



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 10:32 pm BST

PDB ID : 3PCQ

Title : Femtosecond X-ray protein Nanocrystallography

Authors : Chapman, H.N.; Fromme, P.; Barty, A.; White, T.A.; Kirian, R.A.; Aquila, A.; Hunter, M.S.; Schulz, J.; Deponte, D.P.; Weierstall, U.; Doak, R.B.; Maia, F.R.N.C.; Martin, A.V.; Schlichting, I.; Lomb, L.; Coppola, N.; Shoeman, R.L.; Epp, S.W.; Hartmann, R.; Rolles, D.; Rudenko, A.; Foucar, L.; Kimmel, N.; Weidenspointner, G.; Holl, P.; Liang, M.; Barthelmess, M.; Caleman, C.; Boutet, S.; Bogan, M.J.; Krzywinski, J.; Bostedt, C.; Bajt, S.; Gumprecht, L.; Rudek, B.; Erk, B.; Schmidt, C.; Homke, A.; Reich, C.; Pietschner, D.; Struder, L.; Hauser, G.; Gorke, H.; Ullrich, J.; Herrmann, S.; Schaller, G.; Schopper, F.; Soltau, H.; Kuhn, K.-U.; Messerschmidt, M.; Bozek, J.D.; Hau-Riege, S.P.; Frank, M.; Hampton, C.Y.; Sierra, R.; Starodub, D.; Williams, G.J.; Hajdu, J.; Timneanu, N.; Seibert, M.M.; Andreasson, J.; Rocker, A.; Jonsson, O.; Svenda, M.; Stern, S.; Nass, K.; Andritschke, R.; Schroter, C.-D.; Krasniqi, F.; Bott, M.; Schmidt, K.E.; Wang, X.; Grotjohann, I.; Holton, J.M.; Barends, T.R.M.; Neutze, R.; Marchesini, S.; Fromme, R.; Schorb, S.; Rupp, D.; Adolph, M.; Gorkhover, T.; Andersson, I.; Hirsemann, H.; Potdevin, G.; Graafsma, H.; Nilsson, B.; Spence, J.C.H.

Deposited on : 2010-10-21

Resolution : 8.98 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

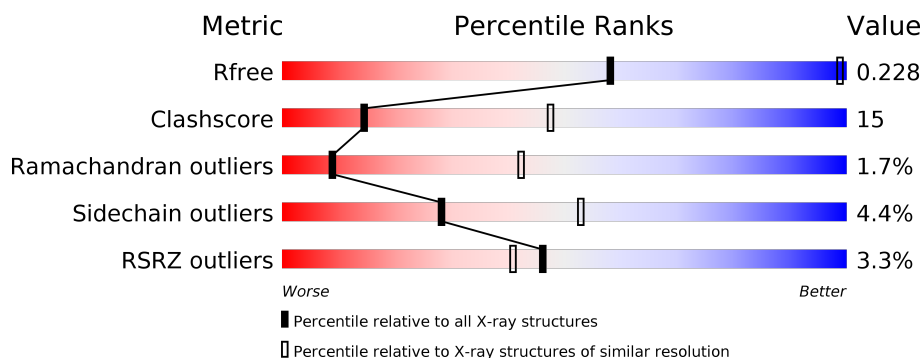
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.98 Å.



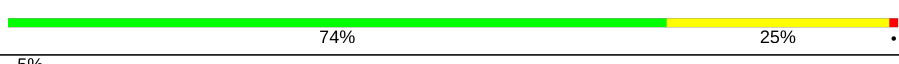



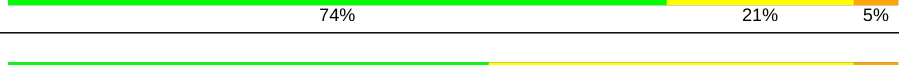
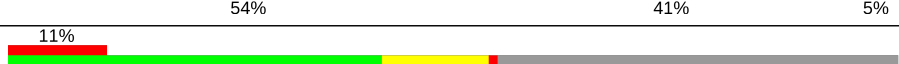
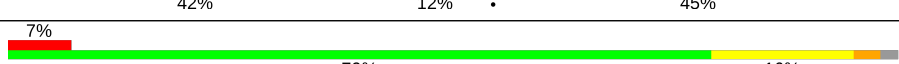
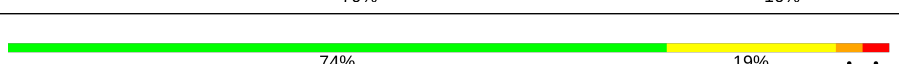


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

Mol	Chain	Length	Quality of chain
1	A	755	
2	B	740	
3	C	80	
4	D	138	
5	E	75	
6	F	164	
7	I	38	
8	J	41	
9	K	83	
10	L	154	
11	M	31	
12	X	35	

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
13	CLA	A	801	X	-	-	-
13	CLA	A	802	X	-	-	-
13	CLA	A	803	X	-	-	-
13	CLA	A	804	X	-	-	-
13	CLA	A	805	X	-	-	-
13	CLA	A	806	X	-	-	-
13	CLA	A	807	X	-	-	-
13	CLA	A	808	X	-	-	-
13	CLA	A	809	X	-	-	-
13	CLA	A	810	X	-	-	-
13	CLA	A	812	X	-	-	-
13	CLA	A	813	X	-	-	-
13	CLA	A	814	X	-	-	-
13	CLA	A	815	X	-	-	-
13	CLA	A	816	X	-	-	X
13	CLA	A	817	X	-	-	-
13	CLA	A	818	X	-	-	-
13	CLA	A	819	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	820	X	-	-	-
13	CLA	A	821	X	-	-	-
13	CLA	A	822	X	-	-	X
13	CLA	A	823	X	-	-	X
13	CLA	A	824	X	-	-	X
13	CLA	A	825	X	-	-	-
13	CLA	A	826	X	-	-	-
13	CLA	A	827	X	-	-	X
13	CLA	A	828	X	-	-	-
13	CLA	A	829	X	-	-	-
13	CLA	A	830	X	-	-	-
13	CLA	A	831	X	-	-	-
13	CLA	A	832	X	-	-	-
13	CLA	A	833	X	-	-	-
13	CLA	A	835	X	-	-	-
13	CLA	A	836	X	-	-	-
13	CLA	A	837	X	-	-	-
13	CLA	A	838	X	-	-	-
13	CLA	A	839	X	-	-	-
13	CLA	A	840	X	-	-	-
13	CLA	A	841	X	-	-	-
13	CLA	A	842	X	-	-	-
13	CLA	A	843	X	-	-	-
13	CLA	A	844	X	-	-	X
13	CLA	A	845	X	-	-	X
13	CLA	A	846	X	-	-	-
13	CLA	B	801	X	-	-	-
13	CLA	B	802	X	-	-	-
13	CLA	B	803	X	-	-	-
13	CLA	B	804	X	-	-	-
13	CLA	B	805	X	-	-	-
13	CLA	B	806	X	-	-	-
13	CLA	B	807	X	-	-	-
13	CLA	B	808	X	-	-	-
13	CLA	B	809	X	-	-	-
13	CLA	B	810	X	-	-	-
13	CLA	B	811	X	-	-	-
13	CLA	B	812	X	-	-	X
13	CLA	B	813	X	-	-	-
13	CLA	B	814	X	-	-	-
13	CLA	B	815	X	-	-	X
13	CLA	B	816	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	817	X	-	-	-
13	CLA	B	818	X	-	-	-
13	CLA	B	819	X	-	-	-
13	CLA	B	820	X	-	-	X
13	CLA	B	821	X	-	-	X
13	CLA	B	822	X	-	-	-
13	CLA	B	823	X	-	-	-
13	CLA	B	824	X	-	-	-
13	CLA	B	825	X	-	-	-
13	CLA	B	826	X	-	-	-
13	CLA	B	827	X	-	-	-
13	CLA	B	828	X	-	-	-
13	CLA	B	829	X	-	-	-
13	CLA	B	830	X	-	-	-
13	CLA	B	831	X	-	-	-
13	CLA	B	832	X	-	-	-
13	CLA	B	833	X	-	-	X
13	CLA	B	834	X	-	-	-
13	CLA	B	835	X	-	-	-
13	CLA	B	836	X	-	-	-
13	CLA	B	837	X	-	-	-
13	CLA	B	838	X	-	-	-
13	CLA	B	840	X	-	-	X
13	CLA	B	841	X	-	-	-
13	CLA	F	1301	X	-	-	-
13	CLA	J	101	X	-	-	X
13	CLA	J	102	X	-	-	X
13	CLA	K	1401	X	-	-	X
13	CLA	L	1002	X	-	-	-
13	CLA	L	1003	X	-	-	-
13	CLA	L	1004	X	-	-	-
13	CLA	M	1601	X	-	-	X
13	CLA	X	1701	X	-	-	-
16	BCR	A	850	-	-	-	X
16	BCR	A	851	-	-	-	X
16	BCR	A	852	-	-	-	X
16	BCR	A	853	-	-	-	X
16	BCR	B	843	-	-	-	X
16	BCR	B	844	-	-	-	X
16	BCR	B	845	-	-	-	X
16	BCR	J	105	-	-	-	X
17	LHG	A	855	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	LHG	A	856	X	-	-	-
18	LMG	B	850	-	-	-	X

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 24196 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	A	740	Total	C	N	O	S	0	0	0
			5784	3794	988	976	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	739	Total	C	N	O	S	0	0	0
			5879	3867	986	1005	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			598	367	103	117	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	138	Total	C	N	O	S	0	0	0
			1075	682	186	204	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	69	Total	C	N	O	0	0	0
			539	342	93	104			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	141	Total	C	N	O	S	0	0	0
			1065	680	184	197	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	38	Total	C	N	O	S	0	0	0
			301	208	40	48	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	41	Total	C	N	O	S	0	0	0
			338	231	51	54	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	46	Total	C	N	O		0	0	0
			222	130	46	46				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	151	Total	C	N	O	S	0	0	0
			1119	735	179	201	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	143	LEU	SER	CONFLICT	UNP Q8DGB4

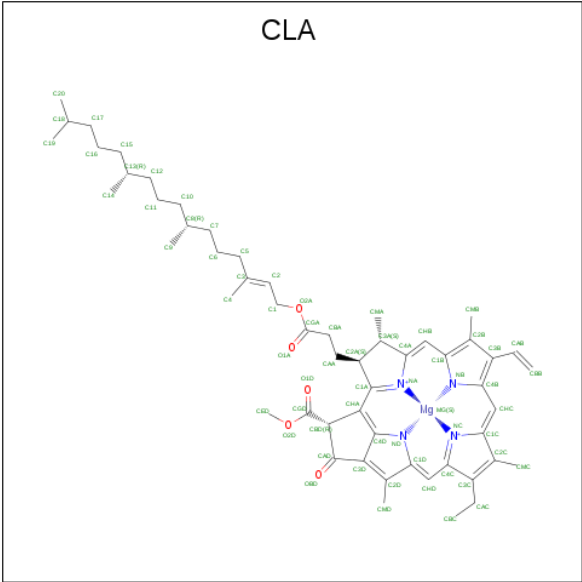
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	M	31	Total	C	N	O	S	0	0	0
			241	161	36	43	1			

- Molecule 12 is a protein called Photosystem I 4.8K protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	X	29	Total	C	N	O		0	0	0
			232	163	34	35				

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	A	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
13	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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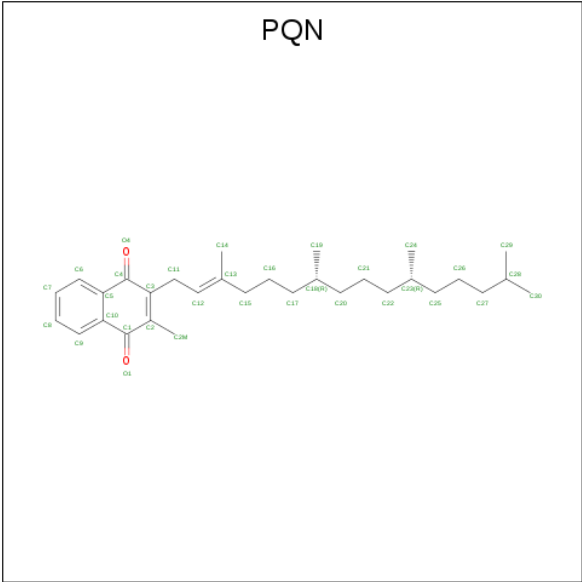
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

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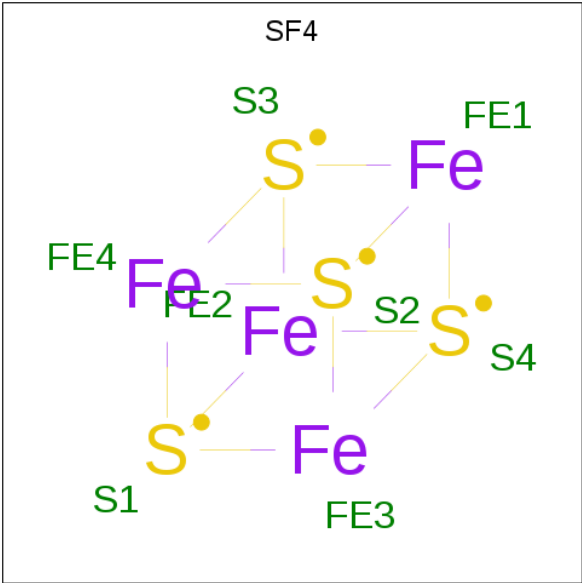
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	J	1	Total	C	Mg	N	O	0	0
			37	31	1	4	1		
13	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	M	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	X	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		

- Molecule 14 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 15 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

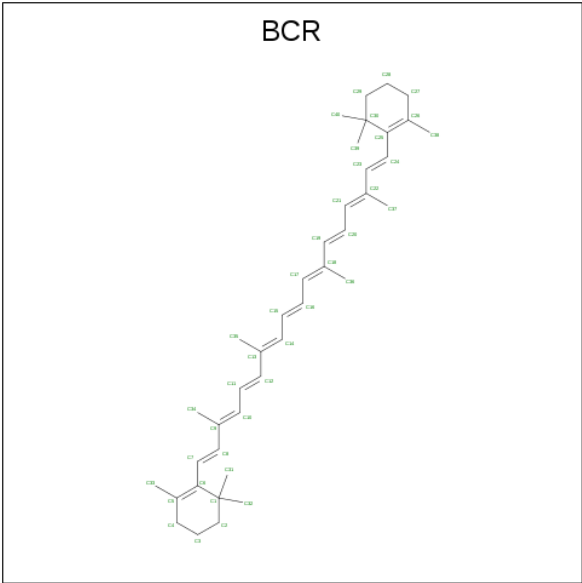


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	Fe	S	0	0
			8	4	4		
15	C	1	Total	Fe	S	0	0
			8	4	4		

Continued from previous page...

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

- Molecule 16 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



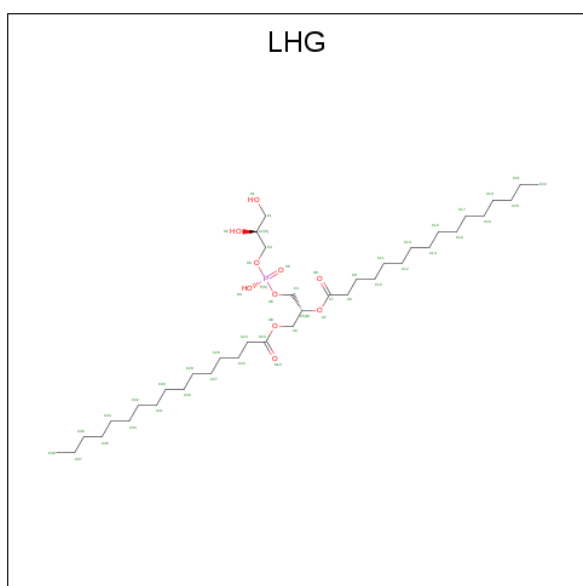
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	C	0	0
			40	40		
16	A	1	Total	C	0	0
			40	40		
16	A	1	Total	C	0	0
			40	40		
16	A	1	Total	C	0	0
			40	40		
16	A	1	Total	C	0	0
			40	40		
16	A	1	Total	C	0	0
			40	40		
16	B	1	Total	C	0	0
			40	40		
16	B	1	Total	C	0	0
			40	40		
16	B	1	Total	C	0	0
			40	40		
16	B	1	Total	C	0	0
			25	25		

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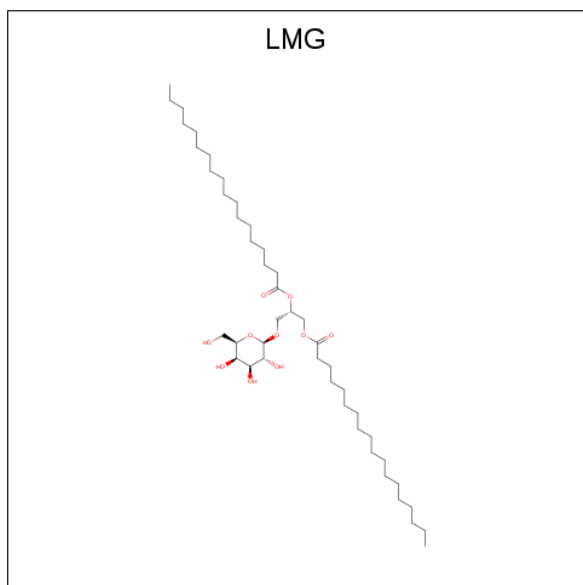
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	F	1	Total C 40 40	0	0
16	I	1	Total C 40 40	0	0
16	I	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	L	1	Total C 40 40	0	0
16	L	1	Total C 40 40	0	0
16	M	1	Total C 40 40	0	0

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	O	P	0	0
			49	38	10	1		
17	A	1	Total	C	O	P	0	0
			27	16	10	1		
17	B	1	Total	C	O	P	0	0
			23	12	10	1		

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	B	1	Total	C	O	0	0
			55	45	10		

- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	L	1	Total	Ca	0	0
			1	1		

- Molecule 20 is water.

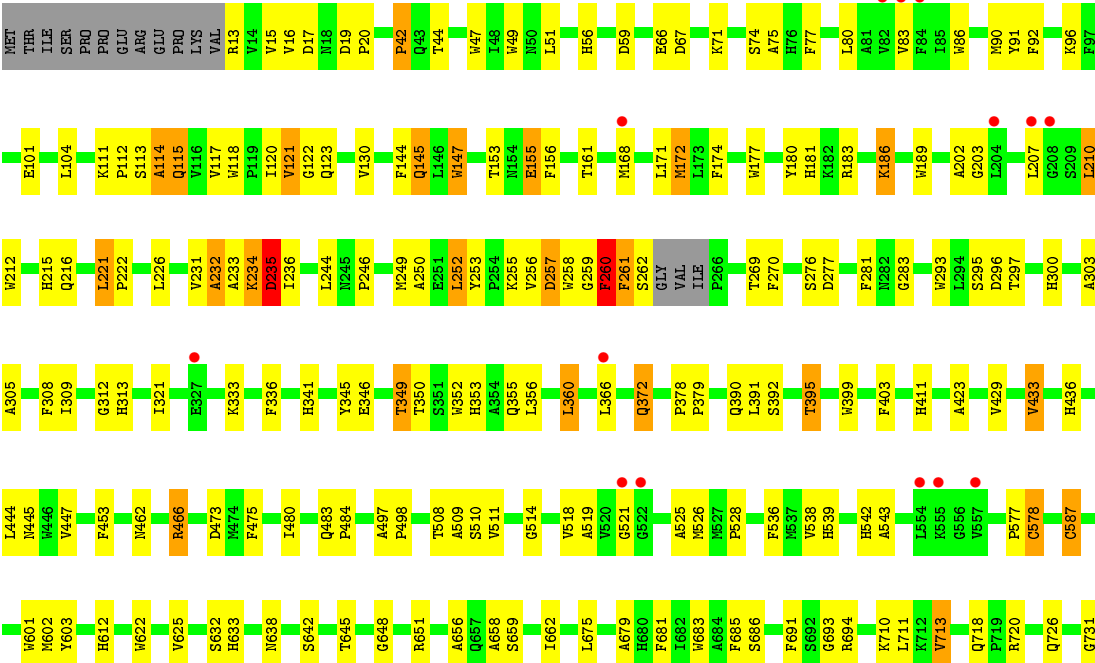
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	53	Total	O	0	0
			53	53		
20	B	65	Total	O	0	0
			65	65		

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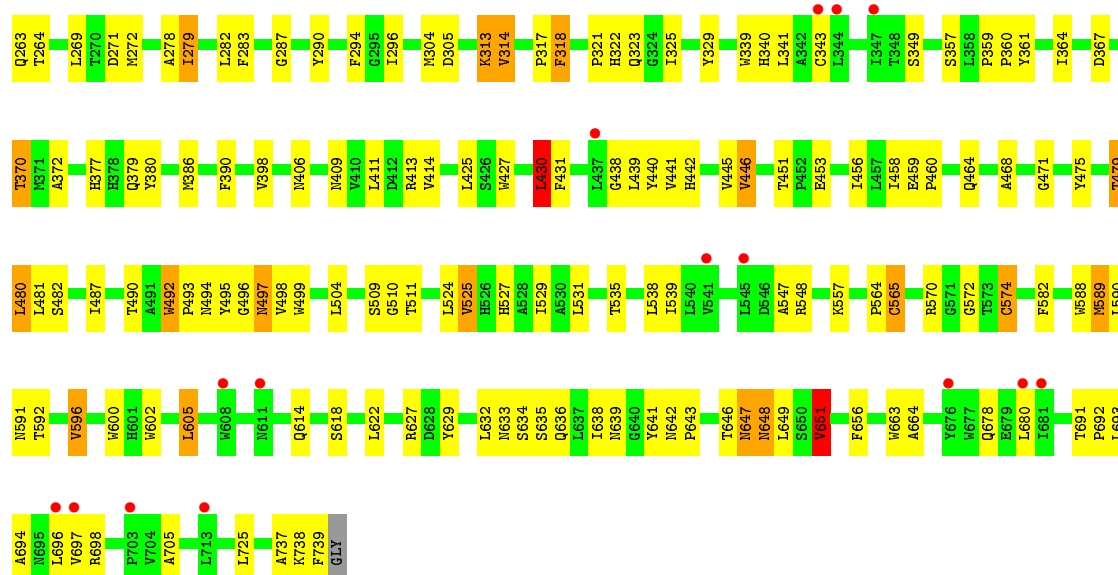
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	C	21	Total 21	O 21	0	0
20	D	17	Total 17	O 17	0	0
20	E	5	Total 5	O 5	0	0
20	F	6	Total 6	O 6	0	0
20	I	3	Total 3	O 3	0	0
20	J	1	Total 1	O 1	0	0
20	L	27	Total 27	O 27	0	0
20	M	2	Total 2	O 2	0	0

These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

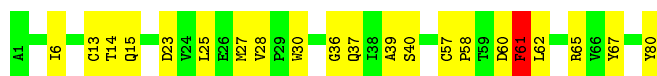
- Chain A: 
- 
- | Position | Amino Acid |
|----------|------------|
| 1 | W34 |
| 2 | H61 |
| 3 | L44 |
| 4 | A305 |
| 5 | W12 |
| 6 | E101 |
| 7 | L104 |
| 8 | K111 |
| 9 | P112 |
| 10 | S113 |
| 11 | A114 |
| 12 | Q115 |
| 13 | V116 |
| 14 | V117 |
| 15 | W118 |
| 16 | P119 |
| 17 | I120 |
| 18 | D125 |
| 19 | V121 |
| 20 | G122 |
| 21 | Q123 |
| 22 | V130 |
| 23 | M249 |
| 24 | F144 |
| 25 | Q145 |
| 26 | L146 |
| 27 | W147 |
| 28 | I148 |
| 29 | W149 |
| 30 | N154 |
| 31 | E155 |
| 32 | F156 |
| 33 | L162 |
| 34 | L675 |
| 35 | A679 |
| 36 | H680 |
| 37 | F681 |
| 38 | I682 |
| 39 | A684 |
| 40 | F685 |
| 41 | S686 |
| 42 | F691 |
| 43 | S692 |
| 44 | G693 |
| 45 | R694 |
| 46 | K710 |
| 47 | L711 |
| 48 | K712 |
| 49 | V713 |
| 50 | Q718 |
| 51 | P719 |
| 52 | R720 |
| 53 | Q726 |
| 54 | G731 |
| 55 | H734 |
| 56 | L737 |
| 57 | G738 |
| 58 | A741 |
| 59 | W744 |
| 60 | G755 |
| 61 | L444 |
| 62 | N445 |
| 63 | W446 |
| 64 | V447 |
| 65 | F308 |
| 66 | I309 |
| 67 | H215 |
| 68 | Q216 |
| 69 | G312 |
| 70 | H313 |
| 71 | I321 |
| 72 | F453 |
| 73 | N462 |
| 74 | R466 |
| 75 | D473 |
| 76 | W474 |
| 77 | F475 |
| 78 | N638 |
| 79 | S642 |
| 80 | T645 |
| 81 | G648 |
| 82 | R651 |
| 83 | T508 |
| 84 | A509 |
| 85 | Q557 |
| 86 | S510 |
| 87 | H353 |
| 88 | V511 |
| 89 | G514 |
| 90 | V518 |
| 91 | A519 |
| 92 | V520 |
| 93 | G521 |
| 94 | G522 |
| 95 | A525 |
| 96 | N526 |
| 97 | N527 |
| 98 | P528 |
| 99 | F536 |
| 100 | N537 |
| 101 | V538 |
| 102 | H539 |
| 103 | H542 |
| 104 | A543 |
| 105 | L554 |
| 106 | K555 |
| 107 | G556 |
| 108 | V557 |
| 109 | P577 |
| 110 | C578 |
| 111 | C587 |
| 112 | H590 |
| 113 | F403 |
| 114 | H411 |
| 115 | A423 |
| 116 | V429 |
| 117 | V433 |
| 118 | H436 |
| 119 | H442 |
| 120 | F281 |
| 121 | G282 |
| 122 | G283 |
| 123 | W293 |
| 124 | L294 |
| 125 | S295 |
| 126 | D296 |
| 127 | T297 |
| 128 | H300 |
| 129 | G208 |
| 130 | S209 |
| 131 | L210 |
| 132 | F514 |
| 133 | K186 |
| 134 | W189 |
| 135 | A202 |
| 136 | G203 |
| 137 | L204 |
| 138 | L207 |
| 139 | F92 |
| 140 | K96 |
| 141 | F97 |
| 142 | S98 |
| 143 | L80 |
| 144 | A81 |
| 145 | V82 |
| 146 | V83 |
| 147 | F84 |
| 148 | I85 |
| 149 | N86 |
| 150 | N90 |
| 151 | Y91 |
| 152 | F92 |
| 153 | K96 |
| 154 | F97 |
| 155 | S98 |
| 156 | L80 |
| 157 | A81 |
| 158 | V82 |
| 159 | V83 |
| 160 | F84 |
| 161 | I85 |
| 162 | N86 |
| 163 | N90 |
| 164 | Y91 |
| 165 | F92 |
| 166 | K96 |
| 167 | F97 |
| 168 | S98 |
| 169 | L80 |
| 170 | A81 |
| 171 | V82 |
| 172 | V83 |
| 173 | F84 |
| 174 | I85 |
| 175 | N86 |
| 176 | N90 |
| 177 | Y91 |
| 178 | F92 |
| 179 | K96 |
| 180 | F97 |
| 181 | S98 |
| 182 | L80 |
| 183 | A81 |
| 184 | V82 |
| 185 | V83 |
| 186 | F84 |
| 187 | I85 |
| 188 | N86 |
| 189 | N90 |
| 190 | Y91 |
| 191 | F92 |
| 192 | K96 |

- Chain B:
-



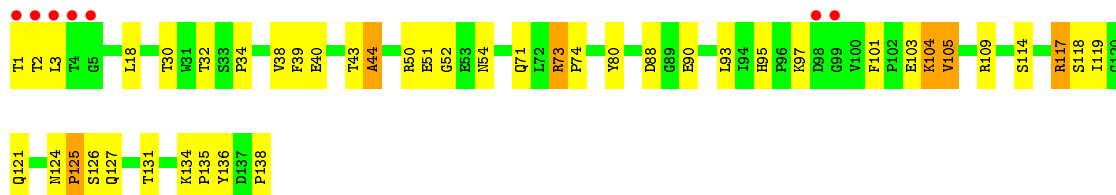
• Molecule 3: Photosystem I iron-sulfur center

Chain C: 74% 25%



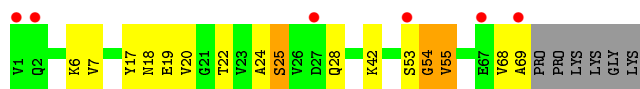
• Molecule 4: Photosystem I reaction center subunit II

Chain D: 5% 68% 28%



• Molecule 5: Photosystem I reaction center subunit IV

Chain E: 8% 71% 17% 8%



• Molecule 6: Photosystem I reaction center subunit III

Chain F: 57% 28% 14%





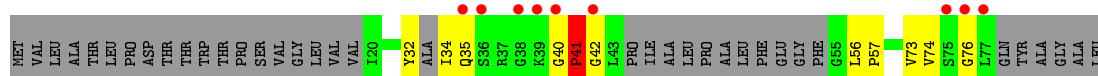
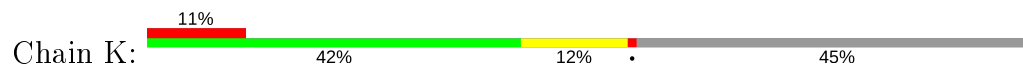
- Molecule 7: Photosystem I reaction center subunit VIII



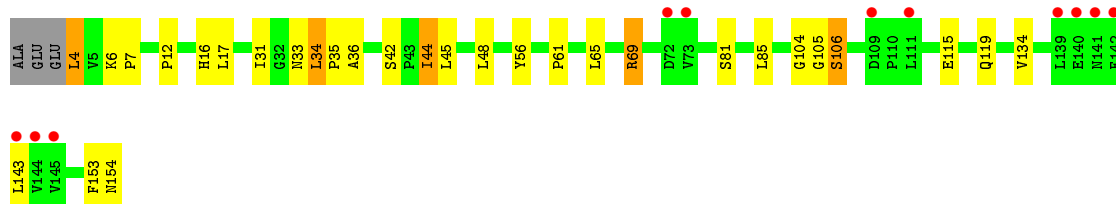
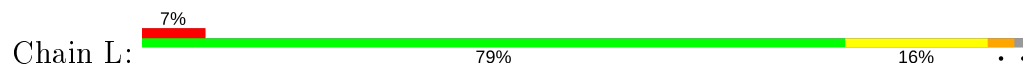
- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 9: Photosystem I reaction center subunit PsaK



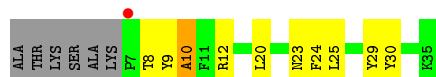
- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 12: Photosystem I 4.8K protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	281.00Å 281.00Å 165.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	81.12 – 8.98 81.12 – 9.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (81.12-8.98) 99.1 (81.12-9.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.89 (at 8.41Å)	Xtriage
Refinement program	REFMAC 5.6.0076	Depositor
R, R_{free}	0.252 , 0.232 0.246 , 0.228	Depositor DCC
R_{free} test set	187 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	203.6	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.16$, $\langle L^2 \rangle = 0.04$	Xtriage
Estimated twinning fraction	0.499 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.500 for H, K, L 0.500 for K, H, -L	Depositor
Outliers	0 of 5591 reflections	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	24196	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, SF4, CLA, PQN, CA, BCR, LMG

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	0.51	0/5983	0.66	2/8158 (0.0%)
2	B	0.56	0/6096	0.67	2/8332 (0.0%)
3	C	0.74	0/608	0.96	4/824 (0.5%)
4	D	0.57	0/1101	0.81	1/1492 (0.1%)
5	E	0.57	0/551	0.84	2/750 (0.3%)
6	F	0.47	0/1087	0.66	0/1476
7	I	0.67	0/312	0.75	0/425
8	J	0.45	0/350	0.65	0/477
9	K	0.52	0/219	0.86	3/297 (1.0%)
10	L	0.67	0/1148	0.75	0/1558
11	M	0.63	0/244	0.85	1/332 (0.3%)
12	X	0.54	0/241	0.67	0/330
All	All	0.55	0/17940	0.70	15/24451 (0.1%)

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

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

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	80	TYR	CA-C-O	9.93	140.96	120.10
11	M	30	TYR	N-CA-C	7.84	132.17	111.00
4	D	131	THR	N-CA-C	-7.83	89.86	111.00
5	E	54	GLY	N-CA-C	7.51	131.88	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	521	GLY	N-CA-C	-6.42	97.05	113.10
3	C	60	ASP	CA-C-N	-6.26	103.42	117.20
9	K	57	PRO	N-CA-CB	6.15	110.69	103.30
3	C	60	ASP	C-N-CA	5.90	136.45	121.70
3	C	61	PHE	N-CA-CB	5.87	121.16	110.60
1	A	114	ALA	N-CA-C	-5.85	95.21	111.00
9	K	41	PRO	N-CA-CB	5.73	110.17	103.30
9	K	35	GLN	N-CA-C	5.36	125.47	111.00
2	B	430	LEU	CA-CB-CG	5.11	127.05	115.30
2	B	651	VAL	CB-CA-C	-5.09	101.73	111.40
5	E	55	VAL	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	61	PHE	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5784	0	5639	214	0
2	B	5879	0	5632	238	0
3	C	598	0	580	16	0
4	D	1075	0	1077	39	0
5	E	539	0	528	10	1
6	F	1065	0	1079	41	1
7	I	301	0	306	7	0
8	J	338	0	347	23	0
9	K	222	0	110	4	0
10	L	1119	0	1125	22	2
11	M	241	0	264	13	0
12	X	232	0	220	6	0
13	A	2687	0	2675	139	0
13	B	2349	0	2304	151	0
13	F	45	0	33	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	J	82	0	58	1	0
13	K	45	0	33	1	0
13	L	195	0	216	11	0
13	M	45	0	33	1	0
13	X	45	0	33	1	0
14	A	33	0	46	1	0
14	B	33	0	46	1	0
15	A	8	0	0	0	0
15	C	16	0	0	0	0
16	A	240	0	336	22	0
16	B	265	0	369	17	0
16	F	40	0	56	2	0
16	I	80	0	112	3	0
16	J	120	0	168	16	0
16	L	80	0	112	1	0
16	M	40	0	56	2	0
17	A	76	0	98	6	0
17	B	23	0	16	1	0
18	B	55	0	86	5	0
19	L	1	0	0	0	1
20	A	53	0	0	5	1
20	B	65	0	0	3	0
20	C	21	0	0	3	0
20	D	17	0	0	1	0
20	E	5	0	0	0	0
20	F	6	0	0	1	0
20	I	3	0	0	0	0
20	J	1	0	0	0	0
20	L	27	0	0	1	2
20	M	2	0	0	1	0
All	All	24196	0	23793	736	5

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 15.

All (736) 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)
8:J:31:ARG:HD3	16:J:104:BCR:H312	1.26	1.17
2:B:622:LEU:HD12	13:B:802:CLA:H11	1.28	1.15
1:A:508:THR:HG22	1:A:510:SER:H	1.18	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:LYS:H	2:B:159:LYS:HD2	1.18	1.04
4:D:50:ARG:H	4:D:54:ASN:HD21	1.06	1.01
2:B:243:PHE:H	2:B:263:GLN:HE22	1.07	1.01
2:B:231:VAL:O	2:B:234:GLN:HG2	1.62	0.99
1:A:536:PHE:HA	13:A:839:CLA:HED1	1.45	0.96
2:B:406:ASN:HD22	2:B:409:ASN:HD21	0.98	0.96
2:B:494:ASN:HD22	2:B:496:GLY:H	1.13	0.93
11:M:31:LYS:O	11:M:31:LYS:HG2	1.70	0.92
1:A:353:HIS:HD2	1:A:411:HIS:HD1	1.21	0.88
4:D:117:ARG:HG3	4:D:121:GLN:HB2	1.54	0.88
16:A:854:BCR:H362	13:B:802:CLA:H42	1.55	0.87
1:A:117:VAL:HG13	1:A:123:GLN:HE21	1.42	0.84
4:D:101:PHE:HB2	4:D:104:LYS:HE2	1.59	0.83
2:B:406:ASN:ND2	2:B:409:ASN:HD21	1.76	0.83
8:J:24:GLY:HA3	13:J:101:CLA:HBB1	1.61	0.83
8:J:31:ARG:HD3	16:J:104:BCR:C31	2.08	0.83
1:A:333:LYS:O	13:A:846:CLA:HBC3	1.81	0.81
2:B:509:SER:O	2:B:511:THR:N	2.12	0.81
1:A:203:GLY:HA2	13:A:821:CLA:HBC1	1.62	0.80
1:A:391:LEU:O	1:A:395:THR:HG23	1.81	0.80
2:B:642:ASN:HB2	2:B:643:PRO:CD	2.12	0.80
6:F:88:VAL:HG11	6:F:97:LYS:HB2	1.64	0.79
6:F:88:VAL:HG12	6:F:94:ALA:HA	1.63	0.79
2:B:494:ASN:ND2	2:B:496:GLY:H	1.80	0.78
2:B:459:GLU:HG3	6:F:5:LEU:HD11	1.63	0.78
1:A:345:TYR:O	1:A:349:THR:HB	1.84	0.78
2:B:243:PHE:H	2:B:263:GLN:NE2	1.82	0.78
1:A:508:THR:HG22	1:A:510:SER:N	1.96	0.77
2:B:313:LYS:O	2:B:314:VAL:HG22	1.85	0.77
3:C:37:GLN:NE2	4:D:105:VAL:HG22	1.99	0.77
2:B:278:ALA:HB2	13:B:817:CLA:HBB1	1.66	0.77
2:B:339:TRP:HE1	13:B:824:CLA:C2B	1.99	0.76
2:B:25:ALA:HB2	18:B:850:LMG:H121	1.67	0.76
13:A:801:CLA:HBB1	13:B:802:CLA:HED1	1.67	0.75
1:A:231:VAL:O	1:A:232:ALA:HB3	1.87	0.75
2:B:367:ASP:CG	2:B:370:THR:HG23	2.06	0.75
2:B:647:ASN:HD22	2:B:649:LEU:H	1.35	0.75
13:A:829:CLA:H192	16:J:103:BCR:H14C	1.69	0.75
13:B:818:CLA:HBB1	13:B:818:CLA:HMB1	1.68	0.75
13:B:825:CLA:HAA2	13:B:826:CLA:OBD	1.87	0.74
13:A:829:CLA:H93	16:J:103:BCR:H361	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:PHE:O	13:A:835:CLA:HBB2	1.88	0.74
2:B:639:ASN:HD22	2:B:642:ASN:HD22	1.36	0.74
2:B:497:ASN:O	2:B:498:VAL:HB	1.87	0.73
2:B:229:TRP:HB2	13:B:816:CLA:H12	1.70	0.73
4:D:50:ARG:N	4:D:54:ASN:HD21	1.84	0.73
2:B:159:LYS:CD	2:B:159:LYS:H	1.92	0.72
2:B:494:ASN:HD22	2:B:496:GLY:N	1.84	0.72
2:B:181:LEU:HG	13:B:813:CLA:H43	1.70	0.72
2:B:622:LEU:HD12	13:B:802:CLA:C1	2.15	0.72
2:B:425:LEU:HG	13:B:839:CLA:CBB	2.20	0.72
2:B:329:TYR:OH	2:B:340:HIS:HE1	1.71	0.72
2:B:725:LEU:HD11	13:B:829:CLA:H203	1.70	0.72
11:M:31:LYS:O	11:M:31:LYS:CG	2.34	0.72
2:B:343:CYS:HB3	13:B:824:CLA:H42	1.72	0.72
13:B:819:CLA:HAA2	13:B:824:CLA:HBB1	1.72	0.72
3:C:39:ALA:O	20:C:209:HOH:O	2.07	0.72
2:B:36:MET:HE3	2:B:40:ASN:HB2	1.72	0.71
1:A:202:ALA:HB2	1:A:312:GLY:HA3	1.72	0.70
1:A:221:LEU:HB2	1:A:222:PRO:HD3	1.73	0.70
1:A:341:HIS:HE1	17:A:856:LHG:HC11	1.56	0.70
5:E:68:VAL:HG23	5:E:69:ALA:H	1.56	0.69
1:A:255:LYS:HB2	1:A:277:ASP:OD2	1.92	0.69
2:B:222:ALA:HB3	2:B:223:PRO:HD3	1.74	0.69
2:B:589:MET:HE1	2:B:590:LEU:HA	1.75	0.69
1:A:13:ARG:HE	1:A:15:VAL:CG2	2.05	0.68
2:B:602:TRP:HE1	2:B:614:GLN:HE21	1.40	0.68
13:A:839:CLA:H101	13:L:1003:CLA:H191	1.75	0.68
6:F:52:VAL:HG12	6:F:54:ASP:HB2	1.76	0.68
1:A:221:LEU:HD11	1:A:295:SER:HA	1.76	0.68
1:A:399:TRP:CD1	13:A:829:CLA:HAB	2.29	0.68
1:A:117:VAL:HG13	1:A:123:GLN:NE2	2.07	0.67
2:B:25:ALA:HA	13:B:829:CLA:H42	1.75	0.67
1:A:101:GLU:OE2	1:A:155:GLU:HG2	1.95	0.67
2:B:339:TRP:HZ2	13:B:824:CLA:HAB	1.58	0.66
6:F:102:ASP:OD2	6:F:105:LEU:HB2	1.94	0.66
1:A:336:PHE:HB2	17:A:856:LHG:HC41	1.78	0.66
3:C:65:ARG:HG2	3:C:67:TYR:CZ	2.31	0.66
14:A:847:PQN:H172	16:B:848:BCR:H382	1.77	0.66
9:K:73:VAL:HA	13:K:1401:CLA:HBB1	1.77	0.66
2:B:188:ALA:HA	13:B:815:CLA:CBB	2.26	0.66
4:D:50:ARG:H	4:D:54:ASN:ND2	1.88	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:TRP:HB3	13:A:806:CLA:HAC1	1.77	0.65
2:B:210:ASN:O	2:B:214:THR:HG23	1.96	0.65
2:B:318:PHE:CD1	13:B:822:CLA:HAB	2.32	0.65
6:F:63:PHE:C	6:F:66:PRO:HD2	2.17	0.65
2:B:41:LEU:O	2:B:45:ILE:HG12	1.97	0.65
1:A:257:ASP:OD1	1:A:262:SER:HB3	1.96	0.65
2:B:318:PHE:HB2	13:B:823:CLA:HMA1	1.78	0.65
1:A:249:MET:O	1:A:252:LEU:O	2.15	0.65
2:B:313:LYS:O	2:B:314:VAL:HG13	1.97	0.65
1:A:269:THR:O	1:A:270:PHE:HB2	1.96	0.65
10:L:6:LYS:HB2	10:L:7:PRO:HD2	1.78	0.65
2:B:492:TRP:CE3	2:B:493:PRO:HD3	2.32	0.65
6:F:54:ASP:OD2	12:X:30:TYR:CE2	2.50	0.65
13:A:844:CLA:H191	13:L:1003:CLA:HBB1	1.78	0.64
6:F:65:ILE:HB	6:F:66:PRO:HD3	1.78	0.64
13:B:829:CLA:HBB1	13:B:829:CLA:HMB1	1.78	0.64
2:B:304:MET:HG3	2:B:322:HIS:O	1.97	0.64
2:B:647:ASN:ND2	2:B:649:LEU:H	1.95	0.64
10:L:61:PRO:HB3	13:L:1004:CLA:HBB1	1.78	0.64
1:A:473:ASP:OD1	10:L:69:ARG:NH2	2.31	0.64
8:J:12:PRO:HB2	16:J:104:BCR:H391	1.78	0.64
2:B:641:TYR:HB2	2:B:646:THR:HG22	1.79	0.64
13:B:806:CLA:H162	13:B:828:CLA:HBB2	1.80	0.64
6:F:103:VAL:HB	6:F:104:PRO:HD3	1.79	0.63
3:C:23:ASP:OD2	4:D:95:HIS:HD2	1.81	0.63
13:B:803:CLA:H111	16:B:849:BCR:H362	1.79	0.63
6:F:63:PHE:O	6:F:66:PRO:HD2	1.97	0.63
2:B:318:PHE:HA	13:B:822:CLA:CAB	2.28	0.63
1:A:177:TRP:HB2	13:A:812:CLA:HMC3	1.80	0.63
2:B:622:LEU:CD1	13:B:802:CLA:H11	2.16	0.63
4:D:117:ARG:HG2	4:D:118:SER:O	1.98	0.63
13:A:801:CLA:HAB	13:B:801:CLA:NA	2.14	0.62
11:M:29:LEU:O	11:M:30:TYR:HB2	1.99	0.62
1:A:104:LEU:HD11	1:A:153:THR:HA	1.81	0.62
1:A:651:ARG:HB2	2:B:638:ILE:HG23	1.81	0.62
6:F:60:ALA:O	6:F:65:ILE:HG12	1.98	0.62
2:B:166:TRP:CZ2	13:B:811:CLA:HMA1	2.33	0.62
2:B:321:PRO:HB2	2:B:409:ASN:HA	1.80	0.62
2:B:228:ASN:O	2:B:231:VAL:HG23	2.00	0.62
1:A:86:TRP:HA	13:A:808:CLA:HBB2	1.82	0.62
2:B:136:GLN:HE22	2:B:208:TRP:HE1	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:647:ASN:HD21	2:B:649:LEU:HB2	1.64	0.62
1:A:356:LEU:O	1:A:360:LEU:HB2	1.99	0.62
1:A:602:MET:HG2	13:A:827:CLA:HBC1	1.80	0.62
2:B:480:LEU:C	2:B:482:SER:H	2.02	0.62
1:A:353:HIS:CD2	1:A:411:HIS:HD1	2.11	0.62
2:B:278:ALA:CB	13:B:817:CLA:HBB1	2.29	0.61
1:A:429:VAL:O	1:A:433:VAL:HG13	1.99	0.61
1:A:90:MET:HE3	13:A:809:CLA:HED2	1.82	0.61
13:A:827:CLA:HAA2	13:A:828:CLA:OBD	2.01	0.61
1:A:42:PRO:HG2	6:F:99:ILE:HD13	1.83	0.61
13:A:844:CLA:HMA1	2:B:694:ALA:CB	2.30	0.61
1:A:543:ALA:HB1	13:A:839:CLA:HMB3	1.83	0.61
1:A:726:GLN:HG3	17:A:855:LHG:O9	2.01	0.61
2:B:438:GLY:HA3	13:B:833:CLA:CBB	2.31	0.61
11:M:24:ARG:HG3	11:M:24:ARG:HH11	1.64	0.61
1:A:601:TRP:HH2	13:A:802:CLA:HBB1	1.66	0.61
13:A:846:CLA:HBD	13:A:846:CLA:H61	1.83	0.61
10:L:153:PHE:O	10:L:154:ASN:HB2	1.99	0.61
1:A:518:VAL:HG22	1:A:525:ALA:HB3	1.82	0.60
1:A:453:PHE:O	13:A:835:CLA:CBB	2.48	0.60
13:B:806:CLA:H151	13:B:806:CLA:H102	1.84	0.60
3:C:30:TRP:O	3:C:36:GLY:HA2	2.00	0.60
1:A:303:ALA:HB2	13:A:819:CLA:HBB1	1.83	0.60
13:B:837:CLA:HMB2	13:B:839:CLA:HED1	1.82	0.60
9:K:32:TYR:O	9:K:34:ILE:N	2.34	0.60
1:A:484:PRO:HB3	13:A:839:CLA:HED3	1.83	0.60
13:A:801:CLA:HBB1	13:B:802:CLA:CED	2.31	0.60
13:A:803:CLA:H71	13:A:843:CLA:HMC3	1.82	0.60
1:A:168:MET:CE	1:A:171:LEU:HD23	2.31	0.60
1:A:300:HIS:O	1:A:304:ILE:HG12	2.02	0.59
1:A:19:ASP:HA	1:A:181:HIS:O	2.02	0.59
1:A:210:LEU:HD21	16:A:849:BCR:H342	1.84	0.59
1:A:259:GLY:O	1:A:261:PHE:N	2.35	0.59
2:B:642:ASN:HB2	2:B:643:PRO:HD2	1.84	0.59
2:B:181:LEU:HD21	13:B:813:CLA:H12	1.85	0.59
2:B:36:MET:CE	2:B:41:LEU:N	2.66	0.59
2:B:589:MET:HE2	2:B:589:MET:O	2.02	0.59
7:I:7:ALA:HB1	7:I:10:LEU:HD22	1.83	0.59
1:A:257:ASP:CG	1:A:258:TRP:N	2.56	0.59
13:B:830:CLA:HBC1	16:B:846:BCR:H23C	1.83	0.59
1:A:16:VAL:HG12	1:A:17:ASP:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:40:GLU:H	4:D:71:GLN:NE2	2.01	0.59
13:A:841:CLA:H43	13:B:832:CLA:HAA2	1.84	0.59
1:A:231:VAL:O	1:A:232:ALA:CB	2.50	0.58
10:L:36:ALA:HB2	13:L:1003:CLA:HMD1	1.84	0.58
2:B:591:ASN:HB2	13:B:802:CLA:HBC2	1.83	0.58
7:I:37:GLU:C	7:I:38:ALA:OXT	2.41	0.58
1:A:145:GLN:NE2	1:A:145:GLN:H	2.02	0.58
1:A:207:LEU:HD22	16:A:850:BCR:H361	1.85	0.58
2:B:438:GLY:HA3	13:B:833:CLA:HBB1	1.86	0.58
1:A:86:TRP:HA	13:A:808:CLA:CBB	2.33	0.58
13:A:809:CLA:HMC2	13:A:829:CLA:H142	1.84	0.58
2:B:243:PHE:N	2:B:263:GLN:HE22	1.90	0.58
13:B:833:CLA:O1D	8:J:35:ASP:HA	2.02	0.58
13:A:824:CLA:HMA1	13:A:846:CLA:HAC2	1.85	0.58
2:B:367:ASP:OD1	2:B:370:THR:HG23	2.03	0.58
2:B:648:ASN:HD22	2:B:648:ASN:N	2.02	0.58
1:A:744:TRP:HB2	13:A:829:CLA:HBB1	1.87	0.57
16:A:854:BCR:HC8	16:A:854:BCR:H321	1.84	0.57
1:A:91:TYR:CZ	1:A:147:TRP:CZ3	2.91	0.57
1:A:392:SER:HB3	13:A:829:CLA:HMA1	1.87	0.57
2:B:380:TYR:CD1	13:B:827:CLA:HBB1	2.39	0.57
6:F:82:ARG:O	6:F:86:ILE:HG12	2.04	0.57
13:A:803:CLA:H12	2:B:430:LEU:HD12	1.85	0.57
2:B:414:VAL:HG11	16:B:846:BCR:H401	1.85	0.57
2:B:557:LYS:HD2	4:D:124:ASN:OD1	2.04	0.57
1:A:542:HIS:HB3	13:A:838:CLA:HBB1	1.87	0.57
1:A:349:THR:HG22	1:A:350:THR:HG23	1.87	0.57
5:E:24:ALA:O	5:E:25:SER:HB3	2.05	0.56
1:A:694:ARG:HD3	2:B:572:GLY:HA3	1.86	0.56
2:B:678:GLN:NE2	2:B:705:ALA:H	2.03	0.56
8:J:15:ALA:O	8:J:19:MET:HB2	2.05	0.56
1:A:67:ASP:O	1:A:71:LYS:HG3	2.05	0.56
1:A:355:GLN:HG3	13:A:826:CLA:H152	1.87	0.56
13:A:809:CLA:H112	13:A:831:CLA:H203	1.87	0.56
2:B:279:ILE:HD11	13:B:817:CLA:CBC	2.35	0.56
2:B:282:LEU:HD12	13:B:819:CLA:HMC1	1.87	0.56
6:F:37:ARG:O	6:F:40:GLN:HG2	2.04	0.56
1:A:233:ALA:O	1:A:235:ASP:N	2.36	0.56
2:B:234:GLN:OE1	2:B:234:GLN:HA	2.06	0.56
2:B:339:TRP:CZ2	13:B:824:CLA:HAB	2.39	0.56
2:B:480:LEU:O	2:B:482:SER:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:ILE:HG23	2:B:283:PHE:CE2	2.41	0.56
6:F:76:TRP:CE2	6:F:113:GLY:HA3	2.40	0.56
1:A:189:TRP:CZ2	13:A:811:CLA:HMA1	2.40	0.56
2:B:339:TRP:CH2	16:B:846:BCR:H372	2.40	0.56
12:X:9:TYR:O	12:X:10:ALA:HB2	2.05	0.56
12:X:20:LEU:HD11	12:X:24:PHE:HE1	1.71	0.56
1:A:66:GLU:OE2	1:A:186:LYS:HG3	2.04	0.56
1:A:366:LEU:HD11	13:A:820:CLA:H71	1.86	0.56
1:A:741:ALA:HB2	16:A:854:BCR:H323	1.88	0.56
13:A:801:CLA:HAB	13:B:801:CLA:C1A	2.37	0.55
1:A:297:THR:O	1:A:300:HIS:HB3	2.06	0.55
13:A:833:CLA:H12	13:L:1003:CLA:H93	1.86	0.55
2:B:588:TRP:HH2	13:B:802:CLA:CBB	2.19	0.55
4:D:117:ARG:CG	4:D:121:GLN:HB2	2.33	0.55
13:A:805:CLA:HMC3	13:A:807:CLA:HED2	1.86	0.55
9:K:40:GLY:O	9:K:41:PRO:C	2.45	0.55
2:B:425:LEU:HD13	2:B:538:LEU:HA	1.89	0.55
2:B:398:VAL:CG2	2:B:547:ALA:HB1	2.37	0.55
2:B:589:MET:HE2	2:B:589:MET:C	2.27	0.55
1:A:681:PHE:CD2	16:A:854:BCR:H363	2.42	0.55
13:B:827:CLA:HBC3	18:B:850:LMG:H421	1.88	0.55
1:A:433:VAL:HA	1:A:436:HIS:CE1	2.41	0.55
2:B:233:ALA:O	2:B:234:GLN:O	2.24	0.55
13:B:828:CLA:H51	16:B:845:BCR:H392	1.88	0.55
2:B:261:HIS:CD2	2:B:264:THR:H	2.25	0.55
13:A:819:CLA:H41	13:A:836:CLA:HAA2	1.88	0.55
16:A:852:BCR:H333	16:A:853:BCR:H333	1.88	0.55
2:B:589:MET:HE1	2:B:590:LEU:CA	2.37	0.55
2:B:525:VAL:HG13	13:B:801:CLA:H141	1.89	0.55
1:A:372:GLN:HG3	13:A:827:CLA:CED	2.37	0.54
13:B:840:CLA:H18	16:I:101:BCR:H362	1.89	0.54
1:A:244:LEU:O	1:A:246:PRO:HD3	2.06	0.54
1:A:681:PHE:CG	16:A:854:BCR:H363	2.43	0.54
2:B:205:HIS:ND1	20:B:947:HOH:O	2.23	0.54
13:A:844:CLA:HMA1	2:B:694:ALA:HB1	1.88	0.54
10:L:35:PRO:HG3	13:L:1003:CLA:HED2	1.88	0.54
1:A:390:GLN:HA	1:A:390:GLN:HE21	1.71	0.54
2:B:179:ALA:HB2	2:B:287:GLY:HA3	1.89	0.54
4:D:43:THR:O	4:D:44:ALA:HB3	2.07	0.54
1:A:403:PHE:HB3	13:A:807:CLA:H112	1.90	0.54
2:B:592:THR:O	2:B:596:VAL:HG13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:819:CLA:HMB2	13:B:824:CLA:HMA3	1.89	0.54
2:B:413:ARG:HD3	13:B:830:CLA:OBD	2.07	0.54
1:A:308:PHE:HE2	13:A:822:CLA:HAB	1.72	0.54
2:B:614:GLN:O	2:B:618:SER:HB2	2.07	0.54
12:X:25:LEU:O	12:X:29:TYR:HD1	1.89	0.54
2:B:171:GLU:HB3	2:B:290:TYR:HB3	1.90	0.54
2:B:318:PHE:HA	13:B:822:CLA:HAB	1.88	0.54
2:B:157:GLN:O	2:B:161:ARG:HG3	2.08	0.54
6:F:52:VAL:CG1	6:F:54:ASP:HB2	2.36	0.54
1:A:42:PRO:HG3	1:A:47:TRP:CE3	2.42	0.54
2:B:212:LEU:HD21	16:B:845:BCR:H341	1.90	0.54
2:B:103:PHE:CZ	2:B:651:VAL:HG22	2.42	0.53
1:A:305:ALA:O	1:A:309:ILE:HG12	2.08	0.53
13:A:804:CLA:HED1	8:J:12:PRO:HA	1.90	0.53
5:E:6:LYS:HD3	5:E:22:THR:HG22	1.90	0.53
13:A:803:CLA:H142	16:A:854:BCR:H402	1.89	0.53
13:A:802:CLA:OBD	13:B:801:CLA:HMB3	2.08	0.53
11:M:24:ARG:HH11	11:M:24:ARG:CG	2.21	0.53
13:A:828:CLA:HBB1	13:A:836:CLA:HMA2	1.90	0.53
1:A:466:ARG:O	2:B:646:THR:HG21	2.09	0.53
13:A:801:CLA:HMB3	13:B:802:CLA:OBD	2.09	0.53
13:B:829:CLA:H143	18:B:850:LMG:H231	1.89	0.53
6:F:88:VAL:HG11	6:F:97:LYS:CB	2.37	0.53
8:J:19:MET:CE	8:J:19:MET:HA	2.38	0.53
1:A:13:ARG:HE	1:A:15:VAL:HG22	1.72	0.53
2:B:479:THR:O	2:B:480:LEU:O	2.27	0.53
10:L:16:HIS:CD2	10:L:17:LEU:H	2.27	0.53
13:A:822:CLA:HMB2	13:A:826:CLA:HMA3	1.91	0.53
6:F:53:VAL:HG12	6:F:63:PHE:HB2	1.90	0.53
1:A:296:ASP:HB3	13:A:819:CLA:HMA1	1.90	0.53
13:A:803:CLA:O1A	2:B:531:LEU:HD11	2.09	0.53
13:A:831:CLA:H111	17:A:855:LHG:H202	1.90	0.52
13:A:827:CLA:H162	16:A:852:BCR:H272	1.91	0.52
1:A:59:ASP:OD2	1:A:353:HIS:HE1	1.91	0.52
1:A:622:TRP:O	1:A:633:HIS:HD2	1.92	0.52
2:B:406:ASN:HD22	2:B:409:ASN:ND2	1.84	0.52
1:A:90:MET:CE	13:A:809:CLA:HED2	2.39	0.52
6:F:40:GLN:OE1	8:J:40:PRO:O	2.26	0.52
1:A:221:LEU:HD11	1:A:295:SER:CA	2.39	0.52
1:A:244:LEU:C	1:A:246:PRO:HD3	2.30	0.52
2:B:78:GLN:OE1	2:B:78:GLN:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LEU:HG	1:A:360:LEU:HD22	1.91	0.52
2:B:90:ILE:HB	2:B:111:PRO:HB2	1.91	0.52
6:F:79:TRP:CH2	6:F:120:ALA:HA	2.44	0.52
1:A:578:CYS:HB3	1:A:587:CYS:HA	1.91	0.52
2:B:36:MET:HE2	2:B:41:LEU:N	2.24	0.52
13:A:836:CLA:HMD2	13:A:837:CLA:HBB1	1.91	0.52
2:B:217:HIS:CG	2:B:218:PRO:HD2	2.44	0.52
8:J:28:GLU:OE1	8:J:28:GLU:HA	2.09	0.52
2:B:430:LEU:HB3	13:B:832:CLA:HED3	1.90	0.52
1:A:744:TRP:CZ2	13:A:829:CLA:H43	2.44	0.52
2:B:634:SER:O	2:B:638:ILE:HB	2.10	0.52
2:B:294:PHE:HE1	13:B:812:CLA:HMA1	1.75	0.52
10:L:31:ILE:HA	10:L:34:LEU:HD22	1.92	0.52
1:A:16:VAL:HG11	1:A:183:ARG:HB3	1.92	0.51
1:A:718:GLN:NE2	5:E:42:LYS:HD3	2.25	0.51
1:A:77:PHE:CE2	13:A:811:CLA:HBB1	2.45	0.51
1:A:83:VAL:HG11	13:A:806:CLA:H72	1.92	0.51
1:A:168:MET:HE1	1:A:171:LEU:HD23	1.92	0.51
1:A:226:LEU:HD22	1:A:231:VAL:HG21	1.93	0.51
1:A:259:GLY:C	1:A:261:PHE:H	2.13	0.51
1:A:71:LYS:NZ	20:A:931:HOH:O	2.43	0.51
1:A:542:HIS:HE1	1:A:612:HIS:ND1	2.08	0.51
2:B:279:ILE:HD11	13:B:817:CLA:HBC2	1.92	0.51
2:B:456:ILE:HG22	2:B:458:ILE:CD1	2.40	0.51
13:A:828:CLA:HMB3	13:A:836:CLA:H12	1.93	0.51
2:B:398:VAL:HG23	2:B:547:ALA:HB1	1.93	0.51
1:A:257:ASP:O	1:A:258:TRP:HB2	2.11	0.51
1:A:444:LEU:HB2	13:A:840:CLA:CBB	2.40	0.51
1:A:303:ALA:CB	13:A:819:CLA:HBB1	2.40	0.51
2:B:159:LYS:HD2	2:B:159:LYS:N	2.04	0.51
1:A:453:PHE:C	13:A:835:CLA:HBB2	2.31	0.51
2:B:379:GLN:HA	2:B:379:GLN:OE1	2.11	0.51
13:B:840:CLA:HBB2	14:B:842:PQN:H141	1.91	0.51
2:B:453:GLU:HA	6:F:48:LEU:HD22	1.93	0.51
4:D:117:ARG:HG2	4:D:118:SER:N	2.26	0.50
7:I:30:LEU:O	7:I:34:ILE:HG12	2.11	0.50
1:A:16:VAL:CG1	1:A:17:ASP:N	2.74	0.50
1:A:118:TRP:CB	16:J:104:BCR:H323	2.41	0.50
2:B:464:GLN:HG2	2:B:475:TYR:CE2	2.47	0.50
2:B:638:ILE:HD11	2:B:656:PHE:CE2	2.46	0.50
13:B:819:CLA:HMD1	13:B:821:CLA:HBB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:823:CLA:HBB1	13:B:830:CLA:HMD2	1.94	0.50
3:C:14:THR:HG22	3:C:27:MET:HG3	1.94	0.50
11:M:30:TYR:O	11:M:31:LYS:OXT	2.29	0.50
2:B:339:TRP:HE1	13:B:824:CLA:C3B	2.23	0.50
2:B:588:TRP:HH2	13:B:802:CLA:HBB1	1.77	0.50
13:A:803:CLA:HBB1	13:B:802:CLA:NB	2.27	0.50
13:B:824:CLA:H61	13:B:826:CLA:H42	1.93	0.50
4:D:32:THR:HA	4:D:52:GLY:O	2.12	0.50
2:B:431:PHE:CZ	16:J:105:BCR:HC41	2.46	0.50
13:B:829:CLA:H8	18:B:850:LMG:H242	1.94	0.49
4:D:101:PHE:HB3	4:D:103:GLU:OE2	2.11	0.49
2:B:459:GLU:OE2	6:F:50:HIS:ND1	2.40	0.49
2:B:548:ARG:HH22	4:D:124:ASN:ND2	2.10	0.49
5:E:68:VAL:O	5:E:69:ALA:O	2.30	0.49
2:B:548:ARG:HH22	4:D:124:ASN:CG	2.15	0.49
2:B:664:ALA:C	13:B:803:CLA:HBB1	2.31	0.49
7:I:9:PHE:CE1	7:I:10:LEU:HD13	2.46	0.49
2:B:340:HIS:HD2	13:B:805:CLA:OBD	1.96	0.49
13:A:844:CLA:H52	13:B:840:CLA:H43	1.93	0.49
1:A:691:PHE:HB2	13:A:803:CLA:HBC2	1.95	0.49
2:B:114:ILE:O	13:B:808:CLA:HMD3	2.12	0.49
10:L:105:GLY:O	10:L:106:SER:HB2	2.11	0.49
13:A:820:CLA:HMB1	13:A:820:CLA:HBB1	1.93	0.49
6:F:80:VAL:HG22	6:F:109:CYS:O	2.13	0.49
2:B:458:ILE:N	2:B:458:ILE:HD12	2.28	0.49
5:E:7:VAL:O	5:E:20:VAL:HA	2.13	0.49
6:F:84:TYR:O	6:F:88:VAL:HG23	2.12	0.49
2:B:162:PRO:HB2	2:B:167:PHE:CE1	2.48	0.49
13:B:801:CLA:H72	13:B:802:CLA:CED	2.42	0.49
13:B:819:CLA:CMB	13:B:824:CLA:HMA3	2.41	0.49
4:D:30:THR:O	4:D:80:TYR:HA	2.13	0.49
2:B:261:HIS:CD2	2:B:263:GLN:H	2.31	0.49
2:B:294:PHE:O	2:B:296:ILE:HG22	2.13	0.49
2:B:390:PHE:CE1	16:B:847:BCR:H373	2.48	0.49
2:B:425:LEU:HG	13:B:839:CLA:HBB1	1.94	0.49
2:B:446:VAL:HG13	2:B:451:THR:O	2.13	0.49
2:B:182:PHE:CE2	13:B:813:CLA:H61	2.48	0.49
1:A:651:ARG:HG3	2:B:638:ILE:CG2	2.43	0.48
13:B:806:CLA:H143	13:B:828:CLA:HBB2	1.95	0.48
1:A:293:TRP:O	1:A:296:ASP:HB2	2.13	0.48
1:A:662:ILE:HD12	2:B:627:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:803:CLA:H71	13:A:843:CLA:CMC	2.42	0.48
2:B:261:HIS:HD2	2:B:263:GLN:H	1.62	0.48
10:L:143:LEU:HD12	10:L:143:LEU:HA	1.61	0.48
1:A:120:ILE:C	1:A:122:GLY:H	2.16	0.48
1:A:444:LEU:HB2	13:A:840:CLA:HBB1	1.96	0.48
2:B:271:ASP:HB3	13:B:817:CLA:HMA1	1.95	0.48
2:B:487:ILE:HG12	13:B:835:CLA:HMD3	1.95	0.48
13:B:806:CLA:H91	18:B:850:LMG:H401	1.96	0.48
13:A:810:CLA:HMA1	8:J:27:ILE:HD13	1.95	0.48
1:A:283:GLY:O	1:A:508:THR:O	2.32	0.48
1:A:399:TRP:NE1	13:A:829:CLA:HAB	2.27	0.48
6:F:109:CYS:O	6:F:112:THR:HB	2.13	0.48
8:J:33:TYR:N	8:J:34:PRO:HD3	2.28	0.48
1:A:118:TRP:HB3	16:J:104:BCR:H323	1.94	0.48
1:A:658:ALA:O	1:A:662:ILE:HG12	2.14	0.48
6:F:88:VAL:HG13	6:F:97:LYS:HD2	1.95	0.48
6:F:73:ILE:O	6:F:76:TRP:HB3	2.14	0.48
1:A:693:GLY:HA3	2:B:574:CYS:HB2	1.95	0.48
8:J:31:ARG:CD	16:J:104:BCR:H312	2.19	0.48
1:A:497:ALA:N	1:A:498:PRO:CD	2.76	0.48
1:A:360:LEU:CD1	13:A:831:CLA:HBB1	2.44	0.48
2:B:180:GLY:HA3	13:B:813:CLA:HBB1	1.96	0.48
1:A:203:GLY:O	1:A:207:LEU:HB2	2.13	0.47
1:A:577:PRO:O	1:A:578:CYS:HB3	2.14	0.47
9:K:74:VAL:C	9:K:76:GLY:H	2.17	0.47
2:B:329:TYR:OH	2:B:340:HIS:CE1	2.61	0.47
6:F:10:ASP:HB3	20:F:1406:HOH:O	2.14	0.47
11:M:24:ARG:NH1	20:M:1702:HOH:O	2.46	0.47
1:A:168:MET:O	1:A:172:MET:HB2	2.14	0.47
2:B:647:ASN:HD22	2:B:649:LEU:N	2.08	0.47
13:B:824:CLA:H41	13:B:824:CLA:H61	1.68	0.47
13:B:814:CLA:HAB	13:B:828:CLA:H13	1.96	0.47
4:D:124:ASN:O	4:D:127:GLN:HB2	2.13	0.47
1:A:74:SER:OG	1:A:180:TYR:HB2	2.15	0.47
1:A:686:SER:HB3	1:A:734:HIS:HB2	1.96	0.47
13:A:815:CLA:HBA2	13:A:817:CLA:HMB3	1.96	0.47
1:A:56:HIS:CG	13:A:806:CLA:HAB	2.49	0.47
1:A:691:PHE:HB2	13:A:803:CLA:CBC	2.45	0.47
1:A:121:VAL:HB	13:B:833:CLA:HMD1	1.96	0.47
2:B:693:LEU:HD12	13:L:1003:CLA:H11	1.96	0.47
2:B:525:VAL:CG1	13:B:801:CLA:H141	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:808:CLA:H142	13:B:808:CLA:HMB2	1.97	0.47
1:A:399:TRP:HB3	13:A:829:CLA:HMC3	1.96	0.47
1:A:447:VAL:HG21	13:A:840:CLA:C2C	2.44	0.47
13:A:804:CLA:H8	8:J:16:ALA:HA	1.97	0.47
2:B:589:MET:CE	2:B:589:MET:C	2.83	0.47
8:J:40:PRO:O	8:J:41:LEU:HB2	2.14	0.47
1:A:174:PHE:HD2	13:A:811:CLA:CBC	2.28	0.47
13:A:806:CLA:HMC3	13:A:831:CLA:HMA1	1.97	0.47
1:A:379:PRO:HB2	13:A:820:CLA:HAA2	1.96	0.47
2:B:313:LYS:O	2:B:314:VAL:CG2	2.60	0.47
6:F:88:VAL:CG1	6:F:97:LYS:HB2	2.41	0.47
2:B:641:TYR:CB	2:B:646:THR:HG22	2.42	0.47
3:C:65:ARG:HG2	3:C:67:TYR:OH	2.14	0.47
13:A:843:CLA:H172	8:J:19:MET:HG3	1.97	0.47
11:M:24:ARG:NH1	11:M:24:ARG:CG	2.78	0.47
13:A:843:CLA:H2	13:A:843:CLA:O1A	2.15	0.46
3:C:57:CYS:HA	3:C:58:PRO:HD3	1.71	0.46
2:B:696:LEU:HD11	10:L:36:ALA:HB1	1.97	0.46
13:B:810:CLA:H42	10:L:81:SER:HA	1.97	0.46
1:A:638:ASN:O	1:A:642:SER:HB2	2.16	0.46
13:B:820:CLA:HBB1	16:B:843:BCR:H14C	1.97	0.46
1:A:603:TYR:OH	13:A:801:CLA:HED1	2.15	0.46
13:A:822:CLA:CMB	13:A:826:CLA:HMA3	2.46	0.46
2:B:39:GLU:O	2:B:43:GLN:HG3	2.15	0.46
3:C:61:PHE:HD2	4:D:119:ILE:HG21	1.81	0.46
13:B:838:CLA:H203	6:F:67:SER:HB3	1.98	0.46
1:A:90:MET:HE1	13:A:809:CLA:HAA2	1.98	0.46
13:A:821:CLA:HBC2	13:A:821:CLA:HMC1	1.97	0.46
2:B:198:ILE:HB	2:B:199:PRO:HD3	1.96	0.46
2:B:361:TYR:O	2:B:364:ILE:HG22	2.15	0.46
13:B:802:CLA:H41	13:B:802:CLA:H61	1.56	0.46
13:B:828:CLA:HBA2	13:B:828:CLA:H3A	1.64	0.46
2:B:589:MET:HE1	2:B:590:LEU:HD23	1.96	0.46
2:B:386:MET:HE1	16:B:847:BCR:H361	1.98	0.46
6:F:80:VAL:HG11	6:F:110:MET:HG2	1.97	0.46
10:L:33:ASN:HB3	13:L:1002:CLA:HAC1	1.98	0.46
11:M:17:LEU:HB3	11:M:18:PRO:CD	2.46	0.46
1:A:656:ALA:O	1:A:659:SER:HB2	2.16	0.46
1:A:744:TRP:CG	16:A:854:BCR:HC22	2.51	0.46
2:B:642:ASN:HB2	2:B:643:PRO:HD3	1.95	0.46
2:B:738:LYS:O	2:B:739:PHE:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ASN:ND2	13:B:803:CLA:HED2	2.31	0.46
13:B:810:CLA:HBB1	13:B:810:CLA:HHC	1.96	0.46
3:C:23:ASP:OD2	4:D:95:HIS:CD2	2.67	0.46
4:D:34:PRO:O	4:D:51:GLU:HG3	2.16	0.46
11:M:13:VAL:HG23	16:M:1602:BCR:H402	1.98	0.46
1:A:168:MET:HE2	1:A:171:LEU:HD23	1.96	0.46
1:A:686:SER:HB3	1:A:734:HIS:CB	2.46	0.46
13:A:801:CLA:HED1	20:A:908:HOH:O	2.15	0.46
16:A:854:BCR:H381	13:B:832:CLA:HMA1	1.97	0.46
1:A:91:TYR:CZ	1:A:147:TRP:HZ3	2.33	0.46
1:A:19:ASP:N	1:A:20:PRO:HD3	2.31	0.46
13:B:807:CLA:H102	16:I:101:BCR:HC31	1.98	0.46
4:D:124:ASN:HB2	4:D:127:GLN:NE2	2.31	0.46
1:A:257:ASP:OD2	1:A:262:SER:C	2.55	0.45
1:A:475:PHE:HA	1:A:480:ILE:O	2.15	0.45
1:A:508:THR:HG21	20:A:930:HOH:O	2.15	0.45
2:B:189:TRP:CA	13:B:814:CLA:HBB1	2.45	0.45
2:B:479:THR:H	2:B:482:SER:HB3	1.79	0.45
13:B:828:CLA:H12	16:B:844:BCR:H393	1.97	0.45
13:B:830:CLA:H3A	13:B:830:CLA:HBA2	1.49	0.45
1:A:44:THR:HB	1:A:720:ARG:HG2	1.98	0.45
13:A:826:CLA:HAB	16:A:852:BCR:H341	1.98	0.45
2:B:36:MET:CE	2:B:40:ASN:HB2	2.45	0.45
2:B:468:ALA:O	2:B:482:SER:HB2	2.16	0.45
2:B:509:SER:O	2:B:509:SER:OG	2.25	0.45
8:J:22:THR:O	8:J:26:LEU:HD13	2.15	0.45
13:L:1002:CLA:C1B	13:L:1003:CLA:HED1	2.46	0.45
1:A:313:HIS:CE1	16:A:849:BCR:H363	2.51	0.45
13:A:821:CLA:H3A	13:A:821:CLA:HBA2	1.83	0.45
13:A:823:CLA:HBA2	13:A:823:CLA:H3A	1.44	0.45
1:A:91:TYR:CE2	1:A:161:THR:HG21	2.51	0.45
2:B:220:GLY:HA3	13:B:815:CLA:HMD1	1.98	0.45
13:B:818:CLA:H41	13:B:818:CLA:H62	1.69	0.45
1:A:539:HIS:CG	13:A:839:CLA:HED2	2.51	0.45
2:B:471:GLY:HA3	2:B:504:LEU:CD2	2.46	0.45
2:B:64:LEU:HD11	16:B:845:BCR:H271	1.98	0.45
13:B:820:CLA:HBA2	13:B:820:CLA:H3A	1.64	0.45
1:A:112:PRO:HB3	1:A:144:PHE:CD1	2.51	0.45
13:B:816:CLA:H41	13:B:816:CLA:H62	1.71	0.45
10:L:115:GLU:O	10:L:119:GLN:HG3	2.17	0.45
2:B:339:TRP:CZ3	16:B:846:BCR:H372	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ALA:HB1	13:A:806:CLA:HBB1	1.98	0.45
2:B:445:VAL:HG21	13:B:833:CLA:HAC2	1.97	0.45
4:D:39:PHE:HB2	4:D:71:GLN:HE21	1.81	0.45
1:A:250:ALA:HA	1:A:258:TRP:CD1	2.52	0.45
1:A:508:THR:HG22	1:A:509:ALA:N	2.31	0.45
1:A:737:LEU:HD22	13:A:843:CLA:HMA1	1.99	0.45
2:B:570:ARG:HH11	2:B:570:ARG:HG3	1.81	0.45
13:B:832:CLA:HBB1	13:B:833:CLA:HMB2	1.98	0.45
1:A:711:LEU:HD23	6:F:130:THR:HG22	1.98	0.45
8:J:1:MET:O	8:J:1:MET:HE2	2.17	0.45
11:M:17:LEU:HB3	11:M:18:PRO:HD3	1.98	0.45
2:B:50:PHE:HB3	2:B:148:ALA:O	2.17	0.45
4:D:114:SER:N	20:D:206:HOH:O	2.50	0.45
4:D:134:LYS:HG2	4:D:136:TYR:CZ	2.52	0.45
1:A:445:ASN:ND2	2:B:680:LEU:HD21	2.33	0.45
1:A:321:ILE:HD11	13:A:821:CLA:H2A	1.99	0.45
1:A:86:TRP:HE1	13:A:809:CLA:HBA1	1.82	0.45
2:B:497:ASN:O	2:B:499:TRP:CE3	2.70	0.45
2:B:557:LYS:NZ	4:D:124:ASN:OD1	2.43	0.45
13:A:801:CLA:NA	13:B:801:CLA:HAB	2.31	0.44
1:A:92:PHE:CZ	1:A:96:LYS:HG3	2.52	0.44
2:B:215:MET:HA	2:B:216:PRO:HD3	1.83	0.44
2:B:480:LEU:C	2:B:482:SER:N	2.69	0.44
2:B:48:SER:HB3	13:B:805:CLA:HBB1	1.98	0.44
13:B:827:CLA:CGA	13:B:827:CLA:H3A	2.47	0.44
13:A:807:CLA:H3A	13:A:831:CLA:HAB	1.99	0.44
1:A:90:MET:HE2	13:A:829:CLA:HED1	1.99	0.44
2:B:531:LEU:HD21	13:B:802:CLA:HBB1	1.99	0.44
13:B:814:CLA:HBA1	16:B:845:BCR:H383	2.00	0.44
13:A:806:CLA:H71	16:A:851:BCR:H402	1.99	0.44
2:B:79:ASP:OD2	2:B:82:ASN:HB2	2.18	0.44
13:B:835:CLA:HMB1	16:B:847:BCR:HC31	1.98	0.44
13:M:1601:CLA:H3A	13:M:1601:CLA:HBA2	1.69	0.44
1:A:484:PRO:HB3	13:A:839:CLA:CED	2.46	0.44
1:A:212:TRP:N	13:A:815:CLA:HBB1	2.32	0.44
2:B:370:THR:HG21	20:B:922:HOH:O	2.16	0.44
2:B:441:VAL:O	2:B:445:VAL:HG23	2.17	0.44
13:B:810:CLA:CED	13:B:810:CLA:H43	2.47	0.44
3:C:6:ILE:HD12	3:C:6:ILE:N	2.33	0.44
4:D:125:PRO:HG3	4:D:135:PRO:HG3	2.00	0.44
13:B:831:CLA:HBC3	16:F:1302:BCR:H362	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:6:LYS:CD	5:E:22:THR:HG22	2.47	0.44
10:L:56:TYR:OH	13:L:1004:CLA:HED2	2.18	0.44
13:A:810:CLA:HBC2	13:A:829:CLA:H141	1.98	0.44
3:C:65:ARG:HD2	4:D:119:ILE:CD1	2.48	0.44
1:A:98:SER:HB2	1:A:113:SER:O	2.18	0.44
6:F:132:LYS:HB2	6:F:135:GLU:HG3	1.99	0.44
1:A:642:SER:O	1:A:648:GLY:HA3	2.17	0.44
16:A:854:BCR:H23C	16:A:854:BCR:H403	1.99	0.44
1:A:111:LYS:HB2	1:A:130:VAL:HB	2.00	0.44
1:A:462:ASN:HB3	1:A:645:THR:HG22	1.99	0.44
13:A:843:CLA:H62	13:A:843:CLA:H41	1.73	0.44
2:B:181:LEU:HD13	13:B:813:CLA:HBB	2.00	0.44
2:B:211:PHE:CE2	2:B:212:LEU:HG	2.53	0.44
13:B:809:CLA:H102	13:B:827:CLA:H193	1.98	0.44
5:E:17:TYR:O	5:E:18:ASN:HB2	2.18	0.43
1:A:519:ALA:HB2	1:A:625:VAL:HG21	2.00	0.43
2:B:317:PRO:HB3	20:B:949:HOH:O	2.18	0.43
13:B:806:CLA:H61	13:B:806:CLA:H41	1.60	0.43
8:J:1:MET:HE2	8:J:5:LEU:HG	2.00	0.43
10:L:7:PRO:HB3	10:L:12:PRO:HA	2.00	0.43
2:B:427:TRP:CE2	13:B:831:CLA:HBB1	2.53	0.43
2:B:430:LEU:HB3	13:B:832:CLA:CED	2.48	0.43
13:A:820:CLA:HMB1	13:A:820:CLA:CBB	2.48	0.43
2:B:231:VAL:C	2:B:234:GLN:HG2	2.36	0.43
2:B:234:GLN:O	2:B:236:PRO:HD3	2.18	0.43
2:B:339:TRP:CE2	13:B:826:CLA:H91	2.54	0.43
2:B:36:MET:HE1	2:B:41:LEU:N	2.33	0.43
2:B:531:LEU:HD21	13:B:802:CLA:CBB	2.48	0.43
2:B:431:PHE:HD2	13:B:838:CLA:HBB2	1.84	0.43
1:A:221:LEU:CB	1:A:222:PRO:HD3	2.45	0.43
2:B:236:PRO:O	2:B:250:GLY:HA3	2.18	0.43
2:B:305:ASP:OD1	2:B:323:GLN:HA	2.18	0.43
2:B:636:GLN:HG3	2:B:737:ALA:CB	2.49	0.43
13:B:835:CLA:HBA2	13:B:836:CLA:HMB3	2.00	0.43
2:B:529:ILE:HG21	13:B:837:CLA:HAB	1.99	0.43
13:B:839:CLA:HBC2	13:X:1701:CLA:HBC3	2.00	0.43
1:A:91:TYR:CE2	1:A:147:TRP:CZ3	3.07	0.43
1:A:215:HIS:HB2	13:A:815:CLA:C1C	2.48	0.43
1:A:443:HIS:CD2	13:A:832:CLA:HMB1	2.53	0.43
2:B:439:LEU:HD11	16:J:105:BCR:H342	2.00	0.43
6:F:21:ALA:HB2	6:F:35:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:VAL:HG11	1:A:236:ILE:HG12	1.99	0.43
1:A:261:PHE:O	1:A:261:PHE:CD2	2.72	0.43
1:A:212:TRP:CA	13:A:815:CLA:HBB1	2.49	0.43
6:F:116:TRP:CG	6:F:117:PRO:HD3	2.54	0.43
13:A:844:CLA:H62	13:A:844:CLA:H41	1.62	0.43
2:B:325:ILE:HD12	2:B:409:ASN:ND2	2.34	0.43
16:J:105:BCR:H20C	16:J:105:BCR:H361	1.89	0.43
13:A:820:CLA:O1A	13:A:830:CLA:HMD1	2.19	0.43
2:B:36:MET:HE1	2:B:40:ASN:C	2.39	0.43
2:B:360:PRO:HG3	13:B:818:CLA:HBA1	2.00	0.43
4:D:18:LEU:HA	4:D:18:LEU:HD23	1.86	0.43
4:D:73:ARG:HB2	4:D:74:PRO:HD3	2.00	0.43
1:A:683:TRP:CE3	13:A:801:CLA:HMA1	2.54	0.42
13:A:845:CLA:HBA2	13:A:845:CLA:H3A	1.74	0.42
13:B:832:CLA:H61	16:F:1302:BCR:H312	2.00	0.42
1:A:215:HIS:CD2	1:A:215:HIS:C	2.92	0.42
1:A:257:ASP:OD1	1:A:262:SER:CB	2.66	0.42
1:A:514:GLY:HA2	1:A:528:PRO:HB3	2.01	0.42
2:B:24:ILE:HA	13:B:804:CLA:HMD3	2.01	0.42
13:B:808:CLA:O1A	13:B:827:CLA:HBD	2.20	0.42
13:B:810:CLA:CBB	7:I:19:CYS:HB3	2.50	0.42
8:J:39:HIS:HA	16:J:105:BCR:H21C	2.00	0.42
1:A:711:LEU:O	1:A:713:VAL:HG22	2.20	0.42
13:B:817:CLA:H3A	13:B:817:CLA:HBA2	1.39	0.42
5:E:6:LYS:NZ	5:E:22:THR:HG21	2.35	0.42
10:L:4:LEU:HD22	10:L:4:LEU:N	2.35	0.42
2:B:357:SER:C	2:B:359:PRO:HD3	2.40	0.42
2:B:325:ILE:CD1	2:B:409:ASN:ND2	2.82	0.42
2:B:535:THR:O	2:B:539:ILE:HG13	2.19	0.42
2:B:103:PHE:HZ	2:B:651:VAL:HG22	1.83	0.42
4:D:95:HIS:HA	4:D:97:LYS:N	2.34	0.42
1:A:256:VAL:HG12	1:A:257:ASP:N	2.34	0.42
1:A:403:PHE:CB	13:A:807:CLA:H112	2.49	0.42
13:A:810:CLA:H11	16:J:103:BCR:H19C	2.02	0.42
2:B:458:ILE:CD1	2:B:458:ILE:N	2.82	0.42
2:B:492:TRP:CZ3	13:B:836:CLA:HMD3	2.54	0.42
2:B:588:TRP:CH2	13:B:802:CLA:CBB	3.02	0.42
13:B:829:CLA:CBB	13:B:829:CLA:HMB1	2.48	0.42
1:A:120:ILE:O	1:A:122:GLY:N	2.52	0.42
1:A:360:LEU:HD11	13:A:831:CLA:HBB1	2.02	0.42
16:A:854:BCR:H362	13:B:802:CLA:C4	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LYS:H	1:A:234:LYS:HG2	1.69	0.42
1:A:542:HIS:HD2	20:A:926:HOH:O	2.03	0.42
1:A:679:ALA:HB1	1:A:738:GLY:O	2.20	0.42
13:A:825:CLA:H92	16:A:852:BCR:H14C	2.01	0.42
2:B:341:LEU:HD21	13:B:829:CLA:HAB	2.02	0.42
8:J:19:MET:HE2	8:J:19:MET:HA	2.00	0.42
1:A:145:GLN:CD	1:A:145:GLN:H	2.22	0.42
1:A:47:TRP:CZ3	1:A:51:LEU:HD12	2.54	0.42
1:A:511:VAL:HB	1:A:526:MET:HG3	2.02	0.42
13:A:827:CLA:H51	13:A:838:CLA:H43	2.00	0.42
13:B:806:CLA:H143	13:B:828:CLA:CBB	2.50	0.42
1:A:423:ALA:HA	4:D:38:VAL:HG11	2.02	0.42
6:F:103:VAL:O	6:F:107:ILE:HG13	2.20	0.42
2:B:6:LYS:HD2	11:M:31:LYS:HB3	2.02	0.42
2:B:261:HIS:HD2	2:B:264:THR:H	1.67	0.42
1:A:156:PHE:CE2	13:A:817:CLA:HAA2	2.55	0.42
1:A:336:PHE:CD2	10:L:4:LEU:HD21	2.55	0.42
13:A:811:CLA:H3A	13:A:811:CLA:HBA2	1.63	0.42
1:A:741:ALA:CB	16:A:854:BCR:H323	2.50	0.42
2:B:414:VAL:HG11	16:B:846:BCR:C40	2.50	0.42
2:B:372:ALA:HA	2:B:600:TRP:CZ3	2.55	0.42
7:I:22:MET:O	7:I:26:VAL:HG13	2.19	0.42
2:B:527:HIS:CD2	16:J:105:BCR:H322	2.55	0.42
13:A:829:CLA:H93	16:J:103:BCR:H20C	2.02	0.41
3:C:28:VAL:HG12	4:D:109:ARG:HB3	2.02	0.41
1:A:42:PRO:CG	6:F:99:ILE:HD13	2.50	0.41
17:B:851:LHG:HC5	12:X:12:ARG:HB3	2.02	0.41
1:A:346:GLU:N	1:A:346:GLU:OE1	2.47	0.41
1:A:686:SER:HB2	1:A:731:GLY:O	2.20	0.41
1:A:685:PHE:HA	13:A:803:CLA:HAB	2.01	0.41
1:A:744:TRP:NE1	13:A:829:CLA:H11	2.35	0.41
13:A:837:CLA:HBA2	13:A:837:CLA:H3A	1.72	0.41
13:A:846:CLA:H12	13:A:846:CLA:HBA2	1.85	0.41
2:B:189:TRP:HA	13:B:814:CLA:HBB1	2.02	0.41
3:C:25:LEU:HA	3:C:40:SER:O	2.20	0.41
11:M:9:TYR:HB3	16:M:1602:BCR:H401	2.02	0.41
1:A:483:GLN:HA	1:A:484:PRO:HD3	1.70	0.41
1:A:203:GLY:HA3	13:A:814:CLA:HBB1	2.02	0.41
1:A:49:TRP:CZ3	17:A:855:LHG:H121	2.56	0.41
2:B:136:GLN:HE21	13:B:814:CLA:HAA1	1.85	0.41
2:B:663:TRP:CE3	13:B:801:CLA:HMA1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:LYS:O	1:A:710:LYS:HD2	2.20	0.41
2:B:178:LEU:O	2:B:283:PHE:HB3	2.21	0.41
1:A:378:PRO:HA	1:A:379:PRO:HD3	1.83	0.41
1:A:49:TRP:HZ3	17:A:855:LHG:H121	1.86	0.41
1:A:212:TRP:HA	13:A:815:CLA:HBB1	2.01	0.41
1:A:202:ALA:C	13:A:821:CLA:HBC3	2.41	0.41
6:F:54:ASP:OD2	12:X:30:TYR:HE2	1.98	0.41
2:B:529:ILE:HG21	13:B:837:CLA:CAB	2.51	0.41
2:B:691:THR:HA	2:B:692:PRO:HD3	1.90	0.41
13:B:816:CLA:H3A	13:B:816:CLA:HBA2	1.68	0.41
3:C:13:CYS:SG	3:C:15:GLN:HB2	2.60	0.41
4:D:50:ARG:NH1	4:D:50:ARG:HG3	2.35	0.41
13:L:1003:CLA:H152	13:L:1003:CLA:H111	1.99	0.41
13:A:820:CLA:HBA2	13:A:820:CLA:H3A	1.89	0.41
1:A:161:THR:HG22	16:A:850:BCR:HC32	2.02	0.41
2:B:442:HIS:CD2	2:B:456:ILE:HG13	2.56	0.41
13:B:805:CLA:H3A	13:B:805:CLA:HBA1	1.74	0.41
13:B:825:CLA:H3A	13:B:825:CLA:HBA2	1.69	0.41
6:F:73:ILE:O	6:F:77:ILE:HG13	2.21	0.41
6:F:24:THR:HG21	8:J:35:ASP:OD1	2.20	0.41
1:A:112:PRO:HA	1:A:144:PHE:CE1	2.55	0.41
1:A:260:PHE:O	1:A:261:PHE:HB2	2.21	0.41
13:A:802:CLA:H3A	13:A:802:CLA:O1A	2.21	0.41
13:A:822:CLA:HMD1	13:A:823:CLA:HBB1	2.02	0.41
2:B:30:PHE:CD1	2:B:45:ILE:HD13	2.56	0.41
4:D:104:LYS:HG2	4:D:104:LYS:H	1.51	0.41
13:B:803:CLA:H122	16:I:101:BCR:H281	2.03	0.41
10:L:44:ILE:HG23	10:L:45:LEU:N	2.36	0.41
1:A:80:LEU:HA	1:A:80:LEU:HD23	1.82	0.41
13:B:818:CLA:H3A	13:B:818:CLA:CGA	2.51	0.41
13:B:814:CLA:HMA2	16:B:845:BCR:H282	2.03	0.41
4:D:43:THR:O	4:D:44:ALA:CB	2.68	0.41
1:A:713:VAL:HG11	13:A:841:CLA:HMB3	2.03	0.41
13:A:843:CLA:H203	13:F:1301:CLA:CBB	2.52	0.41
2:B:440:TYR:CZ	2:B:524:LEU:HB3	2.56	0.41
6:F:80:VAL:HG21	6:F:110:MET:HA	2.03	0.41
13:A:843:CLA:H52	13:A:843:CLA:NC	2.36	0.40
13:A:803:CLA:C14	16:A:854:BCR:H402	2.51	0.40
2:B:193:LEU:HA	2:B:197:ALA:HB3	2.03	0.40
13:B:809:CLA:H203	7:I:26:VAL:CG2	2.51	0.40
13:B:810:CLA:O2A	13:B:810:CLA:H2A	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:19:GLU:OE1	5:E:42:LYS:NZ	2.52	0.40
20:A:944:HOH:O	10:L:16:HIS:HE1	2.04	0.40
13:A:835:CLA:HED2	10:L:65:LEU:O	2.21	0.40
1:A:114:ALA:O	1:A:115:GLN:O	2.39	0.40
1:A:118:TRP:HB3	16:J:104:BCR:C32	2.51	0.40
1:A:212:TRP:O	1:A:216:GLN:HG3	2.22	0.40
1:A:360:LEU:HA	1:A:360:LEU:HD12	1.93	0.40
2:B:313:LYS:O	2:B:314:VAL:CG1	2.68	0.40
2:B:459:GLU:HA	2:B:460:PRO:HD3	1.82	0.40
2:B:490:THR:O	2:B:495:TYR:HA	2.21	0.40
2:B:589:MET:HE1	2:B:590:LEU:N	2.36	0.40
2:B:629:TYR:O	2:B:633:ASN:HB2	2.21	0.40
10:L:44:ILE:HB	20:L:1123:HOH:O	2.20	0.40
13:A:825:CLA:HBB	13:A:846:CLA:HBB1	2.02	0.40
2:B:269:LEU:HD23	2:B:272:MET:HE3	2.02	0.40
2:B:564:PRO:O	2:B:565:CYS:HB3	2.22	0.40
2:B:33:HIS:HE1	13:B:804:CLA:HED1	1.85	0.40
13:B:817:CLA:O1D	13:B:818:CLA:HMA1	2.21	0.40
2:B:318:PHE:H	13:B:822:CLA:C2B	2.34	0.40
13:A:810:CLA:CBB	13:B:833:CLA:HMD2	2.51	0.40
8:J:30:ASN:O	8:J:34:PRO:HG3	2.21	0.40
16:L:1006:BCR:H361	16:L:1006:BCR:H20C	1.88	0.40
2:B:176:HIS:CG	13:B:813:CLA:HMC2	2.56	0.40
2:B:36:MET:HE3	2:B:40:ASN:CB	2.47	0.40
2:B:377:HIS:HE2	13:B:828:CLA:C1B	2.35	0.40
2:B:496:GLY:O	2:B:497:ASN:C	2.59	0.40
2:B:605:LEU:HA	2:B:605:LEU:HD12	1.80	0.40
2:B:279:ILE:HD11	13:B:817:CLA:HBC3	2.02	0.40
13:B:823:CLA:CBB	13:B:830:CLA:HMD2	2.51	0.40
20:C:210:HOH:O	4:D:138:PRO:HG3	2.21	0.40
1:A:120:ILE:HG12	1:A:121:VAL:N	2.36	0.40
1:A:741:ALA:CB	16:A:854:BCR:C32	2.99	0.40
2:B:53:LEU:HA	2:B:53:LEU:HD12	1.83	0.40
2:B:642:ASN:CB	2:B:643:PRO:CD	2.88	0.40
3:C:40:SER:HA	20:C:209:HOH:O	2.21	0.40
4:D:88:ASP:HB3	4:D:90:GLU:H	1.86	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:1126:HOH:O	20:L:1126:HOH:O[2_655]	1.08	1.12
10:L:153:PHE:O	19:L:1001:CA:CA[3_665]	1.57	0.63
5:E:28:GLN:OE1	6:F:1:ASP:N[4_664]	2.00	0.20
10:L:154:ASN:OXT	20:A:950:HOH:O[3_665]	2.07	0.13
20:L:1108:HOH:O	20:L:1117:HOH:O[2_655]	2.07	0.13

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	736/755 (98%)	695 (94%)	31 (4%)	10 (1%)	11	46
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	13	50
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	12	48
4	D	136/138 (99%)	125 (92%)	8 (6%)	3 (2%)	6	35
5	E	67/75 (89%)	59 (88%)	4 (6%)	4 (6%)	1	17
6	F	139/164 (85%)	128 (92%)	8 (6%)	3 (2%)	6	35
7	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	40/83 (48%)	32 (80%)	5 (12%)	3 (8%)	1	13
10	L	149/154 (97%)	140 (94%)	7 (5%)	2 (1%)	12	48
11	M	29/31 (94%)	28 (97%)	0	1 (3%)	3	26
12	X	27/35 (77%)	22 (82%)	4 (15%)	1 (4%)	3	24
All	All	2213/2334 (95%)	2065 (93%)	111 (5%)	37 (2%)	9	42

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	235	ASP
1	A	260	PHE

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Mol	Chain	Res	Type
1	A	261	PHE
2	B	234	GLN
2	B	313	LYS
2	B	314	VAL
2	B	480	LEU
2	B	492	TRP
2	B	497	ASN
2	B	510	GLY
3	C	62	LEU
4	D	2	THR
6	F	91	SER
9	K	41	PRO
9	K	42	GLY
11	M	30	TYR
12	X	10	ALA
1	A	121	VAL
1	A	578	CYS
2	B	565	CYS
4	D	3	LEU
6	F	60	ALA
6	F	89	ARG
10	L	106	SER
1	A	234	LYS
4	D	44	ALA
5	E	53	SER
10	L	104	GLY
1	A	42	PRO
1	A	232	ALA
2	B	481	LEU
5	E	25	SER
5	E	54	GLY
1	A	276	SER
5	E	55	VAL
9	K	56	LEU

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 X-ray entries followed by that with respect to entries of similar resolution.

