



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 05:17 PM EDT

PDB ID : 3PCQ / pdb_00003pcq

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.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

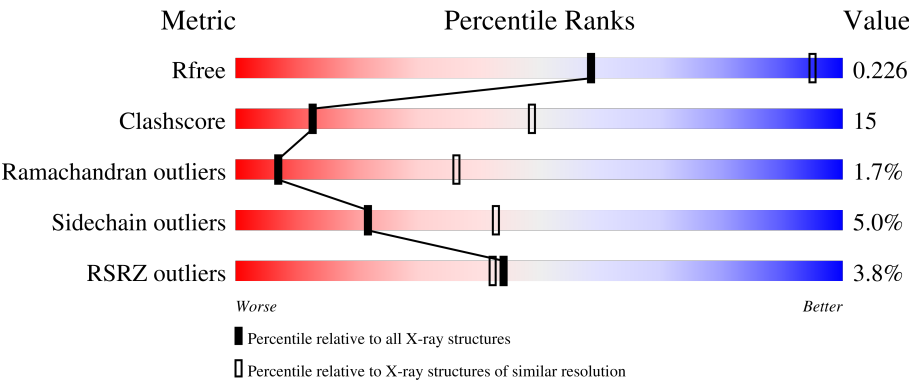
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

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}	180053	1168 (11.50-4.00)
Clashscore	190562	1001 (11.50-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

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 of 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.

Mol	Chain	Length	Quality of chain
1	A	755	4% 67% 26%
2	B	740	4% 68% 27% 5%
3	C	80	68% 28%
4	D	138	5% 64% 30%
5	E	75	3% 65% 23% 8%

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Mol	Chain	Length	Quality of chain
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
17	LHG	A	856	X	-	-	-

2 Entry composition

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	S	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

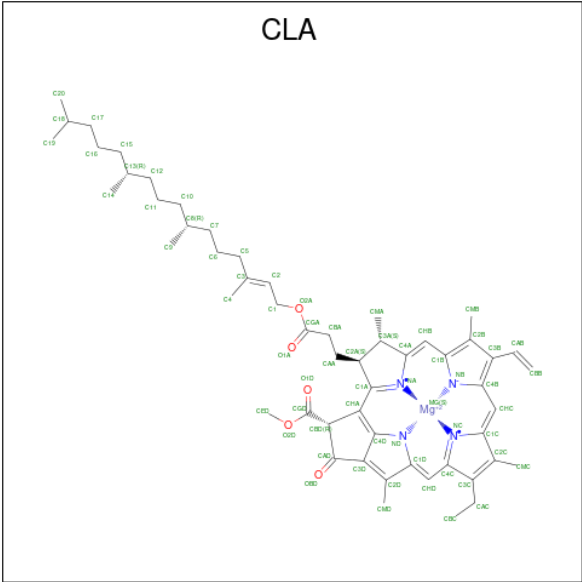
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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	S	0	0	0
			232	163	34	35				

- Molecule 13 is CHLOROPHYLL A (CCD ID: 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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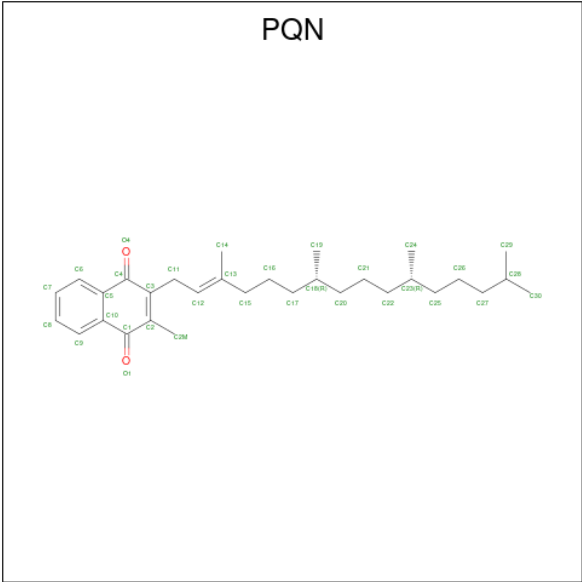
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
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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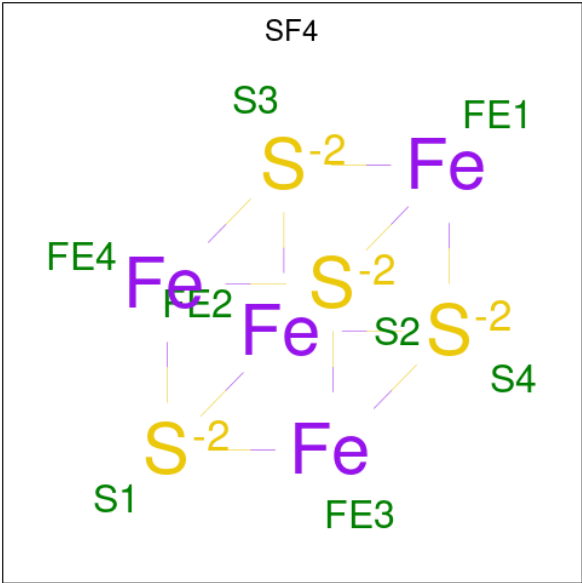
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
13	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
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 (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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 (CCD ID: SF4) (formula: Fe₄S₄).



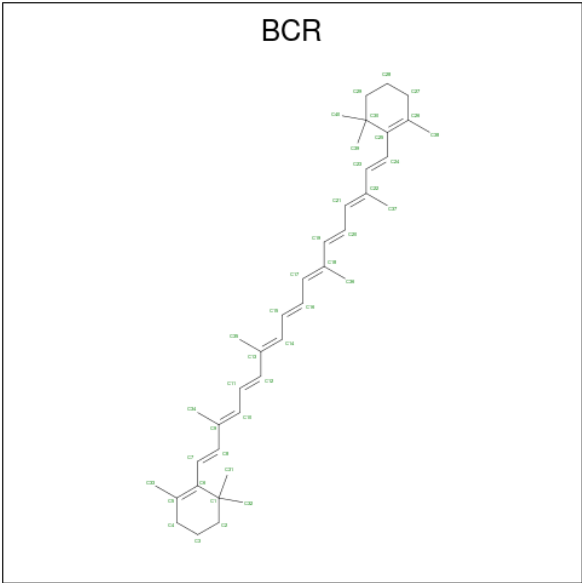
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	A	1	Total	Fe	S	0	0
			8	4	4		
15	C	1	Total	Fe	S	0	0
			8	4	4		

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

- Molecule 16 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



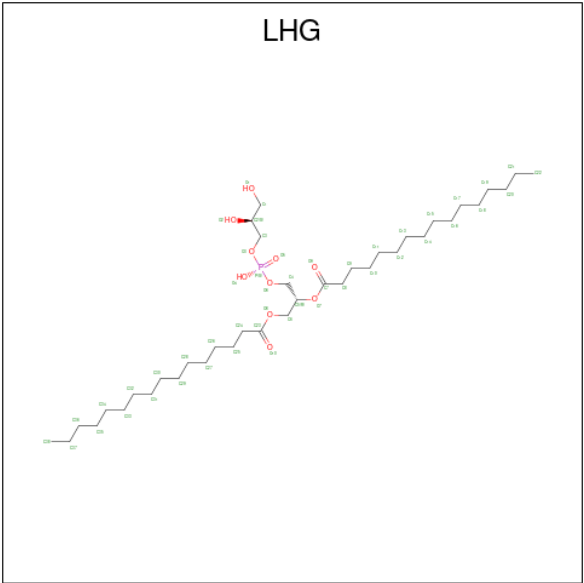
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	C	0	0
			40	40		
16	A	1	Total	C	0	0
			40	40		
16	A	1	Total	C	0	0
			40	40		
16	A	1	Total	C	0	0
			40	40		
16	A	1	Total	C	0	0
			40	40		
16	A	1	Total	C	0	0
			40	40		
16	B	1	Total	C	0	0
			40	40		
16	B	1	Total	C	0	0
			40	40		
16	B	1	Total	C	0	0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

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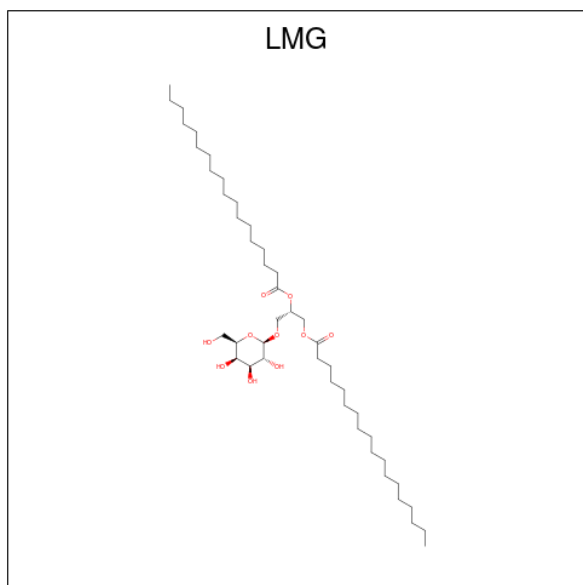
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	B	1	Total C 40 40	0	0
16	F	1	Total C 40 40	0	0
16	I	1	Total C 40 40	0	0
16	I	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	J	1	Total C 40 40	0	0
16	L	1	Total C 40 40	0	0
16	L	1	Total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

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



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 (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

- Molecule 19 is CALCIUM ION (CCD ID: 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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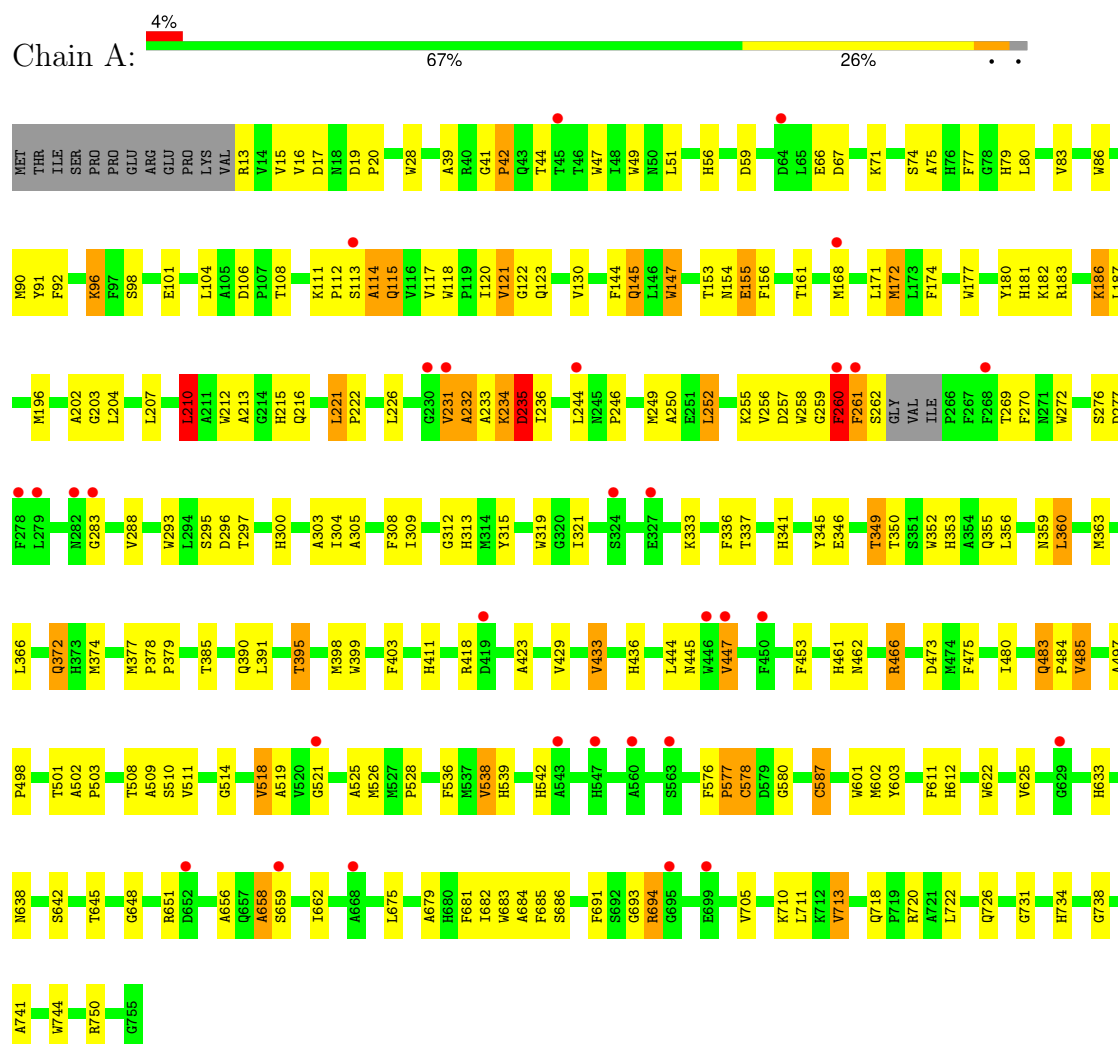
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	C	21	Total 21	O 21	0	0
20	D	17	Total 17	O 17	0	0
20	E	5	Total 5	O 5	0	0
20	F	6	Total 6	O 6	0	0
20	I	3	Total 3	O 3	0	0
20	J	1	Total 1	O 1	0	0
20	L	27	Total 27	O 27	0	0
20	M	2	Total 2	O 2	0	0

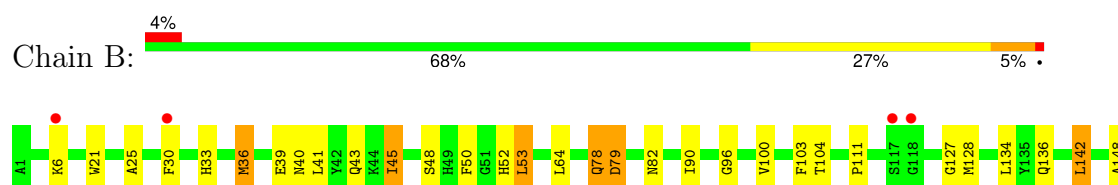
3 Residue-property plots [i](#)

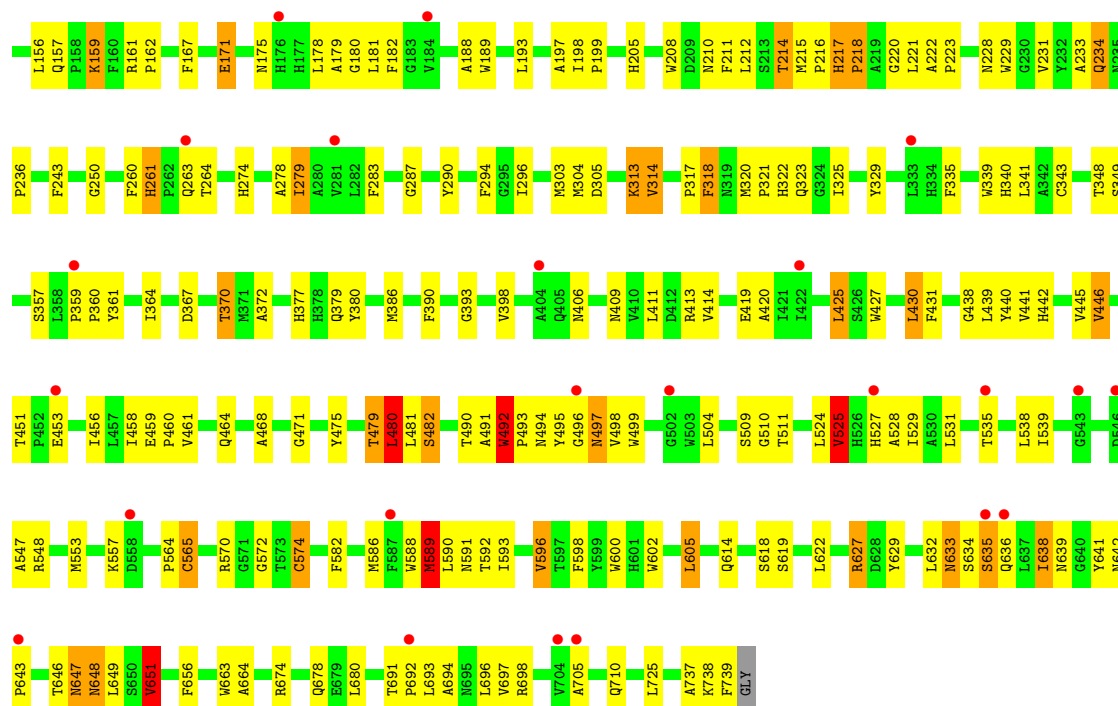
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 ($RSRZ > 2$). 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.

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

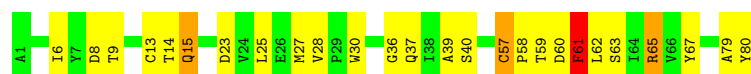


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

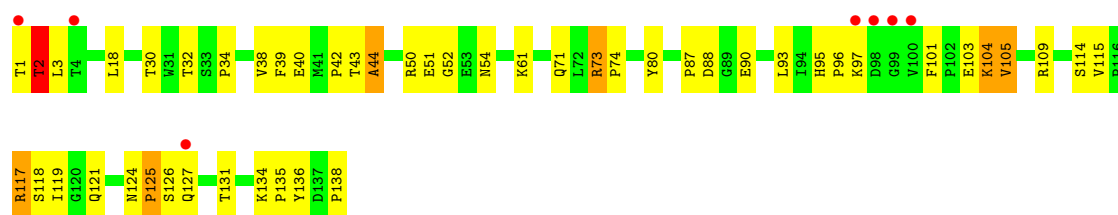




• Molecule 3: Photosystem I iron-sulfur center



• Molecule 4: Photosystem I reaction center subunit II

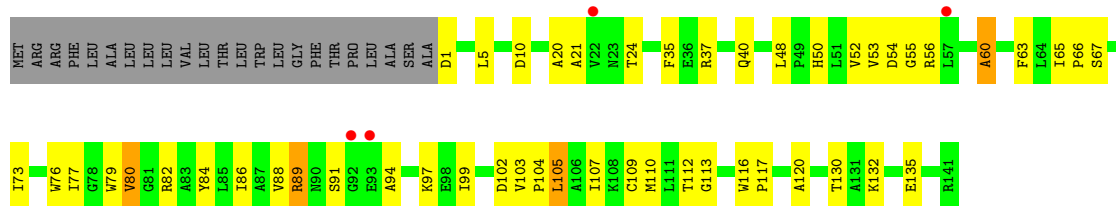


• Molecule 5: Photosystem I reaction center subunit IV

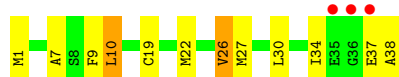


• Molecule 6: Photosystem I reaction center subunit III





• Molecule 7: Photosystem I reaction center subunit VIII



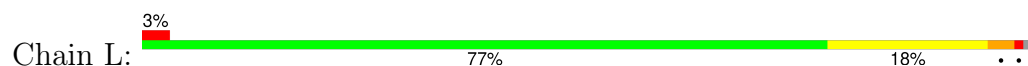
• Molecule 8: Photosystem I reaction center subunit IX



• Molecule 9: Photosystem I reaction center subunit PsaK



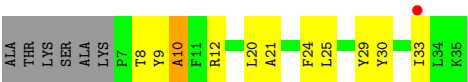
• Molecule 10: Photosystem I reaction center subunit XI



• 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 – 8.98	Depositor EDS
% Data completeness (in resolution range)	98.5 (81.12-8.98) 99.1 (81.12-8.98)	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 0.243 , 0.226	Depositor DCC
R_{free} test set	207 reflections (3.10%)	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)	0.25 , 0.0	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	0.82	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: BCR, PQN, CLA, SF4, LMG, LHG, CA

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	0.60	0/5983	1.04	39/8158 (0.5%)
2	B	0.66	2/6096 (0.0%)	1.03	34/8332 (0.4%)
3	C	0.91	0/608	1.29	12/824 (1.5%)
4	D	0.65	0/1101	1.19	7/1492 (0.5%)
5	E	0.64	0/551	1.25	8/750 (1.1%)
6	F	0.55	0/1087	1.03	1/1476 (0.1%)
7	I	0.85	0/312	1.15	1/425 (0.2%)
8	J	0.49	0/350	1.18	4/477 (0.8%)
9	K	0.72	0/219	1.51	5/297 (1.7%)
10	L	0.77	0/1148	1.04	3/1558 (0.2%)
11	M	0.75	0/244	1.13	1/332 (0.3%)
12	X	0.54	0/241	1.07	2/330 (0.6%)
All	All	0.65	2/17940 (0.0%)	1.07	117/24451 (0.5%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	589	MET	SD-CE	-8.59	1.58	1.79
2	B	36	MET	SD-CE	-7.70	1.60	1.79

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	131	THR	N-CA-C	-13.95	89.86	109.95
9	K	35	GLN	N-CA-C	10.57	125.47	109.62
11	M	30	TYR	N-CA-C	10.03	132.17	110.80
2	B	482	SER	N-CA-C	-8.80	102.56	113.38
2	B	553	MET	CA-C-N	8.35	128.47	119.28
2	B	553	MET	C-N-CA	8.35	128.47	119.28
5	E	34	TYR	CA-C-N	8.32	128.01	119.19
5	E	34	TYR	C-N-CA	8.32	128.01	119.19
3	C	63	SER	N-CA-C	-8.21	103.40	113.50
2	B	651	VAL	CB-CA-C	-8.06	101.73	111.81
1	A	521	GLY	N-CA-C	-8.05	97.05	112.02
2	B	674	ARG	N-CA-C	7.94	124.40	111.37
5	E	54	GLY	N-CA-C	7.89	131.88	113.18
3	C	60	ASP	CA-C-N	7.81	136.45	121.54
3	C	60	ASP	C-N-CA	7.81	136.45	121.54
8	J	2	LYS	N-CA-C	-7.79	102.87	111.36
6	F	55	GLY	N-CA-C	-7.74	105.27	114.48
1	A	231	VAL	N-CA-C	7.44	118.20	110.62
1	A	319	TRP	N-CA-C	7.33	120.26	110.88
5	E	55	VAL	N-CA-C	7.30	124.53	109.34
1	A	577	PRO	N-CA-C	7.28	123.10	113.57
1	A	114	ALA	N-CA-C	-7.26	95.21	108.65
5	E	33	LYS	N-CA-C	7.26	119.28	111.36
8	J	35	ASP	N-CA-C	7.26	121.41	111.54
10	L	34	LEU	N-CA-C	-7.00	100.42	110.08
2	B	461	VAL	N-CA-C	6.99	117.75	110.62
8	J	39	HIS	CA-C-N	6.92	128.49	119.84
8	J	39	HIS	C-N-CA	6.92	128.49	119.84
2	B	528	ALA	N-CA-C	-6.83	103.92	111.36
2	B	261	HIS	N-CA-C	-6.81	99.67	109.48
1	A	580	GLY	CA-C-N	6.78	126.47	119.82
1	A	580	GLY	C-N-CA	6.78	126.47	119.82
1	A	418	ARG	N-CA-C	6.76	121.85	112.45
2	B	217	HIS	CA-C-N	6.76	128.28	119.84
2	B	217	HIS	C-N-CA	6.76	128.28	119.84
9	K	57	PRO	N-CA-CB	6.69	110.69	103.33
1	A	41	GLY	CA-C-N	6.67	128.18	119.84
1	A	41	GLY	C-N-CA	6.67	128.18	119.84
3	C	80	TYR	CA-C-O	6.65	140.96	121.00
9	K	41	PRO	N-CA-CB	6.60	110.17	103.25
2	B	525	VAL	CB-CA-C	-6.45	103.43	112.14
2	B	635	SER	N-CA-C	6.41	118.84	111.02
1	A	213	ALA	N-CA-C	-6.40	104.35	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	61	PHE	N-CA-CB	6.32	121.16	110.49
1	A	502	ALA	CA-C-N	6.29	127.71	119.84
1	A	502	ALA	C-N-CA	6.29	127.71	119.84
1	A	611	PHE	N-CA-C	-6.28	104.52	111.36
2	B	79	ASP	CA-C-N	6.22	125.91	119.56
2	B	79	ASP	C-N-CA	6.22	125.91	119.56
1	A	461	HIS	N-CA-C	-6.19	104.45	111.07
1	A	485	VAL	N-CA-C	6.12	117.60	110.62
1	A	337	THR	N-CA-C	6.11	120.05	112.59
2	B	619	SER	N-CA-C	6.09	120.32	113.01
1	A	96	LYS	N-CA-C	6.07	120.42	112.89
1	A	39	ALA	N-CA-C	6.03	117.85	111.28
2	B	156	LEU	N-CA-C	-5.99	105.93	113.72
7	I	27	MET	N-CA-C	-5.96	104.87	111.36
2	B	220	GLY	N-CA-C	5.95	121.03	112.82
2	B	142	LEU	N-CA-C	-5.93	104.81	111.28
2	B	598	PHE	N-CA-C	-5.92	104.83	111.28
2	B	335	PHE	N-CA-C	-5.91	104.76	111.14
1	A	694	ARG	N-CA-C	5.84	118.42	111.71
10	L	6	LYS	N-CA-C	5.83	113.26	108.07
4	D	87	PRO	CA-C-N	5.83	128.41	120.54
4	D	87	PRO	C-N-CA	5.83	128.41	120.54
1	A	106	ASP	CA-C-N	5.82	125.51	119.05
1	A	106	ASP	C-N-CA	5.82	125.51	119.05
2	B	651	VAL	N-CA-CB	5.80	116.94	110.62
2	B	260	PHE	N-CA-C	5.76	118.60	109.50
1	A	658	ALA	N-CA-C	-5.75	106.03	113.16
1	A	398	MET	N-CA-C	-5.72	104.96	111.14
4	D	115	VAL	CA-C-N	5.72	126.99	119.84
4	D	115	VAL	C-N-CA	5.72	126.99	119.84
9	K	73	VAL	N-CA-C	-5.69	103.94	111.05
2	B	45	ILE	CB-CA-C	-5.67	104.73	111.81
2	B	492	TRP	N-CA-C	5.63	122.25	109.81
2	B	491	ALA	N-CA-C	-5.61	104.17	111.74
1	A	538	VAL	CB-CA-C	-5.61	103.47	112.16
9	K	62	THR	N-CA-C	-5.56	105.75	112.54
3	C	9	THR	N-CA-C	-5.55	106.09	112.92
2	B	96	GLY	N-CA-C	-5.54	103.04	112.51
1	A	377	MET	CA-C-N	5.51	126.06	120.38
1	A	377	MET	C-N-CA	5.51	126.06	120.38
4	D	42	PRO	N-CA-C	-5.47	107.30	114.03
12	X	33	ILE	N-CA-C	-5.46	104.40	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	60	ASP	CA-C-O	5.45	126.86	120.98
1	A	28	TRP	N-CA-C	-5.43	105.47	111.71
5	E	43	VAL	CB-CA-C	-5.42	105.63	111.59
10	L	5	VAL	N-CA-C	-5.38	100.57	108.11
5	E	11	ARG	CA-C-N	5.35	125.42	119.32
5	E	11	ARG	C-N-CA	5.35	125.42	119.32
1	A	483	GLN	CA-C-N	5.33	126.50	119.84
1	A	483	GLN	C-N-CA	5.33	126.50	119.84
2	B	425	LEU	N-CA-C	-5.32	105.48	111.28
1	A	154	ASN	N-CA-C	5.31	117.14	109.07
2	B	627	ARG	N-CA-C	5.31	117.88	111.40
3	C	60	ASP	O-C-N	5.30	129.67	122.57
3	C	79	ALA	N-CA-C	-5.29	106.69	112.72
1	A	272	TRP	N-CA-C	5.27	118.81	112.38
12	X	21	ALA	N-CA-C	-5.26	105.44	111.07
1	A	315	TYR	N-CA-C	5.22	118.33	109.76
1	A	288	VAL	N-CA-C	5.21	115.88	110.82
1	A	182	LYS	N-CA-C	5.21	117.96	111.24
4	D	2	THR	N-CA-C	5.20	121.88	110.80
2	B	393	GLY	N-CA-C	-5.18	106.14	112.77
2	B	420	ALA	N-CA-C	-5.18	105.55	111.14
3	C	57	CYS	CA-C-N	5.17	126.30	119.84
3	C	57	CYS	C-N-CA	5.17	126.30	119.84
2	B	104	THR	N-CA-C	-5.14	98.66	108.17
1	A	210	LEU	N-CA-C	-5.14	105.57	111.07
1	A	576	PHE	CA-C-N	5.07	124.56	119.19
1	A	576	PHE	C-N-CA	5.07	124.56	119.19
3	C	59	THR	N-CA-C	5.07	117.58	110.23
2	B	348	THR	N-CA-C	-5.06	105.46	111.69
2	B	633	ASN	N-CA-C	5.06	119.32	113.20
2	B	127	GLY	N-CA-C	5.04	122.25	115.00
1	A	750	ARG	N-CA-C	5.00	116.58	111.03

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	219	0
2	B	5879	0	5632	239	0
3	C	598	0	580	17	0
4	D	1075	0	1077	40	0
5	E	539	0	528	10	1
6	F	1065	0	1079	44	1
7	I	301	0	306	8	0
8	J	338	0	347	23	0
9	K	222	0	110	5	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	127	0
13	B	2349	0	2304	131	0
13	F	45	0	33	1	0
13	J	82	0	58	1	0
13	K	45	0	33	1	0
13	L	195	0	216	10	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	21	0
16	B	265	0	369	15	0
16	F	40	0	56	2	0
16	I	80	0	112	4	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	723	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 (723) 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
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
2:B:589:MET:HE2	2:B:589:MET:C	2.02	0.85
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
2:B:128:MET:HE3	2:B:134:LEU:HD23	1.64	0.80
1:A:391:LEU:O	1:A:395:THR:HG23	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:367:ASP:CG	2:B:370:THR:HG23	2.06	0.80
2:B:642:ASN:HB2	2:B:643:PRO:CD	2.12	0.80
8:J:19:MET:HE3	8:J:19:MET:HA	1.63	0.80
1:A:90:MET:HE2	13:A:829:CLA:HED1	1.62	0.79
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:589:MET:HE2	2:B:590:LEU:N	1.98	0.78
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:589:MET:HE3	2:B:593:ILE:HG13	1.65	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
13:A:829:CLA:H192	16:J:103:BCR:H14C	1.69	0.75
2:B:647:ASN:HD22	2:B:649:LEU:H	1.35	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
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
1:A:90:MET:HE1	13:A:809:CLA:HED2	1.71	0.73
2:B:229:TRP:HB2	13:B:816:CLA:H12	1.70	0.73
2:B:497:ASN:O	2:B:498:VAL:HB	1.87	0.73
4:D:50:ARG:N	4:D:54:ASN:HD21	1.84	0.73
2:B:159:LYS:H	2:B:159:LYS:CD	1.92	0.72
2:B:181:LEU:HG	13:B:813:CLA:H43	1.70	0.72
2:B:494:ASN:HD22	2:B:496:GLY:N	1.84	0.72
2:B:425:LEU:HG	13:B:839:CLA:CBB	2.20	0.72
2:B:622:LEU:HD12	13:B:802:CLA:C1	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:838:CLA:HMA2	13:B:839:CLA:HED2	1.73	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
2:B:36:MET:HE2	2:B:41:LEU:N	2.06	0.70
6:F:63:PHE:C	6:F:66:PRO:HD2	2.17	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
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:480:LEU:C	2:B:482:SER:H	2.02	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
2:B:320:MET:HE2	13:B:823:CLA:HBB1	1.78	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
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
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
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
1:A:168:MET:HE2	1:A:171:LEU:HD23	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:65:ILE:HB	6:F:66:PRO:HD3	1.78	0.64
2:B:589:MET:HE2	2:B:590:LEU:CA	2.28	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:589:MET:HE3	2:B:593:ILE:CG1	2.27	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
1:A:257:ASP:CG	1:A:258:TRP:N	2.56	0.64
2:B:36:MET:HE2	2:B:41:LEU:CA	2.28	0.63
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
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
2:B:589:MET:HE2	2:B:590:LEU:HA	1.81	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: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
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
1:A:353:HIS:CD2	1:A:411:HIS:HD1	2.11	0.62
2:B:303:MET:HE2	13:B:823:CLA:HED1	1.80	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:42:PRO:HG2	6:F:99:ILE:HD13	1.83	0.61
13:A:827:CLA:HAA2	13:A:828:CLA:OBD	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:453:PHE:O	13:A:835:CLA:CBB	2.48	0.60
1:A:518:VAL:HG22	1:A:525:ALA:HB3	1.82	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
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
9:K:40:GLY:O	9:K:41:PRO:C	2.45	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
13:B:818:CLA:HBB1	13:B:818:CLA:HMB3	1.83	0.59
2:B:36:MET:CE	2:B:41:LEU:N	2.66	0.59
2:B:181:LEU:HD21	13:B:813:CLA:H12	1.85	0.59
7:I:7:ALA:HB1	7:I:10:LEU:HD22	1.83	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
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
7:I:37:GLU:C	7:I:38:ALA:OXT	2.41	0.59
1:A:231:VAL:O	1:A:232:ALA:CB	2.50	0.58
2:B:591:ASN:HB2	13:B:802:CLA:HBC2	1.83	0.58
1:A:145:GLN:H	1:A:145:GLN:NE2	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
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
2:B:367:ASP:OD1	2:B:370:THR:HG23	2.03	0.58
2:B:648:ASN:N	2:B:648:ASN:HD22	2.02	0.58
1:A:744:TRP:HB2	13:A:829:CLA:HBB1	1.87	0.57
16:A:854:BCR:H321	16:A:854:BCR:HC8	1.84	0.57
1:A:91:TYR:CZ	1:A:147:TRP:CZ3	2.91	0.57
2:B:380:TYR:CD1	13:B:827:CLA:HBB1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:244:LEU:C	1:A:246:PRO:HD3	2.30	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
13:A:822:CLA:HMD3	13:A:823:CLA:HBB1	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
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
1:A:259:GLY:C	1:A:261:PHE:H	2.13	0.56
2:B:234:GLN:HA	2:B:234:GLN:OE1	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
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:363:MET:HE1	13:A:830:CLA:HBC3	1.87	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:827:CLA:H12	13:A:838:CLA:HMA3	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
1:A:453:PHE:C	13:A:835:CLA:HBB2	2.31	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
1:A:79:HIS:CE1	13:A:806:CLA:HMA2	2.42	0.55
2:B:398:VAL:CG2	2:B:547:ALA:HB1	2.37	0.55
2:B:425:LEU:HD13	2:B:538:LEU:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
10:L:35:PRO:HG3	13:L:1003:CLA:HED2	1.88	0.54
1:A:390:GLN:HE21	1:A:390:GLN:HA	1.71	0.54
2:B:179:ALA:HB2	2:B:287:GLY:HA3	1.89	0.54
2:B:274:HIS:HB3	13:B:817:CLA:HMB2	1.90	0.54
2:B:664:ALA:C	13:B:803:CLA:HBB1	2.31	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:413:ARG:HD3	13:B:830:CLA:OBD	2.07	0.54
2:B:592:THR:O	2:B:596:VAL:HG13	2.08	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:52:HIS:CE1	13:B:805:CLA:HMA2	2.42	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:21:TRP:CG	2:B:710:GLN:HE22	2.26	0.53
2:B:103:PHE:CZ	2:B:651:VAL:HG22	2.42	0.53
2:B:548:ARG:HH22	4:D:124:ASN:CG	2.15	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
11:M:24:ARG:HH11	11:M:24:ARG:CG	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ARG:O	2:B:646:THR:HG21	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
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
6:F:53:VAL:HG12	6:F:63:PHE:HB2	1.90	0.53
1:A:120:ILE:C	1:A:122:GLY:H	2.16	0.53
13:A:803:CLA:O1A	2:B:531:LEU:HD11	2.09	0.53
1:A:683:TRP:CD2	13:A:801:CLA:HMA2	2.45	0.52
13:A:827:CLA:H162	16:A:852:BCR:H272	1.91	0.52
13:A:831:CLA:H111	17:A:855:LHG:H202	1.90	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
6:F:40:GLN:OE1	8:J:40:PRO:O	2.26	0.52
9:K:74:VAL:C	9:K:76:GLY:H	2.17	0.52
1:A:221:LEU:HD11	1:A:295:SER:CA	2.39	0.52
2:B:78:GLN:OE1	2:B:78:GLN:HA	2.10	0.52
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:217:HIS:CG	2:B:218:PRO:HD2	2.44	0.52
2:B:430:LEU:HB3	13:B:832:CLA:HED3	1.90	0.52
8:J:28:GLU:OE1	8:J:28:GLU:HA	2.09	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
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: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:718:GLN:NE2	5:E:42:LYS:HD3	2.25	0.51
1:A:71:LYS:NZ	20:A:931:HOH:O	2.43	0.51
1:A:226:LEU:HD22	1:A:231:VAL:HG21	1.93	0.51
1:A:542:HIS:HE1	1:A:612:HIS:ND1	2.08	0.51
2:B:36:MET:HE3	2:B:40:ASN:HB2	1.92	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:90:MET:CE	13:A:809:CLA:HED2	2.39	0.51
2:B:453:GLU:HA	6:F:48:LEU:HD22	1.93	0.51
13:B:840:CLA:HBB2	14:B:842:PQN:H141	1.91	0.51
7:I:30:LEU:O	7:I:34:ILE:HG12	2.11	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
1:A:257:ASP:OD2	1:A:262:SER:C	2.55	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
1:A:16:VAL:CG1	1:A:17:ASP:N	2.74	0.50
2:B:379:GLN:HA	2:B:379:GLN:OE1	2.11	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
7:I:9:PHE:CE1	7:I:10:LEU:HD13	2.46	0.49
13:A:844:CLA:H52	13:B:840:CLA:H43	1.93	0.49
2:B:340:HIS:HD2	13:B:805:CLA:OBD	1.96	0.49
1:A:691:PHE:HB2	13:A:803:CLA:HBC2	1.95	0.49
10:L:105:GLY:O	10:L:106:SER:HB2	2.11	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
2:B:303:MET:HE2	13:B:823:CLA:CED	2.42	0.49
13:B:801:CLA:H72	13:B:802:CLA:CED	2.42	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
13:A:803:CLA:H71	13:A:843:CLA:CMC	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:PHE:CE2	13:B:813:CLA:H61	2.48	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
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
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:444:LEU:HB2	13:A:840:CLA:HBB1	1.96	0.48
13:A:834:CLA:HMA2	16:I:101:BCR:H272	1.96	0.48
13:B:806:CLA:H91	18:B:850:LMG:H401	1.96	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
2:B:231:VAL:C	2:B:234:GLN:HG2	2.36	0.48
6:F:73:ILE:O	6:F:76:TRP:HB3	2.14	0.48
1:A:196:MET:HE1	13:A:826:CLA:H142	1.94	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:360:LEU:CD1	13:A:831:CLA:HBB1	2.44	0.48
1:A:497:ALA:N	1:A:498:PRO:CD	2.76	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
13:A:843:CLA:H172	8:J:19:MET:HE2	1.95	0.47
2:B:329:TYR:OH	2:B:340:HIS:CE1	2.61	0.47
4:D:117:ARG:HG2	4:D:118:SER:N	2.26	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:814:CLA:HAB	13:B:828:CLA:H13	1.96	0.47
13:B:824:CLA:H61	13:B:824:CLA:H41	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:SER:HB3	1:A:734:HIS:HB2	1.96	0.47
2:B:357:SER:C	2:B:359:PRO:HD3	2.40	0.47
1:A:56:HIS:CG	13:A:806:CLA:HAB	2.49	0.47
1:A:215:HIS:C	1:A:215:HIS:CD2	2.92	0.47
1:A:691:PHE:HB2	13:A:803:CLA:CBC	2.45	0.47
1:A:683:TRP:CG	13:A:801:CLA:HMA2	2.50	0.47
13:A:810:CLA:HBB1	13:B:833:CLA:HMD2	1.95	0.47
2:B:525:VAL:CG1	13:B:801:CLA:H141	2.45	0.47
2:B:693:LEU:HD12	13:L:1003:CLA:H11	1.96	0.47
1:A:90:MET:HE2	13:A:829:CLA:CED	2.39	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
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
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
2:B:589:MET:C	2:B:589:MET:CE	2.83	0.47
6:F:88:VAL:CG1	6:F:97:LYS:HB2	2.41	0.47
13:A:843:CLA:H172	8:J:19:MET:HG3	1.97	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
11:M:24:ARG:CG	11:M:24:ARG:NH1	2.78	0.47
1:A:145:GLN:H	1:A:145:GLN:CD	2.22	0.46
13:A:843:CLA:O1A	13:A:843:CLA:H2	2.15	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
3:C:57:CYS:HA	3:C:58:PRO:HD3	1.71	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
2:B:39:GLU:O	2:B:43:GLN:HG3	2.15	0.46
2:B:663:TRP:CD2	13:B:801:CLA:HMA2	2.51	0.46
13:B:838:CLA:H203	6:F:67:SER:HB3	1.98	0.46
3:C:61:PHE:HD2	4:D:119:ILE:HG21	1.81	0.46
1:A:374:MET:HE1	13:A:830:CLA:O1D	2.15	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
1:A:577:PRO:O	1:A:578:CYS:HB3	2.14	0.46
6:F:80:VAL:HG11	6:F:110:MET:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ALA:C	13:A:821:CLA:HBC3	2.41	0.46
2:B:509:SER:O	2:B:509:SER:OG	2.25	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:445:ASN:ND2	13:B:803:CLA:HED2	2.31	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
13:B:810:CLA:HHC	13:B:810:CLA:HBB1	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: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
1:A:19:ASP:N	1:A:20:PRO:HD3	2.31	0.46
1:A:91:TYR:CZ	1:A:147:TRP:HZ3	2.33	0.46
2:B:36:MET:CE	2:B:40:ASN:HB2	2.45	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: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:100:VAL:HG22	7:I:1:MET:HE2	1.98	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:468:ALA:O	2:B:482:SER:HB2	2.16	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:91:TYR:CE2	1:A:161:THR:HG21	2.51	0.45
1:A:313:HIS:CE1	16:A:849:BCR:H363	2.51	0.45
1:A:682:ILE:HD11	13:A:843:CLA:HMB1	1.97	0.45
13:A:821:CLA:HBA2	13:A:821:CLA:H3A	1.83	0.45
13:A:823:CLA:HBA2	13:A:823:CLA:H3A	1.44	0.45
13:A:844:CLA:HMA1	2:B:694:ALA:HB1	1.97	0.45
13:B:818:CLA:H62	13:B:818:CLA:H41	1.69	0.45
1:A:539:HIS:CG	13:A:839:CLA:HED2	2.51	0.45
2:B:64:LEU:HD11	16:B:845:BCR:H271	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:471:GLY:HA3	2:B:504:LEU:CD2	2.46	0.45
13:B:820:CLA:H3A	13:B:820:CLA:HBA2	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
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
2:B:496:GLY:O	2:B:497:ASN:C	2.59	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:711:LEU:HD23	6:F:130:THR:HG22	1.98	0.45
2:B:570:ARG:HG3	2:B:570:ARG:HH11	1.81	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:86:TRP:HE1	13:A:809:CLA:HBA1	1.82	0.45
1:A:321:ILE:HD11	13:A:821:CLA:H2A	1.99	0.45
1:A:445:ASN:ND2	2:B:680:LEU:HD21	2.33	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
1:A:92:PHE:CZ	1:A:96:LYS:HG3	2.52	0.44
13:A:801:CLA:NA	13:B:801:CLA:HAB	2.31	0.44
2:B:48:SER:HB3	13:B:805:CLA:HBB1	1.98	0.44
2:B:215:MET:HA	2:B:216:PRO:HD3	1.83	0.44
13:B:827:CLA:CGA	13:B:827:CLA:H3A	2.47	0.44
6:F:20:ALA:O	6:F:21:ALA:C	2.59	0.44
13:A:807:CLA:H3A	13:A:831:CLA:HAB	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:M:1601:CLA:H3A	13:M:1601:CLA:HBA2	1.69	0.44
1:A:212:TRP:N	13:A:815:CLA:HBB1	2.32	0.44
1:A:484:PRO:HB3	13:A:839:CLA:CED	2.46	0.44
13:A:828:CLA:HMB3	13:A:836:CLA:H12	1.99	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:H43	13:B:810:CLA:CED	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:ILE:N	3:C:6:ILE:HD12	2.33	0.44
4:D:125:PRO:HG3	4:D:135:PRO:HG3	2.00	0.44
8:J:1:MET:HE2	8:J:1:MET:O	2.18	0.44
13:B:831:CLA:HBC3	16:F:1302:BCR:H362	2.00	0.44
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
8:J:32:PHE:C	8:J:34:PRO:HD3	2.42	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:H403	16:A:854:BCR:H23C	1.99	0.44
4:D:96:PRO:O	4:D:97:LYS:C	2.59	0.44
6:F:76:TRP:CD1	6:F:76:TRP:C	2.96	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
2:B:589:MET:HE1	2:B:590:LEU:HD23	2.00	0.44
13:B:809:CLA:H102	13:B:827:CLA:H193	1.98	0.44
1:A:684:ALA:C	13:A:803:CLA:HAB	2.43	0.43
5:E:17:TYR:O	5:E:18:ASN:HB2	2.18	0.43
1:A:501:THR:C	1:A:503:PRO:HD3	2.43	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
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
2:B:492:TRP:O	2:B:493:PRO:C	2.61	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:431:PHE:HD2	13:B:838:CLA:HBB2	1.84	0.43
2:B:531:LEU:HD21	13:B:802:CLA:CBB	2.48	0.43
2:B:622:LEU:HD13	13:B:802:CLA:HMA2	2.00	0.43
8:J:19:MET:HA	8:J:19:MET:CE	2.38	0.43
1:A:221:LEU:CB	1:A:222:PRO:HD3	2.45	0.43
1:A:259:GLY:C	1:A:261:PHE:N	2.76	0.43
2:B:236:PRO:O	2:B:250:GLY:HA3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:ASP:OD1	2:B:323:GLN:HA	2.18	0.43
2:B:529:ILE:HG21	13:B:837:CLA:HAB	1.99	0.43
2:B:636:GLN:HG3	2:B:737:ALA:CB	2.49	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
2:B:175:ASN:HB3	13:B:820:CLA:HMD1	2.01	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
1:A:212:TRP:CA	13:A:815:CLA:HBB1	2.49	0.43
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:359:ASN:CG	13:A:826:CLA:HAA1	2.44	0.43
9:K:59:LEU:C	9:K:61:ALA:H	2.25	0.43
6:F:116:TRP:CG	6:F:117:PRO:HD3	2.54	0.43
1:A:120:ILE:C	1:A:122:GLY:N	2.77	0.43
13:A:844:CLA:H41	13:A:844:CLA:H62	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
2:B:360:PRO:HG3	13:B:818:CLA:HBA1	2.00	0.43
4:D:18:LEU:HD23	4:D:18:LEU:HA	1.86	0.43
4:D:73:ARG:HB2	4:D:74:PRO:HD3	2.00	0.43
13:A:809:CLA:HMC2	13:A:829:CLA:H142	2.01	0.42
13:A:845:CLA:H3A	13:A:845:CLA:HBA2	1.74	0.42
13:B:832:CLA:H61	16:F:1302:BCR:H312	2.00	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
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:HBA2	13:B:817:CLA:H3A	1.39	0.42
5:E:6:LYS:NZ	5:E:22:THR:HG21	2.35	0.42
10:L:4:LEU:N	10:L:4:LEU:HD22	2.35	0.42
2:B:103:PHE:HZ	2:B:651:VAL:HG22	1.83	0.42
2:B:325:ILE:CD1	2:B:409:ASN:ND2	2.82	0.42
2:B:386:MET:HE1	16:B:847:BCR:H361	2.01	0.42
2:B:535:THR:O	2:B:539:ILE:HG13	2.19	0.42
2:B:589:MET:CE	2:B:590:LEU:HA	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:588:TRP:CH2	13:B:802:CLA:CBB	3.02	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
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
1:A:47:TRP:CZ3	1:A:51:LEU:HD12	2.54	0.42
1:A:423:ALA:HA	4:D:38:VAL:HG11	2.02	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
2:B:6:LYS:HD2	11:M:31:LYS:HB3	2.02	0.42
13:B:806:CLA:H143	13:B:828:CLA:CBB	2.50	0.42
6:F:103:VAL:O	6:F:107:ILE:HG13	2.20	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
1:A:741:ALA:CB	16:A:854:BCR:H323	2.50	0.42
13:A:811:CLA:H3A	13:A:811:CLA:HBA2	1.63	0.42
2:B:372:ALA:HA	2:B:600:TRP:CZ3	2.55	0.42
2:B:414:VAL:HG11	16:B:846:BCR:C40	2.50	0.42
2:B:527:HIS:CD2	16:J:105:BCR:H322	2.55	0.42
7:I:22:MET:O	7:I:26:VAL:HG13	2.19	0.42
1:A:42:PRO:CG	6:F:99:ILE:HD13	2.50	0.41
13:A:829:CLA:H93	16:J:103:BCR:H20C	2.02	0.41
2:B:36:MET:HE1	2:B:40:ASN:CB	2.50	0.41
17:B:851:LHG:HC5	12:X:12:ARG:HB3	2.02	0.41
3:C:28:VAL:HG12	4:D:109:ARG:HB3	2.02	0.41
1:A:177:TRP:HB2	13:A:812:CLA:CMC	2.50	0.41
1:A:346:GLU:OE1	1:A:346:GLU:N	2.47	0.41
1:A:685:PHE:HA	13:A:803:CLA:HAB	2.01	0.41
1:A:686:SER:HB2	1:A:731:GLY:O	2.20	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:HBA2	13:A:846:CLA:H12	1.85	0.41
2:B:189:TRP:HA	13:B:814:CLA:HBB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:49:TRP:CZ3	17:A:855:LHG:H121	2.56	0.41
1:A:203:GLY:HA3	13:A:814:CLA:HBB1	2.02	0.41
1:A:483:GLN:HA	1:A:484:PRO:HD3	1.70	0.41
2:B:136:GLN:HE21	13:B:814:CLA:HAA1	1.85	0.41
2:B:586:MET:HE3	2:B:586:MET:HB3	1.96	0.41
1:A:204:LEU:HD13	1:A:204:LEU:C	2.45	0.41
1:A:710:LYS:HD2	1:A:710:LYS:O	2.20	0.41
1:A:722:LEU:HD22	1:A:726:GLN:CD	2.46	0.41
2:B:178:LEU:O	2:B:283:PHE:HB3	2.21	0.41
2:B:367:ASP:CG	2:B:370:THR:CG2	2.87	0.41
6:F:88:VAL:O	6:F:89:ARG:C	2.63	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:378:PRO:HA	1:A:379:PRO:HD3	1.83	0.41
5:E:19:GLU:OE1	5:E:42:LYS:NZ	2.52	0.41
6:F:54:ASP:OD2	12:X:30:TYR:HE2	1.98	0.41
1:A:257:ASP:CG	1:A:258:TRP:H	2.27	0.41
3:C:8:ASP:C	3:C:8:ASP:OD1	2.61	0.41
2:B:313:LYS:C	2:B:314:VAL:HG13	2.45	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:H111	13:L:1003:CLA:H152	1.99	0.41
1:A:161:THR:HG22	16:A:850:BCR:HC32	2.02	0.41
1:A:186:LYS:O	1:A:187:LEU:C	2.62	0.41
13:A:820:CLA:HBA2	13:A:820:CLA:H3A	1.89	0.41
2:B:442:HIS:CD2	2:B:456:ILE:HG13	2.56	0.41
13:B:805:CLA:HBA1	13:B:805:CLA:H3A	1.74	0.41
13:B:825:CLA:HBA2	13:B:825:CLA:H3A	1.69	0.41
6:F:24:THR:HG21	8:J:35:ASP:OD1	2.20	0.41
6:F:73:ILE:O	6:F:77:ILE:HG13	2.21	0.41
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.82	0.41
1:A:112:PRO:HA	1:A:144:PHE:CE1	2.55	0.41
13:A:802:CLA:H3A	13:A:802:CLA:O1A	2.21	0.41
13:A:841:CLA:HAA2	13:B:831:CLA:HMB1	2.02	0.41
2:B:30:PHE:CD1	2:B:45:ILE:HD13	2.56	0.41
13:B:803:CLA:H122	16:I:101:BCR:H281	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:818:CLA:CGA	13:B:818:CLA:H3A	2.51	0.41
4:D:43:THR:O	4:D:44:ALA:CB	2.68	0.41
4:D:104:LYS:H	4:D:104:LYS:HG2	1.51	0.41
10:L:44:ILE:HG23	10:L:45:LEU:N	2.36	0.41
10:L:57:PHE:CD1	10:L:57:PHE:C	2.99	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:803:CLA:C14	16:A:854:BCR:H402	2.51	0.40
13:A:835:CLA:HED2	10:L:65:LEU:O	2.21	0.40
13:A:843:CLA:H52	13:A:843:CLA:NC	2.36	0.40
20:A:944:HOH:O	10:L:16:HIS:HE1	2.04	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:H2A	13:B:810:CLA:O2A	2.20	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:HD12	1:A:360:LEU:HA	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: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:803:CLA:H71	13:A:843:CLA:HMC2	2.03	0.40
13:A:825:CLA:HBB	13:A:846:CLA:HBB1	2.02	0.40
2:B:33:HIS:HE1	13:B:804:CLA:HED1	1.85	0.40
2:B:318:PHE:H	13:B:822:CLA:C2B	2.34	0.40
2:B:564:PRO:O	2:B:565:CYS:HB3	2.22	0.40
8:J:30:ASN:O	8:J:34:PRO:HG3	2.21	0.40
16:L:1006:BCR:H20C	16:L:1006:BCR:H361	1.88	0.40
2:B:279:ILE:HD11	13:B:817:CLA:HBC3	2.02	0.40
2:B:377:HIS:HE2	13:B:828:CLA:C1B	2.35	0.40
2:B:605:LEU:HD12	2:B:605:LEU:HA	1.80	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:260:PHE:O	1:A:261:PHE:HB2	2.21	0.40
1:A:741:ALA:CB	16:A:854:BCR:C32	2.99	0.40
2:B:53:LEU:HD12	2:B:53:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	9	40
2	B	737/740 (100%)	691 (94%)	37 (5%)	9 (1%)	10	44
3	C	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	9	42
4	D	136/138 (99%)	125 (92%)	8 (6%)	3 (2%)	5	29
5	E	67/75 (89%)	59 (88%)	4 (6%)	4 (6%)	1	13
6	F	139/164 (85%)	128 (92%)	8 (6%)	3 (2%)	5	29
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	10
10	L	149/154 (97%)	140 (94%)	7 (5%)	2 (1%)	9	42
11	M	29/31 (94%)	28 (97%)	0	1 (3%)	3	21
12	X	27/35 (77%)	22 (82%)	4 (15%)	1 (4%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2213/2334 (95%)	2065 (93%)	111 (5%)	37 (2%)	7	36

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	235	ASP
1	A	260	PHE
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%)	563 (96%)	26 (4%)	25	47
2	B	595/597 (100%)	563 (95%)	32 (5%)	20	41
3	C	67/67 (100%)	65 (97%)	2 (3%)	36	57
4	D	115/115 (100%)	105 (91%)	10 (9%)	9	29
5	E	59/64 (92%)	59 (100%)	0	100	100
6	F	109/128 (85%)	106 (97%)	3 (3%)	38	60
7	I	32/32 (100%)	30 (94%)	2 (6%)	16	37
8	J	36/36 (100%)	34 (94%)	2 (6%)	19	40
10	L	117/119 (98%)	108 (92%)	9 (8%)	12	32
11	M	26/26 (100%)	24 (92%)	2 (8%)	12	32
12	X	20/27 (74%)	19 (95%)	1 (5%)	22	43
All	All	1765/1814 (97%)	1676 (95%)	89 (5%)	22	43

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	THR
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	260	PHE
1	A	349	THR
1	A	360	LEU
1	A	372	GLN
1	A	385	THR

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Mol	Chain	Res	Type
1	A	395	THR
1	A	433	VAL
1	A	447	VAL
1	A	466	ARG
1	A	485	VAL
1	A	518	VAL
1	A	538	VAL
1	A	587	CYS
1	A	675	LEU
1	A	705	VAL
1	A	713	VAL
2	B	53	LEU
2	B	78	GLN
2	B	142	LEU
2	B	159	LYS
2	B	171	GLU
2	B	214	THR
2	B	218	PRO
2	B	221	LEU
2	B	279	ILE
2	B	318	PHE
2	B	349	SER
2	B	370	THR
2	B	411	LEU
2	B	419	GLU
2	B	430	LEU
2	B	446	VAL
2	B	479	THR
2	B	480	LEU
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	638	ILE
2	B	647	ASN
2	B	648	ASN
2	B	651	VAL
2	B	697	VAL

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Mol	Chain	Res	Type
2	B	698	ARG
3	C	15	GLN
3	C	65	ARG
4	D	1	THR
4	D	2	THR
4	D	61	LYS
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	80	VAL
6	F	105	LEU
7	I	10	LEU
7	I	26	VAL
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	68	LEU
10	L	69	ARG
10	L	85	LEU
10	L	134	VAL
11	M	3	LEU
11	M	17	LEU
12	X	8	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	50	ASN
1	A	79	HIS
1	A	145	GLN
1	A	224	ASN
1	A	353	HIS

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Mol	Chain	Res	Type
1	A	359	ASN
1	A	372	GLN
1	A	390	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
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	70	GLN
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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	A	808	1	55,59,73	1.52	8 (14%)	64,96,113	1.87	8 (12%)
13	CLA	B	839	2	51,55,73	1.45	7 (13%)	60,91,113	1.72	6 (10%)
14	PQN	B	842	-	34,34,34	3.54	17 (50%)	43,45,45	2.03	6 (13%)
13	CLA	B	825	20	50,54,73	1.36	7 (14%)	59,90,113	1.98	9 (15%)
13	CLA	A	829	1	69,73,73	1.25	6 (8%)	82,113,113	1.56	8 (9%)
13	CLA	A	805	13,1	63,67,73	1.34	6 (9%)	74,105,113	1.78	9 (12%)
16	BCR	B	843	-	41,41,41	1.54	5 (12%)	56,56,56	2.08	19 (33%)
13	CLA	K	1401	-	49,53,73	1.47	7 (14%)	58,89,113	1.83	6 (10%)
13	CLA	A	833	1	69,73,73	1.20	6 (8%)	82,113,113	1.79	8 (9%)
13	CLA	A	806	1	69,73,73	1.17	4 (5%)	82,113,113	1.69	11 (13%)
16	BCR	A	851	-	41,41,41	1.44	6 (14%)	56,56,56	1.98	21 (37%)
13	CLA	A	809	1	69,73,73	1.29	8 (11%)	82,113,113	1.71	9 (10%)
13	CLA	B	841	2	69,73,73	1.16	8 (11%)	82,113,113	1.64	7 (8%)
16	BCR	I	102	-	41,41,41	1.27	6 (14%)	56,56,56	1.86	18 (32%)
13	CLA	A	837	1	49,53,73	1.42	7 (14%)	58,89,113	1.98	8 (13%)
13	CLA	A	822	20	69,73,73	1.29	9 (13%)	82,113,113	1.72	10 (12%)
13	CLA	B	835	20	49,53,73	1.55	8 (16%)	58,89,113	1.86	9 (15%)
13	CLA	B	821	2	49,53,73	1.49	9 (18%)	58,89,113	2.05	9 (15%)
13	CLA	A	839	1	69,73,73	1.33	8 (11%)	82,113,113	1.55	7 (8%)
13	CLA	A	813	1	58,62,73	1.34	7 (12%)	68,99,113	1.91	8 (11%)
13	CLA	A	842	20	55,59,73	1.44	6 (10%)	64,96,113	1.81	7 (10%)
13	CLA	A	810	1	69,73,73	1.24	7 (10%)	82,113,113	1.75	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	SF4	C	101	3	0,12,12	-	-	-		
13	CLA	B	805	2	69,73,73	1.29	6 (8%)	82,113,113	1.58	10 (12%)
16	BCR	A	850	-	41,41,41	1.28	5 (12%)	56,56,56	1.81	18 (32%)
16	BCR	J	105	-	41,41,41	1.42	5 (12%)	56,56,56	1.93	15 (26%)
13	CLA	A	820	1	69,73,73	1.33	9 (13%)	82,113,113	1.78	11 (13%)
16	BCR	B	845	-	41,41,41	1.27	5 (12%)	56,56,56	2.06	20 (35%)
13	CLA	A	828	1	69,73,73	1.29	6 (8%)	82,113,113	1.71	10 (12%)
16	BCR	J	104	-	41,41,41	1.28	4 (9%)	56,56,56	1.88	19 (33%)
13	CLA	A	846	17	56,60,73	1.51	11 (19%)	65,97,113	2.05	9 (13%)
13	CLA	B	836	20	49,53,73	1.42	4 (8%)	58,89,113	1.95	8 (13%)
16	BCR	A	854	-	41,41,41	1.38	6 (14%)	56,56,56	2.09	19 (33%)
13	CLA	X	1701	12	49,53,73	1.49	5 (10%)	58,89,113	1.99	7 (12%)
13	CLA	B	831	2	53,57,73	1.36	8 (15%)	61,93,113	1.88	6 (9%)
13	CLA	B	815	2	49,53,73	1.49	9 (18%)	58,89,113	1.89	6 (10%)
13	CLA	A	817	20	53,57,73	1.37	8 (15%)	61,93,113	1.93	8 (13%)
16	BCR	M	1602	-	41,41,41	1.36	6 (14%)	56,56,56	1.84	15 (26%)
13	CLA	B	838	2	69,73,73	1.25	8 (11%)	82,113,113	1.73	10 (12%)
13	CLA	A	840	1	51,55,73	1.51	5 (9%)	60,91,113	1.82	9 (15%)
13	CLA	A	814	1	64,68,73	1.23	6 (9%)	76,107,113	1.77	11 (14%)
13	CLA	B	824	2	58,62,73	1.60	12 (20%)	68,99,113	1.83	9 (13%)
13	CLA	B	818	2	64,68,73	1.38	8 (12%)	76,107,113	1.82	8 (10%)
16	BCR	A	853	-	41,41,41	1.31	8 (19%)	56,56,56	1.94	19 (33%)
13	CLA	A	832	1	54,58,73	1.41	7 (12%)	64,95,113	1.97	10 (15%)
13	CLA	B	813	2	69,73,73	1.34	7 (10%)	82,113,113	1.58	8 (9%)
13	CLA	B	822	20	59,63,73	1.42	8 (13%)	70,101,113	1.82	6 (8%)
13	CLA	A	816	1	49,53,73	1.43	6 (12%)	58,89,113	2.05	9 (15%)
13	CLA	B	801	2	69,73,73	1.27	6 (8%)	82,113,113	1.64	10 (12%)
13	CLA	B	817	2	63,67,73	1.37	7 (11%)	74,105,113	1.73	9 (12%)
16	BCR	J	103	-	41,41,41	1.32	5 (12%)	56,56,56	1.95	17 (30%)
13	CLA	A	818	1	58,62,73	1.46	10 (17%)	68,99,113	1.71	7 (10%)
13	CLA	F	1301	20	49,53,73	1.50	8 (16%)	58,89,113	1.92	8 (13%)
13	CLA	B	809	2	69,73,73	1.19	4 (5%)	82,113,113	1.63	8 (9%)
17	LHG	A	855	-	48,48,48	1.80	7 (14%)	51,54,54	1.30	3 (5%)
13	CLA	A	838	1	55,59,73	1.36	5 (9%)	64,96,113	1.94	9 (14%)
13	CLA	B	807	2	69,73,73	1.17	7 (10%)	82,113,113	1.71	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	PQN	A	847	-	34,34,34	3.62	17 (50%)	43,45,45	2.11	3 (6%)
13	CLA	A	843	1	69,73,73	1.26	9 (13%)	82,113,113	1.71	10 (12%)
13	CLA	B	819	20	69,73,73	1.26	6 (8%)	82,113,113	1.66	8 (9%)
13	CLA	A	827	20	69,73,73	1.21	6 (8%)	82,113,113	1.63	9 (10%)
13	CLA	B	804	2	58,62,73	1.37	8 (13%)	68,99,113	1.90	8 (11%)
16	BCR	B	849	-	41,41,41	1.30	4 (9%)	56,56,56	1.78	19 (33%)
13	CLA	B	829	2	69,73,73	1.30	6 (8%)	82,113,113	1.66	10 (12%)
13	CLA	A	830	1	69,73,73	1.29	6 (8%)	82,113,113	1.61	6 (7%)
13	CLA	A	807	1	69,73,73	1.38	8 (11%)	82,113,113	1.80	11 (13%)
13	CLA	A	812	13,1	69,73,73	1.25	8 (11%)	82,113,113	1.68	8 (9%)
13	CLA	B	828	2	69,73,73	1.44	10 (14%)	82,113,113	1.60	10 (12%)
13	CLA	A	803	-	69,73,73	1.39	9 (13%)	82,113,113	1.64	11 (13%)
13	CLA	A	841	1	69,73,73	1.24	9 (13%)	82,113,113	1.67	9 (10%)
13	CLA	B	808	2	69,73,73	1.27	6 (8%)	82,113,113	1.63	9 (10%)
13	CLA	B	834	2	49,53,73	1.46	9 (18%)	58,89,113	1.91	10 (17%)
16	BCR	B	846	-	25,25,41	1.35	4 (16%)	33,33,56	1.88	11 (33%)
13	CLA	J	102	8	41,45,73	1.65	10 (24%)	50,78,113	1.98	6 (12%)
13	CLA	A	835	1	69,73,73	1.22	6 (8%)	82,113,113	1.64	9 (10%)
16	BCR	F	1302	-	41,41,41	1.28	4 (9%)	56,56,56	1.85	16 (28%)
13	CLA	B	833	2	62,66,73	1.40	12 (19%)	73,104,113	1.85	11 (15%)
13	CLA	A	821	1	65,69,73	1.38	9 (13%)	77,108,113	1.86	10 (12%)
13	CLA	A	823	1	53,57,73	1.39	6 (11%)	61,93,113	1.99	11 (18%)
13	CLA	B	810	2	69,73,73	1.34	8 (11%)	82,113,113	1.70	11 (13%)
13	CLA	M	1601	20	49,53,73	1.49	7 (14%)	58,89,113	2.06	7 (12%)
13	CLA	L	1004	20	69,73,73	1.31	5 (7%)	82,113,113	1.60	6 (7%)
17	LHG	A	856	13	26,26,48	2.37	5 (19%)	29,32,54	1.58	5 (17%)
13	CLA	J	101	8	49,53,73	1.53	6 (12%)	58,89,113	2.02	7 (12%)
13	CLA	L	1002	10	69,73,73	1.38	7 (10%)	82,113,113	1.69	10 (12%)
13	CLA	A	824	1	55,59,73	1.49	8 (14%)	64,96,113	1.85	9 (14%)
15	SF4	C	102	3	0,12,12	-	-	-	-	-
16	BCR	A	852	-	41,41,41	1.35	5 (12%)	56,56,56	1.83	16 (28%)
13	CLA	A	834	1	69,73,73	1.14	4 (5%)	82,113,113	1.58	9 (10%)
13	CLA	A	845	-	45,49,73	1.57	7 (15%)	54,83,113	1.84	6 (11%)
13	CLA	A	825	1	63,67,73	1.25	7 (11%)	74,105,113	1.71	10 (13%)
13	CLA	B	826	2	69,73,73	1.33	6 (8%)	82,113,113	1.69	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	831	1	69,73,73	1.42	9 (13%)	82,113,113	1.61	8 (9%)
16	BCR	B	848	-	41,41,41	1.25	7 (17%)	56,56,56	2.03	22 (39%)
13	CLA	B	823	2	49,53,73	1.48	5 (10%)	58,89,113	1.86	5 (8%)
13	CLA	A	815	1	49,53,73	1.53	9 (18%)	58,89,113	1.89	9 (15%)
13	CLA	A	844	20	69,73,73	1.22	8 (11%)	82,113,113	1.59	8 (9%)
13	CLA	L	1003	10	69,73,73	1.36	9 (13%)	82,113,113	1.66	9 (10%)
13	CLA	B	802	20	69,73,73	1.34	6 (8%)	82,113,113	1.66	10 (12%)
13	CLA	A	826	20	69,73,73	1.32	6 (8%)	82,113,113	1.64	11 (13%)
13	CLA	B	803	-	69,73,73	1.41	9 (13%)	82,113,113	1.57	5 (6%)
15	SF4	A	848	2,1	0,12,12	-	-	-	-	-
13	CLA	A	836	1	58,62,73	1.33	6 (10%)	68,99,113	1.88	9 (13%)
13	CLA	B	812	2	49,53,73	1.44	6 (12%)	58,89,113	2.01	8 (13%)
16	BCR	B	847	-	41,41,41	1.26	6 (14%)	56,56,56	1.92	19 (33%)
13	CLA	B	832	2	69,73,73	1.24	7 (10%)	82,113,113	1.67	7 (8%)
13	CLA	B	814	2	69,73,73	1.27	8 (11%)	82,113,113	1.72	10 (12%)
13	CLA	B	820	2	51,55,73	1.44	6 (11%)	60,91,113	2.09	8 (13%)
16	BCR	I	101	-	41,41,41	1.32	7 (17%)	56,56,56	1.84	16 (28%)
13	CLA	A	801	1	69,73,73	1.29	7 (10%)	82,113,113	1.96	16 (19%)
16	BCR	L	1006	-	41,41,41	1.65	8 (19%)	56,56,56	1.77	14 (25%)
16	BCR	L	1005	-	41,41,41	1.46	9 (21%)	56,56,56	1.86	15 (26%)
18	LMG	B	850	-	55,55,55	0.88	2 (3%)	63,63,63	1.29	3 (4%)
17	LHG	B	851	-	22,22,48	2.86	5 (22%)	25,28,54	1.14	2 (8%)
13	CLA	B	811	2	49,53,73	1.44	7 (14%)	58,89,113	1.87	9 (15%)
13	CLA	A	802	20	69,73,73	1.29	10 (14%)	82,113,113	1.60	9 (10%)
13	CLA	B	806	2	69,73,73	1.28	5 (7%)	82,113,113	1.54	6 (7%)
13	CLA	B	840	20	69,73,73	1.24	6 (8%)	82,113,113	1.58	8 (9%)
13	CLA	A	819	1	58,62,73	1.46	9 (15%)	68,99,113	1.80	9 (13%)
13	CLA	B	816	2	59,63,73	1.47	10 (16%)	70,101,113	1.75	7 (10%)
16	BCR	B	844	-	41,41,41	1.56	7 (17%)	56,56,56	2.15	20 (35%)
13	CLA	A	811	1	49,53,73	1.49	6 (12%)	58,89,113	1.84	8 (13%)
13	CLA	A	804	1	69,73,73	1.22	6 (8%)	82,113,113	1.66	7 (8%)
16	BCR	A	849	-	41,41,41	1.38	5 (12%)	56,56,56	1.93	16 (28%)
13	CLA	B	830	2	49,53,73	1.40	7 (14%)	58,89,113	2.03	11 (18%)
13	CLA	B	837	2	64,68,73	1.42	7 (10%)	76,107,113	1.68	9 (11%)
13	CLA	B	827	2	69,73,73	1.39	9 (13%)	82,113,113	1.76	13 (15%)

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	A	808	1	-	7/23/99/115	-
13	CLA	B	839	2	-	6/18/94/115	-
14	PQN	B	842	-	-	4/23/43/43	0/2/2/2
13	CLA	B	825	20	-	8/17/93/115	-
13	CLA	A	829	1	-	10/39/115/115	-
13	CLA	A	805	13,1	-	13/32/108/115	-
16	BCR	B	843	-	-	0/29/63/63	0/2/2/2
13	CLA	K	1401	-	-	7/15/91/115	-
13	CLA	A	833	1	-	8/39/115/115	-
13	CLA	A	806	1	-	16/39/115/115	-
16	BCR	A	851	-	-	0/29/63/63	0/2/2/2
13	CLA	A	809	1	-	17/39/115/115	-
13	CLA	B	841	2	-	5/39/115/115	-
16	BCR	I	102	-	-	4/29/63/63	0/2/2/2
13	CLA	A	837	1	-	3/15/91/115	-
13	CLA	A	822	20	-	6/39/115/115	-
13	CLA	B	835	20	-	0/15/91/115	-
13	CLA	B	821	2	-	6/15/91/115	-
13	CLA	A	839	1	-	7/39/115/115	-
13	CLA	A	813	1	-	5/26/102/115	-
13	CLA	A	842	20	-	8/23/99/115	-
13	CLA	A	810	1	-	12/39/115/115	-
15	SF4	C	101	3	-	-	0/6/5/5
13	CLA	B	805	2	-	14/39/115/115	-
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	820	1	-	11/39/115/115	-
16	BCR	B	845	-	-	5/29/63/63	0/2/2/2
13	CLA	A	828	1	-	7/39/115/115	-
16	BCR	J	104	-	-	4/29/63/63	0/2/2/2
13	CLA	A	846	17	-	13/24/100/115	-
13	CLA	B	836	20	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	A	854	-	-	8/29/63/63	0/2/2/2
13	CLA	X	1701	12	-	8/15/91/115	-
13	CLA	B	831	2	-	10/20/96/115	-
13	CLA	B	815	2	-	7/15/91/115	-
13	CLA	A	817	20	-	9/20/96/115	-
16	BCR	M	1602	-	-	3/29/63/63	0/2/2/2
13	CLA	B	838	2	-	3/39/115/115	-
13	CLA	A	840	1	-	5/18/94/115	-
13	CLA	A	814	1	-	12/33/109/115	-
13	CLA	B	824	2	-	9/26/102/115	-
13	CLA	B	818	2	-	8/33/109/115	-
16	BCR	A	853	-	-	2/29/63/63	0/2/2/2
13	CLA	A	832	1	-	3/21/97/115	-
13	CLA	B	813	2	-	15/39/115/115	-
13	CLA	B	822	20	-	11/27/103/115	-
13	CLA	A	816	1	-	4/15/91/115	-
13	CLA	B	801	2	-	8/39/115/115	-
13	CLA	B	817	2	-	7/32/108/115	-
16	BCR	J	103	-	-	3/29/63/63	0/2/2/2
13	CLA	A	818	1	-	1/26/102/115	-
13	CLA	F	1301	20	-	4/15/91/115	-
13	CLA	B	809	2	-	12/39/115/115	-
17	LHG	A	855	-	-	17/53/53/53	-
13	CLA	A	838	1	-	6/23/99/115	-
13	CLA	B	807	2	-	0/39/115/115	-
14	PQN	A	847	-	-	6/23/43/43	0/2/2/2
13	CLA	A	843	1	-	8/39/115/115	-
13	CLA	B	819	20	-	4/39/115/115	-
13	CLA	A	827	20	-	13/39/115/115	-
13	CLA	B	804	2	-	5/26/102/115	-
16	BCR	B	849	-	-	2/29/63/63	0/2/2/2
13	CLA	B	829	2	-	9/39/115/115	-
13	CLA	A	830	1	-	9/39/115/115	-
13	CLA	A	807	1	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	812	13,1	-	13/39/115/115	-
13	CLA	B	828	2	-	12/39/115/115	-
13	CLA	A	803	-	-	12/39/115/115	-
13	CLA	A	841	1	-	6/39/115/115	-
13	CLA	B	808	2	-	9/39/115/115	-
13	CLA	B	834	2	-	6/15/91/115	-
16	BCR	B	846	-	-	4/18/35/63	0/1/1/2
13	CLA	J	102	8	-	1/4/76/115	-
13	CLA	A	835	1	-	9/39/115/115	-
16	BCR	F	1302	-	-	5/29/63/63	0/2/2/2
13	CLA	B	833	2	-	8/31/107/115	-
13	CLA	A	821	1	-	15/35/111/115	-
13	CLA	A	823	1	-	11/20/96/115	-
13	CLA	B	810	2	-	7/39/115/115	-
13	CLA	M	1601	20	-	9/15/91/115	-
13	CLA	L	1004	20	-	9/39/115/115	-
17	LHG	A	856	13	1/1/5/5	10/31/31/53	-
13	CLA	J	101	8	-	10/15/91/115	-
13	CLA	L	1002	10	-	12/39/115/115	-
13	CLA	A	824	1	-	10/23/99/115	-
16	BCR	A	852	-	-	2/29/63/63	0/2/2/2
15	SF4	C	102	3	-	-	0/6/5/5
13	CLA	A	834	1	-	7/39/115/115	-
13	CLA	A	845	-	-	4/9/81/115	-
13	CLA	A	825	1	-	10/32/108/115	-
13	CLA	B	826	2	-	10/39/115/115	-
13	CLA	A	831	1	-	9/39/115/115	-
16	BCR	B	848	-	-	1/29/63/63	0/2/2/2
13	CLA	B	823	2	-	4/15/91/115	-
13	CLA	A	815	1	-	3/15/91/115	-
13	CLA	A	844	20	-	9/39/115/115	-
13	CLA	L	1003	10	-	9/39/115/115	-
13	CLA	B	802	20	-	8/39/115/115	-
13	CLA	A	826	20	-	13/39/115/115	-
13	CLA	B	803	-	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SF4	A	848	2,1	-	-	0/6/5/5
13	CLA	A	836	1	-	5/26/102/115	-
13	CLA	B	812	2	-	2/15/91/115	-
16	BCR	B	847	-	-	2/29/63/63	0/2/2/2
13	CLA	B	832	2	-	16/39/115/115	-
13	CLA	B	814	2	-	12/39/115/115	-
13	CLA	B	820	2	-	6/18/94/115	-
16	BCR	I	101	-	-	0/29/63/63	0/2/2/2
13	CLA	A	801	1	-	4/39/115/115	-
16	BCR	L	1006	-	-	1/29/63/63	0/2/2/2
16	BCR	L	1005	-	-	1/29/63/63	0/2/2/2
18	LMG	B	850	-	-	8/50/70/70	0/1/1/1
17	LHG	B	851	-	-	6/26/26/53	-
13	CLA	B	811	2	-	5/15/91/115	-
13	CLA	A	802	20	-	7/39/115/115	-
13	CLA	B	806	2	-	16/39/115/115	-
13	CLA	B	840	20	-	2/39/115/115	-
13	CLA	A	819	1	-	12/26/102/115	-
13	CLA	B	816	2	-	9/27/103/115	-
16	BCR	B	844	-	-	6/29/63/63	0/2/2/2
13	CLA	A	811	1	-	9/15/91/115	-
13	CLA	A	804	1	-	6/39/115/115	-
16	BCR	A	849	-	-	0/29/63/63	0/2/2/2
13	CLA	B	830	2	-	9/15/91/115	-
13	CLA	B	837	2	-	8/33/109/115	-
13	CLA	B	827	2	-	15/39/115/115	-

