Full wwPDB X-ray Structure Validation Report (i)

Mar 29, 2026 – 03:02 AM UTC

PDB ID	:	2WSC / pdb_00002wsc
Title	:	Improved Model of Plant Photosystem I
Authors	:	Amunts, A.; Toporik, H.; Borovikov, A.; Nelson, N.
Deposited on	:	2009-09-04
Resolution	:	3.30 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 (i) 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 (i)) were used in the production of this report:

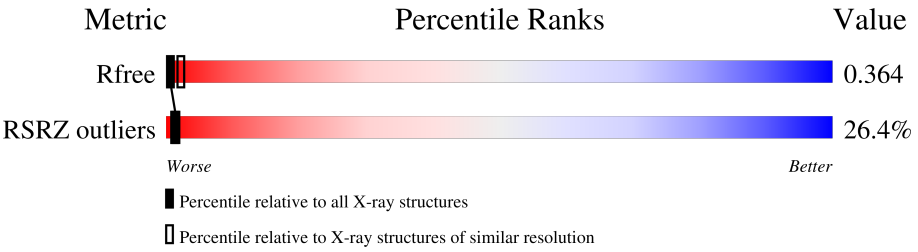
MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.30 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	1169 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 36379 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called AT3G54890.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	165	Total	C	N	O	S	0	0	0
			1264	822	208	230	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-33	ILE	LYS	conflict	UNP Q9C5R7
1	-1	ARG	LYS	conflict	UNP Q9C5R7

- Molecule 2 is a protein called TYPE II CHLOROPHYLL A/B BINDING PROTEIN FROM PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	176	Total	C	N	O	S	0	0	0
			1374	899	226	245	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	195	ALA	-	insertion	UNP Q41038
2	?	-	GLY	deletion	UNP Q41038

- Molecule 3 is a protein called LHCA3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	162	Total	C	N	O	S	0	0	0
			1254	826	203	220	5			

- Molecule 4 is a protein called CHLOROPHYLL A-B BINDING PROTEIN P4, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	166	Total	C	N	O	S	0	0	0
			1319	861	219	236	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	?	-	ALA	deletion	UNP Q9SQL2

- Molecule 5 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	730	Total	C	N	O	S	0	0	0
			5745	3766	974	987	18			

- Molecule 6 is a protein called PHOTOSYSTEM I P700 CHLOROPHYLL A APOPROTEIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	B	733	Total	C	N	O	S	0	0	0
			5848	3843	997	995	13			

- Molecule 7 is a protein called PHOTOSYSTEM I IRON-SULFUR CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	81	Total	C	N	O	S	0	0	0
			619	384	108	115	12			

- Molecule 8 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT II, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	D	138	Total	C	N	O	S	0	0	0
			1095	704	189	198	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-52	GLY	ALA	conflict	UNP P12353
D	-50	PRO	GLN	conflict	UNP P12353
D	-44	ARG	PRO	conflict	UNP P12353
D	-34	GLU	ASP	conflict	UNP P12353
D	-11	LEU	HIS	conflict	UNP P12353

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	THR	SER	conflict	UNP P12353
D	12	THR	PRO	conflict	UNP P12353
D	14	ALA	GLY	conflict	UNP P12353

- Molecule 9 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IV A, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	E	65	Total	C	N	O	0	0	0
			520	332	93	95			

- Molecule 10 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT III, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	F	154	Total	C	N	O	S	0	0	0
			1221	794	207	217	3			

- Molecule 11 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT V, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	G	95	Total	C	N	O	S	0	0	0
			740	481	120	137	2			

- Molecule 12 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	H	69	Total	C	N	O	0	0	0
			529	344	82	103			

- Molecule 13 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	I	30	Total	C	N	O	S	0	0	0
			229	158	34	35	2			

- Molecule 14 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	J	42	Total	C	N	O	S	0	0	0
			338	230	51	56	1			

- Molecule 15 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT PSAK, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	K	84	Total	C	N	O	S	0	0	0
			593	374	102	113	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	47	ILE	LEU	conflict	UNP P36886

- Molecule 16 is a protein called PHOTOSYSTEM I REACTION CENTER SUBUNIT XI, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	161	Total	C	N	O	S	0	0	0
			1203	791	193	214	5			

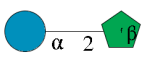
- Molecule 17 is a protein called PHOTOSYSTEM I-N SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	N	85	Total	C	N	O	S	0	0	0
			685	436	113	132	4			

- Molecule 18 is a protein called PHOTOSYSTEM I-N SUBUNIT.

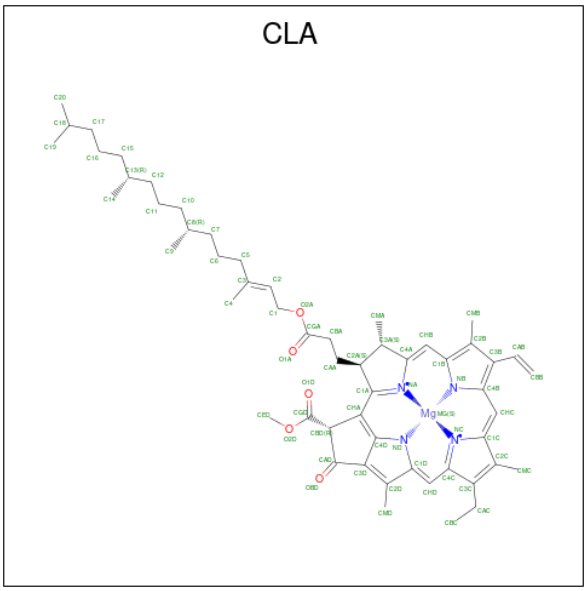
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	53	Total	C	N	O	0	0	0
			265	159	53	53			

- Molecule 19 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	M	2	Total C O 22 12 10	0	0	0
19	O	2	Total C O 23 12 11	0	0	0
19	P	2	Total C O 23 12 11	0	0	0
19	Q	2	Total C O 23 12 11	0	0	0
19	S	2	Total C O 23 12 11	0	0	0
19	T	2	Total C O 23 12 11	0	0	0
19	U	2	Total C O 23 12 11	0	0	0
19	V	2	Total C O 23 12 11	0	0	0
19	W	2	Total C O 23 12 11	0	0	0
19	X	2	Total C O 23 12 11	0	0	0
19	Y	2	Total C O 23 12 11	0	0	0
19	Z	2	Total C O 23 12 11	0	0	0
19	a	2	Total C O 23 12 11	0	0	0

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	1	1	Total C Mg N O 46 36 1 4 5	0	0
20	1	1	Total C Mg N O 47 37 1 4 5	0	0
20	1	1	Total C Mg N O 47 37 1 4 5	0	0
20	1	1	Total C Mg N O 46 36 1 4 5	0	0
20	1	1	Total C Mg N O 36 30 1 4 1	0	0
20	1	1	Total C Mg N O 61 51 1 4 5	0	0
20	1	1	Total C Mg N O 51 41 1 4 5	0	0
20	1	1	Total C Mg N 25 20 1 4	0	0
20	1	1	Total C Mg N O 36 30 1 4 1	0	0
20	1	1	Total C Mg N O 36 30 1 4 1	0	0
20	1	1	Total C Mg N O 51 41 1 4 5	0	0
20	1	1	Total C Mg N O 61 51 1 4 5	0	0
20	1	1	Total C Mg N 25 20 1 4	0	0
20	1	1	Total C Mg N O 51 41 1 4 5	0	0
20	1	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N O 51 41 1 4 5	0	0
20	2	1	Total C Mg N O 56 46 1 4 5	0	0
20	2	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N O 50 40 1 4 5	0	0
20	2	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N O 65 55 1 4 5	0	0
20	2	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	2	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N O 50 40 1 4 5	0	0
20	2	1	Total C Mg N O 50 40 1 4 5	0	0
20	2	1	Total C Mg N O 65 55 1 4 5	0	0
20	2	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N 25 20 1 4	0	0
20	2	1	Total C Mg N O 65 55 1 4 5	0	0
20	2	1	Total C Mg N O 61 51 1 4 5	0	0
20	3	1	Total C Mg N O 56 46 1 4 5	0	0
20	3	1	Total C Mg N O 36 30 1 4 1	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N O 65 55 1 4 5	0	0
20	3	1	Total C Mg N O 65 55 1 4 5	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N O 42 34 1 4 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	3	1	Total C Mg N O 50 40 1 4 5	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N 25 20 1 4	0	0
20	3	1	Total C Mg N O 36 30 1 4 1	0	0
20	3	1	Total C Mg N O 55 45 1 4 5	0	0
20	4	1	Total C Mg N O 55 45 1 4 5	0	0
20	4	1	Total C Mg N O 36 30 1 4 1	0	0
20	4	1	Total C Mg N O 65 55 1 4 5	0	0
20	4	1	Total C Mg N O 55 45 1 4 5	0	0
20	4	1	Total C Mg N O 50 40 1 4 5	0	0
20	4	1	Total C Mg N O 52 42 1 4 5	0	0
20	4	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N O 55 45 1 4 5	0	0
20	4	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N O 36 30 1 4 1	0	0
20	4	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N O 46 36 1 4 5	0	0
20	4	1	Total C Mg N 25 20 1 4	0	0
20	4	1	Total C Mg N O 52 42 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	4	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			42	34	1	4	3		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C Mg N O 46 36 1 4 5	0	0
20	A	1	Total C Mg N O 65 55 1 4 5	0	0
20	A	1	Total C Mg N 25 20 1 4	0	0
20	B	1	Total C Mg N O 45 35 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 54 44 1 4 5	0	0
20	B	1	Total C Mg N O 55 45 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0
20	B	1	Total C Mg N O 60 50 1 4 5	0	0
20	B	1	Total C Mg N O 46 36 1 4 5	0	0
20	B	1	Total C Mg N O 59 49 1 4 5	0	0
20	B	1	Total C Mg N O 60 50 1 4 5	0	0
20	B	1	Total C Mg N O 61 51 1 4 5	0	0
20	B	1	Total C Mg N O 50 40 1 4 5	0	0
20	B	1	Total C Mg N O 46 36 1 4 5	0	0
20	B	1	Total C Mg N O 55 45 1 4 5	0	0
20	B	1	Total C Mg N O 65 55 1 4 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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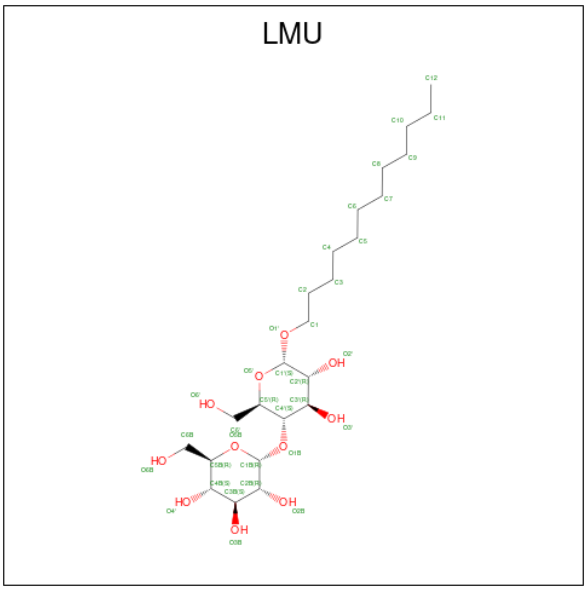
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	F	1	Total	C	Mg	N	O	0	0
			36	30	1	4	1		
20	F	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	F	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
20	G	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	H	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	I	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	J	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
20	J	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	K	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	L	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	R	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
20	R	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	1	1	Total	C	O	0	0
			35	24	11		
21	1	1	Total	C	O	0	0
			35	24	11		
21	1	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		
21	2	1	Total	C	O	0	0
			35	24	11		

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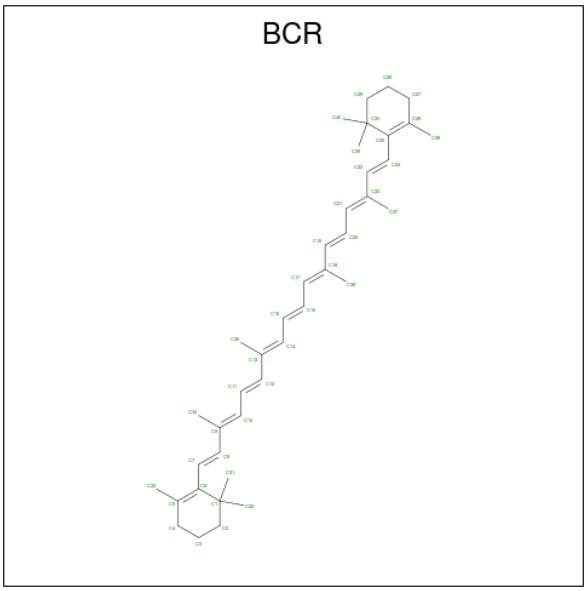
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	2	1	Total C O 35 24 11	0	0
21	3	1	Total C O 35 24 11	0	0
21	3	1	Total C O 35 24 11	0	0
21	4	1	Total C O 35 24 11	0	0
21	4	1	Total C O 35 24 11	0	0
21	4	1	Total C O 34 23 11	0	0
21	4	1	Total C O 35 24 11	0	0
21	4	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	A	1	Total C O 35 24 11	0	0
21	B	1	Total C O 35 24 11	0	0
21	B	1	Total C O 35 24 11	0	0
21	B	1	Total C O 25 14 11	0	0
21	C	1	Total C O 35 24 11	0	0
21	E	1	Total C O 35 24 11	0	0
21	F	1	Total C O 34 23 11	0	0
21	G	1	Total C O 35 24 11	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	H	1	Total C O 35 24 11	0	0
21	H	1	Total C O 35 24 11	0	0
21	H	1	Total C O 35 24 11	0	0
21	H	1	Total C O 35 24 11	0	0
21	K	1	Total C O 35 24 11	0	0
21	K	1	Total C O 35 24 11	0	0
21	K	1	Total C O 35 24 11	0	0
21	L	1	Total C O 35 24 11	0	0
21	L	1	Total C O 35 24 11	0	0
21	L	1	Total C O 35 24 11	0	0
21	R	1	Total C O 35 24 11	0	0
21	R	1	Total C O 35 24 11	0	0
21	R	1	Total C O 35 24 11	0	0
21	R	1	Total C O 35 24 11	0	0
21	R	1	Total C O 35 24 11	0	0
21	R	1	Total C O 35 24 11	0	0
21	R	1	Total C O 35 24 11	0	0

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



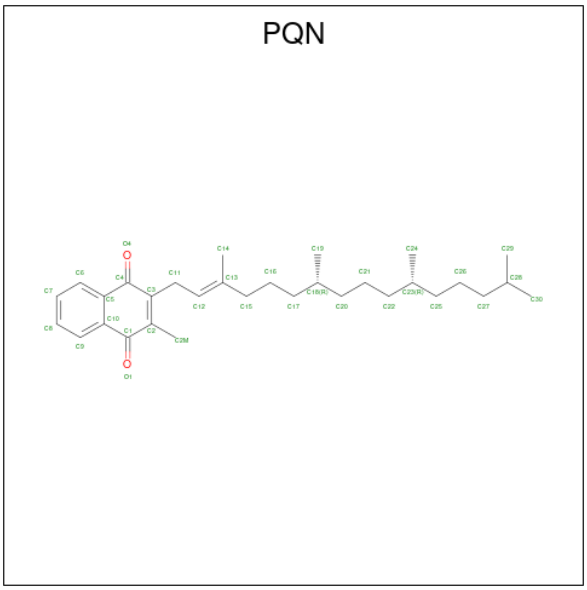
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	3	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	G	1	Total C 40 40	0	0

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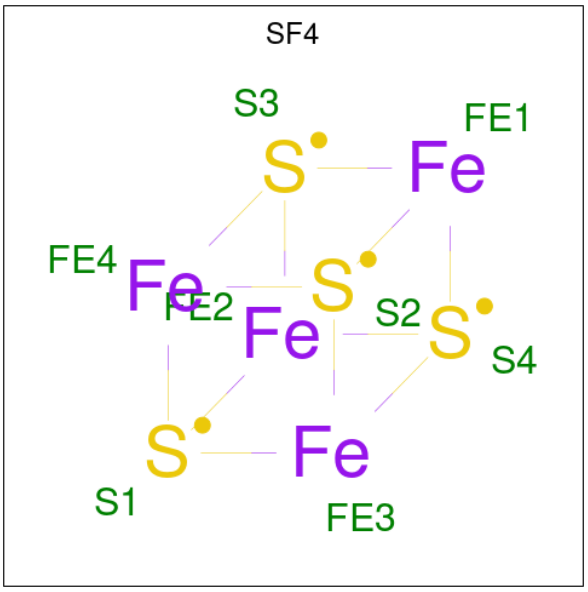
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	I	1	Total C 40 40	0	0
22	I	1	Total C 40 40	0	0
22	J	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



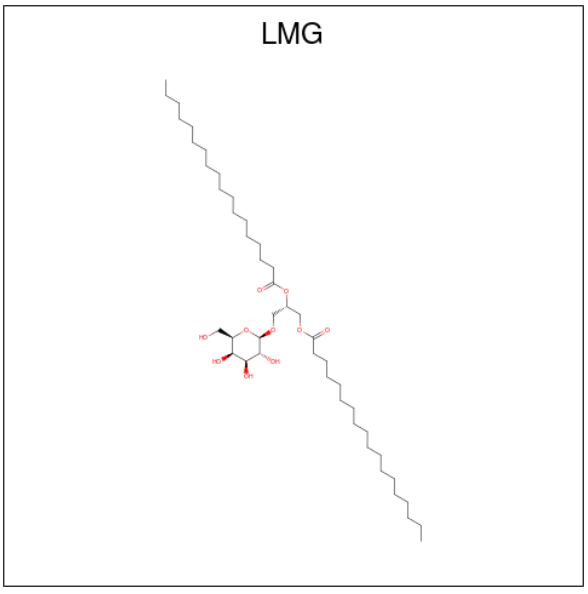
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 33 31 2	0	0
23	B	1	Total C O 33 31 2	0	0

- Molecule 24 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			49	39	10		

- Molecule 26 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	H	1	Total	C	O	0	0
			23	12	11		

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.66Å 189.09Å 129.39Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.30) 99.3 (30.00-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.363 , 0.366 0.359 , 0.364	Depositor DCC
R_{free} test set	4685 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	78.5	Xtriage
Anisotropy	0.655	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.13 , 58.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	36379	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

26 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	GLC	M	1	19	10,10,12	1.47	3 (30%)	14,14,17	2.99	9 (64%)
19	FRU	M	2	19	11,12,12	1.03	1 (9%)	10,18,18	2.30	3 (30%)
19	GLC	O	1	19	11,11,12	0.90	0	15,15,17	3.29	8 (53%)
19	FRU	O	2	19	11,12,12	1.10	1 (9%)	10,18,18	1.70	2 (20%)
19	GLC	P	1	19	11,11,12	0.98	0	15,15,17	2.39	3 (20%)
19	FRU	P	2	19	11,12,12	1.04	1 (9%)	10,18,18	0.98	0
19	GLC	Q	1	19	11,11,12	1.16	1 (9%)	15,15,17	2.07	4 (26%)
19	FRU	Q	2	19	11,12,12	0.99	1 (9%)	10,18,18	1.76	4 (40%)
19	GLC	S	1	19	11,11,12	0.42	0	15,15,17	0.98	1 (6%)
19	FRU	S	2	19,21	11,12,12	0.65	0	10,18,18	1.11	0
19	GLC	T	1	19	11,11,12	1.05	1 (9%)	15,15,17	1.46	2 (13%)
19	FRU	T	2	19	11,12,12	1.94	4 (36%)	10,18,18	2.78	4 (40%)
19	GLC	U	1	19	11,11,12	1.02	1 (9%)	15,15,17	2.43	5 (33%)
19	FRU	U	2	19	11,12,12	0.95	0	10,18,18	1.53	2 (20%)
19	GLC	V	1	19	11,11,12	1.51	2 (18%)	15,15,17	1.79	4 (26%)
19	FRU	V	2	19	11,12,12	0.90	0	10,18,18	1.97	5 (50%)
19	GLC	W	1	19	11,11,12	1.27	2 (18%)	15,15,17	2.73	8 (53%)
19	FRU	W	2	19	11,12,12	1.18	2 (18%)	10,18,18	2.04	2 (20%)
19	GLC	X	1	19	11,11,12	1.17	1 (9%)	15,15,17	1.64	4 (26%)
19	FRU	X	2	19	11,12,12	1.54	2 (18%)	10,18,18	2.34	4 (40%)
19	GLC	Y	1	19	11,11,12	1.08	0	15,15,17	3.33	7 (46%)
19	FRU	Y	2	19	11,12,12	1.14	0	10,18,18	2.25	4 (40%)
19	GLC	Z	1	19	11,11,12	1.70	2 (18%)	15,15,17	4.23	8 (53%)
19	FRU	Z	2	19,21	11,12,12	1.05	1 (9%)	10,18,18	2.32	3 (30%)
19	GLC	a	1	19	11,11,12	1.02	0	15,15,17	1.34	3 (20%)
19	FRU	a	2	19	11,12,12	1.07	0	10,18,18	2.13	3 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	GLC	M	1	19	-	-	0/1/1/1
19	FRU	M	2	19	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	O	1	19	-	1/2/19/22	0/1/1/1
19	FRU	O	2	19	1/1/4/4	4/5/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	GLC	P	1	19	-	2/2/19/22	0/1/1/1
19	FRU	P	2	19	1/1/4/4	2/5/24/24	0/1/1/1
19	GLC	Q	1	19	-	2/2/19/22	0/1/1/1
19	FRU	Q	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	S	1	19	-	1/2/19/22	0/1/1/1
19	FRU	S	2	19,21	1/1/4/4	0/5/24/24	0/1/1/1
19	GLC	T	1	19	-	2/2/19/22	0/1/1/1
19	FRU	T	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	U	1	19	-	2/2/19/22	0/1/1/1
19	FRU	U	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	V	1	19	-	0/2/19/22	0/1/1/1
19	FRU	V	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	W	1	19	-	1/2/19/22	0/1/1/1
19	FRU	W	2	19	1/1/4/4	2/5/24/24	0/1/1/1
19	GLC	X	1	19	-	2/2/19/22	0/1/1/1
19	FRU	X	2	19	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	Y	1	19	-	2/2/19/22	0/1/1/1
19	FRU	Y	2	19	1/1/4/4	1/5/24/24	0/1/1/1
19	GLC	Z	1	19	-	0/2/19/22	0/1/1/1
19	FRU	Z	2	19,21	1/1/4/4	3/5/24/24	0/1/1/1
19	GLC	a	1	19	-	2/2/19/22	0/1/1/1
19	FRU	a	2	19	1/1/4/4	2/5/24/24	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	1	GLC	O5-C1	-3.89	1.37	1.43
19	T	2	FRU	O5-C2	-3.79	1.37	1.43
19	V	1	GLC	O5-C5	-2.74	1.38	1.43
19	M	1	GLC	O5-C5	-2.71	1.38	1.43
19	V	1	GLC	O5-C1	-2.68	1.39	1.43
19	X	2	FRU	O5-C2	-2.67	1.39	1.43
19	P	2	FRU	O2-C2	2.65	1.45	1.40
19	O	2	FRU	O5-C2	-2.65	1.39	1.43
19	X	2	FRU	O2-C2	-2.61	1.36	1.40
19	Z	2	FRU	O5-C2	-2.48	1.39	1.43
19	W	2	FRU	O5-C2	-2.45	1.39	1.43
19	T	2	FRU	C1-C2	-2.43	1.47	1.52
19	X	1	GLC	O5-C1	-2.34	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	T	2	FRU	O2-C2	-2.32	1.36	1.40
19	M	1	GLC	O5-C1	-2.30	1.39	1.43
19	Q	1	GLC	O5-C1	-2.29	1.39	1.43
19	T	2	FRU	O3-C3	-2.29	1.38	1.42
19	W	2	FRU	O5-C5	-2.27	1.38	1.43
19	Q	2	FRU	O5-C2	-2.27	1.39	1.43
19	Z	1	GLC	O5-C5	-2.26	1.39	1.43
19	M	1	GLC	O2-C2	-2.18	1.38	1.43
19	U	1	GLC	C4-C5	-2.10	1.48	1.53
19	M	2	FRU	O5-C5	-2.09	1.39	1.43
19	W	1	GLC	O5-C5	-2.06	1.39	1.43
19	W	1	GLC	O5-C1	-2.05	1.40	1.43
19	T	1	GLC	O5-C5	-2.03	1.39	1.43

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Z	1	GLC	C1-O5-C5	-11.58	96.66	112.19
19	P	1	GLC	C1-O5-C5	7.80	122.64	112.19
19	Y	1	GLC	C1-O5-C5	7.58	122.35	112.19
19	T	2	FRU	O1-C1-C2	-6.73	96.79	111.67
19	M	1	GLC	C1-C2-C3	6.70	119.40	109.64
19	O	1	GLC	O3-C3-C2	6.50	123.32	110.05
19	O	1	GLC	C3-C4-C5	-5.51	100.24	110.23
19	O	1	GLC	C2-C3-C4	-5.43	101.32	110.86
19	Z	1	GLC	C6-C5-C4	5.42	126.33	113.02
19	W	2	FRU	O1-C1-C2	-5.29	99.97	111.67
19	Y	1	GLC	O5-C5-C6	5.27	117.92	107.66
19	U	1	GLC	C6-C5-C4	-5.25	100.13	113.02
19	Z	1	GLC	C3-C4-C5	-5.18	100.84	110.23
19	X	2	FRU	C6-C5-C4	-5.15	102.95	115.10
19	Y	1	GLC	C3-C4-C5	-5.08	101.02	110.23
19	M	1	GLC	O5-C5-C4	-4.98	100.60	109.55
19	W	1	GLC	O3-C3-C4	4.80	121.69	110.38
19	Z	1	GLC	O5-C1-C2	-4.72	99.52	110.79
19	Z	2	FRU	O2-C2-O5	4.63	118.22	109.33
19	Y	1	GLC	C2-C3-C4	-4.59	102.79	110.86
19	Z	2	FRU	O1-C1-C2	-4.59	101.53	111.67
19	U	1	GLC	O5-C5-C6	4.55	116.52	107.66
19	Z	1	GLC	O2-C2-C3	-4.55	100.73	110.15
19	Q	1	GLC	C3-C4-C5	-4.48	102.10	110.23
19	U	1	GLC	C1-O5-C5	4.45	118.15	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	M	2	FRU	O4-C4-C3	-4.31	99.21	112.16
19	Q	1	GLC	C6-C5-C4	-4.30	102.47	113.02
19	O	1	GLC	C1-O5-C5	4.15	117.75	112.19
19	M	2	FRU	O2-C2-O5	-4.14	101.38	109.33
19	W	1	GLC	C2-C3-C4	-3.99	103.85	110.86
19	Y	1	GLC	O3-C3-C2	3.88	117.98	110.05
19	M	2	FRU	O1-C1-C2	3.77	120.01	111.67
19	a	2	FRU	O2-C2-O5	3.77	116.56	109.33
19	Z	1	GLC	C2-C3-C4	-3.68	104.38	110.86
19	V	1	GLC	C1-C2-C3	-3.67	104.31	109.64
19	W	1	GLC	C1-C2-C3	-3.58	104.42	109.64
19	X	2	FRU	O6-C6-C5	-3.52	99.36	111.33
19	X	1	GLC	C2-C3-C4	-3.47	104.77	110.86
19	a	2	FRU	O1-C1-C2	-3.46	104.02	111.67
19	Y	2	FRU	O5-C5-C6	3.45	118.29	108.89
19	Y	2	FRU	O3-C3-C4	-3.44	101.09	113.25
19	T	2	FRU	O3-C3-C4	-3.43	101.12	113.25
19	V	1	GLC	O5-C5-C4	-3.43	102.48	110.83
19	W	1	GLC	O6-C6-C5	-3.42	99.69	111.33
19	W	1	GLC	C3-C4-C5	-3.38	104.11	110.23
19	O	1	GLC	O4-C4-C5	3.32	117.51	109.32
19	M	1	GLC	O2-C2-C1	-3.29	101.69	109.22
19	a	2	FRU	O4-C4-C3	-3.29	102.30	112.16
19	Q	1	GLC	C2-C3-C4	-3.28	105.10	110.86
19	O	1	GLC	O5-C1-C2	3.23	118.50	110.79
19	Z	1	GLC	O5-C5-C4	-3.23	102.96	110.83
19	V	1	GLC	C1-O5-C5	-3.21	107.88	112.19
19	O	1	GLC	O2-C2-C3	3.17	116.72	110.15
19	W	1	GLC	O2-C2-C3	3.16	116.69	110.15
19	M	1	GLC	O3-C3-C2	3.13	116.45	110.05
19	W	1	GLC	C6-C5-C4	-3.13	105.33	113.02
19	O	2	FRU	O2-C2-O5	3.13	115.33	109.33
19	V	2	FRU	O4-C4-C5	3.10	119.98	111.08
19	U	1	GLC	O4-C4-C5	-3.06	101.78	109.32
19	Q	2	FRU	O2-C2-O5	-2.99	103.59	109.33
19	Y	1	GLC	O3-C3-C4	-2.96	103.40	110.38
19	T	1	GLC	O2-C2-C1	2.84	115.73	109.22
19	a	1	GLC	C2-C3-C4	-2.84	105.87	110.86
19	Y	2	FRU	O1-C1-C2	-2.84	105.40	111.67
19	U	2	FRU	O4-C4-C5	-2.82	102.99	111.08
19	T	2	FRU	O2-C2-O5	-2.81	103.92	109.33
19	Y	2	FRU	O6-C6-C5	2.81	120.91	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	W	2	FRU	O2-C2-O5	2.73	114.56	109.33
19	W	1	GLC	O4-C4-C3	2.66	116.64	110.38
19	Q	2	FRU	O4-C4-C5	-2.56	103.72	111.08
19	Q	2	FRU	O5-C5-C6	2.54	115.82	108.89
19	M	1	GLC	C1-O5-C5	-2.53	106.99	112.97
19	T	2	FRU	O4-C4-C3	-2.52	104.61	112.16
19	a	1	GLC	O2-C2-C3	-2.51	104.95	110.15
19	P	1	GLC	O5-C5-C4	2.45	116.78	110.83
19	X	2	FRU	O5-C5-C6	2.44	115.54	108.89
19	S	1	GLC	C1-O5-C5	2.42	115.42	112.19
19	T	1	GLC	C3-C4-C5	2.41	114.60	110.23
19	Z	1	GLC	O4-C4-C3	-2.41	104.70	110.38
19	X	1	GLC	O5-C1-C2	2.37	116.43	110.79
19	P	1	GLC	O3-C3-C2	2.36	114.88	110.05
19	V	2	FRU	O3-C3-C4	-2.36	104.91	113.25
19	Q	1	GLC	O3-C3-C4	-2.36	104.81	110.38
19	M	1	GLC	O4-C4-C5	-2.36	104.53	109.74
19	X	2	FRU	O1-C1-C2	-2.36	106.46	111.67
19	X	1	GLC	C1-O5-C5	2.34	115.32	112.19
19	V	2	FRU	C6-C5-C4	2.31	120.54	115.10
19	a	1	GLC	O5-C5-C6	2.31	112.15	107.66
19	V	2	FRU	O4-C4-C3	-2.28	105.31	112.16
19	M	1	GLC	O3-C3-C4	2.25	115.67	110.38
19	Q	2	FRU	C6-C5-C4	-2.17	109.98	115.10
19	U	1	GLC	C1-C2-C3	2.17	112.80	109.64
19	M	1	GLC	C2-C3-C4	-2.15	107.08	110.86
19	U	2	FRU	O4-C4-C3	-2.14	105.73	112.16
19	Z	2	FRU	C6-C5-C4	-2.11	110.11	115.10
19	O	2	FRU	O1-C1-C2	-2.11	107.00	111.67
19	X	1	GLC	O2-C2-C3	-2.09	105.82	110.15
19	Y	1	GLC	C6-C5-C4	-2.04	108.00	113.02
19	V	1	GLC	O5-C5-C6	2.04	111.63	107.66
19	O	1	GLC	C6-C5-C4	2.04	118.03	113.02
19	V	2	FRU	O1-C1-C2	-2.03	107.19	111.67
19	M	1	GLC	O5-C1-C2	2.01	115.59	110.79

