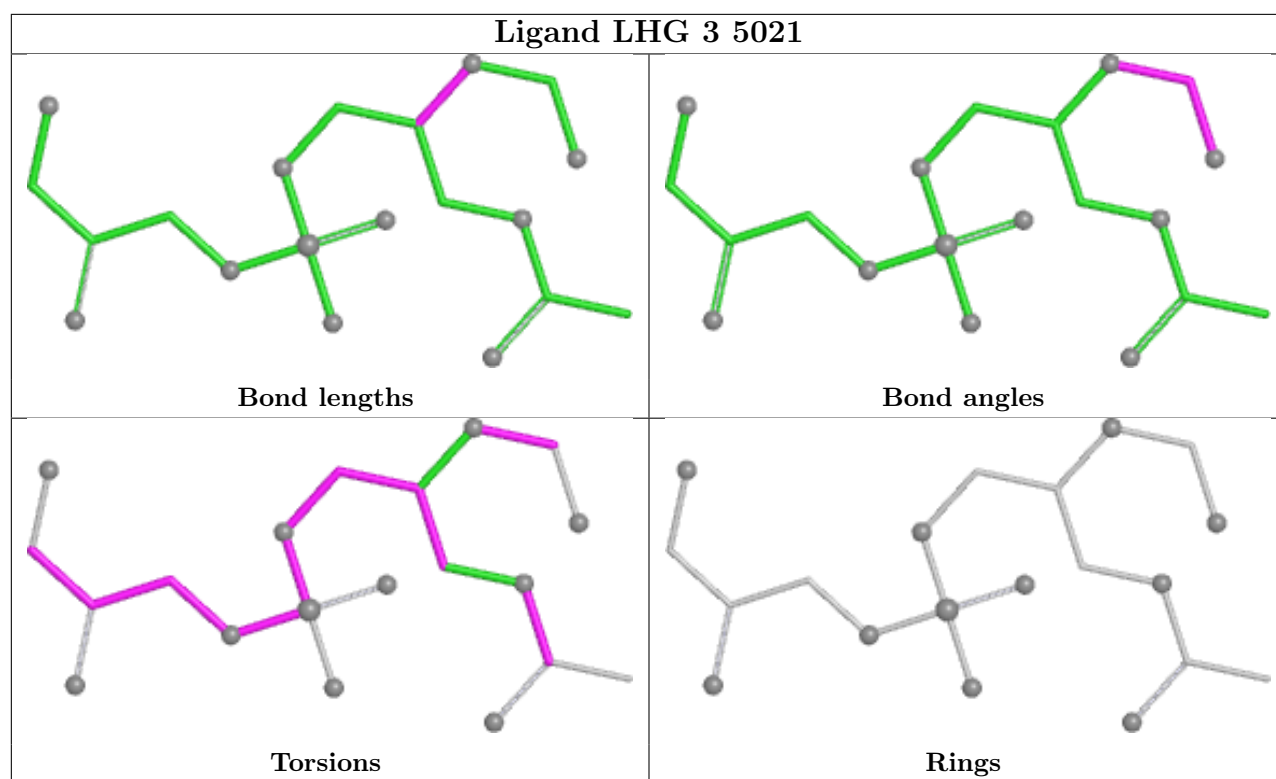


Ligand BCR 5 304	
	
Bond lengths	Bond angles
	
Torsions	Rings

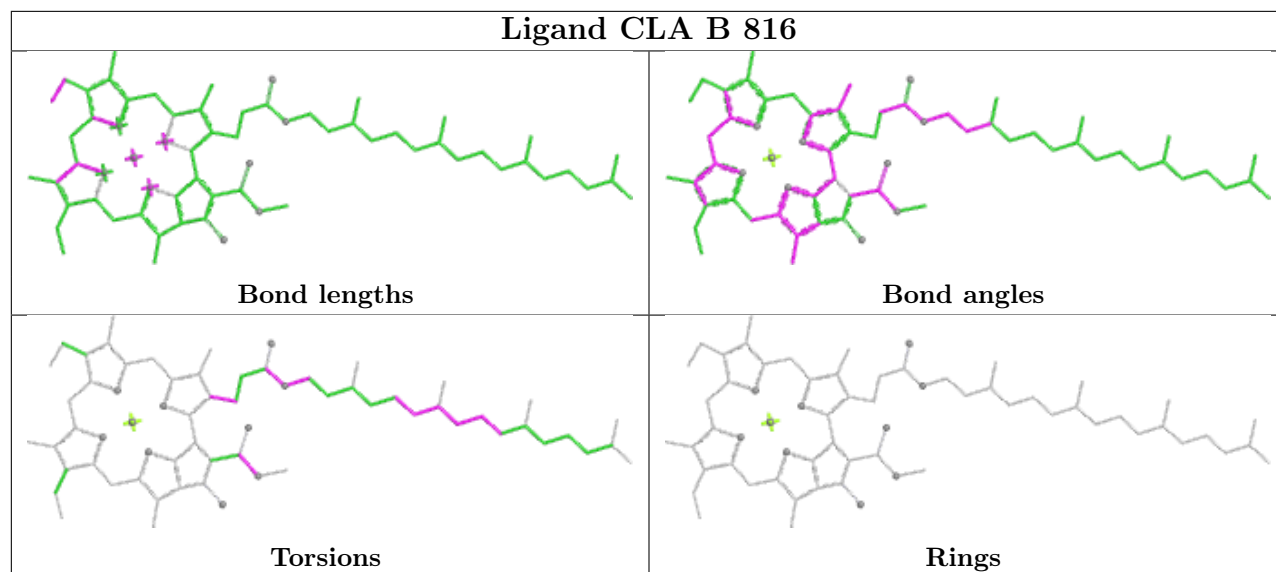
Ligand PLM 7 322	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 5 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

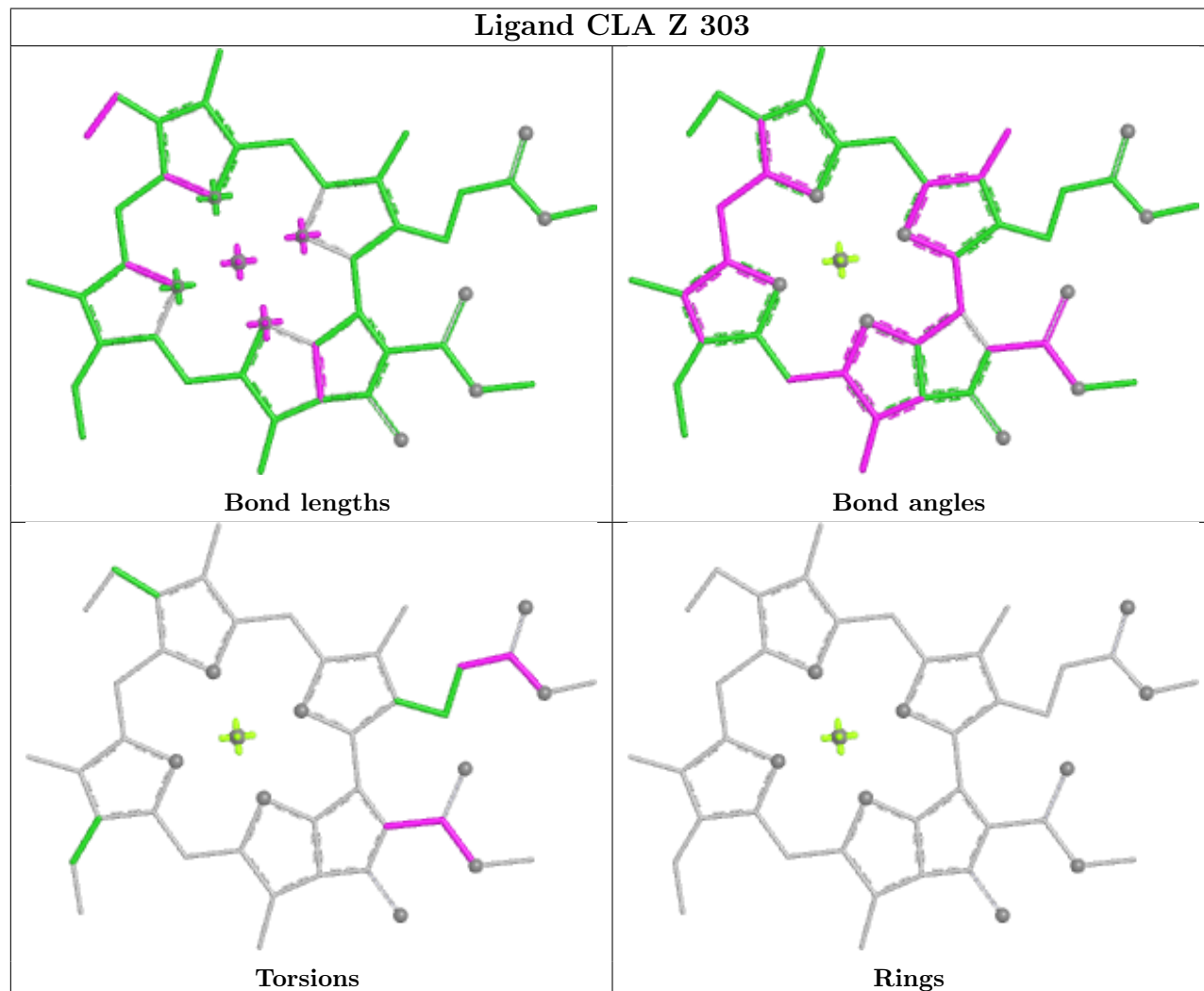




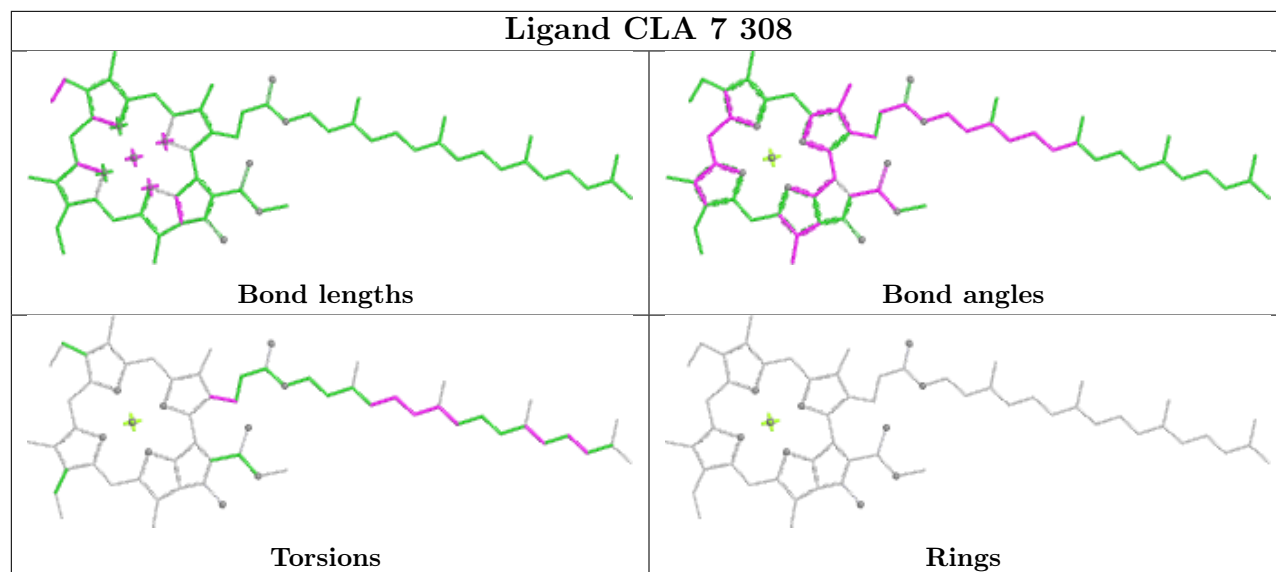
Ligand CLA B 816



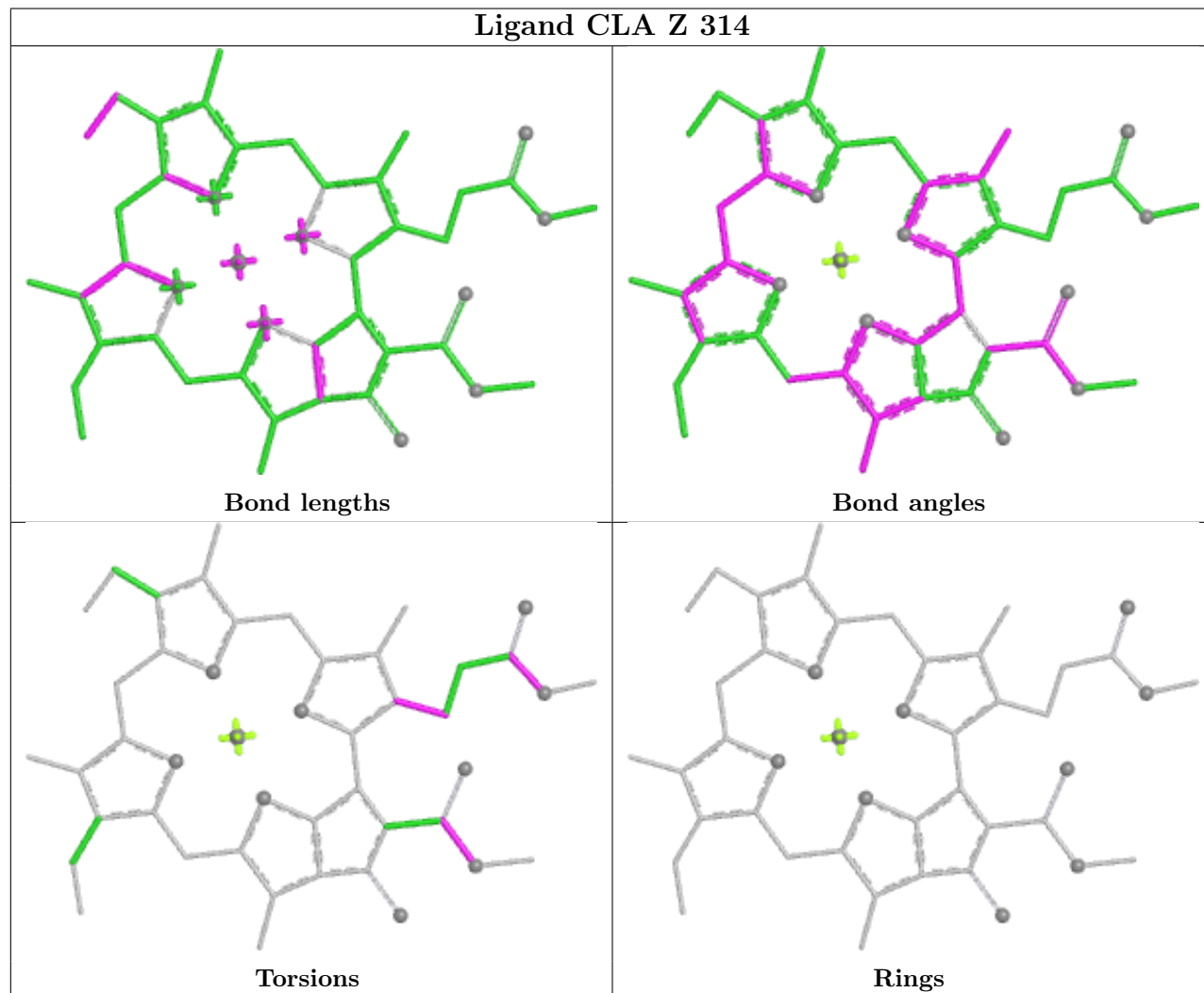
Ligand CLA Z 303

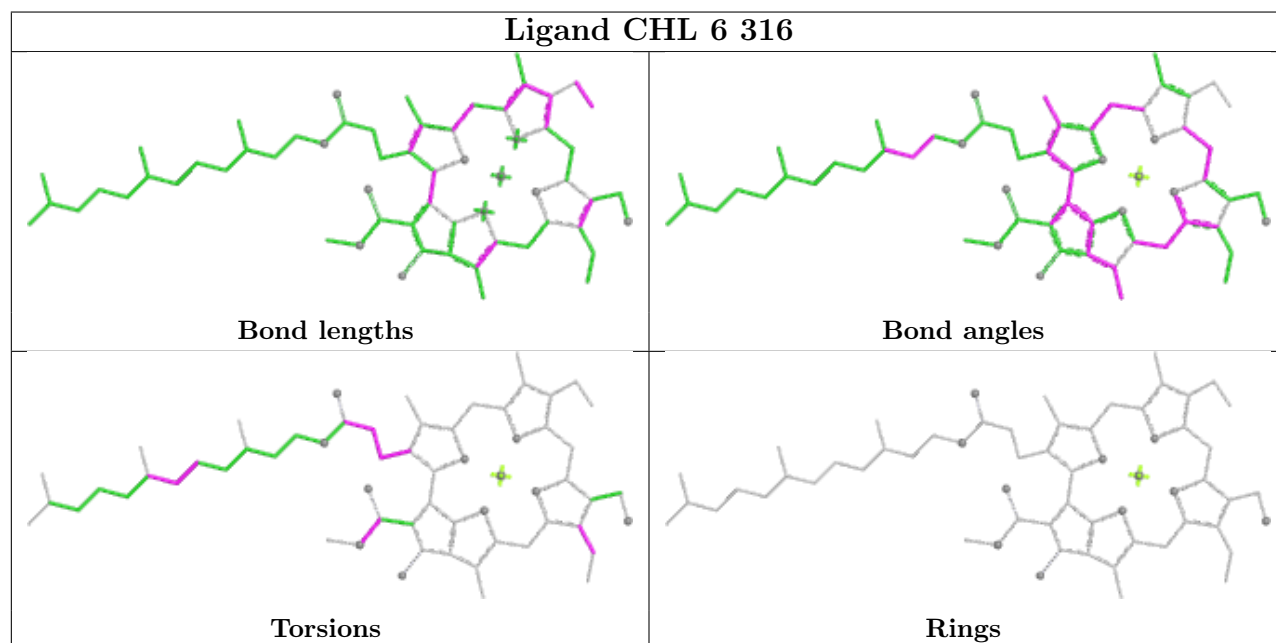
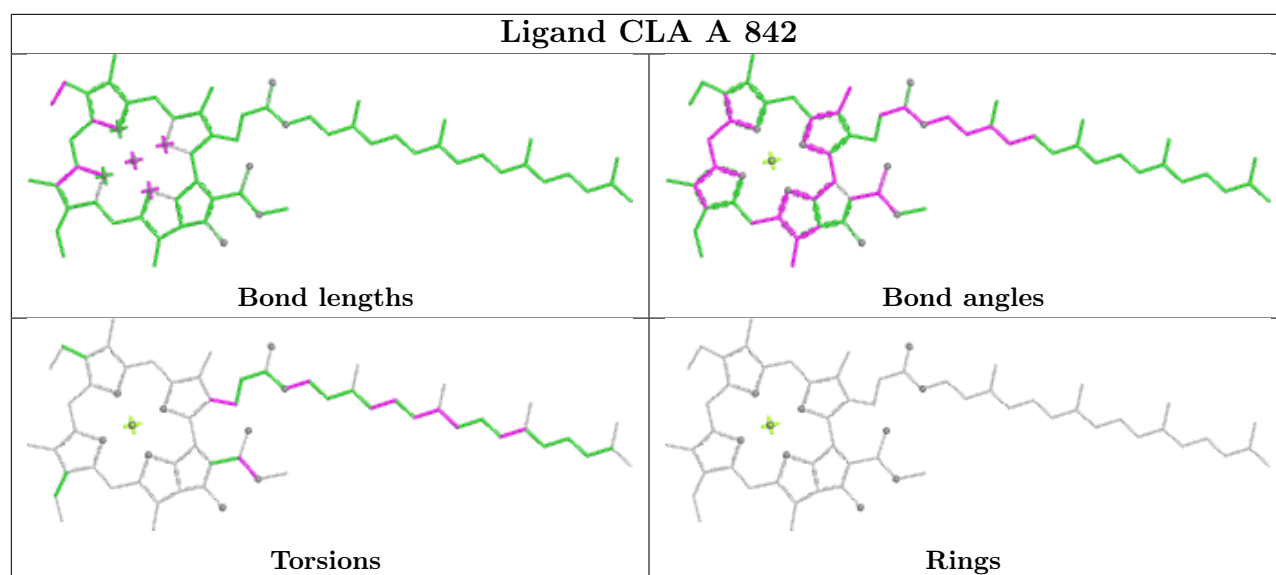


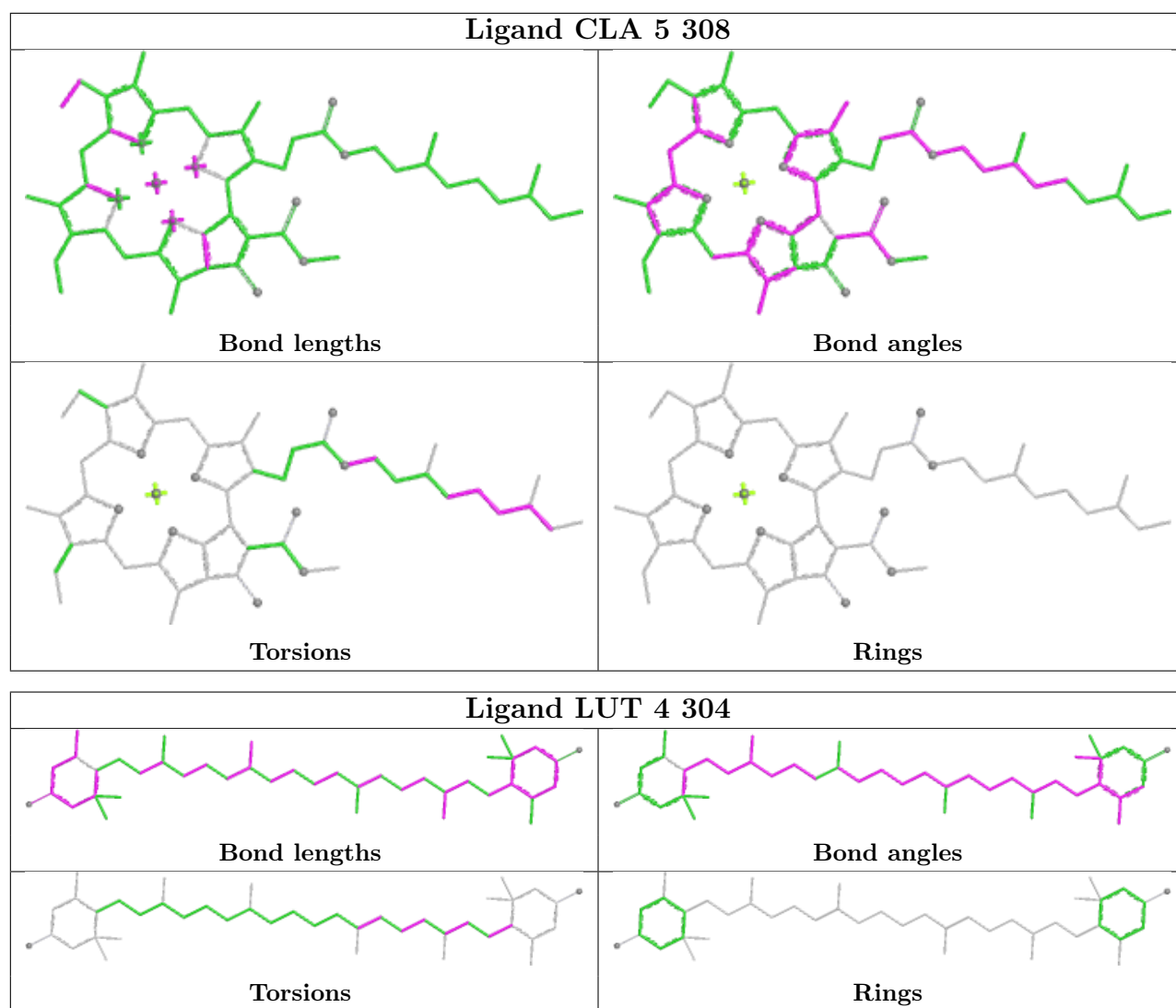
Ligand CLA 7 308



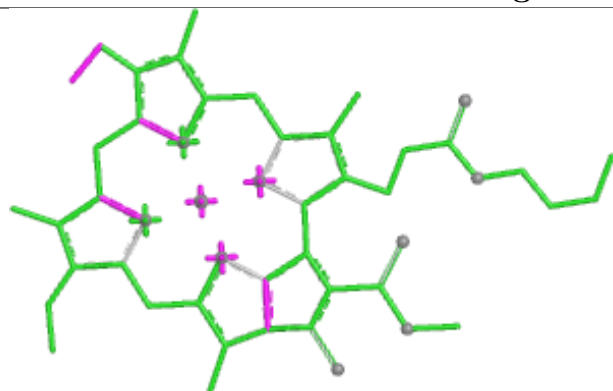
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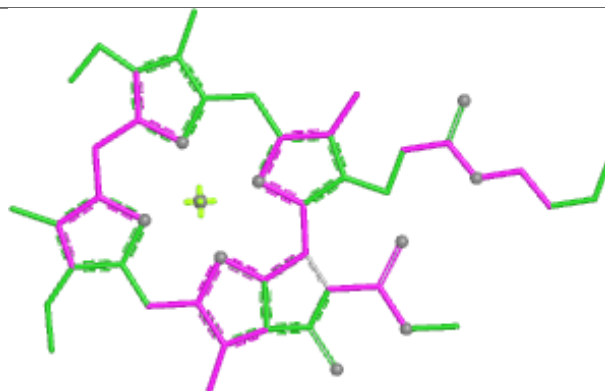




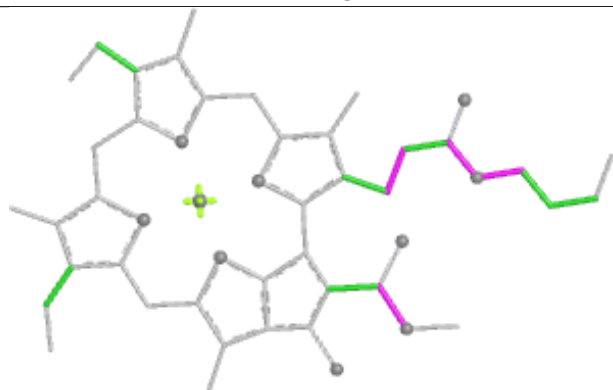
Ligand CLA K 204



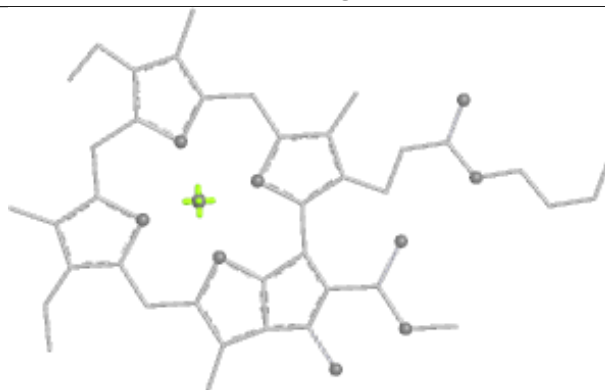
Bond lengths



Bond angles

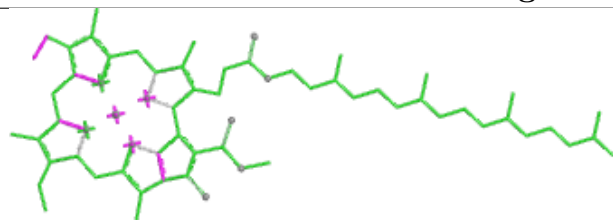


Torsions

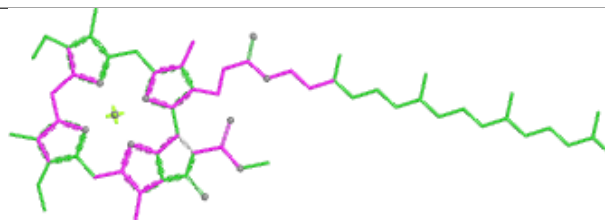


Rings

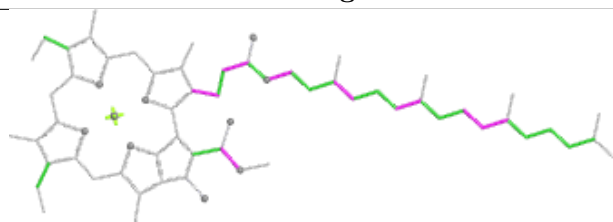
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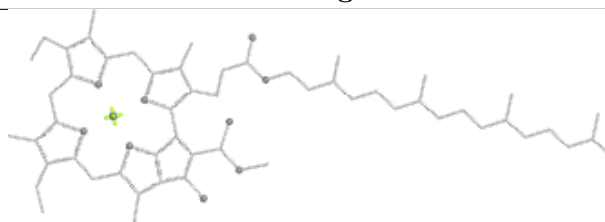
Bond lengths



Bond angles

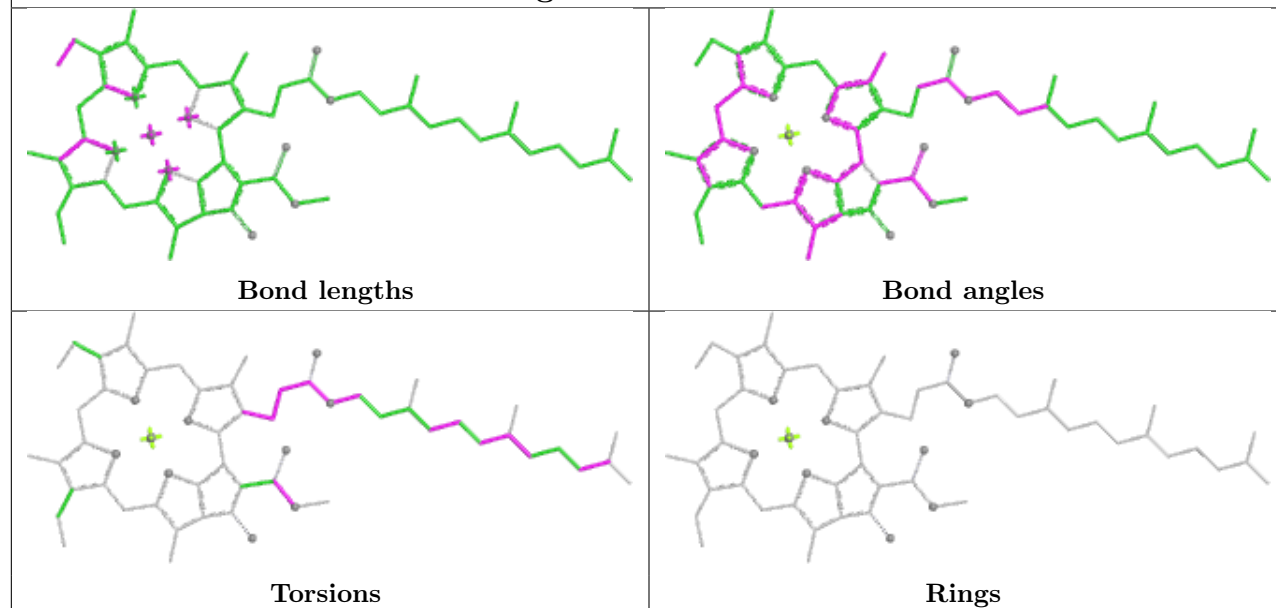


Torsions

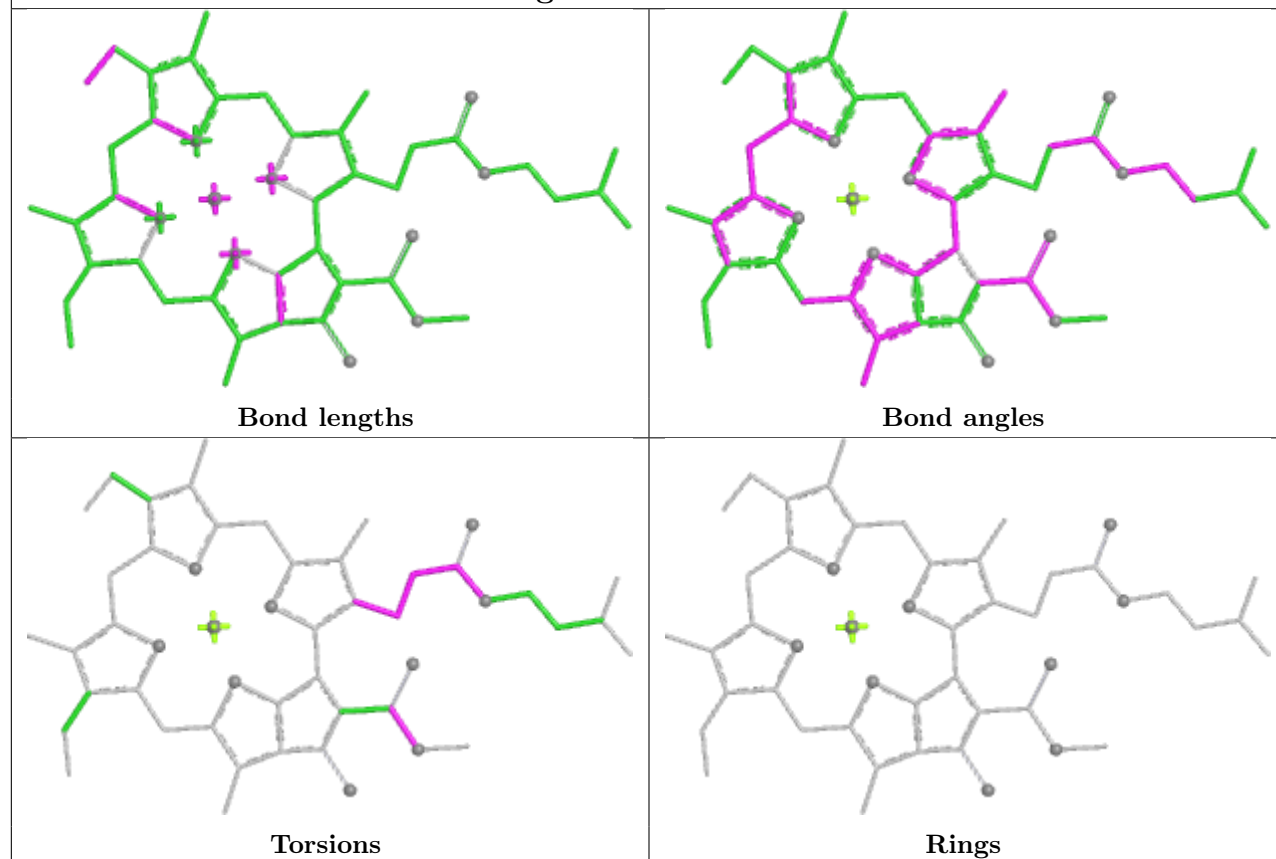


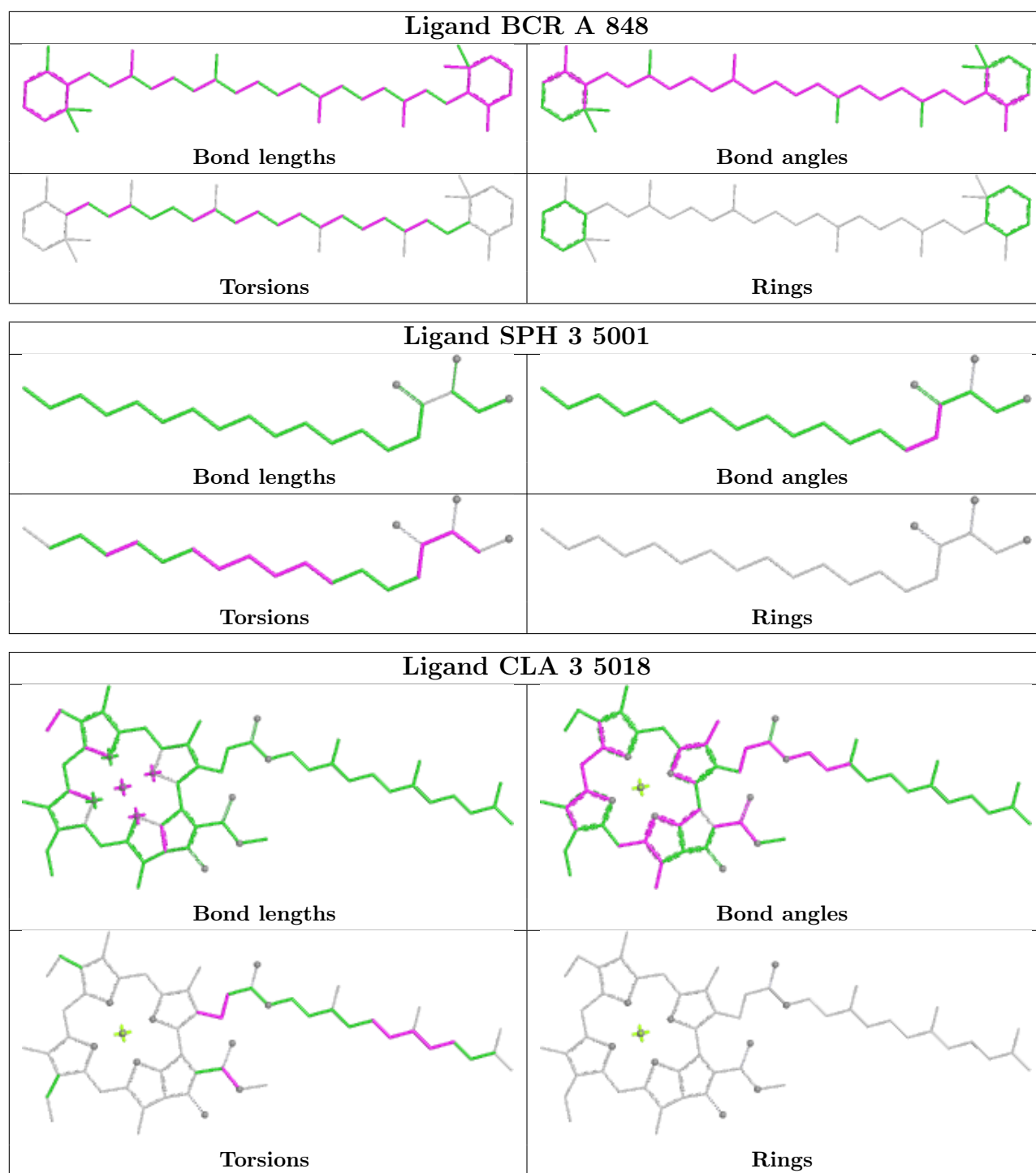
Rings

Ligand CLA 6 302

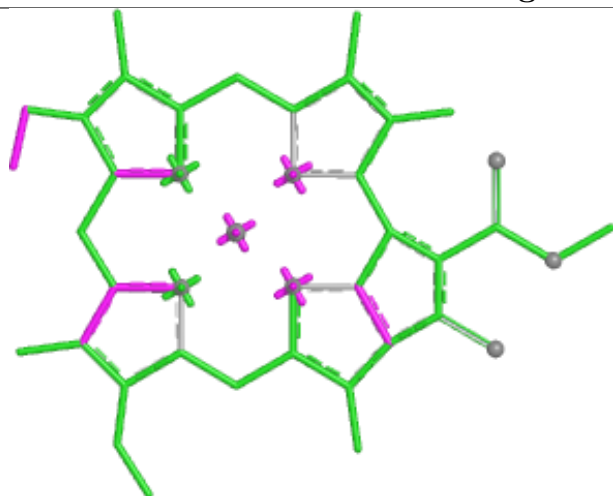


Ligand CLA 5 319

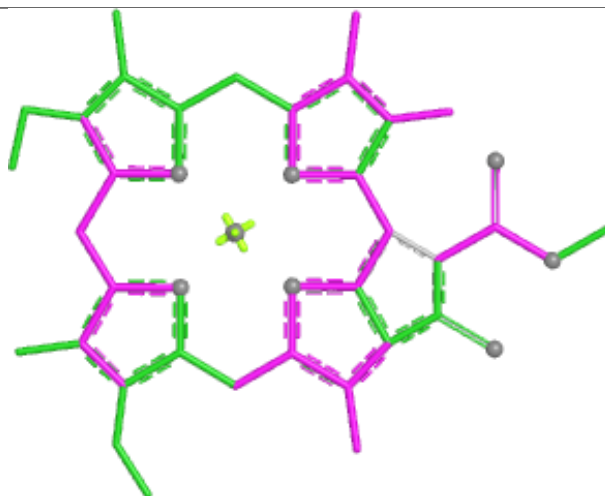




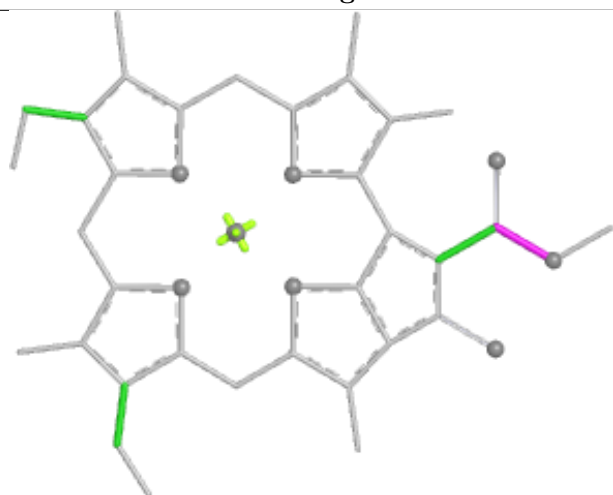
Ligand CLA 4 318



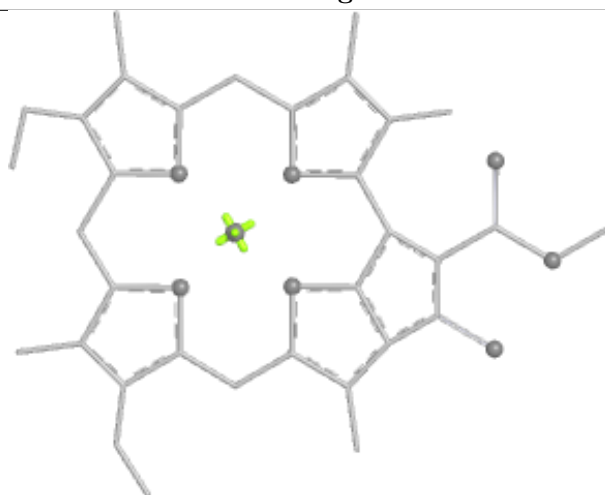
Bond lengths



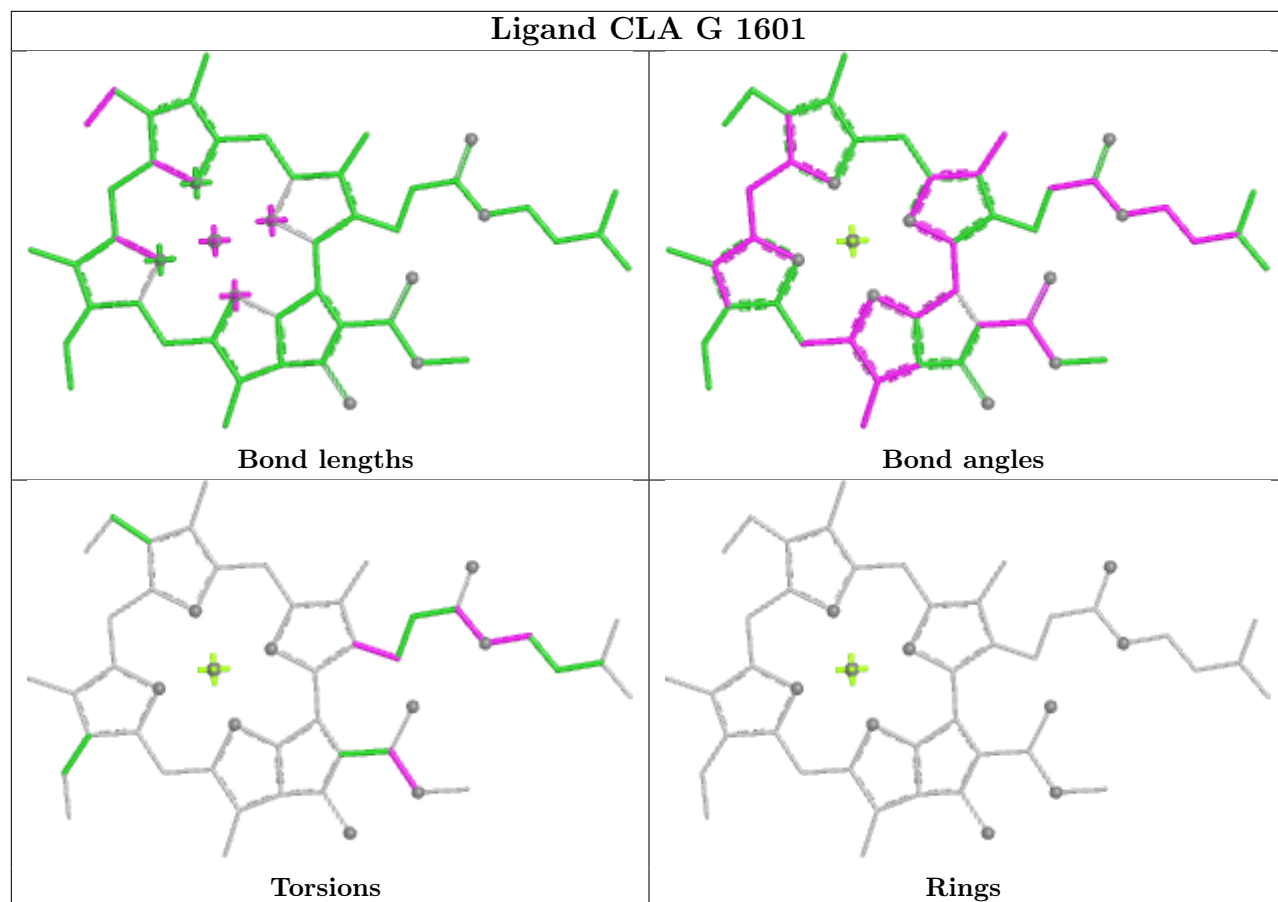
Bond angles

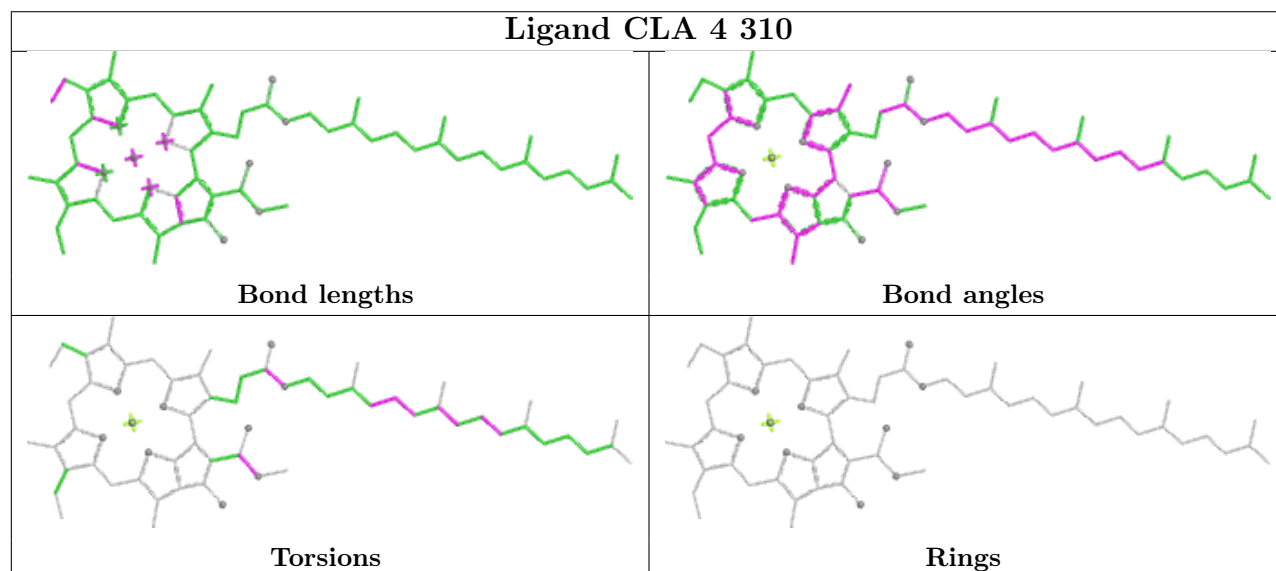
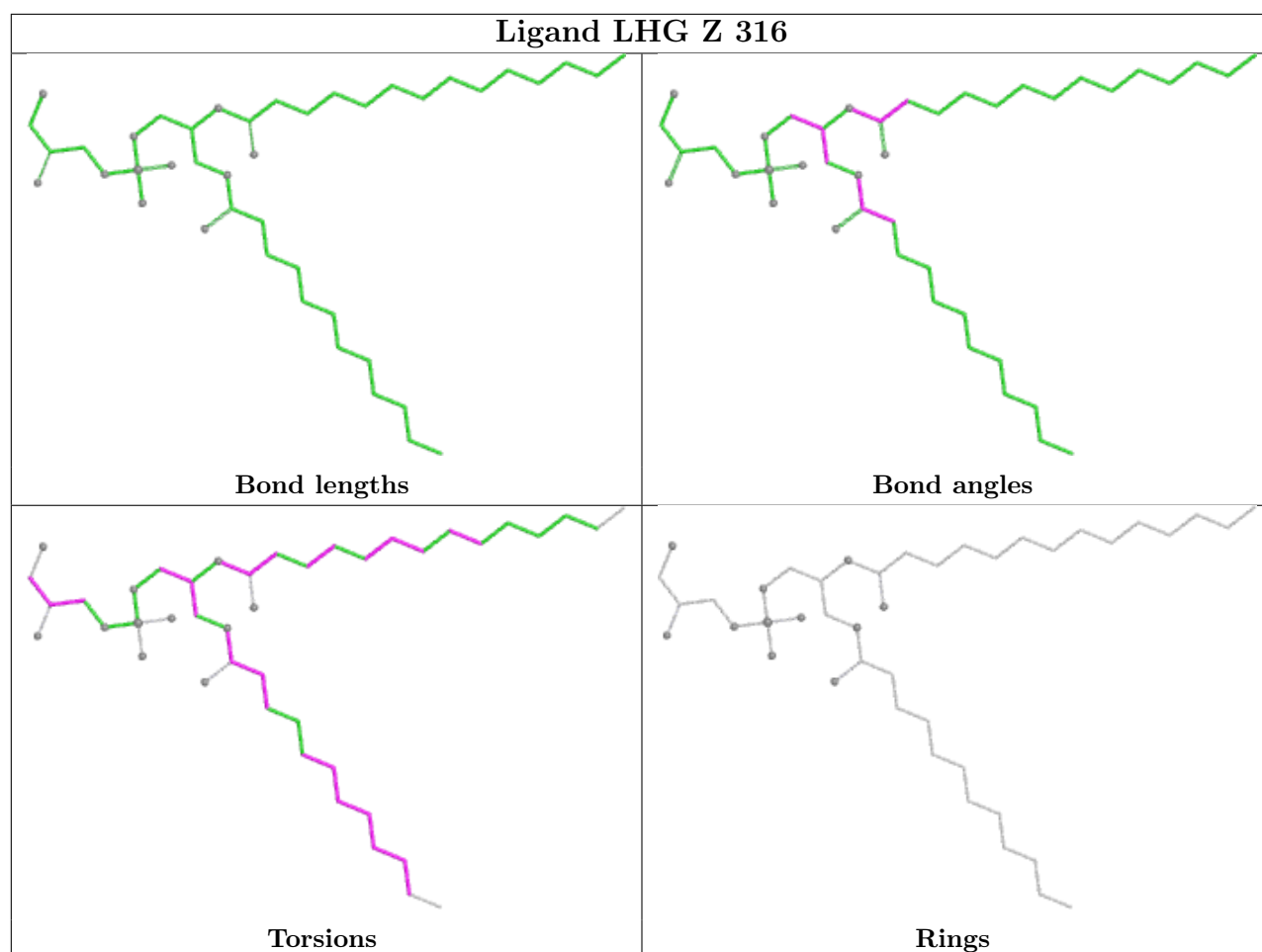


Torsions

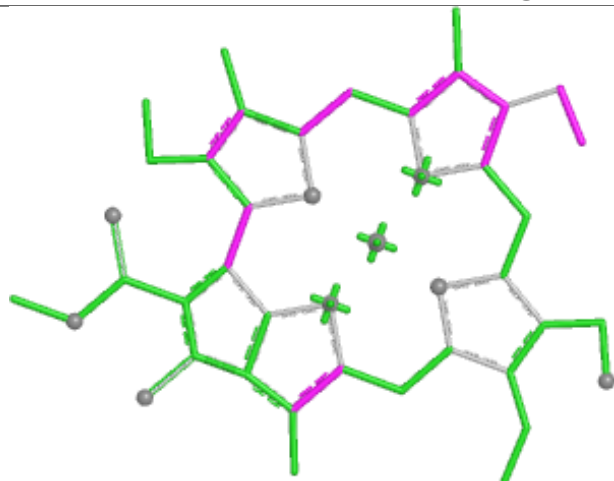


Rings

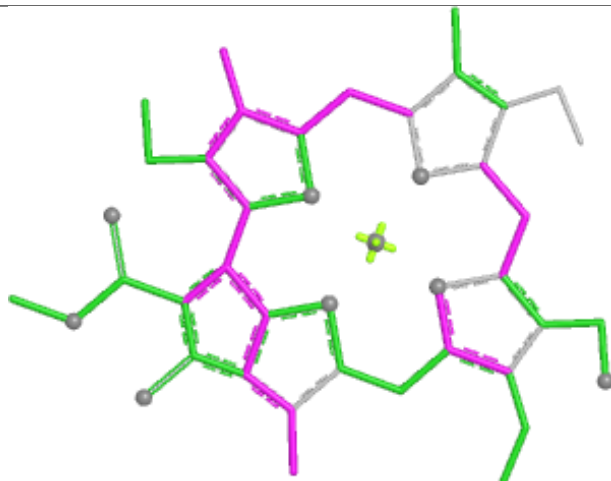




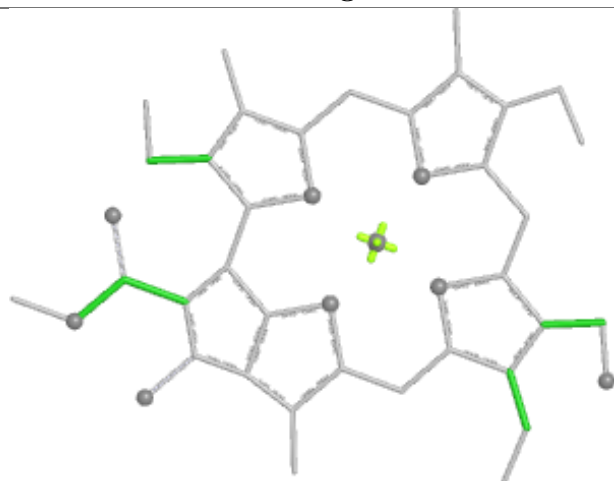
Ligand CHL 4 319



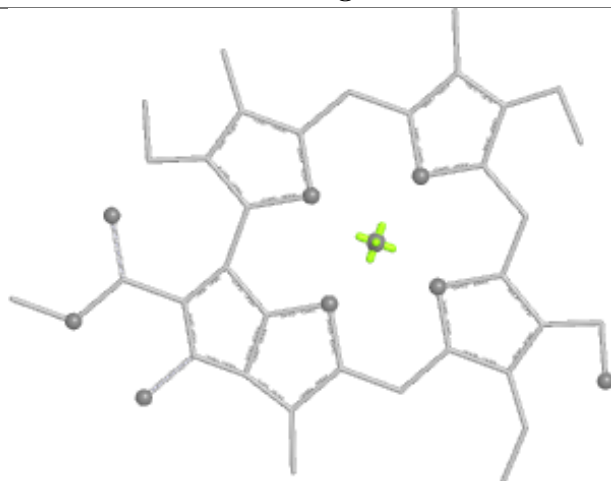
Bond lengths



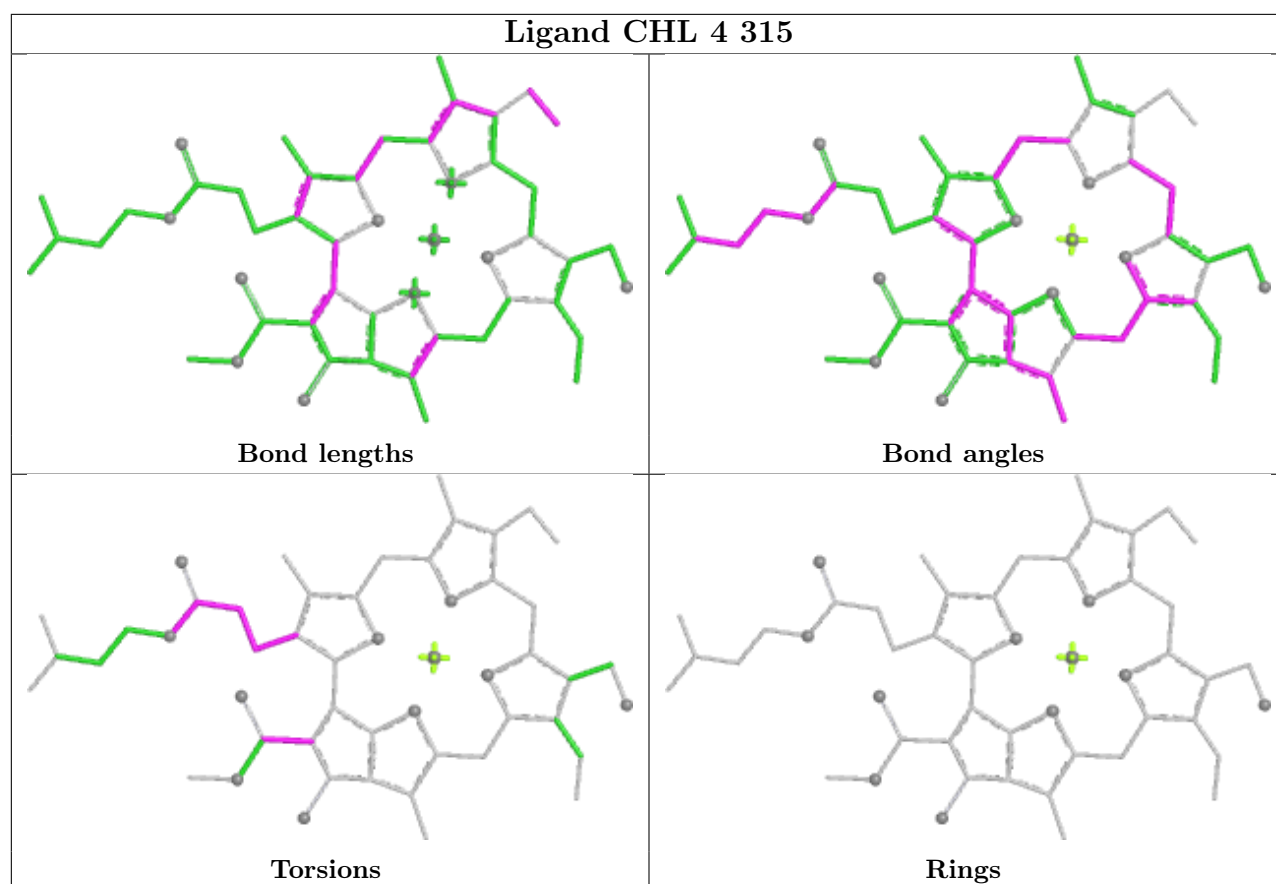
Bond angles



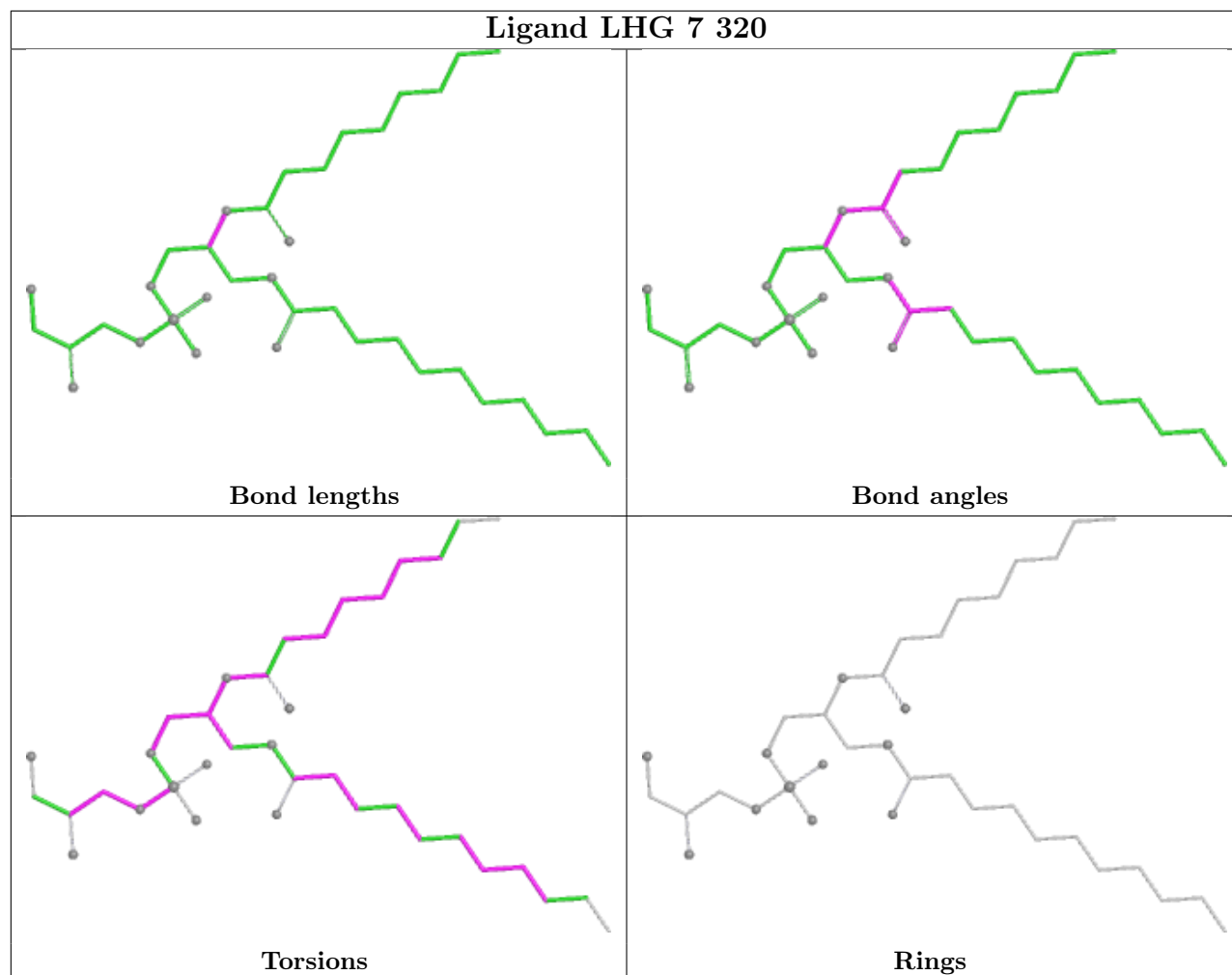
Torsions



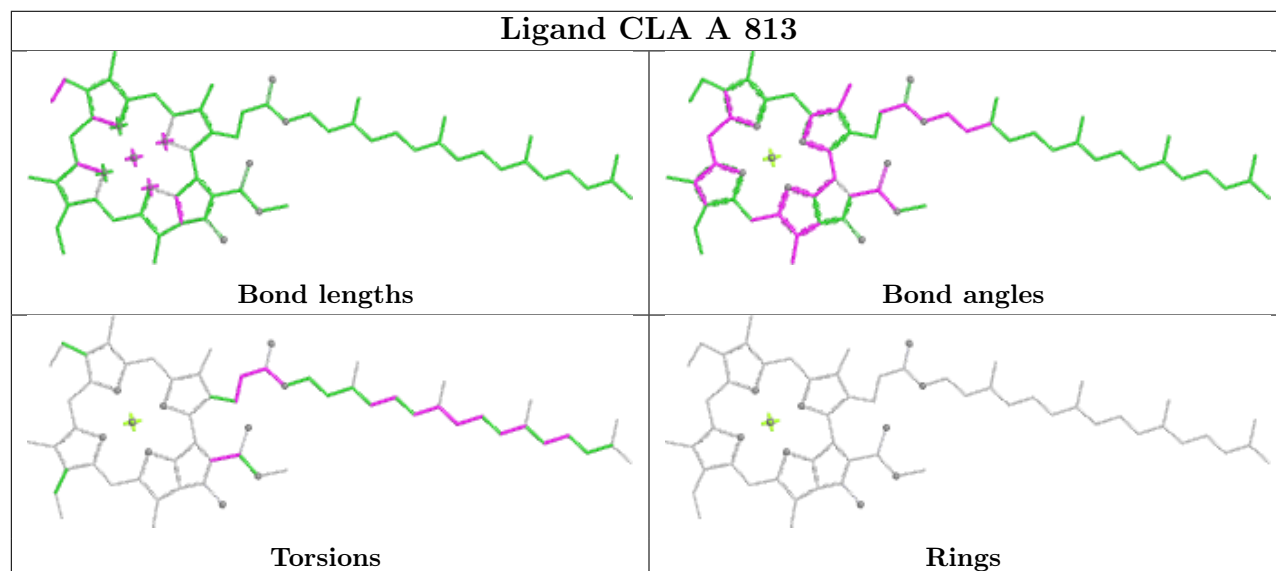
Rings

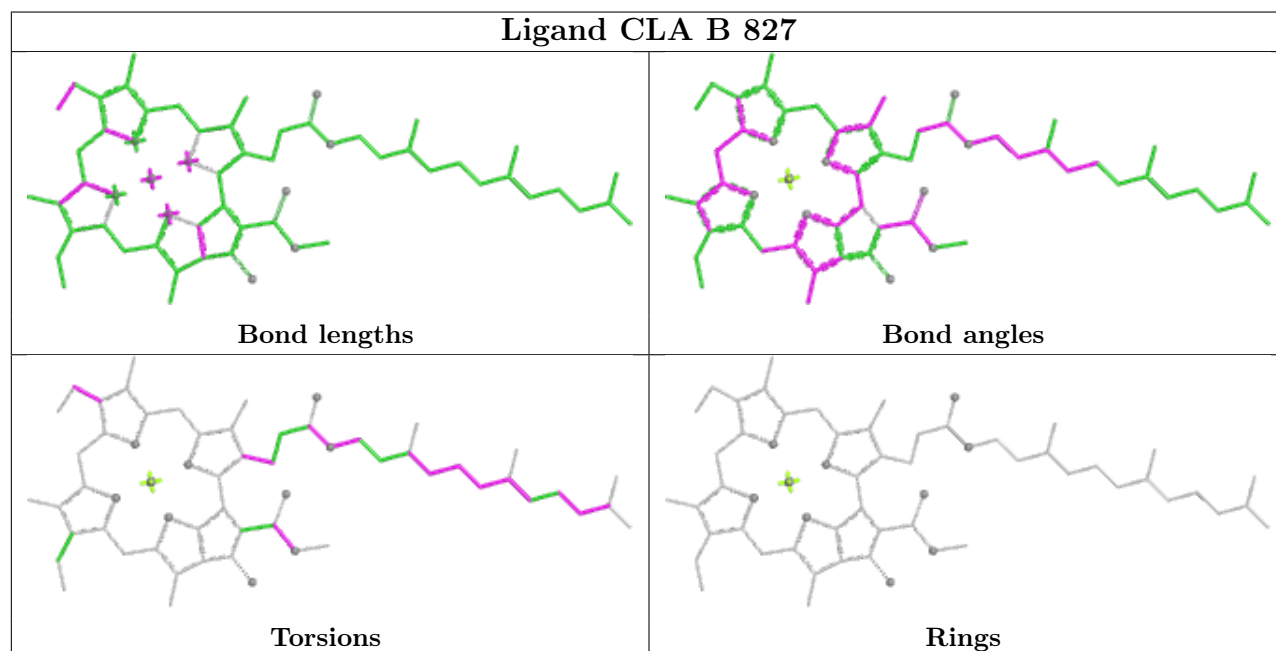
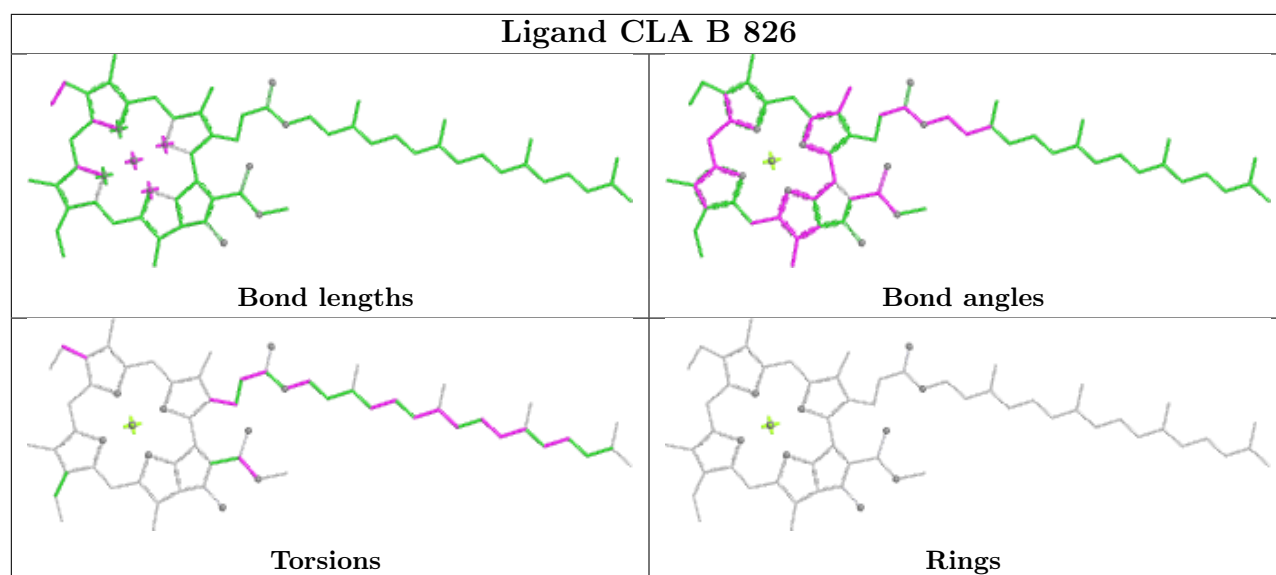