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	589/603 (98%)	565 (96%)	24 (4%)	30	55
2	B	595/597 (100%)	567 (95%)	28 (5%)	26	51
3	C	67/67 (100%)	66 (98%)	1 (2%)	65	80
4	D	115/115 (100%)	107 (93%)	8 (7%)	15	40
5	E	59/64 (92%)	59 (100%)	0	100	100
6	F	109/128 (85%)	107 (98%)	2 (2%)	59	77
7	I	32/32 (100%)	30 (94%)	2 (6%)	18	43
8	J	36/36 (100%)	34 (94%)	2 (6%)	21	46
10	L	117/119 (98%)	109 (93%)	8 (7%)	16	41
11	M	26/26 (100%)	25 (96%)	1 (4%)	33	57
12	X	20/27 (74%)	18 (90%)	2 (10%)	7	26
All	All	1765/1814 (97%)	1687 (96%)	78 (4%)	28	53

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

Mol	Chain	Res	Type
1	A	145	GLN
1	A	147	TRP
1	A	155	GLU
1	A	172	MET
1	A	186	LYS
1	A	210	LEU
1	A	221	LEU
1	A	235	ASP
1	A	252	LEU
1	A	253	TYR
1	A	257	ASP
1	A	260	PHE
1	A	281	PHE
1	A	349	THR
1	A	360	LEU
1	A	372	GLN
1	A	395	THR
1	A	433	VAL
1	A	466	ARG
1	A	538	VAL
1	A	587	CYS
1	A	632	SER
1	A	675	LEU

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Mol	Chain	Res	Type
1	A	713	VAL
2	B	53	LEU
2	B	142	LEU
2	B	159	LYS
2	B	171	GLU
2	B	211	PHE
2	B	214	THR
2	B	256	PHE
2	B	279	ILE
2	B	318	PHE
2	B	349	SER
2	B	370	THR
2	B	411	LEU
2	B	430	LEU
2	B	446	VAL
2	B	479	THR
2	B	525	VAL
2	B	574	CYS
2	B	582	PHE
2	B	589	MET
2	B	596	VAL
2	B	605	LEU
2	B	632	LEU
2	B	635	SER
2	B	647	ASN
2	B	648	ASN
2	B	651	VAL
2	B	697	VAL
2	B	698	ARG
3	C	61	PHE
4	D	1	THR
4	D	73	ARG
4	D	93	LEU
4	D	104	LYS
4	D	105	VAL
4	D	117	ARG
4	D	125	PRO
4	D	126	SER
6	F	56	ARG
6	F	105	LEU
7	I	10	LEU
7	I	26	VAL

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Mol	Chain	Res	Type
8	J	1	MET
8	J	19	MET
10	L	4	LEU
10	L	34	LEU
10	L	42	SER
10	L	44	ILE
10	L	48	LEU
10	L	69	ARG
10	L	85	LEU
10	L	134	VAL
11	M	17	LEU
12	X	8	THR
12	X	23	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	50	ASN
1	A	145	GLN
1	A	353	HIS
1	A	359	ASN
1	A	372	GLN
1	A	390	GLN
1	A	426	GLN
1	A	445	ASN
1	A	542	HIS
1	A	633	HIS
1	A	647	ASN
1	A	718	GLN
2	B	33	HIS
2	B	136	GLN
2	B	261	HIS
2	B	263	GLN
2	B	336	GLN
2	B	340	HIS
2	B	406	ASN
2	B	494	ASN
2	B	611	ASN
2	B	614	GLN
2	B	616	ASN
2	B	639	ASN

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Mol	Chain	Res	Type
2	B	647	ASN
2	B	648	ASN
2	B	678	GLN
2	B	688	HIS
3	C	37	GLN
4	D	54	ASN
4	D	71	GLN
4	D	95	HIS
5	E	18	ASN
6	F	40	GLN
6	F	95	ASN
10	L	16	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 128 ligands modelled in this entry, 1 is monoatomic - leaving 127 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	$\# Z > 2$
13	CLA	L	1004	20	59,73,73	1.42	6 (10%)	67,113,113	1.81	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	A	854	-	41,41,41	1.38	6 (14%)	56,56,56	2.03	19 (33%)
13	CLA	A	829	-	59,73,73	1.25	6 (10%)	67,113,113	1.75	10 (14%)
13	CLA	A	820	-	59,73,73	1.35	10 (16%)	67,113,113	2.02	14 (20%)
13	CLA	A	818	-	48,62,73	1.58	8 (16%)	53,99,113	1.95	8 (15%)
13	CLA	A	804	-	59,73,73	1.27	5 (8%)	67,113,113	1.86	9 (13%)
13	CLA	A	843	-	59,73,73	1.34	9 (15%)	67,113,113	1.91	13 (19%)
13	CLA	B	806	-	59,73,73	1.24	5 (8%)	67,113,113	1.74	10 (14%)
13	CLA	B	811	-	36,53,73	1.59	7 (19%)	39,89,113	2.22	7 (17%)
16	BCR	B	848	-	41,41,41	1.24	5 (12%)	56,56,56	1.99	20 (35%)
13	CLA	J	101	8	36,53,73	1.67	6 (16%)	39,89,113	2.44	9 (23%)
13	CLA	B	836	20	36,53,73	1.54	4 (11%)	39,89,113	2.32	7 (17%)
13	CLA	B	804	-	48,62,73	1.46	7 (14%)	53,99,113	2.14	10 (18%)
13	CLA	A	845	-	32,49,73	1.71	6 (18%)	32,83,113	2.37	6 (18%)
13	CLA	B	825	20	40,54,73	1.38	6 (15%)	44,90,113	2.36	13 (29%)
13	CLA	F	1301	20	36,53,73	1.71	5 (13%)	39,89,113	2.32	7 (17%)
13	CLA	B	838	-	59,73,73	1.29	6 (10%)	67,113,113	1.93	12 (17%)
13	CLA	M	1601	20	36,53,73	1.60	6 (16%)	39,89,113	2.46	7 (17%)
13	CLA	A	839	-	59,73,73	1.36	7 (11%)	67,113,113	1.74	8 (11%)
13	CLA	A	815	-	36,53,73	1.69	6 (16%)	39,89,113	2.26	8 (20%)
13	CLA	B	826	-	59,73,73	1.41	6 (10%)	67,113,113	1.93	12 (17%)
13	CLA	B	823	-	36,53,73	1.62	5 (13%)	39,89,113	2.24	7 (17%)
17	LHG	B	851	-	22,22,48	2.80	5 (22%)	25,28,54	1.13	1 (4%)
13	CLA	A	836	-	48,62,73	1.38	9 (18%)	53,99,113	2.15	11 (20%)
13	CLA	B	839	-	41,55,73	1.55	6 (14%)	45,91,113	2.01	9 (20%)
16	BCR	I	101	-	41,41,41	1.31	7 (17%)	56,56,56	1.79	15 (26%)
13	CLA	A	835	-	59,73,73	1.31	7 (11%)	67,113,113	1.81	10 (14%)
13	CLA	A	830	-	59,73,73	1.39	5 (8%)	67,113,113	1.88	10 (14%)
13	CLA	B	835	20	36,53,73	1.76	7 (19%)	39,89,113	2.24	8 (20%)
13	CLA	A	823	-	43,57,73	1.46	5 (11%)	46,93,113	2.31	13 (28%)
13	CLA	B	829	-	59,73,73	1.37	7 (11%)	67,113,113	1.91	12 (17%)
13	CLA	A	801	-	59,73,73	1.38	5 (8%)	67,113,113	2.40	15 (22%)
13	CLA	B	801	-	59,73,73	1.39	6 (10%)	67,113,113	1.86	12 (17%)
13	CLA	A	826	20	59,73,73	1.41	6 (10%)	67,113,113	1.81	11 (16%)
16	BCR	L	1005	-	41,41,41	1.42	8 (19%)	56,56,56	1.81	15 (26%)
13	CLA	A	825	-	53,67,73	1.32	5 (9%)	59,105,113	1.93	12 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	A	853	-	41,41,41	1.28	8 (19%)	56,56,56	1.90	18 (32%)
13	CLA	A	846	17	46,60,73	1.62	9 (19%)	51,97,113	2.33	12 (23%)
13	CLA	B	822	20	49,63,73	1.46	7 (14%)	55,101,113	2.11	10 (18%)
13	CLA	A	806	-	59,73,73	1.18	4 (6%)	67,113,113	1.92	15 (22%)
13	CLA	B	813	-	59,73,73	1.43	5 (8%)	67,113,113	1.78	11 (16%)
13	CLA	A	811	-	36,53,73	1.65	7 (19%)	39,89,113	2.17	7 (17%)
13	CLA	B	831	-	43,57,73	1.49	6 (13%)	46,93,113	2.17	7 (15%)
16	BCR	M	1602	-	41,41,41	1.33	6 (14%)	56,56,56	1.78	14 (25%)
13	CLA	J	102	-	31,45,73	1.78	4 (12%)	31,78,113	2.56	8 (25%)
13	CLA	B	820	-	41,55,73	1.47	5 (12%)	45,91,113	2.45	12 (26%)
16	BCR	L	1006	-	41,41,41	1.60	8 (19%)	56,56,56	1.72	12 (21%)
13	CLA	B	810	2	59,73,73	1.40	6 (10%)	67,113,113	1.86	13 (19%)
13	CLA	A	816	-	36,53,73	1.53	5 (13%)	39,89,113	2.49	11 (28%)
13	CLA	A	819	-	48,62,73	1.55	8 (16%)	53,99,113	2.08	12 (22%)
13	CLA	A	813	-	48,62,73	1.44	8 (16%)	53,99,113	2.19	10 (18%)
13	CLA	B	833	-	52,66,73	1.42	7 (13%)	58,104,113	2.07	10 (17%)
13	CLA	A	833	-	59,73,73	1.13	4 (6%)	67,113,113	2.05	12 (17%)
13	CLA	B	817	-	53,67,73	1.40	7 (13%)	59,105,113	2.01	14 (23%)
16	BCR	A	849	-	41,41,41	1.36	5 (12%)	56,56,56	1.88	16 (28%)
15	SF4	C	102	3	0,12,12	0.00	-	-	-	-
13	CLA	A	832	-	44,58,73	1.46	5 (11%)	49,95,113	2.27	12 (24%)
13	CLA	B	814	-	59,73,73	1.33	7 (11%)	67,113,113	1.92	12 (17%)
13	CLA	B	830	-	36,53,73	1.55	6 (16%)	39,89,113	2.37	8 (20%)
13	CLA	A	821	-	55,69,73	1.38	7 (12%)	62,108,113	2.10	11 (17%)
13	CLA	B	803	-	59,73,73	1.47	7 (11%)	67,113,113	1.79	9 (13%)
13	CLA	B	805	-	59,73,73	1.30	5 (8%)	67,113,113	1.82	10 (14%)
16	BCR	B	846	-	25,25,41	1.36	4 (16%)	33,33,56	1.85	11 (33%)
13	CLA	B	828	-	59,73,73	1.52	11 (18%)	67,113,113	1.78	12 (17%)
13	CLA	B	827	-	59,73,73	1.57	8 (13%)	67,113,113	1.96	14 (20%)
14	PQN	B	842	-	34,34,34	3.47	16 (47%)	42,45,45	2.10	4 (9%)
16	BCR	B	847	-	41,41,41	1.24	5 (12%)	56,56,56	1.88	19 (33%)
13	CLA	A	803	-	59,73,73	1.28	6 (10%)	67,113,113	1.87	15 (22%)
15	SF4	A	848	1,2	0,12,12	0.00	-	-	-	-
13	CLA	B	808	-	59,73,73	1.33	7 (11%)	67,113,113	1.82	13 (19%)
13	CLA	L	1002	10	59,73,73	1.54	8 (13%)	67,113,113	1.88	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	807	-	59,73,73	1.17	7 (11%)	67,113,113	1.96	12 (17%)
16	BCR	A	851	-	41,41,41	1.41	6 (14%)	56,56,56	1.94	17 (30%)
13	CLA	A	814	-	54,68,73	1.29	5 (9%)	61,107,113	2.02	12 (19%)
13	CLA	A	837	1	36,53,73	1.55	5 (13%)	39,89,113	2.37	8 (20%)
13	CLA	B	824	2	48,62,73	1.74	9 (18%)	53,99,113	2.10	10 (18%)
13	CLA	A	840	-	41,55,73	1.69	8 (19%)	45,91,113	2.10	8 (17%)
13	CLA	B	840	20	59,73,73	1.32	7 (11%)	67,113,113	1.75	11 (16%)
13	CLA	A	844	20	59,73,73	1.30	9 (15%)	67,113,113	1.78	11 (16%)
13	CLA	A	812	13	59,73,73	1.27	7 (11%)	67,113,113	1.89	10 (14%)
13	CLA	B	812	-	36,53,73	1.53	4 (11%)	39,89,113	2.41	8 (20%)
13	CLA	B	818	-	54,68,73	1.36	7 (12%)	61,107,113	2.12	10 (16%)
16	BCR	B	843	-	41,41,41	1.51	5 (12%)	56,56,56	2.02	16 (28%)
13	CLA	A	838	-	45,59,73	1.40	5 (11%)	50,96,113	2.22	12 (24%)
16	BCR	A	850	-	41,41,41	1.27	4 (9%)	56,56,56	1.77	17 (30%)
16	BCR	J	105	-	41,41,41	1.41	5 (12%)	56,56,56	1.88	13 (23%)
13	CLA	A	824	-	45,59,73	1.54	8 (17%)	50,96,113	2.12	10 (20%)
16	BCR	B	849	-	41,41,41	1.28	4 (9%)	56,56,56	1.74	17 (30%)
13	CLA	B	802	20	59,73,73	1.41	4 (6%)	67,113,113	1.89	14 (20%)
13	CLA	L	1003	-	59,73,73	1.39	6 (10%)	67,113,113	1.85	10 (14%)
13	CLA	A	807	-	59,73,73	1.32	6 (10%)	67,113,113	2.05	17 (25%)
13	CLA	A	808	-	45,59,73	1.60	7 (15%)	50,96,113	2.13	9 (18%)
13	CLA	A	831	-	59,73,73	1.55	9 (15%)	67,113,113	1.79	10 (14%)
13	CLA	B	837	-	54,68,73	1.46	7 (12%)	61,107,113	1.89	10 (16%)
18	LMG	B	850	-	55,55,55	0.87	2 (3%)	63,63,63	1.30	3 (4%)
13	CLA	B	816	-	49,63,73	1.57	9 (18%)	55,101,113	2.00	10 (18%)
16	BCR	B	845	-	41,41,41	1.26	5 (12%)	56,56,56	2.01	20 (35%)
13	CLA	A	822	20	59,73,73	1.25	6 (10%)	67,113,113	1.99	13 (19%)
13	CLA	B	841	-	59,73,73	1.08	7 (11%)	67,113,113	1.87	10 (14%)
13	CLA	B	821	-	36,53,73	1.63	6 (16%)	39,89,113	2.47	10 (25%)
16	BCR	I	102	-	41,41,41	1.28	6 (14%)	56,56,56	1.82	17 (30%)
13	CLA	A	805	13	53,67,73	1.34	5 (9%)	59,105,113	2.02	13 (22%)
13	CLA	A	841	-	59,73,73	1.34	5 (8%)	67,113,113	1.85	10 (14%)
16	BCR	A	852	-	41,41,41	1.37	6 (14%)	56,56,56	1.78	14 (25%)
13	CLA	B	819	20	59,73,73	1.33	6 (10%)	67,113,113	1.86	10 (14%)
14	PQN	A	847	-	34,34,34	3.54	17 (50%)	42,45,45	2.21	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	810	1	59,73,73	1.29	5 (8%)	67,113,113	1.94	11 (16%)
13	CLA	B	832	-	59,73,73	1.33	6 (10%)	67,113,113	1.88	8 (11%)
13	CLA	K	1401	-	36,53,73	1.65	6 (16%)	39,89,113	2.18	6 (15%)
13	CLA	A	802	20	59,73,73	1.33	6 (10%)	67,113,113	1.82	10 (14%)
13	CLA	B	809	2	59,73,73	1.32	4 (6%)	67,113,113	1.84	11 (16%)
13	CLA	A	828	-	59,73,73	1.37	6 (10%)	67,113,113	1.88	10 (14%)
16	BCR	F	1302	-	41,41,41	1.28	4 (9%)	56,56,56	1.81	17 (30%)
13	CLA	A	817	20	43,57,73	1.46	7 (16%)	46,93,113	2.25	10 (21%)
13	CLA	B	815	-	36,53,73	1.64	6 (16%)	39,89,113	2.24	8 (20%)
13	CLA	B	834	-	36,53,73	1.58	6 (16%)	39,89,113	2.32	10 (25%)
16	BCR	J	103	-	41,41,41	1.29	5 (12%)	56,56,56	1.90	16 (28%)
13	CLA	A	809	1	59,73,73	1.33	6 (10%)	67,113,113	1.91	9 (13%)
16	BCR	B	844	-	41,41,41	1.56	7 (17%)	56,56,56	2.10	19 (33%)
16	BCR	J	104	-	41,41,41	1.27	4 (9%)	56,56,56	1.83	19 (33%)
13	CLA	A	842	20	45,59,73	1.49	7 (15%)	50,96,113	2.06	10 (20%)
13	CLA	A	834	-	59,73,73	1.18	4 (6%)	67,113,113	1.77	11 (16%)
17	LHG	A	856	13	26,26,48	2.32	5 (19%)	29,32,54	1.58	5 (17%)
17	LHG	A	855	-	48,48,48	1.76	5 (10%)	51,54,54	1.30	3 (5%)
13	CLA	A	827	20	59,73,73	1.17	6 (10%)	67,113,113	1.85	9 (13%)
13	CLA	X	1701	12	36,53,73	1.66	5 (13%)	39,89,113	2.41	8 (20%)
15	SF4	C	101	3	0,12,12	0.00	-	-		

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
13	CLA	L	1004	20	3/3/20/25	8/37/135/135	-
16	BCR	A	854	-	-	8/29/63/63	0/2/2/2
13	CLA	A	829	-	1/1/20/25	8/37/135/135	-
13	CLA	A	820	-	3/3/20/25	14/37/135/135	-
13	CLA	A	818	-	1/1/17/25	1/24/122/135	-
13	CLA	A	804	-	3/3/20/25	6/37/135/135	-
13	CLA	A	843	-	3/3/20/25	8/37/135/135	-
13	CLA	B	806	-	3/3/20/25	15/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	811	-	2/2/16/25	3/11/111/135	-
16	BCR	B	848	-	-	1/29/63/63	0/2/2/2
13	CLA	J	101	8	3/3/16/25	9/11/111/135	-
13	CLA	B	836	20	3/3/16/25	2/11/111/135	-
13	CLA	B	804	-	2/2/17/25	4/24/122/135	-
13	CLA	A	845	-	3/3/14/25	3/5/101/135	-
13	CLA	B	825	20	3/3/16/25	6/15/113/135	-
13	CLA	F	1301	20	3/3/16/25	2/11/111/135	-
13	CLA	B	838	-	3/3/20/25	0/37/135/135	-
13	CLA	M	1601	20	3/3/16/25	7/11/111/135	-
13	CLA	A	839	-	2/2/20/25	8/37/135/135	-
13	CLA	A	815	-	3/3/16/25	1/11/111/135	-
13	CLA	B	826	-	3/3/20/25	12/37/135/135	-
13	CLA	B	823	-	3/3/16/25	1/11/111/135	-
17	LHG	B	851	-	-	7/26/26/53	-
13	CLA	A	836	-	3/3/17/25	6/24/122/135	-
13	CLA	B	839	-	-	4/16/114/135	-
16	BCR	I	101	-	-	0/29/63/63	0/2/2/2
13	CLA	A	835	-	3/3/20/25	8/37/135/135	-
13	CLA	A	830	-	2/2/20/25	9/37/135/135	-
13	CLA	B	835	20	3/3/16/25	0/11/111/135	-
13	CLA	A	823	-	3/3/16/25	10/18/116/135	-
13	CLA	B	829	-	3/3/20/25	9/37/135/135	-
13	CLA	A	801	-	3/3/20/25	2/37/135/135	-
13	CLA	B	801	-	1/1/20/25	10/37/135/135	-
13	CLA	A	826	20	3/3/20/25	11/37/135/135	-
16	BCR	L	1005	-	-	1/29/63/63	0/2/2/2
13	CLA	A	825	-	3/3/18/25	12/30/128/135	-
16	BCR	A	853	-	-	2/29/63/63	0/2/2/2
13	CLA	A	846	17	3/3/17/25	15/22/120/135	-
13	CLA	B	822	20	3/3/18/25	8/25/123/135	-
13	CLA	A	806	-	3/3/20/25	16/37/135/135	-
13	CLA	B	813	-	3/3/20/25	13/37/135/135	-
13	CLA	A	811	-	-	7/11/111/135	-
13	CLA	B	831	-	3/3/16/25	9/18/116/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	M	1602	-	-	4/29/63/63	0/2/2/2
13	CLA	J	102	-	3/3/13/25	0/2/96/135	-
13	CLA	B	820	-	3/3/16/25	6/16/114/135	-
16	BCR	L	1006	-	-	1/29/63/63	0/2/2/2
13	CLA	B	810	2	3/3/20/25	7/37/135/135	-
13	CLA	A	816	-	3/3/16/25	3/11/111/135	-
13	CLA	A	819	-	3/3/17/25	9/24/122/135	-
13	CLA	A	813	-	3/3/17/25	8/24/122/135	-
13	CLA	B	833	-	3/3/18/25	6/29/127/135	-
13	CLA	A	833	-	3/3/20/25	7/37/135/135	-
13	CLA	B	817	-	3/3/18/25	7/30/128/135	-
16	BCR	A	849	-	-	0/29/63/63	0/2/2/2
15	SF4	C	102	3	-	-	0/6/5/5
13	CLA	A	832	-	3/3/17/25	3/19/117/135	-
13	CLA	B	814	-	3/3/20/25	11/37/135/135	-
13	CLA	B	830	-	3/3/16/25	6/11/111/135	-
13	CLA	A	821	-	3/3/19/25	14/33/131/135	-
13	CLA	B	803	-	1/1/20/25	2/37/135/135	-
13	CLA	B	805	-	3/3/20/25	13/37/135/135	-
16	BCR	B	846	-	-	6/18/35/63	0/1/1/2
13	CLA	B	828	-	1/1/20/25	10/37/135/135	-
13	CLA	B	827	-	1/1/20/25	14/37/135/135	-
14	PQN	B	842	-	-	4/23/43/43	0/2/2/2
16	BCR	B	847	-	-	2/29/63/63	0/2/2/2
13	CLA	A	803	-	2/2/20/25	10/37/135/135	-
15	SF4	A	848	1,2	-	-	0/6/5/5
13	CLA	B	808	-	2/2/20/25	9/37/135/135	-
13	CLA	L	1002	10	3/3/20/25	11/37/135/135	-
13	CLA	B	807	-	3/3/20/25	2/37/135/135	-
16	BCR	A	851	-	-	0/29/63/63	0/2/2/2
13	CLA	A	814	-	3/3/19/25	11/31/129/135	-
13	CLA	A	837	1	3/3/16/25	5/11/111/135	-
13	CLA	B	824	2	3/3/17/25	7/24/122/135	-
13	CLA	A	840	-	1/1/16/25	5/16/114/135	-
13	CLA	B	840	20	2/2/20/25	2/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	844	20	3/3/20/25	10/37/135/135	-
13	CLA	A	812	13	3/3/20/25	12/37/135/135	-
13	CLA	B	812	-	3/3/16/25	1/11/111/135	-
13	CLA	B	818	-	3/3/19/25	10/31/129/135	-
16	BCR	B	843	-	-	0/29/63/63	0/2/2/2
13	CLA	A	838	-	3/3/17/25	6/21/119/135	-
16	BCR	A	850	-	-	4/29/63/63	0/2/2/2
16	BCR	J	105	-	-	2/29/63/63	0/2/2/2
13	CLA	A	824	-	2/2/17/25	10/21/119/135	-
16	BCR	B	849	-	-	2/29/63/63	0/2/2/2
13	CLA	B	802	20	2/2/20/25	7/37/135/135	-
13	CLA	L	1003	-	2/2/20/25	7/37/135/135	-
13	CLA	A	807	-	3/3/20/25	14/37/135/135	-
13	CLA	A	808	-	2/2/17/25	6/21/119/135	-
13	CLA	A	831	-	3/3/20/25	6/37/135/135	-
13	CLA	B	837	-	3/3/19/25	9/31/129/135	-
18	LMG	B	850	-	-	8/50/70/70	0/1/1/1
13	CLA	B	816	-	3/3/18/25	8/25/123/135	-
16	BCR	B	845	-	-	6/29/63/63	0/2/2/2
13	CLA	A	822	20	3/3/20/25	6/37/135/135	-
13	CLA	B	841	-	2/2/20/25	8/37/135/135	-
13	CLA	B	821	-	3/3/16/25	3/11/111/135	-
16	BCR	I	102	-	-	4/29/63/63	0/2/2/2
13	CLA	A	805	13	3/3/18/25	12/30/128/135	-
13	CLA	A	841	-	3/3/20/25	7/37/135/135	-
16	BCR	A	852	-	-	2/29/63/63	0/2/2/2
13	CLA	B	819	20	3/3/20/25	4/37/135/135	-
14	PQN	A	847	-	-	6/23/43/43	0/2/2/2
13	CLA	A	810	1	3/3/20/25	13/37/135/135	-
13	CLA	B	832	-	3/3/20/25	16/37/135/135	-
13	CLA	K	1401	-	2/2/16/25	4/11/111/135	-
13	CLA	A	802	20	2/2/20/25	4/37/135/135	-
13	CLA	B	809	2	1/1/20/25	14/37/135/135	-
13	CLA	A	828	-	3/3/20/25	7/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	F	1302	-	-	5/29/63/63	0/2/2/2
13	CLA	A	817	20	3/3/16/25	9/18/116/135	-
13	CLA	B	815	-	2/2/16/25	6/11/111/135	-
13	CLA	B	834	-	3/3/16/25	4/11/111/135	-
16	BCR	J	103	-	-	3/29/63/63	0/2/2/2
13	CLA	A	809	1	3/3/20/25	16/37/135/135	-
16	BCR	B	844	-	-	6/29/63/63	0/2/2/2
16	BCR	J	104	-	-	4/29/63/63	0/2/2/2
13	CLA	A	842	20	3/3/17/25	8/21/119/135	-
13	CLA	A	834	-	-	5/37/135/135	-
17	LHG	A	856	13	1/1/5/5	10/31/31/53	-
17	LHG	A	855	-	-	18/53/53/53	-
13	CLA	A	827	20	3/3/20/25	12/37/135/135	-
13	CLA	X	1701	12	3/3/16/25	3/11/111/135	-
15	SF4	C	101	3	-	-	0/6/5/5

All (780) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	847	PQN	O4-C4	9.27	1.42	1.23
14	B	842	PQN	O4-C4	8.96	1.42	1.23
14	A	847	PQN	O1-C1	8.94	1.42	1.23
17	B	851	LHG	P-O5	8.61	1.81	1.50
14	B	842	PQN	O1-C1	8.43	1.41	1.23
14	A	847	PQN	C12-C13	8.31	1.52	1.33
14	B	842	PQN	C12-C13	8.28	1.52	1.33
17	A	855	LHG	P-O5	8.22	1.80	1.50
17	A	856	LHG	P-O5	7.65	1.78	1.50
14	A	847	PQN	C2M-C2	-6.79	1.36	1.50
13	L	1002	CLA	MG-NA	6.69	2.22	2.06
13	B	824	CLA	MG-NA	6.64	2.22	2.06
13	A	826	CLA	MG-NA	6.60	2.21	2.06
13	A	840	CLA	MG-NA	6.52	2.21	2.06
14	B	842	PQN	C2M-C2	-6.47	1.37	1.50
13	B	810	CLA	MG-NA	6.47	2.21	2.06
13	B	813	CLA	MG-NA	6.46	2.21	2.06
14	B	842	PQN	C3-C2	6.36	1.46	1.35
14	A	847	PQN	C3-C2	6.34	1.46	1.35
13	B	828	CLA	MG-NA	6.33	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	818	CLA	MG-NA	6.25	2.21	2.06
13	A	831	CLA	MG-NA	6.25	2.21	2.06
13	A	824	CLA	MG-NA	6.24	2.21	2.06
13	A	845	CLA	MG-NA	6.24	2.21	2.06
13	B	840	CLA	MG-NA	6.21	2.21	2.06
13	A	815	CLA	MG-NA	6.21	2.21	2.06
13	B	835	CLA	MG-NA	6.20	2.21	2.06
13	B	837	CLA	MG-NA	6.17	2.20	2.06
13	A	811	CLA	MG-NA	6.17	2.20	2.06
13	B	823	CLA	MG-NA	6.17	2.20	2.06
13	B	816	CLA	MG-NA	6.16	2.20	2.06
13	J	102	CLA	MG-NA	6.10	2.20	2.06
13	A	808	CLA	MG-NA	6.08	2.20	2.06
13	B	829	CLA	MG-NA	6.04	2.20	2.06
13	J	101	CLA	MG-NA	6.00	2.20	2.06
13	A	830	CLA	MG-NA	5.99	2.20	2.06
13	A	819	CLA	MG-NA	5.99	2.20	2.06
13	A	838	CLA	MG-NA	5.95	2.20	2.06
13	B	802	CLA	MG-NA	5.91	2.20	2.06
13	X	1701	CLA	MG-NA	5.90	2.20	2.06
13	A	842	CLA	MG-NA	5.89	2.20	2.06
17	B	851	LHG	P-O6	5.88	1.83	1.59
13	A	834	CLA	MG-NA	5.87	2.20	2.06
13	A	829	CLA	MG-NA	5.86	2.20	2.06
13	B	839	CLA	MG-NA	5.84	2.20	2.06
13	B	827	CLA	MG-NA	5.81	2.20	2.06
13	B	826	CLA	MG-NA	5.81	2.20	2.06
13	B	809	CLA	MG-NA	5.80	2.20	2.06
13	B	836	CLA	MG-NA	5.80	2.20	2.06
13	A	816	CLA	MG-NA	5.80	2.20	2.06
13	B	821	CLA	MG-NA	5.78	2.20	2.06
13	B	815	CLA	MG-NA	5.78	2.20	2.06
13	A	805	CLA	MG-NA	5.76	2.20	2.06
13	A	807	CLA	MG-NA	5.76	2.19	2.06
13	L	1004	CLA	MG-NA	5.73	2.19	2.06
13	A	820	CLA	MG-NA	5.72	2.19	2.06
13	B	805	CLA	MG-NA	5.72	2.19	2.06
13	K	1401	CLA	MG-NA	5.71	2.19	2.06
13	A	839	CLA	MG-NA	5.71	2.19	2.06
13	A	817	CLA	MG-NA	5.70	2.19	2.06
13	B	820	CLA	MG-NA	5.69	2.19	2.06
13	B	806	CLA	MG-NA	5.69	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	819	CLA	MG-NA	5.68	2.19	2.06
13	B	811	CLA	MG-NA	5.68	2.19	2.06
13	A	846	CLA	MG-NA	5.66	2.19	2.06
13	A	823	CLA	MG-NA	5.66	2.19	2.06
13	F	1301	CLA	MG-NA	5.66	2.19	2.06
13	A	837	CLA	MG-NA	5.61	2.19	2.06
13	A	804	CLA	MG-NA	5.58	2.19	2.06
13	M	1601	CLA	MG-NA	5.54	2.19	2.06
13	B	812	CLA	MG-NA	5.54	2.19	2.06
13	A	831	CLA	C4B-NB	5.54	1.40	1.35
13	B	830	CLA	MG-NA	5.53	2.19	2.06
13	B	814	CLA	MG-NA	5.49	2.19	2.06
13	A	821	CLA	MG-NA	5.49	2.19	2.06
13	B	818	CLA	MG-NA	5.43	2.19	2.06
13	A	801	CLA	MG-NA	5.42	2.19	2.06
13	A	810	CLA	MG-NA	5.37	2.19	2.06
13	A	828	CLA	MG-NA	5.37	2.19	2.06
13	B	822	CLA	MG-NA	5.36	2.19	2.06
13	B	801	CLA	MG-NA	5.33	2.18	2.06
13	A	841	CLA	C4B-NB	5.33	1.40	1.35
13	B	804	CLA	MG-NA	5.31	2.18	2.06
17	B	851	LHG	P-O3	5.29	1.80	1.59
13	B	833	CLA	MG-NA	5.28	2.18	2.06
13	A	812	CLA	MG-NA	5.28	2.18	2.06
13	L	1003	CLA	MG-NA	5.25	2.18	2.06
17	A	855	LHG	P-O3	5.22	1.80	1.59
13	B	825	CLA	MG-NA	5.21	2.18	2.06
13	A	825	CLA	MG-NA	5.16	2.18	2.06
13	A	836	CLA	MG-NA	5.16	2.18	2.06
13	A	813	CLA	MG-NA	5.14	2.18	2.06
13	L	1002	CLA	C4B-NB	5.14	1.39	1.35
13	B	809	CLA	C4B-NB	5.13	1.39	1.35
13	A	830	CLA	C4B-NB	5.13	1.39	1.35
13	B	827	CLA	C4B-NB	5.11	1.39	1.35
13	A	814	CLA	MG-NA	5.08	2.18	2.06
13	A	822	CLA	MG-NA	5.08	2.18	2.06
13	B	824	CLA	C4B-NB	5.07	1.39	1.35
13	A	802	CLA	MG-NA	5.06	2.18	2.06
13	B	803	CLA	MG-NA	5.06	2.18	2.06
13	F	1301	CLA	C4B-NB	5.04	1.39	1.35
13	A	801	CLA	C4B-NB	5.03	1.39	1.35
13	A	803	CLA	MG-NA	5.01	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	832	CLA	MG-NA	4.99	2.18	2.06
13	A	809	CLA	MG-NA	4.97	2.18	2.06
13	B	817	CLA	MG-NA	4.97	2.18	2.06
13	B	831	CLA	MG-NA	4.94	2.18	2.06
13	B	808	CLA	MG-NA	4.94	2.18	2.06
17	A	856	LHG	P-O6	4.93	1.79	1.59
13	A	841	CLA	MG-NA	4.88	2.17	2.06
16	L	1006	BCR	C1-C6	4.87	1.60	1.53
13	A	832	CLA	MG-NA	4.81	2.17	2.06
13	B	838	CLA	MG-NA	4.77	2.17	2.06
16	B	844	BCR	C1-C6	4.75	1.60	1.53
16	L	1005	BCR	C30-C25	4.74	1.60	1.53
13	A	835	CLA	MG-NA	4.70	2.17	2.06
14	B	842	PQN	C16-C15	-4.68	1.35	1.52
16	B	843	BCR	C30-C25	4.67	1.60	1.53
13	A	827	CLA	MG-NA	4.64	2.17	2.06
13	B	834	CLA	MG-NA	4.63	2.17	2.06
13	A	843	CLA	MG-NA	4.63	2.17	2.06
13	B	803	CLA	C4B-NB	4.60	1.39	1.35
13	B	802	CLA	C4B-NB	4.57	1.39	1.35
13	X	1701	CLA	C4B-NB	4.56	1.39	1.35
14	A	847	PQN	C16-C15	-4.54	1.35	1.52
16	L	1006	BCR	C30-C25	4.52	1.60	1.53
17	A	856	LHG	P-O3	4.49	1.77	1.59
13	B	813	CLA	C4B-NB	4.46	1.39	1.35
13	A	833	CLA	MG-NA	4.46	2.16	2.06
13	B	826	CLA	C4B-NB	4.44	1.39	1.35
13	J	102	CLA	C4B-NB	4.42	1.39	1.35
13	A	828	CLA	C4B-NB	4.41	1.39	1.35
16	A	852	BCR	C30-C25	4.39	1.59	1.53
13	A	806	CLA	MG-NA	4.39	2.16	2.06
13	B	835	CLA	C4B-NB	4.38	1.39	1.35
13	B	832	CLA	C4B-NB	4.34	1.39	1.35
13	A	802	CLA	C4B-NB	4.33	1.39	1.35
13	A	844	CLA	MG-NA	4.32	2.16	2.06
13	B	841	CLA	MG-NA	4.31	2.16	2.06
13	A	810	CLA	C4B-NB	4.30	1.39	1.35
13	A	818	CLA	C4B-NB	4.28	1.39	1.35
13	A	846	CLA	C4B-NB	4.23	1.39	1.35
13	B	834	CLA	C4B-NB	4.22	1.39	1.35
13	B	831	CLA	C4B-NB	4.19	1.38	1.35
13	B	821	CLA	C4B-NB	4.18	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	801	CLA	C4B-NB	4.15	1.38	1.35
17	A	855	LHG	P-O6	4.10	1.75	1.59
13	B	838	CLA	CHC-C1C	4.07	1.45	1.35
13	L	1004	CLA	C4B-NB	4.01	1.38	1.35
13	L	1002	CLA	CHC-C1C	4.00	1.45	1.35
13	A	835	CLA	C4B-NB	3.98	1.38	1.35
13	K	1401	CLA	C4B-NB	3.97	1.38	1.35
13	A	808	CLA	C4B-NB	3.97	1.38	1.35
13	B	807	CLA	MG-NA	3.96	2.15	2.06
13	B	808	CLA	C4B-NB	3.94	1.38	1.35
13	A	840	CLA	C4B-NB	3.93	1.38	1.35
13	M	1601	CLA	C4B-NB	3.89	1.38	1.35
13	B	821	CLA	CHC-C1C	3.88	1.44	1.35
13	A	815	CLA	C4B-NB	3.87	1.38	1.35
13	B	803	CLA	CHC-C1C	3.85	1.44	1.35
13	A	837	CLA	C4B-NB	3.81	1.38	1.35
13	A	841	CLA	CHC-C1C	3.81	1.44	1.35
17	A	856	LHG	O7-C7	3.80	1.45	1.34
13	A	804	CLA	C4B-NB	3.80	1.38	1.35
13	A	831	CLA	CHC-C1C	3.76	1.44	1.35
16	J	104	BCR	C29-C30	3.74	1.62	1.54
13	J	101	CLA	C4B-NB	3.74	1.38	1.35
13	B	820	CLA	C4B-NB	3.74	1.38	1.35
13	A	813	CLA	C4B-NB	3.74	1.38	1.35
13	A	809	CLA	CHC-C1C	3.73	1.44	1.35
13	X	1701	CLA	CHC-C1C	3.73	1.44	1.35
13	B	824	CLA	CHC-C1C	3.72	1.44	1.35
13	B	827	CLA	CHC-C1C	3.72	1.44	1.35
13	B	836	CLA	C4B-NB	3.72	1.38	1.35
13	A	811	CLA	C4B-NB	3.72	1.38	1.35
14	B	842	PQN	C10-C5	3.71	1.46	1.40
13	A	846	CLA	CHC-C1C	3.70	1.44	1.35
16	A	851	BCR	C30-C25	3.70	1.58	1.53
16	A	851	BCR	C1-C6	3.69	1.58	1.53
13	L	1003	CLA	CHC-C1C	3.69	1.44	1.35
13	B	834	CLA	CHC-C1C	3.69	1.44	1.35
13	A	828	CLA	CHC-C1C	3.69	1.44	1.35
13	B	823	CLA	CHC-C1C	3.68	1.44	1.35
13	A	815	CLA	CHC-C1C	3.66	1.44	1.35
13	A	819	CLA	C4B-NB	3.66	1.38	1.35
13	A	845	CLA	C4B-NB	3.64	1.38	1.35
13	A	822	CLA	CHC-C1C	3.64	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	832	CLA	C4B-NB	3.64	1.38	1.35
13	A	826	CLA	C4B-NB	3.64	1.38	1.35
13	B	810	CLA	C1B-NB	3.63	1.38	1.35
13	A	814	CLA	C4B-NB	3.62	1.38	1.35
13	B	807	CLA	C3B-C2B	-3.61	1.35	1.40
13	B	804	CLA	C4B-NB	3.61	1.38	1.35
13	B	817	CLA	C4B-NB	3.60	1.38	1.35
13	B	811	CLA	C4B-NB	3.60	1.38	1.35
13	A	821	CLA	CHC-C1C	3.59	1.44	1.35
13	B	812	CLA	C4B-NB	3.59	1.38	1.35
13	B	835	CLA	CHC-C1C	3.59	1.44	1.35
13	A	823	CLA	CHC-C1C	3.59	1.44	1.35
13	B	802	CLA	CHC-C1C	3.58	1.44	1.35
13	B	815	CLA	CHC-C1C	3.58	1.44	1.35
17	B	851	LHG	O7-C7	3.58	1.44	1.34
13	B	828	CLA	C4B-NB	3.58	1.38	1.35
13	A	826	CLA	CHC-C1C	3.57	1.44	1.35
16	J	105	BCR	C30-C25	3.57	1.58	1.53
13	B	822	CLA	C4B-NB	3.56	1.38	1.35
16	J	104	BCR	C2-C1	3.56	1.62	1.54
13	B	838	CLA	C4B-NB	3.56	1.38	1.35
13	B	837	CLA	CHC-C1C	3.55	1.44	1.35
13	A	817	CLA	C4B-NB	3.54	1.38	1.35
13	A	832	CLA	CHC-C1C	3.54	1.44	1.35
16	A	849	BCR	C30-C25	3.53	1.58	1.53
13	L	1004	CLA	CHC-C1C	3.52	1.44	1.35
16	F	1302	BCR	C2-C1	3.51	1.62	1.54
13	B	827	CLA	MG-NC	3.50	2.14	2.06
16	A	849	BCR	C1-C6	3.49	1.58	1.53
14	B	842	PQN	C11-C12	3.49	1.55	1.50
13	A	825	CLA	C4B-NB	3.49	1.38	1.35
13	L	1004	CLA	C1B-NB	3.49	1.38	1.35
16	A	854	BCR	C30-C25	3.48	1.58	1.53
13	A	839	CLA	CHC-C1C	3.47	1.43	1.35
13	J	101	CLA	CHC-C1C	3.47	1.43	1.35
13	B	823	CLA	C4B-NB	3.47	1.38	1.35
13	B	814	CLA	C4B-NB	3.47	1.38	1.35
13	A	840	CLA	CHC-C1C	3.45	1.43	1.35
13	B	810	CLA	MG-NC	3.45	2.14	2.06
13	F	1301	CLA	CHC-C1C	3.44	1.43	1.35
16	L	1006	BCR	C2-C1	3.43	1.62	1.54
13	A	844	CLA	C1B-NB	3.43	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	805	CLA	CHC-C1C	3.42	1.43	1.35
13	B	833	CLA	C4B-NB	3.42	1.38	1.35
13	A	806	CLA	C4B-NB	3.42	1.38	1.35
13	A	835	CLA	C3B-C2B	-3.40	1.35	1.40
16	A	850	BCR	C30-C25	3.40	1.58	1.53
13	A	843	CLA	C4B-NB	3.39	1.38	1.35
13	B	826	CLA	CHC-C1C	3.39	1.43	1.35
13	B	804	CLA	CHC-C1C	3.38	1.43	1.35
13	A	843	CLA	CHC-C1C	3.37	1.43	1.35
13	A	808	CLA	CHC-C1C	3.37	1.43	1.35
13	B	805	CLA	C4B-NB	3.37	1.38	1.35
13	B	830	CLA	C3B-C2B	-3.36	1.35	1.40
16	J	105	BCR	C1-C6	3.36	1.58	1.53
13	B	831	CLA	CHC-C1C	3.35	1.43	1.35
13	A	806	CLA	CHC-C1C	3.35	1.43	1.35
16	M	1602	BCR	C1-C6	3.35	1.58	1.53
13	B	819	CLA	C4B-NB	3.35	1.38	1.35
13	B	818	CLA	C4B-NB	3.34	1.38	1.35
16	A	853	BCR	C1-C6	3.33	1.58	1.53
13	M	1601	CLA	CHC-C1C	3.33	1.43	1.35
13	A	823	CLA	C4B-NB	3.32	1.38	1.35
13	A	821	CLA	C4B-NB	3.32	1.38	1.35
13	A	819	CLA	CHC-C1C	3.32	1.43	1.35
13	B	817	CLA	CHC-C1C	3.32	1.43	1.35
13	B	822	CLA	CHC-C1C	3.31	1.43	1.35
13	B	815	CLA	C4B-NB	3.29	1.38	1.35
13	A	820	CLA	C4B-NB	3.29	1.38	1.35
13	A	818	CLA	CHC-C1C	3.29	1.43	1.35
13	B	816	CLA	C4B-NB	3.28	1.38	1.35
16	B	843	BCR	C2-C1	3.28	1.61	1.54
16	A	854	BCR	C1-C6	3.27	1.58	1.53
13	J	102	CLA	CHC-C1C	3.26	1.43	1.35
13	B	830	CLA	CHC-C1C	3.26	1.43	1.35
13	A	805	CLA	C4B-NB	3.26	1.38	1.35
13	B	820	CLA	CHC-C1C	3.26	1.43	1.35
13	A	807	CLA	CHC-C1C	3.26	1.43	1.35
16	B	843	BCR	C1-C6	3.24	1.58	1.53
13	A	825	CLA	CHC-C1C	3.24	1.43	1.35
13	A	837	CLA	CHC-C1C	3.23	1.43	1.35
13	B	839	CLA	C4B-NB	3.23	1.38	1.35
16	I	102	BCR	C30-C25	3.23	1.58	1.53
13	B	832	CLA	CHC-C1C	3.23	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	809	CLA	MG-NC	3.22	2.13	2.06
16	B	843	BCR	C26-C25	3.22	1.40	1.34
13	A	802	CLA	CHC-C1C	3.21	1.43	1.35
13	B	812	CLA	CHC-C1C	3.20	1.43	1.35
13	F	1301	CLA	MG-NC	3.20	2.13	2.06
14	A	847	PQN	C10-C5	3.19	1.46	1.40
13	A	838	CLA	MG-NC	3.19	2.13	2.06
13	B	839	CLA	CHC-C1C	3.18	1.43	1.35
13	A	812	CLA	C4B-NB	3.18	1.38	1.35
13	A	816	CLA	C4B-NB	3.18	1.38	1.35
13	L	1003	CLA	C1B-NB	3.18	1.38	1.35
13	B	826	CLA	MG-NC	3.18	2.13	2.06
13	B	829	CLA	MG-NC	3.17	2.13	2.06
13	L	1003	CLA	C4B-NB	3.17	1.38	1.35
13	B	802	CLA	MG-NC	3.17	2.13	2.06
13	A	839	CLA	C4B-NB	3.17	1.38	1.35
13	B	814	CLA	CHC-C1C	3.17	1.43	1.35
13	B	816	CLA	CHC-C1C	3.16	1.43	1.35
13	A	810	CLA	CHC-C1C	3.16	1.43	1.35
13	B	828	CLA	C2-C3	3.15	1.40	1.33
13	K	1401	CLA	CHC-C1C	3.15	1.43	1.35
13	B	813	CLA	MG-NC	3.15	2.13	2.06
13	B	819	CLA	CHC-C1C	3.14	1.43	1.35
13	B	811	CLA	CHC-C1C	3.14	1.43	1.35
16	J	103	BCR	C29-C30	3.13	1.61	1.54
16	F	1302	BCR	C30-C25	3.12	1.58	1.53
16	A	854	BCR	C2-C1	3.12	1.61	1.54
16	B	847	BCR	C30-C25	3.12	1.58	1.53
13	B	829	CLA	C4B-NB	3.12	1.38	1.35
13	L	1002	CLA	C1B-NB	3.11	1.38	1.35
13	A	803	CLA	C4B-NB	3.11	1.38	1.35
16	J	104	BCR	C30-C25	3.10	1.58	1.53
16	A	850	BCR	C2-C1	3.10	1.61	1.54
16	A	852	BCR	C29-C30	3.10	1.61	1.54
16	J	105	BCR	C2-C1	3.10	1.61	1.54
13	A	807	CLA	C4B-NB	3.09	1.38	1.35
13	B	837	CLA	C3B-C2B	-3.08	1.36	1.40
13	A	801	CLA	CHC-C1C	3.08	1.42	1.35
13	B	836	CLA	CHC-C1C	3.08	1.42	1.35
16	B	849	BCR	C2-C1	3.08	1.61	1.54
14	B	842	PQN	C6-C5	3.08	1.44	1.39
13	B	838	CLA	C3B-C2B	-3.08	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	816	CLA	CHC-C1C	3.07	1.42	1.35
13	A	824	CLA	CHC-C1C	3.06	1.42	1.35
13	A	804	CLA	CHC-C1C	3.06	1.42	1.35
13	A	809	CLA	CAA-C2A	3.06	1.59	1.54
13	B	831	CLA	C3B-C2B	-3.05	1.36	1.40
13	A	828	CLA	C5-C3	3.05	1.57	1.51
13	A	836	CLA	CHC-C1C	3.05	1.42	1.35
13	B	808	CLA	CHC-C1C	3.04	1.42	1.35
13	B	837	CLA	C4B-NB	3.04	1.37	1.35
13	B	813	CLA	CHC-C1C	3.03	1.42	1.35
13	A	819	CLA	CAA-C2A	3.03	1.59	1.54
13	A	802	CLA	MG-NC	3.03	2.13	2.06
16	A	851	BCR	C2-C1	3.02	1.61	1.54
13	A	817	CLA	CHC-C1C	3.01	1.42	1.35
13	B	833	CLA	CHC-C1C	3.01	1.42	1.35
16	J	103	BCR	C1-C6	3.00	1.57	1.53
13	A	812	CLA	CHC-C1C	3.00	1.42	1.35
13	B	827	CLA	OBD-CAD	3.00	1.26	1.22
13	B	832	CLA	C3B-C2B	-2.99	1.36	1.40
16	B	848	BCR	C29-C30	2.99	1.61	1.54
13	A	803	CLA	CHC-C1C	2.99	1.42	1.35
13	A	830	CLA	MG-NC	2.99	2.13	2.06
16	M	1602	BCR	C29-C30	2.97	1.60	1.54
14	A	847	PQN	C6-C5	2.97	1.44	1.39
16	A	849	BCR	C29-C30	2.97	1.60	1.54
16	A	850	BCR	C29-C30	2.97	1.60	1.54
13	A	811	CLA	MG-NC	2.96	2.13	2.06
16	B	844	BCR	C2-C1	2.95	1.60	1.54
13	A	814	CLA	CHC-C1C	2.95	1.42	1.35
13	B	825	CLA	CHC-C1C	2.95	1.42	1.35
16	M	1602	BCR	C2-C1	2.95	1.60	1.54
13	B	825	CLA	C4B-NB	2.95	1.37	1.35
13	A	819	CLA	C3B-C2B	-2.94	1.36	1.40
13	A	811	CLA	CHC-C1C	2.94	1.42	1.35
16	B	843	BCR	C29-C30	2.94	1.60	1.54
16	B	846	BCR	C29-C30	2.94	1.60	1.54
13	B	808	CLA	C1B-CHB	-2.93	1.32	1.41
16	B	845	BCR	C30-C25	2.92	1.57	1.53
13	B	824	CLA	C5-C3	2.92	1.57	1.51
13	B	822	CLA	CAA-C2A	2.92	1.59	1.54
13	A	830	CLA	CHC-C1C	2.91	1.42	1.35
16	B	845	BCR	C2-C1	2.91	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	849	BCR	C29-C30	2.91	1.60	1.54
13	A	845	CLA	CHC-C1C	2.91	1.42	1.35
13	B	816	CLA	C5-C3	2.91	1.57	1.51
13	A	822	CLA	C4B-NB	2.90	1.37	1.35
16	B	844	BCR	C30-C25	2.90	1.57	1.53
16	F	1302	BCR	C29-C30	2.90	1.60	1.54
16	J	105	BCR	C29-C30	2.90	1.60	1.54
13	B	831	CLA	C1B-CHB	-2.89	1.32	1.41
17	A	856	LHG	O8-C23	2.89	1.41	1.33
16	B	844	BCR	C26-C25	2.89	1.39	1.34
16	B	847	BCR	C2-C1	2.88	1.60	1.54
13	A	840	CLA	CAA-C2A	2.88	1.59	1.54
13	B	801	CLA	MG-NC	2.88	2.13	2.06
13	B	816	CLA	CAA-C2A	2.87	1.59	1.54
16	B	845	BCR	C29-C30	2.87	1.60	1.54
13	B	827	CLA	CAA-C2A	2.87	1.59	1.54
13	A	826	CLA	C3B-C2B	-2.86	1.36	1.40
16	B	849	BCR	C30-C25	2.86	1.57	1.53
13	A	846	CLA	CAA-C2A	2.86	1.59	1.54
14	B	842	PQN	C11-C3	2.86	1.56	1.51
16	A	854	BCR	C29-C30	2.85	1.60	1.54
13	A	809	CLA	C3B-C2B	-2.85	1.36	1.40
13	A	822	CLA	CAA-C2A	2.85	1.59	1.54
13	J	101	CLA	MG-NC	2.85	2.13	2.06
13	A	836	CLA	C4B-NB	2.85	1.37	1.35
13	B	829	CLA	CAA-C2A	2.84	1.59	1.54
13	A	832	CLA	C3B-C2B	-2.84	1.36	1.40
13	B	815	CLA	MG-NC	2.84	2.13	2.06
13	A	813	CLA	CHC-C1C	2.83	1.42	1.35
13	A	822	CLA	C1B-CHB	-2.83	1.33	1.41
16	J	103	BCR	C30-C25	2.83	1.57	1.53
16	I	102	BCR	C2-C1	2.82	1.60	1.54
16	B	845	BCR	C1-C6	2.82	1.57	1.53
16	L	1005	BCR	C29-C30	2.81	1.60	1.54
13	B	830	CLA	C4B-NB	2.80	1.37	1.35
13	A	833	CLA	MG-NC	2.80	2.12	2.06
13	A	838	CLA	C4B-NB	2.80	1.37	1.35
16	A	853	BCR	C30-C25	2.80	1.57	1.53
13	B	828	CLA	CHC-C1C	2.80	1.42	1.35
13	A	832	CLA	C1B-CHB	-2.79	1.33	1.41
13	B	808	CLA	MG-NC	2.79	2.12	2.06
13	B	817	CLA	CAA-C2A	2.79	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	803	CLA	C1B-CHB	-2.79	1.33	1.41
13	A	808	CLA	MG-NC	2.78	2.12	2.06
16	I	101	BCR	C29-C30	2.78	1.60	1.54
16	J	103	BCR	C2-C1	2.78	1.60	1.54
13	B	811	CLA	C3B-C2B	-2.78	1.36	1.40
13	A	840	CLA	MG-NC	2.77	2.12	2.06
13	B	835	CLA	CAA-C2A	2.77	1.59	1.54
18	B	850	LMG	O8-C28	2.76	1.41	1.33
13	A	824	CLA	C4B-NB	2.76	1.37	1.35
13	B	803	CLA	C1B-CHB	-2.75	1.33	1.41
13	B	807	CLA	C1B-CHB	-2.74	1.33	1.41
16	I	102	BCR	C29-C30	2.74	1.60	1.54
13	B	829	CLA	CHC-C1C	2.74	1.42	1.35
13	B	828	CLA	MG-NC	2.74	2.12	2.06
14	A	847	PQN	C11-C12	2.74	1.54	1.50
13	B	803	CLA	C3B-C2B	-2.73	1.36	1.40
13	A	843	CLA	C1B-NB	2.73	1.37	1.35
16	A	849	BCR	C2-C1	2.73	1.60	1.54
16	B	846	BCR	C30-C25	2.73	1.57	1.53
13	B	801	CLA	C1B-CHB	-2.71	1.33	1.41
16	M	1602	BCR	C30-C25	2.71	1.57	1.53
16	L	1006	BCR	C29-C30	2.71	1.60	1.54
13	A	827	CLA	C1B-CHB	-2.71	1.33	1.41
13	B	808	CLA	C3B-C2B	-2.71	1.36	1.40
14	A	847	PQN	C15-C13	2.70	1.56	1.51
13	A	810	CLA	MG-NC	2.70	2.12	2.06
13	A	831	CLA	C3B-C2B	-2.70	1.36	1.40
17	A	855	LHG	O8-C23	2.70	1.41	1.33
13	B	833	CLA	C5-C3	2.70	1.56	1.51
14	A	847	PQN	C10-C1	-2.68	1.43	1.48
13	B	818	CLA	CHC-C1C	2.68	1.41	1.35
13	A	841	CLA	C1B-CHB	-2.68	1.33	1.41
13	A	809	CLA	C1B-CHB	-2.67	1.33	1.41
13	B	805	CLA	CHC-C1C	2.67	1.41	1.35
16	A	850	BCR	C1-C6	2.67	1.57	1.53
13	B	817	CLA	C1B-CHB	-2.67	1.33	1.41
13	A	808	CLA	C3B-C2B	-2.66	1.36	1.40
13	B	811	CLA	C1B-CHB	-2.66	1.33	1.41
13	B	806	CLA	MG-NC	2.66	2.12	2.06
13	A	829	CLA	MG-NC	2.66	2.12	2.06
13	A	839	CLA	C3B-C2B	-2.65	1.36	1.40
13	L	1002	CLA	MG-NC	2.65	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	839	CLA	MG-NC	2.65	2.12	2.06
13	B	839	CLA	C1B-CHB	-2.64	1.33	1.41
16	A	852	BCR	C1-C6	2.64	1.57	1.53
13	L	1003	CLA	C1B-CHB	-2.64	1.33	1.41
13	B	841	CLA	CHC-C1C	2.64	1.41	1.35
13	B	828	CLA	C5-C3	2.64	1.56	1.51
13	B	801	CLA	C1B-NB	2.64	1.37	1.35
13	B	824	CLA	C1B-CHB	-2.63	1.33	1.41
13	A	805	CLA	CAA-C2A	2.63	1.59	1.54
16	B	848	BCR	C2-C1	2.63	1.60	1.54
17	A	855	LHG	O7-C7	2.62	1.41	1.34
13	B	806	CLA	CHC-C1C	2.62	1.41	1.35
13	B	818	CLA	CAA-C2A	2.62	1.59	1.54
13	B	806	CLA	C4B-NB	2.62	1.37	1.35
13	A	842	CLA	C4B-NB	2.62	1.37	1.35
13	B	826	CLA	C1B-NB	2.61	1.37	1.35
13	A	804	CLA	C1B-CHB	-2.61	1.33	1.41
16	A	852	BCR	C2-C1	2.61	1.60	1.54
13	A	811	CLA	C3B-C2B	-2.60	1.36	1.40
13	A	842	CLA	CHC-C1C	2.60	1.41	1.35
13	A	843	CLA	C1-C2	2.60	1.56	1.49
13	B	834	CLA	C3B-C2B	-2.59	1.36	1.40
13	A	844	CLA	CAA-C2A	2.59	1.58	1.54
13	A	815	CLA	C1B-CHB	-2.58	1.33	1.41
13	B	801	CLA	CHC-C1C	2.58	1.41	1.35
16	A	854	BCR	C23-C22	-2.58	1.40	1.45
13	A	806	CLA	C1B-CHB	-2.58	1.33	1.41
13	B	819	CLA	MG-NC	2.58	2.12	2.06
13	A	824	CLA	C3B-C2B	-2.57	1.36	1.40
13	B	835	CLA	C3B-C2B	-2.57	1.36	1.40
13	B	819	CLA	C3B-C2B	-2.57	1.36	1.40
13	B	803	CLA	MG-NC	2.56	2.12	2.06
13	B	813	CLA	C1B-CHB	-2.56	1.33	1.41
13	A	818	CLA	C1B-CHB	-2.56	1.33	1.41
13	B	839	CLA	C3B-C2B	-2.55	1.36	1.40
16	B	847	BCR	C1-C6	2.55	1.57	1.53
14	A	847	PQN	C11-C3	2.55	1.55	1.51
13	B	838	CLA	C1B-CHB	-2.54	1.33	1.41
13	A	807	CLA	MG-NC	2.54	2.12	2.06
13	A	825	CLA	C1B-CHB	-2.54	1.33	1.41
13	A	839	CLA	C1B-CHB	-2.54	1.33	1.41
13	A	814	CLA	C1B-CHB	-2.54	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	842	PQN	C9-C10	2.54	1.43	1.39
13	A	835	CLA	C1B-CHB	-2.54	1.33	1.41
13	A	835	CLA	CHC-C1C	2.53	1.41	1.35
13	A	812	CLA	C1B-CHB	-2.53	1.34	1.41
13	B	835	CLA	C1B-CHB	-2.53	1.34	1.41
13	A	819	CLA	C5-C3	2.52	1.56	1.51
13	A	809	CLA	C4B-NB	2.52	1.37	1.35
13	B	840	CLA	C3B-C2B	-2.52	1.36	1.40
13	B	828	CLA	C3B-C2B	-2.52	1.36	1.40
13	A	829	CLA	CHC-C1C	2.52	1.41	1.35
13	A	820	CLA	CHC-C1C	2.52	1.41	1.35
13	B	820	CLA	CAA-C2A	2.51	1.58	1.54
13	B	819	CLA	C1B-CHB	-2.51	1.34	1.41
16	A	853	BCR	C29-C30	2.51	1.59	1.54
13	A	833	CLA	C4B-NB	2.51	1.37	1.35
13	B	840	CLA	MG-NC	2.51	2.12	2.06
13	A	829	CLA	C4B-NB	2.51	1.37	1.35
13	A	827	CLA	CHC-C1C	2.51	1.41	1.35
13	A	820	CLA	C2-C3	2.51	1.39	1.33
13	A	831	CLA	C5-C3	2.51	1.56	1.51
13	A	836	CLA	C5-C3	2.50	1.56	1.51
13	M	1601	CLA	CAA-C2A	2.50	1.58	1.54
13	B	824	CLA	MG-NC	2.49	2.12	2.06
13	B	834	CLA	C1B-CHB	-2.49	1.34	1.41
16	J	105	BCR	C5-C6	2.49	1.38	1.34
13	B	829	CLA	C1B-NB	2.49	1.37	1.35
13	B	830	CLA	C1B-CHB	-2.48	1.34	1.41
13	B	814	CLA	C1B-CHB	-2.48	1.34	1.41
13	A	802	CLA	C1B-CHB	-2.48	1.34	1.41
13	A	815	CLA	C3B-C2B	-2.48	1.36	1.40
13	J	102	CLA	MG-NC	2.47	2.12	2.06
13	A	821	CLA	C5-C3	2.47	1.56	1.51
13	A	842	CLA	MG-NC	2.47	2.12	2.06
16	I	101	BCR	C2-C1	2.47	1.59	1.54
13	A	831	CLA	C1B-NB	2.47	1.37	1.35
13	K	1401	CLA	C1B-CHB	-2.47	1.34	1.41
16	B	844	BCR	C29-C30	2.47	1.59	1.54
18	B	850	LMG	O7-C8	-2.46	1.40	1.46
13	L	1004	CLA	MG-NC	2.46	2.12	2.06
16	A	854	BCR	C14-C13	2.46	1.39	1.35
13	A	811	CLA	CAA-C2A	2.45	1.58	1.54
16	M	1602	BCR	C23-C22	-2.45	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	1005	BCR	C19-C18	-2.45	1.40	1.45
13	A	829	CLA	C1B-CHB	-2.45	1.34	1.41
13	A	826	CLA	MG-NC	2.44	2.12	2.06
13	B	805	CLA	MG-NC	2.44	2.12	2.06
13	A	842	CLA	C5-C3	2.44	1.58	1.51
13	A	820	CLA	C1-C2	2.44	1.56	1.49
13	A	844	CLA	C3B-C2B	-2.44	1.37	1.40
13	A	803	CLA	CAA-C2A	2.44	1.58	1.54
13	A	818	CLA	C1B-NB	2.44	1.37	1.35
13	L	1003	CLA	CAA-C2A	2.43	1.58	1.54
13	A	831	CLA	MG-NC	2.43	2.12	2.06
13	B	840	CLA	CHC-C1C	2.43	1.41	1.35
16	L	1005	BCR	C2-C1	2.43	1.59	1.54
16	I	101	BCR	C33-C5	2.43	1.54	1.50
13	A	844	CLA	C1B-CHB	-2.42	1.34	1.41
13	B	828	CLA	CAA-C2A	2.42	1.58	1.54
13	B	810	CLA	C3B-C2B	-2.42	1.37	1.40
13	B	824	CLA	C3B-C2B	-2.42	1.37	1.40
13	B	815	CLA	C1B-CHB	-2.42	1.34	1.41
16	B	844	BCR	C38-C26	2.42	1.54	1.50
13	A	823	CLA	C3B-C2B	-2.42	1.37	1.40
16	A	849	BCR	C26-C25	2.41	1.38	1.34
13	A	820	CLA	CAA-C2A	2.41	1.58	1.54
13	A	827	CLA	MG-NC	2.41	2.12	2.06
13	B	817	CLA	C3B-C2B	-2.41	1.37	1.40
13	A	802	CLA	C3B-C2B	-2.41	1.37	1.40
13	X	1701	CLA	MG-NC	2.41	2.12	2.06
14	A	847	PQN	C9-C10	2.41	1.43	1.39
16	B	846	BCR	C23-C22	-2.40	1.40	1.45
13	A	821	CLA	CAA-C2A	2.40	1.58	1.54
13	A	824	CLA	CAA-C2A	2.39	1.58	1.54
13	A	804	CLA	C3B-C2B	-2.39	1.37	1.40
13	A	834	CLA	MG-NC	2.39	2.11	2.06
13	A	812	CLA	C3B-C2B	-2.39	1.37	1.40
16	B	847	BCR	C29-C30	2.39	1.59	1.54
16	B	849	BCR	C23-C22	-2.39	1.40	1.45
13	B	807	CLA	CAA-C2A	2.38	1.58	1.54
16	L	1006	BCR	C38-C26	2.38	1.54	1.50
13	L	1002	CLA	CAA-C2A	2.38	1.58	1.54
13	A	817	CLA	C1B-CHB	-2.38	1.34	1.41
13	A	813	CLA	CAA-C2A	2.38	1.58	1.54
16	B	848	BCR	C23-C22	-2.38	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	K	1401	CLA	MG-NC	2.37	2.11	2.06
13	B	818	CLA	C3B-CAB	2.37	1.52	1.47
13	A	818	CLA	MG-NC	2.37	2.11	2.06
13	A	846	CLA	C1B-CHB	-2.37	1.34	1.41
13	B	809	CLA	CHC-C1C	2.36	1.41	1.35
13	A	824	CLA	MG-NC	2.36	2.11	2.06
16	L	1006	BCR	C26-C25	2.36	1.38	1.34
13	A	824	CLA	C1B-CHB	-2.36	1.34	1.41
13	B	838	CLA	MG-NC	2.36	2.11	2.06
16	I	101	BCR	C30-C25	2.36	1.57	1.53
13	A	844	CLA	CHC-C1C	2.36	1.41	1.35
13	B	816	CLA	C1B-CHB	-2.35	1.34	1.41
13	A	846	CLA	C5-C3	2.35	1.56	1.51
13	A	811	CLA	C1B-CHB	-2.35	1.34	1.41
13	A	833	CLA	CHC-C1C	2.34	1.41	1.35
13	B	833	CLA	CAA-C2A	2.34	1.58	1.54
13	B	816	CLA	C3B-C2B	-2.33	1.37	1.40
13	A	839	CLA	MG-NC	2.33	2.11	2.06
16	A	851	BCR	C29-C30	2.33	1.59	1.54
13	A	823	CLA	C1B-CHB	-2.33	1.34	1.41
13	B	828	CLA	C1-C2	2.33	1.56	1.49
13	A	813	CLA	C1B-CHB	-2.32	1.34	1.41
13	B	832	CLA	C1B-CHB	-2.32	1.34	1.41
13	B	828	CLA	C1B-CHB	-2.32	1.34	1.41
13	A	812	CLA	MG-NC	2.32	2.11	2.06
13	A	846	CLA	C3B-C2B	-2.32	1.37	1.40
13	B	805	CLA	C5-C3	2.32	1.56	1.51
13	A	813	CLA	C3B-C2B	-2.32	1.37	1.40
13	B	825	CLA	MG-NC	2.31	2.11	2.06
13	A	820	CLA	C1B-CHB	-2.31	1.34	1.41
13	A	844	CLA	CMD-C2D	2.31	1.57	1.51
14	B	842	PQN	C5-C4	-2.30	1.43	1.48
13	A	840	CLA	C3B-C2B	-2.30	1.37	1.40
13	B	814	CLA	C5-C3	2.30	1.56	1.51
13	B	841	CLA	C1C-NC	-2.30	1.34	1.37
16	I	102	BCR	C33-C5	2.29	1.54	1.50
13	A	810	CLA	C1B-CHB	-2.29	1.34	1.41
13	B	815	CLA	C3B-C2B	-2.29	1.37	1.40
13	K	1401	CLA	C3B-C2B	-2.29	1.37	1.40
13	A	844	CLA	C4-C3	2.28	1.56	1.50
13	A	827	CLA	CAA-C2A	2.28	1.58	1.54
13	A	821	CLA	C3B-C2B	-2.28	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	810	CLA	C1B-CHB	-2.27	1.34	1.41
13	B	811	CLA	CAA-C2A	2.27	1.58	1.54
16	B	844	BCR	C29-C28	-2.27	1.47	1.52
16	I	102	BCR	C19-C18	-2.27	1.41	1.45
13	B	818	CLA	C1B-CHB	-2.27	1.34	1.41
14	A	847	PQN	C8-C7	2.26	1.44	1.38
16	J	103	BCR	C26-C25	2.26	1.38	1.34
13	B	829	CLA	OBD-CAD	2.26	1.25	1.22
13	X	1701	CLA	C1B-NB	2.26	1.37	1.35
13	B	840	CLA	CAA-C2A	2.25	1.58	1.54
13	A	819	CLA	MG-NC	2.25	2.11	2.06
13	J	101	CLA	CAA-C2A	2.25	1.58	1.54
13	B	822	CLA	C1B-CHB	-2.25	1.34	1.41
13	B	828	CLA	C1B-NB	2.25	1.37	1.35
13	A	827	CLA	C4B-NB	2.25	1.37	1.35
13	A	836	CLA	MG-NC	2.24	2.11	2.06
13	A	819	CLA	C1B-CHB	-2.24	1.34	1.41
13	A	846	CLA	MG-NC	2.24	2.11	2.06
13	A	828	CLA	MG-NC	2.24	2.11	2.06
13	A	837	CLA	CAA-C2A	2.24	1.58	1.54
14	B	842	PQN	C10-C1	-2.24	1.43	1.48
16	I	101	BCR	C19-C18	-2.24	1.41	1.45
13	A	816	CLA	MG-NC	2.23	2.11	2.06
13	B	833	CLA	MG-NC	2.23	2.11	2.06
16	I	101	BCR	C2-C3	-2.23	1.47	1.52
13	B	840	CLA	C1B-CHB	-2.23	1.34	1.41
13	A	845	CLA	MG-NC	2.23	2.11	2.06
13	B	814	CLA	MG-NC	2.23	2.11	2.06
16	L	1005	BCR	C26-C25	2.22	1.38	1.34
13	B	841	CLA	CAA-CBA	-2.22	1.45	1.52
13	A	803	CLA	MG-NC	2.22	2.11	2.06
13	A	814	CLA	MG-NC	2.22	2.11	2.06
13	A	838	CLA	CHC-C1C	2.22	1.40	1.35
13	A	817	CLA	MG-NC	2.22	2.11	2.06
16	B	848	BCR	C5-C6	2.22	1.38	1.34
13	A	843	CLA	C1B-CHB	-2.22	1.34	1.41
13	A	831	CLA	CAA-C2A	2.21	1.58	1.54
13	B	825	CLA	CAA-C2A	2.21	1.58	1.54
13	B	804	CLA	C1B-CHB	-2.21	1.34	1.41
13	A	842	CLA	C3B-C2B	-2.21	1.37	1.40
13	B	823	CLA	C1B-CHB	-2.21	1.34	1.41
13	B	832	CLA	MG-NC	2.21	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	847	PQN	C8-C9	2.21	1.43	1.38
13	B	804	CLA	CAA-C2A	2.20	1.58	1.54
13	A	845	CLA	CAA-C2A	2.20	1.58	1.54
16	I	102	BCR	C26-C25	2.20	1.38	1.34
13	B	837	CLA	MG-NC	2.20	2.11	2.06
13	A	841	CLA	CAA-C2A	2.20	1.58	1.54
13	B	816	CLA	C4-C3	2.19	1.56	1.50
13	B	824	CLA	C1-C2	2.19	1.55	1.49
13	F	1301	CLA	C1B-CHB	-2.19	1.34	1.41
13	B	812	CLA	C1B-NB	2.19	1.37	1.35
13	B	830	CLA	CAA-C2A	2.19	1.58	1.54
13	A	831	CLA	C1B-CHB	-2.19	1.34	1.41
13	A	836	CLA	C1-C2	2.18	1.55	1.49
13	B	807	CLA	C4B-NB	2.18	1.37	1.35
16	A	853	BCR	C33-C5	2.18	1.54	1.50
13	B	841	CLA	MG-NC	2.18	2.11	2.06
13	B	822	CLA	MG-NC	2.18	2.11	2.06
13	B	841	CLA	C1B-CHB	-2.18	1.34	1.41
13	A	822	CLA	C1-C2	2.18	1.55	1.49
13	B	837	CLA	C5-C3	2.18	1.55	1.51
16	A	853	BCR	C2-C1	2.18	1.59	1.54
13	B	810	CLA	C4B-NB	2.17	1.37	1.35
13	A	808	CLA	C1-C2	2.17	1.55	1.49
14	B	842	PQN	C8-C9	2.17	1.43	1.38
16	L	1005	BCR	C38-C26	2.17	1.54	1.50
16	M	1602	BCR	C2-C3	-2.17	1.47	1.52
13	B	814	CLA	C3B-C2B	-2.16	1.37	1.40
16	L	1006	BCR	C23-C22	-2.16	1.41	1.45
13	A	807	CLA	C1B-CHB	-2.16	1.35	1.41
13	B	826	CLA	C3B-CAB	2.16	1.52	1.47
16	B	848	BCR	C29-C28	-2.16	1.47	1.52
13	A	835	CLA	MG-NC	2.16	2.11	2.06
16	A	852	BCR	C14-C13	2.16	1.38	1.35
13	A	815	CLA	CAA-C2A	2.16	1.58	1.54
13	A	818	CLA	C3B-C2B	-2.15	1.37	1.40
13	B	816	CLA	C1-C2	2.15	1.55	1.49
13	A	812	CLA	CAA-C2A	2.15	1.58	1.54
13	B	818	CLA	OBD-CAD	2.15	1.25	1.22
14	A	847	PQN	C7-C6	2.15	1.43	1.38
16	L	1005	BCR	C29-C28	-2.14	1.47	1.52
13	B	808	CLA	C1B-NB	2.14	1.37	1.35
13	B	807	CLA	C5-C3	2.14	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	842	PQN	C8-C7	2.14	1.43	1.38
13	A	816	CLA	C1B-NB	2.14	1.37	1.35
16	A	851	BCR	C26-C25	2.14	1.38	1.34
13	A	839	CLA	CAA-C2A	2.14	1.58	1.54
13	L	1004	CLA	C1B-CHB	-2.14	1.35	1.41
13	B	827	CLA	C1B-NB	2.14	1.37	1.35
14	A	847	PQN	C5-C4	-2.14	1.44	1.48
13	A	830	CLA	C5-C3	2.14	1.55	1.51
13	B	823	CLA	C3B-C2B	-2.14	1.37	1.40
16	B	845	BCR	C5-C6	2.13	1.38	1.34
13	B	834	CLA	CAA-C2A	2.13	1.58	1.54
16	A	853	BCR	C19-C18	-2.13	1.41	1.45
13	A	846	CLA	C4-C3	2.13	1.56	1.50
13	L	1002	CLA	C1B-CHB	-2.13	1.35	1.41
13	A	843	CLA	C5-C3	2.13	1.55	1.51
16	B	846	BCR	C14-C13	2.13	1.40	1.35
13	B	804	CLA	C1-C2	2.13	1.55	1.49
13	A	801	CLA	C1B-CHB	-2.13	1.35	1.41
13	A	836	CLA	C3B-C2B	-2.12	1.37	1.40
13	A	807	CLA	CAA-CBA	-2.12	1.46	1.52
13	B	836	CLA	C1B-CHB	-2.12	1.35	1.41
13	B	811	CLA	MG-NC	2.12	2.11	2.06
13	A	845	CLA	C1B-CHB	-2.11	1.35	1.41
16	A	851	BCR	C29-C28	-2.11	1.47	1.52
13	B	821	CLA	C1B-CHB	-2.11	1.35	1.41
14	B	842	PQN	C15-C13	2.11	1.55	1.51
13	A	821	CLA	C1B-CHB	-2.11	1.35	1.41
13	A	843	CLA	OBD-CAD	2.10	1.25	1.22
13	B	831	CLA	CAA-C2A	2.10	1.58	1.54
13	A	801	CLA	MG-NC	2.10	2.11	2.06
13	A	820	CLA	OBD-CAD	2.10	1.25	1.22
13	M	1601	CLA	MG-NC	2.10	2.11	2.06
13	A	805	CLA	C1B-CHB	-2.10	1.35	1.41
13	A	813	CLA	C5-C3	2.09	1.55	1.51
13	A	826	CLA	C1B-CHB	-2.09	1.35	1.41
13	B	841	CLA	C3B-C2B	-2.09	1.37	1.40
13	A	834	CLA	C4B-NB	2.09	1.37	1.35
13	A	808	CLA	C1B-CHB	-2.09	1.35	1.41
13	B	835	CLA	MG-NC	2.09	2.11	2.06
13	B	820	CLA	C1B-CHB	-2.09	1.35	1.41
13	A	817	CLA	C3B-C2B	-2.08	1.37	1.40
13	A	818	CLA	CAA-C2A	2.08	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	853	BCR	C29-C28	-2.08	1.47	1.52
13	M	1601	CLA	C1B-CHB	-2.08	1.35	1.41
13	A	835	CLA	C1-C2	2.08	1.55	1.49
13	A	836	CLA	C1B-CHB	-2.07	1.35	1.41
16	L	1005	BCR	C2-C3	-2.07	1.47	1.52
13	B	821	CLA	CAA-C2A	2.07	1.57	1.54
13	B	806	CLA	CAA-C2A	2.06	1.57	1.54
16	F	1302	BCR	C23-C22	-2.06	1.41	1.45
13	A	820	CLA	MG-NC	2.06	2.11	2.06
13	B	825	CLA	C1B-CHB	-2.06	1.35	1.41
13	A	844	CLA	C5-C3	2.06	1.55	1.51
13	A	840	CLA	OBD-CAD	2.06	1.25	1.22
16	J	104	BCR	C1-C6	2.06	1.56	1.53
13	J	101	CLA	C1B-CHB	-2.06	1.35	1.41
13	A	824	CLA	C1-C2	2.06	1.55	1.49
13	A	825	CLA	C5-C3	2.05	1.55	1.51
13	B	803	CLA	C4-C3	2.05	1.56	1.50
13	B	807	CLA	CHC-C1C	2.05	1.40	1.35
16	I	101	BCR	C26-C25	2.05	1.38	1.34
13	A	828	CLA	C1B-CHB	-2.05	1.35	1.41
16	A	853	BCR	C26-C25	2.05	1.38	1.34
13	B	817	CLA	MG-NC	2.05	2.11	2.06
13	A	813	CLA	C4-C3	2.05	1.55	1.50
13	A	829	CLA	C4-C3	2.05	1.55	1.50
13	B	840	CLA	C1-C2	2.04	1.55	1.49
13	A	837	CLA	C1B-CHB	-2.04	1.35	1.41
16	A	852	BCR	C2-C3	-2.04	1.47	1.52
16	B	847	BCR	C5-C6	2.03	1.38	1.34
13	A	817	CLA	CAA-C2A	2.03	1.57	1.54
17	B	851	LHG	O8-C23	2.03	1.43	1.33
13	B	824	CLA	CAA-C2A	2.03	1.57	1.54
13	A	820	CLA	C3B-CAB	2.03	1.52	1.47
13	A	838	CLA	C3D-CAD	-2.03	1.40	1.46
13	B	821	CLA	MG-NC	2.02	2.11	2.06
13	A	842	CLA	C1B-CHB	-2.02	1.35	1.41
16	L	1006	BCR	C5-C6	2.02	1.37	1.34
13	A	834	CLA	CHC-C1C	2.02	1.40	1.35
13	A	840	CLA	C1B-NB	2.02	1.37	1.35
13	L	1002	CLA	C1C-C2C	2.02	1.48	1.44
13	A	843	CLA	CAA-C2A	2.02	1.57	1.54
13	B	833	CLA	C4-C3	2.02	1.55	1.50
13	B	827	CLA	C1B-CHB	-2.02	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	804	CLA	MG-NC	2.01	2.11	2.06
13	B	837	CLA	C4-C3	2.00	1.55	1.50
13	B	822	CLA	C3B-CAB	2.00	1.52	1.47
13	A	836	CLA	CAA-C2A	2.00	1.57	1.54