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	M	2	FRU	C2
19	O	2	FRU	C2
19	P	2	FRU	C2

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Mol	Chain	Res	Type	Atom
19	Q	2	FRU	C2
19	S	2	FRU	C2
19	T	2	FRU	C2
19	U	2	FRU	C2
19	V	2	FRU	C2
19	W	2	FRU	C2
19	X	2	FRU	C2
19	Y	2	FRU	C2
19	Z	2	FRU	C2
19	a	2	FRU	C2

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	O	2	FRU	O1-C1-C2-C3
19	O	2	FRU	O1-C1-C2-O2
19	Q	2	FRU	O1-C1-C2-C3
19	Q	2	FRU	O1-C1-C2-O2
19	Q	2	FRU	O1-C1-C2-O5
19	U	2	FRU	O1-C1-C2-C3
19	U	2	FRU	O1-C1-C2-O2
19	U	2	FRU	O1-C1-C2-O5
19	W	2	FRU	O5-C5-C6-O6
19	Z	2	FRU	C4-C5-C6-O6
19	O	2	FRU	O5-C5-C6-O6
19	T	1	GLC	O5-C5-C6-O6
19	Q	1	GLC	O5-C5-C6-O6
19	a	1	GLC	O5-C5-C6-O6
19	Q	1	GLC	C4-C5-C6-O6
19	Z	2	FRU	O5-C5-C6-O6
19	P	1	GLC	O5-C5-C6-O6
19	P	1	GLC	C4-C5-C6-O6
19	T	1	GLC	C4-C5-C6-O6
19	U	1	GLC	O5-C5-C6-O6
19	O	2	FRU	O1-C1-C2-O5
19	V	2	FRU	O1-C1-C2-O5
19	W	2	FRU	C4-C5-C6-O6
19	Y	1	GLC	O5-C5-C6-O6
19	X	1	GLC	C4-C5-C6-O6
19	X	1	GLC	O5-C5-C6-O6
19	a	1	GLC	C4-C5-C6-O6
19	S	1	GLC	O5-C5-C6-O6

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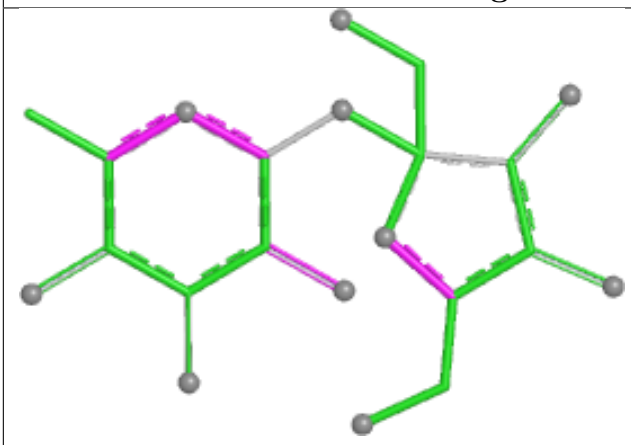
Mol	Chain	Res	Type	Atoms
19	X	2	FRU	O1-C1-C2-O5
19	O	1	GLC	C4-C5-C6-O6
19	P	2	FRU	O5-C5-C6-O6
19	T	2	FRU	C4-C5-C6-O6
19	U	1	GLC	C4-C5-C6-O6
19	V	2	FRU	O1-C1-C2-C3
19	Y	1	GLC	C4-C5-C6-O6
19	P	2	FRU	O1-C1-C2-O5
19	a	2	FRU	O5-C5-C6-O6
19	Y	2	FRU	O1-C1-C2-O5
19	T	2	FRU	O1-C1-C2-C3
19	Z	2	FRU	O1-C1-C2-C3
19	V	2	FRU	O1-C1-C2-O2
19	X	2	FRU	O1-C1-C2-O2
19	T	2	FRU	O5-C5-C6-O6
19	a	2	FRU	C4-C5-C6-O6
19	X	2	FRU	O1-C1-C2-C3
19	W	1	GLC	C4-C5-C6-O6

There are no ring outliers.

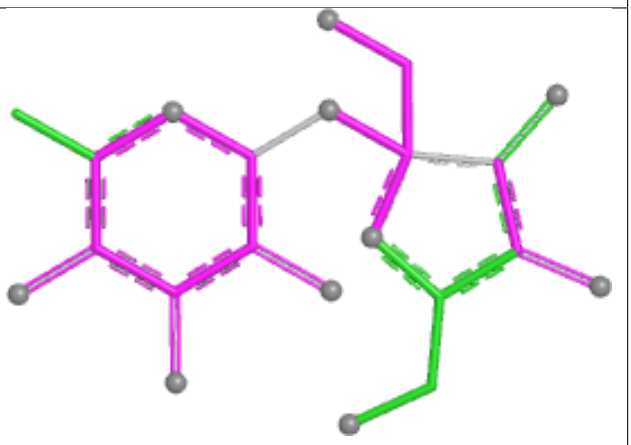
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

