



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:55 AM UTC

PDB ID : 8ASL / pdb_00008asl
EMDB ID : EMD-15618
Title : RCII/PSI complex, class 2
Authors : Zhao, Z.; Vercellino, I.; Knoppova, J.; Sobotka, R.; Murray, J.W.; Nixon, P.J.;
Sazanov, L.A.; Komenda, J.
Deposited on : 2022-08-19
Resolution : 3.15 Å (reported)
Based on initial models : 2XBG, 6WJ6, 5OY0

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

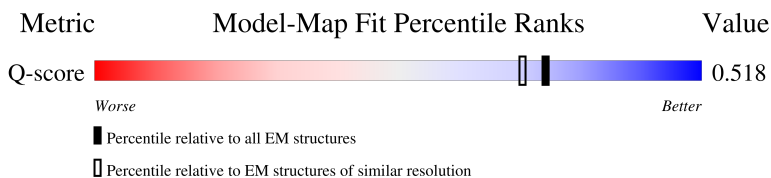
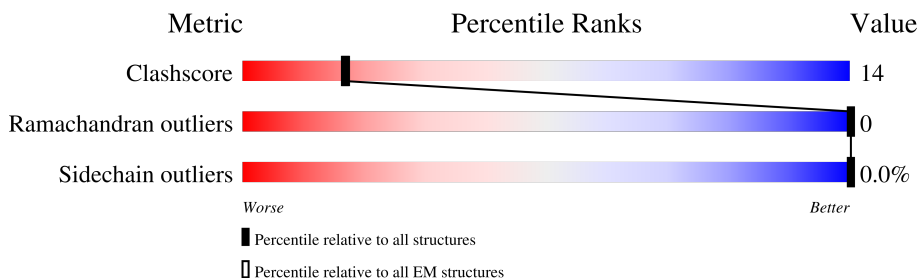
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.15 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	14486 (2.65 - 3.65)

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	 73% 26% .
2	b	731	 79% 21%
3	c	81	 68% 31% .
4	d	141	 78% 21% .

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Mol	Chain	Length	Quality of chain
5	e	74	
6	f	165	
7	i	40	
8	j	40	
9	k	86	
10	l	157	
11	m	31	
12	A	344	
13	D	336	
14	E	81	
15	F	44	
16	I	38	
17	S	342	

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	A	402	X	-	-	-
19	CLA	A	403	X	-	-	-
19	CLA	A	405	X	-	-	-
19	CLA	D	401	X	-	-	-
19	CLA	D	403	X	-	-	-
19	CLA	D	404	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	a	810	X	-	-	-
19	CLA	a	811	X	-	-	-
19	CLA	a	812	X	-	-	-
19	CLA	a	813	X	-	-	-
19	CLA	a	815	X	-	-	-
19	CLA	a	816	X	-	-	-
19	CLA	a	817	X	-	-	-
19	CLA	a	818	X	-	-	-
19	CLA	a	819	X	-	-	-
19	CLA	a	820	X	-	-	-
19	CLA	a	821	X	-	-	-
19	CLA	a	822	X	-	-	-
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	-	-	-
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	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	855	X	-	-	-
19	CLA	a	856	X	-	-	-
19	CLA	a	858	X	-	-	-
19	CLA	b	3002	X	-	-	-
19	CLA	b	3003	X	-	-	-
19	CLA	b	3004	X	-	-	-
19	CLA	b	3005	X	-	-	-
19	CLA	b	3006	X	-	-	-
19	CLA	b	3007	X	-	-	-
19	CLA	b	3008	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	b	3009	X	-	-	-
19	CLA	b	3010	X	-	-	-
19	CLA	b	3011	X	-	-	-
19	CLA	b	3012	X	-	-	-
19	CLA	b	3013	X	-	-	-
19	CLA	b	3014	X	-	-	-
19	CLA	b	3015	X	-	-	-
19	CLA	b	3016	X	-	-	-
19	CLA	b	3017	X	-	-	-
19	CLA	b	3018	X	-	-	-
19	CLA	b	3019	X	-	-	-
19	CLA	b	3020	X	-	-	-
19	CLA	b	3021	X	-	-	-
19	CLA	b	3022	X	-	-	-
19	CLA	b	3023	X	-	-	-
19	CLA	b	3024	X	-	-	-
19	CLA	b	3025	X	-	-	-
19	CLA	b	3026	X	-	-	-
19	CLA	b	3027	X	-	-	-
19	CLA	b	3028	X	-	-	-
19	CLA	b	3029	X	-	-	-
19	CLA	b	3030	X	-	-	-
19	CLA	b	3031	X	-	-	-
19	CLA	b	3032	X	-	-	-
19	CLA	b	3033	X	-	-	-
19	CLA	b	3034	X	-	-	-
19	CLA	b	3035	X	-	-	-
19	CLA	b	3036	X	-	-	-
19	CLA	b	3037	X	-	-	-
19	CLA	b	3038	X	-	-	-
19	CLA	b	3039	X	-	-	-
19	CLA	b	3040	X	-	-	-
19	CLA	b	3041	X	-	-	-
19	CLA	f	201	X	-	-	-
19	CLA	f	203	X	-	-	-
19	CLA	f	204	X	-	-	-
19	CLA	j	102	X	-	-	-
19	CLA	j	103	X	-	-	-
19	CLA	k	4002	X	-	-	-
19	CLA	k	4003	X	-	-	-
19	CLA	l	1501	X	-	-	-
19	CLA	l	1502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	1	1503	X	-	-	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 32739 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	741	Total	C	N	O	S	0	0
			5795	3797	984	987	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	729	Total	C	N	O	S	0	0
			5770	3798	967	990	15		

- 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
			600	369	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	139	Total	C	N	O	S	0	0
			1087	688	188	208	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	e	69	Total	C	N	O	0	0
			538	337	95	106		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	142	Total	C	N	O	S	0	0
			1108	715	184	204	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	40	Total	C	N	O	S	0	0
			311	209	44	55	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	40	Total	C	N	O	S	0	0
			319	215	47	54	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	k	75	Total	C	N	O	S	0	0
			524	343	87	90	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	143	Total	C	N	O	S	0	0
			1069	697	173	197	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

- Molecule 12 is a protein called Photosystem II protein D1 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	289	Total	C	N	O	S	0	0
			2248	1478	366	389	15		

- Molecule 13 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	278	Total	C	N	O	S	0	0
			2188	1465	351	360	12		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	MET	-	initiating methionine	UNP P09192
D	-4	HIS	-	expression tag	UNP P09192
D	-3	HIS	-	expression tag	UNP P09192
D	-2	HIS	-	expression tag	UNP P09192
D	-1	HIS	-	expression tag	UNP P09192
D	0	HIS	-	expression tag	UNP P09192
D	1	HIS	-	expression tag	UNP P09192

- Molecule 14 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	44	Total	C	N	O	S	0	0
			360	245	54	60	1		

- Molecule 15 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	28	Total	C	N	O	S	0	0
			222	149	39	33	1		

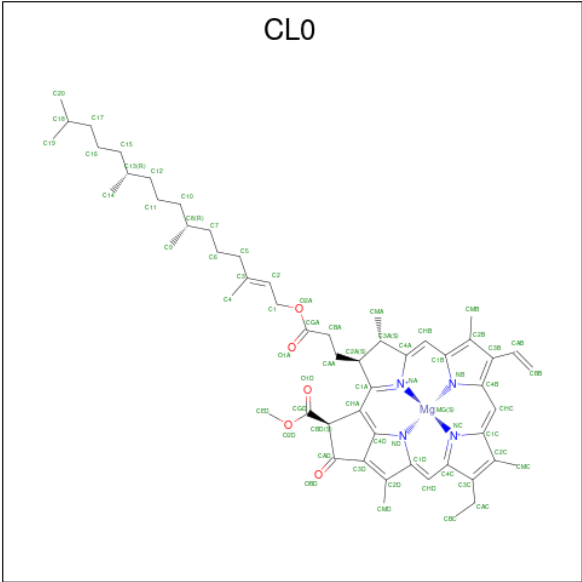
- Molecule 16 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	27	Total	C	N	O		0	0
			211	149	28	34			

- Molecule 17 is a protein called Photosystem II assembly lipoprotein Ycf48.

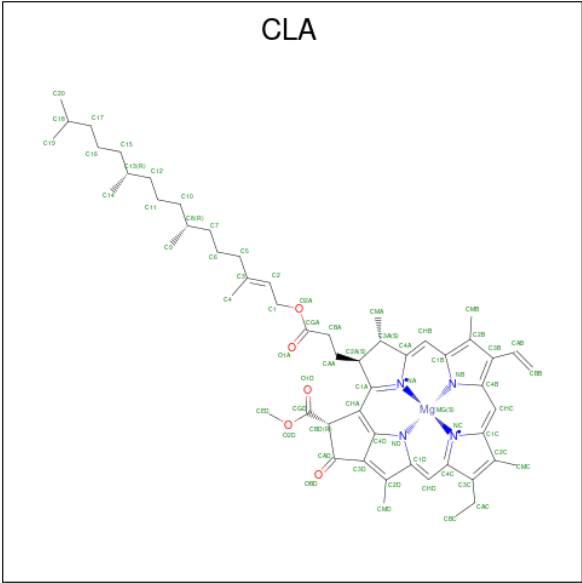
Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	303	Total	C	N	O	S	0	0
			2328	1481	393	451	3		

- Molecule 18 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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) (labeled as "Ligand of Interest" by depositor).



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	

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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
			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
			51	41	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
			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
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			46	36	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
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
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
			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
			56	46	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
			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
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	a	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 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 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	b	1	Total 50	C 40	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 56	C 46	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 60	C 50	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 60	C 50	Mg 1	N 4	O 5	0

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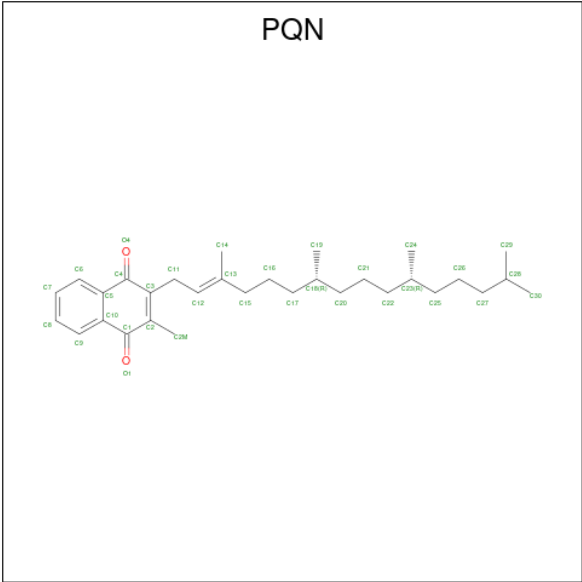
Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	b	1	Total 57	C 47	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	b	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	b	1	Total 50	C 40	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 50	C 40	Mg 1	N 4	O 5	0
19	b	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 50	C 40	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 46	C 36	Mg 1	N 4	O 5	0
19	f	1	Total 65	C 55	Mg 1	N 4	O 5	0

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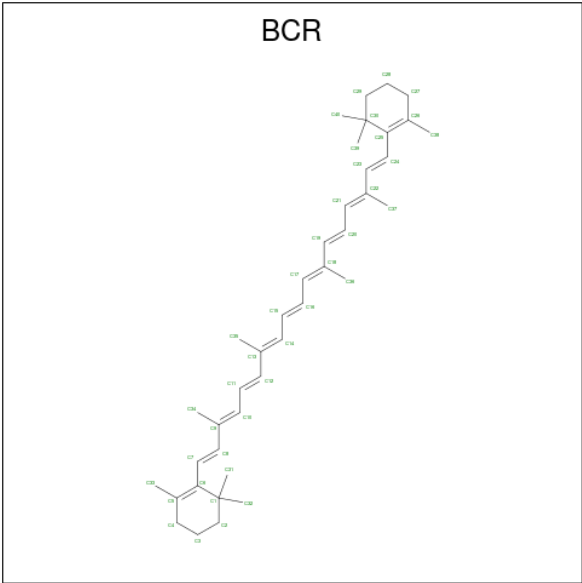
Mol	Chain	Residues	Atoms					AltConf
19	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	k	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			52	42	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
			46	36	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	D	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 20 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



Mol	Chain	Residues	Atoms		AltConf
20	a	1	Total	C	O
			33	31	2
20	b	1	Total	C	O
			33	31	2

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



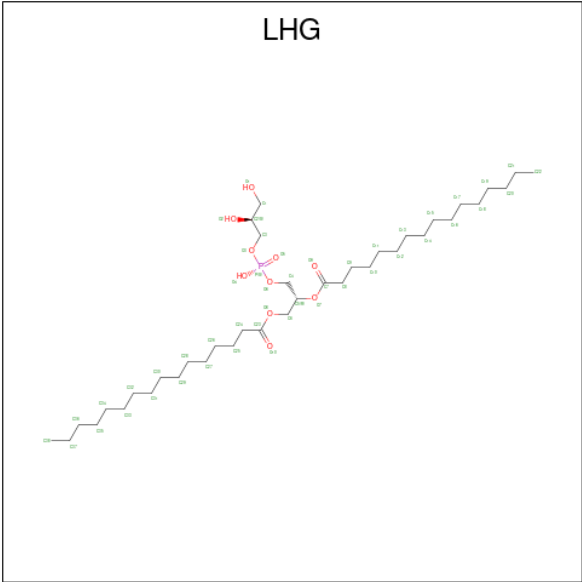
Mol	Chain	Residues	Atoms		AltConf
21	a	1	Total	C	
			40	40	0
21	a	1	Total	C	
			40	40	0

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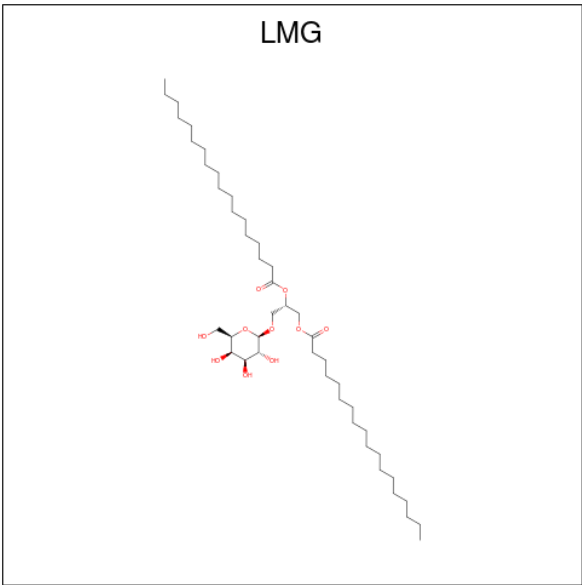
Mol	Chain	Residues	Atoms	AltConf
21	a	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	a	1	Total C 25 25	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	f	1	Total C 40 40	0
21	i	1	Total C 40 40	0
21	j	1	Total C 40 40	0
21	j	1	Total C 40 40	0
21	k	1	Total C 40 40	0
21	k	1	Total C 40 40	0
21	l	1	Total C 40 40	0
21	A	1	Total C 40 40	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



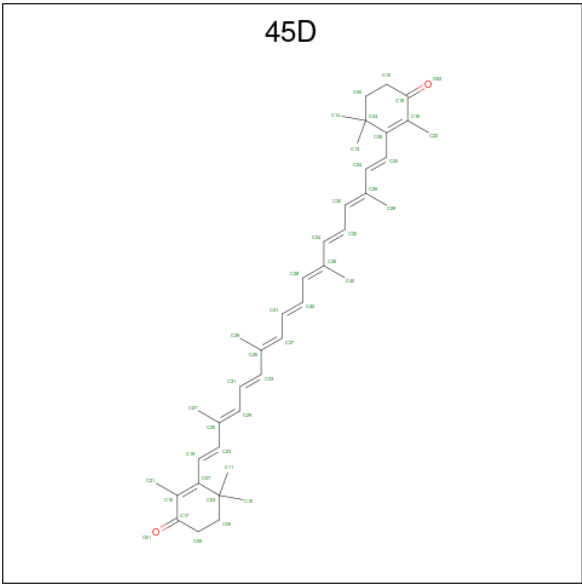
Mol	Chain	Residues	Atoms				AltConf
22	a	1	Total	C	O	P	0
			49	38	10	1	
22	a	1	Total	C	O	P	0
			49	38	10	1	
22	a	1	Total	C	O	P	0
			49	38	10	1	
22	b	1	Total	C	O	P	0
			38	27	10	1	
22	f	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



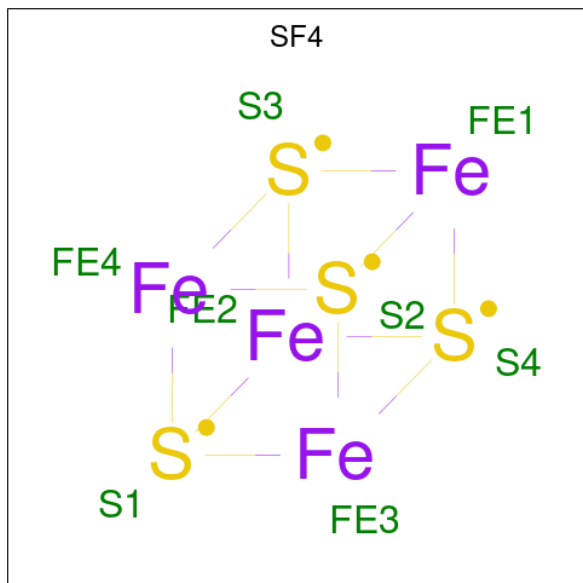
Mol	Chain	Residues	Atoms			AltConf
23	a	1	Total	C	O	0
			50	40	10	
23	a	1	Total	C	O	0
			40	30	10	
23	b	1	Total	C	O	0
			55	45	10	
23	b	1	Total	C	O	0
			55	45	10	

- Molecule 24 is beta,beta-carotene-4,4'-dione (CCD ID: 45D) (formula: C₄₀H₅₂O₂).



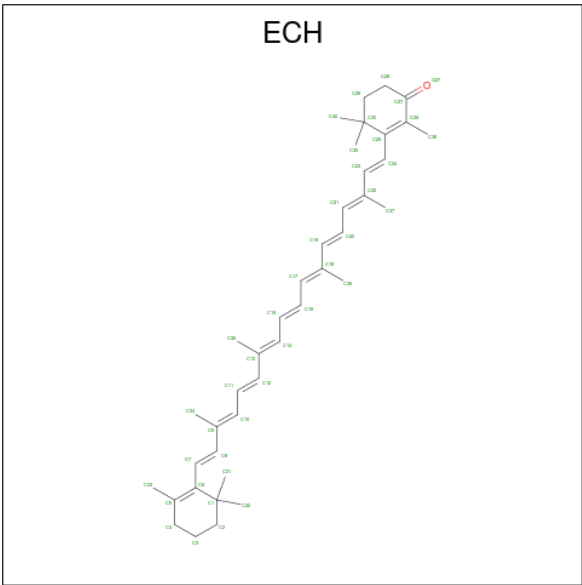
Mol	Chain	Residues	Atoms			AltConf
24	a	1	Total	C	O	0
			42	40	2	

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



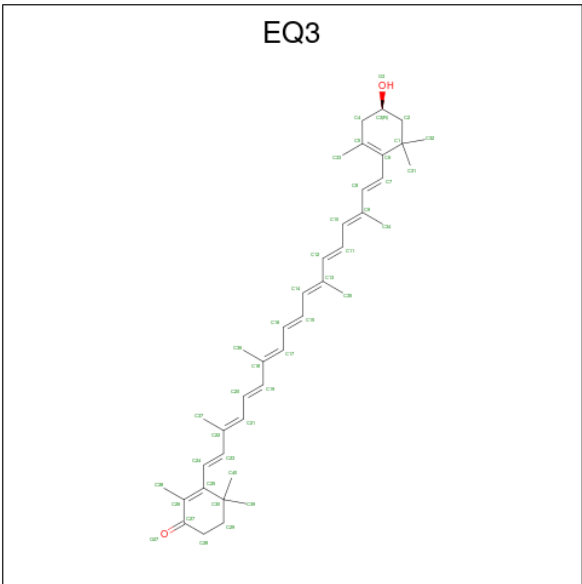
Mol	Chain	Residues	Atoms			AltConf
25	b	1	Total	Fe	S	0
			8	4	4	
25	c	1	Total	Fe	S	0
			8	4	4	
25	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 26 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: $\text{C}_{40}\text{H}_{54}\text{O}$).



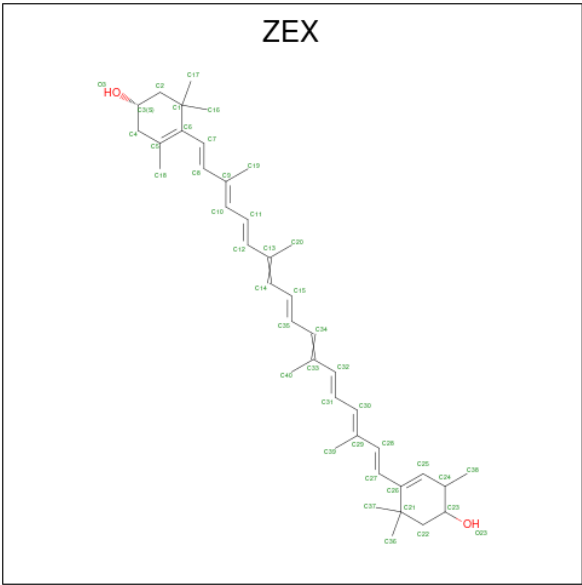
Mol	Chain	Residues	Atoms			AltConf
26	b	1	Total	C	O	0
			41	40	1	
26	m	1	Total	C	O	0
			41	40	1	

- Molecule 27 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (CCD ID: EQ3) (formula: C₄₀H₅₄O₂).



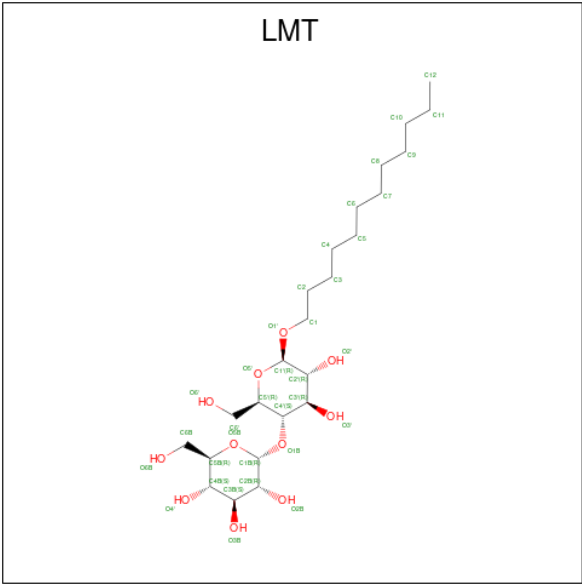
Mol	Chain	Residues	Atoms			AltConf
27	b	1	Total	C	O	0
			42	40	2	

- Molecule 28 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
28	b	1	Total	C	O	0
			42	40	2	
28	f	1	Total	C	O	0
			42	40	2	

- Molecule 29 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).

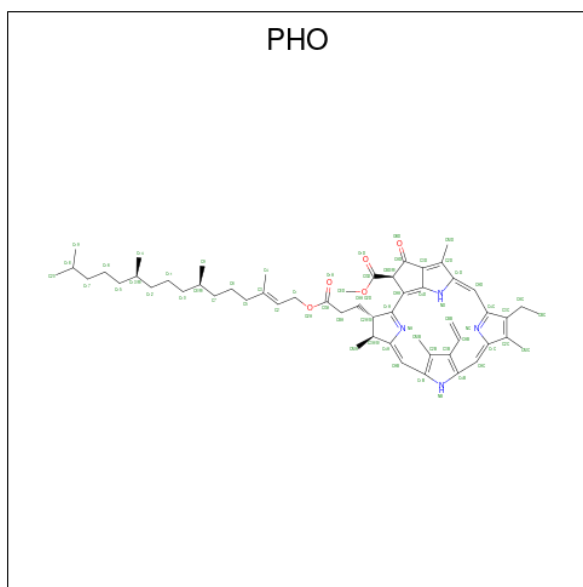


Mol	Chain	Residues	Atoms			AltConf
29	f	1	Total	C	O	0
			35	24	11	

- Molecule 30 is FE (II) ION (CCD ID: FE2) (formula: Fe).

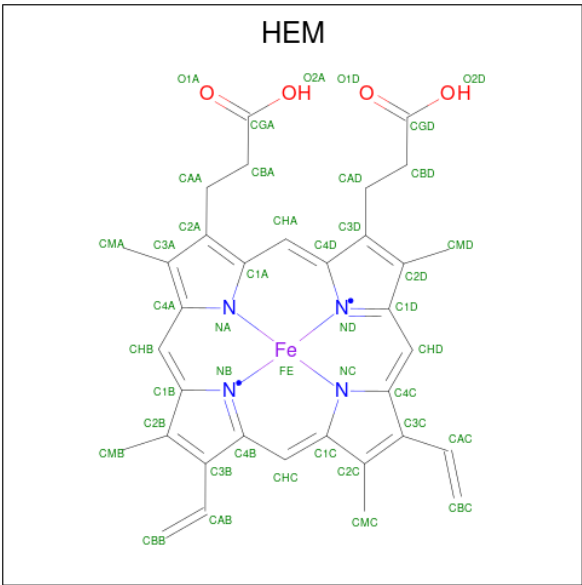
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	Fe		0
			1	1		

- Molecule 31 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



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

- Molecule 32 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).

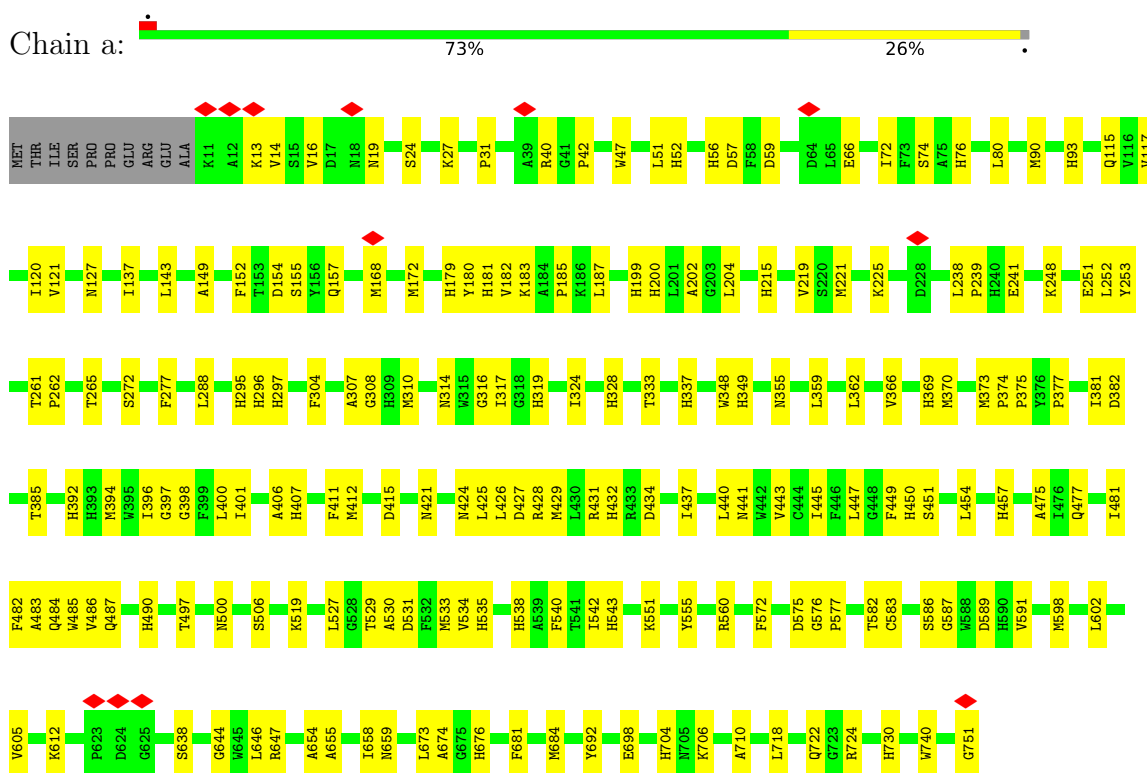


Mol	Chain	Residues	Atoms					AltConf
32	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

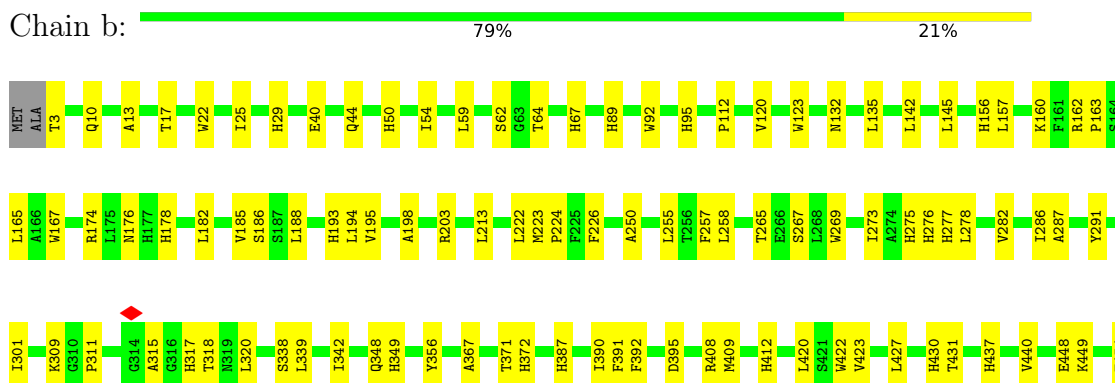
3 Residue-property plots

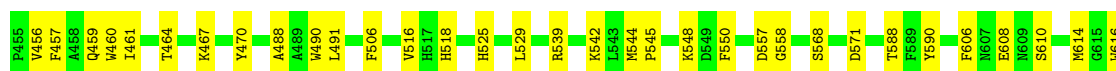
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

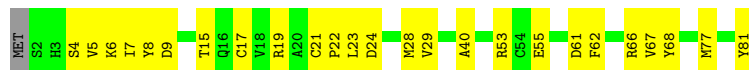


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

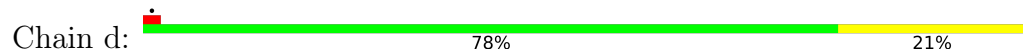




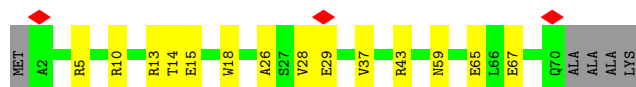
• Molecule 3: Photosystem I iron-sulfur center



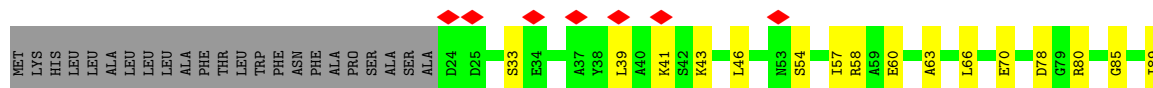
• Molecule 4: Photosystem I reaction center subunit II



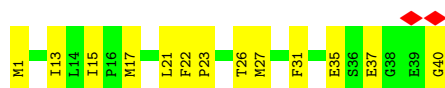
• Molecule 5: Photosystem I reaction center subunit IV



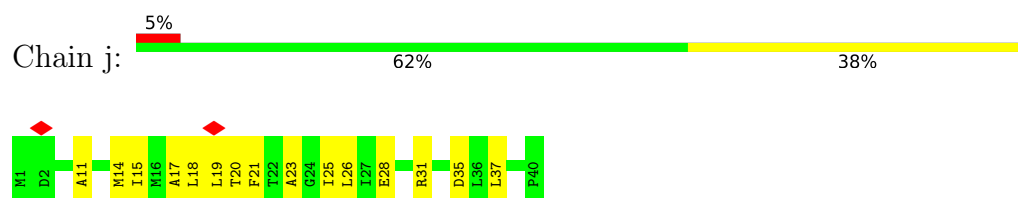
• Molecule 6: Photosystem I reaction center subunit III



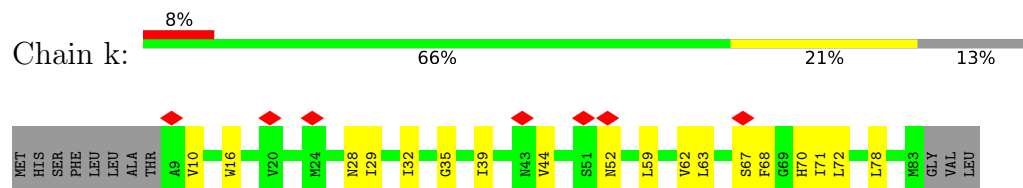
• Molecule 7: Photosystem I reaction center subunit VIII



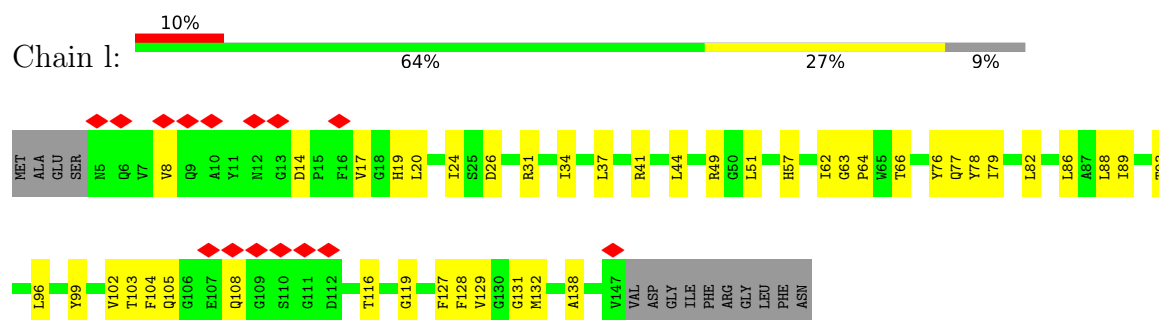
• Molecule 8: Photosystem I reaction center subunit IX



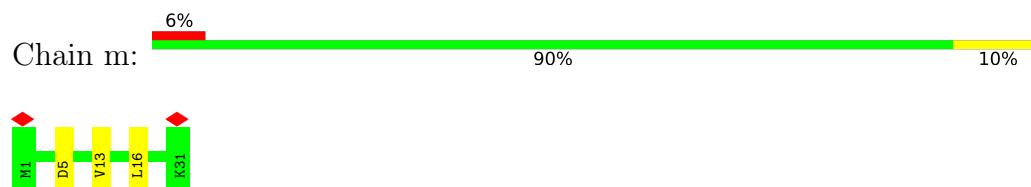
• Molecule 9: Photosystem I reaction center subunit PsaK 1



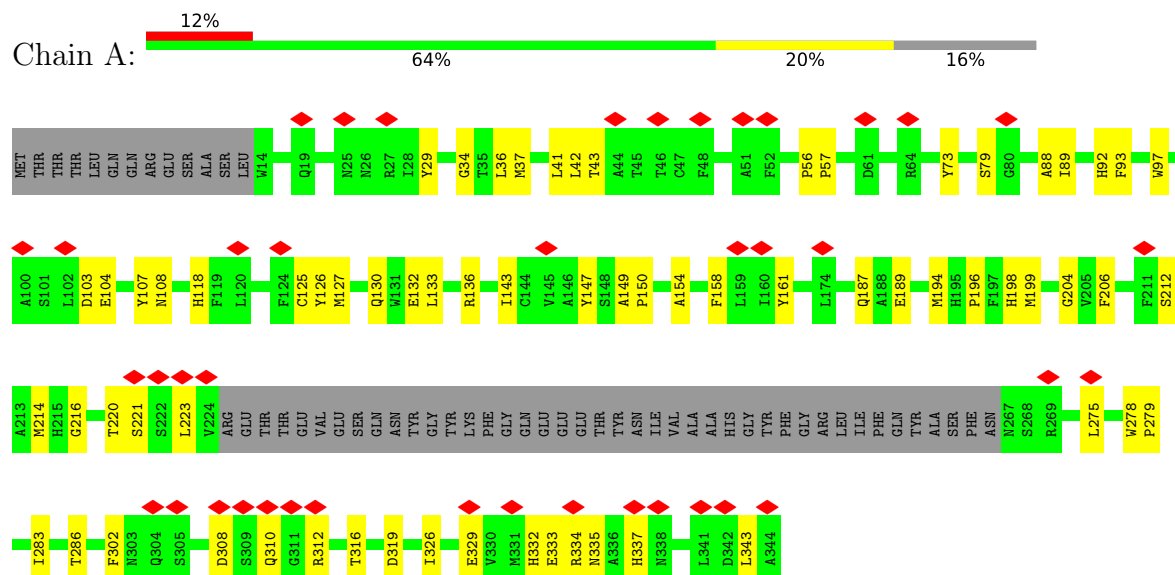
• Molecule 10: Photosystem I reaction center subunit XI



• Molecule 11: Photosystem I reaction center subunit XII



• Molecule 12: Photosystem II protein D1 2



Chain D:

Segment Color	Percentage
Red	18%
Green	62%
Yellow	21%
Grey	17%

Chain E:

7% 30% 25% 46%

MET SER GLY THR THR GLY GLU ARG PRO PHE ASP ASP THR I17 V21 T22 H23 S24 T25 T26 I27 P28 F31 I32 A33 G34 W35 L36 F37 V38 S39 T40 G41 Y44 D45 A46 T49 P50 R51 P52 D53 E54 Y55 F56 THR GLN THR ARG

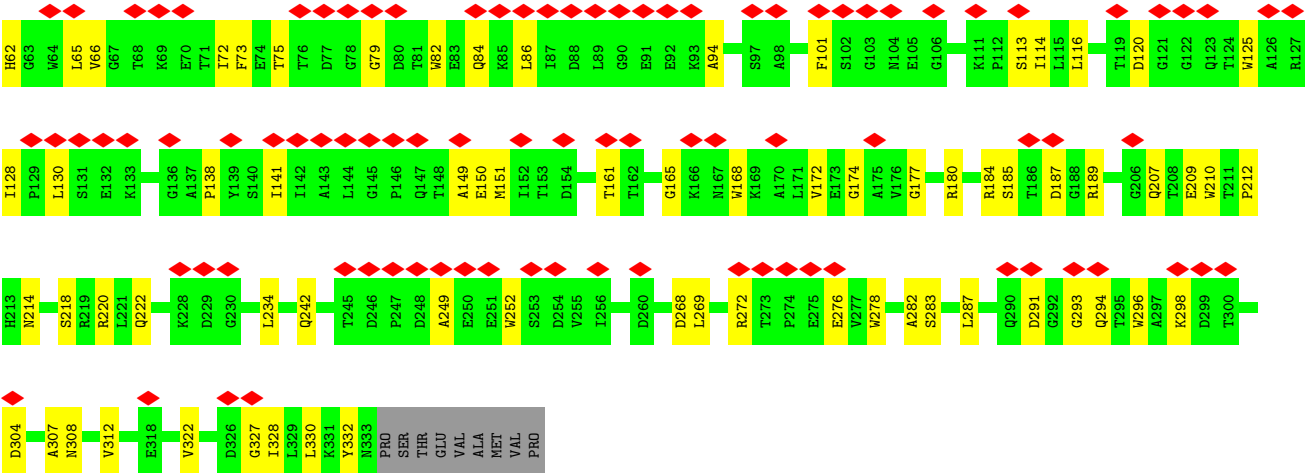
Chain F:

Chain I:

Position	Amino Acid	Conservation (bits)
1	MET	0.10
2	L2	0.10
3	T3	0.10
4	L4	0.10
5	K5	0.10
6	I6	0.10
7	A7	0.10
8	V8	0.10
9	Y9	0.10
10	I10	0.10
11	V11	0.10
12	V12	0.10
13	G13	0.10
14	L14	0.10
15	F15	0.10
16	I16	0.10
17	F23	0.10
18	L24	0.10
19	S25	0.10
20	S26	0.10
21	D27	0.10
22	P28	0.10
23	THR	0.00
24	ARG	0.00
25	ASN	0.00
26	PRO	0.00
27	GLY	0.00
28	ARG	0.00
29	LYS	0.00
30	ASP	0.00
31	PHE	0.00
32	GLU	0.00

Chain S:

Category	Percentage
Red	33%
Green	66%
Yellow	23%
Grey	11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	178513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	90.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.510	Depositor
Minimum map value	-0.112	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0801	Depositor
Map size (Å)	488.0, 488.0, 488.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	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: FE2, BCR, 45D, ZEX, PHO, LHG, HEM, CL0, LMG, SF4, LMT, CLA, EQ3, ECH, PQN

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	0.19	0/5993	0.28	0/8169
2	b	0.18	0/5981	0.29	0/8178
3	c	0.18	0/610	0.36	0/826
4	d	0.15	0/1111	0.29	0/1497
5	e	0.15	0/547	0.33	0/741
6	f	0.14	0/1138	0.28	0/1546
7	i	0.16	0/322	0.36	0/438
8	j	0.14	0/328	0.29	0/443
9	k	0.13	0/535	0.27	0/726
10	l	0.15	0/1097	0.29	0/1493
11	m	0.15	0/241	0.21	0/326
12	A	0.13	0/2322	0.29	0/3169
13	D	0.12	0/2266	0.26	0/3086
14	E	0.14	0/374	0.32	0/513
15	F	0.19	0/228	0.46	0/309
16	I	0.12	0/216	0.29	0/293
17	S	0.11	0/2390	0.27	0/3258
All	All	0.16	0/25699	0.29	0/35011

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	5795	0	5653	182	0
2	b	5770	0	5547	143	0
3	c	600	0	581	21	0
4	d	1087	0	1082	22	0
5	e	538	0	514	9	0
6	f	1108	0	1100	31	0
7	i	311	0	304	12	0
8	j	319	0	328	13	0
9	k	524	0	547	17	0
10	l	1069	0	1044	34	0
11	m	238	0	260	2	0
12	A	2248	0	2170	52	0
13	D	2188	0	2129	57	0
14	E	360	0	352	15	0
15	F	222	0	230	10	0
16	I	211	0	227	4	0
17	S	2328	0	2227	54	0
18	a	65	0	72	4	0
19	A	161	0	144	10	0
19	D	166	0	154	14	0
19	a	2811	0	2986	226	0
19	b	2410	0	2456	160	0
19	f	165	0	150	7	0
19	j	101	0	82	6	0
19	k	91	0	66	4	0
19	l	167	0	154	6	0
20	a	33	0	46	1	0
20	b	33	0	46	1	0
21	A	40	0	56	2	0
21	a	185	0	257	19	0
21	b	200	0	280	21	0
21	f	40	0	56	5	0
21	i	40	0	56	2	0
21	j	80	0	112	10	0
21	k	80	0	112	6	0
21	l	40	0	56	4	0
22	a	147	0	222	11	0
22	b	38	0	49	2	0
22	f	49	0	74	6	0
23	a	90	0	123	5	0
23	b	110	0	172	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	42	0	52	5	0
25	b	8	0	0	0	0
25	c	16	0	0	2	0
26	b	41	0	54	5	0
26	m	41	0	54	4	0
27	b	42	0	0	0	0
28	b	42	0	56	3	0
28	f	42	0	56	0	0
29	f	35	0	45	4	0
30	A	1	0	0	0	0
31	A	64	0	74	5	0
31	D	64	0	74	5	0
32	F	43	0	30	4	0
All	All	32739	0	32771	910	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 14.

All (910) 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)
1:a:392:HIS:HE1	19:a:829:CLA:ND	1.66	0.93
19:b:3020:CLA:HBB1	21:b:3043:BCR:H14C	1.56	0.88
2:b:156:HIS:HE1	19:b:3011:CLA:NC	1.72	0.86
13:D:186:GLN:HB2	19:D:403:CLA:HBC1	1.60	0.83
2:b:275:HIS:HE1	19:b:3016:CLA:ND	1.81	0.79
1:a:407:HIS:HE1	19:a:831:CLA:NA	1.82	0.77
15:F:39:MET:HA	15:F:42:ILE:HG12	1.65	0.77
12:A:133:LEU:HD23	13:D:256:ILE:HG12	1.68	0.76
2:b:387:HIS:HE1	19:b:3029:CLA:NA	1.83	0.76
1:a:457:HIS:HE1	19:a:835:CLA:NA	1.81	0.75
10:l:41:ARG:O	10:l:49:ARG:NH2	2.20	0.75
12:A:143:ILE:HB	13:D:220:ASN:HD21	1.52	0.74
19:a:827:CLA:H52	19:a:838:CLA:H2	1.68	0.73
1:a:304:PHE:HE1	19:a:822:CLA:HAB	1.53	0.73
1:a:93:HIS:HE1	19:a:808:CLA:NA	1.85	0.73
12:A:42:LEU:HB3	21:A:406:BCR:H353	1.69	0.73
19:b:3017:CLA:HBA2	19:b:3026:CLA:HBB2	1.71	0.73
19:a:855:CLA:H11	2:b:648:LEU:HB3	1.71	0.72
1:a:215:HIS:HE1	19:a:815:CLA:NA	1.85	0.72
19:b:3030:CLA:HAC1	21:b:3048:BCR:H383	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:192:THR:HG23	19:D:403:CLA:HBC2	1.72	0.71
19:b:3017:CLA:H161	19:b:3035:CLA:HBA1	1.73	0.70
17:S:62:HIS:HA	17:S:75:THR:O	1.92	0.70
12:A:29:TYR:HB2	13:D:255:GLN:HB3	1.72	0.70
19:a:836:CLA:H42	21:a:848:BCR:H392	1.74	0.70
17:S:138:PRO:HB3	17:S:151:MET:HE1	1.74	0.69
19:a:823:CLA:HMD2	21:k:4001:BCR:H24C	1.74	0.69
10:l:104:PHE:O	10:l:108:GLN:NE2	2.26	0.69
32:F:101:HEM:HBC2	32:F:101:HEM:HHH	1.75	0.69
2:b:659:MET:HG3	19:b:3003:CLA:C1C	2.23	0.69
1:a:52:HIS:HE1	19:a:804:CLA:ND	1.88	0.69
17:S:207:GLN:HG2	17:S:209:GLU:H	1.56	0.68
16:I:6:ILE:O	16:I:10:ILE:HG12	1.94	0.68
13:D:197:HIS:HE1	19:D:403:CLA:NC	1.92	0.67
12:A:198:HIS:HE1	19:A:402:CLA:NB	1.92	0.67
19:a:829:CLA:H61	24:a:857:45D:H221	1.76	0.67
1:a:647:ARG:NH1	2:b:633:ASN:OD1	2.28	0.67
2:b:709:HIS:HE1	19:b:3040:CLA:ND	1.93	0.66
12:A:310:GLN:NE2	14:E:55:TYR:O	2.27	0.66
1:a:586:SER:OG	1:a:589:ASP:OD1	2.13	0.66
12:A:132:GLU:OE2	12:A:136:ARG:NE	2.27	0.66
3:c:8:TYR:HH	3:c:68:TYR:HH	1.37	0.66
2:b:467:LYS:NZ	2:b:506:PHE:O	2.29	0.66
19:a:831:CLA:HBA1	19:a:831:CLA:HBD	1.76	0.66
1:a:355:ASN:ND2	19:a:806:CLA:OBD	2.25	0.65
9:k:29:ILE:HA	9:k:32:ILE:HD12	1.77	0.65
19:b:3029:CLA:HBA1	19:b:3029:CLA:HBD	1.78	0.65
13:D:96:GLU:N	13:D:96:GLU:OE1	2.28	0.65
4:d:61:ARG:NH2	4:d:63:GLU:OE1	2.31	0.64
1:a:295:HIS:HE1	19:a:818:CLA:ND	1.95	0.64
10:l:116:THR:HG23	10:l:119:GLY:H	1.63	0.64
19:a:807:CLA:H42	19:a:831:CLA:H51	1.80	0.64
17:S:58:GLU:HB2	17:S:61:ASN:HB3	1.80	0.64
2:b:659:MET:CG	19:b:3003:CLA:NC	2.62	0.63
19:b:3028:CLA:H8	21:b:3044:BCR:H21C	1.80	0.63
1:a:673:LEU:HB3	19:a:802:CLA:H11	1.81	0.63
2:b:176:ASN:ND2	2:b:291:TYR:O	2.29	0.63
5:e:10:ARG:HB3	5:e:67:GLU:HG2	1.80	0.63
1:a:295:HIS:HE1	19:a:818:CLA:C4D	2.11	0.63
19:a:804:CLA:HBB1	21:j:104:BCR:H292	1.81	0.63
19:a:835:CLA:H2	10:l:64:PRO:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:60:THR:HA	13:D:82:ALA:HB2	1.81	0.63
1:a:457:HIS:HE1	19:a:835:CLA:C1A	2.11	0.62
1:a:704:HIS:HE1	19:a:841:CLA:C4D	2.13	0.62
2:b:608:GLU:HG2	6:f:70:GLU:HG2	1.80	0.62
2:b:667:TYR:OH	19:b:3003:CLA:OBD	2.14	0.62
1:a:704:HIS:HE1	19:a:841:CLA:ND	1.97	0.62
17:S:322:VAL:HB	17:S:330:LEU:HB2	1.81	0.62
2:b:282:VAL:O	2:b:286:ILE:HG12	2.00	0.62
2:b:132:ASN:HA	2:b:135:LEU:HD23	1.82	0.62
2:b:659:MET:HG3	19:b:3003:CLA:NC	2.14	0.62
19:a:834:CLA:H122	20:b:3042:PQN:H191	1.80	0.62
28:b:3053:ZEX:H35	21:f:202:BCR:HC32	1.82	0.62
17:S:113:SER:HB3	17:S:130:LEU:HD12	1.80	0.62
12:A:88:ALA:HB1	17:S:282:ALA:HB2	1.82	0.62
2:b:356:TYR:OH	19:b:3028:CLA:OBD	2.18	0.61
2:b:518:HIS:HE1	19:b:3037:CLA:ND	1.97	0.61
13:D:54:PHE:O	14:E:49:THR:OG1	2.18	0.61
1:a:497:THR:HG21	19:a:836:CLA:HMD1	1.83	0.61
2:b:317:HIS:CD2	19:b:3023:CLA:ND	2.69	0.61
19:a:806:CLA:H72	21:a:846:BCR:H23C	1.82	0.61
10:l:26:ASP:O	10:l:31:ARG:NH1	2.34	0.61
6:f:131:ILE:HG23	19:f:201:CLA:H201	1.81	0.61
12:A:333:GLU:HB3	12:A:337:HIS:HD2	1.65	0.61
1:a:181:HIS:HE1	19:a:812:CLA:NA	1.99	0.61
19:b:3040:CLA:H8	7:i:27:MET:HE1	1.82	0.61
1:a:589:ASP:OD2	1:a:724:ARG:NH1	2.34	0.61
2:b:17:THR:HG21	3:c:77:MET:HE2	1.82	0.61
6:f:46:LEU:O	6:f:58:ARG:NH2	2.32	0.61
2:b:409:MET:HG3	21:b:3048:BCR:H402	1.82	0.60
19:a:824:CLA:H72	22:a:854:LHG:H142	1.84	0.60
15:F:35:ALA:O	15:F:39:MET:HG3	2.02	0.60
1:a:484:GLN:HB3	23:a:853:LMG:HC5	1.83	0.60
19:b:3033:CLA:H71	21:f:202:BCR:H312	1.84	0.60
11:m:5:ASP:OD2	11:m:5:ASP:N	2.34	0.60
2:b:488:ALA:HB3	2:b:491:LEU:HG	1.82	0.60
2:b:694:PRO:O	3:c:81:TYR:OH	2.15	0.60
5:e:13:ARG:HG2	5:e:15:GLU:HG2	1.83	0.60
19:a:837:CLA:H122	19:a:837:CLA:H52	1.83	0.60
2:b:195:VAL:HG21	19:b:3015:CLA:HBC2	1.84	0.60
7:i:22:PHE:O	7:i:26:THR:HG22	2.02	0.60
1:a:519:LYS:NZ	1:a:751:GLY:OXT	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:335:ASN:HA	17:S:174:GLY:HA3	1.84	0.59
22:f:206:LHG:HC5	22:f:206:LHG:H142	1.84	0.59
28:b:3053:ZEX:H391	19:j:103:CLA:HBC2	1.84	0.59
6:f:97:ILE:HG23	19:f:203:CLA:HAA1	1.84	0.59
9:k:62:VAL:HG22	19:k:4003:CLA:HBC3	1.84	0.59
19:a:817:CLA:HBB2	21:a:845:BCR:H352	1.84	0.59
6:f:58:ARG:NH1	8:j:35:ASP:OD2	2.33	0.59
1:a:392:HIS:HE1	19:a:829:CLA:C1D	2.16	0.59
13:D:304:ARG:NH1	13:D:308:ASP:OD2	2.36	0.59
1:a:215:HIS:HB2	19:a:815:CLA:CHC	2.32	0.59
1:a:730:HIS:HE1	19:a:842:CLA:ND	2.01	0.59
19:a:818:CLA:HED3	9:k:10:VAL:HG22	1.83	0.59
1:a:117:VAL:O	1:a:127:ASN:ND2	2.33	0.58
2:b:275:HIS:ND1	19:b:3017:CLA:HAB	2.18	0.58
1:a:692:TYR:OH	19:a:803:CLA:OBD	2.16	0.58
2:b:213:LEU:HD21	26:b:3045:ECH:H34B	1.86	0.58
12:A:221:SER:HB3	13:D:138:ILE:HD12	1.83	0.58
22:f:206:LHG:H282	22:f:206:LHG:H182	1.85	0.58
10:l:128:PHE:O	10:l:132:MET:HG2	2.02	0.58
13:D:325:MET:HE3	13:D:329:MET:HE3	1.85	0.58
10:l:89:ILE:HG12	10:l:131:GLY:HA3	1.86	0.58
2:b:448:GLU:OE2	6:f:58:ARG:NE	2.37	0.58
19:b:3022:CLA:HBB1	21:b:3048:BCR:H323	1.84	0.58
3:c:4:SER:HB3	3:c:6:LYS:HE2	1.85	0.58
8:j:31:ARG:HD3	21:j:104:BCR:H312	1.84	0.58
12:A:161:TYR:OH	12:A:189:GLU:OE2	2.20	0.58
19:a:815:CLA:H52	19:a:815:CLA:H152	1.84	0.58
19:a:831:CLA:H2A	19:a:831:CLA:O2D	2.03	0.58
12:A:108:ASN:OD1	17:S:308:ASN:ND2	2.32	0.58
1:a:59:ASP:OD2	1:a:349:HIS:NE2	2.36	0.58
6:f:119:GLU:OE2	6:f:119:GLU:N	2.32	0.58
10:l:79:ILE:HG12	14:E:17:ILE:HG23	1.85	0.58
13:D:186:GLN:O	13:D:322:ASN:ND2	2.37	0.58
2:b:516:VAL:HG21	2:b:590:TYR:HB2	1.85	0.57
15:F:17:VAL:HG12	15:F:20:LEU:HD12	1.84	0.57
19:a:842:CLA:H171	8:j:19:LEU:HD12	1.85	0.57
1:a:215:HIS:HE1	19:a:815:CLA:C1A	2.17	0.57
19:b:3023:CLA:H52	19:b:3024:CLA:H142	1.86	0.57
13:D:141:TYR:HA	13:D:144:ILE:HG12	1.86	0.57
15:F:17:VAL:HG13	15:F:19:TRP:H	1.70	0.57
1:a:434:ASP:OD2	1:a:560:ARG:NH1	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:824:CLA:HBA1	19:a:824:CLA:HBD	1.86	0.57
1:a:317:ILE:HG22	19:a:823:CLA:HMD1	1.87	0.57
19:b:3005:CLA:H8	19:b:3024:CLA:HBA1	1.86	0.57
17:S:185:SER:OG	17:S:189:ARG:N	2.35	0.57
17:S:249:ALA:O	17:S:252:TRP:NE1	2.38	0.57
12:A:41:LEU:HD22	31:A:404:PHO:H91	1.87	0.56
32:F:101:HEM:HBB2	32:F:101:HEM:HMB1	1.87	0.56
19:A:402:CLA:H61	19:D:401:CLA:HAB	1.87	0.56
1:a:449:PHE:CE1	19:b:3003:CLA:H11	2.40	0.56
19:a:827:CLA:H12	19:a:838:CLA:HMA3	1.87	0.56
2:b:454:GLU:HG3	2:b:459:GLN:HE22	1.70	0.56
7:i:23:PRO:O	7:i:27:MET:HG3	2.05	0.56
12:A:332:HIS:HB3	17:S:177:GLY:HA2	1.87	0.56
19:D:401:CLA:HED3	19:D:401:CLA:H2A	1.86	0.56
1:a:487:GLN:NE2	19:a:838:CLA:OBD	2.39	0.56
19:a:829:CLA:H171	21:j:101:BCR:H12C	1.87	0.56
19:a:829:CLA:H161	21:j:101:BCR:H14C	1.86	0.56
1:a:362:LEU:HD11	19:a:820:CLA:H72	1.87	0.56
2:b:95:HIS:HE1	19:b:3010:CLA:NB	1.98	0.56
2:b:606:PHE:O	2:b:610:SER:OG	2.21	0.56
6:f:96:TYR:OH	6:f:138:PHE:O	2.23	0.56
10:l:57:HIS:HE1	19:l:1502:CLA:C4D	2.07	0.56
13:D:277:THR:O	13:D:281:MET:HG2	2.05	0.56
19:a:815:CLA:H52	19:a:815:CLA:H111	1.88	0.56
2:b:188:LEU:HG	19:b:3015:CLA:HBB2	1.88	0.56
9:k:39:ILE:HD11	21:k:4001:BCR:H291	1.86	0.56
19:a:806:CLA:H41	21:a:846:BCR:H292	1.86	0.56
2:b:89:HIS:CD2	19:b:3008:CLA:NA	2.74	0.56
14:E:23:HIS:NE2	32:F:101:HEM:ND	2.53	0.56
17:S:180:ARG:NH1	17:S:222:GLN:O	2.38	0.56
17:S:287:LEU:HD22	17:S:298:LYS:HA	1.87	0.56
1:a:199:HIS:HE1	19:a:813:CLA:NA	2.04	0.55
2:b:203:ARG:HG2	2:b:250:ALA:HB1	1.88	0.55
2:b:315:ALA:O	2:b:318:THR:OG1	2.20	0.55
2:b:672:ILE:HA	2:b:675:ILE:HD12	1.88	0.55
5:e:29:GLU:OE2	5:e:29:GLU:N	2.39	0.55
17:S:84:GLN:HG2	17:S:86:LEU:HD22	1.87	0.55
1:a:381:ILE:O	1:a:519:LYS:NZ	2.34	0.55
1:a:710:ALA:O	6:f:113:ARG:NH2	2.38	0.55
2:b:614:MET:HE3	2:b:617:PHE:HB3	1.88	0.55
7:i:37:GLU:OE1	10:l:105:GLN:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:88:VAL:HG22	4:d:94:VAL:HG22	1.88	0.55
5:e:28:VAL:HG12	5:e:37:VAL:HA	1.88	0.55
7:i:13:ILE:O	7:i:17:MET:HG3	2.06	0.55
2:b:44:GLN:NE2	2:b:163:PRO:O	2.40	0.55
19:b:3017:CLA:H52	19:b:3034:CLA:HED3	1.89	0.55
19:b:3029:CLA:O2D	19:b:3029:CLA:H2A	2.06	0.55
12:A:126:TYR:HE2	12:A:130:GLN:HE21	1.55	0.55
19:a:832:CLA:HAA2	10:l:8:VAL:HG11	1.88	0.55
6:f:33:SER:OG	6:f:63:ALA:O	2.25	0.55
1:a:74:SER:OG	1:a:180:TYR:HB2	2.07	0.54
2:b:338:SER:O	2:b:342:ILE:HG23	2.06	0.54
12:A:316:THR:N	12:A:319:ASP:OD2	2.38	0.54
14:E:35:TRP:CD1	14:E:39:SER:HG	2.25	0.54
19:a:809:CLA:H121	21:j:101:BCR:H402	1.90	0.54
12:A:104:GLU:O	12:A:108:ASN:ND2	2.34	0.54
3:c:7:ILE:HG12	3:c:40:ALA:HB3	1.89	0.54
2:b:548:LYS:NZ	4:d:127:GLU:OE2	2.38	0.54
19:b:3025:CLA:HAA2	19:b:3026:CLA:OBD	2.07	0.54
1:a:441:ASN:O	1:a:445:ILE:HG13	2.07	0.54
9:k:28:ASN:ND2	19:k:4002:CLA:O1A	2.41	0.54
1:a:304:PHE:CE1	19:a:822:CLA:HAB	2.41	0.54
1:a:429:MET:HE2	19:a:822:CLA:H172	1.90	0.54
19:a:819:CLA:C1B	19:a:819:CLA:H2	2.37	0.54
1:a:366:VAL:O	1:a:370:MET:HB2	2.08	0.54
13:D:201:VAL:HG22	19:D:403:CLA:C1B	2.38	0.54
1:a:337:HIS:CD2	19:a:825:CLA:ND	2.76	0.53
1:a:583:CYS:HB2	2:b:664:TRP:HB3	1.88	0.53
2:b:178:HIS:CD2	19:b:3013:CLA:NB	2.76	0.53
12:A:118:HIS:CD2	19:A:405:CLA:NB	2.74	0.53
1:a:551:LYS:NZ	2:b:670:GLU:OE1	2.41	0.53
2:b:277:HIS:HE1	19:b:3018:CLA:NA	2.05	0.53
1:a:52:HIS:HE1	19:a:804:CLA:C4D	2.22	0.53
1:a:382:ASP:OD2	1:a:385:THR:OG1	2.27	0.53
1:a:42:PRO:HB3	1:a:47:TRP:CE3	2.44	0.53
13:D:161:PRO:HB3	13:D:170:ALA:HB2	1.91	0.53
1:a:316:GLY:HA3	9:k:44:VAL:HG11	1.91	0.53
1:a:500:ASN:HB2	19:a:837:CLA:HED2	1.89	0.53
2:b:371:THR:HG23	2:b:588:THR:HG21	1.91	0.53
1:a:66:GLU:OE2	1:a:187:LEU:N	2.36	0.53
1:a:434:ASP:OD1	1:a:555:TYR:OH	2.27	0.53
12:A:147:TYR:OH	31:A:404:PHO:O1A	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:93:HIS:HE1	19:a:808:CLA:C1A	2.22	0.52
19:a:819:CLA:H193	19:a:828:CLA:H202	1.91	0.52
29:f:207:LMT:H5B	29:f:207:LMT:H6D	1.89	0.52
1:a:56:HIS:HE1	19:a:805:CLA:C1C	2.22	0.52
19:b:3029:CLA:H111	23:b:3049:LMG:H221	1.91	0.52
4:d:39:VAL:HG22	4:d:49:ILE:HG12	1.91	0.52
10:l:79:ILE:HD12	10:l:79:ILE:H	1.74	0.52
17:S:268:ASP:OD2	17:S:312:VAL:N	2.32	0.52
5:e:18:TRP:NE1	5:e:43:ARG:O	2.34	0.52
18:a:801:CL0:CGD	18:a:801:CL0:H8	2.39	0.52
13:D:66:SER:OG	13:D:69:GLU:OE1	2.18	0.52
19:a:827:CLA:HAB	21:a:848:BCR:H311	1.90	0.52
6:f:125:ILE:O	29:f:207:LMT:O2'	2.27	0.52
6:f:127:VAL:HG21	29:f:207:LMT:H61	1.91	0.52
13:D:34:GLY:HA2	13:D:128:ARG:HD2	1.92	0.52
31:A:404:PHO:NC	13:D:209:LEU:HD12	2.24	0.52
1:a:200:HIS:CD2	19:a:814:CLA:NB	2.78	0.52
2:b:349:HIS:CD2	19:b:3026:CLA:NC	2.78	0.52
4:d:77:LYS:HB3	4:d:78:PRO:HD3	1.92	0.52
14:E:34:GLY:O	14:E:38:VAL:HG22	2.10	0.52
2:b:193:HIS:HB2	19:b:3014:CLA:CHC	2.40	0.52
2:b:223:MET:HB3	2:b:224:PRO:HD3	1.91	0.52
2:b:257:PHE:HE1	19:b:3017:CLA:H42	1.75	0.52
13:D:33:SER:HA	13:D:36:LEU:HD13	1.92	0.52
17:S:45:LEU:HD12	17:S:51:PHE:HZ	1.75	0.52
2:b:3:THR:OG1	2:b:13:ALA:O	2.28	0.51
19:a:822:CLA:H61	21:a:847:BCR:H352	1.90	0.51
1:a:425:LEU:HD22	19:a:832:CLA:HMD3	1.92	0.51
13:D:56:THR:HG21	14:E:50:PRO:HD3	1.92	0.51
13:D:279:LEU:HD11	31:D:402:PHO:HMC3	1.92	0.51
1:a:288:LEU:HG	1:a:375:PRO:HA	1.92	0.51
1:a:740:TRP:NE1	19:a:829:CLA:O1A	2.43	0.51
3:c:19:ARG:NH1	4:d:106:GLU:OE1	2.44	0.51
19:a:815:CLA:HAB	21:a:845:BCR:H14C	1.93	0.51
2:b:40:GLU:HG2	2:b:165:LEU:HB2	1.92	0.51
2:b:157:LEU:O	2:b:162:ARG:NH2	2.43	0.51
2:b:456:VAL:HG11	6:f:78:ASP:HB3	1.92	0.51
23:b:3051:LMG:O5	23:b:3051:LMG:O4	2.24	0.51
13:D:102:THR:OG1	14:E:46:ALA:O	2.24	0.51
13:D:288:GLY:O	13:D:292:ASN:N	2.41	0.51
14:E:25:ILE:HG13	14:E:26:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:421:ASN:OD1	1:a:424:ASN:ND2	2.44	0.51
2:b:276:HIS:HB2	19:b:3017:CLA:C1B	2.41	0.51
19:b:3027:CLA:H193	23:b:3049:LMG:H273	1.92	0.51
12:A:143:ILE:HB	13:D:220:ASN:ND2	2.22	0.51
1:a:481:ILE:HB	23:a:853:LMG:H292	1.91	0.51
19:a:839:CLA:H2	19:a:839:CLA:C4D	2.40	0.51
7:i:17:MET:HA	7:i:21:LEU:HB2	1.93	0.51
10:l:96:LEU:HD21	21:l:1504:BCR:H383	1.92	0.51
13:D:111:TRP:HB3	13:D:112:PRO:HD3	1.93	0.51
1:a:40:ARG:HA	1:a:40:ARG:NE	2.26	0.51
24:a:857:45D:H122	24:a:857:45D:H231	1.92	0.51
19:b:3017:CLA:H43	19:b:3017:CLA:HBA1	1.93	0.51
19:b:3033:CLA:HED1	8:j:37:LEU:HD13	1.93	0.51
10:l:99:TYR:O	10:l:103:THR:OG1	2.15	0.51
17:S:150:GLU:OE1	17:S:184:ARG:NH2	2.43	0.51
1:a:221:MET:HG2	1:a:253:TYR:OH	2.11	0.50
1:a:530:ALA:O	1:a:534:VAL:HG23	2.10	0.50
19:b:3005:CLA:HBC2	19:b:3029:CLA:HMA1	1.93	0.50
8:j:26:LEU:HD13	21:j:101:BCR:HC7	1.92	0.50
13:D:191:TRP:CE2	13:D:197:HIS:HB2	2.47	0.50
17:S:57:THR:OG1	17:S:61:ASN:OD1	2.24	0.50
1:a:373:MET:HG3	1:a:506:SER:HB2	1.92	0.50
1:a:477:GLN:H	23:a:851:LMG:HC72	1.75	0.50
2:b:420:LEU:HG	2:b:529:LEU:HB2	1.93	0.50
6:f:99:GLY:HA3	6:f:140:TRP:CZ2	2.46	0.50
12:A:150:PRO:HB2	19:A:402:CLA:H71	1.93	0.50
1:a:531:ASP:OD2	1:a:612:LYS:NZ	2.40	0.50
17:S:185:SER:OG	17:S:187:ASP:OD1	2.26	0.50
1:a:115:GLN:HB3	1:a:137:ILE:HB	1.92	0.50
19:a:827:CLA:HMB1	19:a:840:CLA:HBA1	1.93	0.50
19:b:3031:CLA:HBC2	19:b:3038:CLA:HMC2	1.94	0.50
4:d:120:ARG:NH2	4:d:141:VAL:O	2.41	0.50
19:a:818:CLA:H61	9:k:78:LEU:HD13	1.92	0.50
8:j:21:PHE:O	8:j:25:ILE:HG12	2.12	0.50
13:D:250:ASN:ND2	13:D:261:PHE:O	2.44	0.50
19:a:827:CLA:HAA2	19:a:828:CLA:OBD	2.12	0.50
6:f:114:GLU:HG2	6:f:114:GLU:O	2.11	0.50
10:l:66:THR:HG22	10:l:78:TYR:HA	1.93	0.50
12:A:196:PRO:HA	12:A:199:MET:HE3	1.93	0.50
19:a:835:CLA:O2D	19:a:835:CLA:H2A	2.11	0.50
19:b:3003:CLA:H111	21:b:3047:BCR:H362	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:810:CLA:HBB1	19:a:810:CLA:HMB3	1.94	0.50
12:A:34:GLY:HA2	12:A:37:MET:HB3	1.93	0.50
1:a:277:PHE:HE1	19:a:819:CLA:HAB	1.77	0.50
1:a:333:THR:HB	1:a:425:LEU:HD21	1.94	0.50
1:a:706:LYS:NZ	6:f:157:ASP:OD1	2.38	0.50
1:a:684:MET:HG3	19:a:803:CLA:NC	2.26	0.49
23:a:851:LMG:H322	23:a:851:LMG:HC91	1.93	0.49
2:b:437:HIS:HE1	19:b:3033:CLA:C1A	2.08	0.49
3:c:55:GLU:OE2	3:c:67:VAL:N	2.44	0.49
19:f:201:CLA:H41	8:j:18:LEU:HD13	1.92	0.49
12:A:89:ILE:HD11	12:A:108:ASN:HB3	1.93	0.49
12:A:204:GLY:HA2	12:A:278:TRP:CD1	2.47	0.49
13:D:78:VAL:HB	13:D:173:PHE:HB2	1.93	0.49
17:S:65:LEU:HG	17:S:73:PHE:HB2	1.93	0.49
1:a:179:HIS:HE1	19:a:811:CLA:C1A	2.25	0.49
19:a:811:CLA:O1D	19:a:811:CLA:H2A	2.11	0.49
19:a:837:CLA:H202	19:a:837:CLA:H42	1.94	0.49
10:l:26:ASP:OD2	10:l:26:ASP:N	2.44	0.49
10:l:89:ILE:O	10:l:93:THR:HG23	2.12	0.49
19:A:402:CLA:H122	31:A:404:PHO:H3A	1.95	0.49
1:a:154:ASP:HB3	1:a:157:GLN:HG3	1.95	0.49
10:l:127:PHE:CZ	21:l:1504:BCR:H292	2.47	0.49
1:a:307:ALA:HB2	19:a:822:CLA:HBC2	1.93	0.49
1:a:740:TRP:HD1	19:a:829:CLA:HMB2	1.76	0.49
19:a:823:CLA:H143	19:a:837:CLA:H101	1.93	0.49
10:l:44:LEU:O	10:l:49:ARG:NH1	2.45	0.49
12:A:154:ALA:O	12:A:158:PHE:HB2	2.12	0.49
19:a:824:CLA:CHB	19:a:824:CLA:H2	2.42	0.49
2:b:449:LYS:HB3	19:b:3033:CLA:HED3	1.95	0.49
15:F:17:VAL:HG22	15:F:18:ARG:H	1.78	0.49
19:A:403:CLA:HBC3	13:D:178:ILE:HG23	1.93	0.49
2:b:213:LEU:HD23	19:b:3015:CLA:HMA2	1.94	0.49
3:c:28:MET:HA	3:c:28:MET:HE2	1.93	0.49
12:A:149:ALA:HB1	12:A:283:ILE:HB	1.95	0.49
17:S:161:THR:HB	17:S:168:TRP:CE3	2.47	0.49
1:a:120:ILE:HG13	1:a:121:VAL:HG13	1.95	0.49
1:a:310:MET:HE1	19:a:822:CLA:C3D	2.43	0.49
1:a:655:ALA:O	1:a:659:ASN:ND2	2.46	0.49
7:i:37:GLU:OE1	7:i:37:GLU:N	2.33	0.49
19:a:821:CLA:H141	21:a:845:BCR:H272	1.95	0.49
19:b:3023:CLA:HAB	19:b:3030:CLA:HBC2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:b:3029:CLA:H91	23:b:3049:LMG:H241	1.93	0.49
4:d:21:LYS:HG3	4:d:25:GLU:HB3	1.95	0.49
10:l:66:THR:O	10:l:77:GLN:NE2	2.44	0.49
1:a:427:ASP:OD2	1:a:431:ARG:NE	2.45	0.48
17:S:234:LEU:HG	17:S:242:GLN:HB3	1.94	0.48
19:a:806:CLA:H171	21:a:845:BCR:H343	1.94	0.48
2:b:120:VAL:HG21	19:b:3008:CLA:HED1	1.95	0.48
6:f:131:ILE:HG12	19:f:201:CLA:H191	1.95	0.48
1:a:297:HIS:HE1	19:a:820:CLA:NA	2.11	0.48
19:b:3016:CLA:H2	19:b:3016:CLA:C4D	2.43	0.48
19:b:3025:CLA:HBA2	19:b:3038:CLA:HAA1	1.95	0.48
19:b:3032:CLA:HBB1	21:f:202:BCR:H323	1.95	0.48
1:a:76:HIS:CE1	19:a:806:CLA:ND	2.80	0.48
1:a:248:LYS:O	1:a:251:GLU:HG2	2.13	0.48
1:a:328:HIS:HE1	19:a:824:CLA:ND	2.09	0.48
17:S:66:VAL:HG12	17:S:72:ILE:HG22	1.95	0.48
19:a:818:CLA:C4D	19:a:818:CLA:H12	2.43	0.48
19:a:822:CLA:H102	19:a:825:CLA:H93	1.95	0.48
2:b:637:VAL:HG23	2:b:641:SER:HB2	1.96	0.48
1:a:428:ARG:HH12	10:l:8:VAL:HG21	1.79	0.48
19:a:843:CLA:HBA1	19:a:843:CLA:HBD	1.94	0.48
2:b:412:HIS:CD2	19:b:3030:CLA:C4A	2.97	0.48
1:a:179:HIS:HE1	19:a:811:CLA:NA	2.07	0.48
19:a:835:CLA:H141	19:a:835:CLA:H161	1.71	0.48
19:b:3005:CLA:H122	19:b:3005:CLA:HBD	1.94	0.48
14:E:21:VAL:O	14:E:25:ILE:HG12	2.14	0.48
1:a:406:ALA:HB2	1:a:591:VAL:HG11	1.96	0.48
19:a:828:CLA:H151	19:a:836:CLA:H121	1.95	0.48
8:j:28:GLU:HG3	19:j:102:CLA:C4C	2.43	0.48
9:k:70:HIS:CD2	19:k:4002:CLA:NC	2.81	0.48
13:D:197:HIS:HE1	19:D:403:CLA:C1C	2.26	0.48
1:a:219:VAL:HG13	1:a:239:PRO:HB3	1.95	0.48
2:b:95:HIS:HE1	19:b:3010:CLA:C4B	2.27	0.48
2:b:525:HIS:CD2	19:b:3038:CLA:NB	2.81	0.48
12:A:103:ASP:OD1	12:A:103:ASP:N	2.41	0.48
2:b:64:THR:HG23	19:b:3008:CLA:HED3	1.96	0.47
2:b:568:SER:N	2:b:571:ASP:OD2	2.46	0.47
3:c:9:ASP:OD1	3:c:9:ASP:N	2.47	0.47
19:l:1501:CLA:H3A	19:l:1501:CLA:HBA2	1.38	0.47
19:A:403:CLA:H3A	19:A:403:CLA:HBA2	1.37	0.47
13:D:292:ASN:O	13:D:294:ARG:HD2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:16:VAL:HG12	1:a:185:PRO:HA	1.96	0.47
1:a:440:LEU:O	1:a:443:VAL:HG12	2.14	0.47
2:b:273:ILE:HD12	19:b:3018:CLA:HMA1	1.96	0.47
22:f:206:LHG:H151	22:f:206:LHG:H262	1.96	0.47
12:A:36:LEU:HD22	12:A:125:CYS:SG	2.54	0.47
1:a:543:HIS:CD2	19:a:840:CLA:NB	2.83	0.47
19:a:803:CLA:C2	19:a:803:CLA:H3A	2.45	0.47
19:a:805:CLA:HED1	19:a:812:CLA:HBD	1.96	0.47
19:b:3039:CLA:H3A	19:b:3039:CLA:HBA2	1.57	0.47
3:c:24:ASP:OD1	4:d:105:PRO:HG3	2.14	0.47
13:D:171:PRO:HB3	13:D:181:PHE:CG	2.49	0.47
1:a:676:HIS:CD2	18:a:801:CL0:NB	2.82	0.47
2:b:430:HIS:HE1	19:b:3032:CLA:C4D	2.28	0.47
17:S:40:TRP:HB3	17:S:330:LEU:HB3	1.95	0.47
17:S:276:GLU:OE2	17:S:278:TRP:NE1	2.37	0.47
2:b:50:HIS:CE1	19:b:3005:CLA:ND	2.82	0.47
19:b:3014:CLA:H112	19:b:3014:CLA:H72	1.54	0.47
19:b:3027:CLA:HBA2	19:b:3027:CLA:H3A	1.43	0.47
4:d:101:ASP:OD2	4:d:109:ASN:ND2	2.48	0.47
15:F:30:VAL:HA	15:F:33:VAL:HG22	1.97	0.47
1:a:598:MET:HE3	1:a:598:MET:HB3	1.80	0.47
19:a:806:CLA:HBA1	19:a:806:CLA:H3A	1.43	0.47
2:b:342:ILE:HD11	19:b:3028:CLA:HBC1	1.96	0.47
2:b:518:HIS:HE1	19:b:3037:CLA:C4D	2.28	0.47
19:b:3018:CLA:H142	19:b:3018:CLA:H112	1.78	0.47
19:b:3035:CLA:HBA2	19:b:3035:CLA:H3A	1.46	0.47
3:c:28:MET:O	4:d:112:ARG:NH1	2.46	0.47
3:c:61:ASP:OD1	5:e:59:ASN:ND2	2.48	0.47
4:d:13:GLY:C	10:l:20:LEU:HD21	2.39	0.47
12:A:283:ILE:HA	12:A:286:THR:HG22	1.95	0.47
12:A:308:ASP:OD1	12:A:312:ARG:N	2.45	0.47
1:a:319:HIS:HB3	1:a:324:ILE:HD11	1.97	0.47
1:a:328:HIS:HE1	19:a:824:CLA:C4D	2.27	0.47
1:a:411:PHE:CD1	1:a:415:ASP:HB2	2.49	0.47
1:a:450:HIS:HE1	19:a:834:CLA:NA	2.07	0.47
19:b:3016:CLA:HBA2	19:b:3016:CLA:H3A	1.72	0.47
22:b:3050:LHG:H101	22:b:3050:LHG:H251	1.97	0.47
4:d:109:ASN:O	4:d:112:ARG:HD2	2.14	0.47
2:b:265:THR:OG1	2:b:267:SER:OG	2.25	0.47
19:A:405:CLA:HAB	16:I:15:PHE:HD2	1.79	0.47
17:S:283:SER:O	17:S:283:SER:OG	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:809:CLA:H101	22:a:850:LHG:H223	1.97	0.47
19:a:823:CLA:H62	19:a:823:CLA:H41	1.75	0.47
19:a:856:CLA:H3A	19:a:856:CLA:HBA2	1.57	0.47
2:b:59:LEU:HD12	26:m:101:ECH:H37A	1.97	0.47
2:b:92:TRP:HB2	19:b:3007:CLA:HED1	1.96	0.47
2:b:301:ILE:HG21	19:b:3024:CLA:HAC1	1.96	0.47
2:b:123:TRP:CZ2	19:b:3013:CLA:H201	2.49	0.46
2:b:408:ARG:HD3	19:b:3030:CLA:OBD	2.15	0.46
21:b:3046:BCR:H383	21:b:3048:BCR:H291	1.97	0.46
1:a:168:MET:O	1:a:172:MET:HG2	2.15	0.46
1:a:225:LYS:HG2	1:a:252:LEU:HD12	1.97	0.46
1:a:654:ALA:O	1:a:658:ILE:HG12	2.15	0.46
19:a:813:CLA:H71	19:a:813:CLA:H112	1.60	0.46
2:b:174:ARG:HB2	19:b:3013:CLA:HBC2	1.96	0.46
6:f:118:PRO:O	6:f:122:GLU:HG3	2.15	0.46
19:f:201:CLA:H151	8:j:21:PHE:CD2	2.49	0.46
17:S:116:LEU:HD22	17:S:125:TRP:HB3	1.98	0.46
1:a:450:HIS:O	1:a:454:LEU:HG	2.14	0.46
2:b:590:TYR:HA	2:b:616:TRP:HH2	1.80	0.46
19:l:1502:CLA:H91	19:l:1502:CLA:H112	1.67	0.46
13:D:263:ASN:OD1	13:D:264:LYS:N	2.48	0.46
1:a:27:LYS:HE2	19:a:812:CLA:HAA2	1.96	0.46
21:a:845:BCR:H392	21:k:4001:BCR:HC8	1.98	0.46
17:S:128:ILE:HD13	17:S:165:GLY:HA3	1.96	0.46
6:f:93:LEU:HD13	19:j:103:CLA:HBB2	1.96	0.46
19:D:403:CLA:H62	19:D:403:CLA:H41	1.72	0.46
17:S:172:VAL:HG21	17:S:210:TRP:CD1	2.50	0.46
1:a:241:GLU:HB3	1:a:248:LYS:NZ	2.31	0.46
1:a:450:HIS:HE1	19:a:834:CLA:C1A	2.28	0.46
19:a:841:CLA:CHA	19:a:841:CLA:H11	2.46	0.46
2:b:193:HIS:HE1	19:b:3014:CLA:C1A	2.20	0.46
10:l:76:TYR:HA	10:l:79:ILE:HD13	1.98	0.46
13:D:191:TRP:CE3	13:D:289:LEU:HD11	2.51	0.46
19:b:3004:CLA:H91	19:b:3004:CLA:H112	1.71	0.46
19:b:3015:CLA:HBA1	19:b:3015:CLA:CHA	2.45	0.46
19:b:3037:CLA:H41	19:b:3037:CLA:H62	1.48	0.46
13:D:276:VAL:HG12	31:D:402:PHO:HBC1	1.98	0.46
19:D:401:CLA:CHA	19:D:401:CLA:HBA1	2.45	0.46
1:a:14:VAL:HG21	19:a:811:CLA:HAA2	1.96	0.46
19:a:805:CLA:H3A	19:a:805:CLA:HBA2	1.68	0.46
19:b:3008:CLA:O1A	19:b:3027:CLA:HBD	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:3046:BCR:H15C	21:b:3046:BCR:H351	1.81	0.46
9:k:72:LEU:HD12	9:k:72:LEU:HA	1.81	0.46
1:a:450:HIS:HE1	19:a:834:CLA:C4D	2.29	0.46
1:a:718:LEU:HD21	20:a:844:PQN:H151	1.98	0.46
19:a:808:CLA:H91	19:a:808:CLA:H111	1.63	0.46
19:a:814:CLA:H62	19:a:814:CLA:H102	1.83	0.46
19:a:833:CLA:H3A	19:a:833:CLA:HBA2	1.49	0.46
6:f:41:LYS:HD2	6:f:41:LYS:HA	1.73	0.46
10:l:37:LEU:HD22	19:l:1502:CLA:HBD	1.96	0.46
13:D:125:PHE:HE2	31:D:402:PHO:HBD	1.81	0.46
13:D:152:VAL:HG21	13:D:279:LEU:HD22	1.97	0.46
19:D:404:CLA:H3A	19:D:404:CLA:O1A	2.16	0.46
1:a:482:PHE:HB3	19:a:838:CLA:H42	1.98	0.46
1:a:681:PHE:HZ	19:a:842:CLA:HBC2	1.80	0.46
2:b:182:LEU:O	2:b:186:SER:OG	2.20	0.46
2:b:701:GLN:HB2	23:b:3049:LMG:H111	1.98	0.46
19:b:3017:CLA:H101	19:b:3017:CLA:H62	1.79	0.46
21:b:3046:BCR:H23C	21:b:3048:BCR:H393	1.98	0.46
12:A:275:LEU:HG	13:D:211:CYS:SG	2.55	0.46
17:S:73:PHE:HD2	17:S:82:TRP:HB3	1.81	0.46
1:a:398:GLY:HA3	1:a:602:LEU:HD11	1.99	0.45
19:b:3003:CLA:HBC2	19:b:3003:CLA:HHD	1.97	0.45
19:b:3007:CLA:H3A	19:b:3007:CLA:HBA2	1.70	0.45
19:b:3033:CLA:H101	19:b:3033:CLA:H61	1.56	0.45
3:c:29:VAL:HG21	4:d:114:ALA:HB2	1.98	0.45
19:j:102:CLA:H3A	19:j:102:CLA:HBA2	1.67	0.45
1:a:19:ASN:N	1:a:182:VAL:O	2.40	0.45
2:b:545:PRO:HB3	6:f:164:PRO:HG2	1.98	0.45
19:b:3020:CLA:H61	19:b:3020:CLA:H102	1.51	0.45
19:b:3029:CLA:H122	19:b:3040:CLA:HED1	1.98	0.45
4:d:85:ILE:HD12	4:d:98:HIS:HB3	1.97	0.45
18:a:801:CL0:H41	18:a:801:CL0:H49	1.76	0.45
19:a:814:CLA:H43	21:a:846:BCR:H19C	1.97	0.45
21:a:845:BCR:H20C	21:a:845:BCR:H361	1.83	0.45
2:b:29:HIS:HE1	19:b:3004:CLA:C4B	2.29	0.45
2:b:92:TRP:N	19:b:3009:CLA:O1D	2.45	0.45
19:b:3034:CLA:H3A	19:b:3034:CLA:HBA2	1.42	0.45
13:D:322:ASN:O	13:D:326:ARG:HG2	2.17	0.45
1:a:120:ILE:HG23	1:a:121:VAL:HG22	1.98	0.45
1:a:369:HIS:CD2	19:a:828:CLA:NC	2.85	0.45
1:a:577:PRO:HD3	2:b:558:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:287:ALA:HB2	19:b:3019:CLA:HBC2	1.99	0.45
17:S:57:THR:HG22	17:S:101:PHE:CD2	2.51	0.45
1:a:451:SER:O	1:a:454:LEU:HB2	2.16	0.45
1:a:730:HIS:HE1	19:a:842:CLA:C4D	2.29	0.45
2:b:160:LYS:HG2	17:S:218:SER:HB3	1.99	0.45
19:b:3014:CLA:H62	19:b:3014:CLA:H41	1.70	0.45
1:a:152:PHE:CD1	19:a:815:CLA:HED1	2.51	0.45
19:a:834:CLA:H101	19:a:834:CLA:H62	1.82	0.45
2:b:62:SER:HB3	2:b:142:LEU:HB3	1.98	0.45
19:b:3003:CLA:H41	19:b:3003:CLA:H62	1.62	0.45
19:b:3015:CLA:HBB1	21:b:3043:BCR:H323	1.97	0.45
12:A:220:THR:HA	12:A:223:LEU:HG	1.98	0.45
15:F:27:VAL:HG12	15:F:28:PRO:HD3	1.98	0.45
15:F:32:PHE:O	15:F:36:ILE:HG13	2.16	0.45
17:S:291:ASP:CG	17:S:294:GLN:HB2	2.41	0.45
19:a:817:CLA:H3A	19:a:817:CLA:HBA2	1.44	0.45
19:b:3019:CLA:H11	19:b:3023:CLA:H11	1.98	0.45
19:b:3029:CLA:H8	23:b:3049:LMG:H221	1.99	0.45
6:f:127:VAL:HG22	8:j:14:MET:HE2	1.98	0.45
1:a:204:LEU:HD11	19:a:814:CLA:H42	1.99	0.45
1:a:485:TRP:HA	23:a:853:LMG:HC92	1.99	0.45
19:a:818:CLA:H112	19:a:818:CLA:H142	1.71	0.45
24:a:857:45D:H311	24:a:857:45D:H273	1.88	0.45
19:b:3013:CLA:H143	19:b:3013:CLA:H111	1.66	0.45
19:b:3014:CLA:H3A	26:b:3045:ECH:H38B	1.98	0.45
6:f:156:LYS:HA	6:f:156:LYS:HD3	1.85	0.45
12:A:216:GLY:HA3	13:D:272:LEU:HB2	1.99	0.45
17:S:79:GLY:O	17:S:82:TRP:NE1	2.50	0.45
19:a:828:CLA:H152	19:a:828:CLA:H111	1.55	0.45
19:a:838:CLA:H51	22:a:852:LHG:H371	1.99	0.45
2:b:545:PRO:HD2	3:c:62:PHE:CE1	2.52	0.45
19:b:3029:CLA:H61	19:b:3029:CLA:H41	1.63	0.45
21:j:101:BCR:H15C	21:j:101:BCR:H351	1.85	0.45
26:m:101:ECH:H20	26:m:101:ECH:H36	1.86	0.45
2:b:25:ILE:HG12	21:l:1504:BCR:HC41	1.99	0.45
19:b:3030:CLA:H3A	19:b:3030:CLA:HBA2	1.57	0.45
6:f:39:LEU:O	6:f:43:LYS:NZ	2.47	0.45
12:A:57:PRO:HD3	12:A:73:TYR:CZ	2.52	0.45
12:A:212:SER:OG	13:D:211:CYS:HB2	2.17	0.45
15:F:38:ALA:O	15:F:42:ILE:HG23	2.17	0.45
1:a:497:THR:HG21	19:a:836:CLA:CMD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:827:CLA:H2	19:a:827:CLA:H61	1.81	0.44
19:a:842:CLA:H202	19:a:842:CLA:H162	1.82	0.44
2:b:222:LEU:HD12	2:b:226:PHE:CE2	2.52	0.44
28:b:3053:ZEX:H373	19:j:103:CLA:HBC3	1.99	0.44
6:f:156:LYS:HB2	6:f:159:GLU:HG2	1.99	0.44
1:a:120:ILE:HD13	21:j:104:BCR:H313	1.99	0.44
2:b:311:PRO:HG3	19:b:3041:CLA:C2D	2.46	0.44
2:b:642:VAL:HG21	19:b:3008:CLA:HAC1	1.99	0.44
22:f:206:LHG:H172	22:f:206:LHG:H201	1.73	0.44
19:a:832:CLA:HBA2	19:a:832:CLA:H3A	1.50	0.44
2:b:348:GLN:HG3	19:b:3025:CLA:HED1	1.98	0.44
19:b:3025:CLA:HMB1	19:b:3025:CLA:HBB1	1.98	0.44
21:b:3044:BCR:H15C	21:b:3044:BCR:H351	1.86	0.44
5:e:5:ARG:NE	5:e:26:ALA:O	2.49	0.44
12:A:187:GLN:HB2	19:A:402:CLA:HAC2	1.99	0.44
12:A:214:MET:HE2	12:A:214:MET:HB3	1.78	0.44
17:S:272:ARG:HE	17:S:332:TYR:HE2	1.65	0.44
19:a:822:CLA:H101	21:a:848:BCR:H10C	2.00	0.44
2:b:387:HIS:HA	2:b:390:ILE:HD12	1.99	0.44
19:b:3005:CLA:H202	19:b:3005:CLA:H161	1.68	0.44
19:b:3017:CLA:H101	19:b:3017:CLA:H41	1.98	0.44
19:b:3027:CLA:H143	19:b:3027:CLA:H161	1.79	0.44
12:A:343:LEU:HB2	17:S:168:TRP:HB2	2.00	0.44
17:S:45:LEU:HD12	17:S:51:PHE:CZ	2.52	0.44
17:S:304:ASP:OD1	17:S:304:ASP:N	2.49	0.44
1:a:13:LYS:HG3	1:a:314:ASN:HD21	1.83	0.44
19:a:809:CLA:HAB	19:a:829:CLA:H142	1.98	0.44
19:a:841:CLA:H91	19:a:841:CLA:H112	1.73	0.44
19:b:3003:CLA:H143	21:b:3047:BCR:H362	1.99	0.44
19:b:3027:CLA:H141	19:b:3029:CLA:H151	1.98	0.44
19:b:3037:CLA:H112	19:b:3037:CLA:H142	1.79	0.44
21:b:3046:BCR:H20C	21:b:3046:BCR:H361	1.84	0.44
8:j:11:ALA:O	8:j:15:ILE:HG22	2.18	0.44
1:a:718:LEU:HB3	1:a:722:GLN:HG2	1.99	0.44
19:a:815:CLA:HMB1	21:a:845:BCR:HC8	1.99	0.44
19:a:819:CLA:H92	19:a:819:CLA:H61	1.78	0.44
19:a:841:CLA:HBA2	19:a:841:CLA:H3A	1.76	0.44
2:b:550:PHE:HE2	3:c:66:ARG:NH2	2.16	0.44
21:b:3044:BCR:H20C	21:b:3044:BCR:H361	1.86	0.44
19:a:809:CLA:H2	19:a:829:CLA:H43	1.99	0.44
19:a:815:CLA:HBA2	19:a:815:CLA:H3A	1.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:837:CLA:H12	19:a:858:CLA:H51	1.99	0.44
2:b:269:TRP:O	2:b:273:ILE:HG12	2.18	0.44
19:b:3003:CLA:CGA	19:b:3003:CLA:H3A	2.48	0.44
17:S:291:ASP:OD1	17:S:291:ASP:N	2.51	0.44
17:S:307:ALA:HB2	17:S:328:ILE:HD12	1.99	0.44
19:a:808:CLA:H3A	19:a:808:CLA:HBA2	1.54	0.44
19:a:815:CLA:C1B	21:a:845:BCR:H10C	2.48	0.44
2:b:658:PHE:CB	19:b:3003:CLA:HMC2	2.48	0.44
19:b:3003:CLA:H111	19:b:3003:CLA:H143	1.69	0.44
19:b:3019:CLA:H91	19:b:3019:CLA:H112	1.76	0.44
21:i:101:BCR:H20C	21:i:101:BCR:H361	1.85	0.44
13:D:53:THR:HA	13:D:67:TYR:H	1.82	0.44
1:a:31:PRO:HB2	1:a:51:LEU:HD11	1.99	0.44
19:a:818:CLA:HBA2	19:a:818:CLA:H3A	1.82	0.44
19:a:821:CLA:H3A	19:a:821:CLA:HBA2	1.41	0.44
19:a:833:CLA:C4D	10:l:24:ILE:HD11	2.47	0.44
19:a:840:CLA:H2A	19:a:840:CLA:O2D	2.17	0.44
2:b:420:LEU:O	2:b:423:VAL:HG12	2.18	0.44
21:j:104:BCR:H15C	21:j:104:BCR:H351	1.85	0.44
12:A:189:GLU:OE1	17:S:220:ARG:NH1	2.51	0.44
13:D:109:GLY:C	13:D:112:PRO:HD2	2.42	0.44
1:a:370:MET:HE1	19:a:830:CLA:CGD	2.48	0.43
1:a:490:HIS:CD2	19:a:836:CLA:ND	2.85	0.43
2:b:391:PHE:CD1	2:b:395:ASP:HB2	2.53	0.43
19:b:3021:CLA:H3A	19:b:3021:CLA:HBA2	1.47	0.43
3:c:17:CYS:HB3	25:c:102:SF4:S4	2.58	0.43
7:i:31:PHE:CZ	10:l:102:VAL:HG21	2.53	0.43
1:a:538:HIS:CE1	1:a:605:VAL:HA	2.53	0.43
19:a:815:CLA:H152	19:a:815:CLA:H111	1.73	0.43
19:a:819:CLA:HBA2	19:a:819:CLA:H3A	1.43	0.43
2:b:457:PHE:O	2:b:461:ILE:HG12	2.18	0.43
19:b:3026:CLA:H152	21:b:3046:BCR:H17C	2.00	0.43
22:b:3050:LHG:H251	22:b:3050:LHG:H282	1.63	0.43
19:j:103:CLA:HED3	19:j:103:CLA:H2A	2.00	0.43
21:l:1504:BCR:H20C	21:l:1504:BCR:H361	1.83	0.43
12:A:79:SER:HB2	13:D:313:THR:HG21	1.99	0.43
12:A:92:HIS:ND1	12:A:93:PHE:O	2.49	0.43
1:a:587:GLY:O	1:a:591:VAL:HG23	2.17	0.43
19:a:834:CLA:H2	19:a:834:CLA:H61	1.83	0.43
22:a:852:LHG:H192	22:a:852:LHG:H332	2.01	0.43
24:a:857:45D:O01	21:f:202:BCR:H14C	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:b:3026:CLA:H41	19:b:3026:CLA:H62	1.66	0.43
3:c:5:VAL:HG22	3:c:67:VAL:HG22	1.99	0.43
1:a:90:MET:HE2	19:a:829:CLA:HED1	2.00	0.43
19:a:813:CLA:HBB1	19:a:821:CLA:HBC2	2.00	0.43
2:b:185:VAL:HG11	21:b:3044:BCR:H341	2.00	0.43
12:A:326:ILE:O	12:A:329:GLU:HG3	2.18	0.43
13:D:91:PHE:HE1	19:D:404:CLA:HAA1	1.83	0.43
1:a:57:ASP:HB2	19:a:831:CLA:HAA1	2.00	0.43
1:a:149:ALA:HB2	1:a:377:PRO:HD2	2.01	0.43
1:a:411:PHE:HD1	1:a:415:ASP:HB2	1.83	0.43
19:a:812:CLA:H3A	19:a:812:CLA:HBA2	1.75	0.43
19:a:841:CLA:O2D	2:b:422:TRP:HB2	2.18	0.43
19:b:3027:CLA:H152	19:b:3029:CLA:H171	2.00	0.43
19:b:3037:CLA:HMB3	19:b:3037:CLA:HBB1	1.99	0.43
12:A:97:TRP:CG	16:I:5:LYS:HB2	2.53	0.43
12:A:194:MET:HE1	12:A:302:PHE:CD2	2.53	0.43
1:a:381:ILE:HG13	1:a:519:LYS:HB2	2.00	0.43
1:a:638:SER:O	1:a:644:GLY:HA3	2.18	0.43
19:a:840:CLA:H92	19:a:840:CLA:H61	1.79	0.43
4:d:7:GLN:HG2	4:d:51:ASN:ND2	2.34	0.43
5:e:13:ARG:NE	5:e:65:GLU:OE2	2.43	0.43
6:f:78:ASP:OD2	6:f:80:ARG:NE	2.51	0.43
26:m:101:ECH:H11	26:m:101:ECH:H34	1.93	0.43
13:D:90:LEU:HD22	13:D:107:ILE:HD12	1.99	0.43
1:a:143:LEU:HD12	19:a:809:CLA:HED1	2.00	0.43
19:a:831:CLA:H61	19:a:831:CLA:H41	1.68	0.43
3:c:21:CYS:HA	25:c:101:SF4:S4	2.59	0.43
4:d:28:TYR:OH	4:d:87:ARG:NH2	2.41	0.43
9:k:29:ILE:HD12	9:k:32:ILE:HD12	2.01	0.43
19:a:818:CLA:HBC1	19:a:819:CLA:H122	2.01	0.43
19:a:821:CLA:H151	21:a:845:BCR:H383	1.99	0.43
19:a:856:CLA:H62	19:a:856:CLA:H41	1.41	0.43
2:b:222:LEU:HD11	21:b:3043:BCR:HC42	2.00	0.43
2:b:460:TRP:CZ2	22:f:206:LHG:H272	2.53	0.43
19:b:3017:CLA:H62	19:b:3017:CLA:H41	1.59	0.43
7:i:35:GLU:OE2	7:i:35:GLU:HA	2.19	0.43
13:D:50:THR:HG22	15:F:32:PHE:HZ	1.83	0.43
18:a:801:CL0:H22	2:b:622:TRP:HD1	1.82	0.43
19:a:804:CLA:H102	19:a:804:CLA:H62	1.89	0.43
2:b:658:PHE:HB3	19:b:3003:CLA:HMC2	2.00	0.43
19:b:3033:CLA:H3A	19:b:3033:CLA:HBA2	1.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:b:3047:BCR:H15C	21:b:3047:BCR:H351	1.90	0.43
17:S:149:ALA:HB3	17:S:161:THR:HG22	2.00	0.43
17:S:214:ASN:OD1	17:S:214:ASN:N	2.52	0.43
1:a:261:THR:OG1	1:a:262:PRO:HD3	2.19	0.43
19:a:829:CLA:H62	19:a:829:CLA:H92	1.74	0.43
2:b:178:HIS:O	2:b:182:LEU:HB3	2.19	0.43
9:k:52:ASN:OD1	9:k:52:ASN:N	2.52	0.43
1:a:80:LEU:HD12	19:a:814:CLA:HED1	1.99	0.42
1:a:143:LEU:HD23	1:a:143:LEU:HA	1.86	0.42
1:a:374:PRO:HA	1:a:375:PRO:HD3	1.89	0.42
1:a:407:HIS:HE1	19:a:831:CLA:C4A	2.32	0.42
19:a:813:CLA:H2	19:a:813:CLA:H61	1.83	0.42
19:a:840:CLA:H111	19:a:840:CLA:H93	1.70	0.42
2:b:167:TRP:CZ2	19:b:3011:CLA:HHB	2.53	0.42
2:b:539:ARG:NH2	4:d:127:GLU:OE1	2.51	0.42
19:b:3033:CLA:H141	19:b:3033:CLA:H162	1.78	0.42
19:f:204:CLA:NB	22:f:206:LHG:H171	2.34	0.42
9:k:68:PHE:HD1	21:k:4001:BCR:H23C	1.83	0.42
17:S:45:LEU:HD21	17:S:82:TRP:HB2	2.00	0.42
1:a:437:ILE:HG13	1:a:555:TYR:HE1	1.84	0.42
1:a:740:TRP:CD1	19:a:829:CLA:HMB2	2.54	0.42
2:b:167:TRP:CH2	19:b:3011:CLA:HHB	2.54	0.42
2:b:339:LEU:HD12	2:b:339:LEU:HA	1.86	0.42
2:b:409:MET:HE1	19:b:3030:CLA:CHD	2.49	0.42
26:b:3045:ECH:H24	26:b:3045:ECH:H21	1.85	0.42
9:k:67:SER:O	9:k:71:ILE:HG13	2.20	0.42
10:l:63:GLY:O	10:l:66:THR:OG1	2.33	0.42
12:A:334:ARG:HH22	17:S:212:PRO:HG3	1.84	0.42
13:D:201:VAL:HG22	19:D:403:CLA:C2B	2.48	0.42
17:S:141:ILE:HD11	17:S:149:ALA:HB1	2.00	0.42
1:a:202:ALA:HB2	1:a:308:GLY:HA3	2.02	0.42
1:a:319:HIS:HE1	19:a:823:CLA:C4A	2.31	0.42
1:a:359:LEU:HD23	1:a:400:LEU:HD13	2.01	0.42
19:a:809:CLA:H143	19:a:809:CLA:H112	1.72	0.42
19:a:822:CLA:HMA2	19:a:826:CLA:NC	2.33	0.42
19:a:831:CLA:H122	19:a:831:CLA:H161	1.77	0.42
2:b:67:HIS:HE1	19:b:3007:CLA:C4D	2.32	0.42
2:b:123:TRP:CH2	26:b:3045:ECH:H29	2.54	0.42
21:b:3047:BCR:H20C	21:b:3047:BCR:H361	1.84	0.42
3:c:22:PRO:HG2	3:c:23:LEU:HD12	2.01	0.42
1:a:219:VAL:HG21	19:a:815:CLA:C1D	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:535:HIS:CD2	19:a:838:CLA:NB	2.88	0.42
19:a:803:CLA:H3A	19:a:803:CLA:CGA	2.49	0.42
19:a:808:CLA:H162	19:a:808:CLA:H202	1.77	0.42
19:a:839:CLA:H3A	19:a:839:CLA:HBA2	1.64	0.42
2:b:188:LEU:HG	19:b:3015:CLA:CBB	2.49	0.42
2:b:372:HIS:HB2	19:b:3027:CLA:C1B	2.50	0.42
2:b:412:HIS:CE1	19:b:3030:CLA:ND	2.87	0.42
19:b:3018:CLA:HBB2	19:b:3018:CLA:H111	2.02	0.42
13:D:40:CYS:HB2	19:D:404:CLA:HBB1	2.02	0.42
1:a:576:GLY:O	1:a:582:THR:OG1	2.35	0.42
19:a:827:CLA:HBA2	19:a:827:CLA:H3A	1.76	0.42
19:a:833:CLA:H61	19:l:1502:CLA:H43	2.01	0.42
2:b:255:LEU:HD21	2:b:278:LEU:HD13	2.01	0.42
19:b:3015:CLA:H41	19:b:3015:CLA:H62	1.69	0.42
4:d:132:LYS:HB2	4:d:132:LYS:HE3	1.77	0.42
19:f:201:CLA:H41	19:f:201:CLA:H61	1.44	0.42
11:m:13:VAL:O	11:m:16:LEU:HB2	2.20	0.42
19:a:807:CLA:H41	19:a:807:CLA:H62	1.55	0.42
2:b:544:MET:HE1	2:b:557:ASP:HB2	2.01	0.42
19:b:3003:CLA:H141	19:b:3003:CLA:H162	1.78	0.42
19:b:3008:CLA:H111	19:b:3008:CLA:H2	2.00	0.42
19:D:401:CLA:H2A	19:D:401:CLA:CED	2.49	0.42
17:S:268:ASP:OD1	17:S:269:LEU:N	2.53	0.42
1:a:394:MET:HE3	1:a:605:VAL:HG11	2.01	0.42
19:a:821:CLA:H91	19:a:821:CLA:H111	1.75	0.42
2:b:22:TRP:CG	2:b:701:GLN:HE22	2.37	0.42
21:i:101:BCR:H15C	21:i:101:BCR:H351	1.88	0.42
9:k:35:GLY:O	9:k:39:ILE:HG12	2.19	0.42
12:A:279:PRO:O	12:A:283:ILE:HG12	2.19	0.42
17:S:293:GLY:HA2	17:S:296:TRP:CE2	2.54	0.42
1:a:381:ILE:HG12	1:a:519:LYS:HD3	2.02	0.42
1:a:431:ARG:HD2	4:d:13:GLY:O	2.19	0.42
19:a:836:CLA:H143	19:a:836:CLA:H161	1.85	0.42
6:f:54:SER:HA	6:f:57:ILE:HD12	2.02	0.42
1:a:296:HIS:HB2	19:a:819:CLA:C1B	2.49	0.42
1:a:392:HIS:O	1:a:396:ILE:HG12	2.20	0.42
1:a:426:LEU:HD12	1:a:426:LEU:HA	1.92	0.42
1:a:447:LEU:HB3	1:a:540:PHE:HB2	2.00	0.42
19:a:819:CLA:H62	19:a:819:CLA:H41	1.70	0.42
19:b:3024:CLA:H162	19:b:3024:CLA:H192	1.76	0.42
10:l:14:ASP:O	10:l:17:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:157:PHE:CD1	13:D:171:PRO:HG2	2.54	0.42
1:a:238:LEU:HD23	1:a:238:LEU:HA	1.92	0.42
19:a:830:CLA:H91	19:a:830:CLA:H111	1.72	0.42
2:b:50:HIS:O	2:b:54:ILE:HG13	2.20	0.42
2:b:309:LYS:HB3	2:b:309:LYS:HE3	1.83	0.42
19:b:3018:CLA:H3A	19:b:3018:CLA:HBA2	1.50	0.42
5:e:13:ARG:O	5:e:14:THR:HB	2.19	0.42
9:k:59:LEU:HD12	9:k:63:LEU:HD23	2.02	0.42
13:D:279:LEU:HD12	31:D:402:PHO:HBC3	2.02	0.42
14:E:27:ILE:HB	14:E:28:PRO:HD3	2.02	0.42
1:a:272:SER:HB2	9:k:10:VAL:HG21	2.01	0.41
1:a:475:ALA:O	1:a:477:GLN:HG3	2.19	0.41
1:a:698:GLU:CD	2:b:542:LYS:HB2	2.44	0.41
19:a:856:CLA:H91	19:a:856:CLA:H111	1.72	0.41
2:b:320:LEU:HD23	2:b:320:LEU:HA	1.90	0.41
2:b:367:ALA:HB1	2:b:722:LEU:HD11	2.02	0.41
2:b:392:PHE:CE2	21:b:3046:BCR:H271	2.55	0.41
19:b:3032:CLA:H62	19:b:3032:CLA:H2	1.85	0.41
6:f:66:LEU:HD23	6:f:66:LEU:HA	1.88	0.41
31:A:404:PHO:H3A	31:A:404:PHO:HBA2	1.70	0.41
17:S:120:ASP:OD1	17:S:120:ASP:N	2.52	0.41
19:a:806:CLA:H141	19:a:806:CLA:H162	1.79	0.41
19:a:832:CLA:H93	22:a:852:LHG:H272	2.02	0.41
19:a:842:CLA:H172	8:j:23:ALA:HB2	2.02	0.41
2:b:10:GLN:NE2	7:i:40:GLY:O	2.34	0.41
2:b:440:VAL:HG21	19:b:3033:CLA:HAC2	2.01	0.41
19:b:3007:CLA:H62	19:b:3007:CLA:H41	1.72	0.41
19:b:3009:CLA:H162	19:b:3009:CLA:H141	1.67	0.41
19:b:3024:CLA:H112	19:b:3024:CLA:H152	1.62	0.41
19:k:4002:CLA:HBA2	19:k:4002:CLA:H3A	1.46	0.41
12:A:127:MET:HE3	12:A:147:TYR:HD2	1.86	0.41
17:S:37:PHE:HE2	17:S:39:PRO:HB3	1.85	0.41
1:a:168:MET:HE3	1:a:168:MET:HB3	1.85	0.41
19:a:802:CLA:HMA1	19:b:3002:CLA:H202	2.01	0.41
19:a:804:CLA:H141	19:a:804:CLA:H162	1.85	0.41
19:a:842:CLA:H162	19:a:842:CLA:H141	1.59	0.41
19:a:843:CLA:HAA1	22:a:854:LHG:H383	2.02	0.41
19:b:3020:CLA:HBA2	19:b:3020:CLA:H3A	1.37	0.41
4:d:32:TRP:NE1	4:d:50:MET:SD	2.81	0.41
19:l:1502:CLA:H141	19:l:1502:CLA:H161	1.90	0.41
1:a:348:TRP:HB3	19:a:806:CLA:HAC1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:432:HIS:CD2	19:a:832:CLA:C4A	3.04	0.41
19:a:808:CLA:H62	19:a:808:CLA:H41	1.88	0.41
19:a:809:CLA:HMC3	19:a:810:CLA:HMD1	2.01	0.41
6:f:78:ASP:OD1	6:f:78:ASP:N	2.54	0.41
21:k:4004:BCR:H15C	21:k:4004:BCR:H351	1.86	0.41
19:a:803:CLA:H111	19:a:803:CLA:H142	1.82	0.41
19:a:825:CLA:H61	19:a:825:CLA:H41	1.87	0.41
19:a:827:CLA:CHB	19:a:840:CLA:HAA2	2.49	0.41
19:a:842:CLA:H142	19:a:842:CLA:H111	1.80	0.41
19:b:3004:CLA:HHC	19:b:3006:CLA:OBD	2.21	0.41
3:c:15:THR:HG22	3:c:28:MET:SD	2.61	0.41
6:f:57:ILE:O	6:f:60:GLU:HG3	2.21	0.41
8:j:17:ALA:O	8:j:20:THR:HG22	2.20	0.41
14:E:27:ILE:HG12	32:F:101:HEM:HMC2	2.03	0.41
1:a:646:LEU:HD22	2:b:648:LEU:HD21	2.02	0.41
19:a:809:CLA:H91	19:a:809:CLA:H111	1.62	0.41
19:a:814:CLA:H192	19:a:814:CLA:H162	1.84	0.41
21:a:846:BCR:H24C	21:a:846:BCR:H371	1.91	0.41
2:b:709:HIS:CE1	19:b:3040:CLA:C4D	3.03	0.41
19:b:3020:CLA:H141	19:b:3020:CLA:H161	1.76	0.41
14:E:31:PHE:CD1	14:E:31:PHE:C	2.98	0.41
17:S:42:GLU:HA	17:S:330:LEU:HD23	2.02	0.41
1:a:425:LEU:HD23	1:a:425:LEU:HA	1.84	0.41
19:a:815:CLA:O1A	21:a:845:BCR:HC7	2.20	0.41
19:a:825:CLA:H141	22:a:852:LHG:H171	2.01	0.41
2:b:278:LEU:HD21	19:b:3016:CLA:CAB	2.50	0.41
19:b:3017:CLA:H141	19:b:3017:CLA:H162	1.88	0.41
19:b:3018:CLA:H11	19:b:3018:CLA:H52	1.87	0.41
29:f:207:LMT:H92	29:f:207:LMT:H62	1.75	0.41
21:k:4001:BCR:H15C	21:k:4001:BCR:H351	1.88	0.41
12:A:43:THR:HG23	21:A:406:BCR:H362	2.02	0.41
14:E:44:TYR:CD2	14:E:51:ARG:HG2	2.56	0.41
1:a:182:VAL:HG12	1:a:183:LYS:HG2	2.02	0.41
1:a:397:GLY:O	1:a:401:ILE:HG13	2.20	0.41
1:a:542:ILE:HD11	19:a:838:CLA:HBB1	2.02	0.41
6:f:85:GLY:HA2	6:f:89:ILE:HD12	2.03	0.41
1:a:72:ILE:HG12	19:a:806:CLA:C2C	2.51	0.41
1:a:154:ASP:OD1	1:a:155:SER:N	2.54	0.41
1:a:483:ALA:O	1:a:486:VAL:HG12	2.21	0.41
1:a:527:LEU:HA	1:a:531:ASP:OD2	2.21	0.41
1:a:529:THR:HG22	1:a:533:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:802:CLA:H161	19:a:802:CLA:H122	1.92	0.41
19:a:826:CLA:H101	19:a:826:CLA:H61	1.91	0.41
19:a:843:CLA:H3A	22:a:854:LHG:H371	2.03	0.41
2:b:258:LEU:HD12	2:b:258:LEU:HA	1.86	0.41
2:b:649:PHE:O	2:b:653:VAL:HG23	2.20	0.41
19:b:3012:CLA:H3A	19:b:3012:CLA:HBA2	1.71	0.41
19:b:3026:CLA:H121	21:b:3048:BCR:C20	2.51	0.41
19:b:3027:CLA:H111	19:b:3027:CLA:H93	1.71	0.41
4:d:109:ASN:HB3	4:d:112:ARG:CZ	2.51	0.41
21:f:202:BCR:H20C	21:f:202:BCR:H361	1.89	0.41
21:j:104:BCR:H20C	21:j:104:BCR:H361	1.81	0.41
19:A:405:CLA:HAB	16:I:15:PHE:CD2	2.55	0.41
13:D:189:HIS:ND1	13:D:289:LEU:HD13	2.36	0.41
1:a:265:THR:HB	9:k:16:TRP:HB2	2.03	0.41
1:a:392:HIS:HB2	19:a:829:CLA:CHB	2.51	0.41
1:a:572:PHE:CE1	1:a:586:SER:HB3	2.55	0.41
1:a:575:ASP:CG	3:c:53:ARG:HH21	2.29	0.41
19:a:843:CLA:HMA1	22:a:852:LHG:HC62	2.03	0.41
2:b:460:TRP:O	2:b:464:THR:HG23	2.21	0.41
2:b:709:HIS:HE1	19:b:3040:CLA:C4D	2.34	0.41
19:b:3008:CLA:CGA	19:b:3008:CLA:C1A	2.99	0.41
19:b:3037:CLA:H3A	19:b:3037:CLA:HBA2	1.70	0.41
10:l:62:ILE:HG21	10:l:138:ALA:HB1	2.03	0.41
1:a:429:MET:CE	19:a:832:CLA:HBC3	2.51	0.40
19:a:824:CLA:H2	19:a:824:CLA:C4A	2.50	0.40
2:b:112:PRO:HG2	7:i:1:MET:SD	2.61	0.40
19:b:3025:CLA:HED3	19:b:3026:CLA:CAD	2.51	0.40
10:l:86:LEU:HA	10:l:89:ILE:HG22	2.02	0.40
10:l:88:LEU:HD12	10:l:88:LEU:HA	1.82	0.40
1:a:24:SER:O	19:a:812:CLA:HHB	2.22	0.40
1:a:412:MET:HE2	1:a:412:MET:HB2	1.90	0.40
1:a:457:HIS:HE1	19:a:835:CLA:CHA	2.35	0.40
1:a:704:HIS:CE1	19:a:841:CLA:C4D	3.00	0.40
2:b:490:TRP:CD1	19:b:3034:CLA:HED1	2.55	0.40
26:m:101:ECH:H15	26:m:101:ECH:H35	1.98	0.40
12:A:206:PHE:CD2	31:D:402:PHO:HBB2	2.56	0.40
13:D:293:LEU:HD21	13:D:295:ALA:HB3	2.02	0.40
17:S:94:ALA:HB1	17:S:114:ILE:HG21	2.03	0.40
1:a:674:ALA:HB1	24:a:857:45D:H421	2.02	0.40
19:a:824:CLA:H11	22:a:854:LHG:H101	2.03	0.40
19:a:826:CLA:HBA1	19:a:830:CLA:H191	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:840:CLA:H142	21:a:847:BCR:H281	2.03	0.40
19:a:841:CLA:H72	19:b:3032:CLA:H11	2.03	0.40
19:a:842:CLA:H51	19:a:842:CLA:H8	1.93	0.40
22:a:854:LHG:O10	22:a:854:LHG:O2	2.38	0.40
2:b:59:LEU:HD23	2:b:59:LEU:HA	1.93	0.40
2:b:92:TRP:HB3	7:i:15:ILE:HD12	2.03	0.40
19:b:3008:CLA:H151	19:b:3027:CLA:H162	2.04	0.40
19:b:3014:CLA:H141	19:b:3014:CLA:H193	2.02	0.40
26:b:3045:ECH:H20	26:b:3045:ECH:H36	1.76	0.40
10:l:51:LEU:HD13	10:l:129:VAL:HG23	2.04	0.40
12:A:56:PRO:HB2	12:A:107:TYR:CE1	2.57	0.40
1:a:373:MET:HE2	19:a:828:CLA:HMC2	2.02	0.40
19:a:806:CLA:HBC2	19:a:831:CLA:HMA1	2.02	0.40
19:a:833:CLA:H62	19:a:833:CLA:H102	1.69	0.40
19:a:837:CLA:H121	19:a:858:CLA:HBC2	2.04	0.40
2:b:194:LEU:HA	2:b:198:ALA:HB3	2.03	0.40
2:b:427:LEU:O	2:b:431:THR:OG1	2.26	0.40
2:b:459:GLN:HG2	2:b:470:TYR:CE1	2.56	0.40
10:l:62:ILE:HD11	10:l:82:LEU:HA	2.03	0.40
14:E:36:LEU:O	14:E:40:THR:HG22	2.21	0.40
1:a:56:HIS:HE1	19:a:805:CLA:CHC	2.34	0.40
19:a:837:CLA:C1C	19:a:858:CLA:H42	2.51	0.40
2:b:145:LEU:HD23	2:b:145:LEU:HA	1.92	0.40
19:b:3009:CLA:H41	19:b:3009:CLA:H61	1.88	0.40
19:b:3017:CLA:H93	19:b:3034:CLA:H43	2.02	0.40
10:l:34:ILE:HD13	10:l:34:ILE:HA	1.93	0.40
13:D:69:GLU:OE1	13:D:69:GLU:N	2.44	0.40
13:D:313:THR:HB	13:D:316:THR:HG23	2.04	0.40
17:S:51:PHE:CZ	17:S:327:GLY:HA2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	739/751 (98%)	711 (96%)	28 (4%)	0	100	100
2	b	727/731 (100%)	707 (97%)	20 (3%)	0	100	100
3	c	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	d	137/141 (97%)	128 (93%)	9 (7%)	0	100	100
5	e	67/74 (90%)	64 (96%)	3 (4%)	0	100	100
6	f	140/165 (85%)	135 (96%)	5 (4%)	0	100	100
7	i	38/40 (95%)	38 (100%)	0	0	100	100
8	j	38/40 (95%)	38 (100%)	0	0	100	100
9	k	73/86 (85%)	72 (99%)	1 (1%)	0	100	100
10	l	141/157 (90%)	137 (97%)	4 (3%)	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
12	A	285/344 (83%)	273 (96%)	12 (4%)	0	100	100
13	D	274/336 (82%)	268 (98%)	6 (2%)	0	100	100
14	E	42/81 (52%)	42 (100%)	0	0	100	100
15	F	26/44 (59%)	24 (92%)	2 (8%)	0	100	100
16	I	25/38 (66%)	24 (96%)	1 (4%)	0	100	100
17	S	301/342 (88%)	295 (98%)	6 (2%)	0	100	100
All	All	3160/3482 (91%)	3058 (97%)	102 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	593/603 (98%)	593 (100%)	0	100	100
2	b	582/583 (100%)	582 (100%)	0	100	100
3	c	68/69 (99%)	68 (100%)	0	100	100
4	d	114/116 (98%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	57/60 (95%)	57 (100%)	0	100	100
6	f	119/137 (87%)	119 (100%)	0	100	100
7	i	32/32 (100%)	32 (100%)	0	100	100
8	j	35/35 (100%)	35 (100%)	0	100	100
9	k	53/62 (86%)	53 (100%)	0	100	100
10	l	107/118 (91%)	106 (99%)	1 (1%)	70	77
11	m	25/25 (100%)	25 (100%)	0	100	100
12	A	235/283 (83%)	235 (100%)	0	100	100
13	D	220/271 (81%)	220 (100%)	0	100	100
14	E	38/73 (52%)	38 (100%)	0	100	100
15	F	22/37 (60%)	22 (100%)	0	100	100
16	I	24/34 (71%)	24 (100%)	0	100	100
17	S	239/279 (86%)	239 (100%)	0	100	100
All	All	2563/2817 (91%)	2562 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	l	19	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	157	GLN
1	a	488	HIS
1	a	659	ASN
2	b	361	GLN
2	b	478	ASN
2	b	607	ASN
2	b	630	ASN
3	c	16	GLN
4	d	38	GLN
7	i	33	HIS
10	l	105	GLN
12	A	165	GLN
12	A	298	ASN