All (1377) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	820	CLA	C4A-NA-C1A	12.37	112.27	106.71
13	A	833	CLA	C4A-NA-C1A	12.20	112.19	106.71
13	M	1601	CLA	C4A-NA-C1A	12.08	112.14	106.71
13	A	813	CLA	C4A-NA-C1A	11.91	112.06	106.71
13	A	821	CLA	C4A-NA-C1A	11.90	112.06	106.71
13	A	816	CLA	C4A-NA-C1A	11.86	112.04	106.71
13	B	812	CLA	C4A-NA-C1A	11.84	112.03	106.71
13	X	1701	CLA	C4A-NA-C1A	11.83	112.03	106.71
13	B	821	CLA	C4A-NA-C1A	11.81	112.02	106.71
13	J	101	CLA	C4A-NA-C1A	11.73	111.98	106.71
13	A	846	CLA	C4A-NA-C1A	11.64	111.94	106.71
13	B	836	CLA	C4A-NA-C1A	11.52	111.89	106.71
13	A	812	CLA	C4A-NA-C1A	11.50	111.87	106.71
13	A	837	CLA	C4A-NA-C1A	11.48	111.87	106.71
13	B	830	CLA	C4A-NA-C1A	11.44	111.85	106.71
13	B	818	CLA	C4A-NA-C1A	11.42	111.84	106.71
13	A	817	CLA	C4A-NA-C1A	11.36	111.81	106.71
13	F	1301	CLA	C4A-NA-C1A	11.34	111.81	106.71
13	B	822	CLA	C4A-NA-C1A	11.29	111.78	106.71
13	J	102	CLA	C4A-NA-C1A	11.26	111.77	106.71
13	A	823	CLA	C4A-NA-C1A	11.24	111.76	106.71
13	B	807	CLA	C4A-NA-C1A	11.21	111.75	106.71
13	B	804	CLA	C4A-NA-C1A	11.17	111.73	106.71
13	A	820	CLA	C4A-NA-C1A	11.16	111.72	106.71
13	A	814	CLA	C4A-NA-C1A	11.15	111.72	106.71
13	B	825	CLA	C4A-NA-C1A	11.13	111.71	106.71
13	B	833	CLA	C4A-NA-C1A	11.11	111.70	106.71
13	A	810	CLA	C4A-NA-C1A	11.10	111.70	106.71
13	A	808	CLA	C4A-NA-C1A	11.06	111.68	106.71
13	A	845	CLA	C4A-NA-C1A	11.03	111.67	106.71
13	A	841	CLA	C4A-NA-C1A	11.00	111.65	106.71
13	A	832	CLA	C4A-NA-C1A	10.99	111.65	106.71
13	A	836	CLA	C4A-NA-C1A	10.98	111.64	106.71
13	B	826	CLA	C4A-NA-C1A	10.97	111.64	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	810	CLA	C4A-NA-C1A	10.97	111.64	106.71
13	A	809	CLA	C4A-NA-C1A	10.93	111.62	106.71
13	A	828	CLA	C4A-NA-C1A	10.92	111.62	106.71
13	A	838	CLA	C4A-NA-C1A	10.87	111.59	106.71
13	B	838	CLA	C4A-NA-C1A	10.84	111.58	106.71
13	B	819	CLA	C4A-NA-C1A	10.81	111.57	106.71
13	B	841	CLA	C4A-NA-C1A	10.76	111.54	106.71
13	A	805	CLA	C4A-NA-C1A	10.76	111.54	106.71
13	A	819	CLA	C4A-NA-C1A	10.71	111.52	106.71
13	B	831	CLA	C4A-NA-C1A	10.71	111.52	106.71
13	B	817	CLA	C4A-NA-C1A	10.67	111.50	106.71
13	B	823	CLA	C4A-NA-C1A	10.64	111.49	106.71
13	B	814	CLA	C4A-NA-C1A	10.63	111.49	106.71
13	A	827	CLA	C4A-NA-C1A	10.60	111.47	106.71
13	A	822	CLA	C4A-NA-C1A	10.57	111.46	106.71
13	B	801	CLA	C4A-NA-C1A	10.57	111.46	106.71
13	B	834	CLA	C4A-NA-C1A	10.56	111.45	106.71
13	B	815	CLA	C4A-NA-C1A	10.52	111.44	106.71
13	A	825	CLA	C4A-NA-C1A	10.51	111.43	106.71
13	B	824	CLA	C4A-NA-C1A	10.46	111.41	106.71
13	A	842	CLA	C4A-NA-C1A	10.45	111.40	106.71
13	A	804	CLA	C4A-NA-C1A	10.44	111.40	106.71
13	B	811	CLA	C4A-NA-C1A	10.44	111.40	106.71
13	A	815	CLA	C4A-NA-C1A	10.43	111.39	106.71
13	B	832	CLA	C4A-NA-C1A	10.41	111.39	106.71
13	L	1003	CLA	C4A-NA-C1A	10.41	111.39	106.71
13	L	1002	CLA	C4A-NA-C1A	10.36	111.36	106.71
13	A	843	CLA	C4A-NA-C1A	10.33	111.35	106.71
13	B	827	CLA	C4A-NA-C1A	10.32	111.35	106.71
13	A	830	CLA	C4A-NA-C1A	10.31	111.34	106.71
13	B	809	CLA	C4A-NA-C1A	10.28	111.33	106.71
13	A	811	CLA	C4A-NA-C1A	10.27	111.32	106.71
13	A	826	CLA	C4A-NA-C1A	10.23	111.31	106.71
13	K	1401	CLA	C4A-NA-C1A	10.22	111.30	106.71
13	B	835	CLA	C4A-NA-C1A	10.20	111.29	106.71
13	A	807	CLA	C4A-NA-C1A	10.13	111.26	106.71
13	B	816	CLA	C4A-NA-C1A	10.12	111.26	106.71
13	A	824	CLA	C4A-NA-C1A	10.08	111.24	106.71
13	A	818	CLA	C4A-NA-C1A	10.02	111.21	106.71
13	L	1004	CLA	C4A-NA-C1A	9.99	111.20	106.71
13	A	839	CLA	C4A-NA-C1A	9.99	111.20	106.71
13	B	837	CLA	C4A-NA-C1A	9.98	111.19	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	840	CLA	C4A-NA-C1A	9.87	111.14	106.71
13	A	806	CLA	C4A-NA-C1A	9.83	111.12	106.71
13	B	829	CLA	C4A-NA-C1A	9.78	111.10	106.71
13	A	831	CLA	C4A-NA-C1A	9.77	111.10	106.71
13	A	834	CLA	C4A-NA-C1A	9.72	111.08	106.71
13	B	803	CLA	C4A-NA-C1A	9.68	111.06	106.71
13	A	829	CLA	C4A-NA-C1A	9.66	111.05	106.71
13	B	806	CLA	C4A-NA-C1A	9.66	111.05	106.71
13	A	844	CLA	C4A-NA-C1A	9.65	111.04	106.71
13	B	802	CLA	C4A-NA-C1A	9.56	111.01	106.71
13	A	835	CLA	C4A-NA-C1A	9.51	110.98	106.71
13	B	805	CLA	C4A-NA-C1A	9.48	110.97	106.71
13	B	839	CLA	C4A-NA-C1A	9.44	110.95	106.71
13	A	840	CLA	C4A-NA-C1A	9.41	110.94	106.71
13	A	803	CLA	C4A-NA-C1A	9.31	110.89	106.71
13	B	813	CLA	C4A-NA-C1A	9.28	110.88	106.71
13	A	802	CLA	C4A-NA-C1A	9.15	110.82	106.71
13	A	801	CLA	C4A-NA-C1A	9.08	110.79	106.71
13	B	828	CLA	C4A-NA-C1A	8.90	110.71	106.71
13	B	808	CLA	C4A-NA-C1A	8.84	110.68	106.71
13	A	801	CLA	O2D-CGD-CBD	8.51	126.39	111.27
14	B	842	PQN	C11-C12-C13	-8.16	113.20	126.79
14	A	847	PQN	C11-C12-C13	-8.06	113.38	126.79
14	A	847	PQN	C14-C13-C15	7.41	127.74	115.27
14	A	847	PQN	C15-C13-C12	-7.25	106.45	121.12
13	A	801	CLA	C4D-C3D-CAD	-7.03	104.55	108.47
13	A	801	CLA	C3D-CAD-CBD	-6.67	98.82	107.61
14	B	842	PQN	C14-C13-C15	6.37	125.98	115.27
17	A	855	LHG	C25-C24-C23	6.20	136.17	113.62
14	B	842	PQN	C15-C13-C12	-6.15	108.68	121.12
18	B	850	LMG	C30-C29-C28	6.13	135.91	113.62
16	B	843	BCR	C38-C26-C25	5.94	131.20	124.53
16	B	844	BCR	C38-C26-C25	5.78	131.02	124.53
16	A	853	BCR	C38-C26-C25	5.55	130.76	124.53
13	A	801	CLA	O1D-CGD-CBD	-5.26	113.72	124.48
16	A	849	BCR	C38-C26-C25	5.11	130.27	124.53
16	B	848	BCR	C33-C5-C6	5.11	130.27	124.53
16	J	103	BCR	C38-C26-C25	5.10	130.26	124.53
16	L	1006	BCR	C33-C5-C6	5.10	130.26	124.53
16	L	1005	BCR	C33-C5-C6	4.88	130.01	124.53
13	B	829	CLA	O2D-CGD-CBD	4.88	119.93	111.27
13	B	802	CLA	O2D-CGD-CBD	4.88	119.93	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	835	CLA	O2D-CGD-CBD	4.84	119.87	111.27
17	A	856	LHG	C25-C24-C23	4.84	137.56	114.15
13	B	804	CLA	O2D-CGD-CBD	4.74	119.69	111.27
16	J	105	BCR	C33-C5-C6	4.73	129.84	124.53
16	B	845	BCR	C33-C5-C6	4.72	129.83	124.53
13	A	807	CLA	CAA-C2A-C3A	-4.71	99.87	112.78
16	I	101	BCR	C33-C5-C6	4.68	129.79	124.53
13	L	1002	CLA	O2D-CGD-CBD	4.66	119.56	111.27
13	A	807	CLA	O2A-CGA-CBA	4.66	126.53	111.91
16	A	851	BCR	C38-C26-C25	4.65	129.75	124.53
16	B	843	BCR	C33-C5-C6	4.65	129.75	124.53
16	B	847	BCR	C33-C5-C6	4.65	129.75	124.53
16	J	105	BCR	C38-C26-C25	4.58	129.68	124.53
13	A	805	CLA	O2D-CGD-CBD	4.57	119.39	111.27
13	B	808	CLA	O2D-CGD-CBD	4.54	119.33	111.27
16	F	1302	BCR	C38-C26-C25	4.50	129.59	124.53
16	A	850	BCR	C38-C26-C25	4.49	129.57	124.53
13	A	846	CLA	O2D-CGD-CBD	4.48	119.24	111.27
13	B	833	CLA	O2D-CGD-CBD	4.48	119.23	111.27
13	A	822	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
13	B	814	CLA	O2D-CGD-CBD	4.46	119.19	111.27
16	L	1006	BCR	C38-C26-C25	4.45	129.52	124.53
16	B	845	BCR	C7-C8-C9	4.43	132.93	126.23
16	M	1602	BCR	C38-C26-C25	4.38	129.44	124.53
13	B	818	CLA	CMB-C2B-C1B	-4.37	121.75	128.46
13	B	827	CLA	O2A-CGA-CBA	4.37	125.61	111.91
13	A	820	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
16	I	101	BCR	C38-C26-C25	4.36	129.42	124.53
16	B	848	BCR	C38-C26-C25	4.36	129.42	124.53
16	A	852	BCR	C38-C26-C25	4.34	129.40	124.53
16	A	851	BCR	C33-C5-C6	4.33	129.39	124.53
13	B	815	CLA	O2D-CGD-CBD	4.32	118.94	111.27
16	B	845	BCR	C38-C26-C25	4.31	129.37	124.53
16	A	849	BCR	C33-C5-C6	4.31	129.37	124.53
16	A	854	BCR	C7-C8-C9	4.30	132.74	126.23
13	A	828	CLA	O2D-CGD-CBD	4.27	118.85	111.27
13	B	825	CLA	O2D-CGD-CBD	4.25	118.82	111.27
16	B	845	BCR	C29-C30-C25	4.25	117.02	110.48
13	A	816	CLA	O2D-CGD-CBD	4.24	118.80	111.27
13	A	826	CLA	O2D-CGD-CBD	4.20	118.73	111.27
16	L	1005	BCR	C38-C26-C25	4.18	129.22	124.53
13	A	804	CLA	O2D-CGD-CBD	4.18	118.69	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	809	CLA	O2D-CGD-CBD	4.15	118.65	111.27
13	A	831	CLA	O2D-CGD-CBD	4.14	118.62	111.27
16	B	844	BCR	C33-C5-C6	4.11	129.15	124.53
13	B	820	CLA	O2D-CGD-CBD	4.11	118.58	111.27
16	B	846	BCR	C38-C26-C25	4.10	129.13	124.53
13	B	829	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
13	B	832	CLA	O2D-CGD-CBD	4.07	118.50	111.27
13	M	1601	CLA	O2D-CGD-CBD	4.07	118.50	111.27
16	I	101	BCR	C2-C1-C6	4.07	116.75	110.48
16	J	103	BCR	C33-C5-C6	4.06	129.09	124.53
13	A	838	CLA	O2A-CGA-CBA	4.06	124.65	111.91
13	A	832	CLA	O2D-CGD-CBD	4.05	118.47	111.27
13	A	801	CLA	OBD-CAD-C3D	4.05	134.70	127.98
16	I	102	BCR	C38-C26-C25	4.04	129.07	124.53
16	A	854	BCR	C33-C5-C6	4.03	129.06	124.53
13	A	840	CLA	O2A-CGA-CBA	4.03	124.56	111.91
13	A	830	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
16	J	105	BCR	C8-C7-C6	4.03	138.51	127.20
13	A	803	CLA	O2A-CGA-CBA	4.03	124.54	111.91
16	A	853	BCR	C38-C26-C27	-4.02	105.90	113.62
13	B	837	CLA	O2D-CGD-CBD	3.99	118.36	111.27
13	B	830	CLA	O2D-CGD-CBD	3.98	118.34	111.27
16	I	102	BCR	C24-C23-C22	3.97	132.24	126.23
16	A	850	BCR	C33-C5-C6	3.97	128.98	124.53
16	F	1302	BCR	C33-C5-C6	3.97	128.98	124.53
13	B	821	CLA	O2D-CGD-CBD	3.96	118.30	111.27
13	B	828	CLA	O2A-CGA-CBA	3.95	124.32	111.91
13	A	824	CLA	O2D-CGD-CBD	3.95	118.29	111.27
13	B	813	CLA	O2D-CGD-CBD	3.95	118.29	111.27
16	B	849	BCR	C33-C5-C6	3.94	128.96	124.53
16	A	854	BCR	C38-C26-C25	3.93	128.94	124.53
13	A	802	CLA	C4D-C3D-CAD	-3.93	106.28	108.47
16	B	847	BCR	C38-C26-C25	3.92	128.93	124.53
13	B	826	CLA	O2D-CGD-CBD	3.92	118.23	111.27
13	J	101	CLA	O2D-CGD-CBD	3.92	118.22	111.27
16	B	843	BCR	C38-C26-C27	-3.90	106.12	113.62
13	B	805	CLA	O2D-CGD-CBD	3.90	118.20	111.27
16	B	849	BCR	C38-C26-C25	3.89	128.90	124.53
16	B	844	BCR	C7-C8-C9	3.88	132.10	126.23
13	K	1401	CLA	O2D-CGD-CBD	3.88	118.16	111.27
13	A	806	CLA	O2D-CGD-CBD	3.87	118.15	111.27
16	A	854	BCR	C24-C23-C22	3.85	132.06	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	J	105	BCR	C2-C1-C6	3.83	116.38	110.48
16	A	852	BCR	C33-C5-C6	3.82	128.82	124.53
13	A	843	CLA	O2A-CGA-CBA	3.82	123.89	111.91
13	A	810	CLA	O2A-CGA-CBA	3.81	123.88	111.91
13	B	827	CLA	CBA-CAA-C2A	3.81	125.12	113.86
13	B	824	CLA	O2D-CGD-CBD	3.81	118.04	111.27
16	M	1602	BCR	C24-C23-C22	3.81	131.99	126.23
13	A	823	CLA	O2D-CGD-CBD	3.80	118.02	111.27
13	A	814	CLA	O2D-CGD-CBD	3.80	118.01	111.27
13	A	821	CLA	O2A-CGA-CBA	3.79	123.81	111.91
13	A	820	CLA	O2A-CGA-CBA	3.79	123.81	111.91
13	B	808	CLA	O2A-CGA-CBA	3.79	123.79	111.91
13	A	844	CLA	O2A-CGA-CBA	3.78	123.78	111.91
13	A	823	CLA	O2A-CGA-CBA	3.78	123.77	111.91
13	B	818	CLA	O2A-CGA-CBA	3.78	123.77	111.91
13	A	832	CLA	C1D-CHD-C4C	3.77	127.53	122.56
13	B	826	CLA	CMB-C2B-C1B	-3.77	122.68	128.46
13	A	846	CLA	O2A-CGA-CBA	3.76	123.72	111.91
16	A	854	BCR	C2-C1-C6	3.76	116.27	110.48
13	B	831	CLA	O2D-CGD-CBD	3.75	117.94	111.27
16	B	848	BCR	C7-C8-C9	3.75	131.90	126.23
13	B	814	CLA	C1-C2-C3	3.74	132.52	126.04
13	B	802	CLA	OBD-CAD-CBD	-3.74	120.56	125.89
13	A	802	CLA	OBD-CAD-CBD	-3.73	120.56	125.89
16	A	854	BCR	C40-C30-C25	3.73	116.34	110.30
13	B	834	CLA	O2D-CGD-CBD	3.72	117.88	111.27
13	A	842	CLA	O2A-CGA-CBA	3.71	123.57	111.91
13	A	846	CLA	C1-C2-C3	3.71	132.46	126.04
16	B	843	BCR	C2-C1-C6	3.71	116.19	110.48
16	J	103	BCR	C29-C30-C25	3.70	116.17	110.48
13	A	807	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
13	A	824	CLA	O2A-CGA-CBA	3.67	123.44	111.91
16	B	844	BCR	C38-C26-C27	-3.67	106.57	113.62
16	A	851	BCR	C29-C30-C25	3.66	116.11	110.48
16	J	104	BCR	C33-C5-C6	3.65	128.63	124.53
13	A	830	CLA	O2A-CGA-CBA	3.65	123.35	111.91
16	B	844	BCR	C30-C25-C26	-3.64	117.48	122.61
13	A	833	CLA	C1D-CHD-C4C	3.64	127.37	122.56
16	B	848	BCR	C33-C5-C4	-3.64	106.62	113.62
16	B	844	BCR	C24-C23-C22	3.63	131.72	126.23
13	B	820	CLA	O2A-CGA-CBA	3.63	123.31	111.91
16	I	102	BCR	C33-C5-C6	3.62	128.59	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	817	CLA	O2A-CGA-CBA	3.61	123.25	111.91
13	B	807	CLA	O2D-CGD-CBD	3.61	117.69	111.27
13	A	830	CLA	O2D-CGD-CBD	3.61	117.68	111.27
16	M	1602	BCR	C33-C5-C6	3.61	128.58	124.53
13	B	835	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
16	A	851	BCR	C38-C26-C27	-3.60	106.70	113.62
13	A	840	CLA	O2D-CGD-CBD	3.59	117.65	111.27
13	A	813	CLA	O2A-CGA-CBA	3.59	123.16	111.91
13	A	819	CLA	O2A-CGA-CBA	3.59	123.16	111.91
13	B	809	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
16	A	852	BCR	C24-C23-C22	3.58	131.64	126.23
16	J	104	BCR	C2-C1-C6	3.57	115.98	110.48
16	J	103	BCR	C38-C26-C27	-3.57	106.77	113.62
16	B	847	BCR	C7-C8-C9	3.56	131.62	126.23
13	L	1004	CLA	O2D-CGD-CBD	3.56	117.60	111.27
13	A	817	CLA	O2D-CGD-CBD	3.56	117.60	111.27
13	B	812	CLA	C1D-CHD-C4C	3.56	127.26	122.56
16	J	105	BCR	C24-C23-C22	3.56	131.61	126.23
13	A	821	CLA	O2D-CGD-CBD	3.55	117.58	111.27
16	A	853	BCR	C33-C5-C6	3.55	128.52	124.53
16	J	104	BCR	C29-C30-C25	3.55	115.95	110.48
16	A	849	BCR	C38-C26-C27	-3.55	106.80	113.62
13	A	837	CLA	C1D-CHD-C4C	3.55	127.24	122.56
13	B	816	CLA	O2D-CGD-CBD	3.54	117.55	111.27
16	A	851	BCR	C24-C23-C22	3.54	131.58	126.23
13	X	1701	CLA	O2D-CGD-CBD	3.53	117.54	111.27
13	A	821	CLA	C1D-CHD-C4C	3.53	127.21	122.56
16	B	845	BCR	C38-C26-C27	-3.53	106.84	113.62
13	A	809	CLA	O2A-CGA-CBA	3.52	122.96	111.91
13	B	812	CLA	O2D-CGD-CBD	3.52	117.52	111.27
13	A	808	CLA	O2A-CGA-CBA	3.52	122.96	111.91
13	A	833	CLA	O2D-CGD-CBD	3.52	117.52	111.27
13	B	804	CLA	O2A-CGA-CBA	3.51	122.92	111.91
13	B	813	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
13	J	102	CLA	OBD-CAD-C3D	3.50	130.76	127.19
13	B	841	CLA	OBD-CAD-CBD	-3.49	120.90	125.89
13	A	822	CLA	CMB-C2B-C3B	3.49	131.21	124.68
13	A	827	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
13	A	833	CLA	C1-C2-C3	3.49	132.07	126.04
17	A	856	LHG	O8-C23-C24	3.48	120.52	111.38
13	L	1003	CLA	O2D-CGD-CBD	3.48	117.46	111.27
13	M	1601	CLA	C1D-CHD-C4C	3.48	127.15	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	102	BCR	C33-C5-C4	-3.48	106.93	113.62
13	B	816	CLA	O2A-CGA-CBA	3.47	122.81	111.91
13	A	834	CLA	O2D-CGD-CBD	3.47	117.44	111.27
13	B	805	CLA	OBD-CAD-CBD	-3.47	120.94	125.89
13	J	101	CLA	C1D-CHD-C4C	3.47	127.14	122.56
16	A	850	BCR	C38-C26-C27	-3.46	106.97	113.62
13	A	815	CLA	O2D-CGD-CBD	3.46	117.41	111.27
13	B	838	CLA	O2D-CGD-CBD	3.46	117.41	111.27
16	I	102	BCR	C38-C26-C27	-3.45	106.98	113.62
13	A	827	CLA	O2D-CGD-CBD	3.44	117.39	111.27
16	B	844	BCR	C29-C30-C25	3.44	115.78	110.48
13	B	827	CLA	O2D-CGD-CBD	3.43	117.36	111.27
13	A	842	CLA	O2D-CGD-CBD	3.42	117.35	111.27
13	B	825	CLA	C1D-CHD-C4C	3.42	127.08	122.56
13	B	830	CLA	C1D-CHD-C4C	3.42	127.07	122.56
13	A	828	CLA	O2A-CGA-CBA	3.42	122.64	111.91
13	B	841	CLA	O2D-CGD-CBD	3.42	117.35	111.27
13	B	820	CLA	C1D-CHD-C4C	3.42	127.07	122.56
13	B	807	CLA	OBD-CAD-CBD	-3.41	121.02	125.89
13	J	102	CLA	C1D-CHD-C4C	3.41	127.06	122.56
13	B	818	CLA	O2D-CGD-CBD	3.41	117.32	111.27
13	A	838	CLA	O2D-CGD-CBD	3.40	117.32	111.27
13	B	823	CLA	O2D-CGD-CBD	3.40	117.31	111.27
16	A	853	BCR	C24-C23-C22	3.40	131.38	126.23
16	J	103	BCR	C2-C1-C6	3.39	115.70	110.48
16	L	1005	BCR	C33-C5-C4	-3.39	107.10	113.62
16	A	854	BCR	C29-C30-C25	3.38	115.69	110.48
13	L	1004	CLA	C1D-CHD-C4C	3.38	127.02	122.56
13	B	825	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
16	B	846	BCR	C20-C21-C22	3.38	132.13	127.31
16	B	848	BCR	C29-C30-C25	3.38	115.68	110.48
13	A	812	CLA	O2A-CGA-CBA	3.37	122.49	111.91
13	A	836	CLA	C1-C2-C3	3.37	131.87	126.04
16	B	845	BCR	C2-C1-C6	3.37	115.67	110.48
13	B	829	CLA	CMB-C2B-C3B	3.37	130.98	124.68
16	F	1302	BCR	C15-C14-C13	3.37	132.12	127.31
13	A	816	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
13	A	802	CLA	O2D-CGD-CBD	3.36	117.24	111.27
16	B	847	BCR	C33-C5-C4	-3.35	107.18	113.62
16	A	849	BCR	C29-C30-C25	3.35	115.64	110.48
13	F	1301	CLA	C1D-CHD-C4C	3.35	126.98	122.56
16	A	850	BCR	C2-C1-C6	3.35	115.63	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	838	CLA	C1-C2-C3	3.34	131.82	126.04
16	J	103	BCR	C23-C24-C25	3.34	136.57	127.20
16	B	846	BCR	C38-C26-C27	-3.34	107.20	113.62
13	A	805	CLA	O2A-CGA-CBA	3.33	122.37	111.91
16	B	845	BCR	C33-C5-C4	-3.33	107.22	113.62
16	J	105	BCR	C38-C26-C27	-3.33	107.22	113.62
16	M	1602	BCR	C2-C1-C6	3.33	115.60	110.48
13	A	837	CLA	O2D-CGD-CBD	3.33	117.18	111.27
13	A	810	CLA	C1D-CHD-C4C	3.33	126.95	122.56
13	X	1701	CLA	C1D-CHD-C4C	3.33	126.95	122.56
13	B	837	CLA	C1-C2-C3	3.32	131.79	126.04
13	A	810	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
16	B	848	BCR	C2-C1-C6	3.32	115.59	110.48
13	L	1002	CLA	O2A-CGA-CBA	3.32	122.33	111.91
16	I	101	BCR	C38-C26-C27	-3.31	107.26	113.62
13	B	838	CLA	O2A-CGA-CBA	3.31	122.29	111.91
16	J	105	BCR	C33-C5-C4	-3.31	107.27	113.62
16	B	843	BCR	C23-C24-C25	3.31	136.49	127.20
16	B	849	BCR	C2-C1-C6	3.30	115.56	110.48
16	B	847	BCR	C2-C1-C6	3.29	115.55	110.48
13	A	846	CLA	C1D-CHD-C4C	3.29	126.91	122.56
13	A	806	CLA	C1D-CHD-C4C	3.29	126.90	122.56
13	B	822	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
13	B	822	CLA	C1-C2-C3	3.28	131.72	126.04
13	A	808	CLA	O2D-CGD-CBD	3.28	117.10	111.27
13	B	840	CLA	C1-C2-C3	3.28	131.72	126.04
13	B	805	CLA	C1-C2-C3	3.28	131.72	126.04
16	J	105	BCR	C29-C30-C25	3.28	115.53	110.48
16	B	843	BCR	C30-C25-C26	-3.27	118.00	122.61
13	A	836	CLA	O2D-CGD-CBD	3.27	117.08	111.27
13	B	805	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
16	B	843	BCR	C33-C5-C4	-3.27	107.34	113.62
13	A	816	CLA	C1D-CHD-C4C	3.27	126.87	122.56
13	A	813	CLA	O2D-CGD-CBD	3.27	117.07	111.27
13	B	802	CLA	C4D-C3D-CAD	-3.26	106.65	108.47
13	A	832	CLA	O2A-CGA-CBA	3.25	122.12	111.91
13	A	804	CLA	O2A-CGA-CBA	3.25	122.11	111.91
13	B	832	CLA	C1D-CHD-C4C	3.25	126.85	122.56
13	A	801	CLA	O2A-CGA-CBA	3.25	122.10	111.91
13	B	817	CLA	OBD-CAD-CBD	-3.24	121.26	125.89
13	A	818	CLA	O2D-CGD-CBD	3.24	117.03	111.27
13	A	817	CLA	O2A-CGA-CBA	3.24	122.09	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	1006	BCR	C2-C1-C6	3.24	115.47	110.48
13	A	829	CLA	O2A-CGA-CBA	3.24	122.08	111.91
16	B	848	BCR	C38-C26-C27	-3.24	107.39	113.62
13	A	822	CLA	C1D-CHD-C4C	3.24	126.83	122.56
16	B	843	BCR	C24-C23-C22	3.24	131.12	126.23
13	A	823	CLA	C1D-CHD-C4C	3.23	126.83	122.56
16	F	1302	BCR	C2-C1-C6	3.23	115.46	110.48
13	A	844	CLA	O2A-CGA-O1A	-3.23	115.44	123.59
13	B	818	CLA	CMB-C2B-C3B	3.23	130.71	124.68
16	L	1006	BCR	C33-C5-C4	-3.22	107.42	113.62
16	A	852	BCR	C38-C26-C27	-3.22	107.42	113.62
13	A	833	CLA	O2A-CGA-CBA	3.22	122.02	111.91
16	F	1302	BCR	C33-C5-C4	-3.22	107.43	113.62
13	B	810	CLA	O2A-CGA-CBA	3.22	122.01	111.91
13	A	806	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
13	B	807	CLA	O2A-CGA-CBA	3.22	122.00	111.91
16	A	853	BCR	C29-C30-C25	3.21	115.43	110.48
13	A	834	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
13	B	836	CLA	O2D-CGD-CBD	3.21	116.97	111.27
17	A	855	LHG	O8-C23-C24	3.21	121.97	111.91
13	A	841	CLA	O2A-CGA-CBA	3.20	121.96	111.91
16	J	104	BCR	C38-C26-C25	3.20	128.13	124.53
16	A	851	BCR	C33-C5-C4	-3.20	107.46	113.62
13	B	821	CLA	C1D-CHD-C4C	3.20	126.78	122.56
13	A	803	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
16	M	1602	BCR	C29-C30-C25	3.20	115.40	110.48
13	B	836	CLA	C1D-CHD-C4C	3.20	126.78	122.56
13	A	836	CLA	O2A-CGA-CBA	3.19	121.93	111.91
16	A	849	BCR	C33-C5-C4	-3.19	107.48	113.62
16	F	1302	BCR	C38-C26-C27	-3.19	107.48	113.62
13	B	807	CLA	C1D-CHD-C4C	3.19	126.77	122.56
13	A	829	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
13	B	817	CLA	C1D-CHD-C4C	3.19	126.76	122.56
16	L	1005	BCR	C38-C26-C27	-3.19	107.50	113.62
13	B	840	CLA	CED-O2D-CGD	3.18	123.14	115.94
13	A	814	CLA	C1D-CHD-C4C	3.18	126.75	122.56
16	B	843	BCR	C29-C30-C25	3.17	115.37	110.48
13	A	802	CLA	C1-C2-C3	3.17	131.53	126.04
13	A	839	CLA	O2A-CGA-CBA	3.17	121.86	111.91
16	A	852	BCR	C29-C30-C25	3.17	115.36	110.48
13	B	826	CLA	O2A-CGA-CBA	3.17	121.85	111.91
16	A	849	BCR	C30-C25-C26	-3.17	118.15	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	822	CLA	C1D-CHD-C4C	3.16	126.73	122.56
13	A	845	CLA	OBD-CAD-C3D	3.16	130.41	127.19
13	A	845	CLA	C1D-CHD-C4C	3.16	126.73	122.56
16	B	844	BCR	C33-C5-C4	-3.15	107.56	113.62
13	A	817	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
13	B	805	CLA	O2A-CGA-CBA	3.15	121.80	111.91
13	A	810	CLA	O2D-CGD-CBD	3.15	116.87	111.27
13	A	805	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
16	J	104	BCR	C7-C8-C9	3.15	130.99	126.23
13	A	806	CLA	O2A-CGA-CBA	3.15	121.79	111.91
13	B	824	CLA	C1D-CHD-C4C	3.15	126.71	122.56
13	A	822	CLA	CED-O2D-CGD	3.15	123.06	115.94
16	F	1302	BCR	C29-C30-C25	3.15	115.32	110.48
13	A	814	CLA	O2A-CGA-CBA	3.15	121.78	111.91
13	B	809	CLA	O2D-CGD-CBD	3.14	116.86	111.27
13	B	832	CLA	O2A-CGA-CBA	3.14	121.76	111.91
13	B	813	CLA	O2A-CGA-CBA	3.13	121.73	111.91
13	B	838	CLA	OBD-CAD-CBD	-3.13	121.42	125.89
13	B	832	CLA	OBD-CAD-CBD	-3.13	121.42	125.89
13	B	802	CLA	O2A-CGA-CBA	3.13	121.72	111.91
13	F	1301	CLA	O2D-CGD-CBD	3.13	116.82	111.27
16	A	854	BCR	C33-C5-C4	-3.13	107.61	113.62
13	B	819	CLA	C1D-CHD-C4C	3.12	126.68	122.56
13	A	841	CLA	CED-O2D-CGD	3.12	122.99	115.94
13	L	1002	CLA	OBD-CAD-CBD	-3.12	121.44	125.89
13	A	820	CLA	C1D-CHD-C4C	3.12	126.67	122.56
13	B	833	CLA	C1-C2-C3	3.12	131.43	126.04
16	A	852	BCR	C2-C1-C6	3.11	115.28	110.48
13	K	1401	CLA	C1D-CHD-C4C	3.11	126.67	122.56
13	B	801	CLA	C7-C6-C5	-3.11	104.91	113.36
13	B	808	CLA	O1D-CGD-CBD	-3.11	118.12	124.48
13	B	827	CLA	OBD-CAD-CBD	-3.11	121.46	125.89
13	A	806	CLA	OBD-CAD-CBD	-3.10	121.47	125.89
13	B	818	CLA	C1D-CHD-C4C	3.10	126.65	122.56
13	A	832	CLA	OBD-CAD-CBD	-3.10	121.47	125.89
13	A	803	CLA	CED-O2D-CGD	3.09	122.94	115.94
13	B	835	CLA	C1D-CHD-C4C	3.09	126.64	122.56
13	A	838	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
13	A	803	CLA	O2A-CGA-O1A	-3.09	115.79	123.59
13	A	804	CLA	C1D-CHD-C4C	3.09	126.64	122.56
16	M	1602	BCR	C38-C26-C27	-3.09	107.69	113.62
13	A	811	CLA	CMB-C2B-C1B	-3.09	123.72	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	824	CLA	C1-C2-C3	3.08	131.38	126.04
13	B	810	CLA	O2D-CGD-CBD	3.08	116.75	111.27
13	A	822	CLA	OBD-CAD-CBD	-3.08	121.49	125.89
16	B	847	BCR	C38-C26-C27	-3.08	107.70	113.62
13	A	817	CLA	C1D-CHD-C4C	3.08	126.62	122.56
13	A	843	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
13	B	839	CLA	O2A-CGA-CBA	3.07	121.55	111.91
13	A	825	CLA	O2D-CGD-CBD	3.07	116.73	111.27
13	B	803	CLA	O2A-CGA-CBA	3.07	121.54	111.91
16	B	843	BCR	C7-C8-C9	3.07	130.87	126.23
13	B	823	CLA	C1D-CHD-C4C	3.07	126.61	122.56
13	A	830	CLA	CMB-C2B-C3B	3.07	130.42	124.68
13	B	819	CLA	O2D-CGD-CBD	3.06	116.71	111.27
18	B	850	LMG	O8-C28-C29	3.06	121.52	111.91
16	J	103	BCR	C30-C25-C26	-3.06	118.30	122.61
13	B	827	CLA	C1D-CHD-C4C	3.06	126.60	122.56
13	A	815	CLA	OBD-CAD-CBD	-3.06	121.52	125.89
16	A	851	BCR	C2-C1-C6	3.06	115.19	110.48
16	A	850	BCR	C33-C5-C4	-3.05	107.75	113.62
16	L	1005	BCR	C24-C23-C22	3.05	130.84	126.23
13	B	834	CLA	C1D-CHD-C4C	3.05	126.58	122.56
13	A	817	CLA	CED-O2D-CGD	3.05	122.83	115.94
13	B	827	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
16	J	105	BCR	C1-C6-C5	-3.05	118.32	122.61
13	B	803	CLA	OBD-CAD-CBD	-3.05	121.54	125.89
13	A	826	CLA	O2A-CGA-CBA	3.05	121.47	111.91
16	A	853	BCR	C30-C25-C26	-3.05	118.32	122.61
13	A	819	CLA	OBD-CAD-CBD	-3.04	121.55	125.89
13	B	829	CLA	O2A-CGA-CBA	3.04	121.44	111.91
13	B	801	CLA	O2A-CGA-CBA	3.04	121.44	111.91
13	A	821	CLA	C1-C2-C3	3.04	131.30	126.04
13	A	819	CLA	C1D-CHD-C4C	3.04	126.56	122.56
13	A	806	CLA	CAA-C2A-C3A	-3.04	104.47	112.78
16	B	849	BCR	C7-C8-C9	3.03	130.82	126.23
13	J	102	CLA	CAA-C2A-C3A	-3.02	109.04	116.10
13	B	837	CLA	C1D-CHD-C4C	3.02	126.55	122.56
13	A	814	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
13	B	822	CLA	O2D-CGD-CBD	3.02	116.64	111.27
13	B	840	CLA	OBD-CAD-CBD	-3.02	121.58	125.89
16	B	849	BCR	C38-C26-C27	-3.02	107.81	113.62
16	A	849	BCR	C2-C1-C6	3.02	115.13	110.48
13	L	1004	CLA	OBD-CAD-CBD	-3.02	121.58	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	823	CLA	OBD-CAD-CBD	-3.02	121.58	125.89
13	B	824	CLA	OBD-CAD-CBD	-3.02	121.59	125.89
13	A	801	CLA	C1D-CHD-C4C	3.02	126.54	122.56
13	A	837	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
13	B	824	CLA	O2A-CGA-CBA	3.01	121.36	111.91
16	A	854	BCR	C38-C26-C27	-3.01	107.83	113.62
13	A	838	CLA	O2A-CGA-O1A	-3.01	116.00	123.59
13	A	830	CLA	C1D-CHD-C4C	3.01	126.53	122.56
13	A	819	CLA	O2D-CGD-CBD	3.01	116.61	111.27
16	B	848	BCR	C8-C9-C10	-3.01	114.33	118.94
16	B	844	BCR	C2-C1-C6	3.00	115.11	110.48
13	B	832	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
16	B	846	BCR	C29-C30-C25	3.00	115.10	110.48
13	A	807	CLA	C1D-CHD-C4C	3.00	126.52	122.56
13	M	1601	CLA	CED-O2D-CGD	3.00	122.72	115.94
13	B	841	CLA	O2A-CGA-CBA	3.00	121.31	111.91
13	B	838	CLA	CED-O2D-CGD	3.00	122.71	115.94
13	B	816	CLA	OBD-CAD-CBD	-2.99	121.62	125.89
13	B	813	CLA	C1D-CHD-C4C	2.99	126.51	122.56
13	B	822	CLA	O2A-CGA-CBA	2.99	121.29	111.91
13	A	811	CLA	O2D-CGD-CBD	2.99	116.58	111.27
13	A	807	CLA	CED-O2D-CGD	2.99	122.69	115.94
13	A	829	CLA	OBD-CAD-CBD	-2.99	121.63	125.89
13	B	815	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
17	B	851	LHG	O7-C7-C8	2.98	117.93	111.50
13	A	823	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
13	B	802	CLA	C1D-CHD-C4C	2.98	126.49	122.56
16	B	844	BCR	C1-C6-C5	-2.98	118.42	122.61
13	B	819	CLA	O2A-CGA-CBA	2.98	121.25	111.91
13	B	821	CLA	CMB-C2B-C1B	-2.97	123.89	128.46
13	B	839	CLA	O2D-CGD-CBD	2.97	116.55	111.27
13	B	806	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
16	B	843	BCR	C1-C6-C5	-2.97	118.43	122.61
13	A	836	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
13	B	834	CLA	OBD-CAD-CBD	-2.96	121.66	125.89
13	B	831	CLA	O2A-CGA-CBA	2.96	121.21	111.91
13	B	819	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
16	B	846	BCR	C24-C23-C22	2.96	130.71	126.23
13	A	815	CLA	C1D-CHD-C4C	2.96	126.47	122.56
13	A	836	CLA	C1D-CHD-C4C	2.96	126.47	122.56
13	B	803	CLA	CED-O2D-CGD	2.96	122.63	115.94
13	A	804	CLA	CMB-C2B-C1B	-2.96	123.91	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	818	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
16	J	104	BCR	C33-C5-C4	-2.96	107.93	113.62
13	B	809	CLA	O2A-CGA-CBA	2.96	121.19	111.91
17	A	855	LHG	O7-C7-C8	2.96	117.87	111.50
16	L	1005	BCR	C2-C1-C6	2.96	115.03	110.48
13	B	833	CLA	O2A-CGA-CBA	2.96	121.19	111.91
16	B	847	BCR	C24-C23-C22	2.96	130.70	126.23
13	A	813	CLA	C1D-CHD-C4C	2.96	126.46	122.56
13	B	814	CLA	C1D-CHD-C4C	2.96	126.46	122.56
13	B	817	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
13	B	814	CLA	OBD-CAD-CBD	-2.95	121.68	125.89
13	A	825	CLA	O2A-CGA-CBA	2.95	121.17	111.91
13	A	807	CLA	CMB-C2B-C3B	2.95	130.20	124.68
13	A	839	CLA	OBD-CAD-CBD	-2.95	121.68	125.89
13	B	801	CLA	OBD-CAD-CBD	-2.95	121.68	125.89
16	B	845	BCR	C24-C23-C22	2.94	130.68	126.23
13	A	846	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
13	L	1003	CLA	OBD-CAD-CBD	-2.94	121.69	125.89
13	A	838	CLA	C4-C3-C5	-2.94	112.62	115.98
16	A	851	BCR	C40-C30-C25	2.94	115.07	110.30
13	J	101	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
13	B	835	CLA	OBD-CAD-CBD	-2.94	121.69	125.89
13	A	821	CLA	OBD-CAD-CBD	-2.94	121.70	125.89
13	A	831	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
13	B	829	CLA	C1D-CHD-C4C	2.94	126.43	122.56
13	B	801	CLA	C1D-CHD-C4C	2.93	126.43	122.56
16	B	849	BCR	C33-C5-C4	-2.93	107.98	113.62
13	A	807	CLA	C2A-C3A-C4A	2.93	106.60	101.87
13	B	831	CLA	C1D-CHD-C4C	2.93	126.42	122.56
13	B	820	CLA	CED-O2D-CGD	2.93	122.56	115.94
13	A	818	CLA	C1D-CHD-C4C	2.93	126.42	122.56
13	B	812	CLA	CMB-C2B-C1B	-2.93	123.97	128.46
13	L	1004	CLA	O2A-CGA-CBA	2.93	121.09	111.91
13	L	1003	CLA	O2A-CGA-CBA	2.93	121.09	111.91
13	B	829	CLA	C1-C2-C3	2.92	131.10	126.04
13	A	827	CLA	CMB-C2B-C3B	2.92	130.15	124.68
13	A	835	CLA	OBD-CAD-CBD	-2.92	121.72	125.89
16	A	852	BCR	C33-C5-C4	-2.92	108.00	113.62
13	B	804	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
13	A	811	CLA	OBD-CAD-CBD	-2.92	121.72	125.89
16	B	849	BCR	C29-C30-C25	2.92	114.98	110.48
13	B	811	CLA	CED-O2D-CGD	2.92	122.54	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	826	CLA	C1D-CHD-C4C	2.92	126.41	122.56
13	B	838	CLA	C1D-CHD-C4C	2.91	126.40	122.56
13	A	822	CLA	C1-C2-C3	2.91	131.08	126.04
16	B	844	BCR	C23-C24-C25	2.91	135.38	127.20
16	L	1005	BCR	C30-C25-C24	2.91	124.01	115.78
16	A	850	BCR	C29-C30-C25	2.91	114.96	110.48
13	A	840	CLA	O2A-CGA-O1A	-2.91	116.25	123.59
13	B	818	CLA	OBD-CAD-CBD	-2.91	121.74	125.89
13	A	844	CLA	C1D-CHD-C4C	2.91	126.40	122.56
13	A	818	CLA	O2A-CGA-CBA	2.91	121.03	111.91
13	A	803	CLA	C1D-CHD-C4C	2.91	126.39	122.56
16	A	854	BCR	C16-C17-C18	2.91	131.46	127.31
13	X	1701	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
13	B	809	CLA	OBD-CAD-CBD	-2.90	121.75	125.89
16	A	852	BCR	C30-C25-C26	-2.90	118.53	122.61
16	J	103	BCR	C33-C5-C4	-2.90	108.05	113.62
16	M	1602	BCR	C1-C6-C5	-2.90	118.53	122.61
13	A	820	CLA	CMB-C2B-C3B	2.89	130.09	124.68
13	B	826	CLA	CMB-C2B-C3B	2.89	130.09	124.68
13	A	813	CLA	C1-C2-C3	2.89	131.04	126.04
13	B	823	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
13	A	824	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
13	B	839	CLA	OBD-CAD-CBD	-2.89	121.77	125.89
13	B	808	CLA	CAA-C2A-C3A	-2.89	104.87	112.78
16	I	101	BCR	C7-C8-C9	2.89	130.60	126.23
13	J	101	CLA	OBD-CAD-CBD	-2.89	121.77	125.89
13	A	820	CLA	O2D-CGD-CBD	2.88	116.39	111.27
16	A	849	BCR	C23-C24-C25	2.88	135.30	127.20
13	B	824	CLA	CED-O2D-CGD	2.88	122.46	115.94
13	B	820	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
13	B	816	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
16	J	103	BCR	C8-C7-C6	2.88	135.28	127.20
13	A	843	CLA	O2D-CGD-CBD	2.88	116.38	111.27
13	B	816	CLA	C1D-CHD-C4C	2.88	126.35	122.56
13	B	807	CLA	C4D-C3D-CAD	-2.87	106.87	108.47
16	B	848	BCR	C12-C13-C14	-2.87	114.53	118.94
13	A	827	CLA	O2A-CGA-CBA	2.87	120.92	111.91
16	M	1602	BCR	C1-C6-C7	2.87	123.90	115.78
13	B	813	CLA	C1-C2-C3	2.87	131.01	126.04
13	B	811	CLA	O2D-CGD-CBD	2.87	116.37	111.27
13	A	825	CLA	C1D-CHD-C4C	2.87	126.35	122.56
13	B	814	CLA	O2A-CGA-CBA	2.87	120.92	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	843	CLA	C1D-CHD-C4C	2.87	126.34	122.56
13	B	839	CLA	CMB-C2B-C1B	-2.87	124.06	128.46
13	B	828	CLA	C4-C3-C5	-2.87	110.45	115.27
16	I	101	BCR	C33-C5-C4	-2.87	108.11	113.62
16	B	845	BCR	C1-C6-C5	-2.87	118.58	122.61
16	F	1302	BCR	C24-C23-C22	2.86	130.56	126.23
13	B	817	CLA	O2D-CGD-CBD	2.86	116.36	111.27
13	L	1004	CLA	CMB-C2B-C1B	-2.86	124.06	128.46
17	A	856	LHG	O7-C7-C8	2.86	117.67	111.50
13	B	833	CLA	CED-O2D-CGD	2.86	122.41	115.94
13	B	806	CLA	O2D-CGD-CBD	2.86	116.35	111.27
13	B	825	CLA	CMB-C2B-C3B	2.86	130.03	124.68
16	A	851	BCR	C7-C8-C9	2.86	130.56	126.23
16	A	849	BCR	C24-C23-C22	2.86	130.56	126.23
13	B	822	CLA	CED-O2D-CGD	2.86	122.40	115.94
13	A	819	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
13	A	828	CLA	C1D-CHD-C4C	2.86	126.33	122.56
13	J	101	CLA	CED-O2D-CGD	2.85	122.38	115.94
13	A	807	CLA	CBA-CAA-C2A	2.85	122.27	113.86
13	A	834	CLA	O2A-CGA-CBA	2.85	120.84	111.91
13	A	809	CLA	OBD-CAD-CBD	-2.84	121.83	125.89
16	A	853	BCR	C2-C1-C6	2.84	114.86	110.48
13	B	816	CLA	C1-C2-C3	2.84	130.96	126.04
13	A	809	CLA	C1D-CHD-C4C	2.84	126.31	122.56
13	B	833	CLA	C1D-CHD-C4C	2.84	126.31	122.56
16	J	104	BCR	C30-C25-C24	2.84	123.82	115.78
13	B	834	CLA	CED-O2D-CGD	2.84	122.36	115.94
13	B	828	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
13	B	813	CLA	CMB-C2B-C3B	2.84	129.99	124.68
13	L	1002	CLA	C1D-CHD-C4C	2.84	126.30	122.56
16	B	848	BCR	C15-C14-C13	2.83	131.36	127.31
16	J	103	BCR	C36-C18-C19	2.83	122.54	118.08
13	A	814	CLA	OBD-CAD-CBD	-2.83	121.85	125.89
13	A	820	CLA	CED-O2D-CGD	2.83	122.34	115.94
13	B	802	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
13	B	841	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
13	A	840	CLA	C1D-CHD-C4C	2.82	126.29	122.56
13	A	824	CLA	C1D-CHD-C4C	2.82	126.29	122.56
13	B	835	CLA	CED-O2D-CGD	2.82	122.33	115.94
16	M	1602	BCR	C33-C5-C4	-2.82	108.19	113.62
13	B	814	CLA	CMB-C2B-C1B	-2.82	124.12	128.46
13	A	815	CLA	CMB-C2B-C1B	-2.82	124.13	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	841	CLA	C1D-CHD-C4C	2.82	126.28	122.56
16	L	1006	BCR	C38-C26-C27	-2.82	108.20	113.62
17	A	856	LHG	C6-C5-C4	-2.82	105.13	111.79
13	A	811	CLA	C1D-CHD-C4C	2.82	126.28	122.56
13	A	834	CLA	OBD-CAD-CBD	-2.81	121.88	125.89
13	B	801	CLA	CED-O2D-CGD	2.81	122.30	115.94
16	A	849	BCR	C1-C6-C5	-2.81	118.65	122.61
13	B	821	CLA	CED-O2D-CGD	2.81	122.29	115.94
16	A	852	BCR	C30-C25-C24	2.81	123.72	115.78
13	B	828	CLA	C5-C3-C2	2.81	126.80	121.12
13	B	808	CLA	O2A-CGA-O1A	-2.81	116.51	123.59
13	K	1401	CLA	CMB-C2B-C1B	-2.80	124.15	128.46
13	B	815	CLA	C1D-CHD-C4C	2.80	126.26	122.56
13	A	807	CLA	C1-C2-C3	2.80	130.88	126.04
16	I	102	BCR	C32-C1-C6	2.80	114.84	110.30
13	A	835	CLA	C1D-CHD-C4C	2.80	126.25	122.56
13	A	829	CLA	O2D-CGD-CBD	2.80	116.24	111.27
13	A	823	CLA	OBD-CAD-CBD	-2.80	121.90	125.89
13	A	802	CLA	CMB-C2B-C1B	-2.80	124.17	128.46
13	A	812	CLA	C1D-CHD-C4C	2.79	126.25	122.56
13	A	806	CLA	CED-O2D-CGD	2.79	122.26	115.94
13	A	817	CLA	OBD-CAD-CBD	-2.79	121.90	125.89
13	A	804	CLA	OBD-CAD-CBD	-2.79	121.91	125.89
13	M	1601	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
13	A	841	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
16	I	102	BCR	C7-C8-C9	2.79	130.44	126.23
13	A	831	CLA	OBD-CAD-CBD	-2.78	121.92	125.89
13	B	808	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
13	A	828	CLA	C1-C2-C3	2.78	130.86	126.04
16	L	1006	BCR	C29-C30-C25	2.78	114.76	110.48
16	J	104	BCR	C38-C26-C27	-2.78	108.28	113.62
13	A	825	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
13	B	804	CLA	C1D-CHD-C4C	2.77	126.21	122.56
16	A	850	BCR	C30-C25-C26	-2.77	118.71	122.61
16	B	845	BCR	C30-C25-C26	-2.77	118.71	122.61
13	A	815	CLA	CED-O2D-CGD	2.77	122.20	115.94
13	B	833	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
16	B	846	BCR	C40-C30-C25	2.77	114.78	110.30
13	A	843	CLA	CED-O2D-CGD	2.77	122.19	115.94
13	A	844	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
13	B	828	CLA	O2D-CGD-CBD	2.76	116.18	111.27
16	L	1006	BCR	C8-C7-C6	2.76	134.96	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	833	CLA	CED-O2D-CGD	2.76	122.18	115.94
13	A	812	CLA	CED-O2D-CGD	2.76	122.17	115.94
16	B	846	BCR	C35-C13-C12	2.76	120.69	114.60
13	A	833	CLA	CMB-C2B-C1B	-2.75	124.23	128.46
16	A	854	BCR	C32-C1-C6	2.75	114.76	110.30
16	A	849	BCR	C8-C7-C6	2.75	134.92	127.20
13	A	835	CLA	O2A-CGA-CBA	2.75	120.53	111.91
16	L	1005	BCR	C30-C25-C26	-2.75	118.74	122.61
13	A	844	CLA	O2D-CGD-CBD	2.75	116.15	111.27
16	A	853	BCR	C23-C24-C25	2.75	134.92	127.20
13	A	819	CLA	CED-O2D-CGD	2.75	122.15	115.94
18	B	850	LMG	C7-O1-C1	2.75	119.10	113.74
13	A	827	CLA	C1D-CHD-C4C	2.75	126.18	122.56
13	A	808	CLA	C1D-CHD-C4C	2.75	126.18	122.56
16	B	844	BCR	C1-C6-C7	2.74	123.54	115.78
13	B	824	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
16	J	105	BCR	C30-C25-C26	-2.74	118.75	122.61
13	A	836	CLA	CED-O2D-CGD	2.74	122.13	115.94
13	B	831	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
13	F	1301	CLA	CMB-C2B-C1B	-2.74	124.26	128.46
16	I	101	BCR	C36-C18-C19	2.74	122.39	118.08
13	A	826	CLA	OBD-CAD-CBD	-2.74	121.99	125.89
13	A	816	CLA	CMB-C2B-C3B	2.73	129.79	124.68
13	B	813	CLA	O1D-CGD-CBD	-2.73	118.89	124.48
16	I	102	BCR	C30-C25-C26	-2.73	118.77	122.61
13	A	822	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
13	A	834	CLA	CMB-C2B-C3B	2.73	129.78	124.68
16	A	851	BCR	C1-C6-C5	-2.72	118.78	122.61
13	M	1601	CLA	OBD-CAD-CBD	-2.72	122.01	125.89
13	B	839	CLA	C1D-CHD-C4C	2.72	126.15	122.56
13	A	805	CLA	C1D-CHD-C4C	2.72	126.14	122.56
13	A	839	CLA	C1D-CHD-C4C	2.72	126.14	122.56
13	A	811	CLA	CED-O2D-CGD	2.72	122.08	115.94
16	B	844	BCR	C20-C21-C22	2.71	131.18	127.31
13	B	811	CLA	CAA-C2A-C3A	-2.71	105.35	112.78
13	B	806	CLA	O2A-CGA-CBA	2.71	120.42	111.91
13	B	808	CLA	OBD-CAD-CBD	-2.71	122.02	125.89
13	X	1701	CLA	OBD-CAD-CBD	-2.71	122.02	125.89
13	A	844	CLA	OBD-CAD-CBD	-2.71	122.02	125.89
16	A	854	BCR	C30-C25-C24	2.71	123.44	115.78
13	A	840	CLA	OBD-CAD-CBD	-2.71	122.03	125.89
13	B	811	CLA	OBD-CAD-CBD	-2.71	122.03	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	817	CLA	CED-O2D-CGD	2.70	122.05	115.94
13	B	821	CLA	OBD-CAD-CBD	-2.70	122.03	125.89
13	B	824	CLA	C1-C2-C3	2.70	130.72	126.04
16	B	847	BCR	C29-C30-C25	2.70	114.64	110.48
13	B	826	CLA	C1D-CHD-C4C	2.70	126.13	122.56
13	A	829	CLA	C1D-CHD-C4C	2.70	126.12	122.56
13	B	837	CLA	O2A-CGA-CBA	2.70	120.38	111.91
13	J	102	CLA	CMB-C2B-C1B	-2.70	124.31	128.46
16	L	1005	BCR	C8-C7-C6	2.70	134.78	127.20
13	B	828	CLA	O2A-C1-C2	2.70	115.73	108.64
16	L	1006	BCR	C30-C25-C26	-2.70	118.81	122.61
13	B	810	CLA	C2A-C1A-CHA	2.70	128.57	123.86
13	B	809	CLA	CED-O2D-CGD	2.69	122.03	115.94
13	A	803	CLA	CMB-C2B-C3B	2.69	129.71	124.68
13	A	801	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
13	B	809	CLA	C1D-CHD-C4C	2.69	126.11	122.56
13	B	801	CLA	C1-C2-C3	2.69	130.69	126.04
13	B	805	CLA	C1D-CHD-C4C	2.69	126.10	122.56
13	A	805	CLA	O1D-CGD-CBD	-2.69	118.99	124.48
13	A	807	CLA	O2A-CGA-O1A	-2.68	116.82	123.59
13	A	843	CLA	OBD-CAD-CBD	-2.68	122.07	125.89
13	A	828	CLA	CMB-C2B-C1B	-2.68	124.35	128.46
13	B	806	CLA	C1D-CHD-C4C	2.68	126.09	122.56
13	A	841	CLA	C1D-CHD-C4C	2.68	126.09	122.56
13	A	810	CLA	C2A-C1A-CHA	2.68	128.54	123.86
13	A	827	CLA	OBD-CAD-CBD	-2.67	122.07	125.89
16	B	848	BCR	C30-C25-C26	-2.67	118.85	122.61
13	B	806	CLA	C1-C2-C3	2.67	130.66	126.04
16	I	101	BCR	C23-C24-C25	2.67	134.69	127.20
13	A	846	CLA	O1D-CGD-CBD	-2.67	119.03	124.48
13	B	813	CLA	CED-O2D-CGD	2.66	121.96	115.94
13	A	837	CLA	CED-O2D-CGD	2.66	121.96	115.94
13	B	840	CLA	O2D-CGD-CBD	2.66	116.00	111.27
16	F	1302	BCR	C1-C6-C5	-2.66	118.86	122.61
16	I	101	BCR	C29-C30-C25	2.66	114.58	110.48
13	A	844	CLA	CAA-C2A-C3A	-2.66	105.49	112.78
16	I	102	BCR	C37-C22-C23	2.66	122.27	118.08
16	B	848	BCR	C32-C1-C6	2.66	114.61	110.30
16	L	1005	BCR	C40-C30-C25	2.66	114.61	110.30
13	B	819	CLA	OBD-CAD-CBD	-2.66	122.10	125.89
13	B	819	CLA	CED-O2D-CGD	2.66	121.95	115.94
13	A	839	CLA	CMB-C2B-C1B	-2.65	124.39	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	831	CLA	O2A-CGA-CBA	2.65	120.23	111.91
13	B	803	CLA	C1D-CHD-C4C	2.65	126.06	122.56
13	A	812	CLA	O2D-CGD-CBD	2.65	115.98	111.27
13	A	818	CLA	CED-O2D-CGD	2.65	121.94	115.94
16	B	847	BCR	C30-C25-C26	-2.65	118.88	122.61
13	F	1301	CLA	OBD-CAD-CBD	-2.65	122.11	125.89
13	A	825	CLA	OBD-CAD-CBD	-2.65	122.11	125.89
13	A	846	CLA	CED-O2D-CGD	2.65	121.93	115.94
13	B	814	CLA	O1D-CGD-CBD	-2.65	119.07	124.48
13	A	845	CLA	CMB-C2B-C1B	-2.65	124.40	128.46
13	B	833	CLA	O1D-CGD-CBD	-2.64	119.07	124.48
13	B	828	CLA	C1D-CHD-C4C	2.64	126.05	122.56
13	A	813	CLA	CMB-C2B-C1B	-2.64	124.40	128.46
13	A	843	CLA	O2A-C1-C2	2.64	115.58	108.64
13	A	830	CLA	OBD-CAD-CBD	-2.64	122.12	125.89
13	A	812	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
13	B	837	CLA	OBD-CAD-CBD	-2.64	122.12	125.89
16	B	847	BCR	C36-C18-C19	2.64	122.23	118.08
13	B	828	CLA	CED-O2D-CGD	2.64	121.90	115.94
13	B	803	CLA	C4D-C3D-CAD	-2.64	107.00	108.47
13	B	836	CLA	OBD-CAD-CBD	-2.64	122.13	125.89
13	B	838	CLA	C1-C2-C3	2.63	130.60	126.04
13	A	814	CLA	O1D-CGD-CBD	-2.63	119.09	124.48
13	B	803	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
13	A	824	CLA	OBD-CAD-CBD	-2.63	122.14	125.89
16	J	103	BCR	C1-C6-C7	2.63	123.22	115.78
13	A	809	CLA	O1D-CGD-CBD	-2.63	119.11	124.48
16	A	853	BCR	C11-C10-C9	2.63	131.06	127.31
13	A	826	CLA	O1D-CGD-CBD	-2.63	119.11	124.48
16	B	849	BCR	C8-C9-C10	-2.62	114.92	118.94
16	J	104	BCR	C23-C24-C25	2.62	134.56	127.20
13	A	832	CLA	O1D-CGD-CBD	-2.62	119.12	124.48
13	B	810	CLA	OBD-CAD-CBD	-2.62	122.15	125.89
13	A	814	CLA	CED-O2D-CGD	2.62	121.86	115.94
13	A	827	CLA	C1-C2-C3	2.62	130.57	126.04
13	B	830	CLA	O1D-CGD-CBD	-2.62	119.13	124.48
13	A	808	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
13	A	806	CLA	CMB-C2B-C3B	2.61	129.57	124.68
13	B	840	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
16	F	1302	BCR	C30-C25-C26	-2.60	118.94	122.61
13	B	831	CLA	OBD-CAD-CBD	-2.60	122.17	125.89
13	A	832	CLA	CED-O2D-CGD	2.60	121.82	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	851	BCR	C30-C25-C26	-2.60	118.95	122.61
13	B	836	CLA	CMB-C2B-C1B	-2.60	124.47	128.46
13	A	808	CLA	CED-O2D-CGD	2.60	121.81	115.94
13	B	820	CLA	OBD-CAD-CBD	-2.60	122.19	125.89
13	A	821	CLA	CMB-C2B-C1B	-2.60	124.47	128.46
16	B	848	BCR	C34-C9-C8	2.60	122.17	118.08
13	A	832	CLA	CAA-C2A-C3A	-2.60	105.67	112.78
16	J	103	BCR	C1-C6-C5	-2.59	118.96	122.61
13	B	806	CLA	CMB-C2B-C3B	2.59	129.53	124.68
13	A	820	CLA	OBD-CAD-CBD	-2.59	122.19	125.89
13	B	810	CLA	CED-O2D-CGD	2.59	121.80	115.94
13	B	811	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
13	A	838	CLA	OBD-CAD-CBD	-2.59	122.20	125.89
13	A	842	CLA	CMB-C2B-C1B	-2.59	124.49	128.46
16	A	854	BCR	C30-C25-C26	-2.59	118.97	122.61
16	M	1602	BCR	C30-C25-C26	-2.58	118.97	122.61
16	B	847	BCR	C30-C25-C24	2.58	123.08	115.78
13	L	1003	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
16	L	1005	BCR	C29-C30-C25	2.58	114.45	110.48
13	B	812	CLA	CED-O2D-CGD	2.58	121.76	115.94
16	B	847	BCR	C16-C17-C18	2.58	130.99	127.31
16	J	104	BCR	C30-C25-C26	-2.57	118.99	122.61
13	B	826	CLA	C1-C2-C3	2.57	130.49	126.04
13	B	819	CLA	C1-C2-C3	2.57	130.49	126.04
13	B	805	CLA	CMB-C2B-C3B	2.57	129.49	124.68
13	B	840	CLA	O2A-CGA-CBA	2.57	119.98	111.91
13	A	822	CLA	CAA-CBA-CGA	2.57	120.76	113.25
13	A	831	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
16	L	1006	BCR	C1-C6-C5	-2.57	119.00	122.61
13	L	1002	CLA	CMB-C2B-C1B	-2.57	124.52	128.46
13	A	835	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
13	A	838	CLA	C1D-CHD-C4C	2.56	125.94	122.56
13	A	826	CLA	CMB-C2B-C1B	-2.56	124.53	128.46
13	A	831	CLA	C1D-CHD-C4C	2.56	125.94	122.56
13	L	1003	CLA	CMB-C2B-C1B	-2.56	124.53	128.46
13	B	811	CLA	C1D-CHD-C4C	2.56	125.94	122.56
16	B	845	BCR	C35-C13-C12	2.56	122.10	118.08
13	A	836	CLA	O2A-CGA-O1A	-2.55	117.14	123.59
13	A	840	CLA	CMB-C2B-C1B	-2.55	124.54	128.46
13	B	822	CLA	CMB-C2B-C3B	2.55	129.45	124.68
16	A	853	BCR	C33-C5-C4	-2.55	108.72	113.62
16	J	104	BCR	C1-C6-C5	-2.55	119.03	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	818	CLA	CED-O2D-CGD	2.55	121.70	115.94
13	B	815	CLA	O1D-CGD-CBD	-2.55	119.28	124.48
13	B	827	CLA	C1-C2-C3	2.54	130.44	126.04
13	A	829	CLA	CMB-C2B-C3B	2.54	129.43	124.68
13	A	813	CLA	OBD-CAD-CBD	-2.54	122.27	125.89
13	B	819	CLA	CAA-C2A-C3A	-2.54	105.82	112.78
13	A	801	CLA	C1-C2-C3	2.54	130.44	126.04
13	B	837	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
13	A	814	CLA	C1-C2-C3	2.54	130.43	126.04
13	B	831	CLA	CED-O2D-CGD	2.54	121.68	115.94
16	M	1602	BCR	C8-C7-C6	2.54	134.32	127.20
13	B	802	CLA	C2A-C1A-CHA	2.54	128.29	123.86
13	A	837	CLA	OBD-CAD-CBD	-2.53	122.28	125.89
13	A	822	CLA	O2D-CGD-CBD	2.53	115.76	111.27
13	A	840	CLA	CED-O2D-CGD	2.53	121.66	115.94
13	B	821	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
13	A	816	CLA	CED-O2D-CGD	2.53	121.65	115.94
13	A	842	CLA	C1-C2-C3	2.53	130.41	126.04
16	A	854	BCR	C15-C14-C13	2.53	130.91	127.31
13	A	823	CLA	CED-O2D-CGD	2.52	121.64	115.94
16	B	849	BCR	C34-C9-C8	2.52	122.05	118.08
13	A	808	CLA	C1-C2-C3	2.52	130.40	126.04
13	B	829	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
13	A	832	CLA	CMB-C2B-C1B	-2.51	124.60	128.46
13	A	828	CLA	O1D-CGD-CBD	-2.51	119.34	124.48
16	B	845	BCR	C23-C24-C25	2.51	134.25	127.20
13	L	1002	CLA	O1D-CGD-CBD	-2.51	119.35	124.48
13	A	841	CLA	O2D-CGD-CBD	2.51	115.72	111.27
16	A	850	BCR	C1-C6-C5	-2.51	119.08	122.61
16	B	848	BCR	C23-C24-C25	2.51	134.24	127.20
13	B	825	CLA	OBD-CAD-CBD	-2.51	122.32	125.89
16	B	847	BCR	C32-C1-C6	2.50	114.36	110.30
13	B	835	CLA	O2D-CGD-CBD	2.50	115.72	111.27
13	A	812	CLA	OBD-CAD-CBD	-2.50	122.32	125.89
13	A	805	CLA	OBD-CAD-CBD	-2.50	122.32	125.89
13	A	833	CLA	CMB-C2B-C3B	2.50	129.36	124.68
13	A	807	CLA	C2A-C1A-CHA	2.50	128.23	123.86
13	A	808	CLA	OBD-CAD-CBD	-2.50	122.33	125.89
13	B	838	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
13	L	1003	CLA	C1D-CHD-C4C	2.50	125.85	122.56
16	B	844	BCR	C32-C1-C6	2.50	114.35	110.30
13	A	803	CLA	C1-O2A-CGA	2.50	123.00	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	816	CLA	CED-O2D-CGD	2.49	121.58	115.94
13	J	102	CLA	C2A-C3A-C4A	2.49	104.97	101.78
16	A	854	BCR	C1-C6-C7	2.49	122.83	115.78
13	A	843	CLA	C1-C2-C3	2.49	130.35	126.04
13	B	832	CLA	C1-C2-C3	2.49	130.35	126.04
13	B	839	CLA	CED-O2D-CGD	2.49	121.57	115.94
13	B	805	CLA	CED-O2D-CGD	2.49	121.57	115.94
13	A	802	CLA	O2A-CGA-CBA	2.49	119.72	111.91
13	B	802	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
16	I	101	BCR	C1-C6-C5	-2.49	119.11	122.61
16	J	104	BCR	C36-C18-C19	2.49	121.99	118.08
13	B	830	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
13	B	834	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
13	B	814	CLA	CED-O2D-CGD	2.49	121.56	115.94
13	B	825	CLA	C2A-C3A-C4A	2.48	105.88	101.87
13	B	817	CLA	C1-C2-C3	2.48	130.34	126.04
13	B	807	CLA	C3C-C4C-NC	-2.48	107.79	110.57
13	A	836	CLA	OBD-CAD-CBD	-2.48	122.36	125.89
16	I	102	BCR	C36-C18-C19	2.48	121.98	118.08
13	A	802	CLA	C1D-CHD-C4C	2.48	125.83	122.56
16	B	846	BCR	C30-C25-C26	-2.48	119.13	122.61
13	A	820	CLA	O2A-CGA-O1A	-2.47	117.35	123.59
13	F	1301	CLA	CED-O2D-CGD	2.47	121.52	115.94
13	B	829	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
13	A	835	CLA	CED-O2D-CGD	2.47	121.52	115.94
13	K	1401	CLA	CED-O2D-CGD	2.47	121.52	115.94
16	A	853	BCR	C1-C6-C7	2.47	122.75	115.78
13	A	809	CLA	O2A-CGA-O1A	-2.47	117.37	123.59
13	A	835	CLA	O1D-CGD-CBD	-2.46	119.44	124.48
13	B	810	CLA	C1-C2-C3	2.46	130.30	126.04
13	A	829	CLA	CED-O2D-CGD	2.46	121.50	115.94
13	A	829	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
13	A	810	CLA	OBD-CAD-CBD	-2.46	122.38	125.89
13	A	822	CLA	C12-C11-C10	-2.46	101.94	113.24
13	A	822	CLA	O2A-CGA-CBA	2.46	119.62	111.91
13	B	816	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
13	A	843	CLA	C1-O2A-CGA	2.46	122.89	116.44
16	A	854	BCR	C1-C6-C5	-2.46	119.16	122.61
13	A	816	CLA	OBD-CAD-CBD	-2.46	122.39	125.89
13	A	838	CLA	CMB-C2B-C3B	2.45	129.27	124.68
13	A	846	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
13	B	822	CLA	OBD-CAD-CBD	-2.45	122.39	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	818	CLA	OBD-CAD-CBD	-2.45	122.39	125.89
16	A	850	BCR	C7-C8-C9	2.45	129.94	126.23
13	A	809	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
16	I	101	BCR	C30-C25-C26	-2.45	119.17	122.61
13	B	804	CLA	O1D-CGD-CBD	-2.44	119.48	124.48
13	A	803	CLA	C1-C2-C3	2.44	130.27	126.04
16	A	850	BCR	C30-C25-C24	2.44	122.69	115.78
13	B	830	CLA	C3C-C4C-NC	-2.44	107.83	110.57
16	B	848	BCR	C35-C13-C12	2.44	121.92	118.08
13	B	807	CLA	CED-O2D-CGD	2.44	121.45	115.94
13	A	833	CLA	OBD-CAD-CBD	-2.43	122.42	125.89
16	A	854	BCR	C23-C22-C21	-2.43	115.21	118.94
16	J	103	BCR	C35-C13-C12	2.43	121.91	118.08
13	A	806	CLA	O1D-CGD-CBD	-2.43	119.51	124.48
13	B	827	CLA	OBD-CAD-C3D	2.43	132.01	127.98
13	B	836	CLA	CED-O2D-CGD	2.43	121.43	115.94
13	A	807	CLA	OBD-CAD-CBD	-2.43	122.42	125.89
16	A	851	BCR	C1-C6-C7	2.43	122.65	115.78
13	A	830	CLA	CED-O2D-CGD	2.43	121.42	115.94
16	A	850	BCR	C24-C23-C22	2.42	129.90	126.23
16	A	851	BCR	C30-C25-C24	2.42	122.64	115.78
13	B	810	CLA	C4D-C3D-CAD	-2.42	107.12	108.47
13	A	821	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
13	A	829	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
13	A	826	CLA	CED-O2D-CGD	2.42	121.41	115.94
13	L	1002	CLA	C4D-C3D-CAD	-2.42	107.12	108.47
13	A	816	CLA	O1D-CGD-CBD	-2.42	119.54	124.48
13	A	831	CLA	CED-O2D-CGD	2.41	121.40	115.94
16	L	1005	BCR	C36-C18-C19	2.41	121.88	118.08
13	A	841	CLA	OBD-CAD-CBD	-2.41	122.45	125.89
16	I	102	BCR	C30-C25-C24	2.41	122.59	115.78
13	B	808	CLA	C7-C6-C5	-2.41	106.82	113.36
13	B	825	CLA	O1D-CGD-CBD	-2.41	119.56	124.48
16	B	847	BCR	C1-C6-C5	-2.40	119.23	122.61
13	A	842	CLA	OBD-CAD-CBD	-2.40	122.47	125.89
13	B	826	CLA	OBD-CAD-CBD	-2.40	122.47	125.89
13	B	818	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
13	L	1003	CLA	C3C-C4C-NC	-2.39	107.89	110.57
16	A	853	BCR	C37-C22-C23	2.39	121.84	118.08
13	A	806	CLA	C1-C2-C3	2.39	130.18	126.04
13	A	844	CLA	CED-O2D-CGD	2.39	121.34	115.94
13	B	820	CLA	O1D-CGD-CBD	-2.39	119.60	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	809	CLA	C12-C11-C10	-2.39	102.27	113.24
13	A	842	CLA	C1D-CHD-C4C	2.38	125.70	122.56
13	B	806	CLA	CED-O2D-CGD	2.38	121.33	115.94
16	F	1302	BCR	C7-C8-C9	2.38	129.83	126.23
13	A	806	CLA	C2A-C3A-C4A	2.38	105.71	101.87
16	A	853	BCR	C8-C9-C10	-2.37	115.30	118.94
16	A	852	BCR	C32-C1-C6	2.37	114.15	110.30
13	B	840	CLA	C3C-C4C-NC	-2.37	107.91	110.57
13	B	830	CLA	CED-O2D-CGD	2.37	121.30	115.94
13	A	820	CLA	C4-C3-C5	-2.37	111.29	115.27
13	A	812	CLA	C1-C2-C3	2.37	130.13	126.04
16	A	853	BCR	C34-C9-C8	2.36	121.80	118.08
13	B	813	CLA	OBD-CAD-CBD	-2.36	122.52	125.89
13	B	828	CLA	CBA-CAA-C2A	2.36	120.83	113.86
13	A	814	CLA	CMB-C2B-C3B	2.36	129.09	124.68
13	B	837	CLA	O1D-CGD-CBD	-2.36	119.66	124.48
13	B	803	CLA	OBD-CAD-C3D	2.36	131.90	127.98
13	A	801	CLA	C2A-C3A-C4A	2.36	105.68	101.87
13	B	812	CLA	OBD-CAD-CBD	-2.36	122.53	125.89
16	B	848	BCR	C36-C18-C19	2.36	121.79	118.08
13	A	813	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
13	B	841	CLA	CMB-C2B-C3B	2.35	129.08	124.68
13	B	801	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
13	B	825	CLA	CED-O2D-CGD	2.35	121.25	115.94
16	A	852	BCR	C1-C6-C5	-2.35	119.31	122.61
16	J	103	BCR	C24-C23-C22	2.35	129.78	126.23
16	A	852	BCR	C1-C6-C7	2.35	122.42	115.78
13	B	822	CLA	C3C-C4C-NC	-2.35	107.94	110.57
13	B	832	CLA	C12-C11-C10	-2.34	102.47	113.24
13	A	805	CLA	CMB-C2B-C3B	2.34	129.06	124.68
13	A	832	CLA	O2A-CGA-O1A	-2.34	117.70	123.59
13	B	837	CLA	CED-O2D-CGD	2.33	121.22	115.94
13	A	846	CLA	OBD-CAD-CBD	-2.33	122.56	125.89
13	J	101	CLA	C2A-C1A-CHA	2.33	127.94	123.86
13	A	839	CLA	CED-O2D-CGD	2.33	121.21	115.94
16	I	102	BCR	C1-C6-C5	-2.33	119.33	122.61
13	A	839	CLA	O2D-CGD-CBD	2.33	115.41	111.27
16	B	845	BCR	C28-C27-C26	2.33	118.23	114.08
13	B	826	CLA	C4D-C3D-CAD	-2.33	107.17	108.47
16	B	844	BCR	C35-C13-C12	2.33	121.74	118.08
13	B	834	CLA	C2A-C3A-C4A	2.32	105.62	101.87
13	B	828	CLA	OBD-CAD-CBD	-2.32	122.58	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	849	BCR	C1-C6-C7	2.32	122.34	115.78
13	B	833	CLA	OBD-CAD-CBD	-2.32	122.58	125.89
13	A	804	CLA	C1-C2-C3	2.32	130.05	126.04
16	A	850	BCR	C23-C24-C25	2.32	133.71	127.20
13	A	833	CLA	CAA-C2A-C3A	-2.32	106.44	112.78
13	A	821	CLA	CED-O2D-CGD	2.31	121.17	115.94
13	B	829	CLA	OBD-CAD-CBD	-2.31	122.59	125.89
13	A	828	CLA	OBD-CAD-CBD	-2.31	122.59	125.89
16	J	105	BCR	C30-C25-C24	2.31	122.31	115.78
13	A	833	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
13	B	824	CLA	C2A-C1A-CHA	2.31	127.90	123.86
13	A	831	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
16	I	102	BCR	C29-C30-C25	2.31	114.03	110.48
13	B	804	CLA	C1-C2-C3	2.30	130.03	126.04
13	B	807	CLA	CMB-C2B-C1B	-2.30	124.92	128.46
13	B	808	CLA	C1D-CHD-C4C	2.30	125.60	122.56
16	A	852	BCR	C40-C30-C25	2.30	114.03	110.30
13	F	1301	CLA	C2A-C1A-CHA	2.30	127.88	123.86
13	A	846	CLA	C2A-C1A-CHA	2.30	127.88	123.86
16	J	104	BCR	C40-C30-C25	2.30	114.03	110.30
13	A	839	CLA	C3C-C4C-NC	-2.30	108.00	110.57
13	B	821	CLA	C2A-C1A-CHA	2.30	127.87	123.86
13	B	830	CLA	OBD-CAD-CBD	-2.29	122.62	125.89
16	A	852	BCR	C23-C24-C25	2.29	133.64	127.20
16	B	843	BCR	C8-C7-C6	2.29	133.64	127.20
13	A	825	CLA	CAA-C2A-C3A	-2.29	106.51	112.78
16	B	844	BCR	C34-C9-C8	2.29	121.68	118.08
13	A	842	CLA	CED-O2D-CGD	2.29	121.11	115.94
13	A	806	CLA	C3C-C4C-NC	-2.29	108.01	110.57
16	L	1005	BCR	C1-C6-C5	-2.28	119.40	122.61
13	B	820	CLA	C2A-C1A-CHA	2.28	127.85	123.86
13	B	840	CLA	C1D-CHD-C4C	2.28	125.57	122.56
13	A	835	CLA	CMB-C2B-C1B	-2.28	124.96	128.46
13	B	829	CLA	CED-O2D-CGD	2.28	121.09	115.94
16	B	844	BCR	C36-C18-C19	2.28	121.67	118.08
13	B	810	CLA	CMB-C2B-C1B	-2.28	124.97	128.46
16	A	849	BCR	C35-C13-C12	2.28	121.66	118.08
13	A	803	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
13	A	803	CLA	O2A-C1-C2	-2.27	102.66	108.64
16	A	850	BCR	C1-C6-C7	2.27	122.21	115.78
13	A	823	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
13	B	806	CLA	OBD-CAD-CBD	-2.27	122.65	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	849	BCR	C24-C23-C22	2.27	129.66	126.23
13	B	824	CLA	O1D-CGD-CBD	-2.26	119.85	124.48
13	A	803	CLA	O2D-CGD-CBD	2.26	115.29	111.27
13	B	841	CLA	OBD-CAD-C3D	2.26	131.74	127.98
16	A	849	BCR	C37-C22-C23	2.26	121.64	118.08
13	B	803	CLA	C12-C11-C10	-2.26	102.84	113.24
13	B	835	CLA	C2A-C1A-CHA	2.26	127.82	123.86
13	A	805	CLA	CED-O2D-CGD	2.26	121.05	115.94
13	A	824	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
16	A	853	BCR	C23-C22-C21	-2.26	115.47	118.94
13	A	820	CLA	C1-C2-C3	2.26	129.94	126.04
16	B	849	BCR	C30-C25-C26	-2.25	119.44	122.61
13	A	825	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
13	B	837	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
13	A	820	CLA	C3C-C4C-NC	-2.25	108.05	110.57
13	A	801	CLA	CAA-C2A-C3A	-2.25	106.63	112.78
13	A	828	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
13	A	808	CLA	C4-C3-C5	-2.24	113.42	115.98
13	A	819	CLA	C1-C2-C3	2.24	129.92	126.04
13	B	827	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
13	X	1701	CLA	CED-O2D-CGD	2.24	121.01	115.94
13	A	832	CLA	C1-C2-C3	2.24	130.38	126.75
13	A	821	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
16	B	849	BCR	C23-C24-C25	2.24	133.49	127.20
13	B	825	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
16	B	845	BCR	C34-C9-C8	2.24	121.60	118.08
16	I	102	BCR	C19-C18-C17	-2.23	115.51	118.94
13	A	807	CLA	CAA-CBA-CGA	2.23	119.78	113.25
13	A	830	CLA	C4D-C3D-CAD	-2.23	107.22	108.47
13	A	807	CLA	C3C-C4C-NC	-2.23	108.07	110.57
16	I	101	BCR	C34-C9-C8	2.23	121.59	118.08
16	I	101	BCR	C19-C18-C17	-2.23	115.52	118.94
16	I	102	BCR	C3-C4-C5	2.23	118.06	114.08
13	A	843	CLA	CMB-C2B-C3B	2.23	128.85	124.68
13	B	814	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
13	A	823	CLA	C3C-C4C-NC	-2.23	108.07	110.57
13	B	825	CLA	O2A-CGA-CBA	2.23	121.03	112.23
13	A	836	CLA	CMB-C2B-C3B	2.22	128.84	124.68
16	A	853	BCR	C1-C6-C5	-2.22	119.48	122.61
16	B	849	BCR	C23-C22-C21	-2.22	115.53	118.94
13	B	835	CLA	CMB-C2B-C3B	2.22	128.84	124.68
13	B	820	CLA	O2A-CGA-O1A	-2.22	117.99	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	1006	BCR	C30-C25-C24	2.22	122.06	115.78
16	I	102	BCR	C1-C6-C7	2.22	122.06	115.78
13	B	817	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
13	A	815	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
13	B	801	CLA	CMB-C2B-C1B	-2.22	125.05	128.46
13	A	844	CLA	CMA-C3A-C2A	-2.22	104.88	113.83
13	B	826	CLA	CED-O2D-CGD	2.22	120.95	115.94
13	L	1003	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
16	J	103	BCR	C37-C22-C23	2.22	121.57	118.08
13	B	809	CLA	C1-C2-C3	2.21	129.87	126.04
16	A	851	BCR	C35-C13-C12	2.21	121.56	118.08
13	J	102	CLA	CMA-C3A-C2A	-2.21	110.94	116.10
13	B	808	CLA	CED-O2D-CGD	2.21	120.93	115.94
16	A	854	BCR	C34-C9-C8	2.21	121.56	118.08
13	A	823	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
14	B	842	PQN	C17-C16-C15	-2.21	107.36	113.36
13	A	813	CLA	C3C-C4C-NC	-2.21	108.10	110.57
16	B	846	BCR	C36-C18-C19	2.21	121.55	118.08
13	A	810	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
16	F	1302	BCR	C30-C25-C24	2.20	122.01	115.78
16	J	104	BCR	C24-C23-C22	2.20	129.56	126.23
16	B	845	BCR	C36-C18-C19	2.20	121.55	118.08
13	B	839	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
13	A	832	CLA	C2C-C1C-NC	-2.20	107.91	109.97
13	A	819	CLA	CBA-CAA-C2A	2.20	120.36	113.86
13	B	839	CLA	CMB-C2B-C3B	2.20	128.79	124.68
13	A	805	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
16	B	846	BCR	C30-C25-C24	2.20	122.00	115.78
13	B	836	CLA	C2A-C1A-CHA	2.20	127.70	123.86
13	B	834	CLA	C3C-C4C-NC	-2.20	108.11	110.57
16	L	1005	BCR	C23-C24-C25	2.20	133.37	127.20
16	B	843	BCR	C1-C6-C7	2.19	121.99	115.78
13	A	813	CLA	CED-O2D-CGD	2.19	120.90	115.94
13	B	807	CLA	OBD-CAD-C3D	2.19	131.62	127.98
13	B	826	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
13	B	808	CLA	CMB-C2B-C3B	2.19	128.77	124.68
16	A	851	BCR	C8-C7-C6	2.19	133.35	127.20
13	A	811	CLA	CMB-C2B-C3B	2.18	128.76	124.68
13	L	1002	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
13	B	841	CLA	CBA-CAA-C2A	2.18	120.31	113.86
16	A	849	BCR	C32-C1-C6	2.18	113.84	110.30
16	J	104	BCR	C1-C6-C7	2.18	121.95	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	821	CLA	C2A-C1A-CHA	2.18	127.67	123.86
13	A	810	CLA	CMB-C2B-C3B	2.18	128.75	124.68
13	A	809	CLA	CED-O2D-CGD	2.18	120.86	115.94
13	A	838	CLA	O1D-CGD-CBD	-2.17	120.03	124.48
16	B	848	BCR	C24-C23-C22	2.17	129.52	126.23
16	B	845	BCR	C1-C6-C7	2.17	121.93	115.78
16	B	845	BCR	C30-C25-C24	2.17	121.92	115.78
13	B	841	CLA	CED-O2D-CGD	2.17	120.85	115.94
13	B	810	CLA	CAA-C2A-C1A	2.17	119.09	111.97
13	A	834	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
13	K	1401	CLA	OBD-CAD-CBD	-2.17	122.80	125.89
13	A	812	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
16	J	104	BCR	C34-C9-C8	2.17	121.49	118.08
13	A	817	CLA	CMB-C2B-C3B	2.17	128.73	124.68
13	B	817	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
16	A	850	BCR	C40-C30-C25	2.16	113.81	110.30
13	A	826	CLA	C1-C2-C3	2.16	129.78	126.04
16	A	853	BCR	C7-C8-C9	2.16	129.50	126.23
16	B	849	BCR	C1-C6-C5	-2.16	119.57	122.61
13	A	842	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
16	L	1005	BCR	C37-C22-C23	2.16	121.48	118.08
13	B	807	CLA	C1-C2-C3	2.16	129.77	126.04
16	B	848	BCR	C1-C6-C5	-2.16	119.58	122.61
16	B	845	BCR	C40-C30-C25	2.15	113.79	110.30
13	B	838	CLA	C3C-C4C-NC	-2.15	108.16	110.57
16	J	104	BCR	C35-C13-C12	2.15	121.47	118.08
13	M	1601	CLA	C2A-C1A-CHA	2.15	127.62	123.86
16	I	101	BCR	C1-C6-C7	2.15	121.86	115.78
13	A	833	CLA	C2A-C3A-C4A	2.15	105.34	101.87
16	A	854	BCR	C37-C22-C23	2.15	121.46	118.08
13	J	102	CLA	C3C-C4C-NC	-2.15	108.16	110.57
13	A	803	CLA	OBD-CAD-CBD	-2.15	122.83	125.89
13	A	802	CLA	CED-O2D-CGD	2.15	120.79	115.94
13	B	827	CLA	CAA-CBA-CGA	2.15	119.53	113.25
13	B	802	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
13	B	810	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
16	B	849	BCR	C15-C14-C13	2.15	130.37	127.31
16	B	847	BCR	C1-C6-C7	2.14	121.84	115.78
16	B	843	BCR	C37-C22-C23	2.14	121.45	118.08
13	A	824	CLA	CMB-C2B-C3B	2.14	128.68	124.68
13	X	1701	CLA	CMB-C2B-C3B	2.14	128.68	124.68
13	A	822	CLA	C3C-C4C-NC	-2.14	108.17	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	816	CLA	CMB-C2B-C3B	2.14	128.68	124.68
13	A	819	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
13	A	834	CLA	C1D-CHD-C4C	2.14	125.38	122.56
13	B	801	CLA	OBD-CAD-C3D	2.14	131.53	127.98
13	A	834	CLA	CED-O2D-CGD	2.14	120.77	115.94
13	A	838	CLA	C2A-C1A-CHA	2.14	127.59	123.86
13	B	805	CLA	C2A-C3A-C4A	2.13	105.32	101.87
13	A	823	CLA	C2A-C1A-CHA	2.13	127.59	123.86
13	B	815	CLA	OBD-CAD-CBD	-2.13	122.85	125.89
13	A	834	CLA	C3C-C4C-NC	-2.13	108.18	110.57
13	A	845	CLA	C2A-C3A-C4A	2.13	105.31	101.87
13	A	825	CLA	CED-O2D-CGD	2.13	120.75	115.94
13	A	814	CLA	C2A-C1A-CHA	2.13	127.58	123.86
16	B	847	BCR	C34-C9-C8	2.13	121.43	118.08
13	B	815	CLA	CMB-C2B-C3B	2.13	128.65	124.68
13	B	833	CLA	CBA-CAA-C2A	2.12	120.13	113.86
13	B	812	CLA	C3C-C4C-NC	-2.12	108.19	110.57
16	B	843	BCR	C34-C9-C8	2.12	121.41	118.08
16	I	101	BCR	C32-C1-C6	2.12	113.73	110.30
13	B	804	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
13	A	846	CLA	CMB-C2B-C3B	2.11	128.63	124.68
16	J	104	BCR	C19-C18-C17	-2.11	115.70	118.94
16	J	105	BCR	C16-C17-C18	2.11	130.33	127.31
13	B	834	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
13	B	813	CLA	C2A-C1A-CHA	2.11	127.55	123.86
13	B	840	CLA	CMB-C2B-C3B	2.11	128.63	124.68
16	A	853	BCR	C8-C7-C6	2.11	133.13	127.20
13	A	823	CLA	CMB-C2B-C3B	2.11	128.63	124.68
13	L	1002	CLA	C12-C11-C10	-2.11	103.55	113.24
13	A	837	CLA	C2A-C1A-CHA	2.11	127.55	123.86
13	B	827	CLA	CED-O2D-CGD	2.11	120.70	115.94
13	A	843	CLA	C12-C11-C10	-2.11	103.55	113.24
13	J	101	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
13	A	805	CLA	C12-C11-C10	-2.11	106.17	113.62
16	B	847	BCR	C19-C18-C17	-2.11	115.71	118.94
13	B	810	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
13	A	841	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
13	A	815	CLA	C2A-C1A-CHA	2.10	127.54	123.86
13	A	820	CLA	CBA-CAA-C2A	2.10	120.07	113.86
13	B	827	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
13	A	827	CLA	CED-O2D-CGD	2.10	120.69	115.94
13	A	843	CLA	CBA-CAA-C2A	2.10	120.06	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	836	CLA	C3C-C4C-NC	-2.10	108.22	110.57
13	A	826	CLA	C7-C6-C5	-2.10	107.66	113.36
13	B	802	CLA	OBD-CAD-C3D	2.10	131.46	127.98
13	A	830	CLA	CMD-C2D-C3D	2.10	128.60	124.68
16	L	1006	BCR	C32-C1-C6	2.10	113.70	110.30
13	A	805	CLA	C2A-C1A-CHA	2.10	127.52	123.86
16	F	1302	BCR	C1-C6-C7	2.10	121.71	115.78
13	B	838	CLA	O1D-CGD-CBD	-2.10	120.20	124.48
13	B	817	CLA	CMB-C2B-C3B	2.10	128.60	124.68
13	A	805	CLA	C1-C2-C3	2.09	129.67	126.04
16	M	1602	BCR	C35-C13-C12	2.09	121.37	118.08
16	F	1302	BCR	C8-C7-C6	2.09	133.07	127.20
13	A	802	CLA	C6-C5-C3	-2.09	107.98	113.45
13	A	810	CLA	CBA-CAA-C2A	2.09	120.02	113.86
16	F	1302	BCR	C36-C18-C19	2.09	121.36	118.08
13	A	801	CLA	CGD-CBD-CAD	2.09	117.49	110.73
13	B	815	CLA	C2A-C1A-CHA	2.09	127.50	123.86
13	B	840	CLA	C12-C11-C10	-2.08	103.67	113.24
13	A	826	CLA	C2A-C1A-CHA	2.08	127.50	123.86
13	A	834	CLA	C2A-C3A-C4A	2.08	105.23	101.87
13	B	820	CLA	C3C-C4C-NC	-2.08	108.24	110.57
13	A	812	CLA	CMB-C2B-C3B	2.08	128.57	124.68
13	A	824	CLA	C4-C3-C5	-2.08	113.61	115.98
13	B	809	CLA	CMB-C2B-C3B	2.08	128.56	124.68
13	X	1701	CLA	C2A-C1A-CHA	2.08	127.49	123.86
13	B	804	CLA	CMB-C2B-C3B	2.07	128.56	124.68
13	A	803	CLA	C2A-C3A-C4A	2.07	105.22	101.87
13	A	825	CLA	C1-C2-C3	2.07	129.63	126.04
16	B	849	BCR	C11-C10-C9	2.07	130.27	127.31
13	L	1004	CLA	CMB-C2B-C3B	2.07	128.55	124.68
13	B	804	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
16	A	850	BCR	C15-C14-C13	2.07	130.26	127.31
16	J	103	BCR	C19-C18-C17	-2.07	115.77	118.94
16	B	845	BCR	C32-C1-C6	2.07	113.65	110.30
13	A	816	CLA	C2A-C1A-CHA	2.07	127.47	123.86
13	B	821	CLA	C3C-C4C-NC	-2.07	108.25	110.57
16	J	104	BCR	C15-C14-C13	2.06	130.26	127.31
13	B	820	CLA	CMB-C2B-C3B	2.06	128.54	124.68
16	I	102	BCR	C35-C13-C12	2.06	121.33	118.08
13	A	820	CLA	C2A-C1A-CHA	2.06	127.47	123.86
16	L	1006	BCR	C23-C24-C25	2.06	133.00	127.20
16	M	1602	BCR	C30-C25-C24	2.06	121.61	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	810	CLA	C1-C2-C3	2.06	129.61	126.04
16	B	843	BCR	C20-C21-C22	2.06	130.25	127.31
13	A	825	CLA	C3C-C4C-NC	-2.06	108.26	110.57
13	B	808	CLA	OBD-CAD-C3D	2.06	131.40	127.98
13	A	823	CLA	C2A-C3A-C4A	2.06	105.20	101.87
16	B	846	BCR	C19-C18-C17	-2.06	115.78	118.94
13	B	806	CLA	C3C-C4C-NC	-2.06	108.27	110.57
13	A	807	CLA	C4D-C3D-CAD	-2.06	107.32	108.47
13	B	838	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
16	A	849	BCR	C30-C25-C24	2.05	121.59	115.78
13	B	809	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
13	J	101	CLA	CMB-C2B-C3B	2.05	128.52	124.68
13	A	837	CLA	CMB-C2B-C3B	2.05	128.52	124.68
13	A	806	CLA	OBD-CAD-C3D	2.05	131.38	127.98
16	A	850	BCR	C35-C13-C12	2.05	121.31	118.08
13	B	801	CLA	C4D-C3D-CAD	-2.05	107.33	108.47
13	A	835	CLA	C1-C2-C3	2.05	129.58	126.04
13	L	1004	CLA	CED-O2D-CGD	2.05	120.56	115.94
13	B	826	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
13	A	819	CLA	C2A-C1A-CHA	2.05	127.44	123.86
13	B	825	CLA	C3C-C4C-NC	-2.04	108.28	110.57
13	A	841	CLA	C3C-C4C-NC	-2.04	108.28	110.57
13	A	828	CLA	C2A-C3A-C4A	2.04	105.17	101.87
13	A	817	CLA	C2A-C1A-CHA	2.04	127.43	123.86
16	B	847	BCR	C23-C24-C25	2.04	132.93	127.20
13	B	838	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
13	B	825	CLA	C2A-C1A-CHA	2.04	127.42	123.86
13	B	817	CLA	OBD-CAD-C3D	2.04	131.36	127.98
17	A	856	LHG	P-O6-C4	-2.04	109.74	121.68
13	A	817	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
16	B	845	BCR	C20-C21-C22	2.03	130.21	127.31
13	B	823	CLA	C3C-C4C-NC	-2.03	108.29	110.57
13	B	817	CLA	C2A-C1A-CHA	2.03	127.42	123.86
13	A	801	CLA	CMB-C2B-C3B	2.03	128.48	124.68
13	A	842	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
16	B	849	BCR	C30-C25-C24	2.03	121.53	115.78
13	B	827	CLA	C12-C11-C10	-2.03	103.91	113.24
13	A	801	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
13	A	804	CLA	CMB-C2B-C3B	2.03	128.47	124.68
16	F	1302	BCR	C35-C13-C14	-2.03	120.08	122.92
13	B	821	CLA	CMB-C2B-C3B	2.03	128.47	124.68
16	F	1302	BCR	C40-C30-C25	2.03	113.59	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	825	CLA	CMB-C2B-C3B	2.03	128.47	124.68
13	B	812	CLA	CMB-C2B-C3B	2.03	128.47	124.68
13	B	802	CLA	CHA-C1A-NA	-2.03	121.76	126.40
13	A	816	CLA	C3C-C4C-NC	-2.02	108.30	110.57
13	B	802	CLA	C1-C2-C3	2.02	129.54	126.04
16	M	1602	BCR	C37-C22-C23	2.02	121.27	118.08
13	B	807	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
13	A	816	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
13	B	801	CLA	C2A-C3A-C4A	2.02	105.14	101.87
13	L	1003	CLA	CED-O2D-CGD	2.02	120.51	115.94
13	A	806	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
16	A	850	BCR	C32-C1-C6	2.02	113.58	110.30
13	A	841	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
16	B	844	BCR	C8-C7-C6	2.02	132.87	127.20
13	B	802	CLA	CMB-C2B-C3B	2.02	128.45	124.68
13	B	819	CLA	CMB-C2B-C3B	2.02	128.45	124.68
13	A	804	CLA	C2A-C1A-CHA	2.02	127.39	123.86
13	A	807	CLA	O2D-CGD-CBD	2.02	114.85	111.27
16	B	848	BCR	C11-C10-C9	2.02	130.19	127.31
13	B	818	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
13	A	814	CLA	C2A-C3A-C4A	2.01	105.12	101.87
13	B	823	CLA	CMB-C2B-C3B	2.01	128.45	124.68
13	B	810	CLA	C3A-C2A-C1A	2.01	104.36	101.34
16	A	851	BCR	C37-C22-C23	2.01	121.25	118.08
16	J	105	BCR	C40-C30-C25	2.01	113.56	110.30
13	A	818	CLA	CMB-C2B-C3B	2.01	128.44	124.68
13	A	819	CLA	CMB-C2B-C3B	2.01	128.44	124.68
13	B	834	CLA	CMA-C3A-C2A	-2.01	105.71	113.83
16	B	844	BCR	C15-C14-C13	2.01	130.18	127.31
13	B	828	CLA	C3A-C2A-C1A	2.01	104.35	101.34
16	B	847	BCR	C20-C21-C22	2.01	130.18	127.31
13	B	829	CLA	C2A-C3A-C4A	2.01	105.11	101.87
13	B	814	CLA	C2A-C3A-C4A	2.01	105.11	101.87
13	A	844	CLA	CMB-C2B-C3B	2.01	128.43	124.68
13	B	817	CLA	C3C-C4C-NC	-2.01	108.32	110.57
13	A	845	CLA	CMB-C2B-C3B	2.01	128.43	124.68
13	B	814	CLA	C3C-C4C-NC	-2.01	108.32	110.57
13	A	803	CLA	C4D-C3D-CAD	-2.00	107.35	108.47
16	B	848	BCR	C40-C30-C25	2.00	113.55	110.30
16	A	851	BCR	C15-C14-C13	2.00	130.17	127.31
13	A	831	CLA	O1D-CGD-CBD	-2.00	120.39	124.48

All (249) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	L	1004	CLA	NC
13	L	1004	CLA	ND
13	L	1004	CLA	NA
13	A	829	CLA	ND
13	A	820	CLA	NC
13	A	820	CLA	ND
13	A	820	CLA	NA
13	A	818	CLA	NA
13	A	804	CLA	NC
13	A	804	CLA	ND
13	A	804	CLA	NA
13	A	843	CLA	NC
13	A	843	CLA	ND
13	A	843	CLA	NA
13	B	806	CLA	NA
13	B	806	CLA	NC
13	B	806	CLA	ND
13	B	811	CLA	ND
13	B	811	CLA	NA
13	J	101	CLA	NC
13	J	101	CLA	ND
13	J	101	CLA	NA
13	B	836	CLA	NC
13	B	836	CLA	ND
13	B	836	CLA	NA
13	B	804	CLA	ND
13	B	804	CLA	NA
13	A	845	CLA	NC
13	A	845	CLA	ND
13	A	845	CLA	NA
13	B	825	CLA	NC
13	B	825	CLA	ND
13	B	825	CLA	NA
13	F	1301	CLA	NC
13	F	1301	CLA	ND
13	F	1301	CLA	NA
13	B	838	CLA	NC
13	B	838	CLA	ND
13	B	838	CLA	NA
13	M	1601	CLA	NC
13	M	1601	CLA	ND
13	M	1601	CLA	NA
13	A	839	CLA	ND

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Mol	Chain	Res	Type	Atom
13	A	839	CLA	NA
13	A	815	CLA	NC
13	A	815	CLA	ND
13	A	815	CLA	NA
13	B	826	CLA	NC
13	B	826	CLA	ND
13	B	826	CLA	NA
13	B	823	CLA	NC
13	B	823	CLA	ND
13	B	823	CLA	NA
13	A	836	CLA	NC
13	A	836	CLA	ND
13	A	836	CLA	NA
13	A	835	CLA	NC
13	A	835	CLA	ND
13	A	835	CLA	NA
13	A	830	CLA	NC
13	A	830	CLA	ND
13	B	835	CLA	NC
13	B	835	CLA	ND
13	B	835	CLA	NA
13	A	823	CLA	NC
13	A	823	CLA	ND
13	A	823	CLA	NA
13	B	829	CLA	NC
13	B	829	CLA	ND
13	B	829	CLA	NA
13	A	801	CLA	NC
13	A	801	CLA	ND
13	A	801	CLA	NA
13	B	801	CLA	ND
13	A	826	CLA	NC
13	A	826	CLA	ND
13	A	826	CLA	NA
13	A	825	CLA	NC
13	A	825	CLA	ND
13	A	825	CLA	NA
13	A	846	CLA	NC
13	A	846	CLA	ND
13	A	846	CLA	NA
13	B	822	CLA	NC
13	B	822	CLA	ND

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Mol	Chain	Res	Type	Atom
13	B	822	CLA	NA
13	A	806	CLA	NA
13	A	806	CLA	NC
13	A	806	CLA	ND
13	B	813	CLA	NA
13	B	813	CLA	NC
13	B	813	CLA	ND
13	B	831	CLA	NC
13	B	831	CLA	ND
13	B	831	CLA	NA
13	J	102	CLA	NC
13	J	102	CLA	ND
13	J	102	CLA	NA
13	B	820	CLA	NC
13	B	820	CLA	ND
13	B	820	CLA	NA
13	B	810	CLA	NC
13	B	810	CLA	ND
13	B	810	CLA	NA
13	A	816	CLA	NC
13	A	816	CLA	ND
13	A	816	CLA	NA
13	A	819	CLA	NC
13	A	819	CLA	ND
13	A	819	CLA	NA
13	A	813	CLA	NC
13	A	813	CLA	ND
13	A	813	CLA	NA
13	B	833	CLA	NC
13	B	833	CLA	ND
13	B	833	CLA	NA
13	A	833	CLA	NC
13	A	833	CLA	ND
13	A	833	CLA	NA
13	B	817	CLA	NC
13	B	817	CLA	ND
13	B	817	CLA	NA
13	A	832	CLA	NC
13	A	832	CLA	ND
13	A	832	CLA	NA
13	B	814	CLA	NC
13	B	814	CLA	ND

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Mol	Chain	Res	Type	Atom
13	B	814	CLA	NA
13	B	830	CLA	NC
13	B	830	CLA	ND
13	B	830	CLA	NA
13	A	821	CLA	NC
13	A	821	CLA	ND
13	A	821	CLA	NA
13	B	803	CLA	NA
13	B	805	CLA	NA
13	B	805	CLA	NC
13	B	805	CLA	ND
13	B	828	CLA	NA
13	B	827	CLA	ND
13	A	803	CLA	ND
13	A	803	CLA	NA
13	B	808	CLA	ND
13	B	808	CLA	NA
13	L	1002	CLA	NC
13	L	1002	CLA	ND
13	L	1002	CLA	NA
13	B	807	CLA	NC
13	B	807	CLA	ND
13	B	807	CLA	NA
13	A	814	CLA	NC
13	A	814	CLA	ND
13	A	814	CLA	NA
13	A	837	CLA	NC
13	A	837	CLA	ND
13	A	837	CLA	NA
13	B	824	CLA	NC
13	B	824	CLA	ND
13	B	824	CLA	NA
13	A	840	CLA	ND
13	B	840	CLA	NC
13	B	840	CLA	ND
13	A	844	CLA	NC
13	A	844	CLA	ND
13	A	844	CLA	NA
13	A	812	CLA	NC
13	A	812	CLA	ND
13	A	812	CLA	NA
13	B	812	CLA	NC

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Mol	Chain	Res	Type	Atom
13	B	812	CLA	ND
13	B	812	CLA	NA
13	B	818	CLA	NC
13	B	818	CLA	ND
13	B	818	CLA	NA
13	A	838	CLA	NC
13	A	838	CLA	ND
13	A	838	CLA	NA
13	A	824	CLA	ND
13	A	824	CLA	NA
13	B	802	CLA	ND
13	B	802	CLA	NA
13	L	1003	CLA	NC
13	L	1003	CLA	NA
13	A	807	CLA	NC
13	A	807	CLA	ND
13	A	807	CLA	NA
13	A	808	CLA	ND
13	A	808	CLA	NA
13	A	831	CLA	NC
13	A	831	CLA	ND
13	A	831	CLA	NA
13	B	837	CLA	NC
13	B	837	CLA	ND
13	B	837	CLA	NA
13	B	816	CLA	NC
13	B	816	CLA	ND
13	B	816	CLA	NA
13	A	822	CLA	NC
13	A	822	CLA	ND
13	A	822	CLA	NA
13	B	841	CLA	NC
13	B	841	CLA	NA
13	B	821	CLA	NC
13	B	821	CLA	ND
13	B	821	CLA	NA
13	A	805	CLA	NC
13	A	805	CLA	ND
13	A	805	CLA	NA
13	A	841	CLA	NC
13	A	841	CLA	ND
13	A	841	CLA	NA

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Mol	Chain	Res	Type	Atom
13	B	819	CLA	NC
13	B	819	CLA	ND
13	B	819	CLA	NA
13	A	810	CLA	NC
13	A	810	CLA	ND
13	A	810	CLA	NA
13	B	832	CLA	NC
13	B	832	CLA	ND
13	B	832	CLA	NA
13	K	1401	CLA	NC
13	K	1401	CLA	NA
13	A	802	CLA	ND
13	A	802	CLA	NA
13	B	809	CLA	ND
13	A	828	CLA	NC
13	A	828	CLA	ND
13	A	828	CLA	NA
13	A	817	CLA	NC
13	A	817	CLA	ND
13	A	817	CLA	NA
13	B	815	CLA	NC
13	B	815	CLA	NA
13	B	834	CLA	NC
13	B	834	CLA	ND
13	B	834	CLA	NA
13	A	809	CLA	NC
13	A	809	CLA	ND
13	A	809	CLA	NA
13	A	842	CLA	NC
13	A	842	CLA	ND
13	A	842	CLA	NA
17	A	856	LHG	C2
13	A	827	CLA	NC
13	A	827	CLA	ND
13	A	827	CLA	NA
13	X	1701	CLA	NC
13	X	1701	CLA	ND
13	X	1701	CLA	NA

All (838) torsion outliers are listed below:

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Mol	Chain	Res	Type	Atoms
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Mol	Chain	Res	Type	Atoms
13	A	829	CLA	C2-C3-C5-C6
13	A	829	CLA	C4-C3-C5-C6
13	A	820	CLA	C1A-C2A-CAA-CBA
13	A	820	CLA	C3A-C2A-CAA-CBA
13	A	843	CLA	C4-C3-C5-C6
13	B	806	CLA	C4-C3-C5-C6
13	B	811	CLA	CBD-CGD-O2D-CED
13	J	101	CLA	C1A-C2A-CAA-CBA
13	J	101	CLA	C3A-C2A-CAA-CBA
13	J	101	CLA	CAD-CBD-CGD-O1D
13	J	101	CLA	CAD-CBD-CGD-O2D
13	J	101	CLA	CBD-CGD-O2D-CED
13	B	836	CLA	CBD-CGD-O2D-CED
13	B	825	CLA	C1A-C2A-CAA-CBA
13	B	825	CLA	CHA-CBD-CGD-O1D
13	B	825	CLA	CHA-CBD-CGD-O2D
13	M	1601	CLA	C1A-C2A-CAA-CBA
13	M	1601	CLA	C3A-C2A-CAA-CBA
13	M	1601	CLA	CAD-CBD-CGD-O1D
13	M	1601	CLA	CAD-CBD-CGD-O2D
17	B	851	LHG	O1-C1-C2-C3
13	A	835	CLA	CHA-CBD-CGD-O1D
13	A	835	CLA	CHA-CBD-CGD-O2D
13	A	823	CLA	C1A-C2A-CAA-CBA
13	A	823	CLA	C3A-C2A-CAA-CBA
13	A	823	CLA	C1-C2-C3-C4
13	B	829	CLA	CHA-CBD-CGD-O1D
13	B	829	CLA	CHA-CBD-CGD-O2D
13	A	846	CLA	C1A-C2A-CAA-CBA
13	A	846	CLA	CBA-CGA-O2A-C1
13	A	846	CLA	O1A-CGA-O2A-C1
13	A	846	CLA	CHA-CBD-CGD-O1D
13	A	846	CLA	CHA-CBD-CGD-O2D
13	A	846	CLA	CAD-CBD-CGD-O1D
13	A	846	CLA	CAD-CBD-CGD-O2D
13	A	846	CLA	CBD-CGD-O2D-CED
13	B	822	CLA	CBD-CGD-O2D-CED
13	A	806	CLA	C1A-C2A-CAA-CBA
13	A	806	CLA	C3A-C2A-CAA-CBA
13	A	806	CLA	CBA-CGA-O2A-C1
13	A	806	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	A	806	CLA	CHA-CBD-CGD-O2D
13	A	806	CLA	CAD-CBD-CGD-O1D
13	A	806	CLA	O2A-C1-C2-C3
13	B	813	CLA	C1A-C2A-CAA-CBA
13	A	811	CLA	C1A-C2A-CAA-CBA
13	A	811	CLA	C3A-C2A-CAA-CBA
13	B	820	CLA	C3A-C2A-CAA-CBA
13	A	819	CLA	C3A-C2A-CAA-CBA
13	A	813	CLA	CBD-CGD-O2D-CED
13	B	817	CLA	C1A-C2A-CAA-CBA
13	B	817	CLA	C3A-C2A-CAA-CBA
13	B	830	CLA	C3A-C2A-CAA-CBA
13	B	830	CLA	C2A-CAA-CBA-CGA
13	B	830	CLA	CBD-CGD-O2D-CED
13	A	821	CLA	C1A-C2A-CAA-CBA
13	A	821	CLA	C3A-C2A-CAA-CBA
13	A	821	CLA	CBD-CGD-O2D-CED
13	B	805	CLA	C1A-C2A-CAA-CBA
13	B	805	CLA	C3A-C2A-CAA-CBA
13	B	828	CLA	C1A-C2A-CAA-CBA
13	B	828	CLA	C3A-C2A-CAA-CBA
13	B	827	CLA	C3A-C2A-CAA-CBA
16	B	847	BCR	C23-C24-C25-C26
16	B	847	BCR	C23-C24-C25-C30
13	A	803	CLA	O2A-C1-C2-C3
13	L	1002	CLA	C1A-C2A-CAA-CBA
13	L	1002	CLA	C3A-C2A-CAA-CBA
13	A	837	CLA	C1A-C2A-CAA-CBA
13	A	837	CLA	CHA-CBD-CGD-O1D
13	A	837	CLA	CHA-CBD-CGD-O2D
13	B	824	CLA	CHA-CBD-CGD-O2D
13	A	844	CLA	C4-C3-C5-C6
13	A	812	CLA	C1A-C2A-CAA-CBA
13	A	812	CLA	C3A-C2A-CAA-CBA
13	B	818	CLA	C3A-C2A-CAA-CBA
13	B	818	CLA	C2-C3-C5-C6
13	B	818	CLA	C4-C3-C5-C6
13	A	838	CLA	C4-C3-C5-C6
16	A	850	BCR	C23-C24-C25-C26
13	A	824	CLA	C4-C3-C5-C6
13	A	807	CLA	C1A-C2A-CAA-CBA
13	A	807	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	A	807	CLA	C4-C3-C5-C6
13	B	816	CLA	C1A-C2A-CAA-CBA
13	B	816	CLA	C3A-C2A-CAA-CBA
13	B	841	CLA	C1A-C2A-CAA-CBA
13	B	841	CLA	C3A-C2A-CAA-CBA
13	B	821	CLA	CBD-CGD-O2D-CED
13	A	805	CLA	C3A-C2A-CAA-CBA
13	A	841	CLA	CHA-CBD-CGD-O1D
13	A	841	CLA	CHA-CBD-CGD-O2D
16	A	852	BCR	C23-C24-C25-C26
16	A	852	BCR	C23-C24-C25-C30
14	A	847	PQN	C14-C13-C15-C16
13	B	832	CLA	C1A-C2A-CAA-CBA
13	B	832	CLA	C3A-C2A-CAA-CBA
13	B	832	CLA	O2A-C1-C2-C3
13	K	1401	CLA	CBD-CGD-O2D-CED
13	A	817	CLA	C1A-C2A-CAA-CBA
13	A	817	CLA	C3A-C2A-CAA-CBA
13	A	817	CLA	CBD-CGD-O2D-CED
13	B	815	CLA	C1A-C2A-CAA-CBA
13	B	815	CLA	C3A-C2A-CAA-CBA
16	J	103	BCR	C1-C6-C7-C8
16	J	103	BCR	C5-C6-C7-C8
13	A	809	CLA	C3A-C2A-CAA-CBA
16	J	104	BCR	C23-C24-C25-C26
16	J	104	BCR	C23-C24-C25-C30
13	A	842	CLA	C1A-C2A-CAA-CBA
13	A	842	CLA	C2-C3-C5-C6
13	A	842	CLA	C4-C3-C5-C6
13	A	817	CLA	O1D-CGD-O2D-CED
13	B	834	CLA	O1D-CGD-O2D-CED
13	A	842	CLA	O1D-CGD-O2D-CED
13	B	804	CLA	CBD-CGD-O2D-CED
13	F	1301	CLA	CBD-CGD-O2D-CED
13	M	1601	CLA	CBD-CGD-O2D-CED
13	B	801	CLA	CBD-CGD-O2D-CED
13	A	811	CLA	CBD-CGD-O2D-CED
13	B	831	CLA	CBD-CGD-O2D-CED
13	A	816	CLA	CBD-CGD-O2D-CED
13	A	812	CLA	CBD-CGD-O2D-CED
13	A	807	CLA	CBD-CGD-O2D-CED
13	A	810	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	B	815	CLA	CBD-CGD-O2D-CED
13	B	834	CLA	CBD-CGD-O2D-CED
13	A	842	CLA	CBD-CGD-O2D-CED
13	A	836	CLA	O1A-CGA-O2A-C1
13	A	806	CLA	O1A-CGA-O2A-C1
13	A	821	CLA	O1A-CGA-O2A-C1
13	B	811	CLA	O1D-CGD-O2D-CED
13	A	846	CLA	O1D-CGD-O2D-CED
13	B	822	CLA	O1D-CGD-O2D-CED
13	K	1401	CLA	O1D-CGD-O2D-CED
13	A	836	CLA	CBA-CGA-O2A-C1
13	A	844	CLA	CBA-CGA-O2A-C1
13	L	1004	CLA	CBD-CGD-O2D-CED
13	A	829	CLA	CBD-CGD-O2D-CED
13	A	843	CLA	CBD-CGD-O2D-CED
13	A	835	CLA	CBD-CGD-O2D-CED
13	A	823	CLA	CBD-CGD-O2D-CED
13	B	833	CLA	CBD-CGD-O2D-CED
13	A	808	CLA	CBD-CGD-O2D-CED
13	A	805	CLA	CBD-CGD-O2D-CED
13	A	809	CLA	CBD-CGD-O2D-CED
13	X	1701	CLA	CBD-CGD-O2D-CED
13	A	813	CLA	O1A-CGA-O2A-C1
13	A	833	CLA	O1A-CGA-O2A-C1
13	A	803	CLA	O1A-CGA-O2A-C1
13	A	844	CLA	O1A-CGA-O2A-C1
13	A	838	CLA	O1A-CGA-O2A-C1
13	J	101	CLA	O1D-CGD-O2D-CED
13	B	836	CLA	O1D-CGD-O2D-CED
13	M	1601	CLA	O1D-CGD-O2D-CED
13	A	813	CLA	O1D-CGD-O2D-CED
13	A	821	CLA	O1D-CGD-O2D-CED
13	A	830	CLA	CBD-CGD-O2D-CED
13	A	825	CLA	CBD-CGD-O2D-CED
13	B	821	CLA	O1D-CGD-O2D-CED
13	A	806	CLA	C3-C5-C6-C7
13	A	813	CLA	C3-C5-C6-C7
13	A	810	CLA	C3-C5-C6-C7
13	B	809	CLA	C3-C5-C6-C7
13	A	820	CLA	CBA-CGA-O2A-C1
13	A	821	CLA	CBA-CGA-O2A-C1
13	L	1002	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	A	840	CLA	CBA-CGA-O2A-C1
13	A	838	CLA	CBA-CGA-O2A-C1
13	A	817	CLA	CBA-CGA-O2A-C1
17	B	851	LHG	C24-C23-O8-C6
13	B	801	CLA	O1D-CGD-O2D-CED
13	B	830	CLA	O1D-CGD-O2D-CED
13	A	843	CLA	C2-C3-C5-C6
13	B	806	CLA	C2-C3-C5-C6
13	A	824	CLA	CBD-CGD-O2D-CED
13	A	830	CLA	C2A-CAA-CBA-CGA
13	B	831	CLA	C2A-CAA-CBA-CGA
13	B	840	CLA	C2A-CAA-CBA-CGA
13	A	825	CLA	CBA-CGA-O2A-C1
13	B	820	CLA	CBA-CGA-O2A-C1
13	A	813	CLA	CBA-CGA-O2A-C1
13	A	833	CLA	CBA-CGA-O2A-C1
13	A	803	CLA	CBA-CGA-O2A-C1
13	B	804	CLA	O1D-CGD-O2D-CED
13	B	806	CLA	CBD-CGD-O2D-CED
13	B	839	CLA	CBD-CGD-O2D-CED
13	F	1301	CLA	O1D-CGD-O2D-CED
13	A	811	CLA	O1D-CGD-O2D-CED
13	A	812	CLA	O1D-CGD-O2D-CED
17	B	851	LHG	O9-C7-O7-C5
13	L	1002	CLA	O1A-CGA-O2A-C1
13	A	824	CLA	O1A-CGA-O2A-C1
13	B	816	CLA	O1A-CGA-O2A-C1
13	A	817	CLA	O1A-CGA-O2A-C1
13	B	815	CLA	C2A-CAA-CBA-CGA
18	B	850	LMG	O6-C5-C6-O5
13	B	810	CLA	CBD-CGD-O2D-CED
13	B	808	CLA	CBD-CGD-O2D-CED
13	B	832	CLA	CBD-CGD-O2D-CED
13	A	826	CLA	C3-C5-C6-C7
13	A	832	CLA	CBA-CGA-O2A-C1
13	L	1003	CLA	CBA-CGA-O2A-C1
13	A	809	CLA	CBA-CGA-O2A-C1
13	A	820	CLA	O1A-CGA-O2A-C1
13	A	840	CLA	O1A-CGA-O2A-C1
13	B	831	CLA	O1D-CGD-O2D-CED
13	A	816	CLA	O1D-CGD-O2D-CED
13	B	815	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
17	B	851	LHG	C8-C7-O7-C5
13	A	806	CLA	CBD-CGD-O2D-CED
13	A	810	CLA	O1D-CGD-O2D-CED
13	B	806	CLA	C3-C5-C6-C7
13	B	808	CLA	C3-C5-C6-C7
13	B	840	CLA	C3-C5-C6-C7
13	A	809	CLA	C3-C5-C6-C7
13	A	824	CLA	CBA-CGA-O2A-C1
13	B	816	CLA	CBA-CGA-O2A-C1
13	A	825	CLA	O1A-CGA-O2A-C1
13	B	820	CLA	O1A-CGA-O2A-C1
13	L	1003	CLA	O1A-CGA-O2A-C1
13	A	809	CLA	O1A-CGA-O2A-C1
13	A	836	CLA	C4-C3-C5-C6
13	B	824	CLA	C4-C3-C5-C6
13	B	802	CLA	C4-C3-C5-C6
13	B	816	CLA	C4-C3-C5-C6
13	A	836	CLA	C2-C3-C5-C6
13	B	824	CLA	C2-C3-C5-C6
13	A	844	CLA	C2-C3-C5-C6
13	B	802	CLA	C2-C3-C5-C6
13	B	816	CLA	C2-C3-C5-C6
14	A	847	PQN	C12-C13-C15-C16
13	B	841	CLA	CBD-CGD-O2D-CED
13	A	807	CLA	O1D-CGD-O2D-CED
13	A	832	CLA	O1A-CGA-O2A-C1
13	B	829	CLA	CBA-CGA-O2A-C1
13	B	818	CLA	CBA-CGA-O2A-C1
13	A	843	CLA	O1D-CGD-O2D-CED
13	A	823	CLA	O1D-CGD-O2D-CED
13	A	829	CLA	O1A-CGA-O2A-C1
13	A	835	CLA	O1D-CGD-O2D-CED
13	B	833	CLA	O1D-CGD-O2D-CED
13	A	808	CLA	O1D-CGD-O2D-CED
13	A	805	CLA	O1D-CGD-O2D-CED
17	B	851	LHG	O10-C23-O8-C6
17	A	856	LHG	C1-C2-C3-O3
13	B	818	CLA	O1A-CGA-O2A-C1
13	B	824	CLA	C3-C5-C6-C7
13	A	829	CLA	CBA-CGA-O2A-C1
13	B	826	CLA	CBA-CGA-O2A-C1
13	A	823	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	B	813	CLA	CBA-CGA-O2A-C1
13	A	812	CLA	CBA-CGA-O2A-C1
13	B	837	CLA	CBA-CGA-O2A-C1
13	A	805	CLA	CBA-CGA-O2A-C1
13	B	805	CLA	CBD-CGD-O2D-CED
13	A	845	CLA	C2A-CAA-CBA-CGA
13	A	843	CLA	C13-C15-C16-C17
13	B	806	CLA	C13-C15-C16-C17
13	A	828	CLA	C10-C11-C12-C13
17	A	856	LHG	O2-C2-C3-O3
13	A	823	CLA	O1A-CGA-O2A-C1
13	B	813	CLA	O1A-CGA-O2A-C1
13	L	1004	CLA	O1D-CGD-O2D-CED
13	X	1701	CLA	O1D-CGD-O2D-CED
13	L	1004	CLA	C5-C6-C7-C8
13	A	812	CLA	O1A-CGA-O2A-C1
13	A	809	CLA	O1D-CGD-O2D-CED
13	A	807	CLA	C15-C16-C17-C18
17	B	851	LHG	O1-C1-C2-O2
13	A	833	CLA	CBD-CGD-O2D-CED
13	A	839	CLA	C8-C10-C11-C12
13	A	843	CLA	C2-C1-O2A-CGA
13	B	810	CLA	C15-C16-C17-C18
13	A	819	CLA	CBD-CGD-O2D-CED
14	B	842	PQN	C25-C26-C27-C28
13	B	801	CLA	C12-C13-C15-C16
13	A	831	CLA	C11-C10-C8-C7
13	B	809	CLA	C12-C13-C15-C16
13	A	807	CLA	C3-C5-C6-C7
13	B	826	CLA	O1A-CGA-O2A-C1
13	A	805	CLA	O1A-CGA-O2A-C1
13	B	804	CLA	C2A-CAA-CBA-CGA
13	A	829	CLA	O1D-CGD-O2D-CED
13	B	829	CLA	O1A-CGA-O2A-C1
13	B	837	CLA	O1A-CGA-O2A-C1
16	B	846	BCR	C18-C19-C20-C21
18	B	850	LMG	C4-C5-C6-O5
13	B	826	CLA	C10-C11-C12-C13
13	B	828	CLA	C15-C16-C17-C18
13	A	810	CLA	C8-C10-C11-C12
13	A	827	CLA	C5-C6-C7-C8
13	B	828	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	B	808	CLA	C13-C15-C16-C17
13	B	837	CLA	C8-C10-C11-C12
13	A	812	CLA	C15-C16-C17-C18
13	A	810	CLA	C13-C15-C16-C17
17	A	855	LHG	C4-O6-P-O3
14	A	847	PQN	C13-C15-C16-C17
13	B	839	CLA	CBA-CGA-O2A-C1
13	A	831	CLA	CBA-CGA-O2A-C1
13	A	842	CLA	CBA-CGA-O2A-C1
13	A	830	CLA	O1D-CGD-O2D-CED
13	B	829	CLA	C13-C15-C16-C17
13	L	1003	CLA	C8-C10-C11-C12
13	B	832	CLA	C10-C11-C12-C13
13	A	825	CLA	O1D-CGD-O2D-CED
13	A	811	CLA	C2A-CAA-CBA-CGA
13	A	837	CLA	C2A-CAA-CBA-CGA
13	A	809	CLA	C5-C6-C7-C8
17	A	855	LHG	C24-C25-C26-C27
13	B	839	CLA	O1D-CGD-O2D-CED
13	A	824	CLA	O1D-CGD-O2D-CED
16	B	846	BCR	C16-C17-C18-C36
16	B	846	BCR	C20-C21-C22-C37
13	B	806	CLA	O1D-CGD-O2D-CED
14	B	842	PQN	C26-C27-C28-C29
13	B	805	CLA	CBA-CGA-O2A-C1
13	B	806	CLA	C10-C11-C12-C13
16	B	846	BCR	C16-C17-C18-C19
16	I	102	BCR	C20-C21-C22-C23
16	B	844	BCR	C11-C10-C9-C8
13	A	833	CLA	C8-C10-C11-C12
13	B	839	CLA	O1A-CGA-O2A-C1
13	A	831	CLA	O1A-CGA-O2A-C1
13	A	842	CLA	O1A-CGA-O2A-C1
13	B	822	CLA	C6-C7-C8-C9
13	A	826	CLA	C4-C3-C5-C6
13	A	826	CLA	C2-C3-C5-C6
13	B	801	CLA	C14-C13-C15-C16
13	A	821	CLA	C6-C7-C8-C9
13	A	823	CLA	C2A-CAA-CBA-CGA
13	A	810	CLA	C2A-CAA-CBA-CGA
13	A	806	CLA	C10-C11-C12-C13
13	B	832	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
17	A	856	LHG	C9-C10-C11-C12
17	A	855	LHG	C28-C29-C30-C31
13	B	822	CLA	C6-C7-C8-C10
14	B	842	PQN	C26-C27-C28-C30
13	B	805	CLA	C13-C15-C16-C17
13	A	804	CLA	CBD-CGD-O2D-CED
13	B	808	CLA	O1D-CGD-O2D-CED
13	M	1601	CLA	C2A-CAA-CBA-CGA
13	X	1701	CLA	C2A-CAA-CBA-CGA
13	A	804	CLA	C3A-C2A-CAA-CBA
13	B	813	CLA	C3A-C2A-CAA-CBA
13	A	837	CLA	C3A-C2A-CAA-CBA
13	A	807	CLA	C3A-C2A-CAA-CBA
13	A	842	CLA	C3A-C2A-CAA-CBA
13	B	824	CLA	O2A-C1-C2-C3
13	B	802	CLA	C3-C5-C6-C7
13	A	834	CLA	C4-C3-C5-C6
13	B	832	CLA	C2-C3-C5-C6
13	A	834	CLA	C2-C3-C5-C6
13	B	810	CLA	O1D-CGD-O2D-CED
13	B	805	CLA	O1A-CGA-O2A-C1
13	B	837	CLA	C5-C6-C7-C8
13	A	821	CLA	C4C-C3C-CAC-CBC
16	A	854	BCR	C1-C6-C7-C8
16	A	854	BCR	C5-C6-C7-C8
16	A	854	BCR	C23-C24-C25-C26
16	A	854	BCR	C23-C24-C25-C30
16	A	853	BCR	C1-C6-C7-C8
16	A	853	BCR	C5-C6-C7-C8
16	M	1602	BCR	C1-C6-C7-C8
16	M	1602	BCR	C5-C6-C7-C8
13	B	818	CLA	C3-C5-C6-C7
16	A	850	BCR	C1-C6-C7-C8
16	A	850	BCR	C5-C6-C7-C8
16	A	850	BCR	C23-C24-C25-C30
16	B	849	BCR	C1-C6-C7-C8
16	I	102	BCR	C23-C24-C25-C26
16	I	102	BCR	C23-C24-C25-C30
16	B	844	BCR	C1-C6-C7-C8
16	B	844	BCR	C5-C6-C7-C8
16	B	844	BCR	C23-C24-C25-C26
16	J	104	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	J	104	BCR	C5-C6-C7-C8
13	A	806	CLA	C8-C10-C11-C12
13	B	801	CLA	C13-C15-C16-C17
13	B	841	CLA	O1D-CGD-O2D-CED
13	A	820	CLA	C11-C12-C13-C15
13	B	826	CLA	C6-C7-C8-C10
13	A	821	CLA	C6-C7-C8-C10
13	L	1003	CLA	C11-C10-C8-C7
13	A	807	CLA	C11-C12-C13-C15
14	A	847	PQN	C16-C17-C18-C20
13	A	834	CLA	C12-C13-C15-C16
13	A	827	CLA	C12-C13-C15-C16
13	A	806	CLA	O1D-CGD-O2D-CED
13	B	819	CLA	C10-C11-C12-C13
13	B	832	CLA	O1D-CGD-O2D-CED
13	B	805	CLA	O1D-CGD-O2D-CED
17	A	855	LHG	C10-C11-C12-C13
13	B	827	CLA	CBD-CGD-O2D-CED
13	A	814	CLA	C3-C5-C6-C7
13	A	843	CLA	C5-C6-C7-C8
13	B	833	CLA	C4-C3-C5-C6
13	B	832	CLA	C4-C3-C5-C6
13	A	846	CLA	C2-C3-C5-C6
13	A	820	CLA	C11-C12-C13-C14
13	B	826	CLA	C6-C7-C8-C9
13	B	826	CLA	C11-C12-C13-C14
13	A	807	CLA	C11-C12-C13-C14
13	A	831	CLA	C11-C10-C8-C9
13	B	809	CLA	C14-C13-C15-C16
13	A	834	CLA	C14-C13-C15-C16
13	A	827	CLA	C14-C13-C15-C16
13	A	804	CLA	C1A-C2A-CAA-CBA
13	B	811	CLA	C1A-C2A-CAA-CBA
13	B	831	CLA	C1A-C2A-CAA-CBA
13	B	820	CLA	C1A-C2A-CAA-CBA
13	A	819	CLA	C1A-C2A-CAA-CBA
13	B	830	CLA	C1A-C2A-CAA-CBA
13	B	827	CLA	C1A-C2A-CAA-CBA
13	A	840	CLA	C1A-C2A-CAA-CBA
13	B	818	CLA	C1A-C2A-CAA-CBA
13	A	805	CLA	C1A-C2A-CAA-CBA
13	B	819	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	K	1401	CLA	C1A-C2A-CAA-CBA
13	A	809	CLA	C1A-C2A-CAA-CBA
13	B	827	CLA	C10-C11-C12-C13
13	A	802	CLA	C15-C16-C17-C18
13	B	813	CLA	C8-C10-C11-C12
13	A	833	CLA	O1D-CGD-O2D-CED
13	A	841	CLA	C5-C6-C7-C8
13	A	846	CLA	C4-C3-C5-C6
13	A	844	CLA	C3-C5-C6-C7
13	B	816	CLA	C3-C5-C6-C7
18	B	850	LMG	C30-C31-C32-C33
13	B	825	CLA	CBA-CGA-O2A-C1
16	I	102	BCR	C20-C21-C22-C37
13	B	831	CLA	CBA-CGA-O2A-C1
13	B	817	CLA	CBA-CGA-O2A-C1
13	B	826	CLA	CBD-CGD-O2D-CED
13	A	817	CLA	C1-C2-C3-C4
13	A	812	CLA	C2A-CAA-CBA-CGA
17	A	855	LHG	C24-C23-O8-C6
13	A	839	CLA	C5-C6-C7-C8
13	A	826	CLA	C8-C10-C11-C12
16	B	848	BCR	C11-C10-C9-C8
13	A	819	CLA	CAA-CBA-CGA-O2A
17	A	856	LHG	C11-C10-C9-C8
13	A	830	CLA	C4-C3-C5-C6
13	B	814	CLA	C4-C3-C5-C6
13	B	828	CLA	C4-C3-C5-C6
13	B	826	CLA	C11-C12-C13-C15
13	B	814	CLA	C2-C3-C5-C6
13	B	805	CLA	C12-C13-C15-C16
13	B	828	CLA	C2-C3-C5-C6
13	A	809	CLA	C11-C10-C8-C7
13	A	820	CLA	C11-C10-C8-C9
13	A	830	CLA	C14-C13-C15-C16
13	L	1003	CLA	C11-C10-C8-C9
14	A	847	PQN	C16-C17-C18-C19
13	A	809	CLA	C11-C10-C8-C9
13	A	828	CLA	CBA-CGA-O2A-C1
13	B	809	CLA	C16-C17-C18-C20
13	A	833	CLA	C3-C5-C6-C7
13	A	819	CLA	O1D-CGD-O2D-CED
13	A	803	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	A	814	CLA	C8-C10-C11-C12
13	A	827	CLA	C15-C16-C17-C18
13	A	804	CLA	O1D-CGD-O2D-CED
13	A	830	CLA	C5-C6-C7-C8
13	B	806	CLA	C15-C16-C17-C18
13	A	826	CLA	C13-C15-C16-C17
13	A	830	CLA	C2-C3-C5-C6
13	L	1002	CLA	C13-C15-C16-C17
13	B	818	CLA	C5-C6-C7-C8
13	A	809	CLA	C15-C16-C17-C18
13	A	809	CLA	C8-C10-C11-C12
13	A	822	CLA	CBA-CGA-O2A-C1
13	A	845	CLA	C3A-C2A-CAA-CBA
13	B	825	CLA	C3A-C2A-CAA-CBA
13	A	846	CLA	C3A-C2A-CAA-CBA
13	B	831	CLA	C3A-C2A-CAA-CBA
13	A	826	CLA	CBA-CGA-O2A-C1
13	A	827	CLA	CBA-CGA-O2A-C1
13	A	827	CLA	C8-C10-C11-C12
13	B	831	CLA	O1A-CGA-O2A-C1
13	A	807	CLA	C16-C17-C18-C19
13	B	809	CLA	C16-C17-C18-C19
13	B	833	CLA	C2-C3-C5-C6
13	A	828	CLA	O1A-CGA-O2A-C1
13	B	801	CLA	C5-C6-C7-C8
13	B	817	CLA	O1A-CGA-O2A-C1
17	A	855	LHG	O10-C23-O8-C6
13	A	814	CLA	C2-C1-O2A-CGA
13	B	802	CLA	C14-C13-C15-C16
13	A	808	CLA	C4-C3-C5-C6
13	A	803	CLA	C2A-CAA-CBA-CGA
13	B	832	CLA	C2A-CAA-CBA-CGA
13	A	817	CLA	O2A-C1-C2-C3
16	M	1602	BCR	C23-C24-C25-C30
16	B	849	BCR	C5-C6-C7-C8
16	F	1302	BCR	C23-C24-C25-C26
16	F	1302	BCR	C23-C24-C25-C30
16	B	844	BCR	C23-C24-C25-C30
13	A	827	CLA	O1A-CGA-O2A-C1
14	A	847	PQN	C15-C16-C17-C18
13	A	835	CLA	C12-C13-C15-C16
13	A	830	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
13	B	813	CLA	C11-C10-C8-C7
13	B	828	CLA	C12-C13-C15-C16
13	B	802	CLA	C12-C13-C15-C16
13	A	841	CLA	C11-C10-C8-C7
13	B	809	CLA	C6-C7-C8-C10
13	A	807	CLA	C16-C17-C18-C20
16	L	1006	BCR	C35-C13-C14-C15
16	F	1302	BCR	C20-C21-C22-C37
16	J	103	BCR	C35-C13-C14-C15
13	A	823	CLA	CAD-CBD-CGD-O2D
13	A	801	CLA	CAD-CBD-CGD-O2D
13	A	816	CLA	CAD-CBD-CGD-O2D
13	B	802	CLA	CAD-CBD-CGD-O2D
13	B	821	CLA	CAD-CBD-CGD-O2D
13	A	827	CLA	CAD-CBD-CGD-O2D
16	L	1005	BCR	C22-C23-C24-C25
13	B	814	CLA	CBA-CGA-O2A-C1
13	A	823	CLA	O2A-C1-C2-C3
13	B	828	CLA	C2A-CAA-CBA-CGA
13	B	805	CLA	CHA-CBD-CGD-O1D
13	B	805	CLA	CHA-CBD-CGD-O2D
13	B	808	CLA	CHA-CBD-CGD-O1D
13	B	808	CLA	CHA-CBD-CGD-O2D
13	B	824	CLA	CHA-CBD-CGD-O1D
13	A	831	CLA	CHA-CBD-CGD-O1D
13	A	831	CLA	CHA-CBD-CGD-O2D
13	B	819	CLA	CHA-CBD-CGD-O1D
13	B	819	CLA	CHA-CBD-CGD-O2D
13	B	834	CLA	CHA-CBD-CGD-O2D
13	A	809	CLA	CHA-CBD-CGD-O1D
13	A	809	CLA	CHA-CBD-CGD-O2D
13	A	826	CLA	O1A-CGA-O2A-C1
13	A	822	CLA	O1A-CGA-O2A-C1
13	A	820	CLA	C16-C17-C18-C20
13	L	1004	CLA	C4-C3-C5-C6
13	B	837	CLA	C4-C3-C5-C6
13	B	837	CLA	C2-C3-C5-C6
13	L	1002	CLA	C11-C10-C8-C9
13	A	810	CLA	C11-C12-C13-C14
13	B	812	CLA	C2A-CAA-CBA-CGA
18	B	850	LMG	C41-C42-C43-C44
13	A	845	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	A	825	CLA	C1A-C2A-CAA-CBA
13	A	844	CLA	C1A-C2A-CAA-CBA
13	A	822	CLA	C1A-C2A-CAA-CBA
13	A	810	CLA	C1A-C2A-CAA-CBA
13	A	844	CLA	O1D-CGD-O2D-CED
13	B	806	CLA	C5-C6-C7-C8
13	B	814	CLA	C3-C5-C6-C7
13	L	1004	CLA	C2-C3-C5-C6
17	A	855	LHG	C4-O6-P-O4
13	B	831	CLA	O2A-C1-C2-C3
13	B	814	CLA	O1A-CGA-O2A-C1
13	B	805	CLA	CAD-CBD-CGD-O1D
13	A	838	CLA	C2-C3-C5-C6
13	A	824	CLA	C2-C3-C5-C6
13	L	1002	CLA	C3-C5-C6-C7
13	B	837	CLA	CBD-CGD-O2D-CED
13	B	826	CLA	O1D-CGD-O2D-CED
13	A	806	CLA	C11-C10-C8-C7
13	B	827	CLA	C6-C7-C8-C10
13	B	827	CLA	C11-C12-C13-C15
13	L	1002	CLA	C11-C10-C8-C7
13	B	832	CLA	C11-C10-C8-C7
13	A	843	CLA	C3-C5-C6-C7
13	B	829	CLA	C10-C11-C12-C13
13	B	820	CLA	C2A-CAA-CBA-CGA
13	B	832	CLA	C16-C17-C18-C20
17	A	855	LHG	C27-C28-C29-C30
13	A	805	CLA	C4-C3-C5-C6
13	A	819	CLA	CBA-CGA-O2A-C1
13	B	806	CLA	C14-C13-C15-C16
13	A	835	CLA	C14-C13-C15-C16
13	A	806	CLA	C11-C10-C8-C9
13	B	813	CLA	C11-C10-C8-C9
13	B	841	CLA	C14-C13-C15-C16
13	A	841	CLA	C11-C10-C8-C9
16	B	845	BCR	C22-C23-C24-C25
13	A	820	CLA	C16-C17-C18-C19
13	B	831	CLA	C1-C2-C3-C4
17	A	855	LHG	C1-C2-C3-O3
13	A	835	CLA	C2A-CAA-CBA-CGA
13	B	814	CLA	C2-C1-O2A-CGA
13	B	841	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
13	B	809	CLA	C2-C1-O2A-CGA
13	B	825	CLA	O1A-CGA-O2A-C1
13	A	819	CLA	O1A-CGA-O2A-C1
13	A	807	CLA	CAA-CBA-CGA-O2A
13	B	813	CLA	C4-C3-C5-C6
13	B	810	CLA	C4-C3-C5-C6
13	B	827	CLA	C4-C3-C5-C6
16	M	1602	BCR	C23-C24-C25-C26
16	J	105	BCR	C23-C24-C25-C30
13	B	803	CLA	C10-C11-C12-C13
18	B	850	LMG	C34-C35-C36-C37
13	A	817	CLA	C2A-CAA-CBA-CGA
16	B	845	BCR	C20-C21-C22-C23
17	B	851	LHG	C3-O3-P-O6
17	A	856	LHG	C3-O3-P-O6
17	A	855	LHG	C3-O3-P-O6
13	B	810	CLA	C13-C15-C16-C17
13	B	802	CLA	C13-C15-C16-C17
13	L	1002	CLA	C4-C3-C5-C6
13	A	820	CLA	C11-C10-C8-C7
13	L	1003	CLA	C12-C13-C15-C16
13	B	841	CLA	C12-C13-C15-C16
13	A	810	CLA	C11-C12-C13-C15
13	B	805	CLA	C14-C13-C15-C16
13	B	828	CLA	C14-C13-C15-C16
13	B	827	CLA	C6-C7-C8-C9
13	B	832	CLA	C11-C10-C8-C9
13	A	844	CLA	C5-C6-C7-C8
13	B	805	CLA	C15-C16-C17-C18
13	L	1004	CLA	C3-C5-C6-C7
13	B	832	CLA	C16-C17-C18-C19
13	B	827	CLA	O1D-CGD-O2D-CED
17	A	855	LHG	C26-C27-C28-C29
13	A	839	CLA	C4-C3-C5-C6
13	A	812	CLA	C10-C11-C12-C13
13	B	828	CLA	C2-C1-O2A-CGA
13	B	827	CLA	C2-C1-O2A-CGA
13	A	809	CLA	C2A-CAA-CBA-CGA
13	A	836	CLA	C3A-C2A-CAA-CBA
13	A	824	CLA	C3A-C2A-CAA-CBA
18	B	850	LMG	C15-C16-C17-C18
13	A	825	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
13	B	814	CLA	C11-C12-C13-C14
16	A	854	BCR	C11-C10-C9-C34
16	A	854	BCR	C16-C17-C18-C36
16	F	1302	BCR	C35-C13-C14-C15
16	B	844	BCR	C11-C10-C9-C34
13	A	810	CLA	C10-C11-C12-C13
13	A	827	CLA	C1A-C2A-CAA-CBA
13	A	814	CLA	C11-C10-C8-C7
18	B	850	LMG	C31-C32-C33-C34
17	A	855	LHG	C19-C20-C21-C22
13	A	827	CLA	O1D-CGD-O2D-CED
13	A	820	CLA	C4-C3-C5-C6
13	A	828	CLA	C4-C3-C5-C6
13	A	805	CLA	C2-C3-C5-C6
13	B	817	CLA	C8-C10-C11-C12
14	B	842	PQN	C23-C25-C26-C27
17	A	855	LHG	O9-C7-O7-C5
16	A	854	BCR	C11-C10-C9-C8
16	A	854	BCR	C16-C17-C18-C19
16	F	1302	BCR	C12-C13-C14-C15
13	A	803	CLA	C8-C10-C11-C12
13	B	808	CLA	C4-C3-C5-C6
13	A	814	CLA	C4-C3-C5-C6
13	A	802	CLA	C4-C3-C5-C6
13	A	846	CLA	C2-C1-O2A-CGA
13	A	838	CLA	C2-C1-O2A-CGA
13	A	822	CLA	C2-C1-O2A-CGA
13	A	805	CLA	C2-C1-O2A-CGA
13	A	810	CLA	C2-C1-O2A-CGA
13	B	813	CLA	C2-C3-C5-C6
13	L	1002	CLA	C2-C3-C5-C6
13	A	839	CLA	C11-C12-C13-C14
13	B	808	CLA	C14-C13-C15-C16
13	J	101	CLA	C2A-CAA-CBA-CGA
13	A	841	CLA	C3-C5-C6-C7
16	B	846	BCR	C23-C24-C25-C30
16	B	845	BCR	C23-C24-C25-C30
13	B	822	CLA	C5-C6-C7-C8
13	B	826	CLA	C4-C3-C5-C6
13	B	810	CLA	C2-C3-C5-C6
13	B	827	CLA	C2-C3-C5-C6
13	A	834	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
13	B	810	CLA	C10-C11-C12-C13
13	A	809	CLA	C4-C3-C5-C6
13	A	819	CLA	CAA-CBA-CGA-O1A
13	B	806	CLA	C12-C13-C15-C16
13	A	839	CLA	C2-C3-C5-C6
13	A	844	CLA	CBD-CGD-O2D-CED
17	A	855	LHG	C11-C10-C9-C8
16	J	105	BCR	C20-C21-C22-C37
16	B	845	BCR	C11-C10-C9-C34
16	B	845	BCR	C20-C21-C22-C37
13	B	829	CLA	C4-C3-C5-C6
13	A	825	CLA	C4-C3-C5-C6
13	A	812	CLA	C4-C3-C5-C6
13	A	810	CLA	C4-C3-C5-C6
13	B	809	CLA	C4-C3-C5-C6
13	A	821	CLA	C8-C10-C11-C12
13	A	820	CLA	C2-C3-C5-C6
13	A	828	CLA	C2-C3-C5-C6
13	B	809	CLA	C6-C7-C8-C9
13	A	828	CLA	C3-C5-C6-C7
13	A	827	CLA	C3A-C2A-CAA-CBA
13	B	804	CLA	CAD-CBD-CGD-O2D
13	A	806	CLA	CAD-CBD-CGD-O2D
13	B	820	CLA	CAD-CBD-CGD-O2D
13	A	813	CLA	CAD-CBD-CGD-O2D
13	A	832	CLA	CAD-CBD-CGD-O2D
13	A	805	CLA	CAD-CBD-CGD-O2D
13	A	828	CLA	CAD-CBD-CGD-O2D
13	B	815	CLA	CAD-CBD-CGD-O2D
13	B	816	CLA	C2A-CAA-CBA-CGA
13	A	826	CLA	CAA-CBA-CGA-O2A
13	B	822	CLA	C4-C3-C5-C6
13	A	819	CLA	C4-C3-C5-C6
13	A	803	CLA	C4-C3-C5-C6
13	A	810	CLA	C2-C3-C5-C6
13	B	809	CLA	C2-C3-C5-C6
13	A	829	CLA	CAA-CBA-CGA-O2A
13	A	805	CLA	CAA-CBA-CGA-O2A
17	A	856	LHG	O7-C7-C8-C9
13	B	806	CLA	CAA-CBA-CGA-O2A
13	B	822	CLA	CAA-CBA-CGA-O2A
13	A	803	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
13	A	826	CLA	O2A-C1-C2-C3
13	A	813	CLA	O2A-C1-C2-C3
13	A	833	CLA	O2A-C1-C2-C3
13	B	817	CLA	O2A-C1-C2-C3
13	B	827	CLA	C2A-CAA-CBA-CGA
13	A	825	CLA	C11-C12-C13-C14
17	A	855	LHG	C11-C12-C13-C14
13	A	820	CLA	CHA-CBD-CGD-O1D
13	A	820	CLA	CHA-CBD-CGD-O2D
13	A	804	CLA	CHA-CBD-CGD-O1D
13	A	804	CLA	CHA-CBD-CGD-O2D
13	J	101	CLA	CHA-CBD-CGD-O1D
13	J	101	CLA	CHA-CBD-CGD-O2D
13	B	801	CLA	CHA-CBD-CGD-O1D
13	B	801	CLA	CHA-CBD-CGD-O2D
13	A	826	CLA	CHA-CBD-CGD-O1D
13	A	825	CLA	CHA-CBD-CGD-O1D
13	A	825	CLA	CHA-CBD-CGD-O2D
13	A	811	CLA	CHA-CBD-CGD-O1D
13	A	811	CLA	CHA-CBD-CGD-O2D
13	B	833	CLA	CHA-CBD-CGD-O1D
13	B	833	CLA	CHA-CBD-CGD-O2D
13	B	814	CLA	CHA-CBD-CGD-O1D
13	B	814	CLA	CHA-CBD-CGD-O2D
13	A	821	CLA	CHA-CBD-CGD-O2D
13	B	807	CLA	CHA-CBD-CGD-O2D
13	A	840	CLA	CHA-CBD-CGD-O1D
13	A	840	CLA	CHA-CBD-CGD-O2D
13	K	1401	CLA	CHA-CBD-CGD-O2D
13	B	809	CLA	CHA-CBD-CGD-O1D
13	B	809	CLA	CHA-CBD-CGD-O2D
13	B	834	CLA	CHA-CBD-CGD-O1D
13	A	822	CLA	C4-C3-C5-C6
13	B	832	CLA	CAA-CBA-CGA-O2A
13	B	829	CLA	C2-C3-C5-C6
16	B	845	BCR	C11-C10-C9-C8
17	A	855	LHG	C13-C14-C15-C16
13	B	806	CLA	C16-C17-C18-C20
13	A	812	CLA	CAA-CBA-CGA-O2A
13	B	824	CLA	C6-C7-C8-C9
13	B	813	CLA	CAA-CBA-CGA-O2A
13	A	808	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	A	808	CLA	CAA-CBA-CGA-O2A
13	A	814	CLA	O1A-CGA-O2A-C1
13	A	839	CLA	C11-C12-C13-C15
13	B	813	CLA	C6-C7-C8-C10
13	A	814	CLA	C2-C3-C5-C6
13	A	846	CLA	CAA-CBA-CGA-O2A
13	A	839	CLA	C14-C13-C15-C16
13	B	813	CLA	C6-C7-C8-C9
13	B	827	CLA	C11-C12-C13-C14
13	A	814	CLA	C11-C10-C8-C9
13	B	818	CLA	C11-C10-C8-C9
13	L	1003	CLA	C14-C13-C15-C16
17	A	855	LHG	C8-C7-O7-C5
13	A	825	CLA	C2A-CAA-CBA-CGA
13	A	807	CLA	C2A-CAA-CBA-CGA
17	A	855	LHG	C25-C26-C27-C28
13	A	827	CLA	C4-C3-C5-C6
17	A	856	LHG	O10-C23-O8-C6
13	B	808	CLA	C2-C3-C5-C6
13	A	802	CLA	C2-C3-C5-C6
13	A	814	CLA	CBA-CGA-O2A-C1
13	L	1004	CLA	C1A-C2A-CAA-CBA
13	B	823	CLA	C1A-C2A-CAA-CBA
13	A	836	CLA	C1A-C2A-CAA-CBA
13	A	814	CLA	C1A-C2A-CAA-CBA
13	A	838	CLA	C1A-C2A-CAA-CBA
13	A	824	CLA	C1A-C2A-CAA-CBA
13	B	837	CLA	C1A-C2A-CAA-CBA
13	A	822	CLA	C13-C15-C16-C17
13	B	801	CLA	C2-C1-O2A-CGA
17	A	856	LHG	C24-C23-O8-C6
13	A	805	CLA	CAA-CBA-CGA-O1A
13	L	1004	CLA	C2A-CAA-CBA-CGA
13	A	802	CLA	C2A-CAA-CBA-CGA
13	B	806	CLA	C16-C17-C18-C19
13	A	835	CLA	C13-C15-C16-C17
13	B	806	CLA	CAA-CBA-CGA-O1A
13	A	826	CLA	CAA-CBA-CGA-O1A
13	A	803	CLA	CAA-CBA-CGA-O1A
16	B	846	BCR	C23-C24-C25-C26
13	A	815	CLA	O1D-CGD-O2D-CED
13	B	829	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
13	A	829	CLA	CAA-CBA-CGA-O1A
13	A	808	CLA	CAA-CBA-CGA-O1A
13	B	814	CLA	CAA-CBA-CGA-O2A
13	B	822	CLA	CAA-CBA-CGA-O1A
13	B	832	CLA	CAA-CBA-CGA-O1A
13	A	812	CLA	CAA-CBA-CGA-O1A
13	A	821	CLA	C4-C3-C5-C6
13	A	803	CLA	C2-C3-C5-C6
13	B	826	CLA	CAD-CBD-CGD-O1D
13	A	825	CLA	CAD-CBD-CGD-O1D
13	B	830	CLA	CAD-CBD-CGD-O1D
13	A	814	CLA	CAD-CBD-CGD-O1D
13	B	818	CLA	CAD-CBD-CGD-O1D
13	B	837	CLA	CAD-CBD-CGD-O1D
13	B	809	CLA	CAD-CBD-CGD-O1D
17	A	856	LHG	O9-C7-C8-C9
13	A	821	CLA	CAA-CBA-CGA-O2A
13	L	1002	CLA	C8-C10-C11-C12
13	B	801	CLA	C11-C10-C8-C9
13	B	809	CLA	C11-C10-C8-C9
13	A	830	CLA	C13-C15-C16-C17
13	A	844	CLA	CAA-CBA-CGA-O2A
13	B	827	CLA	C5-C6-C7-C8
13	A	818	CLA	CAA-CBA-CGA-O2A
13	A	813	CLA	CAA-CBA-CGA-O2A
13	B	803	CLA	CAA-CBA-CGA-O2A
13	A	839	CLA	C12-C13-C15-C16
13	B	814	CLA	C11-C12-C13-C15
13	A	821	CLA	CAA-CBA-CGA-O1A
13	A	824	CLA	CAA-CBA-CGA-O2A
13	B	841	CLA	CAA-CBA-CGA-O2A
17	A	856	LHG	O8-C23-C24-C25
13	B	813	CLA	CAA-CBA-CGA-O1A
13	B	807	CLA	CAA-CBA-CGA-O2A
13	A	841	CLA	CAA-CBA-CGA-O2A
13	A	846	CLA	CAA-CBA-CGA-O1A
13	A	824	CLA	CAA-CBA-CGA-O1A
13	B	817	CLA	C2A-CAA-CBA-CGA
18	B	850	LMG	C16-C17-C18-C19
13	B	826	CLA	CAA-CBA-CGA-O2A
13	A	801	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

114 monomers are involved in 334 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	L	1004	CLA	2	0
16	A	854	BCR	13	0
13	A	829	CLA	13	0
13	A	820	CLA	6	0
13	A	804	CLA	2	0
13	A	843	CLA	8	0
13	B	806	CLA	6	0
13	B	811	CLA	1	0
16	B	848	BCR	1	0
13	J	101	CLA	1	0
13	B	836	CLA	2	0
13	B	804	CLA	2	0
13	A	845	CLA	1	0
13	B	825	CLA	2	0
13	F	1301	CLA	1	0
13	B	838	CLA	2	0
13	M	1601	CLA	1	0
13	A	839	CLA	6	0
13	A	815	CLA	5	0
13	B	826	CLA	3	0
13	B	823	CLA	3	0
17	B	851	LHG	1	0
13	A	836	CLA	4	0
13	B	839	CLA	4	0
16	I	101	BCR	3	0
13	A	835	CLA	4	0
13	A	830	CLA	1	0
13	B	835	CLA	3	0
13	A	823	CLA	2	0
13	B	829	CLA	7	0
13	A	801	CLA	9	0
13	B	801	CLA	8	0
13	A	826	CLA	4	0
13	A	825	CLA	2	0
16	A	853	BCR	1	0
13	A	846	CLA	5	0
13	B	822	CLA	4	0
13	A	806	CLA	6	0
13	B	813	CLA	6	0
13	A	811	CLA	4	0
13	B	831	CLA	2	0
16	M	1602	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	820	CLA	2	0
16	L	1006	BCR	1	0
13	B	810	CLA	5	0
13	A	819	CLA	4	0
13	B	833	CLA	7	0
13	A	833	CLA	1	0
13	B	817	CLA	8	0
16	A	849	BCR	2	0
13	A	832	CLA	1	0
13	B	814	CLA	6	0
13	B	830	CLA	5	0
13	A	821	CLA	5	0
13	B	803	CLA	4	0
13	B	805	CLA	3	0
16	B	846	BCR	5	0
13	B	828	CLA	8	0
13	B	827	CLA	5	0
14	B	842	PQN	1	0
16	B	847	BCR	3	0
13	A	803	CLA	10	0
13	B	808	CLA	3	0
13	L	1002	CLA	2	0
13	B	807	CLA	1	0
16	A	851	BCR	1	0
13	A	814	CLA	1	0
13	A	837	CLA	2	0
13	B	824	CLA	10	0
13	A	840	CLA	3	0
13	B	840	CLA	3	0
13	A	844	CLA	5	0
13	A	812	CLA	1	0
13	B	812	CLA	1	0
13	B	818	CLA	5	0
16	B	843	BCR	1	0
13	A	838	CLA	2	0
16	A	850	BCR	2	0
16	J	105	BCR	5	0
13	A	824	CLA	1	0
16	B	849	BCR	1	0
13	B	802	CLA	17	0
13	L	1003	CLA	8	0
13	A	807	CLA	4	0

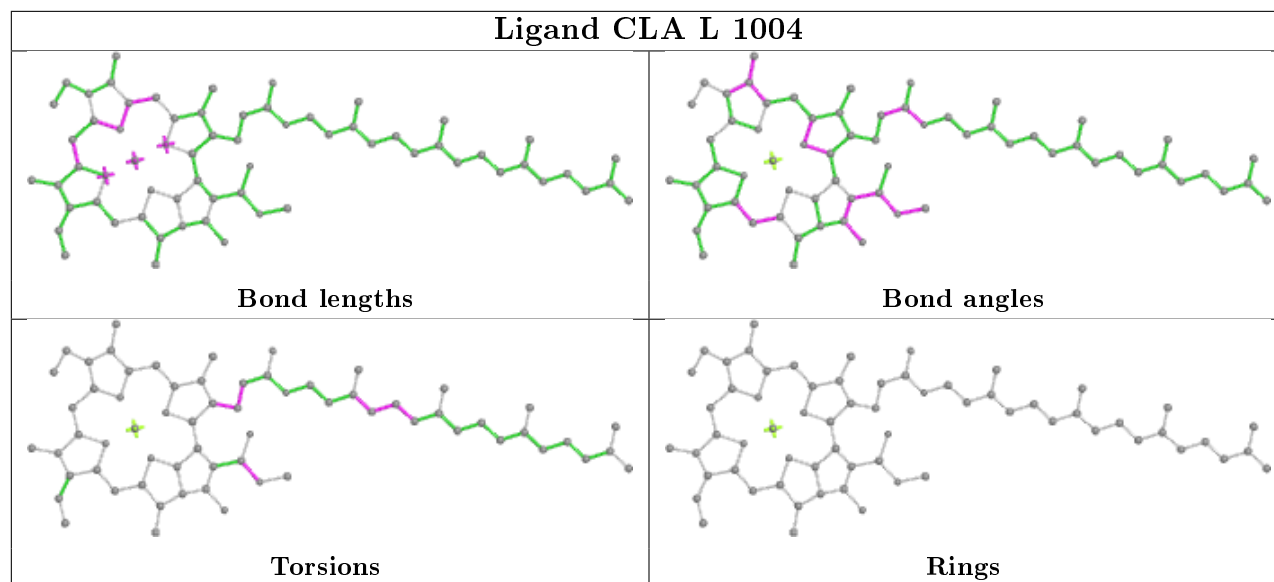
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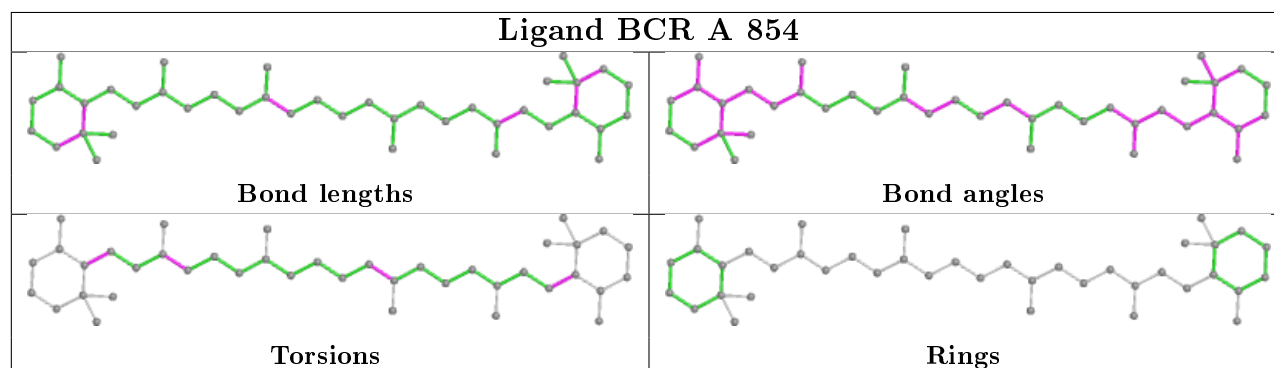
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	808	CLA	2	0
13	A	831	CLA	6	0
13	B	837	CLA	3	0
18	B	850	LMG	5	0
13	B	816	CLA	3	0
16	B	845	BCR	5	0
13	A	822	CLA	4	0
13	B	821	CLA	1	0
13	A	805	CLA	1	0
13	A	841	CLA	2	0
16	A	852	BCR	4	0
13	B	819	CLA	5	0
14	A	847	PQN	1	0
13	A	810	CLA	4	0
13	B	832	CLA	6	0
13	K	1401	CLA	1	0
13	A	802	CLA	3	0
13	B	809	CLA	2	0
13	A	828	CLA	3	0
16	F	1302	BCR	2	0
13	A	817	CLA	2	0
13	B	815	CLA	2	0
16	J	103	BCR	4	0
13	A	809	CLA	6	0
16	B	844	BCR	1	0
16	J	104	BCR	7	0
17	A	856	LHG	2	0
17	A	855	LHG	4	0
13	A	827	CLA	5	0
13	X	1701	CLA	1	0

