Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 04:18 PM EDT

PDB ID	:	7M78 / pdb_00007m78
Title	:	Room Temperature XFEL Crystallography reveals asymmetry in the vicinity of the two phylloquinones in Photosystem I
Authors	:	Keable, S.M.; Simon, P.S.; Kolsch, A.; Kern, J.; Yachandra, V.K.; Zouni, A.; Yano, J.
Deposited on	:	2021-03-26
Resolution	:	3.00 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 ⓘ) were used in the production of this report:

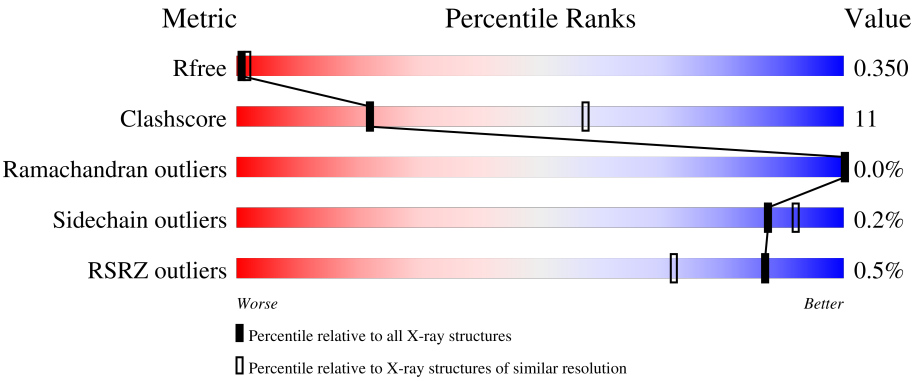
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.00 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.



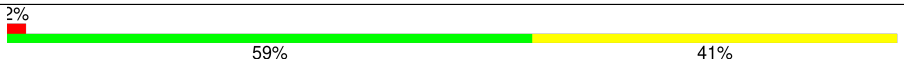
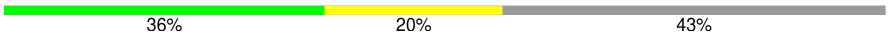
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 <=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	% 73% 25% .
2	B	740	75% 25%
3	C	80	75% 25%
4	D	138	78% 22%

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Mol	Chain	Length	Quality of chain
5	E	75	
6	F	164	
7	I	38	
8	J	41	
9	K	83	
10	L	154	
11	M	31	
12	X	35	

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 48797 atoms, of which 24384 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
			Total	C	H	N	O	S			
1	A	740	11422	3794	5638	988	976	26	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	739	11507	3876	5618	987	1005	21	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	80	1174	367	576	103	117	11	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	138	2152	682	1077	186	204	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
5	E	69	1067	342	528	93	104	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
6	F	141	2141	680	1076	184	197	4	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	I	38	Total	C	H	N	O	S	0	0	0
			607	208	306	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	H	N	O	S	0	0	0
			685	231	347	51	54	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
9	K	47	Total	C	H	N	O	S	0	0	0
			687	217	354	58	57	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
10	L	151	Total	C	H	N	O	S	0	0	0
			2244	735	1125	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

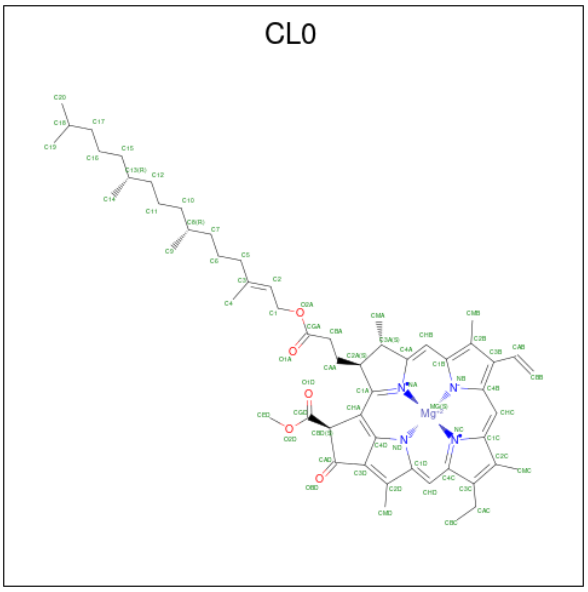
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
11	M	31	Total	C	H	N	O	S	0	0	0
			505	161	264	36	43	1			

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

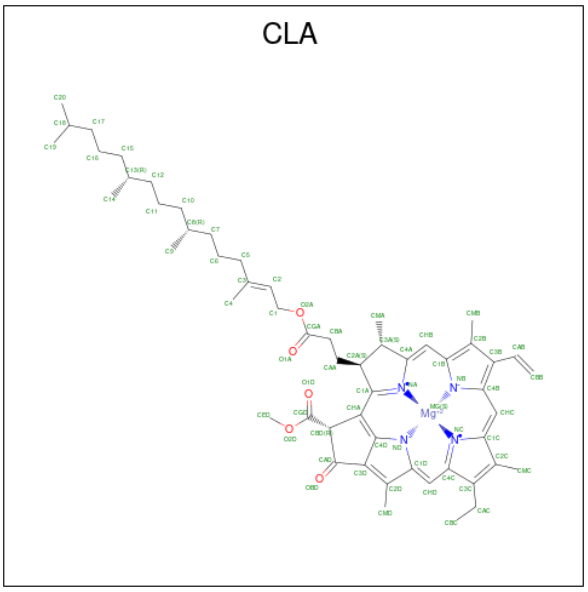
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	X	29	Total	C	H	N	O	0	0	0
			459	172	217	35	35			

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			88	39	39	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			72	35	29	1	4	3		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			88	39	39	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	A	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			89	40	39	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			82	37	35	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			95	42	43	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			104	45	49	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			82	37	35	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			104	45	49	1	4	5		

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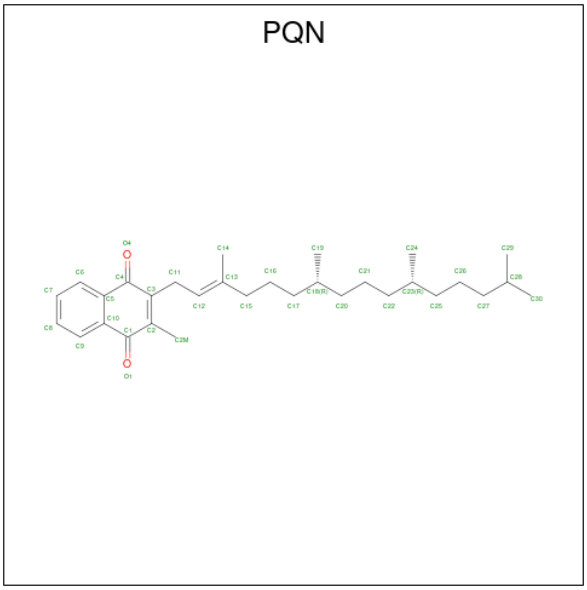
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			102	44	48	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			79	36	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
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			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			88	39	39	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			113	48	55	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			82	37	35	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	F	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		
14	F	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		

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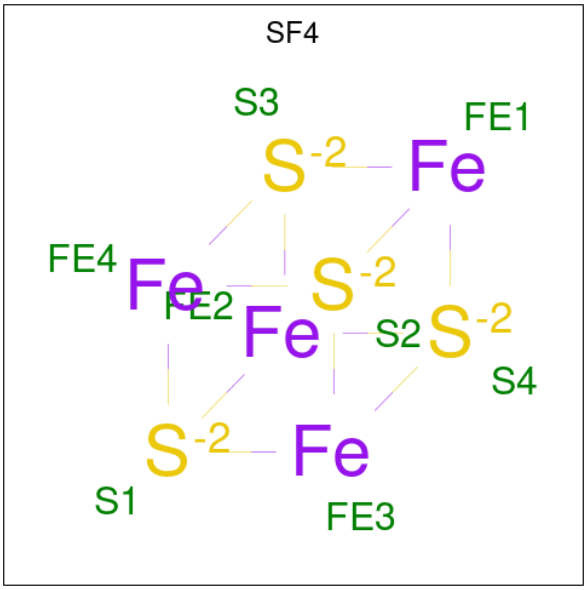
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			78	35	33	1	4	5		
14	J	1	Total	C	H	Mg	N	O	0	0
			62	31	25	1	4	1		
14	K	1	Total	C	H	Mg	N	O	0	0
			70	33	29	1	4	3		
14	K	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	M	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	X	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



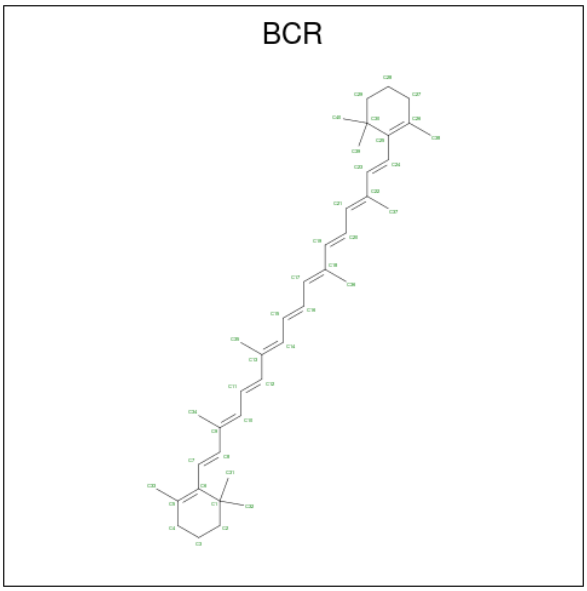
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	A	1	Total	C	H	O	0	0
			79	31	46	2		
15	B	1	Total	C	H	O	0	0
			79	31	46	2		

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



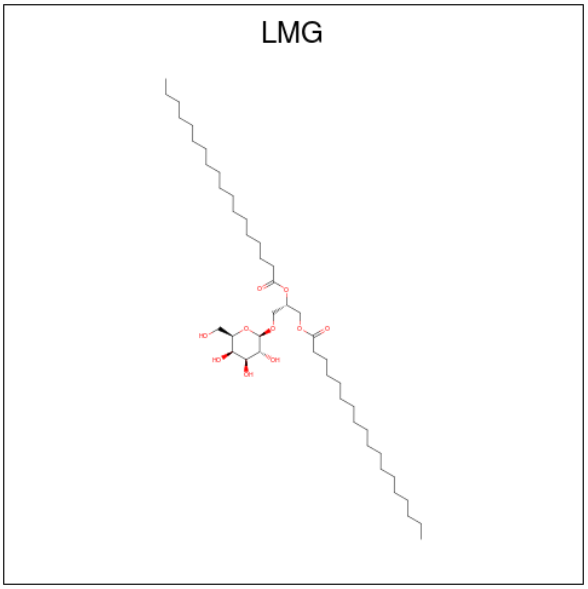
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Fe S 8 4 4	0	0
16	C	1	Total Fe S 8 4 4	0	0
16	C	1	Total Fe S 8 4 4	0	0

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



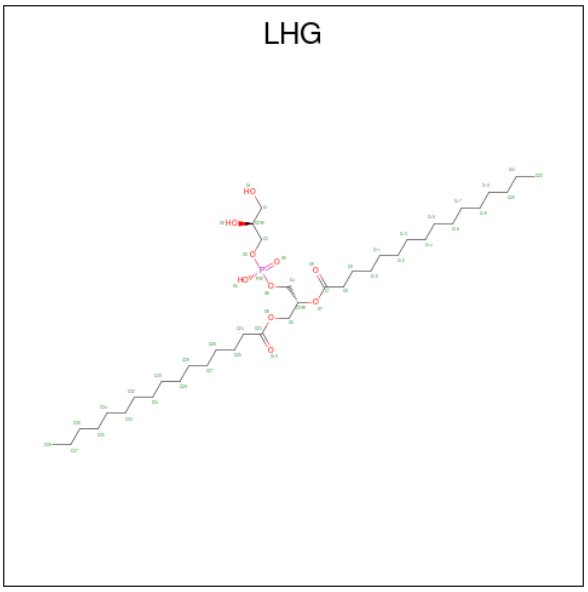
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C H 96 40 56	0	0
17	A	1	Total C H 96 40 56	0	0
17	A	1	Total C H 96 40 56	0	0
17	A	1	Total C H 96 40 56	0	0
17	A	1	Total C H 96 40 56	0	0
17	A	1	Total C H 96 40 56	0	0
17	B	1	Total C H 96 40 56	0	0
17	B	1	Total C H 96 40 56	0	0
17	B	1	Total C H 96 40 56	0	0
17	B	1	Total C H 96 40 56	0	0
17	B	1	Total C H 96 40 56	0	0
17	B	1	Total C H 96 40 56	0	0
17	B	1	Total C H 96 40 56	0	0
17	F	1	Total C H 96 40 56	0	0
17	I	1	Total C H 96 40 56	0	0
17	I	1	Total C H 96 40 56	0	0
17	J	1	Total C H 96 40 56	0	0
17	J	1	Total C H 96 40 56	0	0
17	J	1	Total C H 96 40 56	0	0
17	L	1	Total C H 96 40 56	0	0
17	L	1	Total C H 96 40 56	0	0
17	M	1	Total C H 96 40 56	0	0

- 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	A	1	Total	C	H	O	0	0
			118	38	70	10		
18	A	1	Total	C	H	O	0	0
			67	22	37	8		
18	B	1	Total	C	H	O	0	0
			141	45	86	10		
18	I	1	Total	C	H	O	0	0
			91	30	51	10		

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).

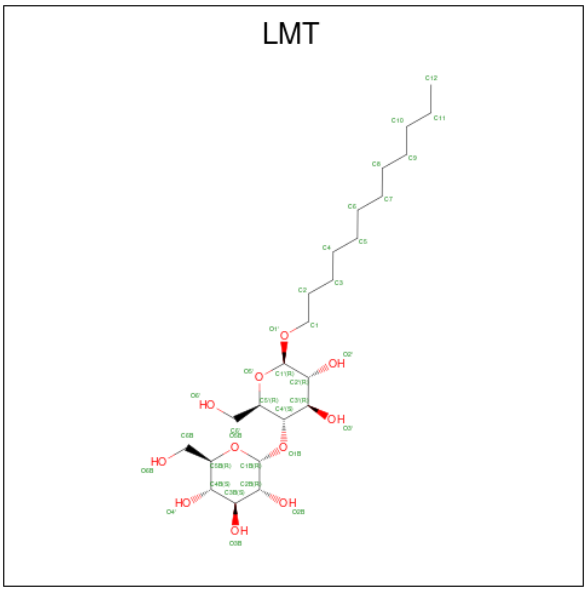


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
19	A	1	Total	C	H	O	P	0	0
			53	16	26	10	1		
19	B	1	Total	C	H	O	P	0	0
			43	12	20	10	1		
19	M	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 20 is CALCIUM ION (CCD ID: CA) (formula: Ca).

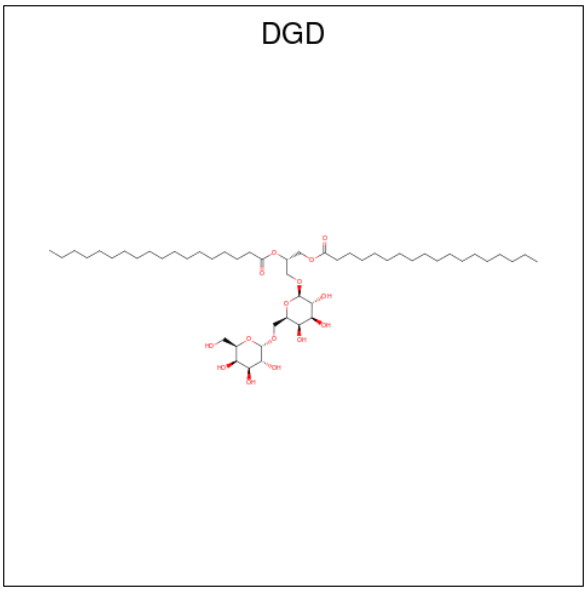
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	B	1	Total	Ca	0	0
			1	1		
20	L	1	Total	Ca	0	0
			1	1		

- Molecule 21 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	L	1	Total	C	H	O	0	0
			81	24	46	11		

- Molecule 22 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	L	1	Total	C	H	O	0	0
			162	51	96	15		

- Molecule 23 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	6	Total O 6 6	0	0
23	B	8	Total O 8 8	0	0
23	F	1	Total O 1 1	0	0
23	J	1	Total O 1 1	0	0
23	L	3	Total O 3 3	0	0
23	M	1	Total O 1 1	0	0

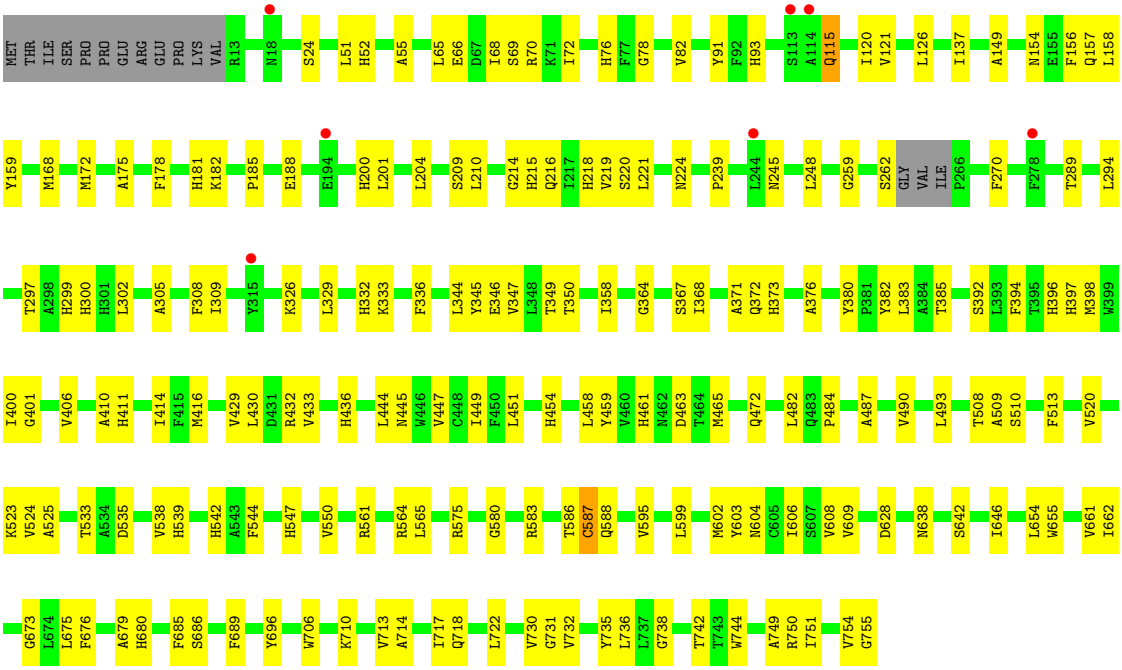
3 Residue-property plots (i)

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

Chain A:

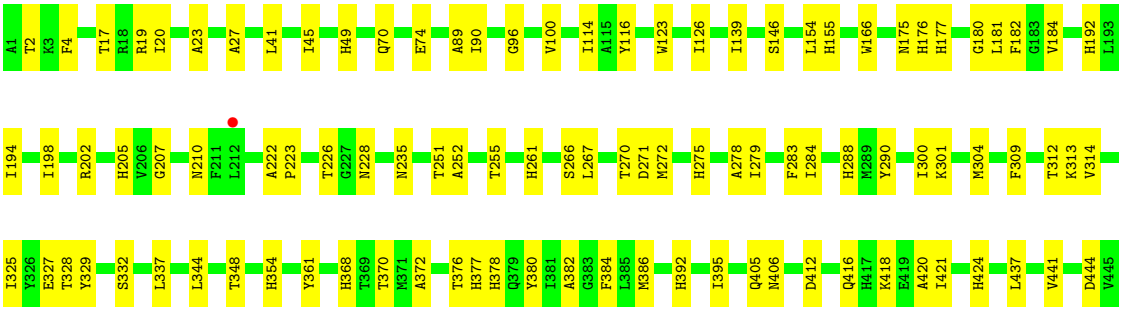


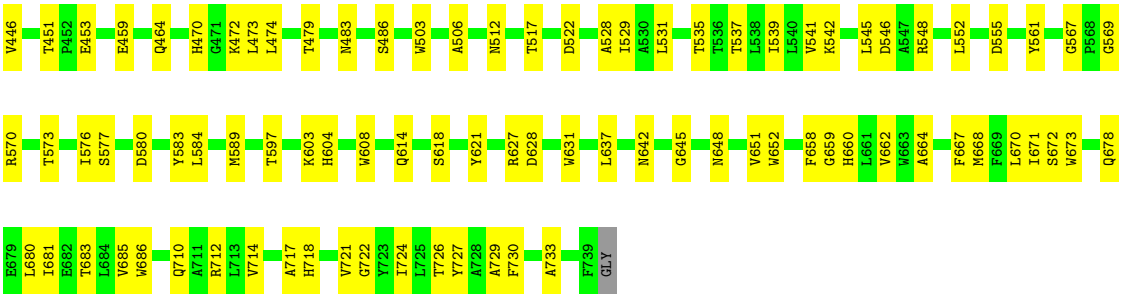


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

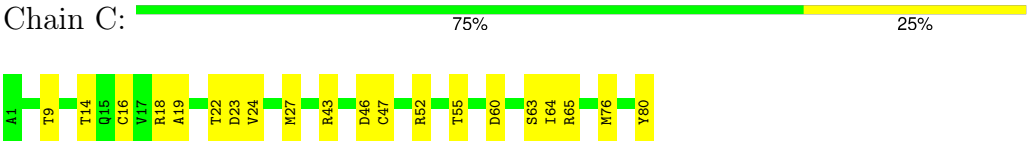
Chain B:



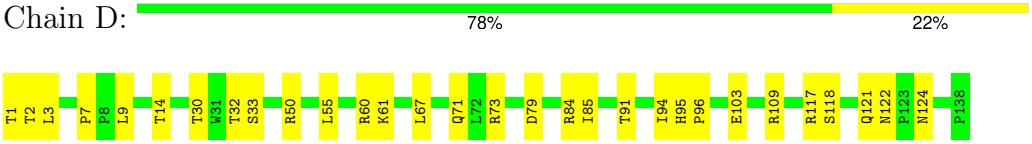




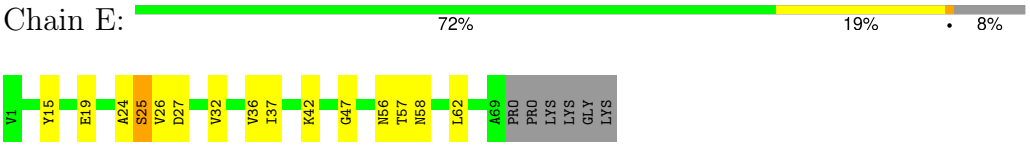
• Molecule 3: Photosystem I iron-sulfur center



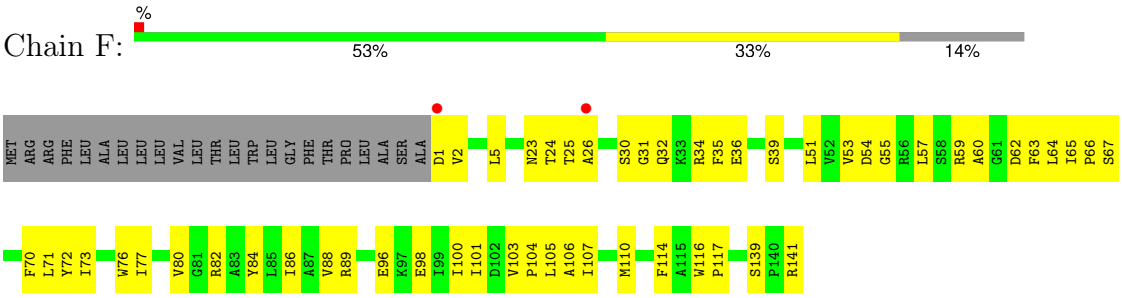
• Molecule 4: Photosystem I reaction center subunit II



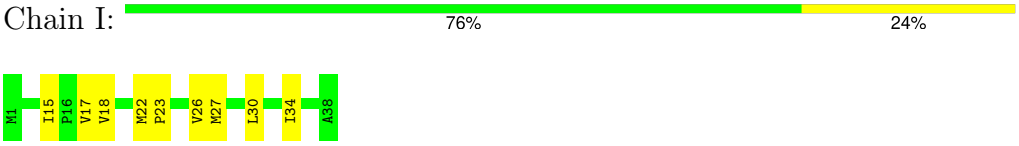
• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 6: Photosystem I reaction center subunit III

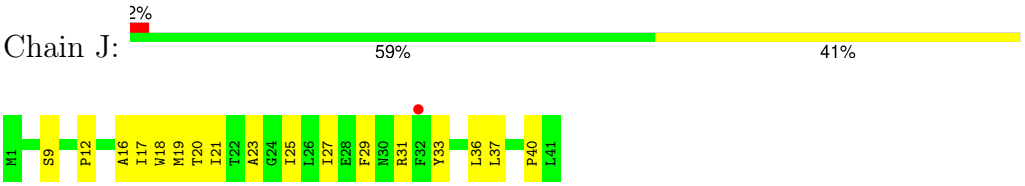


• Molecule 7: Photosystem I reaction center subunit VIII



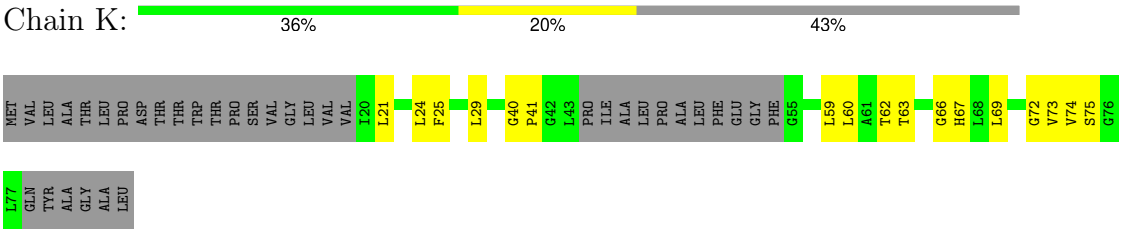
• Molecule 8: Photosystem I reaction center subunit IX

Chain J:



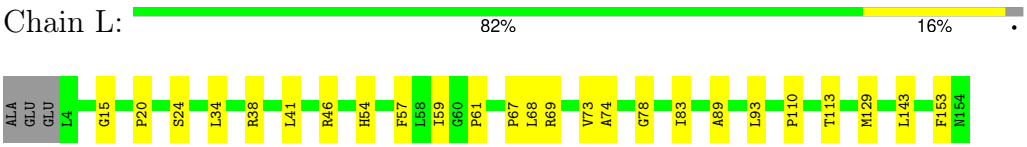
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:



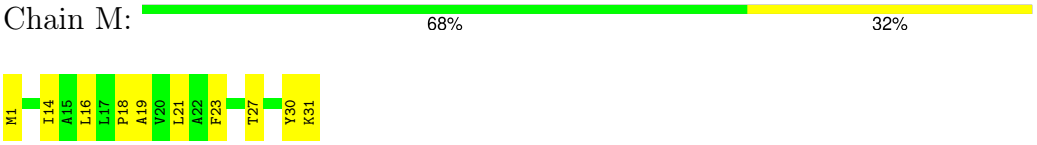
• Molecule 10: Photosystem I reaction center subunit XI

Chain L:



• Molecule 11: Photosystem I reaction center subunit XII

Chain M:



• Molecule 12: Photosystem I 4.8K protein

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	284.86Å 284.86Å 166.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.63 – 3.00 31.63 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.63-3.00) 94.3 (31.63-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.88 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.334 , 0.350 0.335 , 0.350	Depositor DCC
R_{free} test set	1995 reflections (1.30%)	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.13 , 0.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.146 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.73	EDS
Total number of atoms	48797	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PQN, CA, LMG, SF4, CLA, DGD, CL0, BCR, LMT, LHG

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	0.14	0/5983	0.33	0/8158
2	B	0.14	0/6107	0.32	0/8345
3	C	0.12	0/608	0.30	0/824
4	D	0.13	0/1101	0.33	0/1492
5	E	0.12	0/551	0.34	0/750
6	F	0.14	0/1087	0.30	0/1476
7	I	0.17	0/312	0.44	0/425
8	J	0.17	0/350	0.30	0/477
9	K	0.13	0/337	0.35	0/454
10	L	0.15	0/1148	0.31	0/1558
11	M	0.19	0/244	0.36	0/332
12	X	0.14	0/251	0.29	0/342
All	All	0.14	0/18079	0.32	0/24633

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5638	5639	157	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5889	5618	5649	150	0
3	C	598	576	580	16	0
4	D	1075	1077	1077	20	0
5	E	539	528	528	11	0
6	F	1065	1076	1077	41	0
7	I	301	306	306	8	0
8	J	338	347	347	23	0
9	K	333	354	354	16	0
10	L	1119	1125	1125	17	1
11	M	241	264	264	8	0
12	X	242	217	249	10	0
13	A	65	72	72	4	0
14	A	2577	2574	2574	77	0
14	B	2284	2232	2232	55	0
14	F	96	74	74	6	0
14	J	82	58	58	7	0
14	K	86	62	62	5	0
14	L	195	216	216	3	0
14	M	45	33	33	0	0
14	X	45	33	33	4	0
15	A	33	46	46	4	0
15	B	33	46	46	1	0
16	A	8	0	0	0	0
16	C	16	0	0	1	0
17	A	240	336	336	12	0
17	B	280	392	392	14	0
17	F	40	56	56	3	0
17	I	80	112	112	8	0
17	J	120	168	168	16	0
17	L	80	112	112	4	0
17	M	40	56	56	0	0
18	A	78	107	105	1	0
18	B	55	86	86	1	0
18	I	40	51	50	0	0
19	A	76	100	98	1	0
19	B	23	20	16	1	0
19	M	49	74	74	0	0
20	B	1	0	0	0	0
20	L	1	0	0	0	0
21	L	35	46	46	0	0
22	L	66	96	96	2	0
23	A	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	B	8	0	0	0	0
23	F	1	0	0	0	0
23	J	1	0	0	1	0
23	L	3	0	0	1	2
23	M	1	0	0	0	0
All	All	24413	24384	24444	524	2

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 11.

All (524) 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)
10:L:153:PHE:O	23:L:302:HOH:O	1.68	1.10
2:B:583:TYR:OH	2:B:670:LEU:HD22	1.60	1.00
2:B:506:ALA:O	2:B:512:ASN:ND2	1.97	0.98
1:A:336:PHE:O	1:A:432:ARG:NH1	2.10	0.85
6:F:1:ASP:N	6:F:5:LEU:O	2.12	0.83
1:A:376:ALA:O	1:A:510:SER:OG	1.99	0.81
4:D:32:THR:OG1	4:D:79:ASP:OD2	1.97	0.80
5:E:26:VAL:HG22	5:E:36:VAL:HG12	1.61	0.80
2:B:614:GLN:O	2:B:618:SER:OG	2.00	0.80
9:K:72:GLY:O	9:K:75:SER:OG	1.98	0.79
2:B:483:ASN:OD1	2:B:486:SER:N	2.15	0.79
22:L:207:DGD:O5D	22:L:207:DGD:O4D	1.98	0.77
4:D:33:SER:OG	4:D:50:ARG:O	2.02	0.77
2:B:479:THR:HG23	12:X:35:LYS:HG2	1.67	0.76
2:B:446:VAL:O	2:B:451:THR:OG1	2.04	0.76
14:B:832:CLA:H142	17:F:203:BCR:H333	1.68	0.76
14:A:805:CLA:H143	14:A:810:CLA:H143	1.68	0.75
1:A:385:THR:O	1:A:523:LYS:NZ	2.17	0.75
6:F:105:LEU:HD12	6:F:106:ALA:N	2.02	0.75
2:B:304:MET:HE2	2:B:325:ILE:HD11	1.69	0.74
1:A:68:ILE:HD12	1:A:69:SER:N	2.03	0.74
6:F:35:PHE:O	6:F:39:SER:OG	2.06	0.73
2:B:175:ASN:ND2	2:B:290:TYR:O	2.22	0.73
4:D:2:THR:HG22	4:D:3:LEU:H	1.54	0.72
14:B:840:CLA:H193	17:I:101:BCR:H362	1.72	0.72
22:L:207:DGD:O3D	22:L:207:DGD:O1G	2.08	0.71
5:E:27:ASP:OD2	5:E:32:VAL:HG21	1.89	0.71
2:B:710:GLN:O	2:B:714:VAL:HG23	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:GLN:OE1	2:B:406:ASN:ND2	2.24	0.70
4:D:118:SER:OG	4:D:121:GLN:OE1	2.09	0.70
1:A:70:ARG:NH1	1:A:185:PRO:O	2.25	0.69
1:A:149:ALA:O	1:A:220:SER:OG	2.10	0.69
1:A:750:ARG:O	1:A:754:VAL:HG22	1.92	0.69
2:B:255:THR:HG1	2:B:270:THR:HG1	1.13	0.69
9:K:29:LEU:HB3	9:K:62:THR:HG21	1.75	0.68
1:A:215:HIS:O	1:A:219:VAL:N	2.27	0.67
2:B:416:GLN:O	6:F:141:ARG:NH2	2.28	0.67
4:D:117:ARG:NH2	4:D:122:ASN:OD1	2.28	0.67
1:A:416:MET:HE1	1:A:430:LEU:HD11	1.75	0.67
2:B:580:ASP:OD1	2:B:712:ARG:NH1	2.28	0.67
1:A:297:THR:HG23	14:A:820:CLA:HMA3	1.77	0.66
6:F:139:SER:O	6:F:141:ARG:NH1	2.28	0.66
1:A:580:GLY:O	1:A:586:THR:OG1	2.08	0.66
17:A:852:BCR:H362	14:A:857:CLA:C4	2.26	0.66
2:B:552:LEU:O	2:B:570:ARG:NH2	2.30	0.65
14:B:803:CLA:HBB1	14:B:803:CLA:HMB3	1.78	0.65
1:A:454:HIS:O	1:A:458:LEU:HD13	1.96	0.65
2:B:567:GLY:O	2:B:573:THR:HG22	1.96	0.65
1:A:655:TRP:O	2:B:631:TRP:NE1	2.29	0.65
2:B:70:GLN:OE1	2:B:89:ALA:N	2.29	0.65
18:A:856:LMG:O4	18:A:856:LMG:O5	2.03	0.65
2:B:205:HIS:O	2:B:210:ASN:ND2	2.28	0.65
2:B:309:PHE:O	2:B:312:THR:HG22	1.96	0.65
1:A:661:VAL:HG22	1:A:749:ALA:HB3	1.79	0.64
14:B:825:CLA:HMA1	17:B:846:BCR:H14C	1.80	0.64
12:X:23:ASN:HD21	14:X:1701:CLA:CHA	2.11	0.64
1:A:65:LEU:HD12	1:A:68:ILE:HD11	1.79	0.64
2:B:418:LYS:NZ	2:B:546:ASP:OD1	2.21	0.64
2:B:181:LEU:HD21	14:B:813:CLA:H43	1.80	0.63
1:A:115:GLN:HE22	14:A:809:CLA:C1B	2.11	0.63
1:A:564:ARG:NH2	4:D:14:THR:O	2.31	0.63
9:K:25:PHE:O	9:K:29:LEU:HD23	1.98	0.63
2:B:284:ILE:HD13	17:B:843:BCR:H352	1.81	0.62
12:X:23:ASN:ND2	14:X:1701:CLA:O1D	2.32	0.62
1:A:154:ASN:OD1	1:A:157:GLN:NE2	2.32	0.62
9:K:60:LEU:O	9:K:63:THR:HG22	1.99	0.62
2:B:376:THR:HG22	2:B:597:THR:CG2	2.30	0.61
2:B:453:GLU:OE2	6:F:34:ARG:NH2	2.33	0.61
8:J:40:PRO:HD2	17:J:105:BCR:H382	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:392:HIS:HA	2:B:395:ILE:HD12	1.80	0.61
2:B:552:LEU:HD23	2:B:576:ILE:HD12	1.83	0.61
3:C:22:THR:OG1	3:C:24:VAL:HG23	2.00	0.61
8:J:37:LEU:HD23	8:J:37:LEU:O	2.00	0.61
19:B:850:LHG:O3	12:X:12:ARG:NH2	2.34	0.61
2:B:686:TRP:NE1	10:L:15:GLY:O	2.34	0.61
5:E:62:LEU:HD23	5:E:62:LEU:H	1.65	0.60
2:B:255:THR:OG1	2:B:271:ASP:OD1	2.19	0.60
3:C:9:THR:HG1	3:C:63:SER:HG	0.61	0.60
1:A:120:ILE:HG23	1:A:121:VAL:HG22	1.83	0.60
2:B:470:HIS:O	2:B:503:TRP:NE1	2.32	0.60
1:A:463:ASP:OD2	1:A:646:ILE:N	2.33	0.60
1:A:679:ALA:HB1	1:A:738:GLY:O	2.02	0.60
1:A:714:ALA:O	6:F:89:ARG:NH1	2.35	0.60
3:C:27:MET:O	4:D:109:ARG:NH1	2.33	0.60
1:A:333:LYS:O	14:A:844:CLA:HBC3	2.01	0.60
14:A:804:CLA:HED3	15:A:845:PQN:H262	1.84	0.60
1:A:524:VAL:HG12	1:A:525:ALA:N	2.17	0.59
12:X:24:PHE:CD1	14:X:1701:CLA:HMA1	2.37	0.59
6:F:53:VAL:HG13	6:F:63:PHE:CD2	2.37	0.59
14:A:802:CLA:OBD	14:B:802:CLA:HMB2	2.02	0.59
6:F:103:VAL:HG22	6:F:107:ILE:HD12	1.85	0.59
2:B:548:ARG:NH2	4:D:124:ASN:OD1	2.35	0.59
1:A:565:LEU:O	4:D:60:ARG:NH2	2.36	0.59
1:A:66:GLU:OE1	1:A:70:ARG:NH2	2.35	0.59
2:B:472:LYS:NZ	2:B:517:THR:OG1	2.36	0.58
2:B:235:ASN:O	2:B:251:THR:N	2.30	0.58
10:L:68:LEU:HD23	10:L:73:VAL:HG23	1.84	0.58
14:A:842:CLA:H142	17:B:847:BCR:C16	2.34	0.58
1:A:168:MET:O	1:A:172:MET:HG2	2.04	0.58
14:A:822:CLA:H61	17:A:850:BCR:H352	1.86	0.58
2:B:90:ILE:HD11	14:B:809:CLA:HMD1	1.86	0.58
2:B:146:SER:HB3	11:M:21:LEU:HD12	1.85	0.58
14:A:829:CLA:HBB1	14:A:829:CLA:HMB3	1.86	0.58
1:A:410:ALA:HB2	1:A:595:VAL:HG11	1.86	0.57
10:L:61:PRO:HA	14:L:206:CLA:HMB2	1.86	0.57
14:A:827:CLA:HBB1	14:A:827:CLA:HMB3	1.85	0.57
2:B:555:ASP:OD1	3:C:65:ARG:NH1	2.37	0.57
3:C:60:ASP:HB2	5:E:58:ASN:ND2	2.20	0.57
2:B:459:GLU:OE1	2:B:464:GLN:NE2	2.34	0.57
2:B:528:ALA:CB	14:B:802:CLA:H192	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:36:LEU:HD12	17:J:105:BCR:C21	2.34	0.57
14:J:101:CLA:HMD1	17:J:104:BCR:H331	1.84	0.57
14:A:827:CLA:HAB	17:A:851:BCR:H311	1.85	0.57
14:L:204:CLA:H202	14:L:204:CLA:O2A	2.05	0.56
2:B:446:VAL:HG22	2:B:451:THR:OG1	2.05	0.56
1:A:735:TYR:OH	13:A:801:CL0:O1A	2.16	0.56
4:D:3:LEU:HD21	4:D:91:THR:HG21	1.87	0.56
17:B:846:BCR:H331	17:B:846:BCR:C8	2.35	0.56
2:B:479:THR:HG21	12:X:29:TYR:O	2.05	0.56
1:A:305:ALA:O	1:A:309:ILE:HD12	2.06	0.56
1:A:346:GLU:O	1:A:350:THR:OG1	2.12	0.56
8:J:31:ARG:NH2	14:J:101:CLA:O1D	2.34	0.56
1:A:373:HIS:CD2	14:A:828:CLA:NC	2.74	0.55
9:K:69:LEU:O	9:K:73:VAL:HG23	2.07	0.55
14:B:827:CLA:HBB1	14:B:827:CLA:HMB1	1.89	0.55
1:A:710:LYS:NZ	14:B:831:CLA:HED1	2.22	0.55
6:F:73:ILE:O	6:F:77:ILE:HG12	2.07	0.54
2:B:479:THR:HA	12:X:35:LYS:HG2	1.90	0.54
2:B:361:TYR:OH	14:B:828:CLA:OBD	2.22	0.54
9:K:59:LEU:HD12	9:K:59:LEU:O	2.08	0.54
1:A:270:PHE:HE1	14:K:101:CLA:HBC2	1.73	0.54
1:A:368:ILE:HG23	1:A:398:MET:HE3	1.90	0.54
4:D:7:PRO:O	4:D:50:ARG:NH1	2.40	0.54
1:A:445:ASN:ND2	14:A:843:CLA:OBD	2.40	0.54
14:B:812:CLA:HBB1	14:B:820:CLA:HBC2	1.89	0.54
6:F:80:VAL:HG11	14:F:202:CLA:HMD2	1.90	0.54
7:I:22:MET:N	7:I:23:PRO:HD2	2.23	0.53
1:A:524:VAL:HG12	1:A:525:ALA:H	1.74	0.53
2:B:202:ARG:NH2	2:B:252:ALA:O	2.38	0.53
1:A:371:ALA:HB1	1:A:394:PHE:HA	1.89	0.53
2:B:41:LEU:O	2:B:45:ILE:HG12	2.09	0.53
2:B:166:TRP:NE1	14:B:812:CLA:OBD	2.36	0.53
14:B:840:CLA:H193	17:I:101:BCR:C36	2.38	0.53
14:B:809:CLA:H43	17:I:101:BCR:H342	1.90	0.53
1:A:604:ASN:O	1:A:608:VAL:HG23	2.09	0.53
2:B:627:ARG:NH2	2:B:628:ASP:OD2	2.40	0.53
2:B:139:ILE:HD12	11:M:14:ILE:HD13	1.91	0.52
1:A:411:HIS:HE1	14:A:831:CLA:NA	2.07	0.52
1:A:588:GLN:NE2	2:B:671:ILE:O	2.34	0.52
2:B:354:HIS:CD2	14:B:826:CLA:NC	2.77	0.52
1:A:329:LEU:HD12	1:A:345:TYR:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:384:PHE:CD1	2:B:589:MET:HE1	2.45	0.52
2:B:664:ALA:HB3	14:B:803:CLA:HBB2	1.91	0.52
2:B:74:GLU:OE2	11:M:1:MET:N	2.34	0.52
6:F:72:TYR:OH	6:F:114:PHE:O	2.27	0.52
1:A:216:GLN:O	1:A:221:LEU:N	2.37	0.52
14:A:829:CLA:H193	17:J:103:BCR:C14	2.40	0.52
2:B:637:LEU:HD22	2:B:730:PHE:HA	1.92	0.52
5:E:56:ASN:OD1	5:E:57:THR:HG23	2.10	0.51
2:B:529:ILE:HG21	14:B:837:CLA:CBB	2.40	0.51
2:B:678:GLN:NE2	3:C:80:TYR:OH	2.44	0.51
1:A:680:HIS:CE1	1:A:742:THR:HG21	2.46	0.51
2:B:569:GLY:HA3	3:C:55:THR:HG22	1.92	0.51
2:B:642:ASN:OD1	2:B:645:GLY:N	2.42	0.51
6:F:76:TRP:NE1	14:F:202:CLA:OBD	2.44	0.51
2:B:724:ILE:HG23	14:B:827:CLA:HAB	1.92	0.51
6:F:54:ASP:OD1	6:F:55:GLY:N	2.44	0.51
3:C:46:ASP:OD2	4:D:84:ARG:NH2	2.43	0.51
1:A:178:PHE:O	1:A:182:LYS:O	2.28	0.50
6:F:84:TYR:CE1	14:F:201:CLA:HED1	2.46	0.50
4:D:61:LYS:HE3	4:D:94:ILE:HD12	1.91	0.50
1:A:326:LYS:NZ	1:A:346:GLU:OE2	2.44	0.50
14:A:825:CLA:HBB1	14:A:825:CLA:HMB3	1.93	0.50
8:J:17:ILE:HD12	8:J:18:TRP:N	2.25	0.50
6:F:32:GLN:O	6:F:36:GLU:HG3	2.10	0.50
2:B:275:HIS:HE1	14:B:817:CLA:ND	2.08	0.50
6:F:64:LEU:O	6:F:67:SER:OG	2.25	0.50
1:A:372:GLN:HB3	14:A:827:CLA:HED1	1.93	0.50
17:A:848:BCR:H362	17:A:849:BCR:HC8	1.93	0.50
6:F:23:ASN:OD1	6:F:31:GLY:N	2.39	0.50
6:F:59:ARG:NH2	6:F:62:ASP:OD1	2.44	0.50
17:L:201:BCR:H331	17:L:201:BCR:C8	2.41	0.50
1:A:482:LEU:H	1:A:533:THR:HG22	1.77	0.50
9:K:24:LEU:HD13	9:K:69:LEU:HB3	1.93	0.50
2:B:180:GLY:O	2:B:184:VAL:HG22	2.12	0.50
2:B:421:ILE:HG23	14:B:839:CLA:HBB2	1.94	0.50
1:A:539:HIS:CE1	14:A:838:CLA:NC	2.80	0.49
2:B:116:TYR:HA	2:B:370:THR:HG22	1.93	0.49
9:K:59:LEU:HD12	9:K:59:LEU:C	2.37	0.49
2:B:474:LEU:H	2:B:474:LEU:HD22	1.78	0.49
6:F:51:LEU:HD21	8:J:37:LEU:HD21	1.94	0.49
8:J:29:PHE:O	8:J:33:TYR:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1:THR:OG1	4:D:2:THR:N	2.44	0.49
12:X:23:ASN:HD21	14:X:1701:CLA:C1A	2.25	0.49
4:D:30:THR:HG22	4:D:55:LEU:HD13	1.94	0.49
12:X:28:ALA:HA	12:X:33:ILE:HD12	1.94	0.49
1:A:472:GLN:OE1	1:A:472:GLN:N	2.40	0.49
14:B:830:CLA:H3A	14:B:831:CLA:OBD	2.13	0.49
1:A:24:SER:H	14:A:812:CLA:HMA1	1.78	0.49
1:A:259:GLY:N	1:A:262:SER:O	2.45	0.49
1:A:713:VAL:O	1:A:713:VAL:HG22	2.13	0.49
17:J:104:BCR:C8	17:J:104:BCR:H321	2.43	0.49
1:A:344:LEU:HA	1:A:347:VAL:HG22	1.95	0.49
1:A:654:LEU:HD22	13:A:801:CL0:H26	1.94	0.49
1:A:200:HIS:CD2	14:A:814:CLA:NB	2.81	0.49
2:B:279:ILE:HD11	14:B:817:CLA:C3C	2.42	0.49
1:A:204:LEU:O	1:A:204:LEU:HD23	2.13	0.48
1:A:380:TYR:O	1:A:383:LEU:HD22	2.13	0.48
14:A:842:CLA:HBC1	17:B:847:BCR:H392	1.95	0.48
6:F:96:GLU:O	6:F:100:ILE:HD12	2.12	0.48
9:K:67:HIS:CD2	14:K:101:CLA:NC	2.80	0.48
1:A:490:VAL:HA	1:A:493:LEU:CD2	2.43	0.48
1:A:490:VAL:O	1:A:493:LEU:HD23	2.14	0.48
1:A:751:ILE:O	1:A:755:GLY:N	2.45	0.48
1:A:686:SER:HB2	1:A:731:GLY:O	2.13	0.48
17:I:103:BCR:H392	17:I:103:BCR:H23C	1.95	0.48
1:A:706:TRP:CH2	2:B:420:ALA:HB2	2.49	0.48
1:A:717:ILE:HD12	6:F:98:GLU:HB2	1.96	0.48
1:A:51:LEU:C	1:A:51:LEU:HD23	2.38	0.48
1:A:445:ASN:O	1:A:449:ILE:HG13	2.14	0.48
1:A:538:VAL:HG22	1:A:542:HIS:CE1	2.48	0.48
4:D:73:ARG:NH2	4:D:103:GLU:OE2	2.38	0.48
1:A:364:GLY:HA2	1:A:401:GLY:HA2	1.95	0.48
2:B:561:TYR:O	2:B:577:SER:OG	2.30	0.48
3:C:23:ASP:O	3:C:43:ARG:NE	2.40	0.48
8:J:23:ALA:O	8:J:27:ILE:HD12	2.14	0.48
1:A:188:GLU:OE1	1:A:188:GLU:N	2.46	0.48
1:A:201:LEU:HD12	1:A:308:PHE:O	2.14	0.48
2:B:528:ALA:HB1	14:B:802:CLA:H192	1.96	0.48
10:L:41:LEU:O	10:L:46:ARG:NH2	2.47	0.48
2:B:672:SER:O	15:B:842:PQN:H9	2.14	0.48
10:L:110:PRO:O	10:L:113:THR:HG22	2.14	0.48
1:A:628:ASP:N	1:A:628:ASP:OD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:805:CLA:H143	14:A:810:CLA:C14	2.38	0.47
2:B:139:ILE:HD12	11:M:14:ILE:CD1	2.44	0.47
10:L:69:ARG:HA	10:L:74:ALA:HB2	1.96	0.47
2:B:266:SER:OG	2:B:267:LEU:N	2.48	0.47
10:L:57:PHE:CD1	10:L:57:PHE:C	2.92	0.47
2:B:660:HIS:CE1	2:B:726:THR:HG21	2.49	0.47
1:A:513:PHE:HE1	14:A:828:CLA:HBC2	1.80	0.47
2:B:522:ASP:OD2	2:B:603:LYS:NZ	2.39	0.47
14:B:803:CLA:CGA	14:B:803:CLA:H3A	2.45	0.47
6:F:54:ASP:OD2	17:F:203:BCR:H393	2.14	0.47
17:L:208:BCR:H311	17:L:208:BCR:H343	1.96	0.47
1:A:121:VAL:HG21	14:B:833:CLA:HMD2	1.97	0.47
14:A:810:CLA:C2	14:A:810:CLA:H92	2.44	0.47
2:B:300:ILE:O	2:B:304:MET:HG2	2.14	0.47
2:B:479:THR:CG2	12:X:35:LYS:HG2	2.42	0.47
14:B:808:CLA:C1A	14:B:808:CLA:CGA	2.92	0.47
1:A:65:LEU:HD12	1:A:65:LEU:O	2.15	0.47
1:A:638:ASN:O	1:A:642:SER:N	2.42	0.47
1:A:662:ILE:HD12	2:B:627:ARG:HG3	1.96	0.47
1:A:367:SER:OG	1:A:400:ILE:HD11	2.15	0.47
2:B:154:LEU:HD23	2:B:155:HIS:HD1	1.79	0.47
2:B:376:THR:HG22	2:B:597:THR:HG22	1.96	0.47
2:B:652:TRP:O	2:B:729:ALA:HB1	2.15	0.47
10:L:143:LEU:H	10:L:143:LEU:HD22	1.80	0.47
1:A:245:ASN:O	1:A:248:LEU:HD12	2.14	0.47
14:A:804:CLA:H91	8:J:16:ALA:HB2	1.97	0.47
2:B:288:HIS:CD2	14:B:820:CLA:NA	2.82	0.47
1:A:459:TYR:HB3	1:A:646:ILE:HD11	1.96	0.47
14:B:833:CLA:H43	17:J:105:BCR:H361	1.97	0.47
5:E:19:GLU:OE2	5:E:42:LYS:NZ	2.39	0.47
6:F:70:PHE:O	6:F:71:LEU:C	2.57	0.47
6:F:84:TYR:O	6:F:88:VAL:HG23	2.15	0.47
1:A:201:LEU:O	1:A:201:LEU:HD13	2.14	0.47
1:A:587:CYS:HB2	2:B:673:TRP:HB3	1.97	0.47
2:B:17:THR:O	2:B:20:ILE:N	2.47	0.47
17:I:103:BCR:H383	10:L:93:LEU:HD21	1.96	0.47
1:A:689:PHE:CD2	1:A:730:VAL:HG11	2.50	0.46
14:A:820:CLA:H92	14:A:830:CLA:H102	1.98	0.46
2:B:275:HIS:HB2	14:B:817:CLA:C1B	2.46	0.46
10:L:59:ILE:HG22	10:L:78:GLY:O	2.16	0.46
14:A:803:CLA:CGA	14:A:803:CLA:H3A	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:803:CLA:H143	17:B:848:BCR:H362	1.97	0.46
1:A:120:ILE:HG23	1:A:121:VAL:N	2.29	0.46
17:A:852:BCR:H373	2:B:437:LEU:CD1	2.45	0.46
14:B:841:CLA:H8	7:I:27:MET:HE1	1.97	0.46
1:A:451:LEU:HD13	1:A:544:PHE:HA	1.97	0.46
2:B:637:LEU:HD13	2:B:733:ALA:HB3	1.98	0.46
2:B:727:TYR:N	14:B:802:CLA:O1D	2.49	0.46
14:B:825:CLA:HMB3	14:B:825:CLA:HBB1	1.97	0.46
9:K:21:LEU:HD12	14:K:101:CLA:CAD	2.46	0.46
1:A:410:ALA:CB	1:A:595:VAL:HG11	2.45	0.46
1:A:429:VAL:HG23	14:A:825:CLA:HBC2	1.98	0.46
14:A:841:CLA:H143	14:F:202:CLA:HAC1	1.98	0.46
3:C:14:THR:O	3:C:18:ARG:NE	2.46	0.46
8:J:18:TRP:NE1	23:J:201:HOH:O	2.49	0.46
9:K:21:LEU:HD12	14:K:101:CLA:OBD	2.15	0.46
9:K:24:LEU:HD13	9:K:69:LEU:CB	2.46	0.46
1:A:396:HIS:HE1	14:A:829:CLA:ND	2.10	0.46
2:B:329:TYR:CZ	14:B:824:CLA:NC	2.83	0.46
14:L:206:CLA:H51	14:L:206:CLA:H92	1.97	0.46
1:A:396:HIS:HB2	14:A:829:CLA:C1B	2.46	0.46
1:A:547:HIS:CD2	14:A:840:CLA:NB	2.83	0.46
2:B:90:ILE:CD1	14:B:809:CLA:HMD1	2.46	0.46
3:C:60:ASP:HB2	5:E:58:ASN:CG	2.40	0.46
1:A:696:TYR:CE2	2:B:539:ILE:HG23	2.52	0.45
14:A:811:CLA:HBC3	14:A:811:CLA:HHD	1.98	0.45
2:B:337:LEU:HD23	2:B:392:HIS:ND1	2.31	0.45
1:A:175:ALA:HB2	14:A:811:CLA:HBC2	1.98	0.45
1:A:300:HIS:HB2	14:A:819:CLA:C1B	2.46	0.45
1:A:575:ARG:NH1	14:A:831:CLA:O1D	2.46	0.45
3:C:64:ILE:HB	16:C:102:SF4:S3	2.56	0.45
9:K:40:GLY:N	9:K:41:PRO:CD	2.79	0.45
1:A:175:ALA:CA	14:A:811:CLA:HBC2	2.46	0.45
1:A:461:HIS:HE1	14:A:835:CLA:NA	2.13	0.45
14:B:804:CLA:HBC1	18:B:849:LMG:H202	1.98	0.45
17:B:843:BCR:H331	17:B:843:BCR:C8	2.45	0.45
1:A:349:THR:O	1:A:349:THR:HG22	2.16	0.45
17:A:847:BCR:C8	17:A:847:BCR:H331	2.47	0.45
2:B:301:LYS:NZ	2:B:327:GLU:OE2	2.46	0.45
2:B:604:HIS:HB3	2:B:608:TRP:CH2	2.51	0.45
2:B:659:GLY:HA2	2:B:722:GLY:HA2	1.98	0.45
2:B:717:ALA:O	2:B:721:VAL:HG23	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:24:THR:OG1	6:F:34:ARG:NH1	2.50	0.45
8:J:36:LEU:HD11	17:J:105:BCR:C39	2.46	0.45
1:A:126:LEU:HB3	1:A:137:ILE:HD11	1.98	0.45
2:B:96:GLY:O	2:B:100:VAL:HG23	2.16	0.45
2:B:651:VAL:HG13	14:B:809:CLA:HAC1	1.98	0.45
4:D:67:LEU:HD12	4:D:71:GLN:HB2	1.99	0.45
14:A:815:CLA:C1B	17:A:848:BCR:H342	2.46	0.45
2:B:19:ARG:NH2	7:I:34:ILE:O	2.50	0.45
1:A:299:HIS:HE1	14:A:818:CLA:C4D	2.30	0.45
6:F:101:ILE:O	8:J:9:SER:HB3	2.17	0.45
14:F:202:CLA:HBC2	8:J:19:MET:HE3	1.98	0.45
1:A:76:HIS:CE1	14:A:806:CLA:ND	2.84	0.45
1:A:718:GLN:NE2	5:E:15:TYR:OH	2.50	0.45
14:A:841:CLA:H143	14:F:202:CLA:CAC	2.46	0.45
17:A:852:BCR:H372	2:B:441:VAL:HG11	1.99	0.45
17:B:845:BCR:H24C	17:B:845:BCR:H371	1.83	0.45
14:J:101:CLA:HMD1	17:J:104:BCR:C33	2.47	0.45
5:E:24:ALA:O	5:E:25:SER:O	2.35	0.45
2:B:114:ILE:HD11	2:B:116:TYR:CZ	2.52	0.44
2:B:278:ALA:HA	14:B:816:CLA:HMC3	1.99	0.44
6:F:107:ILE:HA	6:F:110:MET:HE3	1.99	0.44
1:A:91:TYR:HD1	1:A:158:LEU:HD23	1.81	0.44
1:A:120:ILE:HD11	8:J:31:ARG:HB2	1.98	0.44
1:A:181:HIS:CD2	14:A:812:CLA:NC	2.85	0.44
1:A:444:LEU:HA	1:A:447:VAL:HG12	1.99	0.44
15:A:845:PQN:H192	17:B:847:BCR:H24C	2.00	0.44
2:B:662:VAL:HG13	2:B:718:HIS:HD2	1.82	0.44
1:A:210:LEU:C	1:A:210:LEU:HD12	2.42	0.44
2:B:176:HIS:O	2:B:180:GLY:N	2.46	0.44
1:A:52:HIS:HB3	14:A:805:CLA:HBC1	1.99	0.44
1:A:68:ILE:O	1:A:72:ILE:HG13	2.17	0.44
1:A:201:LEU:HD13	1:A:201:LEU:C	2.43	0.44
2:B:192:HIS:HB2	14:B:814:CLA:CHC	2.47	0.44
2:B:658:PHE:O	2:B:662:VAL:HG23	2.18	0.44
1:A:52:HIS:HB2	19:A:854:LHG:H111	1.98	0.44
14:A:841:CLA:H93	15:A:845:PQN:H293	1.98	0.44
2:B:662:VAL:HG12	2:B:718:HIS:O	2.17	0.44
1:A:299:HIS:HB3	14:A:819:CLA:HMB1	2.00	0.44
1:A:606:ILE:HA	1:A:609:VAL:HG22	1.99	0.44
14:A:857:CLA:O1D	14:A:857:CLA:H2A	2.18	0.44
2:B:123:TRP:HA	2:B:126:ILE:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:LYS:HE3	2:B:313:LYS:HB2	1.84	0.44
1:A:289:THR:O	1:A:382:TYR:N	2.41	0.44
1:A:299:HIS:HA	1:A:302:LEU:CD2	2.48	0.44
2:B:528:ALA:HB2	14:B:802:CLA:H192	2.00	0.44
6:F:23:ASN:OD1	6:F:30:SER:N	2.51	0.44
1:A:358:ILE:HD11	23:A:901:HOH:O	2.17	0.44
1:A:461:HIS:O	1:A:465:MET:HG2	2.18	0.44
2:B:570:ARG:N	5:E:47:GLY:O	2.50	0.44
14:B:836:CLA:HHC	14:B:836:CLA:HBB1	1.99	0.44
6:F:100:ILE:HG22	6:F:100:ILE:O	2.18	0.44
8:J:12:PRO:HB2	17:J:104:BCR:H401	2.00	0.44
10:L:83:ILE:HD13	10:L:129:MET:SD	2.57	0.44
14:A:802:CLA:H3A	14:A:802:CLA:O1A	2.18	0.43
14:A:805:CLA:C14	14:A:810:CLA:H143	2.45	0.43
2:B:261:HIS:N	2:B:266:SER:O	2.34	0.43
6:F:2:VAL:O	6:F:5:LEU:HD13	2.19	0.43
6:F:57:LEU:HA	6:F:60:ALA:HB2	1.98	0.43
1:A:214:GLY:O	1:A:218:HIS:HB2	2.18	0.43
2:B:328:THR:O	2:B:332:SER:N	2.46	0.43
14:B:814:CLA:H121	14:B:814:CLA:H91	1.99	0.43
6:F:25:THR:OG1	6:F:26:ALA:N	2.51	0.43
8:J:17:ILE:HA	8:J:20:THR:HG22	2.00	0.43
2:B:177:HIS:CD2	14:B:813:CLA:NB	2.85	0.43
2:B:226:THR:OG1	2:B:228:ASN:ND2	2.44	0.43
17:I:101:BCR:H20C	17:I:101:BCR:H361	1.89	0.43
1:A:209:SER:HB3	14:A:820:CLA:HMC2	1.99	0.43
1:A:332:HIS:CD2	14:A:824:CLA:NB	2.86	0.43
1:A:717:ILE:O	1:A:717:ILE:HG22	2.17	0.43
2:B:392:HIS:HE1	14:B:829:CLA:NA	2.15	0.43
2:B:531:LEU:O	2:B:535:THR:HG22	2.19	0.43
6:F:65:ILE:HB	6:F:66:PRO:HD3	2.01	0.43
2:B:49:HIS:CE1	14:B:805:CLA:ND	2.86	0.43
1:A:673:GLY:O	1:A:676:PHE:HB3	2.18	0.43
1:A:717:ILE:HD12	6:F:98:GLU:CB	2.49	0.43
2:B:23:ALA:O	2:B:27:ALA:HB2	2.19	0.43
1:A:416:MET:O	1:A:561:ARG:NE	2.52	0.43
2:B:182:PHE:HB3	2:B:283:PHE:CD2	2.54	0.43
2:B:412:ASP:O	2:B:416:GLN:HG2	2.19	0.43
5:E:37:ILE:N	5:E:37:ILE:HD12	2.33	0.43
8:J:18:TRP:O	8:J:21:ILE:HG13	2.18	0.43
17:L:201:BCR:H15C	17:L:201:BCR:H351	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:VAL:HG13	1:A:239:PRO:HB3	2.01	0.43
1:A:385:THR:CG2	1:A:520:VAL:HB	2.49	0.43
1:A:392:SER:HB3	14:A:829:CLA:HHB	2.01	0.43
14:A:817:CLA:HBB2	17:A:848:BCR:H352	2.01	0.43
2:B:313:LYS:O	2:B:314:VAL:HG13	2.18	0.43
2:B:473:LEU:H	2:B:473:LEU:HD12	1.83	0.43
1:A:550:VAL:HG11	14:A:840:CLA:HMB2	2.01	0.43
2:B:154:LEU:HD23	2:B:155:HIS:ND1	2.34	0.43
14:B:811:CLA:O2D	14:B:811:CLA:H2A	2.19	0.43
7:I:22:MET:O	7:I:26:VAL:HG13	2.18	0.43
14:J:101:CLA:CMD	17:J:104:BCR:H331	2.47	0.43
1:A:484:PRO:HB3	14:A:839:CLA:HED3	2.02	0.42
14:A:813:CLA:HBC2	14:A:813:CLA:HHD	2.01	0.42
8:J:36:LEU:HD11	17:J:105:BCR:H393	2.01	0.42
1:A:219:VAL:CG1	14:A:815:CLA:HED1	2.50	0.42
14:A:805:CLA:HBC2	14:A:831:CLA:H43	2.01	0.42
14:A:807:CLA:HED1	14:A:807:CLA:O1A	2.19	0.42
2:B:344:LEU:O	2:B:348:THR:OG1	2.34	0.42
2:B:418:LYS:CB	2:B:545:LEU:HD13	2.49	0.42
1:A:406:VAL:HG11	1:A:599:LEU:HG	2.01	0.42
1:A:433:VAL:HA	1:A:436:HIS:CE1	2.55	0.42
1:A:685:PHE:HZ	14:A:842:CLA:HBC2	1.85	0.42
14:A:808:CLA:C6	14:J:101:CLA:HBC1	2.50	0.42
2:B:222:ALA:N	2:B:223:PRO:CD	2.83	0.42
2:B:535:THR:O	2:B:539:ILE:HG13	2.20	0.42
4:D:95:HIS:HB3	4:D:96:PRO:CD	2.50	0.42
14:A:833:CLA:HBB1	14:A:833:CLA:HMB3	2.02	0.42
6:F:82:ARG:O	6:F:86:ILE:HG13	2.19	0.42
14:J:101:CLA:HMC1	17:J:104:BCR:H352	2.02	0.42
10:L:34:LEU:O	10:L:38:ARG:N	2.46	0.42
1:A:451:LEU:HB3	1:A:544:PHE:HB2	2.02	0.42
14:A:803:CLA:HMA2	17:B:847:BCR:H401	2.02	0.42
17:A:852:BCR:H393	17:J:103:BCR:H322	2.02	0.42
2:B:382:ALA:O	2:B:386:MET:HG2	2.20	0.42
2:B:680:LEU:O	2:B:683:THR:OG1	2.34	0.42
6:F:103:VAL:HG22	6:F:107:ILE:CD1	2.48	0.42
2:B:372:ALA:O	2:B:376:THR:HG23	2.20	0.42
17:B:847:BCR:C34	6:F:73:ILE:HG21	2.50	0.42
4:D:85:ILE:HG12	4:D:91:THR:HG23	2.01	0.42
7:I:22:MET:HG3	7:I:23:PRO:HD3	2.01	0.42
1:A:544:PHE:CD1	1:A:544:PHE:C	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:ARG:HA	3:C:76:MET:C	2.46	0.41
13:A:801:CL0:H12	14:A:857:CLA:OBD	2.19	0.41
14:A:803:CLA:HMD1	2:B:584:LEU:HB3	2.02	0.41
14:A:806:CLA:H191	17:A:848:BCR:H12C	2.02	0.41
11:M:14:ILE:O	11:M:18:PRO:HD2	2.20	0.41
1:A:93:HIS:HE1	14:A:808:CLA:NC	2.18	0.41
1:A:508:THR:HG22	1:A:509:ALA:N	2.35	0.41
2:B:207:GLY:N	2:B:210:ASN:OD1	2.49	0.41
2:B:272:MET:SD	14:B:818:CLA:HMA2	2.60	0.41
7:I:17:VAL:O	7:I:18:VAL:C	2.63	0.41
1:A:397:HIS:O	1:A:400:ILE:HG13	2.20	0.41
2:B:279:ILE:CG2	2:B:283:PHE:CE2	3.03	0.41
2:B:384:PHE:CE1	2:B:589:MET:HE1	2.56	0.41
3:C:9:THR:HG1	3:C:63:SER:CB	2.22	0.41
17:I:103:BCR:C40	10:L:89:ALA:HB1	2.50	0.41
9:K:24:LEU:HD11	9:K:66:GLY:O	2.21	0.41
2:B:376:THR:O	2:B:380:TYR:HD2	2.04	0.41
2:B:664:ALA:O	2:B:667:PHE:HB2	2.20	0.41
14:B:826:CLA:HBC3	14:B:826:CLA:HHD	2.02	0.41
14:B:805:CLA:HBC2	14:B:829:CLA:HMA1	2.01	0.41
3:C:24:VAL:HG21	3:C:47:CYS:HB2	2.02	0.41
1:A:487:ALA:HA	1:A:490:VAL:HG22	2.02	0.41
2:B:377:HIS:CD2	2:B:378:HIS:HD1	2.38	0.41
3:C:19:ALA:HB1	3:C:52:ARG:HB3	2.02	0.41
10:L:20:PRO:HA	10:L:24:SER:HB3	2.03	0.41
17:L:201:BCR:H20C	17:L:201:BCR:H361	1.93	0.41
11:M:16:LEU:O	11:M:19:ALA:HB3	2.19	0.41
1:A:78:GLY:O	1:A:82:VAL:HG23	2.20	0.41
1:A:675:LEU:HD12	1:A:744:TRP:CZ3	2.56	0.41
2:B:444:ASP:OD1	2:B:621:TYR:HB2	2.21	0.41
6:F:116:TRP:N	6:F:117:PRO:CD	2.83	0.41
17:I:103:BCR:H15C	17:I:103:BCR:H351	1.88	0.41
8:J:21:ILE:O	8:J:25:ILE:HD12	2.20	0.41
1:A:120:ILE:CG2	1:A:121:VAL:N	2.84	0.41
1:A:215:HIS:HB2	14:A:815:CLA:CHC	2.50	0.41
1:A:410:ALA:O	1:A:414:ILE:HG13	2.21	0.41
1:A:722:LEU:HD12	15:A:845:PQN:C4	2.50	0.41
14:A:810:CLA:CMB	8:J:27:ILE:HG12	2.51	0.41
2:B:424:HIS:CD2	14:B:831:CLA:NC	2.89	0.41
14:B:825:CLA:HBA1	14:B:826:CLA:HED3	2.03	0.41
6:F:66:PRO:HG3	17:J:105:BCR:H362	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:36:LEU:HD12	17:J:105:BCR:H21C	2.03	0.41
9:K:74:VAL:O	9:K:74:VAL:HG12	2.20	0.41
1:A:333:LYS:H	14:A:844:CLA:HBC3	1.86	0.41
1:A:513:PHE:N	1:A:513:PHE:CD1	2.89	0.41
1:A:602:MET:O	1:A:606:ILE:HG12	2.21	0.41
2:B:194:ILE:HA	2:B:198:ILE:HD12	2.03	0.41
2:B:337:LEU:HD23	2:B:392:HIS:CG	2.55	0.41
2:B:441:VAL:HG13	14:B:833:CLA:CMC	2.51	0.41
2:B:503:TRP:CE2	14:B:834:CLA:HED1	2.56	0.41
2:B:681:ILE:O	2:B:685:VAL:HG23	2.19	0.41
6:F:103:VAL:N	6:F:104:PRO:CD	2.84	0.41
11:M:23:PHE:CE1	11:M:27:THR:HG21	2.55	0.41
1:A:436:HIS:O	1:A:436:HIS:CG	2.73	0.41
1:A:603:TYR:OH	13:A:801:CL0:H29	2.22	0.41
2:B:648:ASN:OD1	2:B:648:ASN:N	2.52	0.41
17:F:203:BCR:H20C	17:F:203:BCR:H361	1.92	0.41
11:M:30:TYR:O	11:M:31:LYS:OXT	2.38	0.41
1:A:224:ASN:HD21	1:A:294:LEU:HD13	1.84	0.40
1:A:396:HIS:HE1	14:A:829:CLA:C1D	2.34	0.40
1:A:732:VAL:HG22	1:A:736:LEU:HD12	2.03	0.40
2:B:537:THR:O	2:B:541:VAL:HG22	2.21	0.40
9:K:69:LEU:HA	14:K:102:CLA:HBC2	2.01	0.40
10:L:143:LEU:HD22	10:L:143:LEU:N	2.36	0.40
1:A:587:CYS:HB3	2:B:673:TRP:HE3	1.86	0.40
2:B:2:THR:OG1	2:B:4:PHE:O	2.34	0.40
1:A:156:PHE:O	1:A:159:TYR:N	2.55	0.40
14:A:822:CLA:H141	14:A:822:CLA:H171	2.04	0.40
14:A:843:CLA:HHC	14:A:843:CLA:HBB1	2.02	0.40
17:A:852:BCR:H362	14:A:857:CLA:H42	2.01	0.40
17:B:845:BCR:H20C	17:B:845:BCR:H361	1.92	0.40
7:I:15:ILE:N	7:I:15:ILE:HD12	2.36	0.40
7:I:30:LEU:O	7:I:34:ILE:HG12	2.21	0.40
8:J:31:ARG:HH12	14:J:101:CLA:HED2	1.86	0.40
1:A:55:ALA:HB1	14:A:805:CLA:C1D	2.51	0.40
1:A:535:ASP:HA	1:A:538:VAL:HG12	2.04	0.40
14:A:806:CLA:O1D	14:A:806:CLA:H2A	2.21	0.40
2:B:552:LEU:HD23	2:B:576:ILE:CD1	2.51	0.40
2:B:668:MET:HB2	14:B:803:CLA:CHC	2.52	0.40
17:B:846:BCR:C23	17:B:846:BCR:H403	2.51	0.40
17:B:851:BCR:H20C	17:B:851:BCR:H361	1.96	0.40
4:D:9:LEU:HD22	4:D:9:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:54:HIS:HA	10:L:57:PHE:CD2	2.57	0.40
1:A:696:TYR:CE2	2:B:542:LYS:HD2	2.57	0.40
2:B:368:HIS:HB3	2:B:608:TRP:CH2	2.57	0.40
8:J:33:TYR:CD2	17:J:105:BCR:H401	2.56	0.40

All (2) 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)
23:L:301:HOH:O	23:L:302:HOH:O[3_455]	1.08	1.12
10:L:67:PRO:O	23:L:302:HOH:O[3_455]	2.05	0.15

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	736/755 (98%)	688 (94%)	48 (6%)	0	100	100
2	B	737/740 (100%)	695 (94%)	42 (6%)	0	100	100
3	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
4	D	136/138 (99%)	124 (91%)	12 (9%)	0	100	100
5	E	67/75 (89%)	60 (90%)	6 (9%)	1 (2%)	8	35
6	F	139/164 (85%)	128 (92%)	11 (8%)	0	100	100
7	I	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	K	43/83 (52%)	38 (88%)	5 (12%)	0	100	100
10	L	149/154 (97%)	146 (98%)	3 (2%)	0	100	100
11	M	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
12	X	27/35 (77%)	26 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2216/2334 (95%)	2074 (94%)	141 (6%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	25	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	587 (100%)	2 (0%)	86 91
2	B	597/597 (100%)	597 (100%)	0	100 100
3	C	67/67 (100%)	66 (98%)	1 (2%)	57 80
4	D	115/115 (100%)	115 (100%)	0	100 100
5	E	59/64 (92%)	59 (100%)	0	100 100
6	F	109/128 (85%)	109 (100%)	0	100 100
7	I	32/32 (100%)	32 (100%)	0	100 100
8	J	36/36 (100%)	36 (100%)	0	100 100
9	K	33/61 (54%)	33 (100%)	0	100 100
10	L	117/119 (98%)	117 (100%)	0	100 100
11	M	26/26 (100%)	26 (100%)	0	100 100
12	X	23/27 (85%)	23 (100%)	0	100 100
All	All	1803/1875 (96%)	1800 (100%)	3 (0%)	87 92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	587	CYS
3	C	16	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	318	ASN
1	A	483	GLN
1	A	542	HIS
1	A	618	GLN
1	A	657	GLN
1	A	718	GLN
2	B	33	HIS
2	B	78	GLN
2	B	105	GLN
2	B	204	GLN
2	B	377	HIS
2	B	406	ASN
2	B	591	ASN
2	B	604	HIS
2	B	688	HIS
3	C	37	GLN
4	D	6	GLN
4	D	37	GLN
4	D	71	GLN
5	E	59	ASN
5	E	66	GLN
6	F	134	ASN
10	L	9	ASN
10	L	16	HIS
10	L	75	ASN
10	L	102	GLN
11	M	7	GLN

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 135 ligands modelled in this entry, 2 are monoatomic - leaving 133 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	$\#\|Z\| > 2$
14	CLA	A	822	23	69,73,73	1.18	6 (8%)	82,113,113	1.22	5 (6%)
14	CLA	K	101	9	45,49,73	1.45	8 (17%)	54,83,113	1.32	4 (7%)
14	CLA	B	802	2	69,73,73	1.18	6 (8%)	82,113,113	1.26	4 (4%)
14	CLA	A	823	1	53,57,73	1.34	6 (11%)	61,93,113	1.38	5 (8%)
14	CLA	A	821	1	46,50,73	1.41	6 (13%)	54,84,113	1.47	4 (7%)
14	CLA	B	807	2	69,73,73	1.18	7 (10%)	82,113,113	1.20	4 (4%)
17	BCR	A	849	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	6 (10%)
14	CLA	B	825	23	50,54,73	1.37	6 (12%)	59,90,113	1.35	4 (6%)
14	CLA	A	813	1	58,62,73	1.29	7 (12%)	68,99,113	1.31	5 (7%)
14	CLA	A	809	1	69,73,73	1.18	7 (10%)	82,113,113	1.29	6 (7%)
14	CLA	B	812	2	49,53,73	1.42	7 (14%)	58,89,113	1.38	5 (8%)
18	LMG	A	856	-	30,30,55	1.01	2 (6%)	37,37,63	1.30	5 (13%)
14	CLA	A	806	1	69,73,73	1.18	6 (8%)	82,113,113	1.29	6 (7%)
16	SF4	C	101	3	0,12,12	-	-	-		
18	LMG	A	853	-	48,48,55	0.77	1 (2%)	56,56,63	1.28	6 (10%)
14	CLA	M	102	23	49,53,73	1.42	8 (16%)	58,89,113	1.40	4 (6%)
22	DGD	L	207	-	67,67,67	0.93	2 (2%)	81,81,81	1.40	14 (17%)
17	BCR	L	201	-	41,41,41	1.13	2 (4%)	56,56,56	1.29	8 (14%)
14	CLA	A	804	1	69,73,73	1.19	6 (8%)	82,113,113	1.20	5 (6%)
14	CLA	A	810	1	69,73,73	1.20	8 (11%)	82,113,113	1.26	6 (7%)
14	CLA	B	806	2	69,73,73	1.20	6 (8%)	82,113,113	1.22	4 (4%)
14	CLA	B	804	2	58,62,73	1.28	6 (10%)	68,99,113	1.33	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	B	817	2	63,67,73	1.25	5 (7%)	74,105,113	1.25	6 (8%)
17	BCR	A	850	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	7 (12%)
14	CLA	B	840	23	69,73,73	1.18	6 (8%)	82,113,113	1.23	6 (7%)
14	CLA	A	833	1	69,73,73	1.18	7 (10%)	82,113,113	1.18	4 (4%)
16	SF4	A	846	1,2	0,12,12	-	-	-		
14	CLA	A	811	1	49,53,73	1.41	6 (12%)	58,89,113	1.39	6 (10%)
14	CLA	A	844	19	56,60,73	1.31	6 (10%)	65,97,113	1.38	6 (9%)
17	BCR	J	103	-	41,41,41	1.15	2 (4%)	56,56,56	1.28	7 (12%)
16	SF4	C	102	3	0,12,12	-	-	-		
17	BCR	A	847	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	8 (14%)
14	CLA	B	834	2	49,53,73	1.40	6 (12%)	58,89,113	1.42	4 (6%)
14	CLA	X	1701	12	49,53,73	1.40	6 (12%)	58,89,113	1.34	5 (8%)
18	LMG	B	849	-	55,55,55	0.71	1 (1%)	63,63,63	1.37	8 (12%)
14	CLA	B	829	2	69,73,73	1.17	7 (10%)	82,113,113	1.31	6 (7%)
14	CLA	B	815	2	49,53,73	1.40	6 (12%)	58,89,113	1.35	4 (6%)
14	CLA	F	201	23	55,59,73	1.33	6 (10%)	64,96,113	1.35	6 (9%)
17	BCR	M	103	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	7 (12%)
14	CLA	A	817	23	53,57,73	1.34	7 (13%)	61,93,113	1.31	5 (8%)
14	CLA	B	830	2	49,53,73	1.41	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	A	818	1	58,62,73	1.29	7 (12%)	68,99,113	1.33	5 (7%)
14	CLA	L	206	23	69,73,73	1.18	5 (7%)	82,113,113	1.35	8 (9%)
15	PQN	A	845	-	34,34,34	2.06	7 (20%)	43,45,45	1.23	5 (11%)
14	CLA	A	807	1	69,73,73	1.21	6 (8%)	82,113,113	1.19	4 (4%)
14	CLA	B	805	2	69,73,73	1.18	6 (8%)	82,113,113	1.21	4 (4%)
14	CLA	L	205	10	69,73,73	1.17	8 (11%)	82,113,113	1.26	7 (8%)
14	CLA	A	805	1,14	63,67,73	1.25	6 (9%)	74,105,113	1.24	6 (8%)
17	BCR	J	104	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	10 (17%)
14	CLA	B	837	2	64,68,73	1.24	6 (9%)	76,107,113	1.30	7 (9%)
14	CLA	A	830	1	69,73,73	1.19	6 (8%)	82,113,113	1.23	5 (6%)
14	CLA	F	202	23	49,53,73	1.41	6 (12%)	58,89,113	1.32	4 (6%)
14	CLA	B	813	2	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
14	CLA	A	812	1,14	69,73,73	1.18	6 (8%)	82,113,113	1.19	4 (4%)
14	CLA	B	822	23	59,63,73	1.27	6 (10%)	70,101,113	1.26	5 (7%)
14	CLA	A	834	1	69,73,73	1.19	5 (7%)	82,113,113	1.16	5 (6%)
14	CLA	J	101	8	49,53,73	1.40	6 (12%)	58,89,113	1.40	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	B	811	2	49,53,73	1.40	6 (12%)	58,89,113	1.48	5 (8%)
14	CLA	B	816	2	59,63,73	1.28	6 (10%)	70,101,113	1.28	5 (7%)
17	BCR	B	851	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	7 (12%)
14	CLA	A	825	1	63,67,73	1.24	6 (9%)	74,105,113	1.26	5 (6%)
14	CLA	B	824	2	58,62,73	1.29	7 (12%)	68,99,113	1.29	5 (7%)
17	BCR	J	105	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	9 (16%)
17	BCR	B	848	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	6 (10%)
14	CLA	B	839	2	51,55,73	1.36	8 (15%)	60,91,113	1.33	6 (10%)
14	CLA	B	831	2	53,57,73	1.35	7 (13%)	61,93,113	1.35	6 (9%)
14	CLA	A	816	1	49,53,73	1.40	7 (14%)	58,89,113	1.38	4 (6%)
14	CLA	B	809	2	69,73,73	1.20	8 (11%)	82,113,113	1.32	8 (9%)
14	CLA	B	814	2	69,73,73	1.19	6 (8%)	82,113,113	1.22	5 (6%)
14	CLA	L	204	10	69,73,73	1.17	8 (11%)	82,113,113	1.32	6 (7%)
14	CLA	A	831	1	69,73,73	1.18	7 (10%)	82,113,113	1.22	6 (7%)
14	CLA	A	857	23	69,73,73	1.17	6 (8%)	82,113,113	1.21	5 (6%)
14	CLA	B	810	2	69,73,73	1.18	7 (10%)	82,113,113	1.31	6 (7%)
15	PQN	B	842	-	34,34,34	2.05	7 (20%)	43,45,45	1.17	4 (9%)
14	CLA	A	828	1	69,73,73	1.20	6 (8%)	82,113,113	1.20	5 (6%)
14	CLA	A	815	1	49,53,73	1.42	7 (14%)	58,89,113	1.32	4 (6%)
14	CLA	B	833	2	62,66,73	1.24	6 (9%)	73,104,113	1.27	5 (6%)
17	BCR	A	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.36	8 (14%)
17	BCR	A	851	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	7 (12%)
14	CLA	B	818	2	64,68,73	1.22	6 (9%)	76,107,113	1.25	4 (5%)
14	CLA	B	823	2	49,53,73	1.42	7 (14%)	58,89,113	1.40	4 (6%)
19	LHG	A	854	-	48,48,48	0.63	1 (2%)	51,54,54	1.26	6 (11%)
14	CLA	A	803	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
17	BCR	A	852	-	41,41,41	1.12	2 (4%)	56,56,56	1.39	9 (16%)
21	LMT	L	202	-	36,36,36	1.13	3 (8%)	47,47,47	1.04	2 (4%)
17	BCR	B	847	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	8 (14%)
14	CLA	B	835	23	49,53,73	1.42	7 (14%)	58,89,113	1.37	5 (8%)
14	CLA	A	838	1	55,59,73	1.34	7 (12%)	64,96,113	1.35	5 (7%)
17	BCR	B	845	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	6 (10%)
14	CLA	B	836	23	49,53,73	1.44	7 (14%)	58,89,113	1.36	4 (6%)
14	CLA	A	829	1	69,73,73	1.19	6 (8%)	82,113,113	1.15	4 (4%)
14	CLA	J	102	8	41,45,73	1.49	7 (17%)	50,78,113	1.34	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	B	844	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	9 (16%)
14	CLA	A	808	1	55,59,73	1.35	7 (12%)	64,96,113	1.38	7 (10%)
14	CLA	A	840	1	51,55,73	1.36	7 (13%)	60,91,113	1.36	5 (8%)
14	CLA	B	826	2	69,73,73	1.19	6 (8%)	82,113,113	1.23	5 (6%)
14	CLA	B	808	2	69,73,73	1.19	7 (10%)	82,113,113	1.21	6 (7%)
17	BCR	I	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.30	6 (10%)
14	CLA	B	828	2	69,73,73	1.18	6 (8%)	82,113,113	1.17	5 (6%)
14	CLA	K	102	-	49,53,73	1.40	6 (12%)	58,89,113	1.41	5 (8%)
19	LHG	B	850	-	22,22,48	0.92	2 (9%)	25,28,54	1.23	1 (4%)
14	CLA	A	826	23	69,73,73	1.19	7 (10%)	82,113,113	1.25	4 (4%)
14	CLA	B	841	2	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
14	CLA	A	802	23	69,73,73	1.18	6 (8%)	82,113,113	1.18	3 (3%)
13	CL0	A	801	1	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
19	LHG	A	855	14	26,26,48	0.85	2 (7%)	29,32,54	1.32	3 (10%)
14	CLA	A	843	23	69,73,73	1.20	6 (8%)	82,113,113	1.25	4 (4%)
14	CLA	B	821	2	49,53,73	1.40	7 (14%)	58,89,113	1.39	4 (6%)
14	CLA	B	827	2	69,73,73	1.19	7 (10%)	82,113,113	1.14	5 (6%)
18	LMG	I	102	-	40,40,55	0.89	1 (2%)	48,48,63	1.26	6 (12%)
14	CLA	B	803	-	69,73,73	1.19	6 (8%)	82,113,113	1.21	4 (4%)
14	CLA	B	819	23	69,73,73	1.17	9 (13%)	82,113,113	1.25	5 (6%)
17	BCR	F	203	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	7 (12%)
14	CLA	A	832	1	54,58,73	1.33	7 (12%)	64,95,113	1.34	5 (7%)
17	BCR	B	846	-	41,41,41	1.06	2 (4%)	56,56,56	1.28	7 (12%)
14	CLA	A	820	1	69,73,73	1.17	7 (10%)	82,113,113	1.23	6 (7%)
17	BCR	I	103	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	7 (12%)
14	CLA	A	841	1	69,73,73	1.17	7 (10%)	82,113,113	1.21	4 (4%)
14	CLA	A	836	1	58,62,73	1.31	6 (10%)	68,99,113	1.25	5 (7%)
14	CLA	A	842	1	69,73,73	1.18	7 (10%)	82,113,113	1.29	4 (4%)
14	CLA	A	824	1	55,59,73	1.32	6 (10%)	64,96,113	1.29	6 (9%)
14	CLA	A	837	1	49,53,73	1.41	5 (10%)	58,89,113	1.35	4 (6%)
14	CLA	A	839	1	69,73,73	1.17	7 (10%)	82,113,113	1.24	6 (7%)
14	CLA	B	820	2	51,55,73	1.36	6 (11%)	60,91,113	1.33	4 (6%)
14	CLA	B	838	2	69,73,73	1.20	6 (8%)	82,113,113	1.25	5 (6%)
14	CLA	A	827	23	69,73,73	1.18	6 (8%)	82,113,113	1.21	5 (6%)
19	LHG	M	101	-	48,48,48	0.63	0	51,54,54	1.22	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	A	814	1	64,68,73	1.23	6 (9%)	76,107,113	1.27	6 (7%)
14	CLA	A	819	1	58,62,73	1.31	8 (13%)	68,99,113	1.30	6 (8%)
17	BCR	B	843	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	9 (16%)
14	CLA	B	832	2	69,73,73	1.18	6 (8%)	82,113,113	1.19	5 (6%)
17	BCR	L	208	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	7 (12%)
14	CLA	A	835	1	69,73,73	1.20	6 (8%)	82,113,113	1.20	5 (6%)

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
14	CLA	A	822	23	-	13/39/115/115	-
14	CLA	K	101	9	-	1/9/81/115	-
14	CLA	B	802	2	-	13/39/115/115	-
14	CLA	A	823	1	-	10/20/96/115	-
14	CLA	A	821	1	-	2/10/86/115	-
14	CLA	B	807	2	-	7/39/115/115	-
17	BCR	A	849	-	-	12/29/63/63	0/2/2/2
14	CLA	B	825	23	-	4/17/93/115	-
14	CLA	A	813	1	-	8/26/102/115	-
14	CLA	A	809	1	-	12/39/115/115	-
14	CLA	B	812	2	-	6/15/91/115	-
18	LMG	A	856	-	-	12/23/43/70	0/1/1/1
14	CLA	A	806	1	-	14/39/115/115	-
16	SF4	C	101	3	-	-	0/6/5/5
18	LMG	A	853	-	-	25/43/63/70	0/1/1/1
14	CLA	M	102	23	-	5/15/91/115	-
22	DGD	L	207	-	-	23/55/95/95	0/2/2/2
17	BCR	L	201	-	-	11/29/63/63	0/2/2/2
14	CLA	A	804	1	-	10/39/115/115	-
14	CLA	A	810	1	-	10/39/115/115	-
14	CLA	B	806	2	-	9/39/115/115	-
14	CLA	B	804	2	-	7/26/102/115	-
14	CLA	B	817	2	-	7/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	A	850	-	-	12/29/63/63	0/2/2/2
14	CLA	B	840	23	-	8/39/115/115	-
14	CLA	A	833	1	-	10/39/115/115	-
16	SF4	A	846	1,2	-	-	0/6/5/5
14	CLA	A	811	1	-	8/15/91/115	-
14	CLA	A	844	19	-	6/24/100/115	-
17	BCR	J	103	-	-	18/29/63/63	0/2/2/2
16	SF4	C	102	3	-	-	0/6/5/5
17	BCR	A	847	-	-	11/29/63/63	0/2/2/2
14	CLA	B	834	2	-	6/15/91/115	-
14	CLA	X	1701	12	-	6/15/91/115	-
18	LMG	B	849	-	-	18/50/70/70	0/1/1/1
14	CLA	B	829	2	-	8/39/115/115	-
14	CLA	B	815	2	-	4/15/91/115	-
14	CLA	F	201	23	-	6/23/99/115	-
17	BCR	M	103	-	-	18/29/63/63	0/2/2/2
14	CLA	A	817	23	-	6/20/96/115	-
14	CLA	B	830	2	-	9/15/91/115	-
14	CLA	A	818	1	-	3/26/102/115	-
14	CLA	L	206	23	-	7/39/115/115	-
15	PQN	A	845	-	-	11/23/43/43	0/2/2/2
14	CLA	A	807	1	-	14/39/115/115	-
14	CLA	B	805	2	-	11/39/115/115	-
14	CLA	L	205	10	-	11/39/115/115	-
14	CLA	A	805	1,14	-	6/32/108/115	-
17	BCR	J	104	-	-	13/29/63/63	0/2/2/2
14	CLA	B	837	2	-	5/33/109/115	-
14	CLA	A	830	1	-	14/39/115/115	-
14	CLA	F	202	23	-	4/15/91/115	-
14	CLA	B	813	2	-	18/39/115/115	-
14	CLA	A	812	1,14	-	5/39/115/115	-
14	CLA	B	822	23	-	7/27/103/115	-
14	CLA	A	834	1	-	9/39/115/115	-
14	CLA	J	101	8	-	3/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	811	2	-	2/15/91/115	-
14	CLA	B	816	2	-	6/27/103/115	-
17	BCR	B	851	-	-	8/29/63/63	0/2/2/2
14	CLA	A	825	1	-	10/32/108/115	-
14	CLA	B	824	2	-	7/26/102/115	-
17	BCR	J	105	-	-	10/29/63/63	0/2/2/2
17	BCR	B	848	-	-	6/29/63/63	0/2/2/2
14	CLA	B	839	2	-	4/18/94/115	-
14	CLA	B	831	2	-	7/20/96/115	-
14	CLA	A	816	1	-	5/15/91/115	-
14	CLA	B	809	2	-	14/39/115/115	-
14	CLA	B	814	2	-	13/39/115/115	-
14	CLA	L	204	10	-	13/39/115/115	-
14	CLA	A	831	1	-	10/39/115/115	-
14	CLA	A	857	23	-	17/39/115/115	-
14	CLA	B	810	2	-	16/39/115/115	-
15	PQN	B	842	-	-	8/23/43/43	0/2/2/2
14	CLA	A	828	1	-	11/39/115/115	-
14	CLA	A	815	1	-	3/15/91/115	-
14	CLA	B	833	2	-	4/31/107/115	-
17	BCR	A	848	-	-	17/29/63/63	0/2/2/2
17	BCR	A	851	-	-	7/29/63/63	0/2/2/2
14	CLA	B	818	2	-	10/33/109/115	-
14	CLA	B	823	2	-	6/15/91/115	-
19	LHG	A	854	-	-	21/53/53/53	-
14	CLA	A	803	-	-	6/39/115/115	-
17	BCR	A	852	-	-	19/29/63/63	0/2/2/2
21	LMT	L	202	-	-	12/21/61/61	0/2/2/2
17	BCR	B	847	-	-	13/29/63/63	0/2/2/2
14	CLA	B	835	23	-	7/15/91/115	-
14	CLA	A	838	1	-	5/23/99/115	-
17	BCR	B	845	-	-	9/29/63/63	0/2/2/2
14	CLA	B	836	23	-	4/15/91/115	-
14	CLA	A	829	1	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	J	102	8	-	1/4/76/115	-
17	BCR	B	844	-	-	8/29/63/63	0/2/2/2
14	CLA	A	808	1	-	9/23/99/115	-
14	CLA	A	840	1	-	2/18/94/115	-
14	CLA	B	826	2	-	16/39/115/115	-
14	CLA	B	808	2	-	7/39/115/115	-
17	BCR	I	101	-	-	15/29/63/63	0/2/2/2
14	CLA	B	828	2	-	19/39/115/115	-
14	CLA	K	102	-	-	6/15/91/115	-
19	LHG	B	850	-	-	13/26/26/53	-
14	CLA	A	826	23	-	14/39/115/115	-
14	CLA	B	841	2	-	8/39/115/115	-
14	CLA	A	802	23	-	11/39/115/115	-
13	CL0	A	801	1	-	15/39/115/115	-
19	LHG	A	855	14	-	10/31/31/53	-
14	CLA	A	843	23	-	8/39/115/115	-
14	CLA	B	821	2	-	6/15/91/115	-
14	CLA	B	827	2	-	13/39/115/115	-
18	LMG	I	102	-	-	9/35/55/70	0/1/1/1
14	CLA	B	803	-	-	11/39/115/115	-
14	CLA	B	819	23	-	12/39/115/115	-
17	BCR	F	203	-	-	9/29/63/63	0/2/2/2
14	CLA	A	832	1	-	6/21/97/115	-
17	BCR	B	846	-	-	13/29/63/63	0/2/2/2
14	CLA	A	820	1	-	16/39/115/115	-
17	BCR	I	103	-	-	14/29/63/63	0/2/2/2
14	CLA	A	841	1	-	6/39/115/115	-
14	CLA	A	836	1	-	3/26/102/115	-
14	CLA	A	842	1	-	9/39/115/115	-
14	CLA	A	824	1	-	3/23/99/115	-
14	CLA	A	837	1	-	6/15/91/115	-
14	CLA	A	839	1	-	13/39/115/115	-
14	CLA	B	820	2	-	6/18/94/115	-
14	CLA	B	838	2	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	827	23	-	5/39/115/115	-
19	LHG	M	101	-	-	26/53/53/53	-
14	CLA	A	814	1	-	7/33/109/115	-
14	CLA	A	819	1	-	9/26/102/115	-
17	BCR	B	843	-	-	7/29/63/63	0/2/2/2
14	CLA	B	832	2	-	11/39/115/115	-
17	BCR	L	208	-	-	11/29/63/63	0/2/2/2
14	CLA	A	835	1	-	11/39/115/115	-