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Mol	Chain	Res	Type
12	A	337	HIS
17	S	167	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 145 ligands modelled in this entry, 1 is monoatomic - leaving 144 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	$\# Z > 2$
21	BCR	a	849	-	25,25,41	1.21	1 (4%)	33,33,56	1.34	5 (15%)
19	CLA	a	855	-	69,73,73	1.15	9 (13%)	82,113,113	1.21	6 (7%)
19	CLA	a	802	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	7 (8%)
19	CLA	a	811	-	54,58,73	1.29	8 (14%)	64,95,113	1.48	6 (9%)
19	CLA	b	3004	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
19	CLA	b	3018	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	7 (8%)
19	CLA	b	3019	-	64,68,73	1.19	8 (12%)	76,107,113	1.29	6 (7%)
19	CLA	a	818	-	69,73,73	1.13	8 (11%)	82,113,113	1.33	6 (7%)
21	BCR	l	1504	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	b	3014	-	69,73,73	1.15	8 (11%)	82,113,113	1.32	7 (8%)
19	CLA	b	3037	-	69,73,73	1.14	9 (13%)	82,113,113	1.28	6 (7%)
19	CLA	a	816	-	50,54,73	1.34	9 (18%)	59,90,113	1.42	4 (6%)
19	CLA	a	858	-	69,73,73	1.17	9 (13%)	82,113,113	1.25	5 (6%)
22	LHG	a	854	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
19	CLA	b	3012	-	54,58,73	1.29	9 (16%)	64,95,113	1.36	6 (9%)
19	CLA	a	827	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
19	CLA	b	3036	-	56,60,73	1.28	9 (16%)	65,97,113	1.38	8 (12%)
19	CLA	a	813	-	64,68,73	1.21	8 (12%)	76,107,113	1.27	4 (5%)
23	LMG	b	3049	-	55,55,55	0.69	1 (1%)	63,63,63	1.40	8 (12%)
19	CLA	b	3003	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	8 (9%)
19	CLA	f	201	-	69,73,73	1.16	8 (11%)	82,113,113	1.27	5 (6%)
19	CLA	b	3029	-	69,73,73	1.16	9 (13%)	82,113,113	1.36	7 (8%)
19	CLA	a	856	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	4 (4%)
19	CLA	b	3011	-	60,64,73	1.23	9 (15%)	71,102,113	1.36	5 (7%)
25	SF4	c	101	3	0,12,12	-	-	-	-	-
19	CLA	a	804	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	7 (8%)
19	CLA	a	815	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
19	CLA	a	838	-	55,59,73	1.29	8 (14%)	64,96,113	1.43	9 (14%)
19	CLA	k	4002	-	50,54,73	1.36	9 (18%)	59,90,113	1.39	4 (6%)
21	BCR	b	3048	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	6 (10%)
19	CLA	b	3016	-	60,64,73	1.23	9 (15%)	71,102,113	1.32	5 (7%)
19	CLA	b	3008	-	69,73,73	1.14	9 (13%)	82,113,113	1.29	7 (8%)
21	BCR	a	848	-	41,41,41	1.23	3 (7%)	56,56,56	1.29	7 (12%)
19	CLA	a	840	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	5 (6%)
19	CLA	a	806	-	69,73,73	1.14	9 (13%)	82,113,113	1.36	6 (7%)
19	CLA	a	829	-	69,73,73	1.15	9 (13%)	82,113,113	1.31	7 (8%)
19	CLA	a	834	-	69,73,73	1.15	8 (11%)	82,113,113	1.31	8 (9%)
18	CL0	a	801	-	58,73,73	2.19	12 (20%)	60,113,113	1.65	14 (23%)
19	CLA	b	3013	-	69,73,73	1.15	9 (13%)	82,113,113	1.36	7 (8%)
19	CLA	b	3006	-	69,73,73	1.15	8 (11%)	82,113,113	1.29	6 (7%)
32	HEM	F	101	15,14	50,50,50	1.38	8 (16%)	67,82,82	1.06	1 (1%)
19	CLA	a	842	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	5 (6%)
19	CLA	a	833	-	64,68,73	1.20	9 (14%)	76,107,113	1.30	5 (6%)
19	CLA	b	3031	-	54,58,73	1.29	9 (16%)	64,95,113	1.36	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	BCR	A	406	-	41,41,41	1.18	2 (4%)	56,56,56	1.24	7 (12%)
21	BCR	j	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.28	7 (12%)
23	LMG	b	3051	-	55,55,55	0.76	1 (1%)	63,63,63	1.34	8 (12%)
19	CLA	b	3023	-	61,65,73	1.23	9 (14%)	72,103,113	1.31	6 (8%)
19	CLA	a	823	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	6 (7%)
19	CLA	a	809	1	69,73,73	1.14	9 (13%)	82,113,113	1.30	6 (7%)
25	SF4	c	102	3	0,12,12	-	-	-	-	-
19	CLA	b	3041	22	50,54,73	1.33	8 (16%)	59,90,113	1.38	6 (10%)
19	CLA	b	3030	-	55,59,73	1.30	9 (16%)	64,96,113	1.36	5 (7%)
21	BCR	a	846	-	41,41,41	1.19	3 (7%)	56,56,56	1.23	6 (10%)
19	CLA	a	808	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	8 (9%)
19	CLA	a	822	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
19	CLA	b	3007	-	69,73,73	1.14	8 (11%)	82,113,113	1.26	6 (7%)
19	CLA	b	3021	-	64,68,73	1.20	8 (12%)	76,107,113	1.30	8 (10%)
19	CLA	l	1503	-	56,60,73	1.28	8 (14%)	65,97,113	1.40	5 (7%)
21	BCR	b	3047	-	41,41,41	1.22	3 (7%)	56,56,56	1.20	7 (12%)
19	CLA	b	3039	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	6 (7%)
31	PHO	D	402	-	58,69,69	2.18	11 (18%)	55,99,99	1.53	8 (14%)
19	CLA	b	3038	-	54,58,73	1.30	8 (14%)	64,95,113	1.35	6 (9%)
19	CLA	a	805	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	6 (7%)
19	CLA	j	102	8	59,63,73	1.26	8 (13%)	70,101,113	1.35	6 (8%)
19	CLA	D	404	-	50,54,73	1.35	8 (16%)	59,90,113	1.43	4 (6%)
19	CLA	b	3024	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	7 (8%)
19	CLA	a	830	-	69,73,73	1.15	9 (13%)	82,113,113	1.23	5 (6%)
22	LHG	b	3050	19	37,37,48	0.71	1 (2%)	40,43,54	1.25	4 (10%)
27	EQ3	b	3052	-	43,43,43	1.40	6 (13%)	55,60,60	1.51	14 (25%)
31	PHO	A	404	-	58,69,69	2.13	10 (17%)	55,99,99	1.40	6 (10%)
20	PQN	a	844	-	34,34,34	0.37	0	43,45,45	0.59	1 (2%)
19	CLA	l	1502	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	6 (7%)
22	LHG	a	850	-	48,48,48	0.64	1 (2%)	51,54,54	1.29	6 (11%)
21	BCR	k	4001	-	41,41,41	1.20	2 (4%)	56,56,56	1.30	6 (10%)
19	CLA	a	817	-	50,54,73	1.34	9 (18%)	59,90,113	1.43	4 (6%)
19	CLA	b	3017	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	6 (7%)
19	CLA	a	810	1	55,59,73	1.29	8 (14%)	64,96,113	1.44	6 (9%)
19	CLA	b	3009	2	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LMG	a	853	-	40,40,55	0.81	0	48,48,63	1.33	5 (10%)
19	CLA	D	401	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	4 (4%)
19	CLA	a	807	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
19	CLA	k	4003	9	49,53,73	1.38	8 (16%)	58,89,113	1.40	5 (8%)
24	45D	a	857	-	43,43,43	1.43	9 (20%)	54,60,60	1.54	10 (18%)
21	BCR	i	101	-	41,41,41	1.20	2 (4%)	56,56,56	1.22	5 (8%)
21	BCR	k	4004	-	41,41,41	1.16	2 (4%)	56,56,56	1.27	7 (12%)
26	ECH	b	3045	-	42,42,42	1.41	8 (19%)	55,58,58	2.22	16 (29%)
21	BCR	b	3044	-	41,41,41	1.17	3 (7%)	56,56,56	1.22	6 (10%)
19	CLA	a	831	-	69,73,73	1.14	8 (11%)	82,113,113	1.38	8 (9%)
28	ZEX	f	205	-	43,43,43	1.34	8 (18%)	51,60,60	1.40	9 (17%)
29	LMT	f	207	-	36,36,36	1.16	6 (16%)	47,47,47	1.04	3 (6%)
19	CLA	b	3025	-	59,63,73	1.24	9 (15%)	70,101,113	1.35	6 (8%)
19	CLA	a	826	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	8 (9%)
19	CLA	a	835	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	6 (7%)
19	CLA	a	841	-	69,73,73	1.14	9 (13%)	82,113,113	1.30	5 (6%)
19	CLA	b	3032	-	69,73,73	1.17	9 (13%)	82,113,113	1.24	4 (4%)
19	CLA	a	824	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	4 (4%)
21	BCR	b	3046	-	41,41,41	1.16	2 (4%)	56,56,56	1.27	7 (12%)
19	CLA	b	3015	-	59,63,73	1.26	9 (15%)	70,101,113	1.36	6 (8%)
19	CLA	D	403	-	59,63,73	1.24	8 (13%)	70,101,113	1.35	6 (8%)
22	LHG	a	852	19	48,48,48	0.61	1 (2%)	51,54,54	1.30	6 (11%)
19	CLA	b	3027	-	69,73,73	1.14	9 (13%)	82,113,113	1.27	5 (6%)
19	CLA	b	3033	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	6 (7%)
19	CLA	a	821	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	5 (6%)
19	CLA	a	803	-	69,73,73	1.14	9 (13%)	82,113,113	1.30	5 (6%)
19	CLA	f	204	6	54,58,73	1.32	9 (16%)	64,95,113	1.40	7 (10%)
28	ZEX	b	3053	-	43,43,43	1.35	7 (16%)	51,60,60	1.48	10 (19%)
19	CLA	a	836	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
22	LHG	f	206	-	48,48,48	0.57	0	51,54,54	1.28	6 (11%)
19	CLA	b	3020	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
19	CLA	a	839	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	6 (7%)
19	CLA	b	3026	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
19	CLA	b	3002	-	69,73,73	1.16	9 (13%)	82,113,113	1.22	4 (4%)
19	CLA	a	825	-	64,68,73	1.20	9 (14%)	76,107,113	1.33	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	405	-	54,58,73	1.31	7 (12%)	64,95,113	1.38	5 (7%)
23	LMG	a	851	-	50,50,55	0.76	1 (2%)	58,58,63	1.34	8 (13%)
19	CLA	b	3028	-	69,73,73	1.15	9 (13%)	82,113,113	1.22	4 (4%)
19	CLA	A	402	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	5 (6%)
25	SF4	b	3001	2,1	0,12,12	-	-	-	-	-
21	BCR	a	847	-	41,41,41	1.20	3 (7%)	56,56,56	1.23	6 (10%)
19	CLA	a	820	-	69,73,73	1.15	9 (13%)	82,113,113	1.26	7 (8%)
19	CLA	b	3034	-	69,73,73	1.15	8 (11%)	82,113,113	1.27	7 (8%)
19	CLA	A	403	-	50,54,73	1.34	9 (18%)	59,90,113	1.43	4 (6%)
21	BCR	j	104	-	41,41,41	1.21	3 (7%)	56,56,56	1.24	7 (12%)
19	CLA	a	832	-	60,64,73	1.23	8 (13%)	71,102,113	1.34	4 (5%)
19	CLA	j	103	-	50,54,73	1.36	6 (12%)	59,90,113	1.32	5 (8%)
21	BCR	f	202	-	41,41,41	1.21	3 (7%)	56,56,56	1.20	5 (8%)
19	CLA	b	3022	-	50,54,73	1.34	9 (18%)	59,90,113	1.41	4 (6%)
19	CLA	b	3005	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	7 (8%)
20	PQN	b	3042	-	34,34,34	0.40	0	43,45,45	0.55	1 (2%)
26	ECH	m	101	-	42,42,42	1.47	9 (21%)	55,58,58	1.64	14 (25%)
19	CLA	b	3040	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	5 (6%)
19	CLA	b	3035	-	54,58,73	1.32	8 (14%)	64,95,113	1.42	6 (9%)
19	CLA	a	814	-	69,73,73	1.15	9 (13%)	82,113,113	1.32	8 (9%)
19	CLA	b	3010	-	60,64,73	1.25	9 (15%)	71,102,113	1.31	5 (7%)
21	BCR	b	3043	-	41,41,41	1.25	3 (7%)	56,56,56	1.27	6 (10%)
19	CLA	a	828	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	6 (7%)
19	CLA	f	203	-	54,58,73	1.30	8 (14%)	64,95,113	1.39	7 (10%)
19	CLA	l	1501	-	54,58,73	1.33	7 (12%)	64,95,113	1.42	6 (9%)
19	CLA	a	843	22	60,64,73	1.23	9 (15%)	71,102,113	1.33	7 (9%)
19	CLA	a	837	1	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
19	CLA	a	819	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
19	CLA	a	812	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	7 (8%)
21	BCR	a	845	-	41,41,41	1.21	3 (7%)	56,56,56	1.23	6 (10%)

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
21	BCR	a	849	-	-	3/18/35/63	0/1/1/2
19	CLA	a	855	-	1/1/15/20	8/39/115/115	-
19	CLA	a	802	-	1/1/15/20	15/39/115/115	-
19	CLA	a	811	-	1/1/12/20	9/21/97/115	-
19	CLA	b	3004	-	1/1/15/20	14/39/115/115	-
19	CLA	b	3018	-	1/1/15/20	9/39/115/115	-
19	CLA	b	3019	-	1/1/14/20	8/33/109/115	-
19	CLA	a	818	-	1/1/15/20	10/39/115/115	-
21	BCR	l	1504	-	-	11/29/63/63	0/2/2/2
19	CLA	b	3014	-	1/1/15/20	16/39/115/115	-
19	CLA	b	3037	-	1/1/15/20	13/39/115/115	-
19	CLA	a	816	-	1/1/11/20	7/17/93/115	-
19	CLA	a	858	-	1/1/15/20	13/39/115/115	-
22	LHG	a	854	-	-	24/53/53/53	-
19	CLA	b	3012	-	1/1/12/20	5/21/97/115	-
19	CLA	a	827	-	1/1/15/20	12/39/115/115	-
19	CLA	b	3036	-	1/1/12/20	6/24/100/115	-
19	CLA	a	813	-	1/1/14/20	13/33/109/115	-
23	LMG	b	3049	-	-	27/50/70/70	0/1/1/1
19	CLA	b	3003	-	1/1/15/20	18/39/115/115	-
19	CLA	f	201	-	1/1/15/20	20/39/115/115	-
19	CLA	b	3029	-	1/1/15/20	15/39/115/115	-
19	CLA	a	856	-	1/1/15/20	17/39/115/115	-
19	CLA	b	3011	-	1/1/13/20	10/29/105/115	-
25	SF4	c	101	3	-	-	0/6/5/5
19	CLA	a	804	-	1/1/15/20	7/39/115/115	-
19	CLA	a	815	-	1/1/15/20	10/39/115/115	-
19	CLA	a	838	-	-	4/23/99/115	-
19	CLA	k	4002	-	1/1/11/20	7/17/93/115	-
21	BCR	b	3048	-	-	17/29/63/63	0/2/2/2
19	CLA	b	3016	-	1/1/13/20	8/29/105/115	-
19	CLA	b	3008	-	1/1/15/20	11/39/115/115	-
21	BCR	a	848	-	-	7/29/63/63	0/2/2/2
19	CLA	a	840	-	1/1/15/20	12/39/115/115	-
19	CLA	a	806	-	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	a	829	-	1/1/15/20	7/39/115/115	-
19	CLA	a	834	-	1/1/15/20	7/39/115/115	-
18	CL0	a	801	-	3/3/20/25	10/37/135/135	-
19	CLA	b	3013	-	1/1/15/20	21/39/115/115	-
19	CLA	b	3006	-	1/1/15/20	11/39/115/115	-
32	HEM	F	101	15,14	-	5/14/54/54	-
19	CLA	a	842	-	1/1/15/20	16/39/115/115	-
19	CLA	a	833	-	1/1/14/20	14/33/109/115	-
19	CLA	b	3031	-	1/1/12/20	5/21/97/115	-
21	BCR	A	406	-	-	8/29/63/63	0/2/2/2
21	BCR	j	101	-	-	6/29/63/63	0/2/2/2
23	LMG	b	3051	-	-	29/50/70/70	0/1/1/1
19	CLA	b	3023	-	1/1/13/20	9/30/106/115	-
19	CLA	a	823	-	1/1/15/20	13/39/115/115	-
19	CLA	a	809	1	1/1/15/20	18/39/115/115	-
25	SF4	c	102	3	-	-	0/6/5/5
19	CLA	b	3041	22	1/1/11/20	9/17/93/115	-
19	CLA	b	3030	-	1/1/12/20	9/23/99/115	-
21	BCR	a	846	-	-	5/29/63/63	0/2/2/2
19	CLA	a	808	-	1/1/15/20	13/39/115/115	-
19	CLA	a	822	-	1/1/15/20	12/39/115/115	-
19	CLA	b	3007	-	1/1/15/20	16/39/115/115	-
19	CLA	b	3021	-	1/1/14/20	9/33/109/115	-
19	CLA	l	1503	-	1/1/12/20	7/24/100/115	-
21	BCR	b	3047	-	-	5/29/63/63	0/2/2/2
19	CLA	b	3039	-	1/1/15/20	16/39/115/115	-
31	PHO	D	402	-	-	9/37/103/103	0/5/6/6
19	CLA	b	3038	-	1/1/12/20	6/21/97/115	-
19	CLA	a	805	-	1/1/15/20	11/39/115/115	-
19	CLA	j	102	8	1/1/13/20	10/27/103/115	-
19	CLA	D	404	-	1/1/11/20	5/17/93/115	-
19	CLA	b	3024	-	1/1/15/20	10/39/115/115	-
19	CLA	a	830	-	1/1/15/20	16/39/115/115	-
22	LHG	b	3050	19	-	19/42/42/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	EQ3	b	3052	-	-	3/29/68/68	0/2/2/2
31	PHO	A	404	-	-	11/37/103/103	0/5/6/6
20	PQN	a	844	-	-	1/23/43/43	0/2/2/2
19	CLA	l	1502	-	1/1/15/20	11/39/115/115	-
22	LHG	a	850	-	-	27/53/53/53	-
21	BCR	k	4001	-	-	8/29/63/63	0/2/2/2
19	CLA	a	817	-	1/1/11/20	7/17/93/115	-
19	CLA	b	3017	-	1/1/15/20	12/39/115/115	-
19	CLA	a	810	1	1/1/12/20	3/23/99/115	-
19	CLA	b	3009	2	1/1/15/20	14/39/115/115	-
23	LMG	a	853	-	-	14/35/55/70	0/1/1/1
19	CLA	D	401	-	1/1/15/20	15/39/115/115	-
19	CLA	a	807	-	1/1/15/20	14/39/115/115	-
19	CLA	k	4003	9	1/1/11/20	6/15/91/115	-
24	45D	a	857	-	-	4/29/69/69	0/2/2/2
21	BCR	i	101	-	-	6/29/63/63	0/2/2/2
21	BCR	k	4004	-	-	5/29/63/63	0/2/2/2
26	ECH	b	3045	-	-	9/29/66/66	0/2/2/2
21	BCR	b	3044	-	-	7/29/63/63	0/2/2/2
19	CLA	a	831	-	1/1/15/20	17/39/115/115	-
28	ZEX	f	205	-	-	6/29/67/67	0/2/2/2
29	LMT	f	207	-	-	15/21/61/61	0/2/2/2
19	CLA	b	3025	-	1/1/13/20	7/27/103/115	-
19	CLA	a	826	-	1/1/15/20	15/39/115/115	-
19	CLA	a	835	-	1/1/15/20	14/39/115/115	-
19	CLA	a	841	-	1/1/15/20	12/39/115/115	-
19	CLA	b	3032	-	1/1/15/20	7/39/115/115	-
19	CLA	a	824	-	1/1/15/20	17/39/115/115	-
21	BCR	b	3046	-	-	4/29/63/63	0/2/2/2
19	CLA	b	3015	-	1/1/13/20	11/27/103/115	-
19	CLA	D	403	-	1/1/13/20	10/27/103/115	-
22	LHG	a	852	19	-	21/53/53/53	-
19	CLA	b	3027	-	1/1/15/20	11/39/115/115	-
19	CLA	b	3033	-	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	a	821	-	1/1/15/20	20/39/115/115	-
19	CLA	a	803	-	1/1/15/20	9/39/115/115	-
19	CLA	f	204	6	1/1/12/20	7/21/97/115	-
28	ZEX	b	3053	-	-	4/29/67/67	0/2/2/2
19	CLA	a	836	-	1/1/15/20	12/39/115/115	-
22	LHG	f	206	-	-	28/53/53/53	-
19	CLA	b	3020	-	1/1/15/20	17/39/115/115	-
19	CLA	a	839	-	1/1/15/20	12/39/115/115	-
19	CLA	b	3026	-	1/1/15/20	7/39/115/115	-
19	CLA	b	3002	-	1/1/15/20	13/39/115/115	-
19	CLA	a	825	-	1/1/14/20	11/33/109/115	-
19	CLA	A	405	-	1/1/12/20	5/21/97/115	-
23	LMG	a	851	-	-	27/45/65/70	0/1/1/1
19	CLA	b	3028	-	1/1/15/20	11/39/115/115	-
19	CLA	A	402	-	1/1/15/20	16/39/115/115	-
25	SF4	b	3001	2,1	-	-	0/6/5/5
21	BCR	a	847	-	-	4/29/63/63	0/2/2/2
19	CLA	a	820	-	1/1/15/20	15/39/115/115	-
19	CLA	b	3034	-	1/1/15/20	12/39/115/115	-
19	CLA	A	403	-	1/1/11/20	6/17/93/115	-
21	BCR	j	104	-	-	8/29/63/63	0/2/2/2
19	CLA	a	832	-	1/1/13/20	15/29/105/115	-
19	CLA	j	103	-	1/1/11/20	5/17/93/115	-
21	BCR	f	202	-	-	15/29/63/63	0/2/2/2
19	CLA	b	3022	-	1/1/11/20	3/17/93/115	-
19	CLA	b	3005	-	1/1/15/20	16/39/115/115	-
20	PQN	b	3042	-	-	0/23/43/43	0/2/2/2
26	ECH	m	101	-	-	2/29/66/66	0/2/2/2
19	CLA	b	3040	-	1/1/15/20	8/39/115/115	-
19	CLA	b	3035	-	1/1/12/20	9/21/97/115	-
19	CLA	a	814	-	-	15/39/115/115	-
19	CLA	b	3010	-	1/1/13/20	7/29/105/115	-
21	BCR	b	3043	-	-	10/29/63/63	0/2/2/2
19	CLA	a	828	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	f	203	-	1/1/12/20	4/21/97/115	-
19	CLA	l	1501	-	1/1/12/20	8/21/97/115	-
19	CLA	a	843	22	1/1/13/20	7/29/105/115	-
19	CLA	a	837	1	1/1/15/20	9/39/115/115	-
19	CLA	a	819	-	1/1/15/20	22/39/115/115	-
19	CLA	a	812	-	1/1/15/20	13/39/115/115	-
21	BCR	a	845	-	-	9/29/63/63	0/2/2/2