All (879) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	847	PQN	O4-C4	9.40	1.42	1.23
14	B	842	PQN	O4-C4	9.08	1.42	1.23
14	A	847	PQN	O1-C1	9.06	1.42	1.23
17	B	851	LHG	P-O5	8.84	1.81	1.50
14	A	847	PQN	C12-C13	8.62	1.52	1.33
14	B	842	PQN	C12-C13	8.59	1.52	1.33
14	B	842	PQN	O1-C1	8.55	1.41	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	855	LHG	P-O5	8.44	1.80	1.50
17	A	856	LHG	P-O5	7.85	1.78	1.50
14	A	847	PQN	C2M-C2	-7.00	1.36	1.50
13	L	1002	CLA	MG-NA	6.69	2.22	2.06
14	B	842	PQN	C2M-C2	-6.67	1.37	1.50
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	C3-C2	6.48	1.46	1.35
13	B	810	CLA	MG-NA	6.47	2.21	2.06
14	A	847	PQN	C3-C2	6.46	1.46	1.35
13	B	813	CLA	MG-NA	6.46	2.21	2.06
13	B	828	CLA	MG-NA	6.33	2.21	2.06
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
17	B	851	LHG	P-O6	6.05	1.83	1.59
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
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	A	816	CLA	MG-NA	5.80	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	836	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
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	B	812	CLA	MG-NA	5.54	2.19	2.06
13	M	1601	CLA	MG-NA	5.54	2.19	2.06
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
17	B	851	LHG	P-O3	5.45	1.80	1.59
13	B	818	CLA	MG-NA	5.43	2.19	2.06
13	A	801	CLA	MG-NA	5.42	2.19	2.06
17	A	855	LHG	P-O3	5.37	1.80	1.59
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	B	804	CLA	MG-NA	5.31	2.18	2.06
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
13	B	825	CLA	MG-NA	5.21	2.18	2.06
16	L	1006	BCR	C1-C6	5.21	1.60	1.53
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	814	CLA	MG-NA	5.08	2.18	2.06
16	B	844	BCR	C1-C6	5.08	1.60	1.53
13	A	822	CLA	MG-NA	5.08	2.18	2.06
17	A	856	LHG	P-O6	5.07	1.79	1.59
16	L	1005	BCR	C30-C25	5.07	1.60	1.53
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	A	803	CLA	MG-NA	5.01	2.18	2.06
16	B	843	BCR	C30-C25	4.99	1.60	1.53
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
13	A	841	CLA	MG-NA	4.88	2.17	2.06
16	L	1006	BCR	C30-C25	4.84	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
14	B	842	PQN	C16-C15	-4.71	1.35	1.52
13	A	835	CLA	MG-NA	4.70	2.17	2.06
16	A	852	BCR	C30-C25	4.69	1.59	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
17	A	856	LHG	P-O3	4.62	1.77	1.59
14	A	847	PQN	C16-C15	-4.57	1.35	1.52
13	A	833	CLA	MG-NA	4.46	2.16	2.06
13	B	808	CLA	MG-NB	4.44	2.14	2.05
13	A	806	CLA	MG-NA	4.39	2.16	2.06
13	A	844	CLA	MG-NA	4.32	2.16	2.06
13	B	841	CLA	MG-NA	4.31	2.16	2.06
17	A	855	LHG	P-O6	4.22	1.75	1.59
13	A	803	CLA	MG-NB	4.17	2.14	2.05
13	B	807	CLA	MG-NA	3.96	2.15	2.06
16	A	851	BCR	C30-C25	3.95	1.58	1.53
16	A	851	BCR	C1-C6	3.94	1.58	1.53
13	A	831	CLA	MG-NB	3.86	2.13	2.05
16	J	105	BCR	C30-C25	3.81	1.58	1.53
17	A	856	LHG	O7-C7	3.81	1.45	1.34
16	J	104	BCR	C29-C30	3.79	1.62	1.54
14	B	842	PQN	C10-C5	3.77	1.46	1.40
16	A	849	BCR	C30-C25	3.77	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	849	BCR	C1-C6	3.73	1.58	1.53
16	A	854	BCR	C30-C25	3.72	1.58	1.53
13	L	1003	CLA	MG-NB	3.65	2.13	2.05
13	A	818	CLA	MG-NB	3.65	2.13	2.05
16	A	850	BCR	C30-C25	3.63	1.58	1.53
16	J	104	BCR	C2-C1	3.60	1.62	1.54
13	B	806	CLA	MG-NB	3.60	2.12	2.05
16	J	105	BCR	C1-C6	3.59	1.58	1.53
17	B	851	LHG	O7-C7	3.58	1.44	1.34
16	M	1602	BCR	C1-C6	3.58	1.58	1.53
13	A	808	CLA	MG-NB	3.58	2.12	2.05
13	A	839	CLA	MG-NB	3.57	2.12	2.05
13	B	817	CLA	MG-NB	3.56	2.12	2.05
16	A	853	BCR	C1-C6	3.55	1.58	1.53
16	F	1302	BCR	C2-C1	3.55	1.62	1.54
13	A	806	CLA	MG-NB	3.55	2.12	2.05
13	B	827	CLA	MG-NC	3.50	2.14	2.06
16	A	854	BCR	C1-C6	3.49	1.58	1.53
16	L	1006	BCR	C2-C1	3.47	1.62	1.54
13	A	811	CLA	MG-NB	3.47	2.12	2.05
16	B	843	BCR	C1-C6	3.46	1.58	1.53
13	B	838	CLA	CHC-C1C	3.45	1.45	1.38
16	I	102	BCR	C30-C25	3.45	1.58	1.53
13	B	810	CLA	MG-NC	3.45	2.14	2.06
13	A	838	CLA	MG-NB	3.44	2.12	2.05
13	L	1002	CLA	MG-NB	3.40	2.12	2.05
13	B	805	CLA	MG-NB	3.39	2.12	2.05
13	L	1002	CLA	CHC-C1C	3.37	1.45	1.38
13	A	807	CLA	MG-NB	3.36	2.12	2.05
16	F	1302	BCR	C30-C25	3.34	1.58	1.53
13	A	843	CLA	C1D-ND	-3.33	1.33	1.37
13	B	813	CLA	MG-NB	3.33	2.12	2.05
16	B	847	BCR	C30-C25	3.33	1.58	1.53
16	B	843	BCR	C2-C1	3.32	1.61	1.54
16	J	104	BCR	C30-C25	3.31	1.58	1.53
13	B	815	CLA	MG-NB	3.31	2.12	2.05
13	A	832	CLA	C1D-ND	-3.31	1.33	1.37
13	B	834	CLA	MG-NB	3.30	2.12	2.05
13	B	811	CLA	MG-NB	3.29	2.12	2.05
16	B	843	BCR	C26-C25	3.27	1.40	1.34
14	B	842	PQN	C11-C12	3.27	1.55	1.50
13	B	828	CLA	C2-C3	3.25	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	847	PQN	C10-C5	3.24	1.46	1.40
13	B	822	CLA	MG-NB	3.23	2.12	2.05
13	B	809	CLA	MG-NC	3.22	2.13	2.06
13	B	818	CLA	C1D-ND	-3.22	1.33	1.37
13	B	821	CLA	CHC-C1C	3.21	1.44	1.38
13	A	841	CLA	MG-NB	3.21	2.12	2.05
16	J	103	BCR	C1-C6	3.20	1.57	1.53
13	L	1004	CLA	MG-NB	3.20	2.12	2.05
13	B	823	CLA	MG-NB	3.20	2.12	2.05
14	B	842	PQN	C6-C5	3.20	1.44	1.39
13	F	1301	CLA	MG-NC	3.20	2.13	2.06
13	A	838	CLA	MG-NC	3.19	2.13	2.06
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	B	802	CLA	MG-NC	3.17	2.13	2.06
13	B	837	CLA	MG-NB	3.17	2.12	2.05
16	J	103	BCR	C29-C30	3.17	1.61	1.54
13	B	803	CLA	CHC-C1C	3.17	1.44	1.38
16	A	854	BCR	C2-C1	3.16	1.61	1.54
13	B	838	CLA	MG-NB	3.16	2.12	2.05
13	B	813	CLA	MG-NC	3.15	2.13	2.06
13	A	821	CLA	C1D-ND	-3.14	1.33	1.37
16	A	850	BCR	C2-C1	3.14	1.61	1.54
16	A	852	BCR	C29-C30	3.14	1.61	1.54
16	J	105	BCR	C2-C1	3.14	1.61	1.54
13	B	839	CLA	MG-NB	3.13	2.12	2.05
13	A	809	CLA	CAA-C2A	3.12	1.59	1.54
16	B	845	BCR	C30-C25	3.12	1.57	1.53
16	B	849	BCR	C2-C1	3.12	1.61	1.54
13	A	841	CLA	CHC-C1C	3.12	1.44	1.38
16	B	844	BCR	C30-C25	3.10	1.57	1.53
13	A	819	CLA	CAA-C2A	3.10	1.59	1.54
13	A	822	CLA	C1D-ND	-3.09	1.33	1.37
14	A	847	PQN	C6-C5	3.08	1.44	1.39
13	A	828	CLA	C5-C3	3.07	1.57	1.51
13	B	828	CLA	MG-NB	3.07	2.11	2.05
13	A	844	CLA	CMD-C2D	3.07	1.57	1.50
16	A	851	BCR	C2-C1	3.06	1.61	1.54
13	B	841	CLA	C1D-ND	-3.06	1.33	1.37
13	A	824	CLA	MG-NB	3.06	2.11	2.05
13	X	1701	CLA	MG-NB	3.06	2.11	2.05
13	A	831	CLA	CHC-C1C	3.05	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	849	BCR	C30-C25	3.05	1.57	1.53
16	B	848	BCR	C29-C30	3.03	1.61	1.54
13	A	802	CLA	MG-NC	3.03	2.13	2.06
16	J	103	BCR	C30-C25	3.02	1.57	1.53
13	A	809	CLA	CHC-C1C	3.02	1.44	1.38
13	A	812	CLA	MG-NB	3.01	2.11	2.05
13	X	1701	CLA	CHC-C1C	3.01	1.44	1.38
13	B	824	CLA	CHC-C1C	3.01	1.44	1.38
13	B	827	CLA	CHC-C1C	3.01	1.44	1.38
16	M	1602	BCR	C29-C30	3.01	1.60	1.54
16	B	845	BCR	C1-C6	3.01	1.57	1.53
16	A	849	BCR	C29-C30	3.01	1.60	1.54
13	B	833	CLA	MG-NB	3.01	2.11	2.05
16	A	850	BCR	C29-C30	3.00	1.60	1.54
16	B	844	BCR	C2-C1	2.99	1.60	1.54
16	M	1602	BCR	C2-C1	2.99	1.60	1.54
16	A	853	BCR	C30-C25	2.99	1.57	1.53
13	A	830	CLA	MG-NC	2.99	2.13	2.06
13	B	822	CLA	CAA-C2A	2.98	1.59	1.54
13	A	842	CLA	MG-NB	2.98	2.11	2.05
16	B	843	BCR	C29-C30	2.98	1.60	1.54
16	B	846	BCR	C29-C30	2.97	1.60	1.54
13	A	846	CLA	CHC-C1C	2.97	1.44	1.38
13	L	1003	CLA	CHC-C1C	2.97	1.44	1.38
13	B	834	CLA	CHC-C1C	2.97	1.44	1.38
13	A	828	CLA	CHC-C1C	2.96	1.44	1.38
13	A	811	CLA	MG-NC	2.96	2.13	2.06
16	B	845	BCR	C2-C1	2.95	1.60	1.54
16	B	849	BCR	C29-C30	2.95	1.60	1.54
13	B	823	CLA	CHC-C1C	2.95	1.44	1.38
13	A	816	CLA	MG-NB	2.94	2.11	2.05
13	A	840	CLA	CAA-C2A	2.94	1.59	1.54
13	B	824	CLA	C5-C3	2.94	1.57	1.51
13	A	845	CLA	MG-NB	2.94	2.11	2.05
16	F	1302	BCR	C29-C30	2.94	1.60	1.54
13	B	816	CLA	CAA-C2A	2.94	1.59	1.54
16	J	105	BCR	C29-C30	2.94	1.60	1.54
13	B	827	CLA	CAA-C2A	2.93	1.59	1.54
13	A	810	CLA	C1D-ND	-2.93	1.34	1.37
13	B	808	CLA	CHB-C1B	-2.93	1.32	1.39
13	B	816	CLA	C5-C3	2.93	1.57	1.51
16	B	844	BCR	C26-C25	2.93	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	815	CLA	CHC-C1C	2.93	1.44	1.38
13	A	846	CLA	CAA-C2A	2.92	1.59	1.54
16	B	847	BCR	C2-C1	2.92	1.60	1.54
13	B	812	CLA	MG-NB	2.92	2.11	2.05
13	B	824	CLA	MG-NB	2.92	2.11	2.05
13	A	822	CLA	CAA-C2A	2.92	1.59	1.54
13	B	829	CLA	CAA-C2A	2.91	1.59	1.54
16	B	846	BCR	C30-C25	2.91	1.57	1.53
16	B	845	BCR	C29-C30	2.91	1.60	1.54
13	A	840	CLA	MG-NB	2.91	2.11	2.05
13	A	822	CLA	CHC-C1C	2.91	1.44	1.38
16	M	1602	BCR	C30-C25	2.89	1.57	1.53
16	A	854	BCR	C29-C30	2.89	1.60	1.54
17	A	856	LHG	O8-C23	2.89	1.41	1.33
13	B	831	CLA	CHB-C1B	-2.89	1.32	1.39
13	A	802	CLA	MG-NB	2.88	2.11	2.05
13	B	801	CLA	MG-NC	2.88	2.13	2.06
13	B	821	CLA	MG-NB	2.86	2.11	2.05
16	I	102	BCR	C2-C1	2.86	1.60	1.54
13	B	817	CLA	CAA-C2A	2.86	1.59	1.54
13	F	1301	CLA	MG-NB	2.85	2.11	2.05
13	J	101	CLA	MG-NC	2.85	2.13	2.06
16	A	850	BCR	C1-C6	2.85	1.57	1.53
16	L	1005	BCR	C29-C30	2.85	1.60	1.54
13	B	803	CLA	CHD-C1D	2.85	1.43	1.38
13	A	821	CLA	CHC-C1C	2.84	1.44	1.38
13	B	815	CLA	MG-NC	2.84	2.13	2.06
13	B	835	CLA	CHC-C1C	2.83	1.44	1.38
13	A	823	CLA	CHC-C1C	2.83	1.44	1.38
13	B	835	CLA	CAA-C2A	2.83	1.59	1.54
13	K	1401	CLA	MG-NB	2.83	2.11	2.05
13	B	802	CLA	CHC-C1C	2.83	1.44	1.38
13	B	814	CLA	MG-NB	2.83	2.11	2.05
13	B	815	CLA	CHC-C1C	2.82	1.44	1.38
16	A	852	BCR	C1-C6	2.82	1.57	1.53
16	I	101	BCR	C29-C30	2.82	1.60	1.54
16	J	103	BCR	C2-C1	2.82	1.60	1.54
13	A	826	CLA	CHC-C1C	2.81	1.44	1.38
13	A	822	CLA	CHB-C1B	-2.81	1.33	1.39
13	A	833	CLA	MG-NC	2.80	2.12	2.06
13	B	808	CLA	MG-NC	2.79	2.12	2.06
13	B	837	CLA	CHC-C1C	2.79	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	827	CLA	C1D-ND	-2.79	1.34	1.37
13	A	808	CLA	MG-NC	2.78	2.12	2.06
16	I	102	BCR	C29-C30	2.78	1.60	1.54
13	A	809	CLA	MG-NB	2.77	2.11	2.05
13	A	840	CLA	MG-NC	2.77	2.12	2.06
13	A	832	CLA	CHC-C1C	2.77	1.44	1.38
16	A	849	BCR	C2-C1	2.77	1.60	1.54
13	B	826	CLA	MG-NB	2.76	2.11	2.05
18	B	850	LMG	O8-C28	2.76	1.41	1.33
13	A	832	CLA	CHB-C1B	-2.76	1.33	1.39
13	A	803	CLA	CHB-C1B	-2.76	1.33	1.39
13	L	1004	CLA	CHC-C1C	2.75	1.44	1.38
16	L	1006	BCR	C29-C30	2.75	1.60	1.54
13	J	102	CLA	MG-NB	2.74	2.11	2.05
13	B	828	CLA	MG-NC	2.74	2.12	2.06
13	B	812	CLA	C1D-ND	-2.73	1.34	1.37
13	A	820	CLA	MG-NB	2.73	2.11	2.05
14	A	847	PQN	C8-C9	2.73	1.43	1.38
14	A	847	PQN	C15-C13	2.72	1.56	1.51
13	B	804	CLA	MG-NB	2.72	2.11	2.05
13	A	827	CLA	MG-NB	2.72	2.11	2.05
16	B	847	BCR	C1-C6	2.72	1.57	1.53
13	B	833	CLA	C5-C3	2.72	1.56	1.51
13	J	102	CLA	CHD-C1D	2.71	1.43	1.38
13	B	810	CLA	MG-NB	2.71	2.11	2.05
13	A	843	CLA	C1-C2	2.71	1.56	1.49
13	B	803	CLA	CHB-C1B	-2.70	1.33	1.39
13	B	807	CLA	CHB-C1B	-2.70	1.33	1.39
13	A	819	CLA	MG-NB	2.70	2.11	2.05
13	A	810	CLA	MG-NC	2.70	2.12	2.06
17	A	855	LHG	O8-C23	2.70	1.41	1.33
13	A	807	CLA	MG-ND	-2.70	2.00	2.05
13	A	805	CLA	CAA-C2A	2.69	1.59	1.54
13	A	839	CLA	CHC-C1C	2.69	1.43	1.38
13	B	817	CLA	C1D-ND	-2.69	1.34	1.37
13	J	101	CLA	CHC-C1C	2.69	1.43	1.38
13	B	803	CLA	C3B-C4B	2.68	1.50	1.42
13	B	818	CLA	CAA-C2A	2.68	1.59	1.54
13	J	101	CLA	MG-NB	2.68	2.11	2.05
14	B	842	PQN	C8-C9	2.68	1.43	1.38
13	B	807	CLA	CHD-C1D	2.68	1.43	1.38
13	B	826	CLA	C1D-C2D	-2.68	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	1003	CLA	CMD-C2D	2.67	1.56	1.50
13	A	837	CLA	MG-NB	2.67	2.11	2.05
13	B	801	CLA	CHB-C1B	-2.66	1.33	1.39
16	B	848	BCR	C2-C1	2.66	1.60	1.54
13	A	840	CLA	CHC-C1C	2.66	1.43	1.38
13	A	805	CLA	MG-NB	2.66	2.11	2.05
13	B	828	CLA	C5-C3	2.66	1.56	1.51
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	827	CLA	CHB-C1B	-2.65	1.33	1.39
14	A	847	PQN	C7-C6	2.65	1.43	1.38
13	L	1002	CLA	MG-NC	2.65	2.12	2.06
13	B	839	CLA	MG-NC	2.65	2.12	2.06
13	A	844	CLA	CAA-C2A	2.65	1.58	1.54
16	A	852	BCR	C2-C1	2.64	1.60	1.54
13	F	1301	CLA	CHC-C1C	2.64	1.43	1.38
13	A	801	CLA	C4D-CHA	2.64	1.47	1.38
13	M	1601	CLA	MG-NB	2.64	2.11	2.05
14	B	842	PQN	C9-C10	2.63	1.43	1.39
17	A	855	LHG	O7-C7	2.63	1.41	1.34
13	B	837	CLA	C1D-ND	-2.63	1.34	1.37
13	A	805	CLA	CHC-C1C	2.62	1.43	1.38
18	B	850	LMG	O7-C8	-2.62	1.40	1.46
13	B	841	CLA	MG-NB	2.62	2.11	2.05
14	A	847	PQN	C8-C7	2.62	1.44	1.38
13	B	803	CLA	MG-NB	2.62	2.11	2.05
13	A	841	CLA	CHB-C1B	-2.62	1.33	1.39
13	A	809	CLA	CHB-C1B	-2.61	1.33	1.39
14	A	847	PQN	C10-C1	-2.61	1.43	1.48
13	A	815	CLA	MG-NB	2.61	2.11	2.05
13	A	829	CLA	MG-NB	2.60	2.10	2.05
13	B	817	CLA	CHB-C1B	-2.60	1.33	1.39
13	A	846	CLA	MG-NB	2.60	2.10	2.05
13	A	844	CLA	C1D-ND	-2.60	1.34	1.37
13	B	811	CLA	CHB-C1B	-2.60	1.33	1.39
13	B	805	CLA	CMD-C2D	2.60	1.56	1.50
13	A	809	CLA	C1D-ND	-2.59	1.34	1.37
16	A	854	BCR	C23-C22	-2.59	1.40	1.46
13	A	823	CLA	MG-NB	2.59	2.10	2.05
13	B	826	CLA	CHC-C1C	2.58	1.43	1.38
13	B	816	CLA	MG-NB	2.58	2.10	2.05
13	B	839	CLA	CHB-C1B	-2.58	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	820	CLA	C2-C3	2.58	1.39	1.33
14	A	847	PQN	C11-C12	2.58	1.54	1.50
13	B	819	CLA	MG-NC	2.58	2.12	2.06
13	B	820	CLA	CAA-C2A	2.57	1.58	1.54
13	L	1003	CLA	CHB-C1B	-2.57	1.33	1.39
13	M	1601	CLA	C1D-ND	-2.57	1.34	1.37
13	B	820	CLA	MG-NB	2.57	2.10	2.05
13	B	804	CLA	CHC-C1C	2.57	1.43	1.38
13	B	824	CLA	CHB-C1B	-2.56	1.33	1.39
13	B	803	CLA	MG-NC	2.56	2.12	2.06
13	A	843	CLA	CHC-C1C	2.56	1.43	1.38
13	M	1601	CLA	CAA-C2A	2.56	1.58	1.54
13	A	808	CLA	CHC-C1C	2.56	1.43	1.38
13	A	828	CLA	MG-NB	2.55	2.10	2.05
16	A	853	BCR	C29-C30	2.55	1.59	1.54
13	B	810	CLA	MG-ND	-2.55	2.00	2.05
13	B	806	CLA	CHD-C1D	2.54	1.43	1.38
13	A	807	CLA	MG-NC	2.54	2.12	2.06
13	A	819	CLA	C5-C3	2.54	1.56	1.51
13	A	824	CLA	CHD-C1D	2.54	1.43	1.38
13	A	820	CLA	C1-C2	2.54	1.56	1.49
13	B	802	CLA	C1D-ND	-2.54	1.34	1.37
13	A	842	CLA	C5-C3	2.54	1.58	1.51
13	B	831	CLA	CHC-C1C	2.54	1.43	1.38
13	A	806	CLA	CHC-C1C	2.53	1.43	1.38
13	A	804	CLA	CHB-C1B	-2.53	1.33	1.39
13	A	803	CLA	C1D-ND	-2.53	1.34	1.37
13	A	845	CLA	CBD-CAD	2.52	1.57	1.51
13	A	831	CLA	C5-C3	2.52	1.56	1.51
13	A	836	CLA	C5-C3	2.52	1.56	1.51
13	A	803	CLA	CMD-C2D	2.52	1.55	1.50
13	B	820	CLA	C1D-ND	-2.52	1.34	1.37
14	B	842	PQN	C11-C3	2.52	1.56	1.51
16	I	101	BCR	C30-C25	2.52	1.57	1.53
16	J	105	BCR	C5-C6	2.51	1.38	1.34
13	B	836	CLA	MG-NB	2.51	2.10	2.05
13	A	811	CLA	CAA-C2A	2.51	1.58	1.54
13	B	840	CLA	MG-NC	2.51	2.12	2.06
16	I	101	BCR	C2-C1	2.51	1.59	1.54
13	A	810	CLA	MG-ND	-2.50	2.00	2.05
16	B	844	BCR	C29-C30	2.50	1.59	1.54
16	I	101	BCR	C33-C5	2.50	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	815	CLA	CHB-C1B	-2.50	1.33	1.39
13	M	1601	CLA	CHC-C1C	2.50	1.43	1.38
13	A	803	CLA	CAA-C2A	2.50	1.58	1.54
13	B	824	CLA	MG-NC	2.49	2.12	2.06
13	B	802	CLA	MG-NB	2.49	2.10	2.05
13	A	806	CLA	CHB-C1B	-2.49	1.33	1.39
13	L	1003	CLA	CAA-C2A	2.49	1.58	1.54
14	A	847	PQN	C9-C10	2.49	1.43	1.39
16	B	844	BCR	C38-C26	2.49	1.54	1.50
13	A	821	CLA	C5-C3	2.49	1.56	1.51
13	A	804	CLA	C1D-ND	-2.49	1.34	1.37
13	A	814	CLA	MG-NB	2.49	2.10	2.05
13	A	819	CLA	CHC-C1C	2.49	1.43	1.38
13	B	817	CLA	CHC-C1C	2.49	1.43	1.38
13	B	812	CLA	CHD-C1D	2.49	1.43	1.38
13	B	835	CLA	MG-NB	2.48	2.10	2.05
13	B	828	CLA	CAA-C2A	2.48	1.58	1.54
14	B	842	PQN	C8-C7	2.48	1.43	1.38
13	B	813	CLA	CHB-C1B	-2.47	1.33	1.39
13	J	102	CLA	MG-NC	2.47	2.12	2.06
13	A	818	CLA	CHB-C1B	-2.47	1.33	1.39
13	B	822	CLA	CHC-C1C	2.47	1.43	1.38
13	A	842	CLA	MG-NC	2.47	2.12	2.06
13	A	820	CLA	CAA-C2A	2.47	1.58	1.54
13	A	812	CLA	C1D-ND	-2.47	1.34	1.37
13	B	813	CLA	CMD-C2D	2.47	1.55	1.50
13	L	1002	CLA	CMD-C2D	2.47	1.55	1.50
16	M	1602	BCR	C23-C22	-2.47	1.40	1.46
16	L	1005	BCR	C2-C1	2.46	1.59	1.54
13	A	805	CLA	C1D-ND	-2.46	1.34	1.37
16	L	1005	BCR	C19-C18	-2.46	1.40	1.46
13	L	1004	CLA	MG-NC	2.46	2.12	2.06
13	A	813	CLA	CHD-C1D	2.46	1.43	1.38
16	L	1006	BCR	C38-C26	2.46	1.54	1.50
13	A	821	CLA	CAA-C2A	2.46	1.58	1.54
13	A	818	CLA	C1D-ND	-2.45	1.34	1.37
13	B	838	CLA	CHB-C1B	-2.45	1.33	1.39
13	A	818	CLA	CHC-C1C	2.45	1.43	1.38
13	A	825	CLA	CHB-C1B	-2.45	1.33	1.39
13	A	839	CLA	CHB-C1B	-2.45	1.33	1.39
13	A	814	CLA	CHB-C1B	-2.45	1.33	1.39
13	A	824	CLA	CAA-C2A	2.45	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	801	CLA	MG-NB	2.45	2.10	2.05
13	A	802	CLA	MG-ND	-2.45	2.00	2.05
13	A	835	CLA	CHB-C1B	-2.45	1.33	1.39
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	B	818	CLA	MG-NB	2.44	2.10	2.05
13	B	807	CLA	CAA-C2A	2.44	1.58	1.54
16	A	849	BCR	C26-C25	2.44	1.38	1.34
13	L	1002	CLA	CAA-C2A	2.44	1.58	1.54
13	A	813	CLA	CAA-C2A	2.44	1.58	1.54
13	B	805	CLA	C1D-ND	-2.44	1.34	1.37
13	B	819	CLA	MG-NB	2.44	2.10	2.05
13	A	835	CLA	C1D-ND	-2.43	1.34	1.37
13	A	812	CLA	CHB-C1B	-2.43	1.34	1.39
13	B	827	CLA	CMD-C2D	2.43	1.55	1.50
13	A	831	CLA	MG-NC	2.43	2.12	2.06
13	J	101	CLA	CHD-C1D	2.43	1.43	1.38
13	B	835	CLA	CHB-C1B	-2.43	1.34	1.39
13	B	809	CLA	C1D-ND	-2.43	1.34	1.37
13	B	832	CLA	C1D-ND	-2.43	1.34	1.37
16	B	847	BCR	C29-C30	2.42	1.59	1.54
13	B	828	CLA	C1-C2	2.42	1.56	1.49
13	J	102	CLA	CHC-C1C	2.42	1.43	1.38
13	B	819	CLA	C1D-ND	-2.41	1.34	1.37
13	B	830	CLA	CHC-C1C	2.41	1.43	1.38
13	B	819	CLA	CHB-C1B	-2.41	1.34	1.39
13	B	835	CLA	C3B-C4B	2.41	1.49	1.42
16	B	846	BCR	C23-C22	-2.41	1.40	1.46
13	B	801	CLA	MG-NB	2.41	2.10	2.05
13	B	820	CLA	CHC-C1C	2.41	1.43	1.38
13	B	834	CLA	CHD-C1D	2.41	1.43	1.38
13	B	827	CLA	C1D-ND	-2.41	1.34	1.37
13	A	807	CLA	CHC-C1C	2.41	1.43	1.38
13	B	824	CLA	CHD-C1D	2.41	1.43	1.38
13	A	827	CLA	MG-NC	2.41	2.12	2.06
13	X	1701	CLA	MG-NC	2.41	2.12	2.06
13	A	831	CLA	C3B-C4B	2.40	1.49	1.42
16	B	849	BCR	C23-C22	-2.40	1.40	1.46
13	A	826	CLA	CHD-C1D	2.40	1.43	1.38
13	B	833	CLA	CAA-C2A	2.40	1.58	1.54
13	A	830	CLA	CHD-C1D	2.40	1.43	1.38
13	L	1004	CLA	CMD-C2D	2.40	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	848	BCR	C23-C22	-2.39	1.40	1.46
13	A	817	CLA	MG-NB	2.39	2.10	2.05
13	A	821	CLA	MG-NB	2.39	2.10	2.05
13	B	834	CLA	CHB-C1B	-2.39	1.34	1.39
13	A	834	CLA	MG-NC	2.39	2.11	2.06
13	A	825	CLA	CHC-C1C	2.39	1.43	1.38
13	A	844	CLA	C4-C3	2.39	1.56	1.50
16	L	1006	BCR	C26-C25	2.38	1.38	1.34
13	A	831	CLA	C1D-ND	-2.38	1.34	1.37
13	A	837	CLA	CHC-C1C	2.38	1.43	1.38
16	B	844	BCR	C29-C28	-2.38	1.47	1.52
13	B	830	CLA	CHB-C1B	-2.38	1.34	1.39
13	B	832	CLA	CHC-C1C	2.37	1.43	1.38
13	K	1401	CLA	MG-NC	2.37	2.11	2.06
13	A	802	CLA	CHB-C1B	-2.37	1.34	1.39
13	B	814	CLA	CHB-C1B	-2.37	1.34	1.39
13	B	802	CLA	CMD-C2D	2.37	1.55	1.50
13	A	818	CLA	MG-NC	2.37	2.11	2.06
16	A	851	BCR	C29-C30	2.37	1.59	1.54
13	A	846	CLA	C5-C3	2.37	1.56	1.51
13	A	826	CLA	MG-NB	2.37	2.10	2.05
16	I	102	BCR	C33-C5	2.36	1.54	1.50
13	A	824	CLA	MG-NC	2.36	2.11	2.06
13	B	838	CLA	MG-NC	2.36	2.11	2.06
13	K	1401	CLA	CMD-C2D	2.36	1.55	1.50
13	K	1401	CLA	CHB-C1B	-2.36	1.34	1.39
13	A	802	CLA	CHC-C1C	2.35	1.43	1.38
13	A	835	CLA	MG-ND	-2.35	2.01	2.05
13	B	841	CLA	CAA-CBA	-2.35	1.45	1.52
13	A	833	CLA	CMD-C2D	2.34	1.55	1.50
13	A	819	CLA	C1D-C2D	-2.34	1.40	1.45
13	B	812	CLA	CHC-C1C	2.34	1.43	1.38
13	A	829	CLA	CHB-C1B	-2.33	1.34	1.39
16	I	101	BCR	C2-C3	-2.33	1.47	1.52
13	B	805	CLA	C5-C3	2.33	1.56	1.51
13	A	839	CLA	MG-NC	2.33	2.11	2.06
13	A	827	CLA	CAA-C2A	2.33	1.58	1.54
13	B	832	CLA	MG-NB	2.33	2.10	2.05
14	B	842	PQN	C7-C6	2.33	1.42	1.38
13	B	811	CLA	CAA-C2A	2.32	1.58	1.54
13	B	827	CLA	OBD-CAD	2.32	1.26	1.22
13	A	812	CLA	MG-NC	2.32	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	810	CLA	CMD-C2D	2.32	1.55	1.50
13	A	815	CLA	C1D-ND	-2.32	1.34	1.37
13	A	823	CLA	CHD-C1D	2.32	1.42	1.38
13	B	839	CLA	CHC-C1C	2.32	1.43	1.38
13	B	825	CLA	MG-NC	2.31	2.11	2.06
13	B	814	CLA	C5-C3	2.31	1.56	1.51
13	A	830	CLA	MG-NB	2.31	2.10	2.05
13	J	102	CLA	CBD-CAD	2.31	1.57	1.51
13	B	840	CLA	CAA-C2A	2.31	1.58	1.54
13	J	101	CLA	CAA-C2A	2.30	1.58	1.54
13	A	844	CLA	CHB-C1B	-2.30	1.34	1.39
13	A	816	CLA	CHD-C1D	2.30	1.42	1.38
13	B	814	CLA	CHC-C1C	2.30	1.43	1.38
13	B	816	CLA	C4-C3	2.30	1.56	1.50
13	B	815	CLA	CHB-C1B	-2.30	1.34	1.39
13	A	839	CLA	CHD-C1D	2.29	1.42	1.38
13	A	837	CLA	CAA-C2A	2.29	1.58	1.54
13	A	817	CLA	C1D-ND	-2.29	1.34	1.37
13	B	816	CLA	CHC-C1C	2.29	1.43	1.38
13	B	810	CLA	C1B-C2B	2.29	1.48	1.43
13	A	810	CLA	CHC-C1C	2.28	1.43	1.38
13	A	841	CLA	CMD-C2D	2.28	1.55	1.50
13	B	825	CLA	MG-NB	2.28	2.10	2.05
13	B	824	CLA	C1-C2	2.28	1.55	1.49
13	A	818	CLA	C3B-C4B	2.28	1.49	1.42
16	I	102	BCR	C19-C18	-2.28	1.41	1.46
16	J	103	BCR	C26-C25	2.28	1.38	1.34
13	B	825	CLA	CHD-C1D	2.28	1.42	1.38
13	A	802	CLA	C3B-C4B	2.28	1.49	1.42
13	B	830	CLA	C1D-ND	-2.27	1.34	1.37
13	K	1401	CLA	CHC-C1C	2.27	1.43	1.38
13	A	820	CLA	CMD-C2D	2.27	1.55	1.50
13	A	836	CLA	C1-C2	2.27	1.55	1.49
16	M	1602	BCR	C2-C3	-2.27	1.47	1.52
13	A	801	CLA	MG-ND	-2.27	2.01	2.05
13	A	822	CLA	C1-C2	2.27	1.55	1.49
13	A	831	CLA	CAA-C2A	2.27	1.58	1.54
16	B	848	BCR	C29-C28	-2.26	1.47	1.52
13	B	825	CLA	CAA-C2A	2.26	1.58	1.54
13	A	844	CLA	MG-NB	2.26	2.10	2.05
13	B	819	CLA	CHC-C1C	2.26	1.43	1.38
13	B	811	CLA	CHC-C1C	2.26	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	804	CLA	CAA-C2A	2.26	1.58	1.54
13	A	845	CLA	CAA-C2A	2.26	1.58	1.54
13	A	819	CLA	C1D-ND	-2.26	1.34	1.37
13	A	808	CLA	C1-C2	2.26	1.55	1.49
13	B	803	CLA	CMD-C2D	2.25	1.55	1.50
13	B	829	CLA	CHD-C1D	2.25	1.42	1.38
13	A	819	CLA	MG-NC	2.25	2.11	2.06
13	B	810	CLA	C1D-C2D	-2.25	1.40	1.45
13	B	831	CLA	MG-ND	-2.25	2.01	2.05
13	B	827	CLA	MG-NB	2.25	2.10	2.05
13	A	817	CLA	CHB-C1B	-2.25	1.34	1.39
16	A	853	BCR	C33-C5	2.25	1.54	1.50
16	I	101	BCR	C19-C18	-2.25	1.41	1.46
13	A	841	CLA	CAA-C2A	2.25	1.58	1.54
13	B	815	CLA	C3B-C4B	2.25	1.49	1.42
16	L	1005	BCR	C29-C28	-2.25	1.47	1.52
13	A	838	CLA	CHB-C4A	2.25	1.43	1.37
13	A	836	CLA	MG-NC	2.24	2.11	2.06
13	A	802	CLA	CHD-C1D	2.24	1.42	1.38
13	A	808	CLA	C1D-ND	-2.24	1.34	1.37
13	A	815	CLA	C3B-C4B	2.24	1.49	1.42
16	L	1005	BCR	C26-C25	2.24	1.38	1.34
13	A	846	CLA	MG-NC	2.24	2.11	2.06
13	B	834	CLA	CMD-C2D	2.24	1.55	1.50
14	A	847	PQN	C11-C3	2.24	1.55	1.51
13	A	828	CLA	MG-NC	2.24	2.11	2.06
13	B	830	CLA	CAA-C2A	2.24	1.58	1.54
13	B	813	CLA	CHD-C1D	2.24	1.42	1.38
13	A	807	CLA	CAA-CBA	-2.24	1.46	1.52
14	B	842	PQN	C5-C4	-2.24	1.43	1.48
13	B	841	CLA	C1C-NC	-2.24	1.34	1.37
13	A	825	CLA	MG-NB	2.24	2.10	2.05
13	B	840	CLA	CMD-C2D	2.24	1.55	1.50
16	B	848	BCR	C5-C6	2.24	1.38	1.34
13	B	816	CLA	C1-C2	2.24	1.55	1.49
13	A	822	CLA	CHD-C1D	2.24	1.42	1.38
13	A	846	CLA	CHB-C1B	-2.23	1.34	1.39
16	L	1005	BCR	C38-C26	2.23	1.54	1.50
13	B	835	CLA	C1D-ND	-2.23	1.34	1.37
13	B	830	CLA	MG-NB	2.23	2.10	2.05
13	A	846	CLA	C4-C3	2.23	1.56	1.50
13	A	816	CLA	MG-NC	2.23	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	833	CLA	MG-NC	2.23	2.11	2.06
13	B	833	CLA	CMD-C2D	2.23	1.55	1.50
13	A	845	CLA	MG-NC	2.23	2.11	2.06
13	B	814	CLA	MG-NC	2.23	2.11	2.06
13	B	824	CLA	C3B-C4B	2.22	1.49	1.42
13	A	824	CLA	CHB-C1B	-2.22	1.34	1.39
13	A	837	CLA	C1D-ND	-2.22	1.34	1.37
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	B	821	CLA	CHD-C1D	2.22	1.42	1.38
16	I	102	BCR	C26-C25	2.22	1.38	1.34
13	A	817	CLA	MG-NC	2.22	2.11	2.06
13	B	816	CLA	CHB-C1B	-2.22	1.34	1.39
13	A	839	CLA	C3B-C4B	2.22	1.49	1.42
16	A	851	BCR	C29-C28	-2.21	1.47	1.52
13	A	805	CLA	MG-ND	-2.21	2.01	2.05
16	A	853	BCR	C2-C1	2.21	1.59	1.54
13	B	804	CLA	C1-C2	2.21	1.55	1.49
13	A	811	CLA	CHB-C1B	-2.21	1.34	1.39
13	A	821	CLA	MG-ND	-2.21	2.01	2.05
13	B	841	CLA	CMD-C2D	2.21	1.55	1.50
13	A	815	CLA	CAA-C2A	2.21	1.58	1.54
13	B	832	CLA	MG-NC	2.21	2.11	2.06
13	A	812	CLA	CAA-C2A	2.20	1.58	1.54
13	B	814	CLA	CHD-C1D	2.20	1.42	1.38
13	B	837	CLA	MG-NC	2.20	2.11	2.06
13	B	837	CLA	C5-C3	2.19	1.55	1.51
16	J	104	BCR	C1-C6	2.19	1.56	1.53
13	A	839	CLA	CAA-C2A	2.19	1.58	1.54
13	A	829	CLA	C1D-ND	-2.19	1.35	1.37
13	A	801	CLA	CHC-C1C	2.19	1.42	1.38
13	A	833	CLA	C1D-ND	-2.19	1.35	1.37
13	A	823	CLA	CHB-C1B	-2.19	1.34	1.39
13	K	1401	CLA	CHD-C1D	2.18	1.42	1.38
13	B	841	CLA	MG-NC	2.18	2.11	2.06
13	B	836	CLA	CHC-C1C	2.18	1.42	1.38
13	B	834	CLA	CAA-C2A	2.18	1.58	1.54
13	B	830	CLA	CHD-C1D	2.18	1.42	1.38
13	A	832	CLA	CMD-C2D	2.18	1.55	1.50
13	B	821	CLA	C3B-C4B	2.18	1.49	1.42
13	B	822	CLA	MG-NC	2.18	2.11	2.06
13	X	1701	CLA	C3B-C4B	2.18	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	A	853	BCR	C29-C28	-2.18	1.47	1.52
13	A	843	CLA	MG-NB	2.18	2.10	2.05
13	A	813	CLA	CHB-C1B	-2.18	1.34	1.39
14	B	842	PQN	C10-C1	-2.18	1.43	1.48
13	A	804	CLA	MG-NB	2.18	2.10	2.05
13	A	834	CLA	MG-NB	2.18	2.10	2.05
13	B	832	CLA	CHB-C1B	-2.18	1.34	1.39
13	L	1003	CLA	C1D-ND	-2.18	1.35	1.37
16	L	1006	BCR	C23-C22	-2.18	1.41	1.46
13	B	828	CLA	CHB-C1B	-2.18	1.34	1.39
13	A	816	CLA	CHC-C1C	2.18	1.42	1.38
13	A	830	CLA	C1D-C2D	-2.17	1.41	1.45
13	B	804	CLA	C1D-ND	-2.17	1.35	1.37
13	B	818	CLA	CMD-C2D	2.17	1.55	1.50
13	A	838	CLA	C1B-C2B	2.17	1.48	1.43
13	A	821	CLA	C3B-C4B	2.17	1.49	1.42
16	L	1005	BCR	C2-C3	-2.17	1.47	1.52
13	A	803	CLA	CHD-C1D	2.17	1.42	1.38
13	B	831	CLA	MG-NB	2.17	2.10	2.05
13	B	834	CLA	C1D-ND	-2.16	1.35	1.37
13	A	824	CLA	CHC-C1C	2.16	1.42	1.38
13	B	807	CLA	C5-C3	2.16	1.55	1.51
13	A	835	CLA	MG-NC	2.16	2.11	2.06
13	A	820	CLA	CHB-C1B	-2.16	1.34	1.39
13	B	827	CLA	C3B-C4B	2.16	1.49	1.42
13	A	835	CLA	C1-C2	2.16	1.55	1.49
16	A	851	BCR	C26-C25	2.16	1.38	1.34
13	A	822	CLA	MG-NB	2.16	2.10	2.05
13	A	808	CLA	CMD-C2D	2.15	1.55	1.50
13	A	804	CLA	CHC-C1C	2.15	1.42	1.38
13	A	830	CLA	C5-C3	2.15	1.55	1.51
13	B	803	CLA	C4-C3	2.15	1.56	1.50
16	B	845	BCR	C5-C6	2.15	1.38	1.34
13	B	831	CLA	CAA-C2A	2.15	1.58	1.54
13	A	820	CLA	C1D-ND	-2.15	1.35	1.37
13	A	843	CLA	C5-C3	2.15	1.55	1.51
13	A	813	CLA	C4-C3	2.14	1.55	1.50
13	A	836	CLA	CHC-C1C	2.14	1.42	1.38
16	A	853	BCR	C19-C18	-2.14	1.41	1.46
13	B	838	CLA	C3B-C4B	2.14	1.49	1.42
13	A	833	CLA	C1B-C2B	2.14	1.48	1.43
13	A	829	CLA	C4-C3	2.14	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	810	CLA	CHB-C1B	-2.14	1.34	1.39
13	B	829	CLA	C1D-ND	-2.14	1.35	1.37
13	B	828	CLA	C1D-ND	-2.14	1.35	1.37
13	A	824	CLA	C1-C2	2.14	1.55	1.49
16	A	852	BCR	C2-C3	-2.13	1.47	1.52
13	B	816	CLA	CMD-C2D	2.13	1.55	1.50
13	A	828	CLA	C3B-C4B	2.13	1.49	1.42
13	B	838	CLA	CHD-C1D	2.13	1.42	1.38
13	A	818	CLA	CAA-C2A	2.13	1.58	1.54
13	B	808	CLA	CHC-C1C	2.13	1.42	1.38
13	B	833	CLA	C1D-ND	-2.12	1.35	1.37
14	B	842	PQN	C15-C13	2.12	1.55	1.51
13	B	815	CLA	CMD-C2D	2.12	1.55	1.50
13	B	811	CLA	MG-NC	2.12	2.11	2.06
13	A	837	CLA	CMD-C2D	2.12	1.55	1.50
13	B	840	CLA	C1-C2	2.12	1.55	1.49
13	B	823	CLA	C3B-C4B	2.12	1.48	1.42
13	B	813	CLA	CHC-C1C	2.12	1.42	1.38
13	A	815	CLA	CHD-C1D	2.12	1.42	1.38
13	B	821	CLA	CAA-C2A	2.12	1.57	1.54
13	B	810	CLA	CHB-C1B	-2.12	1.34	1.39
13	A	846	CLA	CHD-C1D	2.11	1.42	1.38
13	B	833	CLA	C4-C3	2.11	1.55	1.50
13	B	806	CLA	CAA-C2A	2.11	1.57	1.54
17	A	855	LHG	O7-C5	-2.11	1.41	1.46
13	A	818	CLA	CMD-C2D	2.11	1.55	1.50
13	A	813	CLA	C5-C3	2.11	1.55	1.51
13	B	824	CLA	CMD-C2D	2.11	1.55	1.50
13	B	818	CLA	C1B-NB	-2.11	1.35	1.37
13	B	818	CLA	CHB-C1B	-2.11	1.34	1.39
13	A	804	CLA	C3B-C4B	2.11	1.48	1.42
13	B	833	CLA	CHD-C1D	2.10	1.42	1.38
13	B	838	CLA	CMD-C2D	2.10	1.55	1.50
16	B	848	BCR	C30-C25	2.10	1.56	1.53
13	A	817	CLA	CHC-C1C	2.10	1.42	1.38
13	A	825	CLA	CHD-C1D	2.10	1.42	1.38
13	A	801	CLA	MG-NC	2.10	2.11	2.06
13	A	814	CLA	CMD-C2D	2.10	1.55	1.50
13	B	807	CLA	C3B-C4B	2.10	1.48	1.42
13	A	841	CLA	C1D-ND	-2.10	1.35	1.37
13	M	1601	CLA	MG-NC	2.10	2.11	2.06
13	B	829	CLA	MG-ND	-2.10	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	837	CLA	C4-C3	2.10	1.55	1.50
13	B	833	CLA	CHC-C1C	2.10	1.42	1.38
13	B	822	CLA	C3B-C4B	2.10	1.48	1.42
13	A	807	CLA	CHD-C1D	2.09	1.42	1.38
13	J	102	CLA	C3B-C4B	2.09	1.48	1.42
13	B	835	CLA	MG-NC	2.09	2.11	2.06
13	B	809	CLA	CMD-C2D	2.09	1.55	1.50
13	B	839	CLA	C1D-C2D	-2.09	1.41	1.45
17	B	851	LHG	O8-C23	2.09	1.43	1.33
13	B	822	CLA	CHB-C1B	-2.08	1.34	1.39
13	A	842	CLA	CHB-C4A	2.08	1.42	1.37
13	A	802	CLA	C1D-C2D	-2.08	1.41	1.45
13	A	817	CLA	CAA-C2A	2.08	1.57	1.54
13	A	819	CLA	CHB-C1B	-2.08	1.34	1.39
13	A	841	CLA	C3B-C4B	2.08	1.48	1.42
13	B	815	CLA	C1D-C2D	-2.08	1.41	1.45
13	B	824	CLA	CAA-C2A	2.08	1.57	1.54
13	A	807	CLA	C4-C3	2.08	1.55	1.50
14	A	847	PQN	C5-C4	-2.08	1.44	1.48
13	A	812	CLA	CHC-C1C	2.08	1.42	1.38
13	B	811	CLA	CHD-C1D	2.08	1.42	1.38
13	B	820	CLA	CHD-C1D	2.08	1.42	1.38
16	F	1302	BCR	C23-C22	-2.08	1.41	1.46
13	A	826	CLA	C3B-C4B	2.08	1.48	1.42
13	A	816	CLA	CMD-C2D	2.07	1.55	1.50
13	A	844	CLA	C5-C3	2.07	1.55	1.51
13	A	812	CLA	CMD-C2D	2.07	1.55	1.50
13	B	831	CLA	CHD-C1D	2.07	1.42	1.38
13	F	1301	CLA	CHD-C1D	2.07	1.42	1.38
13	A	822	CLA	C3B-C4B	2.07	1.48	1.42
13	B	816	CLA	C3B-C4B	2.07	1.48	1.42
13	B	824	CLA	C1D-ND	-2.07	1.35	1.37
13	A	825	CLA	C5-C3	2.07	1.55	1.51
13	B	801	CLA	CAA-CBA	-2.07	1.46	1.52
13	B	833	CLA	C1-C2	2.07	1.55	1.49
13	A	843	CLA	CAA-C2A	2.07	1.57	1.54
13	A	808	CLA	C1D-C2D	-2.07	1.41	1.45
13	L	1003	CLA	C1-C2	2.07	1.55	1.49
13	B	825	CLA	C1D-ND	-2.07	1.35	1.37
13	B	822	CLA	C1-C2	2.06	1.55	1.49
13	A	803	CLA	CHC-C1C	2.06	1.42	1.38
13	A	845	CLA	C1D-ND	-2.06	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	I	101	BCR	C26-C25	2.06	1.38	1.34
13	A	820	CLA	MG-NC	2.06	2.11	2.06
13	A	837	CLA	CHD-C1D	2.06	1.42	1.38
16	A	853	BCR	C26-C25	2.06	1.38	1.34
13	F	1301	CLA	C1D-C2D	-2.06	1.41	1.45
16	B	846	BCR	C14-C13	2.06	1.40	1.34
13	F	1301	CLA	C3B-C4B	2.06	1.48	1.42
13	A	834	CLA	CHD-C1D	2.06	1.42	1.38
13	B	840	CLA	CHB-C1B	-2.06	1.34	1.39
13	A	846	CLA	CMD-C2D	2.05	1.55	1.50
13	B	836	CLA	C1D-ND	-2.05	1.35	1.37
13	B	812	CLA	CHB-C4A	2.05	1.42	1.37
13	A	818	CLA	C1-C2	2.05	1.55	1.49
13	A	833	CLA	C1-C2	2.05	1.55	1.49
13	A	815	CLA	CMD-C2D	2.05	1.55	1.50
13	B	828	CLA	CHD-C1D	2.05	1.42	1.38
13	B	834	CLA	C3B-C4B	2.05	1.48	1.42
13	A	836	CLA	CAA-C2A	2.05	1.57	1.54
13	M	1601	CLA	C3B-C4B	2.05	1.48	1.42
13	B	817	CLA	MG-NC	2.05	2.11	2.06
13	L	1002	CLA	C3B-C4B	2.05	1.48	1.42
13	B	821	CLA	C1D-ND	-2.05	1.35	1.37
16	B	847	BCR	C5-C6	2.05	1.38	1.34
13	A	843	CLA	CHB-C1B	-2.05	1.34	1.39
13	A	845	CLA	CHD-C1D	2.04	1.42	1.38
13	J	102	CLA	CMD-C2D	2.04	1.55	1.50
13	B	821	CLA	CMD-C2D	2.04	1.55	1.50
13	B	826	CLA	CHB-C4A	2.04	1.42	1.37
13	B	831	CLA	C3B-C4B	2.04	1.48	1.42
13	J	102	CLA	C1D-ND	-2.04	1.35	1.37
13	A	809	CLA	C1-C2	2.04	1.55	1.49
13	B	804	CLA	CHB-C1B	-2.04	1.34	1.39
17	A	855	LHG	O8-C6	-2.04	1.40	1.45
13	A	821	CLA	C1-C2	2.04	1.55	1.49
13	A	832	CLA	MG-NB	2.04	2.09	2.05
16	L	1006	BCR	C5-C6	2.04	1.37	1.34
13	A	832	CLA	C3B-C4B	2.04	1.48	1.42
13	B	823	CLA	CHB-C1B	-2.03	1.34	1.39
13	B	814	CLA	CAA-C2A	2.03	1.57	1.54
13	A	817	CLA	CMD-C2D	2.03	1.54	1.50
13	L	1003	CLA	C3D-C4D	-2.03	1.39	1.44
16	A	854	BCR	C39-C30	-2.03	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	848	BCR	C1-C6	2.03	1.56	1.53
13	A	825	CLA	C1D-ND	-2.03	1.35	1.37
13	B	821	CLA	MG-NC	2.02	2.11	2.06
13	B	839	CLA	C3D-C4D	-2.02	1.39	1.44
13	A	801	CLA	C1D-C2D	-2.02	1.41	1.45
16	B	847	BCR	C29-C28	-2.02	1.47	1.52
13	A	814	CLA	CHC-C1C	2.02	1.42	1.38
13	A	813	CLA	MG-NB	2.02	2.09	2.05
16	A	850	BCR	C2-C3	-2.02	1.47	1.52
13	B	825	CLA	CHC-C1C	2.02	1.42	1.38
13	B	818	CLA	CAB-C3B	2.02	1.52	1.47
13	F	1301	CLA	CHB-C1B	-2.02	1.34	1.39
13	B	807	CLA	MG-NB	2.02	2.09	2.05
13	B	808	CLA	CAA-C2A	2.01	1.57	1.54
13	B	804	CLA	MG-NC	2.01	2.11	2.06
13	B	833	CLA	CHB-C4A	2.01	1.42	1.37
13	J	102	CLA	CHB-C4A	2.01	1.42	1.37
13	A	843	CLA	C3B-C4B	2.01	1.48	1.42
13	B	815	CLA	CAA-C2A	2.01	1.57	1.54
13	A	831	CLA	CHB-C1B	-2.01	1.34	1.39
13	A	809	CLA	CMD-C2D	2.01	1.54	1.50
16	L	1005	BCR	C23-C22	-2.01	1.41	1.46
13	A	846	CLA	C3B-C4B	2.01	1.48	1.42
13	A	841	CLA	C4-C3	2.01	1.55	1.50
13	B	832	CLA	C3B-C4B	2.01	1.48	1.42
13	A	810	CLA	CHD-C1D	2.01	1.42	1.38
13	B	801	CLA	C4-C3	2.01	1.55	1.50
13	A	802	CLA	C1D-ND	-2.00	1.35	1.37
13	B	841	CLA	CHB-C1B	-2.00	1.34	1.39
13	A	823	CLA	CAA-C2A	2.00	1.57	1.54
13	A	811	CLA	CHC-C1C	2.00	1.42	1.38
13	A	842	CLA	C4-C3	2.00	1.55	1.50

All (1242) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	820	CLA	C4A-NA-C1A	12.25	112.27	106.68
13	A	833	CLA	C4A-NA-C1A	12.08	112.19	106.68
13	M	1601	CLA	C4A-NA-C1A	11.96	112.14	106.68
13	A	813	CLA	C4A-NA-C1A	11.80	112.06	106.68
13	A	821	CLA	C4A-NA-C1A	11.78	112.06	106.68
13	A	816	CLA	C4A-NA-C1A	11.74	112.04	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	812	CLA	C4A-NA-C1A	11.72	112.03	106.68
13	X	1701	CLA	C4A-NA-C1A	11.72	112.03	106.68
13	B	821	CLA	C4A-NA-C1A	11.70	112.02	106.68
13	J	101	CLA	C4A-NA-C1A	11.62	111.98	106.68
13	A	846	CLA	C4A-NA-C1A	11.53	111.94	106.68
13	B	836	CLA	C4A-NA-C1A	11.41	111.89	106.68
13	A	812	CLA	C4A-NA-C1A	11.39	111.87	106.68
13	A	837	CLA	C4A-NA-C1A	11.38	111.87	106.68
13	B	830	CLA	C4A-NA-C1A	11.33	111.85	106.68
13	B	818	CLA	C4A-NA-C1A	11.32	111.84	106.68
13	A	817	CLA	C4A-NA-C1A	11.26	111.81	106.68
13	F	1301	CLA	C4A-NA-C1A	11.24	111.81	106.68
13	B	822	CLA	C4A-NA-C1A	11.19	111.78	106.68
13	J	102	CLA	C4A-NA-C1A	11.16	111.77	106.68
13	A	823	CLA	C4A-NA-C1A	11.14	111.76	106.68
13	B	807	CLA	C4A-NA-C1A	11.11	111.75	106.68
13	B	804	CLA	C4A-NA-C1A	11.06	111.73	106.68
13	A	820	CLA	C4A-NA-C1A	11.06	111.72	106.68
13	A	814	CLA	C4A-NA-C1A	11.05	111.72	106.68
13	B	825	CLA	C4A-NA-C1A	11.03	111.71	106.68
13	B	833	CLA	C4A-NA-C1A	11.01	111.70	106.68
13	A	810	CLA	C4A-NA-C1A	11.00	111.70	106.68
13	A	808	CLA	C4A-NA-C1A	10.96	111.68	106.68
13	A	845	CLA	C4A-NA-C1A	10.93	111.67	106.68
13	A	841	CLA	C4A-NA-C1A	10.90	111.65	106.68
13	A	832	CLA	C4A-NA-C1A	10.89	111.65	106.68
13	A	836	CLA	C4A-NA-C1A	10.88	111.64	106.68
13	B	826	CLA	C4A-NA-C1A	10.87	111.64	106.68
13	B	810	CLA	C4A-NA-C1A	10.87	111.64	106.68
13	A	809	CLA	C4A-NA-C1A	10.83	111.62	106.68
13	A	828	CLA	C4A-NA-C1A	10.82	111.62	106.68
13	A	838	CLA	C4A-NA-C1A	10.78	111.59	106.68
13	B	838	CLA	C4A-NA-C1A	10.74	111.58	106.68
13	B	819	CLA	C4A-NA-C1A	10.71	111.57	106.68
13	A	805	CLA	C4A-NA-C1A	10.66	111.54	106.68
13	B	841	CLA	C4A-NA-C1A	10.66	111.54	106.68
13	A	819	CLA	C4A-NA-C1A	10.62	111.52	106.68
13	B	831	CLA	C4A-NA-C1A	10.61	111.52	106.68
13	B	817	CLA	C4A-NA-C1A	10.58	111.50	106.68
13	B	823	CLA	C4A-NA-C1A	10.54	111.49	106.68
13	B	814	CLA	C4A-NA-C1A	10.54	111.49	106.68
13	A	827	CLA	C4A-NA-C1A	10.51	111.47	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	822	CLA	C4A-NA-C1A	10.48	111.46	106.68
13	B	801	CLA	C4A-NA-C1A	10.47	111.46	106.68
13	B	834	CLA	C4A-NA-C1A	10.47	111.45	106.68
13	B	815	CLA	C4A-NA-C1A	10.42	111.44	106.68
13	A	825	CLA	C4A-NA-C1A	10.42	111.43	106.68
13	B	824	CLA	C4A-NA-C1A	10.36	111.41	106.68
13	A	842	CLA	C4A-NA-C1A	10.35	111.40	106.68
13	A	804	CLA	C4A-NA-C1A	10.35	111.40	106.68
13	B	811	CLA	C4A-NA-C1A	10.35	111.40	106.68
13	A	815	CLA	C4A-NA-C1A	10.33	111.39	106.68
13	B	832	CLA	C4A-NA-C1A	10.32	111.39	106.68
13	L	1003	CLA	C4A-NA-C1A	10.32	111.39	106.68
13	L	1002	CLA	C4A-NA-C1A	10.27	111.36	106.68
13	A	843	CLA	C4A-NA-C1A	10.24	111.35	106.68
13	B	827	CLA	C4A-NA-C1A	10.23	111.35	106.68
13	A	830	CLA	C4A-NA-C1A	10.22	111.34	106.68
13	B	809	CLA	C4A-NA-C1A	10.19	111.33	106.68
13	A	811	CLA	C4A-NA-C1A	10.18	111.32	106.68
13	A	826	CLA	C4A-NA-C1A	10.14	111.31	106.68
13	K	1401	CLA	C4A-NA-C1A	10.13	111.30	106.68
13	B	835	CLA	C4A-NA-C1A	10.11	111.29	106.68
13	A	807	CLA	C4A-NA-C1A	10.04	111.26	106.68
13	B	816	CLA	C4A-NA-C1A	10.03	111.26	106.68
13	A	824	CLA	C4A-NA-C1A	9.99	111.24	106.68
13	A	818	CLA	C4A-NA-C1A	9.93	111.21	106.68
13	L	1004	CLA	C4A-NA-C1A	9.90	111.20	106.68
13	A	839	CLA	C4A-NA-C1A	9.90	111.20	106.68
13	B	837	CLA	C4A-NA-C1A	9.89	111.19	106.68
13	B	840	CLA	C4A-NA-C1A	9.78	111.14	106.68
13	A	806	CLA	C4A-NA-C1A	9.74	111.12	106.68
13	B	829	CLA	C4A-NA-C1A	9.70	111.10	106.68
13	A	831	CLA	C4A-NA-C1A	9.69	111.10	106.68
13	A	834	CLA	C4A-NA-C1A	9.64	111.08	106.68
13	B	803	CLA	C4A-NA-C1A	9.60	111.06	106.68
13	A	829	CLA	C4A-NA-C1A	9.58	111.05	106.68
13	B	806	CLA	C4A-NA-C1A	9.57	111.05	106.68
13	A	844	CLA	C4A-NA-C1A	9.57	111.04	106.68
13	B	802	CLA	C4A-NA-C1A	9.48	111.01	106.68
13	A	835	CLA	C4A-NA-C1A	9.43	110.98	106.68
13	B	805	CLA	C4A-NA-C1A	9.40	110.97	106.68
13	B	839	CLA	C4A-NA-C1A	9.36	110.95	106.68
13	A	840	CLA	C4A-NA-C1A	9.33	110.94	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	803	CLA	C4A-NA-C1A	9.23	110.89	106.68
13	B	813	CLA	C4A-NA-C1A	9.21	110.88	106.68
13	A	802	CLA	C4A-NA-C1A	9.07	110.82	106.68
13	A	801	CLA	C4A-NA-C1A	9.01	110.79	106.68
13	B	828	CLA	C4A-NA-C1A	8.83	110.71	106.68
13	B	808	CLA	C4A-NA-C1A	8.77	110.68	106.68
13	A	801	CLA	O2D-CGD-CBD	8.67	126.39	111.23
14	B	842	PQN	C11-C12-C13	-7.91	113.20	126.83
14	A	847	PQN	C11-C12-C13	-7.81	113.38	126.83
14	A	847	PQN	C14-C13-C15	7.21	127.74	115.23
14	A	847	PQN	C15-C13-C12	-6.55	106.45	121.17
14	B	842	PQN	C14-C13-C15	6.20	125.98	115.23
16	B	843	BCR	C38-C26-C25	6.15	131.20	124.48
17	A	855	LHG	C25-C24-C23	6.13	136.17	113.69
18	B	850	LMG	C30-C29-C28	6.06	135.91	113.69
16	B	844	BCR	C38-C26-C25	5.99	131.02	124.48
16	A	853	BCR	C38-C26-C25	5.75	130.76	124.48
14	B	842	PQN	C15-C13-C12	-5.56	108.68	121.17
13	A	801	CLA	O1D-CGD-CBD	-5.48	113.72	124.52
16	A	849	BCR	C38-C26-C25	5.30	130.27	124.48
16	B	848	BCR	C33-C5-C6	5.30	130.27	124.48
16	J	103	BCR	C38-C26-C25	5.29	130.26	124.48
16	L	1006	BCR	C33-C5-C6	5.29	130.26	124.48
16	L	1005	BCR	C33-C5-C6	5.07	130.01	124.48
13	B	802	CLA	O2D-CGD-CBD	4.98	119.93	111.23
13	B	829	CLA	O2D-CGD-CBD	4.98	119.93	111.23
17	A	856	LHG	C25-C24-C23	4.95	137.56	114.11
13	A	835	CLA	O2D-CGD-CBD	4.94	119.87	111.23
16	J	105	BCR	C33-C5-C6	4.90	129.84	124.48
16	B	845	BCR	C33-C5-C6	4.90	129.83	124.48
16	I	101	BCR	C33-C5-C6	4.86	129.79	124.48
13	A	807	CLA	CAA-C2A-C3A	-4.86	99.87	113.00
13	B	804	CLA	O2D-CGD-CBD	4.84	119.69	111.23
16	A	851	BCR	C38-C26-C25	4.83	129.75	124.48
16	B	843	BCR	C33-C5-C6	4.82	129.75	124.48
16	B	847	BCR	C33-C5-C6	4.82	129.75	124.48
13	A	807	CLA	O2A-CGA-CBA	4.82	126.53	111.83
13	L	1002	CLA	O2D-CGD-CBD	4.76	119.56	111.23
16	J	105	BCR	C38-C26-C25	4.76	129.68	124.48
16	F	1302	BCR	C38-C26-C25	4.68	129.59	124.48
13	A	805	CLA	O2D-CGD-CBD	4.67	119.39	111.23
16	A	850	BCR	C38-C26-C25	4.66	129.57	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	808	CLA	O2D-CGD-CBD	4.63	119.33	111.23
16	L	1006	BCR	C38-C26-C25	4.62	129.52	124.48
13	A	846	CLA	O2D-CGD-CBD	4.58	119.24	111.23
13	B	833	CLA	O2D-CGD-CBD	4.58	119.23	111.23
13	B	814	CLA	O2D-CGD-CBD	4.55	119.19	111.23
16	M	1602	BCR	C38-C26-C25	4.54	129.44	124.48
16	B	845	BCR	C29-C30-C25	4.53	117.02	110.44
16	I	101	BCR	C38-C26-C25	4.53	129.42	124.48
16	B	845	BCR	C7-C8-C9	4.53	132.93	126.23
16	B	848	BCR	C38-C26-C25	4.52	129.42	124.48
13	B	827	CLA	O2A-CGA-CBA	4.52	125.61	111.83
16	A	852	BCR	C38-C26-C25	4.51	129.40	124.48
16	A	851	BCR	C33-C5-C6	4.50	129.39	124.48
16	B	845	BCR	C38-C26-C25	4.48	129.37	124.48
16	A	849	BCR	C33-C5-C6	4.47	129.37	124.48
13	B	815	CLA	O2D-CGD-CBD	4.41	118.94	111.23
16	A	854	BCR	C7-C8-C9	4.40	132.74	126.23
13	A	828	CLA	O2D-CGD-CBD	4.36	118.85	111.23
16	L	1005	BCR	C38-C26-C25	4.34	129.22	124.48
13	B	825	CLA	O2D-CGD-CBD	4.34	118.82	111.23
16	I	101	BCR	C2-C1-C6	4.34	116.75	110.44
13	A	816	CLA	O2D-CGD-CBD	4.33	118.80	111.23
16	J	105	BCR	C8-C7-C6	4.31	138.51	127.00
13	A	826	CLA	O2D-CGD-CBD	4.29	118.73	111.23
16	B	844	BCR	C33-C5-C6	4.27	129.15	124.48
13	A	804	CLA	O2D-CGD-CBD	4.27	118.69	111.23
16	B	846	BCR	C38-C26-C25	4.26	129.13	124.48
13	A	809	CLA	O2D-CGD-CBD	4.24	118.65	111.23
13	A	831	CLA	O2D-CGD-CBD	4.23	118.62	111.23
16	J	103	BCR	C33-C5-C6	4.22	129.09	124.48
13	B	820	CLA	O2D-CGD-CBD	4.20	118.58	111.23
16	I	102	BCR	C38-C26-C25	4.20	129.07	124.48
13	A	838	CLA	O2A-CGA-CBA	4.20	124.65	111.83
16	A	854	BCR	C33-C5-C6	4.19	129.06	124.48
13	A	840	CLA	O2A-CGA-CBA	4.18	124.56	111.83
13	A	803	CLA	O2A-CGA-CBA	4.17	124.54	111.83
13	B	832	CLA	O2D-CGD-CBD	4.16	118.50	111.23
13	M	1601	CLA	O2D-CGD-CBD	4.16	118.50	111.23
13	A	832	CLA	O2D-CGD-CBD	4.14	118.47	111.23
16	A	850	BCR	C33-C5-C6	4.12	128.98	124.48
16	F	1302	BCR	C33-C5-C6	4.12	128.98	124.48
16	B	849	BCR	C33-C5-C6	4.10	128.96	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	828	CLA	O2A-CGA-CBA	4.09	124.32	111.83
16	A	854	BCR	C38-C26-C25	4.09	128.94	124.48
16	J	105	BCR	C2-C1-C6	4.09	116.38	110.44
13	B	837	CLA	O2D-CGD-CBD	4.08	118.36	111.23
16	B	847	BCR	C38-C26-C25	4.08	128.93	124.48
13	B	830	CLA	O2D-CGD-CBD	4.07	118.34	111.23
16	I	102	BCR	C24-C23-C22	4.06	132.24	126.23
13	B	821	CLA	O2D-CGD-CBD	4.05	118.30	111.23
16	B	849	BCR	C38-C26-C25	4.05	128.90	124.48
13	A	824	CLA	O2D-CGD-CBD	4.04	118.29	111.23
13	B	813	CLA	O2D-CGD-CBD	4.04	118.29	111.23
16	A	854	BCR	C2-C1-C6	4.01	116.27	110.44
13	B	826	CLA	O2D-CGD-CBD	4.01	118.23	111.23
13	J	101	CLA	O2D-CGD-CBD	4.00	118.22	111.23
13	B	805	CLA	O2D-CGD-CBD	3.99	118.20	111.23
16	A	852	BCR	C33-C5-C6	3.98	128.82	124.48
16	B	844	BCR	C7-C8-C9	3.97	132.10	126.23
13	K	1401	CLA	O2D-CGD-CBD	3.96	118.16	111.23
13	A	806	CLA	O2D-CGD-CBD	3.96	118.15	111.23
16	B	843	BCR	C2-C1-C6	3.96	116.19	110.44
13	A	843	CLA	O2A-CGA-CBA	3.95	123.89	111.83
13	A	810	CLA	O2A-CGA-CBA	3.95	123.88	111.83
16	J	103	BCR	C29-C30-C25	3.95	116.17	110.44
16	A	854	BCR	C24-C23-C22	3.94	132.06	126.23
13	A	821	CLA	O2A-CGA-CBA	3.93	123.81	111.83
13	A	820	CLA	O2A-CGA-CBA	3.93	123.81	111.83
13	B	808	CLA	O2A-CGA-CBA	3.92	123.79	111.83
13	A	844	CLA	O2A-CGA-CBA	3.92	123.78	111.83
13	A	823	CLA	O2A-CGA-CBA	3.92	123.77	111.83
13	B	818	CLA	O2A-CGA-CBA	3.91	123.77	111.83
16	A	851	BCR	C29-C30-C25	3.90	116.11	110.44
13	A	846	CLA	O2A-CGA-CBA	3.90	123.72	111.83
13	B	824	CLA	O2D-CGD-CBD	3.89	118.04	111.23
16	A	854	BCR	C40-C30-C25	3.89	116.34	110.24
16	M	1602	BCR	C24-C23-C22	3.89	131.99	126.23
13	A	823	CLA	O2D-CGD-CBD	3.89	118.02	111.23
13	A	814	CLA	O2D-CGD-CBD	3.88	118.01	111.23
13	B	814	CLA	C1-C2-C3	3.86	132.52	126.20
13	A	842	CLA	O2A-CGA-CBA	3.85	123.57	111.83
13	B	831	CLA	O2D-CGD-CBD	3.84	117.94	111.23
16	B	848	BCR	C7-C8-C9	3.83	131.90	126.23
13	A	846	CLA	C1-C2-C3	3.82	132.46	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	J	104	BCR	C2-C1-C6	3.81	115.98	110.44
13	A	802	CLA	C3B-C4B-NB	-3.81	107.13	110.53
13	B	827	CLA	CBA-CAA-C2A	3.81	125.12	113.79
13	A	824	CLA	O2A-CGA-CBA	3.81	123.44	111.83
13	B	834	CLA	O2D-CGD-CBD	3.80	117.88	111.23
16	J	104	BCR	C33-C5-C6	3.80	128.63	124.48
16	J	104	BCR	C29-C30-C25	3.79	115.95	110.44
13	A	830	CLA	O2A-CGA-CBA	3.78	123.35	111.83
16	B	844	BCR	C30-C25-C26	-3.77	117.48	122.64
13	B	820	CLA	O2A-CGA-CBA	3.76	123.31	111.83
16	I	102	BCR	C33-C5-C6	3.76	128.59	124.48
16	M	1602	BCR	C33-C5-C6	3.75	128.58	124.48
13	B	817	CLA	O2A-CGA-CBA	3.74	123.25	111.83
13	A	813	CLA	O2A-CGA-CBA	3.72	123.16	111.83
13	A	819	CLA	O2A-CGA-CBA	3.72	123.16	111.83
16	B	844	BCR	C24-C23-C22	3.71	131.72	126.23
16	A	853	BCR	C33-C5-C6	3.70	128.52	124.48
13	B	807	CLA	O2D-CGD-CBD	3.69	117.69	111.23
13	A	830	CLA	O2D-CGD-CBD	3.69	117.68	111.23
16	B	844	BCR	C29-C30-C25	3.68	115.78	110.44
13	A	840	CLA	O2D-CGD-CBD	3.67	117.65	111.23
16	A	852	BCR	C24-C23-C22	3.65	131.64	126.23
13	A	809	CLA	O2A-CGA-CBA	3.65	122.96	111.83
13	A	808	CLA	O2A-CGA-CBA	3.65	122.96	111.83
13	A	817	CLA	O2D-CGD-CBD	3.64	117.60	111.23
13	L	1004	CLA	O2D-CGD-CBD	3.64	117.60	111.23
16	B	847	BCR	C7-C8-C9	3.64	131.62	126.23
13	B	804	CLA	O2A-CGA-CBA	3.64	122.92	111.83
13	A	821	CLA	O2D-CGD-CBD	3.63	117.58	111.23
16	J	105	BCR	C24-C23-C22	3.63	131.61	126.23
16	J	103	BCR	C2-C1-C6	3.63	115.70	110.44
13	B	816	CLA	O2D-CGD-CBD	3.62	117.55	111.23
16	A	854	BCR	C29-C30-C25	3.61	115.69	110.44
16	A	853	BCR	C38-C26-C27	-3.61	105.90	113.60
16	A	851	BCR	C24-C23-C22	3.61	131.58	126.23
13	X	1701	CLA	O2D-CGD-CBD	3.61	117.54	111.23
16	B	848	BCR	C29-C30-C25	3.61	115.68	110.44
13	B	812	CLA	O2D-CGD-CBD	3.60	117.52	111.23
16	B	845	BCR	C2-C1-C6	3.60	115.67	110.44
13	B	816	CLA	O2A-CGA-CBA	3.60	122.81	111.83
13	A	833	CLA	O2D-CGD-CBD	3.60	117.52	111.23
13	A	833	CLA	C1-C2-C3	3.59	132.07	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	J	103	BCR	C23-C24-C25	3.59	136.57	127.00
16	A	849	BCR	C29-C30-C25	3.58	115.64	110.44
16	A	850	BCR	C2-C1-C6	3.58	115.63	110.44
13	L	1003	CLA	O2D-CGD-CBD	3.56	117.46	111.23
16	M	1602	BCR	C2-C1-C6	3.55	115.60	110.44
16	B	843	BCR	C23-C24-C25	3.55	136.49	127.00
16	B	848	BCR	C2-C1-C6	3.55	115.59	110.44
13	A	834	CLA	O2D-CGD-CBD	3.55	117.44	111.23
13	A	828	CLA	O2A-CGA-CBA	3.54	122.64	111.83
13	A	815	CLA	O2D-CGD-CBD	3.54	117.41	111.23
13	B	838	CLA	O2D-CGD-CBD	3.53	117.41	111.23
13	A	801	CLA	C4D-CHA-C1A	-3.52	117.04	121.24
16	B	849	BCR	C2-C1-C6	3.52	115.56	110.44
13	A	827	CLA	O2D-CGD-CBD	3.52	117.39	111.23
16	B	847	BCR	C2-C1-C6	3.52	115.55	110.44
16	B	843	BCR	C38-C26-C27	-3.51	106.12	113.60
13	B	827	CLA	O2D-CGD-CBD	3.51	117.36	111.23
16	J	105	BCR	C29-C30-C25	3.50	115.53	110.44
13	A	842	CLA	O2D-CGD-CBD	3.50	117.35	111.23
13	B	841	CLA	O2D-CGD-CBD	3.50	117.35	111.23
13	A	812	CLA	O2A-CGA-CBA	3.50	122.49	111.83
13	B	818	CLA	O2D-CGD-CBD	3.49	117.32	111.23
13	A	838	CLA	O2D-CGD-CBD	3.48	117.32	111.23
13	B	823	CLA	O2D-CGD-CBD	3.48	117.31	111.23
16	A	853	BCR	C24-C23-C22	3.48	131.38	126.23
16	L	1006	BCR	C2-C1-C6	3.46	115.47	110.44
13	A	836	CLA	C1-C2-C3	3.46	131.87	126.20
16	B	846	BCR	C20-C21-C22	3.46	132.13	127.28
13	A	805	CLA	O2A-CGA-CBA	3.46	122.37	111.83
16	F	1302	BCR	C2-C1-C6	3.45	115.46	110.44
16	F	1302	BCR	C15-C14-C13	3.45	132.12	127.28
13	L	1002	CLA	O2A-CGA-CBA	3.44	122.33	111.83
13	A	802	CLA	O2D-CGD-CBD	3.44	117.24	111.23
16	A	853	BCR	C29-C30-C25	3.43	115.43	110.44
13	A	838	CLA	C1-C2-C3	3.43	131.82	126.20
13	B	838	CLA	O2A-CGA-CBA	3.43	122.29	111.83
13	A	846	CLA	C3B-C4B-NB	-3.42	107.48	110.53
16	M	1602	BCR	C29-C30-C25	3.42	115.40	110.44
13	B	837	CLA	C1-C2-C3	3.42	131.79	126.20
13	A	837	CLA	O2D-CGD-CBD	3.40	117.18	111.23
16	B	843	BCR	C29-C30-C25	3.39	115.37	110.44
13	A	832	CLA	C3B-C4B-NB	-3.39	107.50	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	852	BCR	C29-C30-C25	3.39	115.36	110.44
16	B	843	BCR	C30-C25-C26	-3.39	118.00	122.64
13	A	832	CLA	O2A-CGA-CBA	3.37	122.12	111.83
13	B	822	CLA	C1-C2-C3	3.37	131.72	126.20
13	B	840	CLA	C1-C2-C3	3.37	131.72	126.20
13	A	804	CLA	O2A-CGA-CBA	3.37	122.11	111.83
13	B	805	CLA	C1-C2-C3	3.37	131.72	126.20
13	A	801	CLA	O2A-CGA-CBA	3.37	122.10	111.83
16	F	1302	BCR	C29-C30-C25	3.36	115.32	110.44
13	A	817	CLA	O2A-CGA-CBA	3.36	122.09	111.83
13	A	829	CLA	O2A-CGA-CBA	3.36	122.08	111.83
13	A	808	CLA	O2D-CGD-CBD	3.36	117.10	111.23
13	A	836	CLA	O2D-CGD-CBD	3.35	117.08	111.23
13	A	813	CLA	O2D-CGD-CBD	3.34	117.07	111.23
13	B	831	CLA	C3B-C4B-NB	-3.34	107.55	110.53
13	A	833	CLA	O2A-CGA-CBA	3.34	122.02	111.83
16	J	104	BCR	C38-C26-C25	3.34	128.13	124.48
13	B	810	CLA	O2A-CGA-CBA	3.34	122.01	111.83
13	B	807	CLA	O2A-CGA-CBA	3.33	122.00	111.83
16	A	852	BCR	C2-C1-C6	3.33	115.28	110.44
17	A	855	LHG	O8-C23-C24	3.32	121.97	111.83
13	B	827	CLA	C3B-C4B-NB	-3.32	107.56	110.53
13	A	841	CLA	O2A-CGA-CBA	3.32	121.96	111.83
13	A	818	CLA	O2D-CGD-CBD	3.32	117.03	111.23
13	A	836	CLA	O2A-CGA-CBA	3.31	121.93	111.83
16	B	843	BCR	C24-C23-C22	3.30	131.12	126.23
16	B	844	BCR	C38-C26-C27	-3.30	106.57	113.60
13	A	839	CLA	O2A-CGA-CBA	3.29	121.86	111.83
13	B	836	CLA	O2D-CGD-CBD	3.29	116.97	111.23
13	B	826	CLA	O2A-CGA-CBA	3.28	121.85	111.83
16	A	849	BCR	C30-C25-C26	-3.28	118.15	122.64
13	A	844	CLA	O2A-CGA-O1A	-3.27	115.44	123.63
13	A	801	CLA	C4D-C3D-CAD	-3.27	104.55	108.11
16	B	848	BCR	C33-C5-C4	-3.27	106.62	113.60
13	B	832	CLA	C3B-C4B-NB	-3.27	107.61	110.53
13	B	835	CLA	C3B-C4B-NB	-3.27	107.61	110.53
16	A	851	BCR	C2-C1-C6	3.27	115.19	110.44
13	B	805	CLA	O2A-CGA-CBA	3.27	121.80	111.83
13	A	806	CLA	O2A-CGA-CBA	3.27	121.79	111.83
13	A	814	CLA	O2A-CGA-CBA	3.26	121.78	111.83
13	A	802	CLA	C1-C2-C3	3.26	131.53	126.20
13	B	832	CLA	O2A-CGA-CBA	3.25	121.76	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	813	CLA	O2A-CGA-CBA	3.25	121.73	111.83
13	B	802	CLA	O2A-CGA-CBA	3.24	121.72	111.83
13	B	808	CLA	O1D-CGD-CBD	-3.24	118.12	124.52
13	B	803	CLA	C3B-C4B-NB	-3.24	107.64	110.53
16	A	851	BCR	C38-C26-C27	-3.23	106.70	113.60
16	A	849	BCR	C2-C1-C6	3.23	115.13	110.44
13	A	810	CLA	O2D-CGD-CBD	3.22	116.87	111.23
13	B	809	CLA	O2D-CGD-CBD	3.22	116.86	111.23
16	J	104	BCR	C7-C8-C9	3.22	130.99	126.23
16	B	844	BCR	C2-C1-C6	3.21	115.11	110.44
16	B	846	BCR	C29-C30-C25	3.21	115.10	110.44
13	B	830	CLA	C3B-C4B-NB	-3.20	107.67	110.53
16	J	103	BCR	C38-C26-C27	-3.20	106.77	113.60
13	B	838	CLA	C3B-C4B-NB	-3.20	107.67	110.53
13	F	1301	CLA	O2D-CGD-CBD	3.20	116.82	111.23
13	B	833	CLA	C1-C2-C3	3.20	131.43	126.20
13	B	839	CLA	O2A-CGA-CBA	3.19	121.55	111.83
16	A	849	BCR	C38-C26-C27	-3.19	106.80	113.60
13	B	803	CLA	O2A-CGA-CBA	3.18	121.54	111.83
13	B	840	CLA	CED-O2D-CGD	3.18	123.14	115.92
13	B	802	CLA	C3B-C4B-NB	-3.18	107.69	110.53
18	B	850	LMG	O8-C28-C29	3.18	121.52	111.83
16	J	103	BCR	C30-C25-C26	-3.17	118.30	122.64
16	B	845	BCR	C38-C26-C27	-3.17	106.84	113.60
16	L	1005	BCR	C2-C1-C6	3.16	115.03	110.44
13	A	824	CLA	C1-C2-C3	3.16	131.38	126.20
13	A	826	CLA	O2A-CGA-CBA	3.16	121.47	111.83
16	J	105	BCR	C1-C6-C5	-3.16	118.32	122.64
13	A	806	CLA	CAA-C2A-C3A	-3.16	104.47	113.00
13	B	810	CLA	O2D-CGD-CBD	3.16	116.75	111.23
16	A	853	BCR	C30-C25-C26	-3.16	118.32	122.64
13	B	829	CLA	O2A-CGA-CBA	3.15	121.44	111.83
13	B	801	CLA	O2A-CGA-CBA	3.15	121.44	111.83
13	A	822	CLA	CED-O2D-CGD	3.15	123.06	115.92
13	A	825	CLA	O2D-CGD-CBD	3.14	116.73	111.23
16	B	844	BCR	C23-C24-C25	3.14	135.38	127.00
13	B	819	CLA	O2D-CGD-CBD	3.14	116.71	111.23
13	B	801	CLA	C7-C6-C5	-3.14	104.91	113.26
13	J	102	CLA	CAA-C2A-C3A	-3.13	109.04	116.23
13	B	824	CLA	C3B-C4B-NB	-3.13	107.73	110.53
13	A	803	CLA	O2A-CGA-O1A	-3.13	115.79	123.63
16	B	843	BCR	C7-C8-C9	3.13	130.87	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	I	102	BCR	C33-C5-C4	-3.13	106.93	113.60
16	B	849	BCR	C29-C30-C25	3.12	114.98	110.44
13	B	824	CLA	O2A-CGA-CBA	3.12	121.36	111.83
13	A	841	CLA	CED-O2D-CGD	3.12	122.99	115.92
16	L	1005	BCR	C24-C23-C22	3.11	130.84	126.23
13	A	821	CLA	C1-C2-C3	3.11	131.30	126.20
16	A	850	BCR	C29-C30-C25	3.11	114.96	110.44
16	A	849	BCR	C23-C24-C25	3.11	135.30	127.00
13	B	841	CLA	O2A-CGA-CBA	3.11	121.31	111.83
16	A	850	BCR	C38-C26-C27	-3.11	106.97	113.60
13	B	822	CLA	O2A-CGA-CBA	3.10	121.29	111.83
16	J	103	BCR	C8-C7-C6	3.10	135.28	127.00
16	I	102	BCR	C38-C26-C27	-3.10	106.98	113.60
16	B	849	BCR	C7-C8-C9	3.10	130.82	126.23
13	A	803	CLA	CED-O2D-CGD	3.10	122.94	115.92
13	B	822	CLA	O2D-CGD-CBD	3.09	116.64	111.23
13	B	819	CLA	O2A-CGA-CBA	3.09	121.25	111.83
16	B	844	BCR	C1-C6-C5	-3.09	118.42	122.64
17	A	856	LHG	O8-C23-C24	3.09	120.52	111.15
16	L	1005	BCR	C30-C25-C24	3.08	124.01	115.65
13	A	819	CLA	O2D-CGD-CBD	3.08	116.61	111.23
16	A	851	BCR	C40-C30-C25	3.08	115.07	110.24
16	B	843	BCR	C1-C6-C5	-3.08	118.43	122.64
13	B	831	CLA	O2A-CGA-CBA	3.08	121.21	111.83
13	B	809	CLA	O2A-CGA-CBA	3.07	121.19	111.83
13	B	833	CLA	O2A-CGA-CBA	3.07	121.19	111.83
13	A	825	CLA	O2A-CGA-CBA	3.06	121.17	111.83
13	A	811	CLA	O2D-CGD-CBD	3.06	116.58	111.23
13	A	838	CLA	O2A-CGA-O1A	-3.05	116.00	123.63
13	A	817	CLA	CED-O2D-CGD	3.05	122.83	115.92
16	L	1005	BCR	C33-C5-C4	-3.04	107.10	113.60
13	B	839	CLA	O2D-CGD-CBD	3.04	116.55	111.23
16	M	1602	BCR	C1-C6-C7	3.04	123.90	115.65
16	A	853	BCR	C2-C1-C6	3.04	114.86	110.44
13	L	1003	CLA	O2A-CGA-CBA	3.03	121.09	111.83
13	L	1004	CLA	O2A-CGA-CBA	3.03	121.09	111.83
16	B	846	BCR	C24-C23-C22	3.03	130.71	126.23
16	B	847	BCR	C24-C23-C22	3.02	130.70	126.23
13	A	818	CLA	O2A-CGA-CBA	3.02	121.03	111.83
13	M	1601	CLA	O2A-CGA-CBA	3.01	123.52	114.00
16	J	104	BCR	C30-C25-C24	3.01	123.82	115.65
16	B	847	BCR	C33-C5-C4	-3.01	107.18	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	808	CLA	CAA-C2A-C3A	-3.01	104.87	113.00
16	B	845	BCR	C24-C23-C22	3.01	130.68	126.23
13	J	101	CLA	C3B-C4B-NB	-3.00	107.85	110.53
16	A	852	BCR	C30-C25-C26	-3.00	118.53	122.64
16	M	1602	BCR	C1-C6-C5	-3.00	118.53	122.64
13	M	1601	CLA	CED-O2D-CGD	3.00	122.72	115.92
16	B	846	BCR	C38-C26-C27	-3.00	107.20	113.60
13	B	838	CLA	CED-O2D-CGD	3.00	122.71	115.92
13	A	835	CLA	C3B-C4B-NB	-3.00	107.86	110.53
13	B	829	CLA	C1-C2-C3	2.99	131.10	126.20
16	B	845	BCR	C33-C5-C4	-2.99	107.22	113.60
13	A	823	CLA	C3B-C4B-NB	-2.99	107.86	110.53
16	J	105	BCR	C38-C26-C27	-2.99	107.22	113.60
13	A	807	CLA	CED-O2D-CGD	2.99	122.69	115.92
13	A	838	CLA	C4-C3-C5	-2.98	112.62	116.13
13	A	822	CLA	C1-C2-C3	2.98	131.08	126.20
17	B	851	LHG	O7-C7-C8	2.98	117.93	111.48
16	A	854	BCR	C16-C17-C18	2.98	131.46	127.28
13	A	827	CLA	O2A-CGA-CBA	2.98	120.92	111.83
16	L	1006	BCR	C8-C7-C6	2.98	134.96	127.00
13	B	814	CLA	O2A-CGA-CBA	2.98	120.92	111.83
16	A	852	BCR	C30-C25-C24	2.98	123.72	115.65
16	B	848	BCR	C8-C9-C10	-2.98	114.33	119.01
16	L	1006	BCR	C29-C30-C25	2.97	114.76	110.44
16	I	101	BCR	C38-C26-C27	-2.97	107.26	113.60
16	B	845	BCR	C1-C6-C5	-2.97	118.58	122.64
16	J	105	BCR	C33-C5-C4	-2.97	107.27	113.60
16	A	849	BCR	C8-C7-C6	2.97	134.92	127.00
16	A	853	BCR	C23-C24-C25	2.97	134.92	127.00
13	B	803	CLA	CED-O2D-CGD	2.96	122.63	115.92
13	A	813	CLA	C1-C2-C3	2.96	131.04	126.20
17	A	855	LHG	O7-C7-C8	2.96	117.87	111.48
13	A	820	CLA	O2D-CGD-CBD	2.95	116.39	111.23
13	A	834	CLA	O2A-CGA-CBA	2.95	120.84	111.83
13	A	840	CLA	O2A-CGA-O1A	-2.95	116.25	123.63
16	I	101	BCR	C7-C8-C9	2.95	130.60	126.23
13	A	843	CLA	O2D-CGD-CBD	2.95	116.38	111.23
13	B	811	CLA	O2D-CGD-CBD	2.94	116.37	111.23
13	B	813	CLA	C1-C2-C3	2.94	131.01	126.20
16	B	843	BCR	C33-C5-C4	-2.93	107.34	113.60
13	B	817	CLA	O2D-CGD-CBD	2.93	116.36	111.23
13	A	807	CLA	C2A-C3A-C4A	2.93	106.60	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	806	CLA	O2D-CGD-CBD	2.93	116.35	111.23
16	I	102	BCR	C32-C1-C6	2.93	114.84	110.24
13	B	820	CLA	CED-O2D-CGD	2.93	122.56	115.92
16	F	1302	BCR	C24-C23-C22	2.93	130.56	126.23
16	A	851	BCR	C7-C8-C9	2.92	130.56	126.23
13	B	811	CLA	CED-O2D-CGD	2.92	122.54	115.92
16	A	849	BCR	C24-C23-C22	2.92	130.56	126.23
16	J	103	BCR	C36-C18-C19	2.92	122.54	118.09
16	L	1005	BCR	C8-C7-C6	2.91	134.78	127.00
16	A	849	BCR	C1-C6-C5	-2.91	118.65	122.64
16	B	848	BCR	C38-C26-C27	-2.91	107.39	113.60
16	B	844	BCR	C1-C6-C7	2.91	123.54	115.65
16	B	848	BCR	C15-C14-C13	2.91	131.36	127.28
13	B	810	CLA	C4D-CHA-C1A	2.91	124.71	121.24
13	B	816	CLA	C1-C2-C3	2.91	130.96	126.20
13	A	821	CLA	C3B-C4B-NB	-2.90	107.94	110.53
16	B	846	BCR	C40-C30-C25	2.90	114.78	110.24
16	L	1006	BCR	C33-C5-C4	-2.89	107.42	113.60
16	A	852	BCR	C38-C26-C27	-2.89	107.42	113.60
16	B	847	BCR	C29-C30-C25	2.89	114.64	110.44
16	F	1302	BCR	C33-C5-C4	-2.89	107.43	113.60
13	B	812	CLA	O2A-CGA-CBA	2.89	123.14	114.00
13	B	824	CLA	CED-O2D-CGD	2.88	122.46	115.92
16	A	854	BCR	C32-C1-C6	2.88	114.76	110.24
16	I	101	BCR	C23-C24-C25	2.88	134.69	127.00
13	J	102	CLA	C2A-C3A-C4A	2.88	104.97	101.59
16	A	851	BCR	C33-C5-C4	-2.88	107.46	113.60
16	A	854	BCR	C30-C25-C24	2.87	123.44	115.65
16	A	850	BCR	C30-C25-C26	-2.87	118.71	122.64
13	B	815	CLA	C3B-C4B-NB	-2.87	107.97	110.53
16	B	845	BCR	C30-C25-C26	-2.87	118.71	122.64
16	A	849	BCR	C33-C5-C4	-2.87	107.48	113.60
13	B	821	CLA	C3B-C4B-NB	-2.87	107.97	110.53
16	F	1302	BCR	C38-C26-C27	-2.87	107.48	113.60
13	A	829	CLA	O2D-CGD-CBD	2.86	116.24	111.23
13	B	833	CLA	CED-O2D-CGD	2.86	122.41	115.92
17	A	856	LHG	O7-C7-C8	2.86	117.67	111.48
13	A	807	CLA	C1-C2-C3	2.86	130.88	126.20
16	L	1005	BCR	C38-C26-C27	-2.86	107.50	113.60
13	B	822	CLA	CED-O2D-CGD	2.86	122.40	115.92
17	A	856	LHG	C6-C5-C4	-2.86	105.13	111.78
13	A	835	CLA	O2A-CGA-CBA	2.85	120.53	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	813	CLA	O1D-CGD-CBD	-2.85	118.89	124.52
16	I	101	BCR	C29-C30-C25	2.85	114.58	110.44
13	J	101	CLA	CED-O2D-CGD	2.85	122.38	115.92
13	B	819	CLA	C3B-C4B-NB	-2.85	107.99	110.53
16	L	1005	BCR	C30-C25-C26	-2.85	118.74	122.64
13	A	807	CLA	CBA-CAA-C2A	2.85	122.27	113.79
13	B	808	CLA	O2A-CGA-O1A	-2.85	116.51	123.63
16	I	102	BCR	C7-C8-C9	2.85	130.44	126.23
13	A	822	CLA	CAA-C2A-C3A	-2.85	105.31	113.00
13	A	826	CLA	C3B-C4B-NB	-2.85	107.99	110.53
16	B	848	BCR	C12-C13-C14	-2.84	114.53	119.01
13	A	828	CLA	C1-C2-C3	2.84	130.86	126.20
13	B	834	CLA	CED-O2D-CGD	2.84	122.36	115.92
16	J	105	BCR	C30-C25-C26	-2.84	118.75	122.64
13	A	820	CLA	CED-O2D-CGD	2.83	122.34	115.92
16	B	844	BCR	C33-C5-C4	-2.83	107.56	113.60
16	J	104	BCR	C23-C24-C25	2.83	134.56	127.00
13	B	811	CLA	CAA-C2A-C3A	-2.83	105.35	113.00
13	B	828	CLA	O2D-CGD-CBD	2.83	116.18	111.23
16	I	102	BCR	C30-C25-C26	-2.83	118.77	122.64
13	B	835	CLA	CED-O2D-CGD	2.83	122.33	115.92
16	A	851	BCR	C1-C6-C5	-2.82	118.78	122.64
13	A	810	CLA	C3B-C4B-NB	-2.82	108.02	110.53
13	A	844	CLA	O2D-CGD-CBD	2.82	116.15	111.23
16	I	101	BCR	C36-C18-C19	2.81	122.39	118.09
13	B	801	CLA	CED-O2D-CGD	2.81	122.30	115.92
13	B	806	CLA	O2A-CGA-CBA	2.81	120.42	111.83
13	B	821	CLA	CED-O2D-CGD	2.81	122.29	115.92
13	A	811	CLA	O2A-CGA-CBA	2.81	122.87	114.00
16	A	854	BCR	C33-C5-C4	-2.81	107.61	113.60
13	B	837	CLA	O2A-CGA-CBA	2.80	120.38	111.83
13	A	805	CLA	O1D-CGD-CBD	-2.80	118.99	124.52
13	A	819	CLA	C3B-C4B-NB	-2.80	108.03	110.53
16	L	1006	BCR	C30-C25-C26	-2.80	118.81	122.64
13	A	806	CLA	CED-O2D-CGD	2.80	122.26	115.92
13	A	841	CLA	C3B-C4B-NB	-2.79	108.04	110.53
16	J	103	BCR	C1-C6-C7	2.79	123.22	115.65
16	B	848	BCR	C32-C1-C6	2.79	114.61	110.24
16	L	1005	BCR	C40-C30-C25	2.79	114.61	110.24
16	B	844	BCR	C20-C21-C22	2.78	131.18	127.28
13	A	846	CLA	O1D-CGD-CBD	-2.78	119.03	124.52
13	A	844	CLA	CAA-C2A-C3A	-2.78	105.49	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	843	CLA	C3B-C4B-NB	-2.77	108.06	110.53
16	M	1602	BCR	C38-C26-C27	-2.77	107.69	113.60
13	A	815	CLA	CED-O2D-CGD	2.77	122.20	115.92
16	B	848	BCR	C30-C25-C26	-2.77	118.85	122.64
16	B	847	BCR	C38-C26-C27	-2.77	107.70	113.60
13	A	843	CLA	CED-O2D-CGD	2.77	122.19	115.92
13	B	836	CLA	O2A-CGA-CBA	2.77	122.74	114.00
13	B	814	CLA	O1D-CGD-CBD	-2.76	119.07	124.52
13	A	833	CLA	CED-O2D-CGD	2.76	122.18	115.92
16	F	1302	BCR	C1-C6-C5	-2.76	118.86	122.64
16	L	1005	BCR	C29-C30-C25	2.76	114.45	110.44
13	B	833	CLA	O1D-CGD-CBD	-2.76	119.07	124.52
13	B	824	CLA	C1-C2-C3	2.76	130.72	126.20
13	A	812	CLA	CED-O2D-CGD	2.76	122.17	115.92
13	M	1601	CLA	C3B-C4B-NB	-2.76	108.07	110.53
13	B	828	CLA	C4-C3-C5	-2.75	110.45	115.23
13	A	831	CLA	O2A-CGA-CBA	2.75	120.23	111.83
13	A	814	CLA	O1D-CGD-CBD	-2.75	119.09	124.52
13	A	819	CLA	CED-O2D-CGD	2.75	122.15	115.92
13	F	1301	CLA	O2A-CGA-CBA	2.75	122.69	114.00
16	B	847	BCR	C30-C25-C26	-2.75	118.88	122.64
13	A	809	CLA	O1D-CGD-CBD	-2.74	119.11	124.52
16	M	1602	BCR	C8-C7-C6	2.74	134.32	127.00
13	A	826	CLA	O1D-CGD-CBD	-2.74	119.11	124.52
13	B	801	CLA	C1-C2-C3	2.74	130.69	126.20
13	A	836	CLA	CED-O2D-CGD	2.74	122.13	115.92
13	X	1701	CLA	O2A-CGA-CBA	2.74	122.66	114.00
16	A	850	BCR	C33-C5-C4	-2.74	107.75	113.60
16	B	847	BCR	C30-C25-C24	2.74	123.08	115.65
16	I	102	BCR	C37-C22-C23	2.74	122.27	118.09
13	A	832	CLA	O1D-CGD-CBD	-2.74	119.12	124.52
13	A	815	CLA	O2A-CGA-CBA	2.73	122.64	114.00
13	A	836	CLA	C3B-C4B-NB	-2.73	108.09	110.53
13	B	830	CLA	O1D-CGD-CBD	-2.73	119.13	124.52
13	B	840	CLA	O2D-CGD-CBD	2.73	116.00	111.23
13	X	1701	CLA	C3B-C4B-NB	-2.73	108.09	110.53
13	B	806	CLA	C1-C2-C3	2.72	130.66	126.20
13	A	807	CLA	O2A-CGA-O1A	-2.72	116.82	123.63
13	A	812	CLA	O2D-CGD-CBD	2.72	115.98	111.23
13	A	811	CLA	CED-O2D-CGD	2.72	122.08	115.92
16	B	845	BCR	C23-C24-C25	2.72	134.25	127.00
13	A	813	CLA	C3B-C4B-NB	-2.71	108.11	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	849	BCR	C38-C26-C27	-2.71	107.81	113.60
13	B	810	CLA	C2A-C1A-CHA	2.71	128.57	123.87
16	B	847	BCR	C36-C18-C19	2.71	122.23	118.09
13	A	832	CLA	CAA-C2A-C3A	-2.71	105.67	113.00
16	B	848	BCR	C23-C24-C25	2.71	134.24	127.00
13	B	817	CLA	CED-O2D-CGD	2.71	122.05	115.92
13	A	837	CLA	C3B-C4B-NB	-2.70	108.12	110.53
16	A	854	BCR	C38-C26-C27	-2.70	107.83	113.60
16	F	1302	BCR	C30-C25-C26	-2.70	118.94	122.64
16	A	853	BCR	C11-C10-C9	2.70	131.06	127.28
16	A	851	BCR	C30-C25-C26	-2.70	118.95	122.64
13	B	807	CLA	C3B-C4B-NB	-2.70	108.12	110.53
13	L	1003	CLA	CAA-C2A-C3A	-2.69	105.72	113.00
13	B	809	CLA	CED-O2D-CGD	2.69	122.03	115.92
13	A	804	CLA	C3B-C4B-NB	-2.69	108.12	110.53
13	A	810	CLA	C2A-C1A-CHA	2.69	128.54	123.87
16	J	103	BCR	C1-C6-C5	-2.69	118.96	122.64
13	A	801	CLA	OBD-CAD-C3D	2.69	134.70	128.42
13	B	838	CLA	C1-C2-C3	2.69	130.60	126.20
13	A	831	CLA	CAA-C2A-C3A	-2.68	105.75	113.00
13	B	820	CLA	C3B-C4B-NB	-2.68	108.13	110.53
16	A	854	BCR	C30-C25-C26	-2.68	118.97	122.64
13	A	835	CLA	CAA-C2A-C3A	-2.68	105.75	113.00
16	M	1602	BCR	C30-C25-C26	-2.68	118.97	122.64
13	A	816	CLA	O2A-CGA-CBA	2.68	122.46	114.00
13	B	840	CLA	O2A-CGA-CBA	2.67	119.98	111.83
16	B	848	BCR	C34-C9-C8	2.67	122.17	118.09
16	J	104	BCR	C30-C25-C26	-2.67	118.99	122.64
13	A	827	CLA	C1-C2-C3	2.67	130.57	126.20
13	A	837	CLA	CED-O2D-CGD	2.67	121.96	115.92
13	B	813	CLA	CED-O2D-CGD	2.67	121.96	115.92
13	A	802	CLA	C4D-CHA-C1A	2.67	124.42	121.24
16	L	1006	BCR	C1-C6-C5	-2.66	119.00	122.64
13	A	822	CLA	CAA-CBA-CGA	2.66	120.76	113.21
13	B	819	CLA	CED-O2D-CGD	2.66	121.95	115.92
13	F	1301	CLA	C3B-C4B-NB	-2.66	108.16	110.53
13	B	815	CLA	O1D-CGD-CBD	-2.66	119.28	124.52
13	B	802	CLA	C4D-CHA-C1A	2.66	124.41	121.24
16	J	104	BCR	C33-C5-C4	-2.66	107.93	113.60
13	B	819	CLA	CAA-C2A-C3A	-2.66	105.82	113.00
13	B	823	CLA	O2A-CGA-CBA	2.66	122.39	114.00
13	A	818	CLA	CED-O2D-CGD	2.65	121.94	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	846	BCR	C35-C13-C12	2.65	120.69	114.59
13	A	809	CLA	C3B-C4B-NB	-2.65	108.16	110.53
13	A	846	CLA	CED-O2D-CGD	2.65	121.93	115.92
16	A	854	BCR	C1-C6-C7	2.65	122.83	115.65
16	B	847	BCR	C16-C17-C18	2.64	130.99	127.28
16	J	104	BCR	C1-C6-C5	-2.64	119.03	122.64
13	B	821	CLA	O1D-CGD-CBD	-2.64	119.31	124.52
13	A	822	CLA	C3B-C4B-NB	-2.64	108.17	110.53
13	B	828	CLA	CED-O2D-CGD	2.64	121.90	115.92
16	B	849	BCR	C33-C5-C4	-2.63	107.98	113.60
13	A	828	CLA	C3B-C4B-NB	-2.63	108.18	110.53
13	B	836	CLA	C3B-C4B-NB	-2.63	108.18	110.53
16	B	845	BCR	C35-C13-C12	2.63	122.10	118.09
16	B	847	BCR	C32-C1-C6	2.63	114.36	110.24
16	A	852	BCR	C33-C5-C4	-2.62	108.00	113.60
13	A	817	CLA	C3B-C4B-NB	-2.62	108.19	110.53
13	A	828	CLA	O1D-CGD-CBD	-2.62	119.34	124.52
13	B	826	CLA	C1-C2-C3	2.62	130.49	126.20
13	B	819	CLA	C1-C2-C3	2.62	130.49	126.20
13	A	803	CLA	C1-O2A-CGA	2.62	123.00	116.65
13	A	814	CLA	CED-O2D-CGD	2.62	121.86	115.92
13	L	1002	CLA	O1D-CGD-CBD	-2.62	119.35	124.52
16	A	853	BCR	C1-C6-C7	2.62	122.75	115.65
16	B	844	BCR	C32-C1-C6	2.62	114.35	110.24
13	J	102	CLA	C3B-C4B-NB	-2.61	108.20	110.53
13	B	821	CLA	O2A-CGA-CBA	2.61	122.23	114.00
13	A	832	CLA	CED-O2D-CGD	2.60	121.82	115.92
16	B	849	BCR	C8-C9-C10	-2.60	114.92	119.01
13	A	808	CLA	CED-O2D-CGD	2.60	121.81	115.92
16	J	103	BCR	C33-C5-C4	-2.60	108.05	113.60
16	A	850	BCR	C1-C6-C5	-2.60	119.08	122.64
13	J	101	CLA	O2A-CGA-CBA	2.60	122.21	114.00
13	B	810	CLA	CED-O2D-CGD	2.59	121.80	115.92
16	A	850	BCR	C30-C25-C24	2.59	122.69	115.65
16	A	854	BCR	C15-C14-C13	2.59	130.91	127.28
16	B	849	BCR	C34-C9-C8	2.59	122.05	118.09
13	A	836	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
13	A	822	CLA	O2D-CGD-CBD	2.59	115.76	111.23
13	B	827	CLA	C1-C2-C3	2.59	130.44	126.20
13	B	815	CLA	O2A-CGA-CBA	2.59	122.18	114.00
13	A	801	CLA	C1-C2-C3	2.59	130.44	126.20
13	A	802	CLA	O2A-CGA-CBA	2.59	119.72	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	814	CLA	C1-C2-C3	2.58	130.43	126.20
16	A	851	BCR	C1-C6-C7	2.58	122.65	115.65
13	B	829	CLA	O1D-CGD-CBD	-2.58	119.43	124.52
16	I	101	BCR	C1-C6-C5	-2.58	119.11	122.64
13	B	812	CLA	CED-O2D-CGD	2.58	121.76	115.92
13	B	812	CLA	C3B-C4B-NB	-2.58	108.23	110.53
13	A	843	CLA	C1-O2A-CGA	2.58	122.89	116.65
16	A	851	BCR	C30-C25-C24	2.58	122.64	115.65
13	A	814	CLA	C4D-CHA-C1A	2.57	124.31	121.24
16	I	101	BCR	C33-C5-C4	-2.57	108.11	113.60
13	A	835	CLA	O1D-CGD-CBD	-2.57	119.44	124.52
13	A	842	CLA	C1-C2-C3	2.57	130.41	126.20
13	A	820	CLA	C4D-CHA-C1A	2.57	124.31	121.24
13	B	830	CLA	O2A-CGA-CBA	2.57	122.12	114.00
13	A	841	CLA	O2D-CGD-CBD	2.57	115.72	111.23
13	A	845	CLA	O2A-CGA-CBA	2.57	122.12	114.00
16	B	846	BCR	C30-C25-C26	-2.57	119.13	122.64
13	B	811	CLA	O2A-CGA-CBA	2.57	122.11	114.00
13	B	835	CLA	O2D-CGD-CBD	2.57	115.72	111.23
13	A	808	CLA	C1-C2-C3	2.57	130.40	126.20
13	B	816	CLA	C3B-C4B-NB	-2.56	108.24	110.53
16	I	102	BCR	C30-C25-C24	2.56	122.59	115.65
13	A	831	CLA	C3B-C4B-NB	-2.56	108.25	110.53
16	J	104	BCR	C36-C18-C19	2.56	121.99	118.09
13	B	829	CLA	O2A-CGA-O1A	-2.55	117.24	123.63
13	A	822	CLA	O2A-CGA-CBA	2.55	119.62	111.83
13	B	804	CLA	O1D-CGD-CBD	-2.55	119.48	124.52
13	B	802	CLA	C2A-C1A-CHA	2.55	128.29	123.87
13	A	815	CLA	C3B-C4B-NB	-2.55	108.25	110.53
13	B	818	CLA	CED-O2D-CGD	2.55	121.70	115.92
13	A	837	CLA	O2A-CGA-CBA	2.55	122.05	114.00
13	B	837	CLA	C3B-C4B-NB	-2.55	108.26	110.53
16	A	854	BCR	C1-C6-C5	-2.55	119.16	122.64
16	I	102	BCR	C36-C18-C19	2.55	121.98	118.09
13	A	840	CLA	C3B-C4B-NB	-2.54	108.26	110.53
13	B	814	CLA	C3B-C4B-NB	-2.54	108.26	110.53
13	A	806	CLA	O1D-CGD-CBD	-2.54	119.51	124.52
13	B	831	CLA	CED-O2D-CGD	2.54	121.68	115.92
13	A	806	CLA	CHD-C1D-ND	-2.54	121.23	124.80
16	I	101	BCR	C30-C25-C26	-2.54	119.17	122.64
13	A	843	CLA	C1-C2-C3	2.54	130.35	126.20
13	B	832	CLA	C1-C2-C3	2.54	130.35	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	M	1602	BCR	C33-C5-C4	-2.54	108.19	113.60
13	A	829	CLA	CAA-C2A-C3A	-2.53	106.15	113.00
16	L	1006	BCR	C38-C26-C27	-2.53	108.20	113.60
13	A	840	CLA	CED-O2D-CGD	2.53	121.66	115.92
13	A	822	CLA	C12-C11-C10	-2.53	101.94	113.28
13	A	816	CLA	CED-O2D-CGD	2.53	121.65	115.92
13	B	834	CLA	C3B-C4B-NB	-2.53	108.27	110.53
13	B	817	CLA	C1-C2-C3	2.53	130.34	126.20
13	B	823	CLA	C3B-C4B-NB	-2.53	108.27	110.53
13	B	802	CLA	O2A-CGA-O1A	-2.53	117.31	123.63
13	A	816	CLA	O1D-CGD-CBD	-2.52	119.54	124.52
13	A	823	CLA	CED-O2D-CGD	2.52	121.64	115.92
13	A	822	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
13	B	811	CLA	C3B-C4B-NB	-2.52	108.28	110.53
13	A	807	CLA	C2A-C1A-CHA	2.51	128.23	123.87
13	B	825	CLA	O1D-CGD-CBD	-2.51	119.56	124.52
16	A	850	BCR	C23-C24-C25	2.51	133.71	127.00
13	A	820	CLA	O2A-CGA-O1A	-2.51	117.35	123.63
13	L	1002	CLA	C3B-C4B-NB	-2.51	108.29	110.53
16	B	848	BCR	C35-C13-C12	2.51	121.92	118.09
13	B	828	CLA	C5-C3-C2	2.51	126.80	121.17
13	B	810	CLA	C1-C2-C3	2.51	130.30	126.20
13	A	809	CLA	O2A-CGA-O1A	-2.50	117.37	123.63
16	A	850	BCR	C7-C8-C9	2.50	129.94	126.23
16	J	103	BCR	C35-C13-C12	2.50	121.91	118.09
13	B	816	CLA	CED-O2D-CGD	2.50	121.58	115.92
13	A	829	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
16	A	852	BCR	C1-C6-C7	2.50	122.42	115.65
13	B	820	CLA	O1D-CGD-CBD	-2.50	119.60	124.52
13	B	816	CLA	O2A-CGA-O1A	-2.49	117.39	123.63
13	B	805	CLA	CED-O2D-CGD	2.49	121.57	115.92
13	B	839	CLA	CED-O2D-CGD	2.49	121.57	115.92
16	J	104	BCR	C38-C26-C27	-2.49	108.28	113.60
16	B	847	BCR	C1-C6-C5	-2.49	119.23	122.64
16	A	852	BCR	C32-C1-C6	2.49	114.15	110.24
13	A	846	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
13	B	840	CLA	C4D-CHA-C1A	2.49	124.21	121.24
13	B	814	CLA	CED-O2D-CGD	2.49	121.56	115.92
16	A	852	BCR	C23-C24-C25	2.49	133.64	127.00
16	B	843	BCR	C8-C7-C6	2.49	133.64	127.00
13	A	803	CLA	C1-C2-C3	2.49	130.27	126.20
13	B	825	CLA	C2A-C3A-C4A	2.48	105.88	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	1005	BCR	C36-C18-C19	2.48	121.88	118.09
16	A	850	BCR	C24-C23-C22	2.48	129.90	126.23
18	B	850	LMG	C7-O1-C1	2.48	119.10	113.80
16	I	102	BCR	C29-C30-C25	2.47	114.03	110.44
13	F	1301	CLA	CED-O2D-CGD	2.47	121.52	115.92
13	A	835	CLA	CED-O2D-CGD	2.47	121.52	115.92
13	K	1401	CLA	CED-O2D-CGD	2.47	121.52	115.92
16	A	849	BCR	C1-C6-C7	2.47	122.34	115.65
13	A	811	CLA	C3B-C4B-NB	-2.47	108.33	110.53
13	B	837	CLA	O1D-CGD-CBD	-2.46	119.66	124.52
13	B	801	CLA	CAA-C2A-C3A	-2.46	106.34	113.00
13	A	829	CLA	CED-O2D-CGD	2.46	121.50	115.92
16	A	853	BCR	C37-C22-C23	2.46	121.84	118.09
13	A	821	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
13	B	809	CLA	C12-C11-C10	-2.46	102.27	113.28
13	B	821	CLA	C4D-CHA-C1A	2.46	124.17	121.24
16	J	105	BCR	C30-C25-C24	2.46	122.31	115.65
13	B	835	CLA	O2A-CGA-CBA	2.45	121.74	114.00
13	A	838	CLA	C4D-CHA-C1A	2.45	124.17	121.24
13	B	807	CLA	CED-O2D-CGD	2.44	121.45	115.92
13	B	828	CLA	C3B-C4B-NB	-2.44	108.35	110.53
13	L	1004	CLA	C3B-C4B-NB	-2.44	108.35	110.53
16	A	852	BCR	C1-C6-C5	-2.44	119.31	122.64
13	K	1401	CLA	O2A-CGA-CBA	2.43	121.69	114.00
13	B	818	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
13	B	836	CLA	CED-O2D-CGD	2.43	121.43	115.92
16	B	849	BCR	C23-C24-C25	2.43	133.49	127.00
16	A	853	BCR	C34-C9-C8	2.43	121.80	118.09
16	F	1302	BCR	C7-C8-C9	2.43	129.83	126.23
13	B	814	CLA	CMD-C2D-C1D	2.43	129.00	124.73
13	A	806	CLA	C1-C2-C3	2.43	130.18	126.20
13	A	833	CLA	CAA-C2A-C3A	-2.43	106.44	113.00
13	A	830	CLA	CED-O2D-CGD	2.43	121.42	115.92
13	B	804	CLA	CMD-C2D-C1D	2.42	129.00	124.73
13	A	826	CLA	CED-O2D-CGD	2.42	121.41	115.92
16	B	848	BCR	C36-C18-C19	2.42	121.79	118.09
13	B	817	CLA	C3B-C4B-NB	-2.42	108.37	110.53
13	B	808	CLA	C7-C6-C5	-2.42	106.82	113.26
16	I	102	BCR	C1-C6-C5	-2.42	119.33	122.64
16	A	850	BCR	C1-C6-C7	2.42	122.21	115.65
16	A	854	BCR	C23-C22-C21	-2.42	115.21	119.01
13	A	831	CLA	CED-O2D-CGD	2.42	121.40	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	852	BCR	C40-C30-C25	2.42	114.03	110.24
13	A	803	CLA	CHD-C1D-ND	-2.41	121.41	124.80
13	B	832	CLA	C12-C11-C10	-2.41	102.47	113.28
16	J	104	BCR	C40-C30-C25	2.41	114.03	110.24
13	B	818	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
13	L	1002	CLA	C4D-CHA-C1A	2.41	124.12	121.24
13	L	1003	CLA	C4D-CHA-C1A	2.40	124.11	121.24
13	A	820	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
13	A	812	CLA	C1-C2-C3	2.40	130.13	126.20
13	A	825	CLA	CAA-C2A-C3A	-2.40	106.51	113.00
16	J	103	BCR	C24-C23-C22	2.40	129.78	126.23
13	A	825	CLA	C3B-C4B-NB	-2.40	108.39	110.53
16	B	844	BCR	C35-C13-C12	2.39	121.74	118.09
13	A	844	CLA	CED-O2D-CGD	2.39	121.34	115.92
13	A	813	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
13	B	834	CLA	O2A-CGA-CBA	2.39	121.55	114.00
13	A	839	CLA	O2D-CGD-CBD	2.39	115.41	111.23
13	A	803	CLA	CAA-C2A-C3A	-2.39	106.55	113.00
13	B	806	CLA	CED-O2D-CGD	2.38	121.33	115.92
16	L	1005	BCR	C23-C24-C25	2.38	133.37	127.00
13	A	806	CLA	C2A-C3A-C4A	2.38	105.71	101.87
16	A	851	BCR	C8-C7-C6	2.38	133.35	127.00
13	A	823	CLA	O1D-CGD-CBD	-2.37	119.84	124.52
13	B	830	CLA	CED-O2D-CGD	2.37	121.30	115.92
13	A	840	CLA	CMD-C2D-C1D	2.37	128.90	124.73
13	A	832	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
16	L	1005	BCR	C1-C6-C5	-2.37	119.40	122.64
13	B	824	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
13	B	835	CLA	O2A-CGA-O1A	-2.37	117.25	123.33
13	B	828	CLA	CBA-CAA-C2A	2.36	120.83	113.79
16	L	1006	BCR	C30-C25-C24	2.36	122.06	115.65
16	I	102	BCR	C1-C6-C7	2.36	122.06	115.65
13	A	806	CLA	CMD-C2D-C1D	2.36	128.89	124.73
16	A	853	BCR	C8-C9-C10	-2.36	115.30	119.01
13	A	801	CLA	CAA-C2A-C3A	-2.36	106.63	113.00
13	A	801	CLA	C2A-C3A-C4A	2.36	105.68	101.87
13	A	828	CLA	C4D-CHA-C1A	2.36	124.06	121.24
13	B	825	CLA	O2A-CGA-CBA	2.35	121.03	112.14
13	A	844	CLA	CMA-C3A-C2A	-2.35	104.88	113.98
13	A	804	CLA	C1-C2-C3	2.35	130.05	126.20
13	B	825	CLA	CED-O2D-CGD	2.35	121.25	115.92
16	B	844	BCR	C34-C9-C8	2.35	121.68	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	825	CLA	CAA-C2A-C3A	-2.35	106.65	113.00
16	F	1302	BCR	C30-C25-C24	2.35	122.01	115.65
13	J	101	CLA	C2A-C1A-CHA	2.34	127.94	123.87
13	A	833	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
13	B	827	CLA	O1D-CGD-CBD	-2.34	119.89	124.52
16	B	845	BCR	C28-C27-C26	2.34	118.23	114.06
13	A	831	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
13	A	821	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
16	B	844	BCR	C36-C18-C19	2.34	121.67	118.09
13	B	814	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
16	B	849	BCR	C30-C25-C26	-2.34	119.44	122.64
16	A	849	BCR	C35-C13-C12	2.34	121.66	118.09
16	B	846	BCR	C30-C25-C24	2.34	122.00	115.65
13	L	1003	CLA	CHD-C1D-ND	-2.34	121.51	124.80
13	B	804	CLA	C1-C2-C3	2.34	130.03	126.20
13	B	837	CLA	CED-O2D-CGD	2.34	121.22	115.92
16	B	843	BCR	C1-C6-C7	2.34	121.99	115.65
13	A	839	CLA	CED-O2D-CGD	2.33	121.21	115.92
13	B	817	CLA	CAA-C2A-C3A	-2.33	106.70	113.00
13	B	830	CLA	CMD-C2D-C1D	2.33	128.83	124.73
13	B	803	CLA	C12-C11-C10	-2.33	102.84	113.28
16	A	849	BCR	C37-C22-C23	2.33	121.64	118.09
13	B	834	CLA	C2A-C3A-C4A	2.32	105.62	101.87
13	A	803	CLA	O2D-CGD-CBD	2.32	115.29	111.23
16	J	104	BCR	C1-C6-C7	2.32	121.95	115.65
13	B	824	CLA	C2A-C1A-CHA	2.32	127.90	123.87
13	A	815	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
13	A	821	CLA	CED-O2D-CGD	2.32	121.17	115.92
16	B	849	BCR	C24-C23-C22	2.32	129.66	126.23
13	A	807	CLA	CAA-CBA-CGA	2.31	119.78	113.21
16	B	845	BCR	C1-C6-C7	2.31	121.93	115.65
16	B	845	BCR	C30-C25-C24	2.31	121.92	115.65
13	F	1301	CLA	C2A-C1A-CHA	2.31	127.88	123.87
13	A	846	CLA	C2A-C1A-CHA	2.31	127.88	123.87
13	B	833	CLA	C4D-CHA-C1A	2.31	124.00	121.24
13	B	821	CLA	C2A-C1A-CHA	2.31	127.87	123.87
13	B	837	CLA	C4D-CHA-C1A	2.31	124.00	121.24
16	A	853	BCR	C1-C6-C5	-2.31	119.48	122.64
13	A	801	CLA	C2D-C1D-ND	2.31	112.41	110.13
13	J	102	CLA	CMA-C3A-C2A	-2.31	110.94	116.23
13	K	1401	CLA	C3B-C4B-NB	-2.30	108.47	110.53
13	A	808	CLA	C4-C3-C5	-2.30	113.42	116.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	824	CLA	C3B-C4B-NB	-2.30	108.47	110.53
13	A	815	CLA	O2A-CGA-O1A	-2.30	117.41	123.33
16	B	845	BCR	C34-C9-C8	2.30	121.60	118.09
13	A	801	CLA	CHA-C4D-ND	2.30	137.29	132.55
13	A	821	CLA	C4D-CHA-C1A	2.30	123.99	121.24
16	A	853	BCR	C8-C7-C6	2.30	133.13	127.00
13	A	824	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
13	B	820	CLA	C2A-C1A-CHA	2.29	127.85	123.87
16	I	101	BCR	C34-C9-C8	2.29	121.59	118.09
13	A	816	CLA	C4D-CHA-C1A	2.29	123.98	121.24
16	A	849	BCR	C32-C1-C6	2.29	113.84	110.24
13	A	844	CLA	C3B-C4B-NB	-2.29	108.48	110.53
13	B	811	CLA	O2A-CGA-O1A	-2.29	117.44	123.33
16	I	101	BCR	C1-C6-C7	2.29	121.86	115.65
13	B	801	CLA	C3B-C4B-NB	-2.29	108.49	110.53
13	B	826	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
13	A	842	CLA	CED-O2D-CGD	2.29	121.11	115.92
13	A	825	CLA	C4D-CHA-C1A	2.29	123.97	121.24
13	M	1601	CLA	O2A-CGA-O1A	-2.29	117.45	123.33
13	B	830	CLA	C4D-CHA-C1A	2.29	123.97	121.24
13	A	825	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
13	A	820	CLA	C1-C2-C3	2.29	129.94	126.20
16	A	853	BCR	C33-C5-C4	-2.29	108.72	113.60
13	B	837	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
13	A	841	CLA	C4D-CHA-C1A	2.29	123.97	121.24
16	B	847	BCR	C1-C6-C7	2.28	121.84	115.65
13	B	833	CLA	C3B-C4B-NB	-2.28	108.49	110.53
13	A	813	CLA	C4D-CHA-C1A	2.28	123.97	121.24
13	B	829	CLA	CED-O2D-CGD	2.28	121.09	115.92
13	A	828	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
16	J	103	BCR	C37-C22-C23	2.28	121.57	118.09
13	A	805	CLA	C3B-C4B-NB	-2.28	108.50	110.53
13	B	835	CLA	C2A-C1A-CHA	2.28	127.82	123.87
13	B	838	CLA	C4D-CHA-C1A	2.28	123.96	121.24
13	A	819	CLA	C1-C2-C3	2.27	129.92	126.20
16	A	850	BCR	C40-C30-C25	2.27	113.81	110.24
13	A	838	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
16	F	1302	BCR	C8-C7-C6	2.27	133.07	127.00
16	A	851	BCR	C35-C13-C12	2.27	121.56	118.09
16	A	854	BCR	C34-C9-C8	2.27	121.56	118.09
13	A	820	CLA	C4-C3-C5	-2.27	111.29	115.23
16	B	846	BCR	C36-C18-C19	2.27	121.55	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	845	BCR	C36-C18-C19	2.26	121.55	118.09
13	A	805	CLA	CED-O2D-CGD	2.26	121.05	115.92
13	A	836	CLA	C4D-CHA-C1A	2.26	123.94	121.24
16	B	845	BCR	C40-C30-C25	2.26	113.79	110.24
13	A	845	CLA	O2A-CGA-O1A	-2.26	117.52	123.33
13	A	837	CLA	O2A-CGA-O1A	-2.26	117.52	123.33
13	A	818	CLA	C3B-C4B-NB	-2.26	108.52	110.53
13	B	820	CLA	O2A-CGA-O1A	-2.26	117.99	123.63
13	A	802	CLA	C6-C5-C3	-2.25	107.98	113.47
13	L	1003	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
16	J	104	BCR	C24-C23-C22	2.25	129.56	126.23
13	B	830	CLA	CHD-C1D-ND	-2.25	121.64	124.80
16	A	853	BCR	C23-C22-C21	-2.25	115.47	119.01
13	B	839	CLA	C3B-C4B-NB	-2.25	108.52	110.53
16	I	102	BCR	C3-C4-C5	2.25	118.06	114.06
16	L	1006	BCR	C23-C24-C25	2.25	133.00	127.00
13	X	1701	CLA	CED-O2D-CGD	2.25	121.01	115.92
13	B	802	CLA	O1D-CGD-CBD	-2.24	120.09	124.52
13	B	809	CLA	C1-C2-C3	2.24	129.87	126.20
13	B	810	CLA	O1D-CGD-CBD	-2.24	120.09	124.52
13	A	823	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
16	B	849	BCR	C1-C6-C5	-2.24	119.57	122.64
13	A	810	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
16	B	848	BCR	C1-C6-C5	-2.24	119.58	122.64
13	A	832	CLA	CHD-C1D-ND	-2.24	121.66	124.80
13	B	839	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
13	A	832	CLA	C1-C2-C3	2.23	130.38	126.76
13	A	826	CLA	C4D-CHA-C1A	2.23	123.91	121.24
16	F	1302	BCR	C1-C6-C7	2.23	121.71	115.65
13	A	839	CLA	CHD-C1D-ND	-2.23	121.66	124.80
13	A	805	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
13	B	833	CLA	CMD-C2D-C1D	2.23	128.66	124.73
16	J	104	BCR	C34-C9-C8	2.23	121.49	118.09
16	I	101	BCR	C32-C1-C6	2.22	113.73	110.24
13	B	827	CLA	CAA-CBA-CGA	2.22	119.53	113.21
13	B	834	CLA	CAA-C2A-C3A	-2.22	106.99	113.00
16	I	102	BCR	C19-C18-C17	-2.22	115.51	119.01
16	B	847	BCR	C23-C24-C25	2.22	132.93	127.00
13	B	826	CLA	CED-O2D-CGD	2.22	120.95	115.92
16	B	848	BCR	C24-C23-C22	2.22	129.52	126.23
16	I	101	BCR	C19-C18-C17	-2.22	115.52	119.01
13	A	829	CLA	CMD-C2D-C1D	2.22	128.63	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	1005	BCR	C37-C22-C23	2.22	121.48	118.09
13	L	1002	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
16	J	104	BCR	C35-C13-C12	2.21	121.47	118.09
14	B	842	PQN	C17-C16-C15	-2.21	107.36	113.26
13	B	808	CLA	CED-O2D-CGD	2.21	120.93	115.92
16	B	849	BCR	C23-C22-C21	-2.21	115.53	119.01
16	A	854	BCR	C37-C22-C23	2.21	121.46	118.09
13	B	836	CLA	C2A-C1A-CHA	2.21	127.70	123.87
13	A	819	CLA	CBA-CAA-C2A	2.21	120.36	113.79
16	B	849	BCR	C15-C14-C13	2.21	130.37	127.28
16	A	853	BCR	C7-C8-C9	2.21	129.50	126.23
13	A	834	CLA	O2A-CGA-O1A	-2.20	118.11	123.63
16	L	1006	BCR	C32-C1-C6	2.20	113.70	110.24
13	J	101	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
16	B	843	BCR	C37-C22-C23	2.20	121.45	118.09
13	A	812	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
13	B	817	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
16	M	1602	BCR	C30-C25-C24	2.20	121.61	115.65
16	B	844	BCR	C8-C7-C6	2.20	132.87	127.00
13	A	813	CLA	CED-O2D-CGD	2.20	120.90	115.92
14	B	842	PQN	C11-C3-C2	-2.20	121.13	124.89
13	B	823	CLA	C4D-CHA-C1A	2.19	123.86	121.24
13	A	842	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
13	B	838	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
13	A	821	CLA	C2A-C1A-CHA	2.19	127.67	123.87
13	A	840	CLA	C4D-CHA-C1A	2.19	123.86	121.24
13	B	824	CLA	C4D-CHA-C1A	2.19	123.86	121.24
13	B	841	CLA	CBA-CAA-C2A	2.19	120.31	113.79
13	A	808	CLA	C3B-C4B-NB	-2.19	108.58	110.53
16	A	849	BCR	C30-C25-C24	2.19	121.59	115.65
13	B	812	CLA	C4D-CHA-C1A	2.19	123.85	121.24
13	A	826	CLA	C1-C2-C3	2.19	129.78	126.20
16	B	847	BCR	C34-C9-C8	2.19	121.43	118.09
13	B	807	CLA	C1-C2-C3	2.18	129.77	126.20
13	A	809	CLA	CED-O2D-CGD	2.18	120.86	115.92
13	B	804	CLA	CAA-C2A-C3A	-2.18	107.11	113.00
16	B	843	BCR	C34-C9-C8	2.18	121.41	118.09
13	B	841	CLA	CED-O2D-CGD	2.18	120.85	115.92
16	B	845	BCR	C32-C1-C6	2.17	113.65	110.24
16	J	105	BCR	C16-C17-C18	2.17	130.33	127.28
13	A	819	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
13	A	808	CLA	C4D-CHA-C1A	2.17	123.83	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	1002	CLA	C12-C11-C10	-2.17	103.55	113.28
13	B	810	CLA	CAA-C2A-C1A	2.17	119.09	111.97
13	B	826	CLA	C4D-CHA-C1A	2.17	123.83	121.24
13	A	843	CLA	C12-C11-C10	-2.17	103.55	113.28
13	A	810	CLA	C4D-CHA-C1A	2.17	123.83	121.24
16	B	849	BCR	C30-C25-C24	2.17	121.53	115.65
13	M	1601	CLA	C2A-C1A-CHA	2.16	127.62	123.87
13	B	809	CLA	CAA-C2A-C3A	-2.16	107.16	113.00
13	F	1301	CLA	O2A-CGA-O1A	-2.16	117.78	123.33
13	A	815	CLA	C4D-CHA-C1A	2.16	123.82	121.24
13	L	1002	CLA	CHB-C1B-NB	2.16	127.28	124.05
13	A	802	CLA	CED-O2D-CGD	2.15	120.79	115.92
13	A	833	CLA	C2A-C3A-C4A	2.15	105.34	101.87
13	A	823	CLA	CHD-C1D-ND	-2.15	121.78	124.80
13	B	838	CLA	CAA-C2A-C3A	-2.15	107.19	113.00
13	B	804	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
13	B	835	CLA	C4D-CHA-C1A	2.15	123.81	121.24
13	B	833	CLA	CHD-C1D-ND	-2.15	121.78	124.80
16	M	1602	BCR	C35-C13-C12	2.15	121.37	118.09
13	A	838	CLA	C2A-C1A-CHA	2.15	127.59	123.87
13	A	834	CLA	C4D-CHA-C1A	2.15	123.80	121.24
13	A	823	CLA	C2A-C1A-CHA	2.15	127.59	123.87
13	A	812	CLA	C2D-C1D-ND	2.15	112.25	110.13
13	B	840	CLA	C12-C11-C10	-2.14	103.67	113.28
16	F	1302	BCR	C36-C18-C19	2.14	121.36	118.09
13	B	840	CLA	CMD-C2D-C1D	2.14	128.50	124.73
13	A	824	CLA	C4-C3-C5	-2.14	113.61	116.13
13	A	834	CLA	CED-O2D-CGD	2.14	120.77	115.92
13	B	834	CLA	CMA-C3A-C2A	-2.14	105.71	113.98
13	B	810	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
13	A	841	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
13	A	814	CLA	C2A-C1A-CHA	2.14	127.58	123.87
13	A	839	CLA	C3B-C4B-NB	-2.14	108.62	110.53
13	B	834	CLA	CHD-C1D-ND	-2.14	121.80	124.80
13	X	1701	CLA	O2A-CGA-O1A	-2.13	117.84	123.33
13	B	805	CLA	C2A-C3A-C4A	2.13	105.32	101.87
13	B	827	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
13	A	816	CLA	CAA-C2A-C3A	-2.13	107.24	113.00
13	B	806	CLA	CMD-C2D-C1D	2.13	128.48	124.73
16	F	1302	BCR	C40-C30-C25	2.13	113.59	110.24
13	A	825	CLA	CED-O2D-CGD	2.13	120.75	115.92
13	B	829	CLA	CMB-C2B-C1B	-2.13	122.17	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	849	BCR	C11-C10-C9	2.13	130.27	127.28
13	A	834	CLA	CMD-C2D-C1D	2.13	128.48	124.73
13	L	1003	CLA	C6-C5-C3	-2.13	108.28	113.47
13	A	845	CLA	C2A-C3A-C4A	2.13	105.31	101.87
13	B	833	CLA	CBA-CAA-C2A	2.13	120.13	113.79
16	A	850	BCR	C15-C14-C13	2.13	130.26	127.28
13	A	841	CLA	CAA-C2A-C3A	-2.13	107.25	113.00
13	A	842	CLA	O1D-CGD-CBD	-2.13	120.33	124.52
16	A	850	BCR	C32-C1-C6	2.13	113.58	110.24
16	J	104	BCR	C15-C14-C13	2.12	130.26	127.28
13	B	813	CLA	C2A-C1A-CHA	2.12	127.55	123.87
13	J	102	CLA	OBD-CAD-CBD	-2.12	121.68	125.94
16	I	102	BCR	C35-C13-C12	2.12	121.33	118.09
16	B	843	BCR	C20-C21-C22	2.12	130.25	127.28
13	A	837	CLA	C2A-C1A-CHA	2.12	127.55	123.87
16	B	848	BCR	C30-C25-C24	2.12	121.40	115.65
13	A	805	CLA	C1-C2-C3	2.12	129.67	126.20
16	J	105	BCR	C40-C30-C25	2.12	113.56	110.24
13	A	825	CLA	CMD-C2D-C1D	2.12	128.46	124.73
13	B	812	CLA	O2A-CGA-O1A	-2.12	117.89	123.33
13	A	815	CLA	C2A-C1A-CHA	2.12	127.54	123.87
13	A	824	CLA	CMD-C2D-C1D	2.11	128.45	124.73
13	A	839	CLA	CMD-C2D-C1D	2.11	128.45	124.73
13	B	825	CLA	CMD-C2D-C1D	2.11	128.45	124.73
13	B	827	CLA	CED-O2D-CGD	2.11	120.70	115.92
13	B	819	CLA	C4D-CHA-C1A	2.11	123.76	121.24
13	A	820	CLA	CBA-CAA-C2A	2.11	120.07	113.79
13	A	801	CLA	CMA-C3A-C2A	-2.11	105.83	113.98
13	A	837	CLA	CHD-C1D-ND	-2.11	121.83	124.80
13	A	843	CLA	CBA-CAA-C2A	2.11	120.06	113.79
13	L	1004	CLA	CHD-C1D-ND	-2.11	121.84	124.80
13	A	805	CLA	C2A-C1A-CHA	2.11	127.52	123.87
13	B	818	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
16	B	848	BCR	C40-C30-C25	2.11	113.55	110.24
16	A	850	BCR	C35-C13-C12	2.11	121.31	118.09
16	J	104	BCR	C19-C18-C17	-2.10	115.70	119.01
13	A	827	CLA	CED-O2D-CGD	2.10	120.69	115.92
16	I	101	BCR	C30-C25-C24	2.10	121.36	115.65
13	A	826	CLA	C7-C6-C5	-2.10	107.66	113.26
13	L	1002	CLA	CMD-C2D-C1D	2.10	128.42	124.73
13	B	805	CLA	CHD-C1D-ND	-2.10	121.85	124.80
16	M	1602	BCR	C32-C1-C6	2.10	113.53	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	847	BCR	C19-C18-C17	-2.10	115.71	119.01
13	A	812	CLA	CHD-C1D-ND	-2.10	121.85	124.80
13	B	815	CLA	C2A-C1A-CHA	2.10	127.50	123.87
13	B	832	CLA	CHD-C1D-ND	-2.10	121.85	124.80
13	A	810	CLA	CBA-CAA-C2A	2.09	120.02	113.79
13	B	836	CLA	O2A-CGA-O1A	-2.09	117.95	123.33
13	A	831	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
13	A	825	CLA	C1-C2-C3	2.09	129.63	126.20
16	B	845	BCR	C20-C21-C22	2.09	130.21	127.28
13	A	811	CLA	O2A-CGA-O1A	-2.09	117.95	123.33
13	A	826	CLA	C2A-C1A-CHA	2.09	127.50	123.87
13	B	827	CLA	C12-C11-C10	-2.09	103.91	113.28
13	B	836	CLA	C4D-CHA-C1A	2.09	123.74	121.24
16	J	105	BCR	C23-C24-C25	2.09	132.58	127.00
13	A	834	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
13	X	1701	CLA	C2A-C1A-CHA	2.09	127.49	123.87
13	B	838	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
13	A	810	CLA	C1-C2-C3	2.08	129.61	126.20
13	B	805	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
16	M	1602	BCR	C37-C22-C23	2.08	121.27	118.09
13	A	834	CLA	C2A-C3A-C4A	2.08	105.23	101.87
13	B	826	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
13	A	810	CLA	CMD-C2D-C1D	2.08	128.39	124.73
13	A	816	CLA	C2A-C1A-CHA	2.08	127.47	123.87
13	A	843	CLA	CMD-C2D-C1D	2.08	128.38	124.73
13	A	840	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
13	A	820	CLA	C2A-C1A-CHA	2.07	127.47	123.87
16	B	844	BCR	C30-C25-C24	2.07	121.28	115.65
13	B	841	CLA	C3B-C4B-NB	-2.07	108.68	110.53
16	B	848	BCR	C11-C10-C9	2.07	130.19	127.28
13	A	803	CLA	C2A-C3A-C4A	2.07	105.22	101.87
13	A	807	CLA	O2D-CGD-CBD	2.07	114.85	111.23
16	I	102	BCR	C23-C24-C25	2.07	132.53	127.00
16	A	852	BCR	C8-C7-C6	2.07	132.53	127.00
16	B	844	BCR	C15-C14-C13	2.07	130.18	127.28
16	A	851	BCR	C37-C22-C23	2.07	121.25	118.09
16	A	853	BCR	C30-C25-C24	2.07	121.26	115.65
13	A	817	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
16	J	103	BCR	C32-C1-C2	-2.07	101.01	108.95
13	A	830	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
13	A	810	CLA	CHB-C1B-NB	2.07	127.15	124.05
16	B	847	BCR	C20-C21-C22	2.07	130.18	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	835	CLA	C1-C2-C3	2.07	129.58	126.20
13	A	803	CLA	CMA-C3A-C2A	-2.07	106.00	113.98
13	B	827	CLA	CHB-C1B-NB	2.06	127.14	124.05
13	A	836	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
16	L	1006	BCR	C1-C6-C7	2.06	121.24	115.65
16	J	103	BCR	C19-C18-C17	-2.06	115.77	119.01
16	A	851	BCR	C15-C14-C13	2.06	130.17	127.28
13	B	809	CLA	C2B-C1B-NB	-2.06	108.19	110.33
13	A	823	CLA	C2A-C3A-C4A	2.06	105.20	101.87
13	A	829	CLA	CHD-C1D-ND	-2.06	121.90	124.80
13	B	807	CLA	C3C-C4C-NC	-2.06	107.79	110.43
13	B	811	CLA	CMD-C2D-C1D	2.06	128.35	124.73
13	A	816	CLA	O2A-CGA-O1A	-2.06	118.04	123.33
13	A	809	CLA	C4D-CHA-C1A	2.06	123.70	121.24
13	B	841	CLA	C4D-CHA-C1A	2.06	123.70	121.24
13	A	819	CLA	C2A-C1A-CHA	2.06	127.44	123.87
13	B	807	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
13	B	830	CLA	O2A-CGA-O1A	-2.06	118.04	123.33
16	B	843	BCR	C40-C30-C25	2.05	113.46	110.24
13	A	827	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
16	B	843	BCR	C35-C13-C12	2.05	121.22	118.09
13	A	806	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
13	A	817	CLA	C2A-C1A-CHA	2.05	127.43	123.87
13	A	801	CLA	CGD-CBD-CAD	2.05	117.49	110.85
13	A	835	CLA	CMD-C2D-C1D	2.05	128.34	124.73
16	B	846	BCR	C19-C18-C17	-2.05	115.78	119.01
13	L	1004	CLA	CED-O2D-CGD	2.05	120.56	115.92
17	B	851	LHG	O8-C23-C24	2.05	121.08	112.38
13	B	805	CLA	C2D-C1D-ND	2.05	112.15	110.13
13	B	825	CLA	C2A-C1A-CHA	2.05	127.42	123.87
13	B	802	CLA	CHA-C1A-NA	-2.05	121.76	126.39
16	A	851	BCR	C34-C9-C8	2.05	121.21	118.09
13	A	828	CLA	CMD-C2D-C1D	2.04	128.33	124.73
13	B	811	CLA	CHD-C1D-ND	-2.04	121.92	124.80
13	B	817	CLA	C2A-C1A-CHA	2.04	127.42	123.87
16	J	105	BCR	C37-C22-C23	2.04	121.21	118.09
13	A	801	CLA	O2D-CGD-O1D	-2.04	119.87	123.85
13	B	802	CLA	C1-C2-C3	2.04	129.54	126.20
13	A	827	CLA	C4D-CHA-C1A	2.04	123.68	121.24
13	B	829	CLA	CAA-C2A-C3A	-2.04	107.48	113.00
13	A	828	CLA	C2A-C3A-C4A	2.04	105.17	101.87
13	A	826	CLA	CMD-C2D-C1D	2.04	128.32	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	851	BCR	C32-C1-C6	2.04	113.44	110.24
13	A	802	CLA	CHB-C1B-NB	2.04	127.11	124.05
16	B	849	BCR	C8-C7-C6	2.04	132.45	127.00
13	A	804	CLA	CMD-C2D-C1D	2.04	128.32	124.73
13	B	801	CLA	O2D-CGD-CBD	2.04	114.80	111.23
13	B	834	CLA	O2A-CGA-O1A	-2.04	118.09	123.33
13	A	801	CLA	C3B-C4B-NB	-2.04	108.71	110.53
14	B	842	PQN	C22-C21-C20	-2.04	104.16	113.28
13	B	818	CLA	CMD-C2D-C1D	2.04	128.31	124.73
16	B	849	BCR	C37-C22-C23	2.04	121.20	118.09
13	B	831	CLA	CHD-C1D-ND	-2.03	121.94	124.80
13	B	801	CLA	CMA-C3A-C2A	-2.03	106.13	113.98
13	B	805	CLA	CMA-C3A-C2A	-2.03	106.13	113.98
13	B	821	CLA	O2A-CGA-O1A	-2.03	118.11	123.33
13	B	827	CLA	CMD-C2D-C1D	2.03	128.30	124.73
13	A	818	CLA	CHD-C1D-ND	-2.03	121.95	124.80
13	A	804	CLA	C2A-C1A-CHA	2.03	127.39	123.87
13	A	817	CLA	C4D-CHA-C1A	2.03	123.66	121.24
13	A	811	CLA	CHD-C1D-ND	-2.03	121.95	124.80
13	B	830	CLA	C3C-C4C-NC	-2.03	107.83	110.43
17	A	856	LHG	P-O6-C4	-2.03	109.74	121.35
13	L	1003	CLA	CED-O2D-CGD	2.02	120.51	115.92
16	A	850	BCR	C8-C7-C6	2.02	132.40	127.00
13	A	823	CLA	C4D-CHA-C1A	2.02	123.66	121.24
13	A	841	CLA	CMD-C2D-C1D	2.02	128.29	124.73
13	A	814	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
13	B	812	CLA	CHD-C1D-ND	-2.02	121.96	124.80
13	B	801	CLA	C2A-C3A-C4A	2.02	105.14	101.87
13	A	827	CLA	CHD-C1D-ND	-2.02	121.96	124.80
13	A	814	CLA	CMD-C2D-C1D	2.02	128.29	124.73
13	B	828	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
13	F	1301	CLA	C4D-CHA-C1A	2.02	123.65	121.24
16	B	843	BCR	C30-C25-C24	2.02	121.13	115.65
13	A	811	CLA	CMD-C2D-C1D	2.02	128.28	124.73
13	B	826	CLA	C12-C11-C10	-2.02	104.24	113.28
13	B	835	CLA	CHB-C1B-NB	2.02	127.07	124.05
13	A	818	CLA	CMD-C2D-C1D	2.02	128.28	124.73
16	B	848	BCR	C1-C6-C7	2.02	121.12	115.65
13	A	814	CLA	C2A-C3A-C4A	2.01	105.12	101.87
13	A	809	CLA	CHD-C1D-ND	-2.01	121.97	124.80
13	B	810	CLA	C3A-C2A-C1A	2.01	104.36	101.34
13	B	813	CLA	C4D-CHA-C1A	2.01	123.64	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	827	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
16	A	851	BCR	C23-C24-C25	2.01	132.37	127.00
16	A	852	BCR	C40-C30-C29	-2.01	101.23	108.95
13	B	828	CLA	C3A-C2A-C1A	2.01	104.35	101.34
13	A	830	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
13	B	807	CLA	CHD-C1D-ND	-2.01	121.98	124.80
16	L	1006	BCR	C35-C13-C12	2.01	121.16	118.09
13	B	814	CLA	C2A-C3A-C4A	2.01	105.11	101.87
13	B	829	CLA	C2A-C3A-C4A	2.01	105.11	101.87
13	B	808	CLA	CMD-C2D-C1D	2.01	128.26	124.73
13	A	845	CLA	OBD-CAD-CBD	-2.01	121.92	125.94
13	A	845	CLA	C3B-C4B-NB	-2.00	108.74	110.53
16	A	851	BCR	C36-C18-C19	2.00	121.15	118.09
13	K	1401	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
13	A	824	CLA	CED-O2D-CGD	2.00	120.46	115.92
13	B	807	CLA	CAA-C2A-C3A	-2.00	107.59	113.00
13	A	810	CLA	CED-O2D-CGD	2.00	120.46	115.92
13	B	822	CLA	CBA-CAA-C2A	2.00	119.75	113.79