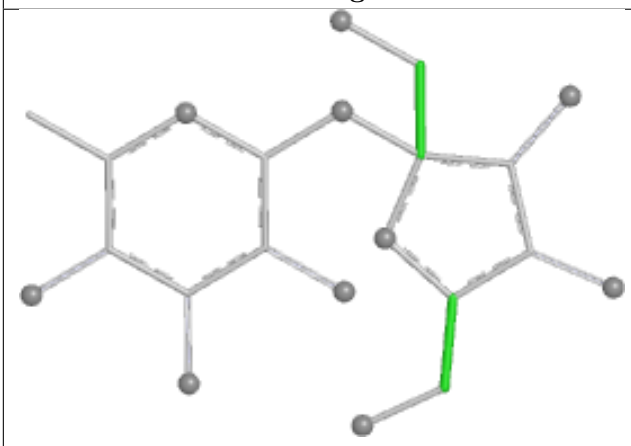
Oligosaccharide Chain M



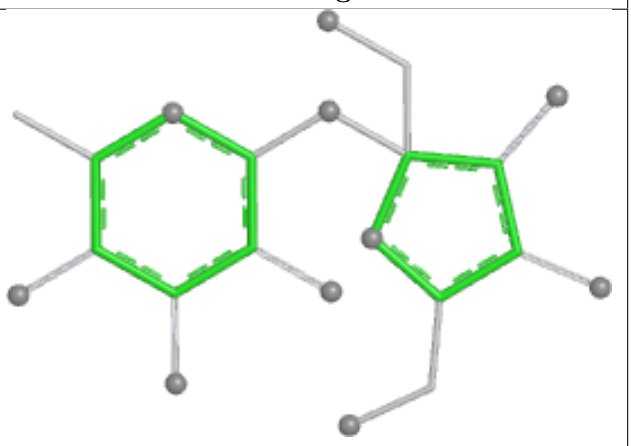
Bond lengths



Bond angles

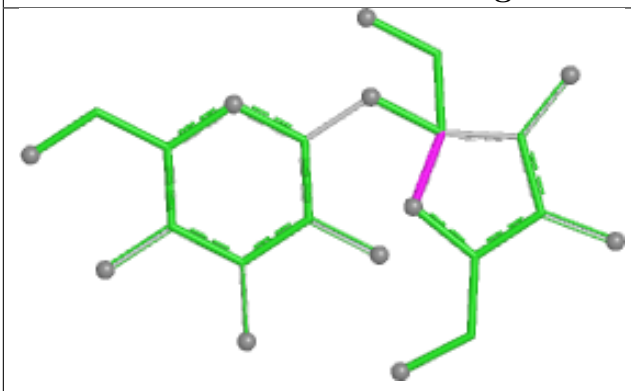


Torsions

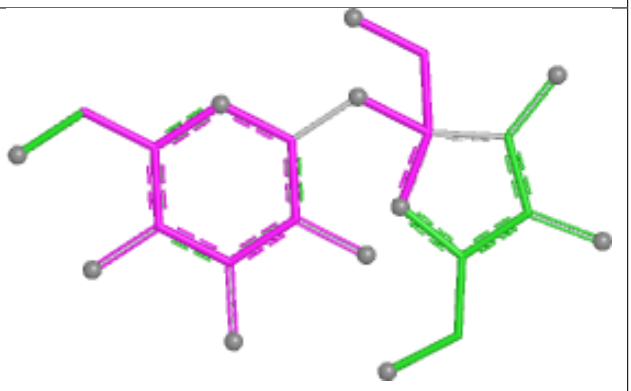


Rings

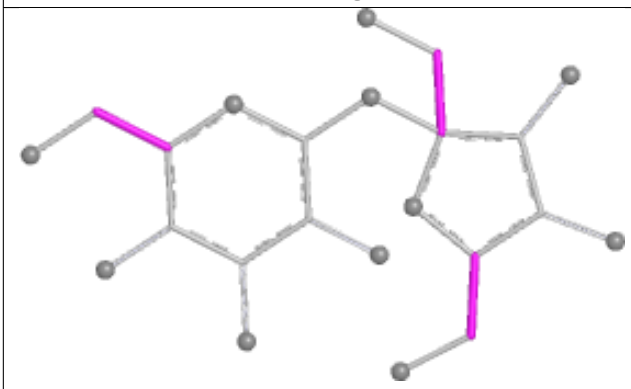
Oligosaccharide Chain O



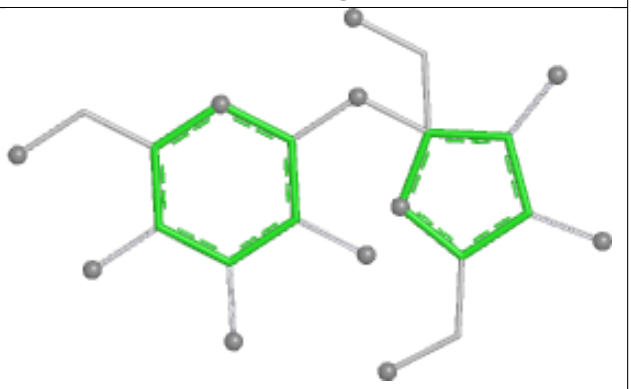
Bond lengths



Bond angles

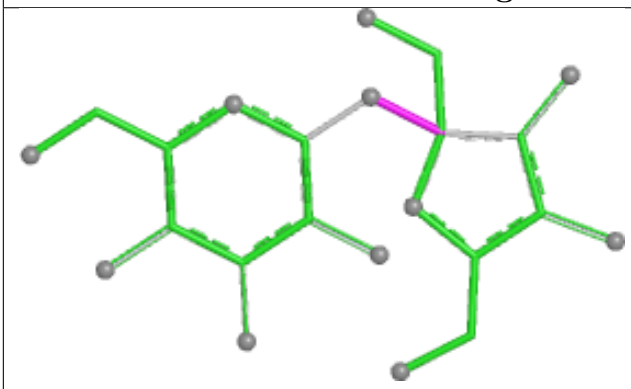


Torsions

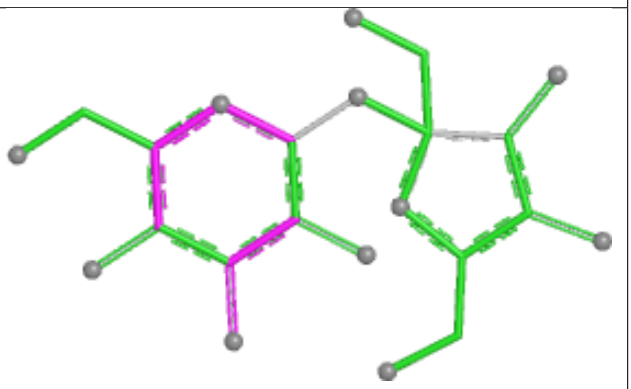


Rings

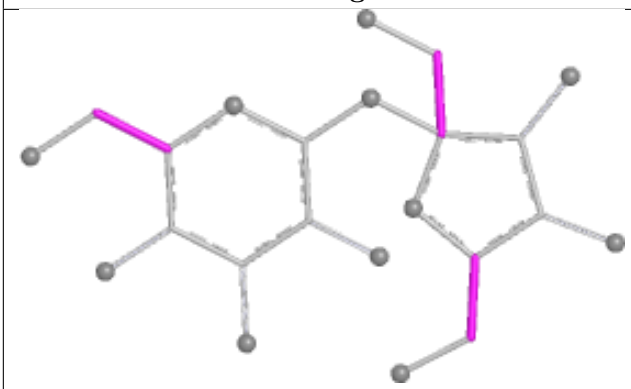
Oligosaccharide Chain P



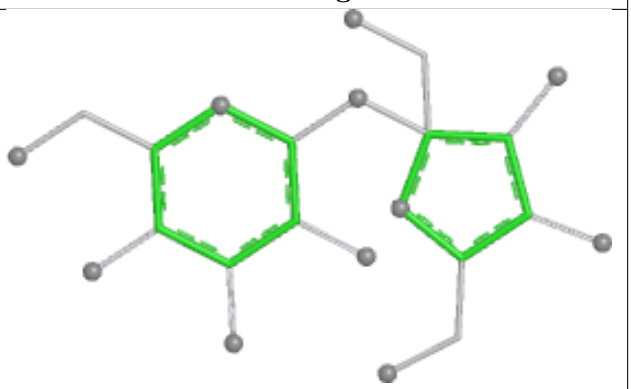
Bond lengths



Bond angles

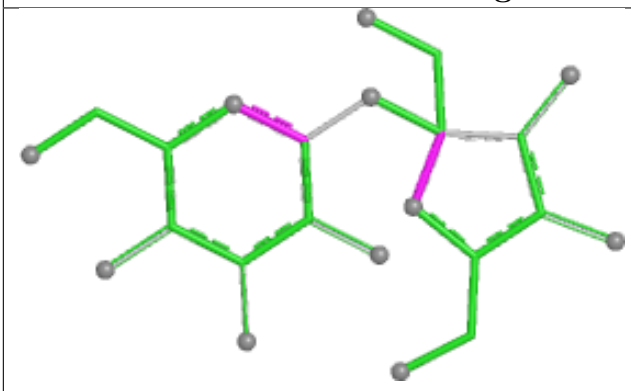


Torsions

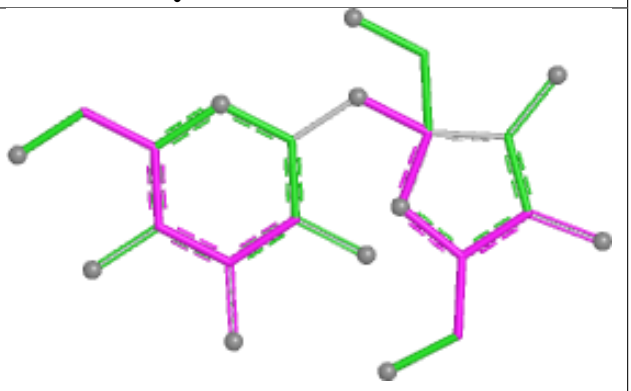


Rings

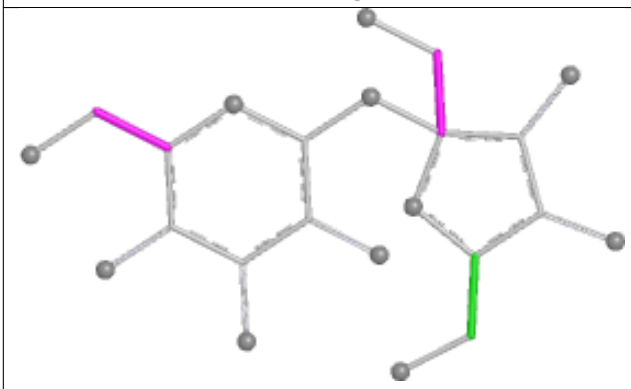
Oligosaccharide Chain Q



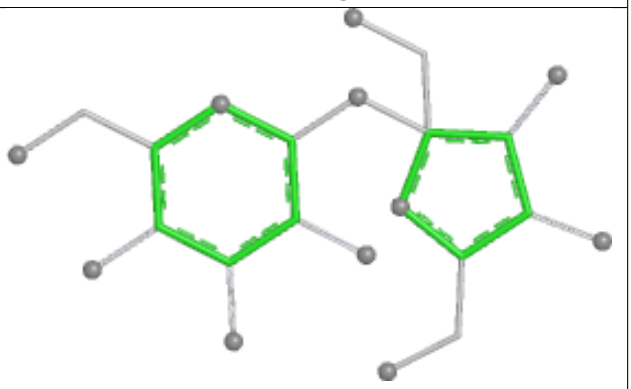
Bond lengths



Bond angles

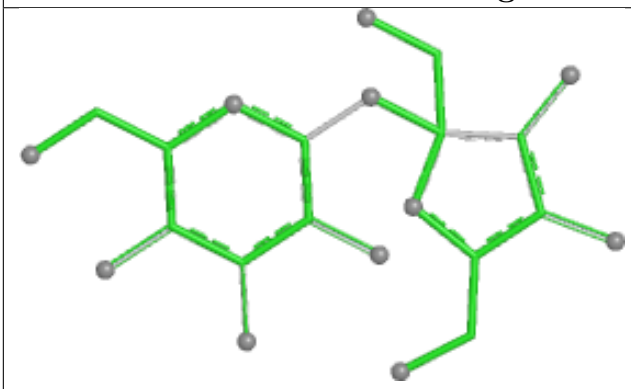


Torsions

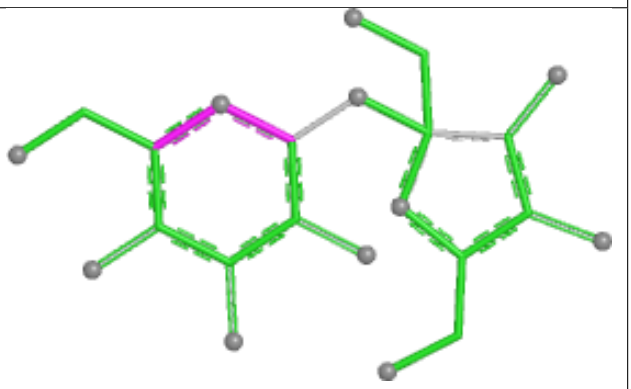


Rings

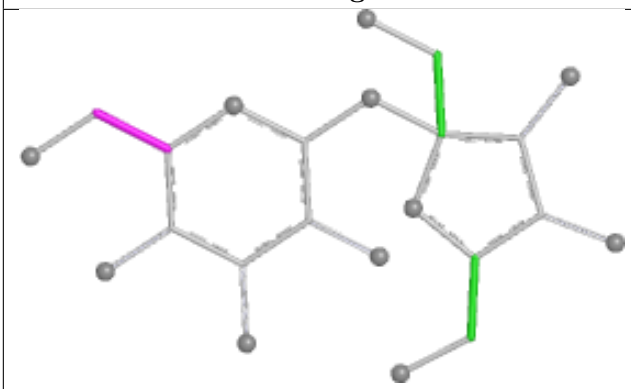
Oligosaccharide Chain S



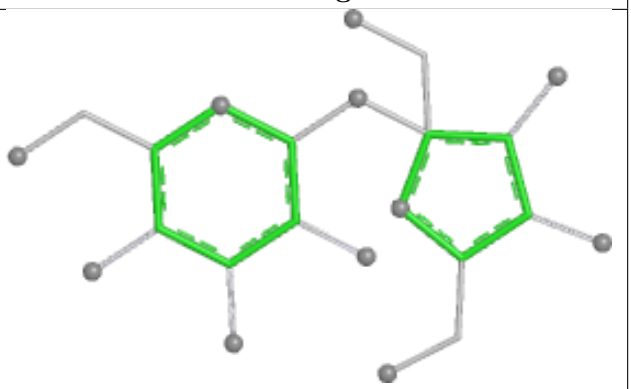
Bond lengths



Bond angles

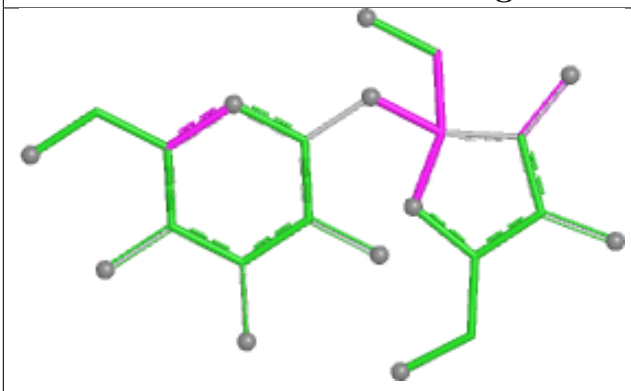


Torsions

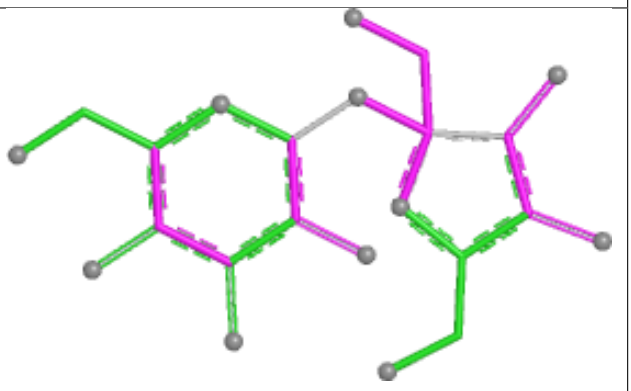


Rings

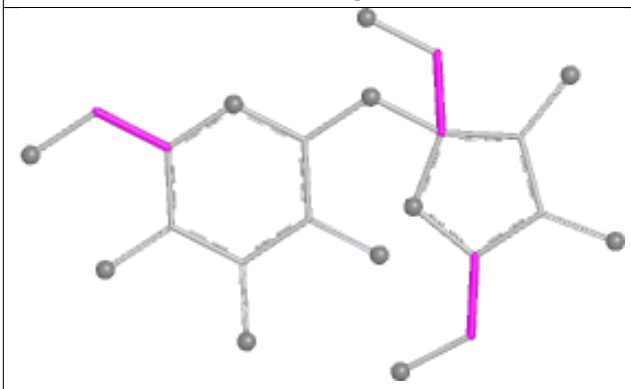
Oligosaccharide Chain T



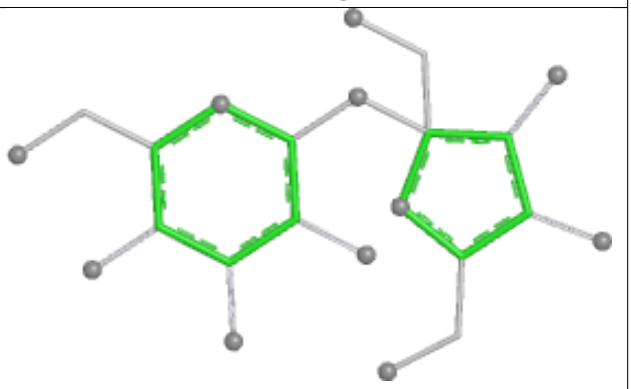
Bond lengths



Bond angles

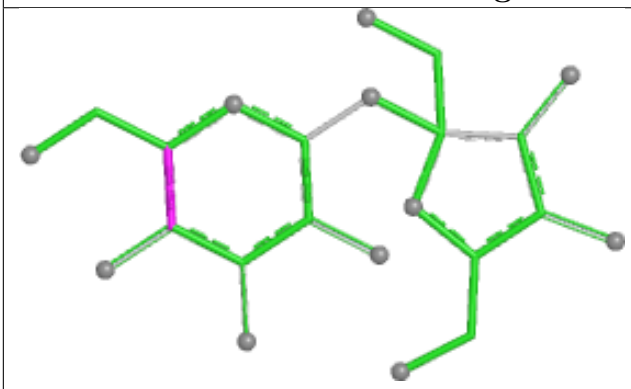


Torsions

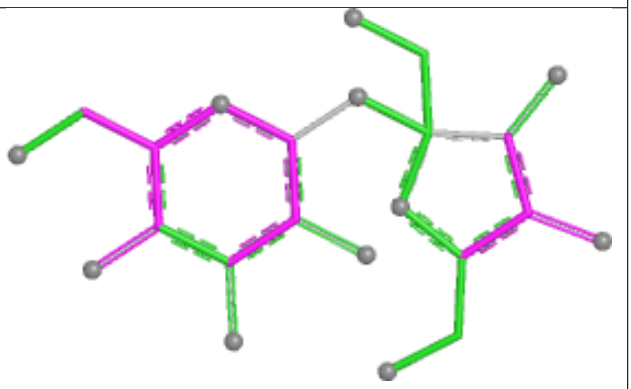


Rings

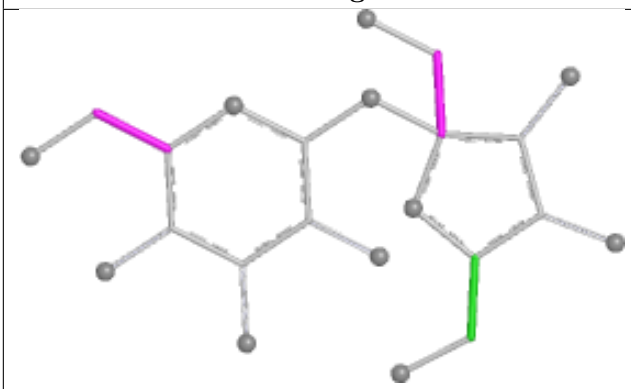
Oligosaccharide Chain U



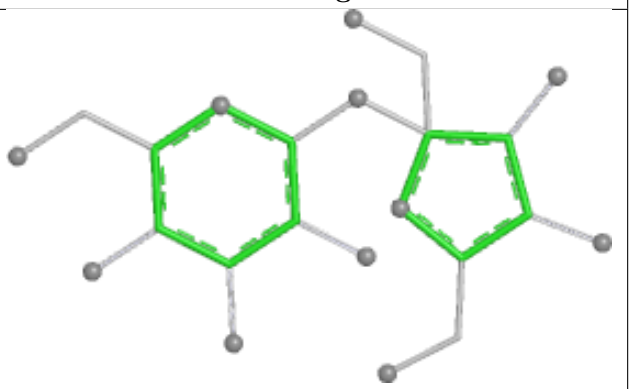
Bond lengths



Bond angles

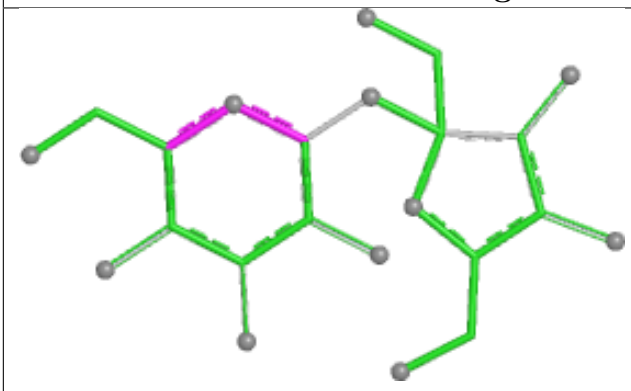


Torsions

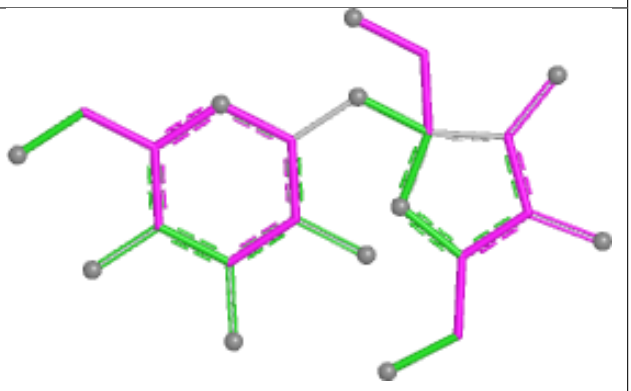


Rings

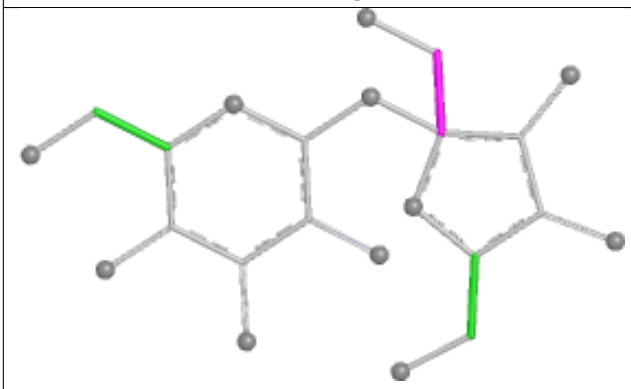
Oligosaccharide Chain V



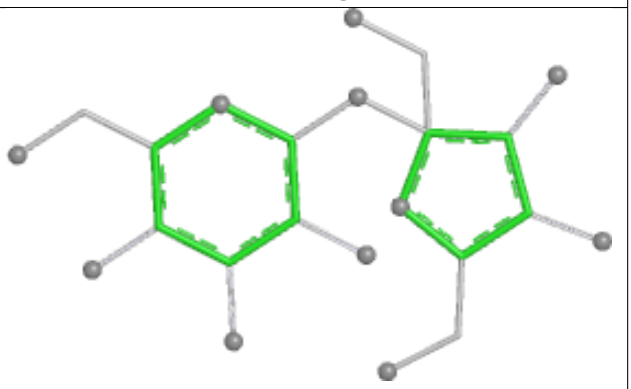
Bond lengths



Bond angles

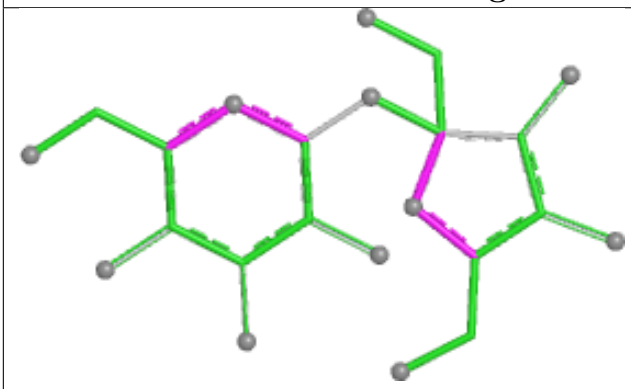


Torsions

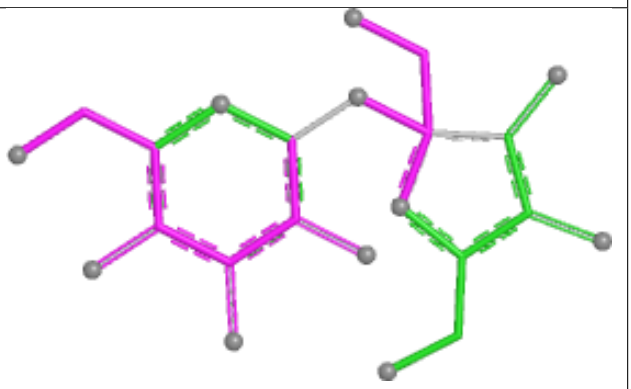


Rings

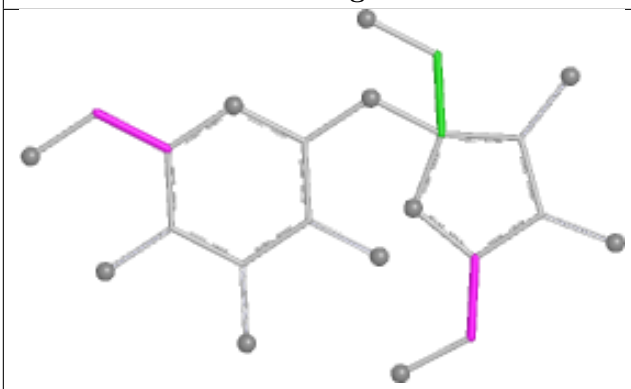
Oligosaccharide Chain W



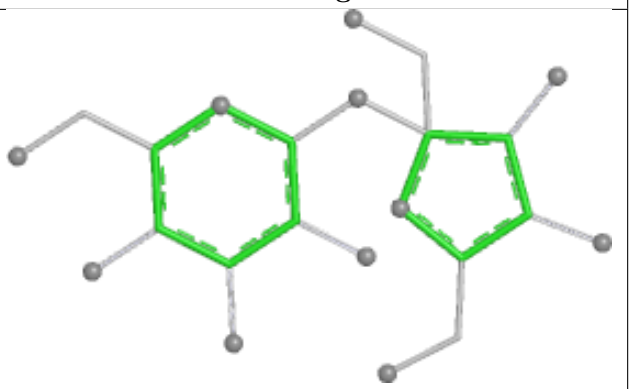
Bond lengths



Bond angles

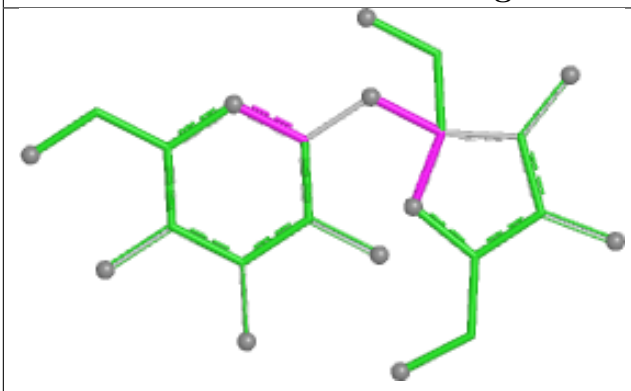


Torsions

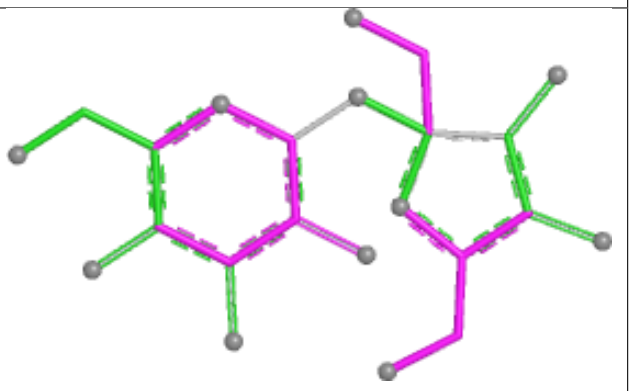


Rings

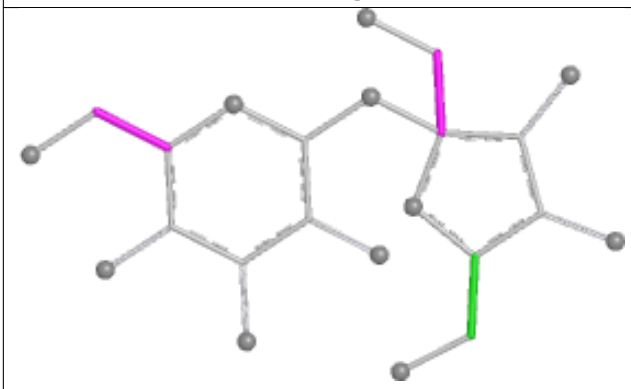
Oligosaccharide Chain X



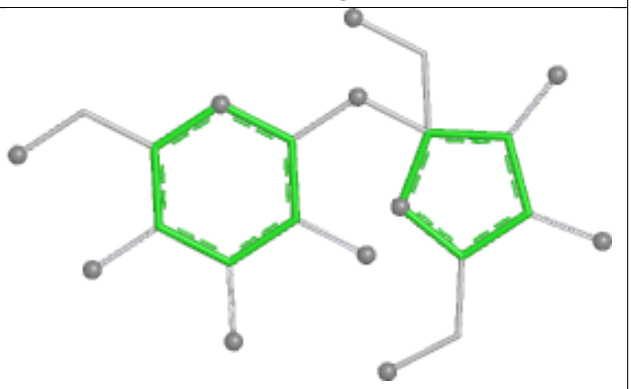
Bond lengths



Bond angles

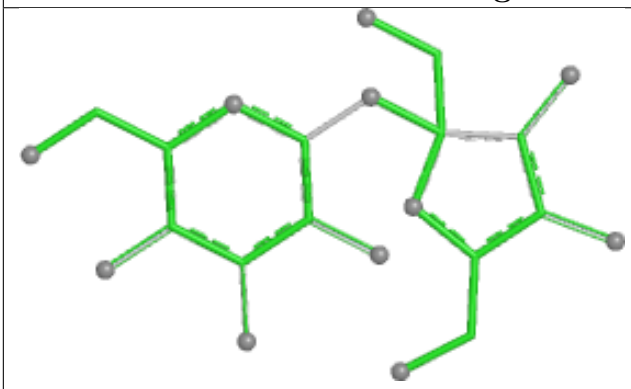


Torsions

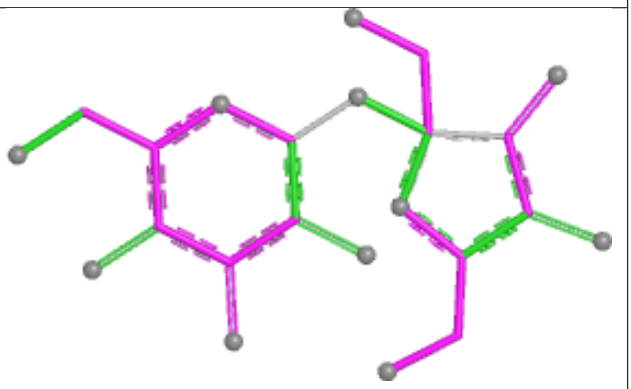


Rings

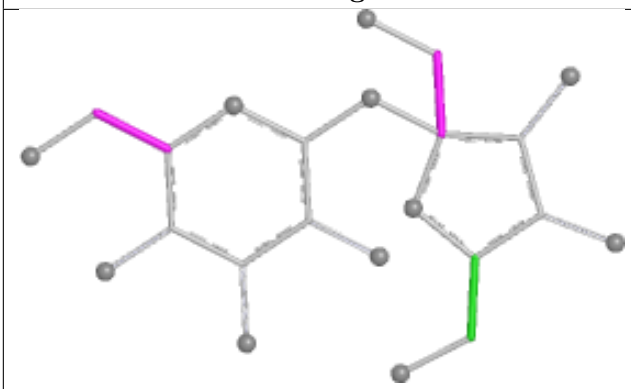
Oligosaccharide Chain Y



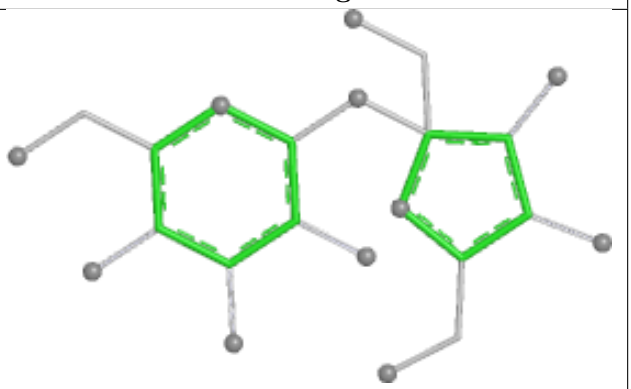
Bond lengths



Bond angles

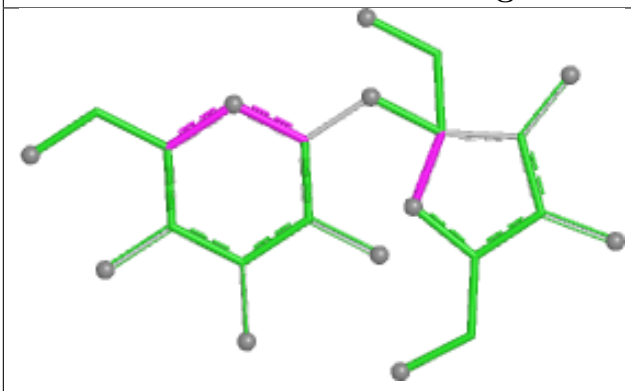


Torsions

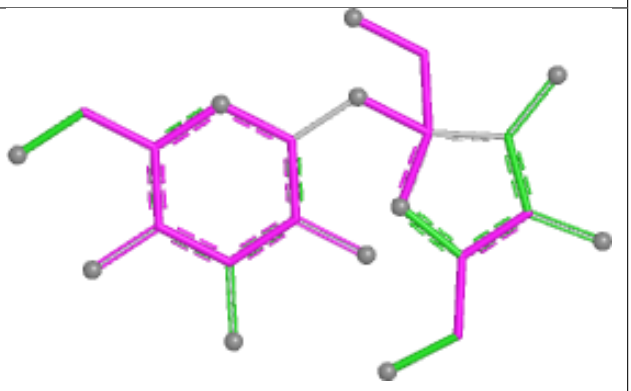


Rings

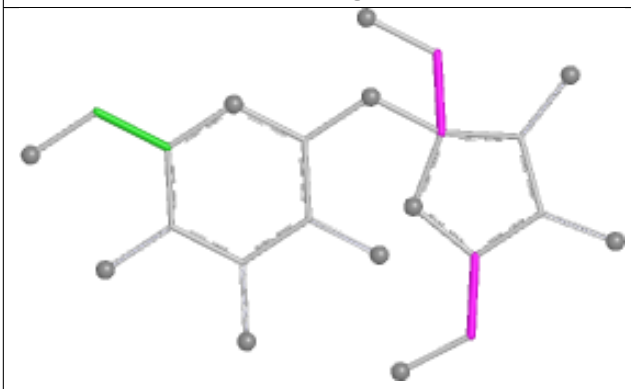
Oligosaccharide Chain Z



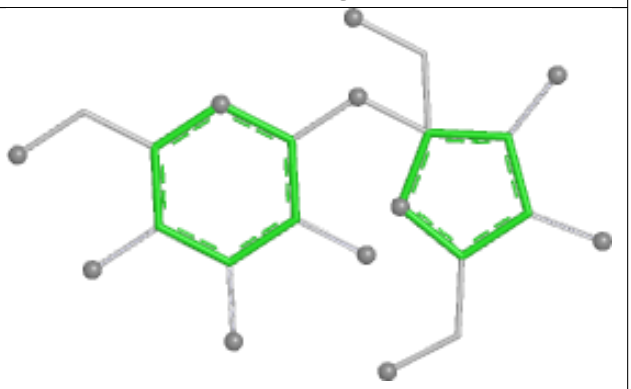
Bond lengths



Bond angles

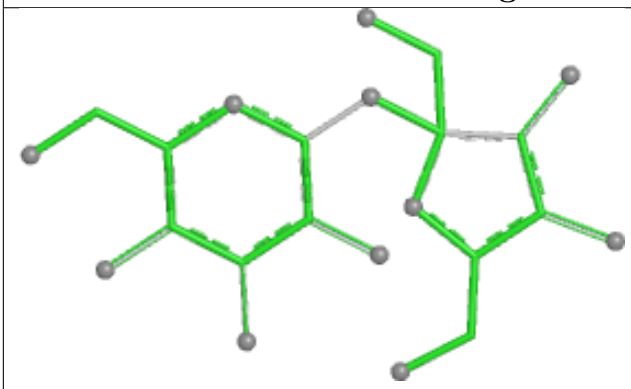


Torsions

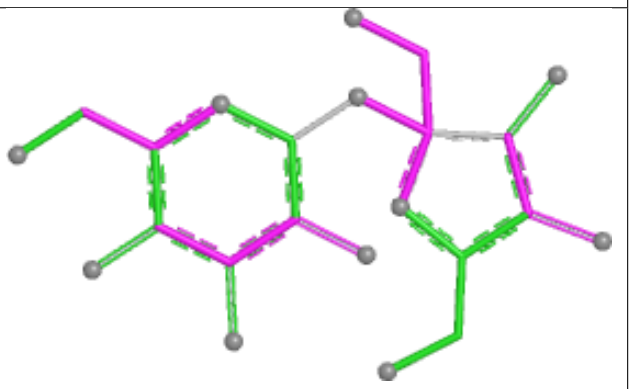


Rings

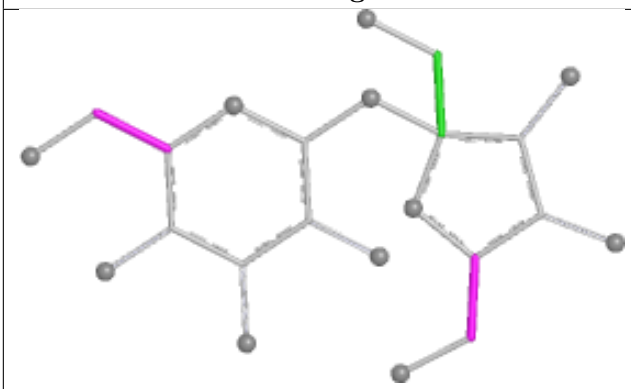
Oligosaccharide Chain a



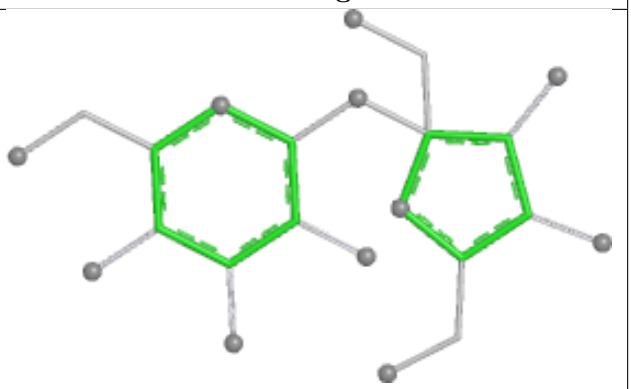
Bond lengths



Bond angles



Torsions



Rings

4.6 Ligand geometry (i)

Of 243 ligands modelled in this entry, 1 is unknown - leaving 242 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	$\#\|Z\| > 2$
20	CLA	1	215	-	24,32,73	2.47	7 (29%)	31,54,113	3.38	19 (61%)
21	LMU	1	217	-	36,36,36	0.45	0	47,47,47	1.65	9 (19%)
20	CLA	4	315	-	50,54,73	2.72	20 (40%)	59,90,113	3.09	25 (42%)
22	BCR	F	203	-	41,41,41	2.48	12 (29%)	56,56,56	6.23	32 (57%)
20	CLA	4	317	-	24,32,73	2.35	8 (33%)	31,54,113	2.71	17 (54%)
20	CLA	4	310	-	59,63,73	2.41	12 (20%)	70,101,113	2.86	28 (40%)
21	LMU	R	109	-	36,36,36	1.15	2 (5%)	47,47,47	2.46	15 (31%)
20	CLA	R	106	-	61,65,73	2.38	13 (21%)	72,103,113	2.91	27 (37%)
20	CLA	A	811	-	58,62,73	2.25	14 (24%)	68,99,113	2.71	25 (36%)
20	CLA	A	815	-	56,60,73	2.46	13 (23%)	65,97,113	3.01	27 (41%)
20	CLA	A	820	-	59,63,73	2.40	14 (23%)	70,101,113	2.82	24 (34%)
20	CLA	3	314	-	46,50,73	2.51	11 (23%)	53,85,113	3.15	27 (50%)
20	CLA	A	813	-	54,58,73	2.57	13 (24%)	64,95,113	2.75	27 (42%)
21	LMU	4	321	-	36,36,36	1.03	1 (2%)	47,47,47	1.42	8 (17%)
20	CLA	A	837	-	69,73,73	2.17	15 (21%)	82,113,113	2.64	23 (28%)
20	CLA	B	822	-	62,66,73	2.29	15 (24%)	73,104,113	2.79	25 (34%)
20	CLA	1	213	-	24,32,73	2.46	8 (33%)	31,54,113	2.89	18 (58%)
20	CLA	B	831	20	49,53,73	2.71	16 (32%)	58,89,113	3.07	20 (34%)
21	LMU	2	318	-	36,36,36	1.12	1 (2%)	47,47,47	1.94	14 (29%)
20	CLA	A	857	-	24,32,73	2.34	10 (41%)	31,54,113	2.81	18 (58%)
20	CLA	L	201	-	69,73,73	2.22	14 (20%)	82,113,113	2.59	27 (32%)
22	BCR	B	843	-	41,41,41	1.68	5 (12%)	56,56,56	6.06	19 (33%)
20	CLA	3	319	-	38,44,73	2.83	11 (28%)	52,78,113	3.35	24 (46%)
20	CLA	A	827	-	54,58,73	2.47	12 (22%)	64,95,113	3.03	28 (43%)
22	BCR	I	103	-	41,41,41	2.45	8 (19%)	56,56,56	6.68	29 (51%)
20	CLA	A	850	-	50,54,73	2.79	15 (30%)	61,90,113	3.93	35 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	3	320	-	59,63,73	2.34	12 (20%)	70,101,113	2.90	26 (37%)
21	LMU	A	852	-	36,36,36	0.62	1 (2%)	47,47,47	1.89	11 (23%)
20	CLA	B	829	-	69,73,73	2.27	16 (23%)	82,113,113	2.92	28 (34%)
22	BCR	I	101	-	41,41,41	2.38	16 (39%)	56,56,56	5.48	31 (55%)
20	CLA	K	103	21	54,58,73	2.46	15 (27%)	64,95,113	2.96	23 (35%)
20	CLA	A	817	-	69,73,73	2.20	16 (23%)	82,113,113	2.59	26 (31%)
20	CLA	L	207	22	51,55,73	2.46	12 (23%)	60,91,113	3.31	27 (45%)
21	LMU	L	205	-	36,36,36	0.70	2 (5%)	47,47,47	2.44	15 (31%)
20	CLA	A	808	-	49,53,73	2.71	13 (26%)	58,89,113	3.20	24 (41%)
22	BCR	B	842	-	41,41,41	1.70	5 (12%)	56,56,56	5.15	23 (41%)
20	CLA	A	821	-	69,73,73	2.11	13 (18%)	82,113,113	2.53	26 (31%)
20	CLA	3	307	-	24,32,73	2.38	9 (37%)	31,54,113	2.76	17 (54%)
20	CLA	B	847	-	69,73,73	2.16	15 (21%)	82,113,113	2.81	36 (43%)
20	CLA	B	815	-	64,68,73	2.19	14 (21%)	76,107,113	2.70	28 (36%)
20	CLA	H	109	16	54,58,73	2.49	12 (22%)	64,95,113	2.84	22 (34%)
20	CLA	A	801	-	54,58,73	2.37	14 (25%)	64,95,113	3.22	28 (43%)
20	CLA	3	315	-	54,58,73	2.50	18 (33%)	64,95,113	3.18	27 (42%)
20	CLA	4	311	-	24,32,73	2.38	9 (37%)	31,54,113	2.92	19 (61%)
21	LMU	A	851	-	36,36,36	0.41	0	47,47,47	0.71	1 (2%)
20	CLA	3	303	-	38,44,73	2.79	10 (26%)	52,78,113	3.04	21 (40%)
20	CLA	L	202	-	69,73,73	2.12	13 (18%)	82,113,113	2.79	29 (35%)
20	CLA	L	204	-	59,63,73	2.85	23 (38%)	70,101,113	3.59	32 (45%)
20	CLA	1	211	-	55,59,73	2.84	24 (43%)	64,96,113	4.11	31 (48%)
20	CLA	H	110	-	59,63,73	2.38	12 (20%)	70,101,113	2.95	25 (35%)
21	LMU	B	802	-	36,36,36	0.96	3 (8%)	47,47,47	2.48	13 (27%)
22	BCR	A	840	-	41,41,41	1.68	4 (9%)	56,56,56	6.06	18 (32%)
20	CLA	A	828	-	69,73,73	2.26	17 (24%)	82,113,113	2.67	23 (28%)
21	LMU	4	322	20	36,36,36	0.85	1 (2%)	47,47,47	1.25	4 (8%)
21	LMU	C	101	-	36,36,36	0.94	1 (2%)	47,47,47	1.36	7 (14%)
20	CLA	A	855	-	69,73,73	2.17	15 (21%)	82,113,113	2.64	23 (28%)
20	CLA	1	214	-	55,59,73	2.90	24 (43%)	64,96,113	3.50	32 (50%)
20	CLA	2	311	-	54,58,73	2.57	14 (25%)	64,95,113	3.01	24 (37%)
20	CLA	B	811	-	69,73,73	2.22	12 (17%)	82,113,113	2.51	28 (34%)
20	CLA	4	314	4	24,32,73	2.37	8 (33%)	31,54,113	2.63	17 (54%)
21	LMU	R	103	-	36,36,36	0.69	0	47,47,47	2.19	17 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	B	818	-	50,54,73	2.50	13 (26%)	59,90,113	3.20	20 (33%)
21	LMU	B	845	-	26,26,36	1.04	1 (3%)	37,37,47	1.44	6 (16%)
22	BCR	G	102	-	41,41,41	1.69	5 (12%)	56,56,56	6.05	19 (33%)
20	CLA	A	812	-	49,53,73	2.63	12 (24%)	58,89,113	2.89	24 (41%)
20	CLA	4	319	21	51,55,73	2.53	15 (29%)	60,91,113	2.98	21 (35%)
20	CLA	3	301	20	60,64,73	2.44	20 (33%)	71,102,113	2.94	27 (38%)
21	LMU	2	313	-	36,36,36	0.90	1 (2%)	47,47,47	0.94	2 (4%)
21	LMU	F	201	-	35,35,36	1.20	4 (11%)	46,46,47	2.36	15 (32%)
20	CLA	R	107	-	69,73,73	2.28	12 (17%)	82,113,113	2.64	30 (36%)
20	CLA	2	303	-	24,32,73	2.35	9 (37%)	31,54,113	2.91	19 (61%)
20	CLA	A	848	-	69,73,73	2.24	18 (26%)	82,113,113	2.62	24 (29%)
20	CLA	B	821	-	58,62,73	2.43	19 (32%)	68,99,113	2.79	28 (41%)
22	BCR	A	843	-	41,41,41	1.68	5 (12%)	56,56,56	6.07	17 (30%)
22	BCR	B	844	-	41,41,41	1.67	5 (12%)	56,56,56	6.07	17 (30%)
20	CLA	2	307	20	69,73,73	2.18	12 (17%)	82,113,113	2.70	28 (34%)
22	BCR	F	202	-	41,41,41	1.68	5 (12%)	56,56,56	6.06	18 (32%)
20	CLA	3	306	-	24,32,73	2.40	9 (37%)	31,54,113	2.97	17 (54%)
20	CLA	B	816	-	65,69,73	2.19	15 (23%)	77,108,113	2.79	27 (35%)
20	CLA	A	819	5	46,50,73	2.59	12 (26%)	53,85,113	3.32	24 (45%)
20	CLA	B	817	-	54,58,73	2.41	13 (24%)	64,95,113	2.96	25 (39%)
20	CLA	A	838	-	54,58,73	2.53	15 (27%)	64,95,113	2.82	23 (35%)
22	BCR	A	842	-	41,41,41	1.68	5 (12%)	56,56,56	6.06	18 (32%)
20	CLA	B	832	20	49,53,73	2.63	13 (26%)	58,89,113	3.13	23 (39%)
22	BCR	A	844	-	41,41,41	1.68	5 (12%)	56,56,56	6.06	18 (32%)
20	CLA	H	107	-	69,73,73	2.26	13 (18%)	82,113,113	2.84	27 (32%)
20	CLA	4	318	-	56,60,73	2.45	13 (23%)	65,97,113	2.93	24 (36%)
20	CLA	4	309	-	24,32,73	2.45	8 (33%)	31,54,113	2.98	18 (58%)
20	CLA	B	849	-	69,73,73	2.26	15 (21%)	82,113,113	2.68	30 (36%)
20	CLA	3	313	-	24,32,73	2.47	9 (37%)	31,54,113	2.84	19 (61%)
20	CLA	A	814	-	69,73,73	2.26	19 (27%)	82,113,113	2.75	28 (34%)
20	CLA	A	847	-	69,73,73	2.20	15 (21%)	82,113,113	2.81	27 (32%)
20	CLA	1	206	-	65,69,73	2.28	15 (23%)	77,108,113	2.59	28 (36%)
21	LMU	H	102	19	36,36,36	1.21	3 (8%)	47,47,47	3.10	22 (46%)
20	CLA	1	207	-	55,59,73	2.53	16 (29%)	64,96,113	3.43	30 (46%)
21	LMU	1	218	-	36,36,36	1.02	3 (8%)	47,47,47	2.30	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	3	304	-	24,32,73	2.42	11 (45%)	31,54,113	3.47	20 (64%)
20	CLA	1	204	-	50,54,73	2.64	14 (28%)	59,90,113	2.78	23 (38%)
20	CLA	3	316	-	24,32,73	2.45	9 (37%)	31,54,113	3.07	19 (61%)
20	CLA	B	839	-	38,44,73	2.88	12 (31%)	52,78,113	3.38	29 (55%)
25	LMG	B	846	-	49,49,55	0.96	2 (4%)	57,57,63	1.02	3 (5%)
21	LMU	E	101	-	36,36,36	0.89	2 (5%)	47,47,47	3.11	22 (46%)
21	LMU	4	320	-	35,35,36	0.41	0	46,46,47	0.71	1 (2%)
20	CLA	B	807	6	69,73,73	2.13	14 (20%)	82,113,113	2.69	24 (29%)
20	CLA	B	805	-	69,73,73	2.21	16 (23%)	82,113,113	3.02	34 (41%)
21	LMU	A	853	-	36,36,36	0.67	1 (2%)	47,47,47	1.96	17 (36%)
20	CLA	B	826	-	69,73,73	2.19	15 (21%)	82,113,113	2.98	27 (32%)
20	CLA	L	208	-	54,58,73	2.65	19 (35%)	64,95,113	3.23	25 (39%)
20	CLA	1	210	1	38,44,73	2.87	12 (31%)	52,78,113	3.10	23 (44%)
20	CLA	K	106	-	54,58,73	2.86	23 (42%)	64,95,113	3.24	30 (46%)
20	CLA	A	830	20	54,58,73	2.43	14 (25%)	64,95,113	2.85	26 (40%)
20	CLA	4	304	-	69,73,73	2.42	27 (39%)	82,113,113	3.52	38 (46%)
20	CLA	B	812	-	64,68,73	2.25	11 (17%)	76,107,113	2.60	26 (34%)
20	CLA	4	308	-	24,32,73	2.45	8 (33%)	31,54,113	2.90	18 (58%)
20	CLA	A	807	-	59,63,73	2.32	12 (20%)	70,101,113	2.98	30 (42%)
20	CLA	3	305	-	24,32,73	2.43	9 (37%)	31,54,113	2.97	17 (54%)
20	CLA	B	823	-	69,73,73	2.18	15 (21%)	82,113,113	2.64	23 (28%)
20	CLA	F	205	20	45,49,73	2.66	15 (33%)	54,84,113	3.14	20 (37%)
20	CLA	G	103	-	55,59,73	2.52	12 (21%)	64,96,113	2.88	26 (40%)
20	CLA	B	813	-	50,54,73	2.51	12 (24%)	59,90,113	2.96	24 (40%)
21	LMU	R	104	-	36,36,36	0.98	2 (5%)	47,47,47	1.64	11 (23%)
23	PQN	B	840	-	34,34,34	1.69	2 (5%)	43,45,45	1.59	6 (13%)
20	CLA	B	838	-	69,73,73	2.11	14 (20%)	82,113,113	2.76	30 (36%)
20	CLA	B	848	-	69,73,73	2.14	13 (18%)	82,113,113	2.76	31 (37%)
21	LMU	3	318	-	36,36,36	0.41	0	47,47,47	0.69	1 (2%)
20	CLA	2	321	20	65,69,73	2.44	25 (38%)	77,108,113	2.97	32 (41%)
20	CLA	A	804	-	61,65,73	2.33	14 (22%)	72,103,113	2.96	29 (40%)
21	LMU	R	108	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
20	CLA	K	107	-	69,73,73	2.21	12 (17%)	82,113,113	2.53	27 (32%)
21	LMU	L	210	-	36,36,36	0.99	3 (8%)	47,47,47	1.49	9 (19%)
21	LMU	1	216	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	2	302	-	60,64,73	2.38	15 (25%)	71,102,113	2.92	31 (43%)
20	CLA	B	827	-	54,58,73	2.67	16 (29%)	64,95,113	2.68	29 (45%)
20	CLA	1	205	-	38,44,73	3.00	12 (31%)	52,78,113	3.27	23 (44%)
20	CLA	A	834	-	51,55,73	2.52	15 (29%)	60,91,113	2.98	21 (35%)
20	CLA	B	810	-	69,73,73	2.24	15 (21%)	82,113,113	2.49	24 (29%)
20	CLA	B	834	-	64,68,73	2.21	13 (20%)	76,107,113	2.99	21 (27%)
21	LMU	2	320	-	36,36,36	1.12	1 (2%)	47,47,47	1.37	4 (8%)
20	CLA	B	835	-	69,73,73	2.13	13 (18%)	82,113,113	2.67	25 (30%)
20	CLA	B	808	-	58,62,73	2.65	14 (24%)	71,100,113	2.80	30 (42%)
21	LMU	R	101	-	36,36,36	0.40	0	47,47,47	1.75	12 (25%)
20	CLA	1	203	-	51,55,73	2.57	13 (25%)	60,91,113	3.26	24 (40%)
20	CLA	2	301	-	55,59,73	2.43	15 (27%)	64,96,113	2.96	23 (35%)
21	LMU	R	105	-	36,36,36	0.96	1 (2%)	47,47,47	1.59	10 (21%)
20	CLA	F	204	-	38,44,73	2.81	12 (31%)	52,78,113	3.20	27 (51%)
20	CLA	4	312	-	24,32,73	2.56	7 (29%)	31,54,113	2.94	20 (64%)
20	CLA	4	307	-	56,60,73	3.06	29 (51%)	65,97,113	3.78	38 (58%)
20	CLA	A	802	-	59,63,73	2.41	16 (27%)	70,101,113	2.81	26 (37%)
20	CLA	B	836	-	51,55,73	2.47	14 (27%)	60,91,113	2.92	26 (43%)
20	CLA	B	837	-	69,73,73	2.17	14 (20%)	82,113,113	2.84	30 (36%)
20	CLA	B	819	-	59,63,73	2.48	15 (25%)	70,101,113	2.76	22 (31%)
22	BCR	A	841	-	41,41,41	1.67	3 (7%)	56,56,56	6.06	17 (30%)
20	CLA	A	824	-	69,73,73	2.17	13 (18%)	82,113,113	2.72	30 (36%)
20	CLA	3	317	-	24,32,73	2.42	7 (29%)	31,54,113	2.82	18 (58%)
20	CLA	1	201	-	50,54,73	2.82	24 (48%)	59,90,113	4.11	36 (61%)
21	LMU	B	801	-	36,36,36	0.64	0	47,47,47	2.42	15 (31%)
20	CLA	3	308	-	24,32,73	2.40	9 (37%)	31,54,113	3.21	18 (58%)
21	LMU	A	854	-	36,36,36	0.83	1 (2%)	47,47,47	1.62	8 (17%)
20	CLA	1	202	-	51,55,73	2.55	14 (27%)	60,91,113	3.00	23 (38%)
20	CLA	4	303	-	38,44,73	3.08	15 (39%)	52,78,113	3.61	24 (46%)
20	CLA	4	305	-	59,63,73	2.31	12 (20%)	70,101,113	2.89	28 (40%)
20	CLA	2	315	-	24,32,73	2.46	8 (33%)	31,54,113	2.71	18 (58%)
20	CLA	B	833	-	55,59,73	2.53	12 (21%)	64,96,113	2.95	25 (39%)
20	CLA	L	203	-	59,63,73	2.43	12 (20%)	70,101,113	2.77	29 (41%)
20	CLA	A	805	-	50,54,73	2.51	12 (24%)	59,90,113	2.91	25 (42%)
20	CLA	2	309	-	24,32,73	2.38	8 (33%)	31,54,113	2.82	18 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	LMU	3	302	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
20	CLA	A	825	-	59,63,73	2.34	15 (25%)	70,101,113	2.78	27 (38%)
20	CLA	3	312	-	24,32,73	2.50	9 (37%)	31,54,113	2.91	20 (64%)
21	LMU	K	102	-	36,36,36	0.47	0	47,47,47	2.08	16 (34%)