All (1018) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	402	PHO	C1B-C2B	9.73	1.50	1.39
31	A	404	PHO	C1B-C2B	9.52	1.50	1.39
18	a	801	CL0	C1B-C2B	8.71	1.49	1.39
31	D	402	PHO	C3B-C4B	8.62	1.50	1.41
31	A	404	PHO	C3B-C4B	8.32	1.49	1.41
18	a	801	CL0	C3B-C4B	7.56	1.48	1.41
18	a	801	CL0	C1D-C2D	7.18	1.47	1.39
31	D	402	PHO	C1D-C2D	4.20	1.44	1.39
21	b	3043	BCR	C1-C6	-4.12	1.48	1.53
18	a	801	CL0	C3D-C4D	4.11	1.47	1.41
21	a	848	BCR	C1-C6	-4.05	1.48	1.53
21	a	847	BCR	C1-C6	-3.95	1.48	1.53
21	k	4001	BCR	C1-C6	-3.94	1.48	1.53
21	j	104	BCR	C1-C6	-3.94	1.48	1.53
21	f	202	BCR	C1-C6	-3.90	1.48	1.53
21	a	849	BCR	C1-C6	-3.90	1.48	1.53
31	A	404	PHO	C1D-C2D	3.90	1.43	1.39
21	b	3047	BCR	C30-C25	-3.85	1.48	1.53
21	a	846	BCR	C1-C6	-3.82	1.48	1.53
21	a	845	BCR	C1-C6	-3.81	1.48	1.53
21	b	3043	BCR	C30-C25	-3.78	1.48	1.53
21	A	406	BCR	C1-C6	-3.75	1.49	1.53
21	j	101	BCR	C1-C6	-3.74	1.49	1.53
21	b	3048	BCR	C1-C6	-3.68	1.49	1.53
31	D	402	PHO	C4D-CHA	3.66	1.45	1.39
21	i	101	BCR	C1-C6	-3.64	1.49	1.53
21	l	1504	BCR	C1-C6	-3.63	1.49	1.53
19	j	102	CLA	C1D-ND	3.63	1.42	1.37
31	A	404	PHO	C4D-CHA	3.63	1.45	1.39
19	j	103	CLA	C1D-ND	3.62	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	l	1501	CLA	C1D-ND	3.62	1.42	1.37
21	b	3044	BCR	C1-C6	-3.61	1.49	1.53
21	a	845	BCR	C30-C25	-3.59	1.49	1.53
21	A	406	BCR	C30-C25	-3.58	1.49	1.53
21	j	104	BCR	C30-C25	-3.58	1.49	1.53
21	i	101	BCR	C30-C25	-3.58	1.49	1.53
19	k	4002	CLA	C1D-ND	3.55	1.42	1.37
19	a	826	CLA	C1D-ND	3.55	1.42	1.37
21	b	3047	BCR	C1-C6	-3.52	1.49	1.53
19	b	3017	CLA	C1D-ND	3.52	1.42	1.37
21	f	202	BCR	C30-C25	-3.51	1.49	1.53
21	k	4004	BCR	C1-C6	-3.50	1.49	1.53
19	f	204	CLA	C1D-ND	3.49	1.42	1.37
21	k	4004	BCR	C30-C25	-3.48	1.49	1.53
19	A	402	CLA	C1D-ND	3.48	1.42	1.37
21	a	848	BCR	C30-C25	-3.47	1.49	1.53
19	a	828	CLA	C1D-ND	3.46	1.42	1.37
21	b	3046	BCR	C1-C6	-3.46	1.49	1.53
19	a	858	CLA	C1D-ND	3.45	1.42	1.37
19	a	822	CLA	C1D-ND	3.44	1.42	1.37
19	a	842	CLA	C1D-ND	3.43	1.42	1.37
21	k	4001	BCR	C30-C25	-3.43	1.49	1.53
26	m	101	ECH	C25-C26	3.42	1.40	1.35
19	b	3035	CLA	C1D-ND	3.42	1.42	1.37
19	a	817	CLA	C1D-ND	3.41	1.42	1.37
19	a	824	CLA	C1D-ND	3.41	1.42	1.37
19	A	405	CLA	C1D-ND	3.40	1.42	1.37
19	D	401	CLA	C1D-ND	3.40	1.42	1.37
19	k	4003	CLA	C1D-ND	3.40	1.42	1.37
19	a	814	CLA	C1D-ND	3.40	1.42	1.37
19	a	823	CLA	C1D-ND	3.40	1.42	1.37
19	a	840	CLA	C1D-ND	3.39	1.42	1.37
19	f	203	CLA	C1D-ND	3.39	1.42	1.37
19	b	3038	CLA	C1D-ND	3.39	1.42	1.37
21	a	847	BCR	C30-C25	-3.39	1.49	1.53
19	a	837	CLA	C1D-ND	3.39	1.42	1.37
19	b	3020	CLA	C1D-ND	3.38	1.42	1.37
19	a	838	CLA	C1D-ND	3.38	1.42	1.37
19	b	3004	CLA	C1D-ND	3.38	1.42	1.37
19	D	404	CLA	C1D-ND	3.37	1.42	1.37
19	b	3002	CLA	C1D-ND	3.37	1.42	1.37
19	A	403	CLA	C1D-ND	3.37	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	3041	CLA	C1D-ND	3.36	1.42	1.37
19	a	815	CLA	C1D-ND	3.36	1.42	1.37
19	a	808	CLA	C1D-ND	3.35	1.42	1.37
19	a	839	CLA	C1D-ND	3.35	1.42	1.37
19	b	3014	CLA	C1D-ND	3.35	1.42	1.37
19	b	3010	CLA	C1D-ND	3.35	1.42	1.37
19	a	856	CLA	C1D-ND	3.34	1.42	1.37
19	b	3021	CLA	C1D-ND	3.34	1.42	1.37
19	b	3022	CLA	C1D-ND	3.34	1.42	1.37
19	a	811	CLA	C1D-ND	3.33	1.42	1.37
19	a	833	CLA	C1D-ND	3.33	1.42	1.37
19	b	3029	CLA	C1D-ND	3.32	1.42	1.37
19	b	3039	CLA	C1D-ND	3.32	1.42	1.37
19	a	816	CLA	C1D-ND	3.32	1.42	1.37
21	b	3048	BCR	C30-C25	-3.31	1.49	1.53
19	a	825	CLA	C1D-ND	3.31	1.42	1.37
19	b	3037	CLA	C1D-ND	3.31	1.42	1.37
19	l	1503	CLA	C1D-ND	3.31	1.42	1.37
19	a	813	CLA	C1D-ND	3.30	1.42	1.37
19	a	829	CLA	C1D-ND	3.30	1.42	1.37
19	a	841	CLA	C1D-ND	3.30	1.42	1.37
19	a	806	CLA	C1D-ND	3.29	1.42	1.37
19	b	3028	CLA	C1D-ND	3.29	1.42	1.37
19	a	835	CLA	C1D-ND	3.29	1.42	1.37
19	b	3013	CLA	C1D-ND	3.29	1.42	1.37
19	a	812	CLA	C1D-ND	3.29	1.42	1.37
19	b	3026	CLA	C1D-ND	3.29	1.42	1.37
19	b	3006	CLA	C1D-ND	3.29	1.42	1.37
19	b	3025	CLA	C1D-ND	3.29	1.42	1.37
19	a	802	CLA	C1D-ND	3.29	1.42	1.37
19	b	3040	CLA	C1D-ND	3.29	1.42	1.37
21	b	3044	BCR	C30-C25	-3.29	1.49	1.53
19	a	821	CLA	C1D-ND	3.29	1.42	1.37
19	b	3016	CLA	C1D-ND	3.28	1.42	1.37
19	b	3018	CLA	C1D-ND	3.28	1.42	1.37
19	b	3034	CLA	C1D-ND	3.28	1.42	1.37
19	b	3030	CLA	C1D-ND	3.27	1.42	1.37
19	b	3036	CLA	C1D-ND	3.27	1.42	1.37
19	b	3031	CLA	C1D-ND	3.27	1.42	1.37
19	a	804	CLA	C1D-ND	3.27	1.42	1.37
19	b	3005	CLA	C1D-ND	3.27	1.42	1.37
19	f	201	CLA	C1D-ND	3.27	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	809	CLA	C1D-ND	3.26	1.42	1.37
21	j	101	BCR	C30-C25	-3.26	1.49	1.53
19	a	855	CLA	C1D-ND	3.26	1.42	1.37
19	a	831	CLA	C1D-ND	3.25	1.42	1.37
21	b	3046	BCR	C30-C25	-3.25	1.49	1.53
19	b	3033	CLA	C1D-ND	3.25	1.42	1.37
19	b	3024	CLA	C1D-ND	3.24	1.42	1.37
19	b	3032	CLA	C1D-ND	3.24	1.42	1.37
19	a	830	CLA	C1D-ND	3.23	1.42	1.37
19	b	3027	CLA	C1D-ND	3.23	1.42	1.37
19	b	3019	CLA	C1D-ND	3.23	1.42	1.37
19	a	819	CLA	C1D-ND	3.22	1.42	1.37
19	a	818	CLA	C1D-ND	3.22	1.42	1.37
19	b	3007	CLA	C1D-ND	3.22	1.42	1.37
19	a	843	CLA	C1D-ND	3.21	1.42	1.37
19	a	803	CLA	C1D-ND	3.21	1.42	1.37
19	b	3015	CLA	C1D-ND	3.21	1.42	1.37
19	D	403	CLA	C1D-ND	3.20	1.42	1.37
19	b	3009	CLA	C1D-ND	3.20	1.42	1.37
21	a	846	BCR	C30-C25	-3.19	1.49	1.53
19	a	827	CLA	C1D-ND	3.19	1.42	1.37
19	b	3023	CLA	C1D-ND	3.18	1.42	1.37
19	b	3011	CLA	C1D-ND	3.18	1.42	1.37
26	b	3045	ECH	C23-C22	-3.18	1.39	1.46
19	a	820	CLA	C1D-ND	3.18	1.42	1.37
19	l	1502	CLA	C1D-ND	3.16	1.42	1.37
19	b	3008	CLA	C1D-ND	3.16	1.42	1.37
19	a	810	CLA	C1D-ND	3.16	1.42	1.37
19	b	3012	CLA	C1D-ND	3.15	1.42	1.37
27	b	3052	EQ3	C8-C9	-3.13	1.39	1.46
19	a	805	CLA	C1D-ND	3.13	1.42	1.37
19	l	1501	CLA	C4B-NB	3.13	1.42	1.37
28	b	3053	ZEX	C8-C9	-3.13	1.39	1.46
19	a	834	CLA	C1D-ND	3.13	1.42	1.37
19	b	3010	CLA	C4B-NB	3.12	1.42	1.37
19	b	3032	CLA	C4B-NB	3.12	1.42	1.37
24	a	857	45D	C24-C26	-3.12	1.39	1.46
19	a	805	CLA	C4B-NB	3.12	1.42	1.37
19	a	840	CLA	C4B-NB	3.11	1.42	1.37
19	a	807	CLA	C1D-ND	3.10	1.41	1.37
19	a	832	CLA	C1D-ND	3.10	1.41	1.37
24	a	857	45D	C23-C25	-3.08	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	405	CLA	C4B-NB	3.07	1.41	1.37
19	j	103	CLA	C4B-NB	3.06	1.41	1.37
32	F	101	HEM	CAB-C3B	3.06	1.55	1.47
19	b	3038	CLA	C4B-NB	3.05	1.41	1.37
26	m	101	ECH	C23-C22	-3.04	1.39	1.46
19	a	836	CLA	C1D-ND	3.04	1.41	1.37
19	k	4003	CLA	C4B-NB	3.03	1.41	1.37
19	b	3022	CLA	C4B-NB	3.03	1.41	1.37
27	b	3052	EQ3	C23-C22	-3.02	1.39	1.46
19	b	3003	CLA	C1D-ND	3.02	1.41	1.37
19	b	3015	CLA	C4B-NB	3.01	1.41	1.37
19	k	4002	CLA	C4B-NB	3.00	1.41	1.37
19	b	3030	CLA	C4B-NB	3.00	1.41	1.37
19	a	813	CLA	C4B-NB	2.99	1.41	1.37
28	f	205	ZEX	C8-C9	-2.99	1.39	1.46
19	a	824	CLA	C4B-NB	2.98	1.41	1.37
21	l	1504	BCR	C30-C25	-2.98	1.50	1.53
19	f	204	CLA	C4B-NB	2.98	1.41	1.37
19	b	3040	CLA	C4B-NB	2.98	1.41	1.37
32	F	101	HEM	CAC-C3C	2.97	1.55	1.47
28	f	205	ZEX	C28-C29	-2.96	1.39	1.46
19	b	3012	CLA	C4B-NB	2.95	1.41	1.37
19	a	819	CLA	C4B-NB	2.95	1.41	1.37
19	b	3035	CLA	C4B-NB	2.95	1.41	1.37
19	D	401	CLA	C4B-NB	2.95	1.41	1.37
26	m	101	ECH	C8-C9	-2.93	1.39	1.46
19	b	3004	CLA	C4B-NB	2.93	1.41	1.37
19	a	821	CLA	C4B-NB	2.92	1.41	1.37
19	j	102	CLA	C4B-NB	2.92	1.41	1.37
28	b	3053	ZEX	C28-C29	-2.91	1.39	1.46
19	b	3002	CLA	C4B-NB	2.91	1.41	1.37
19	b	3033	CLA	C4B-NB	2.90	1.41	1.37
19	a	858	CLA	C4B-NB	2.90	1.41	1.37
19	a	837	CLA	C4B-NB	2.90	1.41	1.37
32	F	101	HEM	FE-ND	2.89	2.03	1.94
19	b	3020	CLA	C4B-NB	2.89	1.41	1.37
19	a	856	CLA	C4B-NB	2.89	1.41	1.37
19	a	815	CLA	C4B-NB	2.88	1.41	1.37
19	f	201	CLA	C4B-NB	2.87	1.41	1.37
19	l	1502	CLA	C4B-NB	2.87	1.41	1.37
19	A	403	CLA	C4B-NB	2.86	1.41	1.37
19	a	842	CLA	C4B-NB	2.86	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	3009	CLA	C4B-NB	2.86	1.41	1.37
27	b	3052	EQ3	C25-C26	2.86	1.39	1.35
19	b	3029	CLA	C4B-NB	2.85	1.41	1.37
19	a	820	CLA	C4B-NB	2.85	1.41	1.37
19	b	3039	CLA	C4B-NB	2.84	1.41	1.37
19	a	843	CLA	C4B-NB	2.84	1.41	1.37
19	b	3026	CLA	C4B-NB	2.84	1.41	1.37
19	b	3034	CLA	C4B-NB	2.84	1.41	1.37
19	a	823	CLA	C4B-NB	2.84	1.41	1.37
19	l	1503	CLA	C4B-NB	2.84	1.41	1.37
26	b	3045	ECH	C8-C9	-2.83	1.39	1.46
19	a	841	CLA	C4B-NB	2.83	1.41	1.37
19	a	816	CLA	C4B-NB	2.83	1.41	1.37
19	a	839	CLA	C4B-NB	2.83	1.41	1.37
19	f	203	CLA	C4B-NB	2.83	1.41	1.37
19	D	403	CLA	C4B-NB	2.82	1.41	1.37
19	b	3016	CLA	C4B-NB	2.81	1.41	1.37
19	b	3011	CLA	C4B-NB	2.81	1.41	1.37
19	a	827	CLA	C4B-NB	2.81	1.41	1.37
19	b	3023	CLA	C4B-NB	2.81	1.41	1.37
19	a	807	CLA	C4B-NB	2.80	1.41	1.37
19	A	402	CLA	C4B-NB	2.80	1.41	1.37
32	F	101	HEM	FE-NC	2.80	2.04	1.95
19	a	804	CLA	C4B-NB	2.79	1.41	1.37
19	b	3041	CLA	C4B-NB	2.79	1.41	1.37
19	b	3003	CLA	C4B-NB	2.79	1.41	1.37
19	a	802	CLA	C4B-NB	2.78	1.41	1.37
19	b	3019	CLA	C4B-NB	2.78	1.41	1.37
19	D	404	CLA	C4B-NB	2.78	1.41	1.37
19	a	825	CLA	C4B-NB	2.77	1.41	1.37
19	b	3027	CLA	C4B-NB	2.77	1.41	1.37
19	a	810	CLA	C4B-NB	2.76	1.41	1.37
19	b	3018	CLA	C4B-NB	2.75	1.41	1.37
19	D	403	CLA	C1B-C2B	2.75	1.49	1.43
19	a	855	CLA	C4B-NB	2.75	1.41	1.37
19	a	812	CLA	C4B-NB	2.75	1.41	1.37
19	b	3036	CLA	C4B-NB	2.74	1.41	1.37
19	a	817	CLA	C4B-NB	2.74	1.41	1.37
19	a	811	CLA	C4B-NB	2.74	1.41	1.37
19	a	836	CLA	C4B-NB	2.73	1.41	1.37
19	a	830	CLA	C4B-NB	2.73	1.41	1.37
19	a	831	CLA	C4B-NB	2.73	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	l	1501	CLA	C1B-C2B	2.73	1.49	1.43
18	a	801	CL0	CMD-C2D	-2.73	1.46	1.51
32	F	101	HEM	FE-NA	2.73	2.04	1.95
19	a	809	CLA	C4B-NB	2.72	1.41	1.37
19	a	838	CLA	C4B-NB	2.72	1.41	1.37
19	a	832	CLA	C4B-NB	2.72	1.41	1.37
19	a	829	CLA	C4B-NB	2.71	1.41	1.37
19	a	835	CLA	C4B-NB	2.70	1.41	1.37
19	a	808	CLA	C4B-NB	2.70	1.41	1.37
19	b	3024	CLA	C4B-NB	2.70	1.41	1.37
19	b	3021	CLA	C4B-NB	2.70	1.41	1.37
19	b	3017	CLA	C4B-NB	2.69	1.41	1.37
19	a	826	CLA	C4B-NB	2.69	1.41	1.37
19	b	3014	CLA	C4B-NB	2.69	1.41	1.37
19	A	402	CLA	C1B-C2B	2.69	1.49	1.43
18	a	801	CL0	CMB-C2B	-2.69	1.46	1.51
19	b	3033	CLA	C1B-C2B	2.69	1.49	1.43
19	b	3030	CLA	C1B-C2B	2.69	1.49	1.43
32	F	101	HEM	FE-NB	2.69	2.03	1.94
19	a	822	CLA	C4B-NB	2.69	1.41	1.37
19	b	3025	CLA	C4B-NB	2.69	1.41	1.37
19	A	403	CLA	C1B-C2B	2.68	1.49	1.43
19	b	3008	CLA	C4B-NB	2.68	1.41	1.37
19	a	815	CLA	C1B-C2B	2.68	1.49	1.43
19	A	405	CLA	C1B-C2B	2.67	1.49	1.43
19	b	3007	CLA	C4B-NB	2.67	1.41	1.37
24	a	857	45D	C08-C16	2.67	1.39	1.35
19	a	821	CLA	C1B-C2B	2.67	1.49	1.43
31	A	404	PHO	CMC-C2C	-2.66	1.46	1.50
19	b	3005	CLA	C4B-NB	2.66	1.41	1.37
19	b	3007	CLA	C1B-C2B	2.66	1.49	1.43
19	b	3031	CLA	C4B-NB	2.66	1.41	1.37
19	a	843	CLA	C1B-C2B	2.65	1.49	1.43
19	a	805	CLA	C1B-C2B	2.65	1.49	1.43
19	a	810	CLA	C1B-C2B	2.65	1.49	1.43
19	a	841	CLA	C1B-C2B	2.65	1.49	1.43
19	l	1502	CLA	C1B-C2B	2.65	1.49	1.43
19	b	3025	CLA	C1B-C2B	2.65	1.49	1.43
19	D	404	CLA	C1B-C2B	2.64	1.49	1.43
19	a	818	CLA	C4B-NB	2.64	1.41	1.37
28	b	3053	ZEX	C32-C33	-2.64	1.40	1.46
19	b	3022	CLA	C1B-C2B	2.64	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	816	CLA	C1B-C2B	2.64	1.49	1.43
19	a	814	CLA	C4B-NB	2.63	1.41	1.37
19	b	3041	CLA	C1B-C2B	2.63	1.49	1.43
19	b	3013	CLA	C4B-NB	2.63	1.41	1.37
19	a	830	CLA	C1B-C2B	2.63	1.49	1.43
19	a	811	CLA	C1B-C2B	2.63	1.49	1.43
19	b	3006	CLA	C4B-NB	2.63	1.41	1.37
19	f	204	CLA	C1B-C2B	2.63	1.49	1.43
23	b	3051	LMG	O7-C8	-2.63	1.40	1.46
19	b	3034	CLA	C1B-C2B	2.62	1.49	1.43
19	b	3031	CLA	C1B-C2B	2.62	1.49	1.43
19	a	817	CLA	C1B-C2B	2.62	1.49	1.43
19	a	834	CLA	C4B-NB	2.62	1.41	1.37
31	D	402	PHO	CMC-C2C	-2.62	1.46	1.50
19	b	3004	CLA	C1B-C2B	2.62	1.49	1.43
19	a	837	CLA	C1B-C2B	2.62	1.49	1.43
19	b	3021	CLA	C1B-C2B	2.62	1.49	1.43
19	k	4003	CLA	C1B-C2B	2.61	1.49	1.43
26	b	3045	ECH	C19-C18	-2.61	1.40	1.46
19	b	3006	CLA	C1B-C2B	2.61	1.49	1.43
19	a	818	CLA	C1B-C2B	2.61	1.49	1.43
19	a	825	CLA	C1B-C2B	2.61	1.49	1.43
19	b	3010	CLA	C1B-C2B	2.61	1.49	1.43
19	l	1503	CLA	C1B-C2B	2.60	1.49	1.43
19	j	103	CLA	C1B-C2B	2.60	1.49	1.43
19	b	3028	CLA	C4B-NB	2.59	1.41	1.37
27	b	3052	EQ3	C12-C13	-2.59	1.40	1.46
19	a	806	CLA	C1B-C2B	2.59	1.49	1.43
19	f	201	CLA	C1B-C2B	2.59	1.49	1.43
19	a	832	CLA	C1B-C2B	2.59	1.49	1.43
19	b	3037	CLA	C4B-NB	2.59	1.41	1.37
19	a	858	CLA	C1B-C2B	2.59	1.49	1.43
19	k	4002	CLA	C1B-C2B	2.59	1.49	1.43
19	a	842	CLA	C1B-C2B	2.59	1.49	1.43
28	b	3053	ZEX	C12-C13	-2.59	1.40	1.46
27	b	3052	EQ3	C19-C18	-2.59	1.40	1.46
19	j	102	CLA	C1B-C2B	2.59	1.49	1.43
19	a	823	CLA	C1B-C2B	2.59	1.49	1.43
29	f	207	LMT	O3'-C3'	-2.58	1.36	1.43
19	b	3016	CLA	C1B-C2B	2.58	1.49	1.43
19	a	838	CLA	C1B-C2B	2.58	1.49	1.43
19	b	3023	CLA	C1B-C2B	2.58	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	803	CLA	C4B-NB	2.58	1.41	1.37
26	b	3045	ECH	C12-C13	-2.58	1.40	1.46
19	b	3017	CLA	C1B-C2B	2.58	1.49	1.43
19	a	806	CLA	C4B-NB	2.58	1.41	1.37
24	a	857	45D	C33-C35	-2.57	1.40	1.46
19	a	824	CLA	C1B-C2B	2.57	1.49	1.43
19	a	813	CLA	C1B-C2B	2.57	1.49	1.43
19	a	812	CLA	C1B-C2B	2.56	1.49	1.43
19	D	401	CLA	C1B-C2B	2.56	1.49	1.43
19	b	3009	CLA	C1B-C2B	2.56	1.49	1.43
19	f	203	CLA	C1B-C2B	2.56	1.49	1.43
19	a	807	CLA	C1B-C2B	2.55	1.49	1.43
19	b	3011	CLA	C1B-C2B	2.55	1.49	1.43
19	a	827	CLA	C1B-C2B	2.55	1.49	1.43
19	a	828	CLA	C4B-NB	2.55	1.41	1.37
19	b	3037	CLA	C1B-C2B	2.55	1.49	1.43
19	b	3029	CLA	C1B-C2B	2.55	1.49	1.43
19	b	3039	CLA	C1B-C2B	2.54	1.49	1.43
19	b	3005	CLA	C1B-C2B	2.54	1.49	1.43
19	b	3035	CLA	C1B-C2B	2.54	1.49	1.43
19	a	833	CLA	C4B-NB	2.54	1.41	1.37
19	a	829	CLA	C1B-C2B	2.53	1.49	1.43
19	a	809	CLA	C1B-C2B	2.53	1.49	1.43
31	D	402	PHO	C3D-C4D	2.53	1.44	1.41
19	b	3028	CLA	C1B-C2B	2.53	1.49	1.43
19	b	3013	CLA	C1B-C2B	2.53	1.49	1.43
28	f	205	ZEX	C12-C13	-2.53	1.40	1.46
19	b	3003	CLA	CMC-C2C	-2.53	1.45	1.50
19	b	3018	CLA	C1B-C2B	2.52	1.49	1.43
19	b	3008	CLA	C1B-C2B	2.52	1.49	1.43
19	b	3019	CLA	C1B-C2B	2.52	1.49	1.43
19	a	828	CLA	C1B-C2B	2.52	1.49	1.43
18	a	801	CL0	CMC-C2C	-2.52	1.46	1.50
19	a	814	CLA	C1B-C2B	2.52	1.49	1.43
19	b	3027	CLA	C1B-C2B	2.51	1.49	1.43
31	D	402	PHO	CMB-C2B	-2.51	1.46	1.51
31	D	402	PHO	CMD-C2D	-2.51	1.46	1.51
19	a	831	CLA	C1B-C2B	2.51	1.49	1.43
19	b	3020	CLA	C1B-C2B	2.50	1.49	1.43
31	A	404	PHO	CMD-C2D	-2.50	1.46	1.51
19	b	3014	CLA	C1B-C2B	2.50	1.49	1.43
19	a	836	CLA	C1B-C2B	2.50	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	833	CLA	C1B-C2B	2.50	1.49	1.43
19	a	803	CLA	C1B-C2B	2.49	1.49	1.43
18	a	801	CL0	CAC-C3C	-2.49	1.47	1.51
19	b	3002	CLA	C1B-C2B	2.49	1.49	1.43
19	a	856	CLA	C1B-C2B	2.48	1.49	1.43
19	b	3003	CLA	C1B-C2B	2.48	1.49	1.43
19	a	808	CLA	C1B-C2B	2.48	1.48	1.43
19	a	835	CLA	C1B-C2B	2.48	1.48	1.43
19	b	3032	CLA	C3B-C4B	2.48	1.50	1.42
19	b	3038	CLA	C1B-C2B	2.48	1.48	1.43
19	a	804	CLA	C1B-C2B	2.48	1.48	1.43
19	a	802	CLA	C1B-C2B	2.48	1.48	1.43
31	A	404	PHO	CMB-C2B	-2.48	1.46	1.51
19	b	3015	CLA	C1B-C2B	2.47	1.48	1.43
19	a	839	CLA	C1B-C2B	2.47	1.48	1.43
26	m	101	ECH	C12-C13	-2.46	1.40	1.46
19	a	840	CLA	C1B-C2B	2.46	1.48	1.43
19	b	3032	CLA	C1B-C2B	2.46	1.48	1.43
24	a	857	45D	C34-C36	-2.46	1.40	1.46
31	D	402	PHO	CAC-C3C	-2.46	1.47	1.51
19	a	855	CLA	C1B-C2B	2.45	1.48	1.43
19	a	826	CLA	C1B-C2B	2.45	1.48	1.43
19	b	3040	CLA	C1B-C2B	2.44	1.48	1.43
22	a	850	LHG	O7-C5	-2.44	1.40	1.46
19	b	3012	CLA	C1B-C2B	2.44	1.48	1.43
19	b	3036	CLA	C1B-C2B	2.44	1.48	1.43
28	f	205	ZEX	C32-C33	-2.43	1.40	1.46
29	f	207	LMT	O2'-C2'	-2.43	1.36	1.43
18	a	801	CL0	C1A-CHA	-2.42	1.37	1.40
19	b	3026	CLA	C1B-C2B	2.42	1.48	1.43
19	b	3009	CLA	CMB-C2B	-2.42	1.45	1.50
19	a	820	CLA	C1B-C2B	2.41	1.48	1.43
19	b	3022	CLA	C3B-C4B	2.40	1.49	1.42
19	a	822	CLA	C1B-C2B	2.40	1.48	1.43
19	b	3040	CLA	CMB-C2B	-2.39	1.45	1.50
19	b	3024	CLA	C1B-C2B	2.38	1.48	1.43
19	b	3012	CLA	C3B-C4B	2.38	1.49	1.42
19	a	834	CLA	C1B-C2B	2.38	1.48	1.43
19	b	3015	CLA	C3B-C4B	2.38	1.49	1.42
22	b	3050	LHG	O7-C5	-2.37	1.41	1.46
19	a	819	CLA	C1B-C2B	2.37	1.48	1.43
19	l	1501	CLA	C3B-C4B	2.37	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	3009	CLA	MG-NB	-2.37	2.01	2.05
31	A	404	PHO	C3D-C4D	2.37	1.44	1.41
19	j	102	CLA	C3B-C4B	2.37	1.49	1.42
31	A	404	PHO	CAC-C3C	-2.37	1.47	1.51
19	a	833	CLA	MG-NB	-2.36	2.01	2.05
19	a	840	CLA	C3B-C4B	2.36	1.49	1.42
19	a	834	CLA	MG-NB	-2.36	2.01	2.05
19	a	813	CLA	C3B-C4B	2.36	1.49	1.42
19	a	805	CLA	CHC-C1C	2.36	1.43	1.38
19	j	103	CLA	C3B-C4B	2.35	1.49	1.42
19	a	832	CLA	MG-NB	-2.35	2.01	2.05
19	b	3013	CLA	MG-NB	-2.35	2.01	2.05
19	b	3010	CLA	C3B-C4B	2.35	1.49	1.42
19	f	204	CLA	C3B-C4B	2.34	1.49	1.42
19	a	810	CLA	CMD-C2D	-2.34	1.46	1.50
19	j	103	CLA	CHC-C1C	2.33	1.43	1.38
19	b	3018	CLA	MG-NB	-2.33	2.01	2.05
19	k	4002	CLA	C3B-C4B	2.33	1.49	1.42
19	b	3014	CLA	MG-NB	-2.32	2.01	2.05
19	b	3036	CLA	MG-NB	-2.32	2.01	2.05
19	b	3037	CLA	MG-NB	-2.32	2.01	2.05
19	a	804	CLA	C3B-C4B	2.31	1.49	1.42
19	A	403	CLA	C3B-C4B	2.31	1.49	1.42
19	a	822	CLA	CMB-C2B	-2.31	1.46	1.50
19	D	401	CLA	C3B-C4B	2.31	1.49	1.42
19	a	834	CLA	CMB-C2B	-2.31	1.46	1.50
19	a	808	CLA	C3B-C4B	2.31	1.49	1.42
19	b	3026	CLA	MG-NB	-2.31	2.01	2.05
19	a	802	CLA	MG-NB	-2.31	2.01	2.05
19	a	836	CLA	MG-NB	-2.30	2.01	2.05
19	a	822	CLA	C3B-C4B	2.30	1.49	1.42
19	D	403	CLA	MG-NB	-2.30	2.01	2.05
19	a	820	CLA	CMB-C2B	-2.30	1.46	1.50
26	m	101	ECH	C21-C22	2.30	1.41	1.35
19	b	3028	CLA	CMD-C2D	-2.30	1.46	1.50
19	b	3023	CLA	C3B-C4B	2.29	1.49	1.42
19	b	3038	CLA	MG-NB	-2.29	2.01	2.05
19	b	3028	CLA	MG-NB	-2.29	2.01	2.05
19	b	3016	CLA	MG-NB	-2.29	2.01	2.05
19	b	3027	CLA	MG-NB	-2.29	2.01	2.05
26	m	101	ECH	C19-C18	-2.29	1.41	1.46
19	b	3035	CLA	CMB-C2B	-2.29	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	803	CLA	C3B-C4B	2.29	1.49	1.42
19	b	3024	CLA	MG-NB	-2.29	2.01	2.05
19	b	3020	CLA	C3B-C4B	2.29	1.49	1.42
19	f	201	CLA	C3B-C4B	2.29	1.49	1.42
19	a	827	CLA	MG-NB	-2.28	2.01	2.05
19	b	3008	CLA	MG-NB	-2.28	2.01	2.05
19	b	3029	CLA	CMD-C2D	-2.28	1.46	1.50
19	a	836	CLA	CMB-C2B	-2.28	1.46	1.50
18	a	801	CL0	MG-NB	-2.28	2.01	2.05
19	a	856	CLA	CMB-C2B	-2.28	1.46	1.50
19	a	810	CLA	MG-NB	-2.28	2.01	2.05
19	a	828	CLA	MG-NB	-2.28	2.01	2.05
19	a	855	CLA	MG-NB	-2.28	2.01	2.05
19	a	856	CLA	MG-NB	-2.28	2.01	2.05
19	f	201	CLA	CMD-C2D	-2.28	1.46	1.50
19	a	823	CLA	MG-NB	-2.28	2.01	2.05
19	b	3021	CLA	MG-NB	-2.27	2.01	2.05
19	D	404	CLA	C3B-C4B	2.27	1.49	1.42
19	a	819	CLA	C3B-C4B	2.27	1.49	1.42
19	D	401	CLA	CHC-C1C	2.27	1.43	1.38
29	f	207	LMT	O2B-C2B	-2.27	1.37	1.43
19	b	3004	CLA	CHC-C1C	2.27	1.43	1.38
19	b	3024	CLA	C3B-C4B	2.27	1.49	1.42
19	b	3041	CLA	C3B-C4B	2.27	1.49	1.42
19	b	3006	CLA	MG-NB	-2.27	2.01	2.05
19	a	826	CLA	C3B-C4B	2.27	1.49	1.42
19	b	3019	CLA	MG-NB	-2.27	2.01	2.05
19	a	843	CLA	C3B-C4B	2.27	1.49	1.42
19	a	826	CLA	MG-NB	-2.26	2.01	2.05
19	b	3008	CLA	CMD-C2D	-2.26	1.46	1.50
19	a	807	CLA	MG-NB	-2.26	2.01	2.05
19	a	842	CLA	MG-NB	-2.26	2.01	2.05
19	b	3026	CLA	CMC-C2C	-2.26	1.46	1.50
19	a	836	CLA	CMD-C2D	-2.26	1.46	1.50
19	b	3033	CLA	MG-NB	-2.26	2.01	2.05
19	a	806	CLA	CMD-C2D	-2.26	1.46	1.50
19	a	838	CLA	MG-NB	-2.26	2.01	2.05
19	A	405	CLA	MG-NB	-2.26	2.01	2.05
26	m	101	ECH	C14-C13	2.26	1.41	1.35
19	l	1503	CLA	MG-NB	-2.26	2.01	2.05
19	a	835	CLA	MG-NB	-2.26	2.01	2.05
19	a	805	CLA	MG-NB	-2.26	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	820	CLA	MG-NB	-2.26	2.01	2.05
19	b	3017	CLA	MG-NB	-2.25	2.01	2.05
19	a	858	CLA	C3B-C4B	2.25	1.49	1.42
19	l	1501	CLA	CHC-C1C	2.25	1.43	1.38
19	a	815	CLA	MG-NB	-2.25	2.01	2.05
19	f	203	CLA	C3B-C4B	2.25	1.49	1.42
19	b	3025	CLA	MG-NB	-2.25	2.01	2.05
19	b	3034	CLA	MG-NB	-2.25	2.01	2.05
19	a	839	CLA	MG-NB	-2.25	2.01	2.05
19	b	3023	CLA	CHC-C1C	2.25	1.43	1.38
19	a	827	CLA	CMD-C2D	-2.25	1.46	1.50
19	a	828	CLA	CMC-C2C	-2.25	1.46	1.50
19	a	814	CLA	MG-NB	-2.25	2.01	2.05
19	a	820	CLA	C3B-C4B	2.25	1.49	1.42
19	b	3024	CLA	CHC-C1C	2.25	1.43	1.38
19	a	839	CLA	C3B-C4B	2.25	1.49	1.42
19	b	3029	CLA	C3B-C4B	2.25	1.49	1.42
19	b	3029	CLA	CMB-C2B	-2.24	1.46	1.50
19	a	824	CLA	C3B-C4B	2.24	1.49	1.42
19	b	3019	CLA	C3B-C4B	2.24	1.49	1.42
19	a	836	CLA	C3B-C4B	2.24	1.49	1.42
19	b	3016	CLA	C3B-C4B	2.24	1.49	1.42
19	b	3004	CLA	C3B-C4B	2.24	1.49	1.42
19	a	825	CLA	MG-NB	-2.24	2.01	2.05
19	b	3002	CLA	CMD-C2D	-2.23	1.46	1.50
19	a	827	CLA	C3B-C4B	2.23	1.49	1.42
19	a	809	CLA	MG-NB	-2.23	2.01	2.05
19	j	102	CLA	CHC-C1C	2.23	1.43	1.38
19	a	818	CLA	MG-NB	-2.23	2.01	2.05
26	m	101	ECH	C17-C18	2.23	1.41	1.35
19	b	3035	CLA	C3B-C4B	2.23	1.49	1.42
19	a	814	CLA	C3B-C4B	2.23	1.49	1.42
19	a	842	CLA	CMB-C2B	-2.23	1.46	1.50
19	l	1503	CLA	C3B-C4B	2.23	1.49	1.42
19	b	3015	CLA	CMB-C2B	-2.23	1.46	1.50
19	a	824	CLA	MG-NB	-2.23	2.01	2.05
19	b	3002	CLA	CMB-C2B	-2.23	1.46	1.50
19	b	3023	CLA	MG-NB	-2.23	2.01	2.05
19	b	3040	CLA	MG-NB	-2.23	2.01	2.05
26	b	3045	ECH	C21-C22	2.23	1.40	1.35
19	k	4003	CLA	C3B-C4B	2.23	1.49	1.42
19	b	3013	CLA	CMC-C2C	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	858	CLA	MG-NB	-2.23	2.01	2.05
19	a	803	CLA	CMC-C2C	-2.22	1.46	1.50
19	f	203	CLA	CHC-C1C	2.22	1.42	1.38
19	b	3038	CLA	C3B-C4B	2.22	1.49	1.42
19	a	830	CLA	C3B-C4B	2.22	1.49	1.42
19	a	818	CLA	CMB-C2B	-2.22	1.46	1.50
19	b	3029	CLA	MG-NB	-2.22	2.01	2.05
19	a	808	CLA	CHC-C1C	2.22	1.42	1.38
19	b	3003	CLA	CHC-C1C	2.22	1.42	1.38
19	b	3035	CLA	MG-NB	-2.22	2.01	2.05
19	b	3002	CLA	MG-NB	-2.22	2.01	2.05
19	a	832	CLA	CMD-C2D	-2.22	1.46	1.50
19	b	3039	CLA	MG-NB	-2.22	2.01	2.05
19	b	3021	CLA	C3B-C4B	2.22	1.49	1.42
19	b	3011	CLA	CMB-C2B	-2.22	1.46	1.50
19	b	3024	CLA	CMD-C2D	-2.22	1.46	1.50
19	a	842	CLA	C3B-C4B	2.22	1.49	1.42
19	A	402	CLA	C3B-C4B	2.22	1.49	1.42
19	a	831	CLA	MG-NB	-2.22	2.01	2.05
19	b	3017	CLA	CMD-C2D	-2.21	1.46	1.50
19	b	3010	CLA	CMD-C2D	-2.21	1.46	1.50
19	a	816	CLA	MG-NB	-2.21	2.01	2.05
19	a	837	CLA	MG-NB	-2.21	2.01	2.05
19	b	3031	CLA	MG-NB	-2.21	2.01	2.05
19	b	3033	CLA	CMB-C2B	-2.21	1.46	1.50
19	b	3026	CLA	C3B-C4B	2.21	1.49	1.42
19	b	3032	CLA	CHC-C1C	2.21	1.42	1.38
19	a	803	CLA	CHC-C1C	2.21	1.42	1.38
19	a	804	CLA	CMB-C2B	-2.21	1.46	1.50
19	A	405	CLA	C3B-C4B	2.21	1.49	1.42
19	a	827	CLA	CHC-C1C	2.21	1.42	1.38
22	a	854	LHG	O7-C5	-2.21	1.41	1.46
19	b	3025	CLA	CMD-C2D	-2.21	1.46	1.50
19	b	3032	CLA	CMB-C2B	-2.21	1.46	1.50
19	l	1502	CLA	C3B-C4B	2.21	1.49	1.42
19	a	825	CLA	CMC-C2C	-2.20	1.46	1.50
19	a	813	CLA	CHC-C1C	2.20	1.42	1.38
19	a	819	CLA	CHC-C1C	2.20	1.42	1.38
19	b	3011	CLA	MG-NB	-2.20	2.01	2.05
19	a	823	CLA	C3B-C4B	2.20	1.49	1.42
19	b	3030	CLA	MG-NB	-2.20	2.01	2.05
19	a	826	CLA	CMD-C2D	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	3034	CLA	C3B-C4B	2.20	1.49	1.42
19	a	829	CLA	MG-NB	-2.20	2.01	2.05
19	b	3040	CLA	C3B-C4B	2.20	1.49	1.42
19	a	808	CLA	MG-NB	-2.20	2.01	2.05
19	a	831	CLA	C3B-C4B	2.20	1.49	1.42
19	b	3008	CLA	C3B-C4B	2.20	1.49	1.42
19	b	3015	CLA	CMD-C2D	-2.20	1.46	1.50
19	b	3026	CLA	CHC-C1C	2.20	1.42	1.38
19	a	805	CLA	C3B-C4B	2.20	1.49	1.42
19	b	3039	CLA	C3B-C4B	2.20	1.49	1.42
19	b	3005	CLA	MG-NB	-2.20	2.01	2.05
19	a	813	CLA	CMB-C2B	-2.20	1.46	1.50
19	a	837	CLA	CHC-C1C	2.20	1.42	1.38
19	a	812	CLA	MG-NB	-2.20	2.01	2.05
19	b	3007	CLA	MG-NB	-2.20	2.01	2.05
19	D	401	CLA	MG-NB	-2.20	2.01	2.05
19	a	830	CLA	CMD-C2D	-2.20	1.46	1.50
19	a	835	CLA	CMB-C2B	-2.20	1.46	1.50
19	b	3030	CLA	CMB-C2B	-2.20	1.46	1.50
19	b	3020	CLA	MG-NB	-2.20	2.01	2.05
19	a	807	CLA	CMD-C2D	-2.19	1.46	1.50
19	a	819	CLA	MG-NB	-2.19	2.01	2.05
28	f	205	ZEX	C30-C29	2.19	1.40	1.35
19	a	841	CLA	MG-NB	-2.19	2.01	2.05
19	a	829	CLA	C3B-C4B	2.19	1.49	1.42
19	b	3017	CLA	C3B-C4B	2.19	1.49	1.42
19	b	3022	CLA	CHC-C1C	2.19	1.42	1.38
19	b	3013	CLA	CMD-C2D	-2.19	1.46	1.50
19	b	3039	CLA	CMD-C2D	-2.19	1.46	1.50
19	b	3040	CLA	CMD-C2D	-2.19	1.46	1.50
19	b	3031	CLA	C3B-C4B	2.19	1.49	1.42
19	b	3036	CLA	C3B-C4B	2.19	1.49	1.42
22	a	852	LHG	O7-C5	-2.19	1.41	1.46
19	a	821	CLA	CMB-C2B	-2.19	1.46	1.50
19	k	4003	CLA	CHC-C1C	2.19	1.42	1.38
19	b	3005	CLA	C3B-C4B	2.19	1.49	1.42
19	b	3012	CLA	CMD-C2D	-2.19	1.46	1.50
19	a	809	CLA	C3B-C4B	2.19	1.49	1.42
19	a	803	CLA	CMD-C2D	-2.19	1.46	1.50
19	b	3034	CLA	CHC-C1C	2.19	1.42	1.38
19	a	804	CLA	MG-NB	-2.19	2.01	2.05
19	A	403	CLA	CHC-C1C	2.19	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	3003	CLA	C3B-C4B	2.19	1.49	1.42
19	a	821	CLA	C3B-C4B	2.19	1.49	1.42
19	b	3005	CLA	CHC-C1C	2.19	1.42	1.38
19	a	829	CLA	CMD-C2D	-2.19	1.46	1.50
19	b	3020	CLA	CHC-C1C	2.19	1.42	1.38
19	b	3019	CLA	CMB-C2B	-2.19	1.46	1.50
19	a	856	CLA	C3B-C4B	2.19	1.49	1.42
19	b	3027	CLA	CMD-C2D	-2.18	1.46	1.50
19	a	832	CLA	CMB-C2B	-2.18	1.46	1.50
19	b	3031	CLA	CHC-C1C	2.18	1.42	1.38
19	b	3004	CLA	CMC-C2C	-2.18	1.46	1.50
19	b	3014	CLA	C3B-C4B	2.18	1.49	1.42
19	a	822	CLA	MG-NB	-2.18	2.01	2.05
19	l	1502	CLA	CMD-C2D	-2.18	1.46	1.50
19	a	821	CLA	MG-NB	-2.18	2.01	2.05
19	a	831	CLA	CMD-C2D	-2.18	1.46	1.50
19	b	3038	CLA	CMD-C2D	-2.18	1.46	1.50
19	f	201	CLA	CHC-C1C	2.18	1.42	1.38
19	a	839	CLA	CMD-C2D	-2.18	1.46	1.50
19	b	3006	CLA	CMB-C2B	-2.18	1.46	1.50
19	a	855	CLA	CMD-C2D	-2.18	1.46	1.50
19	b	3004	CLA	MG-NB	-2.18	2.01	2.05
19	b	3021	CLA	CHC-C1C	2.18	1.42	1.38
19	a	843	CLA	CMD-C2D	-2.18	1.46	1.50
19	D	403	CLA	CMD-C2D	-2.18	1.46	1.50
19	a	815	CLA	C3B-C4B	2.18	1.49	1.42
19	a	821	CLA	CHC-C1C	2.18	1.42	1.38
19	l	1502	CLA	MG-NB	-2.18	2.01	2.05
19	a	819	CLA	CMC-C2C	-2.18	1.46	1.50
19	b	3007	CLA	CMD-C2D	-2.18	1.46	1.50
19	a	817	CLA	MG-NB	-2.18	2.01	2.05
19	a	838	CLA	CMB-C2B	-2.18	1.46	1.50
19	b	3009	CLA	CMD-C2D	-2.18	1.46	1.50
26	m	101	ECH	C10-C9	2.18	1.40	1.35
19	a	831	CLA	CMB-C2B	-2.17	1.46	1.50
19	a	856	CLA	CMC-C2C	-2.17	1.46	1.50
19	b	3010	CLA	CMB-C2B	-2.17	1.46	1.50
19	a	835	CLA	C3B-C4B	2.17	1.49	1.42
19	a	826	CLA	CHC-C1C	2.17	1.42	1.38
19	b	3041	CLA	CHC-C1C	2.17	1.42	1.38
19	a	816	CLA	C3B-C4B	2.17	1.49	1.42
19	a	803	CLA	MG-NB	-2.17	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	814	CLA	CMD-C2D	-2.17	1.46	1.50
19	b	3015	CLA	CHC-C1C	2.17	1.42	1.38
19	a	810	CLA	C3B-C4B	2.17	1.49	1.42
19	D	403	CLA	C3B-C4B	2.17	1.49	1.42
19	b	3014	CLA	CMD-C2D	-2.17	1.46	1.50
19	a	830	CLA	CHC-C1C	2.17	1.42	1.38
19	a	807	CLA	C3B-C4B	2.17	1.49	1.42
19	a	855	CLA	CMB-C2B	-2.17	1.46	1.50
19	b	3020	CLA	CMD-C2D	-2.17	1.46	1.50
19	f	201	CLA	CMB-C2B	-2.17	1.46	1.50
19	b	3003	CLA	MG-NB	-2.17	2.01	2.05
19	a	836	CLA	CHC-C1C	2.17	1.42	1.38
29	f	207	LMT	O3B-C3B	-2.17	1.37	1.43
19	a	822	CLA	CHC-C1C	2.17	1.42	1.38
19	k	4002	CLA	CHC-C1C	2.17	1.42	1.38
19	a	806	CLA	CMC-C2C	-2.17	1.46	1.50
19	b	3038	CLA	CMB-C2B	-2.17	1.46	1.50
19	a	813	CLA	MG-NB	-2.17	2.01	2.05
19	a	839	CLA	CHC-C1C	2.17	1.42	1.38
19	D	404	CLA	MG-NB	-2.17	2.01	2.05
19	b	3016	CLA	CHC-C1C	2.16	1.42	1.38
19	f	201	CLA	MG-NB	-2.16	2.01	2.05
19	a	817	CLA	CMB-C2B	-2.16	1.46	1.50
19	a	824	CLA	CMB-C2B	-2.16	1.46	1.50
19	f	203	CLA	MG-NB	-2.16	2.01	2.05
19	b	3023	CLA	CMD-C2D	-2.16	1.46	1.50
19	b	3012	CLA	MG-NB	-2.16	2.01	2.05
19	b	3002	CLA	CHC-C1C	2.16	1.42	1.38
19	a	809	CLA	CMB-C2B	-2.16	1.46	1.50
19	a	834	CLA	CMD-C2D	-2.16	1.46	1.50
19	a	820	CLA	CMD-C2D	-2.16	1.46	1.50
19	b	3013	CLA	CMB-C2B	-2.16	1.46	1.50
19	a	813	CLA	CMD-C2D	-2.16	1.46	1.50
19	b	3016	CLA	CMD-C2D	-2.16	1.46	1.50
19	a	812	CLA	C3B-C4B	2.16	1.49	1.42
19	b	3034	CLA	CMD-C2D	-2.16	1.46	1.50
19	b	3018	CLA	C3B-C4B	2.16	1.49	1.42
19	a	809	CLA	CMD-C2D	-2.16	1.46	1.50
19	b	3002	CLA	C3B-C4B	2.15	1.49	1.42
19	A	402	CLA	MG-NB	-2.15	2.01	2.05
19	a	811	CLA	C3B-C4B	2.15	1.49	1.42
19	b	3019	CLA	CHC-C1C	2.15	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	810	CLA	CMB-C2B	-2.15	1.46	1.50
19	b	3014	CLA	CHC-C1C	2.15	1.42	1.38
19	b	3033	CLA	C3B-C4B	2.15	1.49	1.42
19	a	828	CLA	CMB-C2B	-2.15	1.46	1.50
19	b	3030	CLA	CMD-C2D	-2.15	1.46	1.50
19	a	828	CLA	CHC-C1C	2.15	1.42	1.38
19	b	3036	CLA	CHC-C1C	2.15	1.42	1.38
19	a	856	CLA	CMD-C2D	-2.15	1.46	1.50
19	a	837	CLA	CMD-C2D	-2.15	1.46	1.50
19	a	840	CLA	MG-NB	-2.15	2.01	2.05
19	b	3041	CLA	MG-NB	-2.15	2.01	2.05
19	a	805	CLA	CMD-C2D	-2.15	1.46	1.50
19	a	833	CLA	CMD-C2D	-2.15	1.46	1.50
19	b	3012	CLA	CMB-C2B	-2.15	1.46	1.50
19	b	3037	CLA	C3B-C4B	2.15	1.49	1.42
19	a	819	CLA	CMD-C2D	-2.15	1.46	1.50
19	b	3037	CLA	CMB-C2B	-2.15	1.46	1.50
28	f	205	ZEX	C34-C33	2.15	1.40	1.35
19	a	812	CLA	CMD-C2D	-2.15	1.46	1.50
26	b	3045	ECH	C10-C9	2.15	1.40	1.35
19	a	858	CLA	CMD-C2D	-2.15	1.46	1.50
19	b	3004	CLA	CMB-C2B	-2.15	1.46	1.50
19	A	405	CLA	CMD-C2D	-2.15	1.46	1.50
19	a	828	CLA	C3B-C4B	2.15	1.49	1.42
19	a	814	CLA	CHC-C1C	2.15	1.42	1.38
19	k	4002	CLA	MG-NB	-2.15	2.01	2.05
19	a	817	CLA	C3B-C4B	2.15	1.49	1.42
19	f	204	CLA	CHC-C1C	2.14	1.42	1.38
19	a	824	CLA	CMD-C2D	-2.14	1.46	1.50
19	a	827	CLA	CMB-C2B	-2.14	1.46	1.50
19	a	843	CLA	MG-NB	-2.14	2.01	2.05
19	b	3025	CLA	CMB-C2B	-2.14	1.46	1.50
19	b	3028	CLA	C3B-C4B	2.14	1.49	1.42
19	a	826	CLA	CMB-C2B	-2.14	1.46	1.50
19	a	858	CLA	CHC-C1C	2.14	1.42	1.38
19	b	3018	CLA	CMB-C2B	-2.14	1.46	1.50
19	b	3019	CLA	CMD-C2D	-2.14	1.46	1.50
19	a	811	CLA	CMB-C2B	-2.14	1.46	1.50
19	a	825	CLA	CMD-C2D	-2.14	1.46	1.50
19	a	806	CLA	C3B-C4B	2.14	1.49	1.42
19	a	806	CLA	MG-NB	-2.14	2.01	2.05
19	a	815	CLA	CHC-C1C	2.14	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	3012	CLA	CHC-C1C	2.14	1.42	1.38
19	b	3035	CLA	CHC-C1C	2.14	1.42	1.38
19	a	830	CLA	MG-NB	-2.14	2.01	2.05
19	a	829	CLA	CMB-C2B	-2.14	1.46	1.50
24	a	857	45D	C38-C36	2.14	1.40	1.35
19	a	824	CLA	CHC-C1C	2.14	1.42	1.38
19	a	821	CLA	CMD-C2D	-2.14	1.46	1.50
19	a	833	CLA	CMB-C2B	-2.14	1.46	1.50
19	a	819	CLA	CMB-C2B	-2.14	1.46	1.50
19	b	3031	CLA	CMD-C2D	-2.14	1.46	1.50
19	a	842	CLA	CMD-C2D	-2.14	1.46	1.50
19	b	3020	CLA	CMB-C2B	-2.14	1.46	1.50
19	A	402	CLA	CMC-C2C	-2.14	1.46	1.50
19	l	1502	CLA	CMB-C2B	-2.14	1.46	1.50
19	a	835	CLA	CMD-C2D	-2.14	1.46	1.50
19	b	3023	CLA	CMB-C2B	-2.14	1.46	1.50
19	b	3037	CLA	CMD-C2D	-2.14	1.46	1.50
21	j	104	BCR	C33-C5	-2.14	1.47	1.50
19	b	3008	CLA	CHC-C1C	2.14	1.42	1.38
19	b	3022	CLA	MG-NB	-2.14	2.01	2.05
19	a	811	CLA	CMD-C2D	-2.14	1.46	1.50
19	a	822	CLA	CMD-C2D	-2.14	1.46	1.50
19	b	3017	CLA	CMB-C2B	-2.14	1.46	1.50
19	a	825	CLA	C3B-C4B	2.14	1.49	1.42
19	k	4002	CLA	CMD-C2D	-2.13	1.46	1.50
19	b	3003	CLA	CMB-C2B	-2.13	1.46	1.50
19	b	3026	CLA	CMB-C2B	-2.13	1.46	1.50
19	b	3018	CLA	CMD-C2D	-2.13	1.46	1.50
19	l	1502	CLA	CHC-C1C	2.13	1.42	1.38
19	b	3016	CLA	CMB-C2B	-2.13	1.46	1.50
19	b	3026	CLA	CMD-C2D	-2.13	1.46	1.50
19	b	3024	CLA	CMB-C2B	-2.13	1.46	1.50
19	a	843	CLA	CHC-C1C	2.13	1.42	1.38
19	a	841	CLA	C3B-C4B	2.13	1.48	1.42
19	a	841	CLA	CMD-C2D	-2.13	1.46	1.50
19	b	3028	CLA	CHC-C1C	2.13	1.42	1.38
19	b	3005	CLA	CMB-C2B	-2.13	1.46	1.50
19	b	3006	CLA	CMC-C2C	-2.13	1.46	1.50
19	a	811	CLA	MG-NB	-2.13	2.01	2.05
19	a	858	CLA	CMC-C2C	-2.13	1.46	1.50
19	a	856	CLA	CHC-C1C	2.13	1.42	1.38
19	a	837	CLA	C3B-C4B	2.13	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	816	CLA	CMD-C2D	-2.13	1.46	1.50
19	a	825	CLA	CMB-C2B	-2.13	1.46	1.50
19	b	3005	CLA	CMD-C2D	-2.13	1.46	1.50
19	b	3036	CLA	CMD-C2D	-2.13	1.46	1.50
19	a	834	CLA	C3B-C4B	2.13	1.48	1.42
19	A	405	CLA	CHC-C1C	2.12	1.42	1.38
19	a	828	CLA	CMD-C2D	-2.12	1.46	1.50
19	b	3011	CLA	CMD-C2D	-2.12	1.46	1.50
19	b	3010	CLA	MG-NB	-2.12	2.01	2.05
19	a	838	CLA	CMD-C2D	-2.12	1.46	1.50
19	b	3002	CLA	CMC-C2C	-2.12	1.46	1.50
19	b	3003	CLA	CMD-C2D	-2.12	1.46	1.50
19	b	3039	CLA	CMB-C2B	-2.12	1.46	1.50
26	b	3045	ECH	C17-C18	2.12	1.40	1.35
19	b	3008	CLA	CMC-C2C	-2.12	1.46	1.50
19	b	3013	CLA	C3B-C4B	2.12	1.48	1.42
19	D	404	CLA	CHC-C1C	2.12	1.42	1.38
19	a	840	CLA	CMD-C2D	-2.12	1.46	1.50
19	a	802	CLA	C3B-C4B	2.12	1.48	1.42
19	b	3011	CLA	C3B-C4B	2.12	1.48	1.42
19	a	807	CLA	CMB-C2B	-2.12	1.46	1.50
19	b	3008	CLA	CMB-C2B	-2.12	1.46	1.50
19	a	807	CLA	CHC-C1C	2.12	1.42	1.38
19	b	3027	CLA	C3B-C4B	2.12	1.48	1.42
19	a	804	CLA	CMC-C2C	-2.12	1.46	1.50
19	a	818	CLA	CMD-C2D	-2.12	1.46	1.50
19	b	3029	CLA	CHC-C1C	2.12	1.42	1.38
19	b	3005	CLA	CMC-C2C	-2.12	1.46	1.50
19	a	802	CLA	CMB-C2B	-2.12	1.46	1.50
19	a	802	CLA	CMD-C2D	-2.12	1.46	1.50
19	a	817	CLA	CMD-C2D	-2.12	1.46	1.50
19	a	855	CLA	CMC-C2C	-2.12	1.46	1.50
24	a	857	45D	C37-C35	2.12	1.40	1.35
19	a	831	CLA	CHC-C1C	2.12	1.42	1.38
19	b	3006	CLA	CMD-C2D	-2.12	1.46	1.50
19	b	3015	CLA	CMC-C2C	-2.11	1.46	1.50
23	b	3049	LMG	O7-C8	-2.11	1.41	1.46
19	a	809	CLA	CHC-C1C	2.11	1.42	1.38
19	a	812	CLA	CHC-C1C	2.11	1.42	1.38
19	a	808	CLA	CMD-C2D	-2.11	1.46	1.50
19	a	810	CLA	CMC-C2C	-2.11	1.46	1.50
19	a	806	CLA	CMB-C2B	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	840	CLA	CMB-C2B	-2.11	1.46	1.50
19	b	3031	CLA	CMC-C2C	-2.11	1.46	1.50
19	a	817	CLA	CHC-C1C	2.11	1.42	1.38
19	a	823	CLA	CHC-C1C	2.11	1.42	1.38
19	a	830	CLA	CMB-C2B	-2.11	1.46	1.50
19	a	802	CLA	CHC-C1C	2.11	1.42	1.38
19	b	3006	CLA	C3B-C4B	2.11	1.48	1.42
19	a	820	CLA	CMC-C2C	-2.11	1.46	1.50
19	b	3033	CLA	CMD-C2D	-2.11	1.46	1.50
19	a	829	CLA	CHC-C1C	2.11	1.42	1.38
23	a	851	LMG	O7-C8	-2.11	1.41	1.46
19	a	808	CLA	CMC-C2C	-2.11	1.46	1.50
19	a	839	CLA	CMB-C2B	-2.11	1.46	1.50
19	b	3021	CLA	CMD-C2D	-2.11	1.46	1.50
19	f	203	CLA	CMD-C2D	-2.11	1.46	1.50
19	a	823	CLA	CMD-C2D	-2.11	1.46	1.50
19	A	402	CLA	CHC-C1C	2.11	1.42	1.38
19	a	815	CLA	CMD-C2D	-2.11	1.46	1.50
19	a	833	CLA	C3B-C4B	2.11	1.48	1.42
19	j	103	CLA	MG-NB	-2.11	2.01	2.05
19	a	833	CLA	CHC-C1C	2.11	1.42	1.38
19	A	403	CLA	MG-NB	-2.11	2.01	2.05
19	b	3039	CLA	CHC-C1C	2.10	1.42	1.38
28	b	3053	ZEX	C34-C33	2.10	1.40	1.35
19	b	3027	CLA	CMB-C2B	-2.10	1.46	1.50
19	A	403	CLA	CMD-C2D	-2.10	1.46	1.50
19	a	804	CLA	CMD-C2D	-2.10	1.46	1.50
19	f	204	CLA	CMB-C2B	-2.10	1.46	1.50
18	a	801	CL0	CHC-C4B	-2.10	1.36	1.39
19	b	3030	CLA	C3B-C4B	2.10	1.48	1.42
19	b	3033	CLA	CHC-C1C	2.10	1.42	1.38
19	a	816	CLA	CHC-C1C	2.10	1.42	1.38
19	b	3022	CLA	CMB-C2B	-2.10	1.46	1.50
19	a	843	CLA	CMB-C2B	-2.10	1.46	1.50
19	a	838	CLA	CMC-C2C	-2.10	1.46	1.50
19	a	815	CLA	CMB-C2B	-2.10	1.46	1.50
19	a	855	CLA	C3B-C4B	2.10	1.48	1.42
19	a	841	CLA	CMC-C2C	-2.10	1.46	1.50
19	b	3032	CLA	CMD-C2D	-2.10	1.46	1.50
19	b	3041	CLA	CMD-C2D	-2.10	1.46	1.50
19	a	820	CLA	CHC-C1C	2.10	1.42	1.38
19	a	802	CLA	CMC-C2C	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	832	CLA	C3B-C4B	2.10	1.48	1.42
19	a	822	CLA	CMC-C2C	-2.10	1.46	1.50
19	a	805	CLA	CMB-C2B	-2.10	1.46	1.50
19	a	814	CLA	CMB-C2B	-2.10	1.46	1.50
19	a	838	CLA	C3B-C4B	2.10	1.48	1.42
21	a	847	BCR	C33-C5	-2.10	1.47	1.50
19	l	1503	CLA	CHC-C1C	2.10	1.42	1.38
19	b	3004	CLA	CMD-C2D	-2.10	1.46	1.50
19	b	3007	CLA	CMB-C2B	-2.09	1.46	1.50
19	j	102	CLA	MG-NB	-2.09	2.01	2.05
19	D	404	CLA	CMD-C2D	-2.09	1.46	1.50
19	a	841	CLA	CMB-C2B	-2.09	1.46	1.50
29	f	207	LMT	O4'-C4B	-2.09	1.37	1.43
19	b	3027	CLA	CMC-C2C	-2.09	1.46	1.50
19	a	814	CLA	CMC-C2C	-2.09	1.46	1.50
19	b	3034	CLA	CMB-C2B	-2.09	1.46	1.50
19	f	204	CLA	CMD-C2D	-2.09	1.46	1.50
19	a	833	CLA	CMC-C2C	-2.09	1.46	1.50
19	a	837	CLA	CMB-C2B	-2.09	1.46	1.50
19	D	401	CLA	CMB-C2B	-2.09	1.46	1.50
19	b	3030	CLA	CHC-C1C	2.09	1.42	1.38
19	b	3037	CLA	CMC-C2C	-2.09	1.46	1.50
19	j	102	CLA	CMD-C2D	-2.09	1.46	1.50
19	l	1503	CLA	CMD-C2D	-2.09	1.46	1.50
19	a	839	CLA	CMC-C2C	-2.09	1.46	1.50
19	b	3016	CLA	CMC-C2C	-2.09	1.46	1.50
19	a	815	CLA	CMC-C2C	-2.08	1.46	1.50
19	k	4003	CLA	MG-NB	-2.08	2.01	2.05
19	b	3022	CLA	CMD-C2D	-2.08	1.46	1.50
19	b	3028	CLA	CMB-C2B	-2.08	1.46	1.50
19	b	3013	CLA	CHC-C1C	2.08	1.42	1.38
19	b	3020	CLA	CMC-C2C	-2.08	1.46	1.50
19	b	3015	CLA	MG-NB	-2.08	2.01	2.05
19	b	3032	CLA	MG-NB	-2.08	2.01	2.05
19	b	3035	CLA	CMD-C2D	-2.08	1.46	1.50
19	D	403	CLA	CMC-C2C	-2.08	1.46	1.50
19	A	402	CLA	CMD-C2D	-2.08	1.46	1.50
19	a	829	CLA	CMC-C2C	-2.08	1.46	1.50
24	a	857	45D	C30-C26	2.08	1.40	1.35
19	a	836	CLA	CMC-C2C	-2.08	1.46	1.50
19	b	3031	CLA	CMB-C2B	-2.08	1.46	1.50
19	a	806	CLA	CHC-C1C	2.08	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	3036	CLA	CMB-C2B	-2.08	1.46	1.50
19	a	809	CLA	CMC-C2C	-2.08	1.46	1.50
19	l	1502	CLA	CMC-C2C	-2.08	1.46	1.50
19	b	3014	CLA	CMB-C2B	-2.07	1.46	1.50
19	b	3040	CLA	CMC-C2C	-2.07	1.46	1.50
19	b	3033	CLA	CMC-C2C	-2.07	1.46	1.50
19	b	3009	CLA	C3B-C4B	2.07	1.48	1.42
19	b	3028	CLA	CMC-C2C	-2.07	1.46	1.50
19	k	4003	CLA	CMD-C2D	-2.07	1.46	1.50
19	a	818	CLA	C3B-C4B	2.07	1.48	1.42
19	f	204	CLA	MG-NB	-2.07	2.01	2.05
19	a	827	CLA	CMC-C2C	-2.07	1.46	1.50
19	k	4002	CLA	CMB-C2B	-2.07	1.46	1.50
26	b	3045	ECH	C14-C13	2.07	1.40	1.35
19	a	803	CLA	CMB-C2B	-2.07	1.46	1.50
19	b	3037	CLA	CHC-C1C	2.07	1.42	1.38
19	b	3012	CLA	CMC-C2C	-2.07	1.46	1.50
19	b	3025	CLA	C3B-C4B	2.07	1.48	1.42
19	b	3010	CLA	CHC-C1C	2.07	1.42	1.38
28	b	3053	ZEX	C14-C13	2.07	1.40	1.35
19	D	403	CLA	CHC-C1C	2.07	1.42	1.38
19	b	3018	CLA	CHC-C1C	2.06	1.42	1.38
19	a	823	CLA	CMB-C2B	-2.06	1.46	1.50
19	a	843	CLA	CMC-C2C	-2.06	1.46	1.50
19	b	3010	CLA	CMC-C2C	-2.06	1.46	1.50
28	f	205	ZEX	C10-C9	2.06	1.40	1.35
19	a	825	CLA	CHC-C1C	2.06	1.42	1.38
19	b	3038	CLA	CHC-C1C	2.06	1.42	1.38
19	b	3007	CLA	CMC-C2C	-2.06	1.46	1.50
19	a	835	CLA	CHC-C1C	2.06	1.42	1.38
19	a	830	CLA	CMC-C2C	-2.06	1.46	1.50
19	a	858	CLA	CMB-C2B	-2.06	1.46	1.50
19	a	824	CLA	CMC-C2C	-2.06	1.46	1.50
19	b	3029	CLA	CMC-C2C	-2.06	1.46	1.50
19	b	3025	CLA	CHC-C1C	2.06	1.42	1.38
32	F	101	HEM	CMB-C2B	2.06	1.55	1.50
19	j	102	CLA	CMB-C2B	-2.06	1.46	1.50
19	a	842	CLA	CMC-C2C	-2.06	1.46	1.50
27	b	3052	EQ3	C21-C22	2.06	1.40	1.35
19	b	3036	CLA	CMC-C2C	-2.06	1.46	1.50
19	b	3009	CLA	CMC-C2C	-2.06	1.46	1.50
28	f	205	ZEX	C14-C13	2.05	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	F	101	HEM	C2A-C3A	-2.05	1.33	1.38
19	b	3007	CLA	C3B-C4B	2.05	1.48	1.42
19	a	826	CLA	CMC-C2C	-2.05	1.46	1.50
19	a	816	CLA	CMC-C2C	-2.05	1.46	1.50
21	a	848	BCR	C33-C5	-2.05	1.47	1.50
19	l	1503	CLA	CMB-C2B	-2.05	1.46	1.50
19	a	804	CLA	CHC-C1C	2.05	1.42	1.38
19	a	807	CLA	CMC-C2C	-2.05	1.46	1.50
19	a	841	CLA	CHC-C1C	2.05	1.42	1.38
21	a	845	BCR	C33-C5	-2.05	1.47	1.50
19	b	3023	CLA	CMC-C2C	-2.05	1.46	1.50
19	b	3024	CLA	CMC-C2C	-2.04	1.46	1.50
19	D	401	CLA	CMD-C2D	-2.04	1.46	1.50
19	a	805	CLA	CMC-C2C	-2.04	1.46	1.50
19	a	835	CLA	CMC-C2C	-2.04	1.46	1.50
19	k	4003	CLA	CMB-C2B	-2.04	1.46	1.50
19	a	855	CLA	CHC-C1C	2.04	1.42	1.38
19	b	3017	CLA	CMC-C2C	-2.04	1.46	1.50
19	a	821	CLA	CMC-C2C	-2.04	1.46	1.50
19	b	3030	CLA	CMC-C2C	-2.04	1.46	1.50
24	a	857	45D	C29-C25	2.04	1.40	1.35
19	a	823	CLA	CMC-C2C	-2.04	1.46	1.50
31	D	402	PHO	C4D-ND	-2.04	1.35	1.38
19	a	816	CLA	CMB-C2B	-2.04	1.46	1.50
19	b	3021	CLA	CMC-C2C	-2.03	1.46	1.50
19	a	818	CLA	CMC-C2C	-2.03	1.46	1.50
29	f	207	LMT	O1'-C1'	-2.03	1.36	1.40
19	a	832	CLA	CHC-C1C	2.03	1.42	1.38
19	k	4002	CLA	CMC-C2C	-2.03	1.46	1.50
19	b	3011	CLA	CHC-C1C	2.03	1.42	1.38
19	b	3025	CLA	CMC-C2C	-2.03	1.46	1.50
19	b	3032	CLA	CMC-C2C	-2.03	1.46	1.50
19	a	811	CLA	CHC-C1C	2.03	1.42	1.38
19	b	3018	CLA	CMC-C2C	-2.03	1.46	1.50
19	a	812	CLA	CMB-C2B	-2.03	1.46	1.50
19	a	817	CLA	CMC-C2C	-2.03	1.46	1.50
21	a	846	BCR	C33-C5	-2.03	1.47	1.50
19	a	840	CLA	CMC-C2C	-2.03	1.46	1.50
31	D	402	PHO	C3B-C2B	-2.02	1.37	1.40
19	a	812	CLA	CMC-C2C	-2.02	1.46	1.50
19	b	3009	CLA	CHC-C1C	2.02	1.42	1.38
19	a	842	CLA	CHC-C1C	2.02	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	f	203	CLA	CMB-C2B	-2.02	1.46	1.50
19	A	403	CLA	CMC-C2C	-2.02	1.46	1.50
19	D	404	CLA	CMB-C2B	-2.02	1.46	1.50
19	b	3011	CLA	CMC-C2C	-2.02	1.46	1.50
21	b	3043	BCR	C33-C5	-2.02	1.47	1.50
28	b	3053	ZEX	C10-C9	2.01	1.40	1.35
18	a	801	CL0	C3B-C2B	-2.01	1.37	1.40
19	b	3022	CLA	CMC-C2C	-2.01	1.46	1.50
19	a	834	CLA	CHC-C1C	2.01	1.42	1.38
21	b	3044	BCR	C33-C5	-2.01	1.47	1.50
19	A	403	CLA	CMB-C2B	-2.01	1.46	1.50
19	a	808	CLA	CMB-C2B	-2.01	1.46	1.50
31	A	404	PHO	C4D-ND	-2.01	1.35	1.38
19	b	3041	CLA	CMC-C2C	-2.01	1.46	1.50
19	f	204	CLA	CMC-C2C	-2.00	1.46	1.50
19	b	3027	CLA	CHC-C1C	2.00	1.42	1.38
21	b	3047	BCR	C38-C26	-2.00	1.47	1.50
21	f	202	BCR	C33-C5	-2.00	1.47	1.50
19	A	402	CLA	CMB-C2B	-2.00	1.46	1.50
19	l	1501	CLA	MG-NB	-2.00	2.01	2.05
19	b	3039	CLA	CMC-C2C	-2.00	1.46	1.50
19	l	1501	CLA	CMD-C2D	-2.00	1.46	1.50

All (869) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	3045	ECH	C15-C16-C17	8.17	140.25	123.52
19	a	818	CLA	C4A-NA-C1A	7.42	110.07	106.68
19	a	840	CLA	C4A-NA-C1A	7.32	110.02	106.68
19	a	842	CLA	C4A-NA-C1A	7.30	110.01	106.68
19	a	806	CLA	C4A-NA-C1A	7.29	110.00	106.68
19	l	1502	CLA	C4A-NA-C1A	7.23	109.98	106.68
19	b	3040	CLA	C4A-NA-C1A	7.20	109.96	106.68
19	a	841	CLA	C4A-NA-C1A	7.15	109.94	106.68
19	a	810	CLA	C4A-NA-C1A	7.10	109.92	106.68
19	a	811	CLA	C4A-NA-C1A	7.09	109.91	106.68
19	a	835	CLA	C4A-NA-C1A	6.92	109.83	106.68
19	A	403	CLA	C4A-NA-C1A	6.89	109.82	106.68
19	b	3007	CLA	C4A-NA-C1A	6.88	109.82	106.68
19	b	3011	CLA	C4A-NA-C1A	6.88	109.82	106.68
19	b	3033	CLA	C4A-NA-C1A	6.86	109.81	106.68
19	a	824	CLA	C4A-NA-C1A	6.85	109.81	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	j	102	CLA	C4A-NA-C1A	6.84	109.80	106.68
19	b	3005	CLA	C4A-NA-C1A	6.81	109.79	106.68
19	D	403	CLA	C4A-NA-C1A	6.80	109.78	106.68
19	b	3022	CLA	C4A-NA-C1A	6.75	109.76	106.68
19	b	3025	CLA	C4A-NA-C1A	6.73	109.75	106.68
19	a	816	CLA	C4A-NA-C1A	6.72	109.75	106.68
19	a	829	CLA	C4A-NA-C1A	6.71	109.74	106.68
19	a	817	CLA	C4A-NA-C1A	6.71	109.74	106.68
19	b	3017	CLA	C4A-NA-C1A	6.71	109.74	106.68
19	b	3004	CLA	C4A-NA-C1A	6.71	109.74	106.68
19	l	1501	CLA	C4A-NA-C1A	6.69	109.73	106.68
19	A	405	CLA	C4A-NA-C1A	6.68	109.73	106.68
19	a	823	CLA	C4A-NA-C1A	6.68	109.73	106.68
19	b	3035	CLA	C4A-NA-C1A	6.67	109.72	106.68
19	D	404	CLA	C4A-NA-C1A	6.67	109.72	106.68
19	b	3013	CLA	C4A-NA-C1A	6.67	109.72	106.68
19	a	831	CLA	C4A-NA-C1A	6.63	109.70	106.68
19	a	834	CLA	C4A-NA-C1A	6.62	109.70	106.68
19	a	856	CLA	C4A-NA-C1A	6.62	109.70	106.68
19	l	1503	CLA	C4A-NA-C1A	6.61	109.69	106.68
19	a	825	CLA	C4A-NA-C1A	6.61	109.69	106.68
19	b	3037	CLA	C4A-NA-C1A	6.60	109.69	106.68
19	b	3010	CLA	C4A-NA-C1A	6.59	109.69	106.68
19	b	3034	CLA	C4A-NA-C1A	6.58	109.68	106.68
19	a	839	CLA	C4A-NA-C1A	6.57	109.68	106.68
19	a	807	CLA	C4A-NA-C1A	6.57	109.68	106.68
19	b	3016	CLA	C4A-NA-C1A	6.57	109.67	106.68
19	b	3027	CLA	C4A-NA-C1A	6.56	109.67	106.68
19	b	3009	CLA	C4A-NA-C1A	6.56	109.67	106.68
19	a	828	CLA	C4A-NA-C1A	6.56	109.67	106.68
19	b	3039	CLA	C4A-NA-C1A	6.56	109.67	106.68
19	a	821	CLA	C4A-NA-C1A	6.55	109.67	106.68
19	b	3029	CLA	C4A-NA-C1A	6.55	109.67	106.68
19	D	401	CLA	C4A-NA-C1A	6.54	109.66	106.68
19	b	3014	CLA	C4A-NA-C1A	6.54	109.66	106.68
19	a	832	CLA	C4A-NA-C1A	6.53	109.66	106.68
19	b	3008	CLA	C4A-NA-C1A	6.52	109.65	106.68
19	f	201	CLA	C4A-NA-C1A	6.52	109.65	106.68
19	b	3003	CLA	C4A-NA-C1A	6.50	109.64	106.68
19	a	803	CLA	C4A-NA-C1A	6.49	109.64	106.68
19	a	814	CLA	C4A-NA-C1A	6.49	109.64	106.68
19	b	3019	CLA	C4A-NA-C1A	6.49	109.64	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	402	CLA	C4A-NA-C1A	6.49	109.64	106.68
19	a	826	CLA	C4A-NA-C1A	6.46	109.62	106.68
19	a	815	CLA	C4A-NA-C1A	6.46	109.62	106.68
19	a	808	CLA	C4A-NA-C1A	6.45	109.62	106.68
19	k	4002	CLA	C4A-NA-C1A	6.45	109.62	106.68
19	b	3006	CLA	C4A-NA-C1A	6.44	109.61	106.68
19	a	837	CLA	C4A-NA-C1A	6.43	109.61	106.68
19	a	805	CLA	C4A-NA-C1A	6.43	109.61	106.68
19	b	3038	CLA	C4A-NA-C1A	6.42	109.61	106.68
19	a	813	CLA	C4A-NA-C1A	6.41	109.60	106.68
19	a	804	CLA	C4A-NA-C1A	6.41	109.60	106.68
19	b	3020	CLA	C4A-NA-C1A	6.39	109.59	106.68
19	b	3032	CLA	C4A-NA-C1A	6.37	109.58	106.68
19	b	3030	CLA	C4A-NA-C1A	6.37	109.58	106.68
19	a	827	CLA	C4A-NA-C1A	6.33	109.57	106.68
19	a	836	CLA	C4A-NA-C1A	6.31	109.56	106.68
31	D	402	PHO	C4D-CHA-CBD	-6.31	105.43	108.45
19	f	204	CLA	C4A-NA-C1A	6.30	109.55	106.68
19	a	833	CLA	C4A-NA-C1A	6.29	109.55	106.68
19	a	819	CLA	C4A-NA-C1A	6.28	109.54	106.68
19	a	858	CLA	C4A-NA-C1A	6.26	109.54	106.68
19	b	3041	CLA	C4A-NA-C1A	6.26	109.53	106.68
19	b	3018	CLA	C4A-NA-C1A	6.23	109.52	106.68
19	f	203	CLA	C4A-NA-C1A	6.22	109.52	106.68
19	a	809	CLA	C4A-NA-C1A	6.19	109.50	106.68
19	b	3002	CLA	C4A-NA-C1A	6.19	109.50	106.68
19	b	3023	CLA	C4A-NA-C1A	6.18	109.50	106.68
19	b	3024	CLA	C4A-NA-C1A	6.18	109.50	106.68
19	k	4003	CLA	C4A-NA-C1A	6.17	109.50	106.68
19	b	3012	CLA	C4A-NA-C1A	6.17	109.49	106.68
19	a	838	CLA	C4A-NA-C1A	6.15	109.49	106.68
19	b	3015	CLA	C4A-NA-C1A	6.15	109.48	106.68
19	b	3026	CLA	C4A-NA-C1A	6.15	109.48	106.68
19	a	802	CLA	C4A-NA-C1A	6.13	109.48	106.68
19	b	3021	CLA	C4A-NA-C1A	6.13	109.47	106.68
19	b	3031	CLA	C4A-NA-C1A	6.12	109.47	106.68
19	a	812	CLA	C4A-NA-C1A	6.08	109.45	106.68
19	a	822	CLA	C4A-NA-C1A	6.02	109.42	106.68
19	a	830	CLA	C4A-NA-C1A	5.98	109.41	106.68
19	a	843	CLA	C4A-NA-C1A	5.98	109.41	106.68
19	b	3028	CLA	C4A-NA-C1A	5.98	109.41	106.68
19	b	3036	CLA	C4A-NA-C1A	5.96	109.40	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	820	CLA	C4A-NA-C1A	5.94	109.39	106.68
19	a	855	CLA	C4A-NA-C1A	5.82	109.34	106.68
31	A	404	PHO	C4D-CHA-CBD	-5.81	105.67	108.45
18	a	801	CL0	C1B-CHB-C4A	5.80	125.06	121.32
19	j	103	CLA	C4A-NA-C1A	5.69	109.28	106.68
24	a	857	45D	C42-C41-C37	5.32	134.41	123.52
26	m	101	ECH	C15-C16-C17	4.71	133.16	123.52
26	b	3045	ECH	C19-C18-C17	4.63	126.30	119.01
22	a	852	LHG	O4-P-O5	4.51	133.42	112.44
26	b	3045	ECH	C12-C13-C14	4.46	126.02	119.01
26	b	3045	ECH	C1-C6-C5	-4.44	116.57	122.64
22	a	850	LHG	O4-P-O5	4.44	133.08	112.44
22	b	3050	LHG	O4-P-O5	4.43	133.05	112.44
22	a	854	LHG	O4-P-O5	4.43	133.04	112.44
22	f	206	LHG	O4-P-O5	4.42	133.02	112.44
28	f	205	ZEX	C35-C15-C14	4.33	132.39	123.52
26	b	3045	ECH	C24-C23-C22	-3.88	120.50	126.23
31	D	402	PHO	C2B-C1B-NB	-3.74	106.73	109.43
19	b	3013	CLA	O2D-CGD-O1D	-3.72	116.60	123.85
26	b	3045	ECH	C36-C18-C17	-3.65	116.91	122.82
26	b	3045	ECH	C35-C13-C14	-3.59	117.00	122.82
31	A	404	PHO	C2B-C1B-NB	-3.58	106.84	109.43
26	m	101	ECH	C37-C22-C21	-3.53	117.10	122.82
28	b	3053	ZEX	C35-C15-C14	3.51	130.71	123.52
19	b	3029	CLA	CAA-C2A-C3A	-3.51	103.51	113.00
19	a	831	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
24	a	857	45D	C28-C26-C30	-3.48	117.17	122.82
19	a	811	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
28	b	3053	ZEX	C39-C29-C30	-3.46	117.22	122.82
19	a	815	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
19	a	838	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
28	f	205	ZEX	C19-C9-C10	-3.43	117.25	122.82
27	b	3052	EQ3	C15-C16-C17	3.41	130.50	123.52
19	b	3029	CLA	O2D-CGD-O1D	-3.40	117.24	123.85
24	a	857	45D	C27-C25-C29	-3.38	117.34	122.82
28	f	205	ZEX	C39-C29-C30	-3.36	117.37	122.82
28	b	3053	ZEX	C19-C9-C10	-3.35	117.38	122.82
19	a	831	CLA	CAA-C2A-C3A	-3.33	103.99	113.00
26	m	101	ECH	C19-C18-C17	3.33	124.25	119.01
26	m	101	ECH	C34-C9-C10	-3.33	117.42	122.82
26	b	3045	ECH	C10-C11-C12	3.32	132.83	123.20
19	a	814	CLA	O2D-CGD-O1D	-3.32	117.38	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	3045	ECH	C34-C9-C10	-3.30	117.47	122.82
28	b	3053	ZEX	C39-C29-C28	3.29	123.12	118.09
19	b	3033	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
19	a	805	CLA	O2D-CGD-O1D	-3.27	117.47	123.85
27	b	3052	EQ3	C34-C9-C8	3.27	123.08	118.09
19	a	809	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
19	a	833	CLA	C3B-C4B-NB	-3.25	107.63	110.53
31	A	404	PHO	O1D-CGD-CBD	3.23	129.62	124.72
19	D	401	CLA	C3B-C4B-NB	-3.22	107.66	110.53
21	k	4004	BCR	C2-C1-C6	3.21	115.11	110.44
19	b	3019	CLA	C3B-C4B-NB	-3.20	107.67	110.53
19	a	835	CLA	O2D-CGD-O1D	-3.20	117.63	123.85
27	b	3052	EQ3	C37-C22-C21	-3.18	117.66	122.82
19	b	3013	CLA	O2D-CGD-CBD	3.18	116.78	111.23
19	b	3007	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
18	a	801	CL0	O2D-CGD-CBD	3.17	114.42	110.95
27	b	3052	EQ3	C34-C9-C10	-3.16	117.69	122.82
19	a	840	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
19	b	3012	CLA	C3B-C4B-NB	-3.15	107.71	110.53
19	a	839	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
19	b	3014	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
19	a	819	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
19	b	3024	CLA	C3B-C4B-NB	-3.13	107.73	110.53
19	a	804	CLA	C3B-C4B-NB	-3.12	107.74	110.53
26	m	101	ECH	C36-C18-C17	-3.12	117.77	122.82
19	a	804	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
19	b	3032	CLA	C3B-C4B-NB	-3.11	107.76	110.53
26	m	101	ECH	C23-C22-C21	3.10	123.89	119.01
19	b	3016	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
19	a	858	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
19	a	826	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
19	a	841	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
26	b	3045	ECH	C15-C14-C13	3.09	131.61	127.28
28	b	3053	ZEX	C27-C28-C29	3.09	130.80	126.23
21	j	101	BCR	C15-C16-C17	-3.08	117.21	123.52
26	b	3045	ECH	C37-C22-C21	-3.08	117.82	122.82
19	a	843	CLA	CAA-C2A-C3A	-3.08	104.67	113.00
19	a	836	CLA	C3B-C4B-NB	-3.07	107.78	110.53
19	a	803	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
19	a	803	CLA	C3B-C4B-NB	-3.07	107.79	110.53
19	b	3003	CLA	C3B-C4B-NB	-3.07	107.79	110.53
19	a	809	CLA	C3B-C4B-NB	-3.07	107.79	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	818	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
19	a	832	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
19	b	3037	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
19	a	839	CLA	C3B-C4B-NB	-3.06	107.80	110.53
31	D	402	PHO	C4A-C3A-C2A	-3.05	99.93	102.84
19	a	828	CLA	C3B-C4B-NB	-3.05	107.81	110.53
18	a	801	CL0	O2D-CGD-O1D	-3.05	117.91	123.85
19	b	3017	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
19	b	3003	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
19	a	828	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
19	b	3020	CLA	C3B-C4B-NB	-3.03	107.82	110.53
19	b	3023	CLA	C3B-C4B-NB	-3.03	107.82	110.53
19	b	3002	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
19	b	3008	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
19	f	204	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
19	b	3015	CLA	C3B-C4B-NB	-3.03	107.83	110.53
19	a	821	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
19	b	3013	CLA	C3B-C4B-NB	-3.02	107.83	110.53
19	b	3022	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
19	b	3026	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
19	b	3010	CLA	C3B-C4B-NB	-3.02	107.84	110.53
26	b	3045	ECH	C30-C25-C24	3.01	123.82	115.65
19	a	808	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
19	A	403	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
19	b	3025	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
19	a	813	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
19	l	1502	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
19	a	827	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
19	b	3040	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
19	a	827	CLA	C3B-C4B-NB	-2.99	107.86	110.53
21	k	4001	BCR	C15-C14-C13	-2.99	123.08	127.28
19	b	3022	CLA	C3B-C4B-NB	-2.98	107.87	110.53
19	b	3005	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
19	a	822	CLA	C3B-C4B-NB	-2.97	107.88	110.53
19	b	3014	CLA	C3B-C4B-NB	-2.97	107.88	110.53
19	a	855	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
19	a	858	CLA	C3B-C4B-NB	-2.97	107.88	110.53
19	a	836	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
19	b	3039	CLA	C1-C2-C3	-2.96	121.35	126.20
19	b	3004	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
19	a	810	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
21	b	3047	BCR	C2-C1-C6	2.95	114.73	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	3011	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
19	k	4002	CLA	C3B-C4B-NB	-2.95	107.90	110.53
19	A	405	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
19	b	3004	CLA	C3B-C4B-NB	-2.94	107.90	110.53
19	b	3035	CLA	C3B-C4B-NB	-2.94	107.90	110.53
19	a	837	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
19	j	102	CLA	C3B-C4B-NB	-2.93	107.91	110.53
19	f	201	CLA	C3B-C4B-NB	-2.93	107.91	110.53
19	a	824	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
19	a	842	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
21	a	849	BCR	C15-C14-C13	-2.93	123.17	127.28
19	f	204	CLA	C3B-C4B-NB	-2.93	107.92	110.53
21	b	3046	BCR	C2-C1-C6	2.93	114.69	110.44
19	A	402	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
19	a	829	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
19	a	856	CLA	C3B-C4B-NB	-2.92	107.92	110.53
18	a	801	CL0	C4D-CHA-CBD	-2.91	106.03	108.97
21	b	3043	BCR	C33-C5-C6	-2.91	121.31	124.48
19	b	3018	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
19	a	820	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
19	D	404	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
18	a	801	CL0	CHA-C1A-C2A	-2.91	126.48	133.31
19	b	3024	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
19	b	3028	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
19	b	3020	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
19	b	3039	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
19	a	808	CLA	C3B-C4B-NB	-2.89	107.95	110.53
19	a	817	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
21	a	848	BCR	C33-C5-C6	-2.89	121.33	124.48
19	a	831	CLA	C3B-C4B-NB	-2.89	107.95	110.53
19	b	3012	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
21	a	848	BCR	C15-C16-C17	-2.89	117.61	123.52
19	a	856	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
19	b	3030	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
19	b	3010	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
19	a	826	CLA	C3B-C4B-NB	-2.88	107.96	110.53
19	b	3038	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
19	b	3029	CLA	C3B-C4B-NB	-2.87	107.97	110.53
19	l	1503	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
19	a	822	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
21	b	3046	BCR	C15-C16-C17	-2.87	117.65	123.52
19	a	833	CLA	O2D-CGD-O1D	-2.86	118.27	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	3015	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
19	b	3017	CLA	C3B-C4B-NB	-2.86	107.97	110.53
19	k	4002	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
19	b	3008	CLA	C3B-C4B-NB	-2.86	107.98	110.53
23	a	853	LMG	O6-C1-O1	-2.86	103.28	110.04
19	b	3009	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
19	a	831	CLA	CHB-C4A-NA	2.86	128.53	124.40
19	a	834	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
19	a	811	CLA	C1-C2-C3	-2.86	122.14	126.76
21	j	104	BCR	C15-C16-C17	-2.86	117.68	123.52
21	a	847	BCR	C15-C16-C17	-2.85	117.68	123.52
21	a	849	BCR	C15-C16-C17	-2.85	117.68	123.52
19	a	830	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
19	f	203	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
19	a	805	CLA	C3B-C4B-NB	-2.85	107.98	110.53
22	f	206	LHG	O8-C23-C24	2.85	120.52	111.83
19	b	3023	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
19	b	3034	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
19	b	3035	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
26	b	3045	ECH	C37-C22-C23	2.84	122.43	118.09
28	f	205	ZEX	C15-C35-C34	2.84	129.33	123.52
22	b	3050	LHG	O8-C23-C24	2.84	120.50	111.83
19	l	1501	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
24	a	857	45D	C03-C07-C19	2.84	123.34	115.65
19	b	3005	CLA	C3B-C4B-NB	-2.83	108.00	110.53
19	a	813	CLA	C3B-C4B-NB	-2.83	108.00	110.53
19	b	3006	CLA	C3B-C4B-NB	-2.83	108.00	110.53
19	b	3039	CLA	C3B-C4B-NB	-2.83	108.00	110.53
19	a	812	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
19	a	829	CLA	C1-C2-C3	-2.83	121.56	126.20
19	a	835	CLA	CHB-C4A-NA	2.83	128.48	124.40
23	b	3049	LMG	O6-C1-O1	-2.82	103.37	110.04
19	j	103	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
19	b	3030	CLA	C3B-C4B-NB	-2.82	108.02	110.53
21	b	3046	BCR	C15-C14-C13	-2.81	123.33	127.28
19	a	807	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
19	b	3021	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
21	b	3043	BCR	C15-C16-C17	-2.81	117.77	123.52
27	b	3052	EQ3	C37-C22-C23	2.81	122.38	118.09
19	b	3009	CLA	C3B-C4B-NB	-2.80	108.03	110.53
19	a	814	CLA	C3B-C4B-NB	-2.80	108.03	110.53
19	l	1501	CLA	C3B-C4B-NB	-2.80	108.03	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	3029	CLA	CHB-C4A-NA	2.80	128.44	124.40
21	k	4001	BCR	C24-C23-C22	-2.79	122.11	126.23
27	b	3052	EQ3	C16-C15-C14	2.79	129.23	123.52
19	a	819	CLA	C3B-C4B-NB	-2.79	108.04	110.53
29	f	207	LMT	C1'-O5'-C5'	-2.79	108.27	113.72
19	D	404	CLA	CHB-C4A-NA	2.79	128.42	124.40
21	j	101	BCR	C15-C14-C13	-2.78	123.38	127.28
27	b	3052	EQ3	C36-C18-C17	-2.78	118.31	122.82
19	a	825	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
18	a	801	CL0	CAA-CBA-CGA	-2.78	105.32	113.21
19	b	3002	CLA	C3B-C4B-NB	-2.78	108.05	110.53
19	b	3033	CLA	C3B-C4B-NB	-2.78	108.05	110.53
19	b	3041	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
19	a	843	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
20	a	844	PQN	C11-C3-C2	-2.77	120.14	124.89
21	b	3043	BCR	C27-C26-C25	2.77	126.44	122.70
19	a	824	CLA	CHB-C4A-NA	2.77	128.40	124.40
19	a	842	CLA	C3B-C4B-NB	-2.77	108.06	110.53
19	a	806	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
21	b	3043	BCR	C24-C23-C22	-2.76	122.15	126.23
19	b	3027	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
19	a	802	CLA	C1-C2-C3	-2.76	121.68	126.20
18	a	801	CL0	C1C-CHC-C4B	2.76	125.94	116.07
19	a	816	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
31	D	402	PHO	O1D-CGD-CBD	2.75	128.90	124.72
28	b	3053	ZEX	C15-C35-C34	2.75	129.15	123.52
19	a	806	CLA	CHB-C4A-NA	2.75	128.37	124.40
19	a	821	CLA	C3B-C4B-NB	-2.75	108.08	110.53
19	b	3031	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
19	a	807	CLA	C3B-C4B-NB	-2.75	108.08	110.53
31	D	402	PHO	O2D-CGD-O1D	-2.74	118.51	123.85
21	j	104	BCR	C33-C5-C6	-2.74	121.49	124.48
19	b	3032	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
23	a	851	LMG	O6-C1-O1	-2.73	103.58	110.04
19	b	3036	CLA	C3B-C4B-NB	-2.73	108.09	110.53
19	a	806	CLA	C1-C2-C3	-2.73	121.72	126.20
19	l	1502	CLA	C3B-C4B-NB	-2.73	108.09	110.53
19	k	4003	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
19	a	823	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
19	D	401	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
19	a	812	CLA	C3B-C4B-NB	-2.72	108.10	110.53
21	j	104	BCR	C27-C26-C25	2.72	126.38	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	802	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
19	a	834	CLA	CHB-C4A-NA	2.72	128.32	124.40
19	l	1503	CLA	C3B-C4B-NB	-2.72	108.11	110.53
28	f	205	ZEX	C40-C33-C34	-2.71	118.42	122.82
19	b	3026	CLA	C3B-C4B-NB	-2.71	108.11	110.53
18	a	801	CL0	C3D-C4D-CHA	2.71	112.66	108.54
19	a	818	CLA	C3B-C4B-NB	-2.70	108.12	110.53
27	b	3052	EQ3	C35-C13-C14	-2.70	118.44	122.82
21	j	104	BCR	C24-C23-C22	-2.70	122.24	126.23
19	a	811	CLA	CHB-C4A-NA	2.70	128.29	124.40
28	f	205	ZEX	C32-C33-C34	2.70	123.25	119.01
31	A	404	PHO	O2D-CGD-O1D	-2.69	118.62	123.85
19	j	102	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
19	A	403	CLA	C3B-C4B-NB	-2.69	108.13	110.53
21	b	3044	BCR	C33-C5-C6	-2.68	121.56	124.48
19	a	818	CLA	CHB-C4A-NA	2.68	128.26	124.40
22	a	850	LHG	O8-C23-C24	2.68	120.00	111.83
19	b	3017	CLA	CHB-C4A-NA	2.68	128.26	124.40
21	b	3047	BCR	C27-C26-C25	2.67	126.32	122.70
21	a	845	BCR	C24-C23-C22	-2.67	122.29	126.23
19	D	404	CLA	C3B-C4B-NB	-2.67	108.15	110.53
19	a	842	CLA	C1-C2-C3	-2.66	121.83	126.20
19	a	824	CLA	C3B-C4B-NB	-2.66	108.15	110.53
19	f	201	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
21	k	4004	BCR	C24-C23-C22	-2.66	122.30	126.23
19	a	843	CLA	C3B-C4B-NB	-2.66	108.16	110.53
19	D	403	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
19	b	3006	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
19	b	3021	CLA	C3B-C4B-NB	-2.65	108.16	110.53
19	b	3036	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
21	a	849	BCR	C7-C8-C9	-2.65	122.31	126.23
19	a	832	CLA	C3B-C4B-NB	-2.64	108.17	110.53
21	i	101	BCR	C27-C26-C25	2.64	126.28	122.70
19	l	1502	CLA	CHB-C4A-NA	2.64	128.21	124.40
21	k	4001	BCR	C15-C16-C17	-2.64	118.11	123.52
19	b	3034	CLA	C3B-C4B-NB	-2.64	108.17	110.53
27	b	3052	EQ3	C24-C23-C22	2.64	130.14	126.23
19	b	3035	CLA	CHB-C4A-NA	2.64	128.21	124.40
21	l	1504	BCR	C15-C16-C17	-2.63	118.14	123.52
19	b	3019	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
19	f	203	CLA	C1-C2-C3	-2.63	122.51	126.76
21	A	406	BCR	C27-C26-C25	2.62	126.25	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	854	LHG	O8-C23-C24	2.62	119.84	111.83
22	a	852	LHG	O8-C23-C24	2.62	119.83	111.83
19	b	3019	CLA	CHB-C4A-NA	2.62	128.19	124.40
21	a	847	BCR	C15-C14-C13	-2.62	123.60	127.28
19	b	3015	CLA	CHB-C4A-NA	2.62	128.18	124.40
19	D	401	CLA	CHB-C4A-NA	2.62	128.18	124.40
28	b	3053	ZEX	C20-C13-C14	-2.61	118.58	122.82
19	a	826	CLA	O2D-CGD-CBD	2.61	115.80	111.23
19	a	841	CLA	C3B-C4B-NB	-2.61	108.20	110.53
19	a	836	CLA	CHB-C4A-NA	2.61	128.16	124.40
18	a	801	CL0	C1-C2-C3	-2.60	121.93	126.20
21	k	4004	BCR	C27-C26-C25	2.60	126.22	122.70
19	b	3011	CLA	CHB-C4A-NA	2.60	128.16	124.40
19	A	403	CLA	CHB-C4A-NA	2.60	128.16	124.40
19	a	838	CLA	O2D-CGD-CBD	2.60	115.78	111.23
19	a	802	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
21	k	4004	BCR	C15-C16-C17	-2.60	118.20	123.52
31	A	404	PHO	CMB-C2B-C3B	2.60	129.88	124.68
18	a	801	CL0	CMD-C2D-C3D	2.60	129.87	124.68
19	a	817	CLA	C3B-C4B-NB	-2.59	108.22	110.53
19	b	3003	CLA	CAC-C3C-C4C	2.59	128.16	124.79
21	a	845	BCR	C27-C26-C25	2.59	126.20	122.70
19	j	102	CLA	CHB-C4A-NA	2.58	128.13	124.40
27	b	3052	EQ3	C7-C8-C9	2.58	130.06	126.23
19	a	842	CLA	CHB-C4A-NA	2.58	128.12	124.40
19	a	835	CLA	C3B-C4B-NB	-2.58	108.23	110.53
19	a	806	CLA	C3B-C4B-NB	-2.58	108.23	110.53
27	b	3052	EQ3	C12-C13-C14	2.57	123.06	119.01
21	l	1504	BCR	C2-C1-C6	2.57	114.18	110.44
19	b	3040	CLA	CHB-C4A-NA	2.57	128.11	124.40
23	a	853	LMG	O1-C1-C2	-2.57	104.37	108.27
19	a	837	CLA	C3B-C4B-NB	-2.57	108.24	110.53
20	b	3042	PQN	C11-C3-C2	-2.57	120.49	124.89
19	l	1501	CLA	C1-C2-C3	-2.57	122.61	126.76
19	a	825	CLA	C3B-C4B-NB	-2.57	108.24	110.53
19	b	3041	CLA	C3B-C4B-NB	-2.57	108.24	110.53
19	a	826	CLA	CHB-C4A-NA	2.56	128.10	124.40
19	f	204	CLA	CHB-C4A-NA	2.56	128.10	124.40
21	a	847	BCR	C27-C26-C25	2.56	126.17	122.70
21	f	202	BCR	C27-C26-C25	2.56	126.17	122.70
19	a	838	CLA	C3B-C4B-NB	-2.56	108.24	110.53
26	m	101	ECH	C35-C13-C14	-2.56	118.67	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	3044	BCR	C15-C16-C17	-2.56	118.28	123.52
19	k	4002	CLA	CHB-C4A-NA	2.56	128.09	124.40
19	a	831	CLA	O2D-CGD-CBD	2.55	115.69	111.23
19	a	843	CLA	CHB-C4A-NA	2.55	128.09	124.40
19	l	1503	CLA	CHB-C4A-NA	2.55	128.08	124.40
19	l	1501	CLA	CHB-C4A-NA	2.55	128.08	124.40
19	a	808	CLA	CMB-C2B-C1B	-2.55	121.54	125.42
21	a	846	BCR	C33-C5-C6	-2.54	121.71	124.48
21	j	104	BCR	C15-C14-C13	-2.54	123.71	127.28
19	a	840	CLA	CHB-C4A-NA	2.54	128.07	124.40
21	j	101	BCR	C33-C5-C6	-2.54	121.71	124.48
19	a	809	CLA	CHB-C4A-NA	2.54	128.07	124.40
19	b	3011	CLA	C3B-C4B-NB	-2.54	108.26	110.53
21	i	101	BCR	C15-C16-C17	-2.54	118.33	123.52
19	a	818	CLA	O2A-CGA-O1A	-2.54	117.28	123.63
21	a	848	BCR	C27-C26-C25	2.54	126.13	122.70
19	b	3016	CLA	C3B-C4B-NB	-2.54	108.27	110.53
19	a	816	CLA	C3B-C4B-NB	-2.53	108.27	110.53
19	b	3003	CLA	CHB-C4A-NA	2.53	128.05	124.40
22	a	852	LHG	C11-C10-C9	-2.53	101.58	114.37
19	b	3008	CLA	O2A-CGA-O1A	-2.53	117.31	123.63
27	b	3052	EQ3	C19-C18-C17	2.52	122.98	119.01
19	b	3035	CLA	C1-C2-C3	-2.52	122.68	126.76
19	a	820	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
21	a	846	BCR	C27-C26-C25	2.52	126.11	122.70
19	b	3006	CLA	CHB-C4A-NA	2.52	128.04	124.40
19	a	821	CLA	CHB-C4A-NA	2.52	128.03	124.40
19	b	3020	CLA	CHB-C4A-NA	2.52	128.03	124.40
19	a	803	CLA	CHB-C4A-NA	2.52	128.03	124.40
19	a	830	CLA	C3B-C4B-NB	-2.51	108.28	110.53
19	a	810	CLA	CHB-C4A-NA	2.51	128.03	124.40
21	a	845	BCR	C15-C16-C17	-2.51	118.38	123.52
19	a	829	CLA	CHB-C4A-NA	2.51	128.02	124.40
21	b	3046	BCR	C24-C23-C22	-2.51	122.52	126.23
19	a	828	CLA	C1-C2-C3	-2.51	122.08	126.20
28	b	3053	ZEX	C12-C13-C14	2.51	122.96	119.01
21	A	406	BCR	C33-C5-C6	-2.51	121.75	124.48
19	a	823	CLA	CHB-C4A-NA	2.50	128.01	124.40
19	a	820	CLA	C3B-C4B-NB	-2.50	108.30	110.53
19	b	3007	CLA	CHB-C4A-NA	2.50	128.01	124.40
19	a	841	CLA	CHB-C4A-NA	2.50	128.01	124.40
28	b	3053	ZEX	C40-C33-C34	-2.50	118.77	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	836	CLA	C1-C2-C3	-2.50	122.11	126.20
19	b	3013	CLA	CHB-C4A-NA	2.50	128.00	124.40
19	a	815	CLA	C3B-C4B-NB	-2.50	108.30	110.53
23	a	851	LMG	C38-C37-C36	-2.49	101.78	114.37
19	b	3004	CLA	CHB-C4A-NA	2.49	127.99	124.40
19	b	3012	CLA	C1-C2-C3	-2.49	122.74	126.76
19	a	825	CLA	CHB-C4A-NA	2.49	127.99	124.40
19	b	3006	CLA	C1-C2-C3	-2.49	122.12	126.20
22	a	854	LHG	C11-C10-C9	-2.49	101.80	114.37
21	b	3048	BCR	C15-C16-C17	-2.49	118.43	123.52
19	a	804	CLA	CHB-C4A-NA	2.48	127.98	124.40
19	b	3032	CLA	CHB-C4A-NA	2.48	127.98	124.40
19	a	837	CLA	C1-C2-C3	-2.48	122.13	126.20
19	a	805	CLA	CHB-C4A-NA	2.48	127.98	124.40
19	a	814	CLA	CHB-C4A-NA	2.48	127.98	124.40
21	j	101	BCR	C27-C26-C25	2.48	126.06	122.70
19	a	823	CLA	C3B-C4B-NB	-2.48	108.32	110.53
21	A	406	BCR	C24-C23-C22	-2.48	122.57	126.23
19	b	3005	CLA	CHB-C4A-NA	2.48	127.98	124.40
28	f	205	ZEX	C20-C13-C14	-2.48	118.80	122.82
18	a	801	CL0	C4C-CHD-C1D	2.48	124.93	116.07
19	b	3039	CLA	CHB-C4A-NA	2.48	127.97	124.40
21	a	848	BCR	C15-C14-C13	-2.48	123.80	127.28
19	a	816	CLA	CHB-C4A-NA	2.48	127.97	124.40
21	l	1504	BCR	C15-C14-C13	-2.47	123.81	127.28
19	a	807	CLA	CHB-C4A-NA	2.47	127.97	124.40
19	A	402	CLA	CHB-C4A-NA	2.47	127.97	124.40
19	a	817	CLA	CHB-C4A-NA	2.47	127.97	124.40
19	a	814	CLA	O2D-CGD-CBD	2.47	115.55	111.23
19	b	3014	CLA	C1-C2-C3	-2.47	122.15	126.20
19	b	3040	CLA	C3B-C4B-NB	-2.47	108.33	110.53
19	a	819	CLA	CHB-C4A-NA	2.47	127.96	124.40
26	m	101	ECH	C16-C15-C14	2.47	128.56	123.52
19	b	3037	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
19	a	808	CLA	CHB-C4A-NA	2.46	127.95	124.40
19	b	3013	CLA	C1-C2-C3	-2.46	122.16	126.20
19	D	403	CLA	C3B-C4B-NB	-2.46	108.33	110.53
21	k	4001	BCR	C33-C5-C6	-2.46	121.80	124.48
19	a	834	CLA	C3B-C4B-NB	-2.46	108.33	110.53
19	b	3031	CLA	C3B-C4B-NB	-2.46	108.33	110.53
19	b	3037	CLA	C3B-C4B-NB	-2.46	108.34	110.53
21	k	4004	BCR	C15-C14-C13	-2.46	123.83	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	811	CLA	C3B-C4B-NB	-2.45	108.34	110.53
19	b	3027	CLA	CHB-C4A-NA	2.45	127.94	124.40
19	a	858	CLA	CHB-C4A-NA	2.45	127.93	124.40
19	A	402	CLA	C3B-C4B-NB	-2.45	108.34	110.53
19	a	834	CLA	C1-C2-C3	-2.44	122.20	126.20
23	a	853	LMG	O1-C7-C8	-2.44	104.89	110.82
19	b	3023	CLA	CHB-C4A-NA	2.44	127.92	124.40
19	a	813	CLA	CHB-C4A-NA	2.44	127.92	124.40
19	b	3034	CLA	CHB-C4A-NA	2.44	127.92	124.40
21	b	3048	BCR	C15-C14-C13	-2.44	123.86	127.28
19	a	833	CLA	CHB-C4A-NA	2.44	127.91	124.40
24	a	857	45D	C40-C36-C38	-2.43	118.87	122.82
19	b	3022	CLA	CHB-C4A-NA	2.43	127.91	124.40
21	j	101	BCR	C24-C23-C22	-2.43	122.63	126.23
19	b	3029	CLA	O2D-CGD-CBD	2.43	115.48	111.23
19	a	840	CLA	O2D-CGD-CBD	2.43	115.48	111.23
19	b	3036	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
19	a	822	CLA	CHB-C4A-NA	2.43	127.91	124.40
21	l	1504	BCR	C11-C10-C9	-2.43	123.87	127.28
21	A	406	BCR	C15-C14-C13	-2.43	123.87	127.28
22	f	206	LHG	C11-C10-C9	-2.43	102.09	114.37
23	b	3051	LMG	C40-C39-C38	-2.43	102.11	114.37
21	l	1504	BCR	C28-C27-C26	-2.42	109.73	114.06
19	a	856	CLA	CHB-C4A-NA	2.42	127.89	124.40
19	b	3025	CLA	CHB-C4A-NA	2.42	127.89	124.40
19	b	3036	CLA	CHB-C4A-NA	2.42	127.89	124.40
21	b	3048	BCR	C27-C26-C25	2.42	125.97	122.70
22	a	850	LHG	C20-C19-C18	-2.42	102.15	114.37
19	b	3014	CLA	CHB-C4A-NA	2.42	127.89	124.40
19	b	3026	CLA	CHB-C4A-NA	2.41	127.89	124.40
19	b	3041	CLA	CHB-C4A-NA	2.41	127.88	124.40
23	b	3049	LMG	O1-C7-C8	-2.41	104.95	110.82
19	a	810	CLA	C1-C2-C3	-2.41	122.25	126.20
19	b	3028	CLA	C3B-C4B-NB	-2.41	108.38	110.53
19	b	3033	CLA	O2D-CGD-CBD	2.41	115.44	111.23
29	f	207	LMT	C3'-C4'-C5'	-2.41	105.59	110.93
19	a	828	CLA	CHB-C4A-NA	2.41	127.87	124.40
19	a	809	CLA	C1-C2-C3	-2.41	122.25	126.20
19	b	3024	CLA	CHB-C4A-NA	2.40	127.87	124.40
19	A	405	CLA	C3B-C4B-NB	-2.40	108.39	110.53
19	D	403	CLA	CHB-C4A-NA	2.40	127.87	124.40
23	a	853	LMG	O2-C2-C1	-2.40	104.35	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	3008	CLA	CHB-C4A-NA	2.39	127.86	124.40
19	k	4003	CLA	C3B-C4B-NB	-2.39	108.39	110.53
21	b	3046	BCR	C27-C26-C25	2.39	125.94	122.70
19	b	3018	CLA	CHB-C4A-NA	2.39	127.85	124.40
21	A	406	BCR	C11-C10-C9	-2.39	123.92	127.28
19	a	834	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
21	l	1504	BCR	C33-C5-C6	-2.39	121.88	124.48
19	a	840	CLA	C3B-C4B-NB	-2.39	108.40	110.53
19	a	837	CLA	CHB-C4A-NA	2.39	127.84	124.40
19	a	827	CLA	CHB-C4A-NA	2.39	127.84	124.40
22	f	206	LHG	C20-C19-C18	-2.38	102.32	114.37
19	b	3021	CLA	CMB-C2B-C1B	-2.38	121.79	125.42
26	m	101	ECH	C12-C13-C14	2.38	122.75	119.01
19	b	3016	CLA	CHB-C4A-NA	2.38	127.83	124.40
19	b	3028	CLA	CHB-C4A-NA	2.38	127.83	124.40
19	j	103	CLA	C3B-C4B-NB	-2.37	108.41	110.53
19	a	820	CLA	CHB-C4A-NA	2.37	127.83	124.40
19	b	3025	CLA	C3B-C4B-NB	-2.37	108.41	110.53
19	b	3020	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
23	b	3051	LMG	O6-C1-O1	-2.37	104.45	110.04
23	b	3051	LMG	C38-C37-C36	-2.37	102.39	114.37
18	a	801	CL0	CMB-C2B-C3B	2.37	129.42	124.68
21	a	845	BCR	C33-C5-C6	-2.37	121.90	124.48
19	b	3027	CLA	C3B-C4B-NB	-2.37	108.42	110.53
19	a	839	CLA	CHB-C4A-NA	2.37	127.81	124.40
19	b	3016	CLA	O2A-CGA-O1A	-2.36	117.71	123.63
21	a	847	BCR	C33-C5-C6	-2.36	121.91	124.48
19	b	3031	CLA	C1-C2-C3	-2.36	122.94	126.76
23	b	3049	LMG	C40-C39-C38	-2.36	102.44	114.37
19	a	805	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
19	b	3031	CLA	CHB-C4A-NA	2.36	127.80	124.40
19	a	814	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
19	a	812	CLA	CHB-C4A-NA	2.35	127.80	124.40
21	b	3047	BCR	C15-C16-C17	-2.35	118.71	123.52
19	a	833	CLA	C1-C2-C3	-2.35	122.35	126.20
19	f	201	CLA	CHB-C4A-NA	2.35	127.79	124.40
19	a	838	CLA	CHB-C4A-NA	2.35	127.79	124.40
19	a	855	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
19	f	204	CLA	C1-C2-C3	-2.35	122.97	126.76
19	f	203	CLA	C3B-C4B-NB	-2.34	108.44	110.53
19	A	405	CLA	CHB-C4A-NA	2.34	127.78	124.40
22	a	852	LHG	C20-C19-C18	-2.34	102.53	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	3012	CLA	CHB-C4A-NA	2.34	127.78	124.40
19	a	802	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
19	b	3010	CLA	CHB-C4A-NA	2.34	127.77	124.40
22	a	850	LHG	C11-C10-C9	-2.33	102.58	114.37
19	a	830	CLA	CHB-C4A-NA	2.33	127.77	124.40
19	b	3033	CLA	CHB-C4A-NA	2.33	127.76	124.40
21	b	3043	BCR	C15-C14-C13	-2.33	124.01	127.28
19	a	839	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
19	b	3018	CLA	C3B-C4B-NB	-2.33	108.45	110.53
19	b	3014	CLA	CMB-C2B-C1B	-2.33	121.88	125.42
21	b	3048	BCR	C33-C5-C6	-2.32	121.95	124.48
19	a	803	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
23	b	3049	LMG	O1-C1-C2	-2.32	104.76	108.27
19	b	3021	CLA	CHB-C4A-NA	2.31	127.73	124.40
21	b	3044	BCR	C15-C14-C13	-2.31	124.04	127.28
28	b	3053	ZEX	C32-C33-C34	2.31	122.64	119.01
22	a	854	LHG	C20-C19-C18	-2.31	102.71	114.37
21	k	4001	BCR	C27-C26-C25	2.31	125.82	122.70
21	A	406	BCR	C15-C16-C17	-2.31	118.80	123.52
19	f	203	CLA	CHB-C4A-NA	2.30	127.72	124.40
21	a	846	BCR	C7-C8-C9	-2.30	122.83	126.23
24	a	857	45D	C39-C35-C37	-2.30	119.09	122.82
21	l	1504	BCR	C29-C30-C25	2.30	113.78	110.44
19	a	823	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
21	i	101	BCR	C33-C5-C6	-2.29	121.98	124.48
19	a	815	CLA	O2D-CGD-CBD	2.29	115.24	111.23
23	b	3049	LMG	C38-C37-C36	-2.29	102.78	114.37
19	b	3009	CLA	CHB-C4A-NA	2.29	127.71	124.40
23	b	3051	LMG	O3-C3-C2	-2.29	104.98	110.38
19	k	4003	CLA	CHB-C4A-NA	2.29	127.70	124.40
24	a	857	45D	C24-C26-C30	2.29	122.61	119.01
21	a	846	BCR	C11-C10-C9	-2.29	124.07	127.28
19	a	838	CLA	CMB-C2B-C1B	-2.29	121.94	125.42
19	b	3018	CLA	CMB-C2B-C1B	-2.29	121.94	125.42
19	a	832	CLA	CHB-C4A-NA	2.29	127.70	124.40
21	f	202	BCR	C24-C23-C22	-2.28	122.86	126.23
19	a	826	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
19	b	3034	CLA	C1-C2-C3	-2.28	122.46	126.20
19	a	835	CLA	C1-C2-C3	-2.28	122.46	126.20
19	b	3007	CLA	C3B-C4B-NB	-2.27	108.50	110.53
23	a	851	LMG	O3-C3-C2	-2.27	105.03	110.38
22	f	206	LHG	C18-C17-C16	-2.27	102.89	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	845	BCR	C15-C14-C13	-2.27	124.10	127.28
22	b	3050	LHG	C27-C26-C25	-2.27	102.90	114.37
22	a	852	LHG	C27-C26-C25	-2.27	102.90	114.37
19	a	811	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
23	b	3049	LMG	O2-C2-C1	-2.27	104.67	110.08
19	f	203	CLA	CMB-C2B-C1B	-2.27	121.97	125.42
19	a	835	CLA	O2D-CGD-CBD	2.26	115.19	111.23
19	b	3024	CLA	C1-C2-C3	-2.26	122.49	126.20
21	b	3044	BCR	C2-C1-C6	2.26	113.73	110.44
19	b	3038	CLA	C1-C2-C3	-2.26	123.10	126.76
19	a	808	CLA	CMB-C2B-C3B	2.26	131.87	126.55
19	a	810	CLA	C3B-C4B-NB	-2.26	108.51	110.53
23	b	3051	LMG	C42-C41-C40	-2.26	102.94	114.37
19	b	3005	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
19	a	815	CLA	CHB-C4A-NA	2.26	127.66	124.40
19	b	3017	CLA	C1-C2-C3	-2.26	122.50	126.20
21	a	849	BCR	C11-C10-C9	-2.25	124.12	127.28
19	b	3039	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
21	b	3044	BCR	C28-C27-C26	-2.25	110.04	114.06
21	b	3047	BCR	C24-C23-C22	-2.25	122.91	126.23
28	f	205	ZEX	C12-C13-C14	2.24	122.54	119.01
21	a	847	BCR	C24-C23-C22	-2.24	122.92	126.23
21	b	3046	BCR	C33-C5-C6	-2.24	122.04	124.48
23	b	3051	LMG	O7-C10-O9	-2.24	118.47	123.70
21	a	849	BCR	C33-C5-C6	-2.24	122.04	124.48
19	b	3041	CLA	CMB-C2B-C1B	-2.24	122.02	125.42
21	b	3047	BCR	C10-C11-C12	-2.24	116.72	123.20
26	m	101	ECH	C29-C30-C25	2.24	113.69	110.44
19	b	3021	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
19	b	3036	CLA	CMB-C2B-C3B	2.23	131.80	126.55
19	l	1502	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
19	a	830	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
19	b	3030	CLA	CHB-C4A-NA	2.23	127.62	124.40
21	f	202	BCR	C8-C7-C6	-2.23	121.05	127.00
21	f	202	BCR	C33-C5-C6	-2.23	122.05	124.48
31	D	402	PHO	O2A-CGA-O1A	-2.23	118.06	123.63
19	b	3004	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
22	a	854	LHG	C27-C26-C25	-2.22	103.16	114.37
18	a	801	CL0	C3C-C4C-NC	-2.22	109.23	114.65
19	b	3037	CLA	CHB-C4A-NA	2.21	127.60	124.40
19	a	829	CLA	C3B-C4B-NB	-2.21	108.55	110.53
22	a	852	LHG	C18-C17-C16	-2.21	103.18	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	f	206	LHG	C27-C26-C25	-2.21	103.18	114.37
19	a	837	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
19	b	3007	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
19	j	102	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
19	b	3034	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
23	b	3049	LMG	O3-C3-C2	-2.20	105.18	110.38
19	b	3021	CLA	C1-C2-C3	-2.20	122.59	126.20
19	a	826	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
26	m	101	ECH	C21-C20-C19	2.20	129.58	123.20
19	D	403	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
19	a	804	CLA	C1-C2-C3	-2.20	122.60	126.20
19	b	3007	CLA	O2D-CGD-CBD	2.20	115.07	111.23
19	b	3003	CLA	CMB-C2B-C1B	-2.20	122.08	125.42
19	a	807	CLA	CMB-C2B-C1B	-2.20	122.08	125.42
19	a	810	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
21	b	3046	BCR	C11-C10-C9	-2.19	124.20	127.28
21	j	101	BCR	C11-C10-C9	-2.19	124.20	127.28
19	b	3038	CLA	CHB-C4A-NA	2.19	127.56	124.40
23	a	851	LMG	C40-C39-C38	-2.19	103.30	114.37
21	i	101	BCR	C15-C14-C13	-2.19	124.21	127.28
19	a	802	CLA	CMB-C2B-C3B	2.19	131.69	126.55
22	a	850	LHG	C27-C26-C25	-2.19	103.32	114.37
31	A	404	PHO	O2A-CGA-O1A	-2.18	118.16	123.63
19	a	809	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
19	a	819	CLA	CAA-CBA-CGA	-2.18	107.01	113.21
19	b	3025	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
19	b	3036	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
19	a	802	CLA	CHB-C4A-NA	2.18	127.55	124.40
19	A	405	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
23	b	3049	LMG	C42-C41-C40	-2.18	103.36	114.37
19	a	838	CLA	O2A-CGA-O1A	-2.18	118.19	123.63
21	b	3047	BCR	C15-C14-C13	-2.18	124.23	127.28
19	a	836	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
21	a	846	BCR	C15-C16-C17	-2.17	119.07	123.52
31	D	402	PHO	CMB-C2B-C3B	2.17	129.02	124.68
19	b	3011	CLA	C1-C2-C3	-2.17	122.64	126.20
24	a	857	45D	C33-C35-C37	2.17	122.42	119.01
19	a	822	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
21	b	3043	BCR	C7-C8-C9	-2.16	123.03	126.23
21	a	846	BCR	C15-C14-C13	-2.16	124.25	127.28
21	k	4001	BCR	C11-C10-C9	-2.16	124.25	127.28
19	l	1502	CLA	C1-C2-C3	-2.16	122.66	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	a	804	CLA	O2D-CGD-CBD	2.16	115.01	111.23
19	b	3021	CLA	CMB-C2B-C3B	2.16	131.63	126.55
19	a	829	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
19	a	838	CLA	C1-C2-C3	-2.16	122.66	126.20
23	a	853	LMG	O3-C3-C2	-2.15	105.30	110.38
19	a	812	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
19	a	831	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
19	b	3003	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
22	a	850	LHG	C18-C17-C16	-2.15	103.52	114.37
19	a	806	CLA	CMB-C2B-C1B	-2.14	122.15	125.42
19	a	822	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
19	a	843	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
19	f	201	CLA	C1-C2-C3	-2.14	122.69	126.20
19	l	1501	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
19	b	3013	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
19	a	827	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
23	b	3051	LMG	O2-C2-C1	-2.14	104.98	110.08
19	a	815	CLA	C1-C2-C3	-2.14	122.70	126.20
19	j	103	CLA	CHB-C4A-NA	2.13	127.48	124.40
19	b	3008	CLA	O1D-CGD-CBD	2.13	128.73	124.52
19	a	825	CLA	C1-C2-C3	-2.13	122.70	126.20
19	a	820	CLA	CMB-C2B-C3B	2.13	131.56	126.55
19	a	807	CLA	C1-C2-C3	-2.13	122.71	126.20
23	a	851	LMG	O1-C7-C8	-2.13	105.65	110.82
19	f	204	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
19	a	841	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
19	b	3038	CLA	C3B-C4B-NB	-2.12	108.64	110.53
19	a	812	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
19	b	3015	CLA	CAC-C3C-C4C	2.12	127.55	124.79
19	b	3023	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
19	b	3012	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
19	b	3031	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
19	b	3038	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
21	k	4004	BCR	C7-C8-C9	-2.12	123.10	126.23
19	b	3026	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
19	j	102	CLA	C1-C2-C3	-2.11	122.73	126.20
26	m	101	ECH	C28-C29-C30	-2.11	110.12	113.21
19	b	3031	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
19	b	3037	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
19	a	808	CLA	C1-C2-C3	-2.11	122.74	126.20
21	f	202	BCR	C16-C15-C14	-2.11	119.21	123.52
19	a	829	CLA	CMB-C2B-C3B	2.11	131.51	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	3045	ECH	C21-C20-C19	2.11	129.30	123.20
19	b	3036	CLA	C1-C2-C3	-2.10	122.75	126.20
19	j	103	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
24	a	857	45D	C34-C36-C38	2.10	122.32	119.01
21	l	1504	BCR	C24-C23-C22	-2.10	123.12	126.23
19	a	834	CLA	CMB-C2B-C3B	2.10	131.49	126.55
19	b	3026	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
19	b	3029	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
19	a	855	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
19	b	3009	CLA	CAA-CBA-CGA	-2.10	107.26	113.21
26	m	101	ECH	C1-C6-C5	-2.09	119.77	122.64
23	a	851	LMG	O2-C2-C1	-2.09	105.09	110.08
19	a	814	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
23	a	851	LMG	C42-C41-C40	-2.09	103.79	114.37
19	a	814	CLA	CMB-C2B-C3B	2.09	131.47	126.55
24	a	857	45D	C10-C06-C04	-2.09	110.15	113.21
19	b	3018	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
21	b	3044	BCR	C27-C26-C25	2.09	125.53	122.70
27	b	3052	EQ3	C28-C29-C30	-2.09	110.16	113.21
19	b	3035	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
19	b	3006	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
21	i	101	BCR	C8-C7-C6	-2.08	121.44	127.00
19	D	403	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
19	b	3034	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
26	m	101	ECH	C34-C9-C8	2.08	121.26	118.09
26	b	3045	ECH	C4-C5-C6	-2.07	119.90	122.70
18	a	801	CL0	O2A-CGA-O1A	-2.07	118.45	123.63
19	b	3002	CLA	CHB-C4A-NA	2.07	127.39	124.40
19	b	3018	CLA	CMB-C2B-C3B	2.07	131.41	126.55
19	b	3008	CLA	C1-C2-C3	-2.07	122.81	126.20
19	a	834	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
21	b	3048	BCR	C1-C6-C5	-2.06	119.81	122.64
26	b	3045	ECH	C34-C9-C8	2.06	121.24	118.09
19	b	3040	CLA	C1-C2-C3	-2.06	122.82	126.20
21	a	847	BCR	C7-C8-C9	-2.06	123.19	126.23
22	a	854	LHG	C18-C17-C16	-2.06	103.96	114.37
21	j	104	BCR	C38-C26-C25	-2.06	122.24	124.48
19	b	3014	CLA	CMB-C2B-C3B	2.06	131.39	126.55
19	b	3024	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
21	a	848	BCR	C8-C7-C6	-2.05	121.52	127.00
19	b	3033	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
21	j	104	BCR	C8-C7-C6	-2.05	121.52	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	b	3017	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
19	a	821	CLA	CAA-CBA-CGA	-2.05	107.40	113.21
21	a	848	BCR	C38-C26-C25	-2.05	122.25	124.48
19	f	203	CLA	CMB-C2B-C3B	2.05	131.36	126.55
19	b	3023	CLA	C1-C2-C3	-2.04	122.85	126.20
19	k	4003	CLA	CAC-C3C-C4C	2.04	127.45	124.79
19	a	820	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
19	a	823	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
32	F	101	HEM	C4D-ND-C1D	2.04	107.62	105.21
21	a	845	BCR	C11-C10-C9	-2.04	124.42	127.28
19	a	826	CLA	CMB-C2B-C3B	2.04	131.35	126.55
19	b	3025	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
21	a	848	BCR	C24-C23-C22	-2.04	123.22	126.23
23	b	3051	LMG	O1-C7-C8	-2.04	105.86	110.82
21	b	3047	BCR	C8-C7-C6	-2.04	121.56	127.00
19	b	3019	CLA	C1-C2-C3	-2.04	122.86	126.20
19	b	3004	CLA	C1-C2-C3	-2.04	122.86	126.20
21	j	101	BCR	C8-C7-C6	-2.04	121.56	127.00
19	a	828	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
19	f	204	CLA	O2D-CGD-CBD	2.04	114.79	111.23
19	a	858	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
19	a	843	CLA	C1-C2-C3	-2.03	122.87	126.20
19	a	855	CLA	C1-C2-C3	-2.03	122.87	126.20
19	b	3027	CLA	C1-C2-C3	-2.03	122.87	126.20
19	b	3005	CLA	CMB-C2B-C3B	2.03	131.32	126.55
19	a	804	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
19	b	3009	CLA	C1-C2-C3	-2.02	122.88	126.20
19	a	808	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
19	b	3015	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
19	b	3005	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
21	l	1504	BCR	C7-C8-C9	-2.02	123.24	126.23
19	a	838	CLA	CMB-C2B-C3B	2.02	131.31	126.55
19	b	3030	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
28	f	205	ZEX	C28-C29-C30	2.02	122.19	119.01
19	a	805	CLA	O2D-CGD-CBD	2.02	114.76	111.23
19	a	818	CLA	C1-C2-C3	-2.02	122.89	126.20
19	b	3010	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
19	A	402	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
19	b	3019	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
29	f	207	LMT	C3B-C4B-C5B	-2.02	106.58	110.23
19	a	855	CLA	CMB-C2B-C3B	2.02	131.29	126.55
19	b	3003	CLA	CMB-C2B-C3B	2.02	131.29	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	l	1503	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
21	A	406	BCR	C8-C7-C6	-2.02	121.61	127.00
19	b	3041	CLA	CMB-C2B-C3B	2.01	131.29	126.55
23	a	851	LMG	O7-C10-O9	-2.01	119.00	123.70
27	b	3052	EQ3	C10-C11-C12	2.01	129.02	123.20
19	a	839	CLA	O2D-CGD-CBD	2.01	114.74	111.23
21	k	4004	BCR	C33-C5-C6	-2.01	122.29	124.48
19	a	812	CLA	C1-C2-C3	-2.01	122.91	126.20
19	a	831	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
19	b	3024	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
31	D	402	PHO	C1A-C2A-C3A	-2.00	100.93	102.84
21	b	3048	BCR	C24-C23-C22	-2.00	123.27	126.23
22	b	3050	LHG	C5-O7-C7	-2.00	113.01	117.80