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

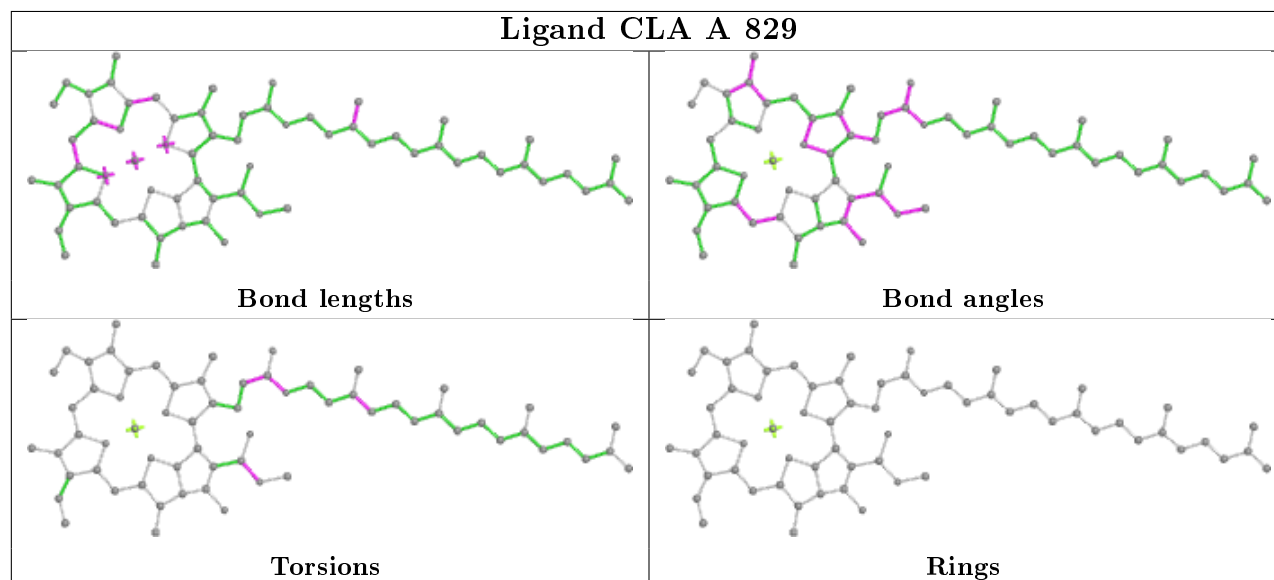
Ligand CLA L 1004



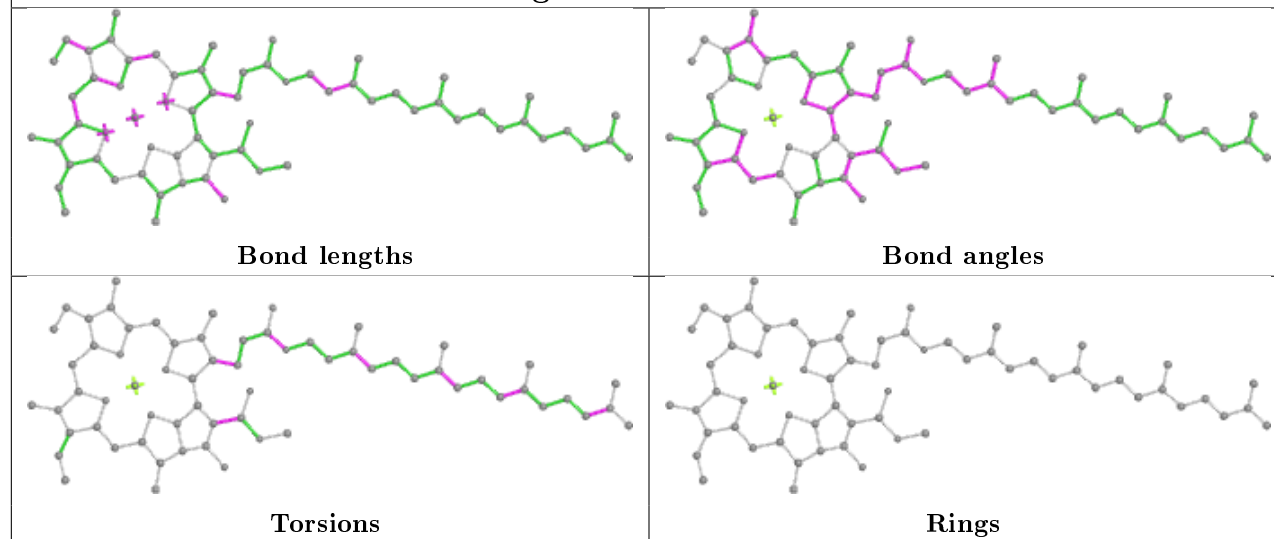
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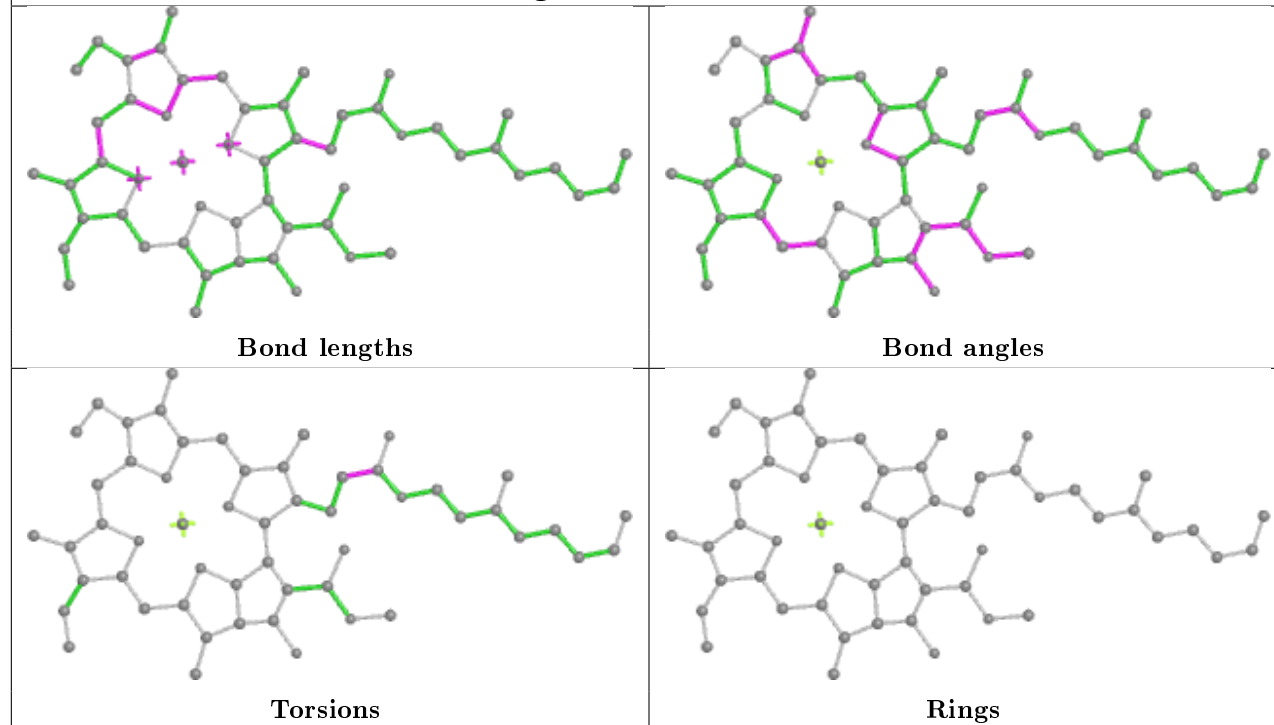
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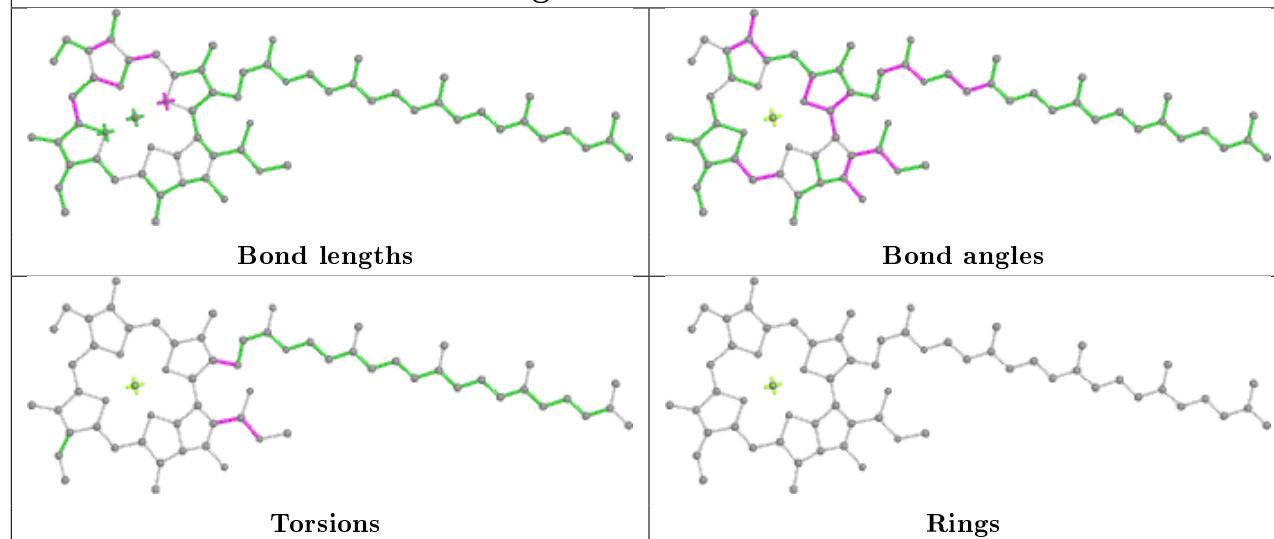
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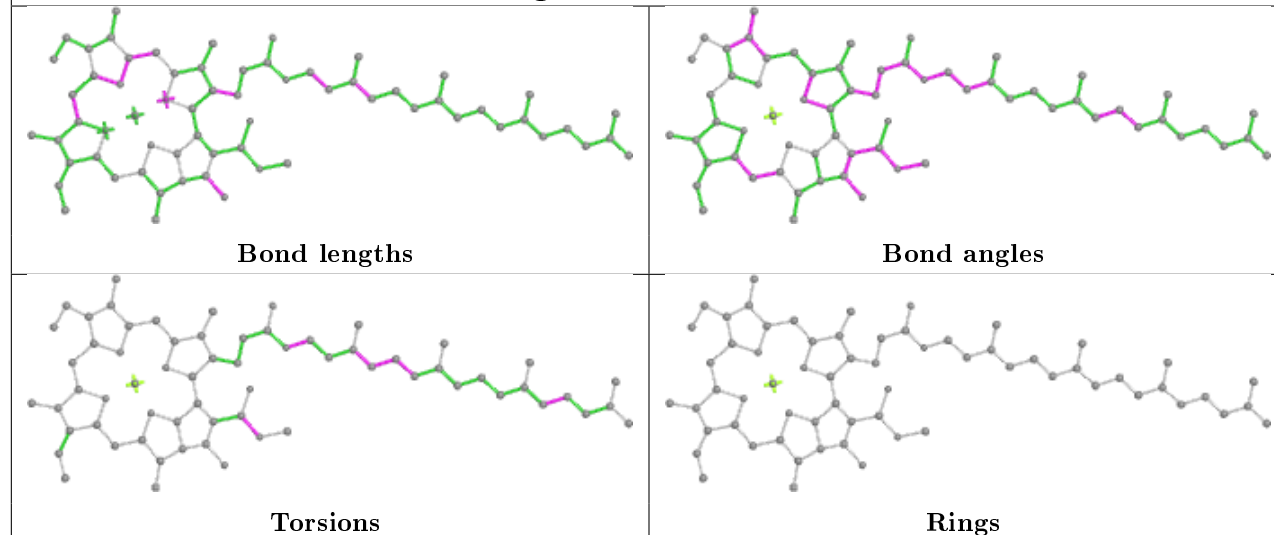
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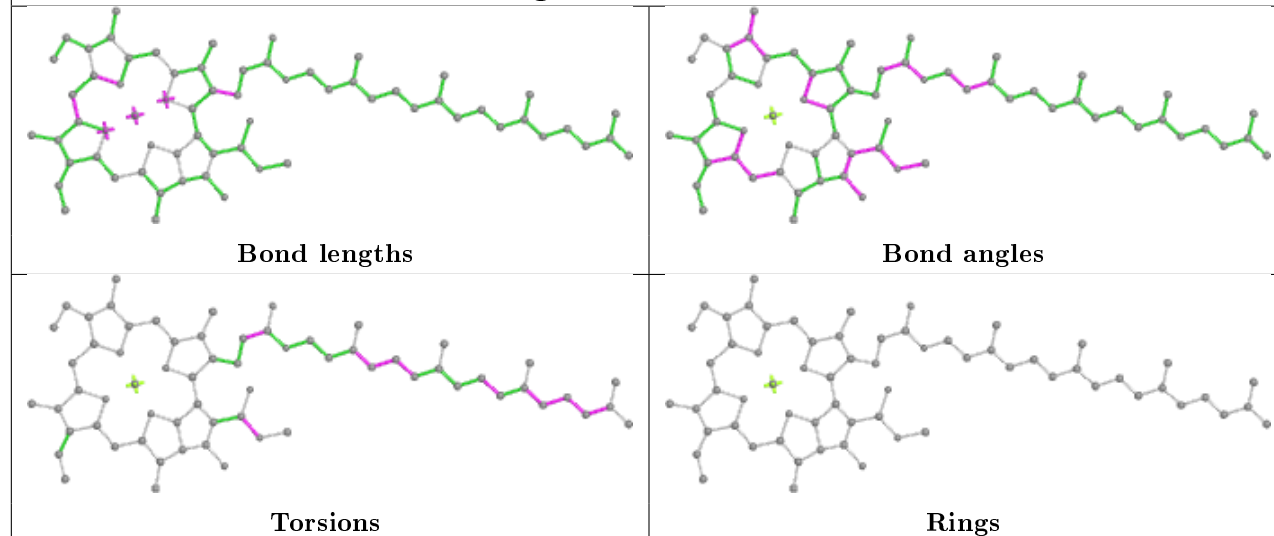
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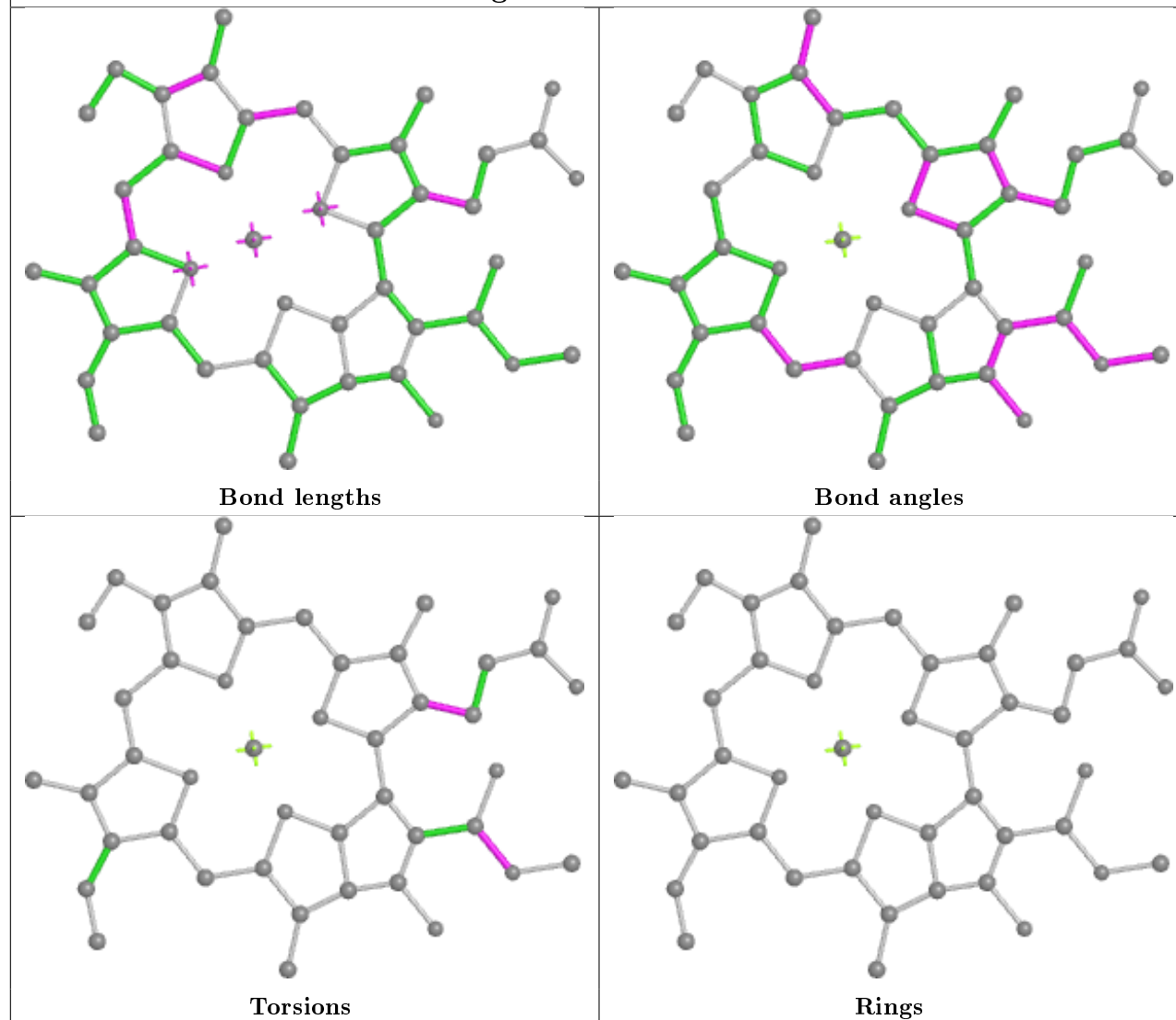
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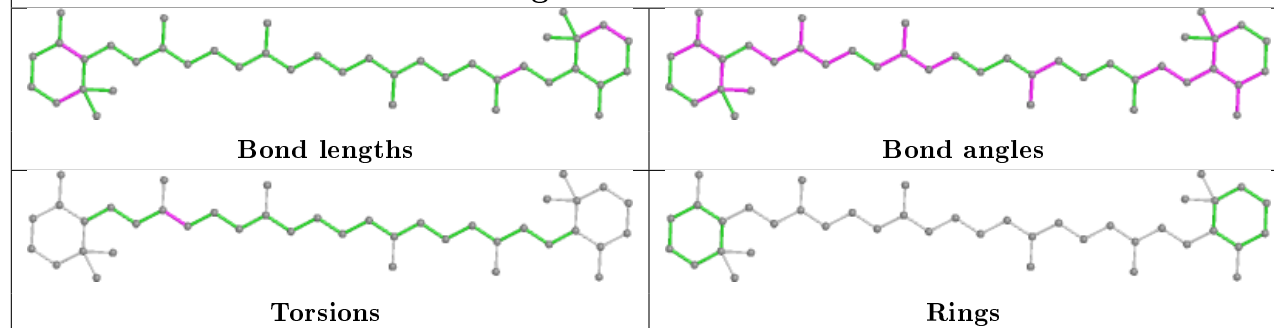
Ligand CLA B 806



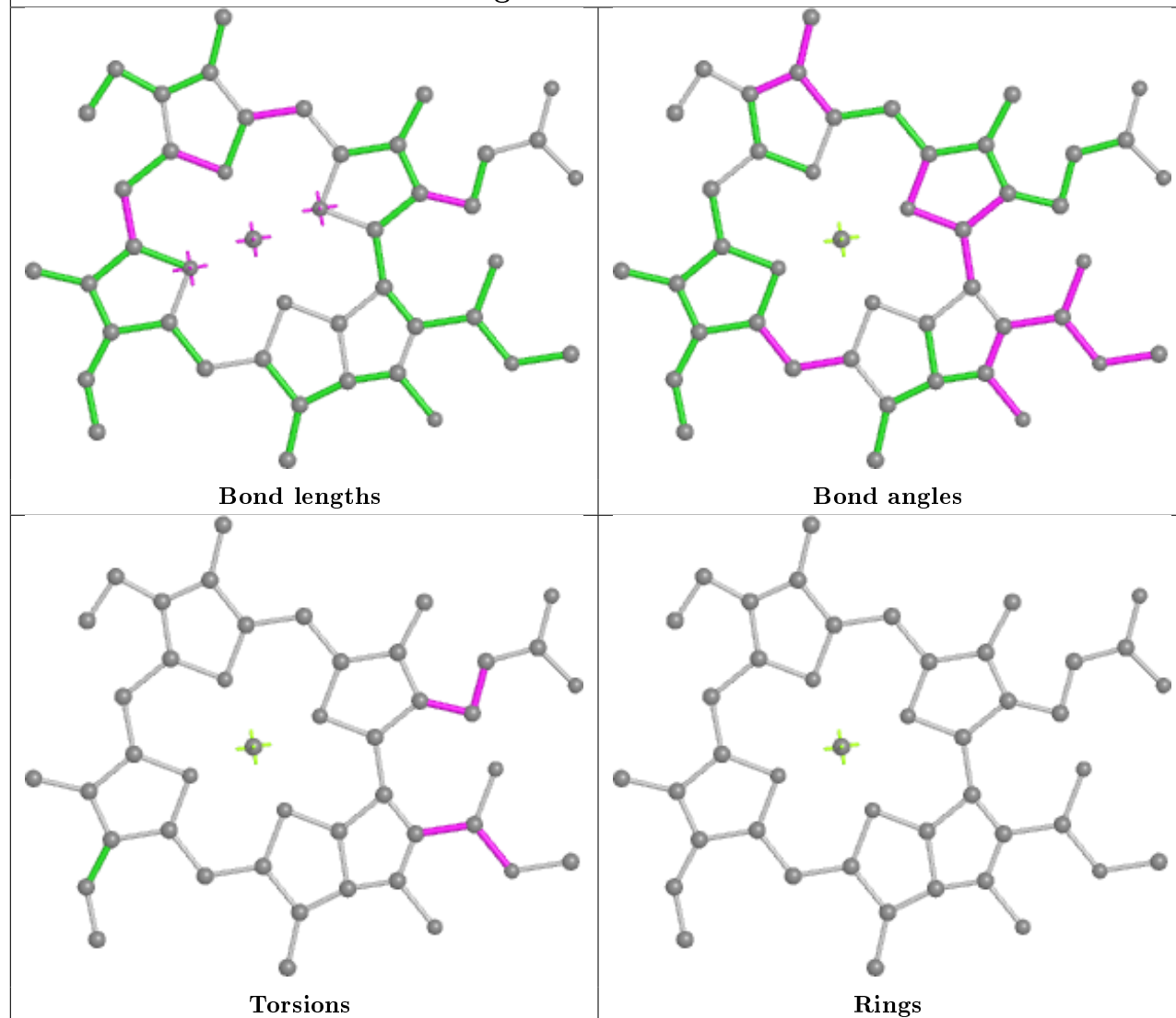
Ligand CLA B 811



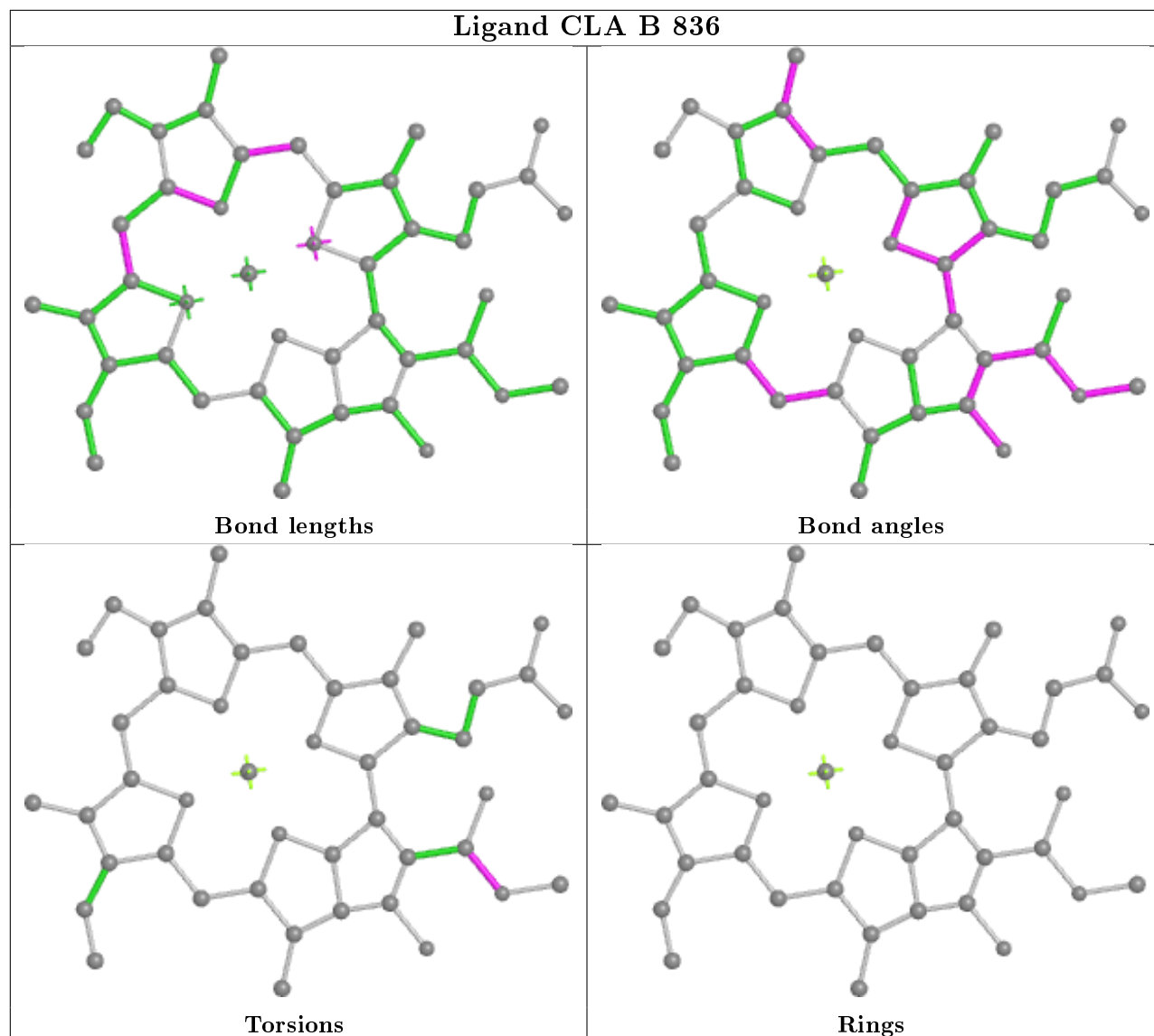
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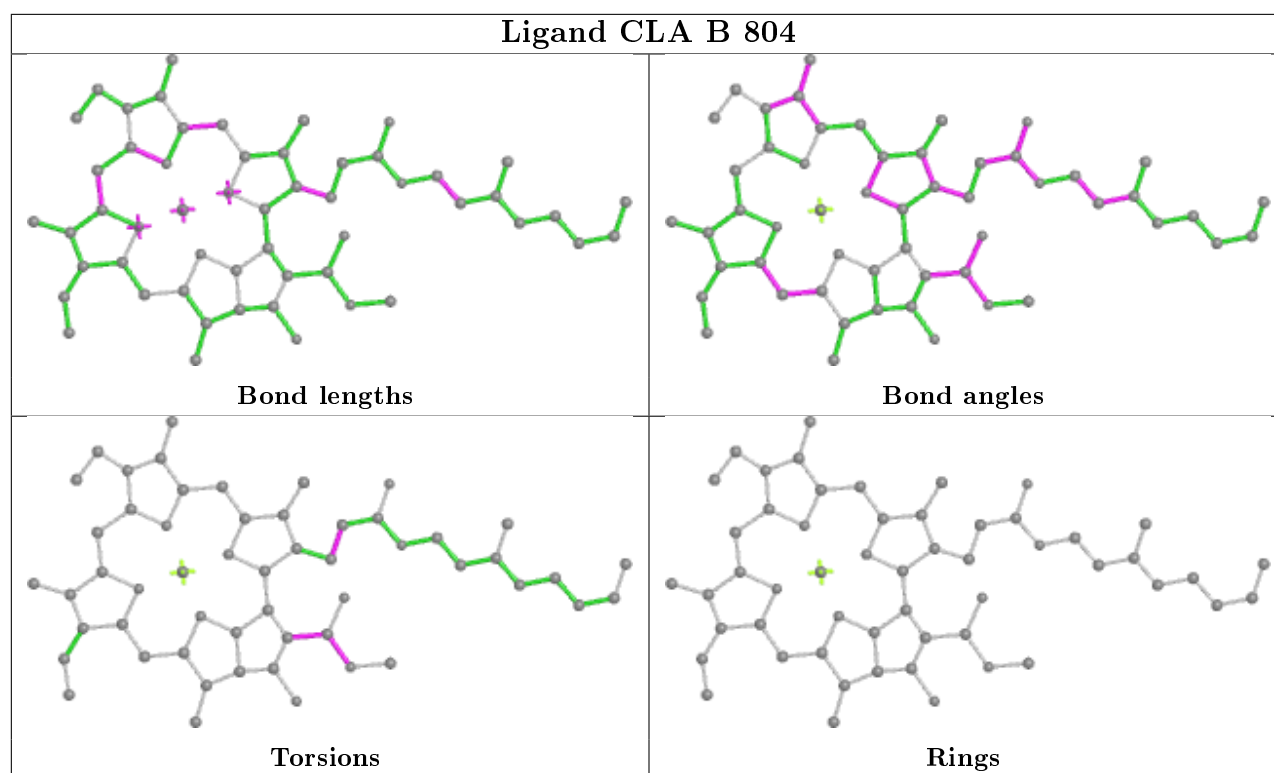


Ligand CLA J 101

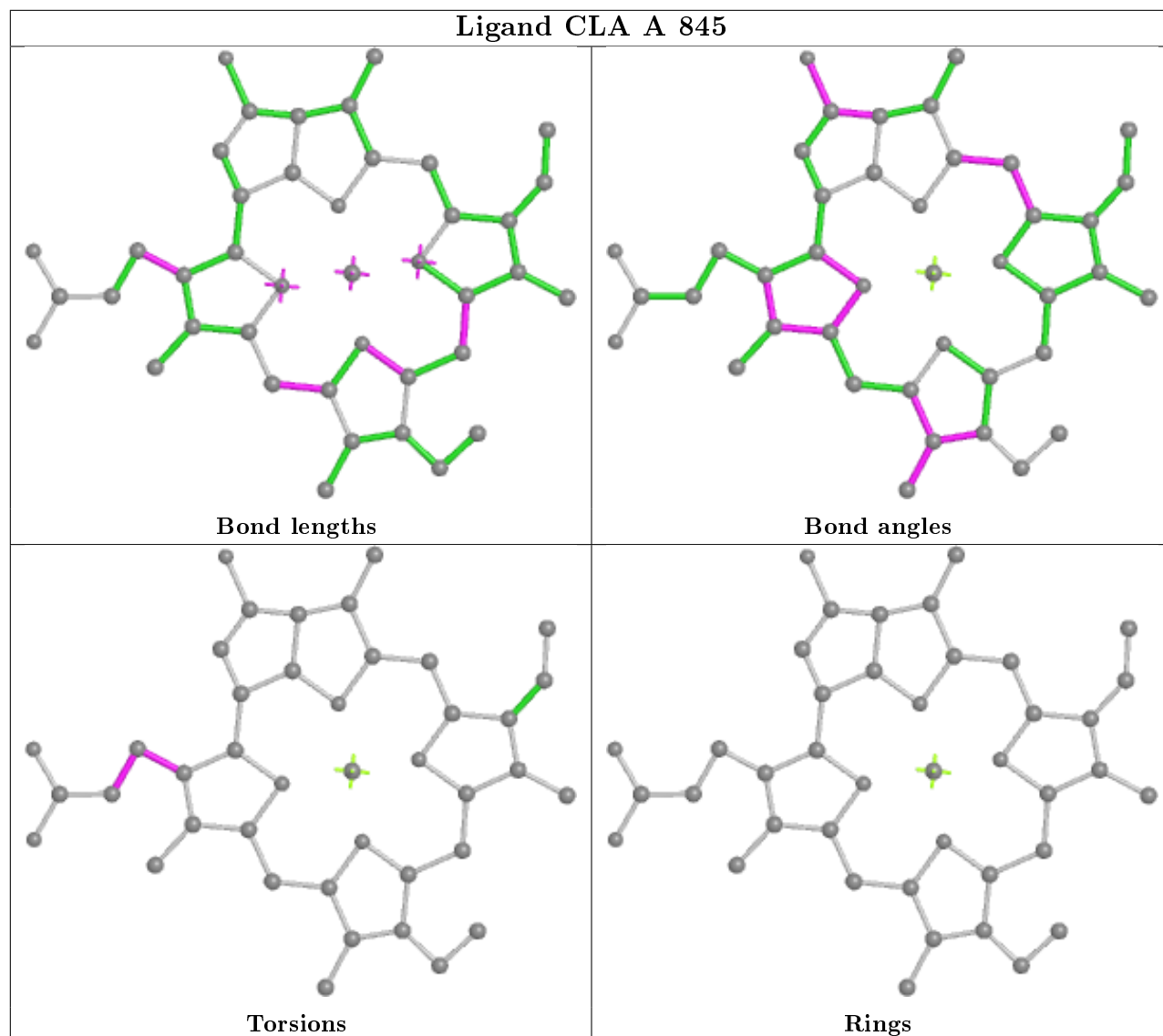


Ligand CLA B 836

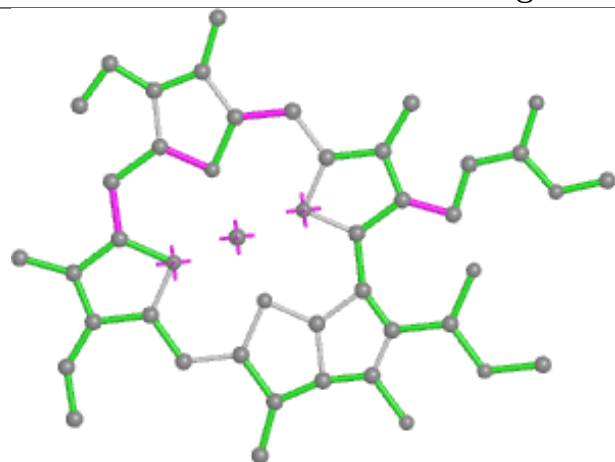




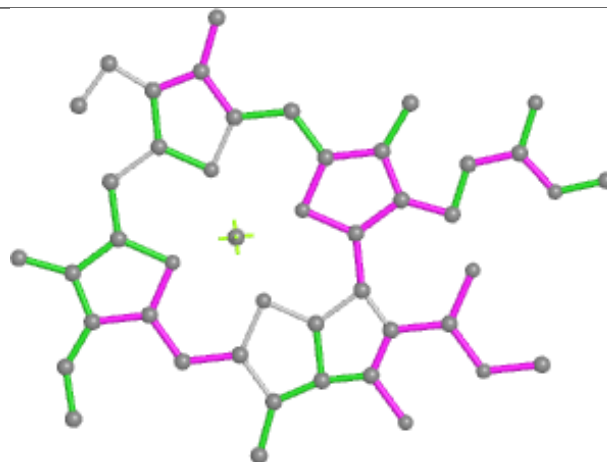
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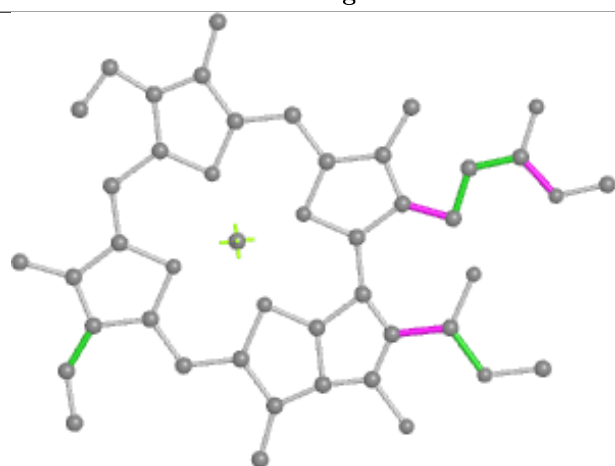
Ligand CLA B 825



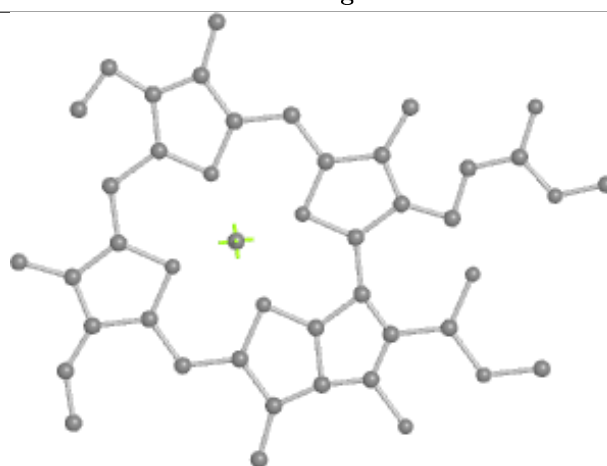
Bond lengths



Bond angles

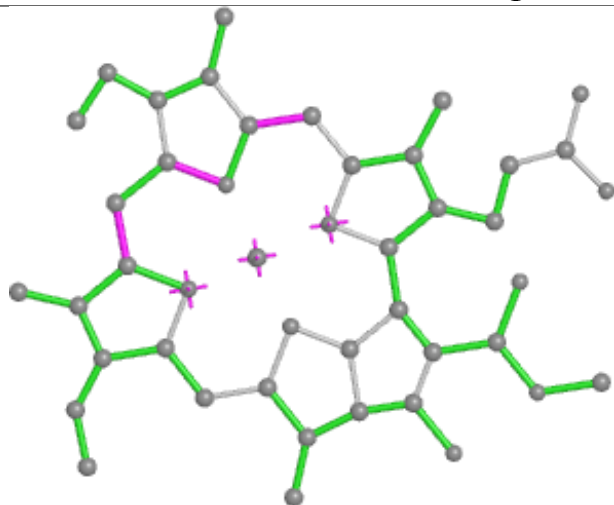


Torsions

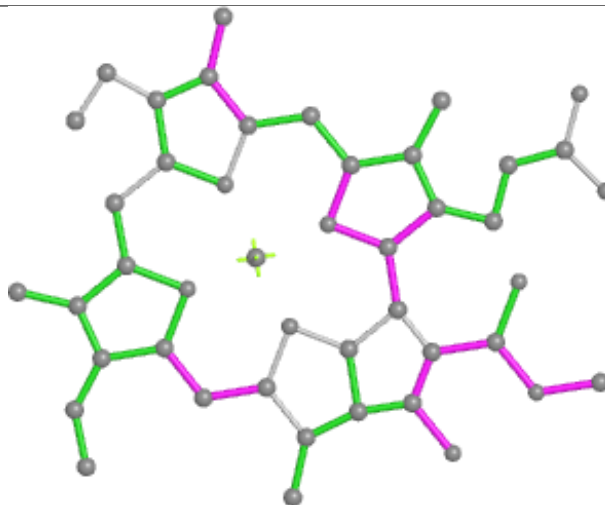


Rings

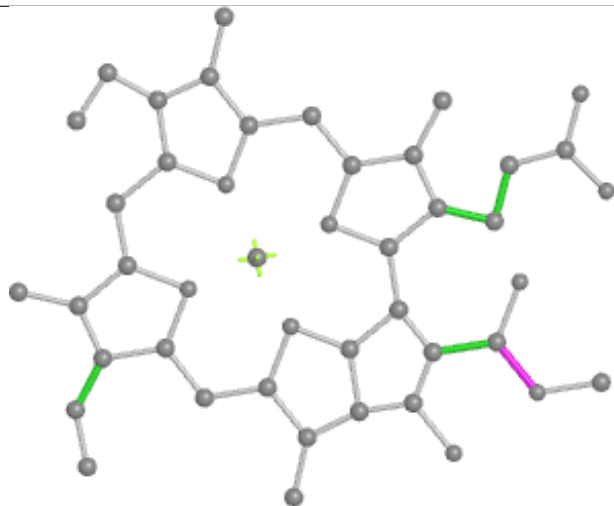
Ligand CLA F 1301



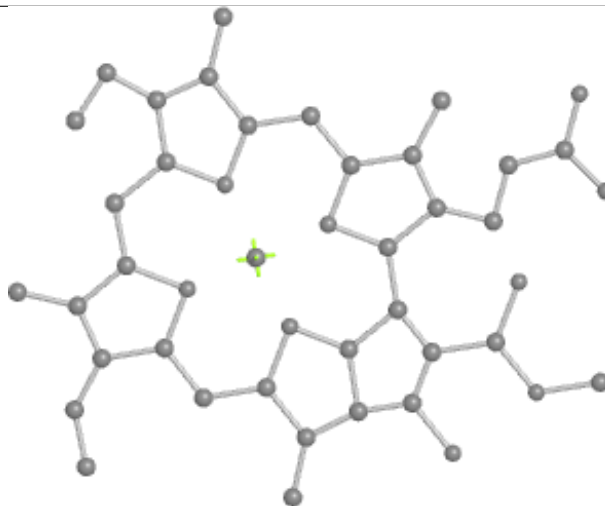
Bond lengths



Bond angles

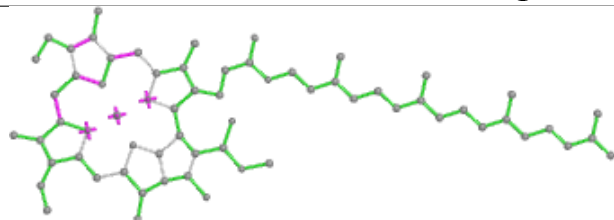


Torsions

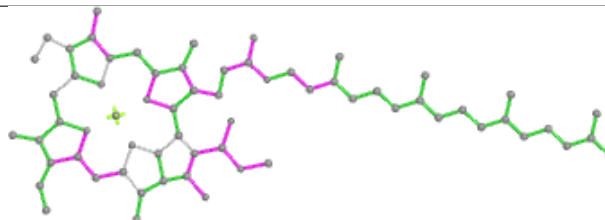


Rings

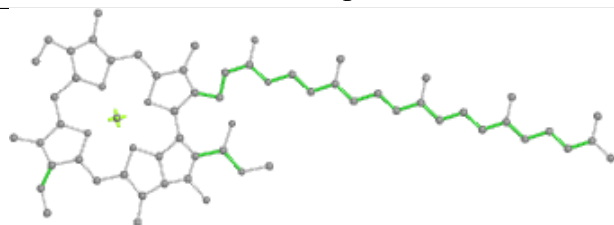
Ligand CLA B 838



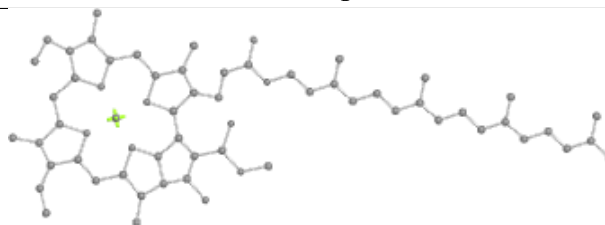
Bond lengths



Bond angles

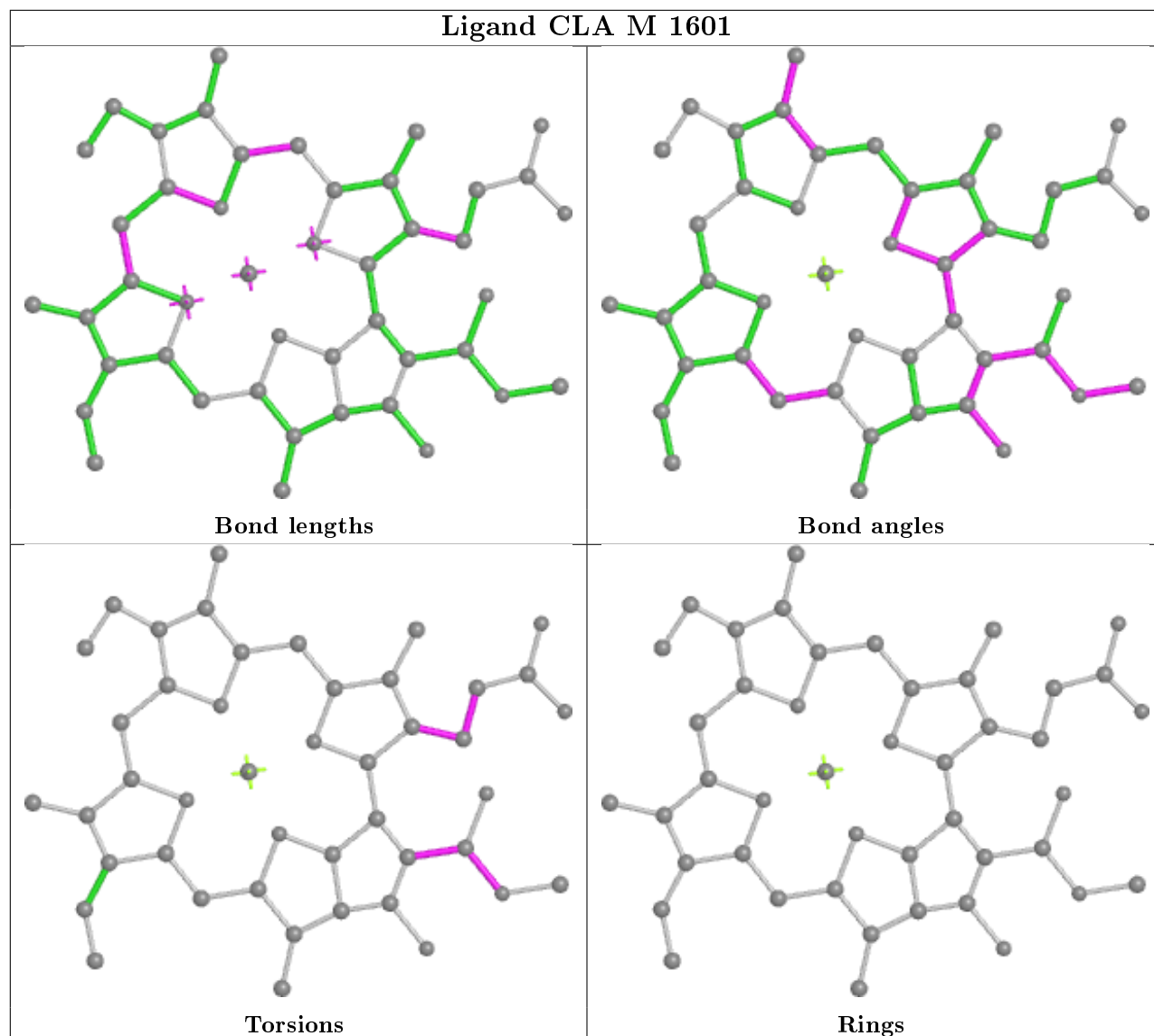


Torsions

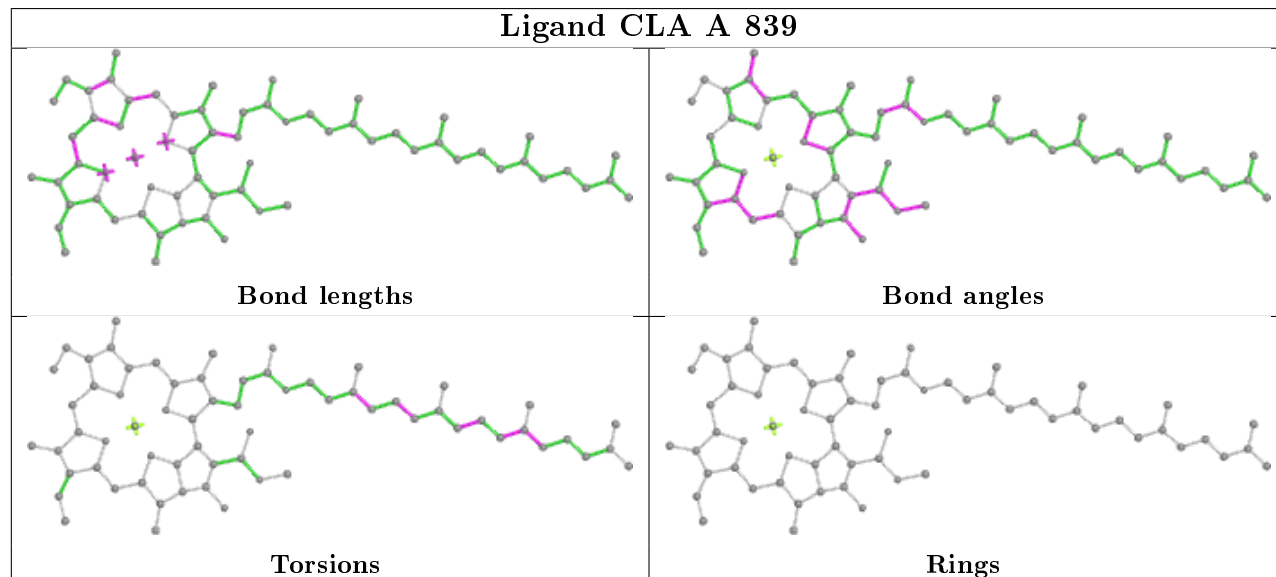


Rings

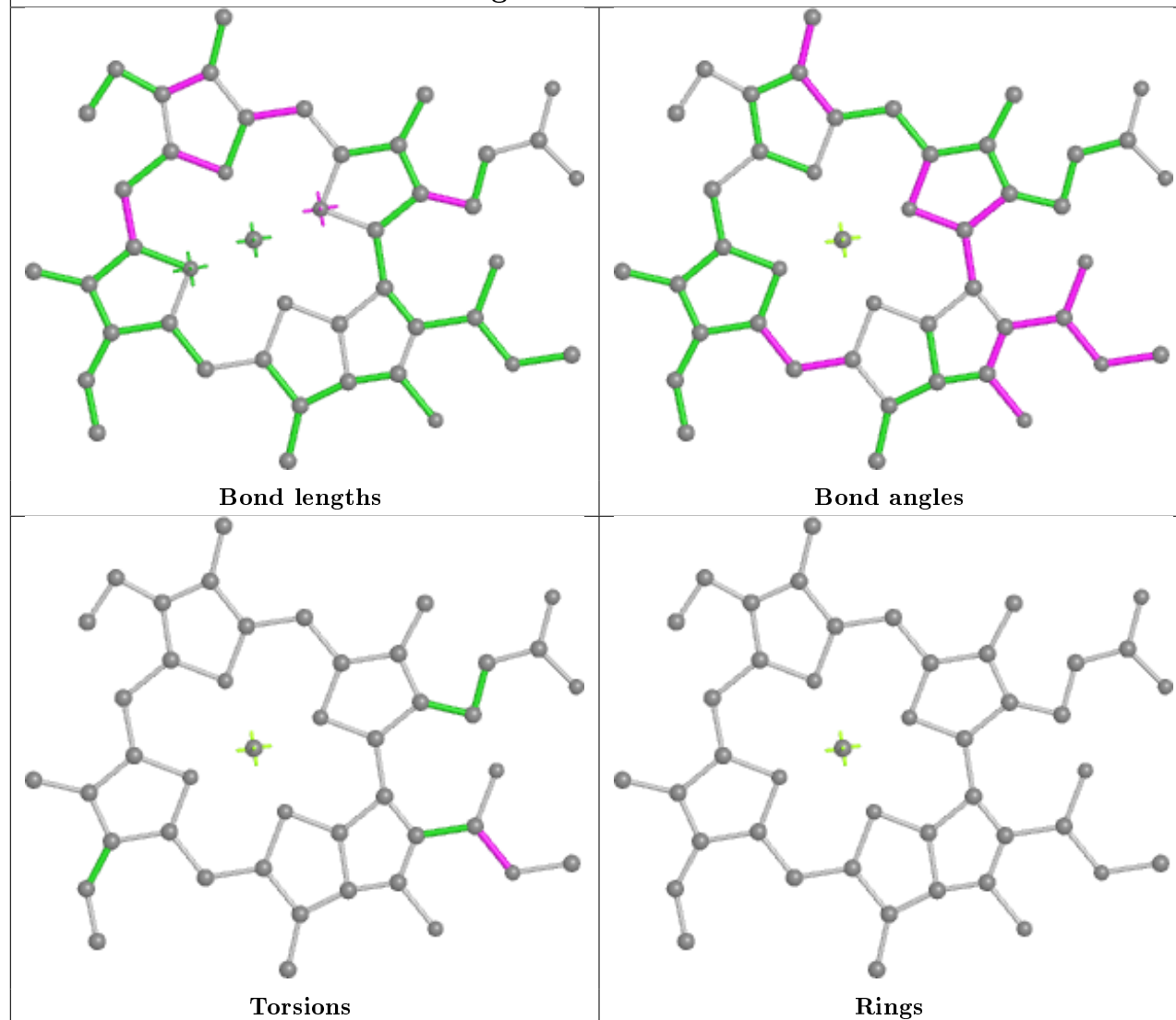
Ligand CLA M 1601



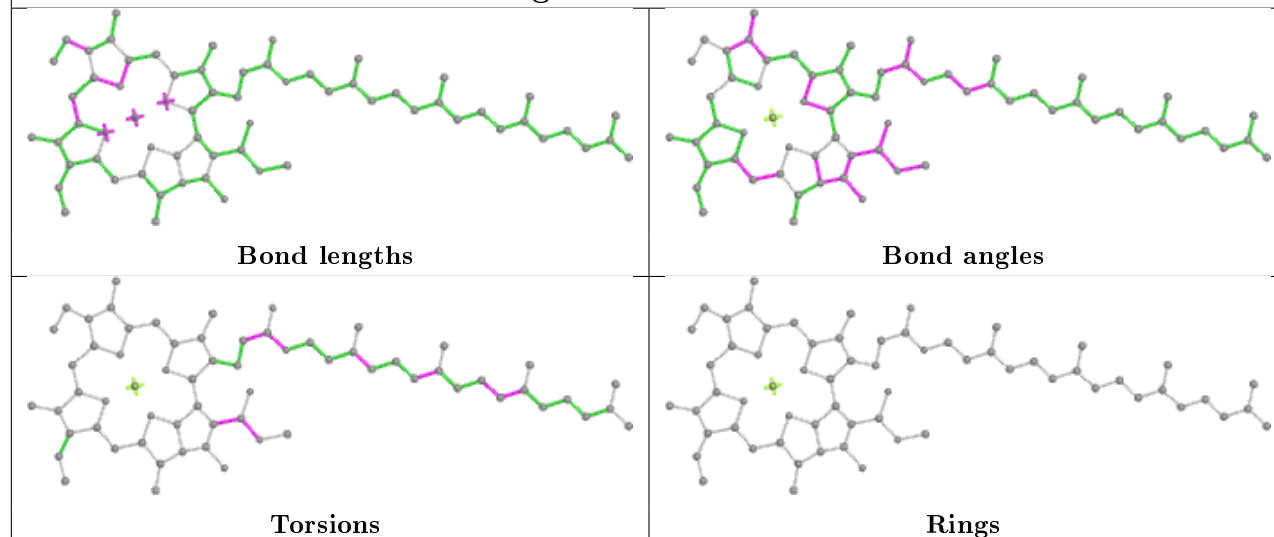
Ligand CLA A 839



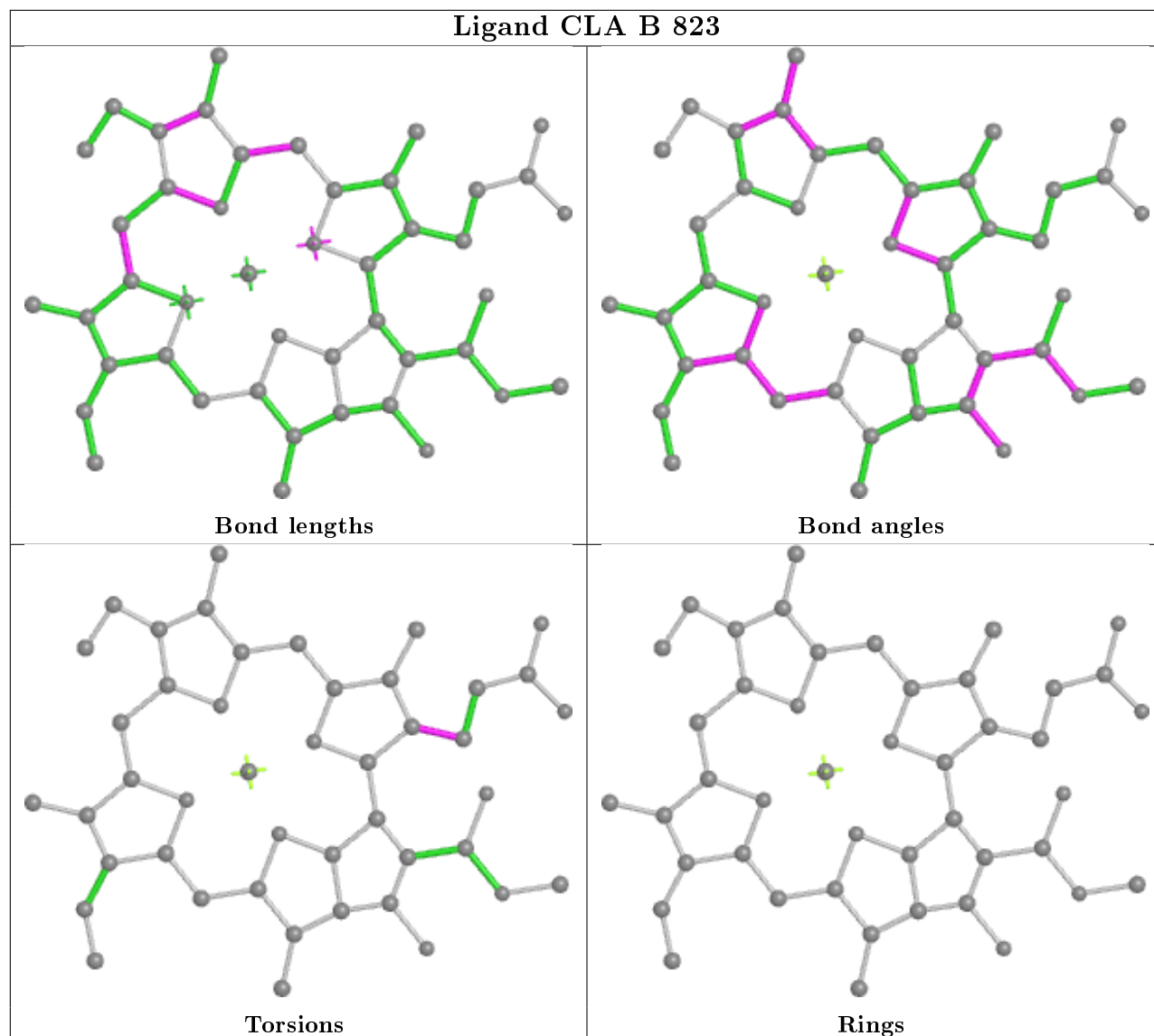
Ligand CLA A 815

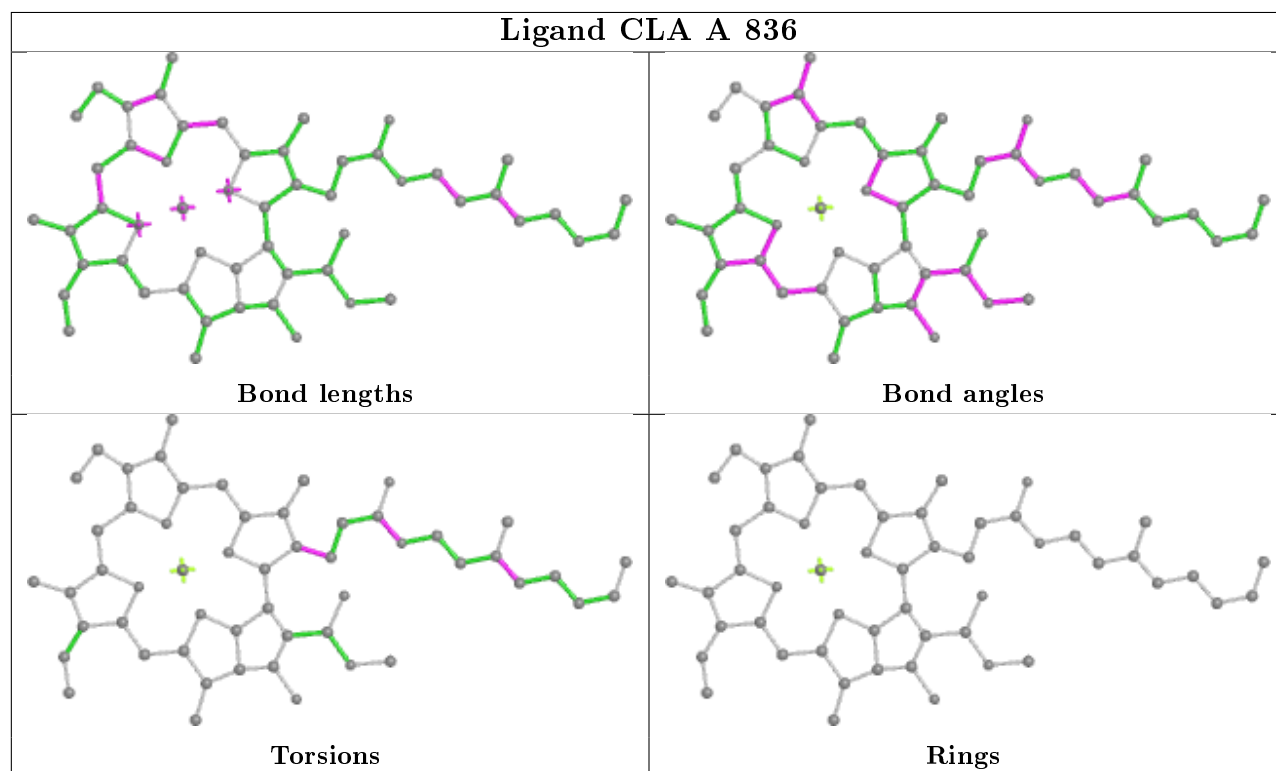
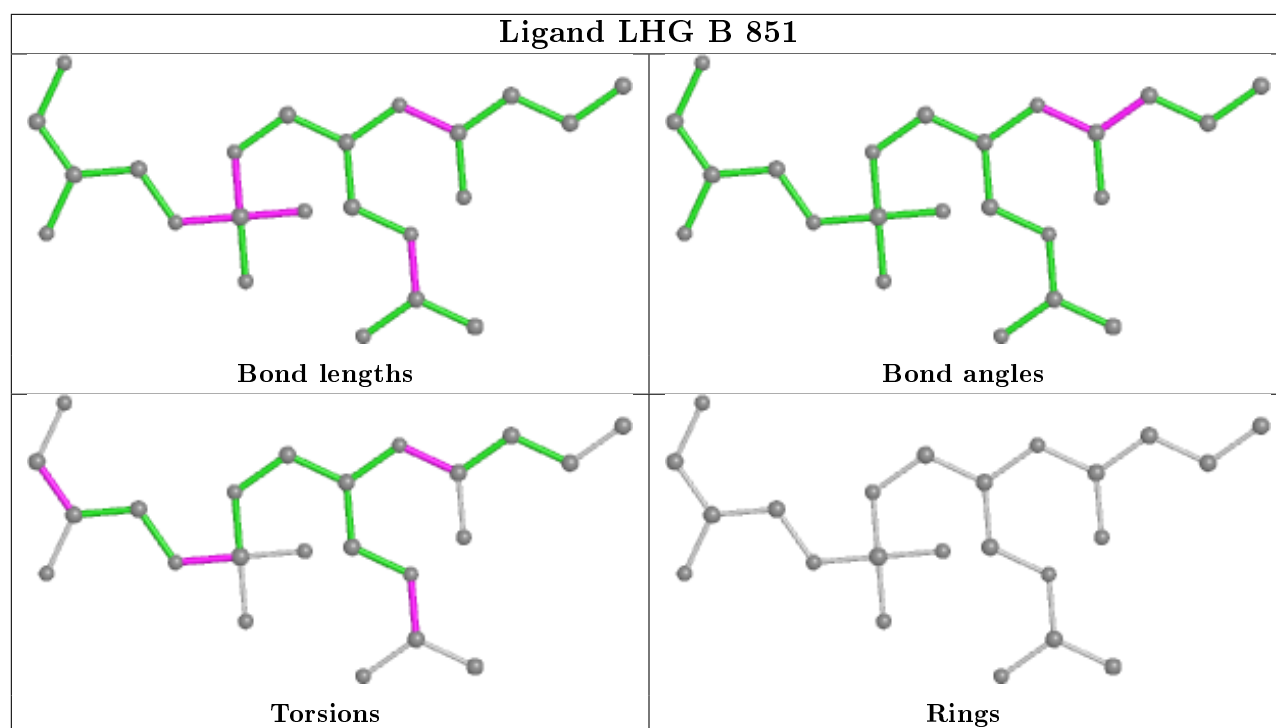