20	CLA	A	803	-	69,73,73	2.13	12 (17%)	82,113,113	2.76	30 (36%)
21	LMU	4	301	-	36,36,36	0.40	0	47,47,47	0.70	1 (2%)
21	LMU	R	102	-	36,36,36	0.75	0	47,47,47	2.09	14 (29%)
22	BCR	L	209	-	41,41,41	2.17	10 (24%)	56,56,56	5.87	20 (35%)
20	CLA	A	818	-	55,59,73	2.50	14 (25%)	64,96,113	2.93	23 (35%)
20	CLA	4	302	-	59,63,73	2.35	15 (25%)	70,101,113	2.84	24 (34%)
20	CLA	B	809	-	59,63,73	2.28	15 (25%)	70,101,113	2.76	28 (40%)
20	CLA	K	105	-	49,53,73	2.56	16 (32%)	58,89,113	3.02	20 (34%)
21	LMU	A	845	-	36,36,36	0.94	0	47,47,47	1.40	6 (12%)
20	CLA	A	810	-	58,62,73	2.36	13 (22%)	68,99,113	2.57	23 (33%)
20	CLA	A	835	-	55,59,73	2.43	15 (27%)	64,96,113	2.96	23 (35%)
23	PQN	A	839	-	34,34,34	1.80	3 (8%)	43,45,45	1.49	9 (20%)
20	CLA	4	306	-	54,58,73	2.58	12 (22%)	64,95,113	2.75	21 (32%)
20	CLA	2	312	-	69,73,73	2.23	14 (20%)	82,113,113	2.70	25 (30%)
20	CLA	2	317	-	69,73,73	2.15	15 (21%)	82,113,113	2.50	22 (26%)
20	CLA	2	304	-	54,58,73	2.47	13 (24%)	64,95,113	2.67	24 (37%)
20	CLA	B	820	-	69,73,73	2.90	30 (43%)	82,113,113	2.92	28 (34%)
21	LMU	H	105	19	36,36,36	0.76	0	47,47,47	2.27	16 (34%)
20	CLA	2	308	-	24,32,73	2.40	8 (33%)	31,54,113	2.98	19 (61%)
20	CLA	H	108	-	59,63,73	2.42	12 (20%)	70,101,113	2.79	24 (34%)
20	CLA	A	822	-	69,73,73	2.17	15 (21%)	82,113,113	2.65	24 (29%)
20	CLA	4	313	-	38,44,73	2.71	11 (28%)	52,78,113	3.51	26 (50%)
20	CLA	J	102	-	65,69,73	2.23	15 (23%)	77,108,113	2.71	23 (29%)
22	BCR	B	841	-	41,41,41	1.69	5 (12%)	56,56,56	6.05	19 (33%)
20	CLA	A	831	5	49,53,73	2.57	15 (30%)	58,89,113	3.03	20 (34%)
20	CLA	A	806	5	69,73,73	2.21	15 (21%)	82,113,113	2.93	32 (39%)
20	CLA	A	849	-	69,73,73	2.34	16 (23%)	82,113,113	2.86	27 (32%)
20	CLA	B	824	-	69,73,73	2.34	14 (20%)	82,113,113	2.85	26 (31%)
20	CLA	2	306	-	69,73,73	2.21	13 (18%)	82,113,113	2.76	25 (30%)
20	CLA	3	310	-	69,73,73	2.16	15 (21%)	82,113,113	2.64	23 (28%)
20	CLA	F	206	20	57,61,73	2.73	24 (42%)	67,98,113	2.83	26 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	B	825	-	69,73,73	2.15	14 (20%)	82,113,113	2.85	30 (36%)
21	LMU	2	316	-	36,36,36	0.39	0	47,47,47	0.70	1 (2%)
20	CLA	1	209	-	38,44,73	3.57	22 (57%)	52,78,113	4.04	26 (50%)
21	LMU	4	316	-	36,36,36	0.86	1 (2%)	47,47,47	1.19	3 (6%)
20	CLA	2	305	-	24,32,73	2.42	11 (45%)	31,54,113	3.11	20 (64%)
20	CLA	A	829	-	69,73,73	2.24	13 (18%)	82,113,113	2.93	32 (39%)
20	CLA	B	830	-	54,58,73	2.59	18 (33%)	64,95,113	3.14	27 (42%)
22	BCR	J	101	-	41,41,41	1.67	5 (12%)	56,56,56	6.06	18 (32%)
20	CLA	H	101	-	59,63,73	2.43	15 (25%)	70,101,113	2.96	29 (41%)
20	CLA	B	814	-	63,67,73	2.31	14 (22%)	74,105,113	2.41	24 (32%)
20	CLA	1	208	-	24,32,73	2.33	8 (33%)	31,54,113	2.76	19 (61%)
21	LMU	G	101	-	36,36,36	0.98	2 (5%)	47,47,47	2.60	13 (27%)
20	CLA	B	828	-	54,58,73	2.34	11 (20%)	64,95,113	3.02	29 (45%)
22	BCR	3	311	-	41,41,41	1.79	5 (12%)	56,56,56	6.05	22 (39%)
22	BCR	B	850	20	41,41,41	2.74	18 (43%)	56,56,56	6.57	27 (48%)
20	CLA	3	309	-	69,73,73	2.48	23 (33%)	82,113,113	3.15	29 (35%)
24	SF4	C	103	7	0,12,12	-	-	-		
20	CLA	J	103	20	59,63,73	2.47	20 (33%)	70,101,113	2.99	27 (38%)
20	CLA	A	833	-	69,73,73	2.17	15 (21%)	82,113,113	2.65	23 (28%)
20	CLA	B	806	-	69,73,73	2.24	13 (18%)	82,113,113	2.78	29 (35%)
20	CLA	A	826	-	69,73,73	2.18	15 (21%)	82,113,113	2.65	30 (36%)
24	SF4	C	102	7	0,12,12	-	-	-		
20	CLA	A	816	-	69,73,73	2.17	15 (21%)	82,113,113	2.61	30 (36%)
24	SF4	A	856	5,6	0,12,12	-	-	-		
20	CLA	2	310	2	54,58,73	2.46	13 (24%)	64,95,113	2.98	25 (39%)
21	LMU	A	846	-	36,36,36	0.95	1 (2%)	47,47,47	1.66	11 (23%)
20	CLA	B	803	-	49,53,73	2.62	16 (32%)	58,89,113	3.13	22 (37%)
20	CLA	A	836	-	69,73,73	2.17	15 (21%)	82,113,113	2.64	23 (28%)
21	LMU	K	104	20	36,36,36	0.75	0	47,47,47	2.28	12 (25%)
20	CLA	1	212	-	65,69,73	2.33	21 (32%)	77,108,113	2.84	29 (37%)
20	CLA	B	804	-	69,73,73	2.16	14 (20%)	82,113,113	3.00	33 (40%)
20	CLA	A	832	-	55,59,73	2.44	15 (27%)	64,96,113	2.96	23 (35%)
21	LMU	2	319	-	36,36,36	1.09	1 (2%)	47,47,47	1.31	6 (12%)
20	CLA	I	102	-	64,68,73	2.31	15 (23%)	76,107,113	2.79	24 (31%)
21	LMU	H	104	-	36,36,36	0.98	3 (8%)	47,47,47	2.76	20 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	CLA	A	823	20	69,73,73	2.17	16 (23%)	82,113,113	2.64	23 (28%)
20	CLA	2	314	-	24,32,73	2.44	11 (45%)	31,54,113	3.04	21 (67%)
21	LMU	H	103	-	36,36,36	0.89	1 (2%)	47,47,47	2.30	16 (34%)
21	LMU	K	101	-	36,36,36	0.61	0	47,47,47	1.91	14 (29%)
21	LMU	L	206	-	36,36,36	0.73	2 (5%)	47,47,47	1.91	17 (36%)
20	CLA	A	809	-	69,73,73	2.19	12 (17%)	82,113,113	3.02	31 (37%)

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
20	CLA	1	215	-	1/1/4/20	-	-
21	LMU	1	217	-	-	10/21/61/61	0/2/2/2
20	CLA	4	315	-	1/1/11/20	10/17/93/115	-
22	BCR	F	203	-	-	12/29/63/63	0/2/2/2
20	CLA	4	317	-	1/1/4/20	-	-
20	CLA	4	310	-	2/2/13/20	14/27/103/115	-
21	LMU	R	109	-	1/1/10/10	11/21/61/61	0/2/2/2
20	CLA	R	106	-	2/2/13/20	15/30/106/115	-
20	CLA	A	811	-	1/1/12/20	10/26/102/115	-
20	CLA	A	815	-	1/1/12/20	11/24/100/115	-
20	CLA	A	820	-	2/2/13/20	10/27/103/115	-
20	CLA	3	314	-	1/1/10/20	5/12/88/115	-
20	CLA	A	813	-	1/1/12/20	10/21/97/115	-
21	LMU	4	321	-	-	15/21/61/61	0/2/2/2
20	CLA	A	837	-	2/2/15/20	17/39/115/115	-
20	CLA	B	822	-	2/2/13/20	16/31/107/115	-
20	CLA	1	213	-	1/1/4/20	-	-
20	CLA	B	831	20	1/1/11/20	11/15/91/115	-
21	LMU	2	318	-	-	13/21/61/61	0/2/2/2
20	CLA	A	857	-	1/1/4/20	-	-
20	CLA	L	201	-	2/2/15/20	14/39/115/115	-
22	BCR	B	843	-	-	13/29/63/63	0/2/2/2
20	CLA	3	319	-	1/1/9/20	-	-
20	CLA	A	827	-	1/1/12/20	4/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	I	103	-	-	13/29/63/63	0/2/2/2
20	CLA	A	850	-	3/3/11/20	12/16/92/115	-
20	CLA	3	320	-	2/2/13/20	8/27/103/115	-
21	LMU	A	852	-	-	11/21/61/61	0/2/2/2
20	CLA	B	829	-	2/2/15/20	21/39/115/115	-
22	BCR	I	101	-	-	7/29/63/63	0/2/2/2
20	CLA	K	103	21	1/1/12/20	5/21/97/115	-
20	CLA	A	817	-	2/2/15/20	13/39/115/115	-
20	CLA	L	207	22	1/1/11/20	11/18/94/115	-
21	LMU	L	205	-	-	15/21/61/61	0/2/2/2
20	CLA	A	808	-	1/1/11/20	4/15/91/115	-
22	BCR	B	842	-	-	11/29/63/63	0/2/2/2
20	CLA	A	821	-	2/2/15/20	20/39/115/115	-
20	CLA	3	307	-	1/1/4/20	-	-
20	CLA	B	847	-	2/2/15/20	16/39/115/115	-
20	CLA	B	815	-	2/2/14/20	15/33/109/115	-
20	CLA	H	109	16	1/1/12/20	10/21/97/115	-
20	CLA	A	801	-	1/1/12/20	4/21/97/115	-
20	CLA	3	315	-	1/1/12/20	6/21/97/115	-
20	CLA	4	311	-	1/1/4/20	-	-
21	LMU	A	851	-	-	19/21/61/61	0/2/2/2
20	CLA	3	303	-	1/1/9/20	-	-
20	CLA	L	202	-	2/2/15/20	14/39/115/115	-
20	CLA	L	204	-	3/3/13/20	14/27/103/115	-
20	CLA	1	211	-	2/2/12/20	9/23/99/115	-
20	CLA	H	110	-	2/2/13/20	14/27/103/115	-
21	LMU	B	802	-	-	11/21/61/61	0/2/2/2
22	BCR	A	840	-	-	12/29/63/63	0/2/2/2
20	CLA	A	828	-	2/2/15/20	21/39/115/115	-
21	LMU	4	322	20	-	14/21/61/61	0/2/2/2
21	LMU	C	101	-	-	14/21/61/61	0/2/2/2
20	CLA	A	855	-	2/2/15/20	20/39/115/115	-
20	CLA	1	214	-	3/3/12/20	13/23/99/115	-
20	CLA	2	311	-	1/1/12/20	9/21/97/115	-
20	CLA	B	811	-	2/2/15/20	25/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	314	4	1/1/4/20	-	-
21	LMU	R	103	-	-	17/21/61/61	0/2/2/2
20	CLA	B	818	-	1/1/11/20	14/17/93/115	-
21	LMU	B	845	-	-	4/11/51/61	0/2/2/2
22	BCR	G	102	-	-	10/29/63/63	0/2/2/2
20	CLA	A	812	-	1/1/11/20	13/15/91/115	-
20	CLA	4	319	21	1/1/11/20	9/18/94/115	-
20	CLA	3	301	20	2/2/13/20	14/29/105/115	-
21	LMU	2	313	-	-	16/21/61/61	0/2/2/2
21	LMU	F	201	-	-	14/20/60/61	0/2/2/2
20	CLA	R	107	-	2/2/15/20	21/39/115/115	-
20	CLA	2	303	-	1/1/4/20	-	-
20	CLA	A	848	-	2/2/15/20	16/39/115/115	-
20	CLA	B	821	-	1/1/12/20	7/26/102/115	-
22	BCR	A	843	-	-	15/29/63/63	0/2/2/2
22	BCR	B	844	-	-	14/29/63/63	0/2/2/2
20	CLA	2	307	20	2/2/15/20	14/39/115/115	-
22	BCR	F	202	-	-	12/29/63/63	0/2/2/2
20	CLA	3	306	-	1/1/4/20	-	-
20	CLA	B	816	-	2/2/14/20	17/35/111/115	-
20	CLA	A	819	5	1/1/10/20	3/12/88/115	-
20	CLA	B	817	-	1/1/12/20	7/21/97/115	-
20	CLA	A	838	-	1/1/12/20	10/21/97/115	-
22	BCR	A	842	-	-	17/29/63/63	0/2/2/2
20	CLA	B	832	20	1/1/11/20	7/15/91/115	-
22	BCR	A	844	-	-	10/29/63/63	0/2/2/2
20	CLA	H	107	-	2/2/15/20	19/39/115/115	-
20	CLA	4	318	-	1/1/12/20	8/24/100/115	-
20	CLA	4	309	-	1/1/4/20	-	-
20	CLA	B	849	-	2/2/15/20	18/39/115/115	-
20	CLA	3	313	-	1/1/4/20	-	-
20	CLA	A	814	-	2/2/15/20	17/39/115/115	-
20	CLA	A	847	-	2/2/15/20	21/39/115/115	-
20	CLA	1	206	-	2/2/14/20	21/35/111/115	-
21	LMU	H	102	19	-	14/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	207	-	2/2/12/20	9/23/99/115	-
21	LMU	1	218	-	-	13/21/61/61	0/2/2/2
20	CLA	3	304	-	1/1/4/20	-	-
20	CLA	1	204	-	1/1/11/20	8/17/93/115	-
20	CLA	3	316	-	1/1/4/20	-	-
20	CLA	B	839	-	1/1/9/20	-	-
25	LMG	B	846	-	-	23/44/64/70	0/1/1/1
21	LMU	E	101	-	-	14/21/61/61	0/2/2/2
21	LMU	4	320	-	-	15/20/60/61	0/2/2/2
20	CLA	B	807	6	2/2/15/20	20/39/115/115	-
20	CLA	B	805	-	2/2/15/20	19/39/115/115	-
21	LMU	A	853	-	-	14/21/61/61	0/2/2/2
20	CLA	B	826	-	2/2/15/20	25/39/115/115	-
20	CLA	L	208	-	2/2/12/20	10/21/97/115	-
20	CLA	1	210	1	1/1/9/20	-	-
20	CLA	K	106	-	1/1/12/20	9/21/97/115	-
20	CLA	A	830	20	1/1/12/20	13/21/97/115	-
20	CLA	4	304	-	3/3/15/20	18/39/115/115	-
20	CLA	B	812	-	2/2/14/20	11/33/109/115	-
20	CLA	4	308	-	1/1/4/20	-	-
20	CLA	A	807	-	2/2/13/20	12/27/103/115	-
20	CLA	3	305	-	1/1/4/20	-	-
20	CLA	B	823	-	2/2/15/20	21/39/115/115	-
20	CLA	F	205	20	1/1/10/20	5/10/86/115	-
20	CLA	G	103	-	1/1/12/20	11/23/99/115	-
20	CLA	B	813	-	1/1/11/20	9/17/93/115	-
21	LMU	R	104	-	-	15/21/61/61	0/2/2/2
23	PQN	B	840	-	1/1/8/9	10/23/43/43	0/2/2/2
20	CLA	B	838	-	2/2/15/20	16/39/115/115	-
20	CLA	B	848	-	2/2/15/20	16/39/115/115	-
21	LMU	3	318	-	-	17/21/61/61	0/2/2/2
20	CLA	2	321	20	2/2/14/20	20/35/111/115	-
20	CLA	A	804	-	2/2/13/20	8/30/106/115	-
21	LMU	R	108	-	-	16/21/61/61	0/2/2/2
20	CLA	K	107	-	2/2/15/20	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMU	L	210	-	-	14/21/61/61	0/2/2/2
21	LMU	1	216	-	-	13/21/61/61	0/2/2/2
20	CLA	2	302	-	2/2/13/20	12/29/105/115	-
20	CLA	B	827	-	1/1/12/20	8/21/97/115	-
20	CLA	1	205	-	1/1/9/20	-	-
20	CLA	A	834	-	1/1/11/20	8/18/94/115	-
20	CLA	B	810	-	2/2/15/20	20/39/115/115	-
20	CLA	B	834	-	2/2/14/20	17/33/109/115	-
21	LMU	2	320	-	-	8/21/61/61	0/2/2/2
20	CLA	B	835	-	2/2/15/20	12/39/115/115	-
20	CLA	B	808	-	2/2/13/20	11/25/101/115	-
21	LMU	R	101	-	-	11/21/61/61	0/2/2/2
20	CLA	1	203	-	1/1/11/20	8/18/94/115	-
20	CLA	2	301	-	1/1/12/20	11/23/99/115	-
21	LMU	R	105	-	-	13/21/61/61	0/2/2/2
20	CLA	F	204	-	1/1/9/20	-	-
20	CLA	4	312	-	1/1/4/20	-	-
20	CLA	4	307	-	2/2/12/20	7/24/100/115	-
20	CLA	A	802	-	2/2/13/20	11/27/103/115	-
20	CLA	B	836	-	1/1/11/20	7/18/94/115	-
20	CLA	B	837	-	2/2/15/20	17/39/115/115	-
20	CLA	B	819	-	2/2/13/20	9/27/103/115	-
22	BCR	A	841	-	-	13/29/63/63	0/2/2/2
20	CLA	A	824	-	2/2/15/20	18/39/115/115	-
20	CLA	3	317	-	1/1/4/20	-	-
20	CLA	1	201	-	1/1/11/20	12/17/93/115	-
21	LMU	B	801	-	-	16/21/61/61	0/2/2/2
20	CLA	3	308	-	1/1/4/20	-	-
21	LMU	A	854	-	-	14/21/61/61	0/2/2/2
20	CLA	1	202	-	1/1/11/20	9/18/94/115	-
20	CLA	4	303	-	1/1/9/20	-	-
20	CLA	4	305	-	2/2/13/20	13/27/103/115	-
20	CLA	2	315	-	1/1/4/20	-	-
20	CLA	B	833	-	1/1/12/20	8/23/99/115	-
20	CLA	L	203	-	2/2/13/20	8/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	805	-	1/1/11/20	7/17/93/115	-
20	CLA	2	309	-	1/1/4/20	-	-
21	LMU	3	302	-	-	11/21/61/61	0/2/2/2
20	CLA	A	825	-	2/2/13/20	9/27/103/115	-
20	CLA	3	312	-	1/1/4/20	-	-
21	LMU	K	102	-	-	18/21/61/61	0/2/2/2
20	CLA	A	803	-	2/2/15/20	22/39/115/115	-
21	LMU	4	301	-	-	13/21/61/61	0/2/2/2
21	LMU	R	102	-	-	13/21/61/61	0/2/2/2
22	BCR	L	209	-	-	12/29/63/63	0/2/2/2
20	CLA	A	818	-	1/1/12/20	9/23/99/115	-
20	CLA	4	302	-	2/2/13/20	14/27/103/115	-
20	CLA	B	809	-	2/2/13/20	11/27/103/115	-
20	CLA	K	105	-	1/1/11/20	5/15/91/115	-
21	LMU	A	845	-	-	16/21/61/61	0/2/2/2
20	CLA	A	810	-	1/1/12/20	13/26/102/115	-
20	CLA	A	835	-	1/1/12/20	13/23/99/115	-
23	PQN	A	839	-	1/1/8/9	11/23/43/43	0/2/2/2
20	CLA	4	306	-	1/1/12/20	6/21/97/115	-
20	CLA	2	312	-	2/2/15/20	18/39/115/115	-
20	CLA	2	317	-	2/2/15/20	20/39/115/115	-
20	CLA	2	304	-	1/1/12/20	9/21/97/115	-
20	CLA	B	820	-	1/1/15/20	18/39/115/115	-
21	LMU	H	105	19	-	11/21/61/61	0/2/2/2
20	CLA	2	308	-	1/1/4/20	-	-
20	CLA	H	108	-	2/2/13/20	10/27/103/115	-
20	CLA	A	822	-	2/2/15/20	18/39/115/115	-
20	CLA	4	313	-	1/1/9/20	-	-
20	CLA	J	102	-	2/2/14/20	25/35/111/115	-
22	BCR	B	841	-	-	8/29/63/63	0/2/2/2
20	CLA	A	831	5	1/1/11/20	8/15/91/115	-
20	CLA	A	806	5	2/2/15/20	19/39/115/115	-
20	CLA	A	849	-	2/2/15/20	22/39/115/115	-
20	CLA	B	824	-	2/2/15/20	17/39/115/115	-
20	CLA	2	306	-	2/2/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	3	310	-	2/2/15/20	22/39/115/115	-
20	CLA	F	206	20	4/4/12/20	11/25/101/115	-
20	CLA	B	825	-	2/2/15/20	15/39/115/115	-
21	LMU	2	316	-	-	14/21/61/61	0/2/2/2
20	CLA	1	209	-	1/1/9/20	-	-
21	LMU	4	316	-	-	13/21/61/61	0/2/2/2
20	CLA	2	305	-	1/1/4/20	-	-
20	CLA	A	829	-	2/2/15/20	23/39/115/115	-
20	CLA	B	830	-	1/1/12/20	8/21/97/115	-
22	BCR	J	101	-	-	12/29/63/63	0/2/2/2
20	CLA	H	101	-	3/3/13/20	14/27/103/115	-
20	CLA	B	814	-	2/2/13/20	12/32/108/115	-
20	CLA	1	208	-	1/1/4/20	-	-
21	LMU	G	101	-	-	14/21/61/61	0/2/2/2
20	CLA	B	828	-	1/1/12/20	13/21/97/115	-
22	BCR	3	311	-	-	13/29/63/63	0/2/2/2
22	BCR	B	850	20	-	12/29/63/63	0/2/2/2
20	CLA	3	309	-	2/2/15/20	20/39/115/115	-
24	SF4	C	103	7	-	-	0/6/5/5
20	CLA	J	103	20	2/2/13/20	13/27/103/115	-
20	CLA	A	833	-	2/2/15/20	15/39/115/115	-
20	CLA	B	806	-	2/2/15/20	12/39/115/115	-
20	CLA	A	826	-	2/2/15/20	17/39/115/115	-
24	SF4	C	102	7	-	-	0/6/5/5
20	CLA	A	816	-	2/2/15/20	19/39/115/115	-
24	SF4	A	856	5,6	-	-	0/6/5/5
20	CLA	2	310	2	1/1/12/20	6/21/97/115	-
21	LMU	A	846	-	-	13/21/61/61	0/2/2/2
20	CLA	B	803	-	1/1/11/20	6/15/91/115	-
20	CLA	A	836	-	2/2/15/20	15/39/115/115	-
21	LMU	K	104	20	-	12/21/61/61	0/2/2/2
20	CLA	1	212	-	2/2/14/20	15/35/111/115	-
20	CLA	B	804	-	2/2/15/20	18/39/115/115	-
20	CLA	A	832	-	1/1/12/20	11/23/99/115	-
21	LMU	2	319	-	-	13/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	I	102	-	2/2/14/20	12/33/109/115	-
21	LMU	H	104	-	-	13/21/61/61	0/2/2/2
20	CLA	A	823	20	2/2/15/20	22/39/115/115	-
20	CLA	2	314	-	1/1/4/20	-	-
21	LMU	H	103	-	-	17/21/61/61	0/2/2/2
21	LMU	K	101	-	-	12/21/61/61	0/2/2/2
21	LMU	L	206	-	-	14/21/61/61	0/2/2/2
20	CLA	A	809	-	2/2/15/20	24/39/115/115	-