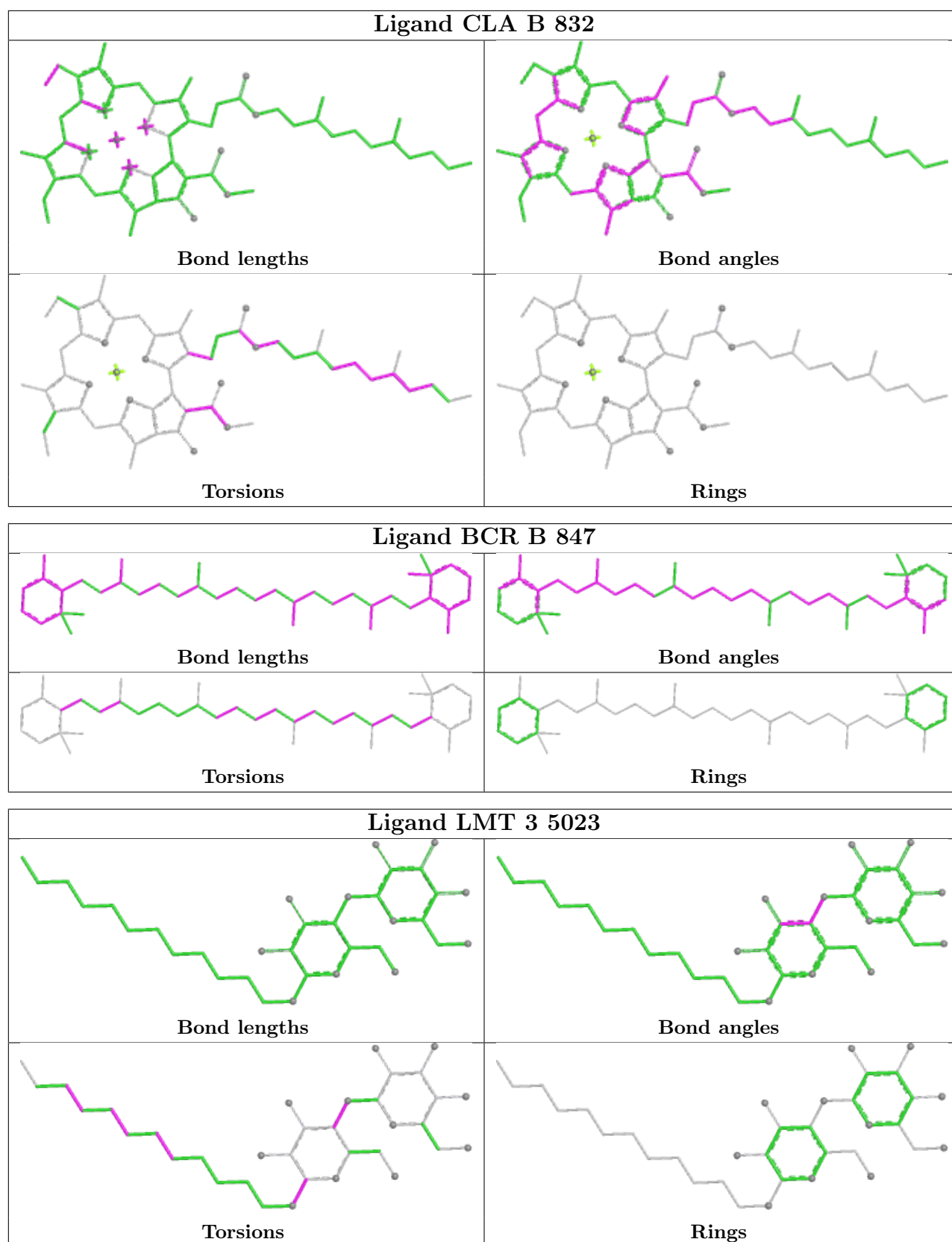
Ligand LHG 7 320

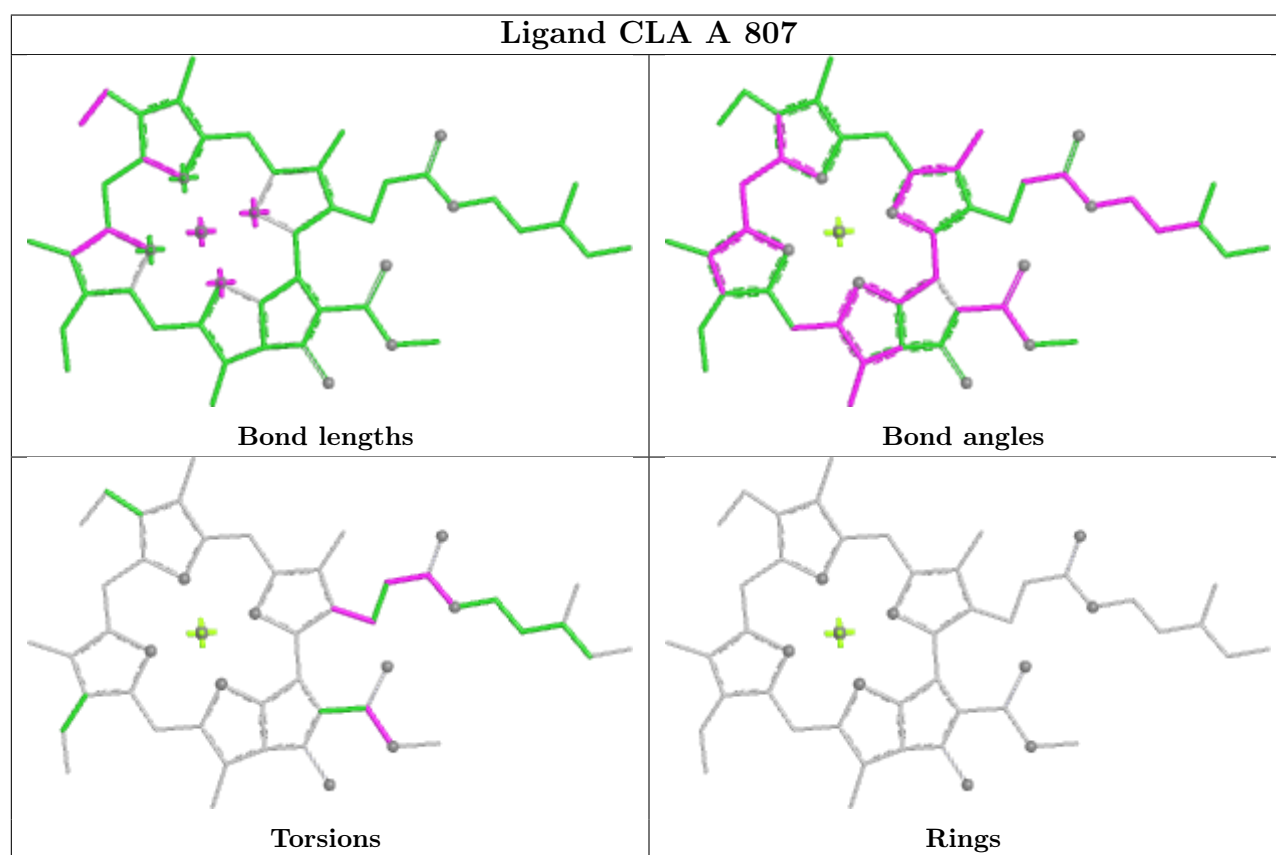
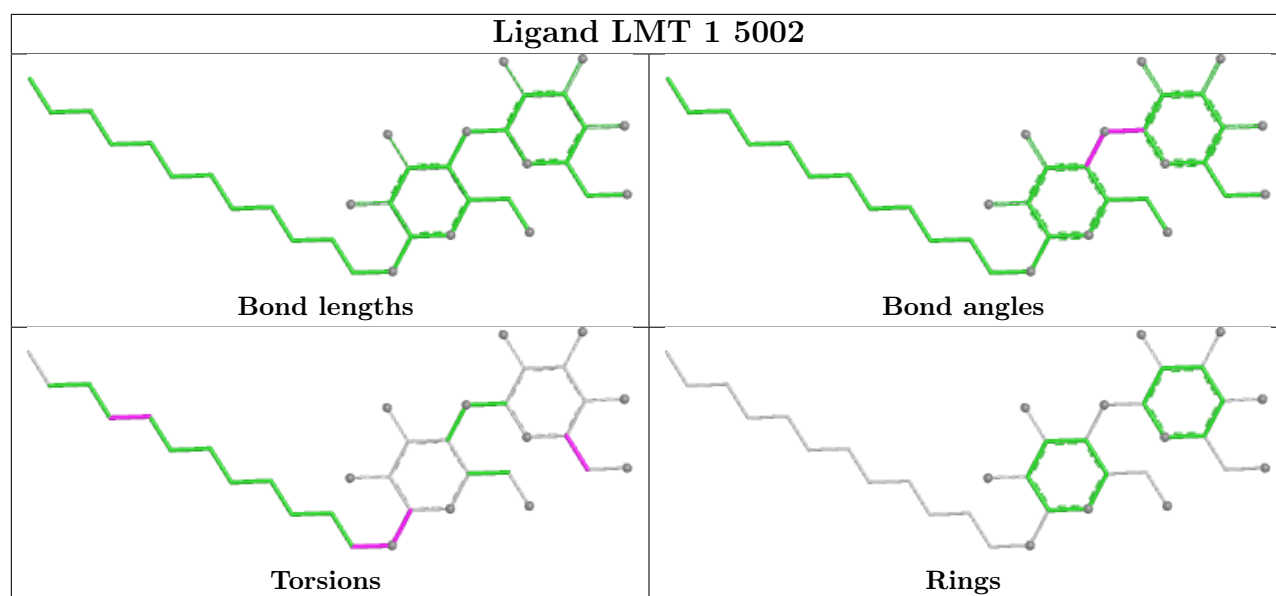


Ligand CLA A 813

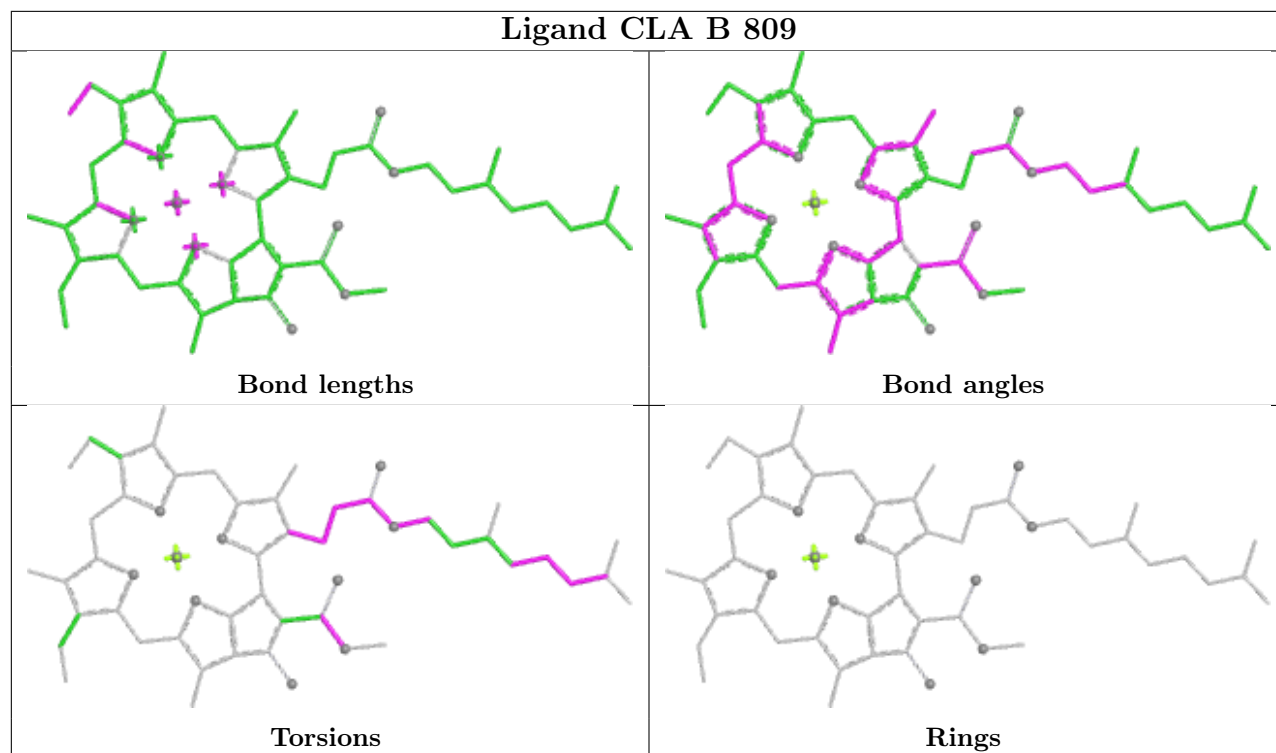




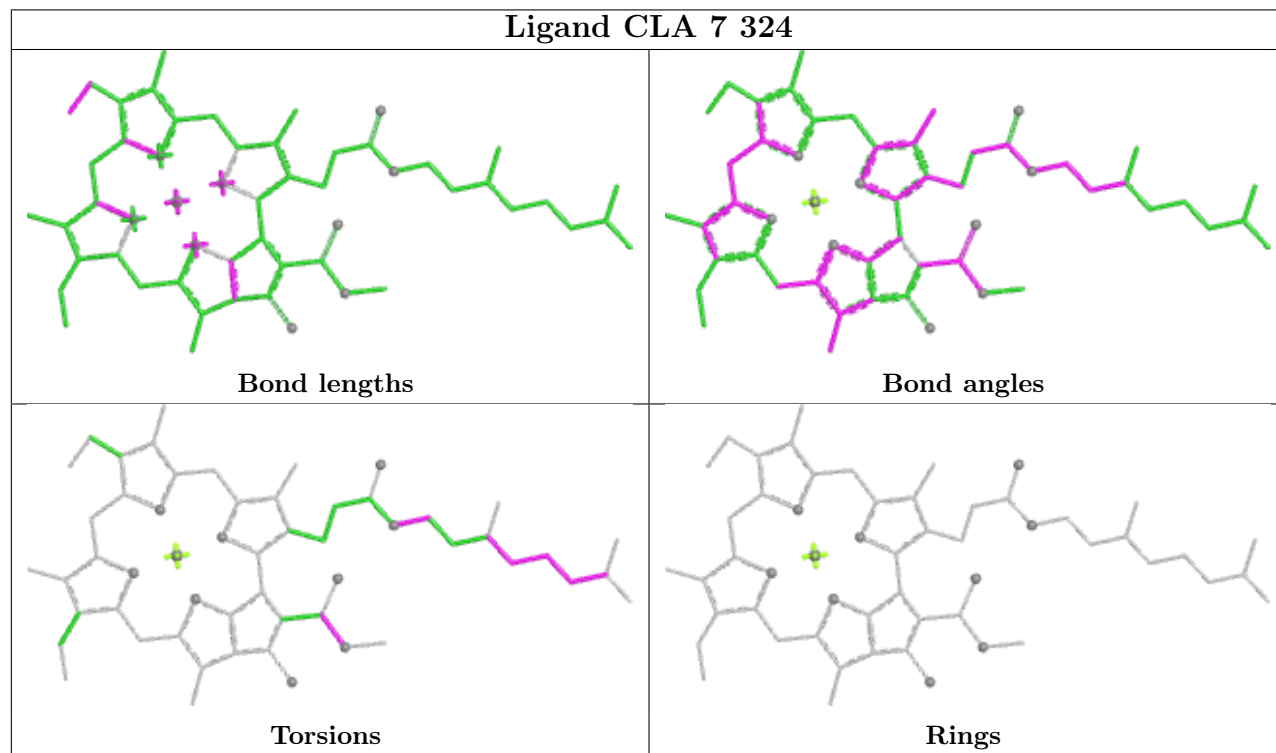


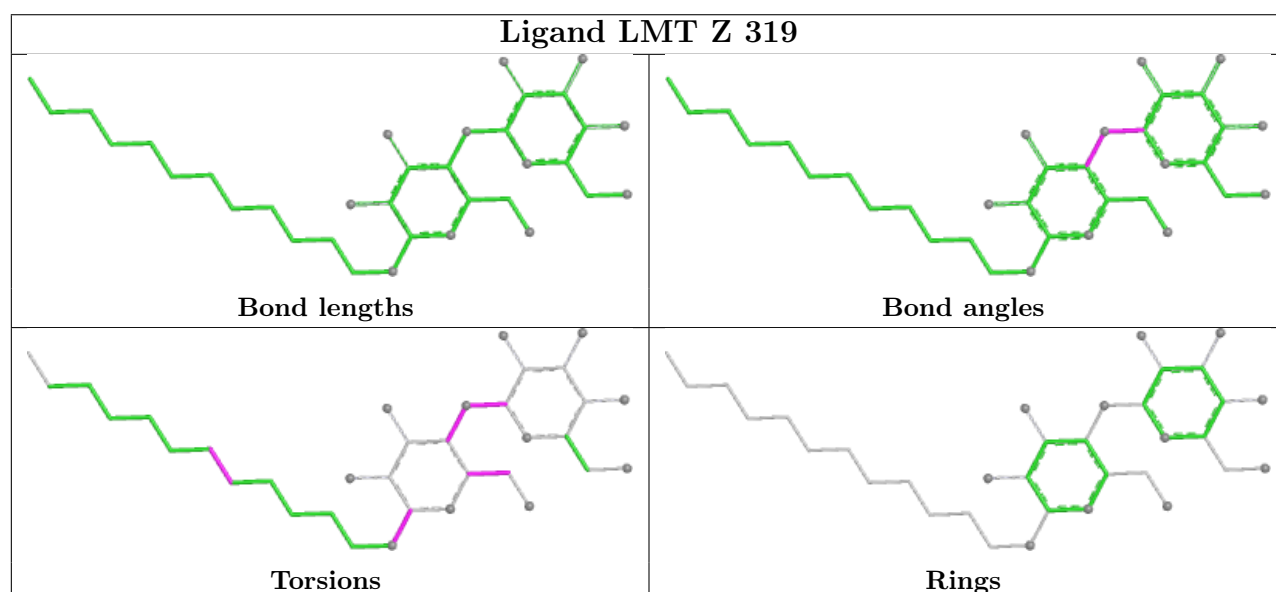
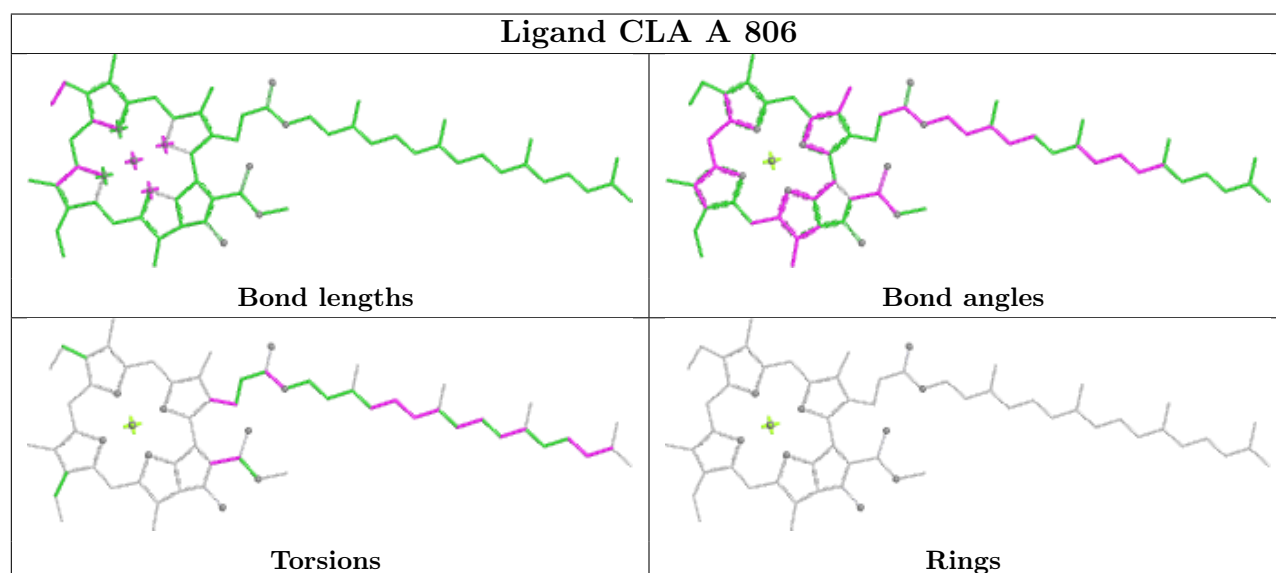
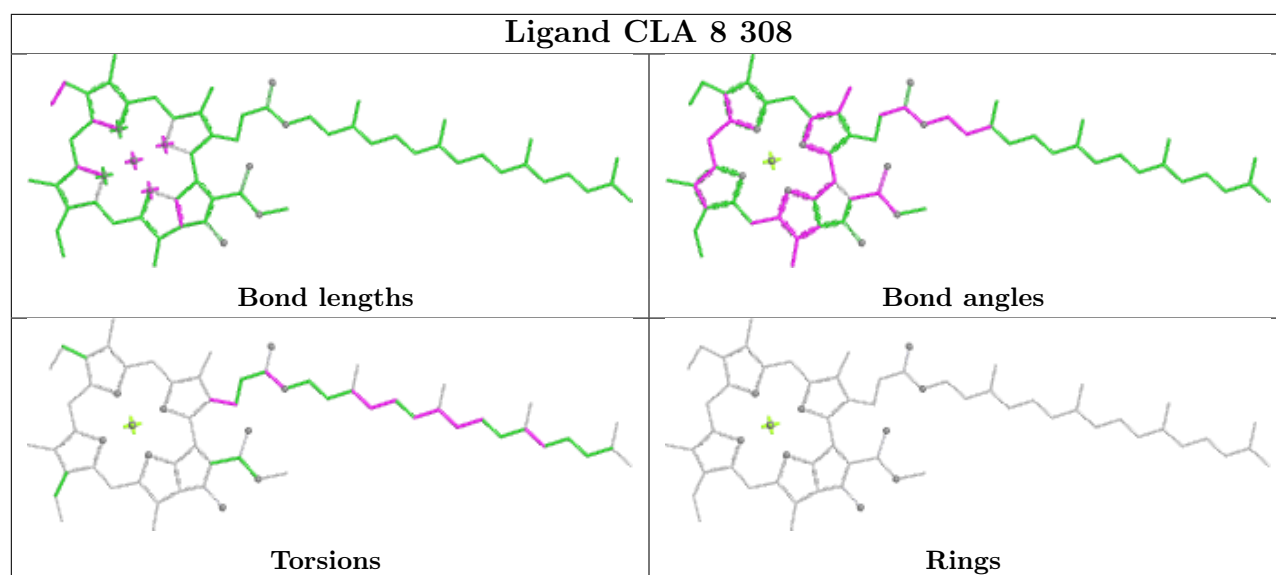


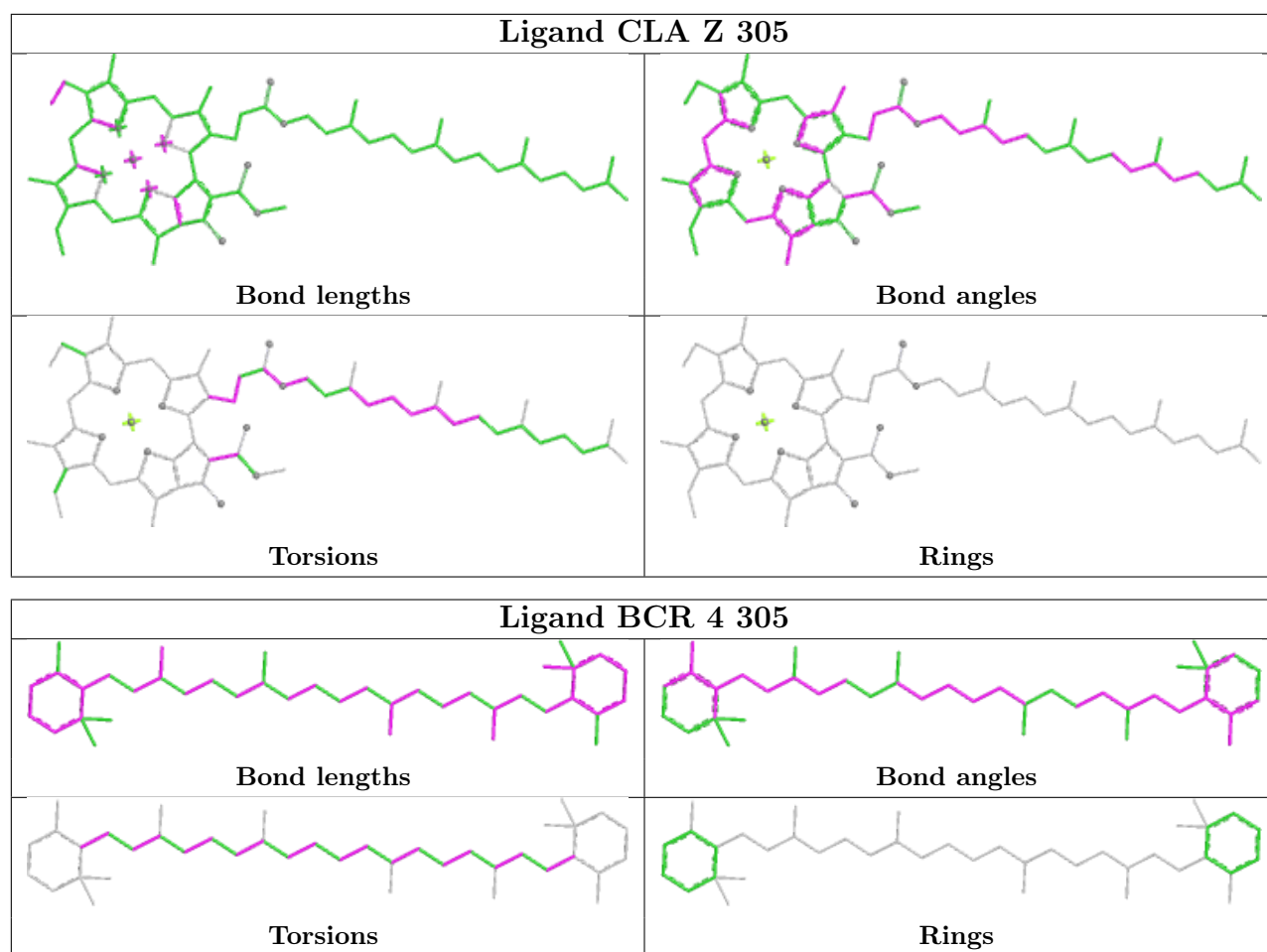
Ligand CLA B 809



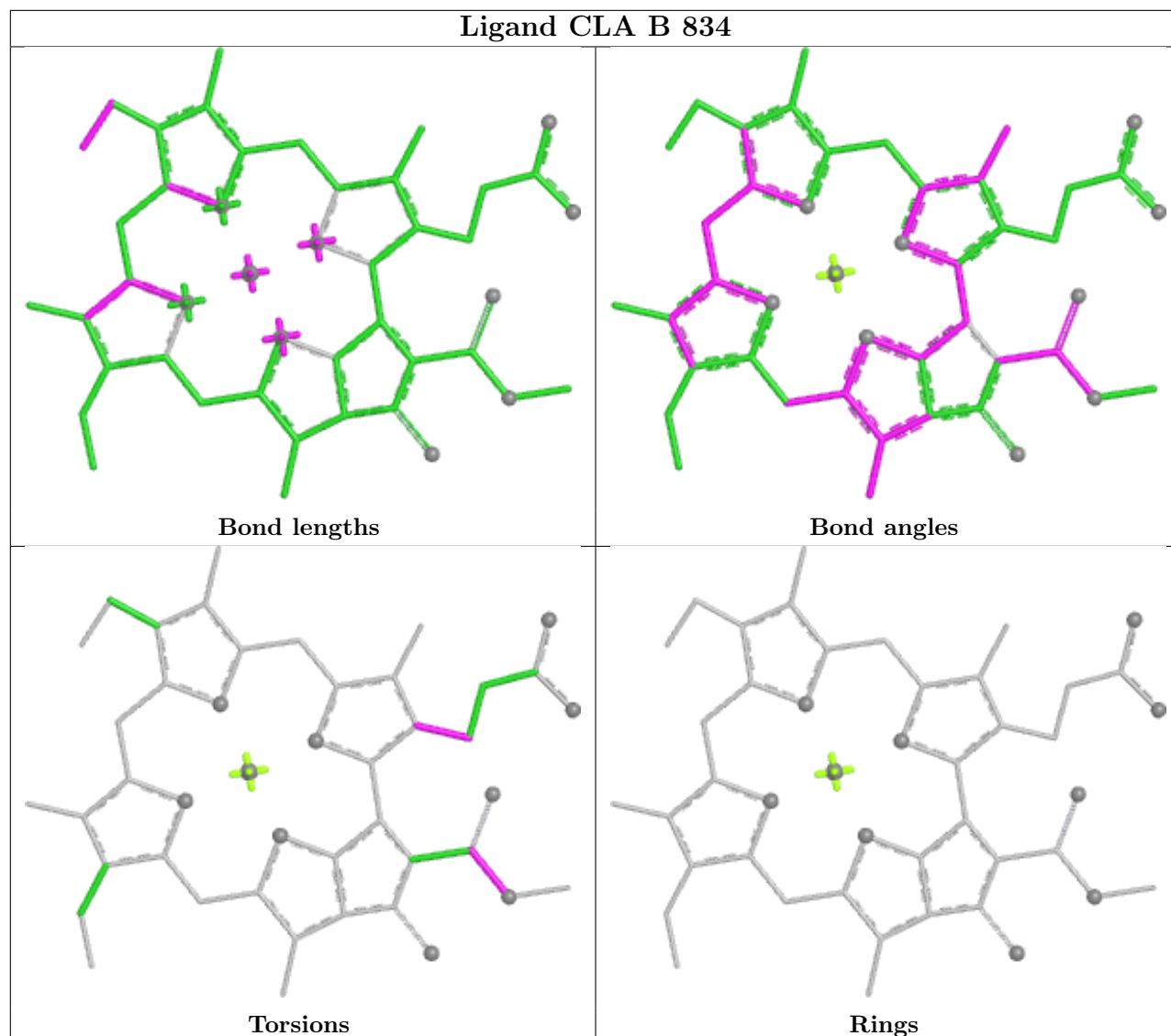
Ligand CLA 7 324



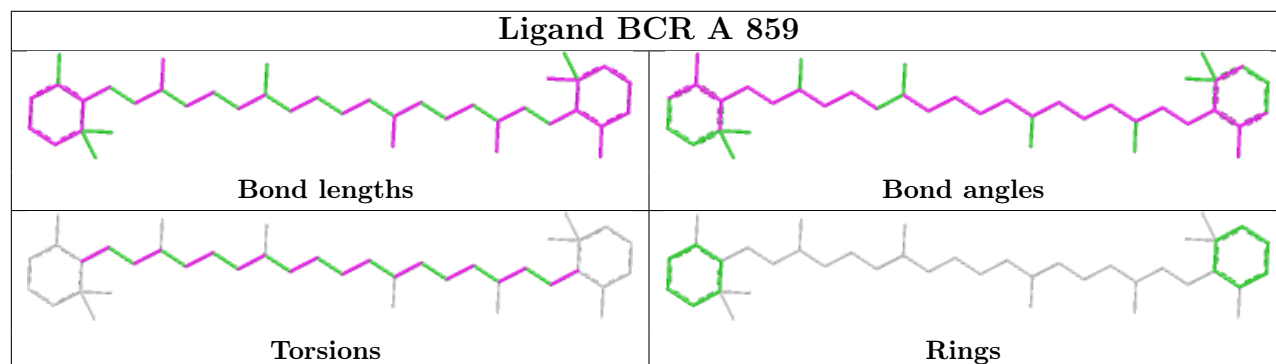


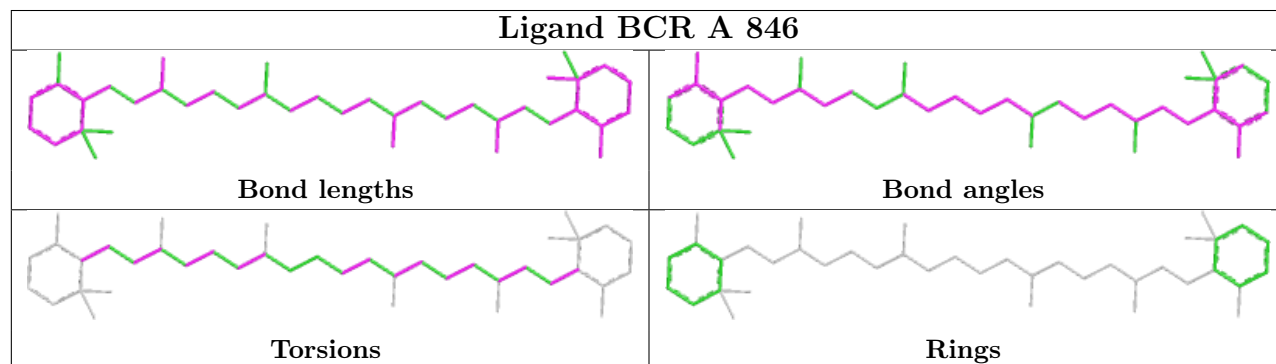
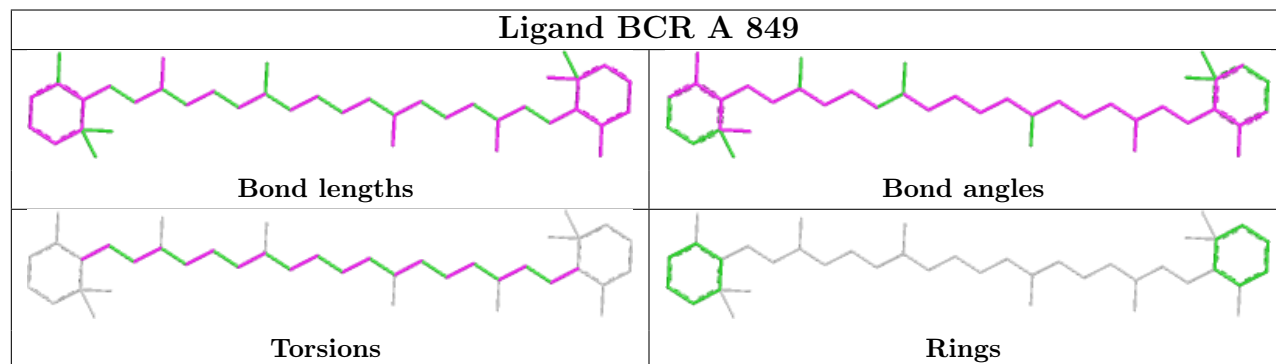
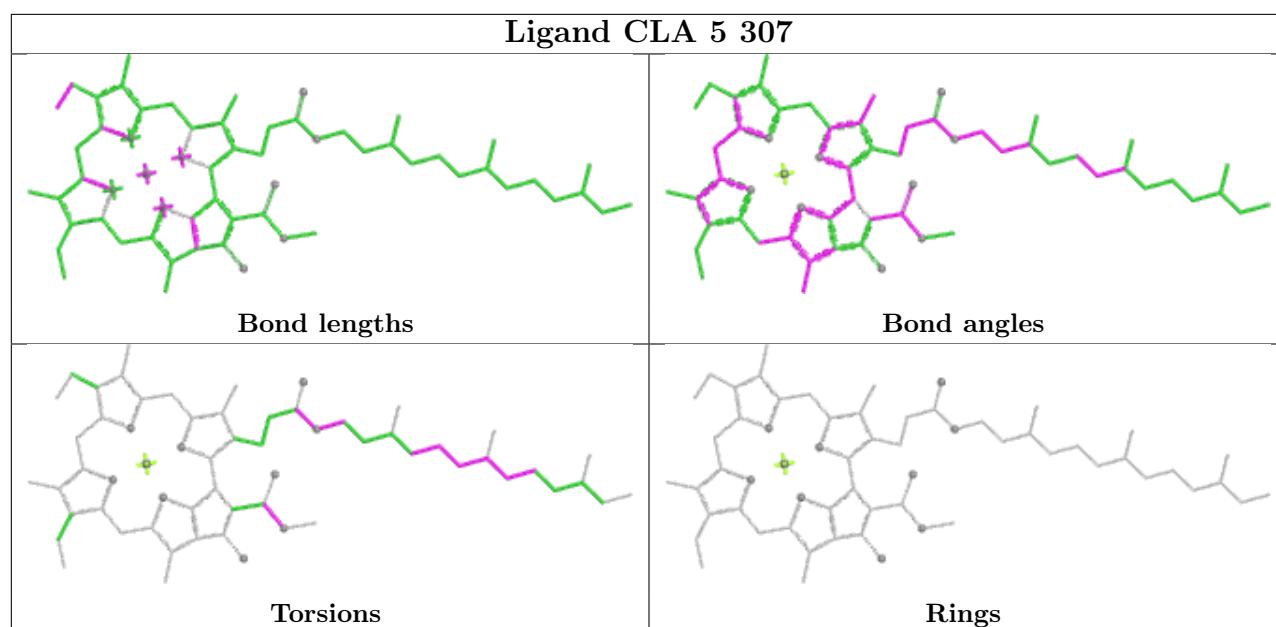


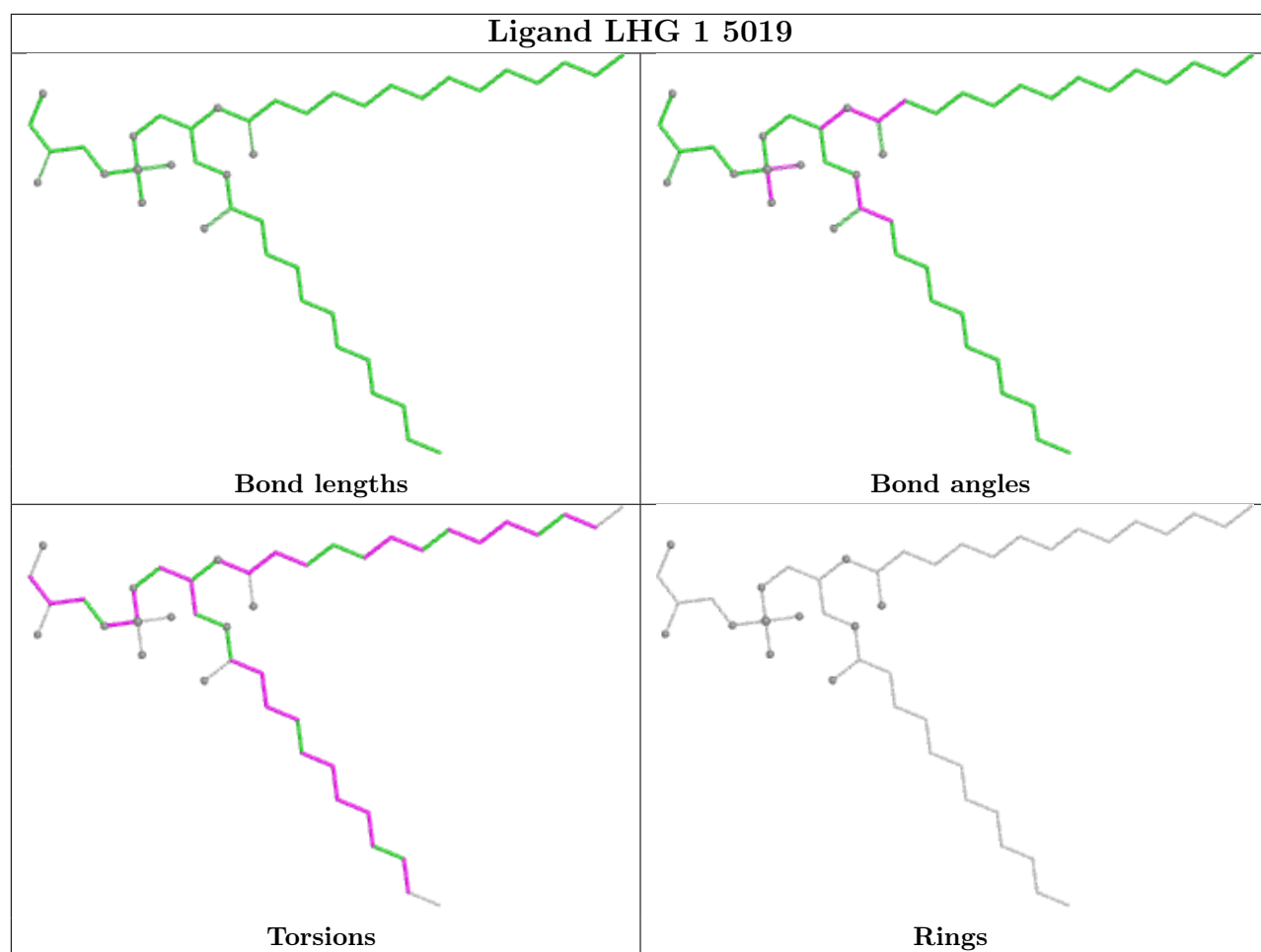
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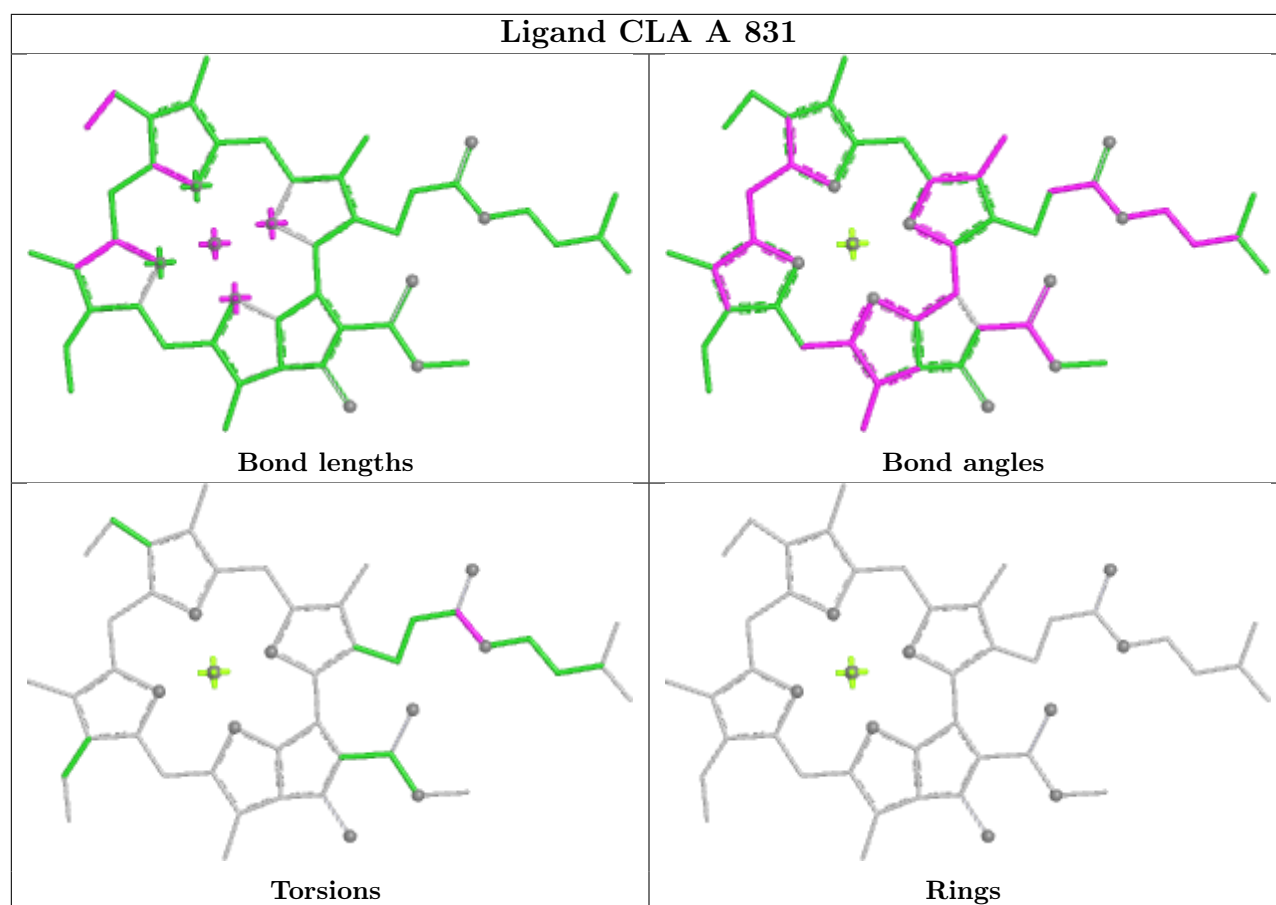


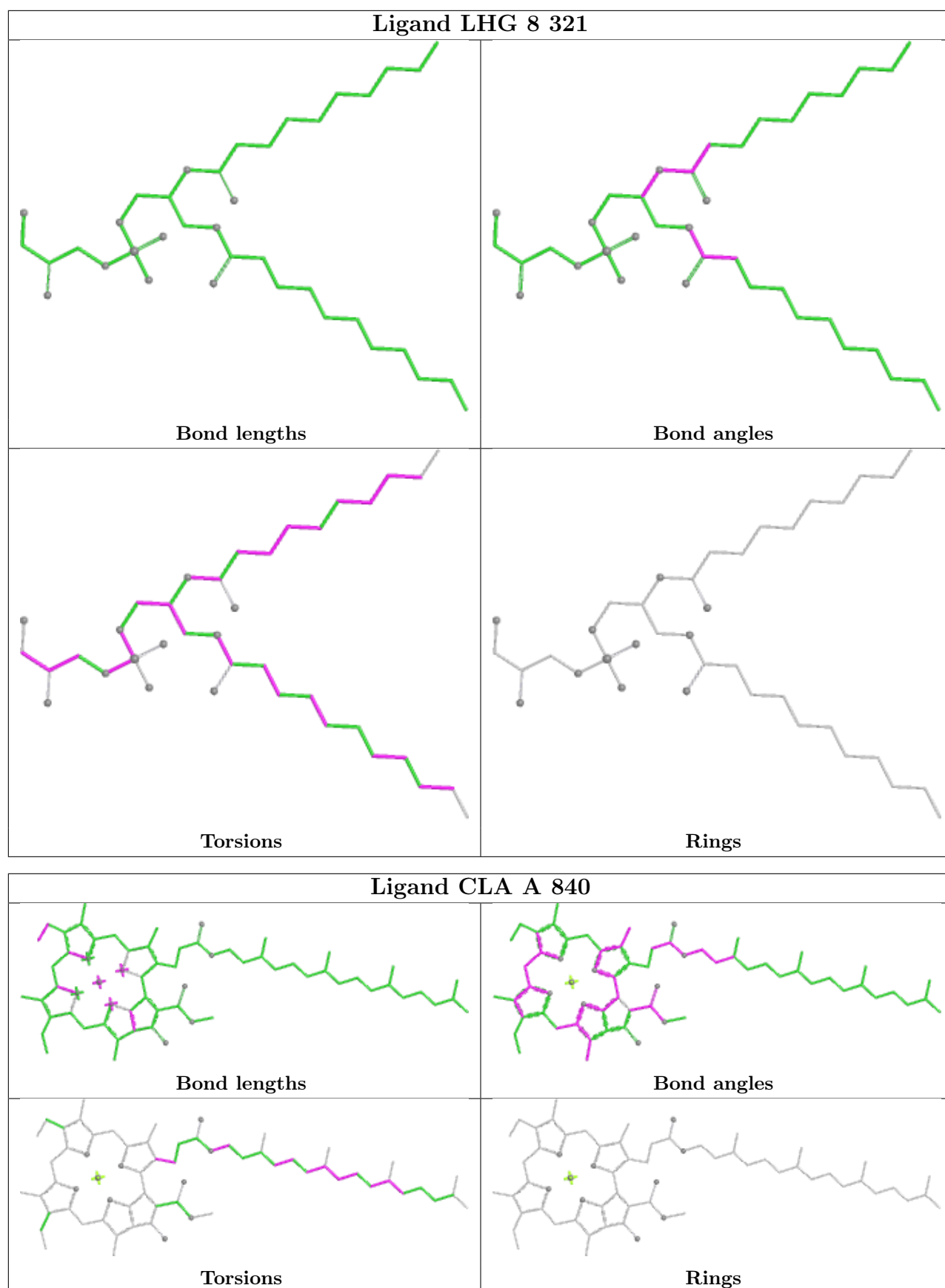
Ligand BCR A 859

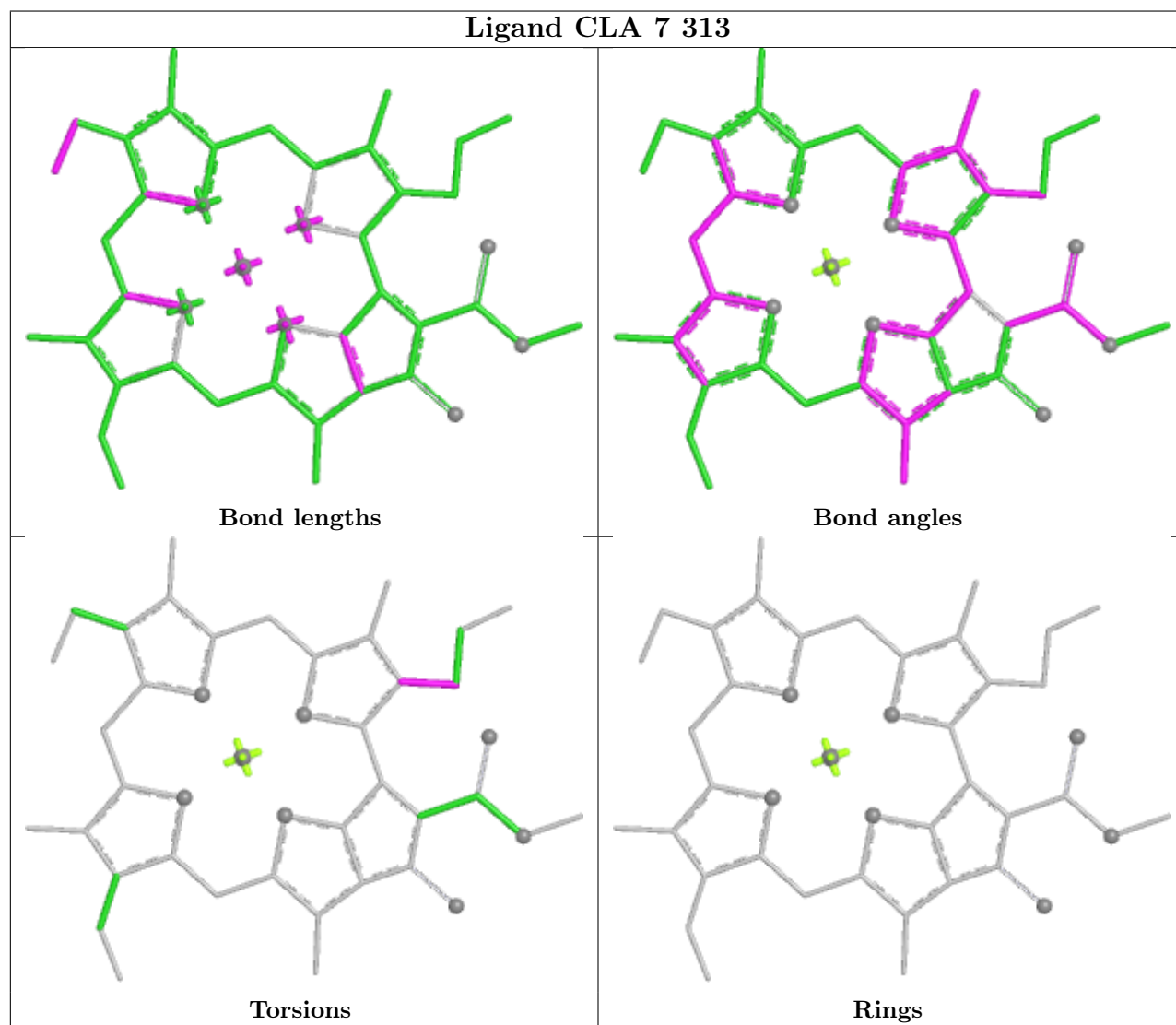
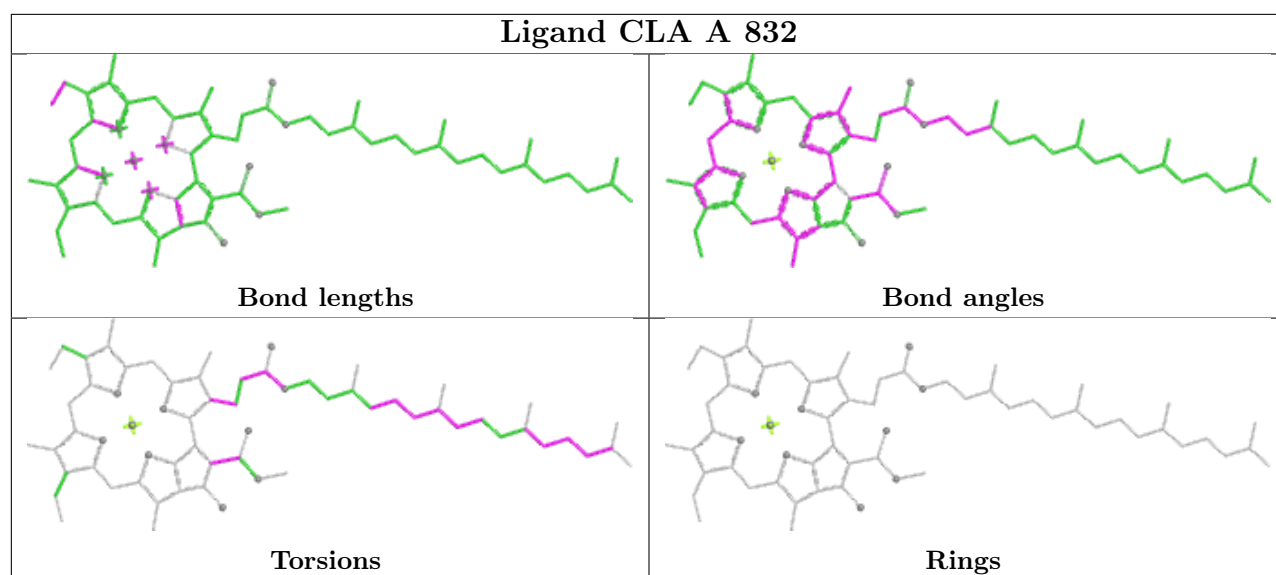


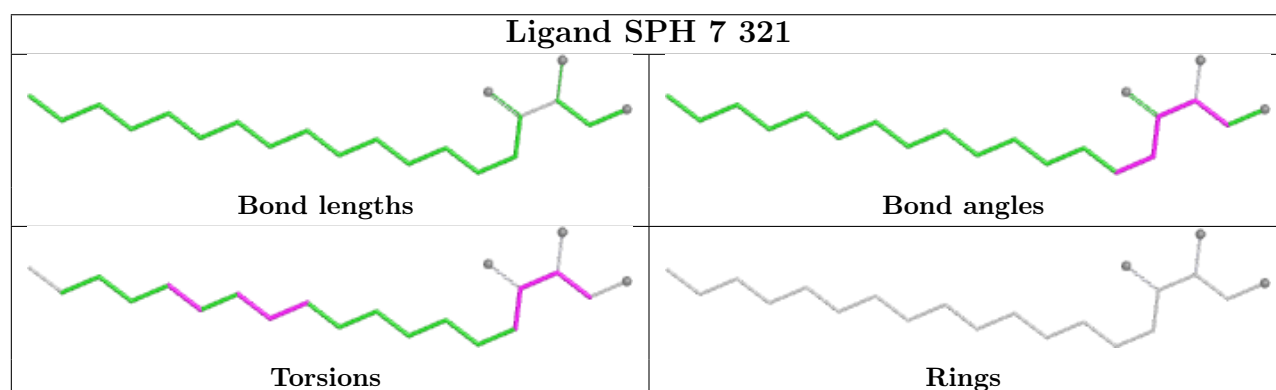
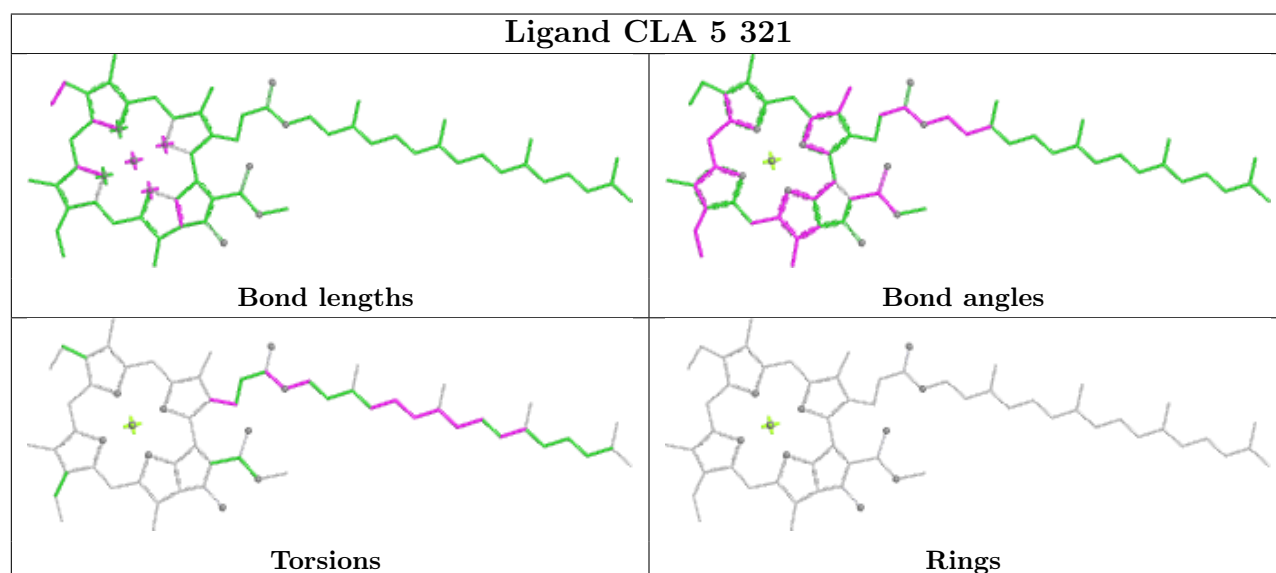
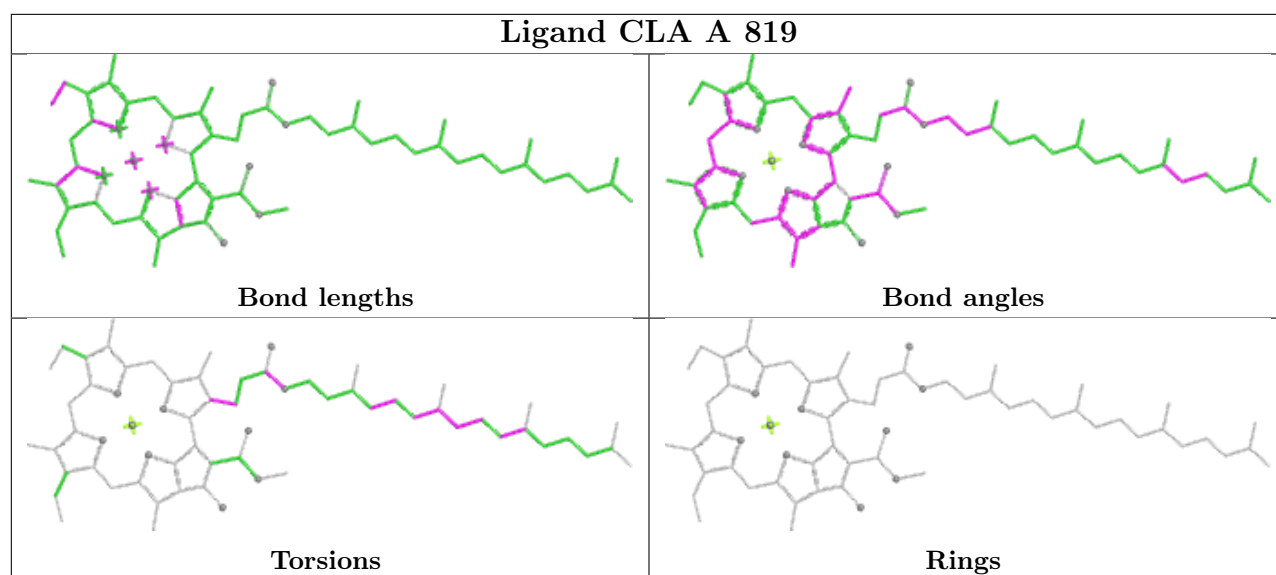


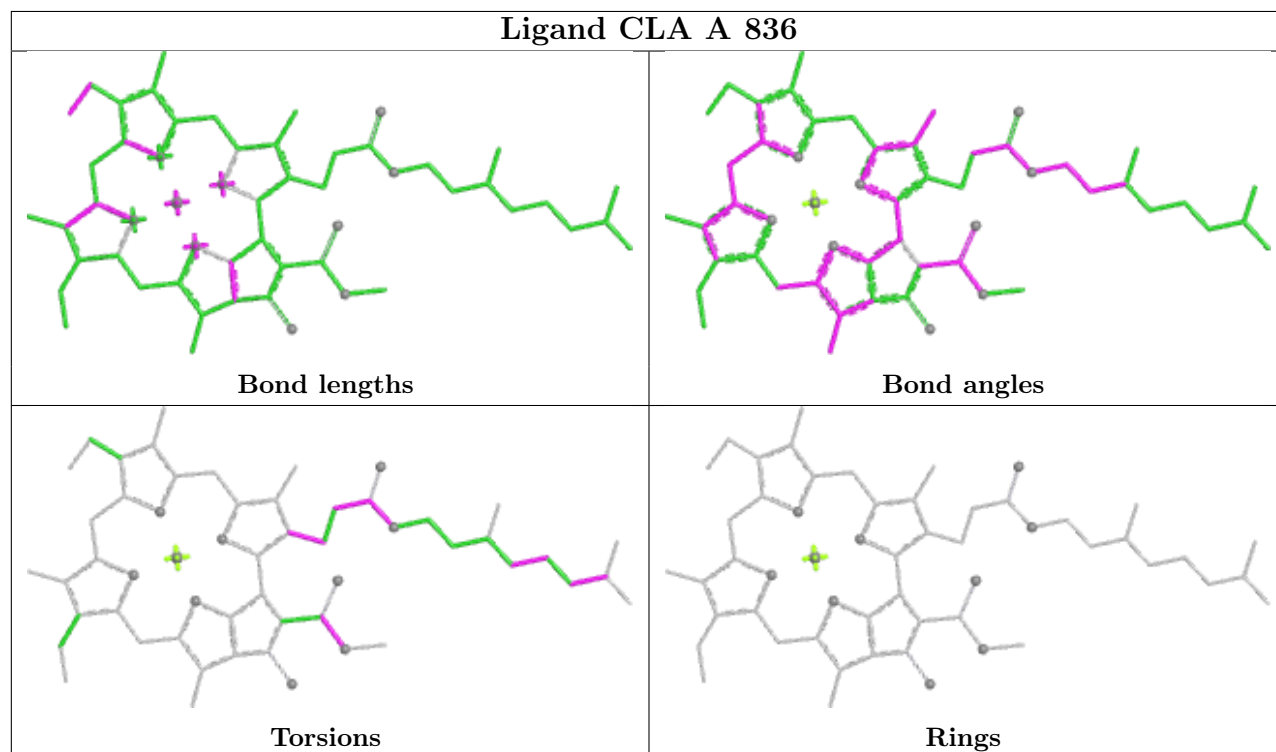
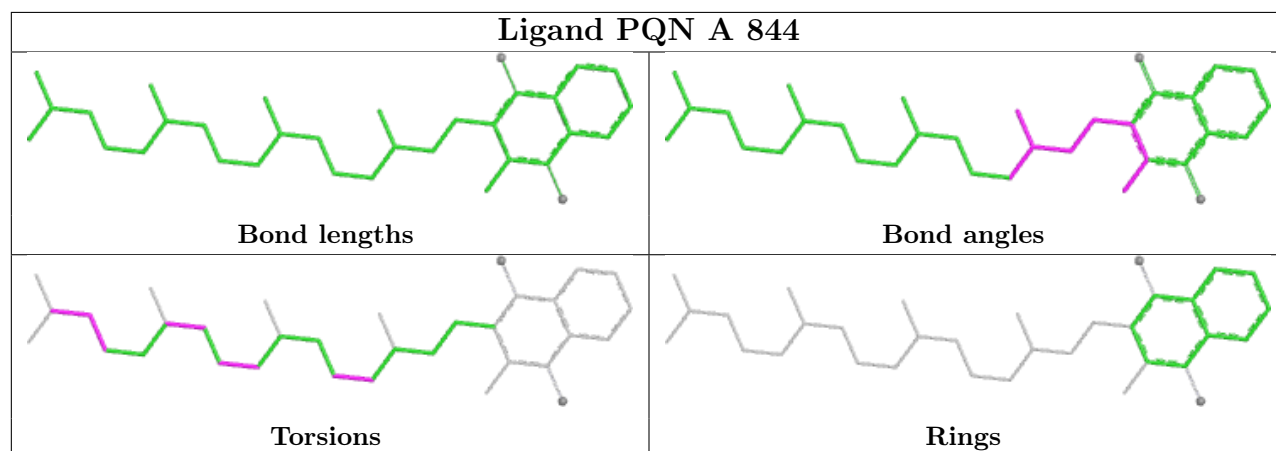
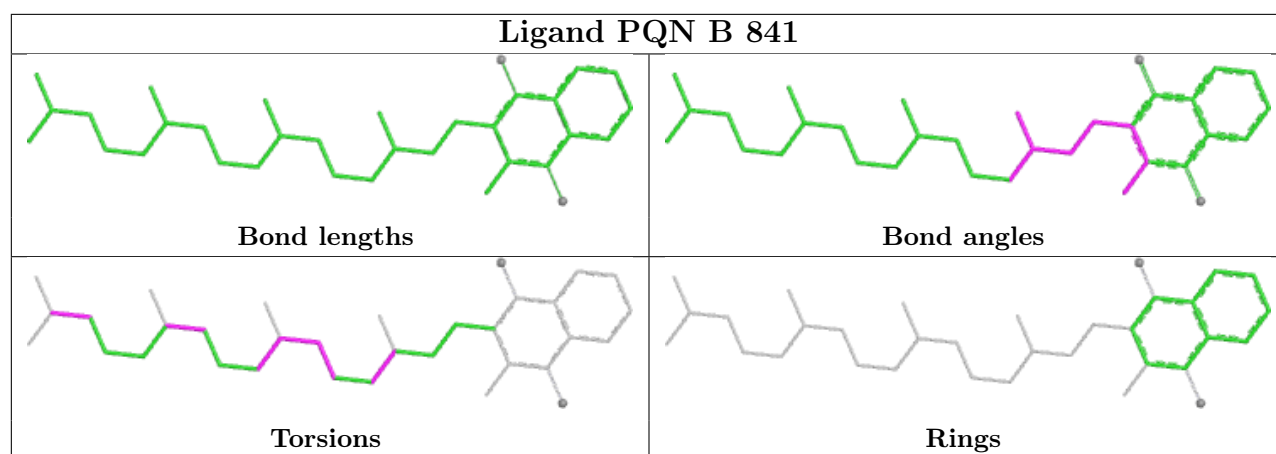


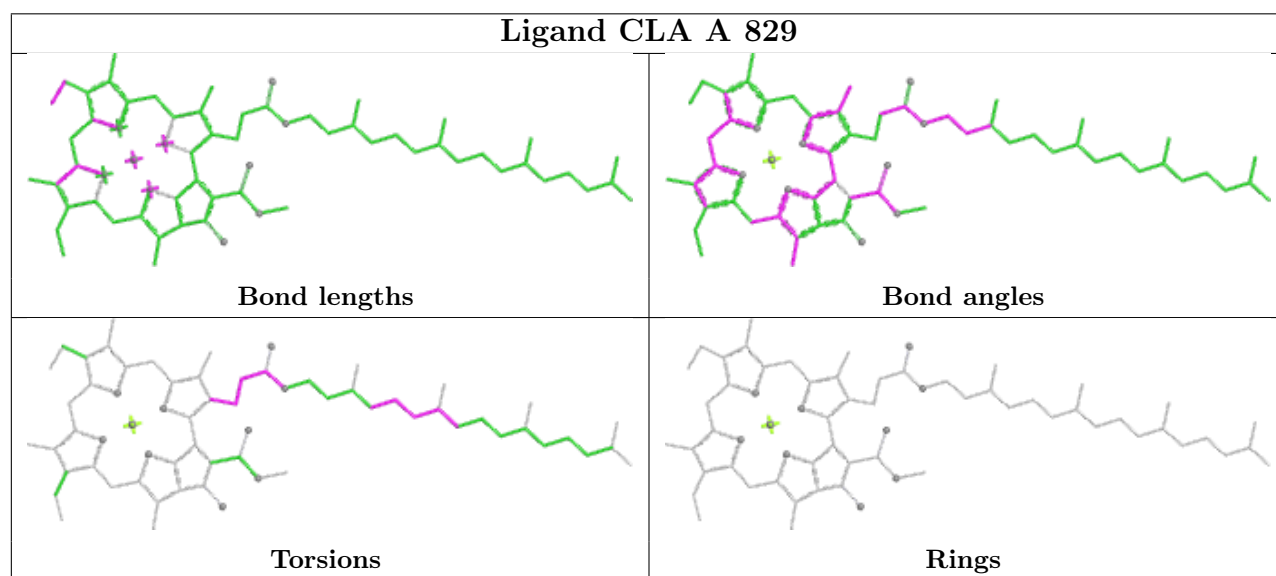
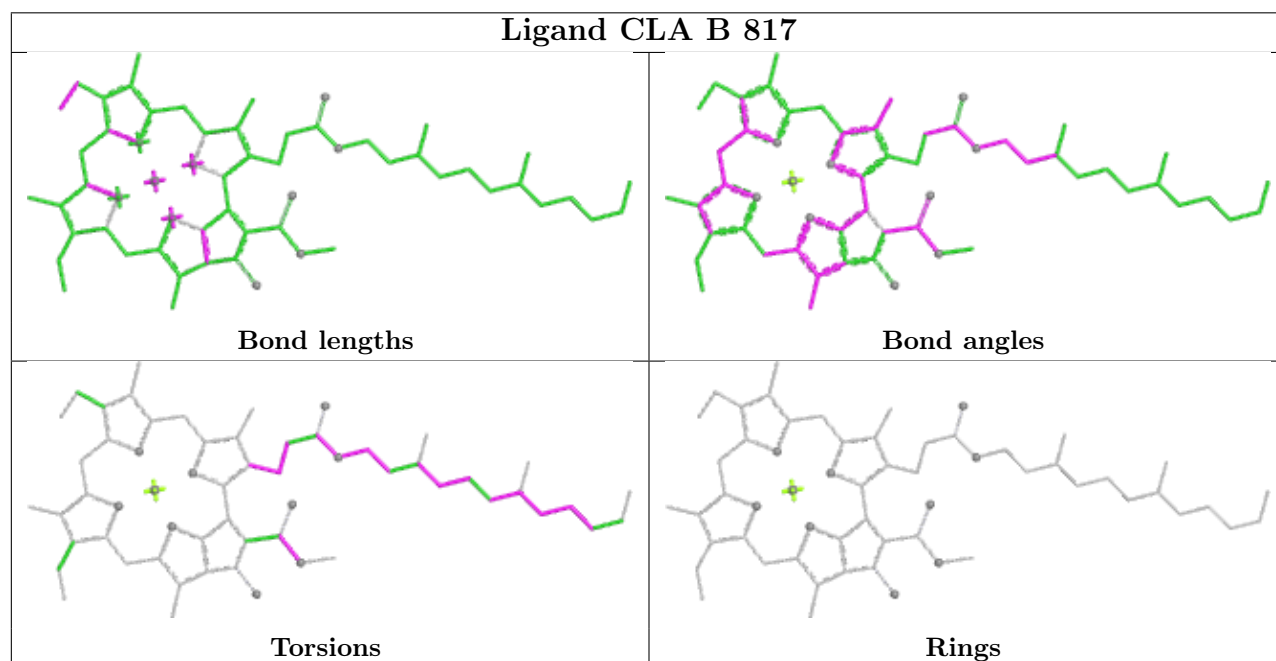
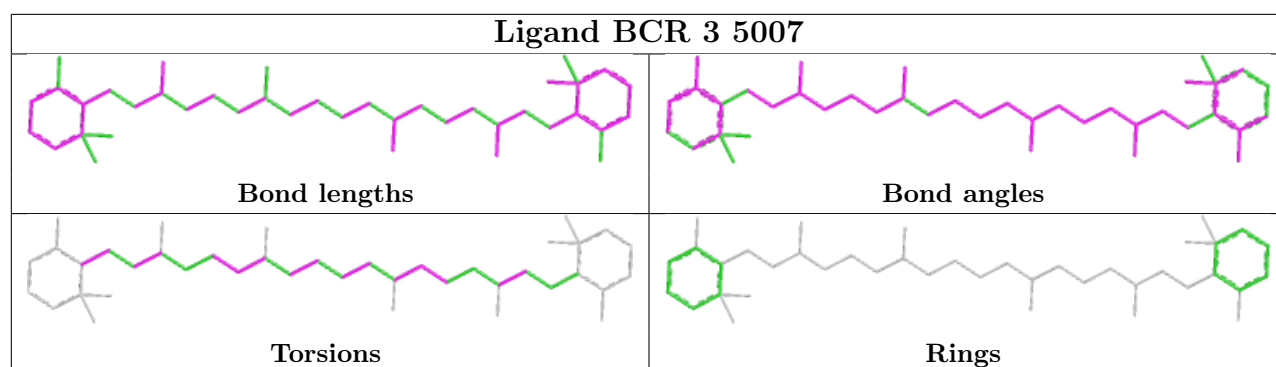