Ligand CLA B 826

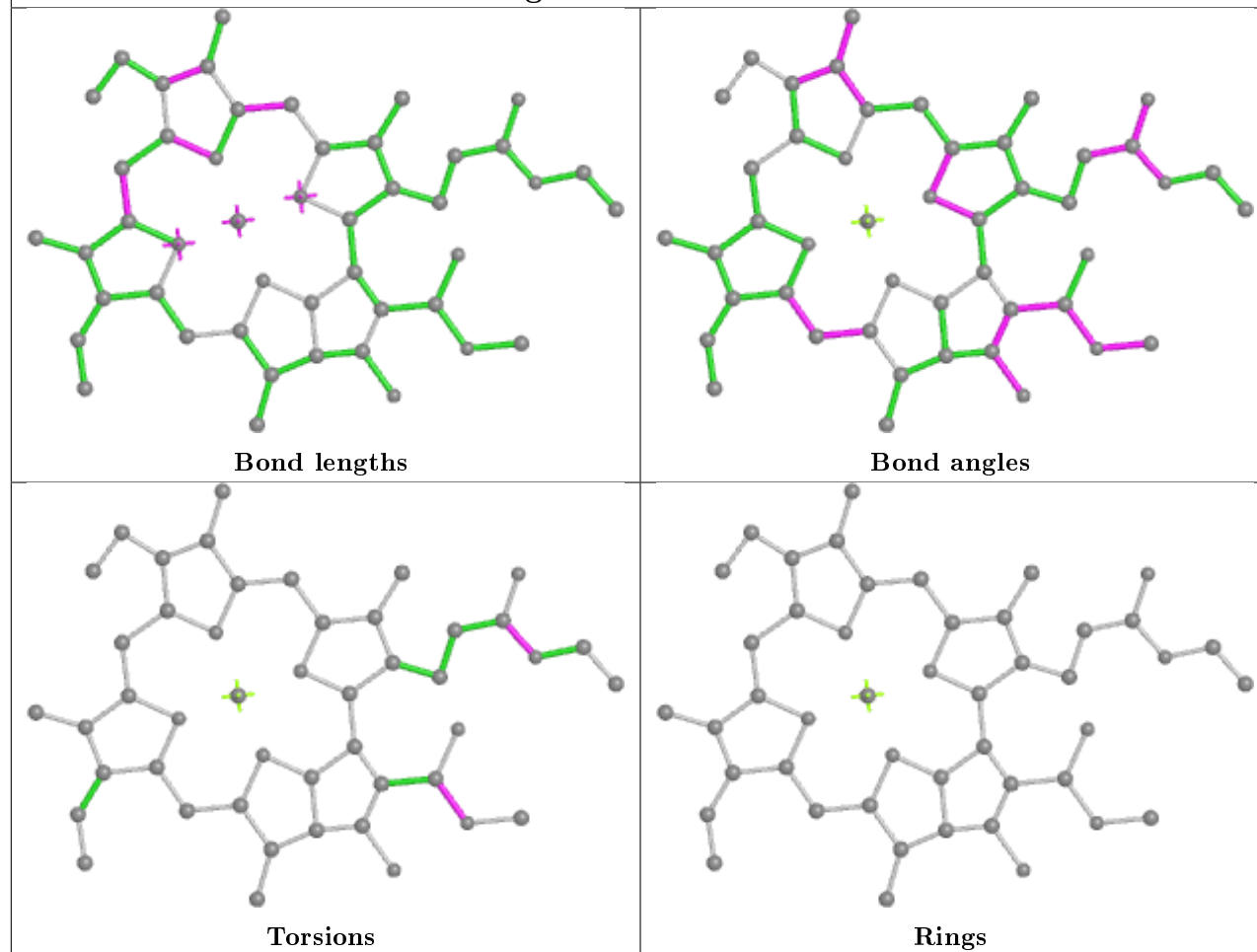


Ligand CLA B 823

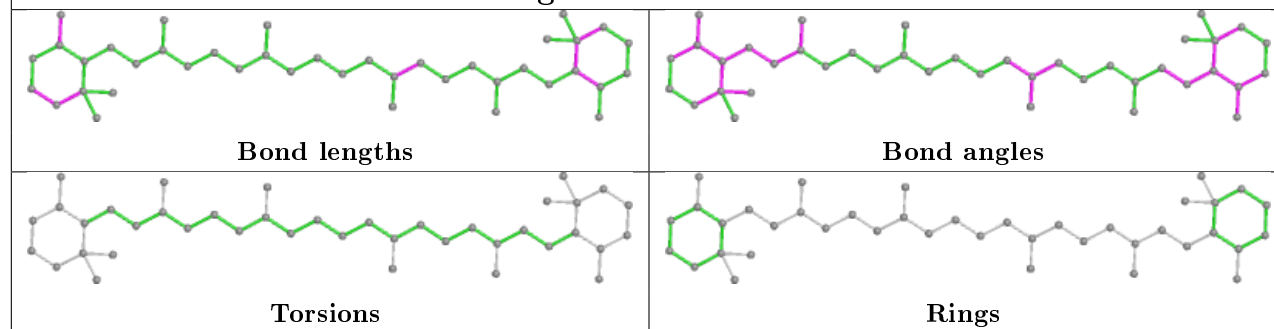




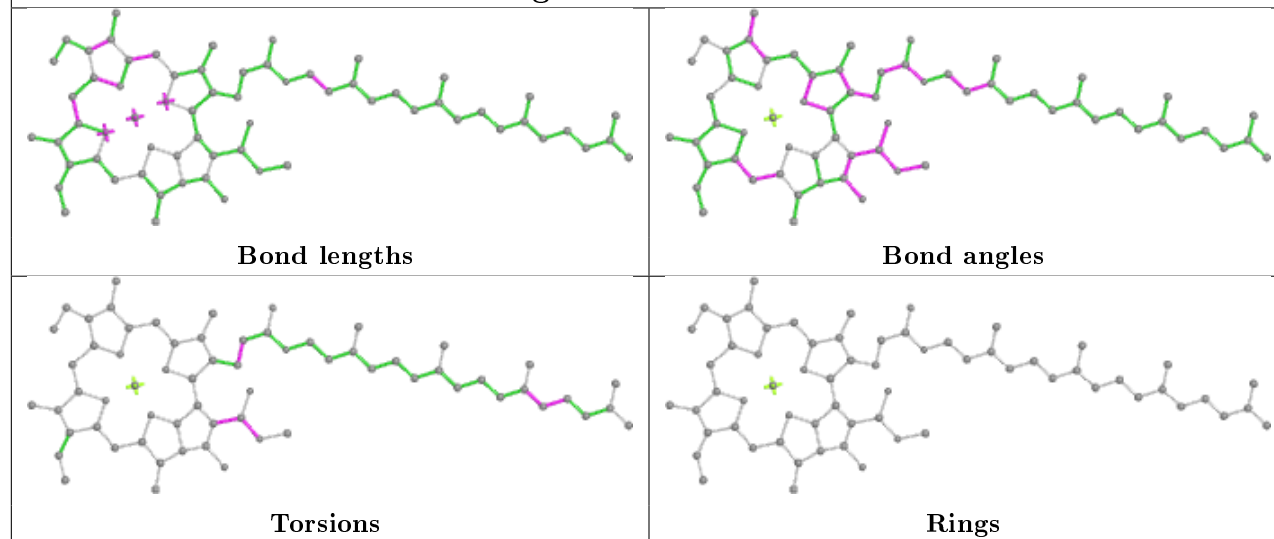
Ligand CLA B 839



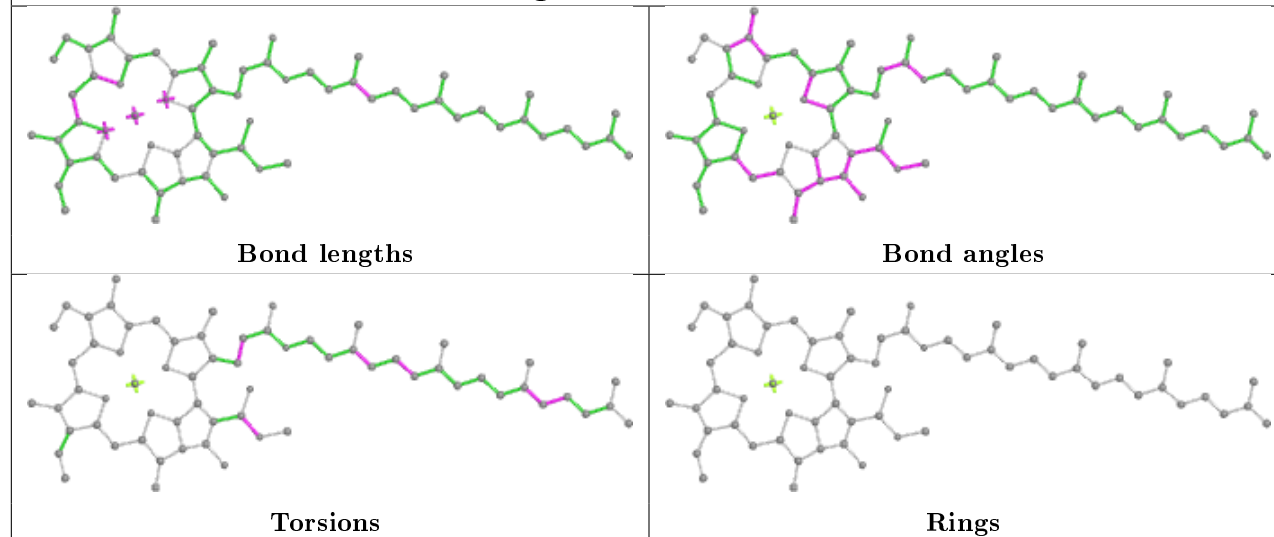
Ligand BCR I 101



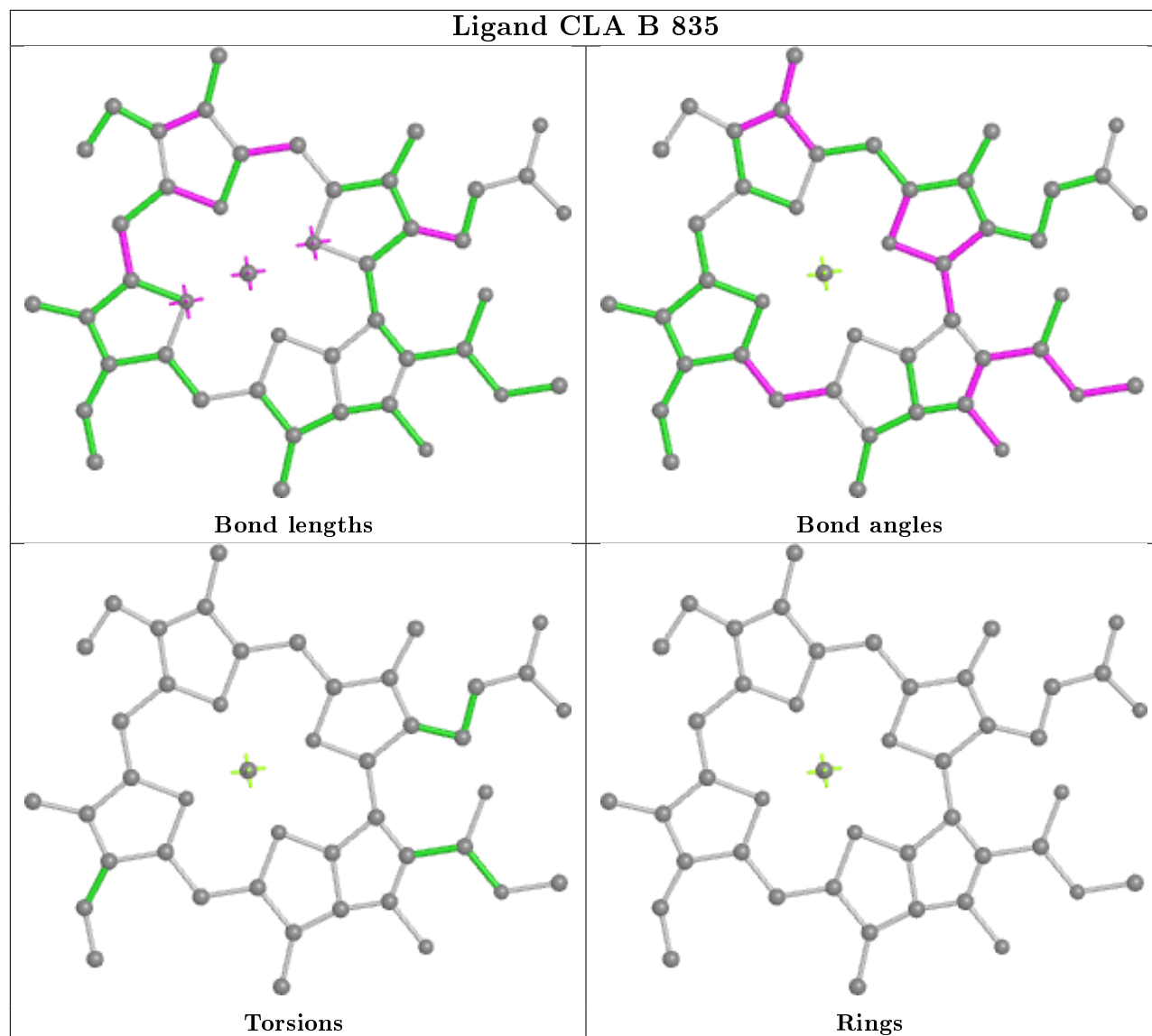
Ligand CLA A 835



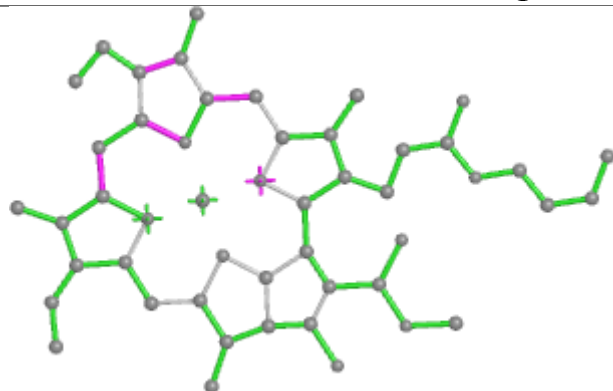
Ligand CLA A 830



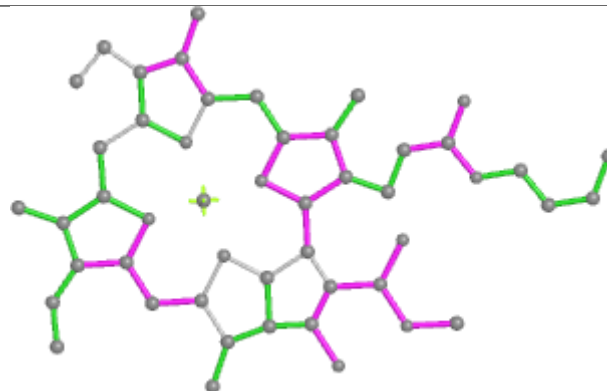
Ligand CLA B 835



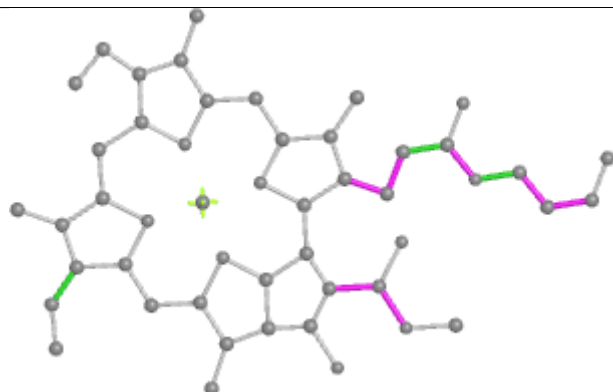
Ligand CLA A 823



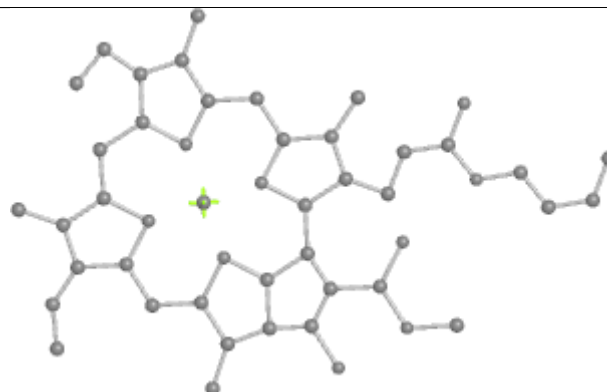
Bond lengths



Bond angles

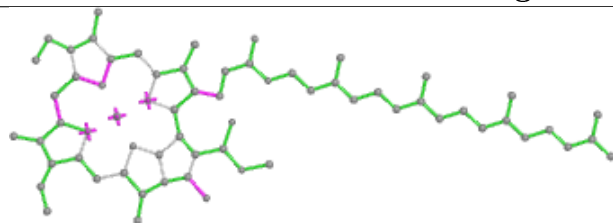


Torsions

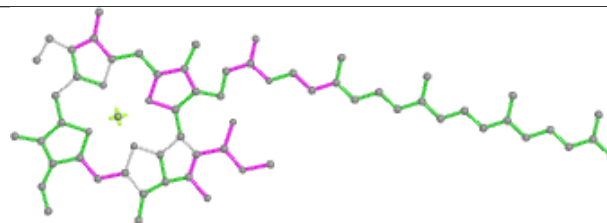


Rings

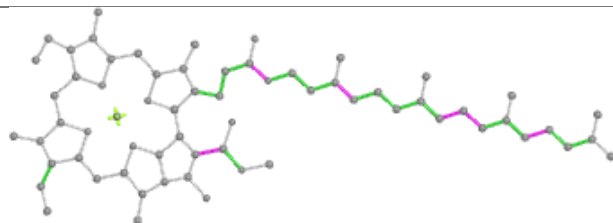
Ligand CLA B 829



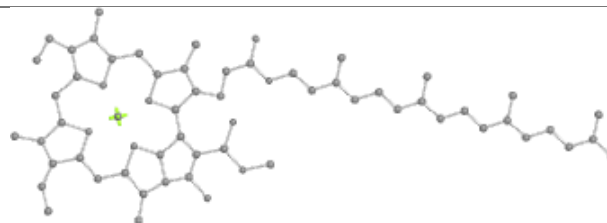
Bond lengths



Bond angles

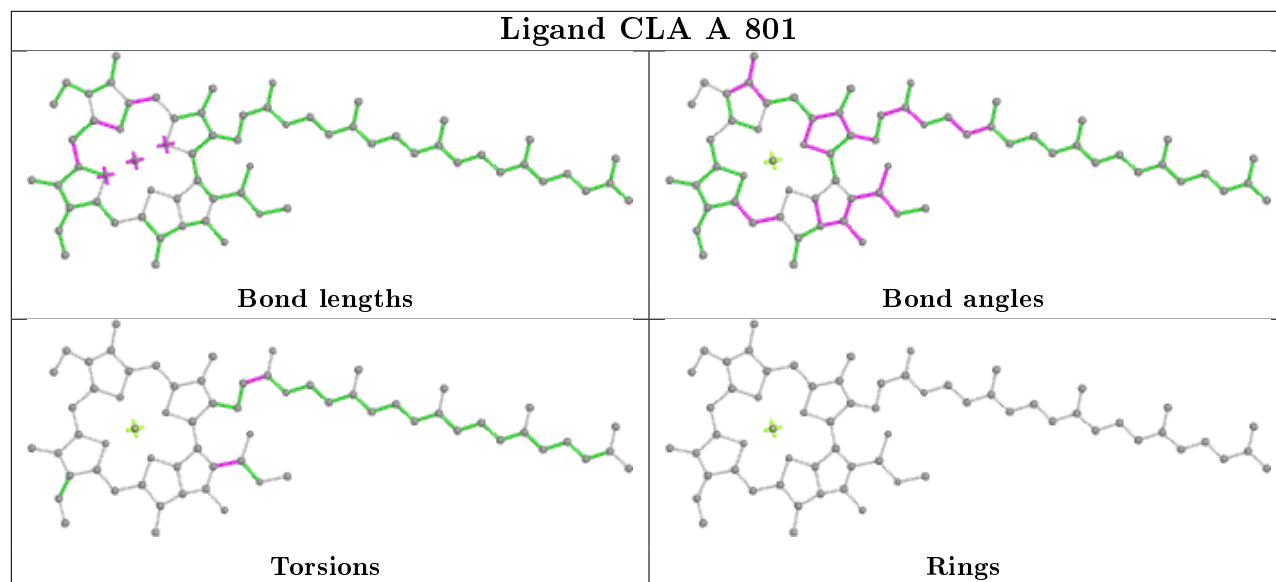


Torsions

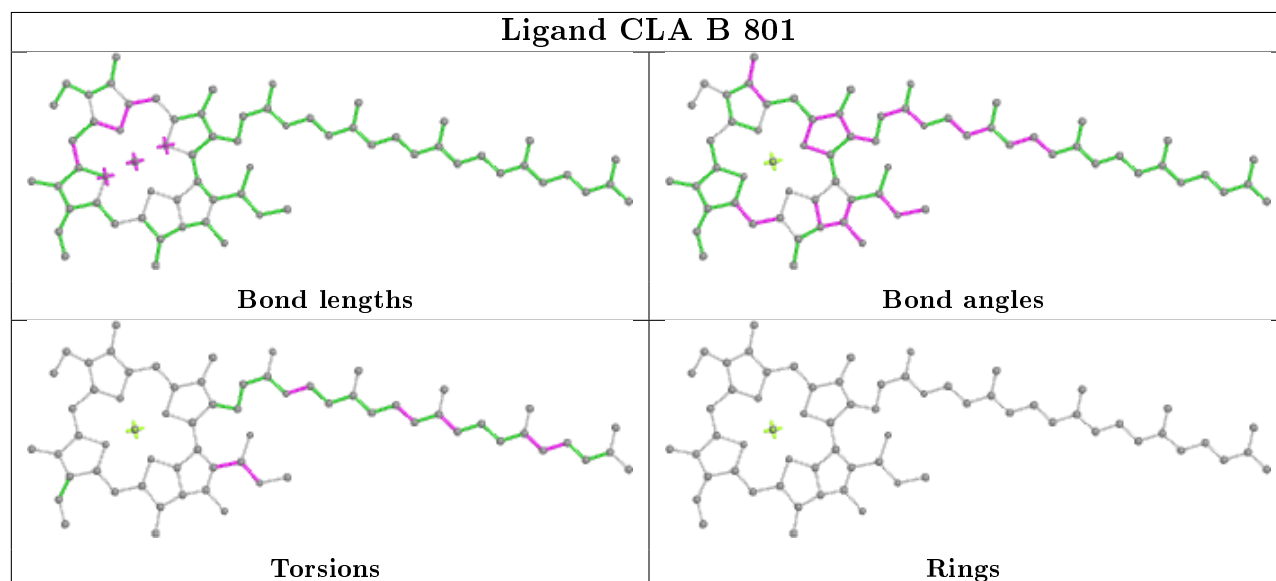


Rings

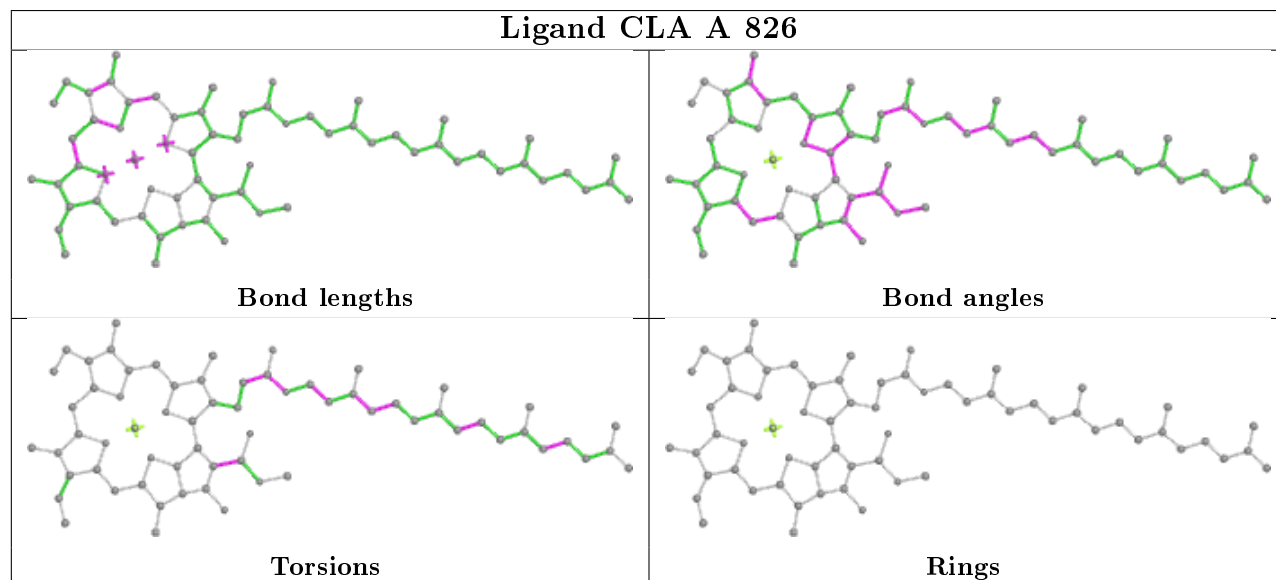
Ligand CLA A 801



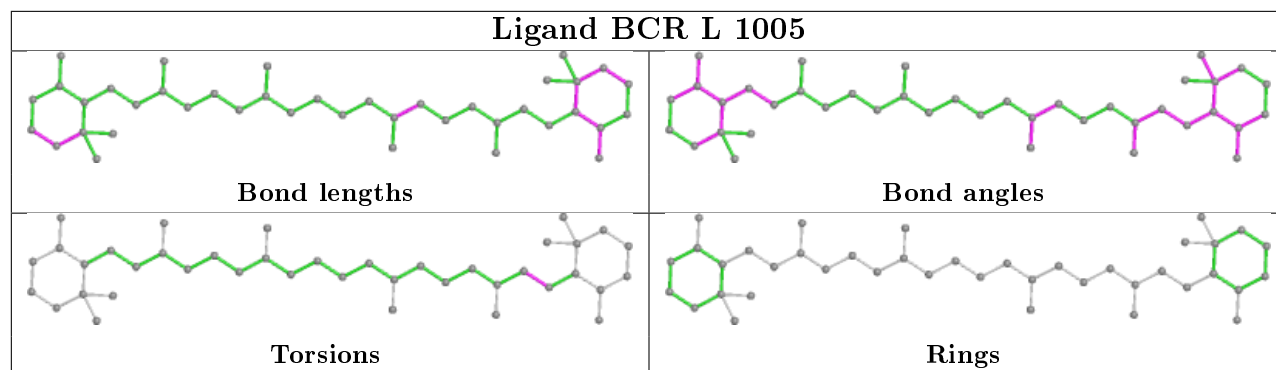
Ligand CLA B 801



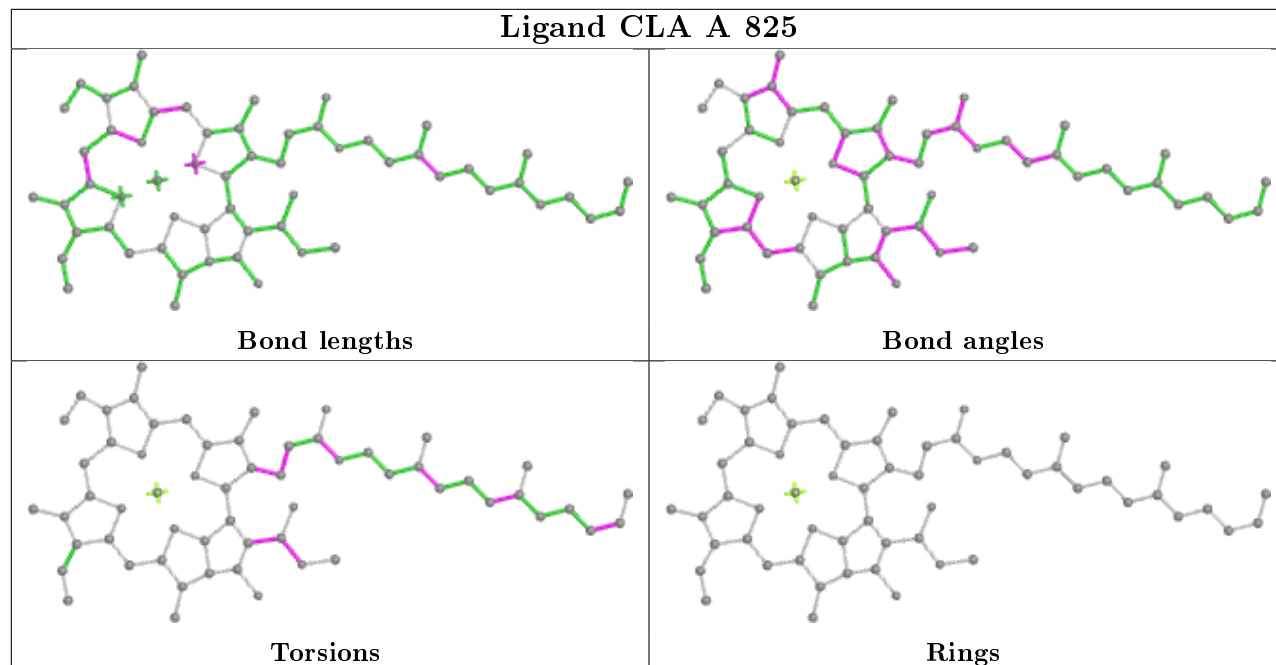
Ligand CLA A 826



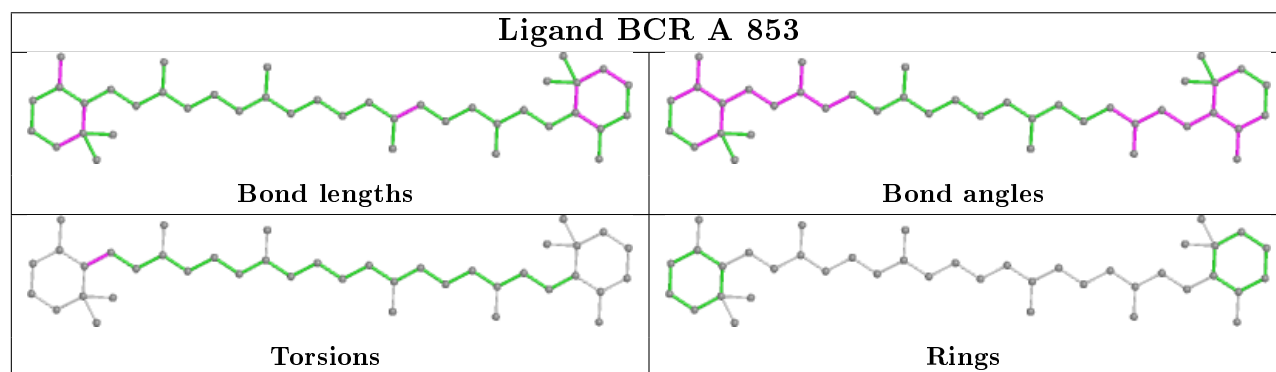
Ligand BCR L 1005



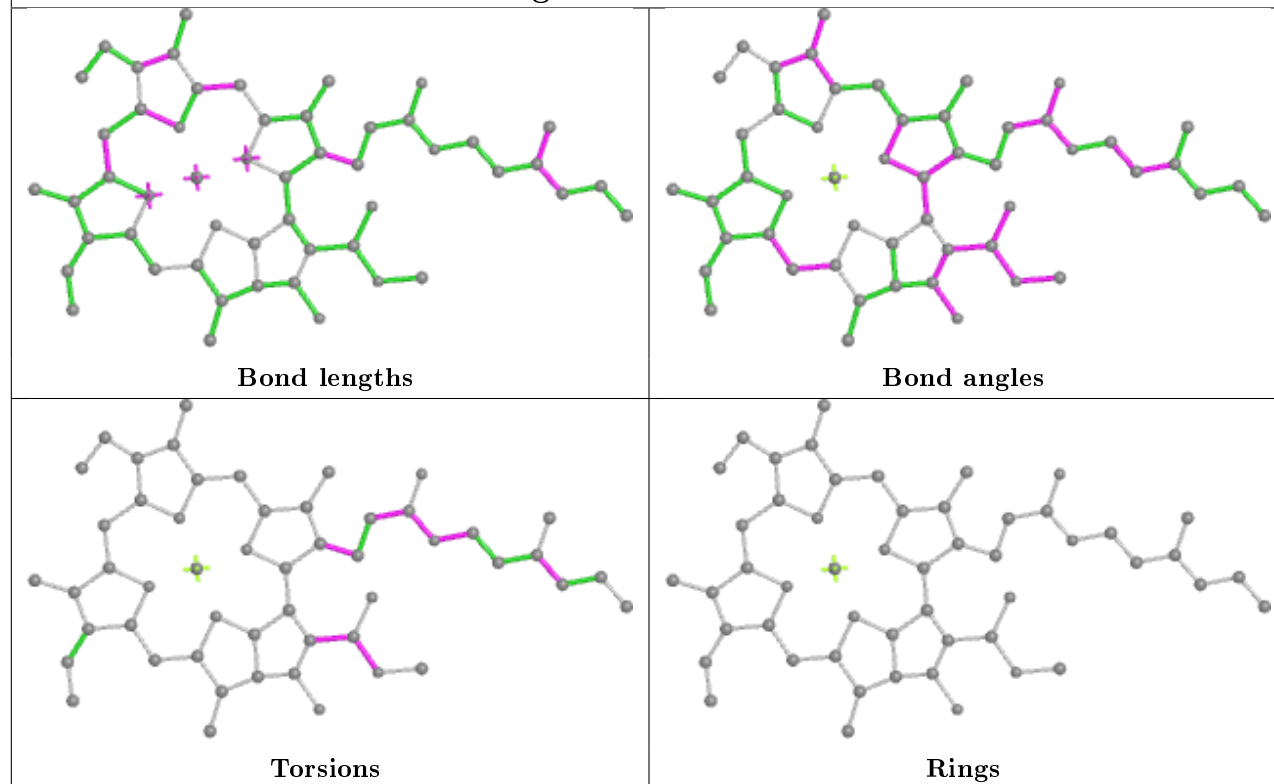
Ligand CLA A 825



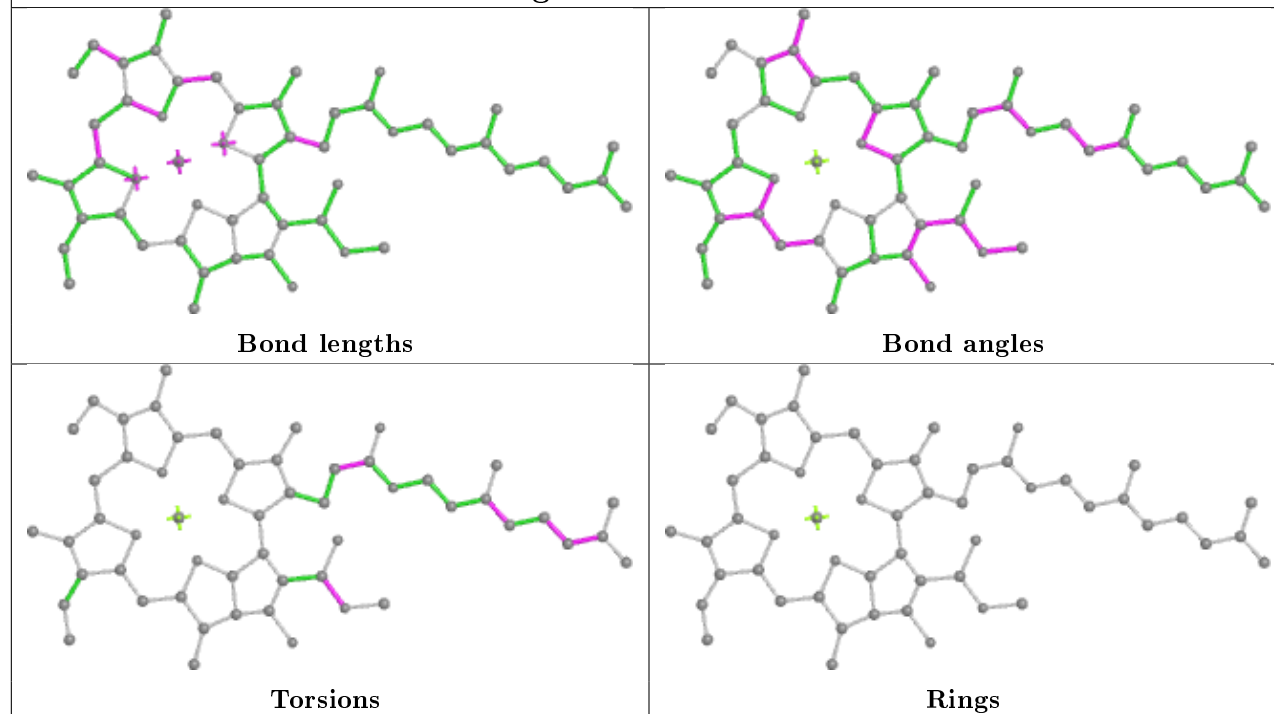
Ligand BCR A 853



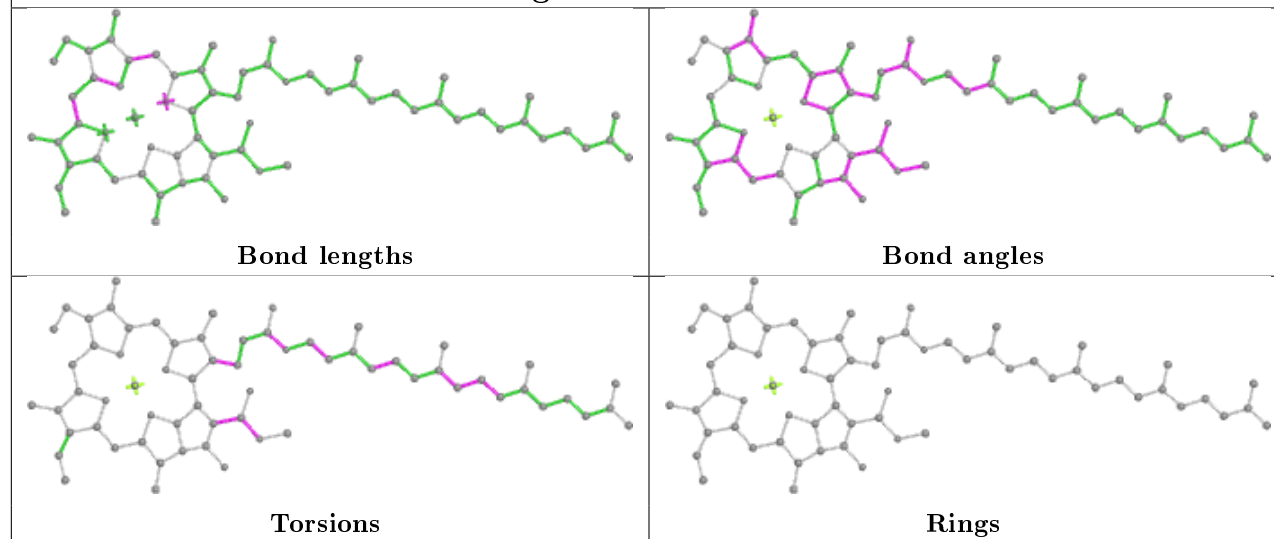
Ligand CLA A 846



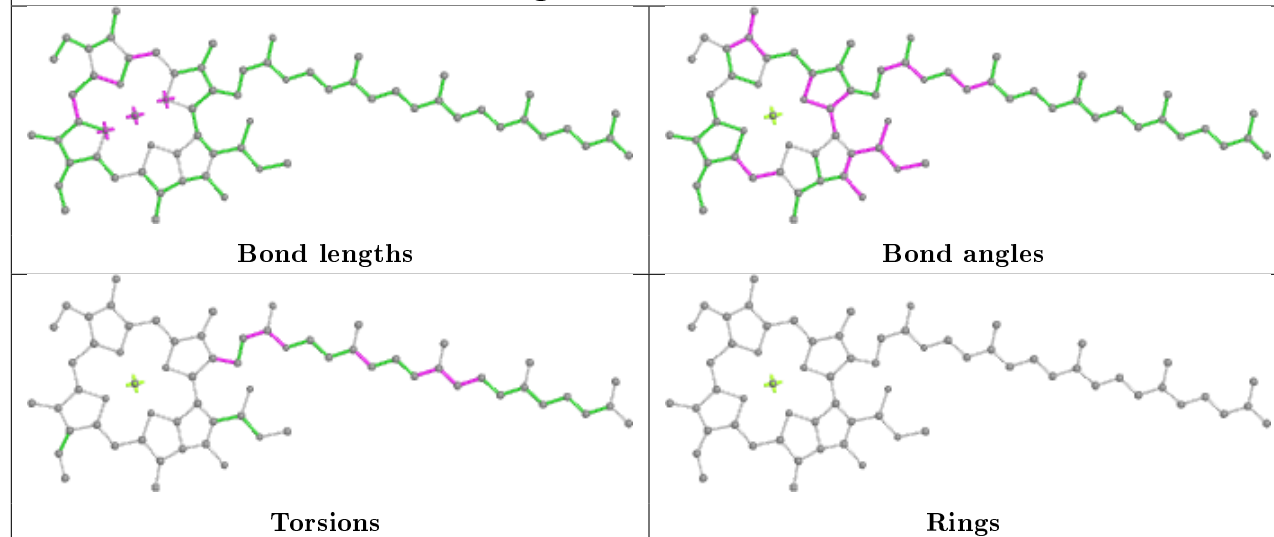
Ligand CLA B 822



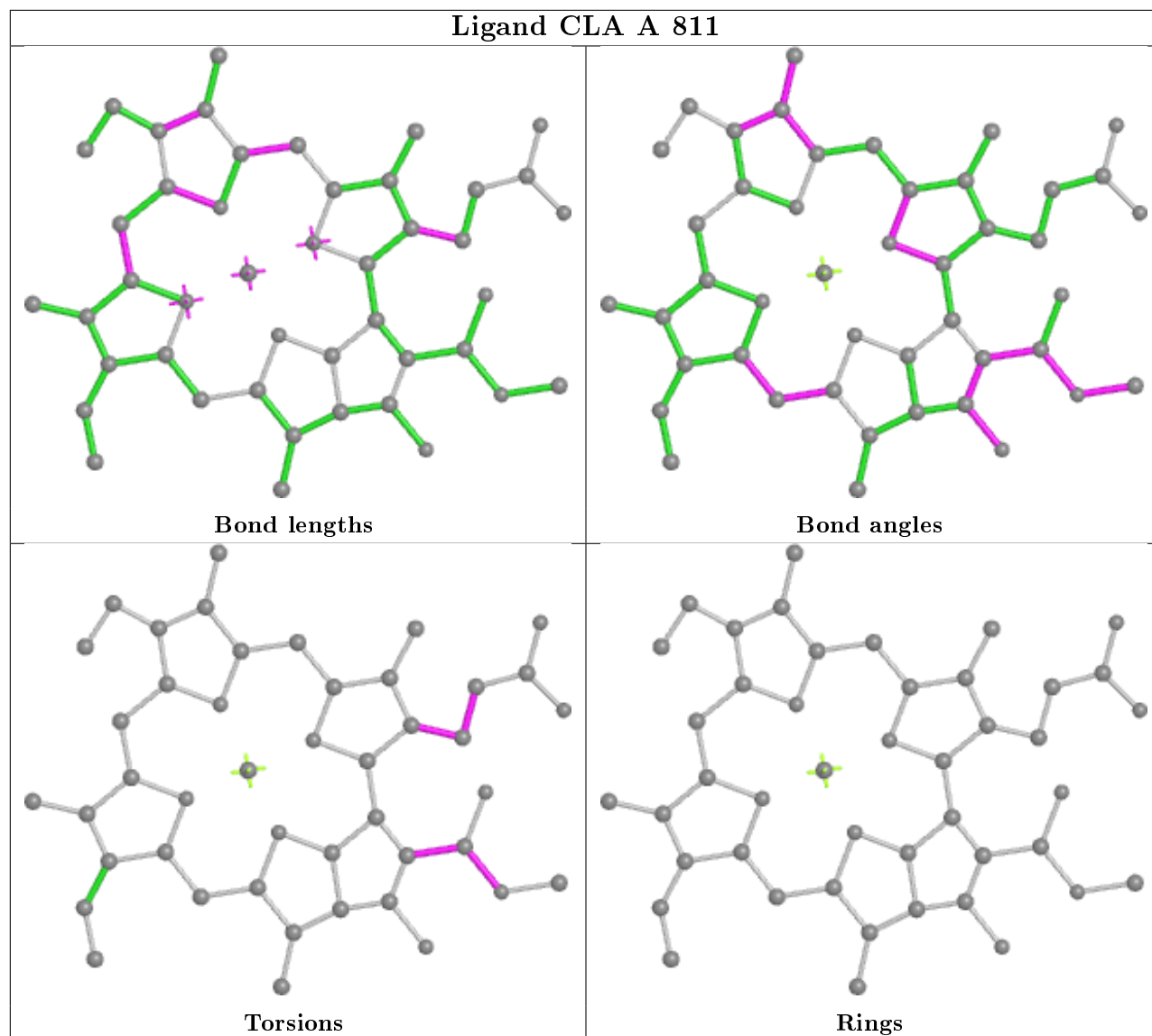
Ligand CLA A 806



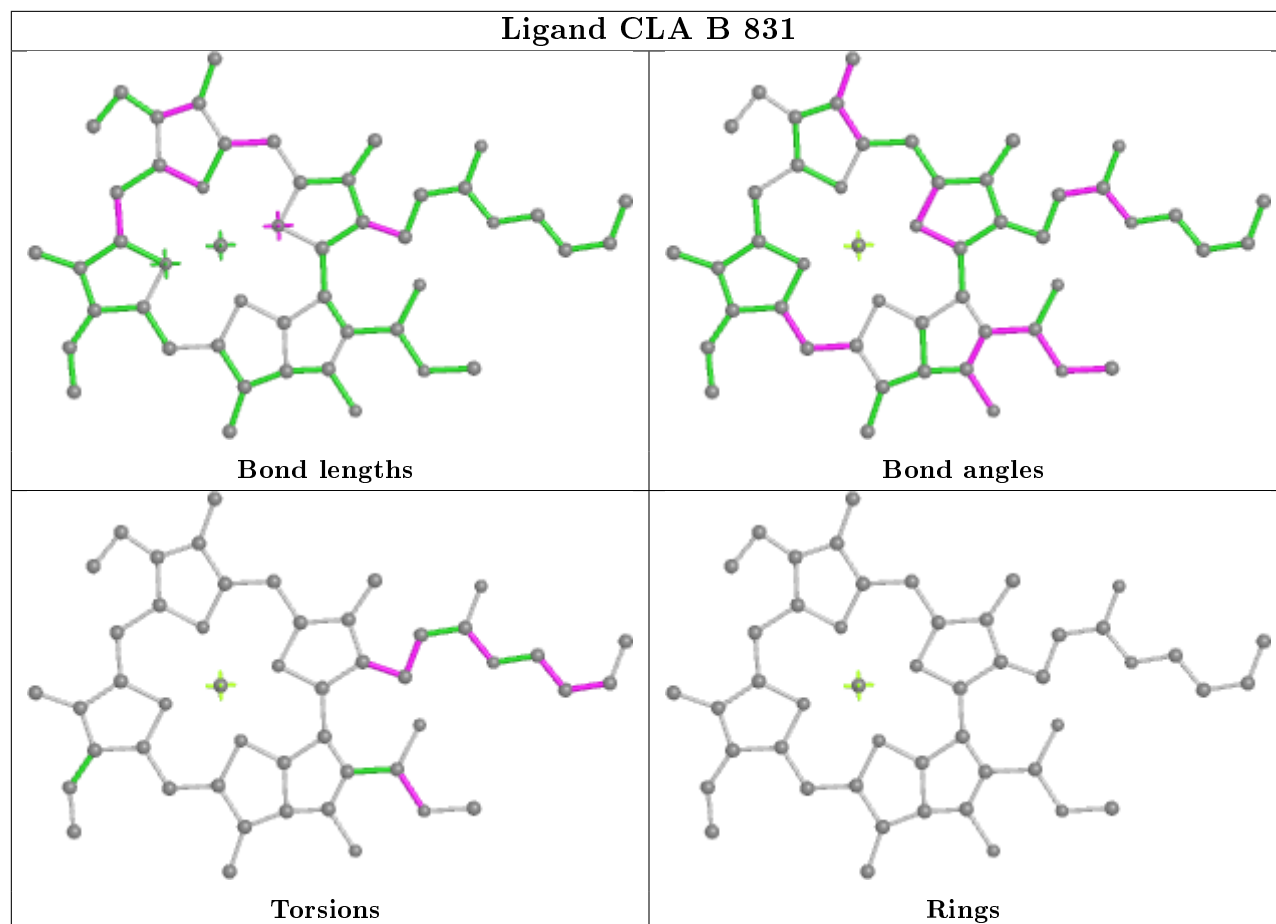
Ligand CLA B 813



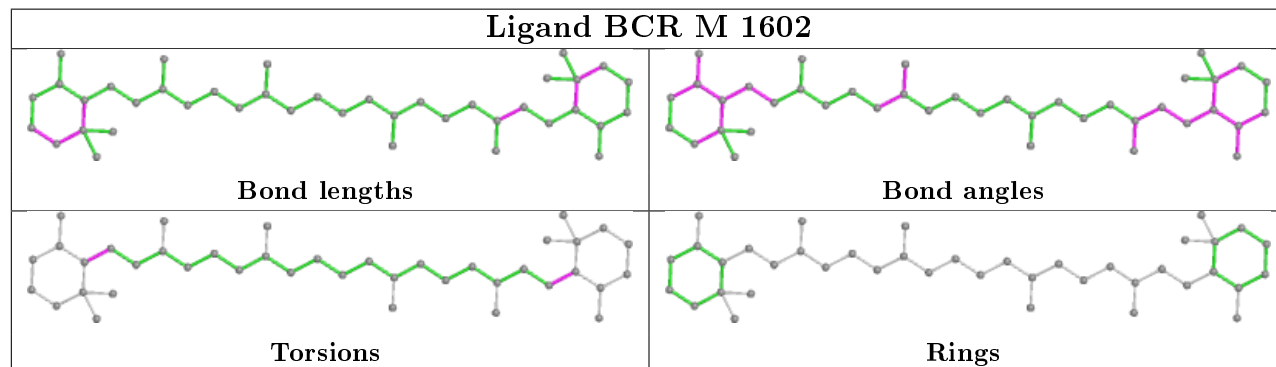
Ligand CLA A 811



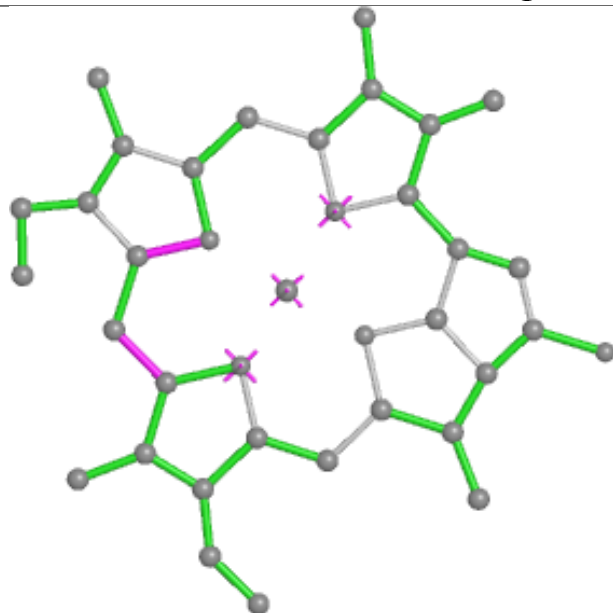
Ligand CLA B 831



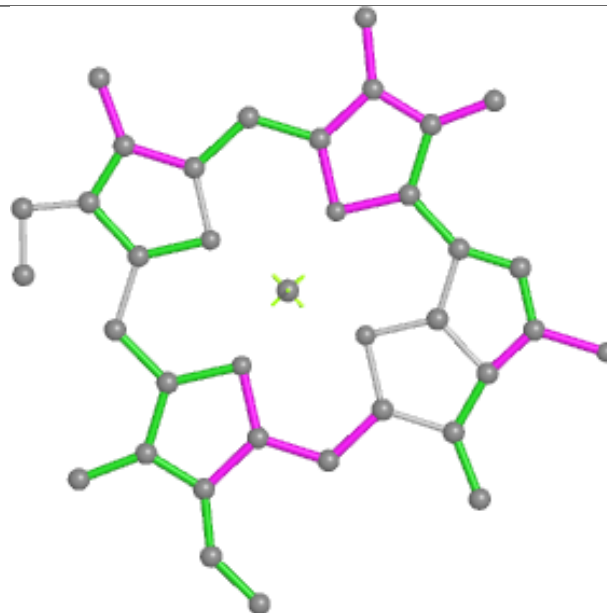
Ligand BCR M 1602



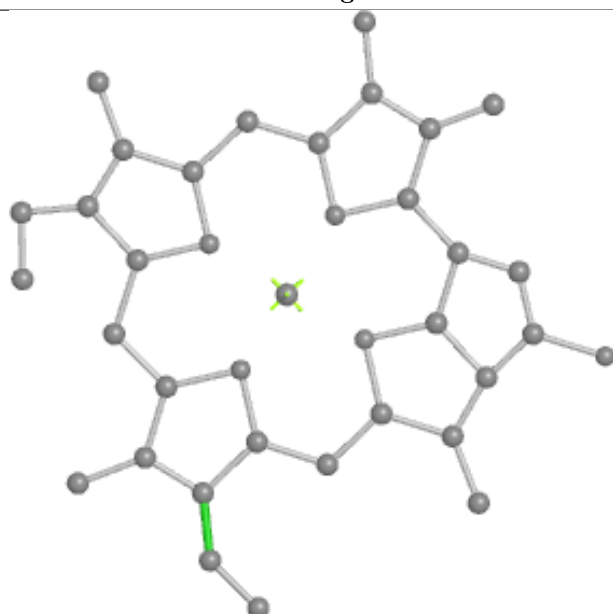
Ligand CLA J 102



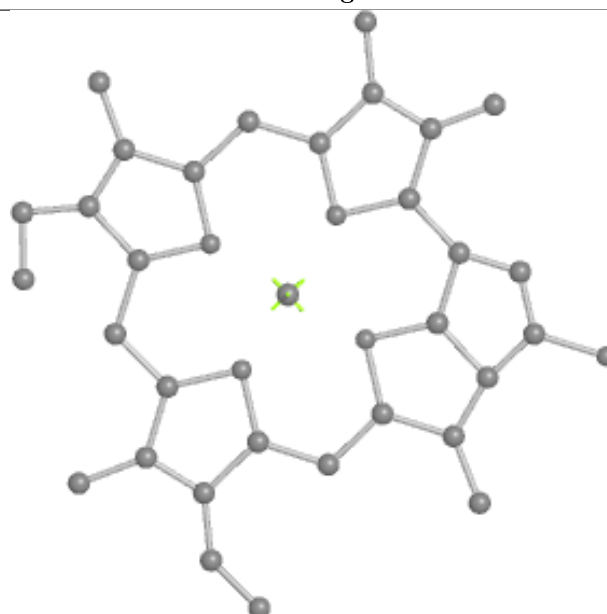
Bond lengths



Bond angles

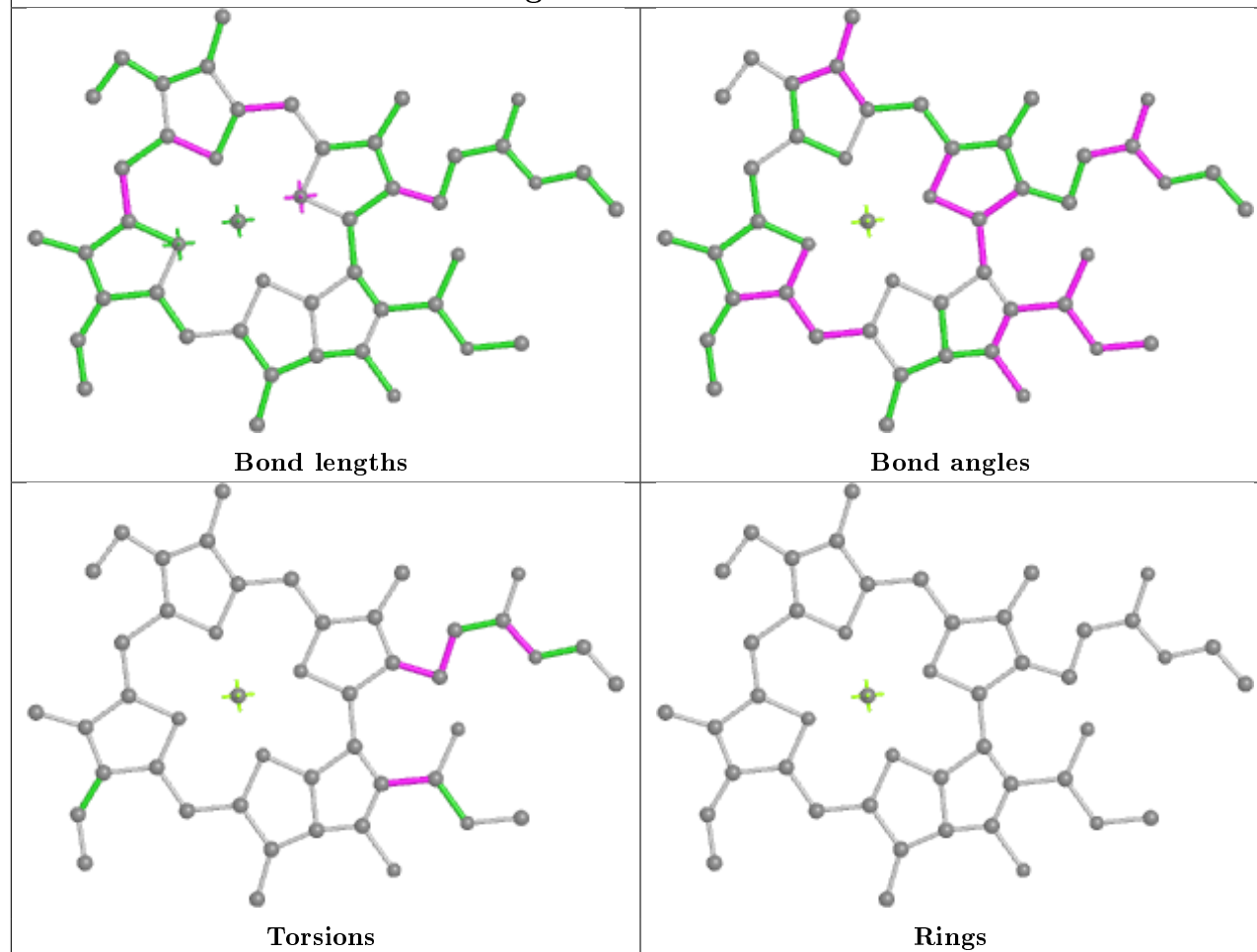


Torsions

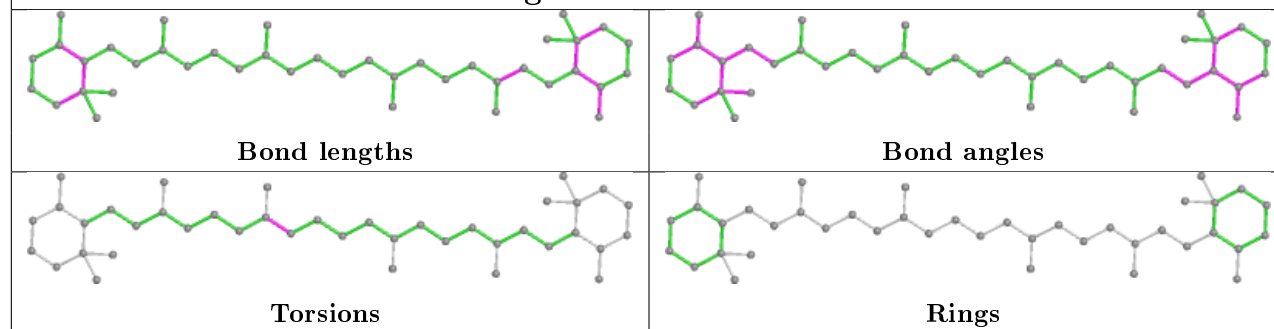


Rings

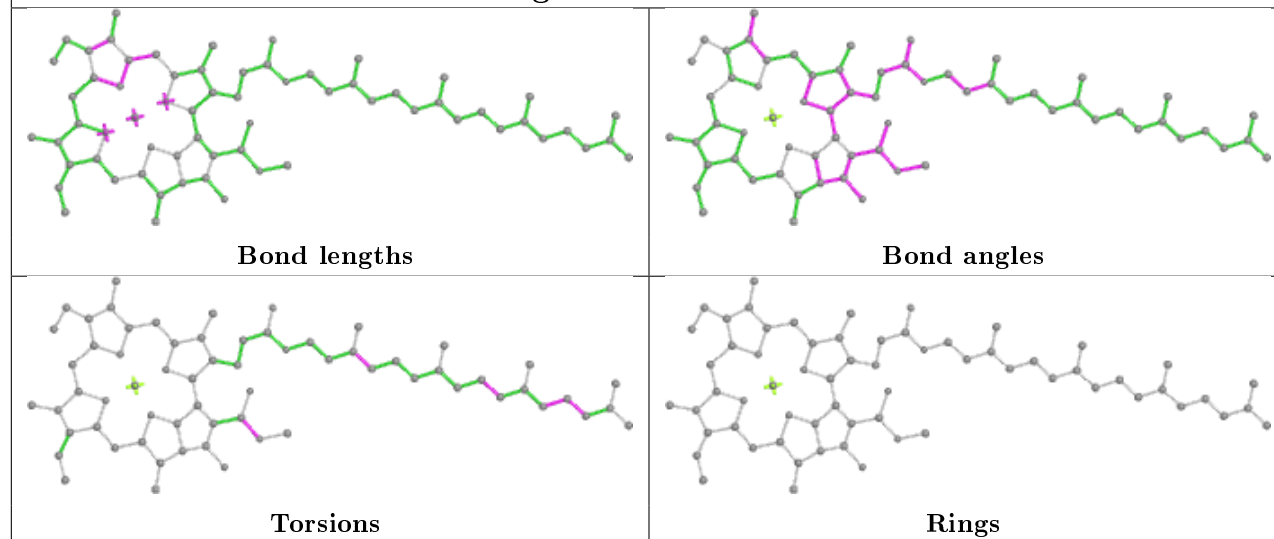
Ligand CLA B 820



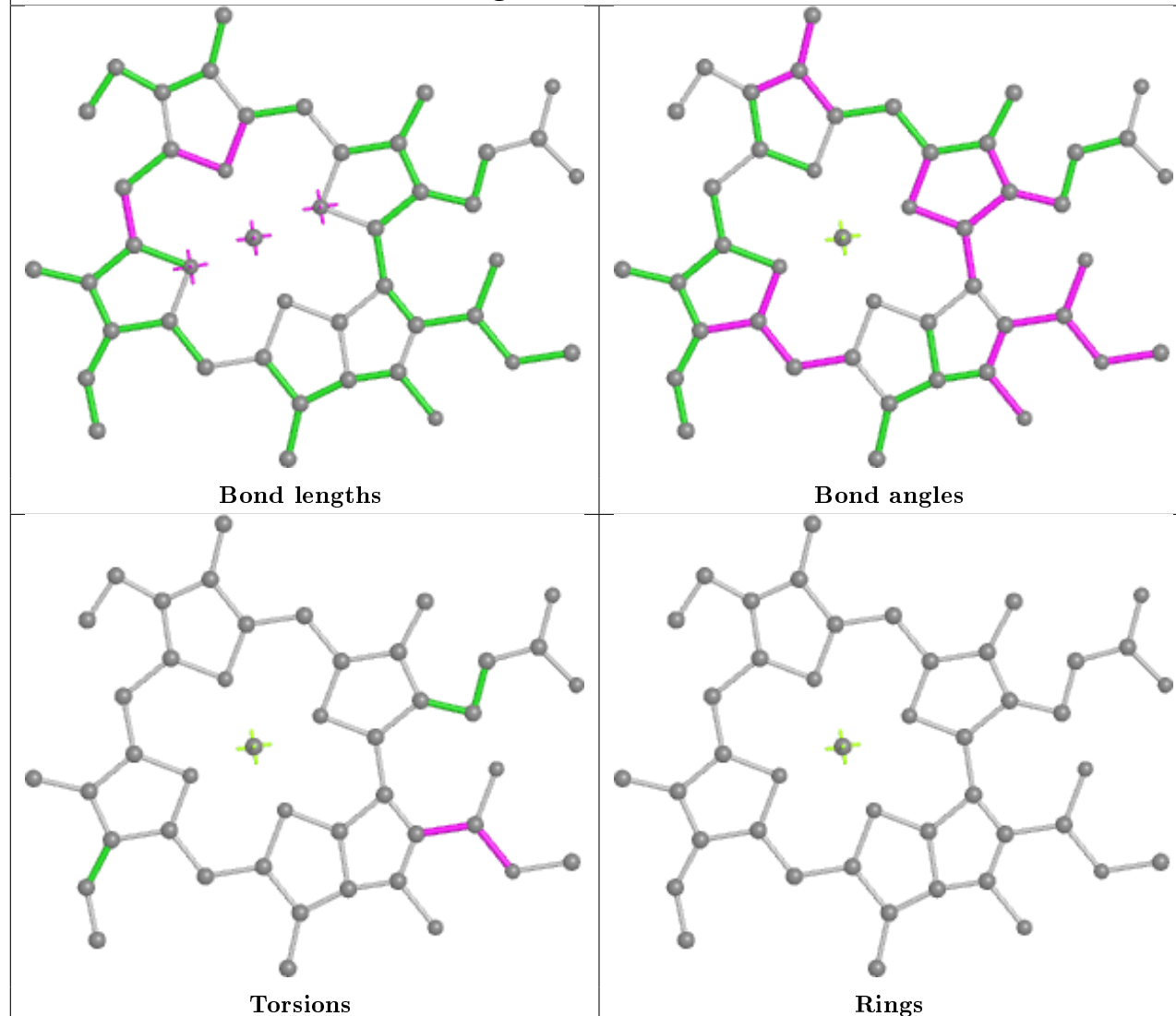
Ligand BCR L 1006



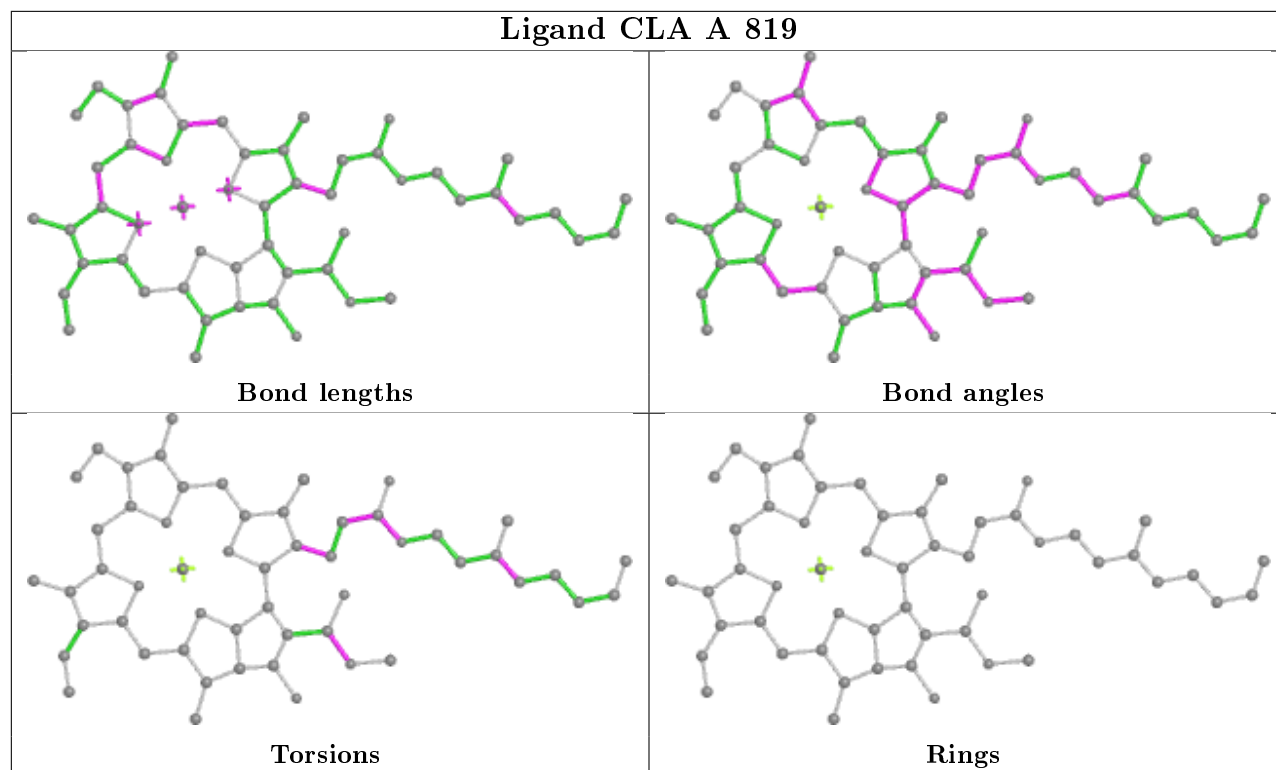
Ligand CLA B 810



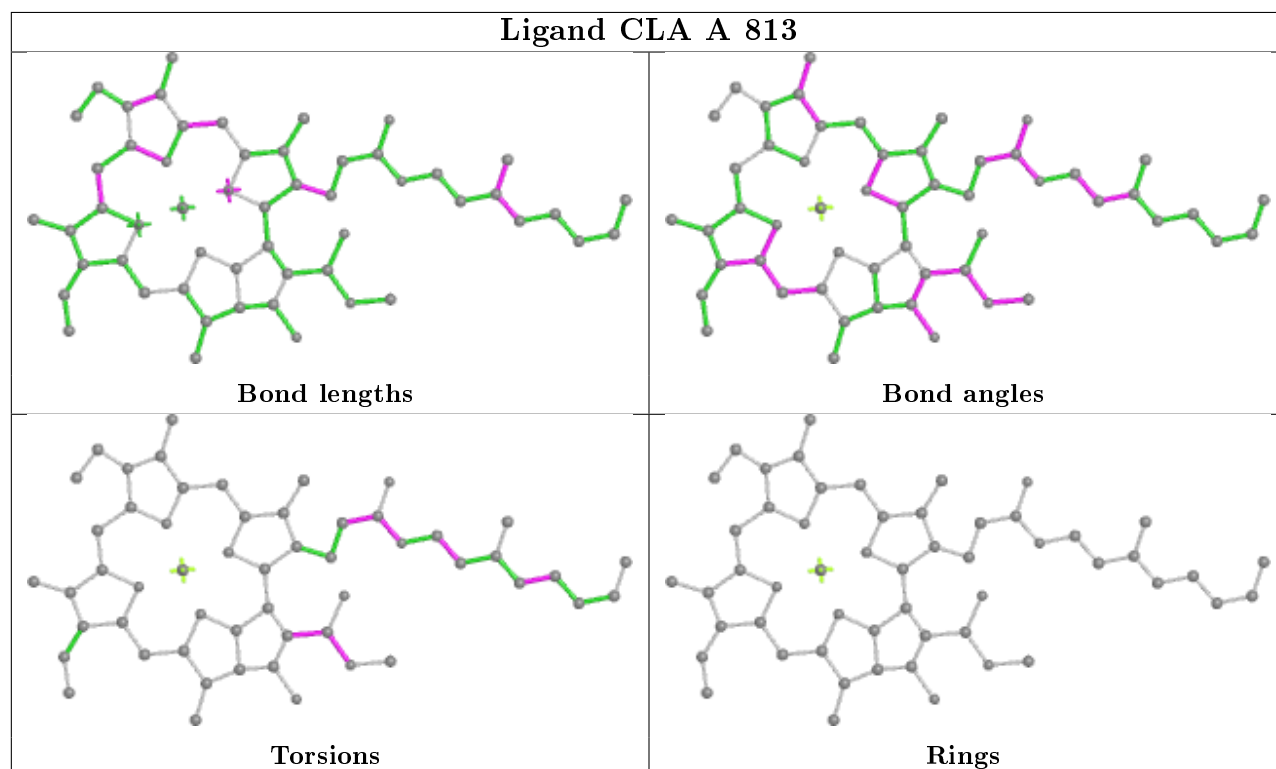
Ligand CLA A 816



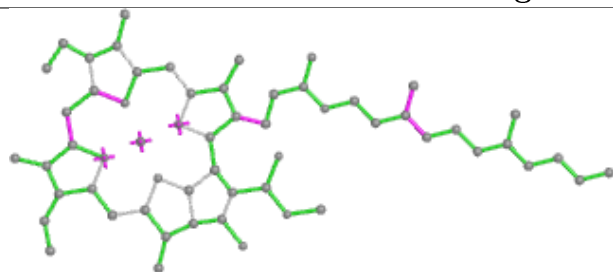
Ligand CLA A 819



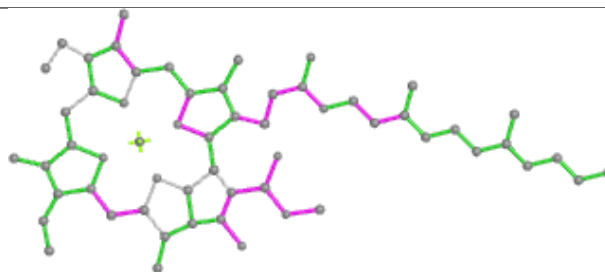
Ligand CLA A 813



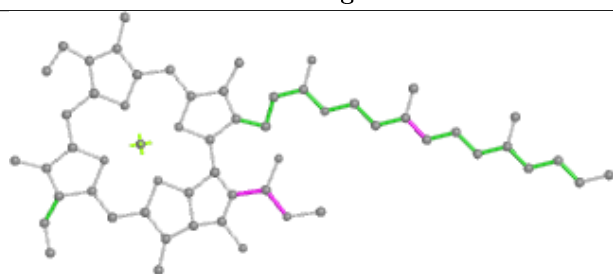
Ligand CLA B 833



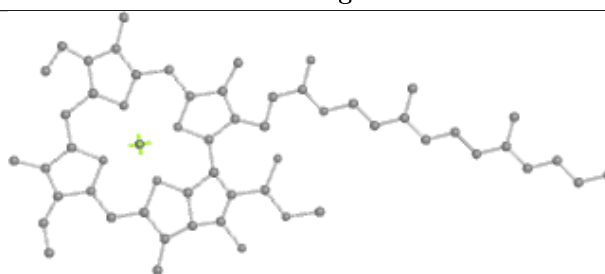
Bond lengths



Bond angles

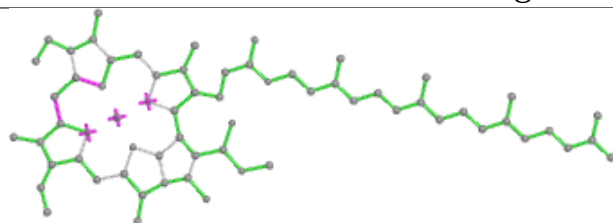


Torsions

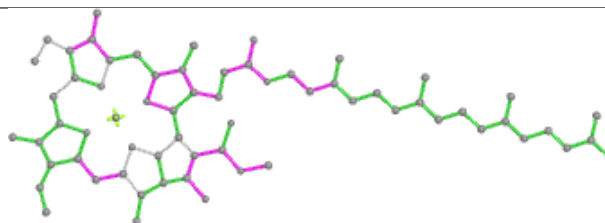


Rings

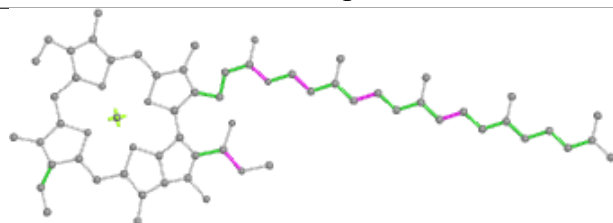
Ligand CLA A 833



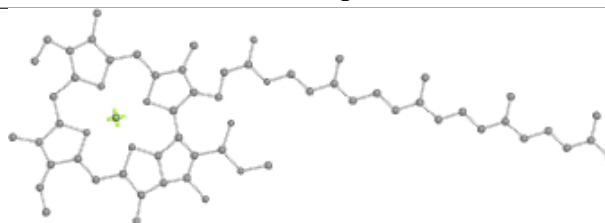
Bond lengths



Bond angles

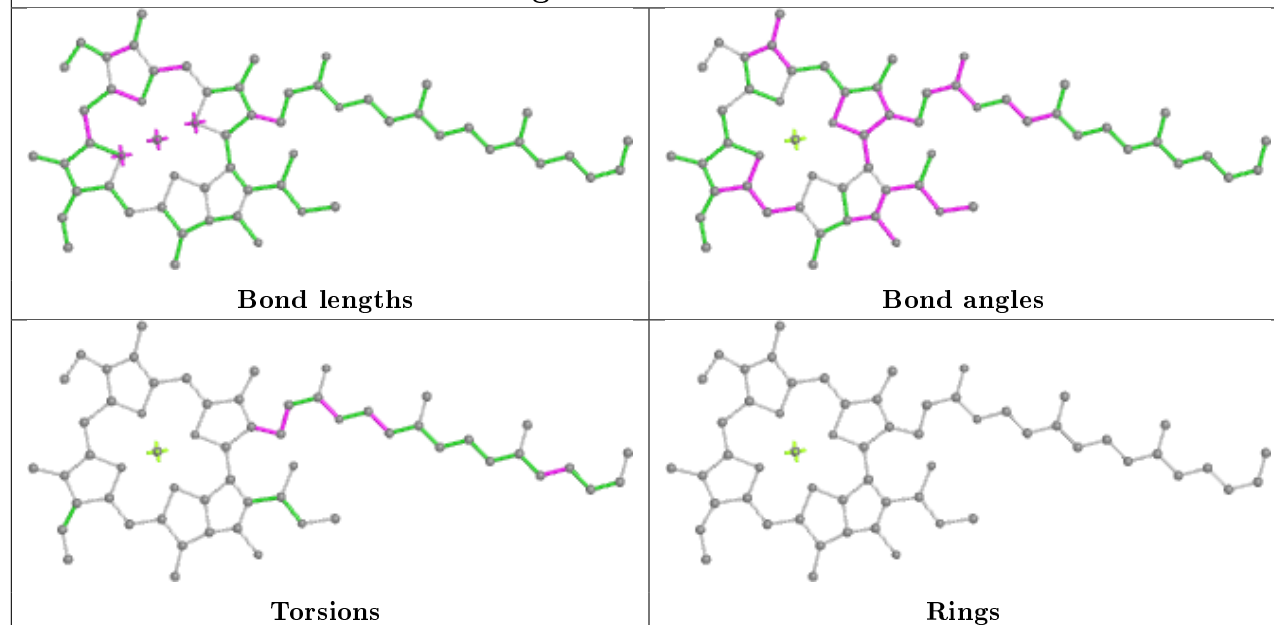


Torsions

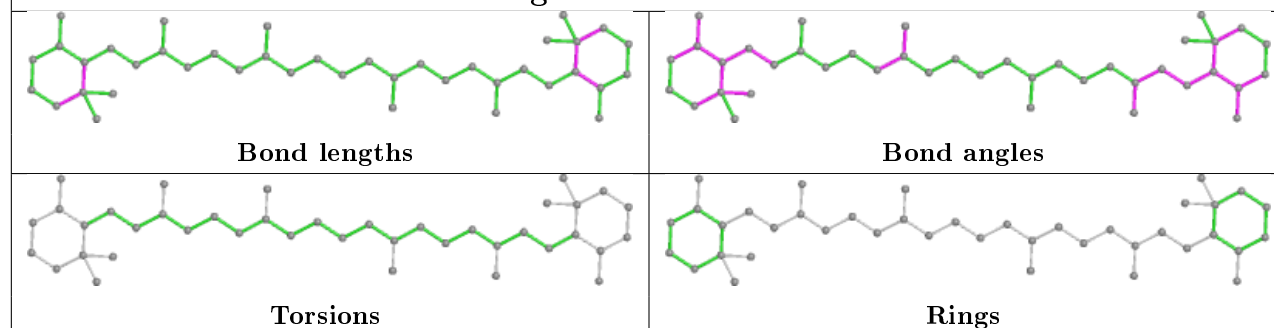


Rings

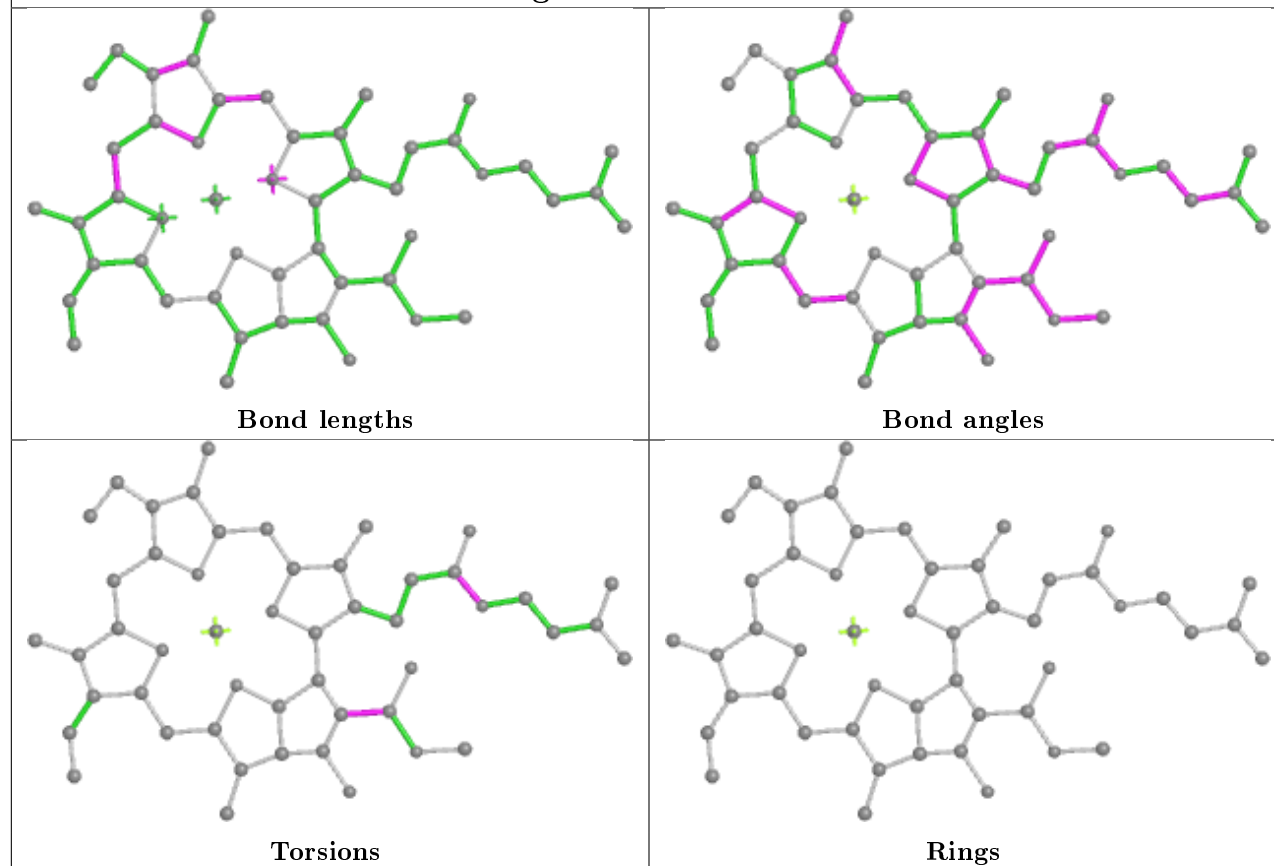
Ligand CLA B 817



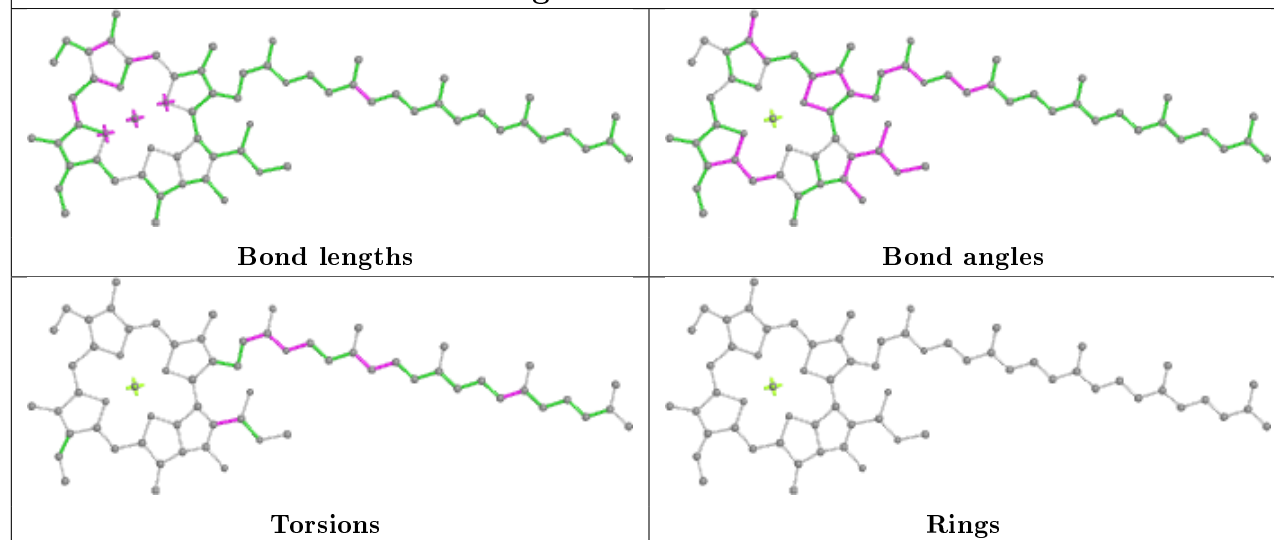
Ligand BCR A 849



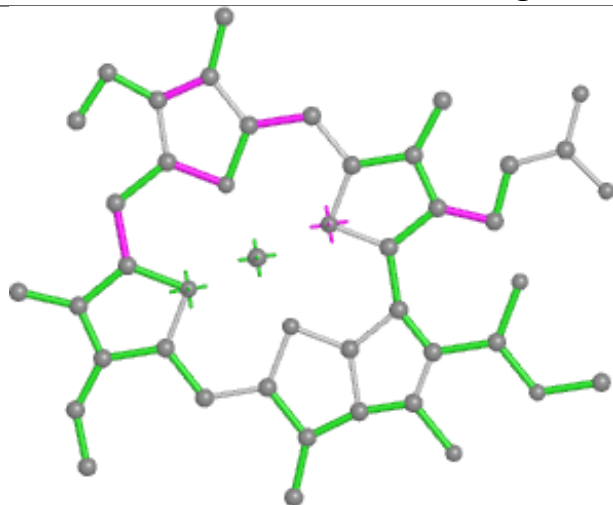
Ligand CLA A 832



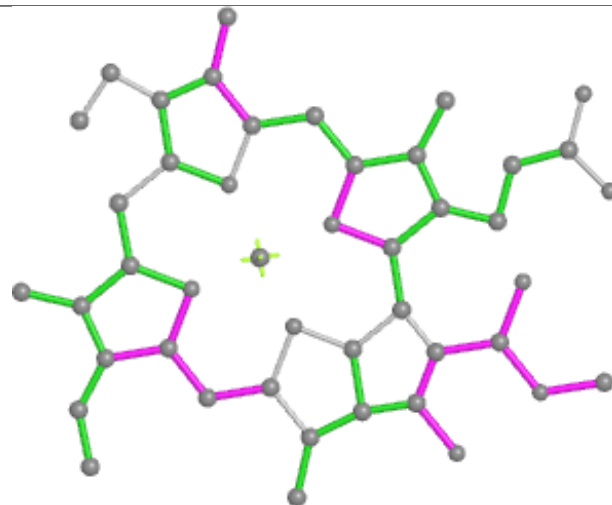
Ligand CLA B 814



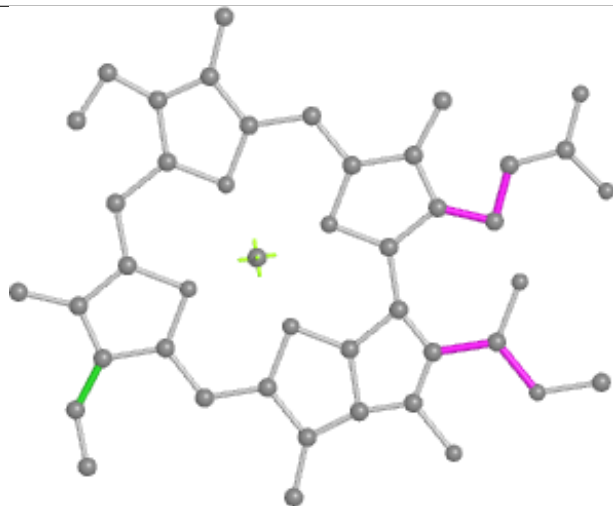
Ligand CLA B 830



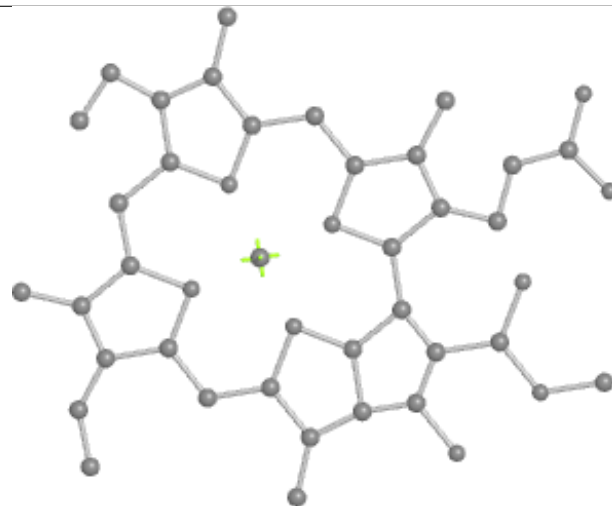
Bond lengths



Bond angles

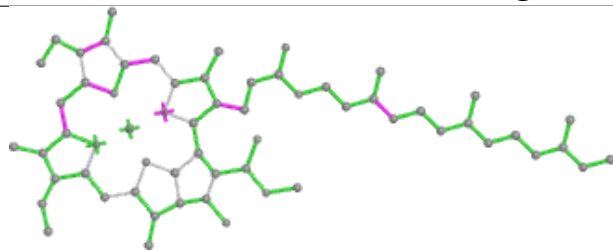


Torsions

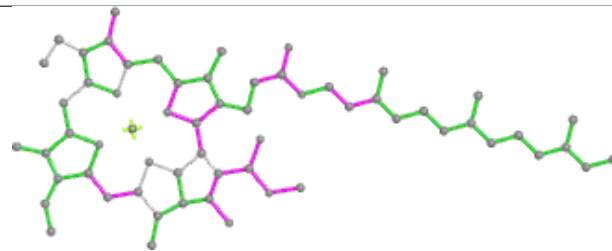


Rings

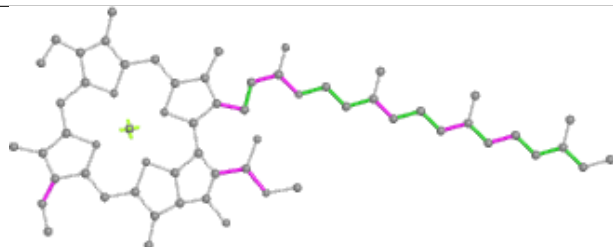
Ligand CLA A 821



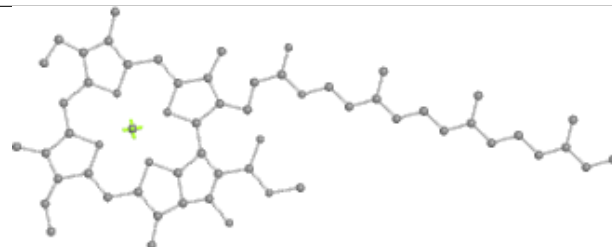
Bond lengths



Bond angles

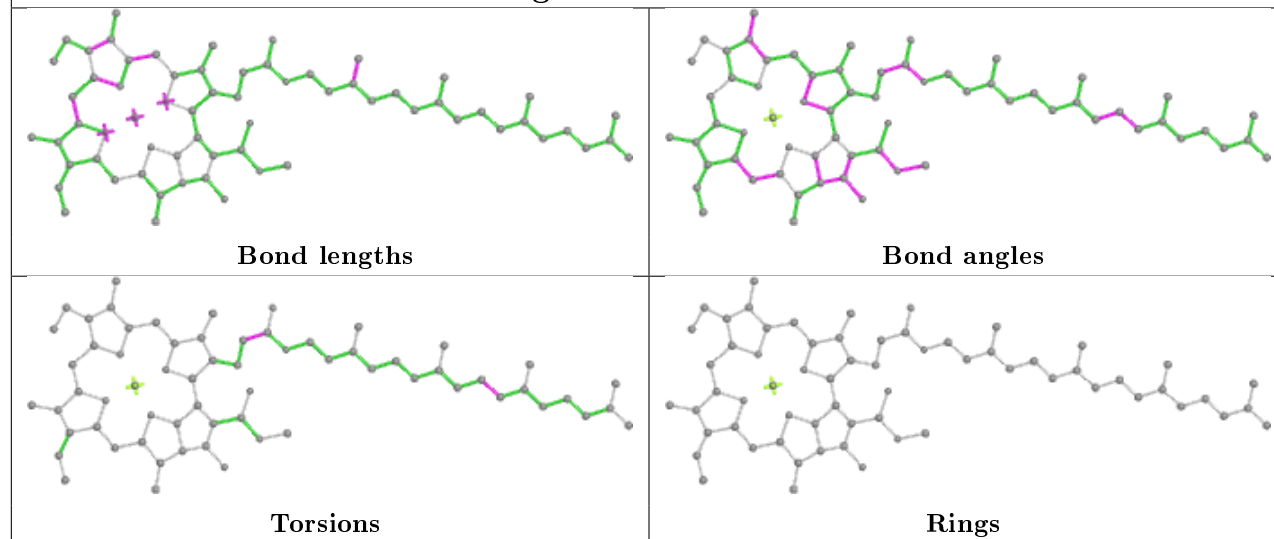


Torsions

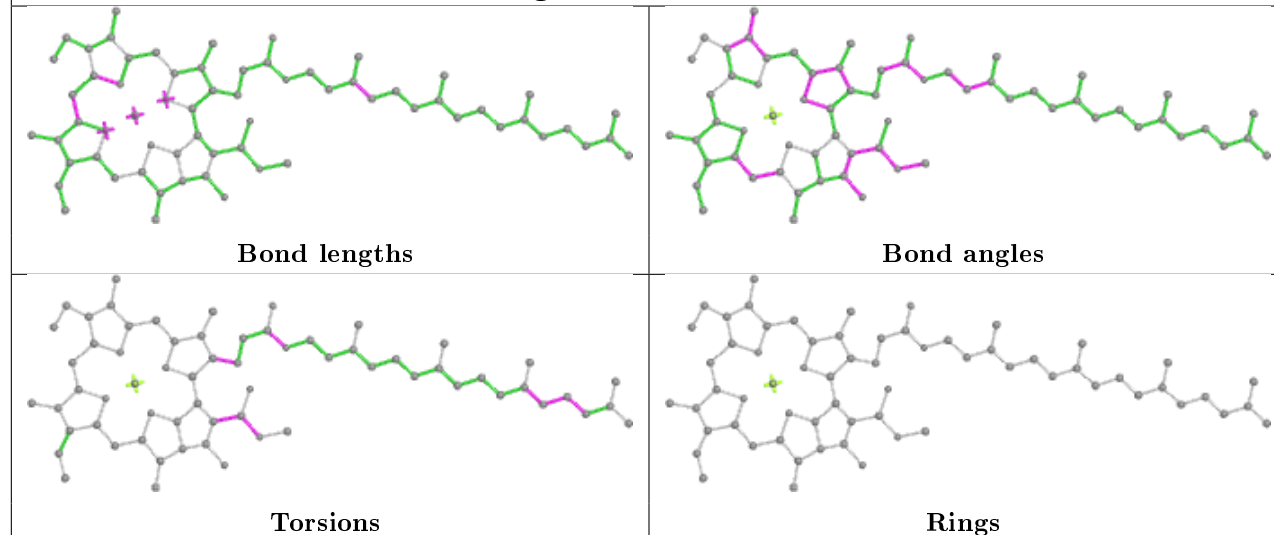


Rings

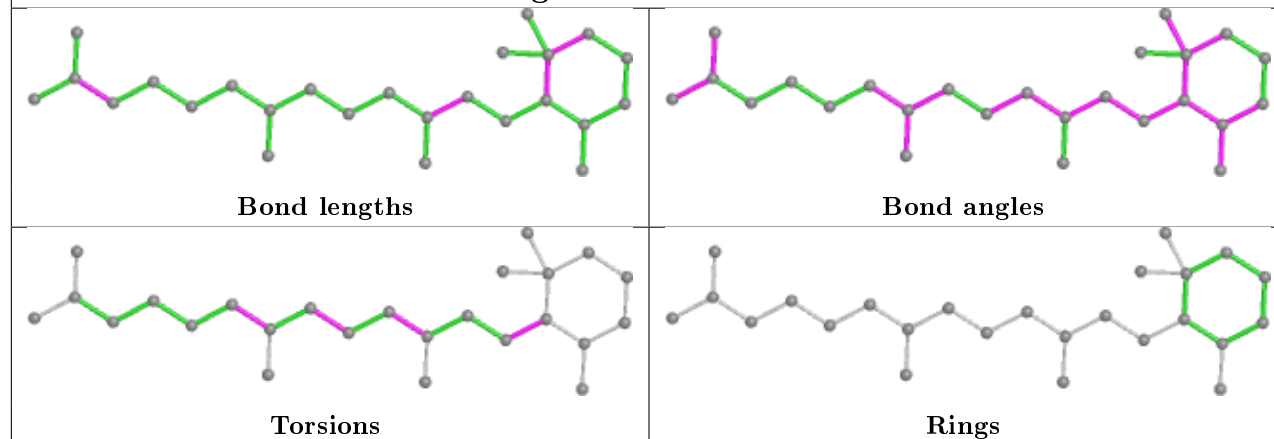
Ligand CLA B 803



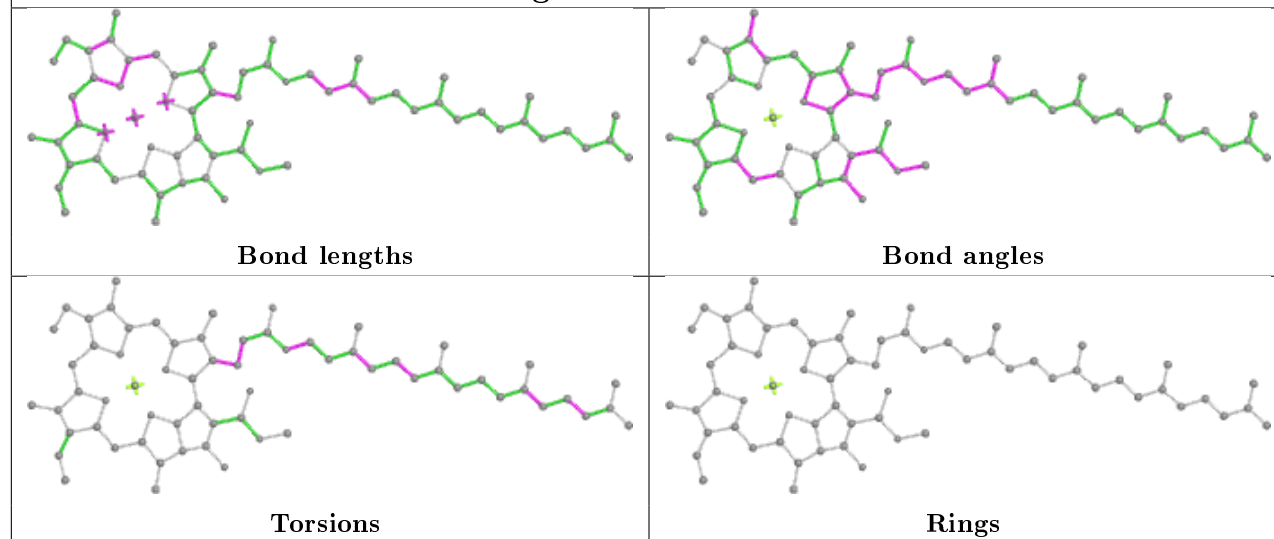
Ligand CLA B 805



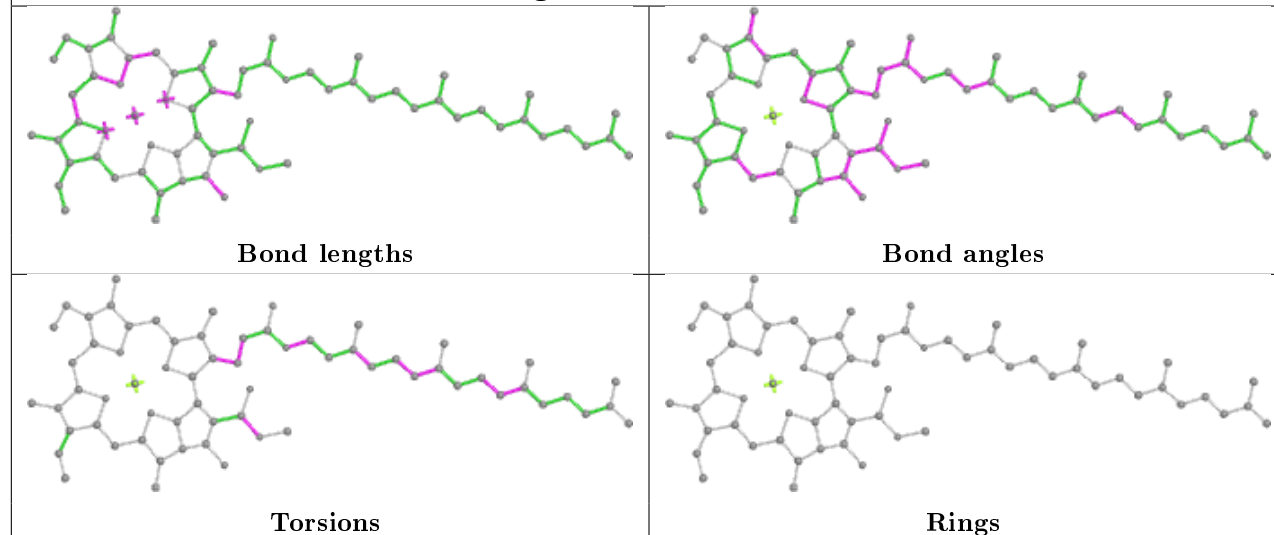
Ligand BCR B 846



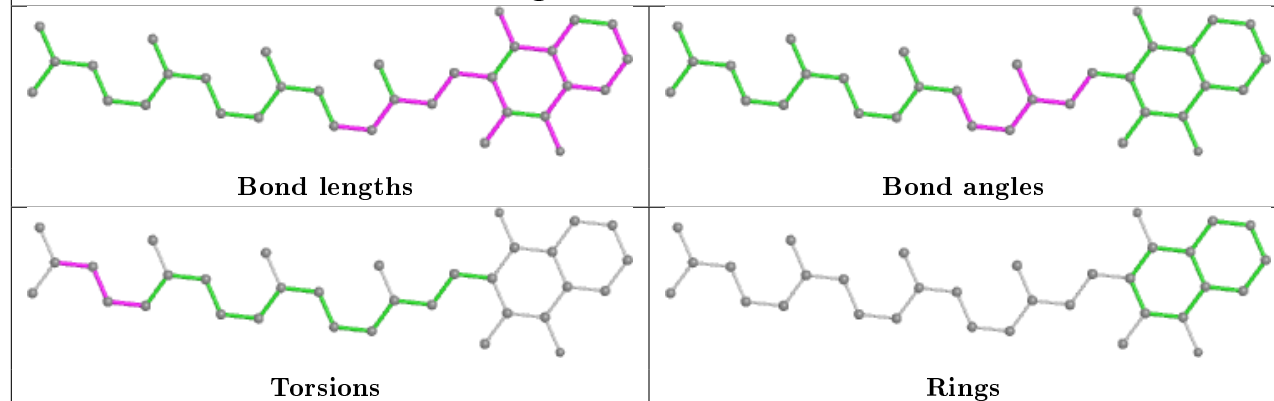
Ligand CLA B 828

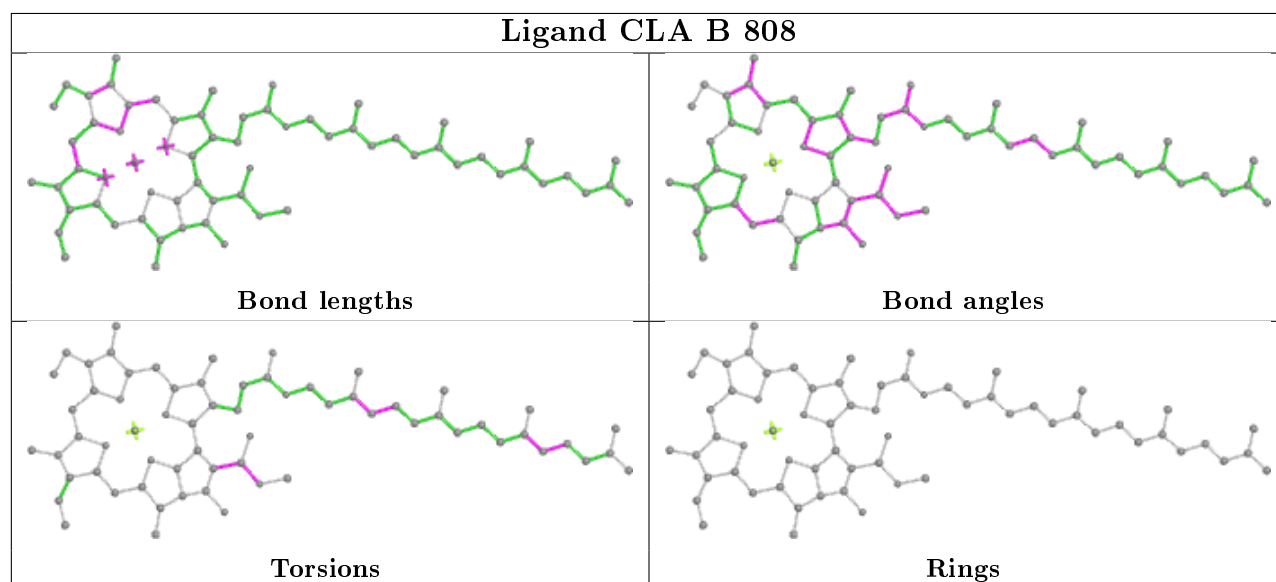
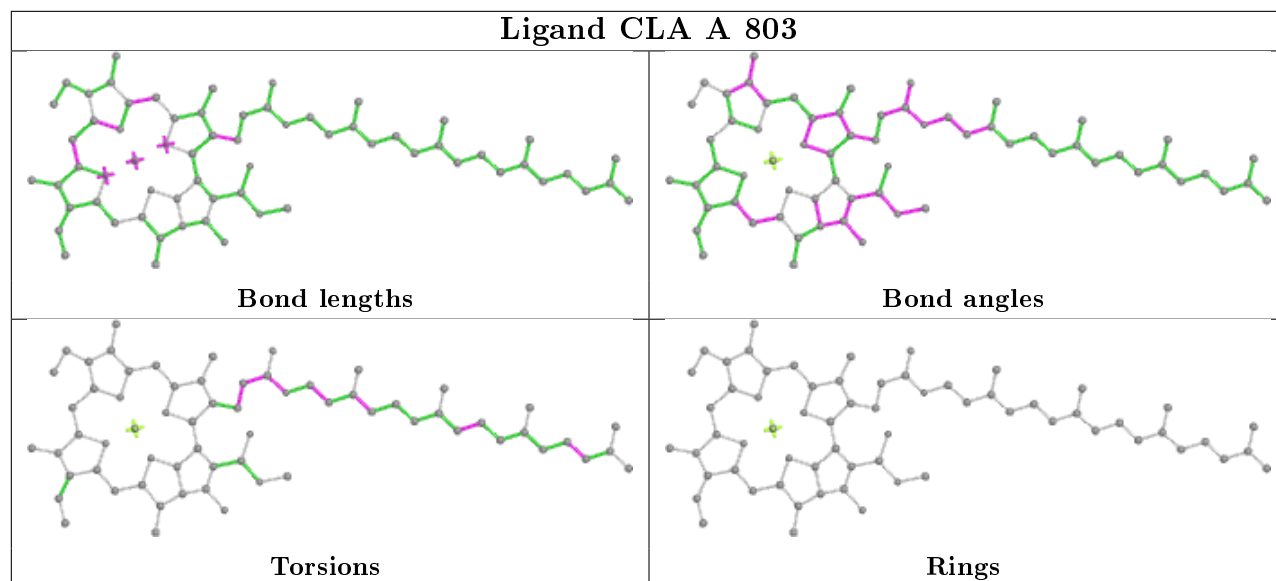
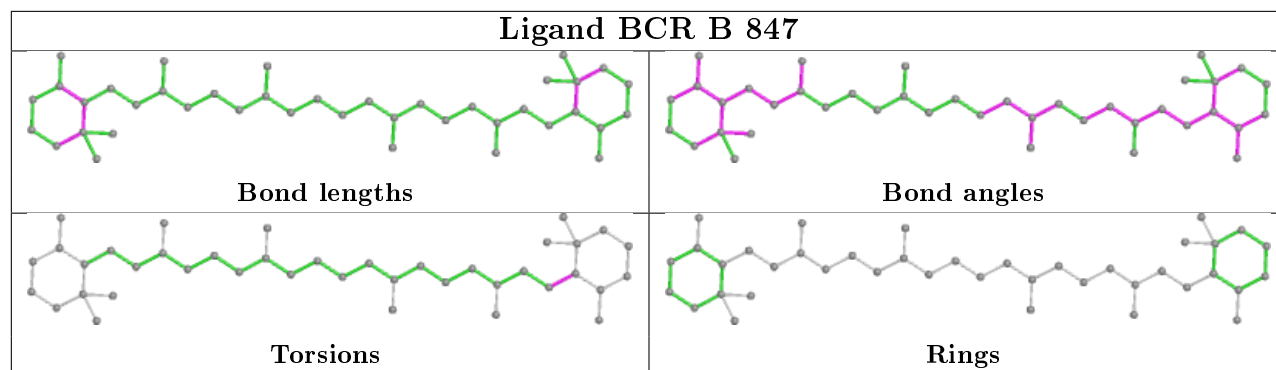


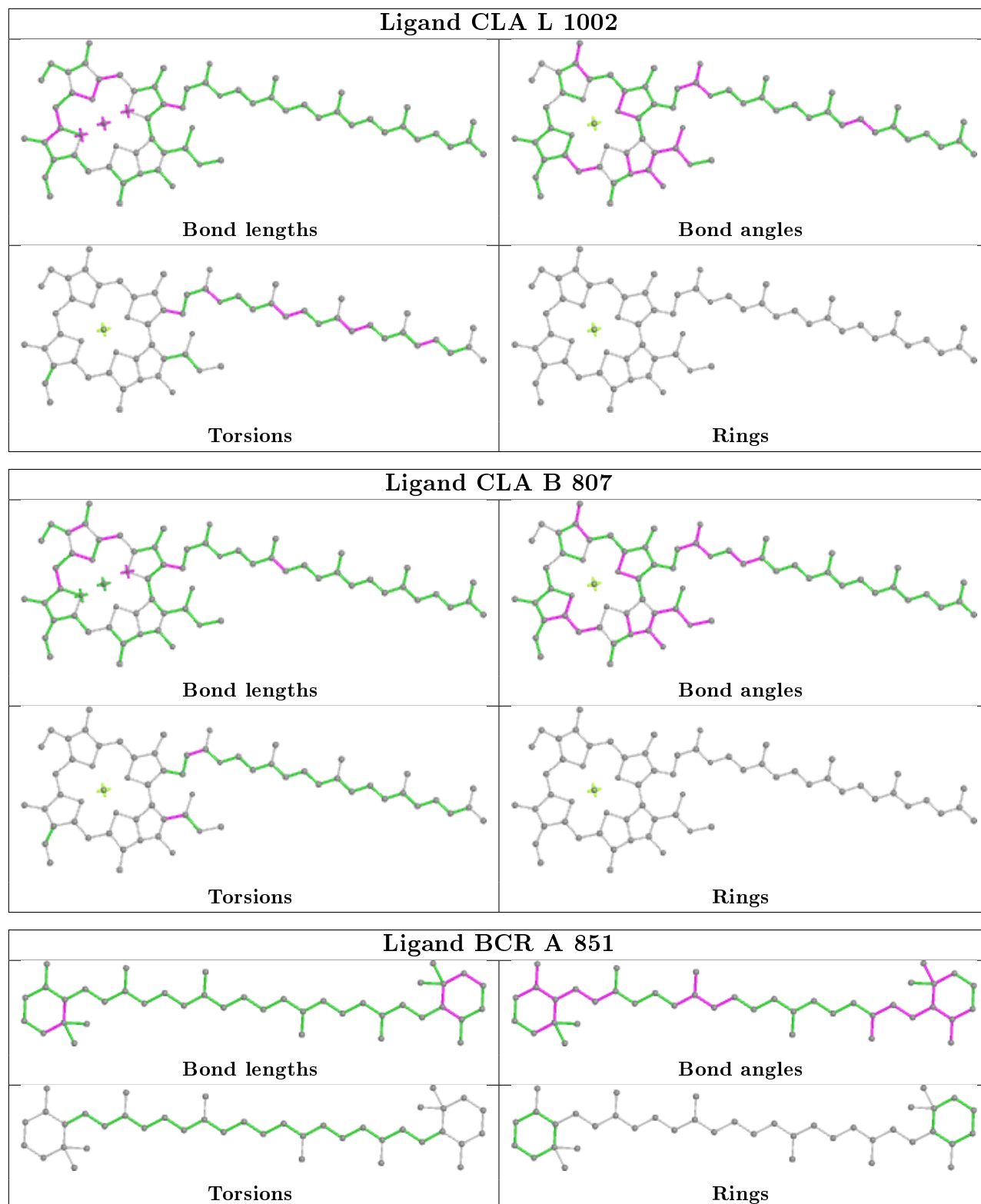
Ligand CLA B 827



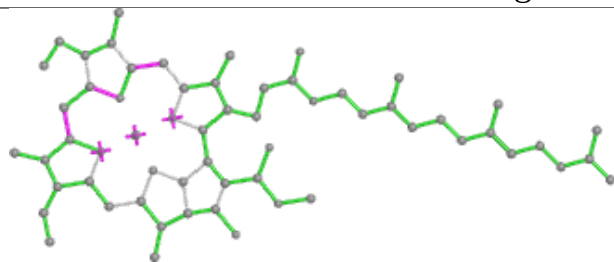
Ligand PQN B 842



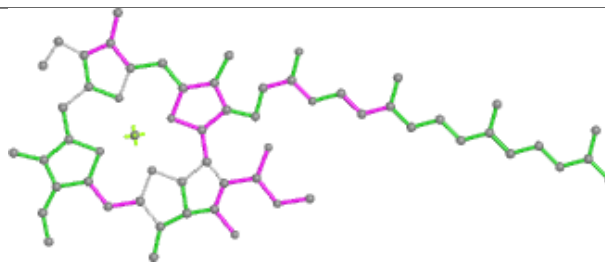




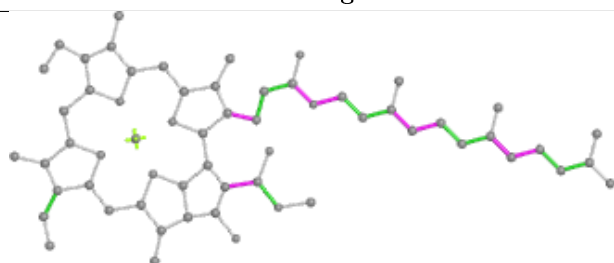
Ligand CLA A 814



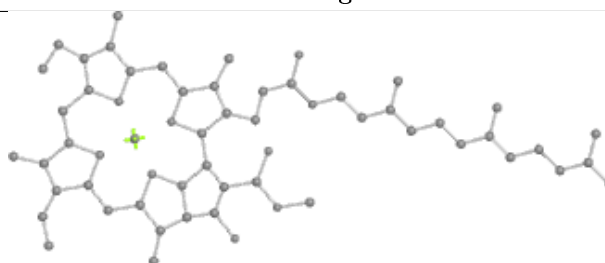
Bond lengths



Bond angles

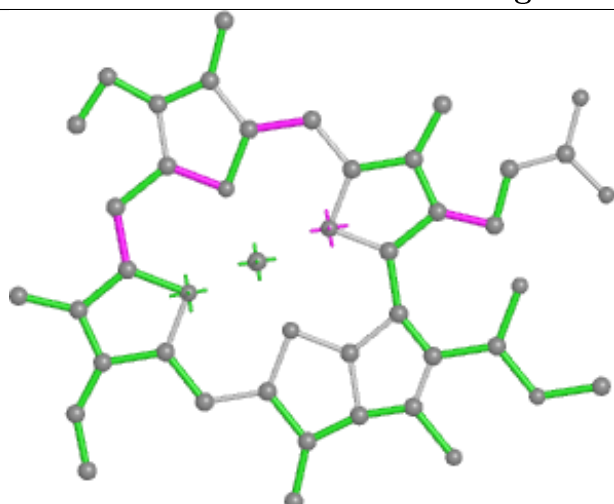


Torsions

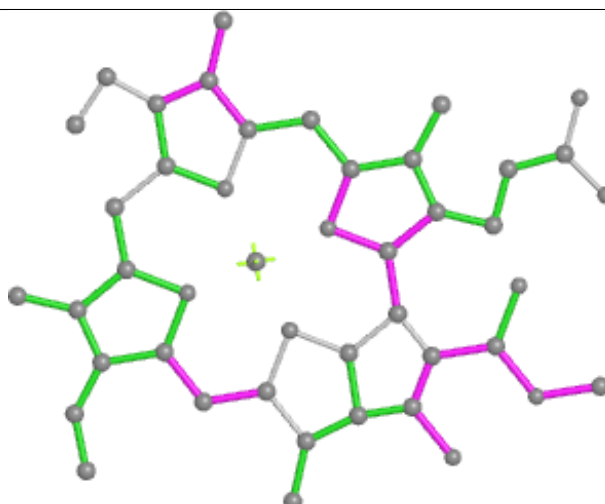


Rings

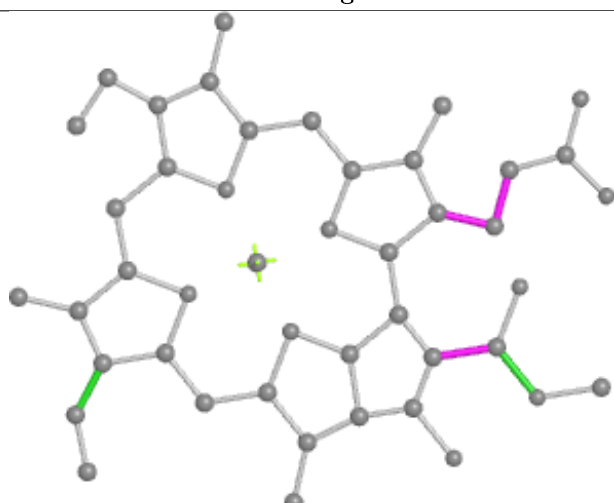
Ligand CLA A 837



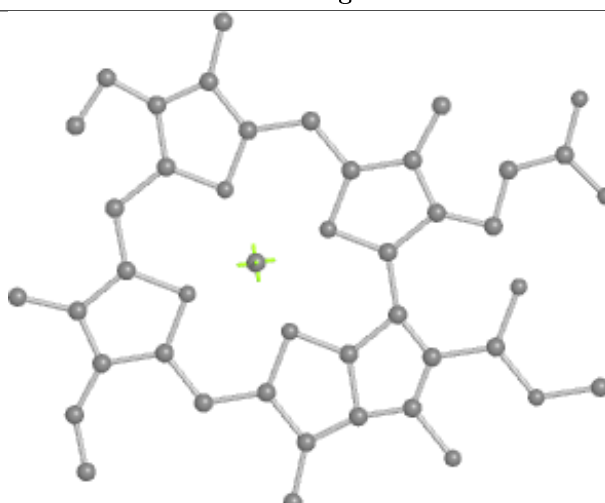
Bond lengths



Bond angles

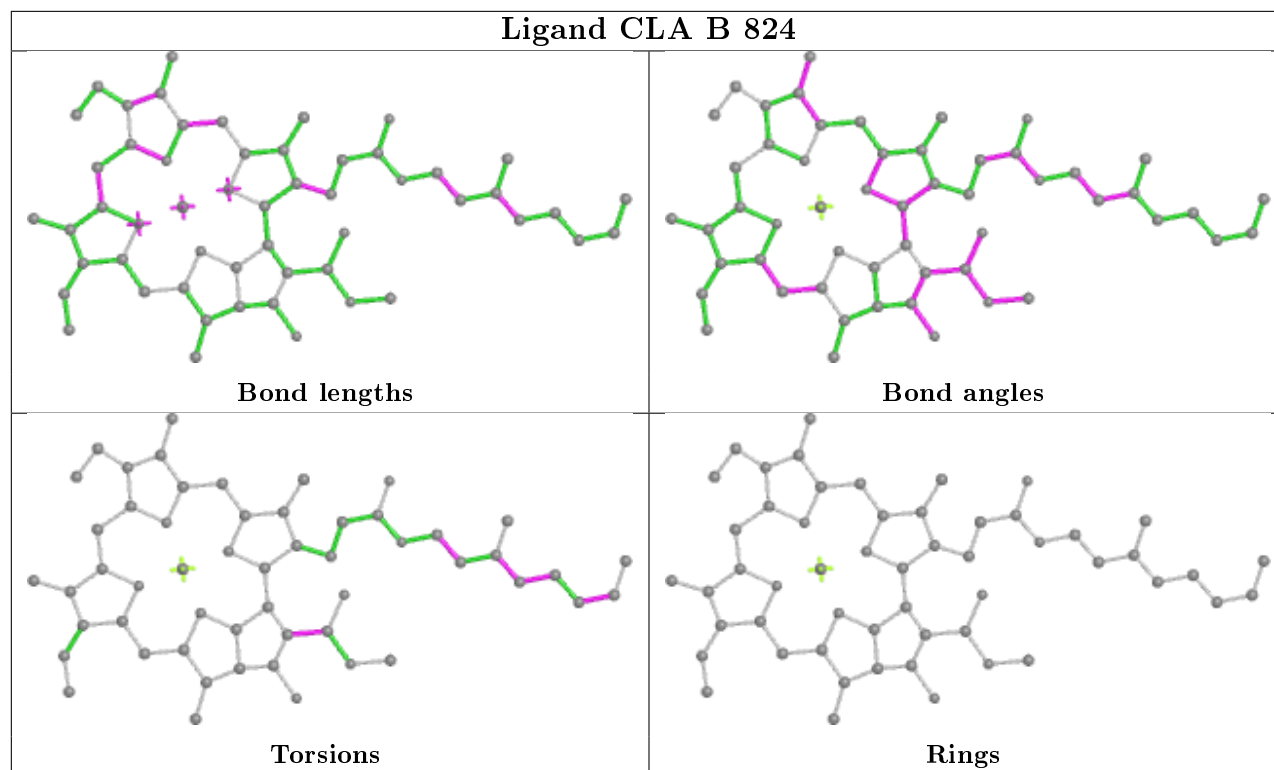


Torsions

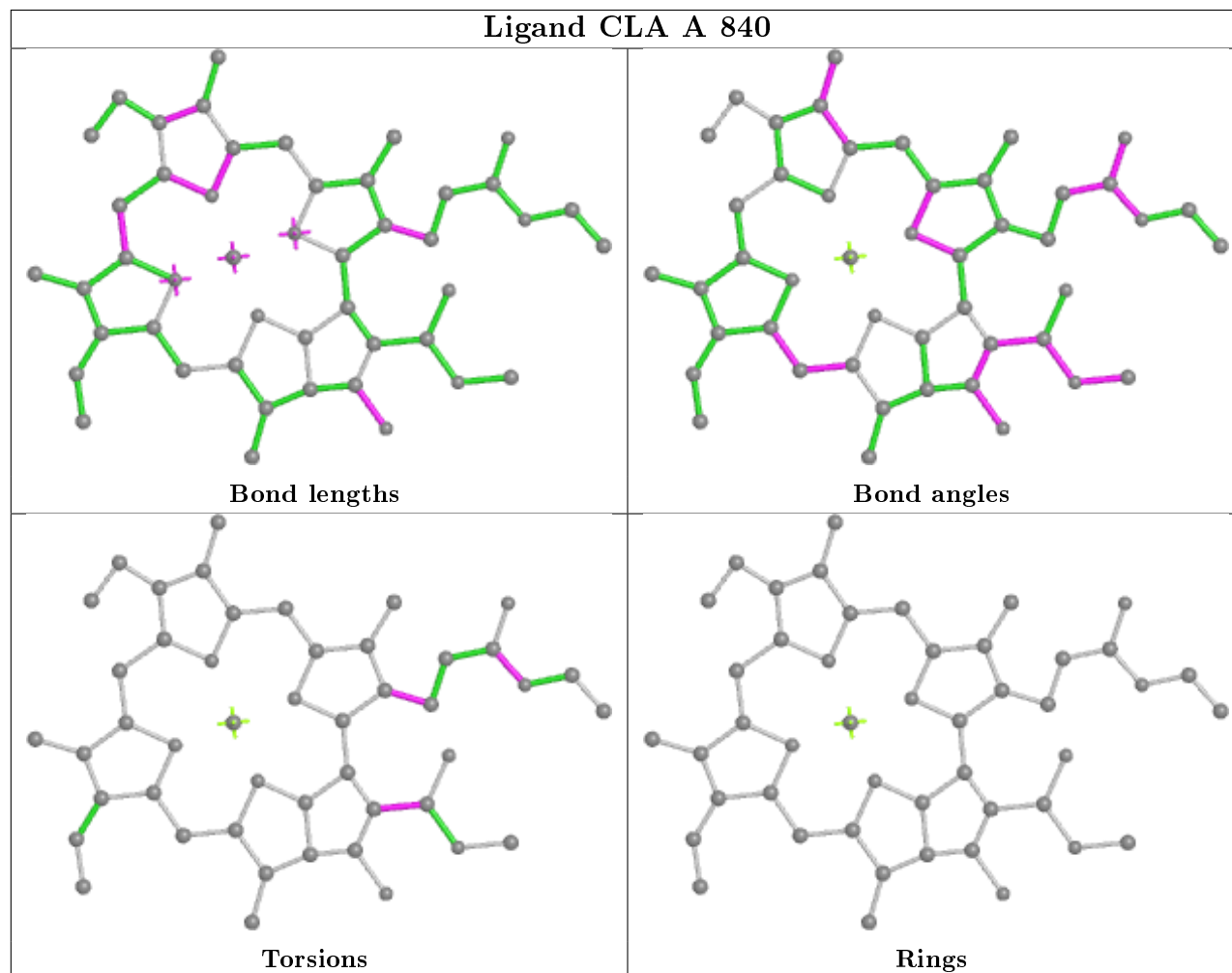


Rings

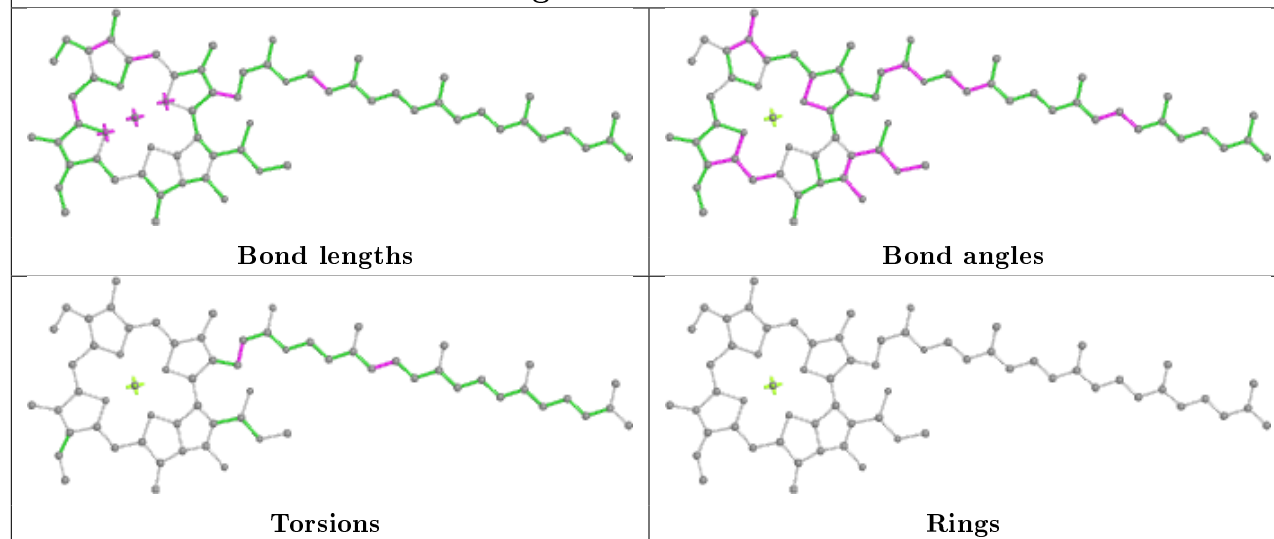
Ligand CLA B 824



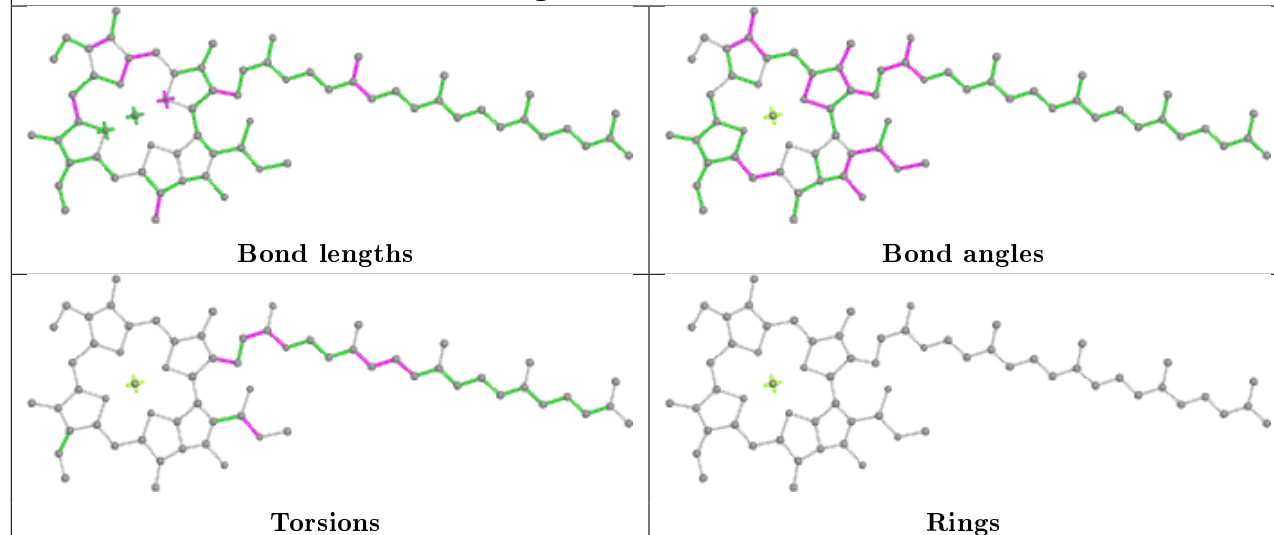
Ligand CLA A 840



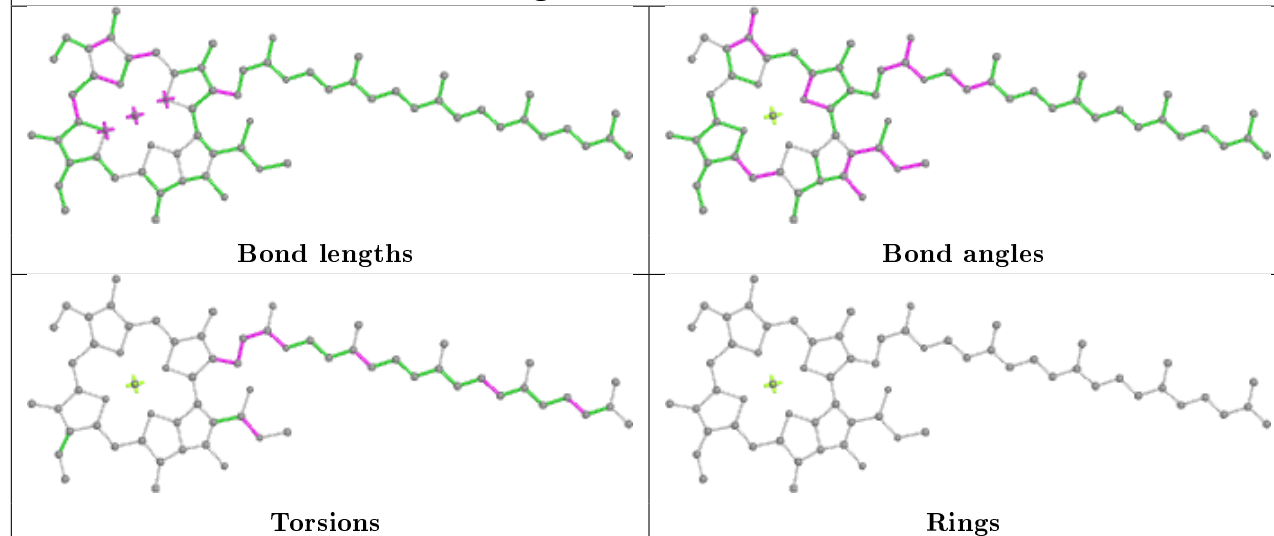
Ligand CLA B 840



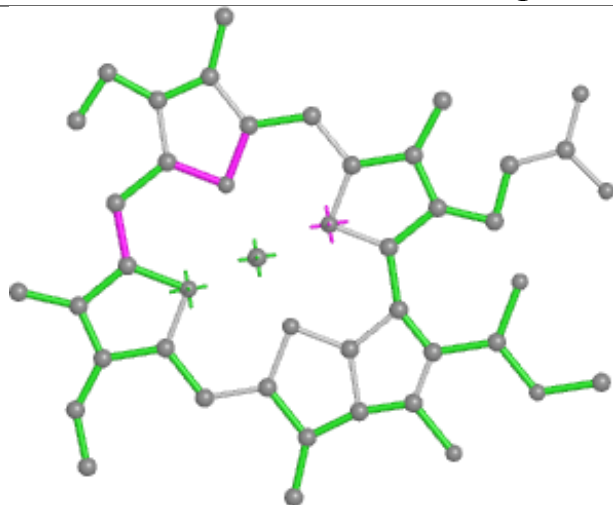
Ligand CLA A 844



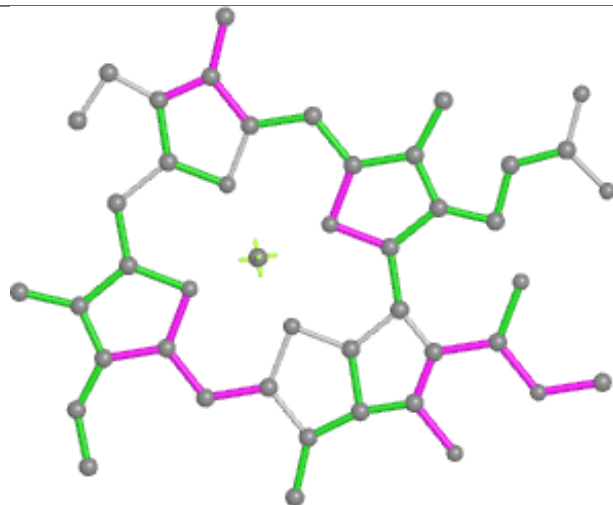
Ligand CLA A 812



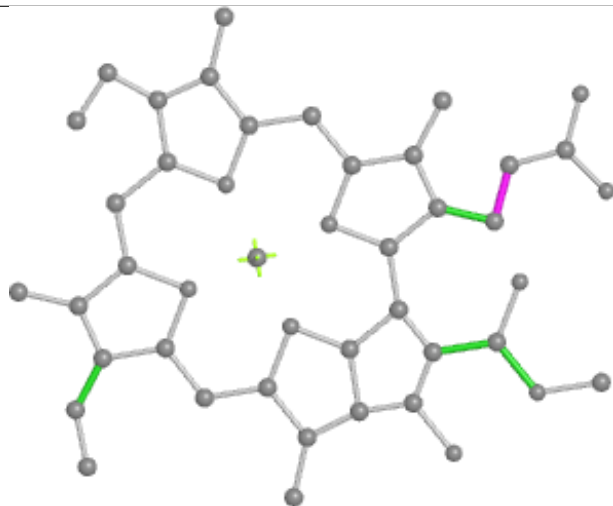
Ligand CLA B 812



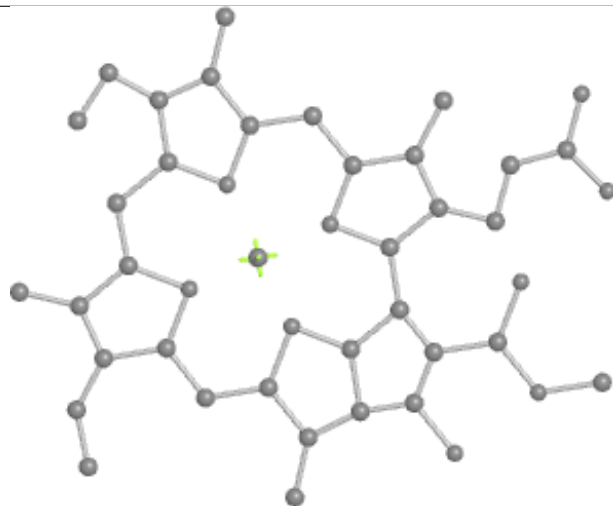
Bond lengths



Bond angles

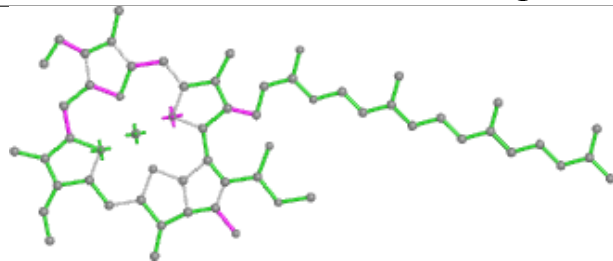


Torsions

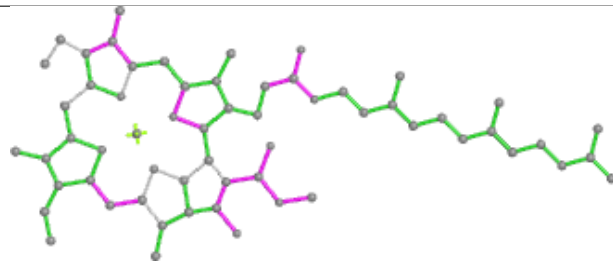


Rings

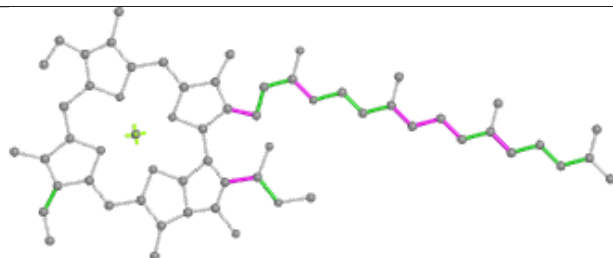
Ligand CLA B 818



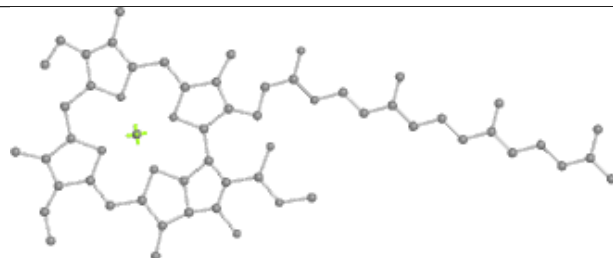
Bond lengths



Bond angles

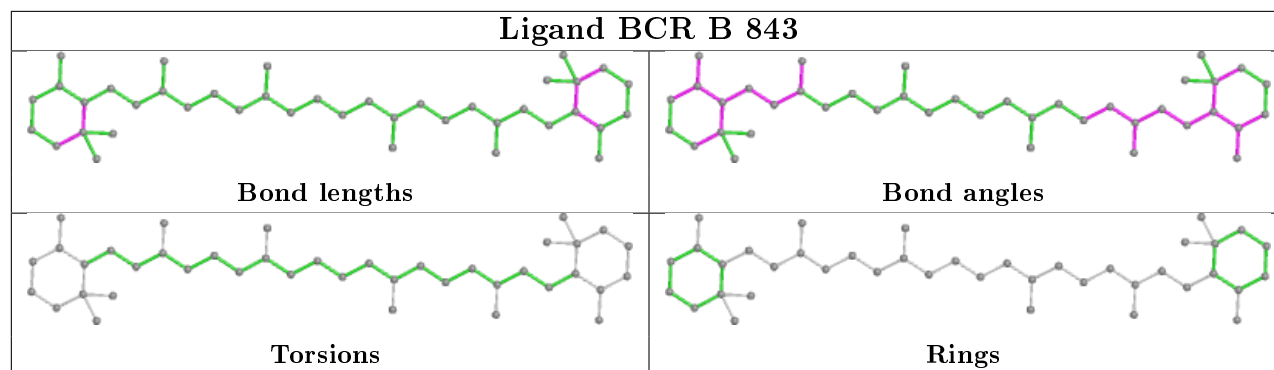


Torsions

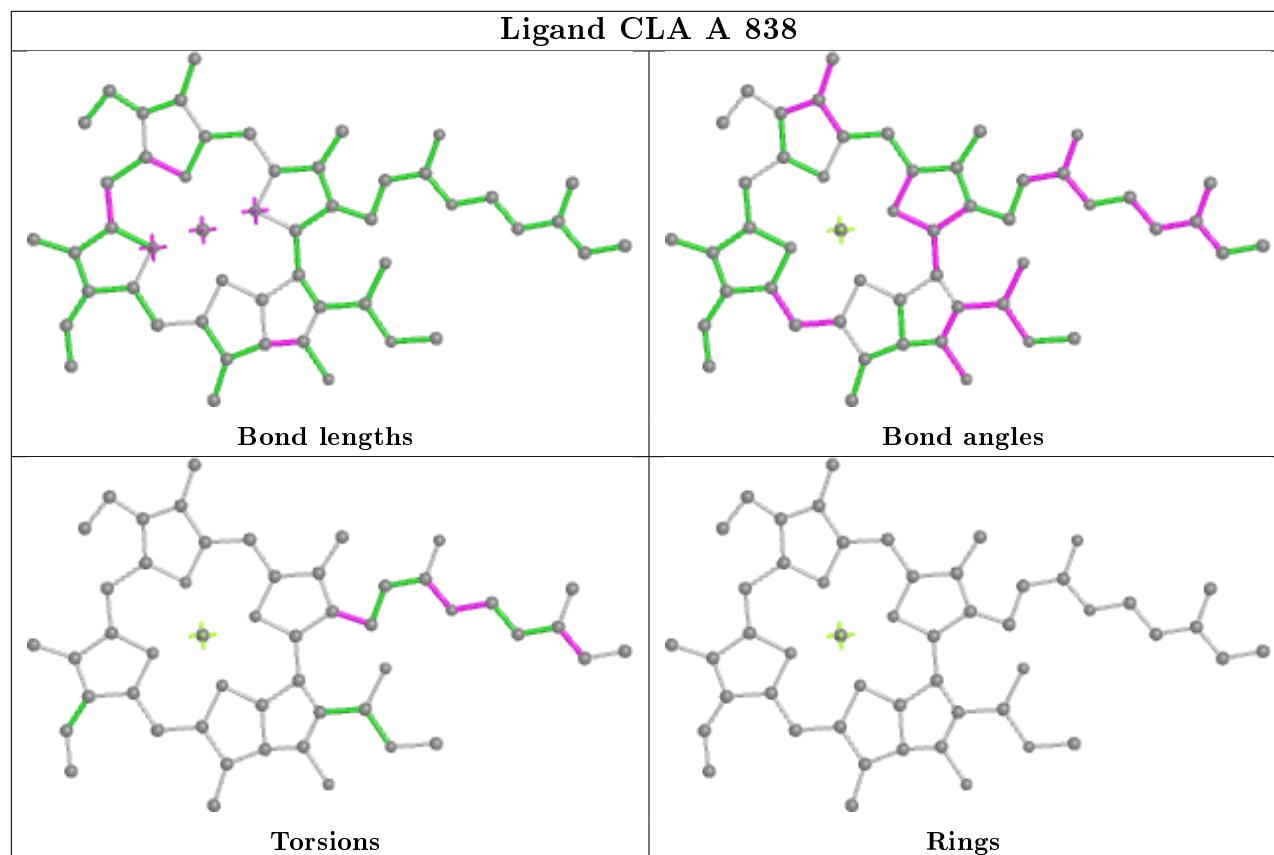


Rings

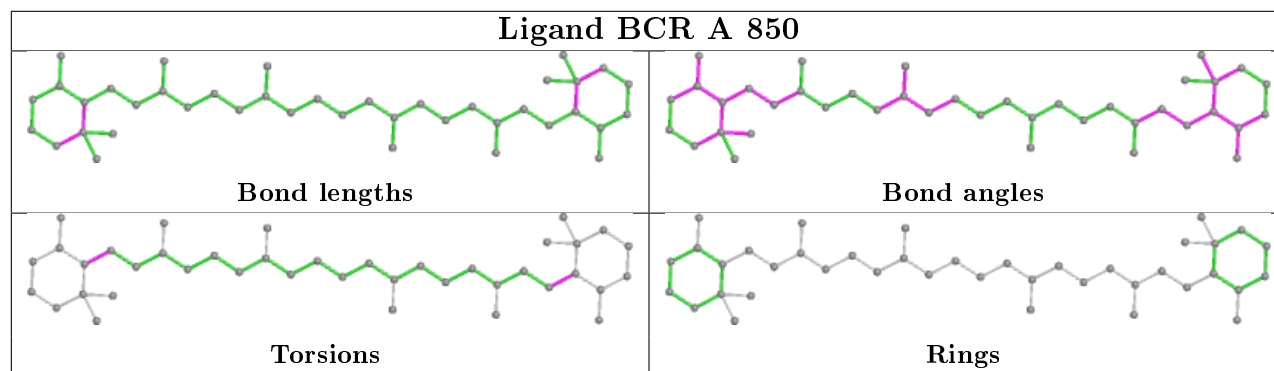
Ligand BCR B 843



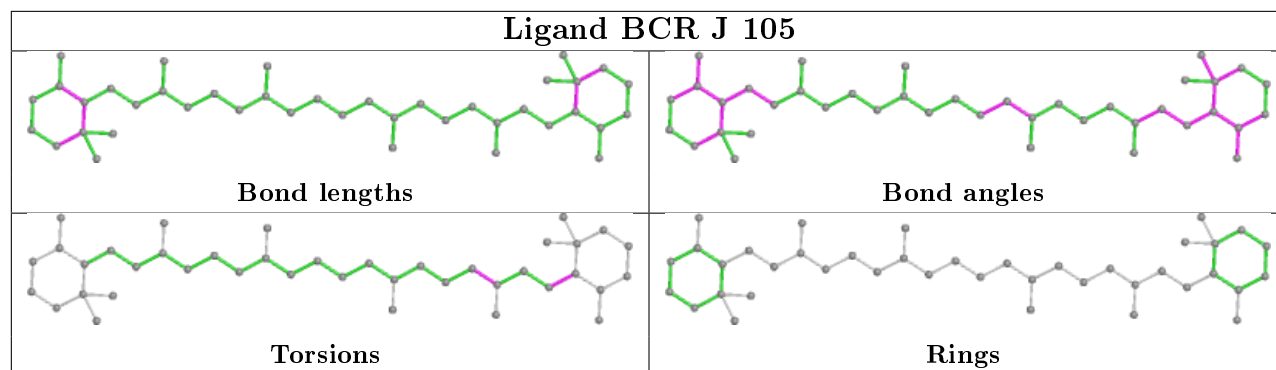
Ligand CLA A 838



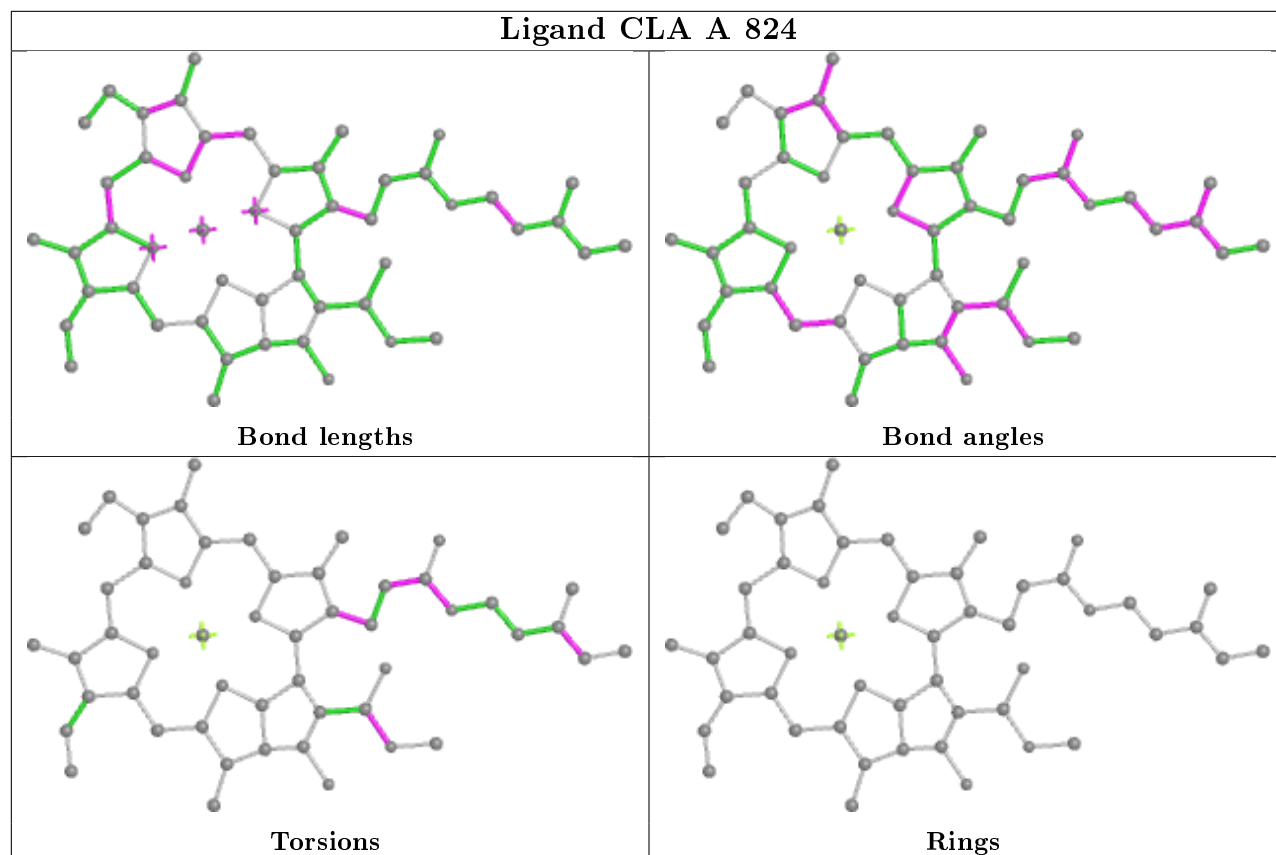
Ligand BCR A 850



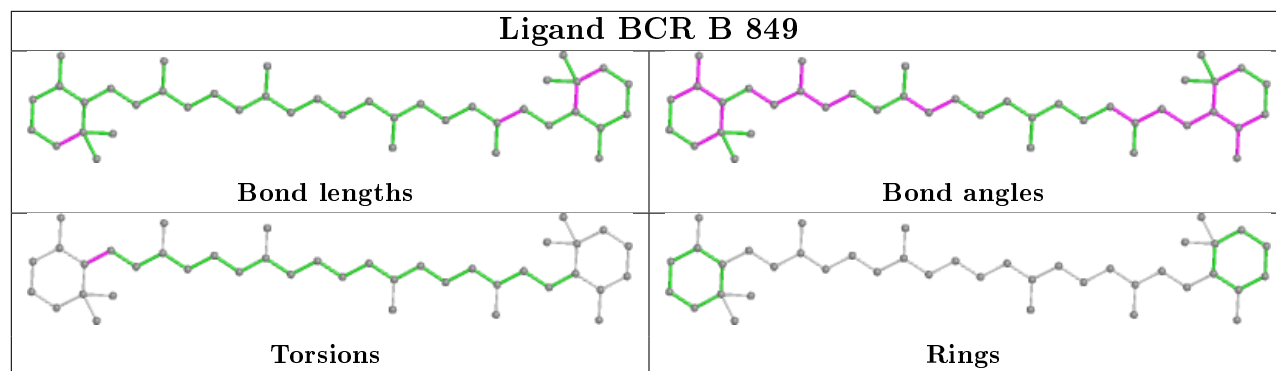
Ligand BCR J 105



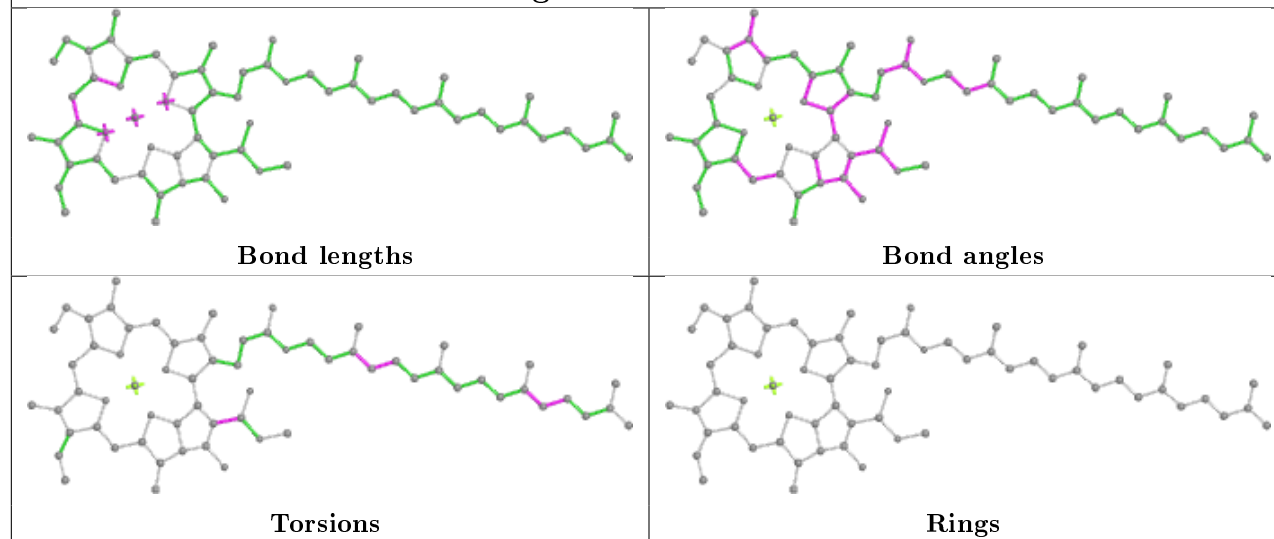
Ligand CLA A 824



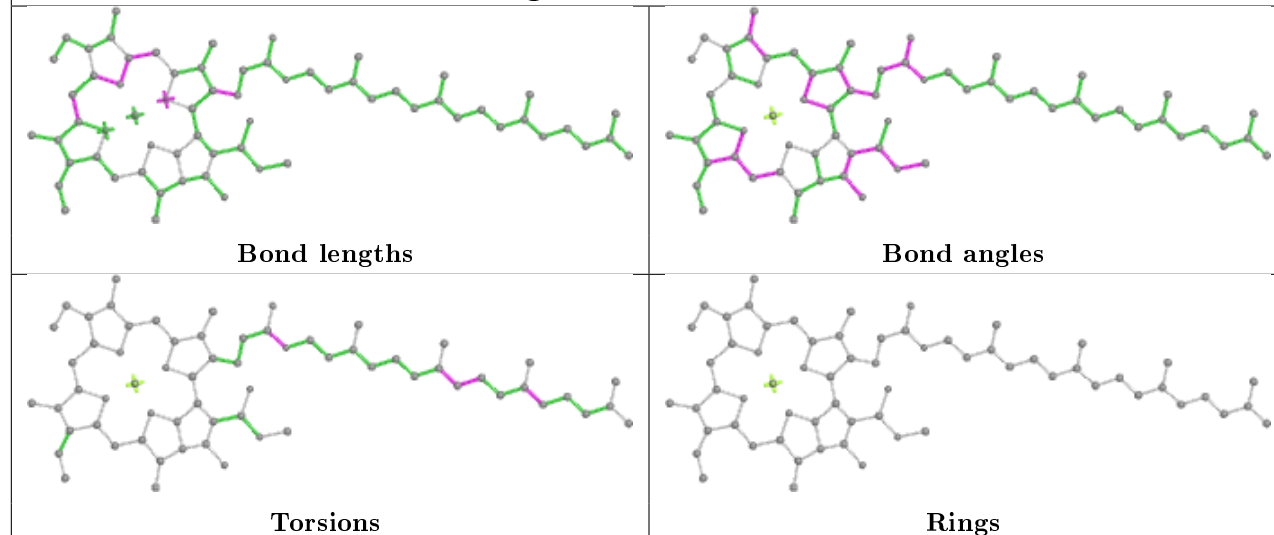
Ligand BCR B 849



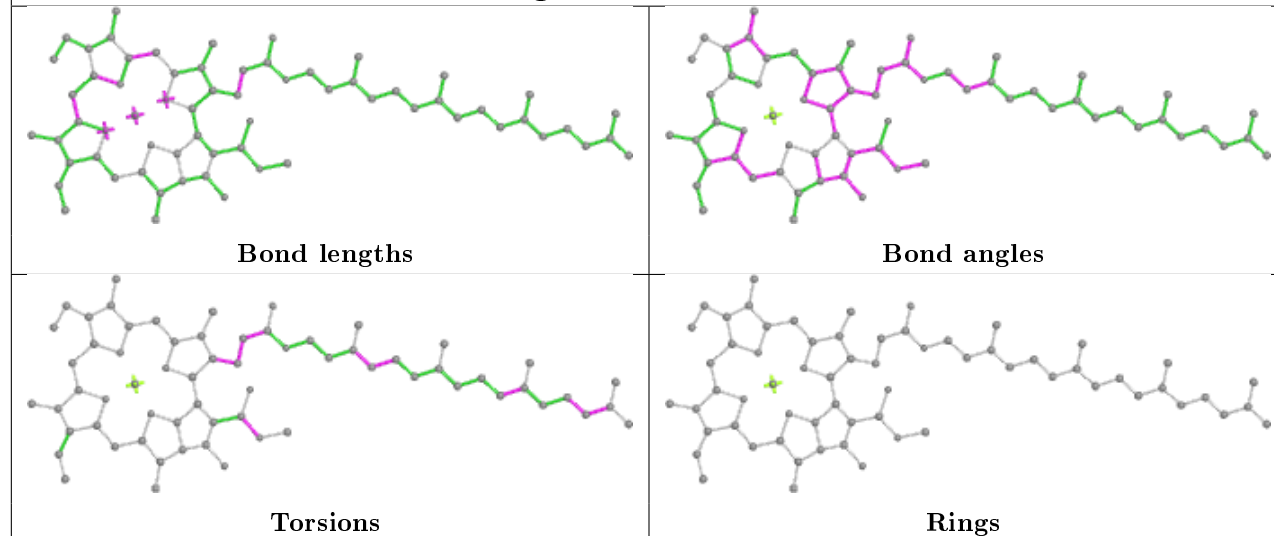
Ligand CLA B 802



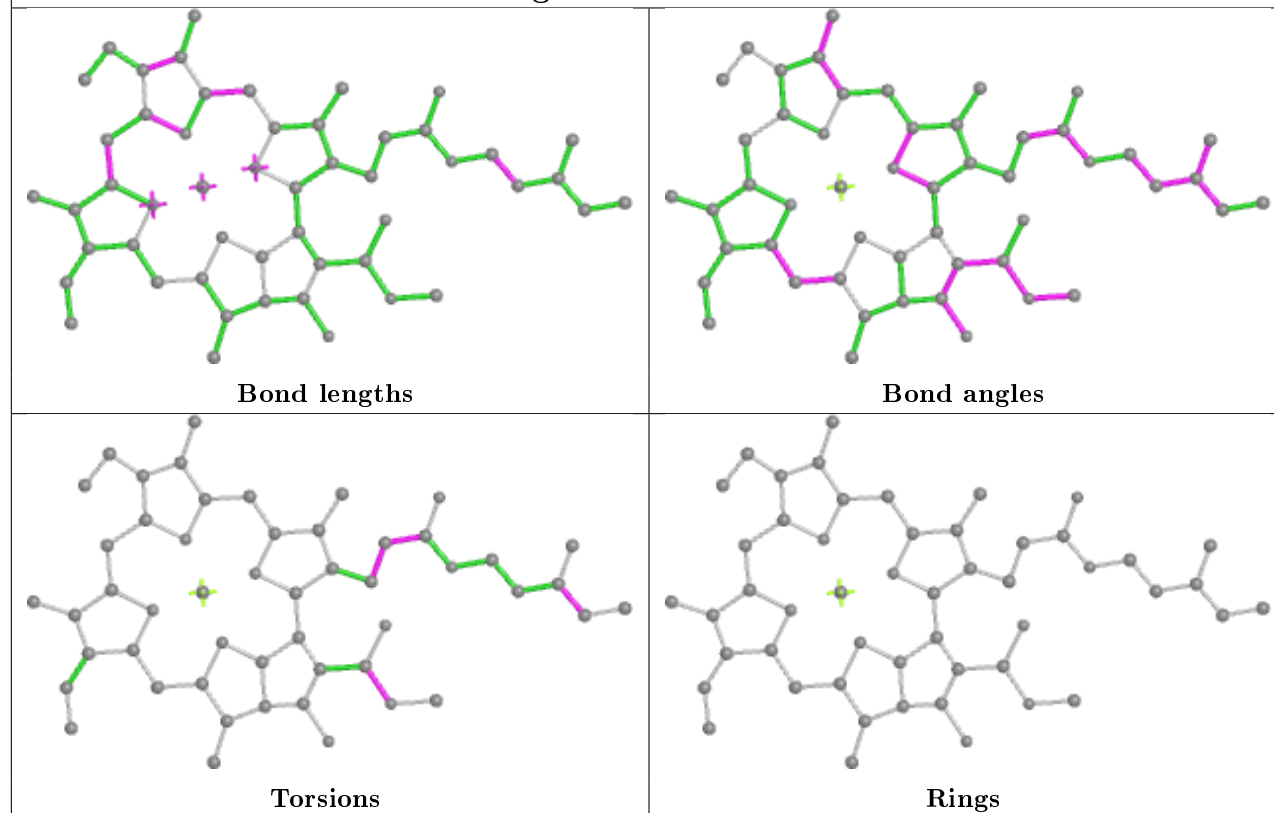
Ligand CLA L 1003



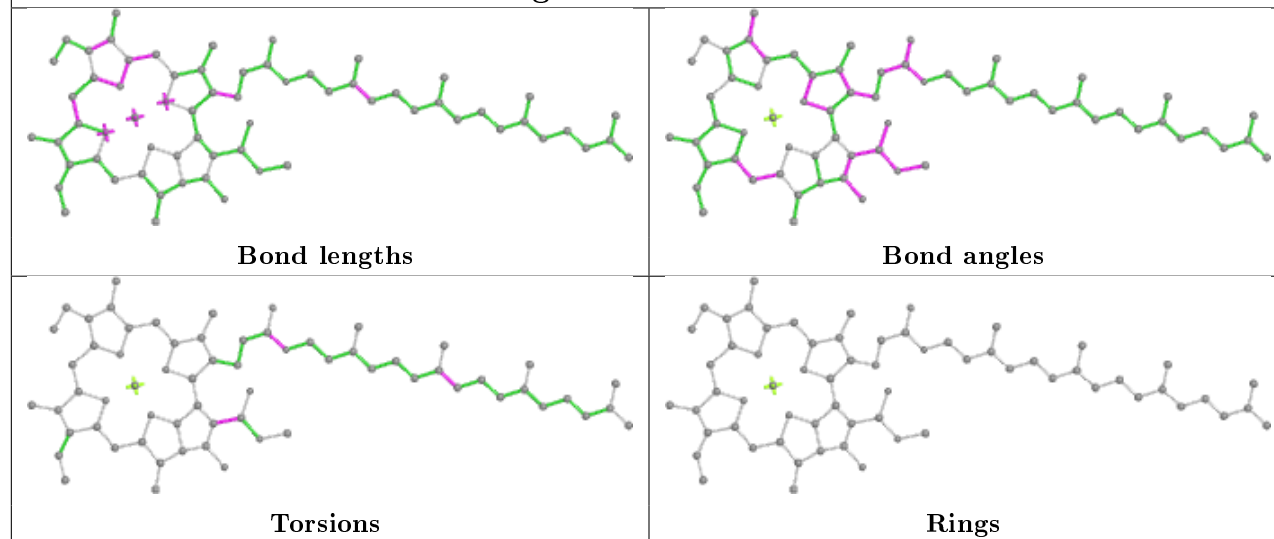
Ligand CLA A 807

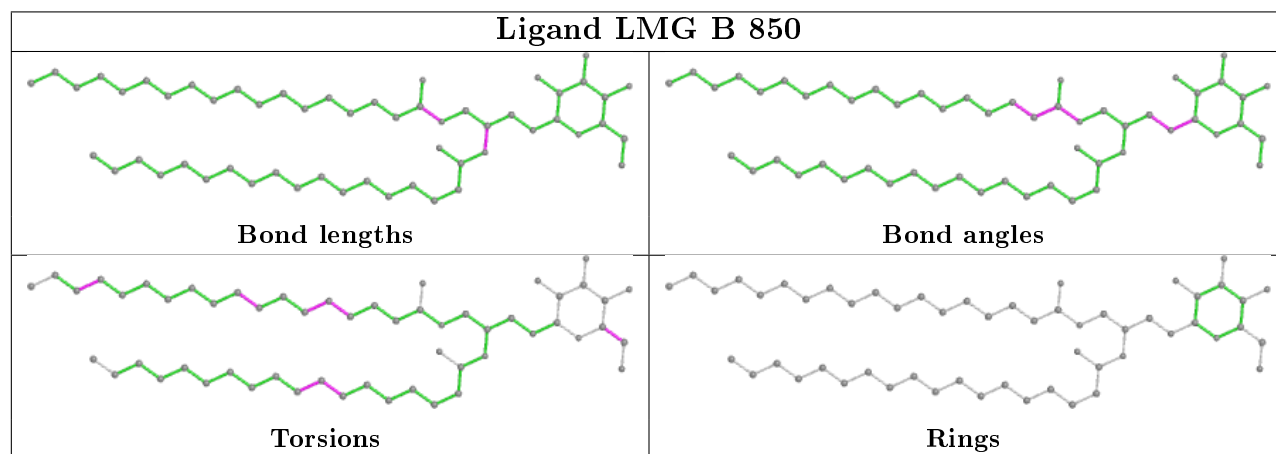
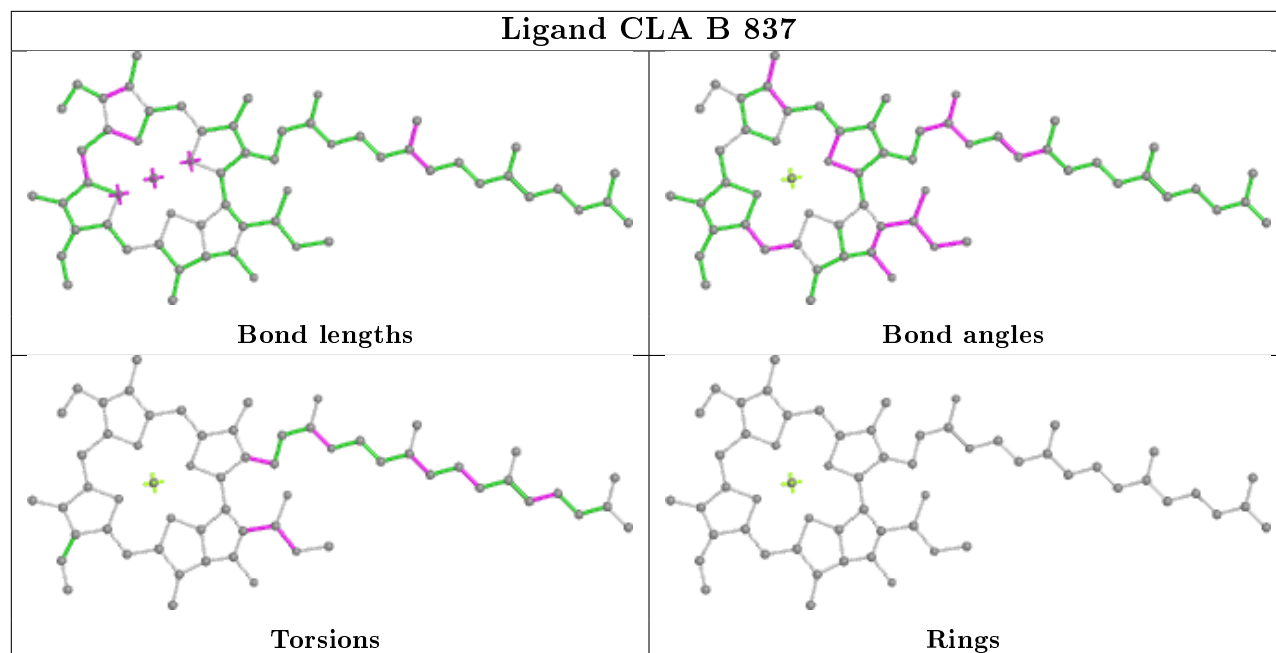