All (2618) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	209	CLA	CAB-C3B	-9.95	1.30	1.50
22	B	850	BCR	C20-C21	-9.80	1.12	1.43
22	L	209	BCR	C20-C21	-8.72	1.16	1.43
20	1	205	CLA	CAB-C3B	-8.54	1.33	1.50
22	F	203	BCR	C20-C21	-8.32	1.17	1.43
20	4	303	CLA	CAB-C3B	-8.22	1.33	1.50
22	3	311	BCR	C20-C21	-8.12	1.18	1.43
22	A	843	BCR	C20-C21	-8.04	1.18	1.43
22	B	841	BCR	C20-C21	-8.02	1.18	1.43
22	I	101	BCR	C20-C21	-8.01	1.18	1.43
22	F	202	BCR	C20-C21	-8.00	1.18	1.43
22	B	843	BCR	C20-C21	-7.99	1.18	1.43
23	A	839	PQN	C3-C2	7.98	1.49	1.35
22	A	840	BCR	C20-C21	-7.98	1.18	1.43
22	A	844	BCR	C20-C21	-7.97	1.18	1.43
20	B	820	CLA	C4C-C3C	-7.96	1.31	1.45
22	J	101	BCR	C20-C21	-7.96	1.18	1.43
22	A	842	BCR	C20-C21	-7.94	1.18	1.43
22	B	844	BCR	C20-C21	-7.94	1.18	1.43
22	G	102	BCR	C20-C21	-7.93	1.18	1.43
22	A	841	BCR	C20-C21	-7.92	1.18	1.43
20	A	807	CLA	CHD-C1D	7.90	1.53	1.38
20	B	808	CLA	CAB-C3B	-7.90	1.34	1.50
20	B	820	CLA	C1B-NB	-7.79	1.27	1.37
20	1	210	CLA	CAB-C3B	-7.76	1.34	1.50
20	B	839	CLA	CAB-C3B	-7.72	1.34	1.50
23	B	840	PQN	C3-C2	7.65	1.48	1.35
20	4	313	CLA	CAB-C3B	-7.65	1.35	1.50
22	I	103	BCR	C20-C21	-7.60	1.19	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	306	CLA	CHC-C1C	7.55	1.53	1.38
20	3	319	CLA	CAB-C3B	-7.54	1.35	1.50
22	B	842	BCR	C20-C21	-7.50	1.19	1.43
20	4	307	CLA	C4C-C3C	-7.49	1.32	1.45
22	I	103	BCR	C30-C25	-7.40	1.44	1.53
20	A	850	CLA	CAB-C3B	-7.37	1.35	1.50
20	A	838	CLA	CHD-C1D	7.31	1.52	1.38
20	B	810	CLA	CHC-C1C	7.28	1.53	1.38
20	2	304	CLA	CHC-C1C	7.26	1.53	1.38
20	A	808	CLA	CHC-C1C	7.25	1.53	1.38
20	L	204	CLA	C3D-C4D	-7.20	1.28	1.44
20	A	828	CLA	CHD-C1D	7.16	1.52	1.38
20	B	812	CLA	CHC-C1C	7.16	1.52	1.38
20	4	307	CLA	C1B-NB	-7.16	1.28	1.37
20	3	303	CLA	CAB-C3B	-7.12	1.36	1.50
20	B	820	CLA	C3D-C4D	-7.10	1.28	1.44
20	B	827	CLA	CHC-C1C	7.07	1.52	1.38
20	B	836	CLA	CHC-C1C	7.06	1.52	1.38
20	A	817	CLA	CHC-C1C	7.05	1.52	1.38
20	A	813	CLA	CHD-C1D	7.04	1.52	1.38
20	F	204	CLA	CAB-C3B	-7.02	1.36	1.50
20	H	101	CLA	CHD-C1D	7.02	1.52	1.38
20	B	833	CLA	CHC-C1C	7.02	1.52	1.38
20	4	312	CLA	CHC-C1C	6.99	1.52	1.38
20	L	204	CLA	CHC-C1C	6.99	1.52	1.38
20	A	827	CLA	CHC-C1C	6.99	1.52	1.38
20	L	203	CLA	CHC-C1C	6.98	1.52	1.38
20	A	829	CLA	CHD-C1D	6.96	1.52	1.38
20	I	102	CLA	CHC-C1C	6.96	1.52	1.38
20	B	827	CLA	CHD-C1D	6.95	1.52	1.38
20	3	313	CLA	CHC-C1C	6.92	1.52	1.38
20	1	210	CLA	CHC-C1C	6.88	1.52	1.38
20	B	831	CLA	CHC-C1C	6.88	1.52	1.38
20	B	832	CLA	CHC-C1C	6.86	1.52	1.38
20	1	207	CLA	CHC-C1C	6.86	1.52	1.38
20	B	849	CLA	CHD-C1D	6.86	1.51	1.38
20	4	314	CLA	CHC-C1C	6.86	1.52	1.38
20	2	308	CLA	CHC-C1C	6.86	1.52	1.38
20	1	209	CLA	C1B-NB	-6.85	1.28	1.37
20	3	309	CLA	C4C-C3C	-6.84	1.33	1.45
20	B	824	CLA	CHC-C1C	6.84	1.52	1.38
20	A	808	CLA	CHD-C4C	6.82	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	205	CLA	CHC-C1C	6.81	1.52	1.38
20	4	310	CLA	CHC-C1C	6.80	1.52	1.38
20	A	850	CLA	CHD-C1D	6.80	1.51	1.38
20	1	211	CLA	CAB-C3B	-6.78	1.29	1.47
20	B	849	CLA	CHC-C1C	6.78	1.52	1.38
20	2	304	CLA	CHD-C1D	6.77	1.51	1.38
20	4	303	CLA	CHC-C1C	6.75	1.52	1.38
20	1	203	CLA	CHC-C1C	6.75	1.52	1.38
20	A	849	CLA	CHD-C4C	6.75	1.54	1.39
20	B	824	CLA	CHD-C4C	6.74	1.54	1.39
20	H	109	CLA	CHC-C1C	6.74	1.52	1.38
20	F	206	CLA	CAB-C3B	-6.73	1.29	1.47
20	A	818	CLA	CHC-C1C	6.73	1.52	1.38
20	B	808	CLA	CHD-C1D	6.72	1.51	1.38
20	G	103	CLA	CHC-C1C	6.72	1.51	1.38
20	A	849	CLA	CHD-C1D	6.71	1.51	1.38
20	R	107	CLA	CHC-C1C	6.71	1.51	1.38
20	A	806	CLA	CHC-C1C	6.70	1.51	1.38
20	B	829	CLA	CHC-C1C	6.70	1.51	1.38
20	A	808	CLA	CHD-C1D	6.70	1.51	1.38
20	A	812	CLA	CHC-C1C	6.70	1.51	1.38
20	A	826	CLA	CHC-C1C	6.69	1.51	1.38
20	2	311	CLA	CHC-C1C	6.69	1.51	1.38
20	A	824	CLA	CHD-C4C	6.68	1.54	1.39
20	2	310	CLA	CHD-C1D	6.68	1.51	1.38
20	B	815	CLA	CHC-C1C	6.67	1.51	1.38
20	A	813	CLA	CHC-C1C	6.67	1.51	1.38
20	B	837	CLA	CHC-C1C	6.66	1.51	1.38
20	B	817	CLA	CHC-C1C	6.64	1.51	1.38
20	H	101	CLA	CHD-C4C	6.64	1.54	1.39
20	1	205	CLA	CHD-C1D	6.63	1.51	1.38
20	B	806	CLA	CHD-C1D	6.63	1.51	1.38
20	B	824	CLA	CHD-C1D	6.63	1.51	1.38
20	A	827	CLA	CHD-C1D	6.62	1.51	1.38
20	B	803	CLA	CHC-C1C	6.61	1.51	1.38
20	A	819	CLA	CHD-C1D	6.61	1.51	1.38
20	B	803	CLA	CHD-C1D	6.61	1.51	1.38
20	A	850	CLA	O2D-CGD	6.60	1.49	1.33
20	A	805	CLA	CHD-C1D	6.60	1.51	1.38
20	4	313	CLA	CHC-C1C	6.60	1.51	1.38
20	H	110	CLA	CHD-C1D	6.60	1.51	1.38
20	A	802	CLA	CHC-C1C	6.60	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	K	107	CLA	CHC-C1C	6.59	1.51	1.38
20	2	309	CLA	CHC-C1C	6.58	1.51	1.38
20	B	814	CLA	CHC-C1C	6.58	1.51	1.38
20	G	103	CLA	CHD-C1D	6.57	1.51	1.38
20	B	811	CLA	CHC-C1C	6.56	1.51	1.38
20	4	305	CLA	CHD-C1D	6.56	1.51	1.38
20	B	820	CLA	CAB-C3B	-6.55	1.29	1.47
20	3	307	CLA	CHC-C1C	6.54	1.51	1.38
20	3	317	CLA	CHC-C1C	6.53	1.51	1.38
20	3	320	CLA	CHC-C1C	6.53	1.51	1.38
20	H	108	CLA	CHC-C1C	6.52	1.51	1.38
20	A	847	CLA	CHC-C1C	6.52	1.51	1.38
20	B	847	CLA	CHC-C1C	6.52	1.51	1.38
20	H	108	CLA	CHD-C1D	6.52	1.51	1.38
20	A	813	CLA	CHD-C4C	6.51	1.54	1.39
20	A	811	CLA	CHC-C1C	6.51	1.51	1.38
20	2	302	CLA	CHC-C1C	6.51	1.51	1.38
20	2	310	CLA	CHC-C1C	6.50	1.51	1.38
20	1	211	CLA	C3D-C4D	-6.50	1.29	1.44
20	3	312	CLA	CHC-C1C	6.50	1.51	1.38
20	B	819	CLA	CHD-C1D	6.49	1.51	1.38
20	1	214	CLA	C3D-C4D	-6.48	1.29	1.44
20	B	820	CLA	C1D-ND	-6.48	1.29	1.37
20	3	309	CLA	C3D-C4D	-6.47	1.29	1.44
20	3	314	CLA	CHD-C1D	6.47	1.51	1.38
20	H	107	CLA	CHD-C1D	6.47	1.51	1.38
20	1	203	CLA	CHD-C1D	6.47	1.51	1.38
20	A	816	CLA	CHD-C1D	6.47	1.51	1.38
20	I	102	CLA	CHD-C1D	6.46	1.51	1.38
20	A	838	CLA	CHD-C4C	6.46	1.53	1.39
20	A	825	CLA	CHC-C1C	6.46	1.51	1.38
20	B	827	CLA	CHD-C4C	6.45	1.53	1.39
20	B	808	CLA	CHC-C1C	6.45	1.51	1.38
20	A	821	CLA	CHC-C1C	6.45	1.51	1.38
20	H	110	CLA	CHC-C1C	6.45	1.51	1.38
20	3	319	CLA	CHD-C1D	6.44	1.51	1.38
20	B	835	CLA	CHD-C1D	6.44	1.51	1.38
20	A	809	CLA	CHD-C1D	6.44	1.51	1.38
20	A	812	CLA	CHD-C1D	6.43	1.51	1.38
20	A	818	CLA	CHD-C1D	6.42	1.51	1.38
20	4	306	CLA	CHD-C1D	6.42	1.51	1.38
20	2	307	CLA	CHD-C1D	6.42	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	308	CLA	CHC-C1C	6.42	1.51	1.38
20	3	303	CLA	CHD-C1D	6.41	1.51	1.38
20	B	804	CLA	CHD-C4C	6.41	1.53	1.39
20	K	106	CLA	C3D-C4D	-6.41	1.29	1.44
20	A	850	CLA	CHC-C1C	6.41	1.51	1.38
20	B	819	CLA	CHD-C4C	6.40	1.53	1.39
20	F	204	CLA	CHC-C1C	6.40	1.51	1.38
20	R	106	CLA	CHC-C1C	6.40	1.51	1.38
20	1	207	CLA	CHD-C1D	6.40	1.50	1.38
20	H	110	CLA	O2D-CGD	6.38	1.48	1.33
20	R	106	CLA	CHD-C1D	6.38	1.50	1.38
20	B	806	CLA	CHC-C1C	6.38	1.51	1.38
20	1	213	CLA	CHC-C1C	6.37	1.51	1.38
20	A	850	CLA	CHD-C4C	6.37	1.53	1.39
20	R	107	CLA	CHD-C1D	6.37	1.50	1.38
20	L	207	CLA	CHC-C1C	6.37	1.51	1.38
20	B	806	CLA	CHD-C4C	6.37	1.53	1.39
20	H	108	CLA	CHD-C4C	6.36	1.53	1.39
20	A	815	CLA	CHC-C1C	6.36	1.51	1.38
20	2	307	CLA	CHD-C4C	6.36	1.53	1.39
20	1	210	CLA	CHD-C1D	6.36	1.50	1.38
20	1	202	CLA	O2D-CGD	6.36	1.48	1.33
20	B	818	CLA	O2D-CGD	6.36	1.48	1.33
20	2	310	CLA	CHD-C4C	6.35	1.53	1.39
20	B	816	CLA	CHC-C1C	6.35	1.51	1.38
20	4	318	CLA	CHD-C1D	6.35	1.50	1.38
20	4	307	CLA	C3D-C4D	-6.35	1.29	1.44
20	A	820	CLA	CHC-C1C	6.35	1.51	1.38
20	1	204	CLA	CHD-C1D	6.35	1.50	1.38
20	L	201	CLA	CHD-C4C	6.35	1.53	1.39
20	A	824	CLA	CHC-C1C	6.34	1.51	1.38
20	2	315	CLA	CHC-C1C	6.34	1.51	1.38
20	1	211	CLA	C4C-C3C	-6.33	1.34	1.45
22	B	850	BCR	C21-C22	-6.33	1.21	1.35
20	B	804	CLA	CHD-C1D	6.33	1.50	1.38
20	B	826	CLA	CHC-C1C	6.32	1.51	1.38
20	3	309	CLA	O2D-CGD	6.32	1.48	1.33
20	2	306	CLA	O2D-CGD	6.31	1.48	1.33
20	4	309	CLA	CHC-C1C	6.31	1.50	1.38
20	A	807	CLA	CHD-C4C	6.31	1.53	1.39
20	L	201	CLA	CHC-C1C	6.31	1.51	1.38
20	4	306	CLA	O2D-CGD	6.31	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	833	CLA	CHD-C1D	6.30	1.50	1.38
20	1	202	CLA	CHD-C1D	6.30	1.50	1.38
20	B	807	CLA	CHC-C1C	6.30	1.51	1.38
20	2	302	CLA	CHD-C1D	6.30	1.50	1.38
20	B	837	CLA	CHD-C4C	6.30	1.53	1.39
20	A	816	CLA	CHC-C1C	6.29	1.51	1.38
20	B	834	CLA	CHD-C1D	6.29	1.50	1.38
20	1	201	CLA	C3D-C4D	-6.29	1.30	1.44
20	B	835	CLA	CHD-C4C	6.28	1.53	1.39
20	2	307	CLA	CHC-C1C	6.28	1.51	1.38
20	3	303	CLA	CHC-C1C	6.28	1.51	1.38
20	F	204	CLA	CHD-C4C	6.27	1.53	1.39
20	B	848	CLA	CHC-C1C	6.26	1.51	1.38
20	B	837	CLA	CHD-C1D	6.26	1.50	1.38
20	B	814	CLA	CHD-C4C	6.26	1.53	1.39
20	3	320	CLA	CHD-C4C	6.25	1.53	1.39
20	L	208	CLA	CHC-C1C	6.25	1.51	1.38
20	A	830	CLA	CHC-C1C	6.25	1.51	1.38
20	3	305	CLA	CHC-C1C	6.25	1.50	1.38
20	A	818	CLA	CHD-C4C	6.25	1.53	1.39
20	A	809	CLA	CHC-C1C	6.25	1.51	1.38
20	A	806	CLA	CHD-C1D	6.25	1.50	1.38
20	B	834	CLA	CHD-C4C	6.25	1.53	1.39
20	B	809	CLA	CHC-C1C	6.25	1.51	1.38
20	B	808	CLA	CHD-C4C	6.25	1.53	1.39
20	4	302	CLA	CHC-C1C	6.24	1.51	1.38
20	K	103	CLA	CHC-C1C	6.24	1.51	1.38
20	1	206	CLA	O2D-CGD	6.24	1.48	1.33
20	4	318	CLA	O2D-CGD	6.23	1.48	1.33
20	2	302	CLA	CHD-C4C	6.23	1.53	1.39
20	A	815	CLA	CHD-C1D	6.22	1.50	1.38
20	3	319	CLA	CHC-C1C	6.22	1.50	1.38
20	A	820	CLA	CHD-C1D	6.22	1.50	1.38
20	4	304	CLA	CAB-C3B	-6.21	1.30	1.47
20	2	301	CLA	CHC-C1C	6.21	1.50	1.38
20	3	314	CLA	CHC-C1C	6.21	1.50	1.38
20	A	803	CLA	CHD-C4C	6.21	1.53	1.39
20	G	103	CLA	O2D-CGD	6.21	1.48	1.33
20	A	819	CLA	O2D-CGD	6.20	1.48	1.33
20	A	812	CLA	CHD-C4C	6.20	1.53	1.39
20	A	829	CLA	CHD-C4C	6.20	1.53	1.39
20	L	201	CLA	CHD-C1D	6.20	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	H	101	CLA	O2D-CGD	6.19	1.48	1.33
20	A	819	CLA	CHD-C4C	6.19	1.53	1.39
20	4	319	CLA	CHC-C1C	6.19	1.50	1.38
20	B	811	CLA	CHD-C4C	6.18	1.53	1.39
20	A	832	CLA	CHC-C1C	6.18	1.50	1.38
20	L	207	CLA	CHD-C4C	6.18	1.53	1.39
20	B	839	CLA	CHC-C1C	6.18	1.50	1.38
20	H	109	CLA	O2D-CGD	6.18	1.48	1.33
20	B	822	CLA	CHC-C1C	6.18	1.50	1.38
20	2	303	CLA	CHC-C1C	6.18	1.50	1.38
20	H	107	CLA	CHC-C1C	6.17	1.50	1.38
20	B	811	CLA	CHD-C1D	6.17	1.50	1.38
20	A	804	CLA	CHC-C1C	6.17	1.50	1.38
20	A	831	CLA	CHC-C1C	6.16	1.50	1.38
20	A	855	CLA	CHC-C1C	6.16	1.50	1.38
20	B	819	CLA	O2D-CGD	6.16	1.48	1.33
20	A	810	CLA	CHC-C1C	6.16	1.50	1.38
20	B	823	CLA	CHC-C1C	6.16	1.50	1.38
20	A	835	CLA	CHC-C1C	6.16	1.50	1.38
20	A	834	CLA	CHC-C1C	6.15	1.50	1.38
20	J	102	CLA	CHC-C1C	6.15	1.50	1.38
20	K	105	CLA	CHC-C1C	6.15	1.50	1.38
20	A	823	CLA	CHC-C1C	6.15	1.50	1.38
20	2	311	CLA	CHD-C1D	6.14	1.50	1.38
20	A	836	CLA	CHC-C1C	6.14	1.50	1.38
20	A	824	CLA	CHD-C1D	6.14	1.50	1.38
20	A	810	CLA	CHD-C4C	6.14	1.53	1.39
20	B	826	CLA	CHD-C1D	6.14	1.50	1.38
20	2	317	CLA	CHC-C1C	6.14	1.50	1.38
20	3	303	CLA	CHD-C4C	6.14	1.53	1.39
20	A	813	CLA	O2D-CGD	6.14	1.48	1.33
20	F	205	CLA	CHC-C1C	6.14	1.50	1.38
20	4	315	CLA	CHC-C1C	6.13	1.50	1.38
20	1	214	CLA	C1B-NB	-6.13	1.29	1.37
20	A	837	CLA	CHC-C1C	6.13	1.50	1.38
20	B	818	CLA	CHC-C1C	6.13	1.50	1.38
20	1	206	CLA	CHC-C1C	6.13	1.50	1.38
20	A	817	CLA	CHD-C1D	6.13	1.50	1.38
20	A	833	CLA	CHC-C1C	6.13	1.50	1.38
20	A	848	CLA	CHC-C1C	6.13	1.50	1.38
20	A	821	CLA	CHD-C1D	6.13	1.50	1.38
20	B	819	CLA	CHC-C1C	6.13	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	822	CLA	CHC-C1C	6.12	1.50	1.38
20	A	804	CLA	CHD-C4C	6.12	1.53	1.39
20	1	208	CLA	CHC-C1C	6.12	1.50	1.38
20	B	830	CLA	O2D-CGD	6.12	1.48	1.33
20	3	310	CLA	CHC-C1C	6.11	1.50	1.38
20	H	108	CLA	O2D-CGD	6.11	1.48	1.33
20	B	848	CLA	CHD-C1D	6.10	1.50	1.38
20	3	316	CLA	CHC-C1C	6.10	1.50	1.38
20	1	204	CLA	OBD-CAD	6.10	1.33	1.22
20	B	848	CLA	CHD-C4C	6.09	1.53	1.39
20	4	310	CLA	O2D-CGD	6.09	1.48	1.33
20	A	804	CLA	CHD-C1D	6.09	1.50	1.38
20	B	832	CLA	CHD-C1D	6.09	1.50	1.38
20	B	803	CLA	CHD-C4C	6.09	1.53	1.39
20	3	306	CLA	CHC-C1C	6.07	1.50	1.38
20	B	827	CLA	O2D-CGD	6.07	1.48	1.33
20	H	101	CLA	CHC-C1C	6.07	1.50	1.38
20	1	215	CLA	CHC-C1C	6.07	1.50	1.38
20	B	839	CLA	CHD-C1D	6.07	1.50	1.38
20	B	828	CLA	O2D-CGD	6.07	1.48	1.33
20	B	813	CLA	CHC-C1C	6.07	1.50	1.38
20	A	805	CLA	CHC-C1C	6.06	1.50	1.38
20	H	110	CLA	CHD-C4C	6.06	1.53	1.39
20	4	304	CLA	CHD-C4C	6.06	1.53	1.39
20	B	812	CLA	CHD-C1D	6.06	1.50	1.38
20	F	205	CLA	CHD-C1D	6.06	1.50	1.38
20	F	206	CLA	C3D-C4D	-6.06	1.30	1.44
20	L	204	CLA	CHD-C1D	6.05	1.50	1.38
20	2	310	CLA	CAB-C3B	-6.05	1.31	1.47
20	R	107	CLA	O2D-CGD	6.04	1.48	1.33
20	G	103	CLA	CHD-C4C	6.04	1.53	1.39
20	2	312	CLA	CHC-C1C	6.04	1.50	1.38
20	R	106	CLA	CHD-C4C	6.04	1.53	1.39
20	L	203	CLA	O2D-CGD	6.04	1.48	1.33
20	F	204	CLA	CHD-C1D	6.04	1.50	1.38
20	A	828	CLA	CHC-C1C	6.04	1.50	1.38
20	3	314	CLA	O2D-CGD	6.04	1.48	1.33
20	A	847	CLA	O2D-CGD	6.04	1.48	1.33
20	A	815	CLA	O2D-CGD	6.03	1.48	1.33
20	A	806	CLA	CHD-C4C	6.03	1.52	1.39
20	2	311	CLA	O2D-CGD	6.03	1.48	1.33
20	A	830	CLA	CHD-C1D	6.02	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	834	CLA	CHC-C1C	6.02	1.50	1.38
20	B	814	CLA	O2D-CGD	6.01	1.48	1.33
20	3	315	CLA	CHC-C1C	6.01	1.50	1.38
20	L	202	CLA	CHC-C1C	6.01	1.50	1.38
20	4	302	CLA	CHD-C1D	6.01	1.50	1.38
20	1	203	CLA	CHC-C4B	6.01	1.52	1.39
20	A	802	CLA	CHD-C4C	6.00	1.52	1.39
20	R	106	CLA	O2D-CGD	6.00	1.48	1.33
20	K	103	CLA	CHD-C1D	6.00	1.50	1.38
20	A	847	CLA	CHC-C4B	5.99	1.52	1.39
20	A	833	CLA	CHD-C1D	5.99	1.50	1.38
20	2	306	CLA	CHC-C1C	5.99	1.50	1.38
20	A	831	CLA	CHD-C1D	5.99	1.50	1.38
20	B	825	CLA	CHC-C1C	5.99	1.50	1.38
20	4	312	CLA	CHD-C1D	5.99	1.52	1.38
20	4	311	CLA	CHC-C1C	5.98	1.50	1.38
20	A	855	CLA	CHD-C1D	5.98	1.50	1.38
20	A	835	CLA	CHD-C1D	5.98	1.50	1.38
20	4	305	CLA	CHC-C1C	5.98	1.50	1.38
20	1	210	CLA	CHD-C4C	5.98	1.52	1.39
20	A	809	CLA	CHD-C4C	5.98	1.52	1.39
20	A	805	CLA	CHD-C4C	5.98	1.52	1.39
20	A	826	CLA	CHD-C4C	5.98	1.52	1.39
20	3	320	CLA	CHD-C1D	5.98	1.50	1.38
20	A	830	CLA	CHD-C4C	5.98	1.52	1.39
20	A	837	CLA	CHD-C1D	5.98	1.50	1.38
20	A	832	CLA	CHD-C1D	5.97	1.50	1.38
20	B	806	CLA	CAB-C3B	-5.97	1.31	1.47
20	A	834	CLA	CHD-C1D	5.97	1.50	1.38
20	A	836	CLA	CHD-C1D	5.96	1.50	1.38
20	3	320	CLA	O2D-CGD	5.96	1.47	1.33
20	B	805	CLA	CAB-C3B	-5.96	1.31	1.47
20	B	838	CLA	CHD-C1D	5.96	1.50	1.38
20	B	829	CLA	CHD-C1D	5.96	1.50	1.38
20	B	830	CLA	CHD-C1D	5.96	1.50	1.38
20	A	827	CLA	CHD-C4C	5.96	1.52	1.39
20	2	301	CLA	CHD-C1D	5.96	1.50	1.38
20	J	102	CLA	CHD-C1D	5.96	1.50	1.38
20	B	822	CLA	CHD-C1D	5.96	1.50	1.38
20	A	821	CLA	CHD-C4C	5.96	1.52	1.39
20	A	810	CLA	CHD-C1D	5.95	1.50	1.38
20	1	204	CLA	O2D-CGD	5.95	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	810	CLA	CHC-C4B	5.95	1.52	1.39
20	A	803	CLA	O2D-CGD	5.95	1.47	1.33
20	L	204	CLA	C4B-NB	-5.94	1.30	1.37
20	H	107	CLA	CHD-C4C	5.94	1.52	1.39
20	B	824	CLA	C3D-C4D	-5.94	1.30	1.44
20	B	833	CLA	O2D-CGD	5.94	1.47	1.33
20	B	807	CLA	CHD-C4C	5.94	1.52	1.39
20	A	808	CLA	O2D-CGD	5.94	1.47	1.33
20	4	317	CLA	CHC-C1C	5.93	1.50	1.38
20	A	801	CLA	CHC-C1C	5.93	1.50	1.38
20	B	808	CLA	O2A-CGA	5.93	1.50	1.33
20	4	306	CLA	CHD-C4C	5.93	1.52	1.39
20	K	105	CLA	CHD-C1D	5.92	1.50	1.38
20	2	304	CLA	CHD-C4C	5.92	1.52	1.39
20	A	822	CLA	CHD-C1D	5.92	1.50	1.38
20	1	205	CLA	CHD-C4C	5.92	1.52	1.39
20	B	823	CLA	CHD-C1D	5.92	1.50	1.38
20	4	319	CLA	CHD-C1D	5.92	1.50	1.38
20	B	813	CLA	CHD-C4C	5.91	1.52	1.39
20	A	812	CLA	O2D-CGD	5.91	1.47	1.33
20	B	847	CLA	CHD-C1D	5.91	1.50	1.38
20	B	833	CLA	CHD-C4C	5.91	1.52	1.39
20	B	847	CLA	CHD-C4C	5.91	1.52	1.39
20	B	817	CLA	CHD-C1D	5.91	1.50	1.38
20	B	829	CLA	CHC-C4B	5.91	1.52	1.39
20	2	317	CLA	CHD-C1D	5.91	1.50	1.38
20	A	857	CLA	CHC-C1C	5.90	1.50	1.38
20	3	310	CLA	CHD-C1D	5.90	1.50	1.38
20	L	203	CLA	OBD-CAD	5.90	1.32	1.22
20	4	307	CLA	CHC-C1C	5.89	1.50	1.38
20	1	204	CLA	CHC-C1C	5.89	1.50	1.38
20	H	109	CLA	CHD-C1D	5.89	1.49	1.38