All (703) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	845	PQN	O1-C1	6.00	1.35	1.23
15	B	842	PQN	O4-C4	5.96	1.35	1.23
15	B	842	PQN	O1-C1	5.96	1.35	1.23
15	A	845	PQN	O4-C4	5.95	1.35	1.23
15	A	845	PQN	C10-C1	-4.75	1.38	1.48
15	B	842	PQN	C10-C1	-4.56	1.39	1.48
14	B	827	CLA	C1D-ND	3.96	1.43	1.37
17	J	103	BCR	C1-C6	-3.95	1.48	1.53
14	B	817	CLA	C1D-ND	3.93	1.43	1.37
17	I	103	BCR	C1-C6	-3.90	1.48	1.53
14	B	811	CLA	C1D-ND	3.89	1.43	1.37
17	B	845	BCR	C1-C6	-3.88	1.48	1.53
14	A	819	CLA	C1D-ND	3.86	1.42	1.37
17	B	851	BCR	C1-C6	-3.86	1.48	1.53
14	A	835	CLA	C1D-ND	3.83	1.42	1.37
17	A	848	BCR	C1-C6	-3.82	1.48	1.53
14	A	829	CLA	C1D-ND	3.81	1.42	1.37
17	L	201	BCR	C1-C6	-3.77	1.49	1.53
14	B	836	CLA	C1D-ND	3.75	1.42	1.37
14	B	807	CLA	C1D-ND	3.75	1.42	1.37
14	B	808	CLA	C1D-ND	3.75	1.42	1.37
17	B	847	BCR	C1-C6	-3.75	1.49	1.53
14	B	823	CLA	C1D-ND	3.75	1.42	1.37
14	A	836	CLA	C1D-ND	3.74	1.42	1.37
14	B	802	CLA	C1D-ND	3.72	1.42	1.37
14	B	836	CLA	C4B-NB	3.72	1.42	1.37
17	M	103	BCR	C1-C6	-3.72	1.49	1.53
14	A	840	CLA	C1D-ND	3.72	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	202	CLA	C1D-ND	3.72	1.42	1.37
15	B	842	PQN	C5-C4	-3.71	1.40	1.48
14	B	826	CLA	C1D-ND	3.71	1.42	1.37
14	B	838	CLA	C1D-ND	3.71	1.42	1.37
14	A	816	CLA	C1D-ND	3.70	1.42	1.37
14	A	828	CLA	C1D-ND	3.69	1.42	1.37
15	A	845	PQN	C5-C4	-3.68	1.41	1.48
14	A	824	CLA	C1D-ND	3.68	1.42	1.37
14	B	806	CLA	C1D-ND	3.68	1.42	1.37
14	A	806	CLA	C1D-ND	3.68	1.42	1.37
14	B	839	CLA	C1D-ND	3.67	1.42	1.37
14	B	825	CLA	C1D-ND	3.67	1.42	1.37
14	A	809	CLA	C1D-ND	3.67	1.42	1.37
13	A	801	CL0	C1D-ND	3.67	1.42	1.37
14	A	838	CLA	C1D-ND	3.67	1.42	1.37
14	B	813	CLA	C1D-ND	3.66	1.42	1.37
17	A	850	BCR	C1-C6	-3.66	1.49	1.53
14	B	834	CLA	C1D-ND	3.66	1.42	1.37
14	A	837	CLA	C1D-ND	3.66	1.42	1.37
14	B	810	CLA	C1D-ND	3.65	1.42	1.37
14	A	825	CLA	C1D-ND	3.65	1.42	1.37
14	A	843	CLA	C1D-ND	3.65	1.42	1.37
14	A	811	CLA	C1D-ND	3.64	1.42	1.37
14	A	827	CLA	C1D-ND	3.64	1.42	1.37
14	A	839	CLA	C1D-ND	3.64	1.42	1.37
14	J	102	CLA	C1D-ND	3.64	1.42	1.37
14	B	835	CLA	C1D-ND	3.64	1.42	1.37
14	K	102	CLA	C1D-ND	3.63	1.42	1.37
14	A	807	CLA	C1D-ND	3.63	1.42	1.37
17	A	849	BCR	C1-C6	-3.63	1.49	1.53
14	B	841	CLA	C1D-ND	3.63	1.42	1.37
14	B	837	CLA	C1D-ND	3.63	1.42	1.37
14	A	818	CLA	C1D-ND	3.63	1.42	1.37
14	B	812	CLA	C1D-ND	3.63	1.42	1.37
14	B	805	CLA	C1D-ND	3.63	1.42	1.37
14	B	828	CLA	C1D-ND	3.62	1.42	1.37
14	A	808	CLA	C1D-ND	3.62	1.42	1.37
14	A	810	CLA	C1D-ND	3.62	1.42	1.37
14	B	816	CLA	C1D-ND	3.62	1.42	1.37
14	B	818	CLA	C1D-ND	3.62	1.42	1.37
14	B	821	CLA	C1D-ND	3.62	1.42	1.37
14	L	206	CLA	C1D-ND	3.61	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	J	104	BCR	C1-C6	-3.61	1.49	1.53
14	B	831	CLA	C1D-ND	3.60	1.42	1.37
17	B	848	BCR	C30-C25	-3.60	1.49	1.53
14	A	823	CLA	C1D-ND	3.59	1.42	1.37
14	F	201	CLA	C1D-ND	3.59	1.42	1.37
14	A	826	CLA	C1D-ND	3.59	1.42	1.37
14	B	832	CLA	C1D-ND	3.59	1.42	1.37
17	I	101	BCR	C30-C25	-3.59	1.49	1.53
14	A	832	CLA	C1D-ND	3.59	1.42	1.37
14	B	840	CLA	C1D-ND	3.58	1.42	1.37
14	B	815	CLA	C1D-ND	3.58	1.42	1.37
14	B	804	CLA	C1D-ND	3.58	1.42	1.37
14	B	820	CLA	C1D-ND	3.58	1.42	1.37
14	A	817	CLA	C1D-ND	3.58	1.42	1.37
14	A	805	CLA	C1D-ND	3.57	1.42	1.37
14	B	824	CLA	C1D-ND	3.57	1.42	1.37
14	B	803	CLA	C1D-ND	3.57	1.42	1.37
14	A	822	CLA	C1D-ND	3.55	1.42	1.37
14	A	814	CLA	C1D-ND	3.55	1.42	1.37
14	A	821	CLA	C1D-ND	3.55	1.42	1.37
14	A	804	CLA	C1D-ND	3.55	1.42	1.37
14	A	830	CLA	C1D-ND	3.55	1.42	1.37
14	A	815	CLA	C1D-ND	3.54	1.42	1.37
14	A	844	CLA	C1D-ND	3.54	1.42	1.37
14	J	101	CLA	C1D-ND	3.54	1.42	1.37
14	A	841	CLA	C1D-ND	3.54	1.42	1.37
17	A	847	BCR	C1-C6	-3.54	1.49	1.53
17	L	208	BCR	C1-C6	-3.54	1.49	1.53
14	B	830	CLA	C1D-ND	3.53	1.42	1.37
17	L	201	BCR	C30-C25	-3.52	1.49	1.53
14	X	1701	CLA	C1D-ND	3.52	1.42	1.37
14	A	842	CLA	C1D-ND	3.52	1.42	1.37
14	A	820	CLA	C1D-ND	3.52	1.42	1.37
14	K	101	CLA	C1D-ND	3.51	1.42	1.37
14	A	834	CLA	C1D-ND	3.51	1.42	1.37
17	I	101	BCR	C1-C6	-3.51	1.49	1.53
14	B	814	CLA	C1D-ND	3.51	1.42	1.37
14	A	812	CLA	C1D-ND	3.51	1.42	1.37
14	A	833	CLA	C1D-ND	3.50	1.42	1.37
14	A	843	CLA	C4B-NB	3.49	1.42	1.37
14	L	204	CLA	C1D-ND	3.49	1.42	1.37
14	A	813	CLA	C1D-ND	3.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	819	CLA	C1D-ND	3.48	1.42	1.37
14	B	822	CLA	C1D-ND	3.48	1.42	1.37
14	A	831	CLA	C1D-ND	3.48	1.42	1.37
14	B	841	CLA	C4B-NB	3.48	1.42	1.37
17	B	847	BCR	C30-C25	-3.48	1.49	1.53
14	A	834	CLA	C4B-NB	3.47	1.42	1.37
14	A	808	CLA	C4B-NB	3.45	1.42	1.37
17	B	851	BCR	C30-C25	-3.45	1.49	1.53
14	A	807	CLA	C4B-NB	3.43	1.42	1.37
14	A	857	CLA	C1D-ND	3.43	1.42	1.37
17	A	852	BCR	C1-C6	-3.43	1.49	1.53
14	L	205	CLA	C1D-ND	3.43	1.42	1.37
17	B	843	BCR	C1-C6	-3.43	1.49	1.53
14	A	803	CLA	C1D-ND	3.42	1.42	1.37
14	A	802	CLA	C1D-ND	3.41	1.42	1.37
14	B	829	CLA	C1D-ND	3.41	1.42	1.37
14	A	837	CLA	C4B-NB	3.41	1.42	1.37
14	A	836	CLA	C4B-NB	3.39	1.42	1.37
14	B	809	CLA	C1D-ND	3.38	1.42	1.37
14	B	839	CLA	C4B-NB	3.38	1.42	1.37
14	B	835	CLA	C4B-NB	3.37	1.42	1.37
14	X	1701	CLA	C4B-NB	3.36	1.42	1.37
14	A	815	CLA	C4B-NB	3.36	1.42	1.37
17	J	105	BCR	C30-C25	-3.35	1.49	1.53
14	B	833	CLA	C1D-ND	3.35	1.42	1.37
17	F	203	BCR	C30-C25	-3.35	1.49	1.53
14	B	806	CLA	C4B-NB	3.35	1.42	1.37
14	B	838	CLA	C4B-NB	3.34	1.42	1.37
17	A	849	BCR	C30-C25	-3.33	1.49	1.53
14	M	102	CLA	C1D-ND	3.32	1.42	1.37
17	B	848	BCR	C1-C6	-3.32	1.49	1.53
17	B	844	BCR	C1-C6	-3.32	1.49	1.53
17	A	851	BCR	C30-C25	-3.32	1.49	1.53
14	A	823	CLA	C4B-NB	3.31	1.42	1.37
14	B	812	CLA	C4B-NB	3.30	1.42	1.37
17	J	103	BCR	C30-C25	-3.30	1.49	1.53
17	I	103	BCR	C30-C25	-3.30	1.49	1.53
14	A	835	CLA	C4B-NB	3.29	1.42	1.37
14	A	804	CLA	C4B-NB	3.29	1.42	1.37
14	A	842	CLA	C4B-NB	3.28	1.42	1.37
14	A	805	CLA	C4B-NB	3.28	1.42	1.37
14	A	857	CLA	C4B-NB	3.27	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	848	BCR	C30-C25	-3.27	1.49	1.53
17	A	851	BCR	C1-C6	-3.27	1.49	1.53
17	A	847	BCR	C30-C25	-3.27	1.49	1.53
17	B	846	BCR	C1-C6	-3.27	1.49	1.53
17	B	844	BCR	C30-C25	-3.26	1.49	1.53
14	F	202	CLA	C4B-NB	3.26	1.42	1.37
14	A	829	CLA	C4B-NB	3.26	1.42	1.37
15	B	842	PQN	C2-C1	-3.26	1.40	1.47
14	A	816	CLA	C4B-NB	3.26	1.42	1.37
14	F	201	CLA	C4B-NB	3.26	1.42	1.37
17	A	850	BCR	C30-C25	-3.25	1.49	1.53
14	B	814	CLA	C4B-NB	3.25	1.42	1.37
14	B	832	CLA	C4B-NB	3.25	1.42	1.37
14	A	840	CLA	C4B-NB	3.25	1.42	1.37
14	B	828	CLA	C4B-NB	3.24	1.42	1.37
14	B	803	CLA	C4B-NB	3.24	1.42	1.37
14	A	811	CLA	C4B-NB	3.24	1.42	1.37
14	A	802	CLA	C4B-NB	3.24	1.42	1.37
14	A	831	CLA	C4B-NB	3.24	1.42	1.37
14	A	827	CLA	C4B-NB	3.24	1.42	1.37
14	B	804	CLA	C4B-NB	3.24	1.42	1.37
17	F	203	BCR	C1-C6	-3.24	1.49	1.53
14	B	815	CLA	C4B-NB	3.23	1.42	1.37
15	A	845	PQN	C3-C2	3.23	1.41	1.35
14	J	101	CLA	C4B-NB	3.23	1.42	1.37
14	B	823	CLA	C4B-NB	3.22	1.42	1.37
14	A	828	CLA	C4B-NB	3.22	1.42	1.37
17	J	105	BCR	C1-C6	-3.22	1.49	1.53
14	K	102	CLA	C4B-NB	3.22	1.42	1.37
14	B	811	CLA	C4B-NB	3.21	1.42	1.37
14	M	102	CLA	C4B-NB	3.21	1.42	1.37
14	B	807	CLA	C4B-NB	3.21	1.42	1.37
14	B	820	CLA	C4B-NB	3.20	1.42	1.37
14	A	813	CLA	C4B-NB	3.20	1.42	1.37
15	B	842	PQN	C3-C2	3.20	1.40	1.35
14	B	837	CLA	C4B-NB	3.19	1.42	1.37
14	A	814	CLA	C4B-NB	3.19	1.42	1.37
17	M	103	BCR	C30-C25	-3.19	1.49	1.53
14	A	844	CLA	C4B-NB	3.18	1.42	1.37
14	B	830	CLA	C4B-NB	3.18	1.42	1.37
14	B	817	CLA	C4B-NB	3.18	1.42	1.37
14	A	812	CLA	C4B-NB	3.18	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	830	CLA	C4B-NB	3.17	1.42	1.37
14	A	822	CLA	C4B-NB	3.17	1.42	1.37
14	A	841	CLA	C4B-NB	3.16	1.42	1.37
14	A	820	CLA	C4B-NB	3.16	1.42	1.37
14	B	829	CLA	C4B-NB	3.16	1.42	1.37
14	A	810	CLA	C4B-NB	3.16	1.42	1.37
14	B	822	CLA	C4B-NB	3.16	1.42	1.37
17	A	852	BCR	C30-C25	-3.16	1.49	1.53
14	B	805	CLA	C4B-NB	3.15	1.42	1.37
14	A	821	CLA	C4B-NB	3.15	1.42	1.37
14	A	838	CLA	C4B-NB	3.15	1.42	1.37
14	L	206	CLA	C4B-NB	3.14	1.42	1.37
14	B	821	CLA	C4B-NB	3.14	1.42	1.37
17	J	104	BCR	C30-C25	-3.13	1.49	1.53
14	A	806	CLA	C4B-NB	3.13	1.42	1.37
14	A	817	CLA	C4B-NB	3.13	1.42	1.37
14	A	825	CLA	C4B-NB	3.12	1.42	1.37
14	B	816	CLA	C4B-NB	3.12	1.42	1.37
14	K	101	CLA	C4B-NB	3.12	1.42	1.37
14	B	840	CLA	C4B-NB	3.11	1.42	1.37
14	B	831	CLA	C4B-NB	3.11	1.41	1.37
14	B	827	CLA	C4B-NB	3.11	1.41	1.37
14	L	205	CLA	C4B-NB	3.11	1.41	1.37
14	A	826	CLA	C4B-NB	3.10	1.41	1.37
14	A	809	CLA	C4B-NB	3.10	1.41	1.37
14	B	825	CLA	C4B-NB	3.10	1.41	1.37
14	B	833	CLA	C4B-NB	3.10	1.41	1.37
14	J	102	CLA	C4B-NB	3.10	1.41	1.37
14	A	832	CLA	C4B-NB	3.10	1.41	1.37
14	B	834	CLA	C4B-NB	3.09	1.41	1.37
14	A	819	CLA	C4B-NB	3.09	1.41	1.37
14	A	824	CLA	C4B-NB	3.08	1.41	1.37
14	B	826	CLA	C4B-NB	3.08	1.41	1.37
17	B	845	BCR	C30-C25	-3.08	1.49	1.53
14	A	805	CLA	C1B-C2B	3.07	1.50	1.43
14	B	824	CLA	C4B-NB	3.07	1.41	1.37
17	B	843	BCR	C30-C25	-3.07	1.49	1.53
14	A	818	CLA	C4B-NB	3.06	1.41	1.37
14	A	833	CLA	C4B-NB	3.06	1.41	1.37
14	B	813	CLA	C4B-NB	3.05	1.41	1.37
14	B	818	CLA	C4B-NB	3.04	1.41	1.37
13	A	801	CL0	C4B-NB	3.02	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	803	CLA	C4B-NB	3.02	1.41	1.37
14	A	814	CLA	C1B-C2B	3.02	1.50	1.43
14	B	810	CLA	C4B-NB	3.01	1.41	1.37
18	A	856	LMG	O7-C8	-3.00	1.41	1.47
14	B	808	CLA	C4B-NB	3.00	1.41	1.37
14	B	802	CLA	C1B-C2B	3.00	1.50	1.43
15	A	845	PQN	C2-C1	-3.00	1.40	1.47
14	B	805	CLA	C1B-C2B	2.99	1.50	1.43
14	B	822	CLA	C1B-C2B	2.98	1.50	1.43
14	B	802	CLA	C4B-NB	2.98	1.41	1.37
14	A	841	CLA	C1B-C2B	2.97	1.50	1.43
14	B	823	CLA	C1B-C2B	2.96	1.50	1.43
14	B	804	CLA	C1B-C2B	2.95	1.50	1.43
15	B	842	PQN	C3-C4	-2.95	1.39	1.47
14	A	839	CLA	C4B-NB	2.94	1.41	1.37
14	M	102	CLA	C1B-C2B	2.94	1.50	1.43
14	A	811	CLA	C1B-C2B	2.93	1.50	1.43
14	B	832	CLA	C1B-C2B	2.93	1.50	1.43
14	B	827	CLA	C1B-C2B	2.93	1.50	1.43
14	B	825	CLA	C1B-C2B	2.93	1.50	1.43
15	A	845	PQN	C3-C4	-2.93	1.39	1.47
14	B	809	CLA	C4B-NB	2.93	1.41	1.37
14	A	829	CLA	C1B-C2B	2.92	1.50	1.43
14	B	808	CLA	C1B-C2B	2.92	1.50	1.43
14	B	806	CLA	C1B-C2B	2.92	1.50	1.43
14	A	813	CLA	C1B-C2B	2.92	1.50	1.43
14	A	842	CLA	C1B-C2B	2.91	1.50	1.43
14	B	819	CLA	C4B-NB	2.91	1.41	1.37
14	A	812	CLA	C1B-C2B	2.91	1.49	1.43
14	B	815	CLA	C1B-C2B	2.91	1.49	1.43
17	B	846	BCR	C30-C25	-2.90	1.50	1.53
14	A	818	CLA	C1B-C2B	2.90	1.49	1.43
14	J	102	CLA	C1B-C2B	2.90	1.49	1.43
14	A	838	CLA	C1B-C2B	2.90	1.49	1.43
14	A	828	CLA	C1B-C2B	2.88	1.49	1.43
14	B	826	CLA	C1B-C2B	2.88	1.49	1.43
14	A	833	CLA	C1B-C2B	2.88	1.49	1.43
14	B	813	CLA	C1B-C2B	2.88	1.49	1.43
14	A	817	CLA	C1B-C2B	2.88	1.49	1.43
14	K	102	CLA	C1B-C2B	2.88	1.49	1.43
14	B	814	CLA	C1B-C2B	2.87	1.49	1.43
14	X	1701	CLA	C1B-C2B	2.87	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	836	CLA	C1B-C2B	2.87	1.49	1.43
17	L	208	BCR	C30-C25	-2.87	1.50	1.53
14	B	828	CLA	C1B-C2B	2.87	1.49	1.43
14	L	204	CLA	C4B-NB	2.85	1.41	1.37
18	I	102	LMG	C4-C5	2.85	1.59	1.53
14	A	839	CLA	C1B-C2B	2.85	1.49	1.43
14	B	807	CLA	C1B-C2B	2.85	1.49	1.43
14	A	840	CLA	C1B-C2B	2.85	1.49	1.43
14	A	806	CLA	C1B-C2B	2.84	1.49	1.43
14	B	833	CLA	C1B-C2B	2.84	1.49	1.43
14	A	827	CLA	C1B-C2B	2.84	1.49	1.43
14	A	824	CLA	C1B-C2B	2.83	1.49	1.43
14	B	810	CLA	C1B-C2B	2.83	1.49	1.43
14	A	816	CLA	C1B-C2B	2.83	1.49	1.43
14	B	816	CLA	C1B-C2B	2.83	1.49	1.43
14	F	201	CLA	C1B-C2B	2.83	1.49	1.43
14	B	835	CLA	C1B-C2B	2.83	1.49	1.43
14	A	823	CLA	C1B-C2B	2.83	1.49	1.43
14	A	815	CLA	C1B-C2B	2.83	1.49	1.43
14	B	838	CLA	C1B-C2B	2.83	1.49	1.43
14	A	857	CLA	C1B-C2B	2.82	1.49	1.43
14	J	101	CLA	C1B-C2B	2.82	1.49	1.43
13	A	801	CL0	C1B-C2B	2.82	1.49	1.43
14	A	821	CLA	C1B-C2B	2.82	1.49	1.43
14	A	825	CLA	C1B-C2B	2.81	1.49	1.43
14	A	835	CLA	C1B-C2B	2.80	1.49	1.43
14	B	837	CLA	C1B-C2B	2.80	1.49	1.43
14	B	841	CLA	C1B-C2B	2.79	1.49	1.43
14	B	817	CLA	C1B-C2B	2.79	1.49	1.43
14	K	101	CLA	C1B-C2B	2.79	1.49	1.43
14	B	834	CLA	C1B-C2B	2.79	1.49	1.43
14	A	810	CLA	C1B-C2B	2.78	1.49	1.43
14	A	844	CLA	C1B-C2B	2.77	1.49	1.43
14	B	840	CLA	C1B-C2B	2.76	1.49	1.43
14	B	811	CLA	C1B-C2B	2.76	1.49	1.43
14	L	204	CLA	C1B-C2B	2.76	1.49	1.43
14	B	818	CLA	C1B-C2B	2.75	1.49	1.43
14	A	802	CLA	C1B-C2B	2.75	1.49	1.43
14	A	830	CLA	C1B-C2B	2.75	1.49	1.43
14	A	822	CLA	C1B-C2B	2.74	1.49	1.43
14	F	202	CLA	C1B-C2B	2.73	1.49	1.43
14	A	834	CLA	C1B-C2B	2.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	837	CLA	C1B-C2B	2.72	1.49	1.43
14	B	839	CLA	C1B-C2B	2.71	1.49	1.43
14	B	821	CLA	C1B-C2B	2.71	1.49	1.43
14	A	831	CLA	C1B-C2B	2.71	1.49	1.43
14	A	832	CLA	C1B-C2B	2.71	1.49	1.43
14	A	807	CLA	C1B-C2B	2.71	1.49	1.43
14	A	826	CLA	C1B-C2B	2.71	1.49	1.43
14	A	804	CLA	C1B-C2B	2.71	1.49	1.43
14	A	809	CLA	C1B-C2B	2.70	1.49	1.43
14	B	829	CLA	C1B-C2B	2.69	1.49	1.43
14	A	808	CLA	C1B-C2B	2.68	1.49	1.43
14	B	819	CLA	C1B-C2B	2.68	1.49	1.43
14	B	824	CLA	C1B-C2B	2.67	1.49	1.43
14	B	803	CLA	C1B-C2B	2.67	1.49	1.43
14	L	205	CLA	C1B-C2B	2.67	1.49	1.43
14	A	843	CLA	C1B-C2B	2.66	1.49	1.43
14	B	831	CLA	C1B-C2B	2.66	1.49	1.43
14	B	836	CLA	C3B-C4B	2.65	1.50	1.42
14	B	836	CLA	C1B-C2B	2.65	1.49	1.43
14	B	820	CLA	C1B-C2B	2.63	1.49	1.43
14	A	820	CLA	C1B-C2B	2.63	1.49	1.43
14	B	830	CLA	C1B-C2B	2.62	1.49	1.43
14	A	843	CLA	C3B-C4B	2.62	1.50	1.42
14	A	803	CLA	CHC-C1C	2.61	1.43	1.38
14	L	206	CLA	C1B-C2B	2.59	1.49	1.43
14	B	812	CLA	C1B-C2B	2.59	1.49	1.43
14	A	807	CLA	C3B-C4B	2.58	1.50	1.42
14	B	803	CLA	CHC-C1C	2.57	1.43	1.38
22	L	207	DGD	O2G-C2G	-2.57	1.40	1.46
14	B	803	CLA	C3B-C4B	2.56	1.50	1.42
14	A	808	CLA	CHC-C1C	2.56	1.43	1.38
14	B	820	CLA	C3B-C4B	2.56	1.50	1.42
14	B	809	CLA	C1B-C2B	2.56	1.49	1.43
14	A	834	CLA	CHC-C1C	2.53	1.43	1.38
14	A	804	CLA	C3B-C4B	2.52	1.50	1.42
14	L	206	CLA	C3B-C4B	2.52	1.50	1.42
14	A	829	CLA	C3B-C4B	2.49	1.50	1.42
14	B	812	CLA	C3B-C4B	2.49	1.50	1.42
14	A	837	CLA	C3B-C4B	2.49	1.50	1.42
14	A	803	CLA	C3B-C4B	2.49	1.50	1.42
14	B	809	CLA	CMB-C2B	-2.49	1.45	1.50
14	M	102	CLA	CMD-C2D	-2.49	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	834	CLA	C3B-C4B	2.48	1.50	1.42
14	B	828	CLA	C3B-C4B	2.48	1.49	1.42
14	F	202	CLA	C3B-C4B	2.47	1.49	1.42
14	A	857	CLA	C3B-C4B	2.47	1.49	1.42
14	A	827	CLA	C3B-C4B	2.46	1.49	1.42
14	A	819	CLA	CHC-C1C	2.46	1.43	1.38
14	A	825	CLA	C3B-C4B	2.45	1.49	1.42
14	B	822	CLA	C3B-C4B	2.44	1.49	1.42
14	A	807	CLA	CHC-C1C	2.44	1.43	1.38
14	A	828	CLA	CHC-C1C	2.44	1.43	1.38
14	A	844	CLA	C3B-C4B	2.44	1.49	1.42
14	B	827	CLA	C3B-C4B	2.44	1.49	1.42
14	B	838	CLA	C3B-C4B	2.43	1.49	1.42
14	A	809	CLA	CHC-C1C	2.43	1.43	1.38
14	B	824	CLA	C3B-C4B	2.43	1.49	1.42
14	J	101	CLA	C3B-C4B	2.43	1.49	1.42
14	A	802	CLA	C3B-C4B	2.43	1.49	1.42
14	A	826	CLA	C3B-C4B	2.43	1.49	1.42
14	B	839	CLA	C3B-C4B	2.42	1.49	1.42
14	A	833	CLA	C3B-C4B	2.42	1.49	1.42
14	B	825	CLA	C3B-C4B	2.42	1.49	1.42
14	A	819	CLA	C3B-C4B	2.42	1.49	1.42
14	J	101	CLA	CHC-C1C	2.42	1.43	1.38
14	B	840	CLA	C3B-C4B	2.42	1.49	1.42
14	B	812	CLA	CHC-C1C	2.42	1.43	1.38
14	B	837	CLA	CHC-C1C	2.42	1.43	1.38
14	B	837	CLA	C3B-C4B	2.42	1.49	1.42
14	A	823	CLA	C3B-C4B	2.42	1.49	1.42
14	A	815	CLA	CHC-C1C	2.41	1.43	1.38
14	A	819	CLA	C1B-C2B	2.41	1.48	1.43
14	A	830	CLA	C3B-C4B	2.41	1.49	1.42
14	B	824	CLA	CHC-C1C	2.41	1.43	1.38
14	A	836	CLA	C3B-C4B	2.41	1.49	1.42
14	B	816	CLA	CHC-C1C	2.41	1.43	1.38
14	B	817	CLA	C3B-C4B	2.41	1.49	1.42
14	L	205	CLA	C3B-C4B	2.41	1.49	1.42
14	B	830	CLA	CHC-C1C	2.40	1.43	1.38
14	A	826	CLA	CHC-C1C	2.40	1.43	1.38
14	A	824	CLA	C3B-C4B	2.40	1.49	1.42
14	A	804	CLA	CHC-C1C	2.40	1.43	1.38
21	L	202	LMT	O3'-C3'	-2.39	1.37	1.43
14	A	857	CLA	CHC-C1C	2.39	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	814	CLA	CHC-C1C	2.39	1.43	1.38
14	L	205	CLA	CHC-C1C	2.39	1.43	1.38
14	B	830	CLA	C3B-C4B	2.39	1.49	1.42
14	F	201	CLA	C3B-C4B	2.39	1.49	1.42
14	B	816	CLA	C3B-C4B	2.39	1.49	1.42
14	A	822	CLA	C3B-C4B	2.39	1.49	1.42
14	B	819	CLA	CHC-C1C	2.39	1.43	1.38
14	B	835	CLA	C3B-C4B	2.38	1.49	1.42
14	A	835	CLA	CHC-C1C	2.38	1.43	1.38
14	B	831	CLA	CHC-C1C	2.38	1.43	1.38
14	A	828	CLA	C3B-C4B	2.38	1.49	1.42
14	A	822	CLA	CHC-C1C	2.38	1.43	1.38
14	L	206	CLA	CHC-C1C	2.38	1.43	1.38
14	A	823	CLA	CHC-C1C	2.37	1.43	1.38
14	A	827	CLA	CHC-C1C	2.37	1.43	1.38
14	B	838	CLA	CHC-C1C	2.37	1.43	1.38
14	B	829	CLA	C3B-C4B	2.37	1.49	1.42
14	B	815	CLA	C3B-C4B	2.37	1.49	1.42
14	B	813	CLA	C3B-C4B	2.37	1.49	1.42
14	A	803	CLA	C1B-C2B	2.37	1.48	1.43
14	B	834	CLA	C3B-C4B	2.37	1.49	1.42
14	A	842	CLA	C3B-C4B	2.37	1.49	1.42
14	B	831	CLA	C3B-C4B	2.37	1.49	1.42
14	A	820	CLA	CHC-C1C	2.37	1.43	1.38
14	A	809	CLA	C3B-C4B	2.36	1.49	1.42
14	B	806	CLA	C3B-C4B	2.36	1.49	1.42
14	B	832	CLA	C3B-C4B	2.36	1.49	1.42
14	A	835	CLA	C3B-C4B	2.36	1.49	1.42
14	B	823	CLA	CHC-C1C	2.36	1.43	1.38
14	F	201	CLA	CHC-C1C	2.36	1.43	1.38
14	B	826	CLA	C3B-C4B	2.35	1.49	1.42
14	B	827	CLA	CHC-C1C	2.35	1.43	1.38
14	F	202	CLA	CHC-C1C	2.35	1.43	1.38
14	B	833	CLA	CHC-C1C	2.35	1.43	1.38
14	A	821	CLA	C3B-C4B	2.35	1.49	1.42
14	A	842	CLA	CHC-C1C	2.35	1.43	1.38
14	A	820	CLA	C3B-C4B	2.34	1.49	1.42
14	A	813	CLA	C3B-C4B	2.34	1.49	1.42
14	K	101	CLA	C3B-C4B	2.34	1.49	1.42
14	X	1701	CLA	C3B-C4B	2.34	1.49	1.42
14	B	819	CLA	C3B-C4B	2.34	1.49	1.42
14	K	101	CLA	CHC-C1C	2.33	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	817	CLA	CHC-C1C	2.33	1.43	1.38
14	A	806	CLA	C3B-C4B	2.33	1.49	1.42
14	A	840	CLA	C3B-C4B	2.33	1.49	1.42
14	A	824	CLA	CHC-C1C	2.33	1.43	1.38
14	B	820	CLA	CHC-C1C	2.33	1.43	1.38
14	A	830	CLA	CHC-C1C	2.33	1.43	1.38
14	A	825	CLA	CHC-C1C	2.33	1.43	1.38
14	A	829	CLA	CHC-C1C	2.33	1.43	1.38
14	B	834	CLA	CHC-C1C	2.33	1.43	1.38
14	A	831	CLA	CMB-C2B	-2.32	1.46	1.50
14	B	828	CLA	CHC-C1C	2.32	1.43	1.38
14	B	835	CLA	CHC-C1C	2.32	1.43	1.38
14	A	811	CLA	C3B-C4B	2.32	1.49	1.42
14	A	805	CLA	CHC-C1C	2.32	1.43	1.38
14	A	821	CLA	CHC-C1C	2.32	1.43	1.38
14	A	812	CLA	C3B-C4B	2.31	1.49	1.42
14	A	814	CLA	C3B-C4B	2.31	1.49	1.42
14	K	102	CLA	C3B-C4B	2.31	1.49	1.42
14	B	833	CLA	C3B-C4B	2.31	1.49	1.42
14	A	806	CLA	CHC-C1C	2.31	1.43	1.38
14	A	810	CLA	CMB-C2B	-2.30	1.46	1.50
14	A	810	CLA	C3B-C4B	2.30	1.49	1.42
14	A	837	CLA	CHC-C1C	2.30	1.43	1.38
14	B	832	CLA	CHC-C1C	2.30	1.43	1.38
14	B	840	CLA	CHC-C1C	2.30	1.43	1.38
14	A	831	CLA	C3B-C4B	2.30	1.49	1.42
14	A	839	CLA	C3B-C4B	2.30	1.49	1.42
14	B	804	CLA	C3B-C4B	2.30	1.49	1.42
14	A	815	CLA	C3B-C4B	2.30	1.49	1.42
14	B	806	CLA	CHC-C1C	2.30	1.43	1.38
18	B	849	LMG	O7-C8	-2.29	1.41	1.46
14	A	844	CLA	CHC-C1C	2.29	1.43	1.38
14	A	816	CLA	C3B-C4B	2.29	1.49	1.42
14	A	808	CLA	C3B-C4B	2.29	1.49	1.42
14	B	823	CLA	C3B-C4B	2.29	1.49	1.42
14	B	826	CLA	CHC-C1C	2.28	1.43	1.38
14	K	102	CLA	CHC-C1C	2.28	1.43	1.38
14	B	813	CLA	CHC-C1C	2.28	1.43	1.38
14	A	833	CLA	CHC-C1C	2.28	1.43	1.38
14	A	832	CLA	C3B-C4B	2.28	1.49	1.42
14	A	811	CLA	CHC-C1C	2.28	1.43	1.38
14	B	805	CLA	C3B-C4B	2.28	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	839	CLA	CHC-C1C	2.28	1.43	1.38
14	B	818	CLA	CHC-C1C	2.27	1.43	1.38
14	B	807	CLA	C3B-C4B	2.27	1.49	1.42
14	A	816	CLA	CHC-C1C	2.27	1.43	1.38
14	A	818	CLA	CHC-C1C	2.27	1.43	1.38
14	B	809	CLA	MG-NB	-2.27	2.01	2.05
14	A	814	CLA	CHC-C1C	2.27	1.43	1.38
14	B	818	CLA	C3B-C4B	2.26	1.49	1.42
14	A	841	CLA	CHC-C1C	2.26	1.43	1.38
19	A	855	LHG	P-O6	2.26	1.68	1.59
14	A	841	CLA	C3B-C4B	2.26	1.49	1.42
14	J	102	CLA	CHC-C1C	2.26	1.43	1.38
14	B	808	CLA	C3B-C4B	2.26	1.49	1.42
19	B	850	LHG	P-O6	2.26	1.68	1.59
14	B	836	CLA	CHC-C1C	2.25	1.43	1.38
14	J	102	CLA	C3B-C4B	2.25	1.49	1.42
14	B	822	CLA	CHC-C1C	2.25	1.43	1.38
14	B	833	CLA	CMD-C2D	-2.25	1.46	1.50
14	B	828	CLA	CMD-C2D	-2.25	1.46	1.50
14	B	802	CLA	CHC-C1C	2.24	1.43	1.38
14	B	811	CLA	C3B-C4B	2.24	1.49	1.42
14	B	810	CLA	C3B-C4B	2.24	1.49	1.42
14	B	804	CLA	CHC-C1C	2.24	1.43	1.38
14	A	805	CLA	C3B-C4B	2.24	1.49	1.42
14	A	802	CLA	CHC-C1C	2.24	1.43	1.38
14	B	814	CLA	C3B-C4B	2.24	1.49	1.42
14	B	841	CLA	C3B-C4B	2.24	1.49	1.42
14	A	817	CLA	CHC-C1C	2.23	1.43	1.38
14	J	102	CLA	CBD-CAD	2.23	1.56	1.51
14	A	838	CLA	C3B-C4B	2.23	1.49	1.42
14	A	818	CLA	C3B-C4B	2.23	1.49	1.42
14	A	813	CLA	CHC-C1C	2.23	1.43	1.38
14	B	821	CLA	C3B-C4B	2.22	1.49	1.42
14	A	819	CLA	MG-NB	-2.22	2.01	2.05
14	A	839	CLA	CHC-C1C	2.22	1.42	1.38
14	B	808	CLA	CHC-C1C	2.22	1.42	1.38
14	B	802	CLA	C3B-C4B	2.22	1.49	1.42
14	B	841	CLA	CMB-C2B	-2.21	1.46	1.50
14	A	817	CLA	C3B-C4B	2.21	1.49	1.42
14	A	813	CLA	CMD-C2D	-2.21	1.46	1.50
14	B	815	CLA	CHC-C1C	2.21	1.42	1.38
14	A	812	CLA	CHC-C1C	2.21	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	207	DGD	O5D-C6D	-2.20	1.39	1.43
13	A	801	CL0	C3B-C4B	2.20	1.49	1.42
14	M	102	CLA	CMB-C2B	-2.20	1.46	1.50
14	B	812	CLA	CMB-C2B	-2.20	1.46	1.50
13	A	801	CL0	CHC-C1C	2.19	1.42	1.38
14	A	838	CLA	CHC-C1C	2.19	1.42	1.38
14	B	821	CLA	CMB-C2B	-2.19	1.46	1.50
14	A	832	CLA	CMB-C2B	-2.19	1.46	1.50
14	A	802	CLA	CMD-C2D	-2.19	1.46	1.50
14	M	102	CLA	CHC-C1C	2.19	1.42	1.38
14	B	811	CLA	CHC-C1C	2.19	1.42	1.38
14	B	829	CLA	CMB-C2B	-2.18	1.46	1.50
14	A	805	CLA	CMD-C2D	-2.18	1.46	1.50
14	B	830	CLA	CMB-C2B	-2.18	1.46	1.50
14	B	805	CLA	CHC-C1C	2.18	1.42	1.38
14	K	101	CLA	CBD-CAD	2.18	1.56	1.51
14	B	829	CLA	CHC-C1C	2.18	1.42	1.38
14	A	836	CLA	CHC-C1C	2.18	1.42	1.38
14	A	810	CLA	CHC-C1C	2.17	1.42	1.38
13	A	801	CL0	CMB-C2B	-2.17	1.46	1.50
14	B	825	CLA	CHC-C1C	2.17	1.42	1.38
14	X	1701	CLA	CHC-C1C	2.17	1.42	1.38
14	A	833	CLA	MG-NB	-2.16	2.01	2.05
14	L	204	CLA	C3B-C4B	2.16	1.49	1.42
14	A	830	CLA	CMD-C2D	-2.16	1.46	1.50
14	A	832	CLA	CHC-C1C	2.16	1.42	1.38
14	B	821	CLA	CHC-C1C	2.15	1.42	1.38
14	A	857	CLA	CMD-C2D	-2.15	1.46	1.50
21	L	202	LMT	O2B-C2B	-2.15	1.37	1.43
14	A	842	CLA	CMC-C2C	-2.15	1.46	1.50
19	B	850	LHG	O7-C5	-2.15	1.41	1.46
14	B	829	CLA	CMD-C2D	-2.14	1.46	1.50
14	A	814	CLA	CMD-C2D	-2.14	1.46	1.50
14	B	841	CLA	MG-NB	-2.14	2.01	2.05
14	A	803	CLA	CMD-C2D	-2.14	1.46	1.50
14	L	204	CLA	MG-NB	-2.14	2.01	2.05
14	M	102	CLA	MG-NB	-2.13	2.01	2.05
14	A	840	CLA	CHC-C1C	2.13	1.42	1.38
14	A	832	CLA	MG-NB	-2.13	2.01	2.05
14	B	807	CLA	CHC-C1C	2.12	1.42	1.38
14	B	819	CLA	MG-NB	-2.12	2.01	2.05
14	A	815	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	843	CLA	CHC-C1C	2.12	1.42	1.38
14	A	831	CLA	CHC-C1C	2.12	1.42	1.38
14	B	810	CLA	CHC-C1C	2.12	1.42	1.38
14	L	204	CLA	CHC-C1C	2.11	1.42	1.38
14	A	819	CLA	CMB-C2B	-2.11	1.46	1.50
14	B	823	CLA	CMD-C2D	-2.11	1.46	1.50
14	A	842	CLA	CMD-C2D	-2.11	1.46	1.50
19	A	855	LHG	O7-C5	-2.11	1.41	1.46
14	A	818	CLA	MG-NB	-2.11	2.01	2.05
14	A	803	CLA	MG-NB	-2.11	2.01	2.05
14	M	102	CLA	C3B-C4B	2.11	1.48	1.42
14	B	811	CLA	CMB-C2B	-2.10	1.46	1.50
21	L	202	LMT	O3B-C3B	-2.10	1.37	1.43
14	B	827	CLA	CMC-C2C	-2.10	1.46	1.50
18	A	856	LMG	C7-C8	2.10	1.55	1.50
14	A	826	CLA	CMD-C2D	-2.10	1.46	1.50
14	B	827	CLA	CMD-C2D	-2.09	1.46	1.50
14	A	821	CLA	CMD-C2D	-2.09	1.46	1.50
14	B	840	CLA	CMB-C2B	-2.09	1.46	1.50
14	A	804	CLA	CMD-C2D	-2.09	1.46	1.50
14	B	807	CLA	MG-NB	-2.09	2.01	2.05
14	B	809	CLA	CHC-C1C	2.09	1.42	1.38
13	A	801	CL0	MG-NB	-2.09	2.01	2.05
14	A	808	CLA	CMB-C2B	-2.09	1.46	1.50
14	B	808	CLA	CMD-C2D	-2.09	1.46	1.50
14	B	830	CLA	CMD-C2D	-2.09	1.46	1.50
14	A	822	CLA	CMD-C2D	-2.09	1.46	1.50
14	B	807	CLA	CMB-C2B	-2.09	1.46	1.50
14	A	839	CLA	MG-NB	-2.08	2.01	2.05
14	B	822	CLA	CMD-C2D	-2.08	1.46	1.50
14	B	809	CLA	C3B-C4B	2.08	1.48	1.42
14	A	833	CLA	CMD-C2D	-2.08	1.46	1.50
14	B	804	CLA	CMD-C2D	-2.08	1.46	1.50
14	A	827	CLA	CMD-C2D	-2.08	1.46	1.50
14	B	810	CLA	CMC-C2C	-2.08	1.46	1.50
14	A	812	CLA	CMD-C2D	-2.08	1.46	1.50
14	B	814	CLA	CMD-C2D	-2.08	1.46	1.50
14	B	819	CLA	CMD-C2D	-2.08	1.46	1.50
14	B	806	CLA	CMD-C2D	-2.08	1.46	1.50
14	L	204	CLA	CMD-C2D	-2.08	1.46	1.50
14	B	820	CLA	CMD-C2D	-2.08	1.46	1.50
19	A	854	LHG	P-O6	2.08	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	831	CLA	MG-NB	-2.08	2.01	2.05
14	A	803	CLA	CMB-C2B	-2.07	1.46	1.50
14	B	835	CLA	CMB-C2B	-2.07	1.46	1.50
14	B	824	CLA	CMD-C2D	-2.07	1.46	1.50
14	A	819	CLA	CMD-C2D	-2.07	1.46	1.50
14	K	101	CLA	CMD-C2D	-2.07	1.46	1.50
14	B	816	CLA	CMD-C2D	-2.07	1.46	1.50
14	A	840	CLA	MG-NB	-2.07	2.01	2.05
14	B	815	CLA	CMD-C2D	-2.06	1.46	1.50
14	B	838	CLA	CMD-C2D	-2.06	1.46	1.50
14	A	807	CLA	CMD-C2D	-2.06	1.46	1.50
14	B	819	CLA	CMC-C2C	-2.06	1.46	1.50
14	B	808	CLA	CMC-C2C	-2.06	1.46	1.50
14	B	836	CLA	CMD-C2D	-2.06	1.46	1.50
14	A	828	CLA	CMD-C2D	-2.06	1.46	1.50
14	A	843	CLA	CMB-C2B	-2.06	1.46	1.50
14	A	810	CLA	CMD-C2D	-2.06	1.46	1.50
14	F	201	CLA	CMD-C2D	-2.06	1.46	1.50
14	A	839	CLA	CMD-C2D	-2.06	1.46	1.50
14	B	831	CLA	CMD-C2D	-2.05	1.46	1.50
14	A	817	CLA	CMB-C2B	-2.05	1.46	1.50
14	B	839	CLA	MG-NB	-2.05	2.01	2.05
14	B	826	CLA	CMD-C2D	-2.05	1.46	1.50
14	K	101	CLA	MG-NB	-2.05	2.01	2.05
14	A	818	CLA	CMD-C2D	-2.05	1.46	1.50
14	B	830	CLA	MG-NB	-2.05	2.01	2.05
14	A	841	CLA	CMC-C2C	-2.05	1.46	1.50
14	B	813	CLA	CMC-C2C	-2.05	1.46	1.50
14	A	835	CLA	CMD-C2D	-2.05	1.46	1.50
14	B	813	CLA	MG-NB	-2.05	2.01	2.05
14	A	817	CLA	MG-NB	-2.05	2.01	2.05
14	B	837	CLA	CMD-C2D	-2.04	1.46	1.50
14	B	834	CLA	CMB-C2B	-2.04	1.46	1.50
14	A	809	CLA	CMB-C2B	-2.04	1.46	1.50
14	B	813	CLA	CMD-C2D	-2.04	1.46	1.50
14	A	841	CLA	CMD-C2D	-2.04	1.46	1.50
14	A	813	CLA	MG-NB	-2.04	2.01	2.05
14	A	829	CLA	CMD-C2D	-2.04	1.46	1.50
14	L	204	CLA	CMB-C2B	-2.04	1.46	1.50
14	A	824	CLA	CMD-C2D	-2.04	1.46	1.50
13	A	801	CL0	CMD-C2D	-2.04	1.46	1.50
14	A	831	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	836	CLA	CMB-C2B	-2.04	1.46	1.50
14	A	825	CLA	CMD-C2D	-2.04	1.46	1.50
14	A	838	CLA	CMD-C2D	-2.03	1.46	1.50
14	B	809	CLA	CMD-C2D	-2.03	1.46	1.50
14	K	102	CLA	CMD-C2D	-2.03	1.46	1.50
14	A	823	CLA	CMD-C2D	-2.03	1.46	1.50
14	B	825	CLA	CMD-C2D	-2.03	1.46	1.50
14	B	805	CLA	CMD-C2D	-2.03	1.46	1.50
14	A	838	CLA	CMB-C2B	-2.03	1.46	1.50
14	A	808	CLA	CMD-C2D	-2.03	1.46	1.50
14	F	202	CLA	CMD-C2D	-2.03	1.46	1.50
14	B	832	CLA	CMD-C2D	-2.03	1.46	1.50
14	B	835	CLA	CMD-C2D	-2.03	1.46	1.50
14	J	101	CLA	CMD-C2D	-2.03	1.46	1.50
14	A	844	CLA	CMD-C2D	-2.02	1.46	1.50
14	B	802	CLA	CMD-C2D	-2.02	1.46	1.50
18	A	853	LMG	O7-C8	-2.02	1.41	1.46
14	B	841	CLA	CHC-C1C	2.02	1.42	1.38
14	A	809	CLA	CMD-C2D	-2.02	1.46	1.50
14	L	205	CLA	CMD-C2D	-2.02	1.46	1.50
14	B	823	CLA	CMB-C2B	-2.02	1.46	1.50
14	A	815	CLA	MG-NB	-2.01	2.01	2.05
14	A	806	CLA	CMD-C2D	-2.01	1.46	1.50
14	B	824	CLA	CMB-C2B	-2.01	1.46	1.50
14	L	205	CLA	CMB-C2B	-2.01	1.46	1.50
14	A	820	CLA	CMB-C2B	-2.01	1.46	1.50
14	B	810	CLA	CMD-C2D	-2.01	1.46	1.50
14	B	819	CLA	CMB-C2B	-2.01	1.46	1.50
14	B	818	CLA	MG-NB	-2.01	2.01	2.05
14	J	102	CLA	MG-NB	-2.01	2.01	2.05
14	A	816	CLA	CMC-C2C	-2.01	1.46	1.50
14	A	816	CLA	CMD-C2D	-2.01	1.46	1.50
14	B	803	CLA	CMD-C2D	-2.01	1.46	1.50
14	L	205	CLA	MG-NB	-2.01	2.01	2.05
14	A	811	CLA	CMD-C2D	-2.01	1.46	1.50
14	B	839	CLA	CMD-C2D	-2.01	1.46	1.50
14	A	836	CLA	CMD-C2D	-2.00	1.46	1.50
14	B	821	CLA	MG-NB	-2.00	2.01	2.05
14	A	826	CLA	CMB-C2B	-2.00	1.46	1.50
14	A	820	CLA	CMD-C2D	-2.00	1.46	1.50
14	X	1701	CLA	CMD-C2D	-2.00	1.46	1.50
14	A	840	CLA	CMD-C2D	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	812	CLA	CMD-C2D	-2.00	1.46	1.50
14	B	839	CLA	CMB-C2B	-2.00	1.46	1.50
14	A	810	CLA	MG-NB	-2.00	2.01	2.05

All (715) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	842	CLA	C4A-NA-C1A	7.29	110.00	106.68
14	B	802	CLA	C4A-NA-C1A	7.21	109.97	106.68
14	B	810	CLA	C4A-NA-C1A	7.10	109.92	106.68
14	B	811	CLA	C4A-NA-C1A	6.92	109.83	106.68
14	L	204	CLA	C4A-NA-C1A	6.83	109.79	106.68
14	A	806	CLA	C4A-NA-C1A	6.82	109.79	106.68
14	A	840	CLA	C4A-NA-C1A	6.80	109.78	106.68
13	A	801	CL0	C4A-NA-C1A	6.74	109.75	106.68
14	B	804	CLA	C4A-NA-C1A	6.67	109.72	106.68
14	B	805	CLA	C4A-NA-C1A	6.66	109.72	106.68
14	B	841	CLA	C4A-NA-C1A	6.65	109.71	106.68
14	B	838	CLA	C4A-NA-C1A	6.64	109.71	106.68
14	B	814	CLA	C4A-NA-C1A	6.62	109.70	106.68
14	B	832	CLA	C4A-NA-C1A	6.55	109.67	106.68
14	B	807	CLA	C4A-NA-C1A	6.50	109.64	106.68
14	B	835	CLA	C4A-NA-C1A	6.49	109.64	106.68
14	J	101	CLA	C4A-NA-C1A	6.49	109.64	106.68
14	B	837	CLA	C4A-NA-C1A	6.49	109.64	106.68
14	A	818	CLA	C4A-NA-C1A	6.47	109.63	106.68
14	L	206	CLA	C4A-NA-C1A	6.46	109.63	106.68
14	A	814	CLA	C4A-NA-C1A	6.44	109.62	106.68
14	B	819	CLA	C4A-NA-C1A	6.40	109.60	106.68
14	A	844	CLA	C4A-NA-C1A	6.40	109.60	106.68
14	B	826	CLA	C4A-NA-C1A	6.36	109.58	106.68
14	A	816	CLA	C4A-NA-C1A	6.35	109.58	106.68
14	A	839	CLA	C4A-NA-C1A	6.35	109.58	106.68
14	B	840	CLA	C4A-NA-C1A	6.35	109.58	106.68
14	F	201	CLA	C4A-NA-C1A	6.34	109.57	106.68
14	B	822	CLA	C4A-NA-C1A	6.34	109.57	106.68
14	B	834	CLA	C4A-NA-C1A	6.33	109.57	106.68
14	A	809	CLA	C4A-NA-C1A	6.33	109.57	106.68
14	M	102	CLA	C4A-NA-C1A	6.31	109.56	106.68
14	K	102	CLA	C4A-NA-C1A	6.31	109.56	106.68
14	B	809	CLA	C4A-NA-C1A	6.31	109.56	106.68
14	A	825	CLA	C4A-NA-C1A	6.30	109.55	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	812	CLA	C4A-NA-C1A	6.29	109.55	106.68
14	B	808	CLA	C4A-NA-C1A	6.28	109.55	106.68
14	A	811	CLA	C4A-NA-C1A	6.28	109.54	106.68
14	A	830	CLA	C4A-NA-C1A	6.27	109.54	106.68
14	A	810	CLA	C4A-NA-C1A	6.27	109.54	106.68
14	A	823	CLA	C4A-NA-C1A	6.26	109.53	106.68
14	A	813	CLA	C4A-NA-C1A	6.26	109.53	106.68
14	A	831	CLA	C4A-NA-C1A	6.25	109.53	106.68
14	A	843	CLA	C4A-NA-C1A	6.25	109.53	106.68
14	A	841	CLA	C4A-NA-C1A	6.25	109.53	106.68
14	A	826	CLA	C4A-NA-C1A	6.24	109.52	106.68
14	B	816	CLA	C4A-NA-C1A	6.23	109.52	106.68
14	A	821	CLA	C4A-NA-C1A	6.23	109.52	106.68
14	B	818	CLA	C4A-NA-C1A	6.23	109.52	106.68
14	B	821	CLA	C4A-NA-C1A	6.22	109.52	106.68
14	A	812	CLA	C4A-NA-C1A	6.20	109.51	106.68
14	B	830	CLA	C4A-NA-C1A	6.18	109.50	106.68
14	B	806	CLA	C4A-NA-C1A	6.15	109.48	106.68
14	B	839	CLA	C4A-NA-C1A	6.14	109.48	106.68
14	B	813	CLA	C4A-NA-C1A	6.14	109.48	106.68
14	B	836	CLA	C4A-NA-C1A	6.14	109.48	106.68
14	L	205	CLA	C4A-NA-C1A	6.13	109.48	106.68
14	A	804	CLA	C4A-NA-C1A	6.13	109.47	106.68
14	A	807	CLA	C4A-NA-C1A	6.12	109.47	106.68
14	A	832	CLA	C4A-NA-C1A	6.11	109.47	106.68
14	X	1701	CLA	C4A-NA-C1A	6.11	109.47	106.68
14	A	822	CLA	C4A-NA-C1A	6.10	109.46	106.68
14	A	817	CLA	C4A-NA-C1A	6.09	109.46	106.68
14	K	101	CLA	C4A-NA-C1A	6.09	109.46	106.68
14	A	837	CLA	C4A-NA-C1A	6.07	109.45	106.68
14	B	823	CLA	C4A-NA-C1A	6.07	109.45	106.68
14	B	833	CLA	C4A-NA-C1A	6.06	109.44	106.68
14	A	838	CLA	C4A-NA-C1A	6.06	109.44	106.68
14	A	808	CLA	C4A-NA-C1A	6.02	109.42	106.68
14	J	102	CLA	C4A-NA-C1A	6.02	109.42	106.68
14	A	857	CLA	C4A-NA-C1A	6.00	109.42	106.68
14	A	827	CLA	C4A-NA-C1A	5.97	109.40	106.68
14	B	820	CLA	C4A-NA-C1A	5.96	109.40	106.68
14	B	803	CLA	C4A-NA-C1A	5.95	109.39	106.68
14	B	829	CLA	C4A-NA-C1A	5.95	109.39	106.68
14	A	833	CLA	C4A-NA-C1A	5.90	109.37	106.68
14	A	805	CLA	C4A-NA-C1A	5.90	109.37	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	825	CLA	C4A-NA-C1A	5.84	109.34	106.68
14	A	828	CLA	C4A-NA-C1A	5.82	109.33	106.68
14	B	815	CLA	C4A-NA-C1A	5.80	109.32	106.68
14	A	820	CLA	C4A-NA-C1A	5.79	109.32	106.68
14	A	815	CLA	C4A-NA-C1A	5.74	109.30	106.68
14	A	829	CLA	C4A-NA-C1A	5.69	109.27	106.68
14	A	803	CLA	C4A-NA-C1A	5.68	109.27	106.68
14	B	824	CLA	C4A-NA-C1A	5.65	109.26	106.68
14	A	824	CLA	C4A-NA-C1A	5.64	109.25	106.68
14	B	817	CLA	C4A-NA-C1A	5.61	109.24	106.68
14	A	836	CLA	C4A-NA-C1A	5.55	109.21	106.68
14	A	834	CLA	C4A-NA-C1A	5.52	109.20	106.68
14	B	831	CLA	C4A-NA-C1A	5.51	109.19	106.68
14	F	202	CLA	C4A-NA-C1A	5.49	109.18	106.68
14	B	828	CLA	C4A-NA-C1A	5.43	109.16	106.68
14	B	827	CLA	C4A-NA-C1A	5.37	109.13	106.68
14	A	802	CLA	C4A-NA-C1A	5.34	109.12	106.68
14	A	835	CLA	C4A-NA-C1A	5.33	109.11	106.68
14	A	819	CLA	C4A-NA-C1A	4.99	108.96	106.68
19	M	101	LHG	O4-P-O5	4.43	133.03	112.44
19	B	850	LHG	O4-P-O5	4.38	132.80	112.44
19	A	854	LHG	O4-P-O5	4.36	132.74	112.44
19	A	855	LHG	O4-P-O5	4.35	132.67	112.44
22	L	207	DGD	O3G-C3G-C2G	-4.14	100.75	110.82
17	A	852	BCR	C2-C1-C6	3.84	116.02	110.44
14	A	819	CLA	C3B-C4B-NB	-3.68	107.24	110.53
17	B	846	BCR	C15-C16-C17	-3.63	116.08	123.52
22	L	207	DGD	O6D-C1D-O3G	-3.58	101.58	110.04
14	B	829	CLA	CAA-C2A-C3A	-3.58	103.33	113.00
14	A	839	CLA	O2D-CGD-O1D	-3.57	116.89	123.85
14	A	803	CLA	C3B-C4B-NB	-3.50	107.41	110.53
14	B	803	CLA	C3B-C4B-NB	-3.48	107.42	110.53
14	K	102	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
14	A	836	CLA	O2D-CGD-O1D	-3.43	117.16	123.85
14	B	828	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
14	A	831	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
14	B	830	CLA	C3B-C4B-NB	-3.40	107.50	110.53
17	A	847	BCR	C2-C1-C6	3.38	115.35	110.44
14	A	808	CLA	C3B-C4B-NB	-3.38	107.52	110.53
14	L	206	CLA	CMB-C2B-C1B	-3.34	120.33	125.42
14	B	832	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
14	A	811	CLA	O2D-CGD-O1D	-3.30	117.43	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	I	103	BCR	C15-C16-C17	-3.29	116.79	123.52
14	B	839	CLA	O2D-CGD-O1D	-3.29	117.45	123.85
13	A	801	CL0	C3B-C4B-NB	-3.28	107.60	110.53
14	A	857	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
17	A	851	BCR	C15-C16-C17	-3.26	116.86	123.52
14	B	826	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
14	A	802	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
14	B	810	CLA	CHB-C4A-NA	3.24	129.08	124.40
17	A	848	BCR	C15-C16-C17	-3.23	116.90	123.52
14	B	827	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
14	A	814	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
14	B	811	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
14	B	819	CLA	C3B-C4B-NB	-3.23	107.65	110.53
14	B	837	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
14	A	821	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
14	A	834	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
14	L	205	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
14	B	840	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
19	A	855	LHG	O8-C23-C24	3.20	120.86	111.15
14	A	818	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
14	B	807	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
14	B	823	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
17	I	103	BCR	C24-C23-C22	-3.18	121.54	126.23
14	B	824	CLA	C3B-C4B-NB	-3.17	107.70	110.53
14	A	807	CLA	C3B-C4B-NB	-3.17	107.70	110.53
14	A	809	CLA	C3B-C4B-NB	-3.17	107.70	110.53
17	A	850	BCR	C15-C14-C13	-3.16	122.84	127.28
14	B	812	CLA	C3B-C4B-NB	-3.16	107.71	110.53
17	L	201	BCR	C15-C14-C13	-3.16	122.85	127.28
14	A	828	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
17	J	105	BCR	C7-C8-C9	-3.14	121.58	126.23
14	A	813	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
17	L	201	BCR	C15-C16-C17	-3.14	117.09	123.52
14	A	828	CLA	C3B-C4B-NB	-3.14	107.73	110.53
14	A	832	CLA	C3B-C4B-NB	-3.14	107.73	110.53
14	A	809	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
14	A	829	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
14	A	830	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
14	B	814	CLA	C3B-C4B-NB	-3.11	107.76	110.53
14	A	822	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
14	B	821	CLA	O2D-CGD-O1D	-3.09	117.82	123.85
14	A	806	CLA	O2D-CGD-O1D	-3.09	117.83	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	838	CLA	C3B-C4B-NB	-3.09	107.77	110.53
14	A	812	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
14	B	834	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
14	A	844	CLA	C3B-C4B-NB	-3.09	107.78	110.53
14	F	201	CLA	C3B-C4B-NB	-3.07	107.79	110.53
14	X	1701	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
14	B	819	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
14	A	803	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
14	A	813	CLA	C3B-C4B-NB	-3.06	107.80	110.53
17	J	105	BCR	C15-C16-C17	-3.06	117.26	123.52
14	L	206	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
14	B	841	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
14	A	817	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
14	A	805	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
14	K	101	CLA	C3B-C4B-NB	-3.02	107.84	110.53
14	F	202	CLA	C3B-C4B-NB	-3.01	107.84	110.53
14	B	820	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
14	B	805	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
14	A	835	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
14	A	826	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
14	B	824	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
14	B	817	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
14	A	808	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
14	A	819	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
17	B	844	BCR	C2-C1-C6	3.00	114.79	110.44
14	A	804	CLA	C3B-C4B-NB	-3.00	107.86	110.53
17	J	103	BCR	C15-C14-C13	-2.99	123.08	127.28
14	A	842	CLA	C3B-C4B-NB	-2.99	107.86	110.53
14	A	823	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
14	A	840	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
14	A	833	CLA	C3B-C4B-NB	-2.99	107.86	110.53
14	A	818	CLA	C3B-C4B-NB	-2.99	107.86	110.53
14	B	831	CLA	O2D-CGD-O1D	-2.98	118.04	123.85
14	L	205	CLA	C3B-C4B-NB	-2.98	107.87	110.53
14	A	816	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
14	A	838	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
14	B	815	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
14	B	838	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
14	A	824	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
14	A	837	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
17	J	104	BCR	C15-C16-C17	-2.96	117.46	123.52
14	A	843	CLA	C3B-C4B-NB	-2.96	107.89	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	J	103	BCR	C15-C16-C17	-2.96	117.47	123.52
14	B	836	CLA	O2D-CGD-O1D	-2.96	118.10	123.85
17	A	847	BCR	C15-C16-C17	-2.95	117.48	123.52
14	A	826	CLA	C3B-C4B-NB	-2.95	107.89	110.53
14	J	101	CLA	C3B-C4B-NB	-2.95	107.90	110.53
14	B	830	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
14	A	804	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
14	B	806	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
14	B	818	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
18	B	849	LMG	O6-C1-O1	-2.93	103.12	110.04
18	I	102	LMG	O6-C1-O1	-2.92	103.13	110.04
17	A	850	BCR	C15-C16-C17	-2.92	117.54	123.52
14	B	817	CLA	C3B-C4B-NB	-2.92	107.92	110.53
17	I	103	BCR	C27-C26-C25	2.92	126.65	122.70
14	F	202	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
14	A	825	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
17	F	203	BCR	C35-C13-C14	-2.91	118.11	122.82
14	B	810	CLA	C3B-C4B-NB	-2.91	107.94	110.53
14	B	823	CLA	C3B-C4B-NB	-2.90	107.94	110.53
14	A	807	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
14	B	834	CLA	C3B-C4B-NB	-2.90	107.94	110.53
17	J	103	BCR	C33-C5-C6	-2.90	121.32	124.48
17	M	103	BCR	C33-C5-C6	-2.89	121.33	124.48
14	B	813	CLA	C3B-C4B-NB	-2.89	107.95	110.53
17	B	845	BCR	C15-C16-C17	-2.89	117.61	123.52
14	A	839	CLA	C3B-C4B-NB	-2.89	107.95	110.53
17	J	104	BCR	C24-C23-C22	-2.89	121.97	126.23
14	A	832	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
17	A	848	BCR	C33-C5-C6	-2.88	121.34	124.48
14	B	813	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
14	A	820	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
14	B	820	CLA	C3B-C4B-NB	-2.88	107.96	110.53
17	A	852	BCR	C15-C16-C17	-2.88	117.63	123.52
14	B	809	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
14	M	102	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
14	A	827	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
14	B	816	CLA	C3B-C4B-NB	-2.87	107.97	110.53
14	J	101	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
14	B	809	CLA	C3B-C4B-NB	-2.86	107.97	110.53
14	B	837	CLA	C3B-C4B-NB	-2.86	107.97	110.53
17	B	851	BCR	C33-C5-C6	-2.86	121.36	124.48
14	A	843	CLA	O2D-CGD-O1D	-2.86	118.28	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	847	BCR	C24-C23-C22	-2.85	122.02	126.23
14	B	825	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
14	A	842	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
14	A	844	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
14	M	102	CLA	C3B-C4B-NB	-2.84	108.00	110.53
17	B	846	BCR	C2-C1-C6	2.84	114.56	110.44
14	A	810	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
17	I	101	BCR	C27-C26-C25	2.84	126.54	122.70
17	J	105	BCR	C2-C1-C6	2.83	114.55	110.44
14	B	833	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
14	A	806	CLA	C3B-C4B-NB	-2.83	108.01	110.53
14	B	840	CLA	C3B-C4B-NB	-2.82	108.01	110.53
14	B	803	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
19	M	101	LHG	O8-C23-C24	2.81	120.41	111.83
17	B	845	BCR	C33-C5-C6	-2.81	121.42	124.48
17	B	847	BCR	C2-C1-C6	2.81	114.52	110.44
17	B	843	BCR	C24-C23-C22	-2.80	122.09	126.23
14	A	815	CLA	C3B-C4B-NB	-2.80	108.03	110.53
14	B	806	CLA	C3B-C4B-NB	-2.80	108.03	110.53
14	A	830	CLA	C3B-C4B-NB	-2.79	108.04	110.53
17	B	851	BCR	C27-C26-C25	2.79	126.48	122.70
17	B	851	BCR	C15-C16-C17	-2.79	117.81	123.52
17	I	103	BCR	C33-C5-C6	-2.79	121.44	124.48
17	B	843	BCR	C15-C16-C17	-2.78	117.83	123.52
14	B	831	CLA	C3B-C4B-NB	-2.78	108.05	110.53
15	A	845	PQN	O1-C1-C10	-2.78	117.13	121.57
14	B	818	CLA	C3B-C4B-NB	-2.77	108.05	110.53
17	A	852	BCR	C33-C5-C6	-2.77	121.46	124.48
14	L	204	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
14	B	835	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
14	F	201	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
17	A	850	BCR	C27-C26-C25	2.76	126.43	122.70
14	L	206	CLA	CMB-C2B-C3B	2.76	133.04	126.55
14	B	822	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
14	A	841	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
14	A	825	CLA	C3B-C4B-NB	-2.75	108.08	110.53
14	B	835	CLA	C3B-C4B-NB	-2.75	108.08	110.53
14	A	834	CLA	C3B-C4B-NB	-2.75	108.08	110.53
13	A	801	CL0	O2D-CGD-O1D	-2.75	118.50	123.85
14	B	814	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
17	A	847	BCR	C27-C26-C25	2.74	126.41	122.70
17	L	208	BCR	C2-C1-C6	2.74	114.42	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	849	BCR	C33-C5-C6	-2.74	121.49	124.48
14	A	838	CLA	C3B-C4B-NB	-2.74	108.08	110.53
14	B	802	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
14	A	823	CLA	C3B-C4B-NB	-2.74	108.09	110.53
14	B	826	CLA	C3B-C4B-NB	-2.74	108.09	110.53
17	A	849	BCR	C27-C26-C25	2.73	126.40	122.70
15	B	842	PQN	O1-C1-C10	-2.73	117.20	121.57
17	A	848	BCR	C15-C14-C13	-2.73	123.45	127.28
14	B	802	CLA	C3B-C4B-NB	-2.73	108.09	110.53
14	B	833	CLA	C3B-C4B-NB	-2.73	108.09	110.53
17	B	848	BCR	C2-C1-C6	2.73	114.40	110.44
17	I	101	BCR	C15-C16-C17	-2.73	117.94	123.52
14	A	821	CLA	C3B-C4B-NB	-2.73	108.09	110.53
14	L	204	CLA	O2A-CGA-O1A	-2.72	116.81	123.63
17	A	850	BCR	C24-C23-C22	-2.72	122.21	126.23
14	A	842	CLA	CHB-C4A-NA	2.72	128.32	124.40
17	L	201	BCR	C24-C23-C22	-2.72	122.21	126.23
14	B	804	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
14	B	803	CLA	CHB-C4A-NA	2.71	128.31	124.40
17	L	201	BCR	C27-C26-C25	2.71	126.36	122.70
17	L	208	BCR	C15-C16-C17	-2.70	118.00	123.52
14	B	829	CLA	CHB-C4A-NA	2.70	128.29	124.40
17	F	203	BCR	C33-C5-C6	-2.69	121.55	124.48
14	L	204	CLA	C3B-C4B-NB	-2.69	108.13	110.53
14	J	102	CLA	C3B-C4B-NB	-2.69	108.13	110.53
17	J	104	BCR	C33-C5-C6	-2.68	121.56	124.48
17	A	848	BCR	C11-C10-C9	-2.68	123.52	127.28
14	L	205	CLA	O2D-CGD-CBD	2.68	115.92	111.23
19	A	854	LHG	O8-C23-C24	2.67	119.99	111.83
14	A	832	CLA	CHB-C4A-NA	2.67	128.25	124.40
17	A	852	BCR	C15-C14-C13	-2.67	123.54	127.28
14	B	839	CLA	C3B-C4B-NB	-2.66	108.15	110.53
17	A	851	BCR	C33-C5-C6	-2.66	121.58	124.48
17	I	103	BCR	C15-C14-C13	-2.66	123.55	127.28
14	B	817	CLA	CHB-C4A-NA	2.66	128.24	124.40
14	B	834	CLA	CHB-C4A-NA	2.65	128.23	124.40
17	A	850	BCR	C33-C5-C6	-2.65	121.59	124.48
14	B	829	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
17	I	101	BCR	C24-C23-C22	-2.64	122.33	126.23
14	A	806	CLA	CHB-C4A-NA	2.64	128.21	124.40
14	A	833	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
14	B	808	CLA	O2D-CGD-O1D	-2.64	118.72	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	825	CLA	CHB-C4A-NA	2.63	128.20	124.40
17	L	208	BCR	C8-C7-C6	-2.63	119.96	127.00
14	A	840	CLA	C3B-C4B-NB	-2.63	108.18	110.53
14	A	820	CLA	C1-C2-C3	-2.63	121.89	126.20
14	B	816	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
17	I	101	BCR	C33-C5-C6	-2.62	121.62	124.48
14	B	824	CLA	CHB-C4A-NA	2.62	128.18	124.40
14	L	204	CLA	CHB-C4A-NA	2.62	128.18	124.40
14	A	827	CLA	C3B-C4B-NB	-2.61	108.20	110.53
14	B	810	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
14	A	817	CLA	C3B-C4B-NB	-2.61	108.20	110.53
17	B	847	BCR	C27-C26-C25	2.60	126.22	122.70
14	A	811	CLA	C3B-C4B-NB	-2.60	108.21	110.53
14	L	206	CLA	C1-C2-C3	-2.60	121.94	126.20
17	B	846	BCR	C24-C23-C22	-2.59	122.41	126.23
14	B	812	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
14	B	805	CLA	C3B-C4B-NB	-2.59	108.22	110.53
17	M	103	BCR	C24-C23-C22	-2.59	122.41	126.23
18	A	856	LMG	O6-C1-O1	-2.58	103.94	110.04
14	B	829	CLA	C3B-C4B-NB	-2.58	108.22	110.53
18	I	102	LMG	O1-C1-C2	-2.58	104.35	108.27
17	B	843	BCR	C2-C1-C6	2.58	114.19	110.44
14	L	206	CLA	CHB-C4A-NA	2.58	128.12	124.40
17	F	203	BCR	C16-C15-C14	-2.58	118.25	123.52
17	M	103	BCR	C15-C16-C17	-2.57	118.25	123.52
14	A	815	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
14	B	835	CLA	CHB-C4A-NA	2.57	128.11	124.40
14	B	811	CLA	CHB-C4A-NA	2.57	128.11	124.40
14	B	808	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
14	A	814	CLA	CHB-C4A-NA	2.57	128.10	124.40
14	A	809	CLA	CHB-C4A-NA	2.56	128.10	124.40
14	A	814	CLA	C3B-C4B-NB	-2.56	108.25	110.53
17	B	847	BCR	C33-C5-C6	-2.56	121.69	124.48
14	B	809	CLA	O1D-CGD-CBD	2.56	129.56	124.52
14	A	822	CLA	C3B-C4B-NB	-2.56	108.25	110.53
17	J	105	BCR	C27-C26-C25	2.56	126.16	122.70
14	A	838	CLA	CHB-C4A-NA	2.55	128.08	124.40
14	B	841	CLA	C3B-C4B-NB	-2.55	108.25	110.53
17	B	847	BCR	C16-C15-C14	-2.55	118.30	123.52
14	B	804	CLA	C3B-C4B-NB	-2.55	108.25	110.53
14	A	836	CLA	C3B-C4B-NB	-2.54	108.27	110.53
14	A	826	CLA	CHB-C4A-NA	2.53	128.05	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	821	CLA	C3B-C4B-NB	-2.53	108.28	110.53
14	B	836	CLA	C3B-C4B-NB	-2.52	108.28	110.53
14	A	805	CLA	C3B-C4B-NB	-2.52	108.28	110.53
14	B	822	CLA	C3B-C4B-NB	-2.52	108.28	110.53
17	B	848	BCR	C16-C15-C14	-2.51	118.38	123.52
15	A	845	PQN	C2M-C2-C3	-2.51	120.33	124.45
17	B	847	BCR	C24-C23-C22	-2.51	122.53	126.23
17	B	847	BCR	C15-C16-C17	-2.51	118.39	123.52
14	B	808	CLA	C3B-C4B-NB	-2.51	108.29	110.53
18	B	849	LMG	O1-C7-C8	-2.50	104.73	110.82
14	B	826	CLA	CHB-C4A-NA	2.50	128.01	124.40
14	A	807	CLA	CHB-C4A-NA	2.50	128.01	124.40
17	L	208	BCR	C33-C5-C6	-2.50	121.76	124.48
17	L	201	BCR	C33-C5-C6	-2.50	121.76	124.48
17	F	203	BCR	C2-C1-C6	2.49	114.06	110.44
17	F	203	BCR	C27-C26-C25	2.49	126.07	122.70
14	B	828	CLA	C3B-C4B-NB	-2.49	108.31	110.53
14	A	827	CLA	CHB-C4A-NA	2.49	127.99	124.40
14	B	840	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
14	A	830	CLA	CHB-C4A-NA	2.48	127.97	124.40
14	K	102	CLA	C3B-C4B-NB	-2.47	108.32	110.53
17	A	848	BCR	C24-C23-C22	-2.47	122.58	126.23
17	I	101	BCR	C11-C10-C9	-2.47	123.81	127.28
14	B	840	CLA	CHB-C4A-NA	2.47	127.96	124.40
14	K	102	CLA	O2D-CGD-CBD	2.47	115.54	111.23
17	M	103	BCR	C15-C14-C13	-2.47	123.82	127.28
14	B	829	CLA	C1-C2-C3	-2.47	122.16	126.20
14	X	1701	CLA	CHB-C4A-NA	2.46	127.96	124.40
14	B	806	CLA	CHB-C4A-NA	2.46	127.94	124.40
17	B	848	BCR	C27-C26-C25	2.45	126.02	122.70
14	B	815	CLA	C3B-C4B-NB	-2.45	108.34	110.53
14	J	101	CLA	CHB-C4A-NA	2.45	127.94	124.40
14	A	837	CLA	C3B-C4B-NB	-2.45	108.34	110.53
17	B	848	BCR	C15-C16-C17	-2.45	118.51	123.52
14	B	804	CLA	CHB-C4A-NA	2.45	127.93	124.40
13	A	801	CL0	CHB-C4A-NA	2.45	127.93	124.40
14	A	844	CLA	C1-C2-C3	-2.44	122.19	126.20
17	J	104	BCR	C20-C21-C22	-2.44	123.85	127.28
14	B	807	CLA	O2D-CGD-CBD	2.44	115.50	111.23
14	B	832	CLA	C3B-C4B-NB	-2.44	108.36	110.53
14	L	204	CLA	C1-C2-C3	-2.43	122.21	126.20
17	B	844	BCR	C8-C7-C6	-2.43	120.50	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	836	CLA	O2D-CGD-CBD	2.43	115.48	111.23
14	A	820	CLA	C3B-C4B-NB	-2.43	108.36	110.53
14	A	835	CLA	C3B-C4B-NB	-2.43	108.36	110.53
14	B	815	CLA	CHB-C4A-NA	2.43	127.90	124.40
17	B	843	BCR	C29-C30-C25	2.43	113.97	110.44
14	B	814	CLA	CHB-C4A-NA	2.43	127.90	124.40
14	B	830	CLA	CHB-C4A-NA	2.43	127.90	124.40
17	B	847	BCR	C8-C7-C6	-2.42	120.52	127.00
14	F	201	CLA	CHB-C4A-NA	2.42	127.90	124.40
14	A	803	CLA	CHB-C4A-NA	2.42	127.89	124.40
14	A	805	CLA	C1-C2-C3	-2.42	122.23	126.20
14	A	823	CLA	CHB-C4A-NA	2.42	127.89	124.40
17	A	847	BCR	C33-C5-C6	-2.42	121.85	124.48
14	B	832	CLA	O2D-CGD-CBD	2.42	115.45	111.23
17	B	845	BCR	C27-C26-C25	2.42	125.97	122.70
14	A	810	CLA	C3B-C4B-NB	-2.41	108.38	110.53
14	A	825	CLA	CHB-C4A-NA	2.41	127.88	124.40
14	B	802	CLA	CHB-C4A-NA	2.41	127.88	124.40
17	A	852	BCR	C27-C26-C25	2.41	125.95	122.70
17	A	847	BCR	C15-C14-C13	-2.41	123.91	127.28
14	A	818	CLA	CHB-C4A-NA	2.40	127.87	124.40
14	A	835	CLA	CHB-C4A-NA	2.40	127.87	124.40
22	L	207	DGD	O3G-C1D-C2D	-2.40	104.62	108.27
14	B	839	CLA	O2D-CGD-CBD	2.40	115.43	111.23
14	L	206	CLA	C3B-C4B-NB	-2.40	108.39	110.53
17	B	846	BCR	C15-C14-C13	-2.40	123.91	127.28
14	B	818	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	A	810	CLA	CHB-C4A-NA	2.39	127.85	124.40
17	B	844	BCR	C33-C5-C6	-2.39	121.88	124.48
14	K	102	CLA	CHB-C4A-NA	2.39	127.85	124.40
17	B	847	BCR	C10-C11-C12	-2.39	116.28	123.20
14	B	819	CLA	CHB-C4A-NA	2.39	127.85	124.40
14	B	821	CLA	CHB-C4A-NA	2.39	127.84	124.40
14	A	838	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
17	A	851	BCR	C27-C26-C25	2.39	125.93	122.70
14	A	816	CLA	CHB-C4A-NA	2.39	127.84	124.40
17	A	852	BCR	C8-C7-C6	-2.38	120.63	127.00
17	J	104	BCR	C15-C14-C13	-2.38	123.94	127.28
14	B	813	CLA	CHB-C4A-NA	2.37	127.82	124.40
17	B	844	BCR	C27-C26-C25	2.37	125.90	122.70
14	A	844	CLA	CHB-C4A-NA	2.37	127.81	124.40
17	B	848	BCR	C33-C5-C6	-2.36	121.91	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	848	BCR	C27-C26-C25	2.36	125.89	122.70
19	A	854	LHG	C18-C17-C16	-2.35	102.47	114.37
17	B	843	BCR	C28-C27-C26	-2.35	109.87	114.06
14	A	857	CLA	O2D-CGD-CBD	2.35	115.33	111.23
14	A	808	CLA	CHB-C4A-NA	2.35	127.79	124.40
14	F	202	CLA	CHB-C4A-NA	2.34	127.78	124.40
19	M	101	LHG	C20-C19-C18	-2.34	102.53	114.37
14	F	201	CLA	C1-C2-C3	-2.34	122.36	126.20
14	B	833	CLA	CHB-C4A-NA	2.34	127.78	124.40
17	M	103	BCR	C28-C27-C26	-2.34	109.88	114.06
14	B	813	CLA	CAC-C3C-C4C	2.34	127.83	124.79
17	A	852	BCR	C24-C23-C22	-2.34	122.78	126.23
14	B	822	CLA	CHB-C4A-NA	2.34	127.77	124.40
17	B	845	BCR	C8-C7-C6	-2.34	120.76	127.00
14	A	808	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
17	A	850	BCR	C8-C7-C6	-2.34	120.76	127.00
14	A	828	CLA	CHB-C4A-NA	2.34	127.77	124.40
14	B	837	CLA	CHB-C4A-NA	2.33	127.77	124.40
14	A	827	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
14	A	828	CLA	O2A-CGA-O1A	-2.33	117.79	123.63
14	A	820	CLA	CAA-C2A-C1A	-2.33	104.33	111.97
14	B	838	CLA	CHB-C4A-NA	2.32	127.75	124.40
14	A	805	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
14	A	839	CLA	CHB-C4A-NA	2.32	127.75	124.40
14	B	804	CLA	C1-C2-C3	-2.32	122.40	126.20
14	B	827	CLA	C3B-C4B-NB	-2.32	108.46	110.53
22	L	207	DGD	CAB-C9B-C8B	-2.31	102.67	114.37
15	B	842	PQN	C2M-C2-C3	-2.31	120.65	124.45
14	B	823	CLA	CHB-C4A-NA	2.31	127.74	124.40
18	I	102	LMG	O2-C2-C1	-2.31	104.57	110.08
22	L	207	DGD	C3G-C2G-C1G	-2.31	106.41	111.78
18	B	849	LMG	C40-C39-C38	-2.30	102.72	114.37
14	A	804	CLA	CHB-C4A-NA	2.30	127.72	124.40
14	A	829	CLA	C3B-C4B-NB	-2.30	108.48	110.53
14	B	812	CLA	CHB-C4A-NA	2.30	127.71	124.40
19	M	101	LHG	C11-C10-C9	-2.30	102.77	114.37
14	B	811	CLA	C3B-C4B-NB	-2.29	108.48	110.53
14	K	101	CLA	CHB-C4A-NA	2.29	127.71	124.40
14	A	831	CLA	C3B-C4B-NB	-2.29	108.48	110.53
19	A	855	LHG	C11-C10-C9	-2.29	102.80	114.37
14	A	819	CLA	CHB-C4A-NA	2.29	127.70	124.40
14	A	834	CLA	CHB-C4A-NA	2.28	127.69	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	B	832	CLA	CHB-C4A-NA	2.28	127.69	124.40
14	A	821	CLA	CHB-C4A-NA	2.28	127.69	124.40
17	A	849	BCR	C8-C7-C6	-2.28	120.91	127.00
17	A	847	BCR	C11-C10-C9	-2.28	124.08	127.28
17	A	852	BCR	C38-C26-C25	-2.28	122.00	124.48
14	B	809	CLA	CHB-C4A-NA	2.28	127.69	124.40
14	A	843	CLA	CHB-C4A-NA	2.27	127.68	124.40
17	B	845	BCR	C15-C14-C13	-2.27	124.09	127.28
14	A	812	CLA	CHB-C4A-NA	2.27	127.68	124.40
14	A	823	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
18	A	853	LMG	O1-C7-C8	-2.27	105.29	110.82
14	B	827	CLA	O1D-CGD-CBD	2.27	129.00	124.52
14	B	837	CLA	O2D-CGD-CBD	2.27	115.20	111.23
17	B	844	BCR	C16-C15-C14	-2.27	118.88	123.52
22	L	207	DGD	CDB-CCB-CBB	-2.26	102.92	114.37
21	L	202	LMT	C1'-O5'-C5'	-2.26	109.30	113.72
14	A	809	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
14	B	837	CLA	C1-C2-C3	-2.26	122.49	126.20
17	B	845	BCR	C38-C26-C25	-2.26	122.02	124.48
15	B	842	PQN	C10-C1-C2	2.26	122.11	118.97
14	A	822	CLA	CHB-C4A-NA	2.26	127.66	124.40
14	A	813	CLA	CHB-C4A-NA	2.26	127.66	124.40
14	A	837	CLA	CHB-C4A-NA	2.26	127.66	124.40
14	B	816	CLA	CHB-C4A-NA	2.25	127.65	124.40
17	B	843	BCR	C33-C5-C6	-2.25	122.03	124.48
14	A	805	CLA	CHB-C4A-NA	2.25	127.65	124.40
14	L	205	CLA	CHB-C4A-NA	2.25	127.65	124.40
14	B	805	CLA	CHB-C4A-NA	2.25	127.65	124.40
17	A	851	BCR	C8-C7-C6	-2.25	120.99	127.00
17	B	846	BCR	C33-C5-C6	-2.25	122.03	124.48
14	L	205	CLA	C1-C2-C3	-2.25	122.52	126.20
14	B	804	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
17	J	103	BCR	C38-C26-C25	-2.25	122.03	124.48
14	A	857	CLA	O2A-CGA-O1A	-2.25	118.01	123.63
17	B	844	BCR	C35-C13-C12	2.24	121.51	118.09
15	A	845	PQN	C10-C1-C2	2.24	122.08	118.97
14	A	814	CLA	O2D-CGD-CBD	2.24	115.14	111.23
17	B	848	BCR	C8-C7-C6	-2.24	121.02	127.00
15	B	842	PQN	O4-C4-C3	-2.24	117.08	120.67
18	A	856	LMG	O1-C7-C8	-2.23	105.39	110.82
19	A	854	LHG	C11-C10-C9	-2.23	103.08	114.37
17	L	208	BCR	C27-C26-C25	2.23	125.72	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	L	207	DGD	O5D-C6D-C5D	-2.23	104.39	109.42
14	B	807	CLA	CHB-C4A-NA	2.23	127.62	124.40
17	I	103	BCR	C11-C10-C9	-2.23	124.15	127.28
14	A	811	CLA	CHB-C4A-NA	2.23	127.62	124.40
14	B	841	CLA	O2D-CGD-CBD	2.23	115.13	111.23
14	B	808	CLA	CHB-C4A-NA	2.23	127.62	124.40
17	J	105	BCR	C24-C23-C22	-2.23	122.94	126.23
17	L	201	BCR	C8-C7-C6	-2.23	121.05	127.00
14	A	831	CLA	O2D-CGD-CBD	2.23	115.12	111.23
14	J	102	CLA	CHB-C4A-NA	2.23	127.61	124.40
17	J	103	BCR	C27-C26-C25	2.23	125.71	122.70
14	A	825	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
14	A	808	CLA	O2D-CGD-CBD	2.22	115.11	111.23
17	I	103	BCR	C7-C8-C9	-2.22	122.95	126.23
14	A	819	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
14	K	101	CLA	O2A-CGA-O1A	-2.22	117.63	123.33
19	A	854	LHG	C20-C19-C18	-2.21	103.17	114.37
14	B	811	CLA	O2D-CGD-CBD	2.21	115.10	111.23
14	A	816	CLA	C3B-C4B-NB	-2.21	108.55	110.53
14	M	102	CLA	CHB-C4A-NA	2.21	127.59	124.40
18	B	849	LMG	O2-C2-C1	-2.21	104.80	110.08
14	A	836	CLA	CHB-C4A-NA	2.21	127.58	124.40
17	M	103	BCR	C8-C7-C6	-2.20	121.11	127.00
14	X	1701	CLA	C3B-C4B-NB	-2.20	108.56	110.53
15	A	845	PQN	O4-C4-C3	-2.20	117.14	120.67
14	A	824	CLA	C3B-C4B-NB	-2.20	108.57	110.53
14	B	836	CLA	CHB-C4A-NA	2.20	127.57	124.40
17	B	846	BCR	C27-C26-C25	2.19	125.67	122.70
17	A	848	BCR	C8-C7-C6	-2.19	121.14	127.00
17	J	103	BCR	C24-C23-C22	-2.19	122.99	126.23
14	B	809	CLA	CAC-C3C-C4C	2.19	127.64	124.79
18	A	853	LMG	O3-C3-C2	-2.19	105.21	110.38
14	B	804	CLA	O2D-CGD-CBD	2.19	115.06	111.23
14	B	820	CLA	CHB-C4A-NA	2.19	127.56	124.40
14	B	810	CLA	C2A-C1A-CHA	2.19	127.67	123.87
14	B	825	CLA	C3B-C4B-NB	-2.19	108.58	110.53
17	J	105	BCR	C33-C5-C6	-2.19	122.10	124.48
18	I	102	LMG	O1-C7-C8	-2.19	105.50	110.82
18	I	102	LMG	O6-C5-C4	2.18	113.64	109.70
18	A	853	LMG	C1-O6-C5	-2.18	109.46	113.72
17	B	844	BCR	C3-C4-C5	-2.18	110.16	114.06
17	J	104	BCR	C27-C26-C25	2.18	125.65	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	856	LMG	O2-C2-C1	-2.18	104.88	110.08
17	A	851	BCR	C11-C10-C9	-2.18	124.22	127.28
14	B	808	CLA	C1-C2-C3	-2.18	122.62	126.20
17	B	843	BCR	C15-C14-C13	-2.18	124.22	127.28
17	A	851	BCR	C15-C14-C13	-2.18	124.23	127.28
14	A	810	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
14	A	857	CLA	C3B-C4B-NB	-2.17	108.59	110.53
17	B	846	BCR	C8-C7-C6	-2.17	121.21	127.00
18	B	849	LMG	C42-C41-C40	-2.17	103.42	114.37
14	L	206	CLA	O2D-CGD-CBD	2.17	115.02	111.23
17	J	104	BCR	C8-C7-C6	-2.16	121.22	127.00
18	A	856	LMG	O3-C3-C2	-2.16	105.28	110.38
14	A	803	CLA	CAA-C2A-C1A	-2.16	104.90	111.97
14	B	814	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
14	A	831	CLA	CHB-C4A-NA	2.16	127.51	124.40
14	A	811	CLA	O2D-CGD-CBD	2.16	115.00	111.23
17	L	208	BCR	C24-C23-C22	-2.15	123.05	126.23
14	B	828	CLA	CHB-C4A-NA	2.15	127.51	124.40
14	B	831	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
18	I	102	LMG	O3-C3-C2	-2.15	105.32	110.38
14	B	831	CLA	CHB-C4A-NA	2.15	127.50	124.40
17	L	208	BCR	C15-C14-C13	-2.14	124.27	127.28
14	A	809	CLA	C1-C2-C3	-2.14	122.68	126.20
14	A	840	CLA	CHB-C4A-NA	2.14	127.49	124.40
22	L	207	DGD	CFB-CEB-CDB	-2.14	103.54	114.37
14	A	808	CLA	C1-C2-C3	-2.14	122.69	126.20
21	L	202	LMT	C2'-C3'-C4'	2.14	114.54	109.68
14	A	818	CLA	O2D-CGD-CBD	2.14	114.97	111.23
17	B	843	BCR	C8-C7-C6	-2.14	121.28	127.00
14	A	811	CLA	O2A-CGA-O1A	-2.14	117.83	123.33
14	A	817	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
14	A	814	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
18	B	849	LMG	O3-C3-C2	-2.14	105.34	110.38
14	A	817	CLA	CHB-C4A-NA	2.13	127.48	124.40
14	X	1701	CLA	O2D-CGD-CBD	2.13	114.96	111.23
14	A	806	CLA	O1D-CGD-CBD	2.13	128.72	124.52
17	B	844	BCR	C24-C23-C22	-2.13	123.09	126.23
13	A	801	CL0	C1-C2-C3	-2.13	122.71	126.20
14	A	834	CLA	O2D-CGD-CBD	2.12	114.94	111.23
18	A	853	LMG	C1-C2-C3	-2.12	105.54	110.01
14	A	835	CLA	C1-C2-C3	-2.12	122.72	126.20
14	A	844	CLA	O2A-CGA-O1A	-2.12	118.32	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	L	207	DGD	O6D-C5D-C6D	-2.12	102.49	106.69
14	B	819	CLA	O2D-CGD-CBD	2.11	114.92	111.23
14	B	839	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
14	B	838	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
17	J	103	BCR	C8-C7-C6	-2.11	121.37	127.00
14	B	816	CLA	C1-C2-C3	-2.11	122.75	126.20
18	A	853	LMG	O2-C2-C1	-2.11	105.06	110.08
17	J	104	BCR	C38-C26-C25	-2.11	122.19	124.48
15	A	845	PQN	C5-C4-C3	2.11	122.13	118.27
14	B	827	CLA	CHB-C4A-NA	2.10	127.44	124.40
17	I	101	BCR	C8-C7-C6	-2.10	121.38	127.00
14	B	839	CLA	CHB-C4A-NA	2.10	127.43	124.40
22	L	207	DGD	O6E-C1E-O5D	-2.10	105.08	110.04
17	A	851	BCR	C2-C1-C6	2.10	113.49	110.44
17	A	847	BCR	C8-C7-C6	-2.10	121.39	127.00
17	A	850	BCR	C38-C26-C25	-2.09	122.20	124.48
17	J	104	BCR	C11-C10-C9	-2.09	124.34	127.28
14	A	833	CLA	CHB-C4A-NA	2.09	127.42	124.40
14	A	839	CLA	O2D-CGD-CBD	2.09	114.88	111.23
14	A	840	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
18	B	849	LMG	O1-C1-C2	-2.09	105.11	108.27
17	B	843	BCR	C11-C10-C9	-2.08	124.35	127.28
19	A	854	LHG	C27-C26-C25	-2.08	103.83	114.37
14	A	815	CLA	CHB-C4A-NA	2.08	127.41	124.40
14	A	819	CLA	C1-C2-C3	-2.08	122.78	126.20
14	B	812	CLA	O2A-CGA-O1A	-2.08	117.97	123.33
14	F	201	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
14	A	831	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
14	A	806	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
17	B	844	BCR	C15-C16-C17	-2.08	119.27	123.52
18	A	856	LMG	O1-C1-C2	-2.08	105.12	108.27
22	L	207	DGD	O6D-C1D-C2D	2.08	114.63	110.37
22	L	207	DGD	CBB-CAB-C9B	-2.07	103.89	114.37
14	B	809	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
14	A	820	CLA	CHB-C4A-NA	2.07	127.39	124.40
14	B	841	CLA	CHB-C4A-NA	2.07	127.39	124.40
14	A	812	CLA	C3B-C4B-NB	-2.07	108.68	110.53
14	B	810	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
19	M	101	LHG	C18-C17-C16	-2.07	103.91	114.37
14	A	824	CLA	CHB-C4A-NA	2.07	127.39	124.40
17	B	851	BCR	C8-C7-C6	-2.07	121.47	127.00
14	B	840	CLA	O2D-CGD-CBD	2.07	114.85	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	A	849	BCR	C16-C15-C14	-2.07	119.29	123.52
14	B	817	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
14	B	833	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
17	J	105	BCR	C3-C4-C5	-2.07	110.37	114.06
14	A	841	CLA	CHB-C4A-NA	2.06	127.38	124.40
14	L	205	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
17	A	849	BCR	C2-C1-C6	2.06	113.43	110.44
17	J	105	BCR	C15-C14-C13	-2.06	124.39	127.28
17	L	201	BCR	C38-C26-C25	-2.06	122.24	124.48
14	A	830	CLA	O2D-CGD-CBD	2.05	114.82	111.23
14	A	813	CLA	O2D-CGD-CBD	2.05	114.81	111.23
14	A	810	CLA	C1-C2-C3	-2.05	122.84	126.20
14	A	839	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
14	B	813	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
14	B	831	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
14	A	803	CLA	O2D-CGD-CBD	2.04	114.80	111.23
17	F	203	BCR	C38-C26-C25	-2.04	122.26	124.48
22	L	207	DGD	C5B-C4B-C3B	-2.04	104.05	114.37
14	B	828	CLA	O2D-CGD-CBD	2.04	114.80	111.23
17	J	105	BCR	C11-C10-C9	-2.04	124.42	127.28
14	A	822	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
14	B	835	CLA	O2A-CGA-O1A	-2.04	118.09	123.33
17	B	851	BCR	C15-C14-C13	-2.04	124.42	127.28
14	A	841	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
14	A	829	CLA	CHB-C4A-NA	2.04	127.34	124.40
17	M	103	BCR	C16-C15-C14	-2.03	119.36	123.52
17	L	201	BCR	C35-C13-C14	-2.03	119.52	122.82
14	A	824	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
13	A	801	CL0	O2A-CGA-O1A	-2.03	118.54	123.63
14	A	832	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
14	B	824	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
14	B	817	CLA	C1-C2-C3	-2.03	122.88	126.20
19	M	101	LHG	C27-C26-C25	-2.03	104.12	114.37
17	F	203	BCR	C8-C7-C6	-2.03	121.58	127.00
14	B	826	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
17	A	852	BCR	C10-C11-C12	-2.02	117.34	123.20
18	B	849	LMG	O7-C10-O9	-2.02	118.99	123.70
17	J	104	BCR	C2-C1-C6	2.02	113.37	110.44
14	A	824	CLA	C1-C2-C3	-2.02	122.89	126.20
14	B	822	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
22	L	207	DGD	O3E-C3E-C2E	-2.01	105.63	110.38
14	B	809	CLA	O2A-CGA-O1A	-2.01	118.60	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	B	851	BCR	C7-C8-C9	-2.01	123.26	126.23
14	B	837	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
14	A	804	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
17	B	851	BCR	C38-C26-C25	-2.00	122.30	124.48
14	A	802	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
18	A	853	LMG	O6-C1-O1	-2.00	105.31	110.04
17	A	848	BCR	C38-C26-C25	-2.00	122.30	124.48
17	A	849	BCR	C15-C16-C17	-2.00	119.43	123.52

There are no chirality outliers.