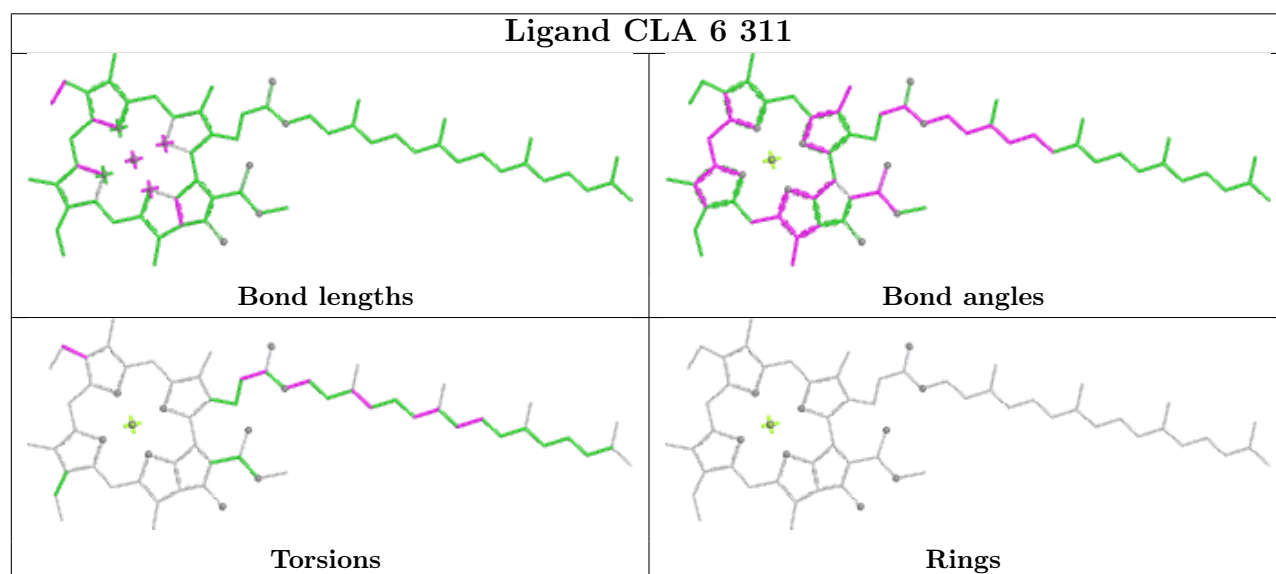
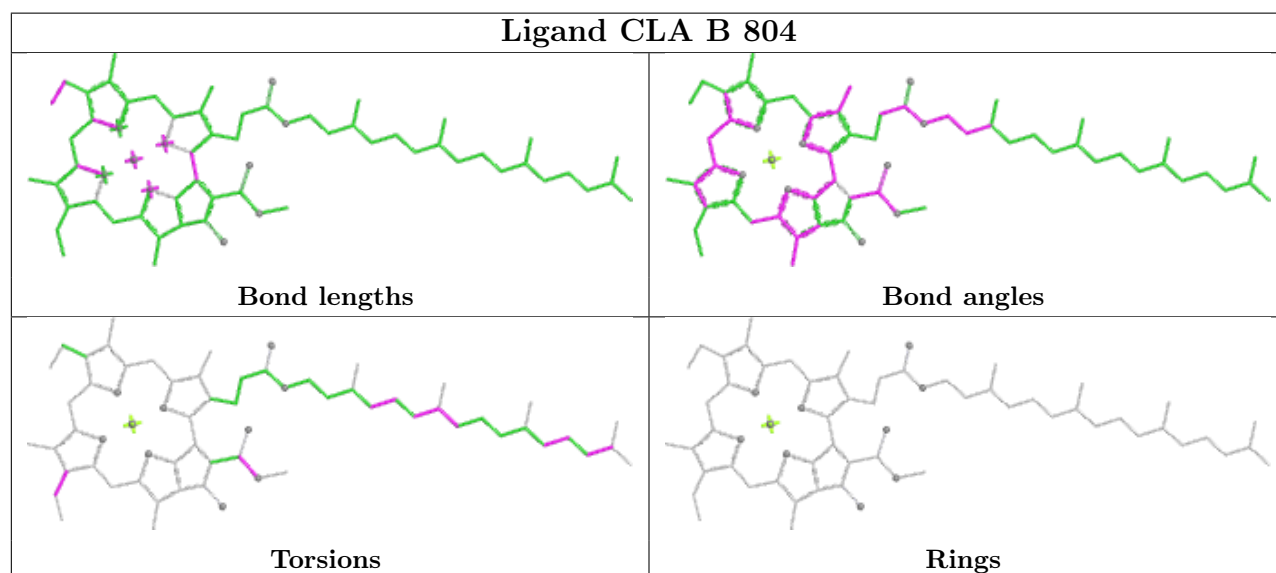
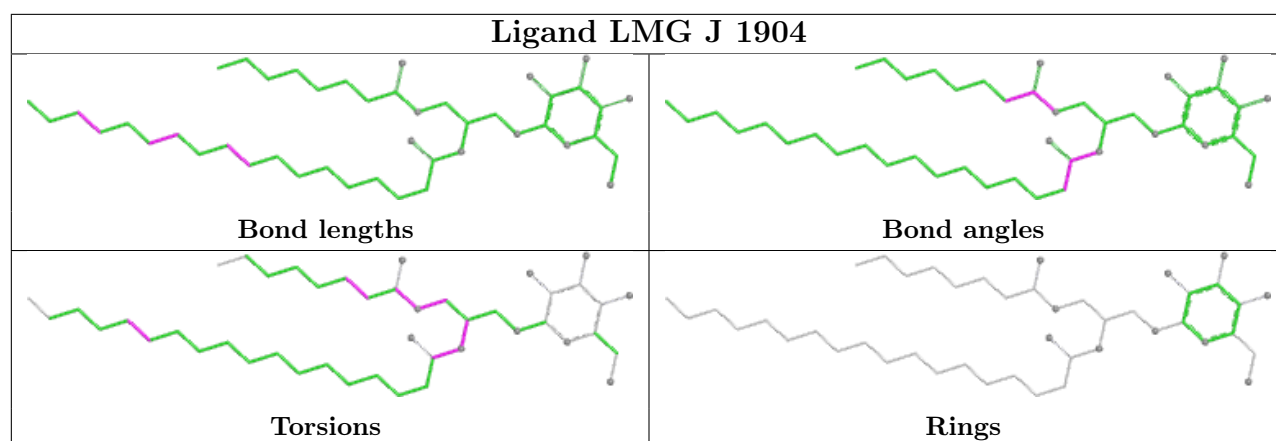


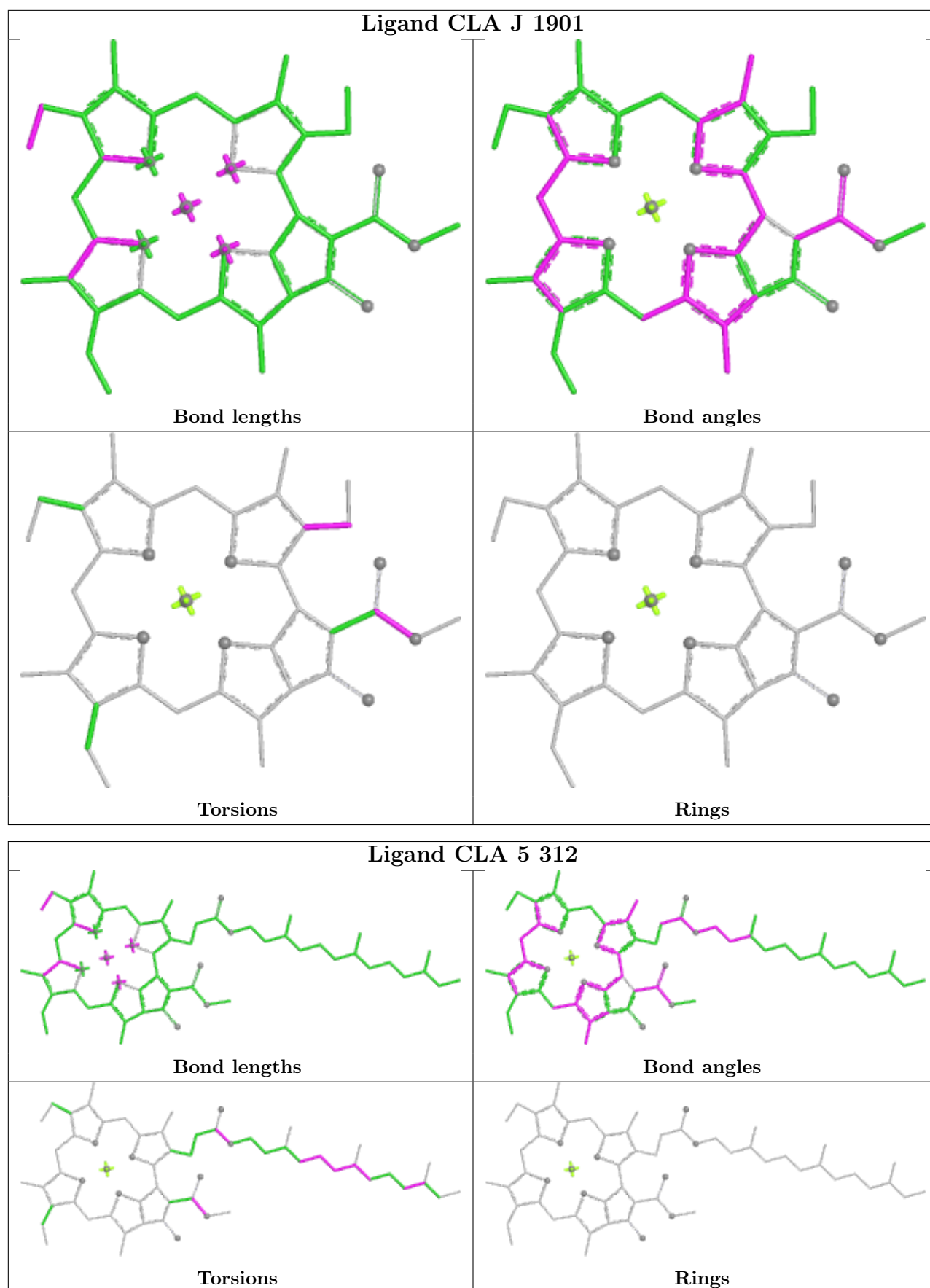


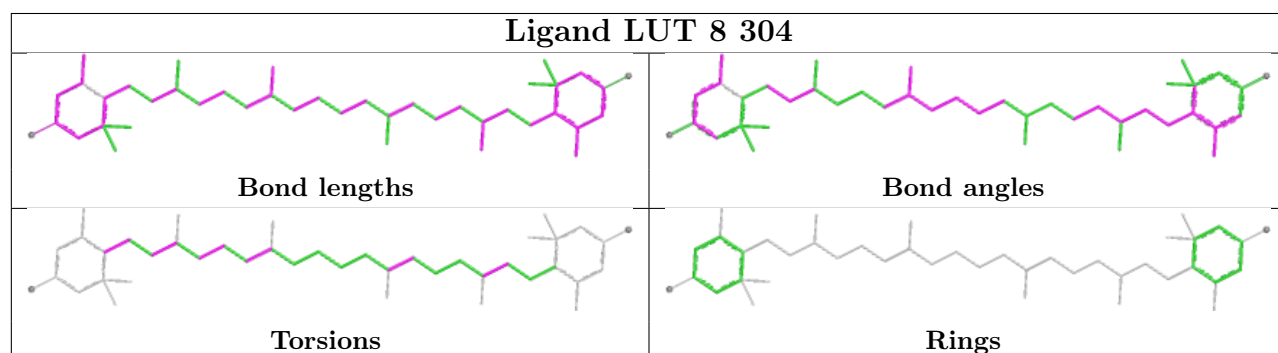
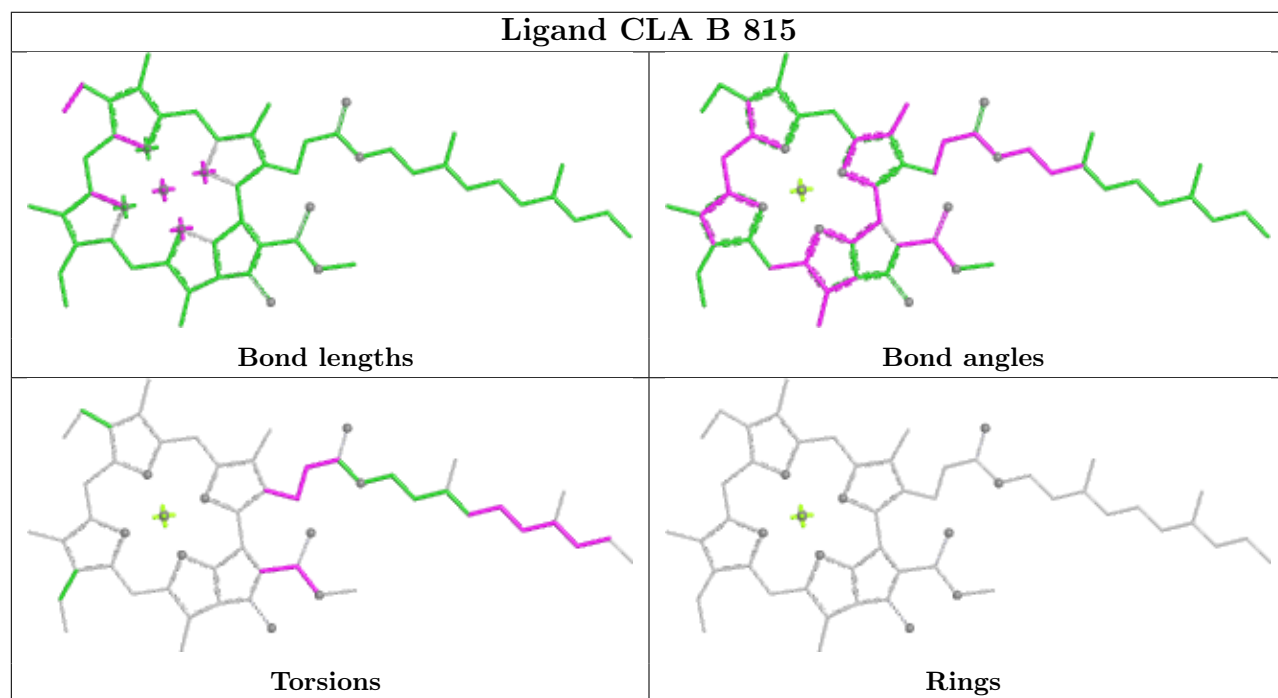
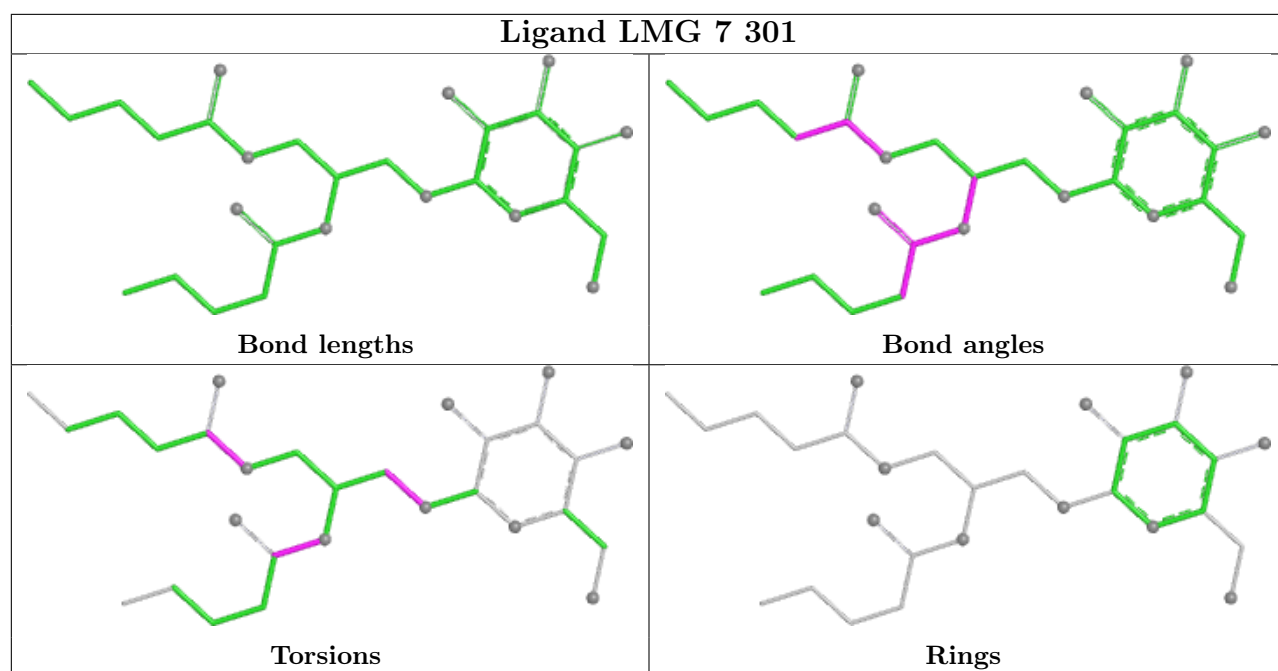


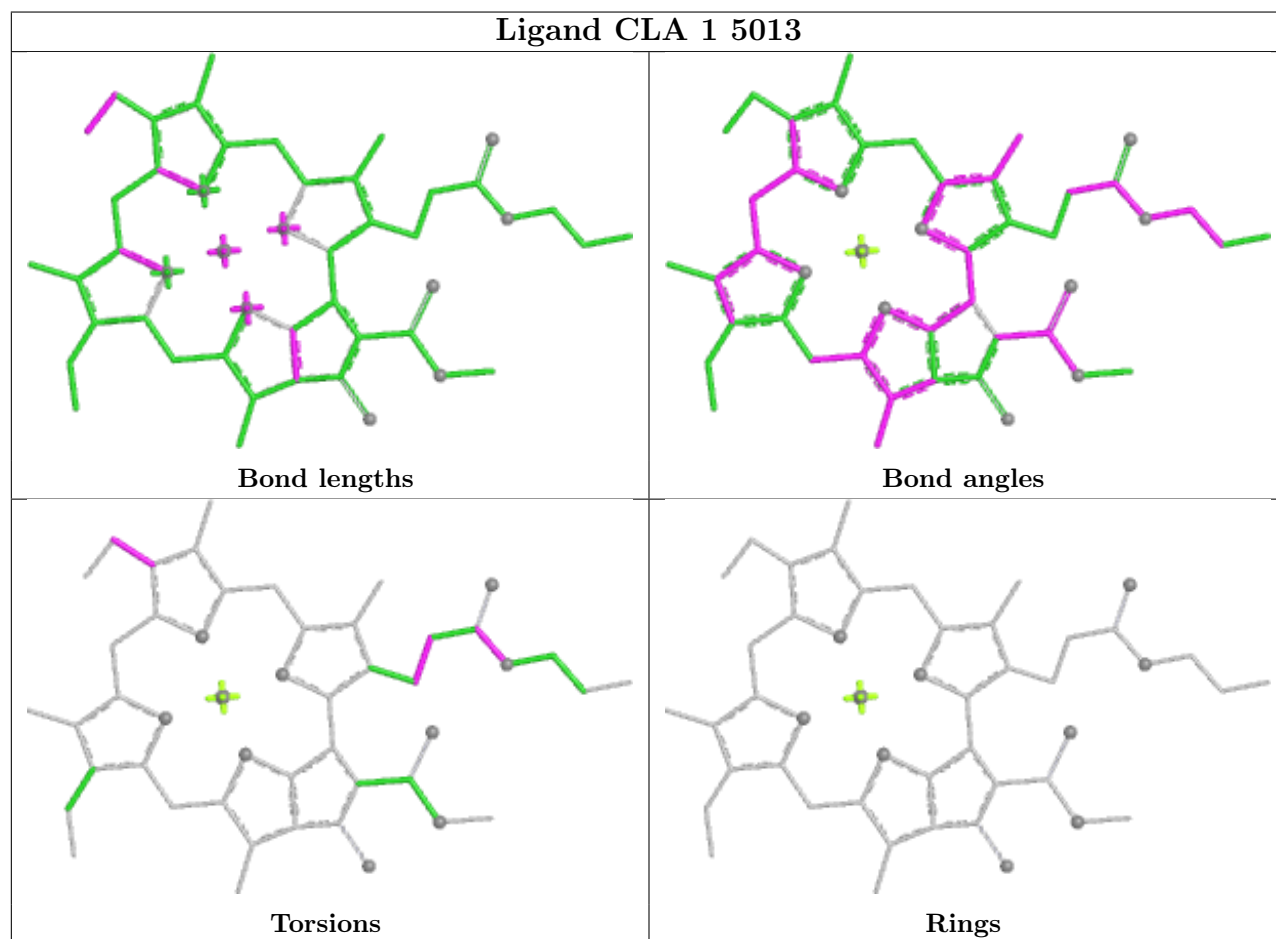
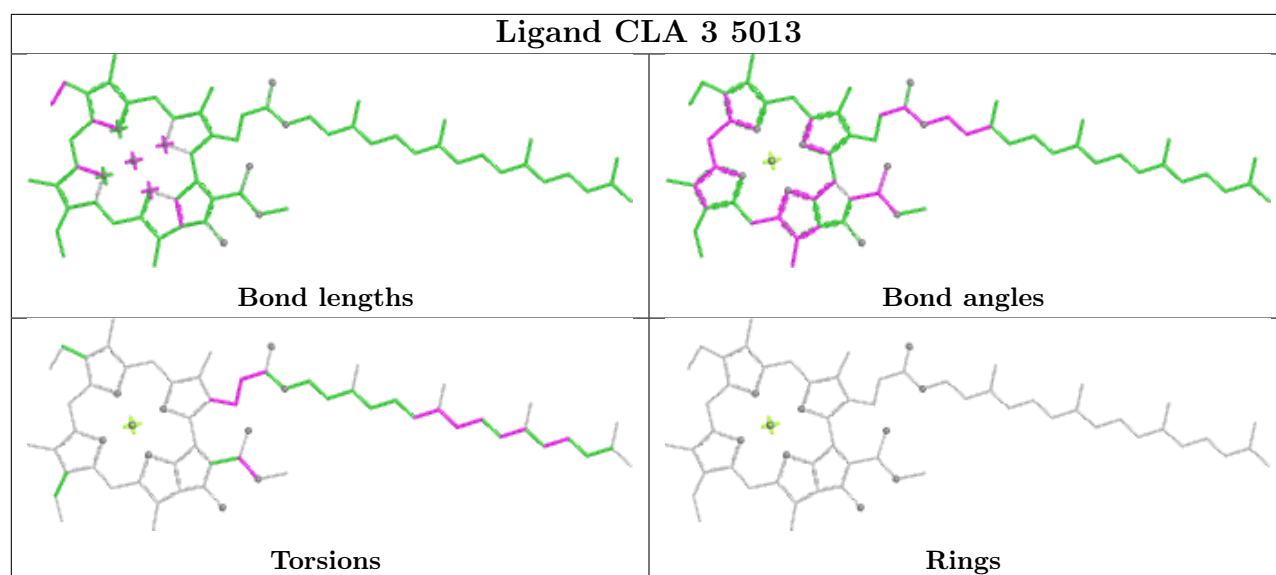


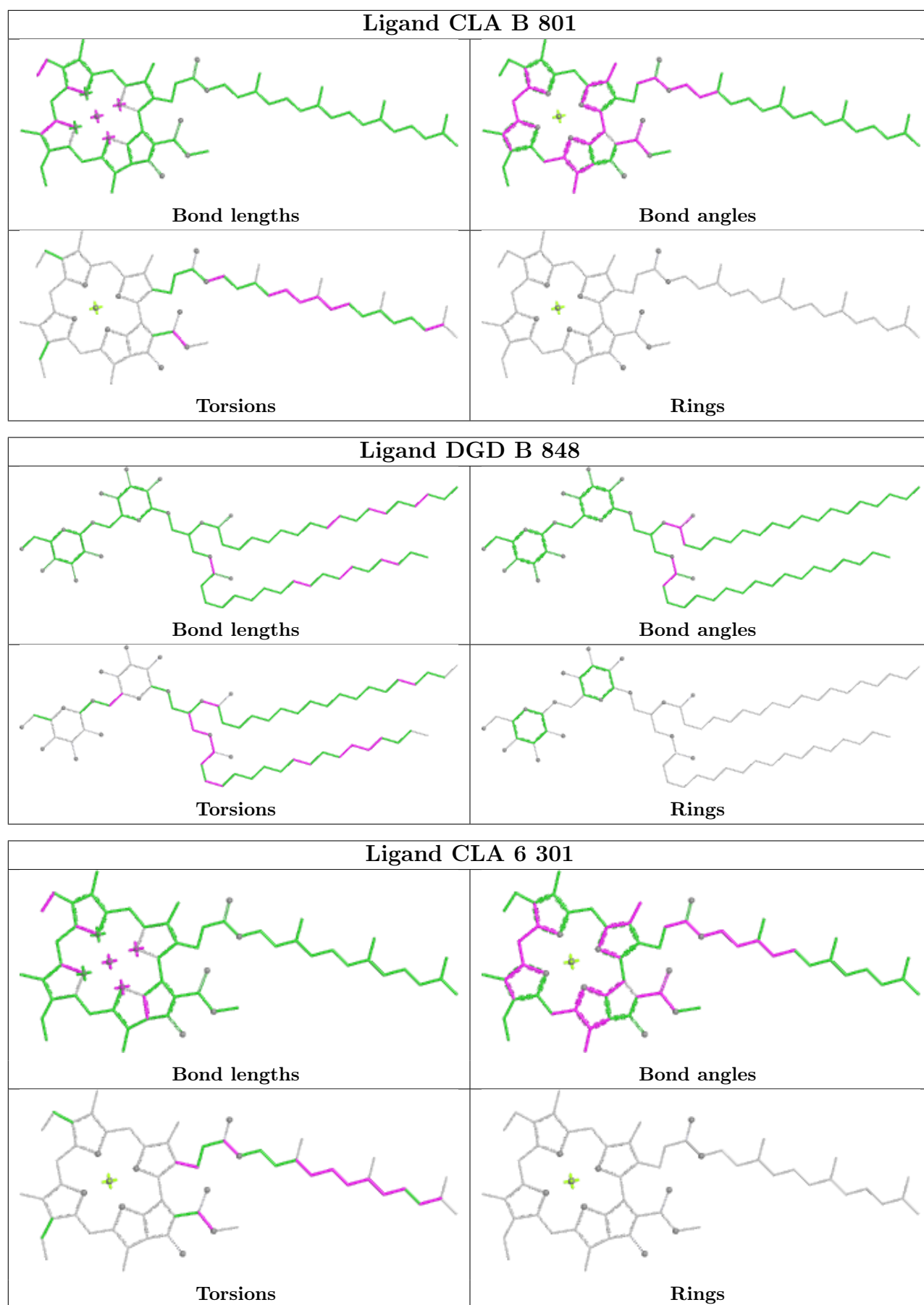


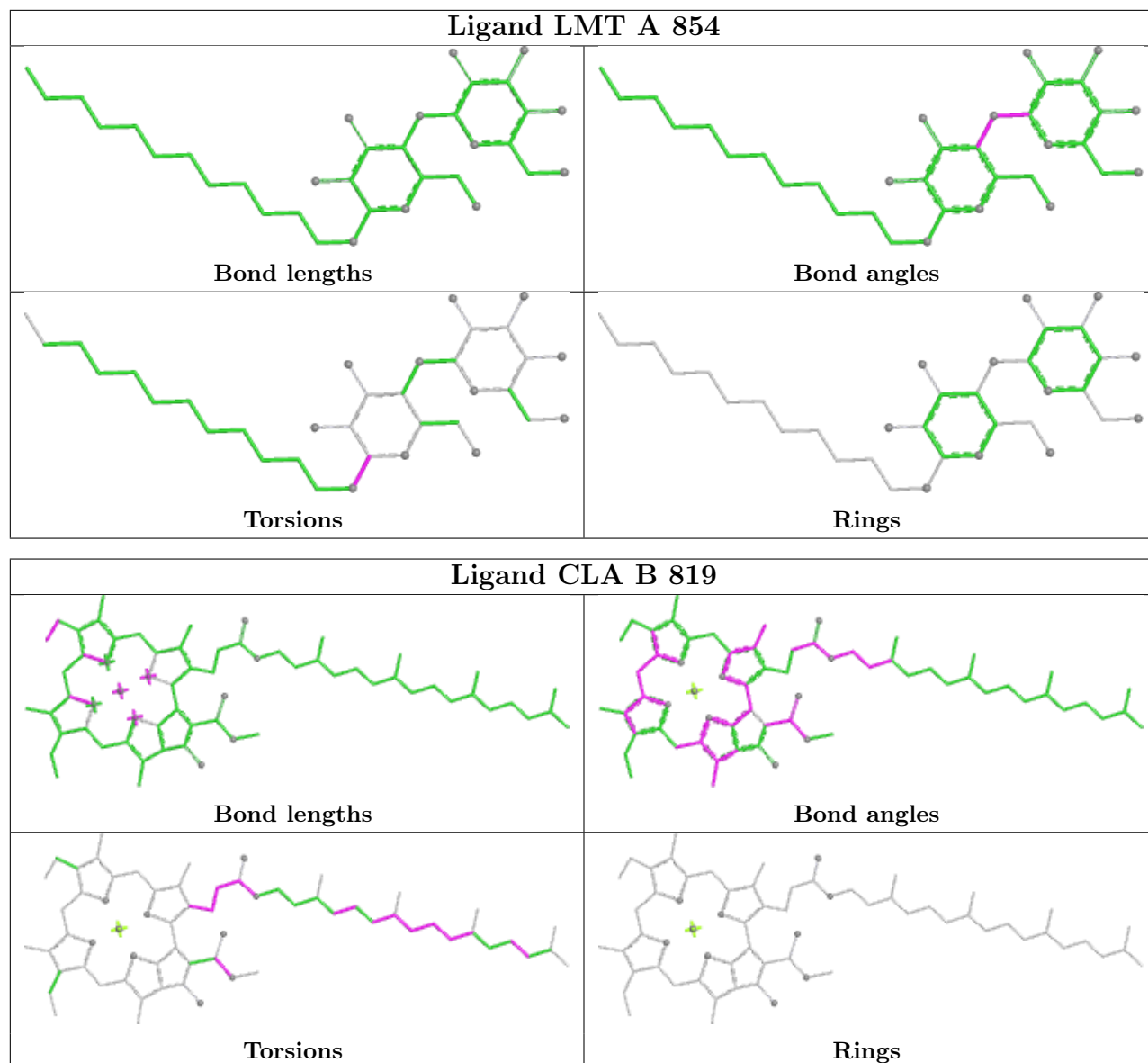


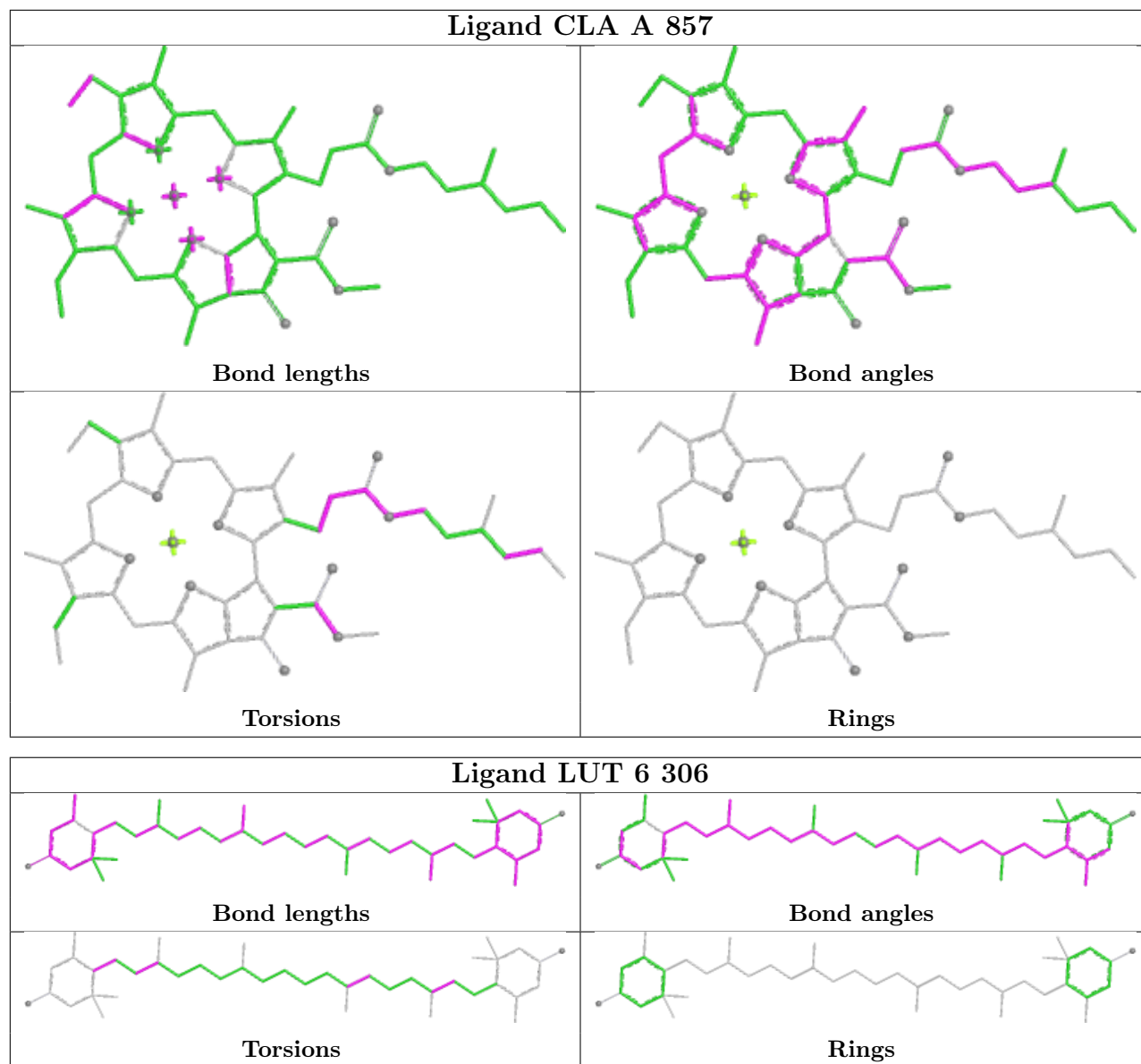




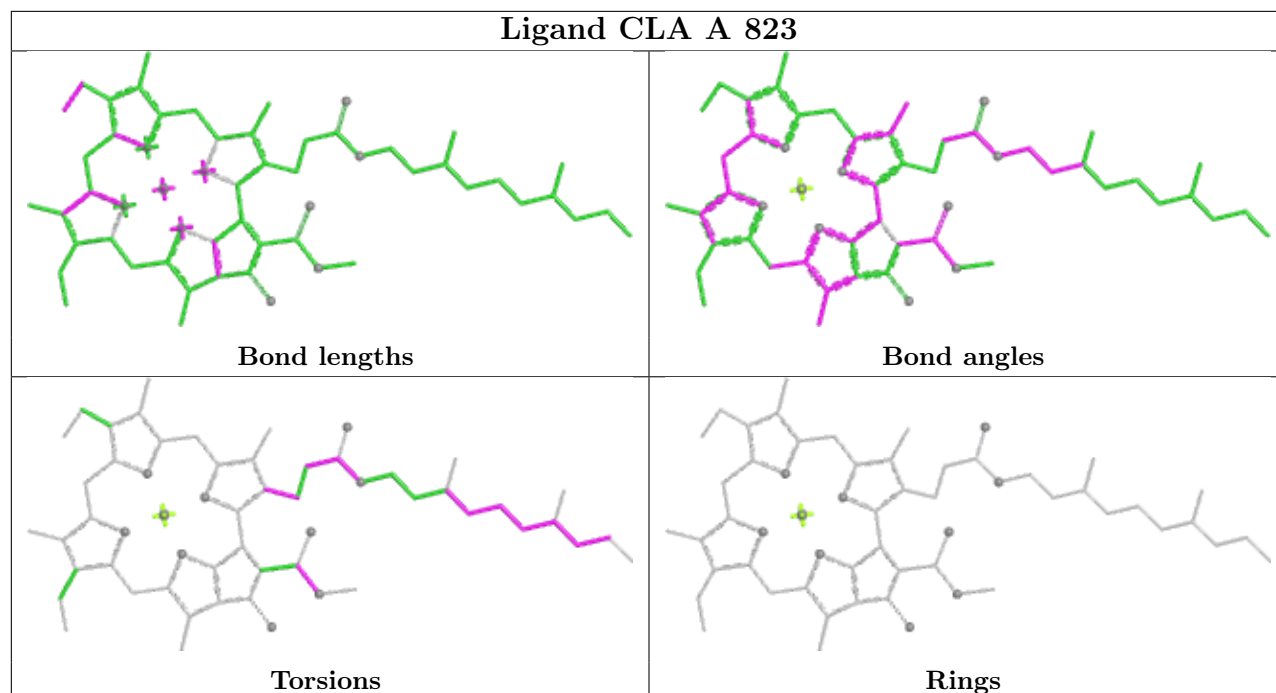




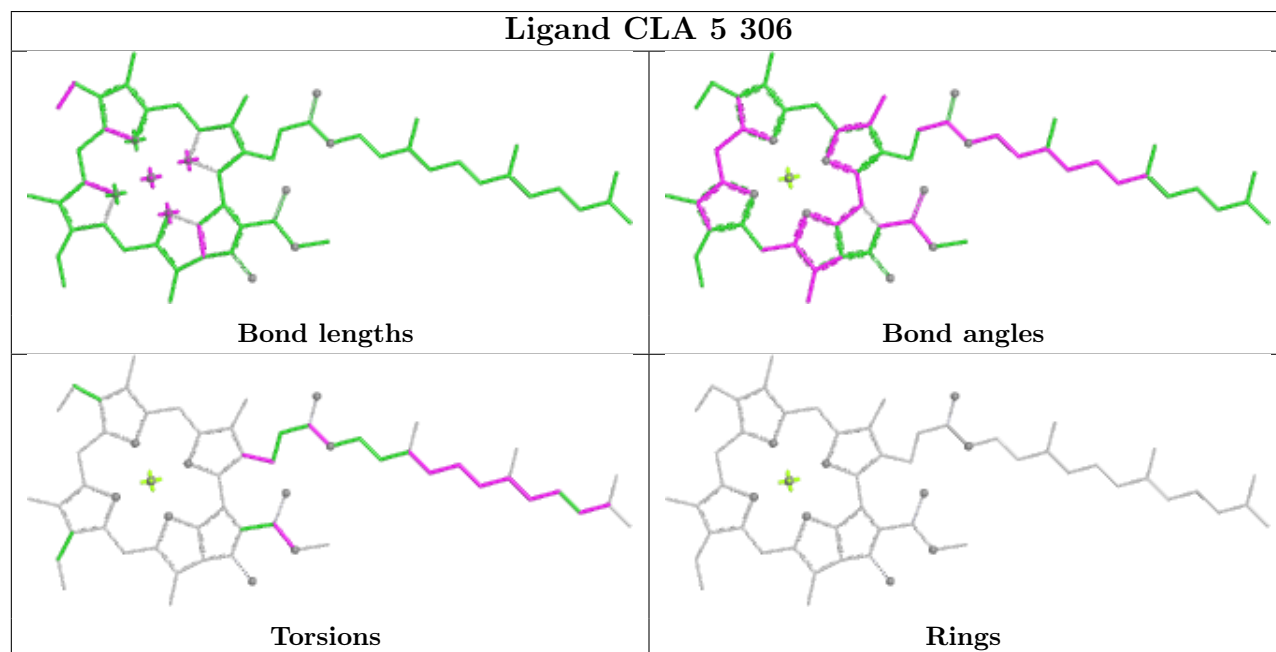


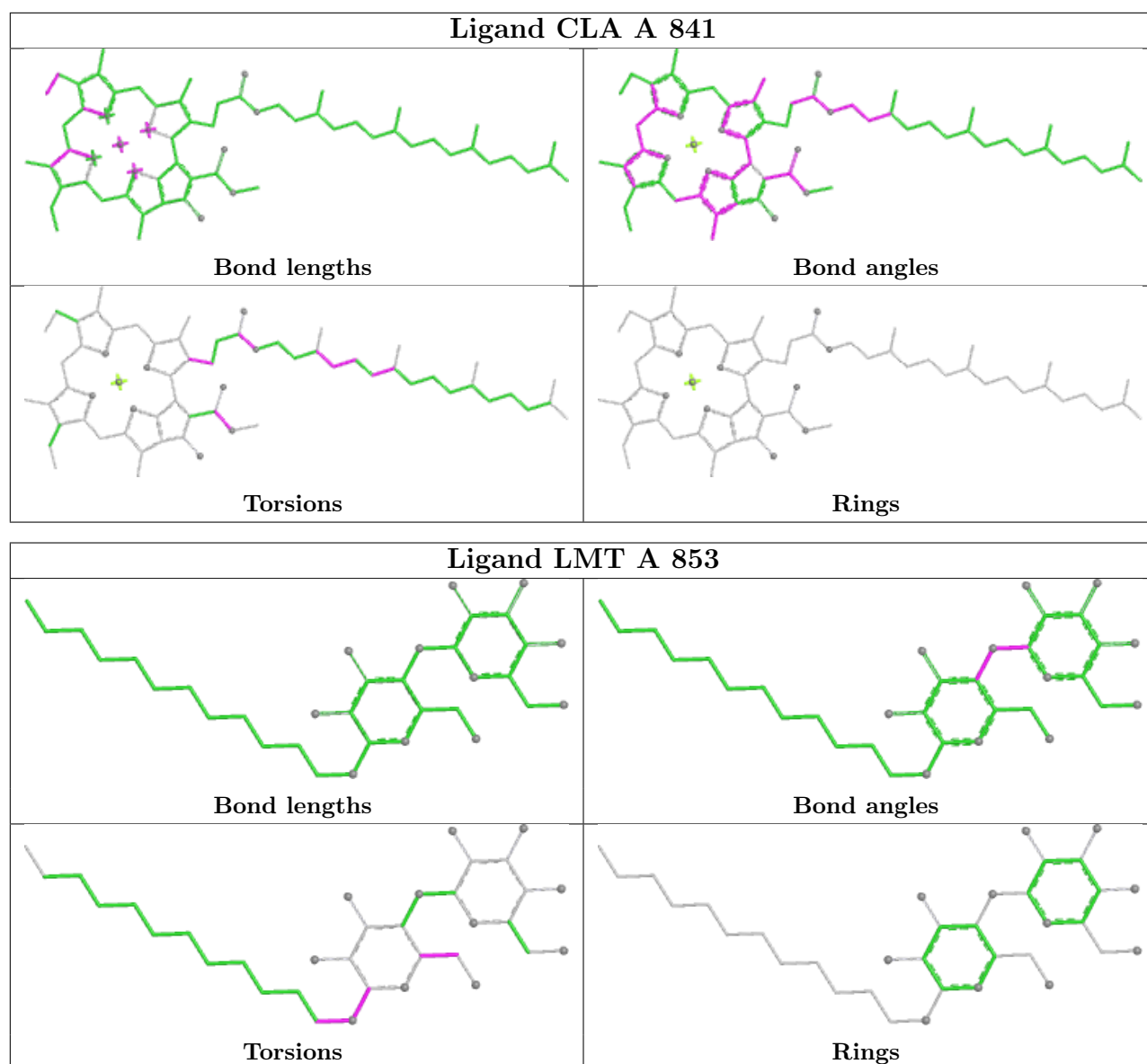


Ligand CLA A 823

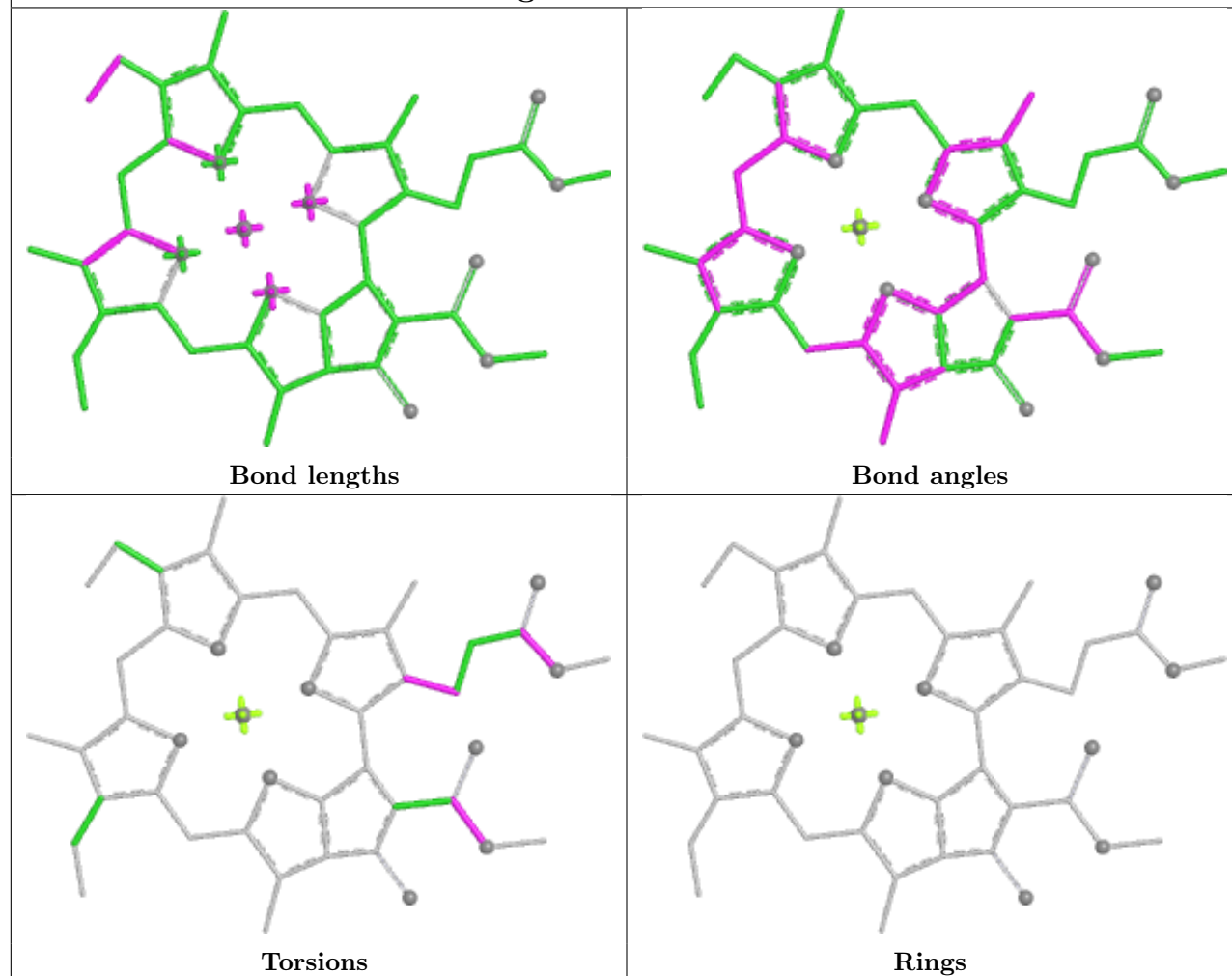


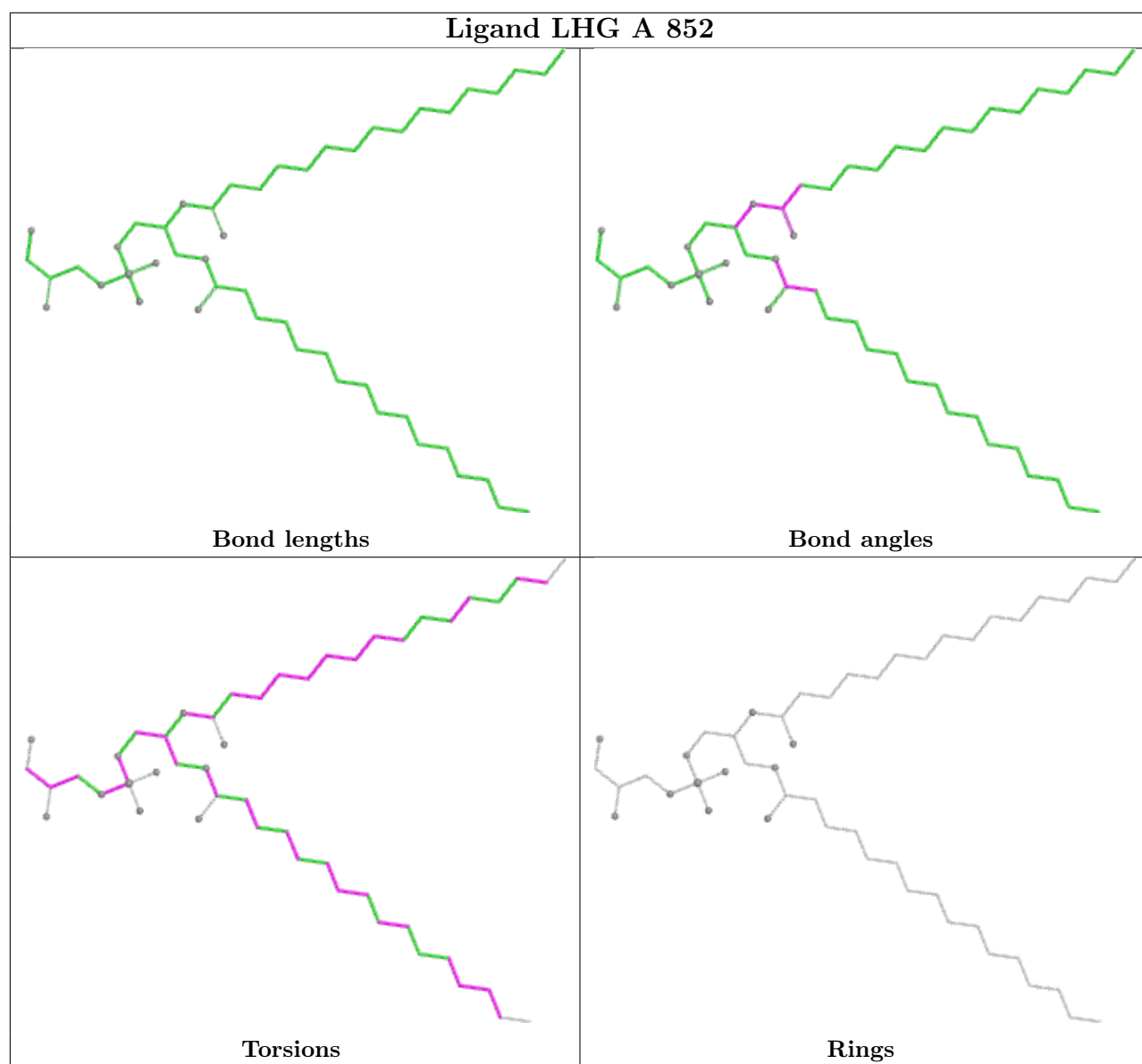
Ligand CLA 5 306

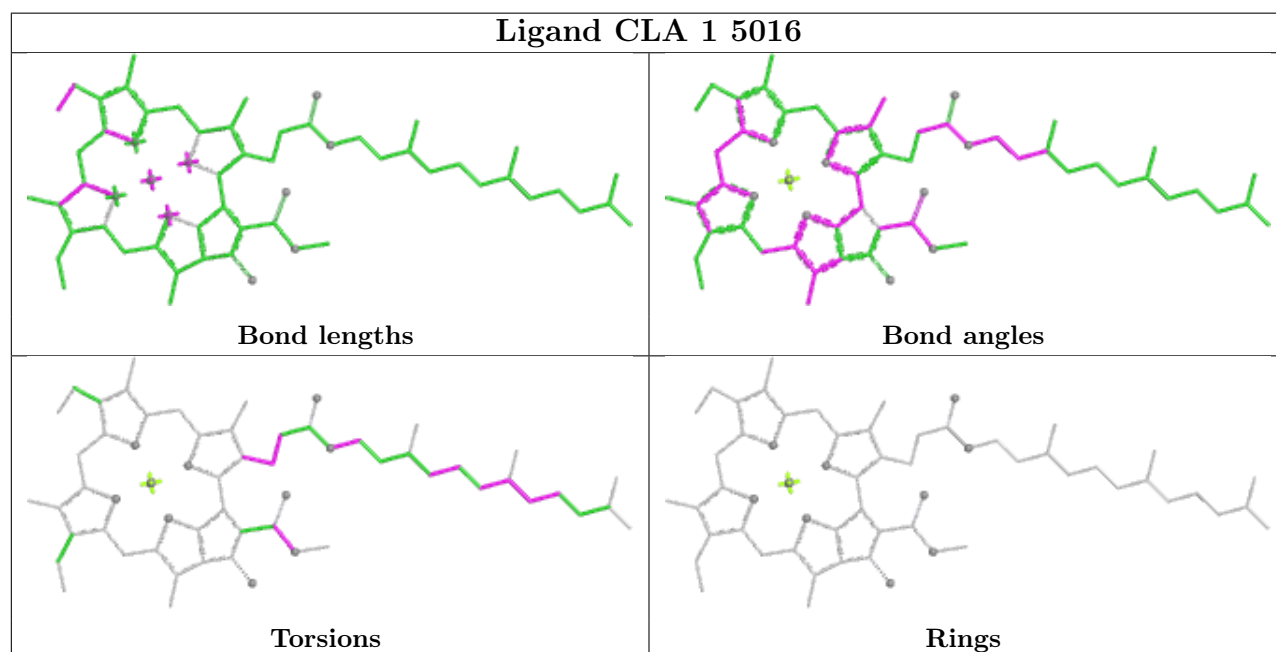
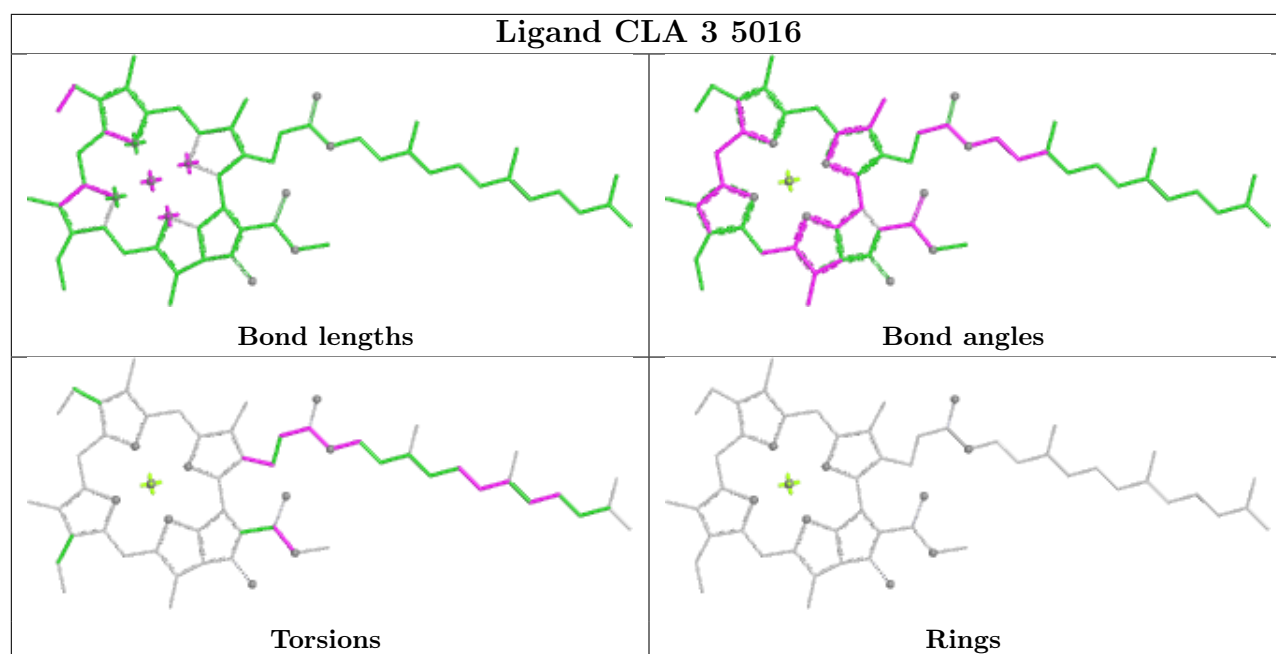


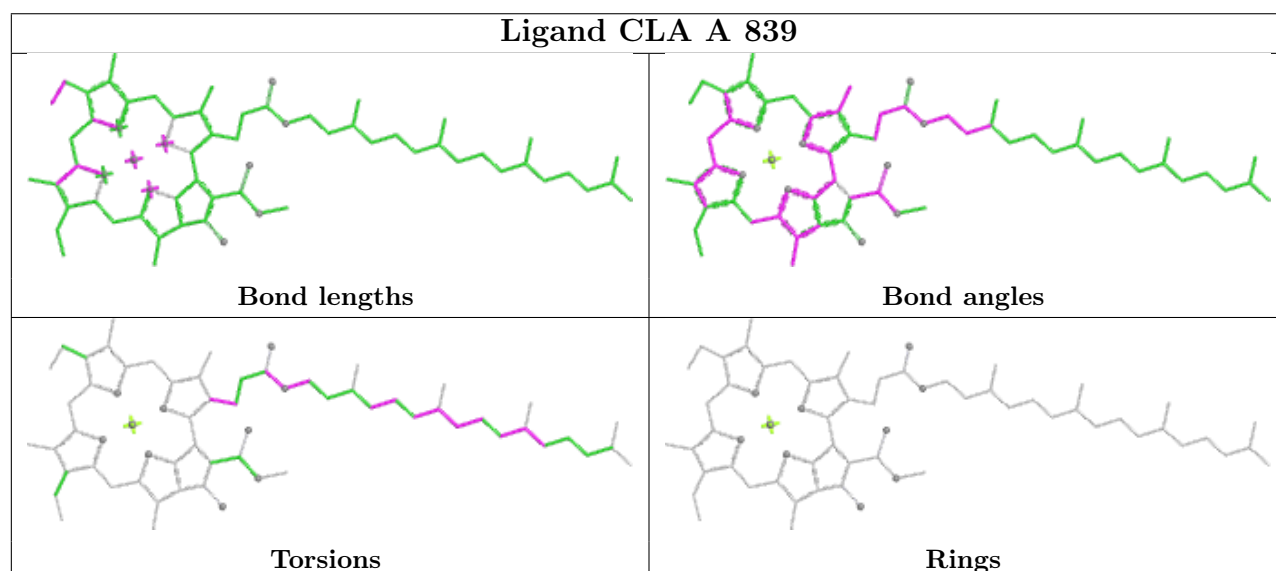
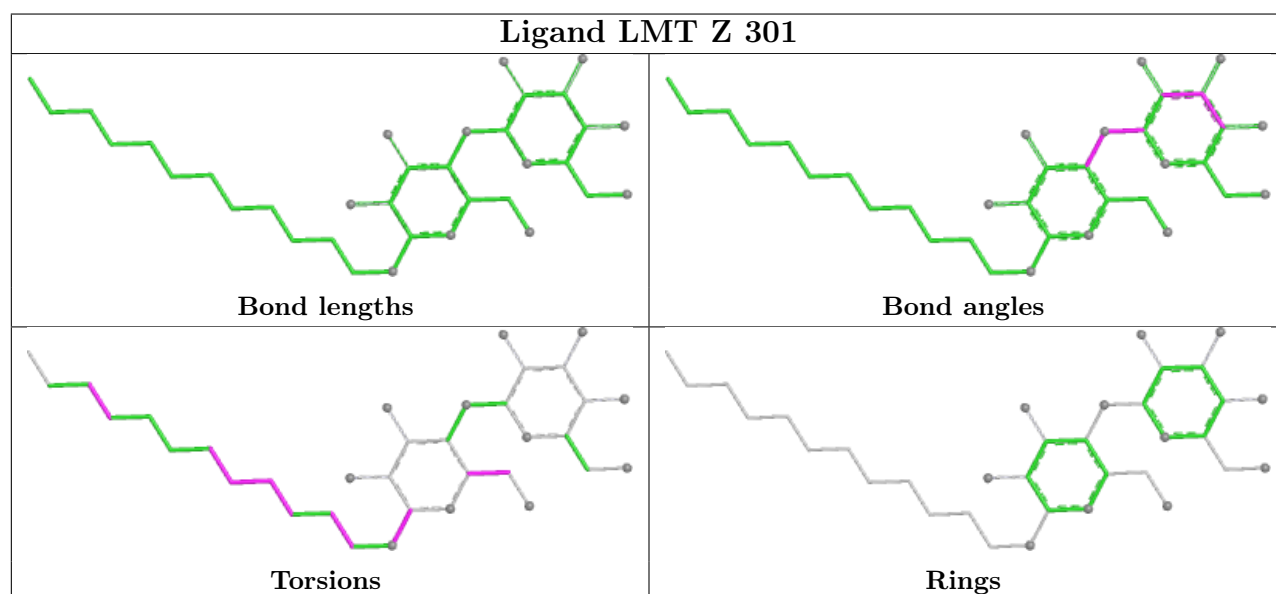
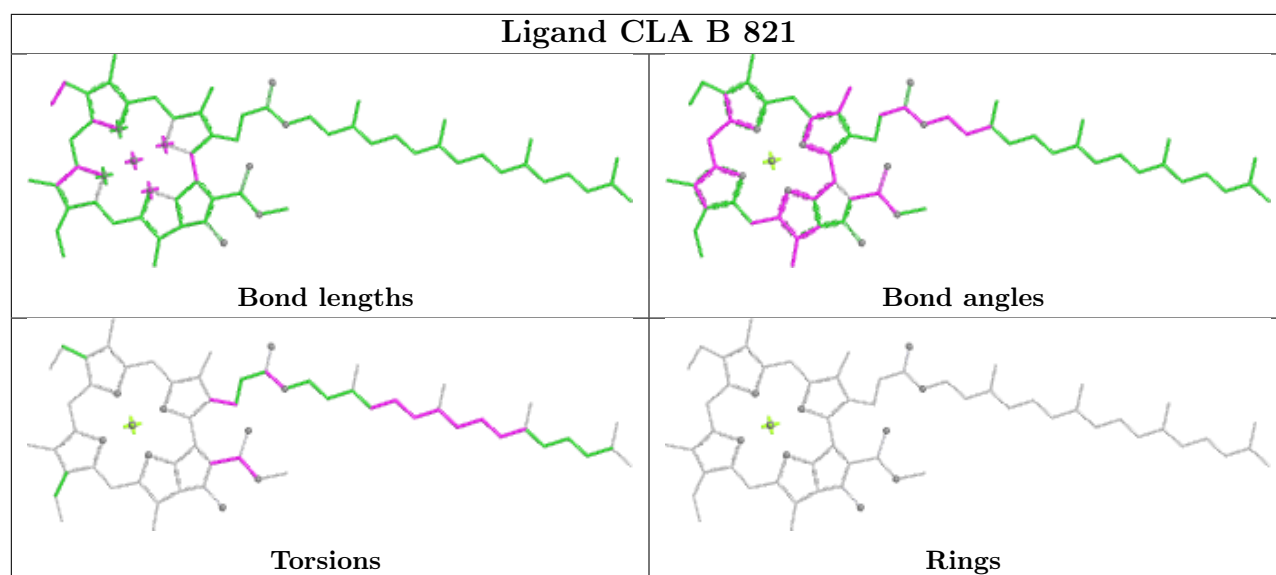


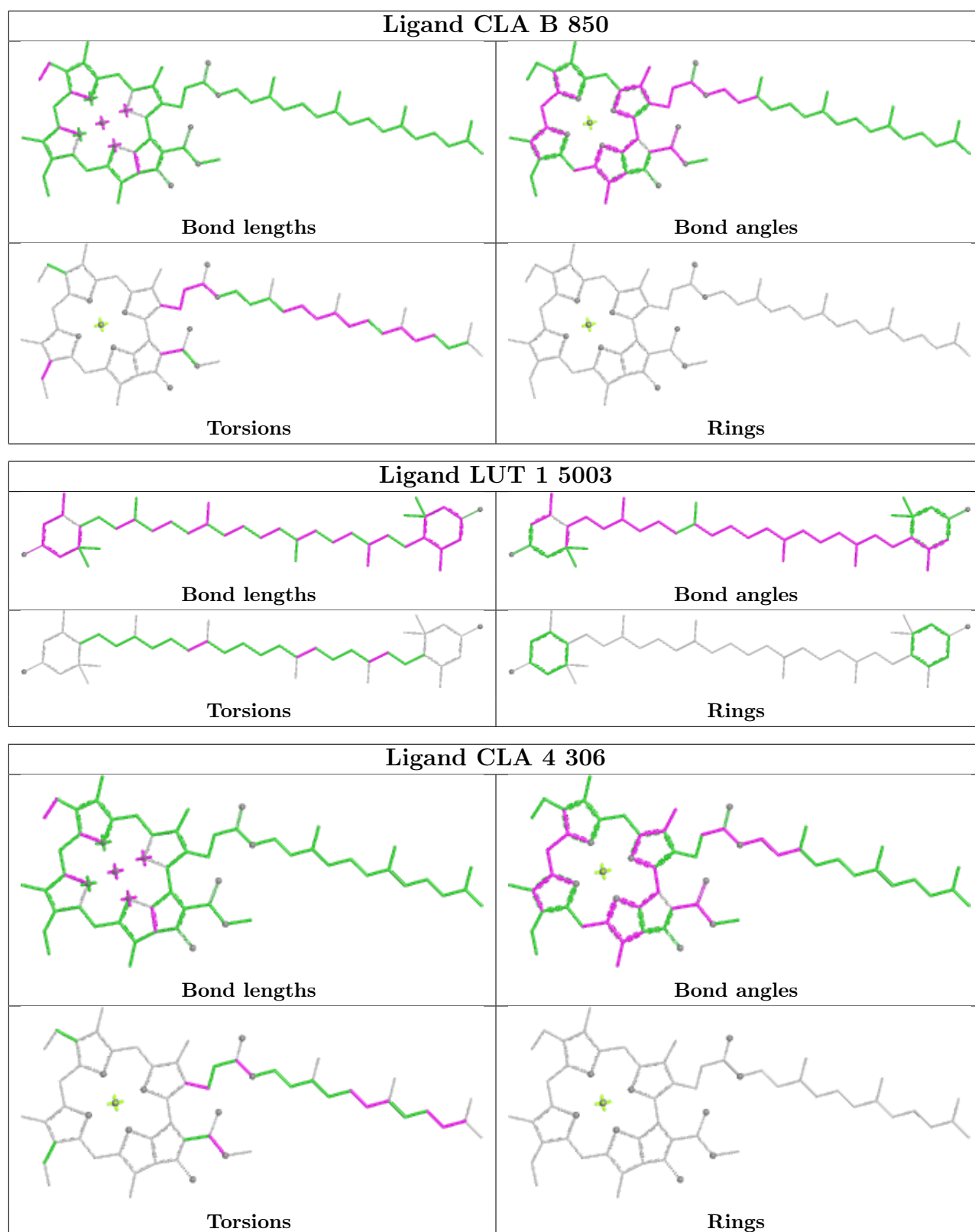
Ligand CLA 8 320

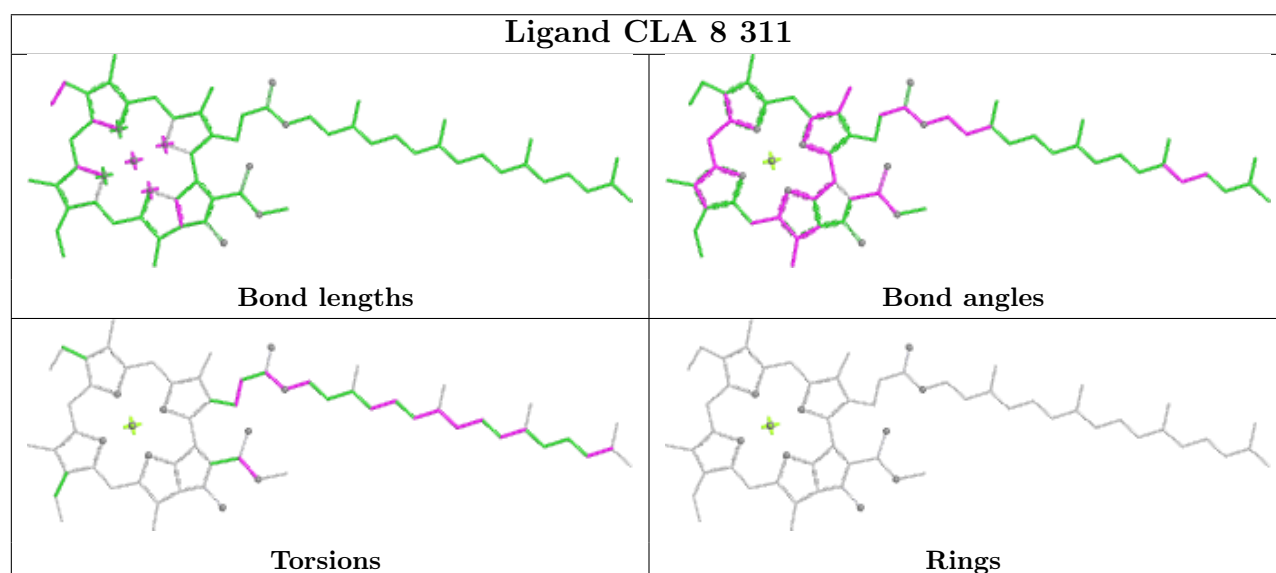
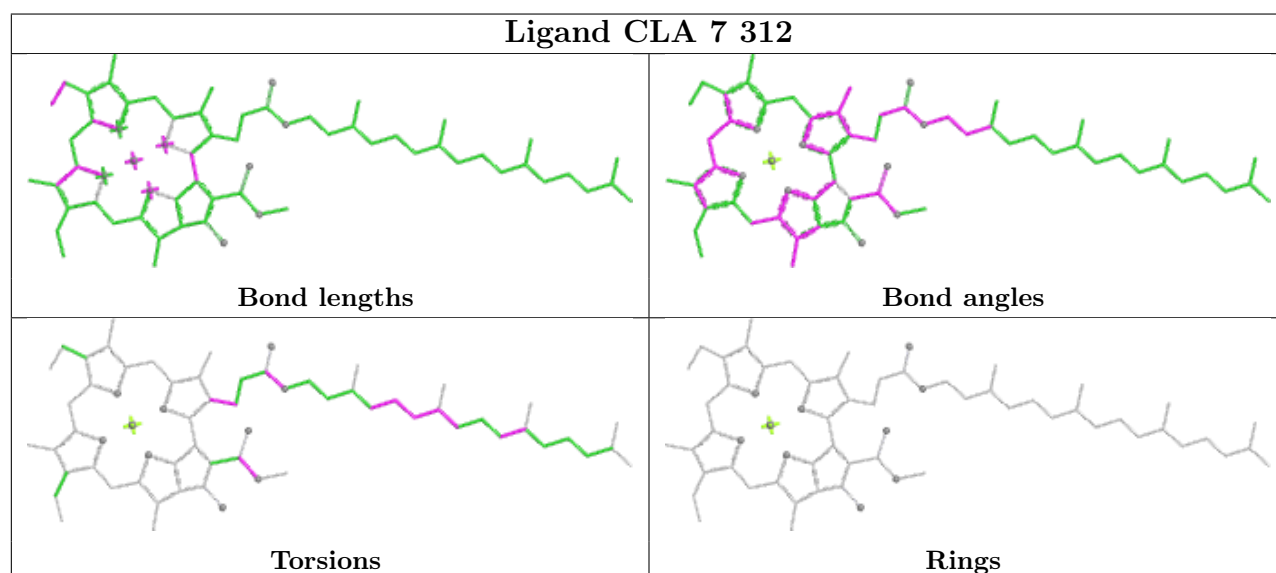
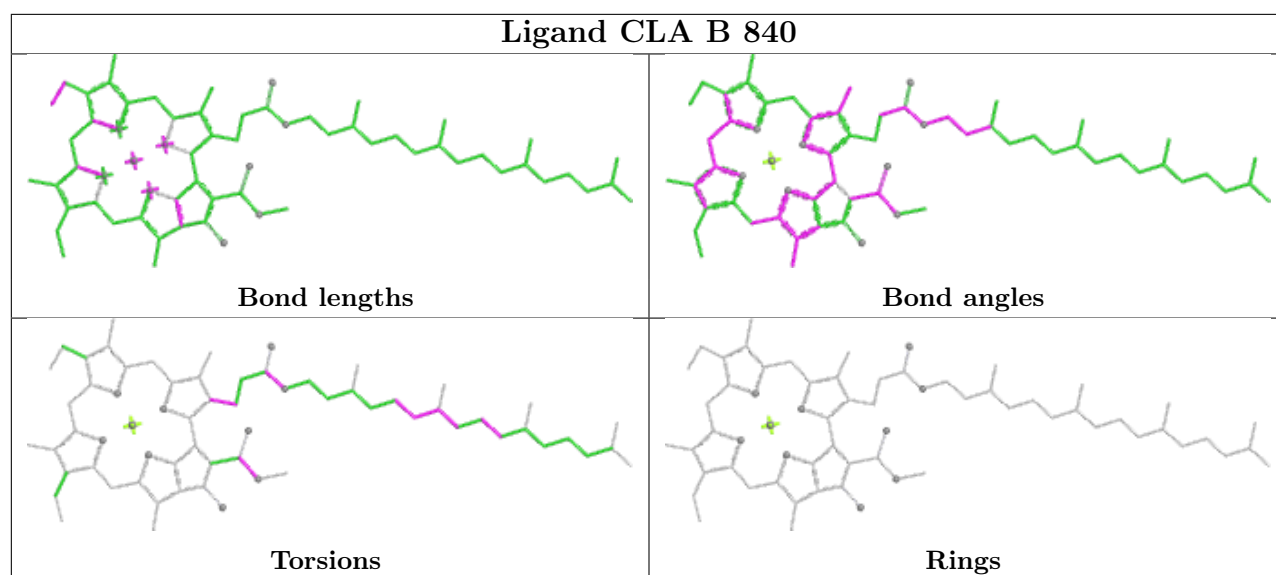