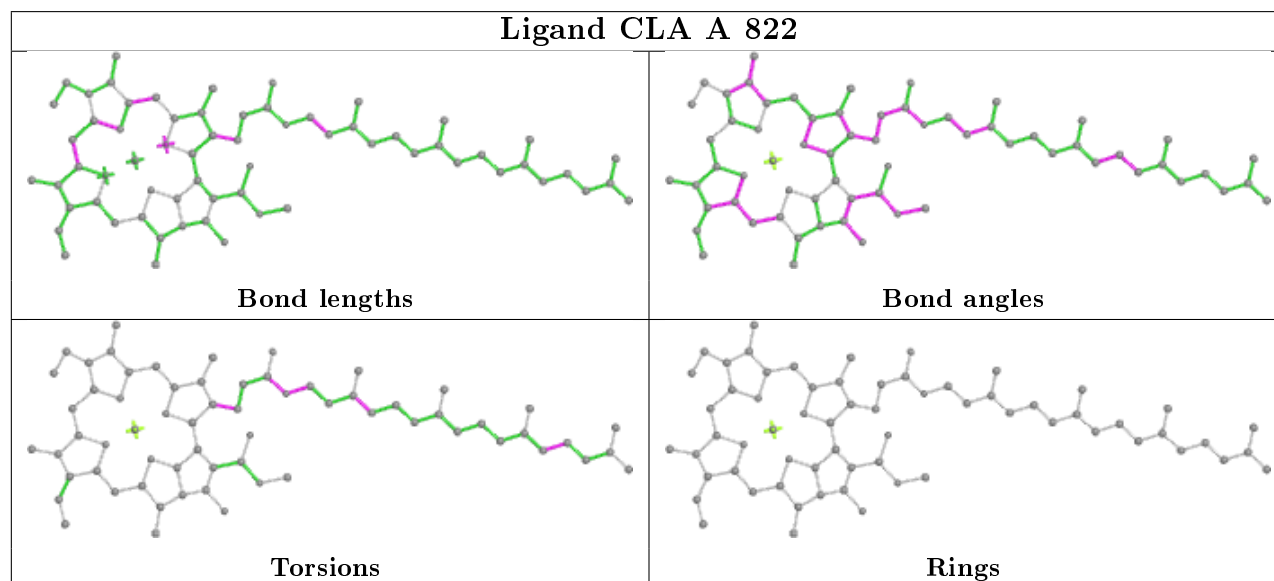
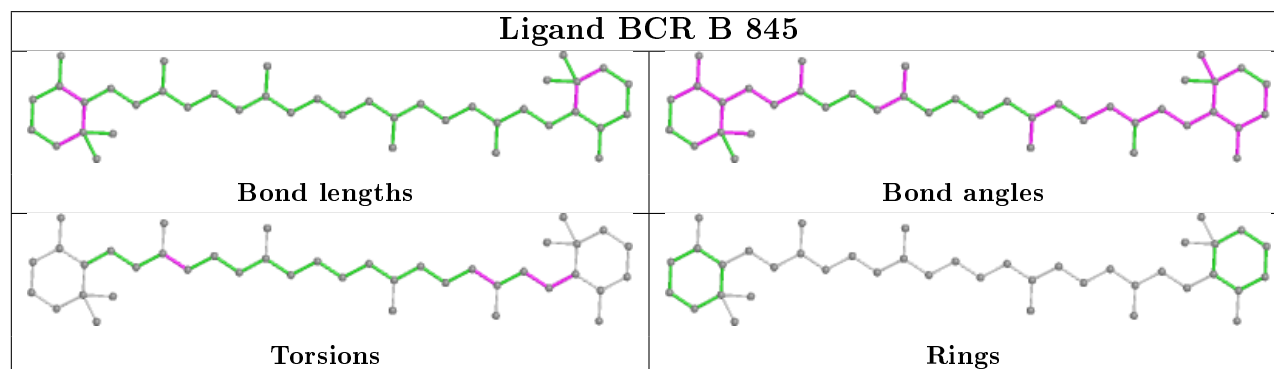
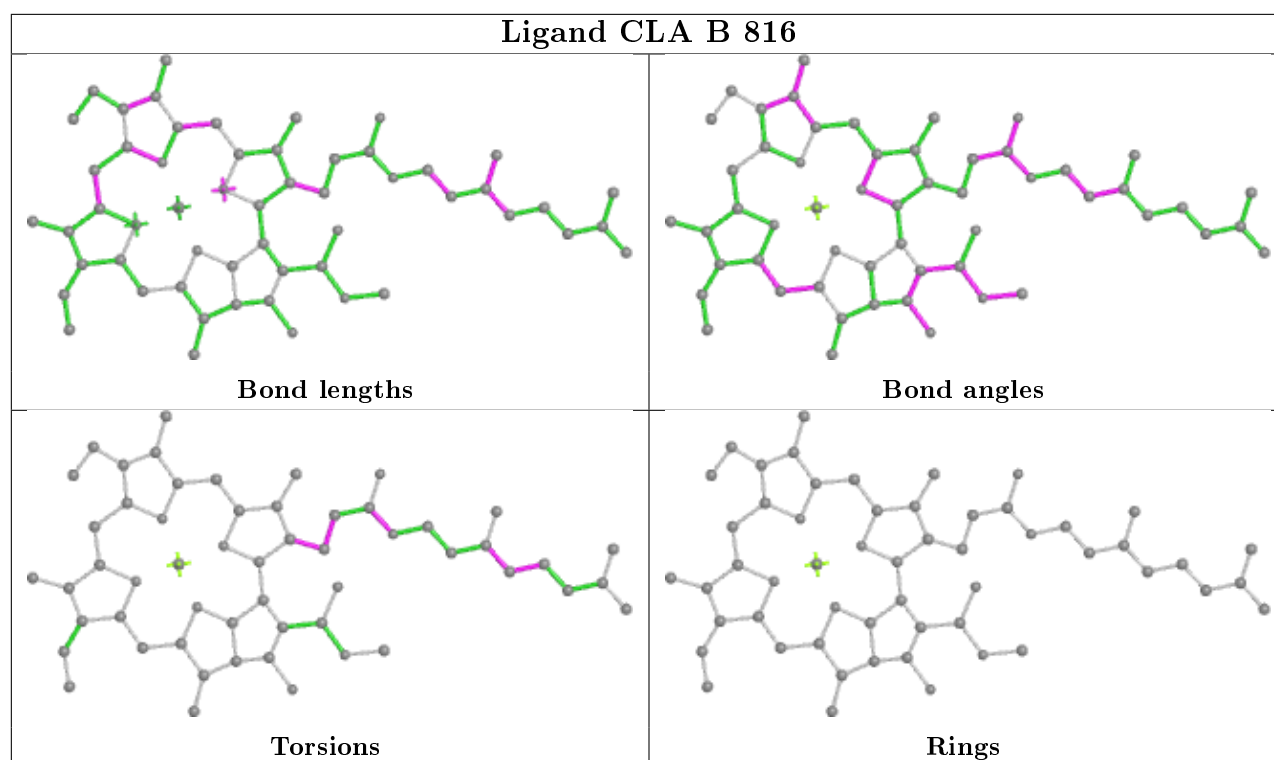
Ligand CLA A 808



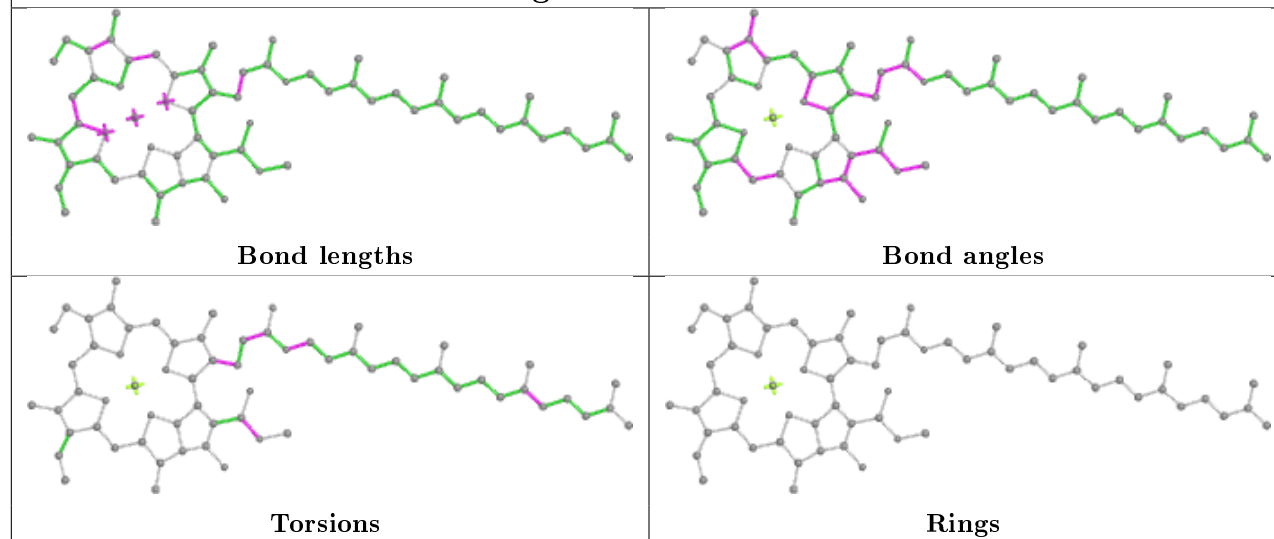
Ligand CLA A 831



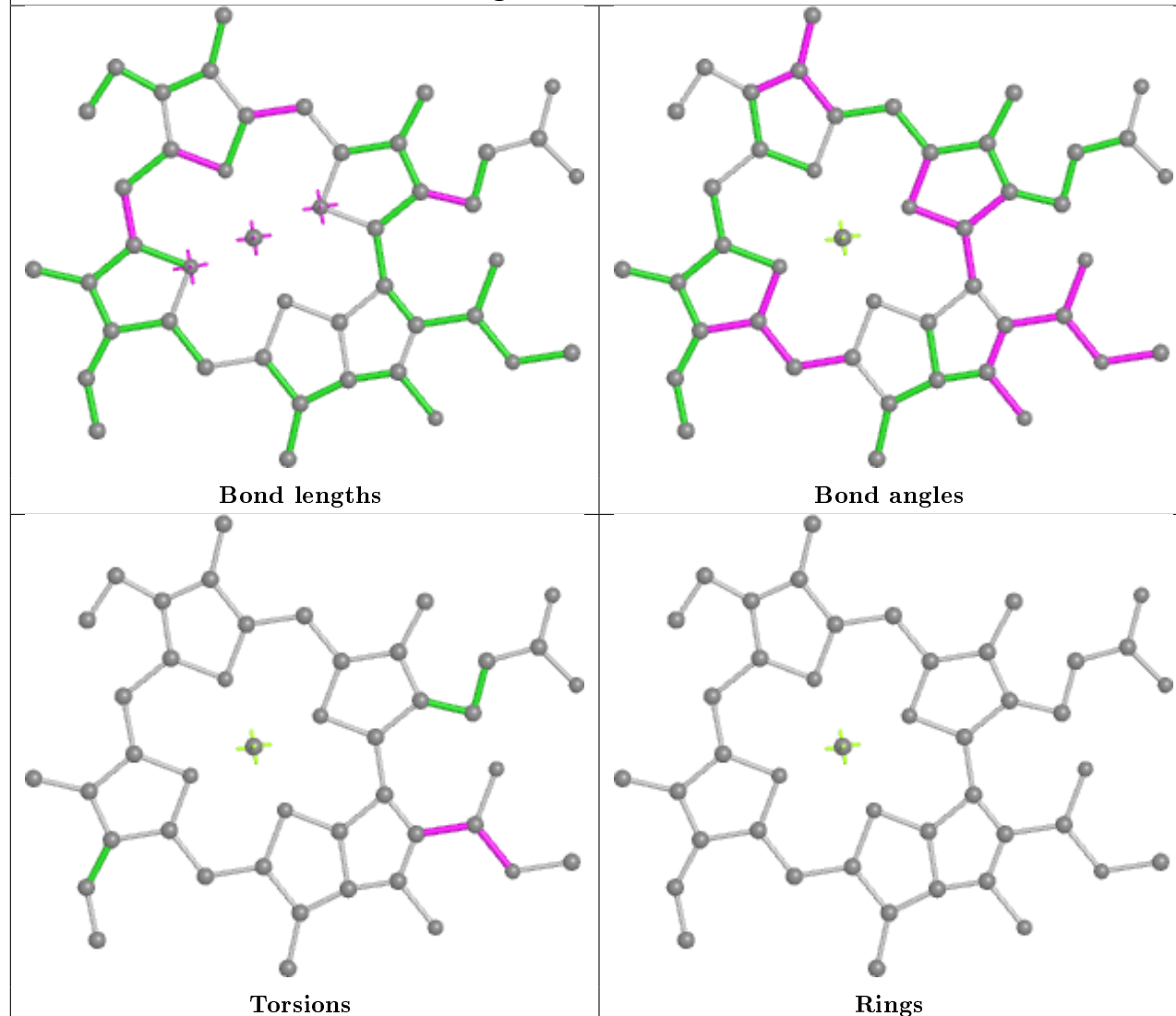




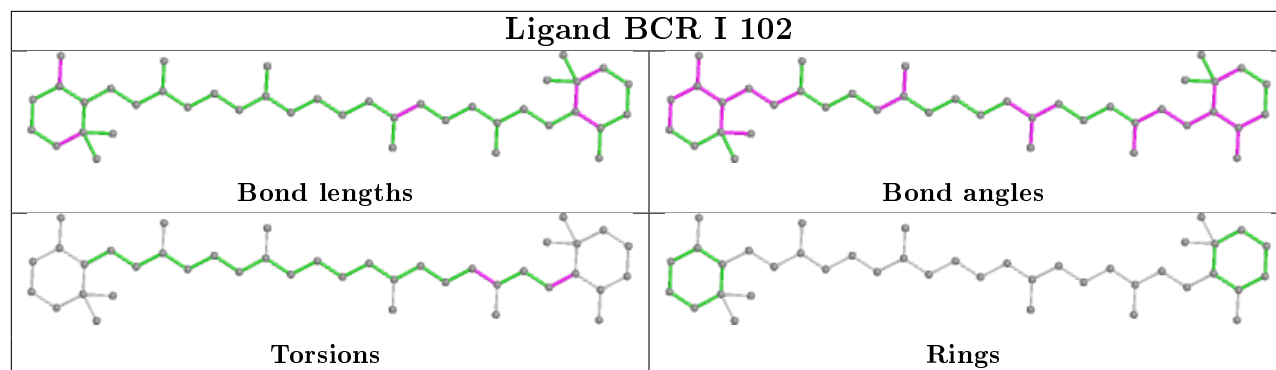
Ligand CLA B 841



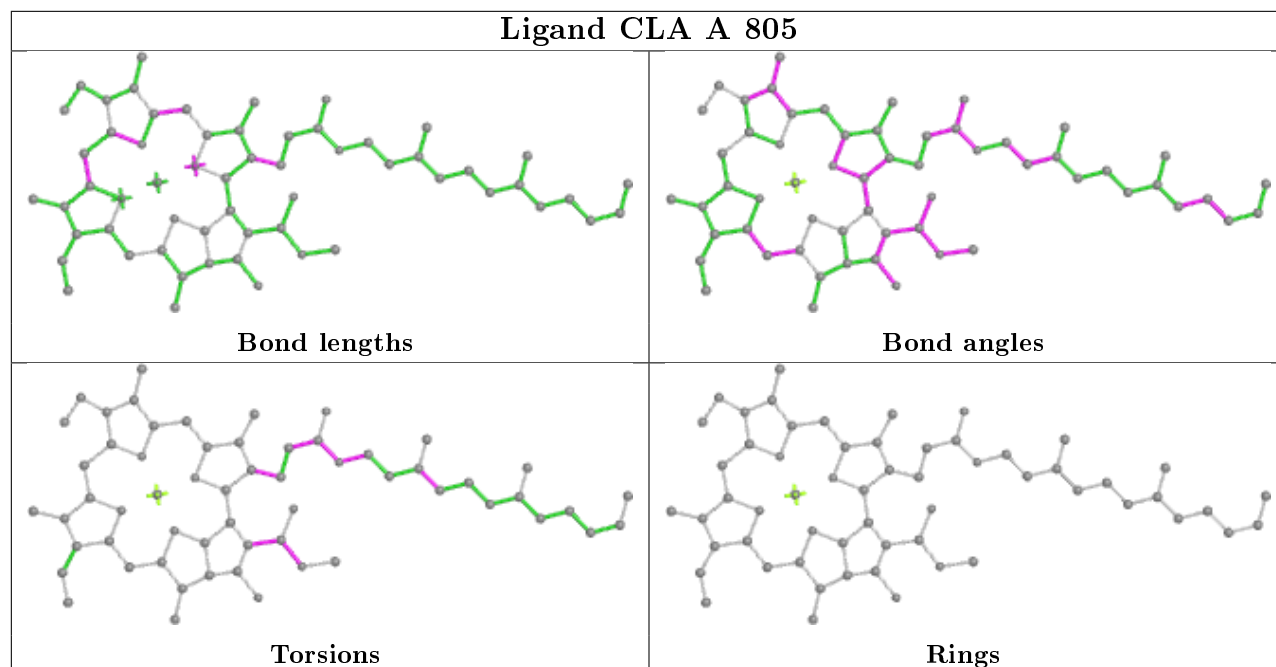
Ligand CLA B 821



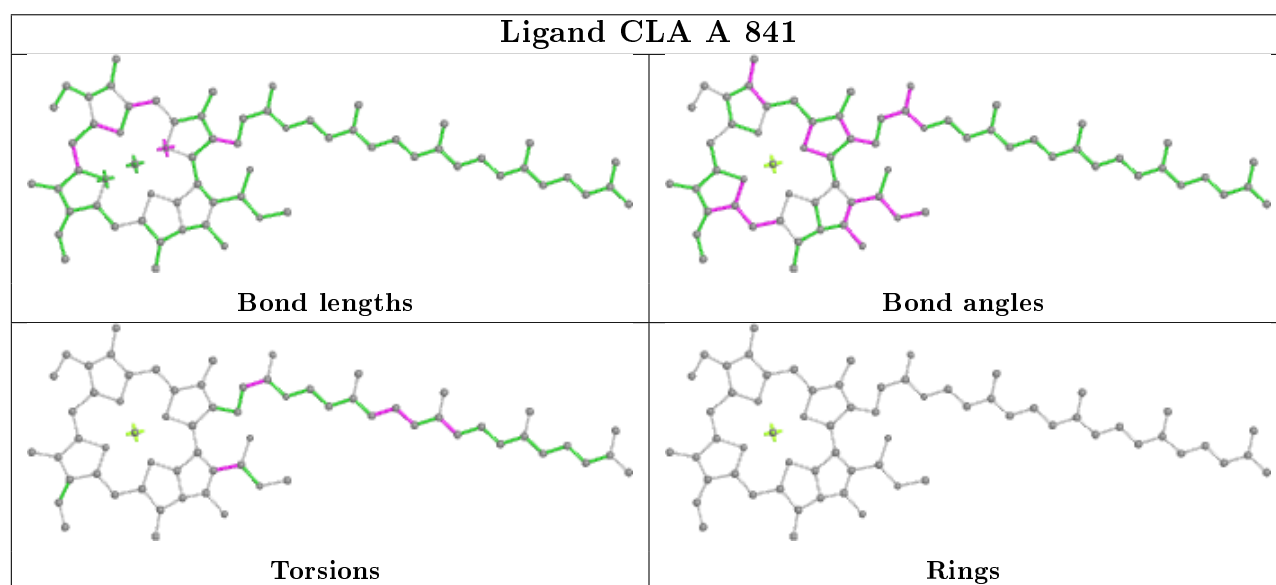
Ligand BCR I 102

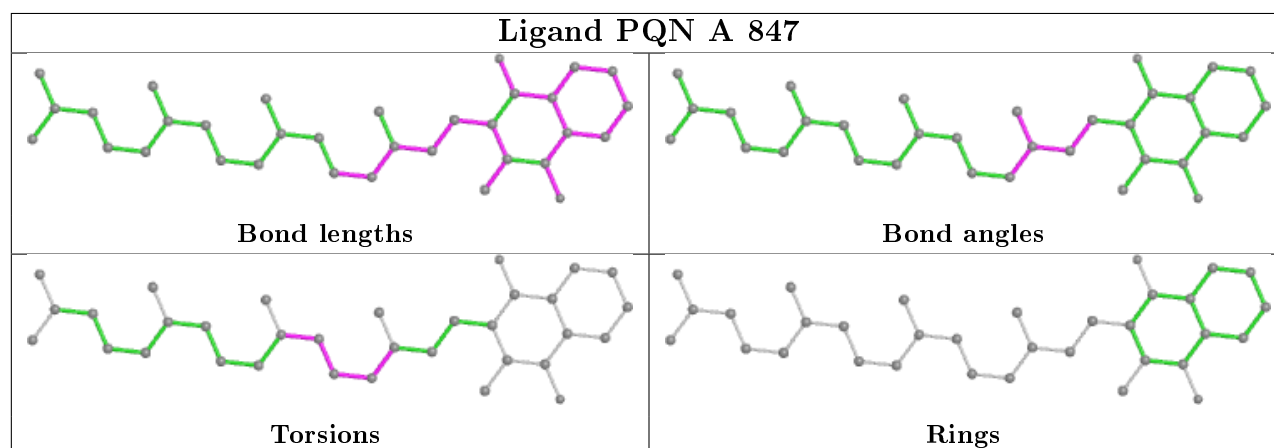
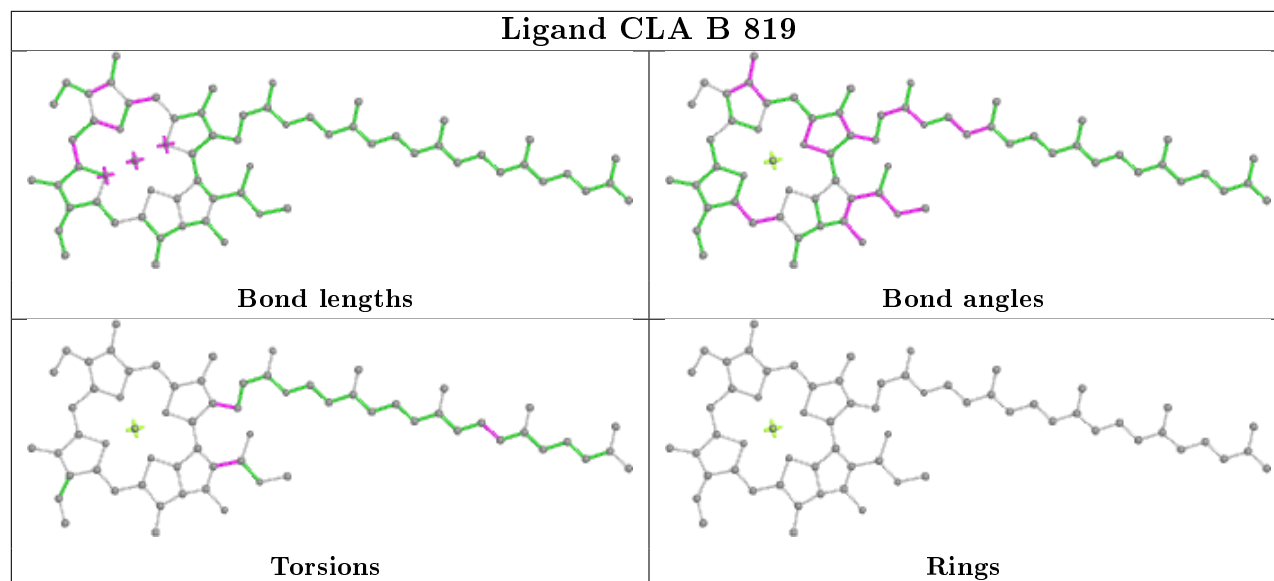
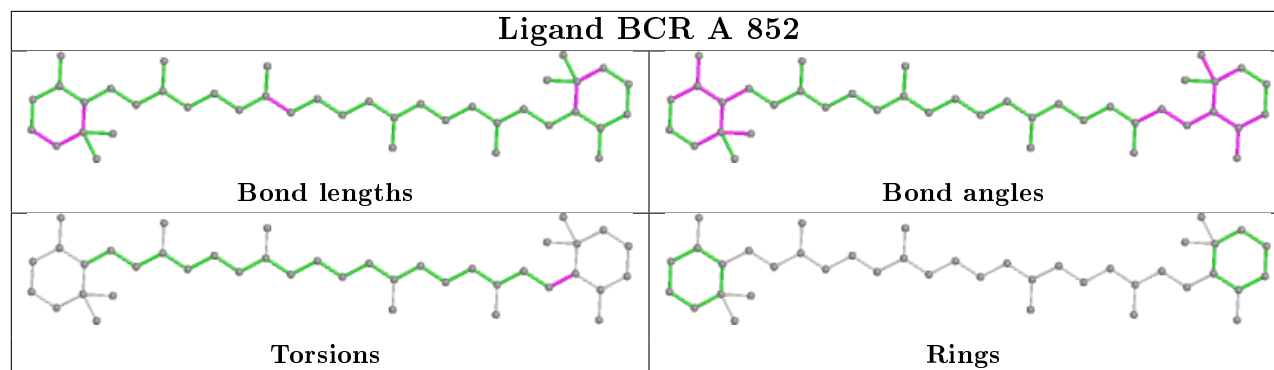


Ligand CLA A 805

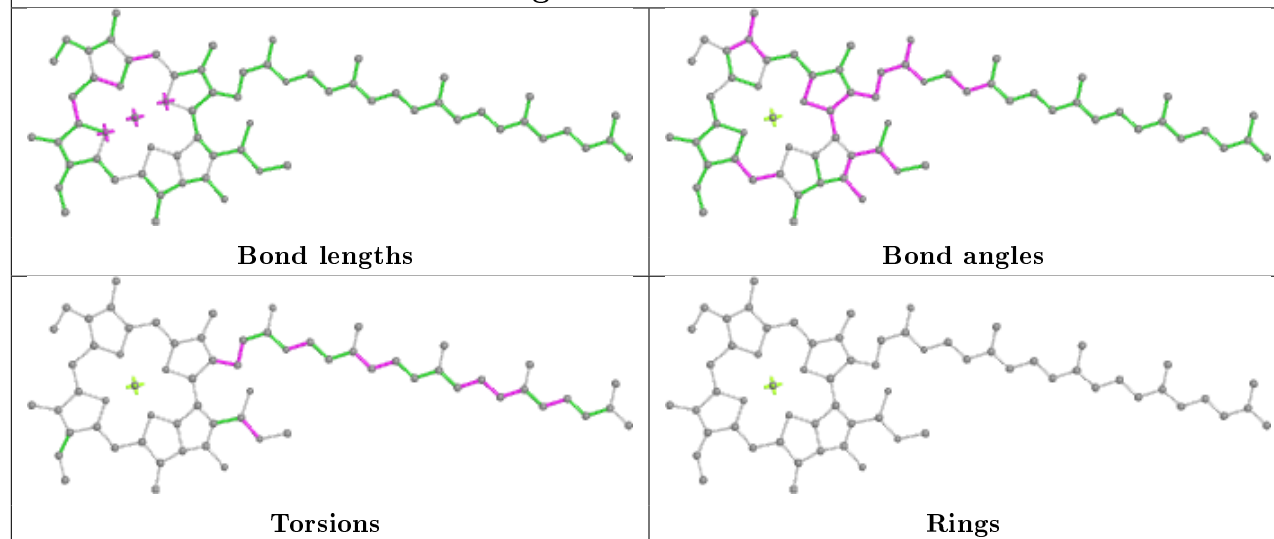


Ligand CLA A 841

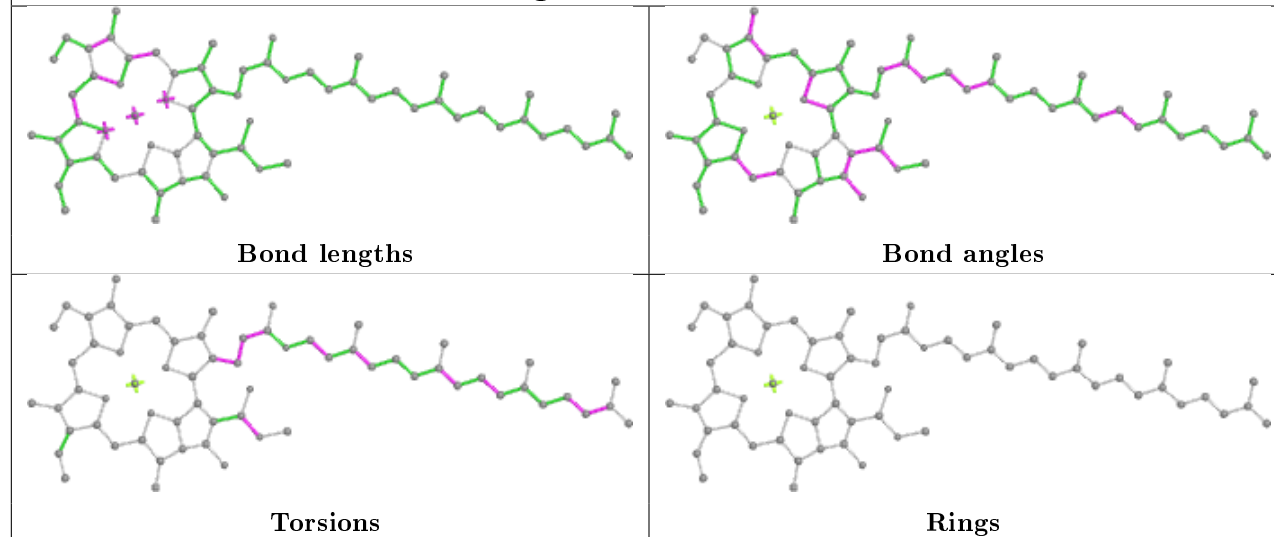




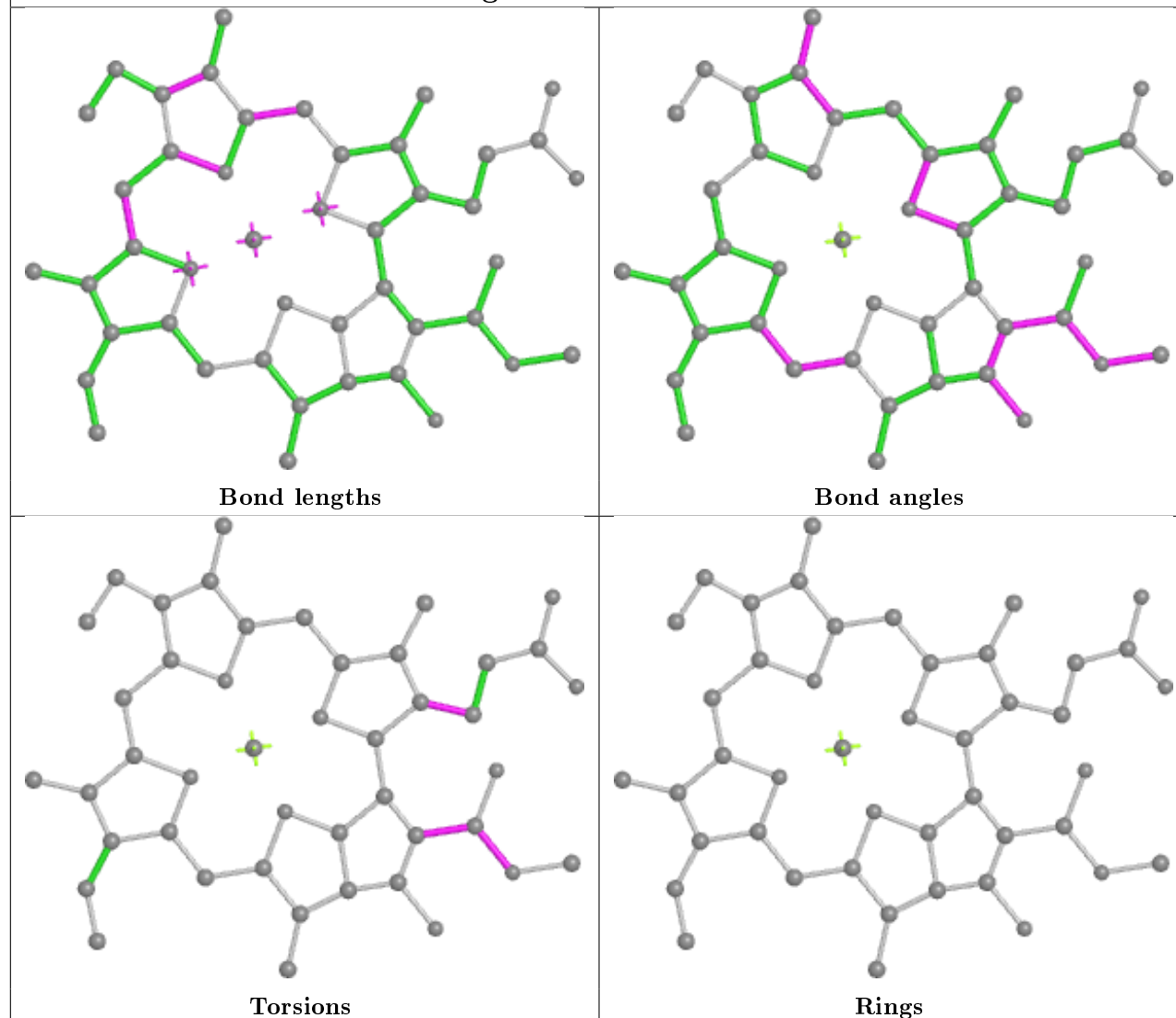
Ligand CLA A 810



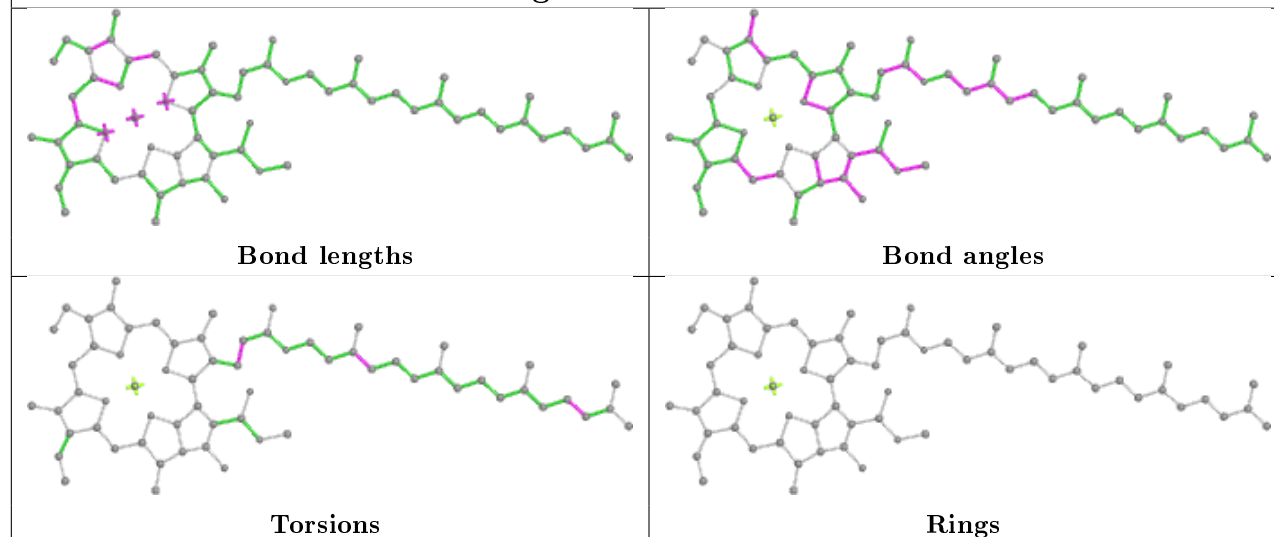
Ligand CLA B 832



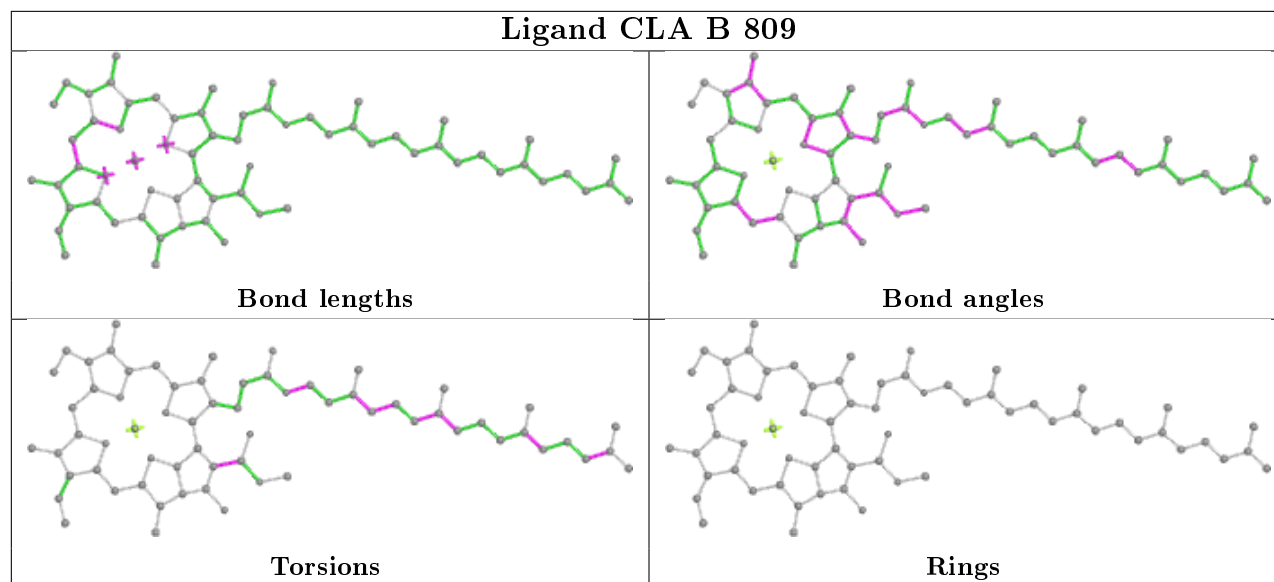
Ligand CLA K 1401



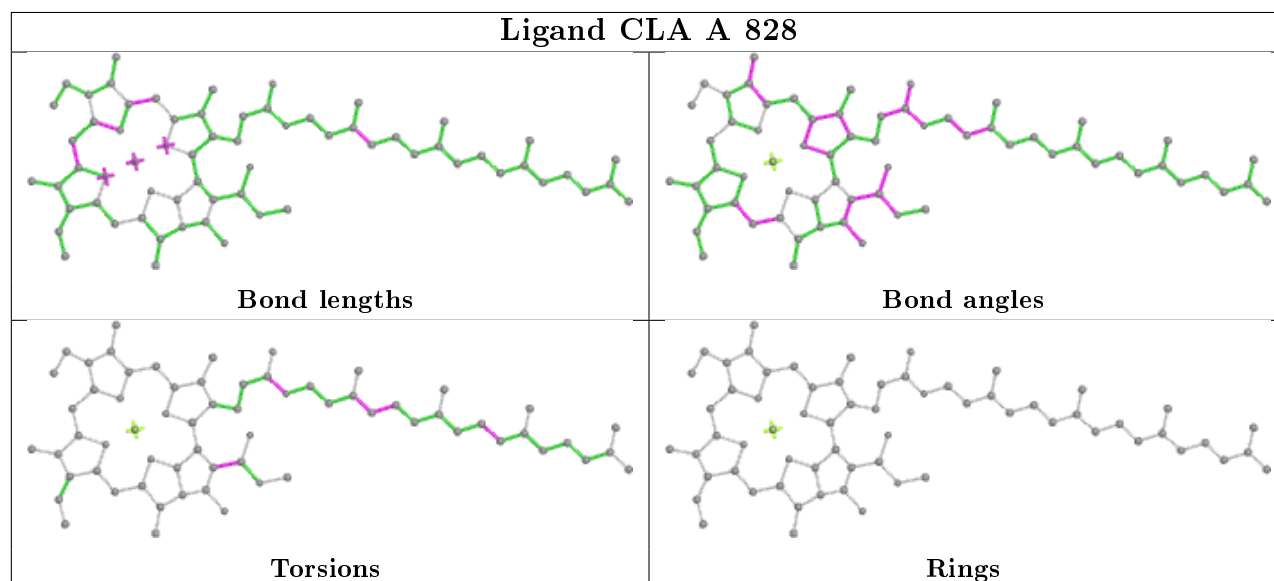
Ligand CLA A 802



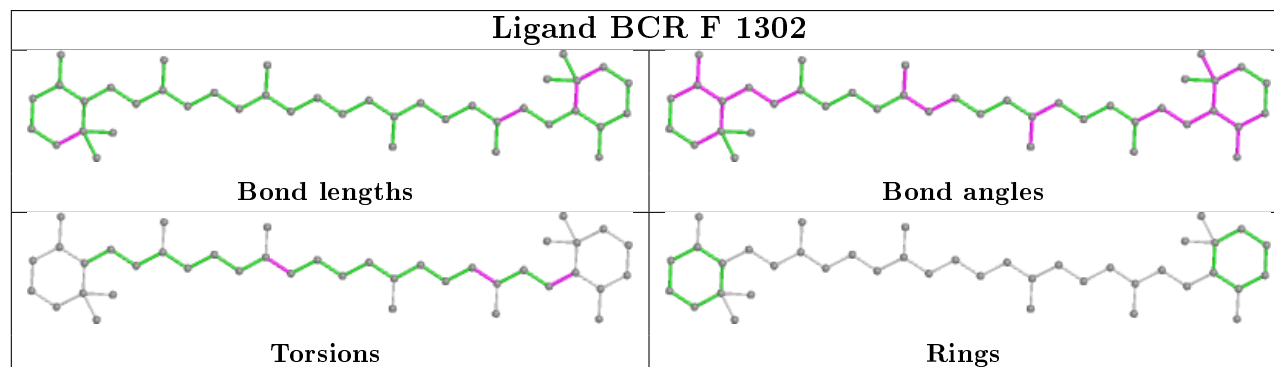
Ligand CLA B 809

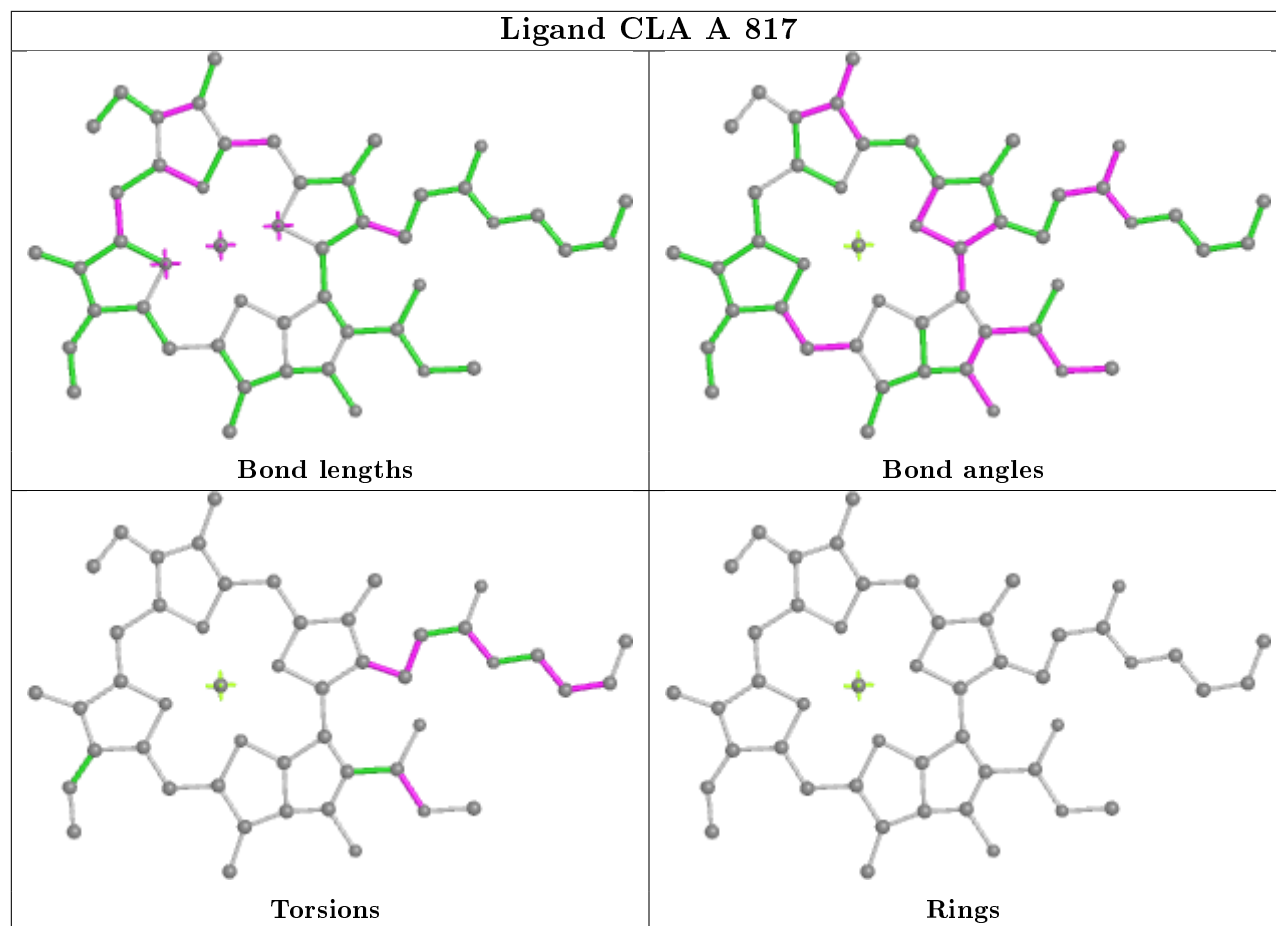


Ligand CLA A 828

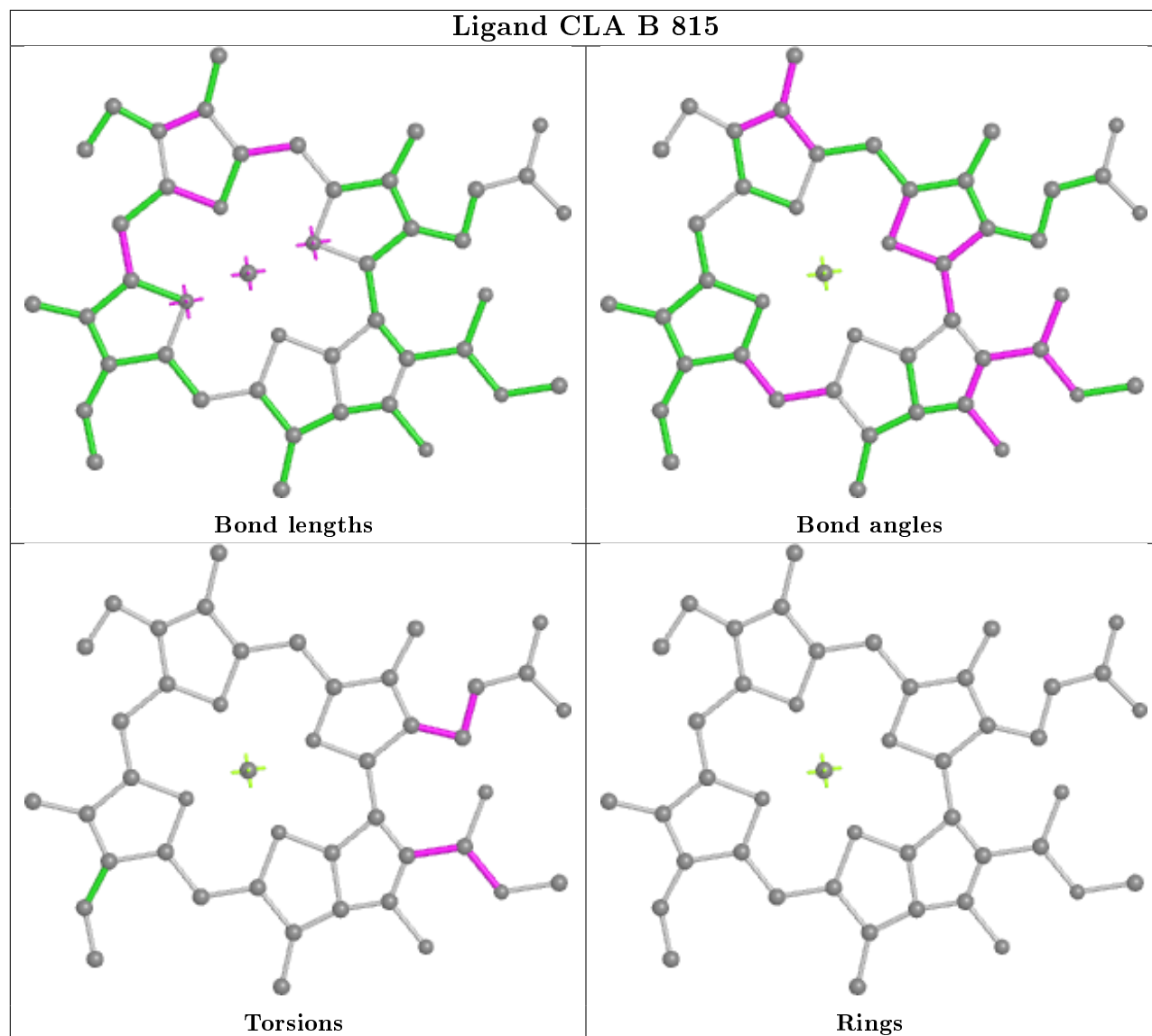


Ligand BCR F 1302

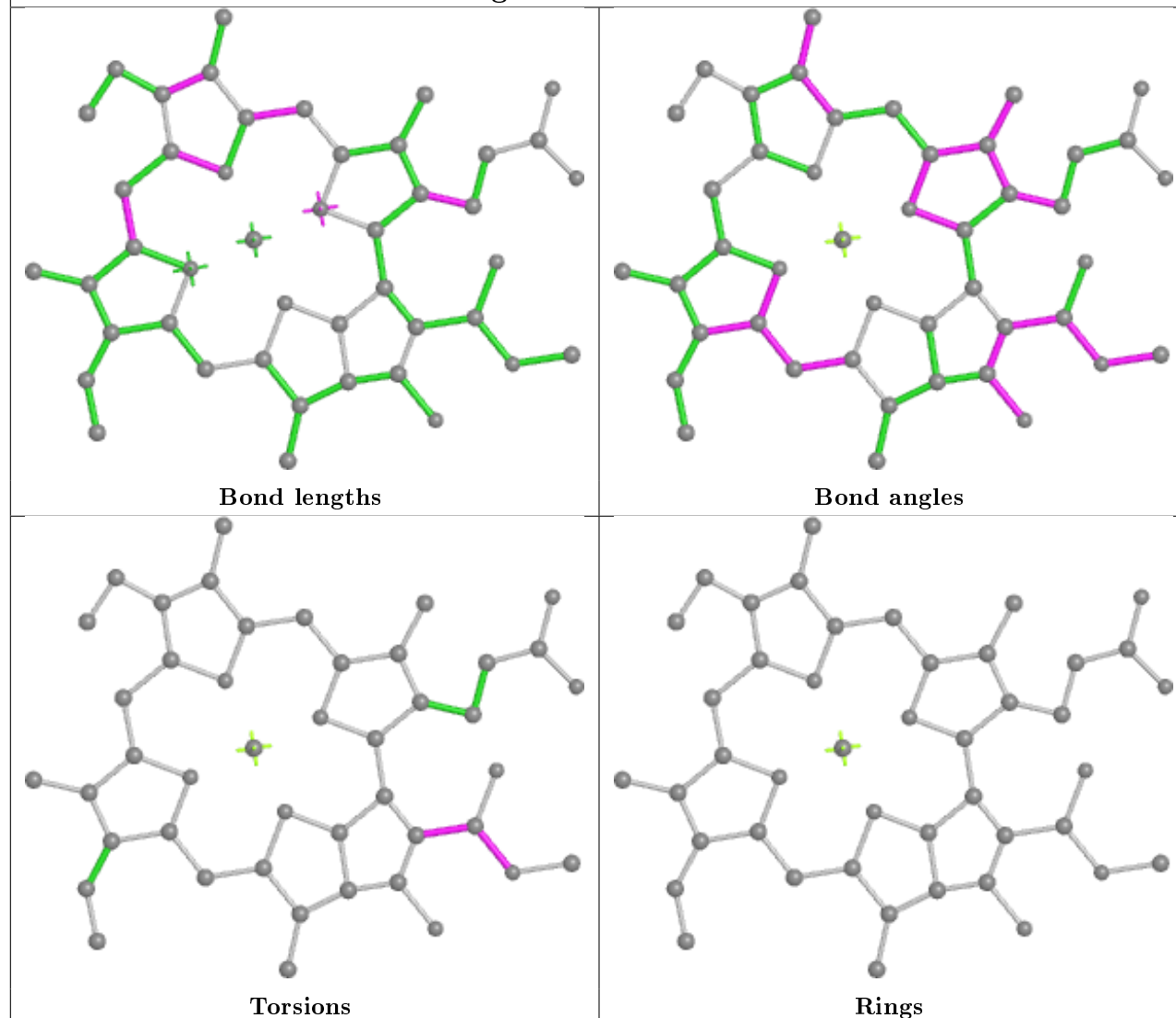




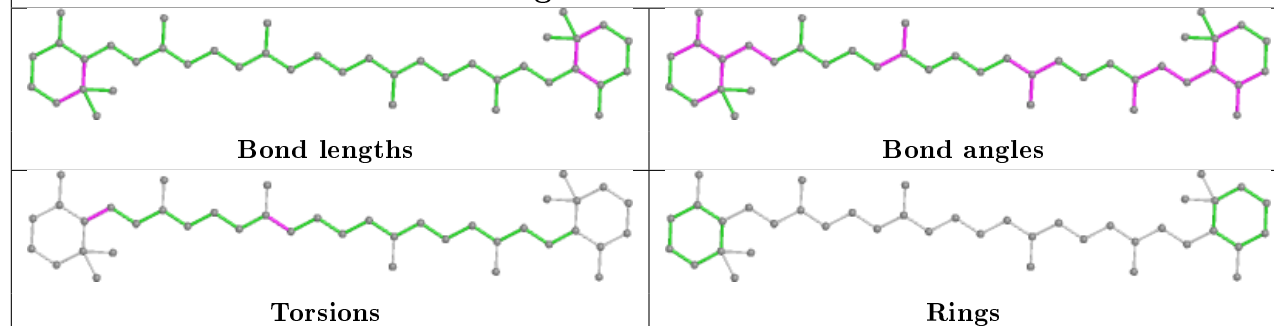
Ligand CLA B 815



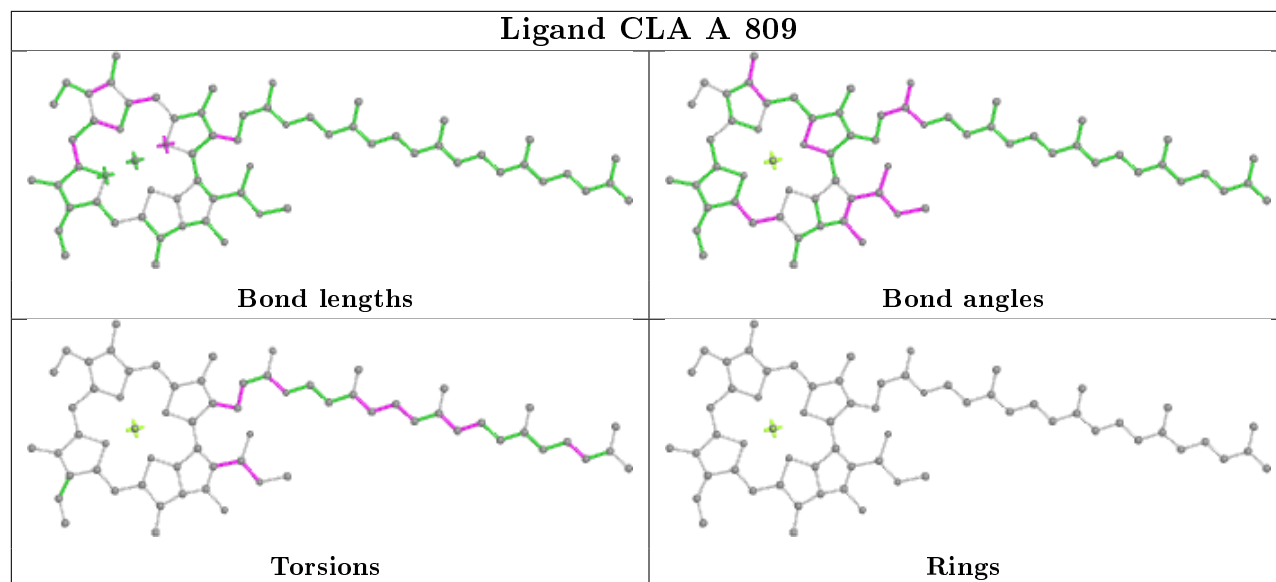
Ligand CLA B 834



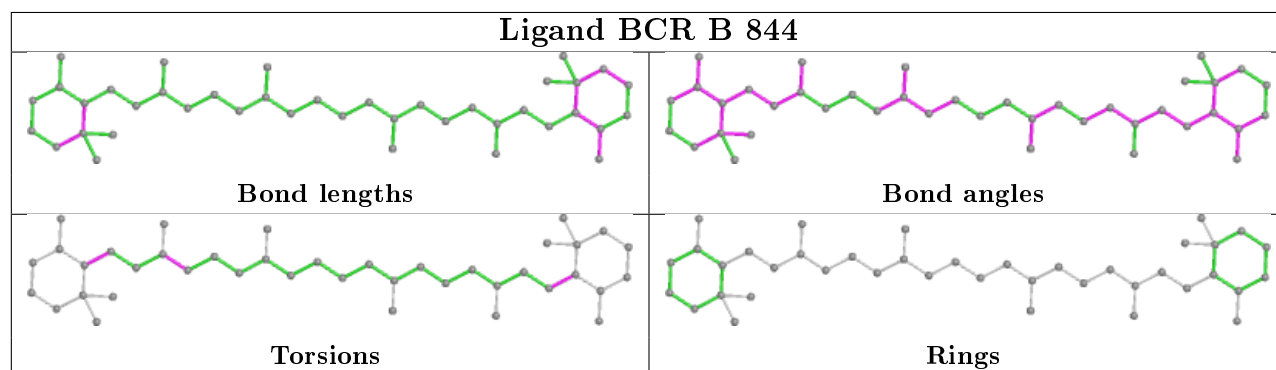
Ligand BCR J 103



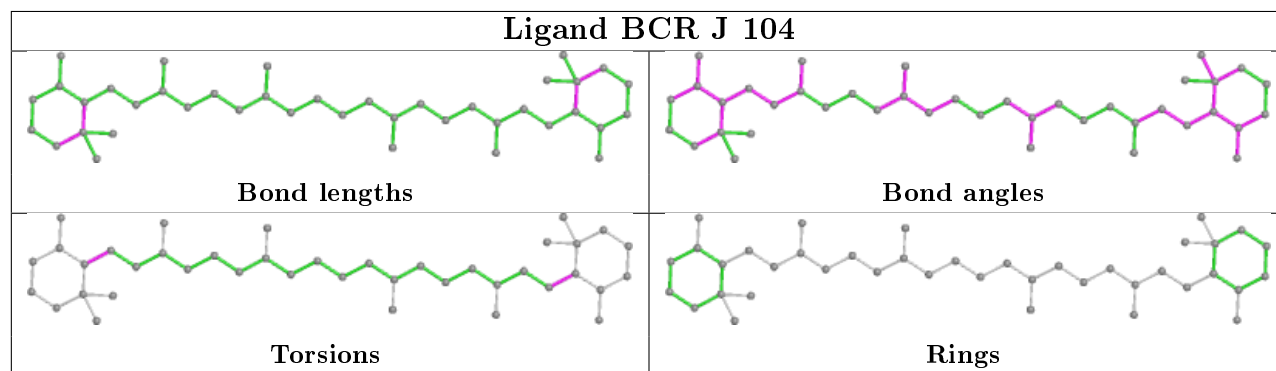
Ligand CLA A 809



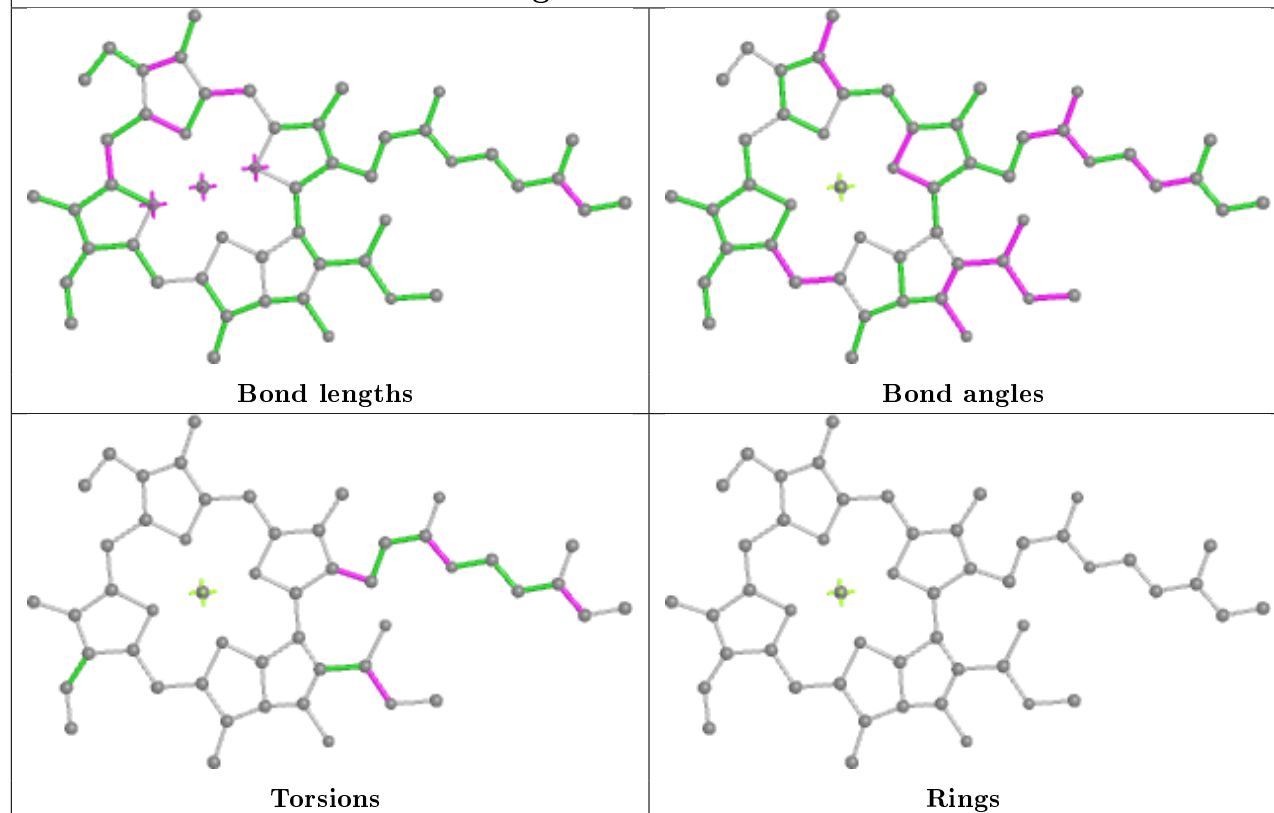
Ligand BCR B 844



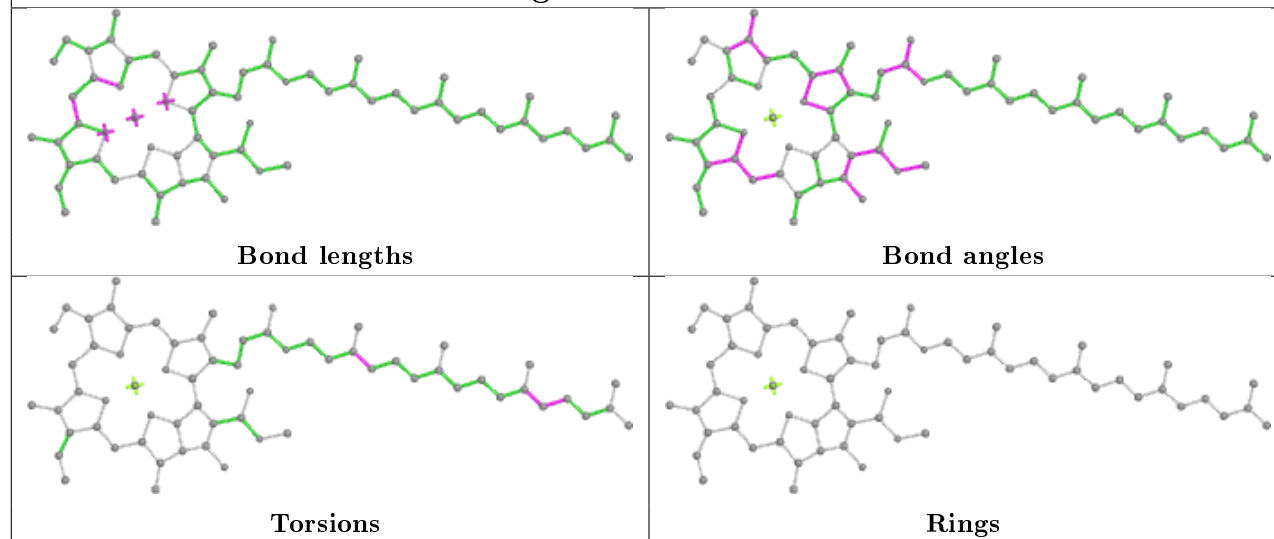
Ligand BCR J 104

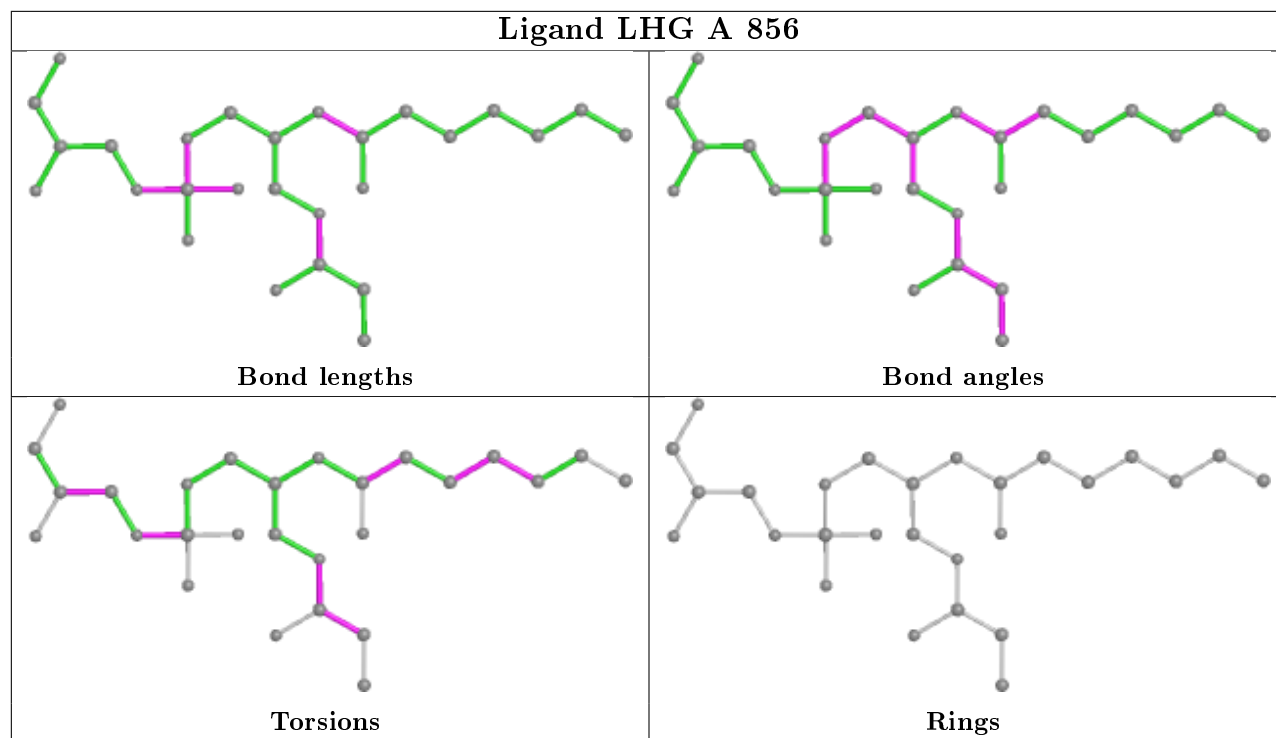


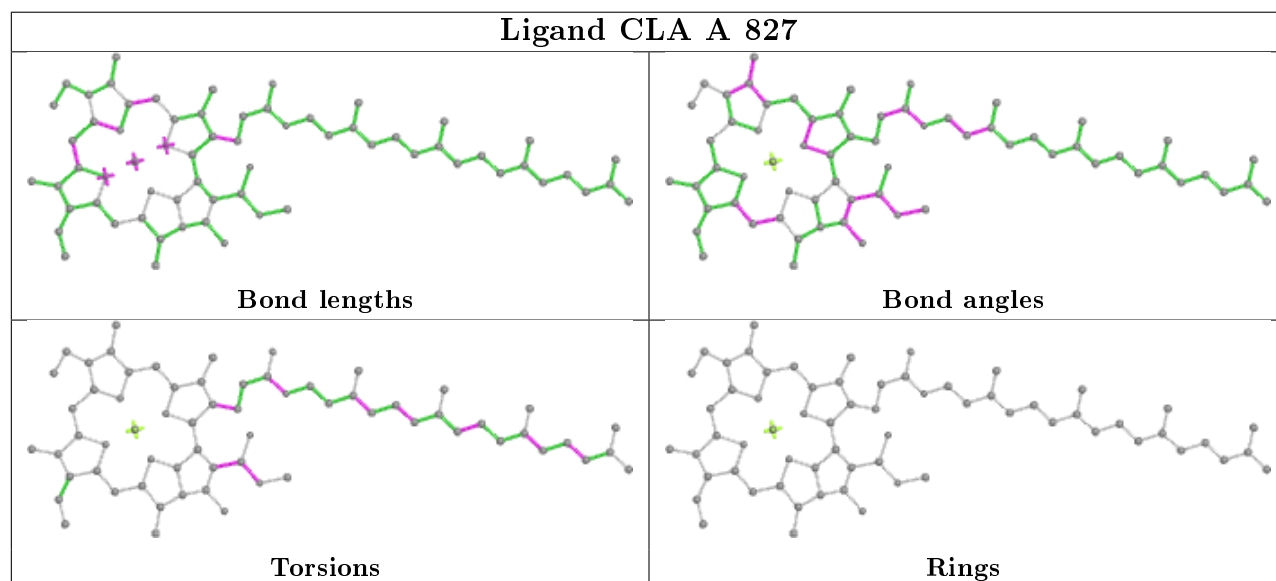
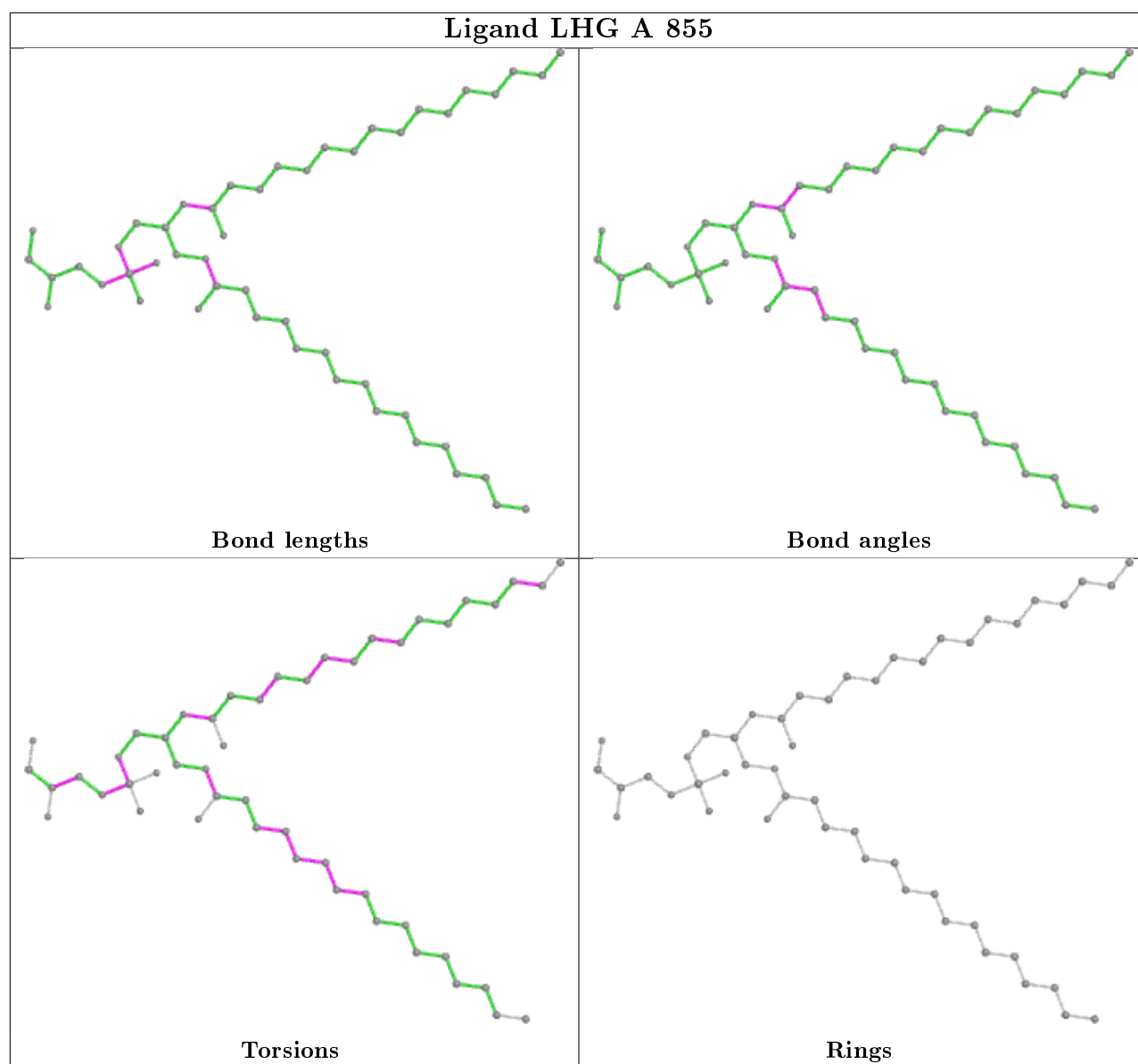
Ligand CLA A 842

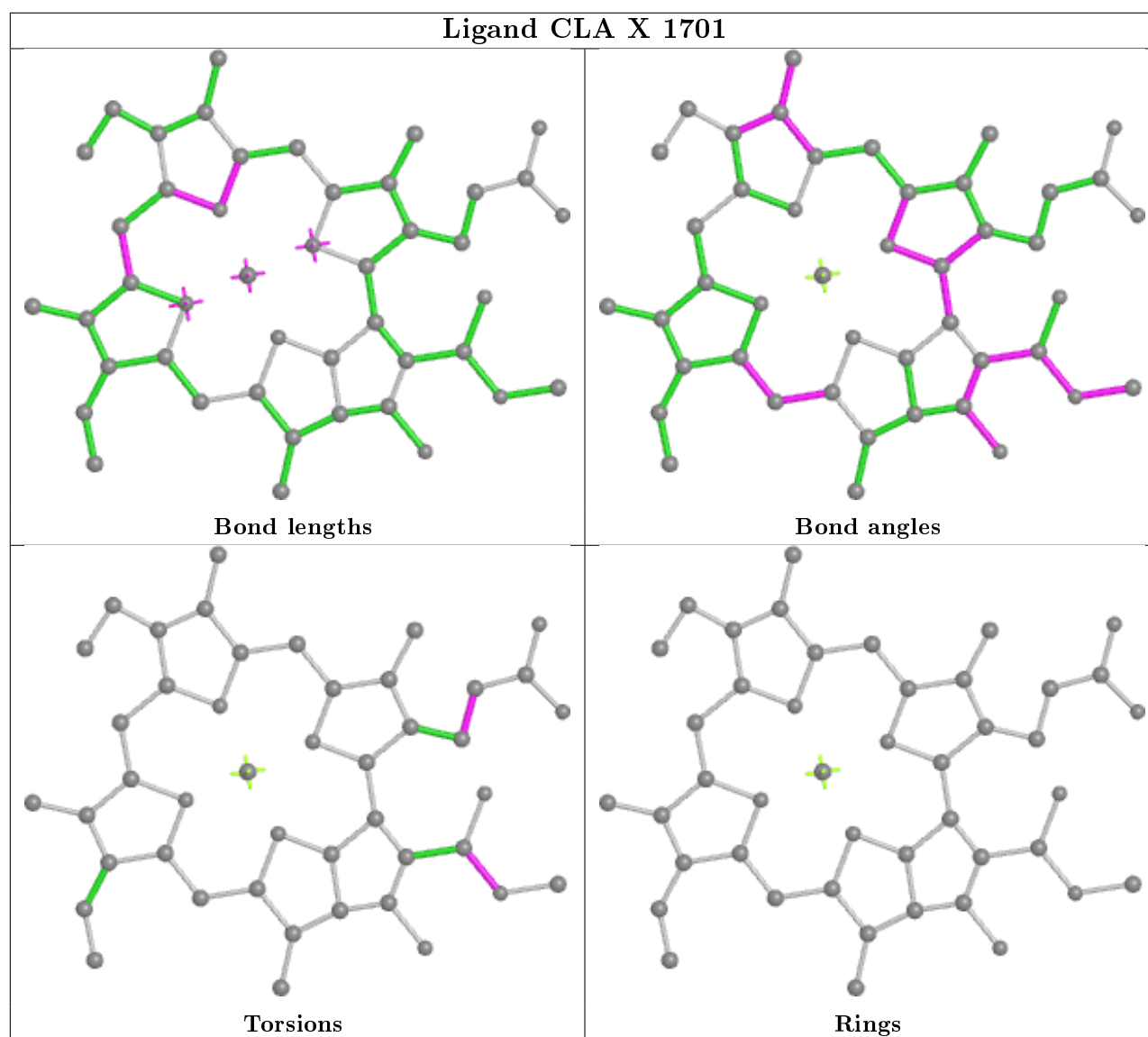


Ligand CLA A 834









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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	740/755 (98%)	-0.24	16 (2%) 62 54	22, 45, 71, 93	0
2	B	739/740 (99%)	-0.14	23 (3%) 49 42	20, 38, 71, 89	0
3	C	80/80 (100%)	-0.61	0 100 100	22, 33, 45, 54	0
4	D	138/138 (100%)	-0.07	7 (5%) 28 27	27, 41, 56, 84	0
5	E	69/75 (92%)	0.41	6 (8%) 10 12	29, 46, 62, 76	0
6	F	141/164 (85%)	-0.24	0 100 100	37, 57, 68, 72	0
7	I	38/38 (100%)	0.34	0 100 100	20, 33, 47, 53	0
8	J	41/41 (100%)	0.01	0 100 100	53, 60, 77, 86	0
9	K	46/83 (55%)	0.98	9 (19%) 1 3	72, 81, 96, 99	0
10	L	151/154 (98%)	0.25	11 (7%) 15 16	19, 26, 47, 67	0
11	M	31/31 (100%)	0.25	0 100 100	30, 38, 52, 62	0
12	X	29/35 (82%)	-0.06	1 (3%) 45 40	58, 63, 81, 88	0
All	All	2243/2334 (96%)	-0.11	73 (3%) 46 41	19, 42, 74, 99	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	2	THR	7.3
4	D	3	LEU	5.9
4	D	4	THR	5.5
1	A	207	LEU	5.4
10	L	144	VAL	4.5
10	L	141	ASN	4.3
5	E	1	VAL	4.2
4	D	1	THR	4.0
1	A	521	GLY	3.8
2	B	697	VAL	3.7
2	B	24	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	181	LEU	3.6
2	B	680	LEU	3.4
10	L	142	PHE	3.3
10	L	72	ASP	3.3
9	K	38	GLY	3.3
9	K	36	SER	3.2
1	A	82	VAL	3.2
2	B	713	LEU	3.1
5	E	2	GLN	3.1
1	A	168	MET	3.1
2	B	184	VAL	3.1
2	B	696	LEU	3.1
1	A	555	LYS	3.0
9	K	77	LEU	3.0
9	K	35	GLN	3.0
1	A	554	LEU	3.0
1	A	208	GLY	2.9
2	B	347	ILE	2.9
1	A	83	VAL	2.9
2	B	21	TRP	2.9
2	B	608	TRP	2.8
10	L	145	VAL	2.8
2	B	541	VAL	2.8
2	B	344	LEU	2.7
2	B	185	SER	2.7
5	E	53	SER	2.7
1	A	522	GLY	2.7
10	L	139	LEU	2.7
2	B	676	TYR	2.6
10	L	140	GLU	2.6
4	D	99	GLY	2.6
9	K	76	GLY	2.6
2	B	182	PHE	2.5
12	X	7	PRO	2.5
2	B	545	LEU	2.5
1	A	204	LEU	2.5
1	A	737	LEU	2.5
1	A	84	PHE	2.5
10	L	109	ASP	2.4
2	B	25	ALA	2.4
10	L	143	LEU	2.4
9	K	39	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	594	HIS	2.3
10	L	73	VAL	2.3
9	K	42	GLY	2.3
4	D	5	GLY	2.3
5	E	69	ALA	2.3
1	A	327	GLU	2.3
9	K	75	SER	2.3
2	B	703	PRO	2.2
1	A	366	LEU	2.2
10	L	111	LEU	2.2
2	B	611	ASN	2.2
2	B	681	ILE	2.2
1	A	557	VAL	2.1
2	B	20	ILE	2.1
9	K	40	GLY	2.1
5	E	67	GLU	2.1
2	B	437	LEU	2.0
5	E	27	ASP	2.0
2	B	343	CYS	2.0
4	D	98	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	BCR	A	852	40/40	0.57	1.14	47,60,96,96	0
13	CLA	J	102	37/65	0.61	0.94	95,96,97,97	0
13	CLA	B	812	45/65	0.62	0.57	66,69,80,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	LMG	B	850	55/55	0.69	1.11	34,40,57,60	0
16	BCR	B	844	40/40	0.69	1.82	56,68,93,93	0
13	CLA	A	823	49/65	0.71	0.50	64,68,82,83	0
13	CLA	J	101	45/65	0.72	0.70	98,99,100,100	0
16	BCR	A	851	40/40	0.73	1.46	47,61,89,89	0
13	CLA	A	845	41/65	0.73	0.82	87,90,92,93	0
16	BCR	J	105	40/40	0.73	0.78	53,67,93,94	0
13	CLA	B	816	55/65	0.74	0.63	54,60,85,87	0
16	BCR	B	845	40/40	0.74	1.29	33,51,87,88	0
13	CLA	B	840	65/65	0.74	1.10	13,18,41,42	0
13	CLA	B	820	47/65	0.74	0.67	88,92,97,97	0
13	CLA	A	822	65/65	0.76	0.83	41,45,55,57	0
16	BCR	A	853	40/40	0.76	1.16	30,37,59,60	0
13	CLA	B	815	45/65	0.76	0.55	57,62,73,77	0
16	BCR	A	850	40/40	0.76	1.29	57,61,79,79	0
13	CLA	B	833	58/65	0.77	0.70	36,47,77,78	0
13	CLA	A	811	45/65	0.77	0.39	68,71,75,76	0
16	BCR	B	843	40/40	0.77	0.86	88,90,97,98	0
13	CLA	A	844	65/65	0.78	0.93	17,22,43,47	0
13	CLA	A	824	51/65	0.78	0.66	53,59,77,77	0
13	CLA	M	1601	45/65	0.78	0.87	96,97,99,100	0
13	CLA	A	816	45/65	0.79	0.63	78,82,83,83	0
19	CA	L	1001	1/1	0.79	0.17	27,27,27,27	0
17	LHG	A	855	49/49	0.79	0.76	39,50,60,63	0
13	CLA	A	827	65/65	0.79	0.64	24,31,83,85	0
13	CLA	B	811	45/65	0.80	0.39	42,49,62,66	0
13	CLA	K	1401	45/65	0.80	0.66	70,74,81,84	0
13	CLA	B	821	45/65	0.80	0.49	80,81,90,93	0
13	CLA	A	808	51/65	0.81	0.46	55,58,79,79	0
13	CLA	A	812	65/65	0.81	0.45	63,65,72,74	0
13	CLA	B	836	45/65	0.81	0.41	78,82,85,87	0
13	CLA	A	846	52/65	0.82	0.54	69,75,97,99	0
13	CLA	B	814	65/65	0.82	0.65	34,43,68,69	0
13	CLA	A	821	61/65	0.82	0.74	56,62,85,85	0
16	BCR	B	846	25/40	0.82	0.98	64,66,69,70	0
13	CLA	F	1301	45/65	0.82	0.53	75,77,82,83	0
16	BCR	M	1602	40/40	0.83	0.88	28,37,59,62	0
13	CLA	B	830	45/65	0.83	0.69	51,54,67,72	0
17	LHG	B	851	23/49	0.83	0.46	79,89,92,93	0
13	CLA	B	831	49/65	0.83	0.82	36,40,63,65	0
16	BCR	A	849	40/40	0.83	0.80	62,69,79,79	0

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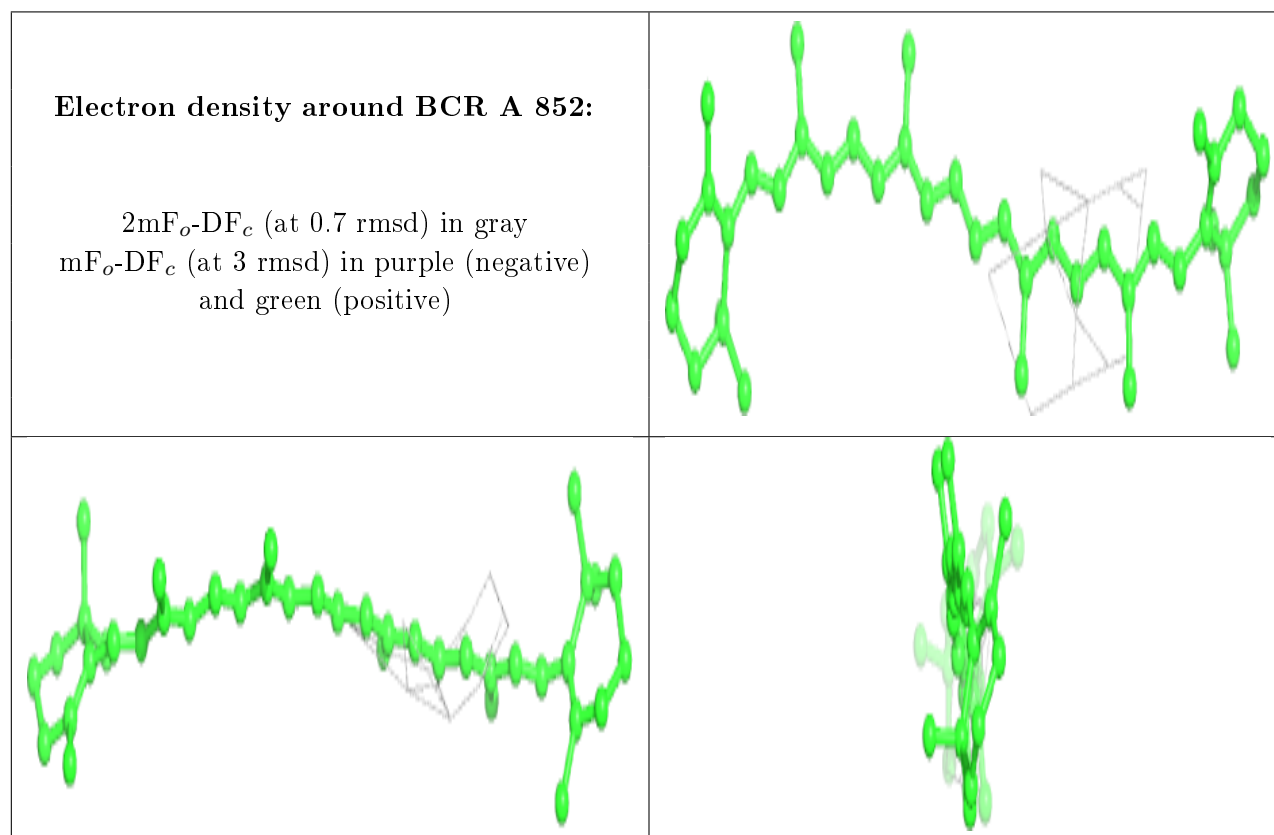
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	CLA	B	839	47/65	0.84	0.55	41,47,55,60	0
13	CLA	B	819	65/65	0.84	0.74	78,82,99,100	0
13	CLA	A	818	54/65	0.84	0.51	63,66,68,69	0
13	CLA	A	828	65/65	0.84	0.56	32,42,66,68	0
16	BCR	L	1005	40/40	0.84	1.37	20,24,29,30	0
13	CLA	L	1004	65/65	0.84	0.82	22,31,61,62	0
13	CLA	A	834	65/65	0.84	1.04	24,28,43,44	0
13	CLA	A	813	54/65	0.84	0.56	44,47,76,77	0
16	BCR	B	849	40/40	0.84	1.07	23,27,30,31	0
13	CLA	A	817	49/65	0.85	0.47	87,90,92,94	0
13	CLA	A	825	59/65	0.85	0.74	34,43,76,76	0
13	CLA	B	826	65/65	0.85	0.65	31,39,63,65	0
13	CLA	A	810	65/65	0.85	0.89	39,43,77,78	0
13	CLA	B	841	65/65	0.85	1.14	22,29,44,50	0
13	CLA	A	840	47/65	0.85	0.70	30,35,52,57	0
16	BCR	J	104	40/40	0.86	0.87	61,69,75,76	0
13	CLA	B	803	65/65	0.86	0.62	24,29,35,36	0
13	CLA	A	838	51/65	0.86	0.34	30,35,45,46	0
16	BCR	I	101	40/40	0.86	0.77	19,27,40,40	0
13	CLA	A	833	65/65	0.87	0.80	20,31,85,88	0
13	CLA	A	839	65/65	0.87	0.70	32,38,58,59	0
13	CLA	A	837	45/65	0.87	0.56	60,68,76,80	0
16	BCR	F	1302	40/40	0.88	0.77	43,49,60,60	0
13	CLA	B	832	65/65	0.88	0.63	37,43,65,66	0
16	BCR	B	847	40/40	0.88	0.97	46,53,61,61	0
13	CLA	A	814	60/65	0.88	0.69	49,53,80,81	0
16	BCR	J	103	40/40	0.89	1.36	55,58,60,60	0
13	CLA	A	805	59/65	0.89	0.46	40,46,85,86	0
13	CLA	L	1003	65/65	0.89	0.78	17,23,66,67	0
16	BCR	L	1006	40/40	0.89	0.45	26,35,66,67	0
13	CLA	B	825	46/65	0.89	0.49	29,36,46,48	0
13	CLA	A	815	45/65	0.89	0.36	64,66,67,68	0
13	CLA	X	1701	45/65	0.89	0.46	77,83,86,88	0
13	CLA	B	810	65/65	0.90	0.53	15,23,43,44	0
13	CLA	A	843	65/65	0.90	1.48	29,35,60,60	0
13	CLA	A	826	65/65	0.90	0.45	45,49,62,63	0
13	CLA	A	806	65/65	0.90	0.61	33,39,68,70	0
13	CLA	B	828	65/65	0.90	1.11	31,35,48,52	0
13	CLA	B	824	54/65	0.91	0.51	54,59,69,71	0
13	CLA	A	807	65/65	0.91	0.77	38,43,51,52	0
13	CLA	B	804	54/65	0.92	0.84	20,29,48,52	0
13	CLA	B	838	65/65	0.92	0.46	38,44,74,78	0

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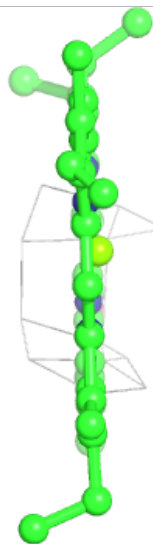
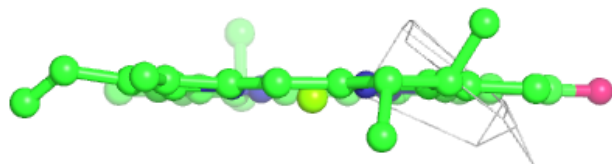
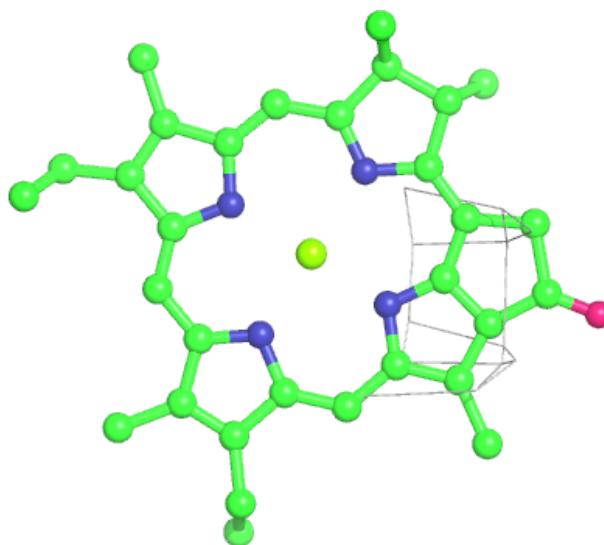
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
13	CLA	A	802	65/65	0.92	0.53	23,26,35,39	0
13	CLA	B	817	59/65	0.92	0.54	39,47,66,70	0
13	CLA	L	1002	65/65	0.92	0.57	21,27,58,61	0
13	CLA	B	807	65/65	0.92	0.52	21,24,50,53	0
13	CLA	B	801	65/65	0.92	0.31	22,30,38,46	0
13	CLA	B	813	65/65	0.92	0.90	49,59,68,70	0
16	BCR	I	102	40/40	0.92	0.59	19,26,31,32	0
13	CLA	A	804	65/65	0.92	0.83	45,50,80,83	0
13	CLA	A	836	54/65	0.92	0.59	46,50,64,64	0
17	LHG	A	856	27/49	0.92	0.40	51,56,60,61	0
16	BCR	B	848	40/40	0.92	0.95	40,52,58,58	0
14	PQN	A	847	33/33	0.92	0.77	41,43,67,68	0
13	CLA	B	805	65/65	0.92	0.65	28,37,66,69	0
13	CLA	B	835	45/65	0.93	0.46	58,61,70,75	0
13	CLA	A	819	54/65	0.93	0.39	44,50,54,56	0
13	CLA	A	820	65/65	0.93	0.59	43,48,56,58	0
13	CLA	A	801	65/65	0.93	0.39	22,27,36,38	0
13	CLA	B	822	55/65	0.93	0.35	69,70,88,89	0
13	CLA	B	823	45/65	0.93	0.36	58,62,70,73	0
16	BCR	A	854	40/40	0.93	1.45	29,39,50,53	0
15	SF4	C	102	8/8	0.93	0.21	33,34,35,35	0
13	CLA	A	830	65/65	0.93	0.72	33,40,52,55	0
13	CLA	B	829	65/65	0.94	0.88	18,29,63,65	0
13	CLA	A	809	65/65	0.94	0.75	33,40,66,67	0
13	CLA	A	831	65/65	0.94	0.53	35,43,52,53	0
13	CLA	A	803	65/65	0.94	0.71	33,41,51,54	0
13	CLA	A	842	51/65	0.94	0.45	38,43,70,71	0
13	CLA	B	809	65/65	0.94	0.71	20,26,61,62	0
13	CLA	A	832	50/65	0.94	0.43	32,37,58,59	0
13	CLA	B	818	60/65	0.94	0.86	33,39,64,66	0
13	CLA	B	806	65/65	0.94	0.98	30,34,53,54	0
14	PQN	B	842	33/33	0.94	0.96	24,29,36,36	0
13	CLA	A	835	65/65	0.95	0.49	14,19,36,40	0
13	CLA	B	837	60/65	0.95	0.33	42,48,70,71	0
13	CLA	B	827	65/65	0.96	0.63	24,31,77,80	0
13	CLA	B	834	45/65	0.96	0.47	40,47,53,56	0
13	CLA	B	808	65/65	0.96	0.56	21,28,49,50	0
13	CLA	B	802	65/65	0.96	0.53	28,39,55,59	0
13	CLA	A	841	65/65	0.97	0.42	33,38,55,55	0
15	SF4	C	101	8/8	0.97	0.24	24,25,26,26	0
13	CLA	A	829	65/65	0.98	0.61	38,46,74,75	0
15	SF4	A	848	8/8	0.99	0.18	25,26,27,27	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



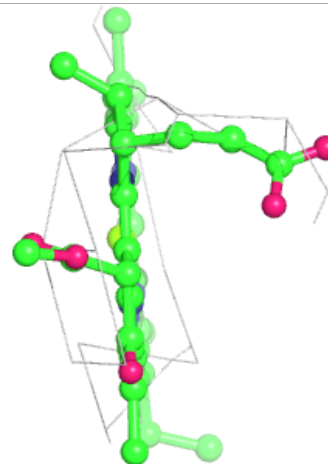
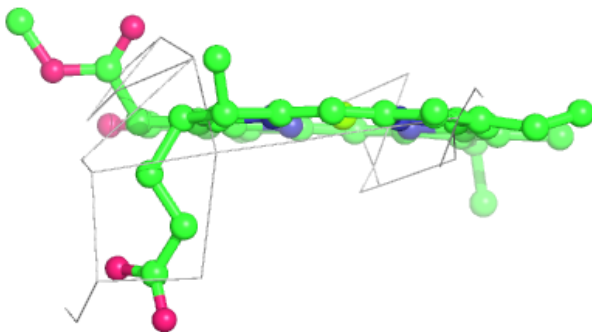
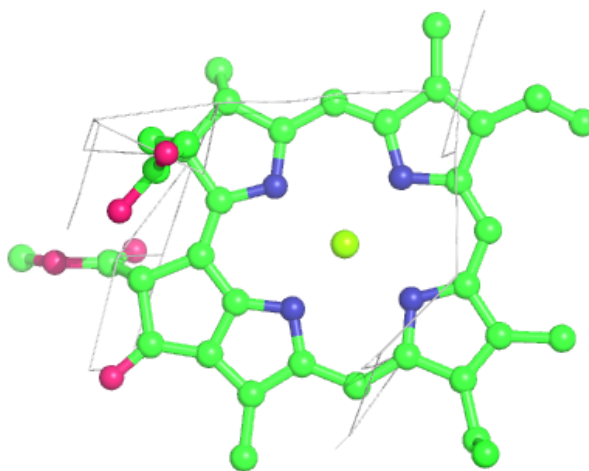
Electron density around CLA J 102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



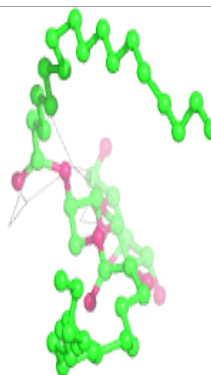
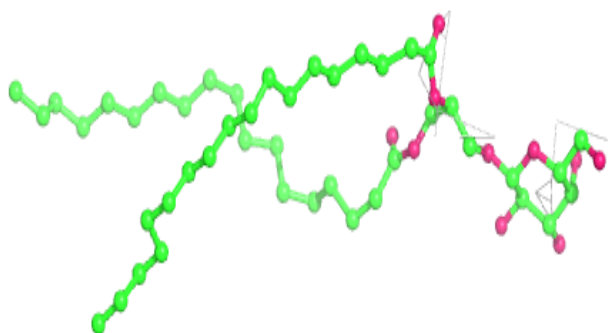
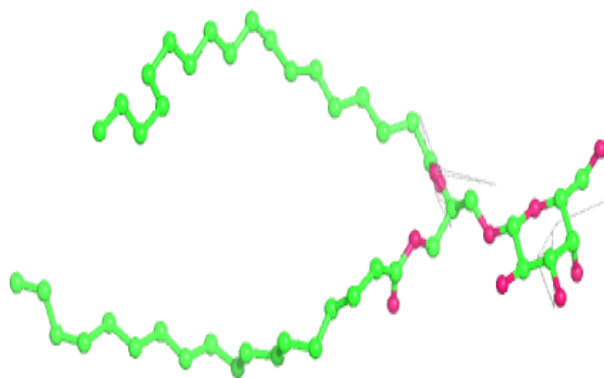
Electron density around CLA B 812:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

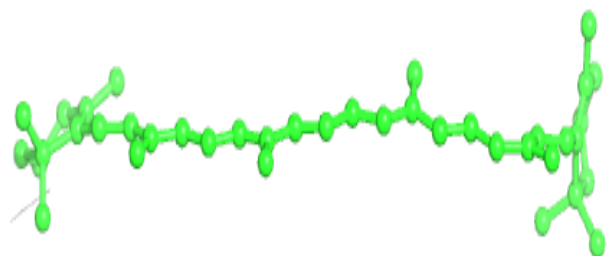
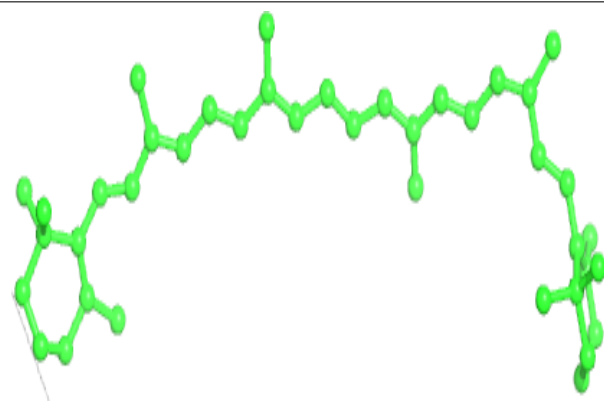


Electron density around LMG B 850:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

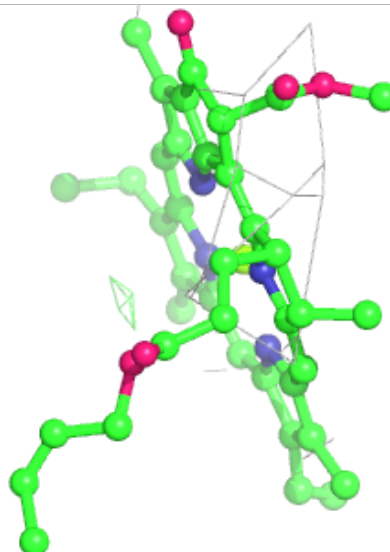
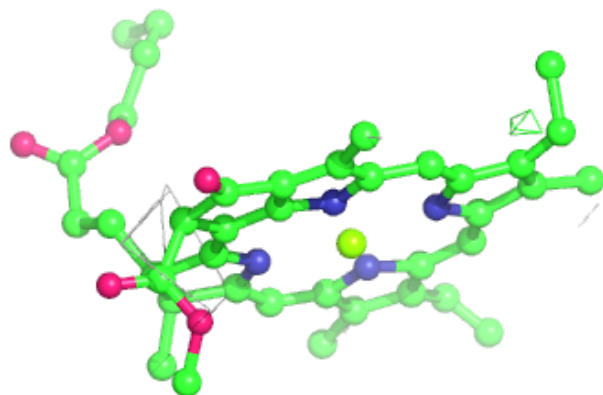
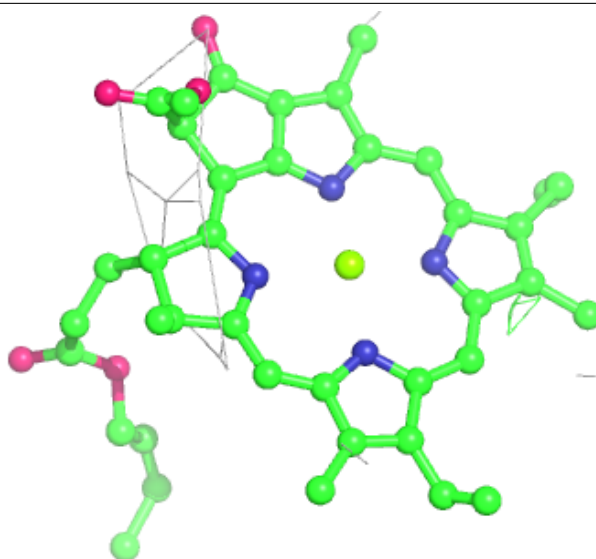
**Electron density around BCR B 844:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



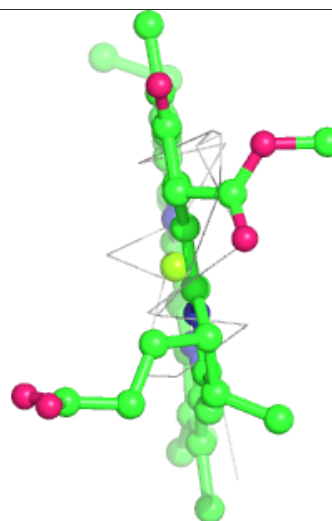
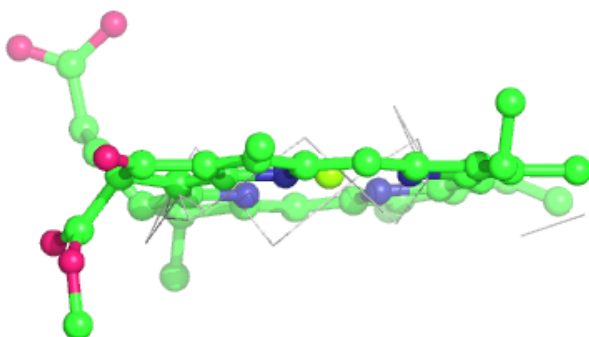
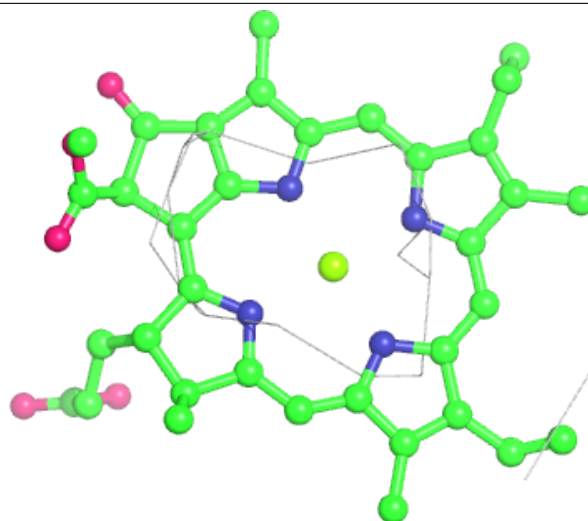
Electron density around CLA A 823:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



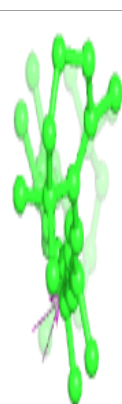
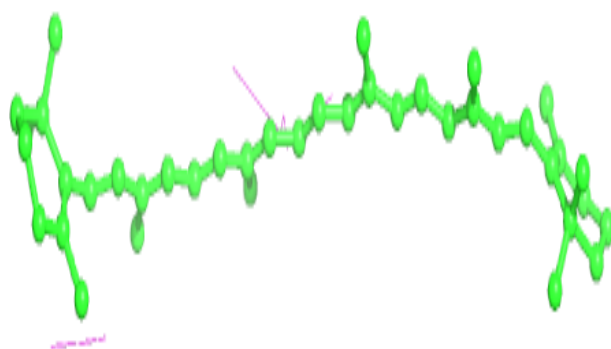
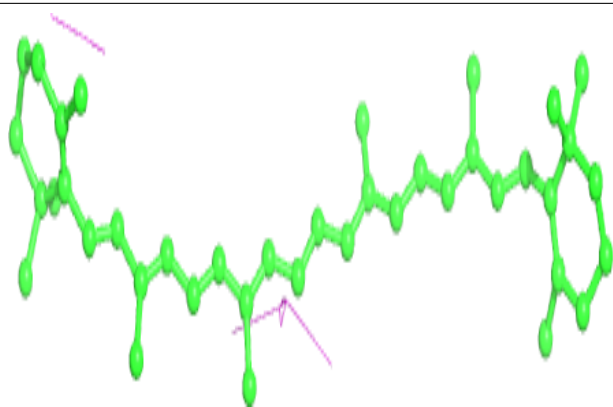
Electron density around CLA J 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