All (102) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
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	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	855	CLA	ND
19	a	856	CLA	ND
19	a	858	CLA	ND
19	b	3002	CLA	ND
19	b	3003	CLA	ND
19	b	3004	CLA	ND
19	b	3005	CLA	ND
19	b	3006	CLA	ND
19	b	3007	CLA	ND
19	b	3008	CLA	ND
19	b	3009	CLA	ND
19	b	3010	CLA	ND
19	b	3011	CLA	ND
19	b	3012	CLA	ND
19	b	3013	CLA	ND
19	b	3014	CLA	ND
19	b	3015	CLA	ND
19	b	3016	CLA	ND
19	b	3017	CLA	ND
19	b	3018	CLA	ND
19	b	3019	CLA	ND
19	b	3020	CLA	ND
19	b	3021	CLA	ND
19	b	3022	CLA	ND

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Mol	Chain	Res	Type	Atom
19	b	3023	CLA	ND
19	b	3024	CLA	ND
19	b	3025	CLA	ND
19	b	3026	CLA	ND
19	b	3027	CLA	ND
19	b	3028	CLA	ND
19	b	3029	CLA	ND
19	b	3030	CLA	ND
19	b	3031	CLA	ND
19	b	3032	CLA	ND
19	b	3033	CLA	ND
19	b	3034	CLA	ND
19	b	3035	CLA	ND
19	b	3036	CLA	ND
19	b	3037	CLA	ND
19	b	3038	CLA	ND
19	b	3039	CLA	ND
19	b	3040	CLA	ND
19	b	3041	CLA	ND
19	f	201	CLA	ND
19	f	203	CLA	ND
19	f	204	CLA	ND
19	j	102	CLA	ND
19	j	103	CLA	ND
19	k	4002	CLA	ND
19	k	4003	CLA	ND
19	l	1501	CLA	ND
19	l	1502	CLA	ND
19	l	1503	CLA	ND
19	A	402	CLA	ND
19	A	403	CLA	ND
19	A	405	CLA	ND
19	D	401	CLA	ND
19	D	403	CLA	ND
19	D	404	CLA	ND

All (1561) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	a	802	CLA	CBD-CGD-O2D-CED
19	a	803	CLA	CBA-CGA-O2A-C1
19	a	803	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	a	805	CLA	C1A-C2A-CAA-CBA
19	a	805	CLA	C3A-C2A-CAA-CBA
19	a	806	CLA	C3A-C2A-CAA-CBA
19	a	808	CLA	C1A-C2A-CAA-CBA
19	a	808	CLA	C3A-C2A-CAA-CBA
19	a	809	CLA	C3A-C2A-CAA-CBA
19	a	811	CLA	CAD-CBD-CGD-O1D
19	a	811	CLA	CAD-CBD-CGD-O2D
19	a	813	CLA	C1A-C2A-CAA-CBA
19	a	813	CLA	C3A-C2A-CAA-CBA
19	a	815	CLA	C3A-C2A-CAA-CBA
19	a	817	CLA	C1A-C2A-CAA-CBA
19	a	817	CLA	C3A-C2A-CAA-CBA
19	a	817	CLA	CBA-CGA-O2A-C1
19	a	818	CLA	C1A-C2A-CAA-CBA
19	a	819	CLA	C1A-C2A-CAA-CBA
19	a	819	CLA	C3A-C2A-CAA-CBA
19	a	819	CLA	C6-C7-C8-C9
19	a	819	CLA	C11-C10-C8-C9
19	a	820	CLA	C1A-C2A-CAA-CBA
19	a	820	CLA	C3A-C2A-CAA-CBA
19	a	821	CLA	C1A-C2A-CAA-CBA
19	a	821	CLA	C3A-C2A-CAA-CBA
19	a	821	CLA	C2-C1-O2A-CGA
19	a	821	CLA	CBD-CGD-O2D-CED
19	a	823	CLA	C1A-C2A-CAA-CBA
19	a	823	CLA	C3A-C2A-CAA-CBA
19	a	823	CLA	CBD-CGD-O2D-CED
19	a	824	CLA	C1A-C2A-CAA-CBA
19	a	827	CLA	C1A-C2A-CAA-CBA
19	a	827	CLA	C3A-C2A-CAA-CBA
19	a	828	CLA	C1A-C2A-CAA-CBA
19	a	828	CLA	C3A-C2A-CAA-CBA
19	a	829	CLA	C1A-C2A-CAA-CBA
19	a	832	CLA	C3A-C2A-CAA-CBA
19	a	833	CLA	C1A-C2A-CAA-CBA
19	a	833	CLA	C3A-C2A-CAA-CBA
19	a	838	CLA	C1A-C2A-CAA-CBA
19	a	839	CLA	C1A-C2A-CAA-CBA
19	a	839	CLA	C3A-C2A-CAA-CBA
19	a	841	CLA	C1A-C2A-CAA-CBA
19	a	841	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	a	842	CLA	C1A-C2A-CAA-CBA
19	a	856	CLA	C1A-C2A-CAA-CBA
19	a	856	CLA	C3A-C2A-CAA-CBA
19	b	3002	CLA	CBD-CGD-O2D-CED
19	b	3003	CLA	CBD-CGD-O2D-CED
19	b	3003	CLA	C2-C3-C5-C6
19	b	3003	CLA	C4-C3-C5-C6
19	b	3004	CLA	C1A-C2A-CAA-CBA
19	b	3005	CLA	O1A-CGA-O2A-C1
19	b	3005	CLA	CAD-CBD-CGD-O1D
19	b	3005	CLA	CAD-CBD-CGD-O2D
19	b	3007	CLA	C1A-C2A-CAA-CBA
19	b	3007	CLA	C3A-C2A-CAA-CBA
19	b	3011	CLA	C1A-C2A-CAA-CBA
19	b	3011	CLA	C3A-C2A-CAA-CBA
19	b	3011	CLA	C2B-C3B-CAB-CBB
19	b	3011	CLA	C4B-C3B-CAB-CBB
19	b	3013	CLA	CHA-CBD-CGD-O2D
19	b	3014	CLA	CAD-CBD-CGD-O2D
19	b	3014	CLA	C4-C3-C5-C6
19	b	3015	CLA	C1A-C2A-CAA-CBA
19	b	3016	CLA	C1A-C2A-CAA-CBA
19	b	3018	CLA	C1A-C2A-CAA-CBA
19	b	3018	CLA	C3A-C2A-CAA-CBA
19	b	3019	CLA	C2B-C3B-CAB-CBB
19	b	3019	CLA	C4B-C3B-CAB-CBB
19	b	3020	CLA	C1A-C2A-CAA-CBA
19	b	3020	CLA	C3A-C2A-CAA-CBA
19	b	3021	CLA	C1A-C2A-CAA-CBA
19	b	3021	CLA	C3A-C2A-CAA-CBA
19	b	3022	CLA	CBA-CGA-O2A-C1
19	b	3022	CLA	O1A-CGA-O2A-C1
19	b	3024	CLA	C1A-C2A-CAA-CBA
19	b	3024	CLA	C3A-C2A-CAA-CBA
19	b	3025	CLA	C1A-C2A-CAA-CBA
19	b	3025	CLA	C3A-C2A-CAA-CBA
19	b	3026	CLA	C1A-C2A-CAA-CBA
19	b	3026	CLA	C3A-C2A-CAA-CBA
19	b	3027	CLA	C1A-C2A-CAA-CBA
19	b	3027	CLA	C3A-C2A-CAA-CBA
19	b	3029	CLA	C4-C3-C5-C6
19	b	3030	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	b	3030	CLA	C3A-C2A-CAA-CBA
19	b	3030	CLA	CBD-CGD-O2D-CED
19	b	3033	CLA	C3A-C2A-CAA-CBA
19	b	3033	CLA	CBA-CGA-O2A-C1
19	b	3033	CLA	CHA-CBD-CGD-O1D
19	b	3033	CLA	CHA-CBD-CGD-O2D
19	b	3034	CLA	C1A-C2A-CAA-CBA
19	b	3034	CLA	C3A-C2A-CAA-CBA
19	b	3035	CLA	C1A-C2A-CAA-CBA
19	b	3035	CLA	C3A-C2A-CAA-CBA
19	b	3035	CLA	C2B-C3B-CAB-CBB
19	b	3035	CLA	C4B-C3B-CAB-CBB
19	b	3035	CLA	CBD-CGD-O2D-CED
19	b	3036	CLA	CAD-CBD-CGD-O1D
19	b	3036	CLA	CAD-CBD-CGD-O2D
19	b	3037	CLA	C1A-C2A-CAA-CBA
19	b	3037	CLA	C3A-C2A-CAA-CBA
19	b	3039	CLA	C1A-C2A-CAA-CBA
19	b	3041	CLA	CAD-CBD-CGD-O1D
19	b	3041	CLA	CAD-CBD-CGD-O2D
19	j	102	CLA	C1A-C2A-CAA-CBA
19	j	102	CLA	CBD-CGD-O2D-CED
19	k	4002	CLA	C3A-C2A-CAA-CBA
19	k	4003	CLA	CBD-CGD-O2D-CED
19	l	1501	CLA	C1A-C2A-CAA-CBA
19	l	1501	CLA	C3A-C2A-CAA-CBA
19	l	1503	CLA	CBD-CGD-O2D-CED
19	A	403	CLA	C1A-C2A-CAA-CBA
19	A	403	CLA	C3A-C2A-CAA-CBA
19	A	403	CLA	CBA-CGA-O2A-C1
19	A	405	CLA	C1A-C2A-CAA-CBA
19	D	401	CLA	C1A-C2A-CAA-CBA
19	D	401	CLA	C4B-C3B-CAB-CBB
19	D	403	CLA	C3A-C2A-CAA-CBA
19	D	404	CLA	CBA-CGA-O2A-C1
19	D	404	CLA	O1A-CGA-O2A-C1
21	a	845	BCR	C6-C7-C8-C9
21	a	845	BCR	C9-C10-C11-C12
21	a	845	BCR	C21-C22-C23-C24
21	a	848	BCR	C14-C15-C16-C17
21	a	848	BCR	C21-C22-C23-C24
21	a	849	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	b	3043	BCR	C6-C7-C8-C9
21	b	3043	BCR	C7-C8-C9-C10
21	b	3043	BCR	C22-C23-C24-C25
21	b	3044	BCR	C7-C8-C9-C10
21	b	3044	BCR	C7-C8-C9-C34
21	b	3046	BCR	C22-C23-C24-C25
21	b	3047	BCR	C11-C12-C13-C35
21	b	3048	BCR	C6-C7-C8-C9
21	b	3048	BCR	C16-C17-C18-C19
21	b	3048	BCR	C16-C17-C18-C36
21	b	3048	BCR	C20-C21-C22-C37
21	b	3048	BCR	C21-C22-C23-C24
21	b	3048	BCR	C37-C22-C23-C24
21	b	3048	BCR	C22-C23-C24-C25
21	f	202	BCR	C7-C8-C9-C34
21	f	202	BCR	C11-C12-C13-C35
21	f	202	BCR	C37-C22-C23-C24
21	i	101	BCR	C10-C11-C12-C13
21	i	101	BCR	C21-C22-C23-C24
21	j	101	BCR	C21-C22-C23-C24
21	k	4001	BCR	C7-C8-C9-C10
21	k	4004	BCR	C17-C18-C19-C20
21	k	4004	BCR	C18-C19-C20-C21
21	k	4004	BCR	C22-C23-C24-C25
21	l	1504	BCR	C7-C8-C9-C10
21	l	1504	BCR	C7-C8-C9-C34
21	l	1504	BCR	C21-C22-C23-C24
21	l	1504	BCR	C23-C24-C25-C26
21	A	406	BCR	C6-C7-C8-C9
21	A	406	BCR	C22-C23-C24-C25
22	a	850	LHG	O1-C1-C2-C3
22	a	850	LHG	C3-O3-P-O4
22	a	850	LHG	C3-O3-P-O6
22	a	850	LHG	O10-C23-O8-C6
22	a	852	LHG	C3-O3-P-O5
22	a	852	LHG	O7-C5-C6-O8
22	a	854	LHG	C4-O6-P-O3
22	a	854	LHG	C4-O6-P-O5
22	a	854	LHG	O9-C7-O7-C5
22	a	854	LHG	C8-C7-O7-C5
22	b	3050	LHG	C3-O3-P-O4
22	b	3050	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
22	f	206	LHG	O1-C1-C2-O2
22	f	206	LHG	C3-O3-P-O4
22	f	206	LHG	C3-O3-P-O6
22	f	206	LHG	C4-O6-P-O4
22	f	206	LHG	O6-C4-C5-O7
23	a	851	LMG	C2-C1-O1-C7
23	a	851	LMG	O6-C1-O1-C7
23	a	851	LMG	O9-C10-O7-C8
23	b	3051	LMG	C2-C1-O1-C7
23	b	3051	LMG	O6-C1-O1-C7
26	b	3045	ECH	C5-C6-C7-C8
26	b	3045	ECH	C22-C23-C24-C25
29	f	207	LMT	O5'-C1'-O1'-C1
31	A	404	PHO	O1A-CGA-O2A-C1
31	A	404	PHO	CBD-CGD-O2D-CED
19	a	811	CLA	O1D-CGD-O2D-CED
19	a	821	CLA	O1D-CGD-O2D-CED
19	b	3015	CLA	O1D-CGD-O2D-CED
19	b	3020	CLA	O1D-CGD-O2D-CED
19	l	1503	CLA	O1D-CGD-O2D-CED
19	a	802	CLA	O1D-CGD-O2D-CED
19	b	3003	CLA	O1D-CGD-O2D-CED
19	a	811	CLA	CBD-CGD-O2D-CED
19	a	816	CLA	CBD-CGD-O2D-CED
19	b	3009	CLA	CBD-CGD-O2D-CED
19	b	3014	CLA	CBD-CGD-O2D-CED
19	b	3015	CLA	CBD-CGD-O2D-CED
19	b	3020	CLA	CBD-CGD-O2D-CED
19	b	3027	CLA	CBD-CGD-O2D-CED
19	b	3034	CLA	CBD-CGD-O2D-CED
19	b	3036	CLA	CBD-CGD-O2D-CED
19	b	3039	CLA	CBD-CGD-O2D-CED
19	f	201	CLA	CBD-CGD-O2D-CED
19	j	103	CLA	CBD-CGD-O2D-CED
19	A	402	CLA	CBD-CGD-O2D-CED
19	a	835	CLA	O1A-CGA-O2A-C1
19	b	3006	CLA	O1A-CGA-O2A-C1
19	b	3011	CLA	O1A-CGA-O2A-C1
19	b	3021	CLA	O1A-CGA-O2A-C1
19	b	3031	CLA	O1A-CGA-O2A-C1
19	b	3033	CLA	O1A-CGA-O2A-C1
19	b	3034	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	a	817	CLA	O1A-CGA-O2A-C1
19	A	403	CLA	O1A-CGA-O2A-C1
19	b	3030	CLA	O1D-CGD-O2D-CED
19	k	4003	CLA	O1D-CGD-O2D-CED
19	f	201	CLA	O1D-CGD-O2D-CED
19	a	835	CLA	CBA-CGA-O2A-C1
19	b	3012	CLA	CBA-CGA-O2A-C1
22	a	850	LHG	C24-C23-O8-C6
19	a	802	CLA	O1A-CGA-O2A-C1
19	a	813	CLA	O1A-CGA-O2A-C1
19	a	820	CLA	O1A-CGA-O2A-C1
19	a	821	CLA	O1A-CGA-O2A-C1
19	a	838	CLA	O1A-CGA-O2A-C1
19	b	3003	CLA	O1A-CGA-O2A-C1
19	b	3012	CLA	O1A-CGA-O2A-C1
19	b	3024	CLA	O1A-CGA-O2A-C1
19	b	3038	CLA	O1A-CGA-O2A-C1
19	b	3039	CLA	O1A-CGA-O2A-C1
19	l	1501	CLA	O1A-CGA-O2A-C1
19	l	1502	CLA	O1A-CGA-O2A-C1
19	l	1503	CLA	O1A-CGA-O2A-C1
19	A	405	CLA	O1A-CGA-O2A-C1
22	f	206	LHG	O10-C23-O8-C6
23	a	853	LMG	O10-C28-O8-C9
19	a	823	CLA	O1D-CGD-O2D-CED
19	b	3002	CLA	O1D-CGD-O2D-CED
19	j	102	CLA	O1D-CGD-O2D-CED
31	A	404	PHO	O1D-CGD-O2D-CED
19	a	841	CLA	CBD-CGD-O2D-CED
19	a	855	CLA	O1A-CGA-O2A-C1
22	f	206	LHG	O9-C7-O7-C5
19	k	4002	CLA	CBA-CGA-O2A-C1
19	b	3041	CLA	O1A-CGA-O2A-C1
19	k	4002	CLA	O1A-CGA-O2A-C1
19	a	809	CLA	C3-C5-C6-C7
19	a	818	CLA	C3-C5-C6-C7
19	a	824	CLA	C3-C5-C6-C7
19	a	826	CLA	C3-C5-C6-C7
19	a	856	CLA	C3-C5-C6-C7
19	b	3007	CLA	C3-C5-C6-C7
19	b	3013	CLA	C3-C5-C6-C7
19	b	3017	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	b	3033	CLA	C3-C5-C6-C7
19	b	3039	CLA	C3-C5-C6-C7
19	a	802	CLA	CBA-CGA-O2A-C1
19	a	819	CLA	CBA-CGA-O2A-C1
19	a	820	CLA	CBA-CGA-O2A-C1
19	a	825	CLA	CBA-CGA-O2A-C1
19	a	828	CLA	CBA-CGA-O2A-C1
19	a	839	CLA	CBA-CGA-O2A-C1
19	a	856	CLA	CBA-CGA-O2A-C1
19	b	3005	CLA	CBA-CGA-O2A-C1
19	b	3006	CLA	CBA-CGA-O2A-C1
19	b	3011	CLA	CBA-CGA-O2A-C1
19	b	3021	CLA	CBA-CGA-O2A-C1
19	b	3031	CLA	CBA-CGA-O2A-C1
19	b	3034	CLA	CBA-CGA-O2A-C1
19	b	3037	CLA	CBA-CGA-O2A-C1
19	j	102	CLA	CBA-CGA-O2A-C1
19	l	1501	CLA	CBA-CGA-O2A-C1
19	A	402	CLA	CBA-CGA-O2A-C1
19	A	405	CLA	CBA-CGA-O2A-C1
31	A	404	PHO	CBA-CGA-O2A-C1
19	a	807	CLA	CBD-CGD-O2D-CED
19	a	810	CLA	CBD-CGD-O2D-CED
19	a	819	CLA	CBD-CGD-O2D-CED
19	a	855	CLA	CBD-CGD-O2D-CED
19	b	3008	CLA	CBD-CGD-O2D-CED
19	b	3023	CLA	CBD-CGD-O2D-CED
19	b	3028	CLA	CBD-CGD-O2D-CED
19	b	3041	CLA	CBD-CGD-O2D-CED
19	f	203	CLA	CBD-CGD-O2D-CED
19	f	204	CLA	CBD-CGD-O2D-CED
19	D	401	CLA	CBD-CGD-O2D-CED
19	D	403	CLA	CBD-CGD-O2D-CED
23	a	851	LMG	C11-C10-O7-C8
19	b	3035	CLA	O1D-CGD-O2D-CED
19	a	843	CLA	O1A-CGA-O2A-C1
19	a	802	CLA	C4-C3-C5-C6
19	a	807	CLA	C4-C3-C5-C6
19	a	836	CLA	C4-C3-C5-C6
19	a	837	CLA	C4-C3-C5-C6
19	a	840	CLA	C4-C3-C5-C6
19	b	3017	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	b	3026	CLA	C4-C3-C5-C6
19	a	807	CLA	C2-C3-C5-C6
19	a	836	CLA	C2-C3-C5-C6
19	a	837	CLA	C2-C3-C5-C6
19	b	3014	CLA	C2-C3-C5-C6
19	b	3017	CLA	C2-C3-C5-C6
19	b	3026	CLA	C2-C3-C5-C6
19	b	3029	CLA	C2-C3-C5-C6
19	b	3041	CLA	CBA-CGA-O2A-C1
19	b	3027	CLA	O1D-CGD-O2D-CED
19	j	103	CLA	O1D-CGD-O2D-CED
19	A	402	CLA	O1D-CGD-O2D-CED
29	f	207	LMT	O5'-C5'-C6'-O6'
18	a	801	CL0	O1A-CGA-O2A-C1
19	a	808	CLA	O1A-CGA-O2A-C1
19	a	827	CLA	C3-C5-C6-C7
19	a	831	CLA	C3-C5-C6-C7
19	a	833	CLA	C3-C5-C6-C7
19	a	841	CLA	C3-C5-C6-C7
19	a	858	CLA	C3-C5-C6-C7
19	b	3006	CLA	C3-C5-C6-C7
31	D	402	PHO	C3-C5-C6-C7
19	a	804	CLA	CBA-CGA-O2A-C1
19	a	808	CLA	CBA-CGA-O2A-C1
19	a	812	CLA	CBA-CGA-O2A-C1
19	a	813	CLA	CBA-CGA-O2A-C1
19	a	821	CLA	CBA-CGA-O2A-C1
19	a	824	CLA	CBA-CGA-O2A-C1
19	a	830	CLA	CBA-CGA-O2A-C1
19	a	838	CLA	CBA-CGA-O2A-C1
19	a	843	CLA	CBA-CGA-O2A-C1
19	a	855	CLA	CBA-CGA-O2A-C1
19	b	3003	CLA	CBA-CGA-O2A-C1
19	b	3007	CLA	CBA-CGA-O2A-C1
19	b	3016	CLA	CBA-CGA-O2A-C1
19	b	3024	CLA	CBA-CGA-O2A-C1
19	b	3030	CLA	CBA-CGA-O2A-C1
19	b	3038	CLA	CBA-CGA-O2A-C1
19	b	3039	CLA	CBA-CGA-O2A-C1
19	f	201	CLA	CBA-CGA-O2A-C1
19	f	203	CLA	CBA-CGA-O2A-C1
19	f	204	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	l	1502	CLA	CBA-CGA-O2A-C1
19	l	1503	CLA	CBA-CGA-O2A-C1
22	f	206	LHG	C24-C23-O8-C6
23	a	853	LMG	C29-C28-O8-C9
19	a	804	CLA	O1A-CGA-O2A-C1
19	a	811	CLA	O1A-CGA-O2A-C1
19	a	812	CLA	O1A-CGA-O2A-C1
19	a	819	CLA	O1A-CGA-O2A-C1
19	a	823	CLA	O1A-CGA-O2A-C1
19	a	824	CLA	O1A-CGA-O2A-C1
19	a	825	CLA	O1A-CGA-O2A-C1
19	a	828	CLA	O1A-CGA-O2A-C1
19	a	839	CLA	O1A-CGA-O2A-C1
19	a	856	CLA	O1A-CGA-O2A-C1
19	b	3002	CLA	O1A-CGA-O2A-C1
19	b	3017	CLA	O1A-CGA-O2A-C1
19	b	3036	CLA	O1A-CGA-O2A-C1
19	b	3037	CLA	O1A-CGA-O2A-C1
19	f	201	CLA	O1A-CGA-O2A-C1
19	f	203	CLA	O1A-CGA-O2A-C1
19	j	102	CLA	O1A-CGA-O2A-C1
19	A	402	CLA	O1A-CGA-O2A-C1
19	a	819	CLA	C3-C5-C6-C7
19	a	835	CLA	C3-C5-C6-C7
19	b	3004	CLA	C3-C5-C6-C7
19	a	824	CLA	CBD-CGD-O2D-CED
19	a	835	CLA	CBD-CGD-O2D-CED
22	a	854	LHG	O2-C2-C3-O3
19	b	3036	CLA	O1D-CGD-O2D-CED
19	a	811	CLA	CBA-CGA-O2A-C1
19	a	815	CLA	CBA-CGA-O2A-C1
19	a	822	CLA	CBA-CGA-O2A-C1
19	a	831	CLA	CBA-CGA-O2A-C1
19	a	832	CLA	CBA-CGA-O2A-C1
19	a	837	CLA	CBA-CGA-O2A-C1
19	a	858	CLA	CBA-CGA-O2A-C1
19	b	3027	CLA	CBA-CGA-O2A-C1
19	a	830	CLA	O1A-CGA-O2A-C1
19	b	3007	CLA	O1A-CGA-O2A-C1
19	b	3027	CLA	O1A-CGA-O2A-C1
19	a	816	CLA	O1D-CGD-O2D-CED
29	f	207	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
19	a	816	CLA	CBA-CGA-O2A-C1
19	b	3034	CLA	O1D-CGD-O2D-CED
23	a	851	LMG	O6-C5-C6-O5
29	f	207	LMT	O5B-C5B-C6B-O6B
19	b	3009	CLA	O1D-CGD-O2D-CED
19	a	803	CLA	C3-C5-C6-C7
19	b	3037	CLA	C3-C5-C6-C7
19	a	832	CLA	CBD-CGD-O2D-CED
19	b	3040	CLA	CBD-CGD-O2D-CED
19	b	3014	CLA	O1D-CGD-O2D-CED
18	a	801	CL0	CBA-CGA-O2A-C1
19	a	823	CLA	CBA-CGA-O2A-C1
19	b	3002	CLA	CBA-CGA-O2A-C1
19	b	3017	CLA	CBA-CGA-O2A-C1
19	b	3028	CLA	CBA-CGA-O2A-C1
19	b	3036	CLA	CBA-CGA-O2A-C1
19	a	831	CLA	C4-C3-C5-C6
19	b	3007	CLA	C4-C3-C5-C6
19	b	3015	CLA	C4-C3-C5-C6
19	b	3037	CLA	C4-C3-C5-C6
19	a	802	CLA	C2-C3-C5-C6
19	a	840	CLA	C2-C3-C5-C6
19	b	3037	CLA	C2-C3-C5-C6
19	f	201	CLA	C2-C3-C5-C6
19	a	815	CLA	O1A-CGA-O2A-C1
19	a	831	CLA	O1A-CGA-O2A-C1
19	b	3016	CLA	O1A-CGA-O2A-C1
19	b	3030	CLA	O1A-CGA-O2A-C1
19	f	204	CLA	O1A-CGA-O2A-C1
19	b	3013	CLA	CBD-CGD-O2D-CED
19	l	1501	CLA	CBD-CGD-O2D-CED
19	a	837	CLA	C2A-CAA-CBA-CGA
19	l	1503	CLA	C3-C5-C6-C7
19	a	822	CLA	O1A-CGA-O2A-C1
19	a	837	CLA	O1A-CGA-O2A-C1
19	a	858	CLA	O1A-CGA-O2A-C1
19	b	3028	CLA	O1A-CGA-O2A-C1
23	a	851	LMG	O10-C28-O8-C9
23	b	3049	LMG	O6-C5-C6-O5
29	f	207	LMT	C4'-C5'-C6'-O6'
19	b	3039	CLA	O1D-CGD-O2D-CED
19	b	3010	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	b	3029	CLA	CBA-CGA-O2A-C1
19	b	3035	CLA	CBA-CGA-O2A-C1
19	a	831	CLA	CBD-CGD-O2D-CED
19	D	404	CLA	CBD-CGD-O2D-CED
23	a	851	LMG	C4-C5-C6-O5
19	a	832	CLA	O1A-CGA-O2A-C1
22	b	3050	LHG	C32-C33-C34-C35
19	a	803	CLA	CBD-CGD-O2D-CED
19	a	814	CLA	CBD-CGD-O2D-CED
19	a	817	CLA	CBD-CGD-O2D-CED
19	f	201	CLA	C3-C5-C6-C7
19	a	841	CLA	O1A-CGA-O2A-C1
19	b	3029	CLA	O1A-CGA-O2A-C1
19	b	3035	CLA	O1A-CGA-O2A-C1
19	a	809	CLA	CBA-CGA-O2A-C1
19	a	826	CLA	CBA-CGA-O2A-C1
19	a	833	CLA	CBA-CGA-O2A-C1
19	a	841	CLA	CBA-CGA-O2A-C1
19	a	842	CLA	CBA-CGA-O2A-C1
19	b	3032	CLA	CBA-CGA-O2A-C1
22	a	852	LHG	C24-C23-O8-C6
23	a	851	LMG	C29-C28-O8-C9
23	b	3051	LMG	C29-C28-O8-C9
22	a	852	LHG	C29-C30-C31-C32
19	a	819	CLA	O1D-CGD-O2D-CED
19	a	841	CLA	O1D-CGD-O2D-CED
19	D	403	CLA	O1D-CGD-O2D-CED
19	a	856	CLA	C4-C3-C5-C6
19	f	201	CLA	C4-C3-C5-C6
19	a	831	CLA	C2-C3-C5-C6
19	a	856	CLA	C2-C3-C5-C6
19	b	3007	CLA	C2-C3-C5-C6
19	b	3015	CLA	C2-C3-C5-C6
19	A	403	CLA	CBD-CGD-O2D-CED
19	a	808	CLA	C6-C7-C8-C9
19	a	818	CLA	C11-C10-C8-C9
19	a	826	CLA	C14-C13-C15-C16
19	a	842	CLA	C11-C12-C13-C14
19	b	3002	CLA	C11-C12-C13-C14
19	b	3003	CLA	C6-C7-C8-C9
19	b	3003	CLA	C11-C12-C13-C14
19	b	3007	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	b	3029	CLA	C11-C12-C13-C14
19	l	1502	CLA	C6-C7-C8-C9
23	b	3049	LMG	C4-C5-C6-O5
19	b	3008	CLA	O1D-CGD-O2D-CED
22	b	3050	LHG	O2-C2-C3-O3
19	a	855	CLA	O1D-CGD-O2D-CED
19	b	3033	CLA	CBD-CGD-O2D-CED
19	a	807	CLA	O1D-CGD-O2D-CED
21	a	845	BCR	C7-C8-C9-C34
21	a	848	BCR	C7-C8-C9-C34
21	b	3043	BCR	C7-C8-C9-C34
21	b	3048	BCR	C11-C12-C13-C35
21	k	4001	BCR	C7-C8-C9-C34
21	l	1504	BCR	C37-C22-C23-C24
26	b	3045	ECH	C37-C22-C23-C24
26	m	101	ECH	C37-C22-C23-C24
21	a	845	BCR	C7-C8-C9-C10
26	m	101	ECH	C21-C22-C23-C24
19	l	1501	CLA	C2A-CAA-CBA-CGA
22	a	852	LHG	C7-C8-C9-C10
19	a	833	CLA	O1A-CGA-O2A-C1
19	b	3013	CLA	C5-C6-C7-C8
19	D	401	CLA	O1D-CGD-O2D-CED
19	a	805	CLA	CBA-CGA-O2A-C1
19	D	401	CLA	CBA-CGA-O2A-C1
19	a	837	CLA	C5-C6-C7-C8
19	a	832	CLA	C2C-C3C-CAC-CBC
19	a	855	CLA	C2-C1-O2A-CGA
19	b	3006	CLA	C2-C1-O2A-CGA
19	b	3021	CLA	C2-C1-O2A-CGA
19	l	1501	CLA	C2-C1-O2A-CGA
19	b	3041	CLA	O1D-CGD-O2D-CED
19	f	204	CLA	O1D-CGD-O2D-CED
19	a	809	CLA	C15-C16-C17-C18
19	a	829	CLA	C10-C11-C12-C13
19	a	810	CLA	O1D-CGD-O2D-CED
19	b	3023	CLA	O1D-CGD-O2D-CED
19	a	816	CLA	O1A-CGA-O2A-C1
19	a	805	CLA	C6-C7-C8-C10
19	a	814	CLA	C6-C7-C8-C10
19	a	821	CLA	C6-C7-C8-C10
19	a	822	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	a	826	CLA	C6-C7-C8-C10
19	a	834	CLA	C6-C7-C8-C10
19	b	3019	CLA	C6-C7-C8-C10
19	b	3024	CLA	C11-C12-C13-C15
19	f	203	CLA	O1D-CGD-O2D-CED
19	b	3028	CLA	O1D-CGD-O2D-CED
19	a	840	CLA	C3-C5-C6-C7
19	a	815	CLA	C5-C6-C7-C8
19	a	815	CLA	C13-C15-C16-C17
19	a	843	CLA	C5-C6-C7-C8
19	a	809	CLA	O1A-CGA-O2A-C1
19	a	842	CLA	O1A-CGA-O2A-C1
19	b	3015	CLA	CBA-CGA-O2A-C1
19	b	3005	CLA	C13-C15-C16-C17
19	b	3013	CLA	C8-C10-C11-C12
19	b	3020	CLA	C10-C11-C12-C13
19	f	201	CLA	C8-C10-C11-C12
19	l	1502	CLA	C10-C11-C12-C13
19	a	809	CLA	C2A-CAA-CBA-CGA
19	a	815	CLA	C2A-CAA-CBA-CGA
19	a	828	CLA	C2A-CAA-CBA-CGA
19	a	842	CLA	C2A-CAA-CBA-CGA
19	a	843	CLA	C2A-CAA-CBA-CGA
19	b	3010	CLA	C2A-CAA-CBA-CGA
19	b	3013	CLA	C2A-CAA-CBA-CGA
19	b	3028	CLA	C2A-CAA-CBA-CGA
19	b	3041	CLA	C2A-CAA-CBA-CGA
19	f	204	CLA	C2A-CAA-CBA-CGA
21	b	3048	BCR	C10-C11-C12-C13
19	a	809	CLA	C8-C10-C11-C12
19	a	822	CLA	C8-C10-C11-C12
19	a	822	CLA	C15-C16-C17-C18
19	a	824	CLA	C5-C6-C7-C8
19	a	839	CLA	C8-C10-C11-C12
19	b	3026	CLA	C8-C10-C11-C12
19	f	201	CLA	C15-C16-C17-C18
19	A	402	CLA	C13-C15-C16-C17
19	A	402	CLA	C15-C16-C17-C18
20	a	844	PQN	C18-C20-C21-C22
22	a	852	LHG	C23-C24-C25-C26
22	b	3050	LHG	C23-C24-C25-C26
22	f	206	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
19	a	826	CLA	O1A-CGA-O2A-C1
19	b	3032	CLA	O1A-CGA-O2A-C1
21	a	846	BCR	C6-C7-C8-C9
21	j	101	BCR	C6-C7-C8-C9
19	a	803	CLA	C10-C11-C12-C13
19	a	805	CLA	C5-C6-C7-C8
19	a	808	CLA	C8-C10-C11-C12
19	a	812	CLA	C13-C15-C16-C17
19	a	819	CLA	C13-C15-C16-C17
19	a	826	CLA	C5-C6-C7-C8
19	a	828	CLA	C15-C16-C17-C18
19	a	834	CLA	C5-C6-C7-C8
19	a	837	CLA	C8-C10-C11-C12
19	b	3004	CLA	C10-C11-C12-C13
19	b	3005	CLA	C15-C16-C17-C18
19	b	3019	CLA	C8-C10-C11-C12
19	b	3029	CLA	C5-C6-C7-C8
22	a	852	LHG	O2-C2-C3-O3
19	b	3010	CLA	O1A-CGA-O2A-C1
19	a	815	CLA	C15-C16-C17-C18
19	a	834	CLA	C13-C15-C16-C17
19	b	3039	CLA	C8-C10-C11-C12
19	a	802	CLA	C3-C5-C6-C7
19	a	840	CLA	C5-C6-C7-C8
19	a	840	CLA	C15-C16-C17-C18
19	a	805	CLA	O1A-CGA-O2A-C1
19	a	824	CLA	O1D-CGD-O2D-CED
19	a	835	CLA	O1D-CGD-O2D-CED
19	a	802	CLA	C15-C16-C17-C18
19	a	858	CLA	C10-C11-C12-C13
19	b	3006	CLA	C15-C16-C17-C18
19	b	3020	CLA	C15-C16-C17-C18
19	b	3027	CLA	C8-C10-C11-C12
19	a	830	CLA	CBD-CGD-O2D-CED
22	f	206	LHG	C8-C7-O7-C5
21	a	849	BCR	C9-C10-C11-C12
21	b	3044	BCR	C19-C20-C21-C22
19	f	201	CLA	C13-C15-C16-C17
28	b	3053	ZEX	C25-C26-C27-C28
28	f	205	ZEX	C25-C26-C27-C28
22	a	852	LHG	C1-C2-C3-O3
19	a	802	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	a	811	CLA	C2A-CAA-CBA-CGA
19	a	825	CLA	C2A-CAA-CBA-CGA
19	D	404	CLA	C2A-CAA-CBA-CGA
19	b	3023	CLA	CBA-CGA-O2A-C1
19	b	3008	CLA	C10-C11-C12-C13
19	b	3014	CLA	C5-C6-C7-C8
19	b	3018	CLA	C10-C11-C12-C13
19	b	3033	CLA	C5-C6-C7-C8
19	a	802	CLA	C5-C6-C7-C8
19	a	824	CLA	C8-C10-C11-C12
19	a	830	CLA	C13-C15-C16-C17
19	a	808	CLA	C5-C6-C7-C8
19	a	822	CLA	C10-C11-C12-C13
19	a	840	CLA	C8-C10-C11-C12
19	b	3017	CLA	C15-C16-C17-C18
19	a	814	CLA	CBA-CGA-O2A-C1
19	a	825	CLA	C4-C3-C5-C6
19	a	809	CLA	C10-C11-C12-C13
19	a	839	CLA	C16-C17-C18-C20
21	a	847	BCR	C16-C17-C18-C36
21	a	848	BCR	C20-C21-C22-C37
21	b	3044	BCR	C16-C17-C18-C36
21	b	3046	BCR	C20-C21-C22-C37
21	b	3047	BCR	C20-C21-C22-C37
21	i	101	BCR	C20-C21-C22-C37
19	b	3039	CLA	C10-C11-C12-C13
21	a	845	BCR	C11-C12-C13-C35
21	a	847	BCR	C7-C8-C9-C34
26	b	3045	ECH	C21-C22-C23-C24
32	F	101	HEM	C2A-CAA-CBA-CGA
19	D	401	CLA	O1A-CGA-O2A-C1
19	a	816	CLA	C2A-CAA-CBA-CGA
19	b	3032	CLA	C2A-CAA-CBA-CGA
19	k	4003	CLA	C2A-CAA-CBA-CGA
19	l	1503	CLA	C2A-CAA-CBA-CGA
22	a	852	LHG	O1-C1-C2-C3
22	f	206	LHG	O1-C1-C2-C3
22	f	206	LHG	C6-C5-O7-C7
22	b	3050	LHG	C30-C31-C32-C33
19	a	802	CLA	C16-C17-C18-C19
19	a	825	CLA	C11-C12-C13-C14
19	b	3014	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
19	b	3015	CLA	O1A-CGA-O2A-C1
18	a	801	CL0	C3-C5-C6-C7
19	b	3018	CLA	C3-C5-C6-C7
21	b	3048	BCR	C11-C10-C9-C8
21	b	3048	BCR	C20-C21-C22-C23
21	f	202	BCR	C12-C13-C14-C15
19	b	3040	CLA	O1D-CGD-O2D-CED
19	a	831	CLA	O1D-CGD-O2D-CED
19	l	1501	CLA	O1D-CGD-O2D-CED
22	a	854	LHG	C28-C29-C30-C31
22	a	854	LHG	C23-C24-C25-C26
18	a	801	CL0	C2-C1-O2A-CGA
19	a	811	CLA	C2-C1-O2A-CGA
19	a	819	CLA	C2-C1-O2A-CGA
19	a	823	CLA	C2-C1-O2A-CGA
19	a	824	CLA	C2-C1-O2A-CGA
19	a	830	CLA	C2-C1-O2A-CGA
19	a	856	CLA	C2-C1-O2A-CGA
19	b	3007	CLA	C2-C1-O2A-CGA
19	b	3038	CLA	C2-C1-O2A-CGA
19	a	805	CLA	C16-C17-C18-C19
19	b	3019	CLA	C11-C12-C13-C15
31	D	402	PHO	C16-C17-C18-C19
19	b	3023	CLA	O1A-CGA-O2A-C1
22	a	850	LHG	C29-C30-C31-C32
22	a	850	LHG	C32-C33-C34-C35
22	a	852	LHG	C28-C29-C30-C31
23	b	3049	LMG	C33-C34-C35-C36
19	a	858	CLA	C5-C6-C7-C8
23	a	851	LMG	C18-C19-C20-C21
23	a	853	LMG	C12-C13-C14-C15
23	b	3049	LMG	C37-C38-C39-C40
19	a	832	CLA	O1D-CGD-O2D-CED
23	b	3051	LMG	C14-C15-C16-C17
23	b	3051	LMG	C15-C16-C17-C18
29	f	207	LMT	C3-C4-C5-C6
22	a	850	LHG	O1-C1-C2-O2
19	a	819	CLA	C4B-C3B-CAB-CBB
19	b	3030	CLA	C4B-C3B-CAB-CBB
23	a	851	LMG	C28-C29-C30-C31
19	a	805	CLA	C16-C17-C18-C20
19	a	822	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
19	a	822	CLA	C16-C17-C18-C20
19	a	825	CLA	C11-C12-C13-C15
19	a	833	CLA	C11-C12-C13-C15
19	a	839	CLA	C16-C17-C18-C19
19	b	3014	CLA	C16-C17-C18-C19
19	b	3039	CLA	C16-C17-C18-C19
19	b	3039	CLA	C16-C17-C18-C20
19	b	3040	CLA	C16-C17-C18-C19
19	a	814	CLA	C2A-CAA-CBA-CGA
22	a	850	LHG	C15-C16-C17-C18
22	a	852	LHG	C32-C33-C34-C35
23	b	3051	LMG	C31-C32-C33-C34
18	a	801	CL0	C5-C6-C7-C8
19	b	3017	CLA	C5-C6-C7-C8
23	b	3051	LMG	C18-C19-C20-C21
18	a	801	CL0	C12-C13-C15-C16
19	a	813	CLA	C11-C10-C8-C7
19	b	3010	CLA	C6-C7-C8-C10
19	b	3018	CLA	C11-C10-C8-C7
19	b	3020	CLA	C6-C7-C8-C10
19	A	402	CLA	C12-C13-C15-C16
23	b	3051	LMG	C28-C29-C30-C31
19	b	3003	CLA	C2C-C3C-CAC-CBC
19	D	401	CLA	C8-C10-C11-C12
22	a	850	LHG	C28-C29-C30-C31
22	a	854	LHG	C32-C33-C34-C35
19	a	814	CLA	O1A-CGA-O2A-C1
19	a	818	CLA	C3A-C2A-CAA-CBA
19	a	824	CLA	C3A-C2A-CAA-CBA
19	a	829	CLA	C3A-C2A-CAA-CBA
19	a	838	CLA	C3A-C2A-CAA-CBA
19	b	3005	CLA	C3A-C2A-CAA-CBA
19	b	3015	CLA	C3A-C2A-CAA-CBA
19	b	3016	CLA	C3A-C2A-CAA-CBA
19	b	3039	CLA	C3A-C2A-CAA-CBA
19	b	3041	CLA	C3A-C2A-CAA-CBA
19	A	402	CLA	C3A-C2A-CAA-CBA
19	D	401	CLA	C3A-C2A-CAA-CBA
31	D	402	PHO	C3A-C2A-CAA-CBA
19	b	3013	CLA	O1D-CGD-O2D-CED
22	f	206	LHG	C29-C30-C31-C32
22	f	206	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
23	a	853	LMG	C32-C33-C34-C35
19	b	3003	CLA	C10-C11-C12-C13
19	a	833	CLA	C11-C12-C13-C14
19	b	3019	CLA	C11-C12-C13-C14
19	b	3040	CLA	C16-C17-C18-C20
19	b	3013	CLA	C10-C11-C12-C13
19	a	840	CLA	CBA-CGA-O2A-C1
22	a	854	LHG	C7-C8-C9-C10
22	a	854	LHG	C11-C10-C9-C8
22	a	854	LHG	C14-C15-C16-C17
22	f	206	LHG	C27-C28-C29-C30
23	b	3051	LMG	C12-C13-C14-C15
19	a	832	CLA	C4C-C3C-CAC-CBC
23	a	851	LMG	C32-C33-C34-C35
19	D	404	CLA	O1D-CGD-O2D-CED
31	D	402	PHO	C16-C17-C18-C20
19	a	819	CLA	C2B-C3B-CAB-CBB
19	D	401	CLA	C2B-C3B-CAB-CBB
21	b	3043	BCR	C1-C6-C7-C8
21	b	3043	BCR	C5-C6-C7-C8
21	j	104	BCR	C1-C6-C7-C8
21	j	104	BCR	C5-C6-C7-C8
21	l	1504	BCR	C23-C24-C25-C30
26	b	3045	ECH	C1-C6-C7-C8
23	b	3051	LMG	C11-C10-O7-C8
19	a	804	CLA	C15-C16-C17-C18
19	a	836	CLA	C3-C5-C6-C7
19	a	804	CLA	C2A-CAA-CBA-CGA
19	a	805	CLA	C2A-CAA-CBA-CGA
19	a	821	CLA	C2A-CAA-CBA-CGA
19	b	3017	CLA	C2A-CAA-CBA-CGA
19	b	3029	CLA	C2A-CAA-CBA-CGA
19	a	812	CLA	C8-C10-C11-C12
19	a	840	CLA	O1A-CGA-O2A-C1
19	b	3005	CLA	CBD-CGD-O2D-CED
19	a	819	CLA	C4-C3-C5-C6
21	b	3048	BCR	C18-C19-C20-C21
21	f	202	BCR	C10-C11-C12-C13
21	k	4001	BCR	C18-C19-C20-C21
22	a	850	LHG	C23-C24-C25-C26
19	a	809	CLA	C11-C12-C13-C14
19	b	3024	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	b	3047	BCR	C6-C7-C8-C9
22	a	854	LHG	C16-C17-C18-C19
22	a	850	LHG	C24-C25-C26-C27
23	b	3051	LMG	C41-C42-C43-C44
21	b	3048	BCR	C13-C14-C15-C16
22	b	3050	LHG	C8-C7-O7-C5
22	f	206	LHG	C30-C31-C32-C33
23	b	3049	LMG	C32-C33-C34-C35
19	b	3026	CLA	C5-C6-C7-C8
23	b	3049	LMG	C19-C20-C21-C22
19	b	3004	CLA	CBD-CGD-O2D-CED
23	b	3049	LMG	C18-C19-C20-C21
23	a	851	LMG	C31-C32-C33-C34
21	f	202	BCR	C11-C12-C13-C14
22	b	3050	LHG	C27-C28-C29-C30
23	b	3051	LMG	C17-C18-C19-C20
19	A	405	CLA	C2A-CAA-CBA-CGA
19	a	802	CLA	C16-C17-C18-C20
19	b	3021	CLA	C11-C12-C13-C14
19	b	3011	CLA	CBD-CGD-O2D-CED
23	b	3049	LMG	C34-C35-C36-C37
19	a	808	CLA	C4-C3-C5-C6
19	a	823	CLA	C4-C3-C5-C6
19	a	827	CLA	C4-C3-C5-C6
23	a	851	LMG	C15-C16-C17-C18
19	a	821	CLA	C10-C11-C12-C13
22	a	850	LHG	C9-C10-C11-C12
23	a	851	LMG	C37-C38-C39-C40
19	a	827	CLA	C5-C6-C7-C8
19	a	830	CLA	C5-C6-C7-C8
19	a	842	CLA	C8-C10-C11-C12
19	a	814	CLA	O1D-CGD-O2D-CED
22	a	850	LHG	C7-C8-C9-C10
23	a	851	LMG	C10-C11-C12-C13
19	a	803	CLA	O1D-CGD-O2D-CED
19	a	817	CLA	O1D-CGD-O2D-CED
22	a	850	LHG	O7-C5-C6-O8
23	b	3049	LMG	O7-C8-C9-O8
19	b	3025	CLA	CBA-CGA-O2A-C1
19	b	3024	CLA	C15-C16-C17-C18
22	a	852	LHG	C34-C35-C36-C37
19	b	3037	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	a	820	CLA	C16-C17-C18-C20
22	f	206	LHG	C2-C3-O3-P
23	a	853	LMG	C15-C16-C17-C18
23	b	3051	LMG	C34-C35-C36-C37
19	b	3033	CLA	O1D-CGD-O2D-CED
19	D	403	CLA	C4-C3-C5-C6
19	a	813	CLA	C3-C5-C6-C7
19	a	803	CLA	C2A-CAA-CBA-CGA
19	a	808	CLA	C2A-CAA-CBA-CGA
19	l	1502	CLA	C2A-CAA-CBA-CGA
19	b	3025	CLA	CBD-CGD-O2D-CED
19	A	403	CLA	O1D-CGD-O2D-CED
19	a	828	CLA	C8-C10-C11-C12
19	b	3028	CLA	C8-C10-C11-C12
22	a	850	LHG	C8-C7-O7-C5
23	b	3051	LMG	O6-C5-C6-O5
23	b	3049	LMG	C23-C24-C25-C26
19	a	806	CLA	C1A-C2A-CAA-CBA
19	a	809	CLA	C1A-C2A-CAA-CBA
19	a	812	CLA	C1A-C2A-CAA-CBA
19	a	815	CLA	C1A-C2A-CAA-CBA
19	a	832	CLA	C1A-C2A-CAA-CBA
19	a	835	CLA	C1A-C2A-CAA-CBA
19	b	3022	CLA	C1A-C2A-CAA-CBA
19	b	3033	CLA	C1A-C2A-CAA-CBA
19	b	3038	CLA	C1A-C2A-CAA-CBA
19	b	3041	CLA	C1A-C2A-CAA-CBA
19	j	103	CLA	C1A-C2A-CAA-CBA
19	k	4002	CLA	C1A-C2A-CAA-CBA
19	A	402	CLA	C1A-C2A-CAA-CBA
19	D	403	CLA	C1A-C2A-CAA-CBA
22	a	850	LHG	C26-C27-C28-C29
22	f	206	LHG	C15-C16-C17-C18
23	a	851	LMG	C30-C31-C32-C33
22	b	3050	LHG	O6-C4-C5-C6
22	f	206	LHG	O6-C4-C5-C6
19	a	807	CLA	C12-C13-C15-C16
19	a	809	CLA	C6-C7-C8-C10
19	a	812	CLA	C11-C10-C8-C7
19	a	812	CLA	C11-C12-C13-C15
19	a	820	CLA	C11-C10-C8-C7
19	a	820	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	a	823	CLA	C11-C10-C8-C7
19	a	831	CLA	C6-C7-C8-C10
19	a	833	CLA	C11-C10-C8-C7
19	a	834	CLA	C11-C12-C13-C15
19	a	842	CLA	C6-C7-C8-C10
19	b	3002	CLA	C11-C12-C13-C15
19	b	3006	CLA	C12-C13-C15-C16
19	b	3009	CLA	C11-C12-C13-C15
19	b	3033	CLA	C6-C7-C8-C10
19	b	3040	CLA	C11-C12-C13-C15
19	f	201	CLA	C11-C12-C13-C15
23	b	3049	LMG	C28-C29-C30-C31
19	a	828	CLA	C4-C3-C5-C6
19	a	827	CLA	C2-C3-C5-C6
19	a	834	CLA	C2-C3-C5-C6
19	a	856	CLA	C5-C6-C7-C8
18	a	801	CL0	C2A-CAA-CBA-CGA
19	a	855	CLA	C2A-CAA-CBA-CGA
19	b	3030	CLA	C2A-CAA-CBA-CGA
19	a	808	CLA	C11-C10-C8-C9
19	a	815	CLA	C6-C7-C8-C9
19	a	820	CLA	C11-C12-C13-C14
19	a	821	CLA	C11-C12-C13-C14
19	a	823	CLA	C11-C10-C8-C9
19	a	827	CLA	C14-C13-C15-C16
19	a	831	CLA	C6-C7-C8-C9
19	a	832	CLA	C6-C7-C8-C9
19	a	839	CLA	C11-C10-C8-C9
19	a	840	CLA	C11-C10-C8-C9
19	a	842	CLA	C6-C7-C8-C9
19	a	856	CLA	C6-C7-C8-C9
19	b	3006	CLA	C14-C13-C15-C16
19	b	3014	CLA	C14-C13-C15-C16
19	b	3020	CLA	C11-C10-C8-C9
19	b	3023	CLA	C6-C7-C8-C9
29	f	207	LMT	C2'-C1'-O1'-C1
23	b	3051	LMG	C30-C31-C32-C33
22	a	852	LHG	C4-C5-C6-O8
22	a	854	LHG	C4-C5-C6-O8
23	a	853	LMG	O1-C7-C8-C9
23	b	3049	LMG	C16-C17-C18-C19
23	b	3051	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
19	a	809	CLA	C5-C6-C7-C8
23	b	3051	LMG	C16-C17-C18-C19
19	a	820	CLA	C16-C17-C18-C19
19	b	3021	CLA	C11-C12-C13-C15
23	b	3049	LMG	C30-C31-C32-C33
23	a	851	LMG	C40-C41-C42-C43
18	a	801	CL0	CHA-CBD-CGD-O1D
18	a	801	CL0	CHA-CBD-CGD-O2D
21	f	202	BCR	C35-C13-C14-C15
31	D	402	PHO	CHA-CBD-CGD-O1D
31	D	402	PHO	CHA-CBD-CGD-O2D
31	A	404	PHO	C5-C6-C7-C8
19	b	3025	CLA	O1A-CGA-O2A-C1
22	a	852	LHG	O10-C23-O8-C6
23	b	3051	LMG	O10-C28-O8-C9
19	b	3032	CLA	C4-C3-C5-C6
19	a	828	CLA	C2-C3-C5-C6
19	b	3032	CLA	C2-C3-C5-C6
23	b	3049	LMG	C17-C18-C19-C20
21	b	3043	BCR	C21-C22-C23-C24
21	f	202	BCR	C21-C22-C23-C24
19	a	804	CLA	C5-C6-C7-C8
19	b	3003	CLA	O2A-C1-C2-C3
22	b	3050	LHG	C28-C29-C30-C31
21	a	845	BCR	C18-C19-C20-C21
19	b	3024	CLA	C10-C11-C12-C13
23	a	851	LMG	C16-C17-C18-C19
19	b	3031	CLA	CBD-CGD-O2D-CED
22	b	3050	LHG	C1-C2-C3-O3
22	a	852	LHG	C27-C28-C29-C30
19	b	3033	CLA	C4-C3-C5-C6
19	a	836	CLA	C16-C17-C18-C20
23	a	851	LMG	C19-C20-C21-C22
19	a	814	CLA	C13-C15-C16-C17
19	b	3007	CLA	C5-C6-C7-C8
23	b	3051	LMG	C21-C22-C23-C24
19	b	3015	CLA	C2C-C3C-CAC-CBC
23	a	853	LMG	C34-C35-C36-C37
23	a	853	LMG	C16-C17-C18-C19
23	b	3051	LMG	C32-C33-C34-C35
29	f	207	LMT	C5-C6-C7-C8
19	a	858	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	a	834	CLA	C4-C3-C5-C6
19	b	3004	CLA	C4-C3-C5-C6
19	b	3034	CLA	C4-C3-C5-C6
19	a	813	CLA	C2-C3-C5-C6
19	a	819	CLA	C5-C6-C7-C8
29	f	207	LMT	C2-C1-O1'-C1'
19	a	805	CLA	C6-C7-C8-C9
19	a	807	CLA	C11-C12-C13-C14
19	a	812	CLA	C11-C12-C13-C14
19	a	820	CLA	C11-C10-C8-C9
19	a	822	CLA	C11-C12-C13-C14
19	a	822	CLA	C14-C13-C15-C16
19	a	833	CLA	C11-C10-C8-C9
19	a	858	CLA	C6-C7-C8-C9
19	b	3002	CLA	C11-C10-C8-C9
19	b	3018	CLA	C6-C7-C8-C9
19	b	3018	CLA	C11-C10-C8-C9
19	b	3034	CLA	C11-C10-C8-C9
19	b	3037	CLA	C6-C7-C8-C9
19	b	3040	CLA	C11-C12-C13-C14
19	f	201	CLA	C11-C12-C13-C14
19	D	401	CLA	C10-C11-C12-C13
19	a	809	CLA	C4B-C3B-CAB-CBB
19	a	828	CLA	C4B-C3B-CAB-CBB
19	a	832	CLA	C4B-C3B-CAB-CBB
19	a	833	CLA	C4B-C3B-CAB-CBB
19	a	856	CLA	C4B-C3B-CAB-CBB
19	b	3008	CLA	C4B-C3B-CAB-CBB
19	b	3033	CLA	C4B-C3B-CAB-CBB
19	b	3039	CLA	C4B-C3B-CAB-CBB
19	l	1502	CLA	C4B-C3B-CAB-CBB
22	a	852	LHG	C24-C25-C26-C27
23	b	3051	LMG	C19-C20-C21-C22
29	f	207	LMT	C4-C5-C6-C7
19	a	814	CLA	C3-C5-C6-C7
19	a	807	CLA	C11-C12-C13-C15
19	a	815	CLA	C6-C7-C8-C10
19	a	821	CLA	C11-C12-C13-C15
19	a	822	CLA	C11-C12-C13-C15
19	a	827	CLA	C12-C13-C15-C16
19	a	837	CLA	C6-C7-C8-C10
19	a	856	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	a	858	CLA	C6-C7-C8-C10
19	b	3002	CLA	C11-C10-C8-C7
19	b	3014	CLA	C12-C13-C15-C16
19	b	3020	CLA	C11-C10-C8-C7
19	b	3023	CLA	C6-C7-C8-C10
19	b	3034	CLA	C11-C10-C8-C7
19	b	3037	CLA	C6-C7-C8-C10
19	a	842	CLA	C10-C11-C12-C13
19	b	3020	CLA	C5-C6-C7-C8
19	a	836	CLA	C16-C17-C18-C19
19	a	803	CLA	C3A-C2A-CAA-CBA
19	a	812	CLA	C3A-C2A-CAA-CBA
19	a	813	CLA	C4-C3-C5-C6
19	a	842	CLA	C3A-C2A-CAA-CBA
19	b	3004	CLA	C3A-C2A-CAA-CBA
19	b	3012	CLA	C3A-C2A-CAA-CBA
19	b	3013	CLA	C4-C3-C5-C6
19	j	102	CLA	C3A-C2A-CAA-CBA
19	A	405	CLA	C3A-C2A-CAA-CBA
19	a	825	CLA	C2-C3-C5-C6
23	b	3049	LMG	C39-C40-C41-C42
31	A	404	PHO	C3-C5-C6-C7
23	b	3051	LMG	C42-C43-C44-C45
19	a	836	CLA	CBD-CGD-O2D-CED
23	b	3049	LMG	C7-C8-C9-O8
19	b	3040	CLA	C15-C16-C17-C18
28	b	3053	ZEX	C21-C26-C27-C28
28	f	205	ZEX	C21-C26-C27-C28
31	D	402	PHO	C1A-C2A-CAA-CBA
19	a	826	CLA	C8-C10-C11-C12
19	a	828	CLA	C10-C11-C12-C13
19	b	3013	CLA	C2-C3-C5-C6
23	b	3049	LMG	C38-C39-C40-C41
19	a	830	CLA	C16-C17-C18-C20
19	b	3028	CLA	C16-C17-C18-C20
22	b	3050	LHG	O6-C4-C5-O7
19	a	856	CLA	C2B-C3B-CAB-CBB
19	b	3002	CLA	C2B-C3B-CAB-CBB
19	b	3008	CLA	C2B-C3B-CAB-CBB
21	a	846	BCR	C1-C6-C7-C8
21	a	848	BCR	C23-C24-C25-C30
21	b	3044	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	j	101	BCR	C1-C6-C7-C8
21	k	4004	BCR	C23-C24-C25-C30
21	A	406	BCR	C1-C6-C7-C8
21	A	406	BCR	C23-C24-C25-C30
27	b	3052	EQ3	C23-C24-C25-C26
19	a	826	CLA	C13-C15-C16-C17
19	a	841	CLA	C8-C10-C11-C12
19	a	812	CLA	C15-C16-C17-C18
19	a	830	CLA	O1D-CGD-O2D-CED
22	a	854	LHG	C13-C14-C15-C16
19	b	3008	CLA	C16-C17-C18-C20
23	b	3051	LMG	O1-C7-C8-O7
19	a	821	CLA	C4-C3-C5-C6
19	a	821	CLA	C5-C6-C7-C8
19	a	835	CLA	C13-C15-C16-C17
19	a	821	CLA	C2-C3-C5-C6
19	b	3034	CLA	C2-C3-C5-C6
23	b	3049	LMG	C15-C16-C17-C18
31	D	402	PHO	CBA-CGA-O2A-C1
19	a	807	CLA	C14-C13-C15-C16
19	a	828	CLA	C11-C10-C8-C9
19	b	3007	CLA	C11-C12-C13-C14
19	b	3009	CLA	C11-C10-C8-C9
21	f	202	BCR	C6-C7-C8-C9
19	a	817	CLA	C2A-CAA-CBA-CGA
22	f	206	LHG	C31-C32-C33-C34
23	a	851	LMG	C42-C43-C44-C45
19	b	3002	CLA	C10-C11-C12-C13
21	b	3048	BCR	C15-C16-C17-C18
19	b	3004	CLA	C2-C3-C5-C6
19	a	830	CLA	C16-C17-C18-C19
19	b	3034	CLA	C13-C15-C16-C17
23	b	3049	LMG	C31-C32-C33-C34
19	b	3005	CLA	C16-C17-C18-C20
19	a	805	CLA	C13-C15-C16-C17
19	a	806	CLA	C13-C15-C16-C17
19	a	825	CLA	C5-C6-C7-C8
21	a	846	BCR	C37-C22-C23-C24
28	b	3053	ZEX	C27-C28-C29-C39
28	f	205	ZEX	C27-C28-C29-C39
19	a	802	CLA	C6-C7-C8-C10
19	a	808	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	a	820	CLA	C6-C7-C8-C10
19	a	828	CLA	C11-C10-C8-C7
19	a	841	CLA	C6-C7-C8-C10
19	a	858	CLA	C12-C13-C15-C16
19	b	3007	CLA	C11-C12-C13-C15
19	b	3008	CLA	C11-C10-C8-C7
19	b	3009	CLA	C11-C10-C8-C7
19	D	401	CLA	C11-C12-C13-C15
22	a	850	LHG	C18-C19-C20-C21
19	a	842	CLA	C13-C15-C16-C17
21	b	3048	BCR	C17-C18-C19-C20
21	f	202	BCR	C7-C8-C9-C10
19	b	3005	CLA	O1D-CGD-O2D-CED
19	b	3011	CLA	O1D-CGD-O2D-CED
31	D	402	PHO	O1A-CGA-O2A-C1
19	a	819	CLA	C2-C3-C5-C6
19	b	3004	CLA	O1D-CGD-O2D-CED
29	f	207	LMT	C11-C10-C9-C8
19	a	856	CLA	O2A-C1-C2-C3
19	b	3008	CLA	C16-C17-C18-C19
19	b	3013	CLA	C16-C17-C18-C19
19	b	3013	CLA	C16-C17-C18-C20
22	f	206	LHG	C32-C33-C34-C35
23	a	851	LMG	C34-C35-C36-C37
21	a	847	BCR	C16-C17-C18-C19
19	b	3025	CLA	O1D-CGD-O2D-CED
23	b	3051	LMG	O1-C7-C8-C9
23	b	3051	LMG	C7-C8-C9-O8
32	F	101	HEM	C4C-C3C-CAC-CBC
19	b	3028	CLA	C16-C17-C18-C19
23	a	851	LMG	C29-C30-C31-C32
19	a	830	CLA	C15-C16-C17-C18
19	a	835	CLA	C4-C3-C5-C6
19	b	3003	CLA	C2A-CAA-CBA-CGA
19	a	823	CLA	C2-C3-C5-C6
19	b	3018	CLA	C5-C6-C7-C8
23	b	3051	LMG	O7-C8-C9-O8
19	a	802	CLA	C6-C7-C8-C9
19	a	809	CLA	C11-C10-C8-C9
19	a	825	CLA	C11-C10-C8-C9
19	a	827	CLA	C11-C10-C8-C9
19	a	837	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	a	841	CLA	C6-C7-C8-C9
19	b	3032	CLA	C14-C13-C15-C16
19	D	401	CLA	C11-C12-C13-C14
22	b	3050	LHG	C24-C25-C26-C27
19	a	833	CLA	C8-C10-C11-C12
19	a	856	CLA	C8-C10-C11-C12
19	b	3029	CLA	C13-C15-C16-C17
19	b	3024	CLA	C2-C1-O2A-CGA
19	b	3031	CLA	O1D-CGD-O2D-CED
22	a	854	LHG	C24-C23-O8-C6
19	a	808	CLA	C2-C3-C5-C6
19	a	820	CLA	C2A-CAA-CBA-CGA
19	b	3005	CLA	C16-C17-C18-C19
19	D	403	CLA	C6-C7-C8-C10
22	b	3050	LHG	C31-C32-C33-C34
19	a	807	CLA	C3-C5-C6-C7
19	a	803	CLA	C1A-C2A-CAA-CBA
19	a	804	CLA	C4B-C3B-CAB-CBB
19	a	810	CLA	C1A-C2A-CAA-CBA
19	a	824	CLA	C4B-C3B-CAB-CBB
19	a	836	CLA	C4B-C3B-CAB-CBB
19	a	842	CLA	C4B-C3B-CAB-CBB
19	a	843	CLA	C1A-C2A-CAA-CBA
19	a	858	CLA	C4B-C3B-CAB-CBB
19	b	3002	CLA	C4B-C3B-CAB-CBB
19	b	3005	CLA	C1A-C2A-CAA-CBA
19	b	3012	CLA	C1A-C2A-CAA-CBA
19	b	3020	CLA	C4B-C3B-CAB-CBB
19	b	3038	CLA	C4B-C3B-CAB-CBB
19	f	201	CLA	C4B-C3B-CAB-CBB
19	f	204	CLA	C4B-C3B-CAB-CBB
19	j	102	CLA	C4B-C3B-CAB-CBB
19	k	4002	CLA	C4B-C3B-CAB-CBB
23	b	3049	LMG	C36-C37-C38-C39
19	j	103	CLA	C2A-CAA-CBA-CGA
19	a	814	CLA	C11-C10-C8-C7
19	a	826	CLA	C11-C12-C13-C15
19	a	827	CLA	C11-C10-C8-C7
19	a	828	CLA	C12-C13-C15-C16
19	b	3003	CLA	C6-C7-C8-C10
19	b	3013	CLA	C6-C7-C8-C10
19	b	3014	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	l	1502	CLA	C6-C7-C8-C10
19	D	401	CLA	C11-C10-C8-C7
19	b	3039	CLA	C4-C3-C5-C6
23	b	3049	LMG	C29-C28-O8-C9
19	a	820	CLA	C6-C7-C8-C9
19	a	821	CLA	C6-C7-C8-C9
19	a	821	CLA	C11-C10-C8-C9
19	a	826	CLA	C6-C7-C8-C9
19	a	834	CLA	C6-C7-C8-C9
19	a	858	CLA	C14-C13-C15-C16
19	l	1502	CLA	C8-C10-C11-C12
19	f	201	CLA	C16-C17-C18-C20
19	a	836	CLA	O1D-CGD-O2D-CED
19	a	832	CLA	C5-C6-C7-C8
22	a	854	LHG	C24-C25-C26-C27
19	b	3008	CLA	C3-C5-C6-C7
22	a	850	LHG	C34-C35-C36-C37
22	a	854	LHG	O7-C5-C6-O8
22	a	850	LHG	C4-C5-C6-O8
23	a	851	LMG	O1-C7-C8-C9
19	b	3009	CLA	C8-C10-C11-C12
19	a	835	CLA	C2-C3-C5-C6
19	a	816	CLA	CAD-CBD-CGD-O2D
19	a	823	CLA	CAD-CBD-CGD-O2D
19	b	3007	CLA	C16-C17-C18-C20
19	a	813	CLA	C2A-CAA-CBA-CGA
19	b	3035	CLA	C2A-CAA-CBA-CGA
22	a	852	LHG	C30-C31-C32-C33
19	a	816	CLA	CAD-CBD-CGD-O1D
19	a	819	CLA	CHA-CBD-CGD-O1D
19	a	823	CLA	CAD-CBD-CGD-O1D
19	b	3013	CLA	CHA-CBD-CGD-O1D
19	b	3014	CLA	CAD-CBD-CGD-O1D
19	b	3025	CLA	CHA-CBD-CGD-O1D
22	a	852	LHG	C3-O3-P-O6
22	b	3050	LHG	C3-O3-P-O5
22	b	3050	LHG	C3-O3-P-O6
22	f	206	LHG	C4-O6-P-O3
31	A	404	PHO	CHA-CBD-CGD-O1D
31	A	404	PHO	CHA-CBD-CGD-O2D
19	b	3005	CLA	C4-C3-C5-C6
19	a	804	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	a	836	CLA	C2B-C3B-CAB-CBB
19	a	858	CLA	C2B-C3B-CAB-CBB
19	b	3020	CLA	C2B-C3B-CAB-CBB
19	b	3030	CLA	C2B-C3B-CAB-CBB
19	b	3038	CLA	C2B-C3B-CAB-CBB
19	f	201	CLA	C2B-C3B-CAB-CBB
19	f	204	CLA	C2B-C3B-CAB-CBB
19	b	3033	CLA	C2-C3-C5-C6
19	D	403	CLA	C2-C3-C5-C6
19	b	3009	CLA	C3-C5-C6-C7
19	a	855	CLA	C5-C6-C7-C8
19	a	818	CLA	C16-C17-C18-C20
19	D	403	CLA	C6-C7-C8-C9
28	f	205	ZEX	C27-C28-C29-C30
22	b	3050	LHG	C7-C8-C9-C10
22	a	854	LHG	C6-C5-O7-C7
22	a	850	LHG	C12-C13-C14-C15
19	a	819	CLA	C16-C17-C18-C20
19	a	807	CLA	C6-C7-C8-C9
19	a	814	CLA	C6-C7-C8-C9
19	a	824	CLA	C14-C13-C15-C16
19	a	827	CLA	C6-C7-C8-C9
19	a	829	CLA	C11-C10-C8-C9
19	a	830	CLA	C14-C13-C15-C16
19	D	401	CLA	C11-C10-C8-C9
19	a	806	CLA	C11-C12-C13-C15
19	b	3007	CLA	C6-C7-C8-C10
19	b	3009	CLA	C6-C7-C8-C10
19	b	3014	CLA	C11-C10-C8-C7
19	A	402	CLA	C6-C7-C8-C10
21	b	3043	BCR	C12-C13-C14-C15
22	a	854	LHG	C1-C2-C3-O3
21	j	104	BCR	C6-C7-C8-C9
19	a	821	CLA	C8-C10-C11-C12
19	a	830	CLA	C8-C10-C11-C12
22	f	206	LHG	O7-C5-C6-O8
23	a	853	LMG	O1-C7-C8-O7
21	A	406	BCR	C9-C10-C11-C12
19	b	3012	CLA	C2A-CAA-CBA-CGA
19	a	841	CLA	C2-C1-O2A-CGA
19	b	3003	CLA	C2-C1-O2A-CGA
19	b	3027	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	a	826	CLA	C16-C17-C18-C20
22	f	206	LHG	C4-C5-C6-O8
21	i	101	BCR	C37-C22-C23-C24
22	a	850	LHG	C11-C10-C9-C8
19	a	841	CLA	C5-C6-C7-C8
19	a	831	CLA	C2A-CAA-CBA-CGA
19	a	832	CLA	C2A-CAA-CBA-CGA
19	a	843	CLA	C4-C3-C5-C6
19	b	3006	CLA	C4-C3-C5-C6
19	b	3005	CLA	C2-C3-C5-C6
22	f	206	LHG	C9-C10-C11-C12
29	f	207	LMT	O5B-C1B-O1B-C4'
19	a	811	CLA	CAA-CBA-CGA-O2A
19	a	806	CLA	C11-C12-C13-C14
19	a	814	CLA	C11-C10-C8-C9
19	a	825	CLA	C6-C7-C8-C9
19	a	828	CLA	C14-C13-C15-C16
19	b	3003	CLA	C11-C10-C8-C9
19	b	3013	CLA	C6-C7-C8-C9
19	b	3020	CLA	C6-C7-C8-C9
19	A	402	CLA	C6-C7-C8-C9
19	b	3006	CLA	C4B-C3B-CAB-CBB
19	b	3040	CLA	C4B-C3B-CAB-CBB
19	k	4003	CLA	C4B-C3B-CAB-CBB
19	b	3037	CLA	O1D-CGD-O2D-CED
19	a	808	CLA	C10-C11-C12-C13
23	a	851	LMG	C38-C39-C40-C41
19	b	3013	CLA	CBA-CGA-O2A-C1
19	f	201	CLA	C16-C17-C18-C19
23	b	3051	LMG	C33-C34-C35-C36
19	a	813	CLA	C8-C10-C11-C12
19	b	3037	CLA	CBD-CGD-O2D-CED
19	D	403	CLA	CBA-CGA-O2A-C1
19	a	819	CLA	C16-C17-C18-C19
19	a	826	CLA	C16-C17-C18-C19
19	b	3007	CLA	C16-C17-C18-C19
19	b	3018	CLA	C8-C10-C11-C12
22	a	850	LHG	C30-C31-C32-C33
19	a	831	CLA	C3A-C2A-CAA-CBA
19	b	3029	CLA	C3A-C2A-CAA-CBA
19	b	3027	CLA	C2-C3-C5-C6
24	a	857	45D	C28-C26-C30-C32

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Mol	Chain	Res	Type	Atoms
24	a	857	45D	C39-C35-C37-C41
26	b	3045	ECH	C11-C10-C9-C34
26	b	3045	ECH	C35-C13-C14-C15
27	b	3052	EQ3	C11-C10-C9-C34
28	f	205	ZEX	C20-C13-C14-C15
19	b	3026	CLA	C2-C1-O2A-CGA
21	l	1504	BCR	C15-C16-C17-C18
19	a	806	CLA	C16-C17-C18-C19
19	b	3014	CLA	C8-C10-C11-C12
21	b	3044	BCR	C37-C22-C23-C24
21	A	406	BCR	C11-C12-C13-C35
19	k	4003	CLA	C2C-C3C-CAC-CBC
19	b	3033	CLA	C16-C17-C18-C20
19	a	822	CLA	C2A-CAA-CBA-CGA
19	b	3009	CLA	C2A-CAA-CBA-CGA
19	a	813	CLA	C6-C7-C8-C9
19	a	824	CLA	C11-C10-C8-C9
19	a	836	CLA	C14-C13-C15-C16
19	a	856	CLA	C11-C10-C8-C9
19	b	3028	CLA	C14-C13-C15-C16
19	l	1502	CLA	C11-C12-C13-C14
19	D	401	CLA	C6-C7-C8-C9
22	a	852	LHG	C26-C27-C28-C29
22	b	3050	LHG	C26-C27-C28-C29
23	b	3049	LMG	C11-C12-C13-C14
19	b	3017	CLA	C16-C17-C18-C20
19	b	3003	CLA	C4C-C3C-CAC-CBC
19	a	843	CLA	C2-C3-C5-C6
19	a	831	CLA	C1A-C2A-CAA-CBA
19	a	858	CLA	C1A-C2A-CAA-CBA
24	a	857	45D	C24-C26-C30-C32
24	a	857	45D	C33-C35-C37-C41
26	b	3045	ECH	C12-C13-C14-C15
27	b	3052	EQ3	C11-C10-C9-C8
28	f	205	ZEX	C12-C13-C14-C15
19	a	839	CLA	C13-C15-C16-C17
19	a	824	CLA	C2B-C3B-CAB-CBB
19	a	842	CLA	C2B-C3B-CAB-CBB
19	b	3033	CLA	C2B-C3B-CAB-CBB
19	b	3039	CLA	C2B-C3B-CAB-CBB
19	j	102	CLA	C2B-C3B-CAB-CBB
19	k	4002	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	k	4003	CLA	C2B-C3B-CAB-CBB
21	a	845	BCR	C1-C6-C7-C8
21	a	846	BCR	C5-C6-C7-C8
21	a	848	BCR	C1-C6-C7-C8
21	a	848	BCR	C23-C24-C25-C26
21	b	3043	BCR	C23-C24-C25-C30
21	b	3044	BCR	C5-C6-C7-C8
21	b	3046	BCR	C23-C24-C25-C30
21	f	202	BCR	C1-C6-C7-C8
21	j	101	BCR	C5-C6-C7-C8
21	j	104	BCR	C23-C24-C25-C30
21	k	4001	BCR	C23-C24-C25-C30
21	l	1504	BCR	C1-C6-C7-C8
21	A	406	BCR	C5-C6-C7-C8
21	A	406	BCR	C23-C24-C25-C26
19	b	3027	CLA	C13-C15-C16-C17
19	b	3019	CLA	C3-C5-C6-C7
23	b	3051	LMG	C13-C14-C15-C16
19	a	824	CLA	C12-C13-C15-C16
19	a	825	CLA	C6-C7-C8-C10
19	a	826	CLA	C12-C13-C15-C16
19	a	830	CLA	C12-C13-C15-C16
19	b	3003	CLA	C11-C10-C8-C7
19	b	3028	CLA	C11-C12-C13-C15
19	b	3029	CLA	C11-C10-C8-C7
19	f	201	CLA	C6-C7-C8-C10
22	f	206	LHG	C18-C19-C20-C21
23	a	851	LMG	O1-C7-C8-O7
19	D	403	CLA	O1A-CGA-O2A-C1
21	j	104	BCR	C7-C8-C9-C34
19	a	806	CLA	CAA-CBA-CGA-O2A
19	a	829	CLA	CAA-CBA-CGA-O2A
19	a	809	CLA	C13-C15-C16-C17
19	a	818	CLA	C10-C11-C12-C13
19	b	3013	CLA	C13-C15-C16-C17
19	b	3013	CLA	O1A-CGA-O2A-C1
22	a	854	LHG	C34-C35-C36-C37
19	a	820	CLA	C13-C15-C16-C17
19	a	820	CLA	C15-C16-C17-C18
21	f	202	BCR	C22-C23-C24-C25
19	b	3023	CLA	C4-C3-C5-C6
19	b	3039	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	a	814	CLA	C15-C16-C17-C18
19	a	829	CLA	C5-C6-C7-C8
19	b	3014	CLA	C15-C16-C17-C18
19	b	3020	CLA	C13-C15-C16-C17
19	a	831	CLA	C13-C15-C16-C17
19	b	3020	CLA	C4-C3-C5-C6
19	b	3032	CLA	C16-C17-C18-C20
19	b	3007	CLA	C4B-C3B-CAB-CBB
19	b	3015	CLA	C4B-C3B-CAB-CBB
22	b	3050	LHG	C34-C35-C36-C37
19	b	3002	CLA	C16-C17-C18-C20
19	A	402	CLA	C16-C17-C18-C19
21	b	3048	BCR	C11-C10-C9-C34
21	f	202	BCR	C20-C21-C22-C37
21	l	1504	BCR	C20-C21-C22-C37
19	A	402	CLA	C4-C3-C5-C6
19	a	842	CLA	O1D-CGD-O2D-CED
19	b	3023	CLA	C2-C3-C5-C6
19	b	3033	CLA	C16-C17-C18-C19
23	b	3049	LMG	C22-C23-C24-C25
19	A	402	CLA	C3-C5-C6-C7
21	b	3048	BCR	C11-C12-C13-C14
18	a	801	CL0	C14-C13-C15-C16
19	a	814	CLA	C11-C12-C13-C14
19	a	836	CLA	C11-C12-C13-C14
19	b	3013	CLA	C14-C13-C15-C16
19	b	3019	CLA	C6-C7-C8-C9
19	b	3034	CLA	C6-C7-C8-C9
21	a	849	BCR	C16-C17-C18-C36
23	a	851	LMG	C8-C7-O1-C1
23	b	3051	LMG	C8-C7-O1-C1
19	b	3004	CLA	C2A-CAA-CBA-CGA
19	a	814	CLA	C2-C1-O2A-CGA
19	a	818	CLA	C2-C1-O2A-CGA
19	b	3004	CLA	C8-C10-C11-C12
19	l	1503	CLA	C3A-C2A-CAA-CBA
19	b	3023	CLA	CAA-CBA-CGA-O2A
23	a	853	LMG	C31-C32-C33-C34
19	a	819	CLA	O2A-C1-C2-C3
19	a	824	CLA	O2A-C1-C2-C3
22	a	854	LHG	C4-C5-O7-C7
21	f	202	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
23	b	3049	LMG	C14-C15-C16-C17
19	a	829	CLA	C2A-CAA-CBA-CGA
19	b	3024	CLA	C3-C5-C6-C7
21	i	101	BCR	C20-C21-C22-C23
21	j	104	BCR	C11-C10-C9-C8
26	b	3045	ECH	C11-C10-C9-C8
19	b	3008	CLA	C5-C6-C7-C8
19	b	3020	CLA	CBA-CGA-O2A-C1
23	a	853	LMG	C7-C8-C9-O8
19	b	3020	CLA	O1A-CGA-O2A-C1
19	a	806	CLA	C10-C11-C12-C13
19	a	821	CLA	C13-C15-C16-C17
19	a	840	CLA	CAA-CBA-CGA-O2A
19	b	3017	CLA	C16-C17-C18-C19
31	A	404	PHO	C15-C16-C17-C18
29	f	207	LMT	C5'-C4'-O1B-C1B
19	a	839	CLA	C6-C7-C8-C9
19	a	840	CLA	C6-C7-C8-C9
19	a	855	CLA	C14-C13-C15-C16
19	b	3008	CLA	C11-C10-C8-C9
19	b	3010	CLA	C6-C7-C8-C9
19	b	3014	CLA	C6-C7-C8-C9
19	a	806	CLA	C16-C17-C18-C20
29	f	207	LMT	C7-C8-C9-C10
19	a	809	CLA	C4-C3-C5-C6
19	a	831	CLA	CAA-CBA-CGA-O2A
23	a	851	LMG	O8-C28-C29-C30
19	a	814	CLA	C11-C12-C13-C15
19	a	818	CLA	C11-C10-C8-C7
19	a	836	CLA	C11-C12-C13-C15
19	a	842	CLA	C11-C12-C13-C15
19	b	3003	CLA	C11-C12-C13-C15
19	b	3013	CLA	C12-C13-C15-C16
19	b	3029	CLA	C11-C12-C13-C15
19	l	1502	CLA	C11-C12-C13-C15
31	A	404	PHO	C11-C10-C8-C7
19	b	3037	CLA	C5-C6-C7-C8
19	a	809	CLA	C2B-C3B-CAB-CBB
19	a	828	CLA	C2B-C3B-CAB-CBB
19	a	832	CLA	C2B-C3B-CAB-CBB
19	a	833	CLA	C2B-C3B-CAB-CBB
19	b	3006	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	l	1502	CLA	C2B-C3B-CAB-CBB
21	a	845	BCR	C5-C6-C7-C8
21	a	846	BCR	C23-C24-C25-C30
21	a	847	BCR	C1-C6-C7-C8
21	b	3043	BCR	C23-C24-C25-C26
21	b	3046	BCR	C23-C24-C25-C26
21	f	202	BCR	C5-C6-C7-C8
21	i	101	BCR	C1-C6-C7-C8
21	j	101	BCR	C23-C24-C25-C30
21	j	104	BCR	C23-C24-C25-C26
21	k	4001	BCR	C1-C6-C7-C8
21	k	4001	BCR	C5-C6-C7-C8
21	k	4001	BCR	C23-C24-C25-C26
21	k	4004	BCR	C23-C24-C25-C26
21	l	1504	BCR	C5-C6-C7-C8
19	a	813	CLA	C2-C1-O2A-CGA
19	b	3010	CLA	C2-C1-O2A-CGA
19	a	842	CLA	CBD-CGD-O2D-CED
19	a	812	CLA	CAA-CBA-CGA-O2A
19	a	856	CLA	C10-C11-C12-C13
19	a	812	CLA	C2A-CAA-CBA-CGA
22	a	852	LHG	C14-C15-C16-C17
19	a	807	CLA	CAA-CBA-CGA-O2A
19	b	3029	CLA	CAA-CBA-CGA-O2A
22	a	854	LHG	C17-C18-C19-C20
19	b	3009	CLA	O1A-CGA-O2A-C1
19	a	832	CLA	CAA-CBA-CGA-O2A
19	b	3006	CLA	C2-C3-C5-C6
19	k	4002	CLA	C2A-CAA-CBA-CGA
19	a	826	CLA	C11-C12-C13-C14
19	a	830	CLA	C11-C10-C8-C9
19	b	3027	CLA	C11-C10-C8-C9
19	b	3028	CLA	C11-C12-C13-C14
19	b	3029	CLA	C11-C10-C8-C9
19	A	402	CLA	C11-C12-C13-C14
21	b	3047	BCR	C7-C8-C9-C34
21	j	104	BCR	C11-C12-C13-C35
19	a	830	CLA	CAA-CBA-CGA-O2A
19	b	3011	CLA	CAA-CBA-CGA-O2A
22	f	206	LHG	O7-C7-C8-C9
19	a	813	CLA	C4B-C3B-CAB-CBB
19	a	818	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
19	a	827	CLA	C4B-C3B-CAB-CBB
19	a	839	CLA	C4B-C3B-CAB-CBB
19	b	3010	CLA	C1A-C2A-CAA-CBA
19	b	3013	CLA	C1A-C2A-CAA-CBA
19	b	3017	CLA	C4B-C3B-CAB-CBB
19	f	201	CLA	C1A-C2A-CAA-CBA
22	f	206	LHG	C24-C25-C26-C27
21	l	1504	BCR	C22-C23-C24-C25
19	a	835	CLA	CAA-CBA-CGA-O2A
21	b	3047	BCR	C11-C12-C13-C14
28	b	3053	ZEX	C27-C28-C29-C30
22	a	854	LHG	C31-C32-C33-C34
19	b	3004	CLA	CAA-CBA-CGA-O2A
19	b	3016	CLA	CAA-CBA-CGA-O2A
23	a	853	LMG	O8-C28-C29-C30
22	a	850	LHG	C25-C26-C27-C28
19	a	818	CLA	C15-C16-C17-C18
32	F	101	HEM	CAA-CBA-CGA-O2A
19	a	807	CLA	O1A-CGA-O2A-C1
23	b	3049	LMG	O7-C10-C11-C12
19	b	3009	CLA	C5-C6-C7-C8
19	a	809	CLA	C2-C1-O2A-CGA
19	a	826	CLA	C2-C1-O2A-CGA
19	a	835	CLA	C2-C1-O2A-CGA
31	A	404	PHO	C2-C1-O2A-CGA
19	j	102	CLA	CAA-CBA-CGA-O2A
19	a	819	CLA	C6-C7-C8-C10
19	a	819	CLA	C11-C10-C8-C7
19	a	828	CLA	C11-C12-C13-C15
19	b	3005	CLA	C12-C13-C15-C16
19	f	201	CLA	C12-C13-C15-C16
19	A	402	CLA	O2A-C1-C2-C3
22	a	850	LHG	C10-C11-C12-C13
19	a	821	CLA	CAA-CBA-CGA-O2A
19	a	835	CLA	C3A-C2A-CAA-CBA
19	b	3017	CLA	C3A-C2A-CAA-CBA
19	b	3004	CLA	O1A-CGA-O2A-C1
21	j	101	BCR	C11-C10-C9-C8
19	a	807	CLA	CBA-CGA-O2A-C1
19	b	3009	CLA	CBA-CGA-O2A-C1
22	a	850	LHG	O6-C4-C5-O7
29	f	207	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
19	a	833	CLA	CAA-CBA-CGA-O2A
19	b	3021	CLA	CAA-CBA-CGA-O2A
23	b	3049	LMG	O9-C10-C11-C12
19	a	833	CLA	C2A-CAA-CBA-CGA
19	b	3005	CLA	C14-C13-C15-C16
19	b	3009	CLA	C11-C12-C13-C14
19	f	201	CLA	C6-C7-C8-C9
19	a	812	CLA	CAA-CBA-CGA-O1A
19	b	3029	CLA	CAA-CBA-CGA-O1A
19	a	831	CLA	C5-C6-C7-C8
23	b	3049	LMG	C29-C30-C31-C32
19	b	3021	CLA	C3-C5-C6-C7
19	b	3002	CLA	C5-C6-C7-C8
19	a	831	CLA	CAA-CBA-CGA-O1A
19	a	840	CLA	CAA-CBA-CGA-O1A
23	a	853	LMG	O10-C28-C29-C30
19	b	3004	CLA	CBA-CGA-O2A-C1
19	a	824	CLA	CAA-CBA-CGA-O2A
19	b	3039	CLA	CAA-CBA-CGA-O2A
21	k	4001	BCR	C21-C22-C23-C24
19	a	807	CLA	CAA-CBA-CGA-O1A
19	b	3004	CLA	CAA-CBA-CGA-O1A
23	a	853	LMG	C13-C14-C15-C16
32	F	101	HEM	CAA-CBA-CGA-O1A
19	a	835	CLA	CAA-CBA-CGA-O1A
19	b	3011	CLA	CAA-CBA-CGA-O1A
19	j	102	CLA	CAA-CBA-CGA-O1A
22	a	852	LHG	C9-C10-C11-C12
19	b	3009	CLA	C13-C15-C16-C17
19	b	3033	CLA	C10-C11-C12-C13
32	F	101	HEM	C2B-C3B-CAB-CBB
19	a	832	CLA	CAA-CBA-CGA-O1A
19	a	831	CLA	CAD-CBD-CGD-O2D
19	b	3016	CLA	CAD-CBD-CGD-O2D
19	b	3029	CLA	CAD-CBD-CGD-O2D
19	a	835	CLA	C4C-C3C-CAC-CBC
19	a	802	CLA	C2-C1-O2A-CGA
19	b	3016	CLA	C2-C1-O2A-CGA
19	a	830	CLA	CAA-CBA-CGA-O1A
19	b	3031	CLA	C2A-CAA-CBA-CGA
19	j	103	CLA	CAA-CBA-CGA-O2A
22	a	854	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
19	b	3016	CLA	CAA-CBA-CGA-O1A
19	a	839	CLA	CAA-CBA-CGA-O2A
19	b	3015	CLA	CAA-CBA-CGA-O2A
22	a	850	LHG	O8-C23-C24-C25

There are no ring outliers.