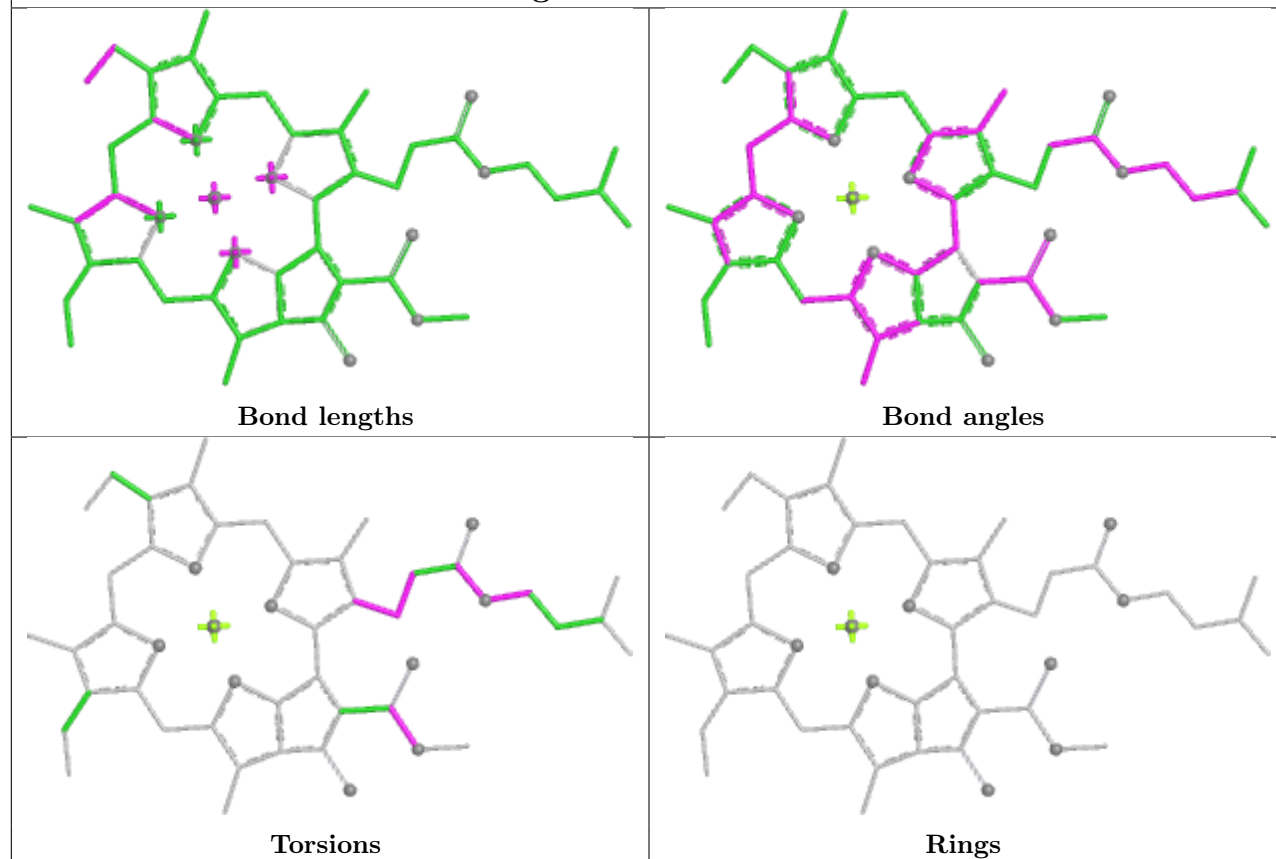




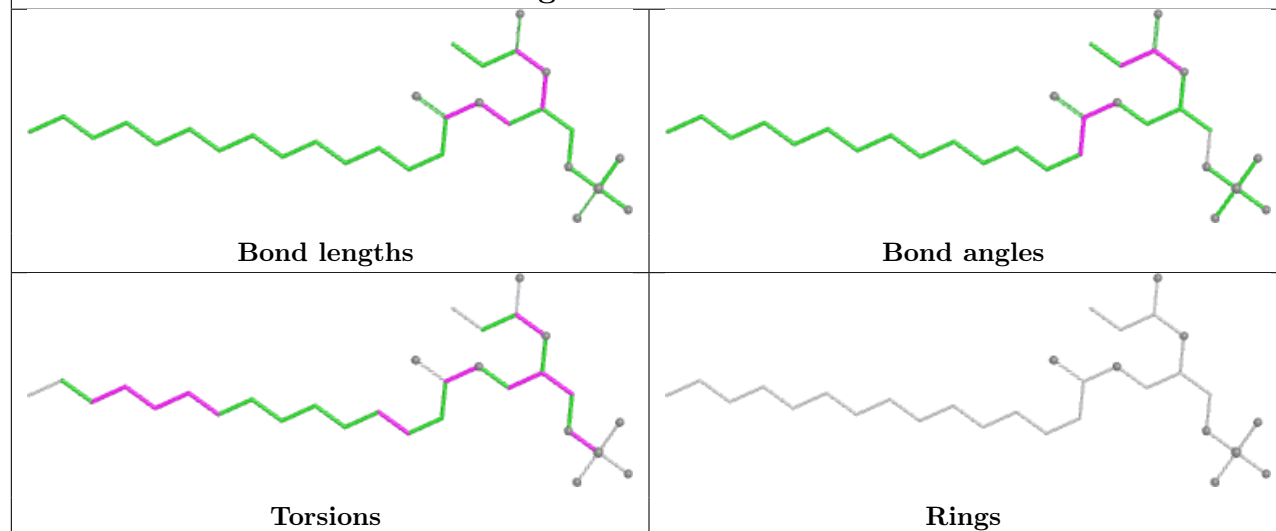




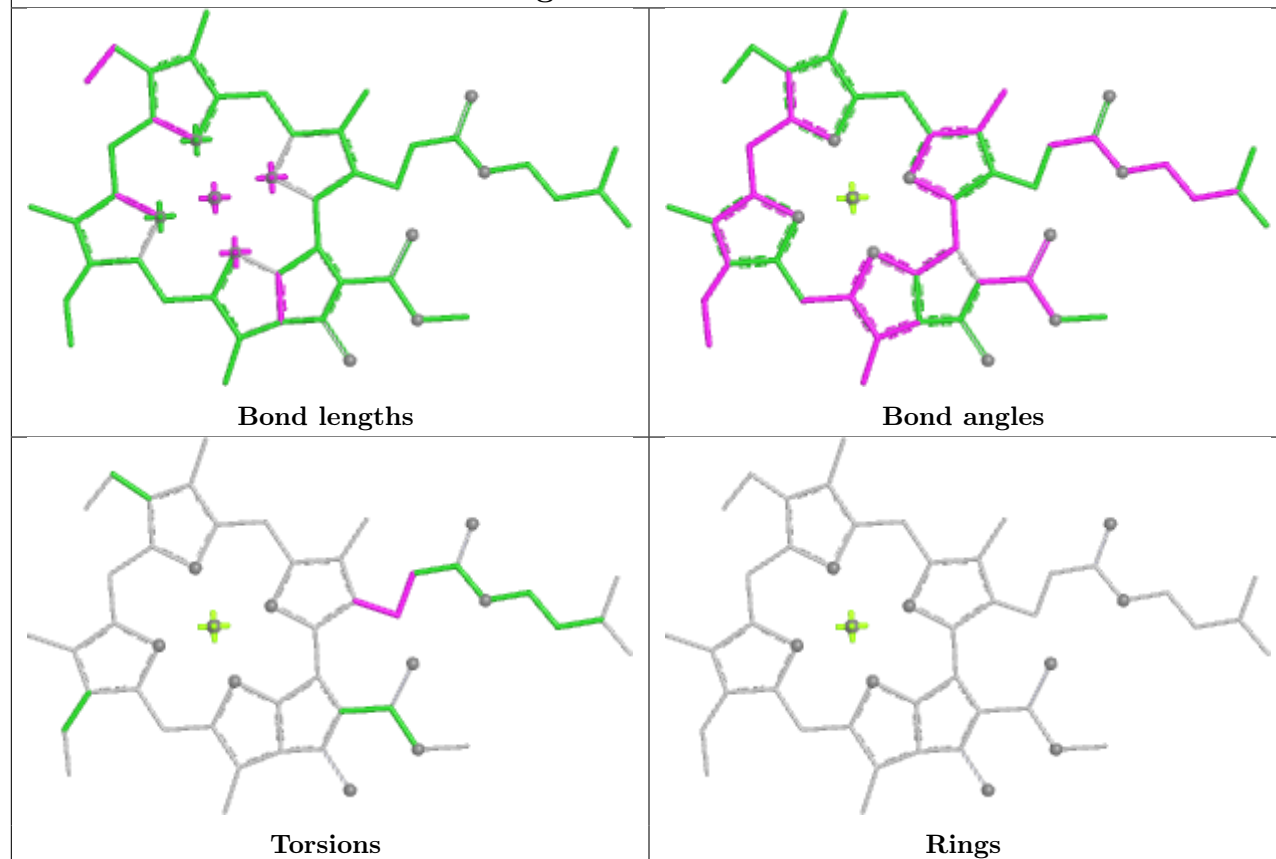
Ligand CLA B 830



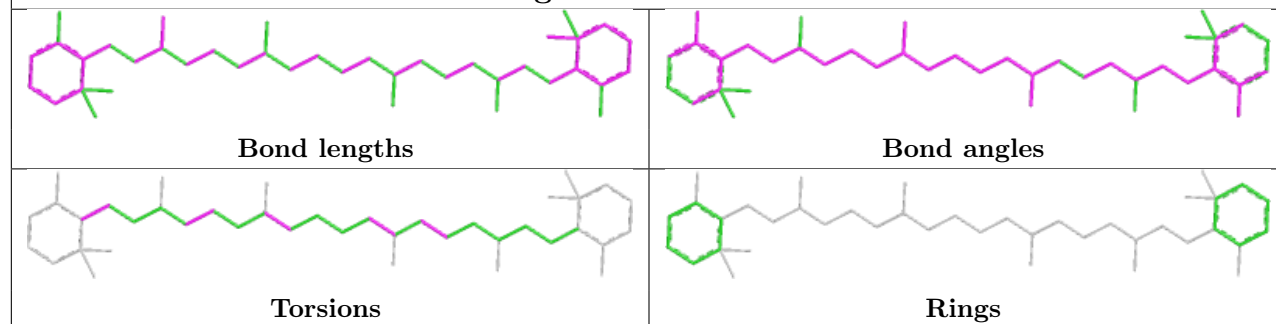
Ligand 3PH 8 322



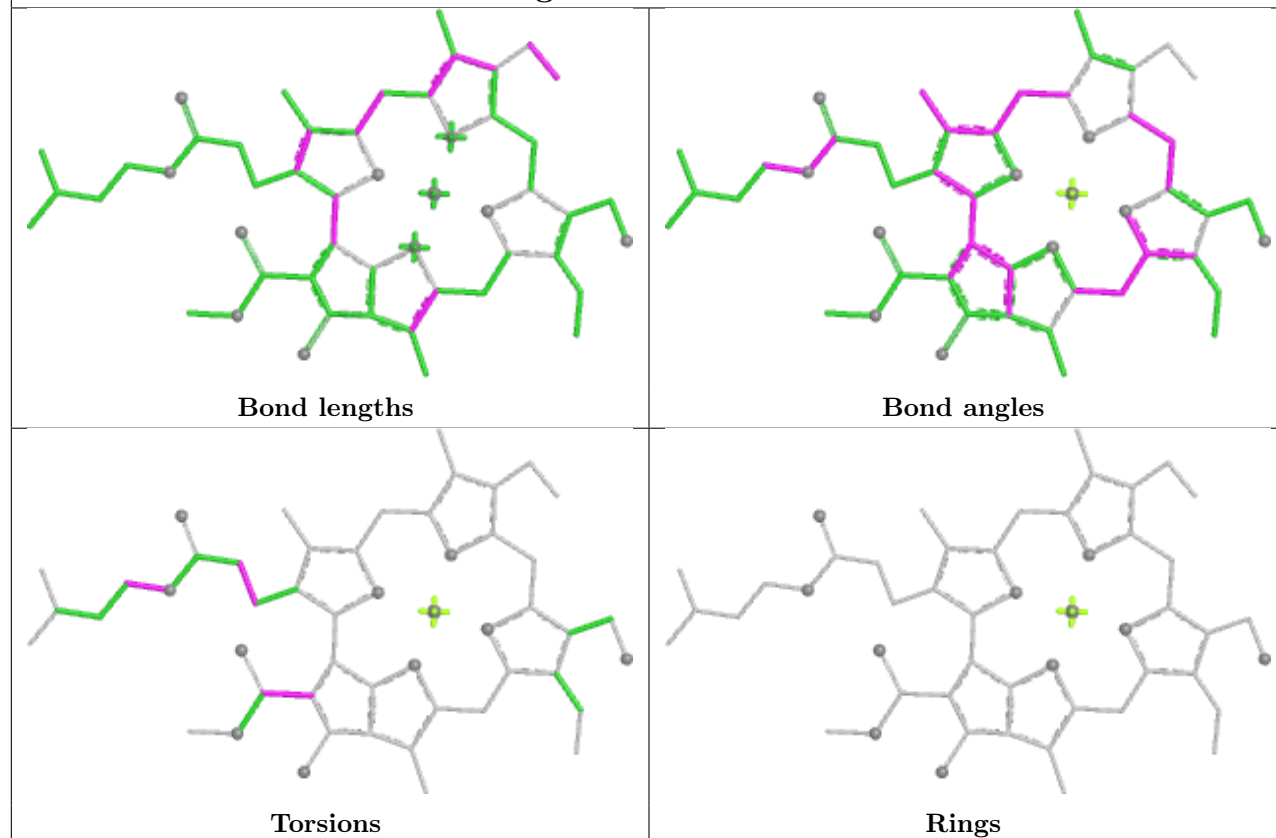
Ligand CLA 6 318



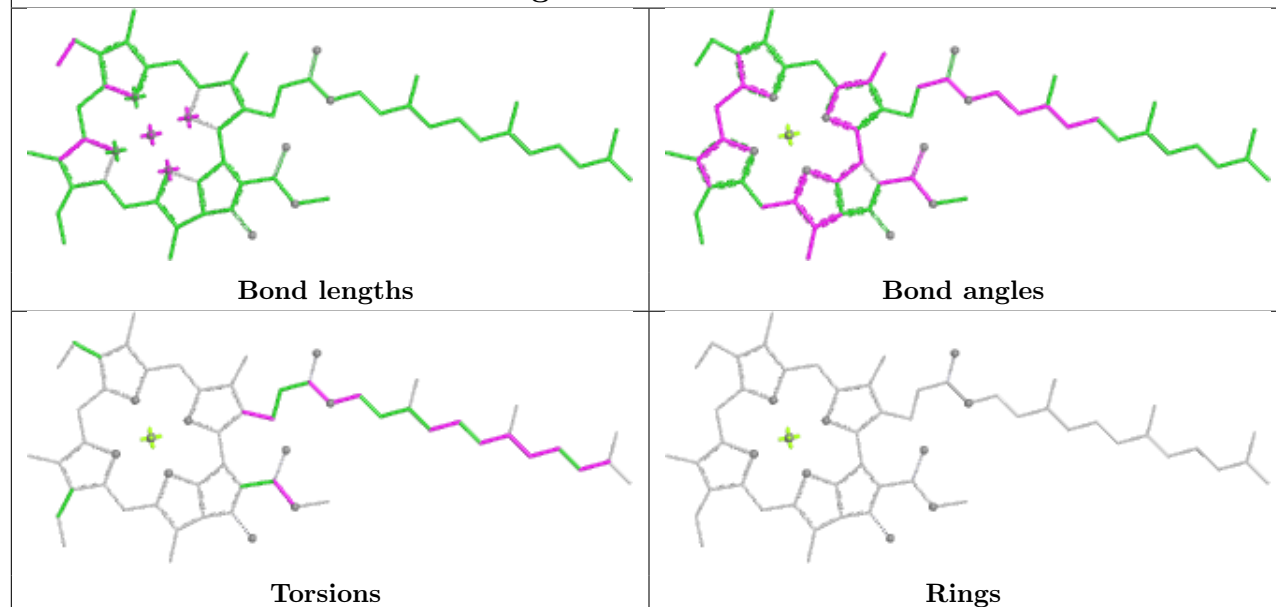
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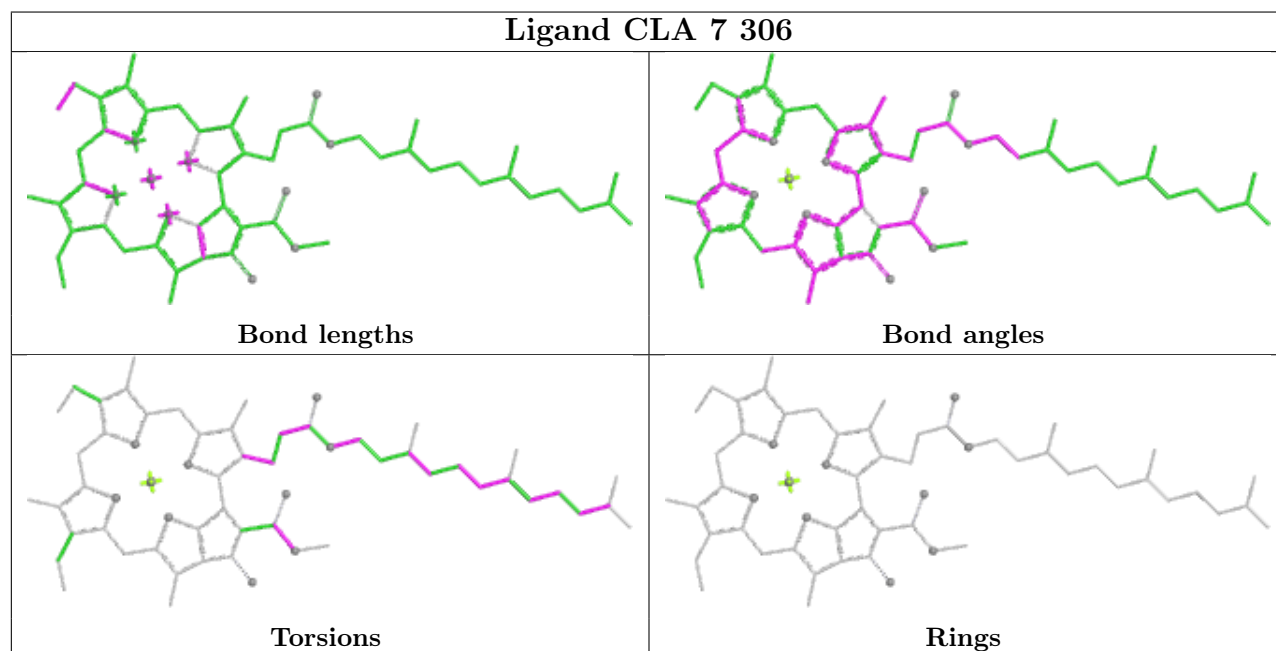
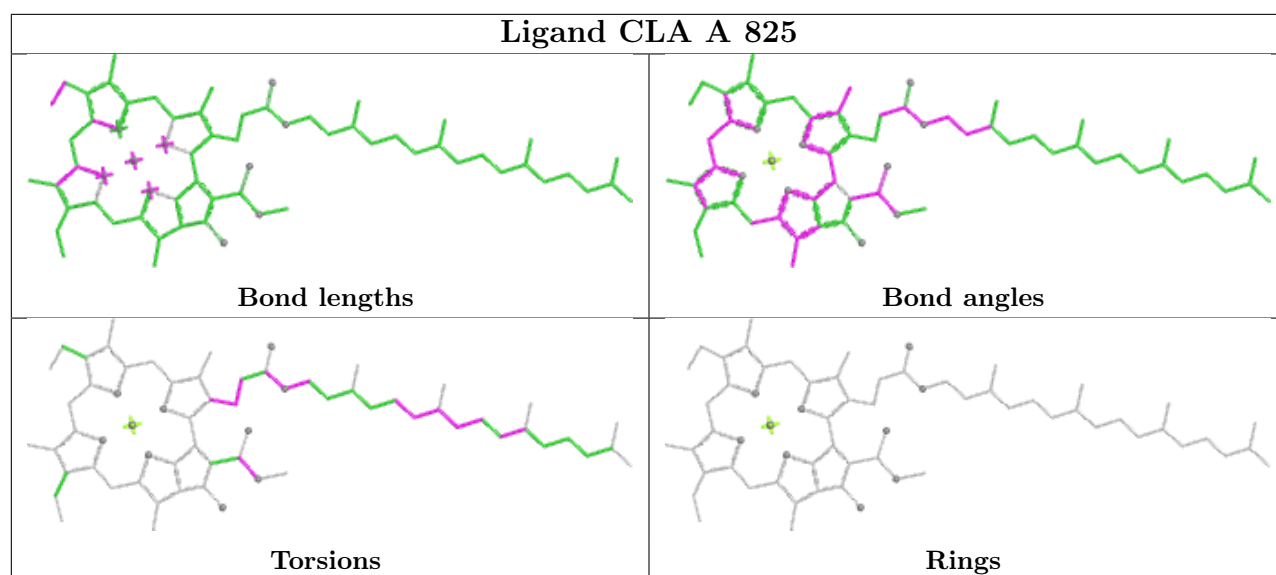


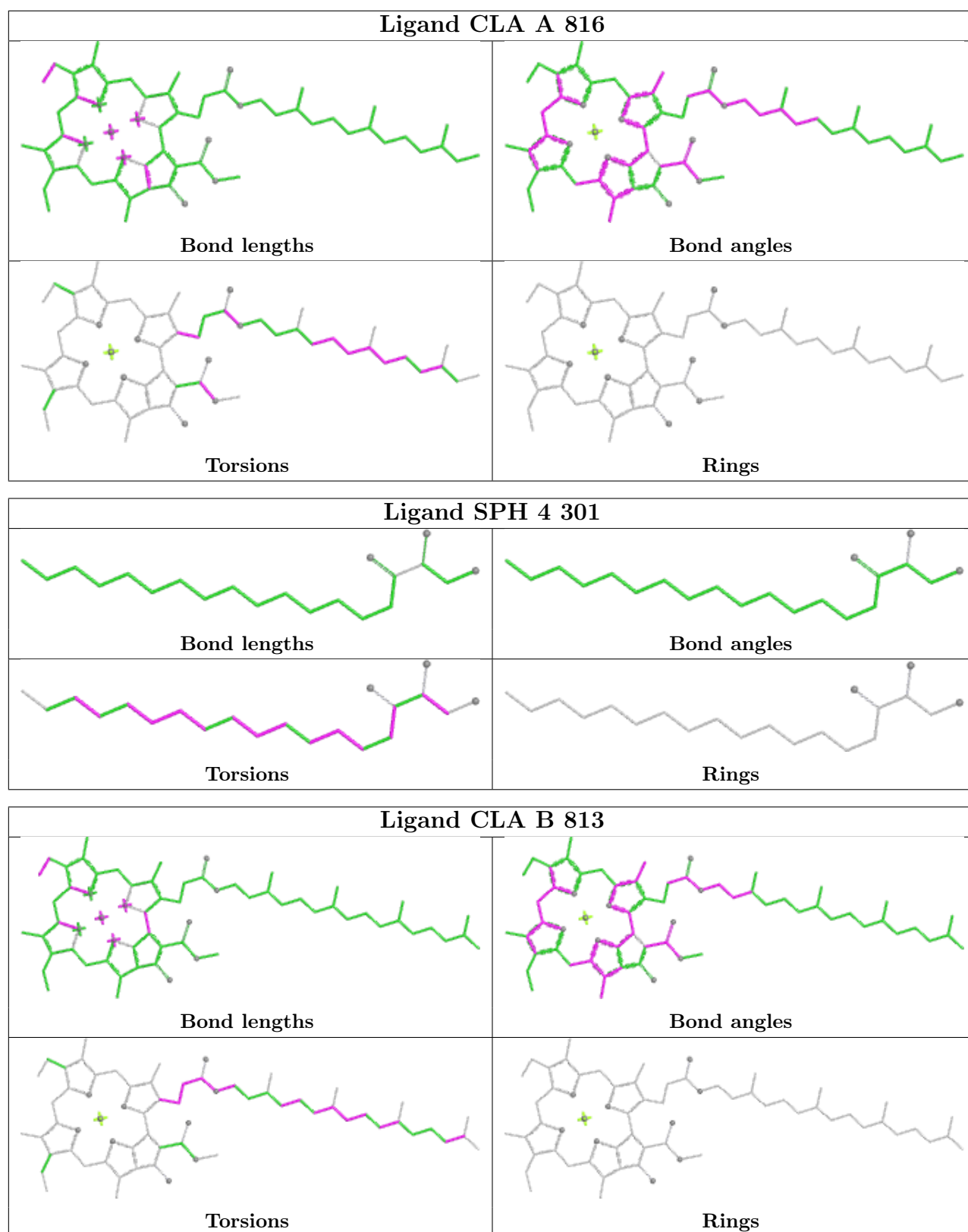
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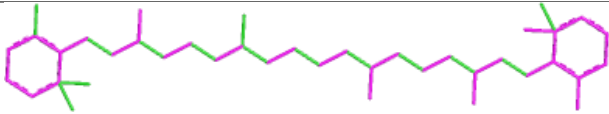
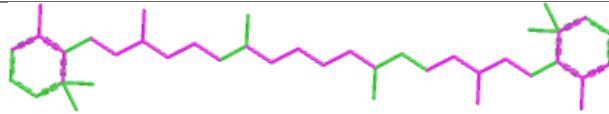
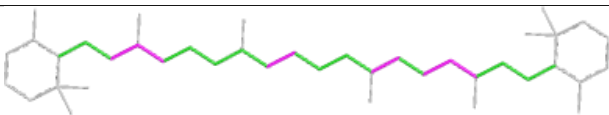
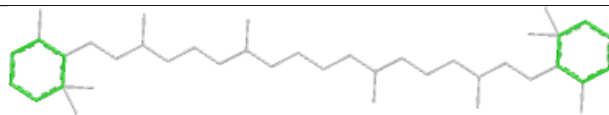


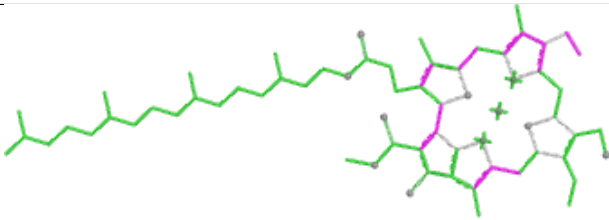
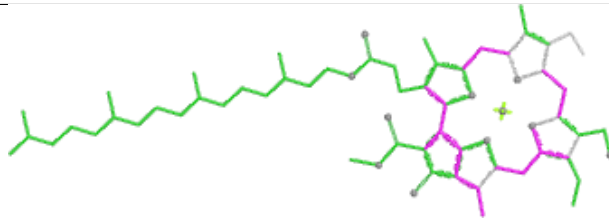
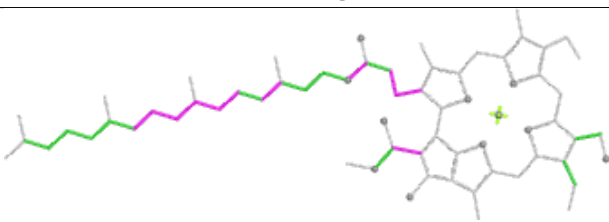
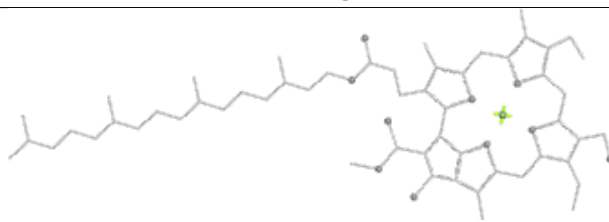
Ligand CLA A 818

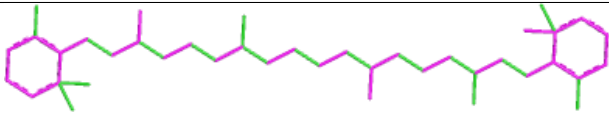
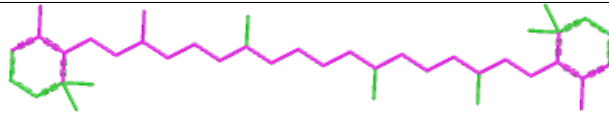
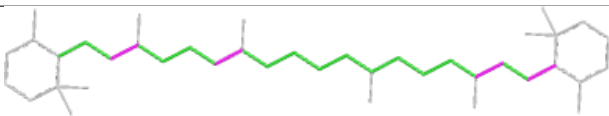
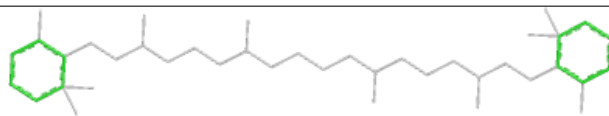


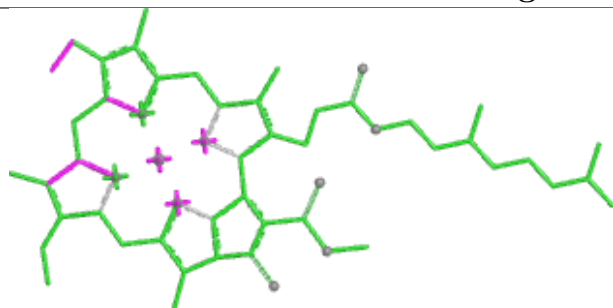




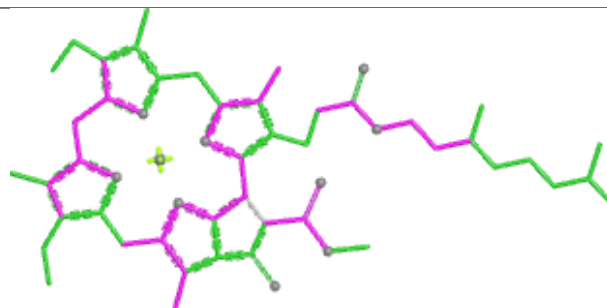
Ligand BCR B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL 7 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

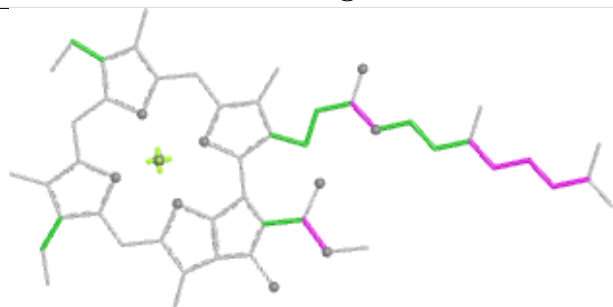
Ligand BCR 3 5005	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 4 312

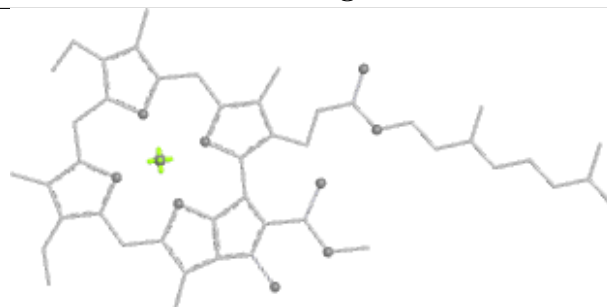
Bond lengths



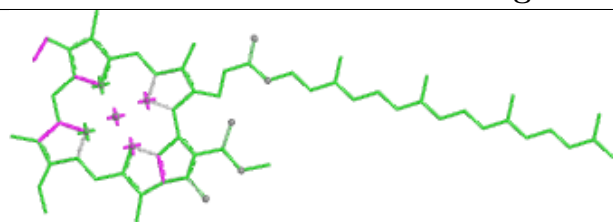
Bond angles



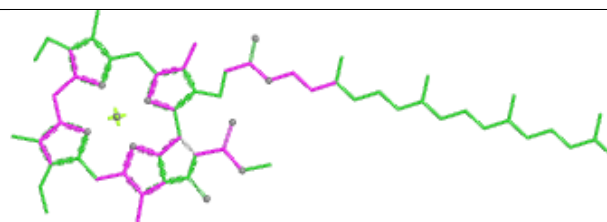
Torsions



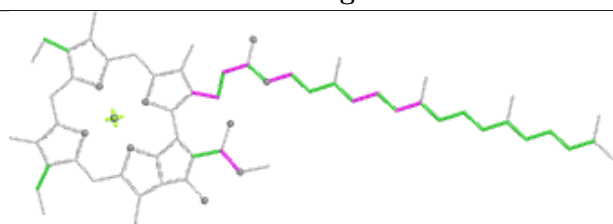
Rings

Ligand CLA A 805

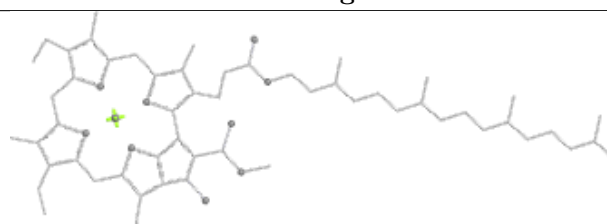
Bond lengths



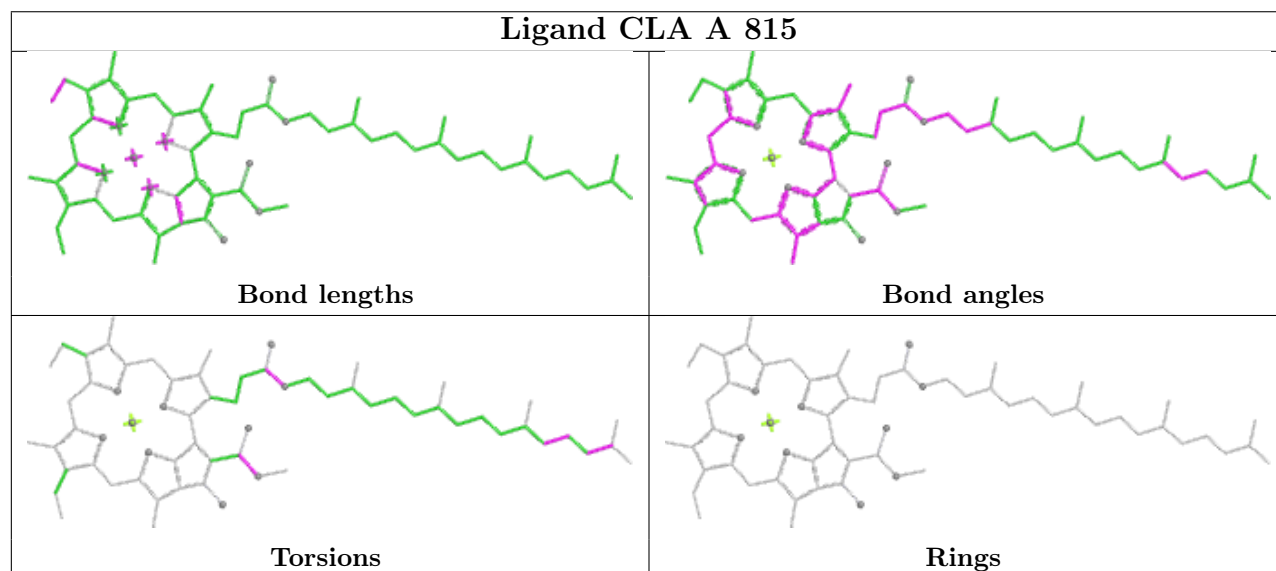
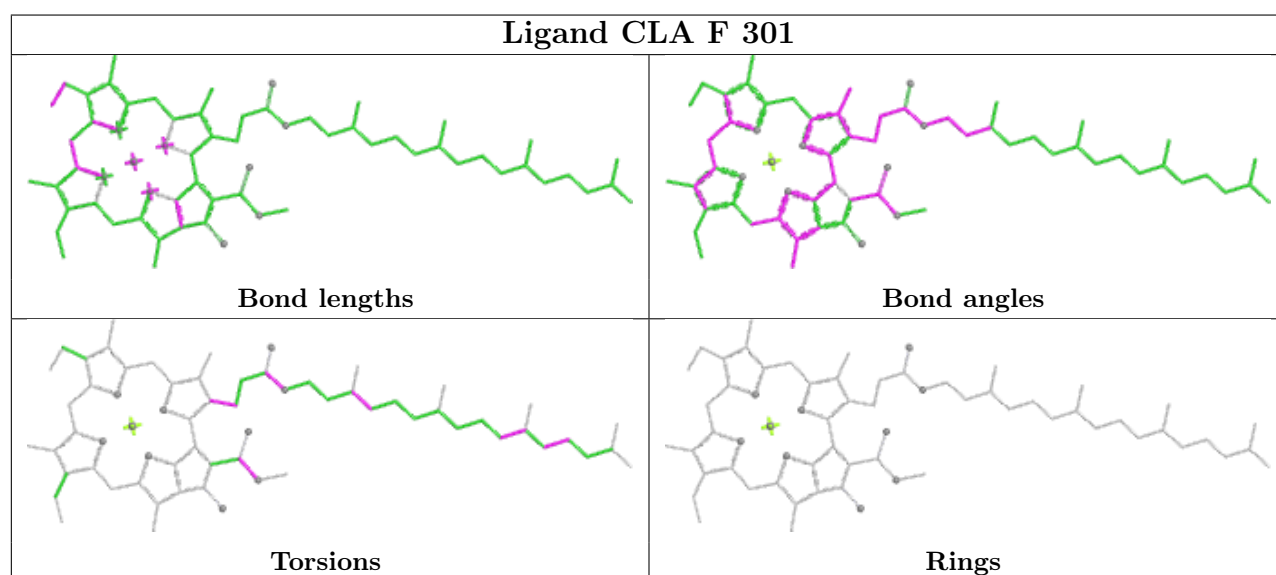
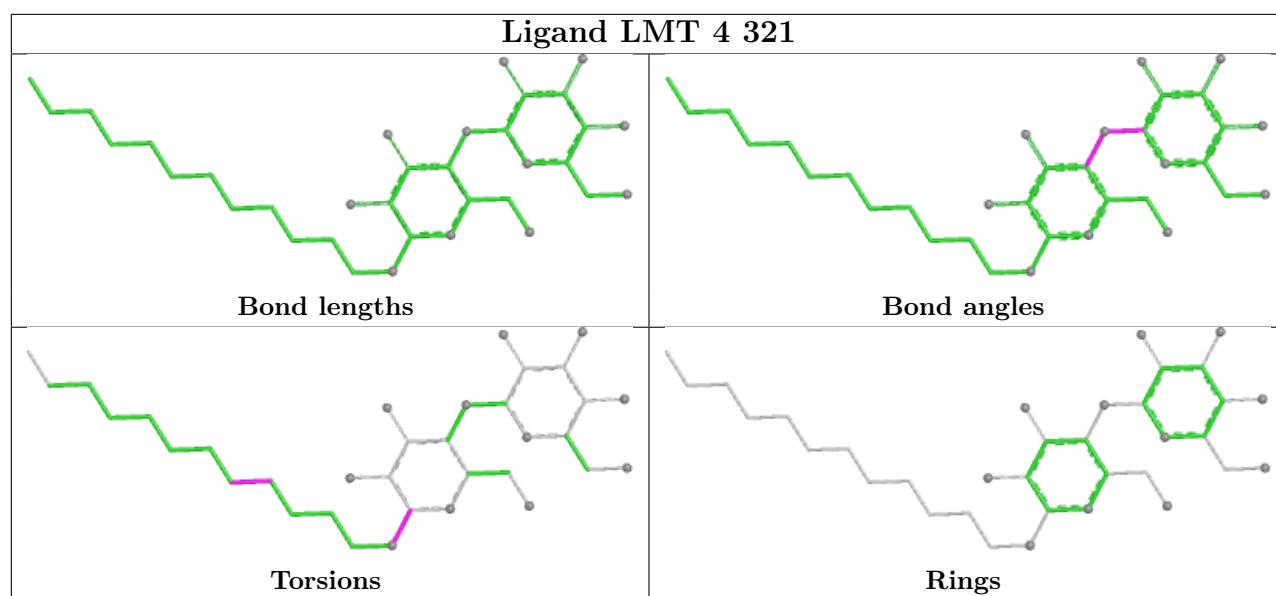
Bond angles

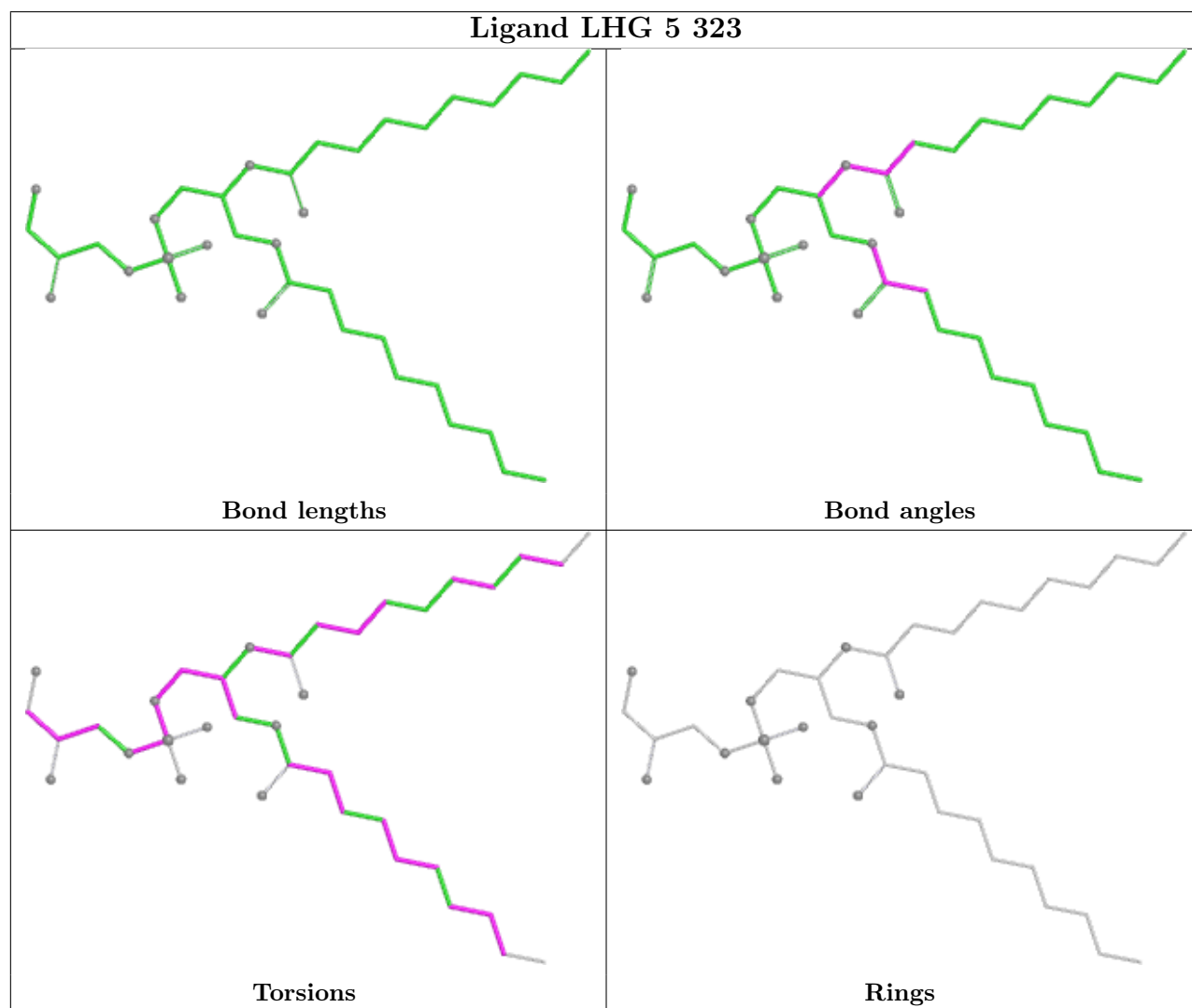
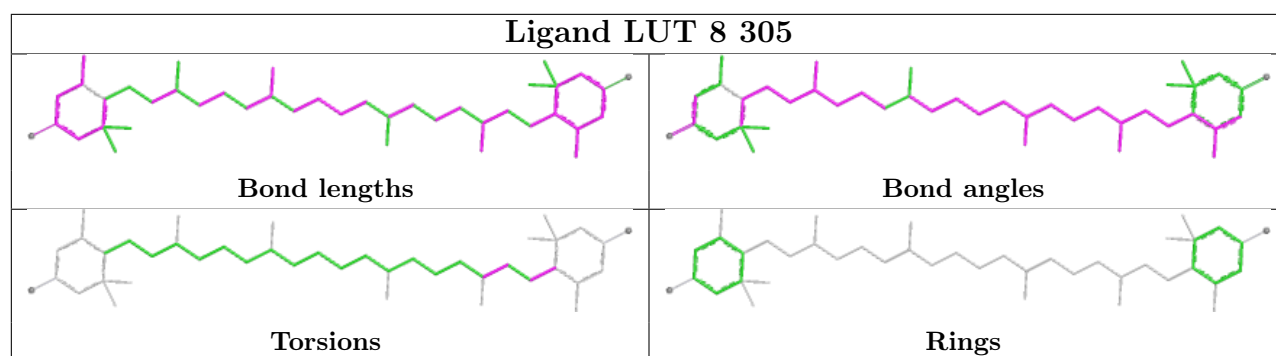


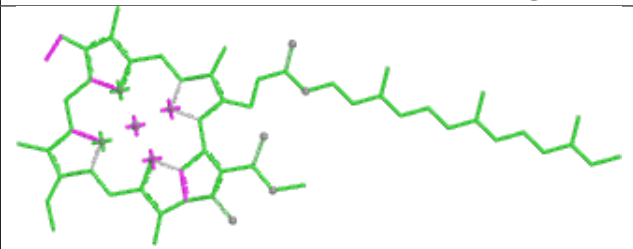
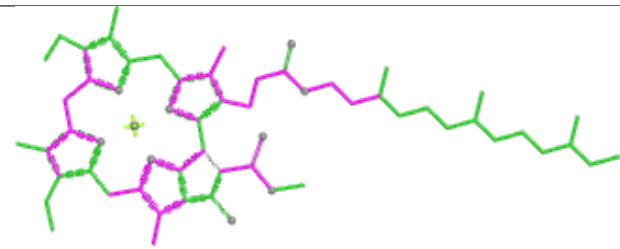
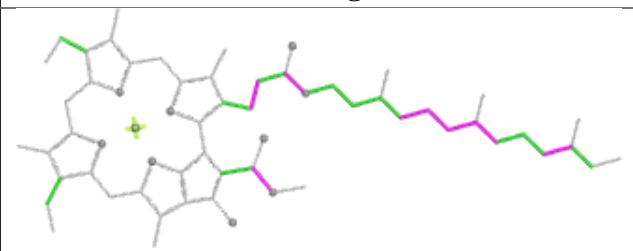
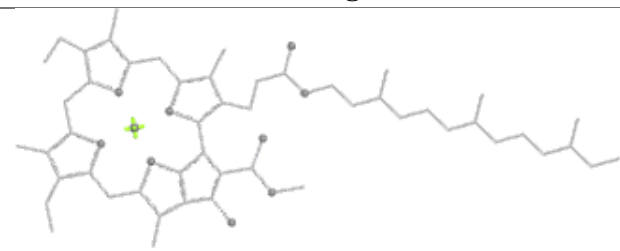
Torsions

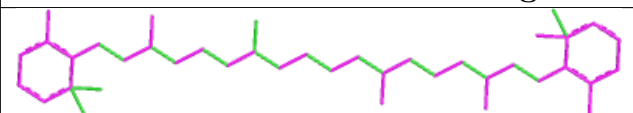
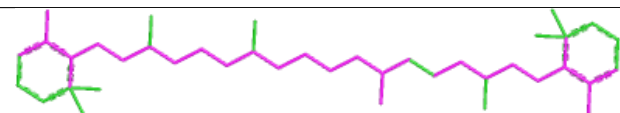
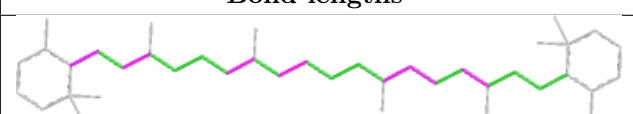
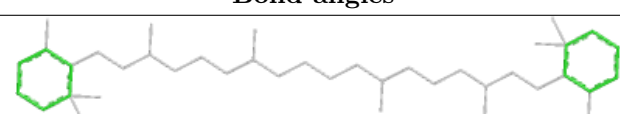


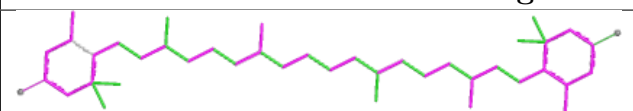
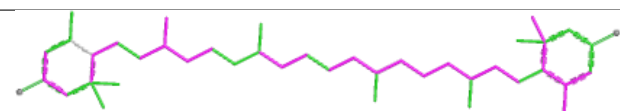
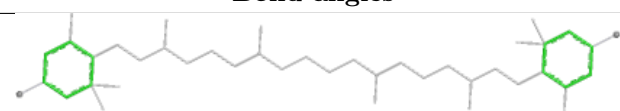
Rings

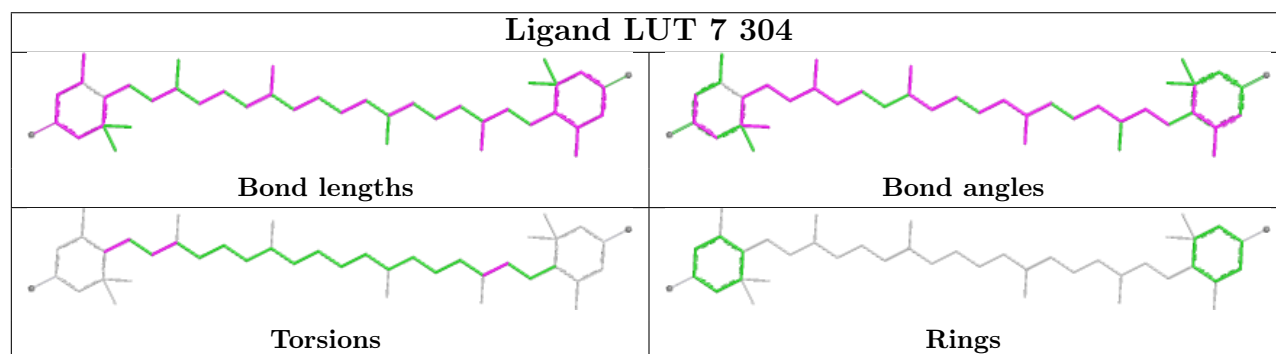
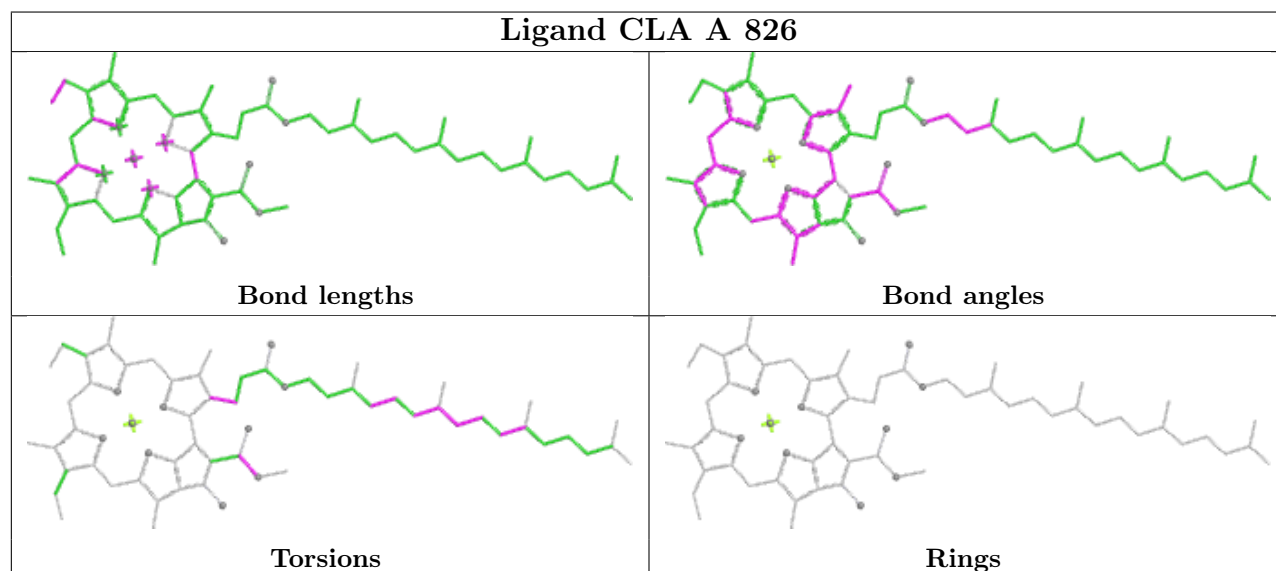
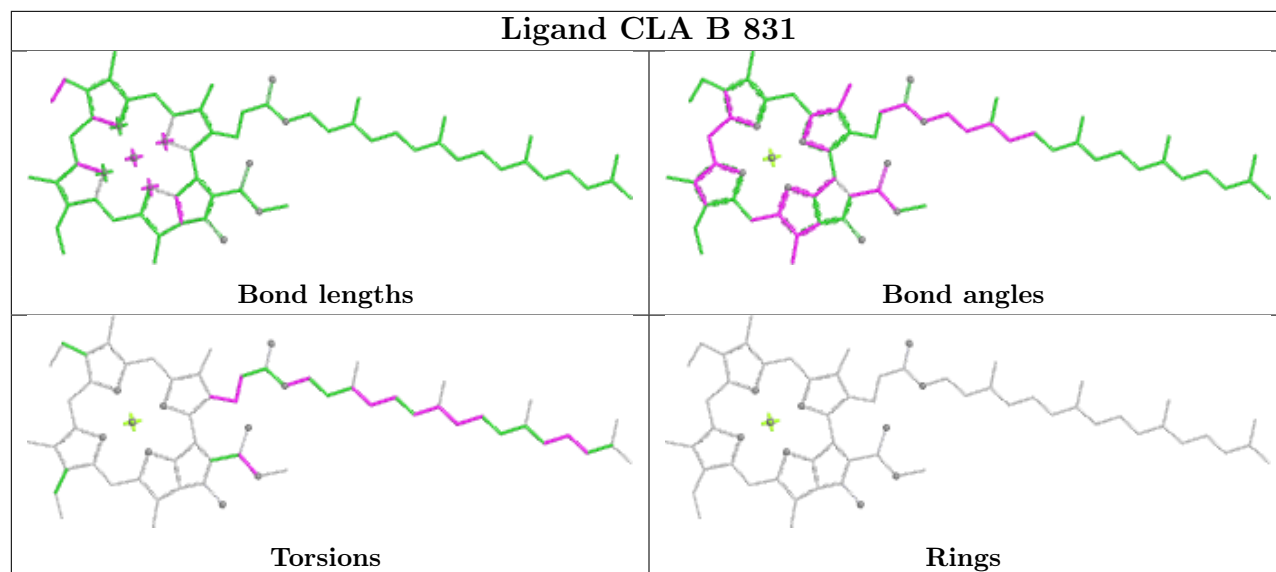


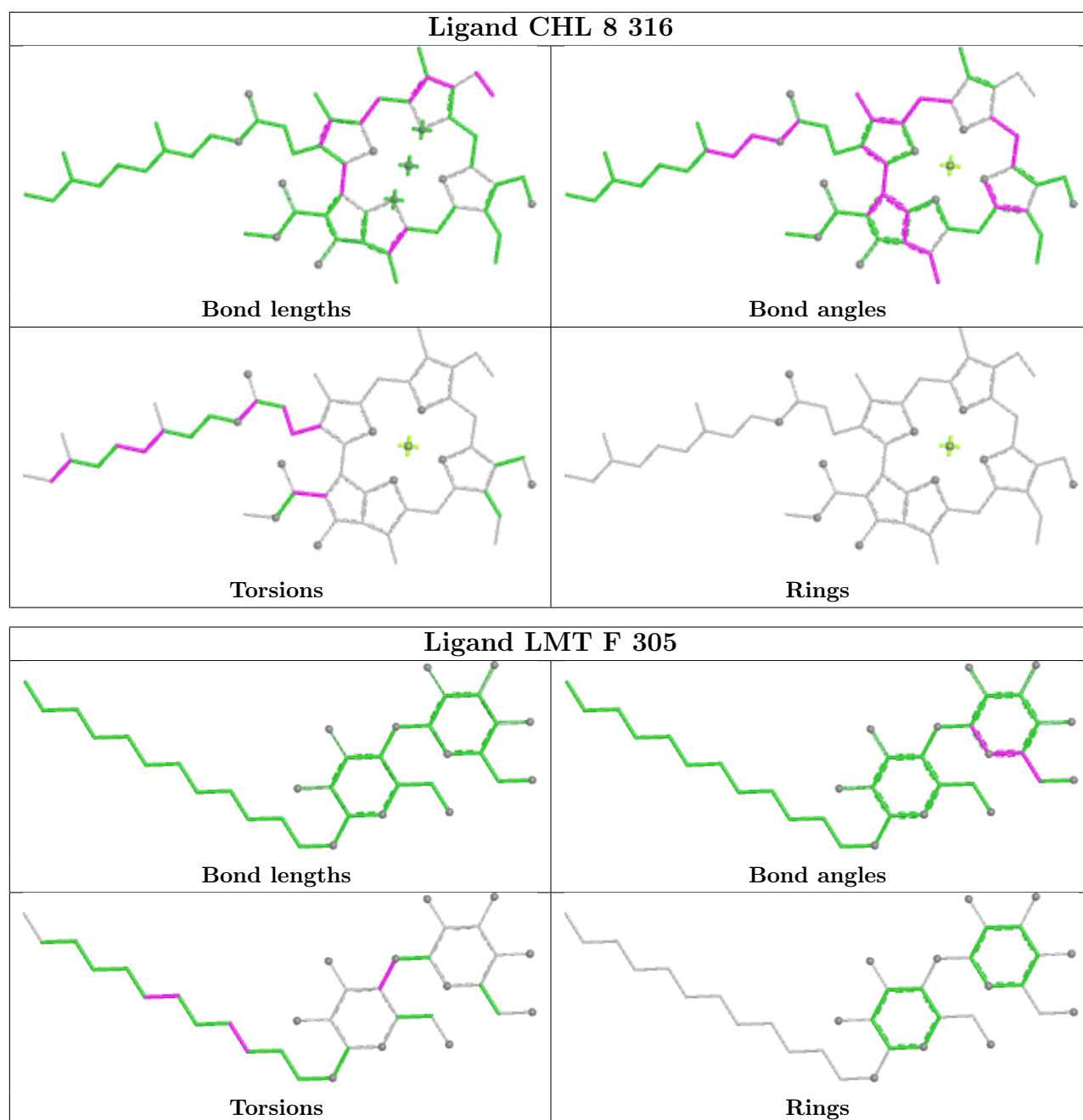


Ligand CLA 7 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

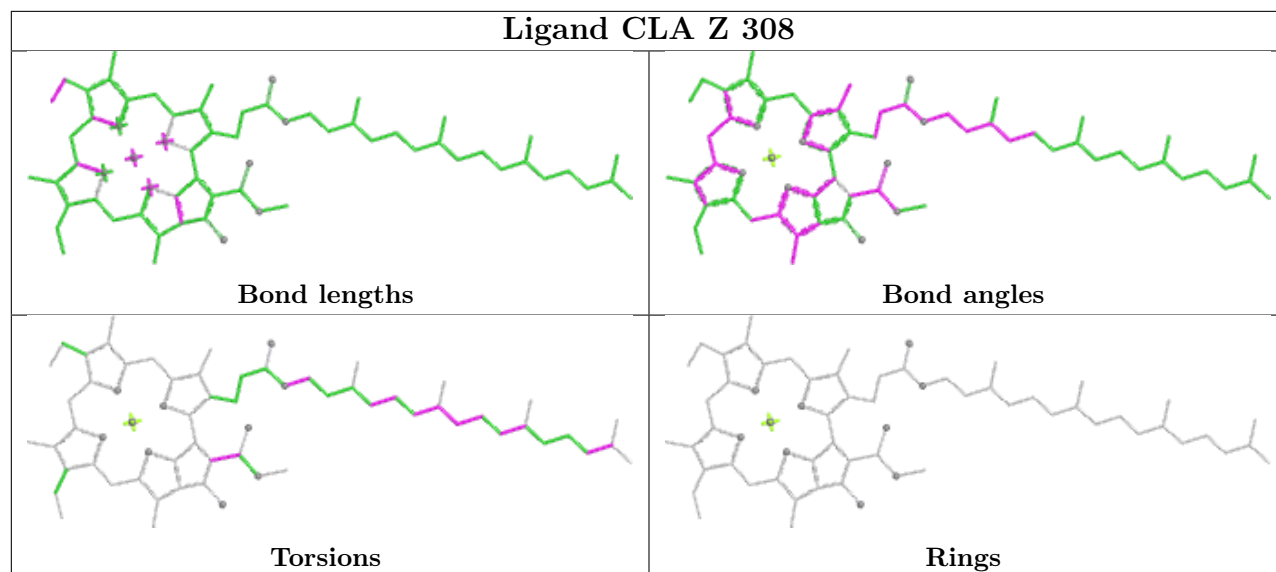
Ligand BCR B 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 3 5003	
	
Bond lengths	Bond angles
	
Torsions	Rings

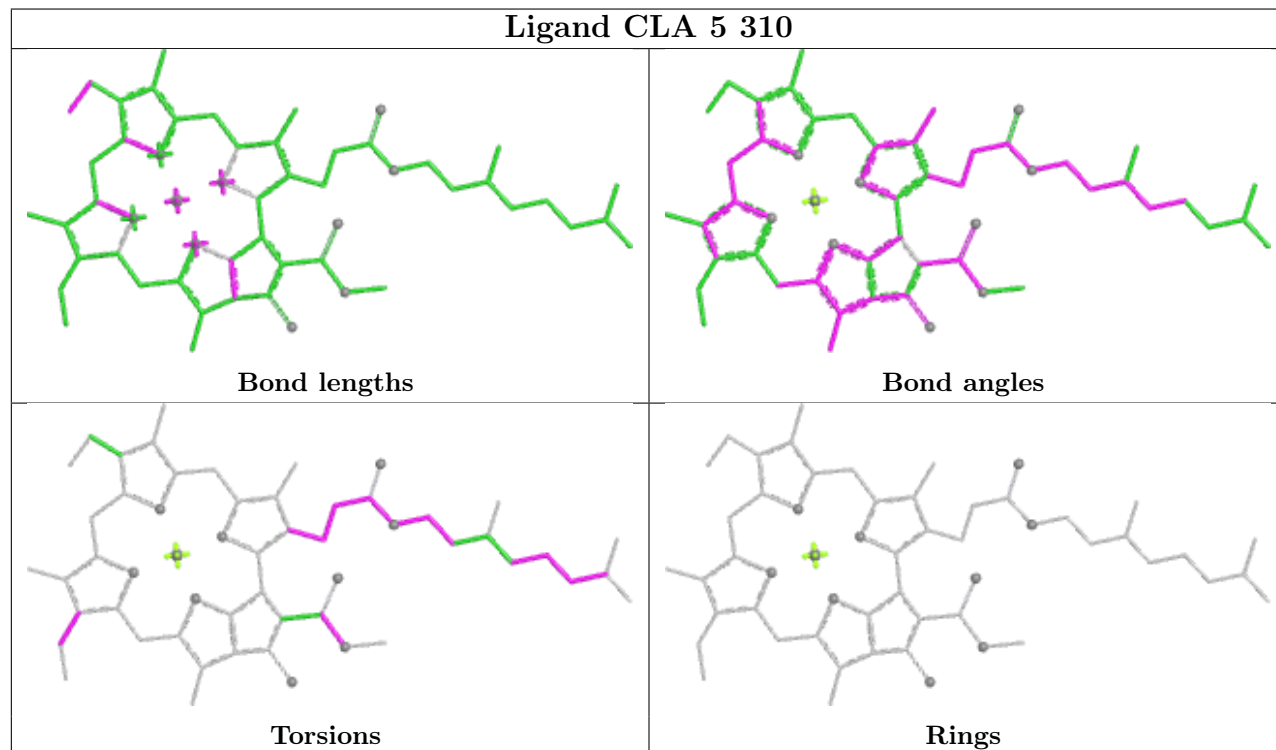


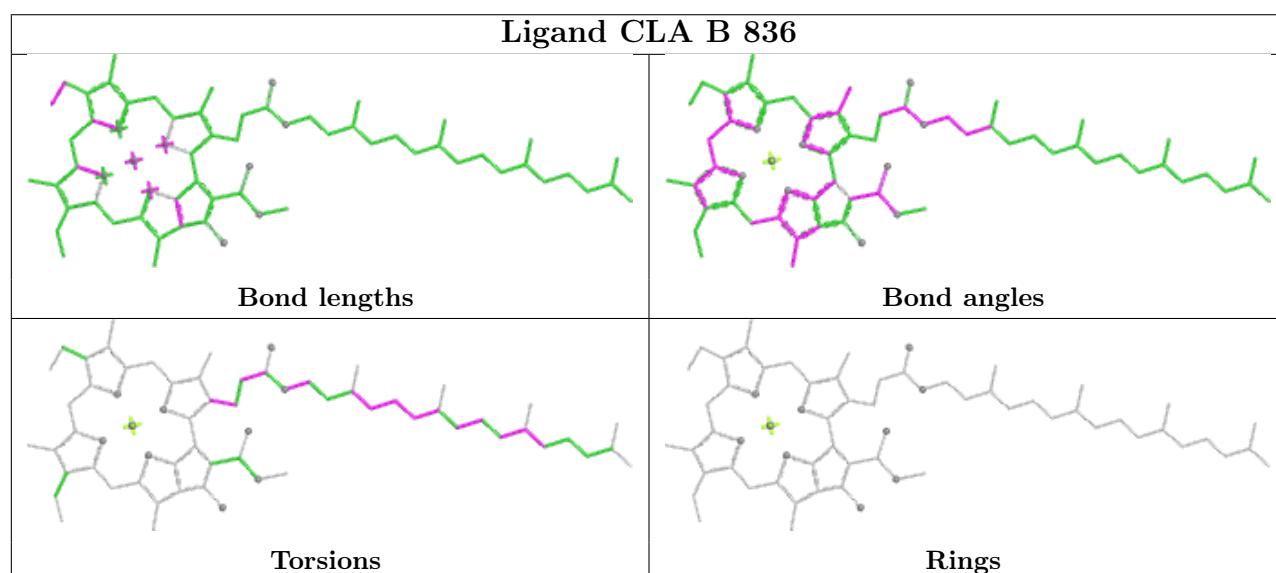
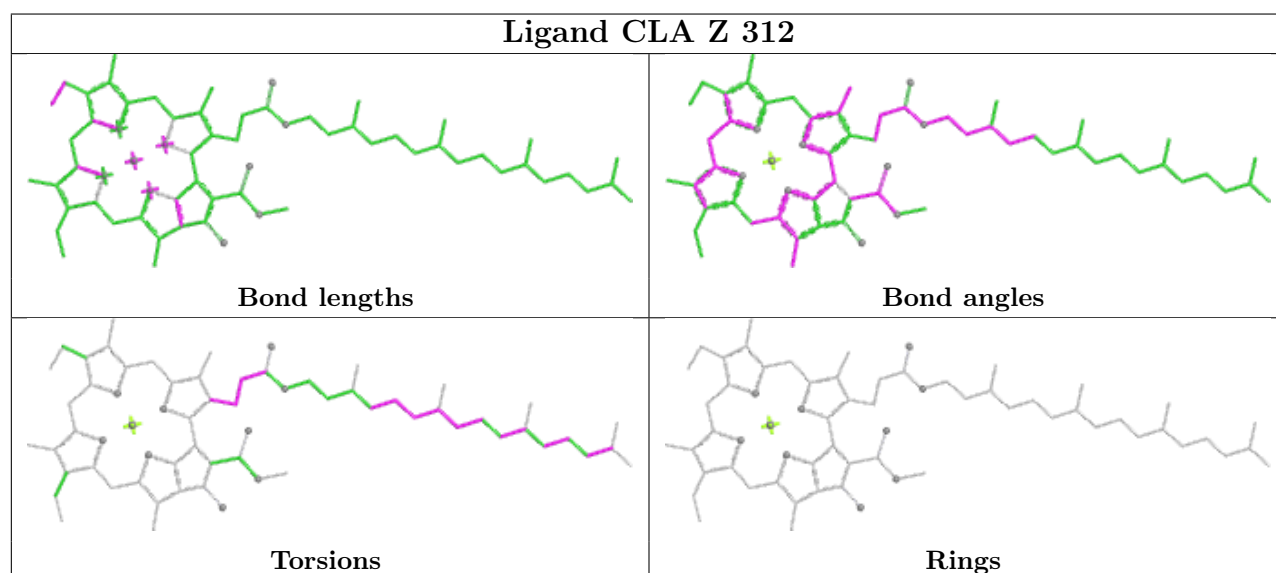
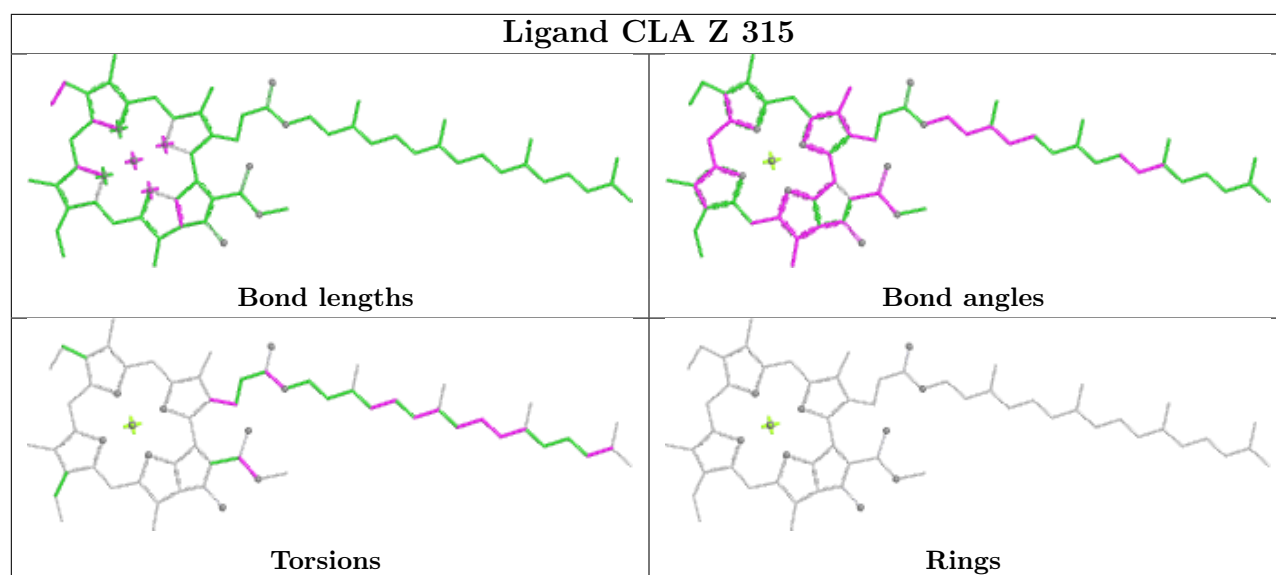