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	856	LHG	C2

All (900) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	801	CLA	C2B-C3B-CAB-CBB
13	A	801	CLA	C4B-C3B-CAB-CBB
13	A	802	CLA	C4B-C3B-CAB-CBB
13	A	805	CLA	C3A-C2A-CAA-CBA
13	A	805	CLA	C2B-C3B-CAB-CBB
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	CAD-CBD-CGD-O1D
13	A	806	CLA	CAD-CBD-CGD-O2D
13	A	807	CLA	C1A-C2A-CAA-CBA
13	A	807	CLA	C2-C3-C5-C6
13	A	807	CLA	C4-C3-C5-C6
13	A	809	CLA	C3A-C2A-CAA-CBA
13	A	809	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	A	809	CLA	CHA-CBD-CGD-O2D
13	A	810	CLA	C2B-C3B-CAB-CBB
13	A	810	CLA	C4B-C3B-CAB-CBB
13	A	811	CLA	C1A-C2A-CAA-CBA
13	A	811	CLA	C3A-C2A-CAA-CBA
13	A	812	CLA	C1A-C2A-CAA-CBA
13	A	812	CLA	C3A-C2A-CAA-CBA
13	A	813	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	A	819	CLA	C3A-C2A-CAA-CBA
13	A	820	CLA	C1A-C2A-CAA-CBA
13	A	820	CLA	C3A-C2A-CAA-CBA
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	A	823	CLA	C1A-C2A-CAA-CBA
13	A	823	CLA	C3A-C2A-CAA-CBA
13	A	823	CLA	C4B-C3B-CAB-CBB
13	A	823	CLA	C1-C2-C3-C4
13	A	824	CLA	C4-C3-C5-C6
13	A	825	CLA	C2B-C3B-CAB-CBB
13	A	825	CLA	C4B-C3B-CAB-CBB
13	A	831	CLA	CHA-CBD-CGD-O1D
13	A	831	CLA	CHA-CBD-CGD-O2D
13	A	834	CLA	C2B-C3B-CAB-CBB
13	A	834	CLA	C4B-C3B-CAB-CBB
13	A	835	CLA	CHA-CBD-CGD-O1D
13	A	835	CLA	CHA-CBD-CGD-O2D
13	A	837	CLA	C1A-C2A-CAA-CBA
13	A	838	CLA	C4-C3-C5-C6
13	A	841	CLA	C4B-C3B-CAB-CBB
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	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	CAD-CBD-CGD-O1D
13	A	846	CLA	CAD-CBD-CGD-O2D
13	A	846	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	B	801	CLA	C2B-C3B-CAB-CBB
13	B	801	CLA	C4B-C3B-CAB-CBB
13	B	802	CLA	C2B-C3B-CAB-CBB
13	B	802	CLA	C4B-C3B-CAB-CBB
13	B	804	CLA	C2B-C3B-CAB-CBB
13	B	804	CLA	C4B-C3B-CAB-CBB
13	B	805	CLA	C1A-C2A-CAA-CBA
13	B	805	CLA	C3A-C2A-CAA-CBA
13	B	808	CLA	CHA-CBD-CGD-O1D
13	B	808	CLA	CHA-CBD-CGD-O2D
13	B	809	CLA	C2B-C3B-CAB-CBB
13	B	809	CLA	C4B-C3B-CAB-CBB
13	B	811	CLA	CBD-CGD-O2D-CED
13	B	813	CLA	C1A-C2A-CAA-CBA
13	B	814	CLA	C2B-C3B-CAB-CBB
13	B	814	CLA	C4B-C3B-CAB-CBB
13	B	814	CLA	CHA-CBD-CGD-O1D
13	B	814	CLA	CHA-CBD-CGD-O2D
13	B	815	CLA	C1A-C2A-CAA-CBA
13	B	815	CLA	C3A-C2A-CAA-CBA
13	B	816	CLA	C1A-C2A-CAA-CBA
13	B	816	CLA	C3A-C2A-CAA-CBA
13	B	817	CLA	C1A-C2A-CAA-CBA
13	B	817	CLA	C3A-C2A-CAA-CBA
13	B	817	CLA	C4B-C3B-CAB-CBB
13	B	818	CLA	C3A-C2A-CAA-CBA
13	B	820	CLA	C3A-C2A-CAA-CBA
13	B	821	CLA	C4B-C3B-CAB-CBB
13	B	821	CLA	CBD-CGD-O2D-CED
13	B	822	CLA	CBD-CGD-O2D-CED
13	B	823	CLA	C4B-C3B-CAB-CBB
13	B	824	CLA	C4B-C3B-CAB-CBB
13	B	824	CLA	CHA-CBD-CGD-O1D
13	B	824	CLA	CHA-CBD-CGD-O2D
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	B	827	CLA	C3A-C2A-CAA-CBA
13	B	828	CLA	C1A-C2A-CAA-CBA
13	B	828	CLA	C3A-C2A-CAA-CBA
13	B	828	CLA	C4B-C3B-CAB-CBB
13	B	829	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	B	829	CLA	CHA-CBD-CGD-O2D
13	B	830	CLA	C3A-C2A-CAA-CBA
13	B	830	CLA	C4B-C3B-CAB-CBB
13	B	830	CLA	CBD-CGD-O2D-CED
13	B	832	CLA	C1A-C2A-CAA-CBA
13	B	832	CLA	C3A-C2A-CAA-CBA
13	B	833	CLA	C4B-C3B-CAB-CBB
13	B	833	CLA	CHA-CBD-CGD-O1D
13	B	833	CLA	CHA-CBD-CGD-O2D
13	B	834	CLA	CHA-CBD-CGD-O1D
13	B	834	CLA	CHA-CBD-CGD-O2D
13	B	836	CLA	CBD-CGD-O2D-CED
13	B	841	CLA	C1A-C2A-CAA-CBA
13	B	841	CLA	C3A-C2A-CAA-CBA
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	K	1401	CLA	CBD-CGD-O2D-CED
13	L	1002	CLA	C1A-C2A-CAA-CBA
13	L	1002	CLA	C3A-C2A-CAA-CBA
13	L	1003	CLA	C2B-C3B-CAB-CBB
13	L	1003	CLA	C4B-C3B-CAB-CBB
13	L	1004	CLA	C2B-C3B-CAB-CBB
13	L	1004	CLA	C4B-C3B-CAB-CBB
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
13	X	1701	CLA	CHA-CBD-CGD-O2D
16	A	850	BCR	C23-C24-C25-C26
16	A	852	BCR	C23-C24-C25-C26
16	A	852	BCR	C23-C24-C25-C30
16	B	847	BCR	C23-C24-C25-C26
16	B	847	BCR	C23-C24-C25-C30
16	J	103	BCR	C1-C6-C7-C8
16	J	103	BCR	C5-C6-C7-C8
16	J	104	BCR	C23-C24-C25-C26
16	J	104	BCR	C23-C24-C25-C30
17	A	855	LHG	C4-O6-P-O3
17	A	855	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
17	B	851	LHG	O1-C1-C2-C3
13	A	817	CLA	O1D-CGD-O2D-CED
13	A	842	CLA	O1D-CGD-O2D-CED
13	B	834	CLA	O1D-CGD-O2D-CED
13	A	810	CLA	CBD-CGD-O2D-CED
13	A	811	CLA	CBD-CGD-O2D-CED
13	A	812	CLA	CBD-CGD-O2D-CED
13	A	816	CLA	CBD-CGD-O2D-CED
13	A	842	CLA	CBD-CGD-O2D-CED
13	B	801	CLA	CBD-CGD-O2D-CED
13	B	804	CLA	CBD-CGD-O2D-CED
13	B	815	CLA	CBD-CGD-O2D-CED
13	B	834	CLA	CBD-CGD-O2D-CED
13	F	1301	CLA	CBD-CGD-O2D-CED
13	M	1601	CLA	CBD-CGD-O2D-CED
13	A	806	CLA	O1A-CGA-O2A-C1
13	A	821	CLA	O1A-CGA-O2A-C1
13	A	836	CLA	O1A-CGA-O2A-C1
13	A	836	CLA	CBA-CGA-O2A-C1
13	A	844	CLA	CBA-CGA-O2A-C1
13	B	831	CLA	CBD-CGD-O2D-CED
13	A	803	CLA	O1A-CGA-O2A-C1
13	A	813	CLA	O1A-CGA-O2A-C1
13	A	833	CLA	O1A-CGA-O2A-C1
13	A	838	CLA	O1A-CGA-O2A-C1
13	A	844	CLA	O1A-CGA-O2A-C1
13	B	822	CLA	O1D-CGD-O2D-CED
13	K	1401	CLA	O1D-CGD-O2D-CED
13	A	846	CLA	O1D-CGD-O2D-CED
13	B	811	CLA	O1D-CGD-O2D-CED
13	A	807	CLA	CBD-CGD-O2D-CED
13	A	806	CLA	C3-C5-C6-C7
13	A	810	CLA	C3-C5-C6-C7
13	A	813	CLA	C3-C5-C6-C7
13	B	809	CLA	C3-C5-C6-C7
13	A	817	CLA	CBA-CGA-O2A-C1
13	A	820	CLA	CBA-CGA-O2A-C1
13	A	821	CLA	CBA-CGA-O2A-C1
13	A	838	CLA	CBA-CGA-O2A-C1
13	A	840	CLA	CBA-CGA-O2A-C1
13	L	1002	CLA	CBA-CGA-O2A-C1
13	A	805	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	A	808	CLA	CBD-CGD-O2D-CED
13	A	809	CLA	CBD-CGD-O2D-CED
13	A	823	CLA	CBD-CGD-O2D-CED
13	A	829	CLA	CBD-CGD-O2D-CED
13	A	835	CLA	CBD-CGD-O2D-CED
13	A	843	CLA	CBD-CGD-O2D-CED
13	B	833	CLA	CBD-CGD-O2D-CED
13	L	1004	CLA	CBD-CGD-O2D-CED
13	X	1701	CLA	CBD-CGD-O2D-CED
13	A	813	CLA	O1D-CGD-O2D-CED
13	A	821	CLA	O1D-CGD-O2D-CED
13	B	836	CLA	O1D-CGD-O2D-CED
13	J	101	CLA	O1D-CGD-O2D-CED
13	M	1601	CLA	O1D-CGD-O2D-CED
13	B	821	CLA	O1D-CGD-O2D-CED
13	A	829	CLA	C4-C3-C5-C6
13	A	843	CLA	C4-C3-C5-C6
13	A	844	CLA	C4-C3-C5-C6
13	B	806	CLA	C4-C3-C5-C6
13	B	818	CLA	C4-C3-C5-C6
14	A	847	PQN	C14-C13-C15-C16
13	A	829	CLA	C2-C3-C5-C6
13	B	818	CLA	C2-C3-C5-C6
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	B	815	CLA	C2A-CAA-CBA-CGA
13	A	803	CLA	CBA-CGA-O2A-C1
13	A	813	CLA	CBA-CGA-O2A-C1
13	A	825	CLA	CBA-CGA-O2A-C1
13	A	833	CLA	CBA-CGA-O2A-C1
13	B	820	CLA	CBA-CGA-O2A-C1
13	A	817	CLA	O1A-CGA-O2A-C1
13	A	824	CLA	O1A-CGA-O2A-C1
13	B	816	CLA	O1A-CGA-O2A-C1
13	L	1002	CLA	O1A-CGA-O2A-C1
17	B	851	LHG	O9-C7-O7-C5
13	B	804	CLA	O1D-CGD-O2D-CED
13	A	826	CLA	C3-C5-C6-C7
13	A	825	CLA	CBD-CGD-O2D-CED
13	A	830	CLA	CBD-CGD-O2D-CED
13	A	811	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	A	812	CLA	O1D-CGD-O2D-CED
13	A	809	CLA	CBA-CGA-O2A-C1
13	A	832	CLA	CBA-CGA-O2A-C1
13	L	1003	CLA	CBA-CGA-O2A-C1
18	B	850	LMG	O6-C5-C6-O5
13	A	820	CLA	O1A-CGA-O2A-C1
13	A	840	CLA	O1A-CGA-O2A-C1
13	F	1301	CLA	O1D-CGD-O2D-CED
17	B	851	LHG	C8-C7-O7-C5
13	A	809	CLA	C3-C5-C6-C7
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	824	CLA	CBD-CGD-O2D-CED
13	A	816	CLA	O1D-CGD-O2D-CED
13	B	815	CLA	O1D-CGD-O2D-CED
13	B	831	CLA	O1D-CGD-O2D-CED
13	A	824	CLA	CBA-CGA-O2A-C1
13	B	816	CLA	CBA-CGA-O2A-C1
13	A	836	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	A	843	CLA	C2-C3-C5-C6
13	B	802	CLA	C2-C3-C5-C6
13	B	806	CLA	C2-C3-C5-C6
13	B	816	CLA	C2-C3-C5-C6
13	A	809	CLA	O1A-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	B	806	CLA	CBD-CGD-O2D-CED
13	B	839	CLA	CBD-CGD-O2D-CED
13	A	810	CLA	O1D-CGD-O2D-CED
13	A	832	CLA	O1A-CGA-O2A-C1
13	B	818	CLA	CBA-CGA-O2A-C1
13	B	829	CLA	CBA-CGA-O2A-C1
13	B	808	CLA	CBD-CGD-O2D-CED
13	B	810	CLA	CBD-CGD-O2D-CED
13	B	832	CLA	CBD-CGD-O2D-CED
13	A	829	CLA	O1A-CGA-O2A-C1
13	A	807	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	B	824	CLA	C3-C5-C6-C7
13	B	818	CLA	O1A-CGA-O2A-C1
17	A	856	LHG	C1-C2-C3-O3
13	A	805	CLA	CBA-CGA-O2A-C1
13	A	812	CLA	CBA-CGA-O2A-C1
13	A	823	CLA	CBA-CGA-O2A-C1
13	A	829	CLA	CBA-CGA-O2A-C1
13	B	813	CLA	CBA-CGA-O2A-C1
13	B	826	CLA	CBA-CGA-O2A-C1
13	B	837	CLA	CBA-CGA-O2A-C1
13	A	806	CLA	CBD-CGD-O2D-CED
13	A	823	CLA	O1D-CGD-O2D-CED
13	A	843	CLA	O1D-CGD-O2D-CED
13	B	824	CLA	C4-C3-C5-C6
13	A	844	CLA	C2-C3-C5-C6
13	B	824	CLA	C2-C3-C5-C6
14	A	847	PQN	C12-C13-C15-C16
17	B	851	LHG	O10-C23-O8-C6
13	A	805	CLA	O1D-CGD-O2D-CED
13	A	835	CLA	O1D-CGD-O2D-CED
13	B	833	CLA	O1D-CGD-O2D-CED
17	A	856	LHG	O2-C2-C3-O3
13	A	808	CLA	O1D-CGD-O2D-CED
13	A	823	CLA	O1A-CGA-O2A-C1
13	B	813	CLA	O1A-CGA-O2A-C1
13	B	841	CLA	CBD-CGD-O2D-CED
13	A	830	CLA	C2A-CAA-CBA-CGA
13	A	812	CLA	O1A-CGA-O2A-C1
13	A	843	CLA	C2-C1-O2A-CGA
13	L	1004	CLA	O1D-CGD-O2D-CED
13	X	1701	CLA	O1D-CGD-O2D-CED
13	A	828	CLA	C10-C11-C12-C13
13	A	843	CLA	C13-C15-C16-C17
13	B	806	CLA	C13-C15-C16-C17
17	B	851	LHG	O1-C1-C2-O2
13	B	805	CLA	CBD-CGD-O2D-CED
13	L	1004	CLA	C5-C6-C7-C8
13	A	809	CLA	O1D-CGD-O2D-CED
13	A	807	CLA	C3-C5-C6-C7
13	A	805	CLA	O1A-CGA-O2A-C1
13	B	826	CLA	O1A-CGA-O2A-C1
13	A	845	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	B	804	CLA	C2A-CAA-CBA-CGA
13	B	830	CLA	C2A-CAA-CBA-CGA
13	B	831	CLA	C2A-CAA-CBA-CGA
13	B	840	CLA	C2A-CAA-CBA-CGA
13	A	807	CLA	C15-C16-C17-C18
18	B	850	LMG	C4-C5-C6-O5
13	B	829	CLA	O1A-CGA-O2A-C1
13	B	837	CLA	O1A-CGA-O2A-C1
13	A	839	CLA	C8-C10-C11-C12
13	B	810	CLA	C15-C16-C17-C18
14	A	847	PQN	C13-C15-C16-C17
13	A	829	CLA	O1D-CGD-O2D-CED
14	B	842	PQN	C25-C26-C27-C28
13	A	833	CLA	CBD-CGD-O2D-CED
13	A	831	CLA	CBA-CGA-O2A-C1
13	A	842	CLA	CBA-CGA-O2A-C1
13	B	839	CLA	CBA-CGA-O2A-C1
13	A	819	CLA	CBD-CGD-O2D-CED
13	A	810	CLA	C8-C10-C11-C12
13	A	827	CLA	C5-C6-C7-C8
13	B	808	CLA	C13-C15-C16-C17
13	B	826	CLA	C10-C11-C12-C13
13	B	828	CLA	C15-C16-C17-C18
13	B	837	CLA	C8-C10-C11-C12
13	A	810	CLA	C13-C15-C16-C17
13	B	828	CLA	C5-C6-C7-C8
13	B	805	CLA	CBA-CGA-O2A-C1
13	A	812	CLA	C15-C16-C17-C18
13	A	830	CLA	O1D-CGD-O2D-CED
13	L	1003	CLA	C8-C10-C11-C12
13	A	825	CLA	O1D-CGD-O2D-CED
16	B	846	BCR	C16-C17-C18-C36
16	B	846	BCR	C20-C21-C22-C37
13	B	829	CLA	C13-C15-C16-C17
13	B	832	CLA	C10-C11-C12-C13
13	A	831	CLA	O1A-CGA-O2A-C1
13	A	842	CLA	O1A-CGA-O2A-C1
13	B	839	CLA	O1A-CGA-O2A-C1
13	A	810	CLA	C2A-CAA-CBA-CGA
13	A	823	CLA	C2A-CAA-CBA-CGA
13	A	824	CLA	O1D-CGD-O2D-CED
13	B	839	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	A	803	CLA	O2A-C1-C2-C3
13	A	806	CLA	O2A-C1-C2-C3
14	B	842	PQN	C26-C27-C28-C29
13	B	806	CLA	O1D-CGD-O2D-CED
16	B	844	BCR	C11-C10-C9-C8
16	B	846	BCR	C16-C17-C18-C19
16	I	102	BCR	C20-C21-C22-C23
13	A	809	CLA	C5-C6-C7-C8
13	B	806	CLA	C10-C11-C12-C13
13	A	833	CLA	C8-C10-C11-C12
13	B	822	CLA	C6-C7-C8-C9
13	B	822	CLA	C6-C7-C8-C10
14	B	842	PQN	C26-C27-C28-C30
17	A	855	LHG	C24-C25-C26-C27
13	A	806	CLA	C10-C11-C12-C13
13	A	805	CLA	C4B-C3B-CAB-CBB
13	A	814	CLA	C4B-C3B-CAB-CBB
13	A	816	CLA	C4B-C3B-CAB-CBB
13	A	826	CLA	C4B-C3B-CAB-CBB
13	A	829	CLA	C4B-C3B-CAB-CBB
13	B	803	CLA	C4B-C3B-CAB-CBB
13	B	806	CLA	C4B-C3B-CAB-CBB
13	B	813	CLA	C4B-C3B-CAB-CBB
13	B	822	CLA	C4B-C3B-CAB-CBB
13	B	825	CLA	C4B-C3B-CAB-CBB
13	B	838	CLA	C4B-C3B-CAB-CBB
13	B	805	CLA	C13-C15-C16-C17
13	B	832	CLA	C15-C16-C17-C18
13	B	805	CLA	O1A-CGA-O2A-C1
13	B	802	CLA	C3-C5-C6-C7
13	A	804	CLA	C3A-C2A-CAA-CBA
13	A	807	CLA	C3A-C2A-CAA-CBA
13	A	837	CLA	C3A-C2A-CAA-CBA
13	A	842	CLA	C3A-C2A-CAA-CBA
13	B	813	CLA	C3A-C2A-CAA-CBA
13	B	808	CLA	O1D-CGD-O2D-CED
13	A	804	CLA	CBD-CGD-O2D-CED
13	A	802	CLA	C2B-C3B-CAB-CBB
13	A	823	CLA	C2B-C3B-CAB-CBB
13	B	821	CLA	C2B-C3B-CAB-CBB
16	A	850	BCR	C1-C6-C7-C8
16	A	850	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
16	A	850	BCR	C23-C24-C25-C30
16	A	853	BCR	C1-C6-C7-C8
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	B	844	BCR	C1-C6-C7-C8
16	B	844	BCR	C5-C6-C7-C8
16	B	844	BCR	C23-C24-C25-C26
16	I	102	BCR	C23-C24-C25-C30
16	J	104	BCR	C1-C6-C7-C8
16	M	1602	BCR	C1-C6-C7-C8
16	M	1602	BCR	C5-C6-C7-C8
13	B	837	CLA	C5-C6-C7-C8
13	B	818	CLA	C3-C5-C6-C7
16	B	846	BCR	C18-C19-C20-C21
13	A	821	CLA	C4C-C3C-CAC-CBC
17	A	855	LHG	C28-C29-C30-C31
13	B	810	CLA	O1D-CGD-O2D-CED
17	A	856	LHG	C9-C10-C11-C12
13	A	806	CLA	C8-C10-C11-C12
13	A	826	CLA	C4-C3-C5-C6
13	B	833	CLA	C4-C3-C5-C6
13	B	801	CLA	C13-C15-C16-C17
13	B	819	CLA	C10-C11-C12-C13
13	A	806	CLA	O1D-CGD-O2D-CED
13	B	841	CLA	O1D-CGD-O2D-CED
13	A	814	CLA	C3-C5-C6-C7
13	B	827	CLA	CBD-CGD-O2D-CED
13	A	826	CLA	C2-C3-C5-C6
13	B	832	CLA	O1D-CGD-O2D-CED
13	B	805	CLA	O1D-CGD-O2D-CED
13	A	804	CLA	C1A-C2A-CAA-CBA
13	A	805	CLA	C1A-C2A-CAA-CBA
13	A	809	CLA	C1A-C2A-CAA-CBA
13	A	819	CLA	C1A-C2A-CAA-CBA
13	A	840	CLA	C1A-C2A-CAA-CBA
13	B	811	CLA	C1A-C2A-CAA-CBA
13	B	818	CLA	C1A-C2A-CAA-CBA
13	B	819	CLA	C1A-C2A-CAA-CBA
13	B	820	CLA	C1A-C2A-CAA-CBA
13	B	827	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	B	830	CLA	C1A-C2A-CAA-CBA
13	B	831	CLA	C1A-C2A-CAA-CBA
13	K	1401	CLA	C1A-C2A-CAA-CBA
13	A	843	CLA	C5-C6-C7-C8
13	B	813	CLA	C8-C10-C11-C12
13	A	844	CLA	C3-C5-C6-C7
13	B	816	CLA	C3-C5-C6-C7
13	A	809	CLA	C11-C10-C8-C7
13	B	826	CLA	C11-C12-C13-C15
13	A	802	CLA	C15-C16-C17-C18
13	B	827	CLA	C10-C11-C12-C13
13	A	834	CLA	C2-C3-C5-C6
13	A	809	CLA	C11-C10-C8-C9
13	B	826	CLA	C11-C12-C13-C14
13	B	817	CLA	CBA-CGA-O2A-C1
13	B	831	CLA	CBA-CGA-O2A-C1
13	A	817	CLA	C1-C2-C3-C4
13	A	841	CLA	C5-C6-C7-C8
17	A	855	LHG	C10-C11-C12-C13
17	A	855	LHG	C24-C23-O8-C6
13	A	833	CLA	O1D-CGD-O2D-CED
16	I	102	BCR	C20-C21-C22-C37
13	A	834	CLA	C4-C3-C5-C6
13	A	812	CLA	C2A-CAA-CBA-CGA
13	A	837	CLA	C2A-CAA-CBA-CGA
13	B	825	CLA	CBA-CGA-O2A-C1
13	A	828	CLA	CBA-CGA-O2A-C1
13	B	824	CLA	O2A-C1-C2-C3
13	B	832	CLA	O2A-C1-C2-C3
13	A	839	CLA	C5-C6-C7-C8
16	B	848	BCR	C11-C10-C9-C8
13	A	846	CLA	C2-C3-C5-C6
13	B	809	CLA	C16-C17-C18-C20
18	B	850	LMG	C30-C31-C32-C33
13	A	833	CLA	C3-C5-C6-C7
13	A	822	CLA	CBA-CGA-O2A-C1
13	B	826	CLA	CBD-CGD-O2D-CED
13	A	827	CLA	C15-C16-C17-C18
17	A	856	LHG	C11-C10-C9-C8
13	A	814	CLA	C8-C10-C11-C12
13	A	830	CLA	C4-C3-C5-C6
13	A	846	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	A	826	CLA	CBA-CGA-O2A-C1
13	A	827	CLA	CBA-CGA-O2A-C1
13	A	830	CLA	C14-C13-C15-C16
13	B	802	CLA	C14-C13-C15-C16
13	A	826	CLA	C8-C10-C11-C12
13	B	806	CLA	C15-C16-C17-C18
13	A	803	CLA	C4B-C3B-CAB-CBB
13	A	815	CLA	C4B-C3B-CAB-CBB
13	A	819	CLA	C4B-C3B-CAB-CBB
13	A	827	CLA	C4B-C3B-CAB-CBB
13	A	832	CLA	C4B-C3B-CAB-CBB
13	A	835	CLA	C4B-C3B-CAB-CBB
13	B	811	CLA	C4B-C3B-CAB-CBB
13	B	834	CLA	C4B-C3B-CAB-CBB
13	A	826	CLA	C13-C15-C16-C17
13	B	809	CLA	C16-C17-C18-C19
13	A	809	CLA	C15-C16-C17-C18
13	A	819	CLA	CAA-CBA-CGA-O2A
13	A	830	CLA	C12-C13-C15-C16
13	A	835	CLA	C12-C13-C15-C16
13	B	802	CLA	C12-C13-C15-C16
13	B	805	CLA	C12-C13-C15-C16
13	A	809	CLA	C8-C10-C11-C12
13	B	831	CLA	O1A-CGA-O2A-C1
13	A	845	CLA	C3A-C2A-CAA-CBA
13	A	846	CLA	C3A-C2A-CAA-CBA
13	B	814	CLA	C4-C3-C5-C6
13	B	825	CLA	C3A-C2A-CAA-CBA
13	B	831	CLA	C3A-C2A-CAA-CBA
13	B	833	CLA	C2-C3-C5-C6
13	A	828	CLA	O1A-CGA-O2A-C1
13	A	803	CLA	C15-C16-C17-C18
13	A	827	CLA	C8-C10-C11-C12
13	A	808	CLA	C4-C3-C5-C6
13	B	817	CLA	O1A-CGA-O2A-C1
17	A	855	LHG	O10-C23-O8-C6
13	A	819	CLA	O1D-CGD-O2D-CED
13	A	830	CLA	C5-C6-C7-C8
13	A	817	CLA	O2A-C1-C2-C3
13	A	804	CLA	O1D-CGD-O2D-CED
13	B	818	CLA	C5-C6-C7-C8
13	L	1002	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
13	B	828	CLA	C4-C3-C5-C6
13	A	830	CLA	C2-C3-C5-C6
13	B	814	CLA	C2-C3-C5-C6
13	A	841	CLA	C2B-C3B-CAB-CBB
13	B	823	CLA	C2B-C3B-CAB-CBB
13	B	833	CLA	C2B-C3B-CAB-CBB
16	J	104	BCR	C5-C6-C7-C8
13	A	827	CLA	O1A-CGA-O2A-C1
13	A	807	CLA	C16-C17-C18-C19
13	B	832	CLA	C2A-CAA-CBA-CGA
13	B	828	CLA	C2-C3-C5-C6
13	B	832	CLA	C2-C3-C5-C6
13	A	807	CLA	C16-C17-C18-C20
13	L	1002	CLA	C11-C10-C8-C9
13	B	801	CLA	C5-C6-C7-C8
16	L	1005	BCR	C22-C23-C24-C25
13	A	823	CLA	O2A-C1-C2-C3
16	F	1302	BCR	C20-C21-C22-C37
16	J	103	BCR	C35-C13-C14-C15
16	L	1006	BCR	C35-C13-C14-C15
13	A	841	CLA	C11-C10-C8-C7
13	B	809	CLA	C6-C7-C8-C10
13	B	813	CLA	C11-C10-C8-C7
13	B	828	CLA	C12-C13-C15-C16
13	L	1002	CLA	C11-C10-C8-C7
14	A	847	PQN	C15-C16-C17-C18
13	B	814	CLA	CBA-CGA-O2A-C1
13	A	803	CLA	C2A-CAA-CBA-CGA
13	A	811	CLA	C2A-CAA-CBA-CGA
13	A	820	CLA	C16-C17-C18-C20
13	B	837	CLA	C4-C3-C5-C6
13	A	826	CLA	O1A-CGA-O2A-C1
13	A	822	CLA	O1A-CGA-O2A-C1
13	B	831	CLA	O2A-C1-C2-C3
13	B	832	CLA	C4-C3-C5-C6
13	L	1004	CLA	C4-C3-C5-C6
13	A	835	CLA	C14-C13-C15-C16
13	B	837	CLA	C2-C3-C5-C6
13	B	828	CLA	C2A-CAA-CBA-CGA
13	B	814	CLA	C3-C5-C6-C7
13	L	1002	CLA	C3-C5-C6-C7
13	B	814	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	A	843	CLA	C3-C5-C6-C7
13	A	809	CLA	C4B-C3B-CAB-CBB
13	A	810	CLA	C1A-C2A-CAA-CBA
13	A	811	CLA	C4B-C3B-CAB-CBB
13	A	821	CLA	C4B-C3B-CAB-CBB
13	A	822	CLA	C1A-C2A-CAA-CBA
13	A	825	CLA	C1A-C2A-CAA-CBA
13	A	828	CLA	C4B-C3B-CAB-CBB
13	A	831	CLA	C4B-C3B-CAB-CBB
13	A	839	CLA	C4B-C3B-CAB-CBB
13	A	840	CLA	C4B-C3B-CAB-CBB
13	A	844	CLA	C1A-C2A-CAA-CBA
13	A	845	CLA	C1A-C2A-CAA-CBA
13	B	819	CLA	C4B-C3B-CAB-CBB
13	B	827	CLA	C4B-C3B-CAB-CBB
13	B	831	CLA	C4B-C3B-CAB-CBB
13	B	839	CLA	C4B-C3B-CAB-CBB
13	K	1401	CLA	C4B-C3B-CAB-CBB
13	L	1002	CLA	C4B-C3B-CAB-CBB
13	A	805	CLA	C4-C3-C5-C6
16	B	845	BCR	C22-C23-C24-C25
13	L	1004	CLA	C2-C3-C5-C6
13	A	824	CLA	C2-C3-C5-C6
13	A	838	CLA	C2-C3-C5-C6
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	B	832	CLA	C11-C10-C8-C7
18	B	850	LMG	C41-C42-C43-C44
13	A	820	CLA	C16-C17-C18-C19
13	B	832	CLA	C16-C17-C18-C20
13	B	806	CLA	C5-C6-C7-C8
13	A	841	CLA	C11-C10-C8-C9
13	B	813	CLA	C11-C10-C8-C9
13	L	1003	CLA	C11-C10-C8-C9
13	A	844	CLA	O1D-CGD-O2D-CED
13	B	831	CLA	C1-C2-C3-C4
13	B	810	CLA	C4-C3-C5-C6
13	B	813	CLA	C4-C3-C5-C6
13	B	827	CLA	C4-C3-C5-C6
13	B	805	CLA	CAD-CBD-CGD-O2D
13	A	819	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	B	812	CLA	C2A-CAA-CBA-CGA
13	B	820	CLA	C2A-CAA-CBA-CGA
17	A	855	LHG	C27-C28-C29-C30
13	A	804	CLA	CHA-CBD-CGD-O1D
13	A	804	CLA	CHA-CBD-CGD-O2D
13	A	826	CLA	CHA-CBD-CGD-O1D
13	A	826	CLA	CHA-CBD-CGD-O2D
13	B	805	CLA	CAD-CBD-CGD-O1D
13	X	1701	CLA	CHA-CBD-CGD-O1D
17	A	856	LHG	C3-O3-P-O5
13	L	1002	CLA	C4-C3-C5-C6
13	A	814	CLA	C2B-C3B-CAB-CBB
13	A	816	CLA	C2B-C3B-CAB-CBB
13	A	821	CLA	C2B-C3B-CAB-CBB
13	A	829	CLA	C2B-C3B-CAB-CBB
13	B	806	CLA	C2B-C3B-CAB-CBB
13	B	813	CLA	C2B-C3B-CAB-CBB
13	B	825	CLA	C2B-C3B-CAB-CBB
16	B	844	BCR	C23-C24-C25-C30
16	B	849	BCR	C1-C6-C7-C8
13	B	829	CLA	C10-C11-C12-C13
13	B	826	CLA	O1D-CGD-O2D-CED
13	B	825	CLA	O1A-CGA-O2A-C1
13	B	837	CLA	CBD-CGD-O2D-CED
13	A	806	CLA	C11-C10-C8-C9
13	A	807	CLA	C11-C12-C13-C14
13	A	827	CLA	C14-C13-C15-C16
13	A	834	CLA	C14-C13-C15-C16
13	B	806	CLA	C14-C13-C15-C16
13	B	827	CLA	C6-C7-C8-C9
13	B	828	CLA	C14-C13-C15-C16
13	B	832	CLA	C11-C10-C8-C9
13	A	807	CLA	C11-C12-C13-C15
13	A	834	CLA	C12-C13-C15-C16
13	L	1003	CLA	C11-C10-C8-C7
13	L	1003	CLA	C12-C13-C15-C16
16	B	845	BCR	C20-C21-C22-C23
13	A	819	CLA	O1A-CGA-O2A-C1
13	B	832	CLA	C16-C17-C18-C19
13	B	805	CLA	C15-C16-C17-C18
13	A	835	CLA	C2A-CAA-CBA-CGA
13	A	839	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	A	807	CLA	CAA-CBA-CGA-O2A
13	B	803	CLA	C10-C11-C12-C13
13	A	817	CLA	C2A-CAA-CBA-CGA
18	B	850	LMG	C34-C35-C36-C37
17	A	855	LHG	C1-C2-C3-O3
13	L	1004	CLA	C3-C5-C6-C7
13	A	820	CLA	C11-C12-C13-C14
13	B	805	CLA	C14-C13-C15-C16
13	B	802	CLA	C13-C15-C16-C17
13	B	810	CLA	C13-C15-C16-C17
13	A	806	CLA	C4B-C3B-CAB-CBB
13	A	818	CLA	C4B-C3B-CAB-CBB
13	B	816	CLA	C4B-C3B-CAB-CBB
13	J	102	CLA	C4B-C3B-CAB-CBB
13	A	844	CLA	C5-C6-C7-C8
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	813	CLA	C2-C3-C5-C6
13	L	1002	CLA	C2-C3-C5-C6
13	B	801	CLA	C12-C13-C15-C16
13	B	809	CLA	C12-C13-C15-C16
13	A	824	CLA	C3A-C2A-CAA-CBA
13	A	836	CLA	C3A-C2A-CAA-CBA
16	A	854	BCR	C11-C10-C9-C34
16	A	854	BCR	C16-C17-C18-C36
16	B	844	BCR	C11-C10-C9-C34
16	F	1302	BCR	C35-C13-C14-C15
13	A	810	CLA	C10-C11-C12-C13
13	A	814	CLA	C2-C1-O2A-CGA
13	B	810	CLA	C2-C3-C5-C6
13	B	827	CLA	C2-C3-C5-C6
13	A	812	CLA	C10-C11-C12-C13
13	M	1601	CLA	C2A-CAA-CBA-CGA
17	A	855	LHG	C26-C27-C28-C29
13	B	827	CLA	O1D-CGD-O2D-CED
13	J	101	CLA	CAA-CBA-CGA-O1A
13	A	825	CLA	C6-C7-C8-C9
13	A	831	CLA	C11-C10-C8-C9
13	B	809	CLA	C14-C13-C15-C16
13	B	814	CLA	C11-C12-C13-C14
13	A	841	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	A	839	CLA	C2-C3-C5-C6
13	B	830	CLA	CAA-CBA-CGA-O2A
13	A	809	CLA	C2A-CAA-CBA-CGA
13	A	827	CLA	C1A-C2A-CAA-CBA
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	B	823	CLA	CAA-CBA-CGA-O2A
18	B	850	LMG	C15-C16-C17-C18
13	A	806	CLA	C2B-C3B-CAB-CBB
13	A	811	CLA	C2B-C3B-CAB-CBB
13	A	815	CLA	C2B-C3B-CAB-CBB
13	A	819	CLA	C2B-C3B-CAB-CBB
13	A	826	CLA	C2B-C3B-CAB-CBB
13	A	833	CLA	C2B-C3B-CAB-CBB
13	A	840	CLA	C2B-C3B-CAB-CBB
13	B	805	CLA	C2B-C3B-CAB-CBB
13	B	811	CLA	C2B-C3B-CAB-CBB
13	B	817	CLA	C2B-C3B-CAB-CBB
13	B	819	CLA	C2B-C3B-CAB-CBB
13	B	822	CLA	C2B-C3B-CAB-CBB
13	B	824	CLA	C2B-C3B-CAB-CBB
13	B	828	CLA	C2B-C3B-CAB-CBB
13	B	830	CLA	C2B-C3B-CAB-CBB
13	B	834	CLA	C2B-C3B-CAB-CBB
13	B	838	CLA	C2B-C3B-CAB-CBB
13	B	839	CLA	C2B-C3B-CAB-CBB
13	K	1401	CLA	C2B-C3B-CAB-CBB
16	A	853	BCR	C5-C6-C7-C8
16	F	1302	BCR	C23-C24-C25-C30
16	I	102	BCR	C23-C24-C25-C26
16	M	1602	BCR	C23-C24-C25-C30
13	B	836	CLA	CAA-CBA-CGA-O2A
13	X	1701	CLA	CAA-CBA-CGA-O2A
13	M	1601	CLA	CAA-CBA-CGA-O1A
13	A	802	CLA	C4-C3-C5-C6
13	A	810	CLA	C4-C3-C5-C6
13	A	814	CLA	C4-C3-C5-C6
13	B	808	CLA	C4-C3-C5-C6
13	B	809	CLA	C4-C3-C5-C6
13	B	826	CLA	C4-C3-C5-C6
13	A	820	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	A	828	CLA	C2-C3-C5-C6
17	A	855	LHG	C19-C20-C21-C22
13	B	830	CLA	CAA-CBA-CGA-O1A
13	B	836	CLA	CAA-CBA-CGA-O1A
18	B	850	LMG	C31-C32-C33-C34
13	A	814	CLA	C11-C10-C8-C7
13	A	820	CLA	C11-C12-C13-C15
13	A	827	CLA	C12-C13-C15-C16
13	B	826	CLA	C6-C7-C8-C10
13	A	803	CLA	C8-C10-C11-C12
13	B	821	CLA	CAA-CBA-CGA-O1A
13	B	821	CLA	CAA-CBA-CGA-O2A
13	X	1701	CLA	CAA-CBA-CGA-O1A
13	A	809	CLA	C4-C3-C5-C6
13	A	810	CLA	C2-C3-C5-C6
13	B	809	CLA	C2-C3-C5-C6
13	B	823	CLA	CAA-CBA-CGA-O1A
13	B	822	CLA	C5-C6-C7-C8
13	J	101	CLA	CAA-CBA-CGA-O2A
13	B	826	CLA	C6-C7-C8-C9
13	A	812	CLA	C4-C3-C5-C6
13	A	825	CLA	C4-C3-C5-C6
13	B	829	CLA	C4-C3-C5-C6
13	M	1601	CLA	CAA-CBA-CGA-O2A
13	B	829	CLA	C2-C3-C5-C6
13	B	817	CLA	C8-C10-C11-C12
14	B	842	PQN	C23-C25-C26-C27
13	A	828	CLA	C3-C5-C6-C7
13	A	834	CLA	C13-C15-C16-C17
13	A	827	CLA	O1D-CGD-O2D-CED
17	A	855	LHG	O9-C7-O7-C5
13	A	803	CLA	C4-C3-C5-C6
13	A	819	CLA	C4-C3-C5-C6
13	B	822	CLA	C4-C3-C5-C6
13	B	810	CLA	C10-C11-C12-C13
13	B	805	CLA	C4B-C3B-CAB-CBB
13	X	1701	CLA	C4B-C3B-CAB-CBB
13	F	1301	CLA	CAA-CBA-CGA-O2A
16	B	845	BCR	C11-C10-C9-C34
16	B	845	BCR	C20-C21-C22-C37
16	J	105	BCR	C20-C21-C22-C37
13	A	822	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	A	814	CLA	C2-C3-C5-C6
13	A	831	CLA	C11-C10-C8-C7
13	A	819	CLA	CAA-CBA-CGA-O1A
13	B	801	CLA	C14-C13-C15-C16
13	B	808	CLA	C14-C13-C15-C16
13	A	827	CLA	C3A-C2A-CAA-CBA
13	A	802	CLA	C2-C3-C5-C6
13	B	808	CLA	C2-C3-C5-C6
17	A	855	LHG	C11-C10-C9-C8
13	F	1301	CLA	CAA-CBA-CGA-O1A
13	B	806	CLA	C16-C17-C18-C20
16	B	845	BCR	C11-C10-C9-C8
13	A	821	CLA	C8-C10-C11-C12
13	A	827	CLA	C4-C3-C5-C6
13	J	101	CLA	C2A-CAA-CBA-CGA
13	A	844	CLA	CBD-CGD-O2D-CED
13	K	1401	CLA	CAA-CBA-CGA-O1A
13	A	821	CLA	C6-C7-C8-C9
13	B	809	CLA	C6-C7-C8-C9
13	A	803	CLA	C2-C3-C5-C6
13	K	1401	CLA	CAA-CBA-CGA-O2A
13	B	816	CLA	C2A-CAA-CBA-CGA
13	A	821	CLA	C6-C7-C8-C10
13	B	813	CLA	C6-C7-C8-C10
14	A	847	PQN	C16-C17-C18-C20
13	A	811	CLA	CAA-CBA-CGA-O1A
13	A	803	CLA	C2B-C3B-CAB-CBB
13	A	807	CLA	C2B-C3B-CAB-CBB
13	A	827	CLA	C2B-C3B-CAB-CBB
13	A	831	CLA	C2B-C3B-CAB-CBB
16	B	849	BCR	C5-C6-C7-C8
16	F	1302	BCR	C23-C24-C25-C26
16	J	105	BCR	C23-C24-C25-C30
13	B	809	CLA	C2-C1-O2A-CGA
13	B	827	CLA	C2-C1-O2A-CGA
13	B	841	CLA	C2-C1-O2A-CGA
17	A	855	LHG	C11-C12-C13-C14
17	A	855	LHG	C13-C14-C15-C16
13	A	821	CLA	C4-C3-C5-C6
17	A	856	LHG	O7-C7-C8-C9
13	X	1701	CLA	C2A-CAA-CBA-CGA
17	A	855	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
13	A	825	CLA	C11-C12-C13-C14
13	A	803	CLA	CAA-CBA-CGA-O2A
13	A	805	CLA	CAA-CBA-CGA-O2A
13	B	806	CLA	CAA-CBA-CGA-O2A
13	B	824	CLA	C6-C7-C8-C9
13	A	814	CLA	O1A-CGA-O2A-C1
13	A	826	CLA	CAA-CBA-CGA-O2A
13	A	829	CLA	CAA-CBA-CGA-O2A
13	B	827	CLA	C2A-CAA-CBA-CGA
13	B	815	CLA	CAA-CBA-CGA-O2A
13	A	835	CLA	C13-C15-C16-C17
13	B	822	CLA	CAA-CBA-CGA-O2A
13	B	832	CLA	CAA-CBA-CGA-O2A
17	A	855	LHG	C25-C26-C27-C28
13	A	812	CLA	CAA-CBA-CGA-O2A
13	B	806	CLA	C16-C17-C18-C19
13	A	807	CLA	C4B-C3B-CAB-CBB
13	A	808	CLA	C4B-C3B-CAB-CBB
13	A	812	CLA	C4B-C3B-CAB-CBB
13	A	814	CLA	C1A-C2A-CAA-CBA
13	A	824	CLA	C1A-C2A-CAA-CBA
13	A	833	CLA	C4B-C3B-CAB-CBB
13	A	838	CLA	C1A-C2A-CAA-CBA
13	A	845	CLA	C4B-C3B-CAB-CBB
13	A	846	CLA	C4B-C3B-CAB-CBB
13	B	820	CLA	C4B-C3B-CAB-CBB
13	B	837	CLA	C1A-C2A-CAA-CBA
13	J	101	CLA	C4B-C3B-CAB-CBB
17	A	856	LHG	O10-C23-O8-C6
13	A	822	CLA	C13-C15-C16-C17
13	B	813	CLA	CAA-CBA-CGA-O2A
13	A	808	CLA	CAA-CBA-CGA-O2A
13	A	846	CLA	CAA-CBA-CGA-O2A
13	A	805	CLA	C2-C1-O2A-CGA
13	A	822	CLA	C2-C1-O2A-CGA
13	A	846	CLA	C2-C1-O2A-CGA
13	B	814	CLA	C2-C1-O2A-CGA
13	B	828	CLA	C2-C1-O2A-CGA
13	A	839	CLA	C12-C13-C15-C16
13	A	819	CLA	C2-C3-C5-C6
13	A	811	CLA	CAA-CBA-CGA-O2A
13	A	802	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	A	807	CLA	C2A-CAA-CBA-CGA
13	L	1004	CLA	C2A-CAA-CBA-CGA
13	B	829	CLA	C8-C10-C11-C12
17	A	856	LHG	O8-C23-C24-C25
13	B	822	CLA	C2-C3-C5-C6
13	B	815	CLA	CAA-CBA-CGA-O1A
13	A	830	CLA	C13-C15-C16-C17
17	A	856	LHG	C24-C23-O8-C6
13	L	1002	CLA	C8-C10-C11-C12
13	A	805	CLA	CAA-CBA-CGA-O1A
13	A	808	CLA	C2A-CAA-CBA-CGA
13	A	814	CLA	CBA-CGA-O2A-C1
13	A	814	CLA	C11-C10-C8-C9
13	A	820	CLA	C11-C10-C8-C9
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	L	1003	CLA	C14-C13-C15-C16
14	A	847	PQN	C16-C17-C18-C19
13	B	827	CLA	C5-C6-C7-C8
13	A	831	CLA	C4-C3-C5-C6
13	B	806	CLA	CAA-CBA-CGA-O1A
13	A	808	CLA	CAA-CBA-CGA-O1A
13	B	832	CLA	CAA-CBA-CGA-O1A
13	B	812	CLA	CAA-CBA-CGA-O1A
13	A	803	CLA	CAA-CBA-CGA-O1A
13	A	829	CLA	CAA-CBA-CGA-O1A
13	A	821	CLA	CAA-CBA-CGA-O2A
13	A	826	CLA	CAA-CBA-CGA-O1A
17	A	856	LHG	O9-C7-C8-C9
13	A	801	CLA	CAD-CBD-CGD-O2D
13	A	838	CLA	C2-C1-O2A-CGA
13	A	815	CLA	O1D-CGD-O2D-CED
13	A	801	CLA	CAA-CBA-CGA-O2A
13	A	824	CLA	CAA-CBA-CGA-O2A
18	B	850	LMG	C16-C17-C18-C19
13	A	824	CLA	CAA-CBA-CGA-O1A
13	B	822	CLA	CAA-CBA-CGA-O1A
13	B	838	CLA	C11-C12-C13-C15
13	B	814	CLA	CAA-CBA-CGA-O2A
13	A	802	CLA	C16-C17-C18-C19
13	A	812	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	A	821	CLA	CAA-CBA-CGA-O1A
13	B	813	CLA	CAA-CBA-CGA-O1A
13	B	803	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

107 monomers are involved in 302 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	808	CLA	2	0
13	B	839	CLA	4	0
14	B	842	PQN	1	0
13	B	825	CLA	2	0
13	A	829	CLA	12	0
16	B	843	BCR	1	0
13	K	1401	CLA	1	0
13	A	833	CLA	1	0
13	A	806	CLA	6	0
16	A	851	BCR	1	0
13	A	809	CLA	5	0
13	A	837	CLA	1	0
13	A	822	CLA	2	0
13	A	839	CLA	5	0
13	A	810	CLA	3	0
13	B	805	CLA	4	0
16	A	850	BCR	2	0
16	J	105	BCR	5	0
13	A	820	CLA	3	0
16	B	845	BCR	4	0
13	A	828	CLA	2	0
16	J	104	BCR	7	0
13	A	846	CLA	4	0
16	A	854	BCR	12	0
13	X	1701	CLA	1	0
13	B	831	CLA	3	0
13	B	815	CLA	1	0
13	A	817	CLA	1	0
16	M	1602	BCR	2	0
13	B	838	CLA	3	0
13	A	840	CLA	3	0
13	A	814	CLA	1	0
13	B	824	CLA	8	0
13	B	818	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	853	BCR	1	0
13	B	813	CLA	5	0
13	B	822	CLA	4	0
13	B	801	CLA	7	0
13	B	817	CLA	7	0
16	J	103	BCR	4	0
13	F	1301	CLA	1	0
13	B	809	CLA	2	0
17	A	855	LHG	4	0
13	A	838	CLA	3	0
13	B	807	CLA	1	0
14	A	847	PQN	1	0
13	A	843	CLA	9	0
13	B	819	CLA	1	0
13	A	827	CLA	6	0
13	B	804	CLA	1	0
16	B	849	BCR	1	0
13	B	829	CLA	5	0
13	A	830	CLA	2	0
13	A	807	CLA	3	0
13	A	812	CLA	1	0
13	B	828	CLA	8	0
13	A	803	CLA	11	0
13	A	841	CLA	2	0
13	B	808	CLA	1	0
16	B	846	BCR	5	0
13	A	835	CLA	4	0
16	F	1302	BCR	2	0
13	B	833	CLA	5	0
13	A	821	CLA	4	0
13	A	823	CLA	2	0
13	B	810	CLA	5	0
13	M	1601	CLA	1	0
13	L	1004	CLA	2	0
17	A	856	LHG	2	0
13	J	101	CLA	1	0
13	L	1002	CLA	2	0
16	A	852	BCR	4	0
13	A	834	CLA	1	0
13	A	845	CLA	1	0
13	A	825	CLA	2	0
13	B	826	CLA	3	0

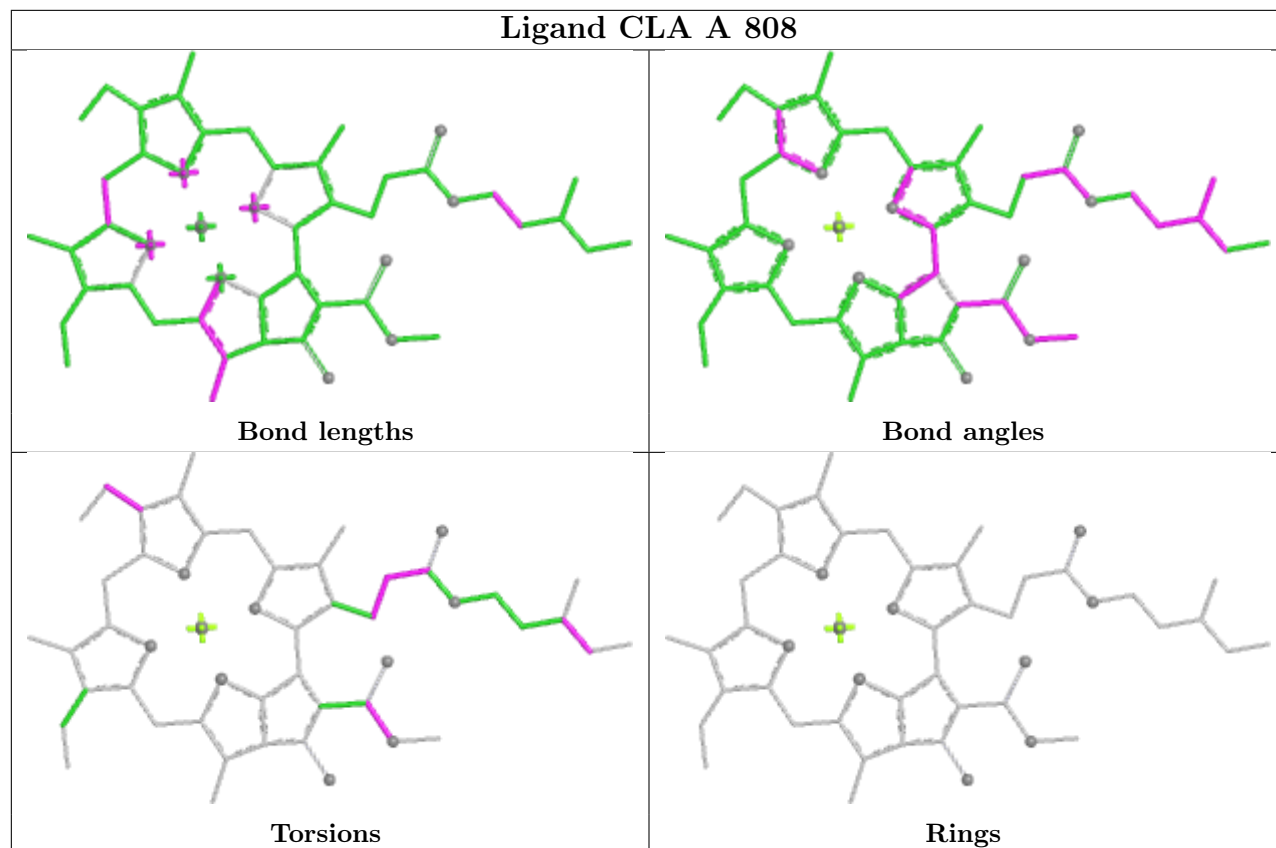
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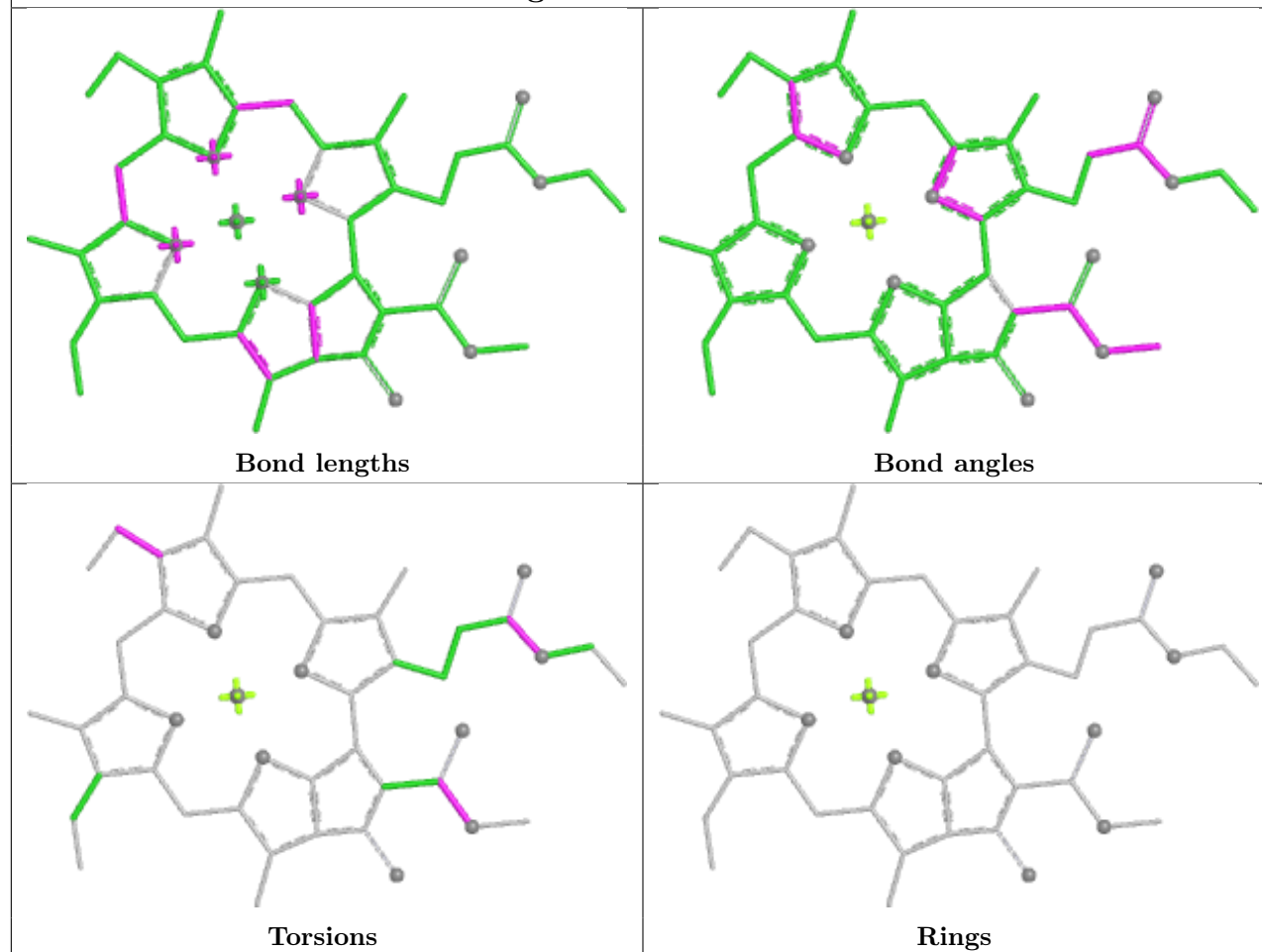
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	831	CLA	5	0
16	B	848	BCR	1	0
13	B	823	CLA	3	0
13	A	815	CLA	4	0
13	A	844	CLA	4	0
13	L	1003	CLA	7	0
13	B	802	CLA	17	0
13	A	826	CLA	4	0
13	B	803	CLA	4	0
13	A	836	CLA	2	0
16	B	847	BCR	2	0
13	B	832	CLA	4	0
13	B	814	CLA	5	0
13	B	820	CLA	3	0
16	I	101	BCR	4	0
13	A	801	CLA	9	0
16	L	1006	BCR	1	0
18	B	850	LMG	5	0
17	B	851	LHG	1	0
13	A	802	CLA	2	0
13	B	806	CLA	6	0
13	B	840	CLA	3	0
13	A	819	CLA	3	0
13	B	816	CLA	3	0
16	B	844	BCR	1	0
13	A	811	CLA	3	0
13	A	804	CLA	2	0
16	A	849	BCR	2	0
13	B	830	CLA	3	0
13	B	837	CLA	2	0
13	B	827	CLA	5	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

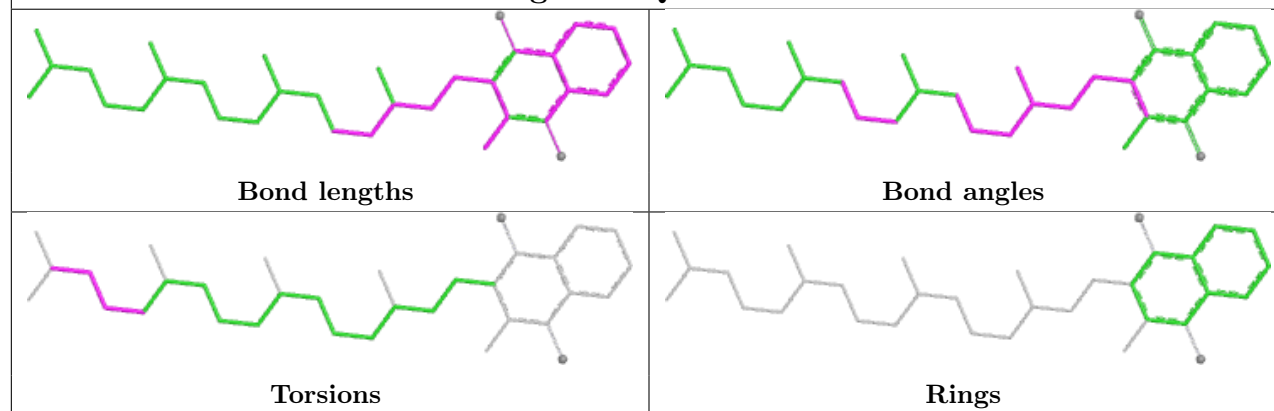
equivalents in the CSD to analyse the geometry.