137 monomers are involved in 516 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	855	CLA	1	0
19	a	802	CLA	3	0
19	a	811	CLA	4	0
19	b	3004	CLA	3	0
19	b	3018	CLA	6	0
19	b	3019	CLA	3	0
19	a	818	CLA	8	0
21	l	1504	BCR	4	0
19	b	3014	CLA	6	0
19	b	3037	CLA	6	0
19	a	858	CLA	3	0
22	a	854	LHG	5	0
19	b	3012	CLA	1	0
19	a	827	CLA	8	0
19	a	813	CLA	4	0
23	b	3049	LMG	5	0
19	b	3003	CLA	14	0
19	f	201	CLA	5	0
19	b	3029	CLA	11	0
19	a	856	CLA	3	0
19	b	3011	CLA	3	0
25	c	101	SF4	1	0
19	a	804	CLA	5	0
19	a	815	CLA	13	0
19	a	838	CLA	7	0
19	k	4002	CLA	3	0
21	b	3048	BCR	6	0
19	b	3016	CLA	4	0
19	b	3008	CLA	8	0
21	a	848	BCR	3	0
19	a	840	CLA	7	0
19	a	806	CLA	10	0
19	a	829	CLA	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	834	CLA	6	0
18	a	801	CL0	4	0
19	b	3013	CLA	4	0
19	b	3006	CLA	1	0
32	F	101	HEM	4	0
19	a	842	CLA	9	0
19	a	833	CLA	4	0
19	b	3031	CLA	1	0
21	A	406	BCR	2	0
21	j	101	BCR	5	0
23	b	3051	LMG	1	0
19	b	3023	CLA	4	0
19	a	823	CLA	5	0
19	a	809	CLA	8	0
25	c	102	SF4	1	0
19	b	3041	CLA	1	0
19	b	3030	CLA	7	0
21	a	846	BCR	4	0
19	a	808	CLA	6	0
19	a	822	CLA	9	0
19	b	3007	CLA	4	0
19	b	3021	CLA	1	0
21	b	3047	BCR	4	0
19	b	3039	CLA	1	0
31	D	402	PHO	5	0
19	b	3038	CLA	3	0
19	a	805	CLA	4	0
19	j	102	CLA	2	0
19	D	404	CLA	3	0
19	b	3024	CLA	5	0
19	a	830	CLA	3	0
22	b	3050	LHG	2	0
31	A	404	PHO	5	0
20	a	844	PQN	1	0
19	l	1502	CLA	5	0
22	a	850	LHG	1	0
21	k	4001	BCR	5	0
19	a	817	CLA	2	0
19	b	3017	CLA	12	0
19	a	810	CLA	2	0
19	b	3009	CLA	3	0
23	a	853	LMG	3	0

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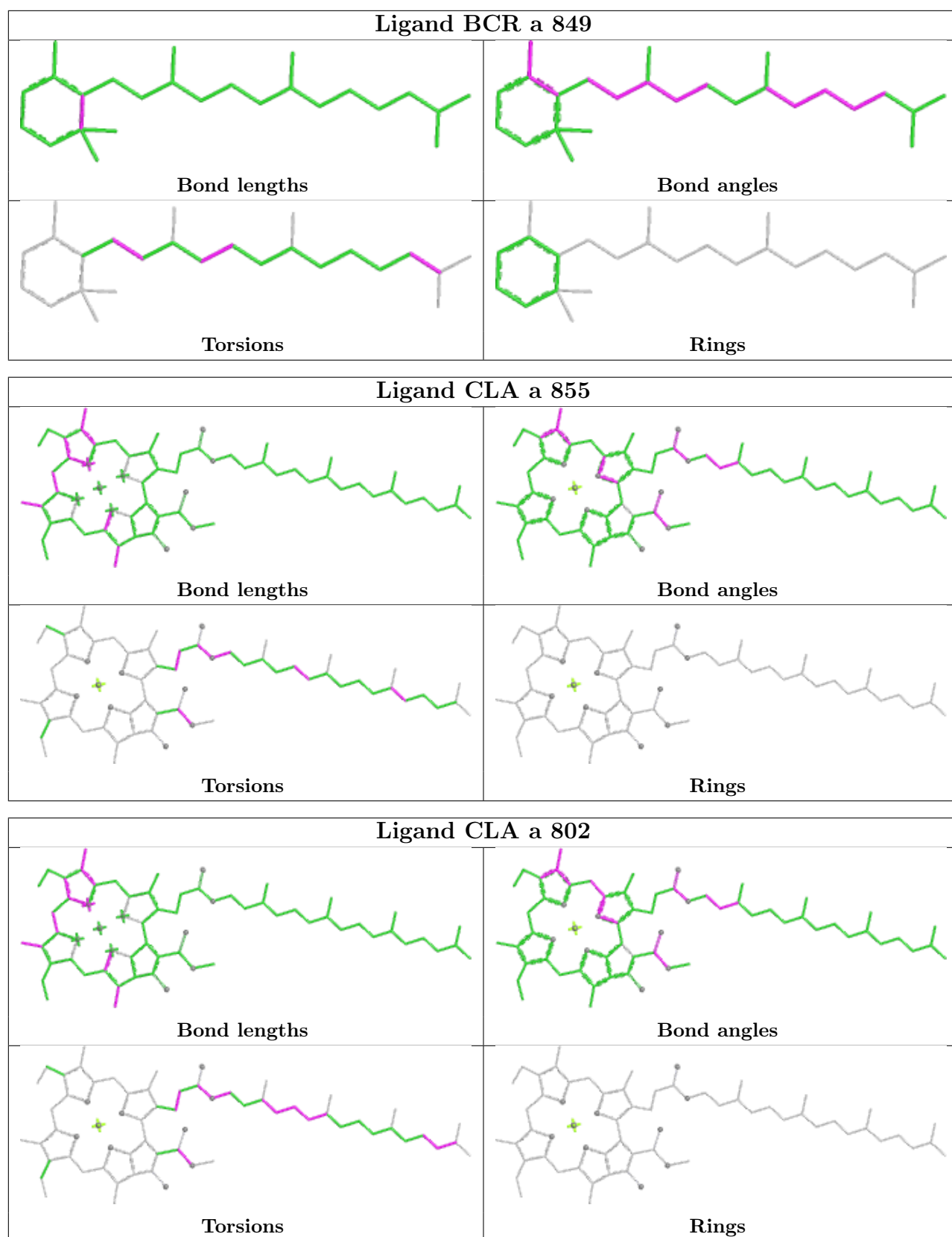
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	D	401	CLA	4	0
19	a	807	CLA	2	0
19	k	4003	CLA	1	0
24	a	857	45D	5	0
21	i	101	BCR	2	0
21	k	4004	BCR	1	0
26	b	3045	ECH	5	0
21	b	3044	BCR	4	0
19	a	831	CLA	9	0
29	f	207	LMT	4	0
19	b	3025	CLA	5	0
19	a	826	CLA	3	0
19	a	835	CLA	6	0
19	a	841	CLA	8	0
19	b	3032	CLA	4	0
19	a	824	CLA	7	0
21	b	3046	BCR	6	0
19	b	3015	CLA	7	0
19	D	403	CLA	7	0
22	a	852	LHG	5	0
19	b	3027	CLA	9	0
19	b	3033	CLA	8	0
19	a	821	CLA	5	0
19	a	803	CLA	5	0
19	f	204	CLA	1	0
28	b	3053	ZEX	3	0
19	a	836	CLA	6	0
22	f	206	LHG	6	0
19	b	3020	CLA	4	0
19	a	839	CLA	2	0
19	b	3026	CLA	7	0
19	b	3002	CLA	1	0
19	a	825	CLA	4	0
19	A	405	CLA	3	0
23	a	851	LMG	2	0
19	b	3028	CLA	3	0
19	A	402	CLA	5	0
21	a	847	BCR	2	0
19	a	820	CLA	2	0
19	b	3034	CLA	4	0
19	A	403	CLA	2	0
21	j	104	BCR	5	0

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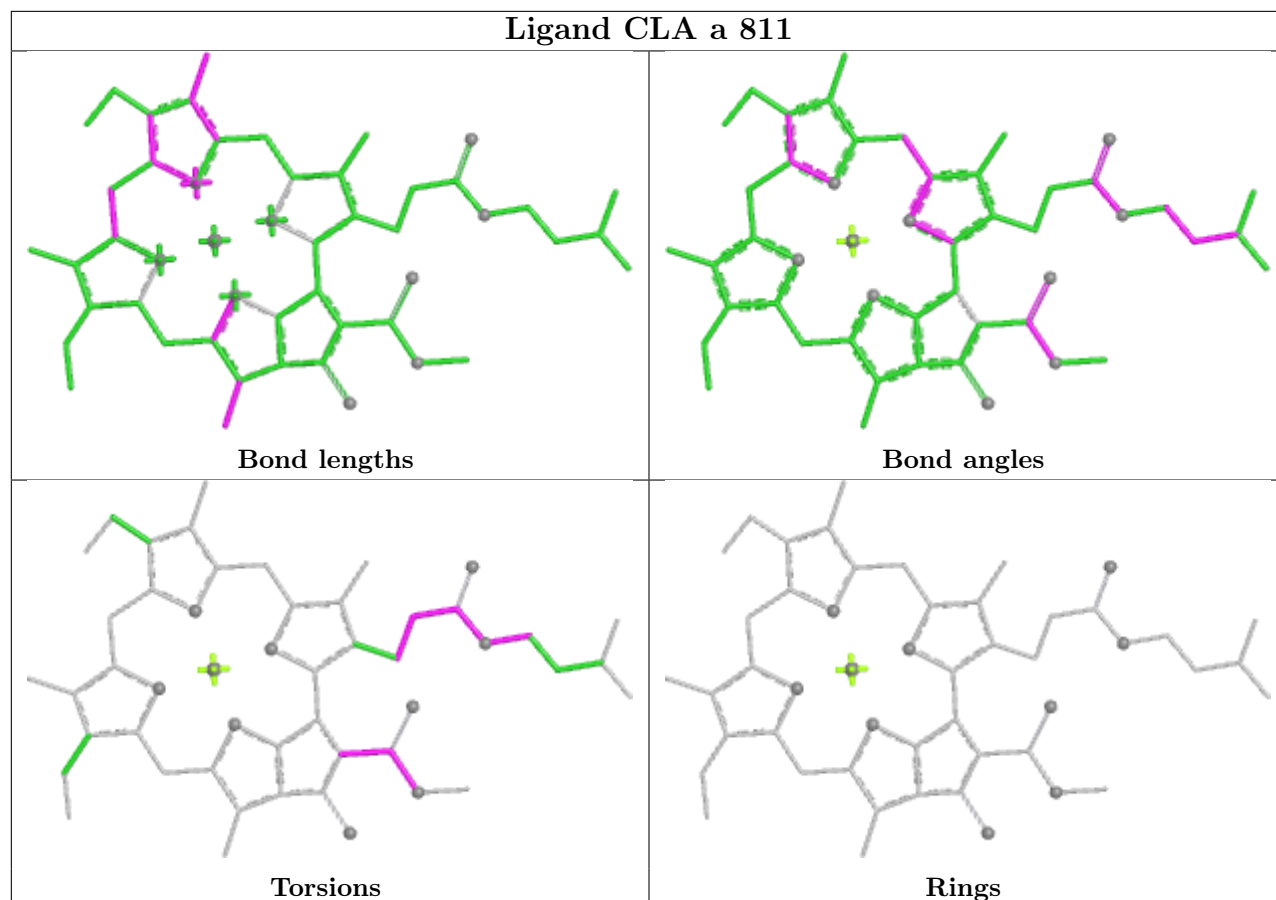
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	a	832	CLA	6	0
19	j	103	CLA	4	0
21	f	202	BCR	5	0
19	b	3022	CLA	1	0
19	b	3005	CLA	5	0
20	b	3042	PQN	1	0
26	m	101	ECH	4	0
19	b	3040	CLA	5	0
19	b	3035	CLA	2	0
19	a	814	CLA	6	0
19	b	3010	CLA	2	0
21	b	3043	BCR	3	0
19	a	828	CLA	6	0
19	f	203	CLA	1	0
19	l	1501	CLA	1	0
19	a	843	CLA	4	0
19	a	837	CLA	7	0
19	a	819	CLA	8	0
19	a	812	CLA	5	0
21	a	845	BCR	10	0

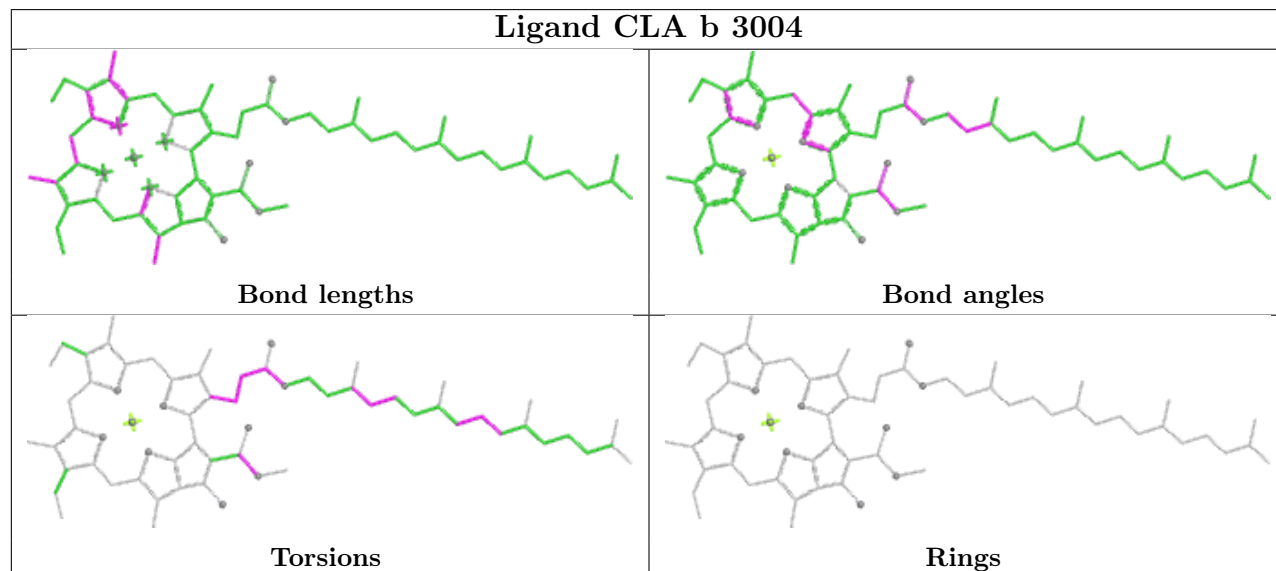
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

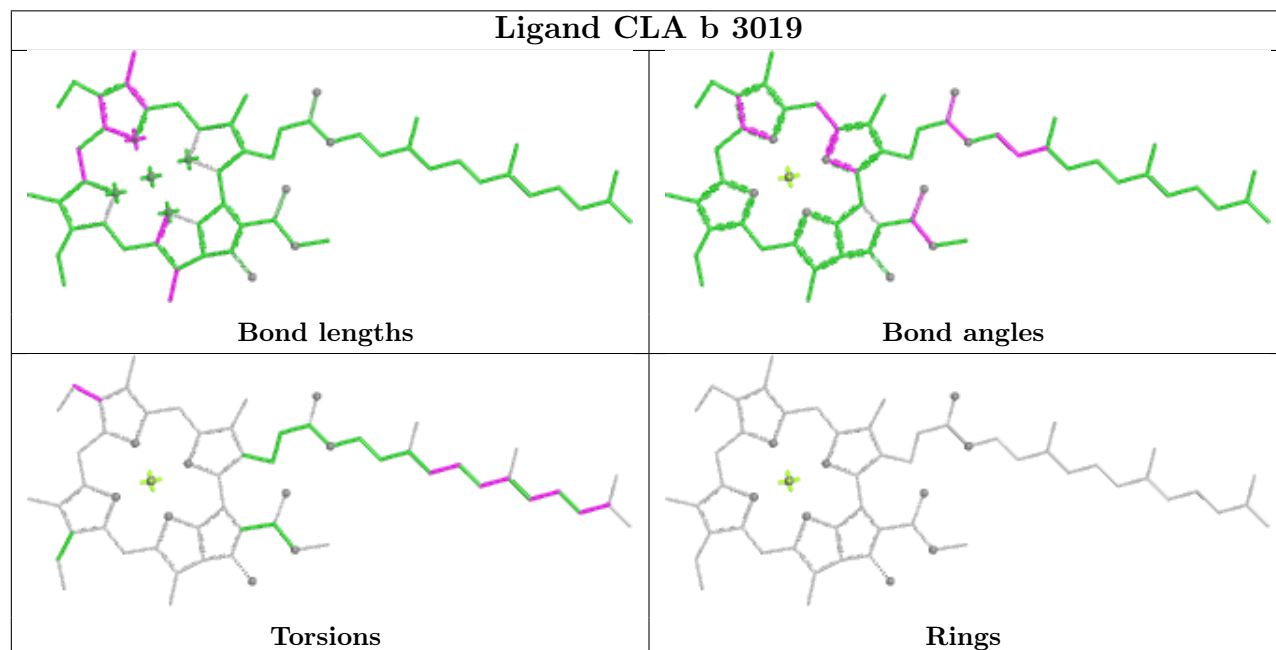
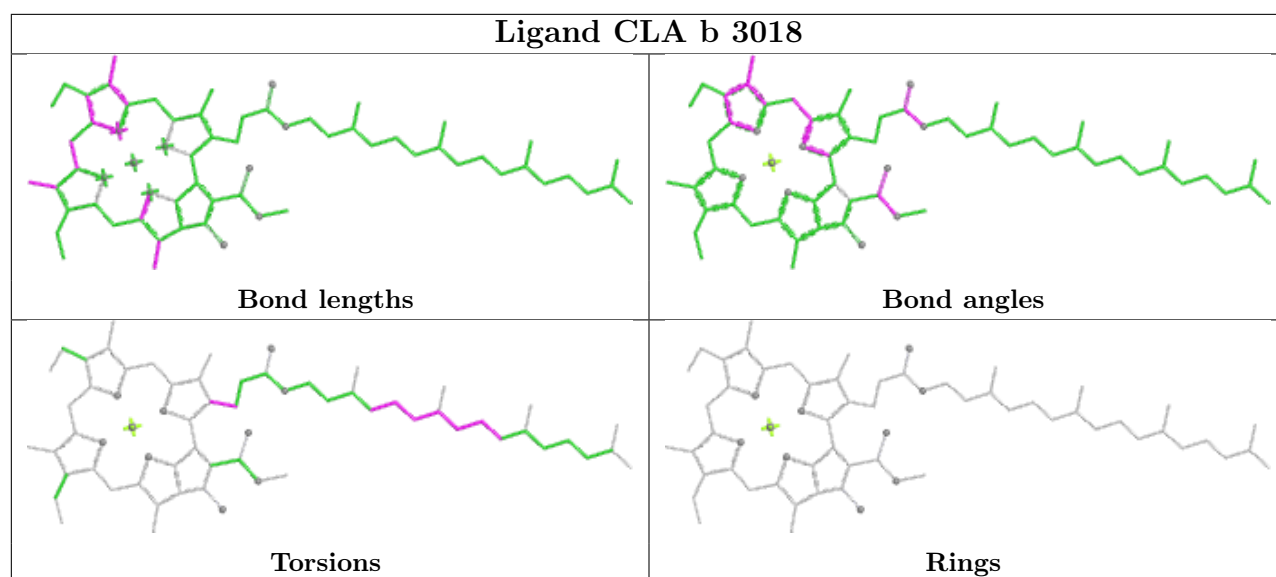


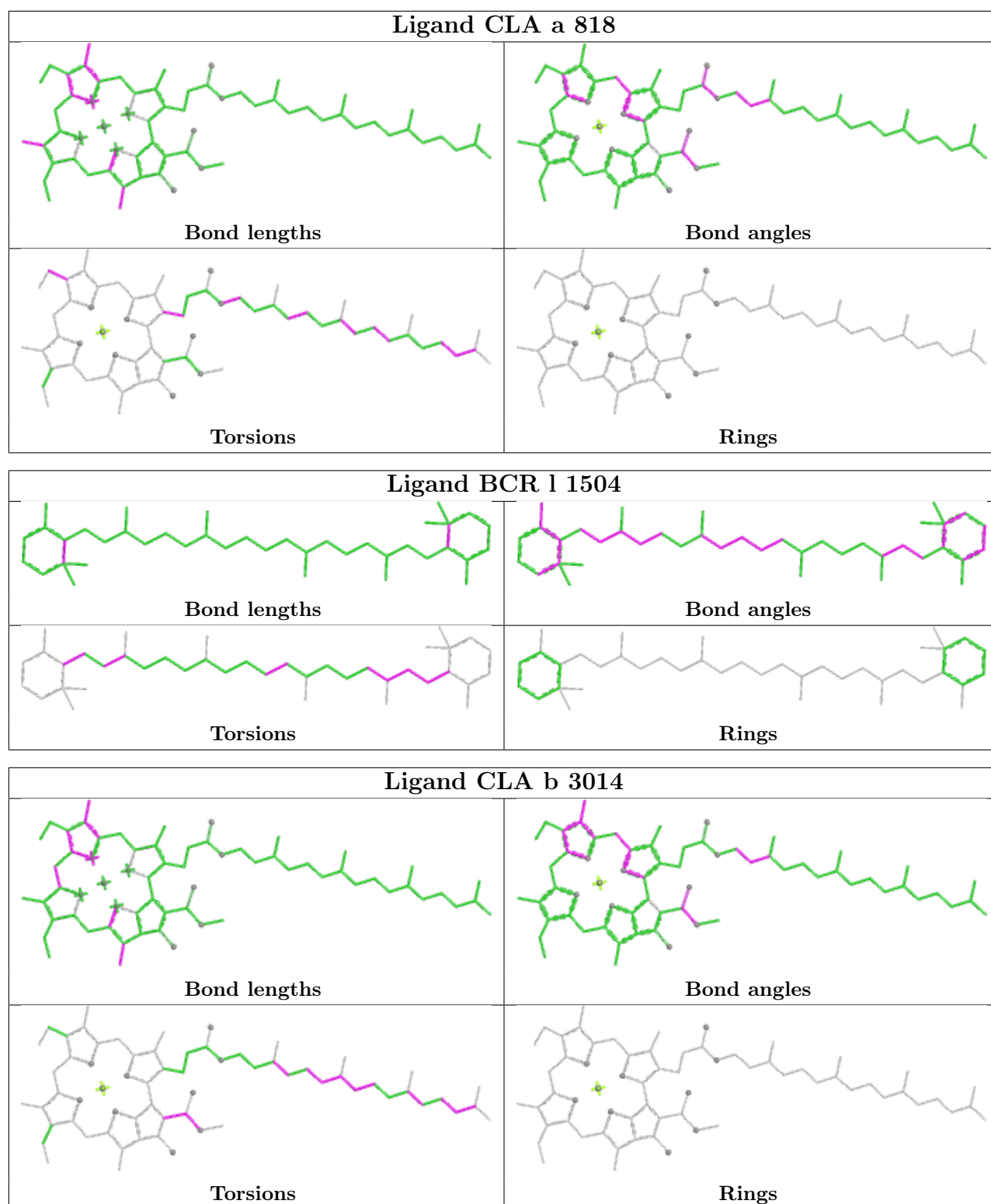
Ligand CLA a 811

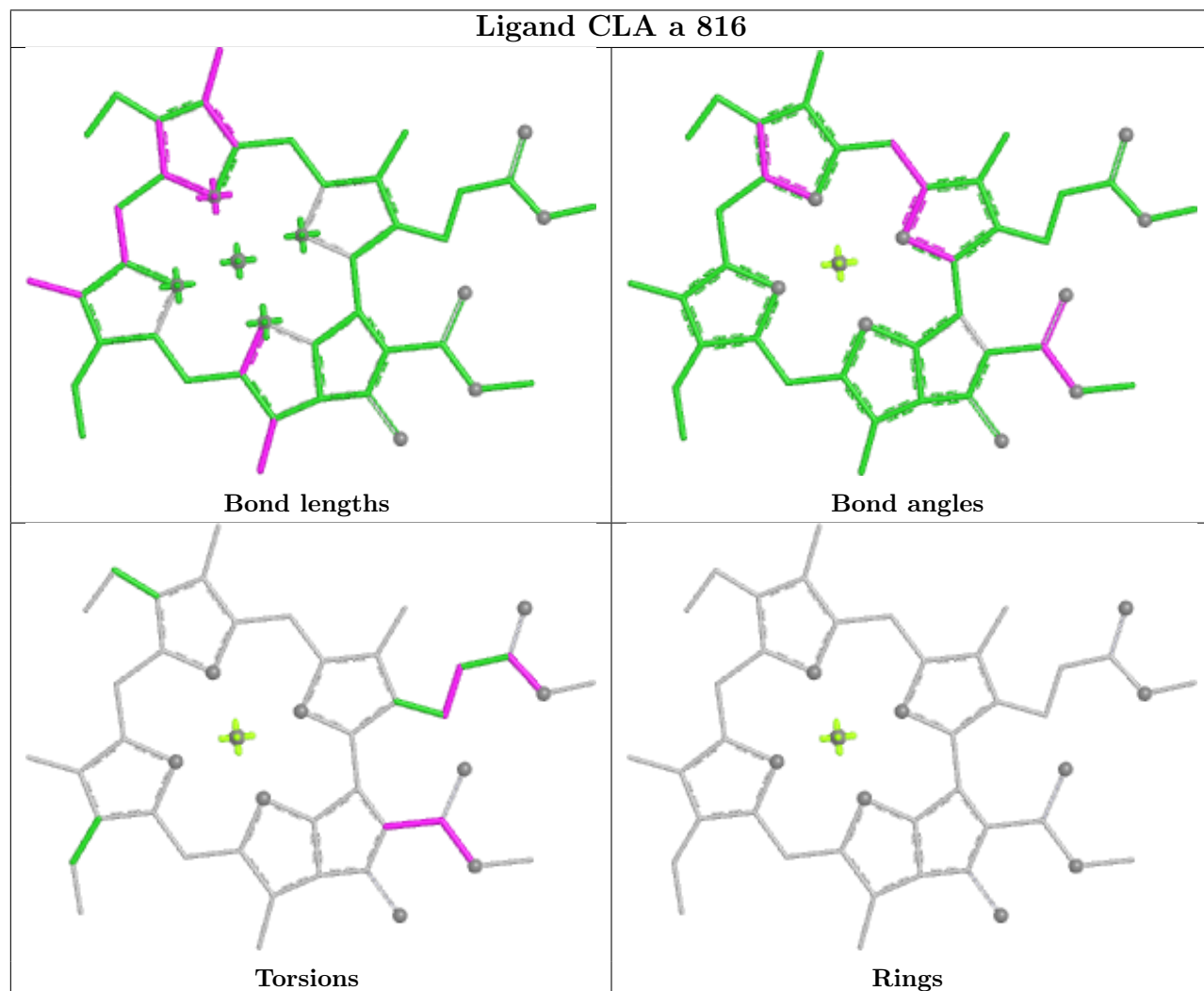
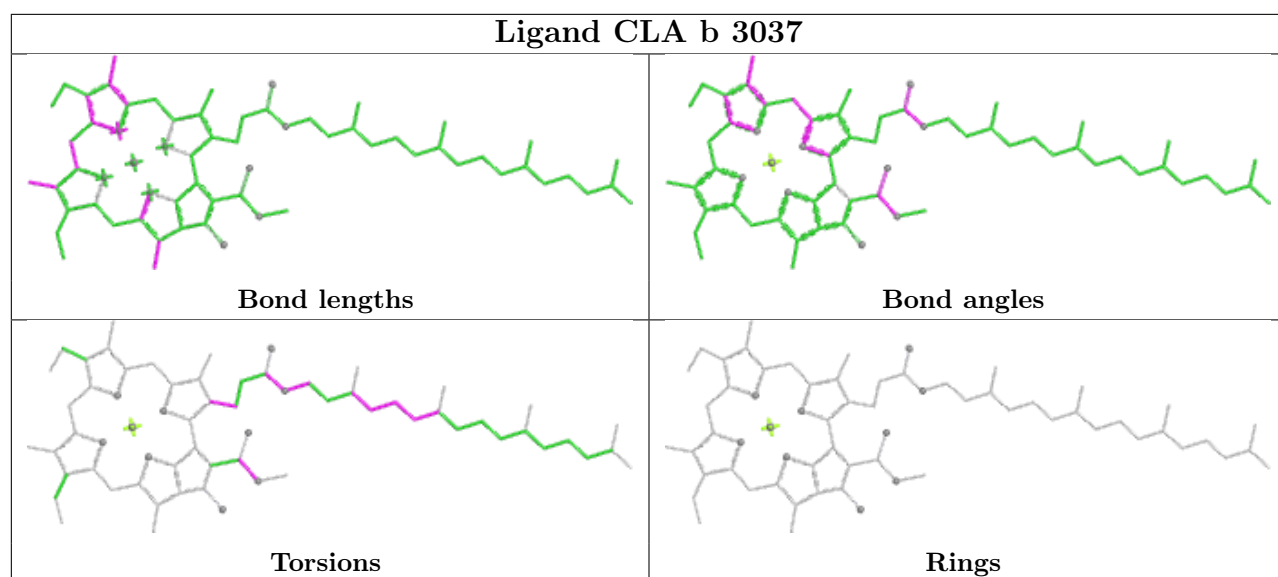


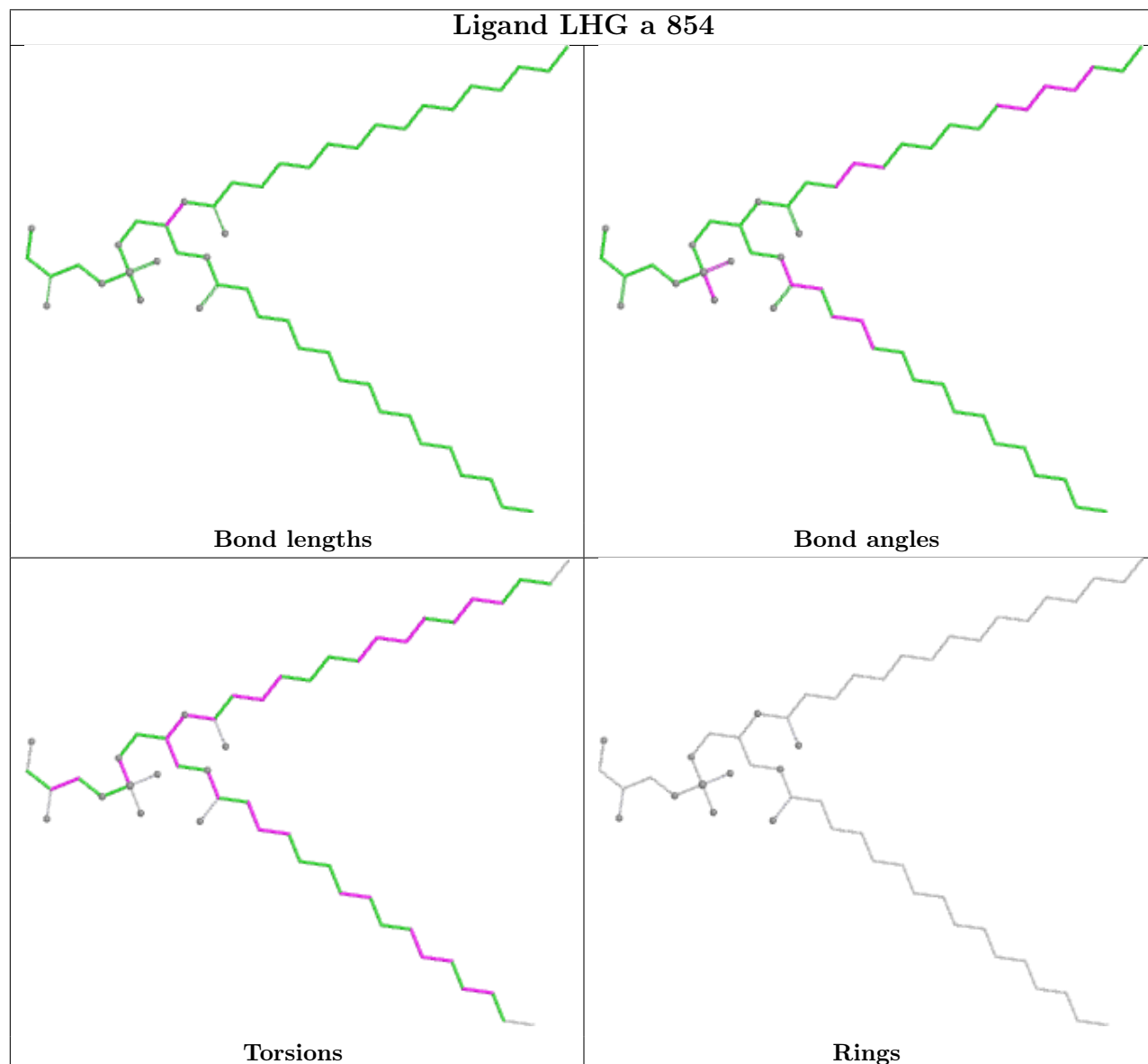
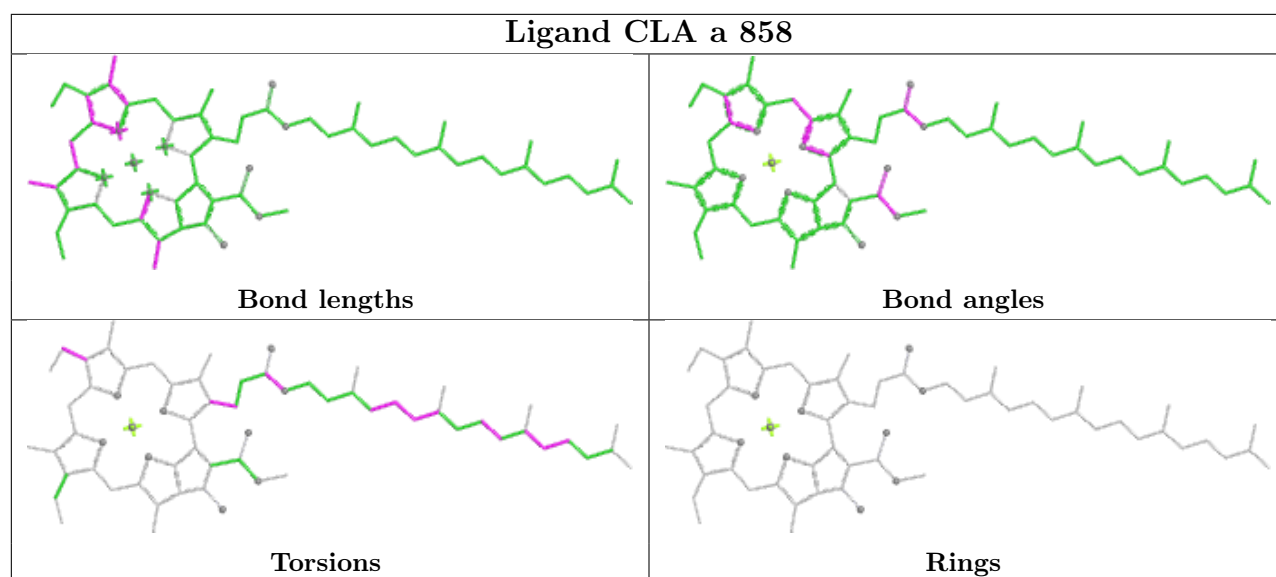
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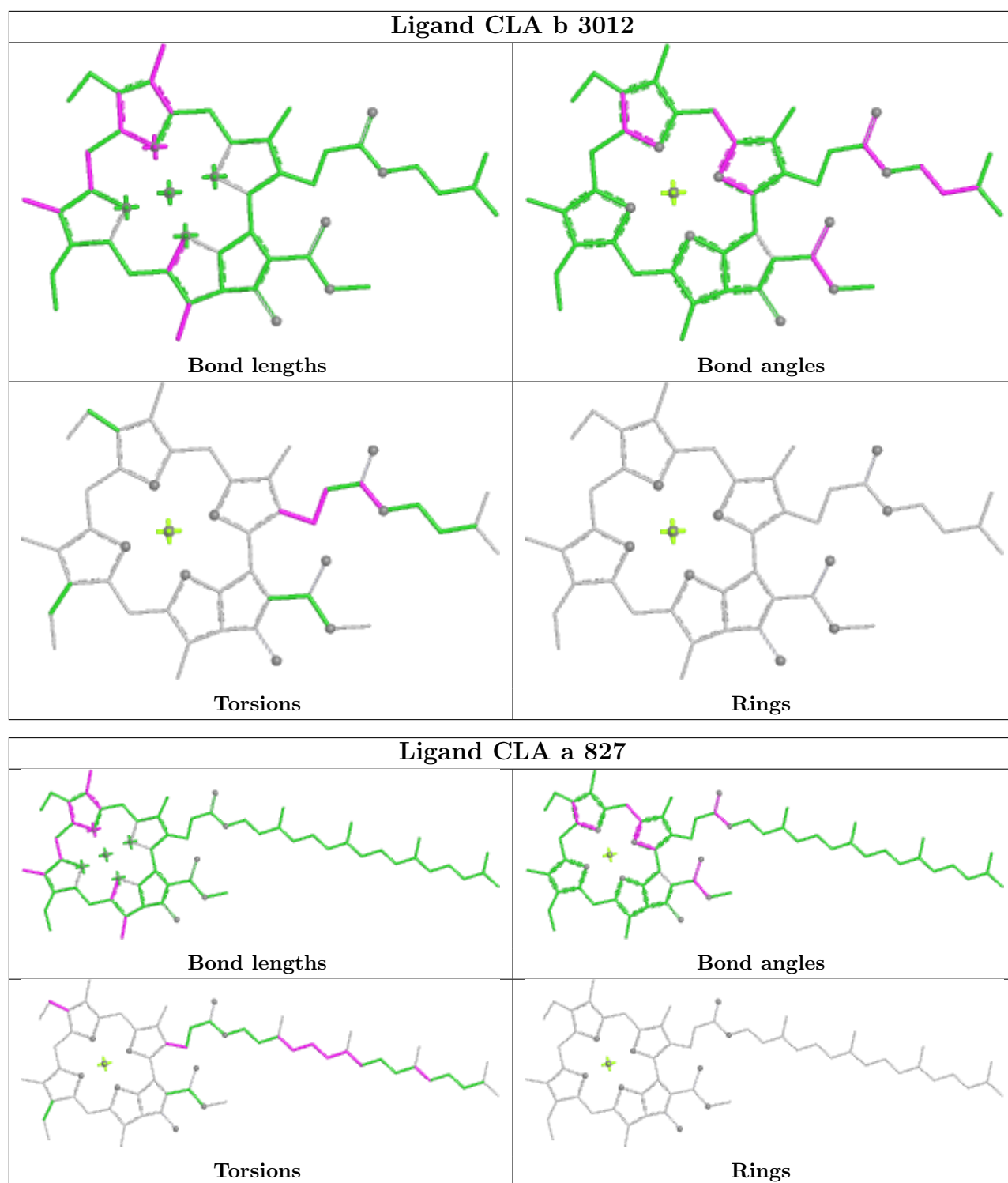


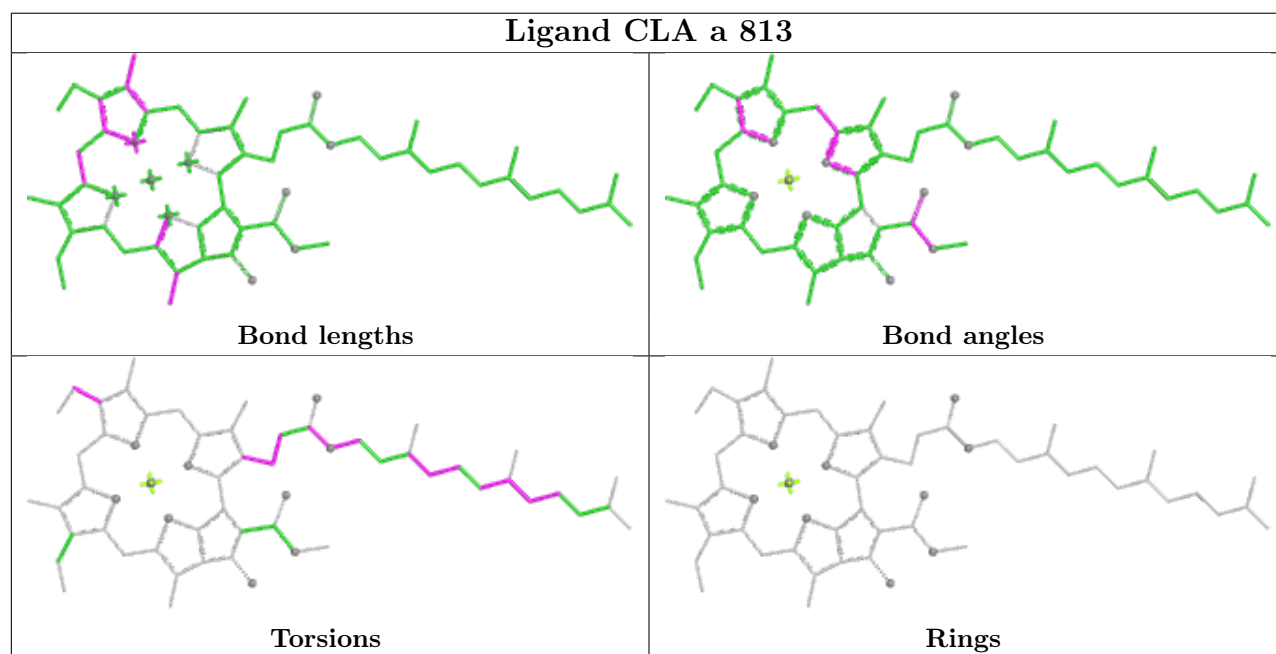
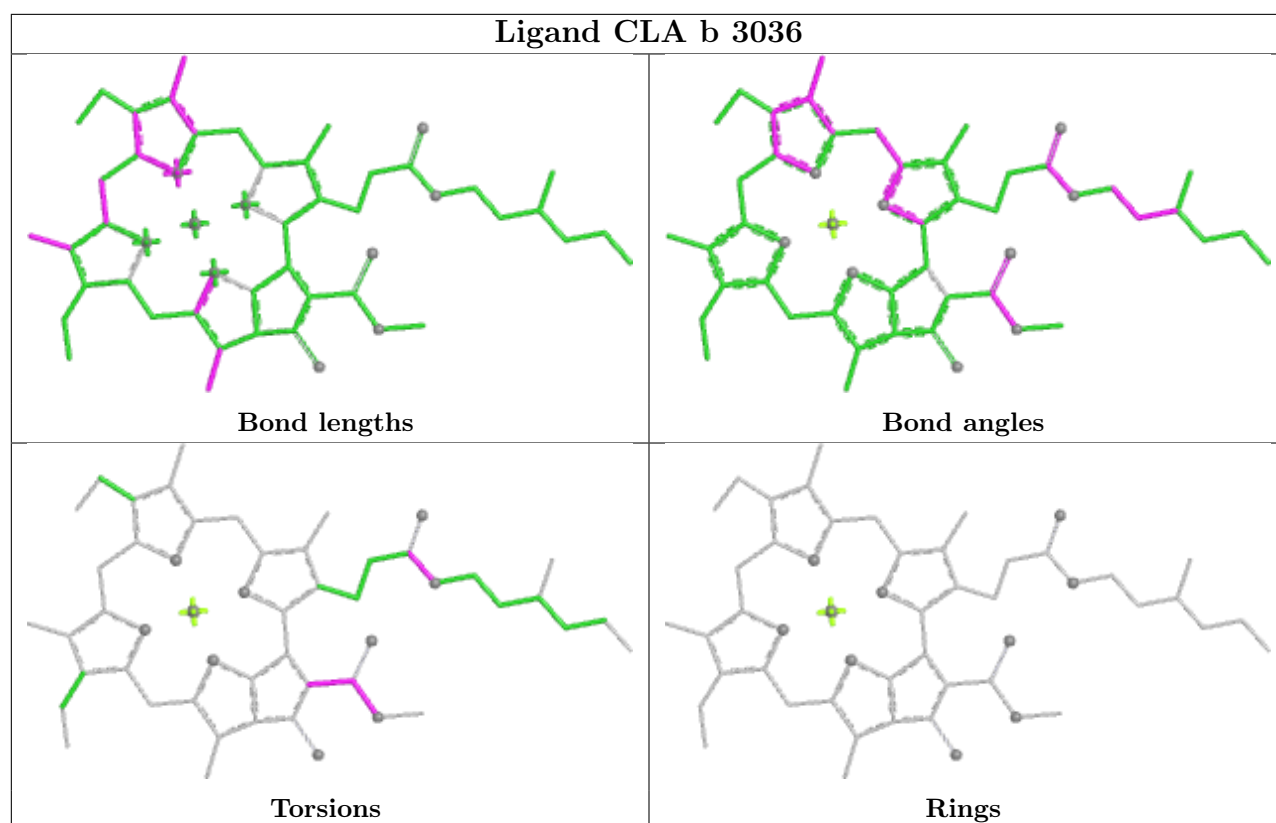


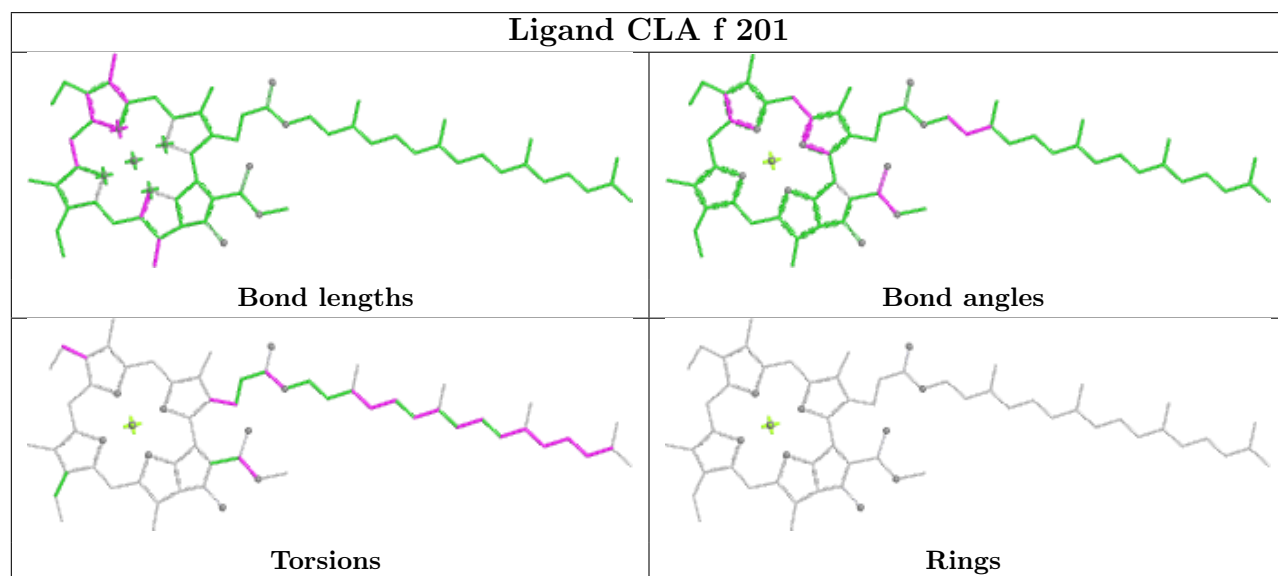
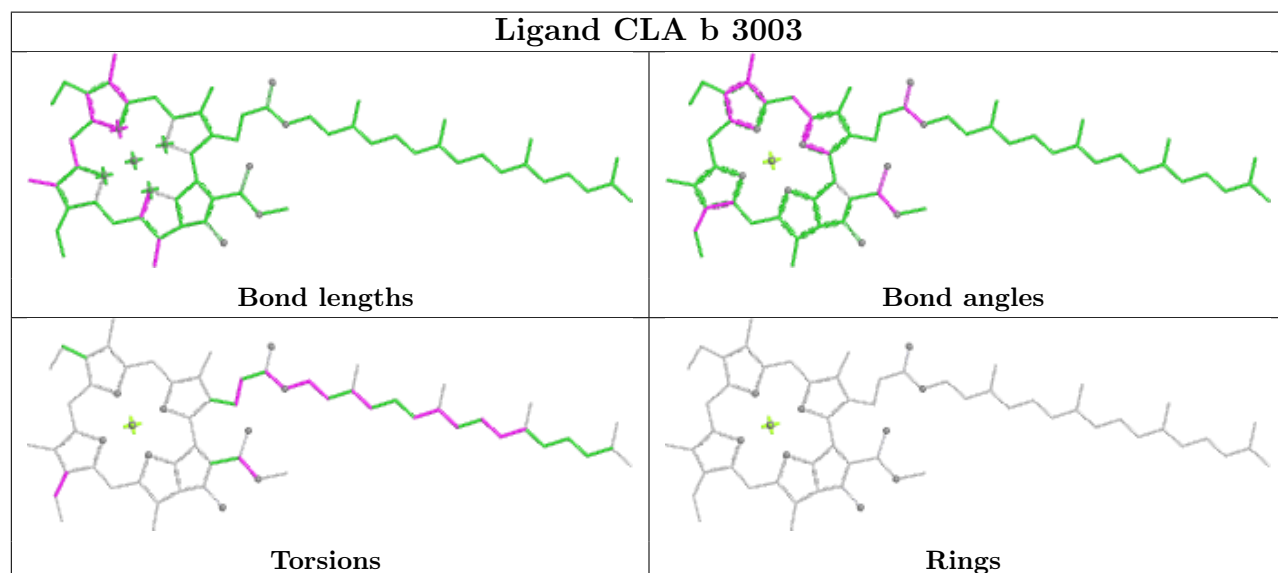
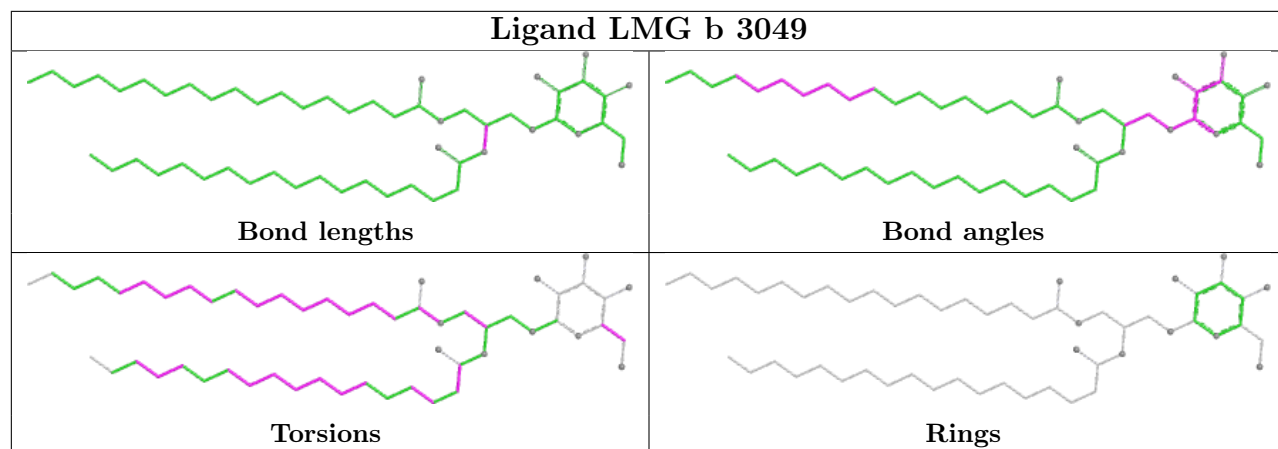


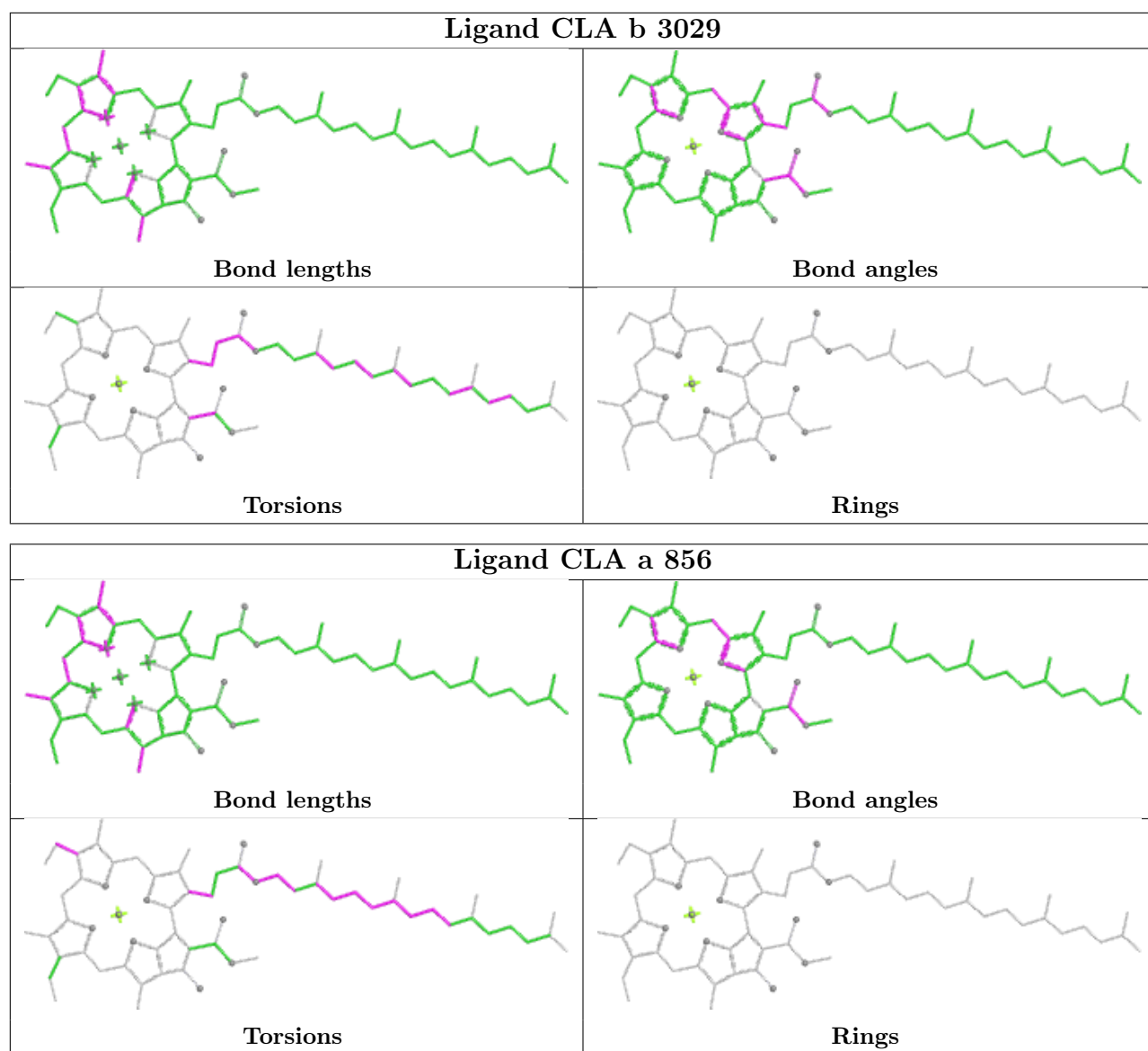


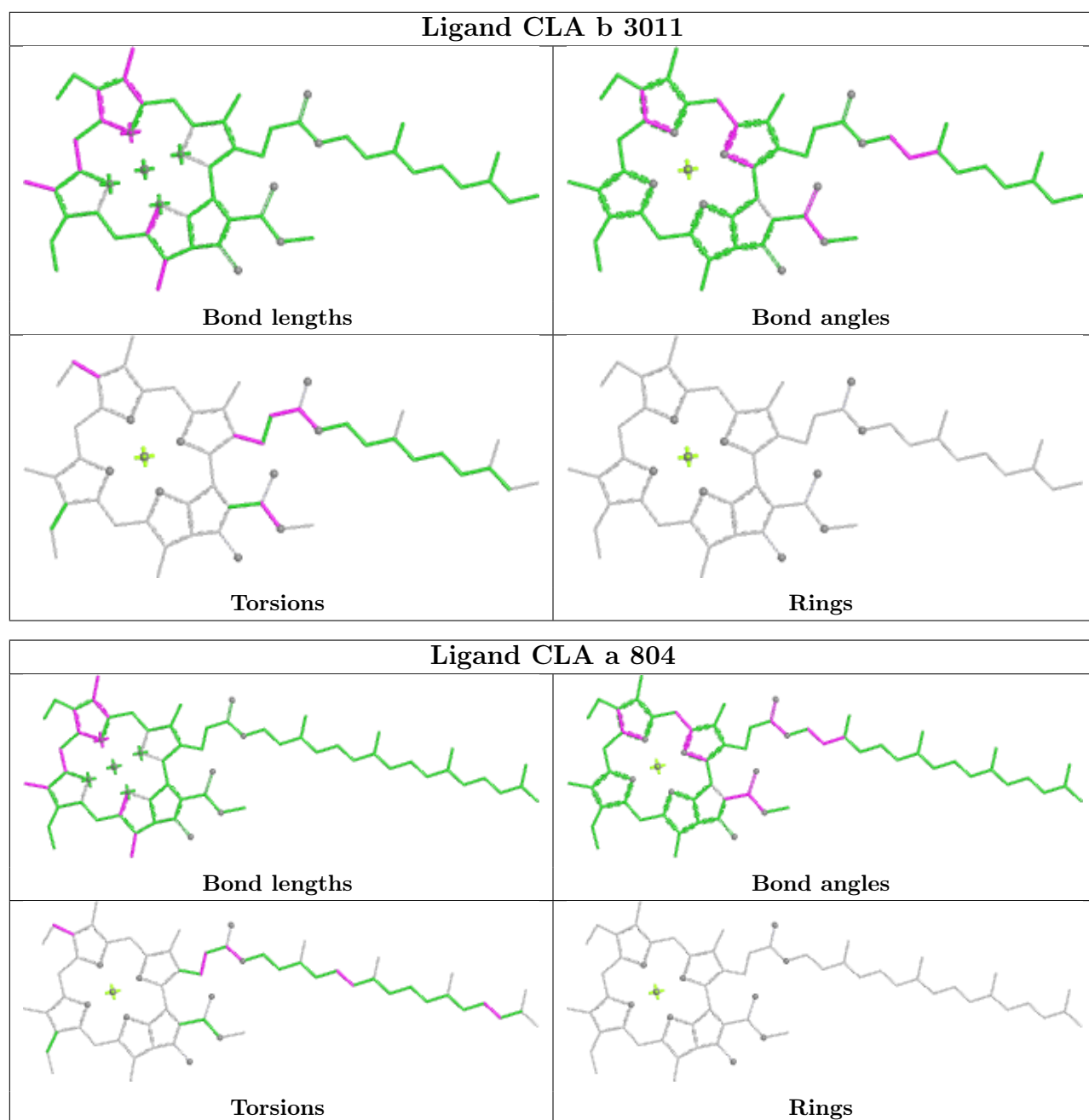


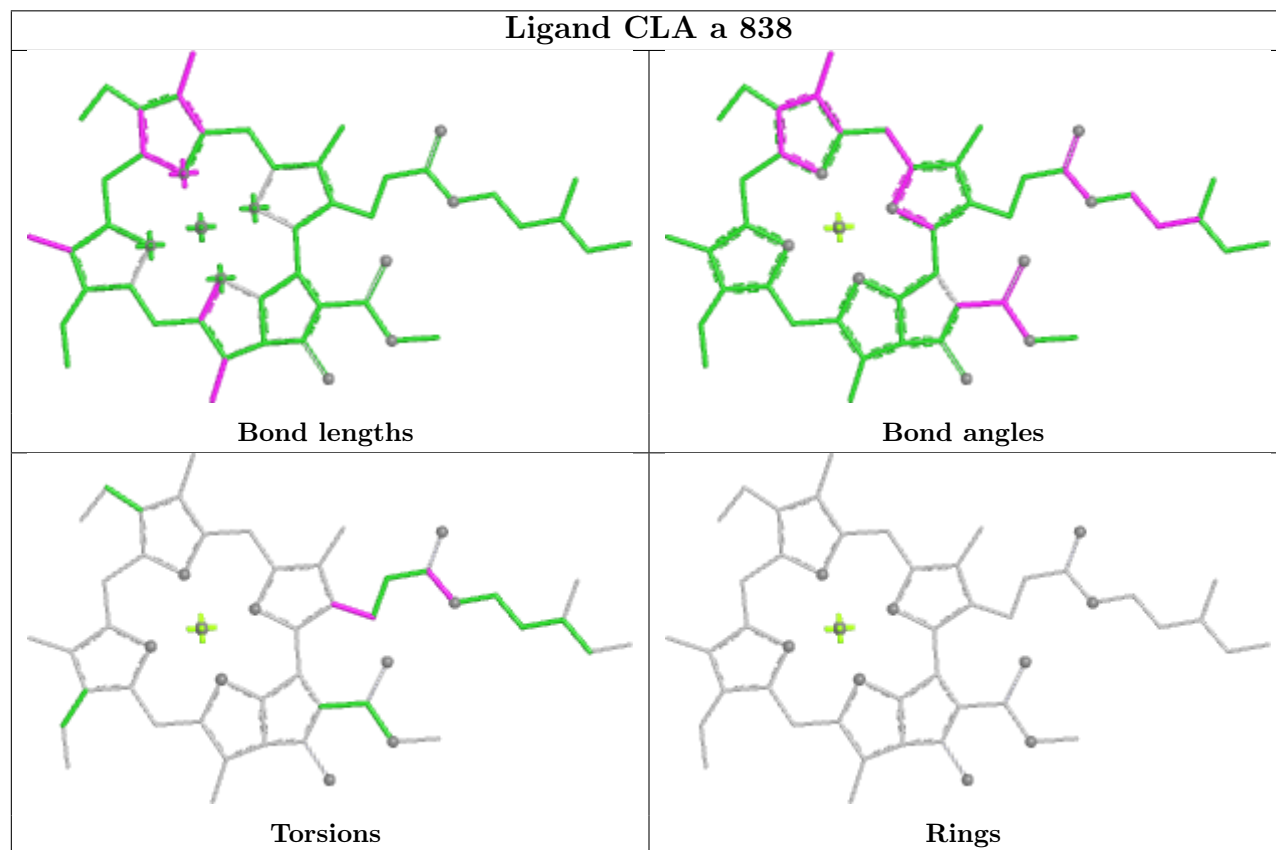
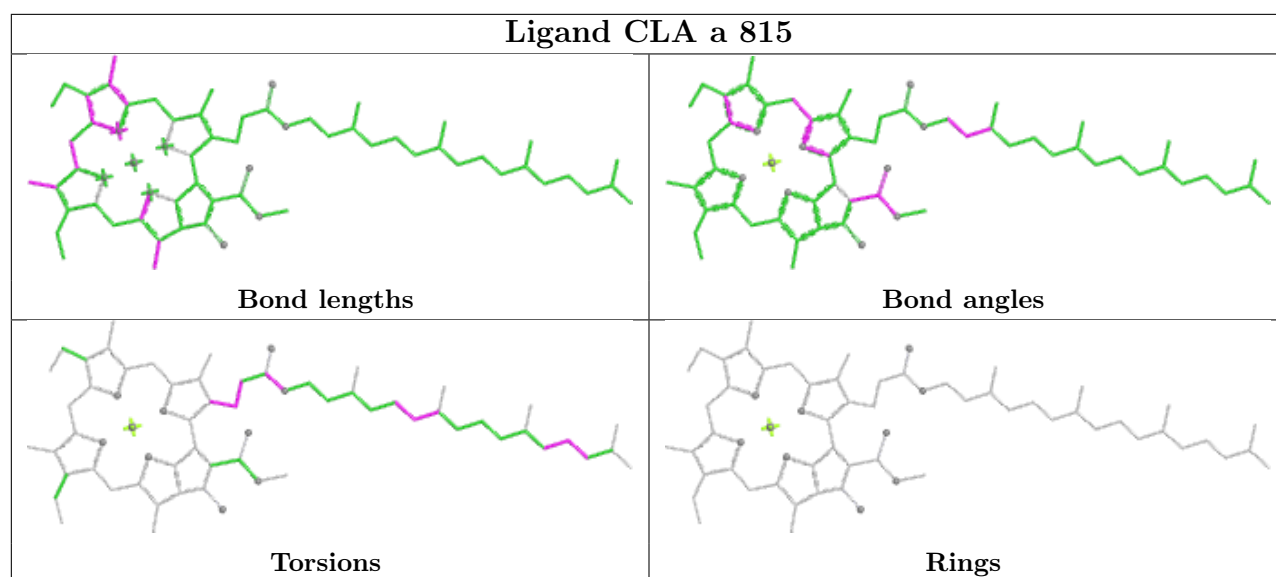


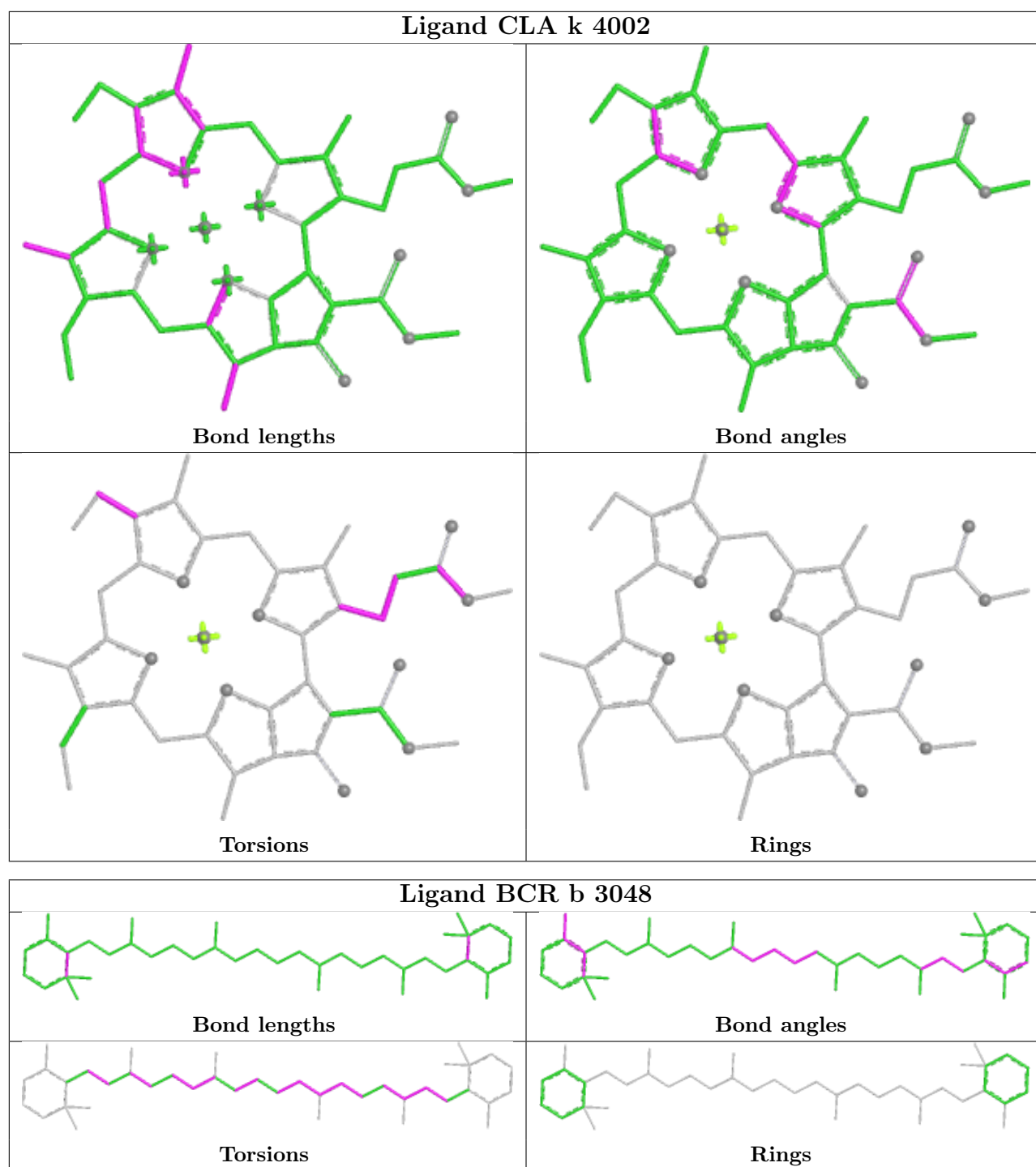


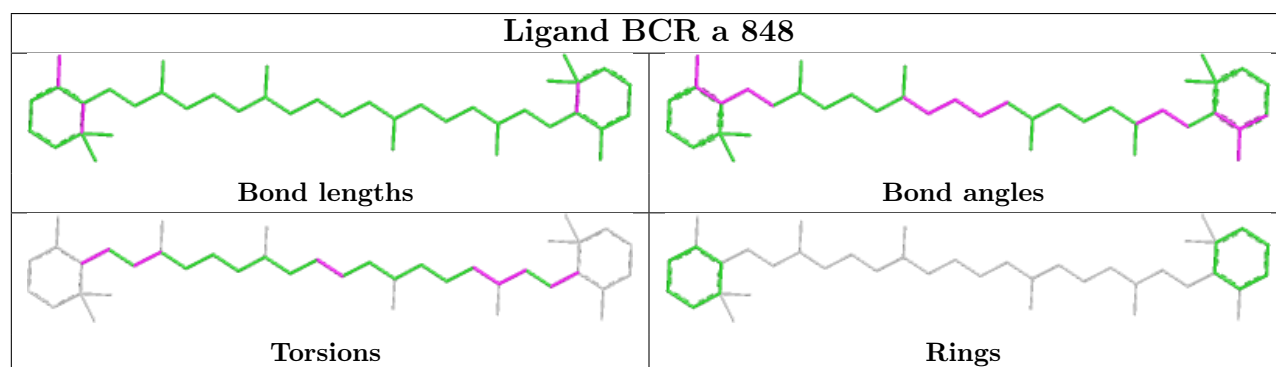
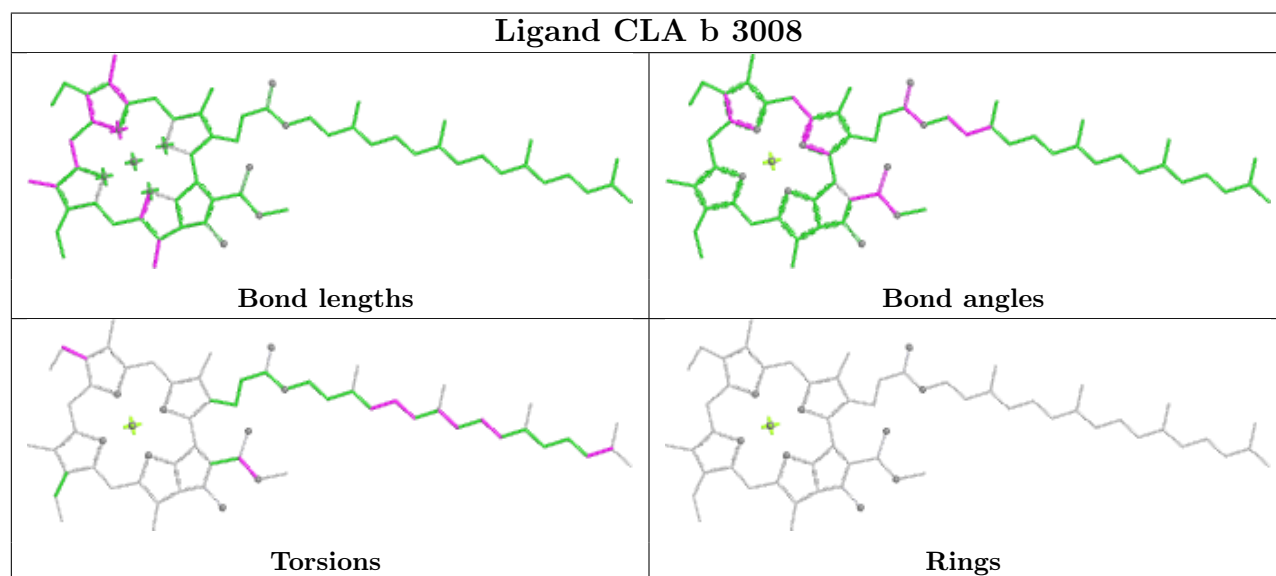
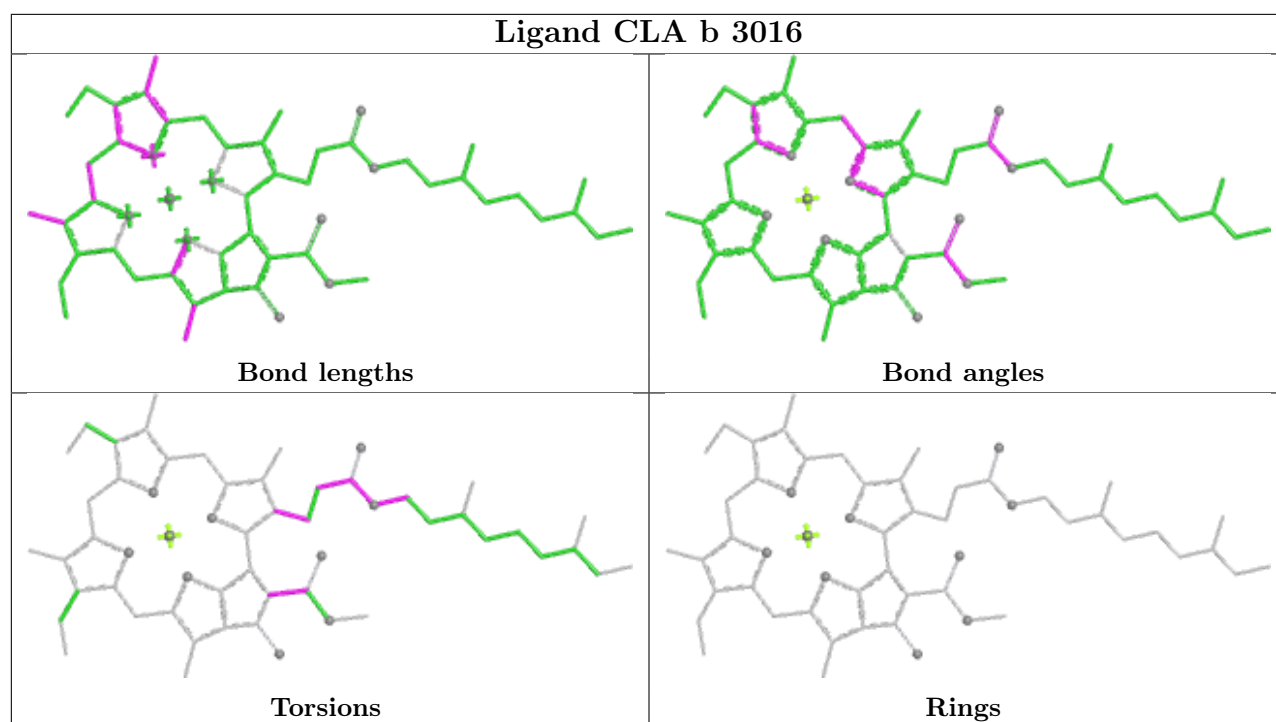


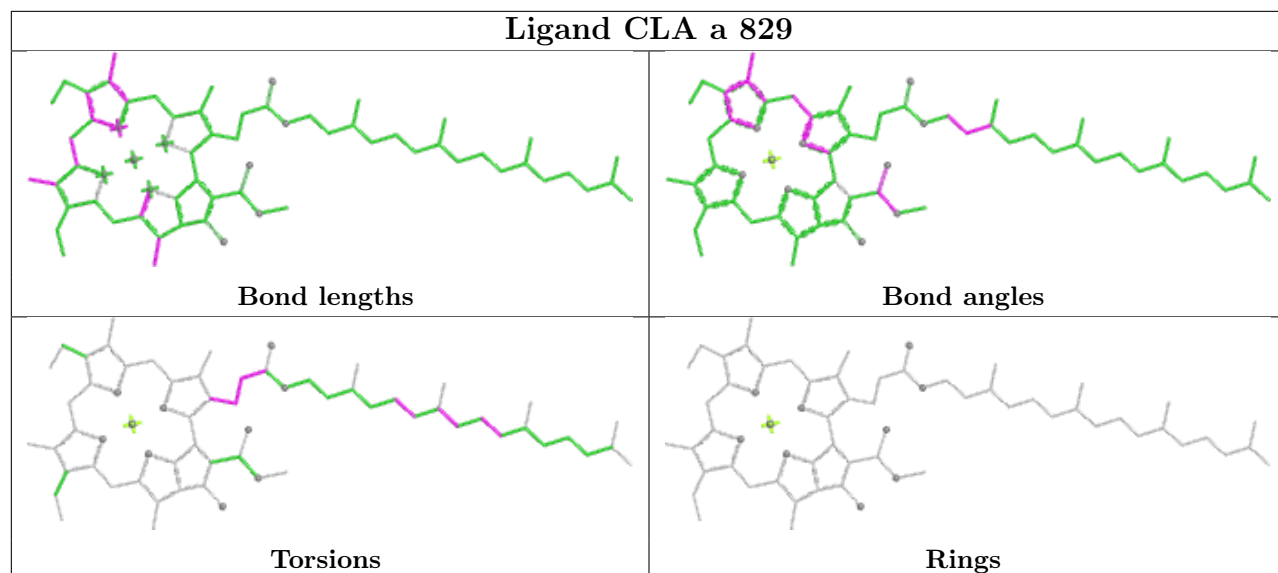
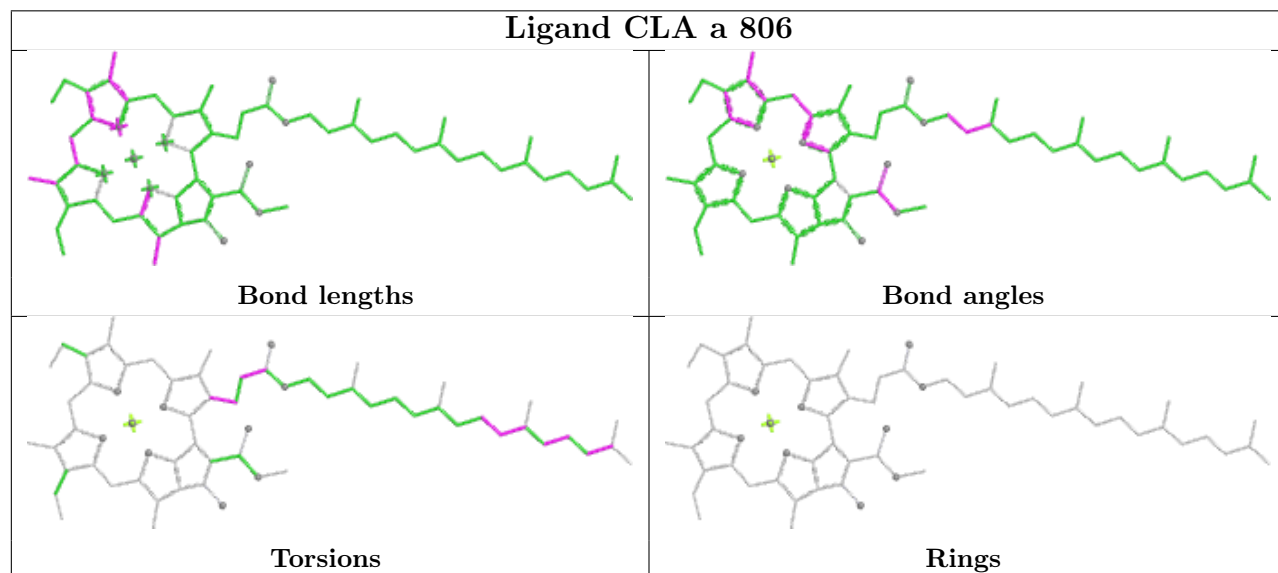
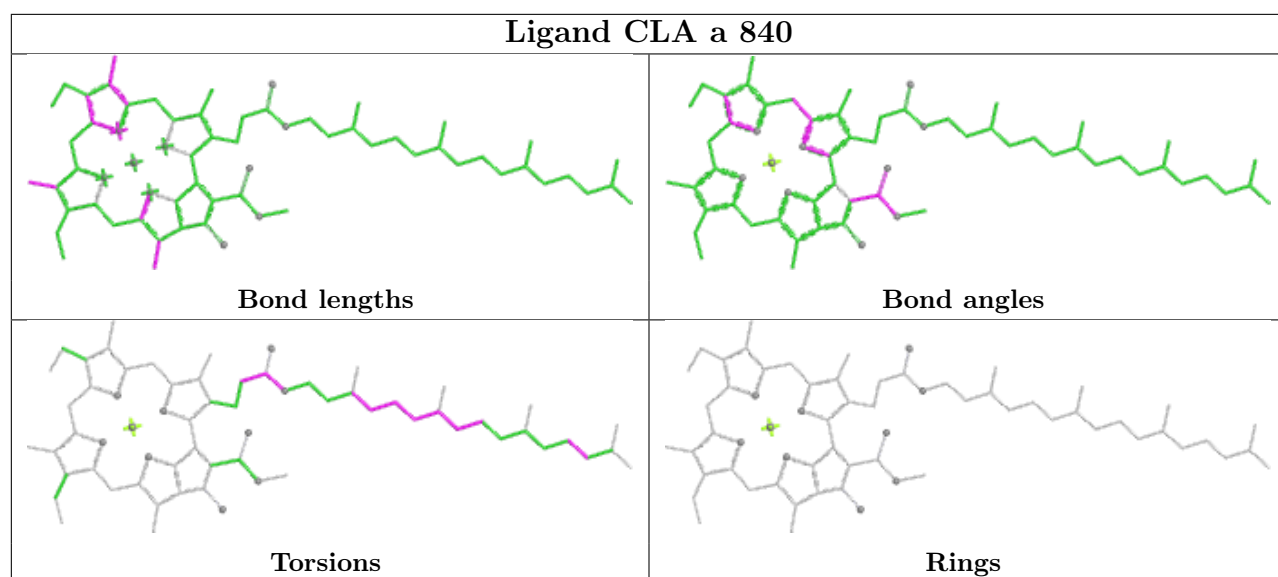


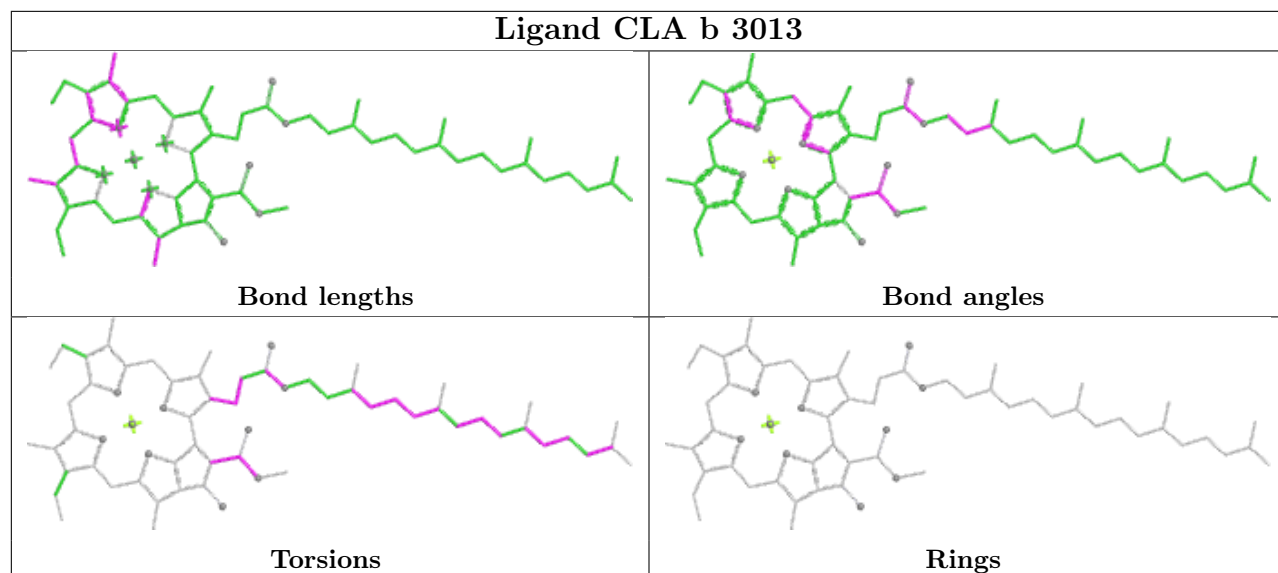
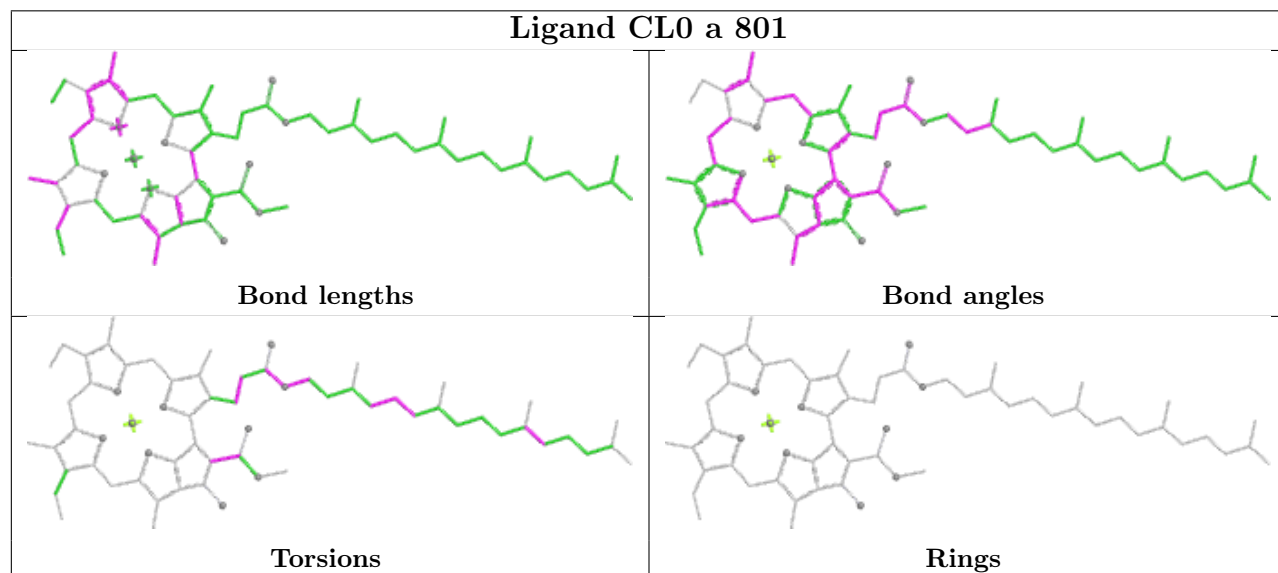
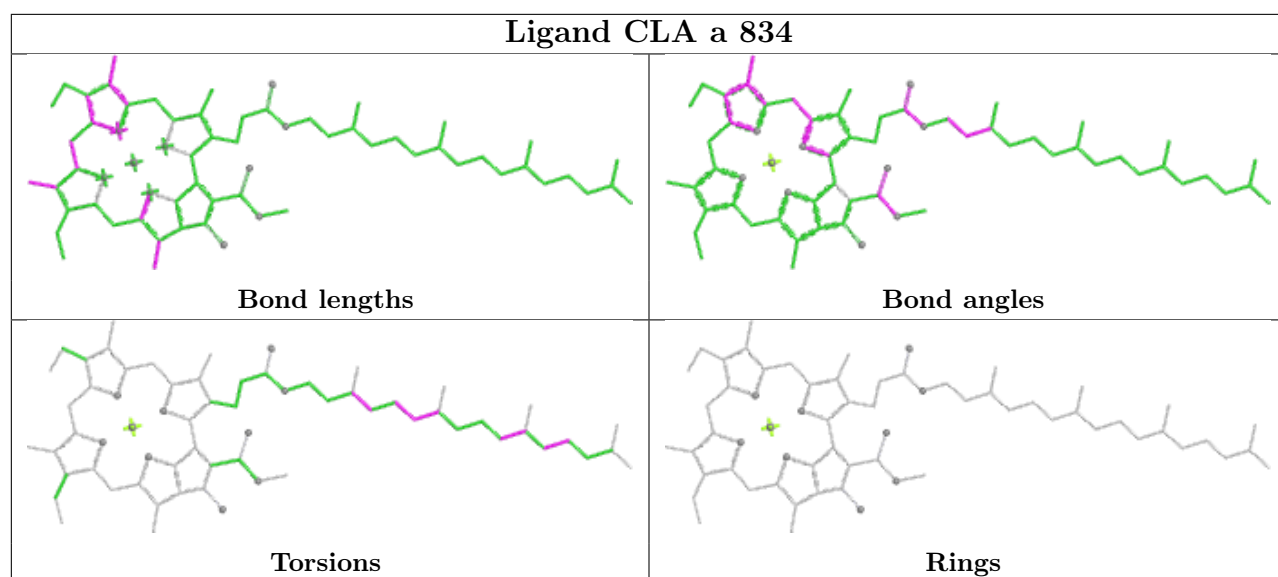