20	A	838	CLA	CHC-C1C	5.89	1.50	1.38
20	A	801	CLA	CHD-C4C	5.89	1.52	1.39
20	A	819	CLA	CHC-C1C	5.89	1.50	1.38
20	A	828	CLA	CHD-C4C	5.89	1.52	1.39
20	3	301	CLA	CHC-C1C	5.89	1.50	1.38
20	A	830	CLA	O2D-CGD	5.88	1.47	1.33
20	A	803	CLA	O2A-CGA	5.88	1.50	1.33
20	B	813	CLA	CHD-C1D	5.88	1.49	1.38
20	4	318	CLA	CHC-C1C	5.88	1.50	1.38
20	B	821	CLA	CHD-C4C	5.88	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	817	CLA	CHD-C4C	5.88	1.52	1.39
20	L	207	CLA	CHD-C1D	5.87	1.49	1.38
20	K	107	CLA	CHD-C1D	5.87	1.49	1.38
20	3	315	CLA	C3D-C4D	-5.87	1.31	1.44
20	K	107	CLA	CHC-C4B	5.87	1.52	1.39
20	A	811	CLA	CHD-C1D	5.86	1.49	1.38
22	F	203	BCR	C30-C25	-5.86	1.46	1.53
20	A	802	CLA	CHD-C1D	5.86	1.49	1.38
20	A	823	CLA	CHD-C1D	5.86	1.49	1.38
20	L	208	CLA	CHD-C4C	5.86	1.52	1.39
20	L	208	CLA	O2D-CGD	5.85	1.47	1.33
20	A	817	CLA	O2D-CGD	5.85	1.47	1.33
20	2	312	CLA	CHD-C1D	5.85	1.49	1.38
20	B	832	CLA	CHD-C4C	5.85	1.52	1.39
20	A	820	CLA	O2D-CGD	5.84	1.47	1.33
20	2	321	CLA	CHC-C1C	5.84	1.50	1.38
20	B	811	CLA	O2D-CGD	5.84	1.47	1.33
20	1	202	CLA	O2A-CGA	5.84	1.50	1.33
20	B	821	CLA	O2D-CGD	5.84	1.47	1.33
20	A	829	CLA	O2D-CGD	5.82	1.47	1.33
20	3	301	CLA	C3D-C4D	-5.82	1.31	1.44
20	2	307	CLA	O2D-CGD	5.82	1.47	1.33
20	A	820	CLA	CHD-C4C	5.82	1.52	1.39
20	4	305	CLA	CHD-C4C	5.81	1.52	1.39
20	B	817	CLA	CHD-C4C	5.81	1.52	1.39
20	H	107	CLA	O2D-CGD	5.81	1.47	1.33
20	1	209	CLA	C3A-C2A	-5.81	1.49	1.54
20	A	804	CLA	O2D-CGD	5.80	1.47	1.33
20	B	813	CLA	O2D-CGD	5.80	1.47	1.33
20	B	810	CLA	CAB-C3B	-5.80	1.31	1.47
20	B	805	CLA	CHD-C1D	5.80	1.49	1.38
20	B	831	CLA	O2D-CGD	5.80	1.47	1.33
20	B	806	CLA	O2D-CGD	5.79	1.47	1.33
20	L	201	CLA	O2D-CGD	5.79	1.47	1.33
20	B	807	CLA	CHD-C1D	5.79	1.49	1.38
20	1	212	CLA	C3D-C4D	-5.78	1.31	1.44
20	A	814	CLA	CHC-C1C	5.78	1.50	1.38
20	A	829	CLA	CHC-C1C	5.77	1.50	1.38
20	A	811	CLA	CHD-C4C	5.77	1.52	1.39
20	2	317	CLA	CHD-C4C	5.77	1.52	1.39
20	1	203	CLA	CHD-C4C	5.77	1.52	1.39
20	1	210	CLA	CHC-C4B	5.77	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	202	CLA	CHD-C4C	5.77	1.52	1.39
20	A	816	CLA	CHD-C4C	5.76	1.52	1.39
20	2	311	CLA	O2A-CGA	5.76	1.50	1.33
20	A	825	CLA	CHD-C1D	5.75	1.49	1.38
20	H	107	CLA	C3D-C4D	-5.75	1.31	1.44
20	A	815	CLA	CHD-C4C	5.75	1.52	1.39
20	B	849	CLA	CHD-C4C	5.75	1.52	1.39
20	A	803	CLA	CHC-C1C	5.75	1.50	1.38
20	B	818	CLA	CHD-C4C	5.75	1.52	1.39
20	B	835	CLA	CHC-C1C	5.74	1.50	1.38
20	A	820	CLA	O2A-CGA	5.74	1.50	1.33
22	I	101	BCR	C21-C22	-5.74	1.22	1.35
20	A	849	CLA	CAB-C3B	-5.73	1.32	1.47
20	B	805	CLA	CHD-C4C	5.73	1.52	1.39
20	4	310	CLA	CHD-C4C	5.72	1.52	1.39
20	1	202	CLA	CHC-C1C	5.72	1.49	1.38
20	2	302	CLA	CHC-C4B	5.72	1.52	1.39
20	2	312	CLA	O2D-CGD	5.71	1.47	1.33
20	3	314	CLA	CHD-C4C	5.71	1.52	1.39
20	B	821	CLA	CHD-C1D	5.70	1.49	1.38
20	B	832	CLA	O2D-CGD	5.70	1.47	1.33
20	B	814	CLA	CHD-C1D	5.70	1.49	1.38
20	B	811	CLA	O2A-CGA	5.70	1.49	1.33
20	B	804	CLA	CHC-C1C	5.70	1.49	1.38
20	R	107	CLA	CHC-C4B	5.69	1.52	1.39
20	A	825	CLA	CHD-C4C	5.68	1.52	1.39
20	3	319	CLA	CHD-C4C	5.68	1.52	1.39
20	K	107	CLA	CHD-C4C	5.68	1.52	1.39
20	1	204	CLA	CHD-C4C	5.68	1.52	1.39
20	B	827	CLA	C3D-C4D	-5.67	1.31	1.44
20	L	203	CLA	CHD-C1D	5.67	1.49	1.38
20	A	806	CLA	CAB-C3B	-5.67	1.32	1.47
20	A	826	CLA	O2D-CGD	5.67	1.47	1.33
20	A	848	CLA	CHD-C4C	5.67	1.52	1.39
20	4	319	CLA	CHD-C4C	5.66	1.52	1.39
20	A	802	CLA	O2A-CGA	5.66	1.49	1.33
20	B	815	CLA	CHD-C1D	5.66	1.49	1.38
20	4	318	CLA	CHD-C4C	5.66	1.52	1.39
20	1	201	CLA	O2D-CGD	5.66	1.47	1.33
20	B	828	CLA	CHD-C4C	5.65	1.52	1.39
20	4	303	CLA	OBD-CAD	5.65	1.32	1.22
20	B	810	CLA	CHD-C4C	5.65	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	205	CLA	CHC-C4B	5.65	1.52	1.39
20	4	315	CLA	CAB-C3B	-5.64	1.32	1.47
20	B	812	CLA	CHC-C4B	5.64	1.52	1.39
20	1	209	CLA	C3D-C4D	-5.64	1.31	1.44
20	B	849	CLA	CAB-C3B	-5.64	1.32	1.47
20	A	801	CLA	CHD-C1D	5.64	1.49	1.38
20	A	803	CLA	CHD-C1D	5.63	1.49	1.38
20	A	814	CLA	C3D-C4D	-5.63	1.31	1.44
20	B	821	CLA	CHC-C1C	5.63	1.49	1.38
20	B	805	CLA	CHC-C1C	5.63	1.49	1.38
20	B	823	CLA	CHD-C4C	5.63	1.52	1.39
20	3	308	CLA	CHD-C1D	5.63	1.52	1.38
20	G	103	CLA	CHC-C4B	5.62	1.52	1.39
20	L	207	CLA	O2D-CGD	5.62	1.47	1.33
20	2	301	CLA	CHD-C4C	5.62	1.52	1.39
20	2	302	CLA	O2D-CGD	5.61	1.47	1.33
20	2	321	CLA	O2D-CGD	5.61	1.47	1.33
20	J	103	CLA	C3D-C4D	-5.61	1.31	1.44
20	A	849	CLA	CHC-C1C	5.61	1.49	1.38
20	1	213	CLA	CHD-C1D	5.60	1.52	1.38
20	B	830	CLA	CHD-C4C	5.60	1.51	1.39
20	R	106	CLA	O2A-CGA	5.60	1.49	1.33
20	1	202	CLA	CHD-C4C	5.60	1.51	1.39
20	B	810	CLA	CHD-C1D	5.59	1.49	1.38
20	B	831	CLA	CHD-C4C	5.59	1.51	1.39
20	A	832	CLA	CHD-C4C	5.59	1.51	1.39
20	K	103	CLA	CHD-C4C	5.59	1.51	1.39
20	3	310	CLA	CHD-C4C	5.59	1.51	1.39
20	4	310	CLA	CHD-C1D	5.59	1.49	1.38
20	A	837	CLA	CHD-C4C	5.59	1.51	1.39
20	A	855	CLA	CHD-C4C	5.58	1.51	1.39
20	K	106	CLA	CHD-C1D	5.58	1.49	1.38
20	3	315	CLA	CHD-C1D	5.58	1.49	1.38
20	1	212	CLA	CHC-C1C	5.58	1.49	1.38
20	4	303	CLA	C3D-C4D	-5.58	1.31	1.44
20	4	302	CLA	CHD-C4C	5.58	1.51	1.39
20	B	828	CLA	CHC-C1C	5.58	1.49	1.38
20	4	308	CLA	CHD-C1D	5.57	1.51	1.38
20	I	102	CLA	O2A-CGA	5.57	1.49	1.33
20	A	835	CLA	CHD-C4C	5.57	1.51	1.39
20	A	833	CLA	CHD-C4C	5.56	1.51	1.39
20	I	102	CLA	CHD-C4C	5.56	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	836	CLA	CHD-C4C	5.56	1.51	1.39
20	A	818	CLA	O2D-CGD	5.56	1.46	1.33
20	1	201	CLA	C1B-NB	-5.56	1.30	1.37
20	A	823	CLA	CHD-C4C	5.56	1.51	1.39
20	F	205	CLA	CHD-C4C	5.56	1.51	1.39
20	F	206	CLA	CHC-C1C	5.56	1.49	1.38
20	4	306	CLA	CHC-C4B	5.56	1.51	1.39
20	B	831	CLA	CAB-C3B	-5.56	1.32	1.47
20	A	822	CLA	CHD-C4C	5.56	1.51	1.39
20	I	102	CLA	CHC-C4B	5.56	1.51	1.39
20	A	847	CLA	CHD-C4C	5.55	1.51	1.39
20	A	805	CLA	O2D-CGD	5.55	1.46	1.33
20	2	306	CLA	OBD-CAD	5.55	1.32	1.22
20	B	809	CLA	CHD-C1D	5.55	1.49	1.38
20	J	103	CLA	CAB-C3B	-5.55	1.32	1.47
20	A	831	CLA	CHD-C4C	5.55	1.51	1.39
20	K	105	CLA	CHD-C4C	5.54	1.51	1.39
20	K	106	CLA	C1B-NB	-5.54	1.30	1.37
20	B	825	CLA	CHD-C1D	5.54	1.49	1.38
20	B	824	CLA	CHC-C4B	5.54	1.51	1.39
20	B	833	CLA	CHC-C4B	5.54	1.51	1.39
20	A	834	CLA	CHD-C4C	5.54	1.51	1.39
20	B	822	CLA	CHD-C4C	5.54	1.51	1.39
20	B	812	CLA	CHD-C4C	5.53	1.51	1.39
20	A	818	CLA	CHC-C4B	5.53	1.51	1.39
20	1	207	CLA	CHD-C4C	5.52	1.51	1.39
20	4	304	CLA	C3D-C4D	-5.52	1.31	1.44
20	B	804	CLA	O2D-CGD	5.52	1.46	1.33
20	4	313	CLA	CHD-C1D	5.52	1.49	1.38
20	A	810	CLA	O2D-CGD	5.52	1.46	1.33
20	B	818	CLA	O2A-CGA	5.51	1.50	1.33
20	B	812	CLA	O2D-CGD	5.51	1.46	1.33
20	2	312	CLA	CHD-C4C	5.51	1.51	1.39
20	F	206	CLA	CHD-C1D	5.51	1.49	1.38
20	L	203	CLA	CHD-C4C	5.51	1.51	1.39
20	2	317	CLA	O2D-CGD	5.51	1.46	1.33
20	L	202	CLA	CHD-C1D	5.51	1.49	1.38
20	A	814	CLA	CHD-C1D	5.50	1.49	1.38
20	J	102	CLA	CHD-C4C	5.50	1.51	1.39
20	L	208	CLA	CHD-C1D	5.50	1.49	1.38
20	B	824	CLA	O2D-CGD	5.49	1.46	1.33
20	H	109	CLA	CHC-C4B	5.49	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	R	107	CLA	CHD-C4C	5.49	1.51	1.39
22	B	850	BCR	C20-C19	-5.49	1.20	1.34
20	A	812	CLA	CHC-C4B	5.49	1.51	1.39
20	2	304	CLA	O2D-CGD	5.48	1.46	1.33
20	A	825	CLA	O2D-CGD	5.48	1.46	1.33
20	A	838	CLA	O2D-CGD	5.48	1.46	1.33
20	2	314	CLA	CHC-C1C	5.48	1.49	1.38
20	3	315	CLA	CHD-C4C	5.48	1.51	1.39
20	2	302	CLA	O2A-CGA	5.47	1.49	1.33
20	H	101	CLA	O2A-CGA	5.46	1.49	1.33
20	J	103	CLA	CHC-C1C	5.46	1.49	1.38
20	B	815	CLA	O2D-CGD	5.46	1.46	1.33
20	3	301	CLA	CHD-C1D	5.45	1.49	1.38
20	A	810	CLA	O2A-CGA	5.45	1.49	1.33
20	A	848	CLA	CHD-C1D	5.45	1.49	1.38
20	B	808	CLA	CHC-C4B	5.45	1.51	1.39
20	H	109	CLA	CHD-C4C	5.44	1.51	1.39
20	B	829	CLA	CHD-C4C	5.44	1.51	1.39
20	A	826	CLA	CHD-C1D	5.44	1.49	1.38
20	A	827	CLA	O2A-CGA	5.43	1.49	1.33
20	L	204	CLA	CHC-C4B	5.42	1.51	1.39
20	A	817	CLA	CHC-C4B	5.42	1.51	1.39
20	A	810	CLA	CHC-C4B	5.42	1.51	1.39
20	B	839	CLA	CHD-C4C	5.42	1.51	1.39
20	B	836	CLA	CHC-C4B	5.42	1.51	1.39
20	B	831	CLA	OBD-CAD	5.42	1.31	1.22
20	4	303	CLA	CHD-C4C	5.42	1.51	1.39
20	B	829	CLA	O2A-CGA	5.41	1.49	1.33
20	B	837	CLA	CHC-C4B	5.41	1.51	1.39
20	2	306	CLA	CHD-C4C	5.41	1.51	1.39
20	B	809	CLA	CHD-C4C	5.41	1.51	1.39
22	F	203	BCR	C21-C22	-5.40	1.23	1.35
20	B	817	CLA	CHC-C4B	5.40	1.51	1.39
20	A	848	CLA	O2D-CGD	5.40	1.46	1.33
20	2	321	CLA	C3D-C4D	-5.39	1.32	1.44
20	B	813	CLA	CHC-C4B	5.38	1.51	1.39
20	A	825	CLA	O2A-CGA	5.38	1.49	1.33
20	B	848	CLA	CHC-C4B	5.38	1.51	1.39
20	4	305	CLA	O2D-CGD	5.38	1.46	1.33
20	A	825	CLA	CAB-C3B	-5.37	1.33	1.47
20	1	212	CLA	CHD-C1D	5.37	1.48	1.38
20	B	803	CLA	O2A-CGA	5.37	1.48	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	207	CLA	O2D-CGD	5.37	1.46	1.33
20	B	827	CLA	O2A-CGA	5.37	1.49	1.33
20	A	804	CLA	OBD-CAD	5.37	1.31	1.22
20	1	212	CLA	O2D-CGD	5.37	1.46	1.33
20	2	315	CLA	CHD-C1D	5.36	1.51	1.38
20	A	824	CLA	CAB-C3B	-5.36	1.33	1.47
20	L	202	CLA	O2D-CGD	5.36	1.46	1.33
20	A	814	CLA	CAB-C3B	-5.35	1.33	1.47
20	3	301	CLA	CAB-C3B	-5.35	1.33	1.47
20	A	820	CLA	CHC-C4B	5.35	1.51	1.39
20	B	827	CLA	CHC-C4B	5.35	1.51	1.39
20	4	303	CLA	CHD-C1D	5.35	1.48	1.38
20	B	835	CLA	CAB-C3B	-5.34	1.33	1.47
20	4	304	CLA	CHC-C1C	5.34	1.49	1.38
20	B	849	CLA	O2D-CGD	5.34	1.46	1.33
20	L	208	CLA	CHC-C4B	5.34	1.51	1.39
20	H	108	CLA	CHC-C4B	5.34	1.51	1.39
20	A	815	CLA	O2A-CGA	5.34	1.48	1.33
20	1	203	CLA	C3D-C4D	-5.33	1.32	1.44
20	K	106	CLA	CAB-C3B	-5.33	1.33	1.47
20	2	305	CLA	CHC-C1C	5.33	1.49	1.38
20	A	802	CLA	CHC-C4B	5.33	1.51	1.39
20	B	838	CLA	CHC-C1C	5.33	1.49	1.38
20	B	814	CLA	O2A-CGA	5.32	1.48	1.33
20	B	831	CLA	CHC-C4B	5.32	1.51	1.39
20	L	204	CLA	CAB-C3B	-5.32	1.33	1.47
20	4	313	CLA	CHD-C4C	5.31	1.51	1.39
20	A	808	CLA	CHC-C4B	5.31	1.51	1.39
20	K	107	CLA	O2D-CGD	5.31	1.46	1.33
20	B	836	CLA	C3D-C4D	-5.30	1.32	1.44
20	H	110	CLA	CHC-C4B	5.30	1.51	1.39
20	B	830	CLA	CHC-C1C	5.30	1.49	1.38
20	2	311	CLA	CHD-C4C	5.29	1.51	1.39
20	R	107	CLA	O2A-CGA	5.28	1.48	1.33
20	B	809	CLA	O2D-CGD	5.28	1.46	1.33
20	B	836	CLA	O2D-CGD	5.28	1.46	1.33
20	B	832	CLA	CHC-C4B	5.27	1.51	1.39
20	A	813	CLA	CHC-C4B	5.27	1.51	1.39
20	B	816	CLA	O2A-CGA	5.27	1.48	1.33
20	B	849	CLA	O2A-CGA	5.27	1.48	1.33
20	B	821	CLA	CAB-C3B	-5.27	1.33	1.47
20	A	829	CLA	C3D-C4D	-5.27	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	206	CLA	OBD-CAD	5.26	1.31	1.22
20	J	103	CLA	CHD-C1D	5.26	1.48	1.38
20	K	103	CLA	C3D-C4D	-5.26	1.32	1.44
20	B	825	CLA	CHD-C4C	5.26	1.51	1.39
20	B	838	CLA	CHD-C4C	5.25	1.51	1.39
20	A	848	CLA	O2A-CGA	5.25	1.48	1.33
20	2	311	CLA	C3D-C4D	-5.25	1.32	1.44
20	1	207	CLA	CHC-C4B	5.25	1.51	1.39
20	B	815	CLA	CHD-C4C	5.25	1.51	1.39
20	B	805	CLA	O2D-CGD	5.25	1.46	1.33
20	B	839	CLA	CHC-C4B	5.25	1.51	1.39
20	B	838	CLA	CAB-C3B	-5.25	1.33	1.47
20	B	817	CLA	O2D-CGD	5.25	1.46	1.33
20	A	815	CLA	CHC-C4B	5.24	1.51	1.39
20	F	205	CLA	C3D-C4D	-5.24	1.32	1.44
20	A	809	CLA	O2A-CGA	5.24	1.48	1.33
20	B	828	CLA	CHD-C1D	5.23	1.48	1.38
20	B	830	CLA	C3D-C4D	-5.23	1.32	1.44
22	I	103	BCR	C26-C25	-5.23	1.25	1.34
20	B	823	CLA	C3D-C4D	-5.23	1.32	1.44
20	B	836	CLA	CHD-C1D	5.23	1.48	1.38
20	1	211	CLA	C1B-NB	-5.23	1.31	1.37
20	B	816	CLA	CHD-C4C	5.22	1.51	1.39
20	A	850	CLA	O2A-CGA	5.22	1.48	1.33
20	4	307	CLA	C1C-C2C	-5.22	1.33	1.44
20	2	304	CLA	CHC-C4B	5.22	1.51	1.39
20	2	306	CLA	CHD-C1D	5.22	1.48	1.38
20	B	804	CLA	O2A-CGA	5.22	1.48	1.33
20	A	806	CLA	C3D-C4D	-5.22	1.32	1.44
20	B	819	CLA	CAB-C3B	-5.22	1.33	1.47
20	4	309	CLA	CHD-C1D	5.22	1.51	1.38
20	A	823	CLA	C3D-C4D	-5.22	1.32	1.44
20	1	212	CLA	CAB-C3B	-5.21	1.33	1.47
20	B	826	CLA	O2D-CGD	5.21	1.46	1.33
22	I	103	BCR	C21-C22	-5.21	1.23	1.35
20	2	321	CLA	CHD-C1D	5.21	1.48	1.38
20	K	106	CLA	O2D-CGD	5.21	1.46	1.33
20	A	816	CLA	O2D-CGD	5.21	1.46	1.33
20	1	203	CLA	O2D-CGD	5.21	1.46	1.33
20	4	313	CLA	CHC-C4B	5.20	1.51	1.39
20	R	107	CLA	CAB-C3B	-5.20	1.33	1.47
20	A	834	CLA	C3D-C4D	-5.20	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	302	CLA	C3D-C4D	-5.20	1.32	1.44
20	2	301	CLA	C3D-C4D	-5.19	1.32	1.44
20	B	817	CLA	O2A-CGA	5.19	1.48	1.33
20	2	312	CLA	O2A-CGA	5.19	1.48	1.33
20	3	312	CLA	CHD-C1D	5.19	1.51	1.38
20	4	319	CLA	C3D-C4D	-5.19	1.32	1.44
20	A	823	CLA	O2D-CGD	5.19	1.46	1.33
20	J	102	CLA	C3D-C4D	-5.19	1.32	1.44
20	1	206	CLA	CHD-C4C	5.19	1.51	1.39
20	A	832	CLA	C3D-C4D	-5.19	1.32	1.44
20	B	829	CLA	CAB-C3B	-5.19	1.33	1.47
20	4	310	CLA	OBD-CAD	5.19	1.31	1.22
20	1	206	CLA	CHC-C4B	5.19	1.51	1.39
20	A	855	CLA	C3D-C4D	-5.18	1.32	1.44
20	4	307	CLA	O2D-CGD	5.18	1.46	1.33
20	B	822	CLA	C3D-C4D	-5.18	1.32	1.44
20	A	822	CLA	C3D-C4D	-5.18	1.32	1.44
20	A	809	CLA	CAB-C3B	-5.18	1.33	1.47
20	3	310	CLA	C3D-C4D	-5.18	1.32	1.44
20	K	106	CLA	CHC-C1C	5.18	1.48	1.38
20	4	302	CLA	O2D-CGD	5.18	1.46	1.33
20	3	317	CLA	CHD-C1D	5.17	1.51	1.38
20	4	319	CLA	O2D-CGD	5.17	1.45	1.33
20	1	211	CLA	CHC-C1C	5.17	1.48	1.38
20	3	301	CLA	O2D-CGD	5.17	1.45	1.33
20	A	833	CLA	C3D-C4D	-5.17	1.32	1.44
20	A	831	CLA	C3D-C4D	-5.17	1.32	1.44
20	B	836	CLA	CHD-C4C	5.16	1.51	1.39
20	A	836	CLA	C3D-C4D	-5.16	1.32	1.44
20	A	829	CLA	CAB-C3B	-5.16	1.33	1.47
20	2	312	CLA	C3D-C4D	-5.16	1.32	1.44
20	B	825	CLA	CHC-C4B	5.16	1.51	1.39
20	K	106	CLA	CHD-C4C	5.16	1.50	1.39
20	B	808	CLA	O2D-CGD	5.16	1.45	1.33
20	A	837	CLA	C3D-C4D	-5.16	1.32	1.44
20	A	834	CLA	O2D-CGD	5.16	1.45	1.33
20	A	836	CLA	O2D-CGD	5.16	1.45	1.33
20	A	819	CLA	OBD-CAD	5.15	1.31	1.22
20	1	204	CLA	C3D-C4D	-5.15	1.32	1.44
20	2	307	CLA	OBD-CAD	5.15	1.31	1.22
20	A	835	CLA	C3D-C4D	-5.15	1.32	1.44
20	A	809	CLA	O2D-CGD	5.15	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	315	CLA	CAB-C3B	-5.15	1.33	1.47
20	A	837	CLA	O2D-CGD	5.14	1.45	1.33
20	A	835	CLA	O2D-CGD	5.14	1.45	1.33
20	A	827	CLA	C3D-C4D	-5.14	1.32	1.44
20	B	834	CLA	CAB-C3B	-5.14	1.33	1.47
20	H	107	CLA	O2A-CGA	5.14	1.48	1.33
20	A	832	CLA	O2D-CGD	5.14	1.45	1.33
20	J	102	CLA	O2D-CGD	5.14	1.45	1.33
20	A	801	CLA	O2D-CGD	5.14	1.45	1.33
20	K	103	CLA	O2D-CGD	5.14	1.45	1.33
20	A	855	CLA	O2D-CGD	5.13	1.45	1.33
20	B	823	CLA	O2D-CGD	5.13	1.45	1.33
20	B	807	CLA	O2D-CGD	5.13	1.45	1.33
20	A	849	CLA	CHC-C4B	5.13	1.50	1.39
20	F	205	CLA	O2D-CGD	5.13	1.45	1.33
20	A	833	CLA	O2D-CGD	5.12	1.45	1.33
20	A	824	CLA	CHC-C4B	5.12	1.50	1.39
20	3	301	CLA	CHD-C4C	5.12	1.50	1.39
20	4	304	CLA	C1B-NB	-5.12	1.31	1.37
20	B	831	CLA	C3D-C4D	-5.12	1.32	1.44
20	A	831	CLA	O2D-CGD	5.12	1.45	1.33
20	B	848	CLA	O2D-CGD	5.12	1.45	1.33
20	A	808	CLA	O2A-CGA	5.12	1.47	1.30
20	A	803	CLA	CAB-C3B	-5.11	1.33	1.47
20	2	314	CLA	CHD-C1D	5.11	1.50	1.38
20	H	109	CLA	O2A-CGA	5.11	1.48	1.33
20	3	313	CLA	CHD-C1D	5.11	1.50	1.38
20	B	816	CLA	CHD-C1D	5.11	1.48	1.38
20	3	315	CLA	O2D-CGD	5.11	1.45	1.33
20	3	310	CLA	O2D-CGD	5.11	1.45	1.33
20	B	831	CLA	CHD-C1D	5.10	1.48	1.38
20	B	829	CLA	C3D-C4D	-5.10	1.32	1.44
20	B	819	CLA	C3D-C4D	-5.10	1.32	1.44
20	A	814	CLA	CHD-C4C	5.09	1.50	1.39
20	A	849	CLA	OBD-CAD	5.09	1.31	1.22
20	B	848	CLA	CAB-C3B	-5.09	1.33	1.47
20	B	826	CLA	C3D-C4D	-5.09	1.32	1.44
20	2	301	CLA	O2D-CGD	5.09	1.45	1.33
20	A	849	CLA	C3D-C4D	-5.09	1.32	1.44
20	B	808	CLA	C3D-C4D	-5.09	1.32	1.44
20	B	831	CLA	O2A-CGA	5.09	1.47	1.30
20	A	826	CLA	C3D-C4D	-5.09	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	839	CLA	OBD-CAD	5.09	1.31	1.22
20	3	303	CLA	CHC-C4B	5.09	1.50	1.39
20	B	807	CLA	CHC-C4B	5.08	1.50	1.39
20	B	838	CLA	O2D-CGD	5.08	1.45	1.33
20	K	106	CLA	C1C-C2C	-5.08	1.34	1.44
20	4	315	CLA	C3D-C4D	-5.08	1.32	1.44
20	K	107	CLA	O2A-CGA	5.08	1.48	1.33
20	K	105	CLA	C3D-C4D	-5.08	1.32	1.44