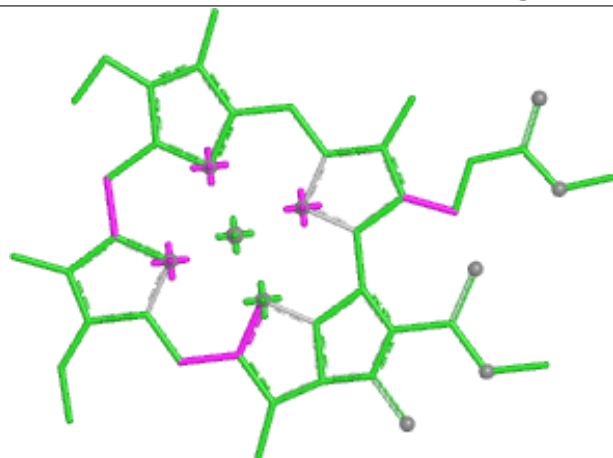
Ligand CLA B 839



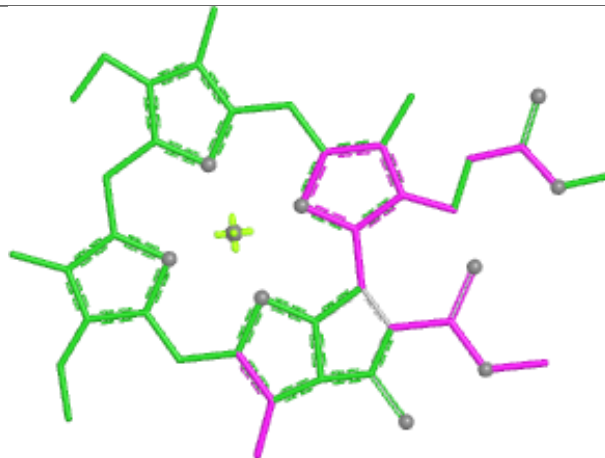
Ligand PQN B 842



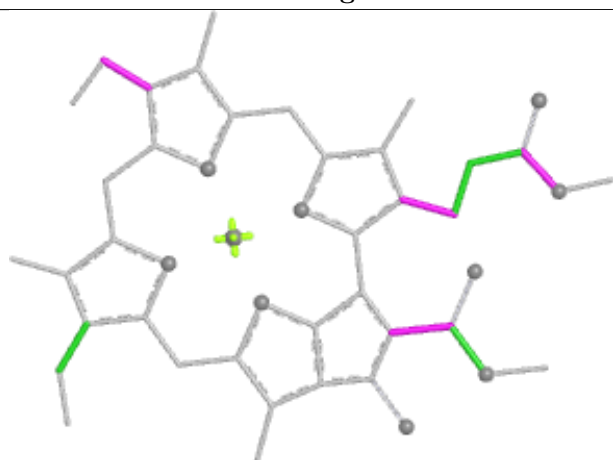
Ligand CLA B 825



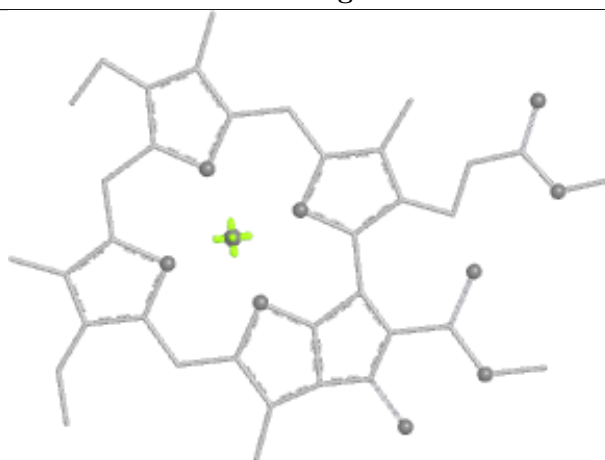
Bond lengths



Bond angles

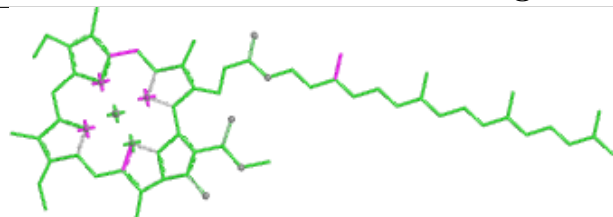


Torsions

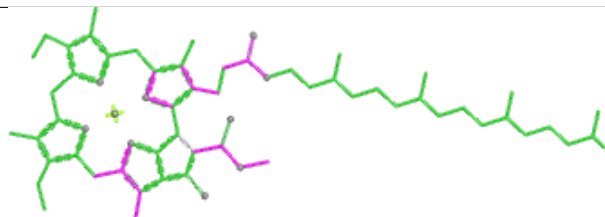


Rings

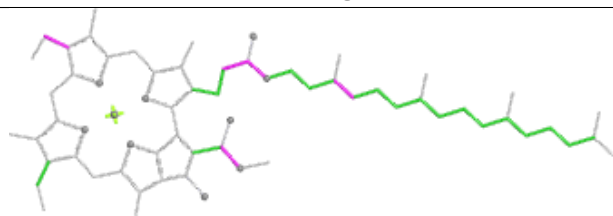
Ligand CLA A 829



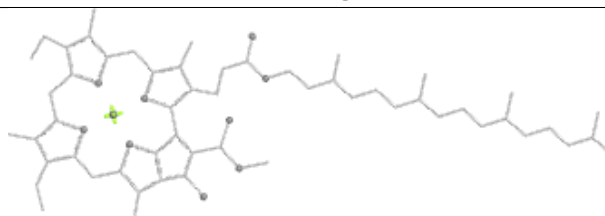
Bond lengths



Bond angles

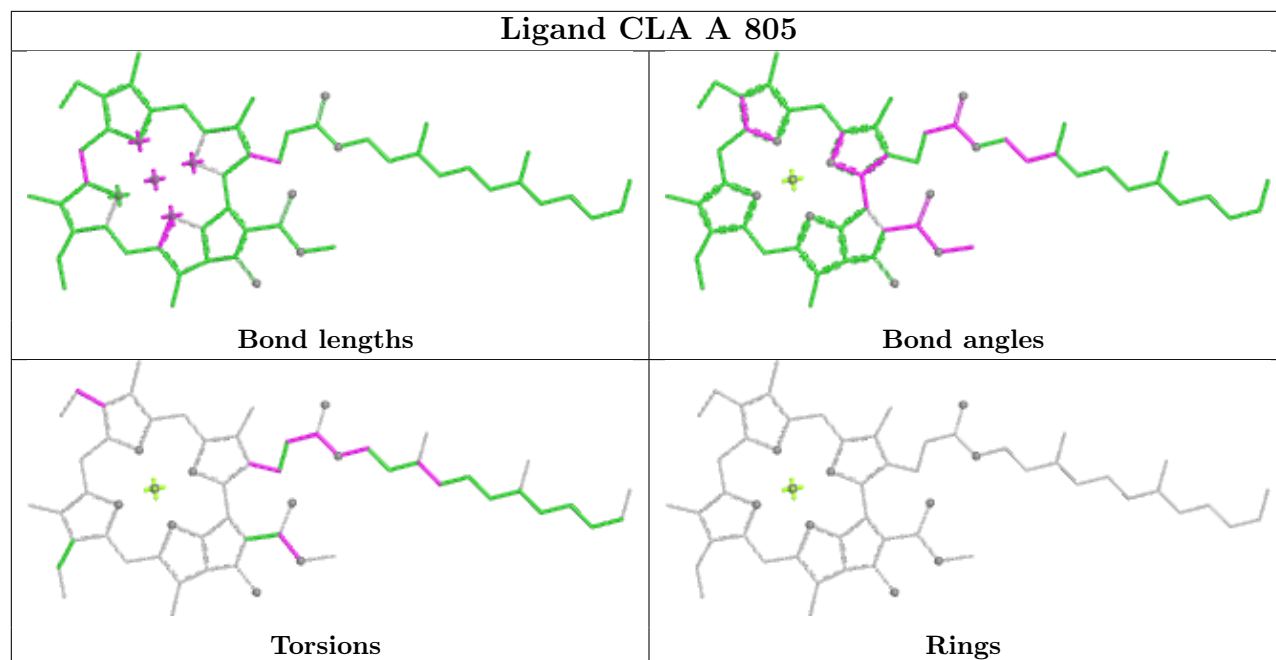


Torsions

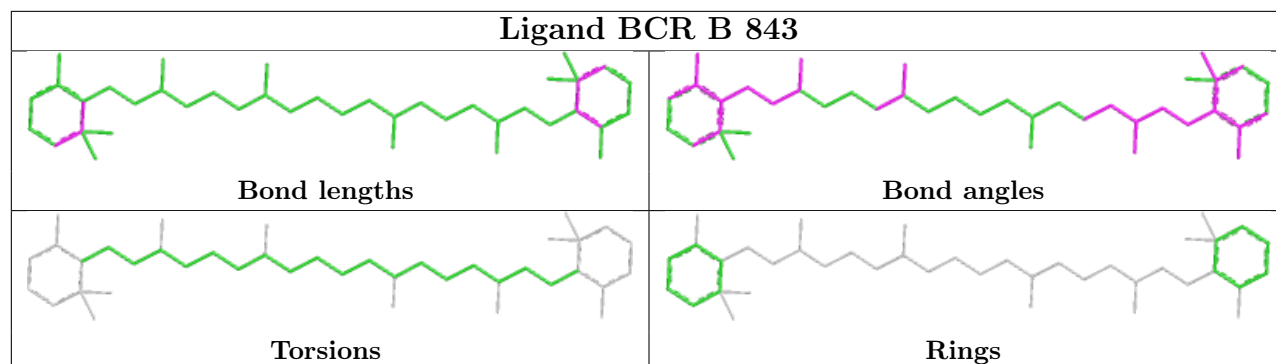


Rings

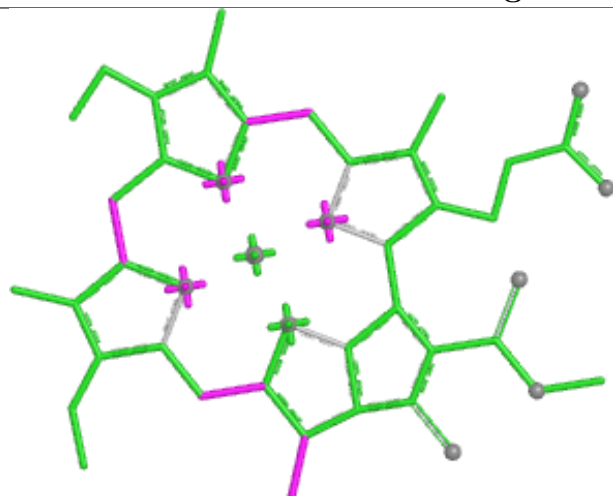
Ligand CLA A 805



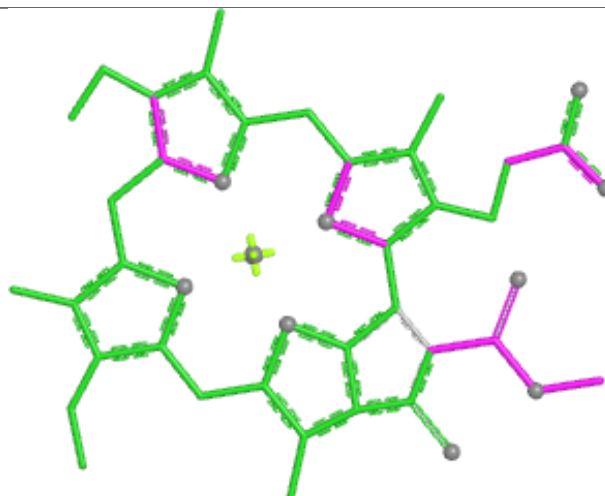
Ligand BCR B 843



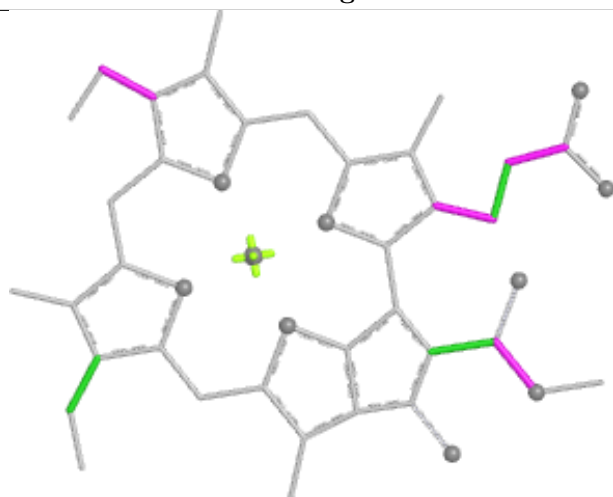
Ligand CLA K 1401



Bond lengths



Bond angles

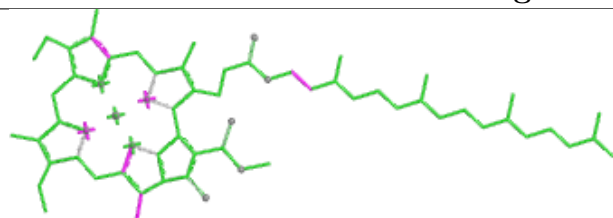


Torsions

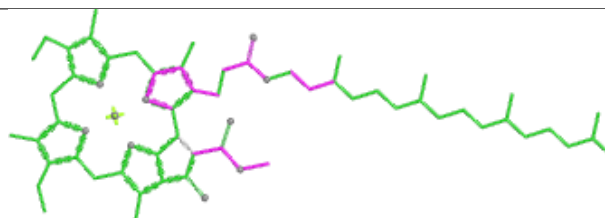


Rings

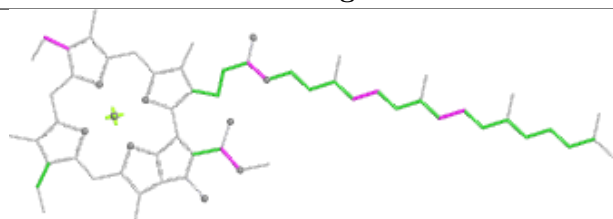
Ligand CLA A 833



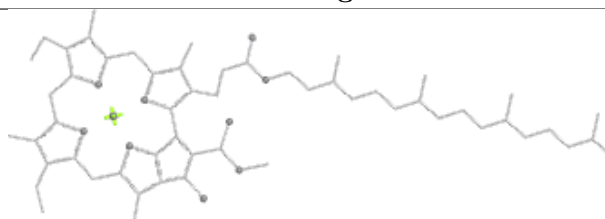
Bond lengths



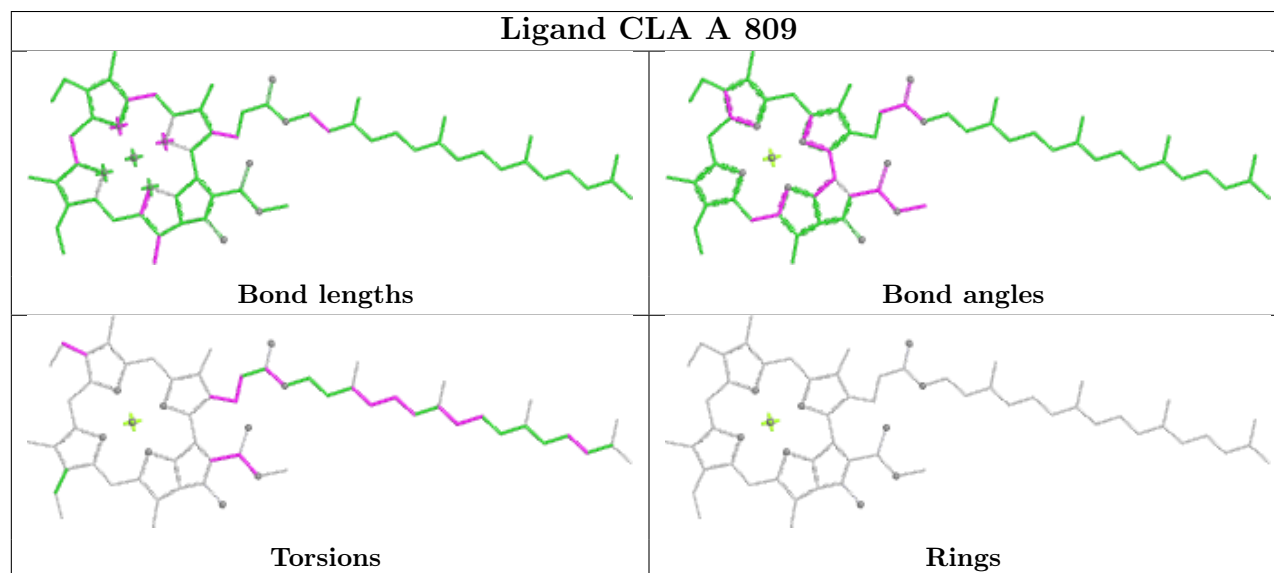
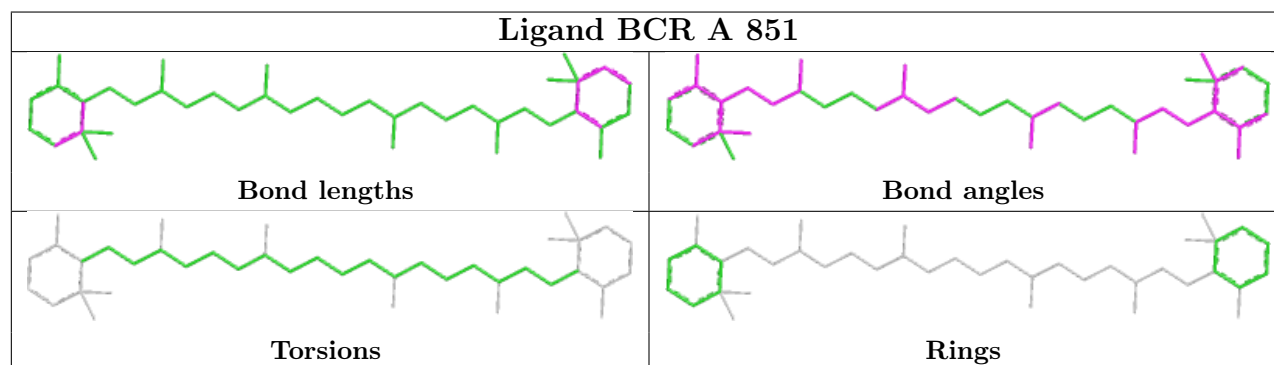
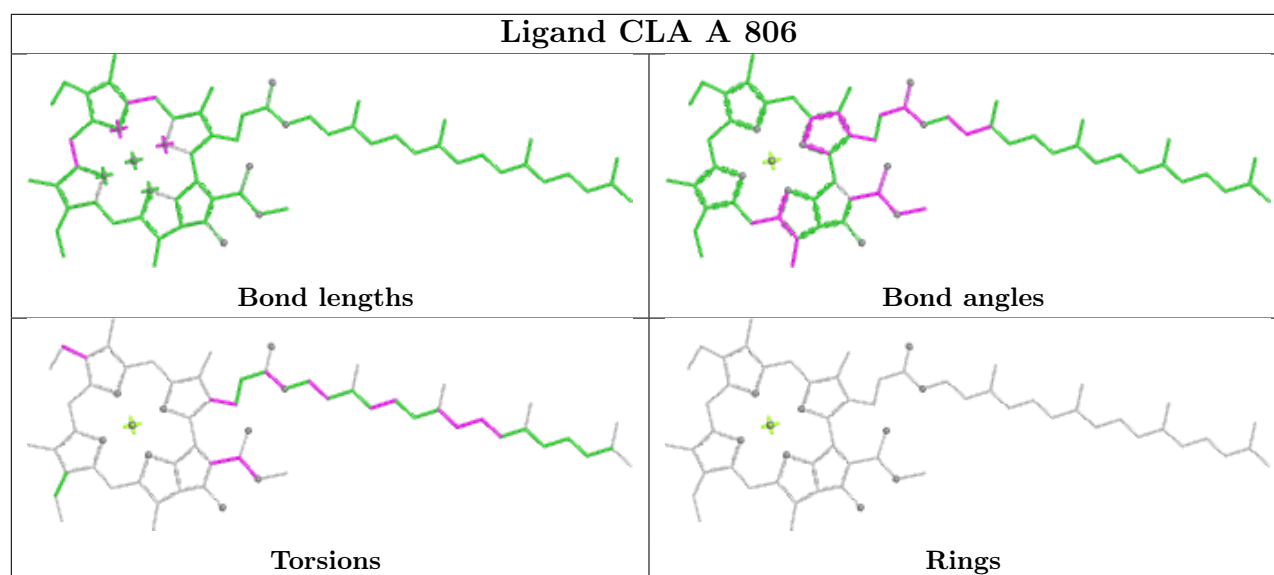
Bond angles

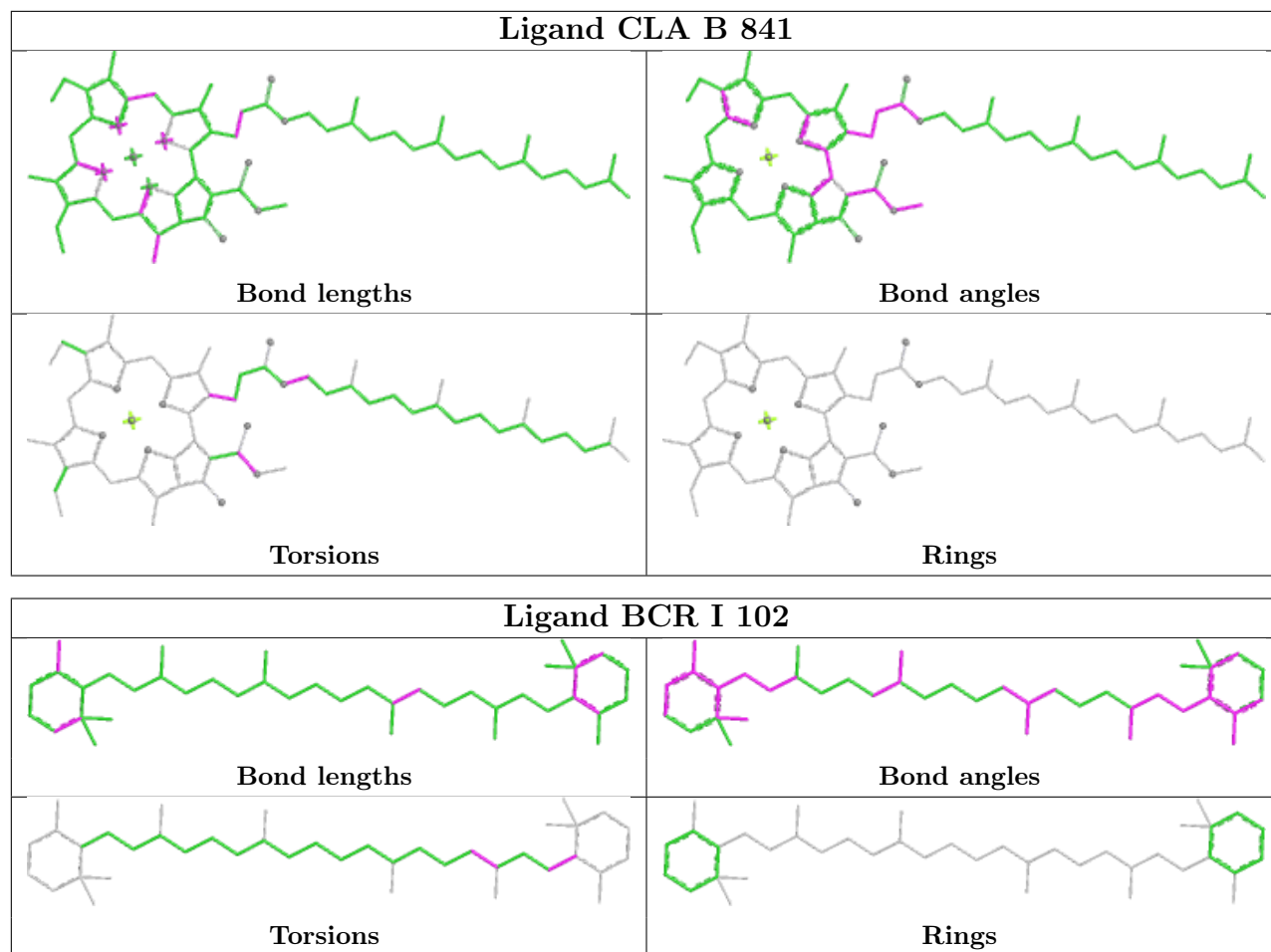


Torsions

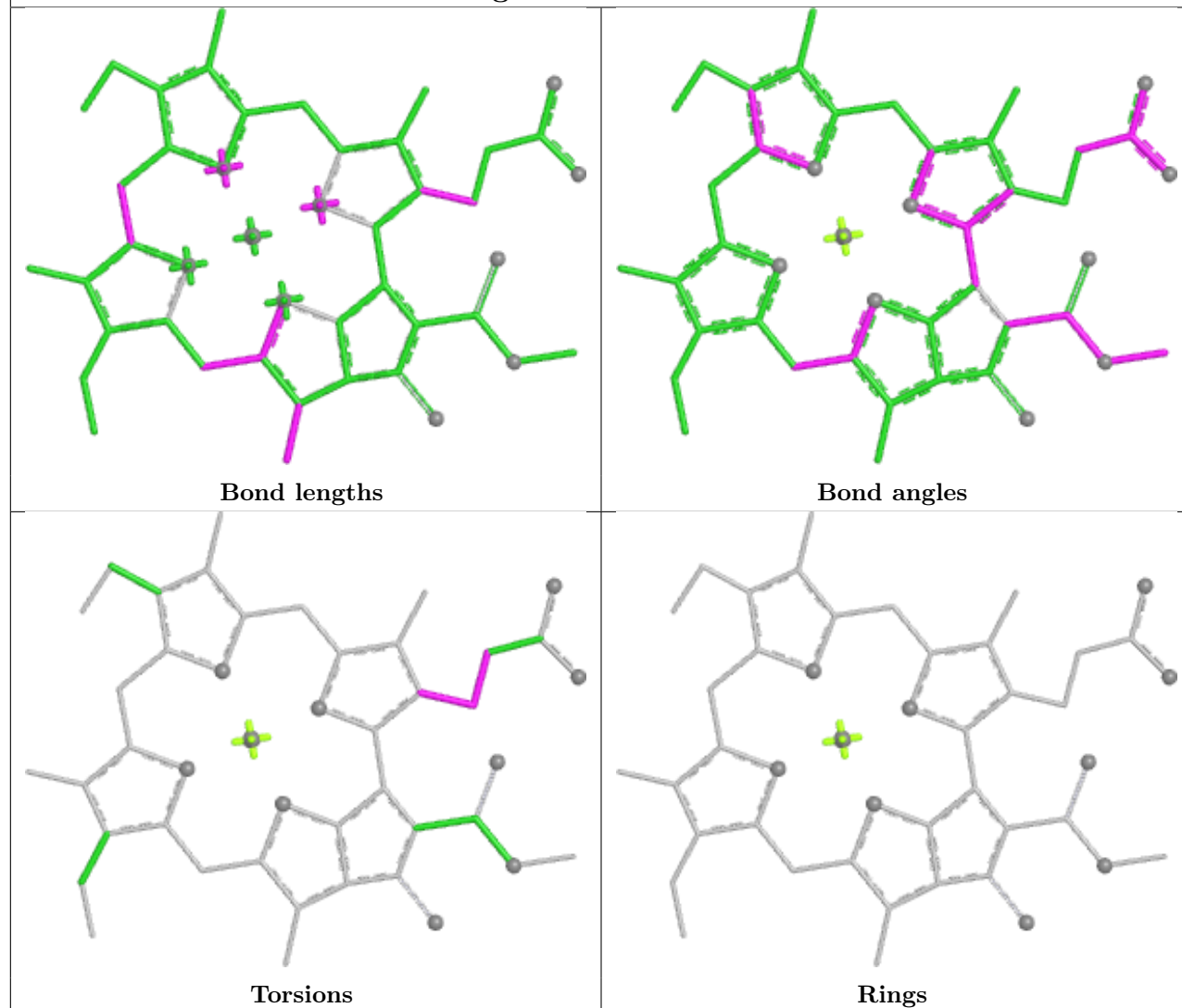


Rings

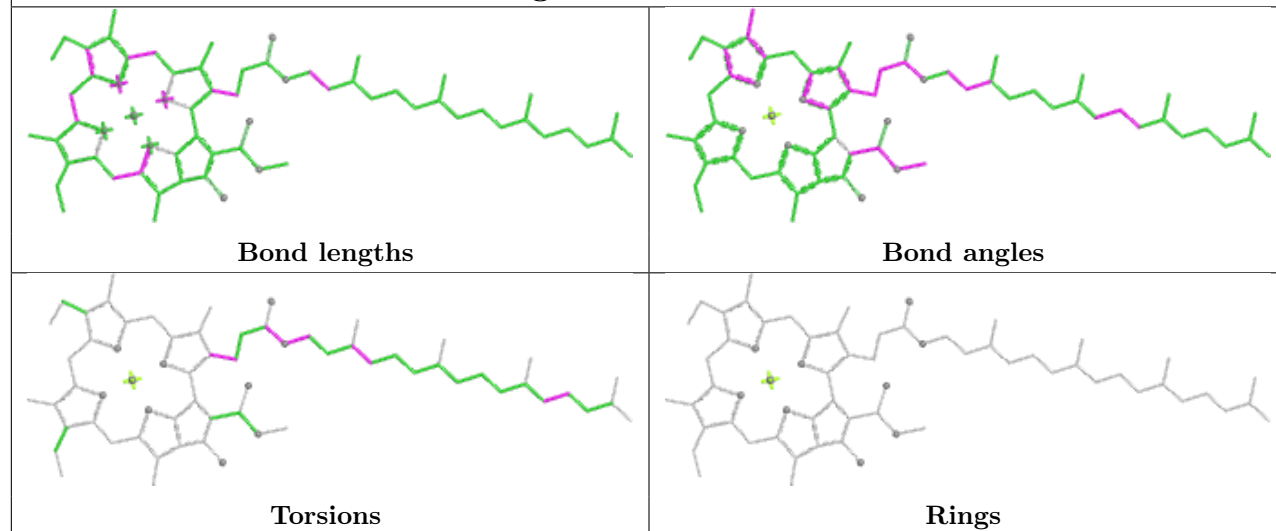




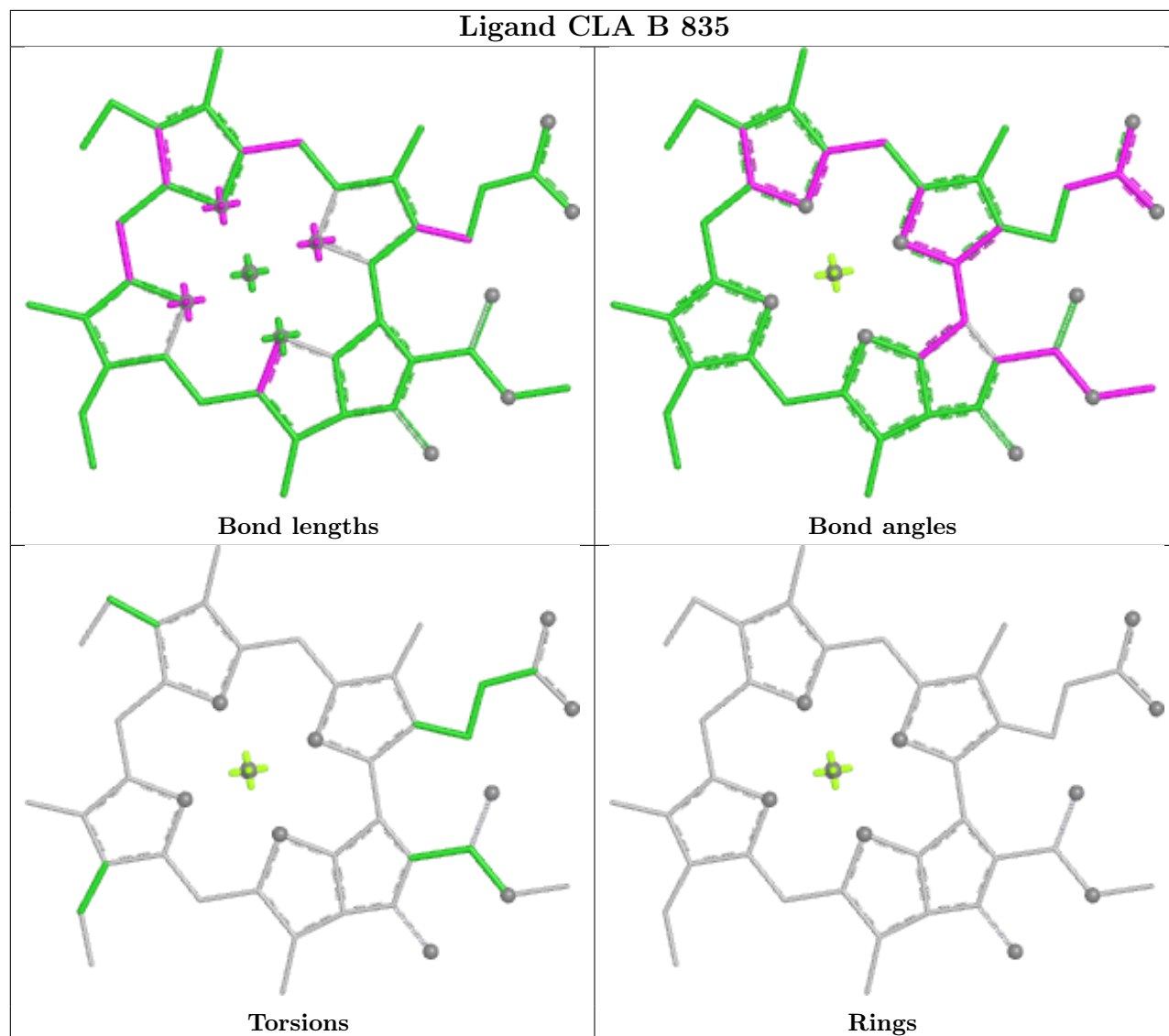
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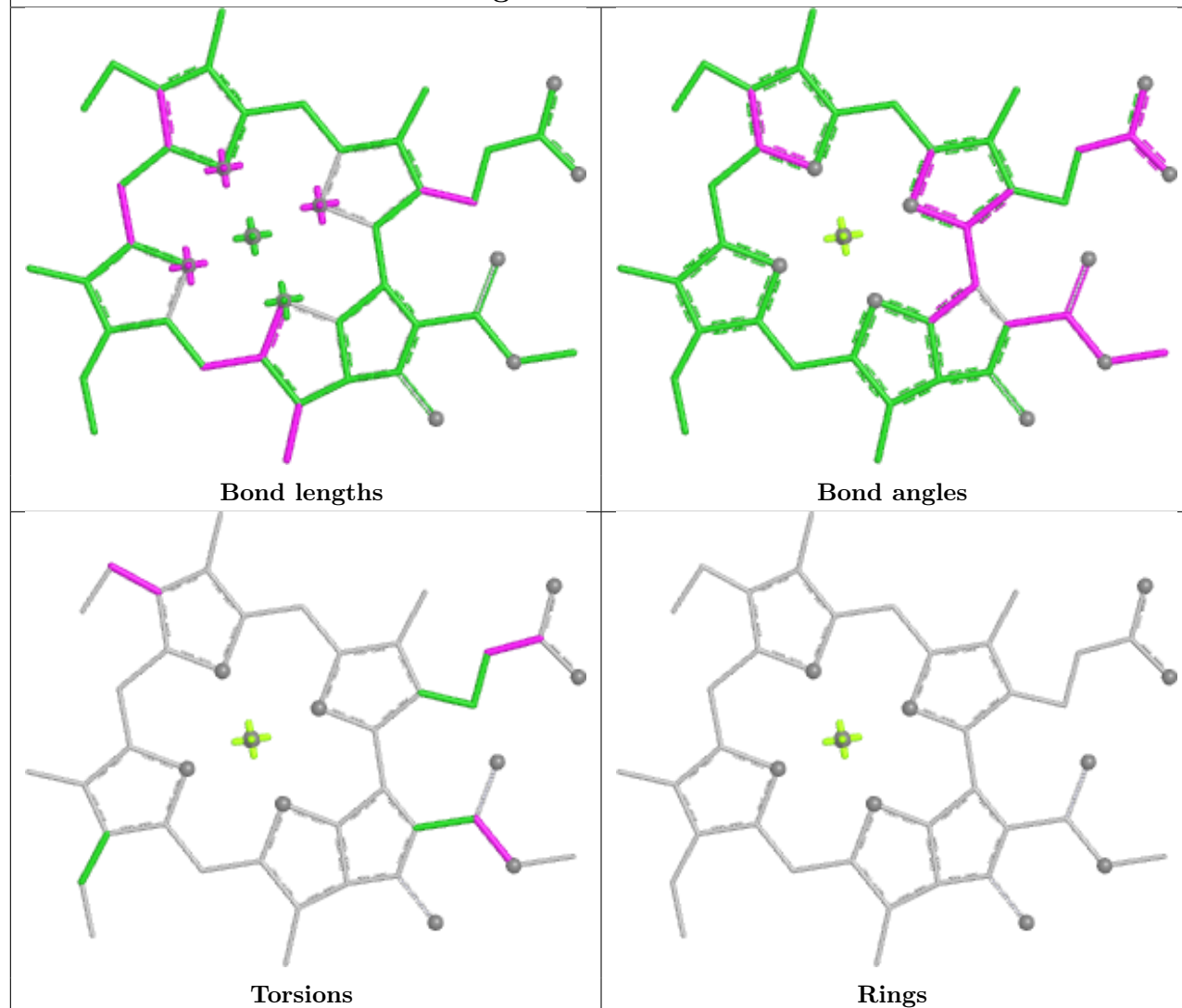
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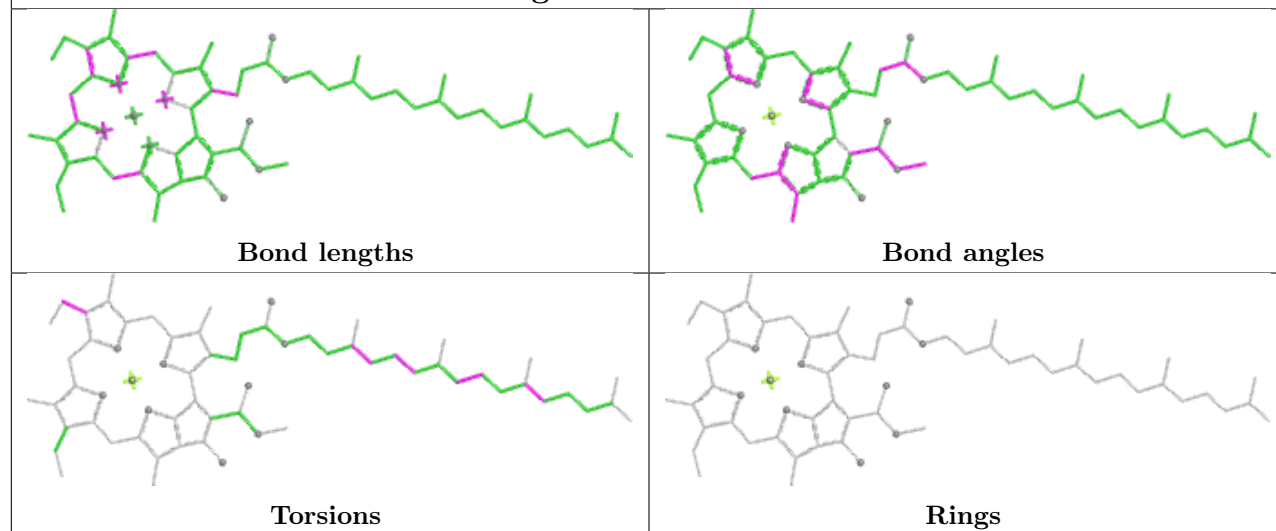
Ligand CLA B 835



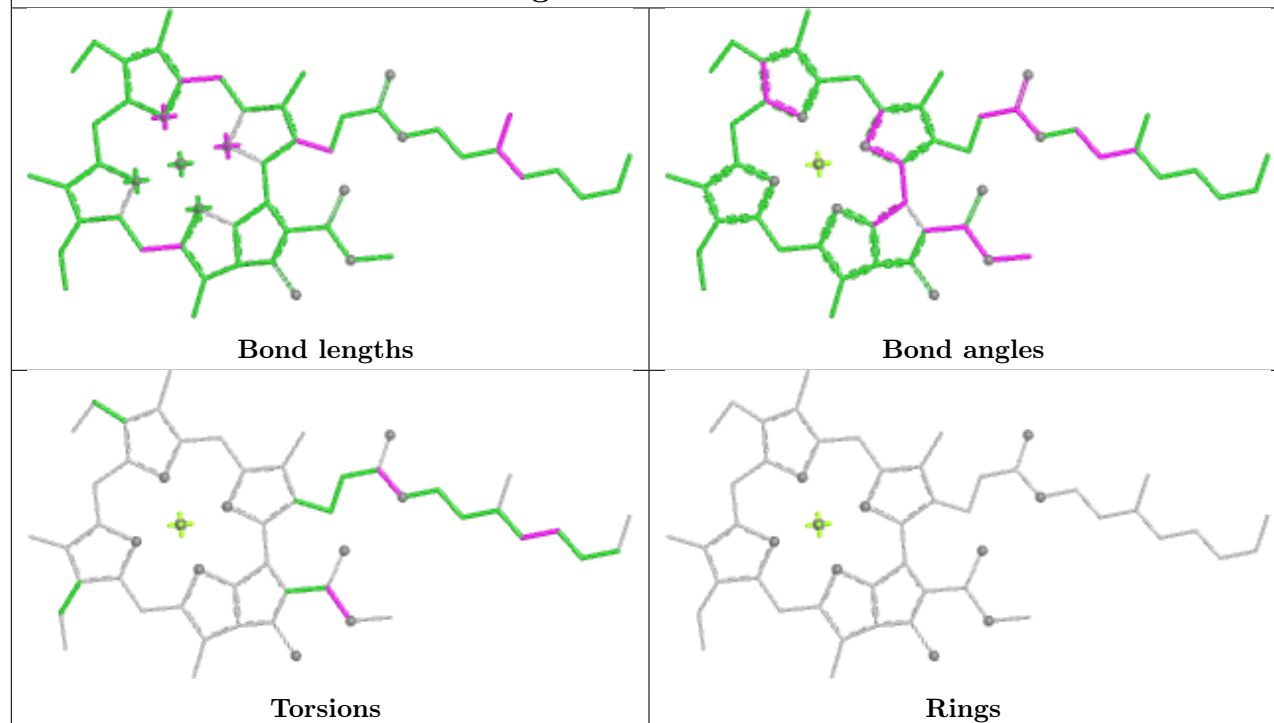
Ligand CLA B 821



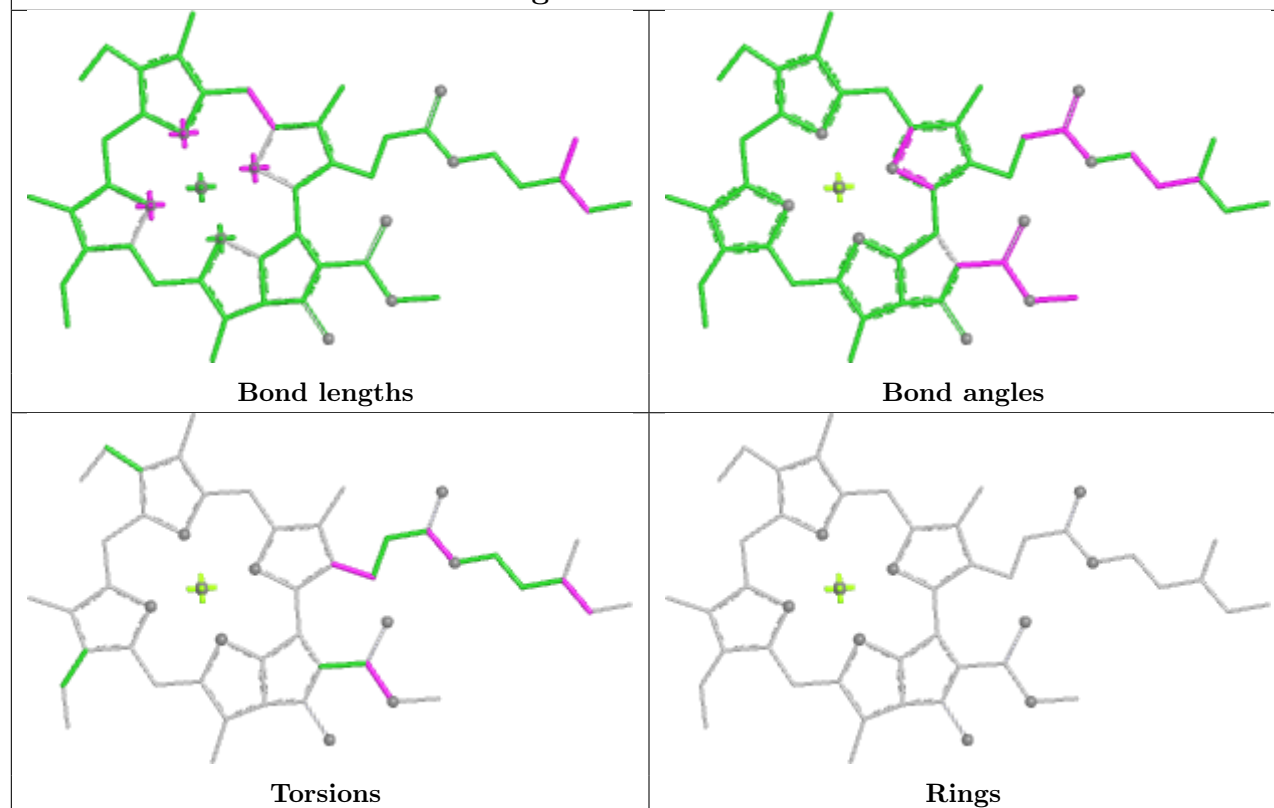
Ligand CLA A 839

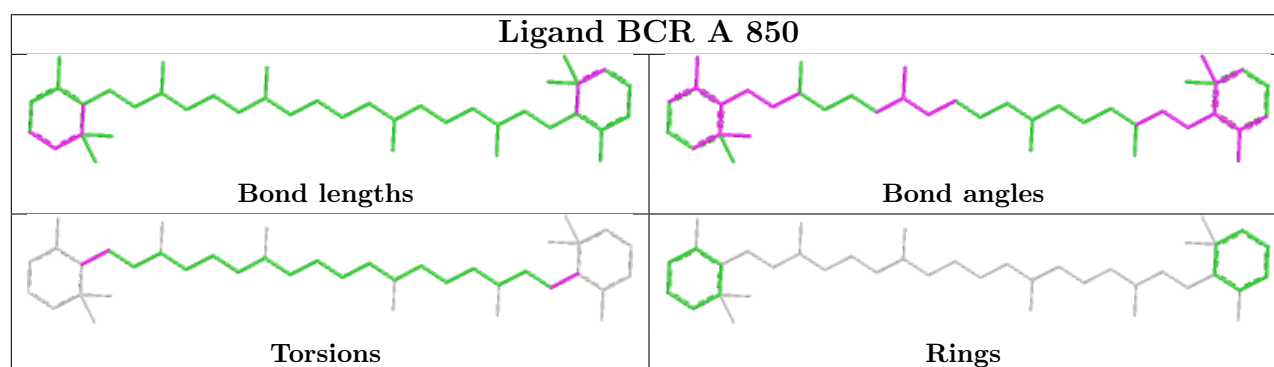
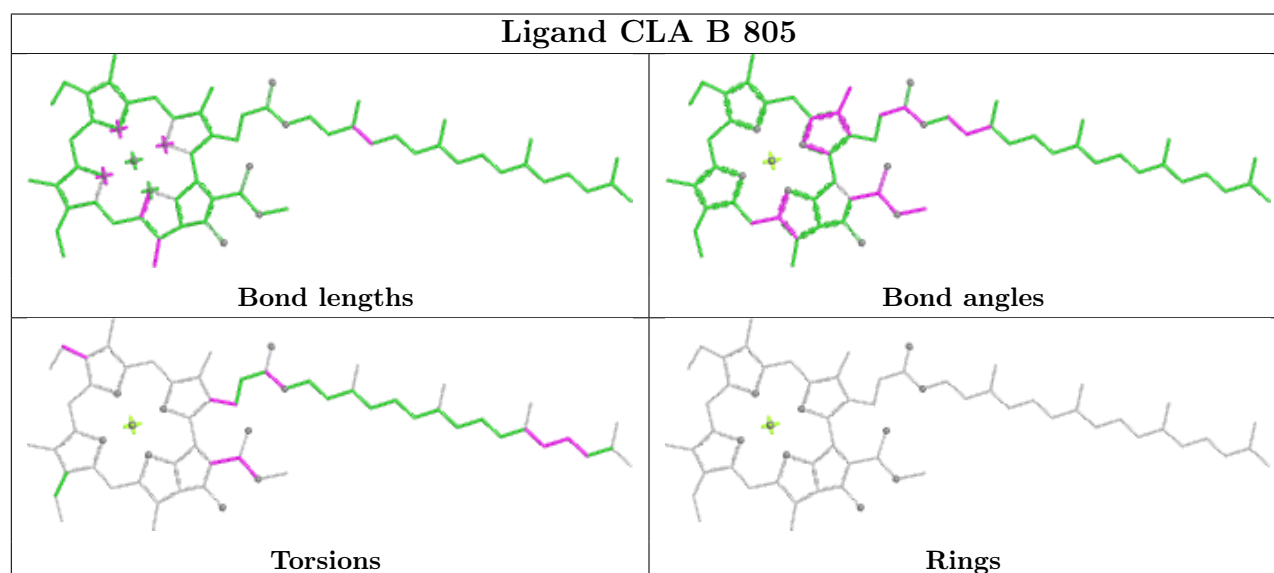
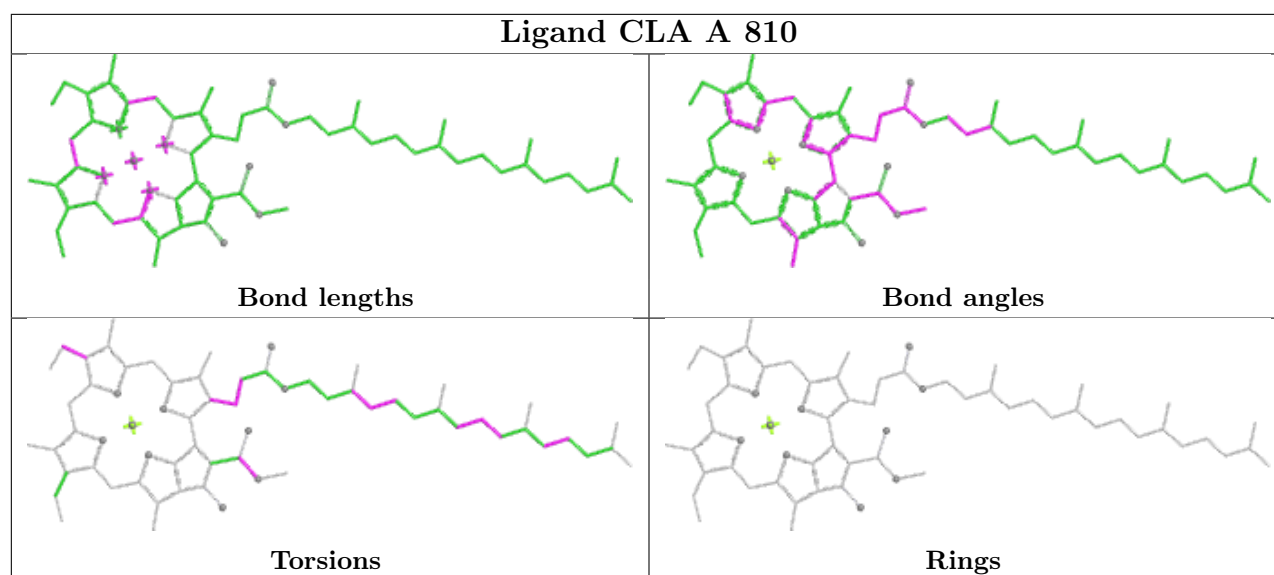


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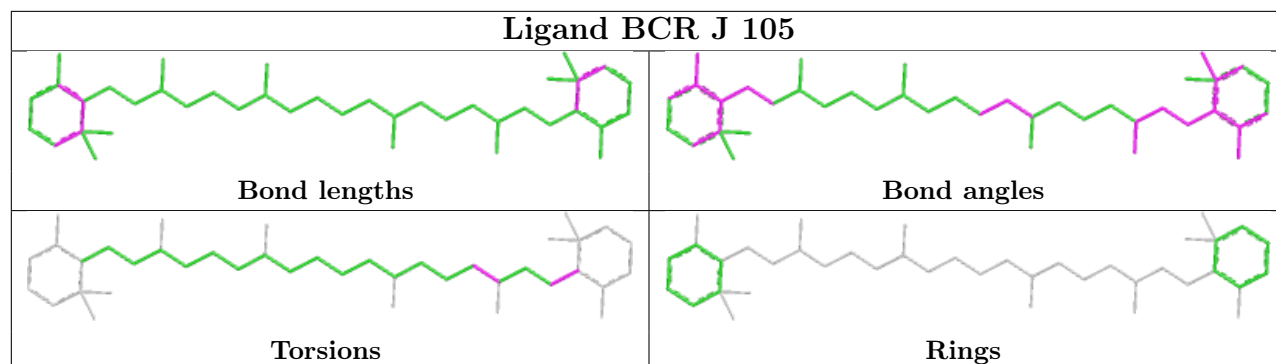


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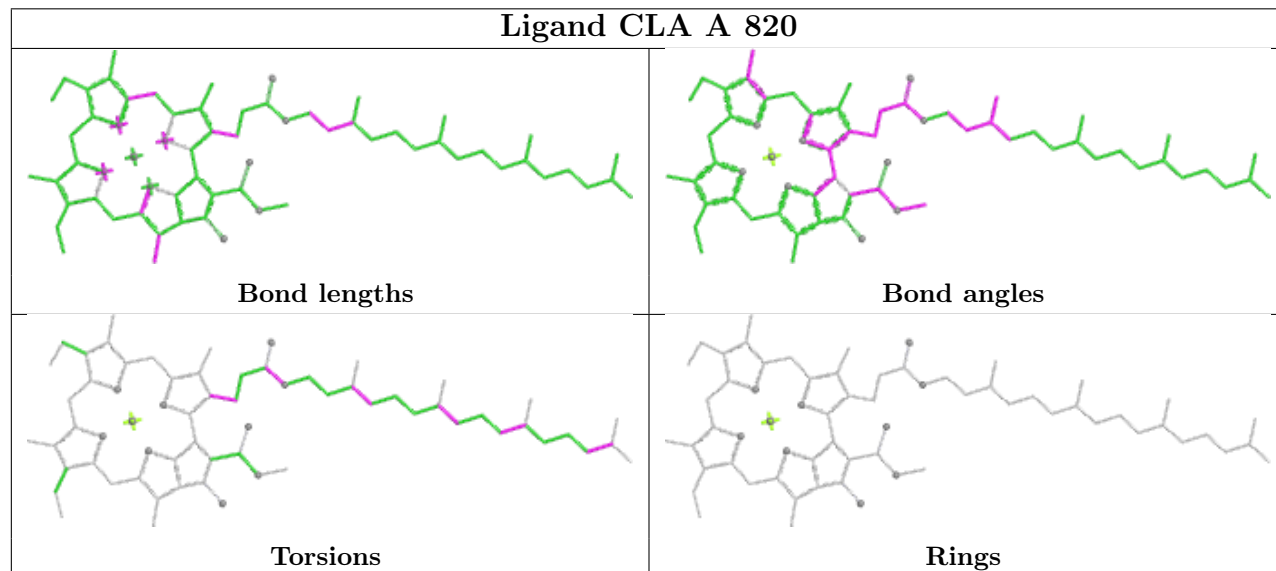




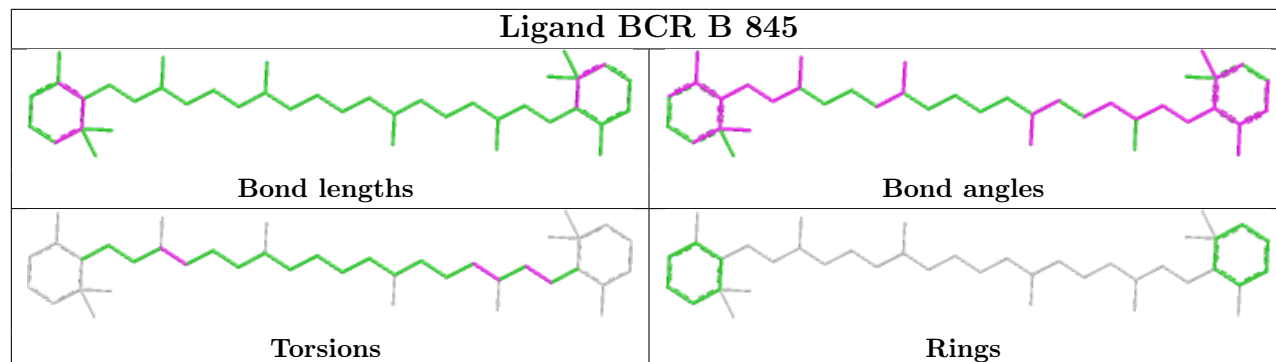
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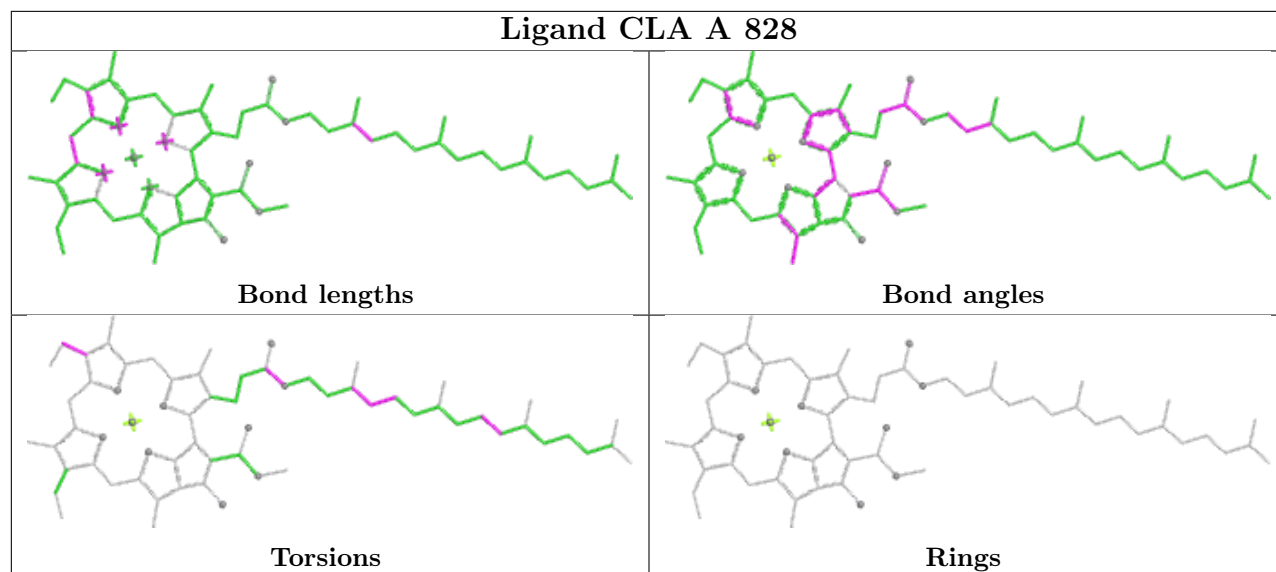
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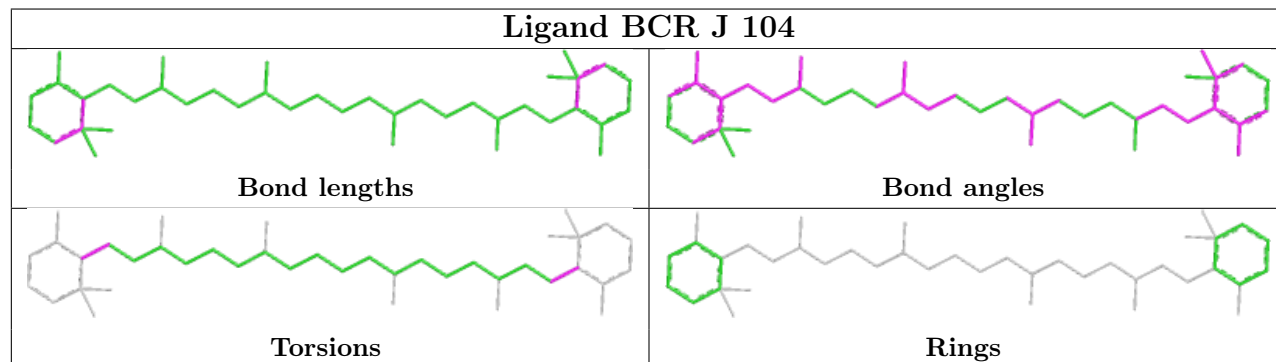
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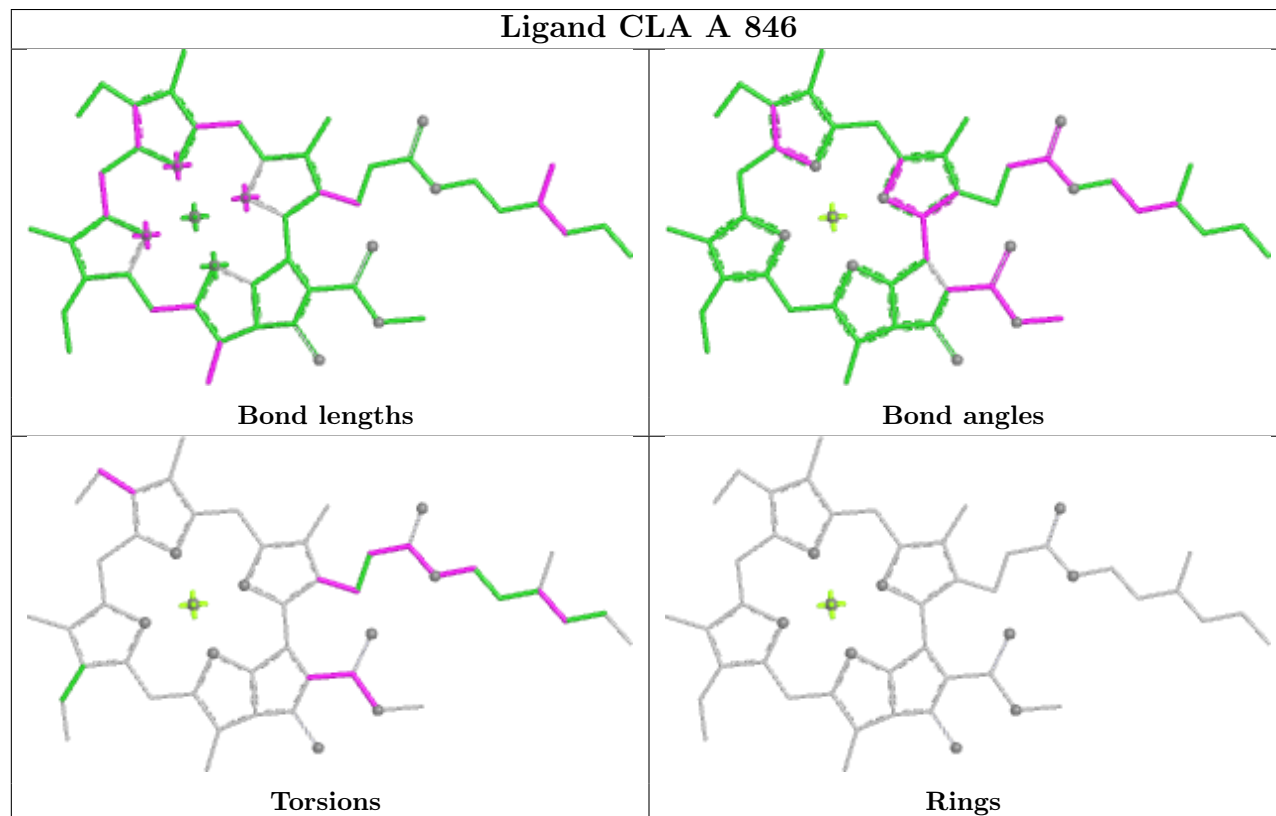
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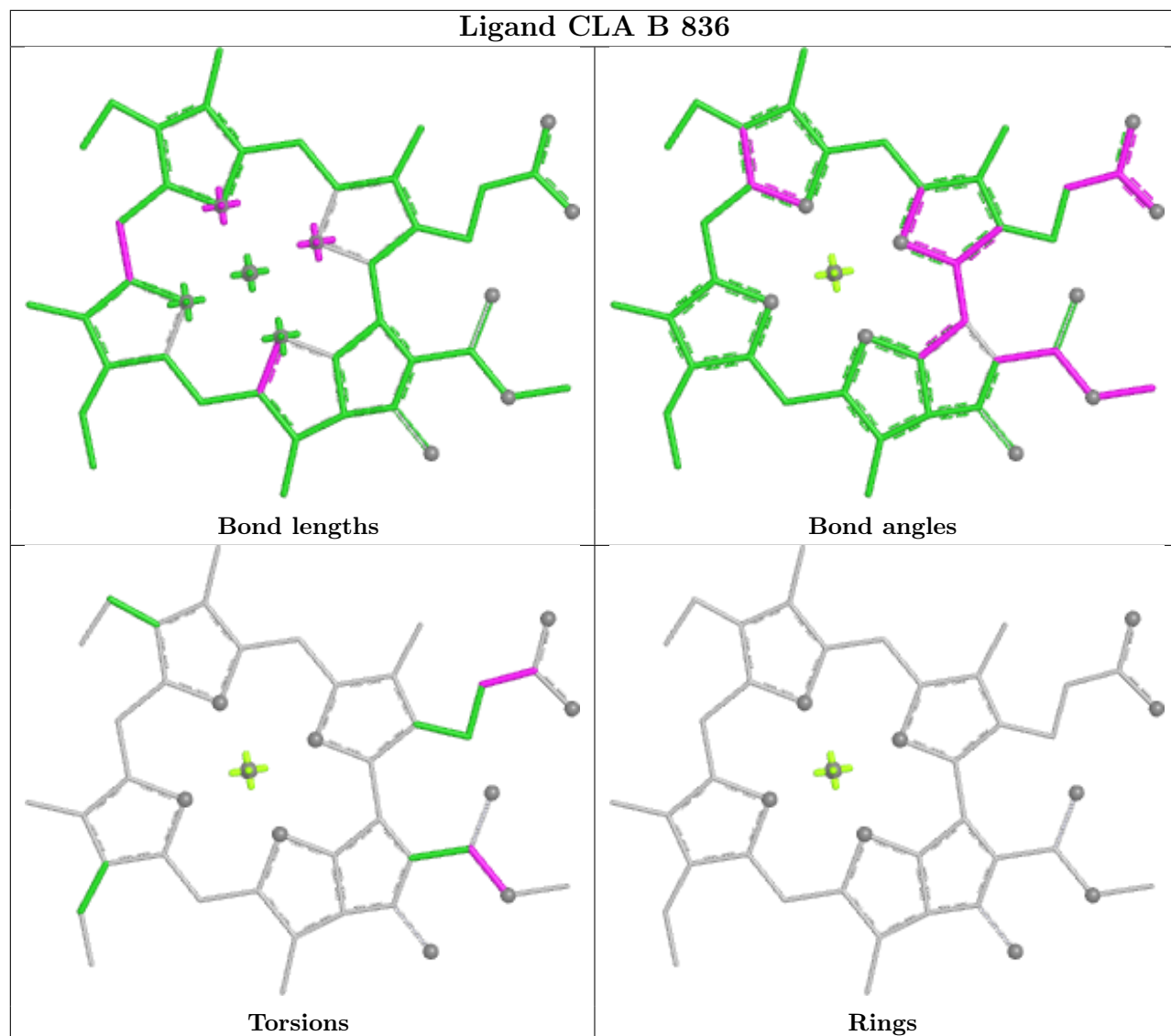
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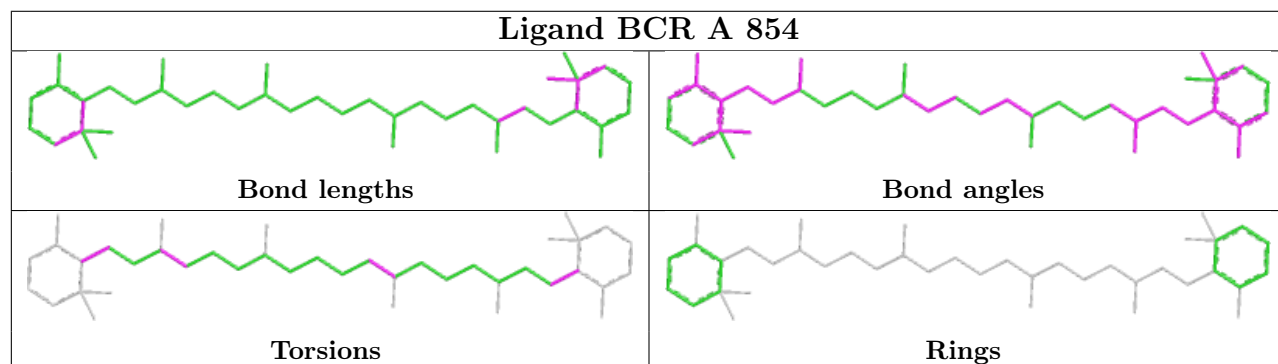
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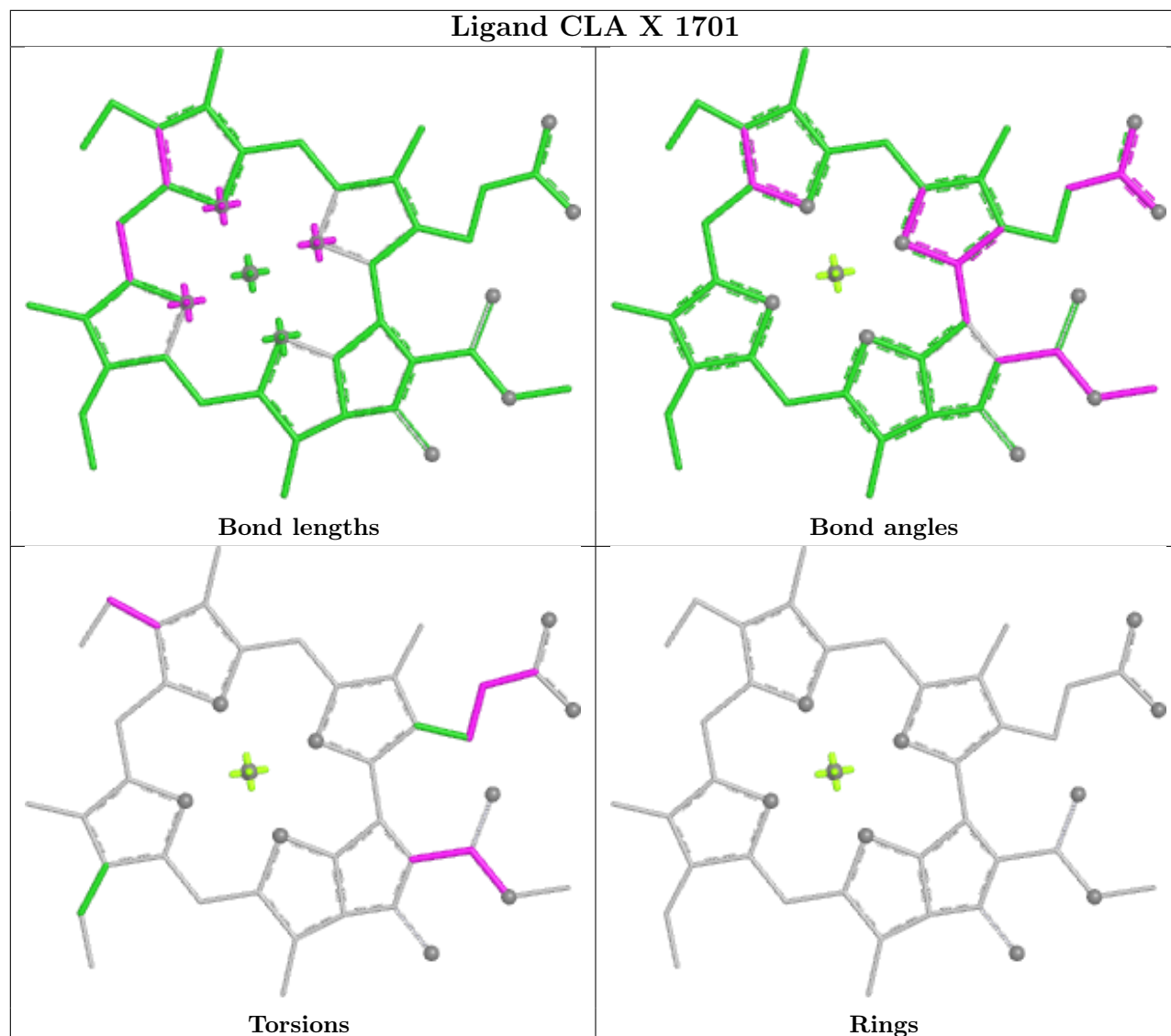
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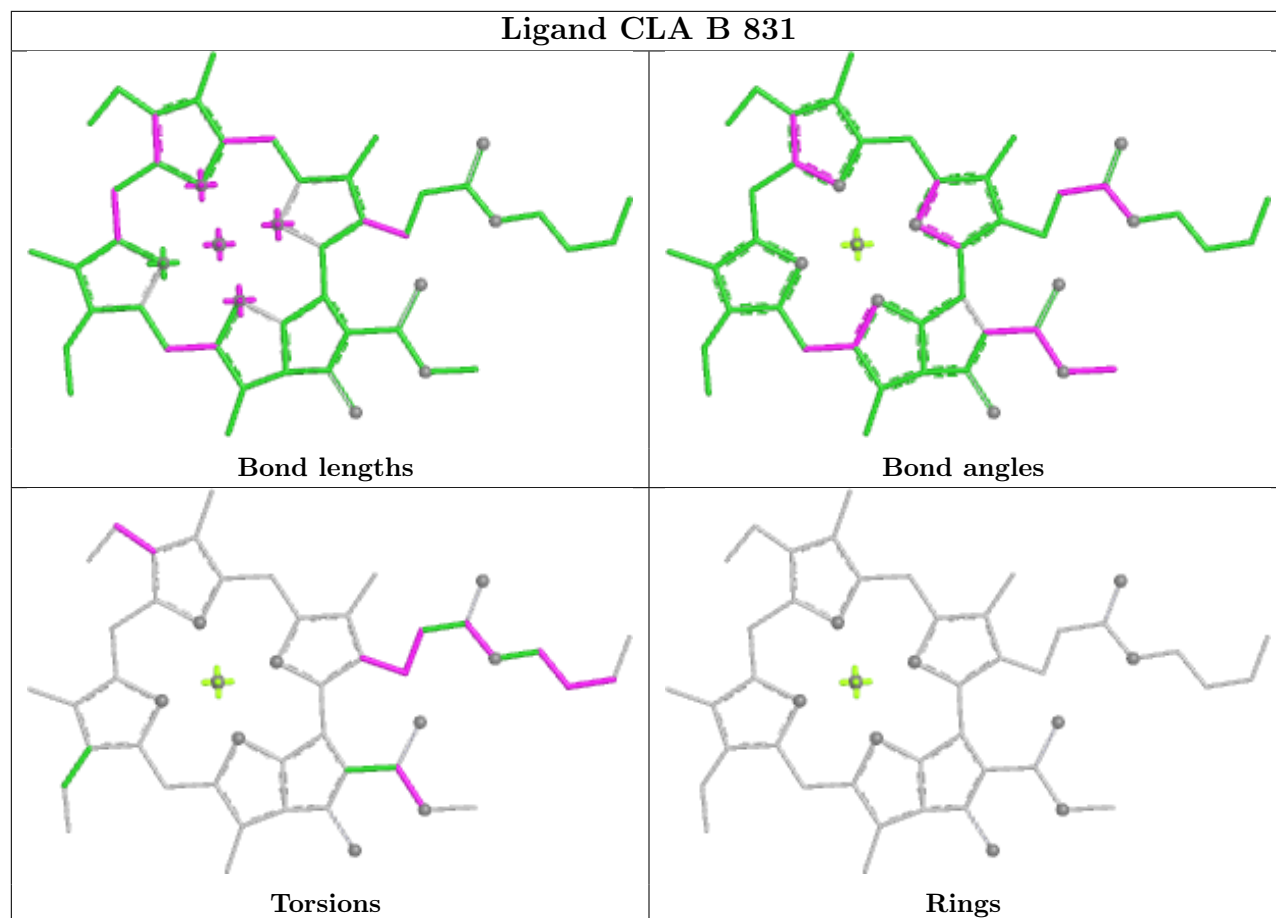
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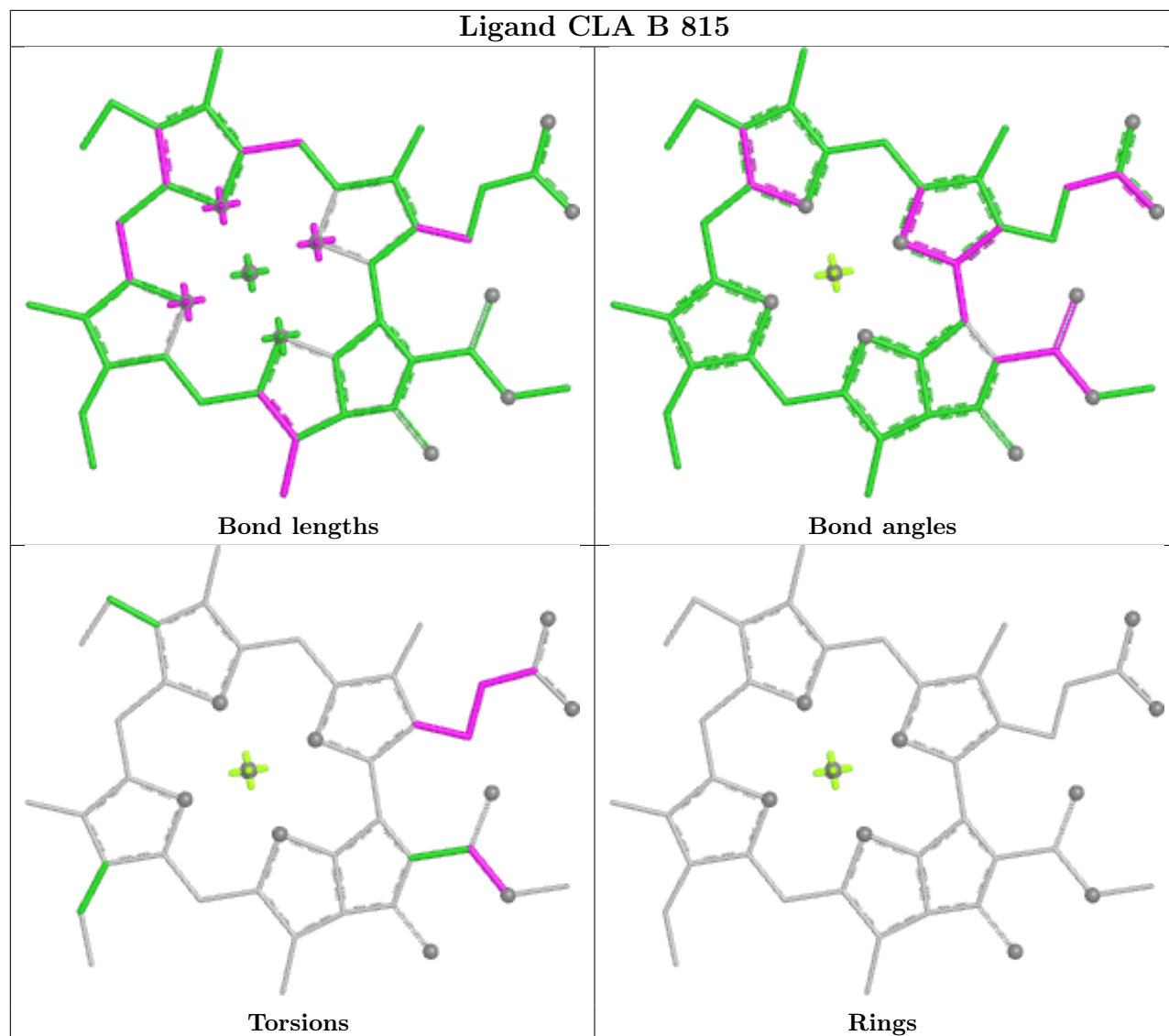
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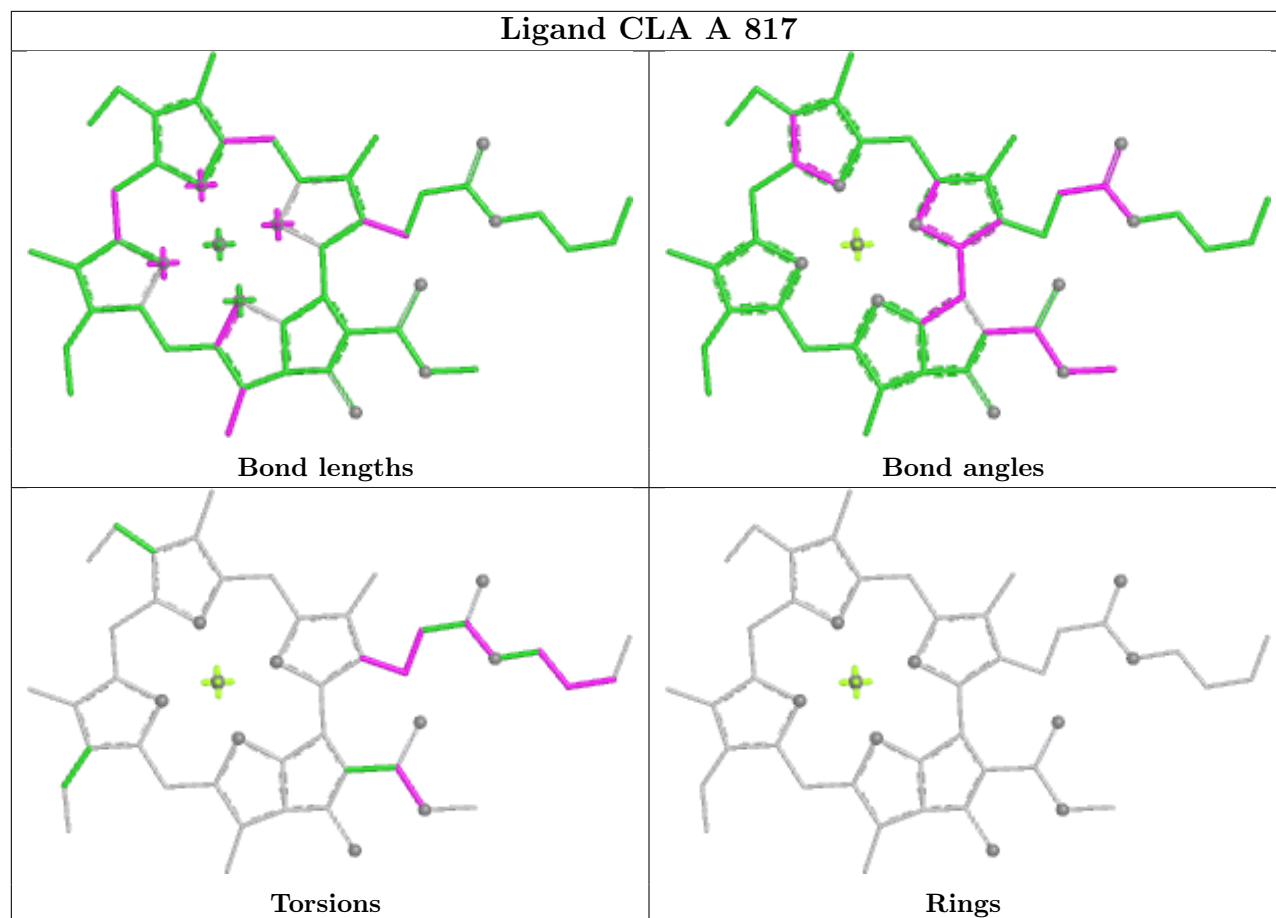
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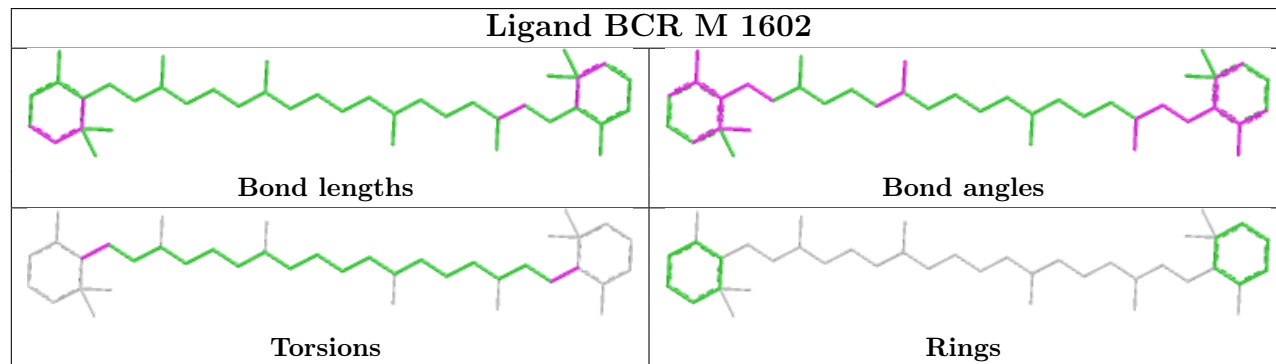
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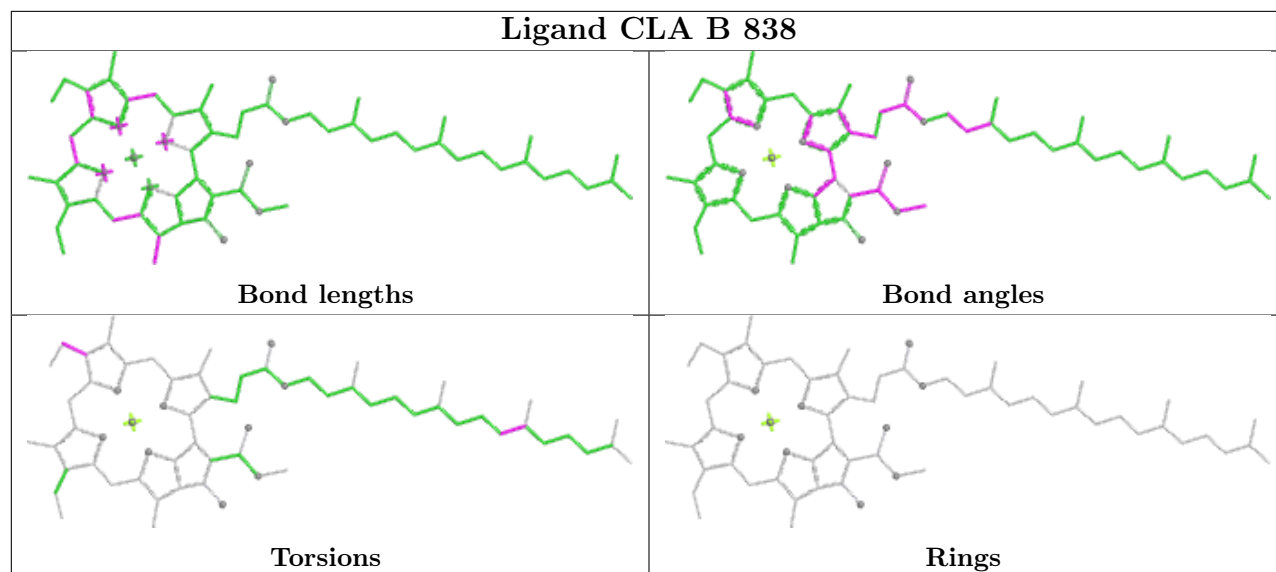
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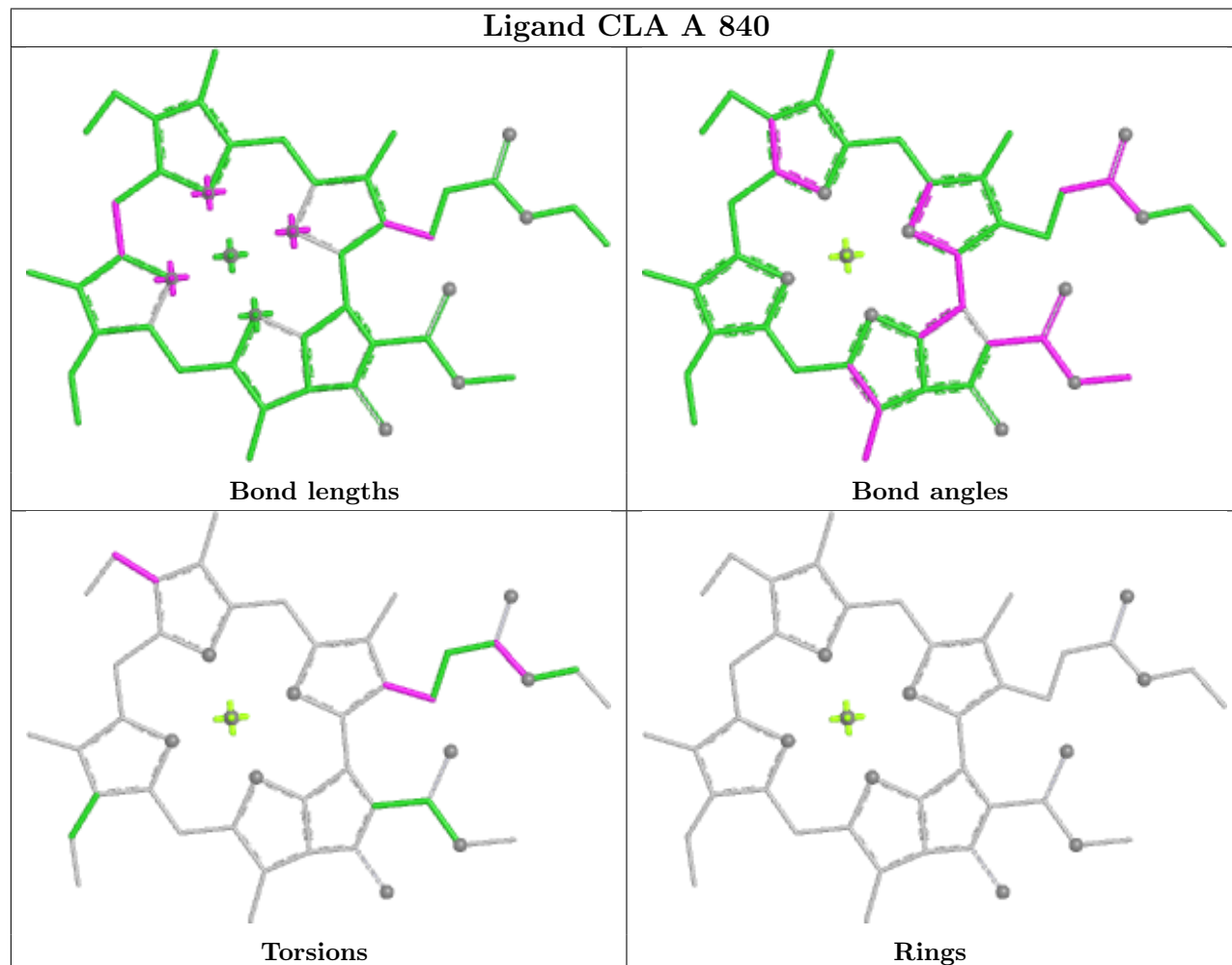
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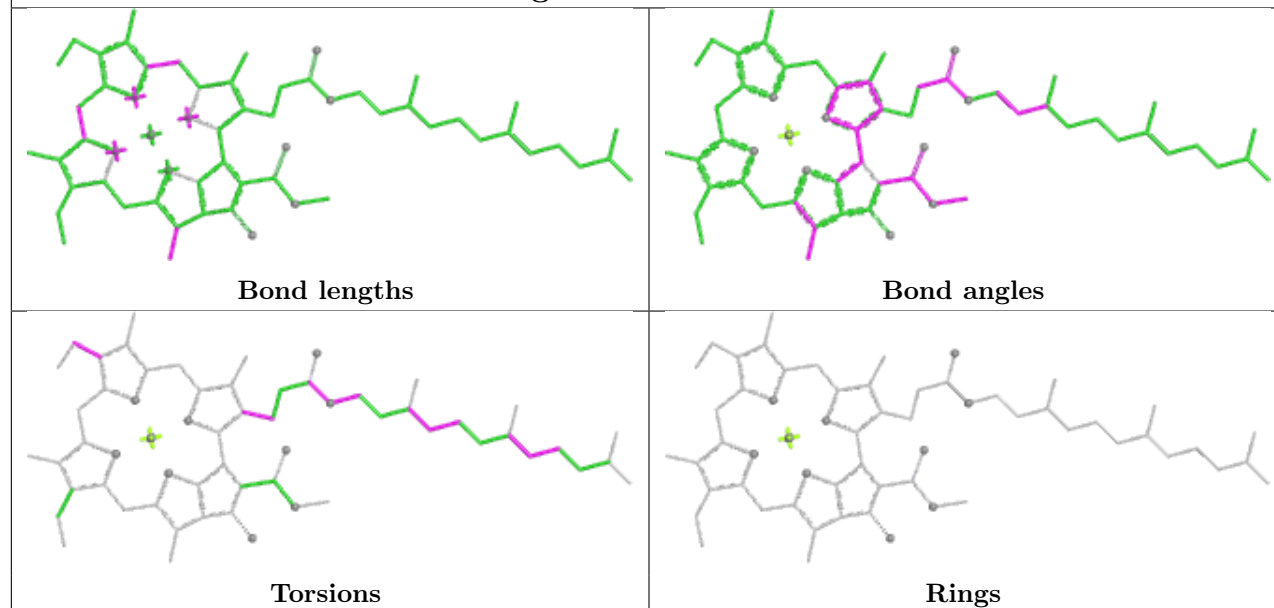
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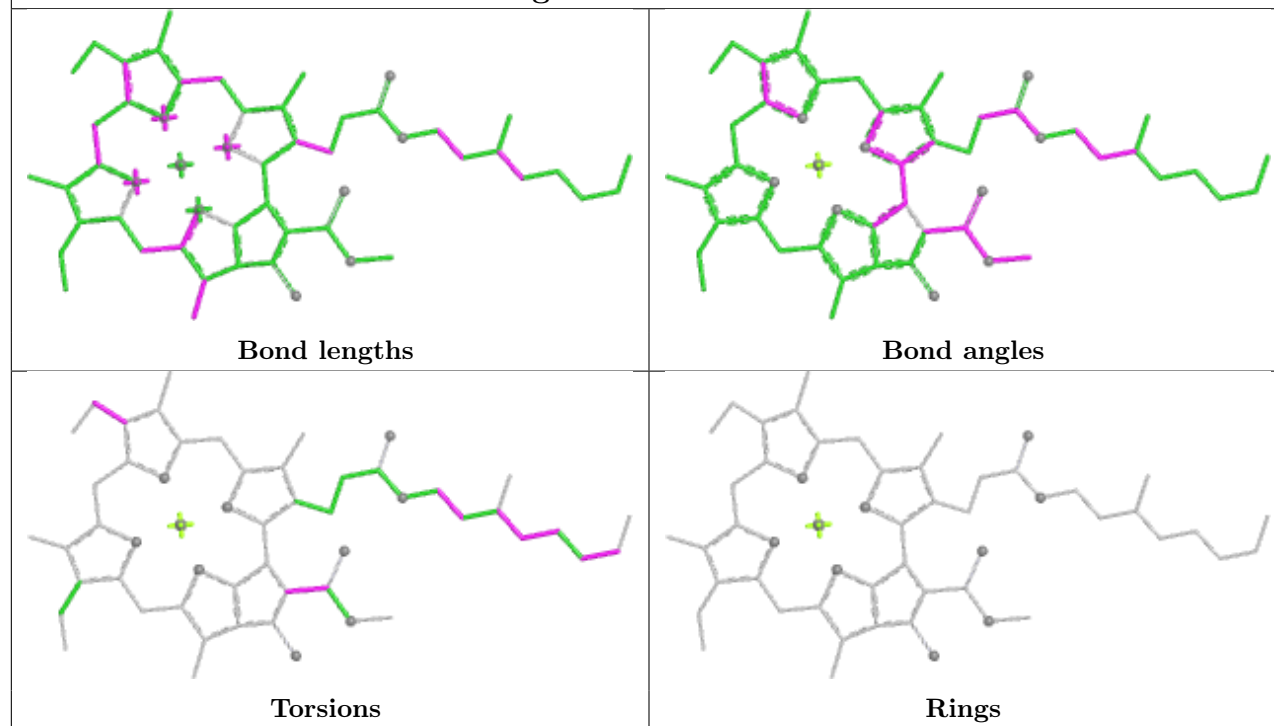
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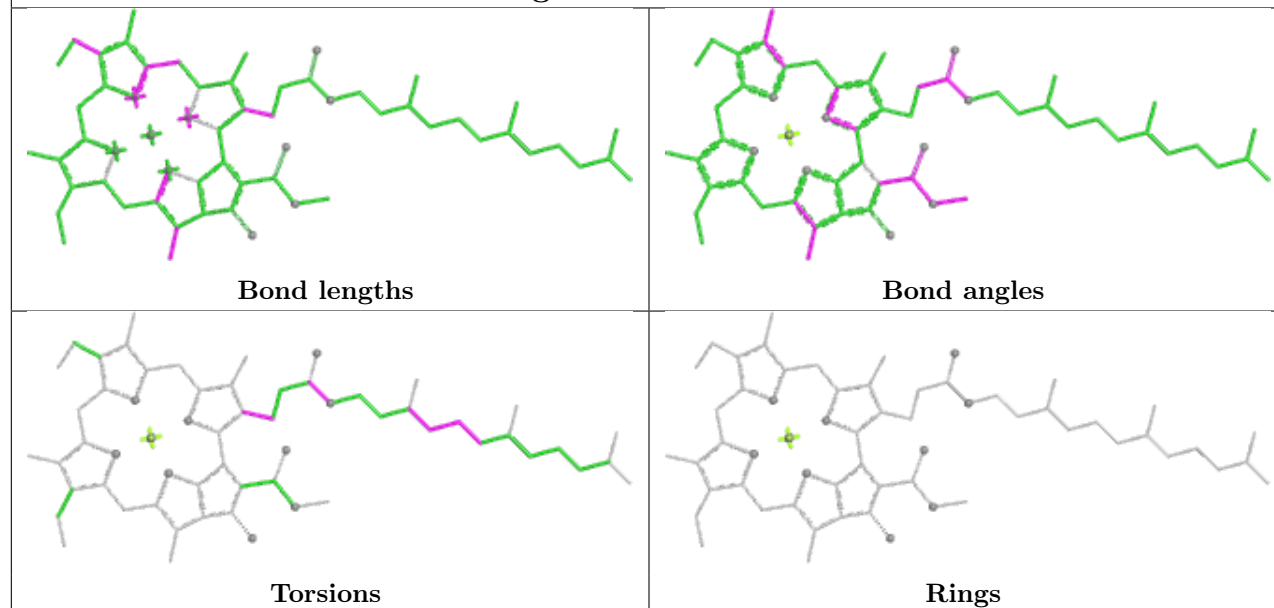
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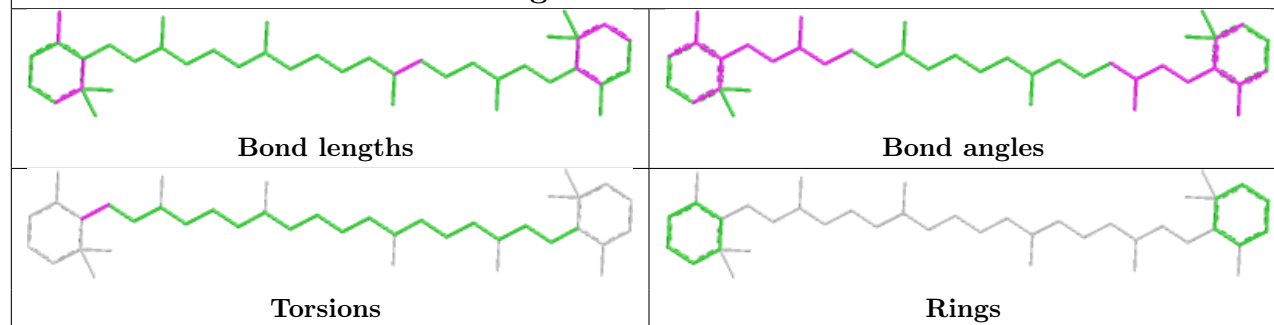
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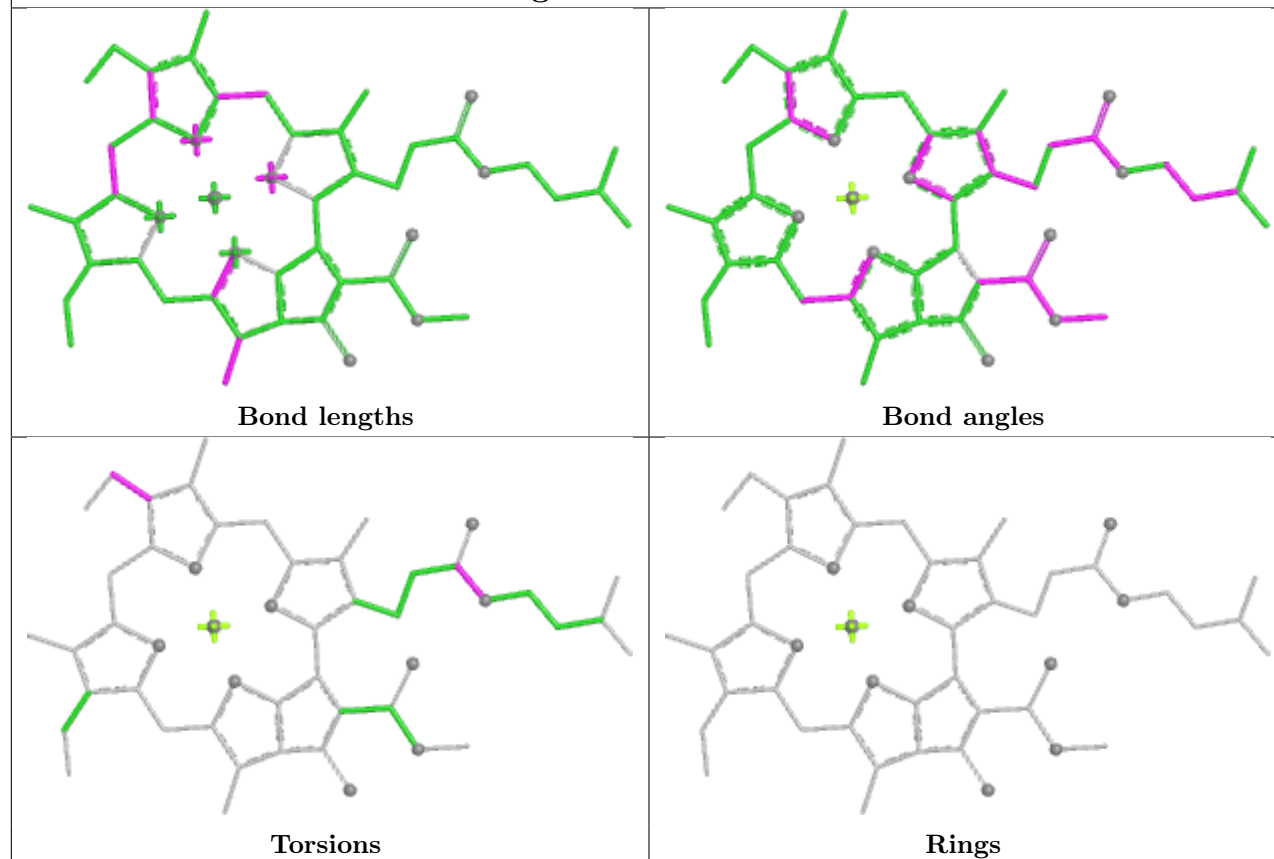
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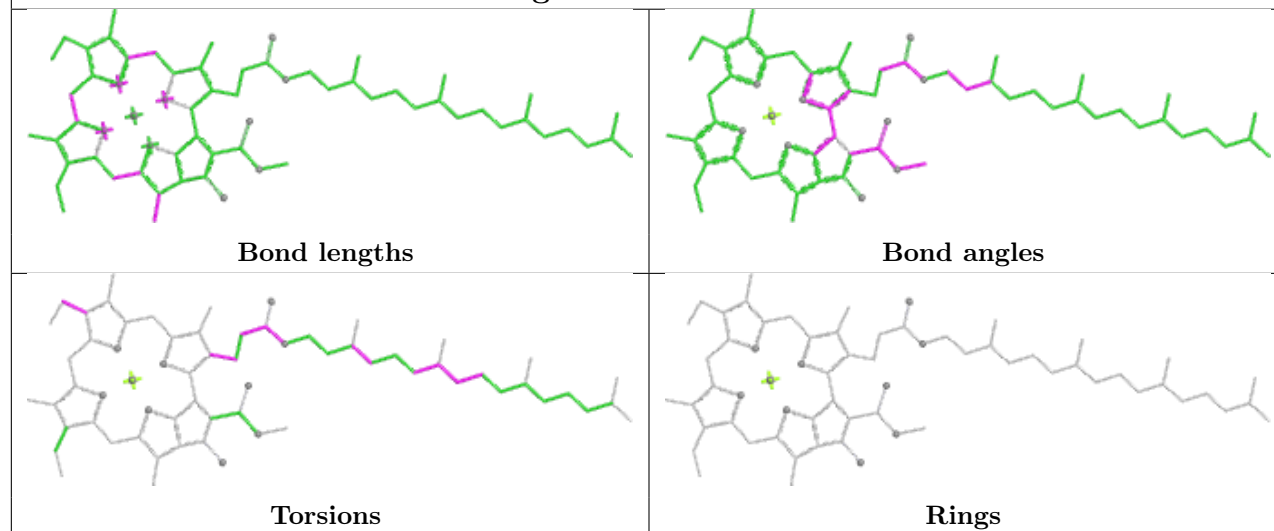
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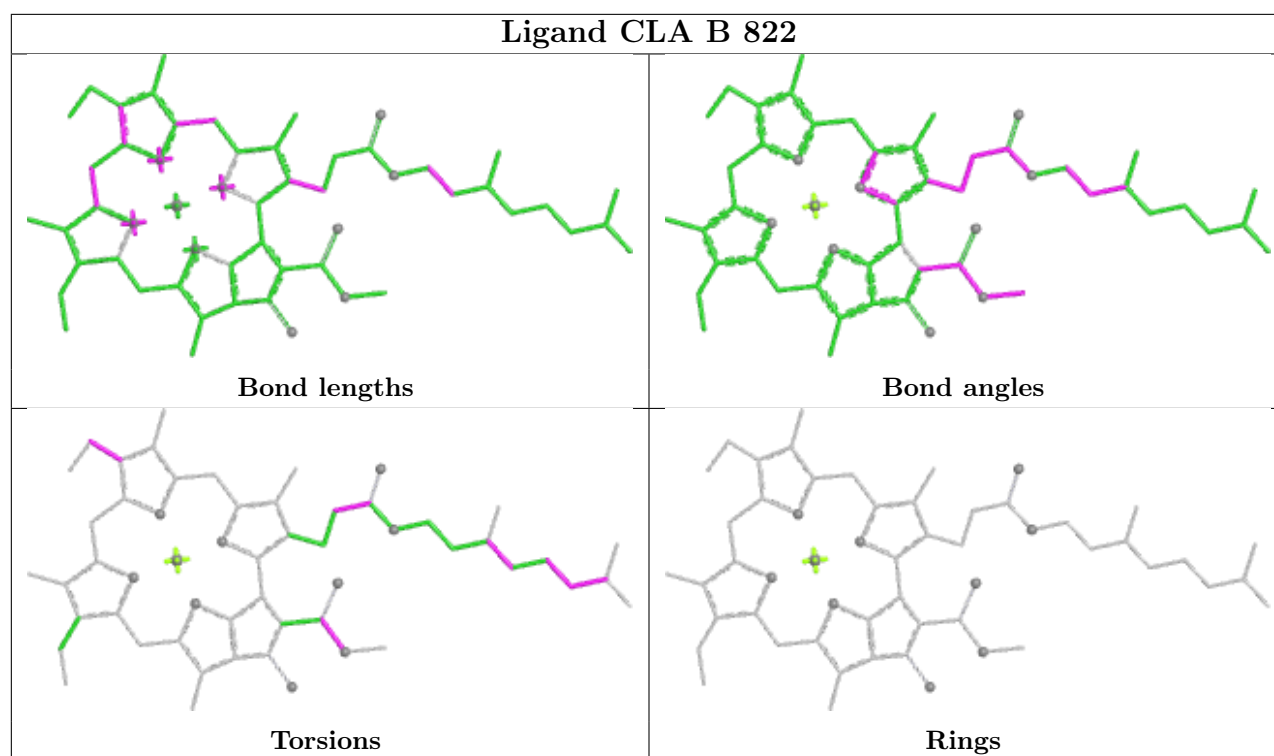