All (1251) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	801	CL0	CBD-CGD-O2D-CED
14	A	804	CLA	C1A-C2A-CAA-CBA
14	A	804	CLA	C3A-C2A-CAA-CBA
14	A	805	CLA	CHA-CBD-CGD-O1D
14	A	805	CLA	CHA-CBD-CGD-O2D
14	A	806	CLA	C1A-C2A-CAA-CBA
14	A	806	CLA	C2-C1-O2A-CGA
14	A	806	CLA	CAD-CBD-CGD-O1D
14	A	806	CLA	CAD-CBD-CGD-O2D
14	A	807	CLA	CBD-CGD-O2D-CED
14	A	808	CLA	C2-C3-C5-C6
14	A	808	CLA	C4-C3-C5-C6
14	A	809	CLA	C1A-C2A-CAA-CBA
14	A	809	CLA	C3A-C2A-CAA-CBA
14	A	809	CLA	CHA-CBD-CGD-O1D
14	A	809	CLA	CHA-CBD-CGD-O2D
14	A	811	CLA	C1A-C2A-CAA-CBA
14	A	811	CLA	C3A-C2A-CAA-CBA
14	A	811	CLA	C2B-C3B-CAB-CBB
14	A	811	CLA	C4B-C3B-CAB-CBB
14	A	816	CLA	CAD-CBD-CGD-O1D
14	A	816	CLA	CAD-CBD-CGD-O2D
14	A	817	CLA	CBD-CGD-O2D-CED
14	A	819	CLA	C1A-C2A-CAA-CBA
14	A	819	CLA	C3A-C2A-CAA-CBA
14	A	820	CLA	C1A-C2A-CAA-CBA
14	A	820	CLA	C3A-C2A-CAA-CBA
14	A	823	CLA	C3A-C2A-CAA-CBA
14	A	823	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
14	A	823	CLA	CAD-CBD-CGD-O2D
14	A	824	CLA	C3A-C2A-CAA-CBA
14	A	826	CLA	C1A-C2A-CAA-CBA
14	A	826	CLA	CHA-CBD-CGD-O2D
14	A	828	CLA	C1A-C2A-CAA-CBA
14	A	829	CLA	CBD-CGD-O2D-CED
14	A	831	CLA	CHA-CBD-CGD-O1D
14	A	831	CLA	CHA-CBD-CGD-O2D
14	A	832	CLA	C1A-C2A-CAA-CBA
14	A	832	CLA	C3A-C2A-CAA-CBA
14	A	834	CLA	C2B-C3B-CAB-CBB
14	A	834	CLA	C4B-C3B-CAB-CBB
14	A	835	CLA	C1A-C2A-CAA-CBA
14	A	835	CLA	C3A-C2A-CAA-CBA
14	A	835	CLA	CHA-CBD-CGD-O1D
14	A	835	CLA	CHA-CBD-CGD-O2D
14	A	841	CLA	CBD-CGD-O2D-CED
14	A	842	CLA	C1A-C2A-CAA-CBA
14	A	842	CLA	C3A-C2A-CAA-CBA
14	A	844	CLA	CBD-CGD-O2D-CED
14	A	844	CLA	O1D-CGD-O2D-CED
14	A	857	CLA	CAD-CBD-CGD-O1D
14	A	857	CLA	CAD-CBD-CGD-O2D
14	A	857	CLA	C2-C3-C5-C6
14	A	857	CLA	C4-C3-C5-C6
14	B	802	CLA	CBD-CGD-O2D-CED
14	B	803	CLA	CBD-CGD-O2D-CED
14	B	804	CLA	CHA-CBD-CGD-O1D
14	B	804	CLA	CHA-CBD-CGD-O2D
14	B	805	CLA	C1A-C2A-CAA-CBA
14	B	805	CLA	C3A-C2A-CAA-CBA
14	B	808	CLA	CHA-CBD-CGD-O1D
14	B	808	CLA	CHA-CBD-CGD-O2D
14	B	813	CLA	CHA-CBD-CGD-O1D
14	B	813	CLA	CHA-CBD-CGD-O2D
14	B	814	CLA	CAD-CBD-CGD-O1D
14	B	814	CLA	CAD-CBD-CGD-O2D
14	B	817	CLA	C3A-C2A-CAA-CBA
14	B	818	CLA	C1A-C2A-CAA-CBA
14	B	818	CLA	C3A-C2A-CAA-CBA
14	B	820	CLA	CAD-CBD-CGD-O1D
14	B	820	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
14	B	821	CLA	CHA-CBD-CGD-O1D
14	B	821	CLA	CHA-CBD-CGD-O2D
14	B	824	CLA	CHA-CBD-CGD-O1D
14	B	824	CLA	CHA-CBD-CGD-O2D
14	B	825	CLA	CHA-CBD-CGD-O1D
14	B	825	CLA	CHA-CBD-CGD-O2D
14	B	827	CLA	C6-C7-C8-C10
14	B	828	CLA	C1A-C2A-CAA-CBA
14	B	828	CLA	C3A-C2A-CAA-CBA
14	B	829	CLA	CHA-CBD-CGD-O1D
14	B	829	CLA	CHA-CBD-CGD-O2D
14	B	830	CLA	C2B-C3B-CAB-CBB
14	B	830	CLA	C4B-C3B-CAB-CBB
14	B	830	CLA	CAD-CBD-CGD-O1D
14	B	830	CLA	CAD-CBD-CGD-O2D
14	B	831	CLA	CBD-CGD-O2D-CED
14	B	834	CLA	CHA-CBD-CGD-O1D
14	B	834	CLA	CHA-CBD-CGD-O2D
14	B	835	CLA	C1A-C2A-CAA-CBA
14	B	835	CLA	C3A-C2A-CAA-CBA
14	B	835	CLA	CBD-CGD-O2D-CED
14	B	836	CLA	CBD-CGD-O2D-CED
14	B	841	CLA	C1A-C2A-CAA-CBA
14	B	841	CLA	C3A-C2A-CAA-CBA
14	F	201	CLA	CBD-CGD-O2D-CED
14	K	102	CLA	C1A-C2A-CAA-CBA
14	K	102	CLA	C3A-C2A-CAA-CBA
14	L	204	CLA	C1A-C2A-CAA-CBA
14	L	204	CLA	C3A-C2A-CAA-CBA
17	A	847	BCR	C16-C17-C18-C36
17	A	848	BCR	C7-C8-C9-C10
17	A	848	BCR	C11-C12-C13-C14
17	A	848	BCR	C11-C12-C13-C35
17	A	848	BCR	C16-C17-C18-C36
17	A	848	BCR	C18-C19-C20-C21
17	A	848	BCR	C20-C21-C22-C37
17	A	850	BCR	C16-C17-C18-C36
17	A	850	BCR	C20-C21-C22-C37
17	A	850	BCR	C22-C23-C24-C25
17	A	851	BCR	C7-C8-C9-C10
17	A	851	BCR	C7-C8-C9-C34
17	A	851	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
17	A	852	BCR	C7-C8-C9-C10
17	A	852	BCR	C7-C8-C9-C34
17	A	852	BCR	C11-C10-C9-C8
17	A	852	BCR	C10-C11-C12-C13
17	A	852	BCR	C11-C12-C13-C14
17	A	852	BCR	C11-C12-C13-C35
17	A	852	BCR	C18-C19-C20-C21
17	A	852	BCR	C20-C21-C22-C23
17	A	852	BCR	C20-C21-C22-C37
17	A	852	BCR	C21-C22-C23-C24
17	A	852	BCR	C37-C22-C23-C24
17	B	843	BCR	C18-C19-C20-C21
17	B	843	BCR	C37-C22-C23-C24
17	B	844	BCR	C6-C7-C8-C9
17	B	844	BCR	C11-C10-C9-C8
17	B	844	BCR	C10-C11-C12-C13
17	B	844	BCR	C16-C17-C18-C36
17	B	844	BCR	C21-C22-C23-C24
17	B	846	BCR	C6-C7-C8-C9
17	B	846	BCR	C11-C12-C13-C35
17	B	846	BCR	C20-C21-C22-C37
17	B	846	BCR	C22-C23-C24-C25
17	B	846	BCR	C23-C24-C25-C26
17	B	847	BCR	C10-C11-C12-C13
17	B	847	BCR	C11-C12-C13-C35
17	B	848	BCR	C20-C21-C22-C37
17	B	851	BCR	C11-C12-C13-C35
17	B	851	BCR	C37-C22-C23-C24
17	F	203	BCR	C16-C17-C18-C36
17	I	101	BCR	C7-C8-C9-C34
17	I	103	BCR	C7-C8-C9-C10
17	I	103	BCR	C11-C10-C9-C34
17	I	103	BCR	C11-C12-C13-C14
17	I	103	BCR	C37-C22-C23-C24
17	I	103	BCR	C23-C24-C25-C26
17	I	103	BCR	C23-C24-C25-C30
17	J	103	BCR	C11-C12-C13-C14
17	J	103	BCR	C12-C13-C14-C15
17	J	103	BCR	C16-C17-C18-C36
17	J	103	BCR	C37-C22-C23-C24
17	J	104	BCR	C1-C6-C7-C8
17	J	104	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
17	J	104	BCR	C6-C7-C8-C9
17	J	104	BCR	C11-C12-C13-C14
17	J	104	BCR	C11-C12-C13-C35
17	J	104	BCR	C20-C21-C22-C23
17	J	104	BCR	C22-C23-C24-C25
17	J	105	BCR	C7-C8-C9-C10
17	J	105	BCR	C22-C23-C24-C25
17	L	201	BCR	C6-C7-C8-C9
17	L	201	BCR	C11-C12-C13-C35
17	L	201	BCR	C22-C23-C24-C25
17	L	208	BCR	C6-C7-C8-C9
17	L	208	BCR	C7-C8-C9-C10
17	L	208	BCR	C7-C8-C9-C34
17	L	208	BCR	C11-C12-C13-C35
17	L	208	BCR	C16-C17-C18-C36
17	M	103	BCR	C5-C6-C7-C8
17	M	103	BCR	C7-C8-C9-C10
17	M	103	BCR	C16-C17-C18-C19
17	M	103	BCR	C16-C17-C18-C36
18	A	853	LMG	O9-C10-O7-C8
18	A	856	LMG	O6-C1-O1-C7
18	A	856	LMG	O9-C10-O7-C8
18	B	849	LMG	C2-C1-O1-C7
18	B	849	LMG	O6-C1-O1-C7
19	A	854	LHG	C3-O3-P-O5
19	A	855	LHG	C1-C2-C3-O3
19	A	855	LHG	C3-O3-P-O5
19	B	850	LHG	O1-C1-C2-C3
19	B	850	LHG	C4-O6-P-O3
19	B	850	LHG	C4-O6-P-O4
19	B	850	LHG	C4-O6-P-O5
19	B	850	LHG	O9-C7-O7-C5
19	B	850	LHG	C8-C7-O7-C5
19	M	101	LHG	C3-O3-P-O4
19	M	101	LHG	C3-O3-P-O5
19	M	101	LHG	C3-O3-P-O6
19	M	101	LHG	C4-O6-P-O3
19	M	101	LHG	C4-O6-P-O5
21	L	202	LMT	O5'-C1'-O1'-C1
22	L	207	DGD	C2B-C1B-O2G-C2G
22	L	207	DGD	O6D-C1D-O3G-C3G
22	L	207	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
22	L	207	DGD	O6E-C1E-O5D-C6D
14	B	811	CLA	O1D-CGD-O2D-CED
14	B	812	CLA	O1D-CGD-O2D-CED
14	B	831	CLA	O1D-CGD-O2D-CED
14	L	204	CLA	O1D-CGD-O2D-CED
13	A	801	CL0	O1D-CGD-O2D-CED
14	A	806	CLA	O1D-CGD-O2D-CED
14	A	807	CLA	O1D-CGD-O2D-CED
14	A	830	CLA	O1D-CGD-O2D-CED
14	A	841	CLA	O1D-CGD-O2D-CED
14	B	802	CLA	O1D-CGD-O2D-CED
14	B	803	CLA	O1D-CGD-O2D-CED
14	B	815	CLA	O1D-CGD-O2D-CED
14	B	822	CLA	O1D-CGD-O2D-CED
14	B	833	CLA	O1D-CGD-O2D-CED
14	A	803	CLA	CBD-CGD-O2D-CED
14	A	806	CLA	CBD-CGD-O2D-CED
14	A	819	CLA	CBD-CGD-O2D-CED
14	A	822	CLA	CBD-CGD-O2D-CED
14	A	823	CLA	CBD-CGD-O2D-CED
14	A	826	CLA	CBD-CGD-O2D-CED
14	A	830	CLA	CBD-CGD-O2D-CED
14	A	838	CLA	CBD-CGD-O2D-CED
14	A	842	CLA	CBD-CGD-O2D-CED
14	B	805	CLA	CBD-CGD-O2D-CED
14	B	810	CLA	CBD-CGD-O2D-CED
14	B	811	CLA	CBD-CGD-O2D-CED
14	B	812	CLA	CBD-CGD-O2D-CED
14	B	815	CLA	CBD-CGD-O2D-CED
14	B	819	CLA	CBD-CGD-O2D-CED
14	B	821	CLA	CBD-CGD-O2D-CED
14	B	822	CLA	CBD-CGD-O2D-CED
14	B	833	CLA	CBD-CGD-O2D-CED
14	B	834	CLA	CBD-CGD-O2D-CED
14	L	204	CLA	CBD-CGD-O2D-CED
14	M	102	CLA	CBD-CGD-O2D-CED
14	A	817	CLA	O1A-CGA-O2A-C1
14	A	820	CLA	O1A-CGA-O2A-C1
19	M	101	LHG	O10-C23-O8-C6
14	A	844	CLA	C4C-C3C-CAC-CBC
14	A	817	CLA	O1D-CGD-O2D-CED
14	A	829	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	B	835	CLA	O1D-CGD-O2D-CED
14	A	823	CLA	O1D-CGD-O2D-CED
14	B	819	CLA	O1D-CGD-O2D-CED
14	B	834	CLA	O1D-CGD-O2D-CED
14	M	102	CLA	O1D-CGD-O2D-CED
14	A	817	CLA	CBA-CGA-O2A-C1
14	A	820	CLA	CBA-CGA-O2A-C1
19	M	101	LHG	C24-C23-O8-C6
14	B	814	CLA	CBD-CGD-O2D-CED
13	A	801	CL0	O1A-CGA-O2A-C1
14	A	806	CLA	O1A-CGA-O2A-C1
14	A	808	CLA	O1A-CGA-O2A-C1
14	A	812	CLA	O1A-CGA-O2A-C1
14	A	825	CLA	O1A-CGA-O2A-C1
14	B	820	CLA	O1A-CGA-O2A-C1
14	L	204	CLA	O1A-CGA-O2A-C1
22	L	207	DGD	O1A-C1A-O1G-C1G
14	A	819	CLA	O1D-CGD-O2D-CED
14	A	838	CLA	O1D-CGD-O2D-CED
14	B	836	CLA	O1D-CGD-O2D-CED
14	F	201	CLA	O1D-CGD-O2D-CED
14	X	1701	CLA	CBD-CGD-O2D-CED
14	A	838	CLA	O1A-CGA-O2A-C1
14	A	844	CLA	C2C-C3C-CAC-CBC
18	I	102	LMG	O6-C5-C6-O5
14	A	802	CLA	C3-C5-C6-C7
14	A	813	CLA	C3-C5-C6-C7
14	A	819	CLA	C3-C5-C6-C7
14	A	830	CLA	C3-C5-C6-C7
14	B	802	CLA	C3-C5-C6-C7
14	B	819	CLA	C3-C5-C6-C7
14	B	840	CLA	C3-C5-C6-C7
14	A	806	CLA	CBA-CGA-O2A-C1
14	A	808	CLA	CBA-CGA-O2A-C1
14	A	809	CLA	CBA-CGA-O2A-C1
14	A	812	CLA	CBA-CGA-O2A-C1
22	L	207	DGD	O6E-C5E-C6E-O5E
14	A	815	CLA	CBD-CGD-O2D-CED
14	A	843	CLA	CBD-CGD-O2D-CED
14	B	809	CLA	CBD-CGD-O2D-CED
14	B	820	CLA	CBD-CGD-O2D-CED
14	B	824	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	B	828	CLA	CBD-CGD-O2D-CED
14	B	830	CLA	CBD-CGD-O2D-CED
18	A	856	LMG	C11-C10-O7-C8
14	B	821	CLA	O1D-CGD-O2D-CED
14	B	824	CLA	C4-C3-C5-C6
14	B	824	CLA	C2-C3-C5-C6
14	B	805	CLA	O1D-CGD-O2D-CED
14	B	826	CLA	C3-C5-C6-C7
14	B	832	CLA	C3-C5-C6-C7
13	A	801	CL0	CBA-CGA-O2A-C1
14	A	805	CLA	CBA-CGA-O2A-C1
14	A	822	CLA	CBA-CGA-O2A-C1
14	A	825	CLA	CBA-CGA-O2A-C1
14	A	838	CLA	CBA-CGA-O2A-C1
14	B	820	CLA	CBA-CGA-O2A-C1
14	B	831	CLA	CBA-CGA-O2A-C1
14	L	204	CLA	CBA-CGA-O2A-C1
22	L	207	DGD	C2A-C1A-O1G-C1G
14	A	805	CLA	O1A-CGA-O2A-C1
14	A	822	CLA	O1A-CGA-O2A-C1
14	A	829	CLA	O1A-CGA-O2A-C1
14	A	844	CLA	O1A-CGA-O2A-C1
14	A	857	CLA	O1A-CGA-O2A-C1
14	B	810	CLA	O1D-CGD-O2D-CED
19	A	854	LHG	O2-C2-C3-O3
19	A	855	LHG	O2-C2-C3-O3
14	A	803	CLA	O1D-CGD-O2D-CED
14	A	828	CLA	CBA-CGA-O2A-C1
14	A	844	CLA	CBA-CGA-O2A-C1
14	A	857	CLA	CBA-CGA-O2A-C1
14	B	817	CLA	CBA-CGA-O2A-C1
22	L	207	DGD	C4D-C5D-C6D-O5D
14	A	809	CLA	O1A-CGA-O2A-C1
18	I	102	LMG	C4-C5-C6-O5
14	A	857	CLA	CBD-CGD-O2D-CED
18	A	853	LMG	C11-C10-O7-C8
14	A	828	CLA	O1A-CGA-O2A-C1
18	B	849	LMG	C4-C5-C6-O5
22	L	207	DGD	C4E-C5E-C6E-O5E
14	A	826	CLA	O1D-CGD-O2D-CED
14	A	829	CLA	C3-C5-C6-C7
14	A	857	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	L	204	CLA	C3-C5-C6-C7
18	B	849	LMG	O6-C5-C6-O5
14	A	822	CLA	O1D-CGD-O2D-CED
14	A	842	CLA	O1D-CGD-O2D-CED
14	A	829	CLA	CBA-CGA-O2A-C1
15	A	845	PQN	C14-C13-C15-C16
15	A	845	PQN	C12-C13-C15-C16
14	B	817	CLA	O1A-CGA-O2A-C1
14	B	831	CLA	O1A-CGA-O2A-C1
19	A	854	LHG	O10-C23-O8-C6
14	A	811	CLA	CBD-CGD-O2D-CED
14	B	826	CLA	CBD-CGD-O2D-CED
14	A	830	CLA	C2A-CAA-CBA-CGA
14	A	842	CLA	CBA-CGA-O2A-C1
14	B	804	CLA	CBA-CGA-O2A-C1
14	B	807	CLA	CBD-CGD-O2D-CED
14	F	202	CLA	CBD-CGD-O2D-CED
21	L	202	LMT	O5'-C5'-C6'-O6'
14	B	814	CLA	O1D-CGD-O2D-CED
14	X	1701	CLA	O1D-CGD-O2D-CED
21	L	202	LMT	C4'-C5'-C6'-O6'
14	A	814	CLA	CBD-CGD-O2D-CED
14	A	825	CLA	CBD-CGD-O2D-CED
14	A	842	CLA	O1A-CGA-O2A-C1
14	B	818	CLA	O1A-CGA-O2A-C1
14	B	809	CLA	O1D-CGD-O2D-CED
14	A	804	CLA	CBA-CGA-O2A-C1
14	A	807	CLA	CBA-CGA-O2A-C1
14	A	832	CLA	CBA-CGA-O2A-C1
14	A	834	CLA	CBA-CGA-O2A-C1
14	A	840	CLA	CBA-CGA-O2A-C1
14	B	818	CLA	CBA-CGA-O2A-C1
14	B	822	CLA	CBA-CGA-O2A-C1
14	B	826	CLA	CBA-CGA-O2A-C1
14	B	839	CLA	CBA-CGA-O2A-C1
18	I	102	LMG	C29-C28-O8-C9
19	A	854	LHG	C24-C23-O8-C6
14	A	815	CLA	O1D-CGD-O2D-CED
14	A	843	CLA	O1D-CGD-O2D-CED
13	A	801	CL0	C3-C5-C6-C7
14	A	820	CLA	C3-C5-C6-C7
14	A	822	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	B	826	CLA	C11-C10-C8-C9
14	B	829	CLA	C6-C7-C8-C9
14	B	840	CLA	C14-C13-C15-C16
15	A	845	PQN	C16-C17-C18-C19
21	L	202	LMT	C3'-C4'-O1B-C1B
14	B	804	CLA	O1A-CGA-O2A-C1
14	B	822	CLA	O1A-CGA-O2A-C1
14	B	813	CLA	CBD-CGD-O2D-CED
17	A	847	BCR	C37-C22-C23-C24
17	A	848	BCR	C36-C18-C19-C20
17	A	849	BCR	C11-C12-C13-C35
17	B	846	BCR	C7-C8-C9-C34
17	B	847	BCR	C36-C18-C19-C20
17	B	847	BCR	C37-C22-C23-C24
17	F	203	BCR	C7-C8-C9-C34
17	I	101	BCR	C11-C12-C13-C35
17	I	101	BCR	C37-C22-C23-C24
17	I	103	BCR	C7-C8-C9-C34
17	I	103	BCR	C11-C12-C13-C35
17	J	103	BCR	C11-C12-C13-C35
17	J	103	BCR	C36-C18-C19-C20
17	J	105	BCR	C7-C8-C9-C34
17	M	103	BCR	C7-C8-C9-C34
17	M	103	BCR	C11-C12-C13-C35
17	M	103	BCR	C36-C18-C19-C20
17	B	843	BCR	C21-C22-C23-C24
17	I	103	BCR	C21-C22-C23-C24
14	B	812	CLA	C2A-CAA-CBA-CGA
14	A	840	CLA	O1A-CGA-O2A-C1
14	B	839	CLA	O1A-CGA-O2A-C1
14	B	823	CLA	CBD-CGD-O2D-CED
19	A	854	LHG	C8-C7-O7-C5
14	A	804	CLA	C10-C11-C12-C13
14	A	828	CLA	C10-C11-C12-C13
14	B	820	CLA	O1D-CGD-O2D-CED
17	B	848	BCR	C14-C15-C16-C17
19	B	850	LHG	O1-C1-C2-O2
14	B	817	CLA	C3-C5-C6-C7
14	A	829	CLA	C13-C15-C16-C17
14	A	837	CLA	CBD-CGD-O2D-CED
14	B	826	CLA	C6-C7-C8-C10
18	A	856	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
14	A	804	CLA	O1A-CGA-O2A-C1
14	B	827	CLA	CBD-CGD-O2D-CED
14	B	803	CLA	C13-C15-C16-C17
14	B	840	CLA	C10-C11-C12-C13
14	B	840	CLA	C15-C16-C17-C18
14	A	857	CLA	C2A-CAA-CBA-CGA
14	B	804	CLA	C2A-CAA-CBA-CGA
14	B	822	CLA	C2A-CAA-CBA-CGA
14	B	828	CLA	C2A-CAA-CBA-CGA
14	B	840	CLA	C2A-CAA-CBA-CGA
17	B	846	BCR	C10-C11-C12-C13
14	A	833	CLA	C13-C15-C16-C17
14	A	843	CLA	C5-C6-C7-C8
19	M	101	LHG	C7-C8-C9-C10
14	B	830	CLA	O1D-CGD-O2D-CED
14	A	807	CLA	O1A-CGA-O2A-C1
14	B	826	CLA	O1A-CGA-O2A-C1
14	A	810	CLA	C3-C5-C6-C7
14	B	804	CLA	C3-C5-C6-C7
13	A	801	CL0	C13-C15-C16-C17
14	A	802	CLA	C10-C11-C12-C13
14	A	809	CLA	C5-C6-C7-C8
14	A	814	CLA	C8-C10-C11-C12
14	A	827	CLA	C13-C15-C16-C17
14	A	834	CLA	C5-C6-C7-C8
14	B	803	CLA	C10-C11-C12-C13
14	B	813	CLA	C13-C15-C16-C17
14	B	827	CLA	C10-C11-C12-C13
14	B	828	CLA	C8-C10-C11-C12
14	B	837	CLA	C5-C6-C7-C8
15	B	842	PQN	C20-C21-C22-C23
15	B	842	PQN	C23-C25-C26-C27
14	A	834	CLA	O1A-CGA-O2A-C1
14	B	825	CLA	CBA-CGA-O2A-C1
14	B	828	CLA	O1D-CGD-O2D-CED
14	A	825	CLA	C5-C6-C7-C8
14	B	807	CLA	C13-C15-C16-C17
14	B	824	CLA	O1D-CGD-O2D-CED
14	A	807	CLA	C5-C6-C7-C8
14	B	827	CLA	C13-C15-C16-C17
14	A	810	CLA	CBA-CGA-O2A-C1
14	A	832	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	B	827	CLA	C8-C10-C11-C12
14	B	803	CLA	C15-C16-C17-C18
14	A	808	CLA	C2A-CAA-CBA-CGA
14	A	833	CLA	CBA-CGA-O2A-C1
13	A	801	CL0	C8-C10-C11-C12
14	A	810	CLA	C15-C16-C17-C18
14	A	812	CLA	C10-C11-C12-C13
14	A	839	CLA	C10-C11-C12-C13
14	B	808	CLA	C15-C16-C17-C18
15	A	845	PQN	C25-C26-C27-C28
14	A	806	CLA	C13-C15-C16-C17
14	A	830	CLA	C8-C10-C11-C12
14	A	830	CLA	C10-C11-C12-C13
14	A	835	CLA	C5-C6-C7-C8
14	B	828	CLA	C15-C16-C17-C18
14	A	826	CLA	C15-C16-C17-C18
18	A	856	LMG	C2-C1-O1-C7
21	L	202	LMT	C2'-C1'-O1'-C1
14	B	805	CLA	C13-C15-C16-C17
14	B	808	CLA	C13-C15-C16-C17
21	L	202	LMT	C5'-C4'-O1B-C1B
14	B	832	CLA	C16-C17-C18-C20
17	A	847	BCR	C11-C10-C9-C34
17	A	847	BCR	C35-C13-C14-C15
17	A	849	BCR	C11-C10-C9-C34
17	A	849	BCR	C20-C21-C22-C37
17	A	851	BCR	C20-C21-C22-C37
17	B	845	BCR	C11-C10-C9-C34
17	B	845	BCR	C35-C13-C14-C15
17	B	845	BCR	C20-C21-C22-C37
17	B	848	BCR	C11-C10-C9-C34
17	B	848	BCR	C16-C17-C18-C36
17	B	851	BCR	C16-C17-C18-C36
17	B	851	BCR	C20-C21-C22-C37
17	F	203	BCR	C20-C21-C22-C37
17	I	101	BCR	C11-C10-C9-C34
17	I	101	BCR	C16-C17-C18-C36
17	I	101	BCR	C20-C21-C22-C37
17	J	103	BCR	C35-C13-C14-C15
17	J	103	BCR	C20-C21-C22-C37
17	J	104	BCR	C11-C10-C9-C34
17	J	104	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
17	J	105	BCR	C20-C21-C22-C37
17	L	201	BCR	C16-C17-C18-C36
17	M	103	BCR	C11-C10-C9-C34
17	M	103	BCR	C20-C21-C22-C37
14	A	857	CLA	O1D-CGD-O2D-CED
14	B	827	CLA	C2C-C3C-CAC-CBC
14	A	822	CLA	C15-C16-C17-C18
17	A	848	BCR	C15-C16-C17-C18
14	B	813	CLA	C16-C17-C18-C19
15	A	845	PQN	C26-C27-C28-C29
17	A	847	BCR	C11-C10-C9-C8
17	A	847	BCR	C12-C13-C14-C15
17	A	848	BCR	C11-C10-C9-C8
17	A	848	BCR	C16-C17-C18-C19
17	A	848	BCR	C20-C21-C22-C23
17	A	849	BCR	C11-C10-C9-C8
17	A	850	BCR	C16-C17-C18-C19
17	A	850	BCR	C20-C21-C22-C23
17	A	852	BCR	C12-C13-C14-C15
17	B	844	BCR	C16-C17-C18-C19
17	B	845	BCR	C11-C10-C9-C8
17	B	845	BCR	C12-C13-C14-C15
17	B	845	BCR	C20-C21-C22-C23
17	B	846	BCR	C20-C21-C22-C23
17	B	848	BCR	C20-C21-C22-C23
17	B	851	BCR	C11-C10-C9-C8
17	F	203	BCR	C11-C10-C9-C8
17	F	203	BCR	C12-C13-C14-C15
17	F	203	BCR	C16-C17-C18-C19
17	I	101	BCR	C16-C17-C18-C19
17	I	101	BCR	C20-C21-C22-C23
17	J	103	BCR	C16-C17-C18-C19
17	J	105	BCR	C11-C10-C9-C8
17	L	201	BCR	C20-C21-C22-C23
14	B	827	CLA	C4C-C3C-CAC-CBC
14	B	826	CLA	O1D-CGD-O2D-CED
14	A	811	CLA	O1D-CGD-O2D-CED
14	B	813	CLA	CBA-CGA-O2A-C1
14	A	820	CLA	C13-C15-C16-C17
14	A	826	CLA	C2-C1-O2A-CGA
14	A	835	CLA	C16-C17-C18-C20
14	B	813	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
14	L	206	CLA	C16-C17-C18-C19
14	L	206	CLA	C16-C17-C18-C20
18	A	853	LMG	O10-C28-O8-C9
19	M	101	LHG	C32-C33-C34-C35
14	A	839	CLA	CBD-CGD-O2D-CED
17	J	104	BCR	C14-C15-C16-C17
17	M	103	BCR	C14-C15-C16-C17
19	M	101	LHG	C14-C15-C16-C17
18	A	853	LMG	C20-C21-C22-C23
14	A	819	CLA	C4B-C3B-CAB-CBB
14	A	806	CLA	C16-C17-C18-C19
14	A	806	CLA	C16-C17-C18-C20
14	A	820	CLA	C16-C17-C18-C20
14	A	833	CLA	C16-C17-C18-C19
14	A	833	CLA	C16-C17-C18-C20
14	B	838	CLA	C16-C17-C18-C20
15	A	845	PQN	C26-C27-C28-C30
14	A	810	CLA	O1A-CGA-O2A-C1
14	K	101	CLA	C2A-CAA-CBA-CGA
14	M	102	CLA	C2A-CAA-CBA-CGA
14	A	809	CLA	C13-C15-C16-C17
14	A	834	CLA	C11-C10-C8-C7
18	A	853	LMG	C17-C18-C19-C20
14	B	832	CLA	C5-C6-C7-C8
14	B	840	CLA	C8-C10-C11-C12
18	A	853	LMG	C30-C31-C32-C33
22	L	207	DGD	C5B-C6B-C7B-C8B
14	A	833	CLA	O1A-CGA-O2A-C1
14	A	806	CLA	C3A-C2A-CAA-CBA
14	A	826	CLA	C3A-C2A-CAA-CBA
14	A	828	CLA	C3A-C2A-CAA-CBA
14	F	201	CLA	C3A-C2A-CAA-CBA
14	B	807	CLA	O1D-CGD-O2D-CED
14	A	803	CLA	C13-C15-C16-C17
14	F	202	CLA	O1D-CGD-O2D-CED
17	A	851	BCR	C15-C16-C17-C18
14	A	820	CLA	C16-C17-C18-C19
14	B	838	CLA	C16-C17-C18-C19
14	B	827	CLA	CBA-CGA-O2A-C1
14	B	828	CLA	CBA-CGA-O2A-C1
14	B	837	CLA	CBA-CGA-O2A-C1
18	B	849	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
18	B	849	LMG	C41-C42-C43-C44
19	M	101	LHG	C30-C31-C32-C33
19	A	854	LHG	C12-C13-C14-C15
14	A	835	CLA	C16-C17-C18-C19
18	I	102	LMG	O10-C28-O8-C9
14	A	819	CLA	C2B-C3B-CAB-CBB
17	A	848	BCR	C23-C24-C25-C26
17	A	848	BCR	C23-C24-C25-C30
17	A	850	BCR	C23-C24-C25-C26
17	A	850	BCR	C23-C24-C25-C30
17	A	852	BCR	C23-C24-C25-C26
17	A	852	BCR	C23-C24-C25-C30
17	B	843	BCR	C23-C24-C25-C26
17	B	843	BCR	C23-C24-C25-C30
17	B	846	BCR	C23-C24-C25-C30
17	B	847	BCR	C23-C24-C25-C30
17	J	103	BCR	C1-C6-C7-C8
17	J	103	BCR	C5-C6-C7-C8
17	J	103	BCR	C23-C24-C25-C26
17	J	103	BCR	C23-C24-C25-C30
17	J	104	BCR	C23-C24-C25-C30
17	L	208	BCR	C23-C24-C25-C26
17	L	208	BCR	C23-C24-C25-C30
17	M	103	BCR	C1-C6-C7-C8
17	M	103	BCR	C23-C24-C25-C26
17	M	103	BCR	C23-C24-C25-C30
14	A	804	CLA	CBD-CGD-O2D-CED
14	A	802	CLA	CBA-CGA-O2A-C1
14	A	818	CLA	CBA-CGA-O2A-C1
14	A	825	CLA	C8-C10-C11-C12
14	A	843	CLA	C15-C16-C17-C18
15	A	845	PQN	C20-C21-C22-C23
18	A	853	LMG	C33-C34-C35-C36
15	A	845	PQN	C15-C16-C17-C18
14	B	813	CLA	O1A-CGA-O2A-C1
14	B	816	CLA	CBD-CGD-O2D-CED
22	L	207	DGD	O1B-C1B-O2G-C2G
18	A	853	LMG	C11-C12-C13-C14
18	B	849	LMG	C35-C36-C37-C38
22	L	207	DGD	CAA-CBA-CCA-CDA
17	A	849	BCR	C18-C19-C20-C21
17	J	103	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
17	L	208	BCR	C10-C11-C12-C13
14	A	839	CLA	C8-C10-C11-C12
14	B	802	CLA	C8-C10-C11-C12
18	A	856	LMG	C18-C19-C20-C21
18	I	102	LMG	C15-C16-C17-C18
14	A	826	CLA	CBA-CGA-O2A-C1
14	B	814	CLA	C15-C16-C17-C18
17	A	847	BCR	C22-C23-C24-C25
17	M	103	BCR	C22-C23-C24-C25
21	L	202	LMT	O5B-C5B-C6B-O6B
19	B	850	LHG	C24-C23-O8-C6
14	B	816	CLA	CBA-CGA-O2A-C1
18	I	102	LMG	C11-C10-O7-C8
19	A	854	LHG	C7-C8-C9-C10
22	L	207	DGD	C9A-CAA-CBA-CCA
14	A	810	CLA	C10-C11-C12-C13
14	A	831	CLA	C10-C11-C12-C13
17	J	105	BCR	C11-C12-C13-C35
18	B	849	LMG	C18-C19-C20-C21
14	A	805	CLA	C10-C11-C12-C13
14	A	820	CLA	C2A-CAA-CBA-CGA
14	B	814	CLA	C2A-CAA-CBA-CGA
14	B	832	CLA	C16-C17-C18-C19
18	A	853	LMG	C14-C15-C16-C17
18	B	849	LMG	C31-C32-C33-C34
14	A	833	CLA	C4-C3-C5-C6
14	B	828	CLA	O1A-CGA-O2A-C1
14	B	827	CLA	O1A-CGA-O2A-C1
14	B	837	CLA	O1A-CGA-O2A-C1
19	A	854	LHG	C27-C28-C29-C30
14	A	818	CLA	O1A-CGA-O2A-C1
18	A	853	LMG	C28-C29-C30-C31
14	A	825	CLA	O1D-CGD-O2D-CED
18	A	853	LMG	C22-C23-C24-C25
19	A	854	LHG	O7-C5-C6-O8
18	B	849	LMG	C17-C18-C19-C20
14	B	837	CLA	C8-C10-C11-C12
18	A	856	LMG	O6-C5-C6-O5
13	A	801	CL0	C16-C17-C18-C20
14	A	804	CLA	C5-C6-C7-C8
14	A	802	CLA	O1A-CGA-O2A-C1
14	B	828	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
19	A	854	LHG	O9-C7-O7-C5
19	M	101	LHG	C34-C35-C36-C37
14	A	835	CLA	CBD-CGD-O2D-CED
14	A	833	CLA	C5-C6-C7-C8
14	A	826	CLA	O1A-CGA-O2A-C1
14	A	823	CLA	C1A-C2A-CAA-CBA
14	A	824	CLA	C1A-C2A-CAA-CBA
14	B	817	CLA	C1A-C2A-CAA-CBA
14	F	201	CLA	C1A-C2A-CAA-CBA
14	J	101	CLA	C1A-C2A-CAA-CBA
14	A	814	CLA	O1D-CGD-O2D-CED
14	A	802	CLA	C11-C10-C8-C7
14	B	802	CLA	C11-C12-C13-C15
14	B	828	CLA	C12-C13-C15-C16
14	B	832	CLA	C11-C12-C13-C15
14	B	838	CLA	C11-C12-C13-C15
14	B	809	CLA	C16-C17-C18-C20
14	A	831	CLA	C13-C15-C16-C17
19	A	854	LHG	C23-C24-C25-C26
14	B	813	CLA	O1D-CGD-O2D-CED
14	A	817	CLA	C2A-CAA-CBA-CGA
13	A	801	CL0	C11-C12-C13-C14
14	A	802	CLA	C11-C10-C8-C9
14	A	805	CLA	C6-C7-C8-C9
14	A	834	CLA	C11-C10-C8-C9
14	A	841	CLA	C6-C7-C8-C9
14	A	857	CLA	C11-C10-C8-C9
14	B	818	CLA	C6-C7-C8-C9
14	B	828	CLA	C14-C13-C15-C16
14	B	838	CLA	C11-C12-C13-C14
18	I	102	LMG	C28-C29-C30-C31
14	B	822	CLA	C5-C6-C7-C8
14	B	823	CLA	O1D-CGD-O2D-CED
19	A	854	LHG	C4-C5-C6-O8
22	L	207	DGD	CEB-CFB-CGB-CHB
14	B	809	CLA	C16-C17-C18-C19
14	B	828	CLA	C5-C6-C7-C8
14	B	816	CLA	O1A-CGA-O2A-C1
14	A	837	CLA	O1D-CGD-O2D-CED
17	A	847	BCR	C20-C21-C22-C37
17	B	844	BCR	C11-C10-C9-C34
17	B	851	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
14	A	826	CLA	C4-C3-C5-C6
14	A	826	CLA	C2-C3-C5-C6
13	A	801	CL0	C16-C17-C18-C19
14	A	839	CLA	C16-C17-C18-C20
18	B	849	LMG	C13-C14-C15-C16
14	B	805	CLA	C15-C16-C17-C18
14	B	825	CLA	O1A-CGA-O2A-C1
21	L	202	LMT	O1'-C1-C2-C3
14	B	810	CLA	CBA-CGA-O2A-C1
14	B	833	CLA	CBA-CGA-O2A-C1
14	A	857	CLA	O2A-C1-C2-C3
14	A	830	CLA	C5-C6-C7-C8
14	B	813	CLA	C8-C10-C11-C12
14	B	818	CLA	C8-C10-C11-C12
19	M	101	LHG	C23-C24-C25-C26
17	B	847	BCR	C12-C13-C14-C15
17	M	103	BCR	C11-C10-C9-C8
14	A	823	CLA	CBA-CGA-O2A-C1
14	L	205	CLA	CBA-CGA-O2A-C1
18	B	849	LMG	C30-C31-C32-C33
18	A	856	LMG	C16-C17-C18-C19
14	A	839	CLA	C16-C17-C18-C19
19	M	101	LHG	C11-C10-C9-C8
14	B	809	CLA	CBA-CGA-O2A-C1
14	A	813	CLA	C6-C7-C8-C9
14	A	825	CLA	C11-C12-C13-C14
14	B	827	CLA	O1D-CGD-O2D-CED
14	B	805	CLA	CBA-CGA-O2A-C1
14	B	841	CLA	CBA-CGA-O2A-C1
18	A	853	LMG	C29-C28-O8-C9
14	B	804	CLA	C6-C7-C8-C9
18	A	856	LMG	C13-C14-C15-C16
21	L	202	LMT	C1-C2-C3-C4
22	L	207	DGD	CCA-CDA-CEA-CFA
22	L	207	DGD	O6D-C5D-C6D-O5D
18	A	853	LMG	C18-C19-C20-C21
19	M	101	LHG	C13-C14-C15-C16
19	A	855	LHG	O9-C7-O7-C5
14	A	827	CLA	C11-C10-C8-C9
14	B	802	CLA	C11-C12-C13-C14
14	B	803	CLA	C11-C10-C8-C9
14	B	832	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	A	806	CLA	C5-C6-C7-C8
14	A	857	CLA	C13-C15-C16-C17
14	B	810	CLA	C5-C6-C7-C8
19	A	855	LHG	C2-C3-O3-P
14	A	808	CLA	C4B-C3B-CAB-CBB
14	B	814	CLA	C8-C10-C11-C12
14	L	206	CLA	C10-C11-C12-C13
18	B	849	LMG	C15-C16-C17-C18
13	A	801	CL0	C11-C12-C13-C15
14	A	820	CLA	C11-C10-C8-C7
14	A	822	CLA	C6-C7-C8-C10
14	A	825	CLA	C11-C10-C8-C7
14	A	827	CLA	C11-C10-C8-C7
14	A	829	CLA	C6-C7-C8-C10
14	A	841	CLA	C6-C7-C8-C10
14	A	857	CLA	C11-C10-C8-C7
14	B	803	CLA	C11-C10-C8-C7
14	B	805	CLA	C12-C13-C15-C16
14	B	806	CLA	C11-C12-C13-C15
14	B	810	CLA	C11-C12-C13-C15
14	B	818	CLA	C6-C7-C8-C10
14	A	806	CLA	C10-C11-C12-C13
14	L	205	CLA	C13-C15-C16-C17
14	B	813	CLA	C3A-C2A-CAA-CBA
14	B	819	CLA	C3A-C2A-CAA-CBA
14	B	832	CLA	C4-C3-C5-C6
14	J	101	CLA	C3A-C2A-CAA-CBA
14	L	204	CLA	C4-C3-C5-C6
19	A	855	LHG	C11-C10-C9-C8
19	A	855	LHG	C9-C10-C11-C12
14	B	810	CLA	O1A-CGA-O2A-C1
14	A	826	CLA	C10-C11-C12-C13
17	A	848	BCR	C9-C10-C11-C12
17	B	845	BCR	C9-C10-C11-C12
17	B	847	BCR	C11-C12-C13-C14
14	B	817	CLA	C10-C11-C12-C13
19	A	854	LHG	C34-C35-C36-C37
18	B	849	LMG	O1-C7-C8-C9
19	B	850	LHG	C4-C5-C6-O8
19	M	101	LHG	C4-C5-C6-O8
14	B	828	CLA	C13-C15-C16-C17
14	A	823	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
14	B	833	CLA	O1A-CGA-O2A-C1
14	L	204	CLA	C2-C3-C5-C6
17	A	847	BCR	C23-C24-C25-C30
17	A	848	BCR	C1-C6-C7-C8
17	A	849	BCR	C1-C6-C7-C8
17	A	852	BCR	C1-C6-C7-C8
17	B	847	BCR	C23-C24-C25-C26
17	F	203	BCR	C23-C24-C25-C30
17	I	101	BCR	C1-C6-C7-C8
17	I	103	BCR	C1-C6-C7-C8
17	J	105	BCR	C1-C6-C7-C8
17	L	208	BCR	C1-C6-C7-C8
14	A	804	CLA	O1D-CGD-O2D-CED
14	A	839	CLA	O1D-CGD-O2D-CED
14	A	822	CLA	C4-C3-C5-C6
19	M	101	LHG	C17-C18-C19-C20
17	B	845	BCR	C10-C11-C12-C13
14	A	822	CLA	C2-C3-C5-C6
14	A	813	CLA	C2C-C3C-CAC-CBC
14	A	803	CLA	C14-C13-C15-C16
14	A	825	CLA	C11-C10-C8-C9
14	B	806	CLA	C11-C12-C13-C14
17	A	848	BCR	C22-C23-C24-C25
17	A	849	BCR	C6-C7-C8-C9
17	A	851	BCR	C6-C7-C8-C9
17	I	101	BCR	C22-C23-C24-C25
17	J	105	BCR	C6-C7-C8-C9
17	A	849	BCR	C14-C15-C16-C17
17	B	847	BCR	C14-C15-C16-C17
14	B	816	CLA	O1D-CGD-O2D-CED
14	A	817	CLA	O2A-C1-C2-C3
18	A	853	LMG	C2-C1-O1-C7
14	B	826	CLA	C2C-C3C-CAC-CBC
18	A	856	LMG	C19-C20-C21-C22
17	B	846	BCR	C9-C10-C11-C12
14	B	832	CLA	C2-C3-C5-C6
14	A	811	CLA	C2C-C3C-CAC-CBC
14	B	808	CLA	C8-C10-C11-C12
17	B	843	BCR	C11-C10-C9-C34
17	B	847	BCR	C11-C10-C9-C34
17	J	103	BCR	C11-C10-C9-C34
14	A	807	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
14	B	809	CLA	C11-C10-C8-C7
14	L	204	CLA	C6-C7-C8-C10
14	L	204	CLA	C12-C13-C15-C16
14	L	205	CLA	C11-C10-C8-C7
14	B	838	CLA	C13-C15-C16-C17
17	B	846	BCR	C7-C8-C9-C10
17	I	101	BCR	C21-C22-C23-C24
17	J	105	BCR	C11-C12-C13-C14
19	M	101	LHG	C29-C30-C31-C32
14	B	809	CLA	O1A-CGA-O2A-C1
14	L	205	CLA	O1A-CGA-O2A-C1
13	A	801	CL0	C2A-CAA-CBA-CGA
14	B	805	CLA	O1A-CGA-O2A-C1
14	B	841	CLA	O1A-CGA-O2A-C1
14	B	824	CLA	C5-C6-C7-C8
14	A	814	CLA	C3-C5-C6-C7
14	A	835	CLA	O1D-CGD-O2D-CED
17	A	849	BCR	C12-C13-C14-C15
17	B	847	BCR	C16-C17-C18-C19
17	I	101	BCR	C12-C13-C14-C15
17	M	103	BCR	C12-C13-C14-C15
17	M	103	BCR	C20-C21-C22-C23
14	A	823	CLA	O2A-C1-C2-C3
18	A	853	LMG	C7-C8-C9-O8
19	A	854	LHG	C9-C10-C11-C12
14	B	826	CLA	C2A-CAA-CBA-CGA
14	B	831	CLA	C2A-CAA-CBA-CGA
14	A	833	CLA	C2-C3-C5-C6
22	L	207	DGD	C4B-C5B-C6B-C7B
19	B	850	LHG	O7-C5-C6-O8
19	M	101	LHG	O7-C5-C6-O8
14	B	817	CLA	C6-C7-C8-C9
14	B	829	CLA	C11-C10-C8-C9
14	L	204	CLA	C14-C13-C15-C16
19	A	854	LHG	C18-C19-C20-C21
14	A	820	CLA	C8-C10-C11-C12
14	B	838	CLA	C5-C6-C7-C8
18	I	102	LMG	C11-C12-C13-C14
19	M	101	LHG	C27-C28-C29-C30
17	I	103	BCR	C15-C16-C17-C18
22	L	207	DGD	C2D-C1D-O3G-C3G
14	L	206	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	B	849	LMG	C23-C24-C25-C26
14	A	807	CLA	C3-C5-C6-C7
14	A	825	CLA	C3-C5-C6-C7
14	A	841	CLA	C5-C6-C7-C8
14	B	806	CLA	C4B-C3B-CAB-CBB
14	B	813	CLA	C1A-C2A-CAA-CBA
14	B	816	CLA	C1A-C2A-CAA-CBA
14	B	826	CLA	C1A-C2A-CAA-CBA
14	B	830	CLA	C1A-C2A-CAA-CBA
14	B	834	CLA	C4B-C3B-CAB-CBB
14	F	201	CLA	C4B-C3B-CAB-CBB
17	B	847	BCR	C22-C23-C24-C25
17	B	846	BCR	C11-C12-C13-C14
22	L	207	DGD	CAB-CBB-CCB-CDB
14	A	802	CLA	C6-C7-C8-C10
14	A	831	CLA	C11-C10-C8-C7
14	A	839	CLA	C6-C7-C8-C10
14	B	802	CLA	C11-C10-C8-C7
14	B	814	CLA	C12-C13-C15-C16
14	B	819	CLA	C11-C10-C8-C7
14	B	829	CLA	C12-C13-C15-C16
14	B	838	CLA	C11-C10-C8-C7
14	L	205	CLA	C12-C13-C15-C16
15	B	842	PQN	C22-C23-C25-C26
14	A	814	CLA	CBA-CGA-O2A-C1
14	B	819	CLA	CBA-CGA-O2A-C1
19	A	855	LHG	C24-C23-O8-C6
14	A	802	CLA	C6-C7-C8-C9
14	A	807	CLA	C14-C13-C15-C16
14	A	820	CLA	C11-C10-C8-C9
14	A	822	CLA	C6-C7-C8-C9
14	B	805	CLA	C14-C13-C15-C16
14	B	809	CLA	C11-C10-C8-C9
14	B	810	CLA	C11-C12-C13-C14
14	L	205	CLA	C11-C10-C8-C9
15	B	842	PQN	C24-C23-C25-C26
22	L	207	DGD	C8A-C9A-CAA-CBA
14	A	823	CLA	C1-C2-C3-C4
14	B	831	CLA	C1-C2-C3-C4
14	A	822	CLA	C3-C5-C6-C7
19	A	854	LHG	C19-C20-C21-C22
18	B	849	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
14	B	841	CLA	C2C-C3C-CAC-CBC
14	B	831	CLA	O2A-C1-C2-C3
14	A	843	CLA	C8-C10-C11-C12
14	B	809	CLA	C10-C11-C12-C13
14	B	832	CLA	C10-C11-C12-C13
14	A	814	CLA	O1A-CGA-O2A-C1
18	A	853	LMG	C29-C30-C31-C32
14	A	813	CLA	CBA-CGA-O2A-C1
14	L	206	CLA	CBA-CGA-O2A-C1
14	B	813	CLA	C5-C6-C7-C8
14	A	833	CLA	C3-C5-C6-C7
14	A	802	CLA	C2A-CAA-CBA-CGA
14	A	839	CLA	C5-C6-C7-C8
14	A	813	CLA	O1A-CGA-O2A-C1
14	A	826	CLA	CHA-CBD-CGD-O1D
14	B	812	CLA	CHA-CBD-CGD-O1D
17	B	848	BCR	C13-C14-C15-C16
17	L	201	BCR	C20-C21-C22-C37
19	B	850	LHG	C3-O3-P-O5
14	L	205	CLA	CBD-CGD-O2D-CED
14	A	839	CLA	C4-C3-C5-C6
14	B	810	CLA	C2B-C3B-CAB-CBB
19	M	101	LHG	C2-C3-O3-P
14	A	820	CLA	C15-C16-C17-C18
14	A	810	CLA	C5-C6-C7-C8
14	L	206	CLA	O1A-CGA-O2A-C1
14	A	822	CLA	C13-C15-C16-C17
17	A	849	BCR	C10-C11-C12-C13
17	I	103	BCR	C9-C10-C11-C12
17	L	201	BCR	C13-C14-C15-C16
14	A	829	CLA	C6-C7-C8-C9
14	B	819	CLA	C11-C10-C8-C9
14	B	819	CLA	C11-C12-C13-C14
14	B	826	CLA	C6-C7-C8-C9
14	B	838	CLA	C11-C10-C8-C9
14	B	829	CLA	C11-C10-C8-C7
14	A	807	CLA	C10-C11-C12-C13
17	A	852	BCR	C16-C17-C18-C19
19	A	854	LHG	C1-C2-C3-O3
14	B	819	CLA	O1A-CGA-O2A-C1
14	A	803	CLA	C3-C5-C6-C7
18	A	853	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
17	B	845	BCR	C13-C14-C15-C16
14	A	830	CLA	C4-C3-C5-C6
14	A	827	CLA	C5-C6-C7-C8
14	B	829	CLA	C8-C10-C11-C12
14	B	826	CLA	C16-C17-C18-C20
17	B	851	BCR	C11-C12-C13-C14
18	A	856	LMG	C8-C7-O1-C1
22	L	207	DGD	C5D-C6D-O5D-C1E
14	A	811	CLA	C2A-CAA-CBA-CGA
14	J	101	CLA	C2A-CAA-CBA-CGA
17	J	103	BCR	C9-C10-C11-C12
19	A	854	LHG	C28-C29-C30-C31
14	A	839	CLA	O1A-CGA-O2A-C1
14	A	807	CLA	C11-C12-C13-C14
14	A	839	CLA	CBA-CGA-O2A-C1
22	L	207	DGD	C2B-C3B-C4B-C5B
14	A	821	CLA	C4B-C3B-CAB-CBB
14	A	830	CLA	C2-C3-C5-C6
18	A	853	LMG	C12-C13-C14-C15
14	A	822	CLA	C12-C13-C15-C16
14	A	829	CLA	C11-C12-C13-C15
15	B	842	PQN	C21-C22-C23-C25
21	L	202	LMT	C5-C6-C7-C8
14	B	826	CLA	C16-C17-C18-C19
19	A	854	LHG	C24-C25-C26-C27
14	A	820	CLA	C4-C3-C5-C6
14	A	831	CLA	C3A-C2A-CAA-CBA
14	A	836	CLA	C3A-C2A-CAA-CBA
14	B	821	CLA	C3A-C2A-CAA-CBA
14	B	826	CLA	C3A-C2A-CAA-CBA
14	B	829	CLA	C3A-C2A-CAA-CBA
17	A	851	BCR	C35-C13-C14-C15
17	A	852	BCR	C11-C10-C9-C34
17	F	203	BCR	C35-C13-C14-C15
15	A	845	PQN	C23-C25-C26-C27
19	A	854	LHG	C29-C30-C31-C32
14	A	832	CLA	C2-C1-O2A-CGA
14	A	814	CLA	C5-C6-C7-C8
14	A	824	CLA	C4-C3-C5-C6
14	B	815	CLA	CAA-CBA-CGA-O1A
17	J	103	BCR	C21-C22-C23-C24
14	B	814	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
14	A	829	CLA	C2C-C3C-CAC-CBC
14	A	839	CLA	C2-C3-C5-C6
18	I	102	LMG	C30-C31-C32-C33
14	X	1701	CLA	CAA-CBA-CGA-O2A
14	A	812	CLA	C14-C13-C15-C16
14	A	857	CLA	C11-C12-C13-C14
14	B	826	CLA	C14-C13-C15-C16
14	L	205	CLA	C14-C13-C15-C16
15	A	845	PQN	C21-C22-C23-C24
14	B	815	CLA	CAA-CBA-CGA-O2A
19	M	101	LHG	C25-C26-C27-C28
14	A	836	CLA	CBA-CGA-O2A-C1
14	A	820	CLA	C2-C3-C5-C6
14	A	827	CLA	C3-C5-C6-C7
13	A	801	CL0	C5-C6-C7-C8
14	X	1701	CLA	CAA-CBA-CGA-O1A
14	B	807	CLA	C2C-C3C-CAC-CBC
13	A	801	CL0	C1A-C2A-CAA-CBA
14	B	819	CLA	C1A-C2A-CAA-CBA
14	B	821	CLA	C1A-C2A-CAA-CBA
14	B	827	CLA	C1A-C2A-CAA-CBA
17	I	103	BCR	C11-C10-C9-C8
17	J	104	BCR	C11-C10-C9-C8
18	A	853	LMG	C35-C36-C37-C38
14	A	808	CLA	C2B-C3B-CAB-CBB
14	B	806	CLA	C2B-C3B-CAB-CBB
14	B	823	CLA	C2B-C3B-CAB-CBB
14	B	834	CLA	C2B-C3B-CAB-CBB
14	F	201	CLA	C2B-C3B-CAB-CBB
17	A	848	BCR	C5-C6-C7-C8
17	A	850	BCR	C1-C6-C7-C8
17	A	852	BCR	C5-C6-C7-C8
17	F	203	BCR	C23-C24-C25-C26
17	I	101	BCR	C5-C6-C7-C8
17	I	103	BCR	C5-C6-C7-C8
17	J	104	BCR	C23-C24-C25-C26
17	J	105	BCR	C5-C6-C7-C8
17	L	208	BCR	C5-C6-C7-C8
14	A	830	CLA	C13-C15-C16-C17
14	M	102	CLA	CAA-CBA-CGA-O1A
14	A	802	CLA	C4-C3-C5-C6
14	B	810	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
17	B	846	BCR	C14-C15-C16-C17
14	A	807	CLA	C11-C12-C13-C15
14	A	830	CLA	C6-C7-C8-C10
14	A	831	CLA	C11-C12-C13-C15
14	A	843	CLA	C11-C12-C13-C15
14	B	802	CLA	C12-C13-C15-C16
14	B	808	CLA	C6-C7-C8-C10
14	B	813	CLA	C6-C7-C8-C10
14	B	828	CLA	C6-C7-C8-C10
14	B	840	CLA	C12-C13-C15-C16
14	B	810	CLA	C16-C17-C18-C20
14	A	813	CLA	C2A-CAA-CBA-CGA
14	B	841	CLA	C5-C6-C7-C8
18	A	856	LMG	C17-C18-C19-C20
14	L	205	CLA	O1D-CGD-O2D-CED
14	A	828	CLA	C8-C10-C11-C12
17	A	847	BCR	C36-C18-C19-C20
14	B	823	CLA	CAA-CBA-CGA-O2A
14	B	809	CLA	C15-C16-C17-C18
14	A	837	CLA	CAA-CBA-CGA-O2A
17	M	103	BCR	C17-C18-C19-C20
14	A	810	CLA	C2A-CAA-CBA-CGA
14	B	823	CLA	CAA-CBA-CGA-O1A
14	A	830	CLA	C11-C12-C13-C14
14	A	834	CLA	C14-C13-C15-C16
14	B	806	CLA	C6-C7-C8-C9
14	A	807	CLA	C13-C15-C16-C17
14	B	802	CLA	C4-C3-C5-C6
14	B	814	CLA	C2-C3-C5-C6
14	B	810	CLA	C8-C10-C11-C12
14	M	102	CLA	CAA-CBA-CGA-O2A
14	A	836	CLA	O1A-CGA-O2A-C1
14	B	830	CLA	CAA-CBA-CGA-O2A
14	B	807	CLA	C2A-CAA-CBA-CGA
14	B	827	CLA	C2A-CAA-CBA-CGA
14	K	102	CLA	C2A-CAA-CBA-CGA
15	B	842	PQN	C26-C27-C28-C29
21	L	202	LMT	C2-C1-O1'-C1'
19	A	855	LHG	O6-C4-C5-O7
14	B	822	CLA	C4-C3-C5-C6
14	B	814	CLA	C4B-C3B-CAB-CBB
14	B	818	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
14	B	823	CLA	C4B-C3B-CAB-CBB
17	A	852	BCR	C16-C17-C18-C36
14	A	819	CLA	CAA-CBA-CGA-O2A
19	A	855	LHG	O6-C4-C5-C6
14	B	807	CLA	C4-C3-C5-C6
14	A	830	CLA	C11-C12-C13-C15
14	B	806	CLA	C6-C7-C8-C10
14	B	819	CLA	C12-C13-C15-C16
14	B	826	CLA	C11-C10-C8-C7
17	I	101	BCR	C19-C20-C21-C22
14	A	837	CLA	CAA-CBA-CGA-O1A
17	I	101	BCR	C7-C8-C9-C10
14	B	827	CLA	C6-C7-C8-C9
14	B	836	CLA	CAA-CBA-CGA-O2A
14	L	205	CLA	C2A-CAA-CBA-CGA
14	A	804	CLA	C2-C1-O2A-CGA
13	A	801	CL0	C3A-C2A-CAA-CBA
14	A	815	CLA	C3A-C2A-CAA-CBA
14	A	837	CLA	C3A-C2A-CAA-CBA
14	B	832	CLA	C3A-C2A-CAA-CBA
14	L	205	CLA	C3A-C2A-CAA-CBA
14	A	838	CLA	C2C-C3C-CAC-CBC
21	L	202	LMT	C11-C10-C9-C8
14	A	810	CLA	O2A-C1-C2-C3
17	L	201	BCR	C18-C19-C20-C21
18	A	853	LMG	C10-C11-C12-C13
14	A	829	CLA	C16-C17-C18-C19
14	F	202	CLA	CAA-CBA-CGA-O2A
14	A	816	CLA	C2A-CAA-CBA-CGA
19	M	101	LHG	C24-C25-C26-C27
17	B	843	BCR	C11-C10-C9-C8
17	L	201	BCR	C11-C10-C9-C8
14	B	830	CLA	CAA-CBA-CGA-O1A
17	B	851	BCR	C6-C7-C8-C9
14	B	806	CLA	O1A-CGA-O2A-C1
14	B	836	CLA	CAA-CBA-CGA-O1A
14	B	807	CLA	C2-C3-C5-C6
14	A	857	CLA	C16-C17-C18-C20
14	A	816	CLA	CAA-CBA-CGA-O2A
14	F	202	CLA	CAA-CBA-CGA-O1A
14	B	809	CLA	C2C-C3C-CAC-CBC
14	A	812	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
14	A	831	CLA	C11-C10-C8-C9
14	B	802	CLA	C11-C10-C8-C9
14	B	814	CLA	C14-C13-C15-C16
14	L	204	CLA	C6-C7-C8-C9
15	B	842	PQN	C21-C22-C23-C24
14	A	809	CLA	CAA-CBA-CGA-O2A
19	M	101	LHG	C28-C29-C30-C31
14	A	826	CLA	C11-C10-C8-C7
14	A	828	CLA	C11-C12-C13-C15
14	A	833	CLA	C11-C10-C8-C7
14	A	834	CLA	C12-C13-C15-C16
14	L	206	CLA	C6-C7-C8-C10
15	A	845	PQN	C16-C17-C18-C20
14	A	828	CLA	C5-C6-C7-C8
14	B	803	CLA	O1A-CGA-O2A-C1
14	K	102	CLA	CAA-CBA-CGA-O2A
14	A	821	CLA	C2B-C3B-CAB-CBB
14	B	814	CLA	C2B-C3B-CAB-CBB
14	B	818	CLA	C2B-C3B-CAB-CBB
17	A	847	BCR	C23-C24-C25-C26
17	A	849	BCR	C5-C6-C7-C8
17	A	850	BCR	C5-C6-C7-C8
17	B	844	BCR	C1-C6-C7-C8
17	L	201	BCR	C23-C24-C25-C30
14	A	835	CLA	C2-C1-O2A-CGA
14	B	837	CLA	C2-C1-O2A-CGA
18	A	853	LMG	C21-C22-C23-C24
18	A	853	LMG	O8-C28-C29-C30
14	A	809	CLA	C8-C10-C11-C12
14	B	810	CLA	CAA-CBA-CGA-O2A
14	A	808	CLA	CAA-CBA-CGA-O2A
14	B	803	CLA	CAA-CBA-CGA-O2A
14	A	837	CLA	C2A-CAA-CBA-CGA
14	B	832	CLA	C2A-CAA-CBA-CGA
14	A	816	CLA	CAA-CBA-CGA-O1A
14	B	813	CLA	CAA-CBA-CGA-O2A
14	B	835	CLA	CAA-CBA-CGA-O2A
14	A	843	CLA	C11-C12-C13-C14
14	B	802	CLA	C14-C13-C15-C16
14	B	808	CLA	C6-C7-C8-C9
14	B	828	CLA	C6-C7-C8-C9
17	A	849	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
14	B	839	CLA	CAA-CBA-CGA-O2A
14	A	813	CLA	C4B-C3B-CAB-CBB
14	A	831	CLA	C1A-C2A-CAA-CBA
14	A	842	CLA	C4B-C3B-CAB-CBB
14	B	809	CLA	C1A-C2A-CAA-CBA
14	B	810	CLA	C4B-C3B-CAB-CBB
14	B	835	CLA	C4B-C3B-CAB-CBB
14	B	840	CLA	C4B-C3B-CAB-CBB
14	B	841	CLA	C4B-C3B-CAB-CBB
14	K	102	CLA	C4B-C3B-CAB-CBB
14	X	1701	CLA	C1A-C2A-CAA-CBA
14	X	1701	CLA	C4B-C3B-CAB-CBB
17	A	850	BCR	C6-C7-C8-C9
14	A	802	CLA	C2-C3-C5-C6
14	B	810	CLA	C2-C3-C5-C6
14	B	812	CLA	CAA-CBA-CGA-O1A
17	J	103	BCR	C17-C18-C19-C20
17	L	201	BCR	C11-C12-C13-C14
17	L	208	BCR	C11-C12-C13-C14
17	A	850	BCR	C13-C14-C15-C16
17	B	847	BCR	C15-C16-C17-C18
14	B	812	CLA	CAA-CBA-CGA-O2A
18	A	853	LMG	O7-C10-C11-C12
14	B	838	CLA	C2A-CAA-CBA-CGA
14	A	835	CLA	C11-C12-C13-C15
14	A	842	CLA	C11-C10-C8-C7
14	B	806	CLA	C11-C10-C8-C7
14	A	810	CLA	C8-C10-C11-C12
14	B	838	CLA	C8-C10-C11-C12
14	B	818	CLA	C2C-C3C-CAC-CBC
14	B	809	CLA	CAA-CBA-CGA-O2A
19	B	850	LHG	O7-C7-C8-C9
18	A	853	LMG	C23-C24-C25-C26
14	B	841	CLA	C4C-C3C-CAC-CBC
14	K	102	CLA	CAA-CBA-CGA-O1A
14	B	828	CLA	C4-C3-C5-C6
14	B	809	CLA	C8-C10-C11-C12
14	A	828	CLA	C16-C17-C18-C19
14	B	806	CLA	CBA-CGA-O2A-C1
22	L	207	DGD	C2A-C3A-C4A-C5A
14	B	828	CLA	CAA-CBA-CGA-O2A
14	A	841	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
14	A	819	CLA	C2A-CAA-CBA-CGA
14	A	828	CLA	C11-C12-C13-C14
14	A	830	CLA	C6-C7-C8-C9
14	A	831	CLA	C11-C12-C13-C14
14	A	839	CLA	C6-C7-C8-C9
14	B	813	CLA	C6-C7-C8-C9
19	B	850	LHG	O9-C7-C8-C9
14	B	813	CLA	C15-C16-C17-C18
14	J	102	CLA	C4C-C3C-CAC-CBC
17	A	850	BCR	C19-C20-C21-C22
14	A	857	CLA	C16-C17-C18-C19
14	B	810	CLA	C16-C17-C18-C19
14	A	808	CLA	CAA-CBA-CGA-O1A
14	A	809	CLA	CAA-CBA-CGA-O1A
14	B	835	CLA	CAA-CBA-CGA-O1A
18	A	853	LMG	O9-C10-C11-C12
18	B	849	LMG	O9-C10-C11-C12
14	A	807	CLA	CAA-CBA-CGA-O2A
14	A	820	CLA	CAA-CBA-CGA-O2A
14	A	828	CLA	CAA-CBA-CGA-O2A
14	B	805	CLA	CAA-CBA-CGA-O2A
19	A	854	LHG	O10-C23-C24-C25
19	M	101	LHG	O9-C7-C8-C9
18	B	849	LMG	C22-C23-C24-C25
14	B	803	CLA	CAA-CBA-CGA-O1A
14	B	810	CLA	CAA-CBA-CGA-O1A
14	B	802	CLA	CBA-CGA-O2A-C1
14	B	813	CLA	CAA-CBA-CGA-O1A
14	A	813	CLA	C4-C3-C5-C6
15	B	842	PQN	C25-C26-C27-C28
14	A	803	CLA	CAD-CBD-CGD-O2D
14	A	804	CLA	CAD-CBD-CGD-O2D
14	A	809	CLA	CAD-CBD-CGD-O2D
14	A	810	CLA	CAD-CBD-CGD-O2D
14	B	816	CLA	CAD-CBD-CGD-O2D
14	A	842	CLA	C2-C1-O2A-CGA
14	B	803	CLA	C2-C1-O2A-CGA
14	A	843	CLA	C2A-CAA-CBA-CGA
19	M	101	LHG	C15-C16-C17-C18
14	B	819	CLA	C13-C15-C16-C17
14	A	818	CLA	CAA-CBA-CGA-O2A
14	A	832	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
14	B	802	CLA	CAA-CBA-CGA-O2A
14	A	807	CLA	CAA-CBA-CGA-O1A
14	B	828	CLA	CAA-CBA-CGA-O1A
14	B	839	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

103 monomers are involved in 198 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	822	CLA	2	0
14	K	101	CLA	4	0
14	B	802	CLA	5	0
17	A	849	BCR	1	0
14	B	825	CLA	3	0
14	A	813	CLA	1	0
14	A	809	CLA	1	0
14	B	812	CLA	2	0
18	A	856	LMG	1	0
14	A	806	CLA	3	0
22	L	207	DGD	2	0
17	L	201	BCR	3	0
14	A	804	CLA	2	0
14	A	810	CLA	5	0
14	B	804	CLA	1	0
14	B	817	CLA	3	0
17	A	850	BCR	1	0
14	B	840	CLA	2	0
14	A	833	CLA	1	0
14	A	811	CLA	3	0
14	A	844	CLA	2	0
17	J	103	BCR	2	0
16	C	102	SF4	1	0
17	A	847	BCR	1	0
14	B	834	CLA	1	0
14	X	1701	CLA	4	0
18	B	849	LMG	1	0
14	B	829	CLA	2	0
14	F	201	CLA	1	0
14	A	817	CLA	1	0
14	B	830	CLA	1	0
14	A	818	CLA	1	0
14	L	206	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	845	PQN	4	0
14	A	807	CLA	1	0
14	B	805	CLA	2	0
14	A	805	CLA	6	0
17	J	104	BCR	6	0
14	B	837	CLA	1	0
14	A	830	CLA	1	0
14	F	202	CLA	5	0
14	B	813	CLA	2	0
14	A	812	CLA	2	0
14	J	101	CLA	7	0
14	B	811	CLA	1	0
14	B	816	CLA	1	0
17	B	851	BCR	1	0
14	A	825	CLA	2	0
14	B	824	CLA	1	0
17	J	105	BCR	8	0
17	B	848	BCR	1	0
14	B	839	CLA	1	0
14	B	831	CLA	3	0
14	B	809	CLA	4	0
14	B	814	CLA	2	0
14	L	204	CLA	1	0
14	A	831	CLA	3	0
14	A	857	CLA	4	0
15	B	842	PQN	1	0
14	A	828	CLA	2	0
14	A	815	CLA	3	0
14	B	833	CLA	3	0
17	A	848	BCR	4	0
17	A	851	BCR	1	0
14	B	818	CLA	1	0
19	A	854	LHG	1	0
14	A	803	CLA	3	0
17	A	852	BCR	5	0
17	B	847	BCR	5	0
14	A	838	CLA	1	0
17	B	845	BCR	2	0
14	B	836	CLA	1	0
14	A	829	CLA	6	0
14	A	808	CLA	2	0
14	A	840	CLA	2	0

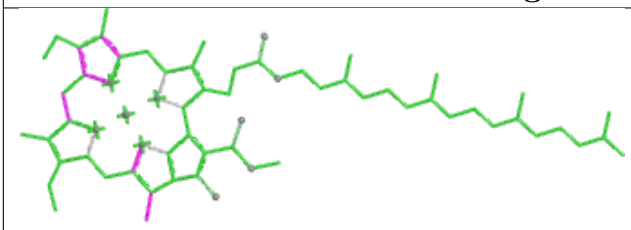
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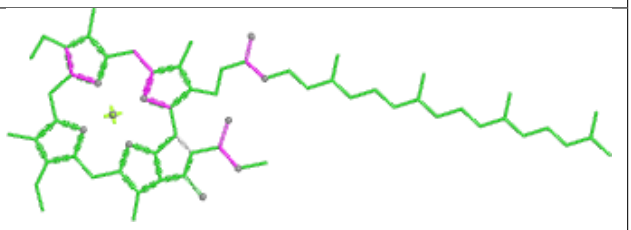
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	826	CLA	3	0
14	B	808	CLA	1	0
17	I	101	BCR	4	0
14	B	828	CLA	1	0
14	K	102	CLA	1	0
19	B	850	LHG	1	0
14	B	841	CLA	1	0
14	A	802	CLA	2	0
13	A	801	CL0	4	0
14	A	843	CLA	2	0
14	B	827	CLA	2	0
14	B	803	CLA	5	0
17	F	203	BCR	3	0
17	B	846	BCR	3	0
14	A	820	CLA	3	0
17	I	103	BCR	4	0
14	A	841	CLA	3	0
14	A	842	CLA	3	0
14	A	824	CLA	1	0
14	A	839	CLA	1	0
14	B	820	CLA	2	0
14	A	827	CLA	3	0
14	A	814	CLA	1	0
14	A	819	CLA	2	0
17	B	843	BCR	2	0
14	B	832	CLA	1	0
17	L	208	BCR	1	0
14	A	835	CLA	1	0

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

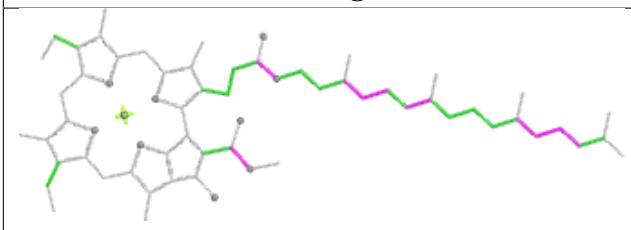
Ligand CLA A 822



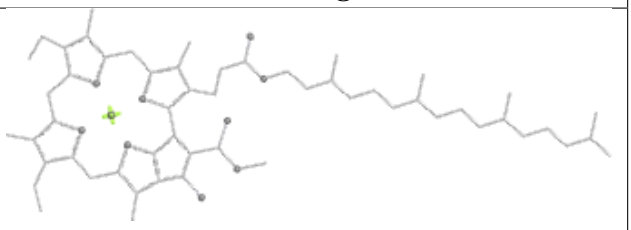
Bond lengths



Bond angles

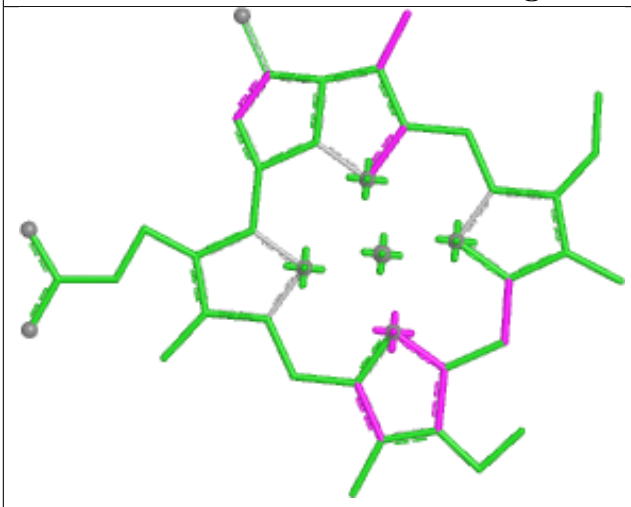


Torsions

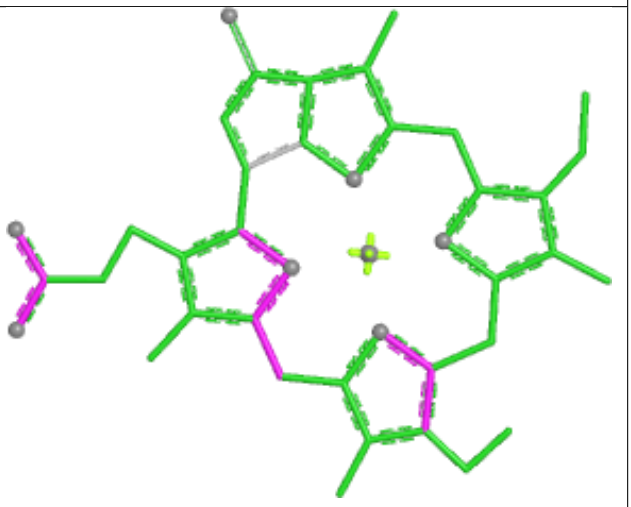


Rings

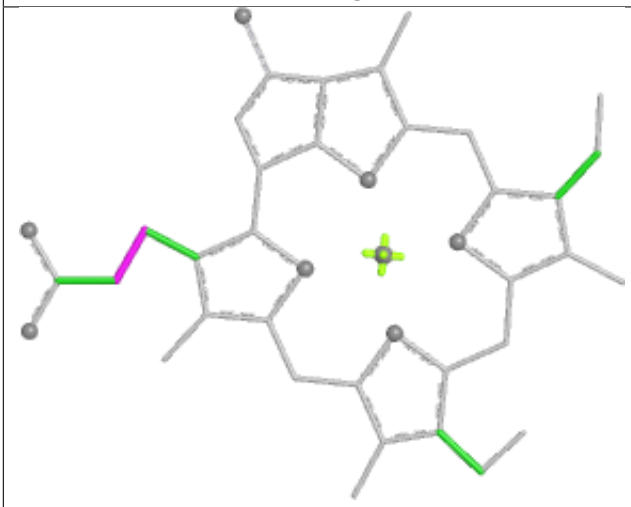
Ligand CLA K 101



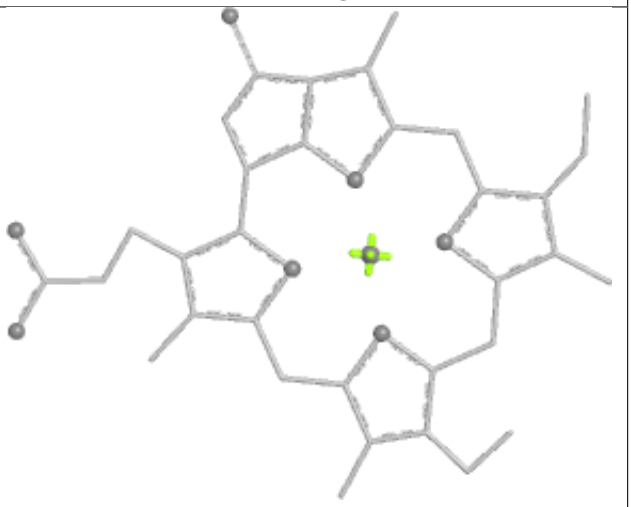
Bond lengths



Bond angles

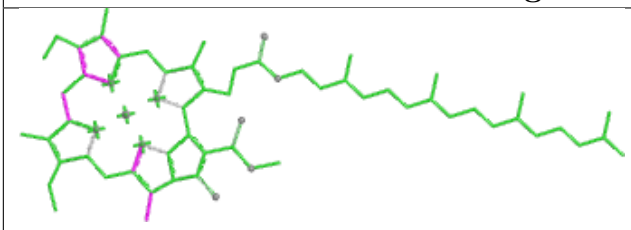


Torsions

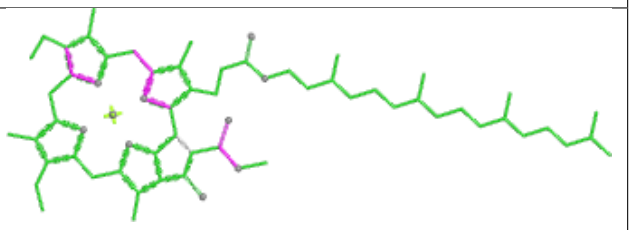


Rings

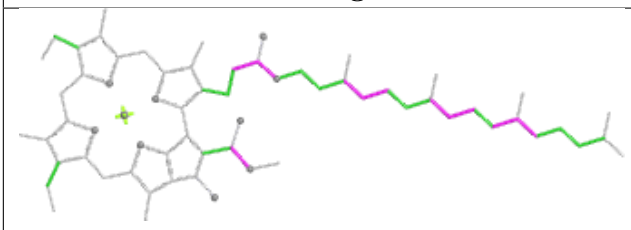
Ligand CLA B 802



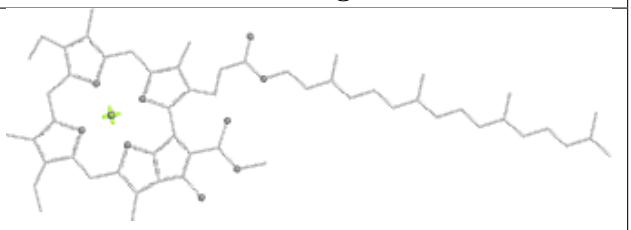
Bond lengths



Bond angles

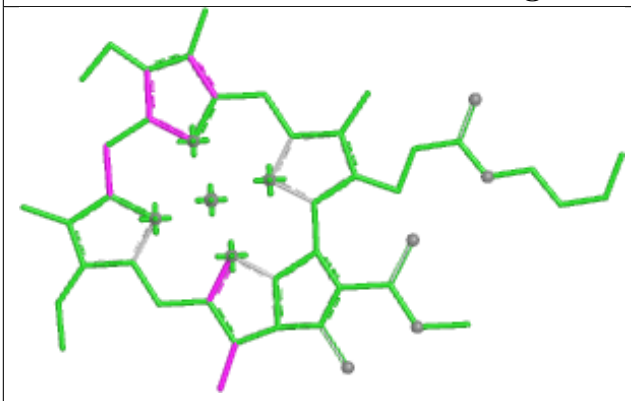


Torsions

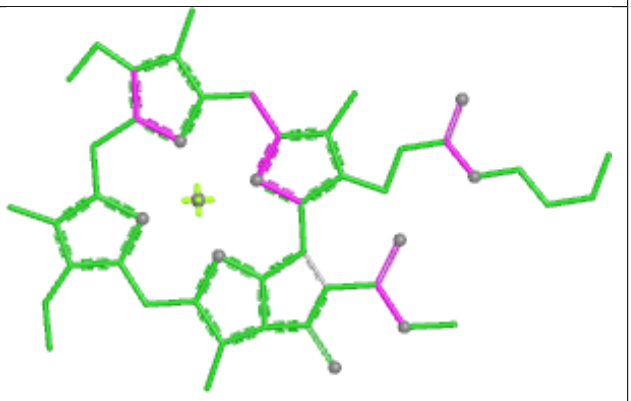


Rings

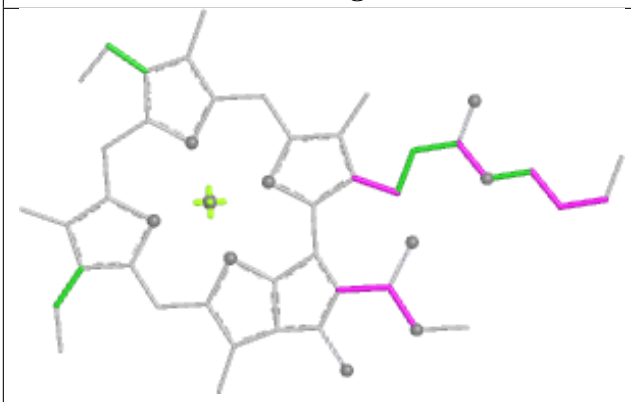
Ligand CLA A 823



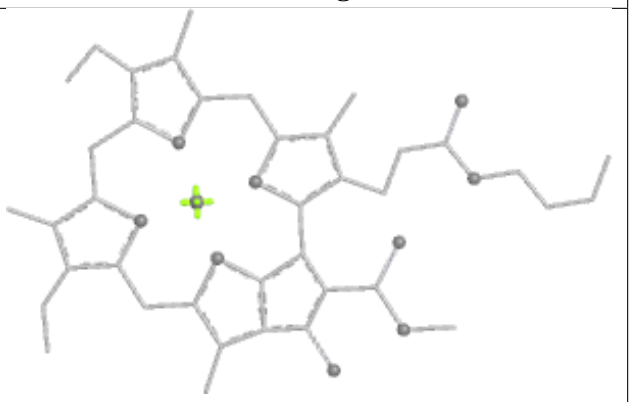
Bond lengths



Bond angles

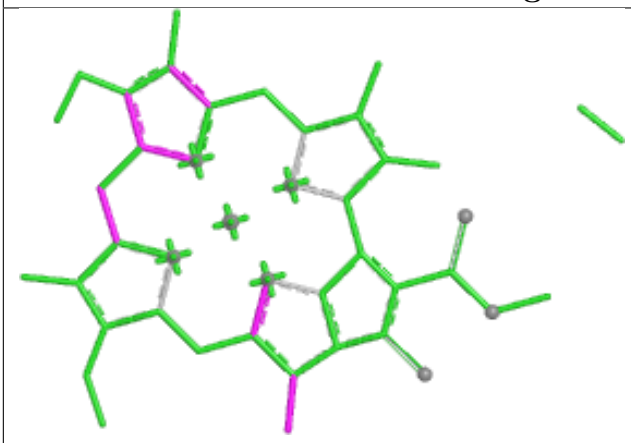


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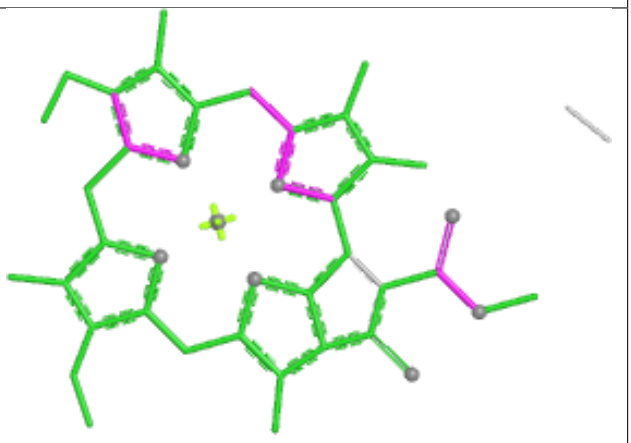


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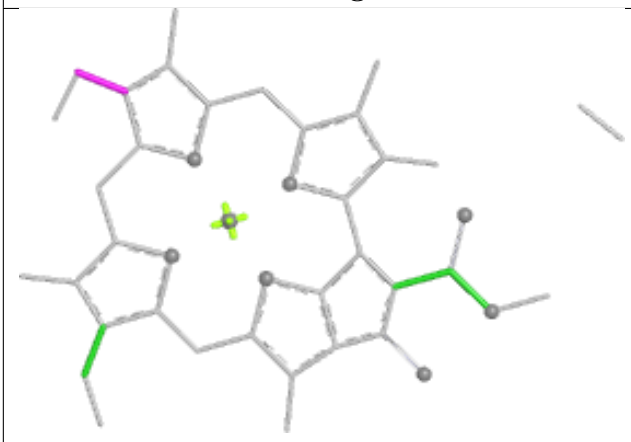
Ligand CLA A 821



Bond lengths



Bond angles

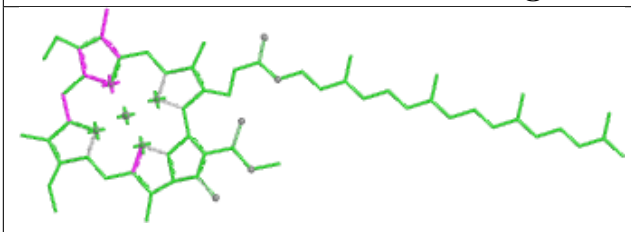


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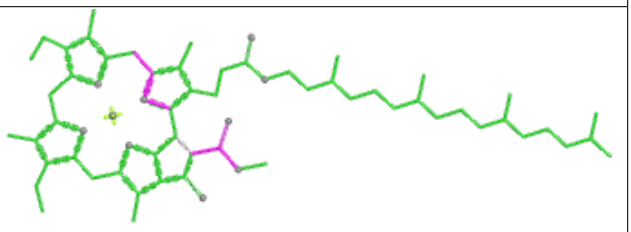


Rings

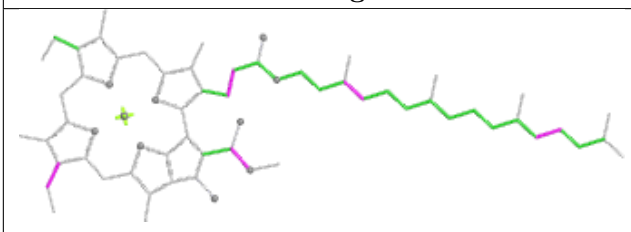
Ligand CLA B 807



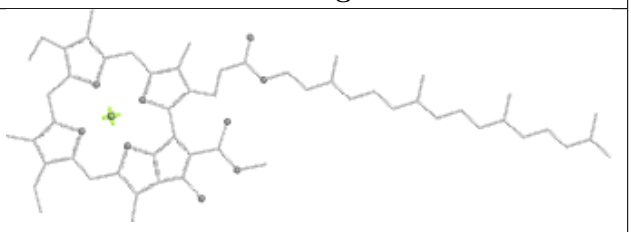
Bond lengths



Bond angles

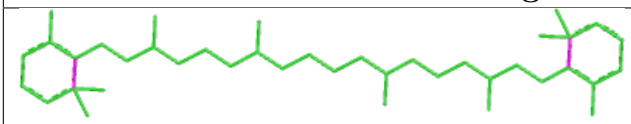


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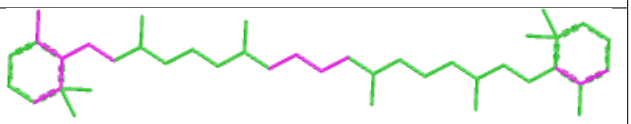


Rings

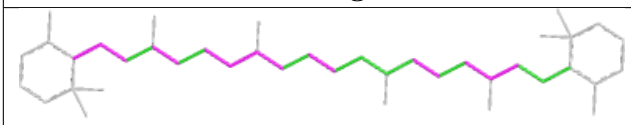
Ligand BCR A 849



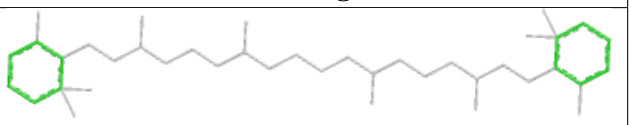
Bond lengths



Bond angles

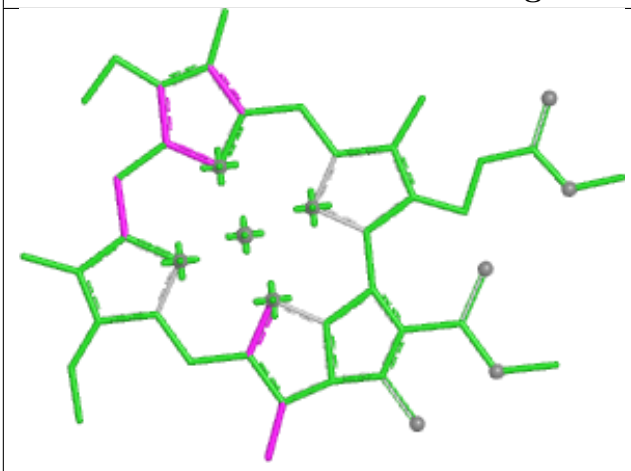


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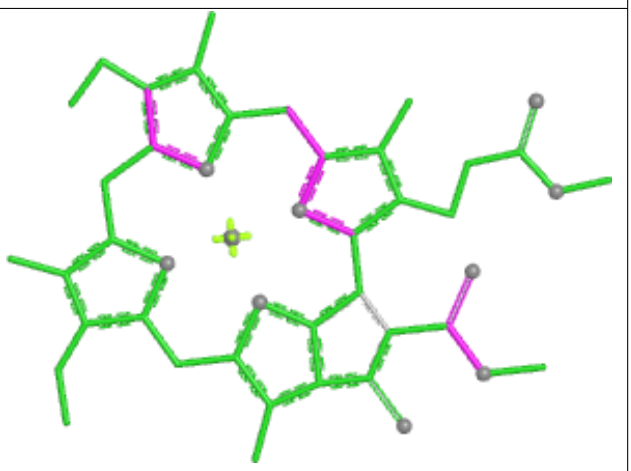


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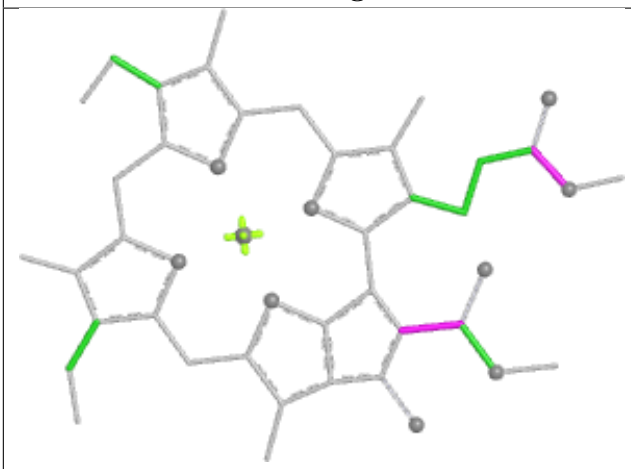
Ligand CLA B 825



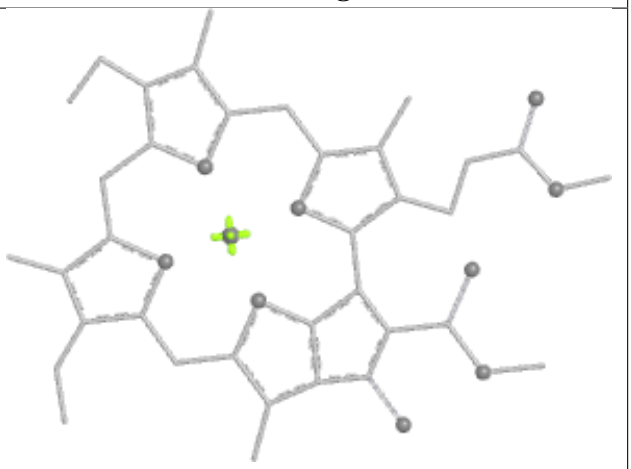
Bond lengths



Bond angles

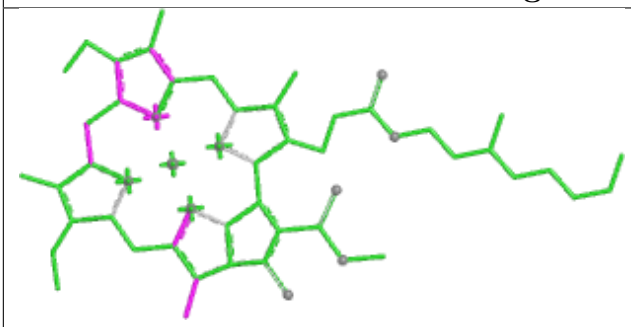


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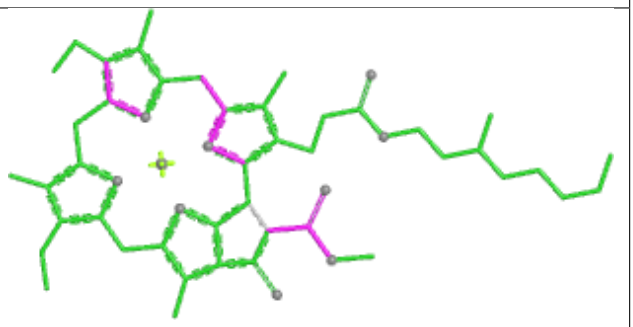


Rings

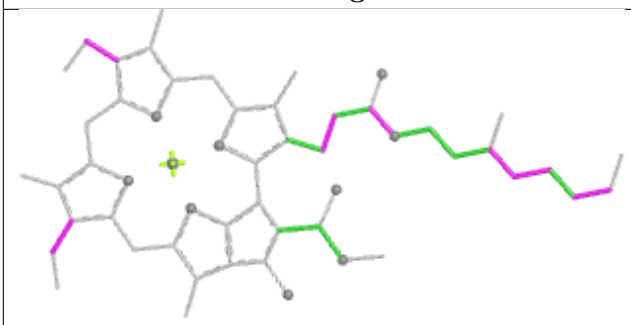
Ligand CLA A 813



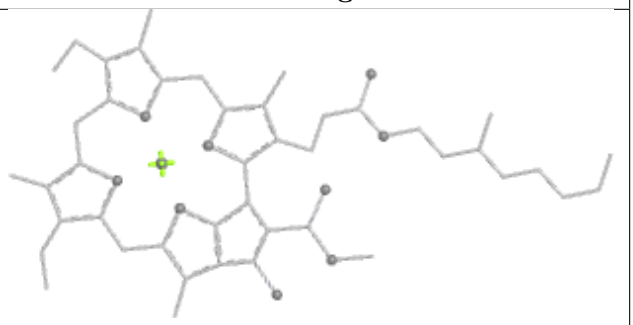
Bond lengths



Bond angles

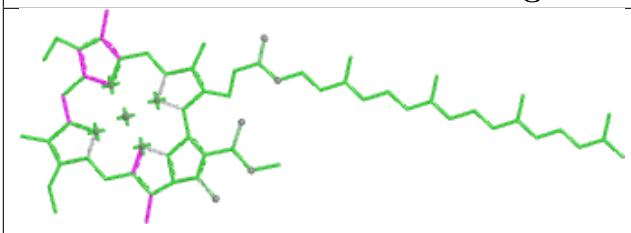


Torsions

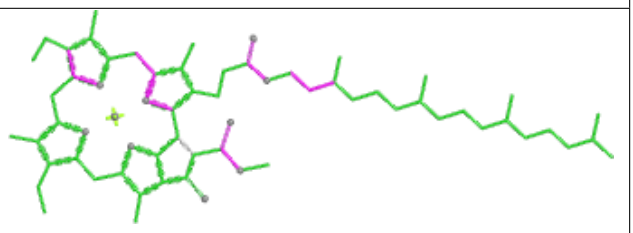


Rings

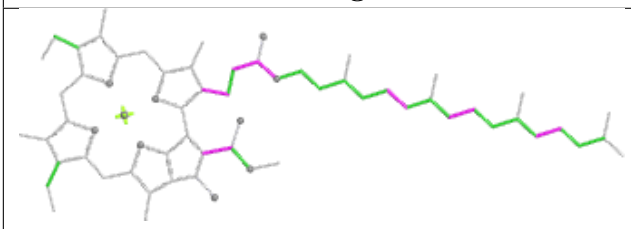
Ligand CLA A 809



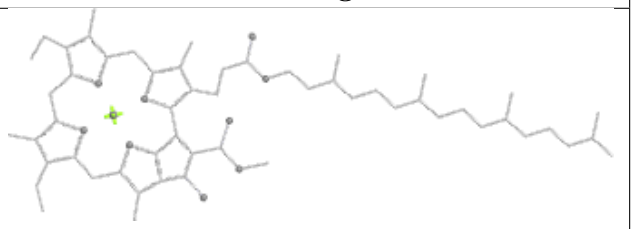
Bond lengths



Bond angles

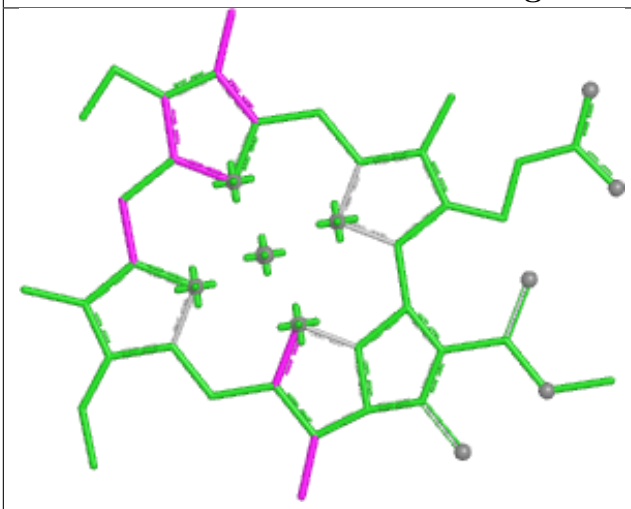


Torsions

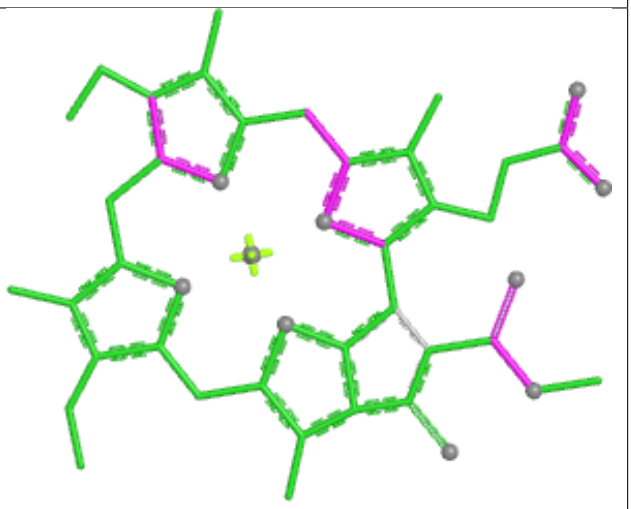


Rings

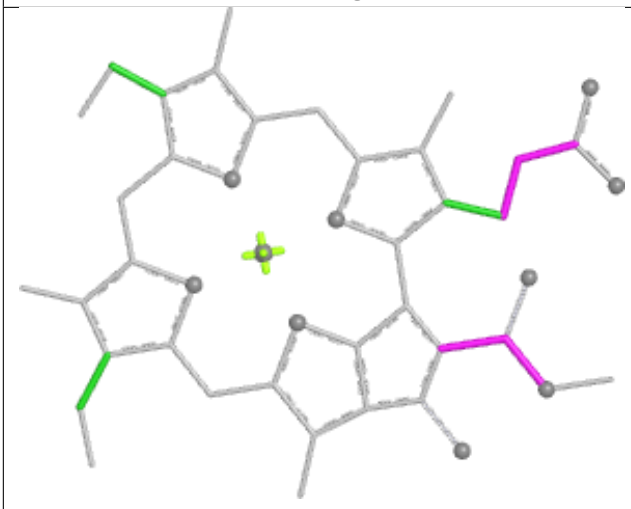
Ligand CLA B 812



Bond lengths



Bond angles

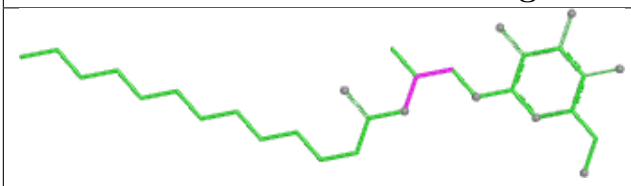


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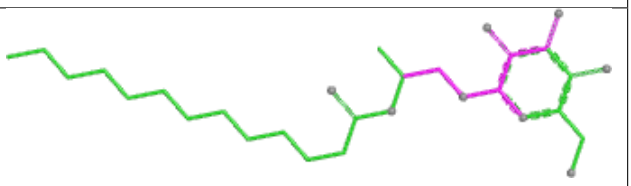


Rings

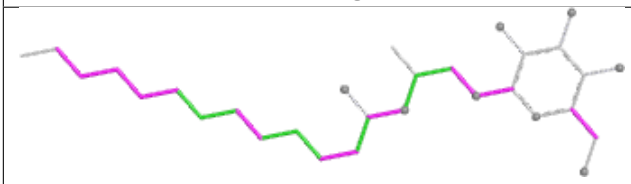
Ligand LMG A 856



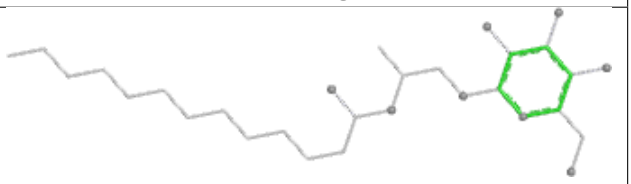
Bond lengths



Bond angles

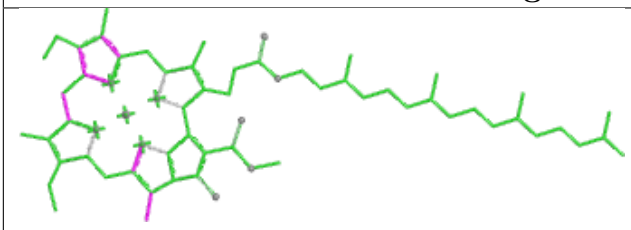


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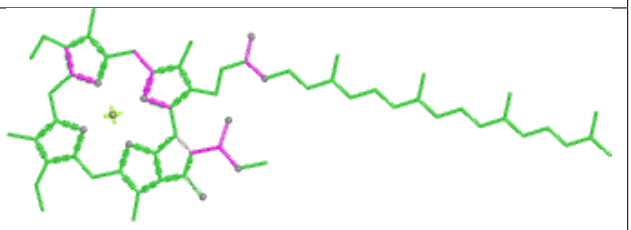


Rings

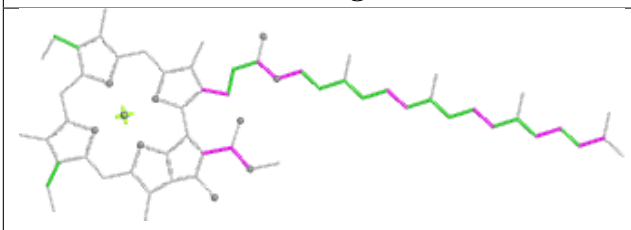
Ligand CLA A 806



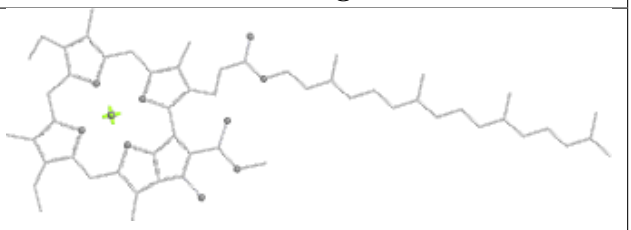
Bond lengths



Bond angles

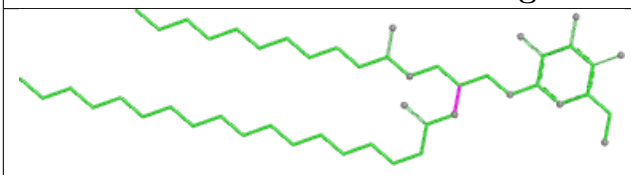


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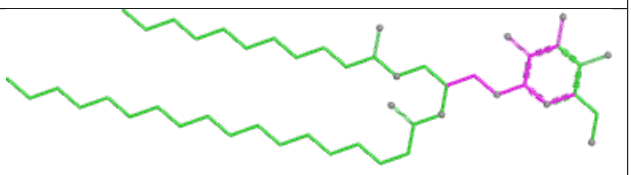


Rings

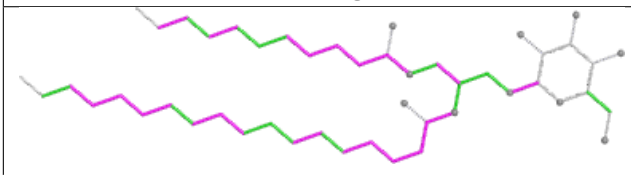
Ligand LMG A 853



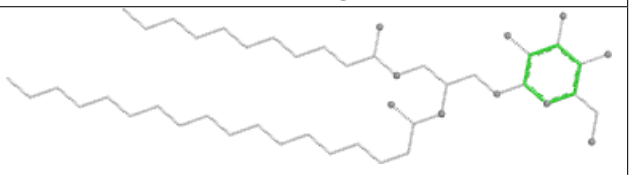
Bond lengths



Bond angles

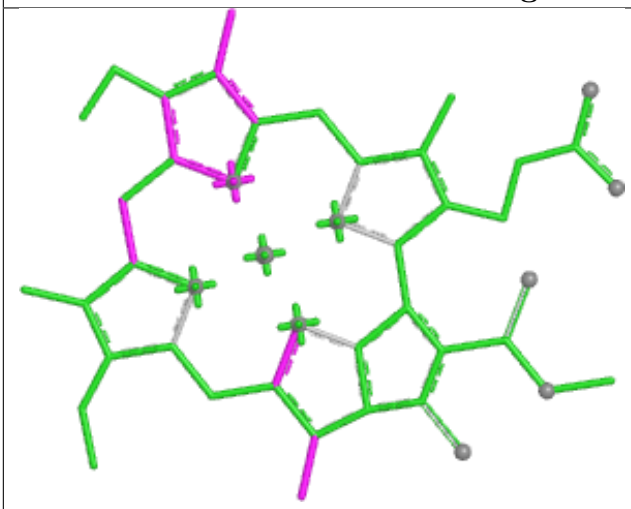


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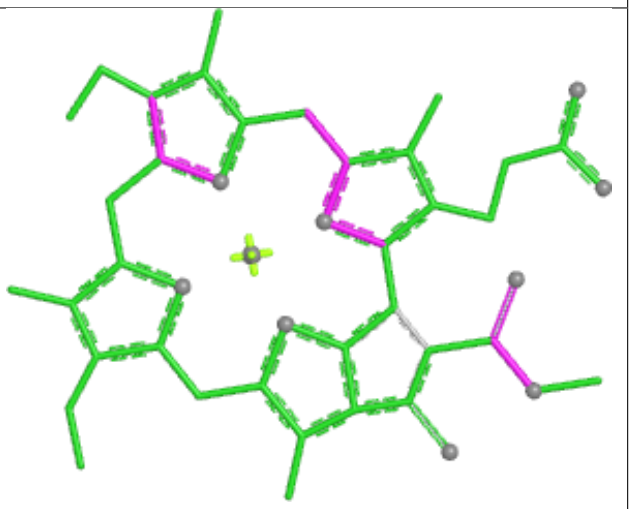


Rings

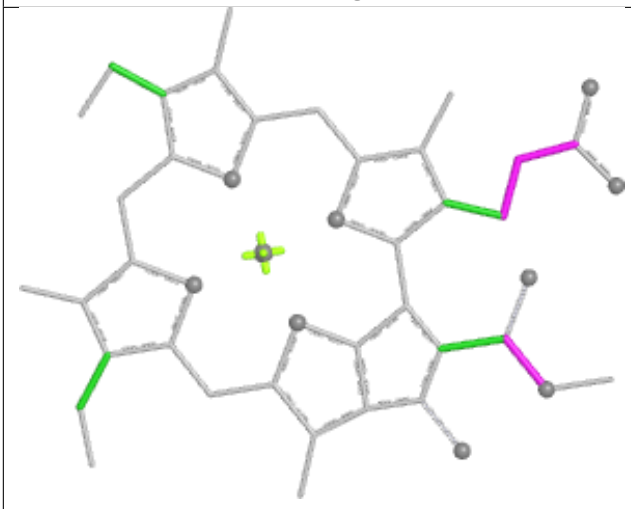
Ligand CLA M 102



Bond lengths



Bond angles

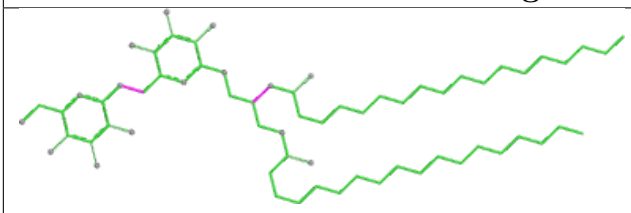


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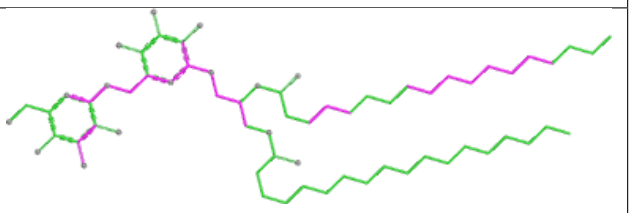


Rings

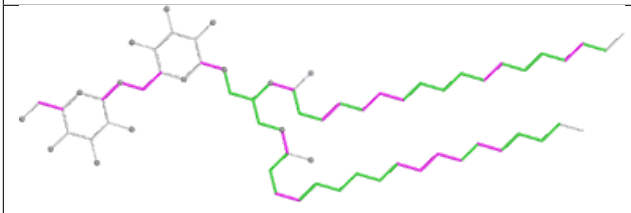
Ligand DGD L 207



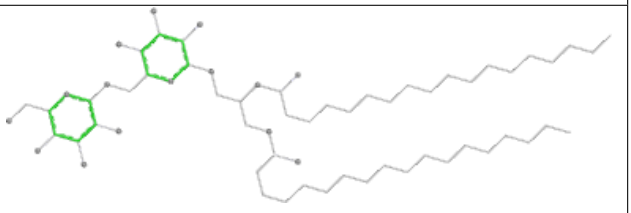
Bond lengths



Bond angles

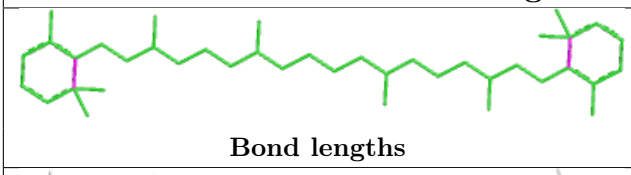


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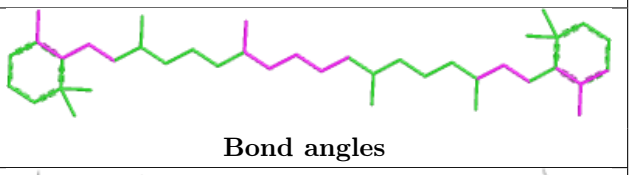