20	A	808	CLA	C3D-C4D	-5.07	1.32	1.44
20	B	827	CLA	CAB-C3B	-5.07	1.33	1.47
20	A	822	CLA	O2D-CGD	5.07	1.45	1.33
20	B	825	CLA	O2D-CGD	5.07	1.45	1.33
20	B	833	CLA	O2A-CGA	5.07	1.48	1.33
20	2	321	CLA	CAB-C3B	-5.07	1.33	1.47
20	A	849	CLA	O2D-CGD	5.06	1.45	1.33
20	K	105	CLA	O2D-CGD	5.06	1.45	1.33
20	4	310	CLA	CHC-C4B	5.06	1.50	1.39
20	B	822	CLA	O2D-CGD	5.06	1.45	1.33
20	2	311	CLA	CHC-C4B	5.06	1.50	1.39
20	B	826	CLA	CHD-C4C	5.06	1.50	1.39
20	3	319	CLA	CHC-C4B	5.06	1.50	1.39
20	B	848	CLA	O2A-CGA	5.06	1.48	1.33
20	L	204	CLA	CHD-C4C	5.06	1.50	1.39
20	3	309	CLA	CAB-C3B	-5.06	1.33	1.47
20	L	207	CLA	CHC-C4B	5.06	1.50	1.39
20	B	833	CLA	C3D-C4D	-5.06	1.32	1.44
20	B	847	CLA	CHC-C4B	5.06	1.50	1.39
20	A	812	CLA	OBD-CAD	5.05	1.31	1.22
20	A	832	CLA	CAB-C3B	-5.05	1.33	1.47
20	A	835	CLA	CAB-C3B	-5.05	1.33	1.47
20	2	306	CLA	CHC-C4B	5.05	1.50	1.39
20	B	818	CLA	CHC-C4B	5.05	1.50	1.39
20	3	310	CLA	CAB-C3B	-5.04	1.33	1.47
20	A	831	CLA	CAB-C3B	-5.04	1.33	1.47
20	B	811	CLA	CAB-C3B	-5.04	1.33	1.47
20	1	214	CLA	O2D-CGD	5.04	1.45	1.33
20	B	816	CLA	O2D-CGD	5.04	1.45	1.33
20	B	814	CLA	CHC-C4B	5.04	1.50	1.39
20	1	214	CLA	CAB-C3B	-5.03	1.34	1.47
20	A	848	CLA	CAB-C3B	-5.03	1.34	1.47
20	2	317	CLA	CHC-C4B	5.03	1.50	1.39
20	A	836	CLA	CAB-C3B	-5.03	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	I	102	CLA	CAB-C3B	-5.03	1.34	1.47
20	F	205	CLA	CAB-C3B	-5.03	1.34	1.47
20	A	834	CLA	CAB-C3B	-5.03	1.34	1.47
20	A	828	CLA	CAB-C3B	-5.02	1.34	1.47
20	4	319	CLA	CAB-C3B	-5.02	1.34	1.47
22	F	203	BCR	C1-C6	-5.02	1.47	1.53
20	A	822	CLA	CAB-C3B	-5.02	1.34	1.47
20	A	833	CLA	CAB-C3B	-5.02	1.34	1.47
20	4	302	CLA	CAB-C3B	-5.02	1.34	1.47
20	A	855	CLA	CAB-C3B	-5.02	1.34	1.47
20	B	834	CLA	O2A-CGA	5.02	1.48	1.33
20	L	204	CLA	C1B-NB	-5.02	1.31	1.37
20	A	837	CLA	CAB-C3B	-5.01	1.34	1.47
20	2	306	CLA	C3D-C4D	-5.01	1.32	1.44
20	B	811	CLA	CHC-C4B	5.01	1.50	1.39
20	2	301	CLA	CAB-C3B	-5.01	1.34	1.47
20	B	823	CLA	CAB-C3B	-5.01	1.34	1.47
20	A	809	CLA	CHC-C4B	5.01	1.50	1.39
20	1	214	CLA	CHD-C4C	5.01	1.50	1.39
20	J	102	CLA	CAB-C3B	-5.01	1.34	1.47
20	K	105	CLA	CAB-C3B	-5.00	1.34	1.47
20	K	107	CLA	OBD-CAD	5.00	1.31	1.22
20	3	306	CLA	CHD-C1D	5.00	1.50	1.38
20	A	805	CLA	CHC-C4B	5.00	1.50	1.39
20	I	102	CLA	C3D-C4D	-5.00	1.32	1.44
20	A	813	CLA	O2A-CGA	5.00	1.47	1.33
20	4	310	CLA	C3D-C4D	-5.00	1.32	1.44
20	L	203	CLA	O2A-CGA	5.00	1.47	1.33
20	B	830	CLA	CHC-C4B	4.99	1.50	1.39
20	1	208	CLA	CHD-C1D	4.99	1.50	1.38
20	4	305	CLA	O2A-CGA	4.99	1.47	1.33
20	K	103	CLA	CAB-C3B	-4.99	1.34	1.47
20	B	810	CLA	O2D-CGD	4.99	1.45	1.33
20	F	206	CLA	C1B-NB	-4.98	1.31	1.37
20	G	103	CLA	C3D-C4D	-4.98	1.33	1.44
20	J	103	CLA	O2D-CGD	4.98	1.45	1.33
20	A	822	CLA	CHC-C4B	4.98	1.50	1.39
20	B	825	CLA	CAB-C3B	-4.98	1.34	1.47
20	3	309	CLA	CHD-C1D	4.98	1.48	1.38
20	A	817	CLA	O2A-CGA	4.97	1.47	1.33
20	A	833	CLA	CHC-C4B	4.97	1.50	1.39
20	3	305	CLA	CHD-C1D	4.97	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	837	CLA	O2D-CGD	4.97	1.45	1.33
20	A	837	CLA	CHC-C4B	4.97	1.50	1.39
20	R	107	CLA	OBD-CAD	4.97	1.31	1.22
20	1	214	CLA	C4C-C3C	-4.96	1.36	1.45
20	A	802	CLA	O2D-CGD	4.96	1.45	1.33
20	B	835	CLA	O2A-CGA	4.96	1.47	1.33
20	1	204	CLA	CHC-C4B	4.96	1.50	1.39
20	B	818	CLA	CHD-C1D	4.96	1.48	1.38
20	B	816	CLA	CHC-C4B	4.96	1.50	1.39
20	A	821	CLA	CHC-C4B	4.96	1.50	1.39
20	A	830	CLA	O2A-CGA	4.95	1.47	1.33
20	A	831	CLA	CHC-C4B	4.95	1.50	1.39
20	I	102	CLA	O2D-CGD	4.95	1.45	1.33
20	A	832	CLA	CHC-C4B	4.95	1.50	1.39
20	A	823	CLA	CAB-C3B	-4.95	1.34	1.47
20	B	828	CLA	O2A-CGA	4.95	1.47	1.33
20	4	302	CLA	CHC-C4B	4.95	1.50	1.39
20	L	203	CLA	CHC-C4B	4.95	1.50	1.39
20	B	819	CLA	OBD-CAD	4.95	1.31	1.22
20	B	822	CLA	CAB-C3B	-4.95	1.34	1.47
20	A	835	CLA	CHC-C4B	4.95	1.50	1.39
20	A	848	CLA	CHC-C4B	4.94	1.50	1.39
20	A	834	CLA	CHC-C4B	4.94	1.50	1.39
20	B	822	CLA	CHC-C4B	4.94	1.50	1.39
20	B	823	CLA	CHC-C4B	4.94	1.50	1.39
20	K	107	CLA	C3D-C4D	-4.94	1.33	1.44
20	1	206	CLA	CHD-C1D	4.94	1.48	1.38
23	A	839	PQN	C10-C5	4.94	1.48	1.40
20	B	815	CLA	C3D-C4D	-4.94	1.33	1.44
20	B	816	CLA	C3D-C4D	-4.94	1.33	1.44
20	A	838	CLA	CHC-C4B	4.94	1.50	1.39
20	A	836	CLA	CHC-C4B	4.93	1.50	1.39
20	L	202	CLA	CAB-C3B	-4.93	1.34	1.47
20	K	105	CLA	CHC-C4B	4.93	1.50	1.39
20	B	824	CLA	CAB-C3B	-4.93	1.34	1.47
20	A	823	CLA	CHC-C4B	4.93	1.50	1.39
20	B	820	CLA	CHD-C1D	4.92	1.48	1.38
20	3	310	CLA	CHC-C4B	4.92	1.50	1.39
20	A	855	CLA	CHC-C4B	4.92	1.50	1.39
20	F	205	CLA	CHC-C4B	4.92	1.50	1.39
20	A	807	CLA	CAB-C3B	-4.92	1.34	1.47
20	4	307	CLA	CHD-C1D	4.92	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	307	CLA	CHD-C1D	4.92	1.50	1.38
20	1	207	CLA	O2A-CGA	4.92	1.47	1.33
20	3	319	CLA	OBD-CAD	4.92	1.30	1.22
20	A	811	CLA	O2D-CGD	4.92	1.45	1.33
20	F	204	CLA	CHC-C4B	4.91	1.50	1.39
20	B	832	CLA	O2A-CGA	4.91	1.47	1.30
20	B	832	CLA	CAB-C3B	-4.91	1.34	1.47
20	K	103	CLA	CHC-C4B	4.91	1.50	1.39
20	A	814	CLA	O2D-CGD	4.91	1.45	1.33
20	4	319	CLA	CHC-C4B	4.91	1.50	1.39
20	A	838	CLA	OBD-CAD	4.91	1.30	1.22
20	B	805	CLA	C3D-C4D	-4.90	1.33	1.44
22	L	209	BCR	C21-C22	-4.90	1.24	1.35
20	2	310	CLA	O2D-CGD	4.90	1.45	1.33
20	A	816	CLA	O2A-CGA	4.90	1.47	1.33
20	3	320	CLA	CHC-C4B	4.90	1.50	1.39
20	A	826	CLA	CHC-C4B	4.90	1.50	1.39
20	L	201	CLA	CHC-C4B	4.90	1.50	1.39
20	A	801	CLA	CAB-C3B	-4.89	1.34	1.47
20	B	820	CLA	CHC-C1C	4.89	1.48	1.38
20	1	201	CLA	OBD-CAD	4.89	1.30	1.22
20	K	106	CLA	C4C-C3C	-4.89	1.36	1.45
20	R	107	CLA	CHB-C1B	4.89	1.50	1.39
20	4	317	CLA	CHD-C1D	4.89	1.50	1.38
20	1	209	CLA	CHC-C1C	4.89	1.48	1.38
20	A	806	CLA	CHC-C4B	4.88	1.50	1.39
20	4	306	CLA	OBD-CAD	4.88	1.30	1.22
20	B	813	CLA	OBD-CAD	4.88	1.30	1.22
20	2	301	CLA	CHC-C4B	4.88	1.50	1.39
20	J	103	CLA	CHD-C4C	4.88	1.50	1.39
20	L	208	CLA	CMA-C3A	4.87	1.63	1.53
20	A	827	CLA	CHC-C4B	4.87	1.50	1.39
20	1	215	CLA	MG-NA	-4.87	1.94	2.06
20	J	103	CLA	C4C-C3C	-4.86	1.36	1.45
20	3	320	CLA	O2A-CGA	4.86	1.47	1.33
20	B	830	CLA	CAB-C3B	-4.86	1.34	1.47
20	A	828	CLA	O2A-CGA	4.86	1.47	1.33
20	A	847	CLA	CHD-C1D	4.85	1.47	1.38
20	2	317	CLA	O2A-CGA	4.85	1.47	1.33
20	B	837	CLA	O2A-CGA	4.85	1.47	1.33
20	B	803	CLA	O2D-CGD	4.85	1.45	1.33
20	F	206	CLA	CHC-C4B	4.85	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	J	102	CLA	CHC-C4B	4.85	1.50	1.39
20	F	204	CLA	C3D-C4D	-4.85	1.33	1.44
20	1	205	CLA	C3D-C4D	-4.84	1.33	1.44
20	1	214	CLA	C4B-NB	-4.84	1.31	1.37
20	K	106	CLA	CHC-C4B	4.84	1.50	1.39
20	B	847	CLA	O2D-CGD	4.84	1.45	1.33
20	1	212	CLA	CHD-C4C	4.84	1.50	1.39
20	B	825	CLA	C3D-C4D	-4.84	1.33	1.44
20	A	818	CLA	C3D-C4D	-4.83	1.33	1.44
20	4	305	CLA	CAB-C3B	-4.83	1.34	1.47
20	B	804	CLA	C3D-C4D	-4.83	1.33	1.44
20	L	207	CLA	CAB-C3B	-4.83	1.34	1.47
20	B	803	CLA	CHC-C4B	4.83	1.50	1.39
20	2	310	CLA	CHC-C4B	4.82	1.50	1.39
20	R	106	CLA	CHC-C4B	4.82	1.50	1.39
20	B	833	CLA	CAB-C3B	-4.82	1.34	1.47
20	4	303	CLA	CHC-C4B	4.82	1.50	1.39
20	4	318	CLA	CHC-C4B	4.82	1.50	1.39
20	B	819	CLA	CHC-C4B	4.81	1.50	1.39
20	4	311	CLA	CHD-C1D	4.81	1.50	1.38
20	A	811	CLA	O2A-CGA	4.81	1.47	1.33
20	B	838	CLA	O2A-CGA	4.81	1.47	1.33
20	B	829	CLA	O2D-CGD	4.81	1.45	1.33
20	B	810	CLA	O2A-CGA	4.81	1.47	1.33
20	1	214	CLA	C1C-C2C	-4.80	1.34	1.44
20	B	821	CLA	OBD-CAD	4.80	1.30	1.22
20	1	201	CLA	CHD-C1D	4.80	1.47	1.38
20	L	201	CLA	OBD-CAD	4.80	1.30	1.22
20	B	828	CLA	CHC-C4B	4.79	1.50	1.39
20	B	820	CLA	CHC-C4B	4.79	1.50	1.39
20	B	847	CLA	CAB-C3B	-4.79	1.34	1.47
20	B	811	CLA	OBD-CAD	4.78	1.30	1.22
20	G	103	CLA	O2A-CGA	4.78	1.47	1.33
20	3	309	CLA	CHD-C4C	4.77	1.50	1.39
20	1	207	CLA	CAB-C3B	-4.77	1.34	1.47
20	B	834	CLA	O2D-CGD	4.77	1.45	1.33
20	A	821	CLA	O2D-CGD	4.77	1.44	1.33
20	2	312	CLA	CHC-C4B	4.76	1.50	1.39
20	H	108	CLA	O2A-CGA	4.76	1.47	1.33
20	H	109	CLA	C3D-C4D	-4.76	1.33	1.44
20	A	804	CLA	CHC-C4B	4.76	1.50	1.39
20	L	202	CLA	CHC-C4B	4.76	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	301	CLA	CHC-C4B	4.76	1.50	1.39
20	B	833	CLA	OBD-CAD	4.76	1.30	1.22
20	B	821	CLA	C3D-C4D	-4.76	1.33	1.44
20	1	209	CLA	CHD-C1D	4.76	1.47	1.38
20	A	818	CLA	O2A-CGA	4.76	1.47	1.33
20	2	305	CLA	CHD-C1D	4.76	1.50	1.38
20	1	205	CLA	OBD-CAD	4.76	1.30	1.22
20	4	307	CLA	CHD-C4C	4.75	1.50	1.39
20	1	201	CLA	CHD-C4C	4.75	1.50	1.39
20	1	211	CLA	CHD-C1D	4.75	1.47	1.38
20	B	836	CLA	O2A-CGA	4.75	1.47	1.33
20	A	830	CLA	C3D-C4D	-4.75	1.33	1.44
20	3	304	CLA	CHC-C1C	4.74	1.47	1.38
20	L	201	CLA	CAB-C3B	-4.74	1.34	1.47
20	2	310	CLA	O2A-CGA	4.74	1.47	1.33
20	A	825	CLA	CHC-C4B	4.74	1.50	1.39
20	3	304	CLA	MG-NA	-4.74	1.95	2.06
20	B	838	CLA	CHC-C4B	4.74	1.50	1.39
20	A	810	CLA	C3D-C4D	-4.74	1.33	1.44
20	L	208	CLA	O2A-CGA	4.74	1.47	1.33
20	2	307	CLA	O2A-CGA	4.74	1.47	1.33
20	A	838	CLA	C3D-C4D	-4.74	1.33	1.44
20	1	201	CLA	CAB-C3B	-4.73	1.34	1.47
20	A	829	CLA	O2A-CGA	4.73	1.47	1.33
20	A	827	CLA	O2D-CGD	4.73	1.44	1.33
20	A	815	CLA	CAB-C3B	-4.73	1.34	1.47
20	A	807	CLA	O2A-CGA	4.72	1.47	1.33
20	B	809	CLA	O2A-CGA	4.72	1.47	1.33
20	2	306	CLA	CAB-C3B	-4.72	1.34	1.47
20	B	821	CLA	O2A-CGA	4.71	1.47	1.33
20	B	812	CLA	O2A-CGA	4.71	1.47	1.33
20	A	805	CLA	C3D-C4D	-4.71	1.33	1.44
20	3	303	CLA	C3D-C4D	-4.71	1.33	1.44
20	L	207	CLA	O2A-CGA	4.71	1.47	1.33
20	A	821	CLA	C3D-C4D	-4.71	1.33	1.44
20	B	815	CLA	CHC-C4B	4.71	1.50	1.39
20	R	106	CLA	C3D-C4D	-4.71	1.33	1.44
20	3	316	CLA	CHD-C1D	4.71	1.49	1.38
20	A	857	CLA	CHD-C1D	4.71	1.49	1.38
20	B	849	CLA	CHC-C4B	4.70	1.50	1.39
20	B	834	CLA	C3D-C4D	-4.70	1.33	1.44
20	1	206	CLA	CAB-C3B	-4.70	1.34	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	811	CLA	CHC-C4B	4.70	1.50	1.39
20	L	202	CLA	C3D-C4D	-4.70	1.33	1.44
20	B	803	CLA	C3D-C4D	-4.70	1.33	1.44
20	B	809	CLA	CHC-C4B	4.70	1.50	1.39
20	L	208	CLA	CAB-C3B	-4.69	1.34	1.47
20	G	103	CLA	OBD-CAD	4.69	1.30	1.22
20	3	314	CLA	C3D-C4D	-4.69	1.33	1.44
20	B	821	CLA	CHC-C4B	4.69	1.49	1.39
20	1	202	CLA	C1B-NB	-4.69	1.31	1.37
20	B	835	CLA	C3D-C4D	-4.69	1.33	1.44
20	2	307	CLA	CHC-C4B	4.69	1.49	1.39
20	2	304	CLA	O2A-CGA	4.69	1.47	1.33
20	L	201	CLA	O2A-CGA	4.68	1.47	1.33
20	H	107	CLA	CHC-C4B	4.68	1.49	1.39
20	A	807	CLA	CHC-C1C	4.68	1.47	1.38
20	1	206	CLA	C3D-C4D	-4.68	1.33	1.44
23	B	840	PQN	C10-C5	4.68	1.48	1.40
20	H	110	CLA	O2A-CGA	4.68	1.47	1.33
20	1	206	CLA	O2A-CGA	4.68	1.47	1.33
20	A	813	CLA	CAB-C3B	-4.68	1.34	1.47
20	4	318	CLA	CAB-C3B	-4.68	1.34	1.47
20	B	803	CLA	OBD-CAD	4.67	1.30	1.22
20	4	318	CLA	OBD-CAD	4.67	1.30	1.22
20	H	108	CLA	CAB-C3B	-4.67	1.34	1.47
20	A	813	CLA	C3D-C4D	-4.66	1.33	1.44
20	B	813	CLA	CAB-C3B	-4.66	1.35	1.47
20	L	208	CLA	C3D-C4D	-4.66	1.33	1.44
20	A	828	CLA	CHC-C4B	4.66	1.49	1.39
20	1	203	CLA	CAB-C3B	-4.66	1.35	1.47
20	B	809	CLA	C3D-C4D	-4.65	1.33	1.44
20	B	847	CLA	C3D-C4D	-4.65	1.33	1.44
20	4	318	CLA	O2A-CGA	4.65	1.46	1.33
20	B	807	CLA	CAB-C3B	-4.65	1.35	1.47
20	3	314	CLA	CHC-C4B	4.65	1.49	1.39
20	B	838	CLA	C3D-C4D	-4.65	1.33	1.44
20	1	203	CLA	OBD-CAD	4.64	1.30	1.22
20	A	827	CLA	CAB-C3B	-4.64	1.35	1.47
20	1	203	CLA	O2A-CGA	4.64	1.46	1.33
20	4	303	CLA	C3A-C2A	-4.63	1.50	1.54
20	B	818	CLA	OBD-CAD	4.63	1.30	1.22
20	4	315	CLA	C4C-C3C	-4.63	1.37	1.45
20	B	806	CLA	CHC-C4B	4.63	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	319	CLA	C3D-C4D	-4.62	1.33	1.44
20	A	816	CLA	CAB-C3B	-4.62	1.35	1.47
20	1	215	CLA	CHD-C1D	4.62	1.49	1.38
20	1	212	CLA	CHC-C4B	4.62	1.49	1.39
20	2	321	CLA	CHC-C4B	4.62	1.49	1.39
20	A	812	CLA	O2A-CGA	4.62	1.46	1.30
20	2	317	CLA	C3D-C4D	-4.62	1.33	1.44
20	4	306	CLA	O2A-CGA	4.62	1.46	1.33
20	B	818	CLA	C3D-C4D	-4.61	1.33	1.44
20	1	204	CLA	CAB-C3B	-4.61	1.35	1.47
20	3	320	CLA	CAB-C3B	-4.61	1.35	1.47
20	2	321	CLA	C1B-NB	-4.61	1.31	1.37
20	4	306	CLA	C3D-C4D	-4.61	1.33	1.44
20	A	802	CLA	OBD-CAD	4.61	1.30	1.22
20	F	206	CLA	OBD-CAD	4.61	1.30	1.22
20	A	815	CLA	C3D-C4D	-4.60	1.33	1.44
20	H	101	CLA	CHC-C4B	4.60	1.49	1.39
20	1	212	CLA	C4C-C3C	-4.60	1.37	1.45
20	2	309	CLA	CHC-C4B	4.60	1.52	1.39
20	1	211	CLA	CHB-C1B	4.60	1.49	1.39
20	3	315	CLA	CHC-C4B	4.59	1.49	1.39
20	H	108	CLA	C3D-C4D	-4.59	1.33	1.44
20	A	828	CLA	C3D-C4D	-4.59	1.33	1.44
20	A	802	CLA	C3D-C4D	-4.58	1.33	1.44
20	A	805	CLA	OBD-CAD	4.58	1.30	1.22
20	F	206	CLA	CHD-C4C	4.58	1.49	1.39
20	A	821	CLA	CAB-C3B	-4.57	1.35	1.47
20	3	304	CLA	CHD-C1D	4.57	1.49	1.38
20	B	832	CLA	C3D-C4D	-4.57	1.33	1.44
20	A	830	CLA	CHC-C4B	4.57	1.49	1.39
20	B	839	CLA	C3D-C4D	-4.57	1.33	1.44
20	F	206	CLA	C4C-C3C	-4.57	1.37	1.45
20	B	817	CLA	CAB-C3B	-4.57	1.35	1.47
20	1	209	CLA	CHD-C4C	4.57	1.49	1.39
20	A	831	CLA	O2A-CGA	4.57	1.45	1.30
20	A	816	CLA	CHC-C4B	4.56	1.49	1.39
20	B	825	CLA	OBD-CAD	4.56	1.30	1.22
20	4	315	CLA	CHC-C4B	4.56	1.49	1.39
20	A	801	CLA	CHC-C4B	4.56	1.49	1.39
20	A	814	CLA	CHC-C4B	4.56	1.49	1.39
20	A	828	CLA	O2D-CGD	4.55	1.44	1.33
20	2	321	CLA	CHD-C4C	4.55	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	819	CLA	CAB-C3B	-4.55	1.35	1.47
20	A	812	CLA	CAB-C3B	-4.53	1.35	1.47
20	K	105	CLA	O2A-CGA	4.53	1.45	1.30
20	H	108	CLA	OBD-CAD	4.53	1.30	1.22
20	2	307	CLA	CAB-C3B	-4.53	1.35	1.47
20	1	209	CLA	MG-NA	-4.53	1.95	2.06
20	2	311	CLA	OBD-CAD	4.53	1.30	1.22
20	1	209	CLA	CHC-C4B	4.53	1.49	1.39
20	3	314	CLA	OBD-CAD	4.52	1.30	1.22
20	A	820	CLA	C3D-C4D	-4.52	1.34	1.44
20	2	304	CLA	C3D-C4D	-4.52	1.34	1.44
20	1	211	CLA	O2D-CGD	4.51	1.44	1.33
20	A	847	CLA	CAB-C3B	-4.51	1.35	1.47
20	1	207	CLA	C3D-C4D	-4.51	1.34	1.44
20	B	814	CLA	C3D-C4D	-4.51	1.34	1.44
20	2	321	CLA	C4B-NB	-4.51	1.31	1.37
20	B	811	CLA	C3D-C4D	-4.51	1.34	1.44
20	B	828	CLA	CAB-C3B	-4.51	1.35	1.47
20	L	208	CLA	OBD-CAD	4.51	1.30	1.22
20	H	109	CLA	CHB-C1B	4.51	1.49	1.39
20	B	813	CLA	C3D-C4D	-4.51	1.34	1.44
20	H	110	CLA	C3D-C4D	-4.50	1.34	1.44
20	B	835	CLA	O2D-CGD	4.50	1.44	1.33
20	A	816	CLA	C3D-C4D	-4.50	1.34	1.44
20	1	204	CLA	O2A-CGA	4.50	1.47	1.33
20	L	203	CLA	CAB-C3B	-4.50	1.35	1.47
20	A	802	CLA	CAB-C3B	-4.49	1.35	1.47
20	L	203	CLA	C3D-C4D	-4.49	1.34	1.44
22	3	311	BCR	C21-C22	-4.49	1.25	1.35
20	B	837	CLA	CAB-C3B	-4.49	1.35	1.47
20	B	819	CLA	O2A-CGA	4.49	1.46	1.33
20	L	207	CLA	C3D-C4D	-4.49	1.34	1.44
20	H	109	CLA	CAB-C3B	-4.49	1.35	1.47
20	1	214	CLA	OBD-CAD	4.48	1.30	1.22
20	4	305	CLA	OBD-CAD	4.48	1.30	1.22
20	J	103	CLA	CHC-C4B	4.48	1.49	1.39
20	L	204	CLA	O2D-CGD	4.48	1.44	1.33
20	A	826	CLA	O2A-CGA	4.48	1.46	1.33
20	1	207	CLA	OBD-CAD	4.47	1.30	1.22
20	B	837	CLA	C3D-C4D	-4.47	1.34	1.44
20	A	804	CLA	O2A-CGA	4.47	1.46	1.33
20	A	819	CLA	CHC-C4B	4.46	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	838	CLA	O2A-CGA	4.46	1.46	1.33
20	B	820	CLA	C4B-NB	-4.46	1.32	1.37
20	A	830	CLA	CAB-C3B	-4.46	1.35	1.47
20	4	318	CLA	CHB-C1B	4.45	1.49	1.39
20	H	107	CLA	OBD-CAD	4.45	1.30	1.22
20	B	826	CLA	CAB-C3B	-4.45	1.35	1.47
20	A	824	CLA	O2D-CGD	4.44	1.44	1.33
20	3	308	CLA	CHC-C1C	4.44	1.47	1.38
20	A	829	CLA	CHC-C4B	4.44	1.49	1.39
20	4	314	CLA	CHD-C1D	4.44	1.49	1.38
20	4	313	CLA	OBD-CAD	4.44	1.30	1.22
20	3	301	CLA	O2A-CGA	4.44	1.46	1.33
20	1	211	CLA	CHD-C4C	4.43	1.49	1.39
22	B	850	BCR	C17-C18	-4.43	1.25	1.35
20	B	848	CLA	C3D-C4D	-4.43	1.34	1.44
20	2	308	CLA	CHD-C1D	4.43	1.49	1.38
20	B	808	CLA	OBD-CAD	4.43	1.30	1.22
20	A	811	CLA	C3D-C4D	-4.43	1.34	1.44
20	4	304	CLA	C1C-C2C	-4.43	1.35	1.44
20	3	301	CLA	C4C-C3C	-4.43	1.37	1.45
20	4	307	CLA	C1B-C2B	-4.43	1.32	1.43
20	A	801	CLA	C3D-C4D	-4.43	1.34	1.44
20	2	312	CLA	CAB-C3B	-4.43	1.35	1.47
20	3	320	CLA	OBD-CAD	4.43	1.30	1.22
20	L	202	CLA	O2A-CGA	4.43	1.46	1.33
20	4	310	CLA	CAB-C3B	-4.42	1.35	1.47