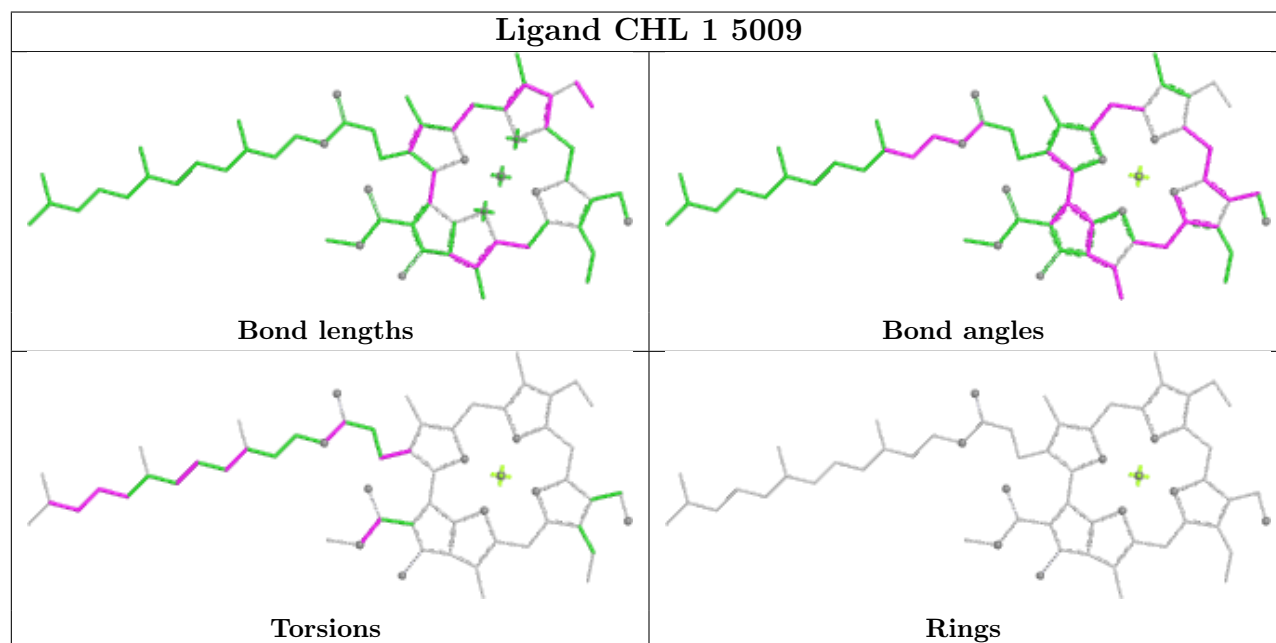
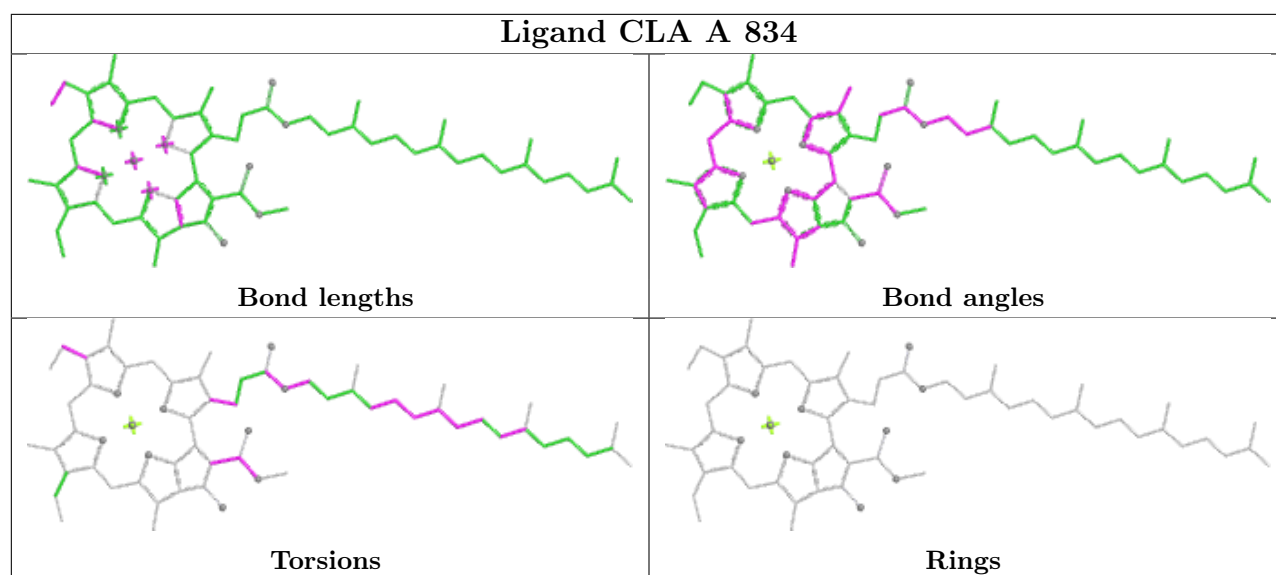
Ligand CLA Z 308

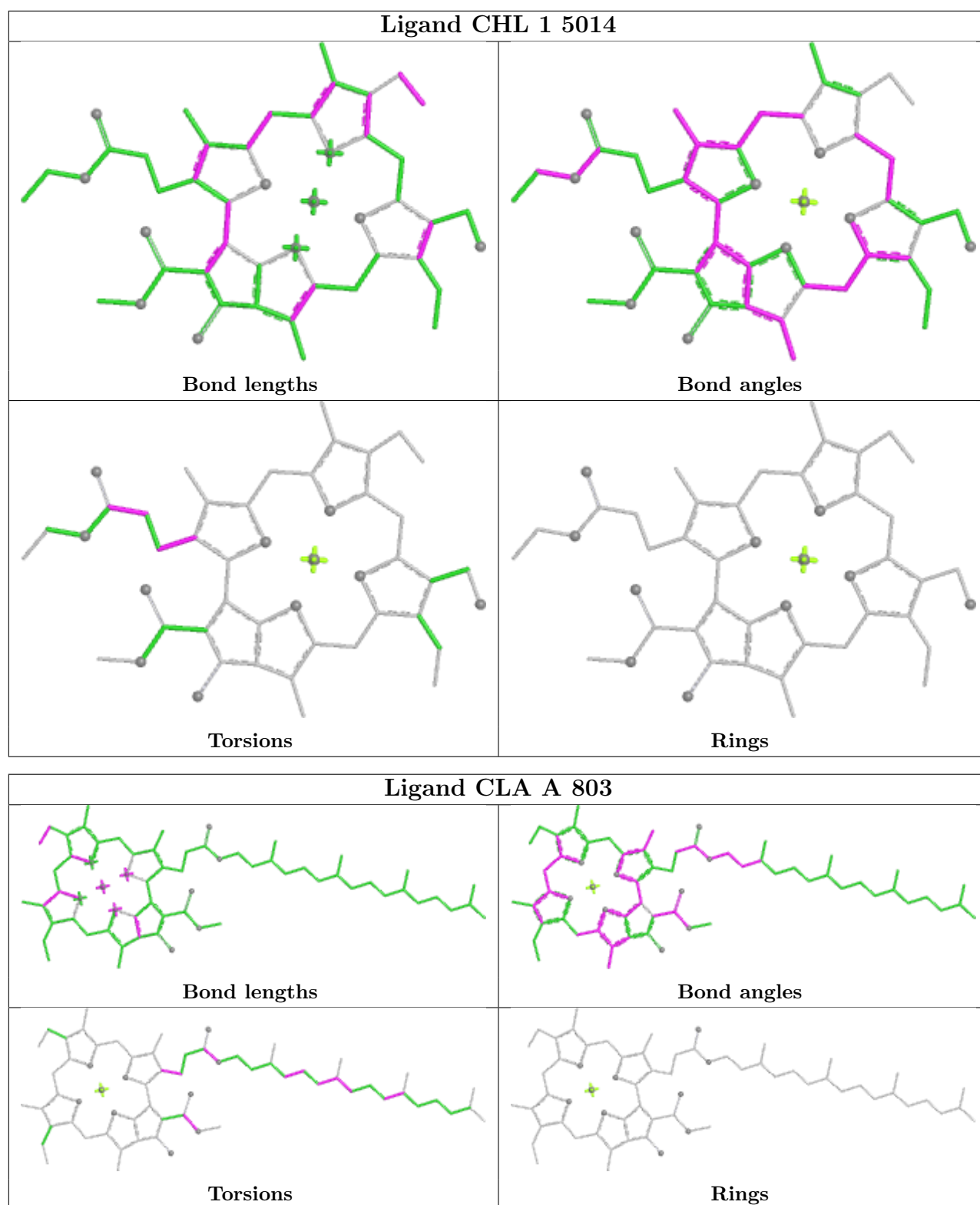


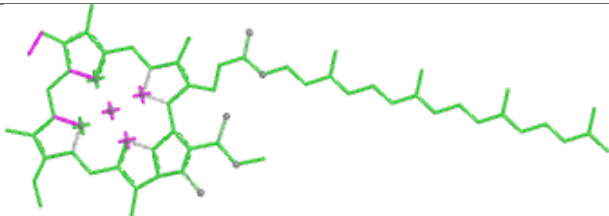
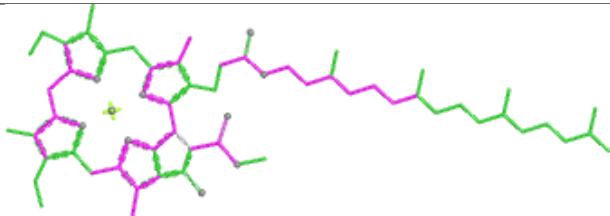
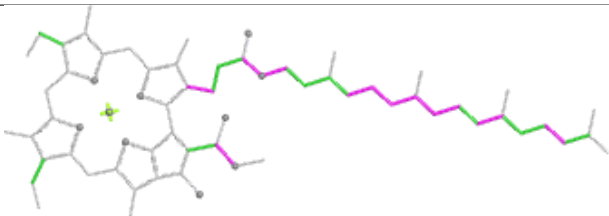
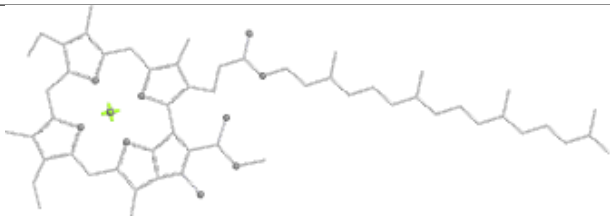
Ligand CLA 5 310

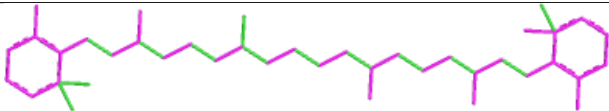
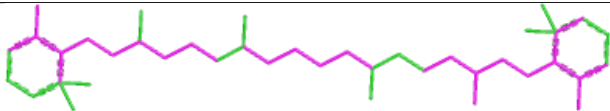
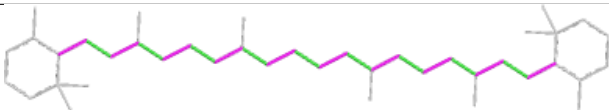
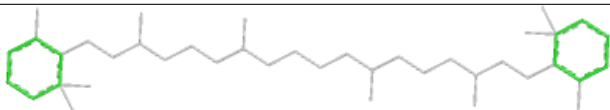


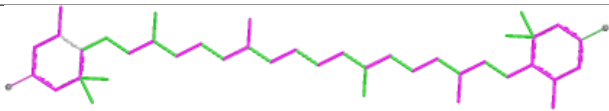
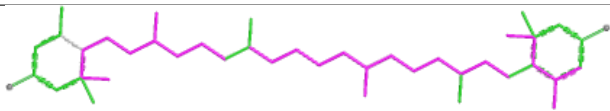
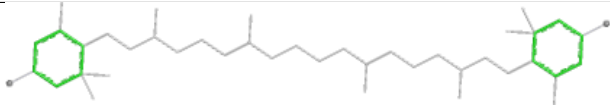




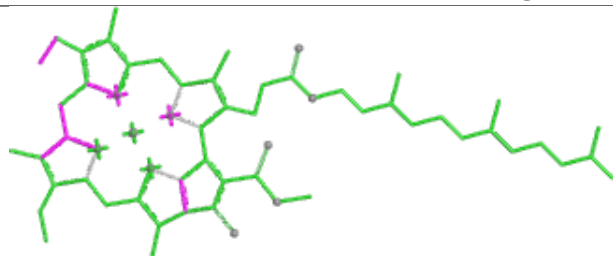


Ligand CLA B 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

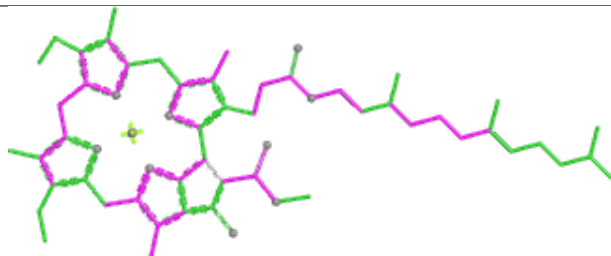
Ligand BCR 7 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 1 5004	
	
Bond lengths	Bond angles
	
Torsions	Rings

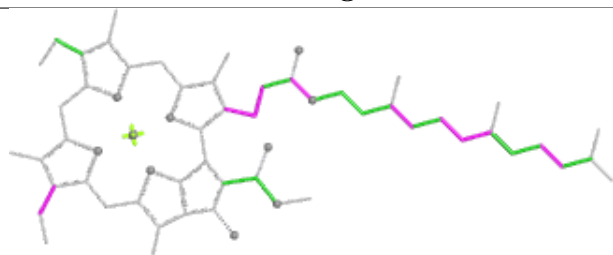
Ligand CLA 8 312



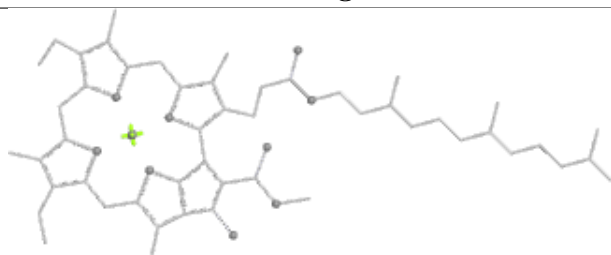
Bond lengths



Bond angles

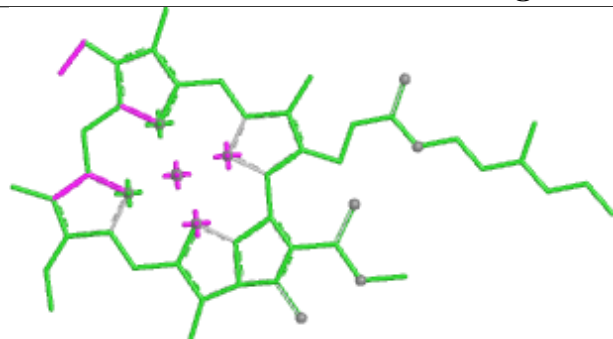


Torsions

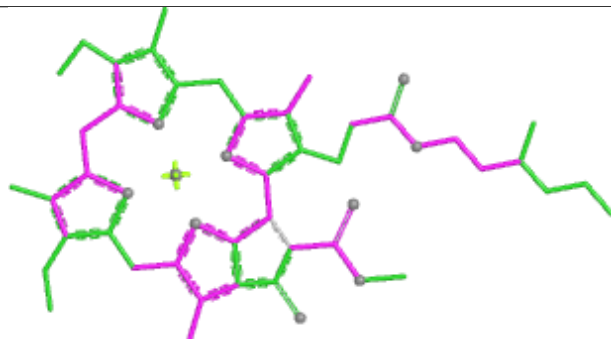


Rings

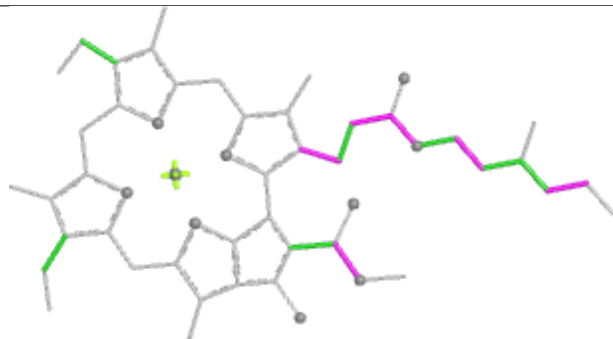
Ligand CLA B 810



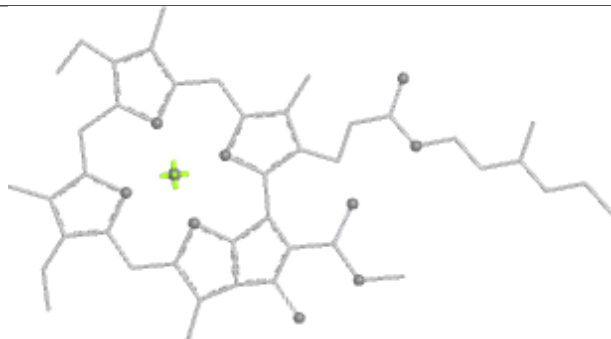
Bond lengths



Bond angles

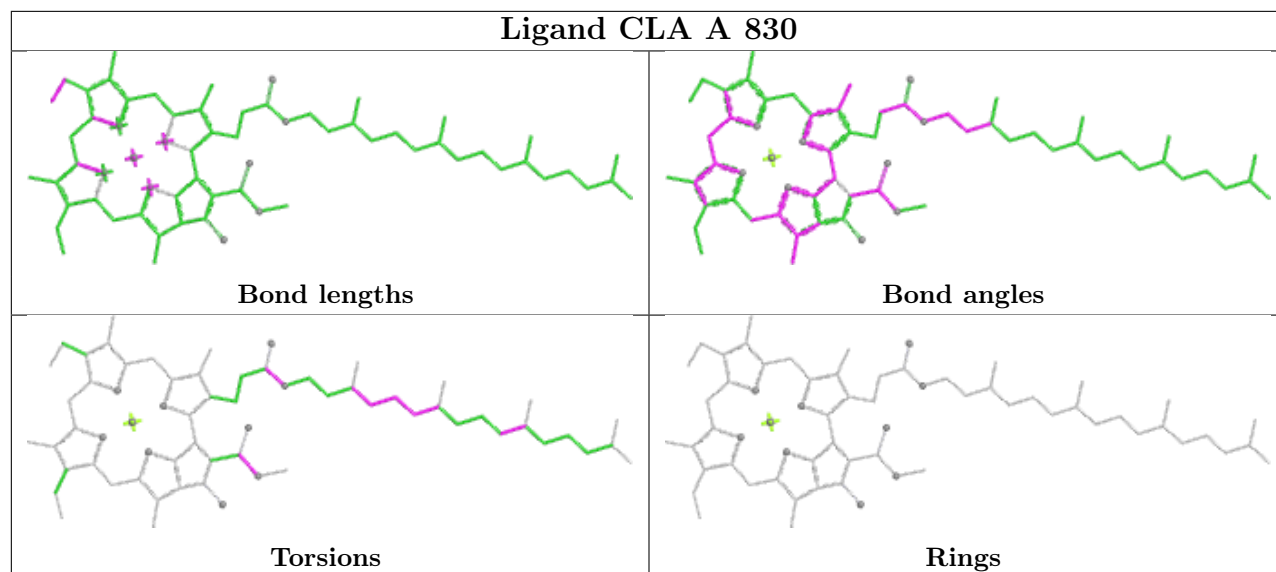


Torsions

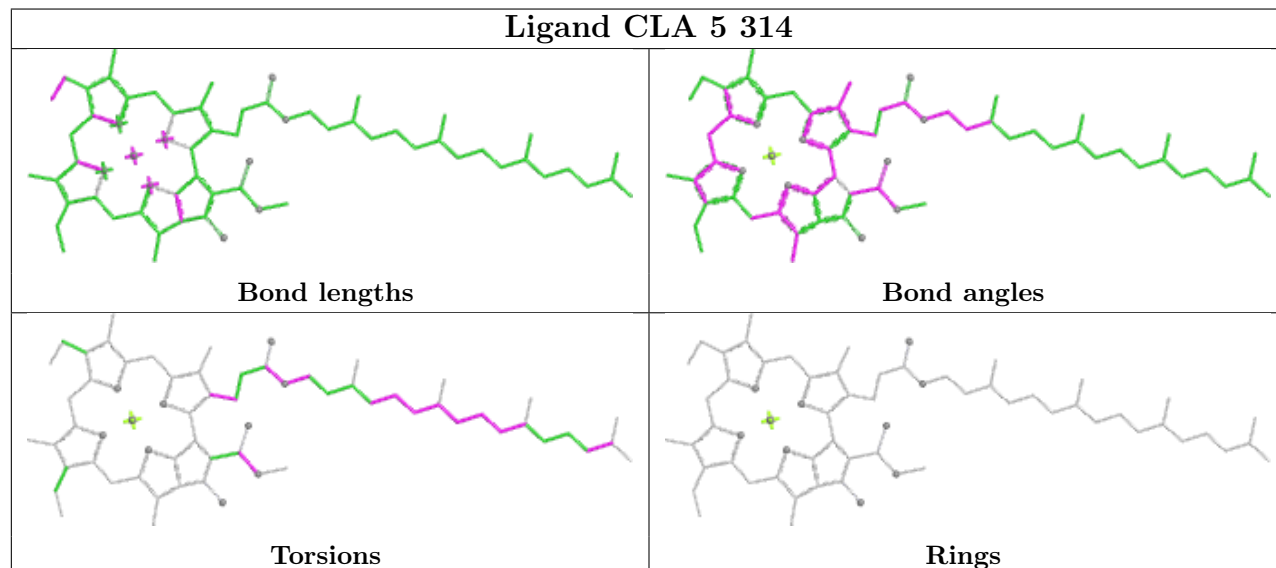


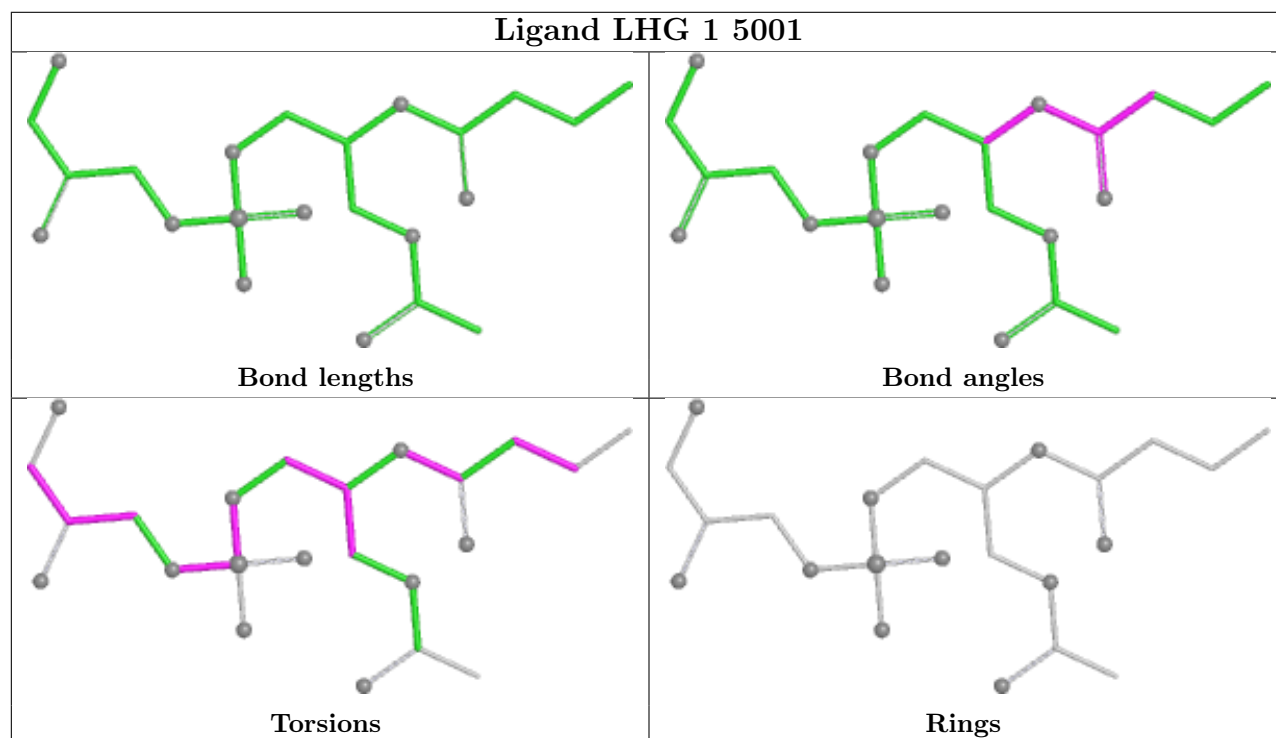
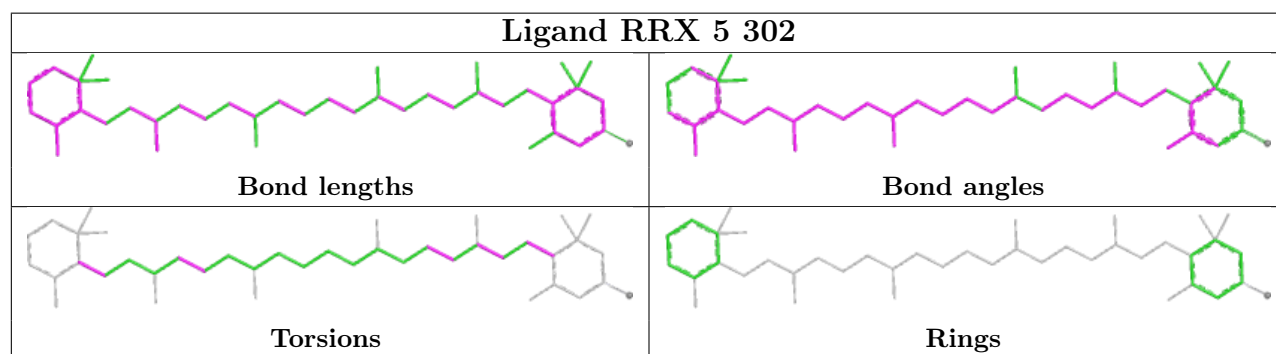
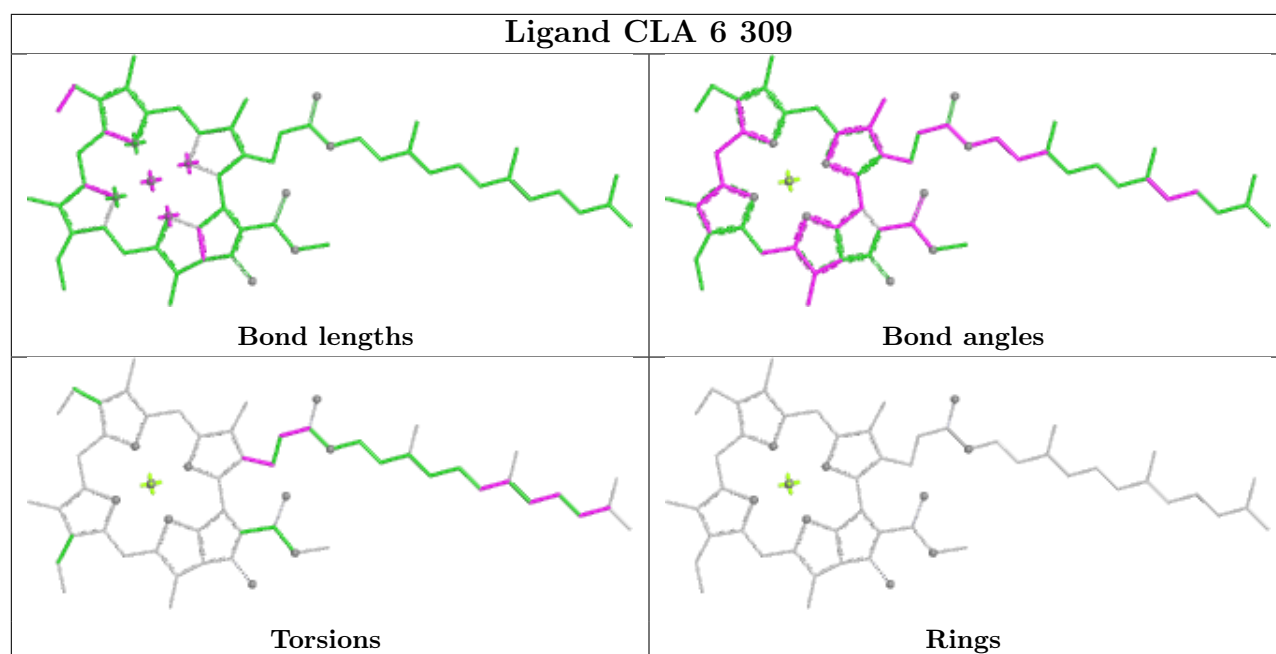
Rings

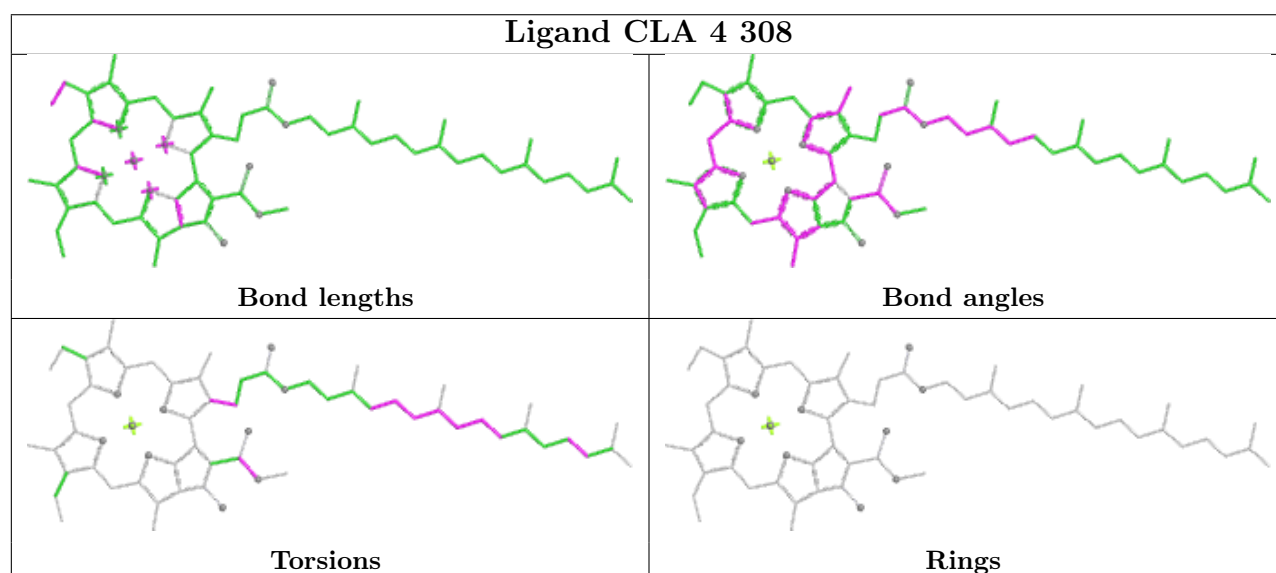
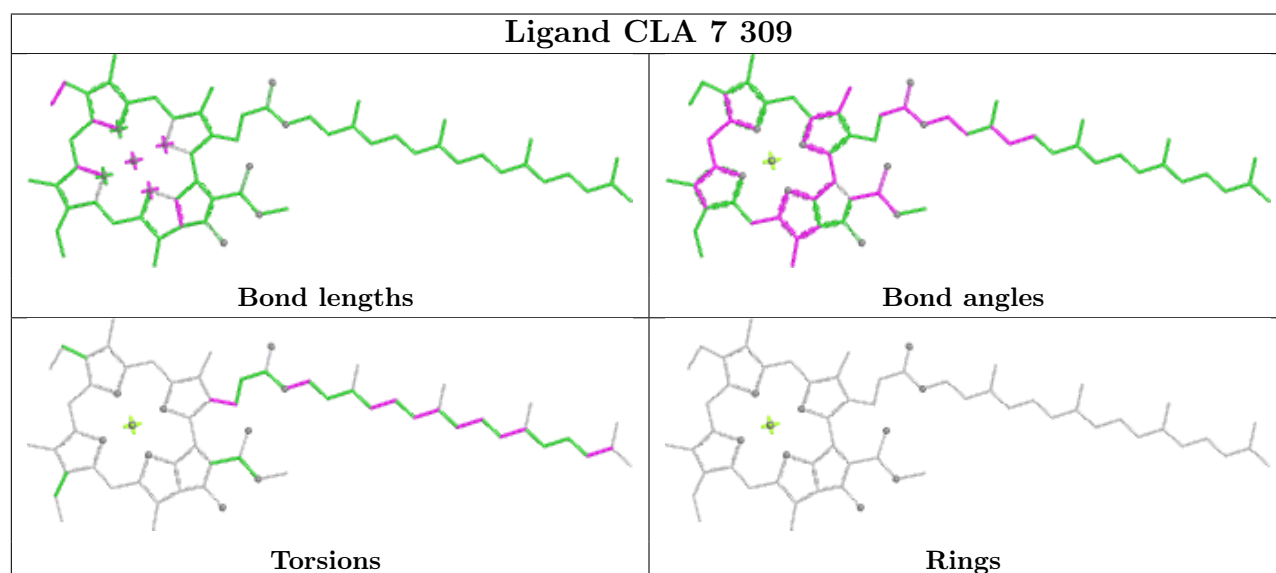
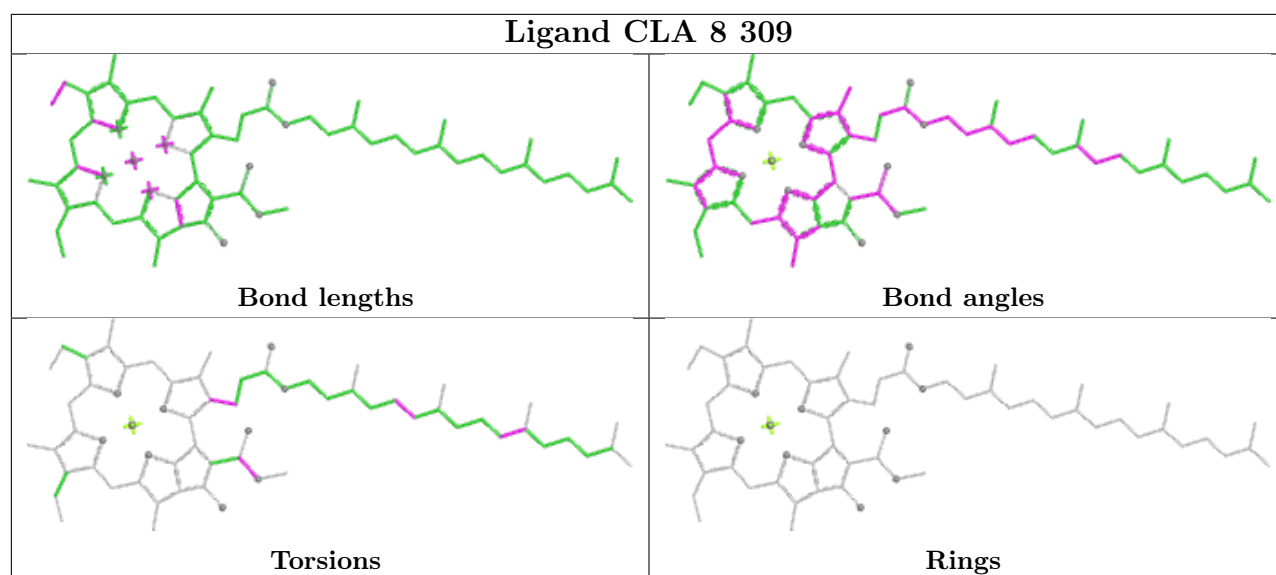
Ligand CLA A 830

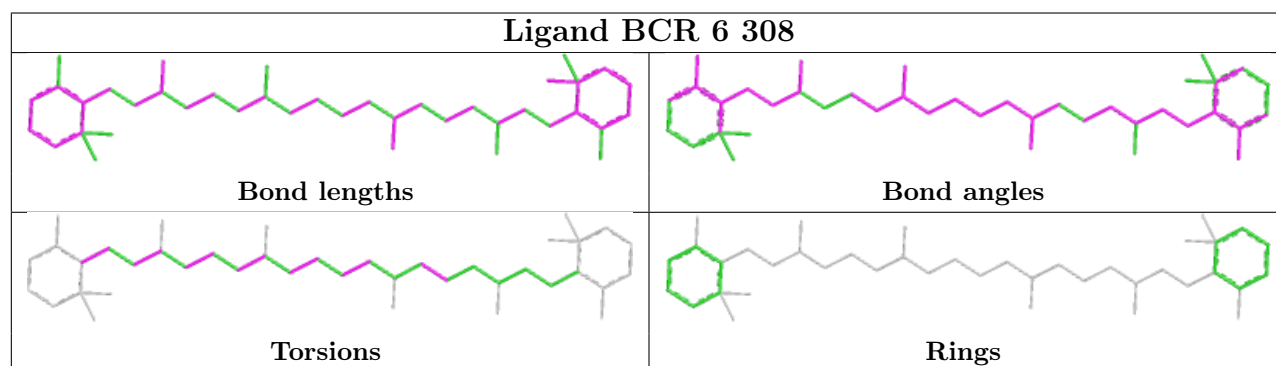
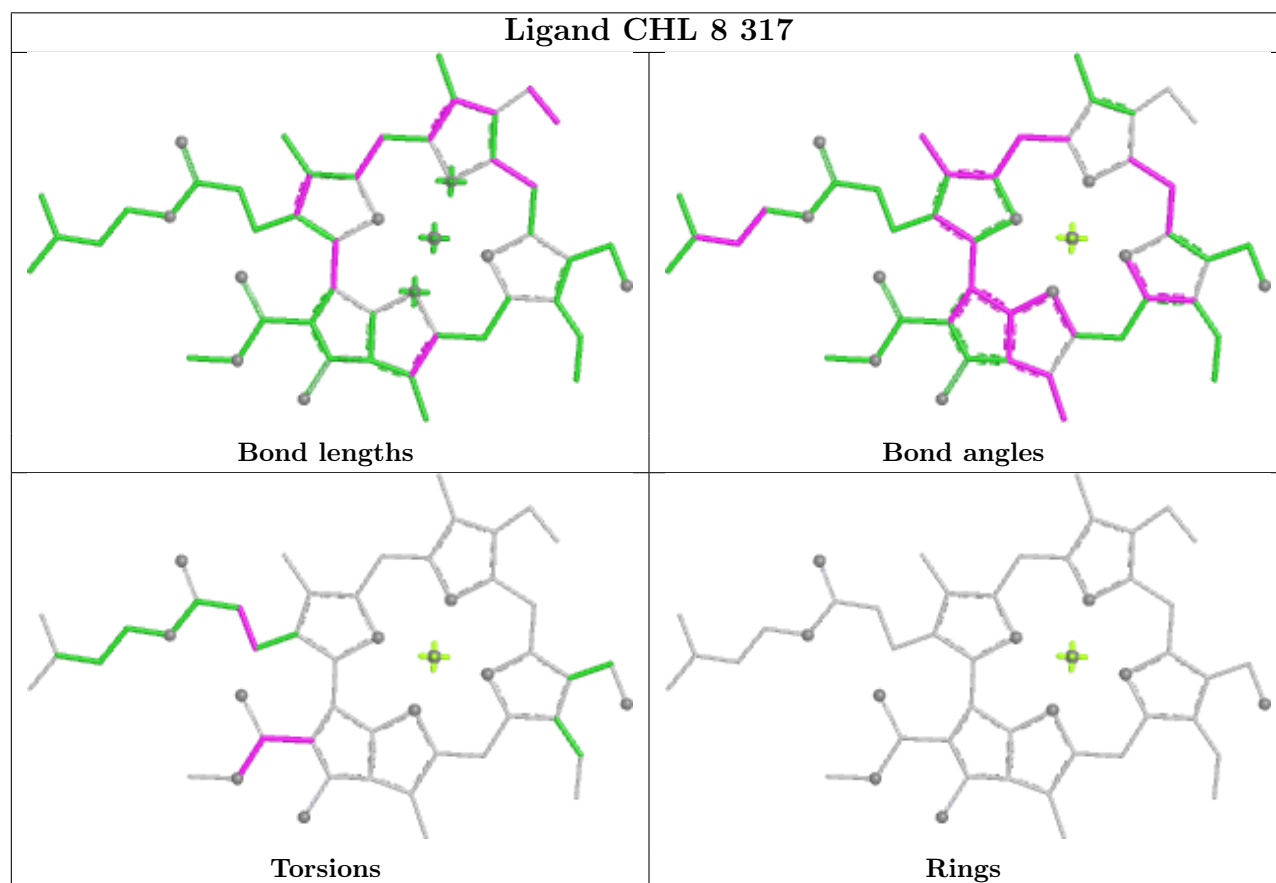
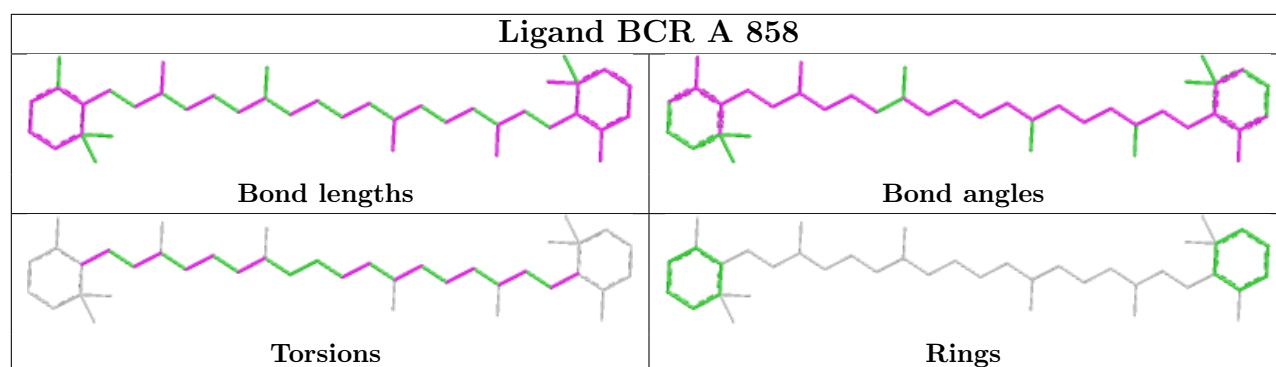


Ligand CLA 5 314

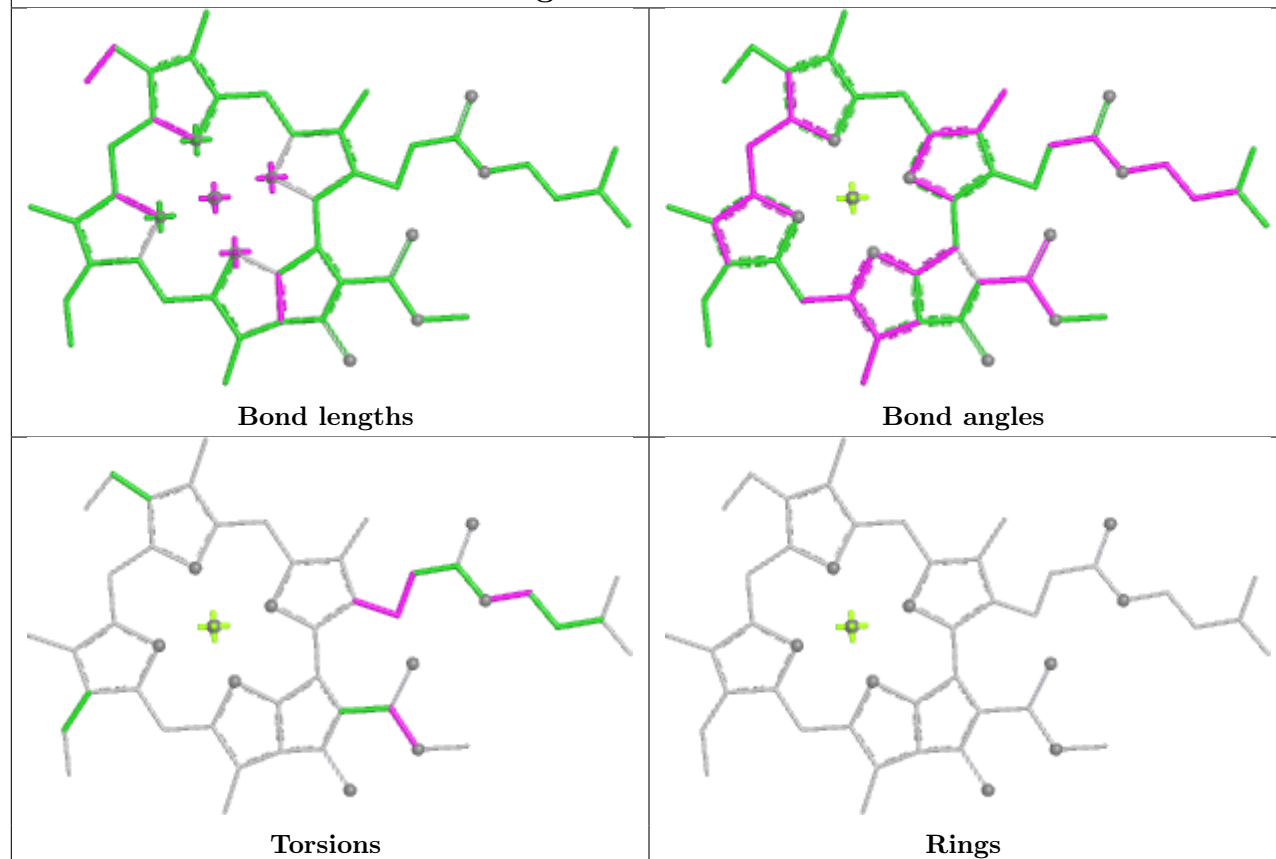




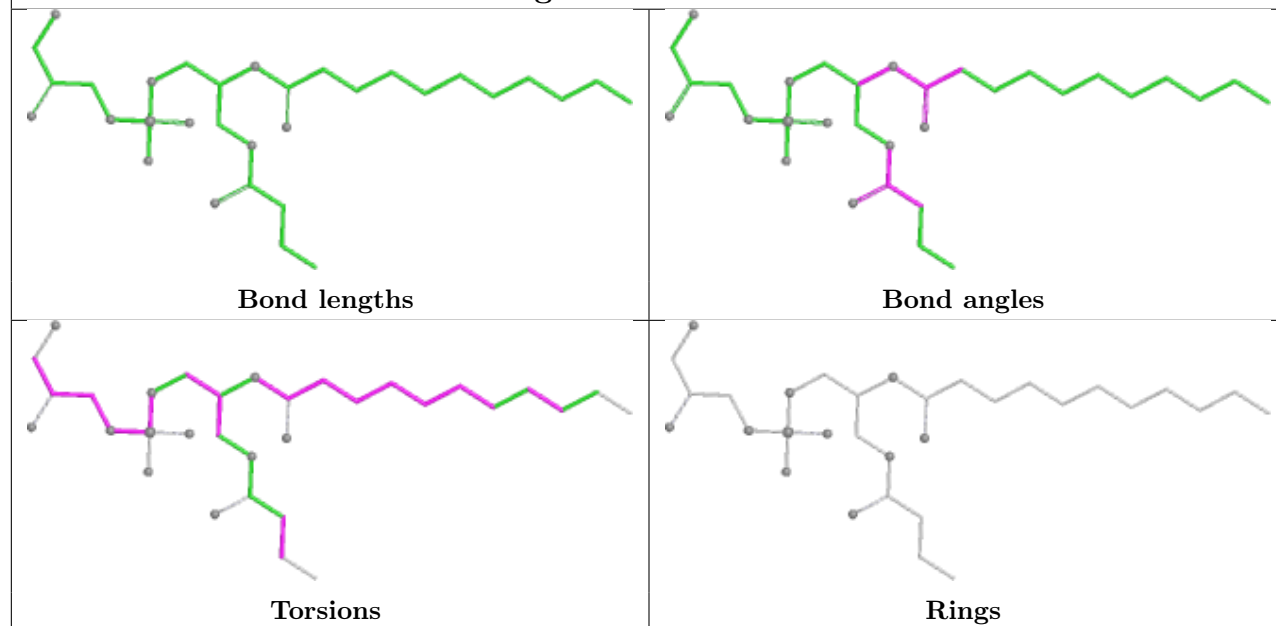


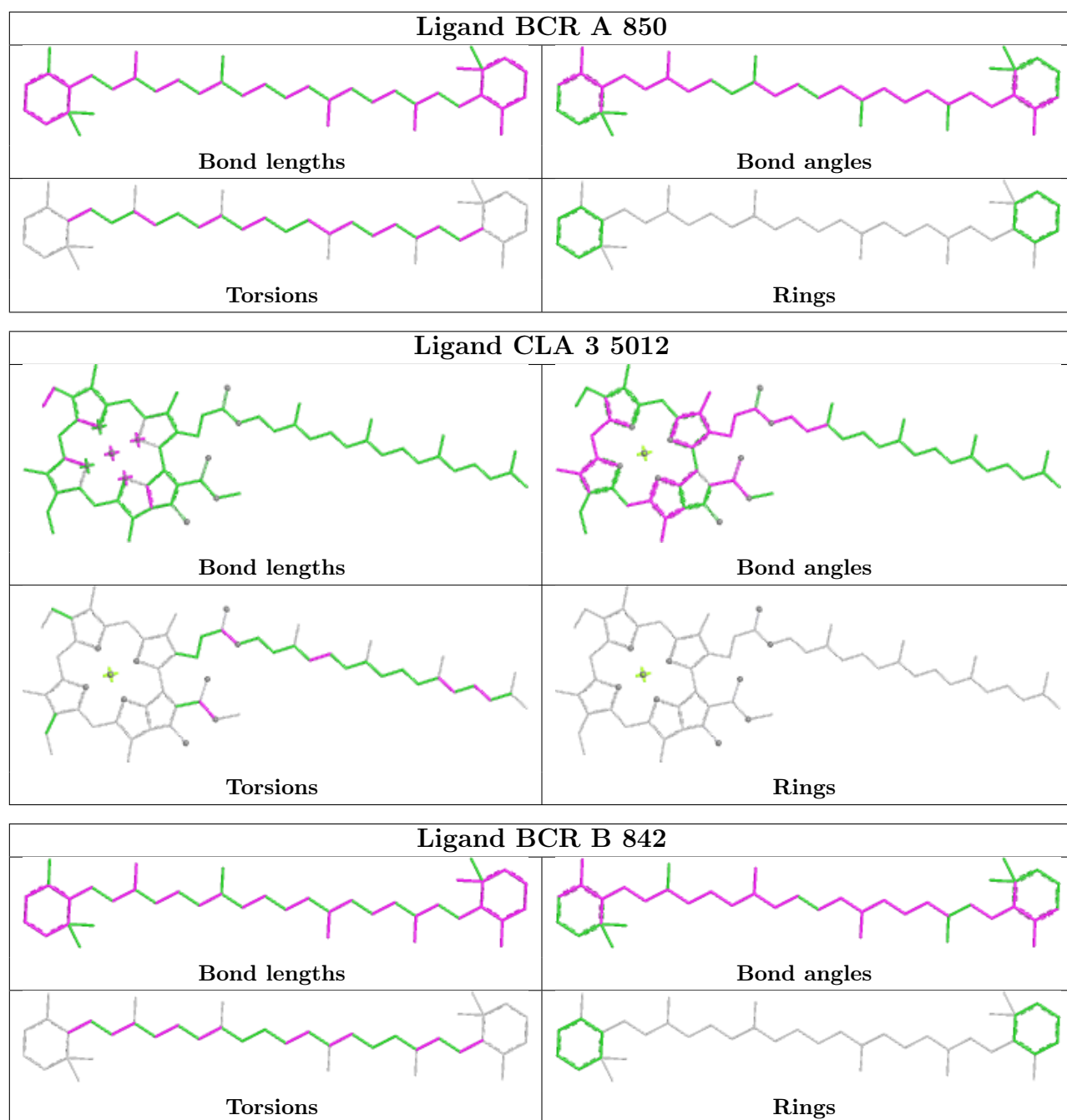


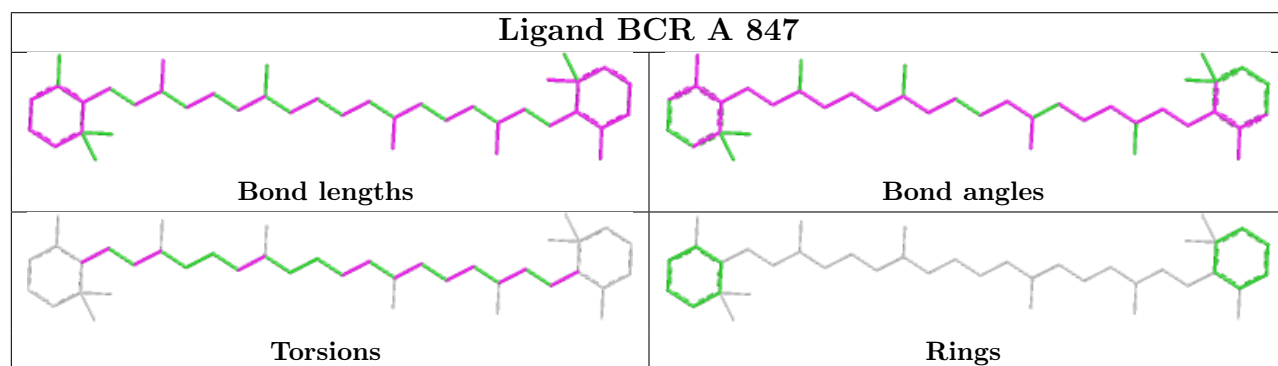
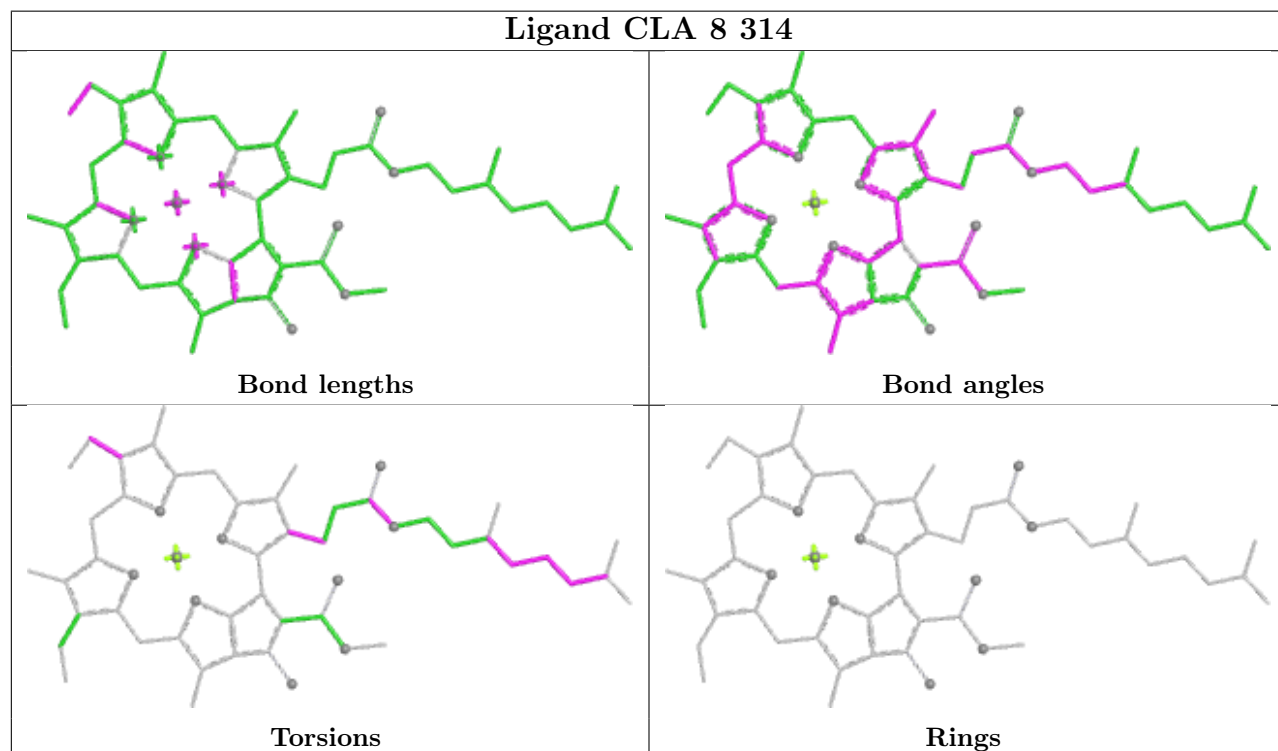
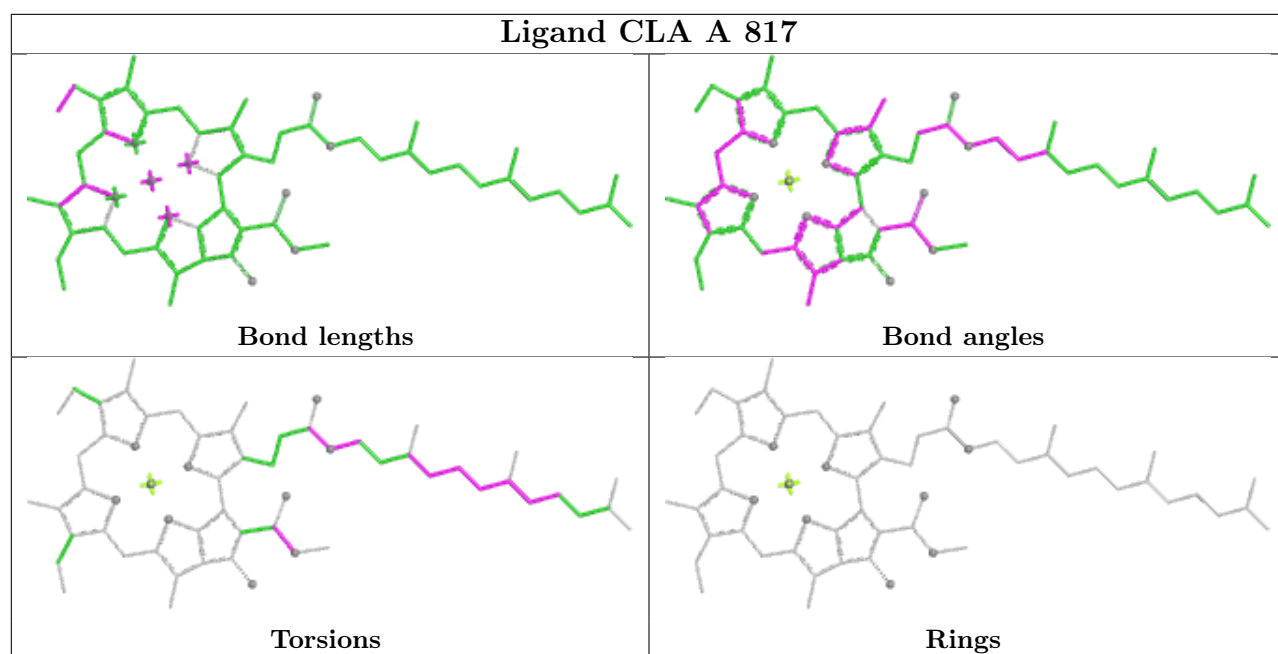
Ligand CLA 7 317