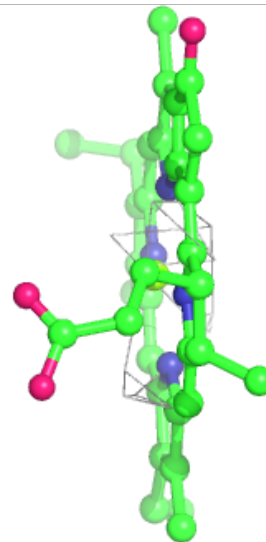
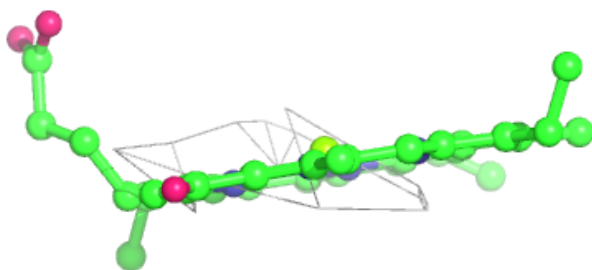
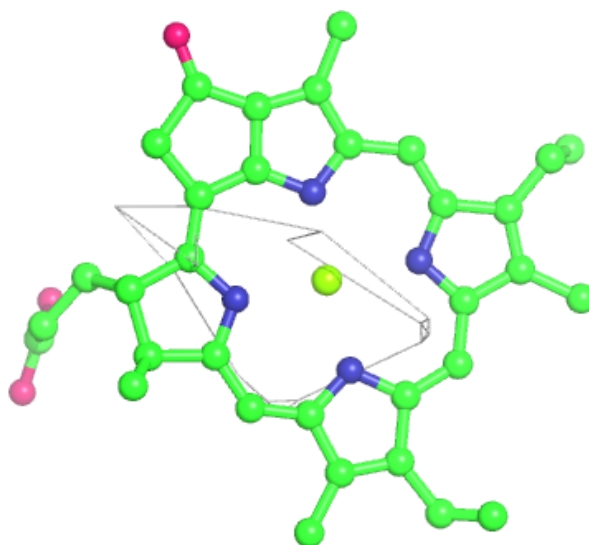
Electron density around BCR A 851:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



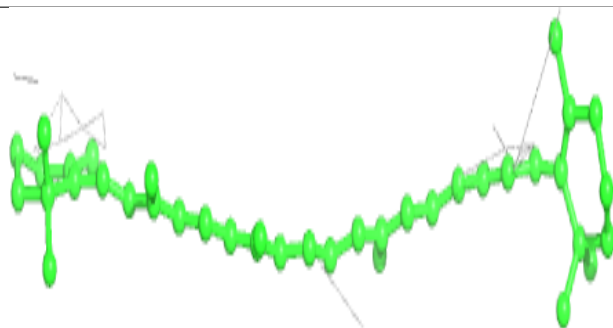
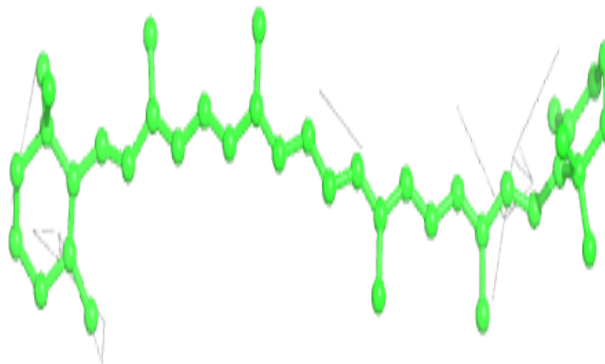
Electron density around CLA A 845:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

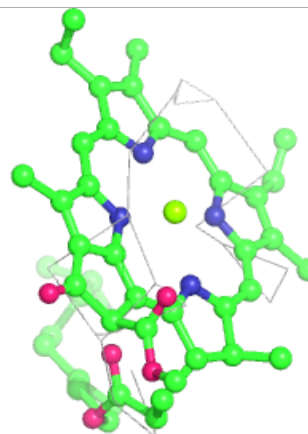
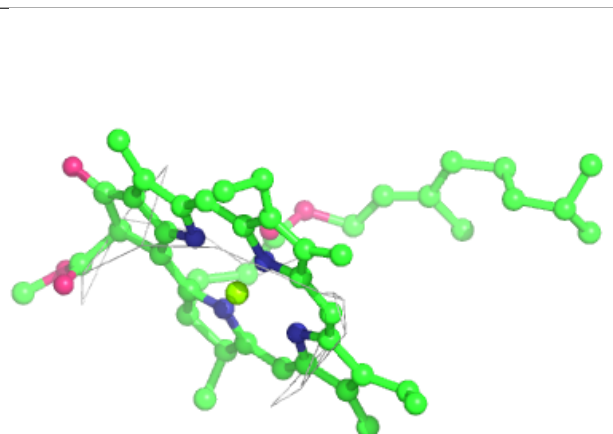
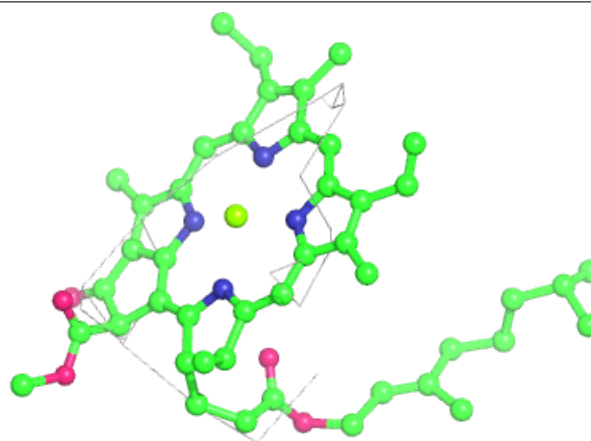


Electron density around BCR J 105:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

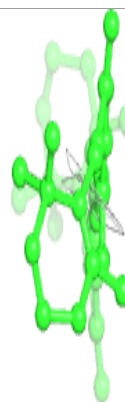
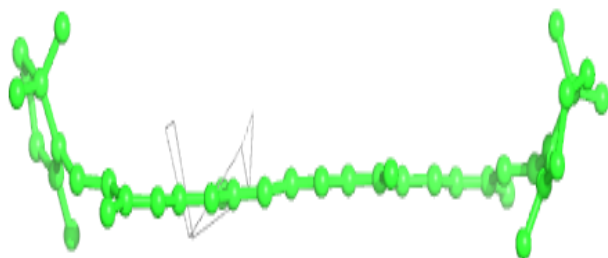
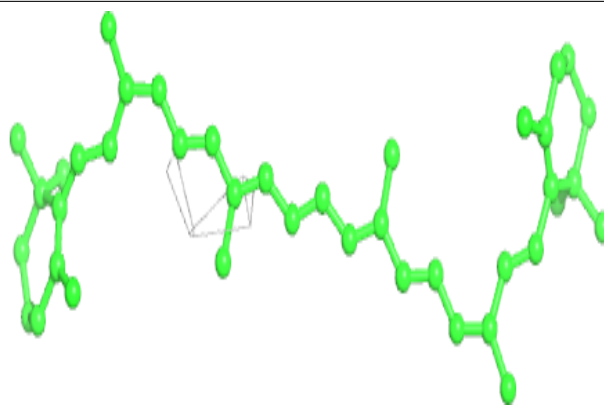
**Electron density around CLA B 816:**

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and green (positive)

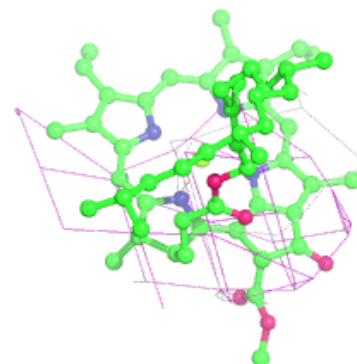
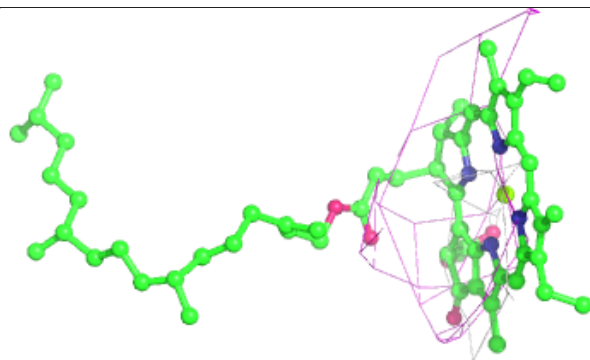
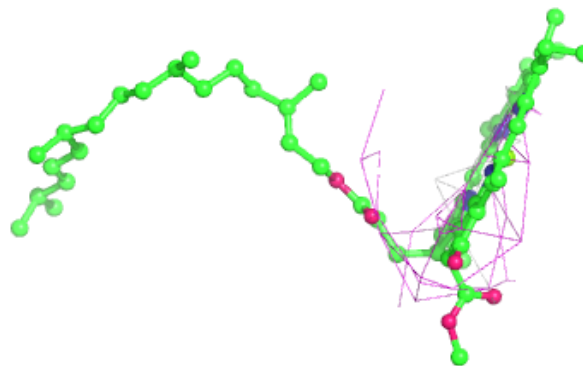


Electron density around BCR B 845:

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and green (positive)

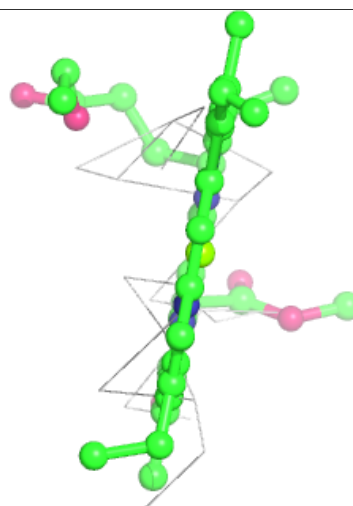
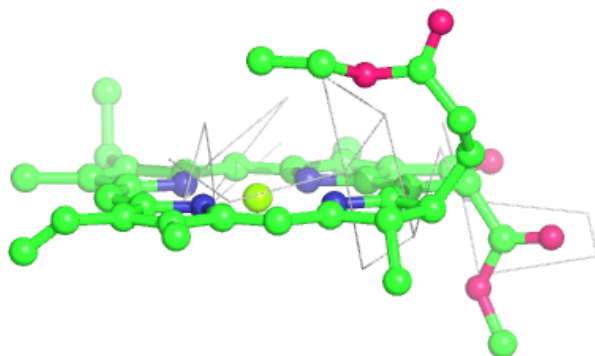
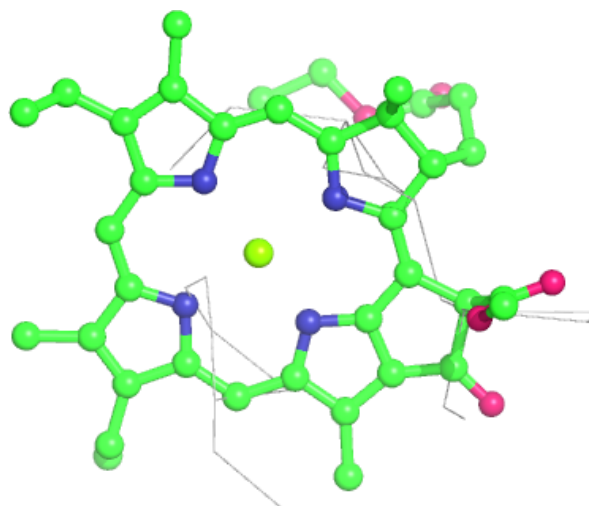
**Electron density around CLA B 840:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



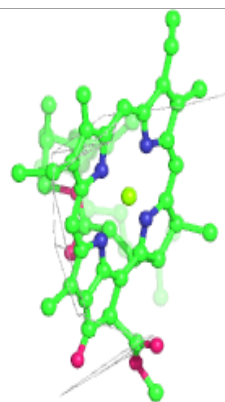
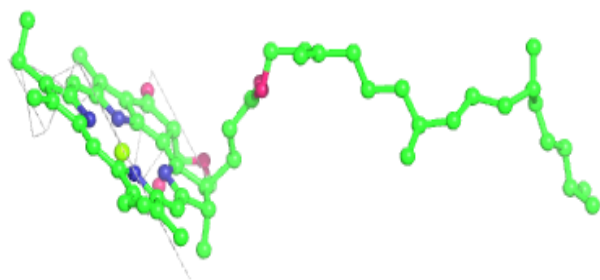
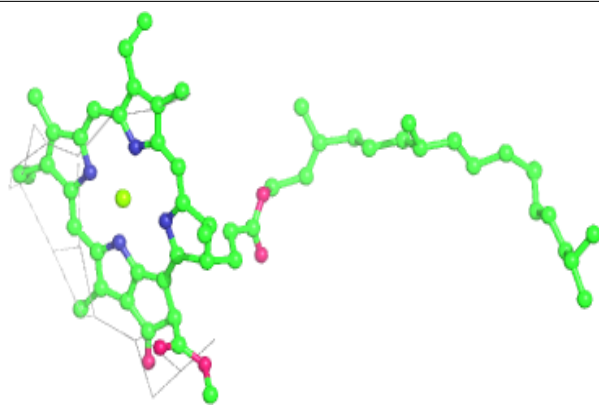
Electron density around CLA B 820:

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and green (positive)

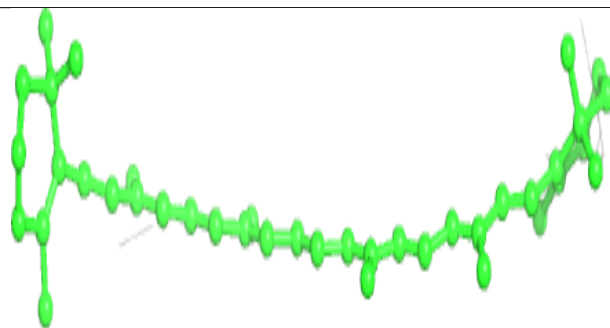
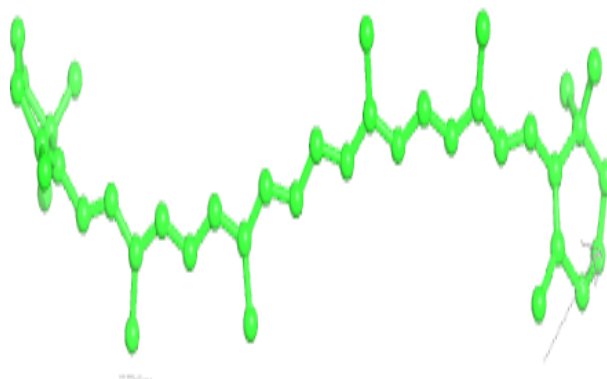


Electron density around CLA A 822:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

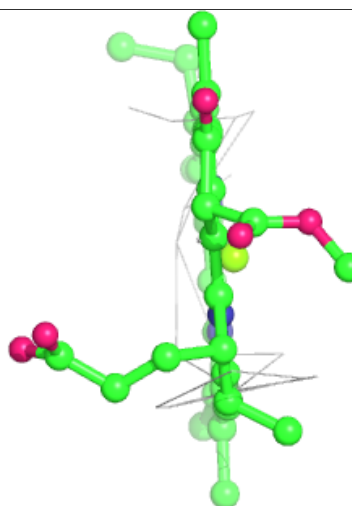
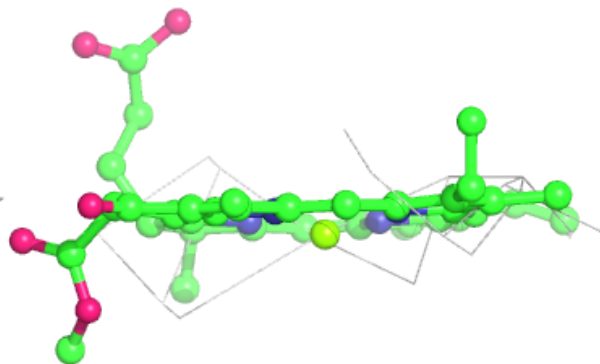
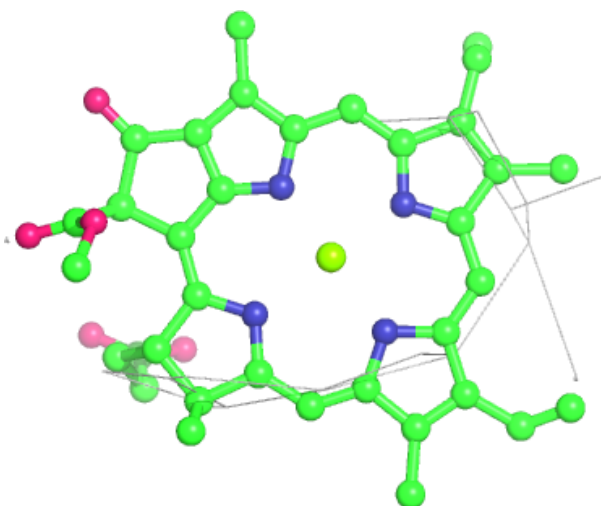
**Electron density around BCR A 853:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



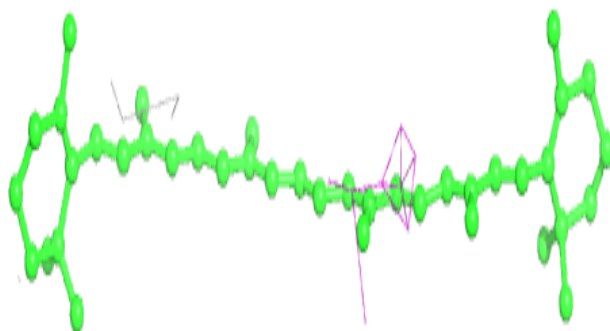
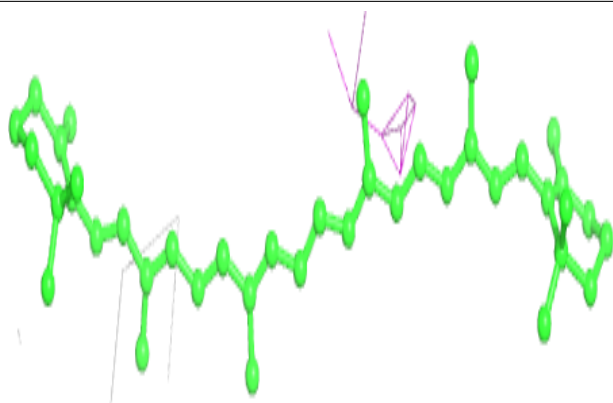
Electron density around CLA B 815:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

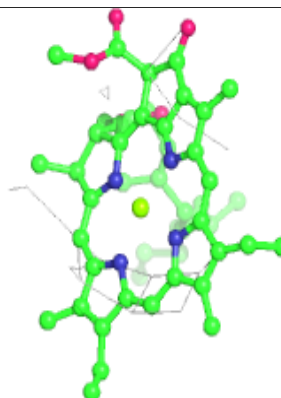
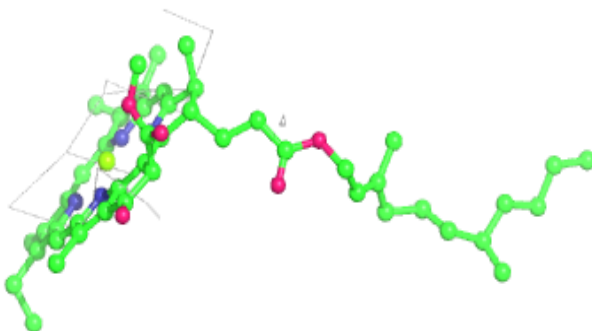
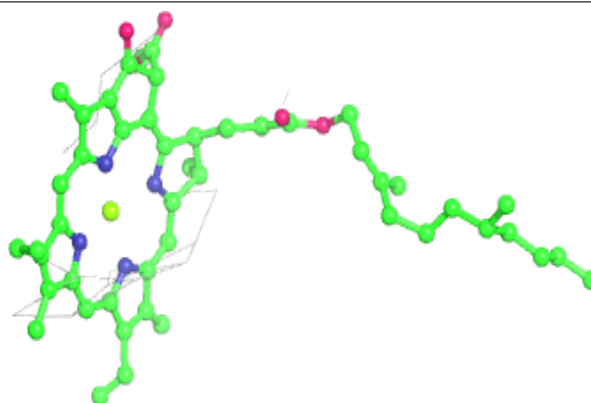


Electron density around BCR A 850:

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and green (positive)

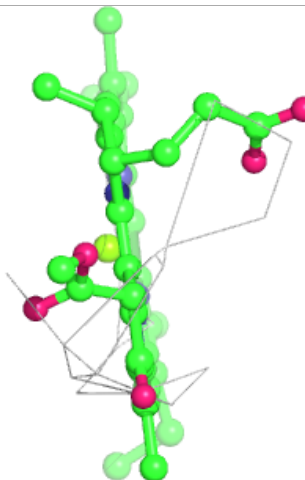
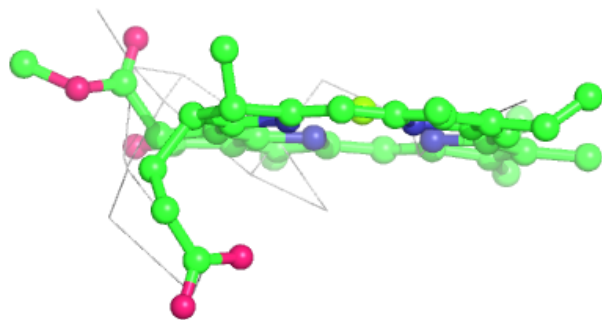
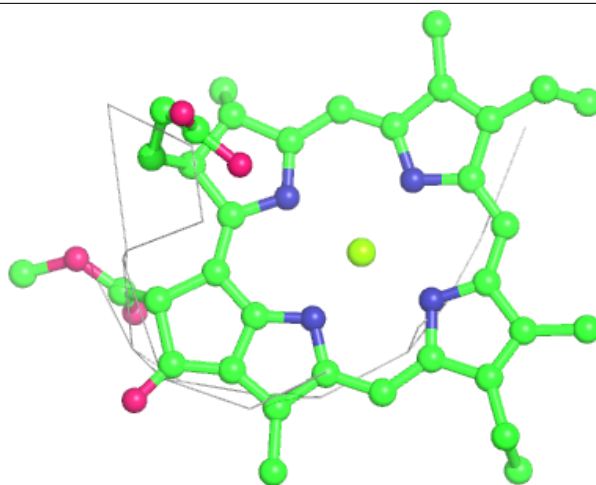
**Electron density around CLA B 833:**

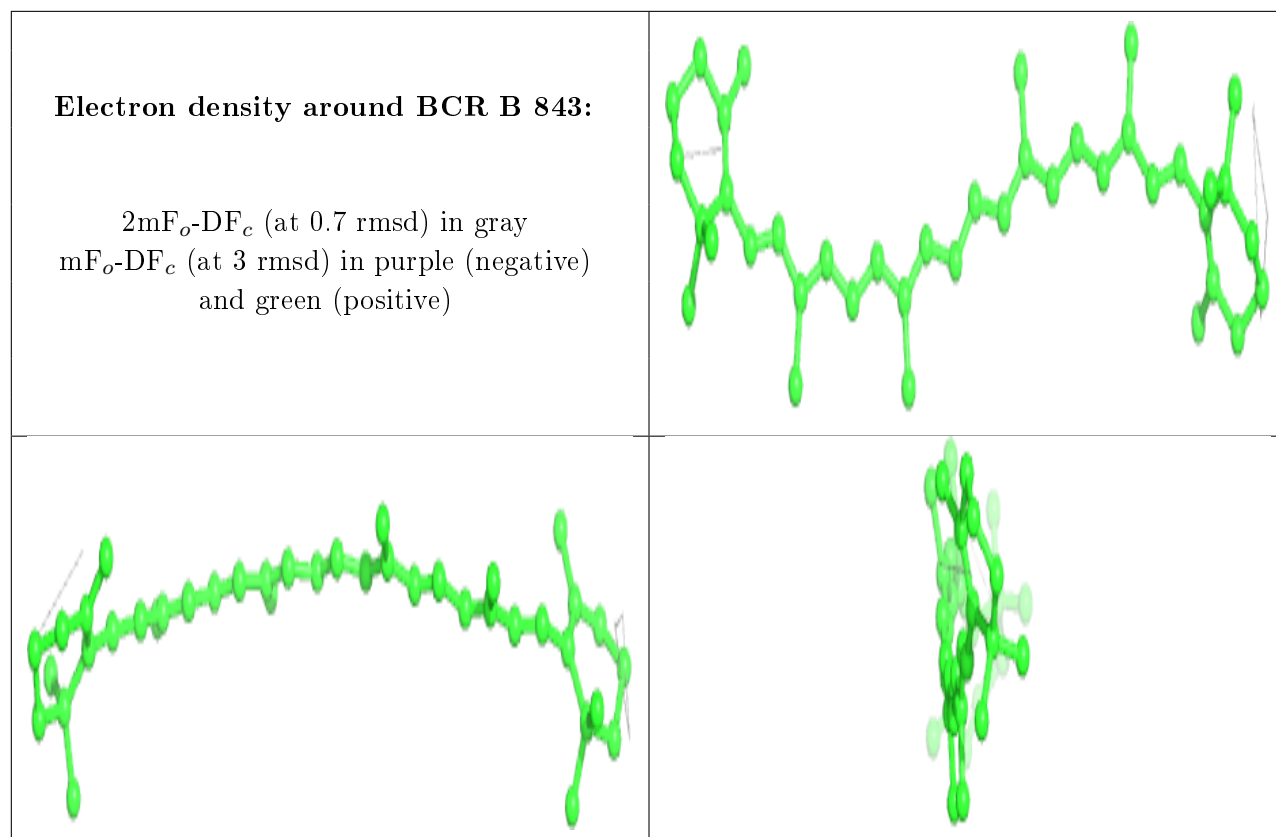
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 811:

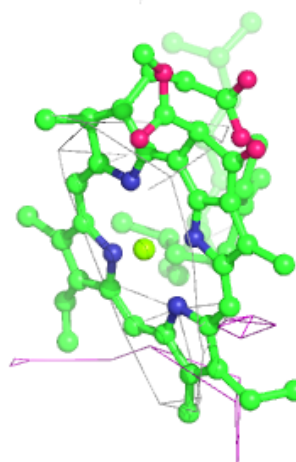
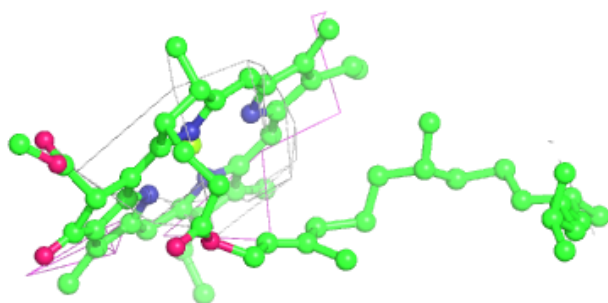
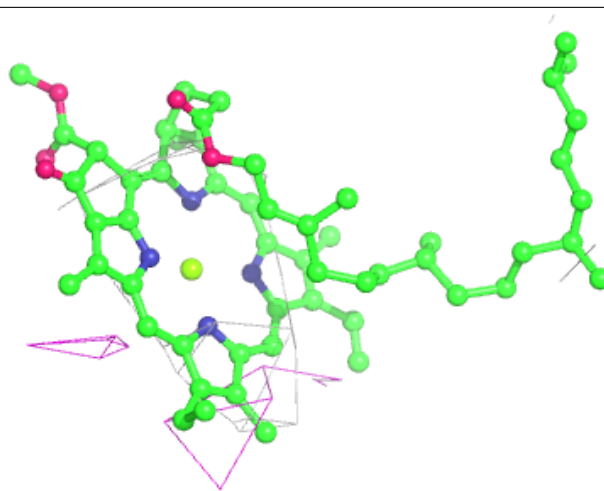
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





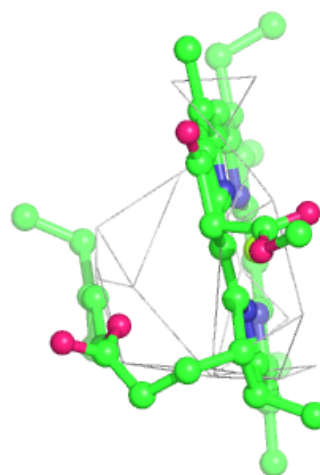
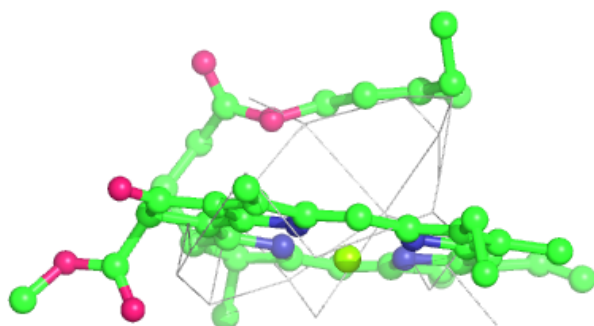
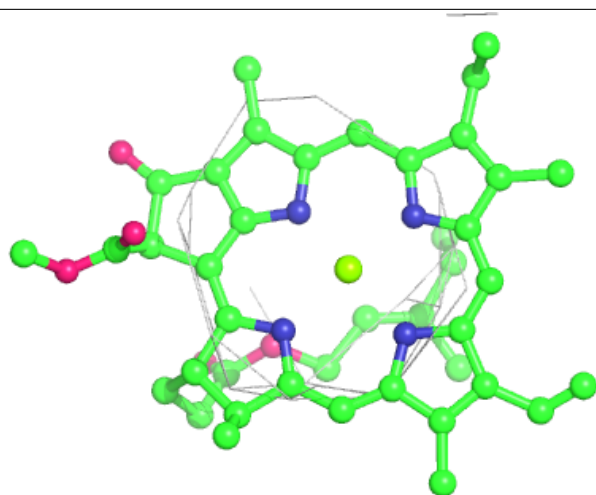
Electron density around CLA A 844:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



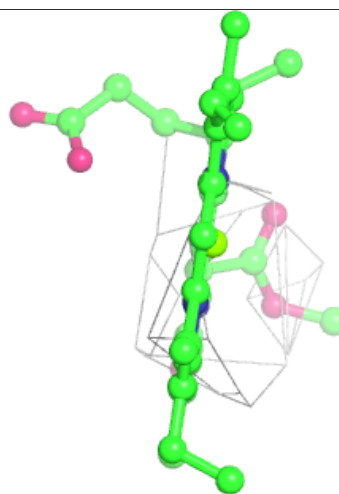
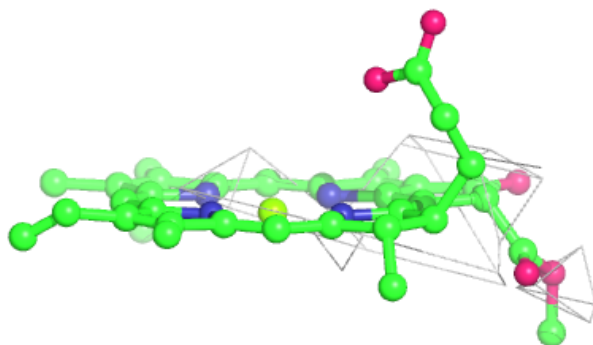
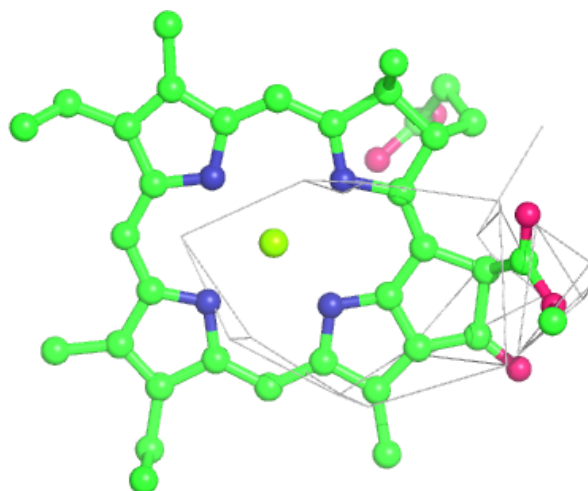
Electron density around CLA A 824:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



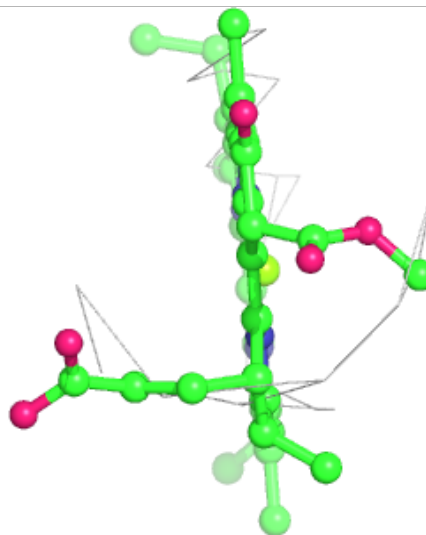
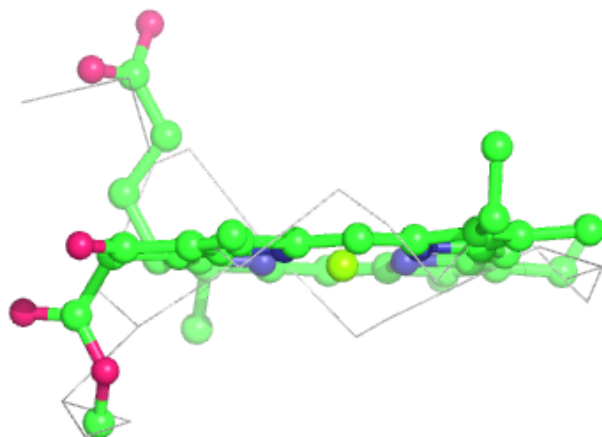
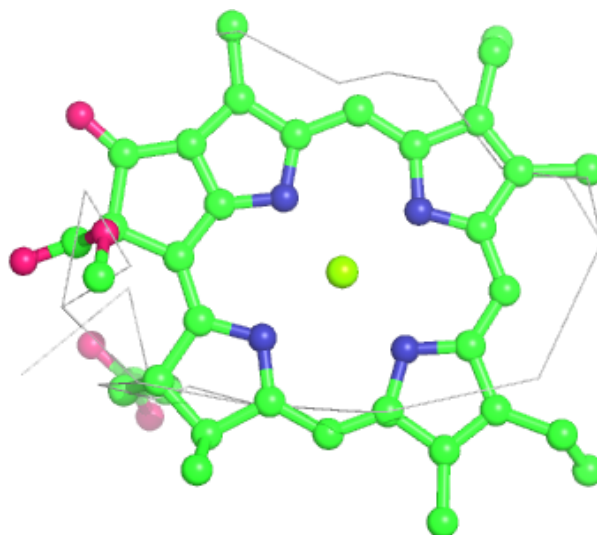
Electron density around CLA M 1601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



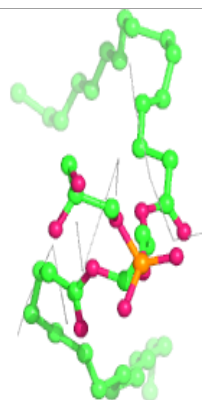
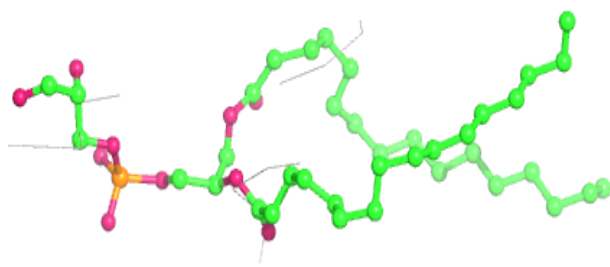
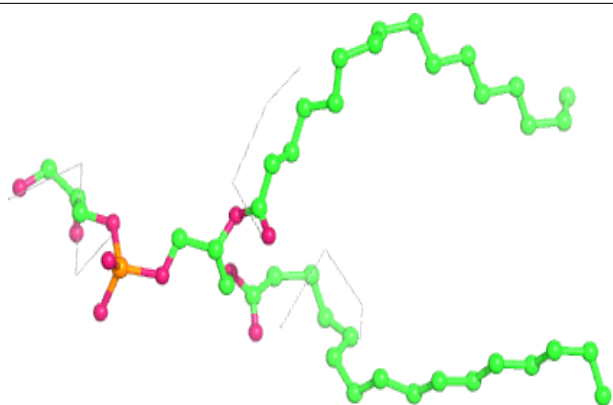
Electron density around CLA A 816:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

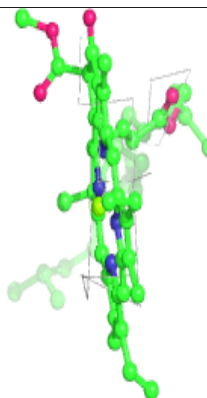
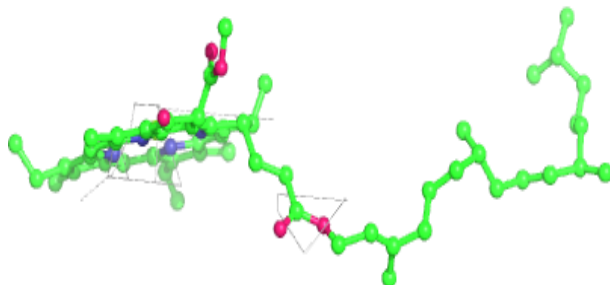
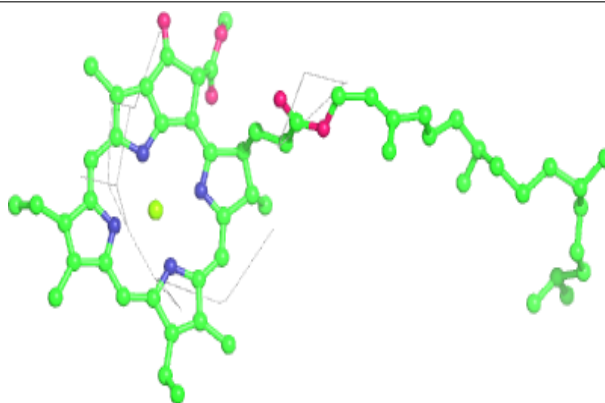


Electron density around LHG A 855:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

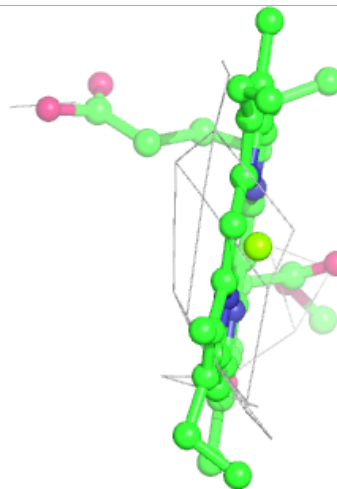
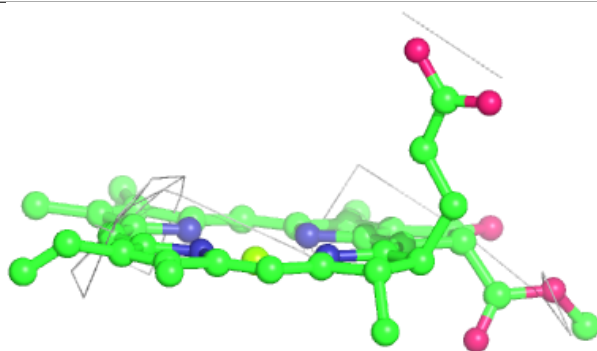
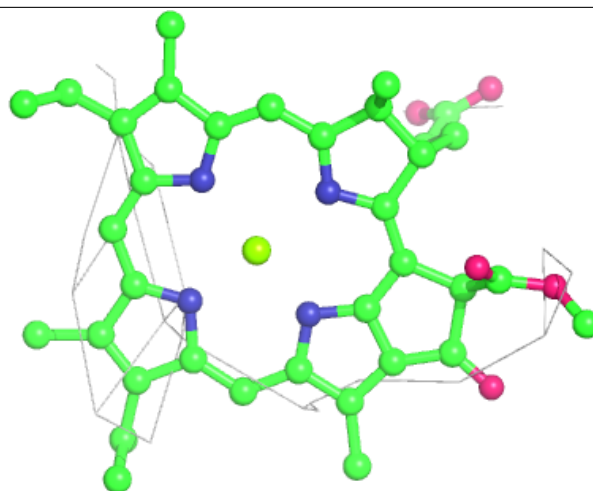
**Electron density around CLA A 827:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



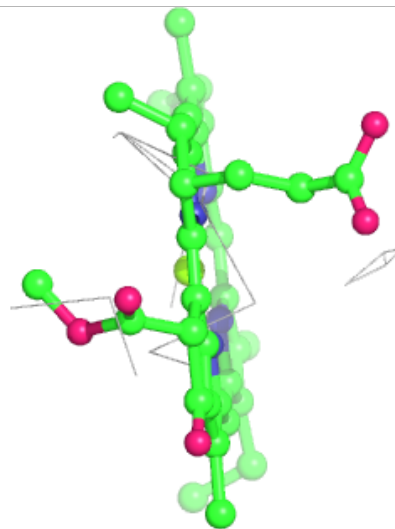
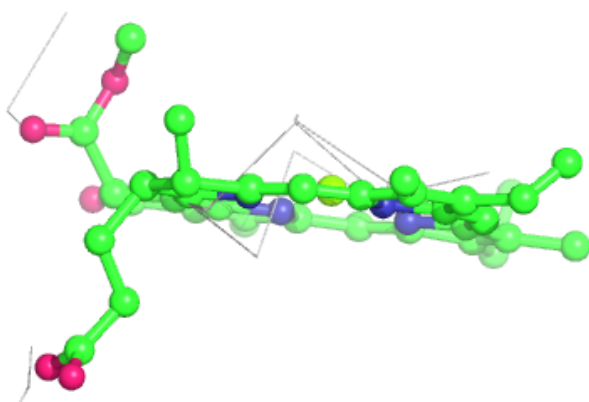
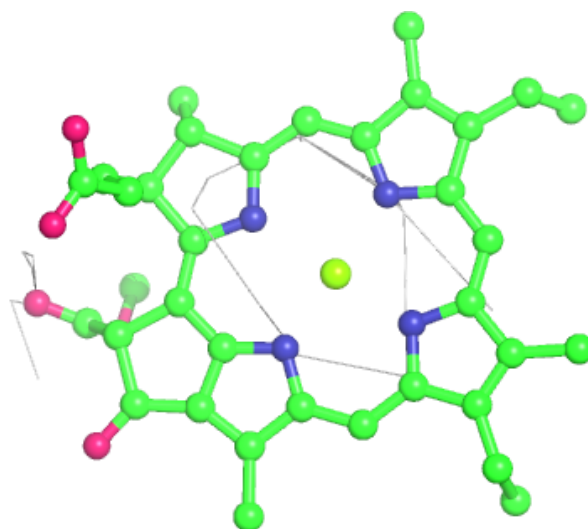
Electron density around CLA B 811:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



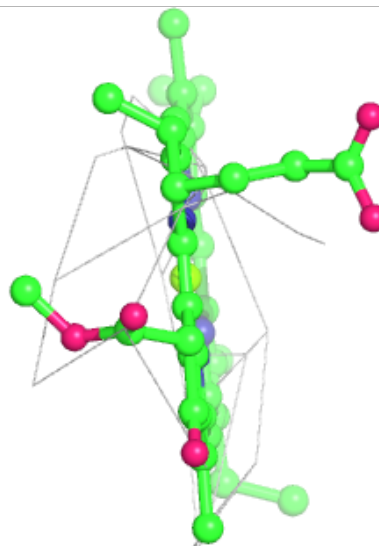
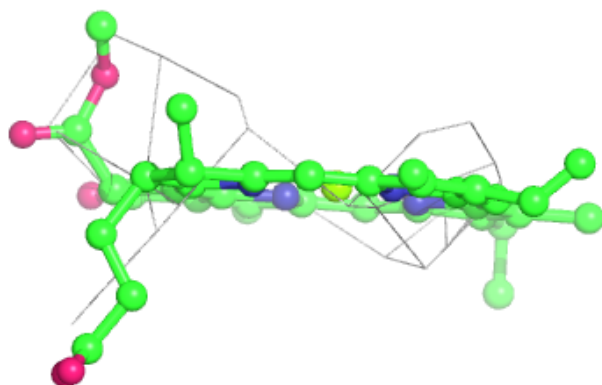
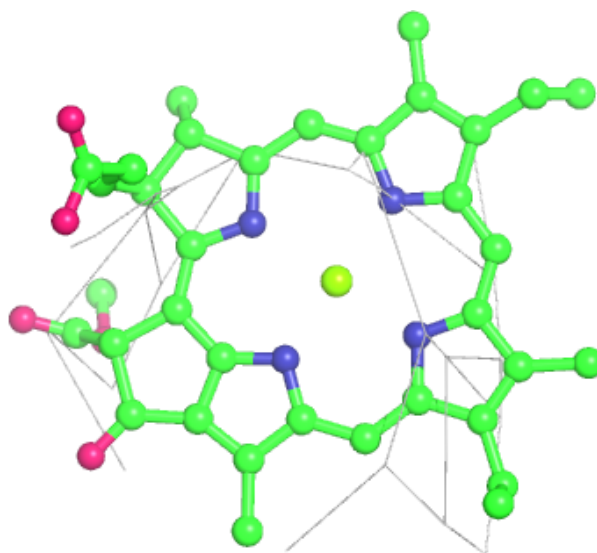
Electron density around CLA K 1401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



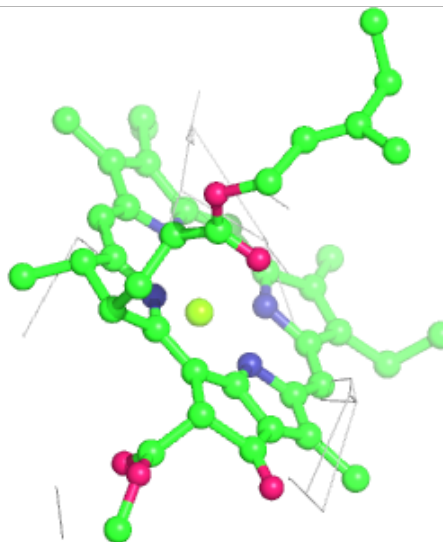
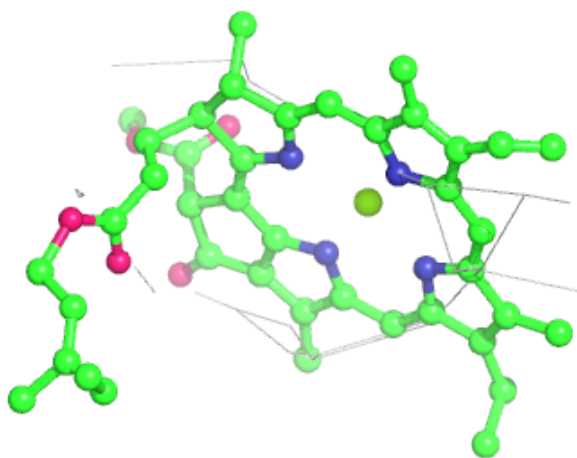
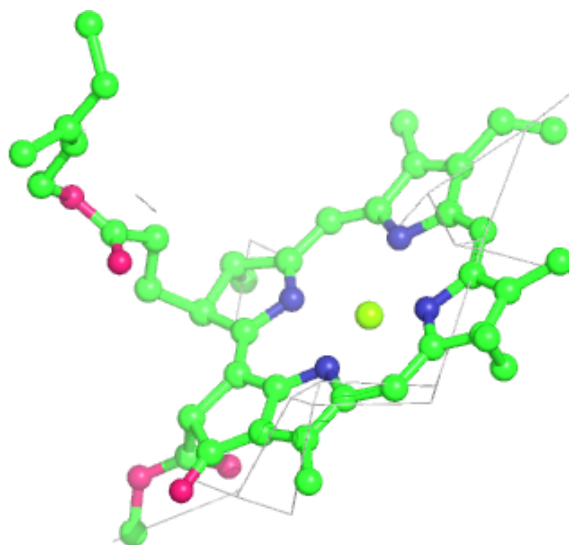
Electron density around CLA B 821:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



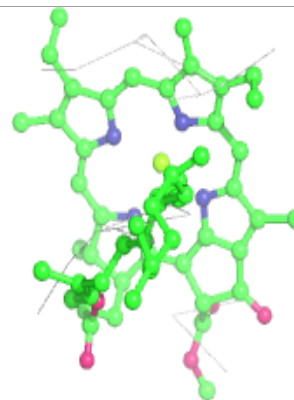
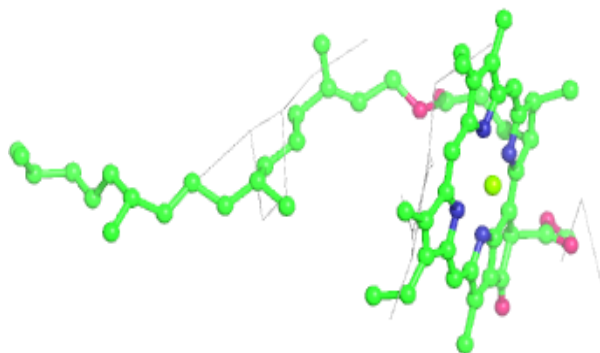
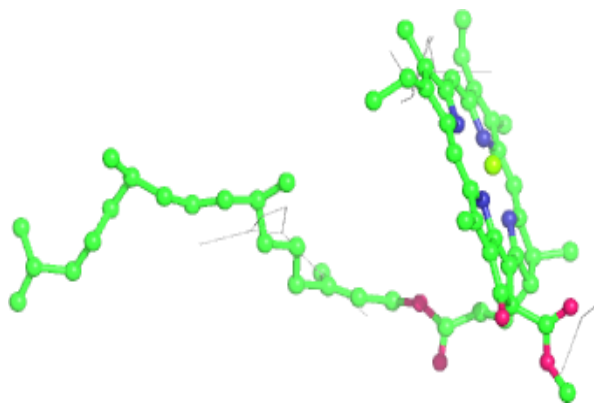
Electron density around CLA A 808:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



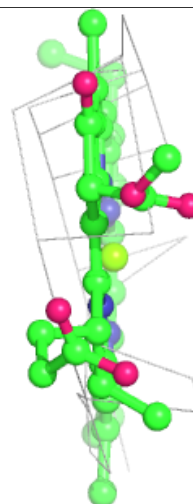
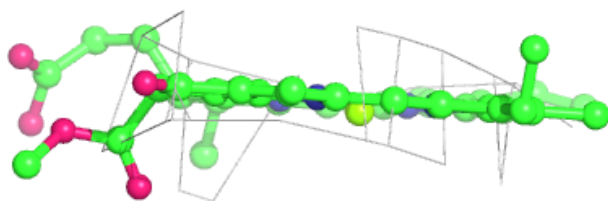
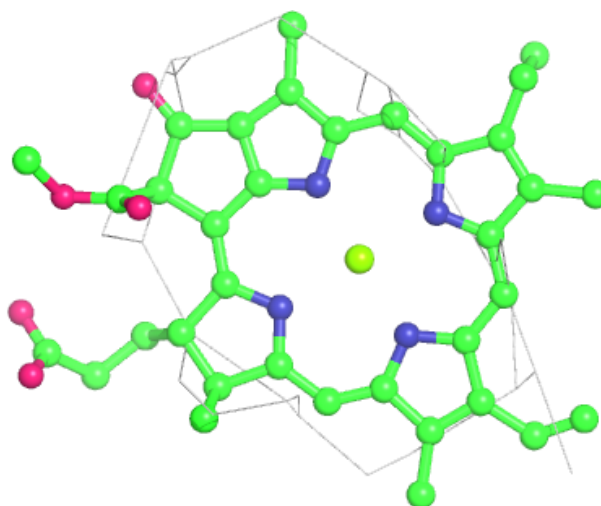
Electron density around CLA A 812:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



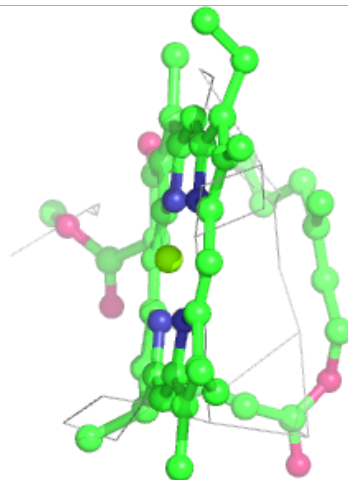
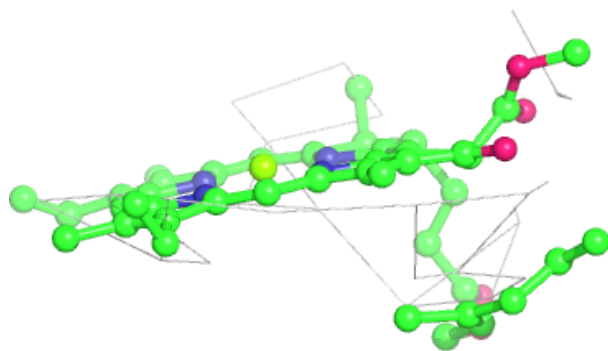
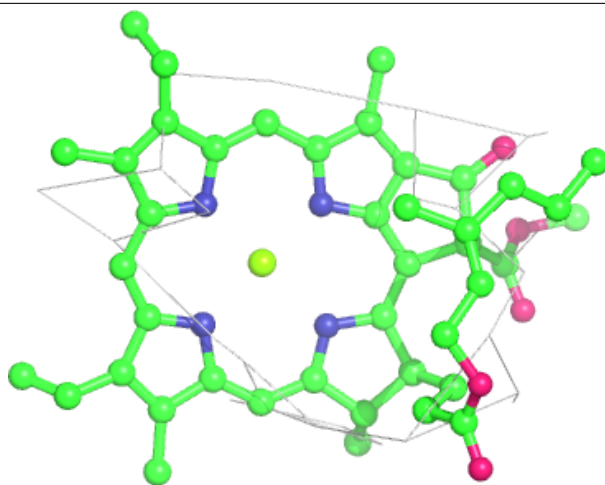
Electron density around CLA B 836:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



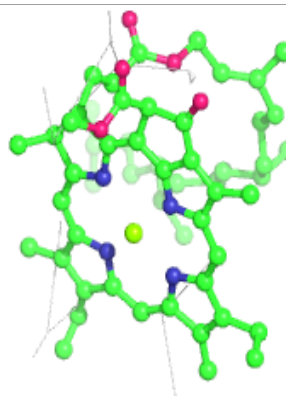
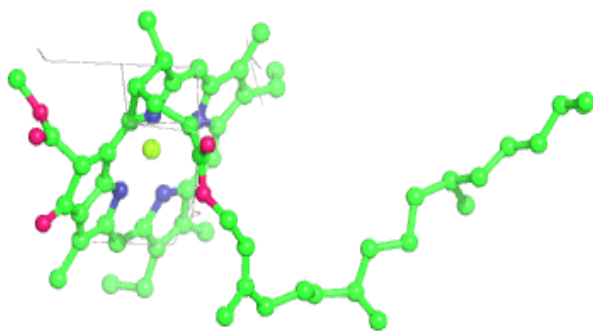
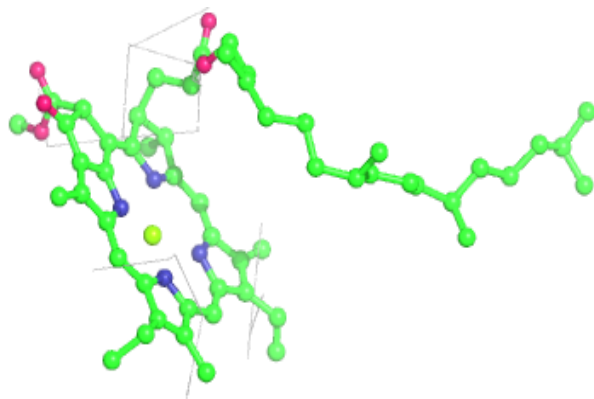
Electron density around CLA A 846:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



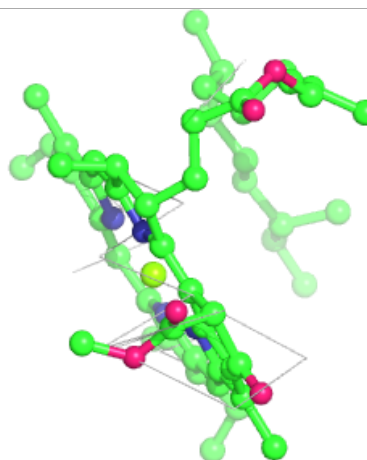
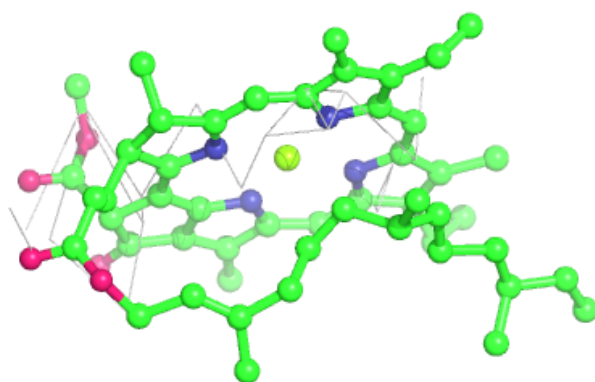
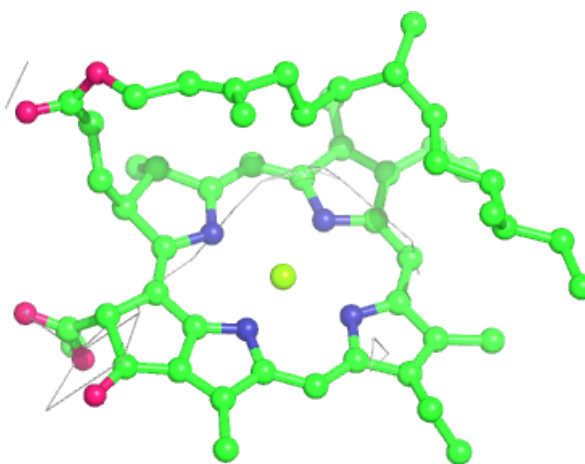
Electron density around CLA B 814:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



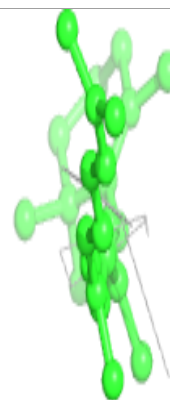
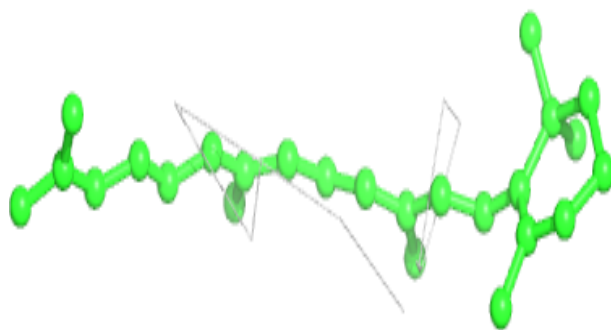
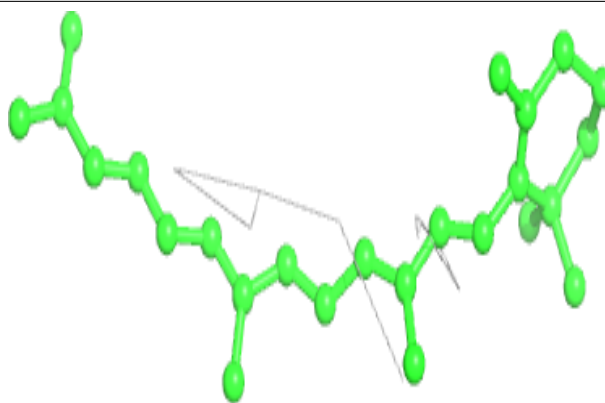
Electron density around CLA A 821:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



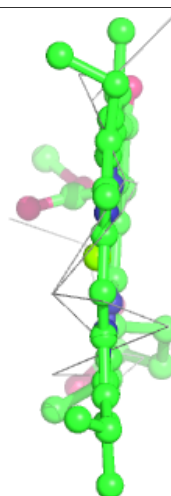
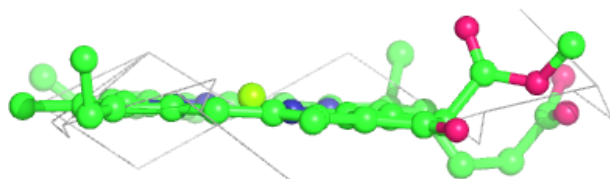
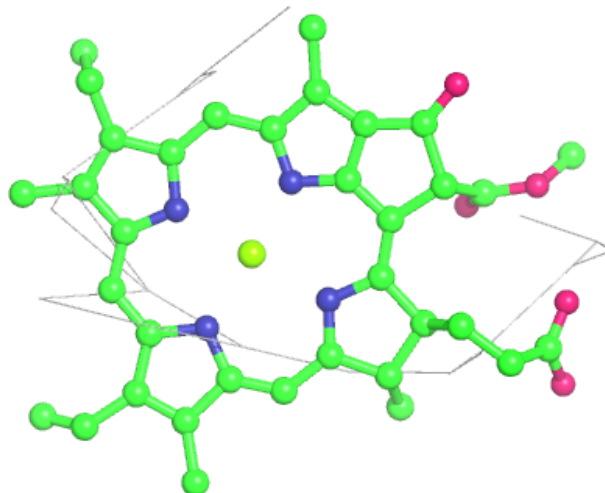
Electron density around BCR B 846:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



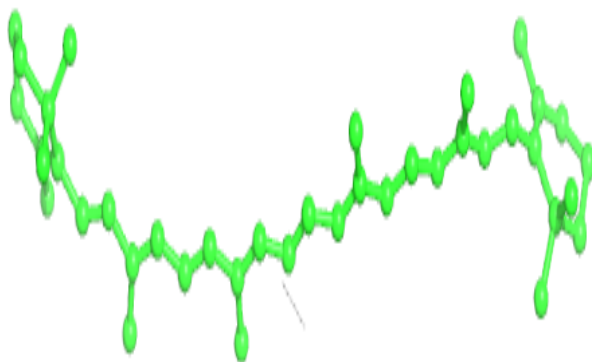
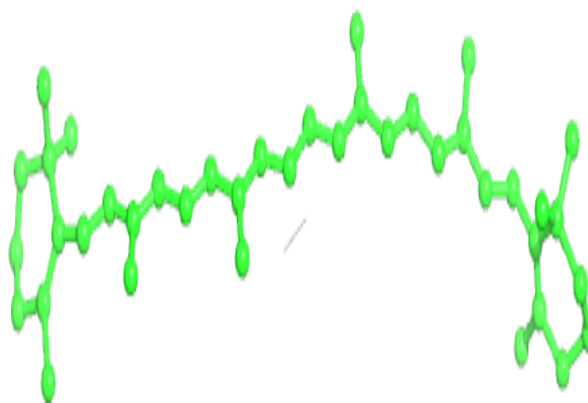
Electron density around CLA F 1301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



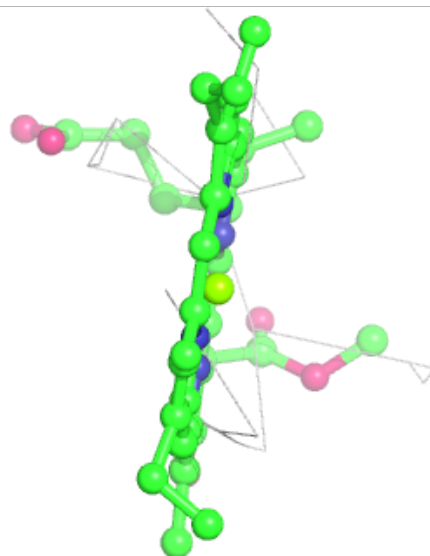
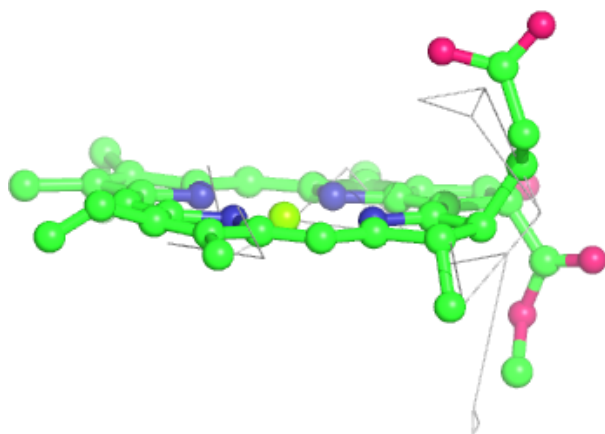
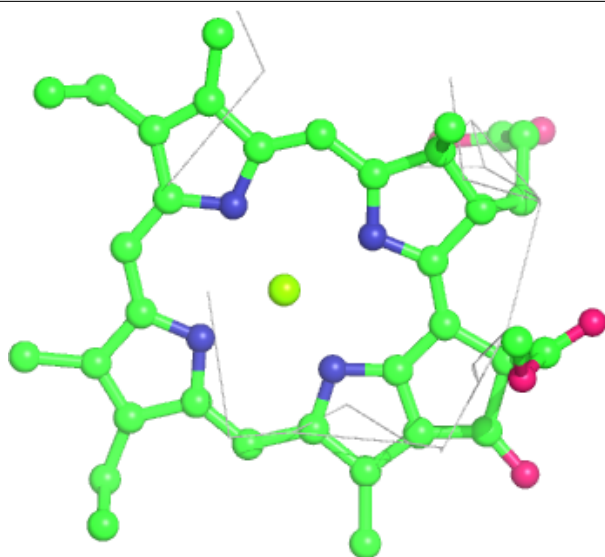
Electron density around BCR M 1602:

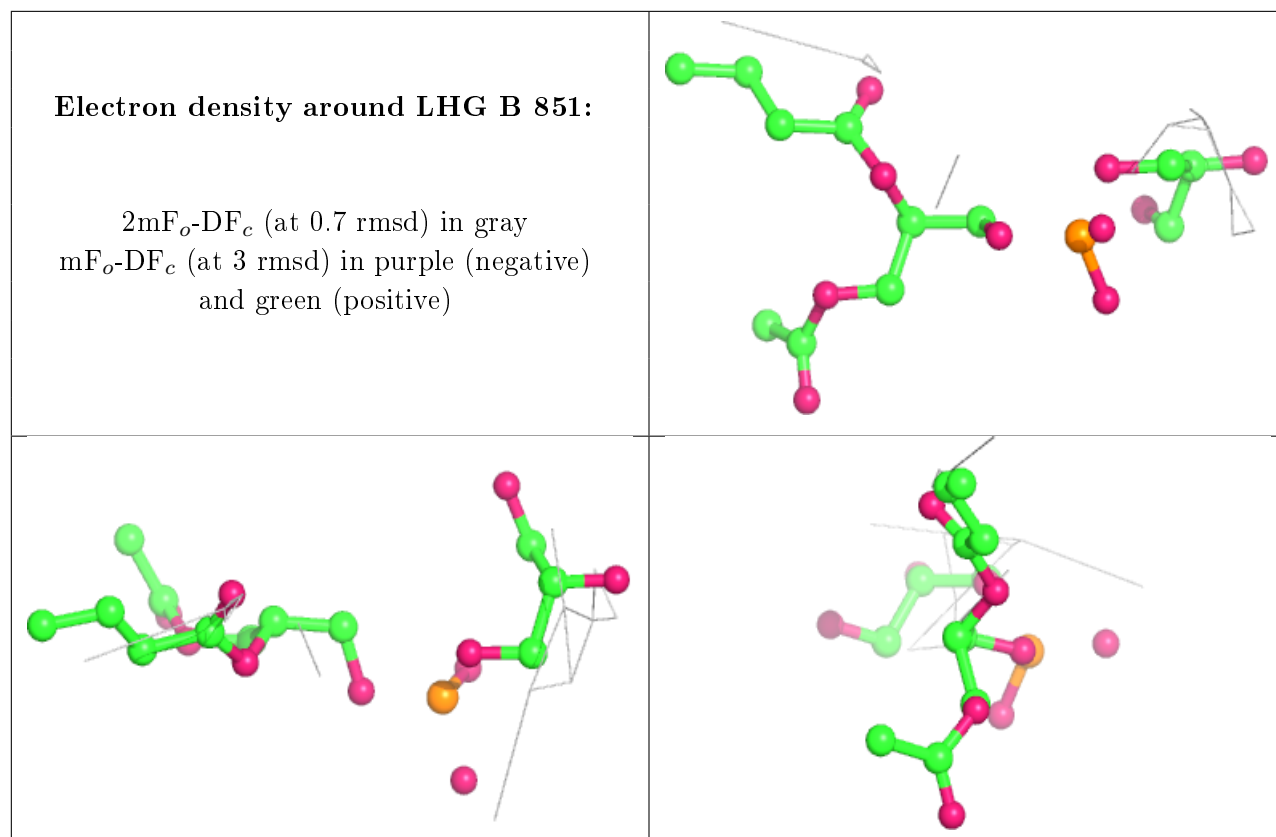
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 830:

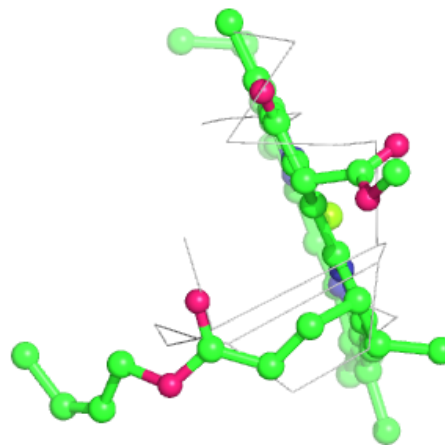
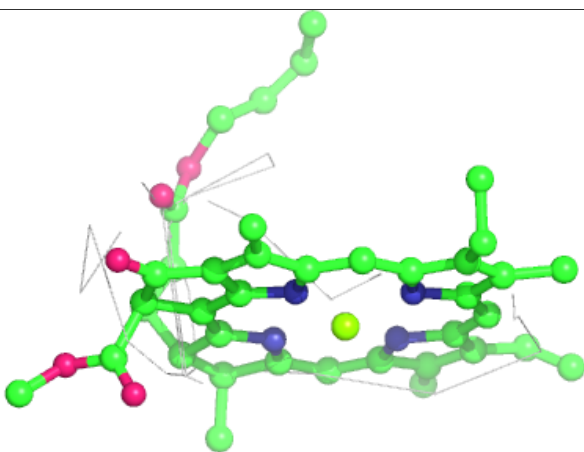
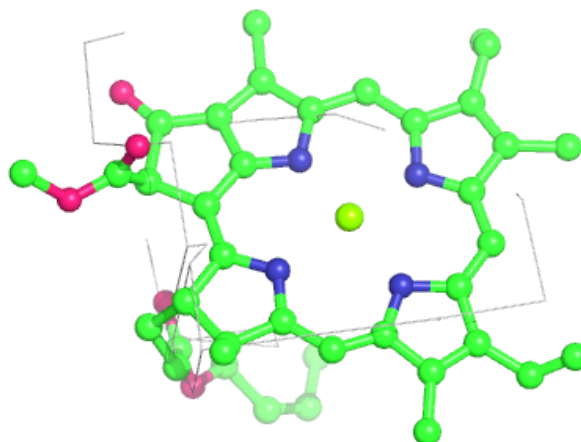
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





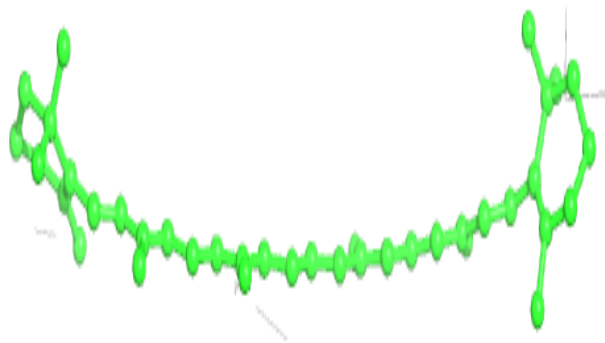
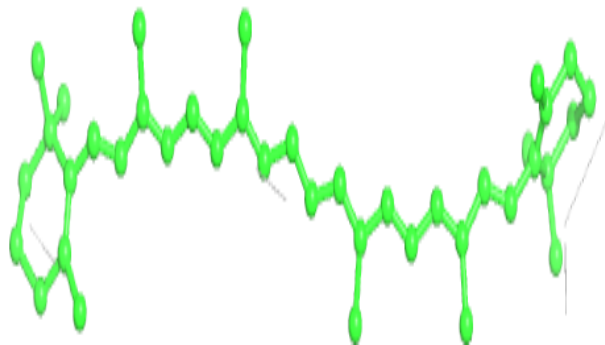
Electron density around CLA B 831:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



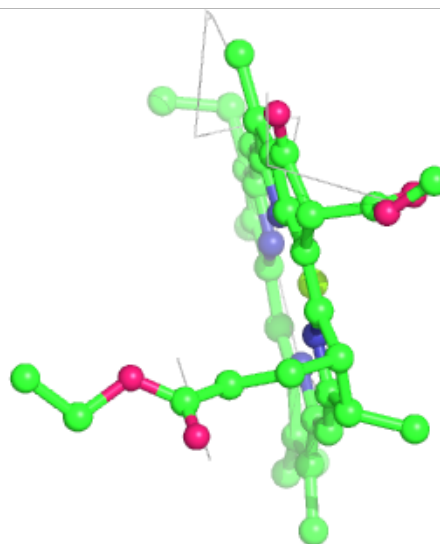
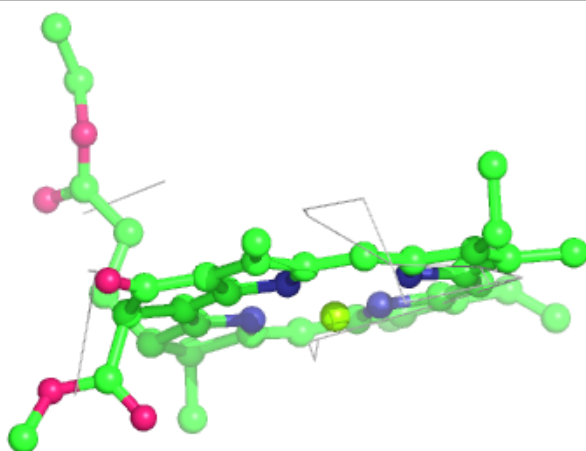
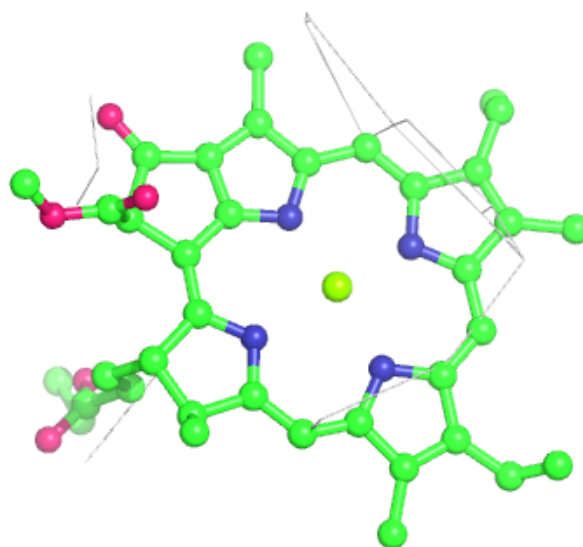
Electron density around BCR A 849:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



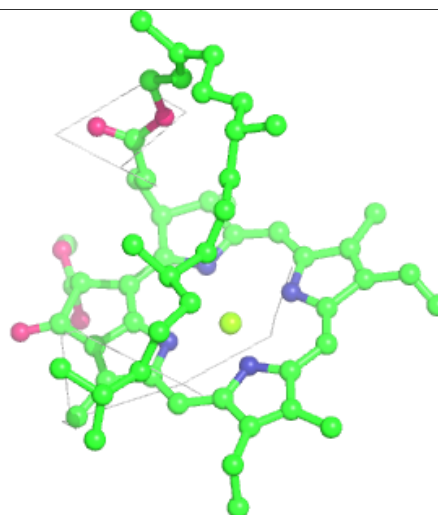
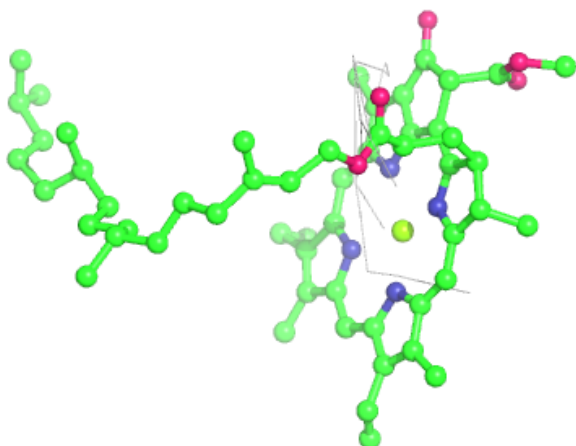
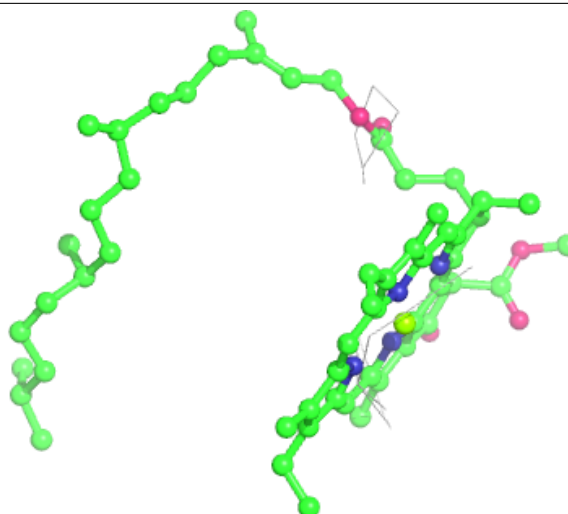
Electron density around CLA B 839:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



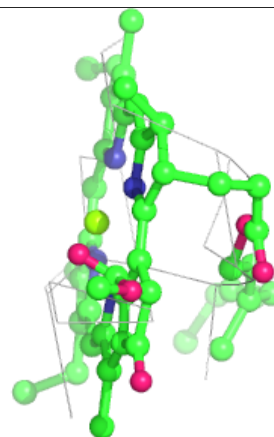
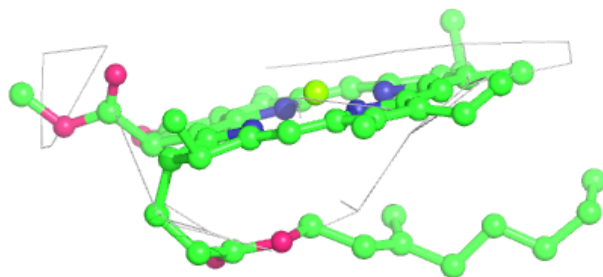
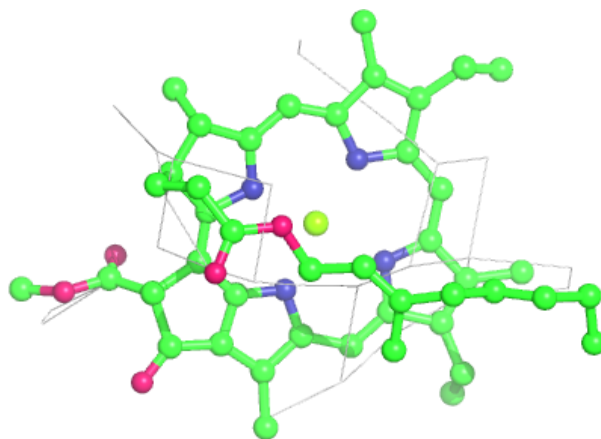
Electron density around CLA B 819:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

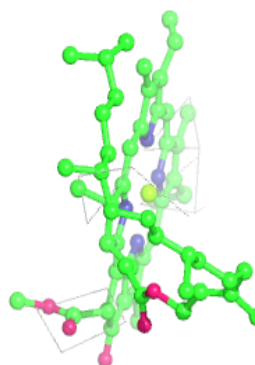
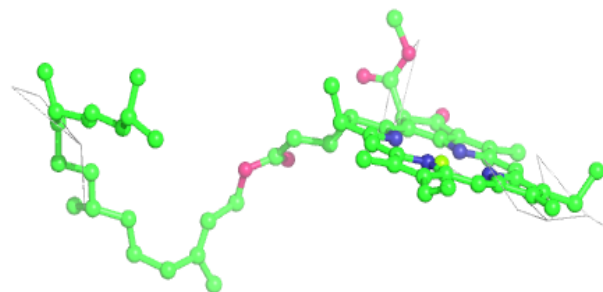
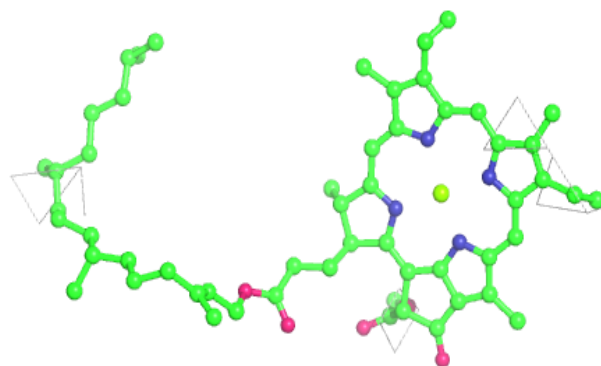


Electron density around CLA A 818:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

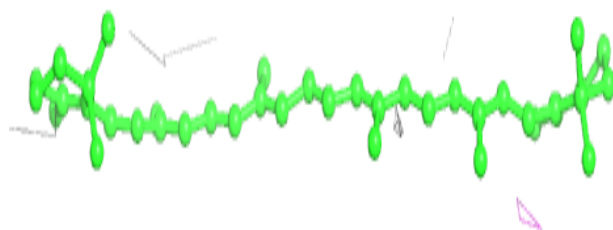
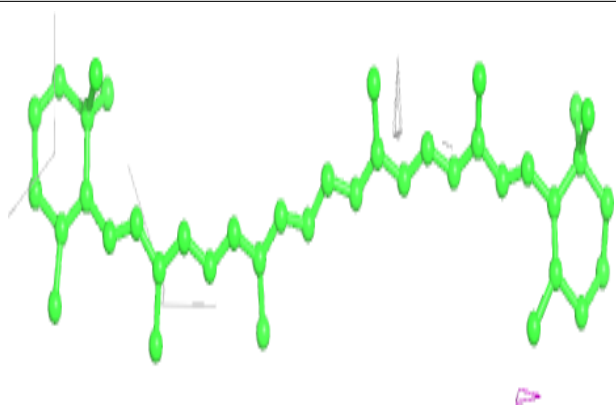
**Electron density around CLA A 828:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

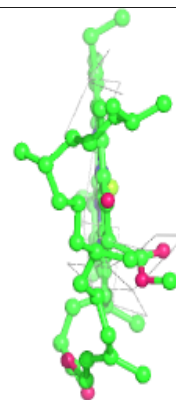
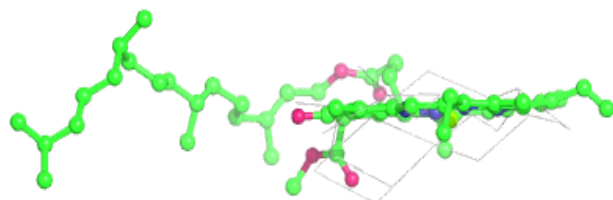
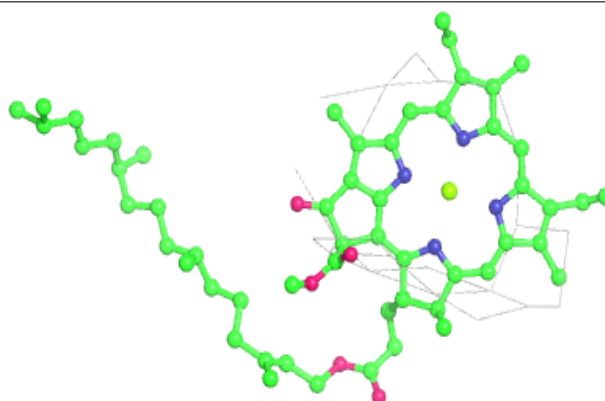


Electron density around BCR L 1005:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

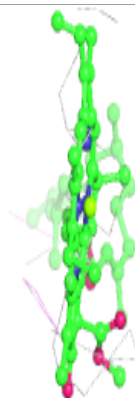
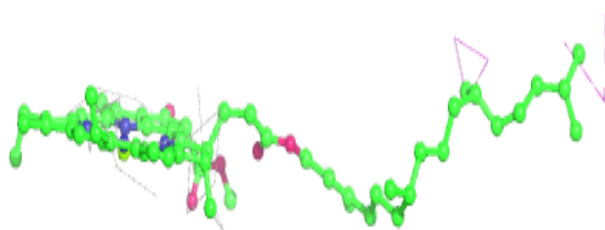
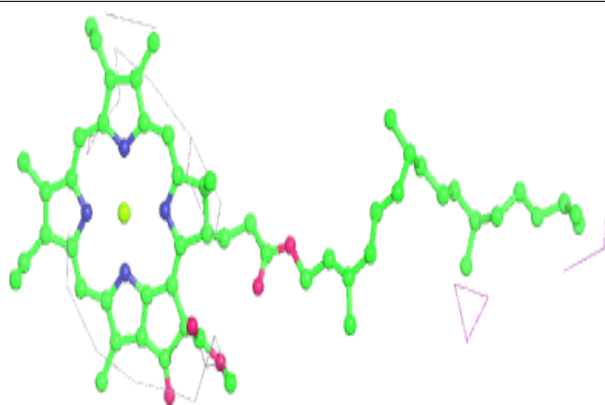
**Electron density around CLA L 1004:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

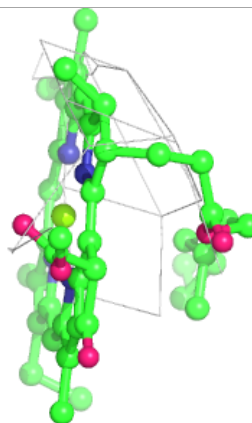
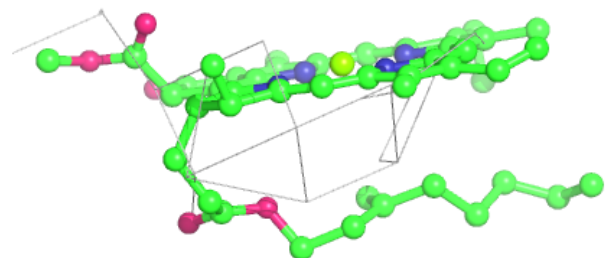
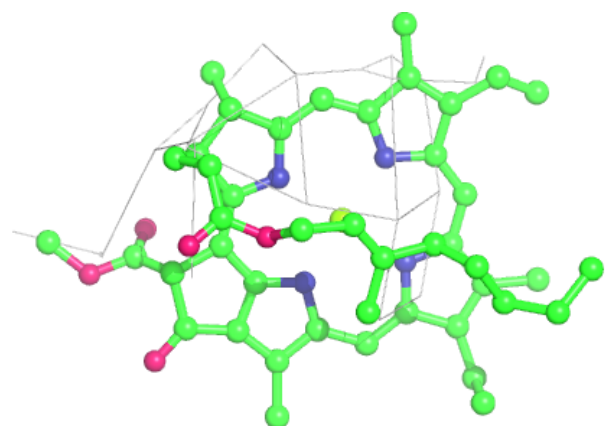


Electron density around CLA A 834:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

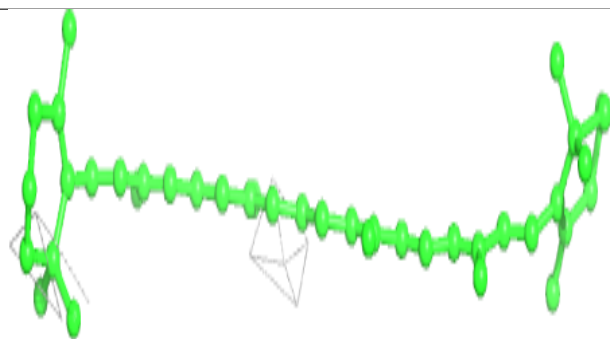
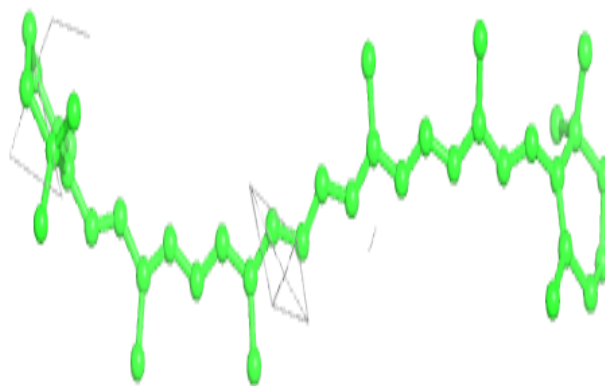
**Electron density around CLA A 813:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



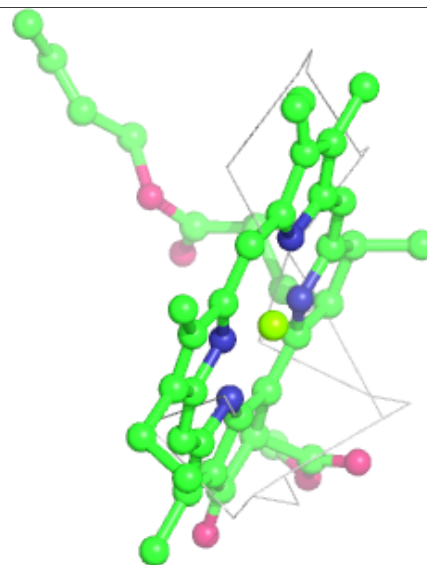
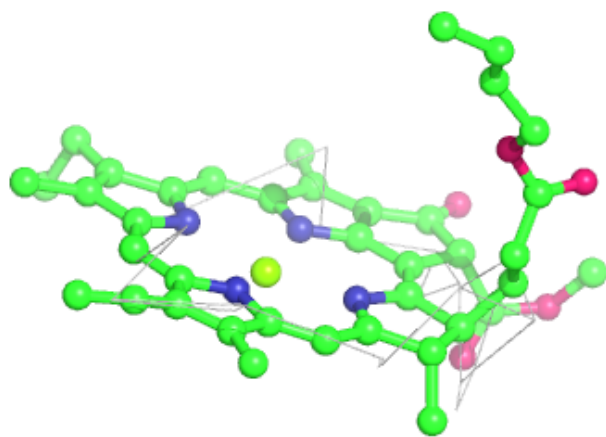
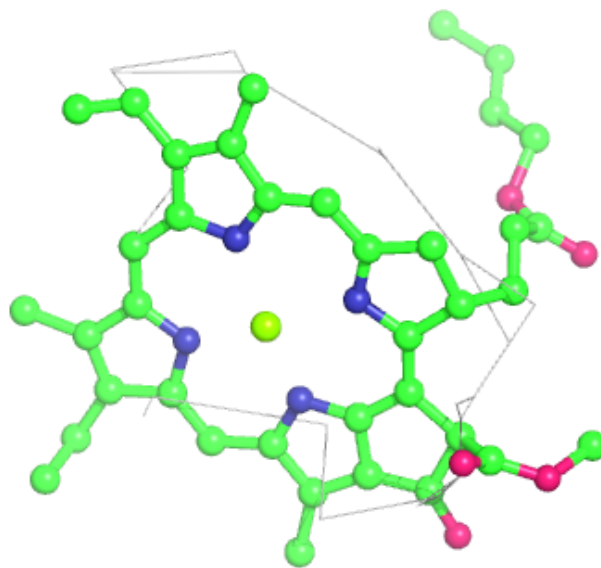
Electron density around BCR B 849:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



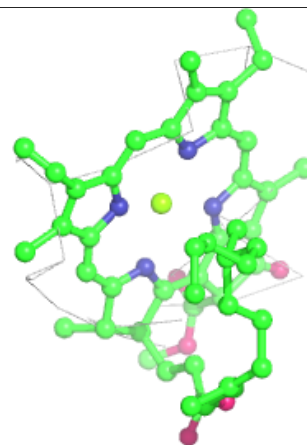
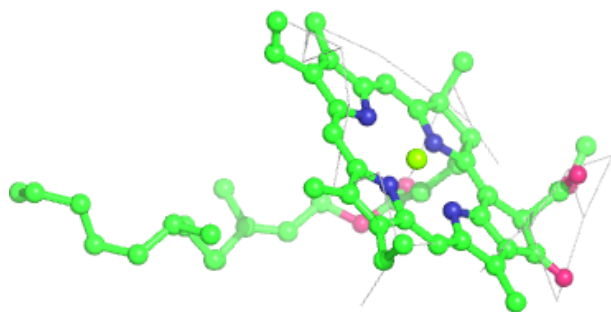
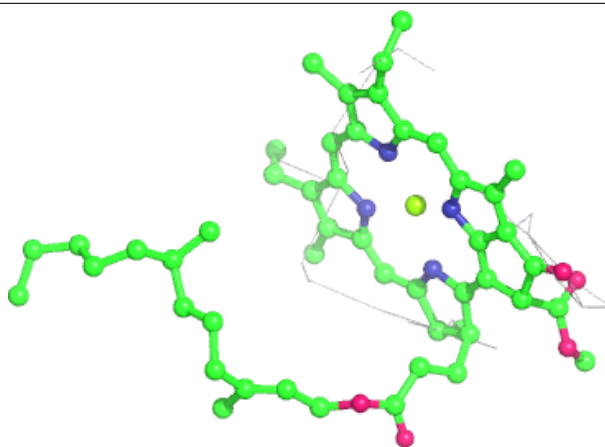
Electron density around CLA A 817:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

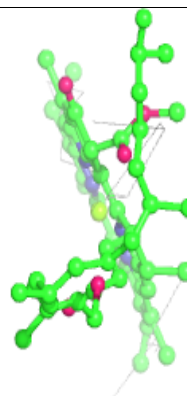
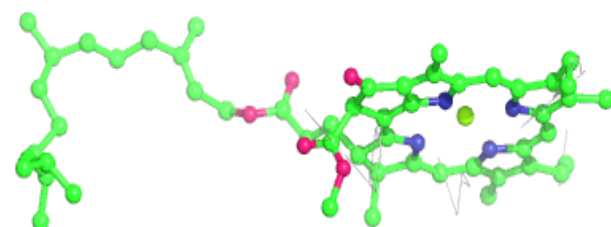
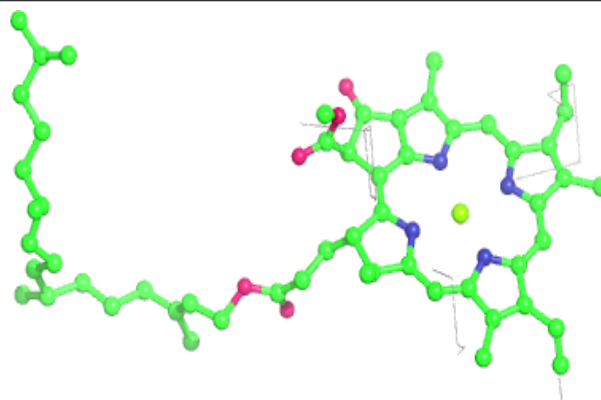


Electron density around CLA A 825:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

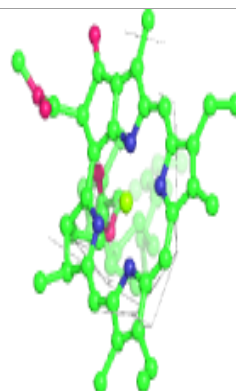
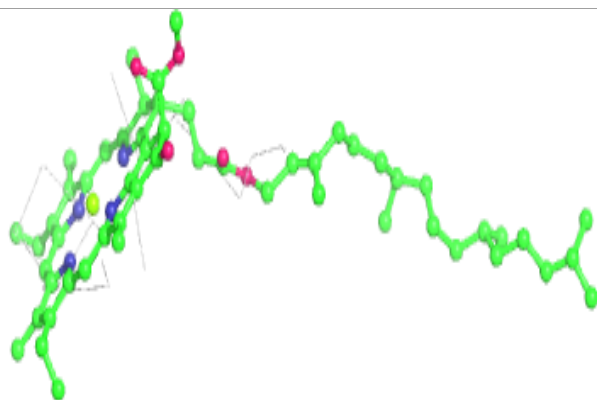
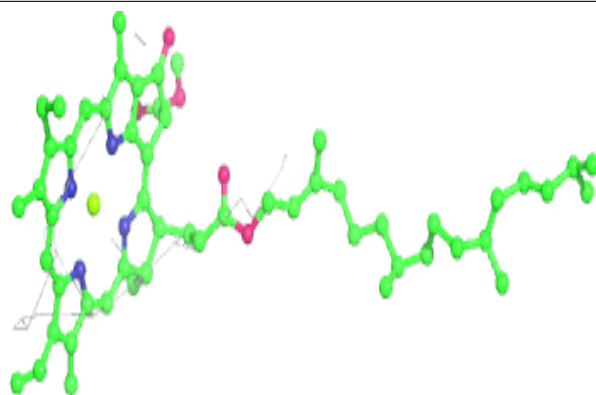
**Electron density around CLA B 826:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

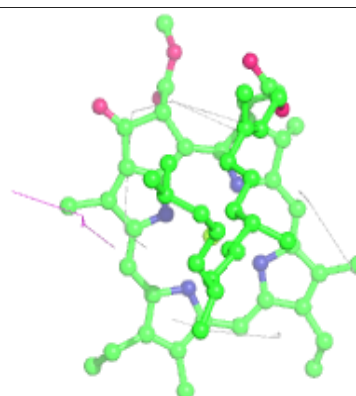
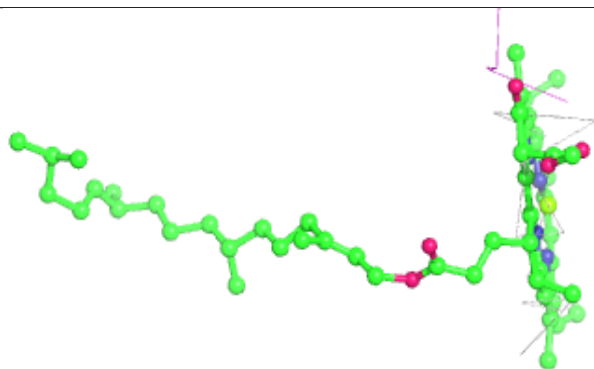
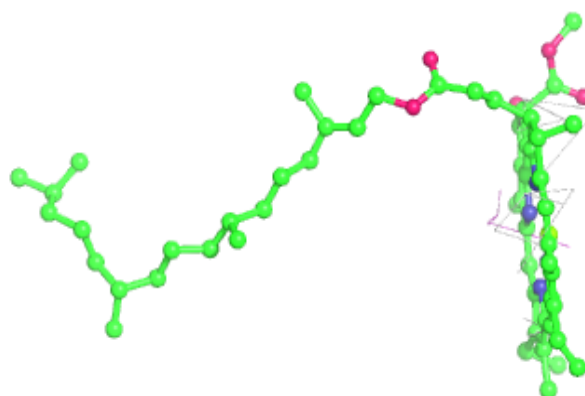


Electron density around CLA A 810:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

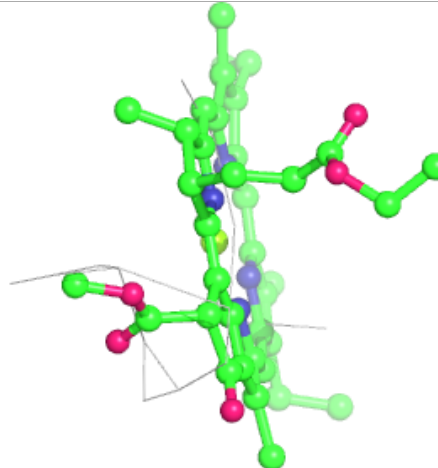
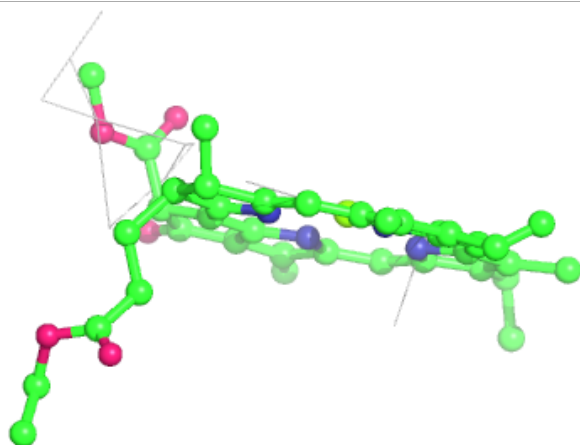
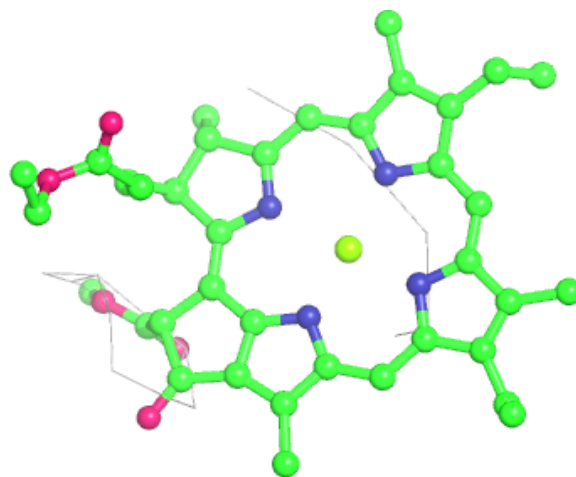
**Electron density around CLA B 841:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



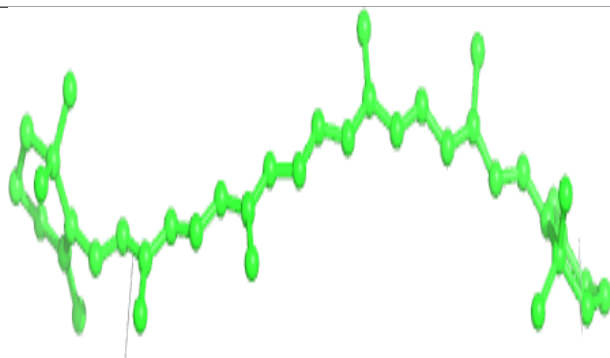
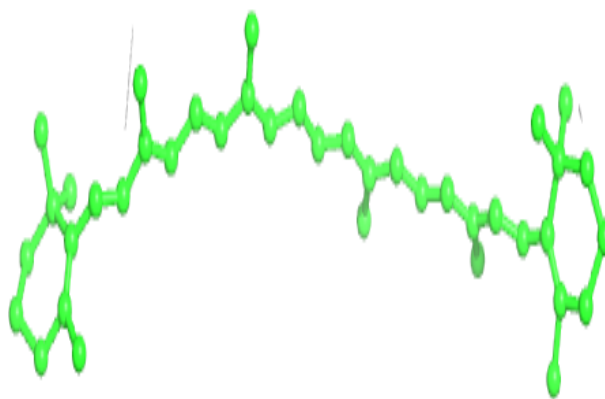
Electron density around CLA A 840:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

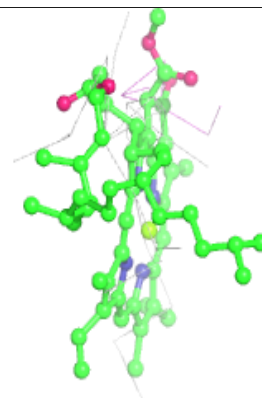
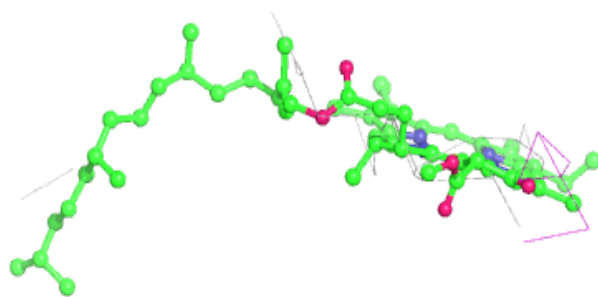
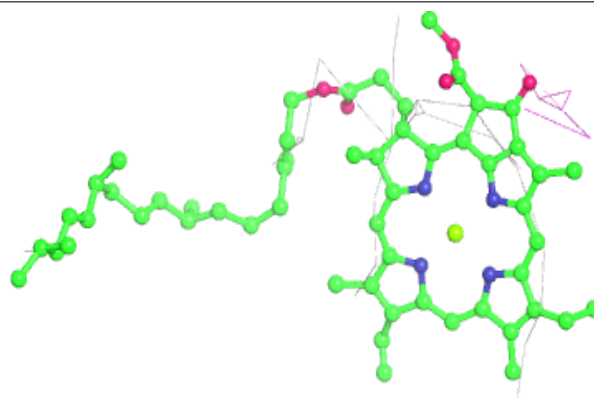


Electron density around BCR J 104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

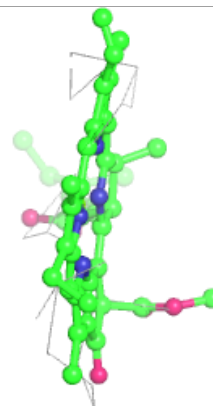
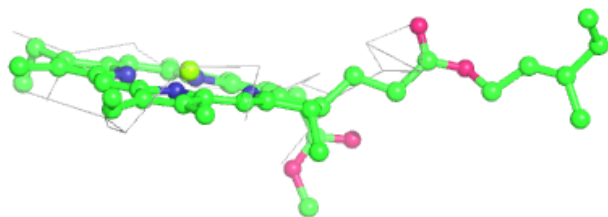
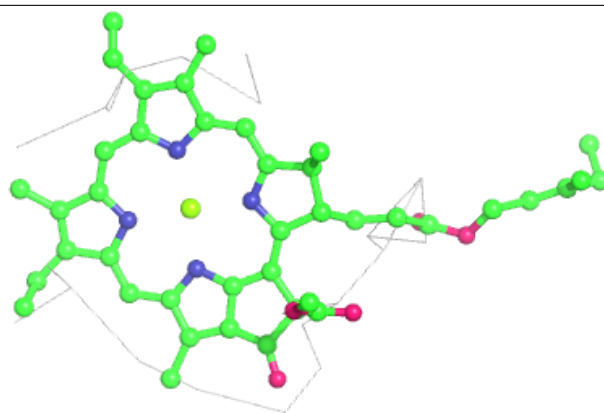
**Electron density around CLA B 803:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

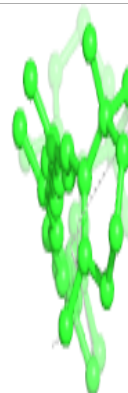
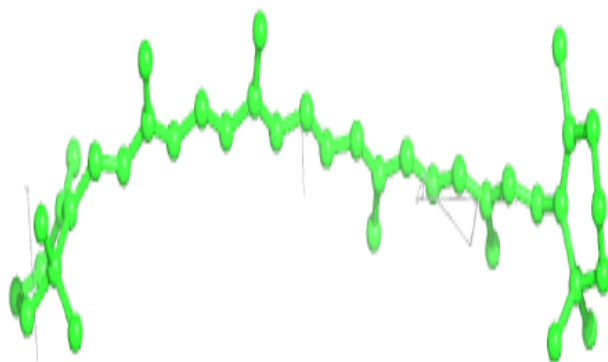
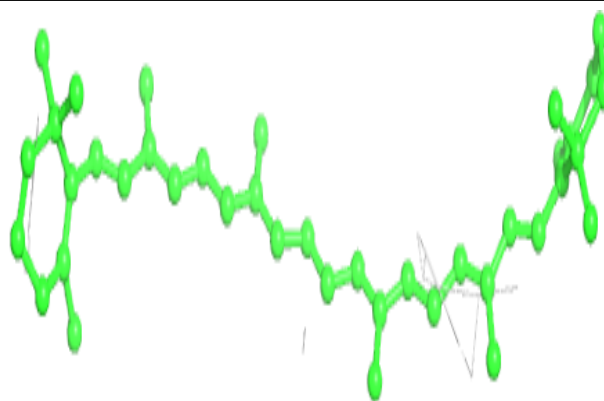


Electron density around CLA A 838:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

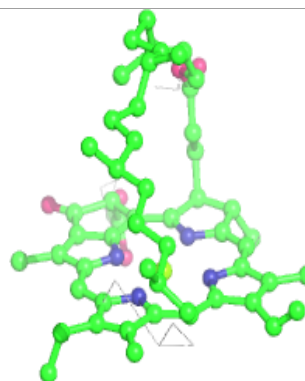
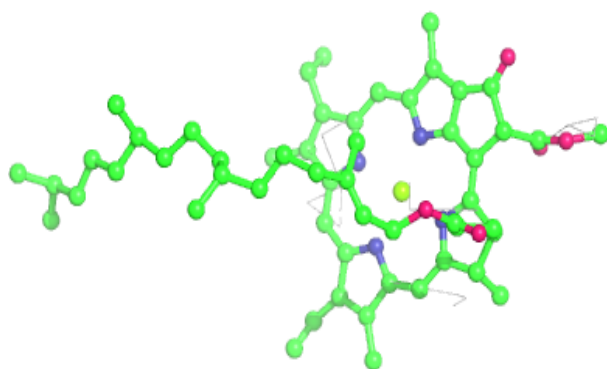
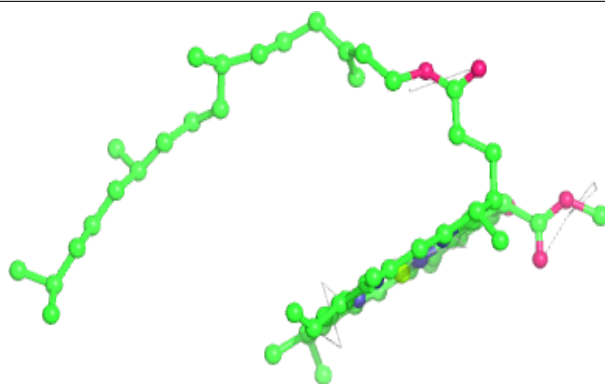
**Electron density around BCR I 101:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

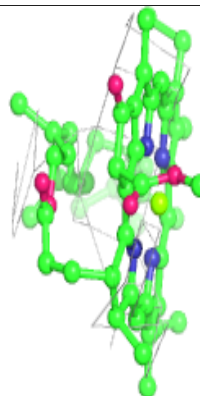
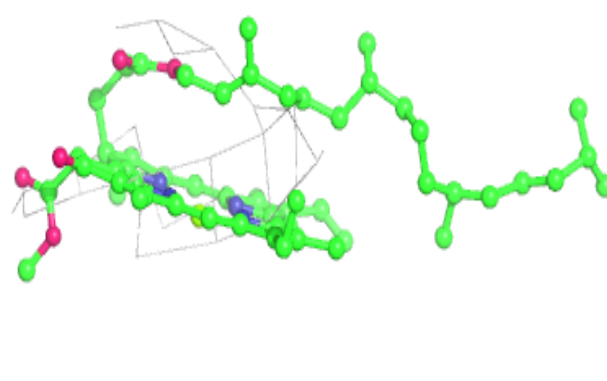
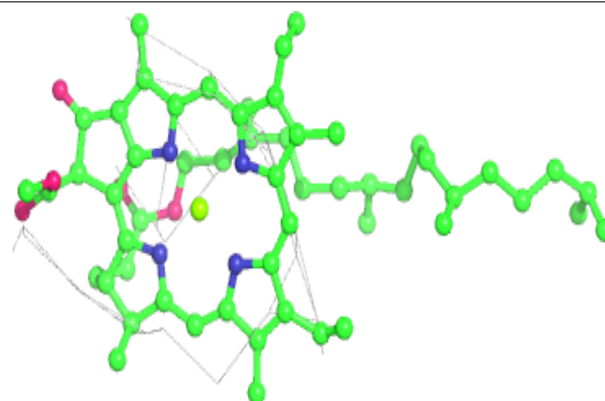


Electron density around CLA A 833:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

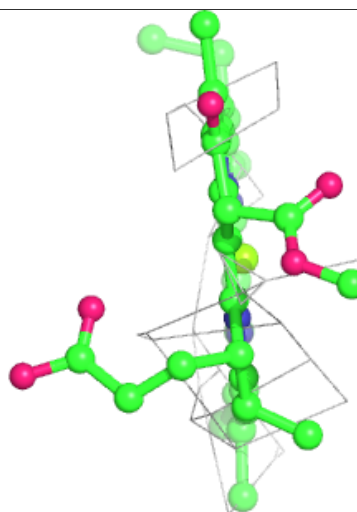
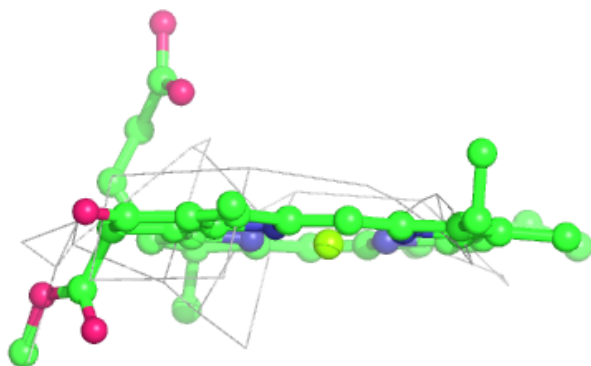
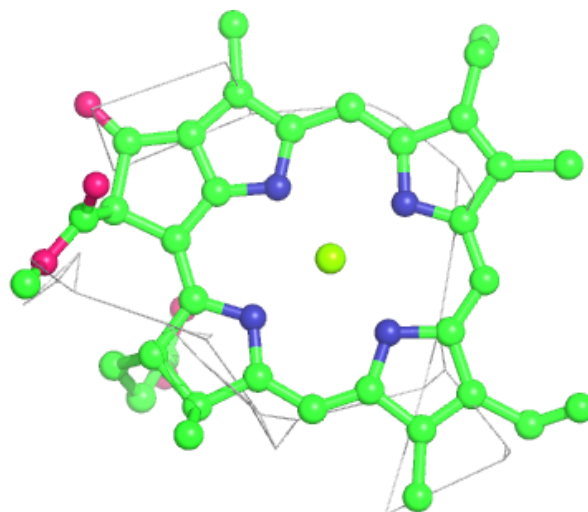
**Electron density around CLA A 839:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