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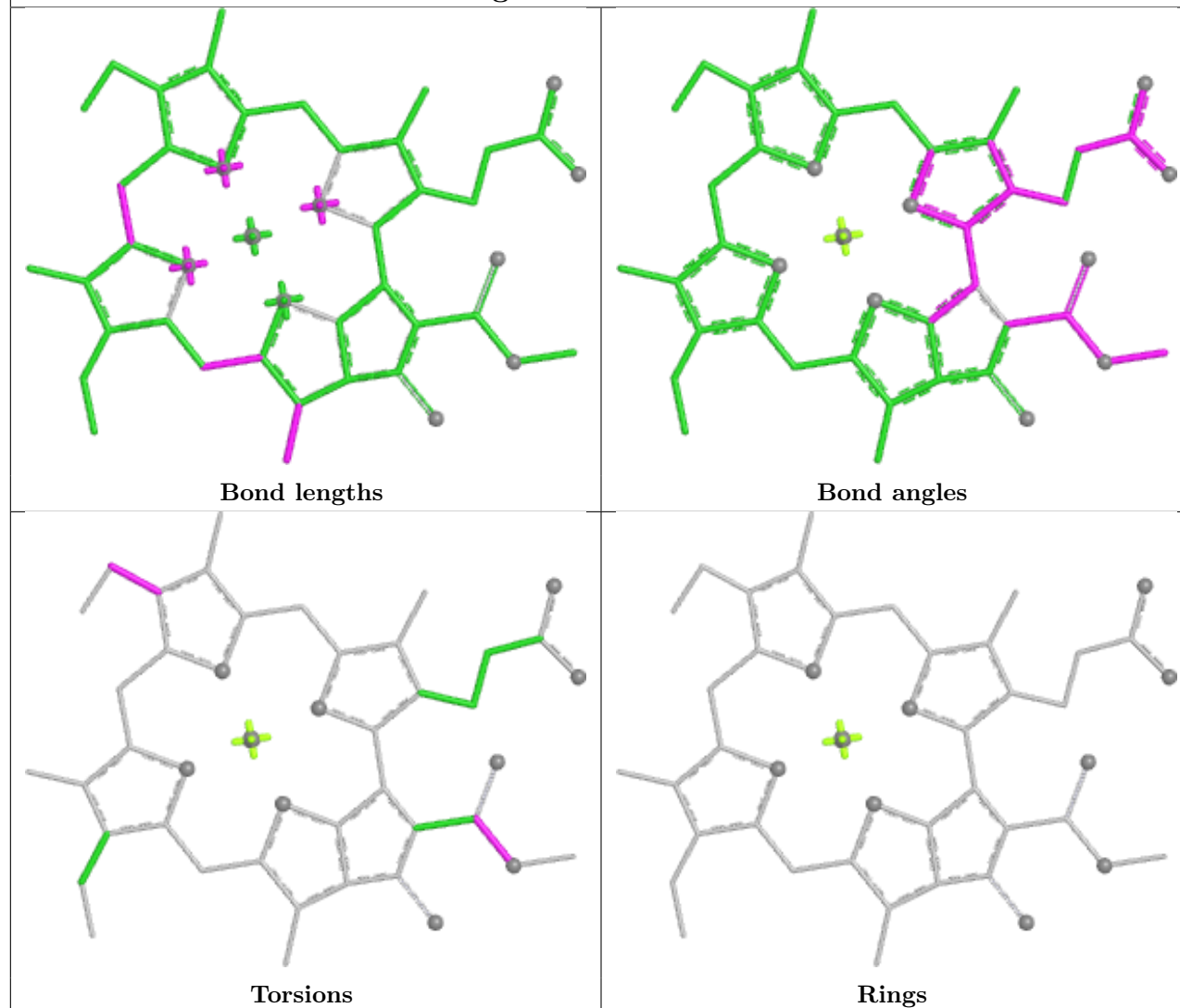


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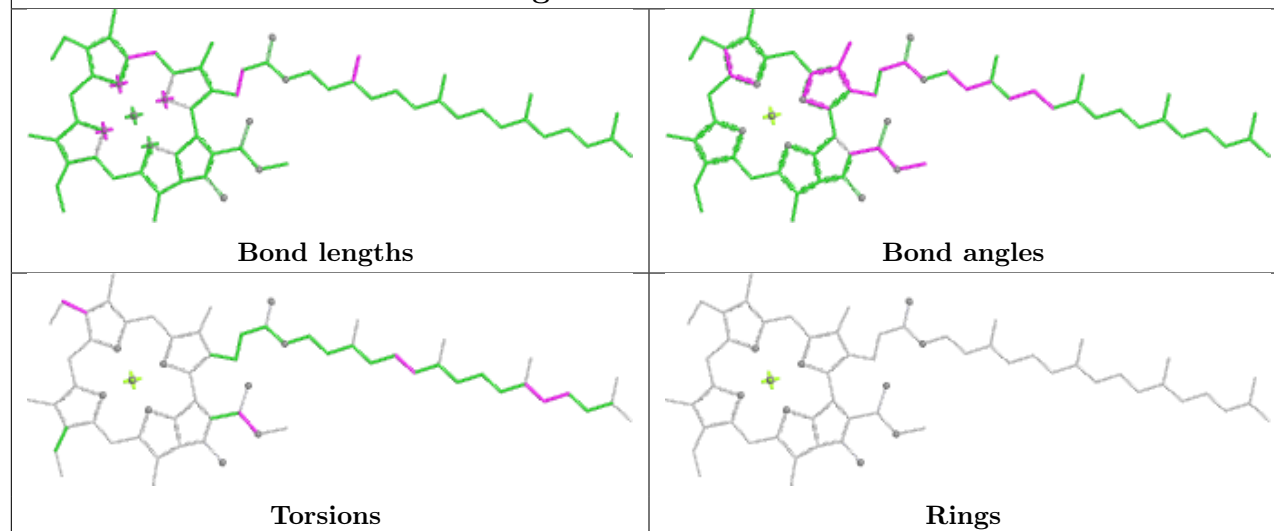




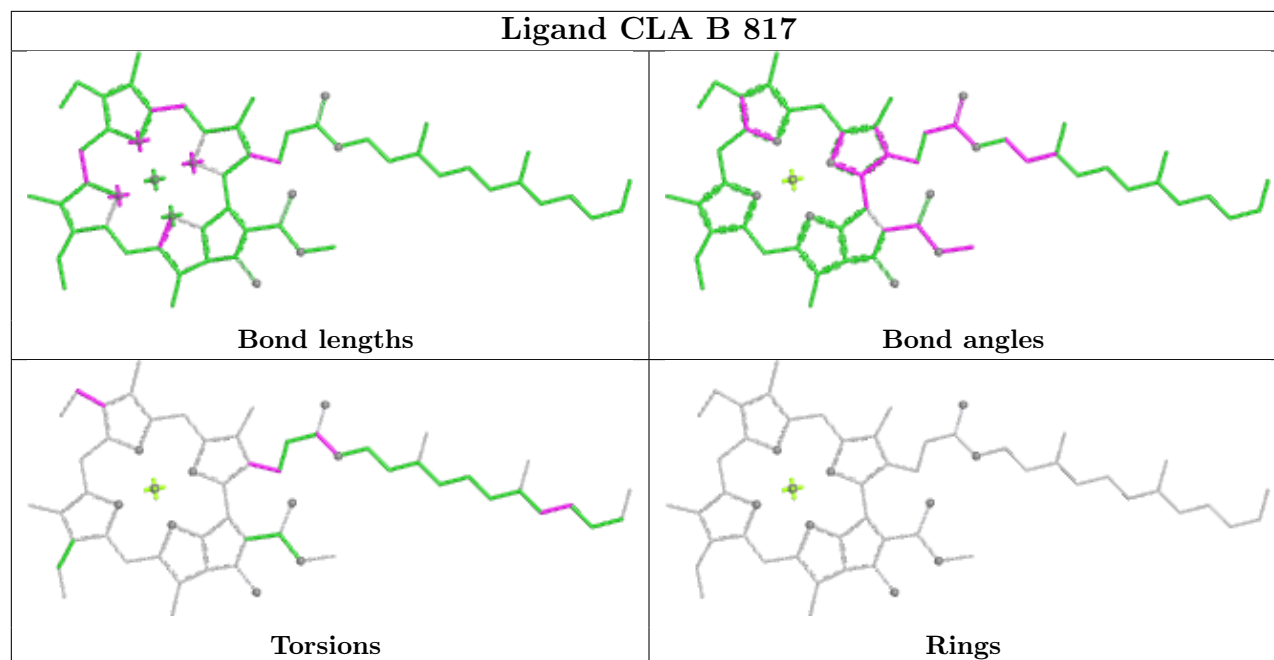
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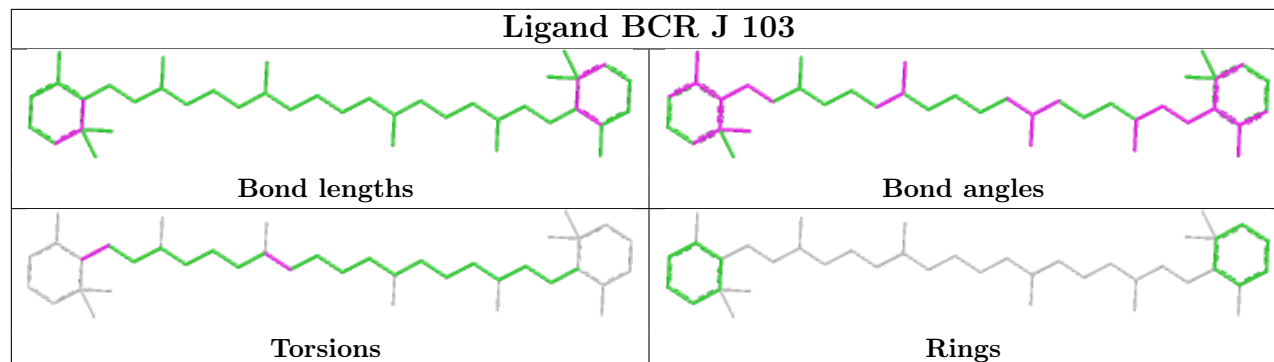
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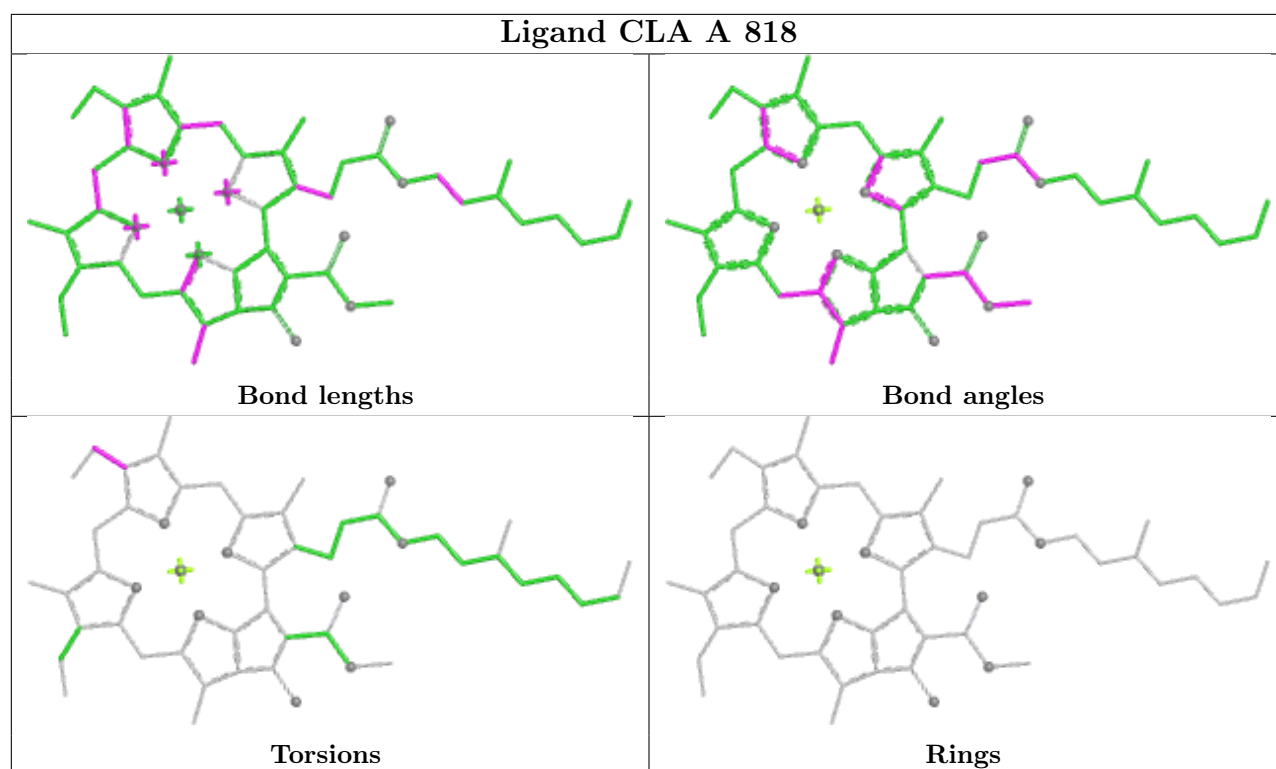


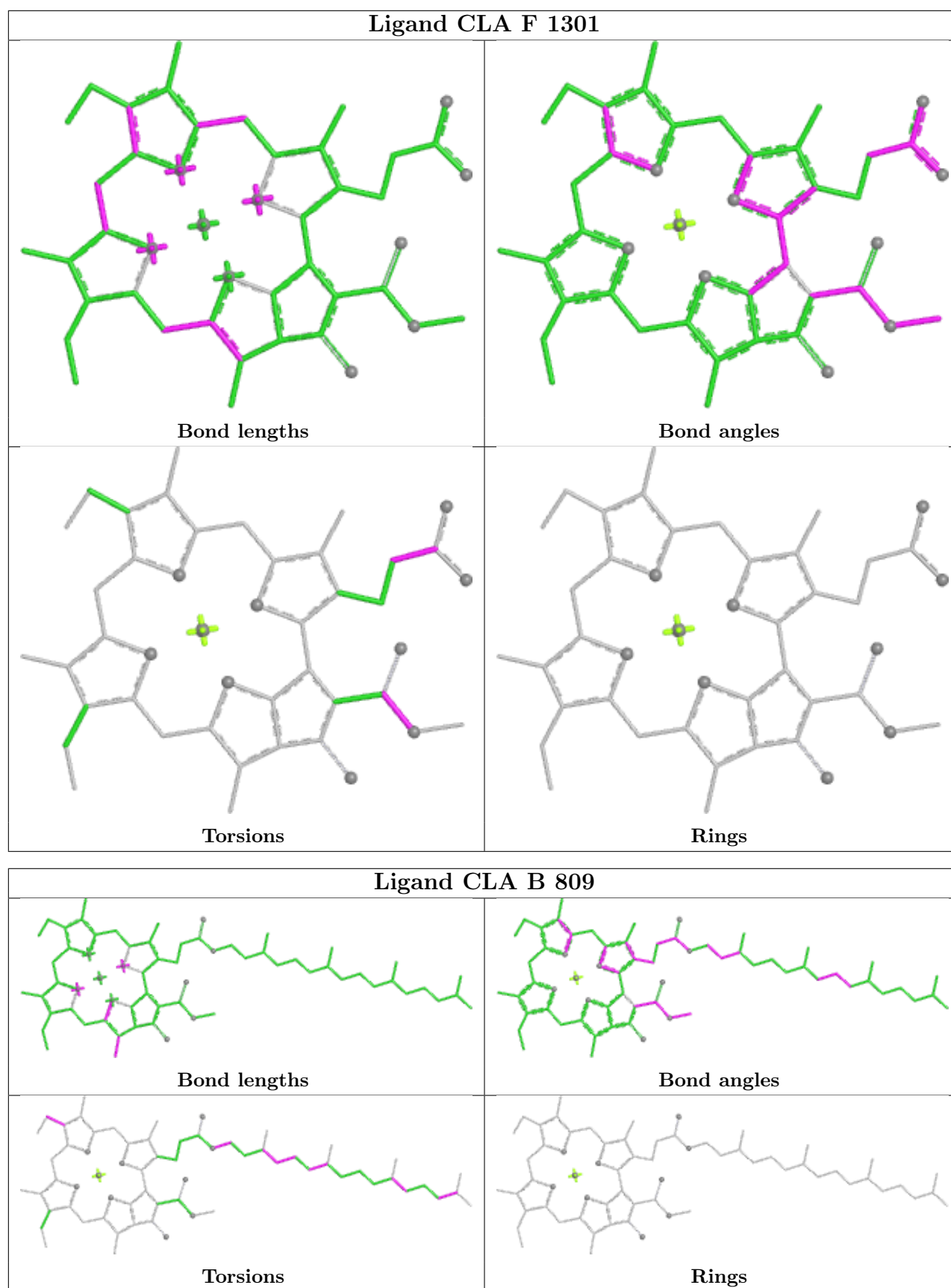
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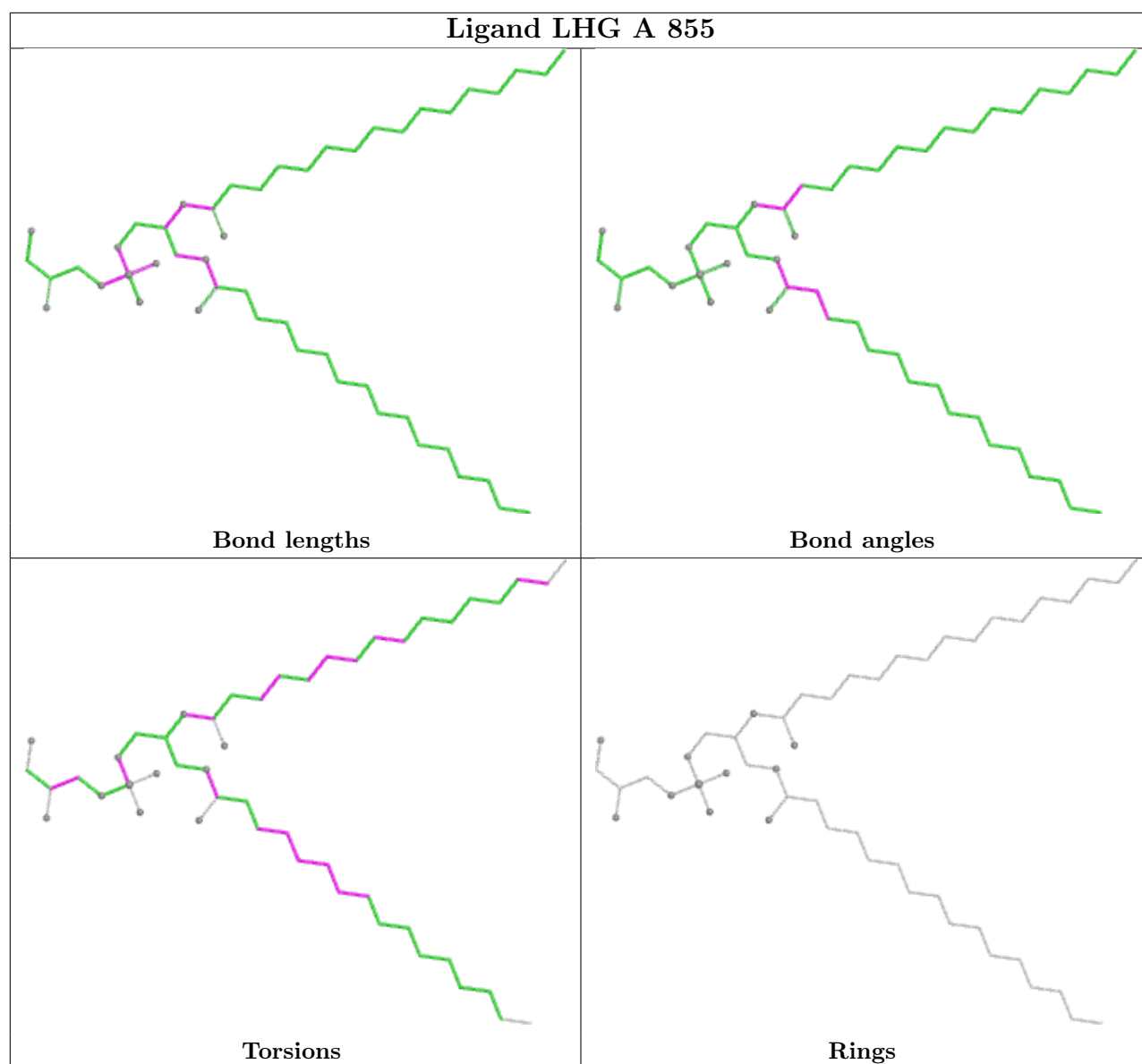


Ligand BCR J 103

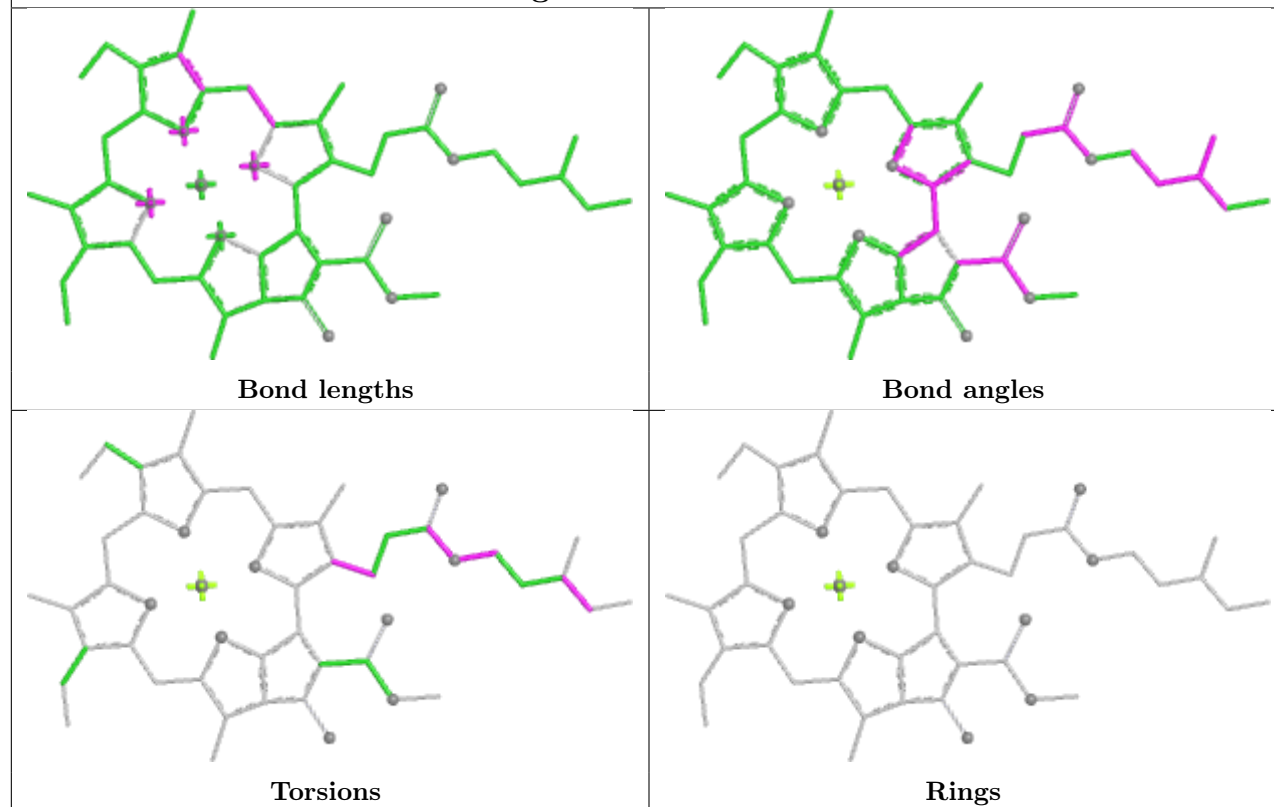




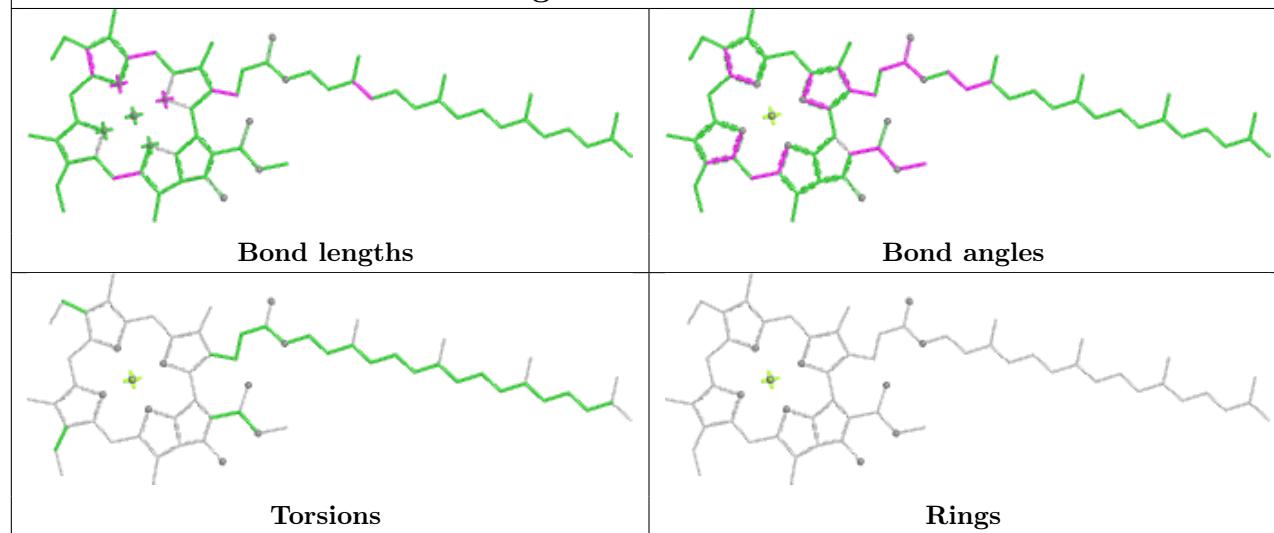


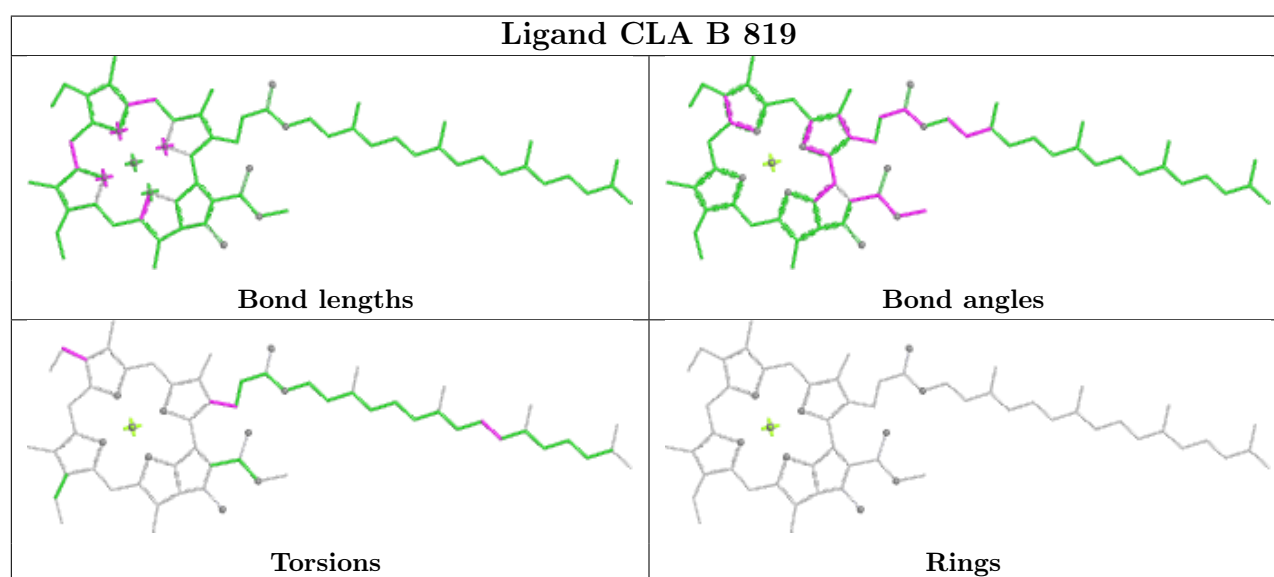
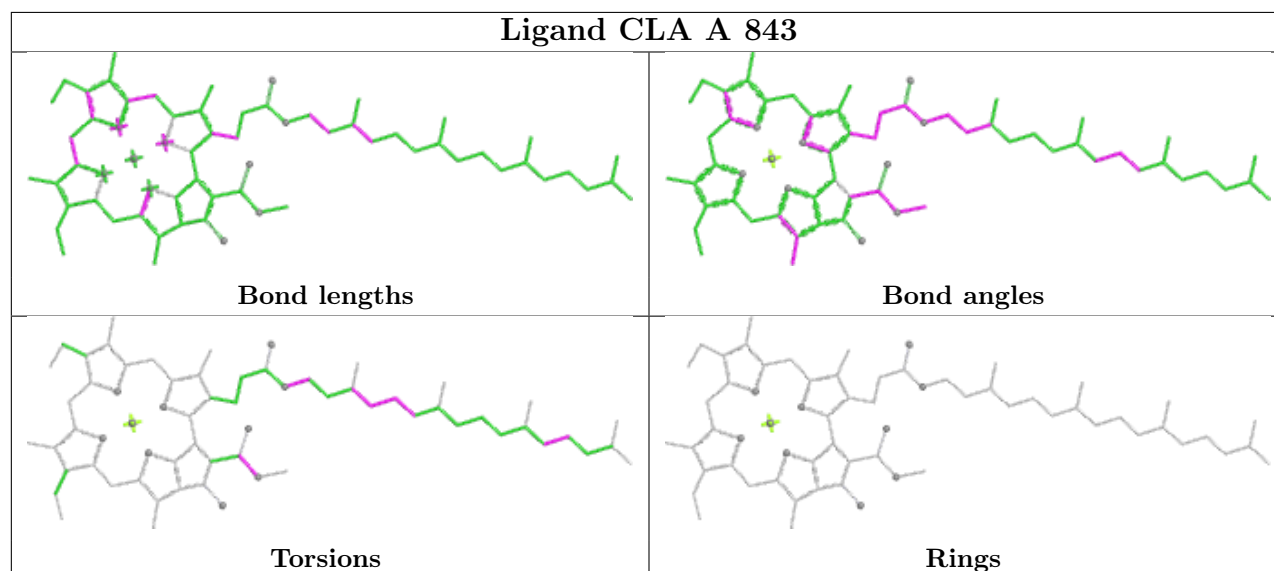
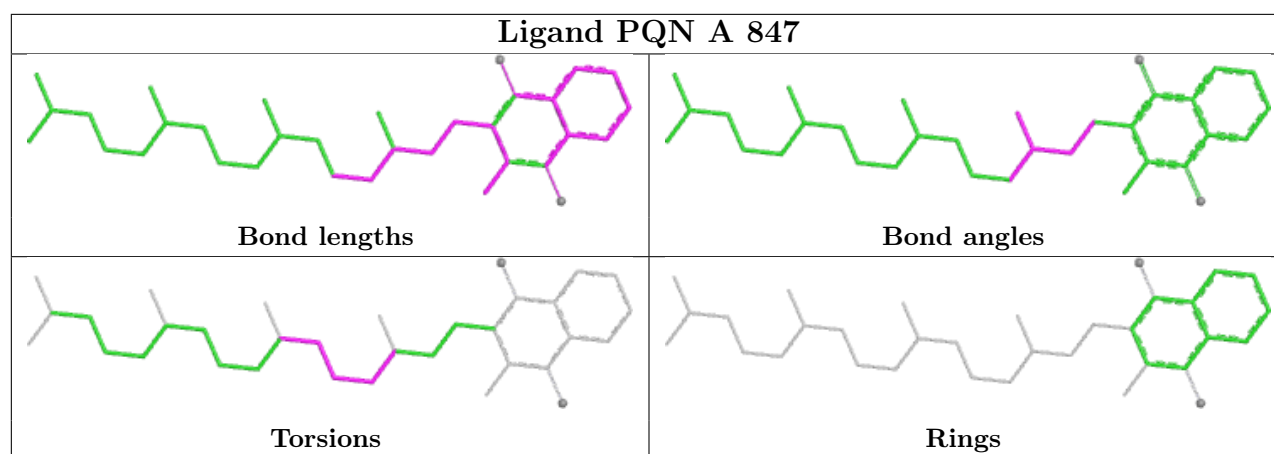


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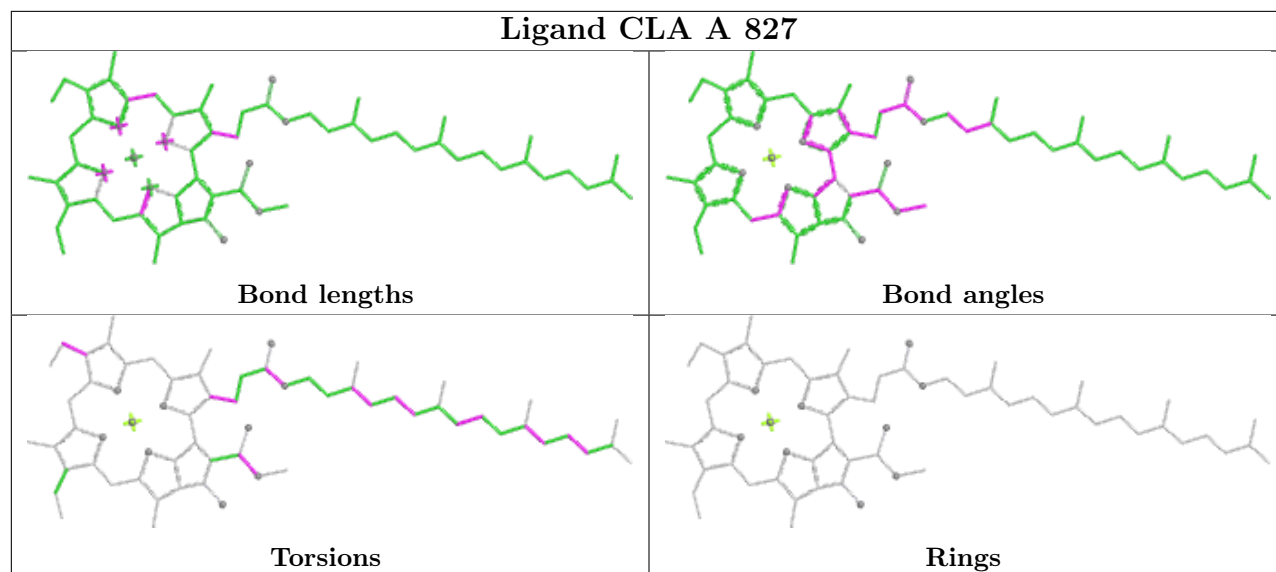


Ligand CLA B 807

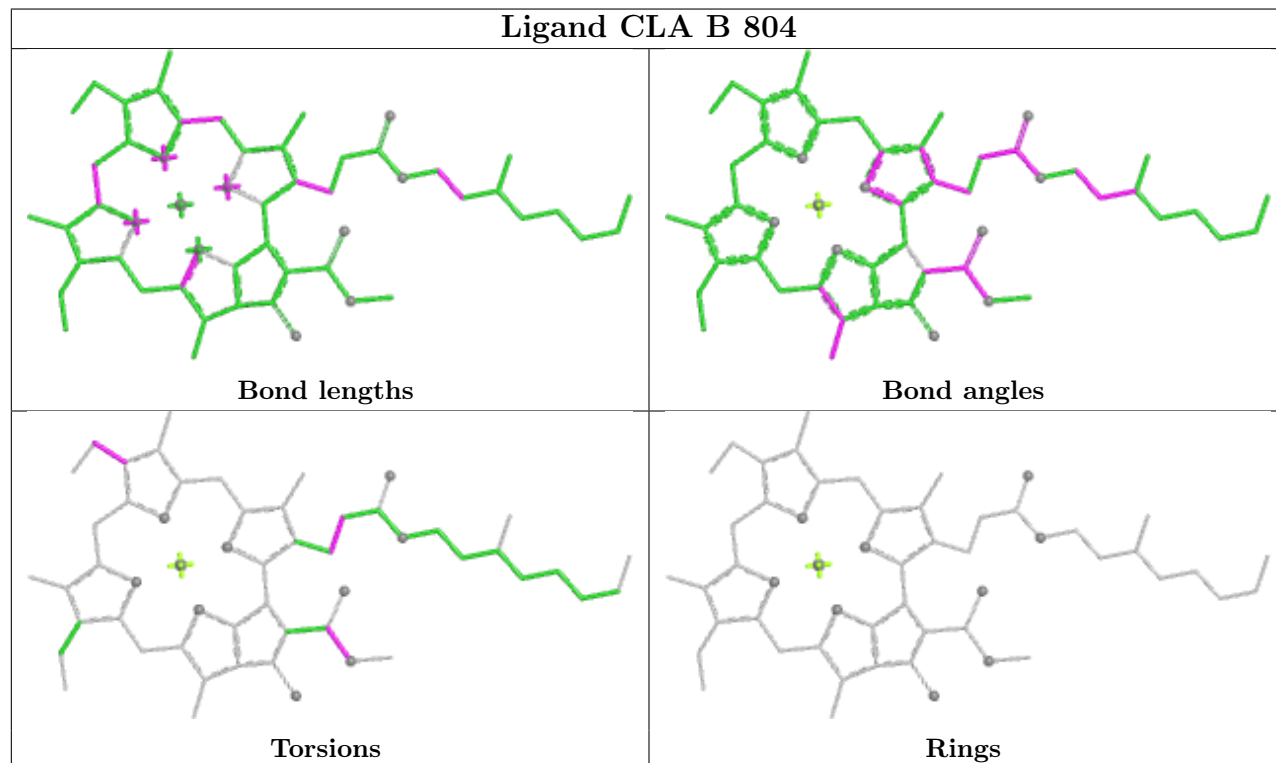




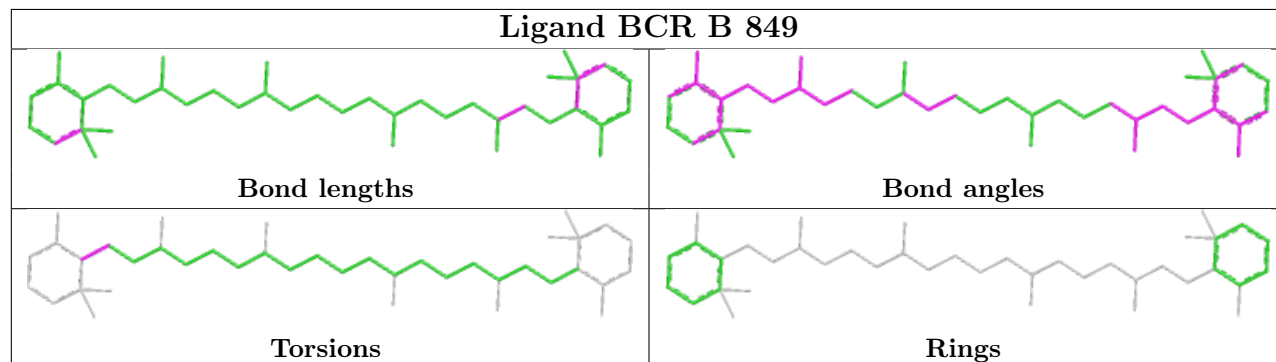
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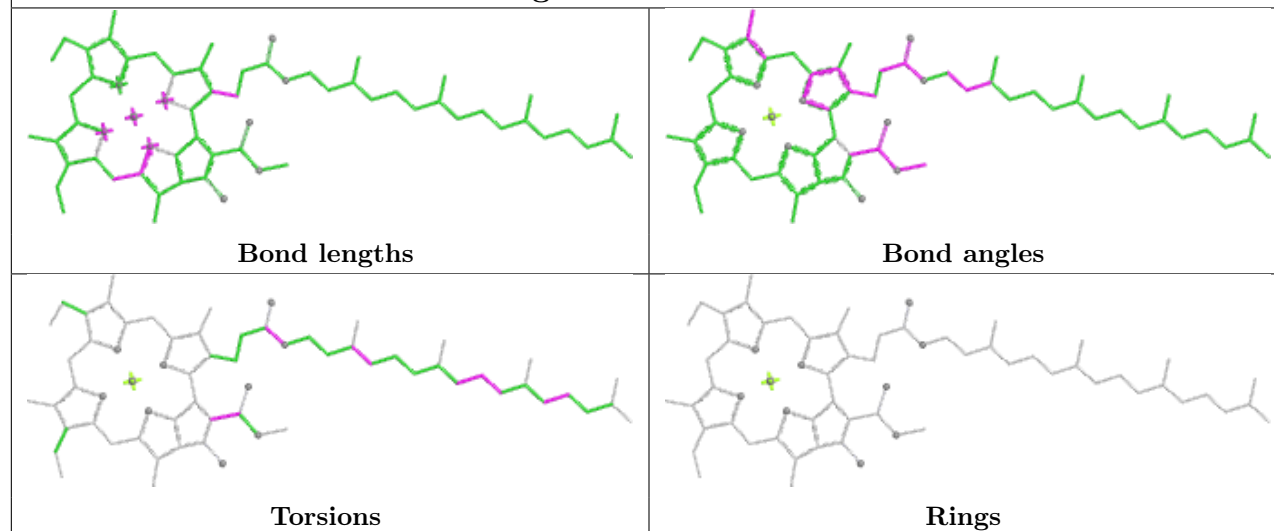
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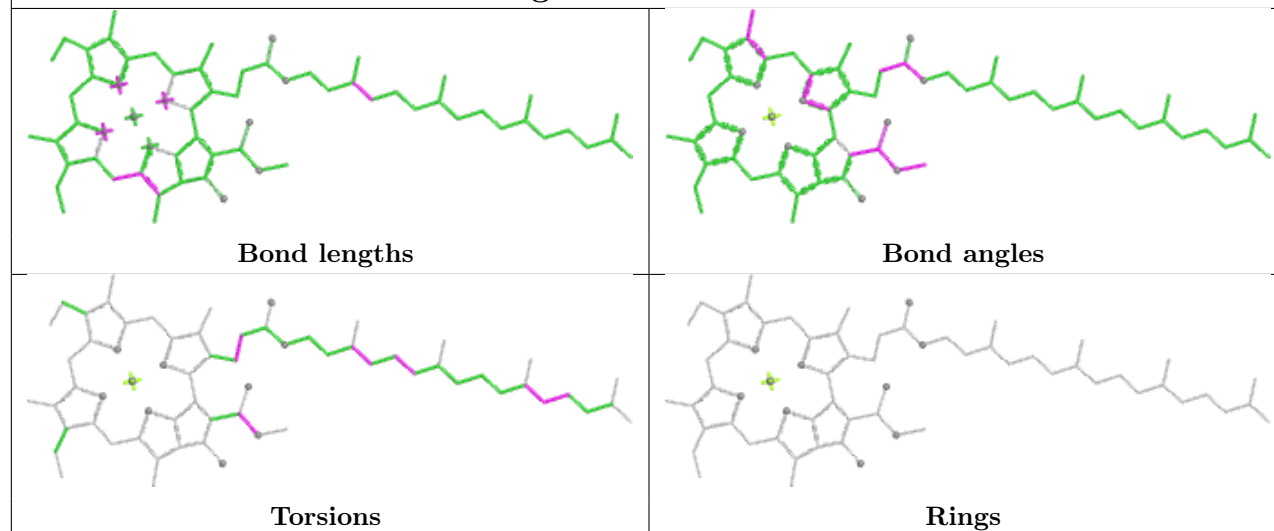
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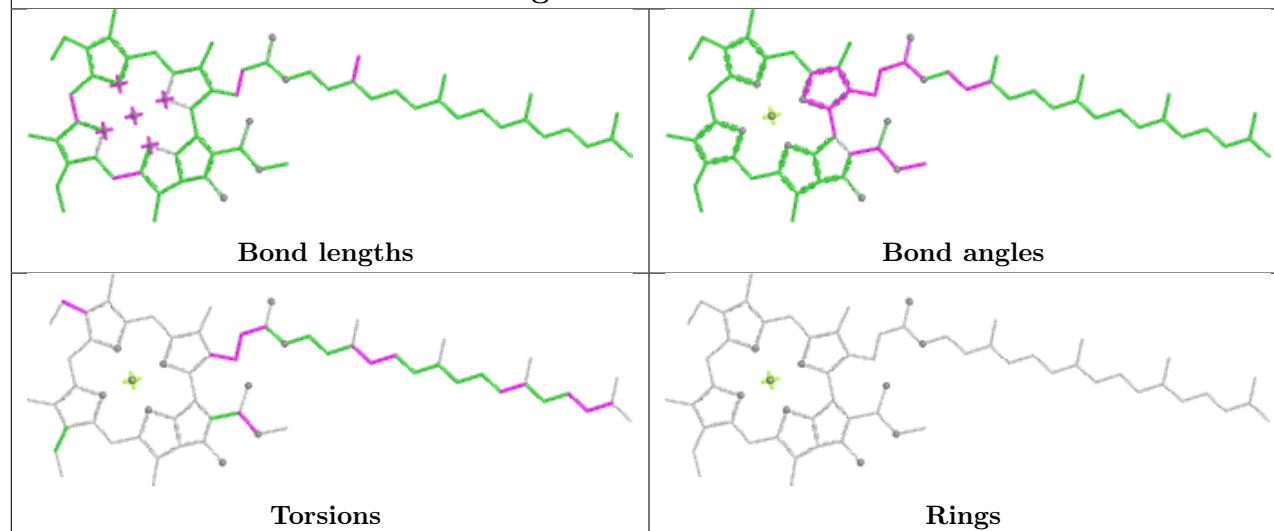
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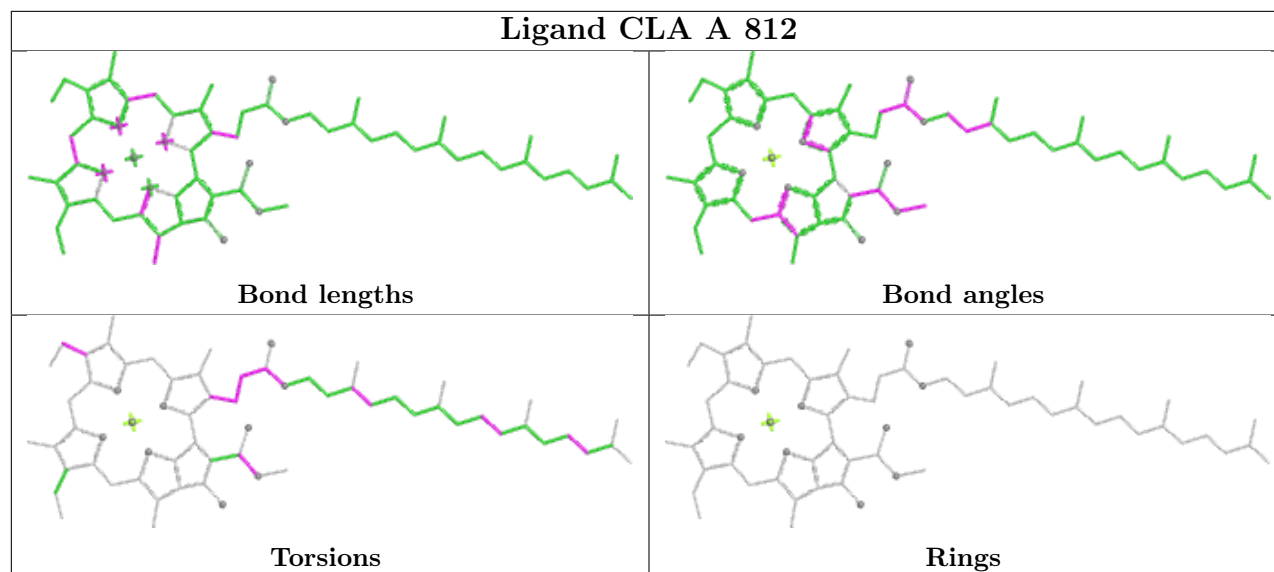
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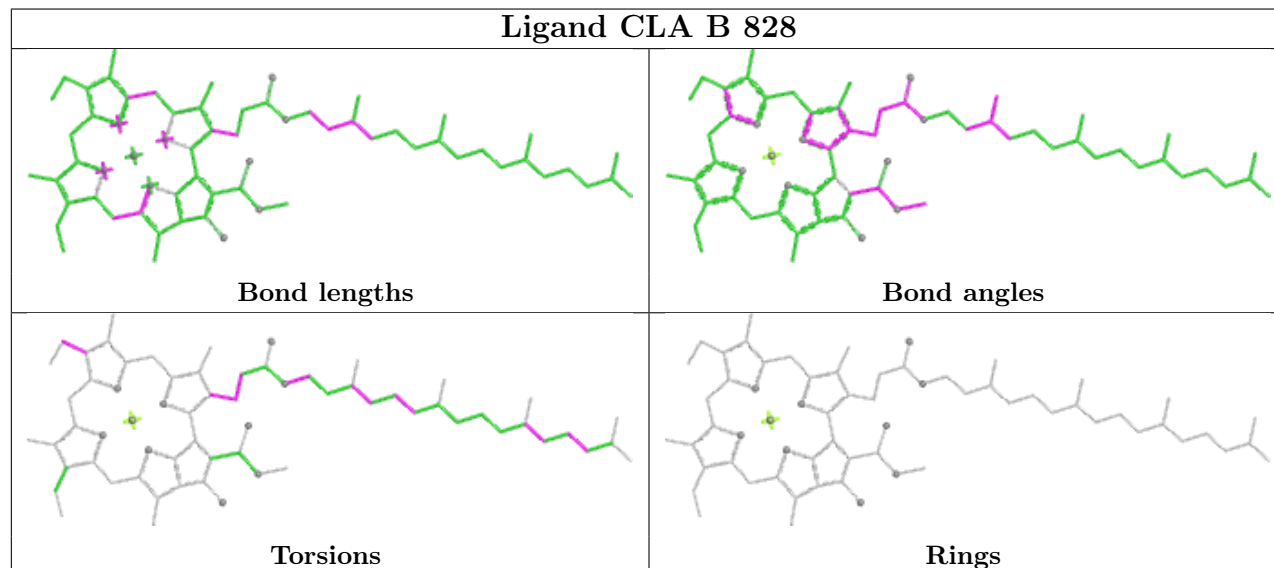
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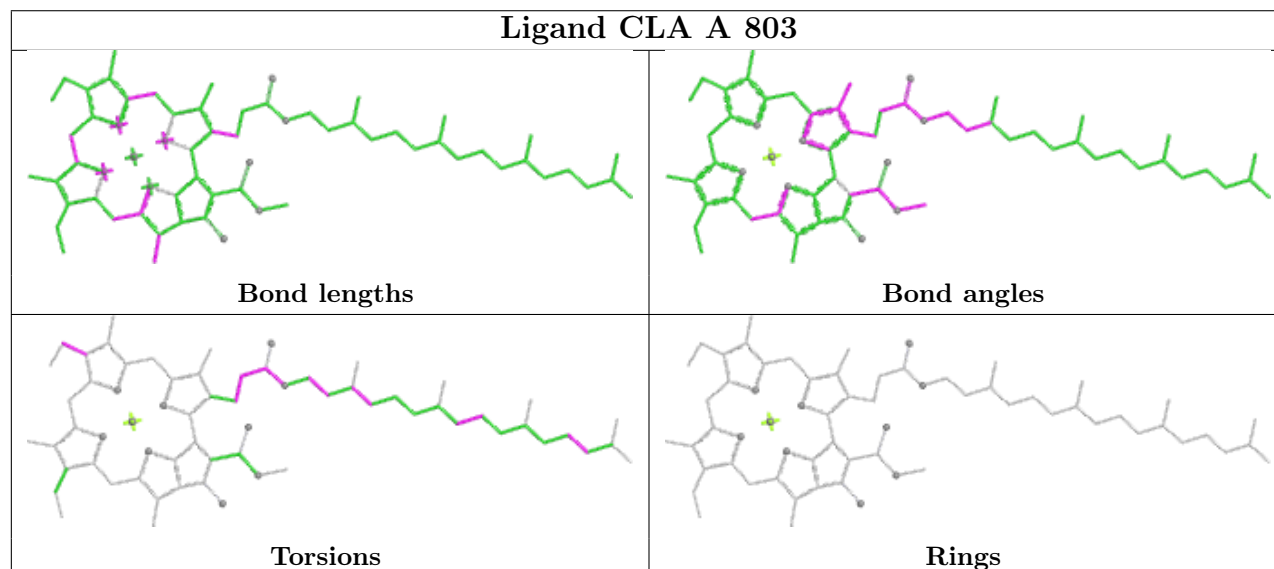
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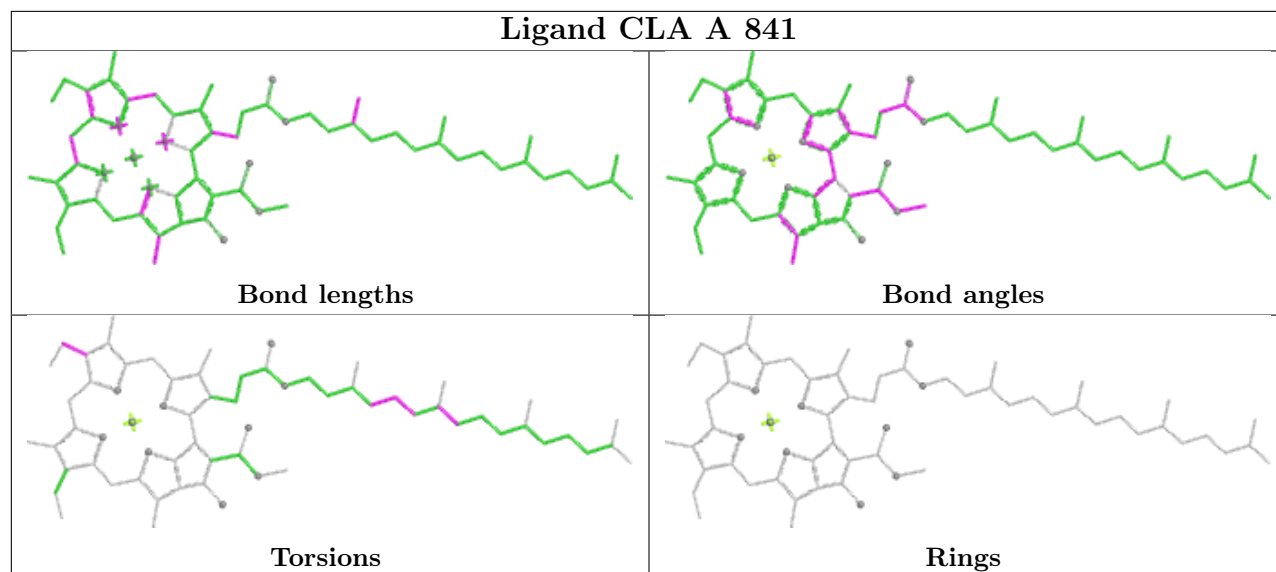
Ligand CLA B 828



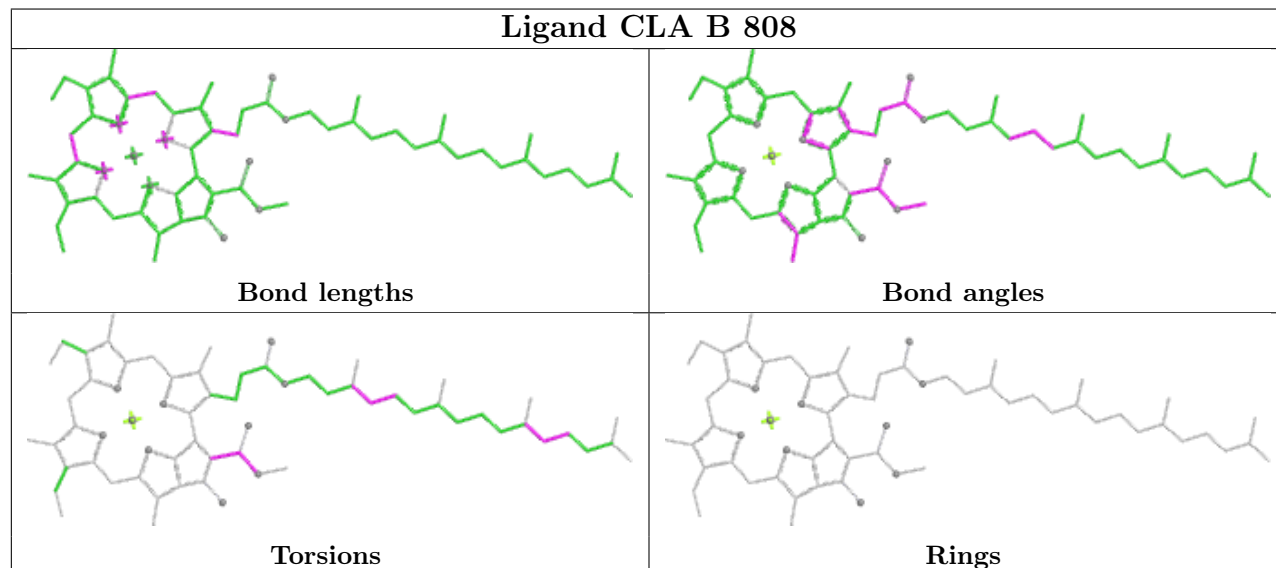
Ligand CLA A 803



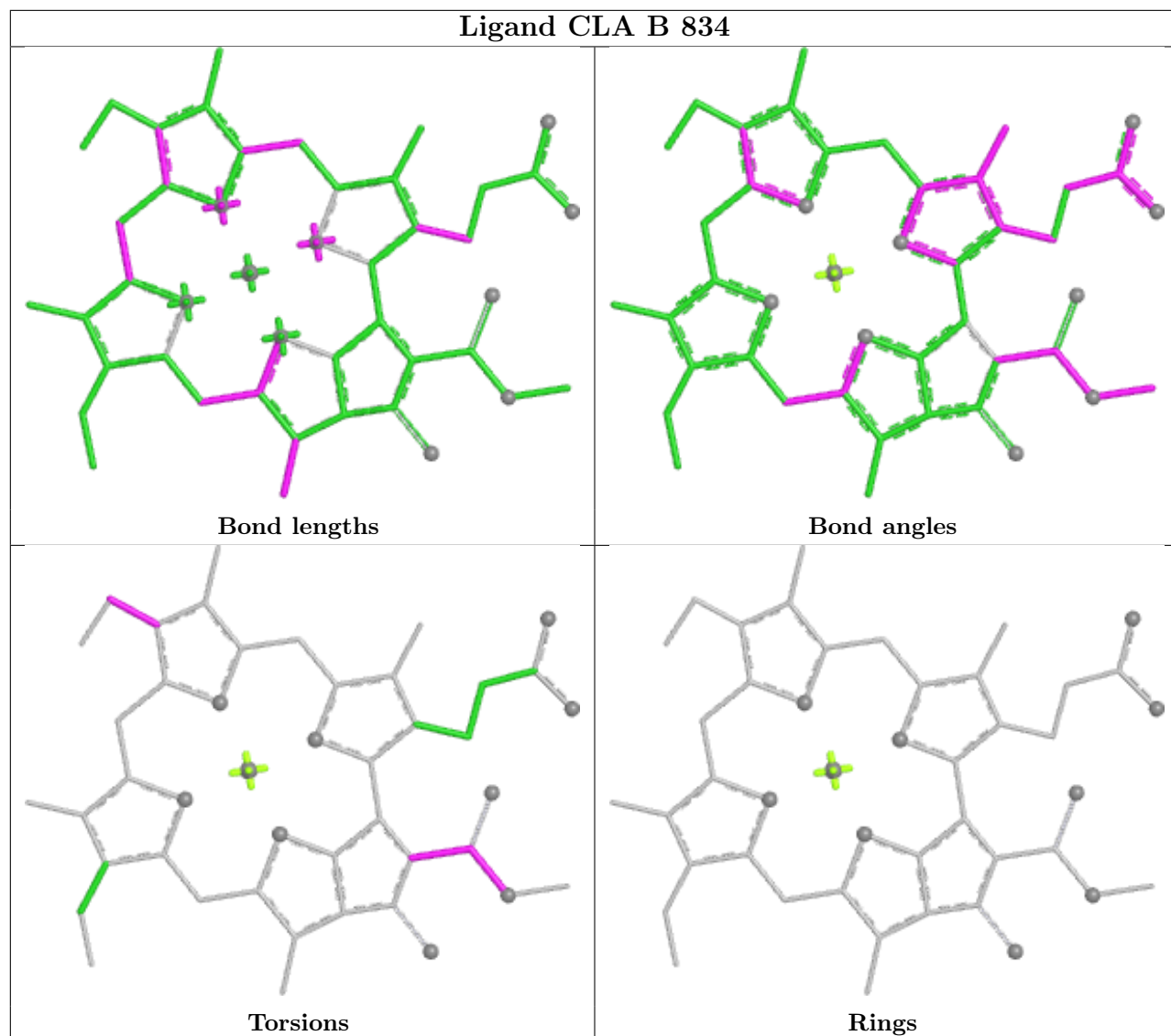
Ligand CLA A 841



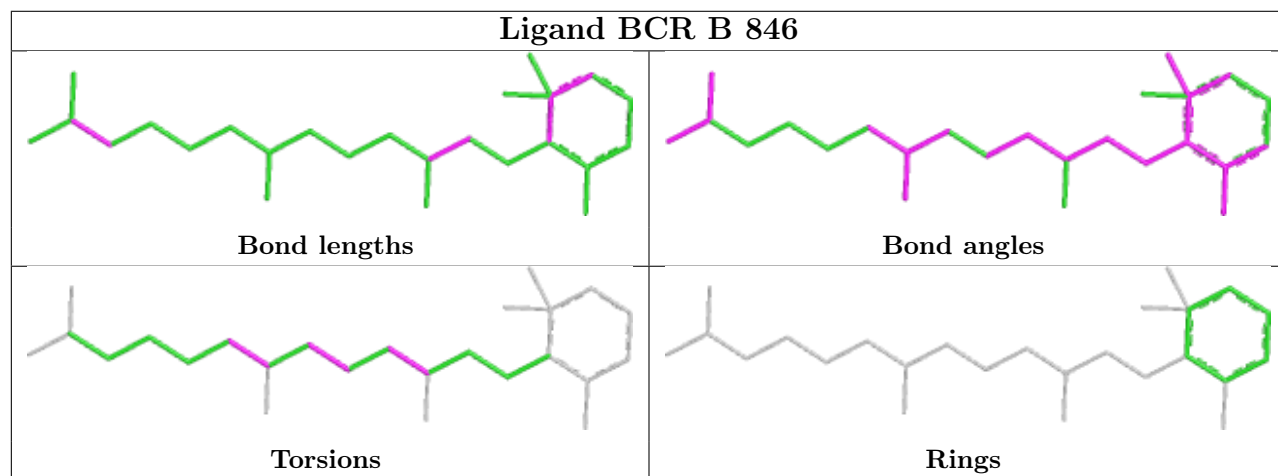
Ligand CLA B 808



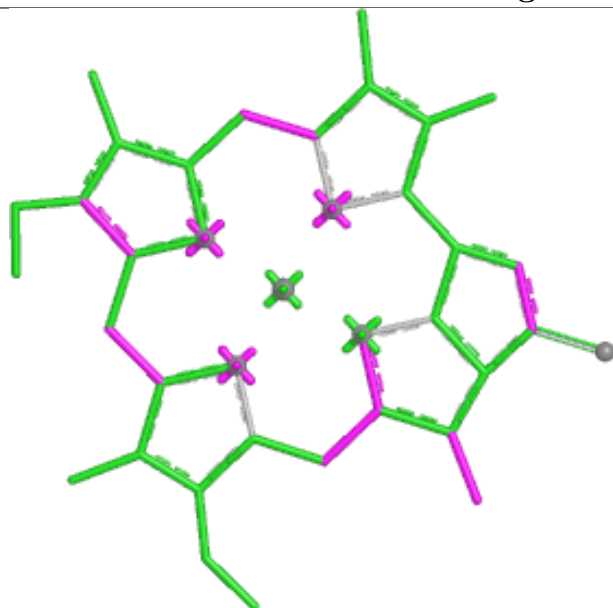
Ligand CLA B 834



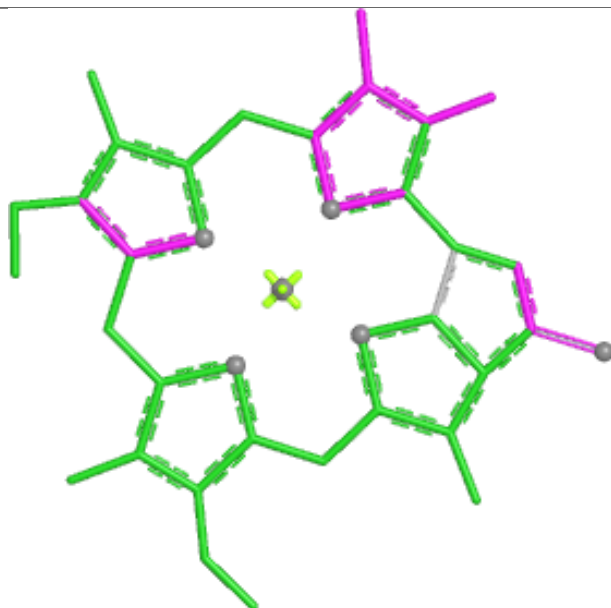
Ligand BCR B 846



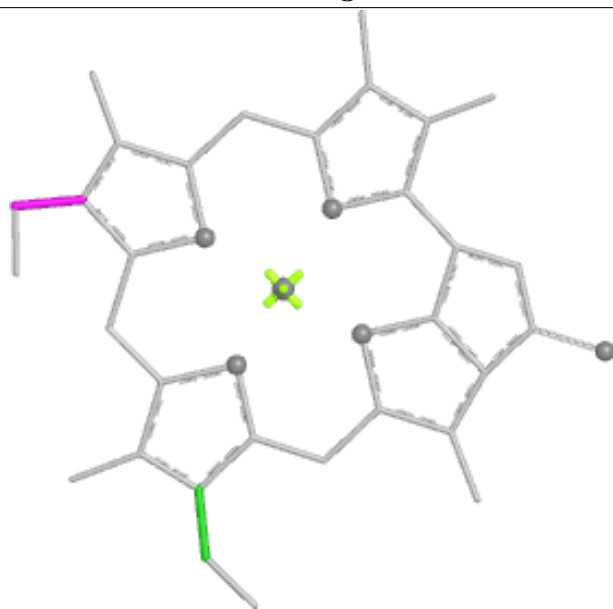
Ligand CLA J 102



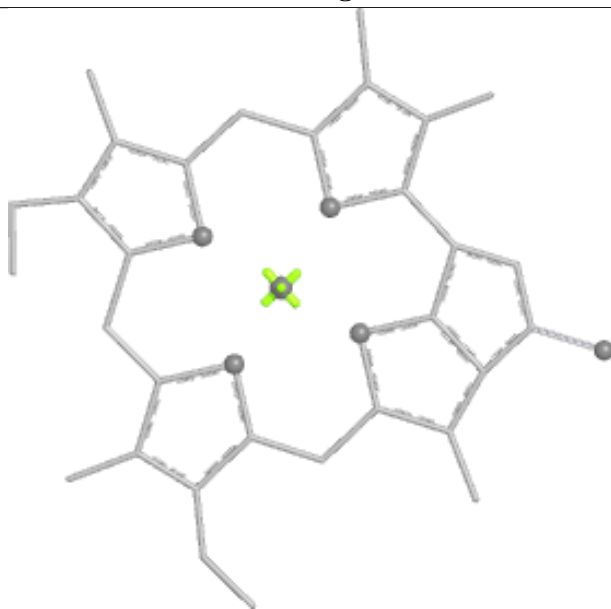
Bond lengths



Bond angles

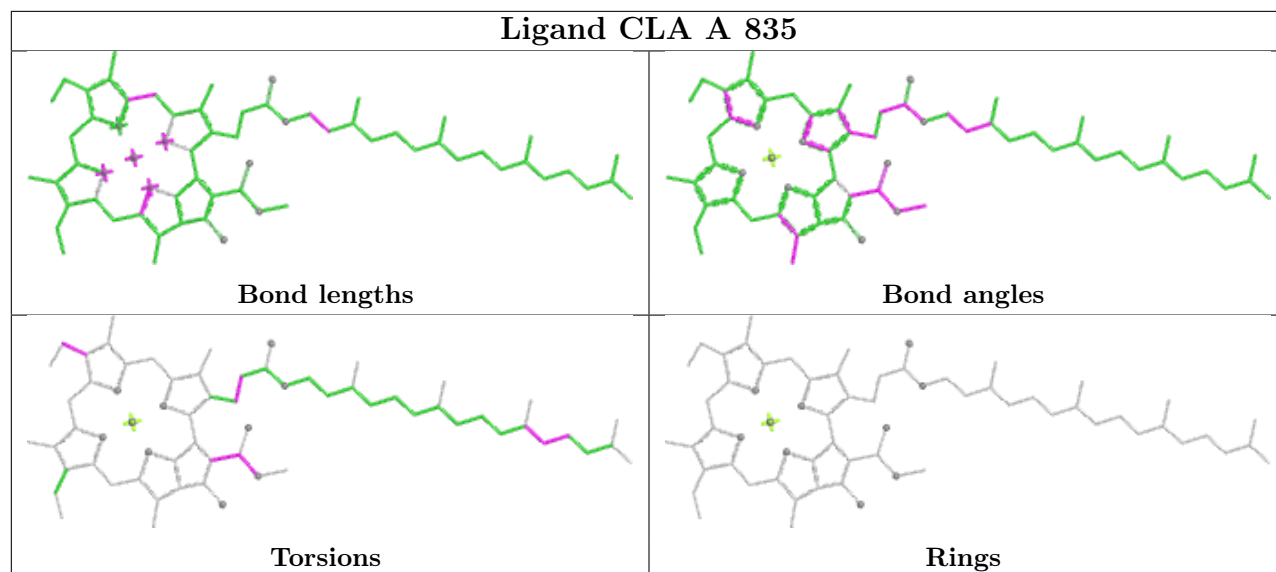


Torsions

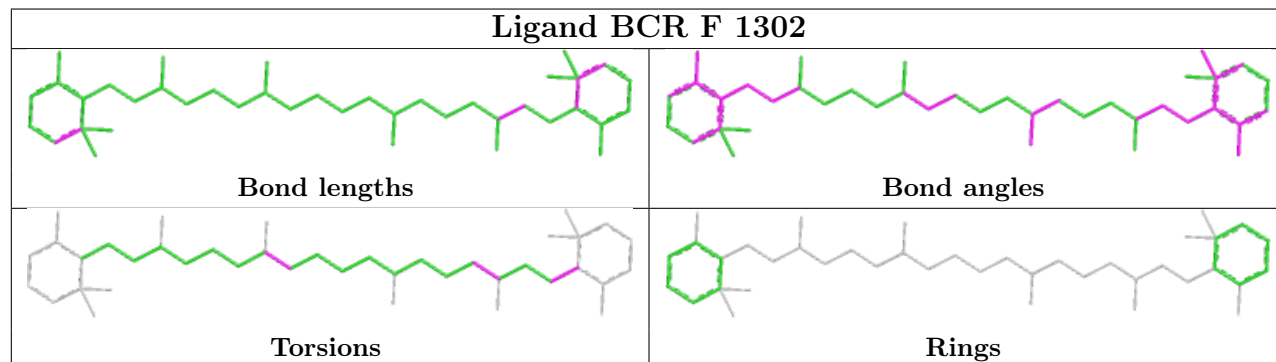


Rings

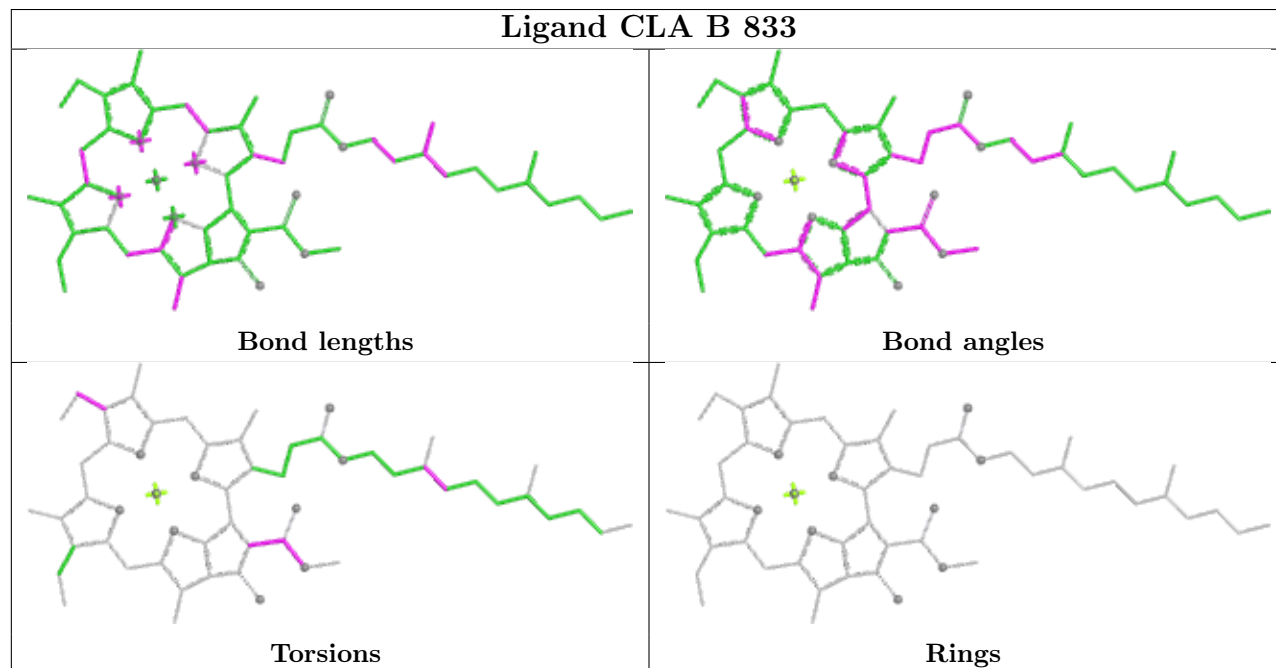
Ligand CLA A 835



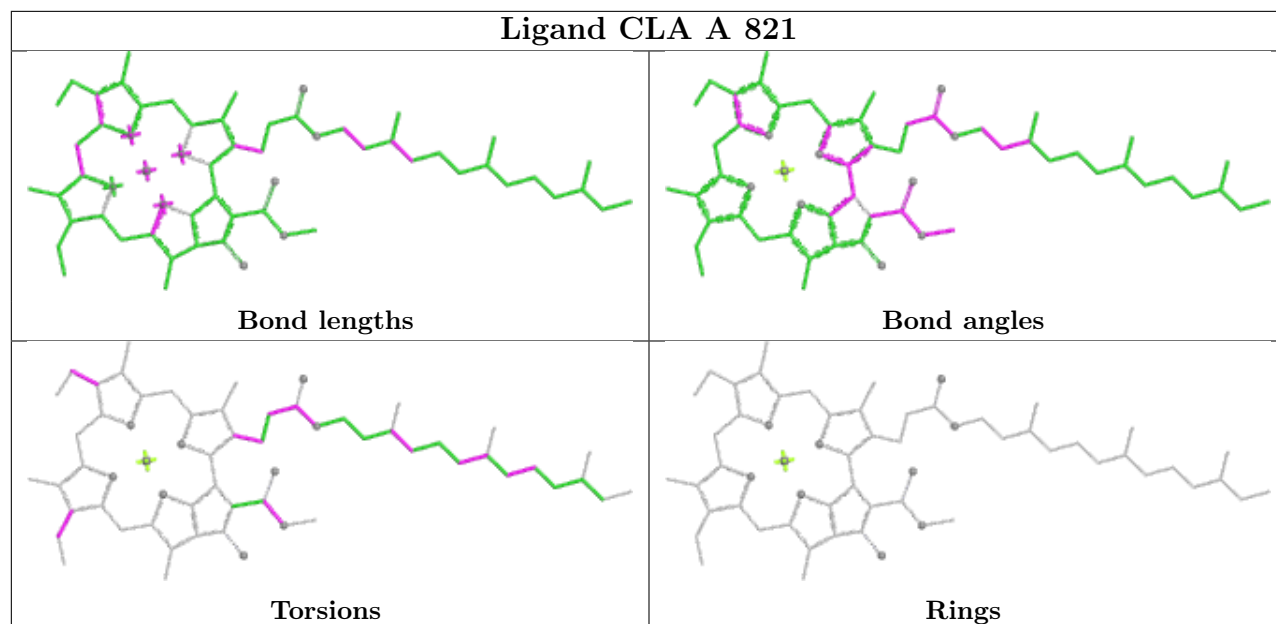
Ligand BCR F 1302



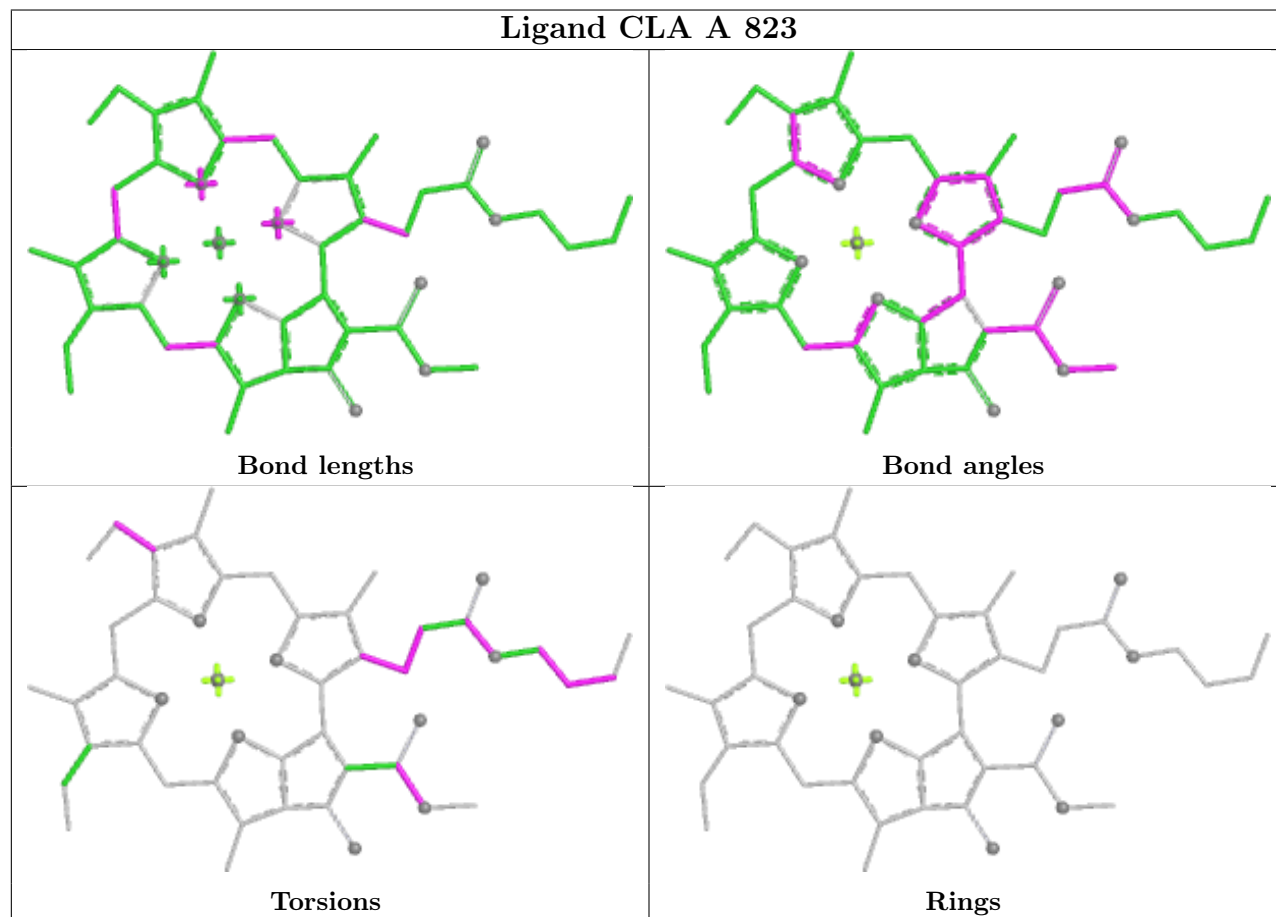
Ligand CLA B 833



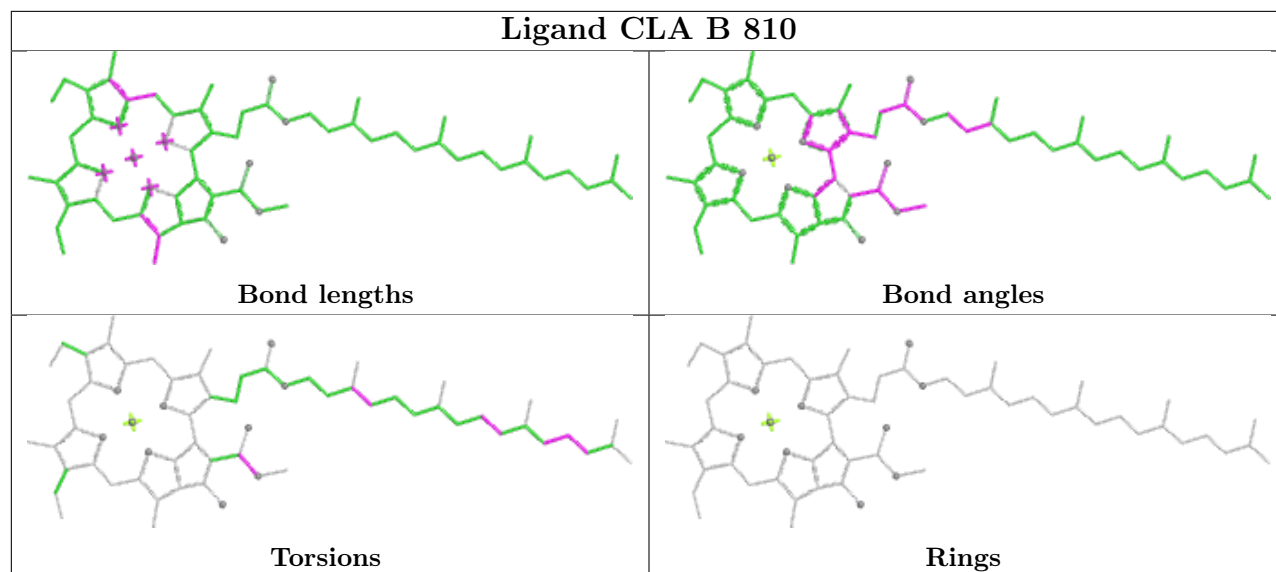
Ligand CLA A 821



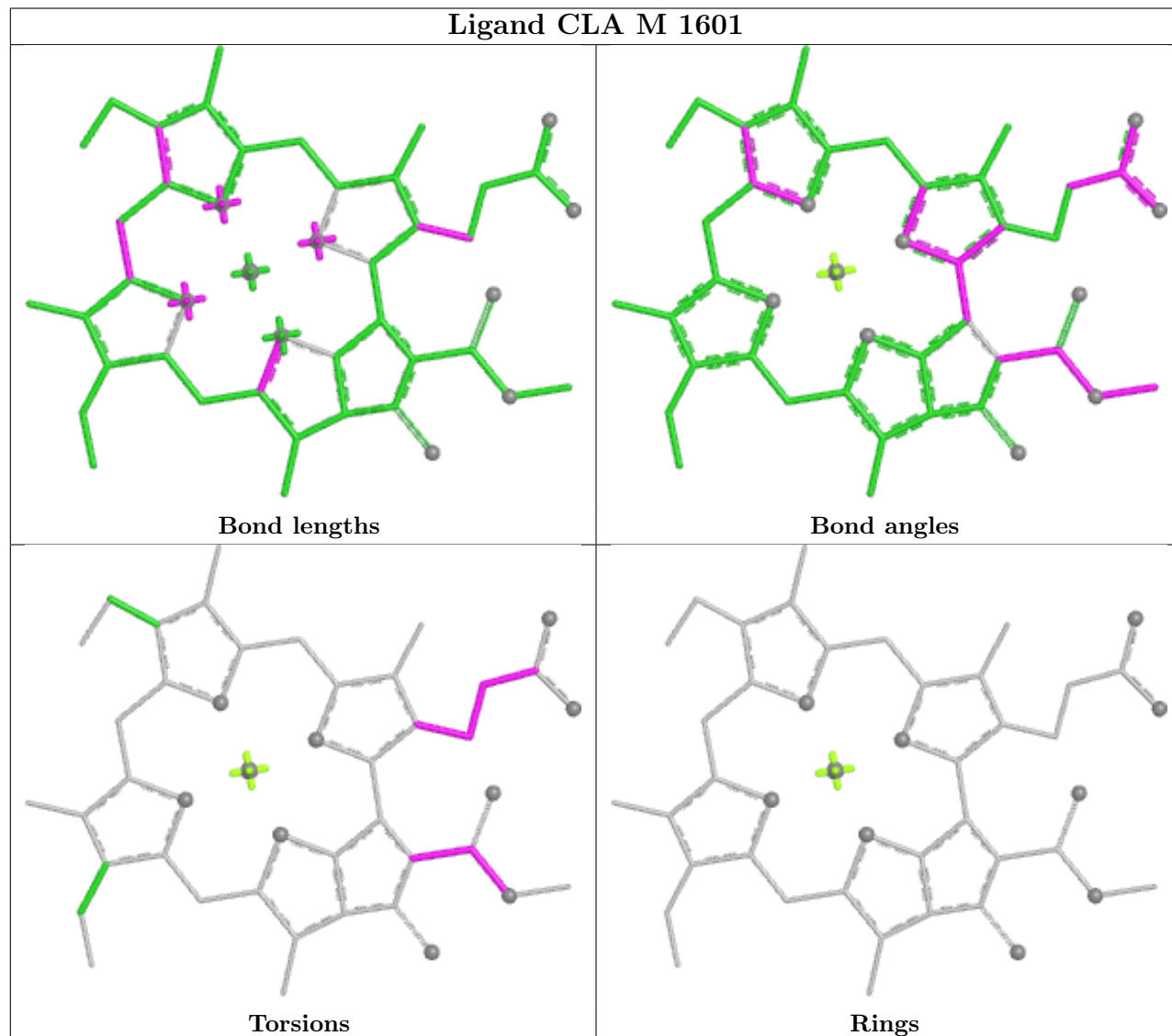
Ligand CLA A 823

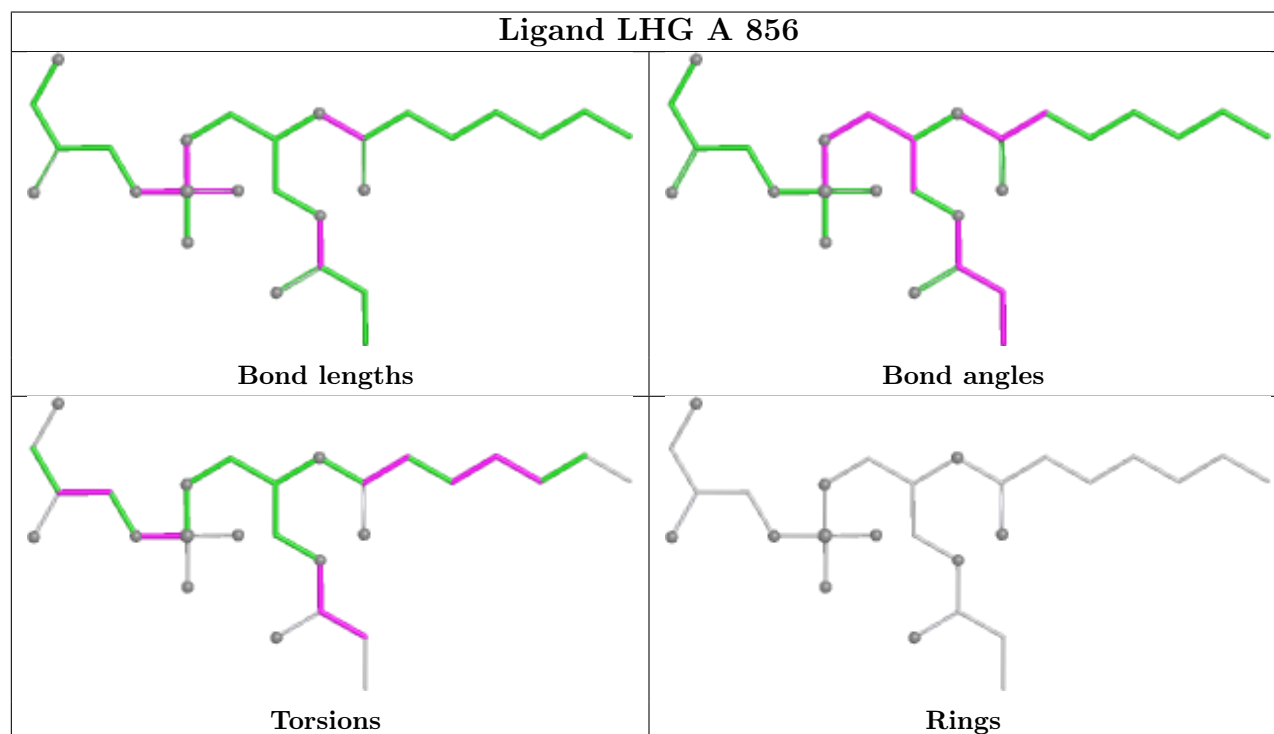
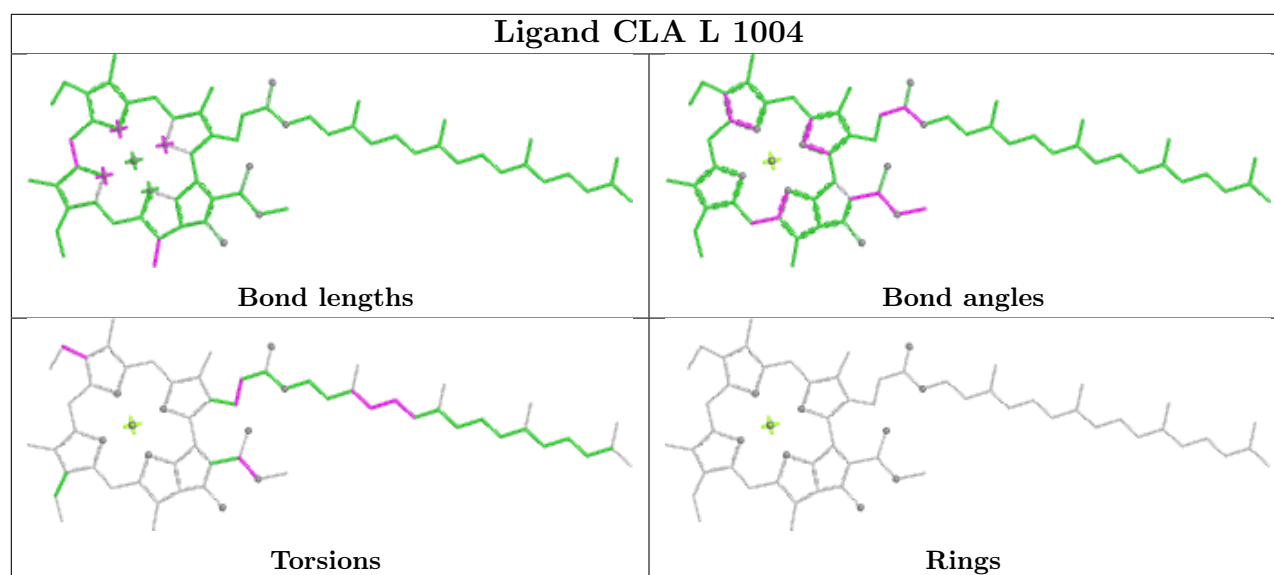