Rings

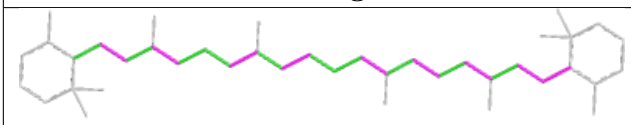
Ligand BCR L 201



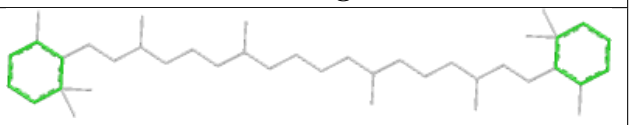
Bond lengths



Bond angles

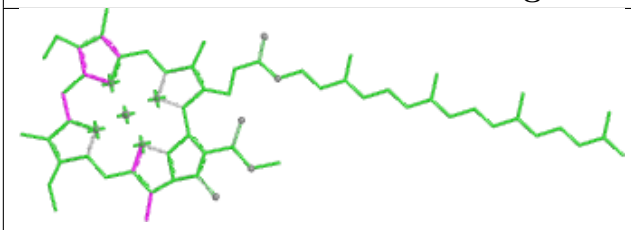


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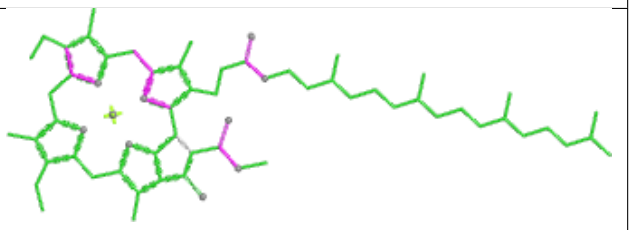


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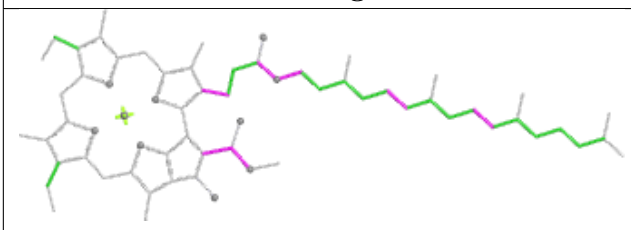
Ligand CLA A 804



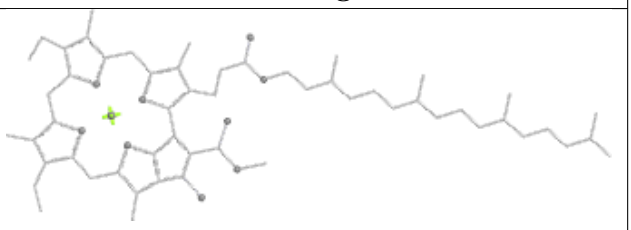
Bond lengths



Bond angles

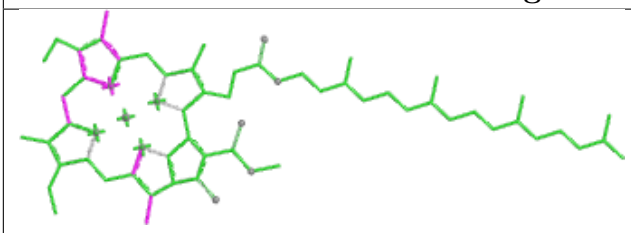


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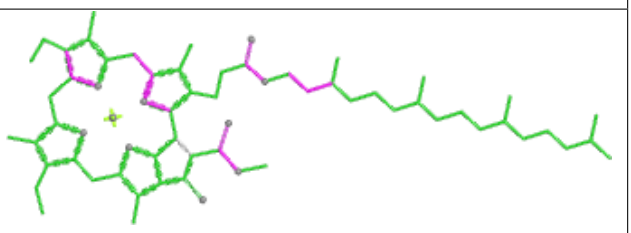


Rings

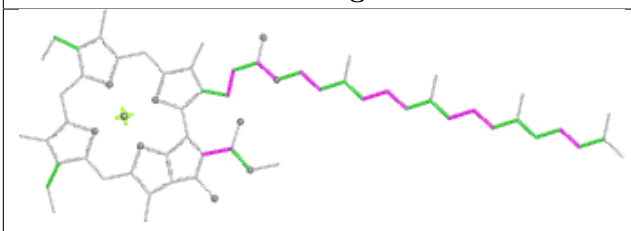
Ligand CLA A 810



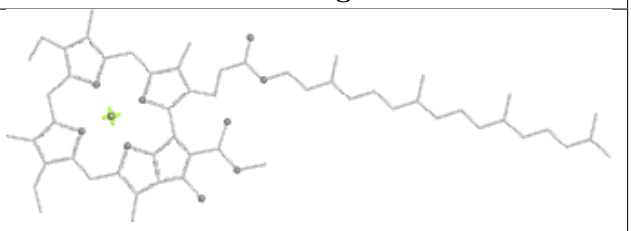
Bond lengths



Bond angles

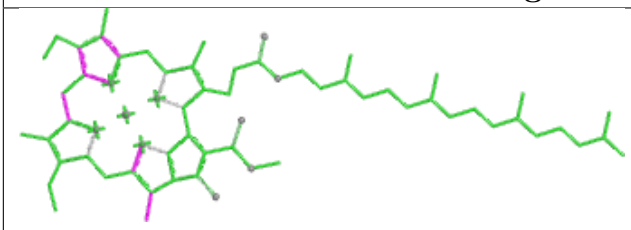


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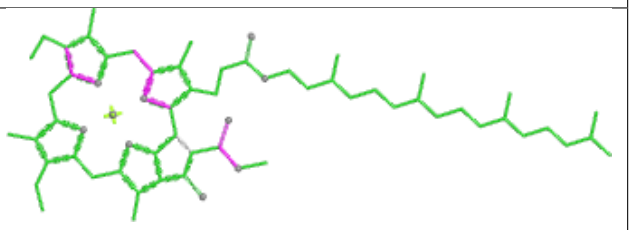


Rings

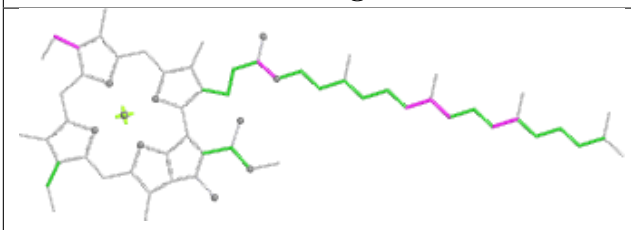
Ligand CLA B 806



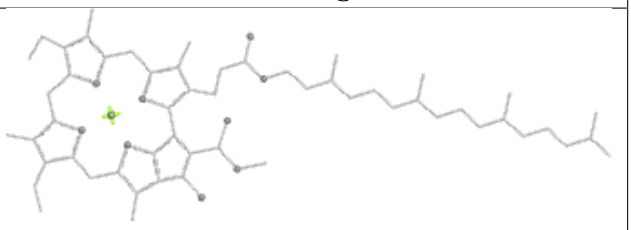
Bond lengths



Bond angles

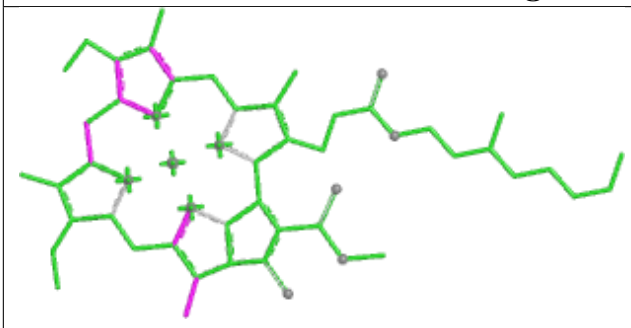


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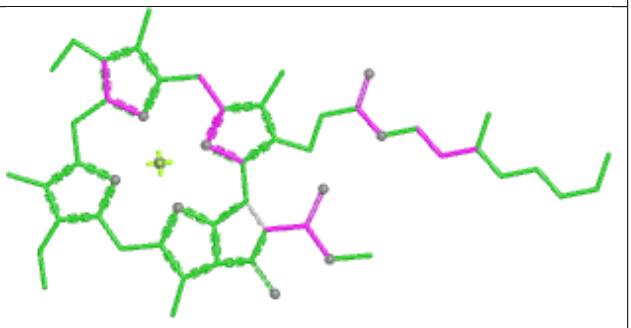


Rings

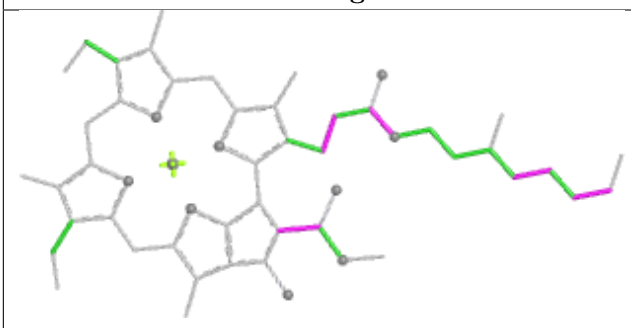
Ligand CLA B 804



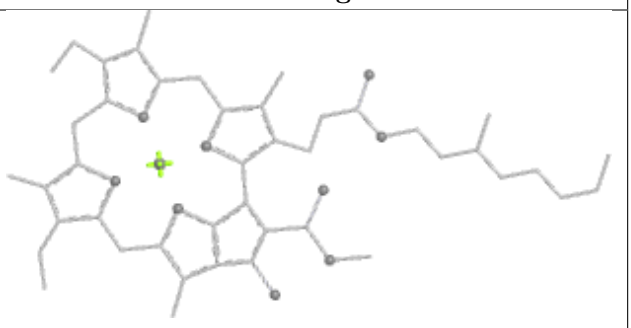
Bond lengths



Bond angles

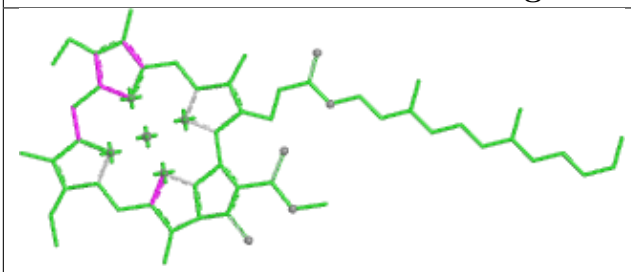


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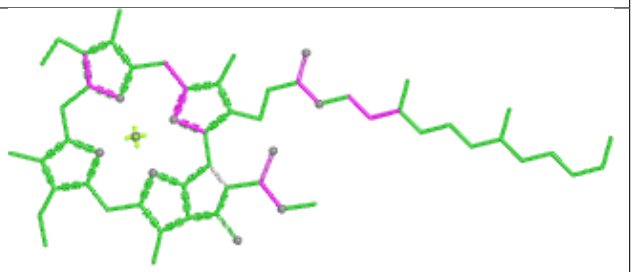


Rings

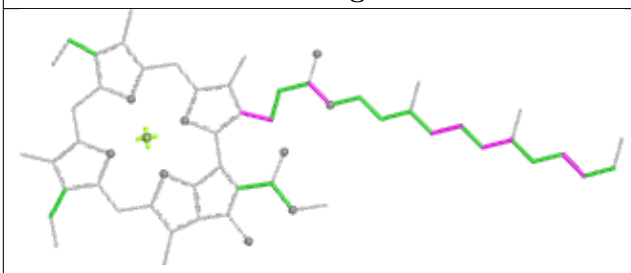
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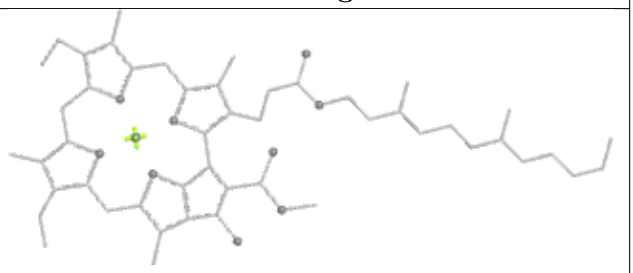
Bond lengths



Bond angles

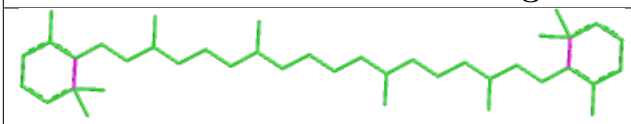


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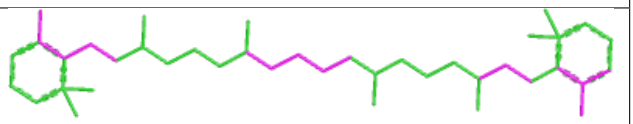


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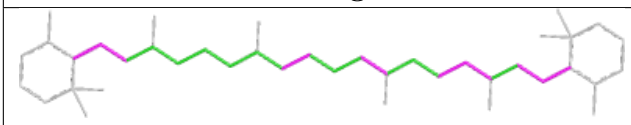
Ligand BCR A 850



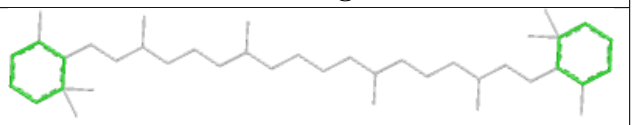
Bond lengths



Bond angles

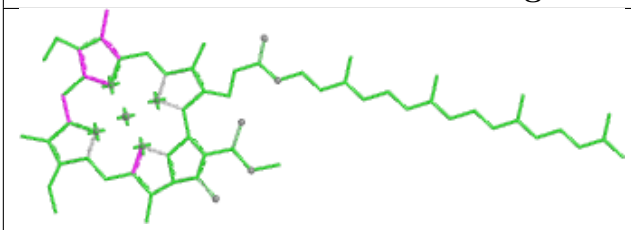


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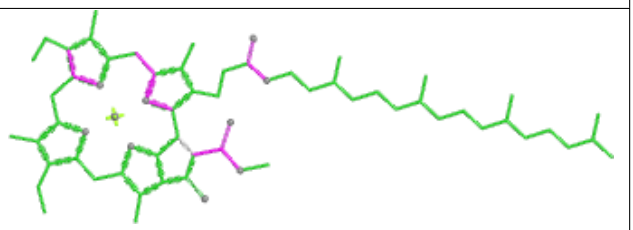


Rings

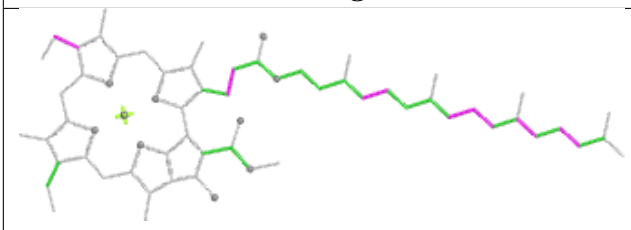
Ligand CLA B 840



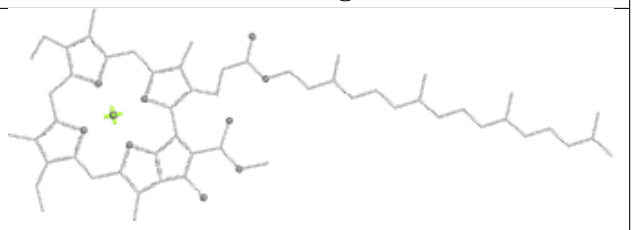
Bond lengths



Bond angles

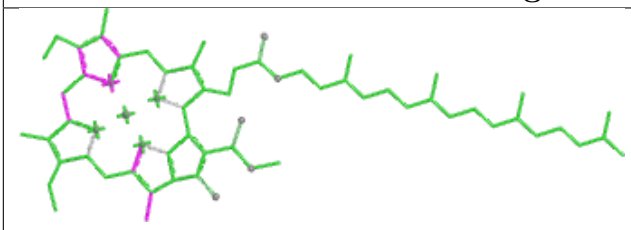


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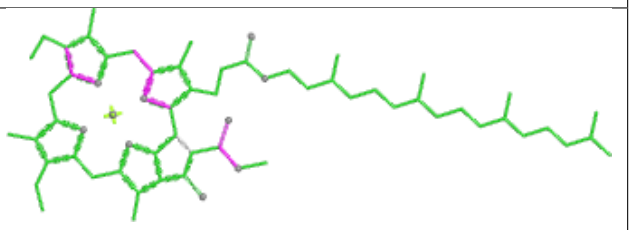


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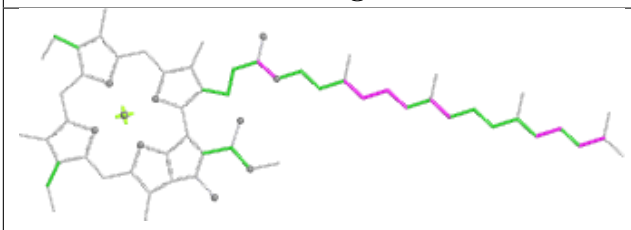
Ligand CLA A 833



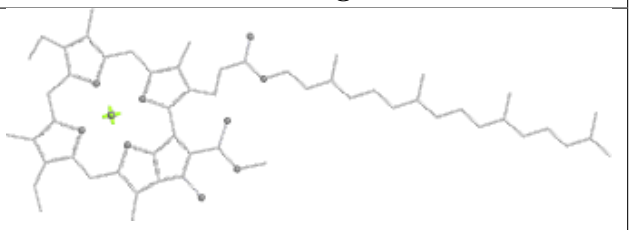
Bond lengths



Bond angles

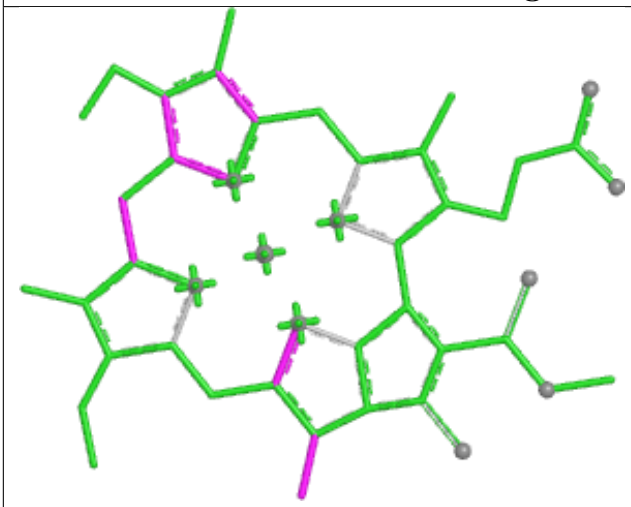


Torsions

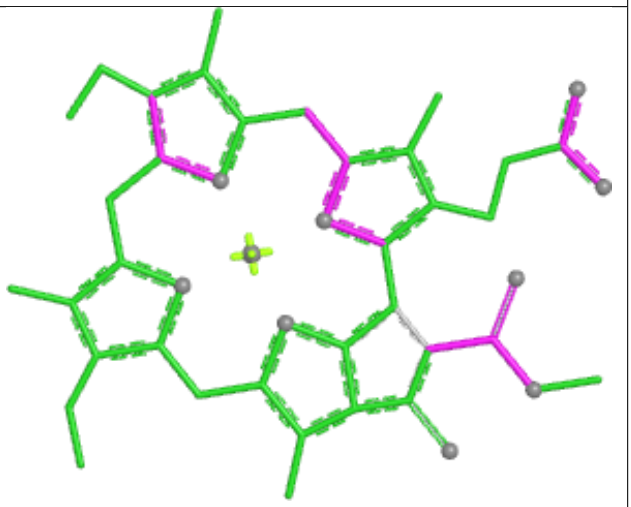


Rings

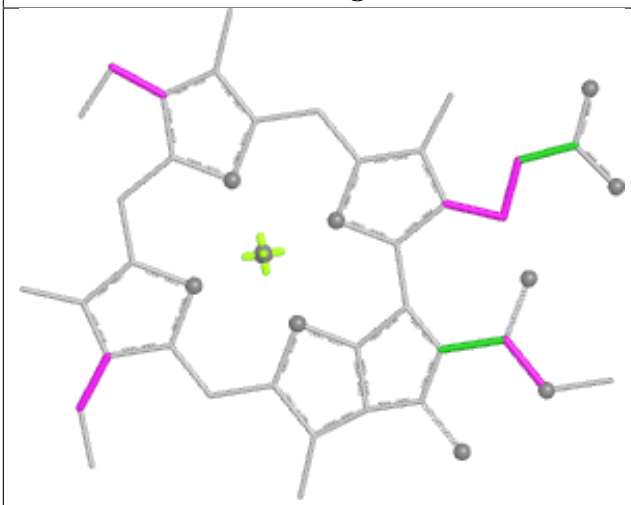
Ligand CLA A 811



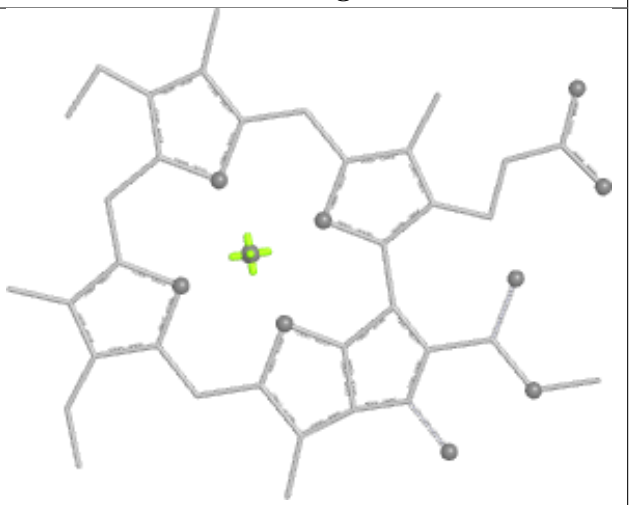
Bond lengths



Bond angles

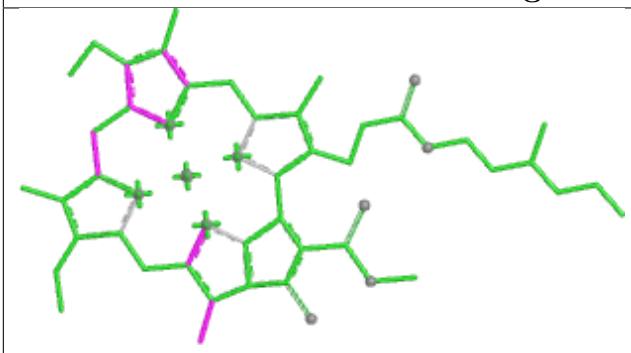


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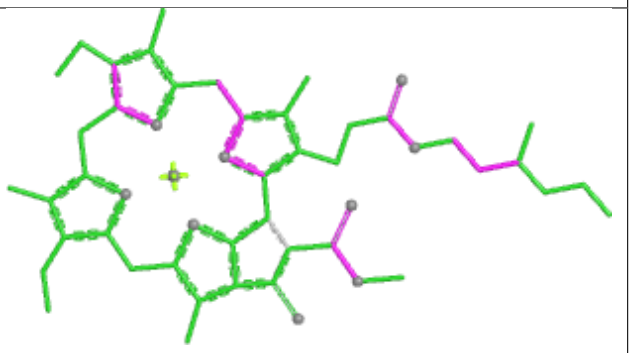


Rings

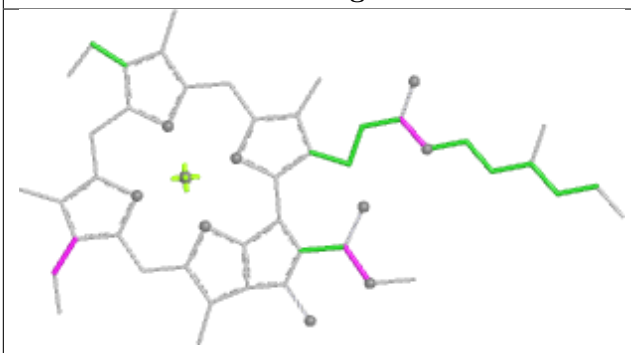
Ligand CLA A 844



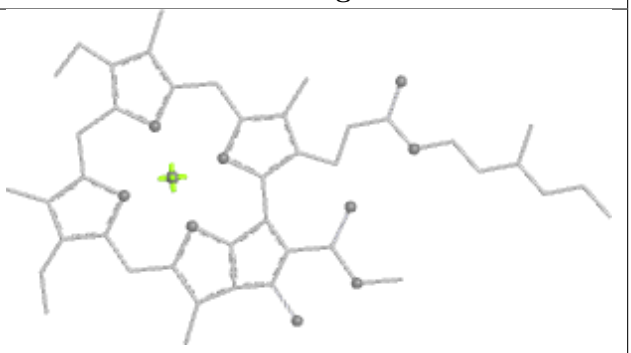
Bond lengths



Bond angles

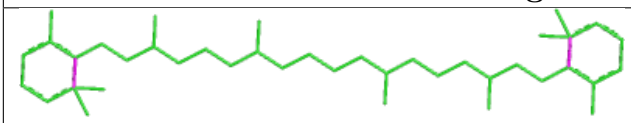


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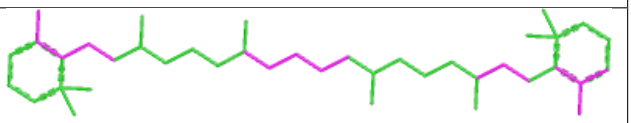


Rings

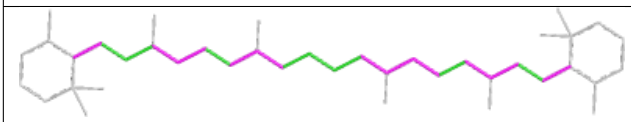
Ligand BCR J 103



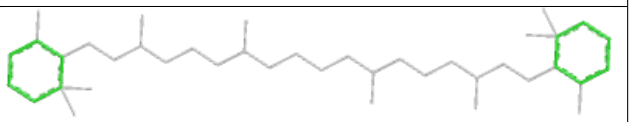
Bond lengths



Bond angles



Torsions

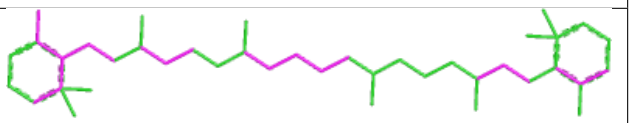


Rings

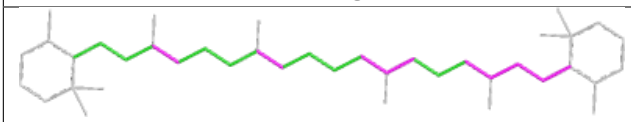
Ligand BCR A 847



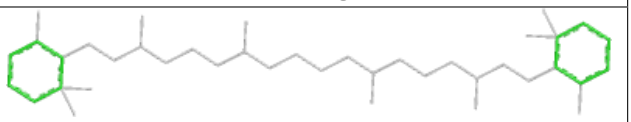
Bond lengths



Bond angles

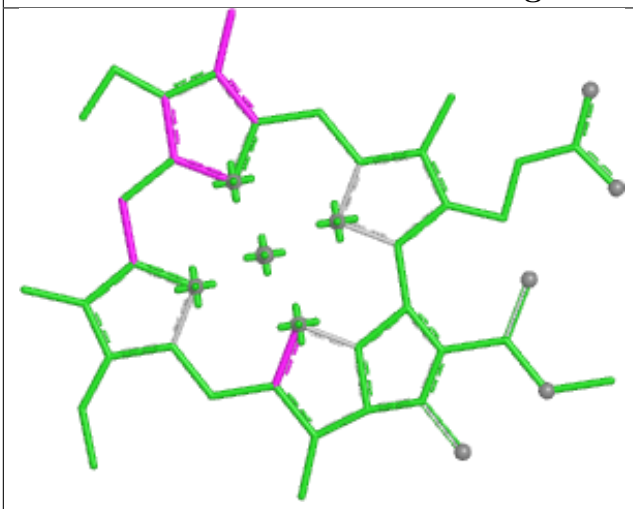


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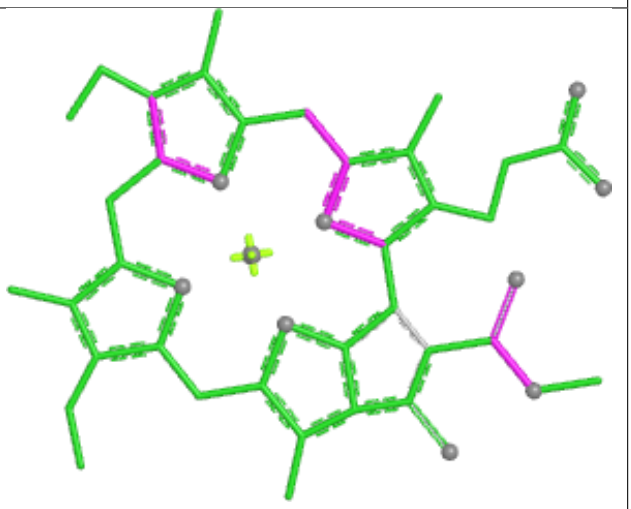


Rings

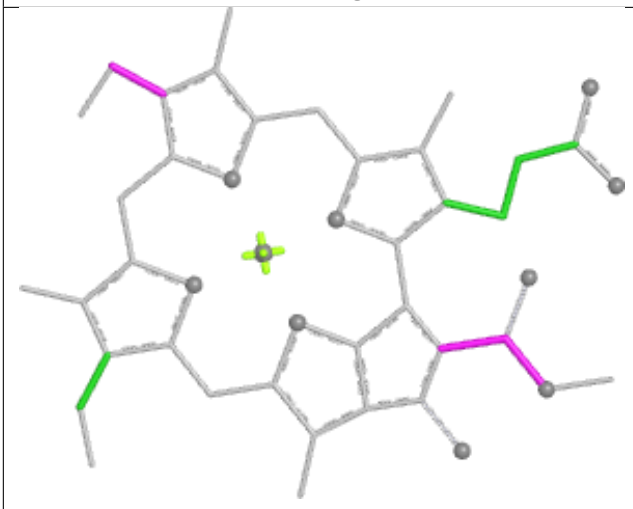
Ligand CLA B 834



Bond lengths



Bond angles

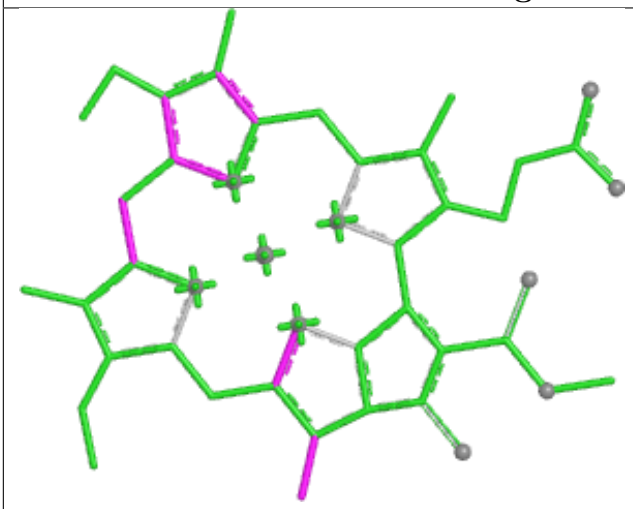


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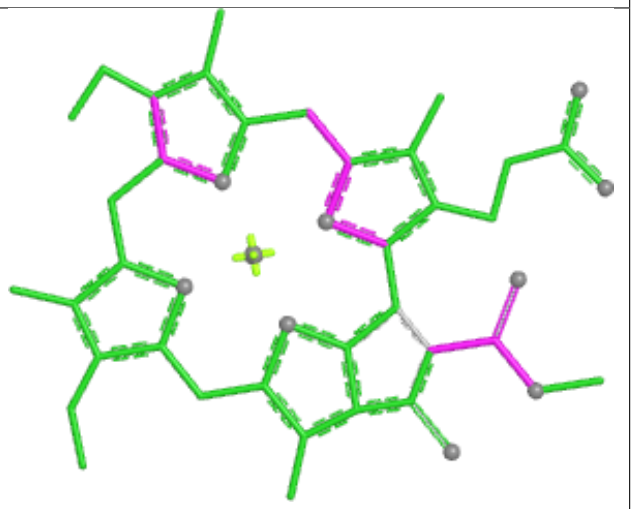


Rings

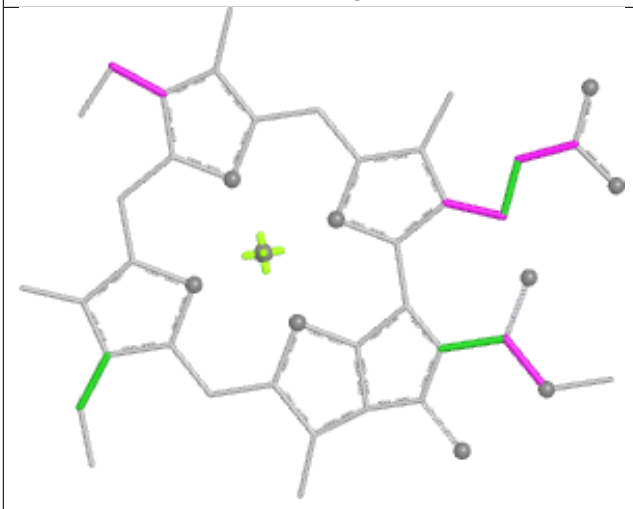
Ligand CLA X 1701



Bond lengths



Bond angles

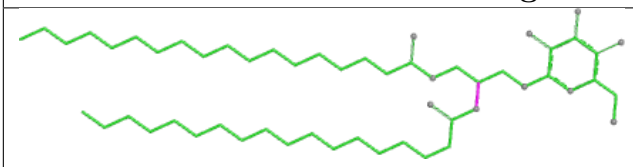


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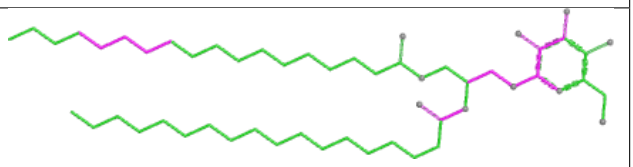


Rings

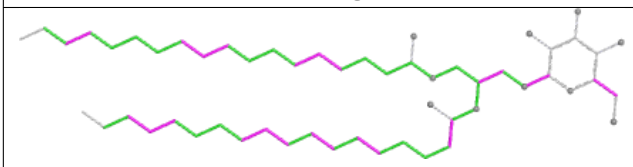
Ligand LMG B 849



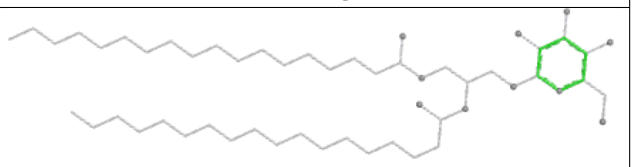
Bond lengths



Bond angles

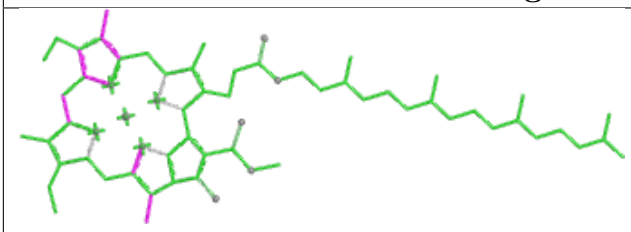


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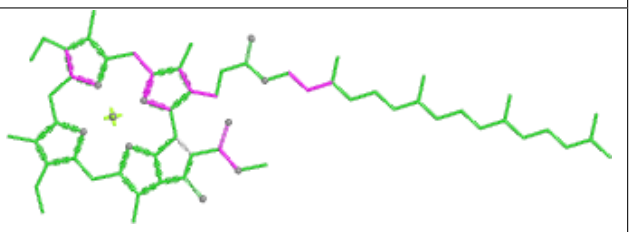


Rings

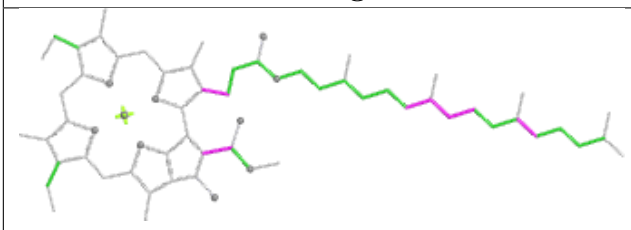
Ligand CLA B 829



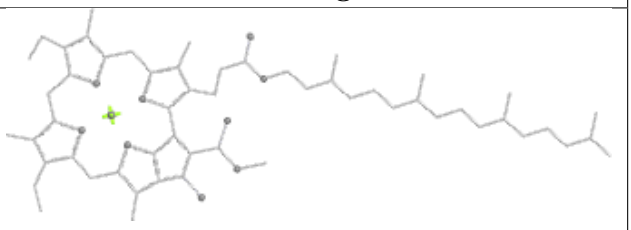
Bond lengths



Bond angles

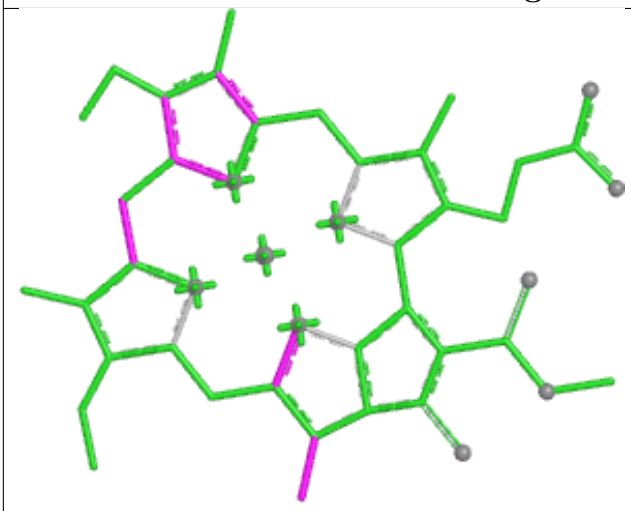


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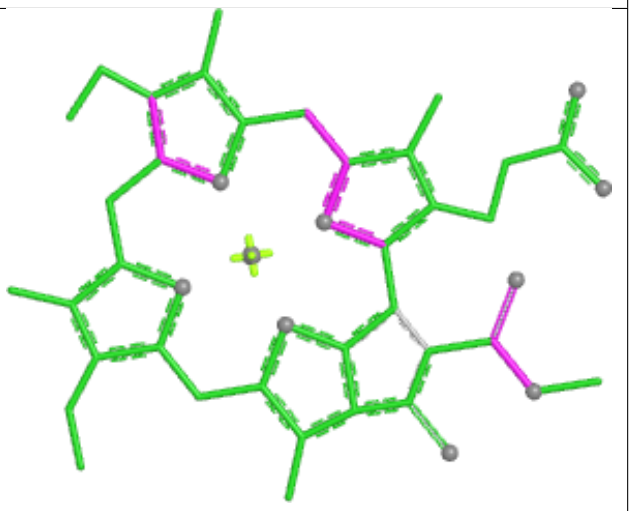


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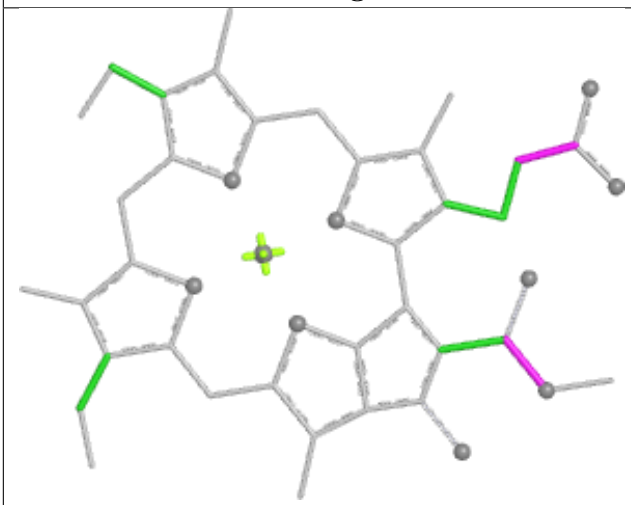
Ligand CLA B 815



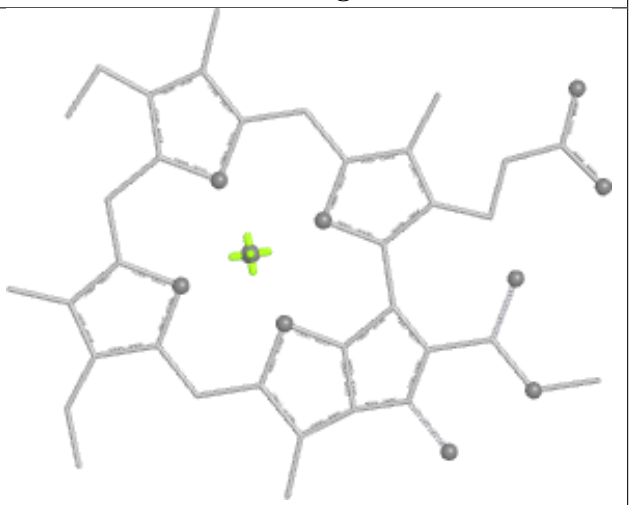
Bond lengths



Bond angles

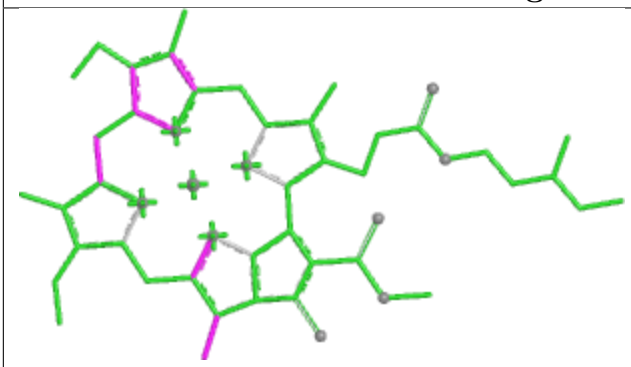


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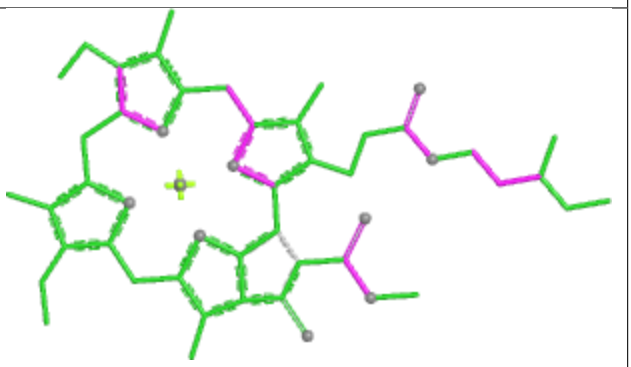


Rings

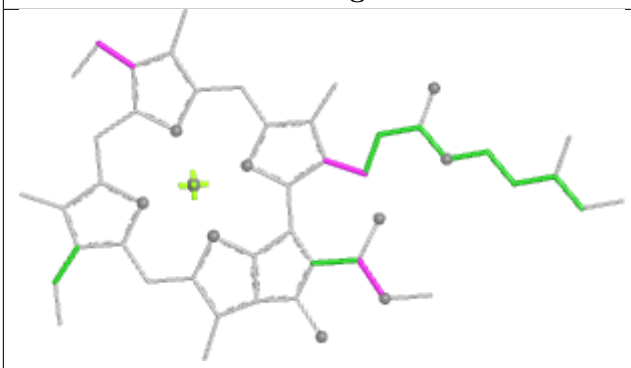
Ligand CLA F 201



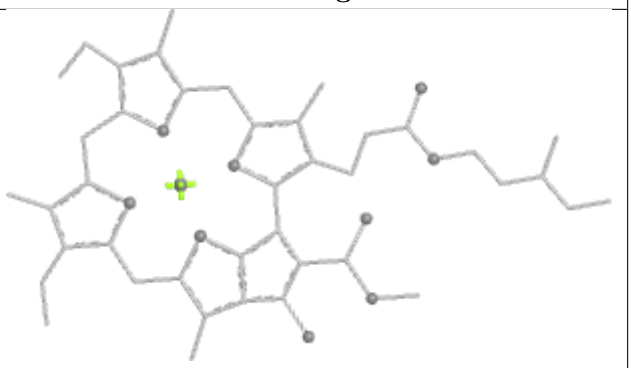
Bond lengths



Bond angles

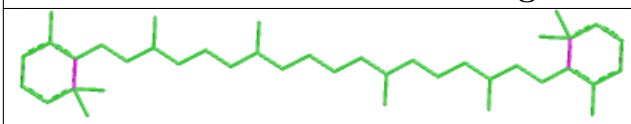


Torsions

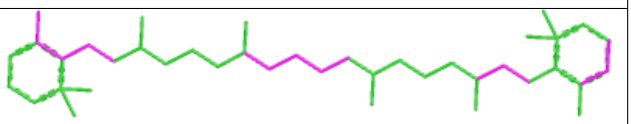


Rings

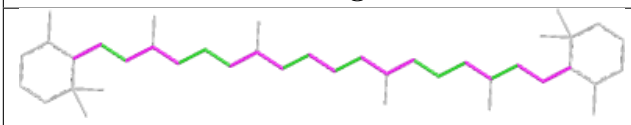
Ligand BCR M 103



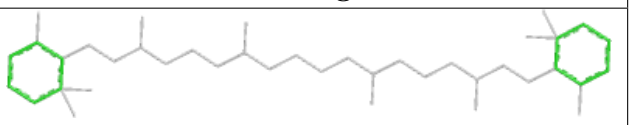
Bond lengths



Bond angles

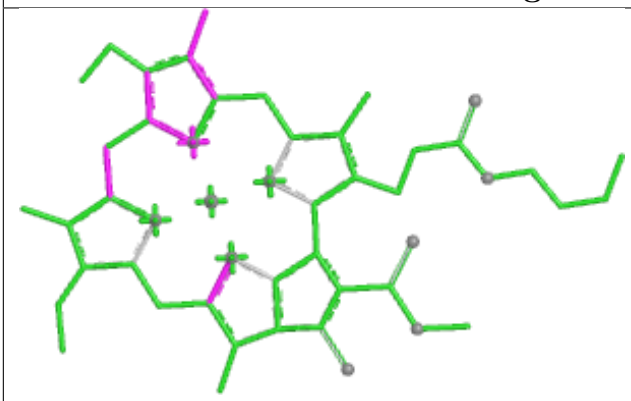


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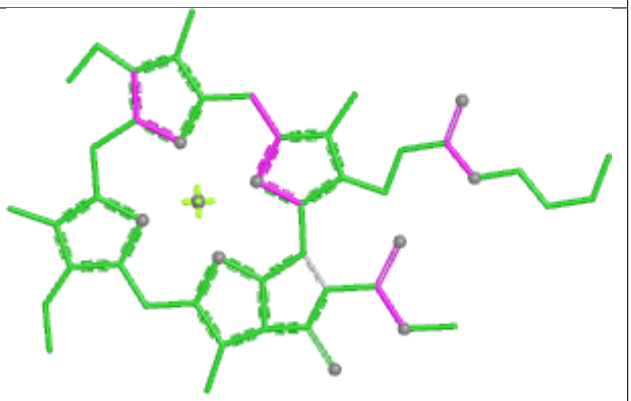


Rings

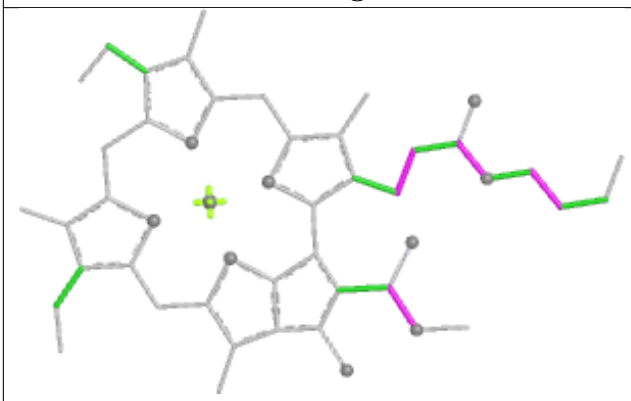
Ligand CLA A 817



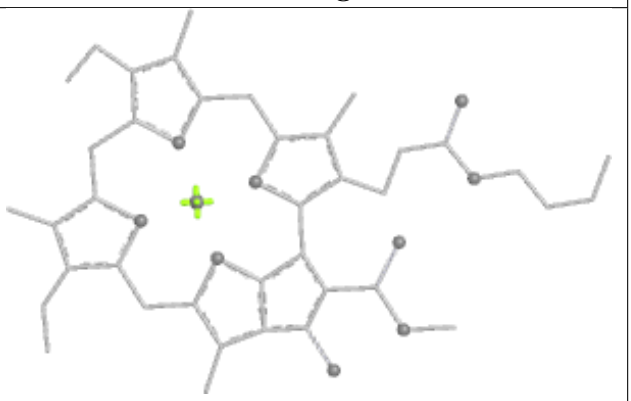
Bond lengths



Bond angles

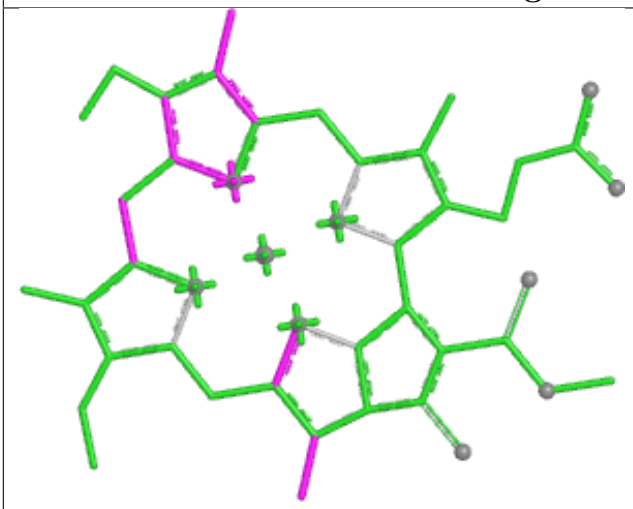


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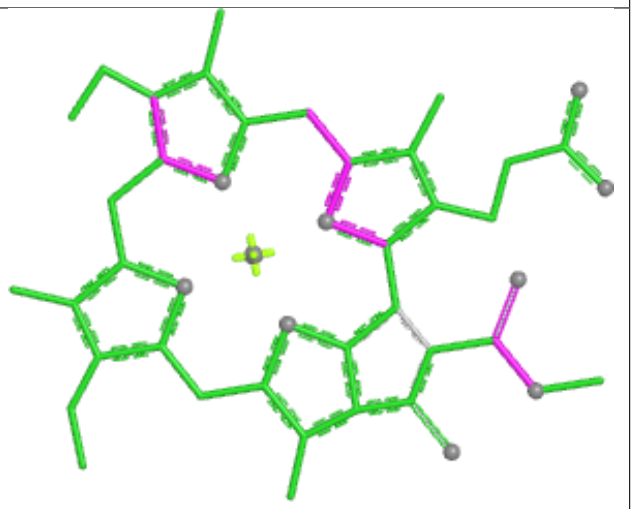


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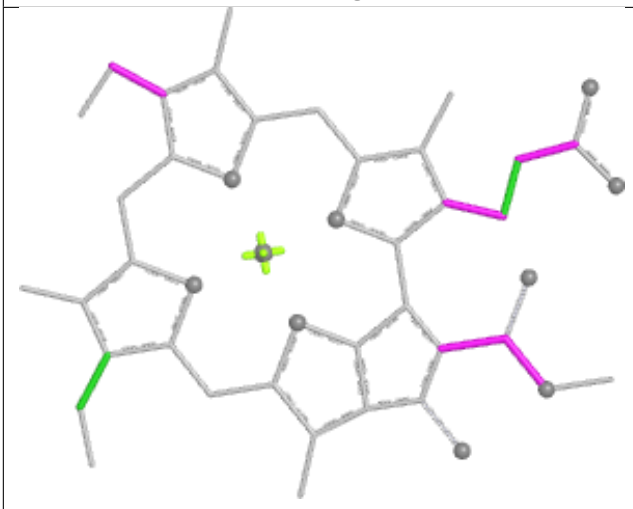
Ligand CLA B 830



Bond lengths



Bond angles

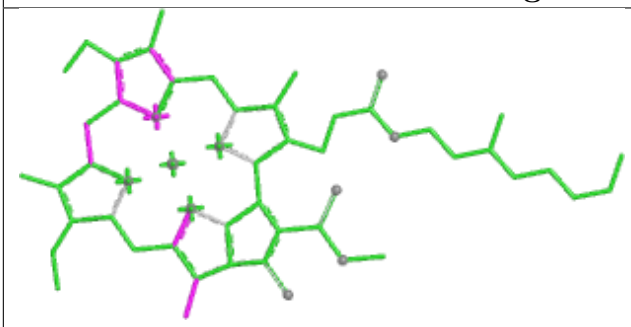


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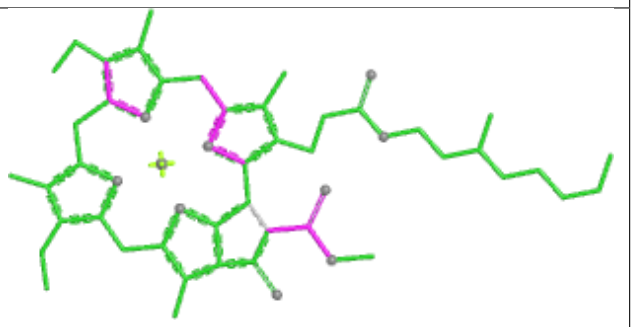


Rings

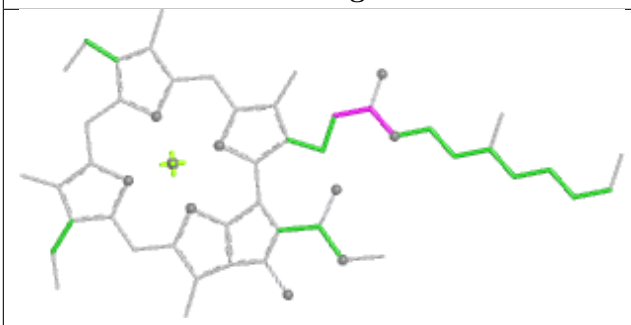
Ligand CLA A 818



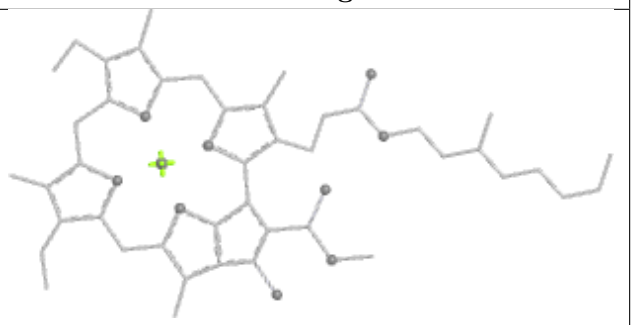
Bond lengths



Bond angles

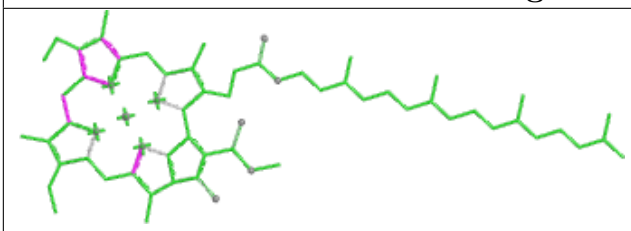


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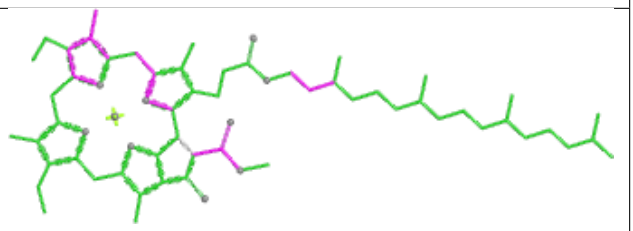


Rings

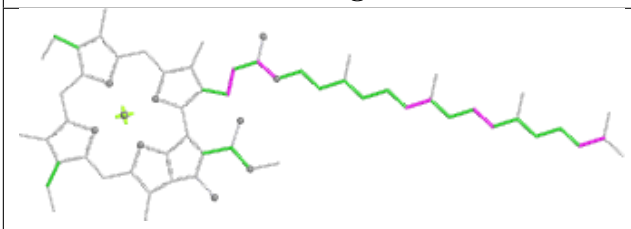
Ligand CLA L 206



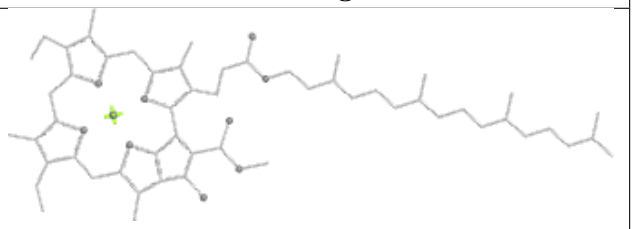
Bond lengths



Bond angles

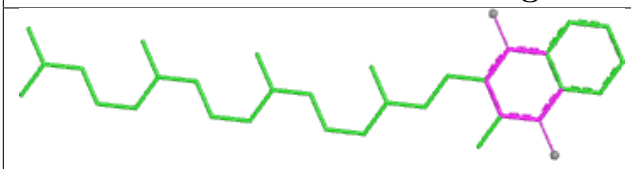


Torsions

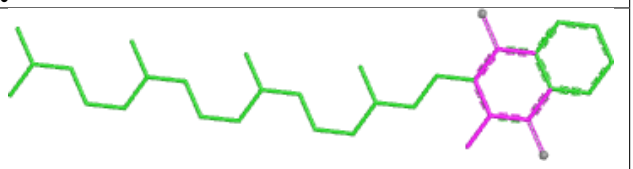


Rings

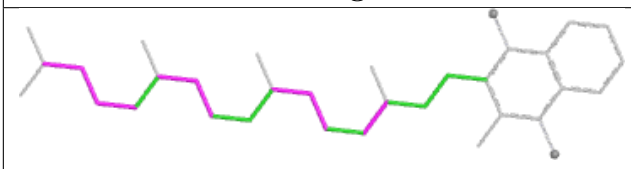
Ligand PQN A 845



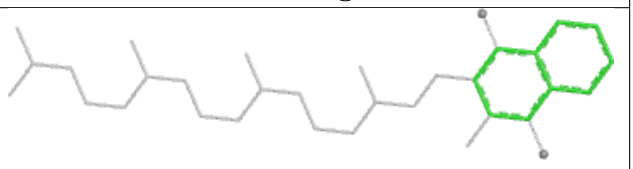
Bond lengths



Bond angles

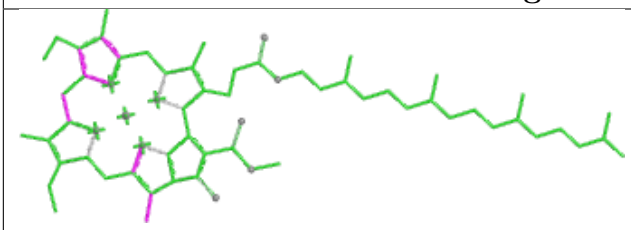


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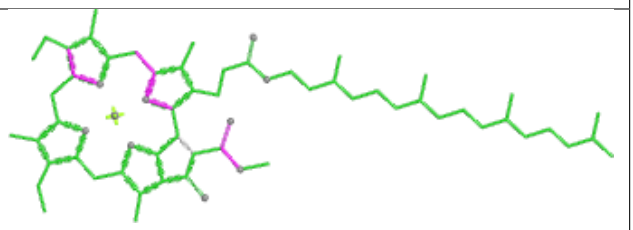


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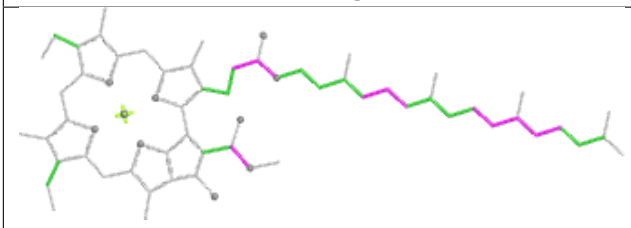
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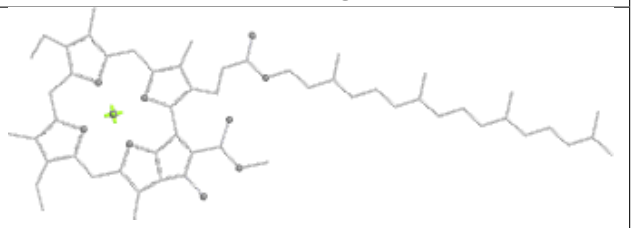
Bond lengths



Bond angles

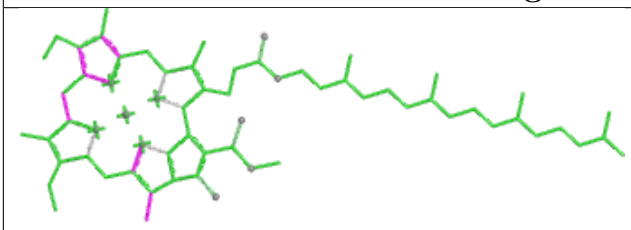


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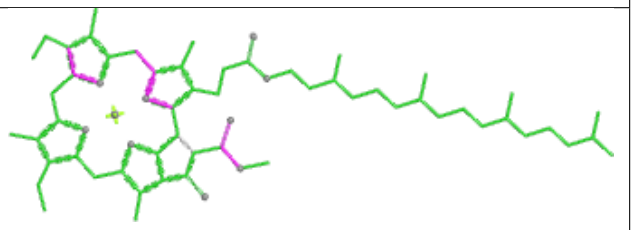


Rings

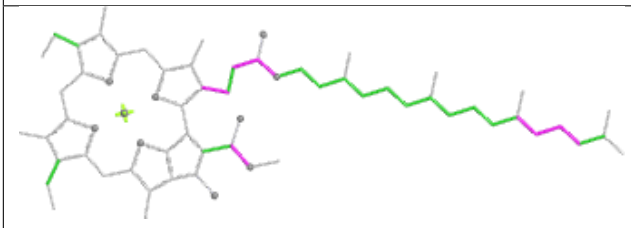
Ligand CLA B 805



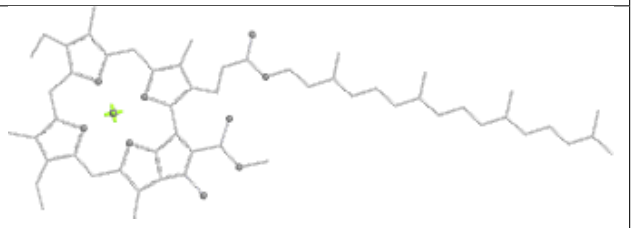
Bond lengths



Bond angles

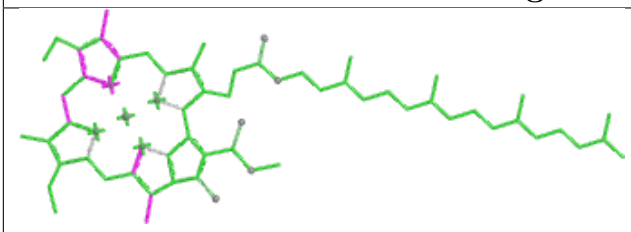


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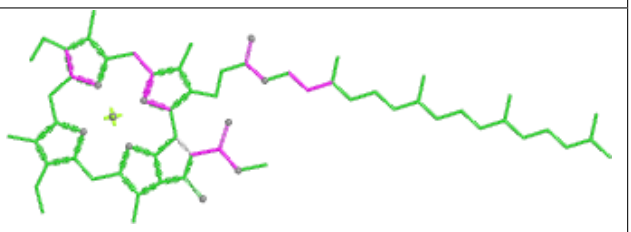


Rings

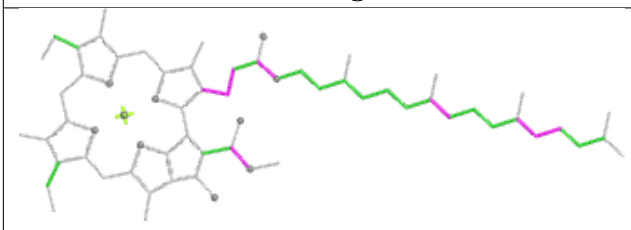
Ligand CLA L 205



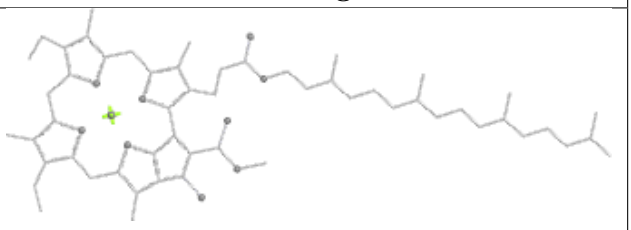
Bond lengths



Bond angles

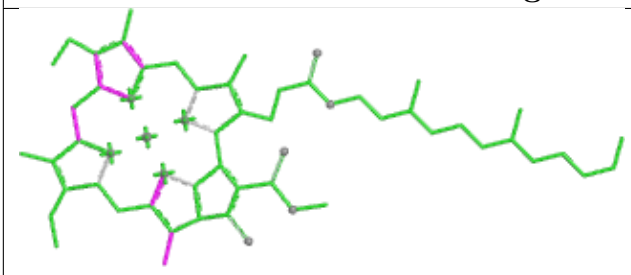


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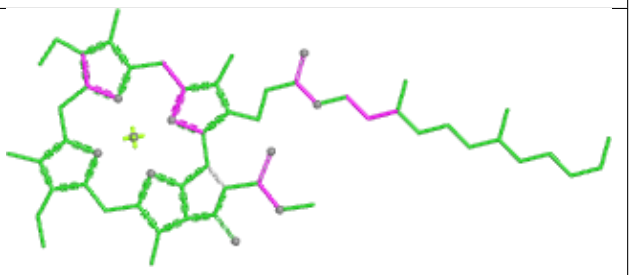


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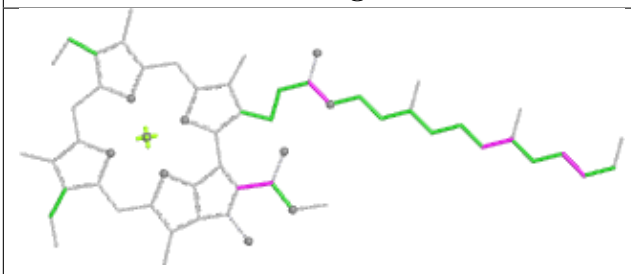
Ligand CLA A 805



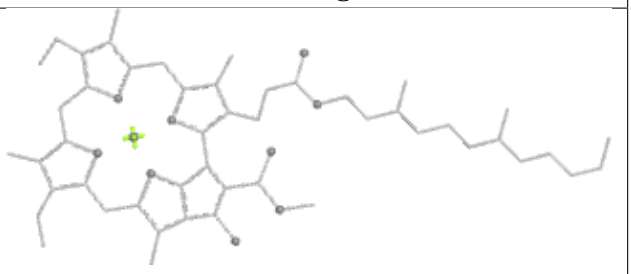
Bond lengths



Bond angles



Torsions

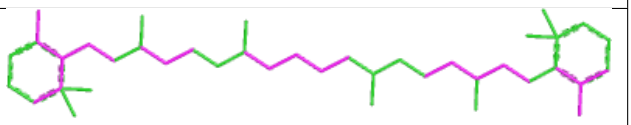


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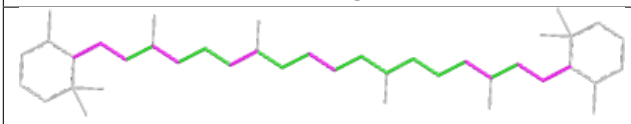
Ligand BCR J 104



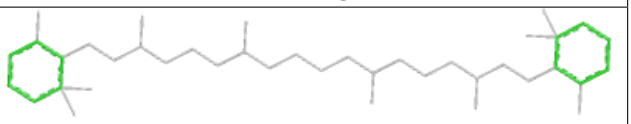
Bond lengths



Bond angles

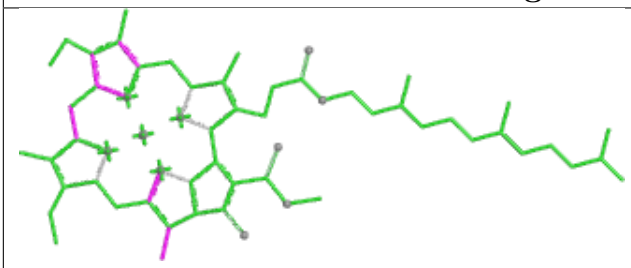


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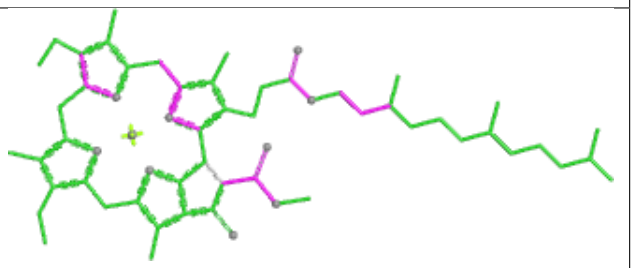


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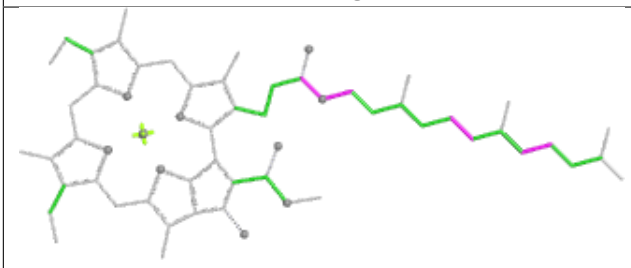
Ligand CLA B 837



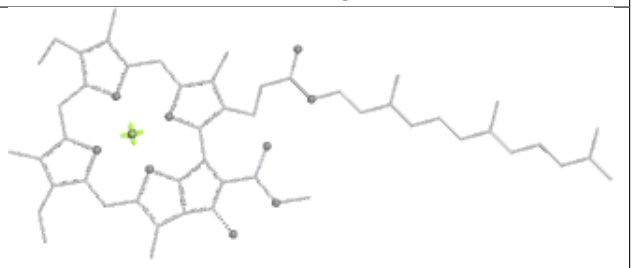
Bond lengths



Bond angles

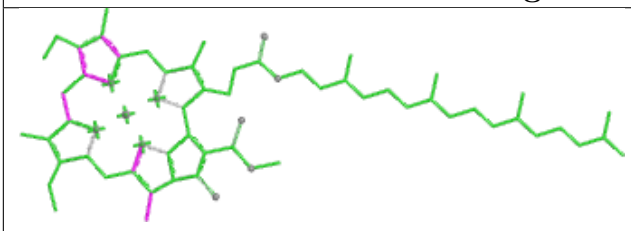


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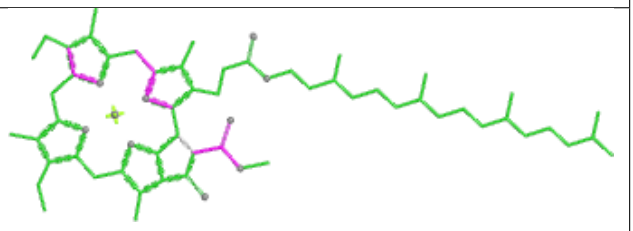


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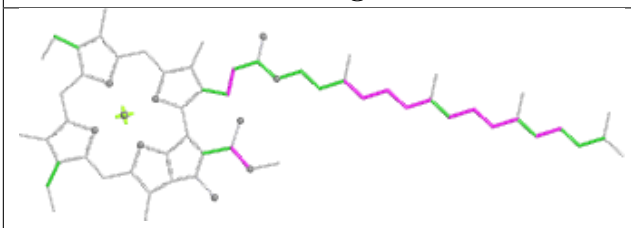
Ligand CLA A 830



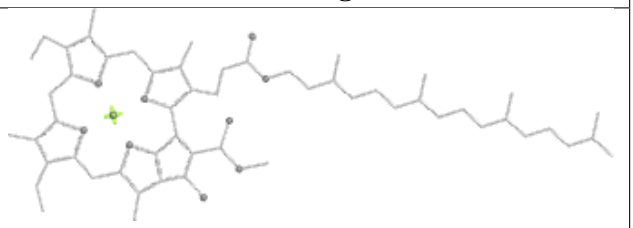
Bond lengths



Bond angles

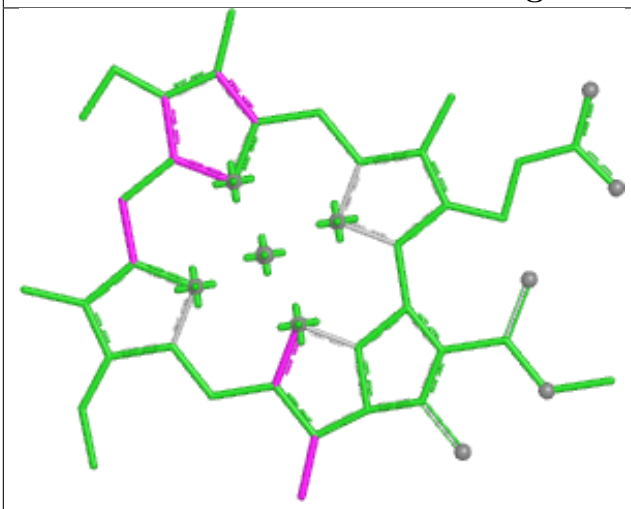


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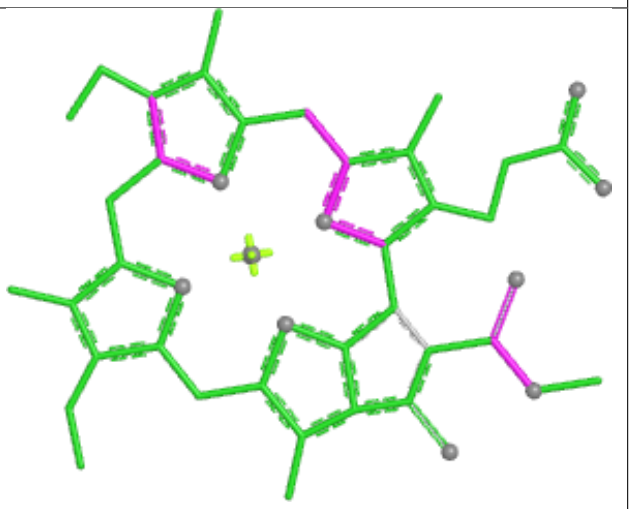


Rings

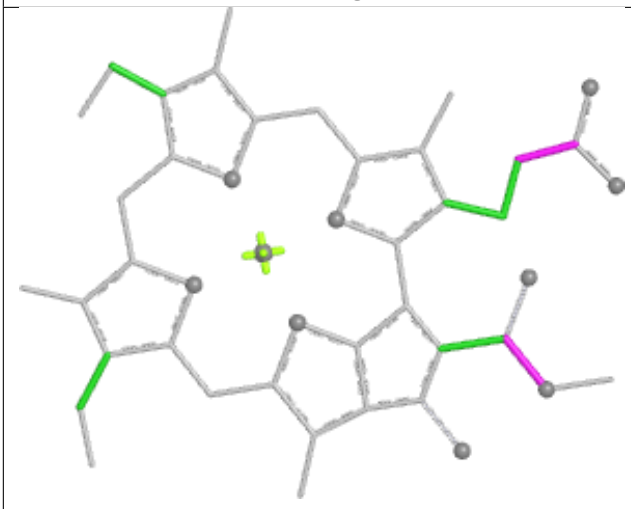
Ligand CLA F 202



Bond lengths



Bond angles

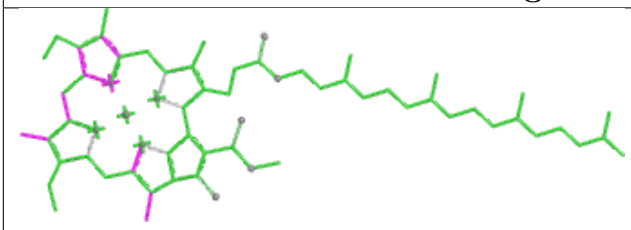


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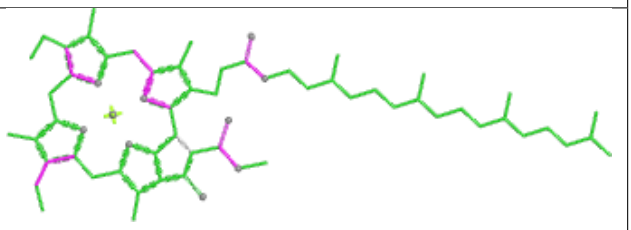


Rings

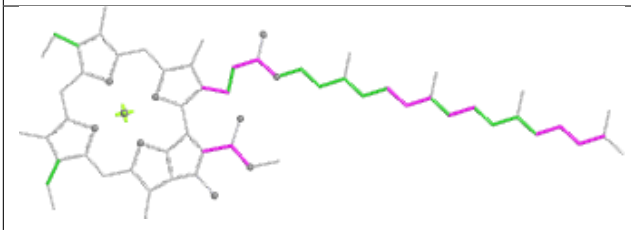
Ligand CLA B 813



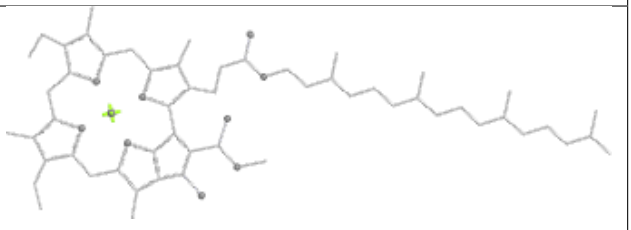
Bond lengths



Bond angles

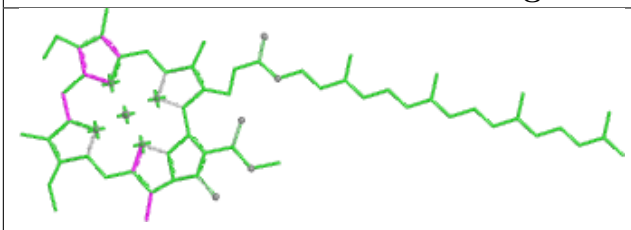


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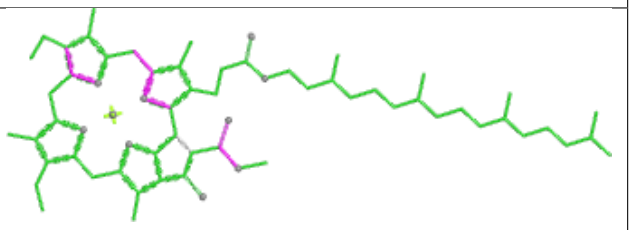


Rings

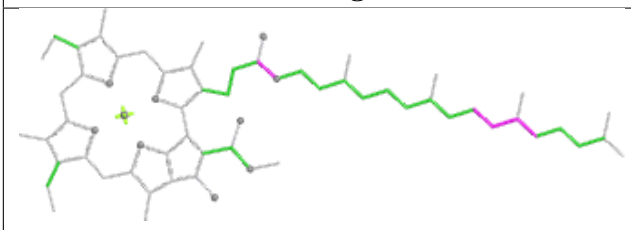
Ligand CLA A 812



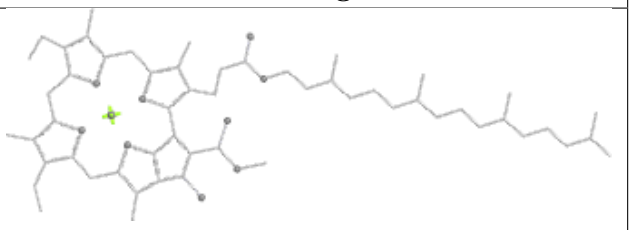
Bond lengths



Bond angles

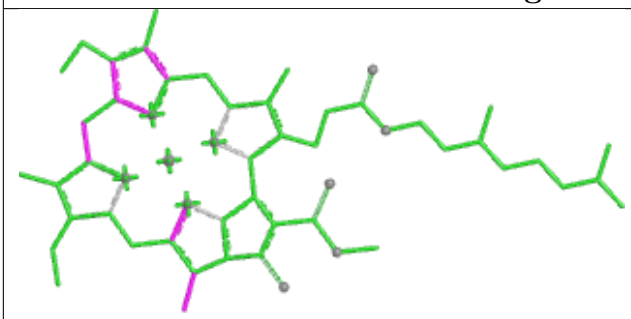


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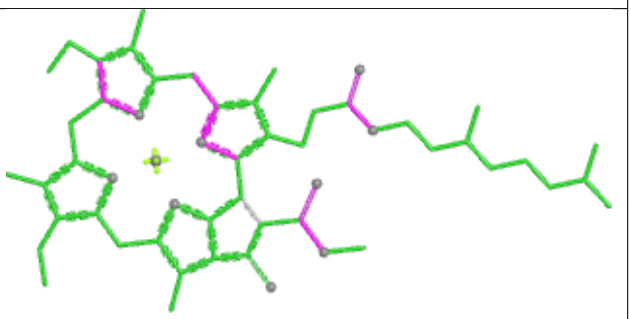


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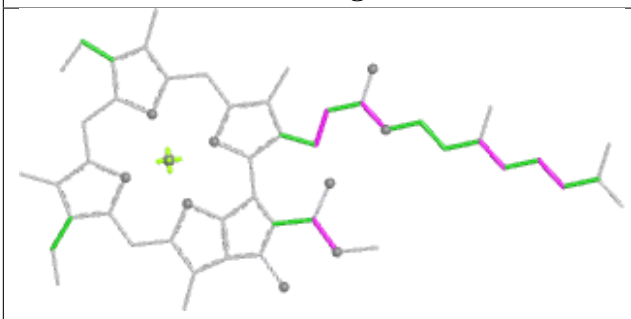
Ligand CLA B 822



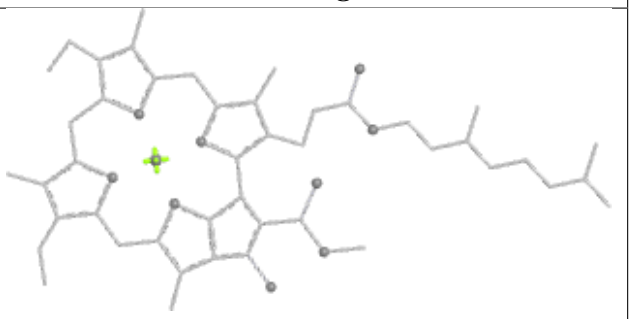
Bond lengths



Bond angles

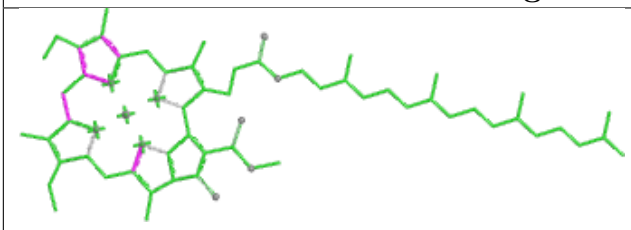


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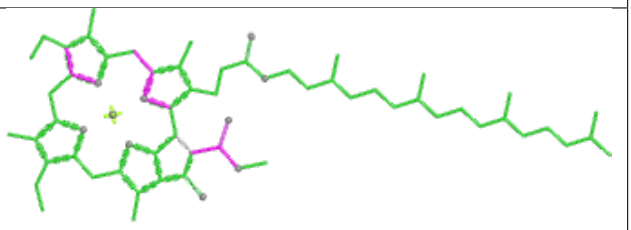


Rings

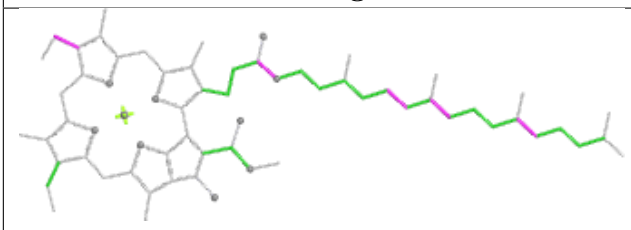
Ligand CLA A 834



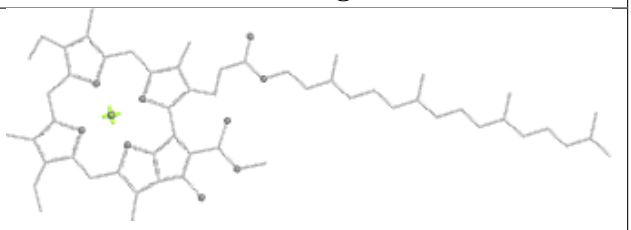
Bond lengths



Bond angles

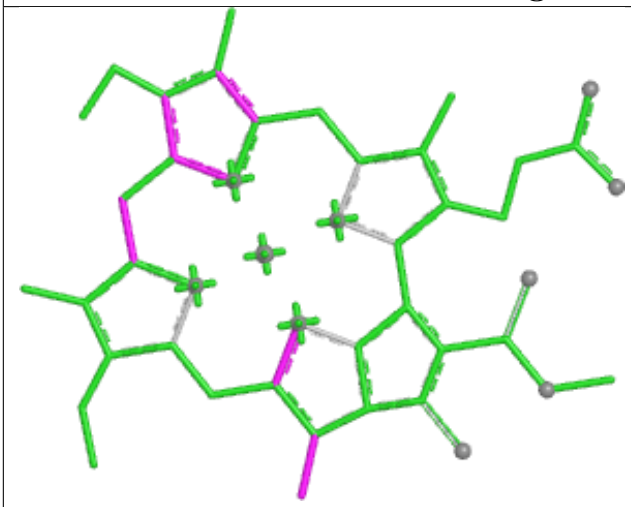


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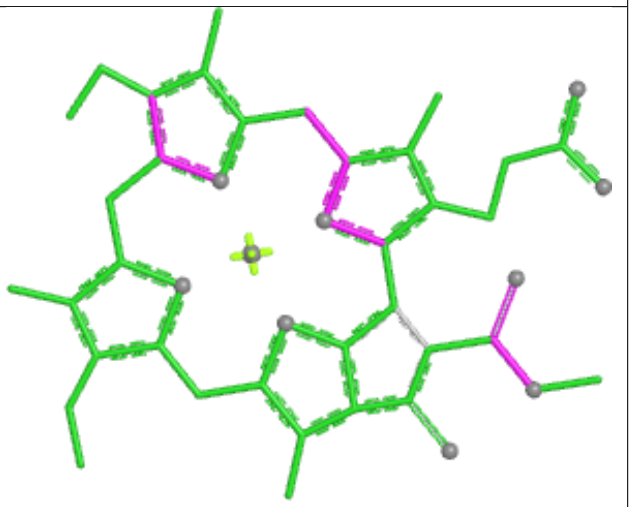


Rings

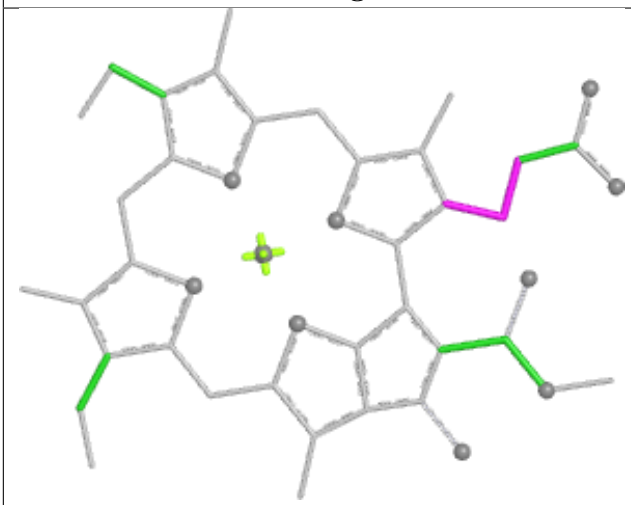
Ligand CLA J 101



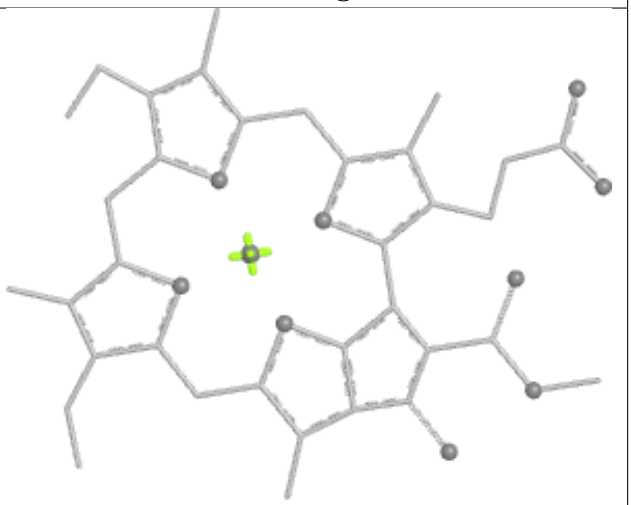
Bond lengths



Bond angles

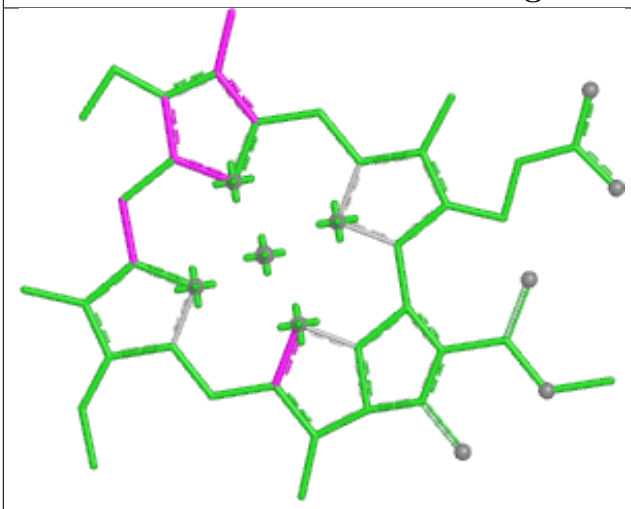


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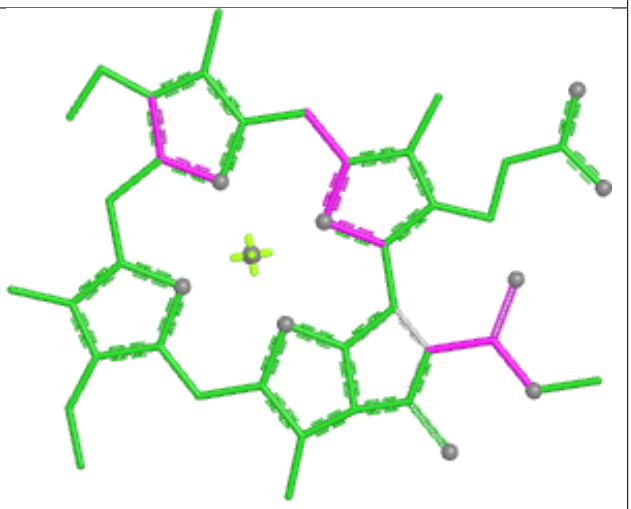


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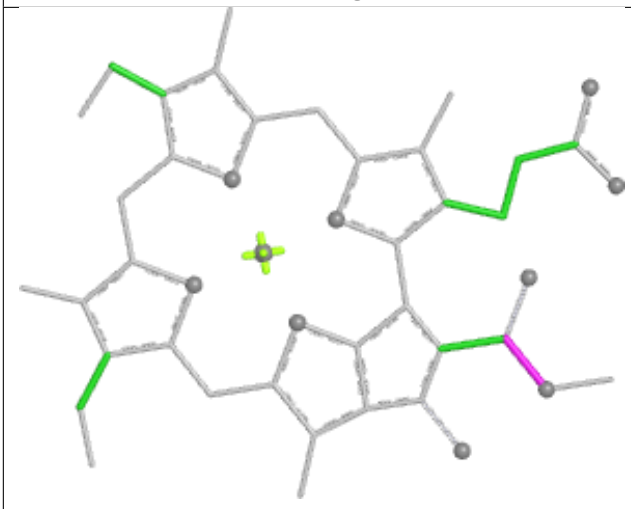
Ligand CLA B 811



Bond lengths



Bond angles

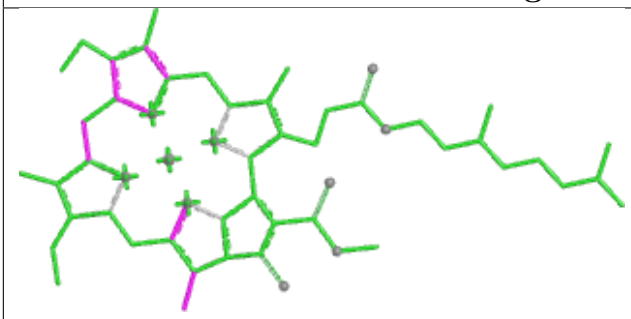


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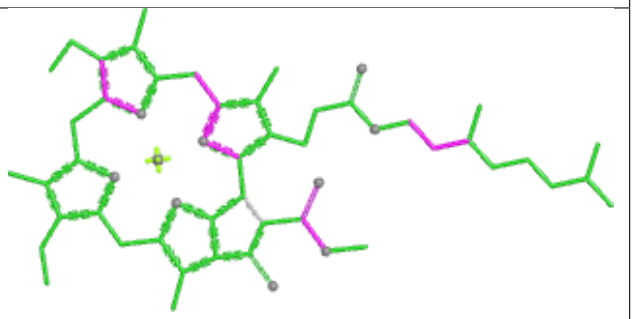


Rings

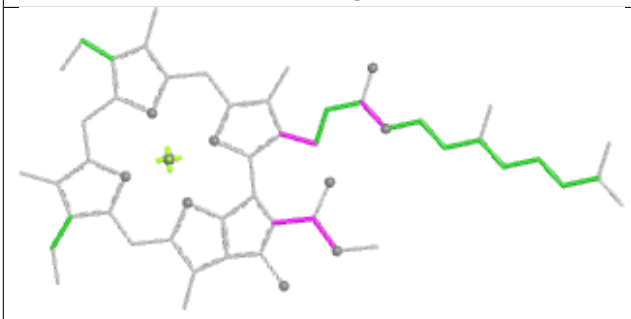
Ligand CLA B 816



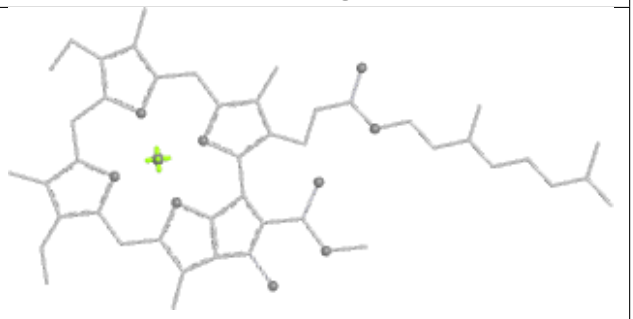
Bond lengths



Bond angles

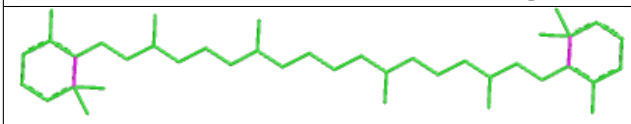


Torsions

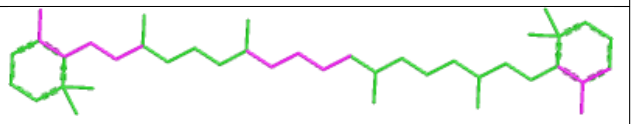


Rings

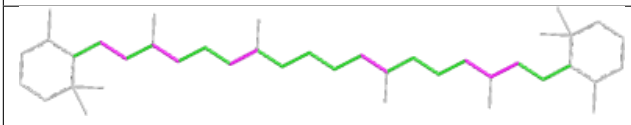
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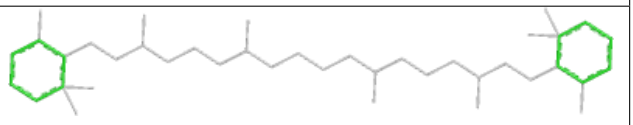
Bond lengths



Bond angles

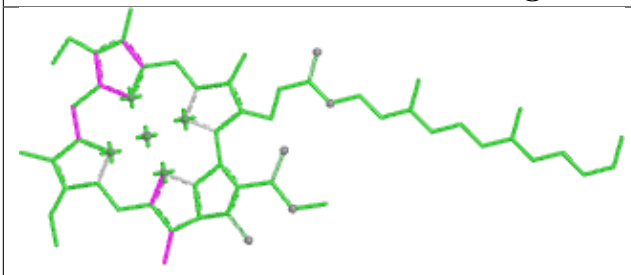


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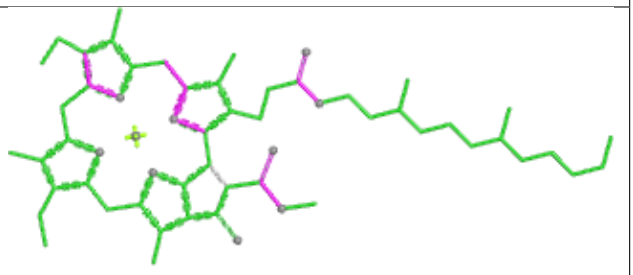


Rings

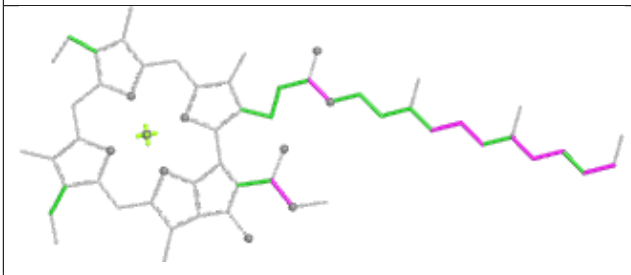
Ligand CLA A 825



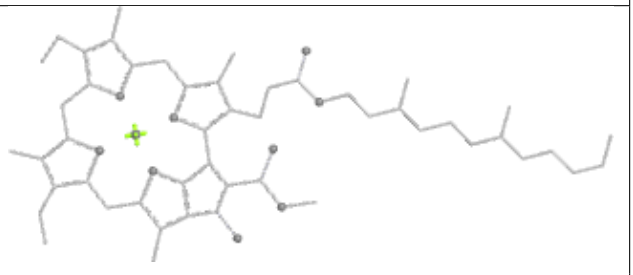
Bond lengths



Bond angles

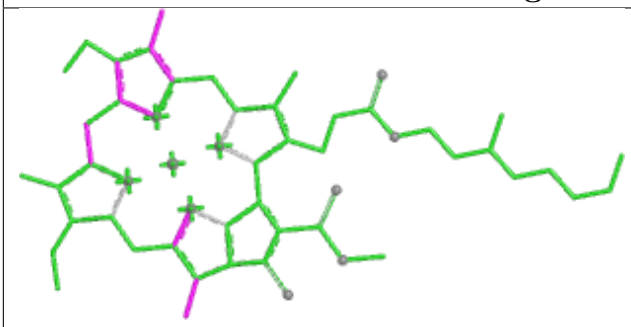


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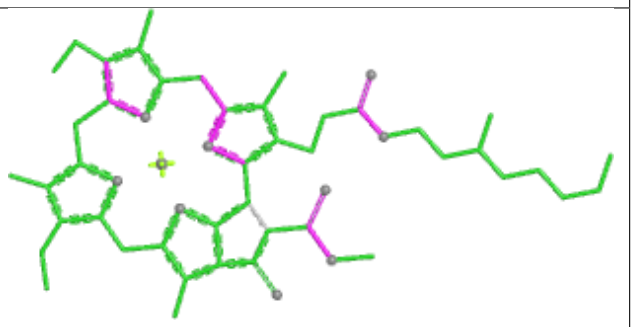


Rings

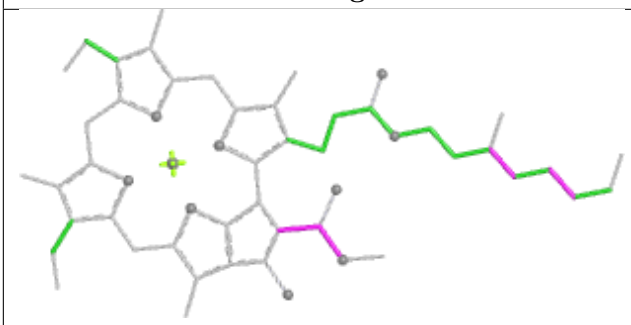
Ligand CLA B 824



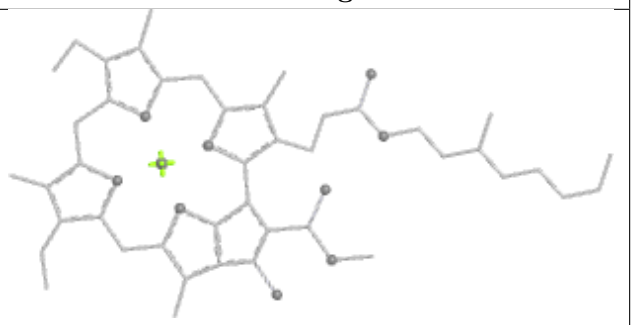
Bond lengths



Bond angles



Torsions

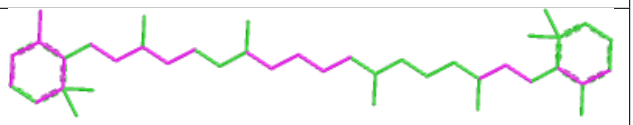


Rings

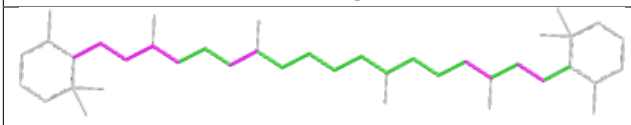
Ligand BCR J 105



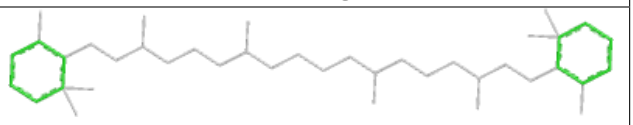
Bond lengths



Bond angles

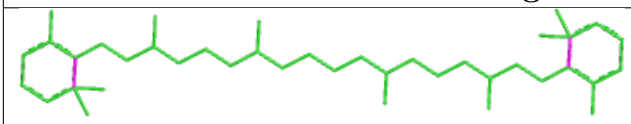


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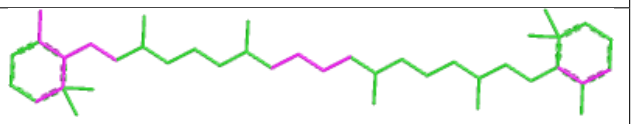