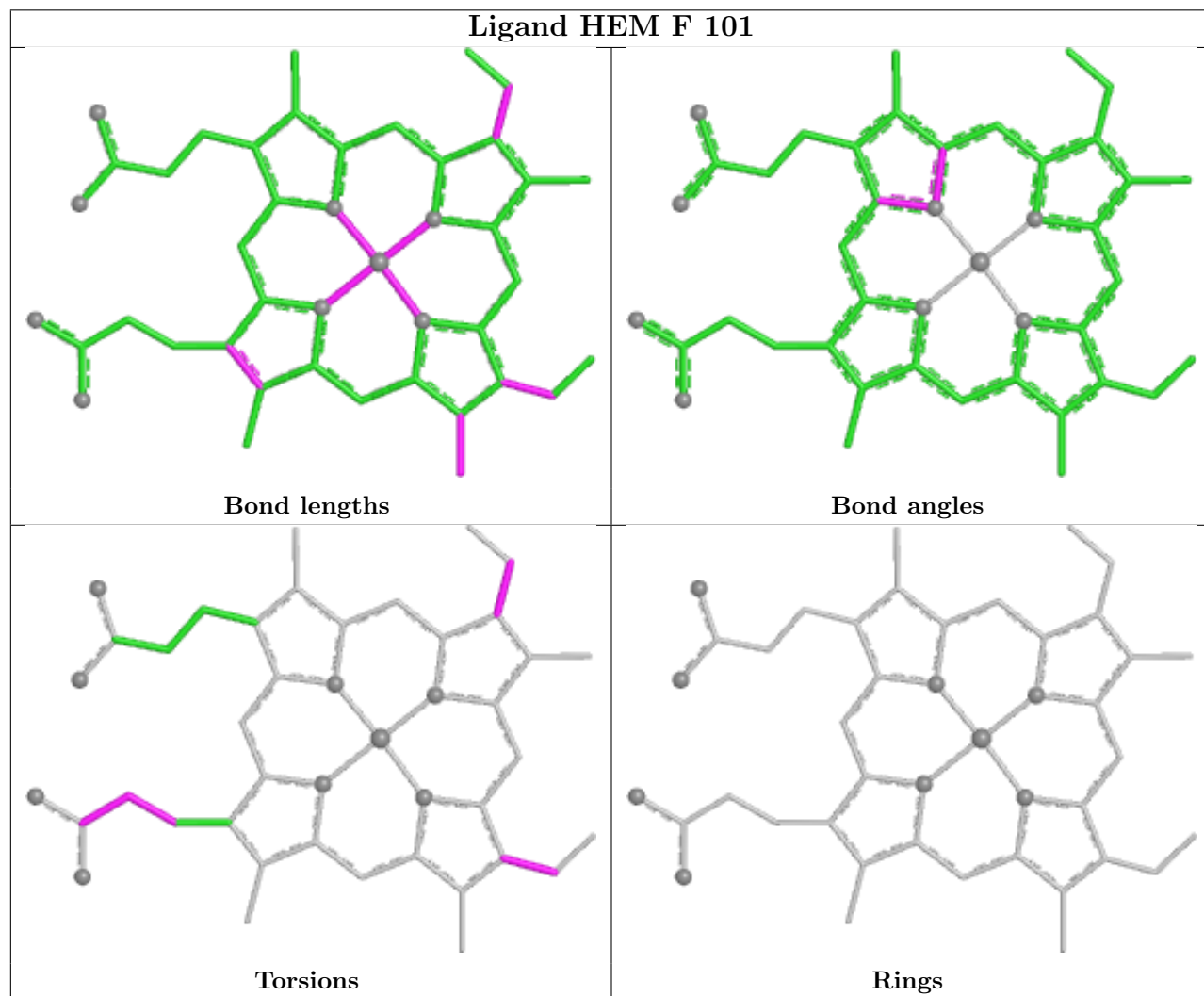
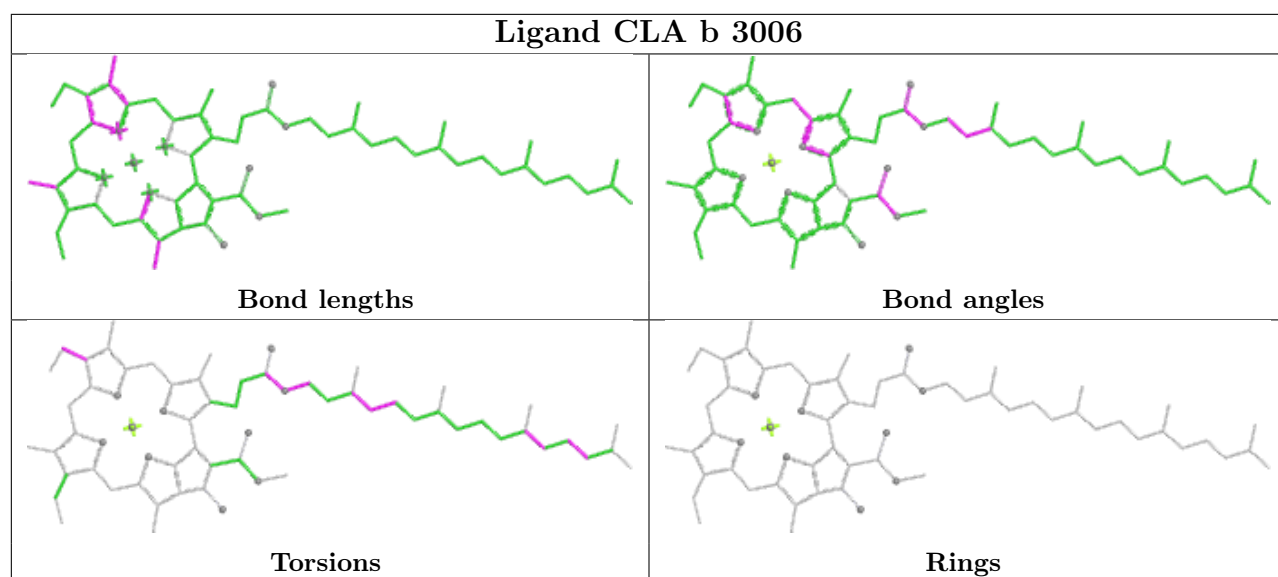


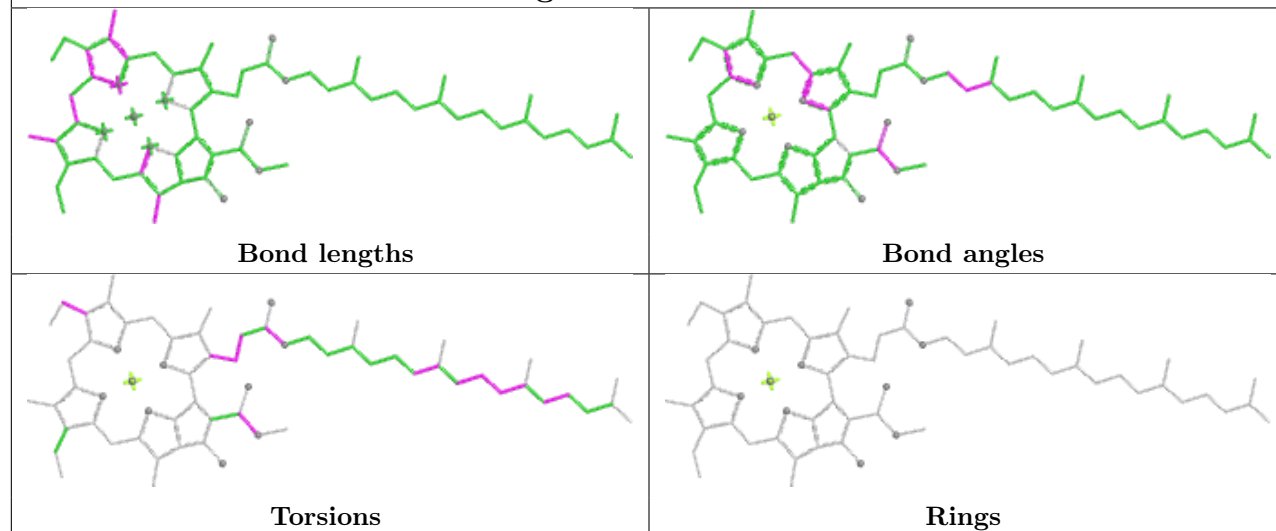
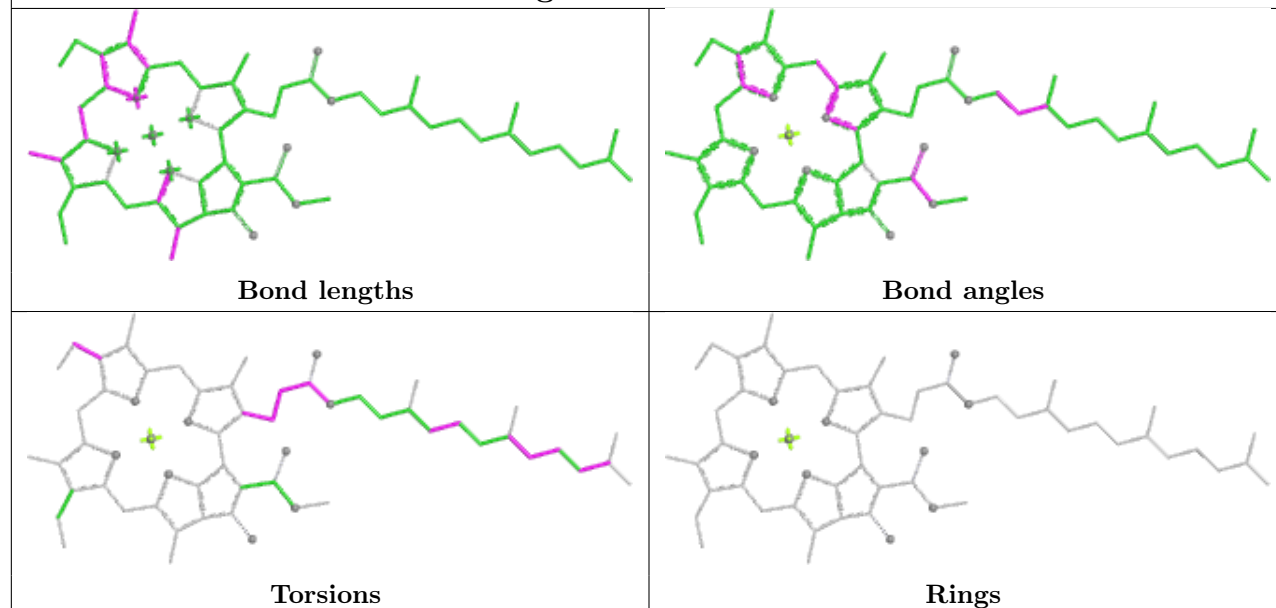


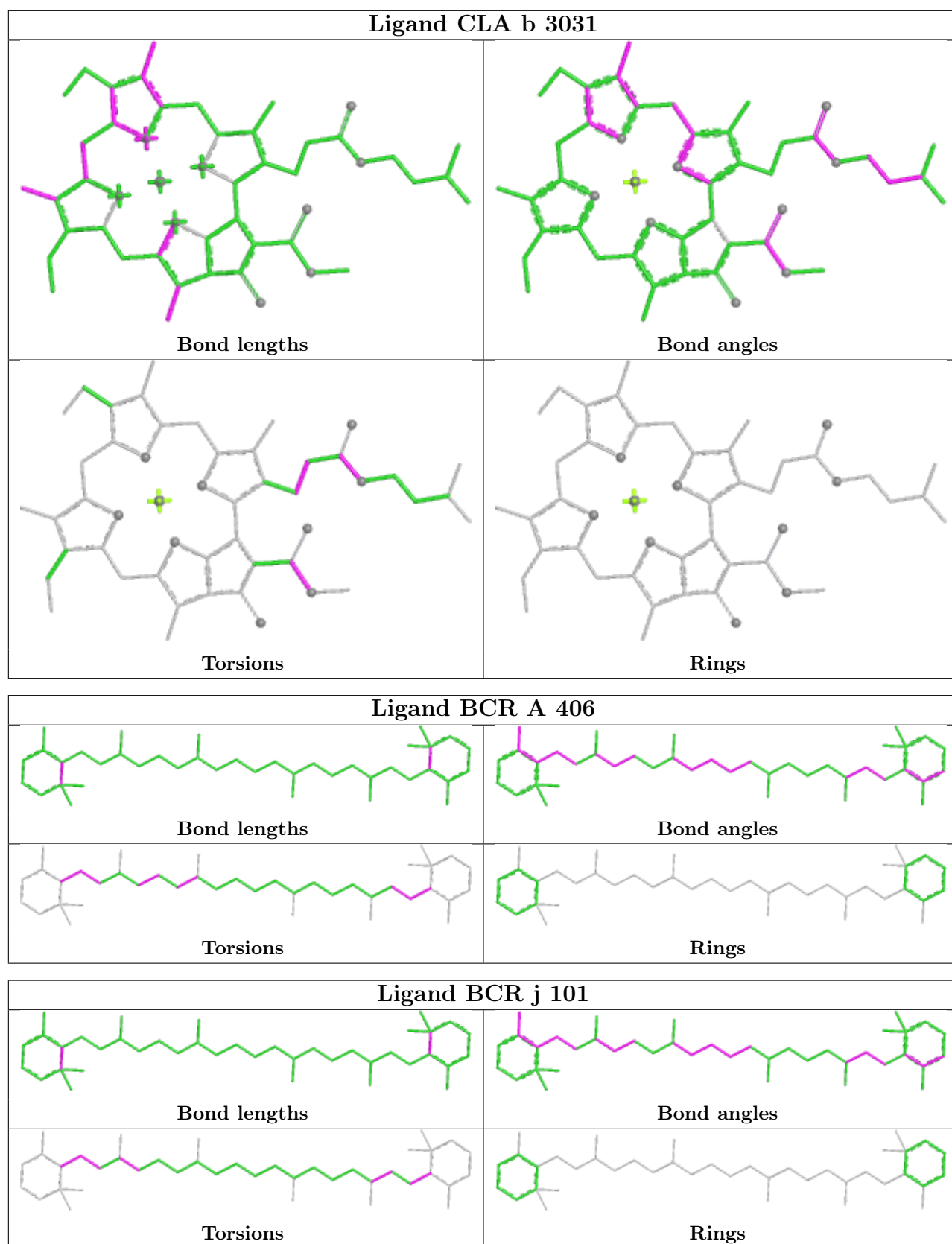


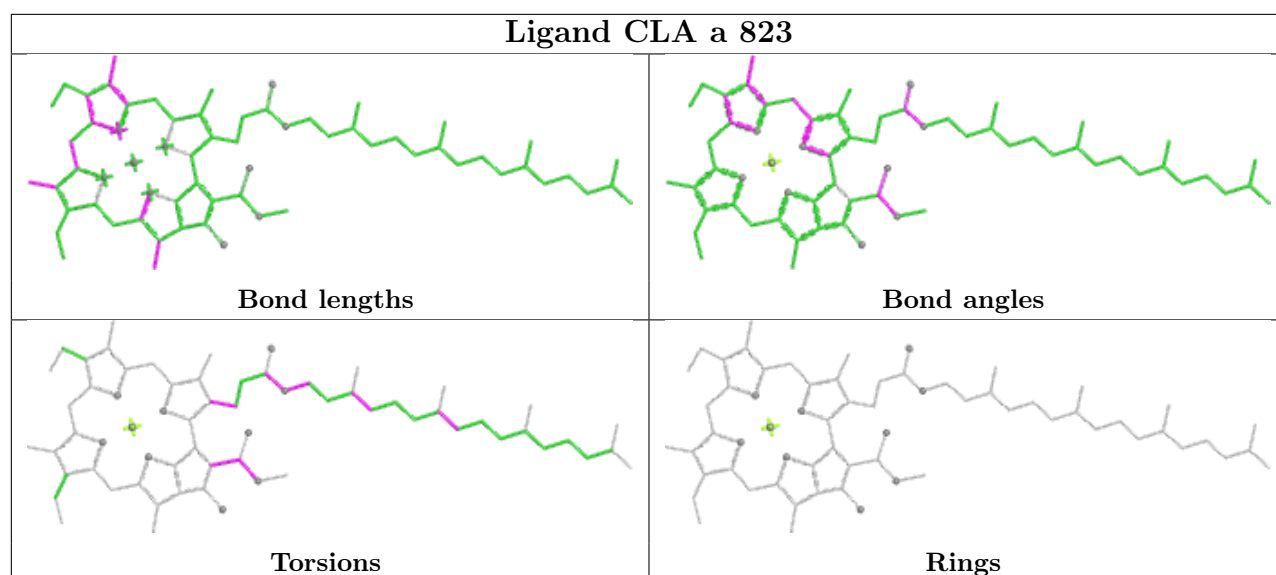
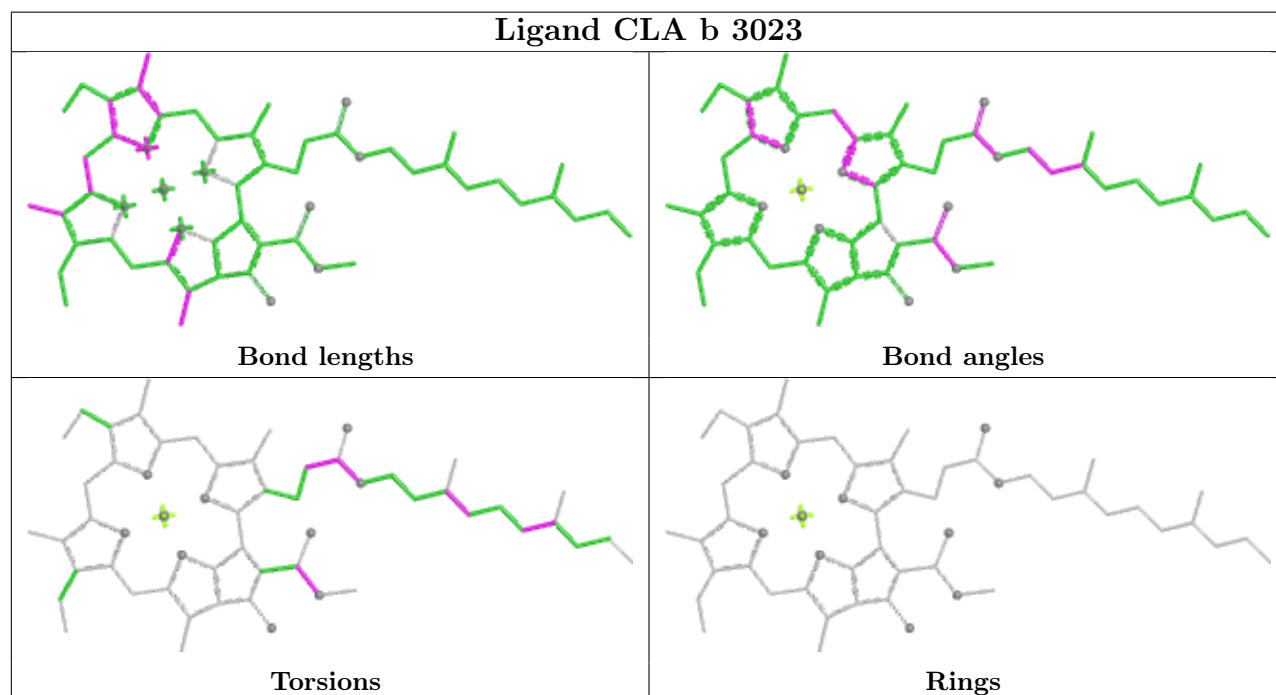
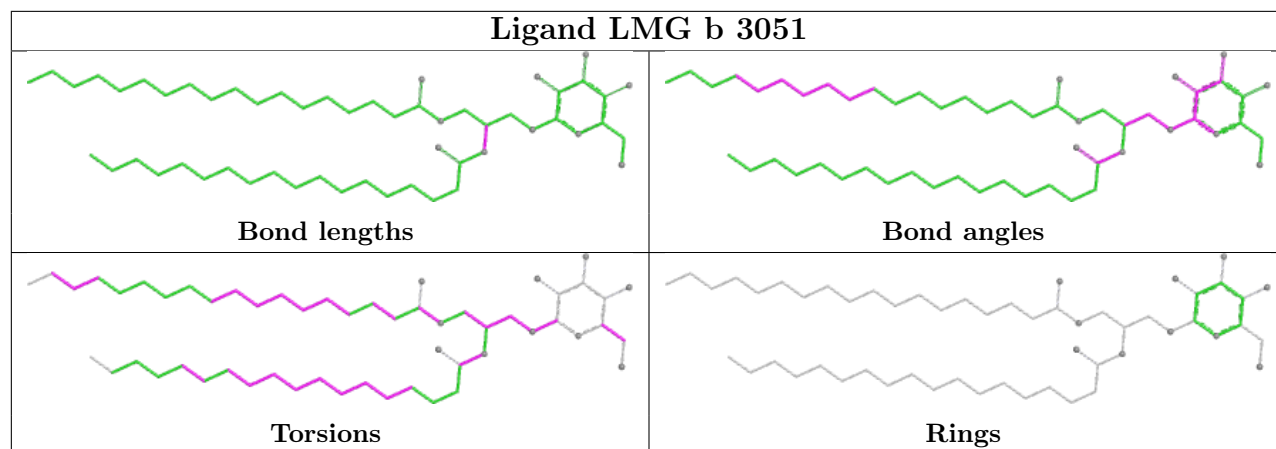




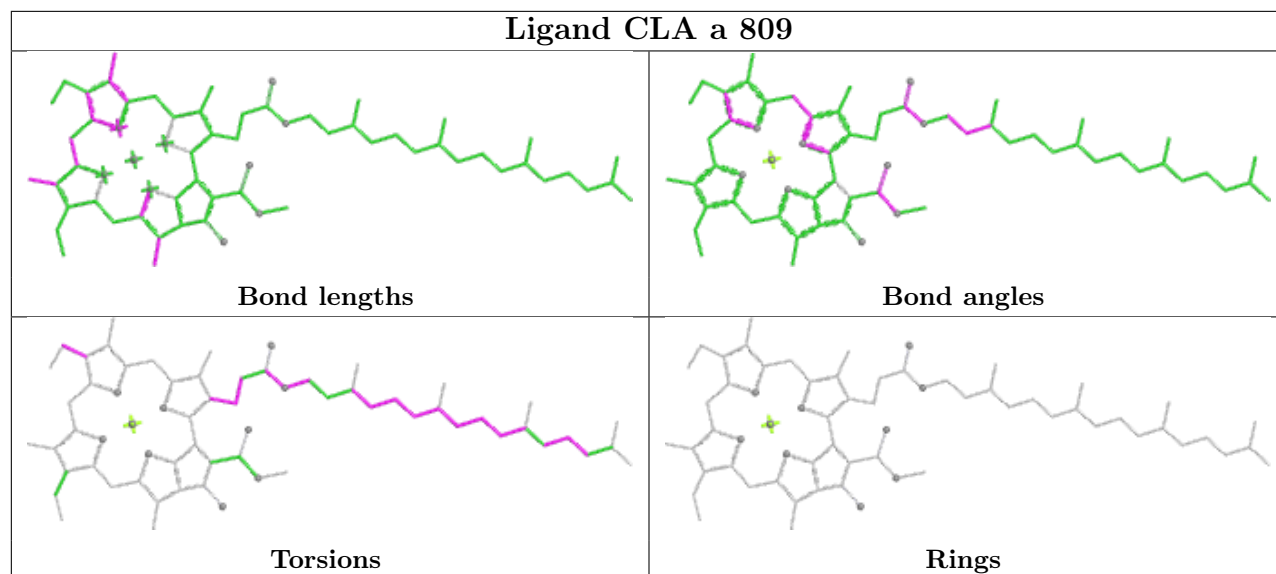


Ligand CLA a 842**Ligand CLA a 833**

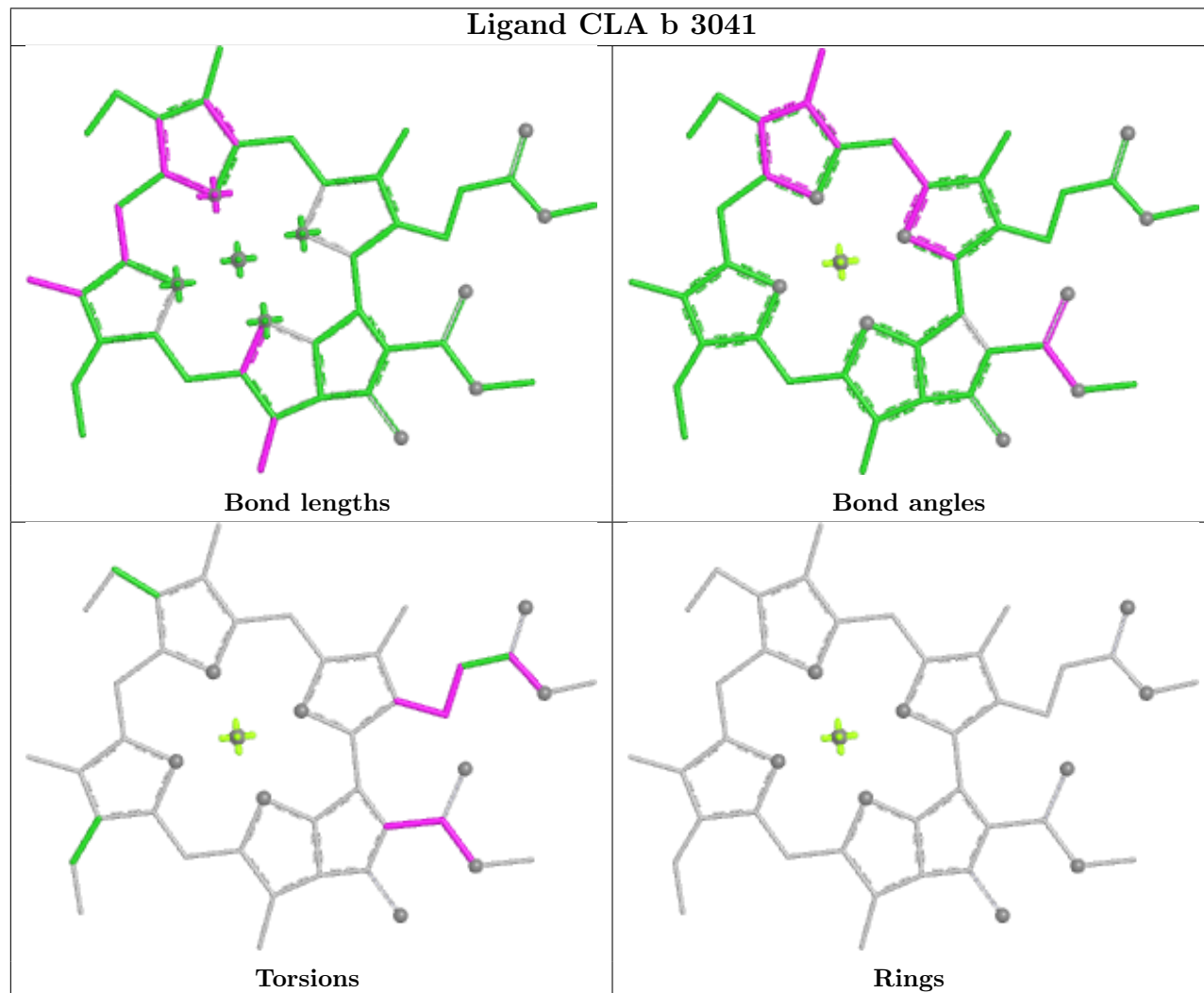


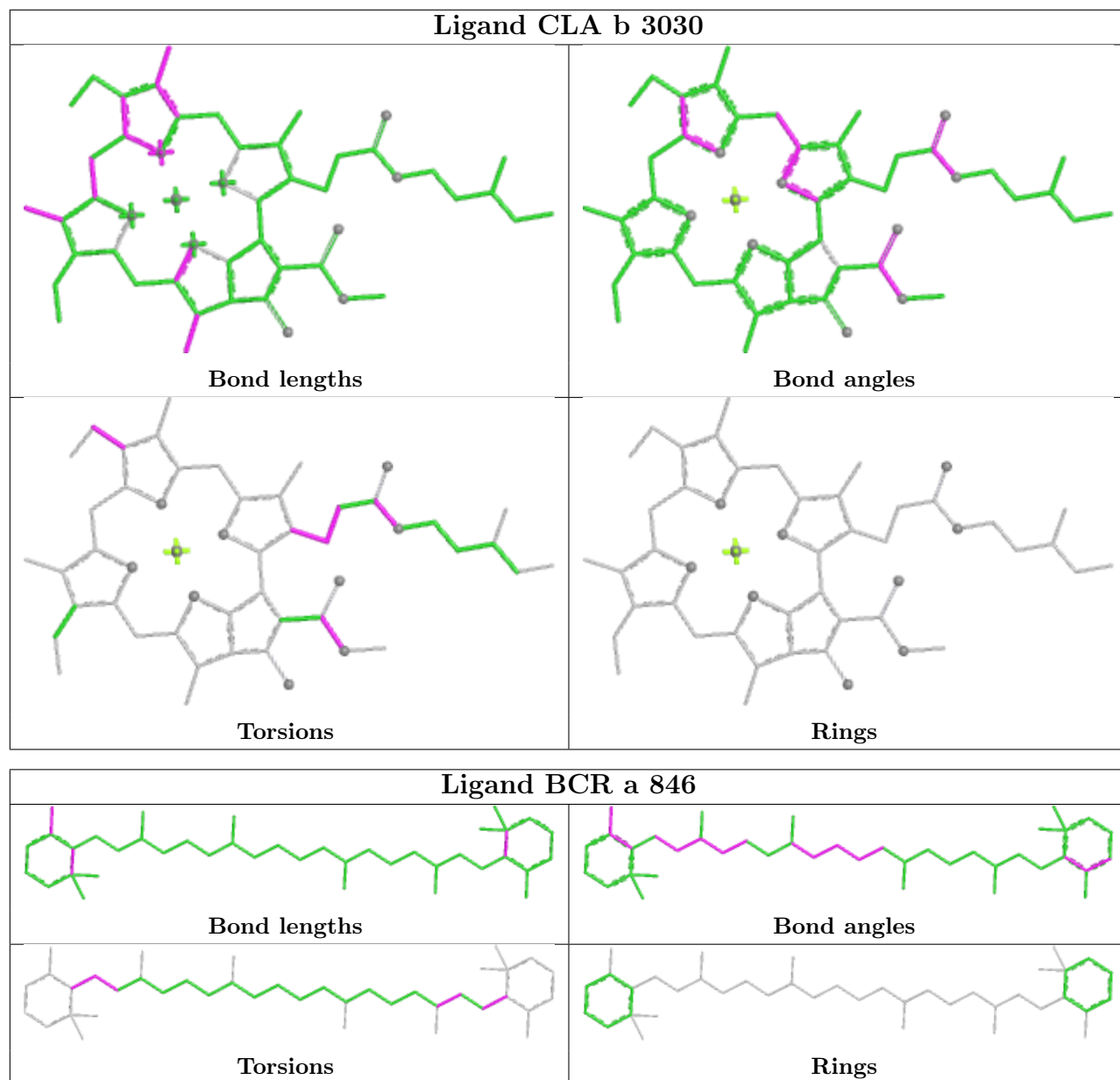


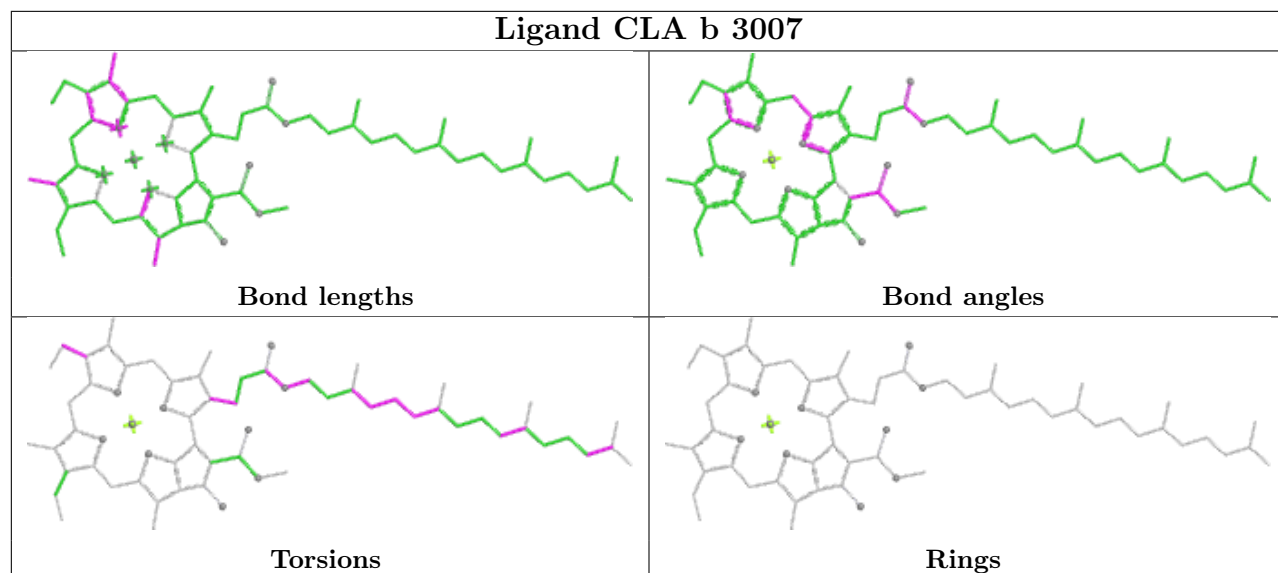
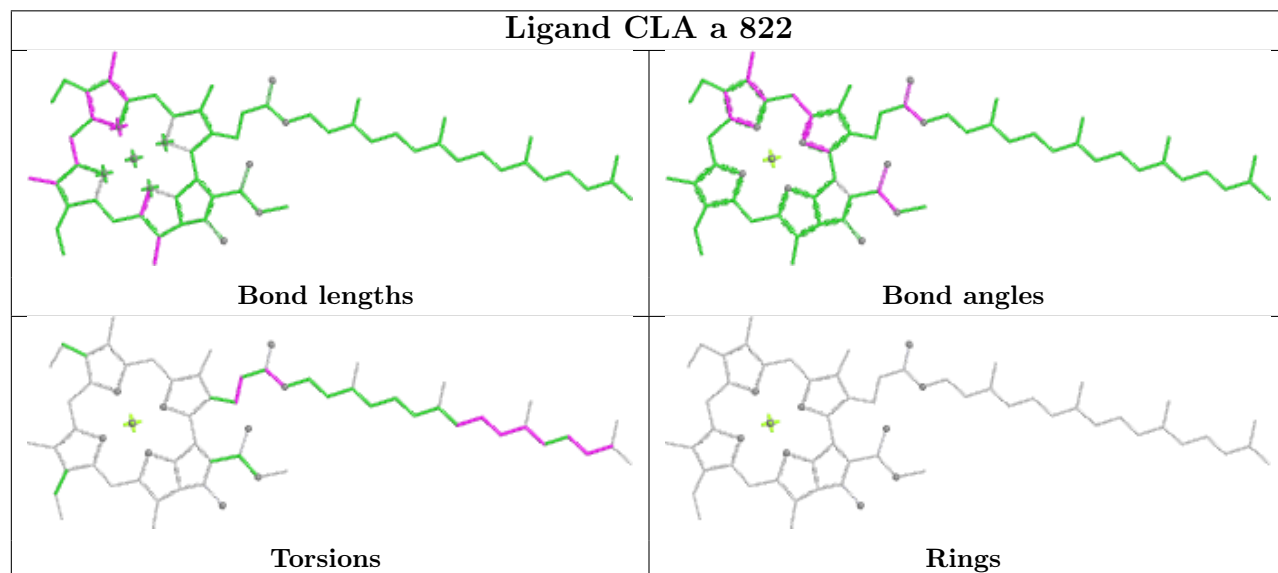
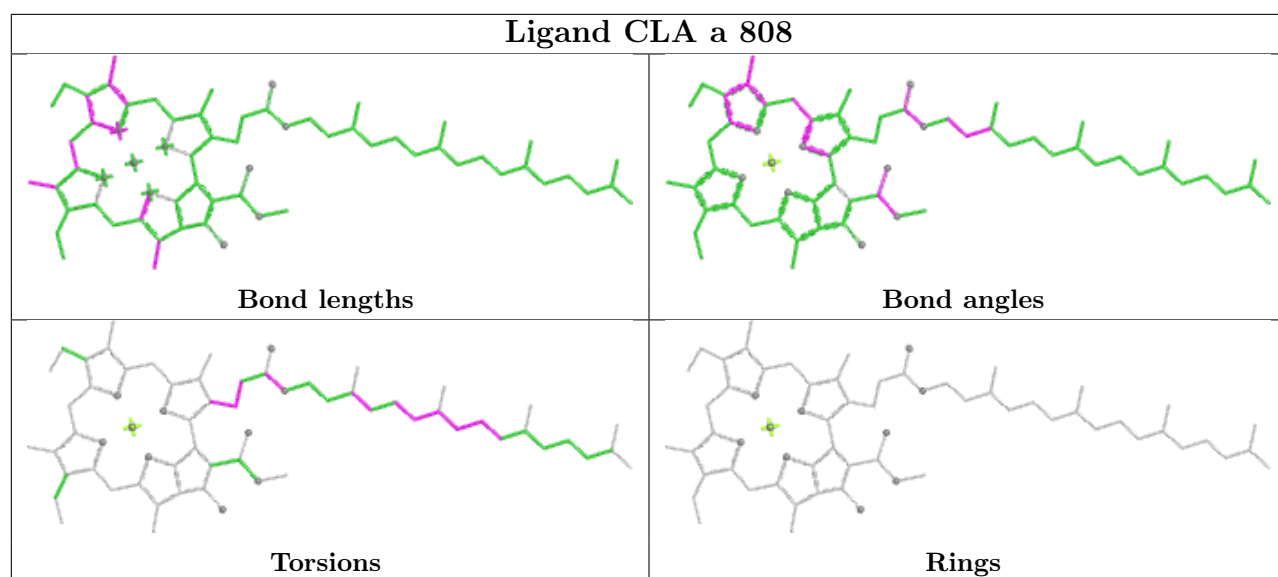
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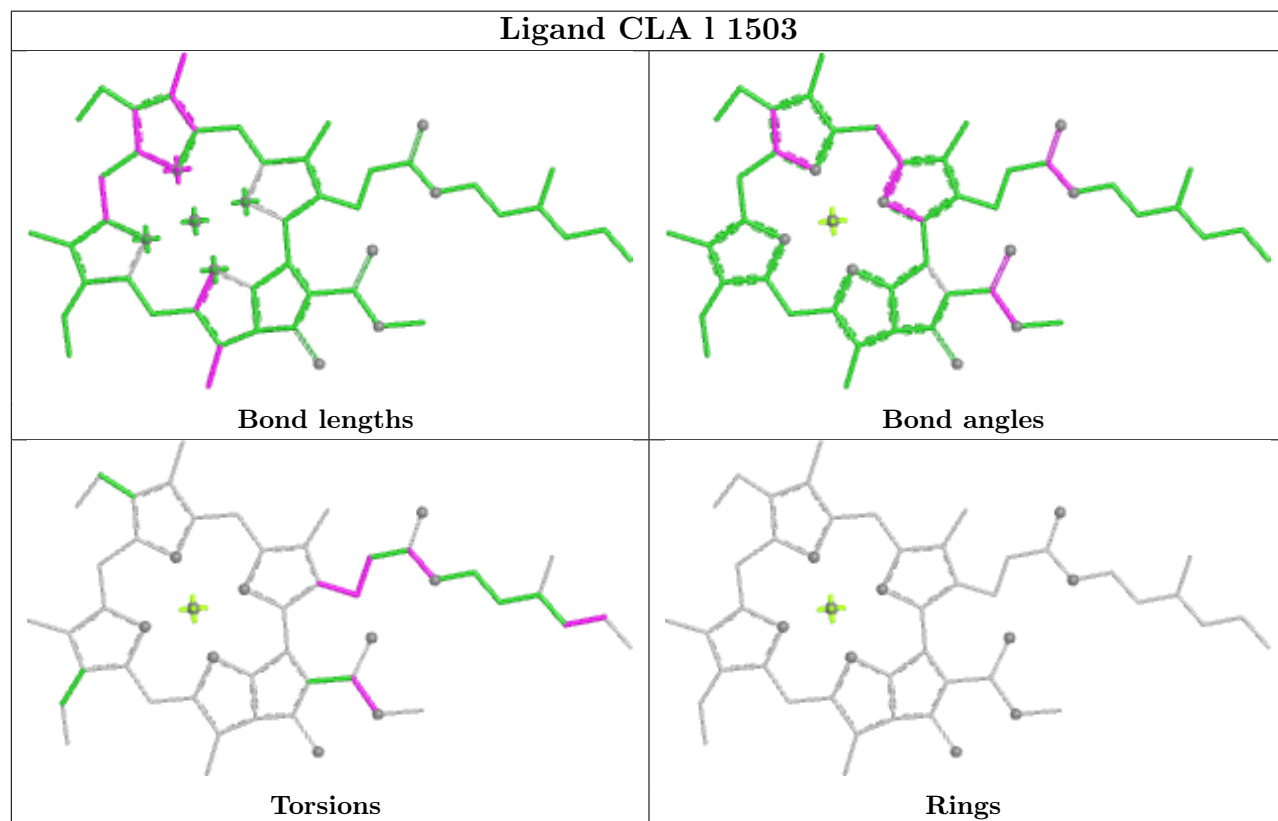
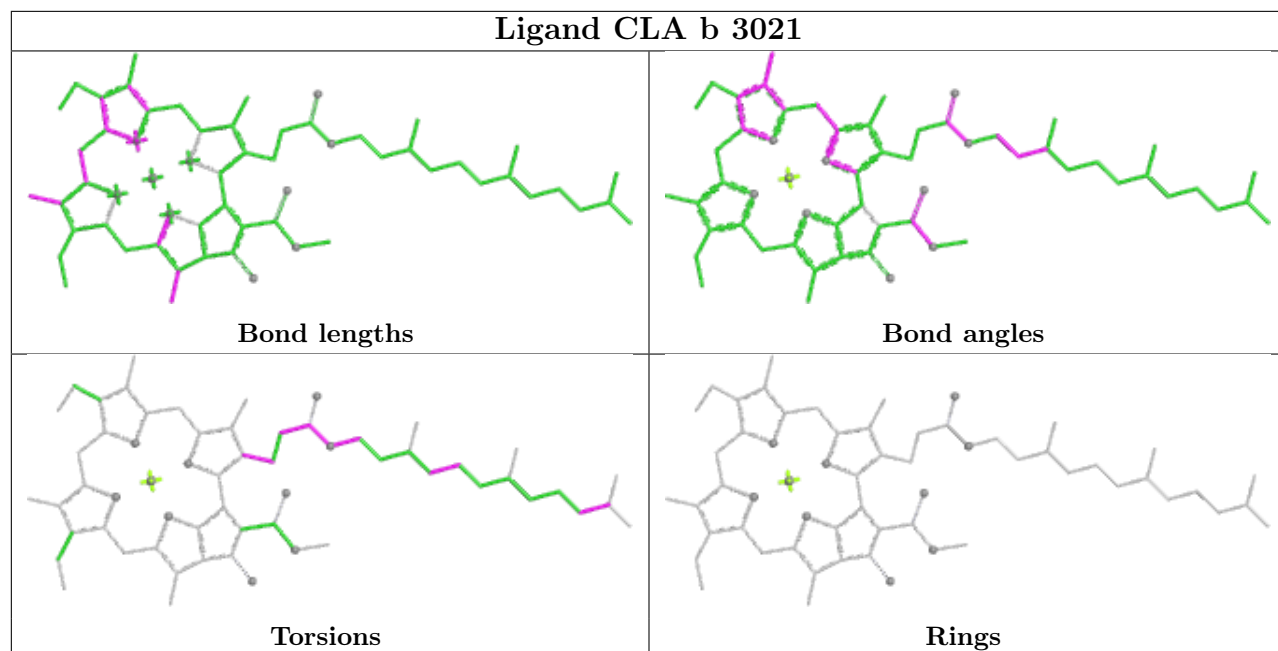


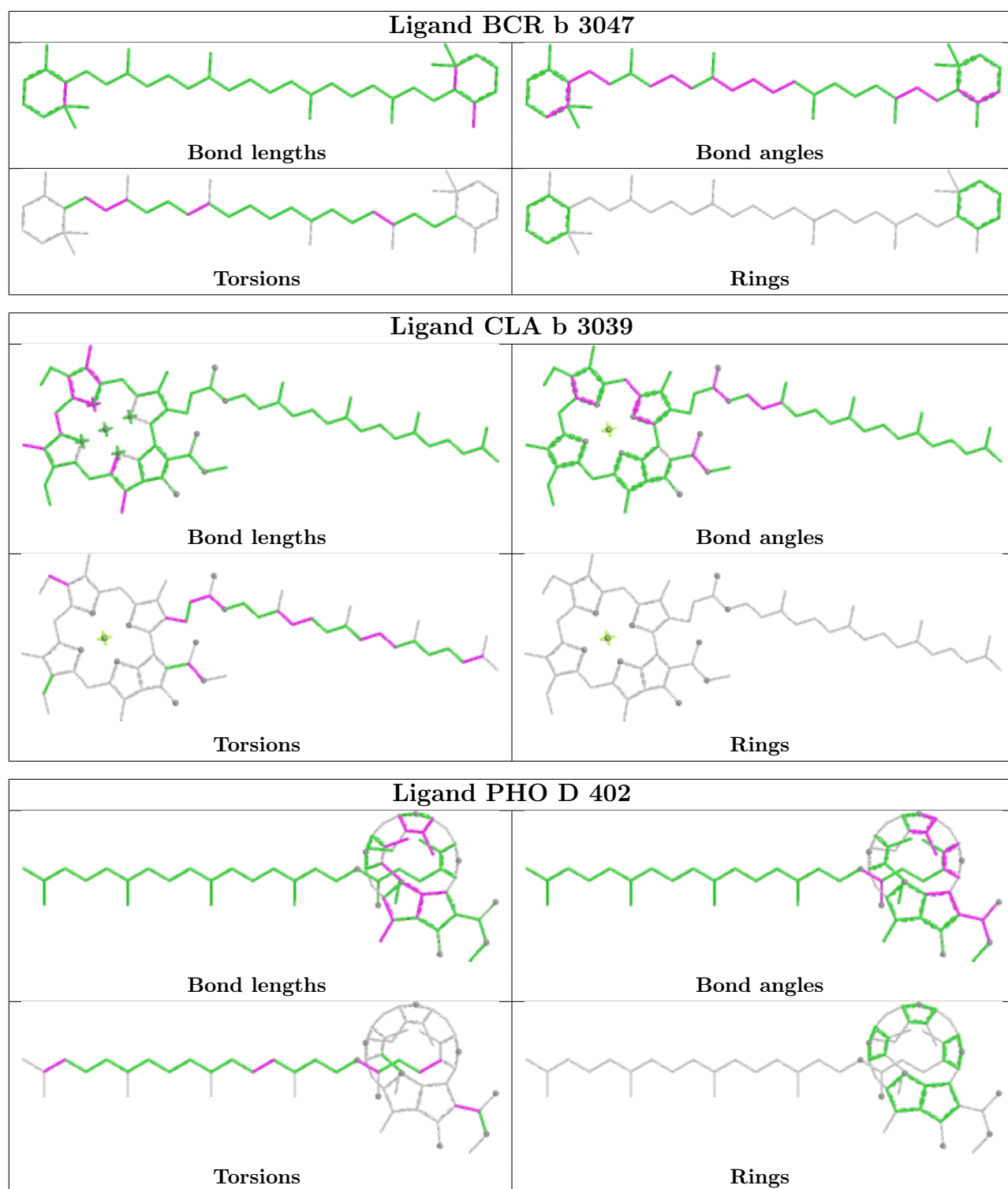
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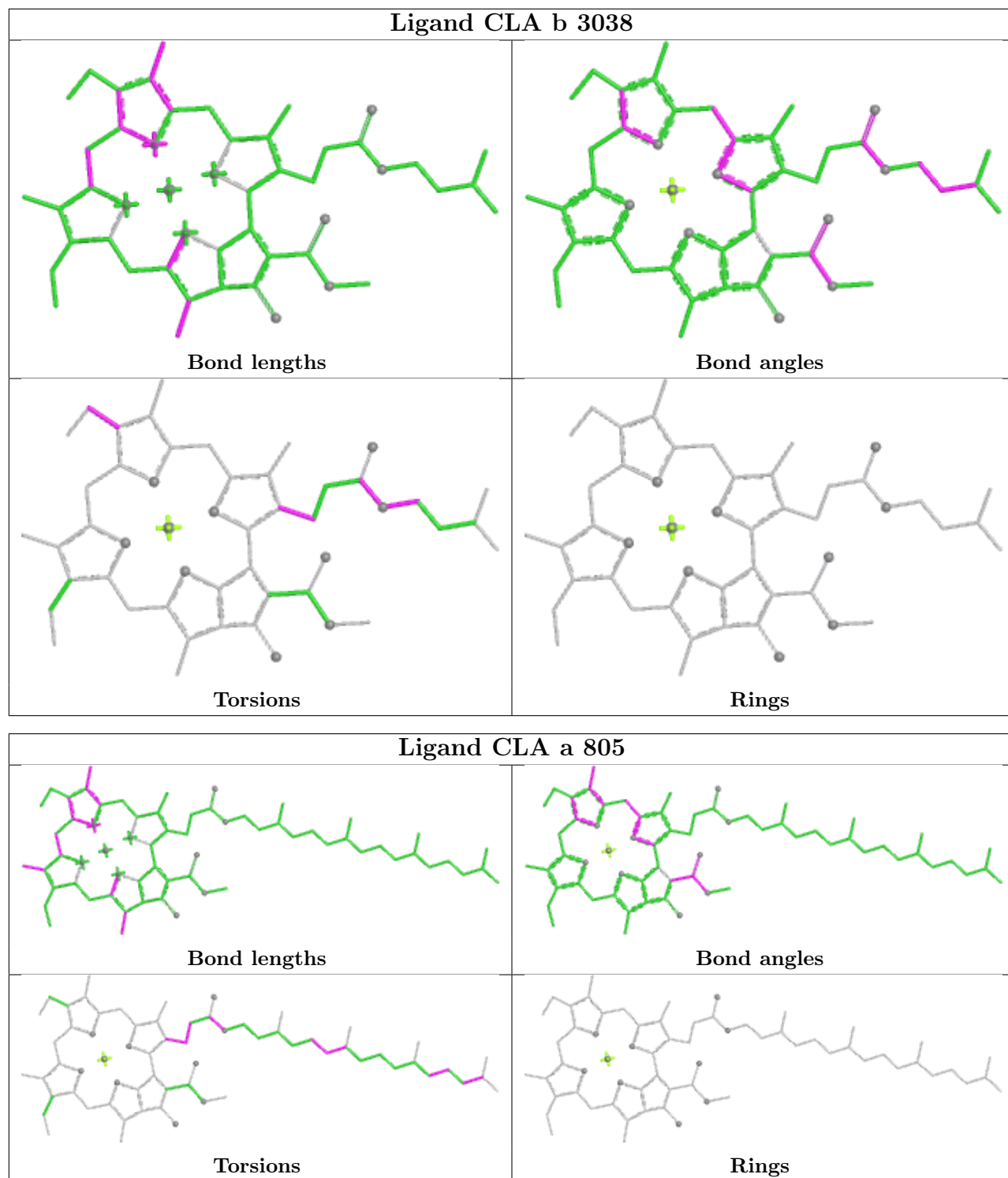


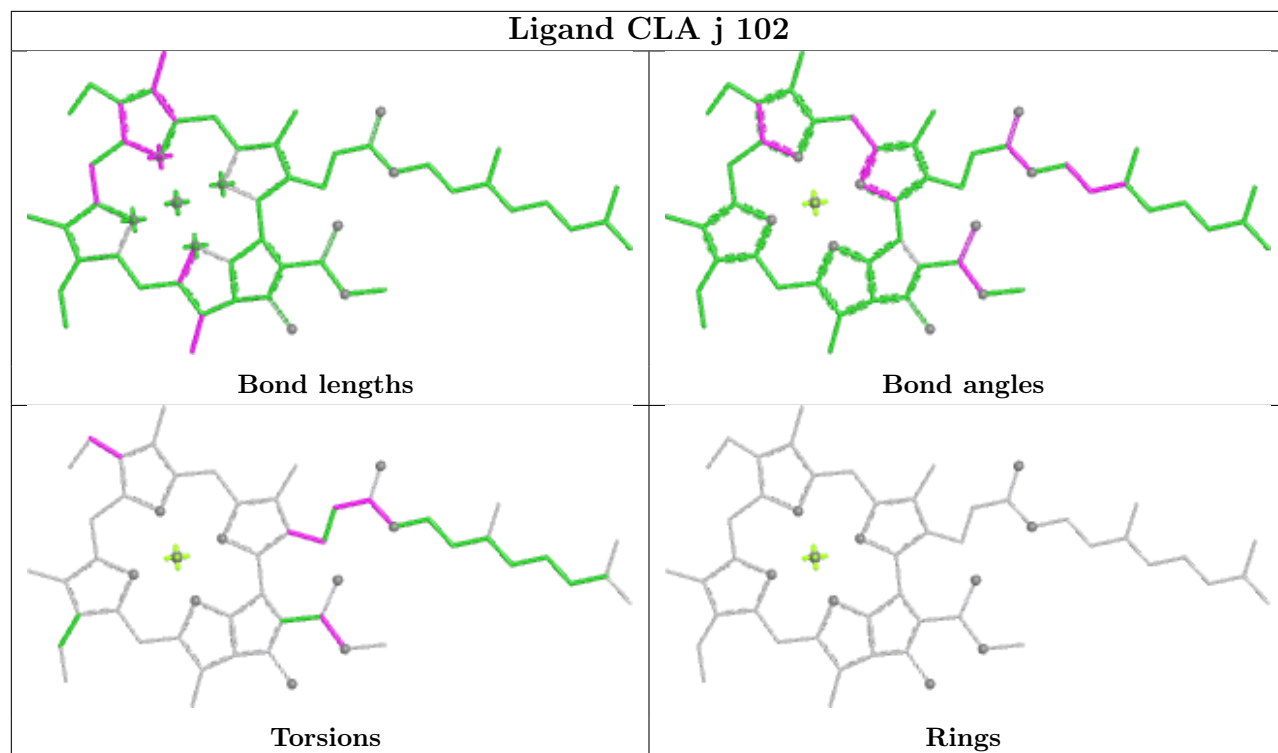




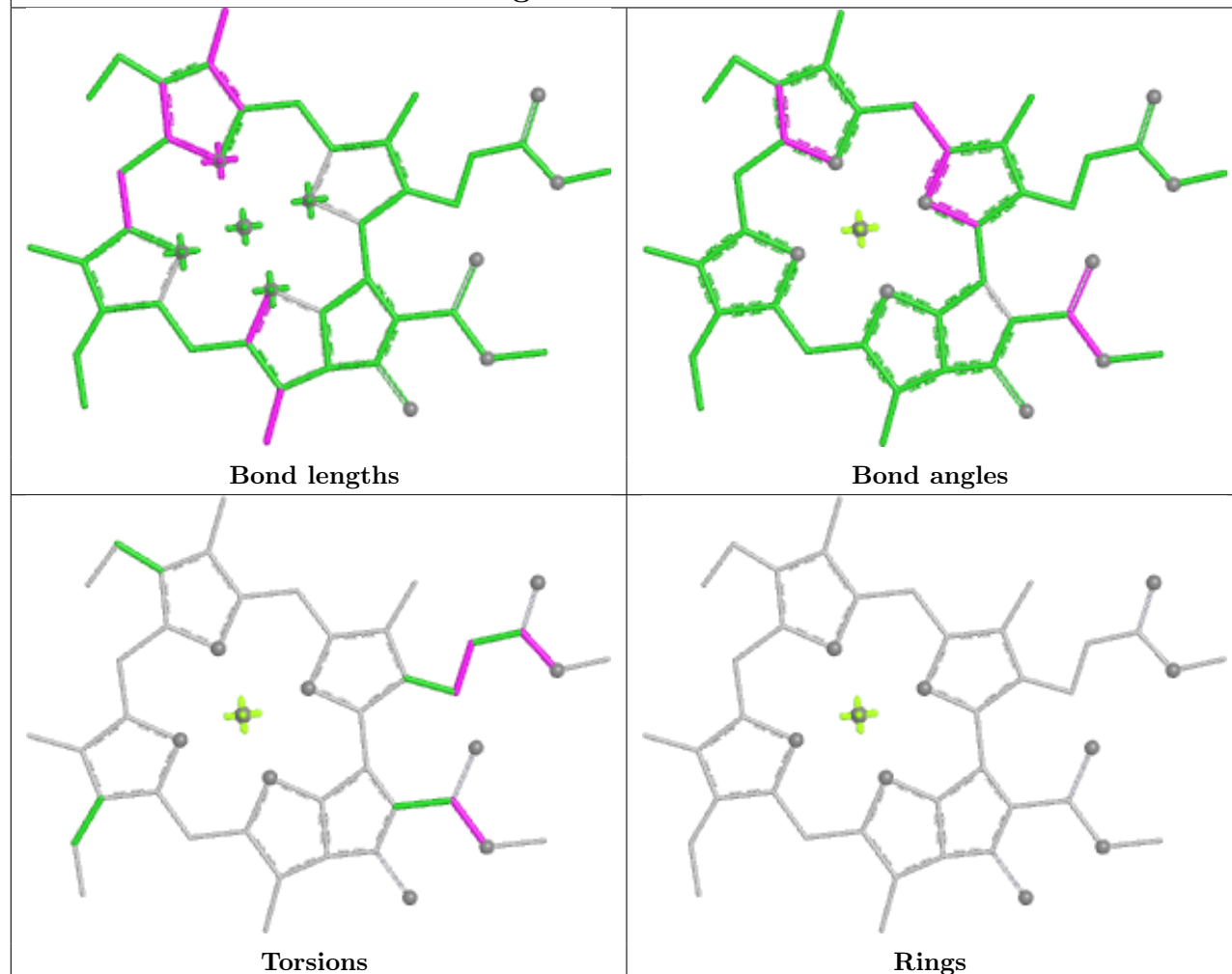




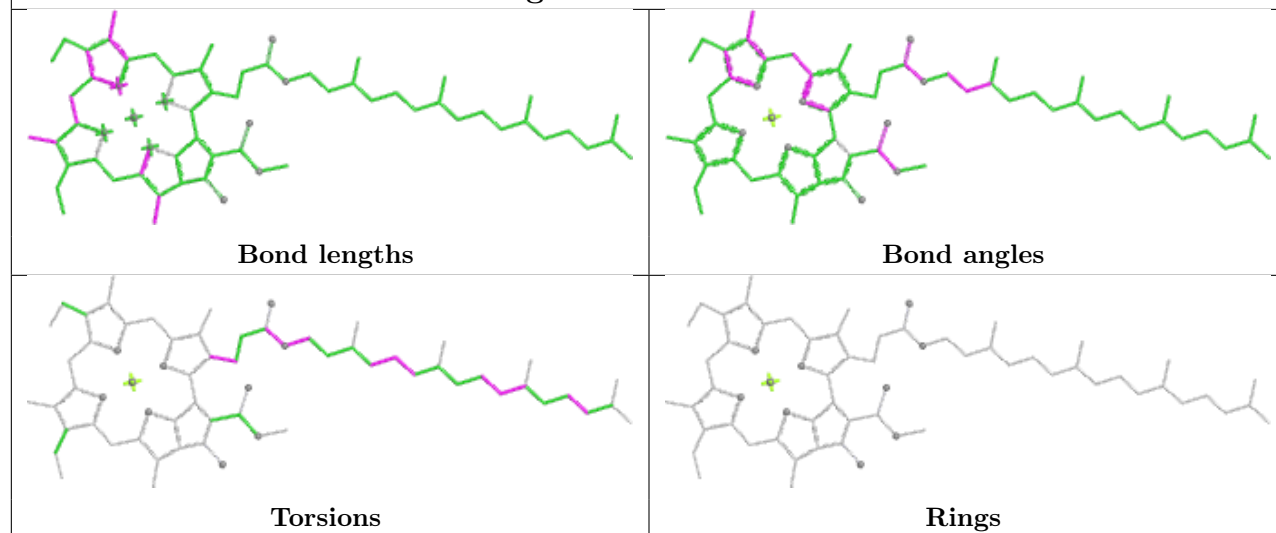


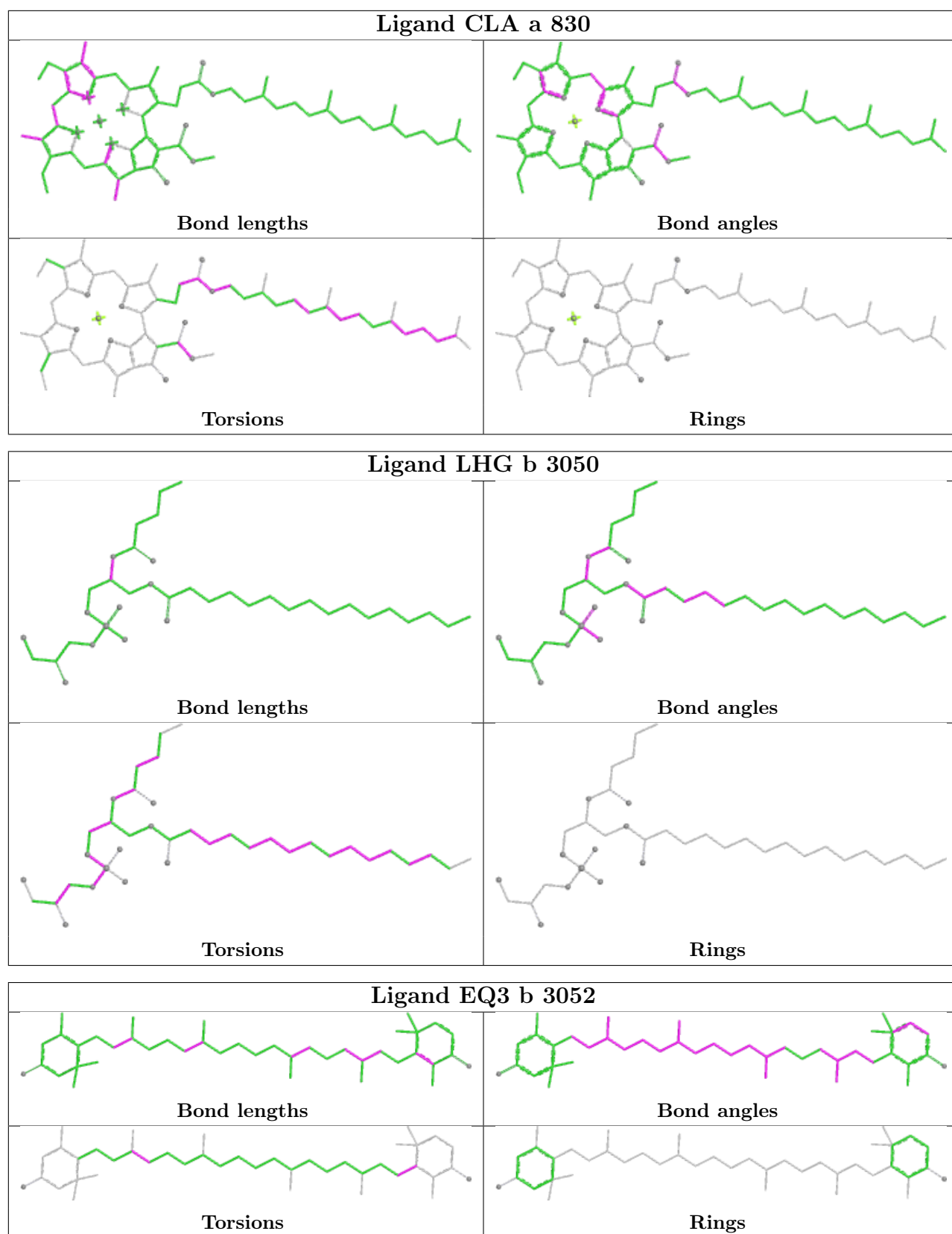


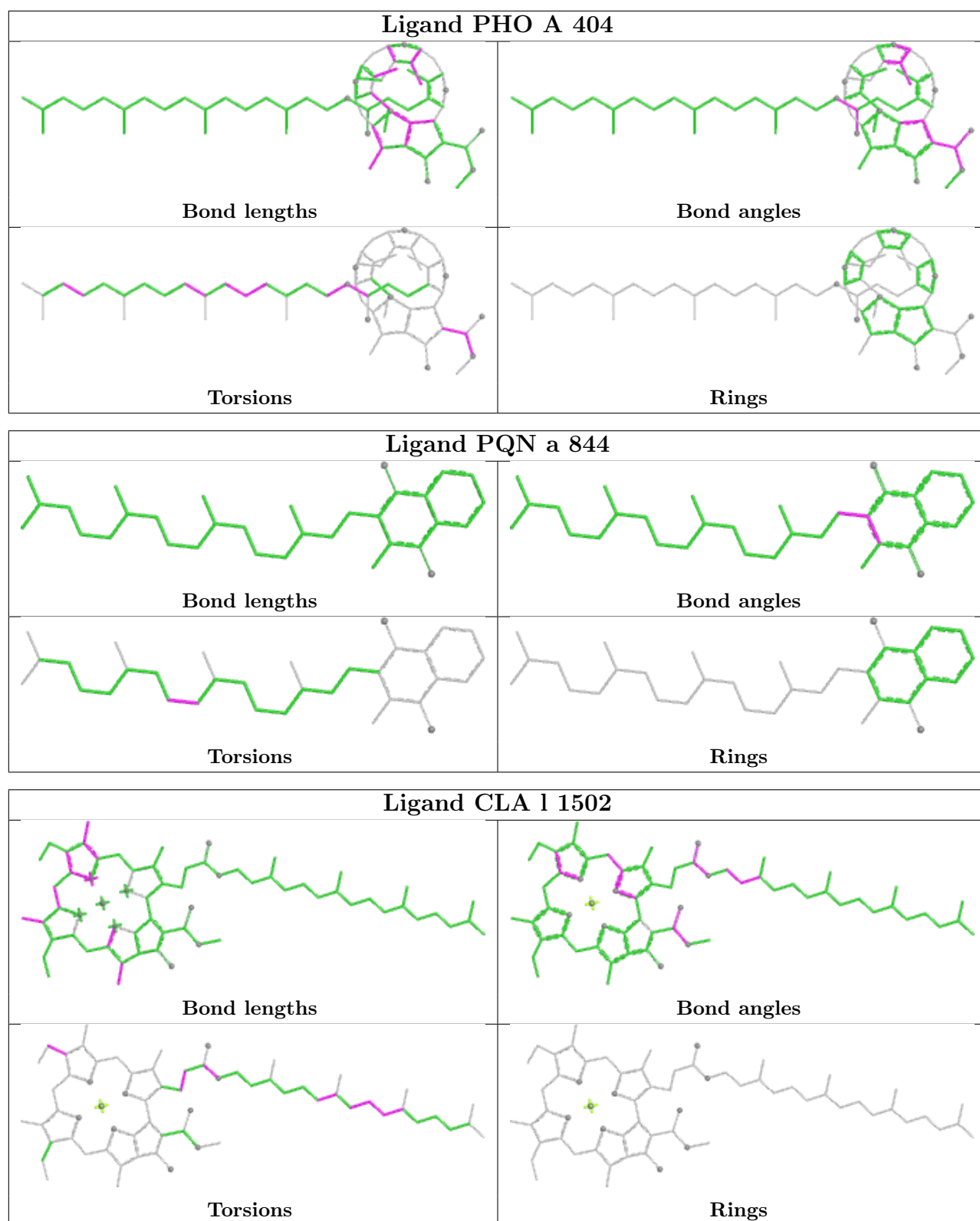
Ligand CLA D 404

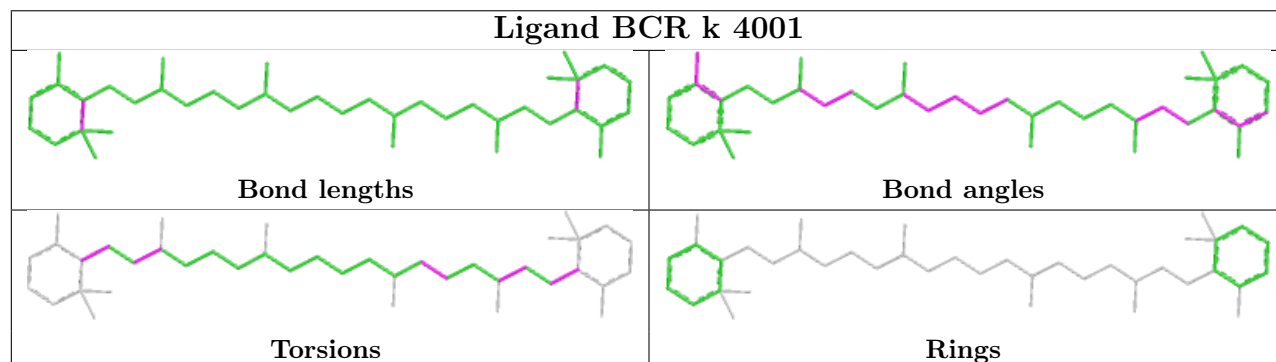
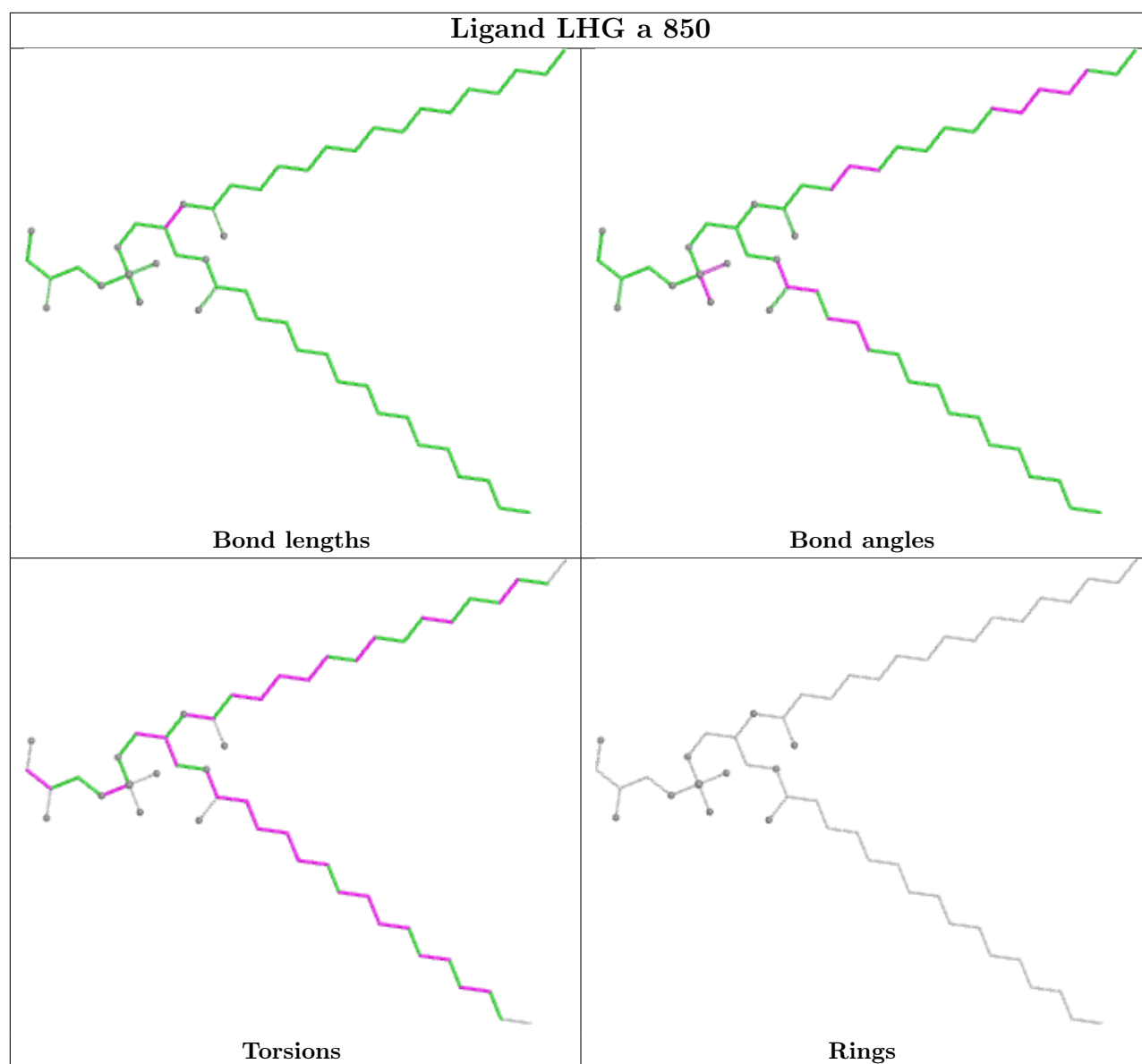


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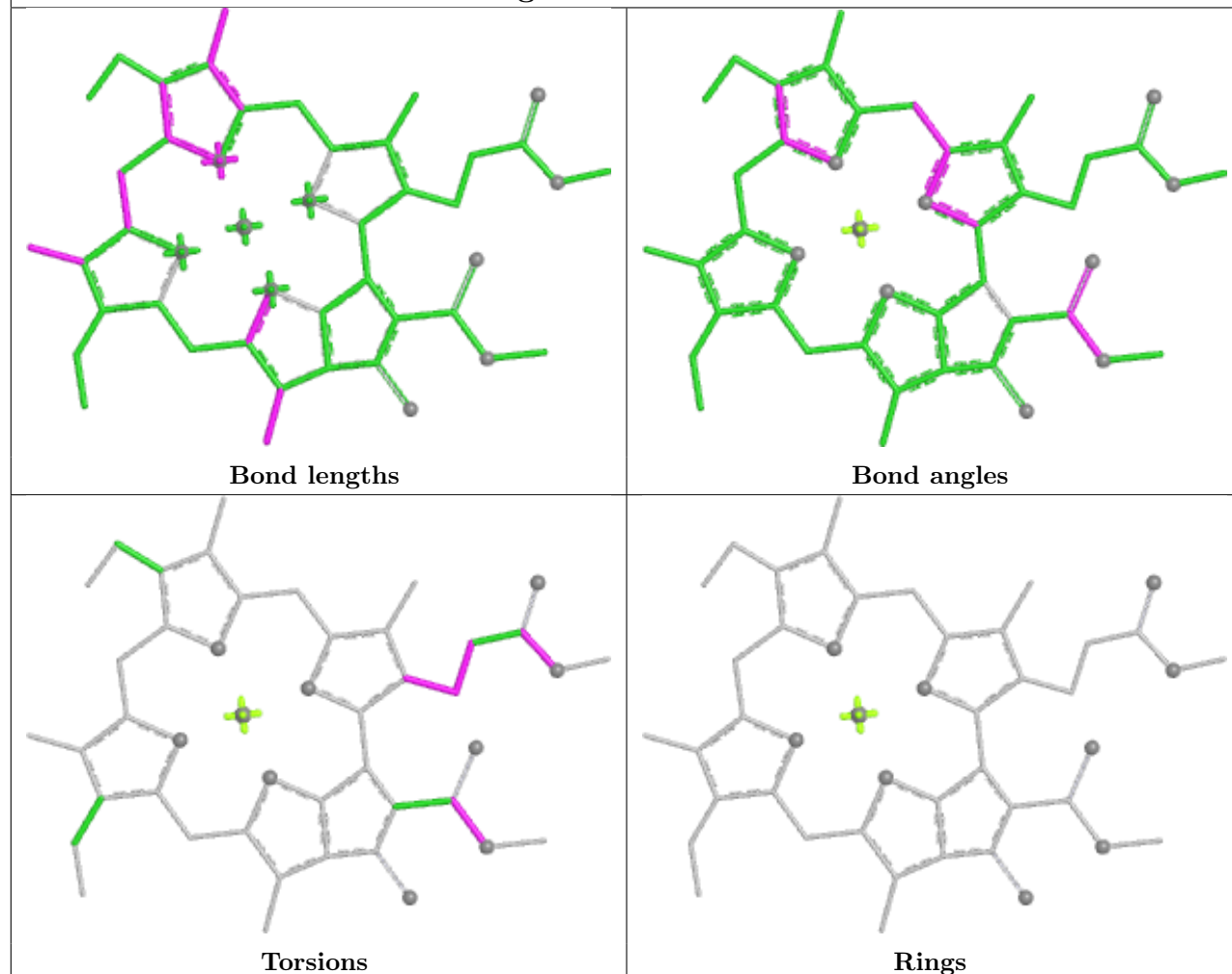




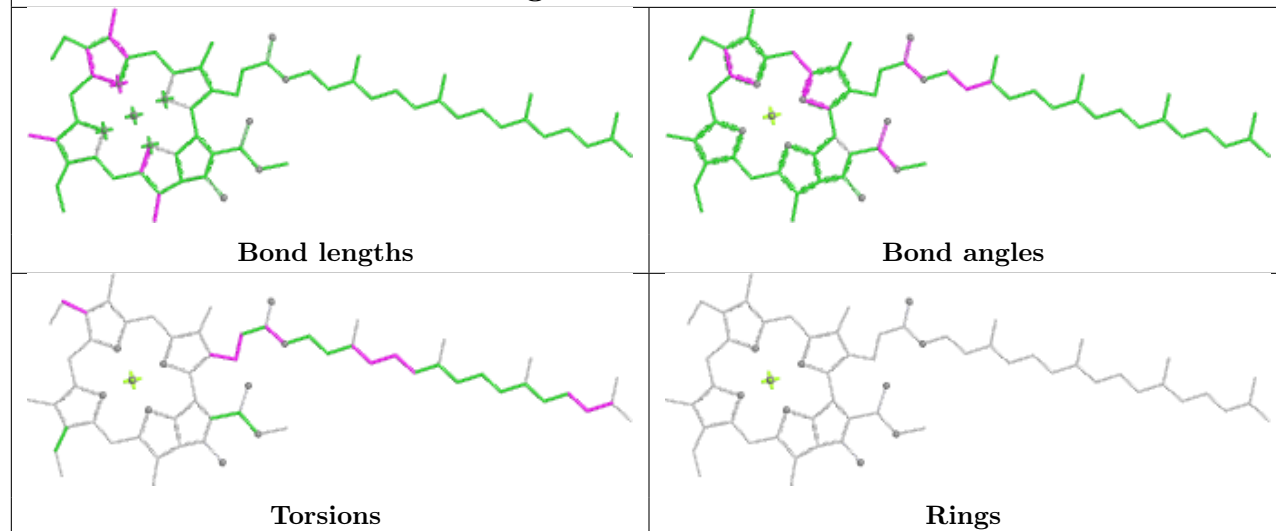




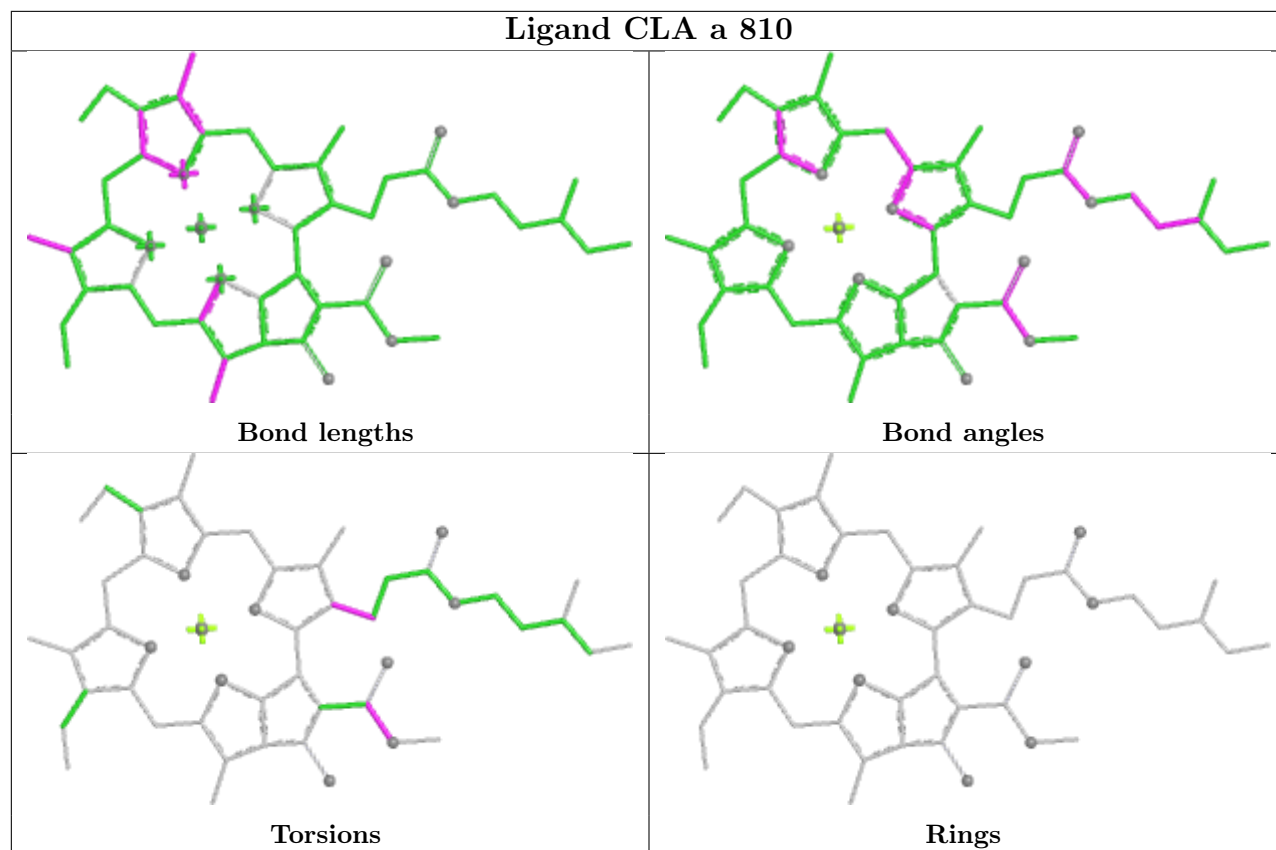
Ligand CLA a 817



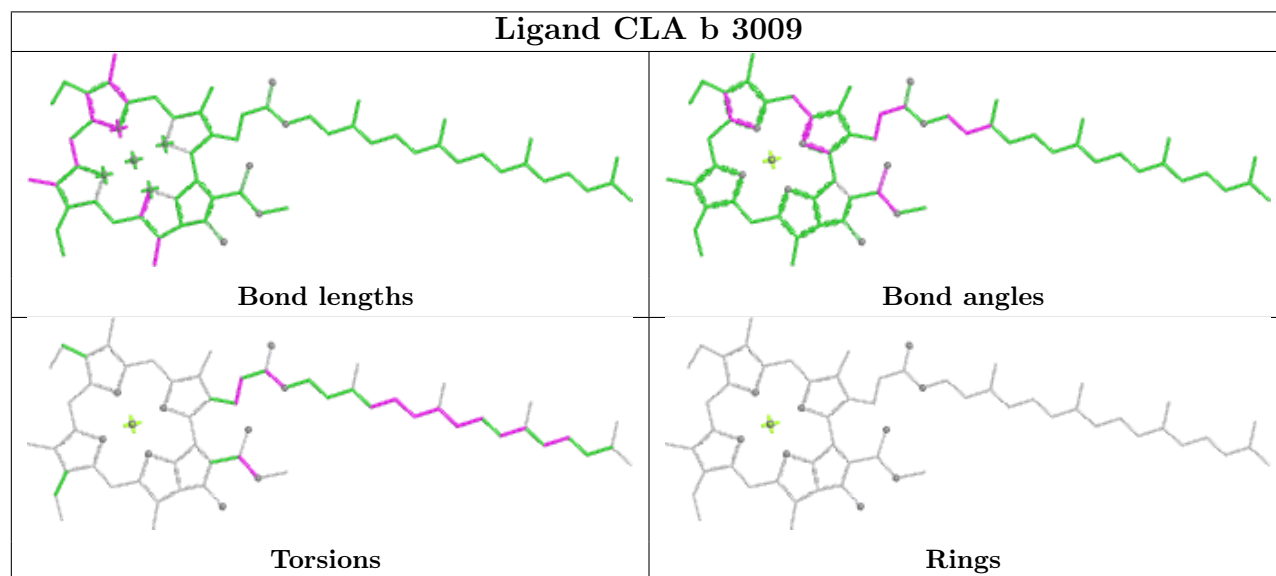
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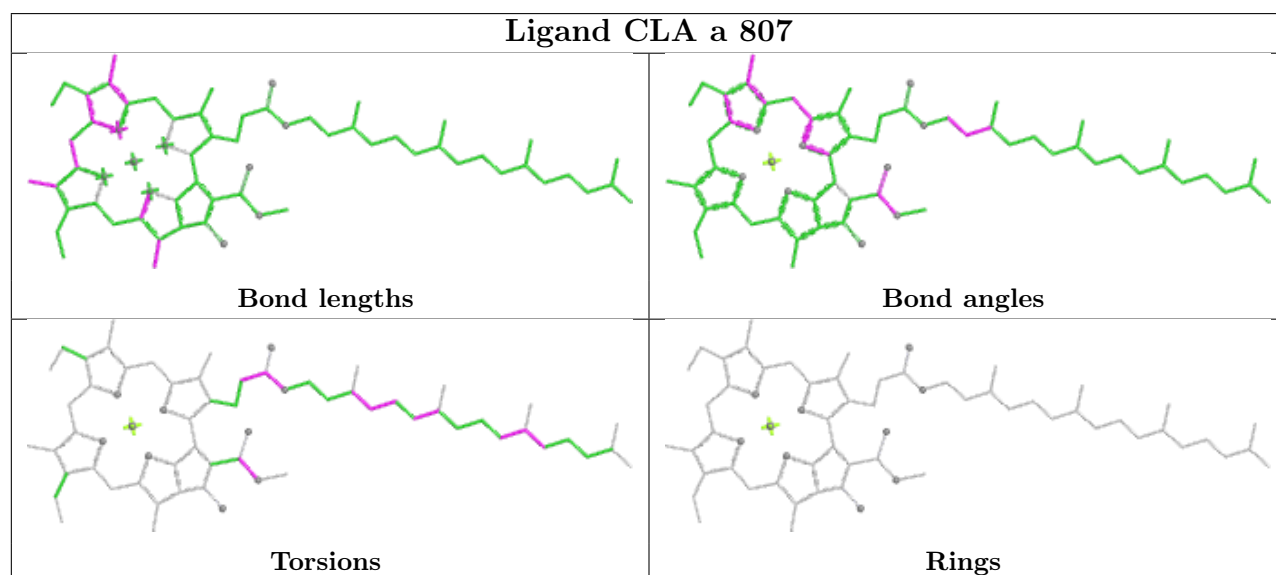
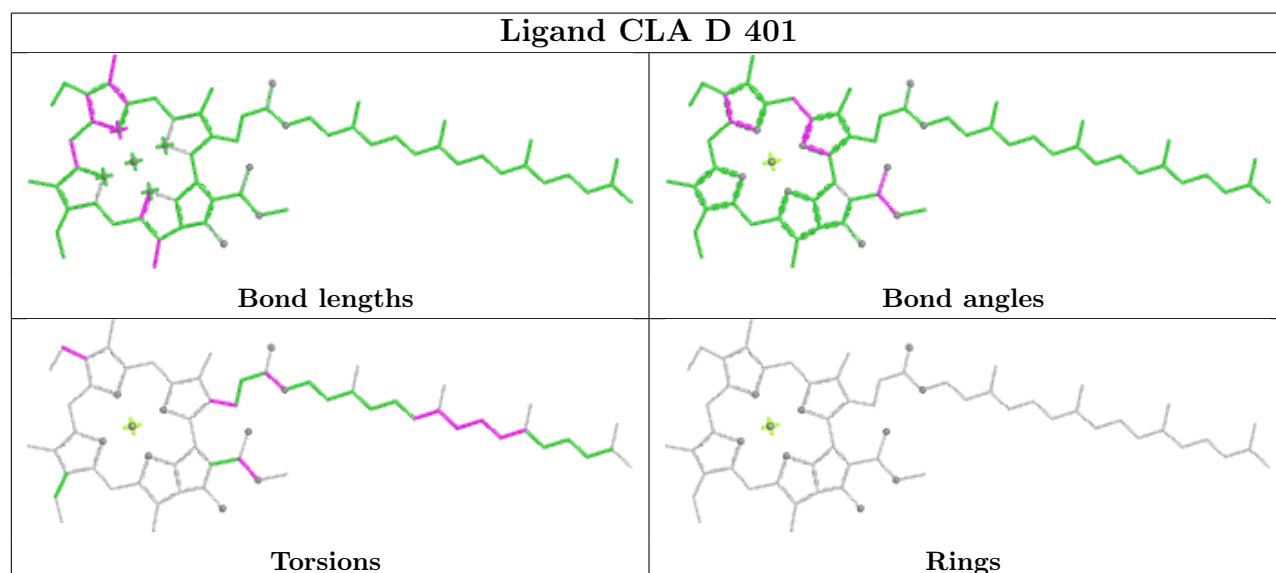
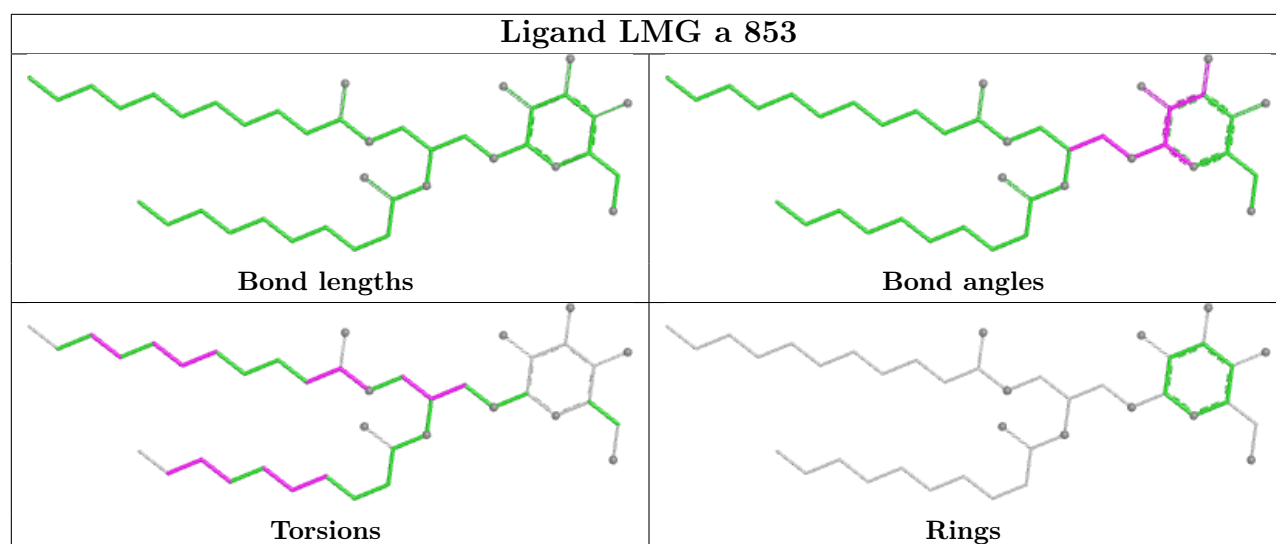