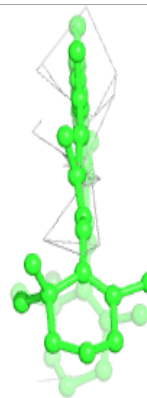
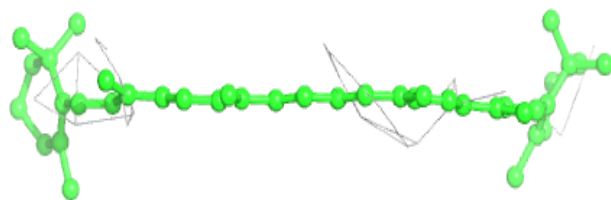
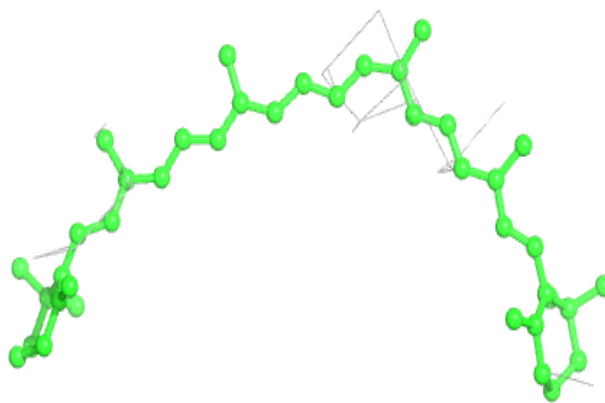
Electron density around CLA A 837:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



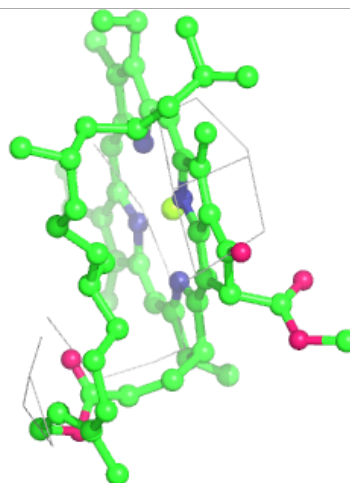
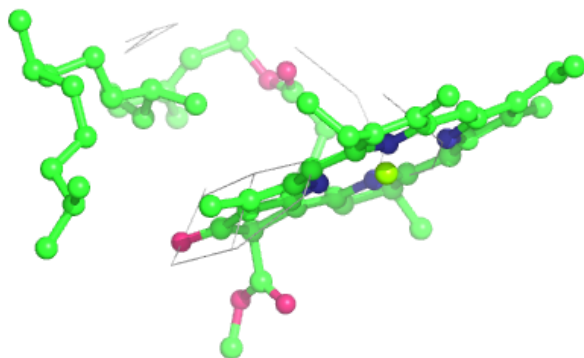
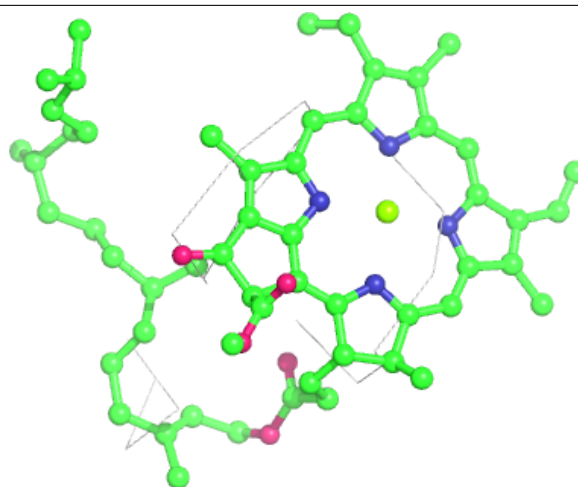
Electron density around BCR F 1302:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



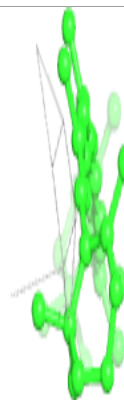
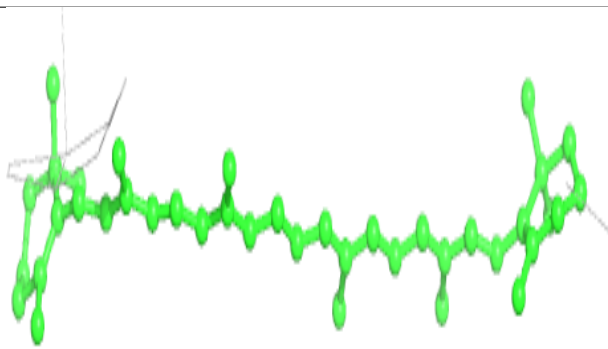
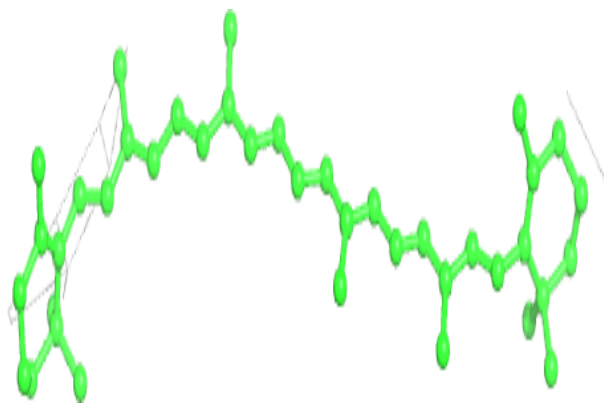
Electron density around CLA B 832:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



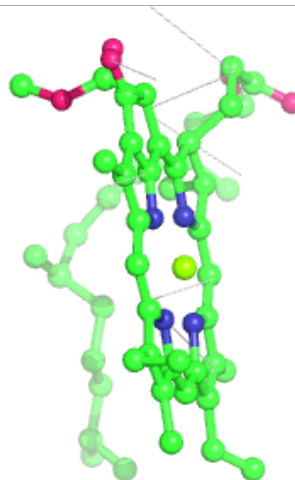
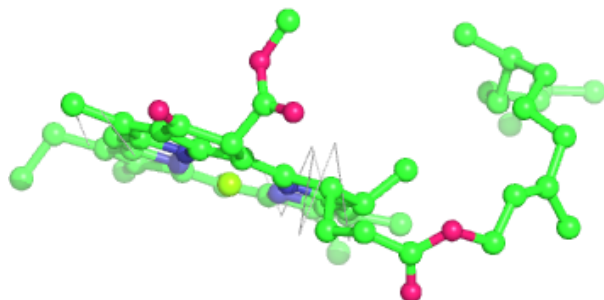
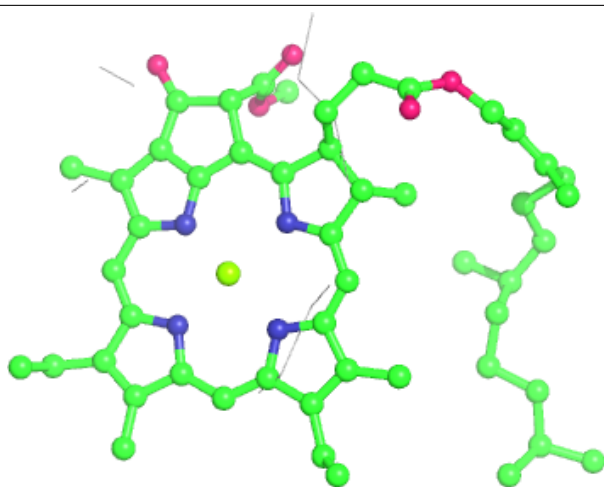
Electron density around BCR B 847:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



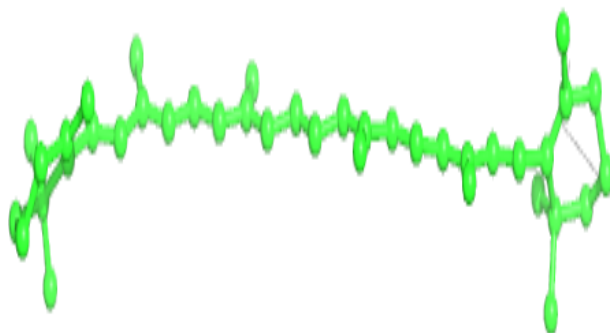
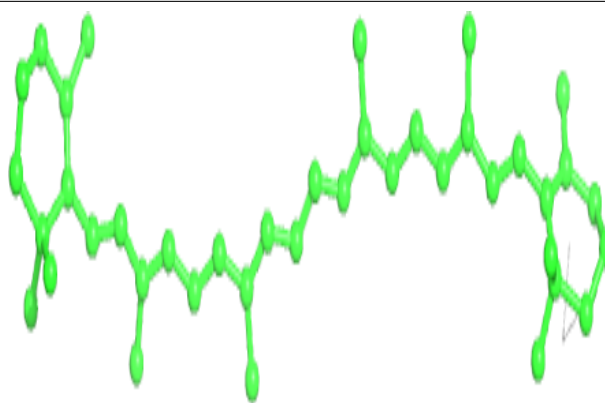
Electron density around CLA A 814:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



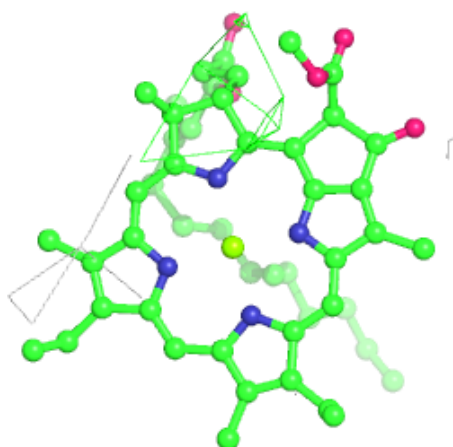
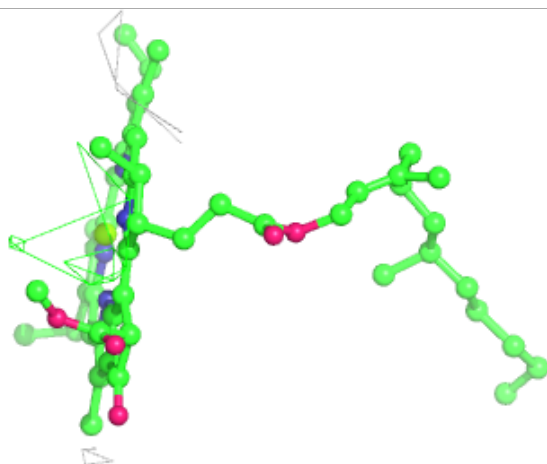
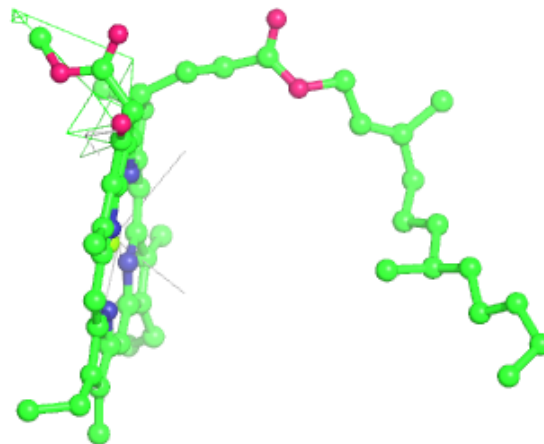
Electron density around BCR J 103:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



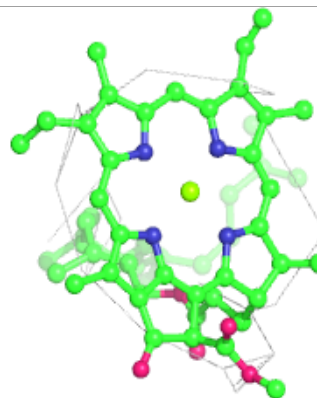
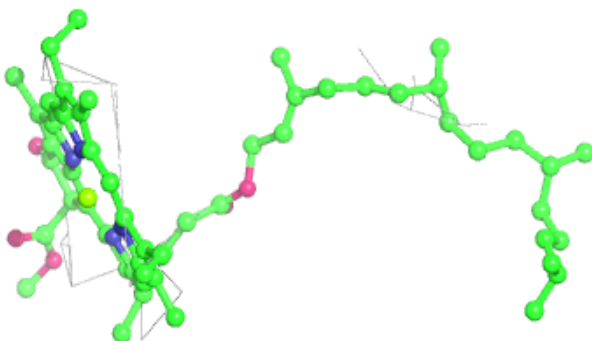
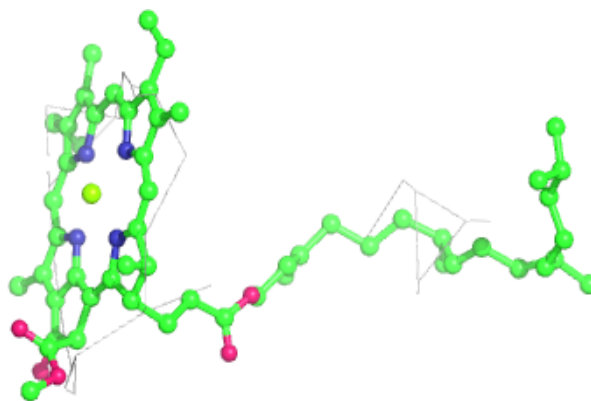
Electron density around CLA A 805:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

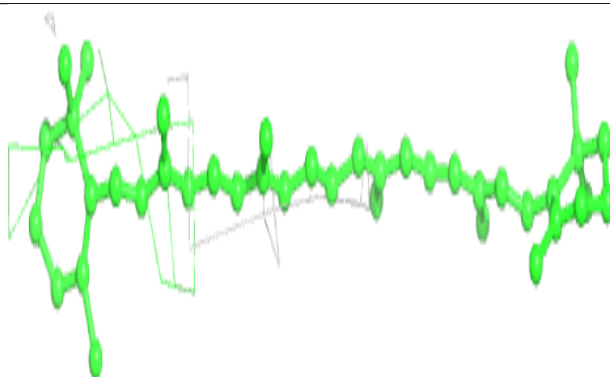
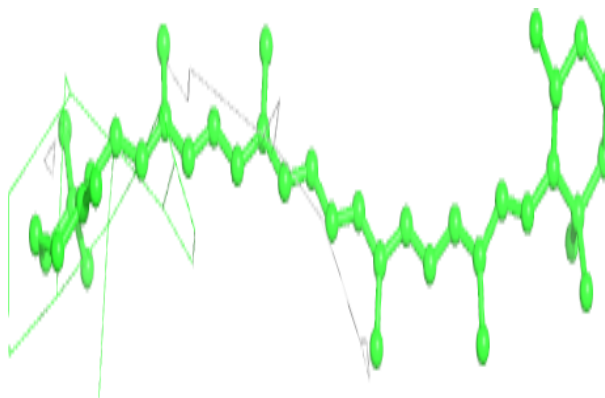


Electron density around CLA L 1003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

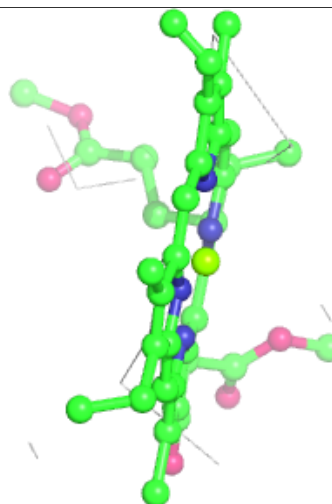
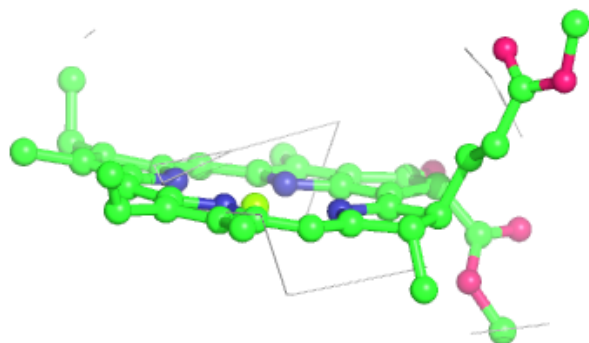
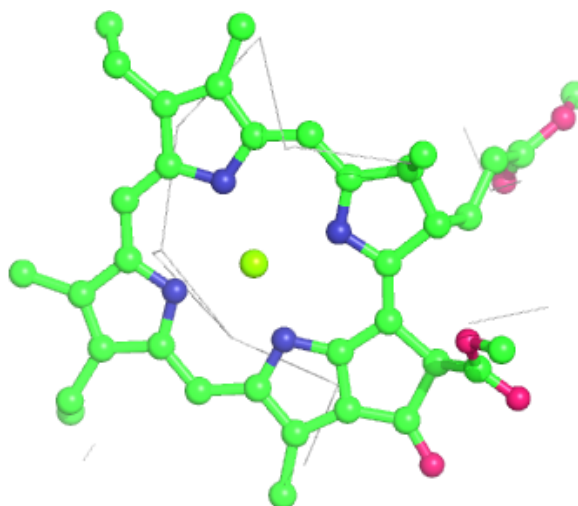
**Electron density around BCR L 1006:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



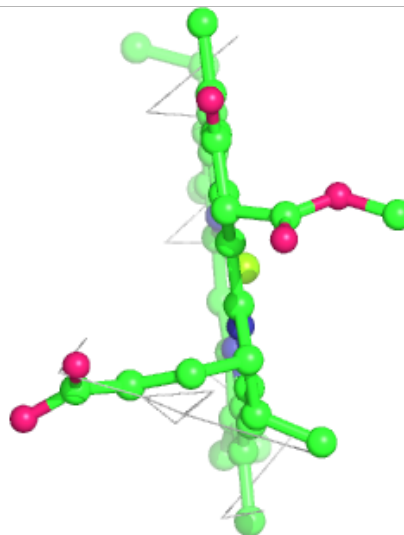
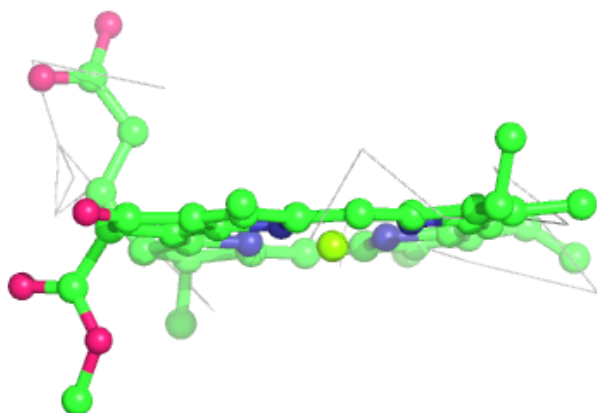
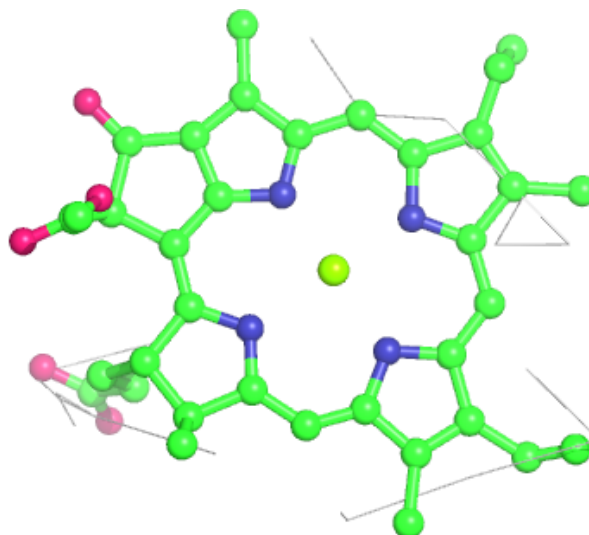
Electron density around CLA B 825:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



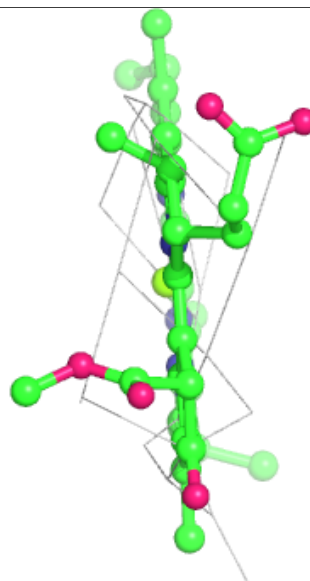
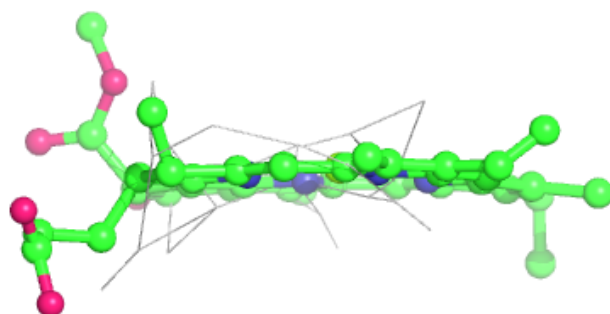
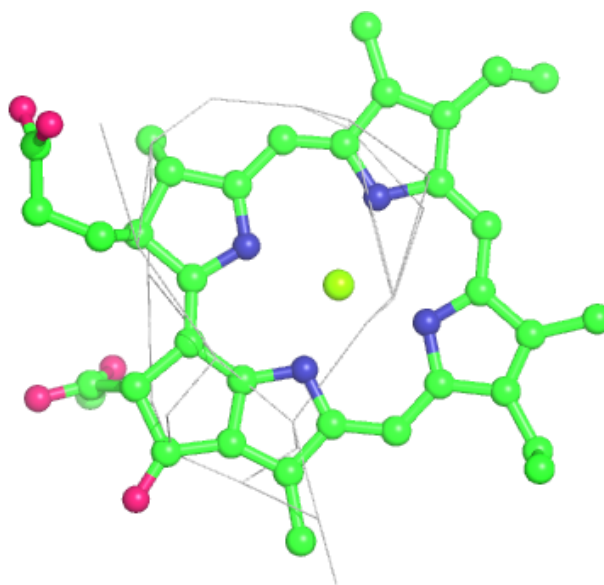
Electron density around CLA A 815:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



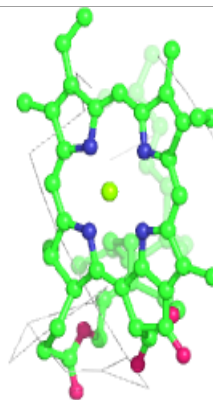
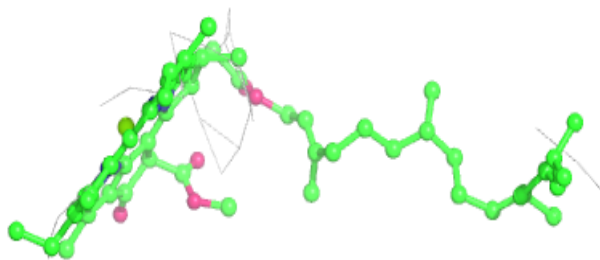
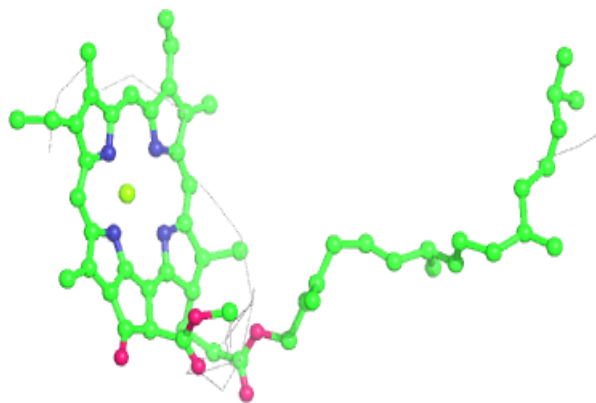
Electron density around CLA X 1701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

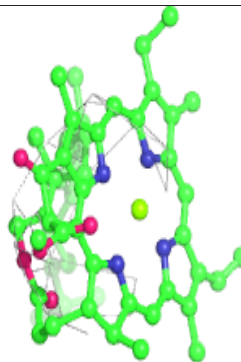
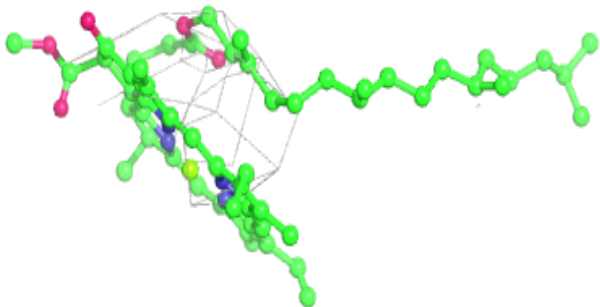
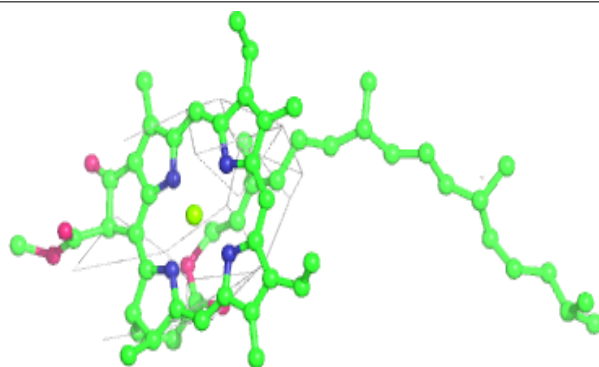


Electron density around CLA B 810:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

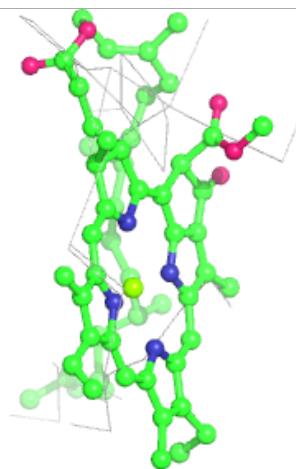
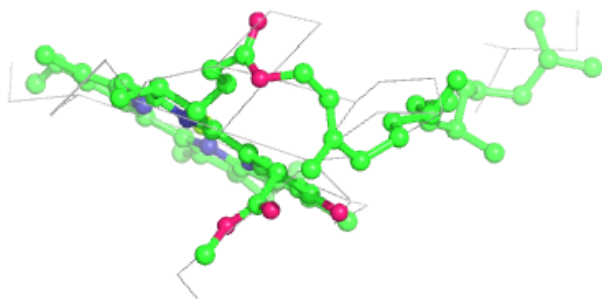
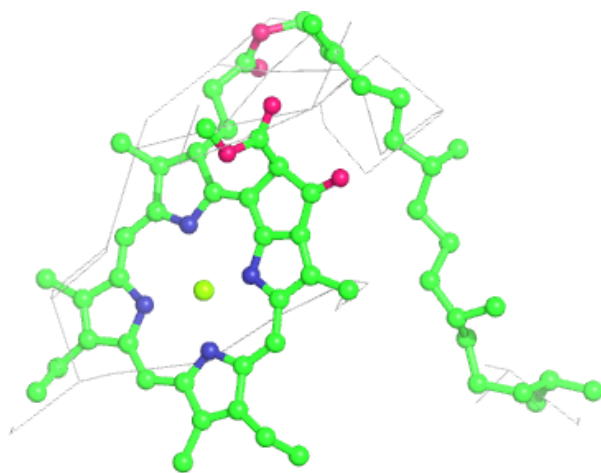
**Electron density around CLA A 843:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



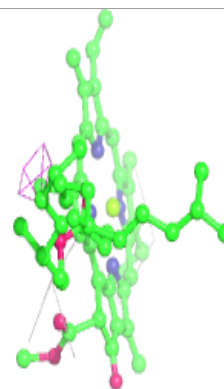
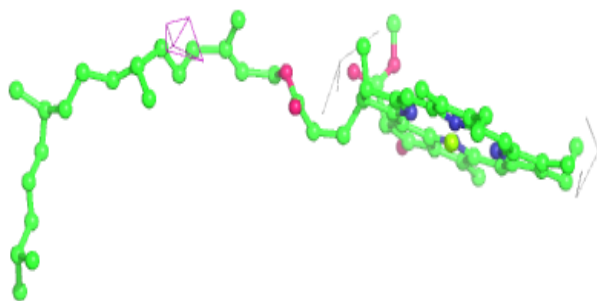
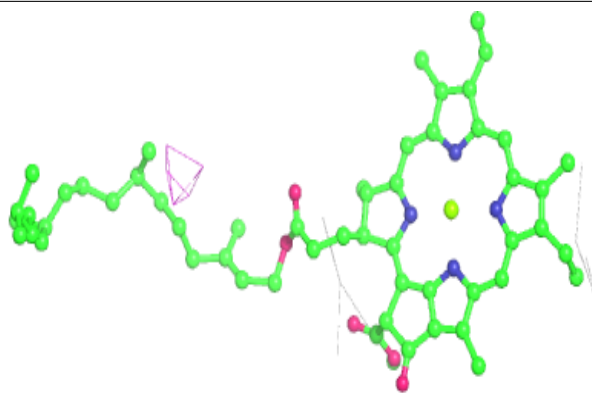
Electron density around CLA A 826:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

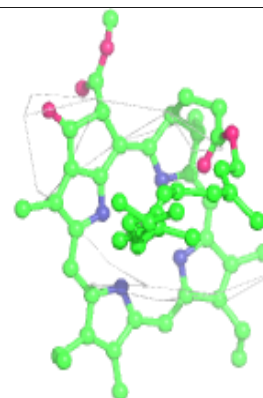
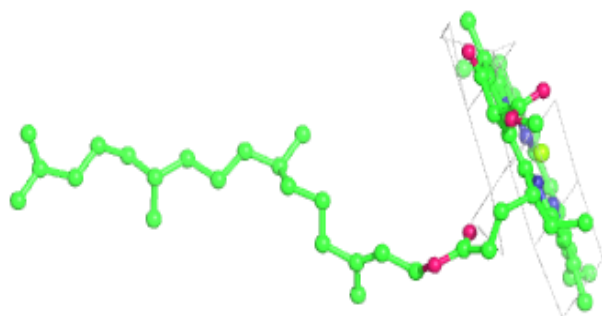
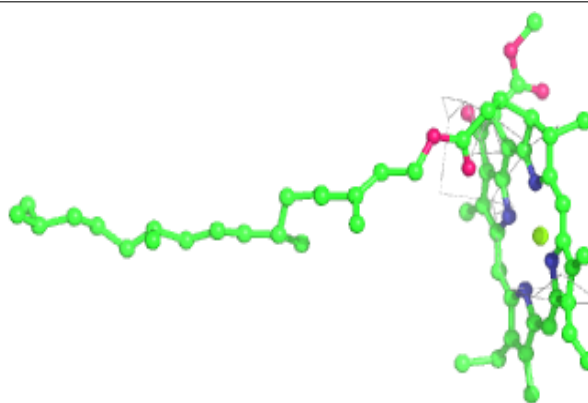


Electron density around CLA A 806:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

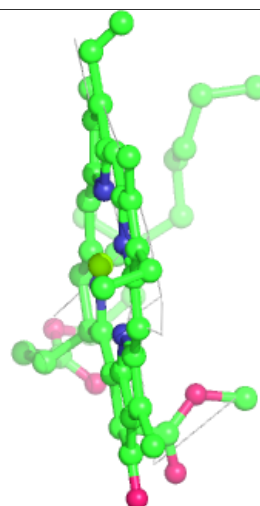
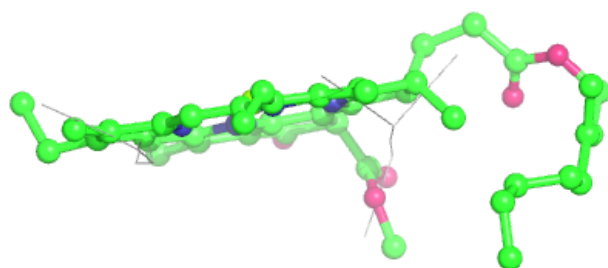
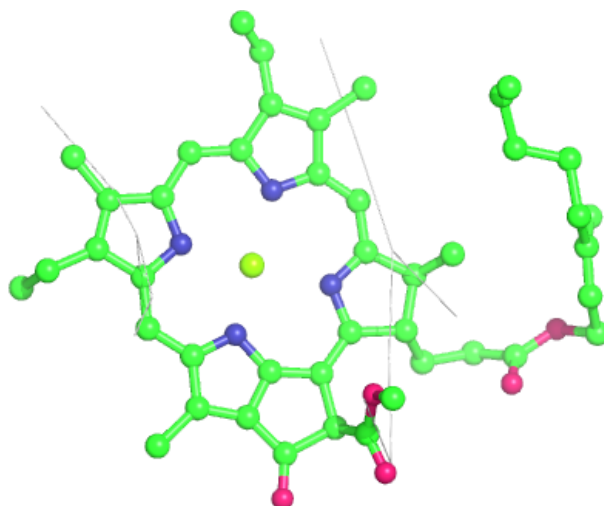
**Electron density around CLA B 828:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



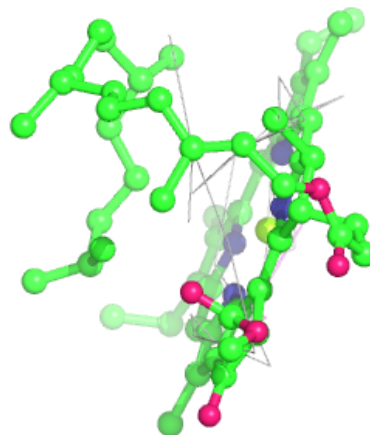
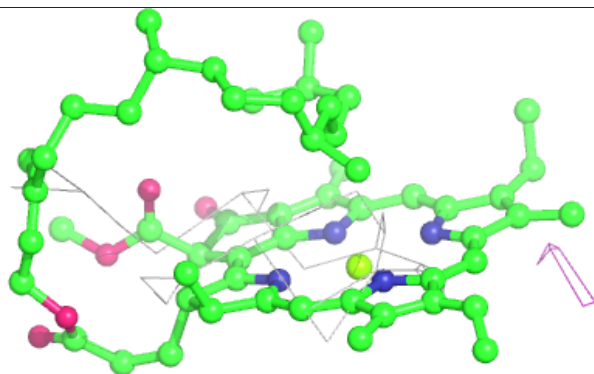
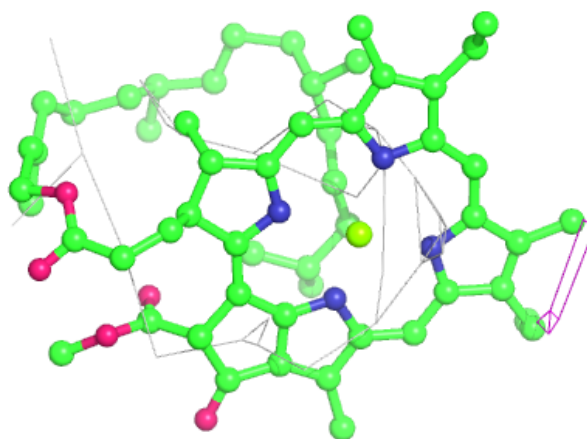
Electron density around CLA B 824:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



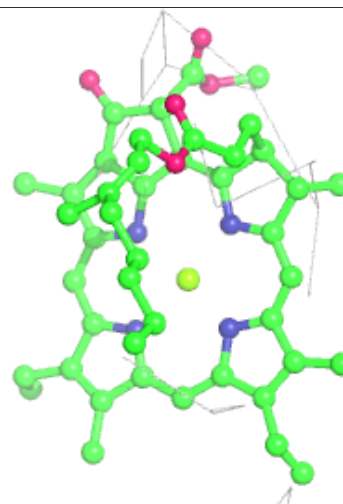
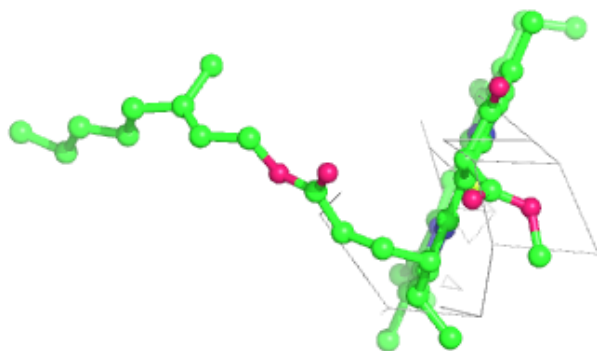
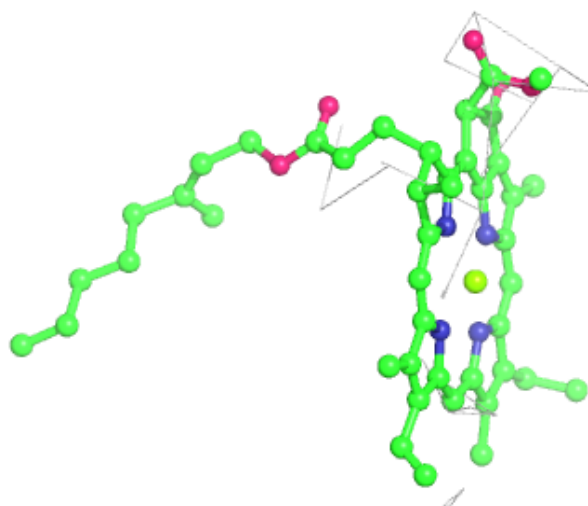
Electron density around CLA A 807:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



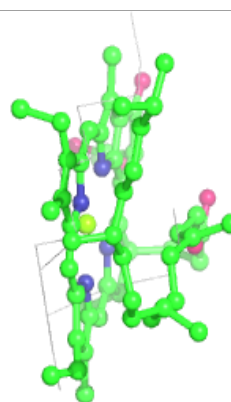
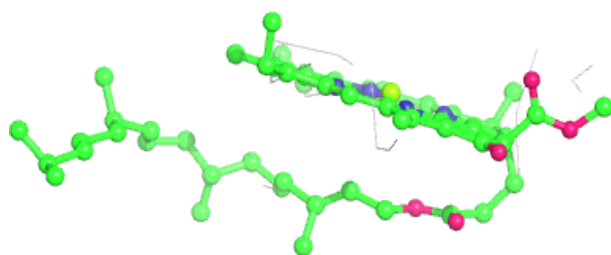
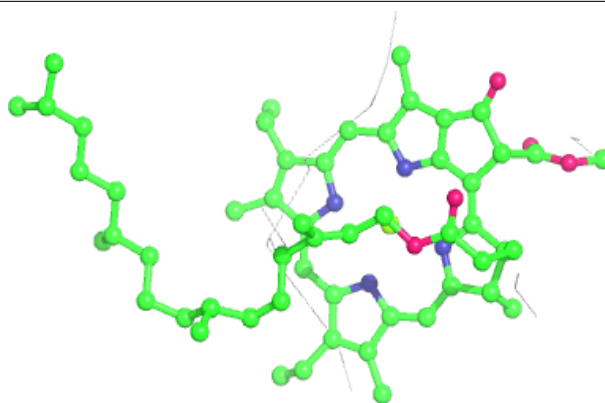
Electron density around CLA B 804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

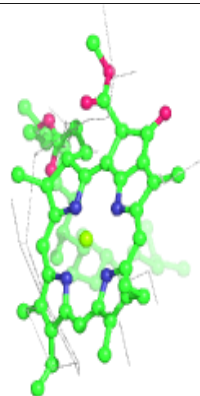
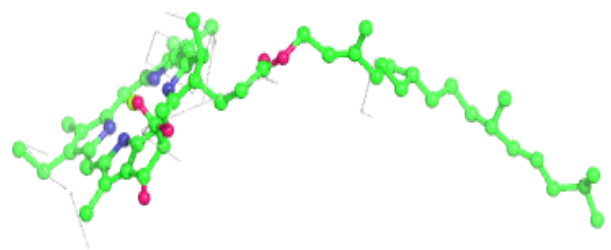
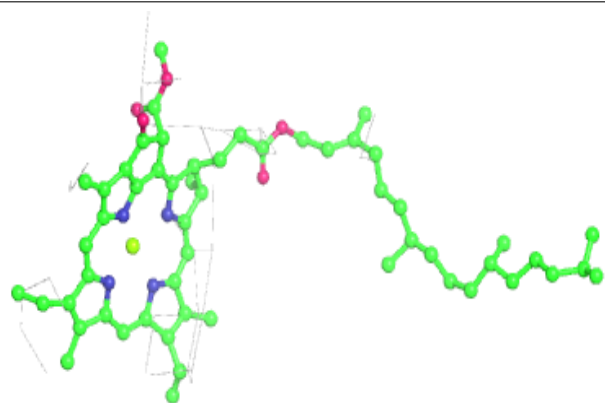


Electron density around CLA B 838:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

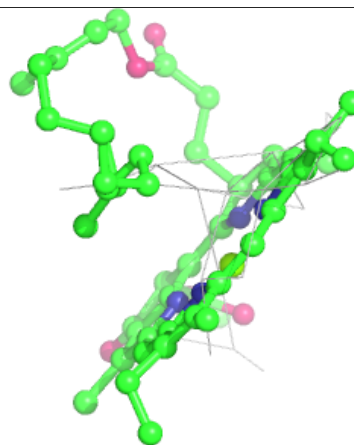
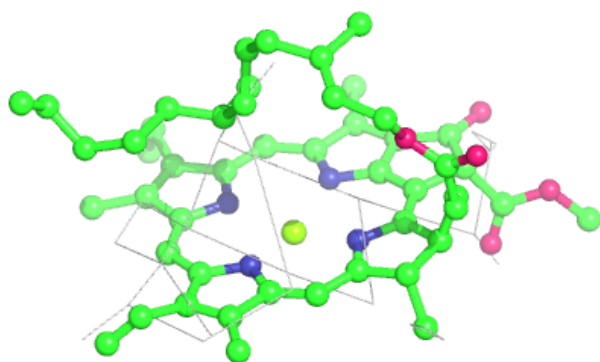
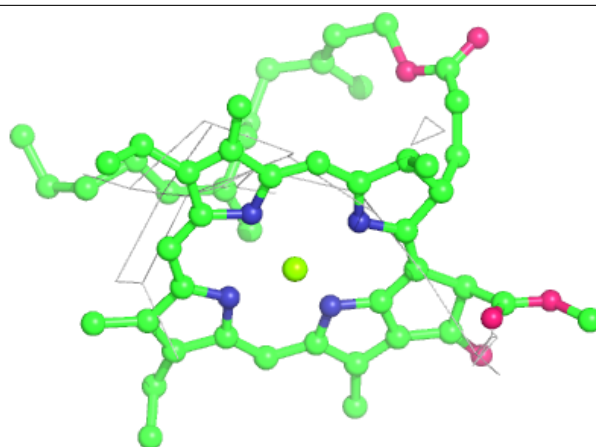
**Electron density around CLA A 802:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



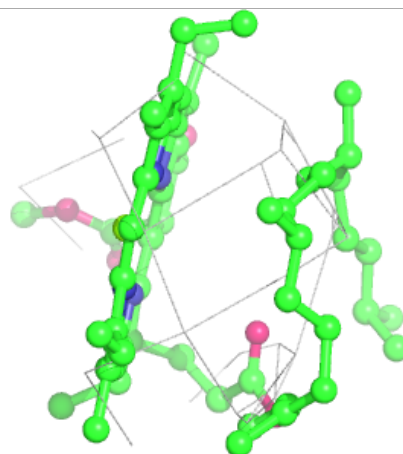
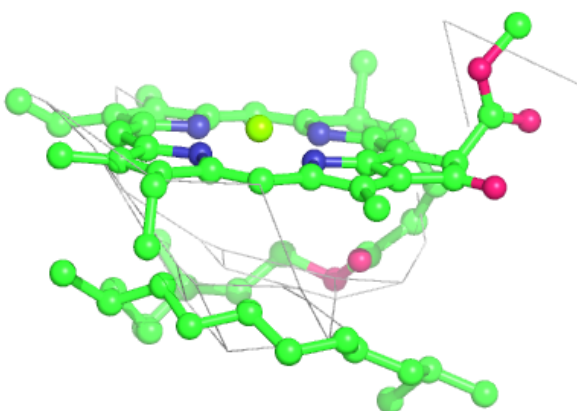
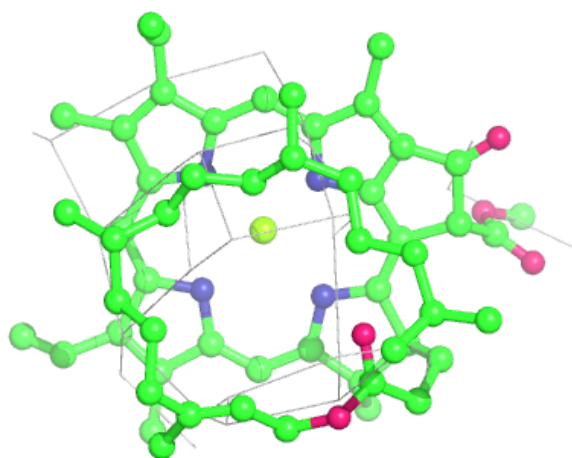
Electron density around CLA B 817:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



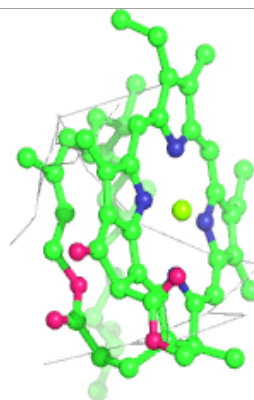
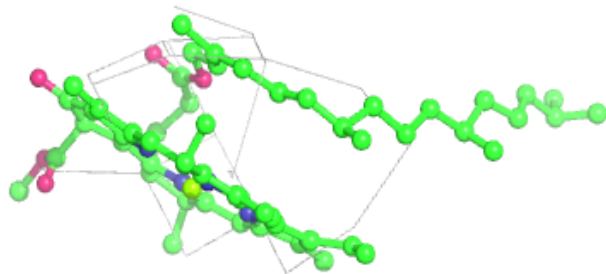
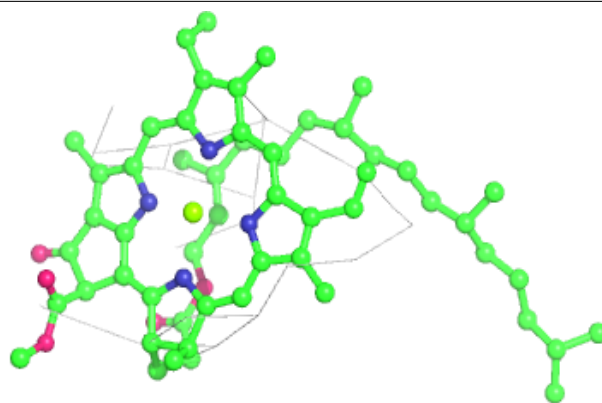
Electron density around CLA L 1002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

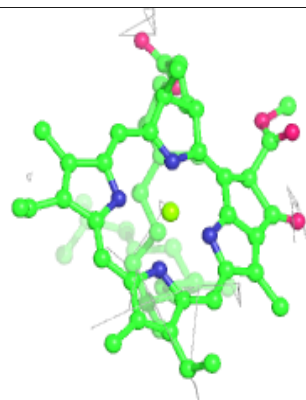
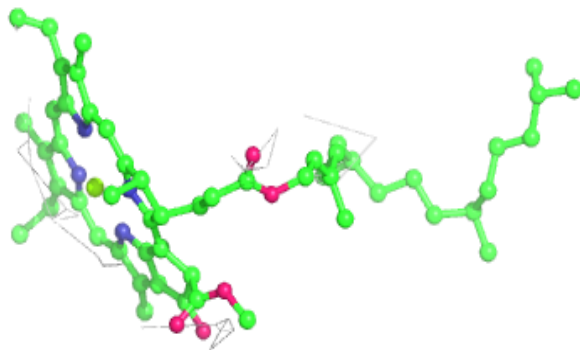
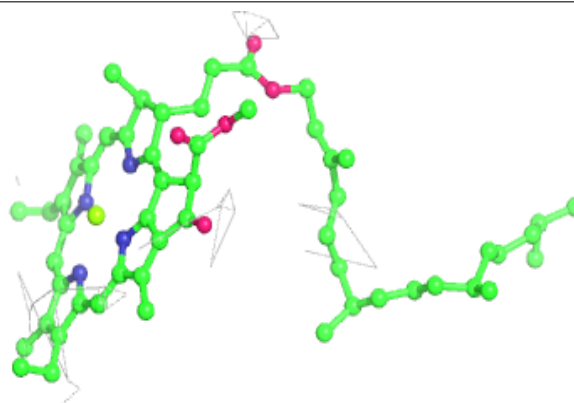


Electron density around CLA B 807:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

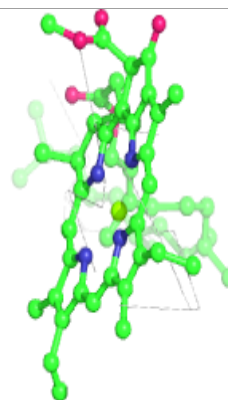
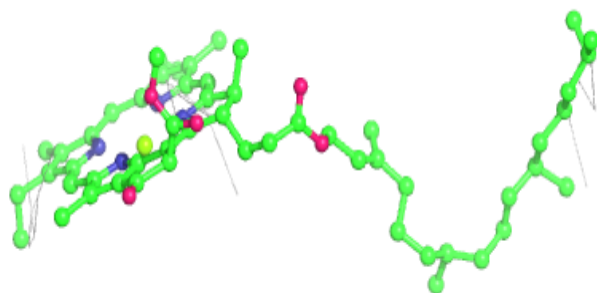
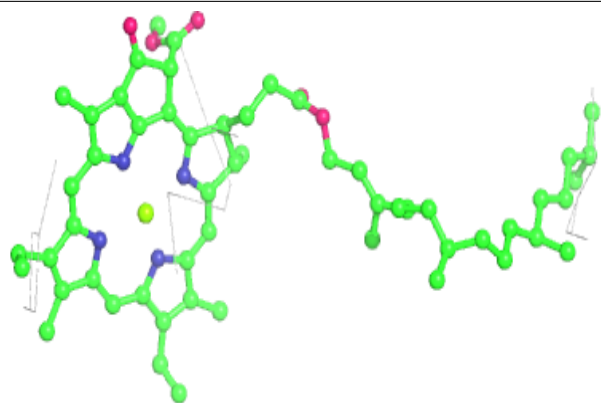
**Electron density around CLA B 801:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

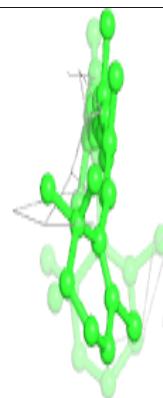
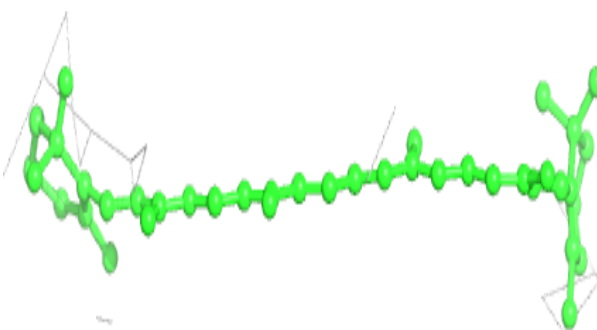
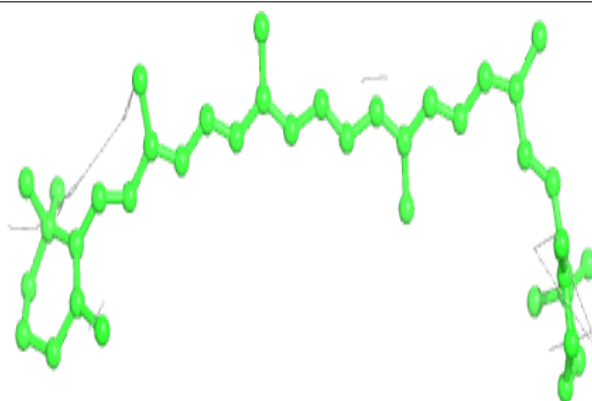


Electron density around CLA B 813:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

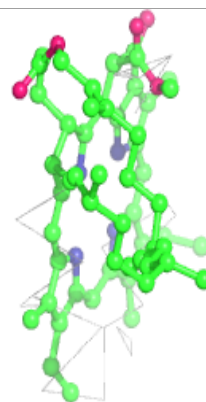
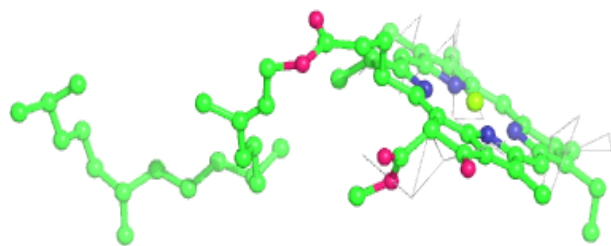
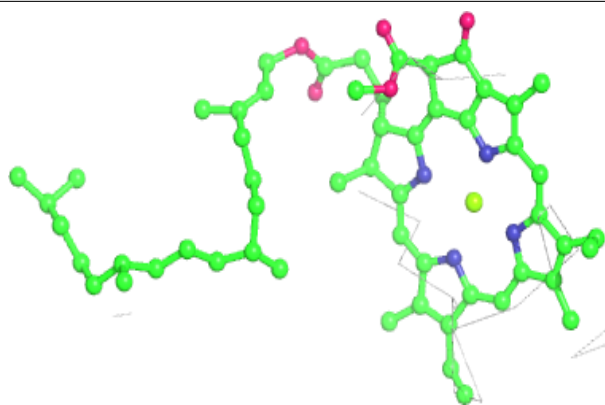
**Electron density around BCR I 102:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



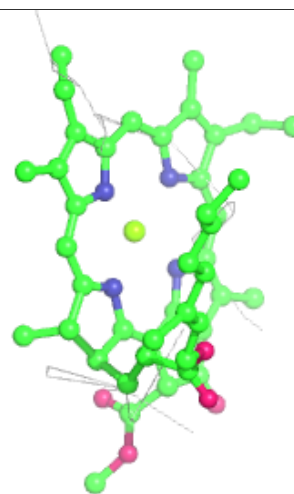
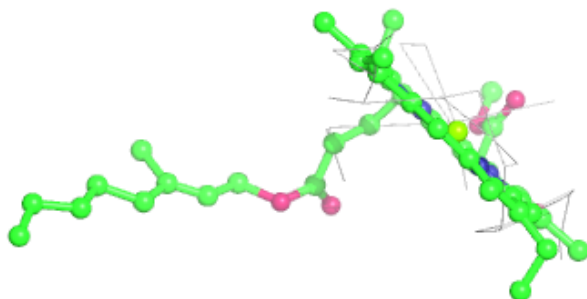
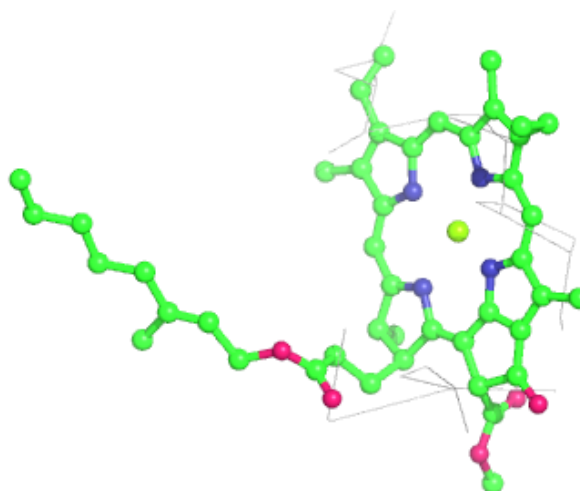
Electron density around CLA A 804:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



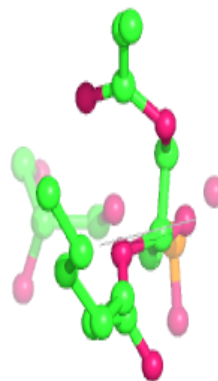
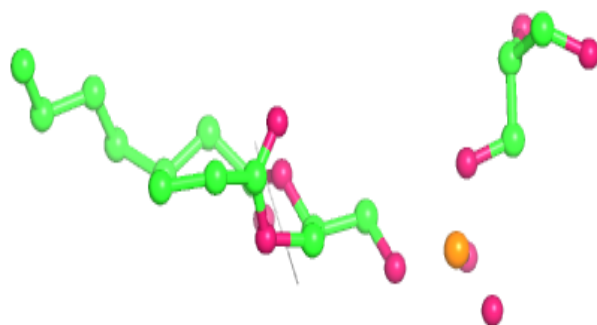
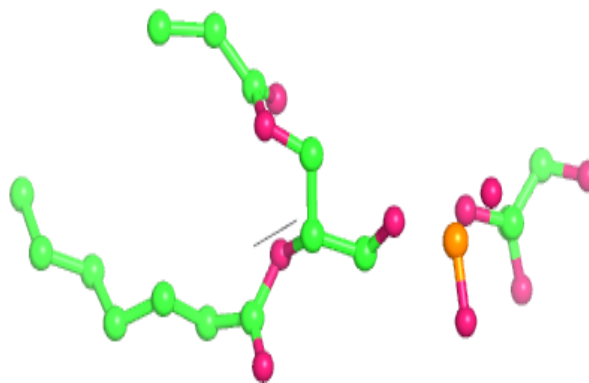
Electron density around CLA A 836:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

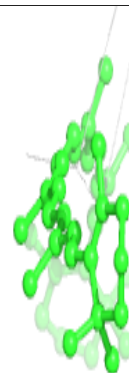
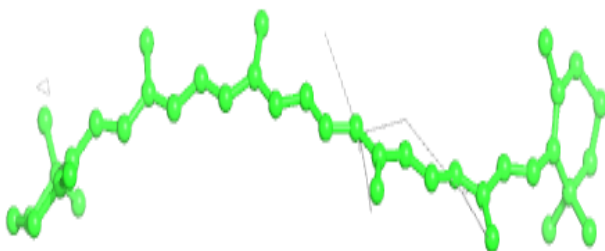
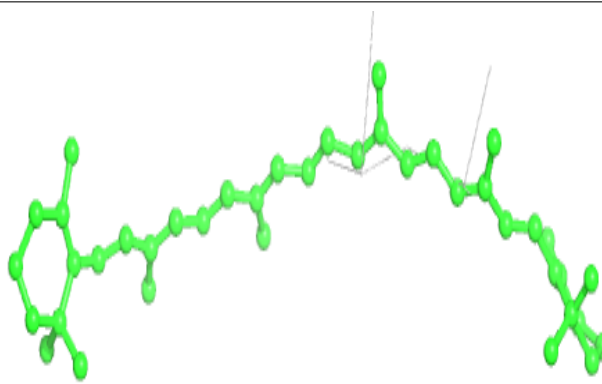


Electron density around LHG A 856:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

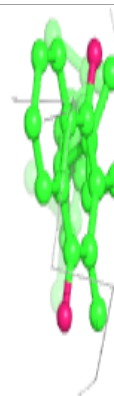
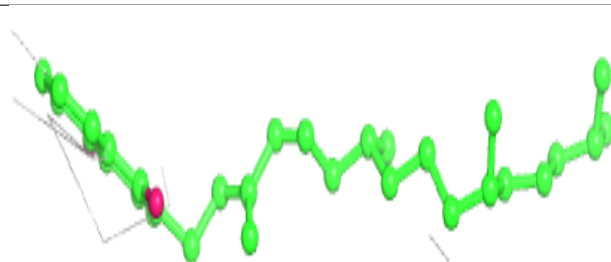
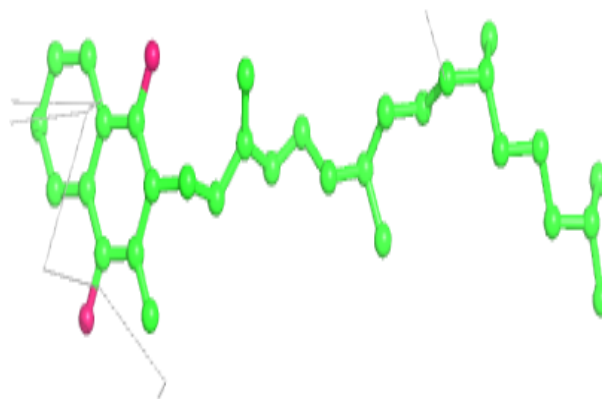
**Electron density around BCR B 848:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



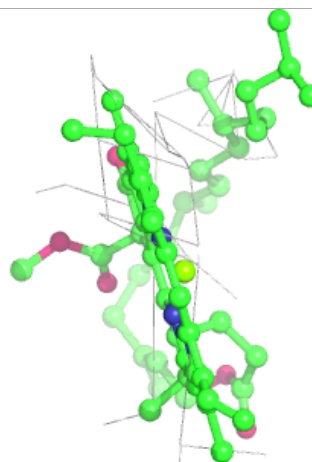
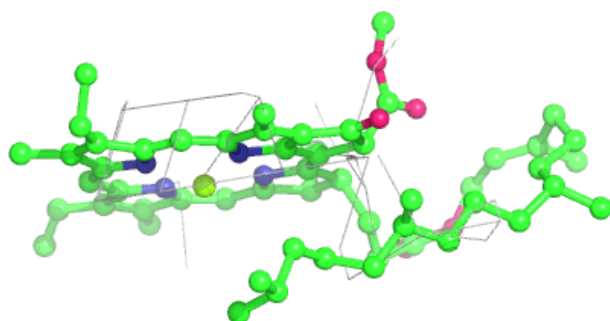
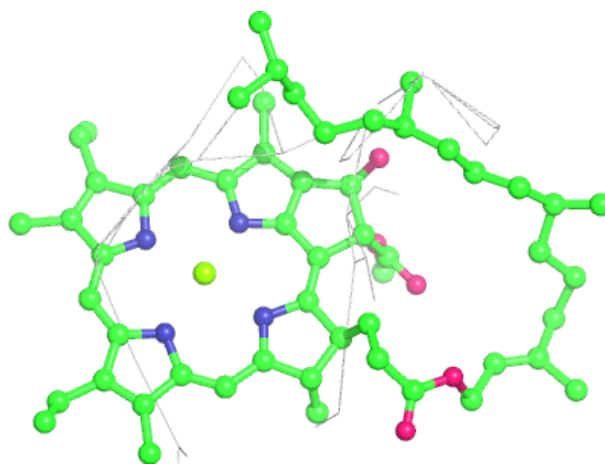
Electron density around PQN A 847:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



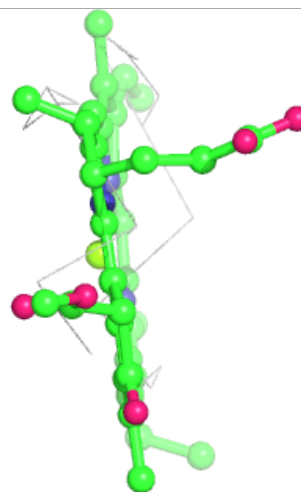
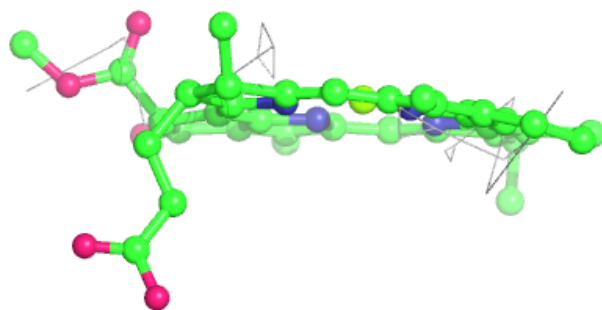
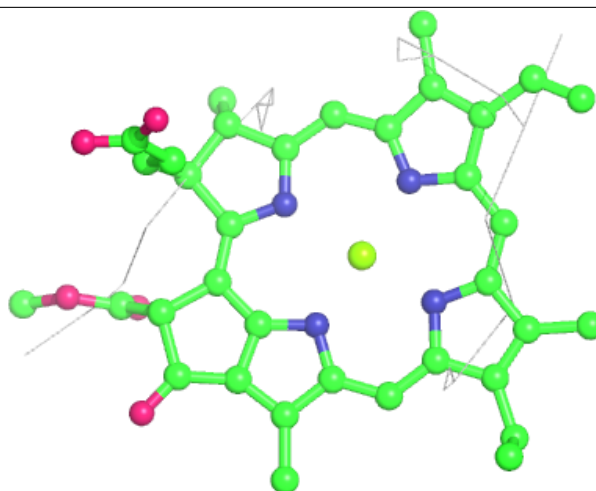
Electron density around CLA B 805:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



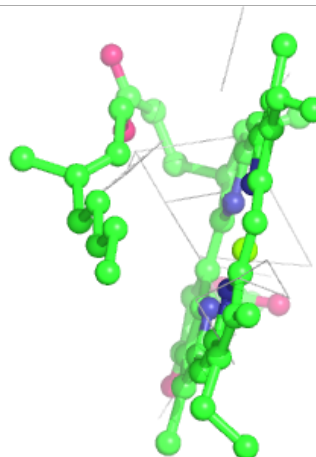
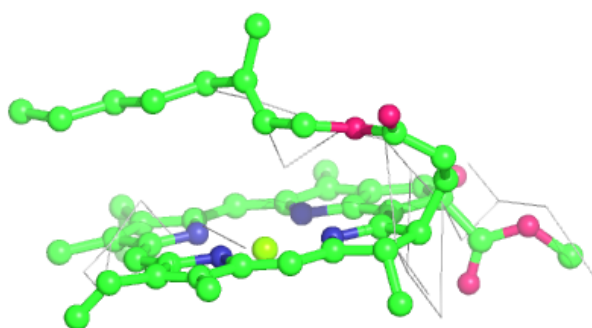
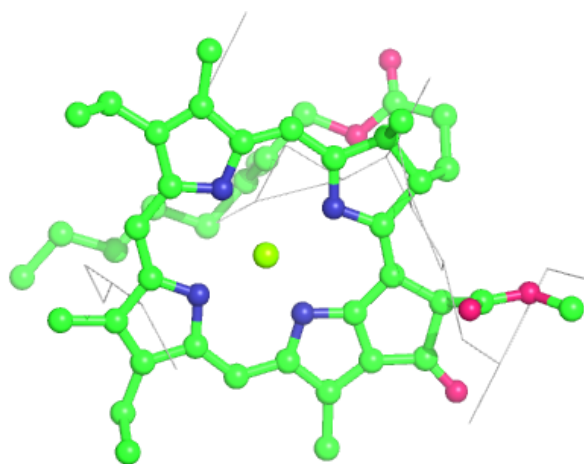
Electron density around CLA B 835:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



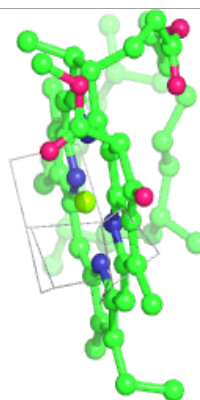
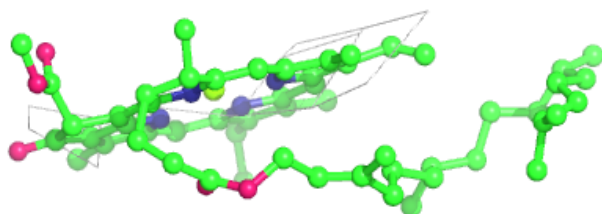
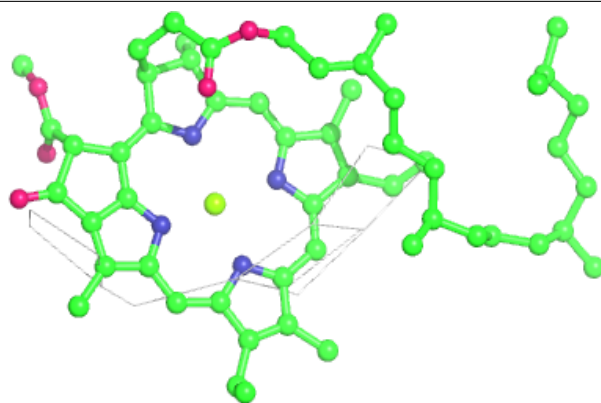
Electron density around CLA A 819:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

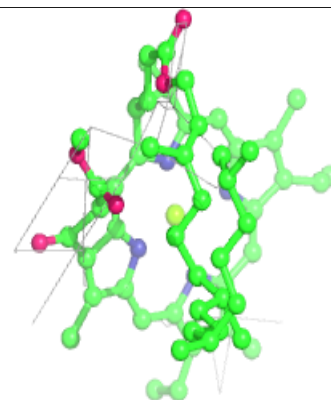
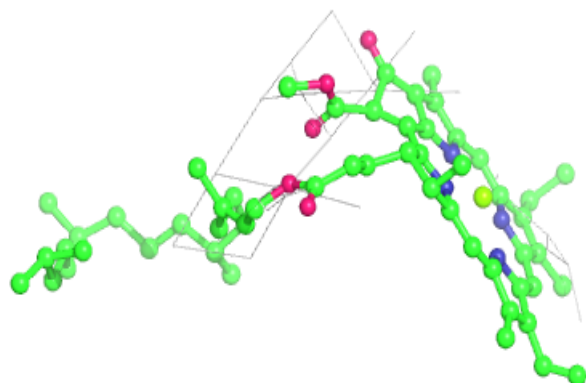
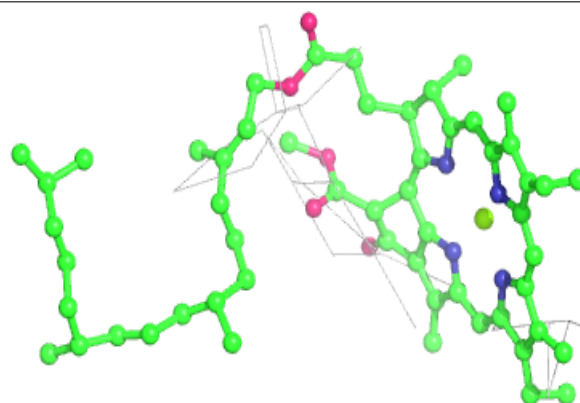


Electron density around CLA A 820:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

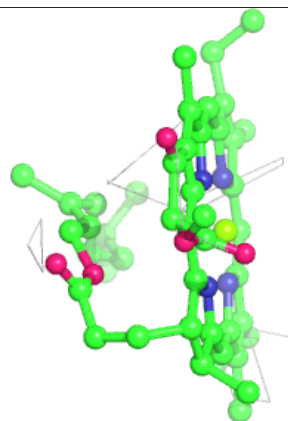
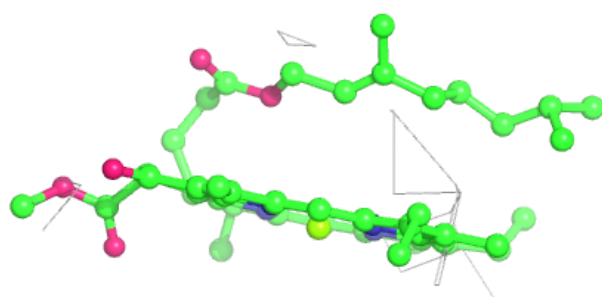
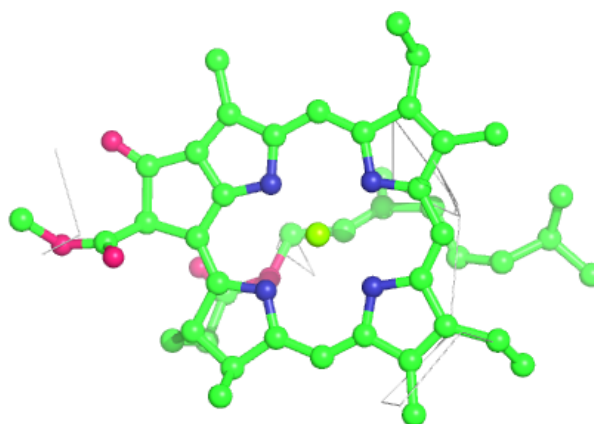
**Electron density around CLA A 801:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



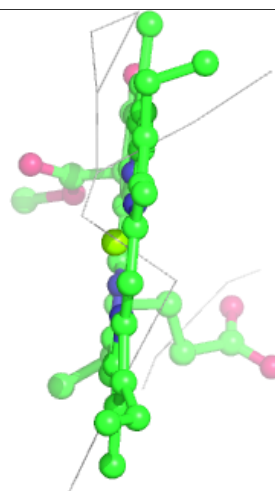
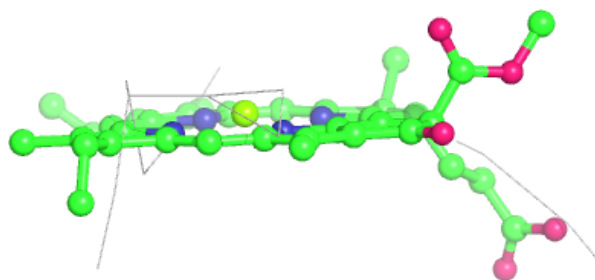
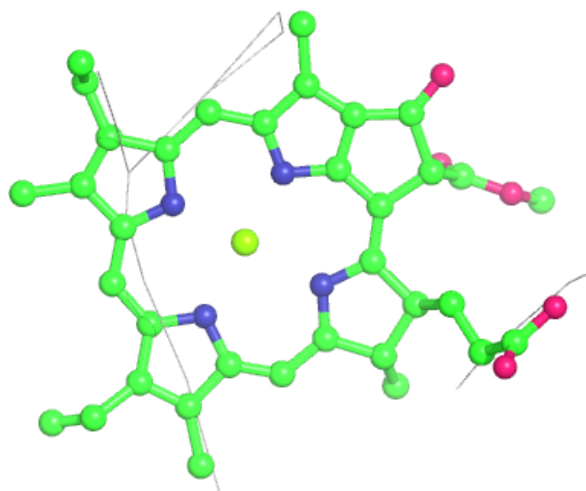
Electron density around CLA B 822:

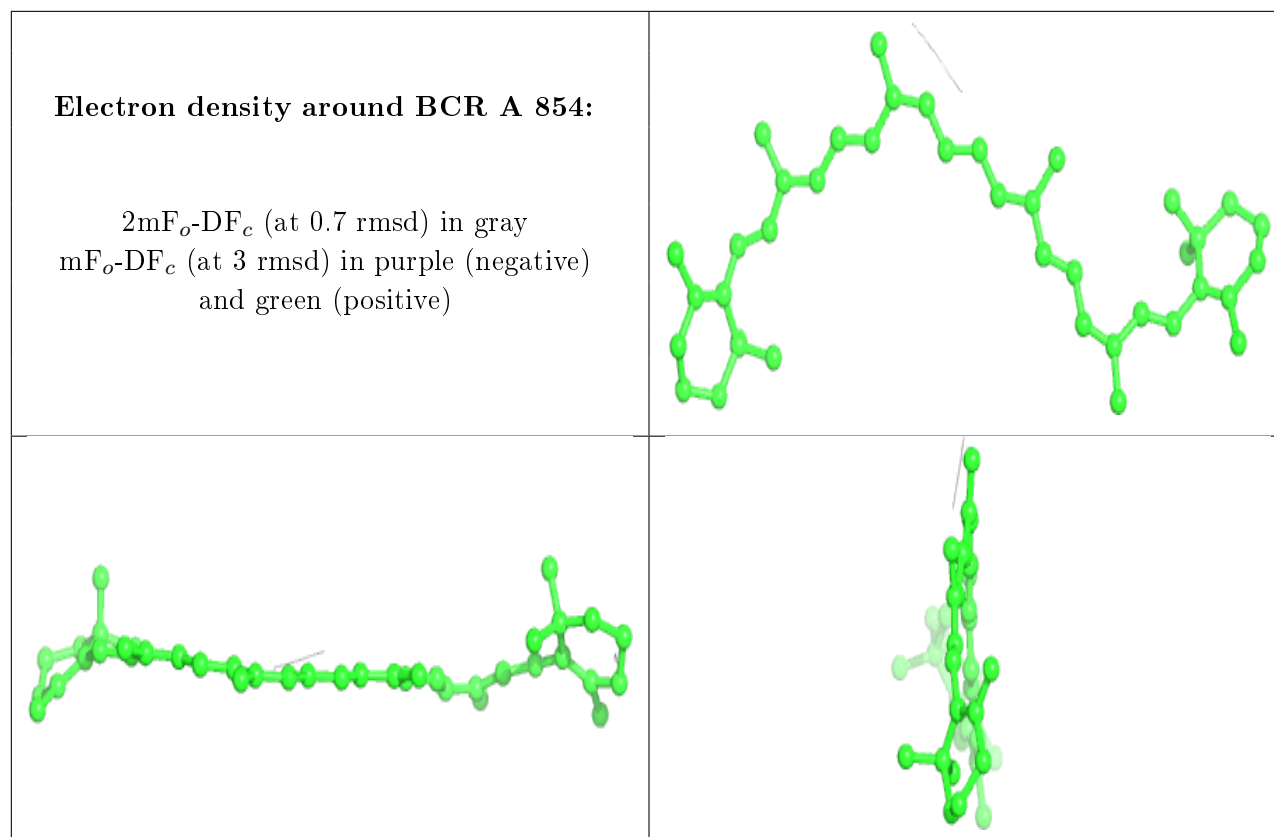
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 823:

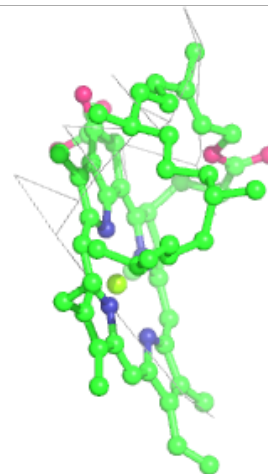
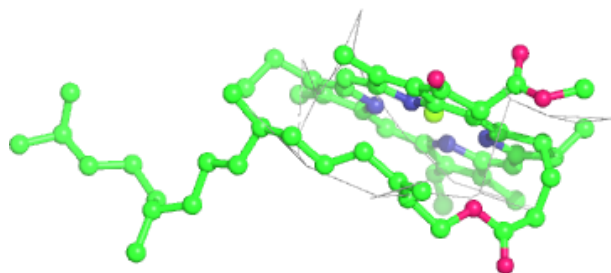
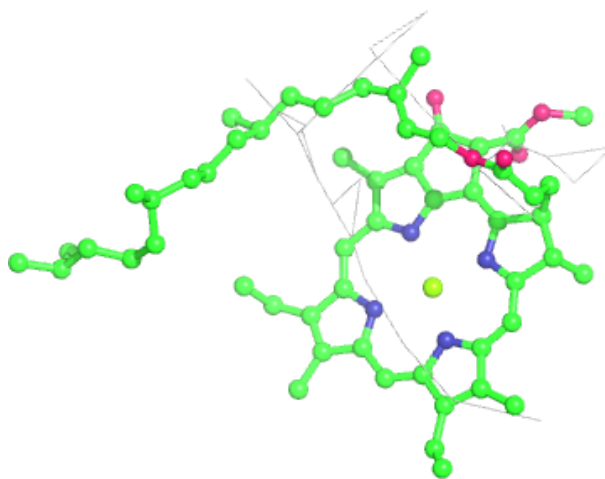
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





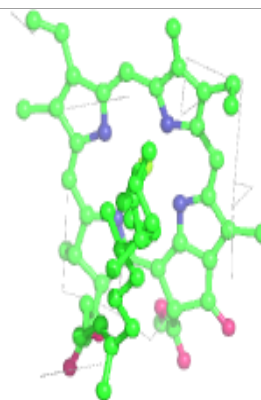
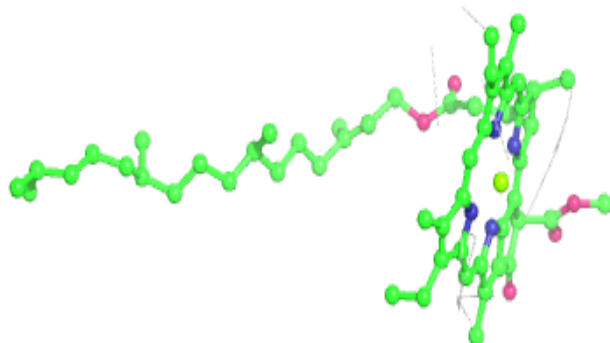
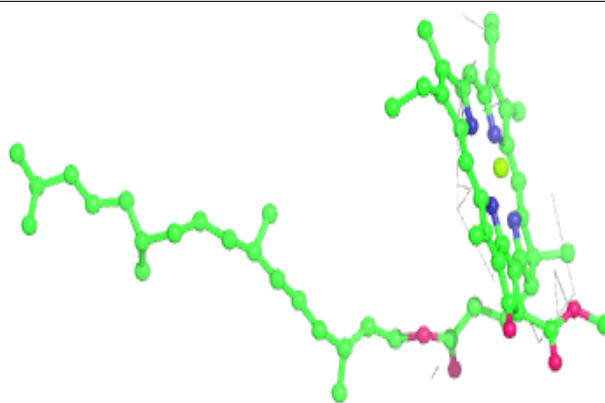
Electron density around CLA A 830:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

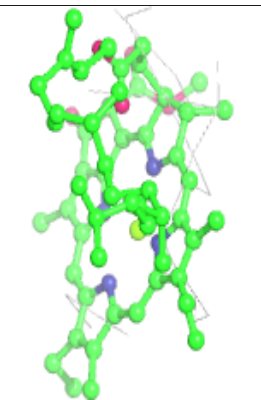
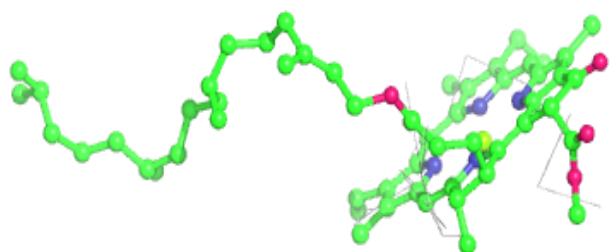
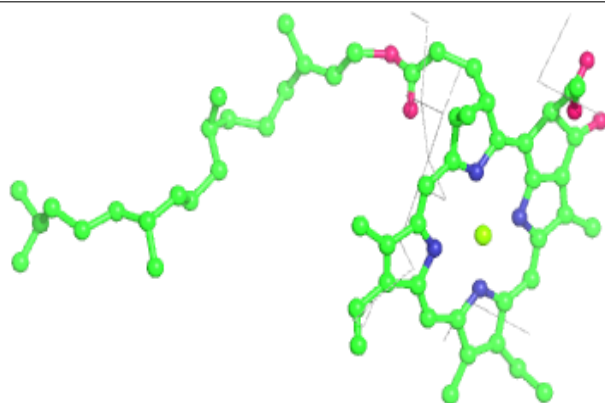


Electron density around CLA B 829:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

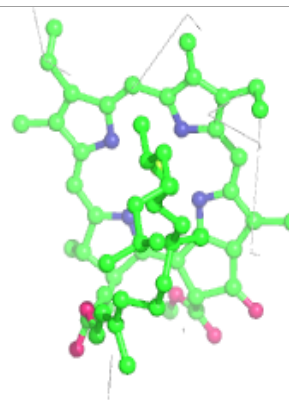
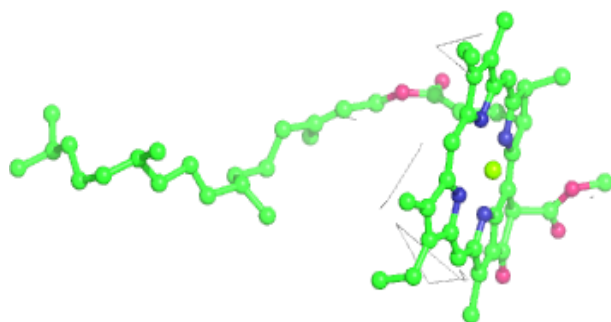
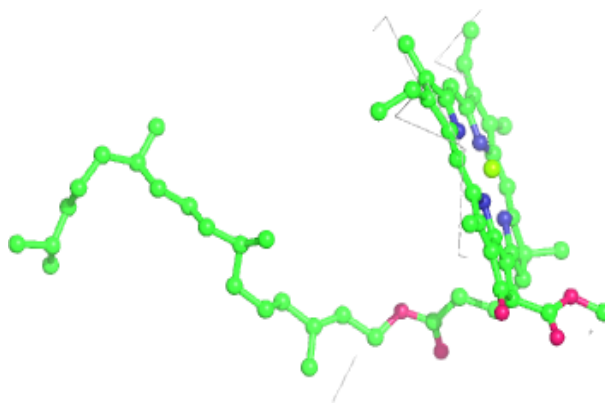
**Electron density around CLA A 809:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

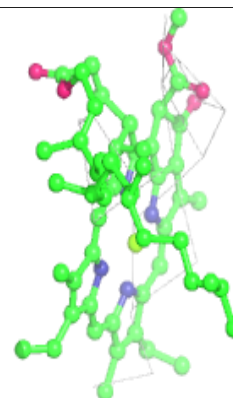
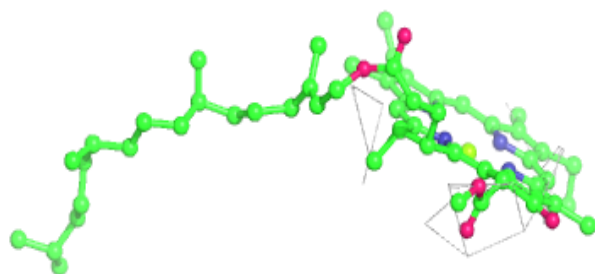
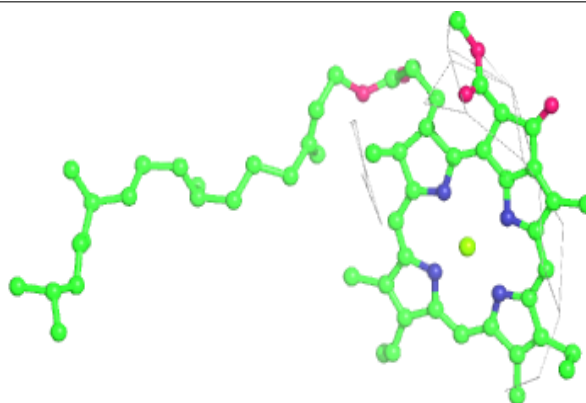


Electron density around CLA A 831:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

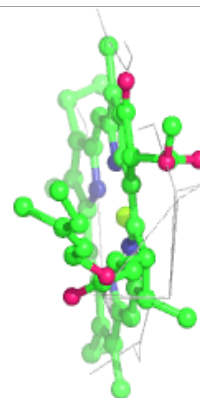
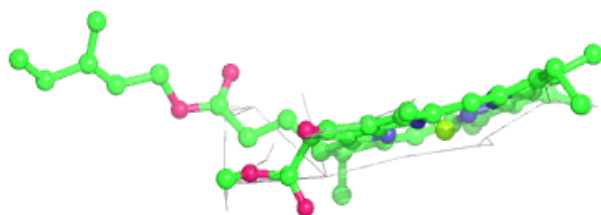
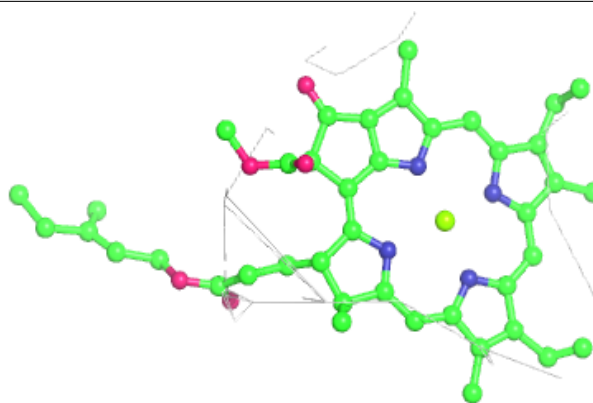
**Electron density around CLA A 803:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

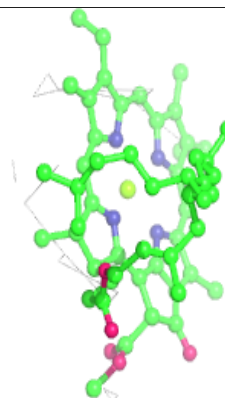
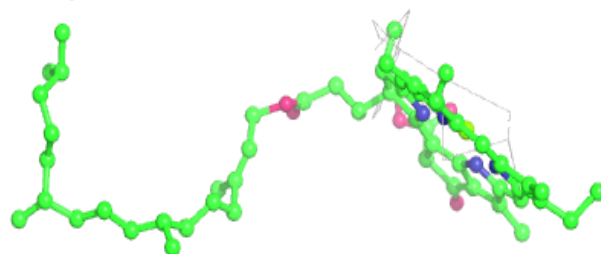
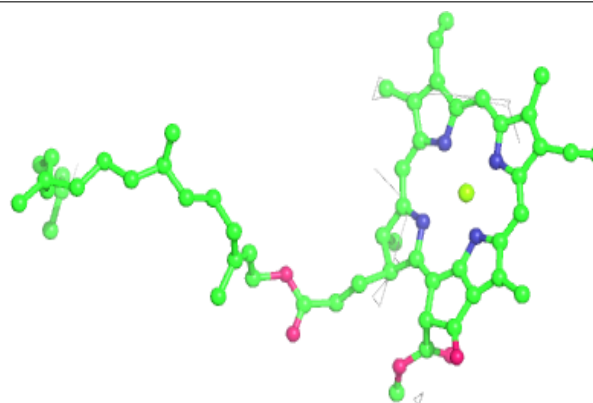


Electron density around CLA A 842:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

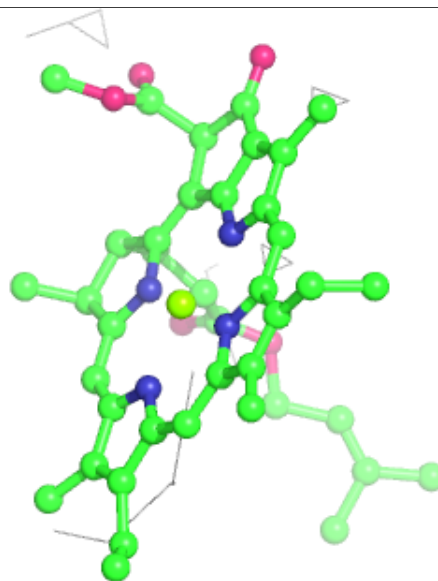
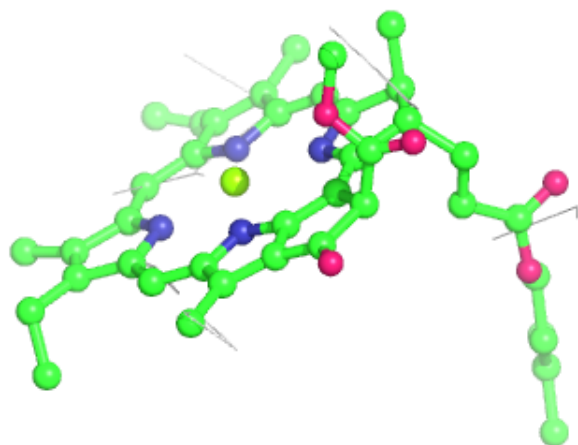
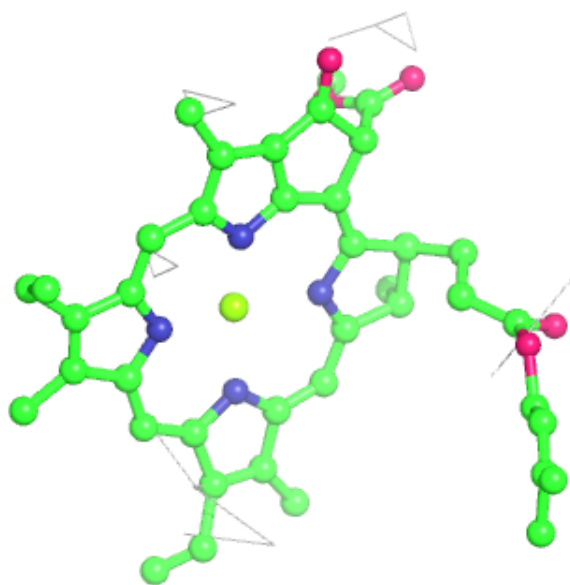
**Electron density around CLA B 809:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



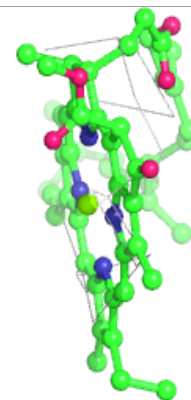
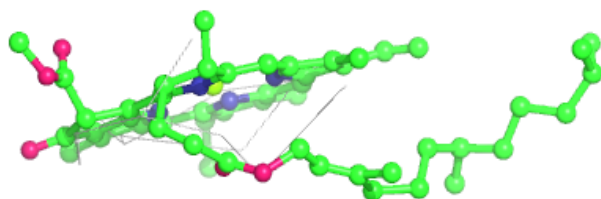
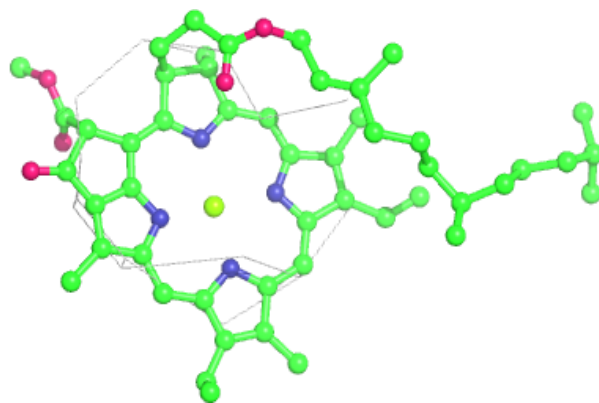
Electron density around CLA A 832:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

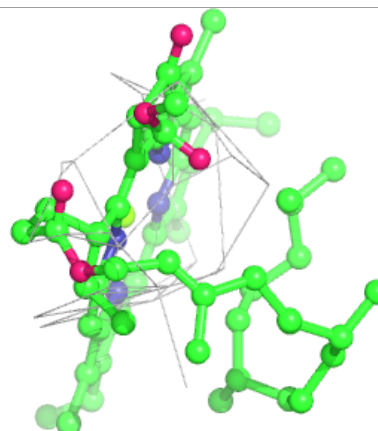
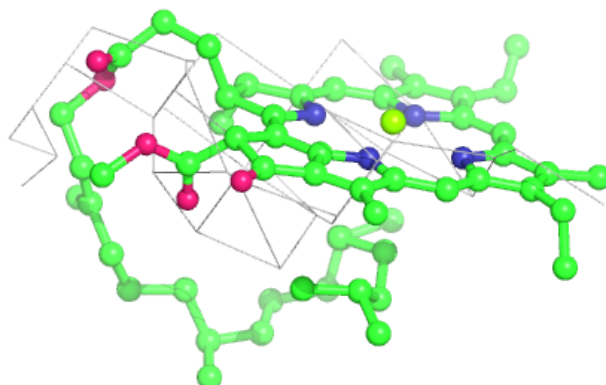
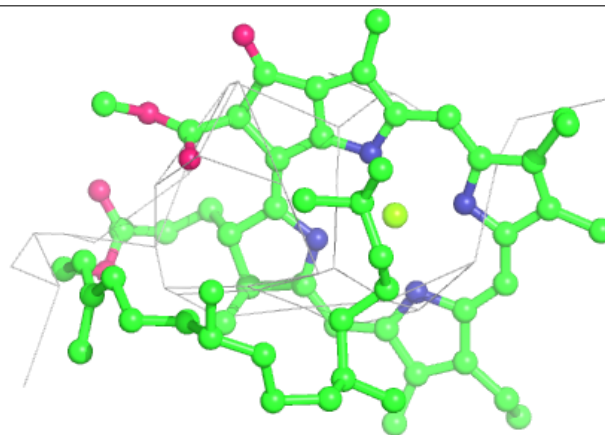


Electron density around CLA B 818:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

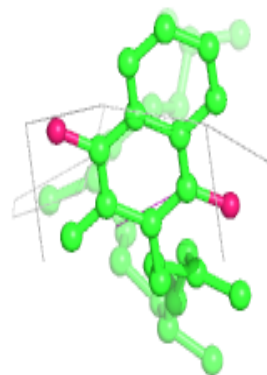
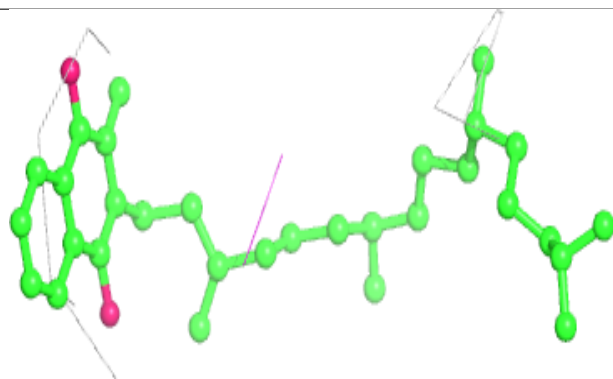
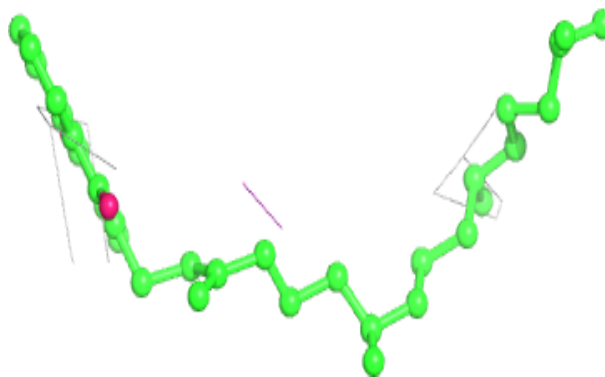
**Electron density around CLA B 806:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

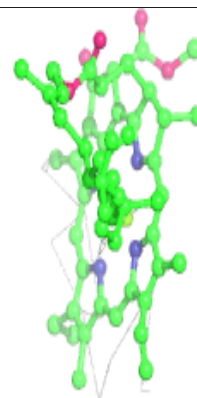
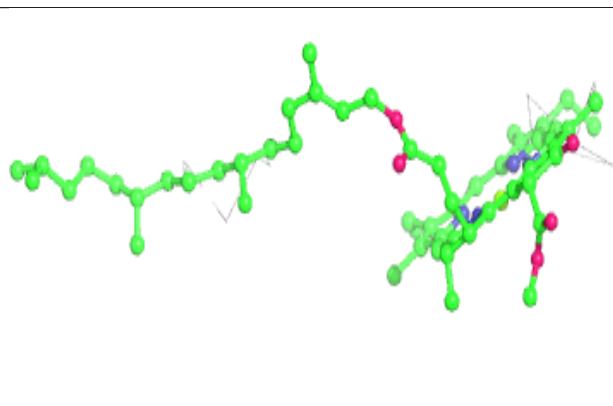
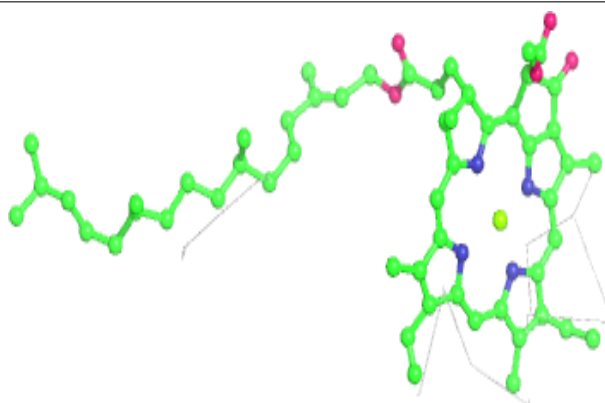


Electron density around PQN B 842:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

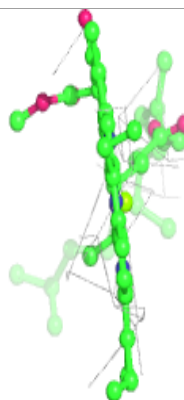
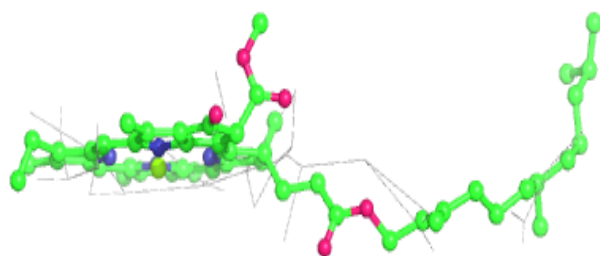
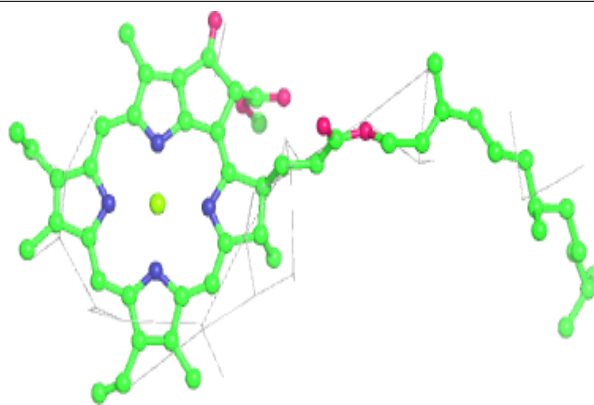
**Electron density around CLA A 835:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



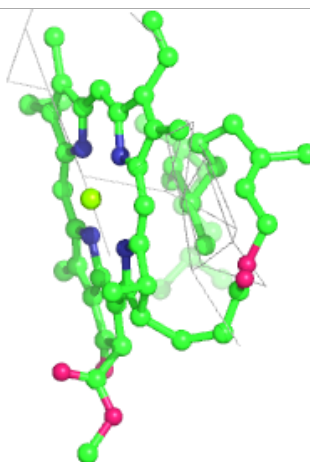
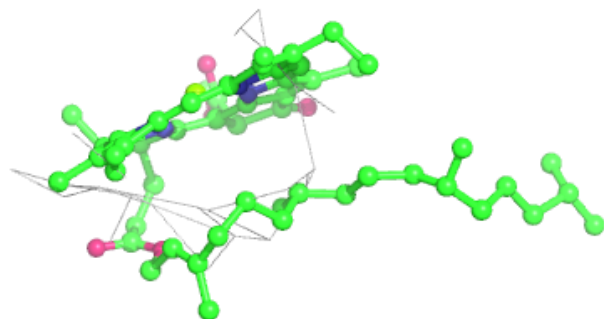
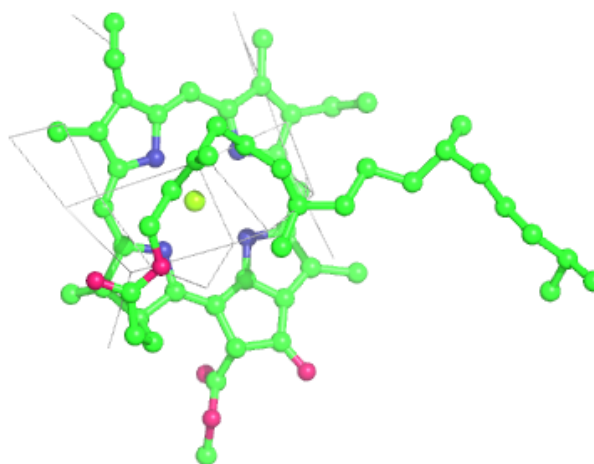
Electron density around CLA B 837:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



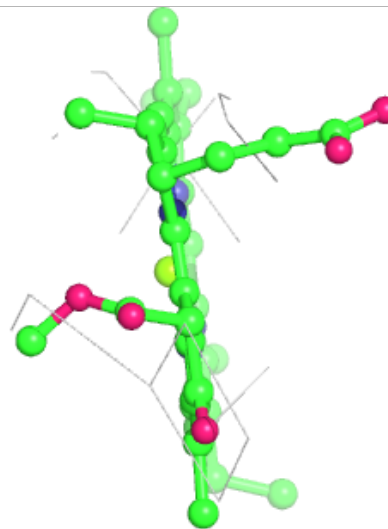
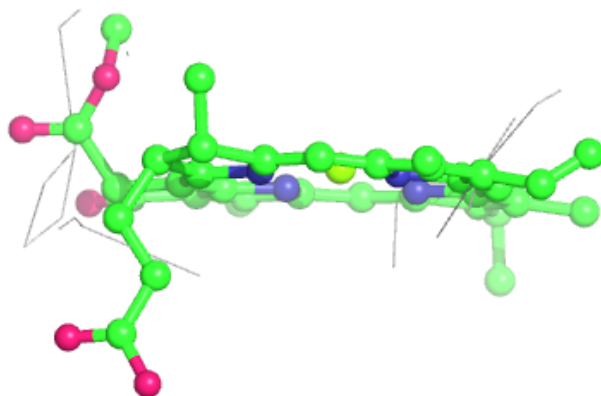
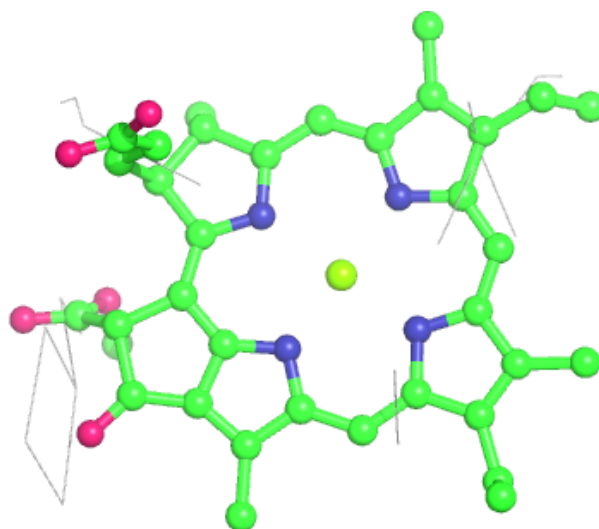
Electron density around CLA B 827:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



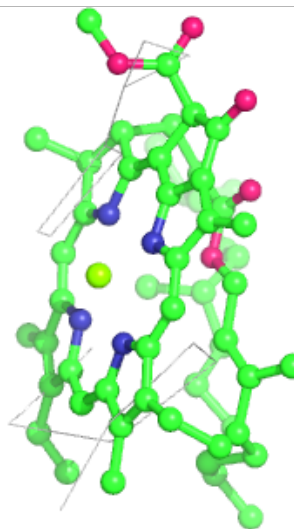
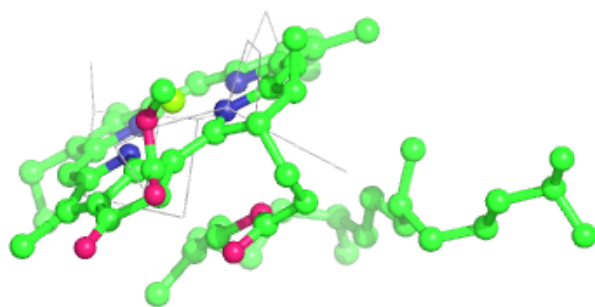
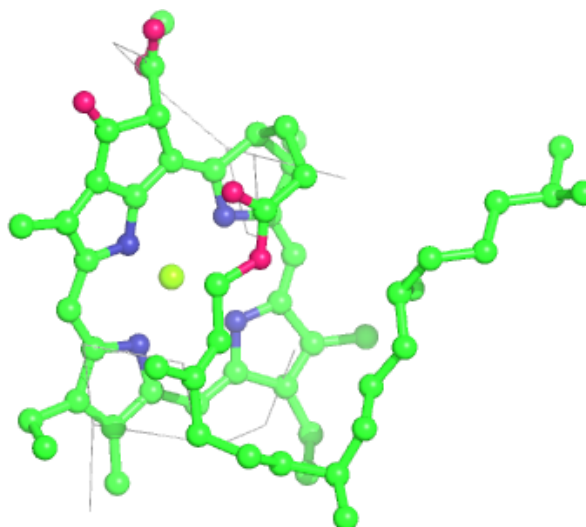
Electron density around CLA B 834:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



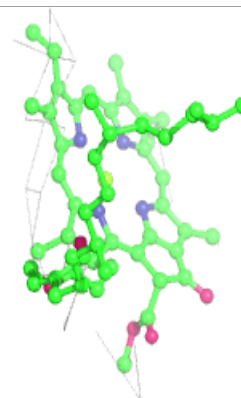
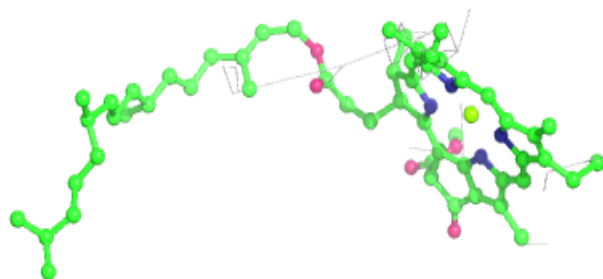
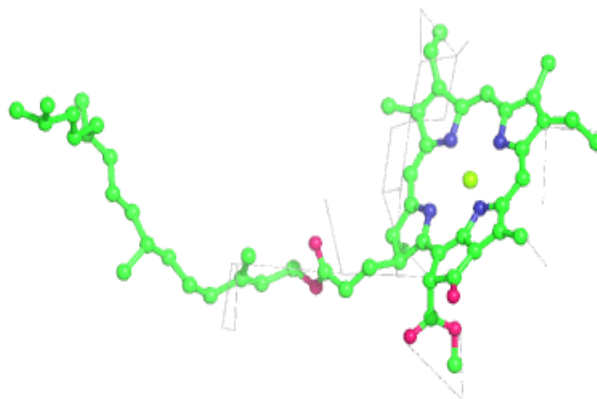
Electron density around CLA B 808:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

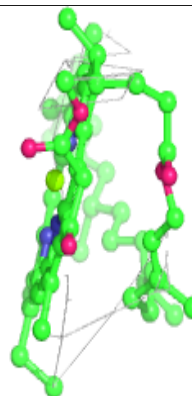
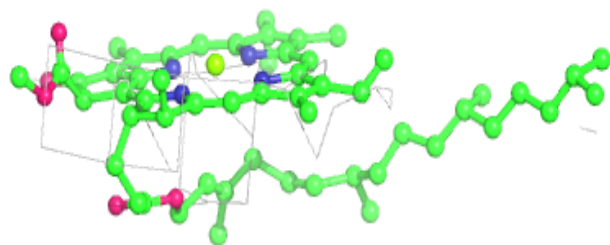
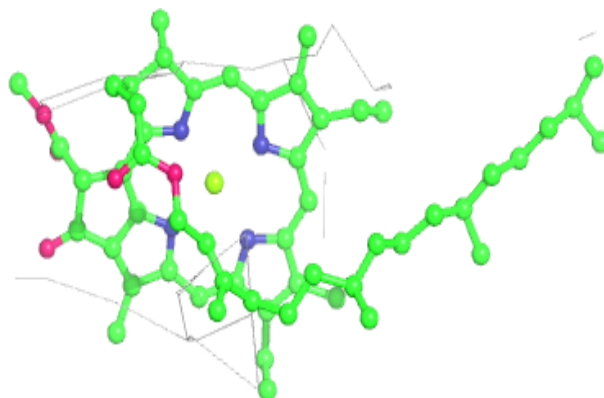


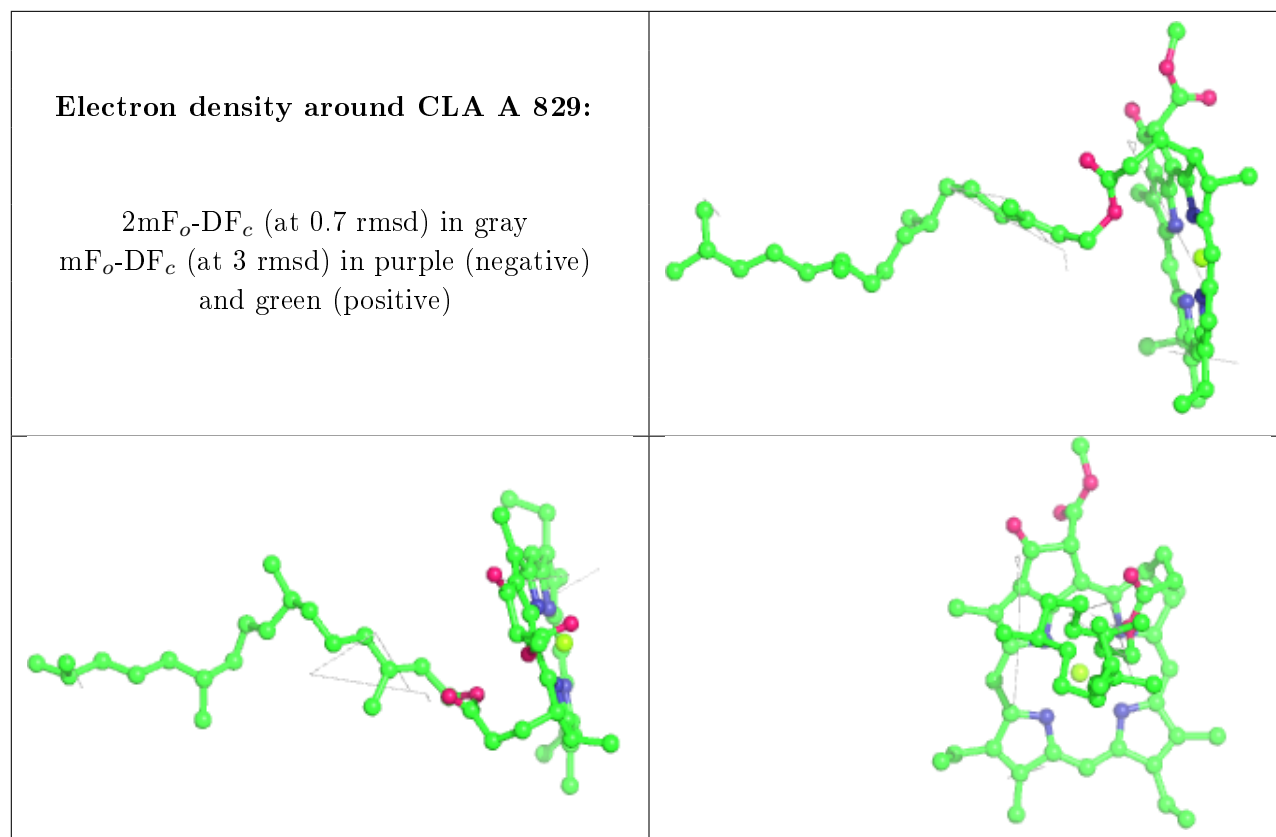
Electron density around CLA B 802:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around CLA A 841:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.