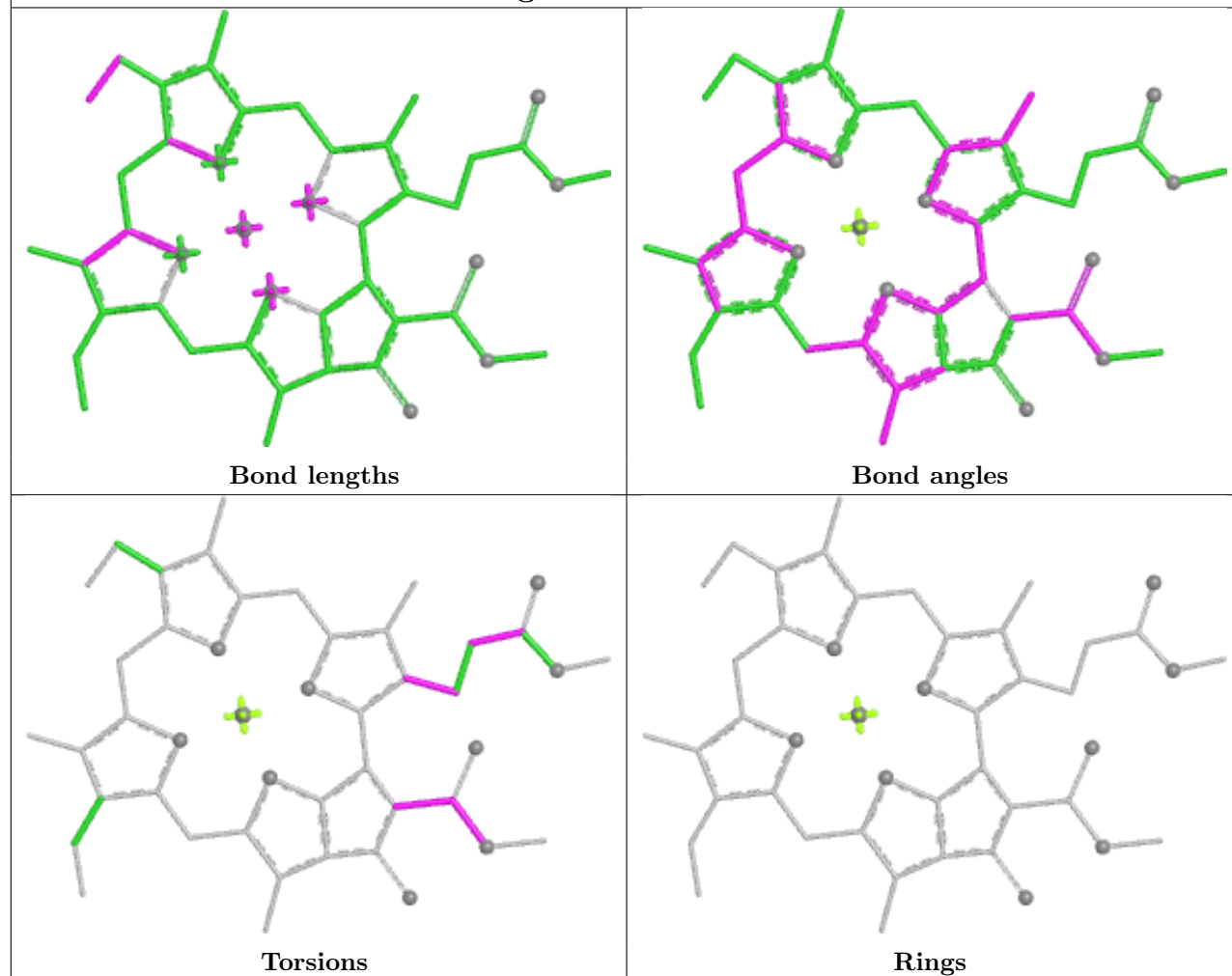
Ligand LHG 6 303

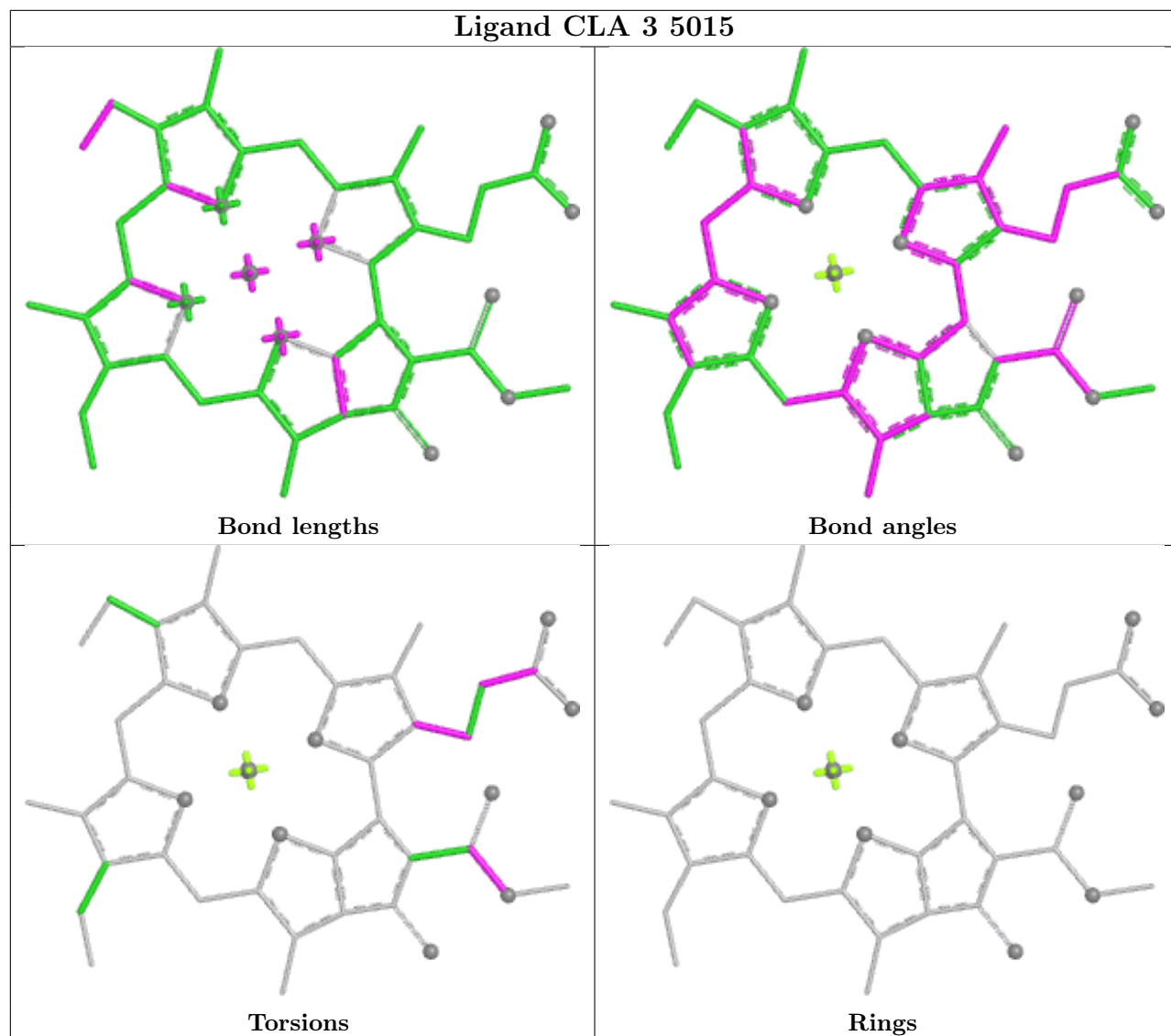


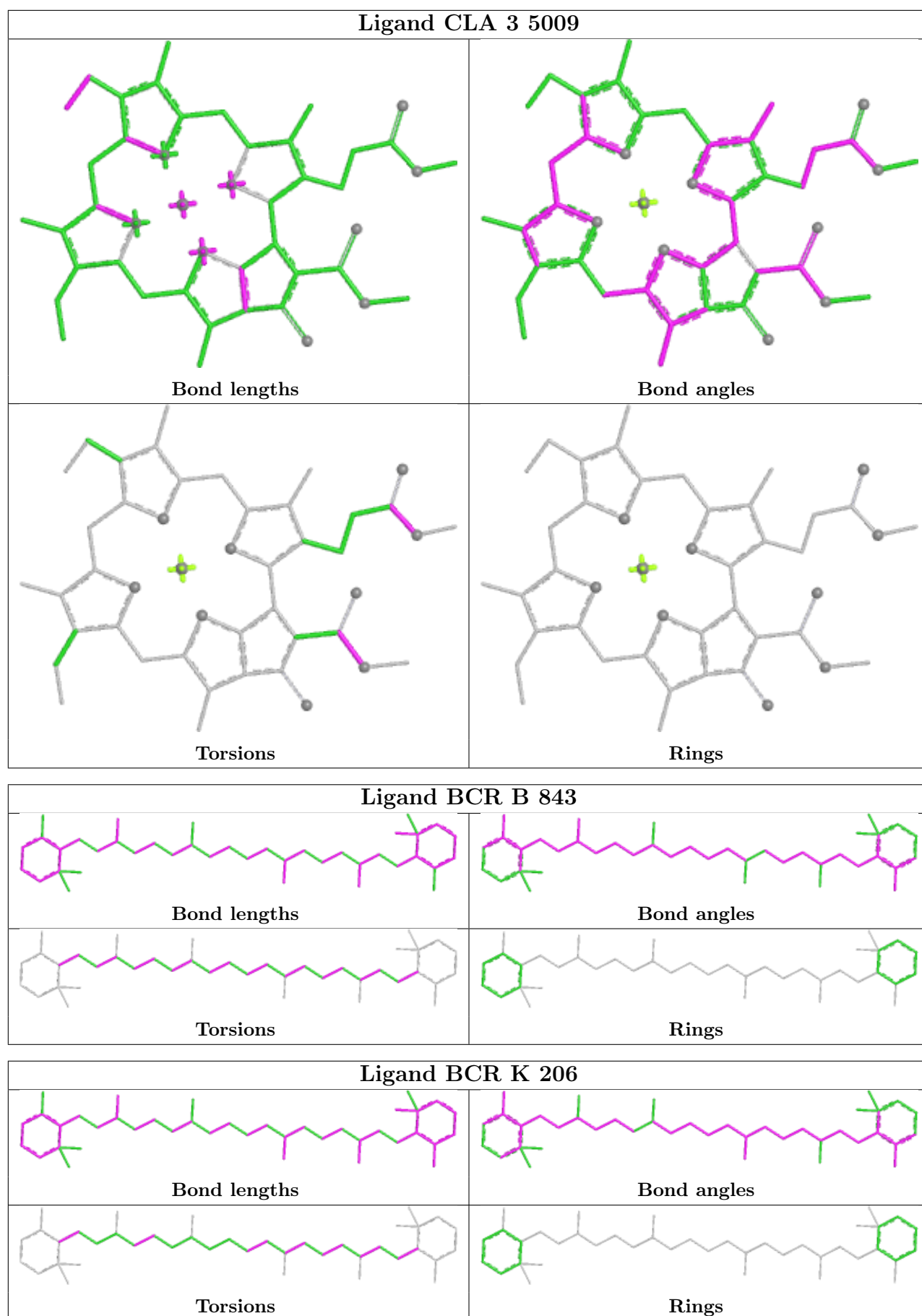


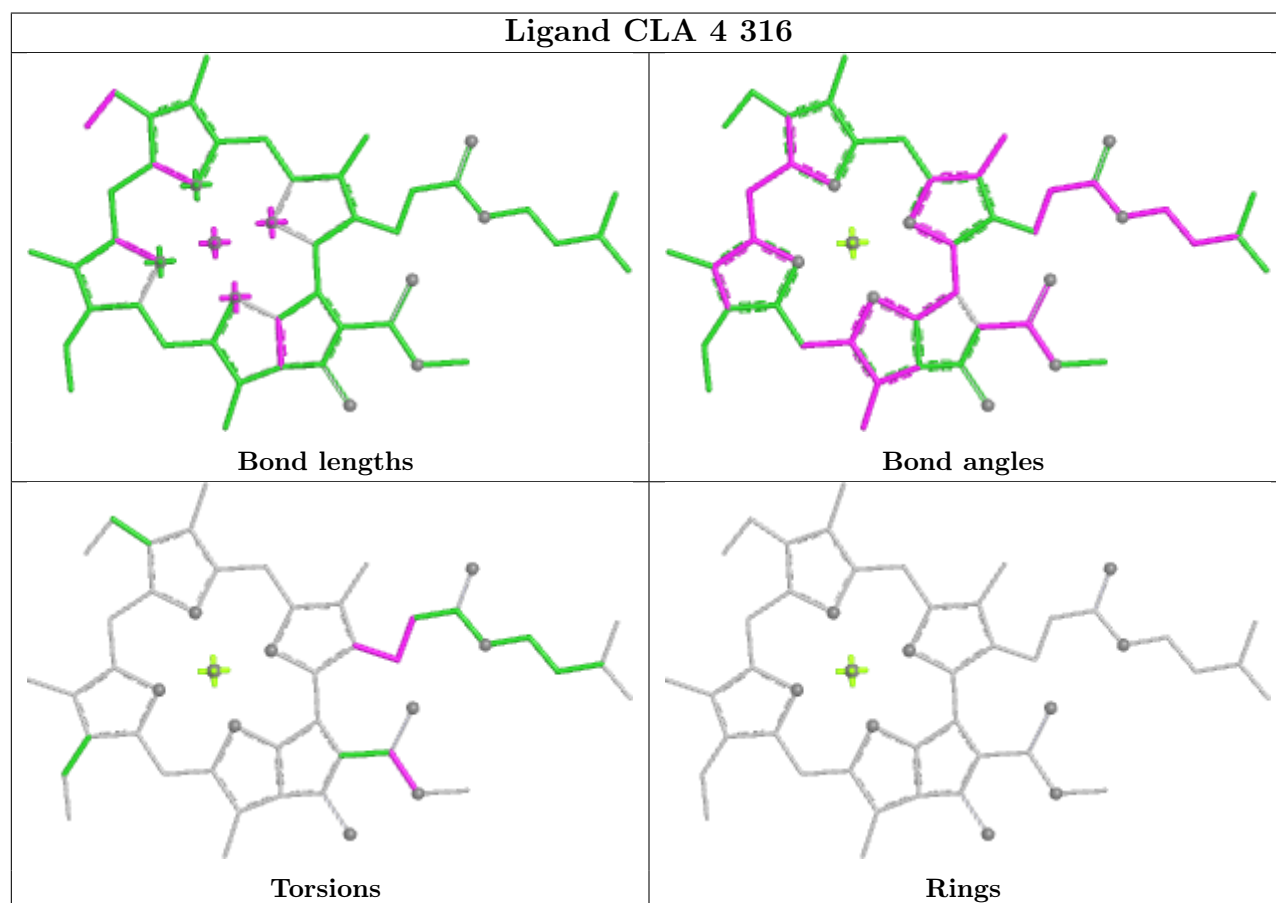
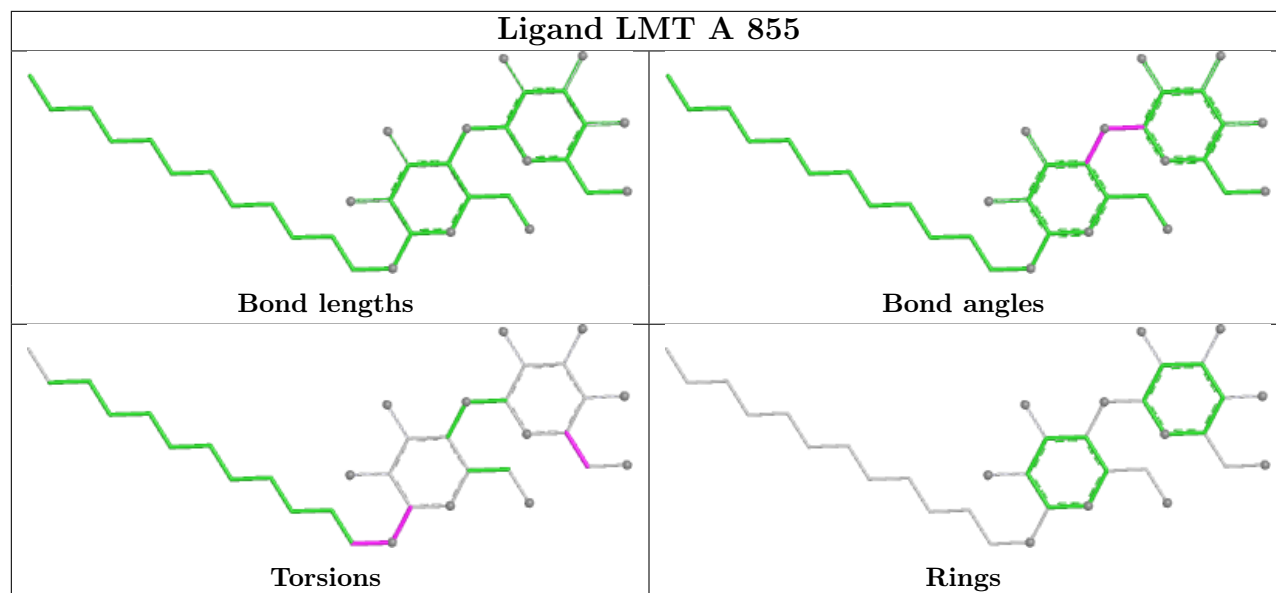


Ligand CLA 5 322

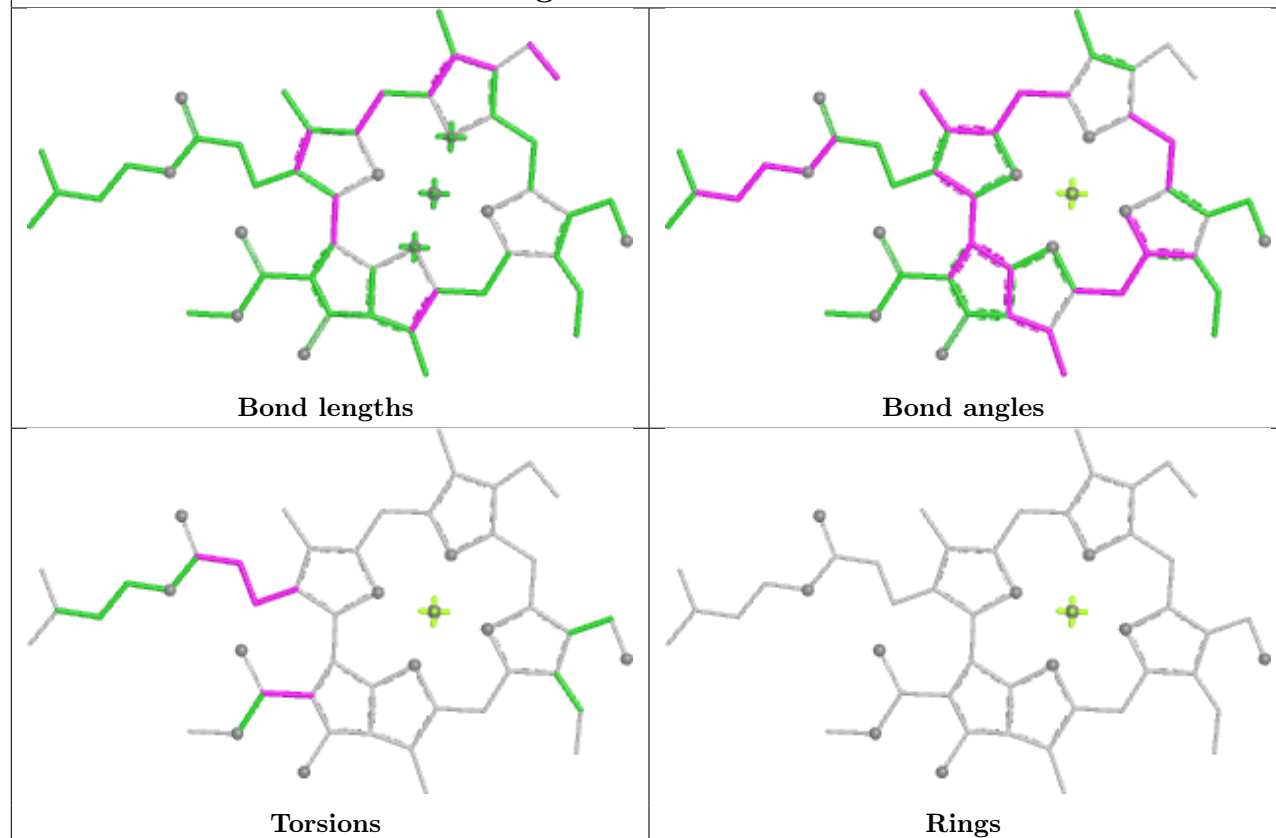




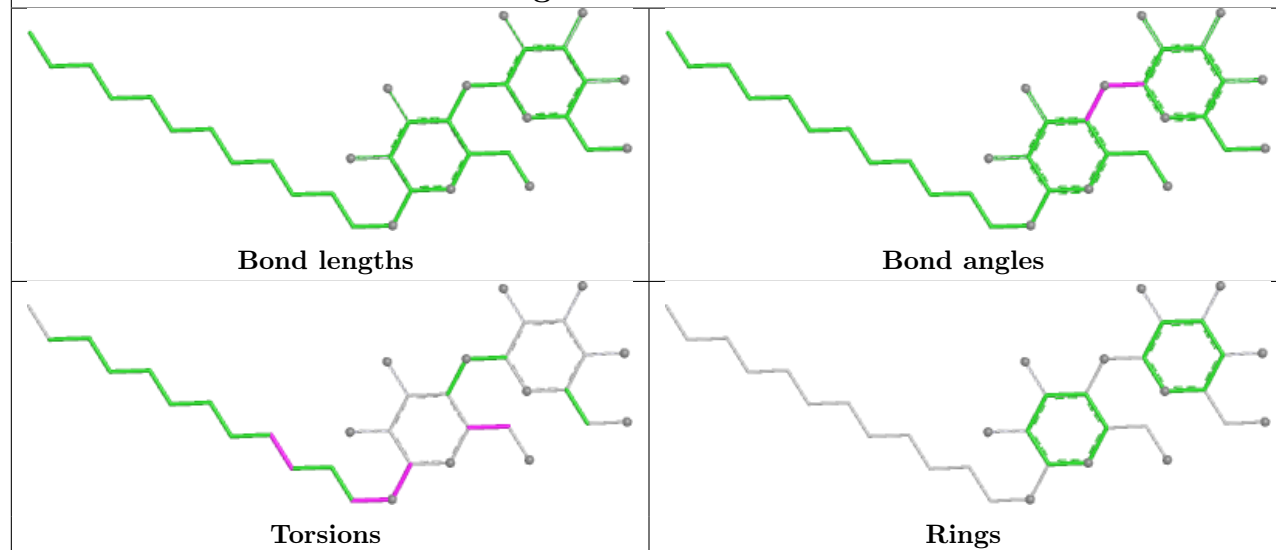




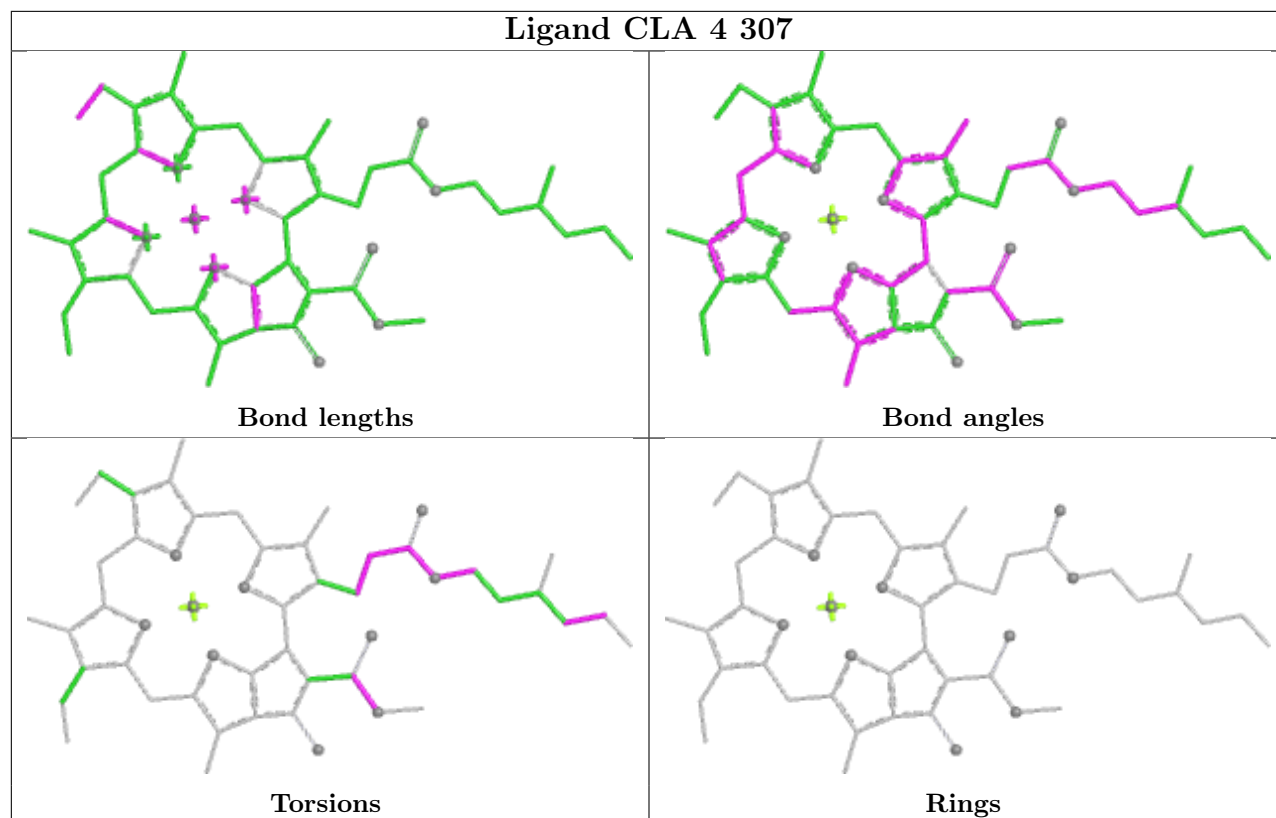
Ligand CHL 4 314



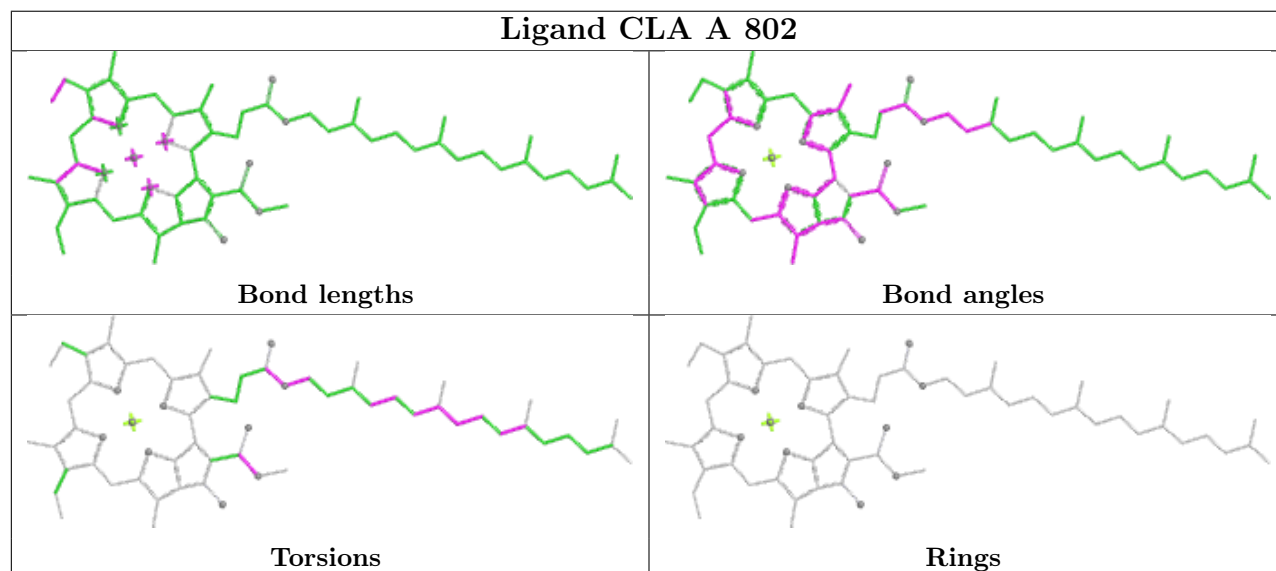
Ligand LMT 4 322

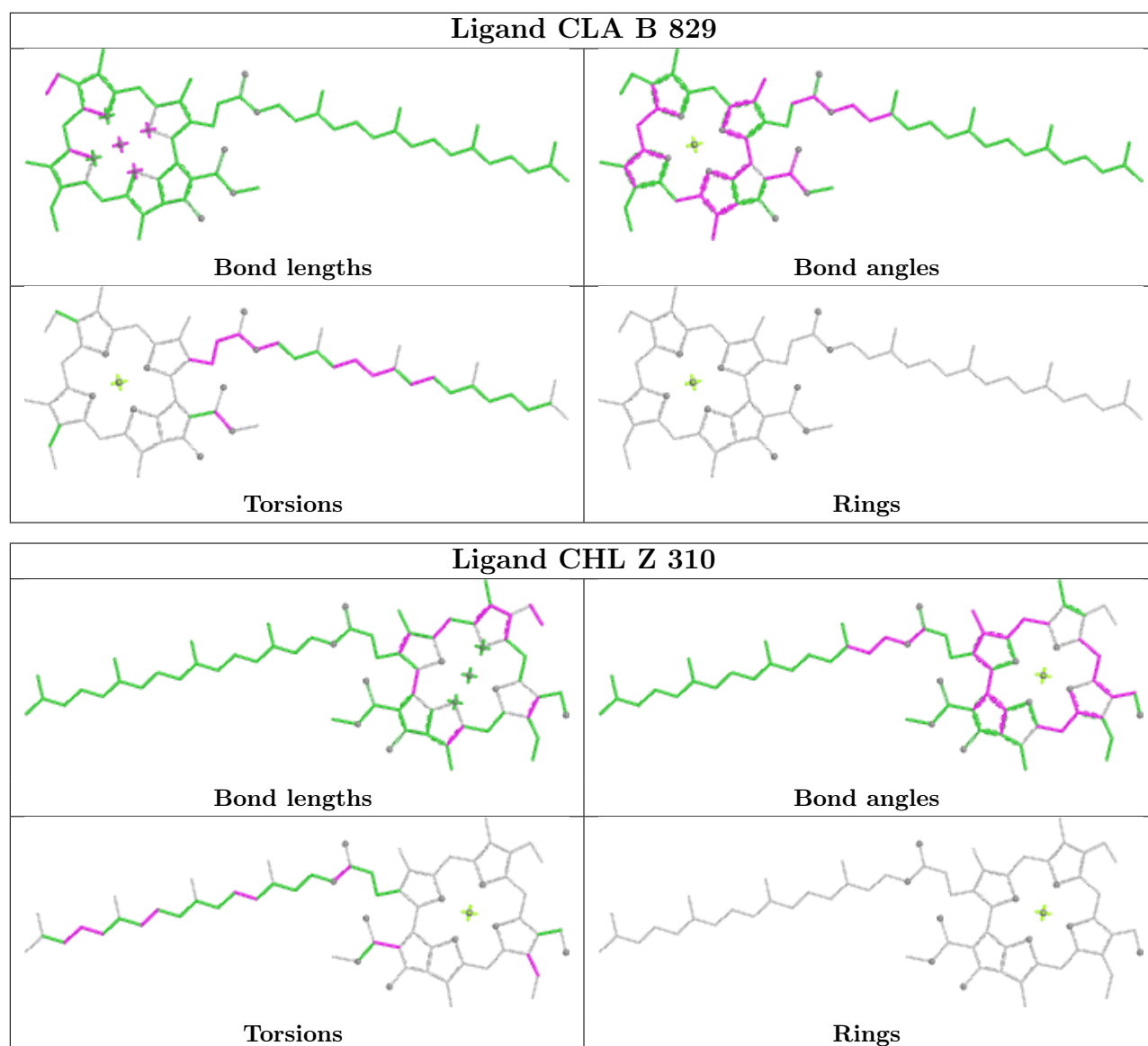


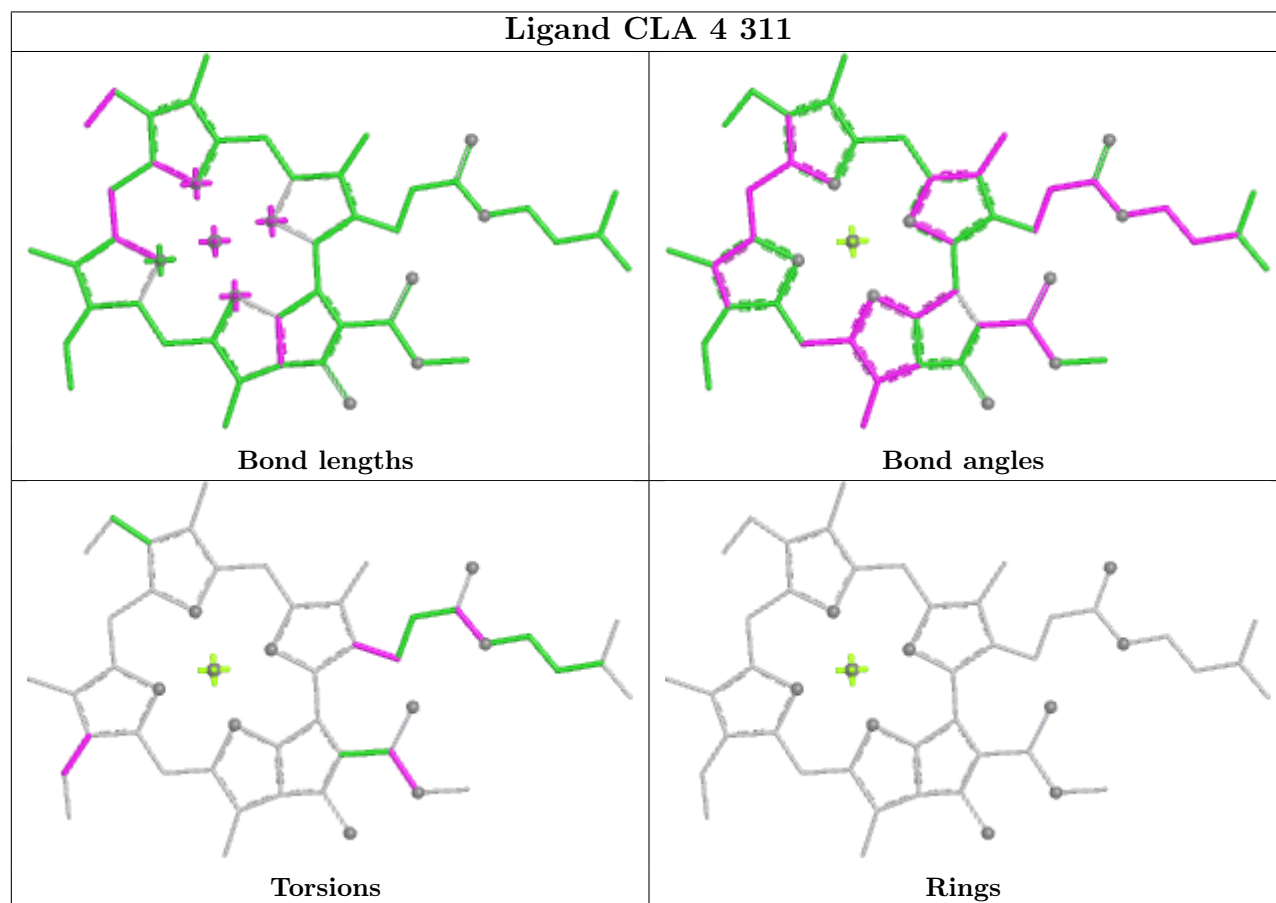
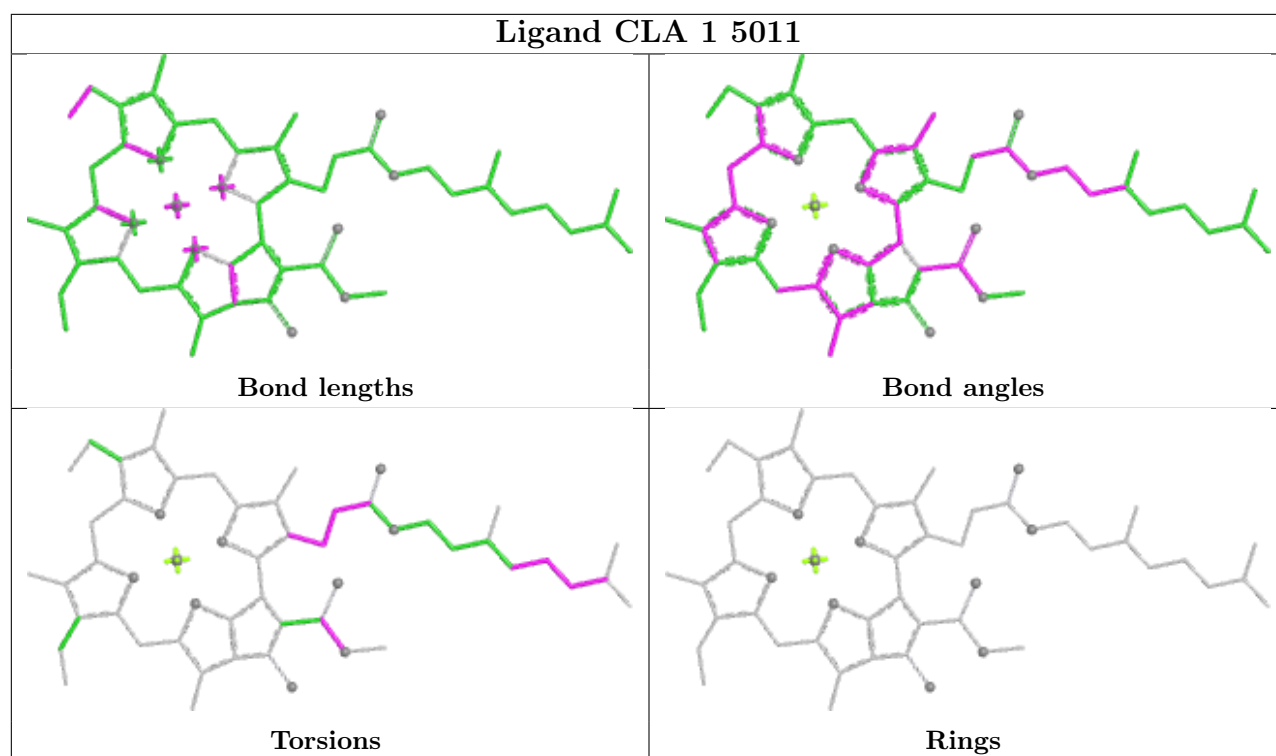
Ligand CLA 4 307

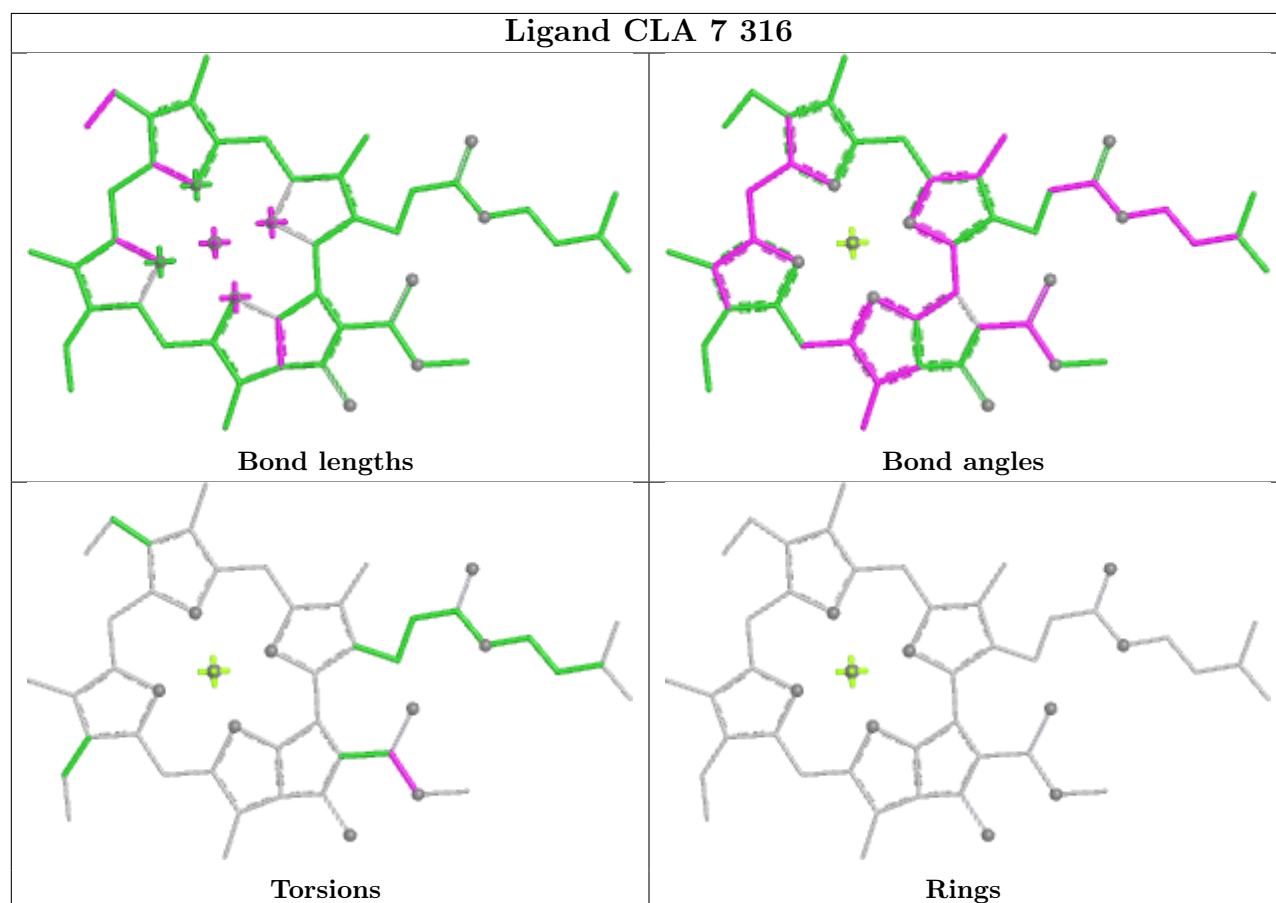
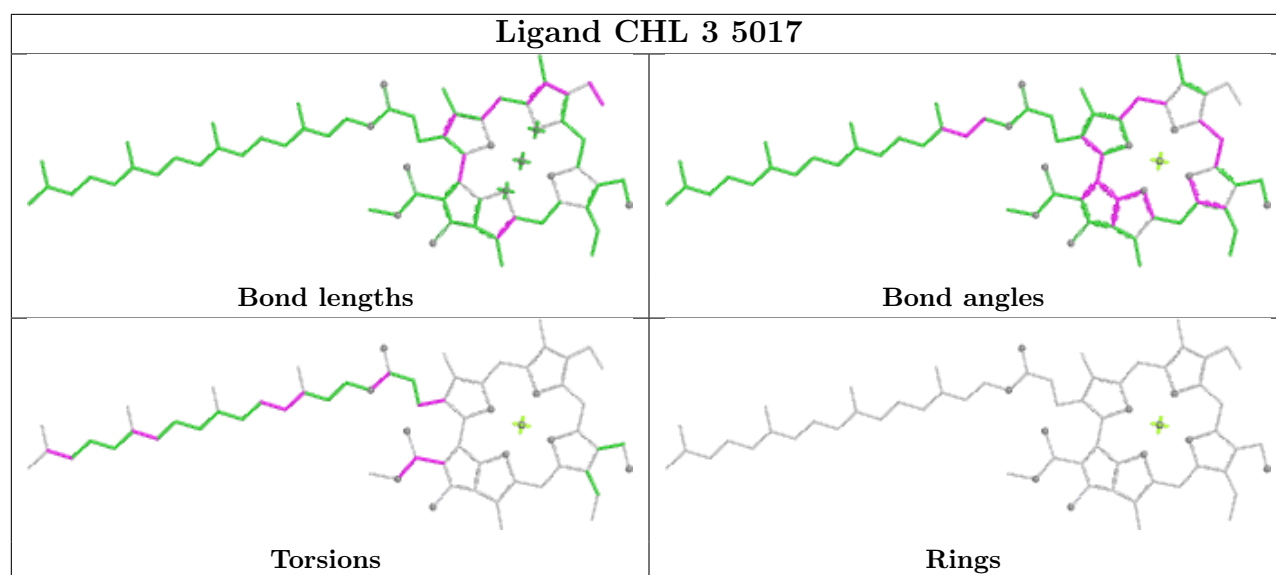


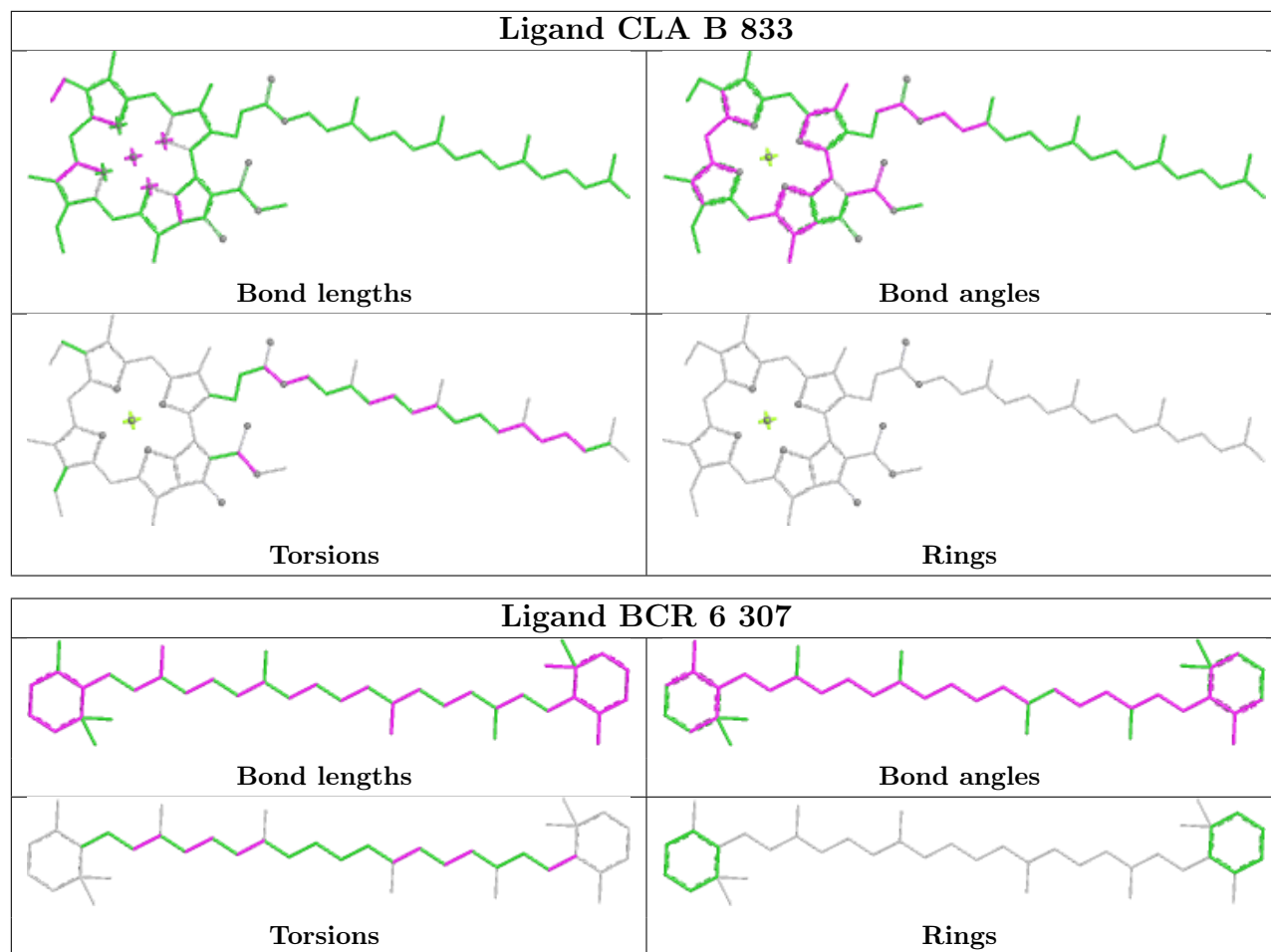
Ligand CLA A 802



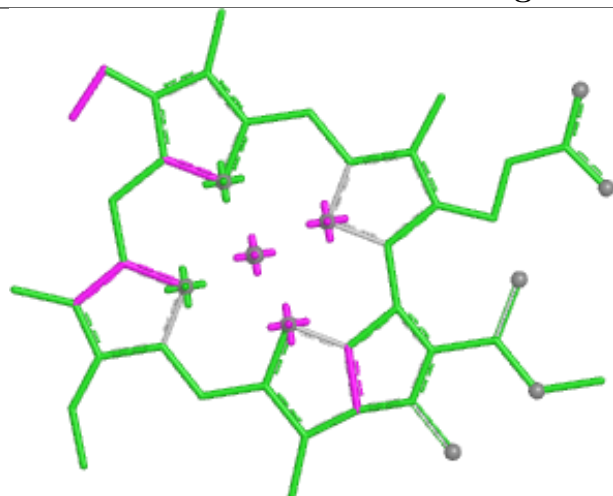




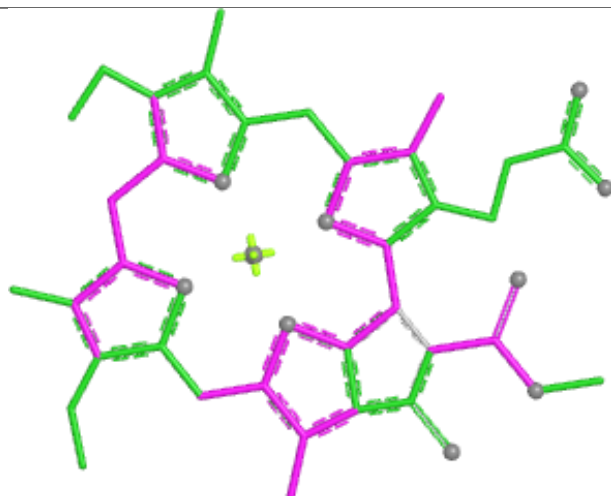




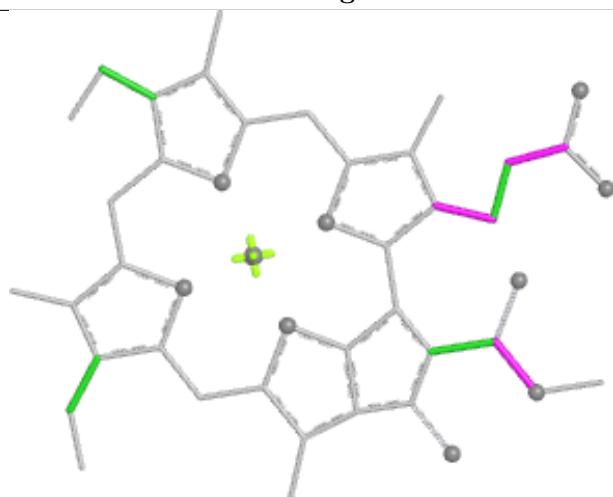
Ligand CLA B 805



Bond lengths



Bond angles

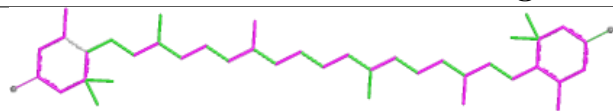


Torsions

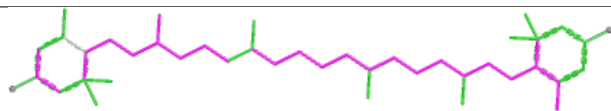


Rings

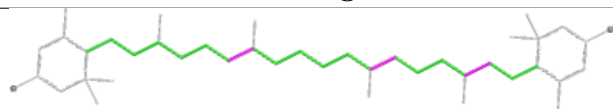
Ligand LUT Z 318



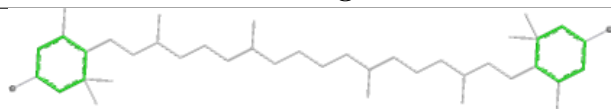
Bond lengths



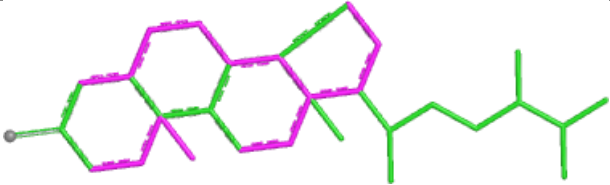
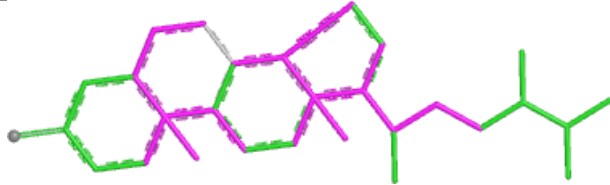
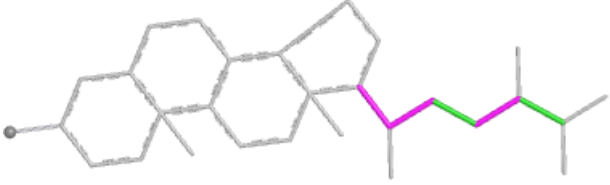
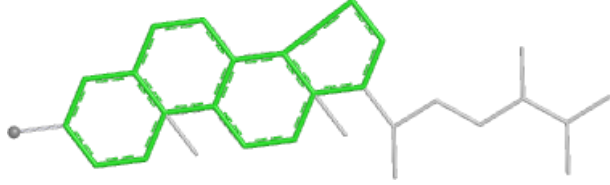
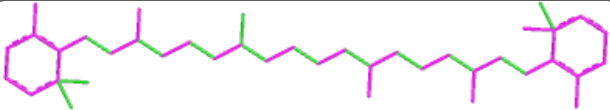
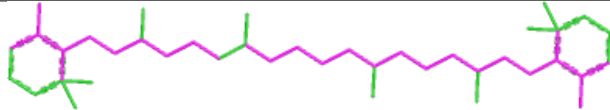
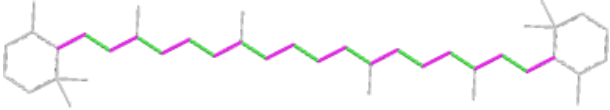
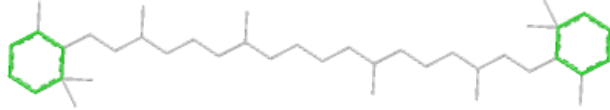
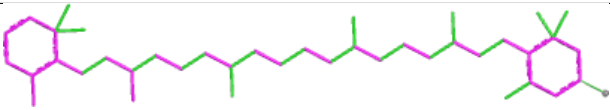
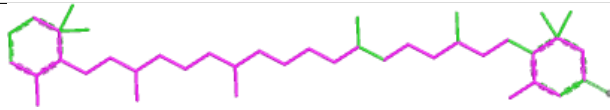
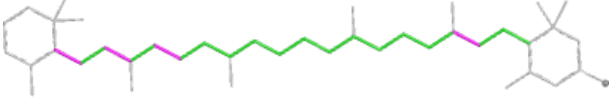
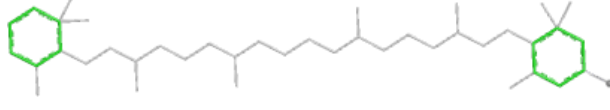
Bond angles



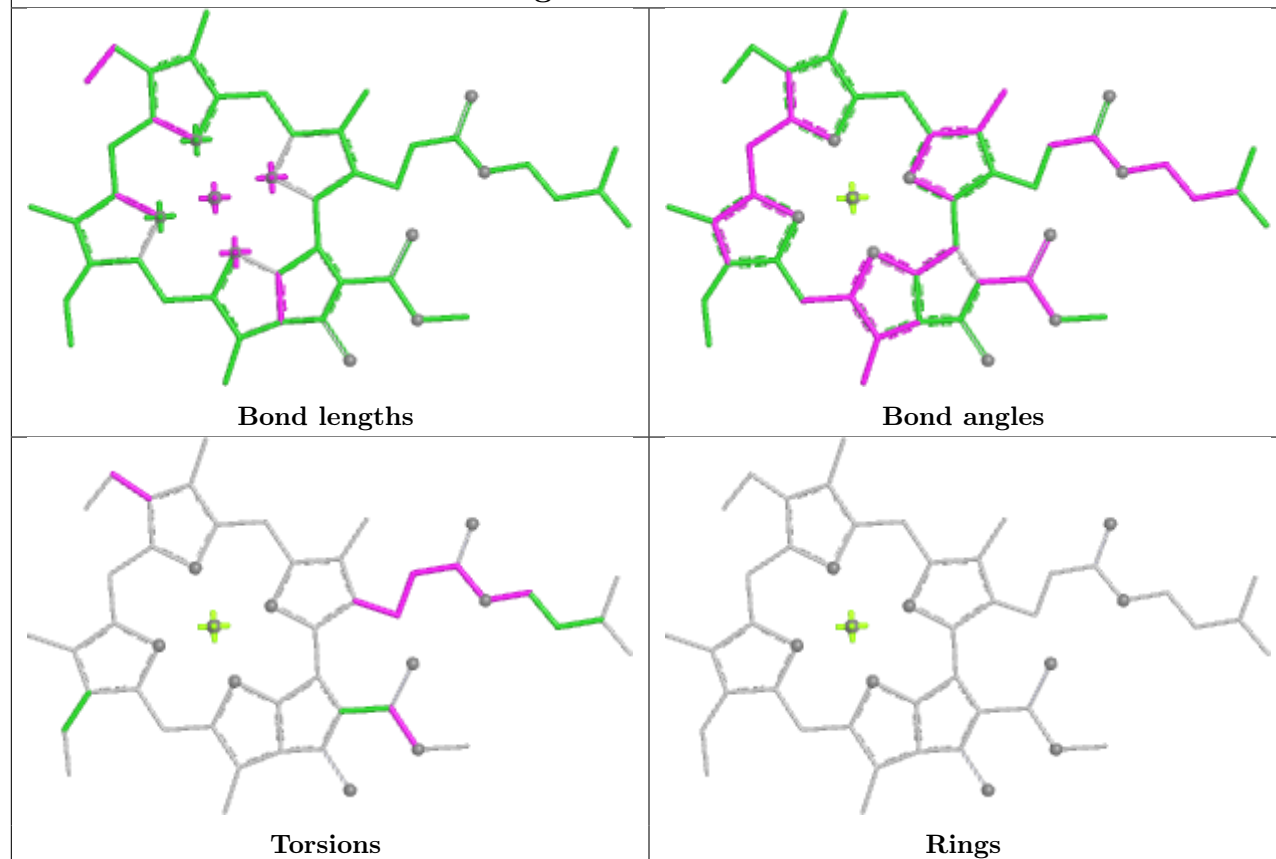
Torsions



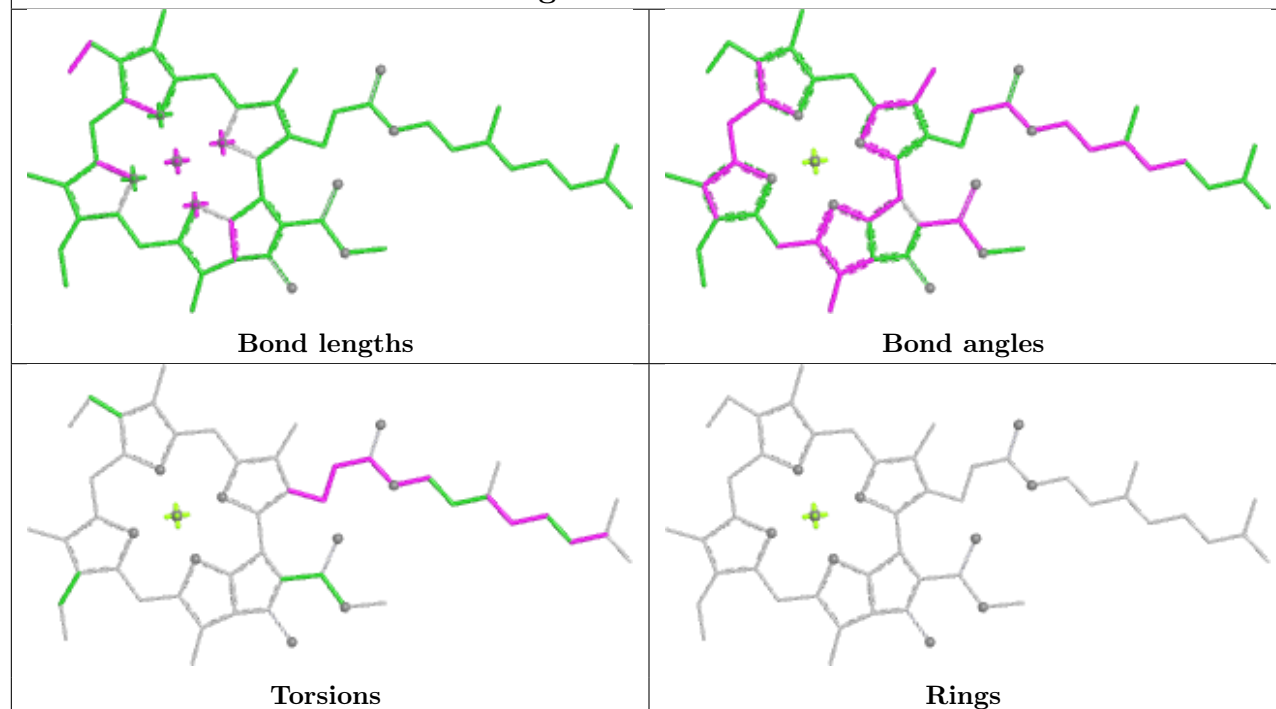
Rings

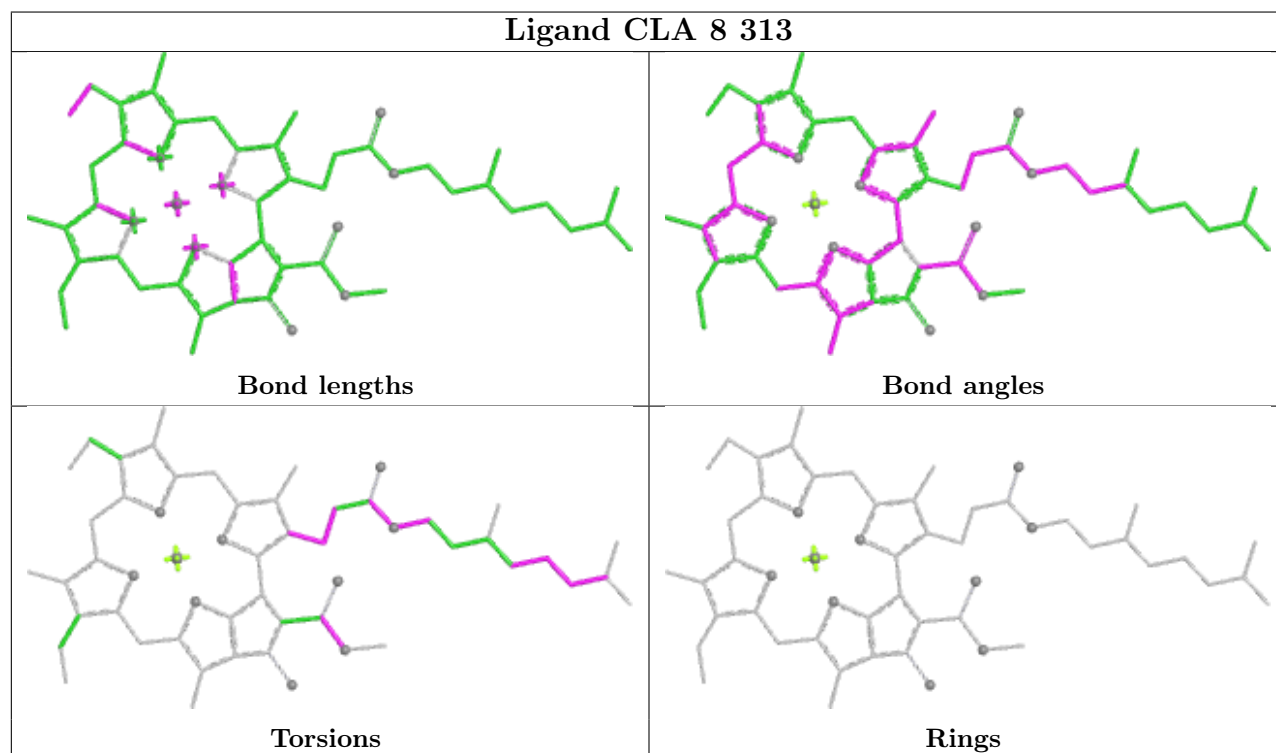
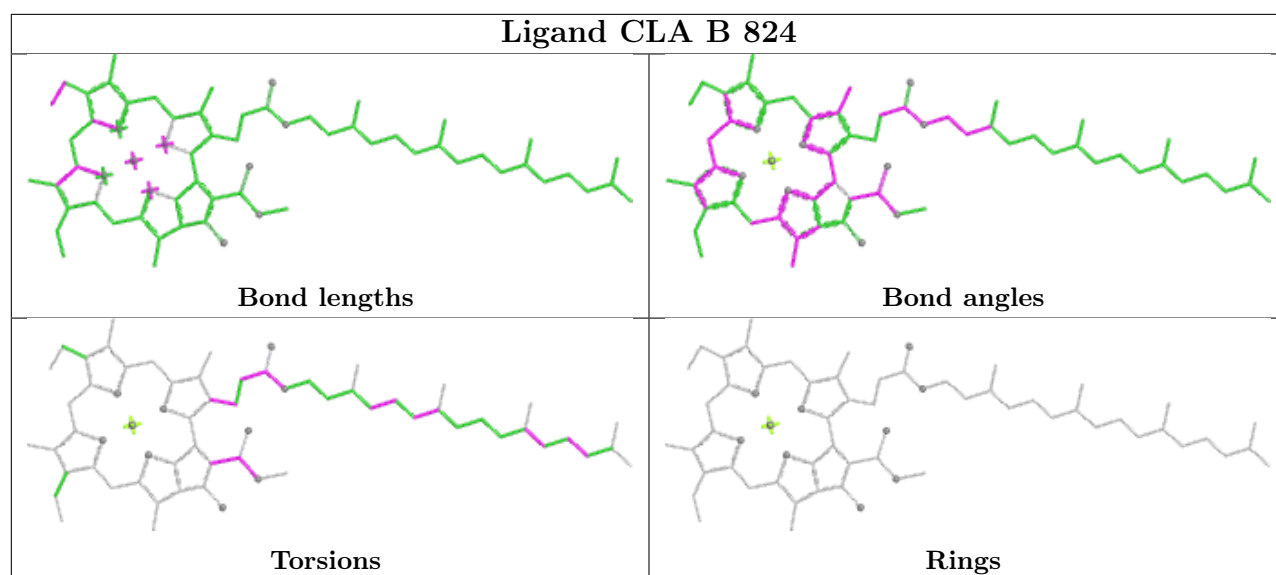
Ligand ERG 6 326	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 3 5006	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand RRX 4 303	
 Bond lengths	 Bond angles
 Torsions	 Rings

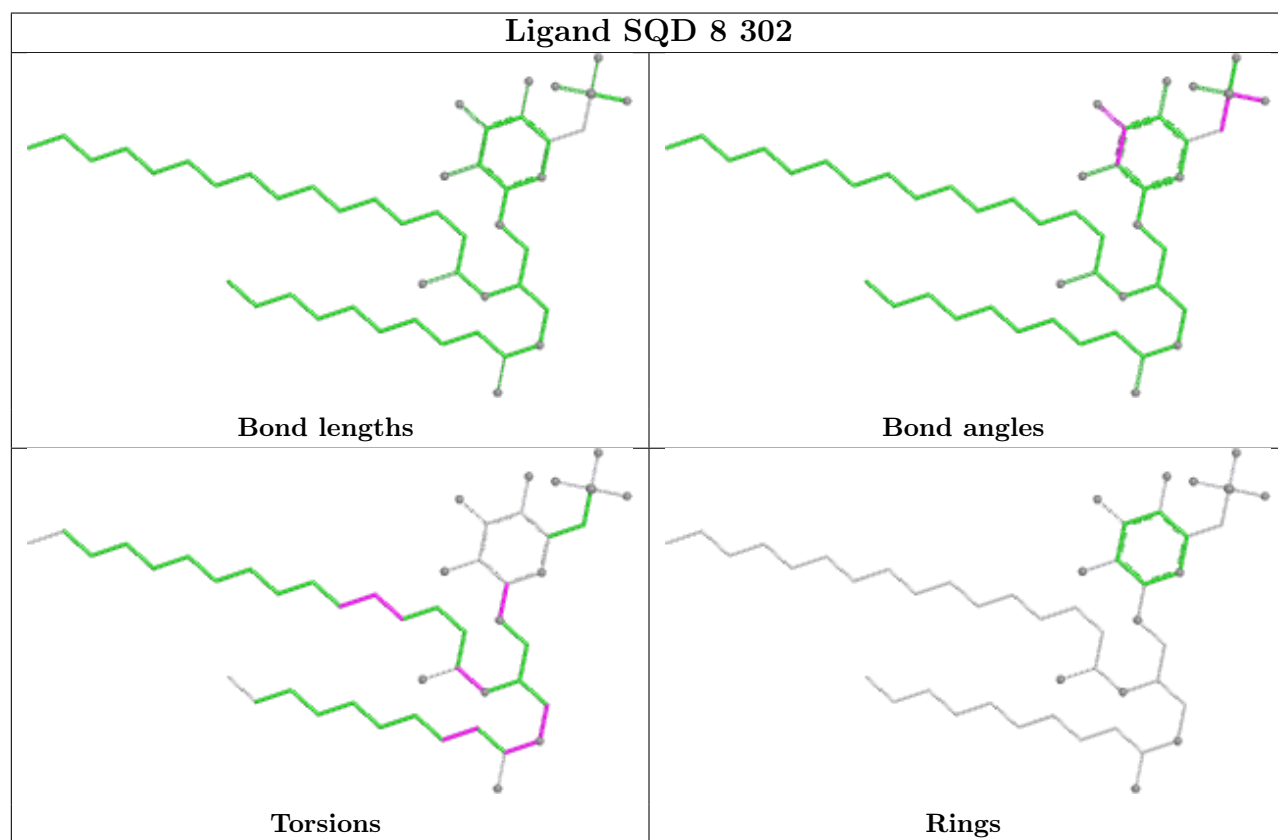
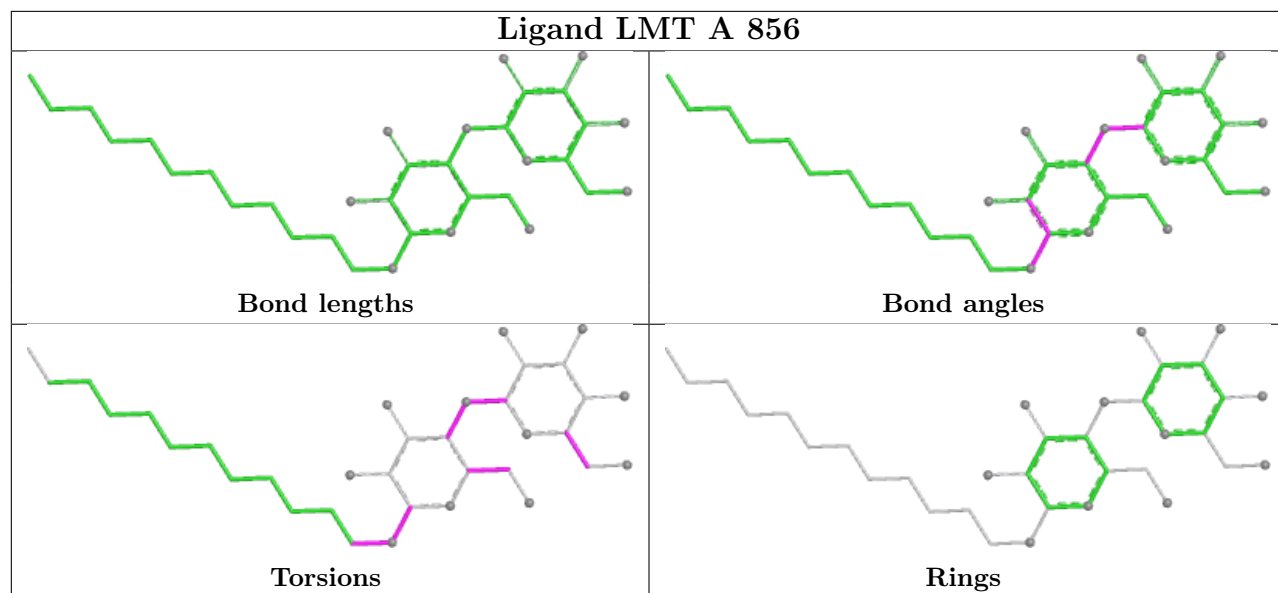
Ligand CLA Z 306

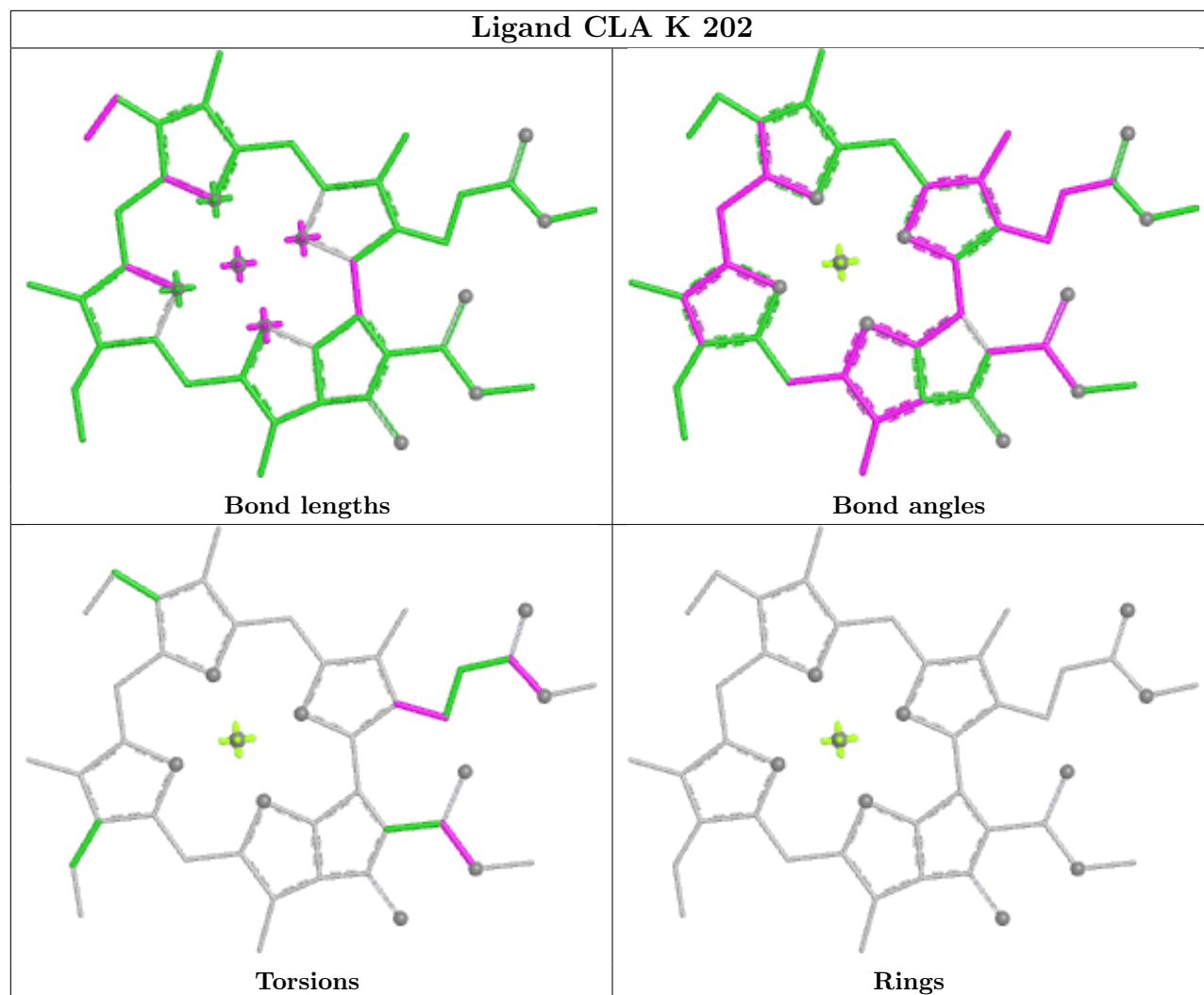


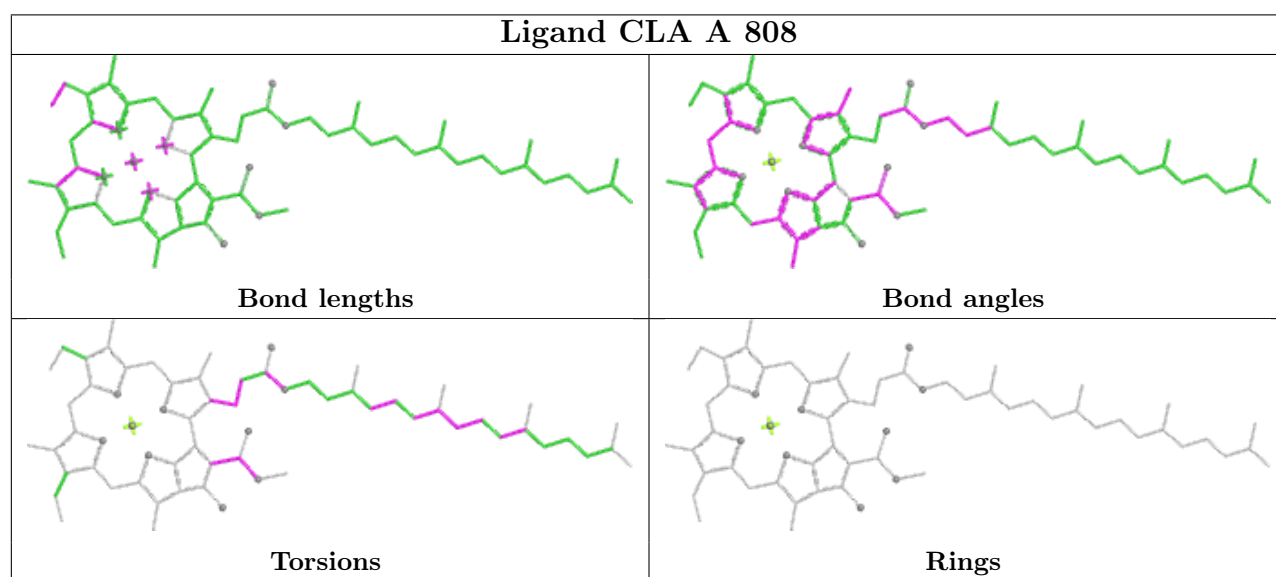
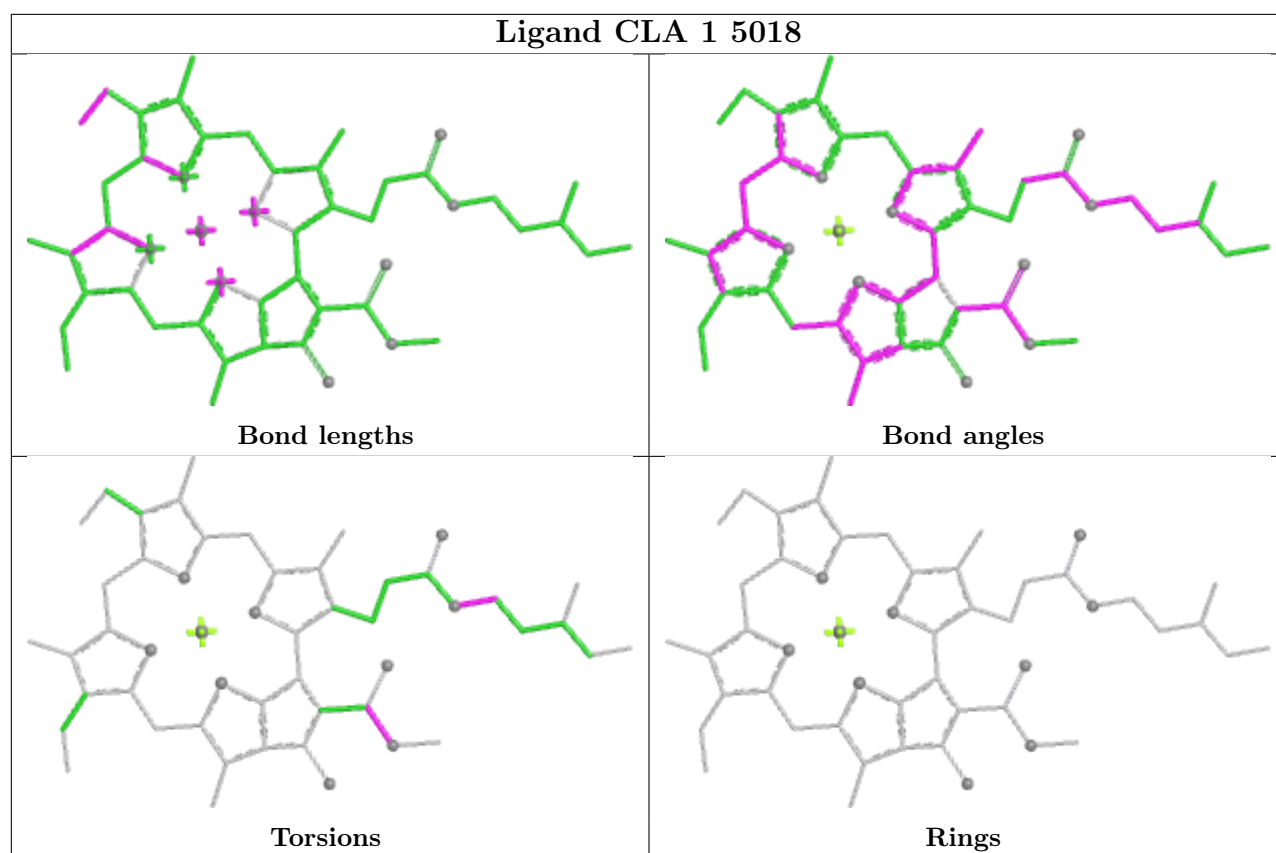
Ligand CLA I 201