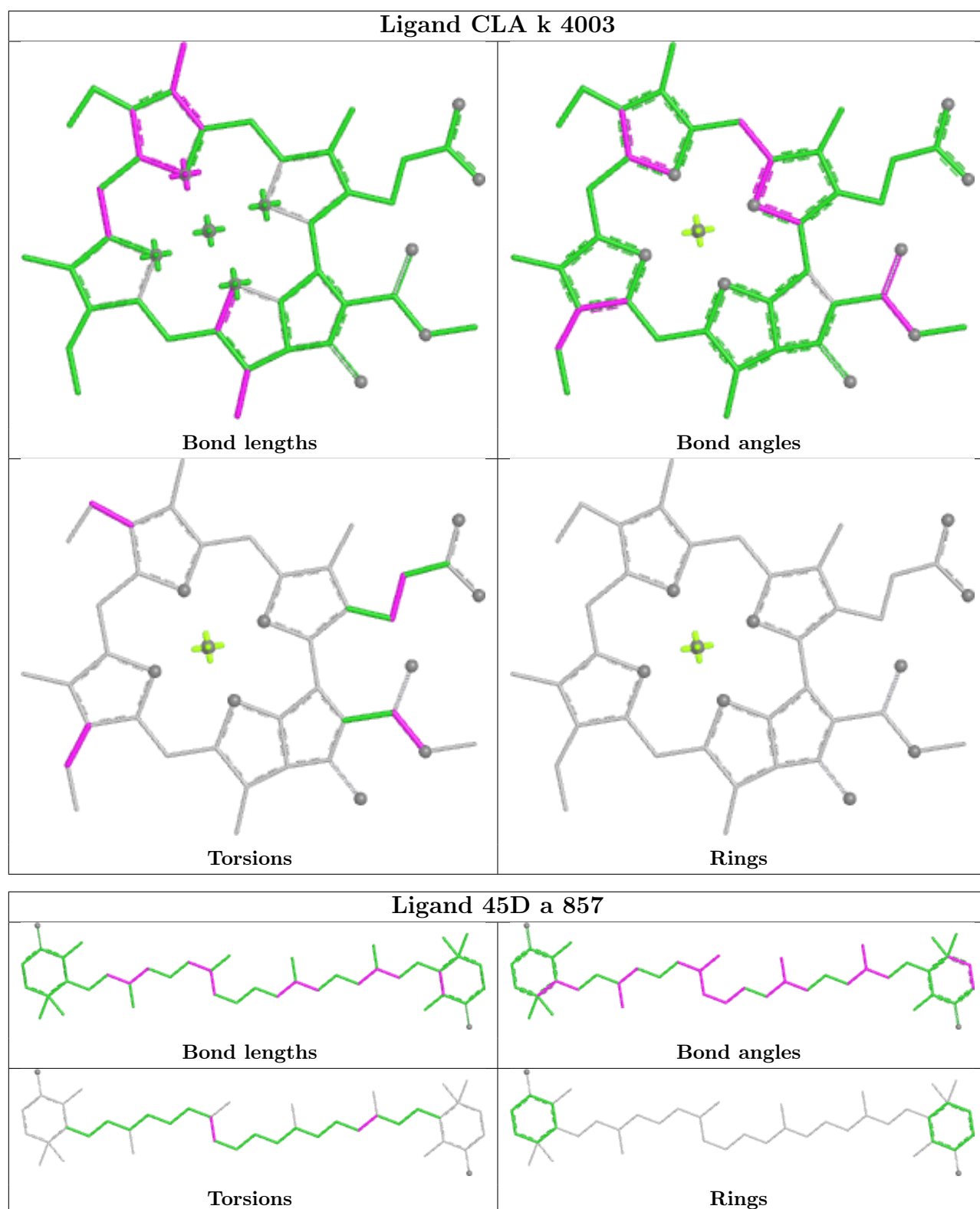
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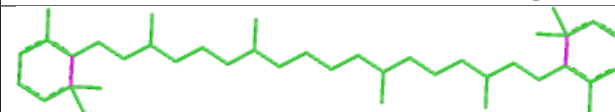
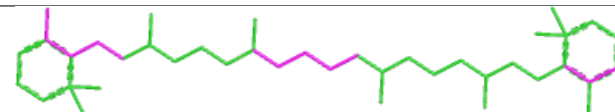
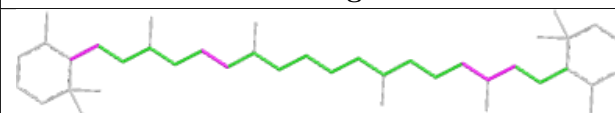
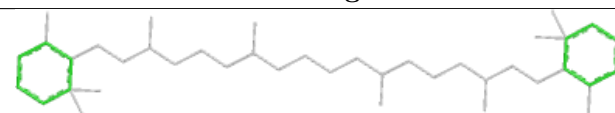


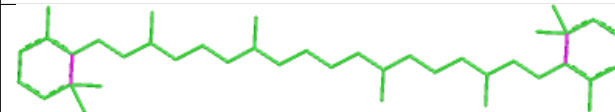
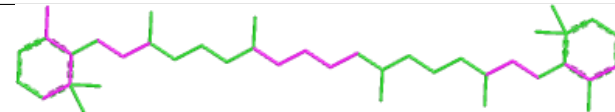
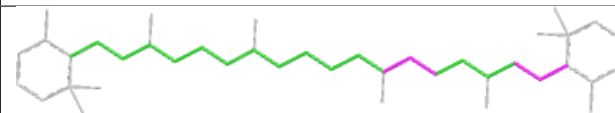
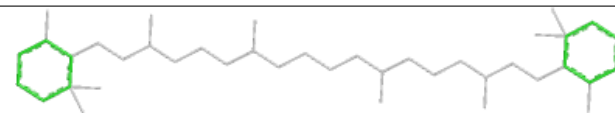
Ligand CLA b 3009

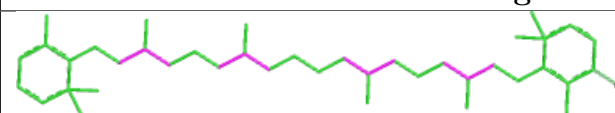
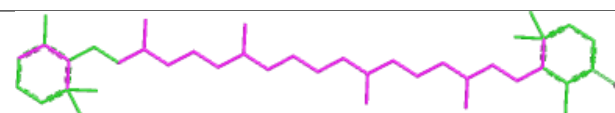
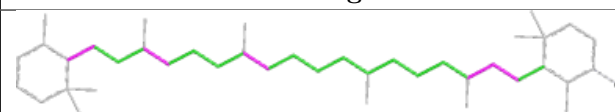
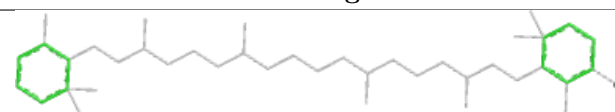


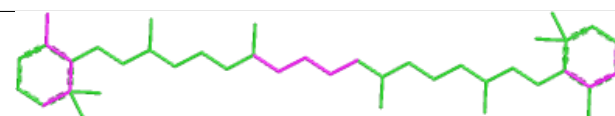
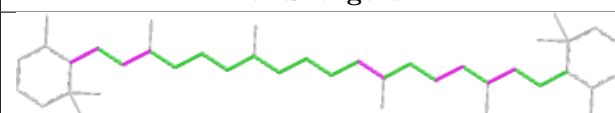
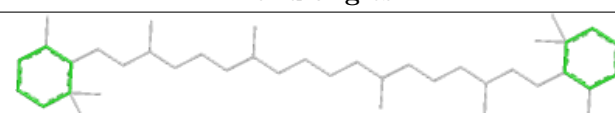


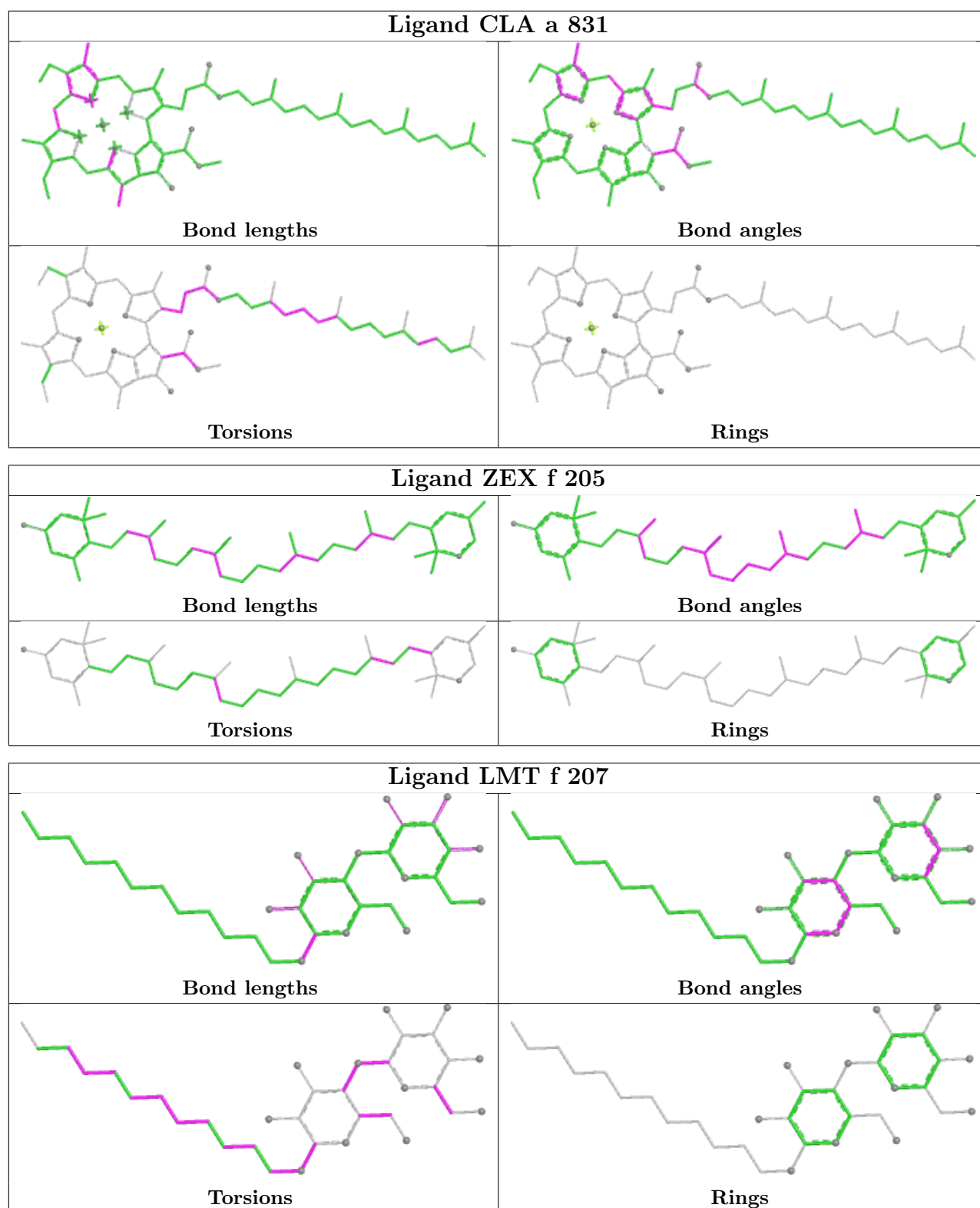


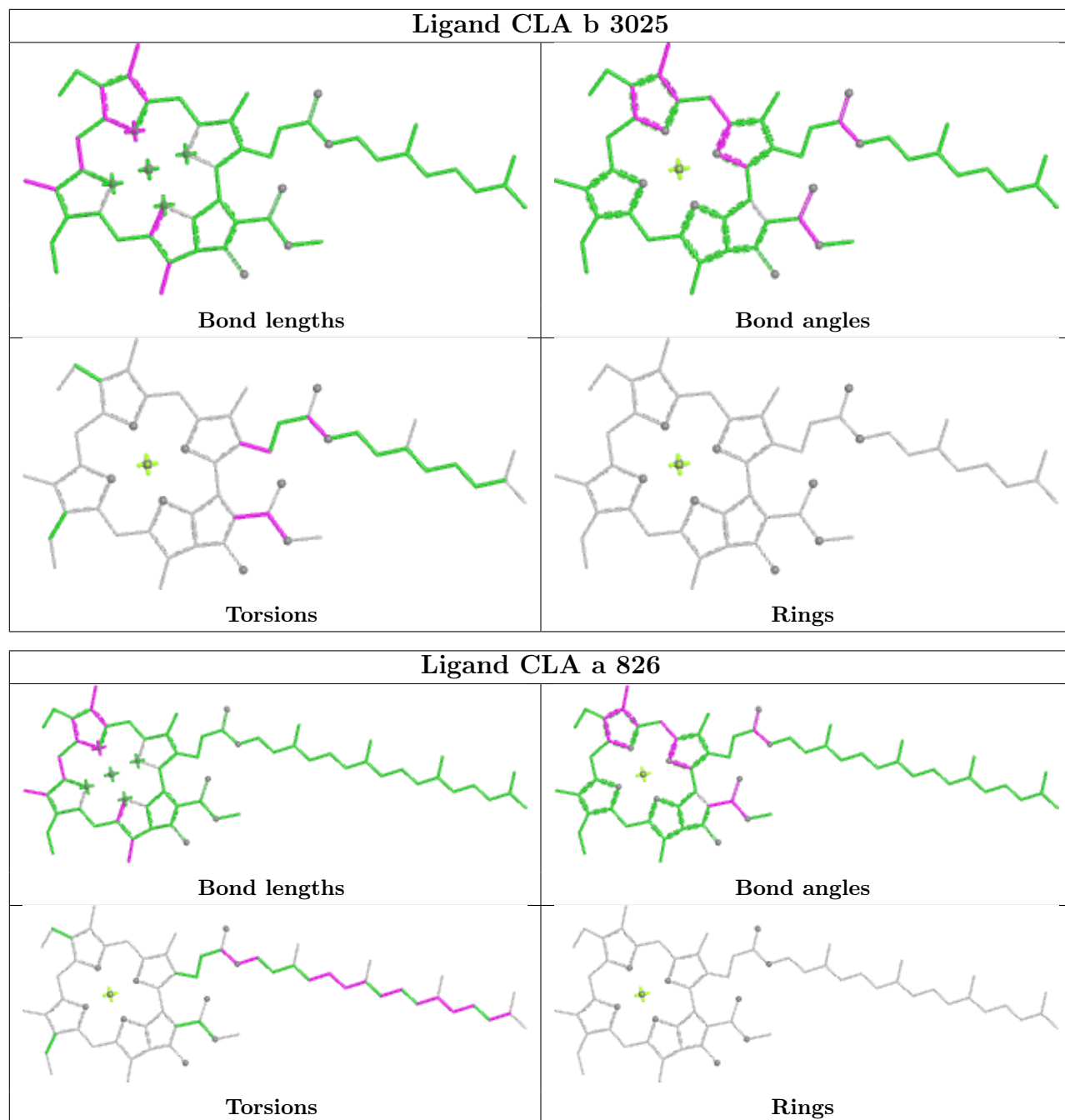
Ligand BCR i 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

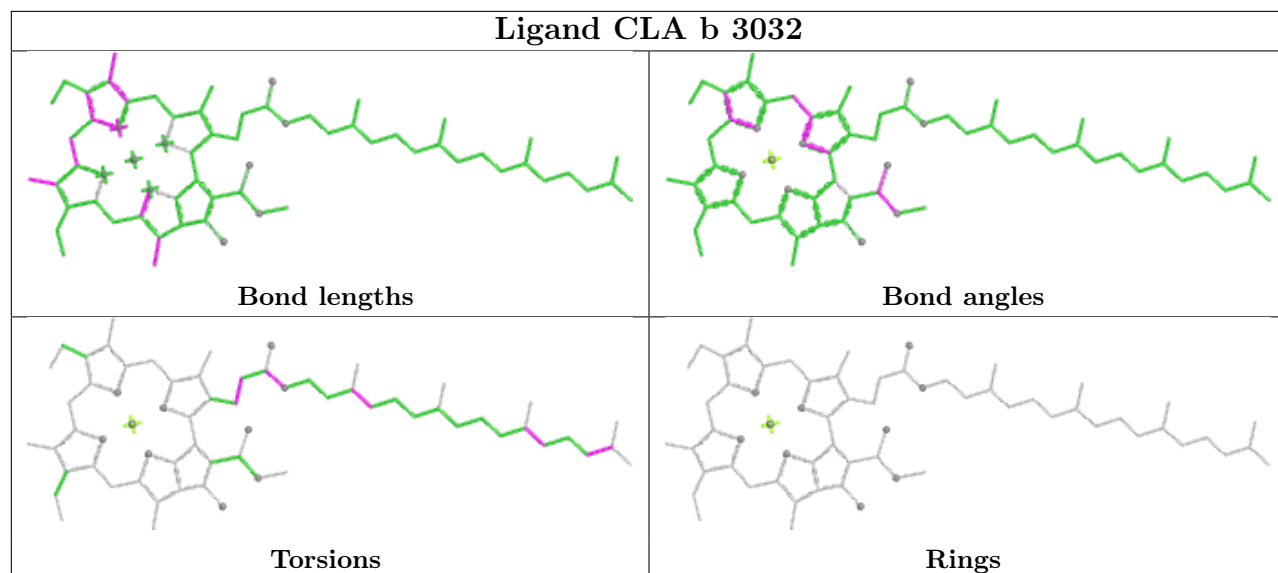
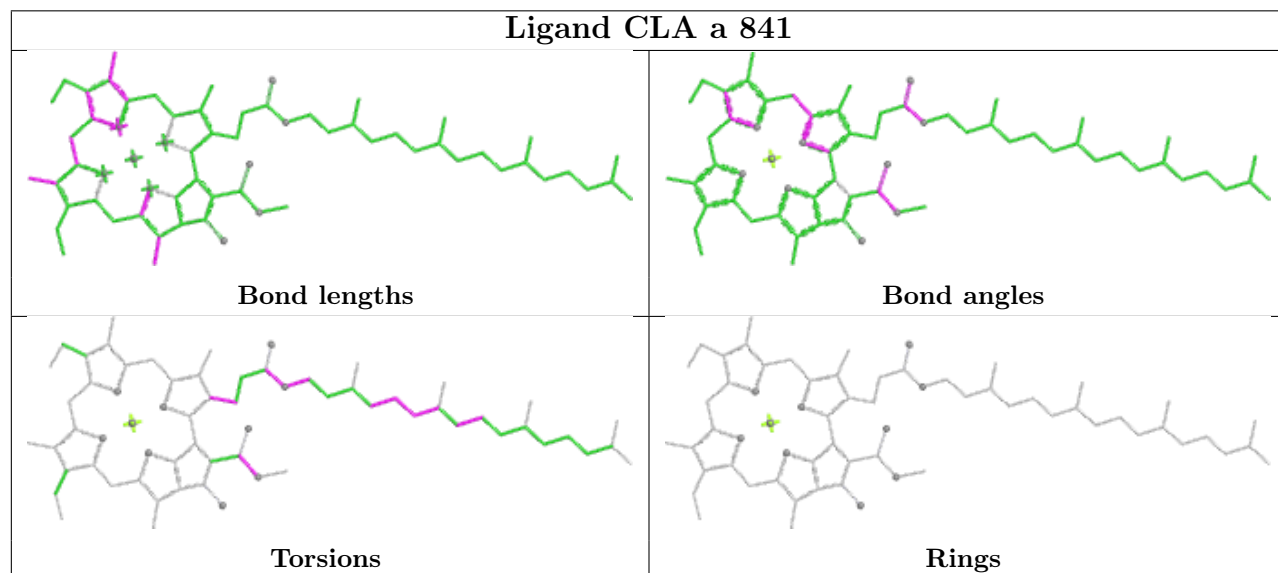
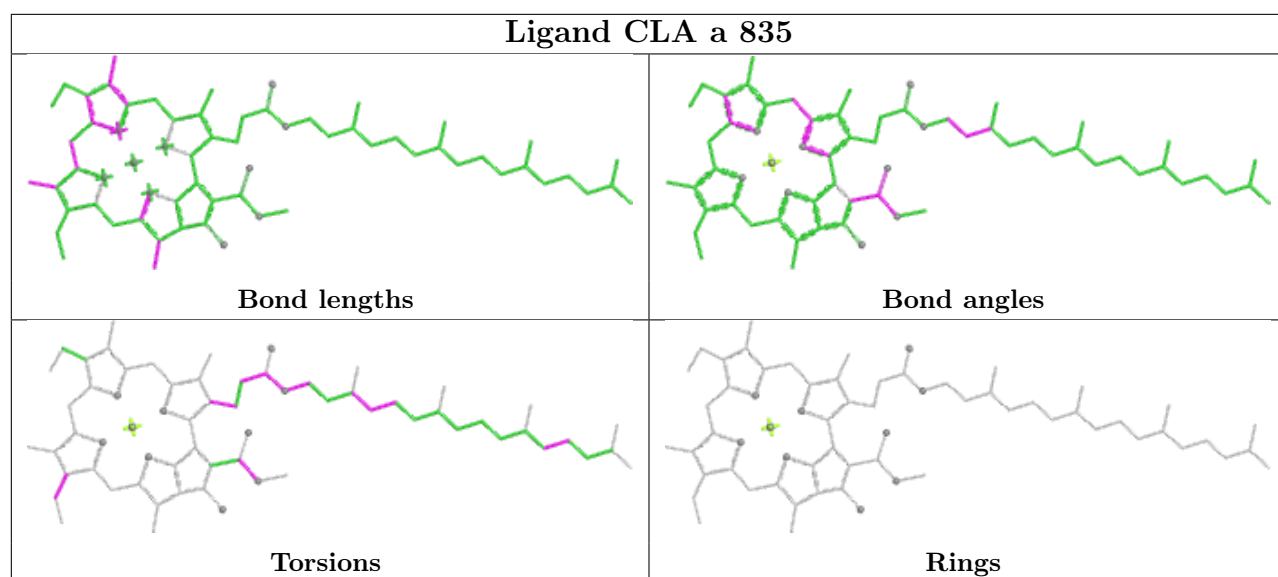
Ligand BCR k 4004	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ECH b 3045	
	
Bond lengths	Bond angles
	
Torsions	Rings

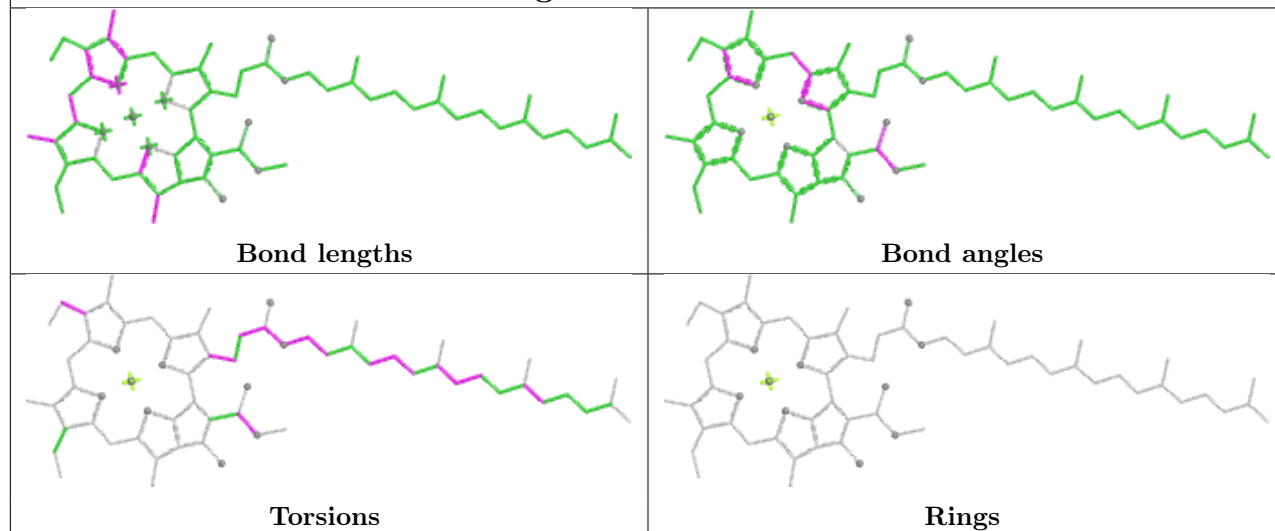
Ligand BCR b 3044	
	
Bond lengths	Bond angles
	
Torsions	Rings



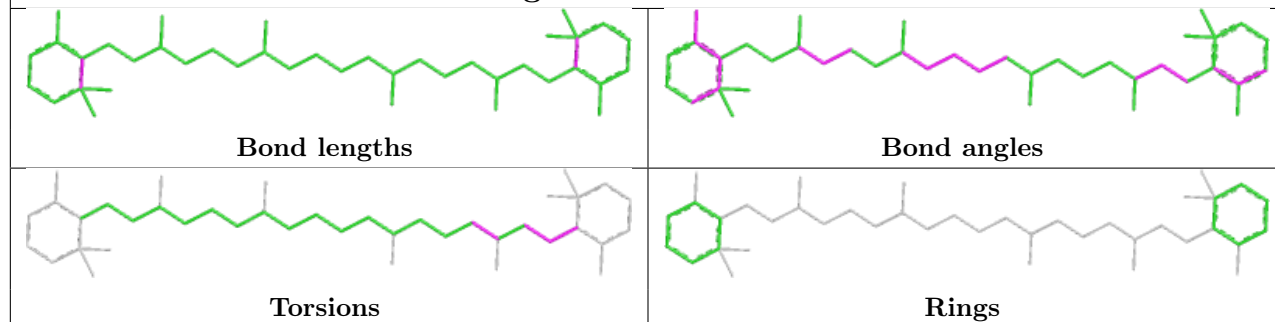




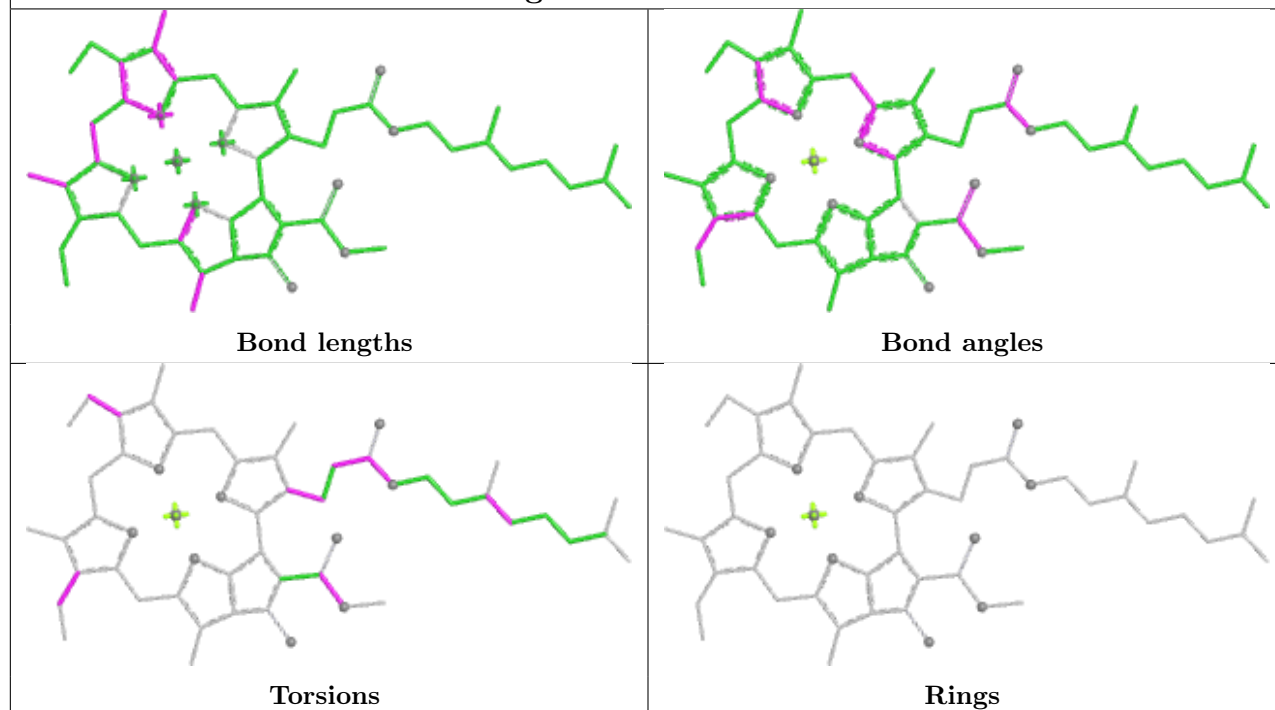
Ligand CLA a 824

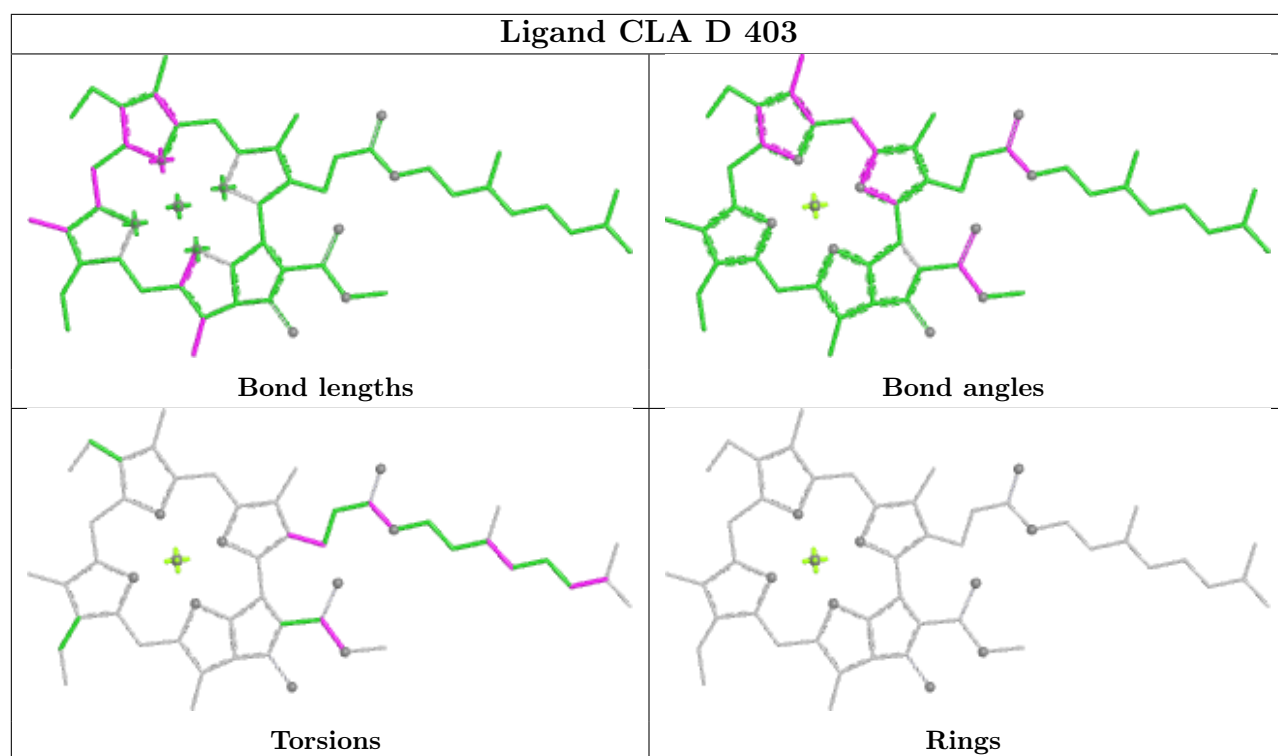


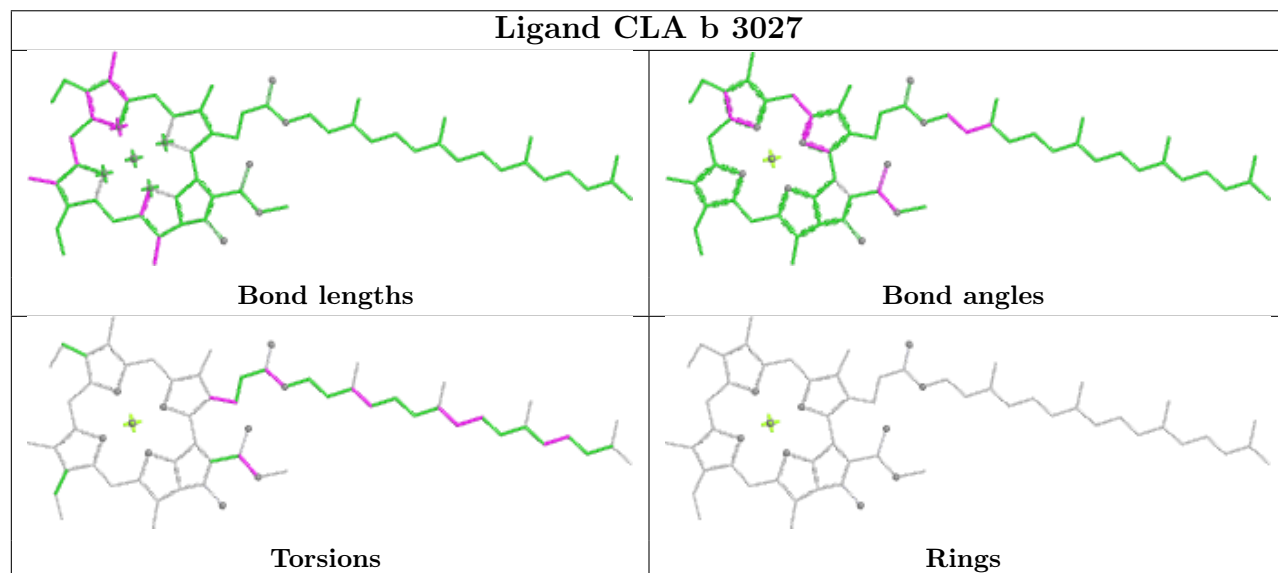
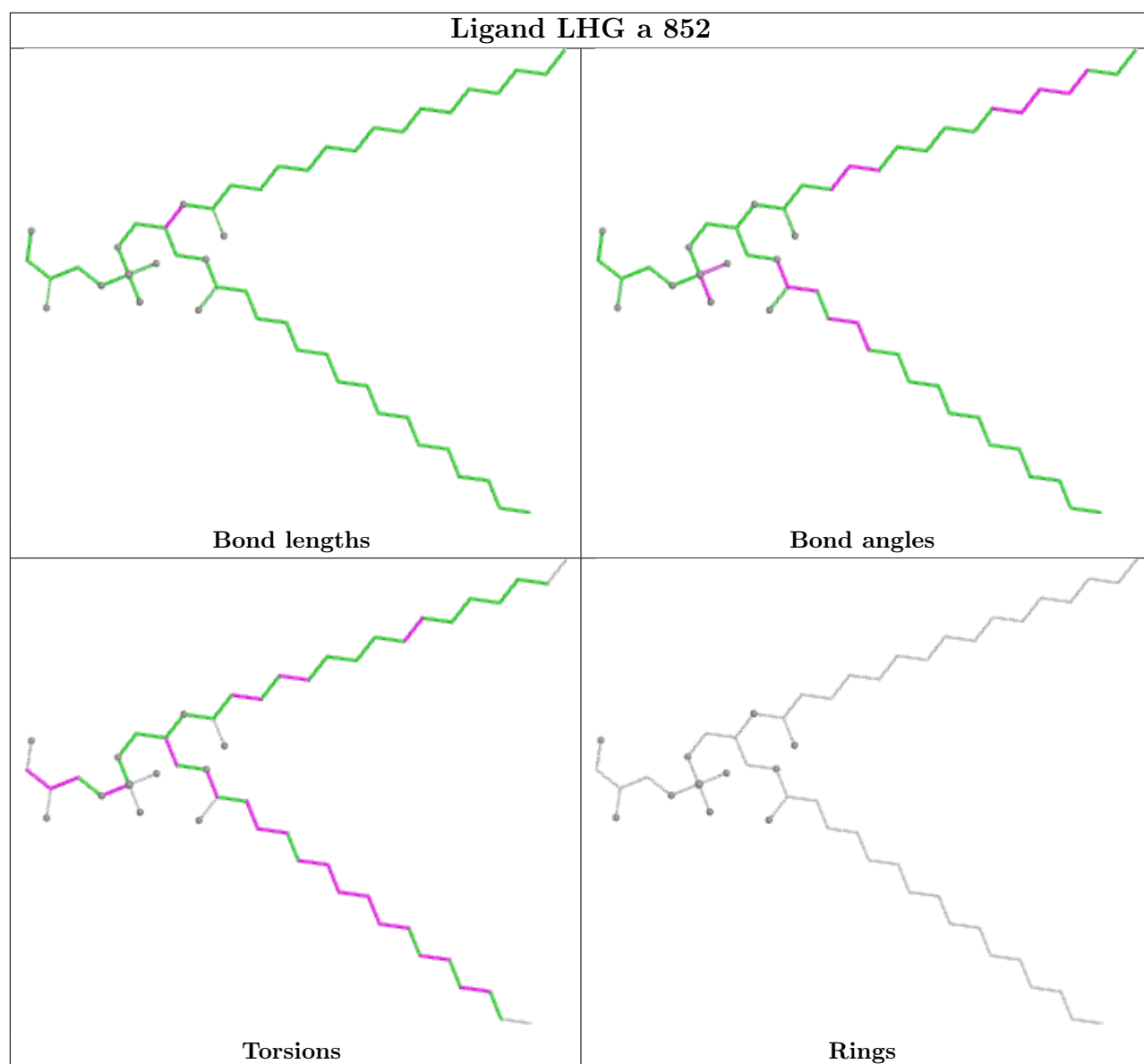
Ligand BCR b 3046

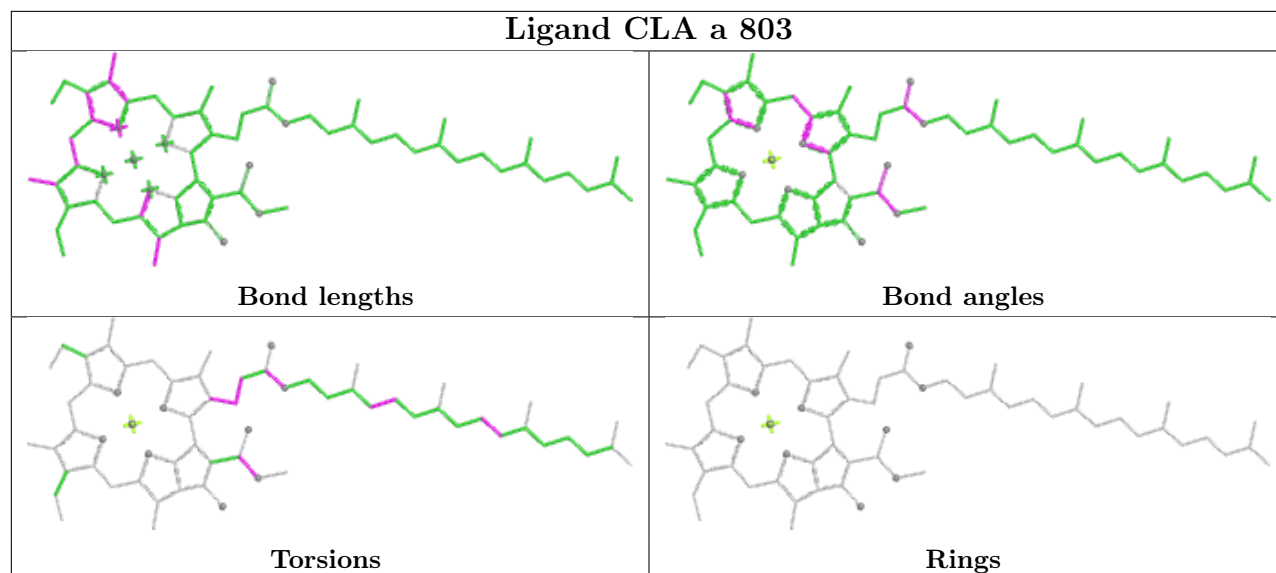
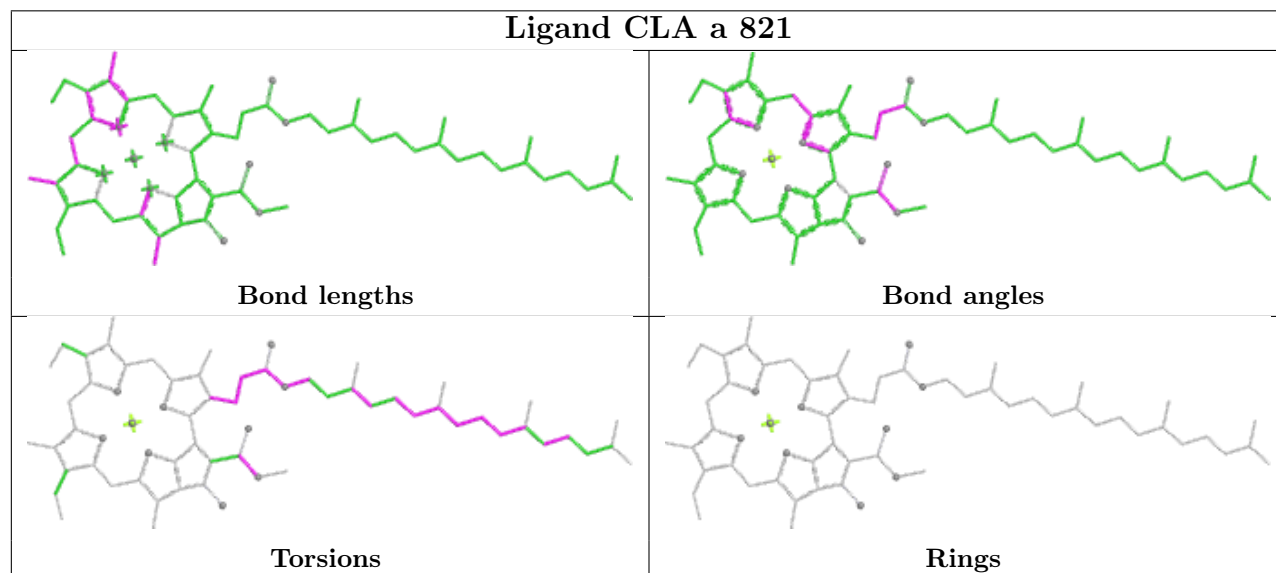
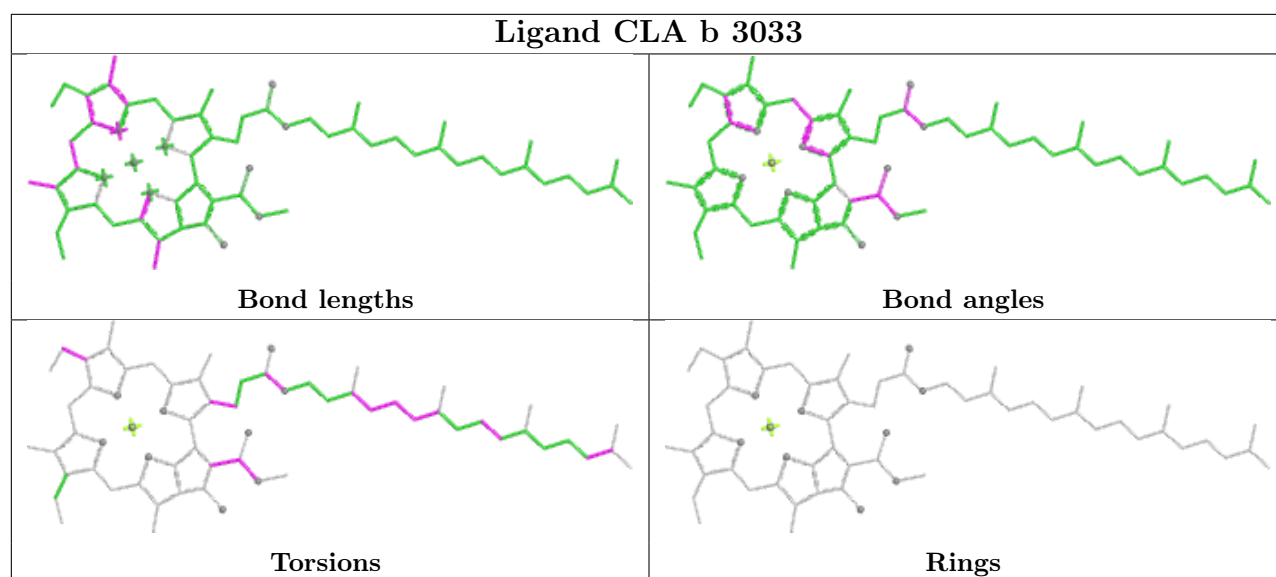


Ligand CLA b 3015

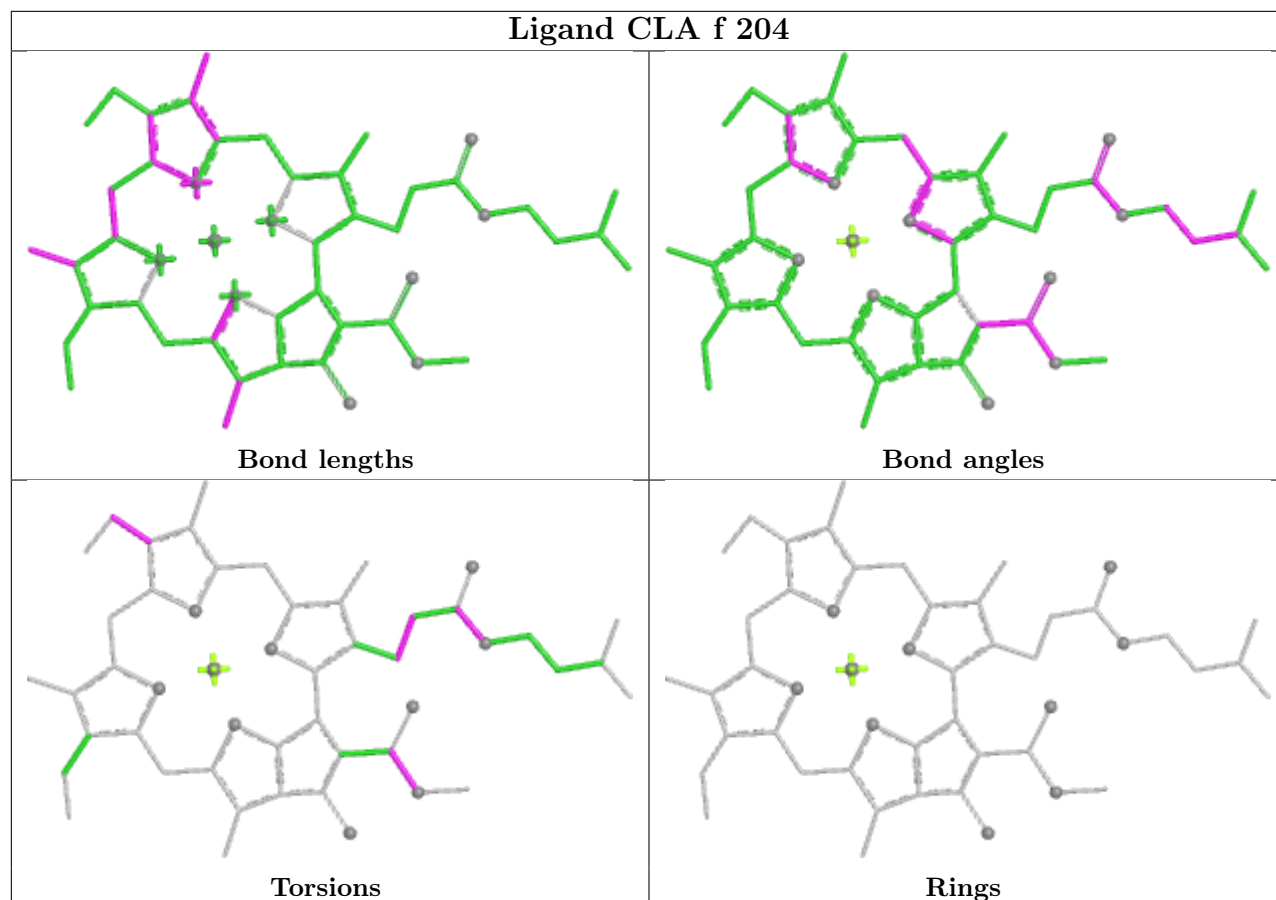




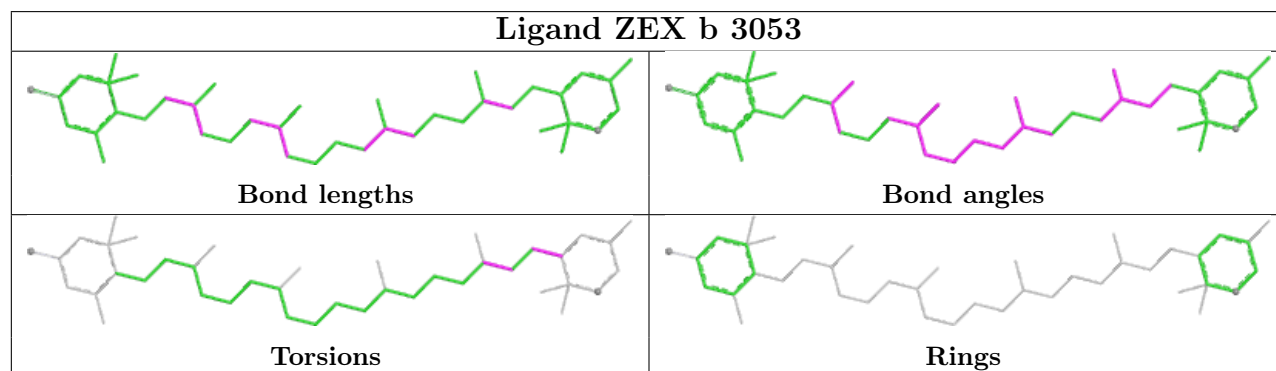


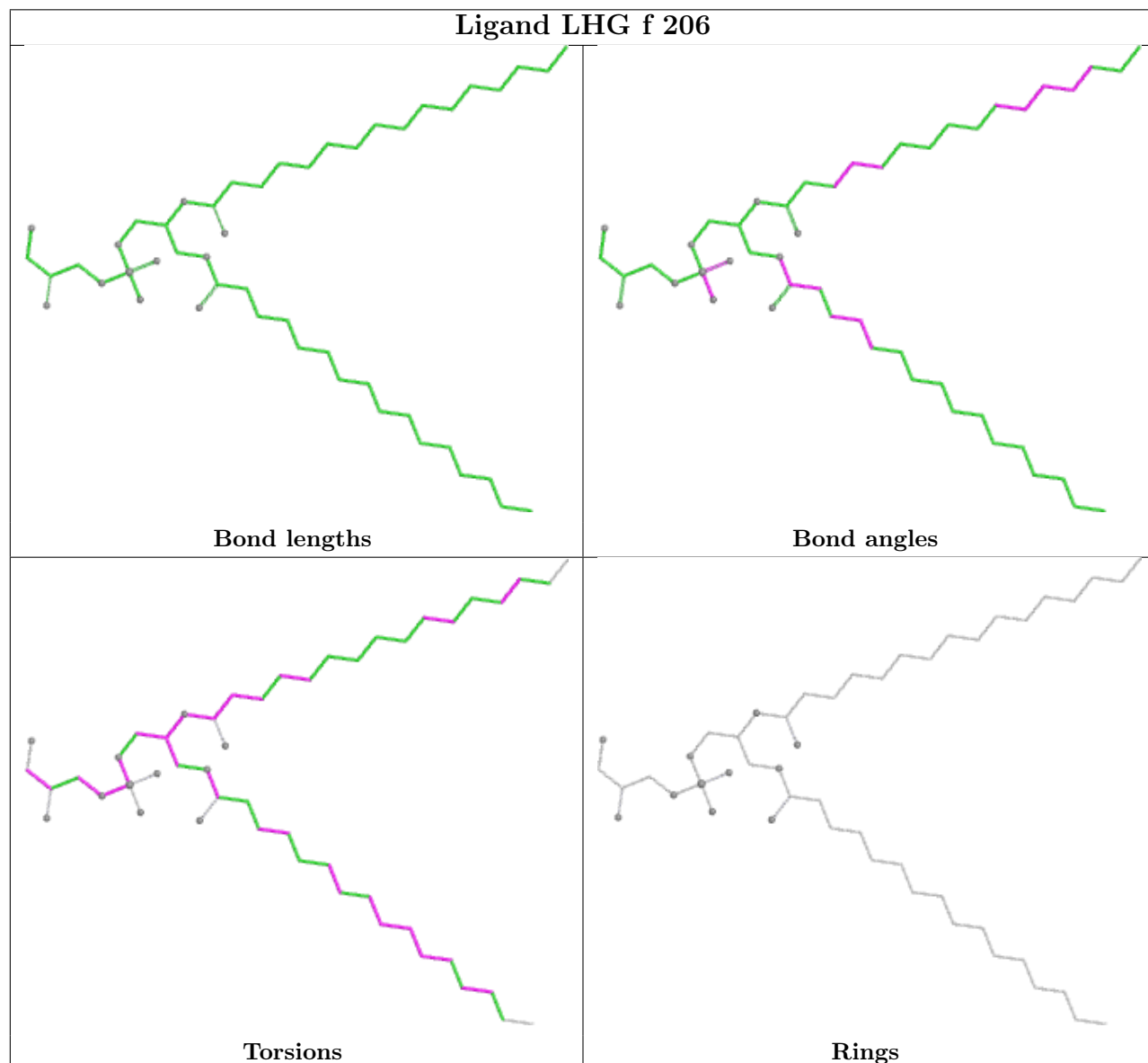
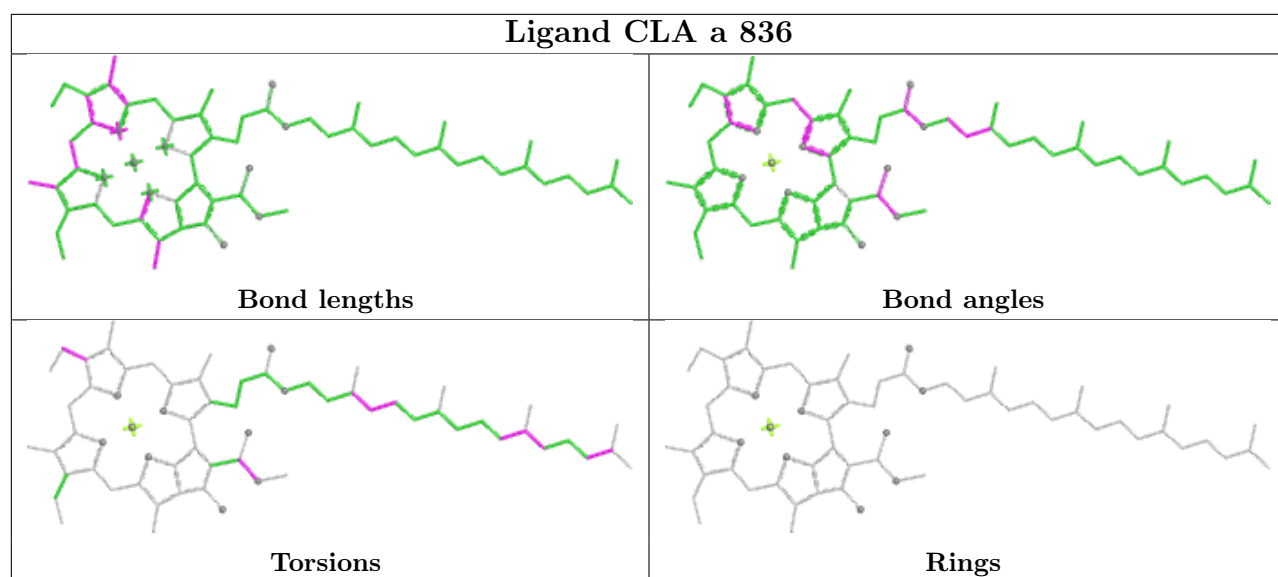


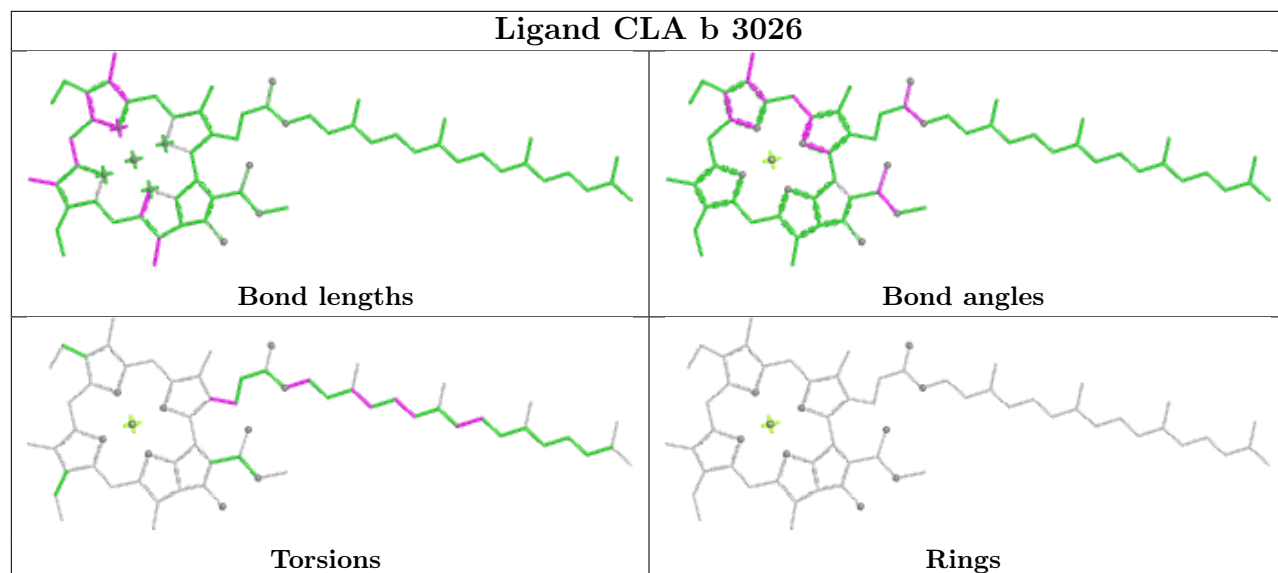
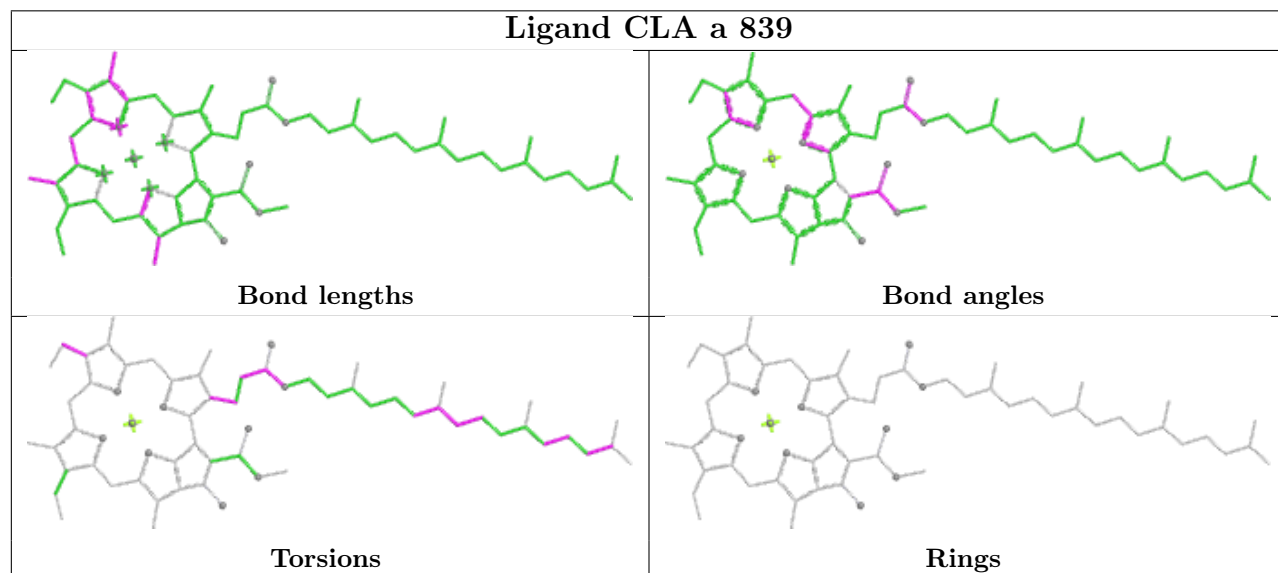
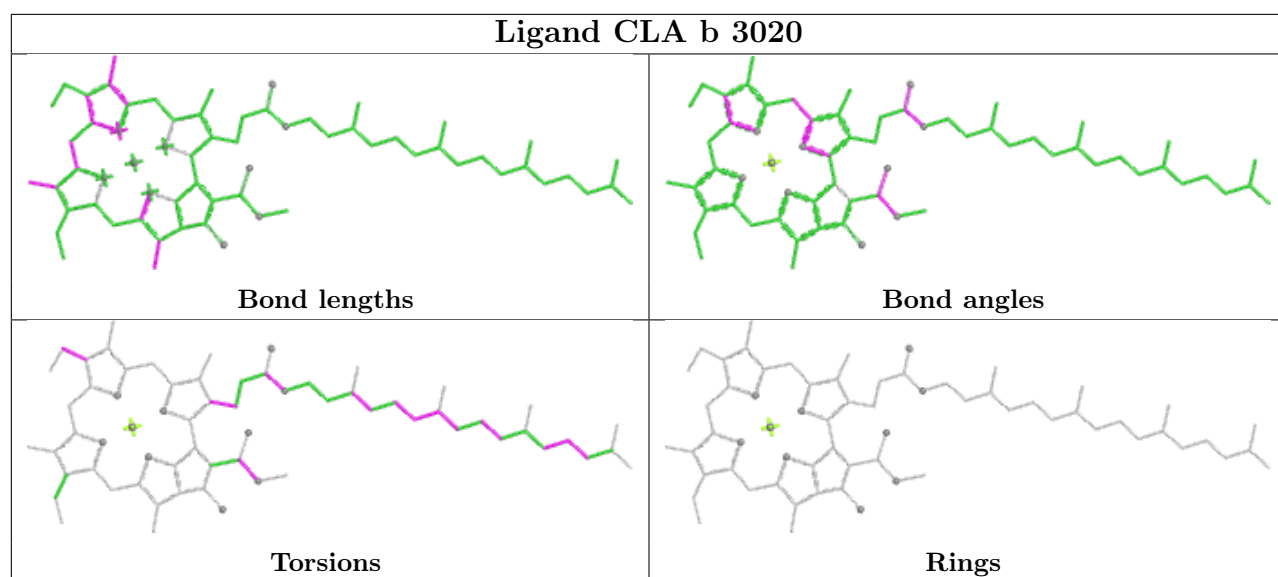
Ligand CLA f 204

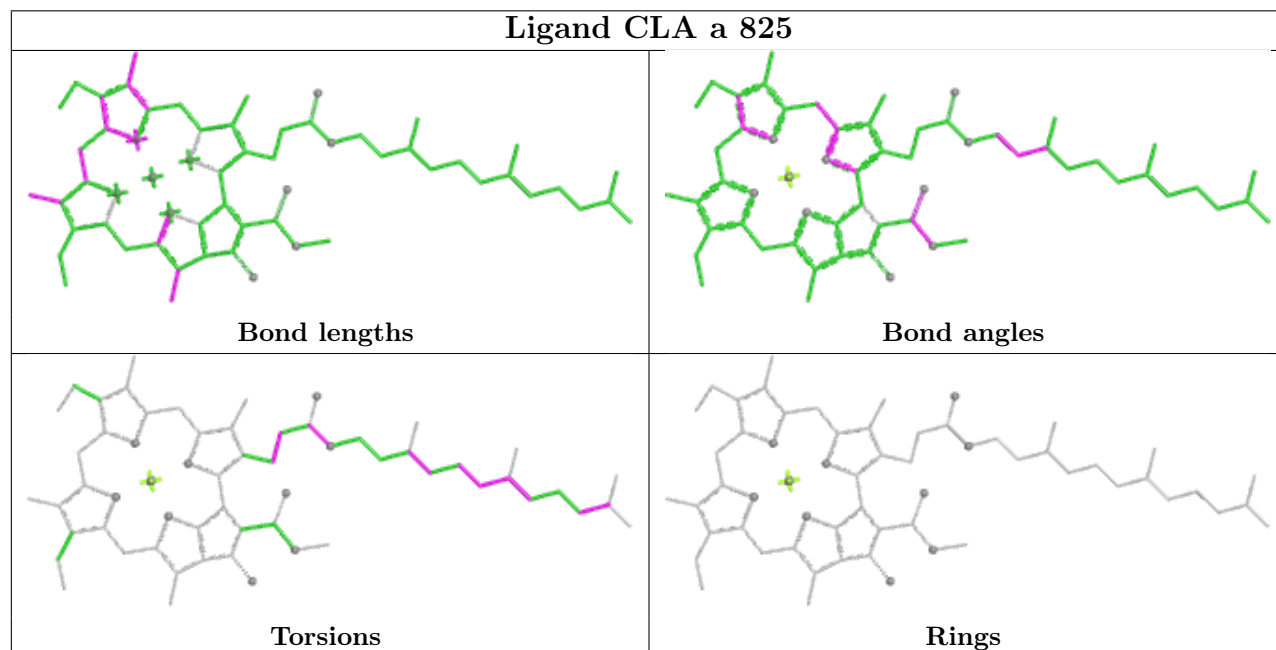
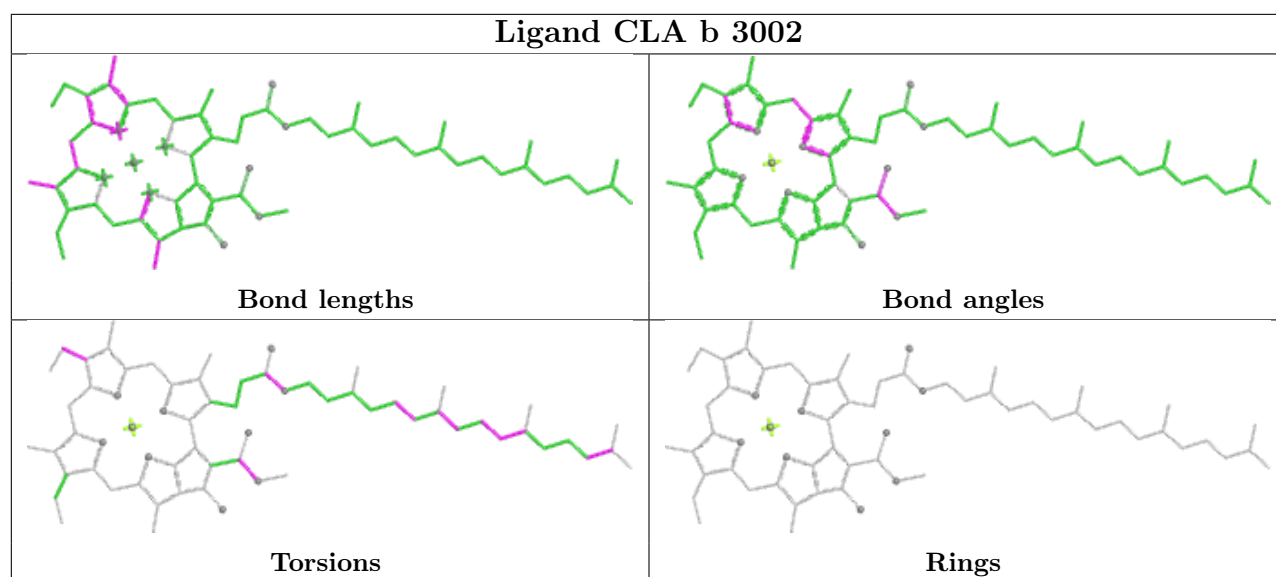


Ligand ZEX b 3053

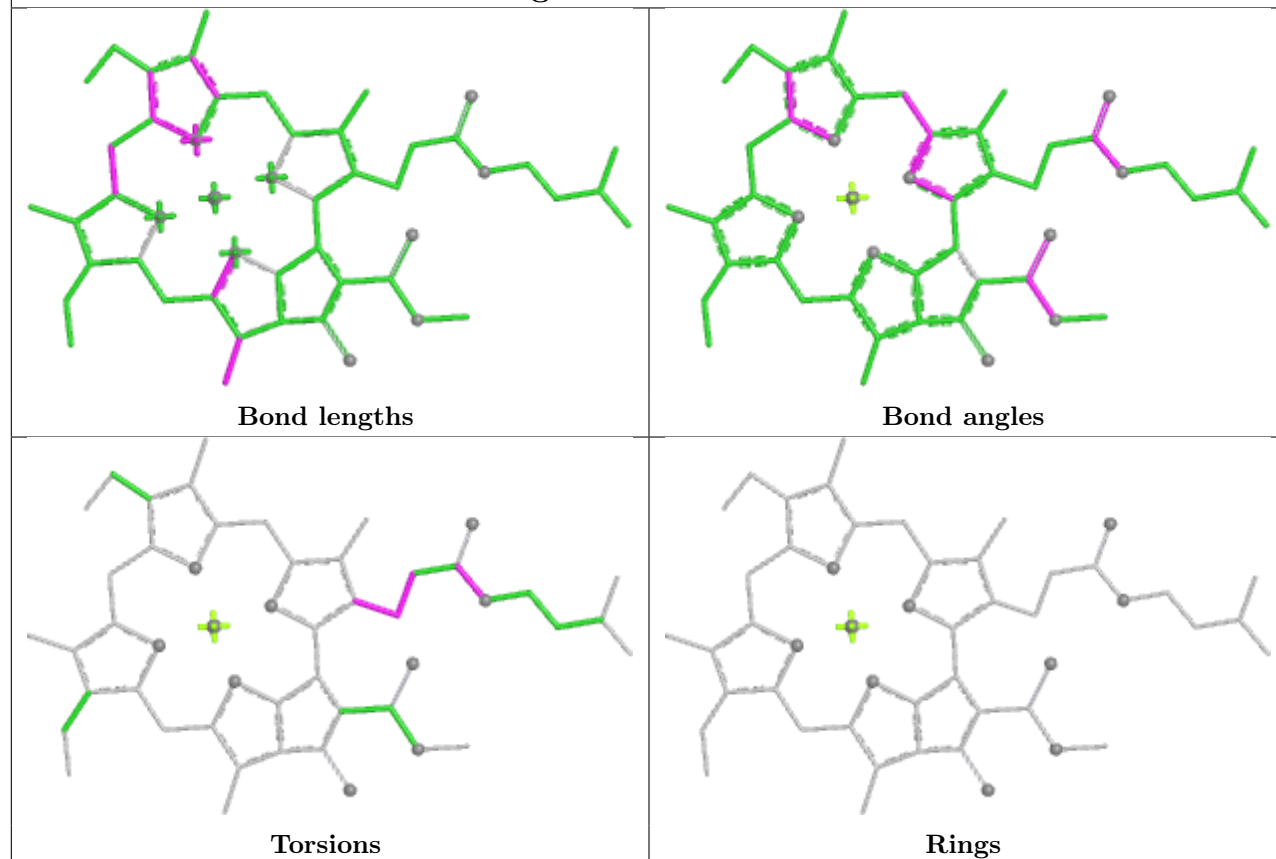




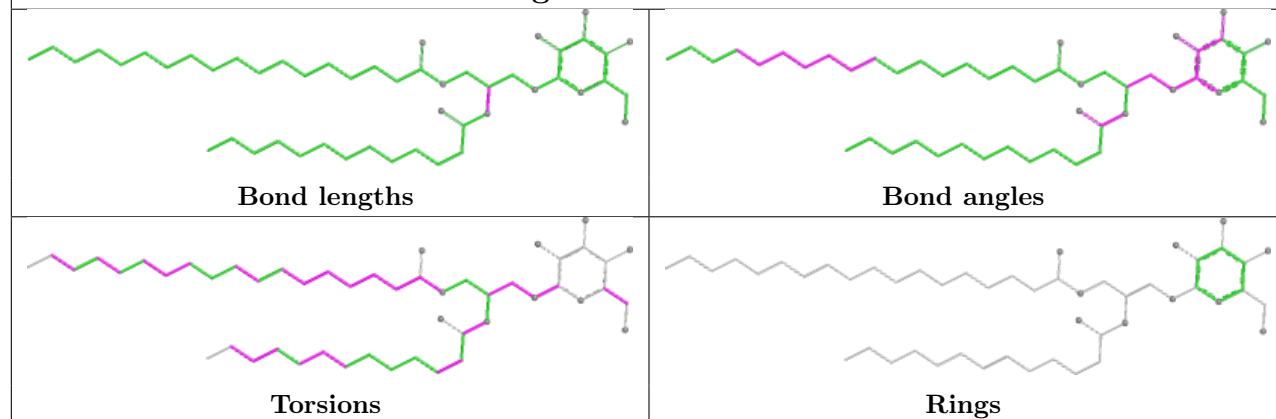


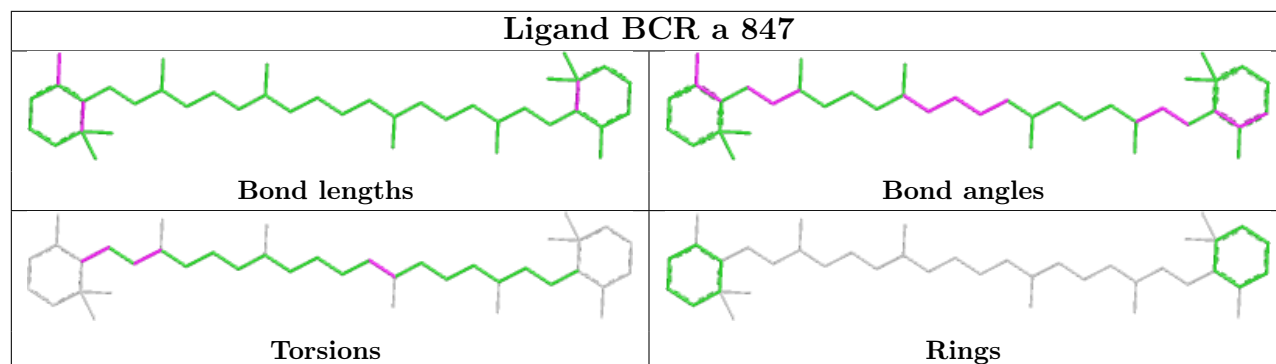
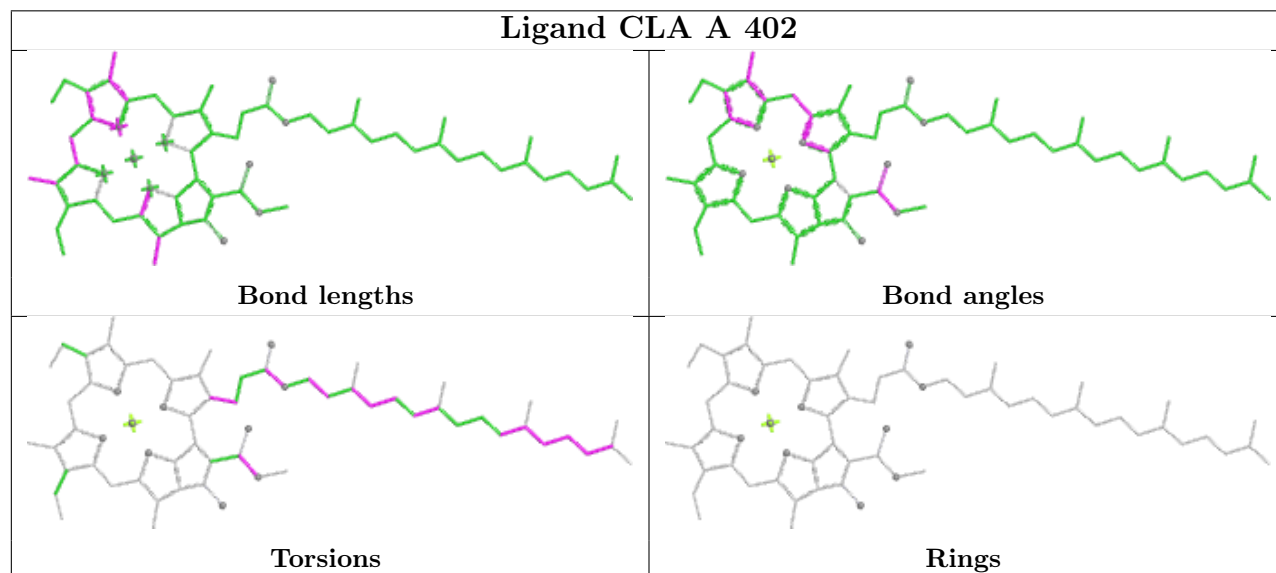
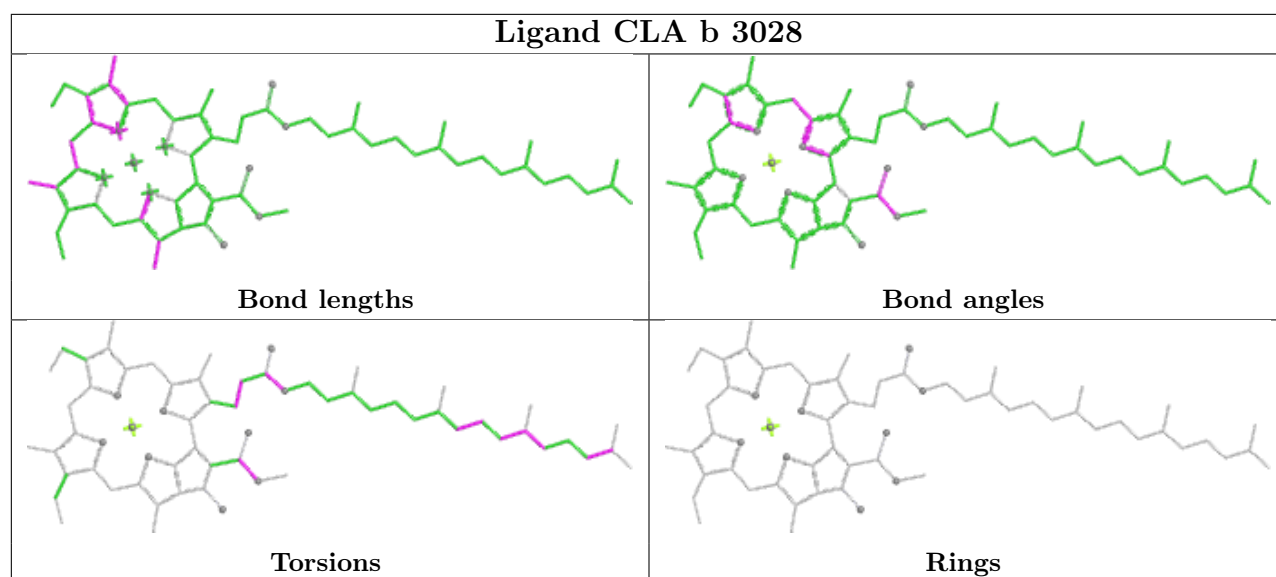


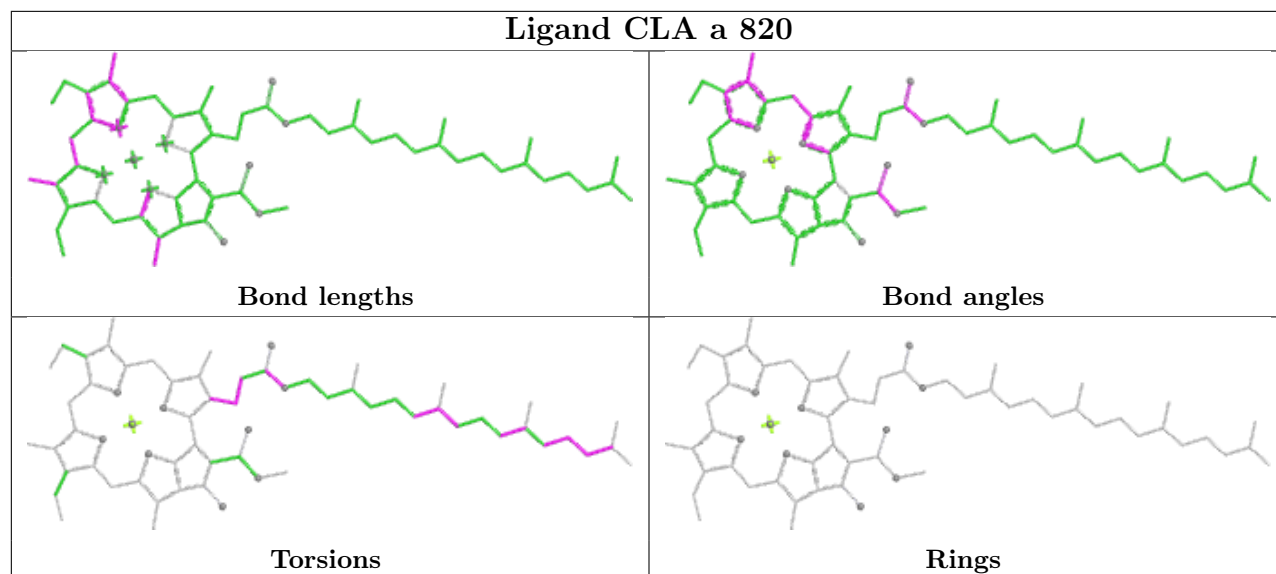
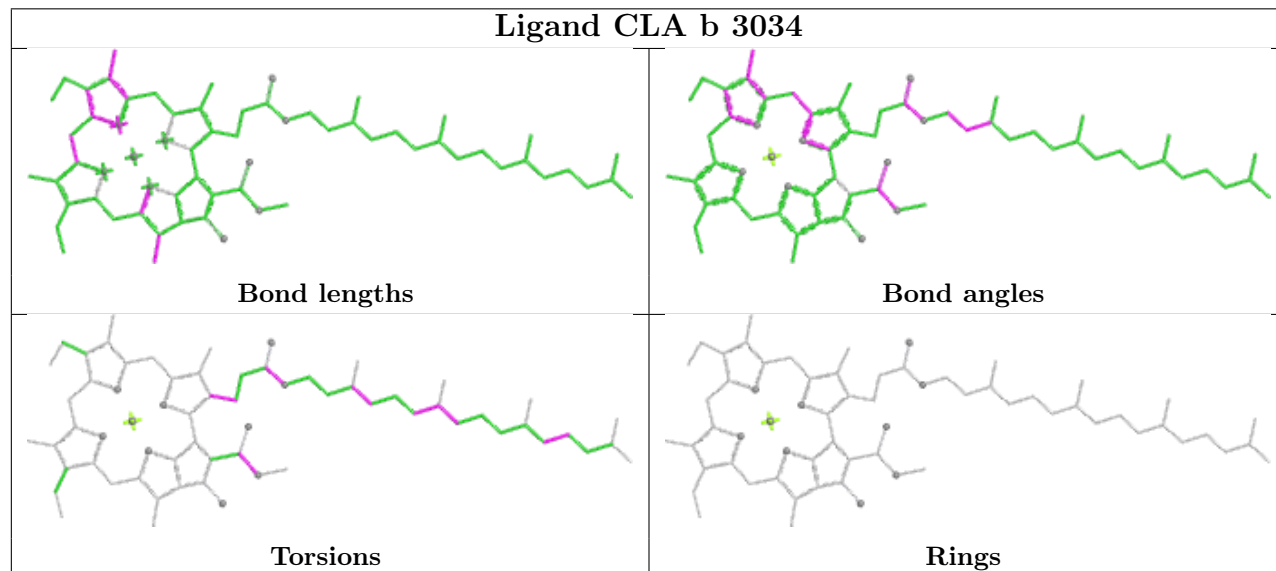
Ligand CLA A 405