Ligand CLA B 810

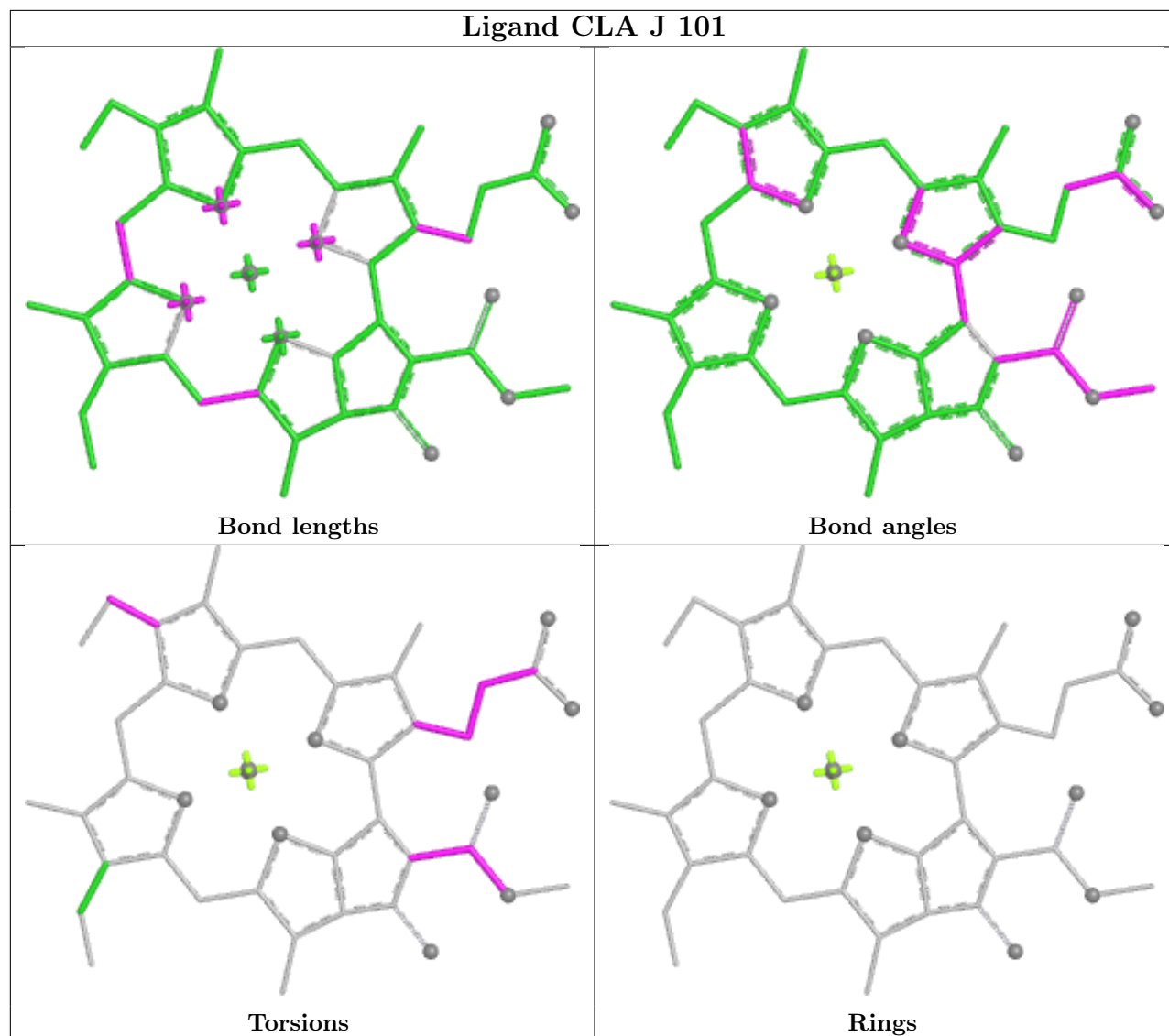


Ligand CLA M 1601

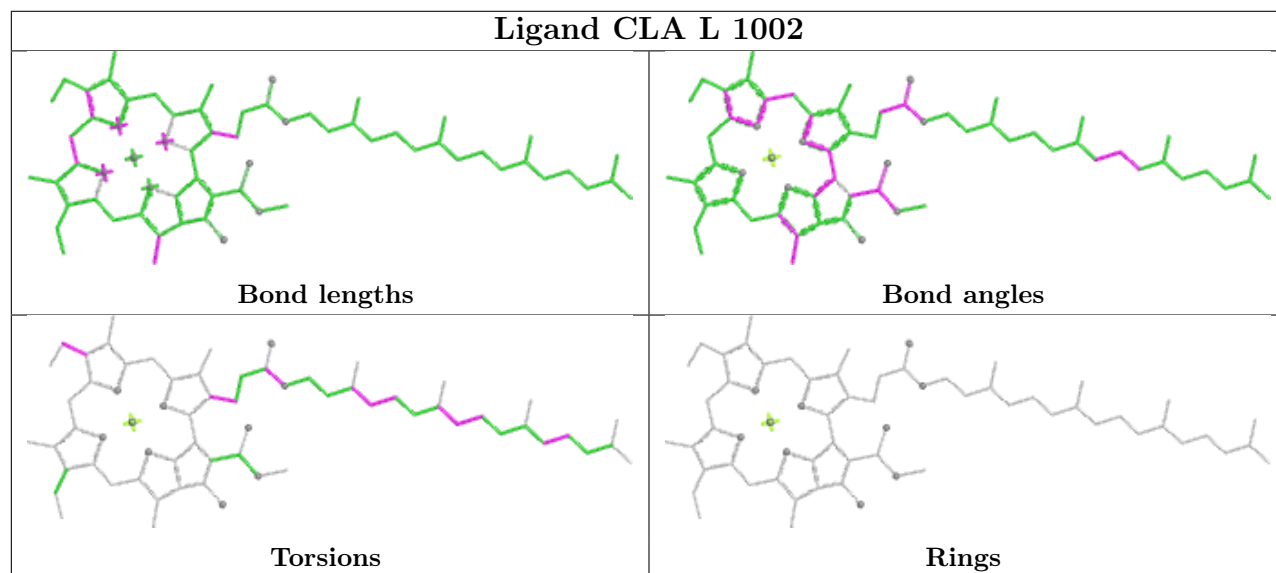




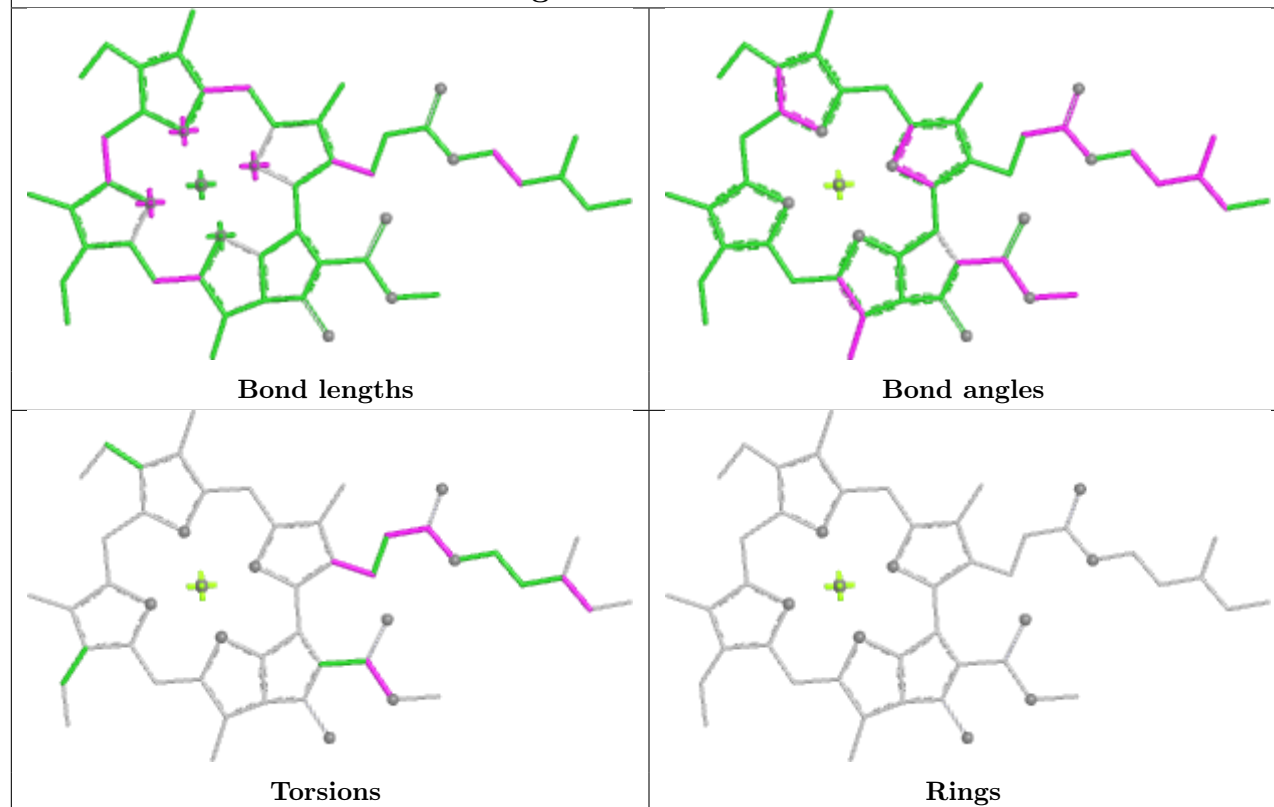
Ligand CLA J 101



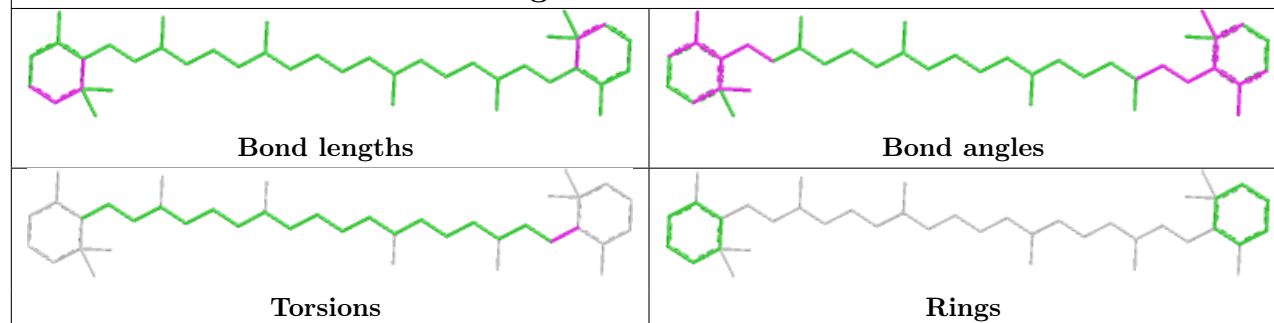
Ligand CLA L 1002



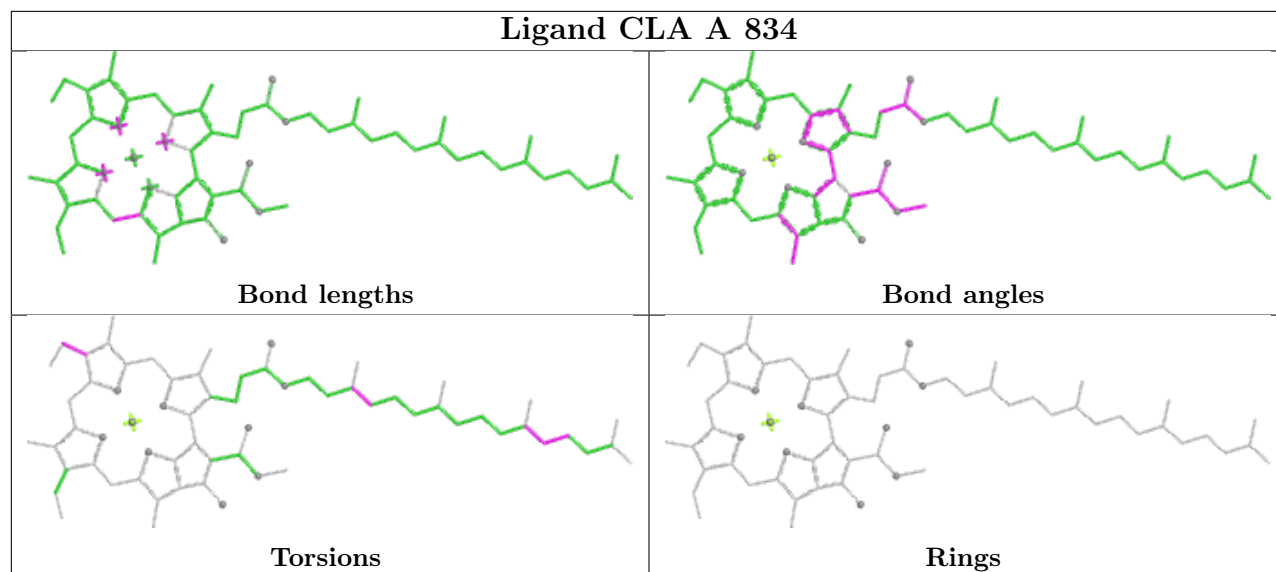
Ligand CLA A 824



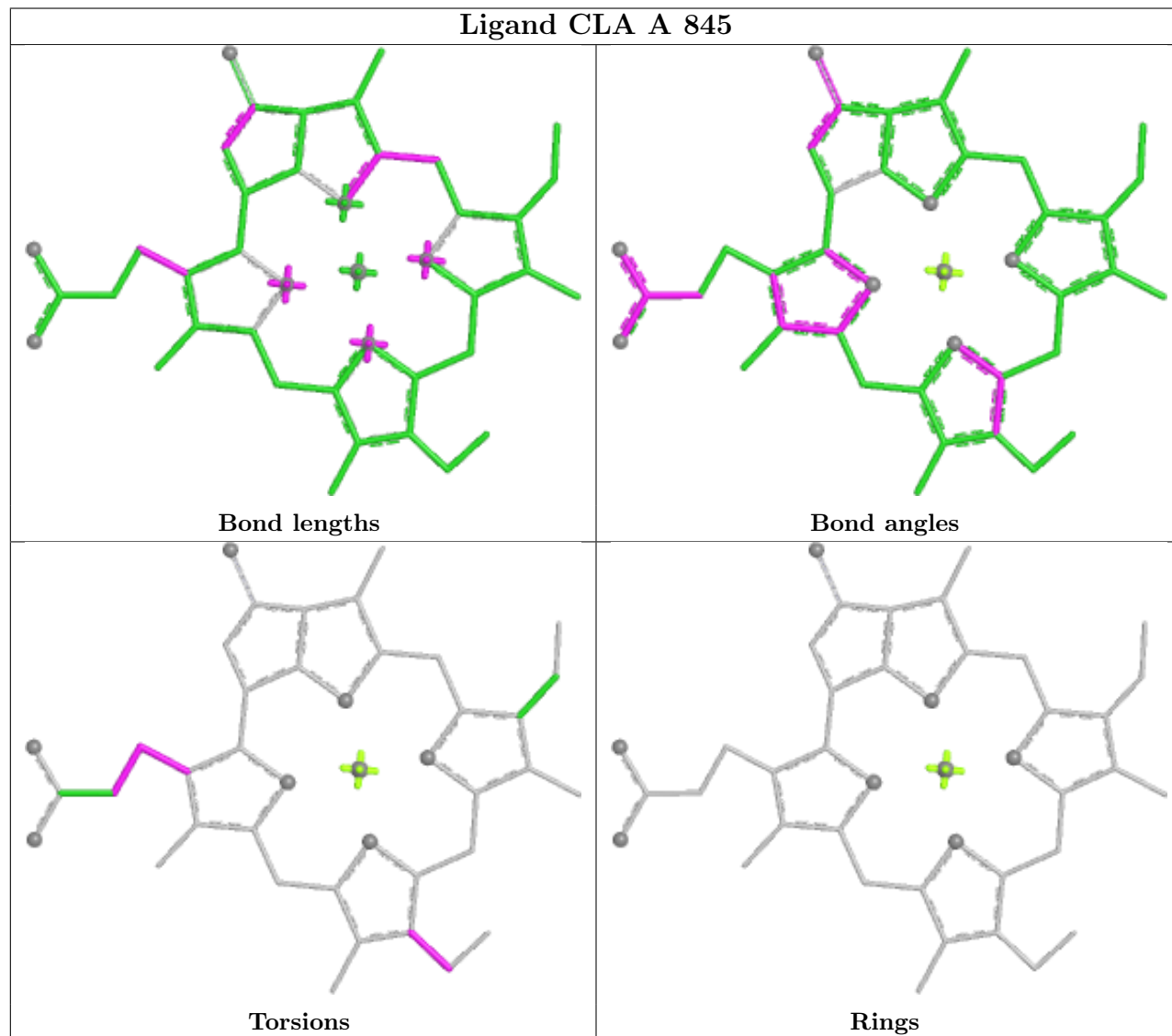
Ligand BCR A 852



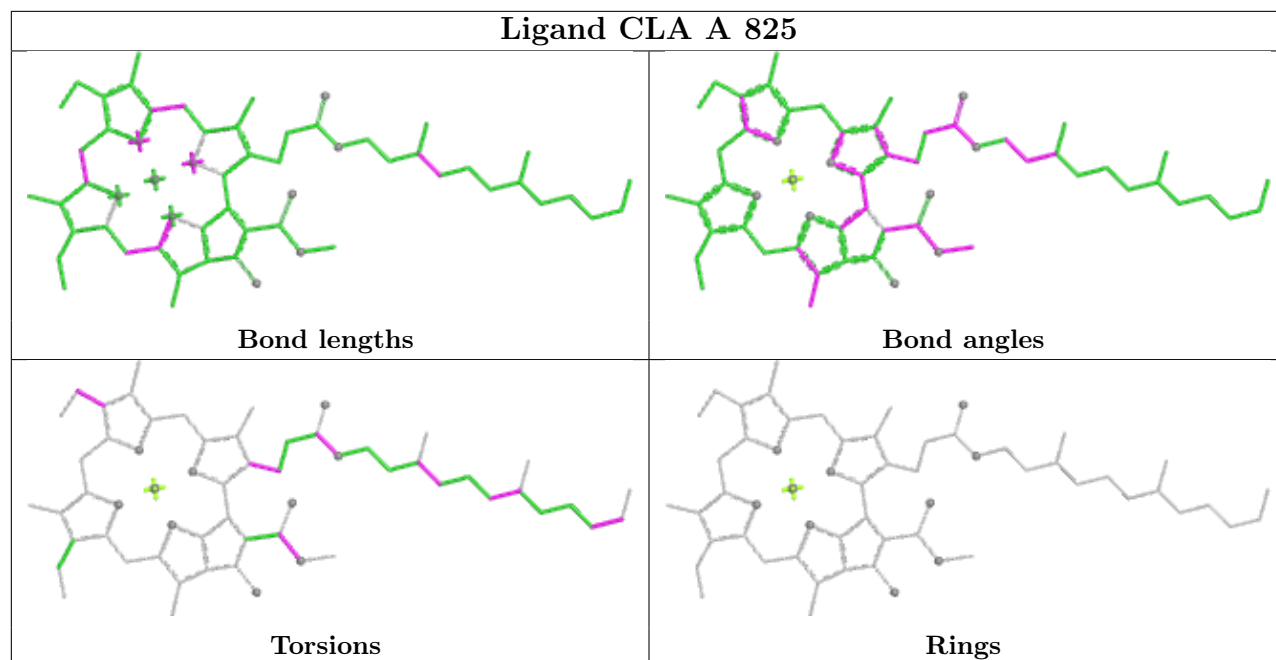
Ligand CLA A 834



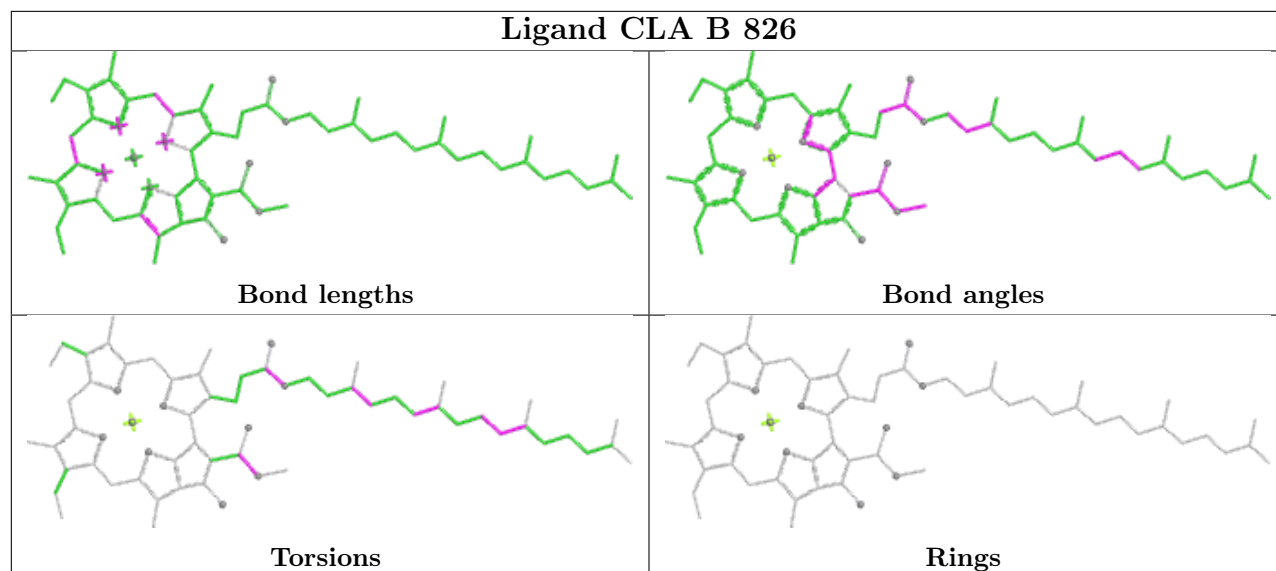
Ligand CLA A 845

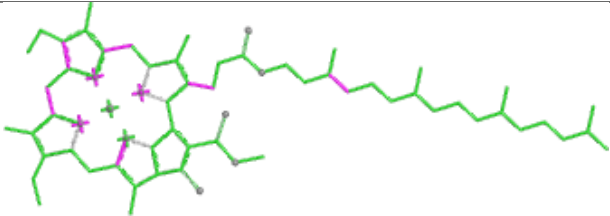
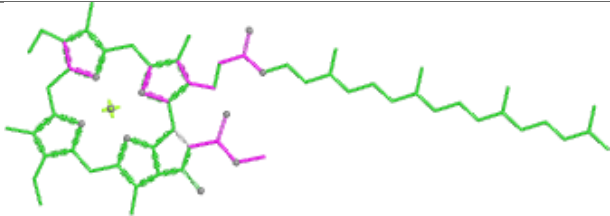
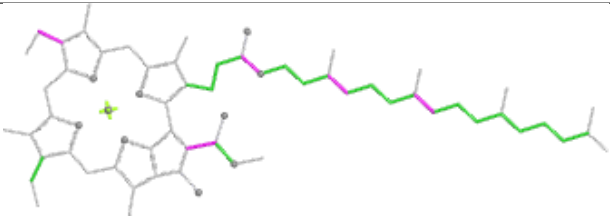
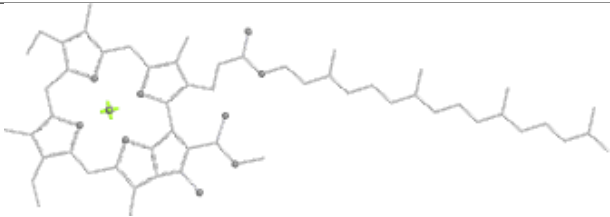
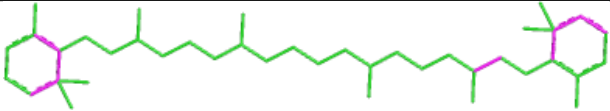
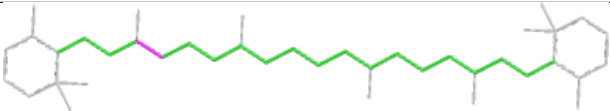
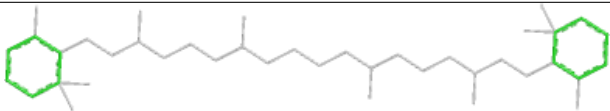


Ligand CLA A 825

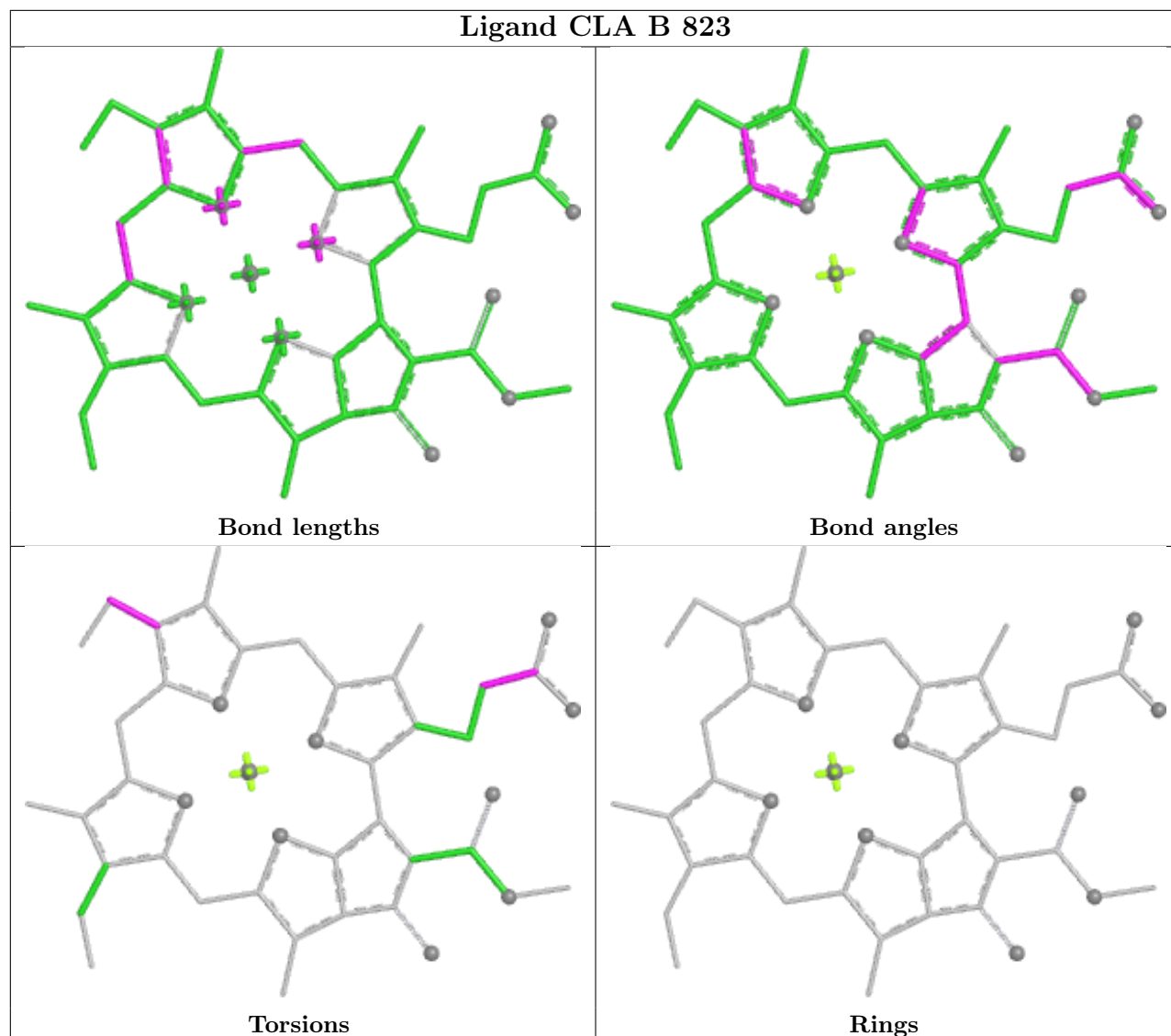


Ligand CLA B 826

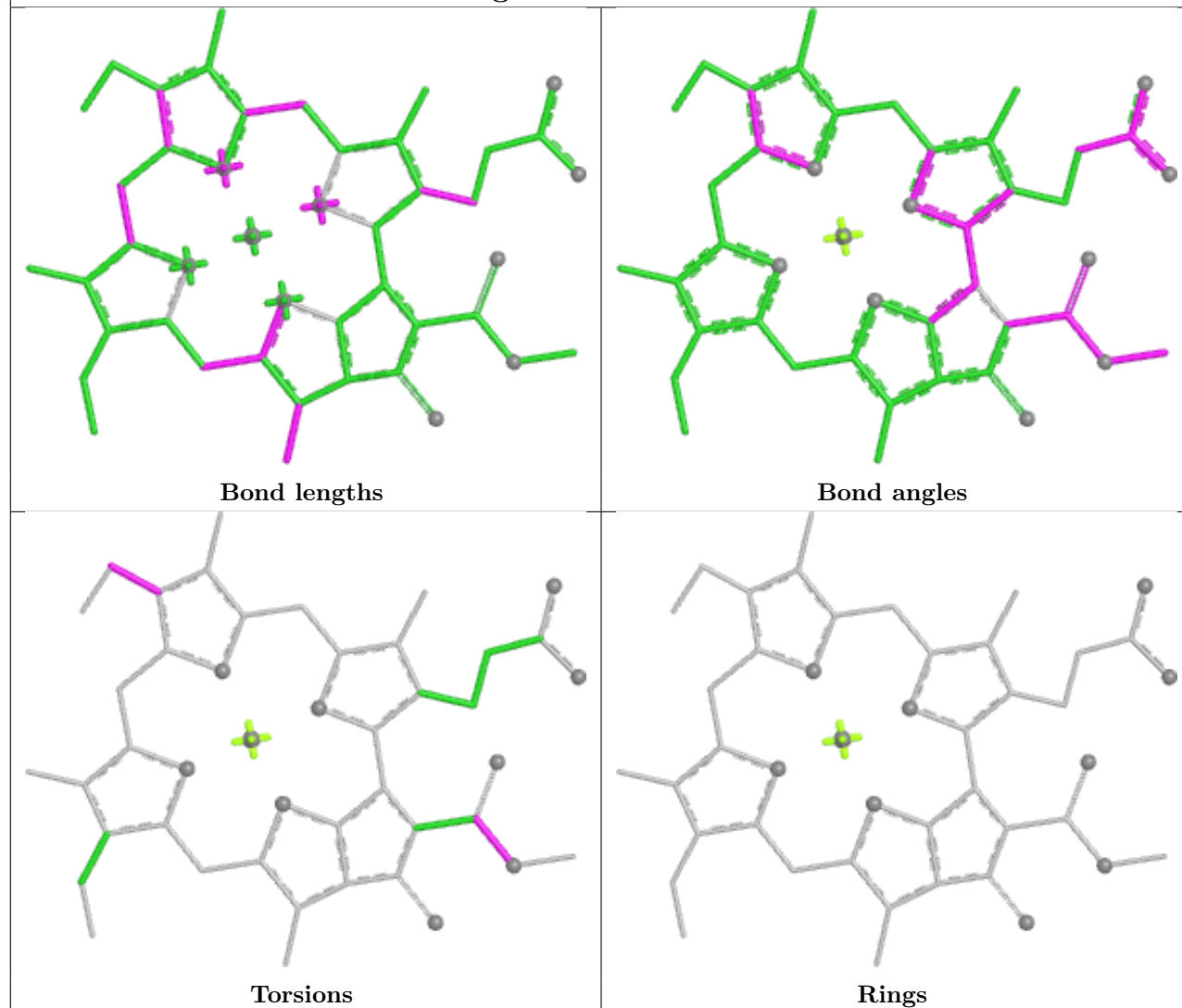


Ligand CLA A 831	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

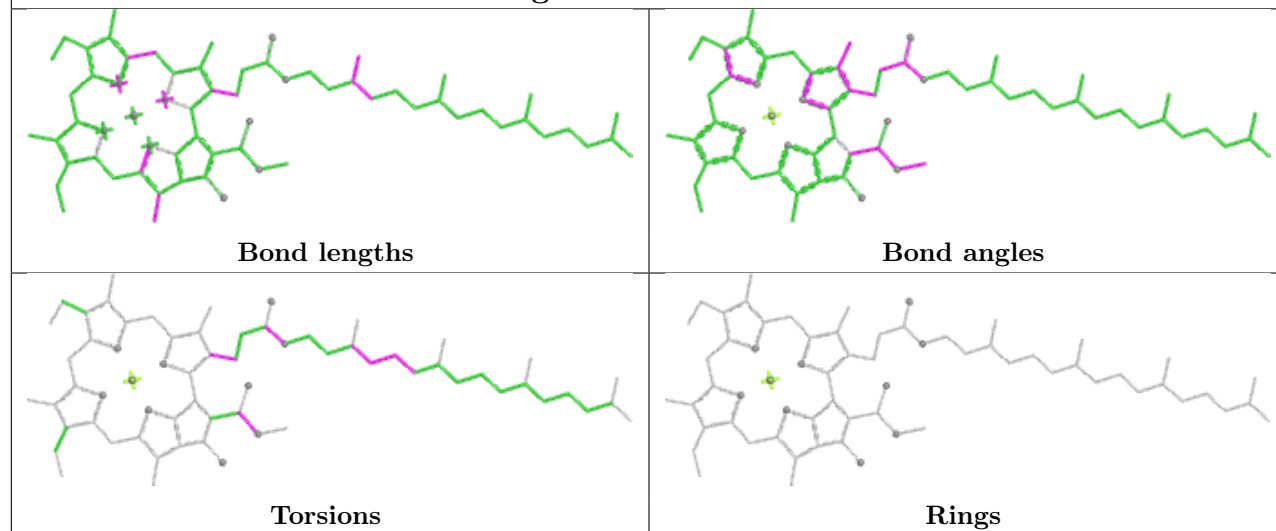
Ligand CLA B 823

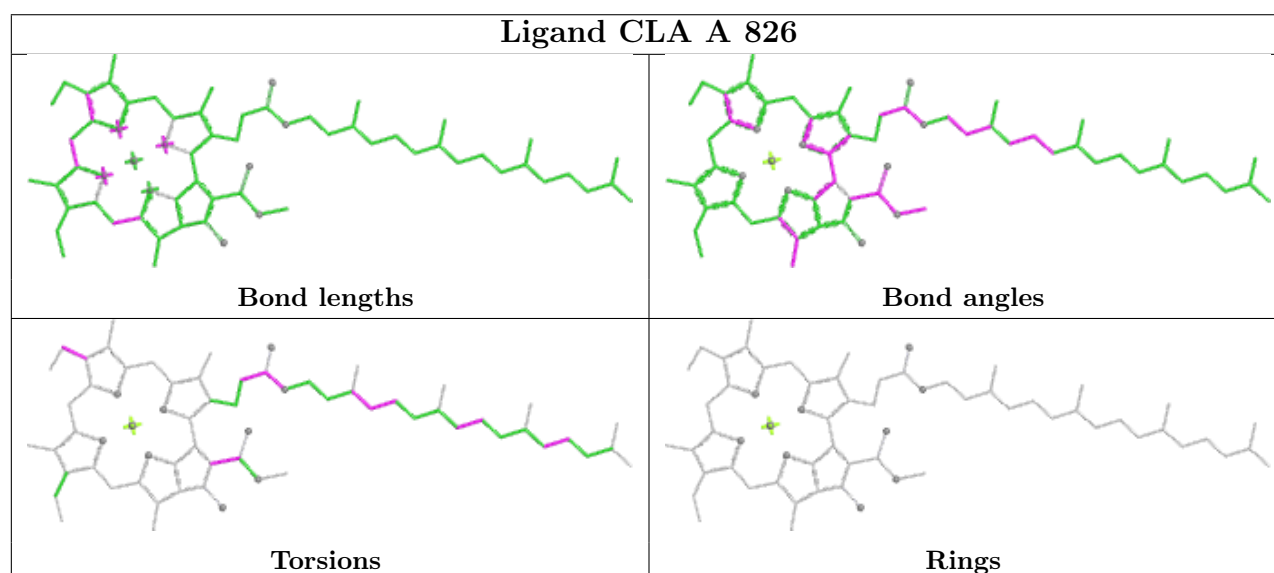
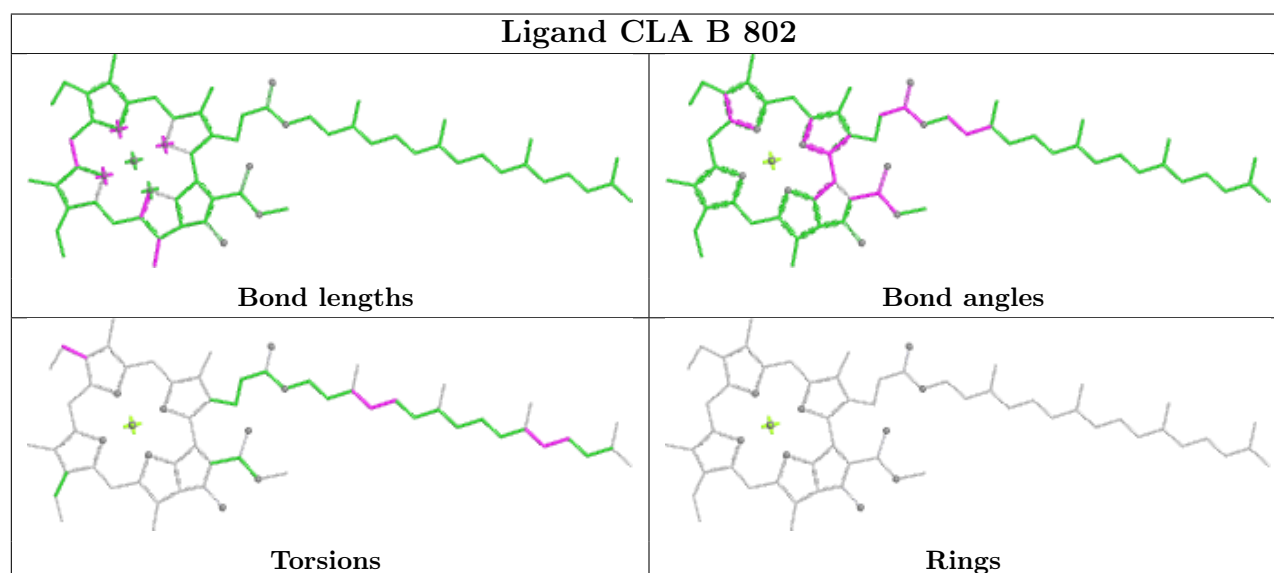
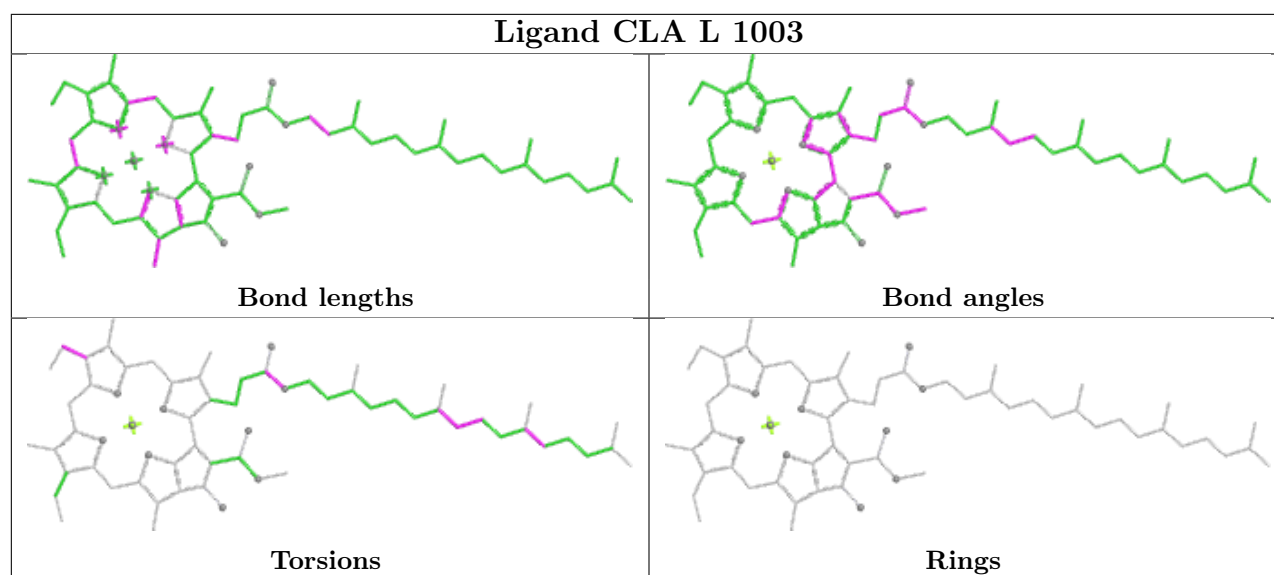


Ligand CLA A 815

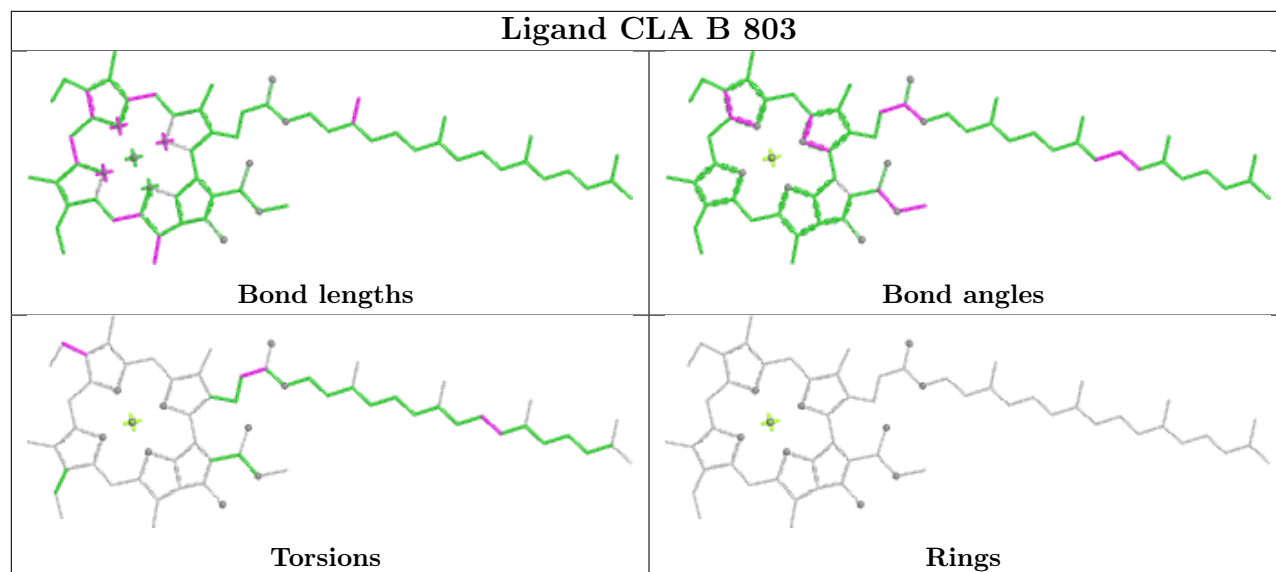


Ligand CLA A 844

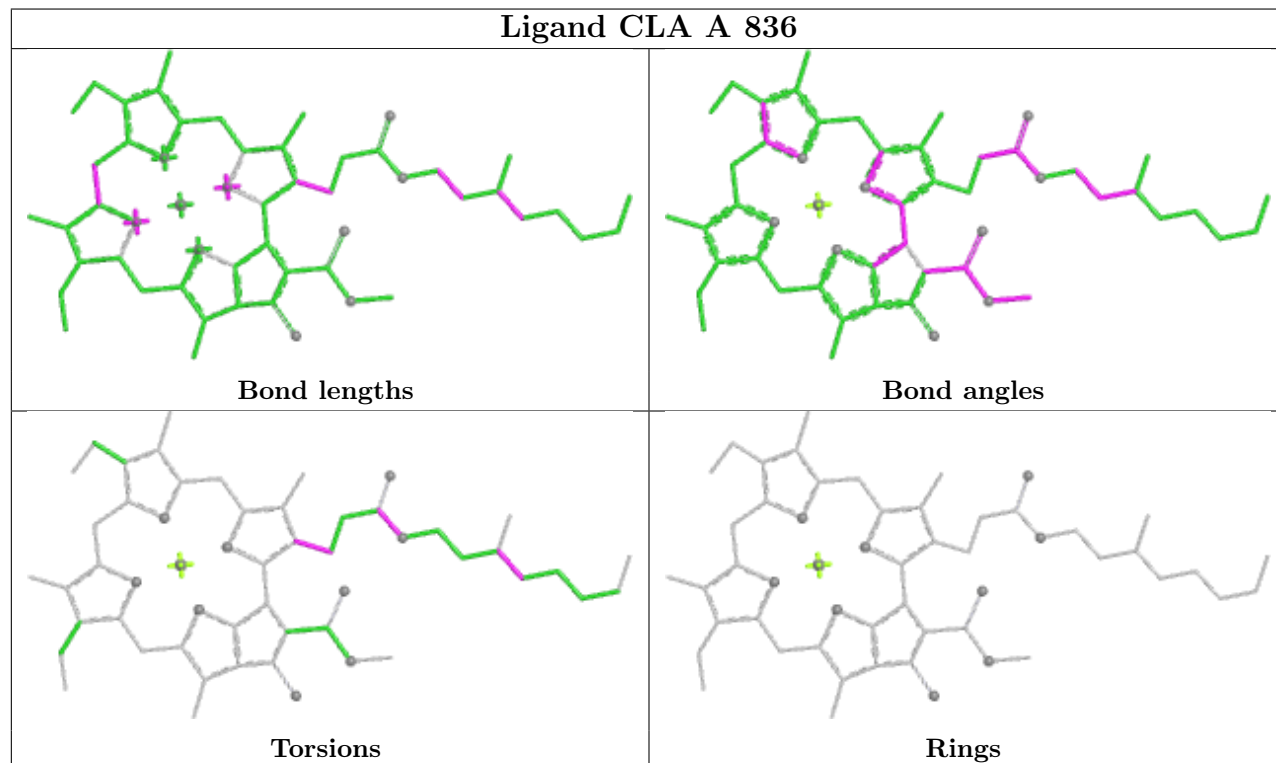




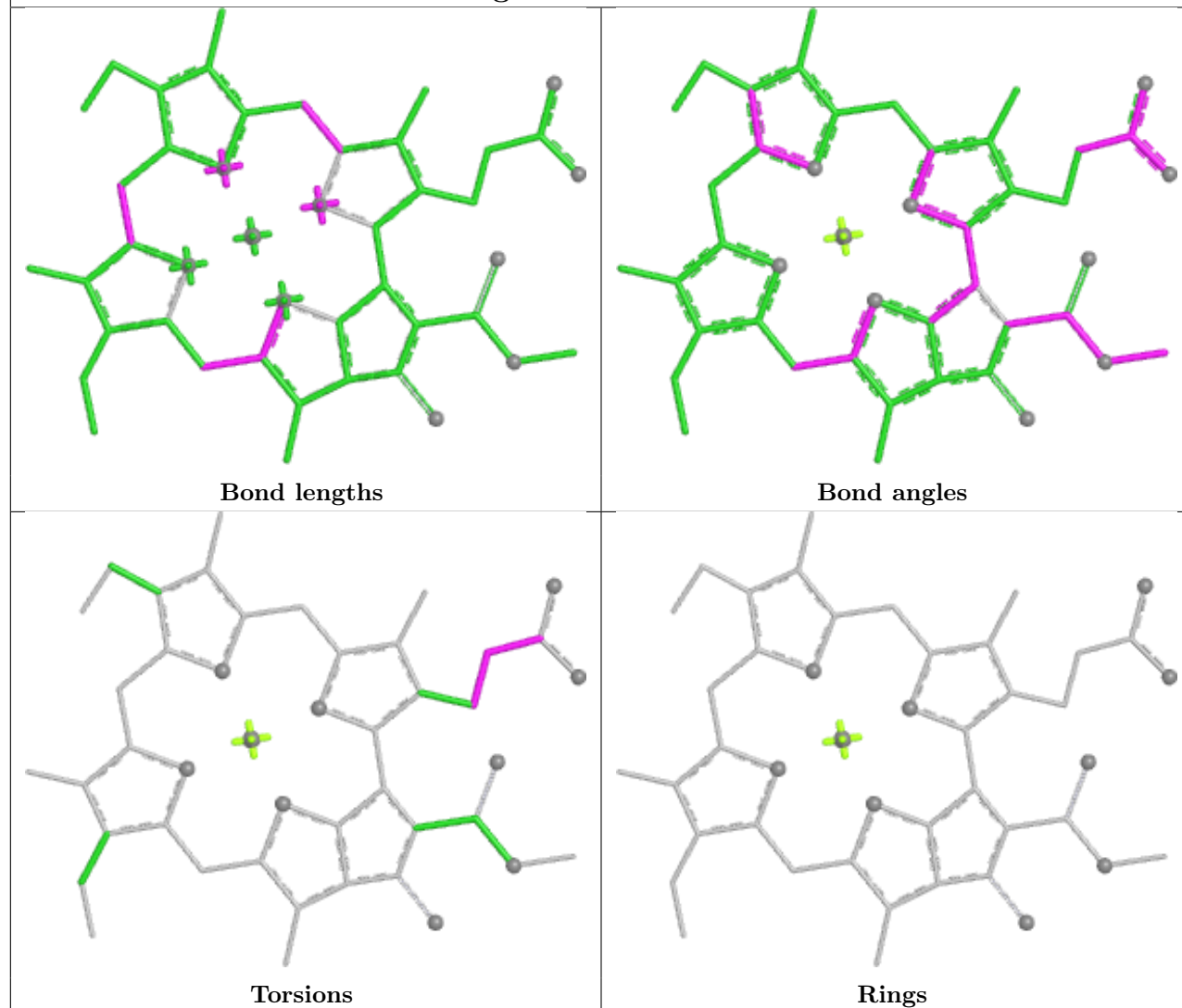
Ligand CLA B 803



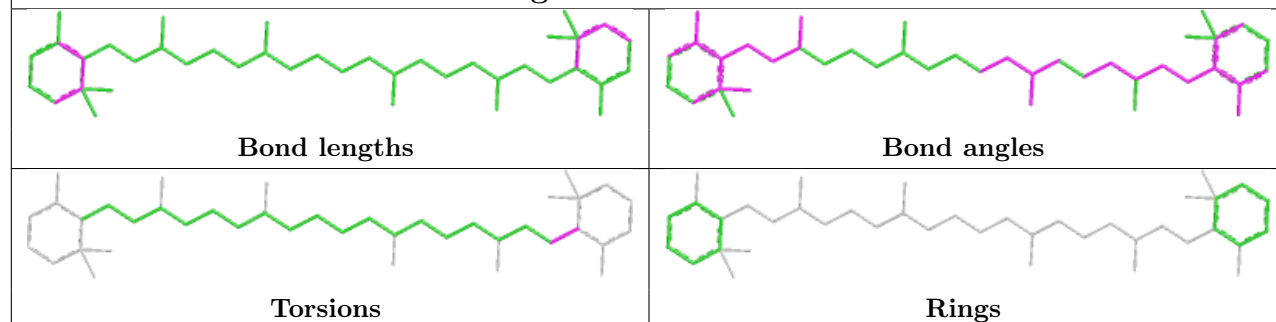
Ligand CLA A 836

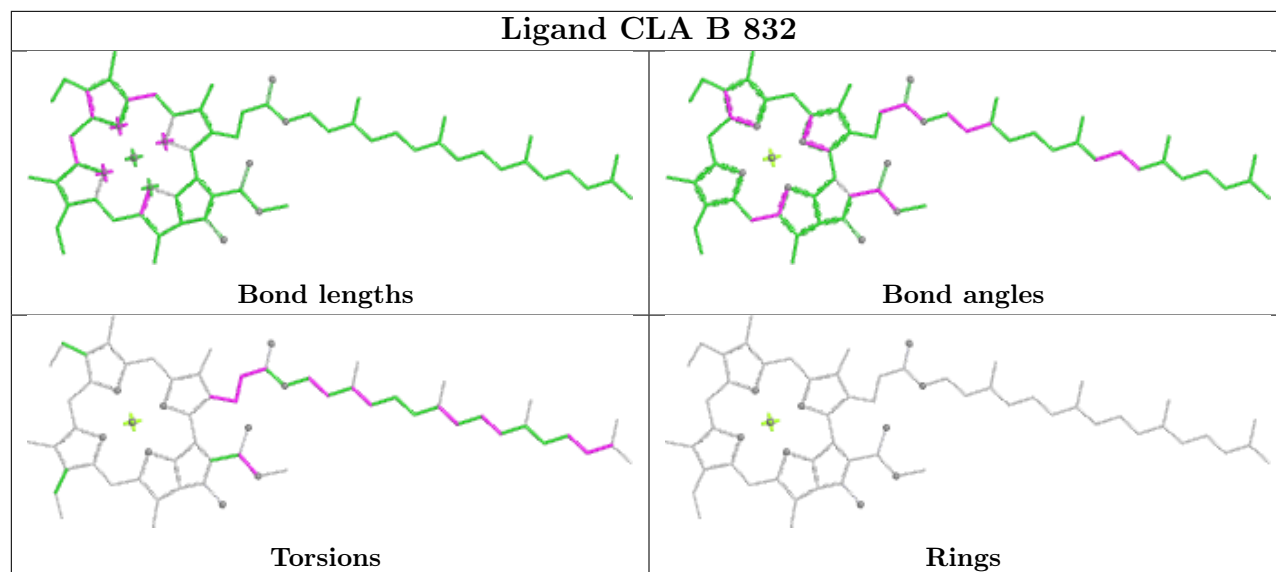
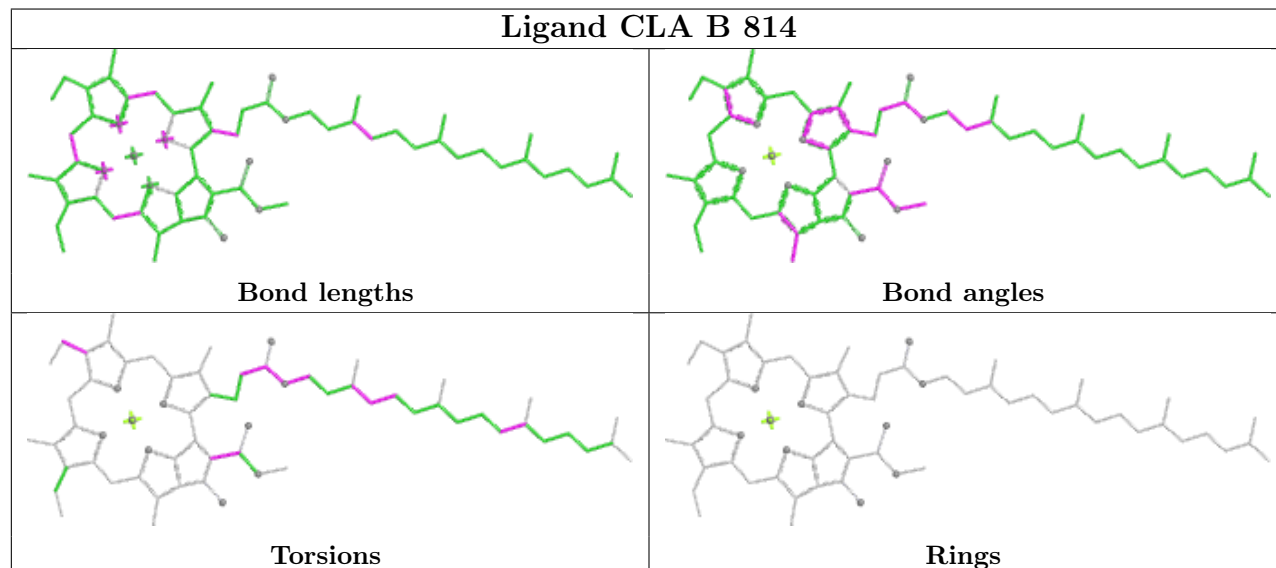


Ligand CLA B 812

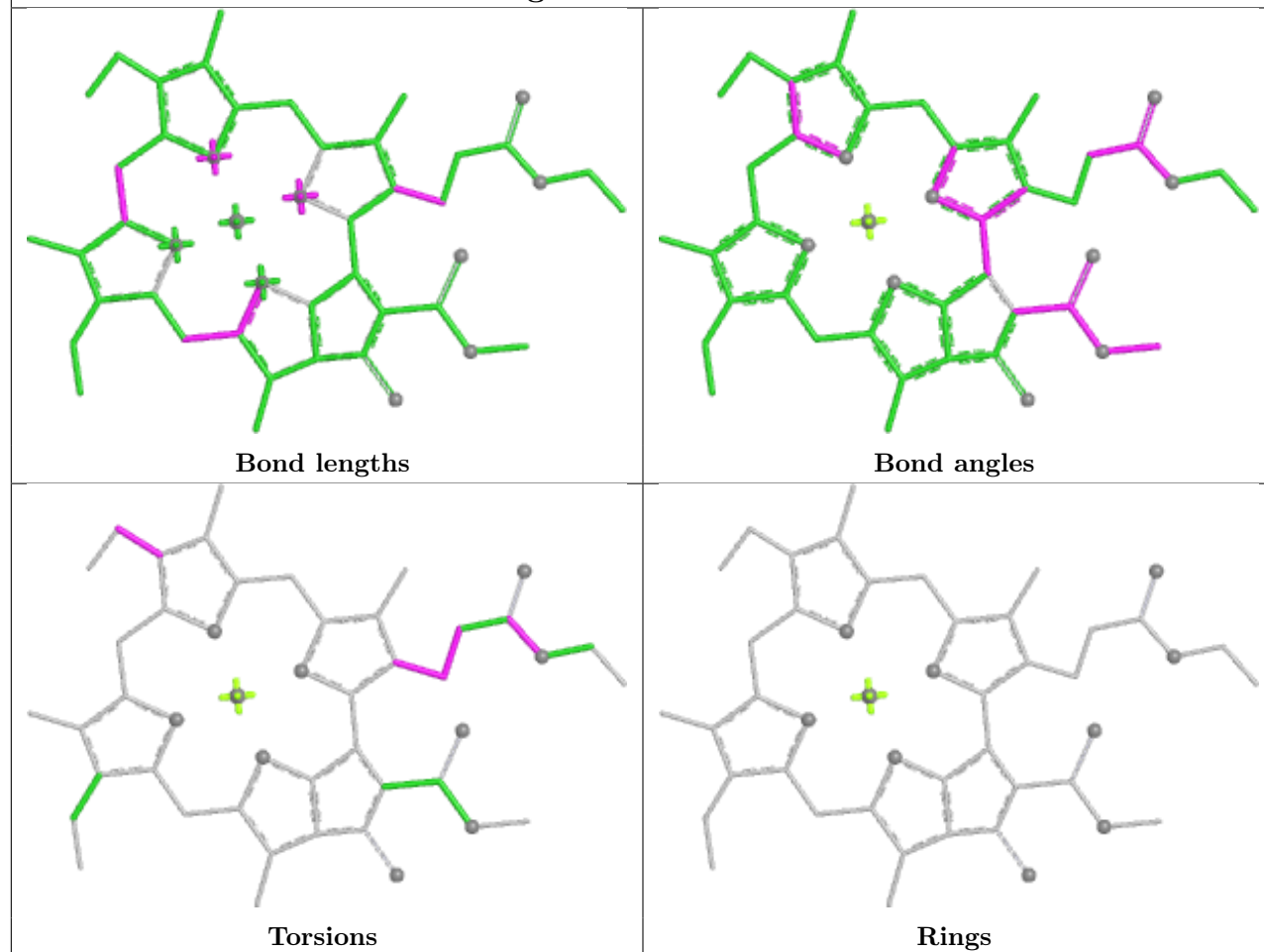


Ligand BCR B 847

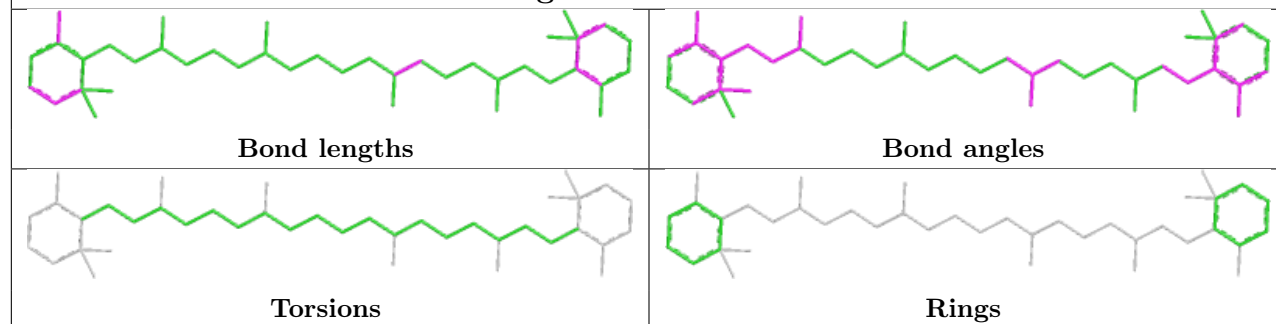


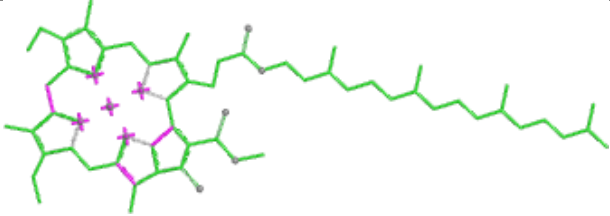
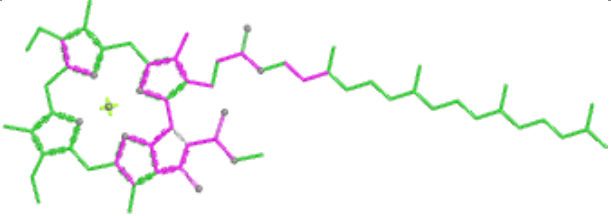
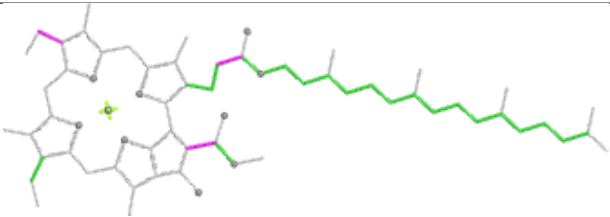
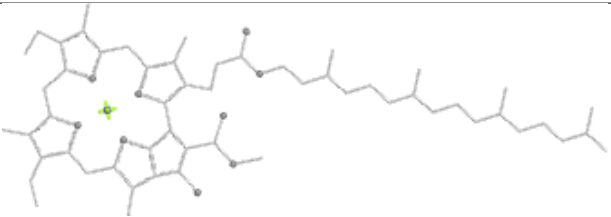
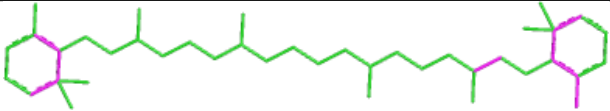
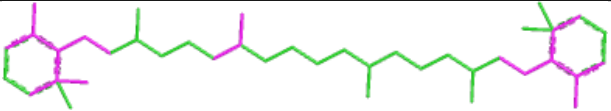
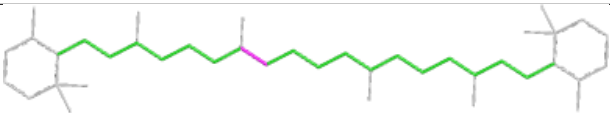
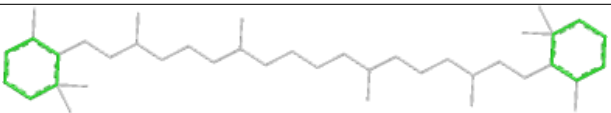
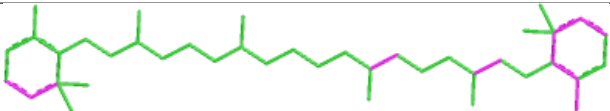
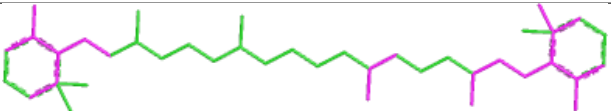
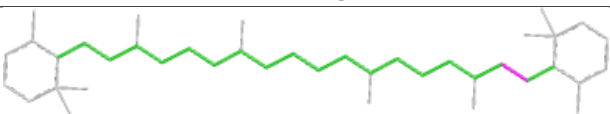
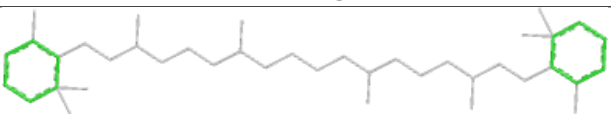
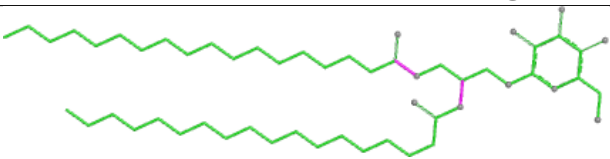
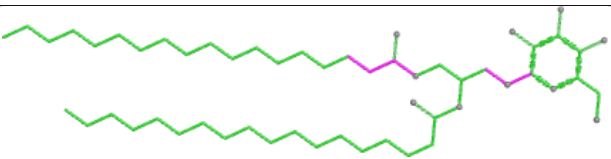
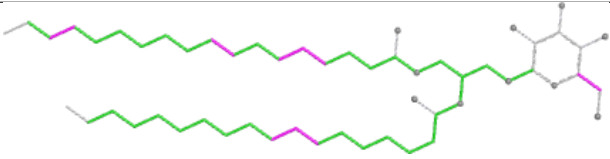
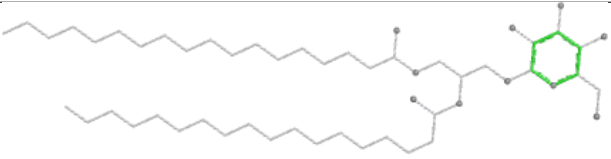
Ligand CLA B 832**Ligand CLA B 814**

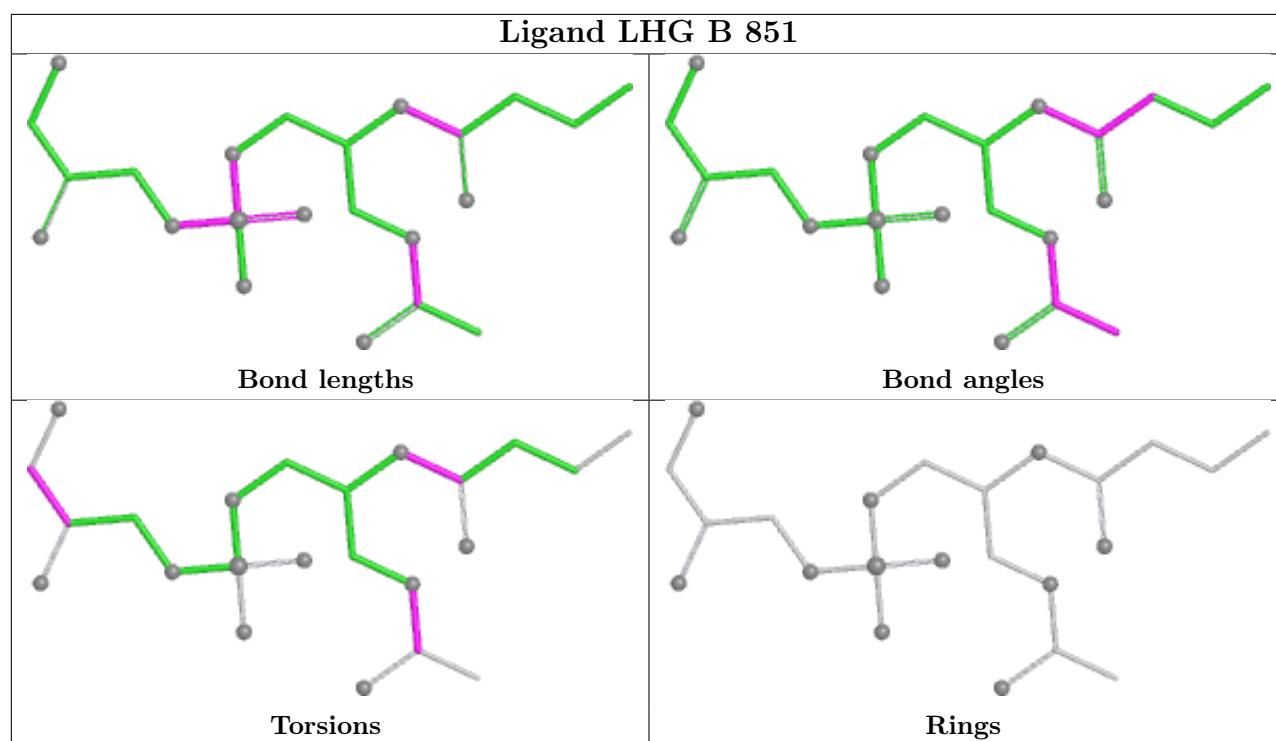
Ligand CLA B 820



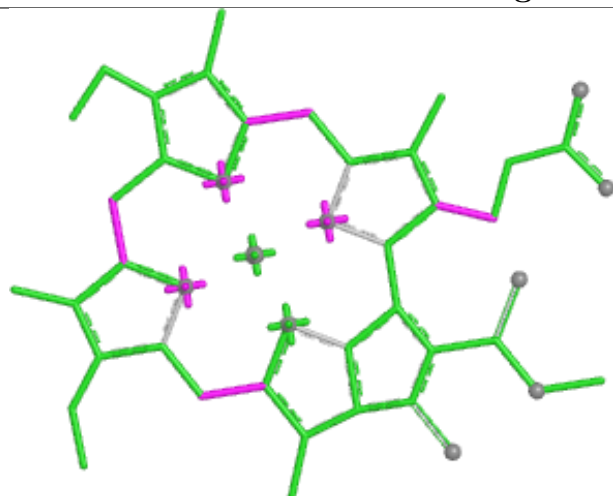
Ligand BCR I 101



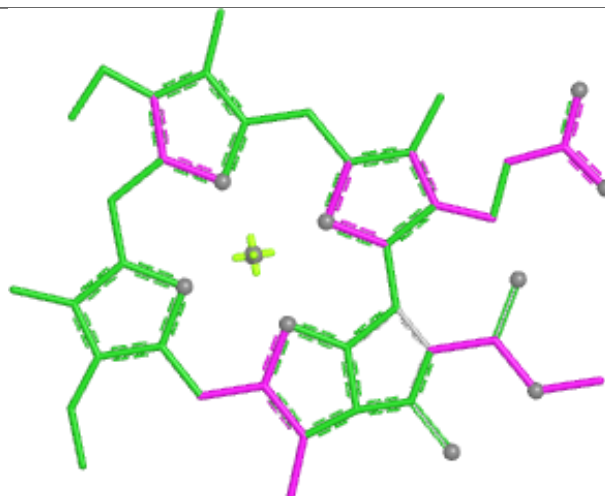
Ligand CLA A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR L 1006	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR L 1005	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG B 850	
 Bond lengths	 Bond angles
 Torsions	 Rings



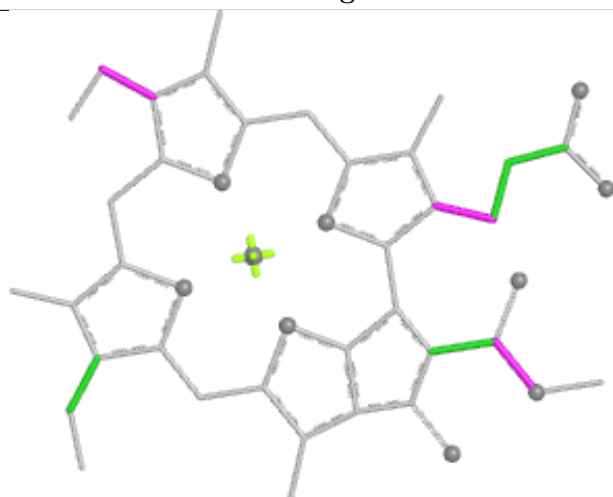
Ligand CLA B 811



Bond lengths



Bond angles

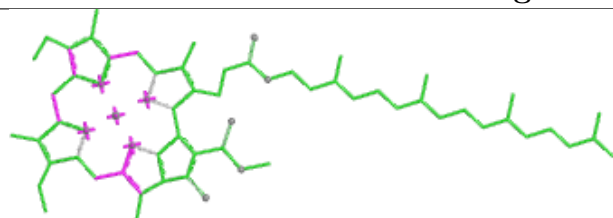


Torsions

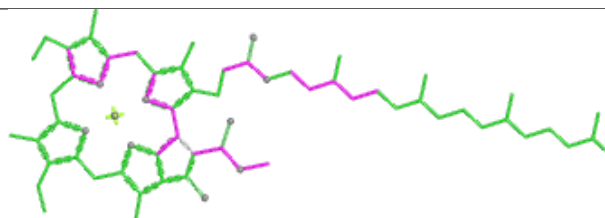


Rings

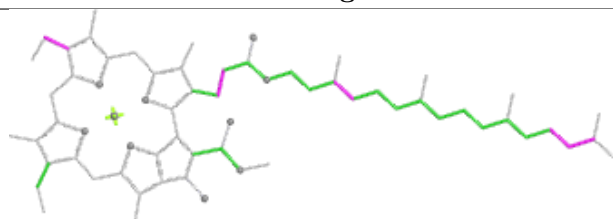
Ligand CLA A 802



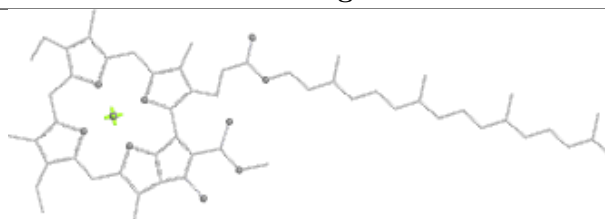
Bond lengths



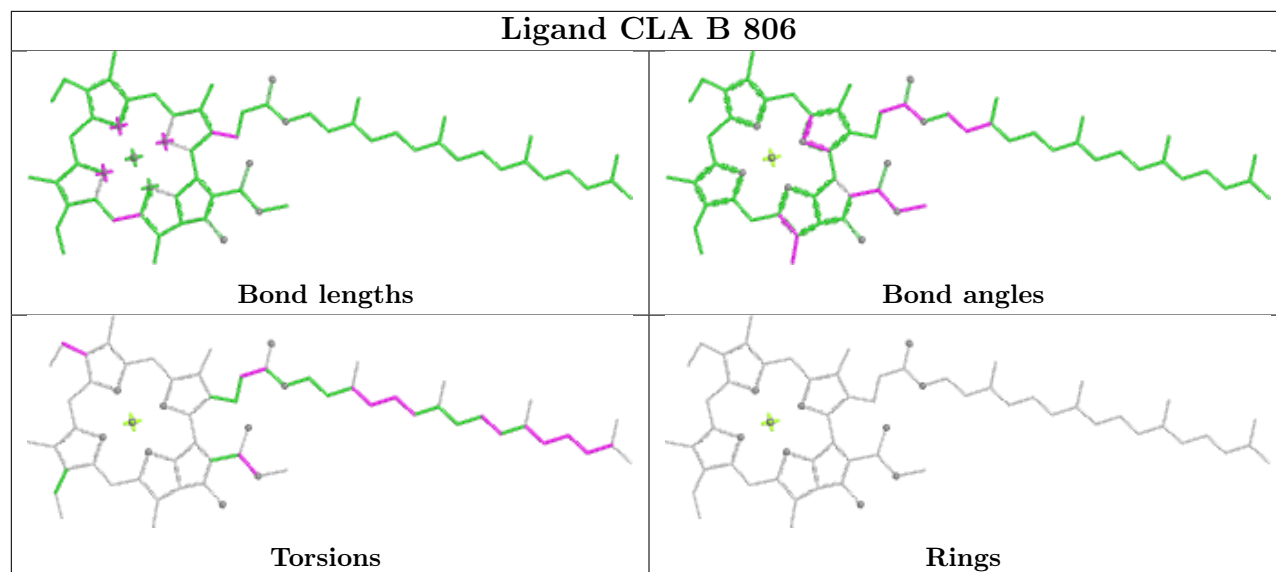
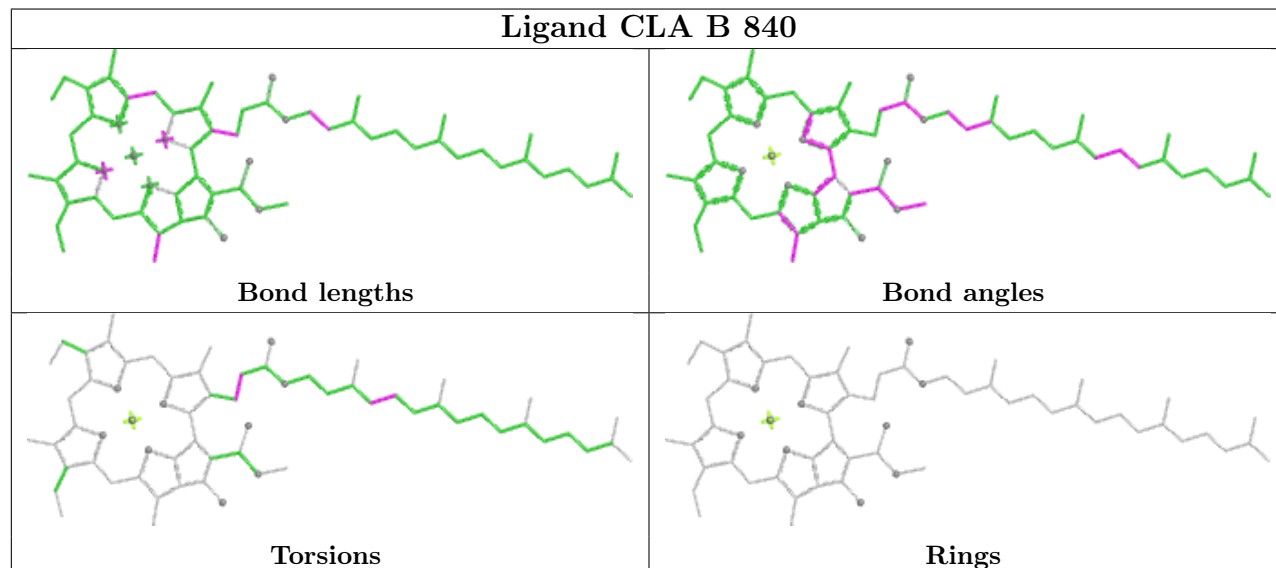
Bond angles



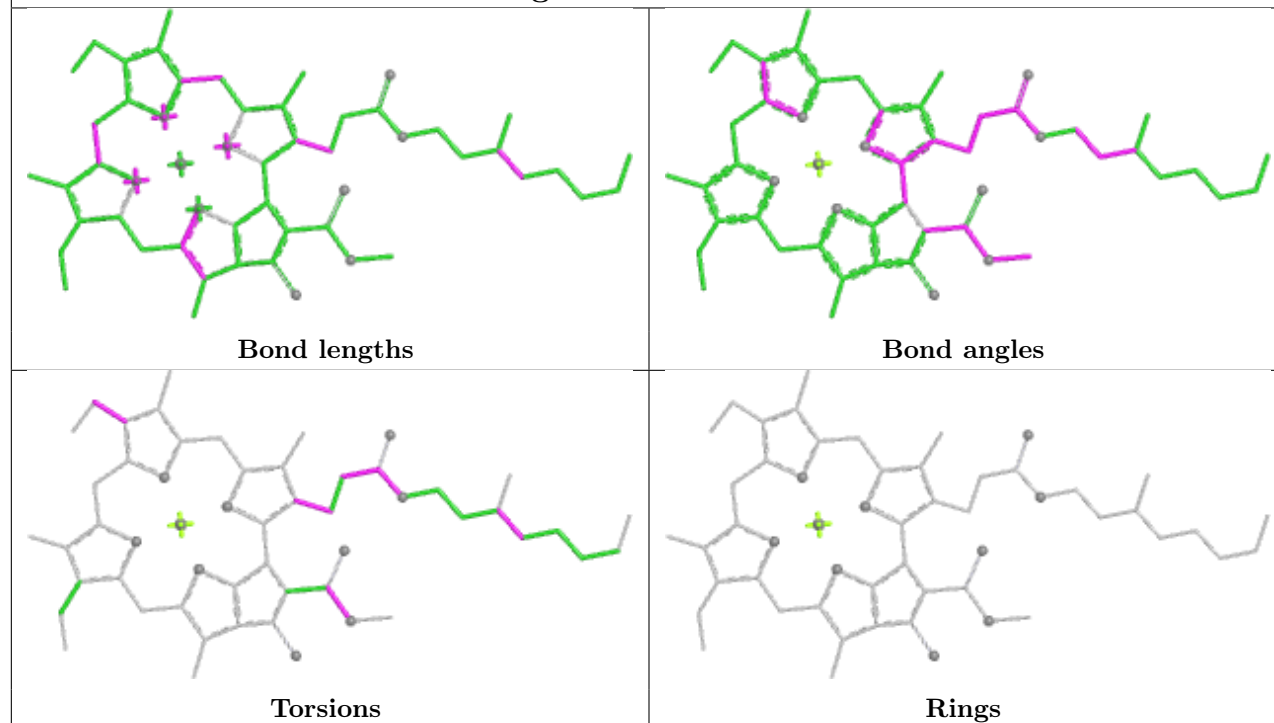
Torsions



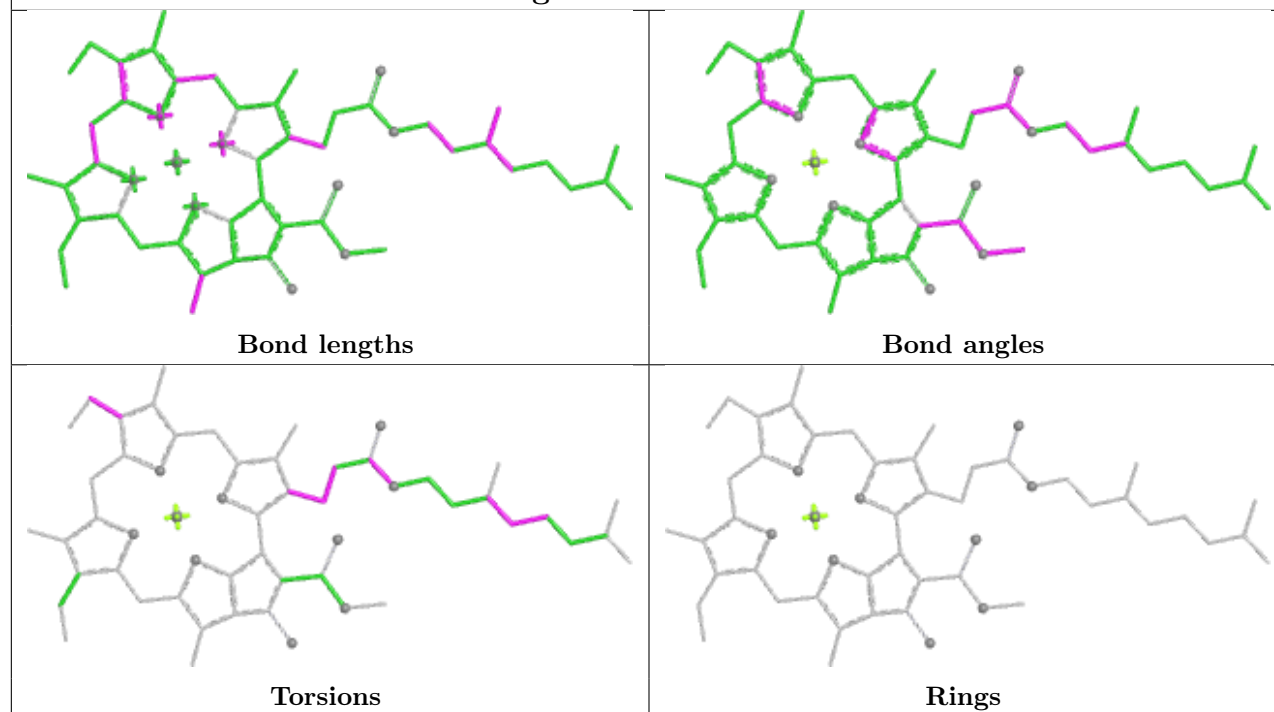
Rings

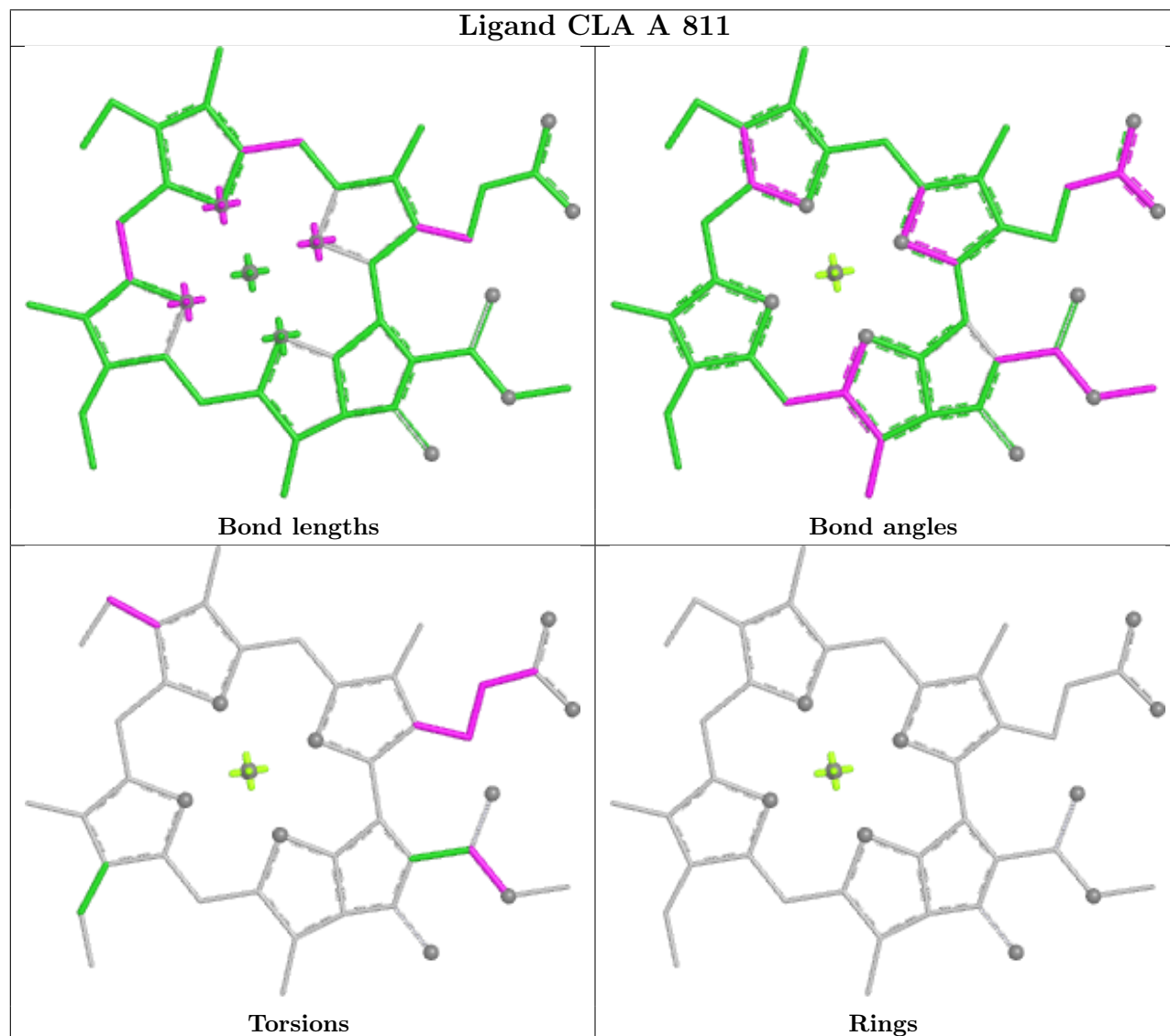
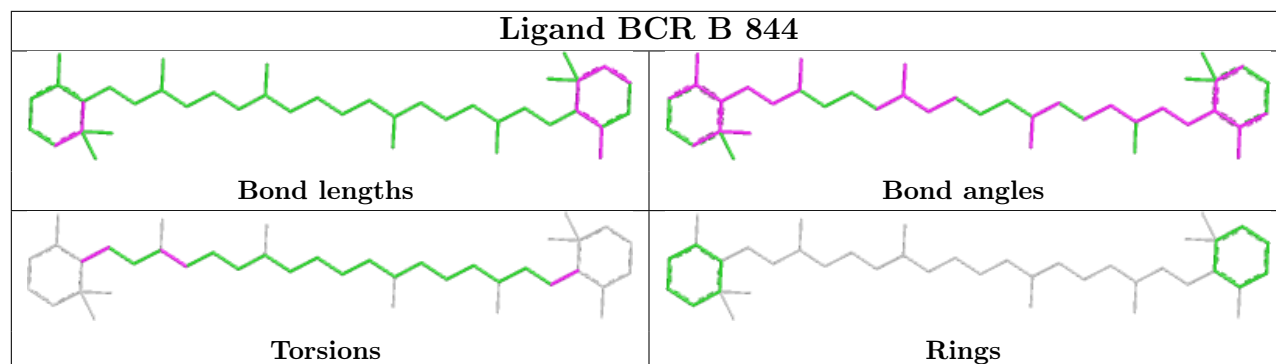
Ligand CLA B 806**Ligand CLA B 840**

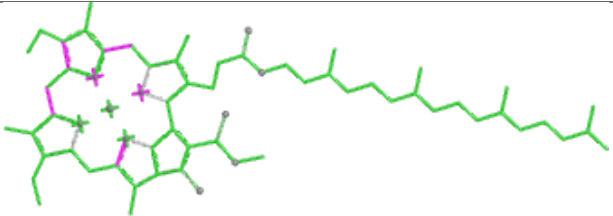
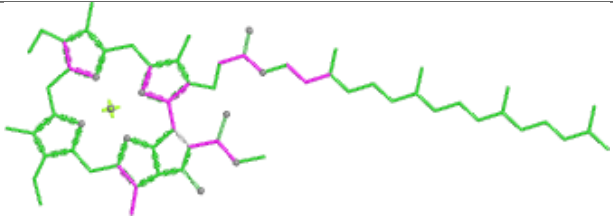
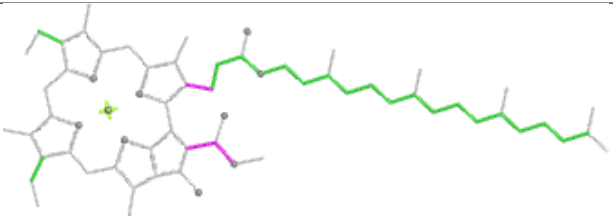
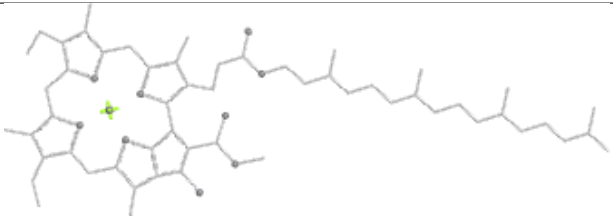
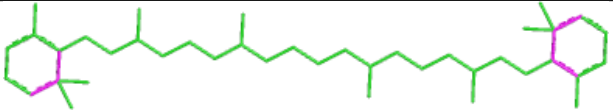
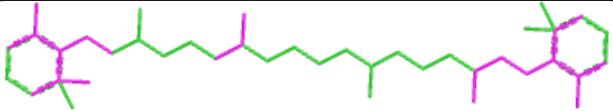
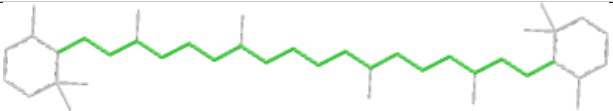
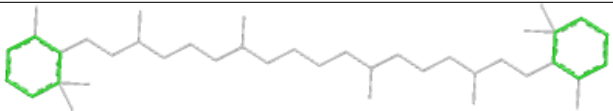
Ligand CLA A 819



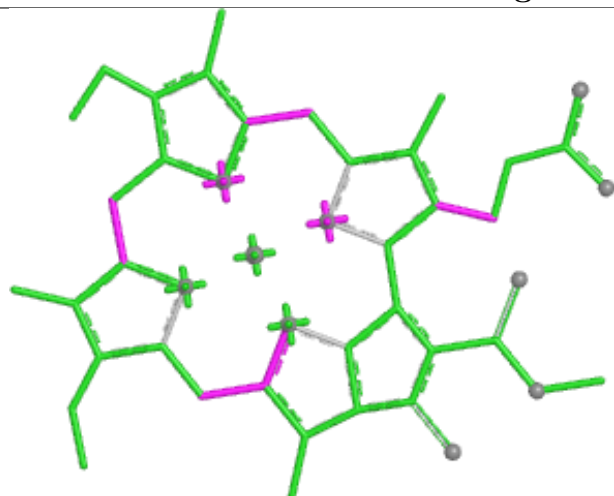
Ligand CLA B 816



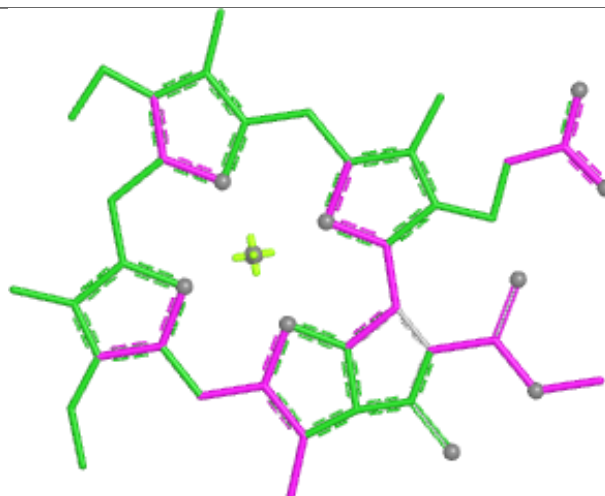


Ligand CLA A 804	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 849	
 Bond lengths	 Bond angles
 Torsions	 Rings

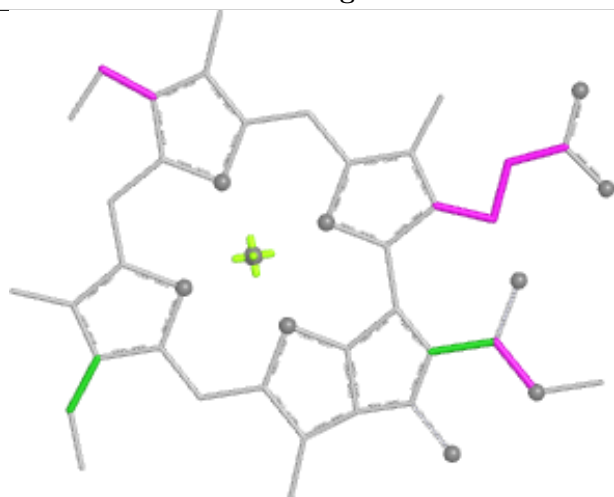
Ligand CLA B 830



Bond lengths



Bond angles

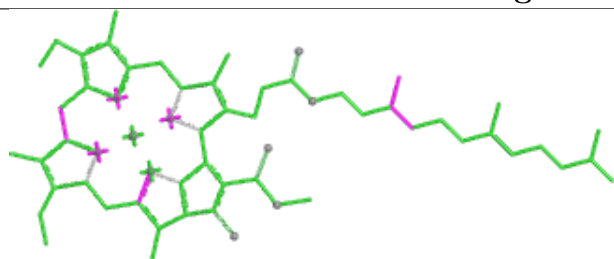


Torsions

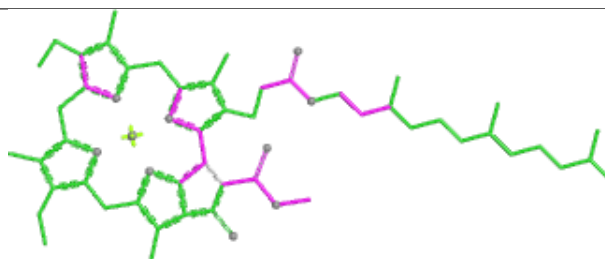


Rings

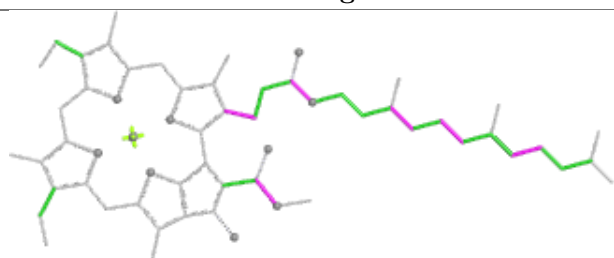
Ligand CLA B 837



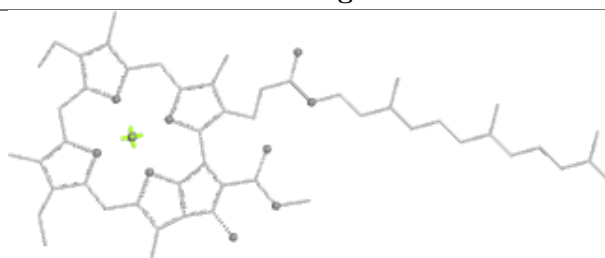
Bond lengths



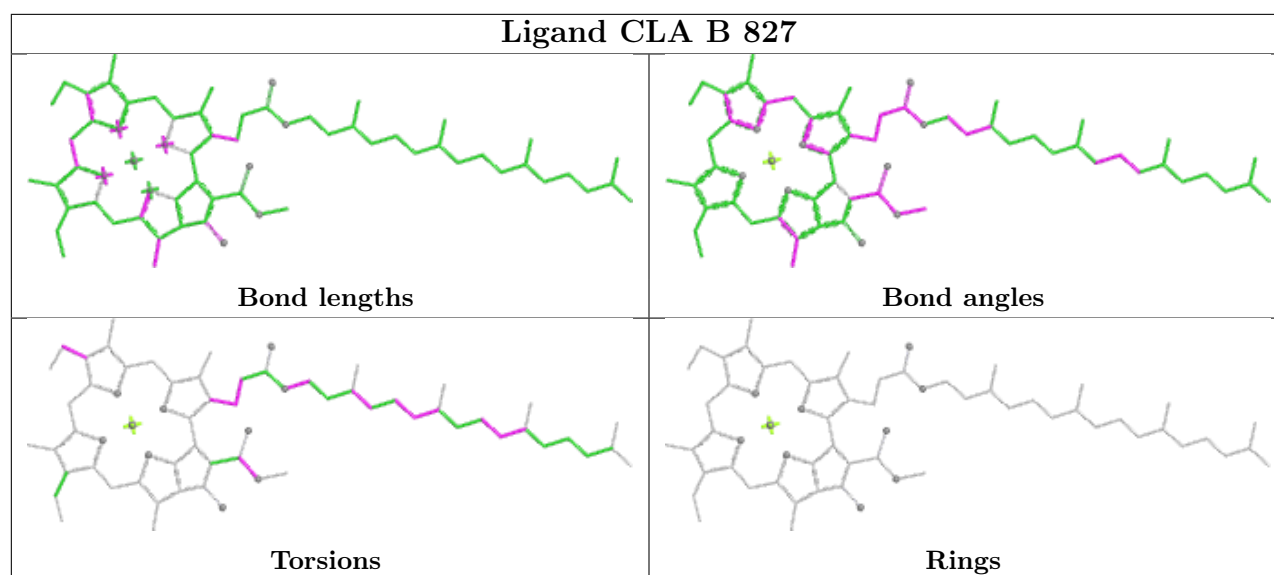
Bond angles



Torsions



Rings



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%)	-0.46	31 (4%) 40 40	22, 45, 71, 93	0
2	B	739/740 (99%)	-0.40	27 (3%) 45 43	20, 38, 71, 89	0
3	C	80/80 (100%)	-0.96	0 100 100	22, 33, 45, 54	0
4	D	138/138 (100%)	-0.41	7 (5%) 33 35	27, 41, 56, 84	0
5	E	69/75 (92%)	-0.24	2 (2%) 53 47	29, 46, 62, 76	0
6	F	141/164 (85%)	-0.47	4 (2%) 55 48	37, 57, 68, 72	0
7	I	38/38 (100%)	-0.19	3 (7%) 18 25	20, 33, 47, 53	0
8	J	41/41 (100%)	-0.37	0 100 100	53, 60, 77, 86	0
9	K	46/83 (55%)	-0.25	3 (6%) 25 30	72, 81, 96, 99	0
10	L	151/154 (98%)	-0.45	5 (3%) 49 45	19, 26, 47, 67	0
11	M	31/31 (100%)	-0.26	2 (6%) 25 30	30, 38, 52, 62	0
12	X	29/35 (82%)	-0.15	1 (3%) 48 44	58, 63, 81, 88	0
All	All	2243/2334 (96%)	-0.43	85 (3%) 44 42	19, 42, 74, 99	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	543	ALA	13.3
1	A	283	GLY	10.4
4	D	99	GLY	8.3
11	M	26	SER	8.0
9	K	35	GLN	7.9
2	B	176	HIS	5.6
2	B	117	SER	5.5
1	A	547	HIS	5.1
2	B	118	GLY	4.8
1	A	324	SER	4.8
1	A	230	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
10	L	94	ALA	4.6
2	B	422	ILE	4.6
4	D	1	THR	4.2
2	B	281	VAL	4.2
1	A	261	PHE	4.1
5	E	67	GLU	3.9
1	A	521	GLY	3.8
2	B	643	PRO	3.8
1	A	113	SER	3.7
6	F	92	GLY	3.7
1	A	327	GLU	3.6
10	L	141	ASN	3.6
2	B	496	GLY	3.5
1	A	231	VAL	3.5
1	A	629	GLY	3.5
2	B	587	PHE	3.5
1	A	260	PHE	3.3
1	A	699	GLU	3.3
2	B	6	LYS	3.1
4	D	98	ASP	3.0
1	A	45	THR	3.0
2	B	535	THR	3.0
2	B	30	PHE	2.9
1	A	695	GLY	2.9
2	B	692	PRO	2.9
4	D	127	GLN	2.8
2	B	704	VAL	2.8
2	B	543	GLY	2.8
2	B	333	LEU	2.8
1	A	282	ASN	2.8
11	M	1	MET	2.8
1	A	668	ALA	2.7
2	B	705	ALA	2.7
7	I	35	GLU	2.7
2	B	263	GLN	2.6
2	B	546	ASP	2.5
10	L	140	GLU	2.5
9	K	31	ARG	2.5
1	A	652	ASP	2.5
2	B	359	PRO	2.5
1	A	278	PHE	2.5
2	B	184	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	64	ASP	2.5
2	B	636	GLN	2.4
1	A	560	ALA	2.4
4	D	4	THR	2.4
1	A	279	LEU	2.4
1	A	268	PHE	2.4
5	E	66	GLN	2.3
4	D	97	LYS	2.3
6	F	22	VAL	2.3
6	F	57	LEU	2.3
2	B	527	HIS	2.3
1	A	446	TRP	2.3
1	A	447	VAL	2.3
7	I	36	GLY	2.2
2	B	453	GLU	2.2
10	L	95	ALA	2.2
4	D	100	VAL	2.2
1	A	168	MET	2.2
9	K	23	ASN	2.1
1	A	563	SER	2.1
2	B	635	SER	2.1
6	F	93	GLU	2.1
7	I	37	GLU	2.1
10	L	139	LEU	2.1
2	B	404	ALA	2.1
1	A	419	ASP	2.0
12	X	33	ILE	2.0
2	B	502	GLY	2.0
2	B	558	ASP	2.0
1	A	244	LEU	2.0
1	A	659	SER	2.0
1	A	450	PHE	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 oligosaccharides in this entry.