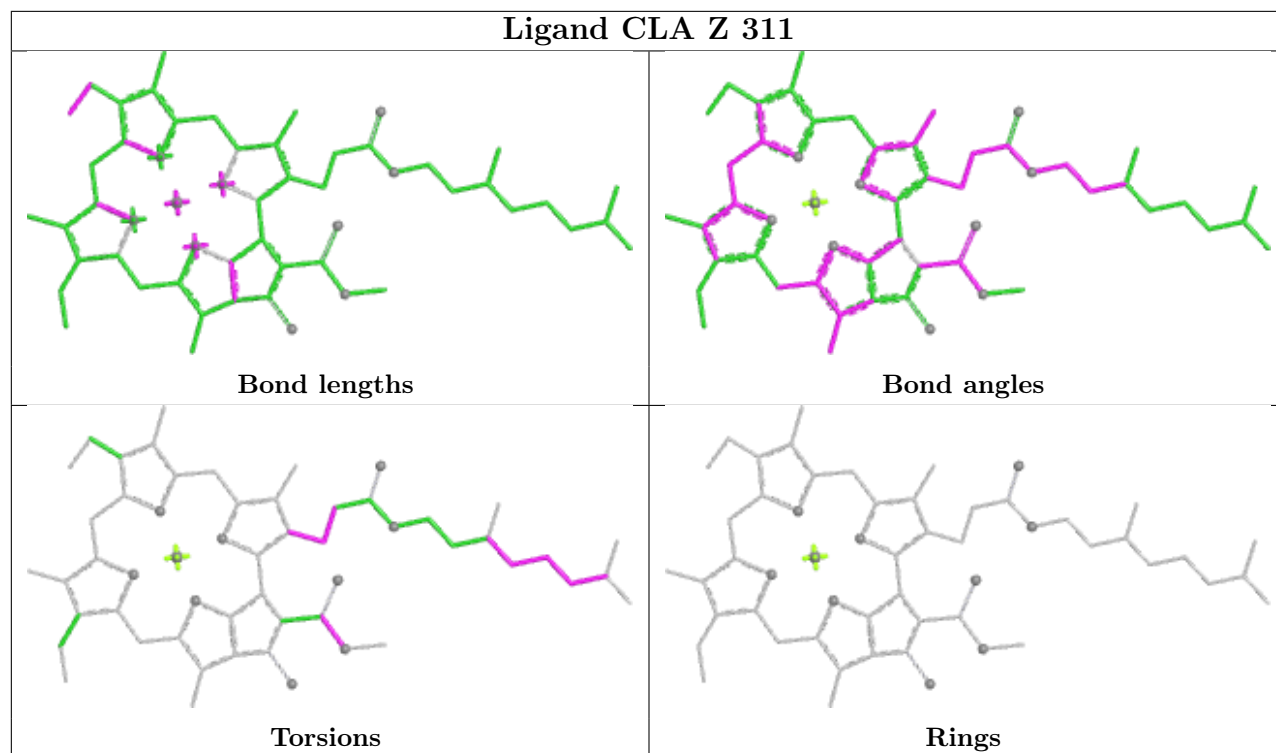




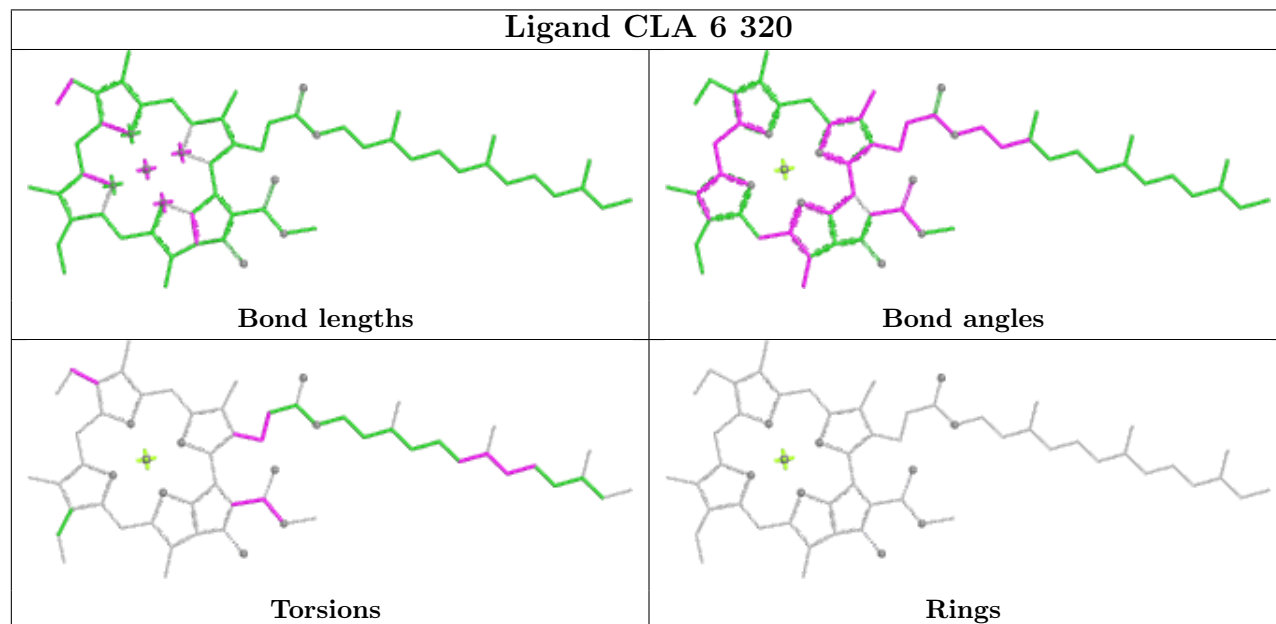


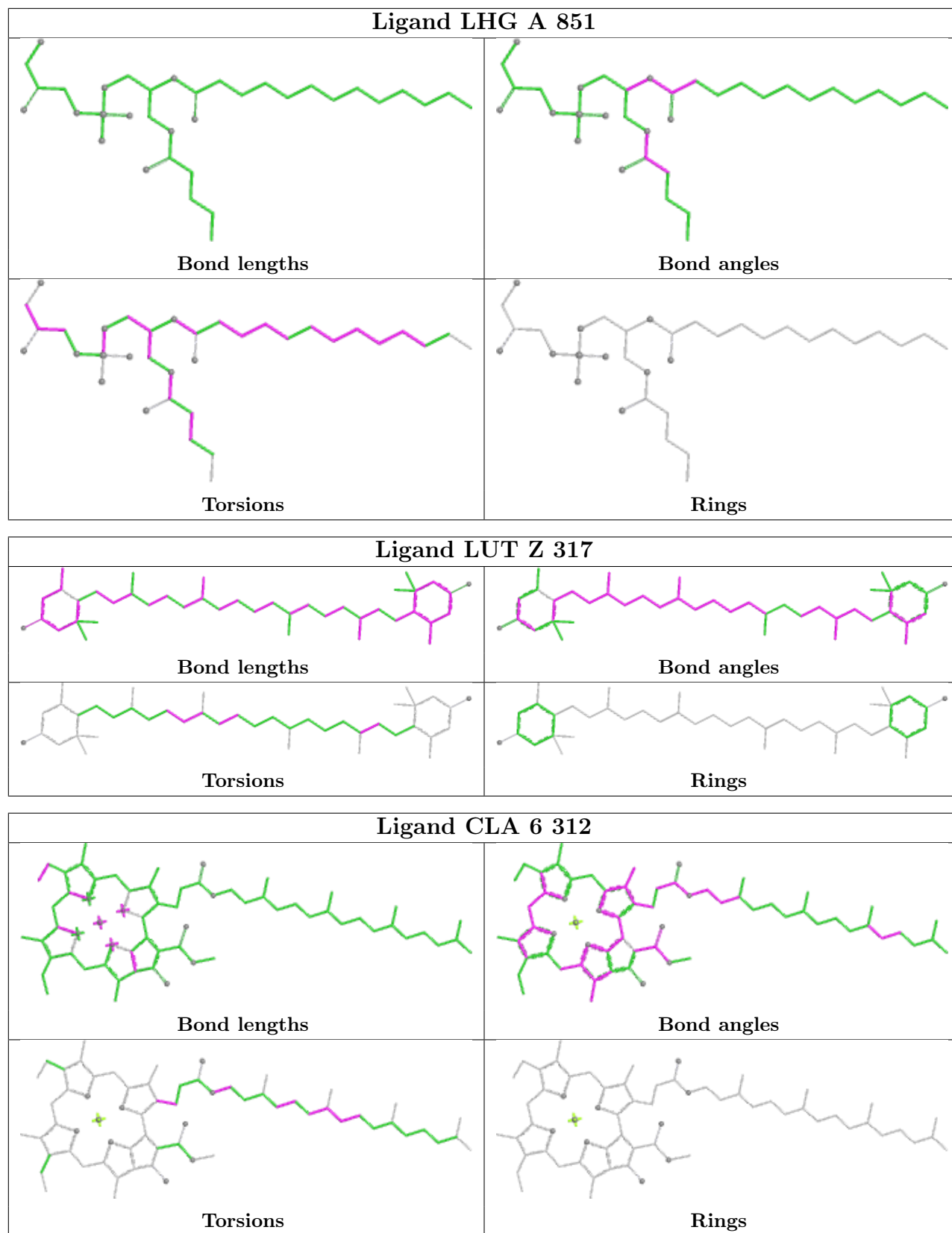


Ligand CLA Z 311

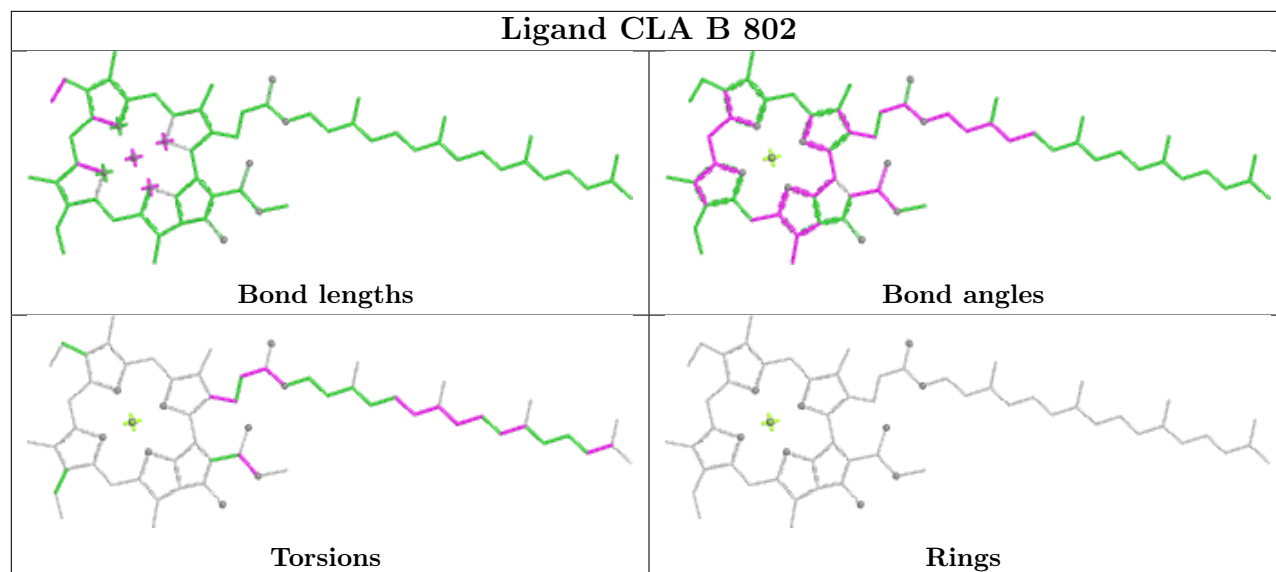


Ligand CLA 6 320

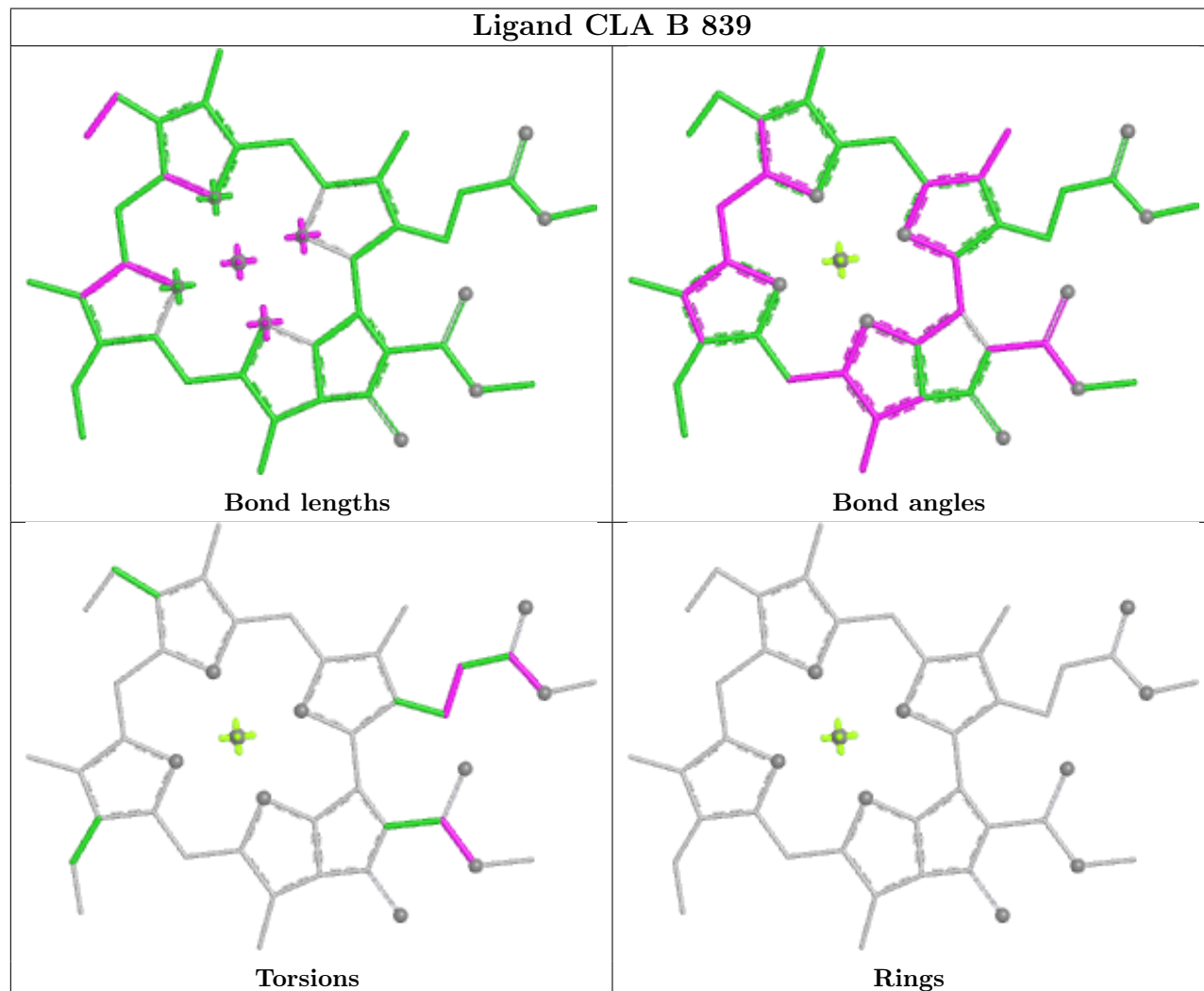




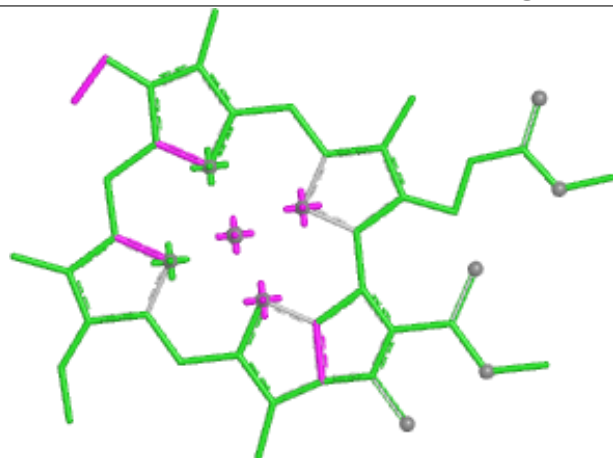
Ligand CLA B 802



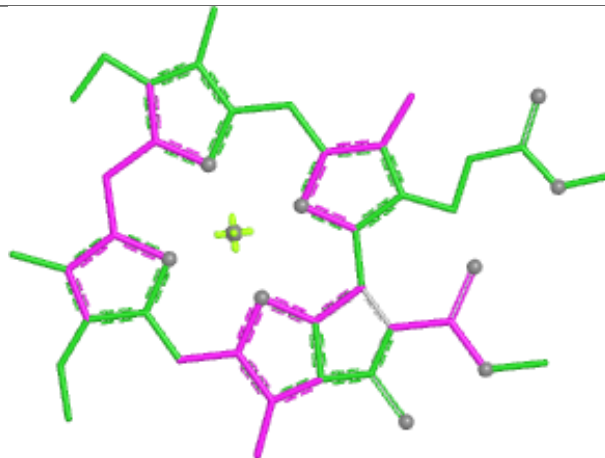
Ligand CLA B 839



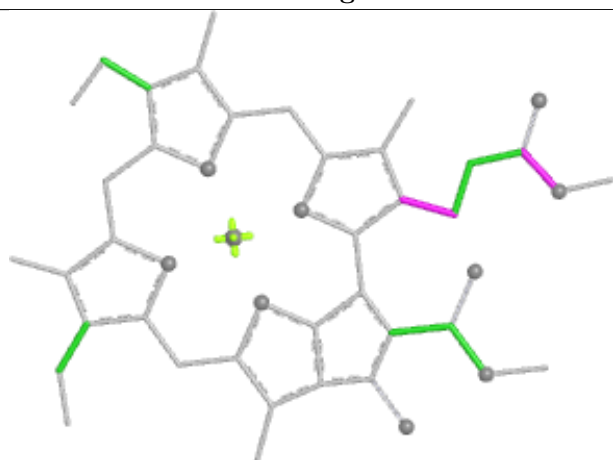
Ligand CLA 6 322



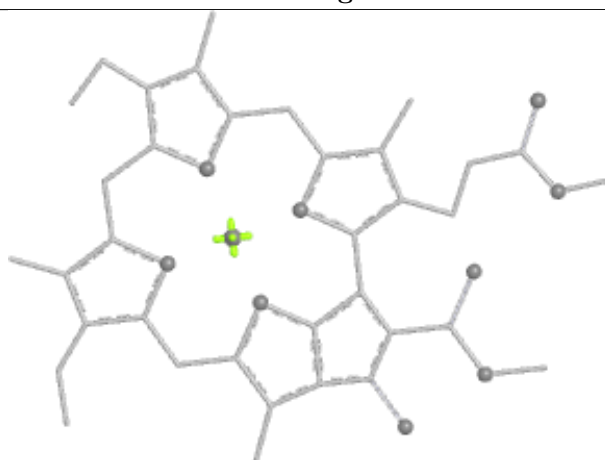
Bond lengths



Bond angles

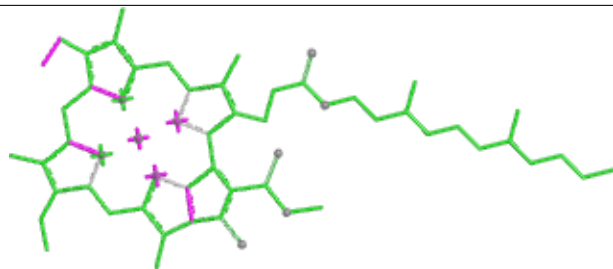


Torsions

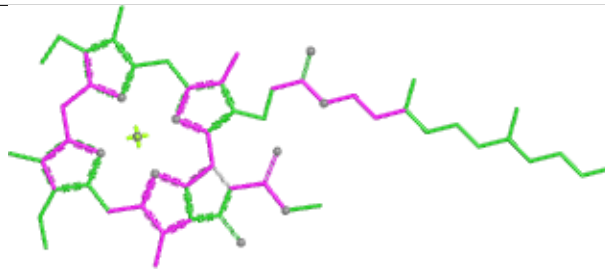


Rings

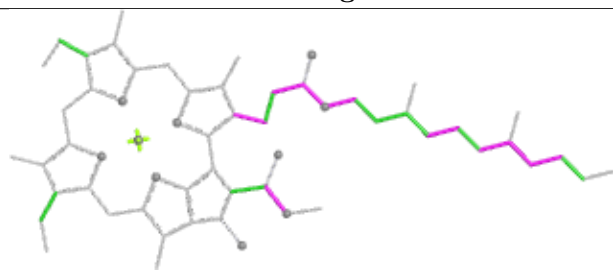
Ligand CLA 7 319



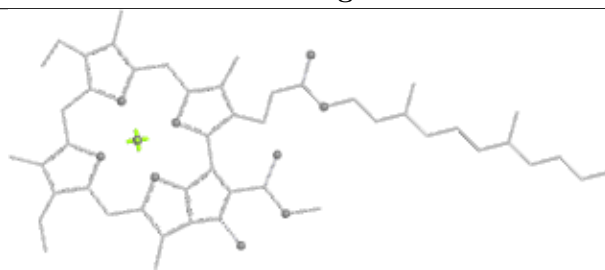
Bond lengths



Bond angles

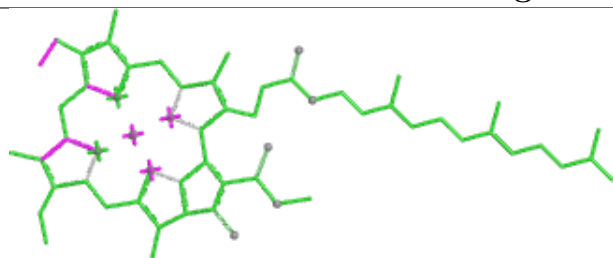


Torsions

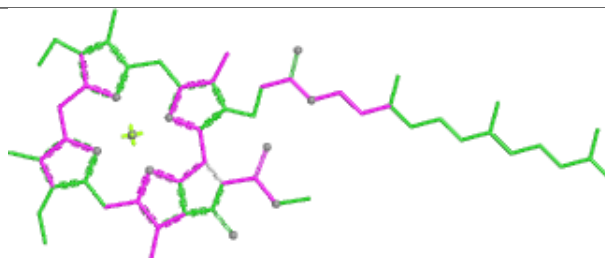


Rings

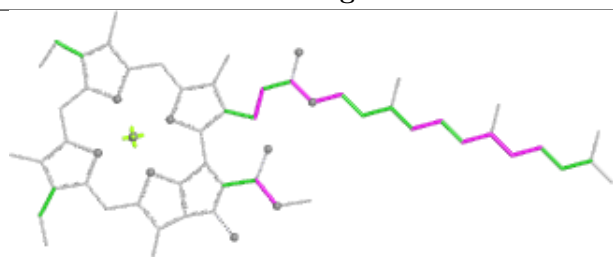
Ligand CLA B 814



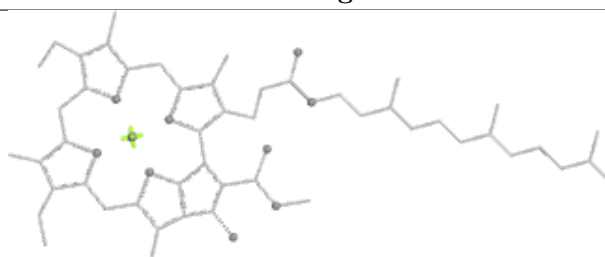
Bond lengths



Bond angles

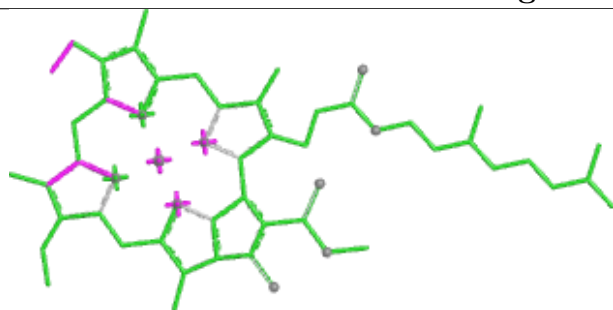


Torsions

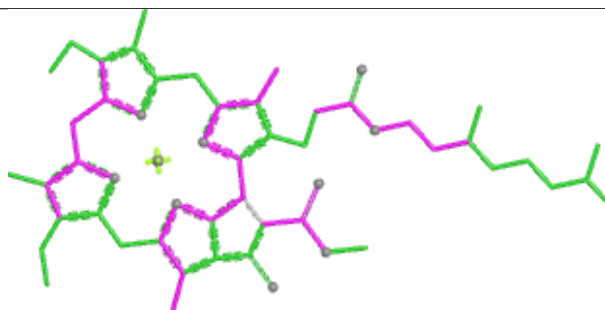


Rings

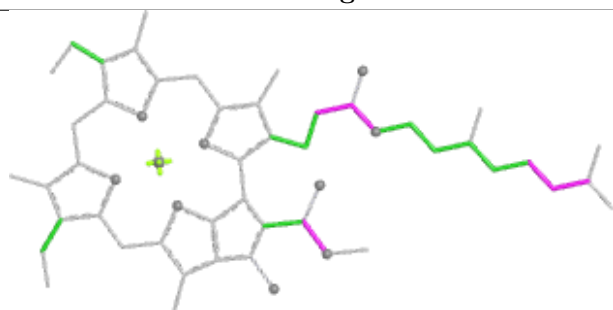
Ligand CLA 6 314



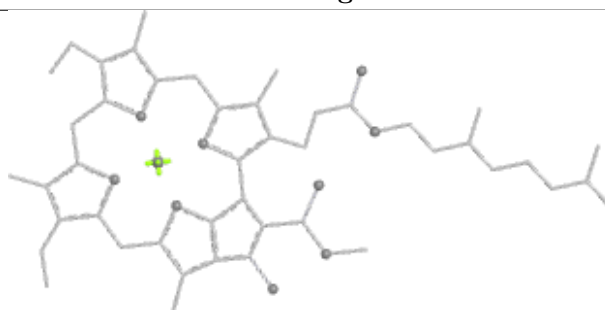
Bond lengths



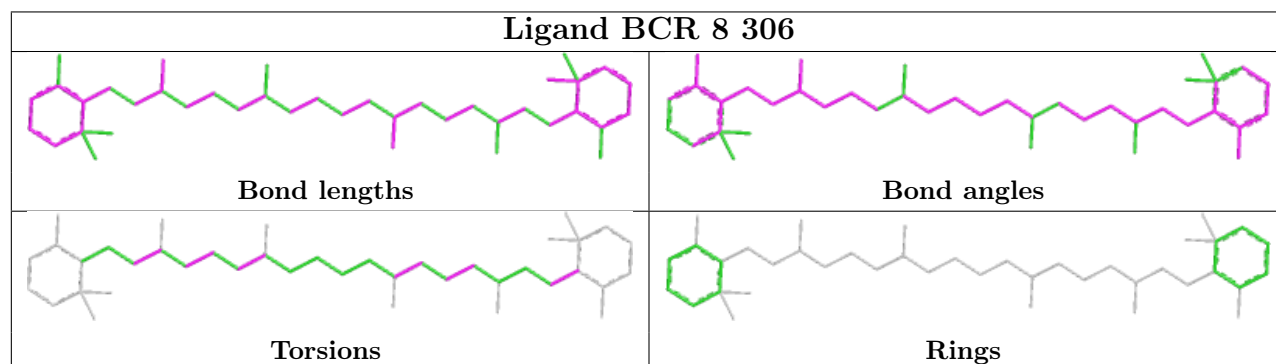
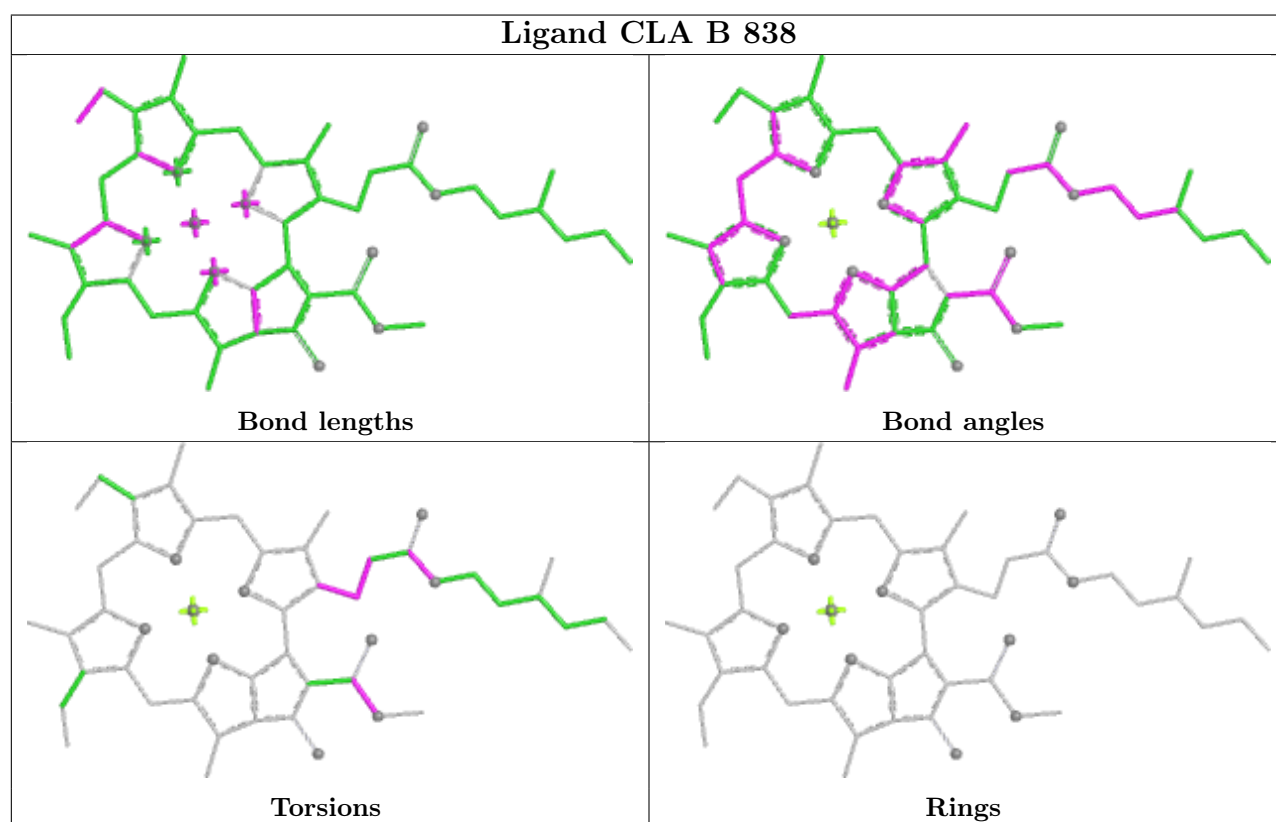
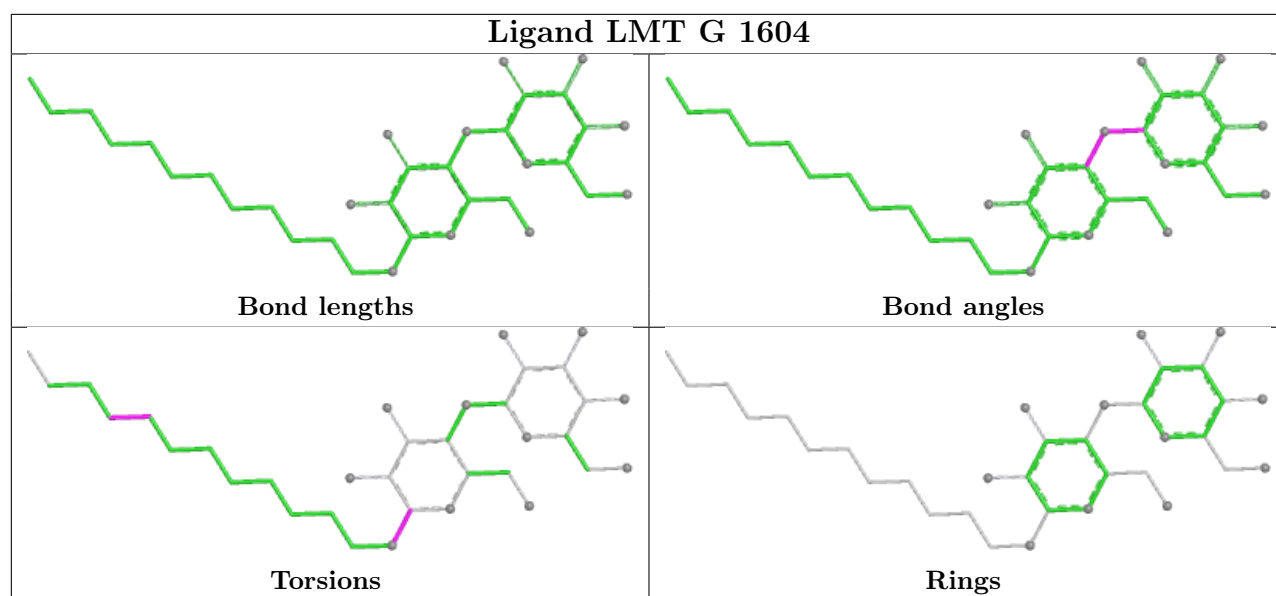
Bond angles

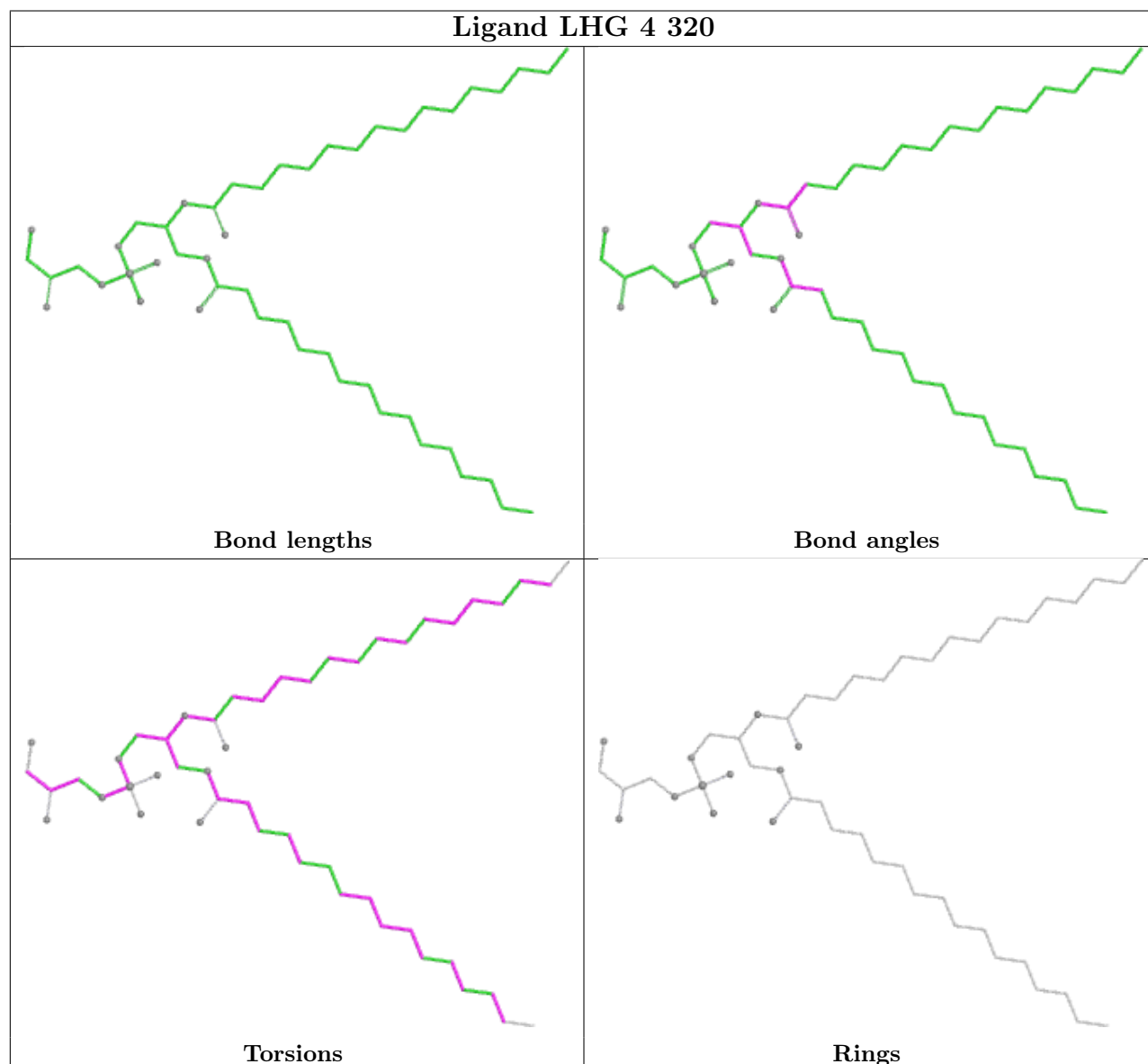
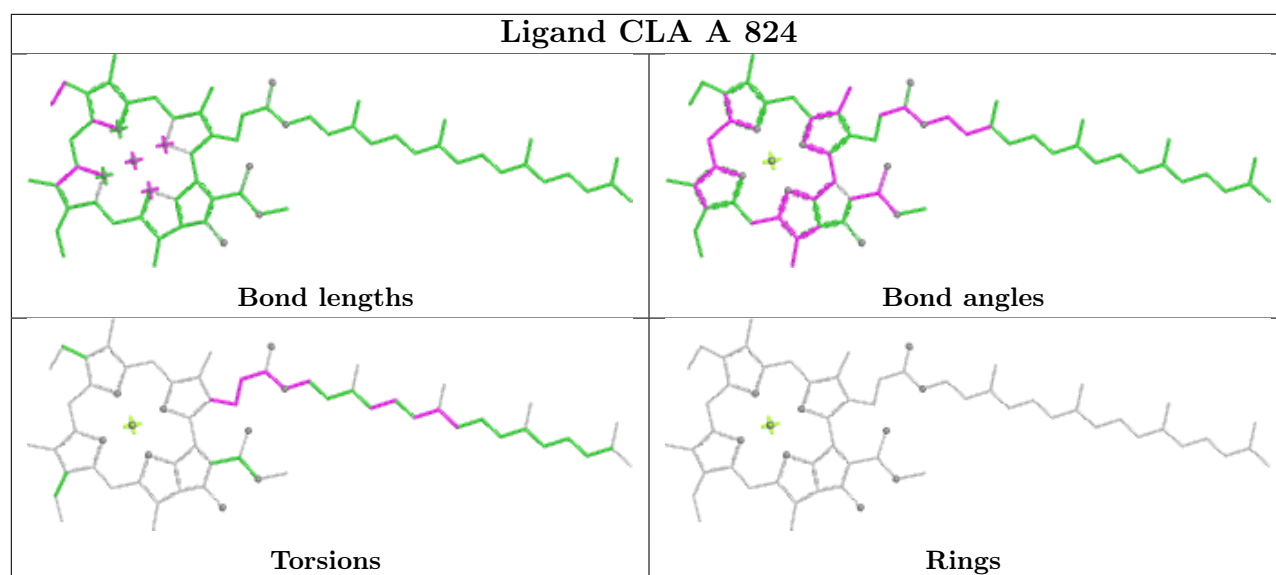


Torsions

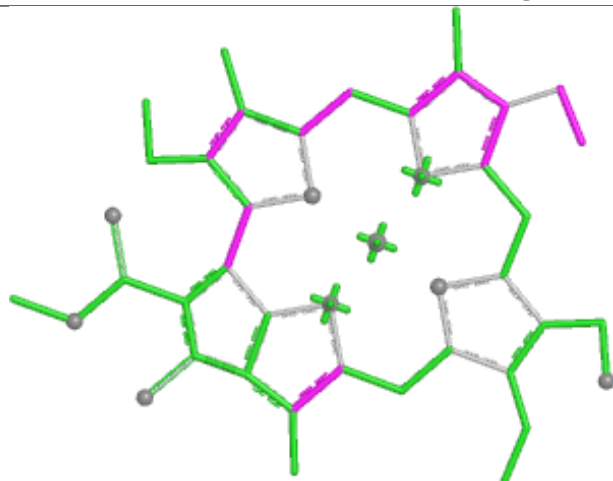


Rings

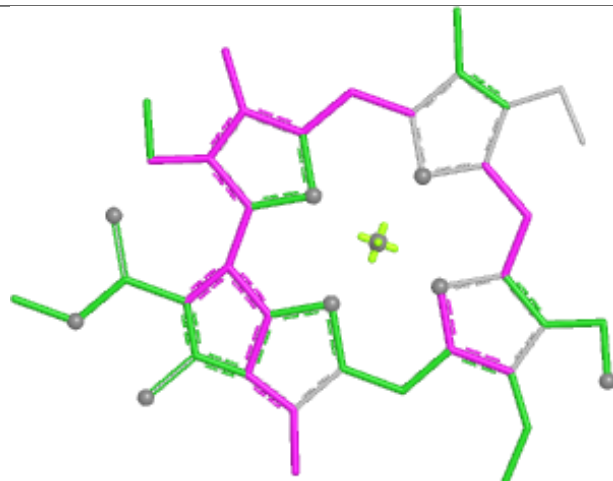




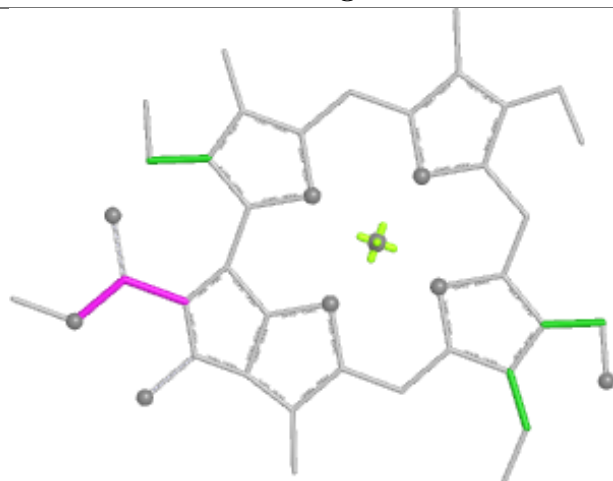
Ligand CHL 6 321



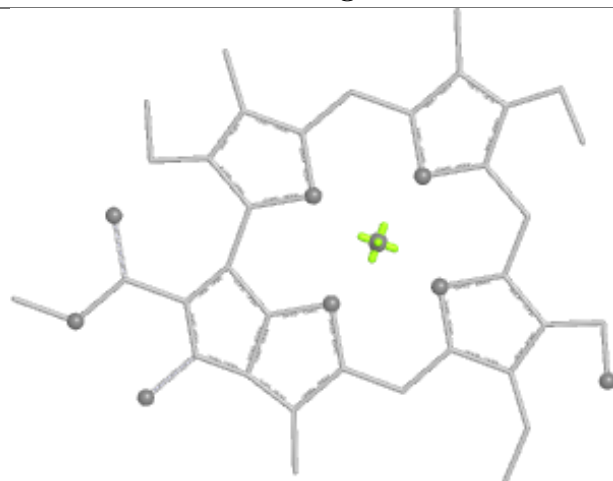
Bond lengths



Bond angles



Torsions

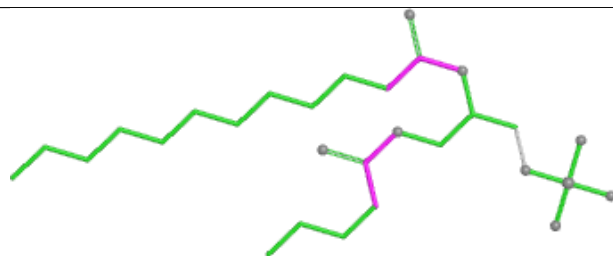


Rings

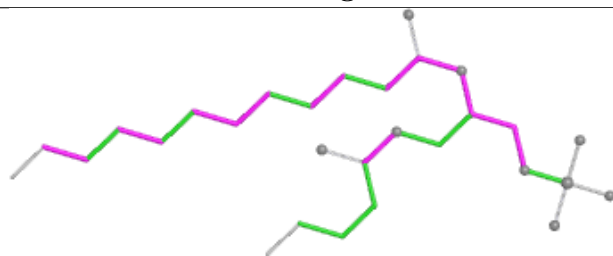
Ligand 3PH 6 325



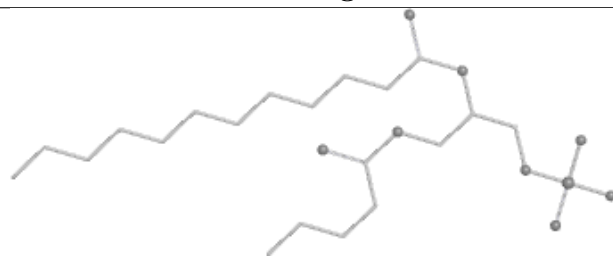
Bond lengths



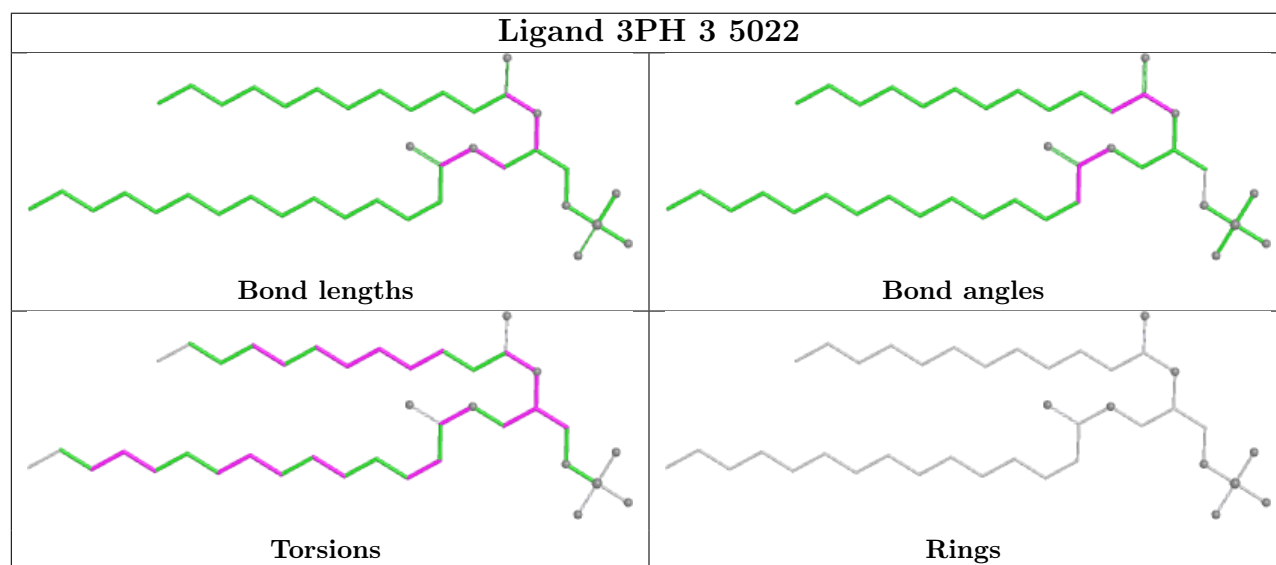
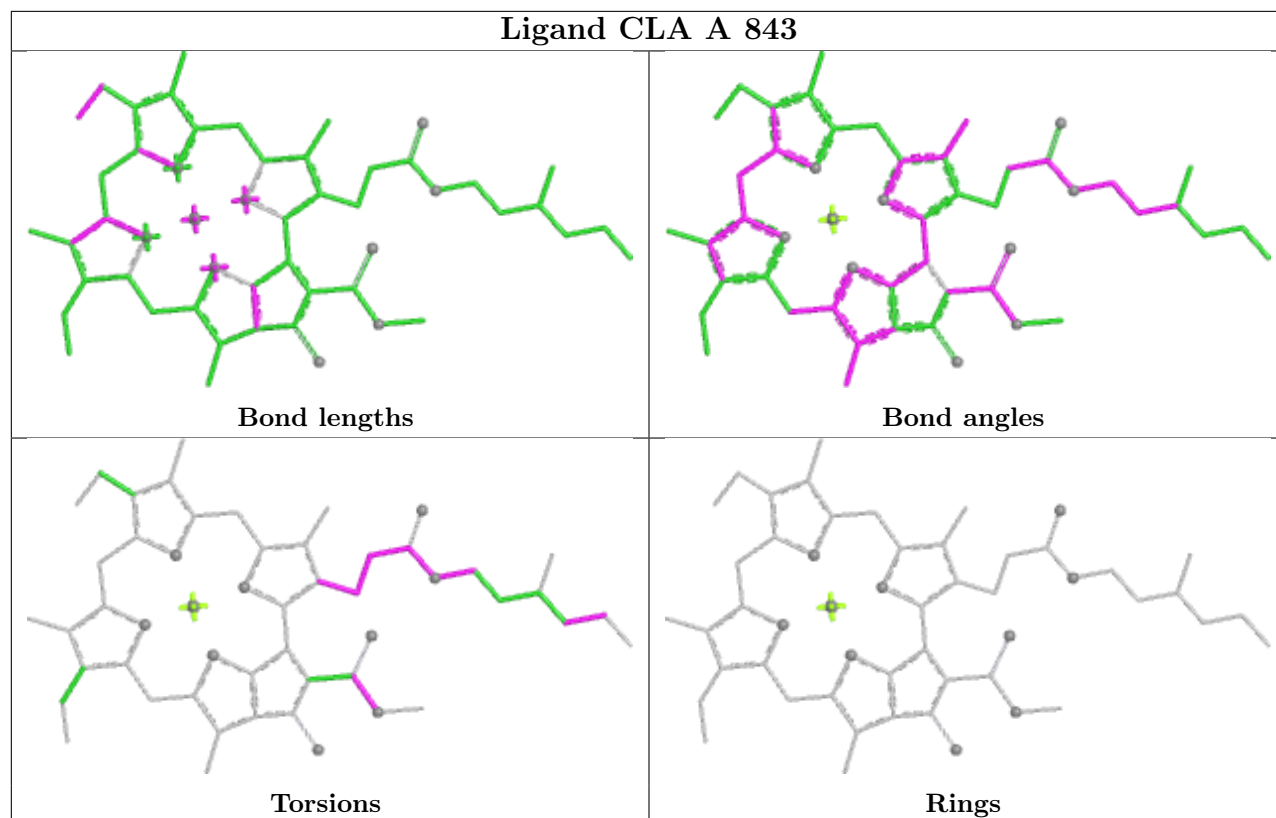
Bond angles

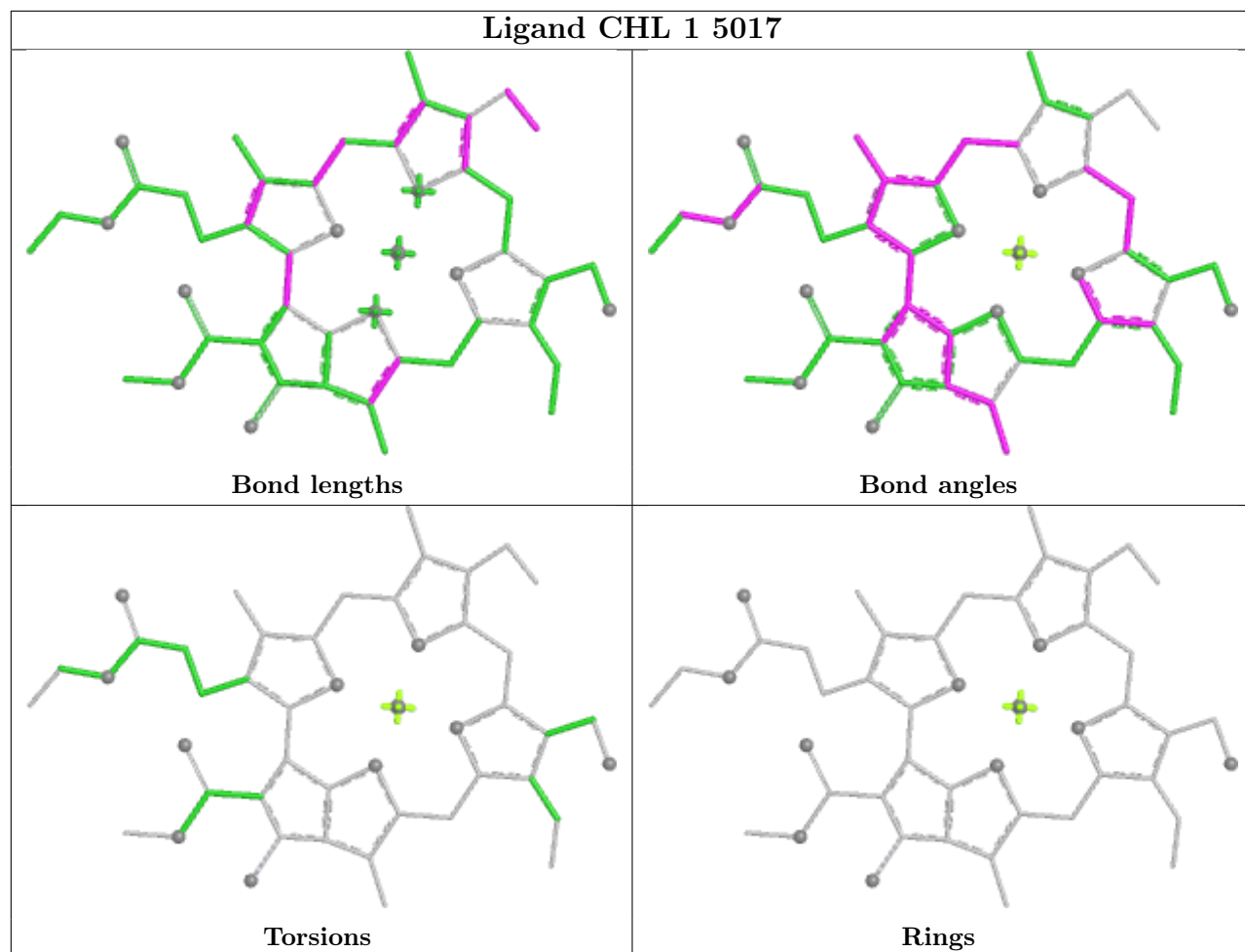


Torsions

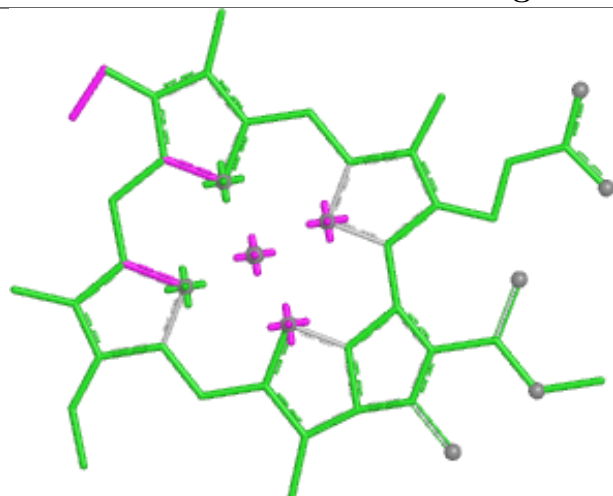


Rings

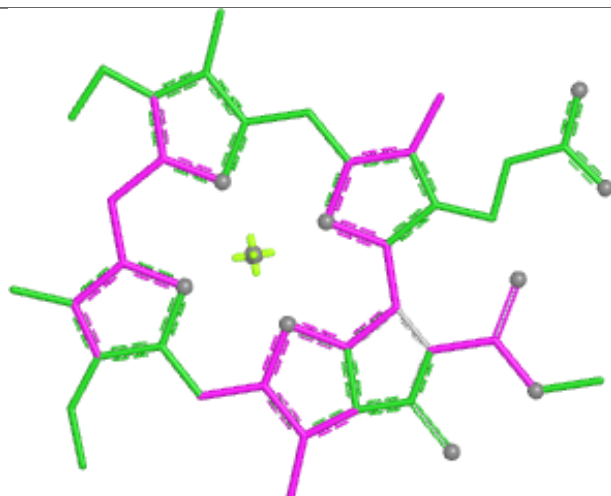




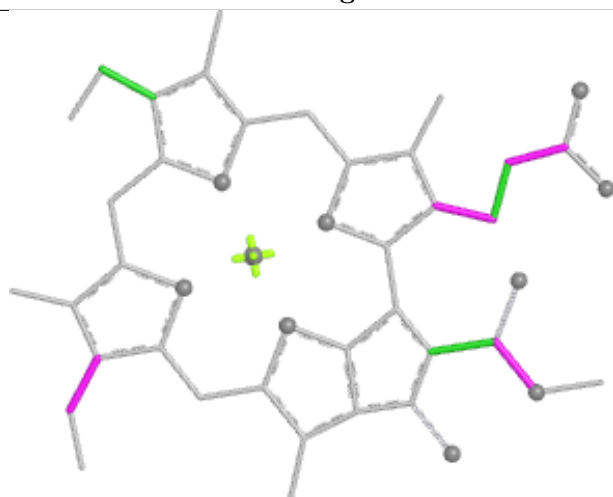
Ligand CLA K 205



Bond lengths



Bond angles

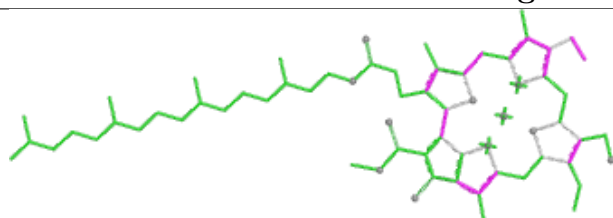


Torsions

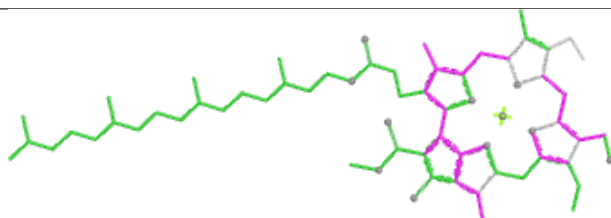


Rings

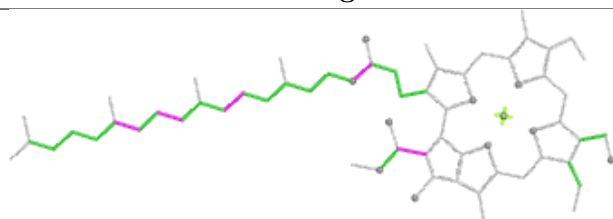
Ligand CHL 4 317



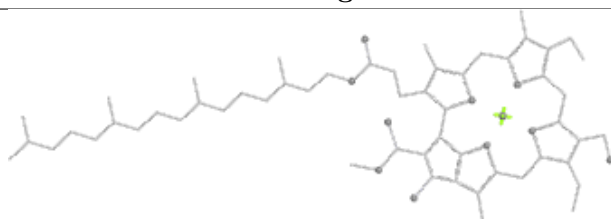
Bond lengths



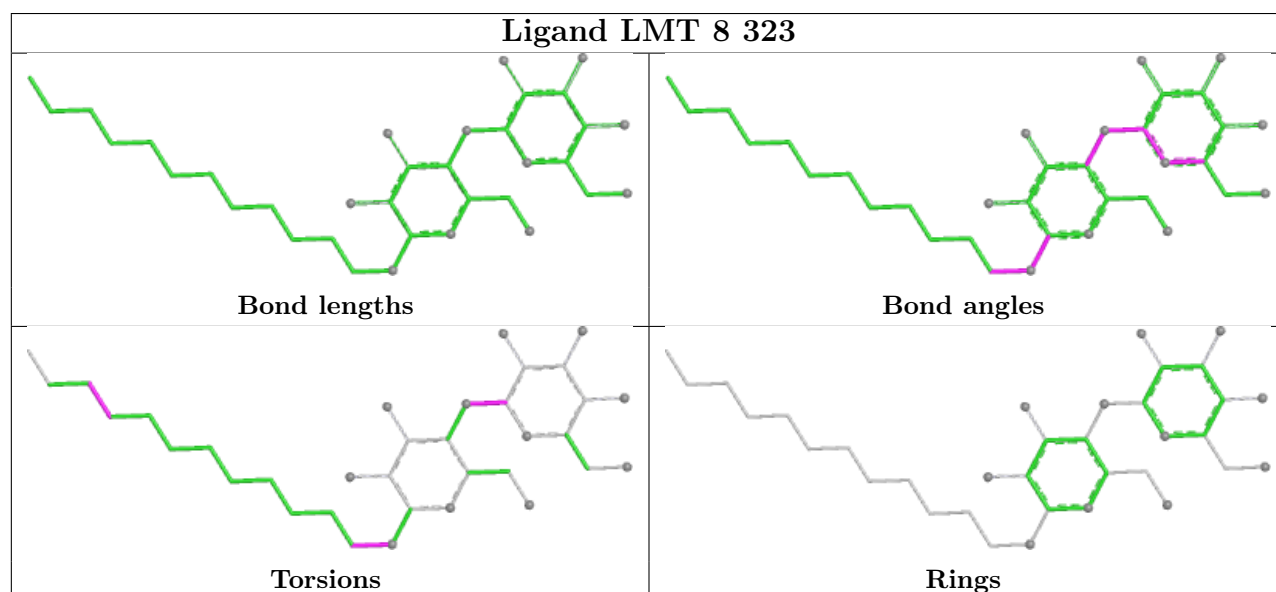
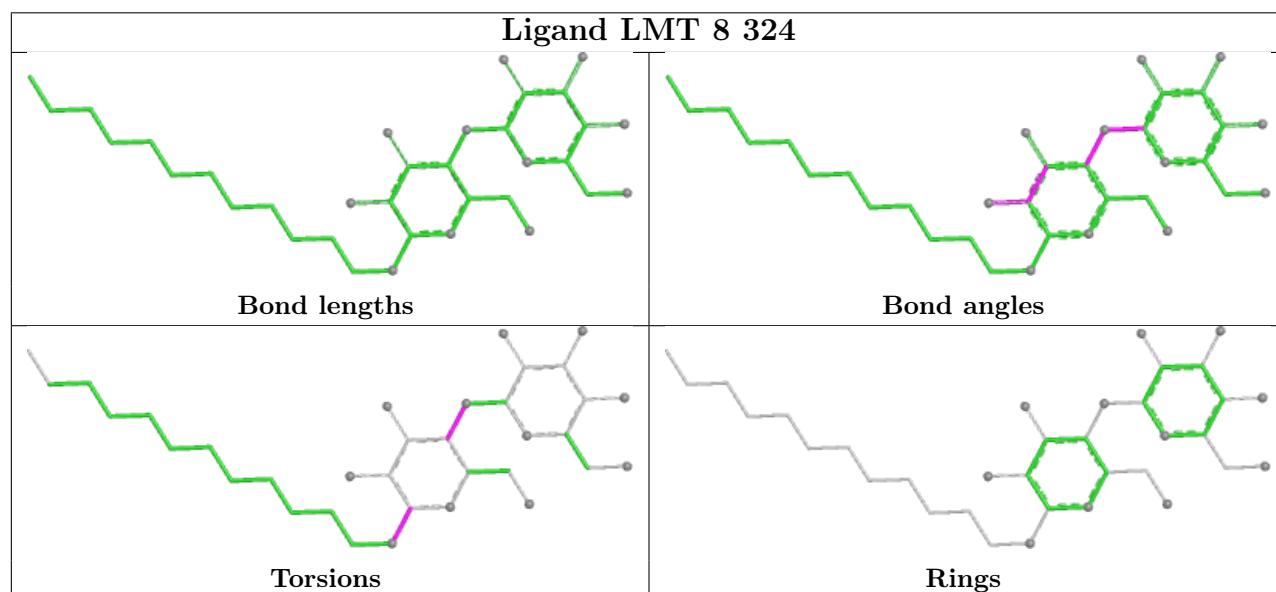
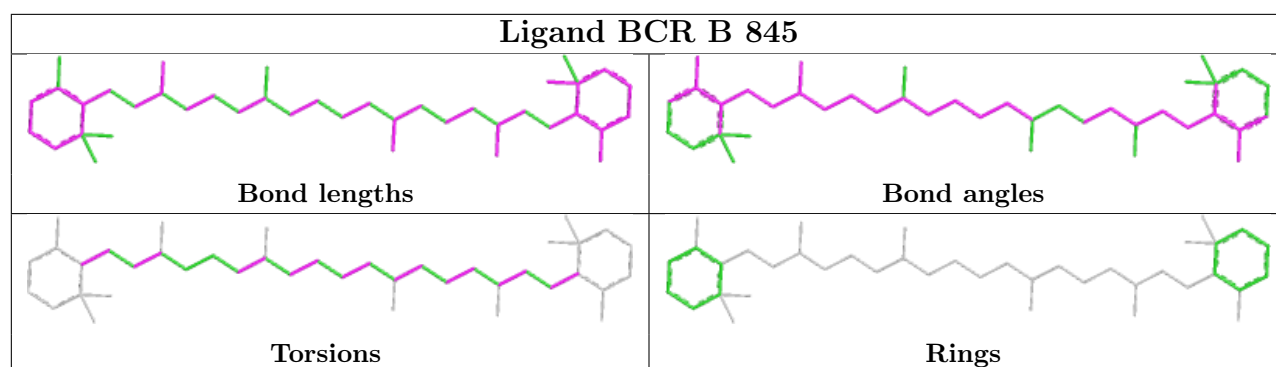
Bond angles