Rings

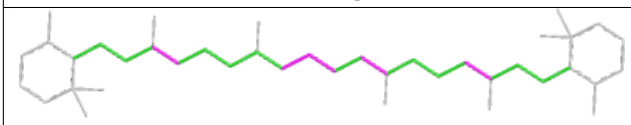
Ligand BCR B 848



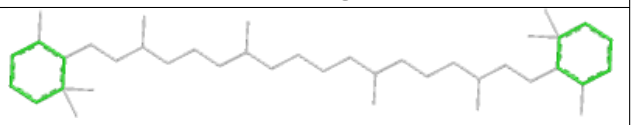
Bond lengths



Bond angles

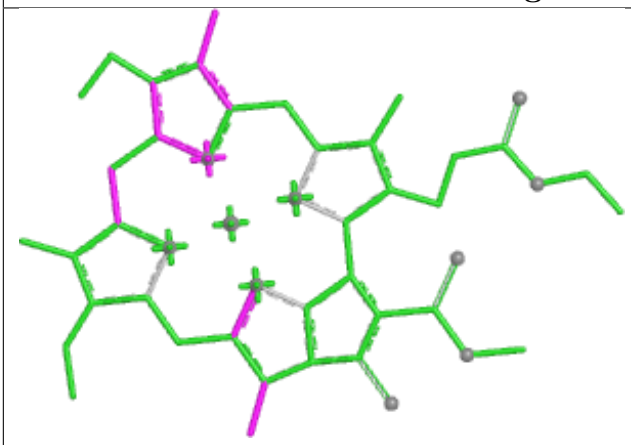


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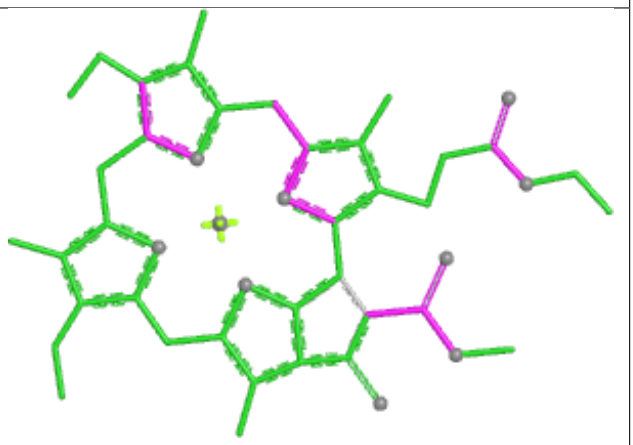


Rings

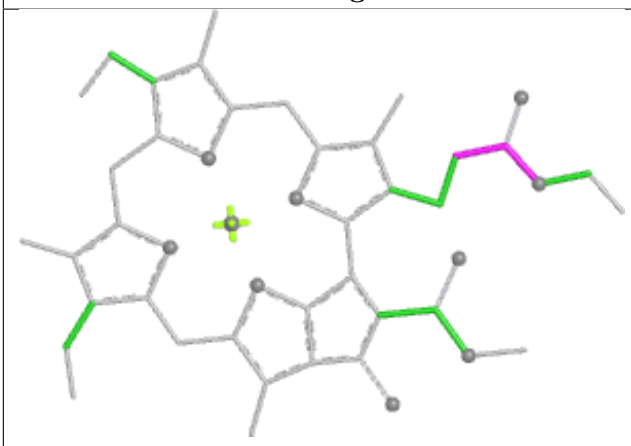
Ligand CLA B 839



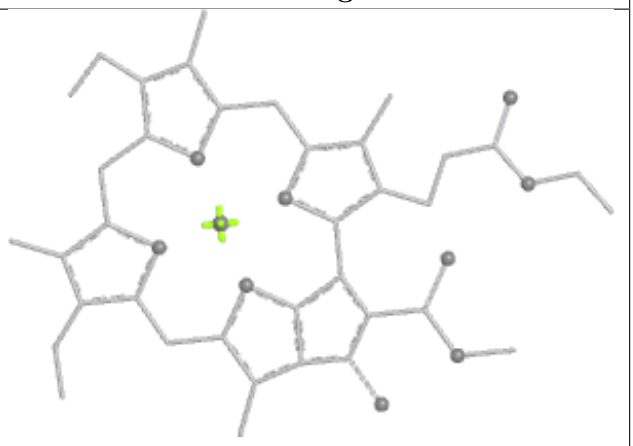
Bond lengths



Bond angles

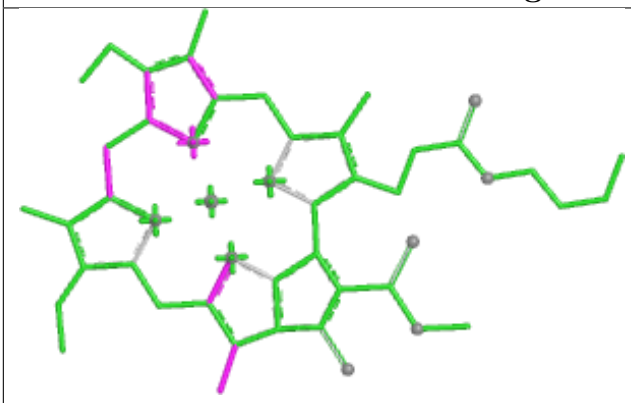


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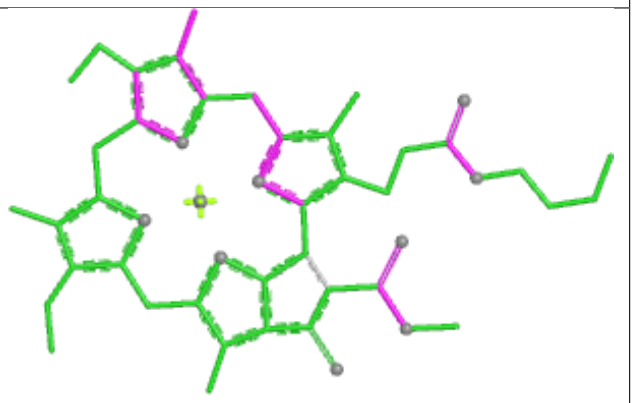


Rings

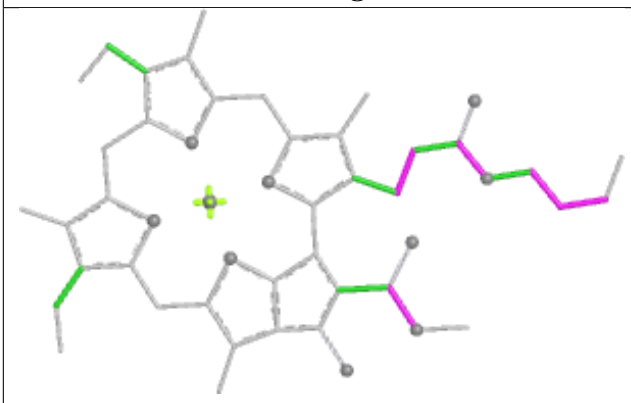
Ligand CLA B 831



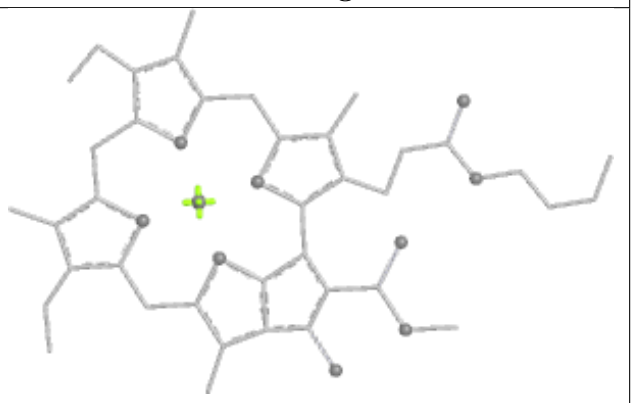
Bond lengths



Bond angles

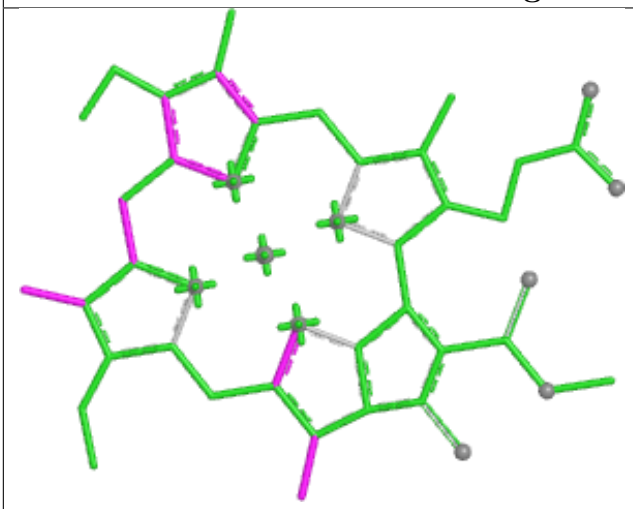


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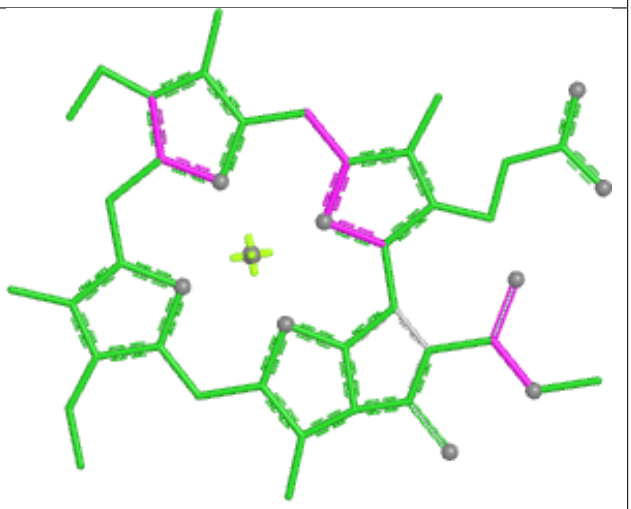


Rings

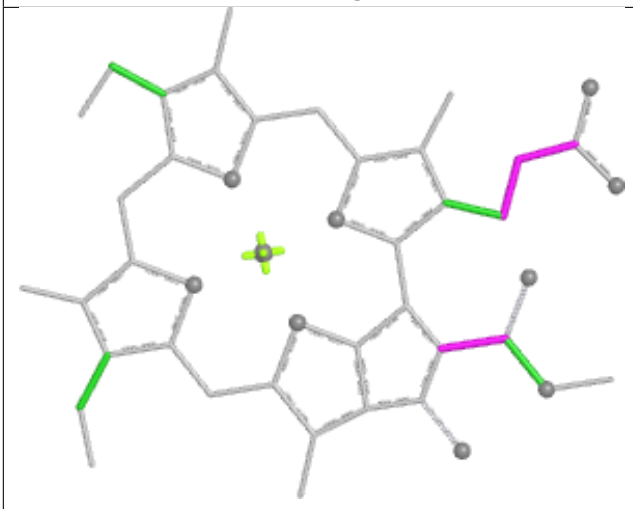
Ligand CLA A 816



Bond lengths



Bond angles

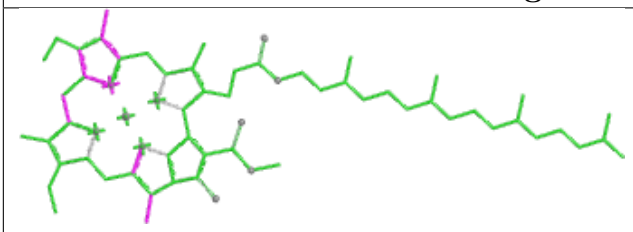


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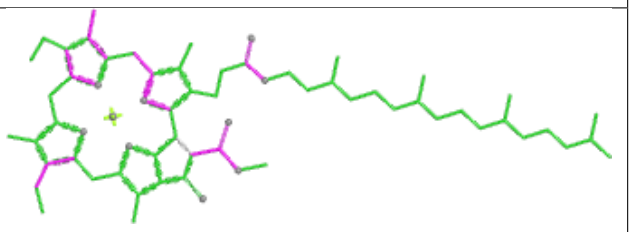


Rings

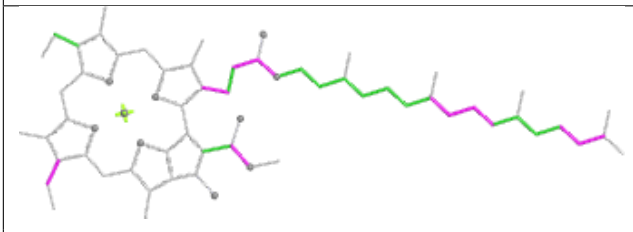
Ligand CLA B 809



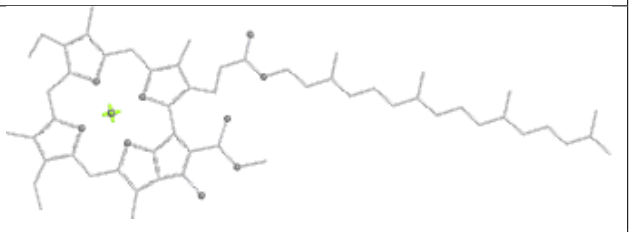
Bond lengths



Bond angles

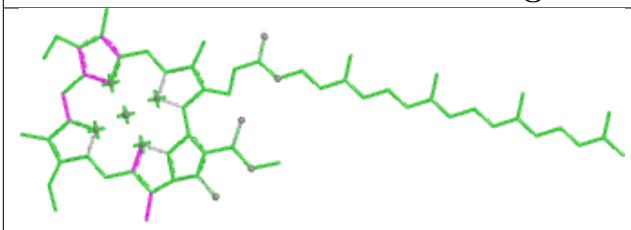


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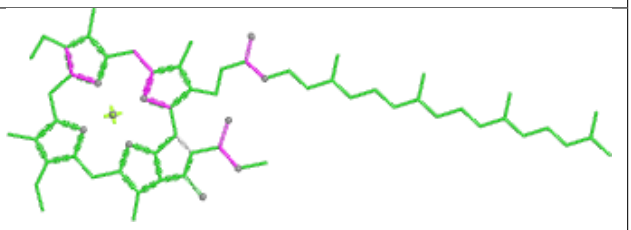


Rings

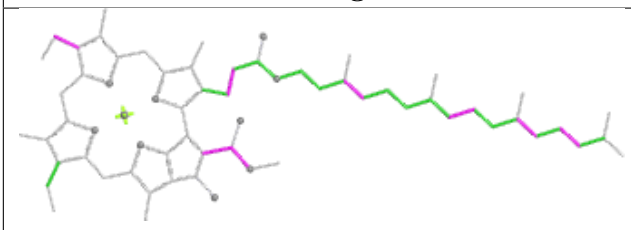
Ligand CLA B 814



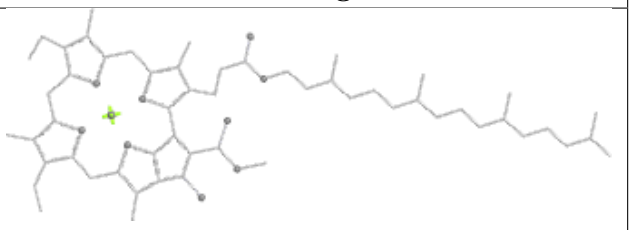
Bond lengths



Bond angles

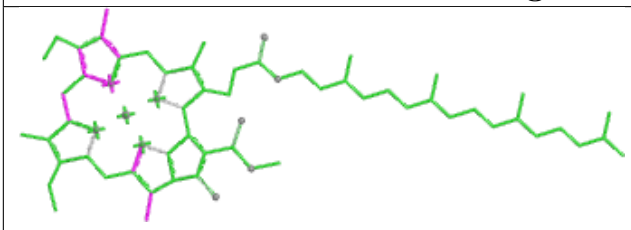


Torsions

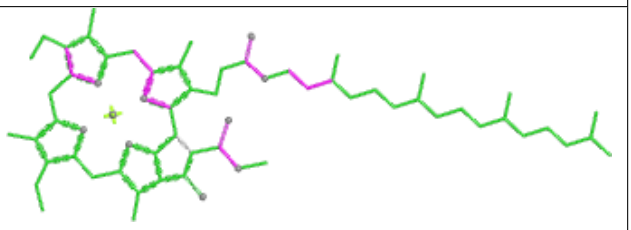


Rings

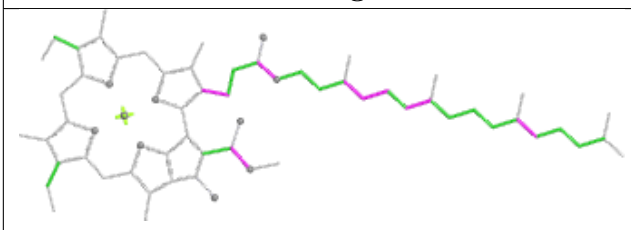
Ligand CLA L 204



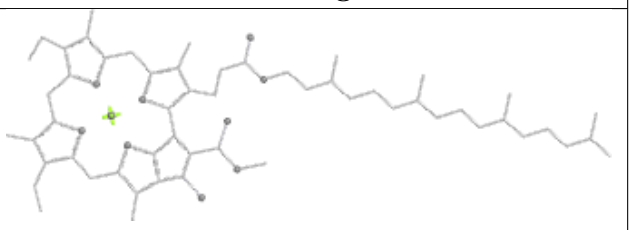
Bond lengths



Bond angles

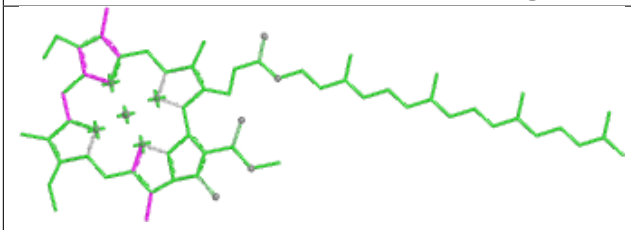


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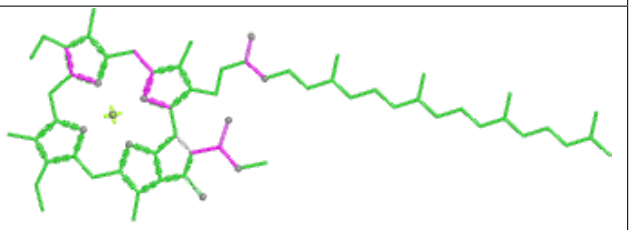


Rings

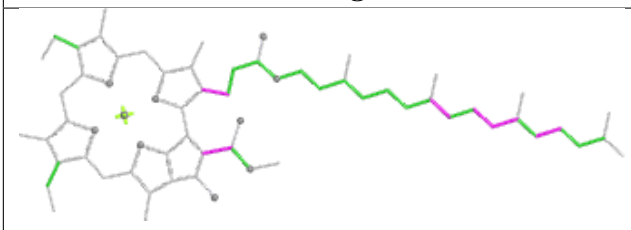
Ligand CLA A 831



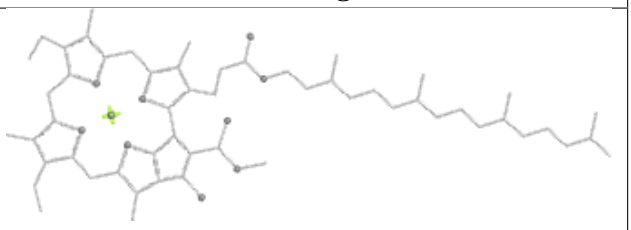
Bond lengths



Bond angles

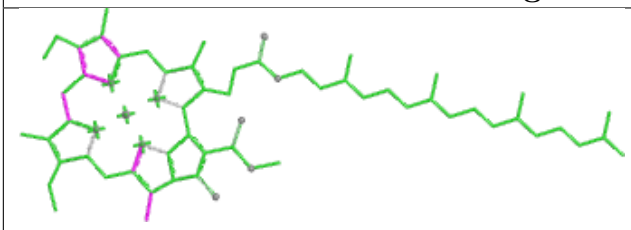


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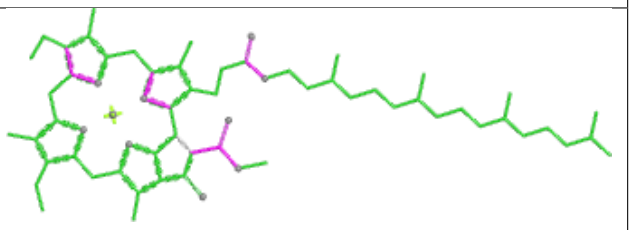


Rings

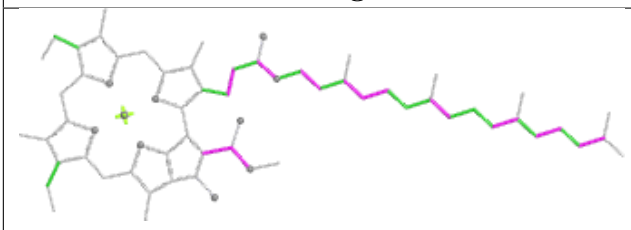
Ligand CLA A 857



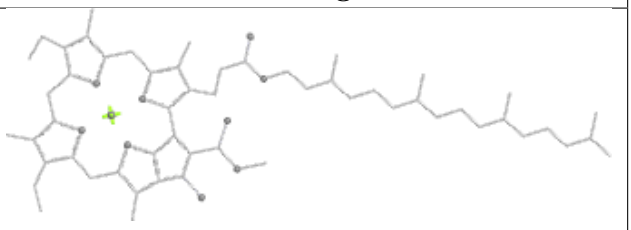
Bond lengths



Bond angles

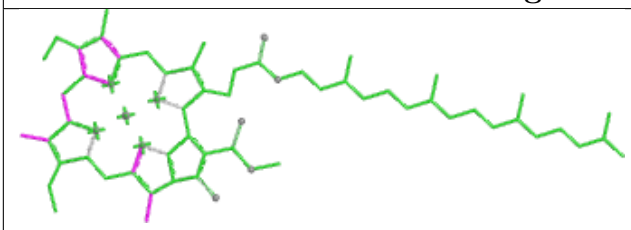


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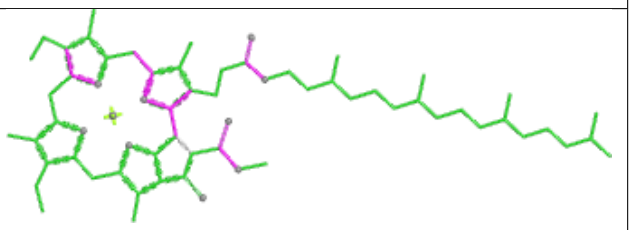


Rings

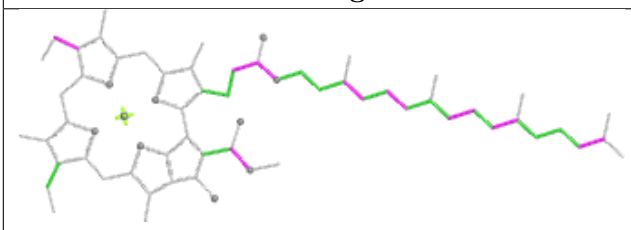
Ligand CLA B 810



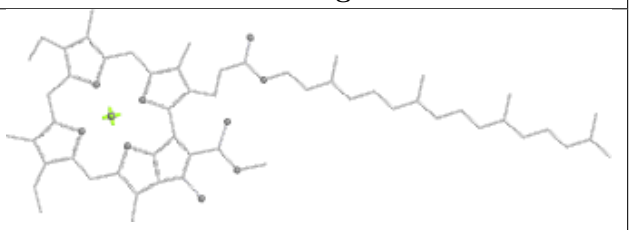
Bond lengths



Bond angles

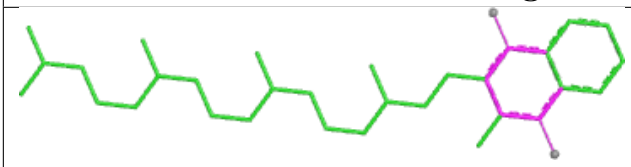


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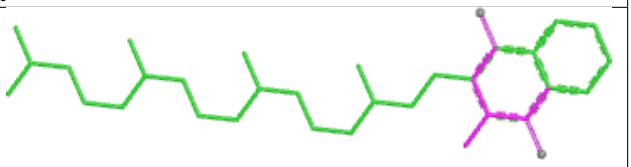


Rings

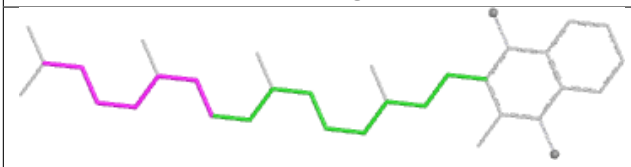
Ligand PQN B 842



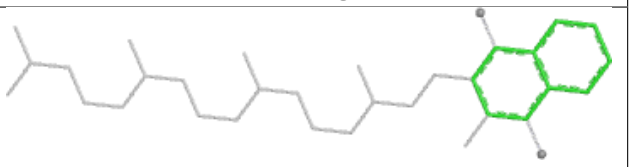
Bond lengths



Bond angles

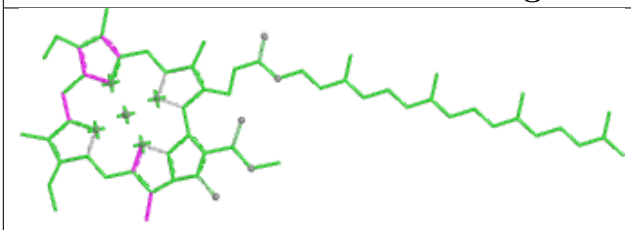


Torsions

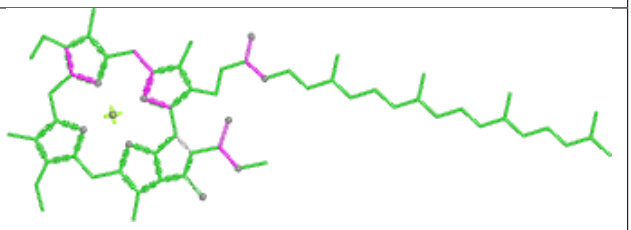


Rings

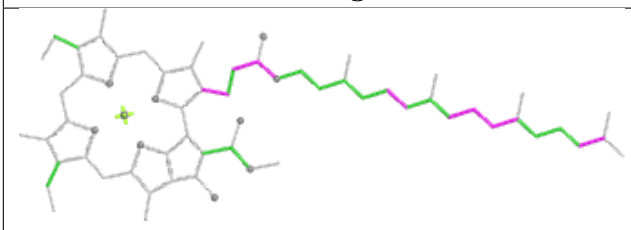
Ligand CLA A 828



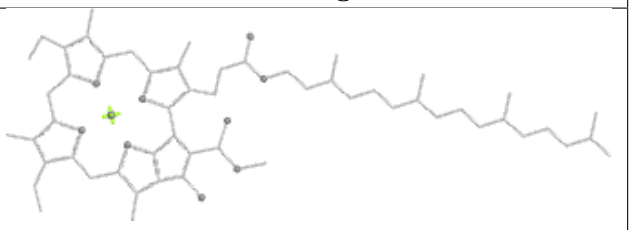
Bond lengths



Bond angles

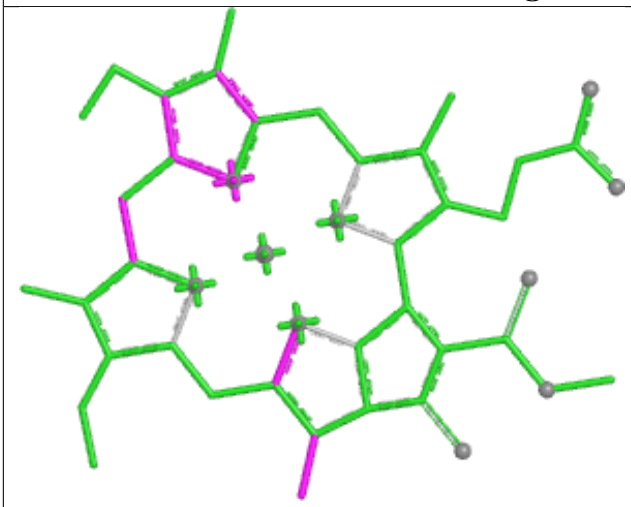


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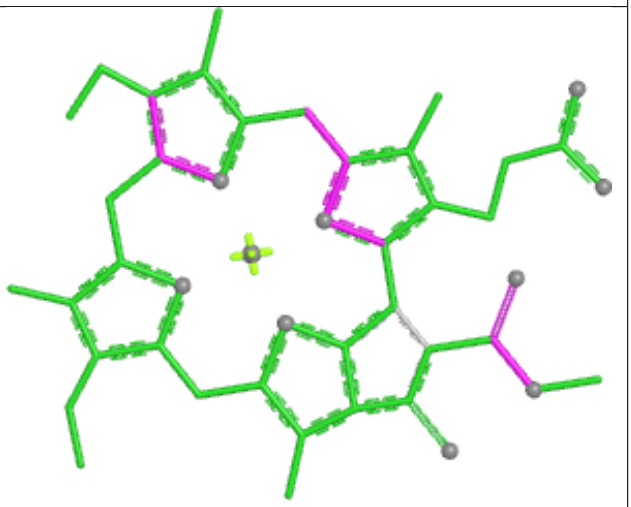


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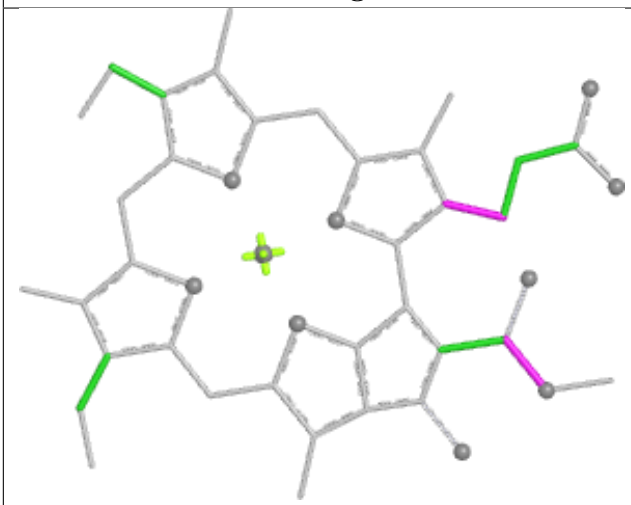
Ligand CLA A 815



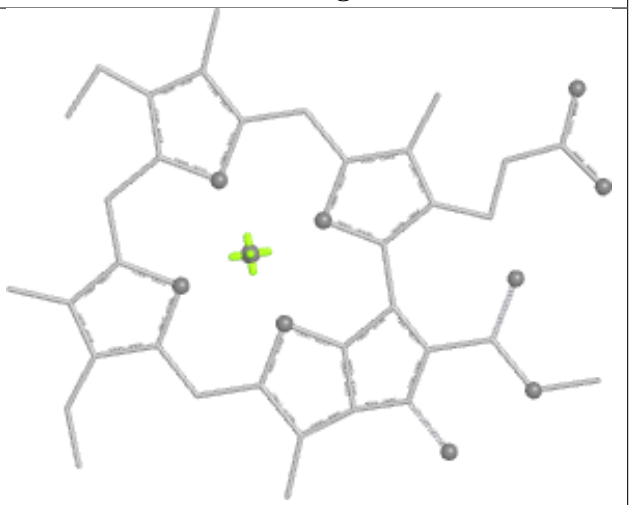
Bond lengths



Bond angles

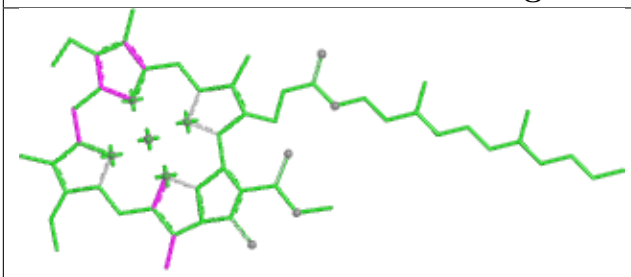


Torsions

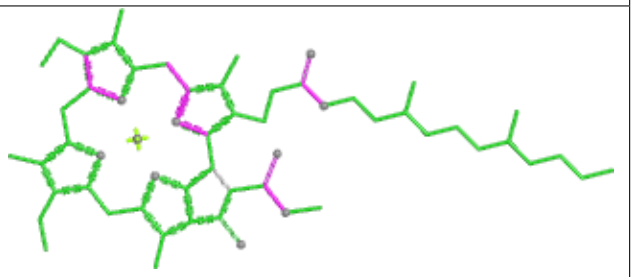


Rings

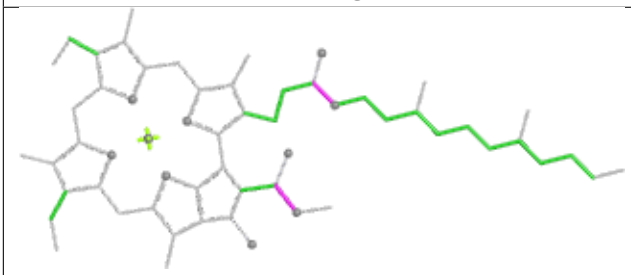
Ligand CLA B 833



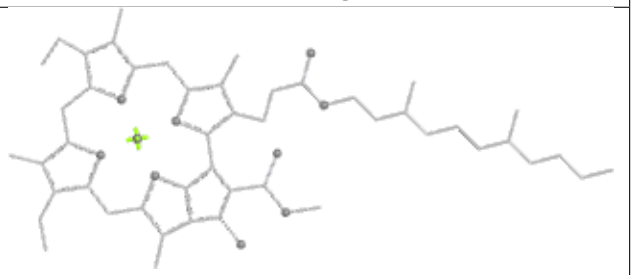
Bond lengths



Bond angles



Torsions

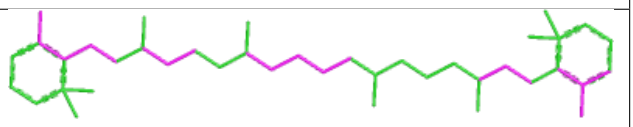


Rings

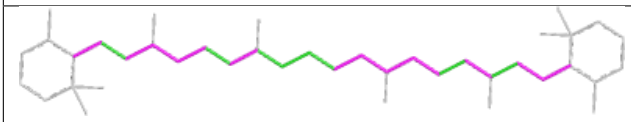
Ligand BCR A 848



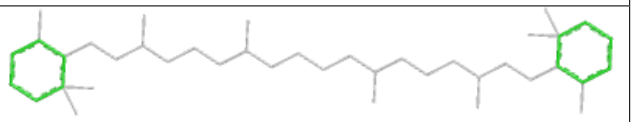
Bond lengths



Bond angles

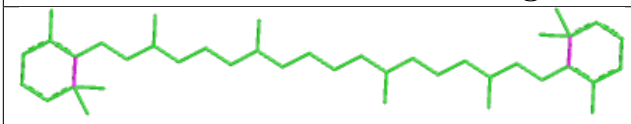


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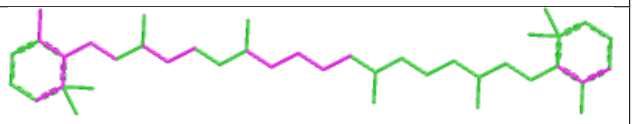


Rings

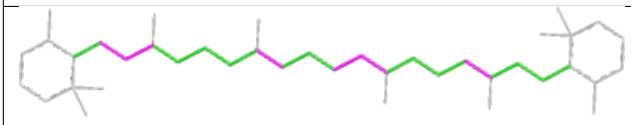
Ligand BCR A 851



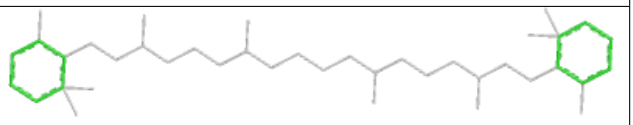
Bond lengths



Bond angles

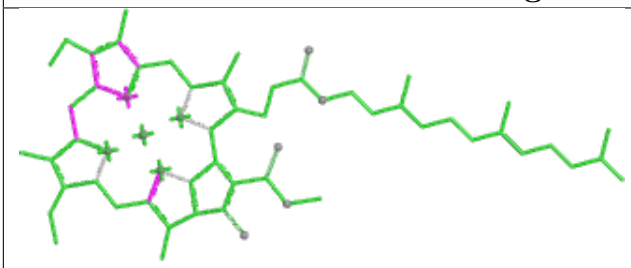


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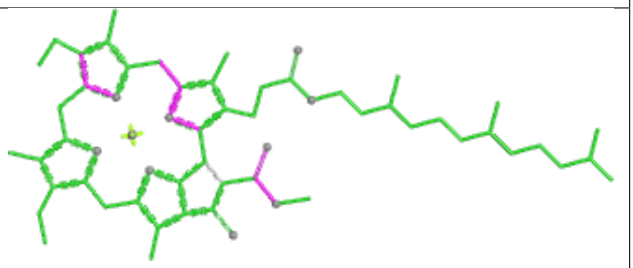


Rings

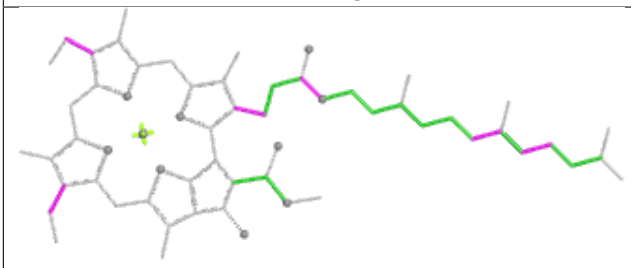
Ligand CLA B 818



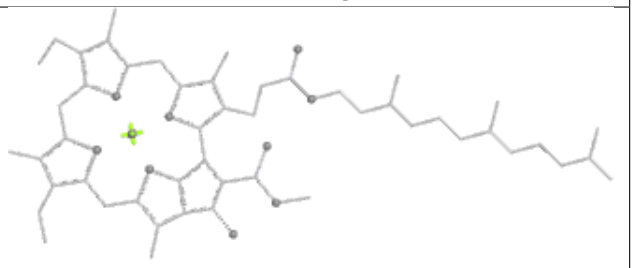
Bond lengths



Bond angles

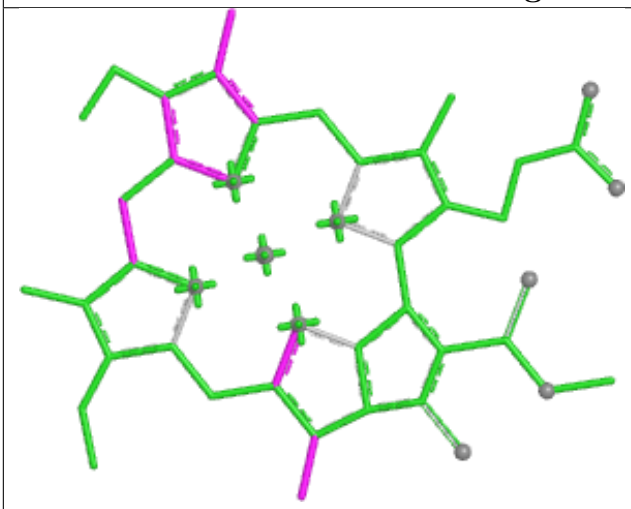


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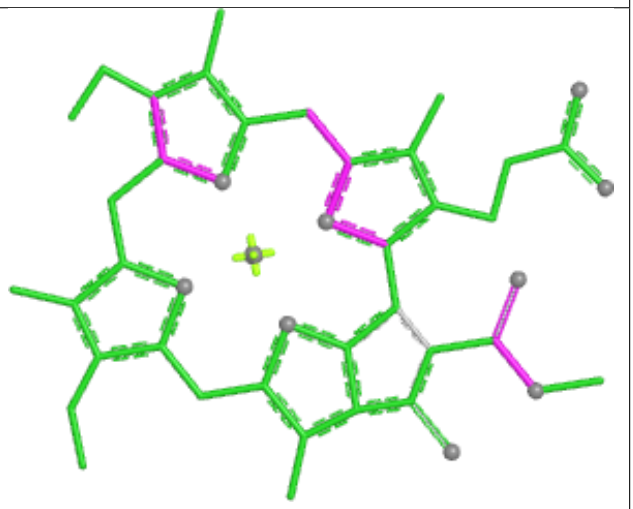


Rings

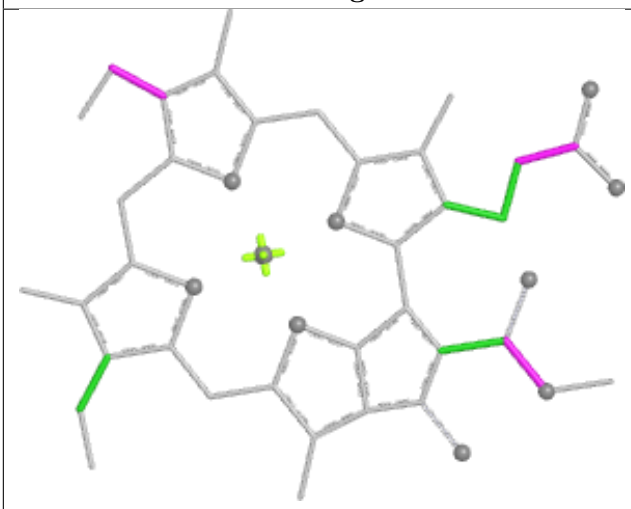
Ligand CLA B 823



Bond lengths



Bond angles

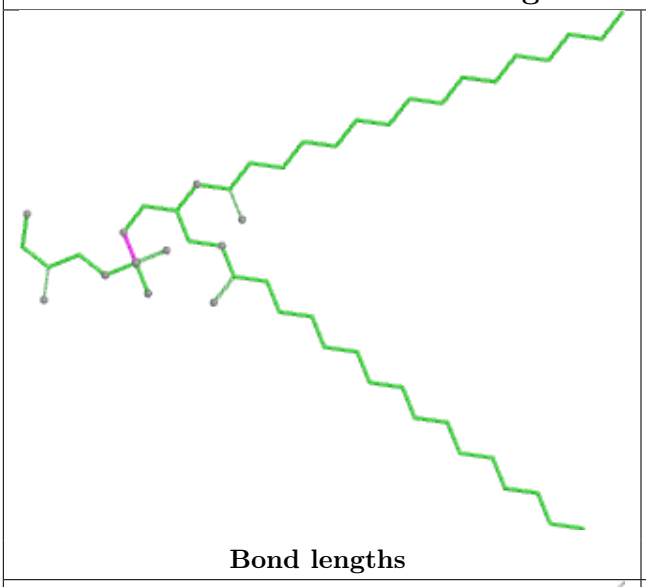


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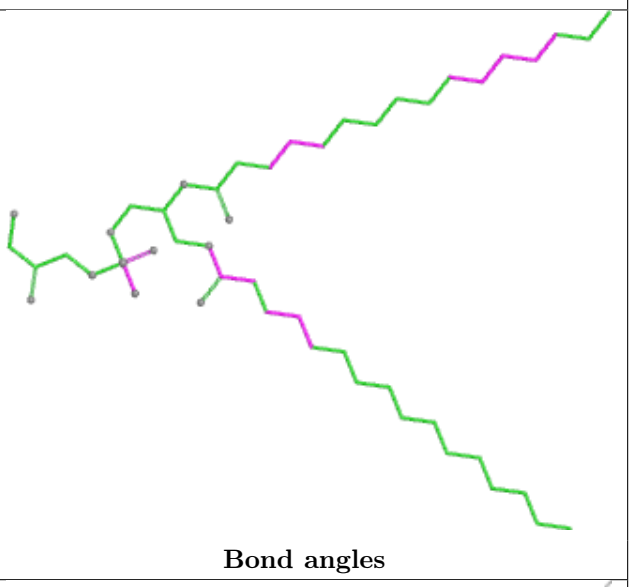


Rings

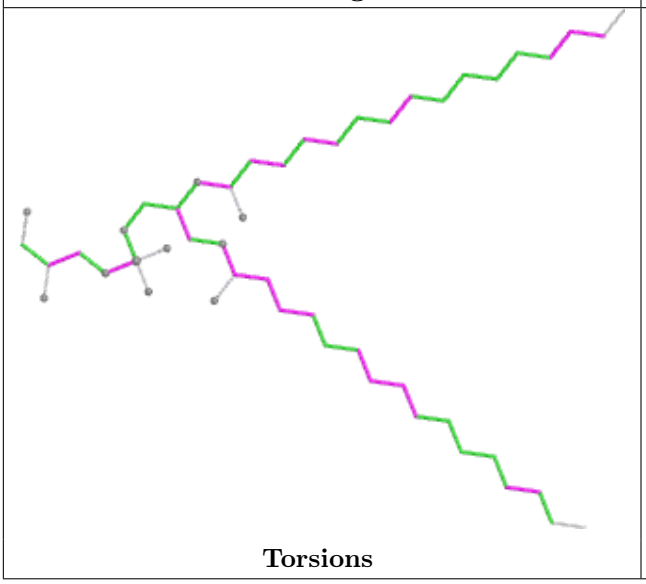
Ligand LHG A 854



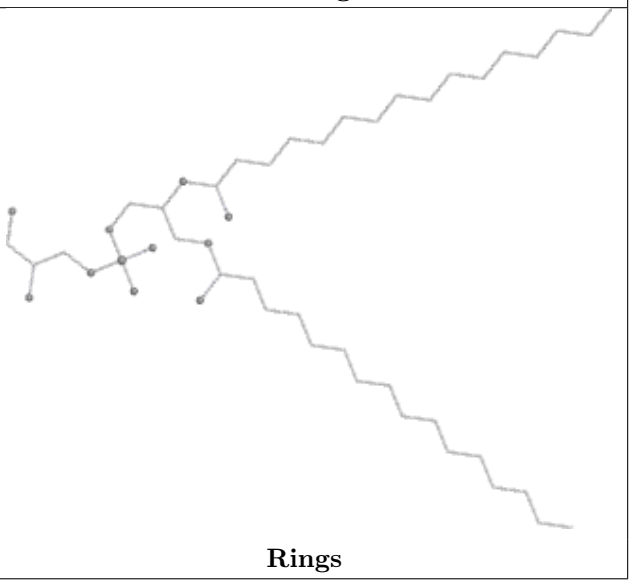
Bond lengths



Bond angles

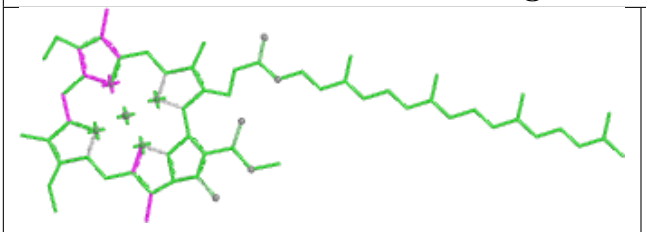


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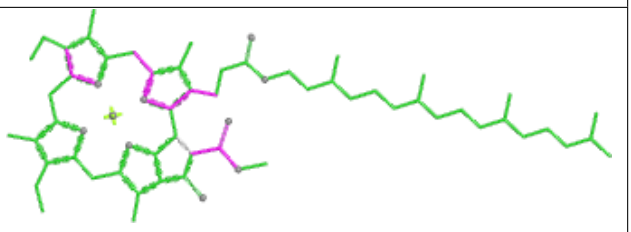


Rings

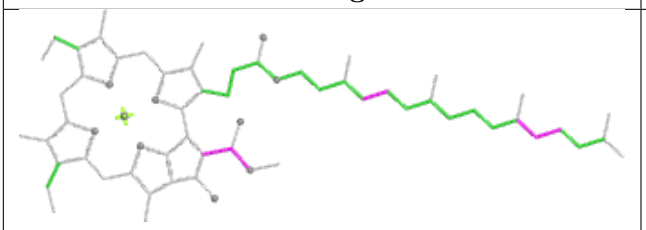
Ligand CLA A 803



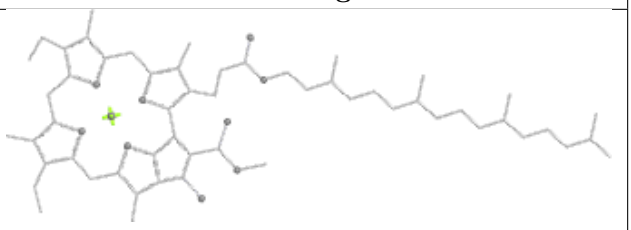
Bond lengths



Bond angles

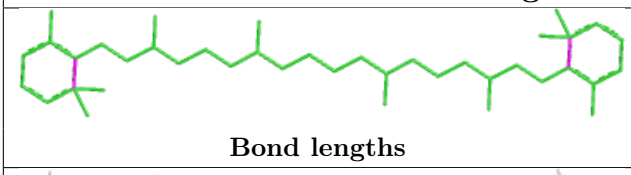


Torsions

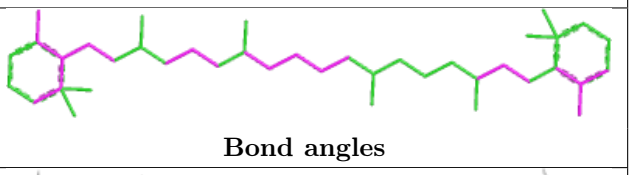


Rings

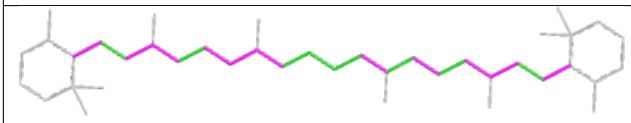
Ligand BCR A 852



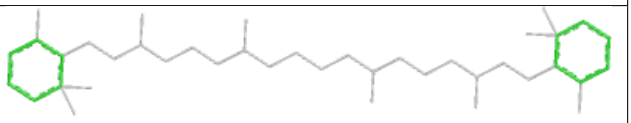
Bond lengths



Bond angles

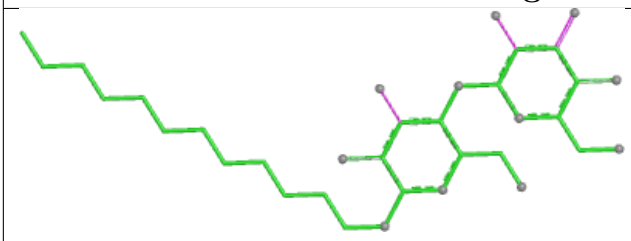


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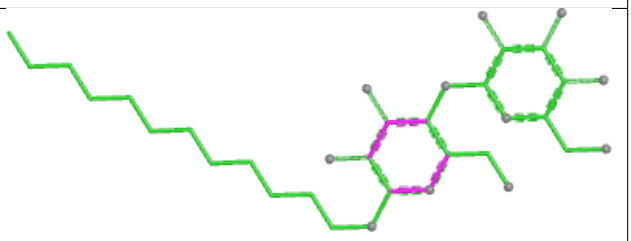


Rings

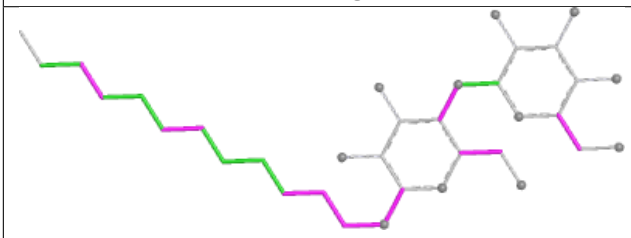
Ligand LMT L 202



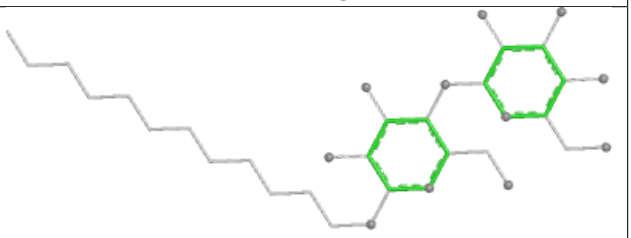
Bond lengths



Bond angles

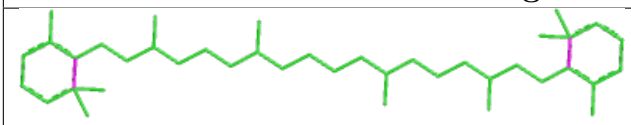


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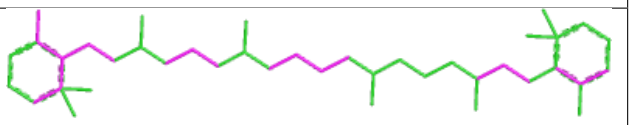


Rings

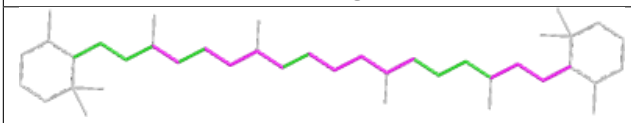
Ligand BCR B 847



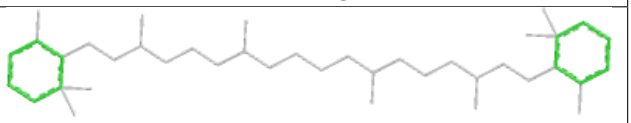
Bond lengths



Bond angles

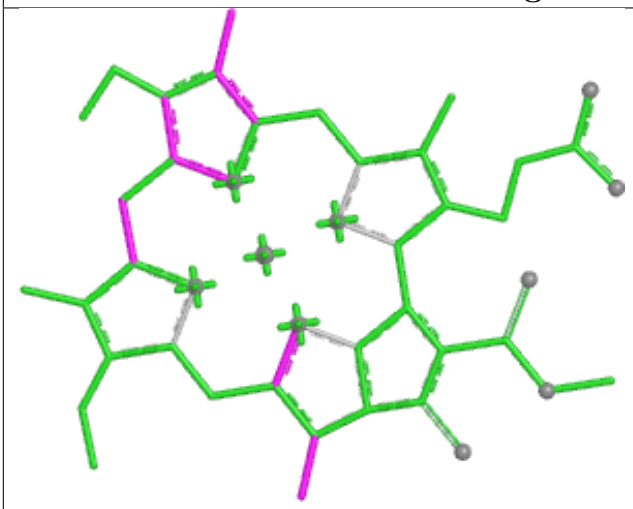


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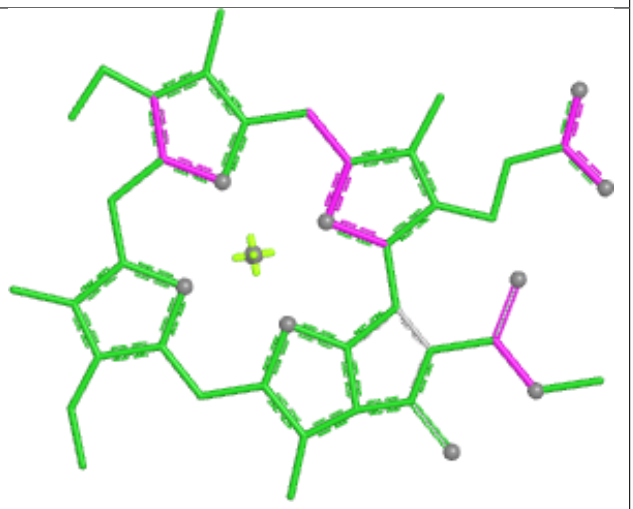


Rings

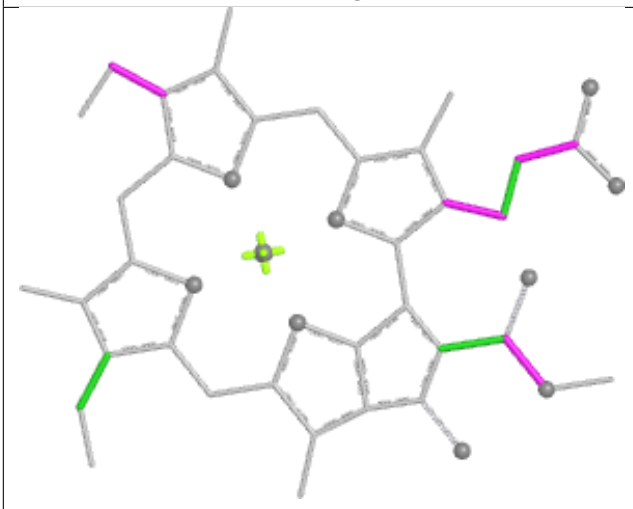
Ligand CLA B 835



Bond lengths



Bond angles

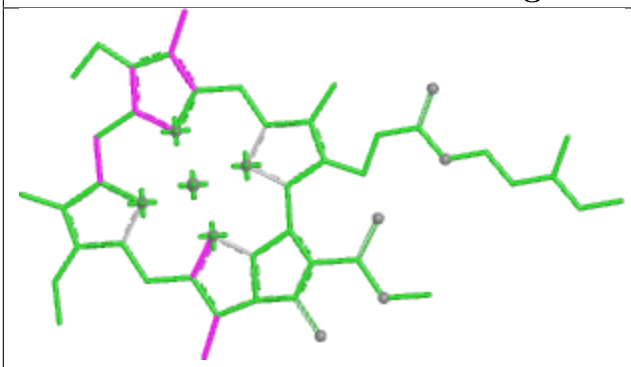


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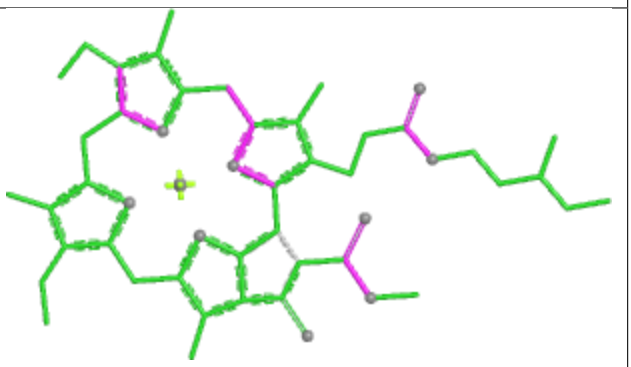


Rings

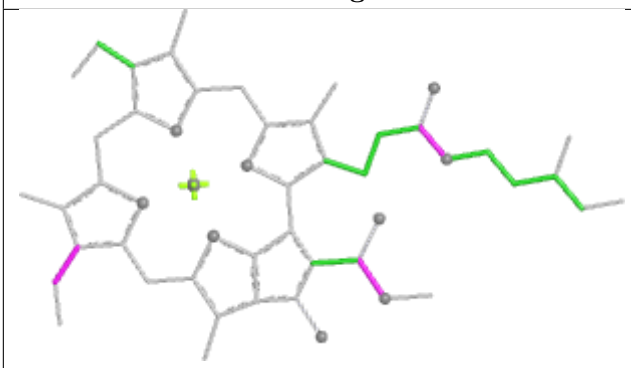
Ligand CLA A 838



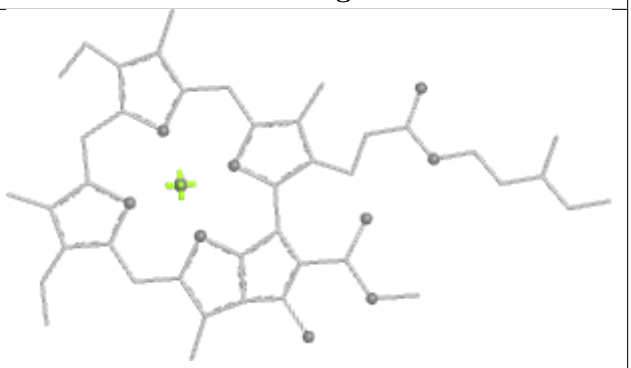
Bond lengths



Bond angles

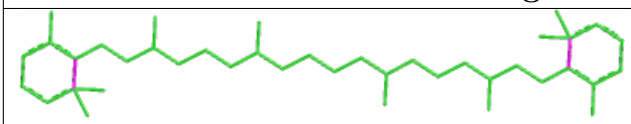


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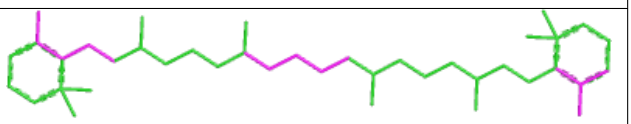


Rings

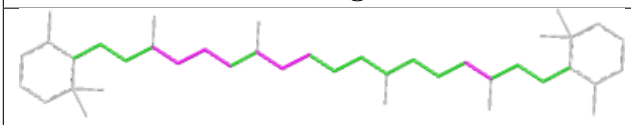
Ligand BCR B 845



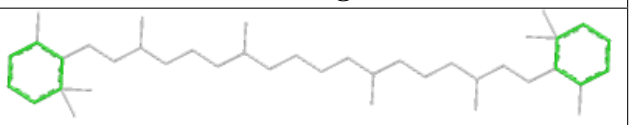
Bond lengths



Bond angles

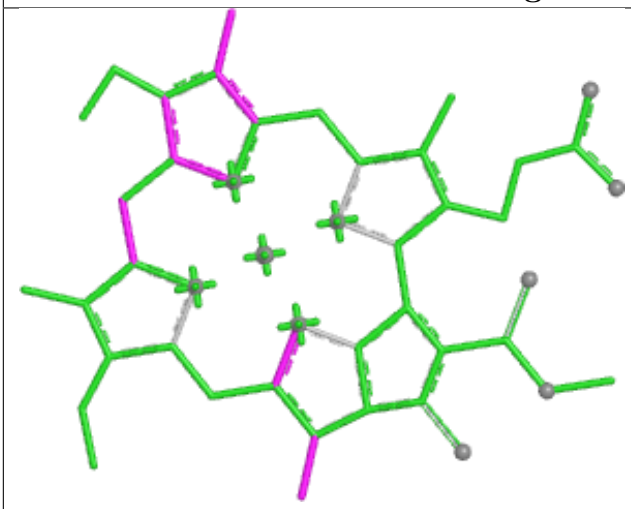


Torsions

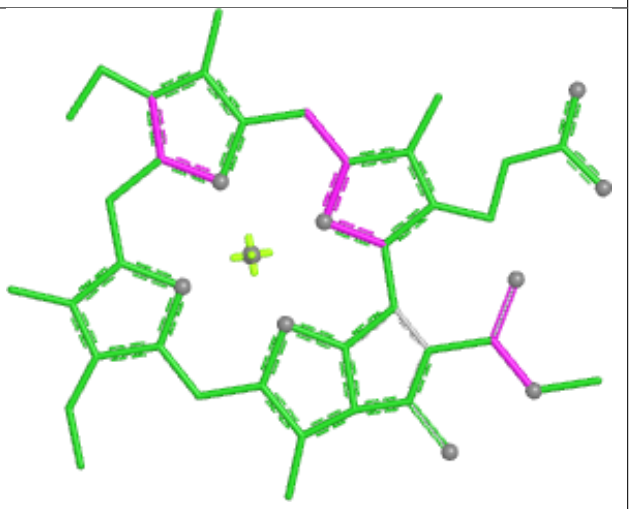


Rings

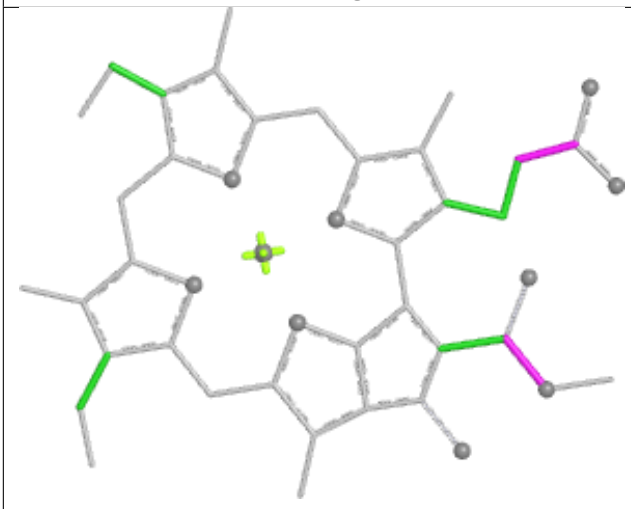
Ligand CLA B 836



Bond lengths



Bond angles

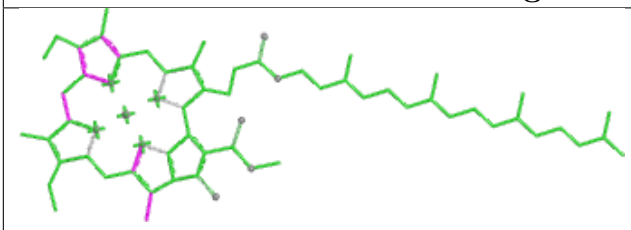


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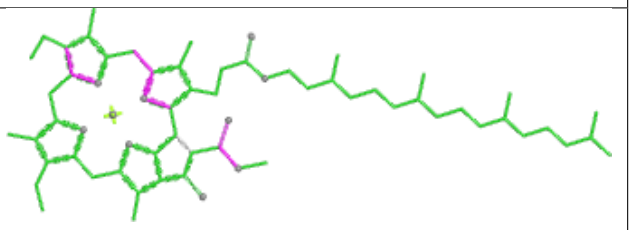


Rings

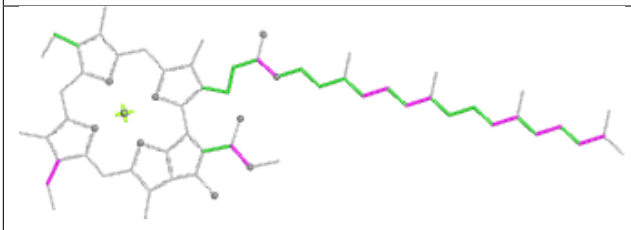
Ligand CLA A 829



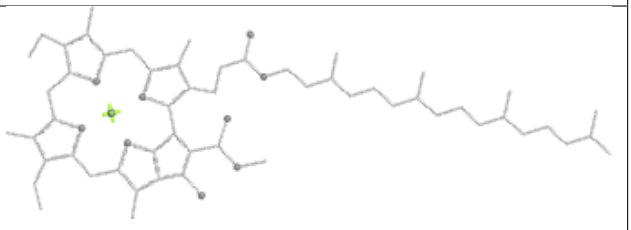
Bond lengths



Bond angles

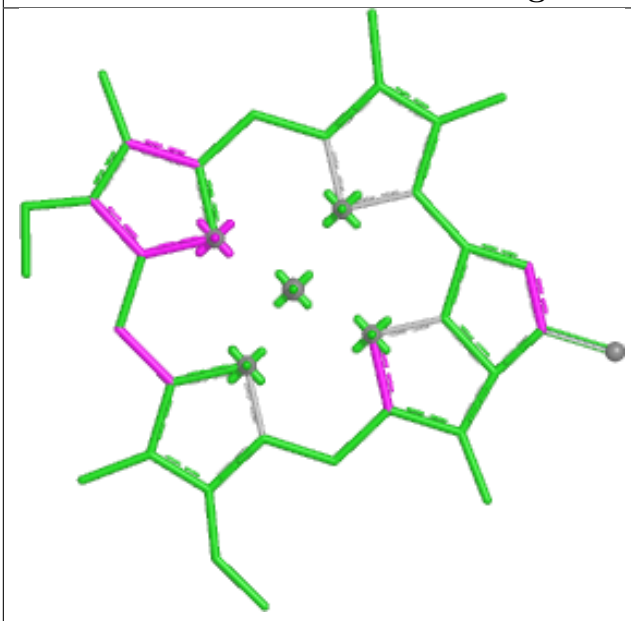


Torsions

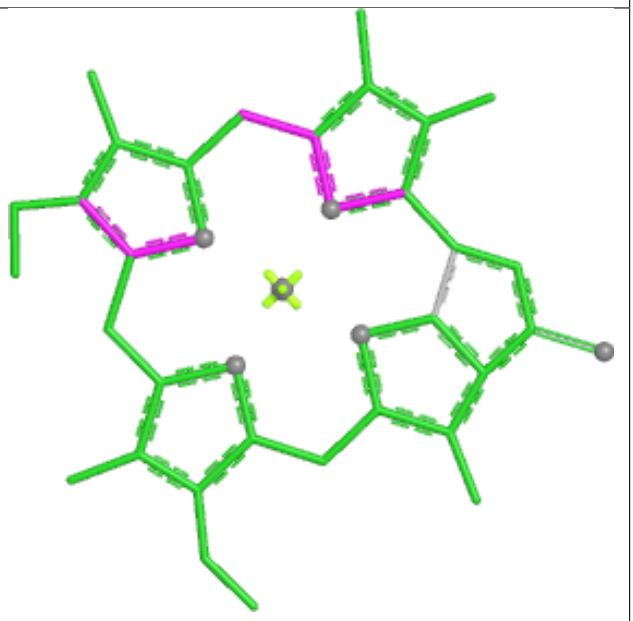


Rings

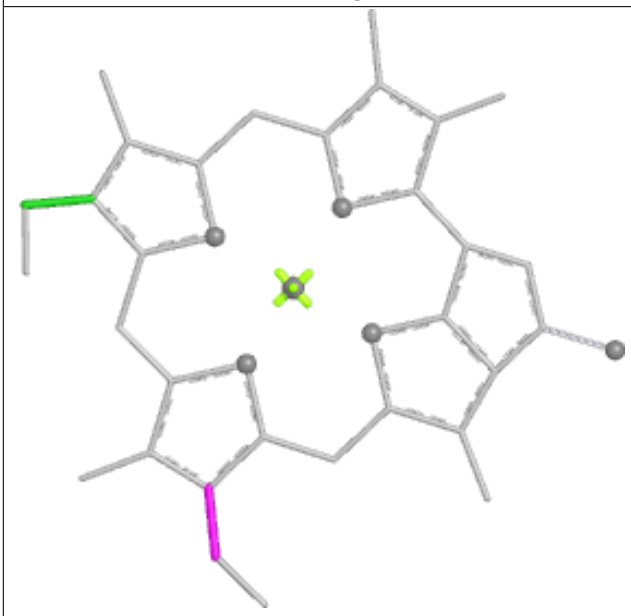
Ligand CLA J 102



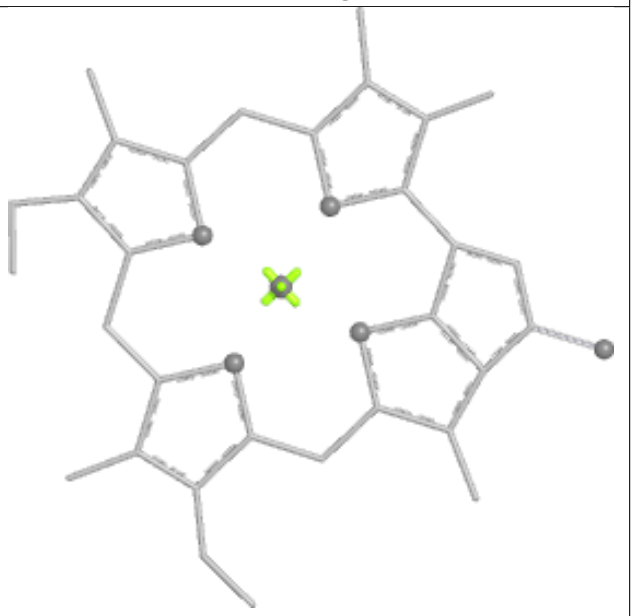
Bond lengths



Bond angles

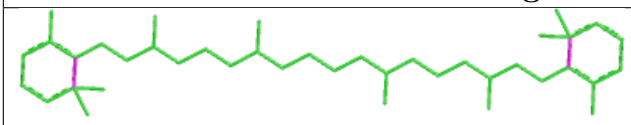


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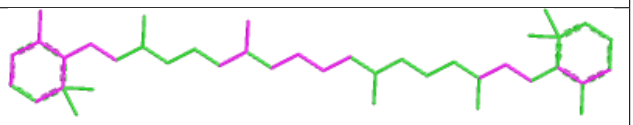


Rings

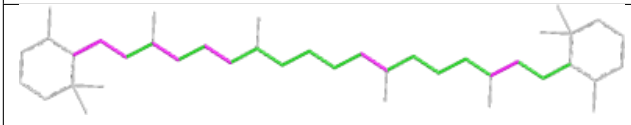
Ligand BCR B 844



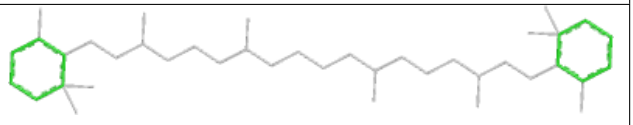
Bond lengths



Bond angles

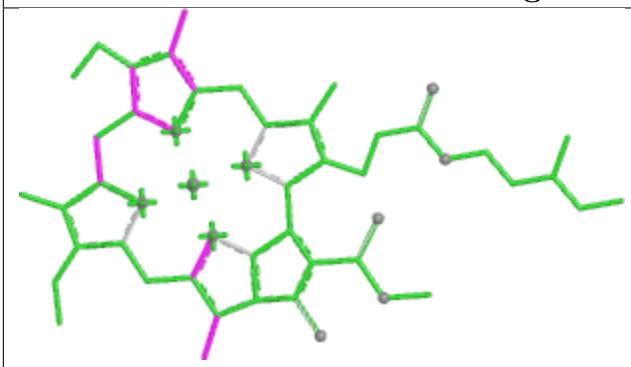


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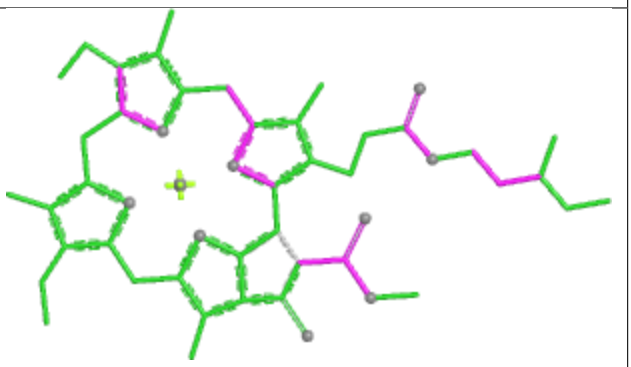


Rings

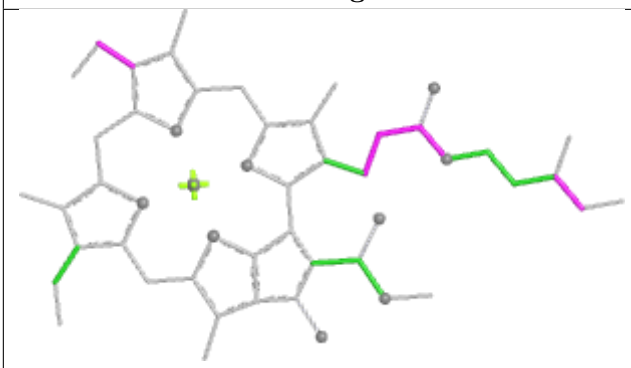
Ligand CLA A 808



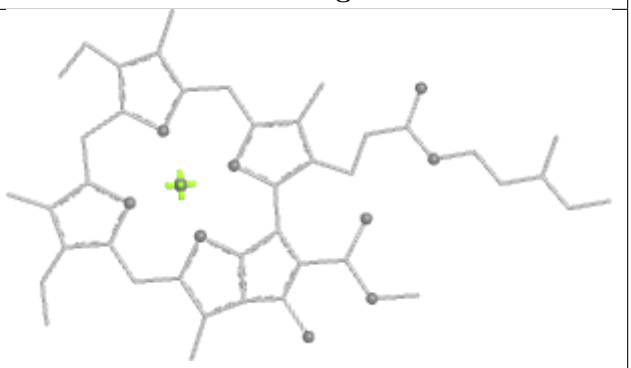
Bond lengths



Bond angles

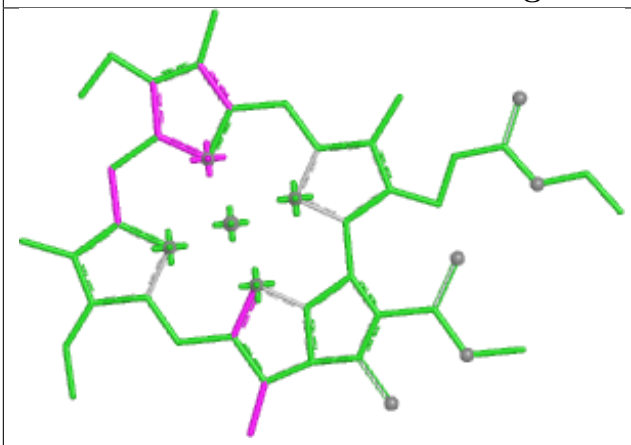


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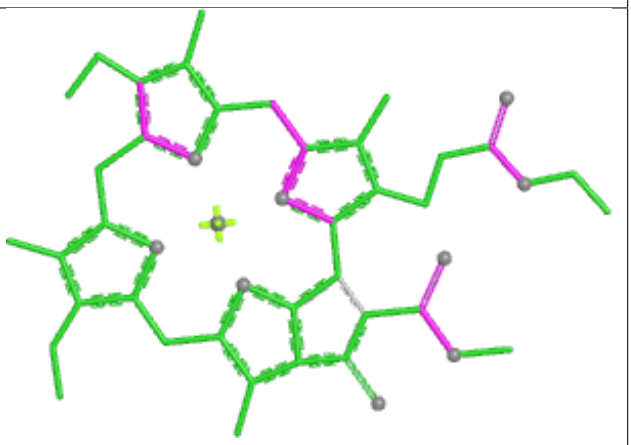


Rings

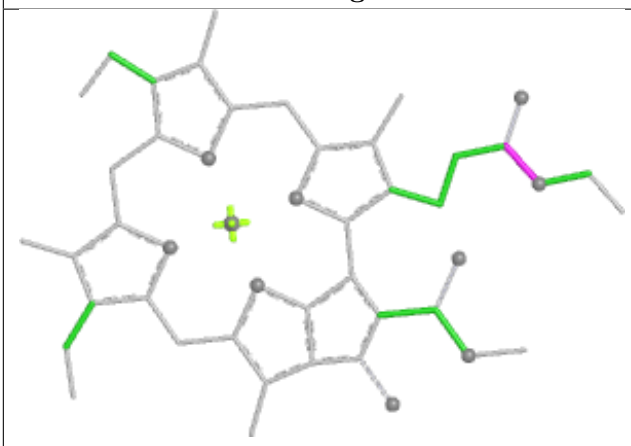
Ligand CLA A 840



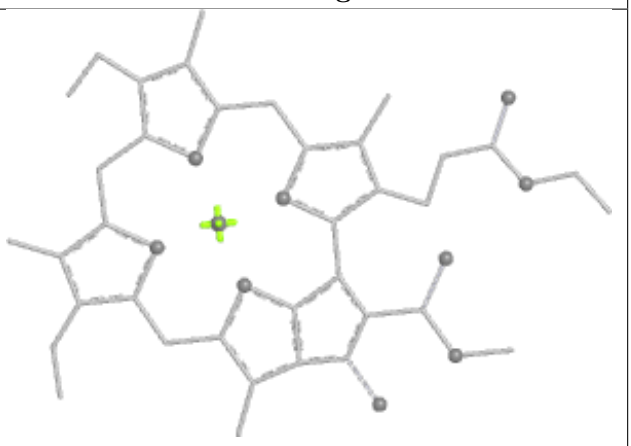
Bond lengths



Bond angles

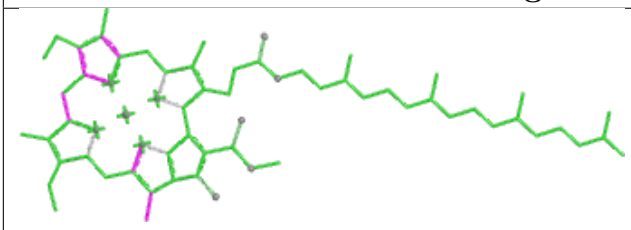


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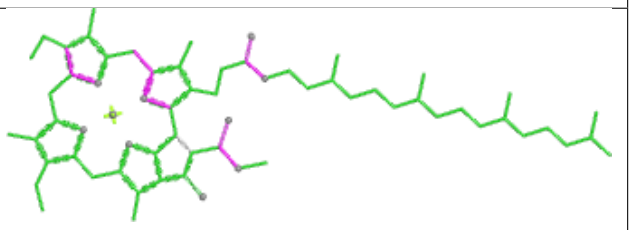


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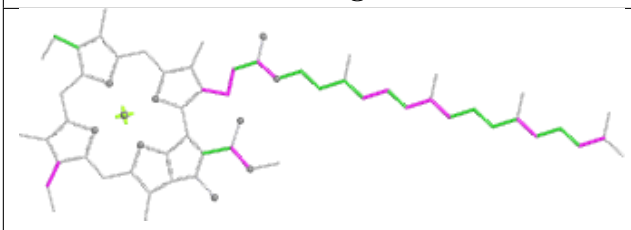
Ligand CLA B 826



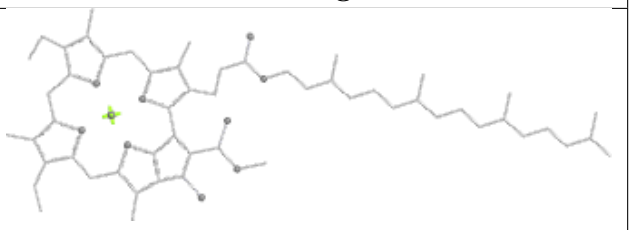
Bond lengths



Bond angles

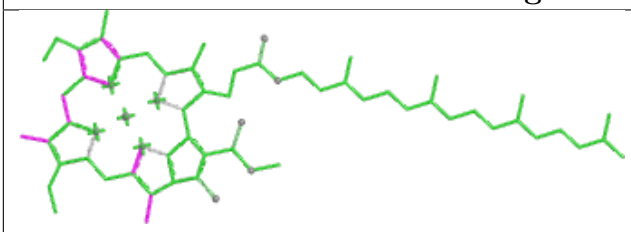


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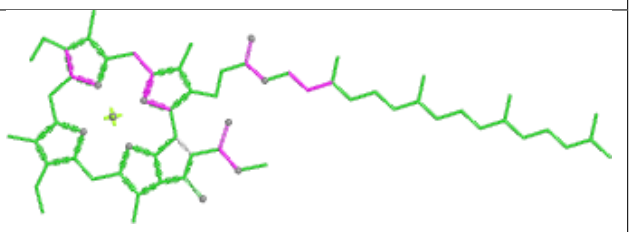


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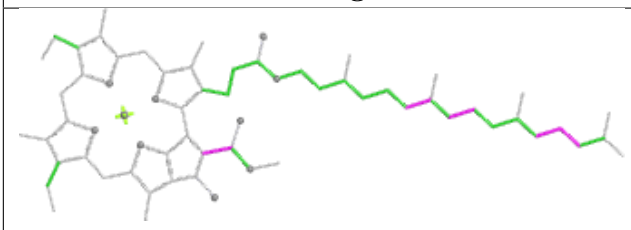
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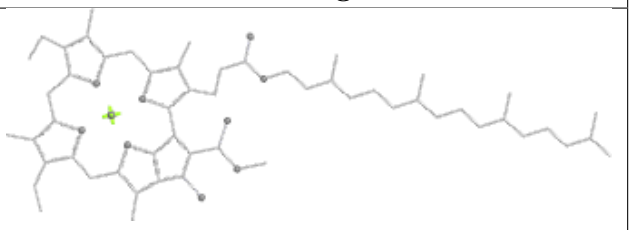
Bond lengths



Bond angles

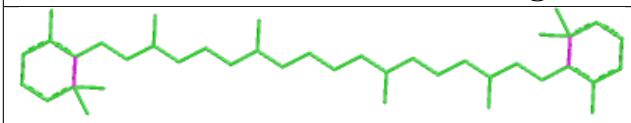


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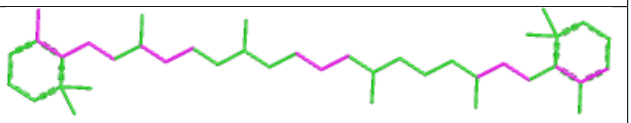


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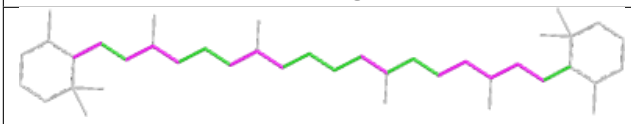
Ligand BCR I 101



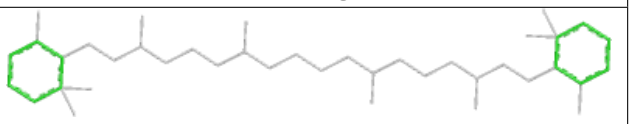
Bond lengths



Bond angles

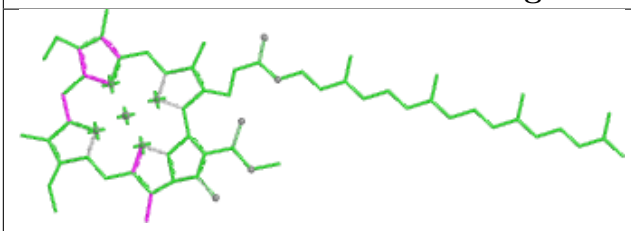


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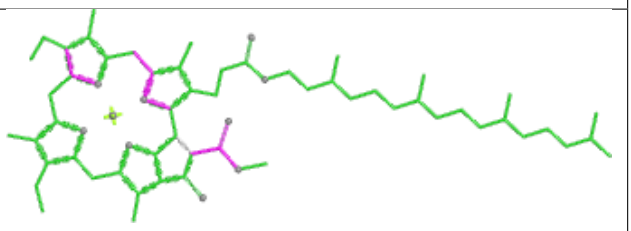


Rings

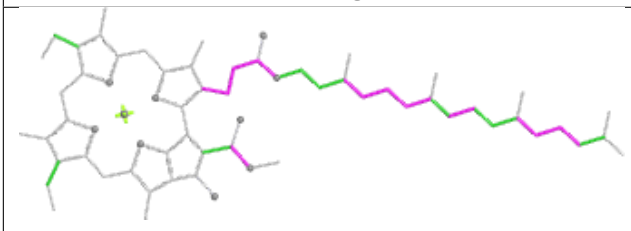
Ligand CLA B 828



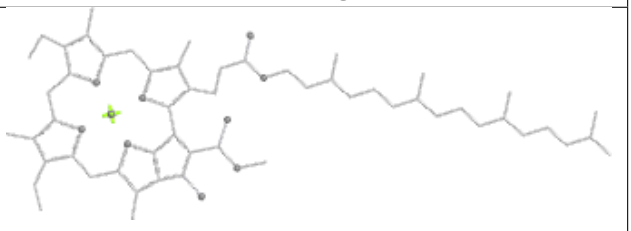
Bond lengths



Bond angles

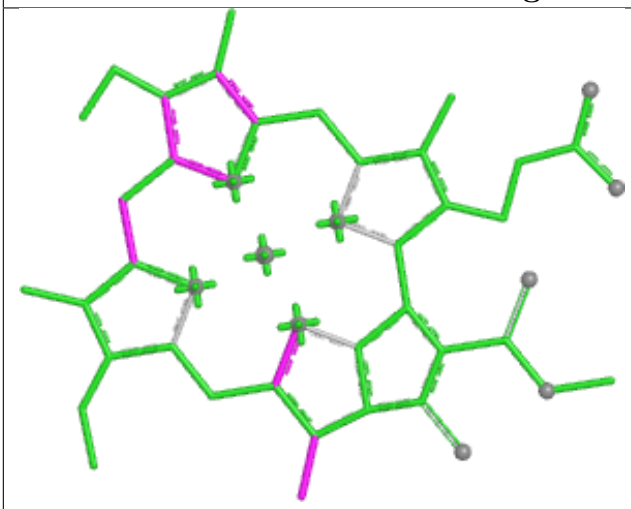


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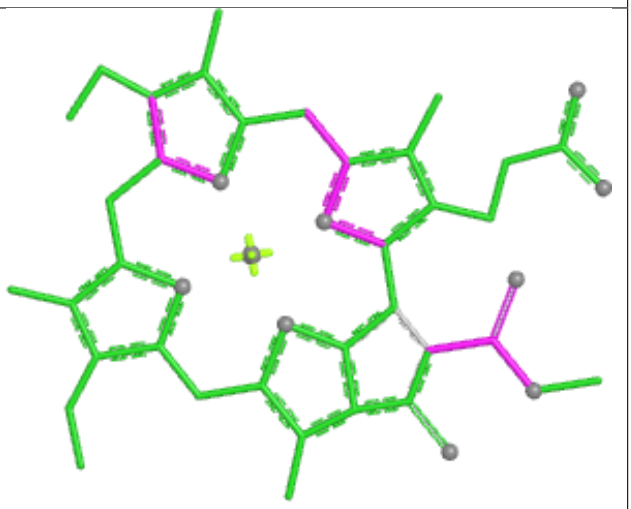


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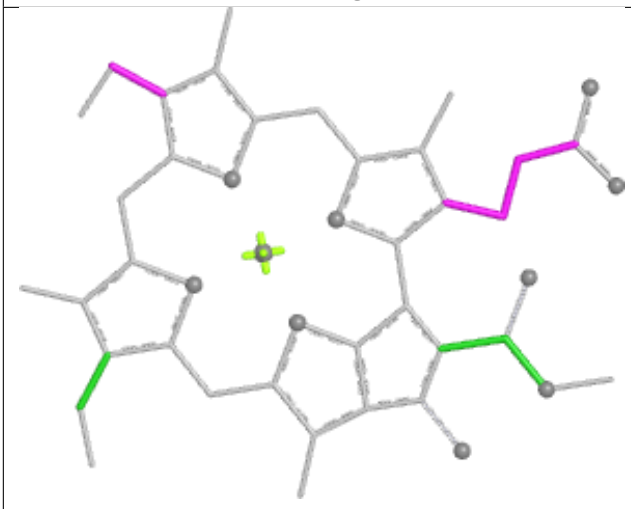
Ligand CLA K 102



Bond lengths



Bond angles

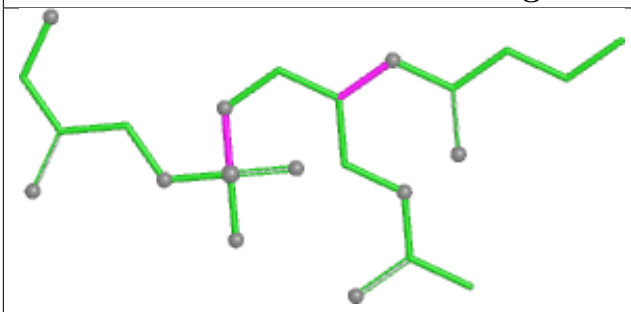


Torsions

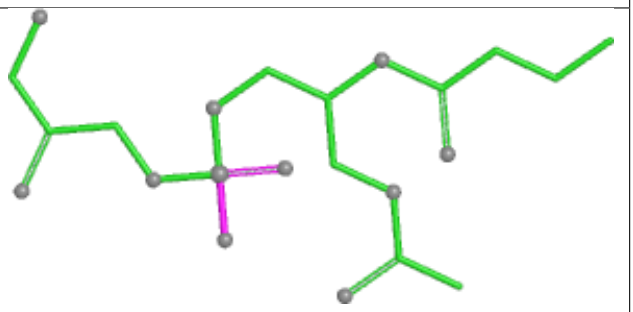


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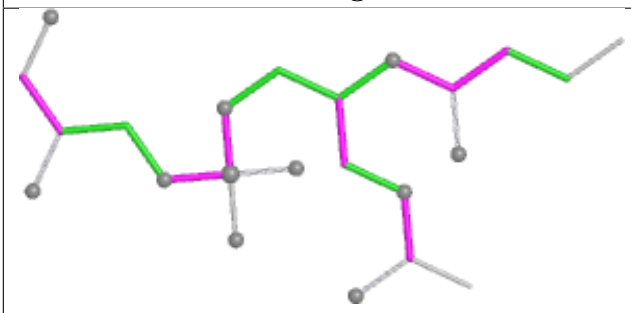
Ligand LHG B 850



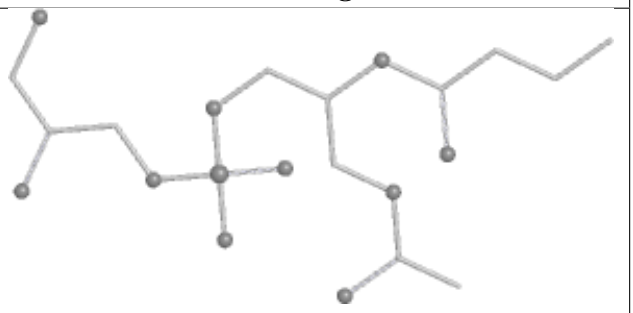
Bond lengths



Bond angles

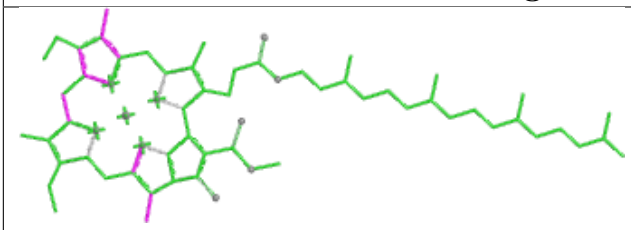


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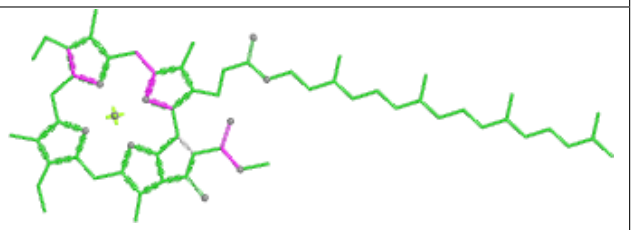


Rings

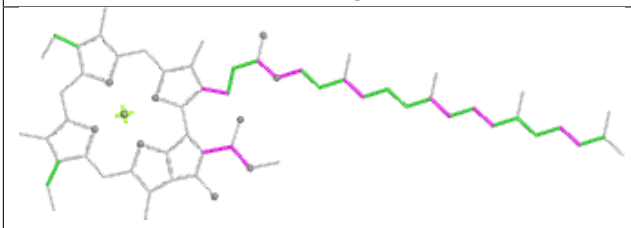
Ligand CLA A 826



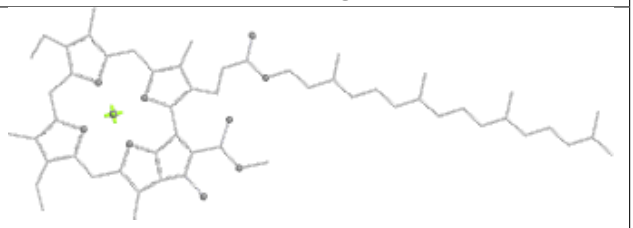
Bond lengths



Bond angles

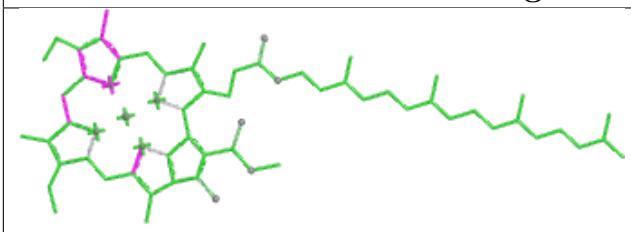


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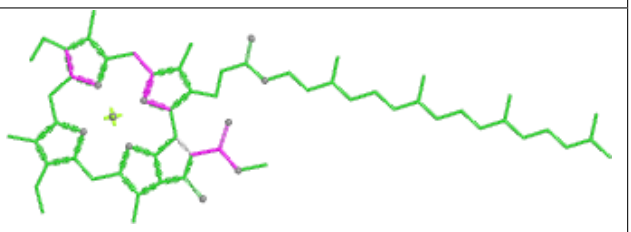


Rings

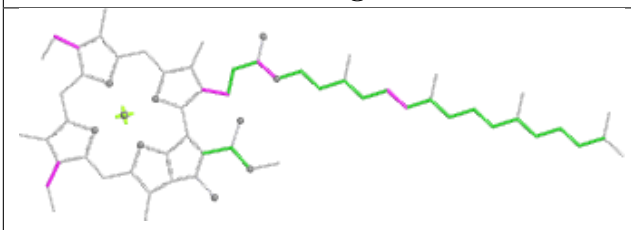
Ligand CLA B 841



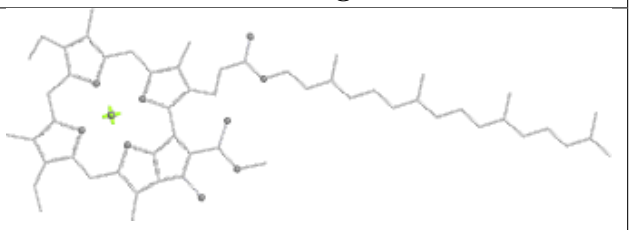
Bond lengths



Bond angles

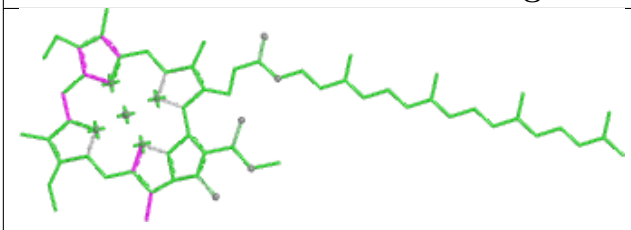


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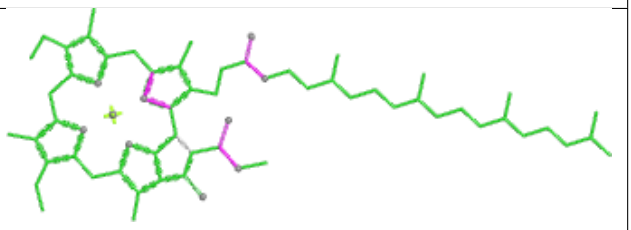


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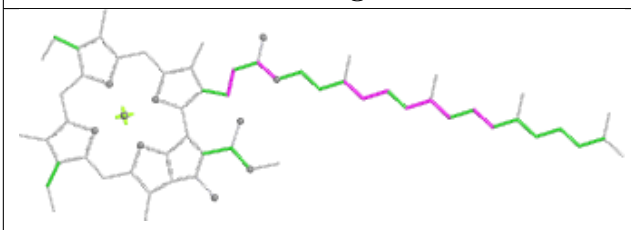
Ligand CLA A 802



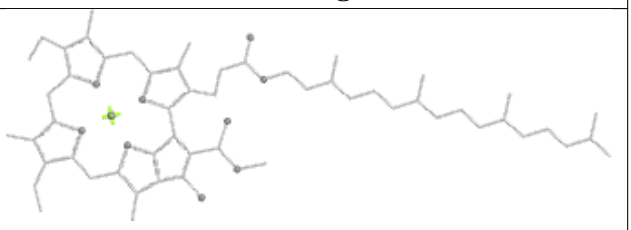
Bond lengths



Bond angles

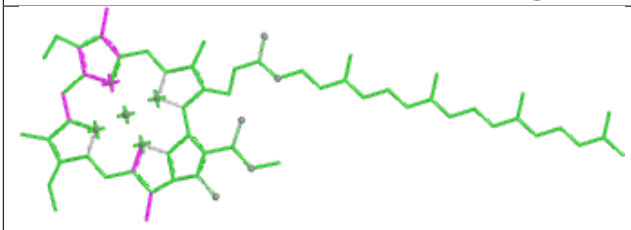


Torsions

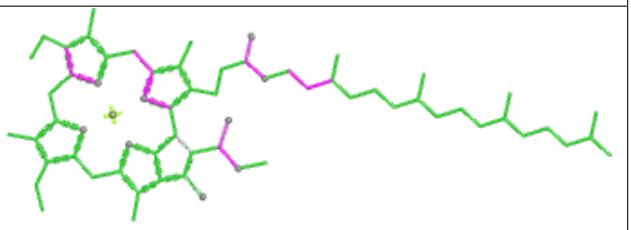


Rings

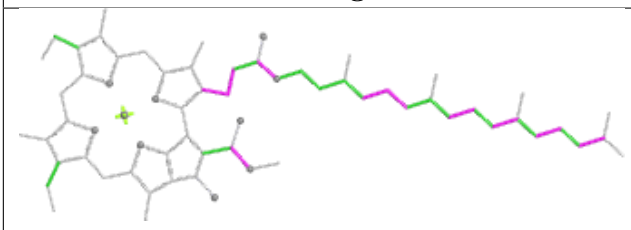
Ligand CL0 A 801



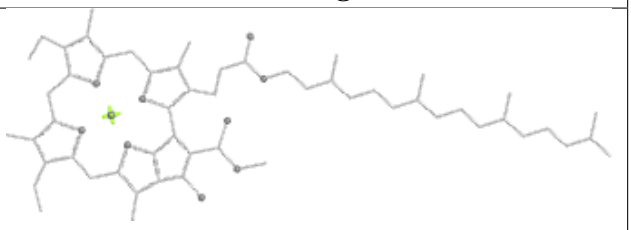
Bond lengths



Bond angles

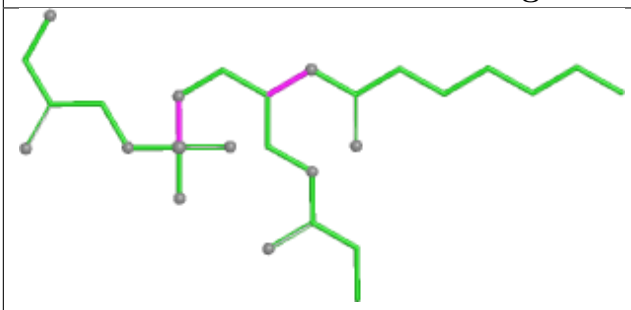


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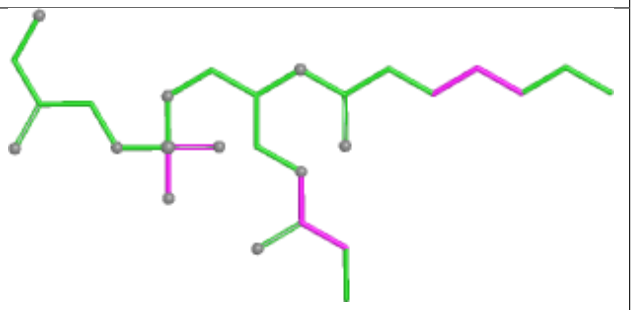