6.4 Ligands

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
13	CLA	A	845	41/65	0.94	0.09	87,90,92,93	0
13	CLA	J	102	37/65	0.95	0.11	95,96,97,97	0
13	CLA	B	812	45/65	0.96	0.14	66,69,80,85	0
16	BCR	J	104	40/40	0.96	0.15	61,69,75,76	0
13	CLA	B	830	45/65	0.97	0.14	51,54,67,72	0
13	CLA	B	841	65/65	0.97	0.16	22,29,44,50	0
13	CLA	B	818	60/65	0.97	0.12	33,39,64,66	0
16	BCR	B	843	40/40	0.97	0.14	88,90,97,98	0
13	CLA	B	820	47/65	0.97	0.13	88,92,97,97	0
17	LHG	B	851	23/49	0.97	0.14	79,89,92,93	0
13	CLA	A	824	51/65	0.98	0.17	53,59,77,77	0
13	CLA	A	826	65/65	0.98	0.06	45,49,62,63	0
13	CLA	A	838	51/65	0.98	0.08	30,35,45,46	0
13	CLA	A	841	65/65	0.98	0.07	33,38,55,55	0
13	CLA	A	801	65/65	0.98	0.09	22,27,36,38	0
13	CLA	B	803	65/65	0.98	0.13	24,29,35,36	0
13	CLA	B	805	65/65	0.98	0.10	28,37,66,69	0
13	CLA	B	806	65/65	0.98	0.10	30,34,53,54	0
13	CLA	B	811	45/65	0.98	0.11	42,49,62,66	0
13	CLA	A	803	65/65	0.98	0.14	33,41,51,54	0
13	CLA	B	813	65/65	0.98	0.10	49,59,68,70	0
13	CLA	B	815	45/65	0.98	0.07	57,62,73,77	0
13	CLA	B	816	55/65	0.98	0.15	54,60,85,87	0
13	CLA	B	817	59/65	0.98	0.08	39,47,66,70	0
13	CLA	A	804	65/65	0.98	0.14	45,50,80,83	0
13	CLA	A	808	51/65	0.98	0.10	55,58,79,79	0
13	CLA	B	825	46/65	0.98	0.10	29,36,46,48	0
13	CLA	B	827	65/65	0.98	0.10	24,31,77,80	0
13	CLA	B	828	65/65	0.98	0.15	31,35,48,52	0
13	CLA	A	812	65/65	0.98	0.08	63,65,72,74	0
13	CLA	B	832	65/65	0.98	0.11	37,43,65,66	0
13	CLA	B	833	58/65	0.98	0.10	36,47,77,78	0
13	CLA	B	836	45/65	0.98	0.11	78,82,85,87	0
13	CLA	B	839	47/65	0.98	0.10	41,47,55,60	0
13	CLA	B	840	65/65	0.98	0.12	13,18,41,42	0
13	CLA	A	813	54/65	0.98	0.09	44,47,76,77	0
13	CLA	F	1301	45/65	0.98	0.08	75,77,82,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	CLA	J	101	45/65	0.98	0.08	98,99,100,100	0
13	CLA	A	817	49/65	0.98	0.11	87,90,92,94	0
13	CLA	L	1002	65/65	0.98	0.10	21,27,58,61	0
13	CLA	M	1601	45/65	0.98	0.15	96,97,99,100	0
13	CLA	X	1701	45/65	0.98	0.11	77,83,86,88	0
16	BCR	A	851	40/40	0.98	0.15	47,61,89,89	0
13	CLA	A	820	65/65	0.98	0.09	43,48,56,58	0
16	BCR	B	844	40/40	0.98	0.16	56,68,93,93	0
16	BCR	B	845	40/40	0.98	0.17	33,51,87,88	0
13	CLA	A	821	61/65	0.98	0.09	56,62,85,85	0
13	CLA	A	823	49/65	0.98	0.11	64,68,82,83	0
13	CLA	B	804	54/65	0.99	0.08	20,29,48,52	0
13	CLA	A	818	54/65	0.99	0.09	63,66,68,69	0
13	CLA	A	819	54/65	0.99	0.08	44,50,54,56	0
13	CLA	B	807	65/65	0.99	0.06	21,24,50,53	0
13	CLA	B	808	65/65	0.99	0.06	21,28,49,50	0
13	CLA	B	809	65/65	0.99	0.08	20,26,61,62	0
13	CLA	B	810	65/65	0.99	0.07	15,23,43,44	0
13	CLA	A	802	65/65	0.99	0.08	23,26,35,39	0
13	CLA	A	809	65/65	0.99	0.09	33,40,66,67	0
13	CLA	A	822	65/65	0.99	0.09	41,45,55,57	0
13	CLA	B	814	65/65	0.99	0.07	34,43,68,69	0
13	CLA	A	810	65/65	0.99	0.08	39,43,77,78	0
13	CLA	A	811	45/65	0.99	0.06	68,71,75,76	0
13	CLA	A	825	59/65	0.99	0.07	34,43,76,76	0
13	CLA	A	805	59/65	0.99	0.07	40,46,85,86	0
13	CLA	B	819	65/65	0.99	0.11	78,82,99,100	0
13	CLA	A	827	65/65	0.99	0.08	24,31,83,85	0
13	CLA	B	821	45/65	0.99	0.07	80,81,90,93	0
13	CLA	B	822	55/65	0.99	0.05	69,70,88,89	0
13	CLA	B	823	45/65	0.99	0.05	58,62,70,73	0
13	CLA	B	824	54/65	0.99	0.06	54,59,69,71	0
13	CLA	A	828	65/65	0.99	0.07	32,42,66,68	0
13	CLA	B	826	65/65	0.99	0.07	31,39,63,65	0
13	CLA	A	829	65/65	0.99	0.11	38,46,74,75	0
13	CLA	A	830	65/65	0.99	0.10	33,40,52,55	0
13	CLA	B	829	65/65	0.99	0.09	18,29,63,65	0
13	CLA	A	831	65/65	0.99	0.08	35,43,52,53	0
13	CLA	B	831	49/65	0.99	0.12	36,40,63,65	0
13	CLA	A	832	50/65	0.99	0.06	32,37,58,59	0
13	CLA	A	833	65/65	0.99	0.08	20,31,85,88	0
13	CLA	B	834	45/65	0.99	0.07	40,47,53,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
13	CLA	B	835	45/65	0.99	0.13	58,61,70,75	0
13	CLA	A	834	65/65	0.99	0.08	24,28,43,44	0
13	CLA	B	837	60/65	0.99	0.12	42,48,70,71	0
13	CLA	B	838	65/65	0.99	0.08	38,44,74,78	0
13	CLA	A	835	65/65	0.99	0.08	14,19,36,40	0
13	CLA	A	836	54/65	0.99	0.08	46,50,64,64	0
13	CLA	A	837	45/65	0.99	0.08	60,68,76,80	0
13	CLA	A	806	65/65	0.99	0.06	33,39,68,70	0
13	CLA	A	839	65/65	0.99	0.06	32,38,58,59	0
13	CLA	A	840	47/65	0.99	0.09	30,35,52,57	0
13	CLA	K	1401	45/65	0.99	0.09	70,74,81,84	0
13	CLA	A	814	60/65	0.99	0.09	49,53,80,81	0
13	CLA	L	1003	65/65	0.99	0.08	17,23,66,67	0
13	CLA	L	1004	65/65	0.99	0.10	22,31,61,62	0
13	CLA	A	842	51/65	0.99	0.08	38,43,70,71	0
13	CLA	A	843	65/65	0.99	0.12	29,35,60,60	0
14	PQN	A	847	33/33	0.99	0.07	41,43,67,68	0
14	PQN	B	842	33/33	0.99	0.15	24,29,36,36	0
16	BCR	A	849	40/40	0.99	0.11	62,69,79,79	0
16	BCR	A	850	40/40	0.99	0.12	57,61,79,79	0
13	CLA	A	844	65/65	0.99	0.08	17,22,43,47	0
16	BCR	A	852	40/40	0.99	0.10	47,60,96,96	0
16	BCR	A	853	40/40	0.99	0.07	30,37,59,60	0
13	CLA	A	816	45/65	0.99	0.07	78,82,83,83	0
13	CLA	A	846	52/65	0.99	0.10	69,75,97,99	0
13	CLA	B	801	65/65	0.99	0.07	22,30,38,46	0
16	BCR	B	846	25/40	0.99	0.14	64,66,69,70	0
16	BCR	B	847	40/40	0.99	0.14	46,53,61,61	0
16	BCR	B	848	40/40	0.99	0.13	40,52,58,58	0
16	BCR	B	849	40/40	0.99	0.09	23,27,30,31	0
16	BCR	F	1302	40/40	0.99	0.10	43,49,60,60	0
16	BCR	I	101	40/40	0.99	0.08	19,27,40,40	0
16	BCR	I	102	40/40	0.99	0.08	19,26,31,32	0
16	BCR	J	103	40/40	0.99	0.10	55,58,60,60	0
13	CLA	B	802	65/65	0.99	0.08	28,39,55,59	0
16	BCR	J	105	40/40	0.99	0.06	53,67,93,94	0
16	BCR	L	1005	40/40	0.99	0.12	20,24,29,30	0
16	BCR	L	1006	40/40	0.99	0.07	26,35,66,67	0
16	BCR	M	1602	40/40	0.99	0.08	28,37,59,62	0
17	LHG	A	855	49/49	0.99	0.07	39,50,60,63	0
13	CLA	A	807	65/65	0.99	0.09	38,43,51,52	0
18	LMG	B	850	55/55	0.99	0.08	34,40,57,60	0

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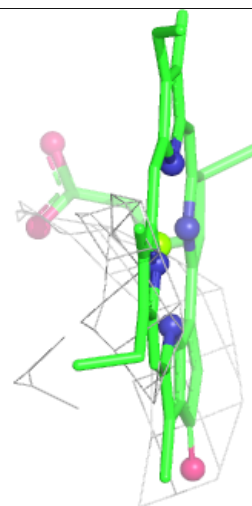
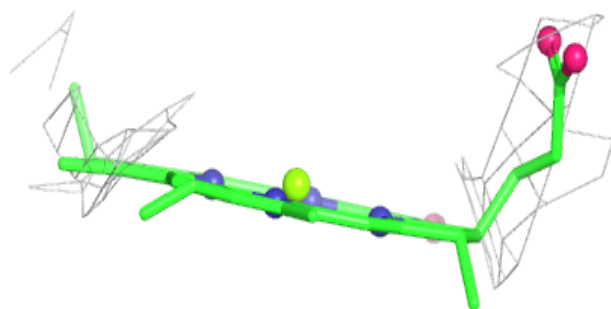
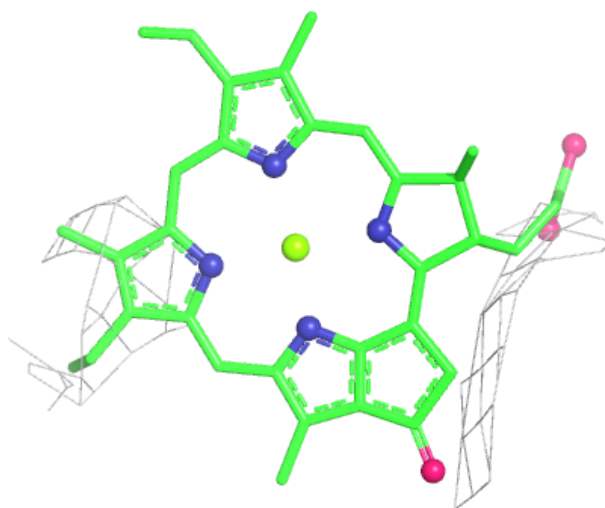
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	BCR	A	854	40/40	1.00	0.07	29,39,50,53	0
15	SF4	A	848	8/8	1.00	0.06	25,26,27,27	0
15	SF4	C	101	8/8	1.00	0.03	24,25,26,26	0
17	LHG	A	856	27/49	1.00	0.08	51,56,60,61	0
15	SF4	C	102	8/8	1.00	0.02	33,34,35,35	0
13	CLA	A	815	45/65	1.00	0.05	64,66,67,68	0
19	CA	L	1001	1/1	1.00	0.00	27,27,27,27	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.

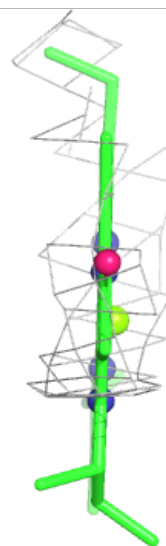
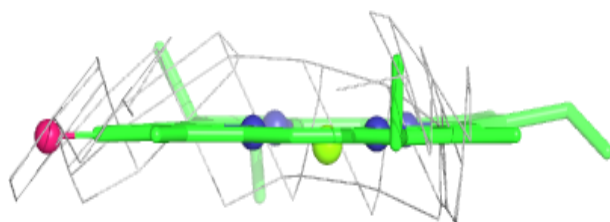
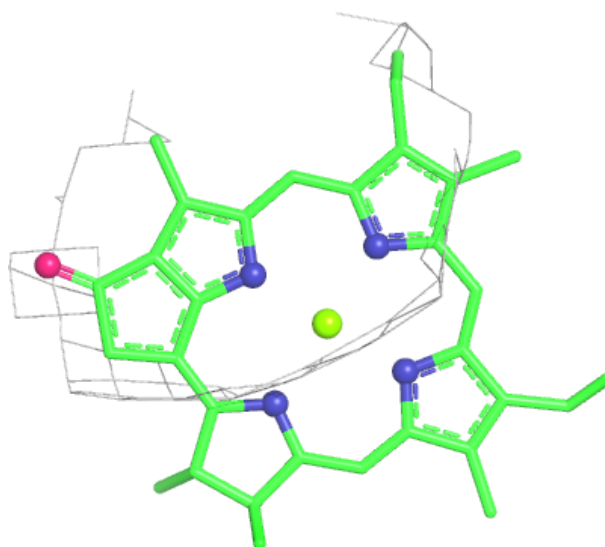
Electron density around CLA A 845:

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



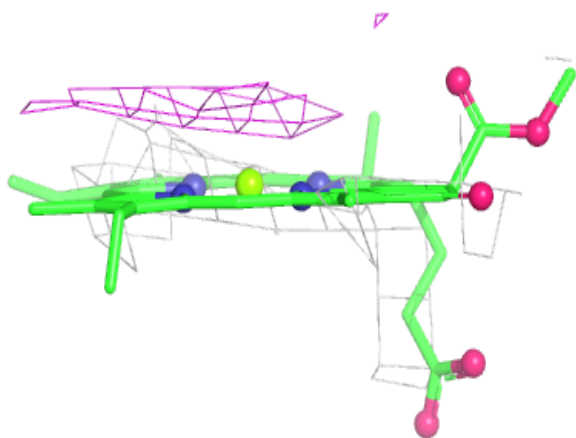
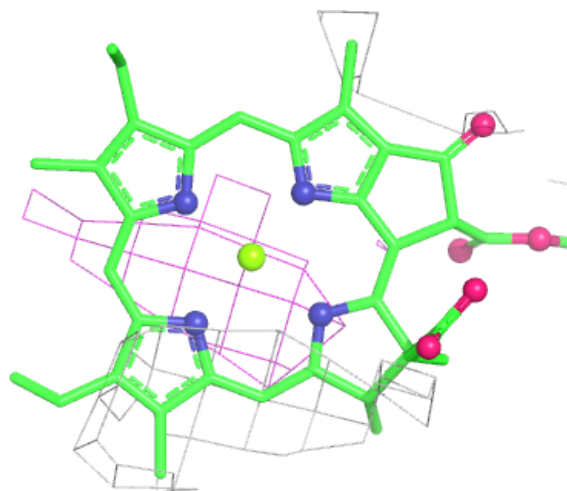
Electron density around CLA J 102:

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



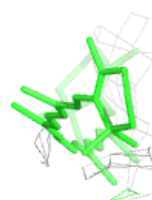
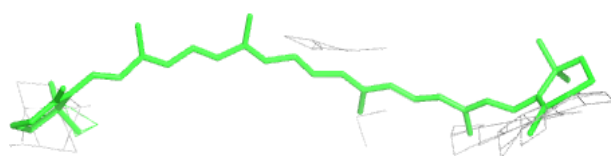
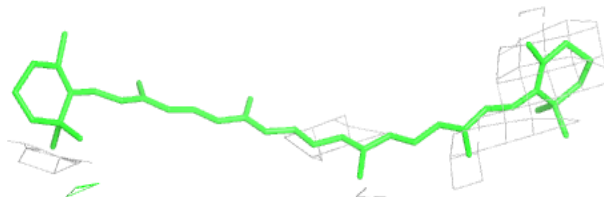
Electron density around CLA B 812:

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



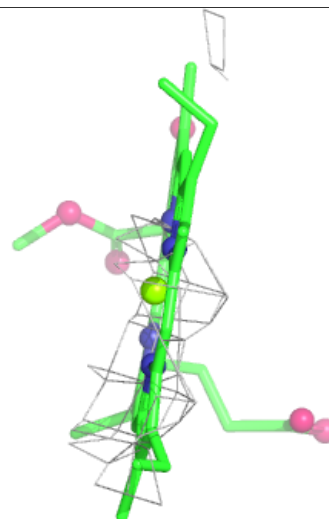
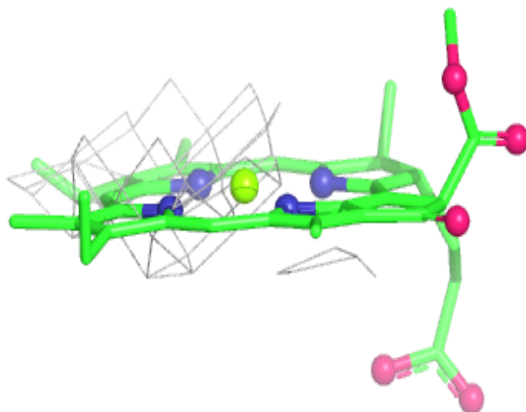
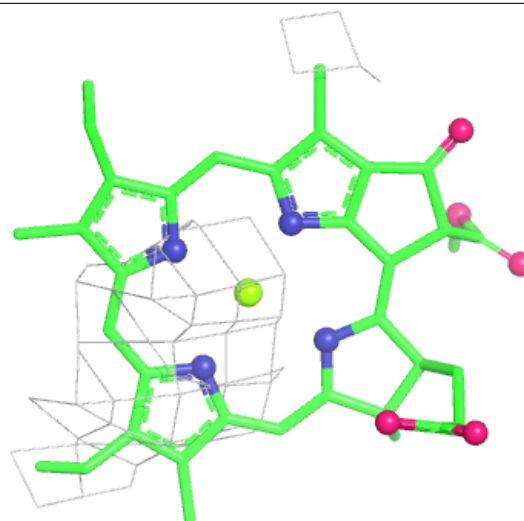
Electron density around BCR J 104:

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



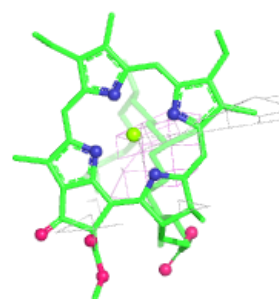
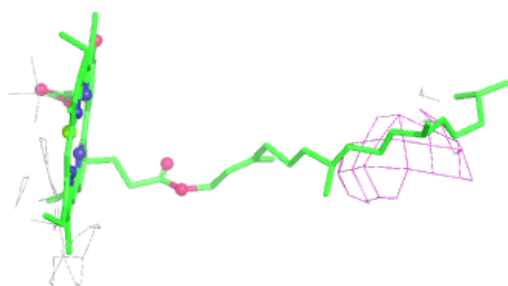
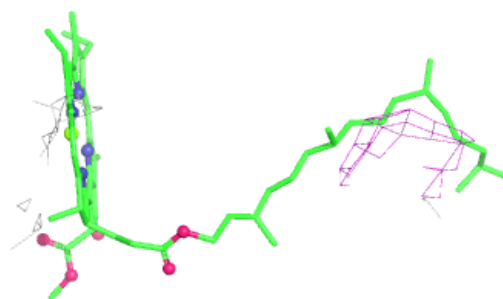
Electron density around CLA B 830:

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

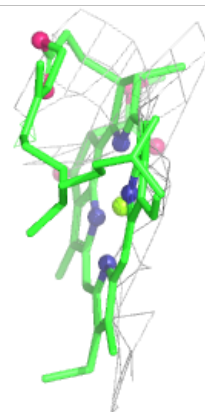
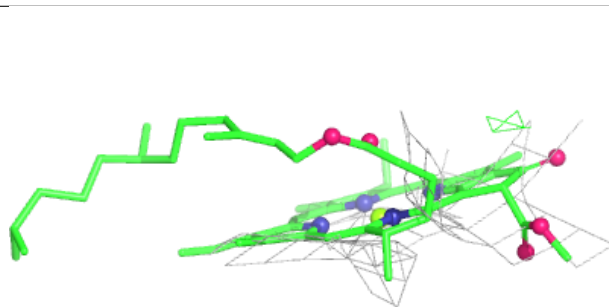
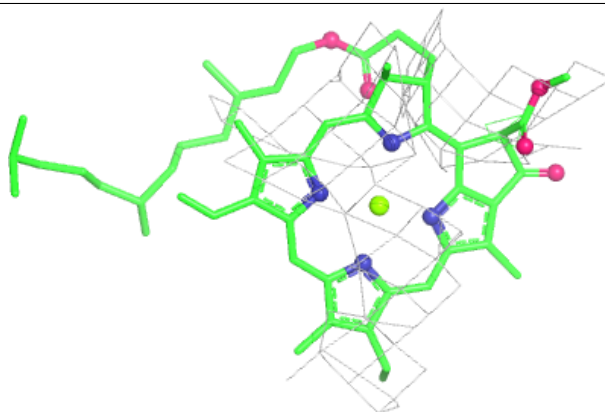


Electron density around CLA B 841:

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

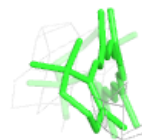
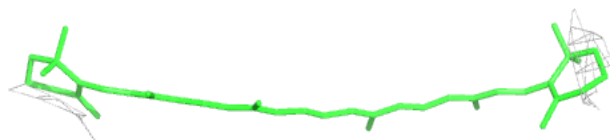
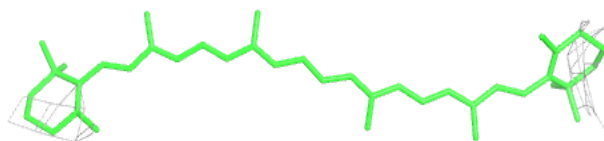
**Electron density around CLA B 818:**

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



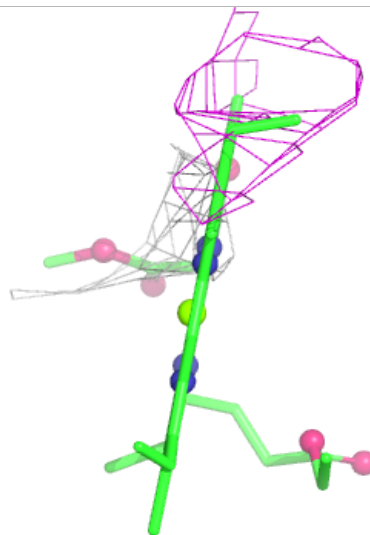
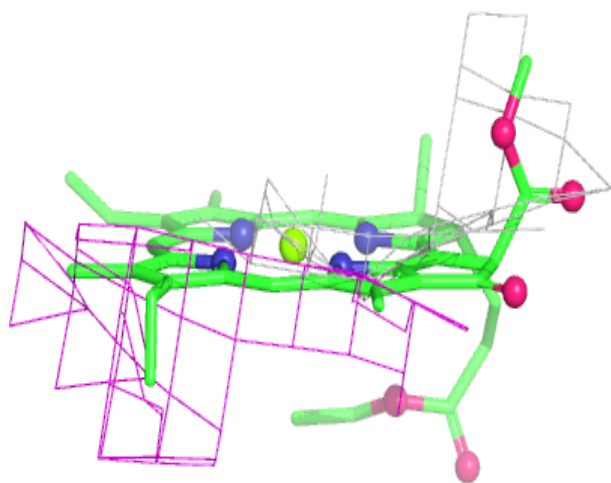
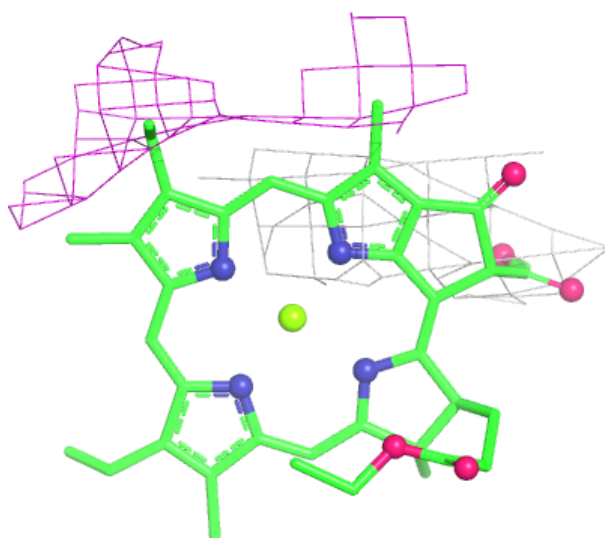
Electron density around BCR B 843:

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



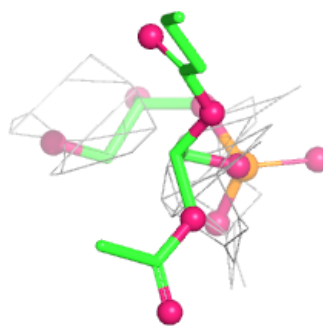
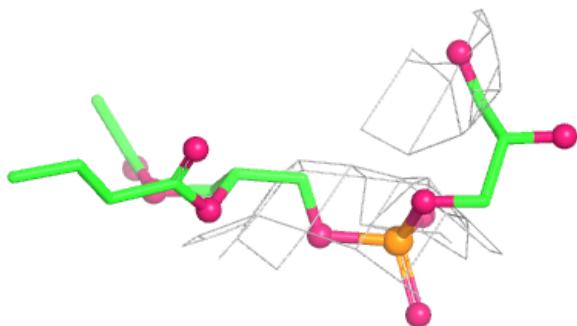
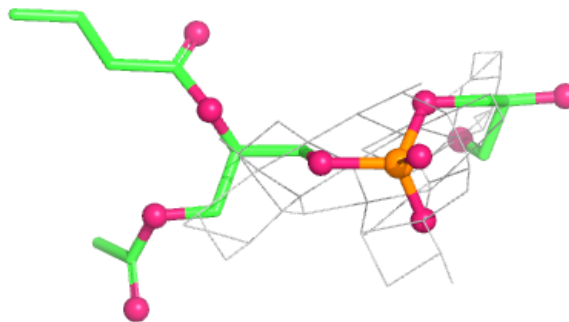
Electron density around CLA B 820:

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



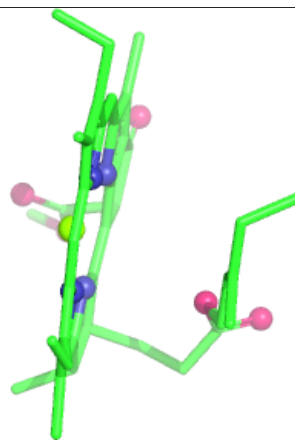
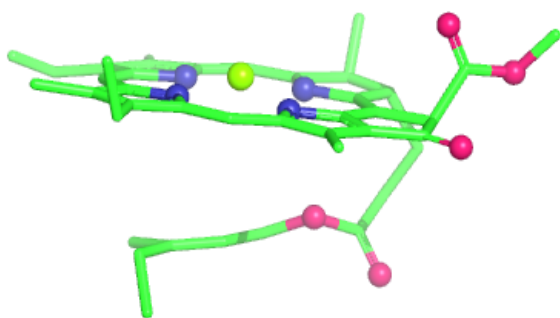
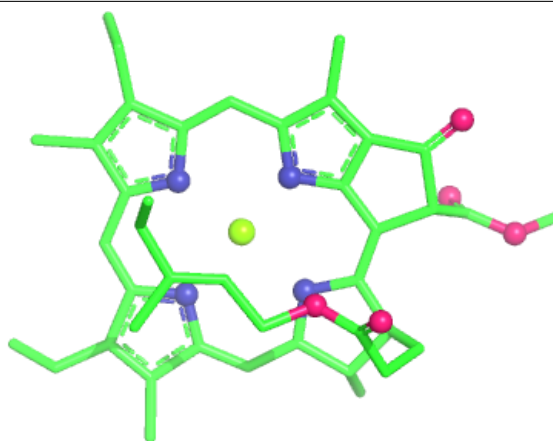
Electron density around LHG B 851:

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



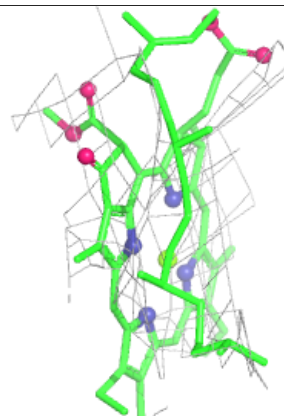
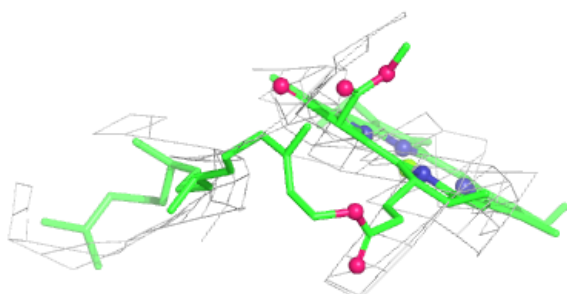
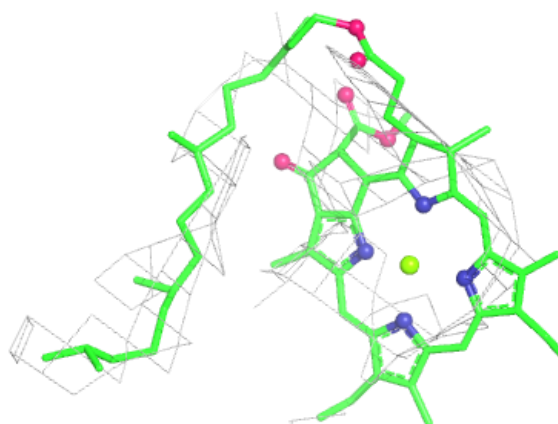
Electron density around CLA A 824:

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

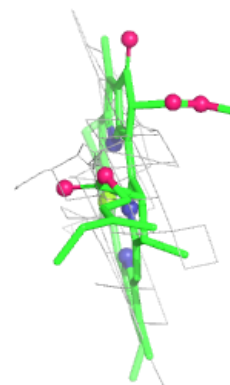
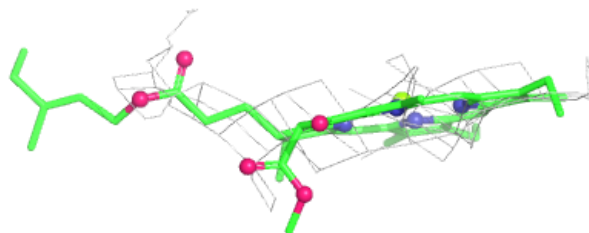
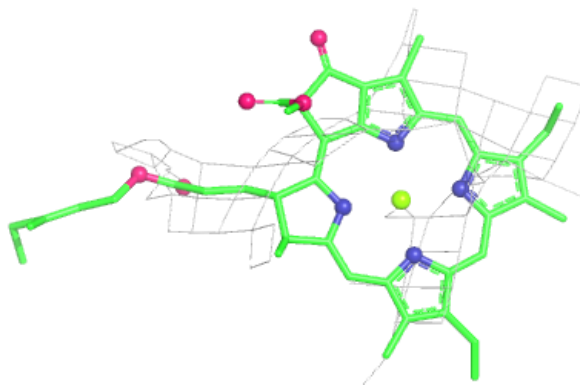


Electron density around CLA A 826:

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

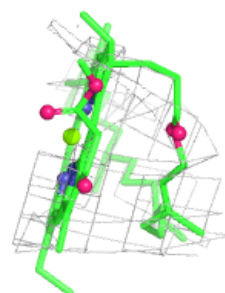
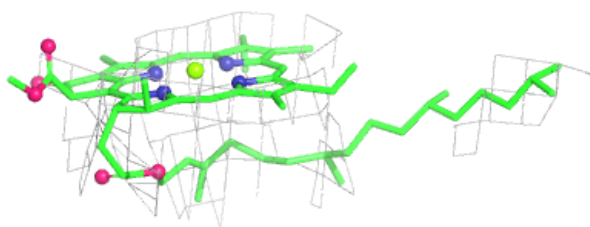
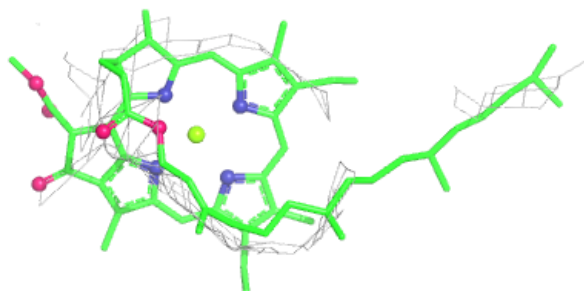
**Electron density around CLA A 838:**

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

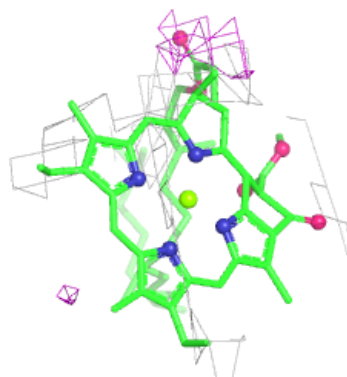
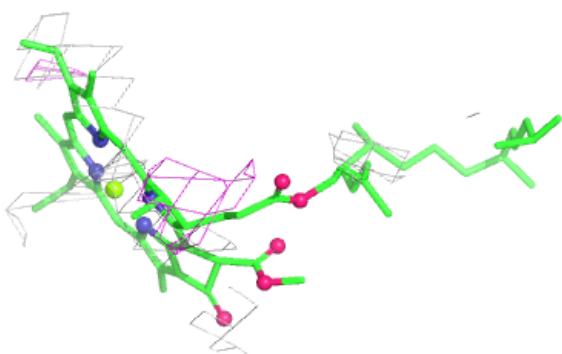
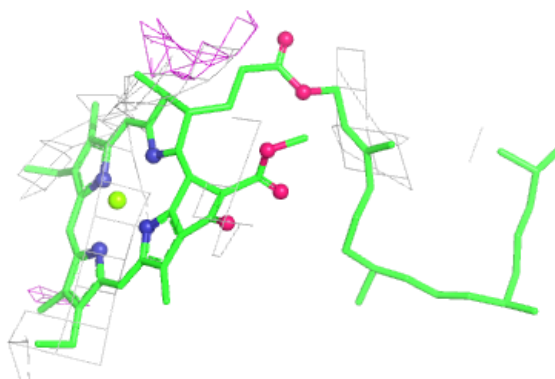


Electron density around CLA A 841:

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

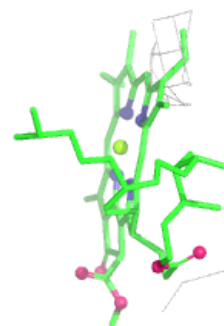
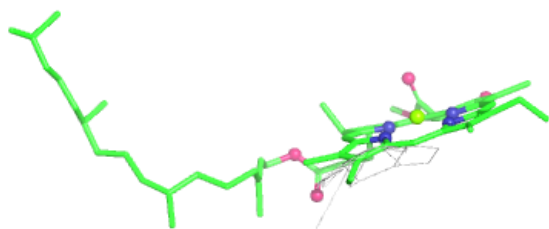
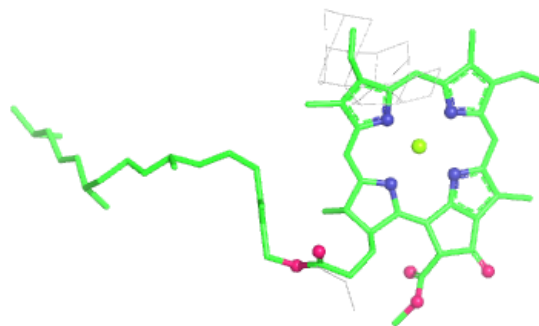
**Electron density around CLA A 801:**

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



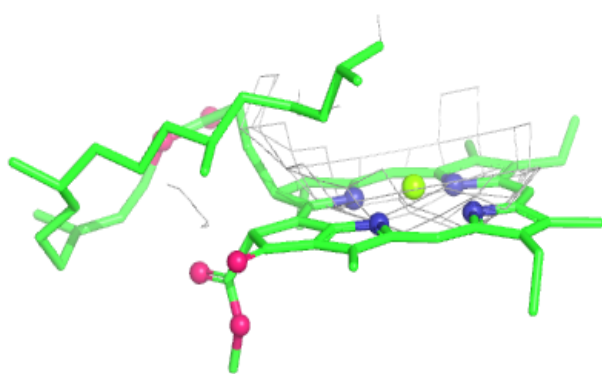
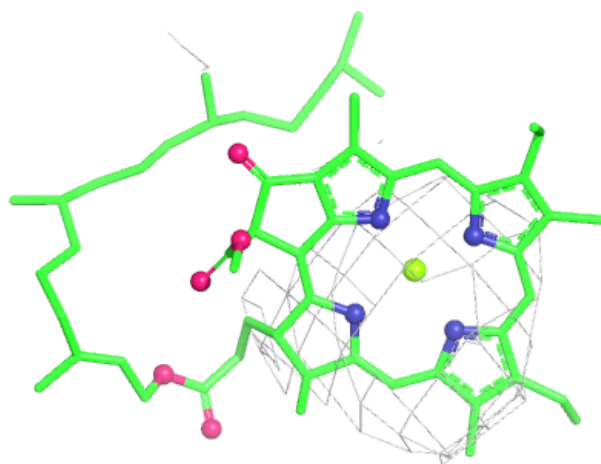
Electron density around CLA B 803:

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



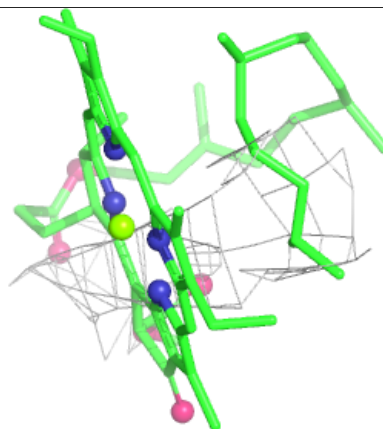
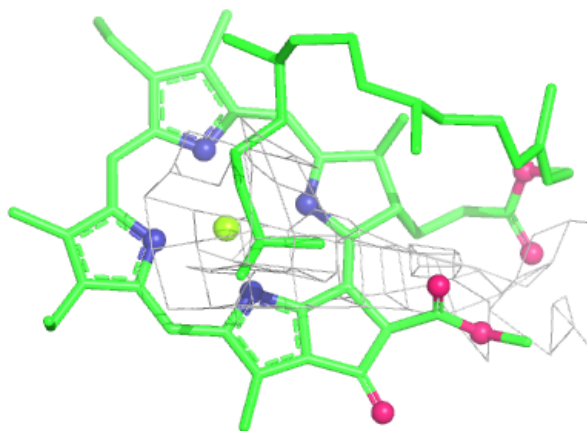
Electron density around CLA B 805:

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



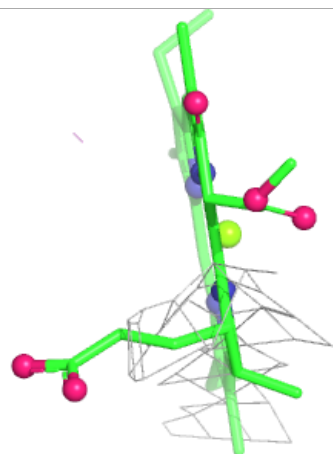
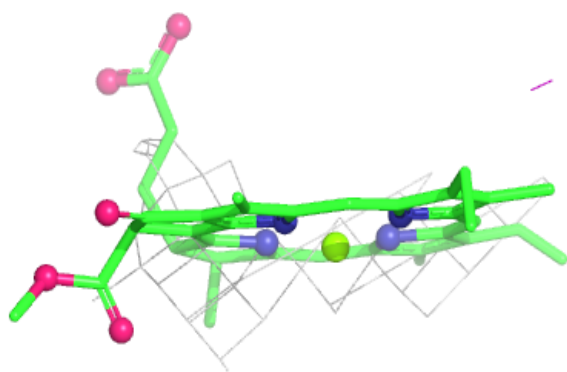
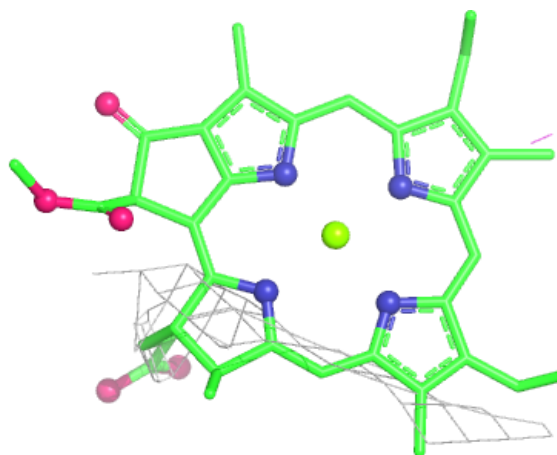
Electron density around CLA B 806:

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



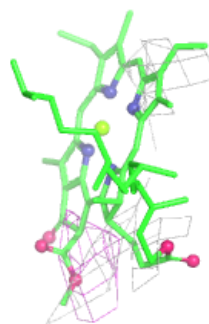
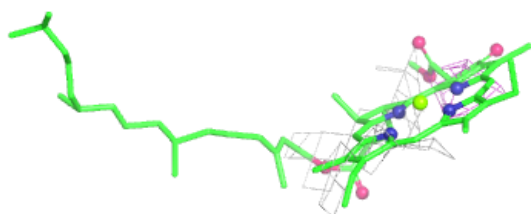
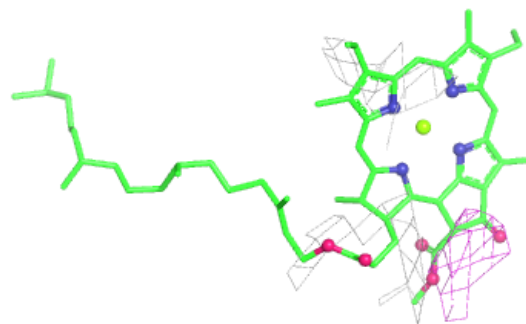
Electron density around CLA B 811:

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

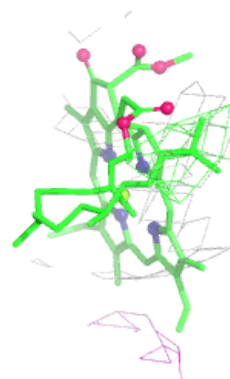
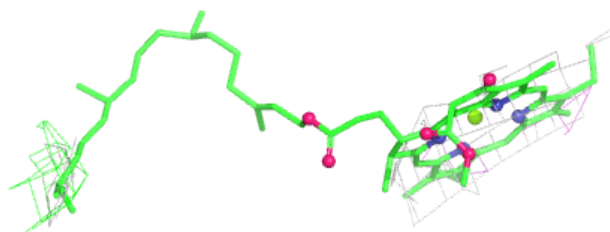
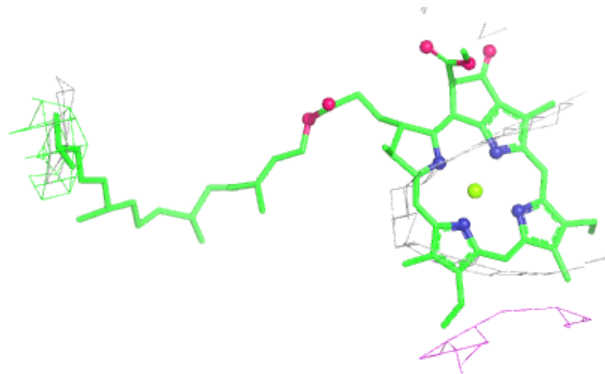


Electron density around CLA A 803:

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

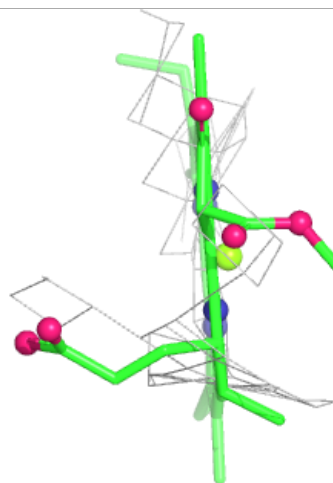
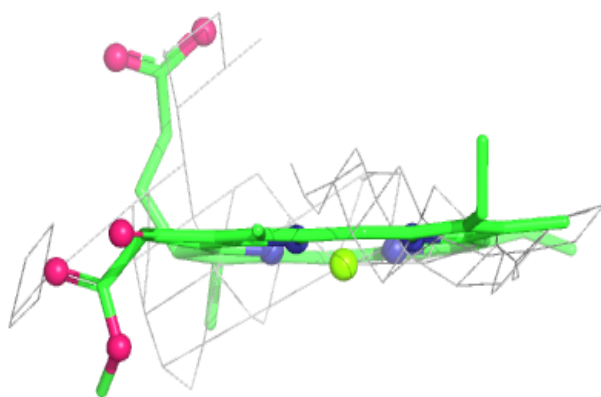
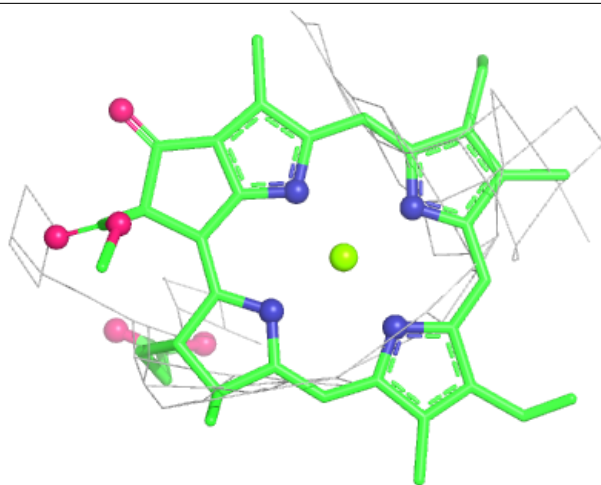
**Electron density around CLA B 813:**

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



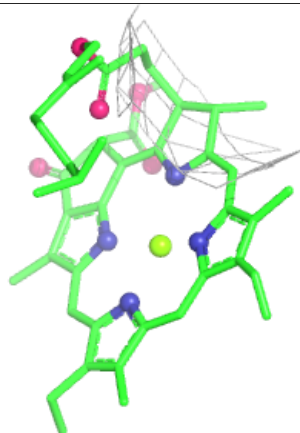
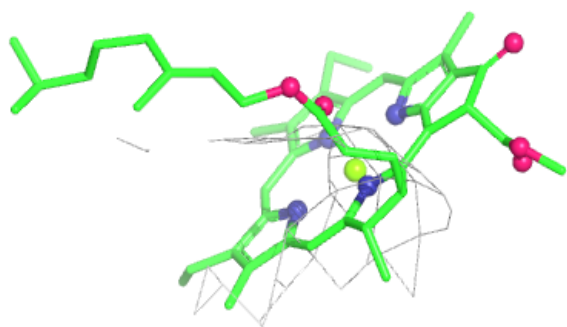
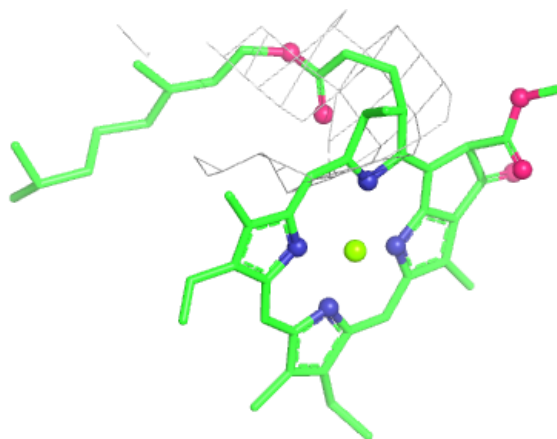
Electron density around CLA B 815:

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



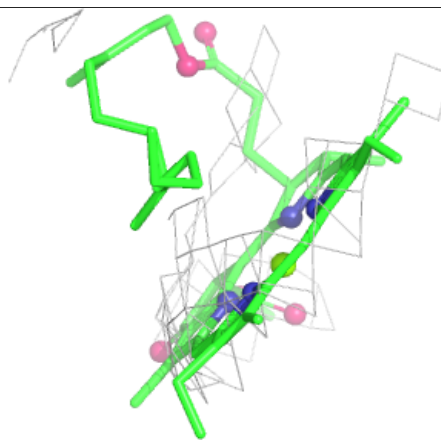
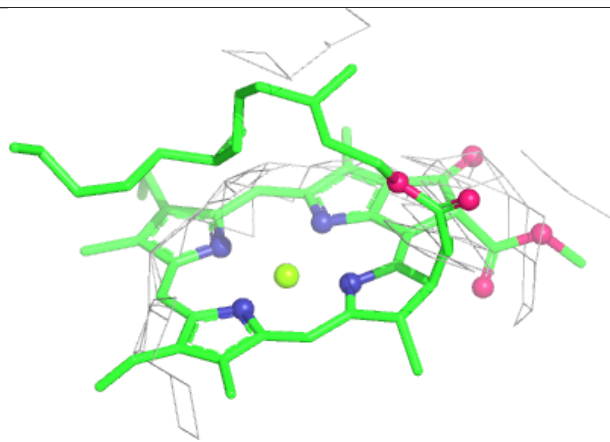
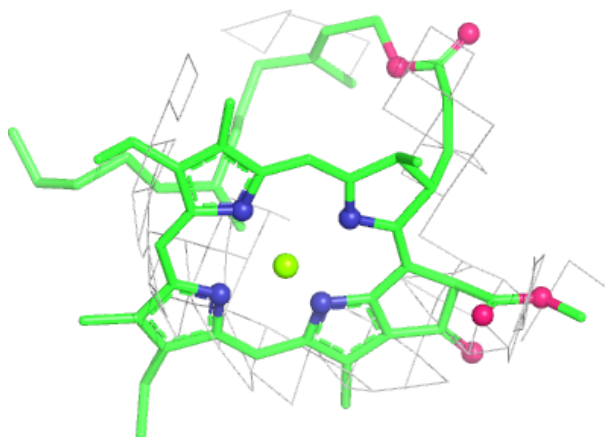
Electron density around CLA B 816:

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



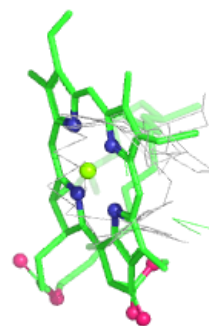
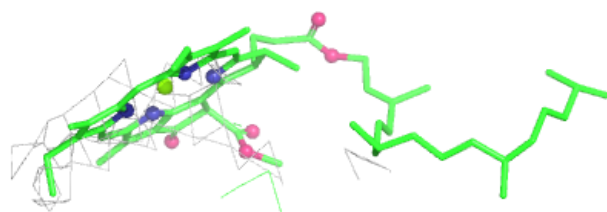
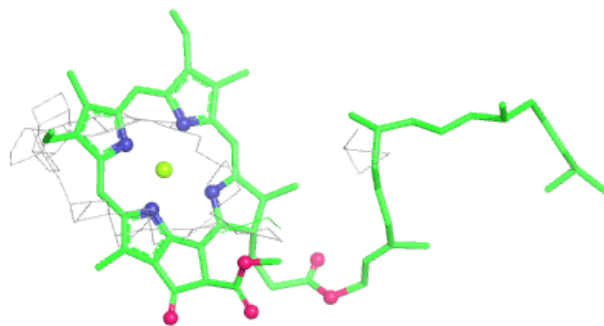
Electron density around CLA B 817:

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



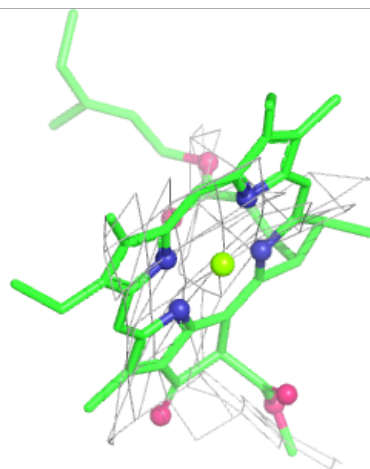
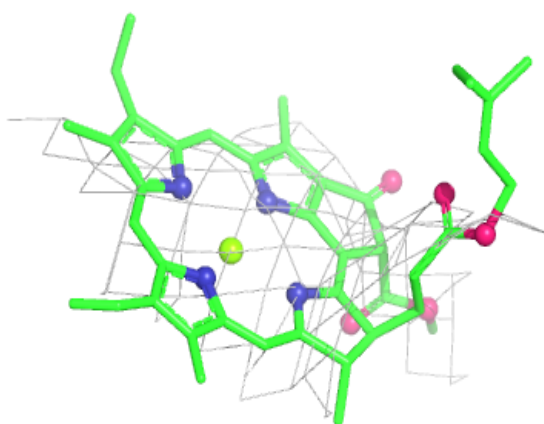
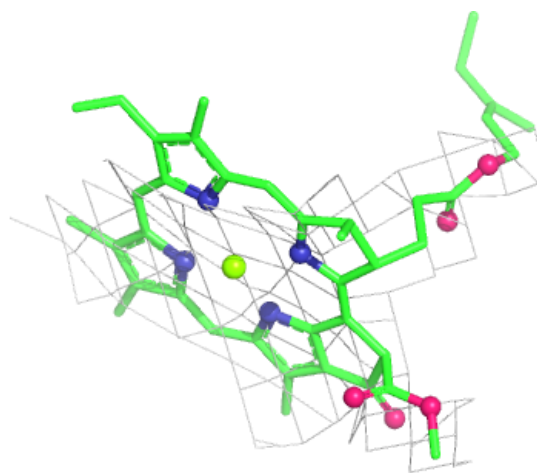
Electron density around CLA A 804:

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



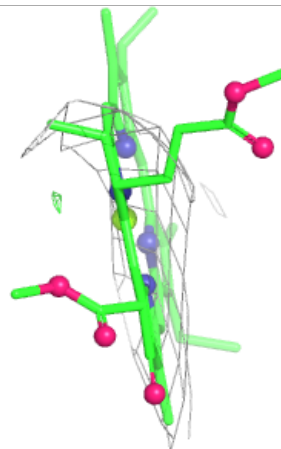
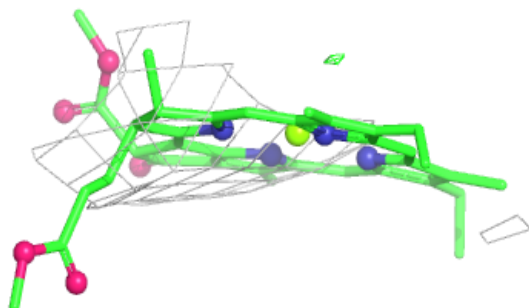
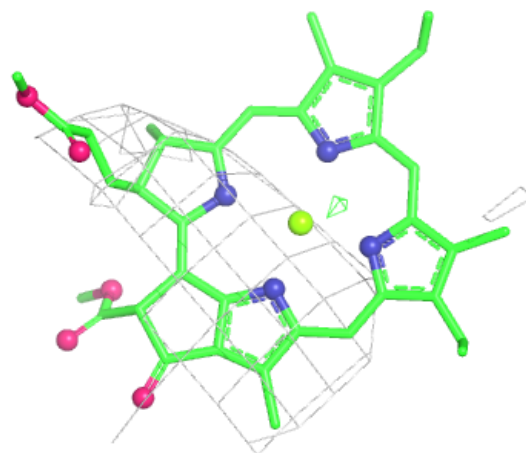
Electron density around CLA A 808:

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



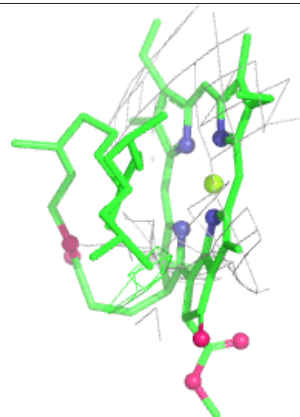
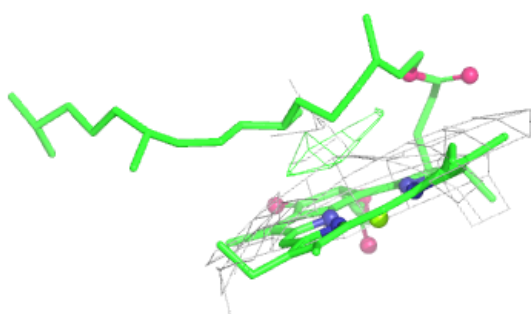
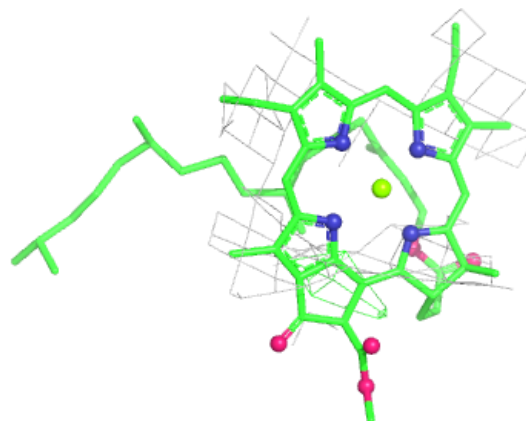
Electron density around CLA B 825:

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

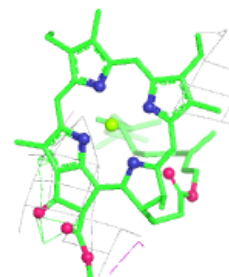
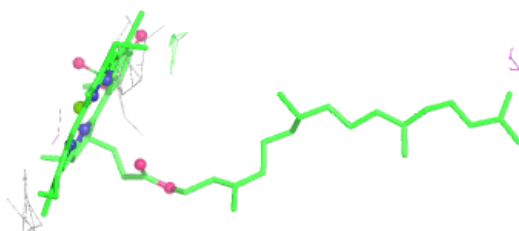
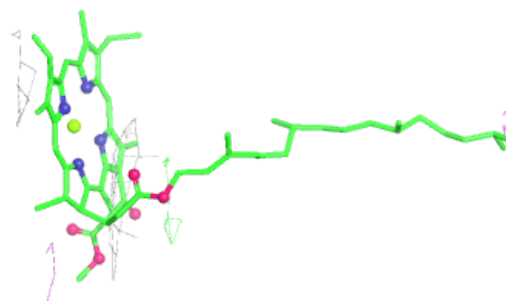


Electron density around CLA B 827:

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

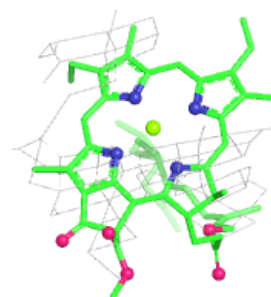
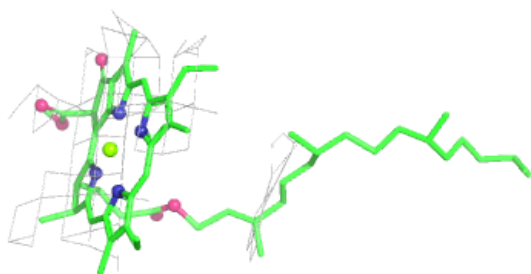
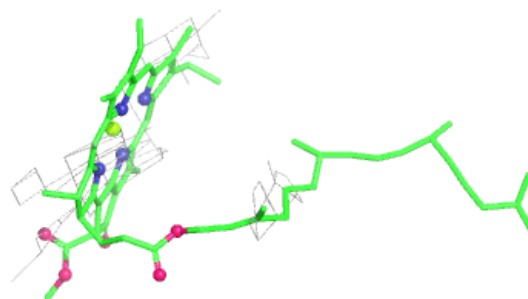
**Electron density around CLA B 828:**

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



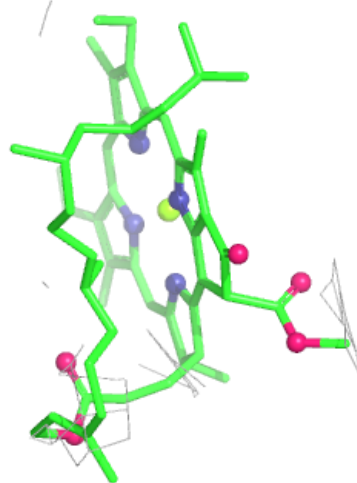
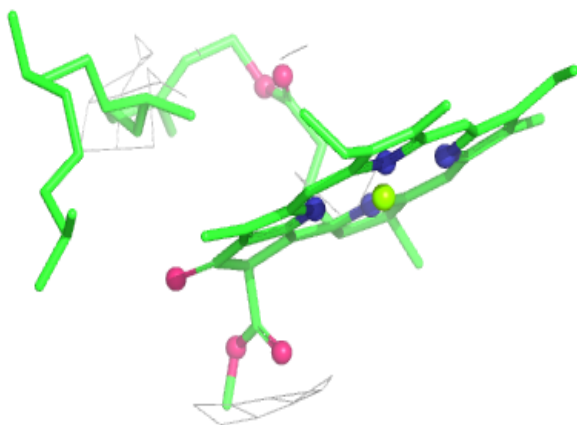
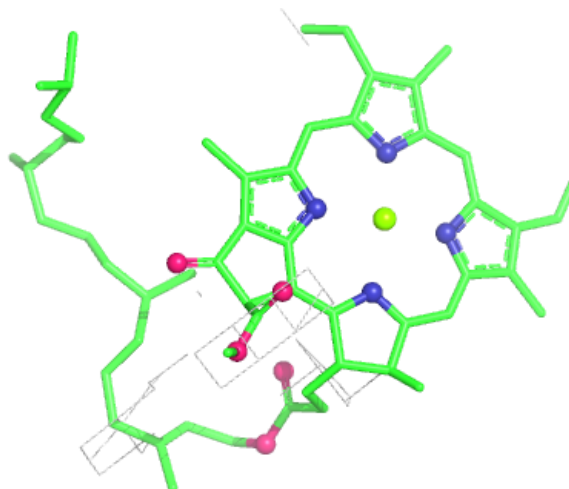
Electron density around CLA A 812:

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



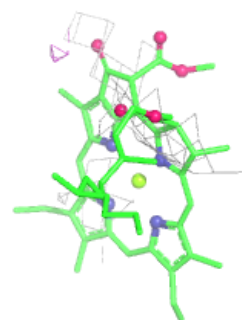
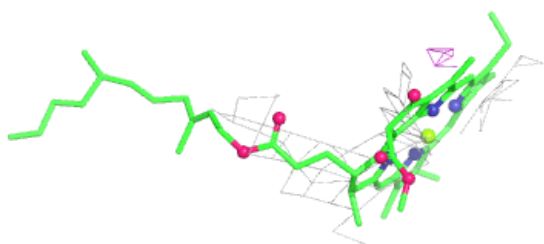
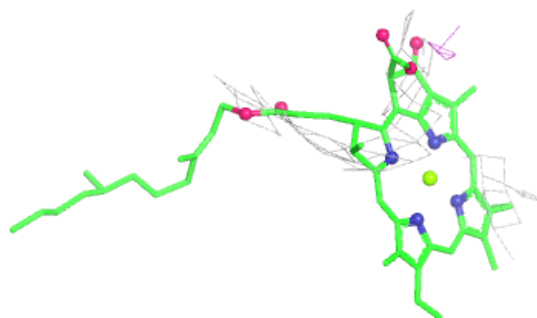
Electron density around CLA B 832:

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



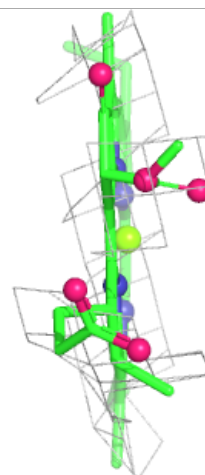
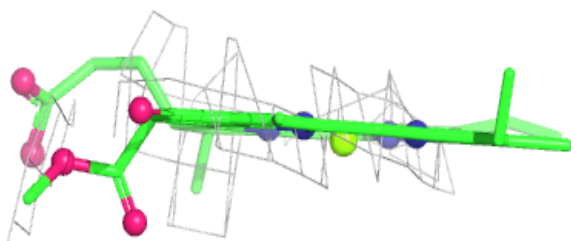
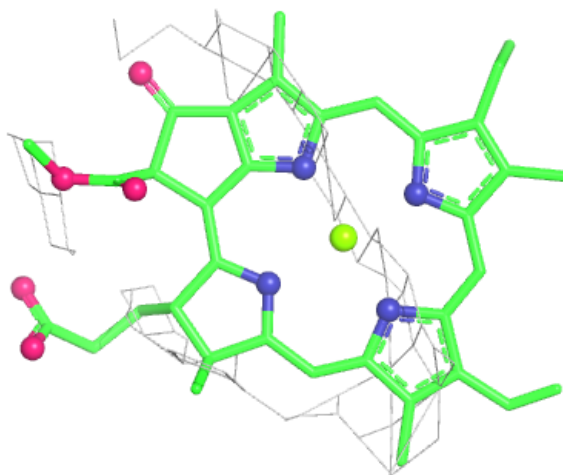
Electron density around CLA B 833:

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



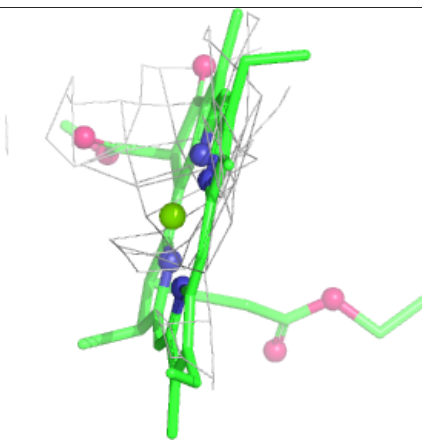
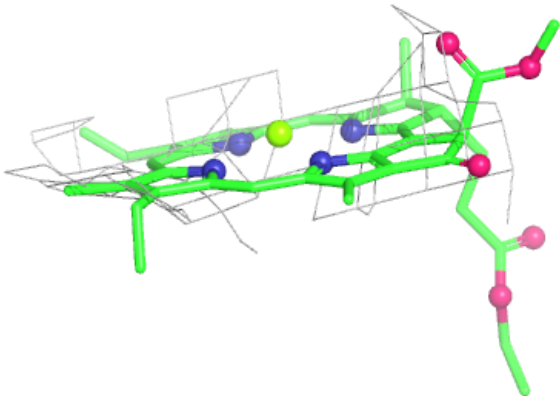
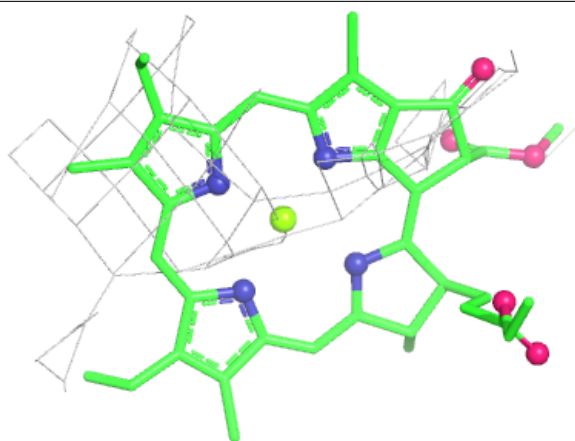
Electron density around CLA B 836:

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



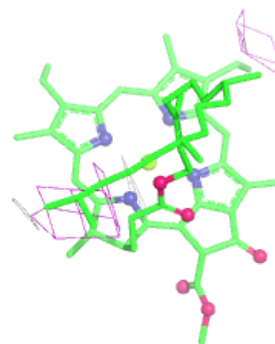
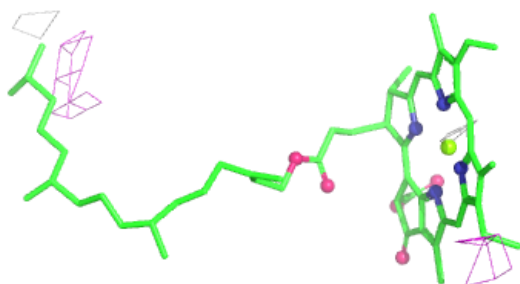
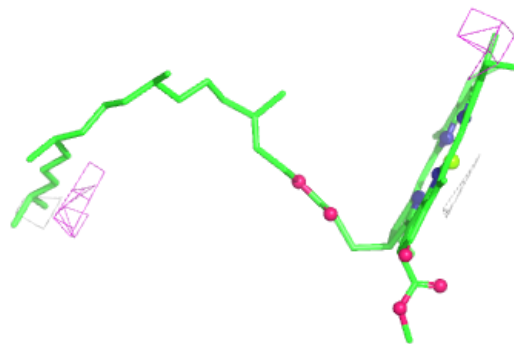
Electron density around CLA B 839:

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



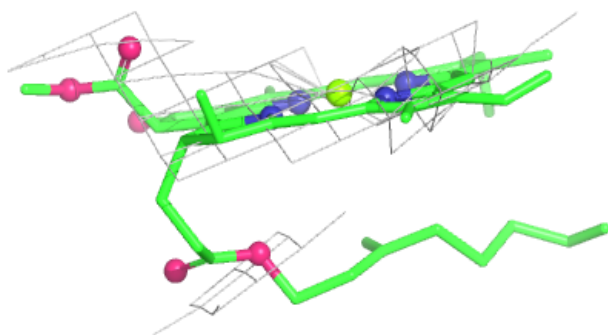
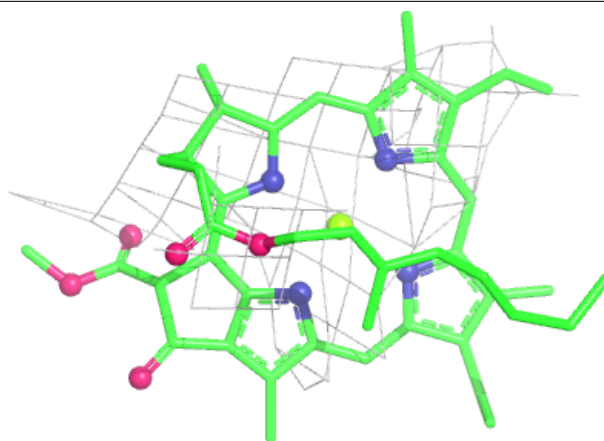
Electron density around CLA B 840:

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



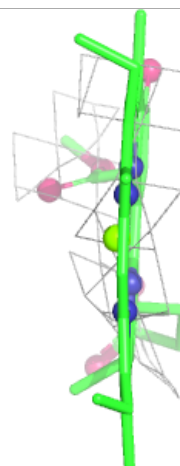
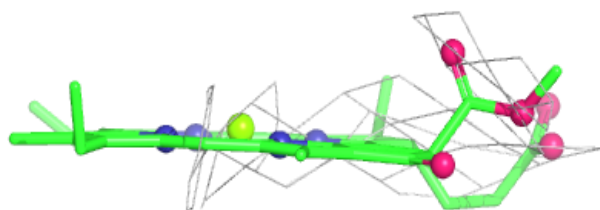
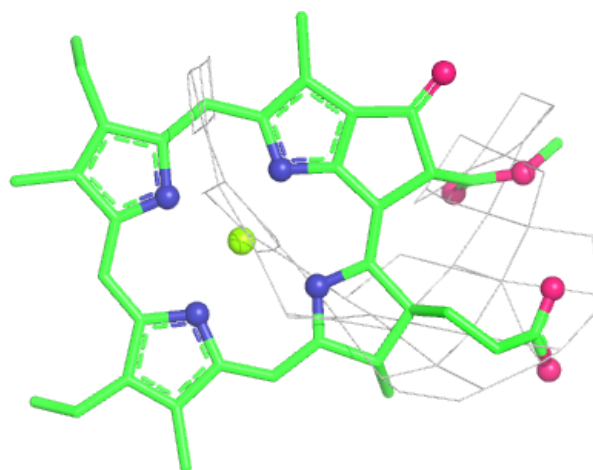
Electron density around CLA A 813:

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



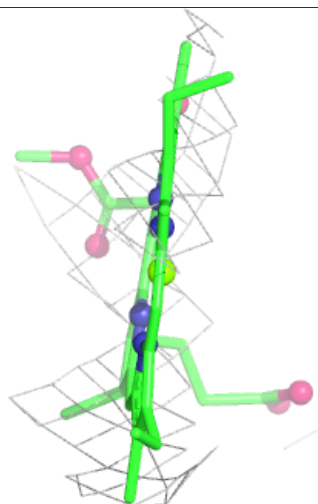
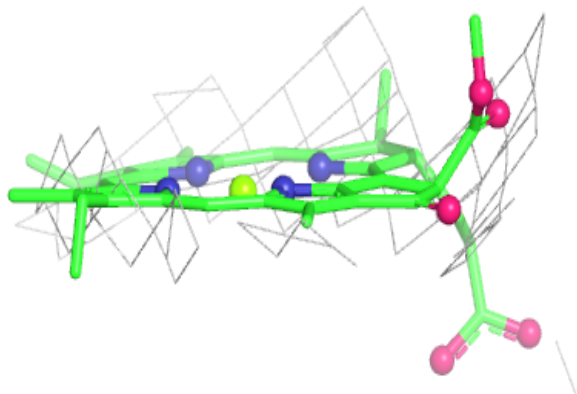
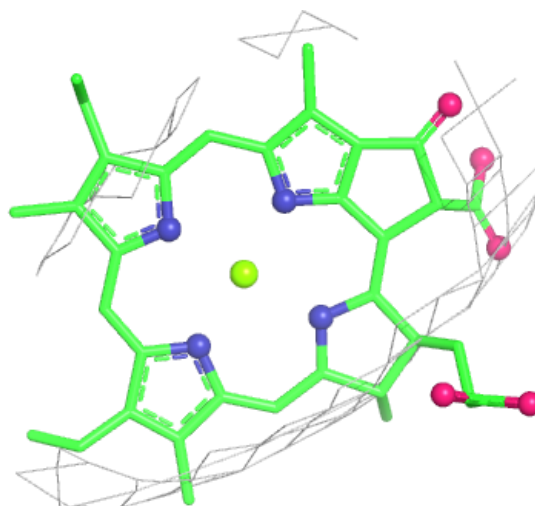
Electron density around CLA F 1301:

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



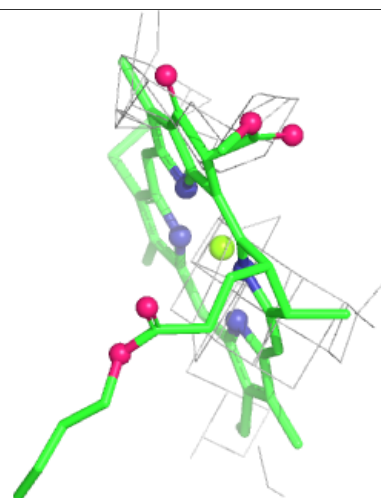
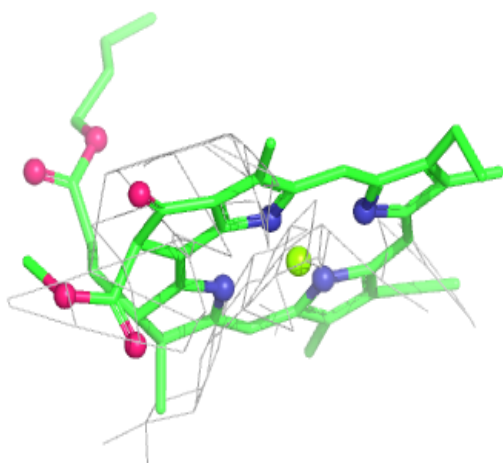
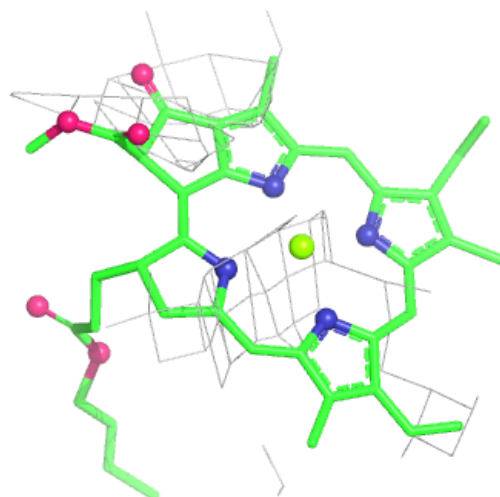
Electron density around CLA J 101:

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



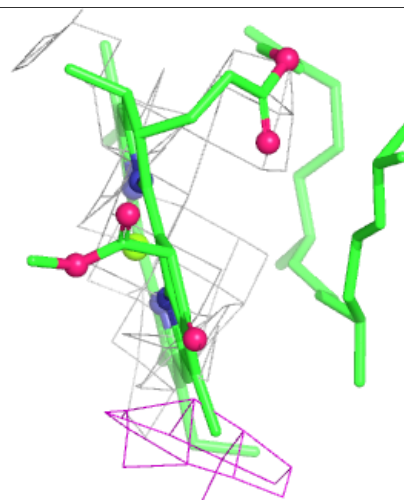
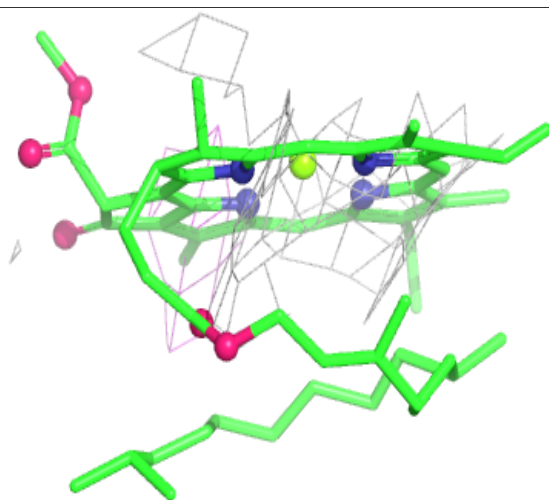
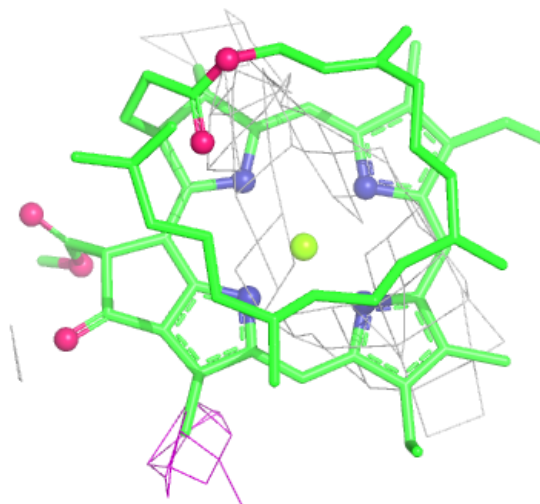
Electron density around CLA A 817:

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



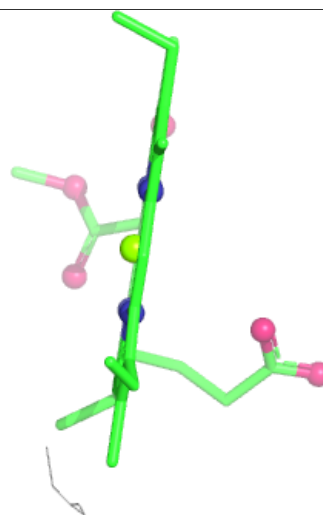
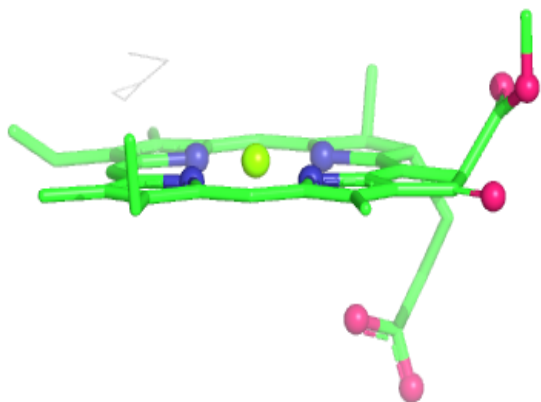
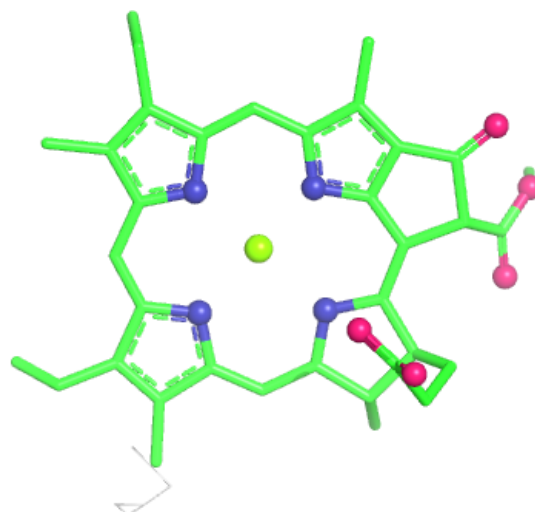
Electron density around CLA L 1002:

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



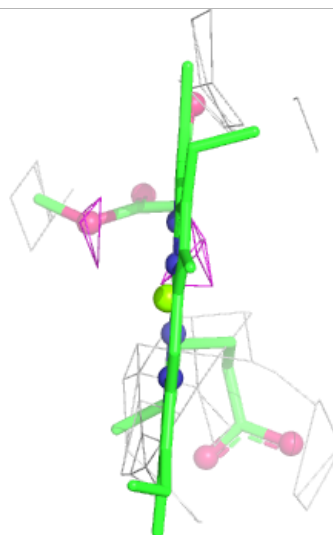
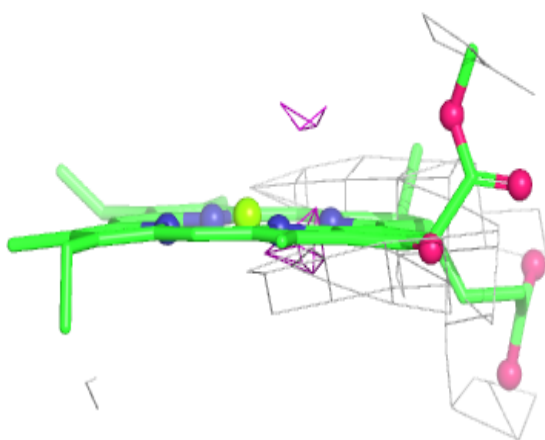
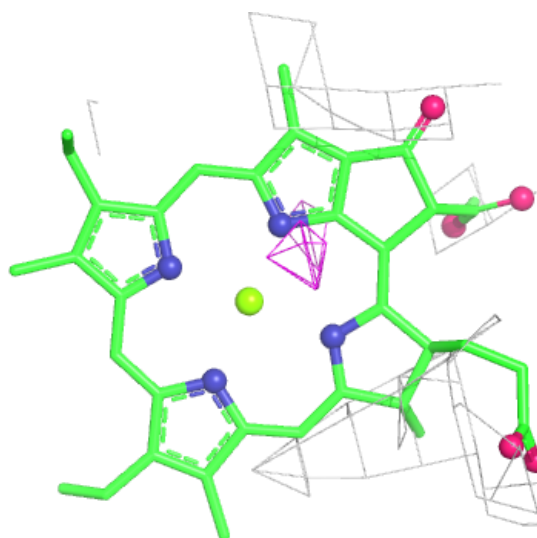
Electron density around CLA M 1601:

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



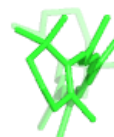
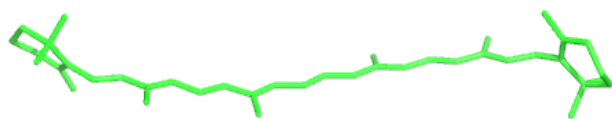
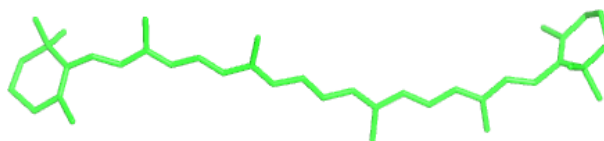
Electron density around CLA X 1701:

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

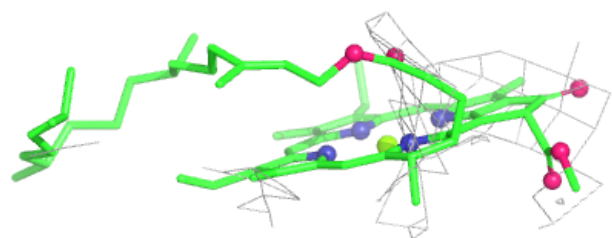
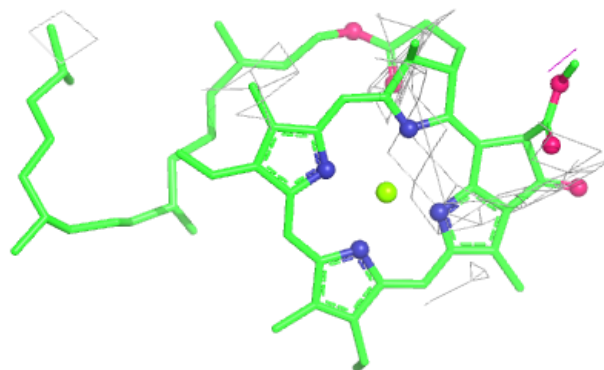


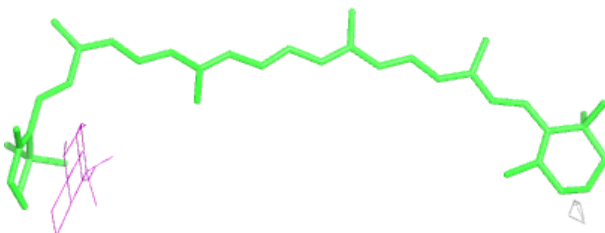
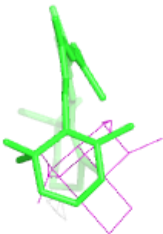
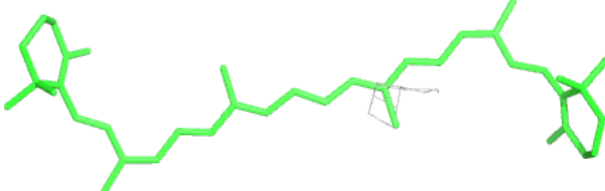
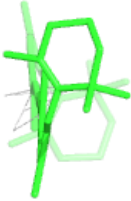
Electron density around BCR A 851:

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

**Electron density around CLA A 820:**

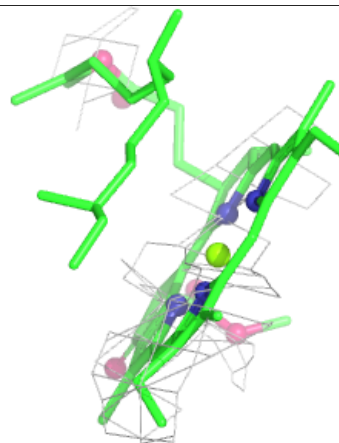
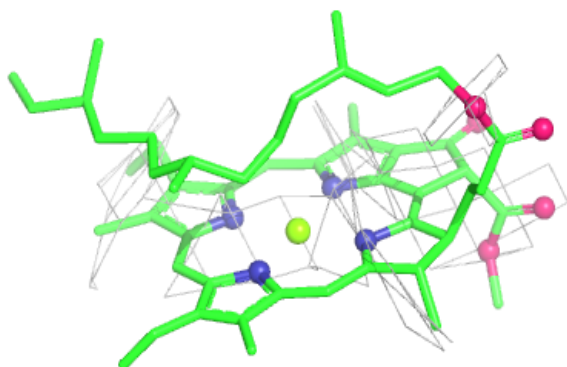
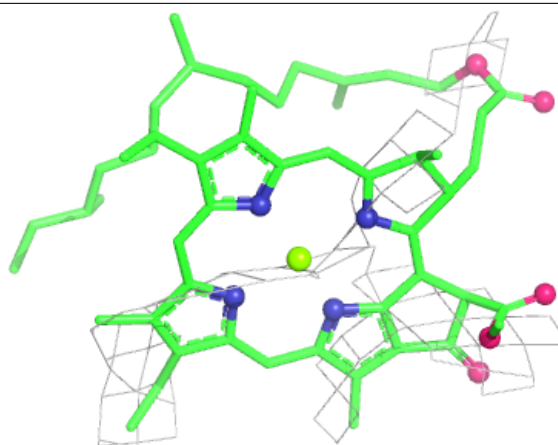
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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 BCR B 845: $2mF_o-DF_c$ (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

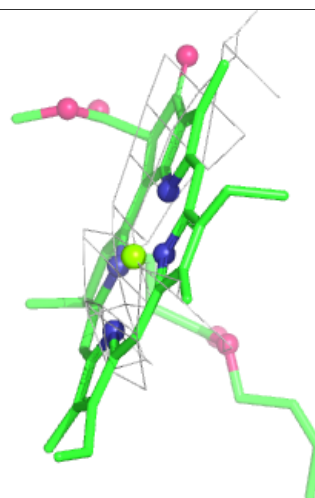
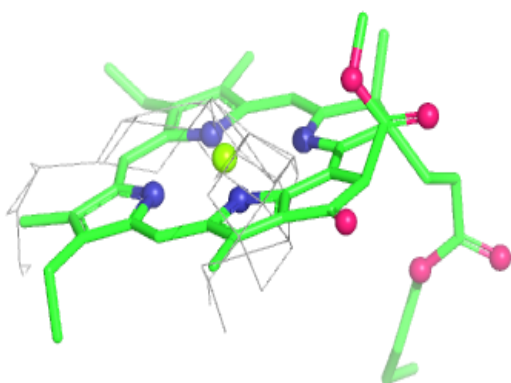
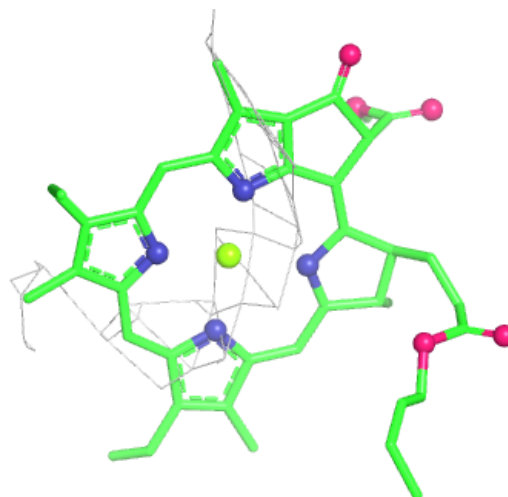
Electron density around CLA A 821:

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



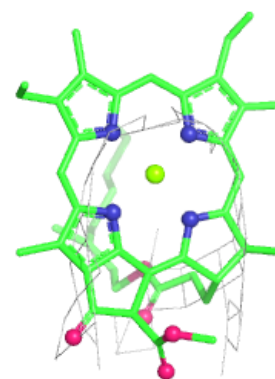
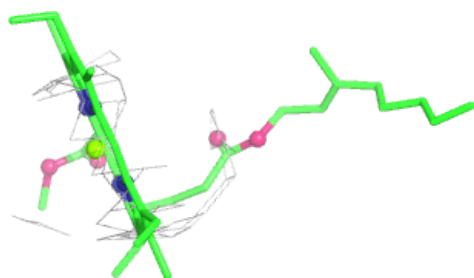
Electron density around CLA A 823:

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

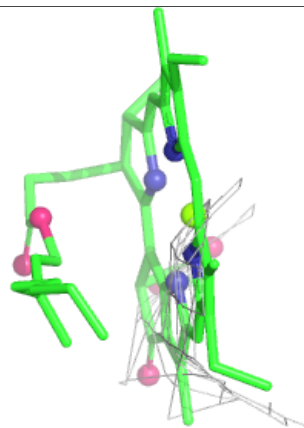
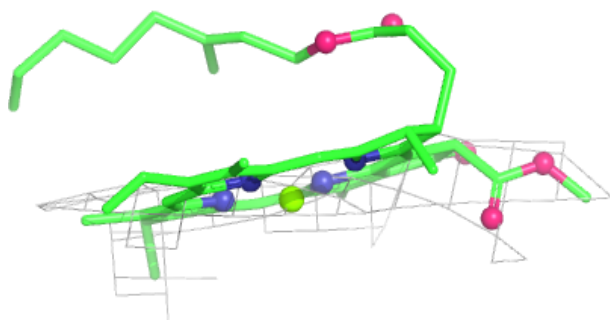
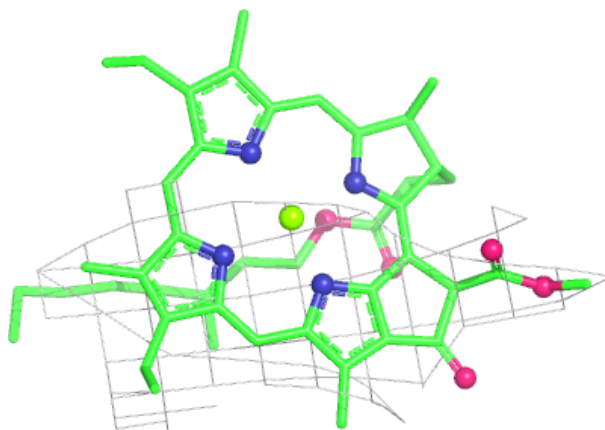


Electron density around CLA B 804:

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

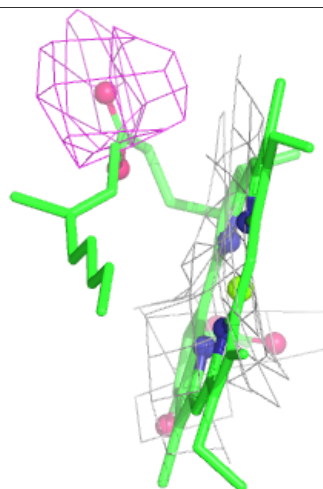
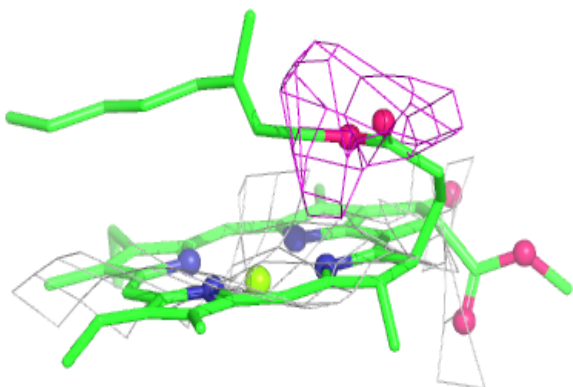
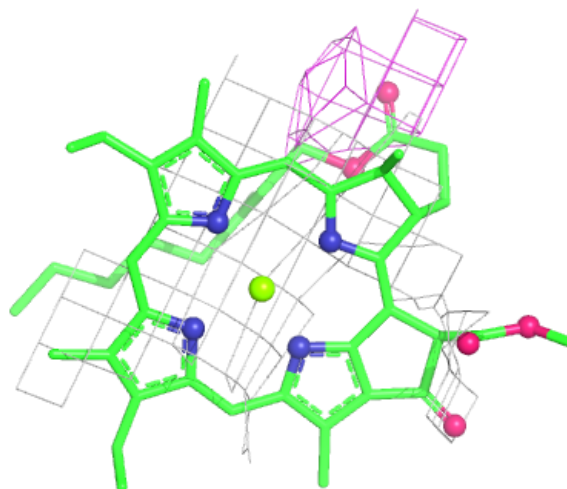
**Electron density around CLA A 818:**