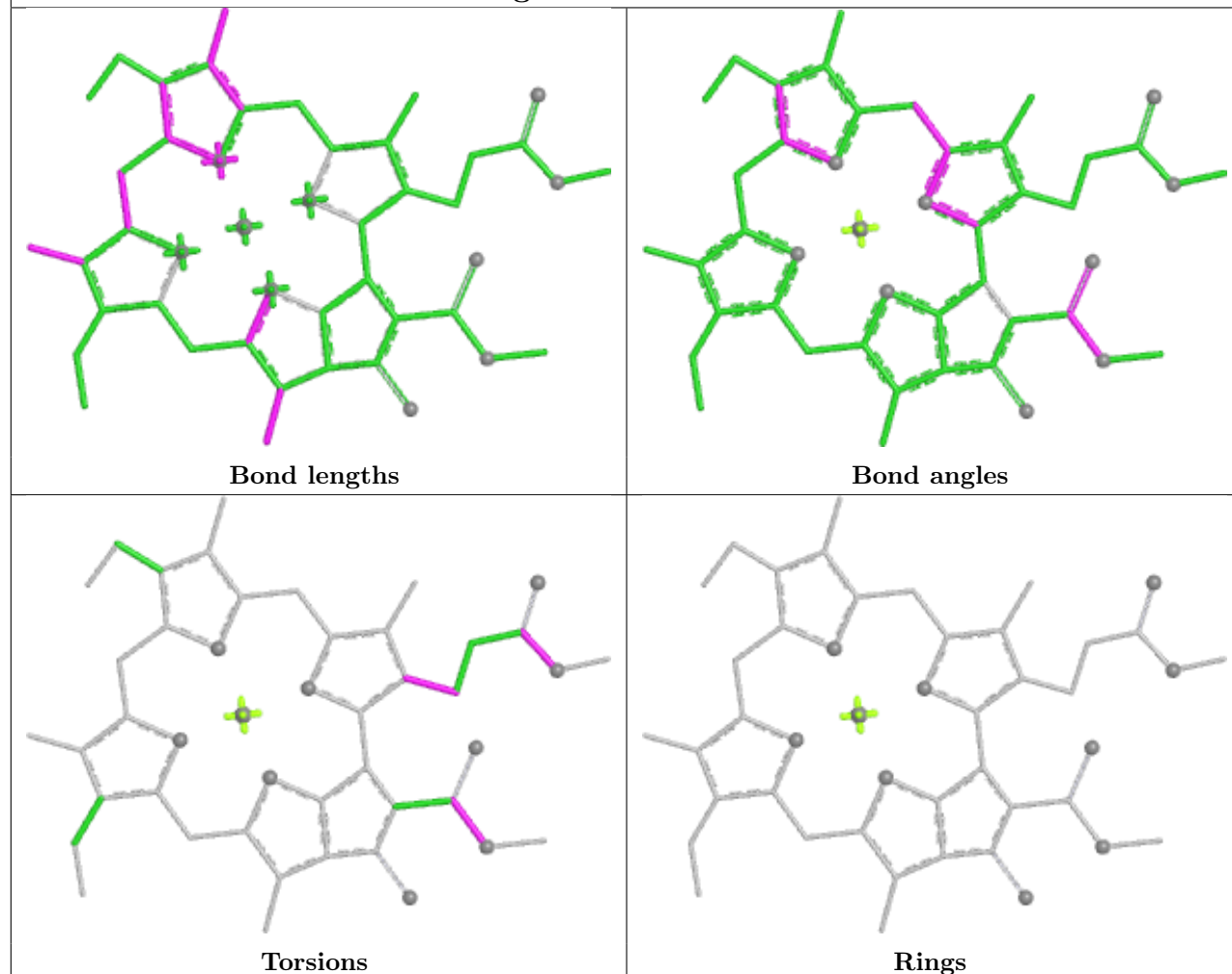
Ligand LMG a 851



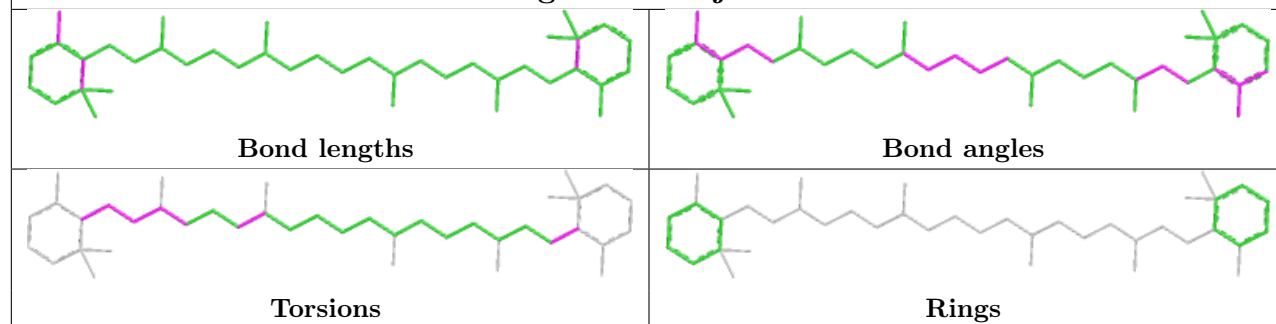


Ligand CLA a 820**Ligand CLA b 3034**

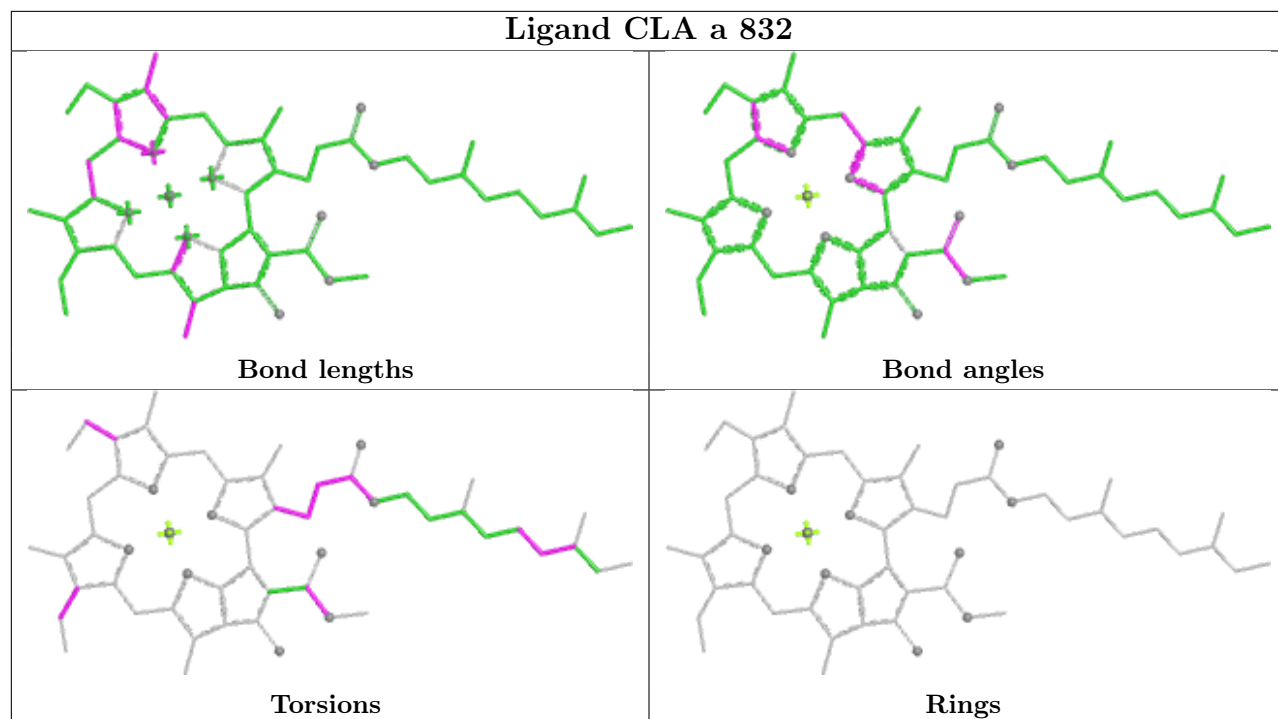
Ligand CLA A 403



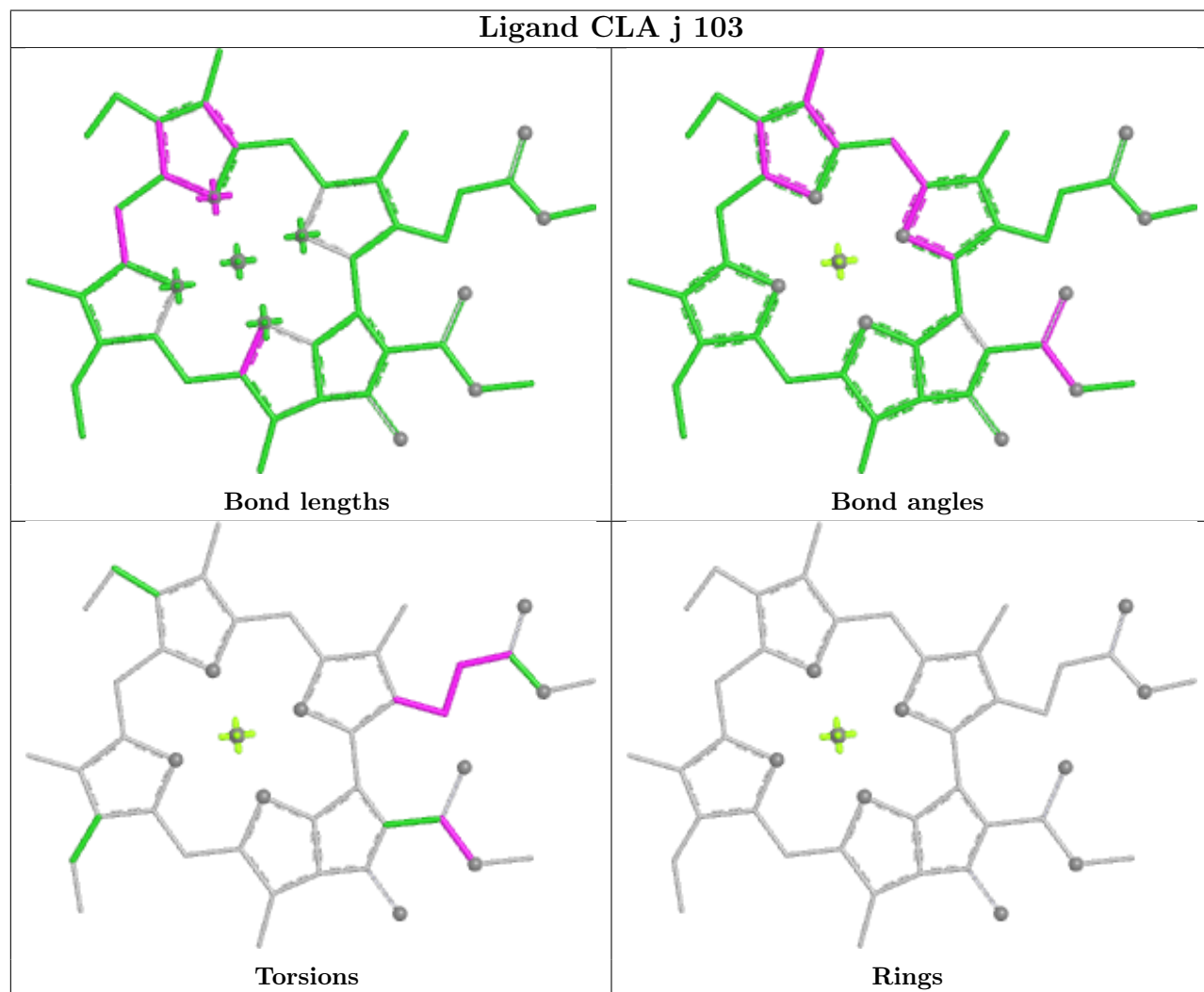
Ligand BCR j 104

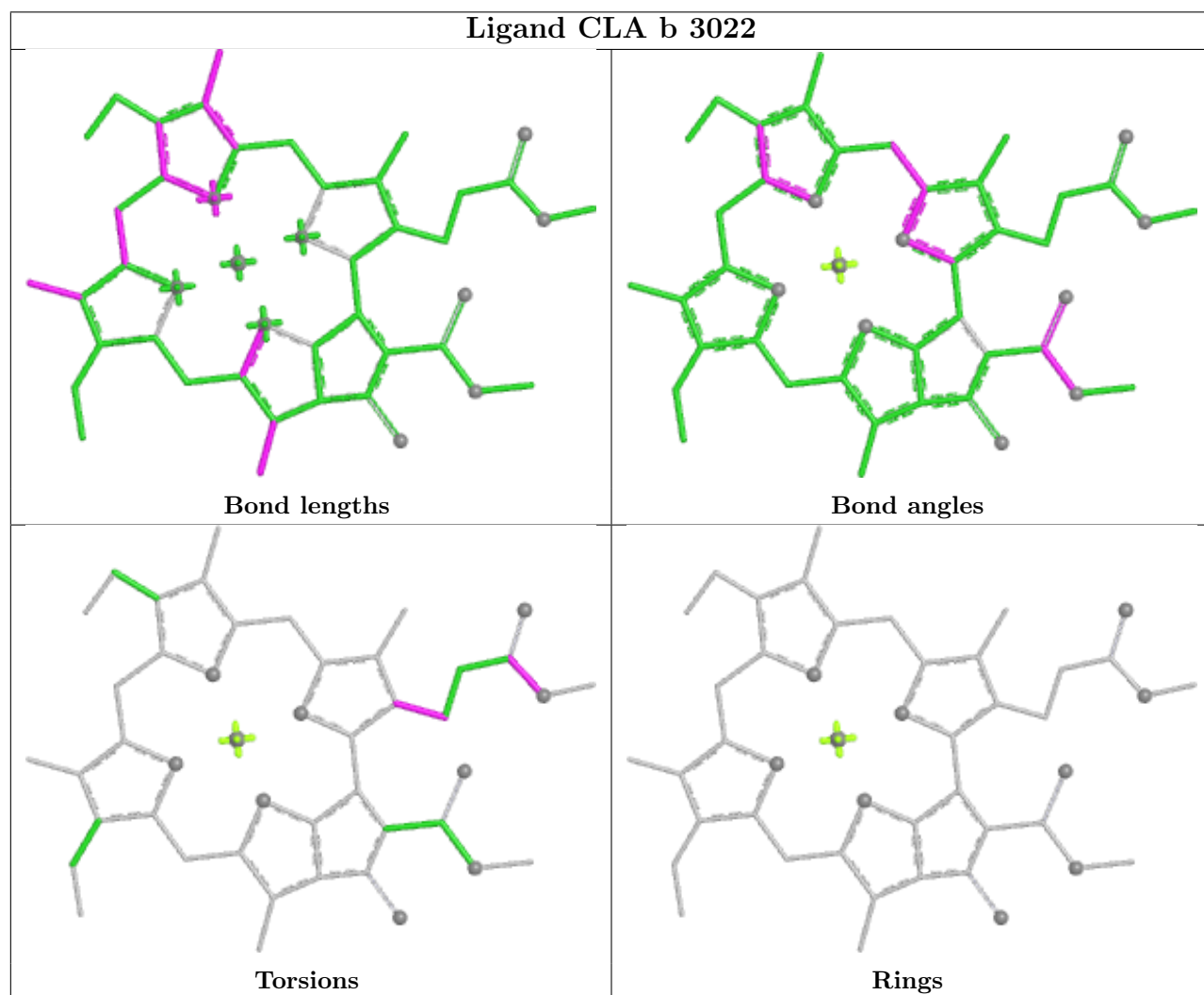
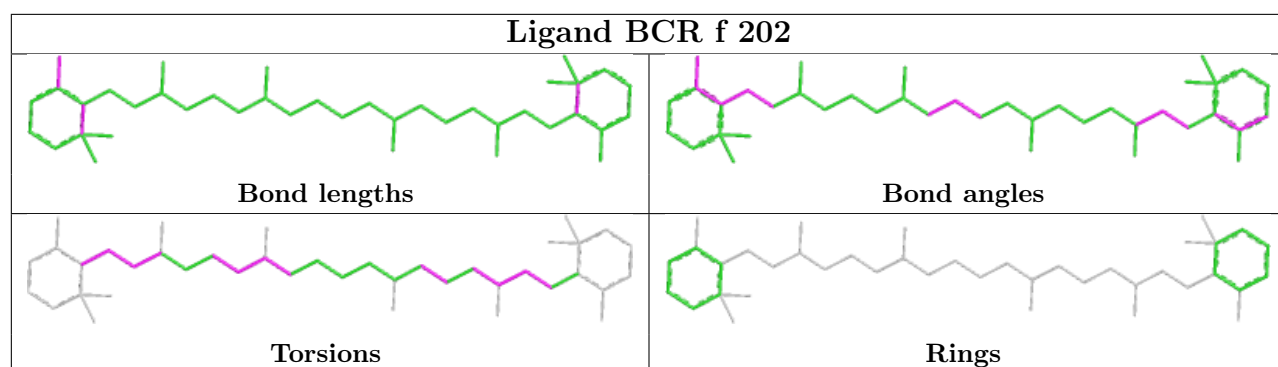


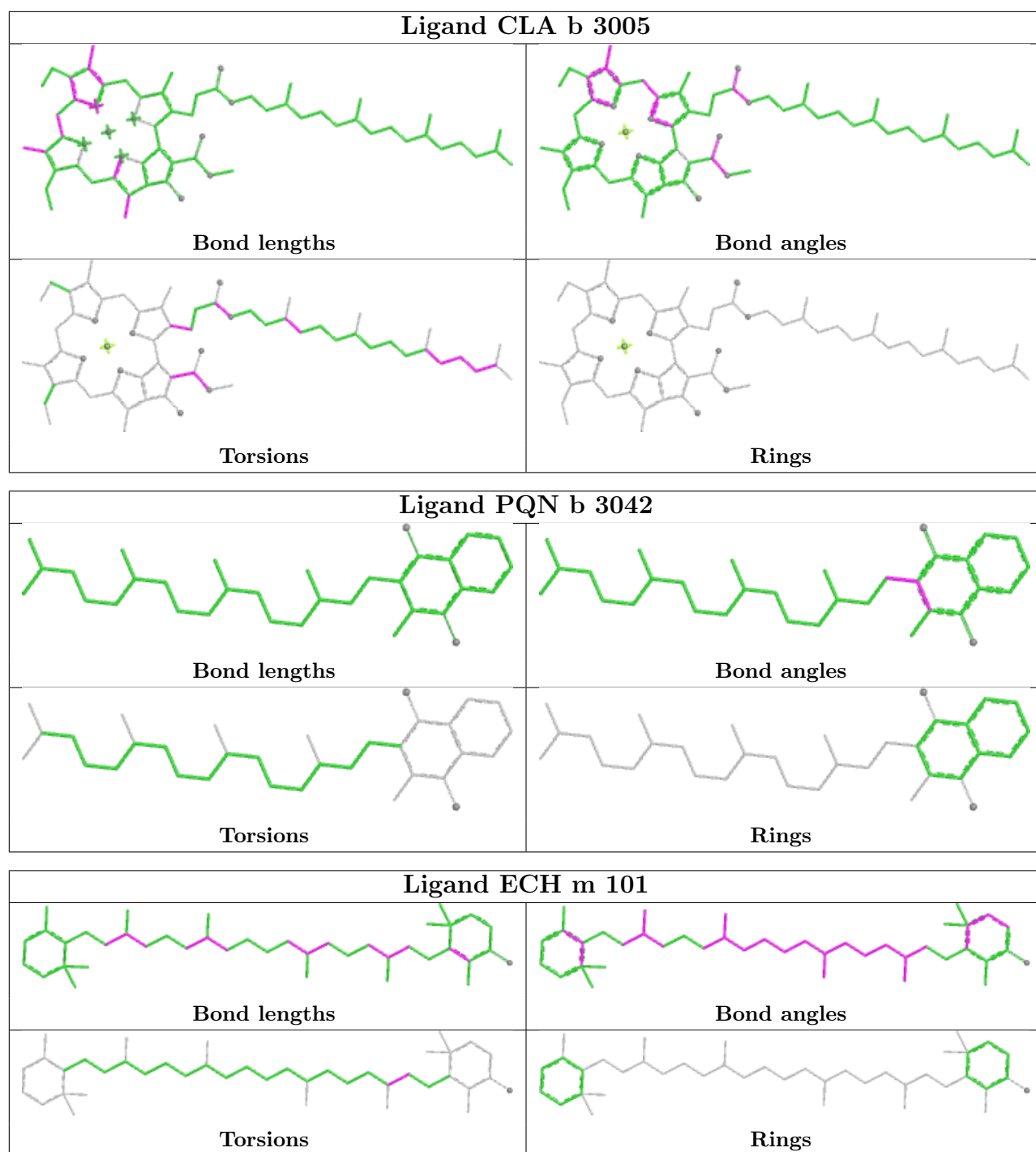
Ligand CLA a 832

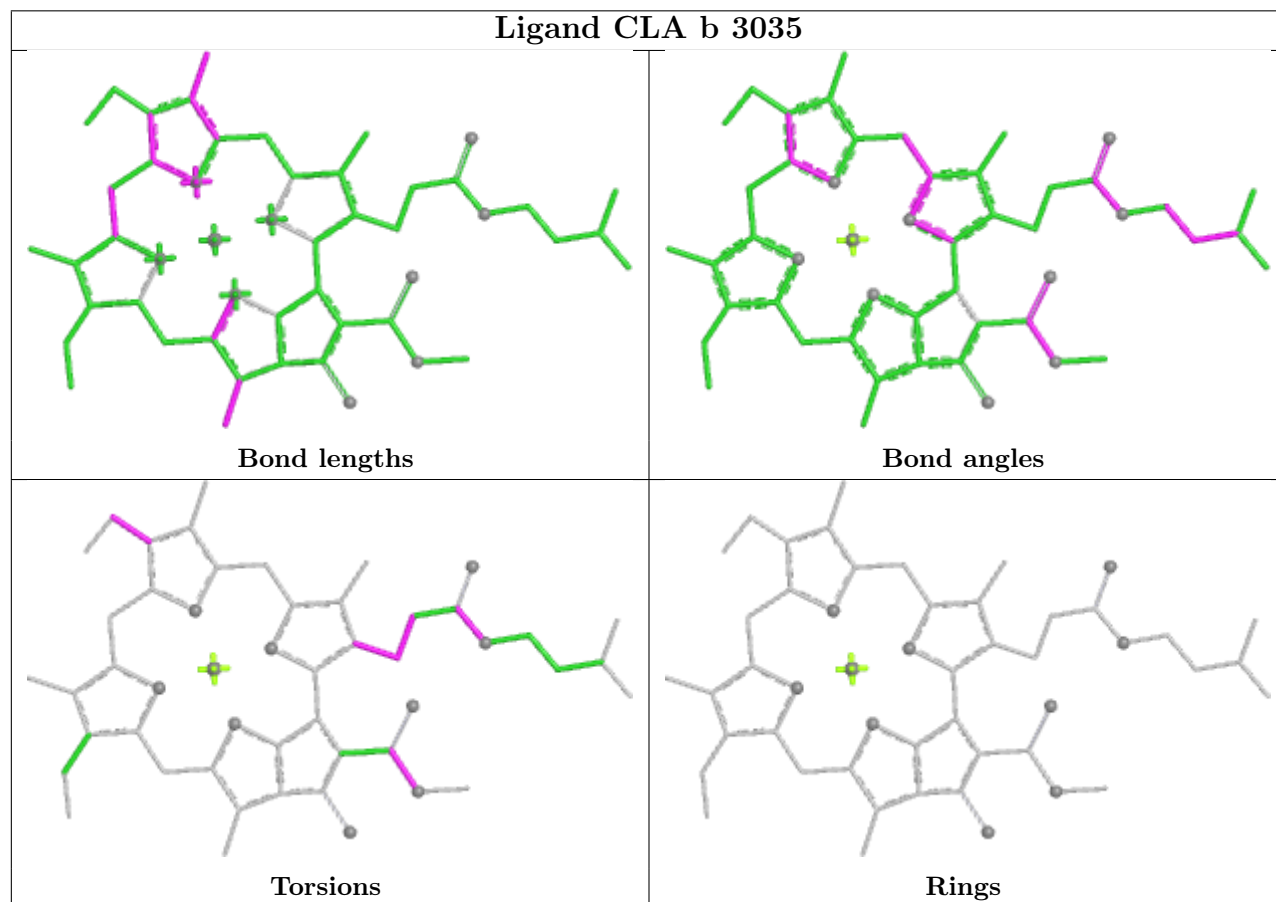
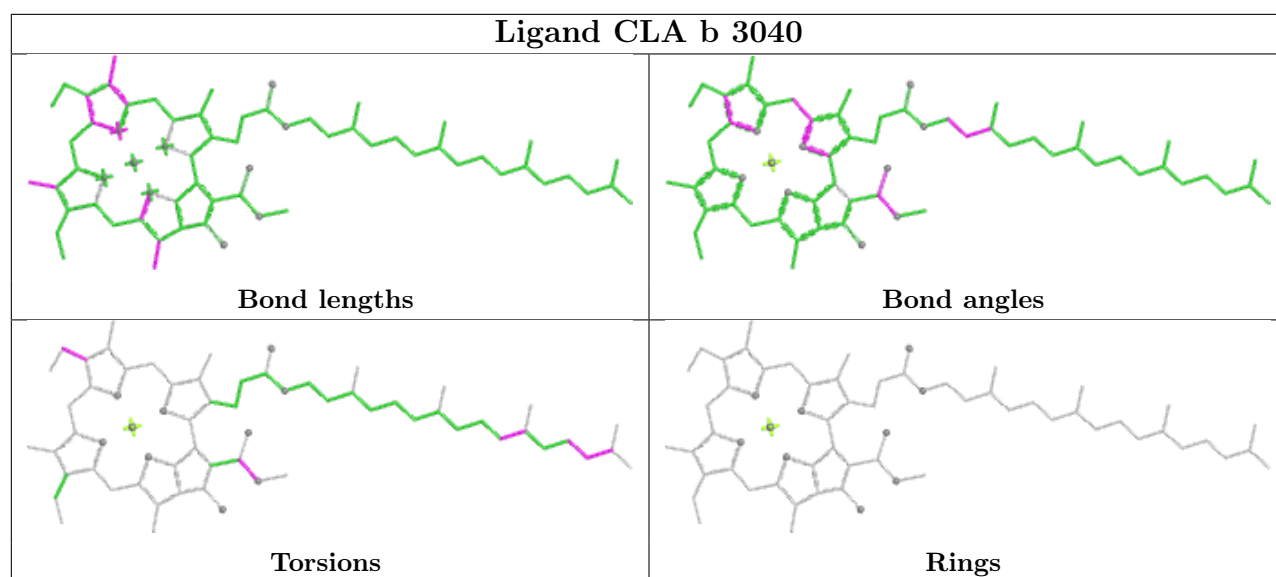


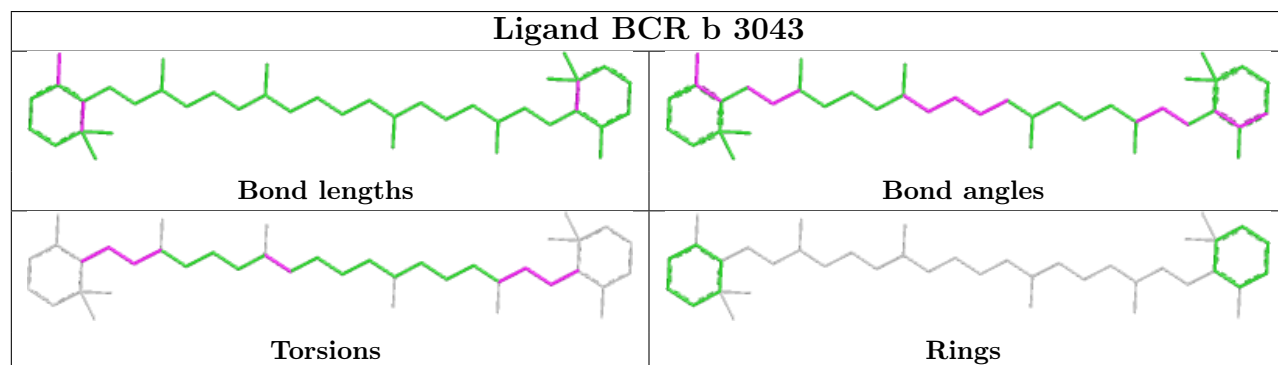
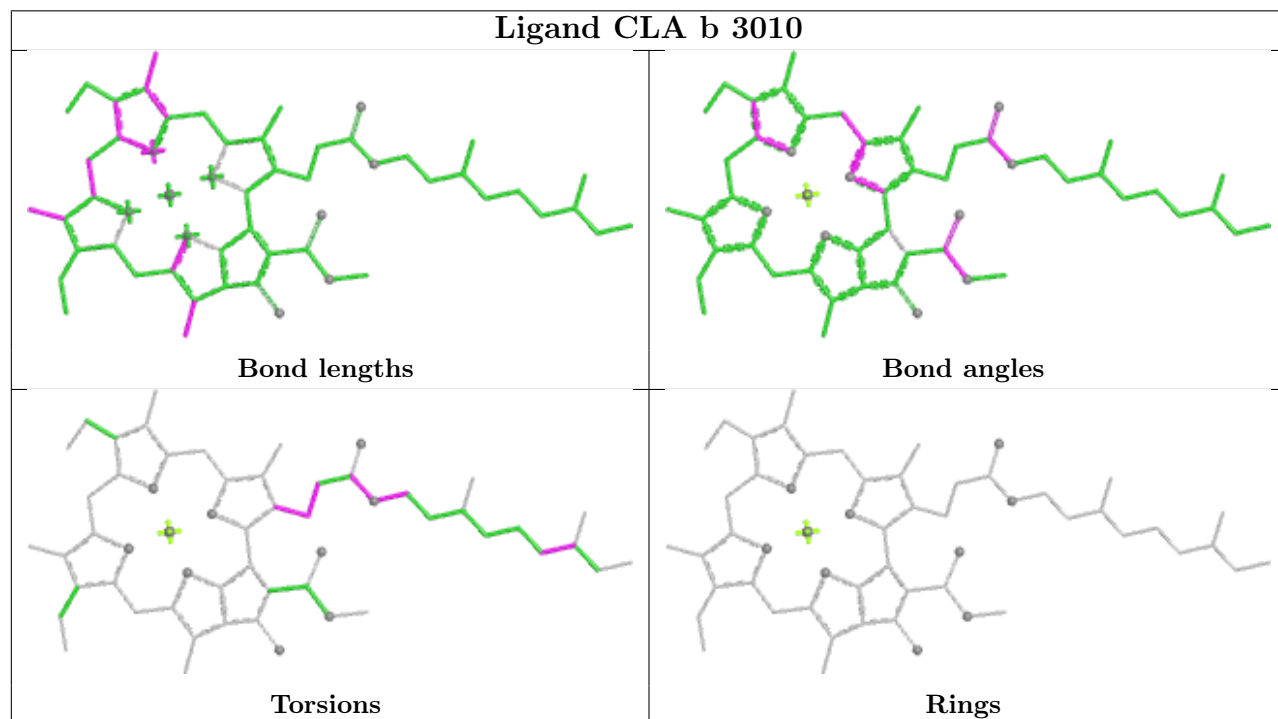
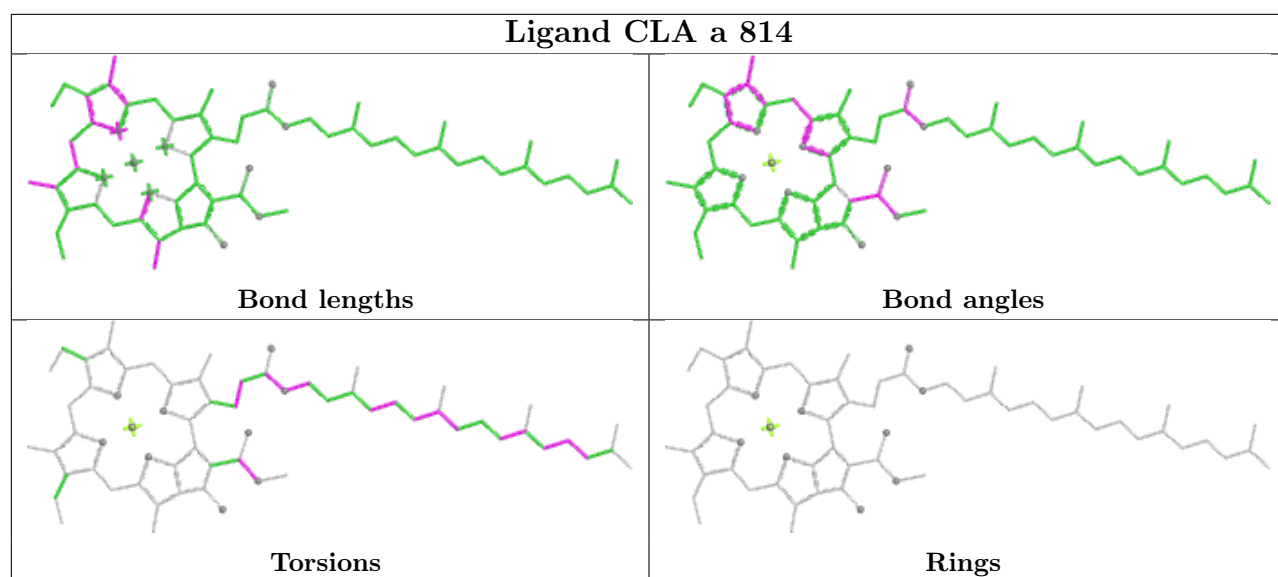
Ligand CLA j 103



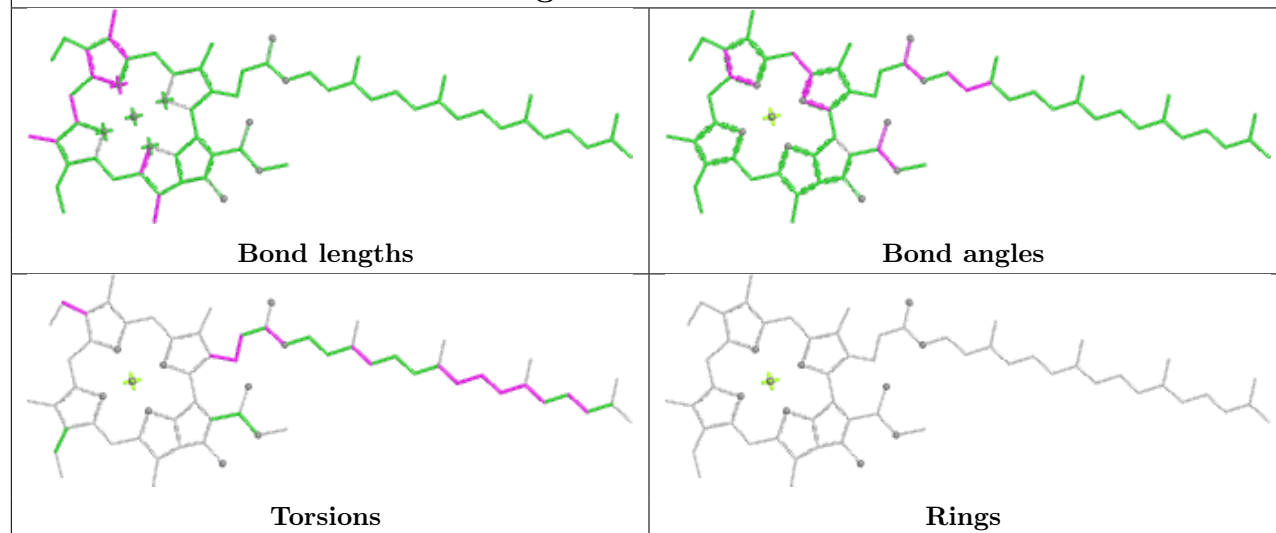




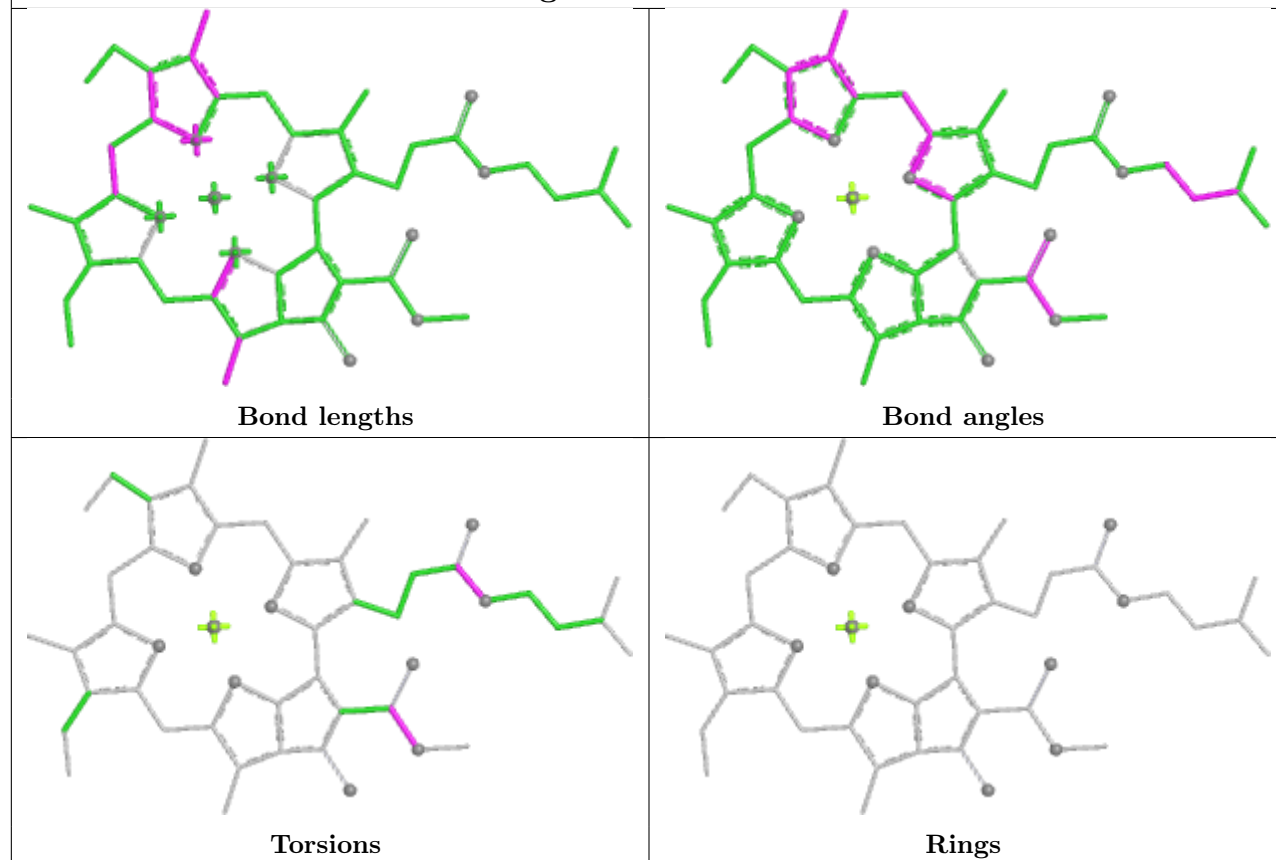




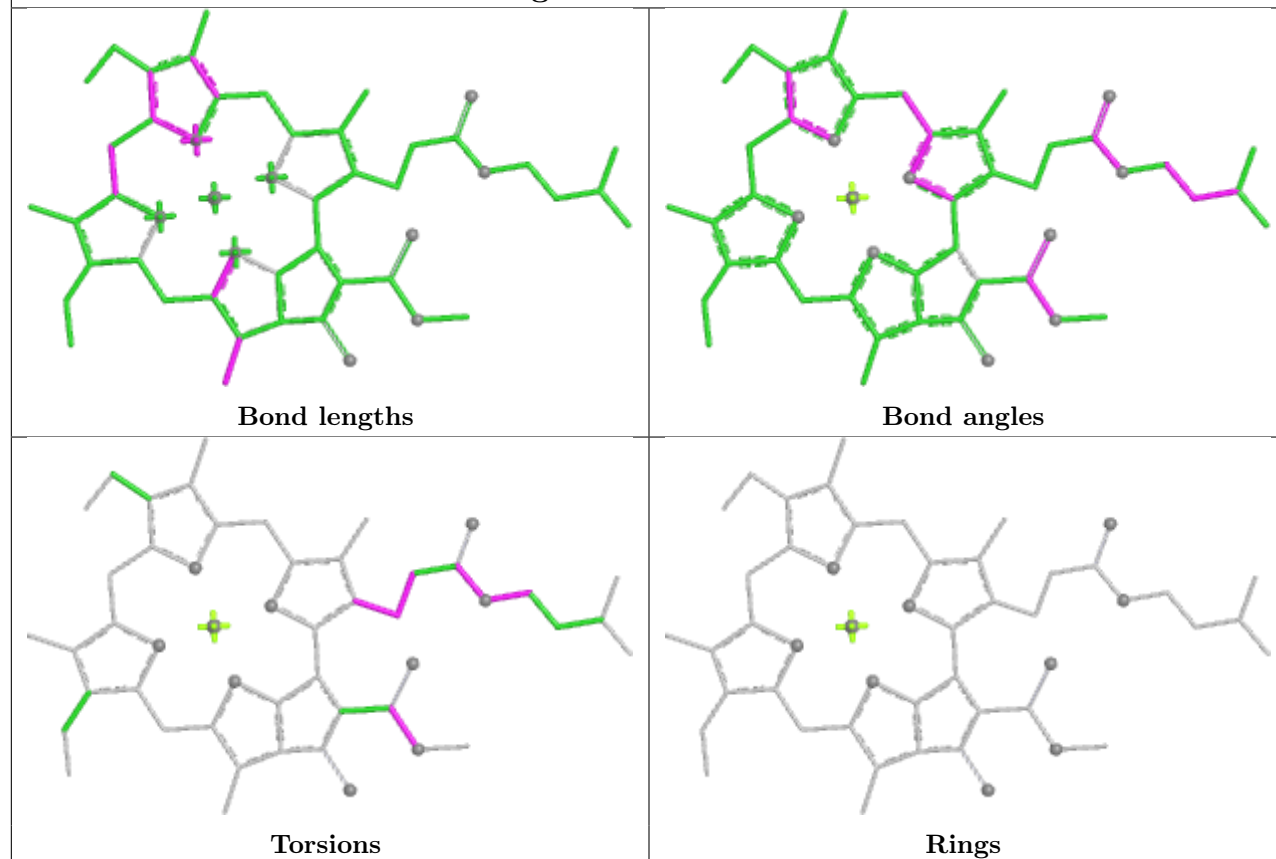
Ligand CLA a 828



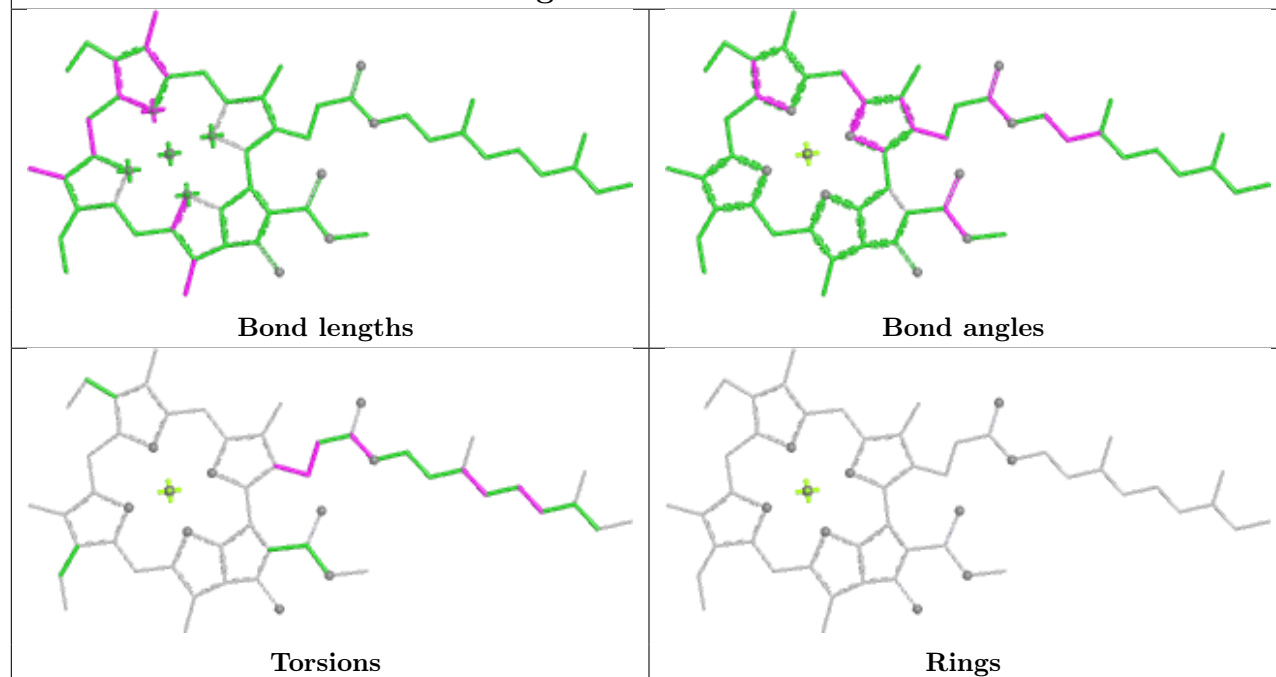
Ligand CLA f 203

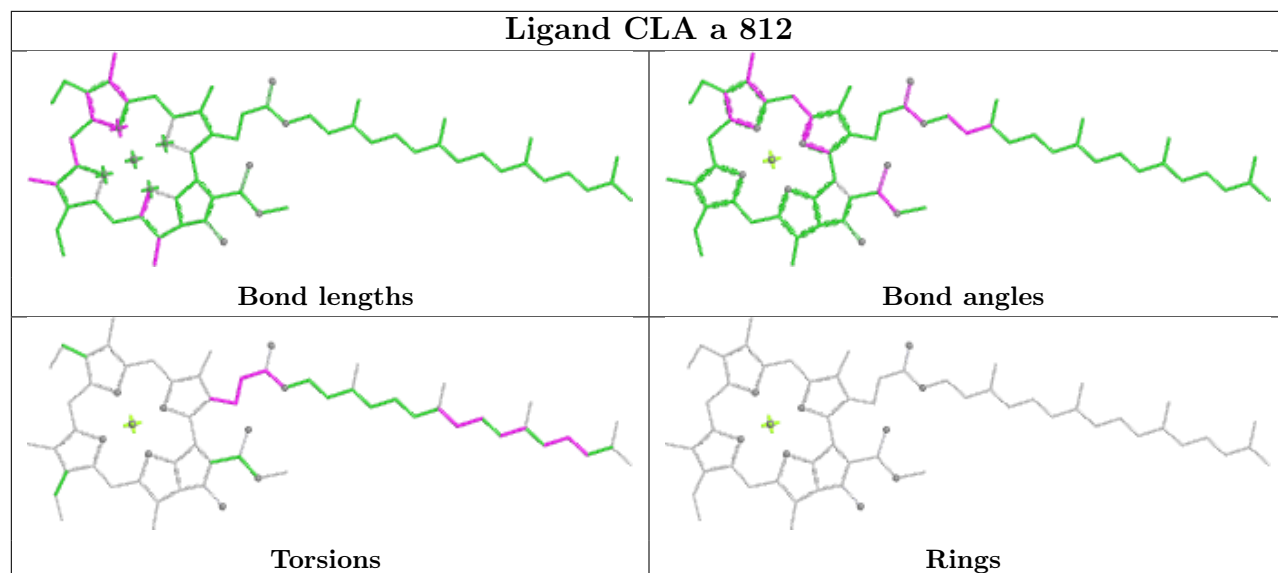
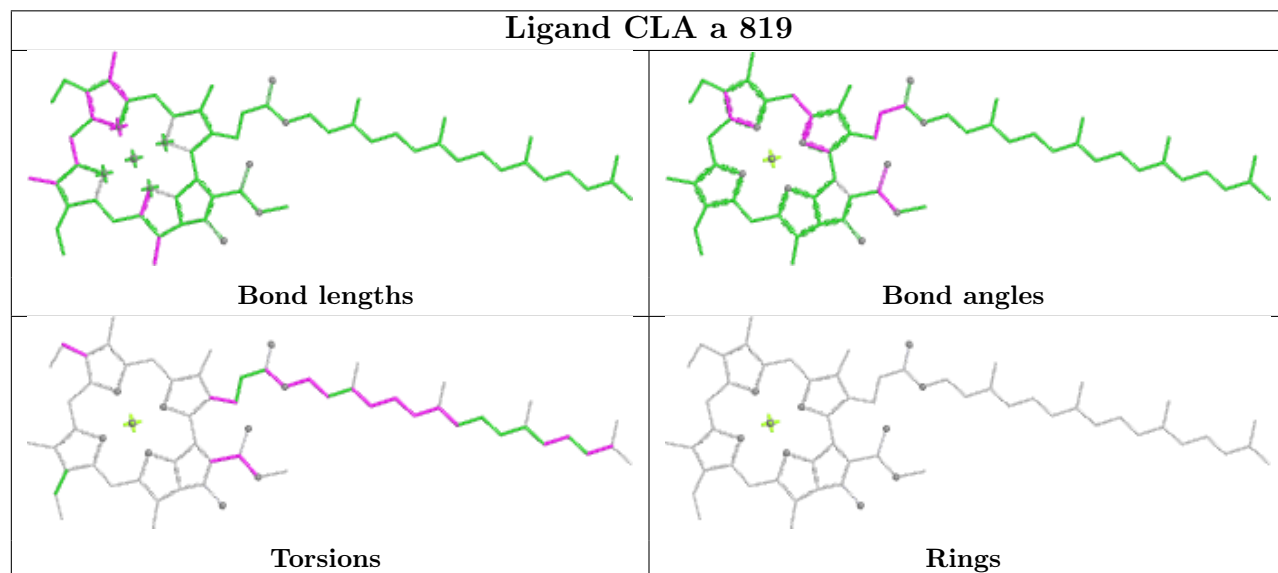
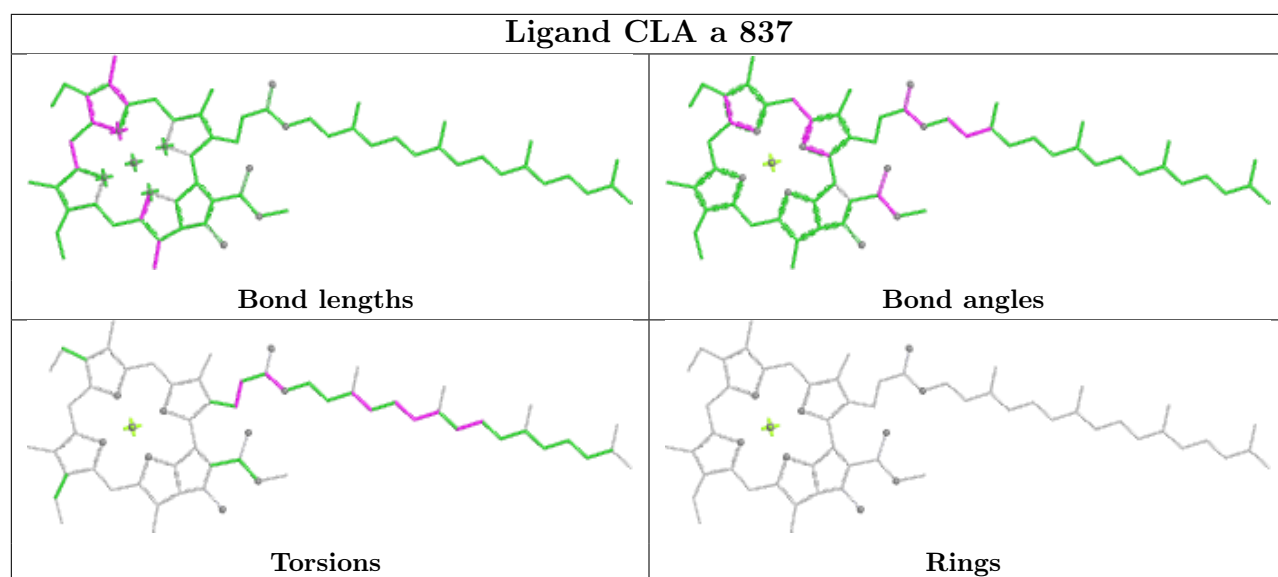


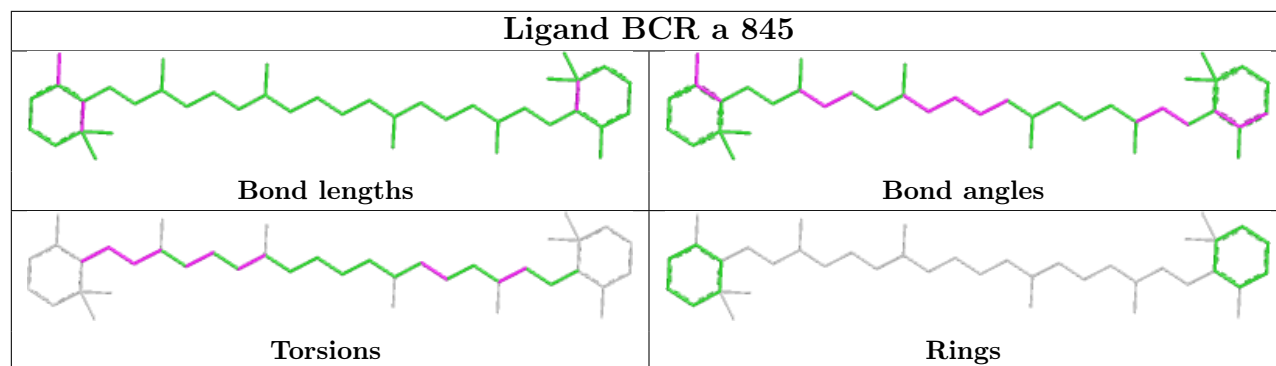
Ligand CLA 1 1501



Ligand CLA a 843







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.

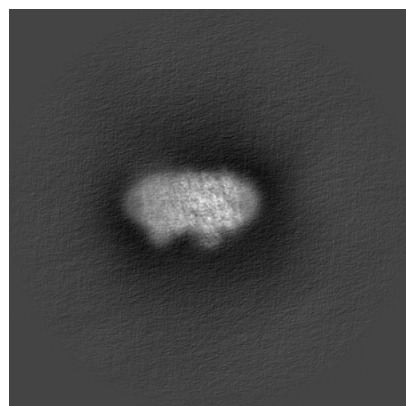
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15618. These allow visual inspection of the internal detail of the map and identification of artifacts.

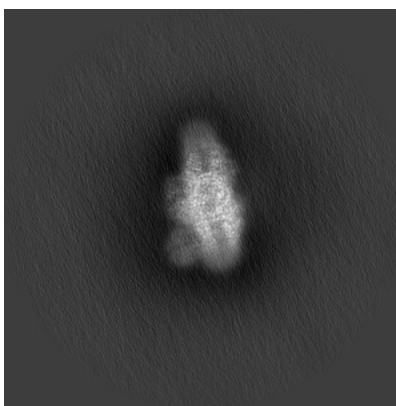
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

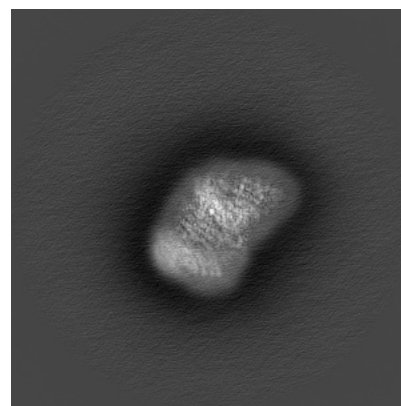
6.1.1 Primary map



X

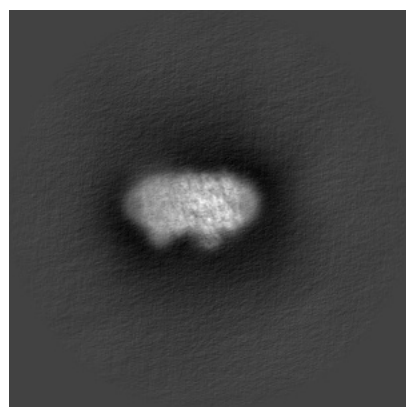


Y

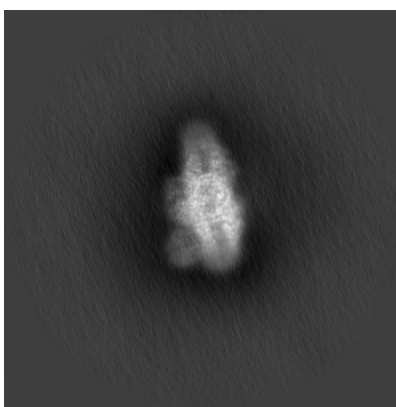


Z

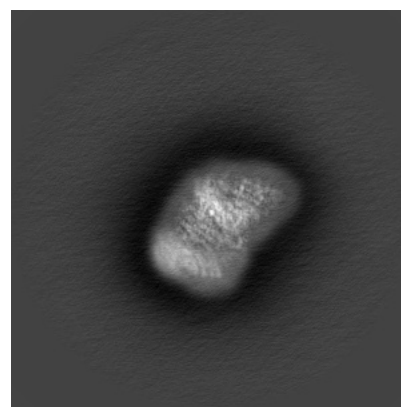
6.1.2 Raw map



X



Y

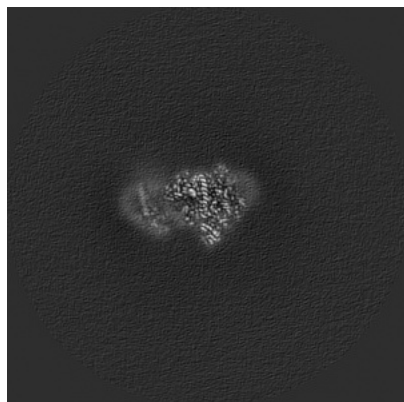


Z

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

6.2 Central slices [i](#)

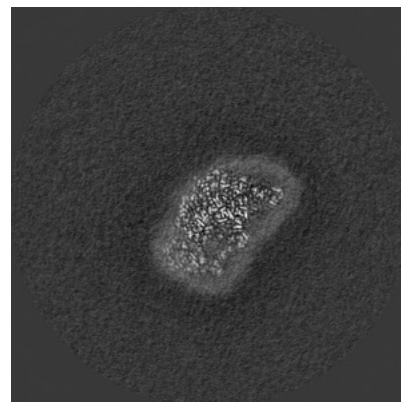
6.2.1 Primary map



X Index: 200

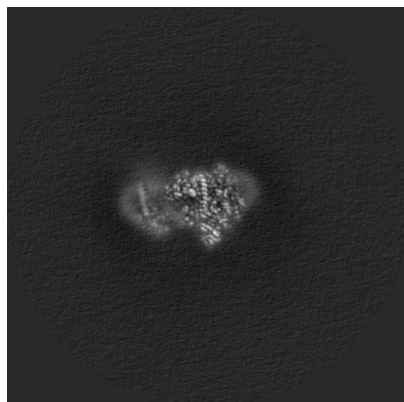


Y Index: 200

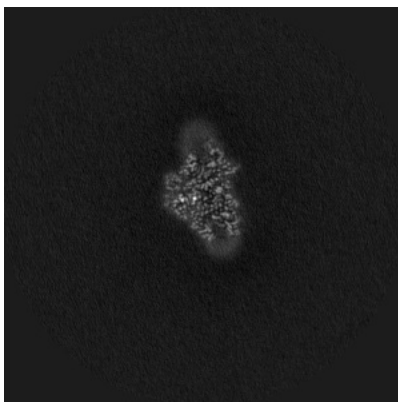


Z Index: 200

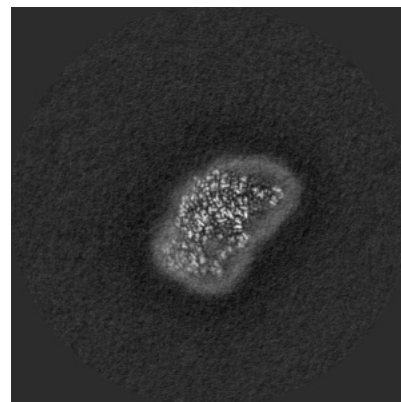
6.2.2 Raw map



X Index: 200



Y Index: 200

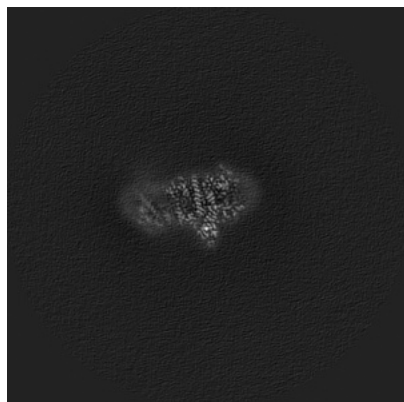


Z Index: 200

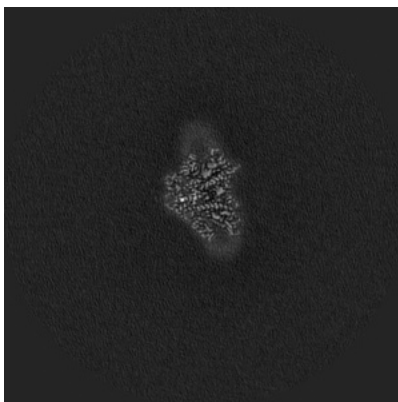
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

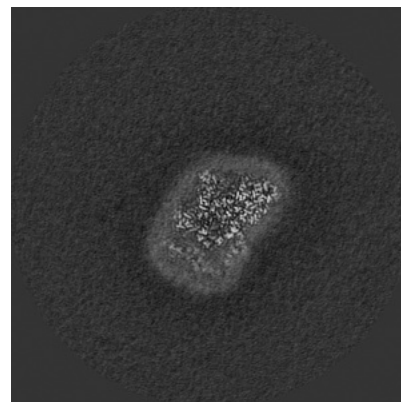
6.3.1 Primary map



X Index: 206

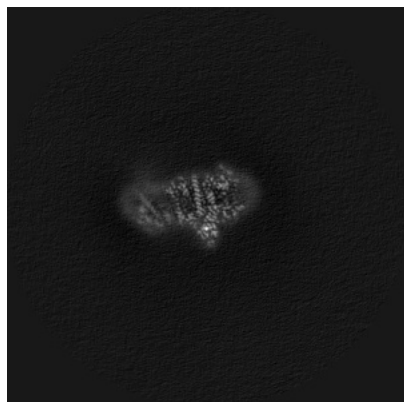


Y Index: 199

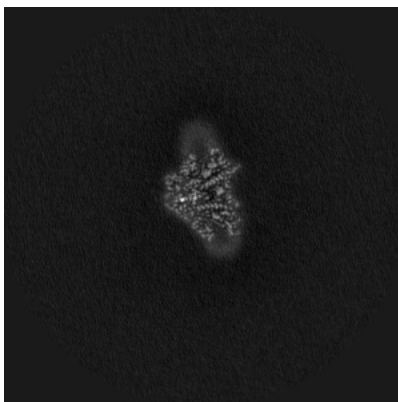


Z Index: 210

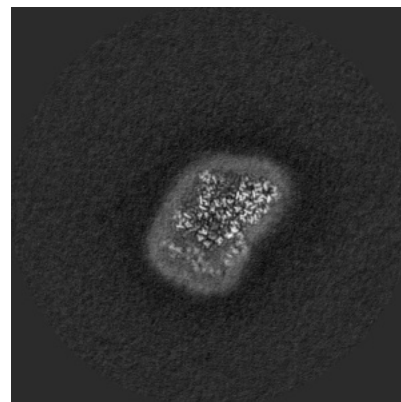
6.3.2 Raw map



X Index: 206



Y Index: 199

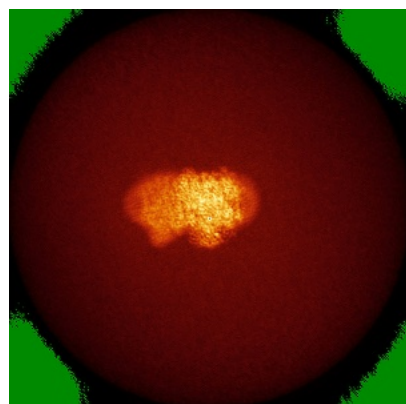


Z Index: 210

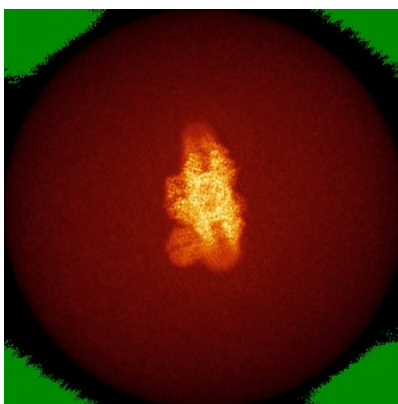
The images above show the largest variance slices of the map in three orthogonal directions.

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

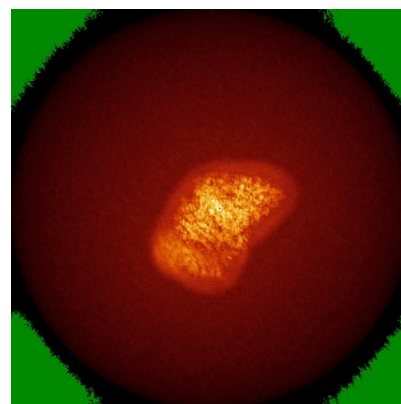
6.4.1 Primary map



X

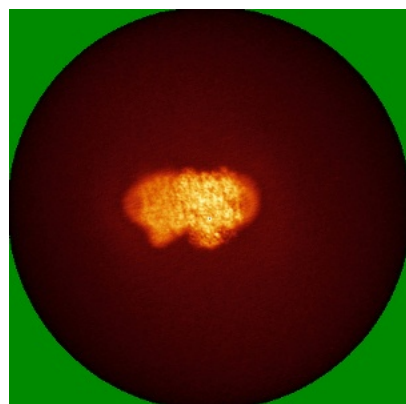


Y

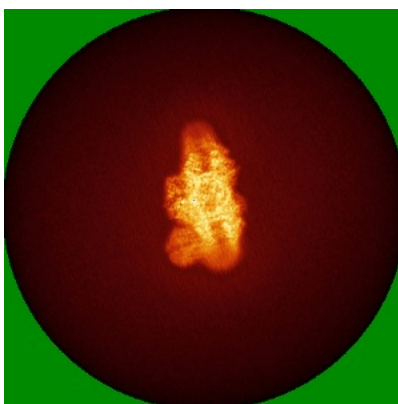


Z

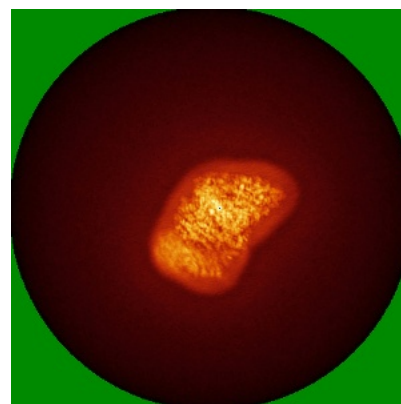
6.4.2 Raw map



X



Y

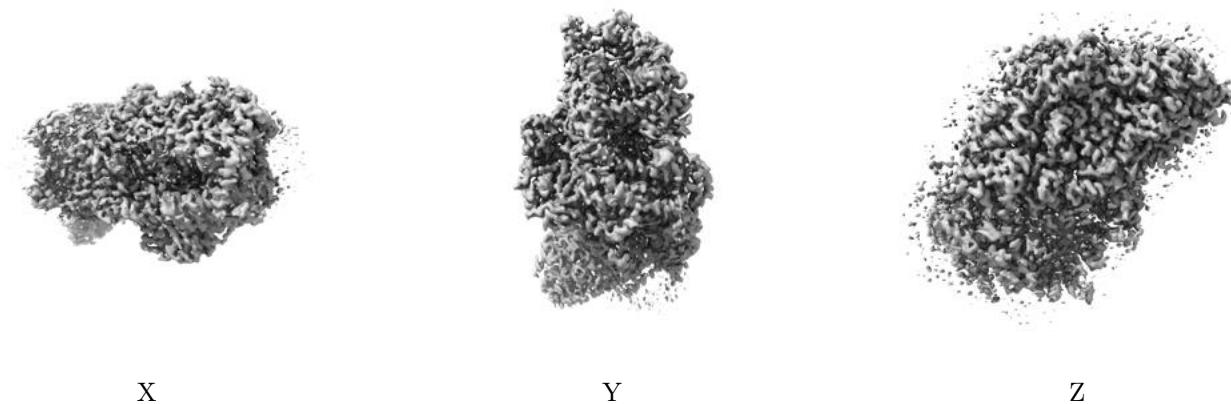


Z

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 0.0801. 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.

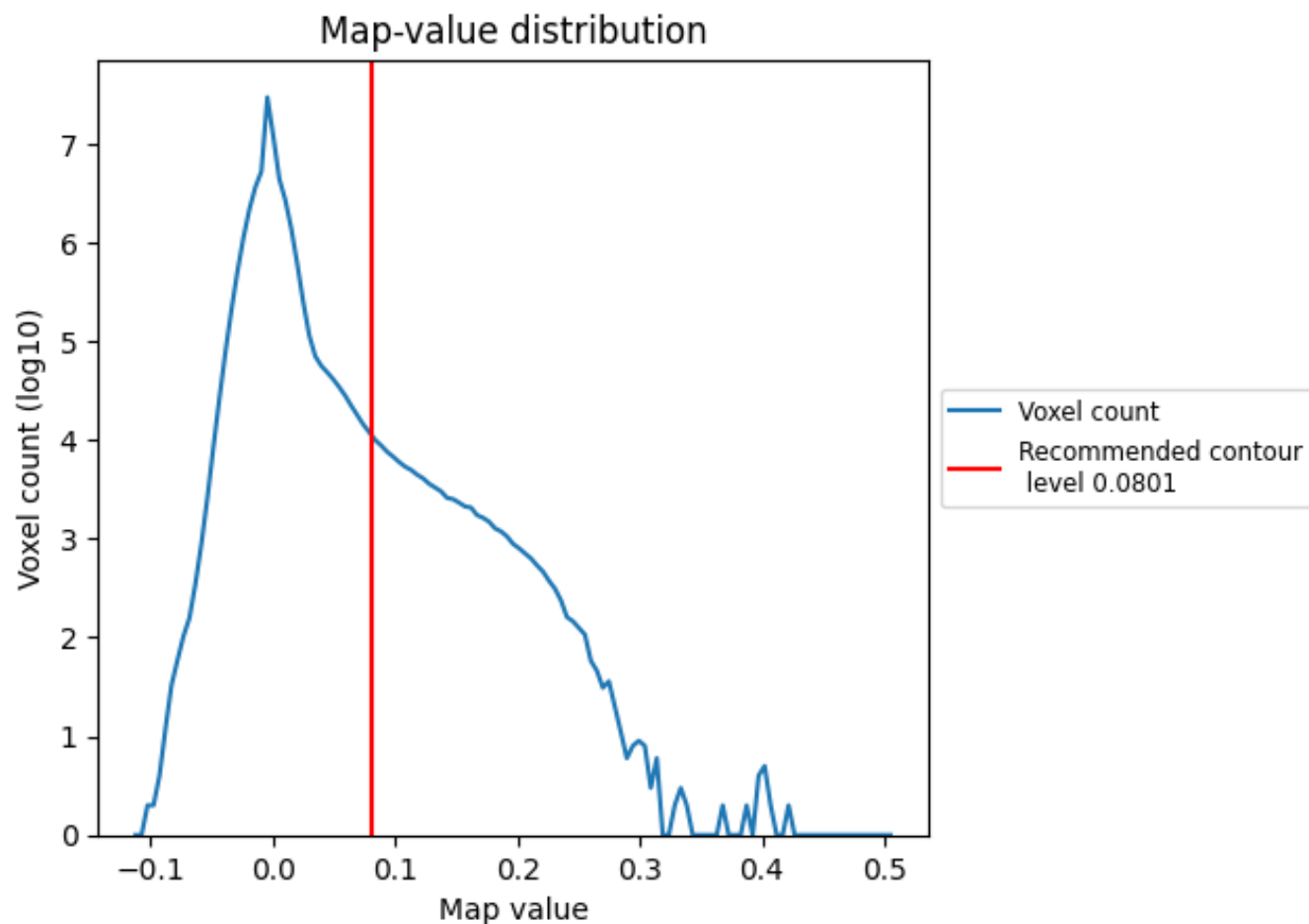
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

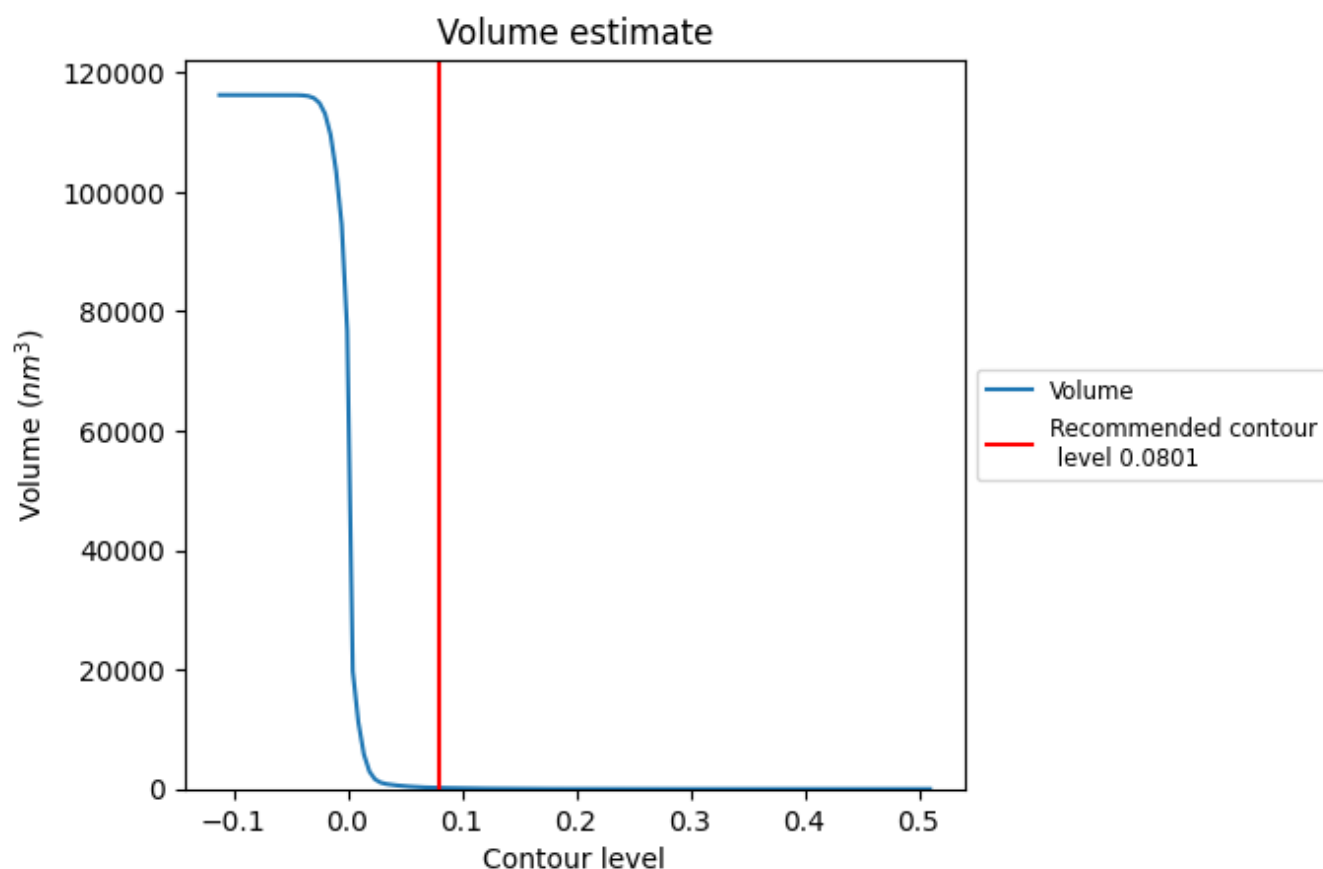
This section contains the results of statistical analysis of the map.

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.

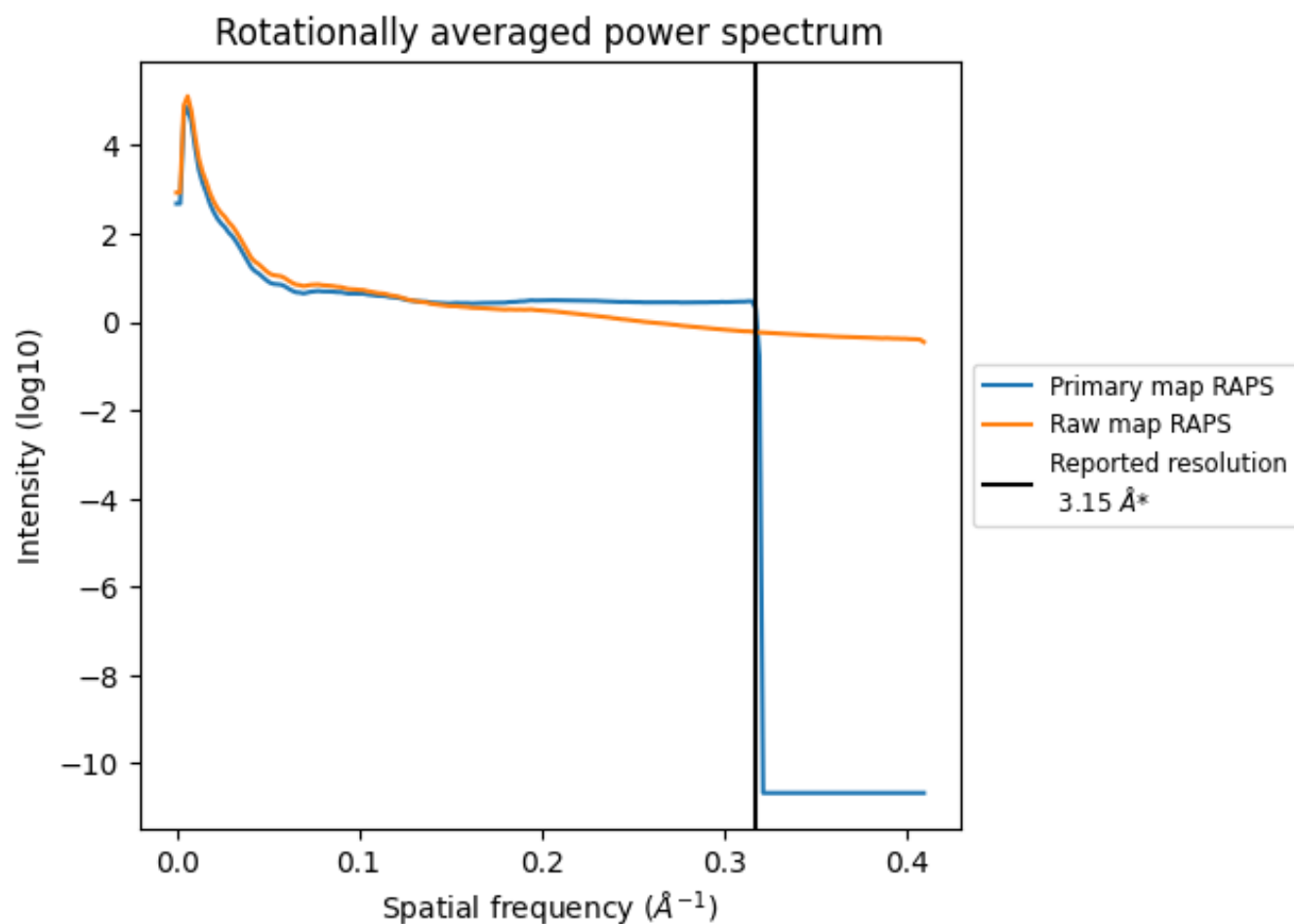
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 187 nm^3 ; this corresponds to an approximate mass of 169 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 ⓘ

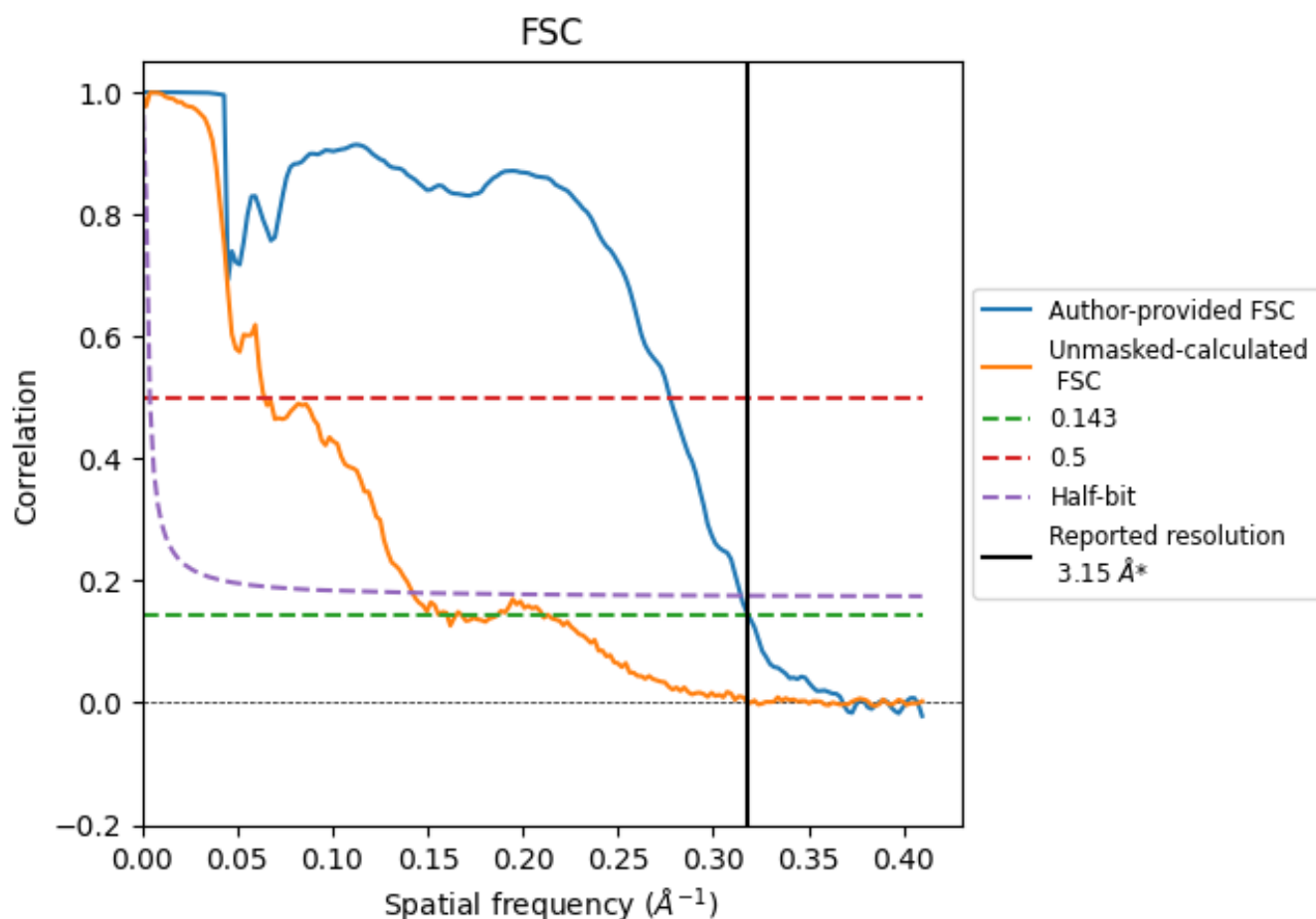


*Reported resolution corresponds to spatial frequency of 0.317 $\text{\AA}^{-1}$

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 0.317 Å⁻¹

8.2 Resolution estimates [i](#)

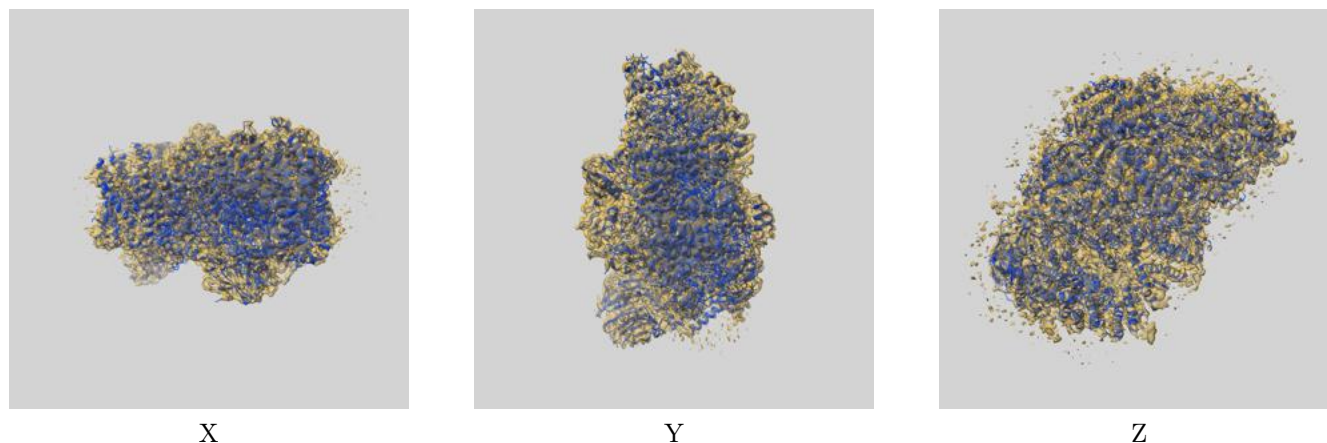
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	3.14	3.60	3.18
Unmasked-calculated*	6.24	15.58	7.04

*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 6.24 differs from the reported value 3.15 by more than 10 %

9 Map-model fit [i](#)

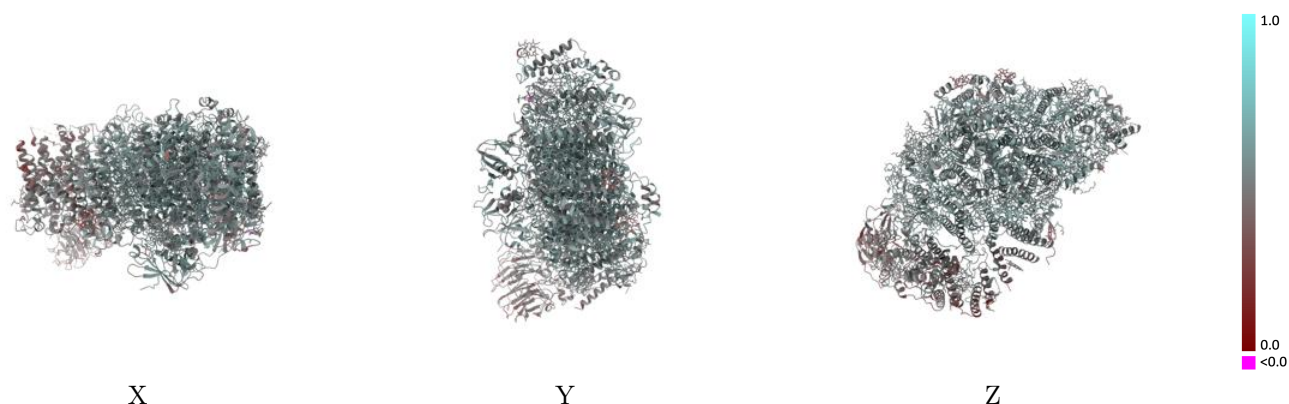
This section contains information regarding the fit between EMDB map EMD-15618 and PDB model 8ASL. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



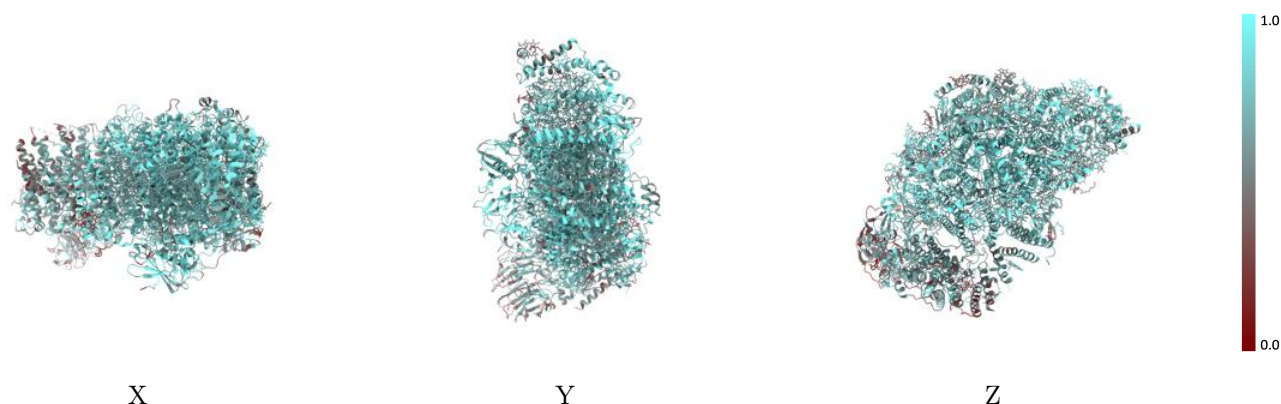
The images above show the 3D surface view of the map at the recommended contour level 0.0801 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



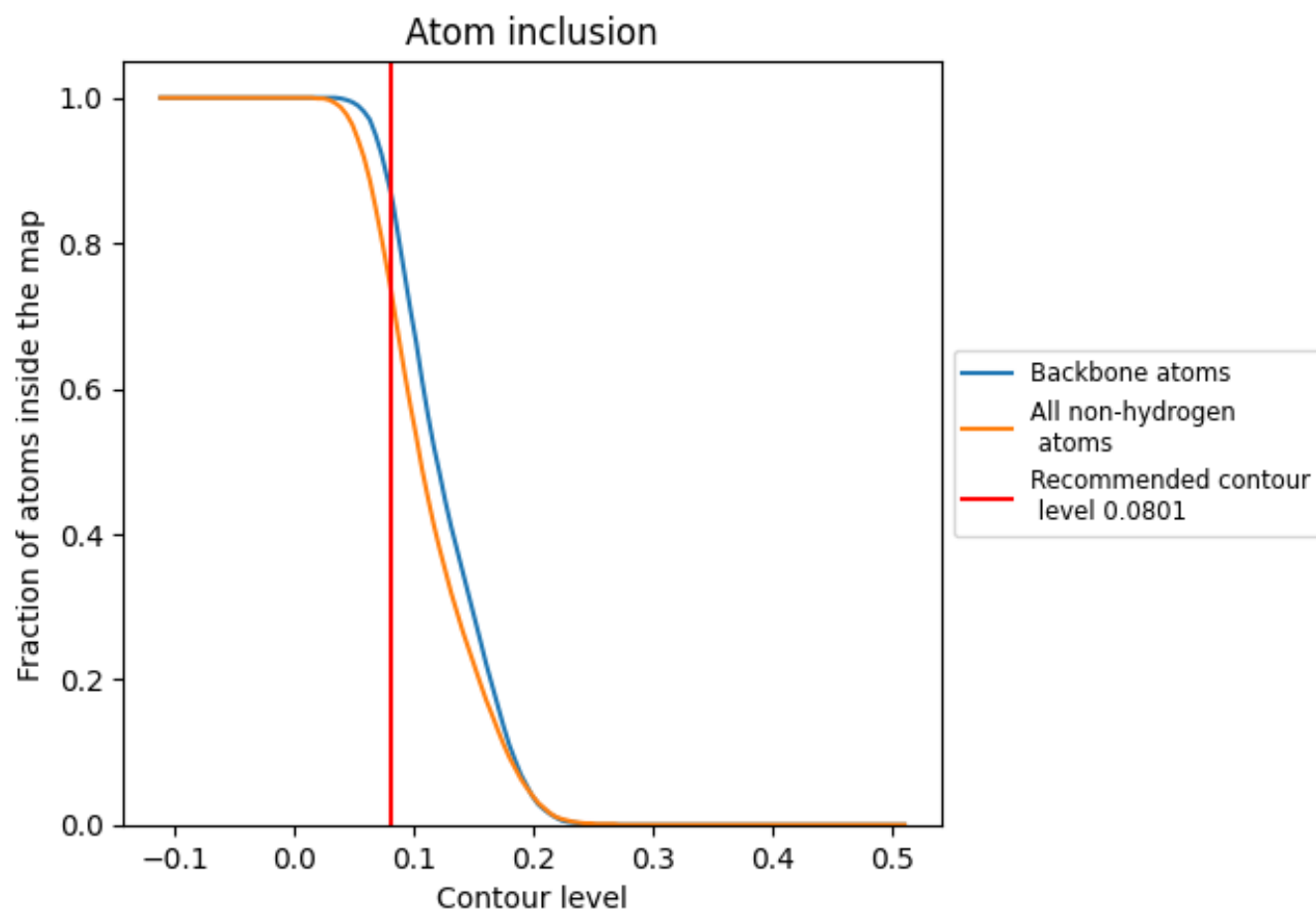
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0801).

9.4 Atom inclusion ⓘ



At the recommended contour level, 87% of all backbone atoms, 74% 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 (0.0801) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7400	0.5180
A	0.6210	0.4580
D	0.5850	0.4470
E	0.6500	0.4520
F	0.6210	0.4440
I	0.4290	0.3910
S	0.5100	0.3970
a	0.8130	0.5560
b	0.8260	0.5550
c	0.9200	0.5460
d	0.8060	0.5380
e	0.7670	0.5320
f	0.6810	0.5230
i	0.7550	0.5400
j	0.6140	0.4920
k	0.6310	0.5060
l	0.7110	0.4970
m	0.7360	0.5420