Rings

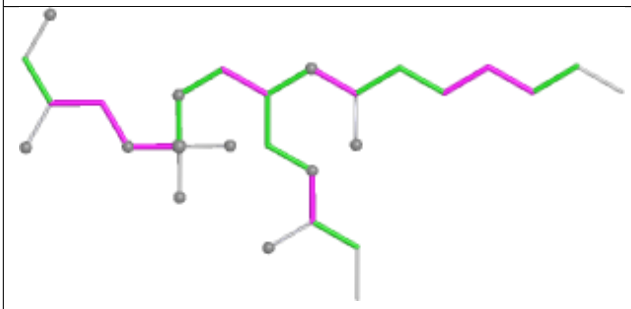
Ligand LHG A 855



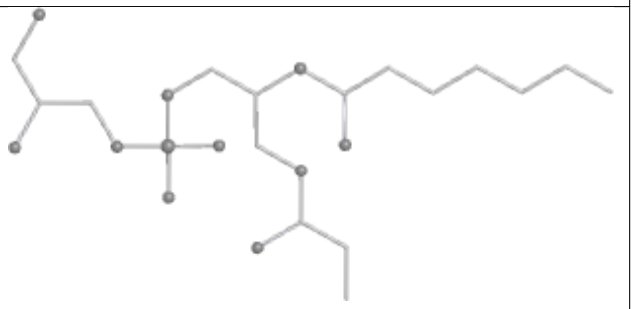
Bond lengths



Bond angles

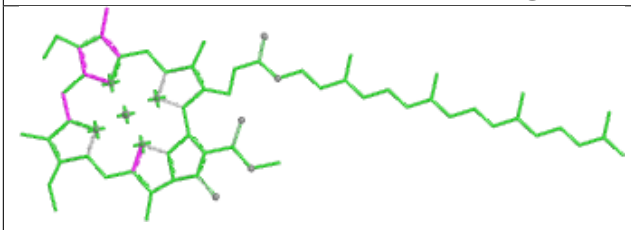


Torsions

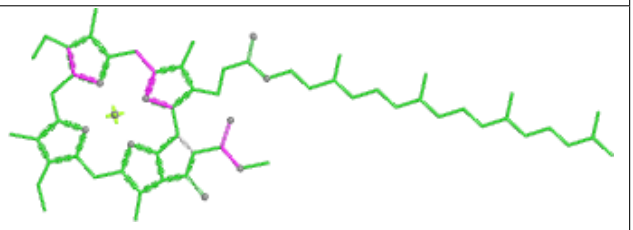


Rings

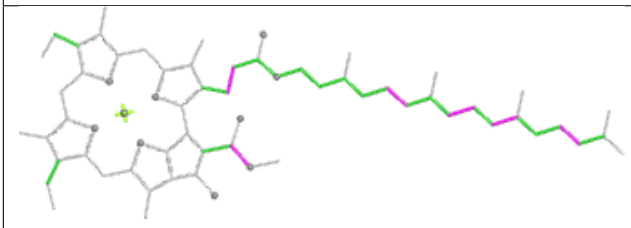
Ligand CLA A 843



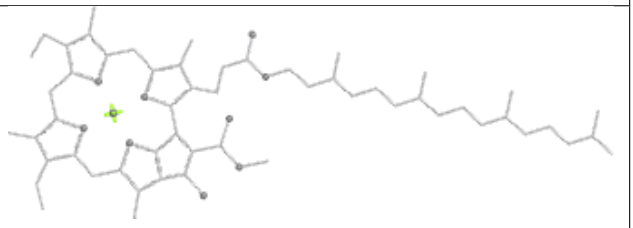
Bond lengths



Bond angles

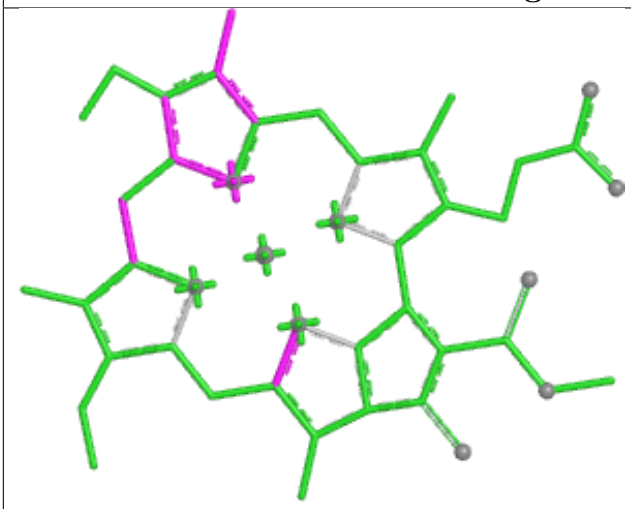


Torsions

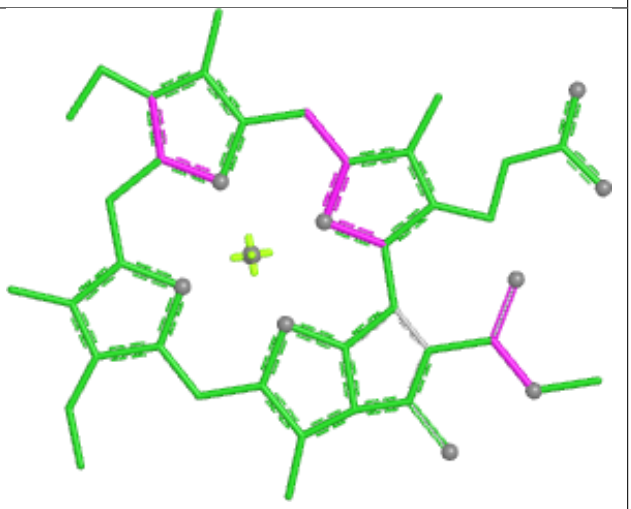


Rings

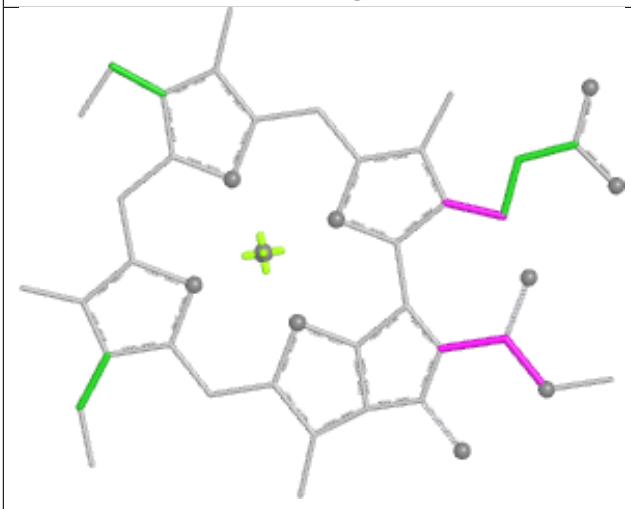
Ligand CLA B 821



Bond lengths



Bond angles

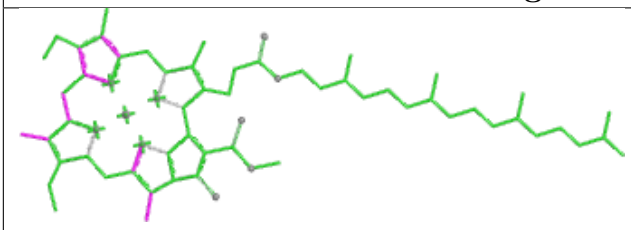


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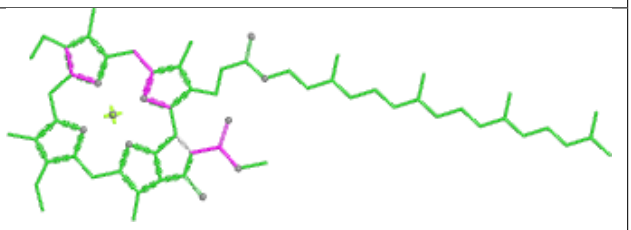


Rings

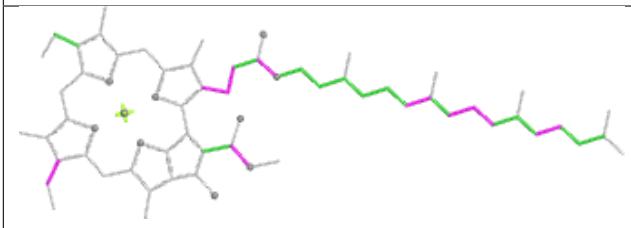
Ligand CLA B 827



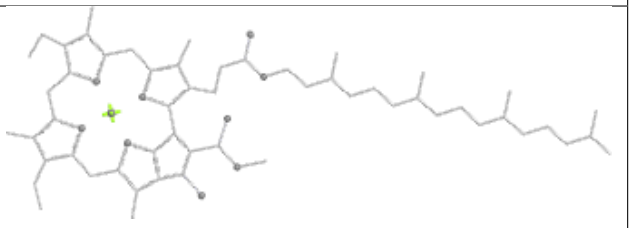
Bond lengths



Bond angles

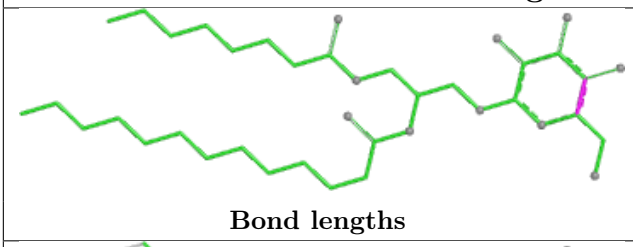


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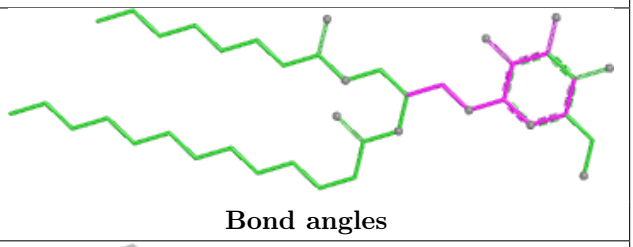


Rings

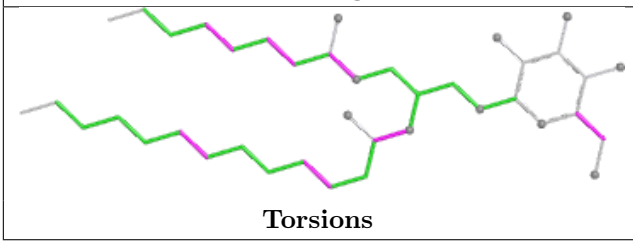
Ligand LMG I 102



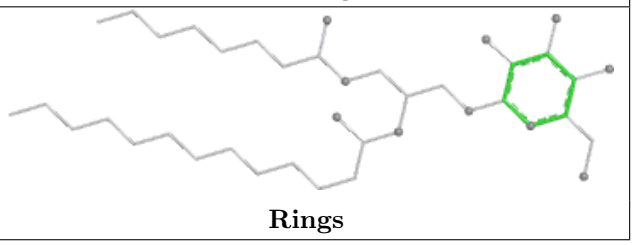
Bond lengths



Bond angles

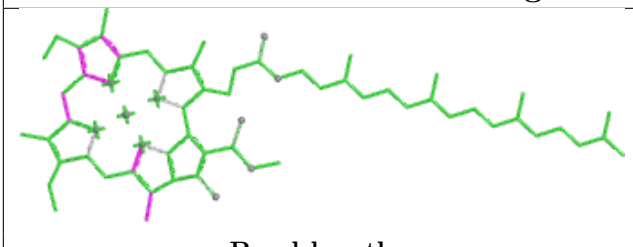


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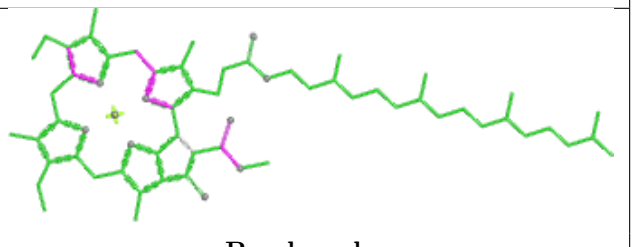


Rings

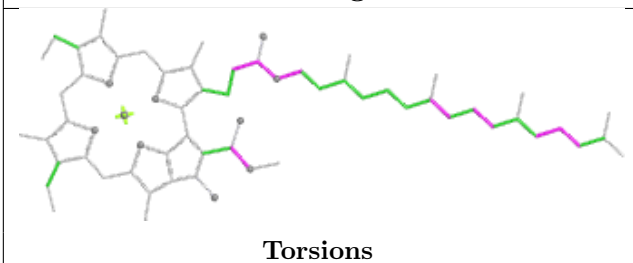
Ligand CLA B 803



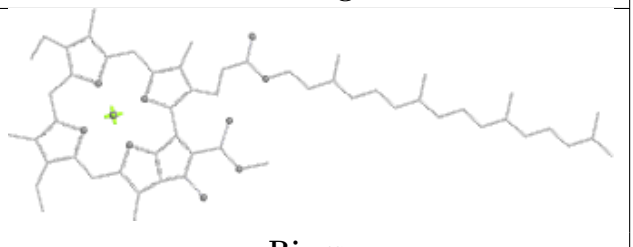
Bond lengths



Bond angles

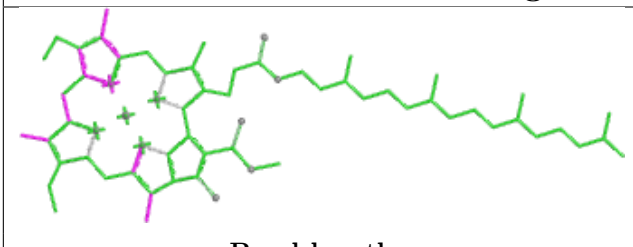


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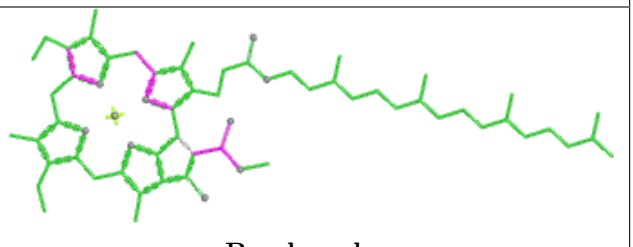


Rings

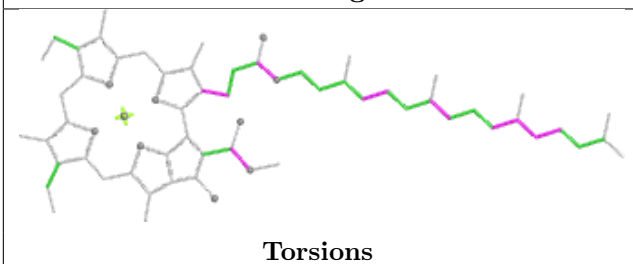
Ligand CLA B 819



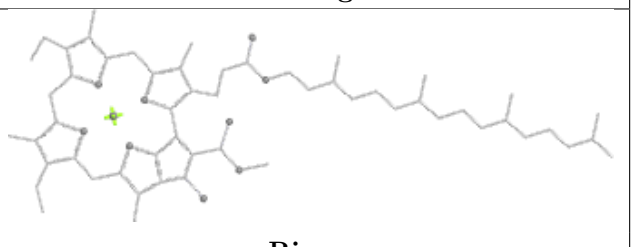
Bond lengths



Bond angles

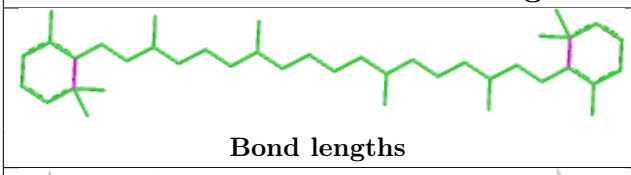


Torsions

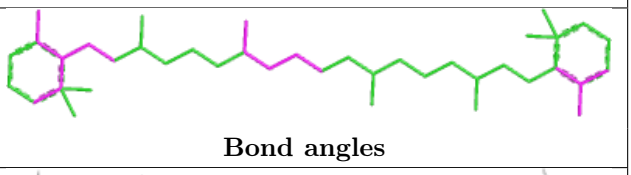


Rings

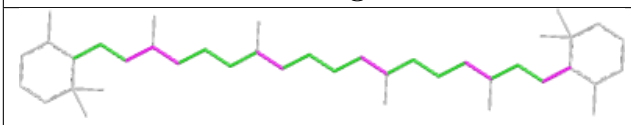
Ligand BCR F 203



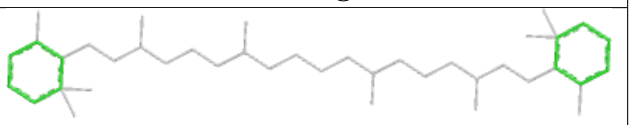
Bond lengths



Bond angles

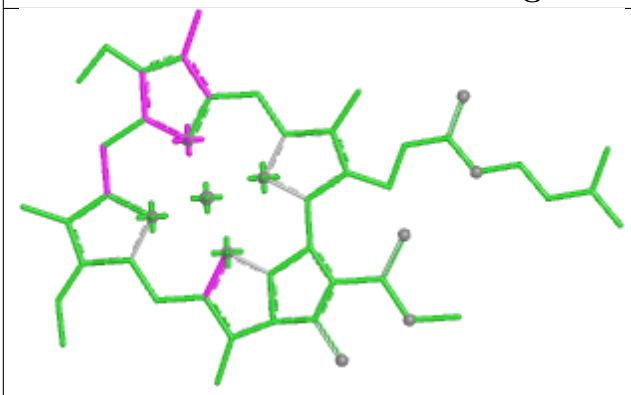


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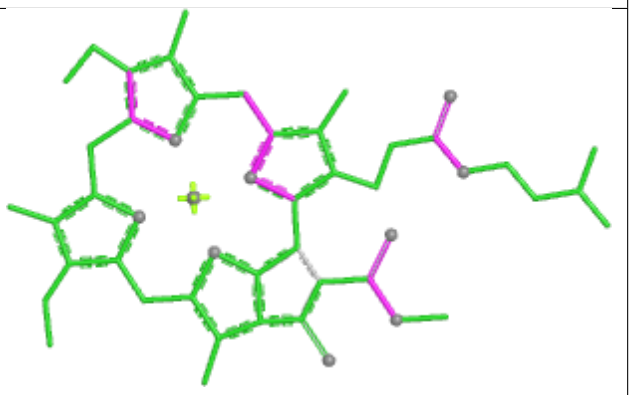


Rings

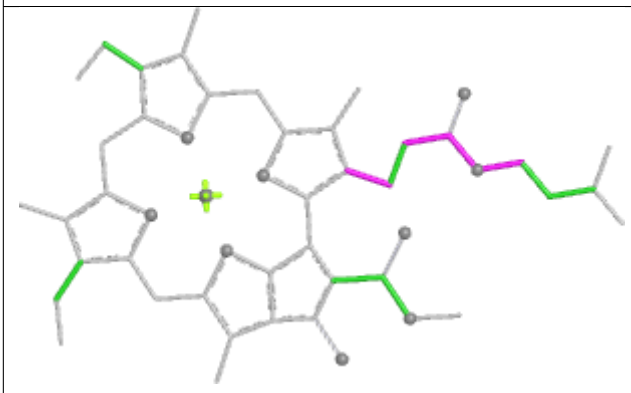
Ligand CLA A 832



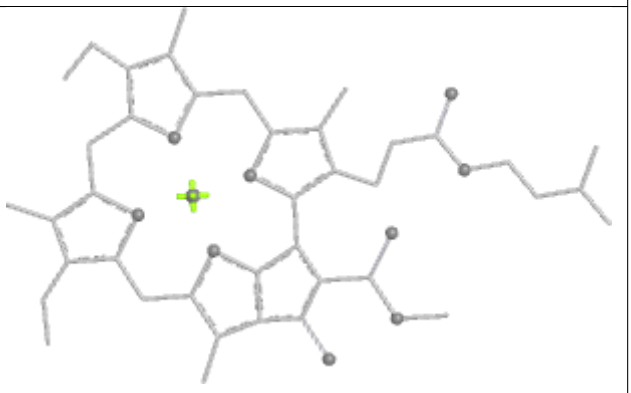
Bond lengths



Bond angles

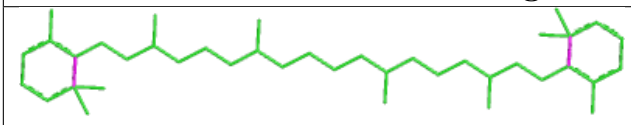


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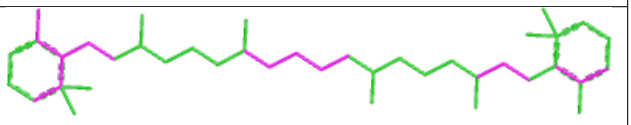


Rings

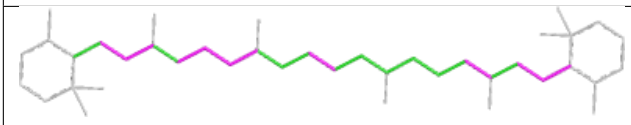
Ligand BCR B 846



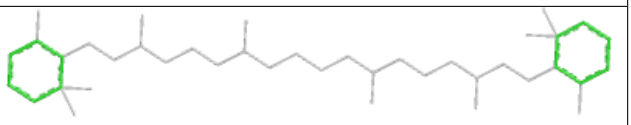
Bond lengths



Bond angles

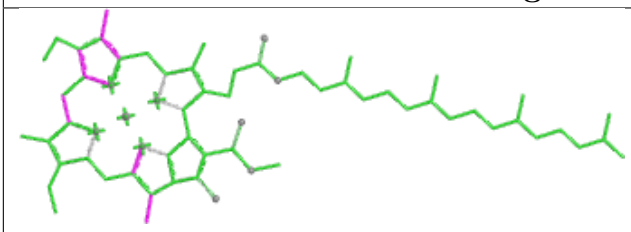


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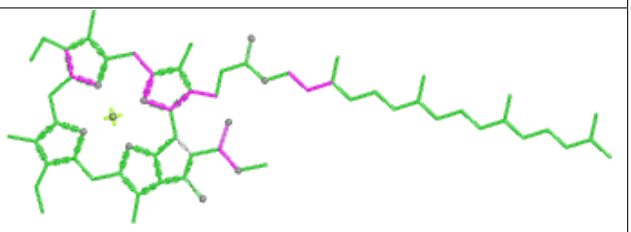


Rings

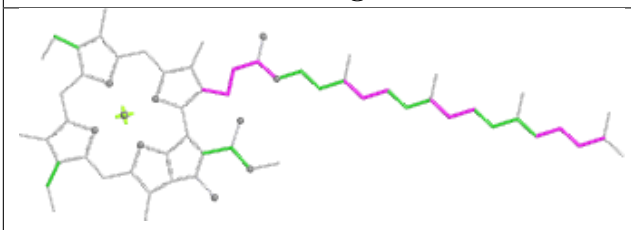
Ligand CLA A 820



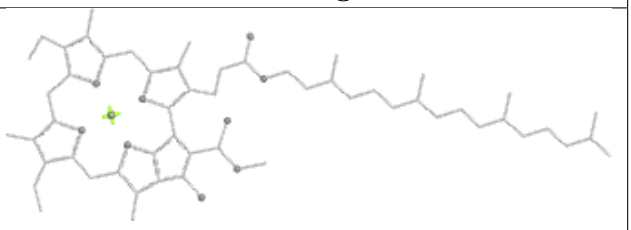
Bond lengths



Bond angles



Torsions

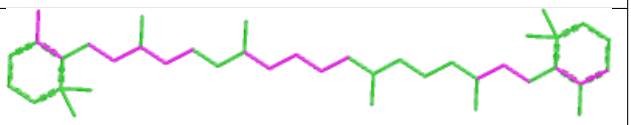


Rings

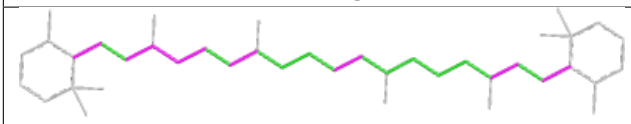
Ligand BCR I 103



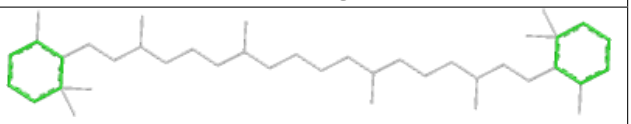
Bond lengths



Bond angles

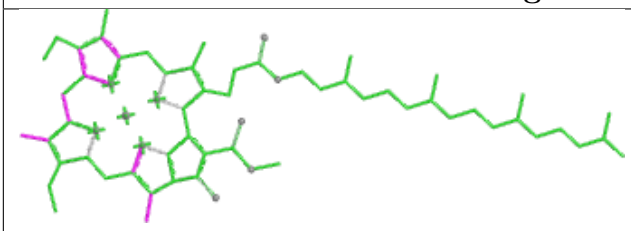


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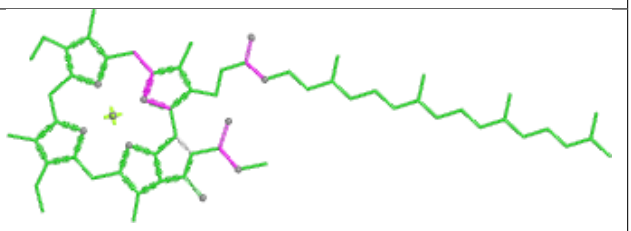


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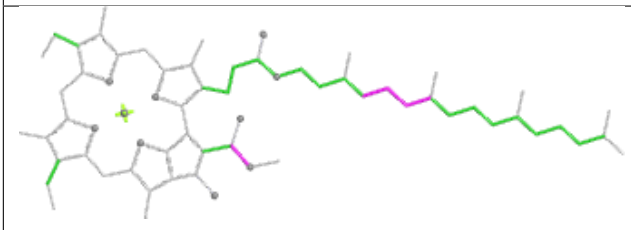
Ligand CLA A 841



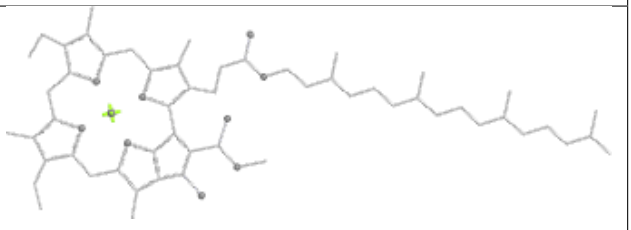
Bond lengths



Bond angles

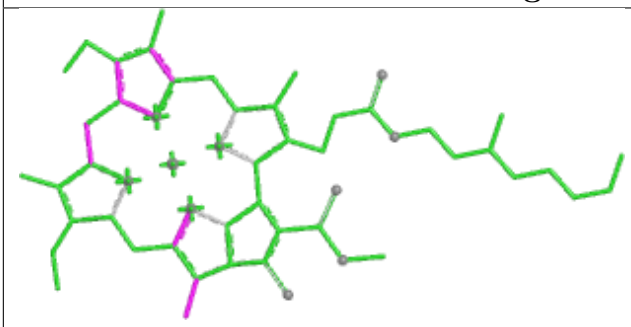


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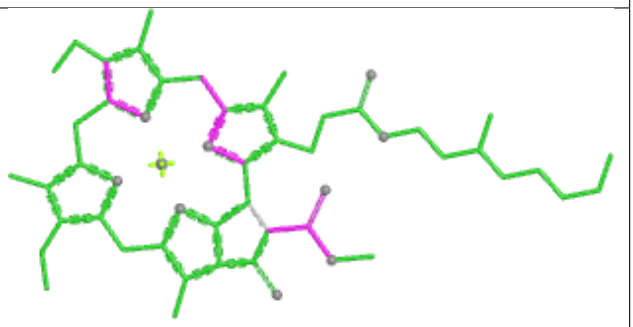


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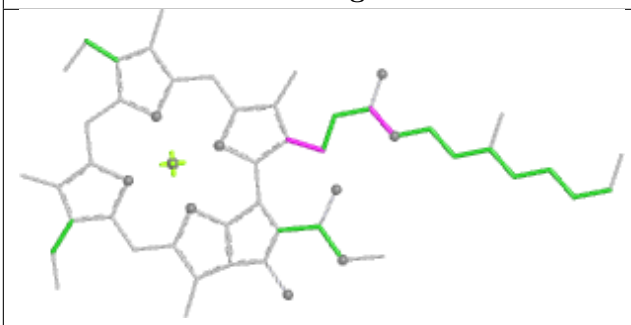
Ligand CLA A 836



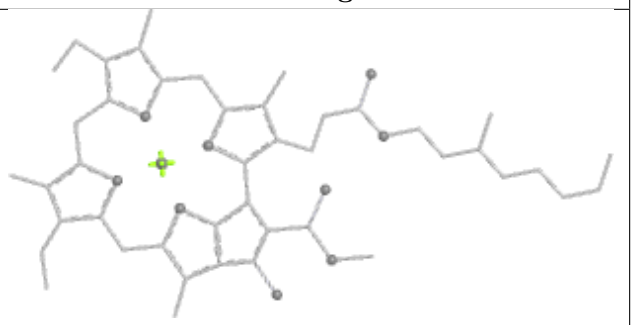
Bond lengths



Bond angles

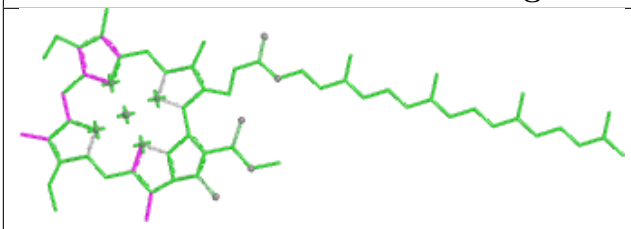


Torsions

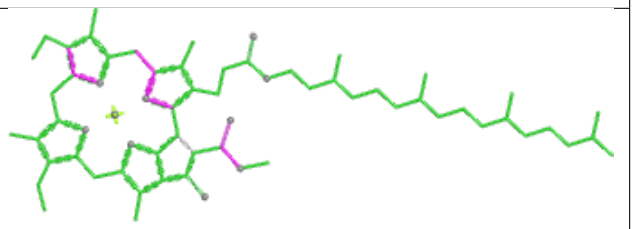


Rings

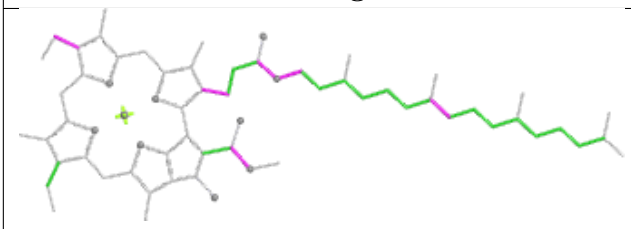
Ligand CLA A 842



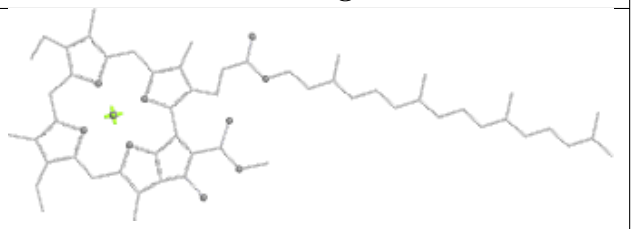
Bond lengths



Bond angles

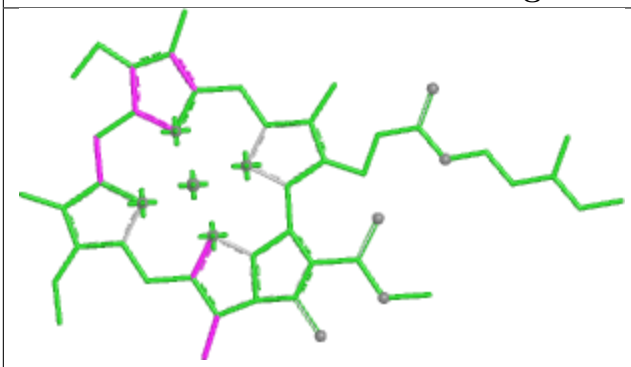


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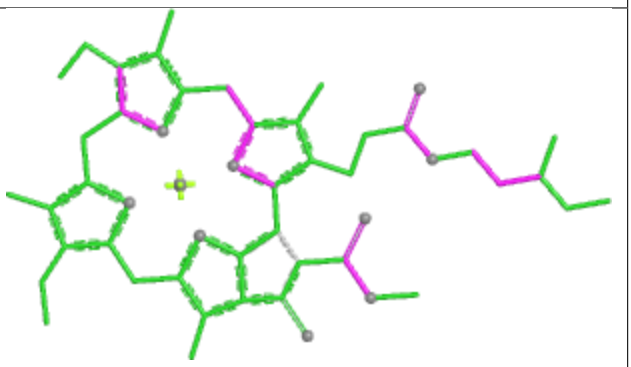


Rings

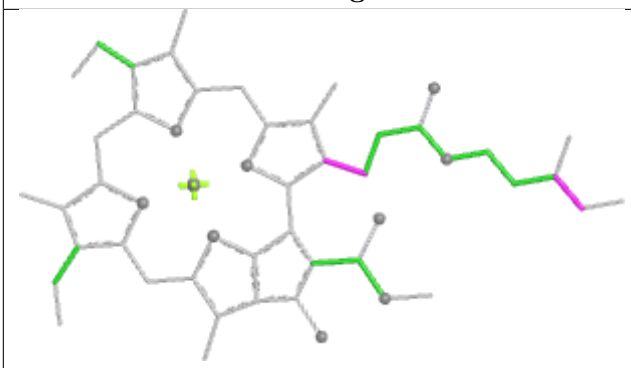
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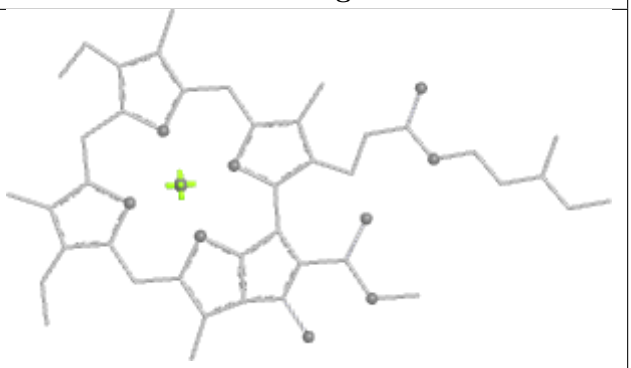
Bond lengths



Bond angles

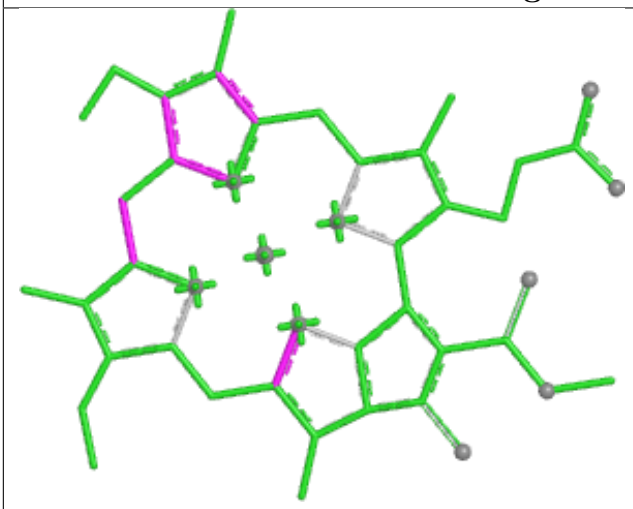


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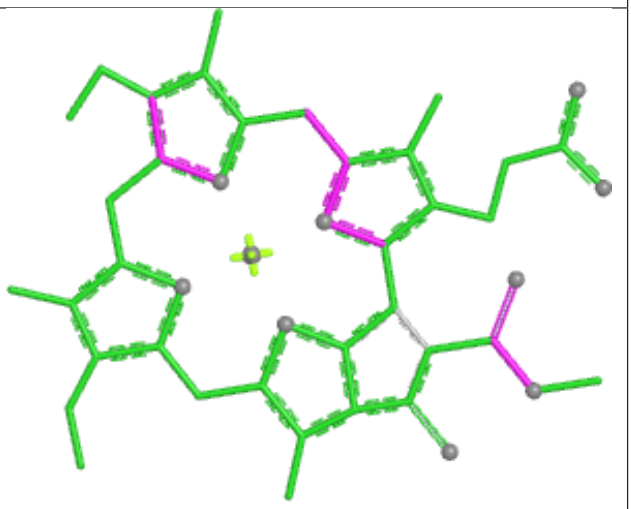


Rings

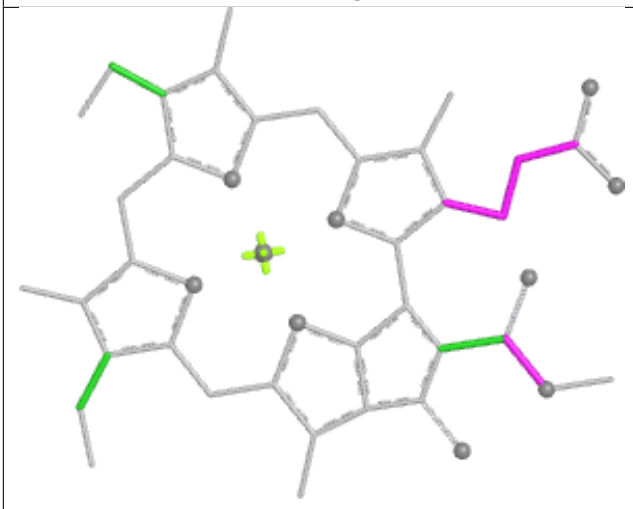
Ligand CLA A 837



Bond lengths



Bond angles

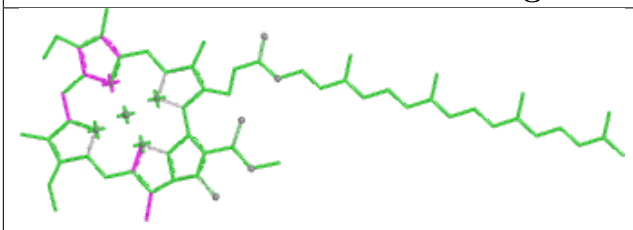


Torsions

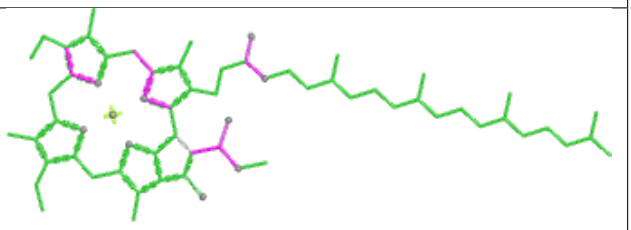


Rings

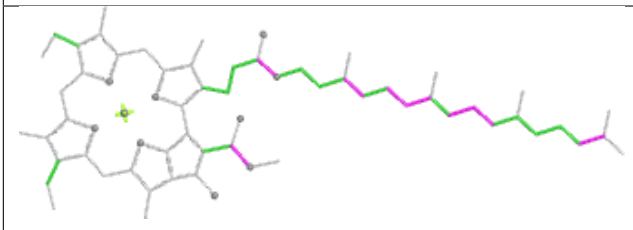
Ligand CLA A 839



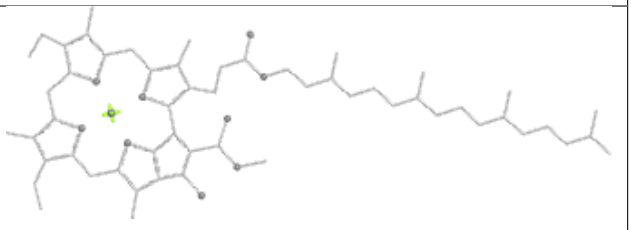
Bond lengths



Bond angles

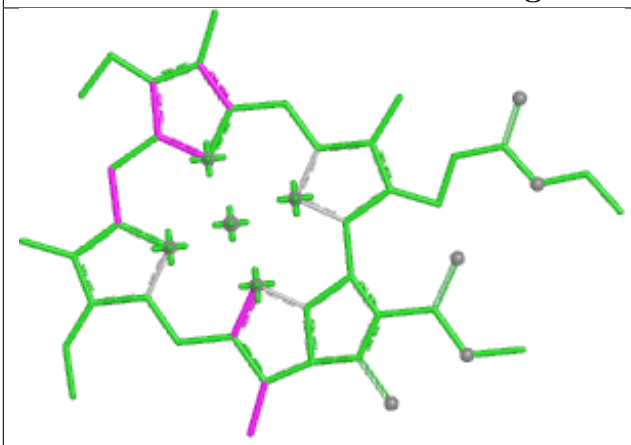


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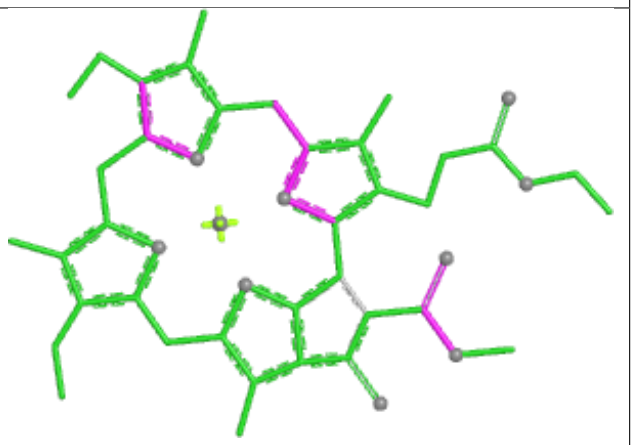


Rings

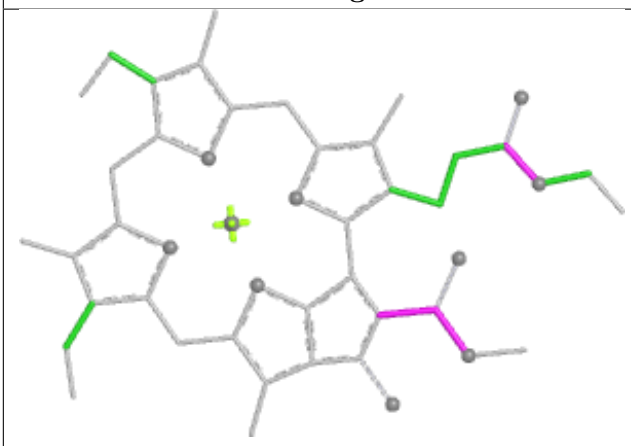
Ligand CLA B 820



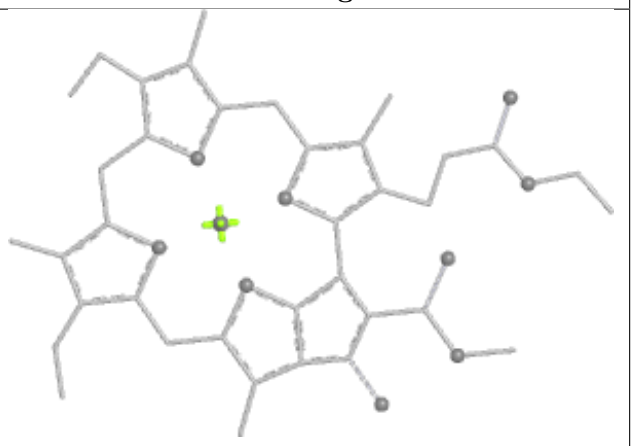
Bond lengths



Bond angles

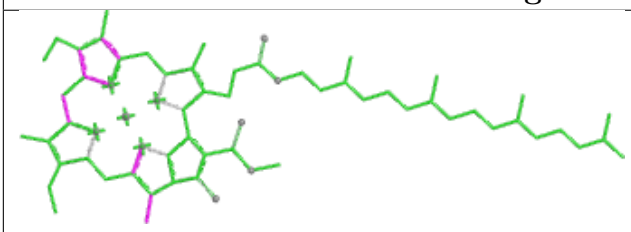


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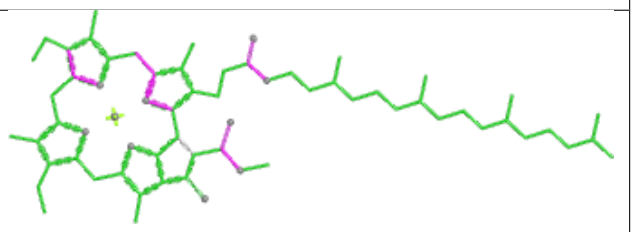


Rings

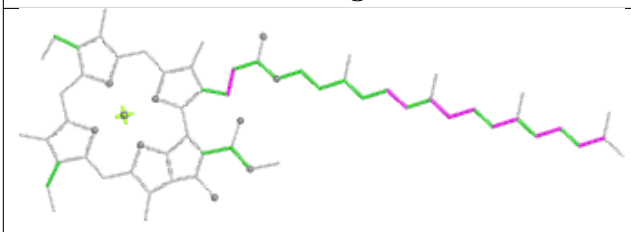
Ligand CLA B 838



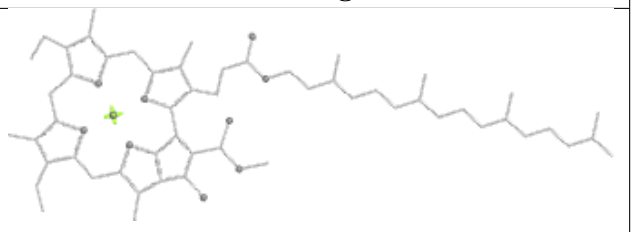
Bond lengths



Bond angles

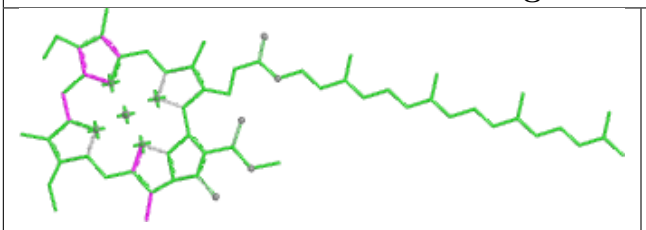


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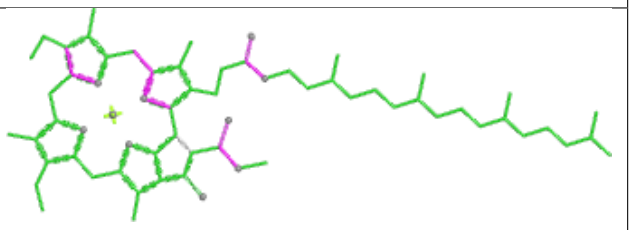


Rings

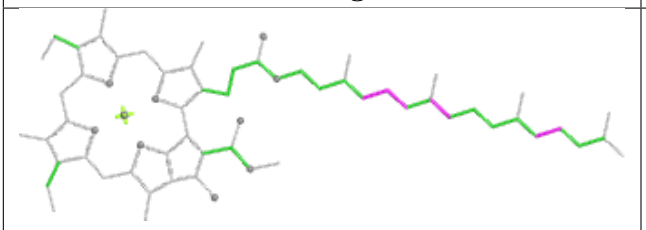
Ligand CLA A 827



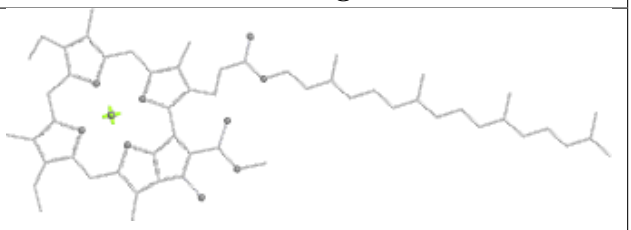
Bond lengths



Bond angles

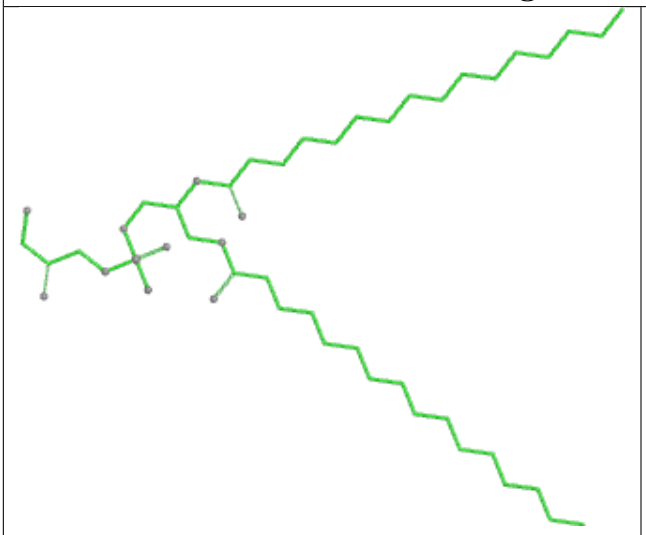


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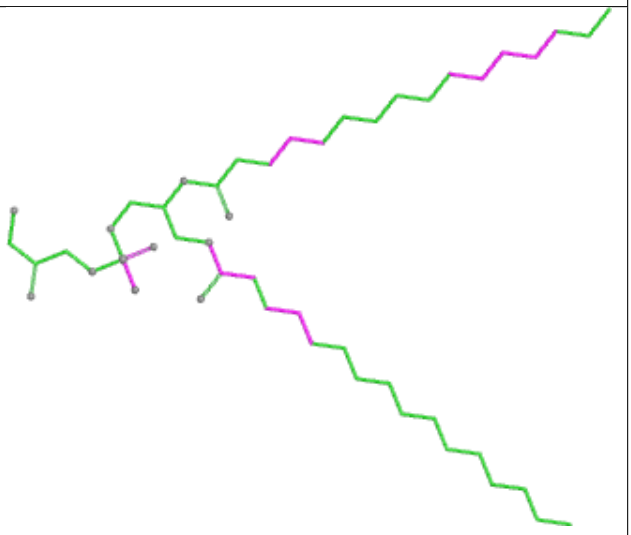


Rings

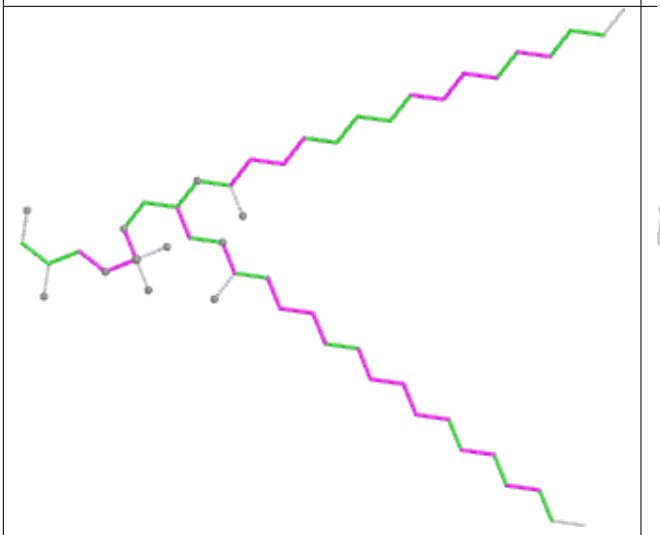
Ligand LHG M 101



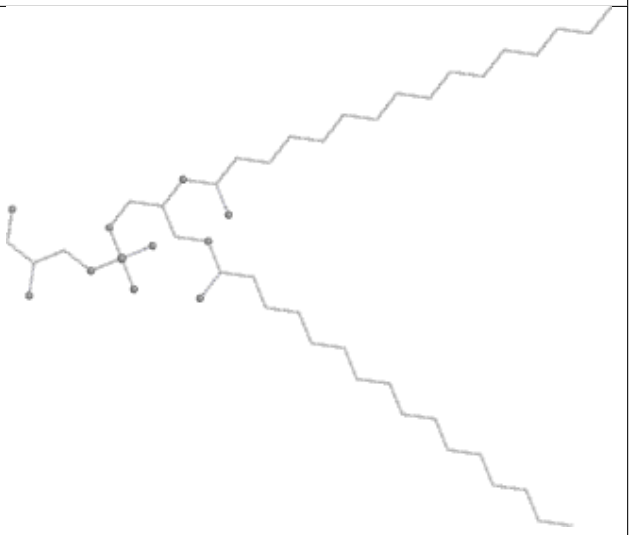
Bond lengths



Bond angles

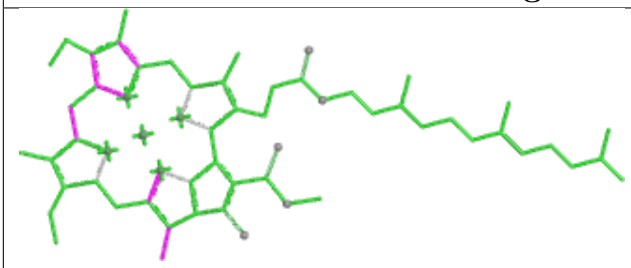


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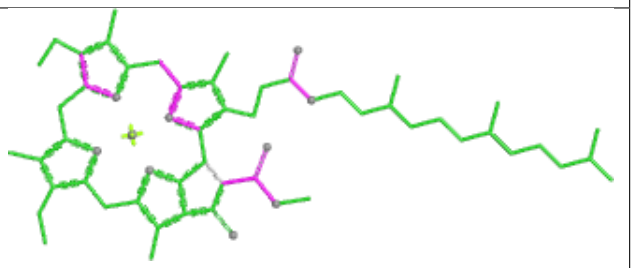


Rings

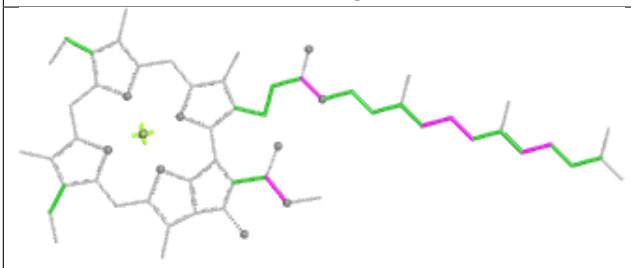
Ligand CLA A 814



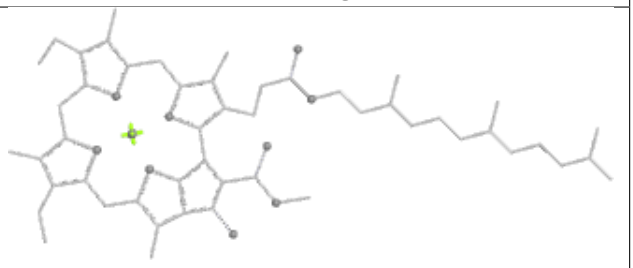
Bond lengths



Bond angles

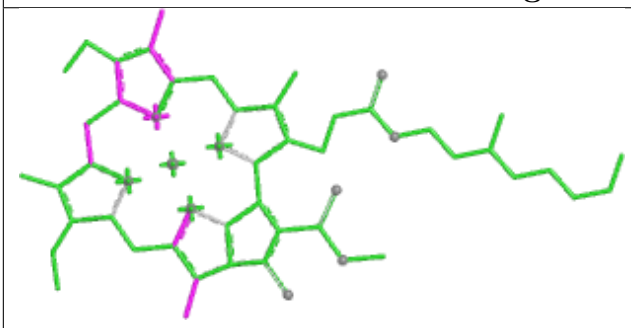


Torsions

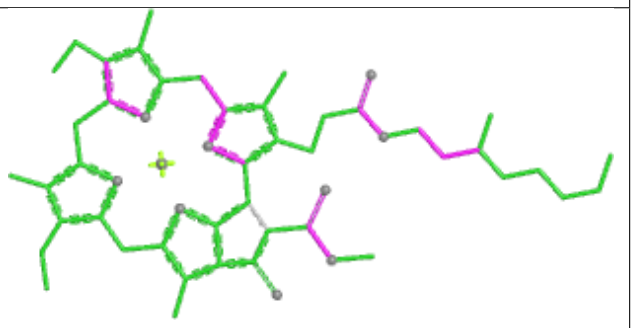


Rings

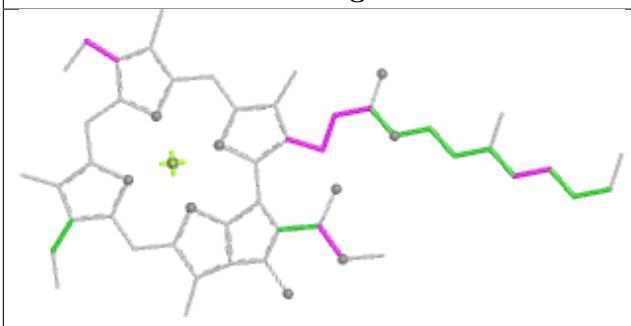
Ligand CLA A 819



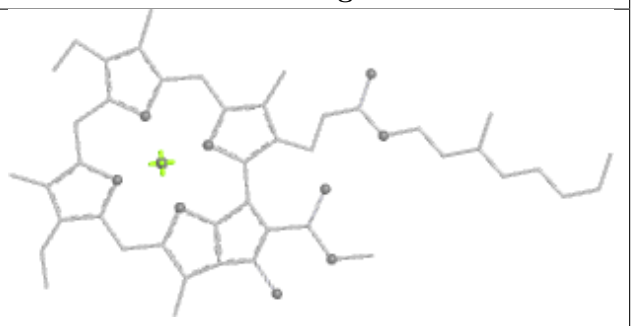
Bond lengths



Bond angles



Torsions

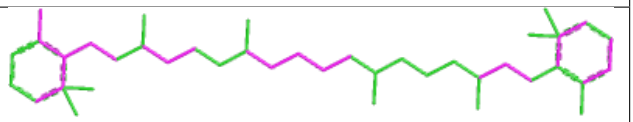


Rings

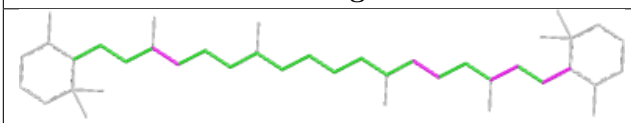
Ligand BCR B 843



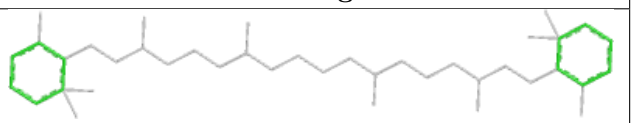
Bond lengths



Bond angles

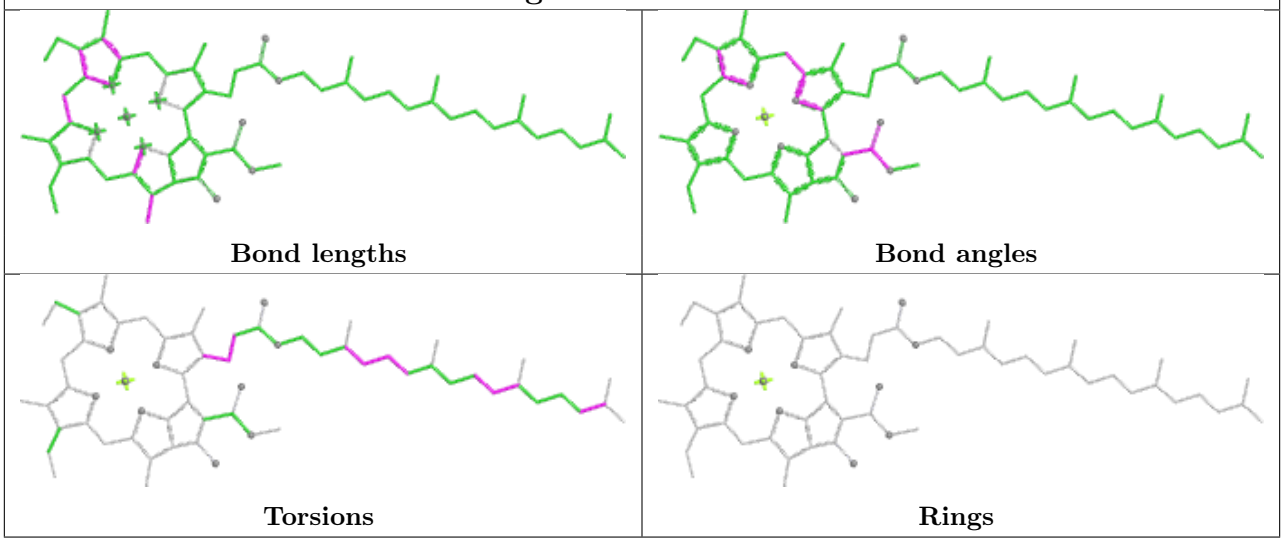


Torsions

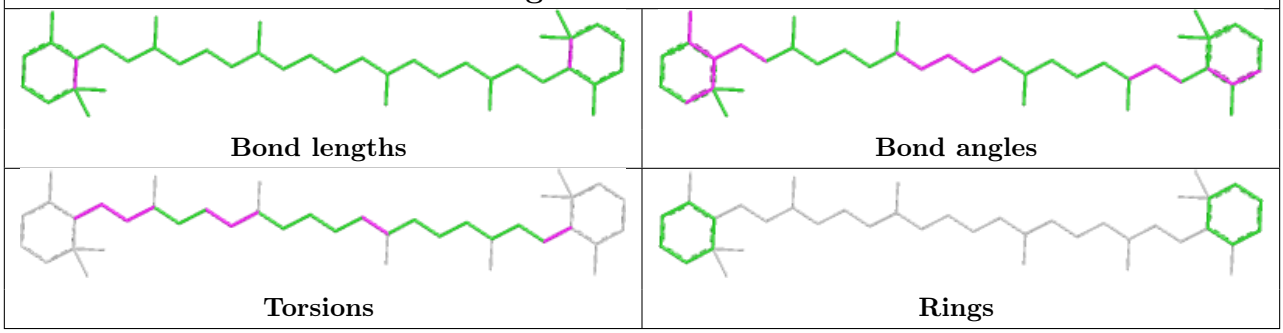


Rings

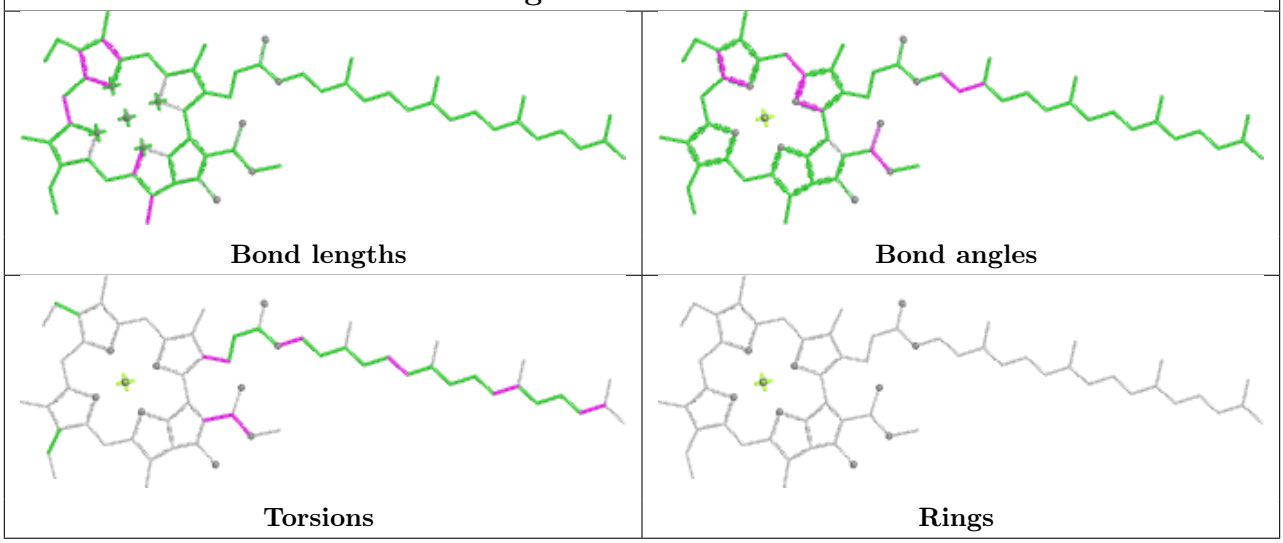
Ligand CLA B 832



Ligand BCR L 208



Ligand CLA A 835



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-0.72	7 (0%) 81 61	3, 61, 113, 158	0
2	B	739/740 (99%)	-1.01	1 (0%) 92 86	2, 34, 80, 114	0
3	C	80/80 (100%)	-1.10	0 100 100	2, 27, 54, 65	0
4	D	138/138 (100%)	-1.10	0 100 100	7, 39, 66, 120	0
5	E	69/75 (92%)	-0.88	0 100 100	27, 56, 78, 94	0
6	F	141/164 (85%)	-0.76	2 (1%) 73 51	27, 80, 99, 107	0
7	I	38/38 (100%)	-1.17	0 100 100	2, 10, 36, 70	0
8	J	41/41 (100%)	-0.81	1 (2%) 59 36	70, 90, 104, 123	0
9	K	47/83 (56%)	-0.61	0 100 100	106, 140, 157, 174	0
10	L	151/154 (98%)	-1.22	0 100 100	2, 10, 46, 94	0
11	M	31/31 (100%)	-1.21	0 100 100	5, 27, 51, 76	0
12	X	29/35 (82%)	-0.97	0 100 100	51, 61, 90, 103	0
All	All	2244/2334 (96%)	-0.91	11 (0%) 87 72	2, 44, 106, 174	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	26	ALA	5.2
1	A	315	TYR	4.4
1	A	114	ALA	3.8
1	A	18	ASN	3.0
1	A	113	SER	3.0
8	J	32	PHE	2.7
2	B	212	LEU	2.6
1	A	278	PHE	2.3
6	F	1	ASP	2.2
1	A	244	LEU	2.1
1	A	194	GLU	2.1

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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
14	CLA	A	816	45/65	0.96	0.10	79,117,143,153	0
14	CLA	A	817	49/65	0.96	0.07	37,101,133,134	0
14	CLA	A	823	49/65	0.96	0.09	52,90,119,131	0
14	CLA	A	824	51/65	0.96	0.08	41,74,106,112	0
14	CLA	A	828	65/65	0.96	0.11	33,66,102,109	0
14	CLA	B	820	47/65	0.96	0.07	43,72,103,108	0
14	CLA	J	101	45/65	0.96	0.09	91,111,145,149	0
14	CLA	J	102	37/65	0.96	0.09	76,99,123,137	0
17	BCR	B	843	40/40	0.96	0.13	49,84,117,135	0
18	LMG	A	856	30/55	0.96	0.10	6,57,119,135	0
18	LMG	I	102	40/55	0.96	0.11	23,59,94,118	0
14	CLA	B	811	45/65	0.97	0.07	18,41,61,84	0
14	CLA	B	816	55/65	0.97	0.08	35,70,107,140	0
14	CLA	B	817	59/65	0.97	0.09	21,55,83,91	0
14	CLA	B	819	65/65	0.97	0.09	22,65,95,106	0
14	CLA	A	818	54/65	0.97	0.08	69,98,125,135	0
14	CLA	B	833	58/65	0.97	0.09	36,72,110,115	0
14	CLA	B	837	60/65	0.97	0.09	15,55,86,96	0
14	CLA	A	814	60/65	0.97	0.10	47,88,113,115	0
14	CLA	A	811	45/65	0.97	0.06	66,99,125,133	0
14	CLA	K	101	41/65	0.97	0.07	86,123,158,168	0
14	CLA	K	102	45/65	0.97	0.08	75,105,138,139	0
14	CLA	M	102	45/65	0.97	0.12	57,105,140,154	0
17	BCR	A	847	40/40	0.97	0.11	81,120,140,149	0
17	BCR	A	848	40/40	0.97	0.10	70,105,135,149	0
17	BCR	A	850	40/40	0.97	0.09	35,65,129,131	0
14	CLA	A	813	54/65	0.97	0.07	47,74,102,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	BCR	B	844	40/40	0.97	0.07	22,48,88,97	0
17	BCR	B	847	40/40	0.97	0.10	19,65,98,106	0
17	BCR	B	851	40/40	0.97	0.09	20,58,101,108	0
17	BCR	J	105	40/40	0.97	0.13	41,87,128,135	0
18	LMG	A	853	48/55	0.97	0.09	30,87,126,134	0
14	CLA	A	836	54/65	0.97	0.07	20,61,102,109	0
14	CLA	A	844	52/65	0.97	0.07	18,57,85,93	0
19	LHG	M	101	49/49	0.97	0.08	21,63,138,155	0
22	DGD	L	207	66/66	0.97	0.08	19,73,129,142	0
14	CLA	B	812	45/65	0.98	0.05	31,63,89,93	0
14	CLA	B	813	65/65	0.98	0.08	15,46,72,76	0
14	CLA	B	815	45/65	0.98	0.06	35,56,89,92	0
14	CLA	A	815	45/65	0.98	0.07	59,88,123,130	0
14	CLA	A	806	65/65	0.98	0.09	40,74,110,115	0
14	CLA	B	818	60/65	0.98	0.08	23,44,74,81	0
14	CLA	A	807	65/65	0.98	0.08	30,58,84,90	0
14	CLA	A	808	51/65	0.98	0.06	55,76,104,107	0
14	CLA	B	821	45/65	0.98	0.05	40,67,93,94	0
14	CLA	B	822	55/65	0.98	0.06	42,68,95,96	0
14	CLA	B	823	45/65	0.98	0.07	4,35,68,80	0
14	CLA	B	825	46/65	0.98	0.07	10,38,62,64	0
14	CLA	B	826	65/65	0.98	0.06	11,39,65,70	0
14	CLA	B	828	65/65	0.98	0.07	2,35,53,71	0
14	CLA	B	830	45/65	0.98	0.06	19,47,69,87	0
14	CLA	B	832	65/65	0.98	0.08	29,60,86,95	0
14	CLA	A	820	65/65	0.98	0.08	39,74,99,107	0
14	CLA	B	834	45/65	0.98	0.07	28,47,69,71	0
14	CLA	B	836	45/65	0.98	0.05	37,62,94,95	0
14	CLA	A	822	65/65	0.98	0.07	25,61,95,101	0
14	CLA	B	838	65/65	0.98	0.07	16,62,101,117	0
14	CLA	F	201	51/65	0.98	0.07	10,49,98,117	0
14	CLA	F	202	45/65	0.98	0.08	60,89,119,125	0
14	CLA	A	809	65/65	0.98	0.08	12,58,97,102	0
14	CLA	A	810	65/65	0.98	0.07	18,73,122,135	0
14	CLA	A	825	59/65	0.98	0.07	23,57,97,109	0
14	CLA	A	826	65/65	0.98	0.08	45,74,105,108	0
14	CLA	L	204	65/65	0.98	0.06	2,15,46,67	0
14	CLA	L	205	65/65	0.98	0.06	2,19,91,104	0
14	CLA	L	206	65/65	0.98	0.06	2,20,49,59	0
14	CLA	A	827	65/65	0.98	0.06	3,42,119,141	0
14	CLA	X	1701	45/65	0.98	0.07	49,78,108,114	0
15	PQN	A	845	33/33	0.98	0.09	61,89,118,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	CLA	A	803	65/65	0.98	0.07	16,41,61,82	0
14	CLA	A	829	65/65	0.98	0.08	33,59,84,91	0
17	BCR	A	849	40/40	0.98	0.11	51,93,145,150	0
14	CLA	A	830	65/65	0.98	0.08	29,62,92,95	0
17	BCR	A	851	40/40	0.98	0.06	15,47,82,98	0
14	CLA	A	831	65/65	0.98	0.08	29,61,84,92	0
14	CLA	A	832	50/65	0.98	0.07	6,35,65,91	0
17	BCR	B	845	40/40	0.98	0.07	16,50,105,117	0
17	BCR	B	846	40/40	0.98	0.07	27,53,73,79	0
14	CLA	A	834	65/65	0.98	0.06	2,11,39,45	0
14	CLA	A	812	65/65	0.98	0.10	55,87,118,120	0
17	BCR	F	203	40/40	0.98	0.10	17,68,100,121	0
17	BCR	I	101	40/40	0.98	0.06	2,2,24,41	0
17	BCR	J	103	40/40	0.98	0.07	34,76,98,103	0
17	BCR	J	104	40/40	0.98	0.07	52,90,119,124	0
14	CLA	A	837	45/65	0.98	0.06	54,78,101,111	0
17	BCR	M	103	40/40	0.98	0.06	2,22,50,56	0
14	CLA	A	838	51/65	0.98	0.07	10,33,53,76	0
14	CLA	A	804	65/65	0.98	0.07	33,72,99,106	0
14	CLA	A	857	65/65	0.98	0.07	12,39,65,76	0
19	LHG	A	854	49/49	0.98	0.09	12,58,82,92	0
19	LHG	B	850	23/49	0.98	0.07	46,85,113,119	0
14	CLA	B	804	54/65	0.98	0.07	2,22,41,48	0
21	LMT	L	202	35/35	0.98	0.07	48,116,152,165	0
14	CLA	A	805	59/65	0.98	0.08	48,72,99,115	0
14	CLA	B	803	65/65	0.99	0.05	2,7,27,38	0
14	CLA	B	824	54/65	0.99	0.05	21,38,60,61	0
14	CLA	A	835	65/65	0.99	0.05	2,6,35,63	0
15	PQN	B	842	33/33	0.99	0.07	27,47,66,70	0
14	CLA	B	805	65/65	0.99	0.06	2,30,63,75	0
14	CLA	B	827	65/65	0.99	0.06	2,22,74,76	0
14	CLA	B	806	65/65	0.99	0.05	2,24,51,64	0
14	CLA	B	829	65/65	0.99	0.05	2,21,53,72	0
14	CLA	B	807	65/65	0.99	0.06	2,9,40,63	0
17	BCR	A	852	40/40	0.99	0.06	2,37,64,66	0
14	CLA	B	831	49/65	0.99	0.05	8,43,70,96	0
14	CLA	B	808	65/65	0.99	0.05	2,13,45,50	0
14	CLA	B	809	65/65	0.99	0.06	2,12,40,63	0
14	CLA	B	810	65/65	0.99	0.05	2,2,33,43	0
14	CLA	B	835	45/65	0.99	0.06	18,53,81,85	0
17	BCR	B	848	40/40	0.99	0.05	2,8,34,35	0
14	CLA	A	802	65/65	0.99	0.05	2,12,28,48	0

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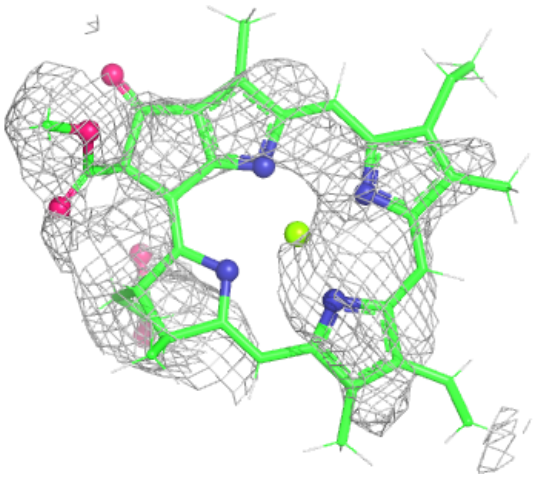
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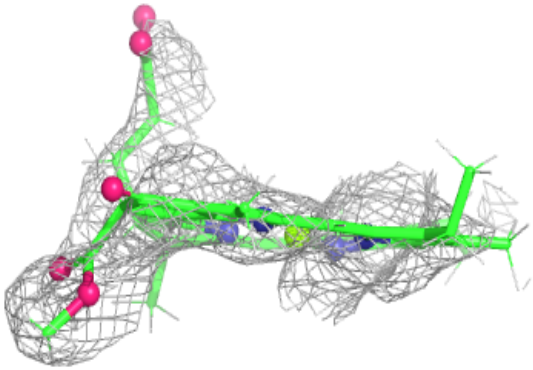
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	CLA	A	819	54/65	0.99	0.06	35,68,90,106	0
13	CL0	A	801	65/65	0.99	0.05	2,20,45,48	0
17	BCR	I	103	40/40	0.99	0.04	2,2,21,39	0
14	CLA	B	839	47/65	0.99	0.06	23,48,67,79	0
14	CLA	B	840	65/65	0.99	0.04	2,2,26,31	0
14	CLA	B	841	65/65	0.99	0.04	2,3,26,29	0
17	BCR	L	201	40/40	0.99	0.04	2,8,33,35	0
17	BCR	L	208	40/40	0.99	0.05	2,12,60,72	0
14	CLA	B	814	65/65	0.99	0.06	19,51,86,91	0
14	CLA	A	839	65/65	0.99	0.05	2,32,71,94	0
14	CLA	A	840	47/65	0.99	0.04	2,28,49,67	0
18	LMG	B	849	55/55	0.99	0.06	2,31,57,61	0
14	CLA	A	841	65/65	0.99	0.07	6,42,97,106	0
14	CLA	A	842	65/65	0.99	0.06	11,47,91,109	0
19	LHG	A	855	27/49	0.99	0.06	20,53,90,91	0
14	CLA	A	843	65/65	0.99	0.05	2,2,24,33	0
14	CLA	A	833	65/65	0.99	0.05	2,37,109,114	0
20	CA	B	801	1/1	0.99	0.07	43,43,43,43	0
14	CLA	A	821	43/65	0.99	0.07	46,104,144,150	0
14	CLA	B	802	65/65	0.99	0.06	2,23,44,50	0
16	SF4	A	846	8/8	1.00	0.02	3,20,62,92	0
20	CA	L	203	1/1	1.00	0.03	2,2,2,2	0
16	SF4	C	101	8/8	1.00	0.02	2,25,32,45	0
16	SF4	C	102	8/8	1.00	0.02	12,19,36,38	0

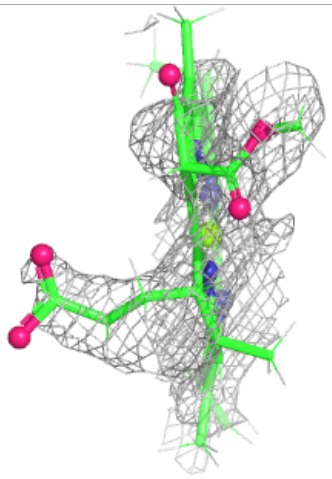
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CLA A 816:

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

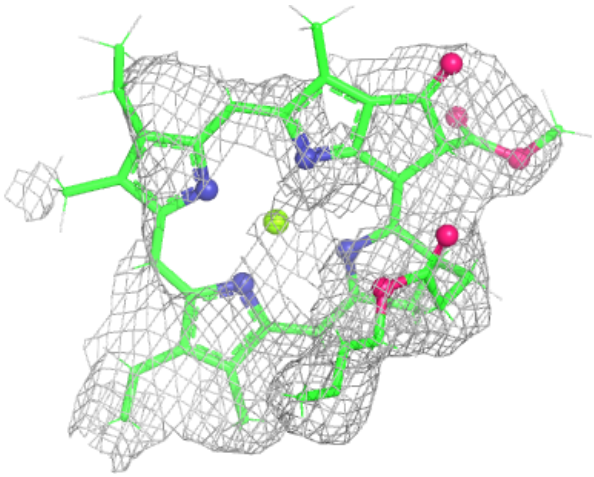


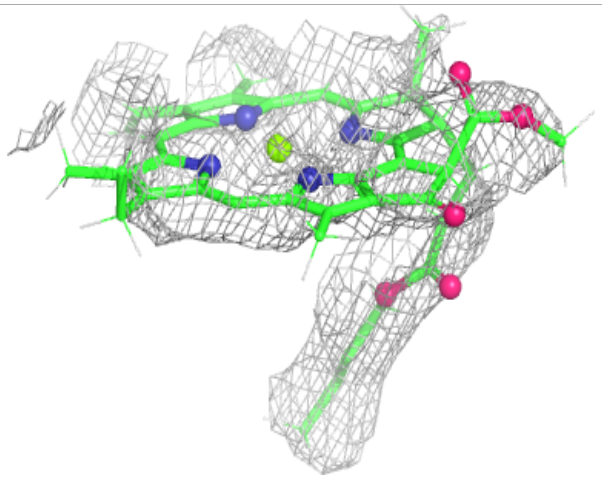


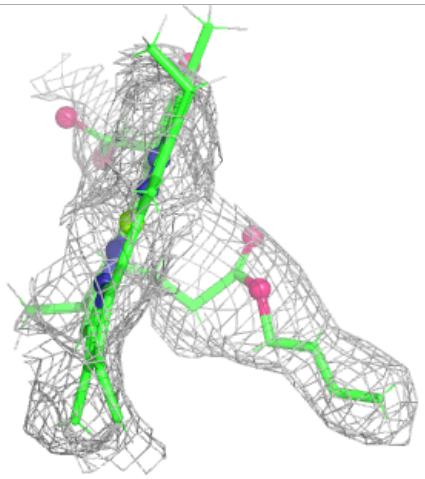


Electron density around CLA A 817:

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

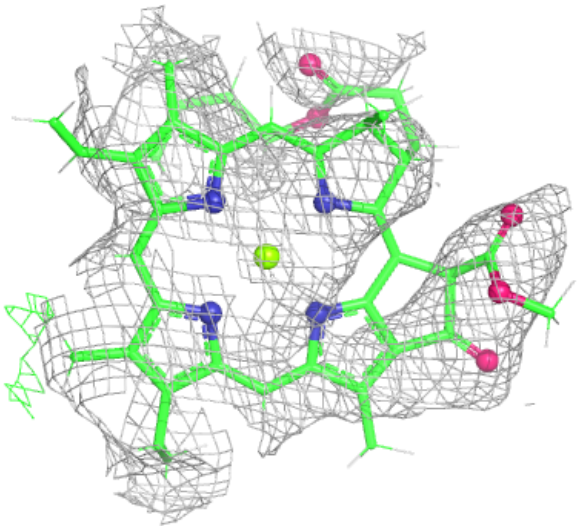


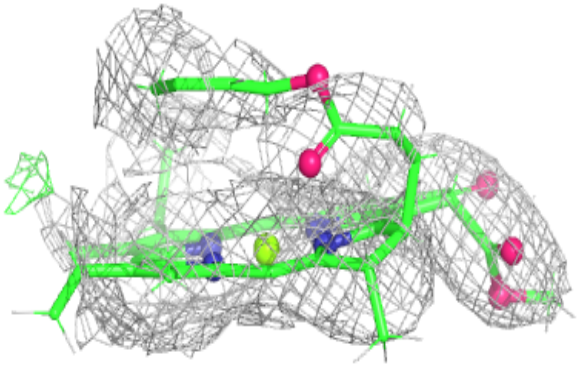


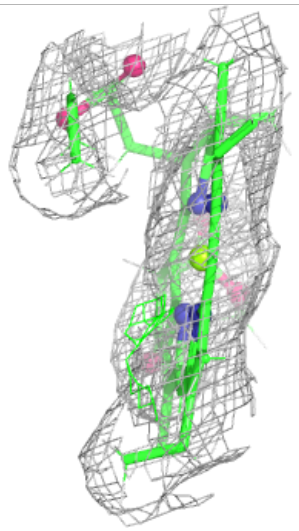


Electron density around CLA A 823:

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

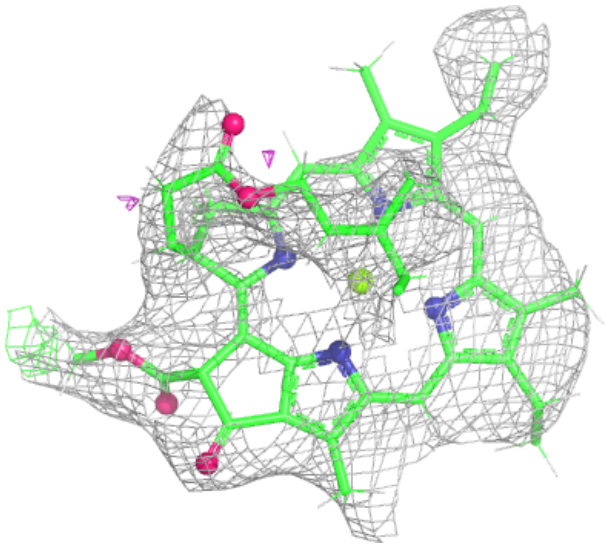


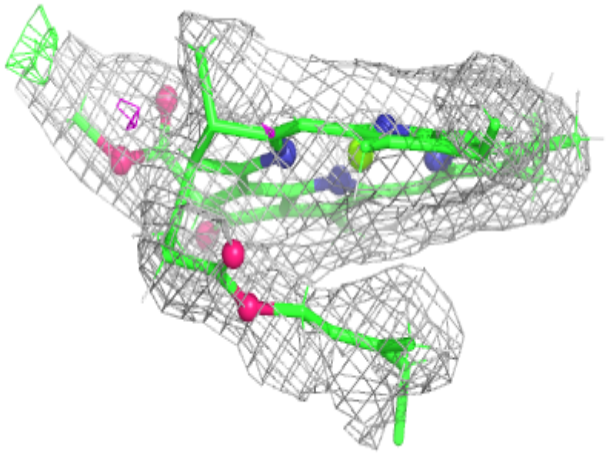


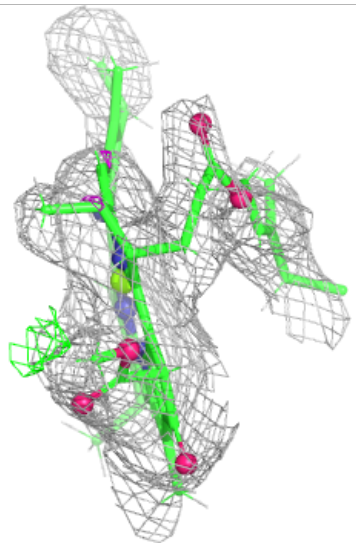


Electron density around CLA A 824:

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

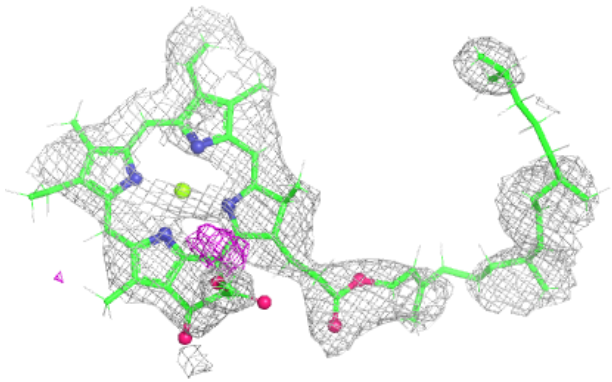


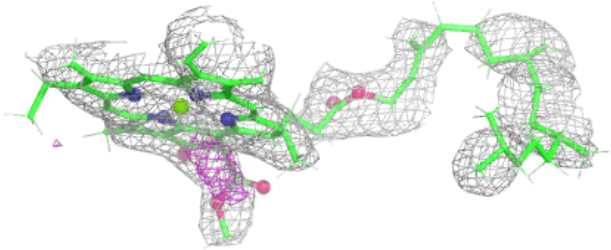


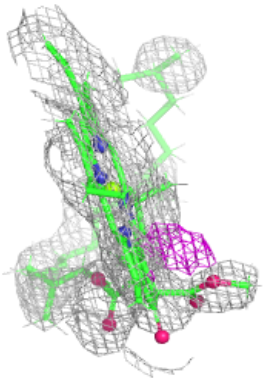


Electron density around CLA A 828:

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

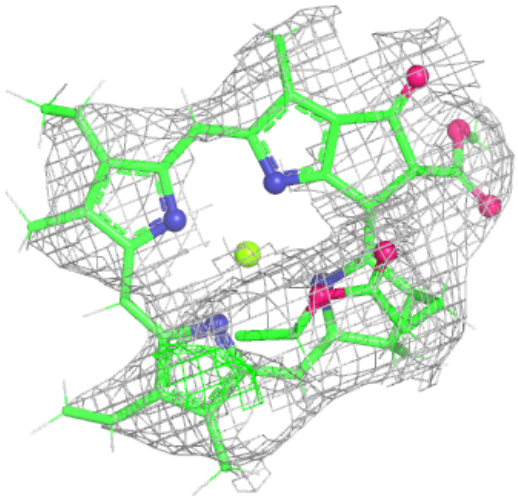


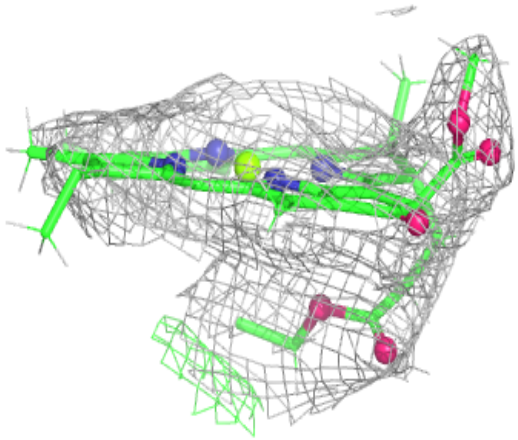


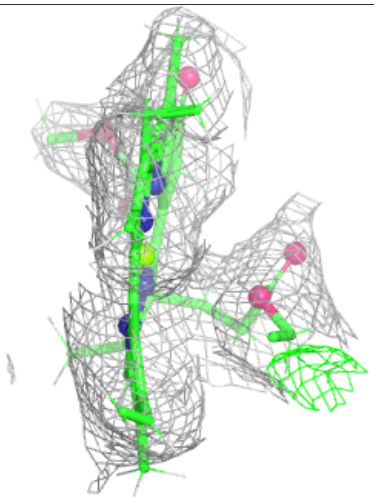


Electron density around CLA B 820:

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

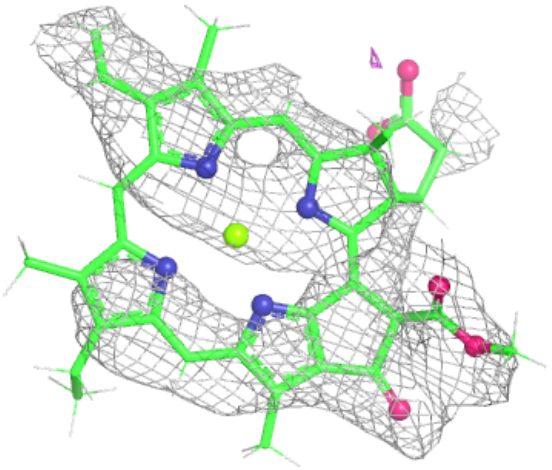


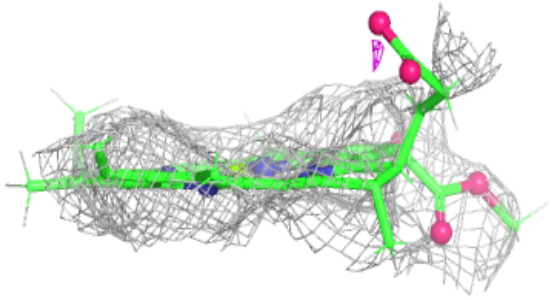


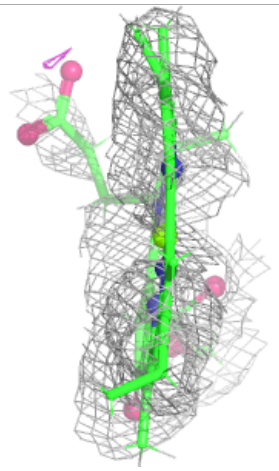


Electron density around CLA J 101:

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

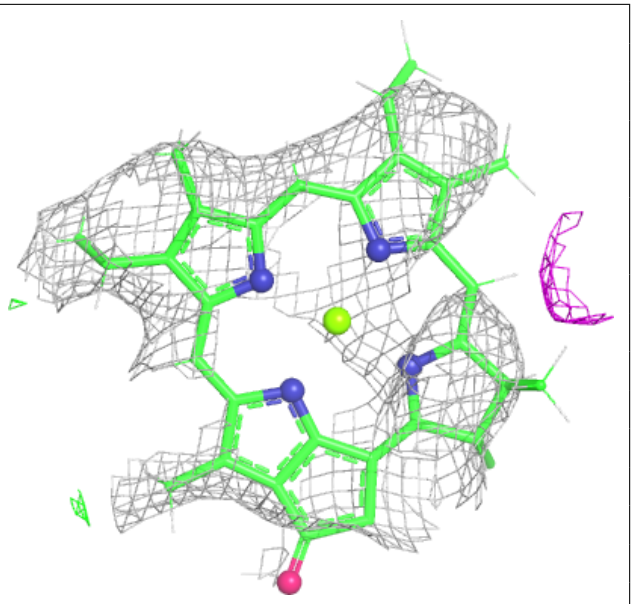


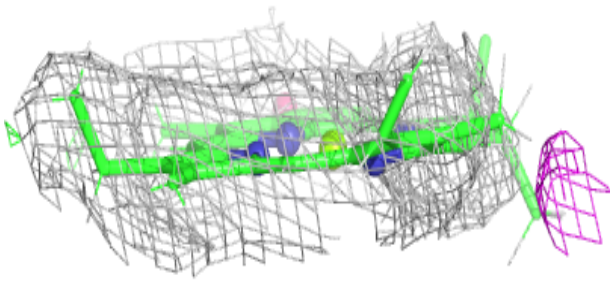


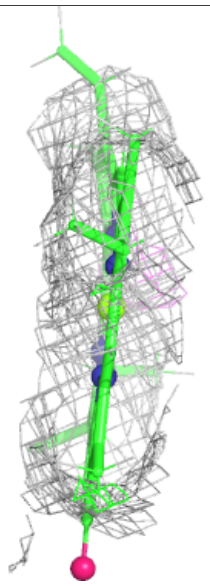


Electron density around CLA J 102:

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

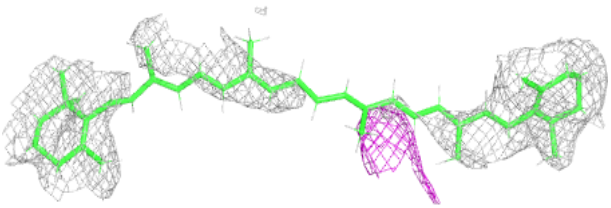


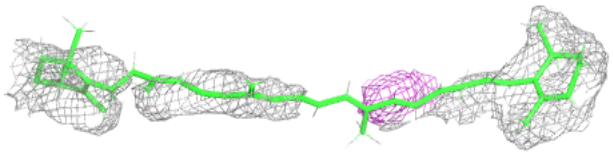


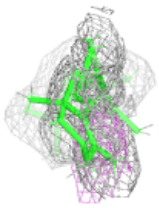


Electron density around BCR B 843:

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

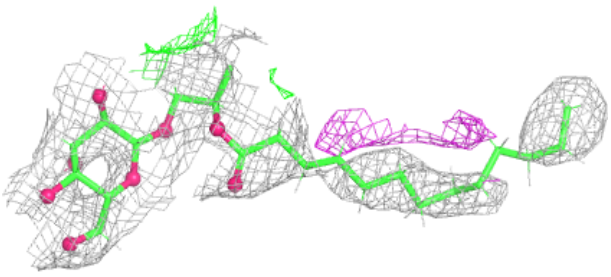


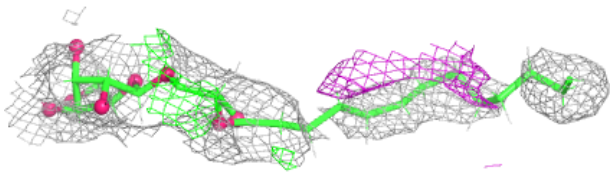


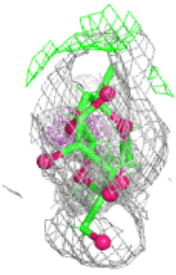


Electron density around LMG A 856:

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

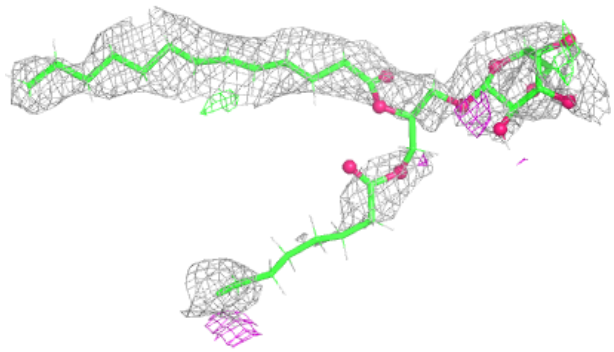


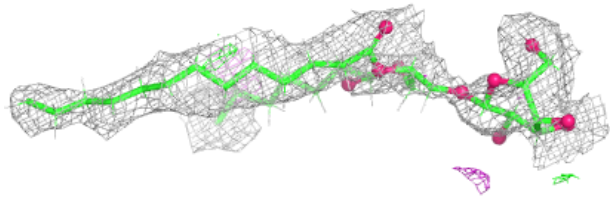


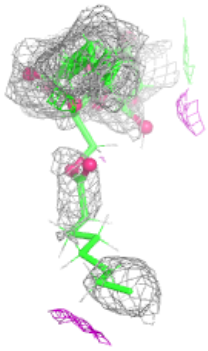


Electron density around LMG I 102:

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

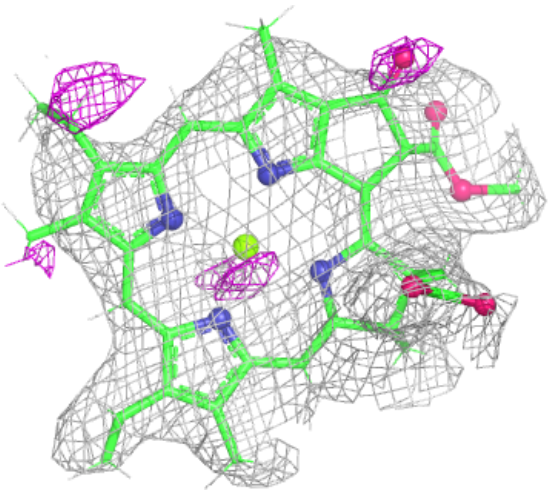


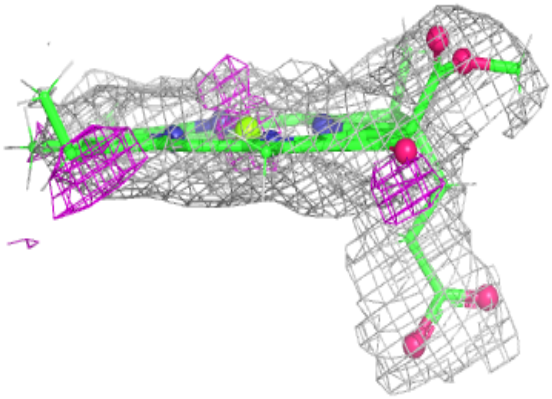




Electron density around CLA B 811:

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

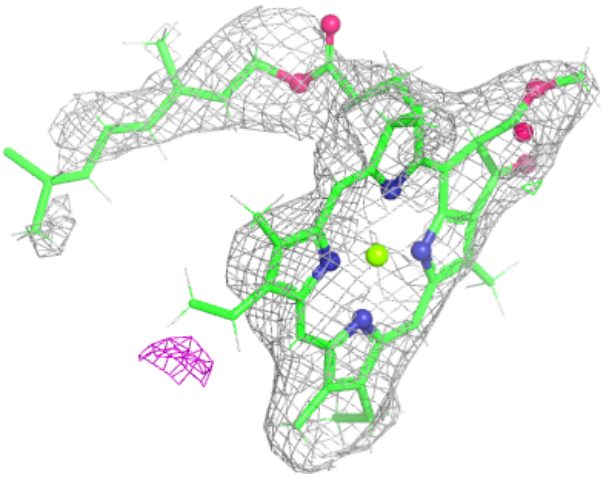


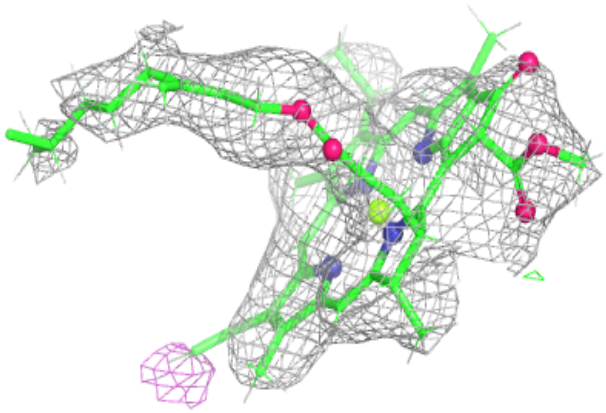


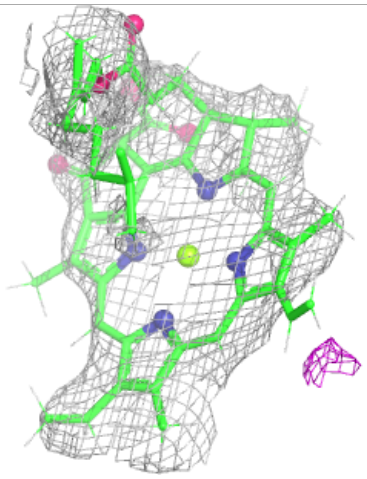


Electron density around CLA B 816:

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

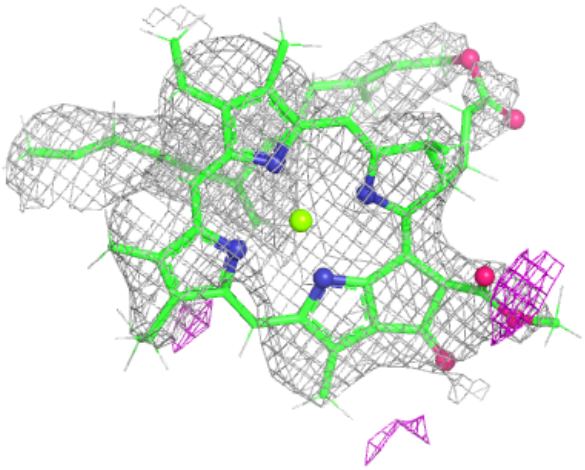


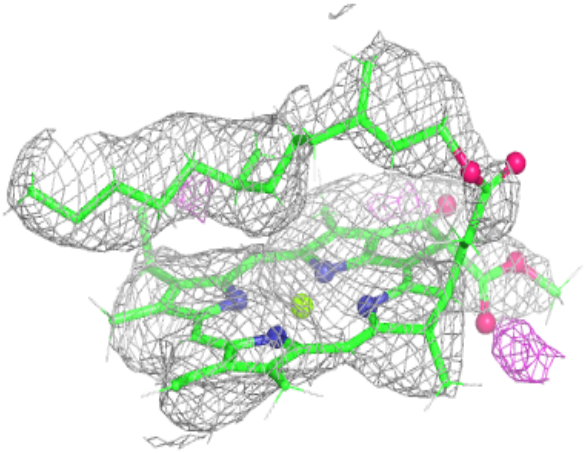


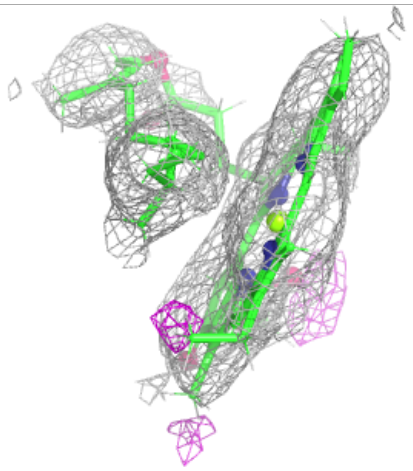


Electron density around CLA B 817:

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

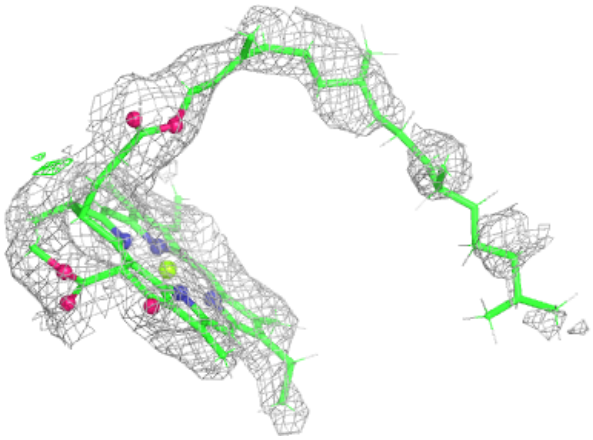


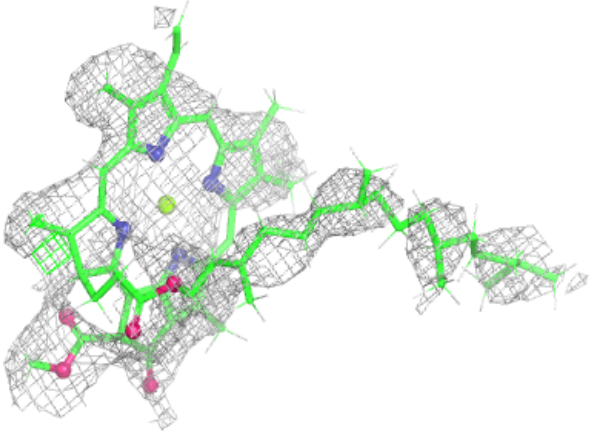


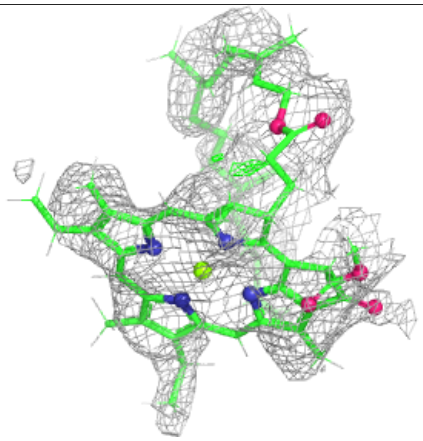


Electron density around CLA B 819:

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

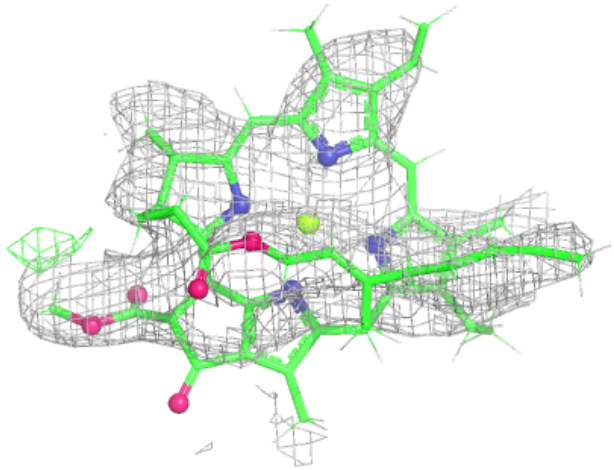




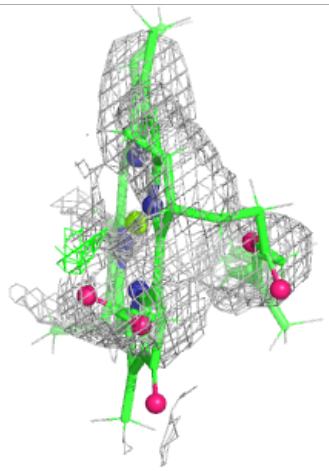


Electron density around CLA A 818:

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

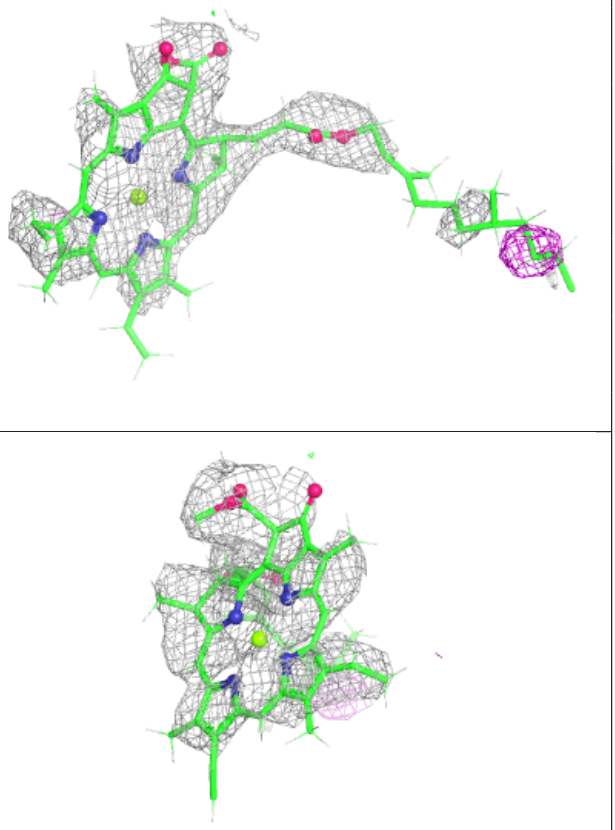






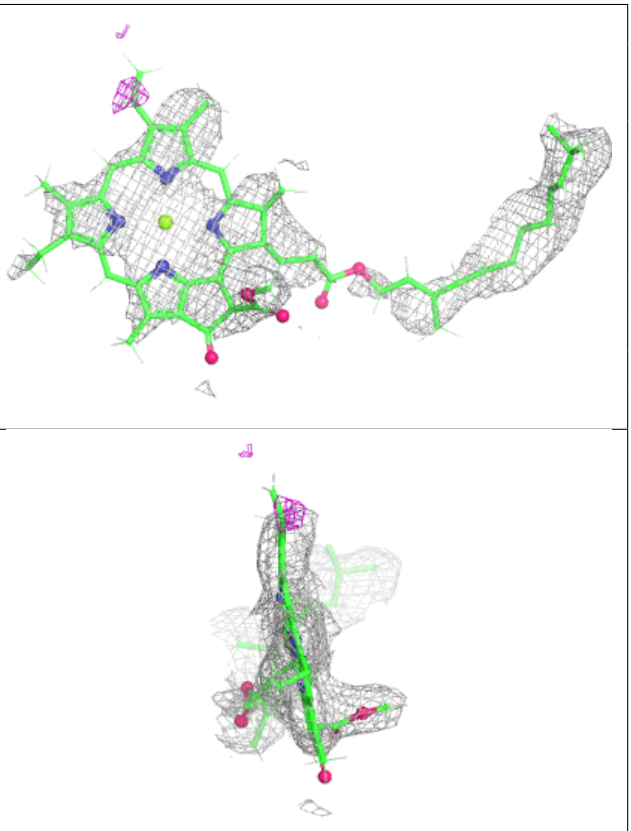
Electron density around CLA B 833:

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



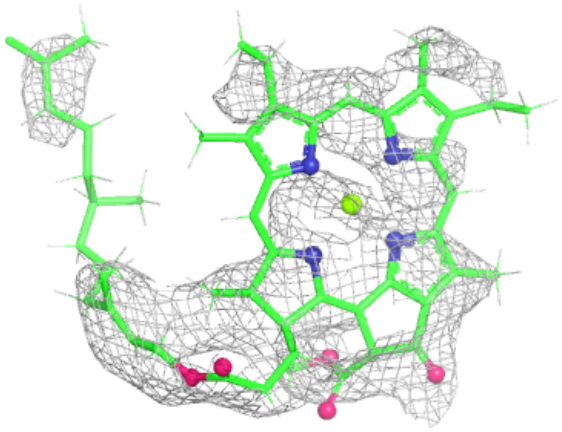
Electron density around CLA B 837:

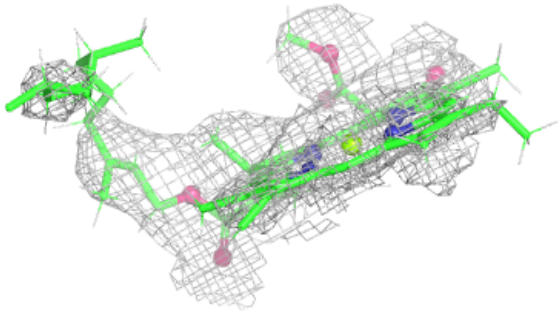
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

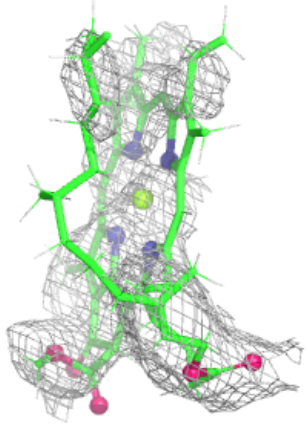


Electron density around CLA A 814:

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

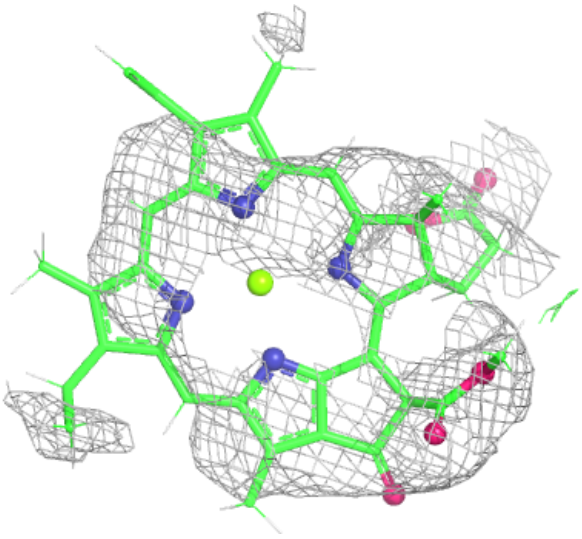


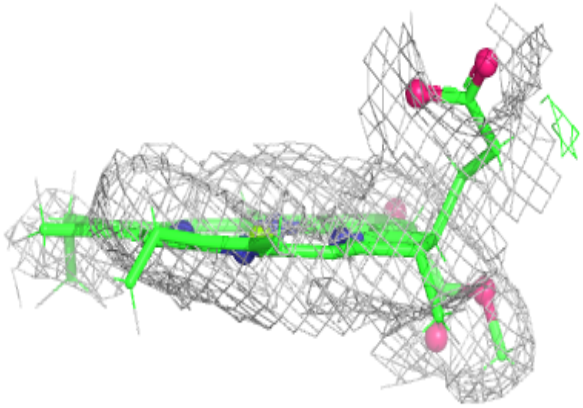


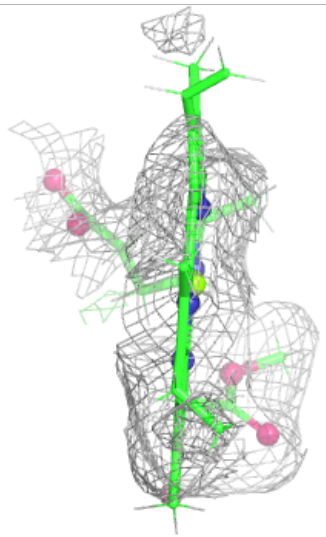


Electron density around CLA A 811:

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

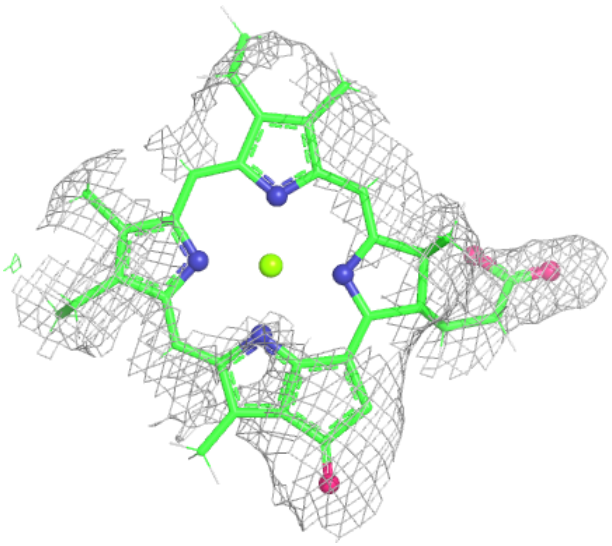


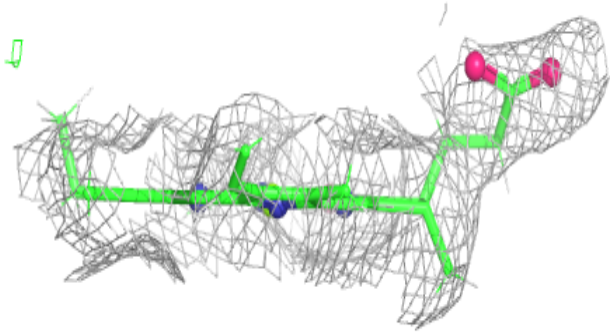


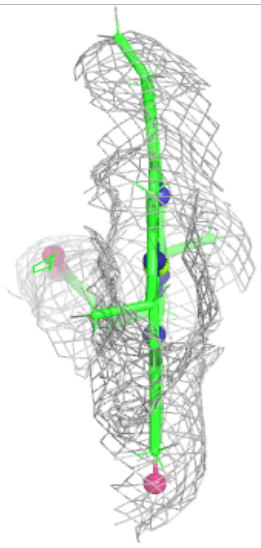


Electron density around CLA K 101:

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

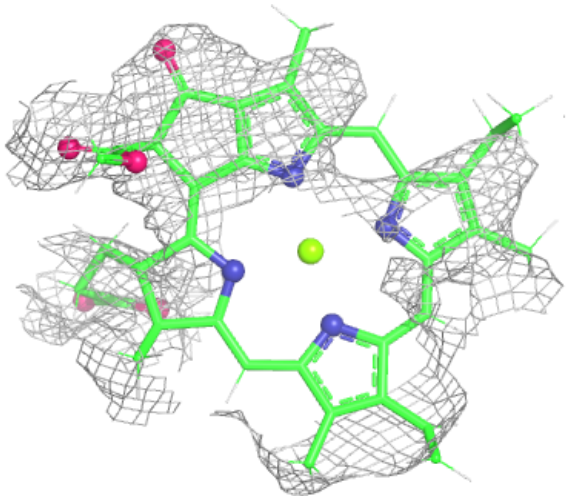


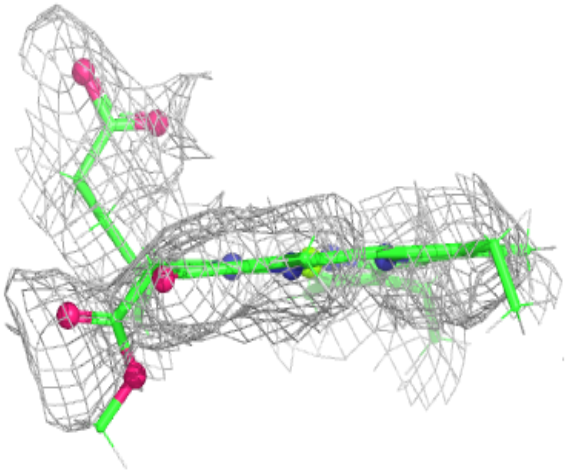


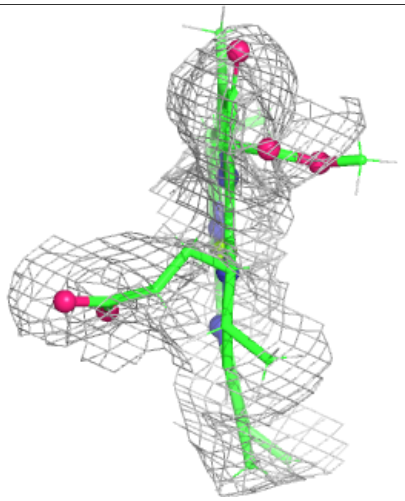


Electron density around CLA K 102:

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

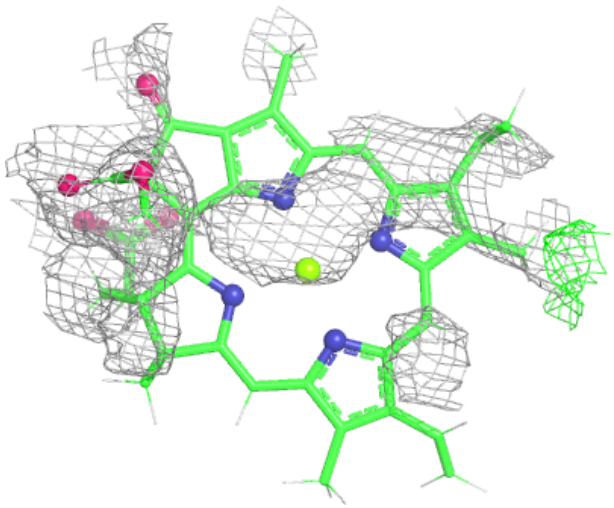


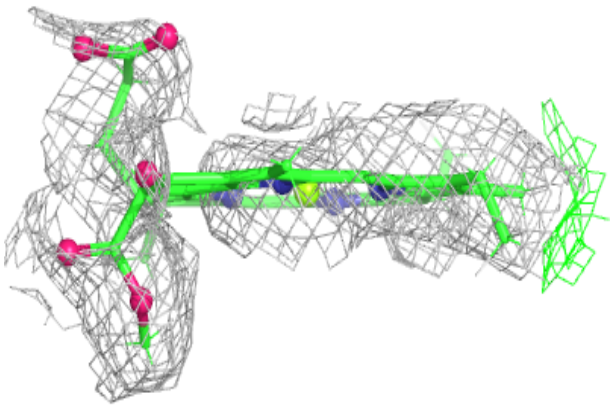


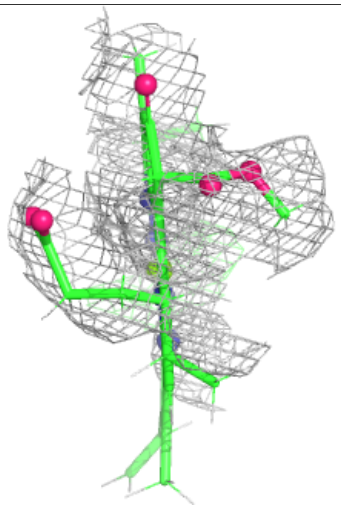


Electron density around CLA M 102:

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

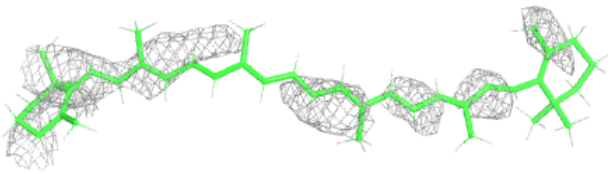


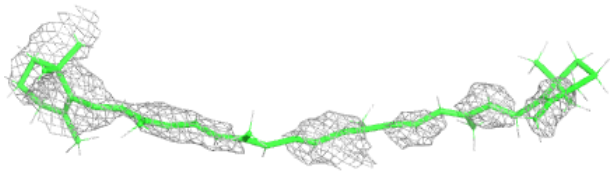


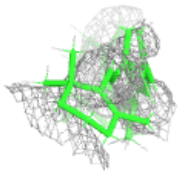


Electron density around BCR A 847:

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

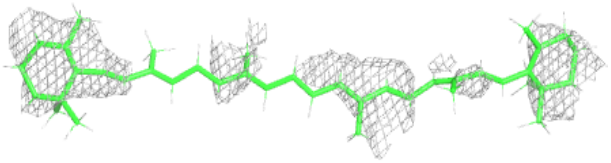


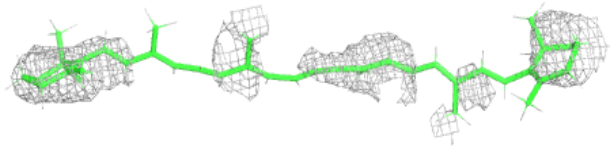


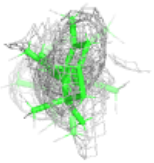


Electron density around BCR A 848:

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

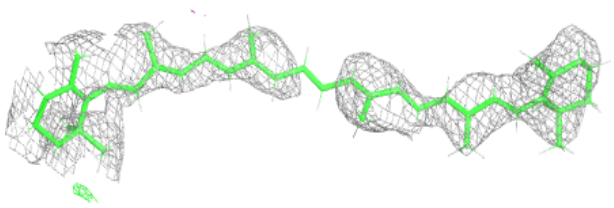


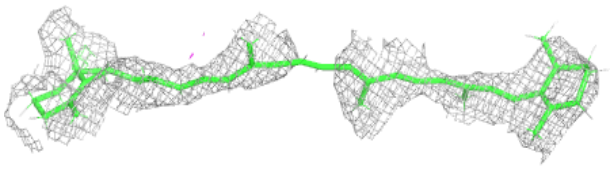


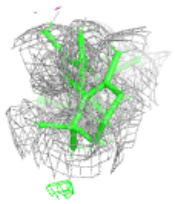


Electron density around BCR A 850:

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

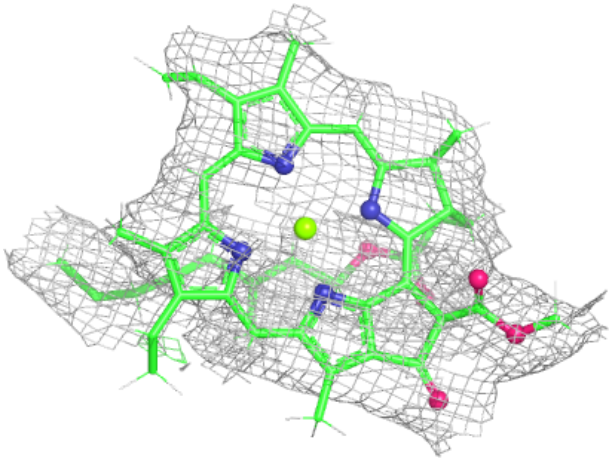


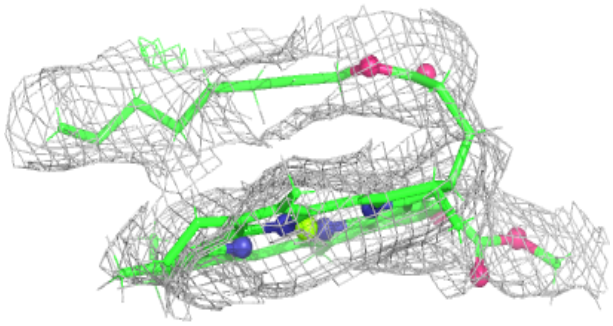




Electron density around CLA A 813:

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

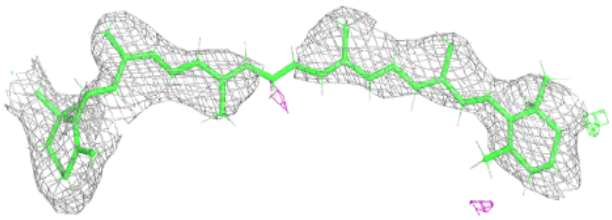


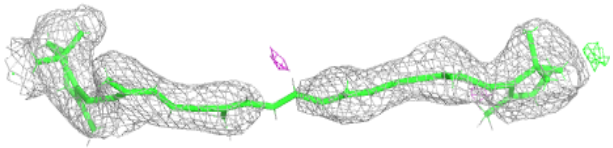


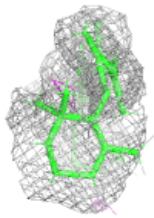


Electron density around BCR B 844:

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

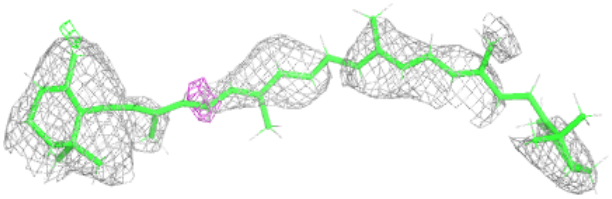


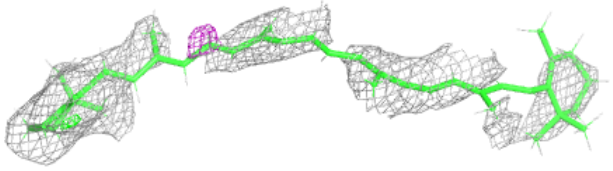


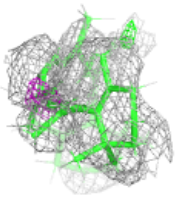


Electron density around BCR B 847:

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

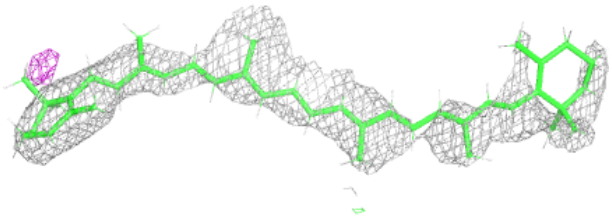


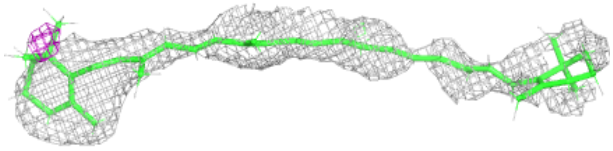


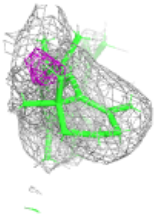


Electron density around BCR B 851:

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

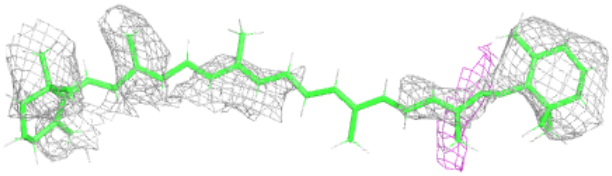


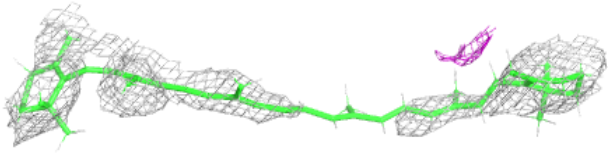


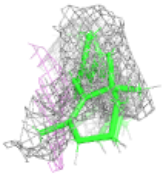


Electron density around BCR J 105:

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

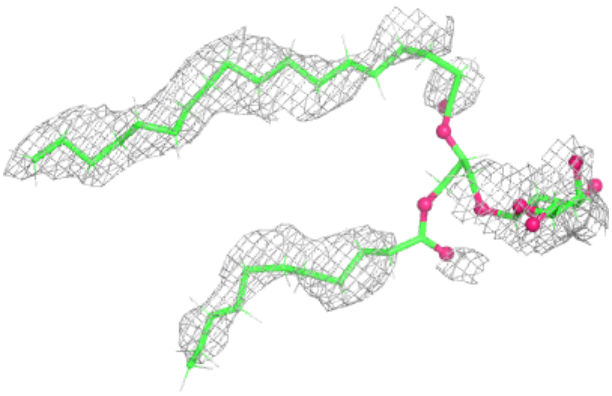


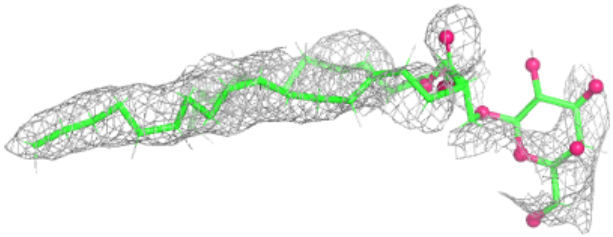


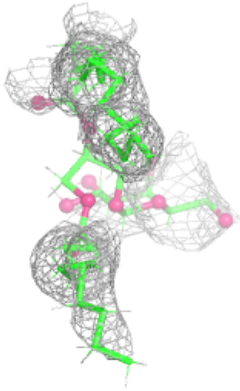


Electron density around LMG A 853:

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

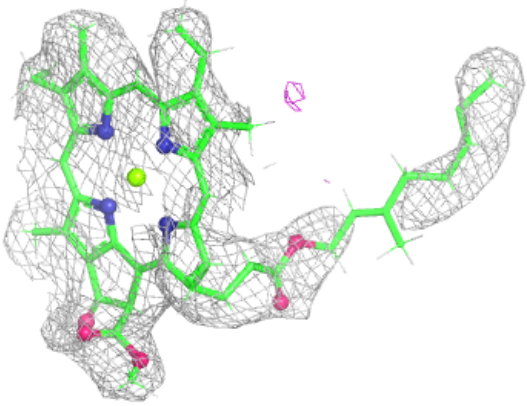


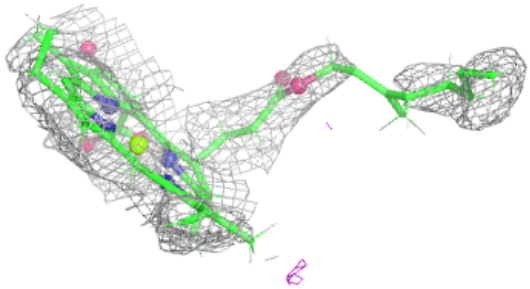


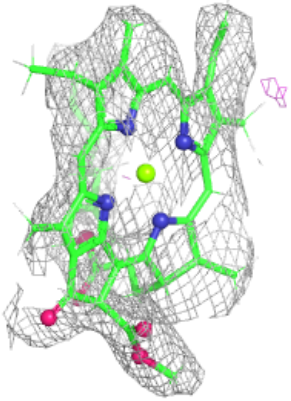


Electron density around CLA A 836:

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

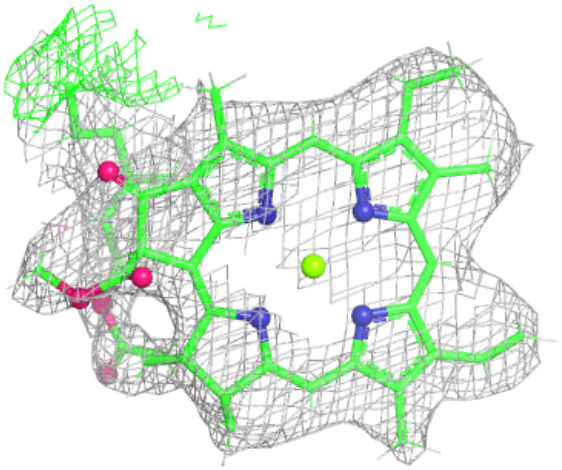


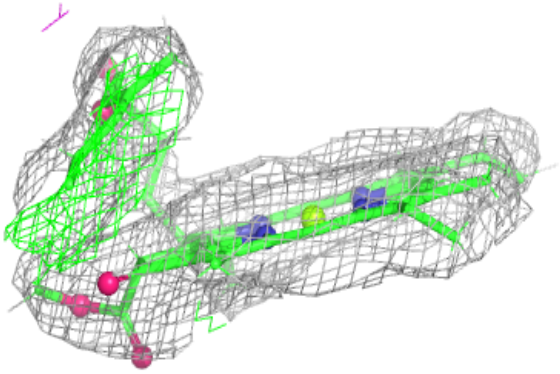


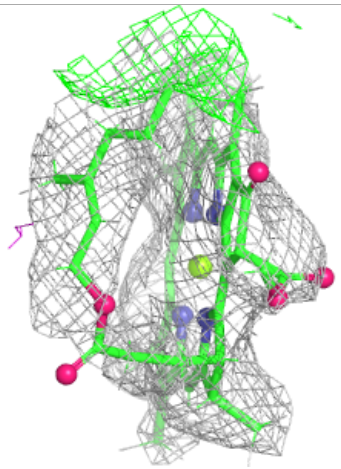


Electron density around CLA A 844:

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

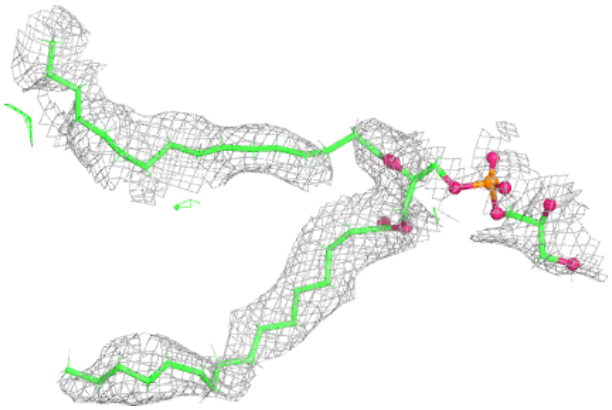


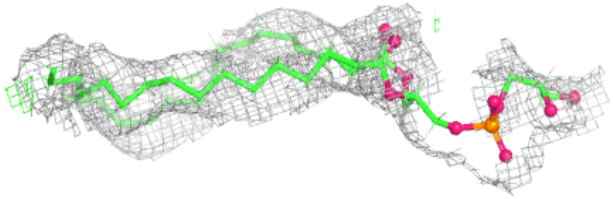


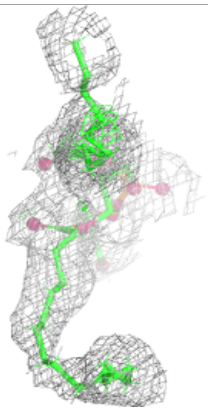


Electron density around LHG M 101:

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

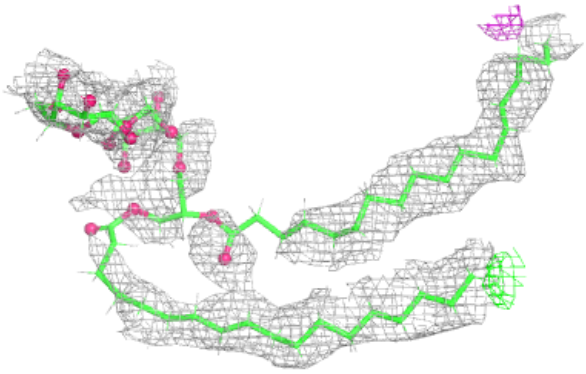


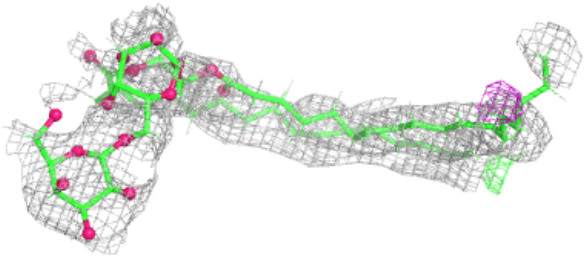




Electron density around DGD L 207:

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

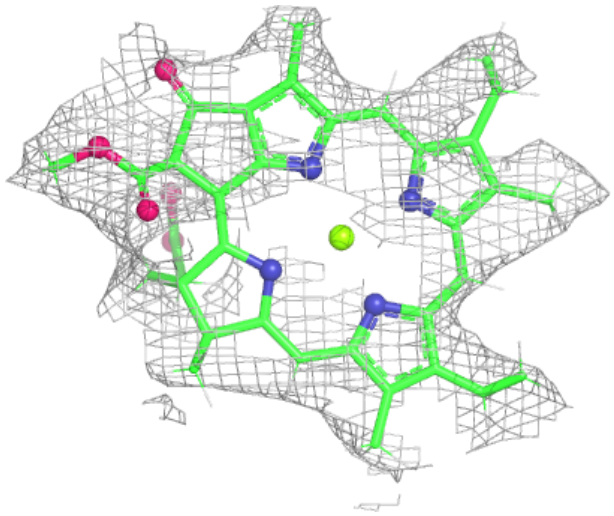


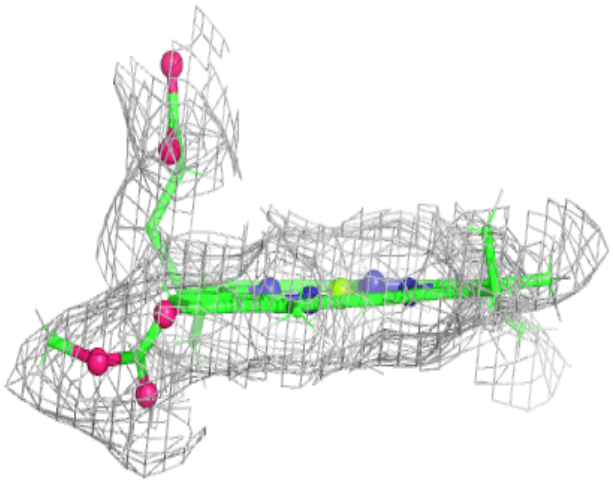


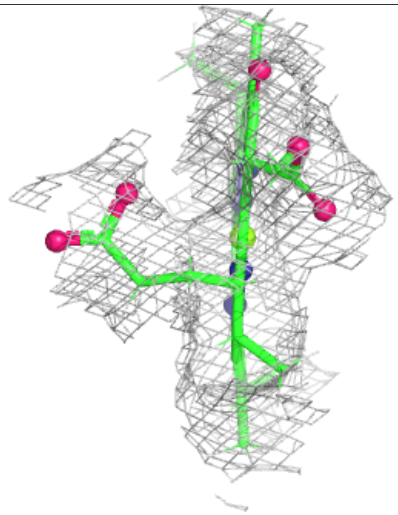


Electron density around CLA B 812:

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

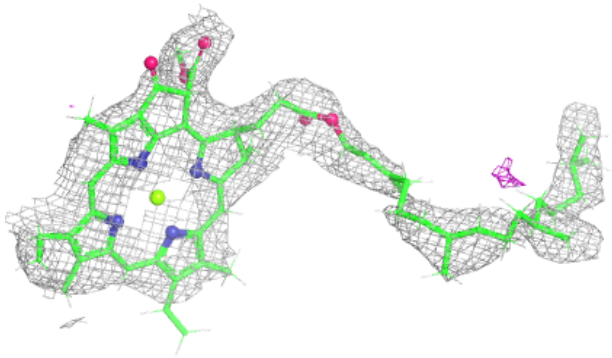


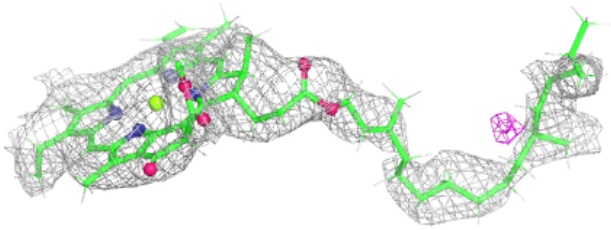


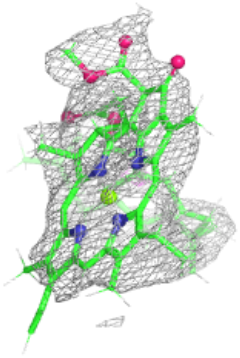


Electron density around CLA B 813:

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

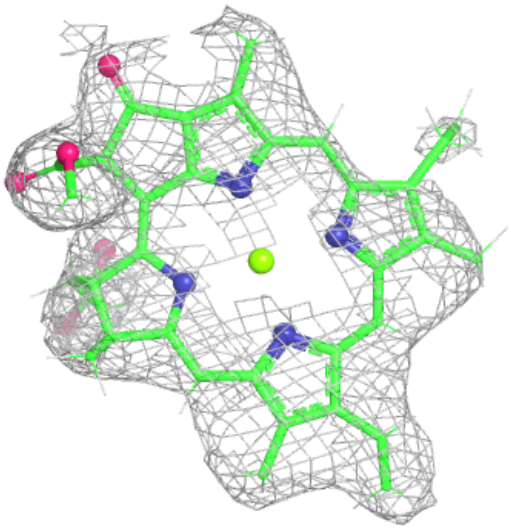


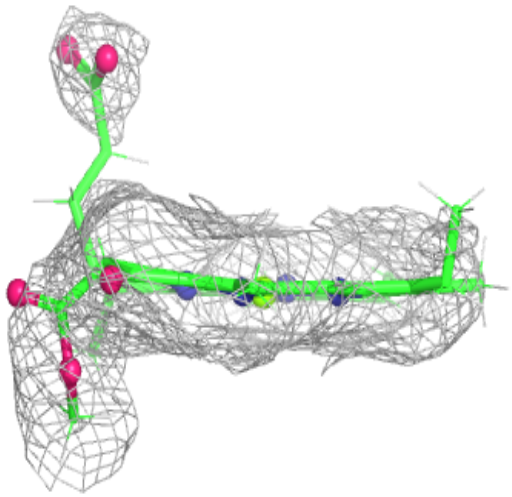


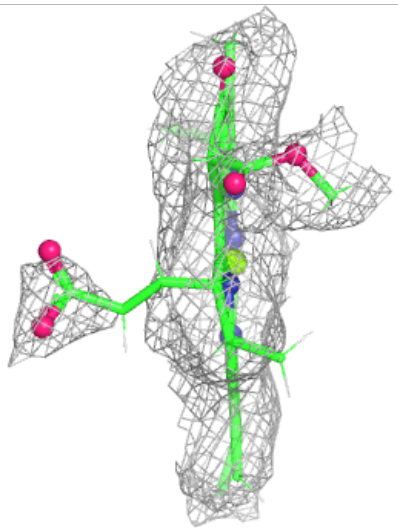


Electron density around CLA B 815:

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

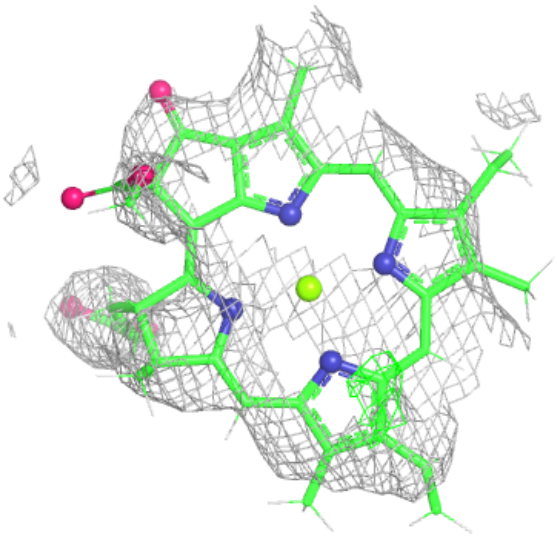


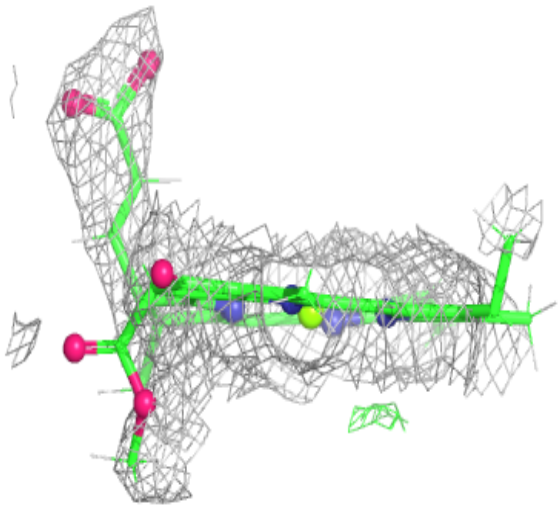


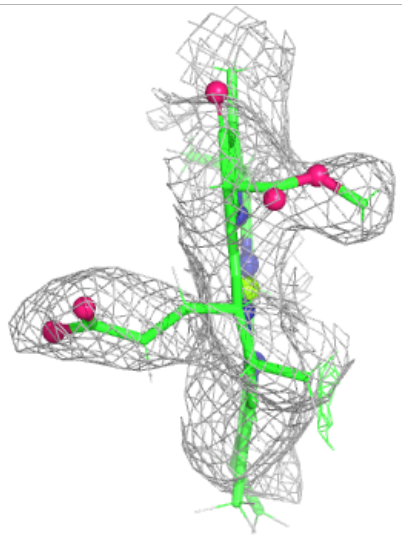


Electron density around CLA A 815:

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

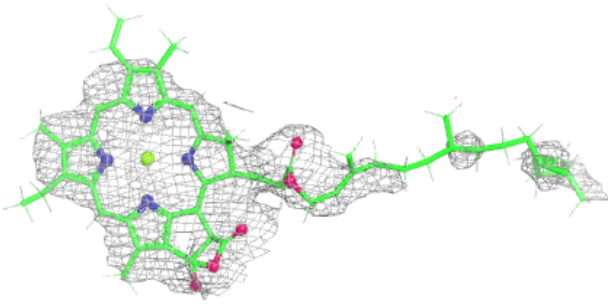


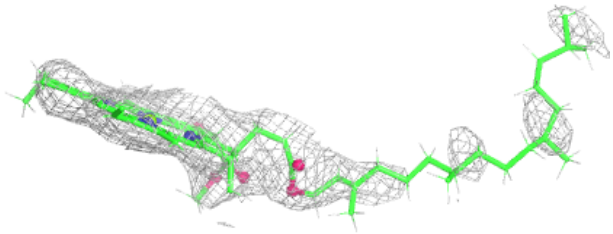


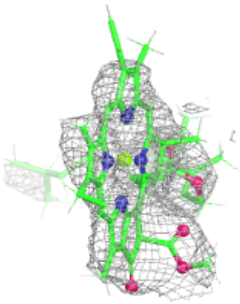


Electron density around CLA A 806:

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

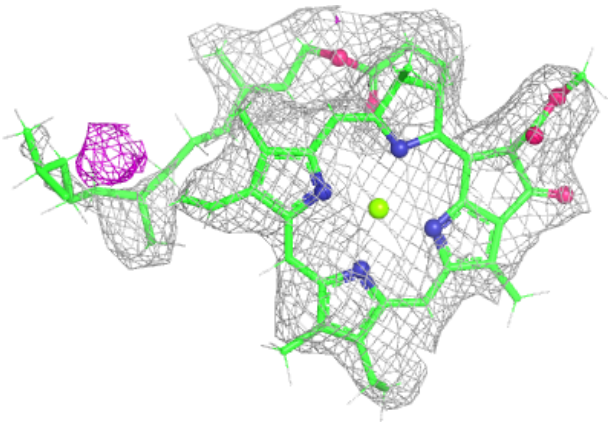


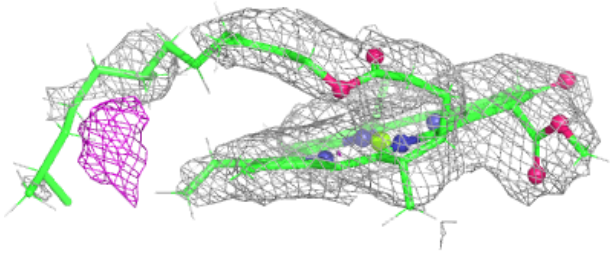


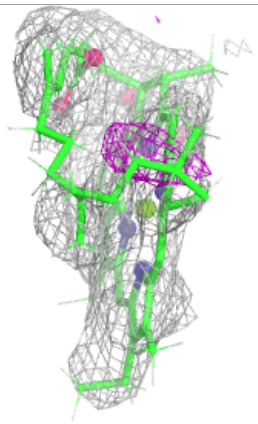


Electron density around CLA B 818:

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

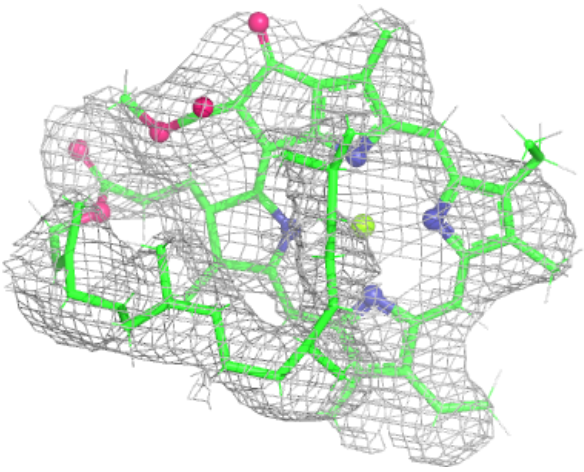


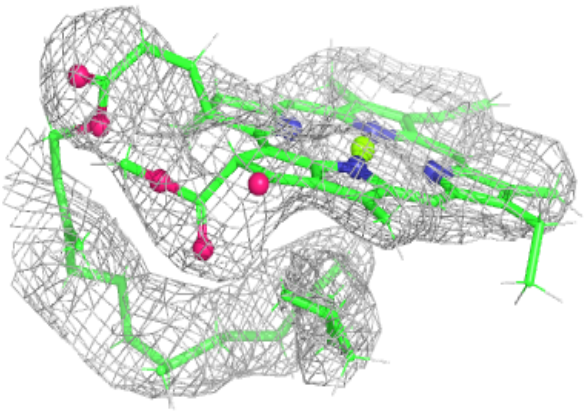


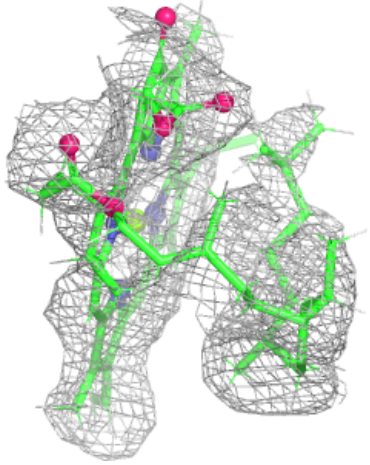


Electron density around CLA A 807:

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

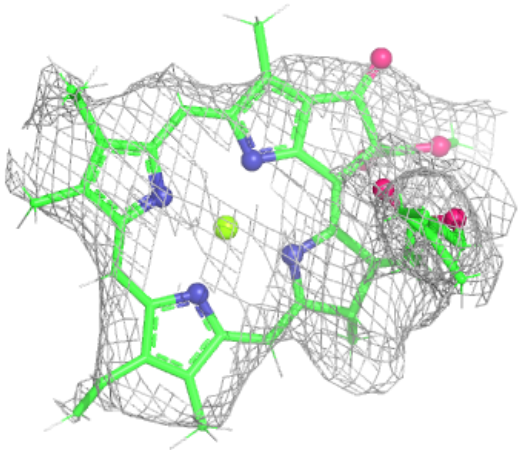


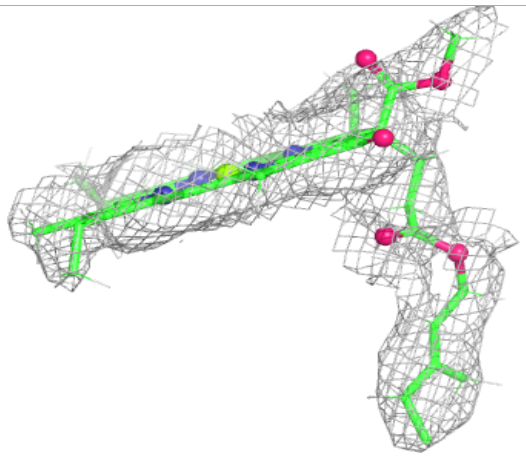


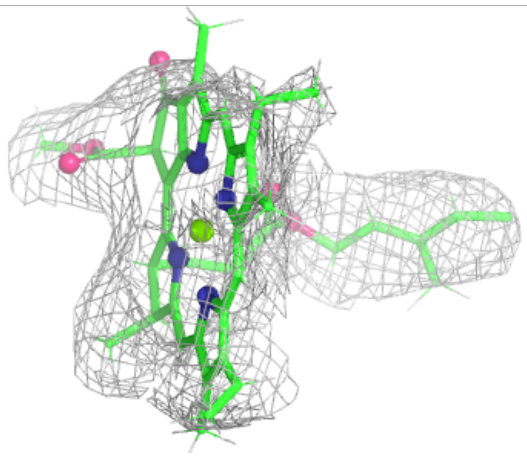


Electron density around CLA A 808:

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

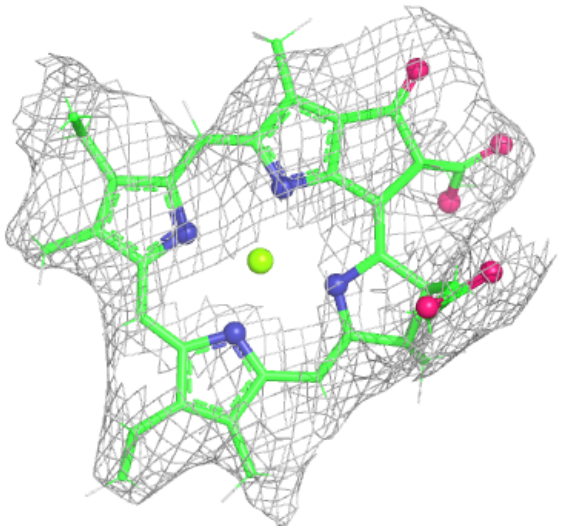


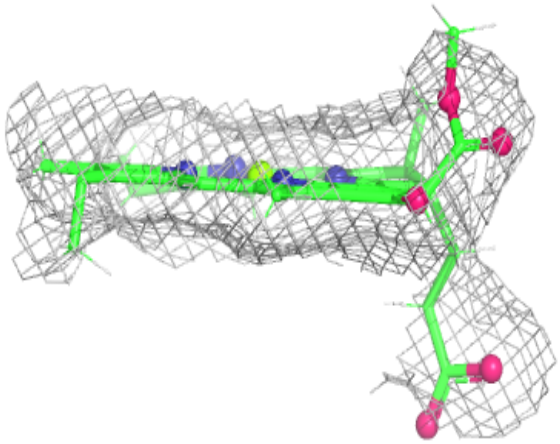


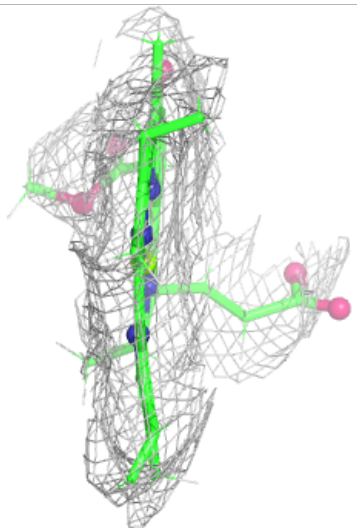


Electron density around CLA B 821:

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

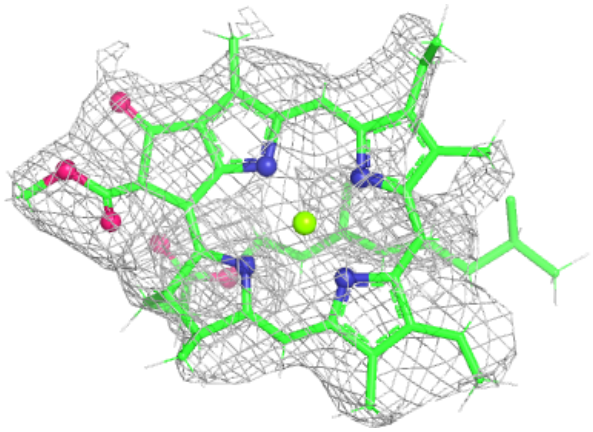


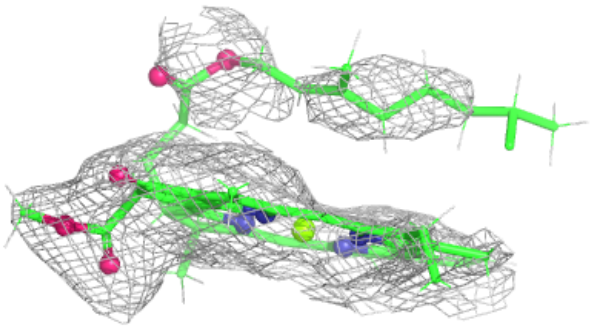


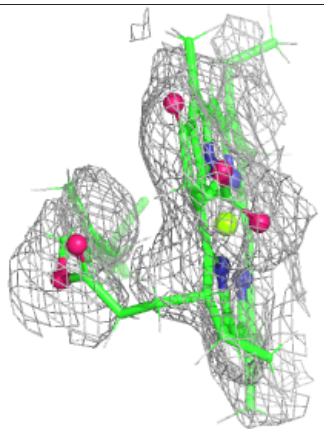


Electron density around CLA B 822:

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

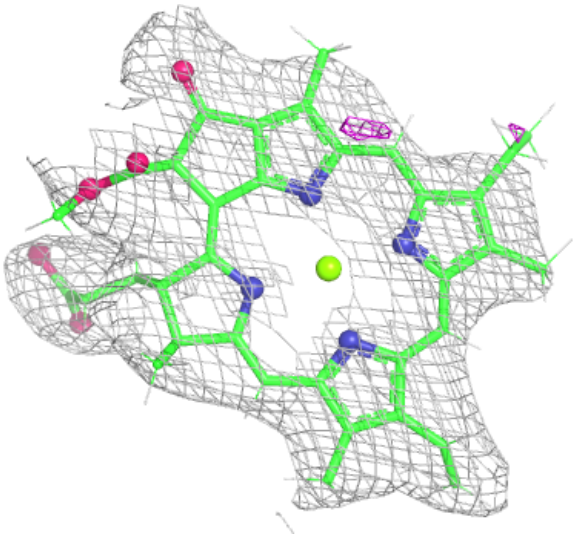


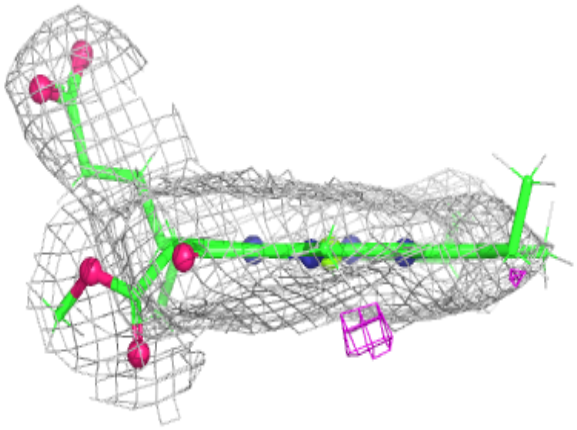


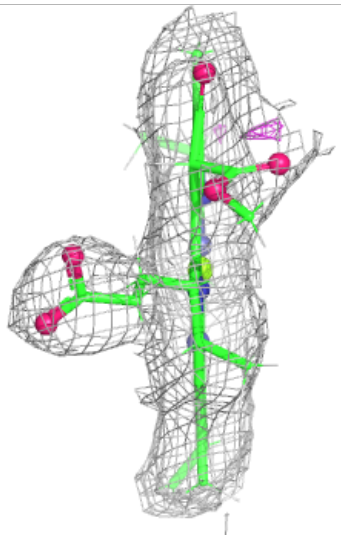


Electron density around CLA B 823:

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

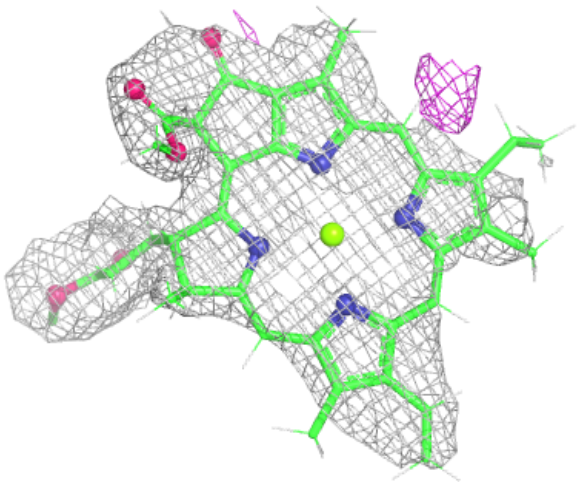


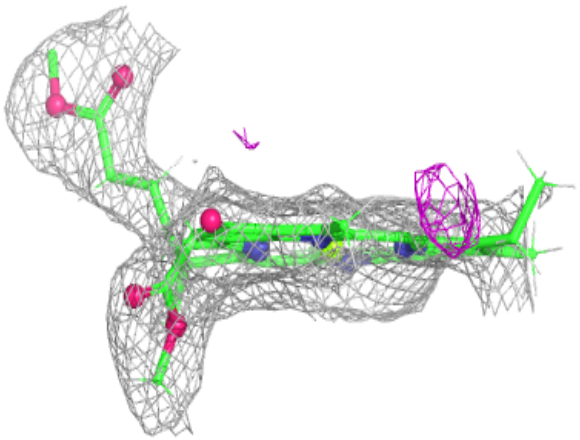


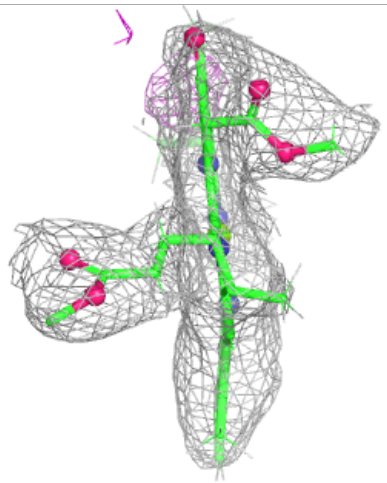


Electron density around CLA B 825:

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

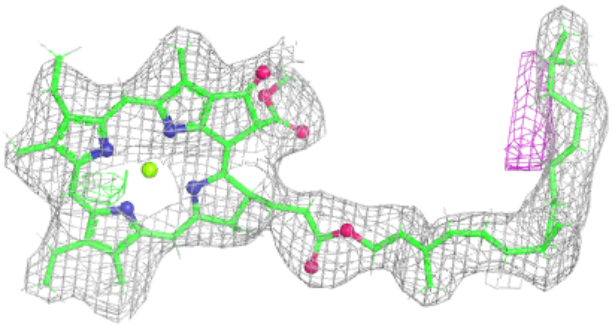


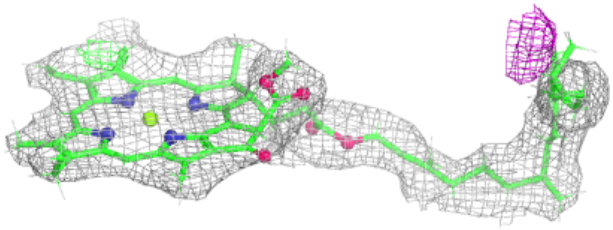


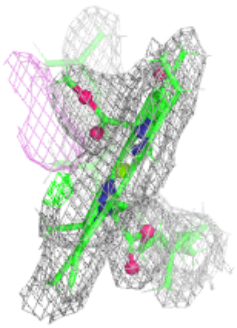


Electron density around CLA B 826:

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

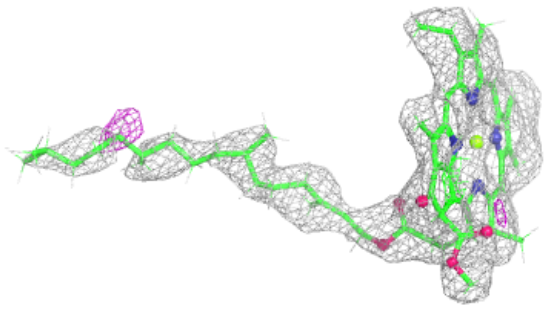


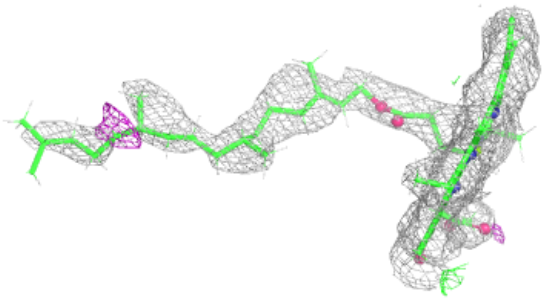


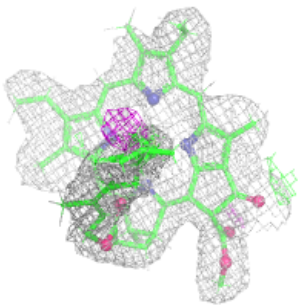


Electron density around CLA B 828:

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

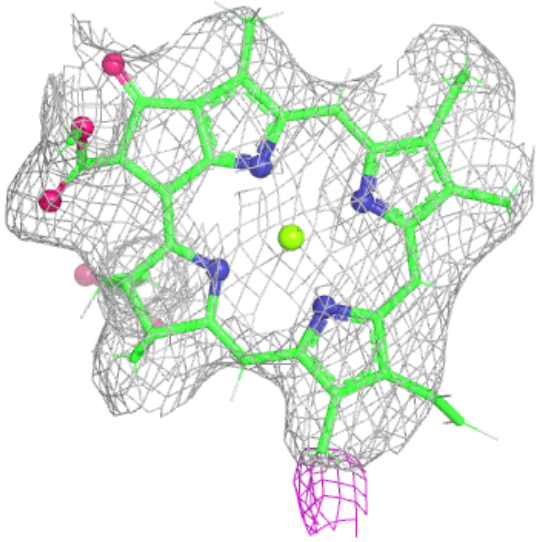


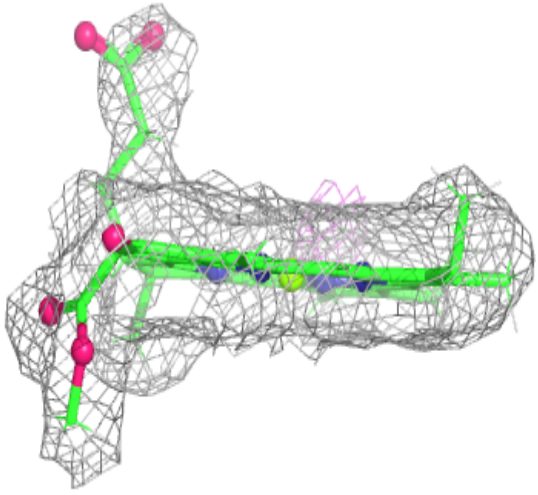


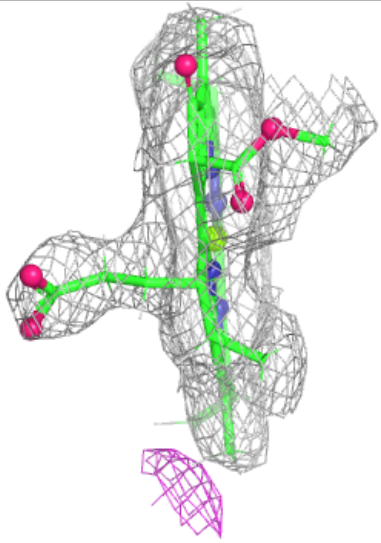


Electron density around CLA B 830:

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

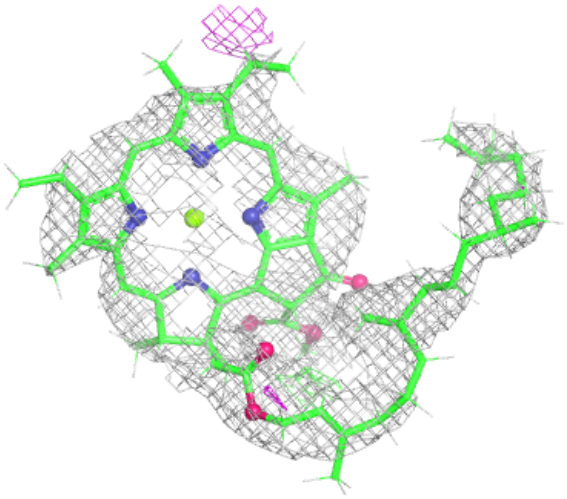


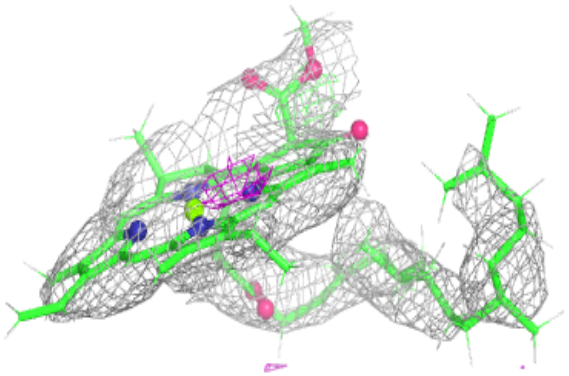


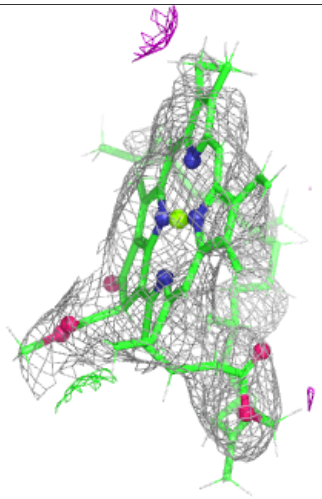


Electron density around CLA B 832:

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

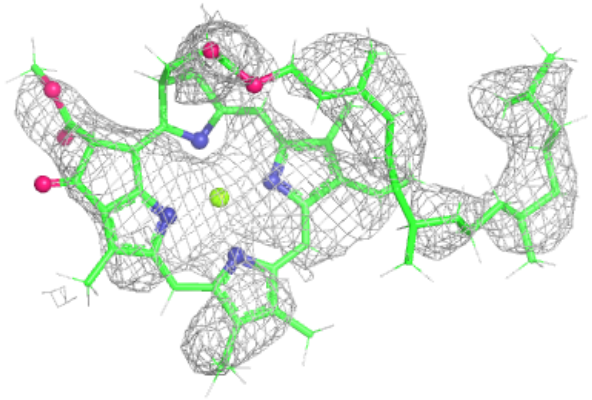


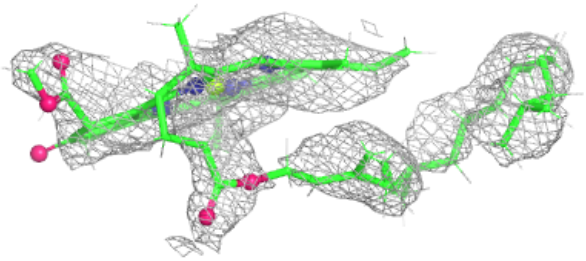


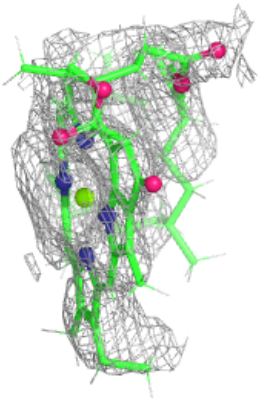


Electron density around CLA A 820:

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

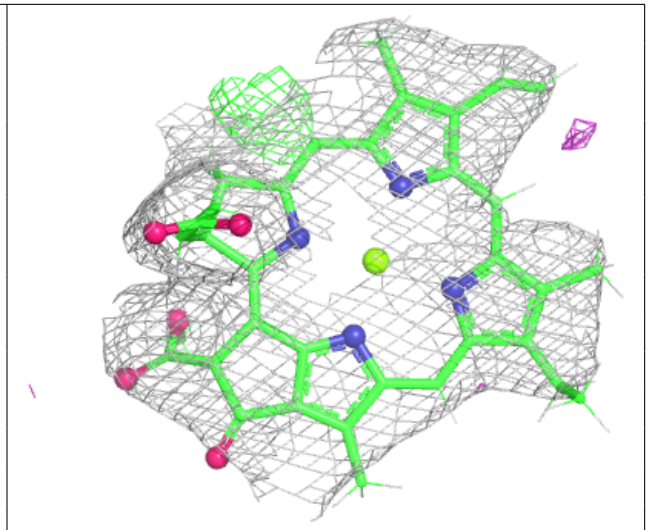


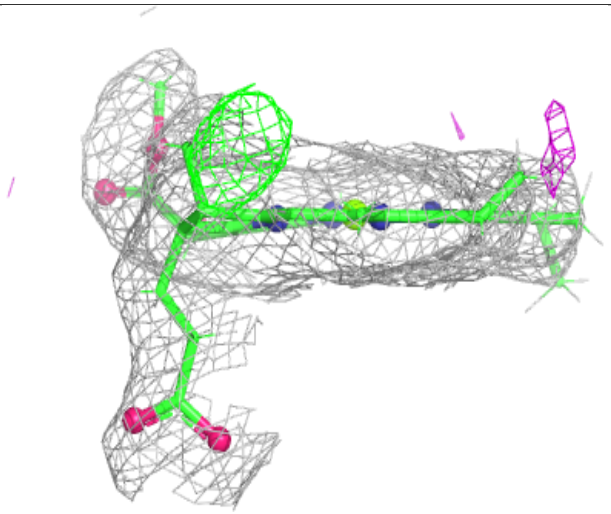


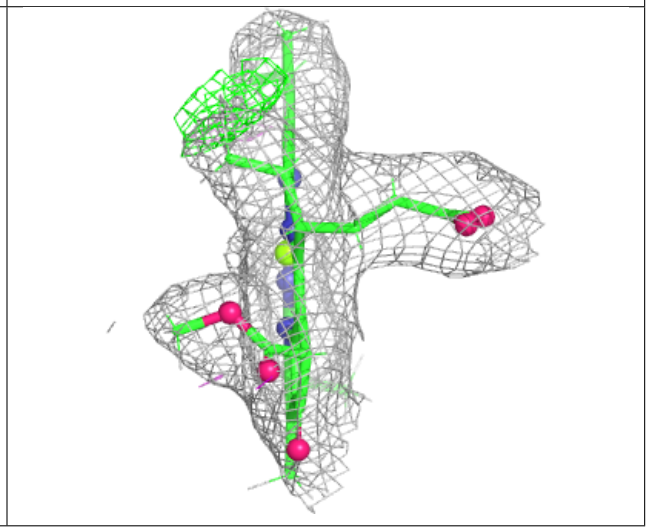


Electron density around CLA B 834:

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

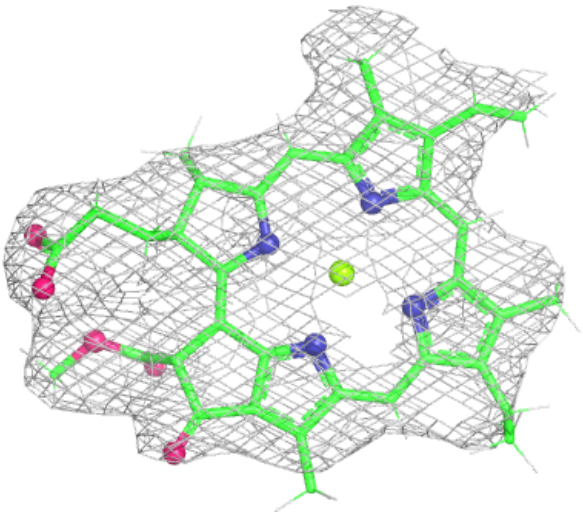


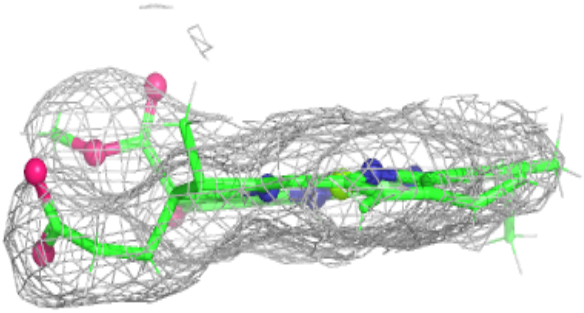




Electron density around CLA B 836:

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

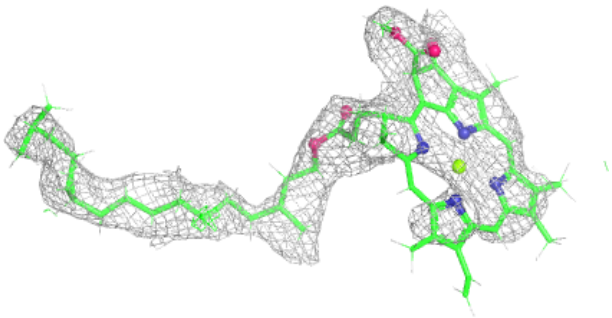


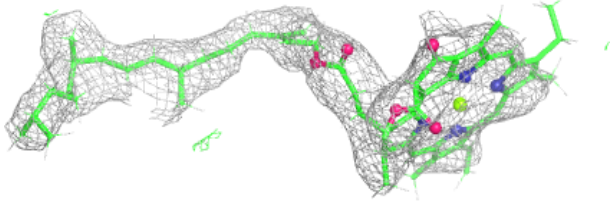




Electron density around CLA A 822:

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

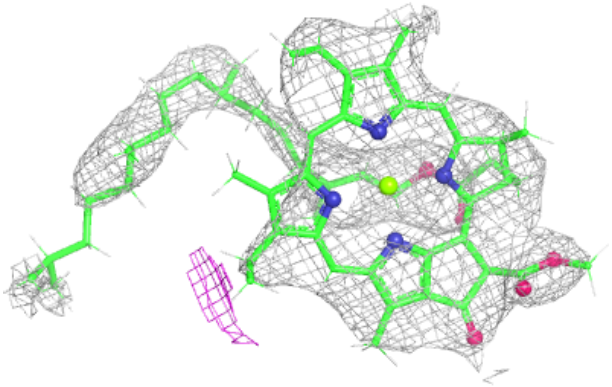


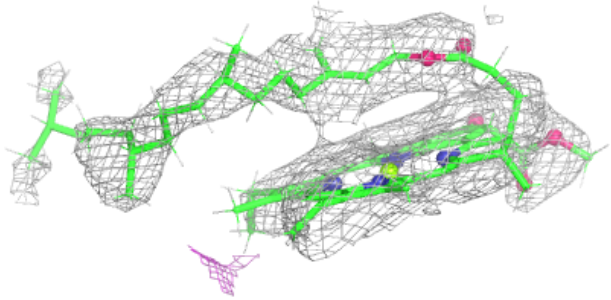




Electron density around CLA B 838:

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

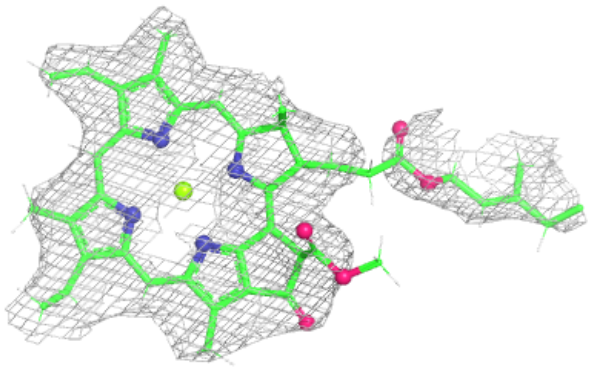


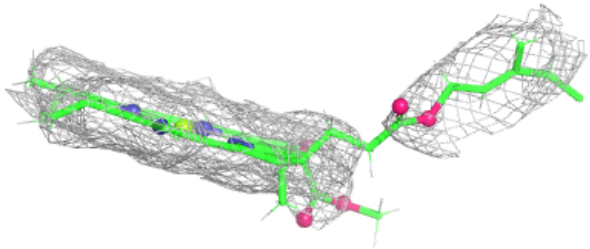


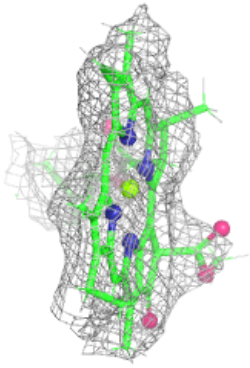


Electron density around CLA F 201:

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

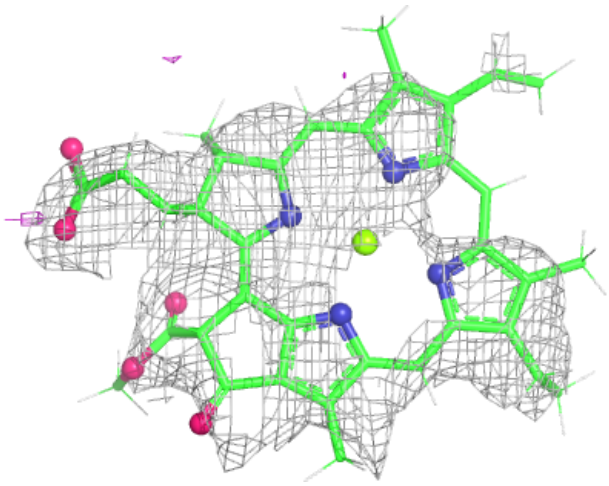


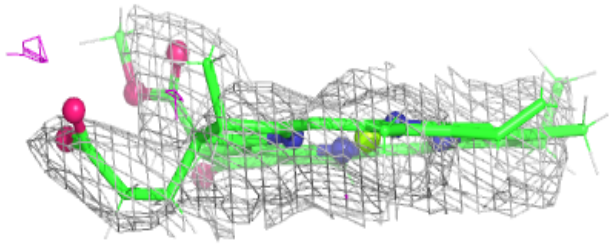


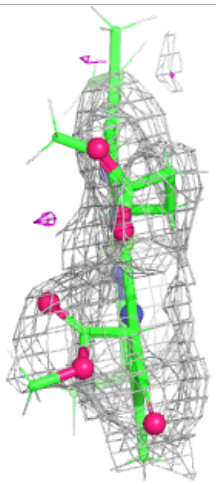


Electron density around CLA F 202:

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

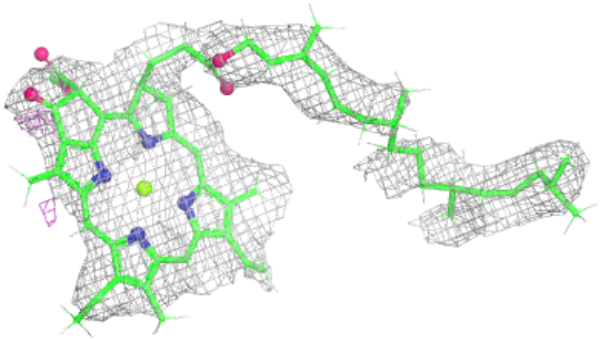


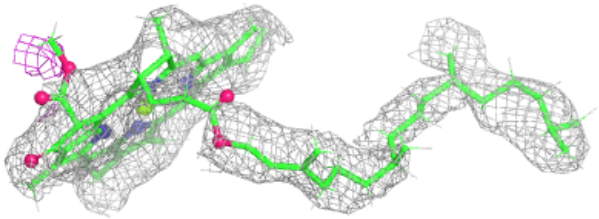


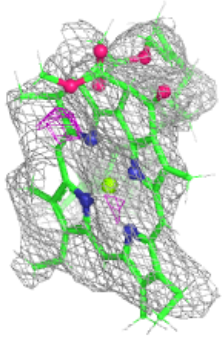


Electron density around CLA A 809:

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

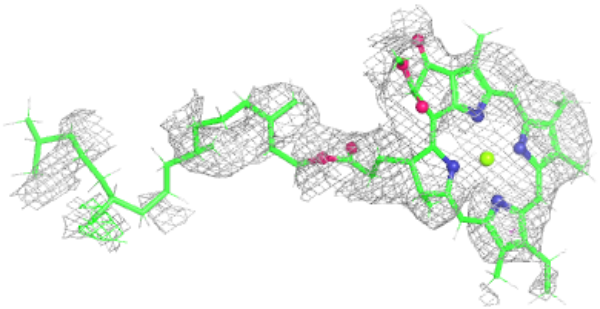


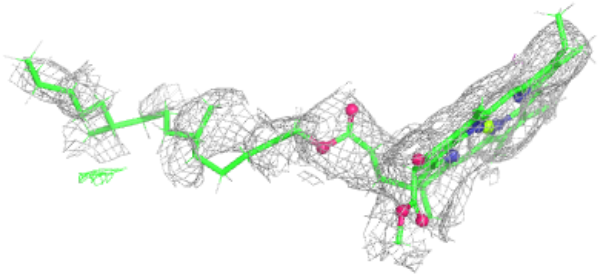


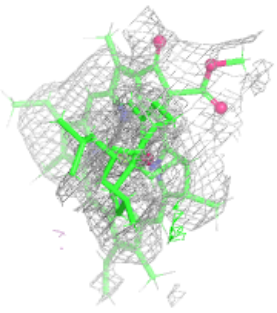


Electron density around CLA A 810:

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

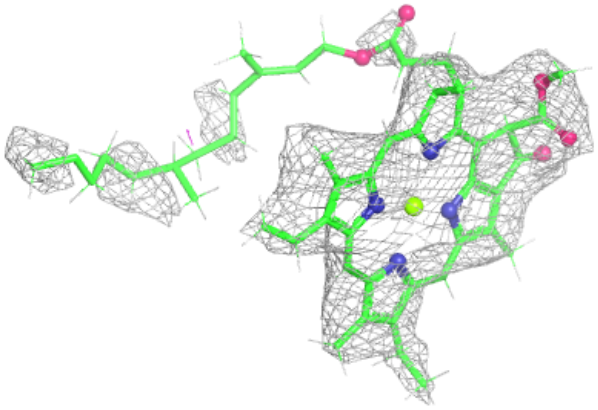


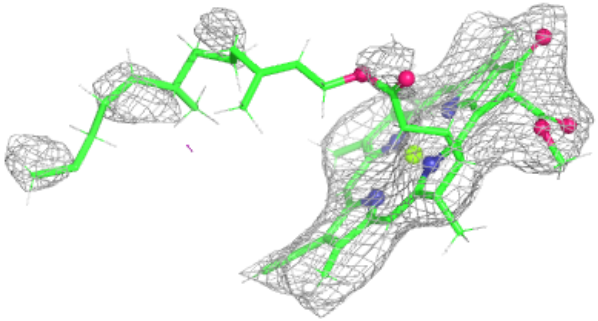


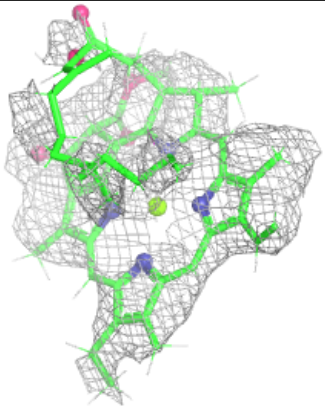


Electron density around CLA A 825:

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

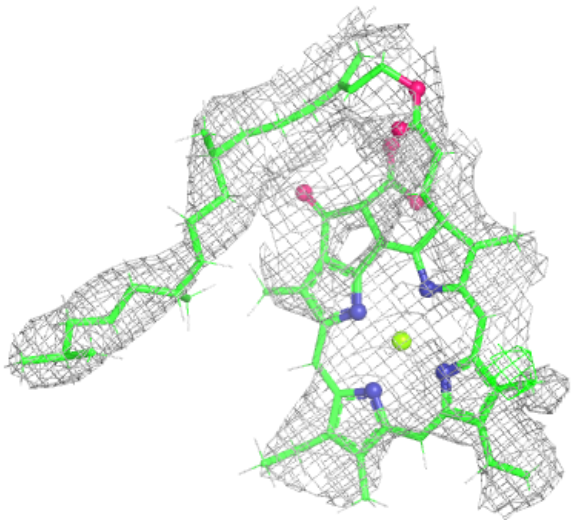


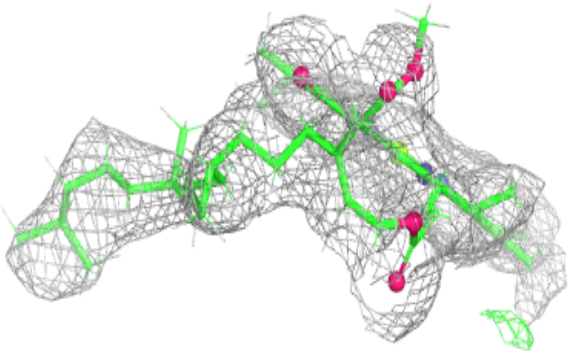




Electron density around CLA A 826:

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

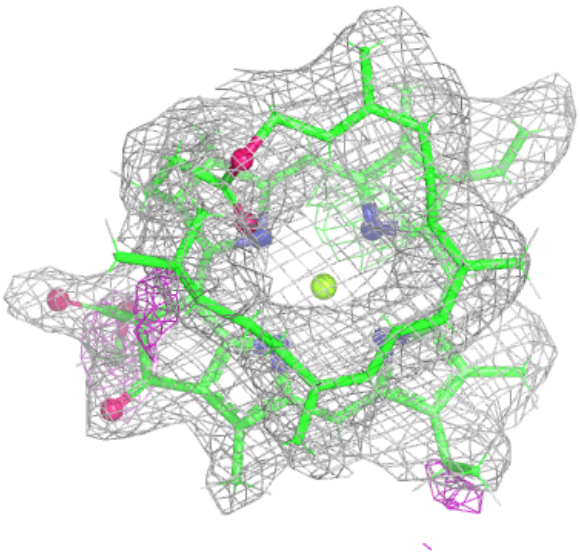


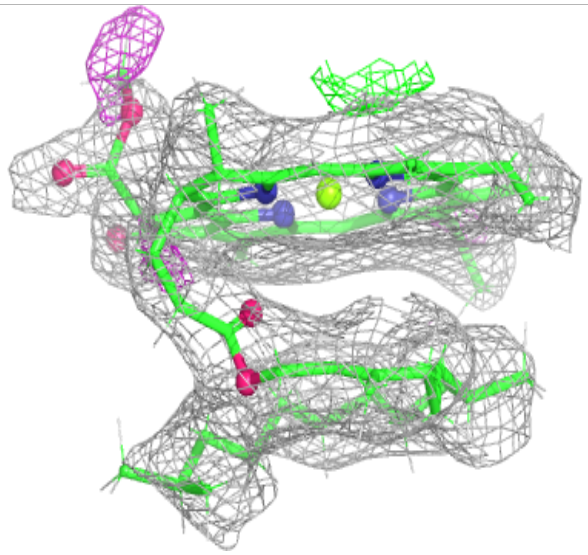


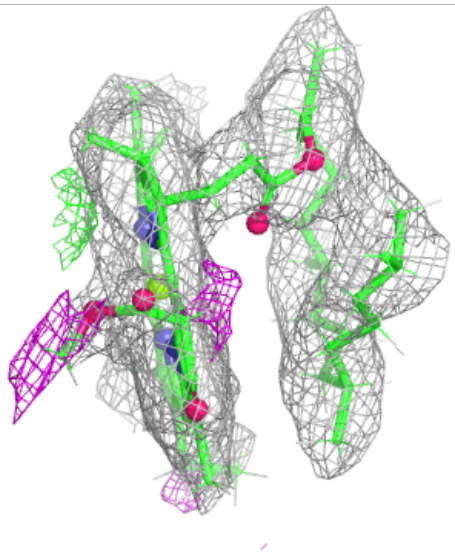


Electron density around CLA L 204:

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

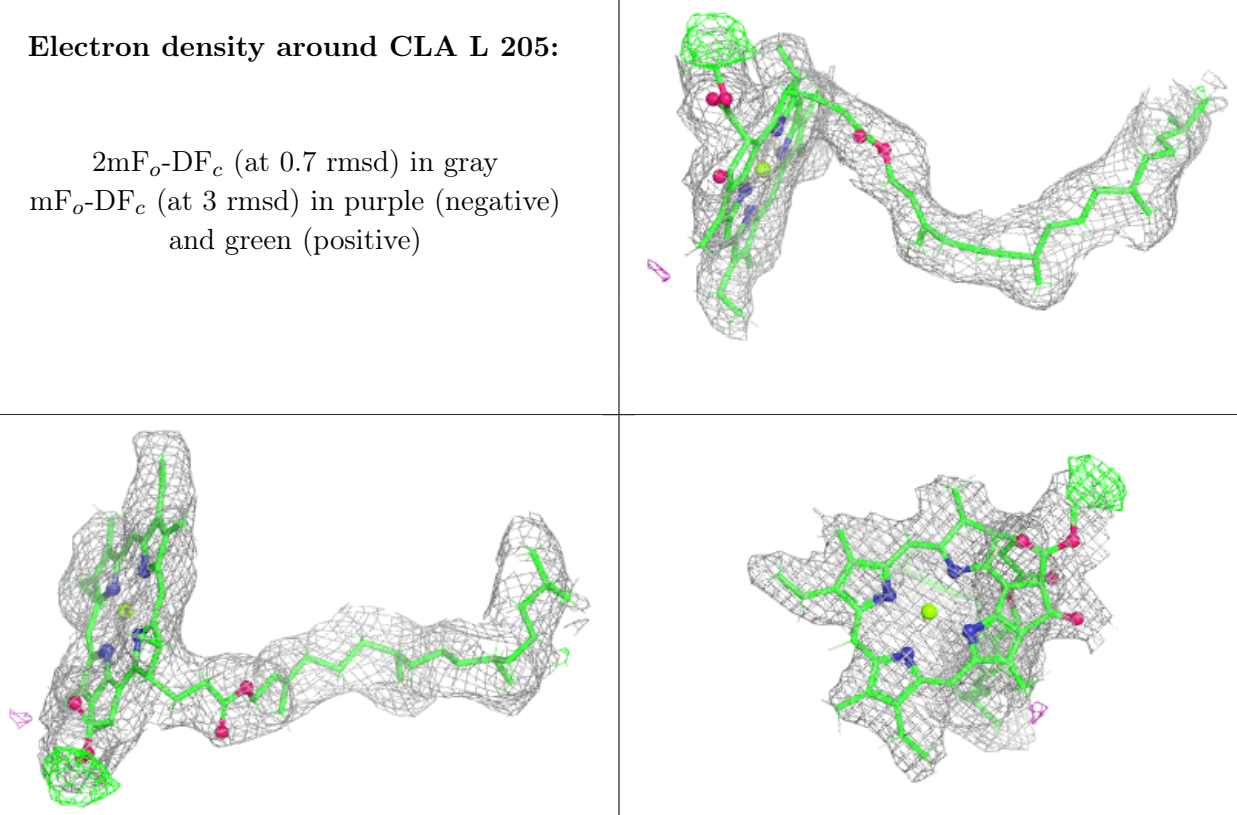






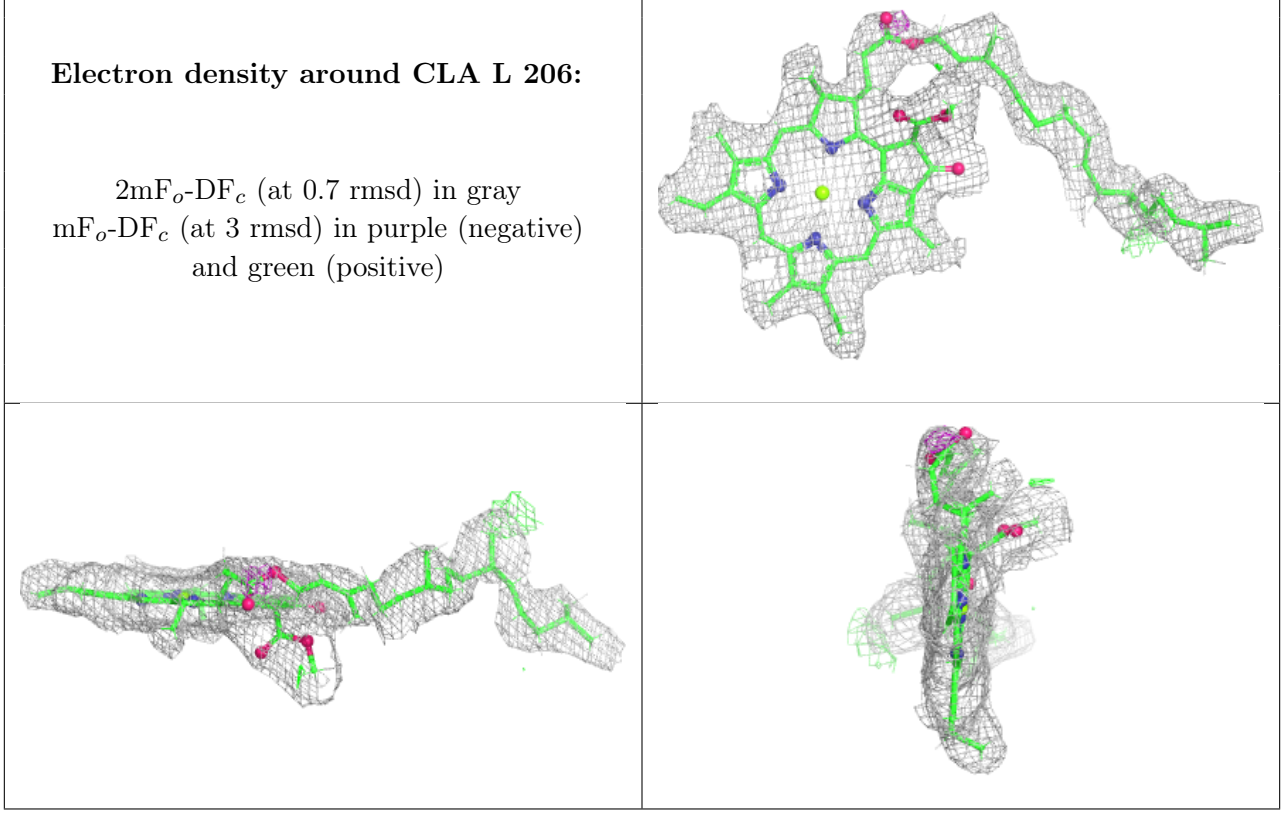
Electron density around CLA L 205:

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



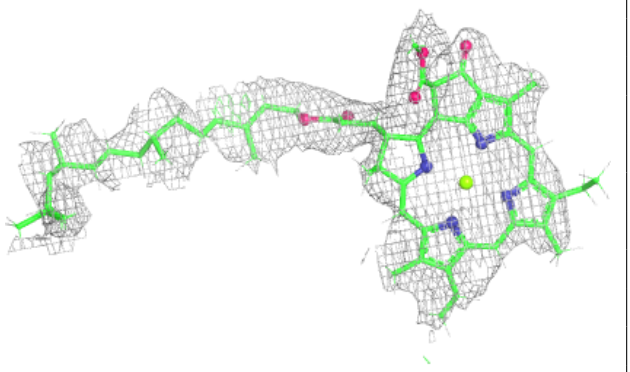
Electron density around CLA L 206:

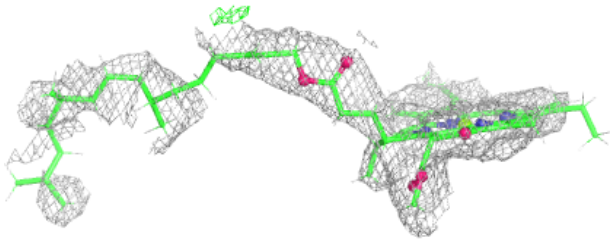
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

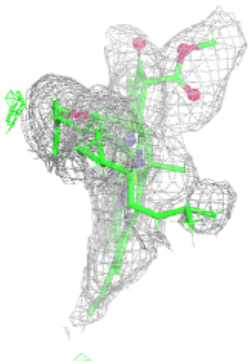


Electron density around CLA A 827:

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

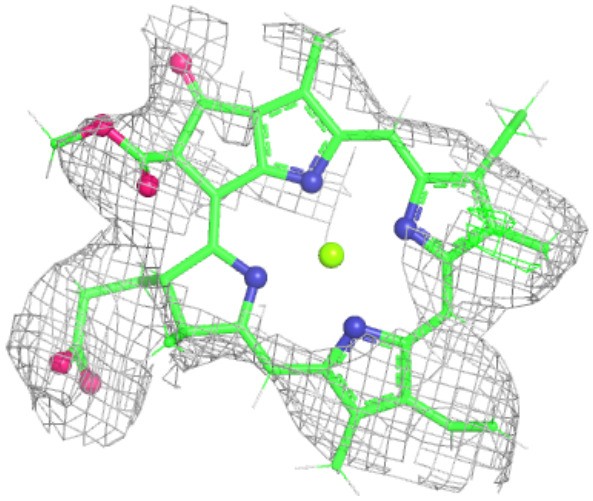


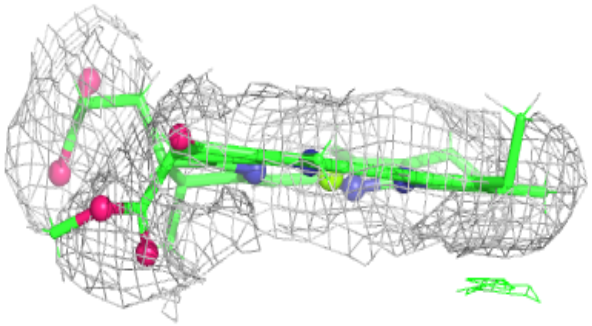


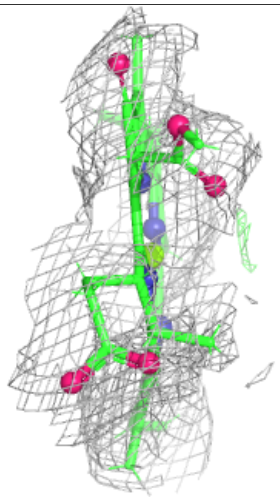


Electron density around CLA X 1701:

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

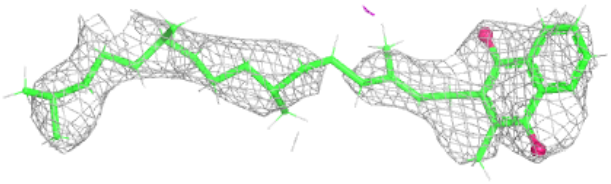


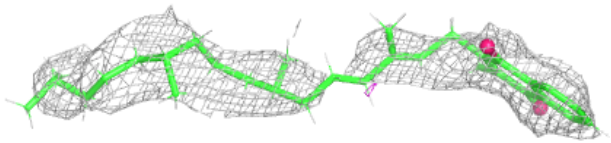


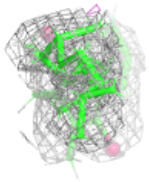


Electron density around PQN A 845:

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

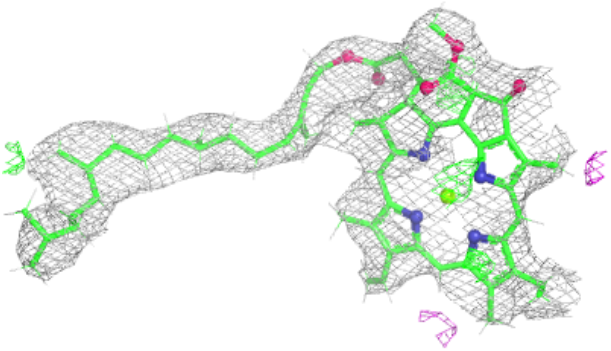


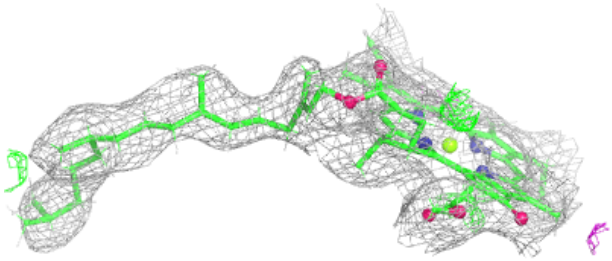


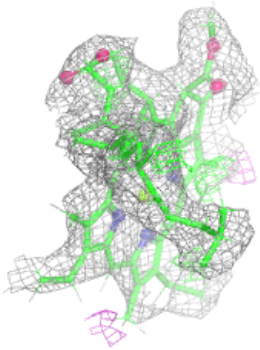


Electron density around CLA A 803:

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

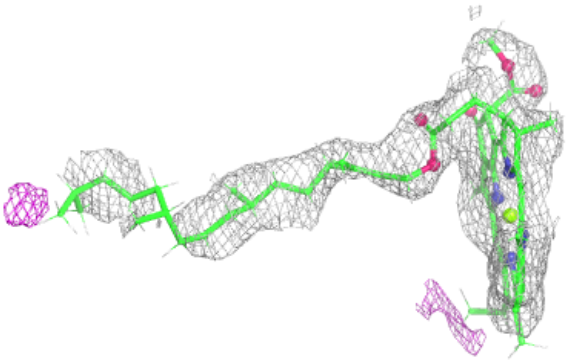


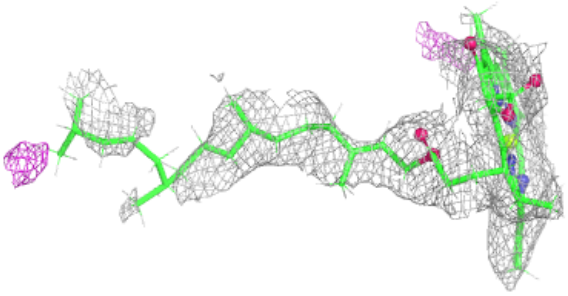


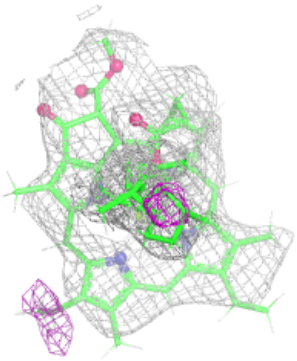


Electron density around CLA A 829:

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

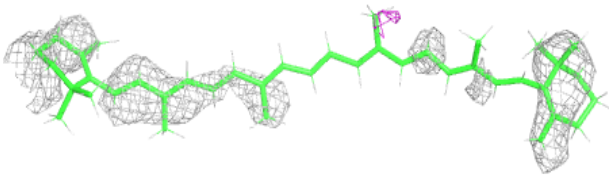


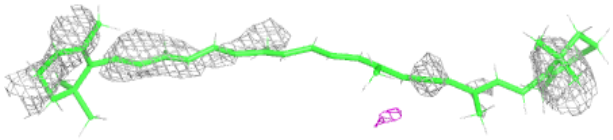


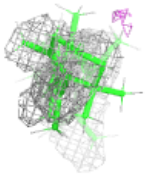


Electron density around BCR A 849:

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

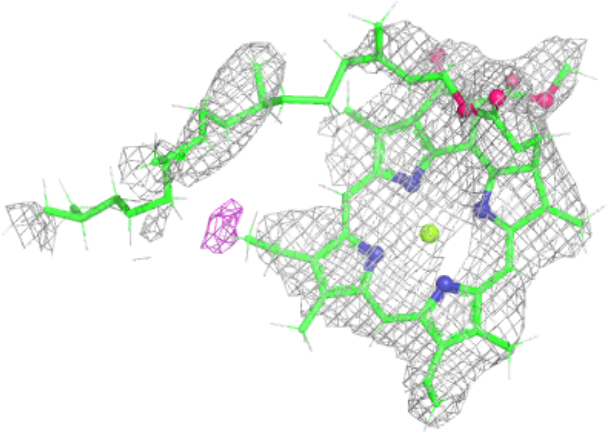


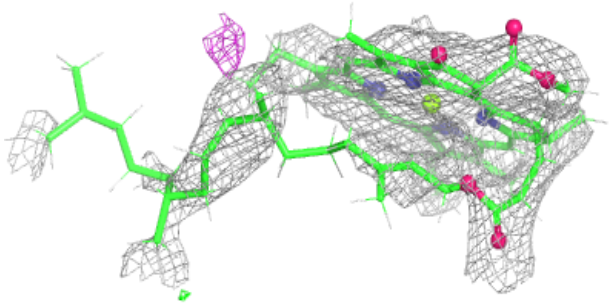


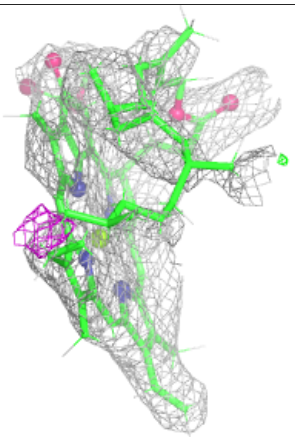


Electron density around CLA A 830:

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

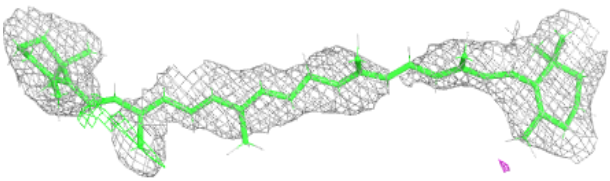


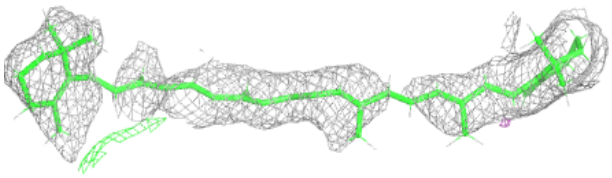


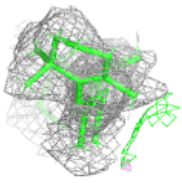


Electron density around BCR A 851:

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

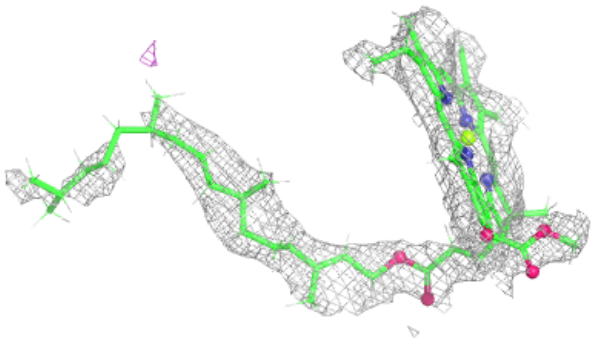


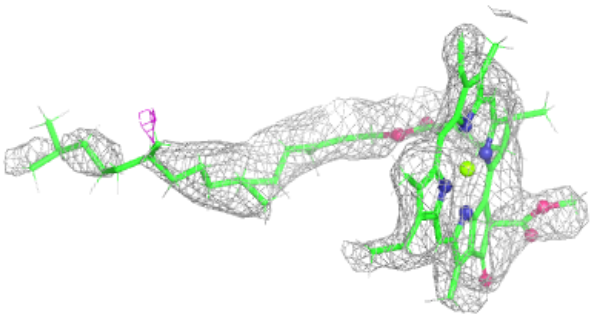


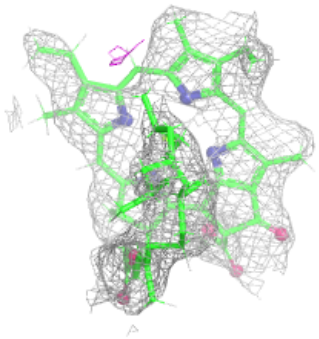


Electron density around CLA A 831:

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

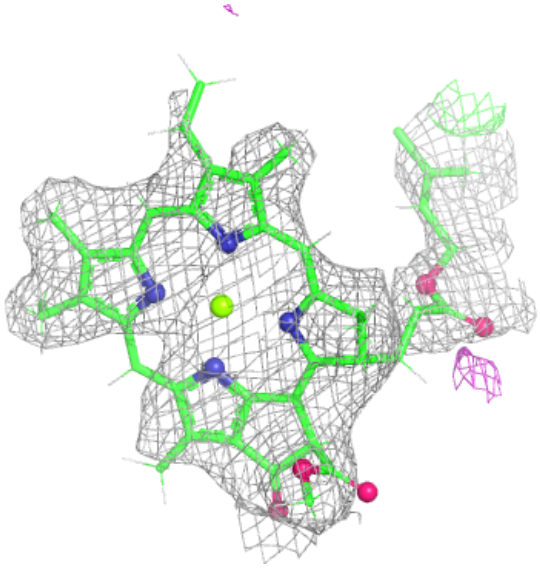


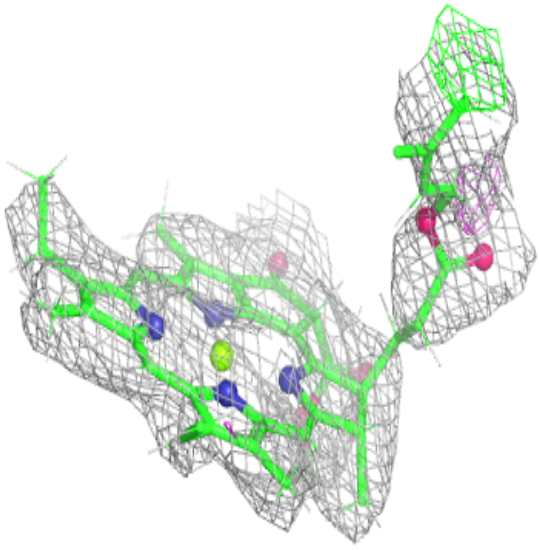


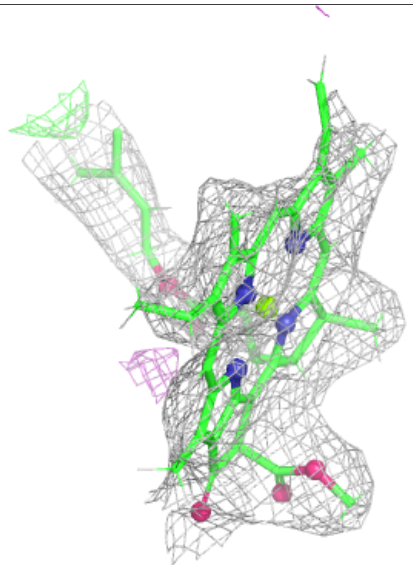


Electron density around CLA A 832:

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

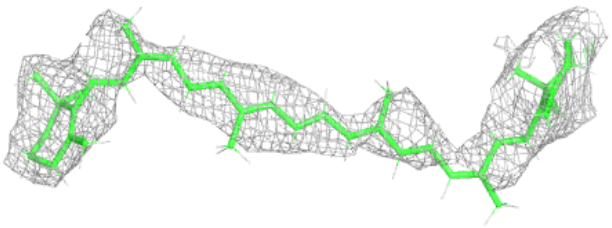


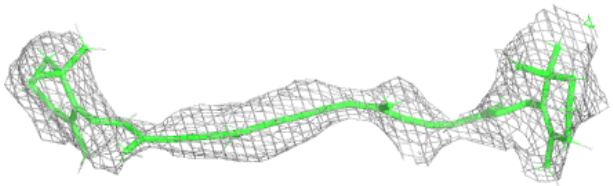


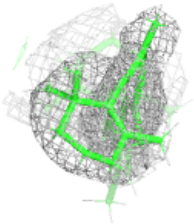


Electron density around BCR B 845:

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

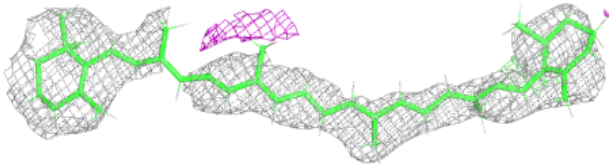


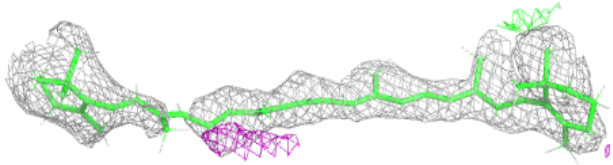


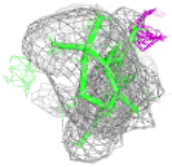


Electron density around BCR B 846:

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

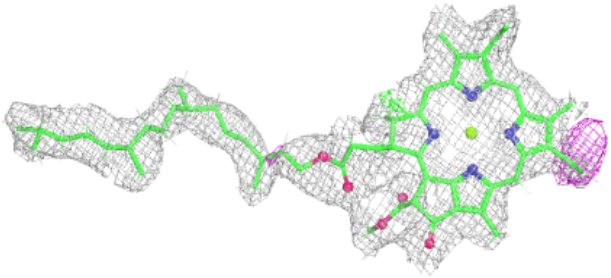


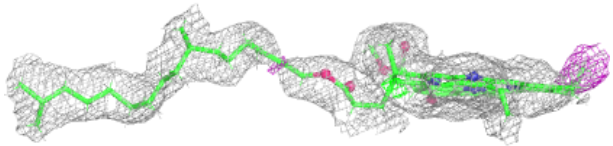


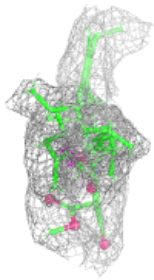


Electron density around CLA A 834:

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

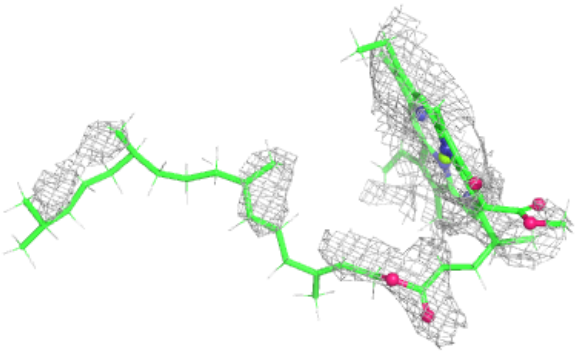


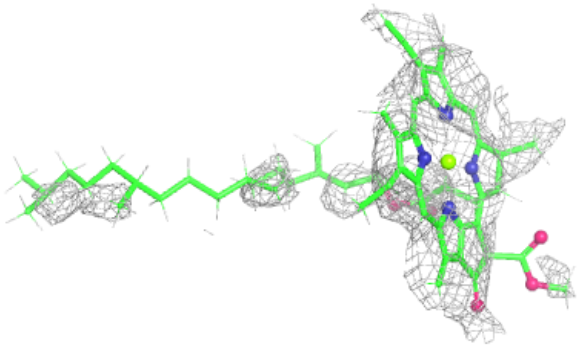


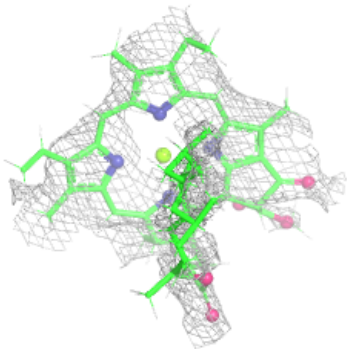


Electron density around CLA A 812:

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

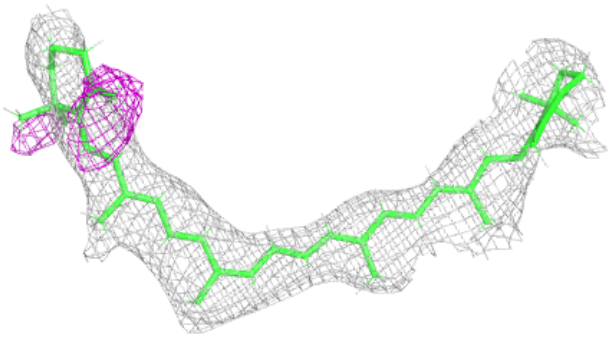


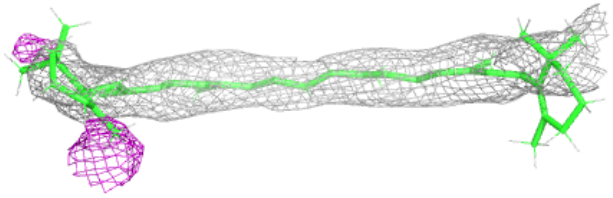


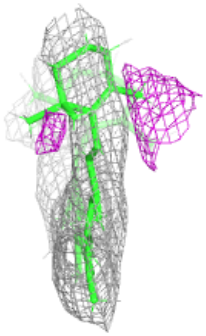


Electron density around BCR F 203:

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



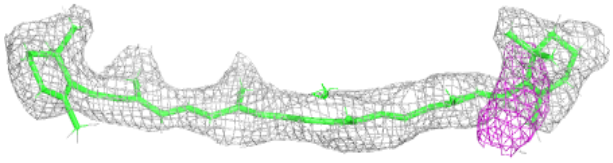


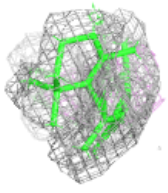


Electron density around BCR I 101:

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

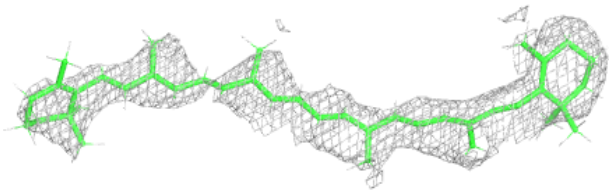


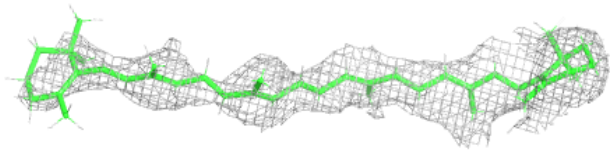


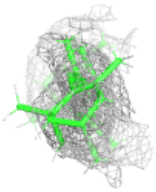


Electron density around BCR J 103:

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

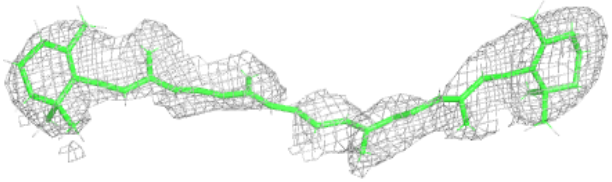


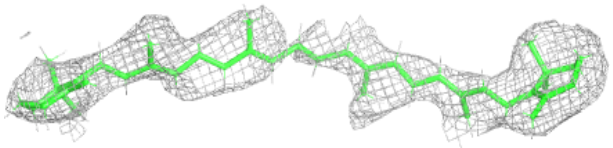


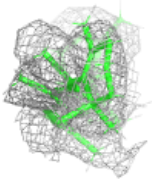


Electron density around BCR J 104:

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

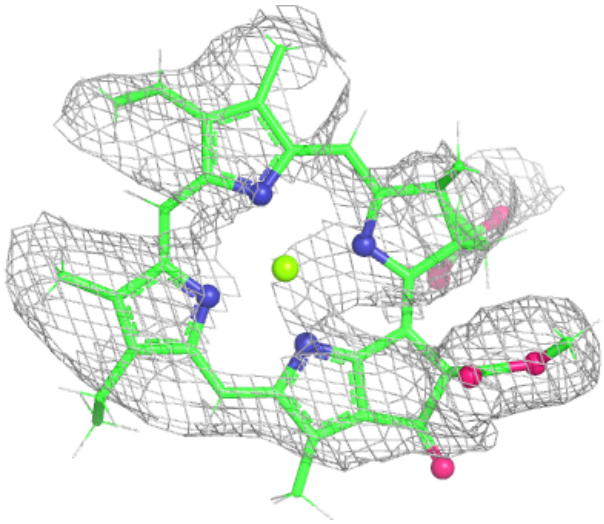


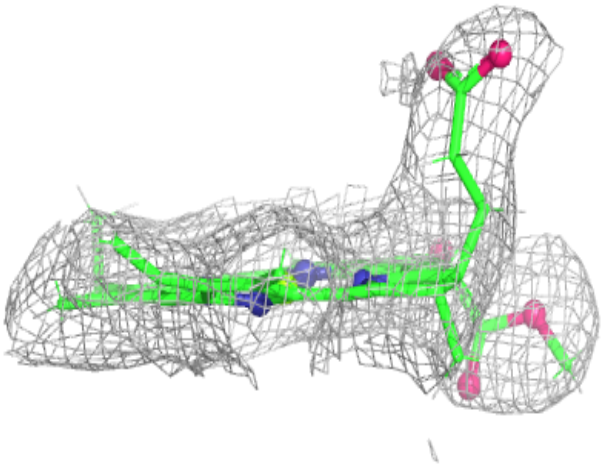


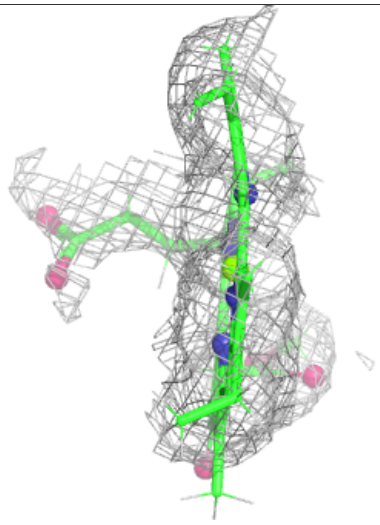


Electron density around CLA A 837:

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

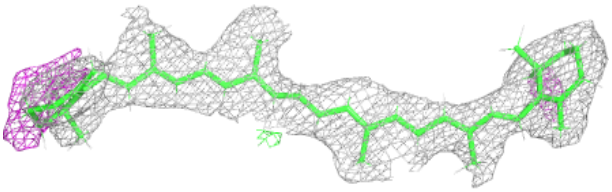


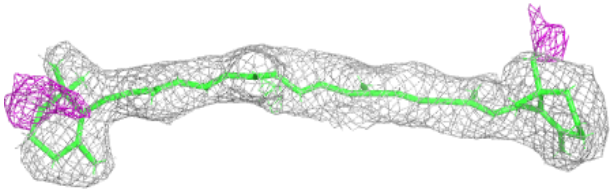


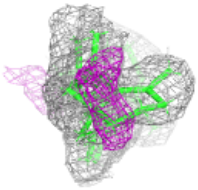


Electron density around BCR M 103:

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

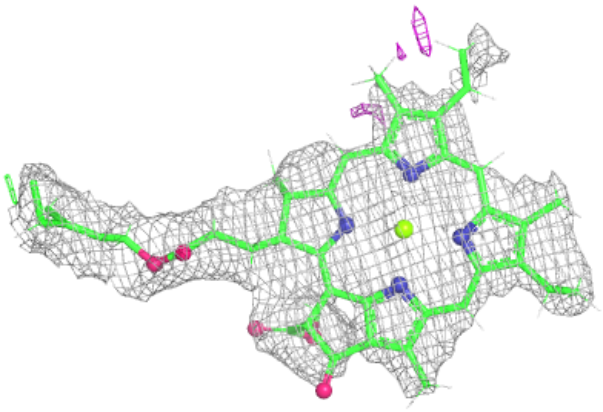


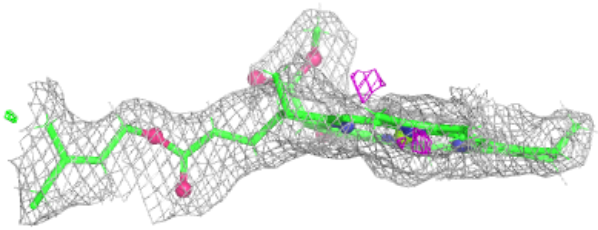


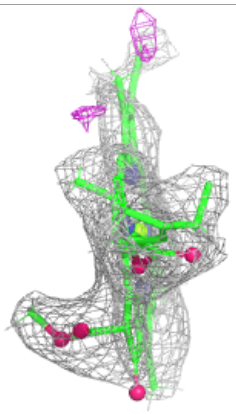


Electron density around CLA A 838:

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

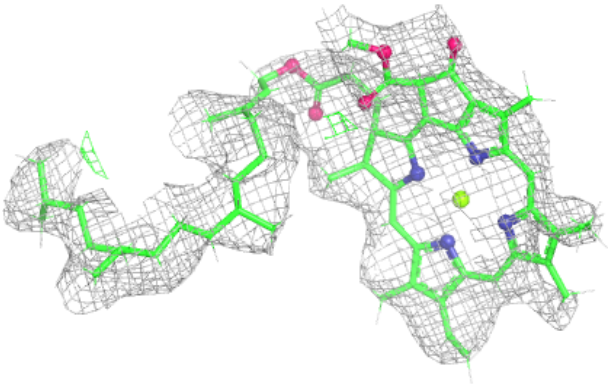


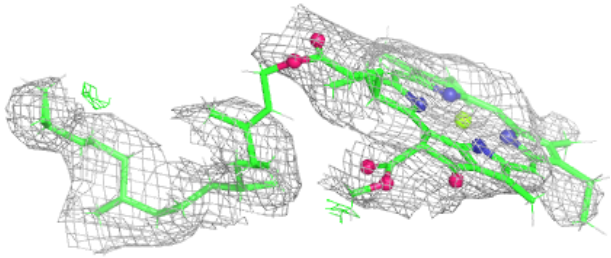


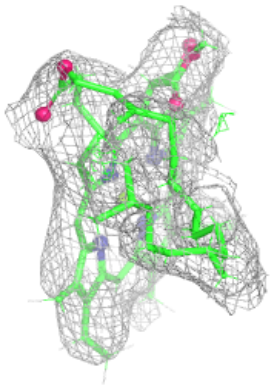


Electron density around CLA A 804:

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

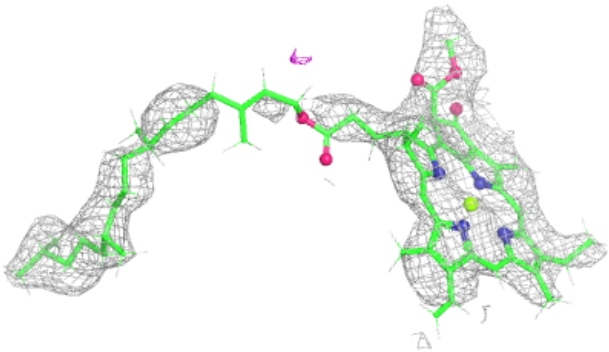


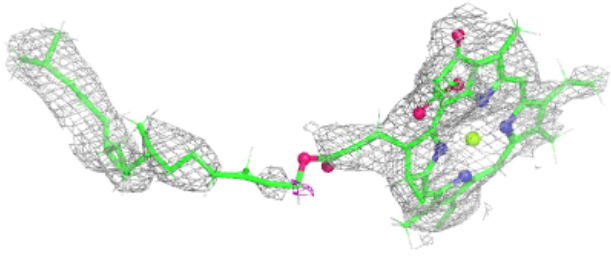




Electron density around CLA A 857:

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

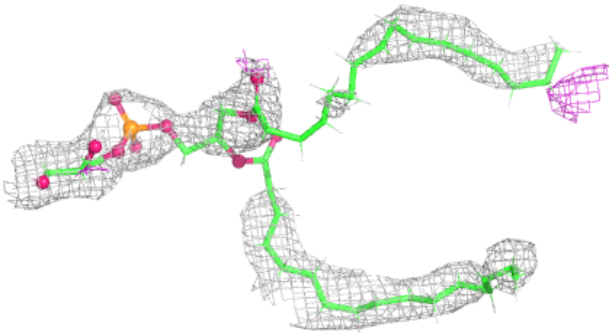


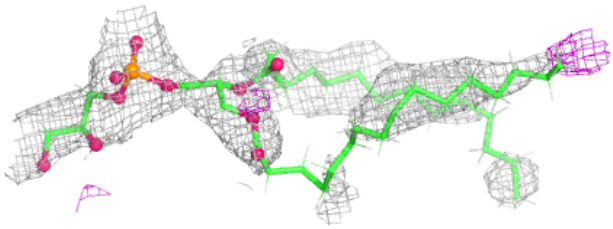


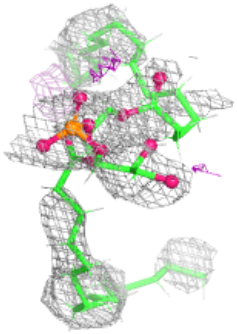


Electron density around LHG A 854:

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

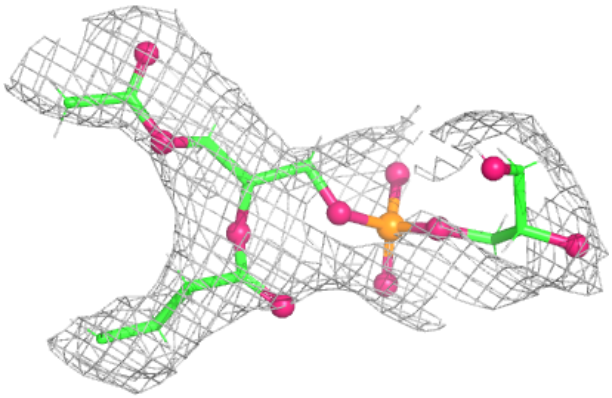


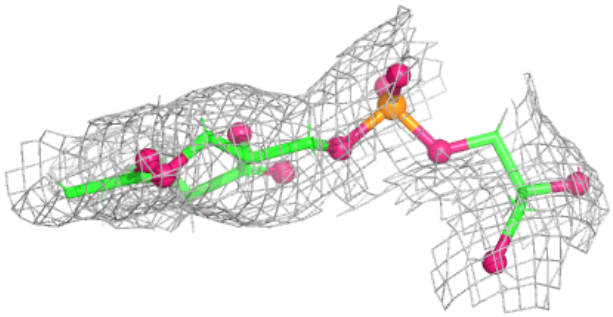


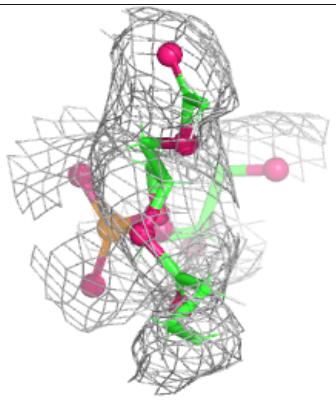


Electron density around LHG B 850:

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

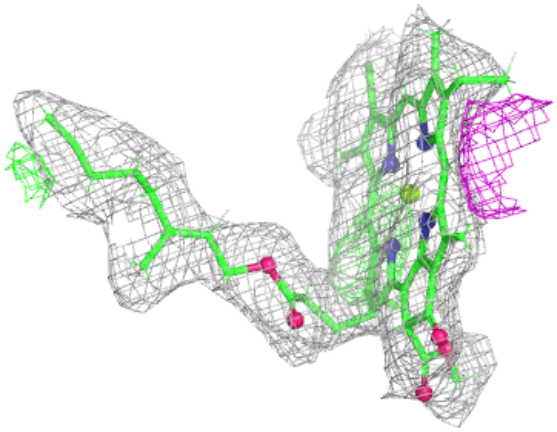


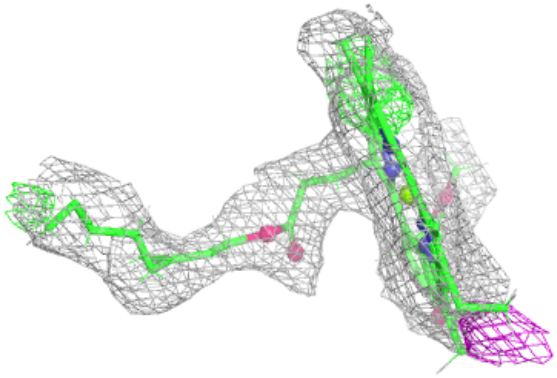


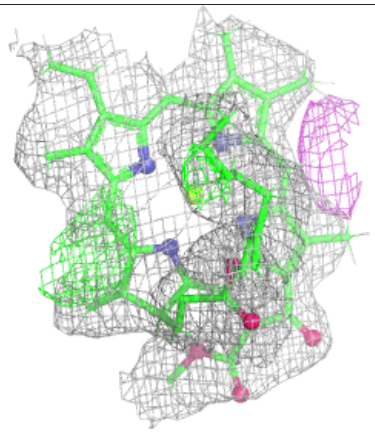


Electron density around CLA B 804:

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

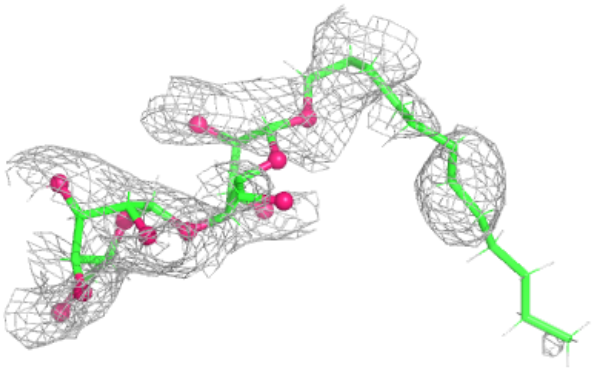


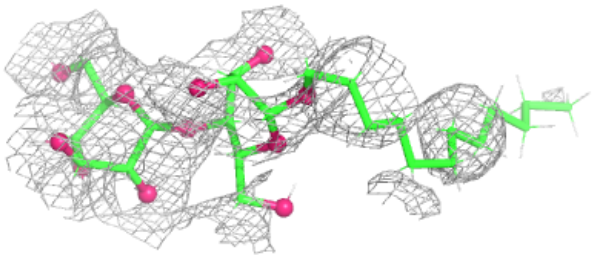


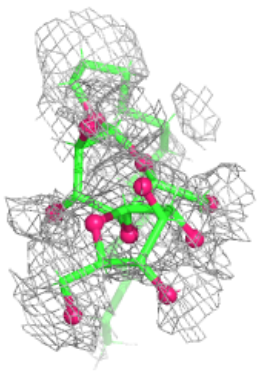


Electron density around LMT L 202:

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

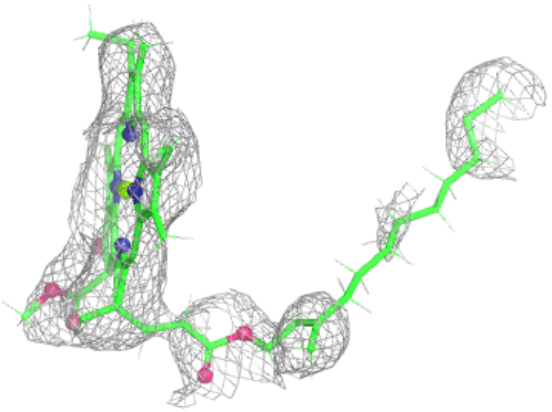


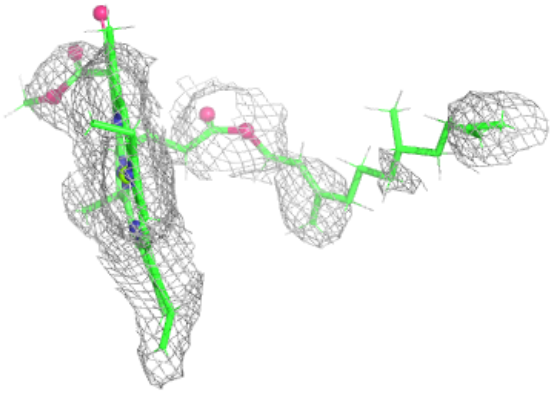


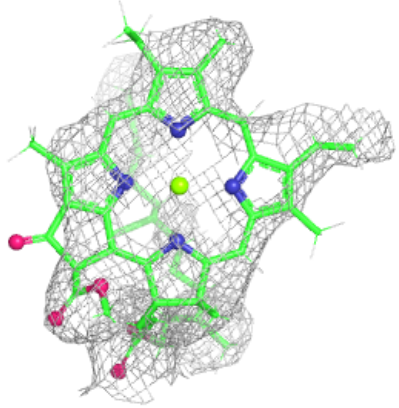


Electron density around CLA A 805:

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

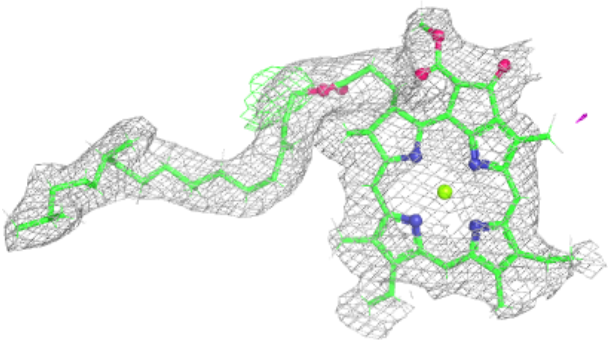


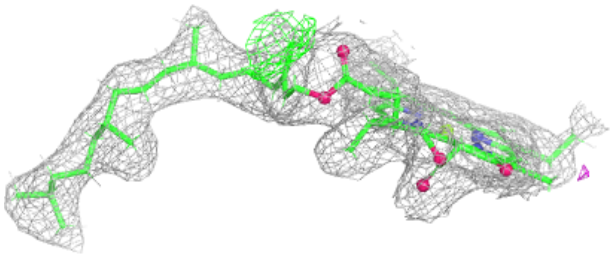


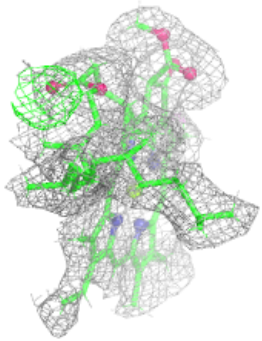


Electron density around CLA B 803:

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

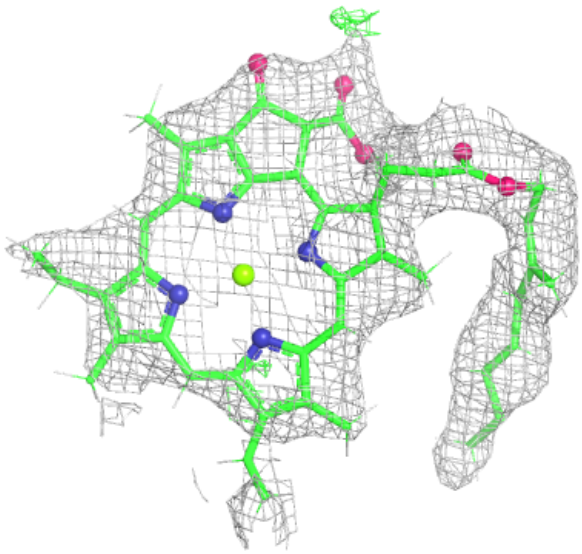


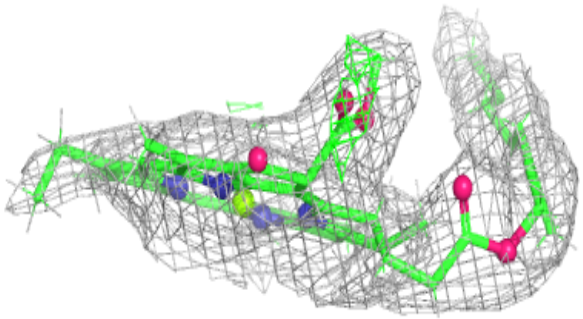


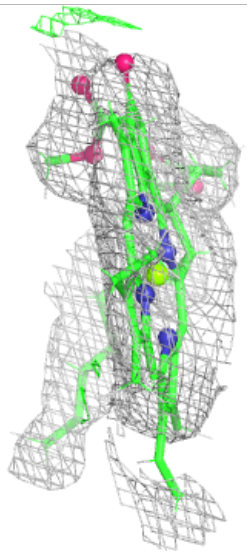


Electron density around CLA B 824:

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

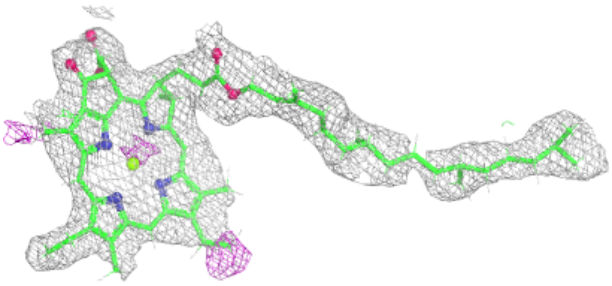


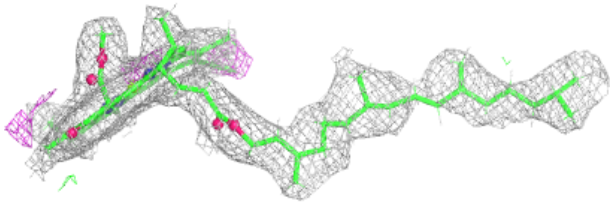


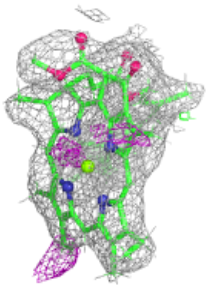


Electron density around CLA A 835:

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

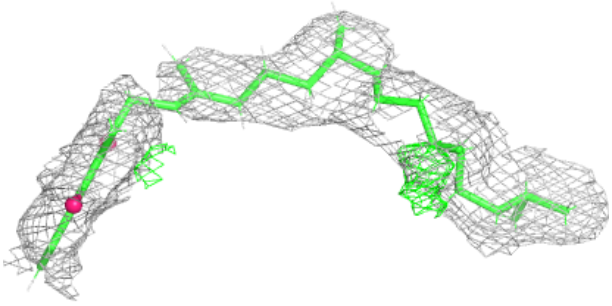


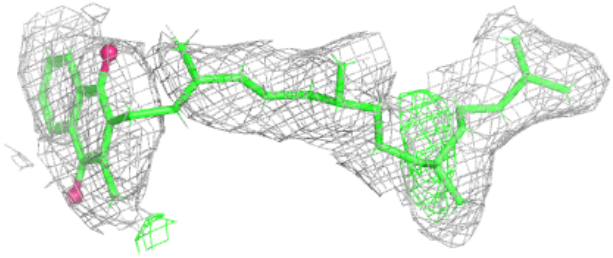




Electron density around PQN B 842:

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

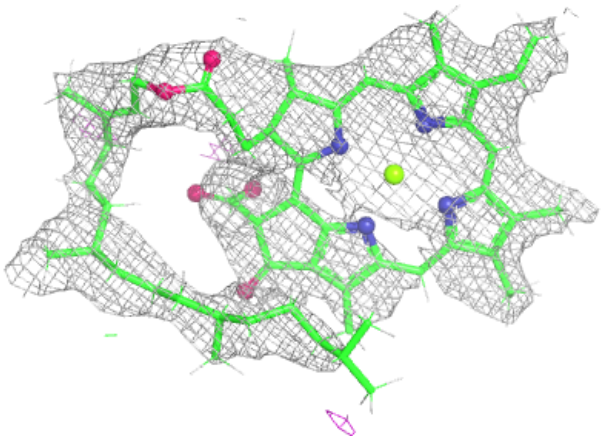


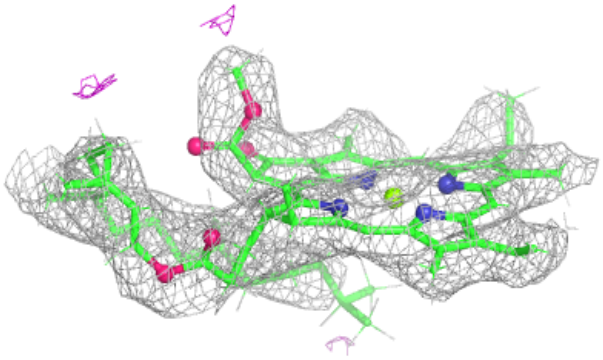


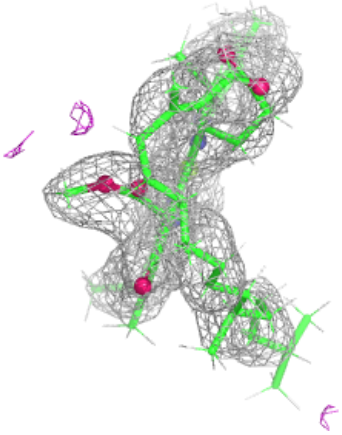


Electron density around CLA B 805:

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

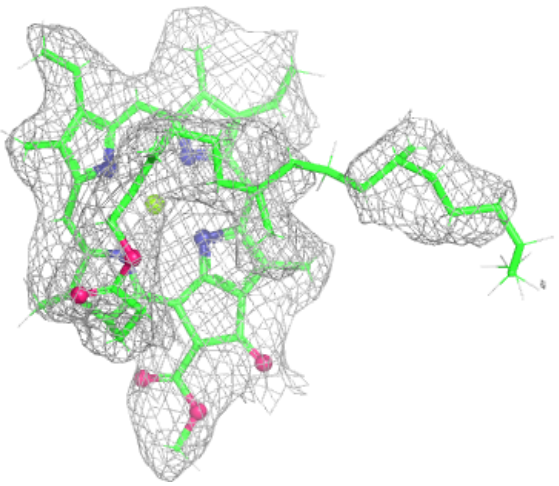


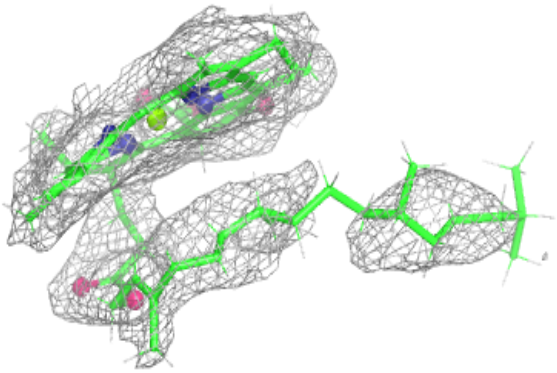


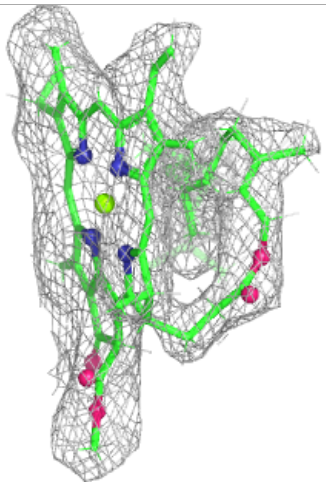


Electron density around CLA B 827:

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

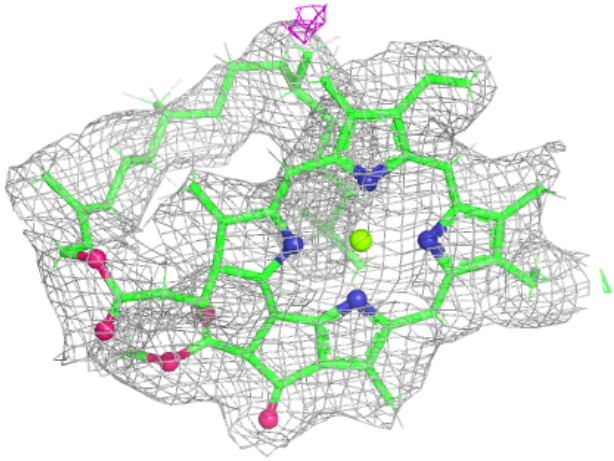


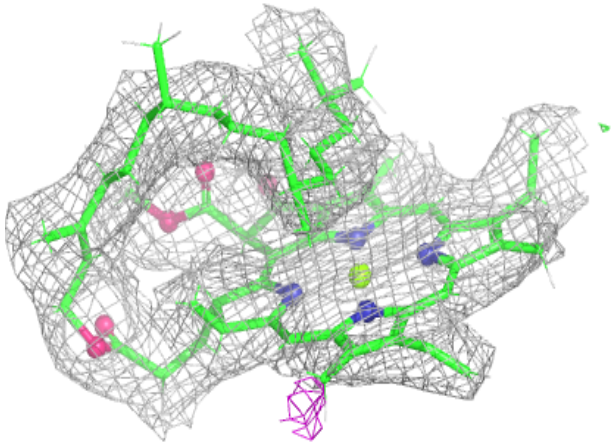


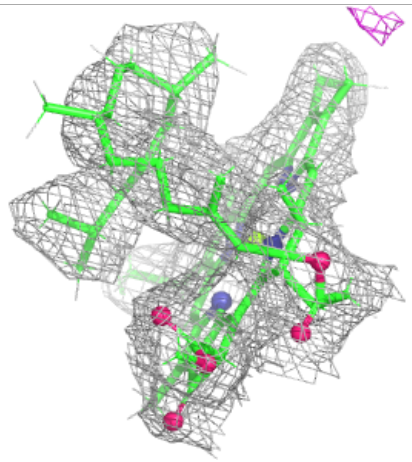


Electron density around CLA B 806:

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

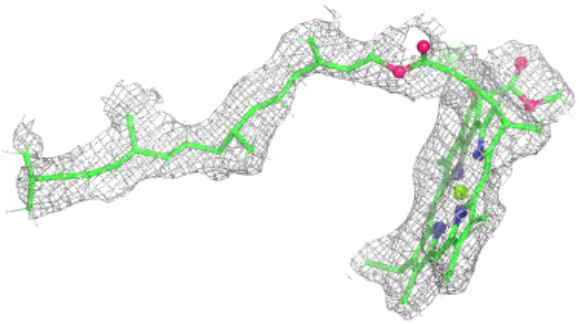


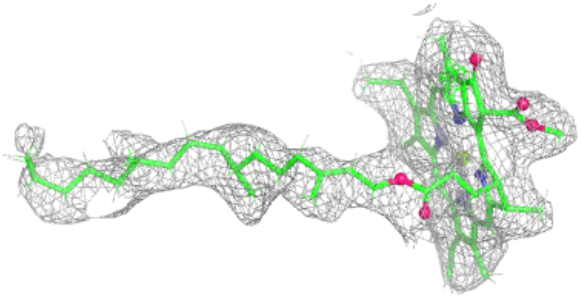


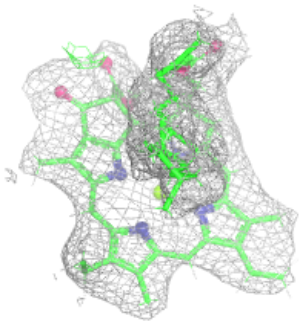


Electron density around CLA B 829:

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

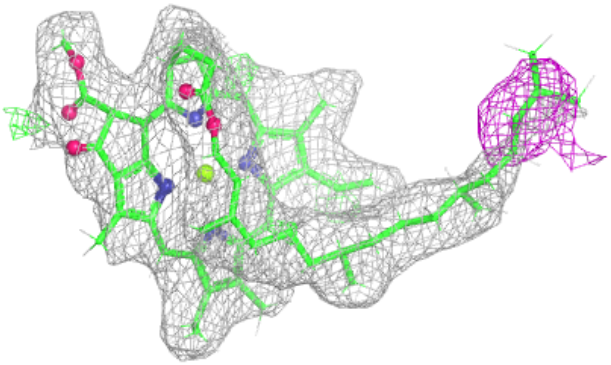


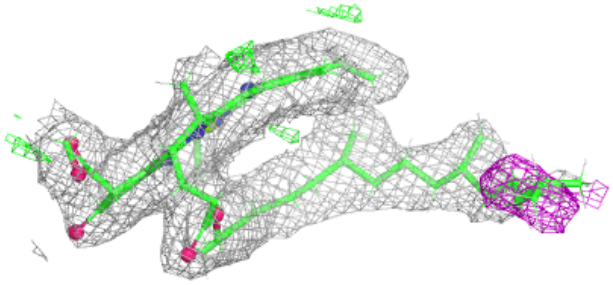


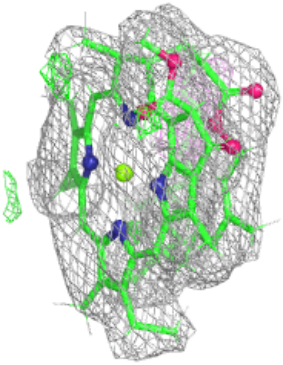


Electron density around CLA B 807:

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

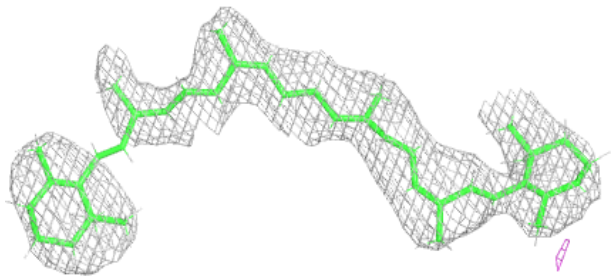


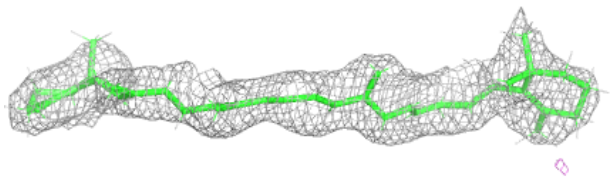


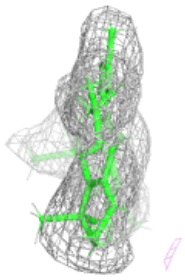


Electron density around BCR A 852:

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

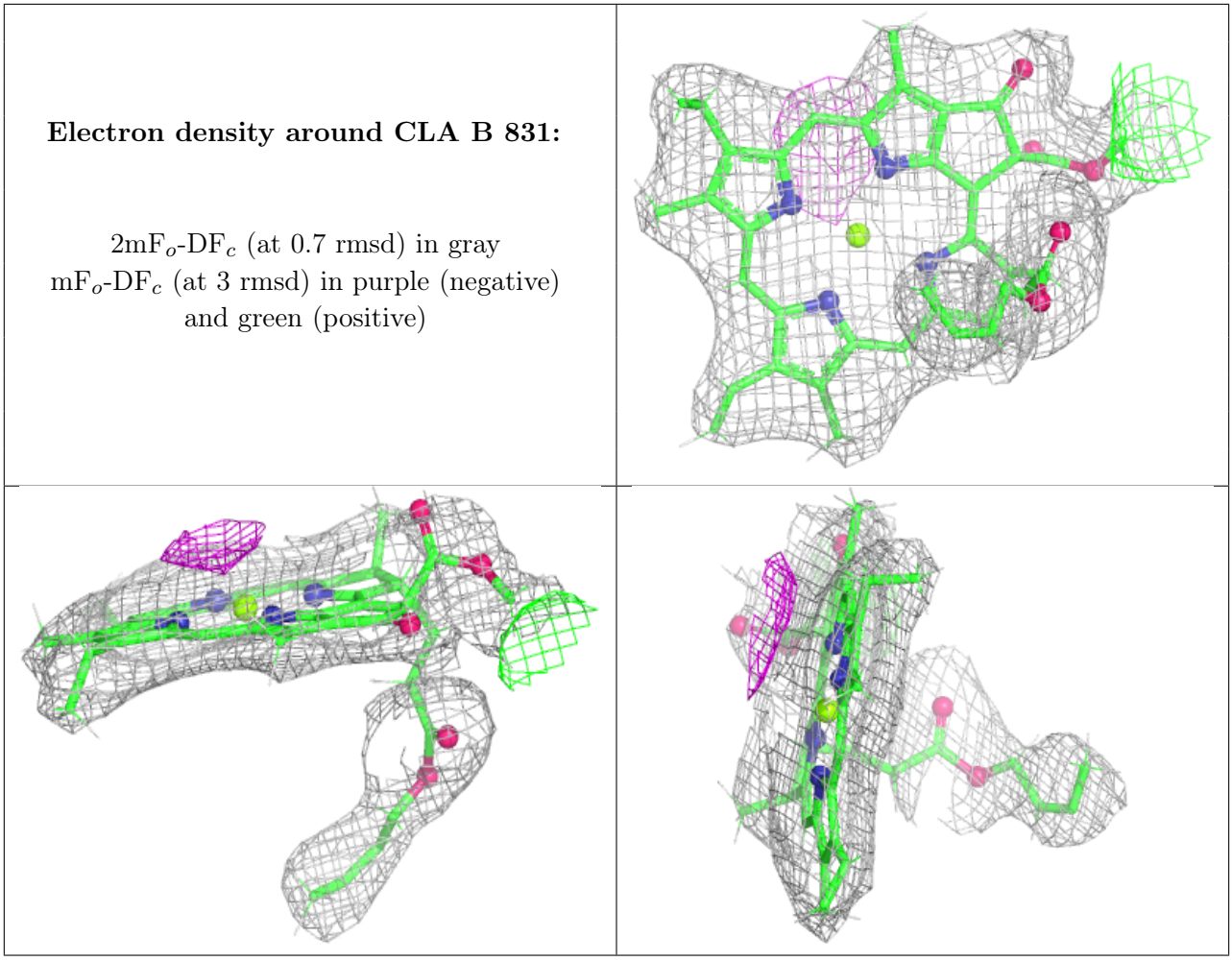






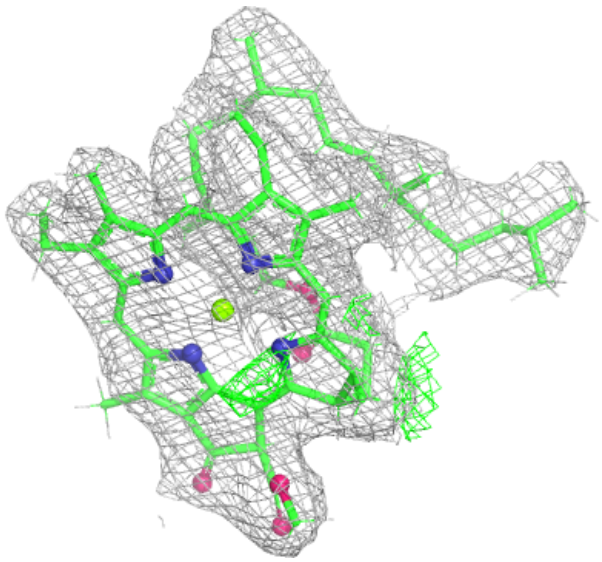
Electron density around CLA B 831:

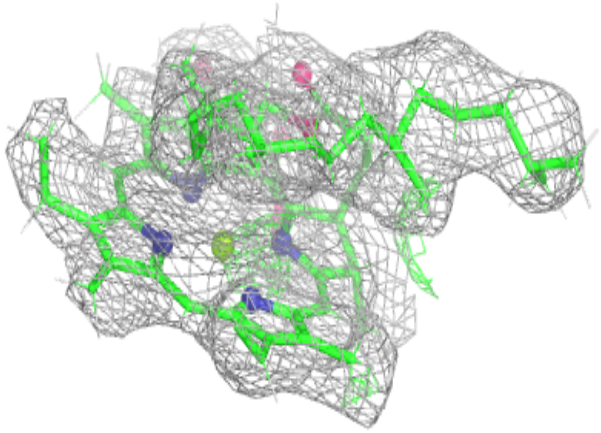
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

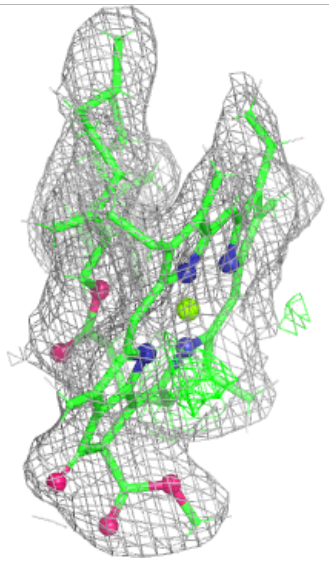


Electron density around CLA B 808:

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

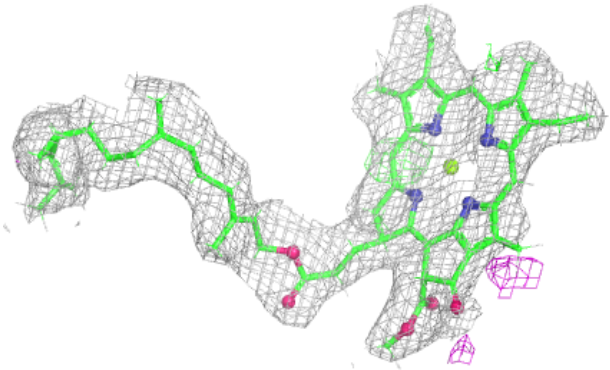


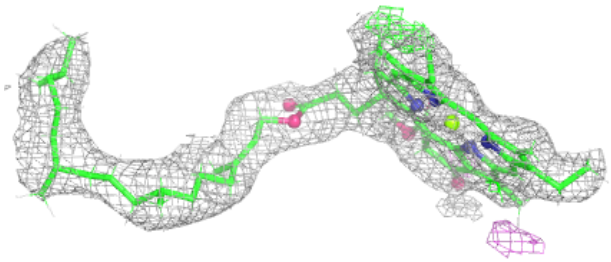


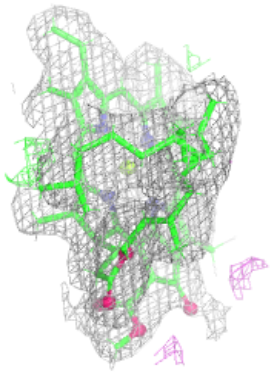


Electron density around CLA B 809:

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

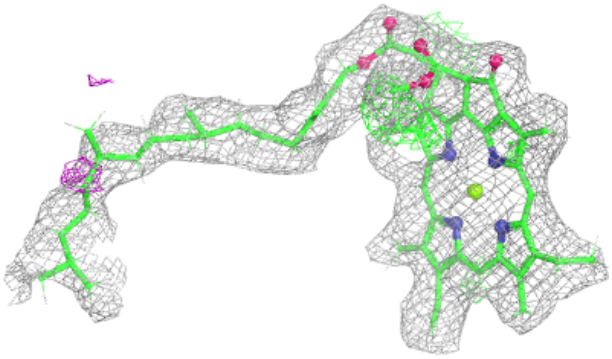


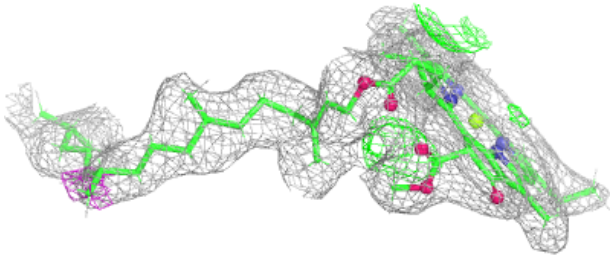


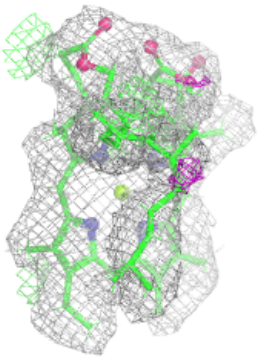


Electron density around CLA B 810:

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

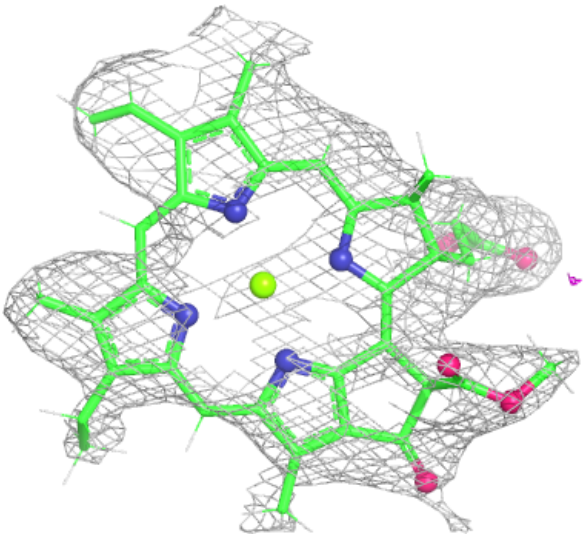


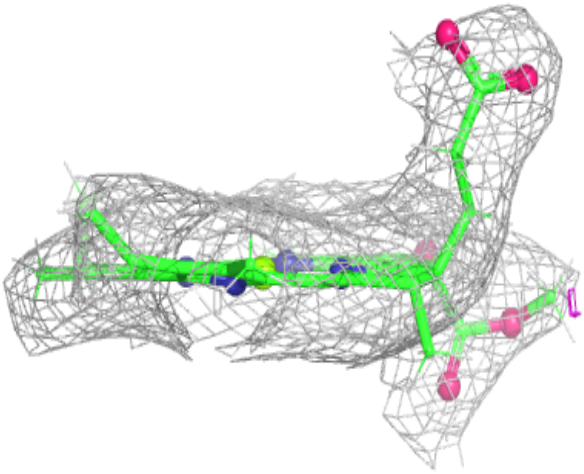


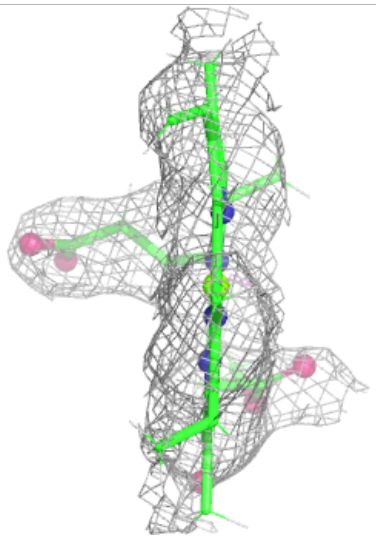


Electron density around CLA B 835:

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

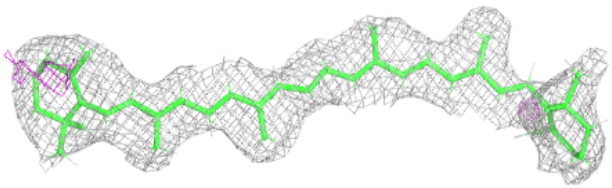


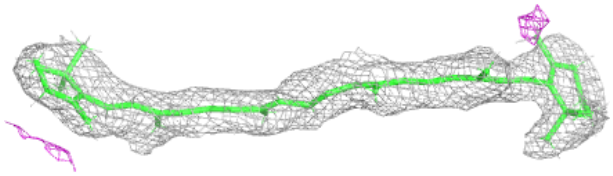


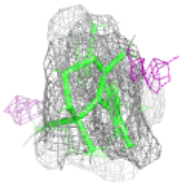


Electron density around BCR B 848:

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

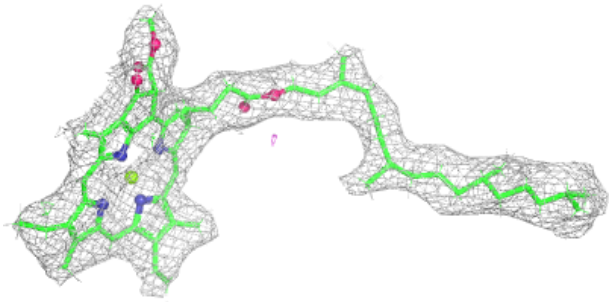


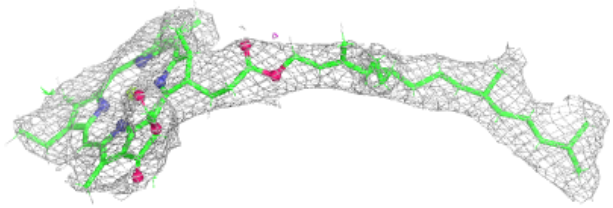


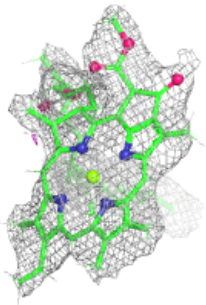


Electron density around CLA A 802:

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

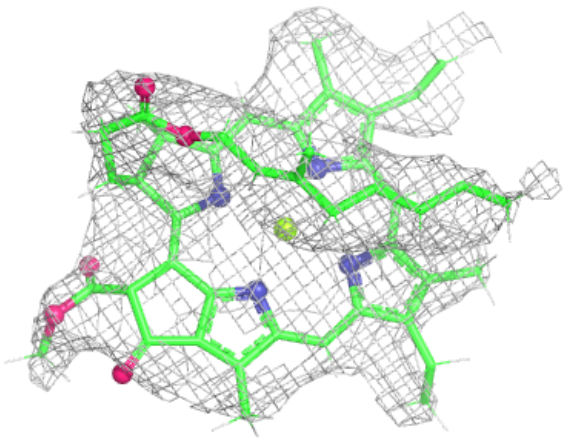


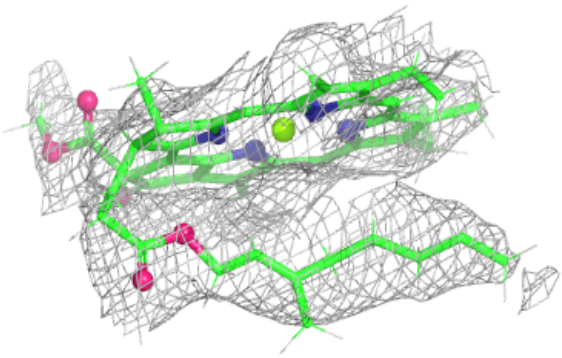


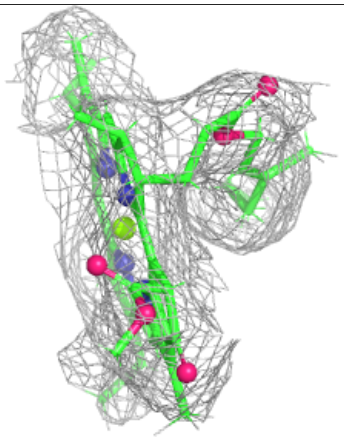


Electron density around CLA A 819:

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

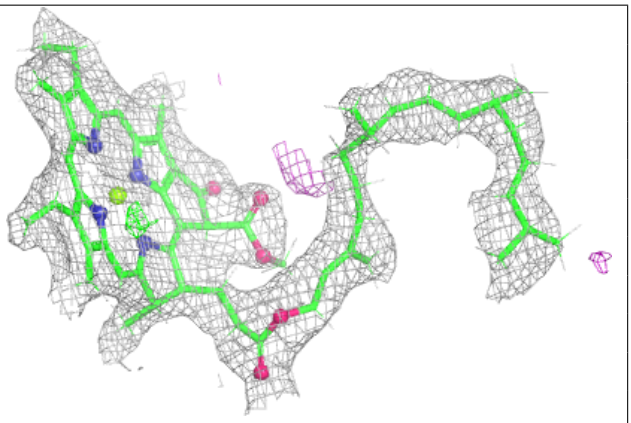


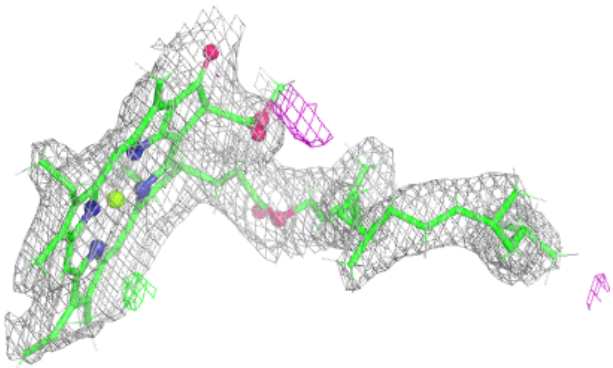


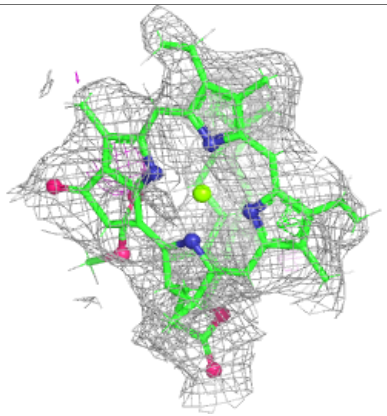


Electron density around CL0 A 801:

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

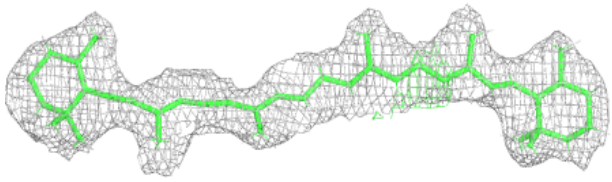


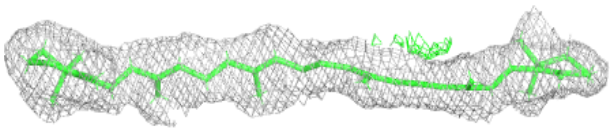


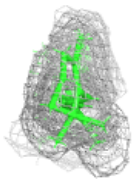


Electron density around BCR I 103:

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

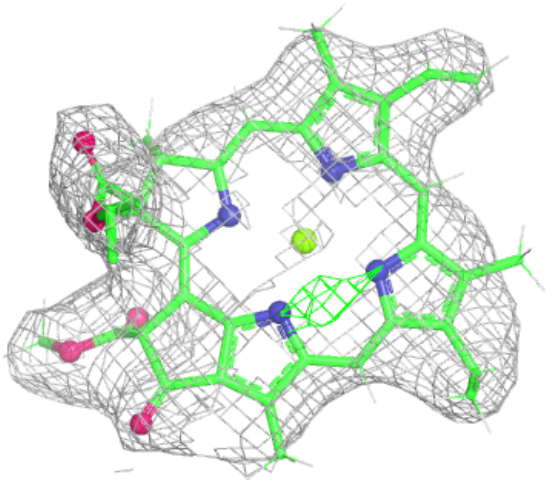


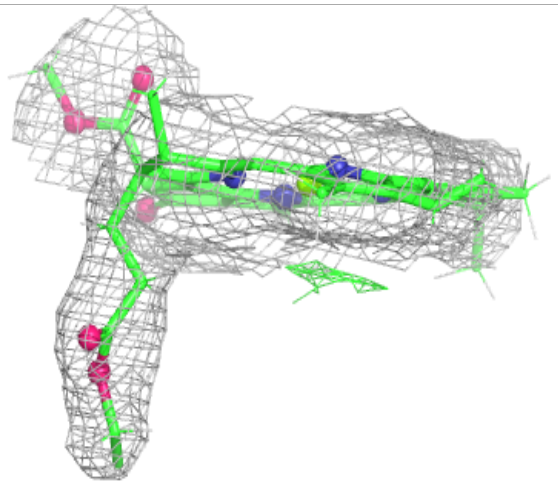


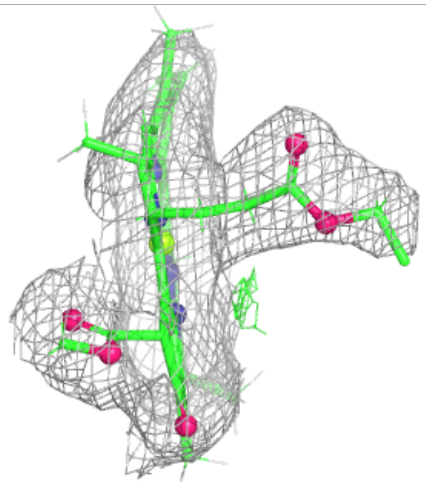


Electron density around CLA B 839:

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

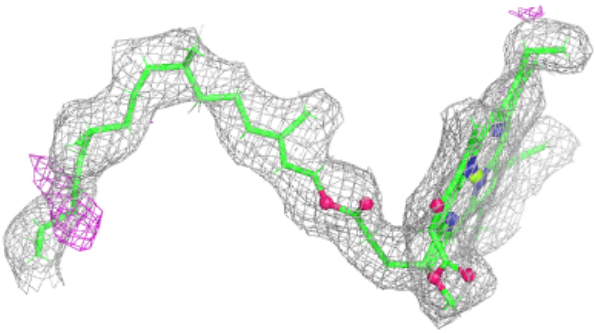


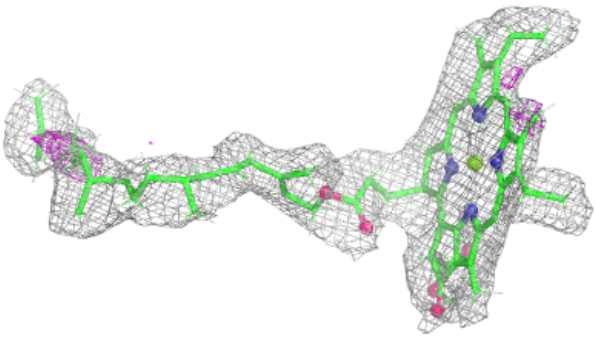


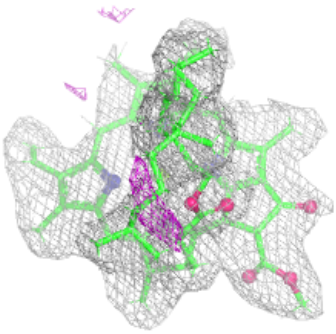


Electron density around CLA B 840:

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

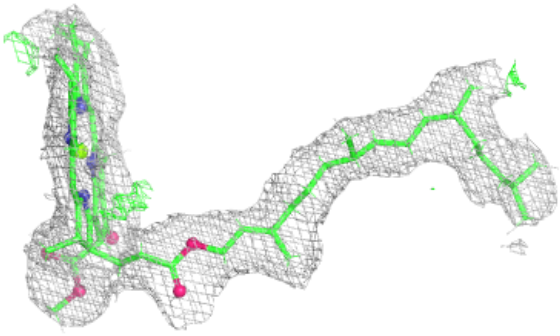


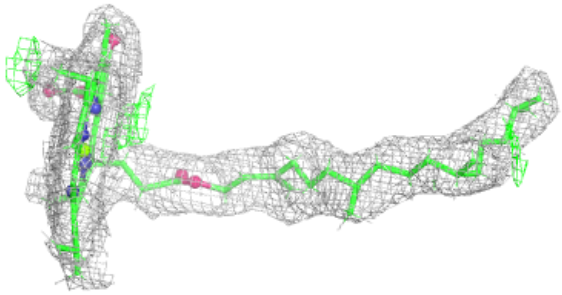


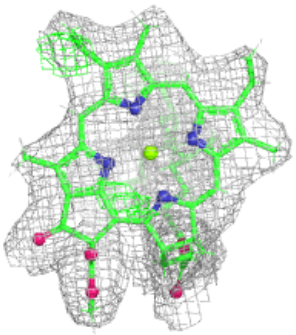


Electron density around CLA B 841:

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

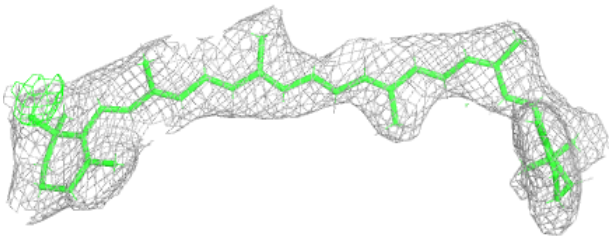


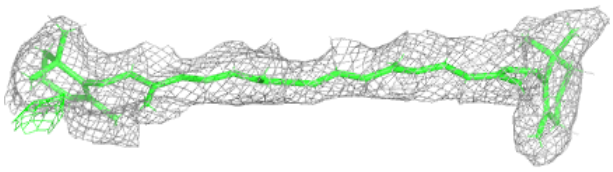


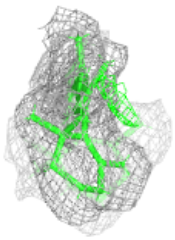


Electron density around BCR L 201:

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

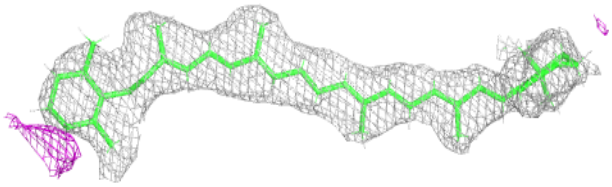


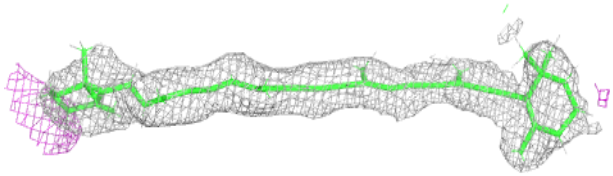


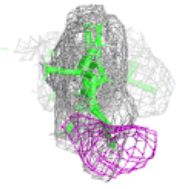


Electron density around BCR L 208:

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

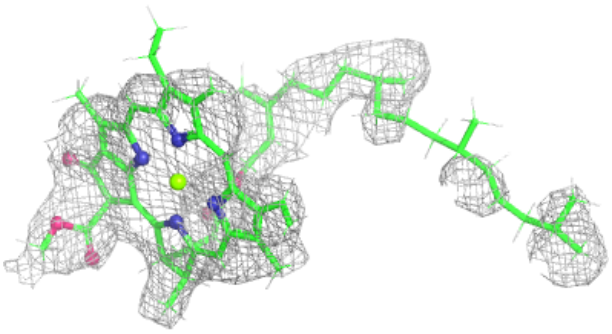


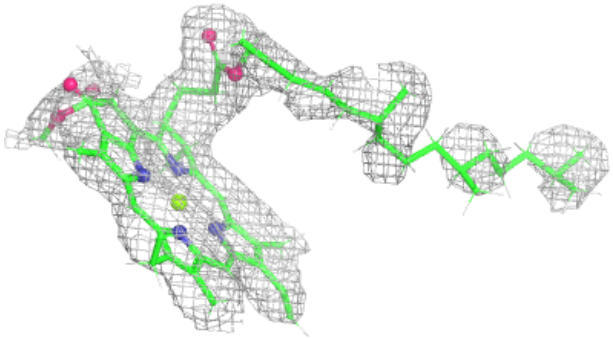


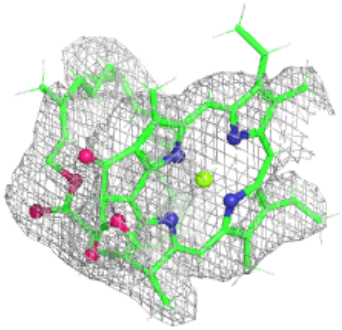


Electron density around CLA B 814:

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

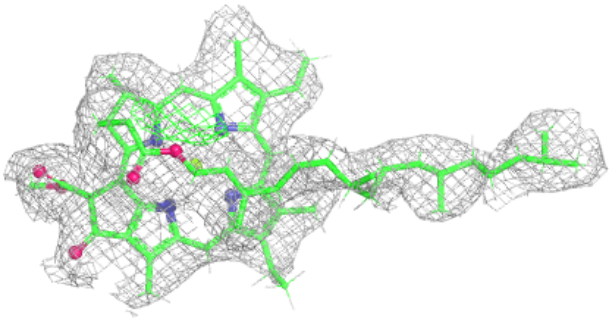


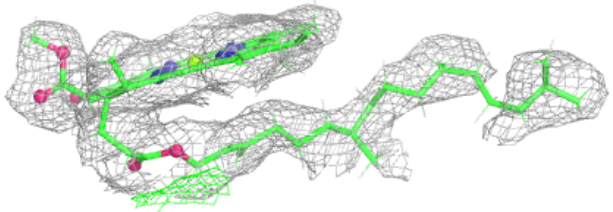


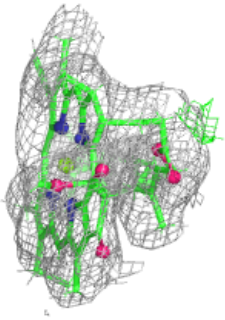


Electron density around CLA A 839:

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

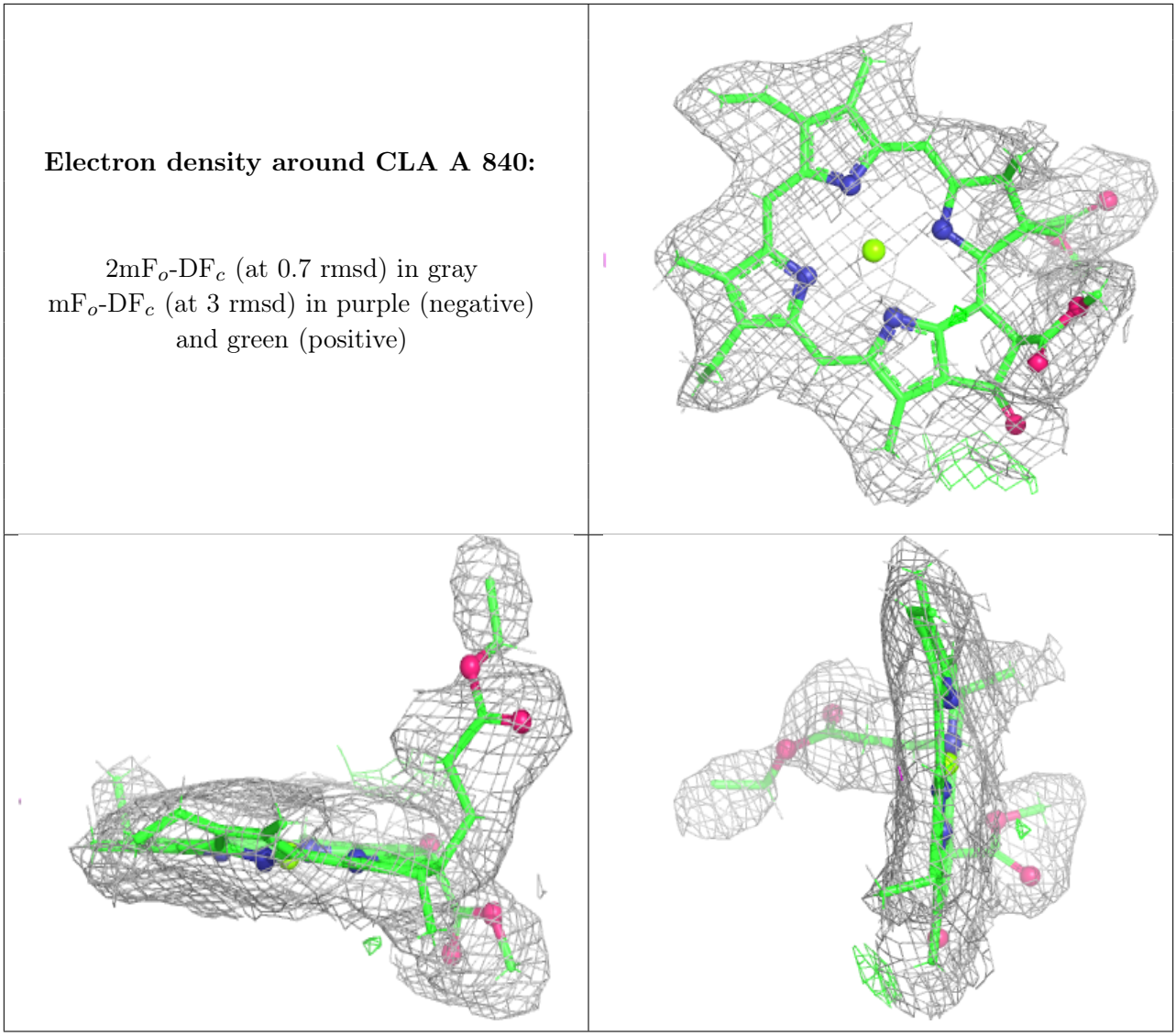






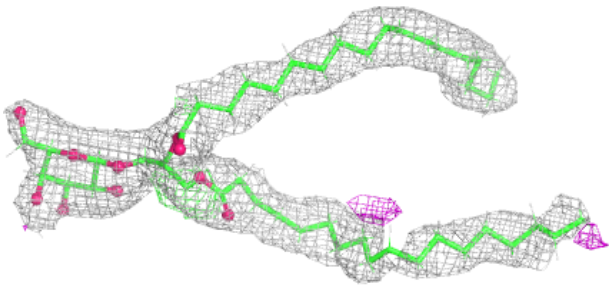
Electron density around CLA A 840:

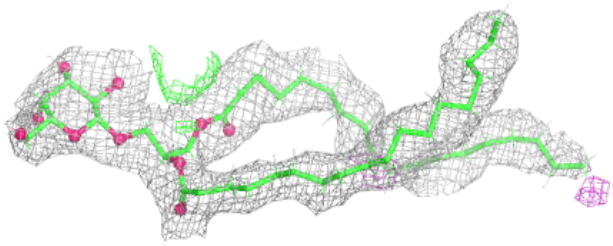
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

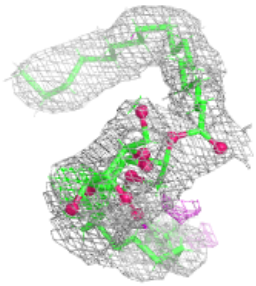


Electron density around LMG B 849:

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

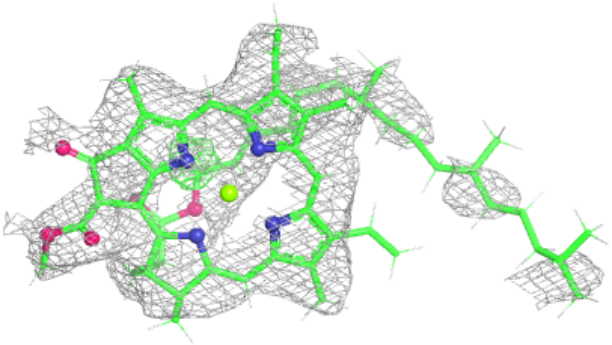


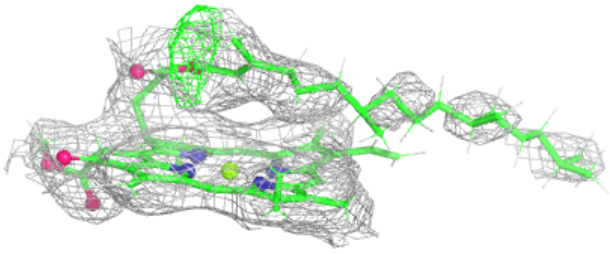


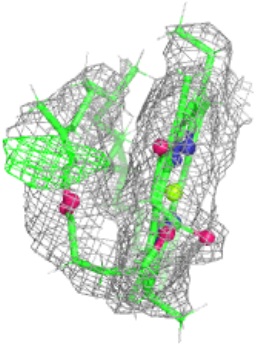


Electron density around CLA A 841:

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

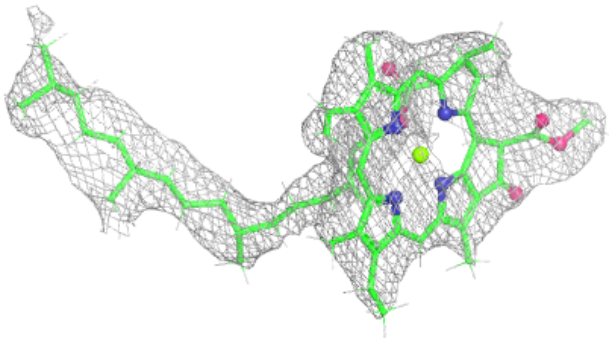


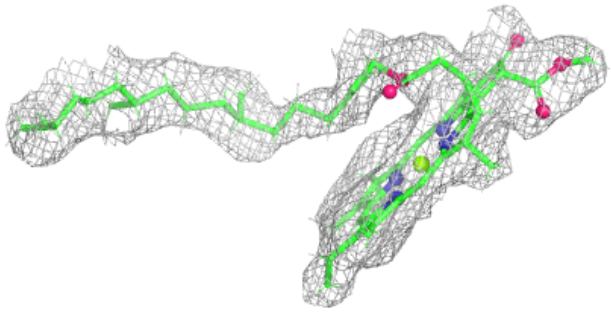


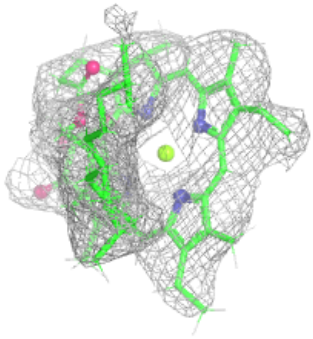


Electron density around CLA A 842:

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

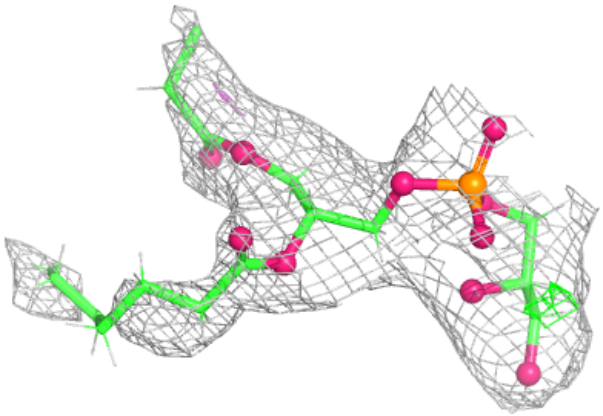


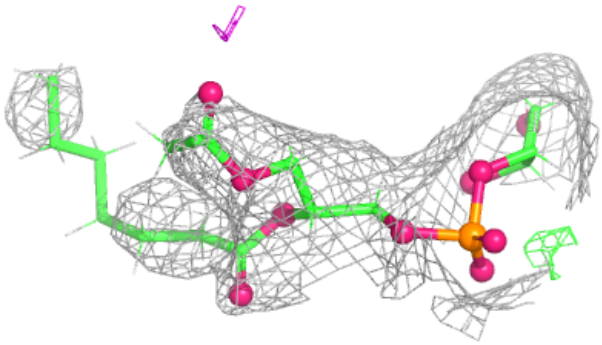


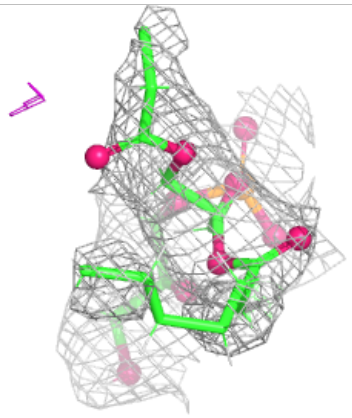


Electron density around LHG A 855:

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

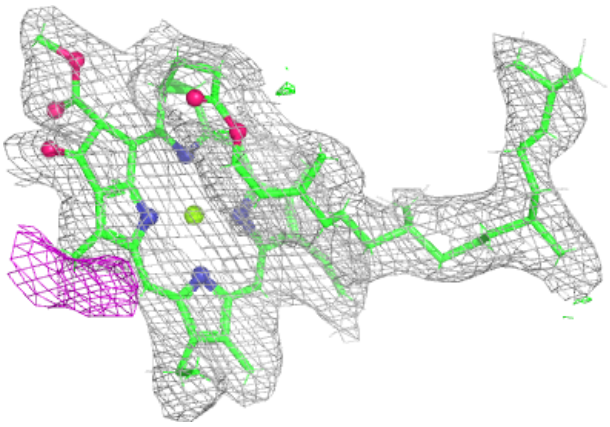


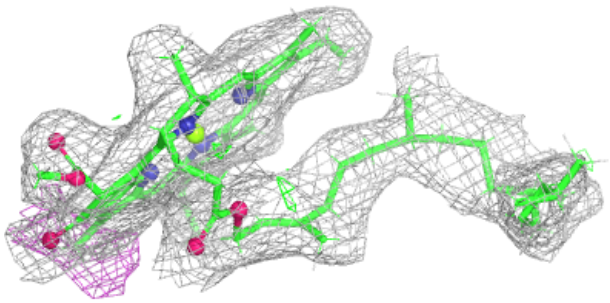


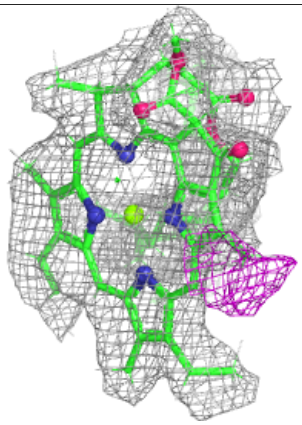


Electron density around CLA A 843:

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

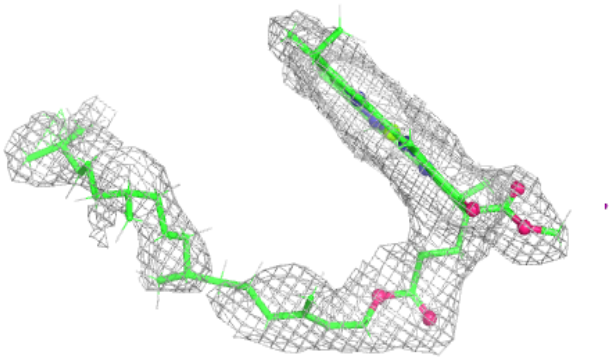


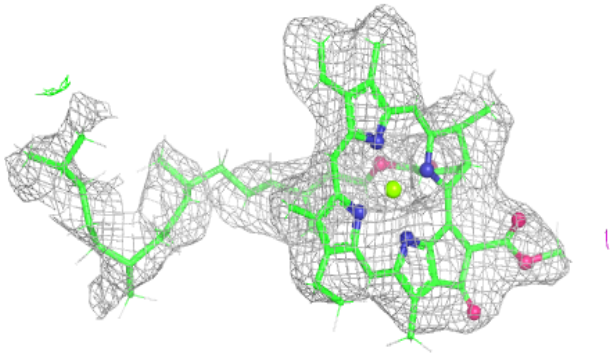


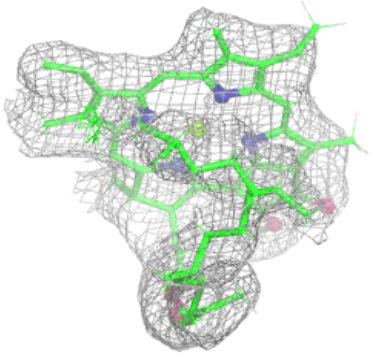


Electron density around CLA A 833:

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

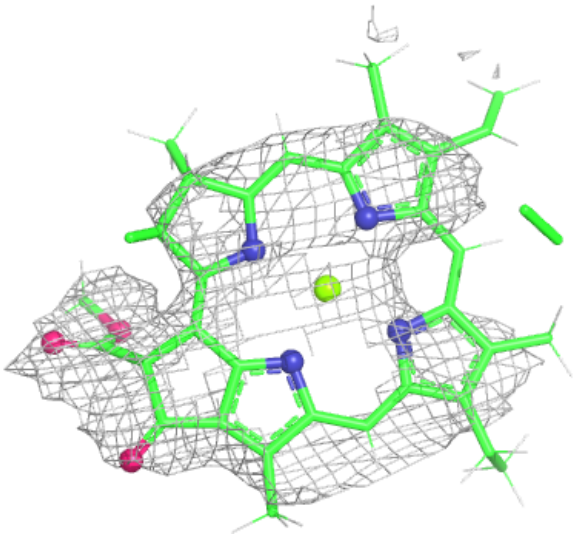


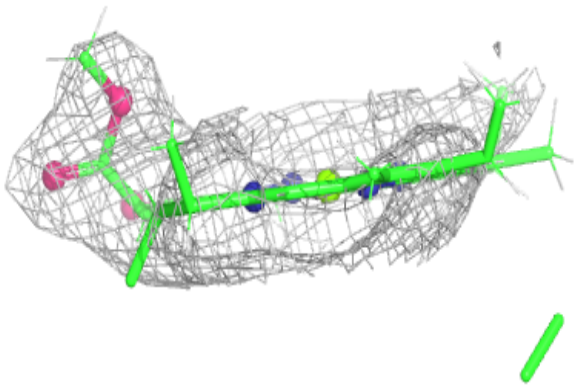


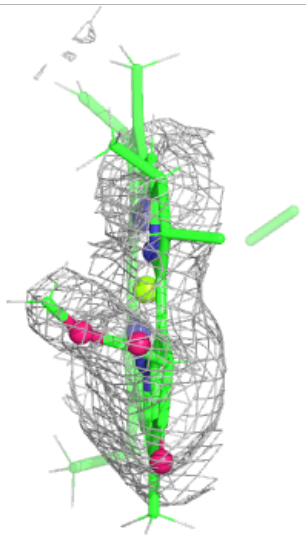


Electron density around CLA A 821:

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

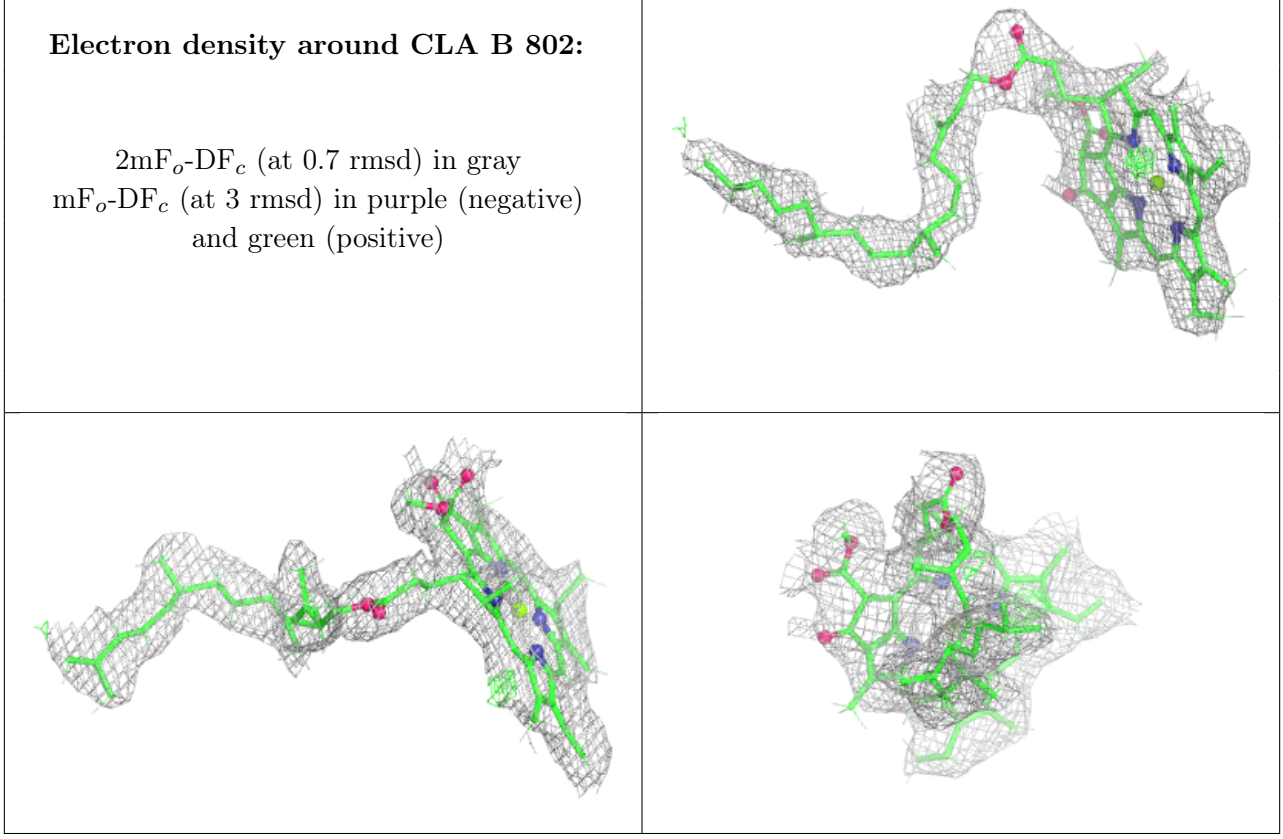






Electron density around CLA B 802:

$2mF_o$-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

There are no such residues in this entry.