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



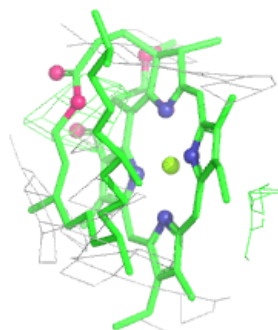
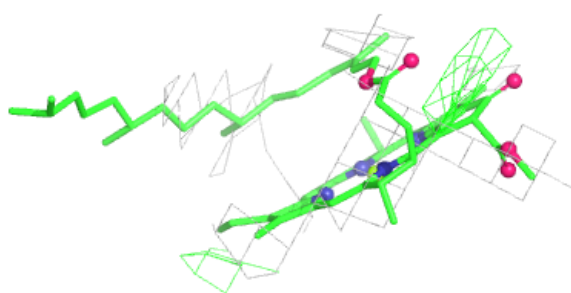
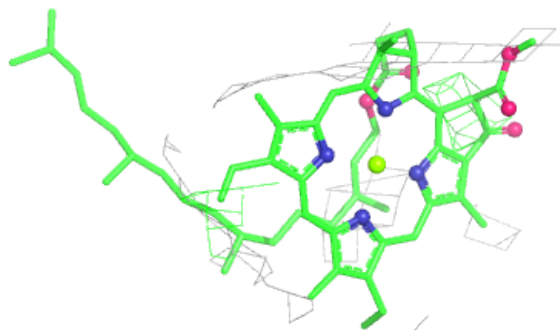
Electron density around CLA A 819:

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



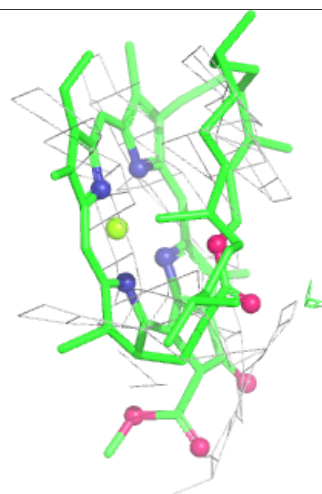
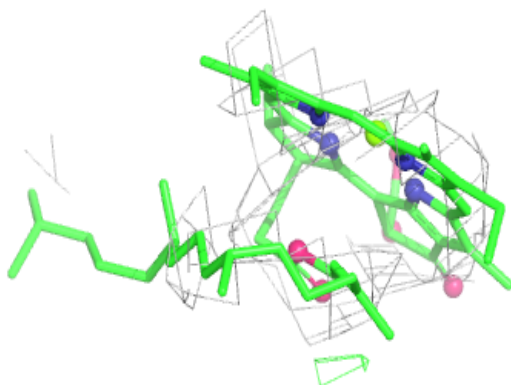
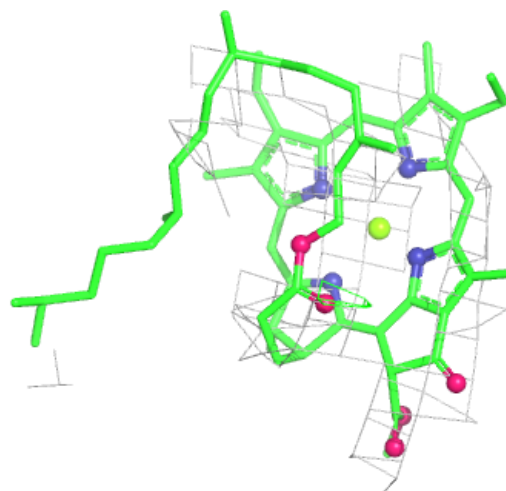
Electron density around CLA B 807:

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



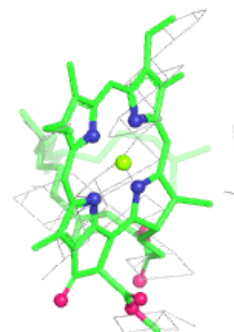
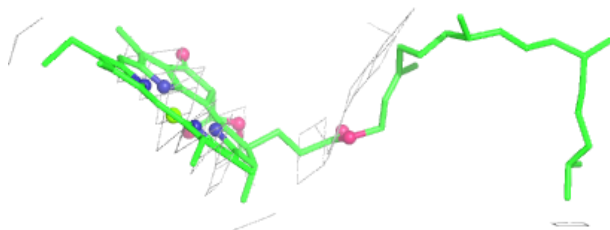
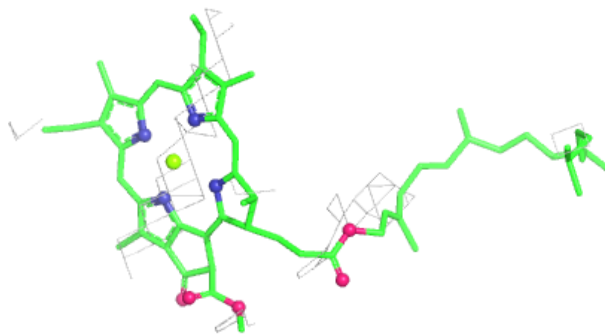
Electron density around CLA B 808:

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

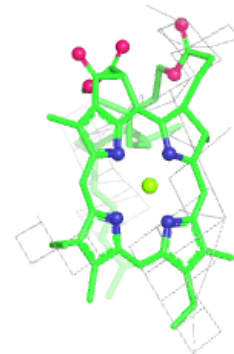
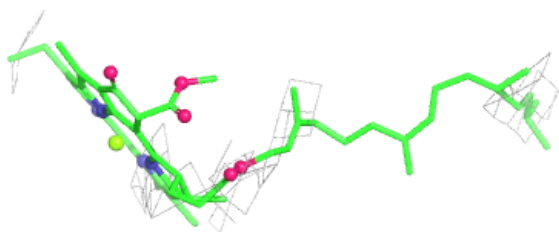
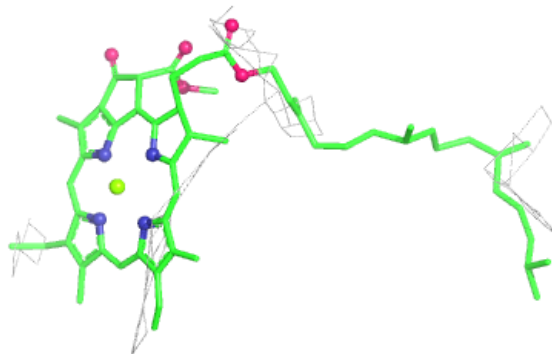


Electron density around CLA B 809:

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

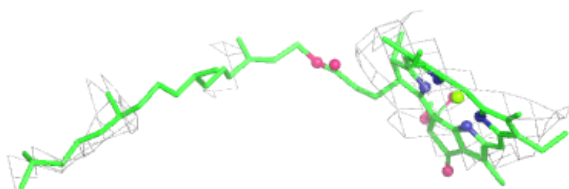
**Electron density around CLA B 810:**

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

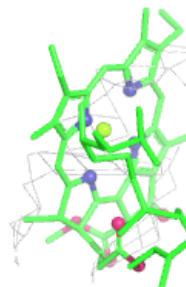
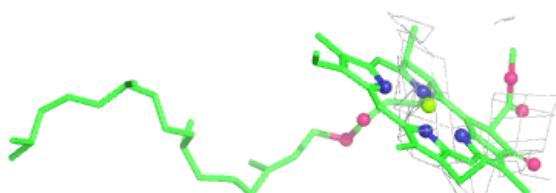
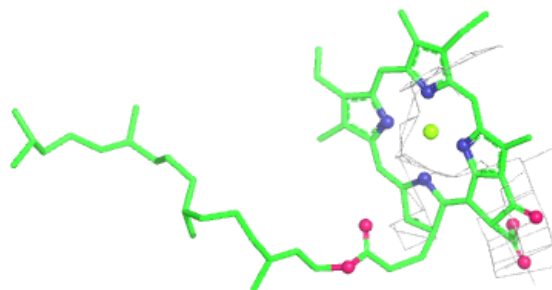


Electron density around CLA A 802:

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

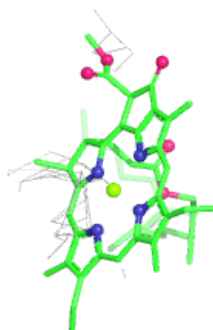
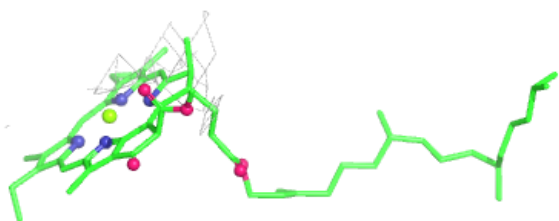
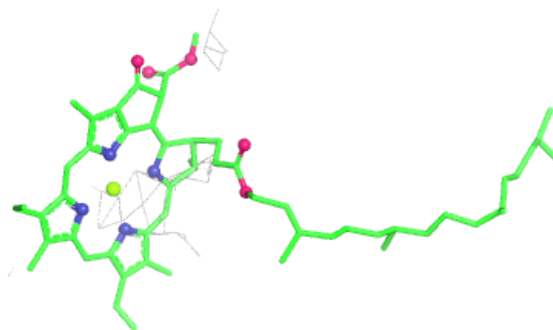
**Electron density around CLA A 809:**

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

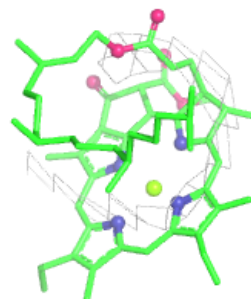
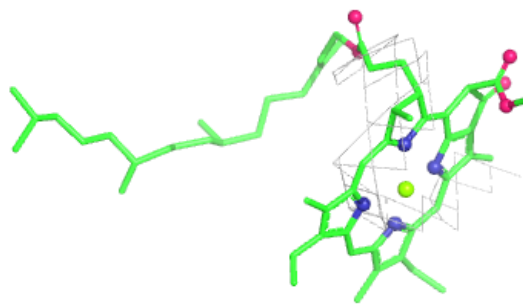


Electron density around CLA A 822:

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

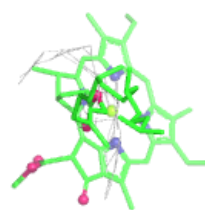
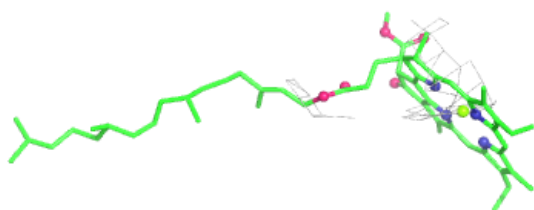
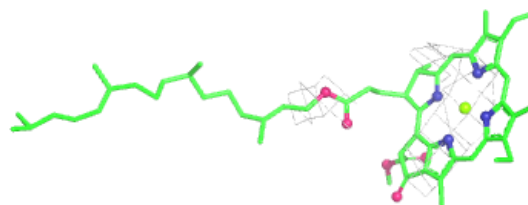
**Electron density around CLA B 814:**

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



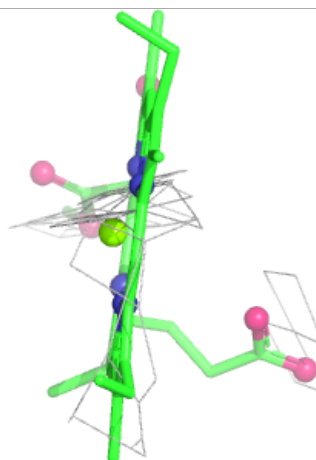
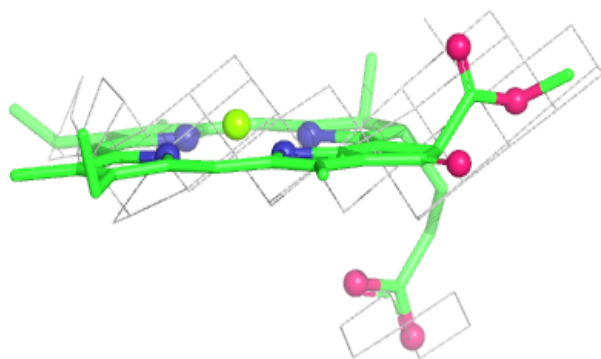
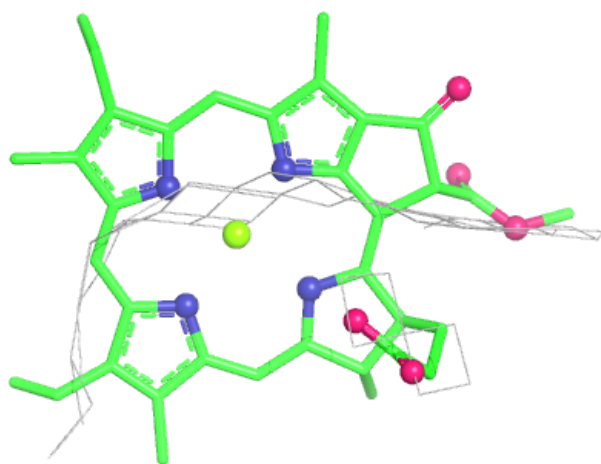
Electron density around CLA A 810:

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



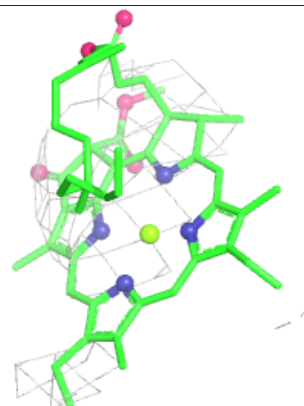
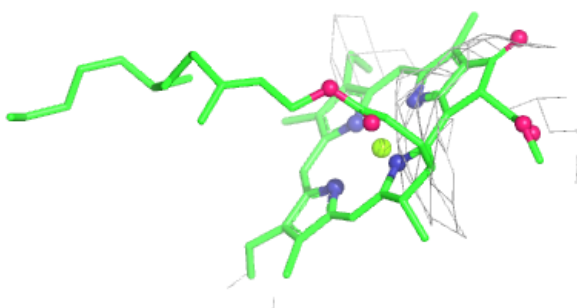
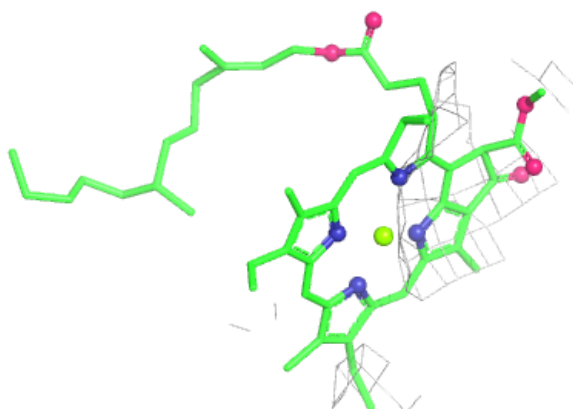
Electron density around CLA A 811:

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

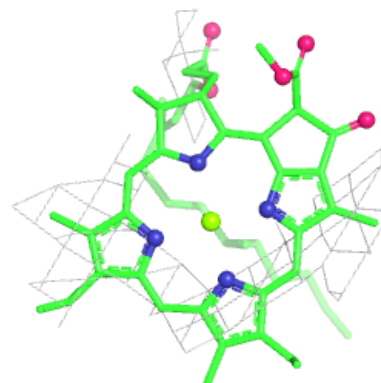
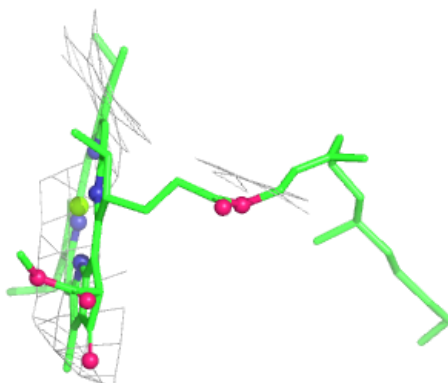
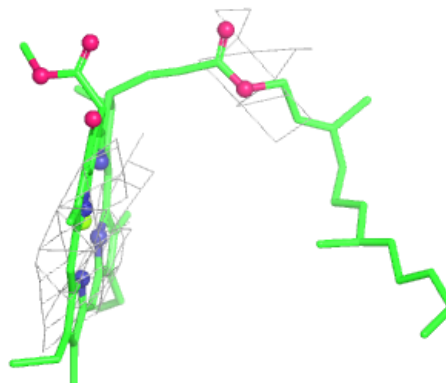


Electron density around CLA A 825:

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

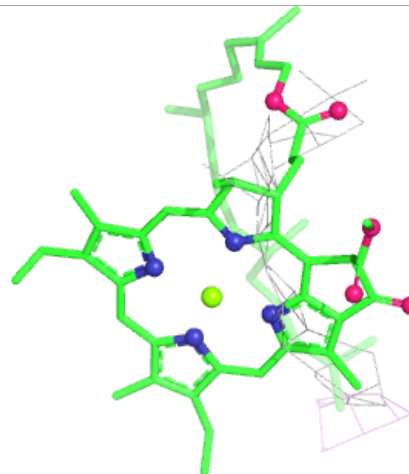
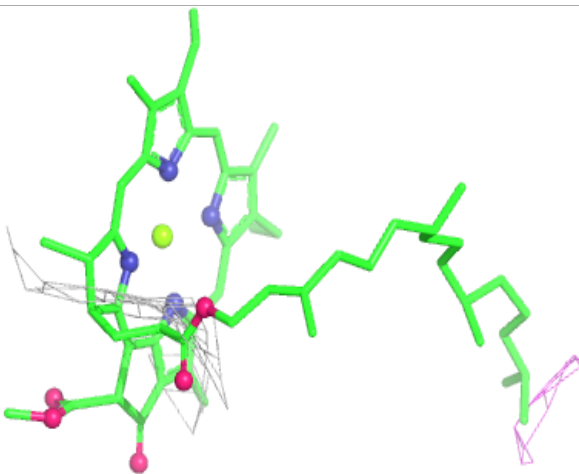
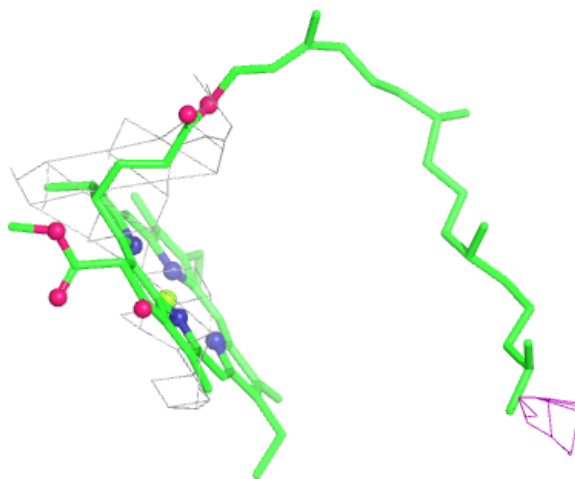
**Electron density around CLA A 805:**

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



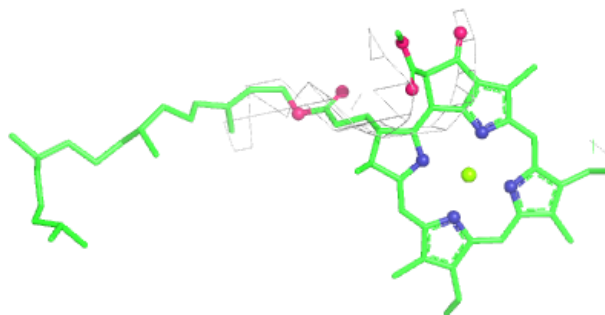
Electron density around CLA B 819:

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



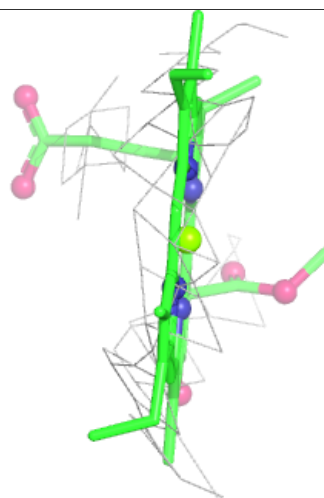
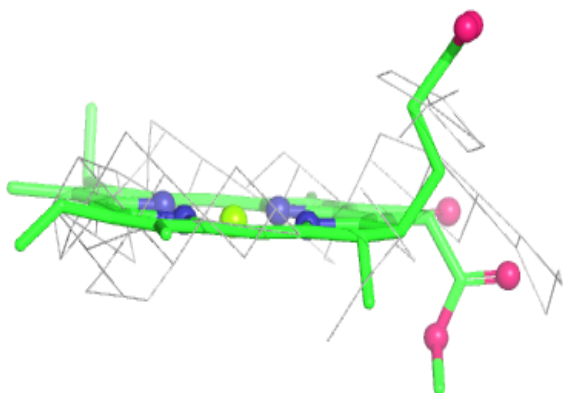
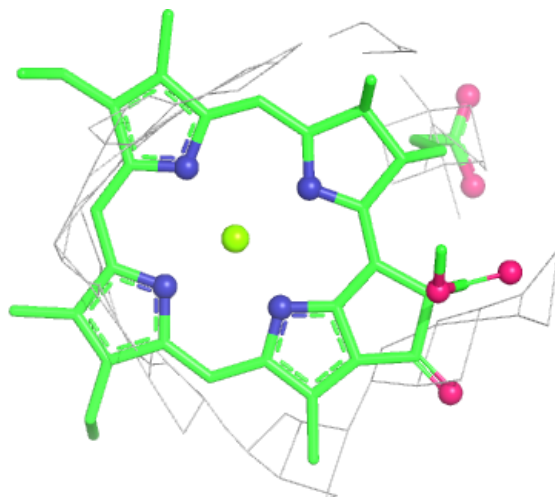
Electron density around CLA A 827:

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



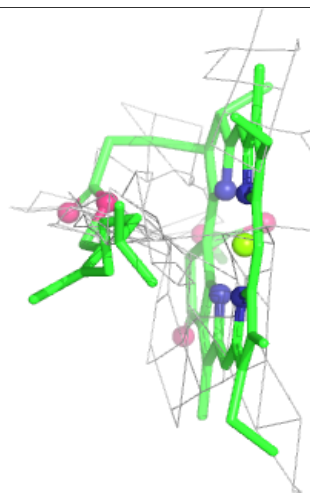
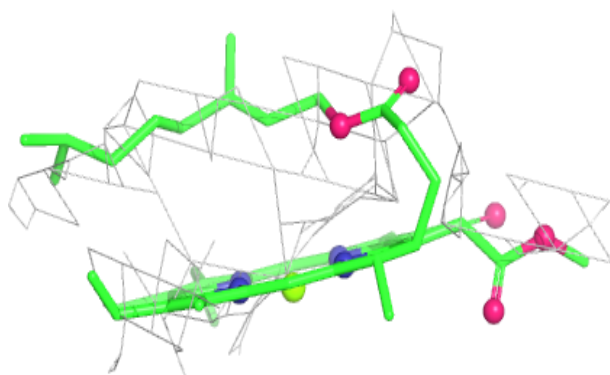
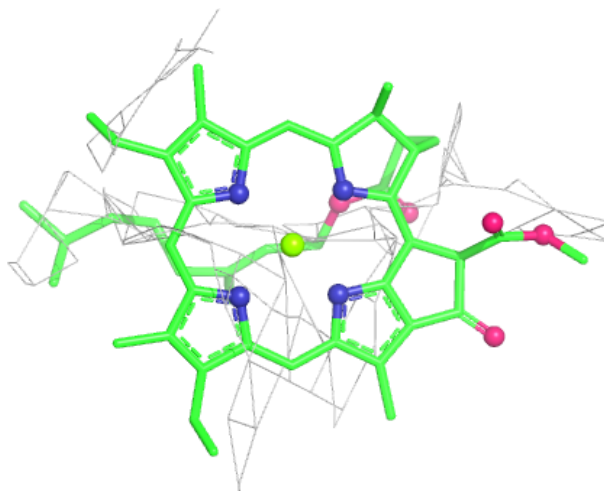
Electron density around CLA B 821:

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



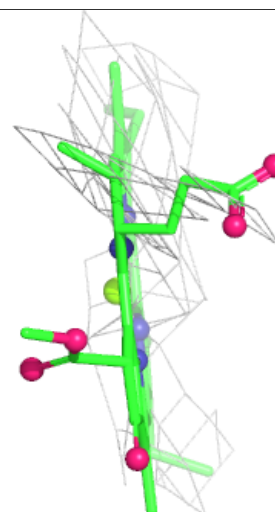
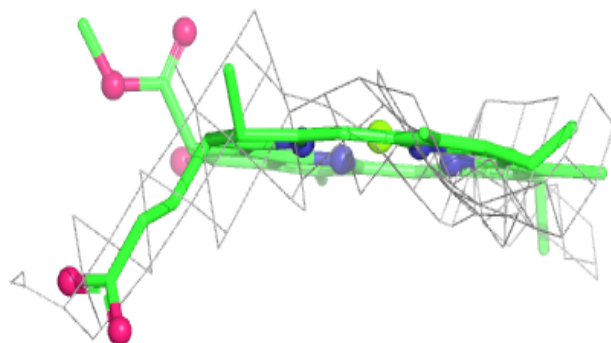
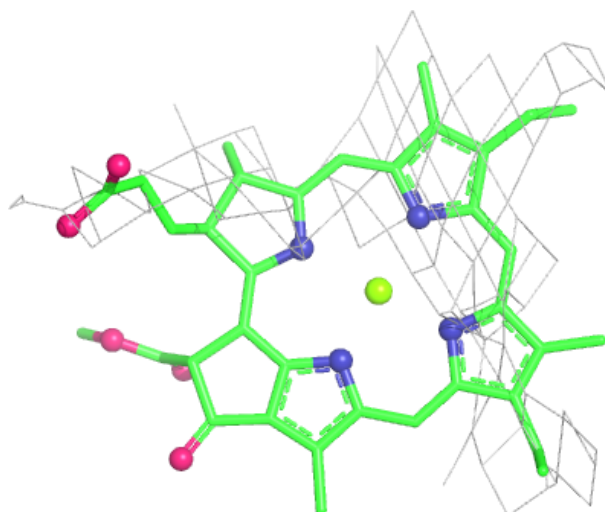
Electron density around CLA B 822:

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



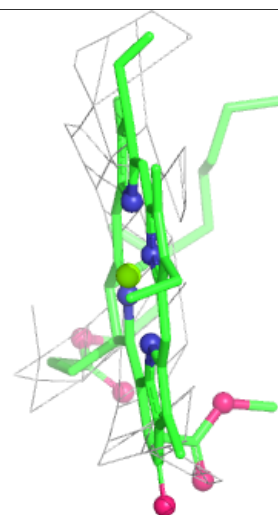
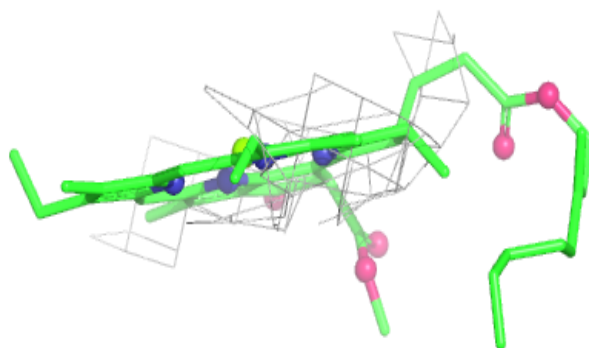
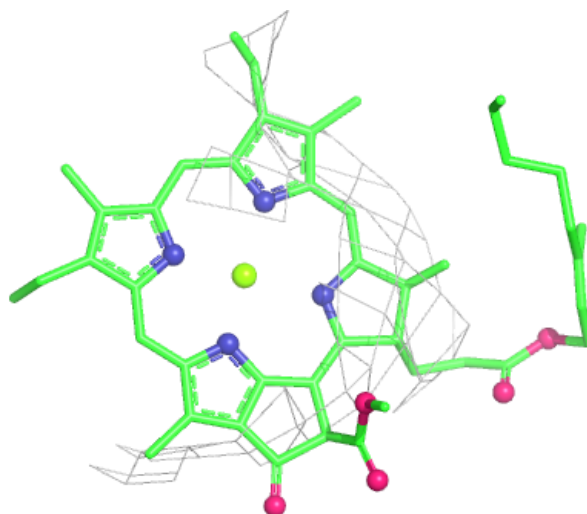
Electron density around CLA B 823:

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



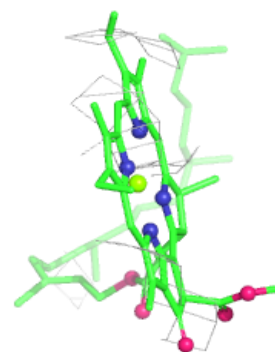
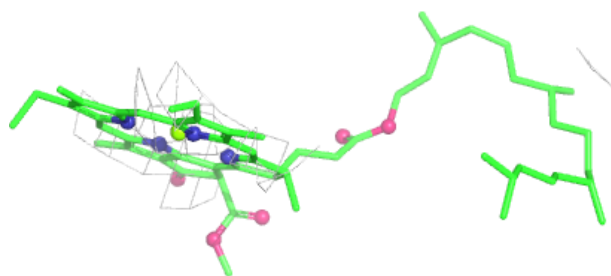
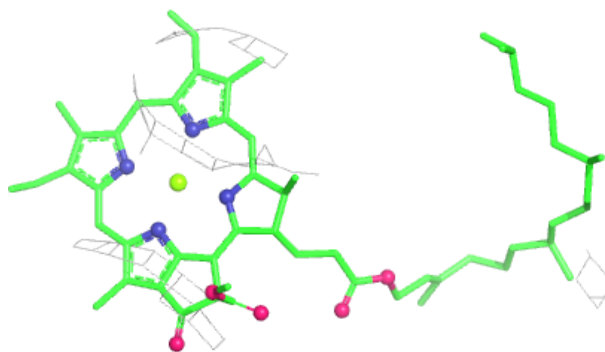
Electron density around CLA B 824:

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

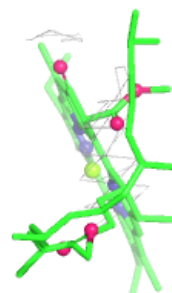
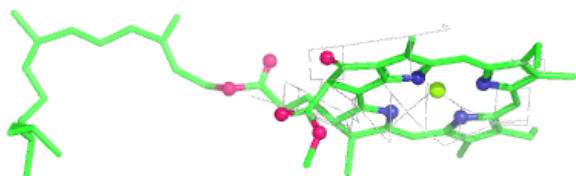
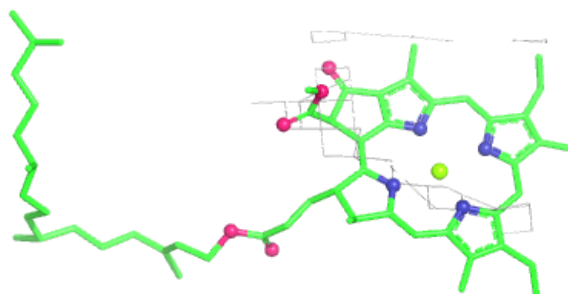


Electron density around CLA A 828:

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

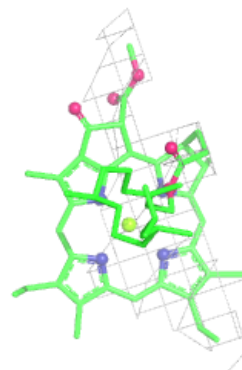
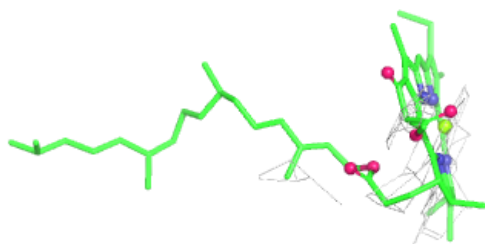
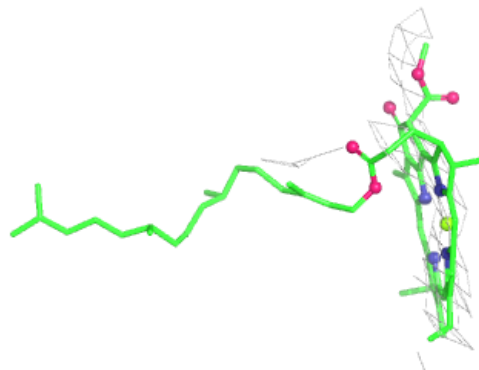
**Electron density around CLA B 826:**

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

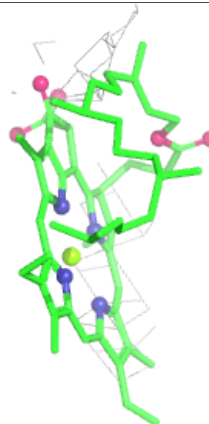
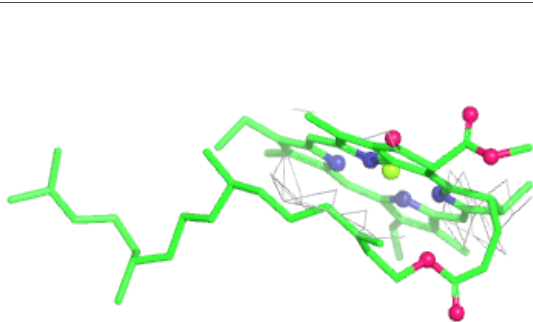
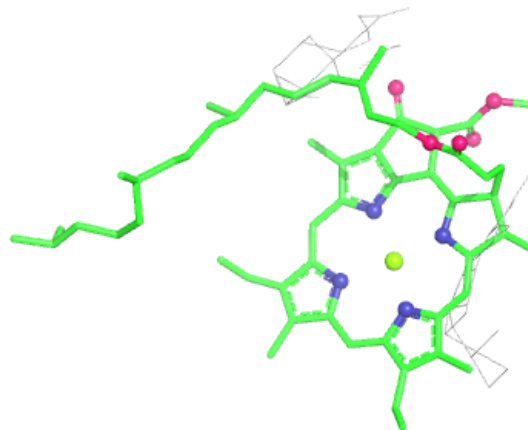


Electron density around CLA A 829:

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

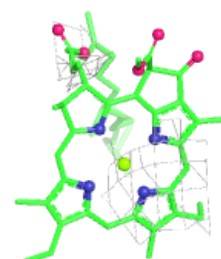
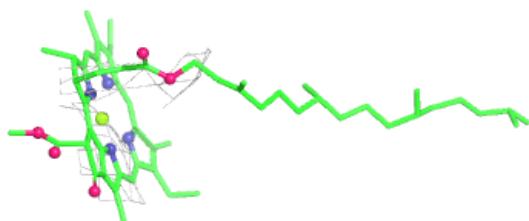
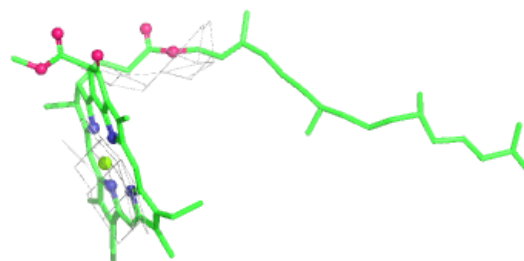
**Electron density around CLA A 830:**

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

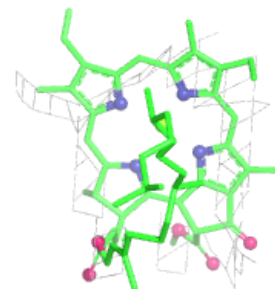
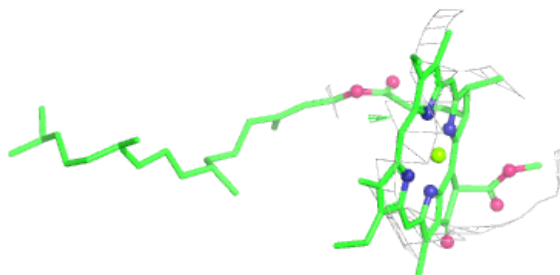
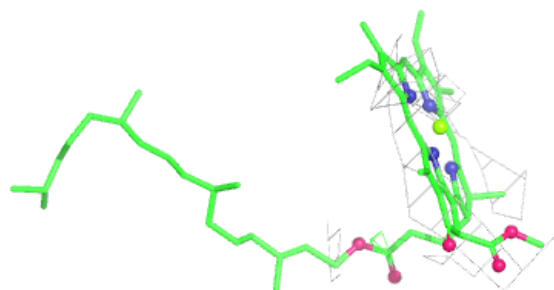


Electron density around CLA B 829:

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

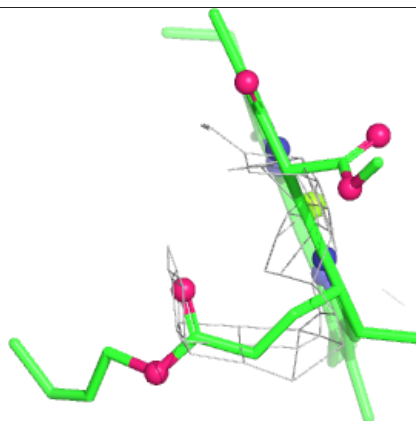
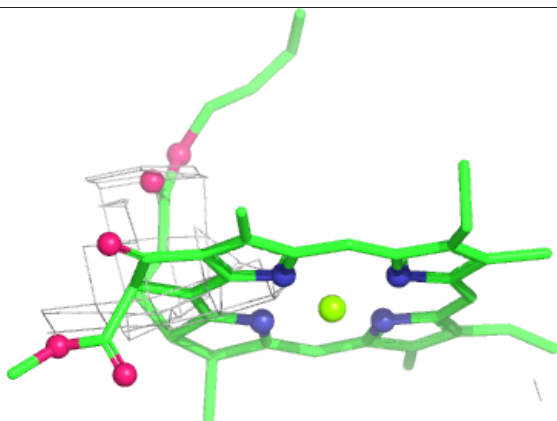
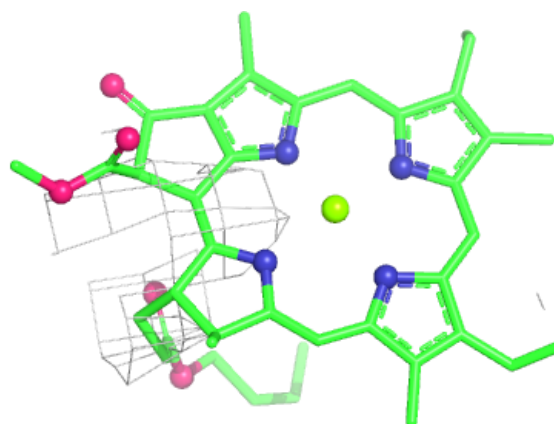
**Electron density around CLA A 831:**

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



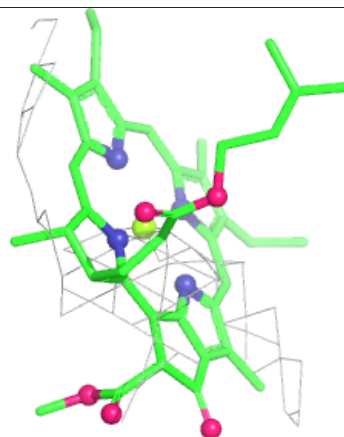
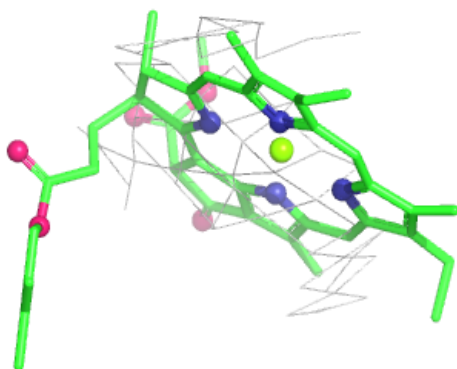
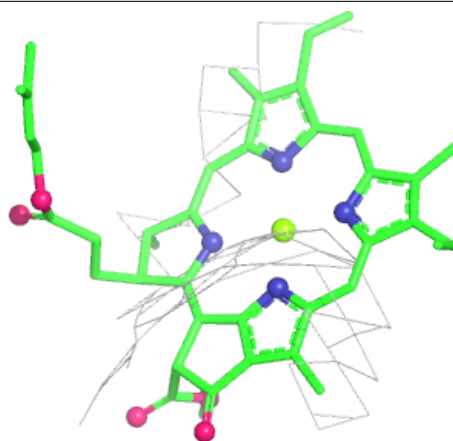
Electron density around CLA B 831:

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



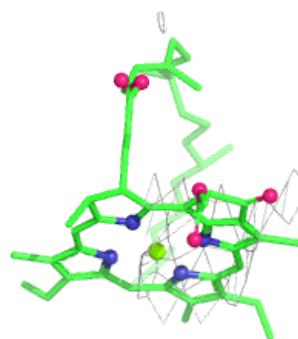
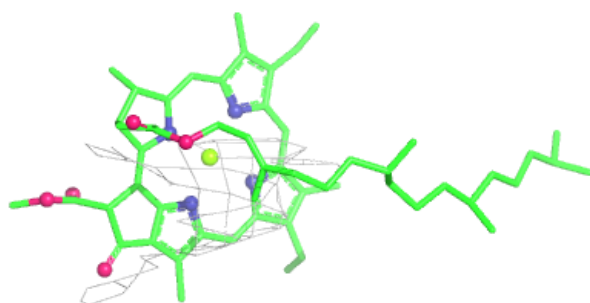
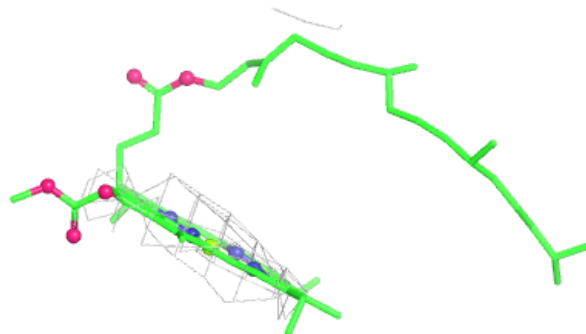
Electron density around CLA A 832:

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



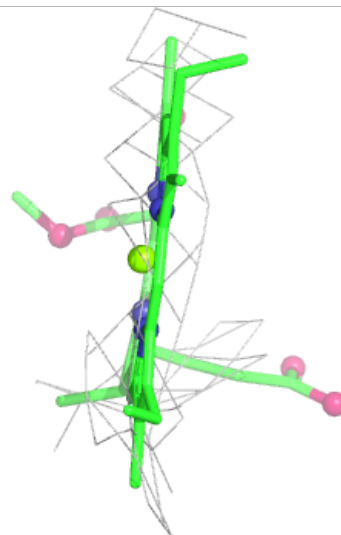
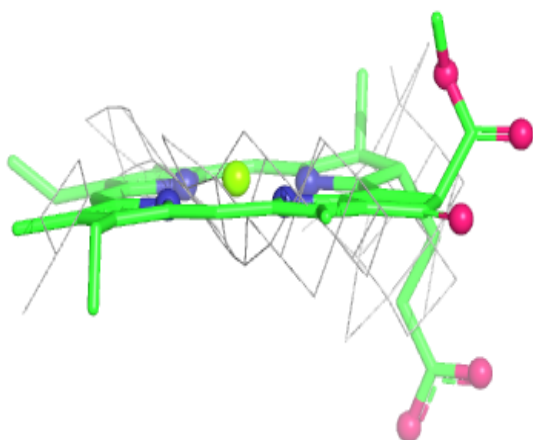
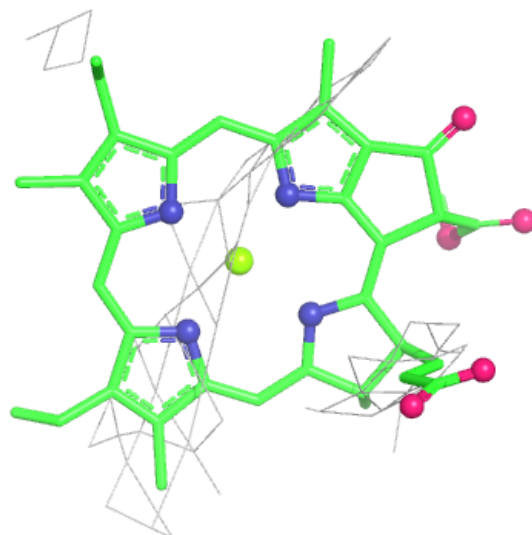
Electron density around CLA A 833:

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



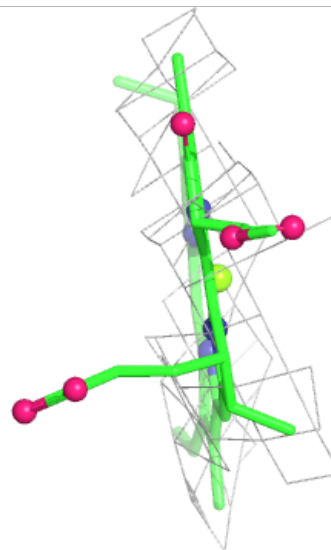
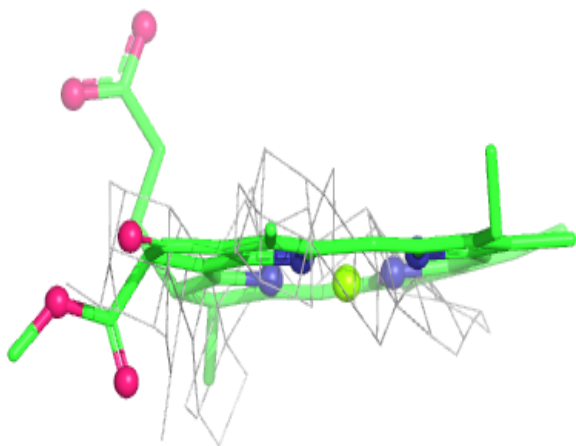
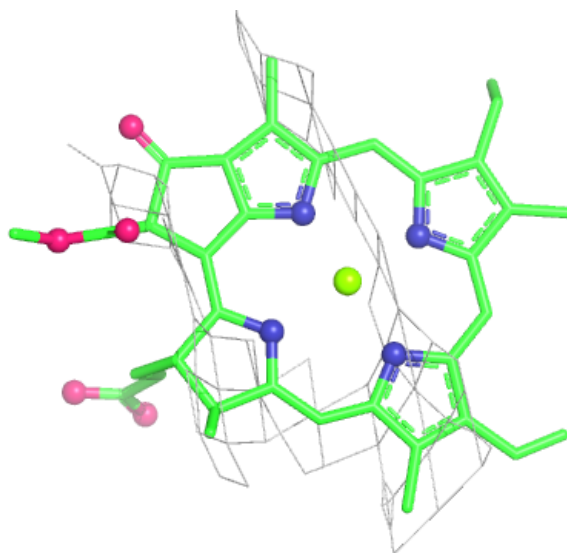
Electron density around CLA B 834:

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



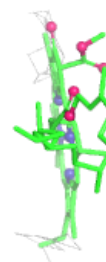
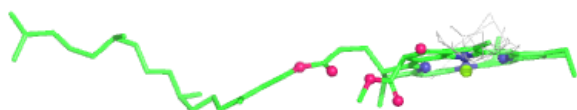
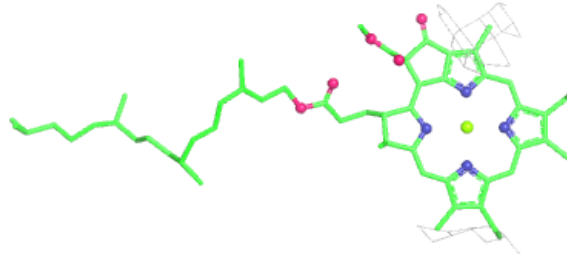
Electron density around CLA B 835:

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

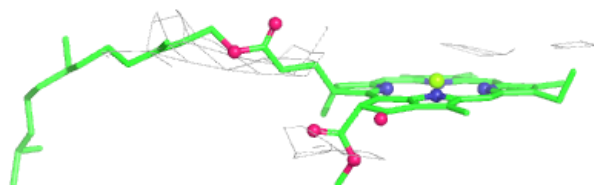
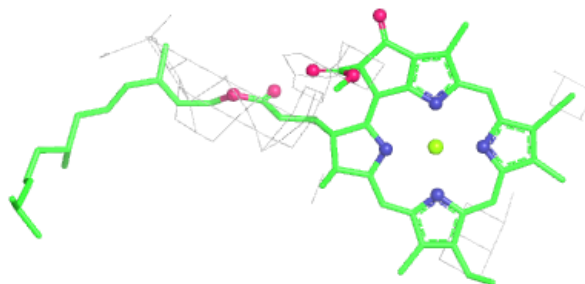


Electron density around CLA A 834:

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

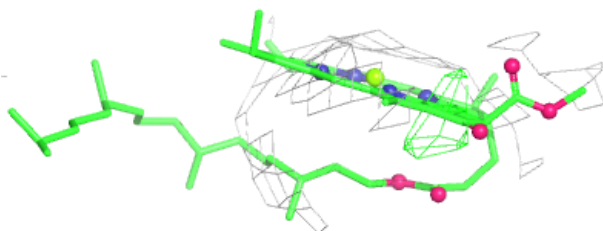
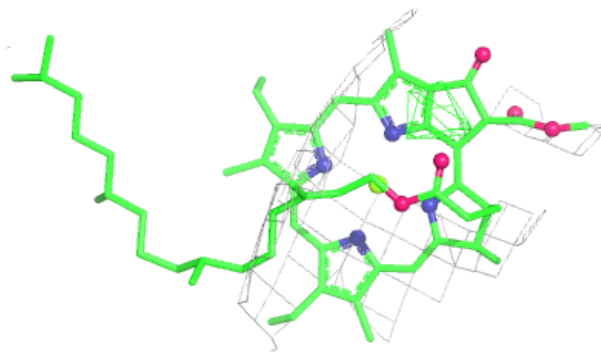
**Electron density around CLA B 837:**

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

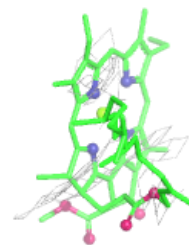
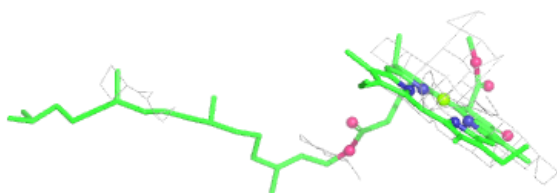
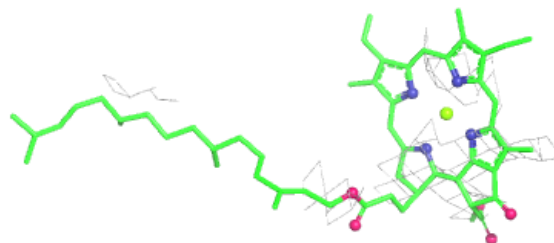


Electron density around CLA B 838:

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

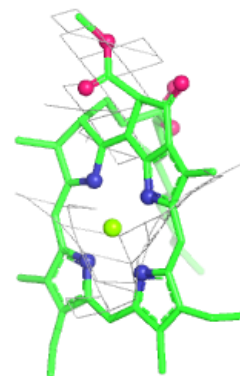
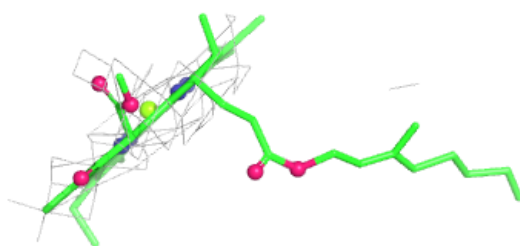
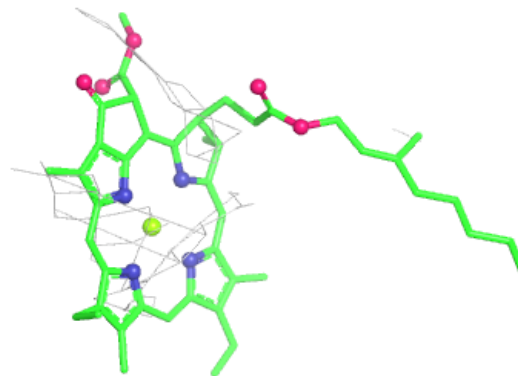
**Electron density around CLA A 835:**

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



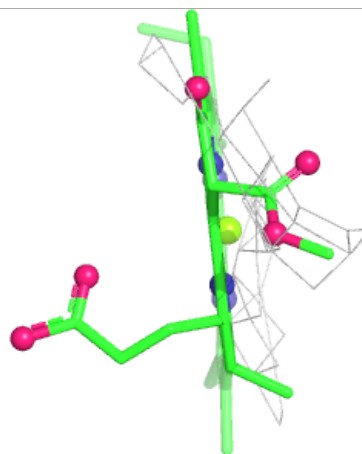
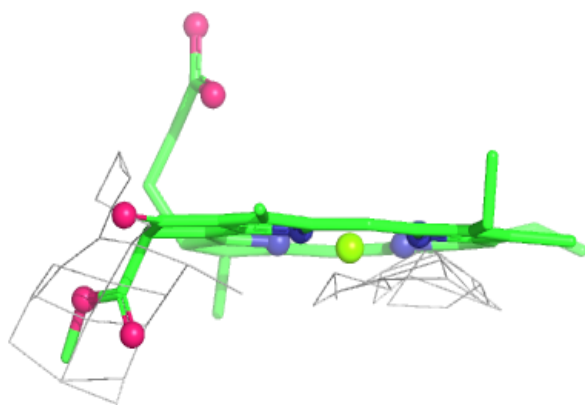
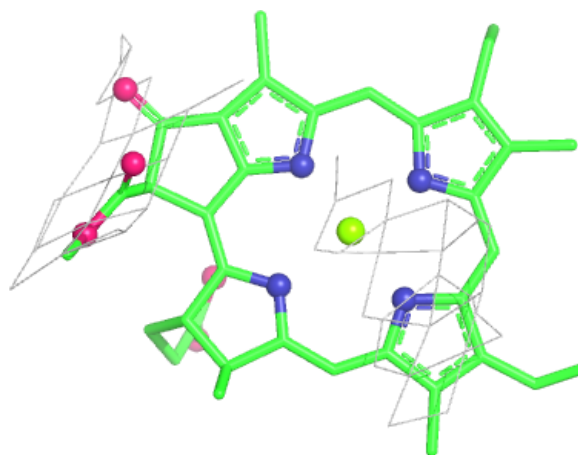
Electron density around CLA A 836:

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



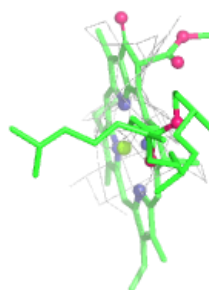
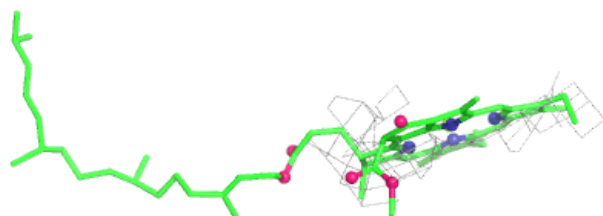
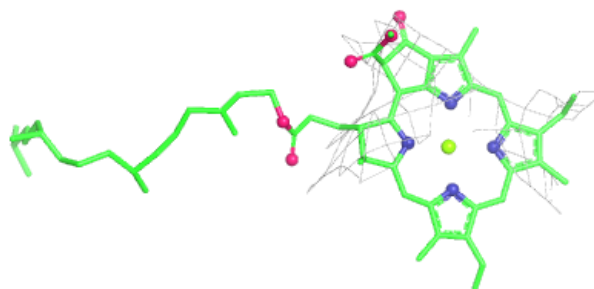
Electron density around CLA A 837:

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

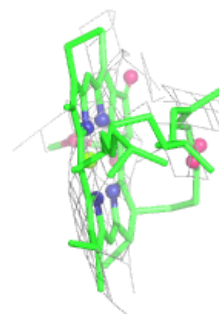
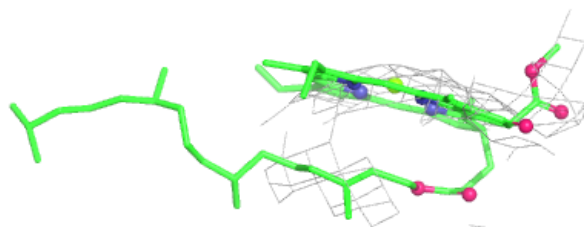
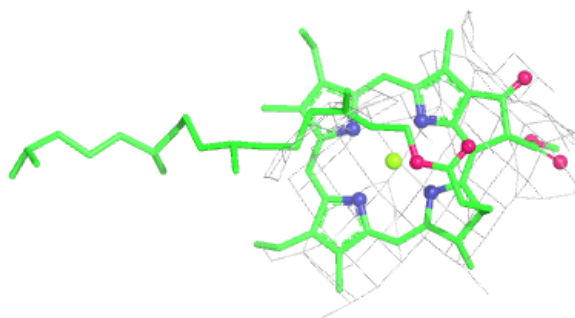


Electron density around CLA A 806:

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

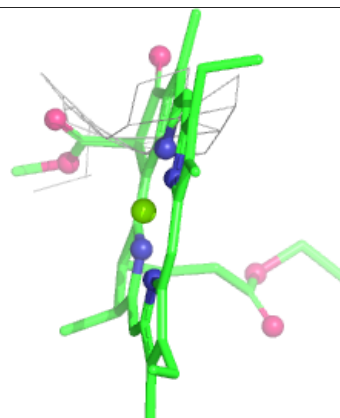
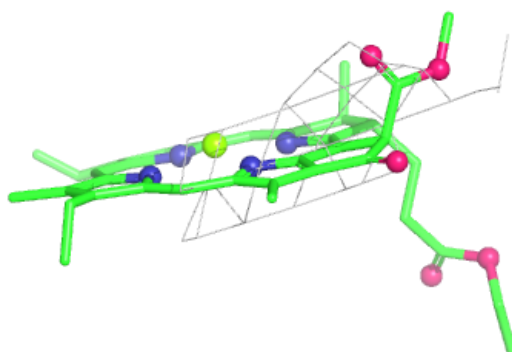
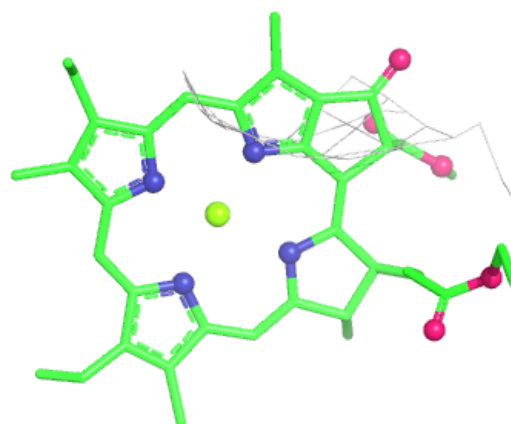
**Electron density around CLA A 839:**

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



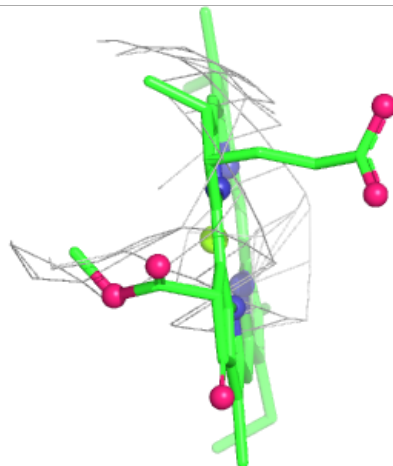
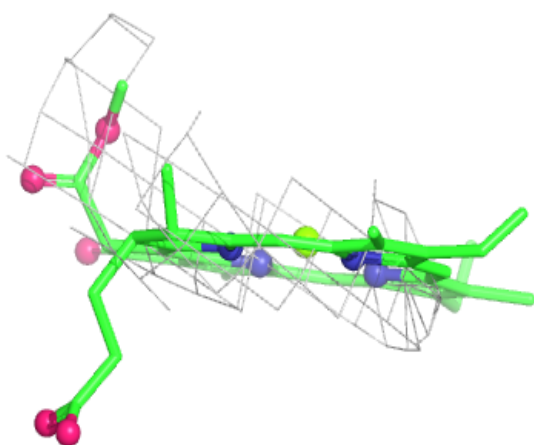
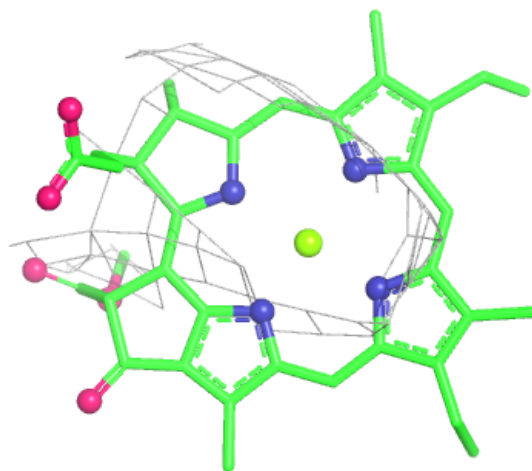
Electron density around CLA A 840:

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



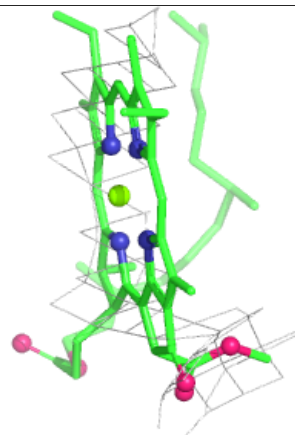
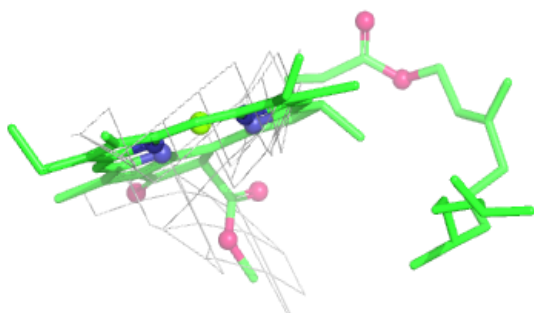
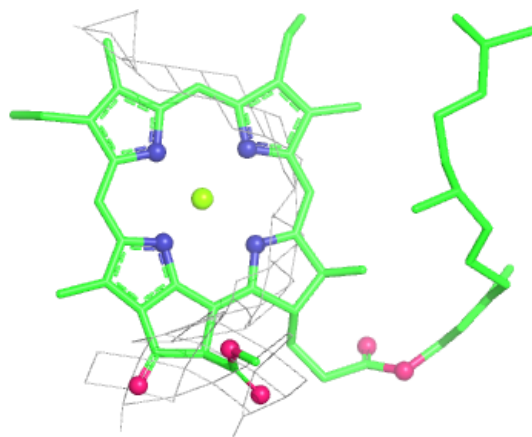
Electron density around CLA K 1401:

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



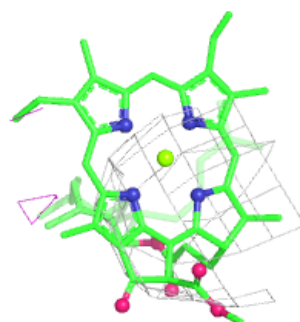
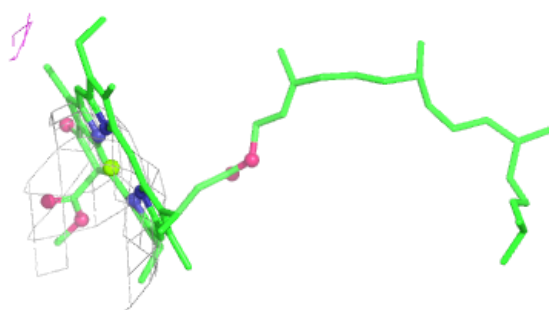
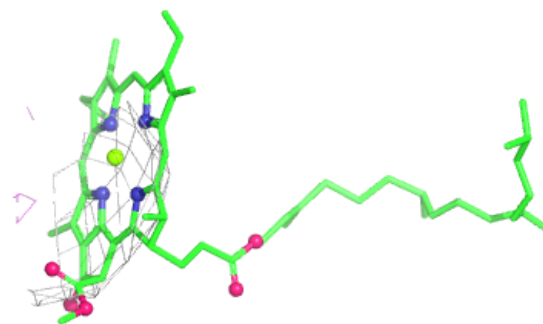
Electron density around CLA A 814:

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

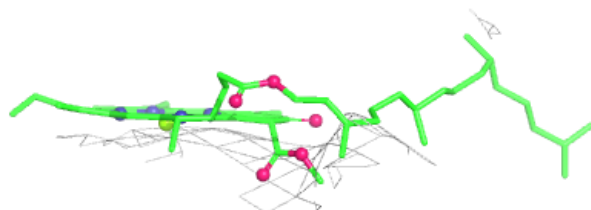
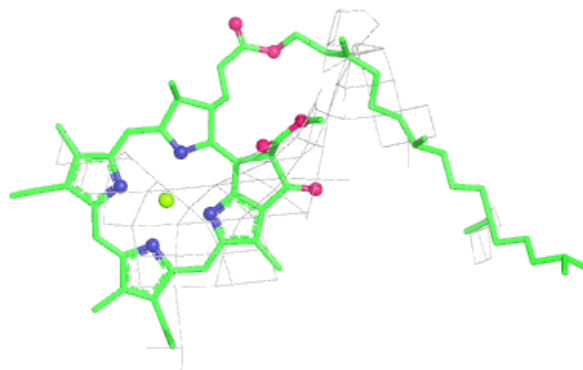


Electron density around CLA L 1003:

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

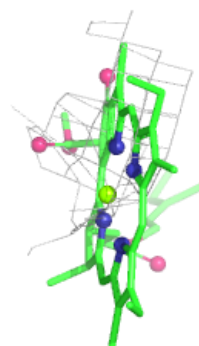
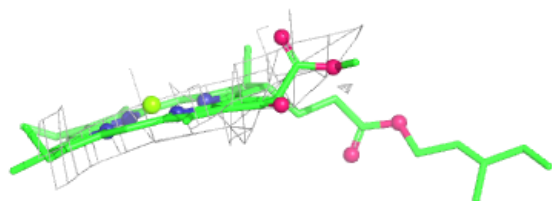
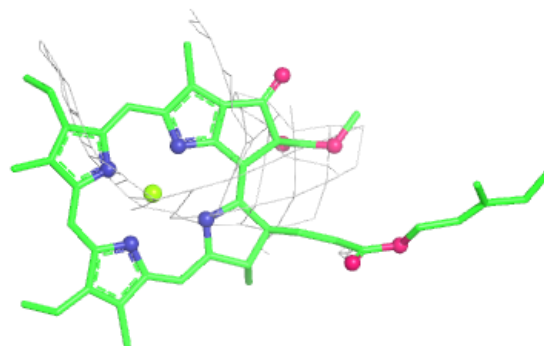
**Electron density around CLA L 1004:**

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

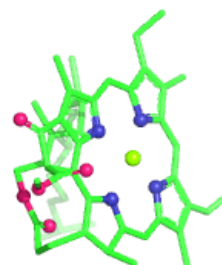
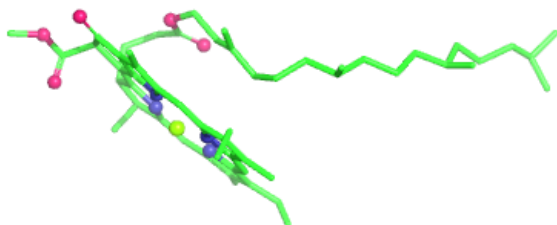
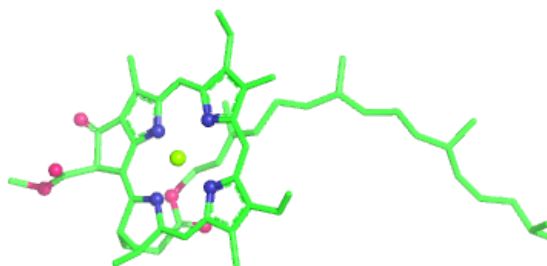


Electron density around CLA A 842:

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

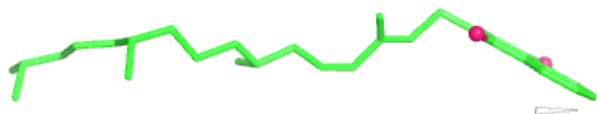
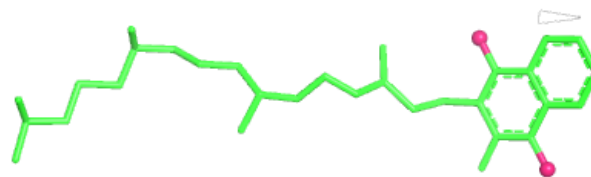
**Electron density around CLA A 843:**

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

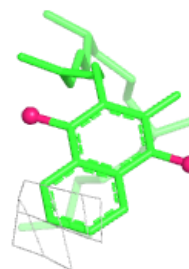
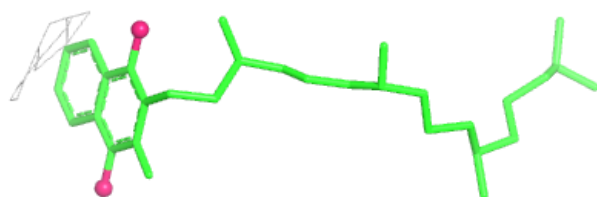
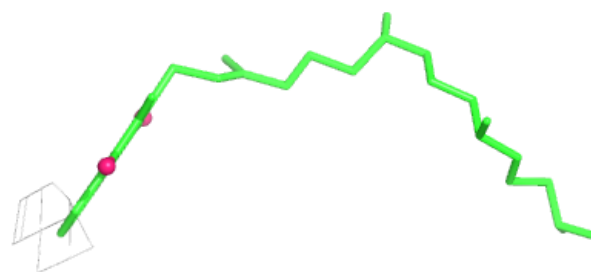


Electron density around PQN A 847:

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

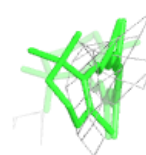
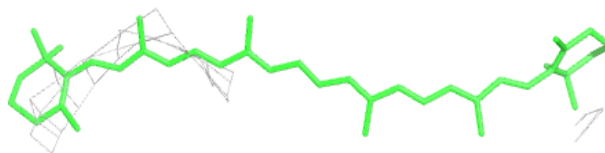
**Electron density around PQN B 842:**

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

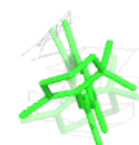
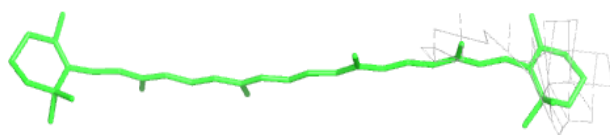
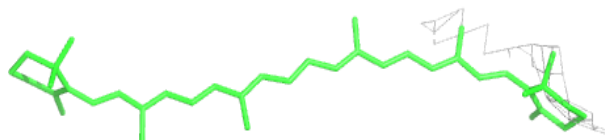


Electron density around BCR A 849:

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

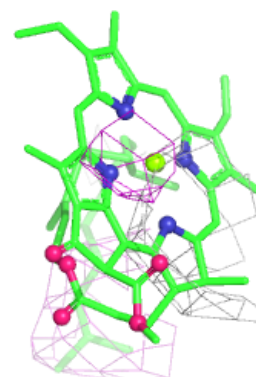
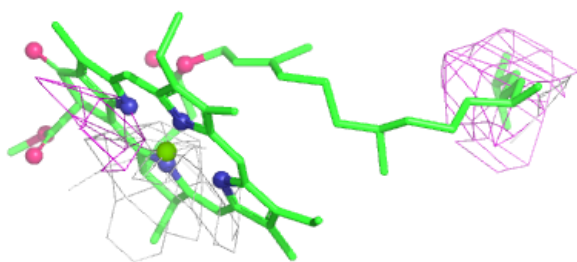
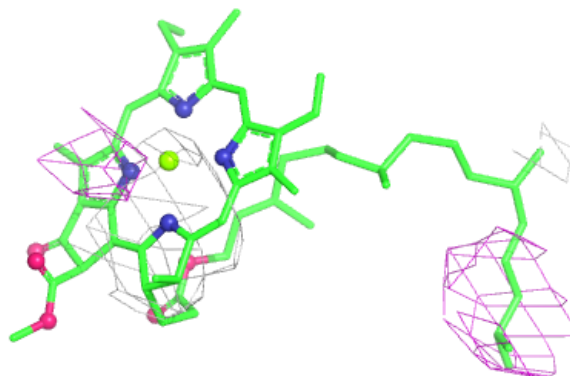
**Electron density around BCR A 850:**

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

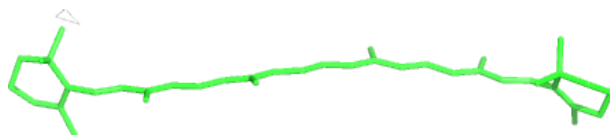
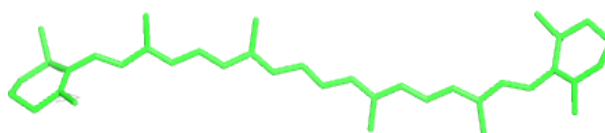


Electron density around CLA A 844:

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

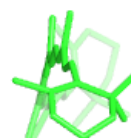
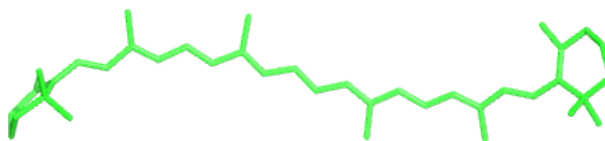
**Electron density around BCR A 852:**

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

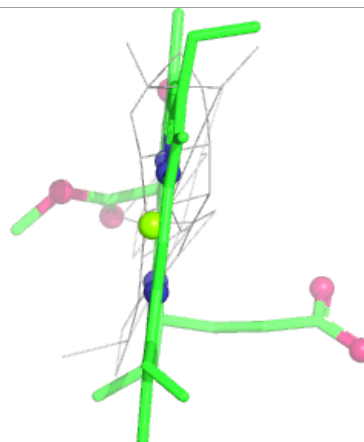
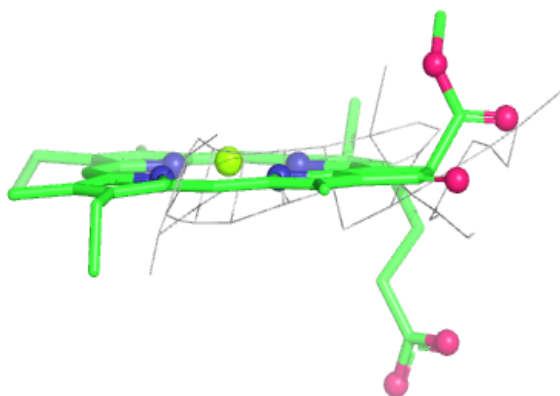
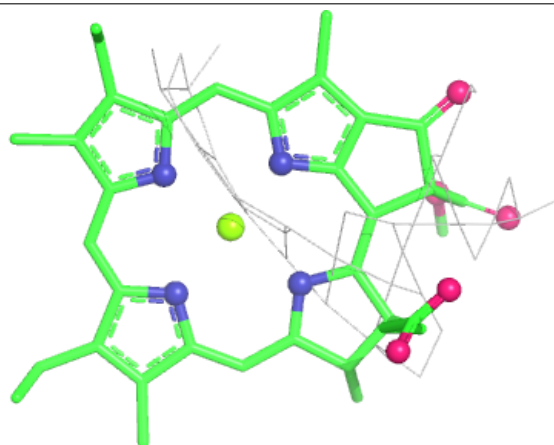


Electron density around BCR A 853:

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

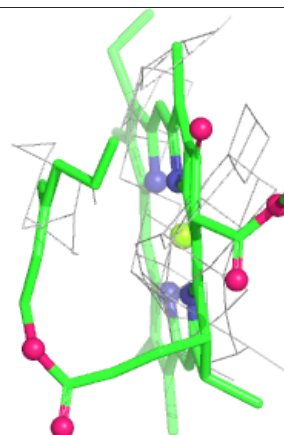
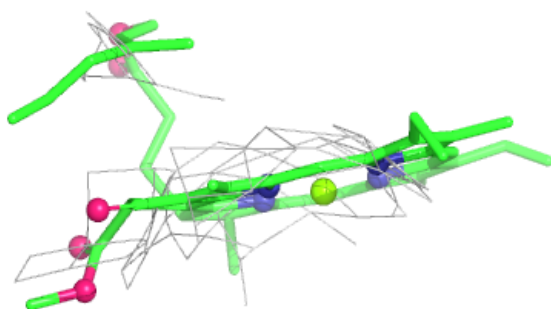
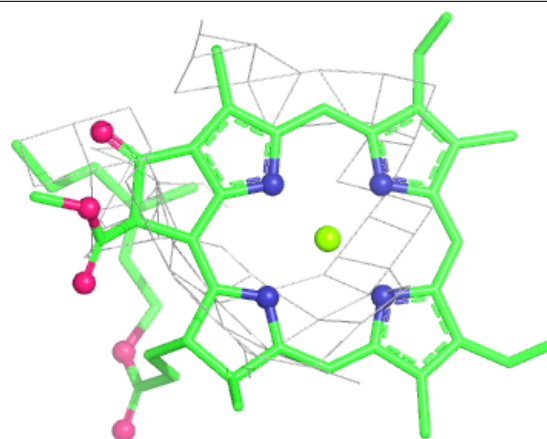
**Electron density around CLA A 816:**

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



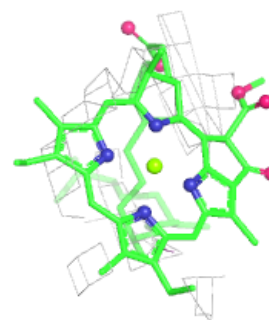
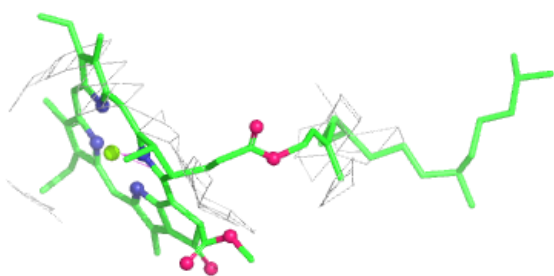
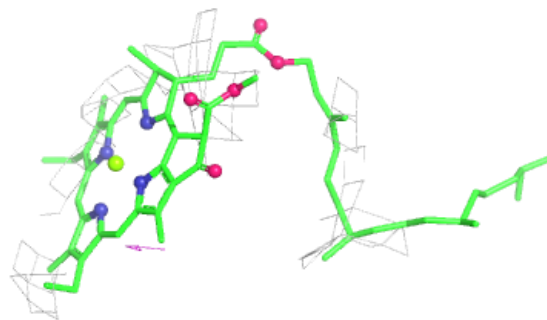
Electron density around CLA A 846:

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

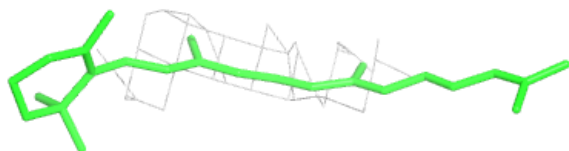
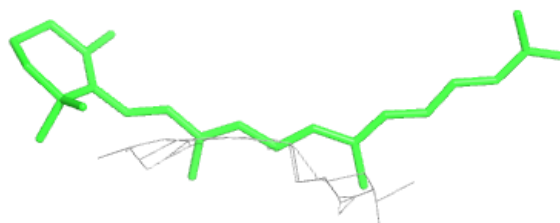


Electron density around CLA B 801:

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

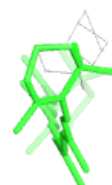
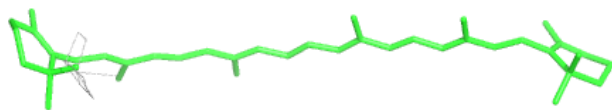
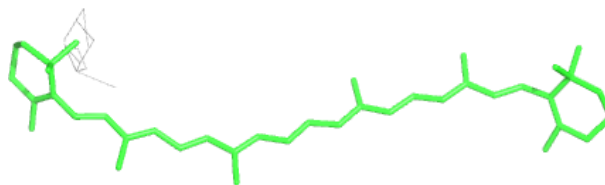
**Electron density around BCR B 846:**

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

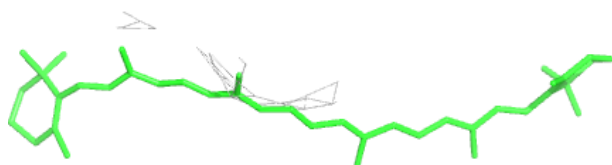


Electron density around BCR B 847:

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

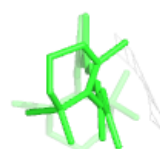
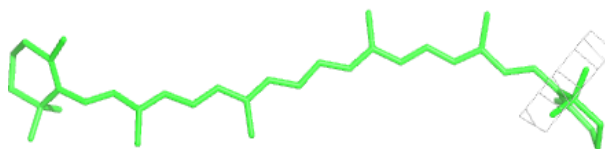
**Electron density around BCR B 848:**

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

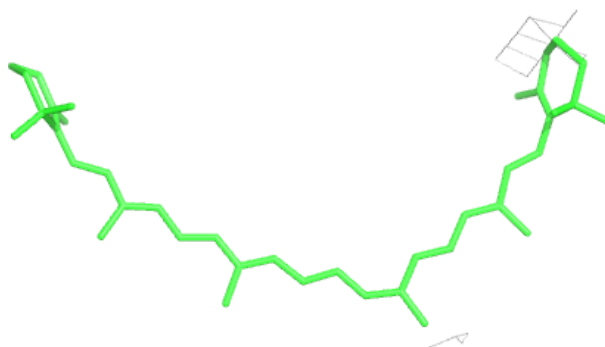


Electron density around BCR B 849:

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

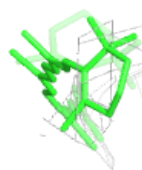
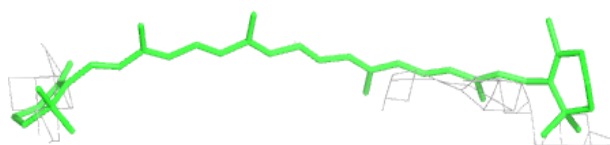
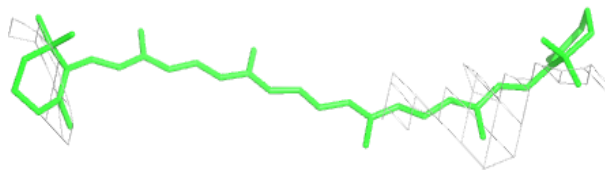
**Electron density around BCR F 1302:**

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

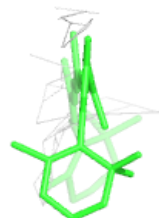
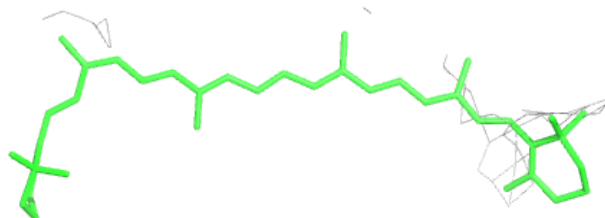


Electron density around BCR I 101:

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

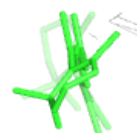
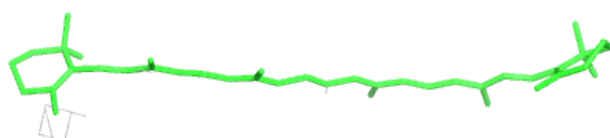
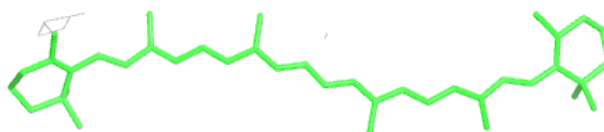
**Electron density around BCR I 102:**

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

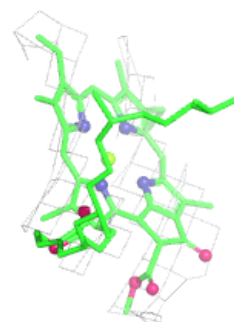
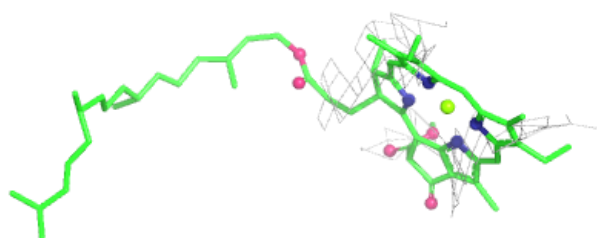
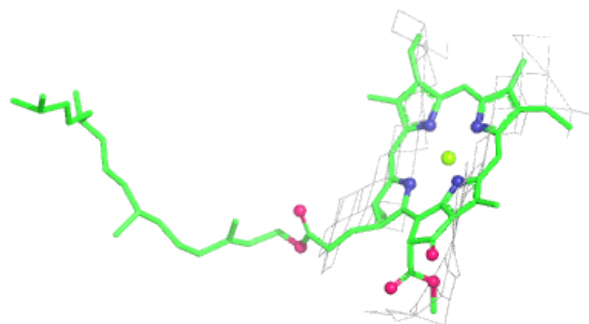


Electron density around BCR J 103:

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

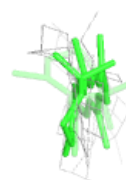
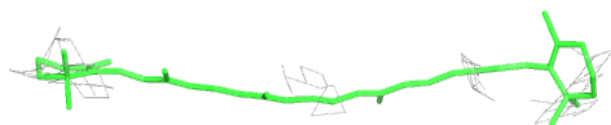
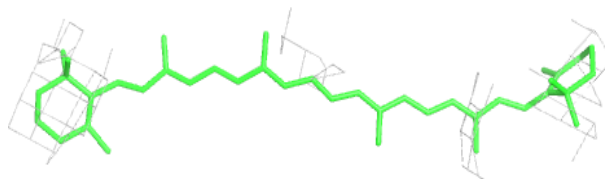
**Electron density around CLA B 802:**

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

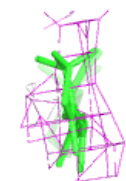
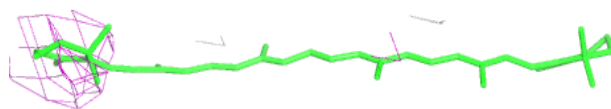
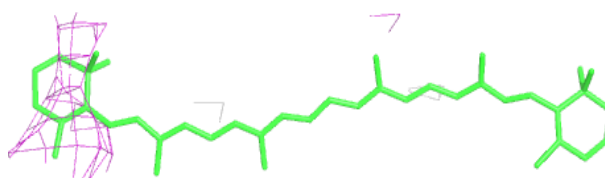


Electron density around BCR J 105:

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

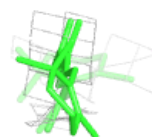
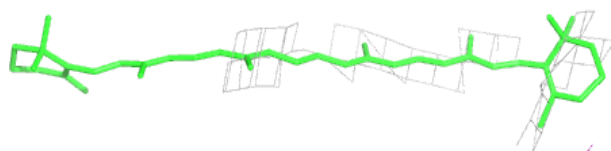
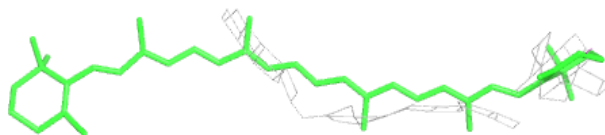
**Electron density around BCR L 1005:**

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

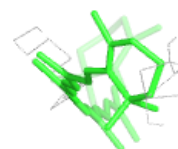
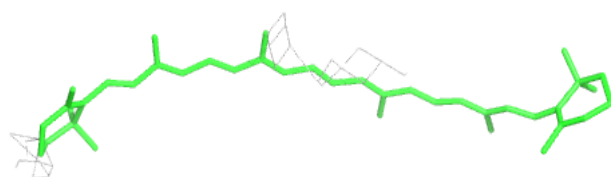
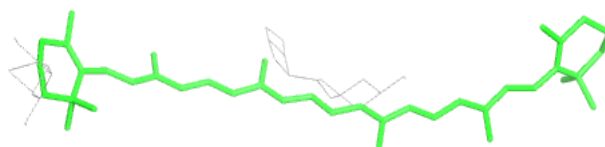


Electron density around BCR L 1006:

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

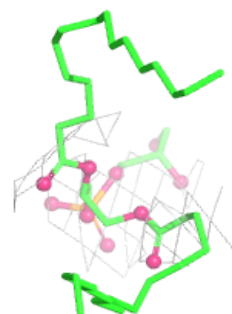
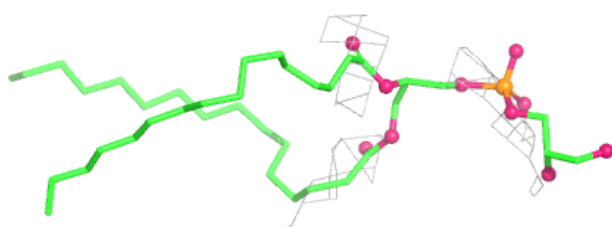
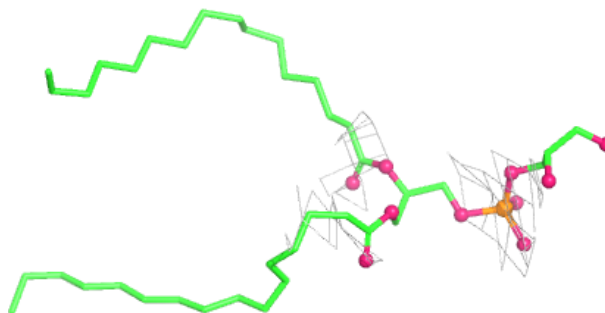
**Electron density around BCR M 1602:**

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

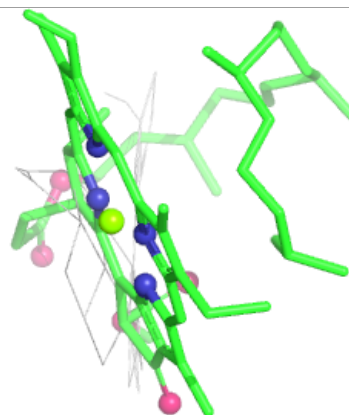
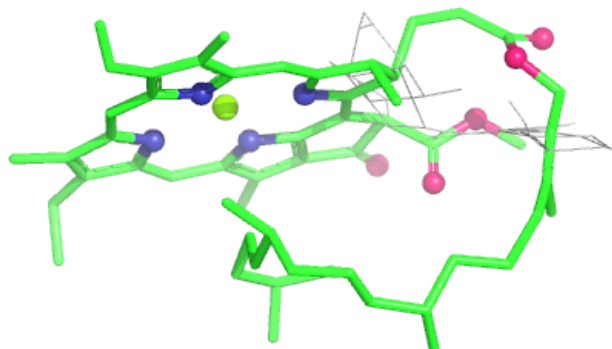
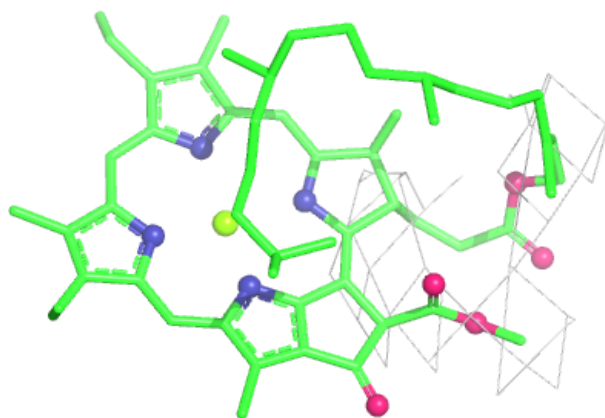


Electron density around LHG A 855:

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

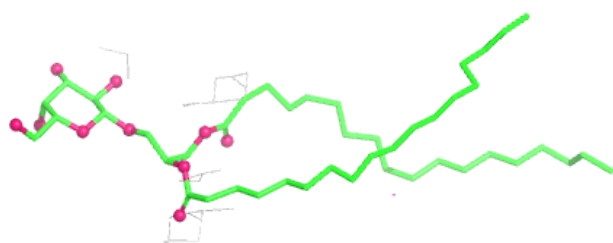
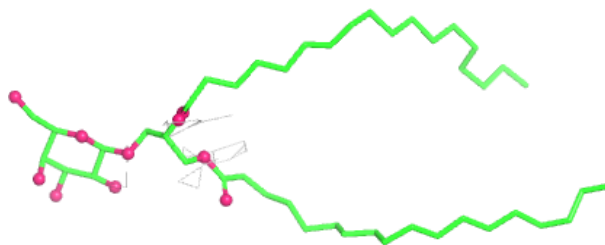
**Electron density around CLA A 807:**

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

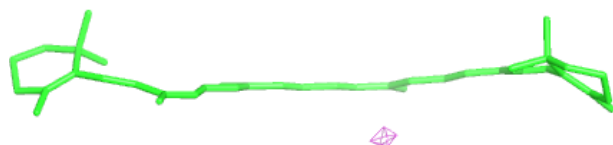
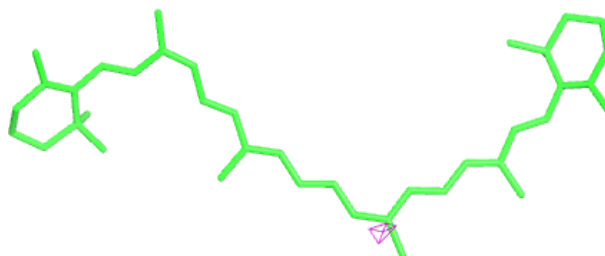


Electron density around LMG B 850:

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

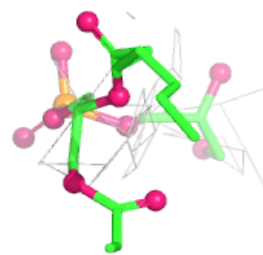
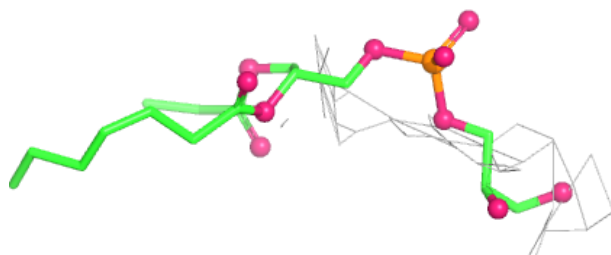
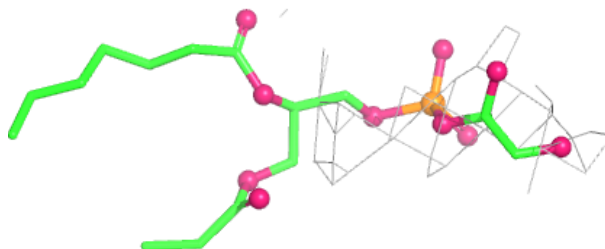
**Electron density around BCR A 854:**

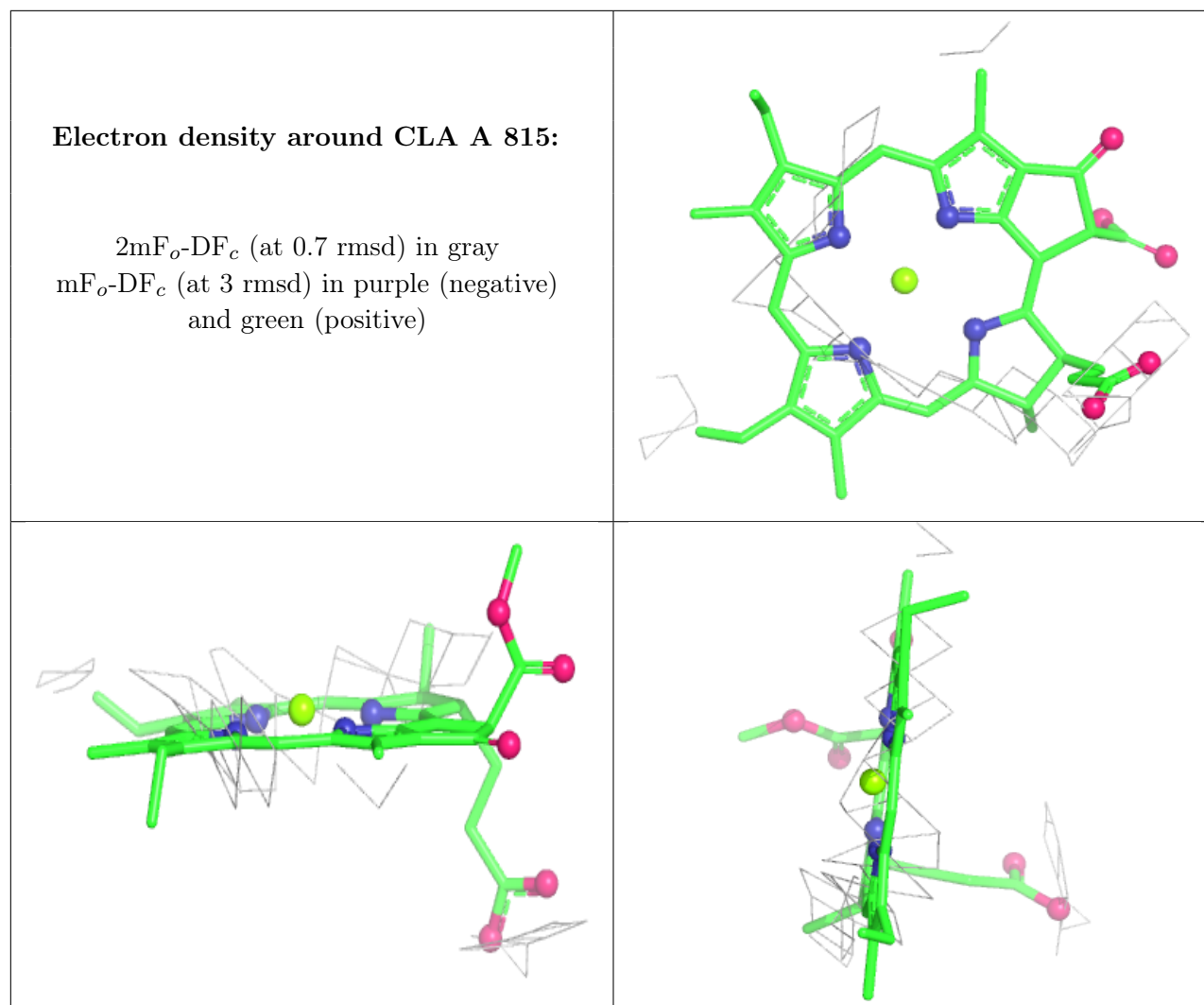
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.