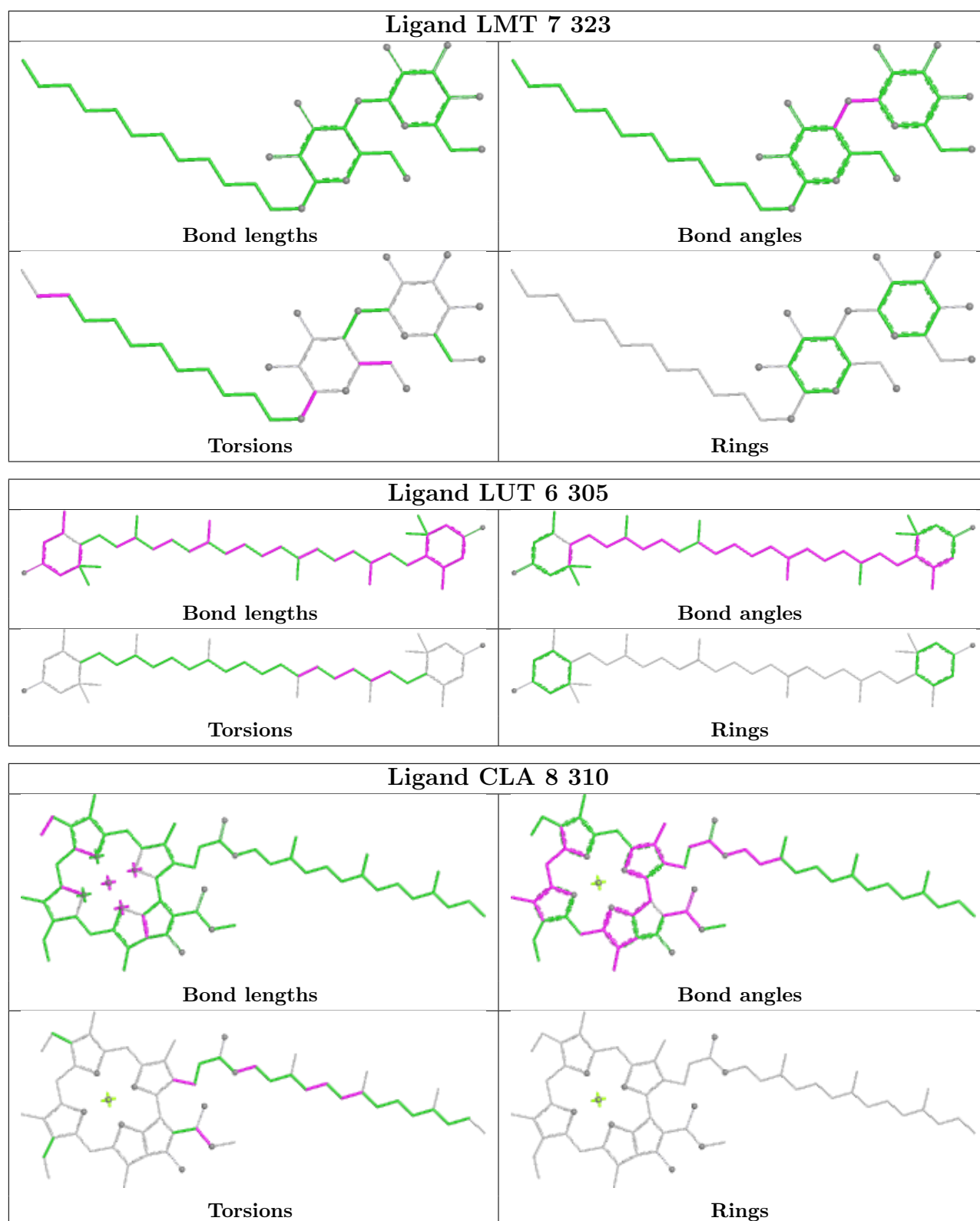


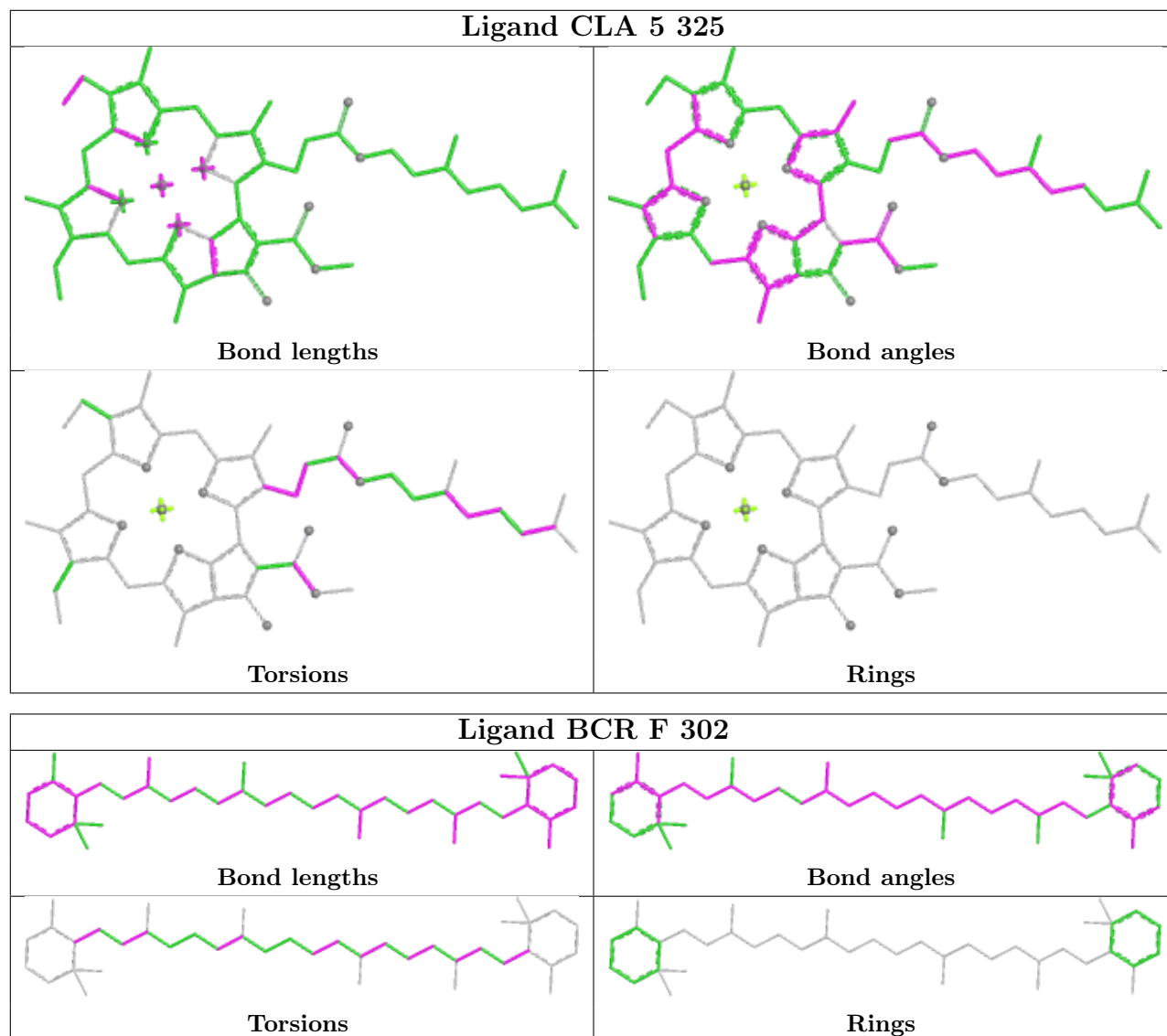
Torsions



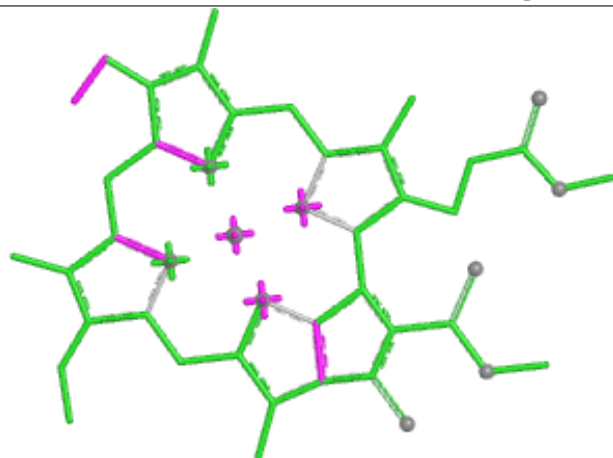
Rings



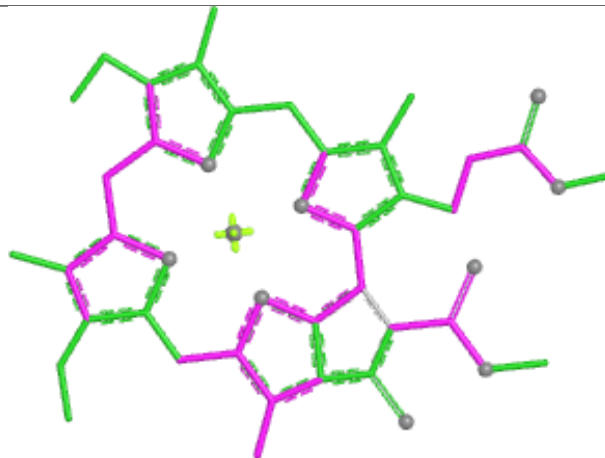




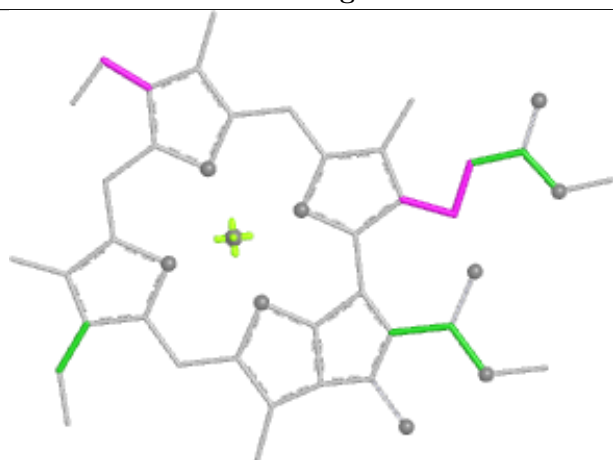
Ligand CLA 8 318



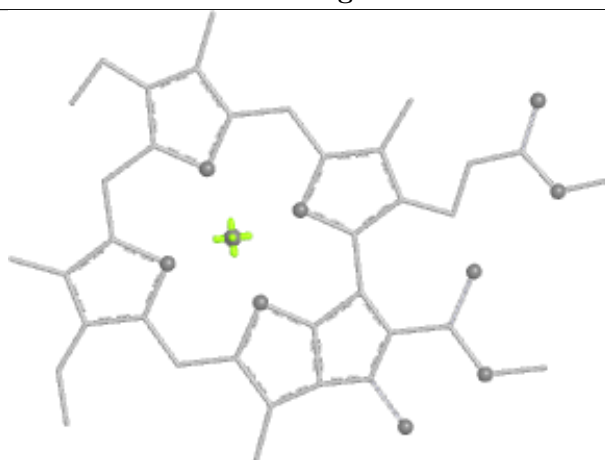
Bond lengths



Bond angles

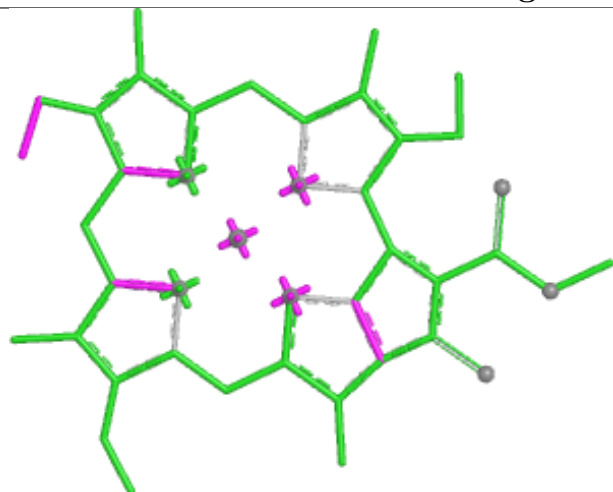


Torsions

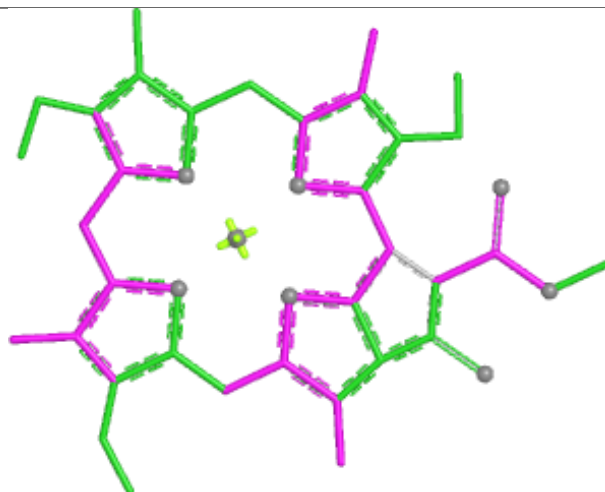


Rings

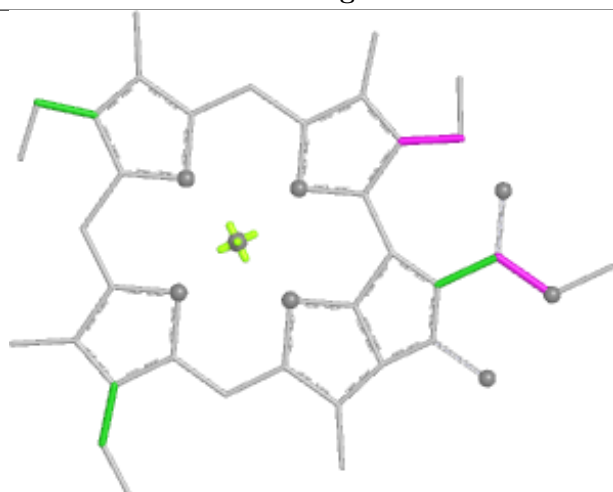
Ligand CLA 7 318



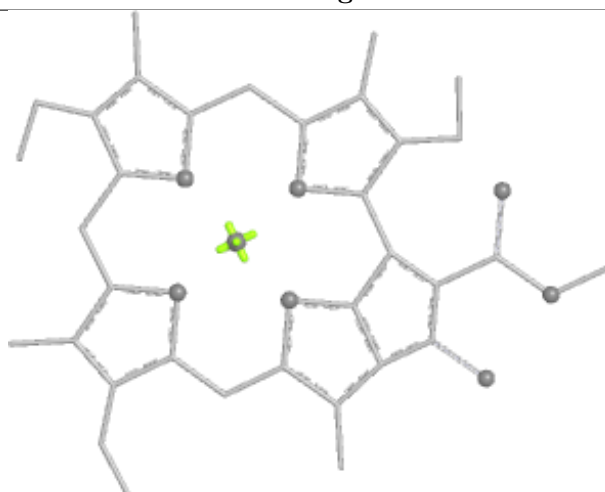
Bond lengths



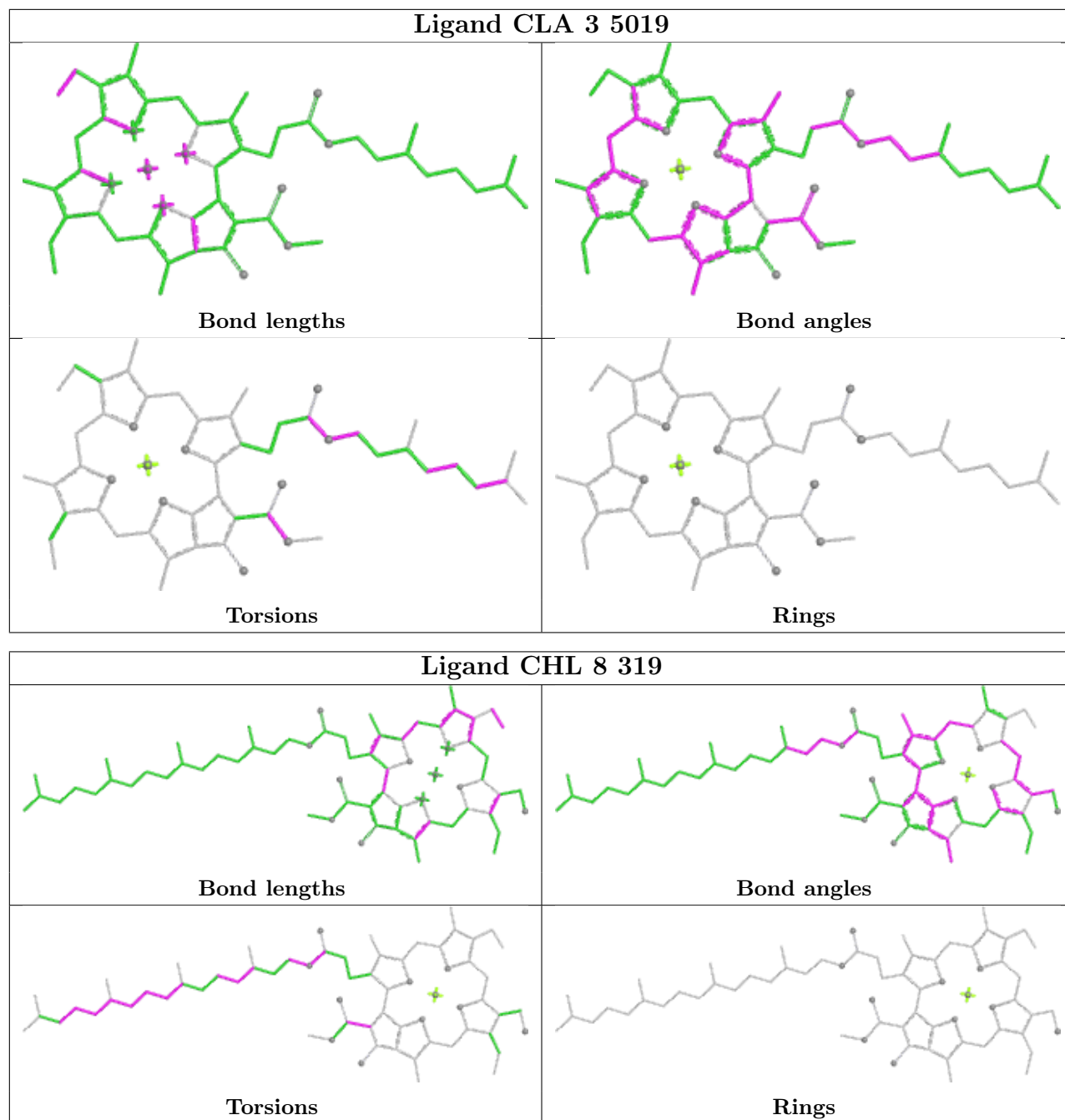
Bond angles



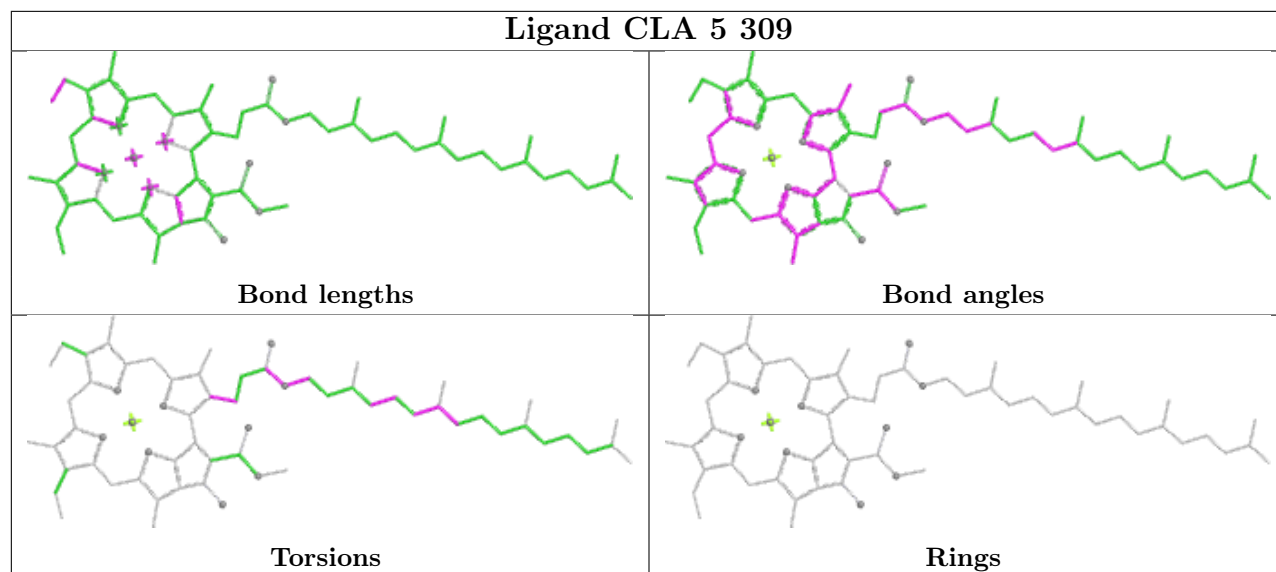
Torsions



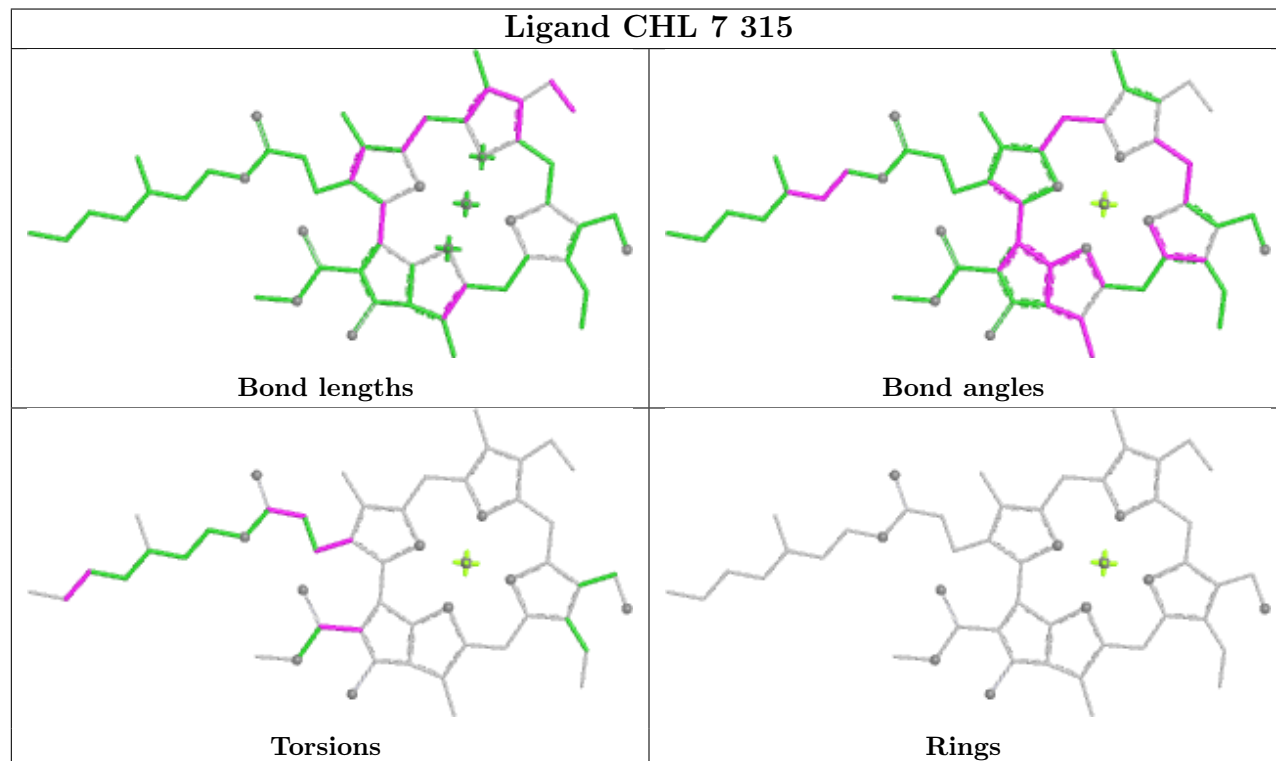
Rings

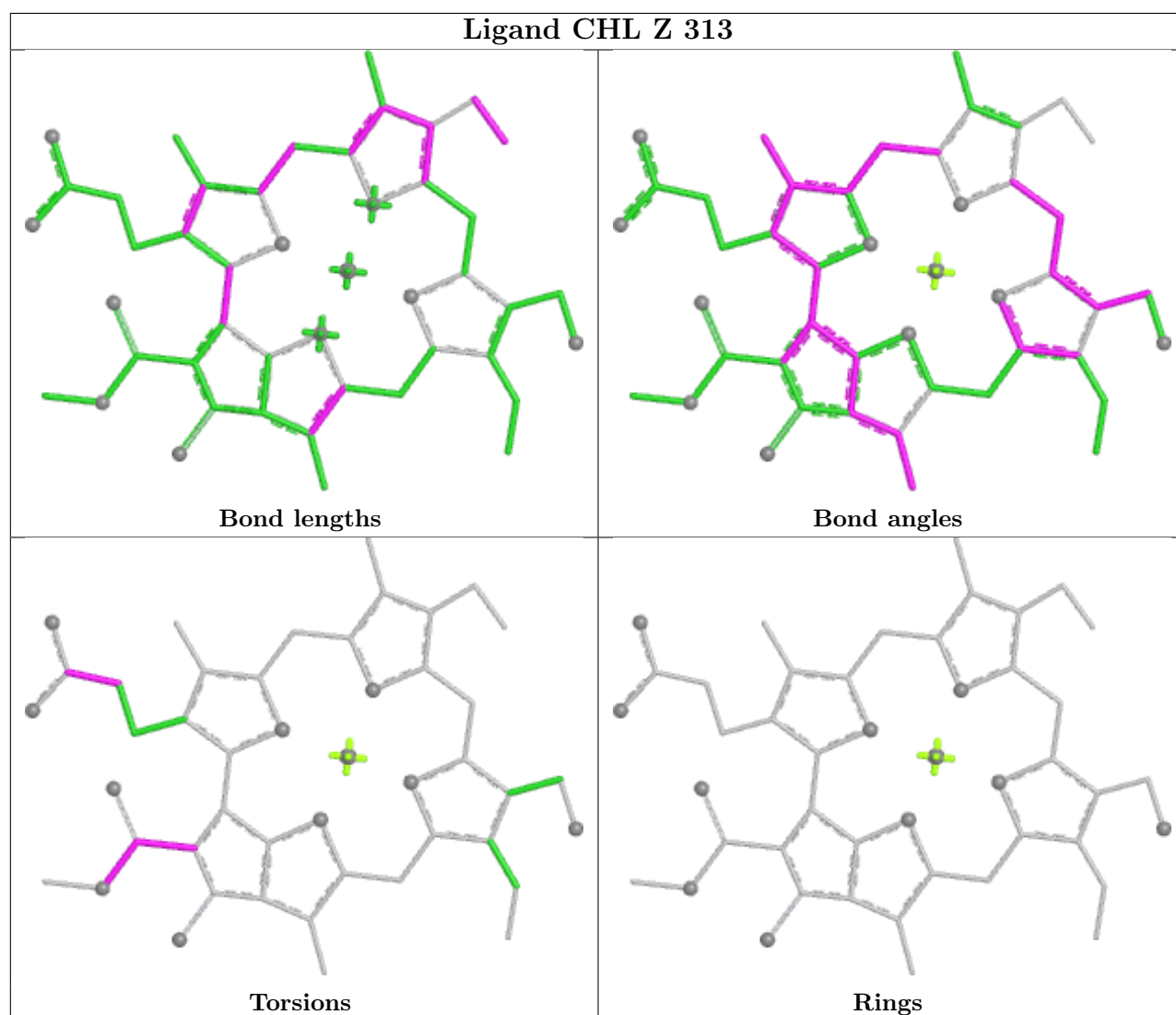
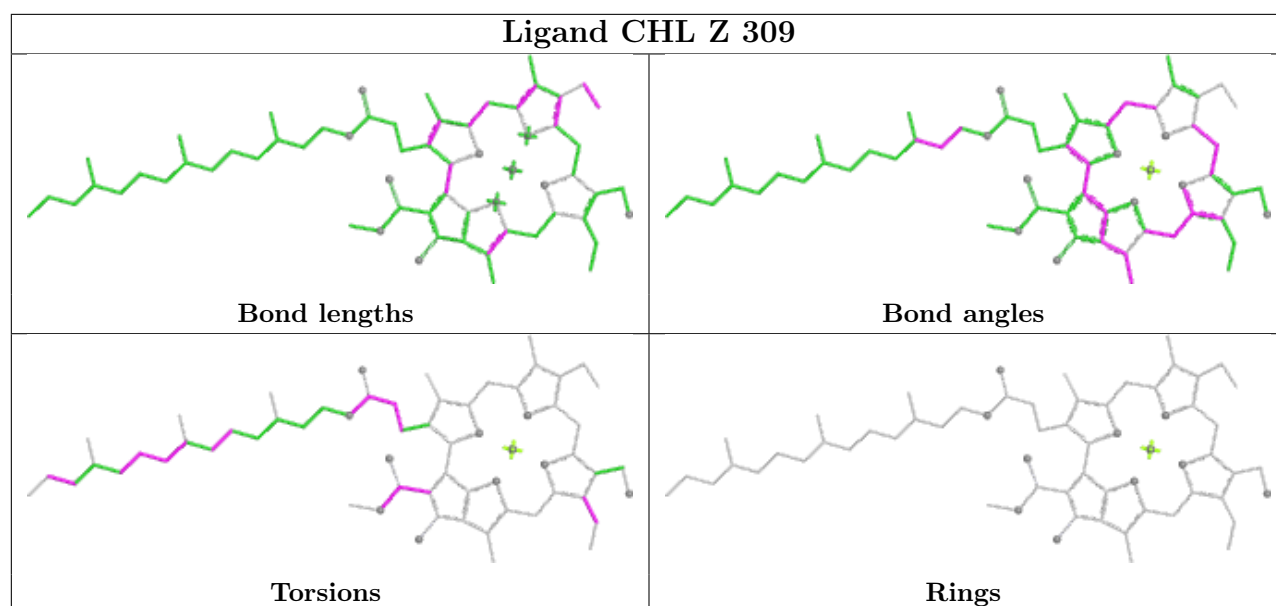


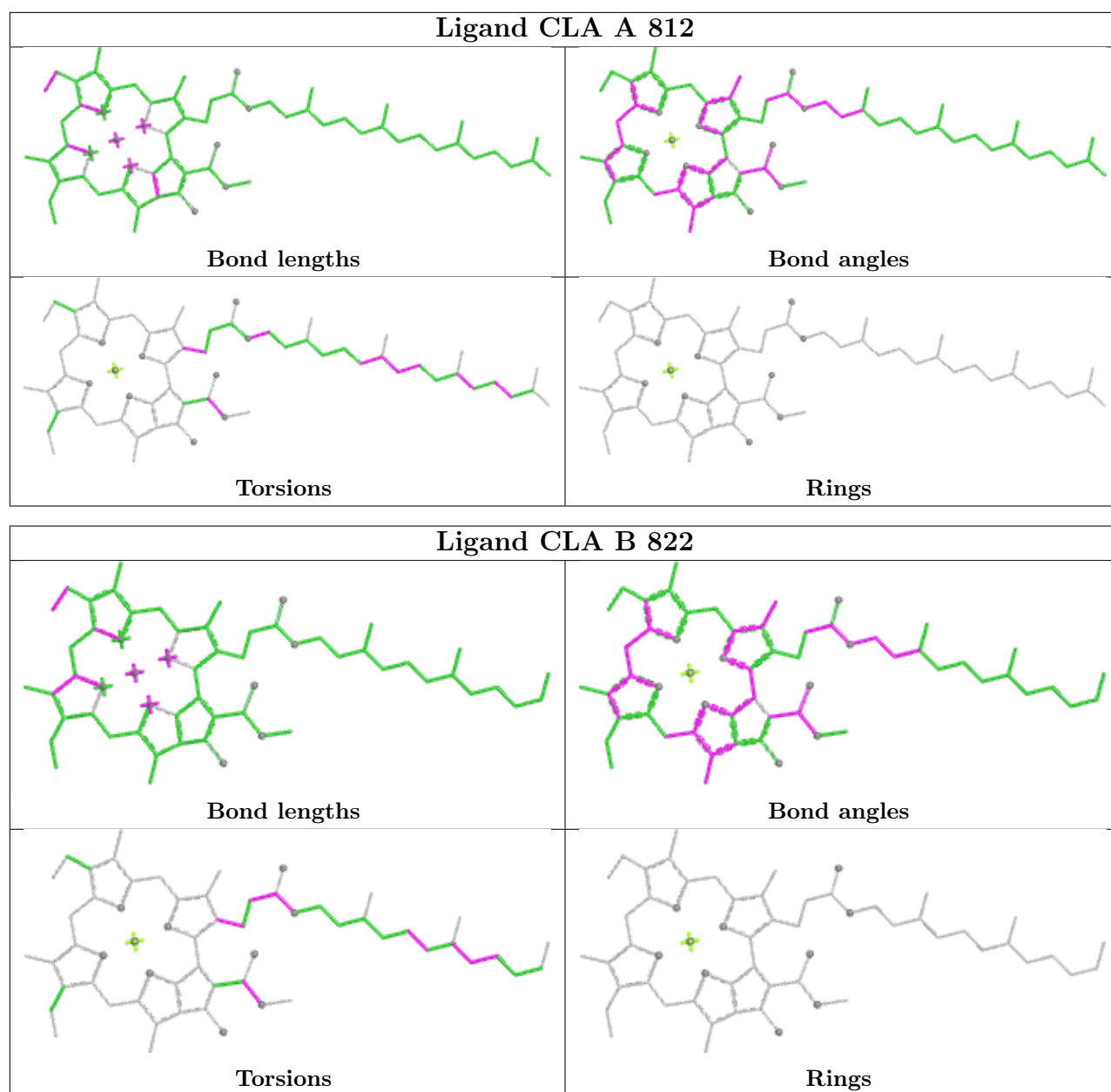
Ligand CLA 5 309



Ligand CHL 7 315







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.

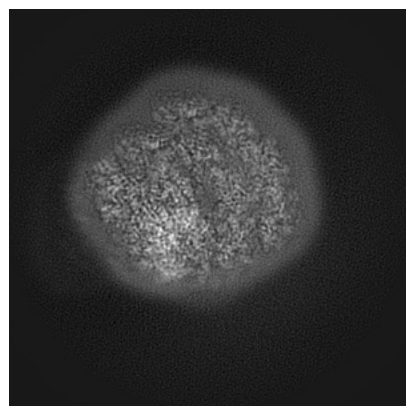
6 Map visualisation [i](#)

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.

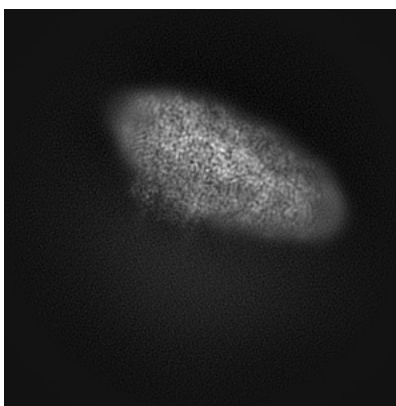
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

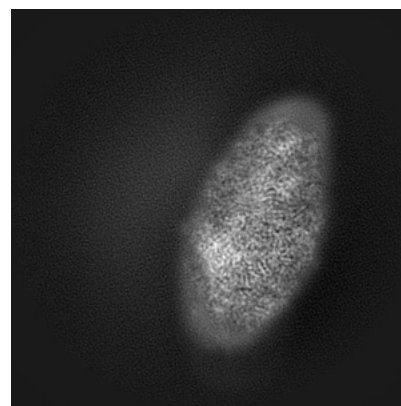
6.1.1 Primary map



X

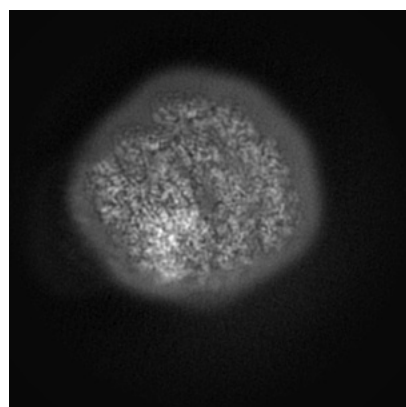


Y

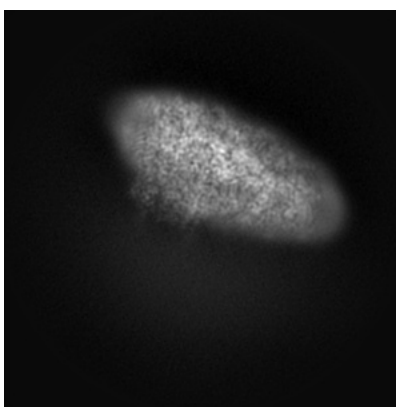


Z

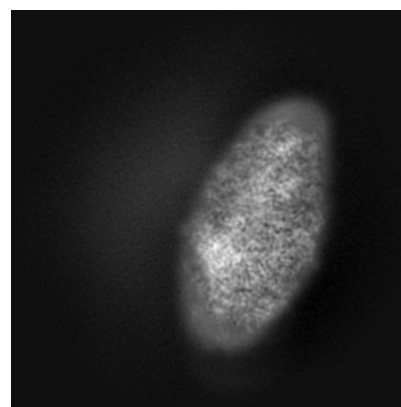
6.1.2 Raw map



X



Y

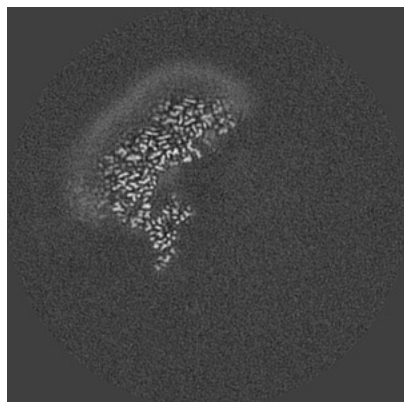


Z

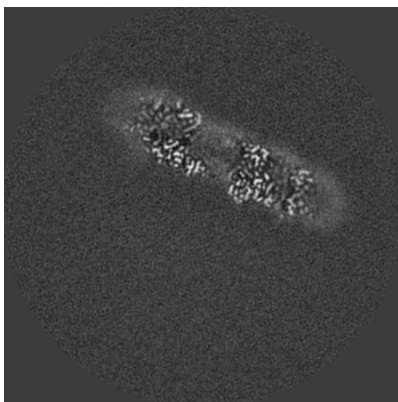
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

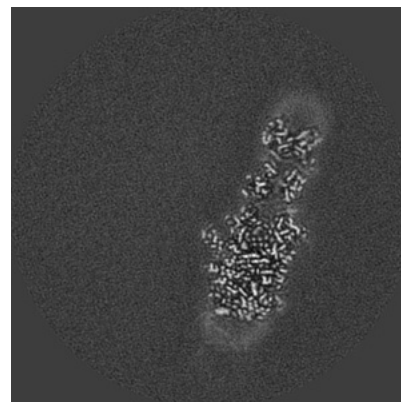
6.2.1 Primary map



X Index: 195

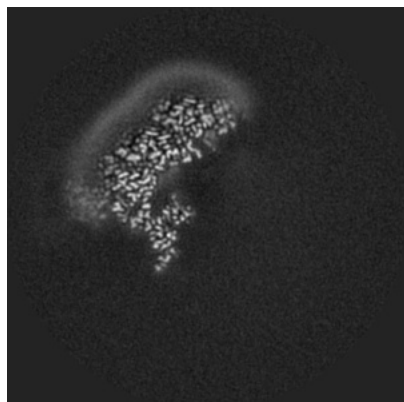


Y Index: 195

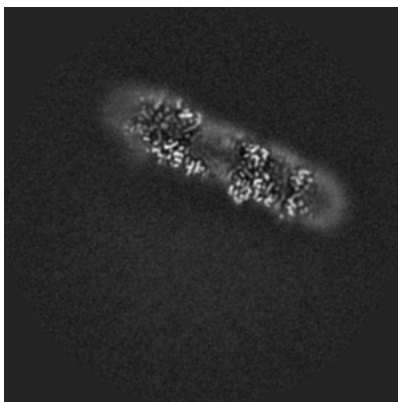


Z Index: 195

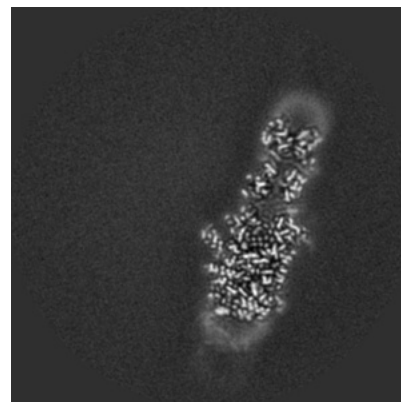
6.2.2 Raw map



X Index: 195



Y Index: 195

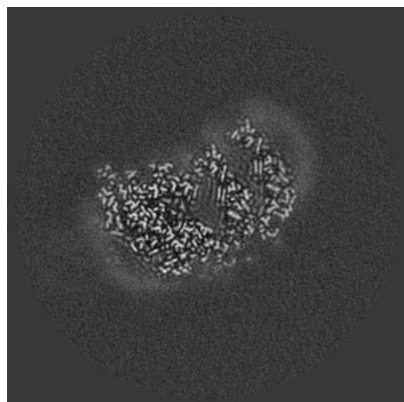


Z Index: 195

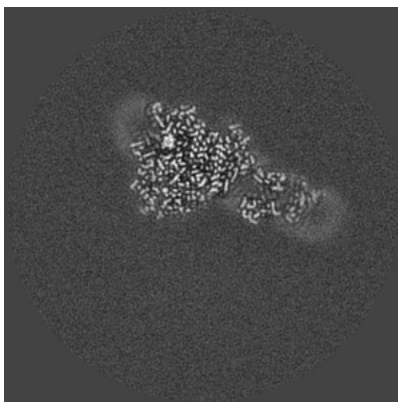
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

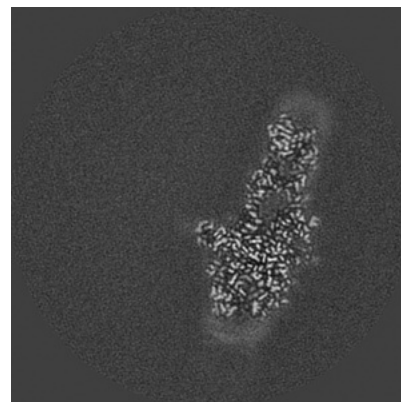
6.3.1 Primary map



X Index: 252

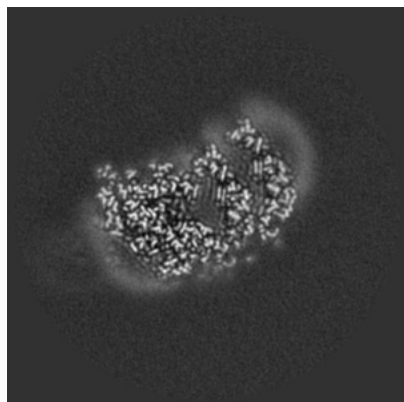


Y Index: 151

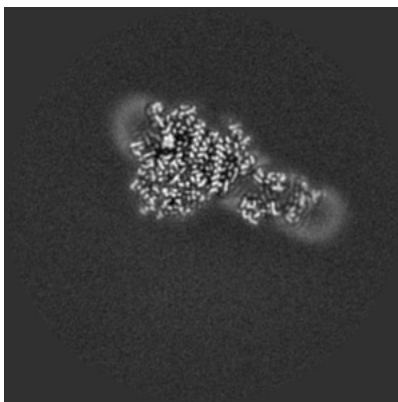


Z Index: 187

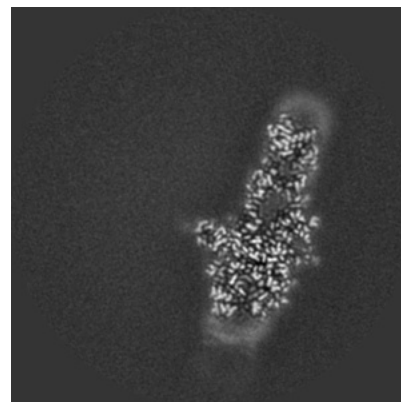
6.3.2 Raw map



X Index: 252



Y Index: 151

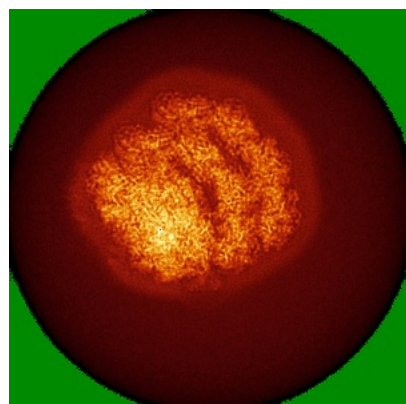


Z Index: 187

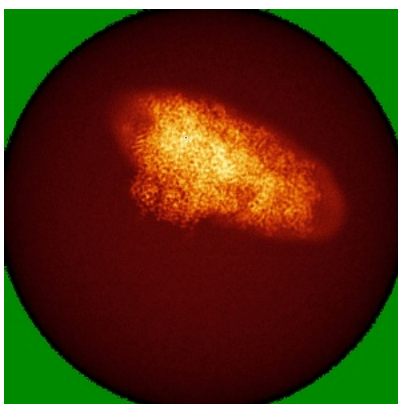
The images above show the largest variance slices of the map in three orthogonal directions.

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

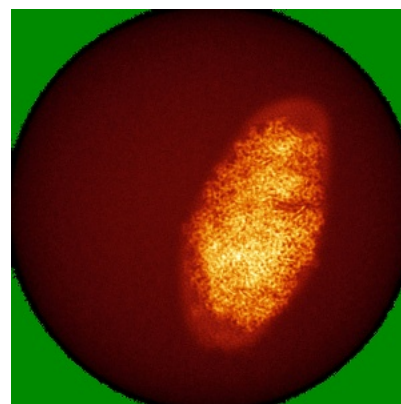
6.4.1 Primary map



X

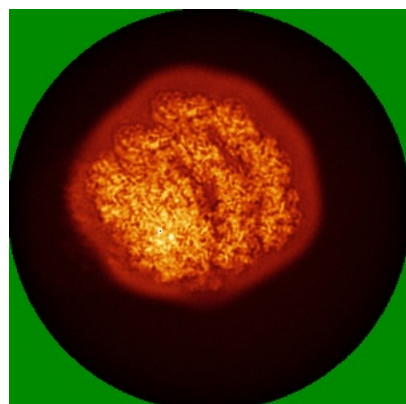


Y



Z

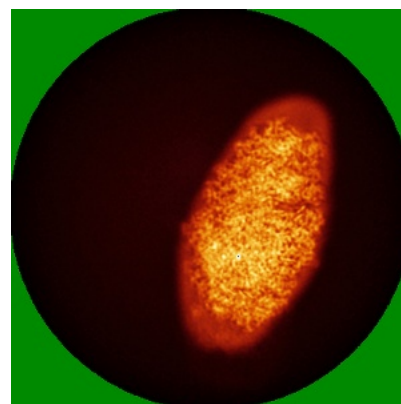
6.4.2 Raw map



X



Y

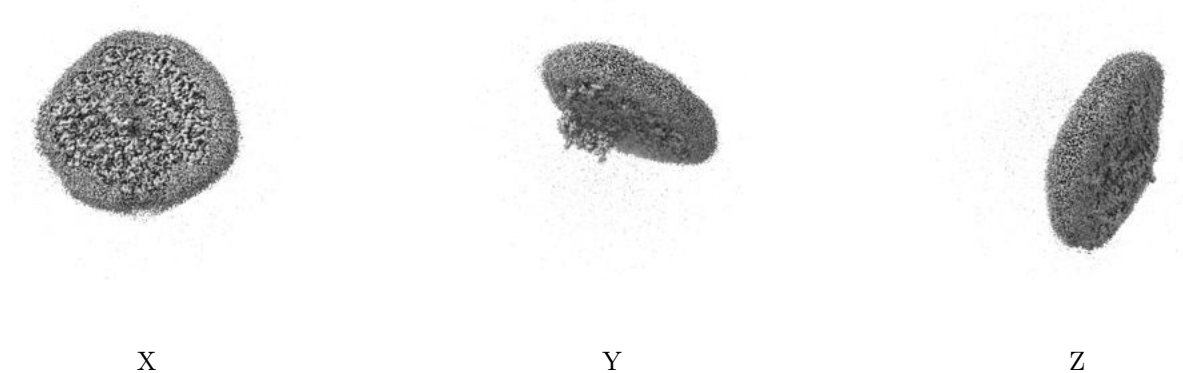


Z

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

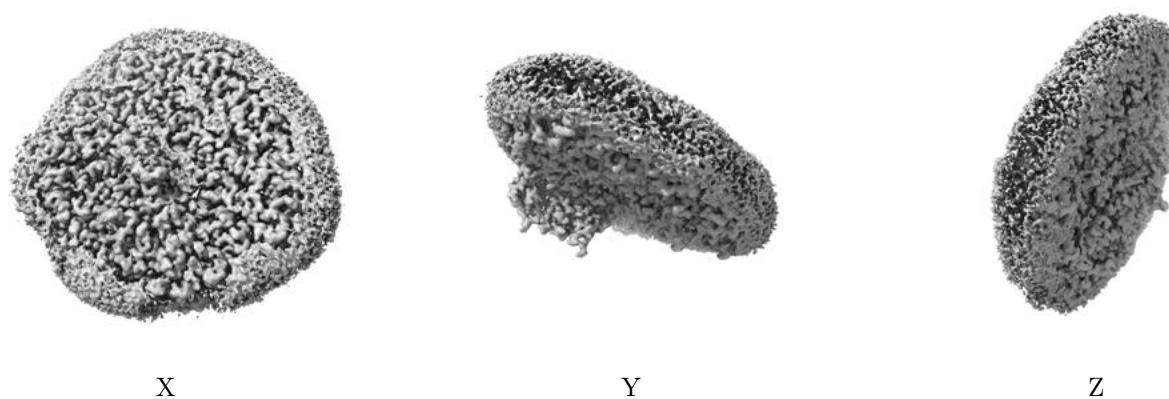
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

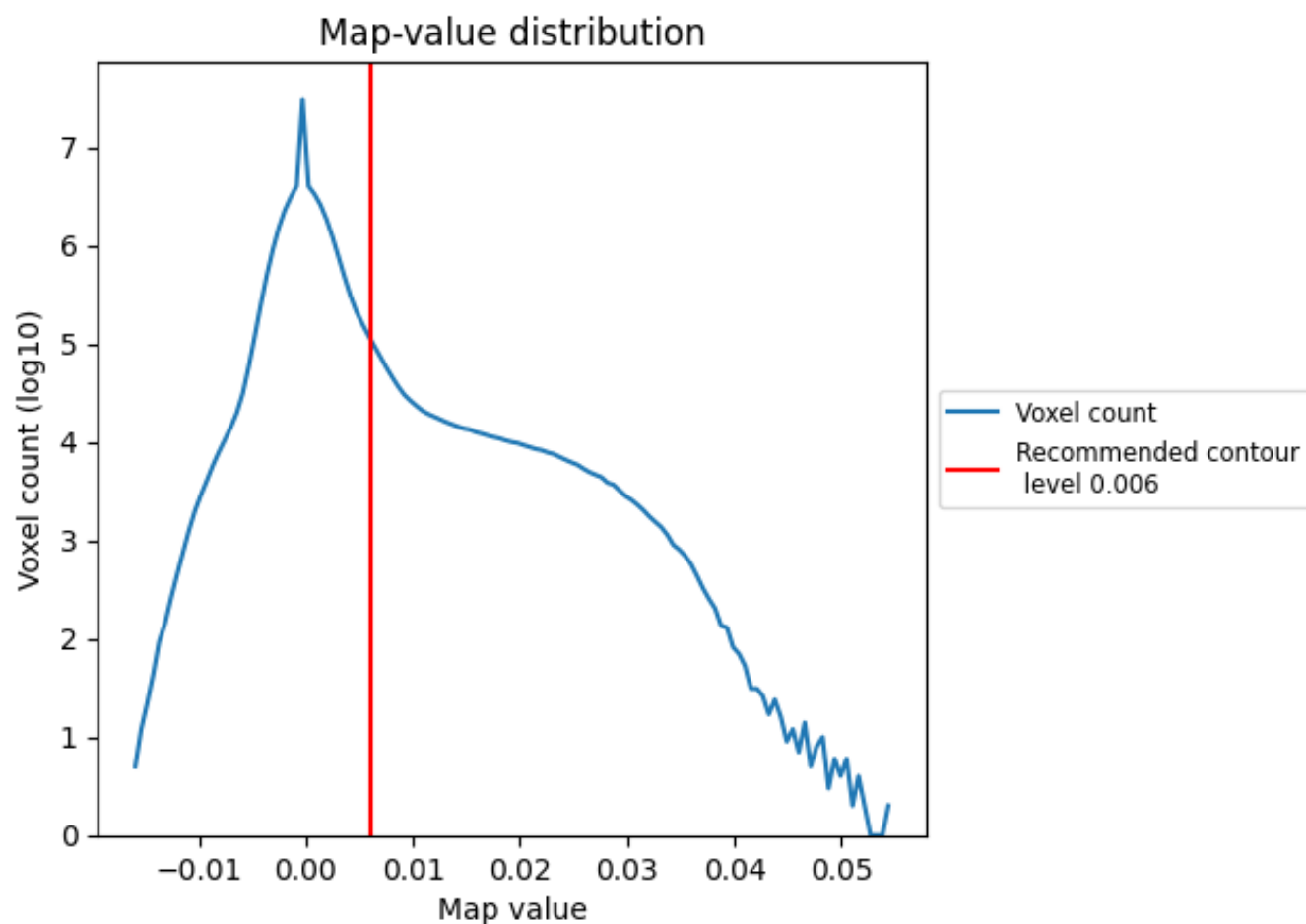
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

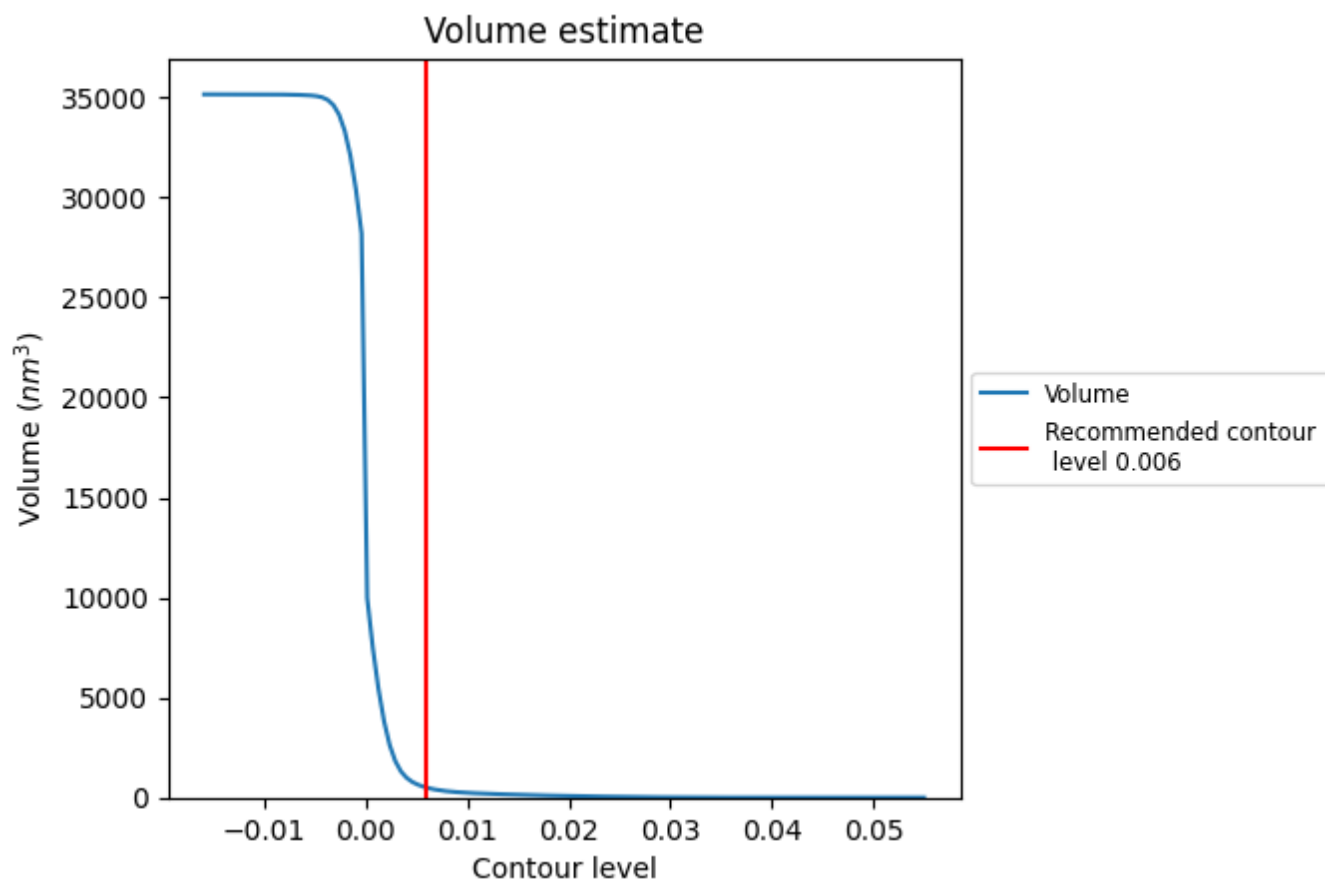
This section contains the results of statistical analysis of the map.

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.

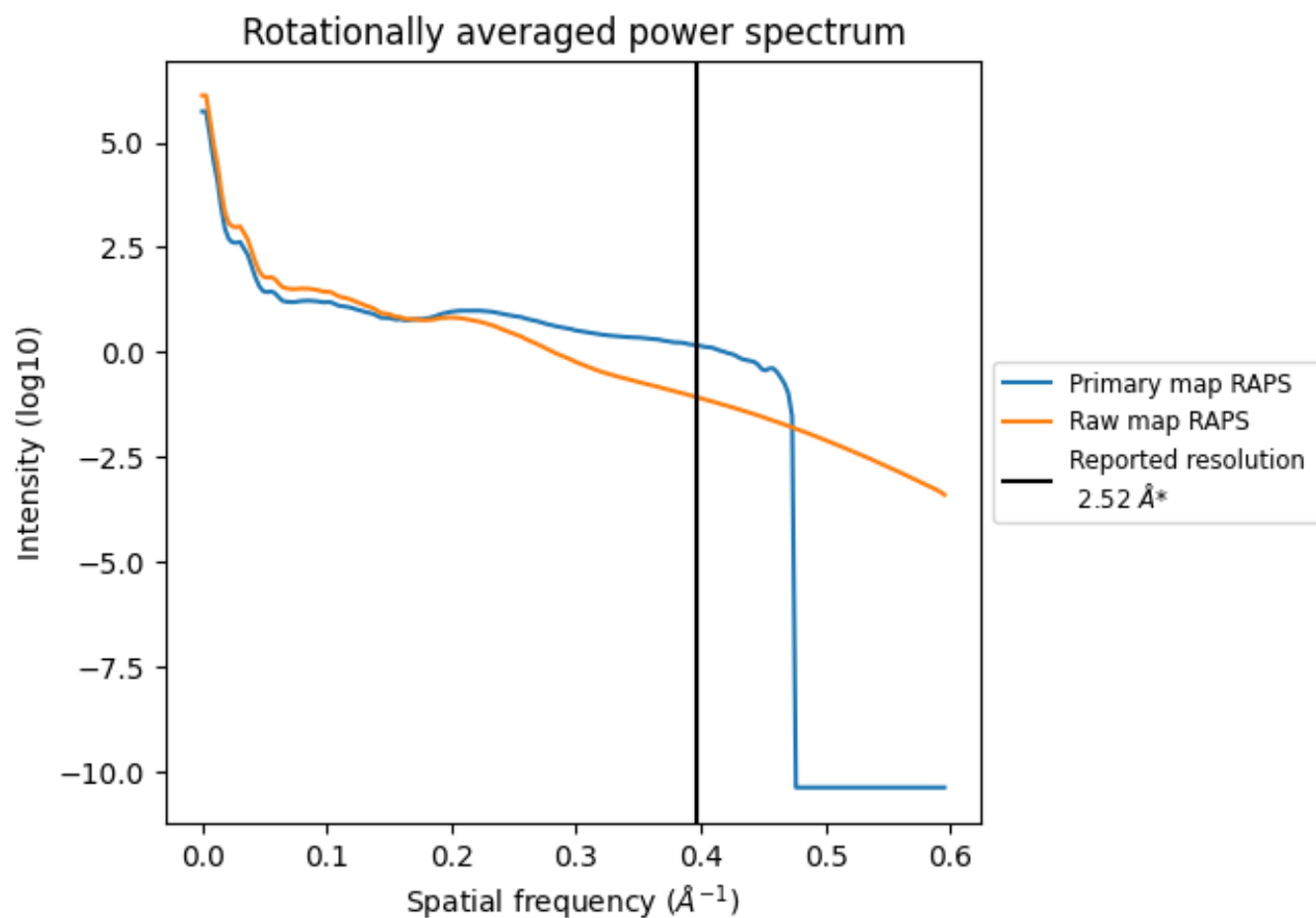
7.2 Volume estimate [i](#)



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 ⓘ

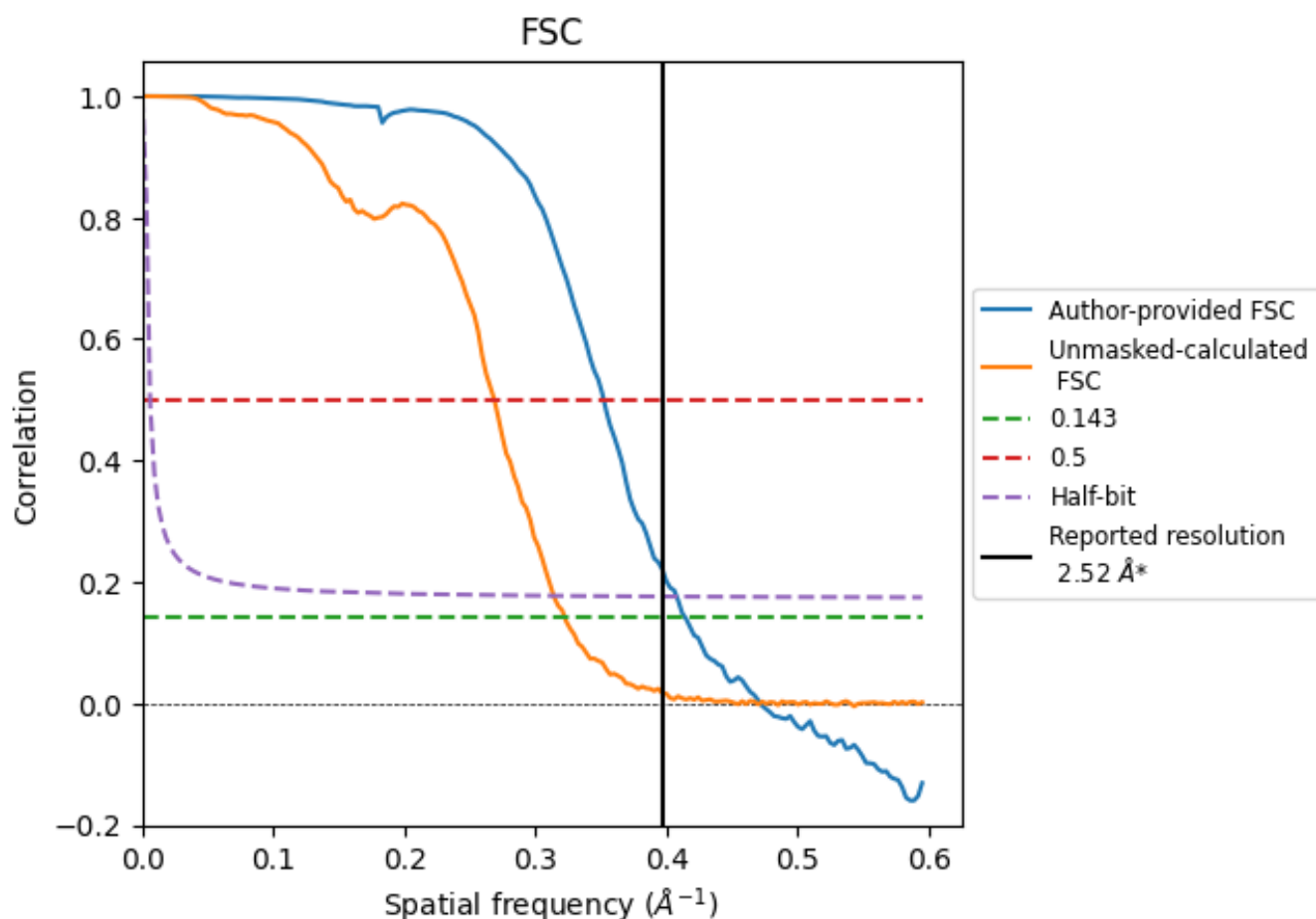


*Reported resolution corresponds to spatial frequency of $0.397 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.397 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

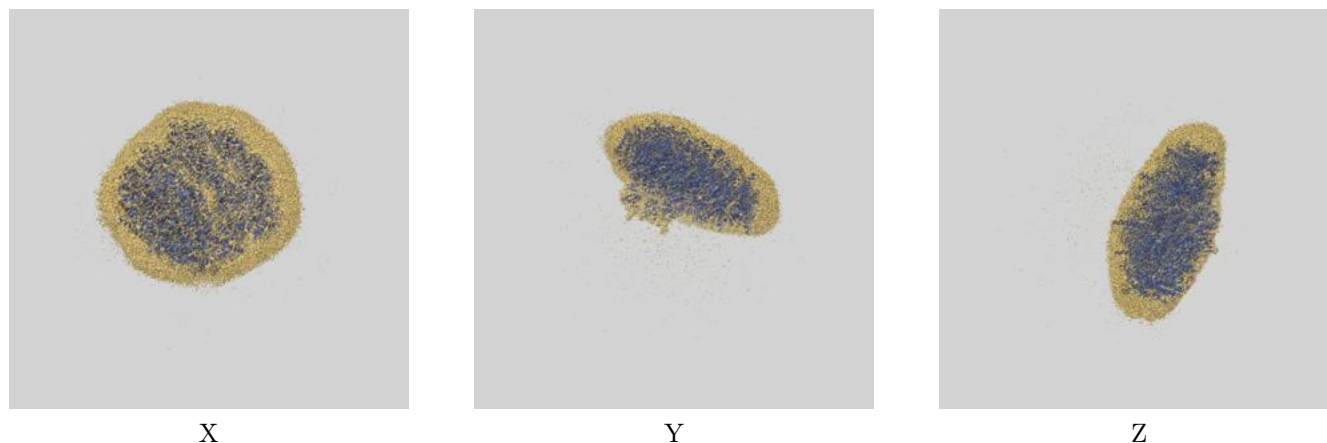
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.52	-	-
Author-provided FSC curve	2.42	2.84	2.45
Unmasked-calculated*	3.10	3.72	3.18

*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](#)

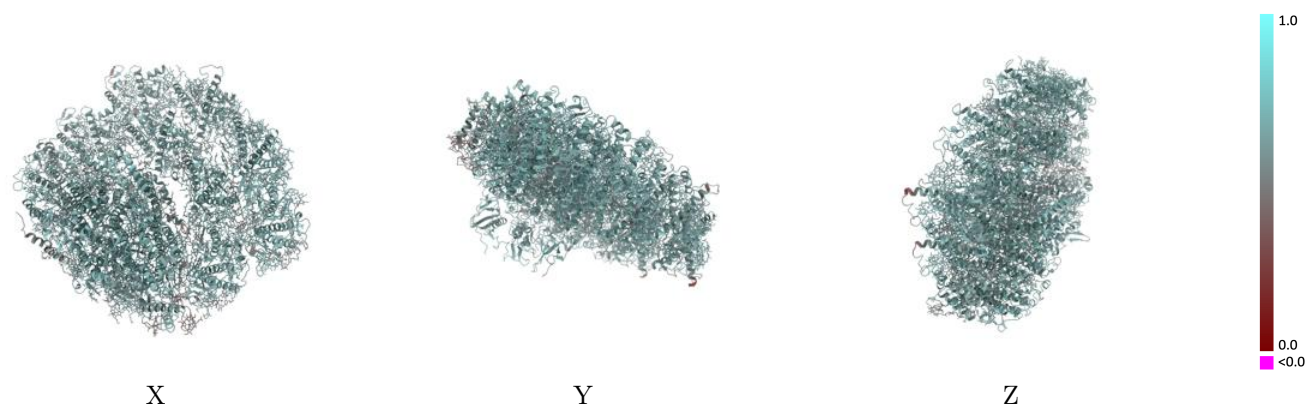
This section contains information regarding the fit between EMDB map EMD-14248 and PDB model 7R3K. Per-residue inclusion information can be found in section [3](#) on page [38](#).

9.1 Map-model overlay [i](#)



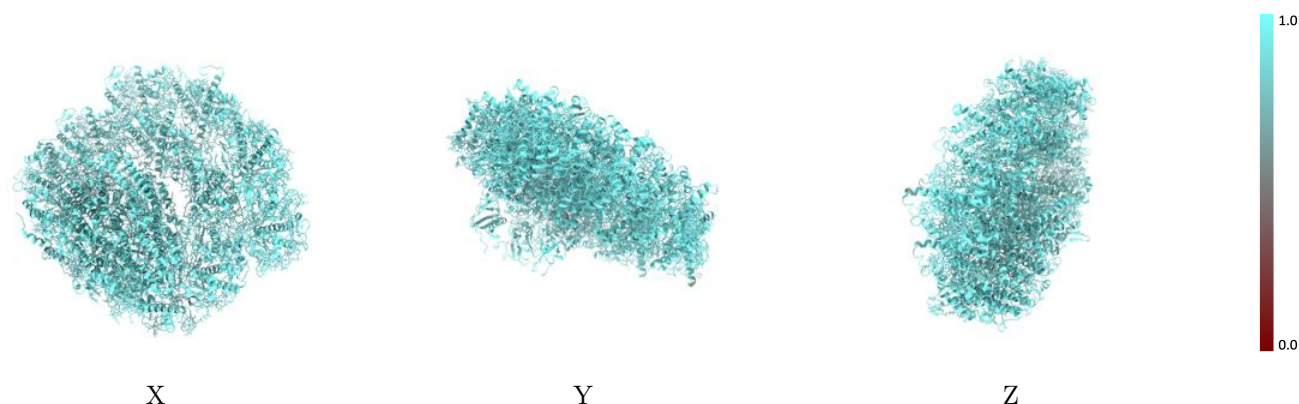
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



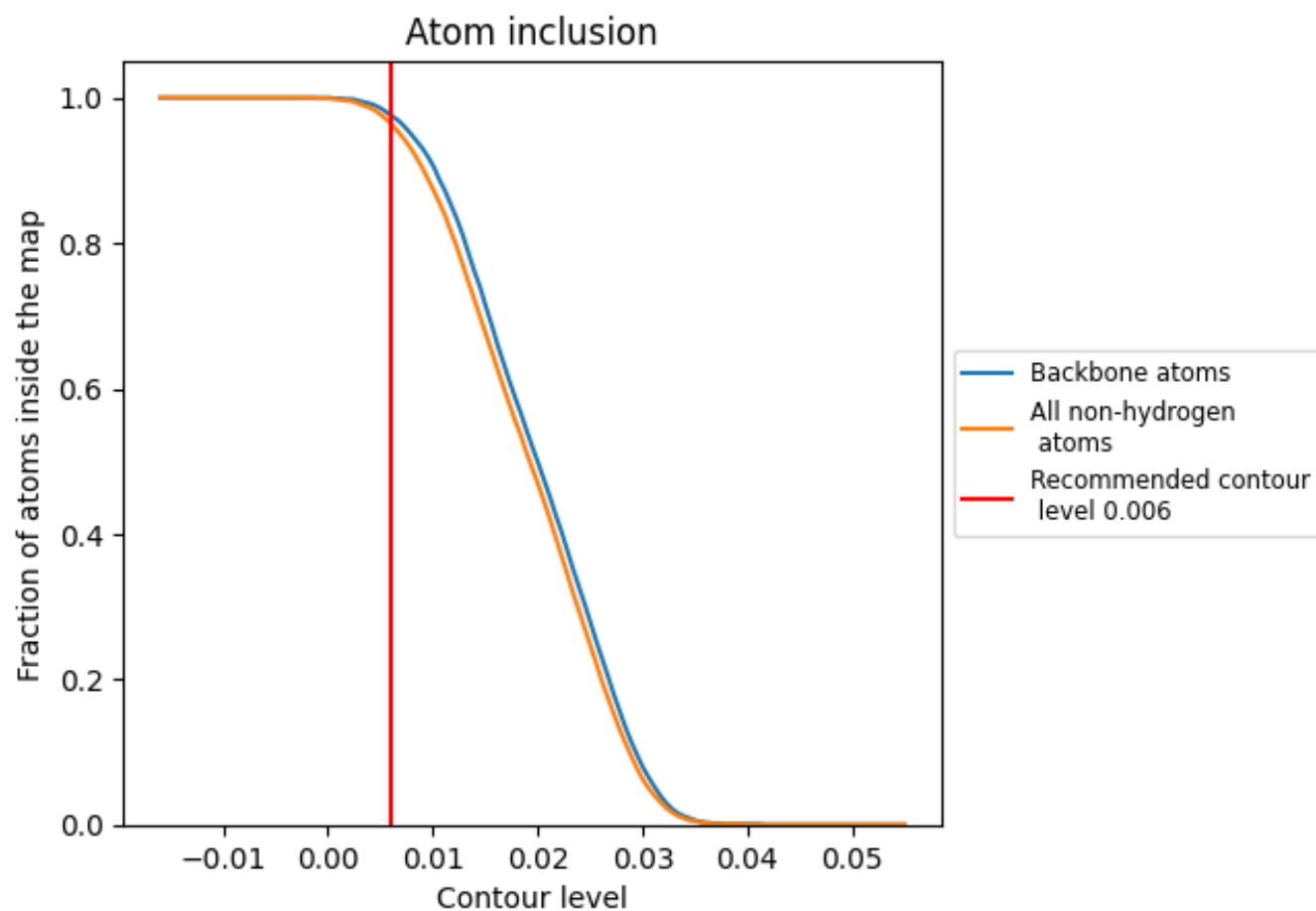
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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