20	A	850	CLA	CHC-C4B	4.42	1.49	1.39
20	1	209	CLA	C4C-C3C	-4.42	1.35	1.44
20	L	202	CLA	CHB-C1B	4.42	1.49	1.39
20	L	203	CLA	CHB-C1B	4.42	1.49	1.39
20	3	303	CLA	OBD-CAD	4.41	1.30	1.22
20	1	214	CLA	CHC-C1C	4.41	1.47	1.38
20	4	310	CLA	O2A-CGA	4.41	1.46	1.33
20	B	804	CLA	CHC-C4B	4.41	1.49	1.39
20	B	806	CLA	O2A-CGA	4.41	1.46	1.33
20	1	209	CLA	C1C-C2C	-4.41	1.35	1.44
20	4	315	CLA	CHD-C1D	4.41	1.47	1.38
20	4	318	CLA	C3D-C4D	-4.40	1.34	1.44
20	B	828	CLA	C3D-C4D	-4.40	1.34	1.44
20	A	803	CLA	C3D-C4D	-4.40	1.34	1.44
20	A	807	CLA	C3D-C4D	-4.40	1.34	1.44
22	L	209	BCR	C20-C19	-4.40	1.23	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	I	103	BCR	C1-C6	-4.40	1.48	1.53
20	A	818	CLA	OBD-CAD	4.40	1.30	1.22
20	B	830	CLA	O2A-CGA	4.40	1.46	1.33
20	K	106	CLA	C1B-C2B	-4.40	1.32	1.43
20	A	806	CLA	O2A-CGA	4.40	1.46	1.33
20	A	812	CLA	C3D-C4D	-4.39	1.34	1.44
20	A	820	CLA	CAB-C3B	-4.39	1.35	1.47
20	B	825	CLA	CHB-C1B	4.39	1.49	1.39
20	2	306	CLA	O2A-CGA	4.39	1.46	1.33
20	3	313	CLA	CHC-C4B	4.39	1.51	1.39
20	A	805	CLA	O2A-CGA	4.39	1.46	1.33
20	3	309	CLA	C1C-C2C	-4.39	1.35	1.44
20	3	312	CLA	CHC-C4B	4.38	1.51	1.39
20	B	834	CLA	CHB-C1B	4.38	1.49	1.39
20	1	214	CLA	C1B-C2B	-4.38	1.32	1.43
20	F	206	CLA	C4B-NB	-4.38	1.32	1.37
20	A	813	CLA	OBD-CAD	4.38	1.30	1.22
20	A	801	CLA	O2A-CGA	4.38	1.46	1.33
20	A	817	CLA	C3D-C4D	-4.38	1.34	1.44
20	3	309	CLA	C4B-NB	-4.37	1.32	1.37
20	2	317	CLA	CAB-C3B	-4.37	1.35	1.47
20	2	302	CLA	C3D-C4D	-4.37	1.34	1.44
20	A	804	CLA	C3D-C4D	-4.37	1.34	1.44
20	2	302	CLA	OBD-CAD	4.37	1.30	1.22
20	B	816	CLA	CAB-C3B	-4.37	1.35	1.47
20	4	311	CLA	CHC-C4B	4.37	1.51	1.39
20	H	101	CLA	CAB-C3B	-4.36	1.35	1.47
20	A	838	CLA	CAB-C3B	-4.36	1.35	1.47
20	B	812	CLA	C3D-C4D	-4.36	1.34	1.44
20	3	309	CLA	C1B-NB	-4.36	1.32	1.37
20	2	311	CLA	CAB-C3B	-4.36	1.35	1.47
20	2	303	CLA	CHD-C1D	4.35	1.49	1.38
20	4	305	CLA	C3D-C4D	-4.35	1.34	1.44
20	2	312	CLA	OBD-CAD	4.35	1.30	1.22
20	A	826	CLA	OBD-CAD	4.35	1.30	1.22
20	A	807	CLA	O2D-CGD	4.35	1.43	1.33
20	A	824	CLA	C3D-C4D	-4.34	1.34	1.44
20	L	204	CLA	C4C-C3C	-4.34	1.37	1.45
20	A	809	CLA	C3D-C4D	-4.34	1.34	1.44
22	B	843	BCR	C21-C22	-4.34	1.25	1.35
20	A	804	CLA	CAB-C3B	-4.33	1.35	1.47
20	A	848	CLA	C3D-C4D	-4.33	1.34	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	206	CLA	CHB-C1B	4.33	1.49	1.39
20	B	815	CLA	CAB-C3B	-4.33	1.35	1.47
20	K	106	CLA	C1D-ND	-4.33	1.32	1.37
20	R	107	CLA	C3D-C4D	-4.33	1.34	1.44
20	1	210	CLA	C3D-C4D	-4.33	1.34	1.44
20	2	309	CLA	CHD-C1D	4.32	1.49	1.38
20	1	211	CLA	O2A-CGA	4.32	1.45	1.33
20	B	822	CLA	O2A-CGA	4.32	1.45	1.33
20	4	310	CLA	CHB-C1B	4.32	1.49	1.39
20	4	319	CLA	O2A-CGA	4.31	1.45	1.33
20	B	810	CLA	C3D-C4D	-4.31	1.34	1.44
20	1	209	CLA	C4B-NB	-4.31	1.32	1.37
20	A	819	CLA	CHB-C1B	4.31	1.49	1.39
20	A	837	CLA	O2A-CGA	4.31	1.45	1.33
20	1	201	CLA	C4C-C3C	-4.31	1.37	1.45
20	A	823	CLA	O2A-CGA	4.31	1.45	1.33
20	B	832	CLA	OBD-CAD	4.31	1.29	1.22
20	L	201	CLA	C3D-C4D	-4.31	1.34	1.44
20	A	821	CLA	O2A-CGA	4.31	1.45	1.33
20	1	214	CLA	MG-ND	-4.31	1.97	2.05
20	B	807	CLA	C3D-C4D	-4.31	1.34	1.44
20	1	202	CLA	CAB-C3B	-4.30	1.35	1.47
20	A	826	CLA	CAB-C3B	-4.30	1.35	1.47
20	A	819	CLA	C3D-C4D	-4.30	1.34	1.44
22	G	102	BCR	C21-C22	-4.30	1.25	1.35
20	B	823	CLA	O2A-CGA	4.30	1.45	1.33
20	A	808	CLA	OBD-CAD	4.30	1.29	1.22
20	A	836	CLA	O2A-CGA	4.30	1.45	1.33
22	A	844	BCR	C21-C22	-4.30	1.25	1.35
20	A	822	CLA	O2A-CGA	4.30	1.45	1.33
20	A	835	CLA	O2A-CGA	4.30	1.45	1.33
20	A	805	CLA	CAB-C3B	-4.30	1.35	1.47
20	A	832	CLA	O2A-CGA	4.30	1.45	1.33
20	4	307	CLA	MG-NA	-4.30	1.96	2.06
20	B	830	CLA	OBD-CAD	4.30	1.29	1.22
20	4	305	CLA	CHC-C4B	4.29	1.49	1.39
22	A	842	BCR	C21-C22	-4.29	1.25	1.35
20	A	834	CLA	O2A-CGA	4.29	1.45	1.33
20	4	306	CLA	CHB-C1B	4.29	1.49	1.39
20	2	310	CLA	C3D-C4D	-4.29	1.34	1.44
20	A	833	CLA	O2A-CGA	4.28	1.45	1.33
20	A	855	CLA	O2A-CGA	4.28	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	814	CLA	CAB-C3B	-4.28	1.36	1.47
22	A	841	BCR	C21-C22	-4.28	1.25	1.35
20	3	310	CLA	O2A-CGA	4.28	1.45	1.33
20	G	103	CLA	CAB-C3B	-4.28	1.36	1.47
20	2	301	CLA	O2A-CGA	4.27	1.45	1.33
22	F	202	BCR	C21-C22	-4.27	1.25	1.35
20	4	315	CLA	CHD-C4C	4.27	1.48	1.39
20	A	820	CLA	OBD-CAD	4.27	1.29	1.22
20	K	107	CLA	CAB-C3B	-4.27	1.36	1.47
20	B	805	CLA	O2A-CGA	4.27	1.45	1.33
20	A	818	CLA	CAB-C3B	-4.26	1.36	1.47
20	A	847	CLA	O2A-CGA	4.26	1.45	1.33
20	J	102	CLA	O2A-CGA	4.26	1.45	1.33
20	1	202	CLA	C3D-C4D	-4.26	1.34	1.44
20	3	314	CLA	CAB-C3B	-4.26	1.36	1.47
20	A	814	CLA	C1B-NB	-4.26	1.32	1.37
20	A	803	CLA	CHC-C4B	4.26	1.49	1.39
20	3	314	CLA	CHB-C1B	4.26	1.49	1.39
20	L	202	CLA	OBD-CAD	4.25	1.29	1.22
20	H	110	CLA	CAB-C3B	-4.25	1.36	1.47
25	B	846	LMG	O8-C28	4.25	1.45	1.33
22	A	840	BCR	C21-C22	-4.25	1.26	1.35
20	B	826	CLA	CHC-C4B	4.25	1.48	1.39
20	4	302	CLA	O2A-CGA	4.25	1.45	1.33
20	1	214	CLA	O2A-CGA	4.25	1.45	1.33
20	4	304	CLA	CHD-C1D	4.24	1.46	1.38
22	B	841	BCR	C21-C22	-4.24	1.26	1.35
20	A	847	CLA	C4C-C3C	-4.24	1.37	1.45
22	J	101	BCR	C21-C22	-4.24	1.26	1.35
20	3	309	CLA	C1C-NC	-4.24	1.31	1.37
20	B	812	CLA	CAB-C3B	-4.24	1.36	1.47
20	A	847	CLA	C3D-C4D	-4.24	1.34	1.44
20	1	208	CLA	CHC-C4B	4.23	1.51	1.39
20	B	820	CLA	MG-NA	-4.23	1.96	2.06
20	4	309	CLA	CHC-C4B	4.23	1.51	1.39
20	B	814	CLA	OBD-CAD	4.23	1.29	1.22
22	A	843	BCR	C21-C22	-4.23	1.26	1.35
22	B	844	BCR	C21-C22	-4.23	1.26	1.35
20	K	103	CLA	O2A-CGA	4.22	1.45	1.33
20	F	204	CLA	OBD-CAD	4.21	1.29	1.22
20	A	806	CLA	O2D-CGD	4.21	1.43	1.33
20	4	304	CLA	C4C-C3C	-4.21	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	313	CLA	C3D-C4D	-4.20	1.34	1.44
20	4	310	CLA	C4C-C3C	-4.20	1.37	1.45
20	A	850	CLA	C3D-C4D	-4.20	1.34	1.44
20	F	206	CLA	O2D-CGD	4.20	1.43	1.33
20	J	103	CLA	C1B-NB	-4.19	1.32	1.37
20	B	804	CLA	CAB-C3B	-4.19	1.36	1.47
20	L	204	CLA	O2A-CGA	4.19	1.45	1.33
20	B	835	CLA	CHB-C1B	4.19	1.48	1.39
20	B	809	CLA	CAB-C3B	-4.19	1.36	1.47
20	B	806	CLA	OBD-CAD	4.19	1.29	1.22
20	B	803	CLA	CAB-C3B	-4.18	1.36	1.47
20	B	826	CLA	O2A-CGA	4.18	1.45	1.33
20	A	808	CLA	CAB-C3B	-4.18	1.36	1.47
20	A	807	CLA	CHB-C1B	4.17	1.48	1.39
20	2	307	CLA	C3D-C4D	-4.17	1.34	1.44
20	B	820	CLA	CHD-C4C	4.17	1.48	1.39
20	H	107	CLA	CAB-C3B	-4.16	1.36	1.47
20	B	805	CLA	CHC-C4B	4.16	1.48	1.39
20	2	306	CLA	CHB-C1B	4.16	1.48	1.39
20	1	212	CLA	O2A-CGA	4.15	1.45	1.33
20	1	210	CLA	OBD-CAD	4.15	1.29	1.22
25	B	846	LMG	O7-C10	4.15	1.46	1.34
20	1	201	CLA	C1D-C2D	-4.14	1.37	1.45
20	3	320	CLA	C3D-C4D	-4.14	1.34	1.44
20	1	211	CLA	C1C-C2C	-4.14	1.36	1.44
20	B	848	CLA	OBD-CAD	4.13	1.29	1.22
20	2	304	CLA	CAB-C3B	-4.13	1.36	1.47
20	A	824	CLA	OBD-CAD	4.13	1.29	1.22
20	B	816	CLA	CHB-C1B	4.12	1.48	1.39
20	4	312	CLA	CHC-C4B	4.12	1.50	1.39
20	3	316	CLA	CHC-C4B	4.12	1.50	1.39
20	A	801	CLA	OBD-CAD	4.12	1.29	1.22
20	4	314	CLA	CHC-C4B	4.11	1.50	1.39
20	B	836	CLA	CHB-C1B	4.11	1.48	1.39
20	H	110	CLA	OBD-CAD	4.10	1.29	1.22
20	B	824	CLA	O2A-CGA	4.09	1.45	1.33
20	R	106	CLA	CAB-C3B	-4.08	1.36	1.47
20	4	315	CLA	O2A-CGA	4.08	1.45	1.33
20	A	850	CLA	CHB-C1B	4.08	1.48	1.39
20	A	807	CLA	C1C-C2C	-4.08	1.36	1.44
20	B	849	CLA	C3D-C4D	-4.07	1.35	1.44
20	2	312	CLA	CHB-C1B	4.07	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	306	CLA	CHC-C4B	4.07	1.50	1.39
20	B	834	CLA	CHC-C4B	4.07	1.48	1.39
20	L	203	CLA	C4C-C3C	-4.06	1.38	1.45
20	B	835	CLA	CHC-C4B	4.06	1.48	1.39
20	3	317	CLA	CHC-C4B	4.06	1.50	1.39
20	B	825	CLA	O2A-CGA	4.05	1.45	1.33
20	B	833	CLA	CHB-C1B	4.05	1.48	1.39
20	A	828	CLA	OBD-CAD	4.04	1.29	1.22
20	L	207	CLA	OBD-CAD	4.04	1.29	1.22
20	B	836	CLA	CAB-C3B	-4.04	1.36	1.47
20	1	201	CLA	C4B-NB	-4.04	1.32	1.37
20	K	107	CLA	CHB-C1B	4.04	1.48	1.39
20	L	204	CLA	C1B-C2B	-4.03	1.33	1.43
20	A	801	CLA	CHB-C1B	4.03	1.48	1.39
20	2	315	CLA	CHC-C4B	4.03	1.50	1.39
20	1	202	CLA	OBD-CAD	4.02	1.29	1.22
20	3	305	CLA	CHC-C4B	4.02	1.50	1.39
20	A	814	CLA	C4C-C3C	-4.02	1.38	1.45
20	A	815	CLA	OBD-CAD	4.02	1.29	1.22
20	B	847	CLA	OBD-CAD	4.02	1.29	1.22
20	A	805	CLA	CHB-C1B	4.01	1.48	1.39
20	1	202	CLA	CHC-C4B	4.01	1.48	1.39
20	1	214	CLA	CHD-C1D	4.01	1.46	1.38
20	4	306	CLA	CAB-C3B	-4.01	1.36	1.47
20	B	813	CLA	O2A-CGA	4.00	1.45	1.33
20	B	817	CLA	CHB-C1B	4.00	1.48	1.39
20	2	317	CLA	OBD-CAD	3.99	1.29	1.22
20	1	214	CLA	C1D-C2D	-3.99	1.37	1.45
20	H	101	CLA	C3D-C4D	-3.99	1.35	1.44
20	A	817	CLA	OBD-CAD	3.99	1.29	1.22
20	1	213	CLA	CHC-C4B	3.98	1.50	1.39
20	B	847	CLA	O2A-CGA	3.98	1.45	1.33
20	R	106	CLA	CHB-C1B	3.98	1.48	1.39
20	B	826	CLA	C4C-C3C	-3.97	1.38	1.45
20	3	309	CLA	CHC-C1C	3.97	1.46	1.38
20	A	811	CLA	CAB-C3B	-3.97	1.36	1.47
20	1	201	CLA	CHC-C1C	3.96	1.46	1.38
20	A	825	CLA	C3D-C4D	-3.96	1.35	1.44
20	4	308	CLA	CHC-C4B	3.96	1.50	1.39
20	H	101	CLA	OBD-CAD	3.95	1.29	1.22
20	F	206	CLA	C1D-ND	-3.94	1.32	1.37
20	3	309	CLA	CHB-C1B	3.94	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	H	109	CLA	OBD-CAD	3.93	1.29	1.22
20	A	849	CLA	O2A-CGA	3.93	1.44	1.33
20	A	809	CLA	OBD-CAD	3.92	1.29	1.22
20	1	211	CLA	C3D-CAD	-3.92	1.32	1.45
20	3	316	CLA	MG-NA	-3.92	1.97	2.06
20	B	810	CLA	C4C-C3C	-3.92	1.38	1.45
20	B	804	CLA	OBD-CAD	3.92	1.29	1.22
20	A	825	CLA	OBD-CAD	3.92	1.29	1.22
20	4	315	CLA	C4B-NB	-3.92	1.32	1.37
20	3	315	CLA	O2A-CGA	3.90	1.44	1.33
20	1	205	CLA	CHB-C1B	3.90	1.48	1.39
20	3	319	CLA	CHB-C1B	3.90	1.48	1.39
20	B	817	CLA	C3D-C4D	-3.90	1.35	1.44
20	3	309	CLA	CHC-C4B	3.89	1.48	1.39
20	A	815	CLA	CHB-C1B	3.89	1.48	1.39
20	B	815	CLA	CHB-C1B	3.89	1.48	1.39
21	2	319	LMU	O1'-C1'	3.88	1.46	1.40
20	A	803	CLA	CHB-C1B	3.88	1.48	1.39
20	2	304	CLA	CHB-C1B	3.88	1.48	1.39
20	A	816	CLA	C4C-C3C	-3.88	1.38	1.45
20	B	815	CLA	O2A-CGA	3.87	1.44	1.33
20	2	310	CLA	CHB-C1B	3.87	1.48	1.39
20	A	827	CLA	CHB-C1B	3.86	1.48	1.39
20	B	813	CLA	CHB-C1B	3.86	1.48	1.39
20	H	110	CLA	CHB-C1B	3.85	1.48	1.39
20	B	839	CLA	CHB-C1B	3.85	1.48	1.39
20	A	817	CLA	CAB-C3B	-3.85	1.37	1.47
20	1	210	CLA	CHB-C1B	3.85	1.48	1.39
20	A	822	CLA	OBD-CAD	3.84	1.29	1.22
20	1	201	CLA	C1C-C2C	-3.84	1.36	1.44
20	1	203	CLA	CHB-C1B	3.83	1.48	1.39
20	4	315	CLA	C1B-NB	-3.83	1.32	1.37
20	A	810	CLA	OBD-CAD	3.83	1.29	1.22
20	3	301	CLA	C1B-NB	-3.83	1.32	1.37
20	4	304	CLA	O2D-CGD	3.82	1.42	1.33
20	A	813	CLA	CHB-C1B	3.82	1.48	1.39
20	B	807	CLA	C1B-NB	-3.82	1.32	1.37
20	4	315	CLA	CHB-C1B	3.81	1.48	1.39
20	B	806	CLA	C3D-C4D	-3.81	1.35	1.44
20	B	820	CLA	C1C-NC	-3.81	1.31	1.37
20	B	805	CLA	C1C-C2C	-3.80	1.36	1.44
20	2	305	CLA	CHC-C4B	3.80	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	834	CLA	OBD-CAD	3.80	1.29	1.22
20	B	849	CLA	C4C-C3C	-3.80	1.38	1.45
20	1	207	CLA	CHB-C1B	3.80	1.47	1.39
22	F	203	BCR	C20-C19	-3.80	1.24	1.34
20	A	807	CLA	CHC-C4B	3.80	1.47	1.39
21	2	320	LMU	O1'-C1'	3.79	1.46	1.40
20	A	833	CLA	OBD-CAD	3.79	1.29	1.22
20	2	314	CLA	MG-NA	-3.79	1.97	2.06
20	B	824	CLA	OBD-CAD	3.78	1.29	1.22
20	B	830	CLA	C1B-NB	-3.78	1.32	1.37
20	1	201	CLA	O2A-CGA	3.78	1.44	1.33
20	J	102	CLA	OBD-CAD	3.78	1.29	1.22
20	F	205	CLA	C3A-C2A	-3.78	1.51	1.54
20	A	832	CLA	OBD-CAD	3.78	1.29	1.22
20	A	849	CLA	C1B-NB	-3.78	1.32	1.37
20	K	103	CLA	OBD-CAD	3.78	1.29	1.22
20	4	302	CLA	OBD-CAD	3.77	1.29	1.22
20	A	855	CLA	OBD-CAD	3.77	1.29	1.22
20	A	824	CLA	O2A-CGA	3.77	1.44	1.33
20	3	303	CLA	CHB-C1B	3.77	1.47	1.39
20	4	309	CLA	CHD-C4C	3.77	1.53	1.40
20	K	106	CLA	MG-NA	-3.77	1.97	2.06
20	B	820	CLA	C1B-C2B	-3.77	1.34	1.43
20	A	807	CLA	OBD-CAD	3.76	1.29	1.22
20	2	303	CLA	CHC-C4B	3.76	1.49	1.39
20	J	103	CLA	O2A-CGA	3.76	1.44	1.33
20	A	837	CLA	OBD-CAD	3.75	1.28	1.22
20	B	822	CLA	OBD-CAD	3.75	1.28	1.22
20	4	319	CLA	OBD-CAD	3.75	1.28	1.22
20	B	823	CLA	OBD-CAD	3.75	1.28	1.22
20	1	214	CLA	C1C-NC	-3.75	1.32	1.37
20	A	835	CLA	OBD-CAD	3.75	1.28	1.22
20	2	302	CLA	CAB-C3B	-3.75	1.37	1.47
20	B	823	CLA	C4C-C3C	-3.75	1.38	1.45
20	B	839	CLA	C3A-C2A	-3.74	1.51	1.54
20	B	832	CLA	CHB-C1B	3.74	1.47	1.39
20	3	310	CLA	OBD-CAD	3.73	1.28	1.22
20	1	211	CLA	CHC-C4B	3.73	1.47	1.39
20	B	805	CLA	C4B-NB	-3.73	1.33	1.37
20	B	812	CLA	OBD-CAD	3.73	1.28	1.22
20	3	315	CLA	C4C-C3C	-3.73	1.38	1.45
20	F	205	CLA	OBD-CAD	3.73	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	836	CLA	OBD-CAD	3.73	1.28	1.22
20	B	826	CLA	CHB-C1B	3.72	1.47	1.39
20	4	305	CLA	CHB-C1B	3.72	1.47	1.39
20	B	828	CLA	OBD-CAD	3.72	1.28	1.22
20	J	103	CLA	C1C-C2C	-3.72	1.37	1.44
20	2	312	CLA	C1B-NB	-3.72	1.33	1.37
20	A	831	CLA	OBD-CAD	3.72	1.28	1.22
20	2	303	CLA	MG-NA	-3.72	1.97	2.06
20	B	838	CLA	CHB-C1B	3.71	1.47	1.39
20	A	830	CLA	OBD-CAD	3.71	1.28	1.22
20	3	307	CLA	CHC-C4B	3.71	1.49	1.39
20	2	321	CLA	OBD-CAD	3.71	1.28	1.22
20	3	315	CLA	C1B-NB	-3.71	1.33	1.37
20	1	204	CLA	CHB-C1B	3.71	1.47	1.39
20	1	211	CLA	C4B-NB	-3.71	1.33	1.37
20	A	857	CLA	CHC-C4B	3.70	1.49	1.39
20	F	205	CLA	C4C-C3C	-3.70	1.38	1.45
20	A	848	CLA	OBD-CAD	3.70	1.28	1.22
20	B	829	CLA	CHB-C1B	3.70	1.47	1.39
20	F	206	CLA	CHB-C1B	3.70	1.47	1.39
20	A	816	CLA	CHB-C1B	3.69	1.47	1.39
20	K	106	CLA	MG-ND	-3.69	1.98	2.05
20	B	831	CLA	C4C-C3C	-3.69	1.38	1.45
20	2	321	CLA	O2A-CGA	3.69	1.44	1.33
20	K	105	CLA	OBD-CAD	3.69	1.28	1.22
20	A	822	CLA	C4C-C3C	-3.69	1.38	1.45
20	B	809	CLA	CHB-C1B	3.68	1.47	1.39
20	A	823	CLA	OBD-CAD	3.68	1.28	1.22
20	B	837	CLA	OBD-CAD	3.68	1.28	1.22
20	A	814	CLA	O2A-CGA	3.68	1.44	1.33
20	B	831	CLA	CHB-C1B	3.68	1.47	1.39
20	2	307	CLA	CHB-C1B	3.68	1.47	1.39
20	1	212	CLA	OBD-CAD	3.68	1.28	1.22
20	A	826	CLA	CHB-C1B	3.68	1.47	1.39
20	L	201	CLA	CHB-C1B	3.68	1.47	1.39
22	I	101	BCR	C20-C19	-3.67	1.25	1.34
20	B	820	CLA	C1C-C2C	-3.67	1.37	1.44
20	4	317	CLA	CHC-C4B	3.67	1.49	1.39
20	A	823	CLA	C4C-C3C	-3.67	1.38	1.45
20	B	809	CLA	OBD-CAD	3.67	1.28	1.22
20	2	308	CLA	CHC-C4B	3.67	1.49	1.39
20	B	830	CLA	CHB-C1B	3.67	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	318	CLA	C4C-C3C	-3.67	1.38	1.45
20	A	832	CLA	C4C-C3C	-3.67	1.38	1.45
20	2	301	CLA	C4C-C3C	-3.66	1.38	1.45
20	A	818	CLA	CHB-C1B	3.66	1.47	1.39
20	4	319	CLA	C4C-C3C	-3.66	1.38	1.45
20	2	311	CLA	C1B-NB	-3.66	1.33	1.37
20	B	830	CLA	C1C-C2C	-3.66	1.37	1.44
20	L	204	CLA	C1C-NC	-3.66	1.32	1.37
20	1	214	CLA	C1D-ND	-3.66	1.33	1.37
20	3	309	CLA	O2A-CGA	3.66	1.44	1.33
20	A	810	CLA	CAB-C3B	-3.65	1.37	1.47
20	2	301	CLA	OBD-CAD	3.65	1.28	1.22
20	B	814	CLA	CHB-C1B	3.65	1.47	1.39
20	2	310	CLA	OBD-CAD	3.65	1.28	1.22
20	G	103	CLA	CHB-C1B	3.65	1.47	1.39
20	B	826	CLA	OBD-CAD	3.64	1.28	1.22
20	4	307	CLA	CAB-C3B	-3.64	1.37	1.47
20	1	209	CLA	C1C-NC	-3.63	1.32	1.37
20	1	212	CLA	C1B-NB	-3.63	1.33	1.37
20	B	808	CLA	CHB-C1B	3.63	1.47	1.39
20	B	815	CLA	C4C-C3C	-3.63	1.38	1.45
20	J	102	CLA	C4C-C3C	-3.63	1.38	1.45
20	A	824	CLA	CHB-C1B	3.63	1.47	1.39
20	3	312	CLA	CHD-C4C	3.63	1.52	1.40
20	A	836	CLA	C4C-C3C	-3.63	1.38	1.45
22	I	101	BCR	C5-C6	-3.63	1.28	1.34
20	A	828	CLA	C4C-C3C	-3.62	1.38	1.45
20	B	810	CLA	C1B-NB	-3.61	1.33	1.37
20	2	304	CLA	OBD-CAD	3.61	1.28	1.22
20	K	105	CLA	C4C-C3C	-3.61	1.38	1.45
20	B	819	CLA	C1B-NB	-3.61	1.33	1.37
20	A	833	CLA	C4C-C3C	-3.61	1.38	1.45
20	B	836	CLA	C4C-C3C	-3.61	1.38	1.45
20	A	855	CLA	C4C-C3C	-3.60	1.38	1.45
20	A	829	CLA	CHB-C1B	3.60	1.47	1.39
20	B	822	CLA	C4C-C3C	-3.60	1.38	1.45
20	A	835	CLA	C4C-C3C	-3.60	1.38	1.45
20	A	850	CLA	OBD-CAD	3.60	1.28	1.22
20	R	106	CLA	OBD-CAD	3.60	1.28	1.22
20	A	825	CLA	CHB-C1B	3.60	1.47	1.39
20	A	808	CLA	CHB-C1B	3.60	1.47	1.39
21	F	201	LMU	O1B-C4'	-3.60	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	308	CLA	CHD-C4C	3.60	1.52	1.40
20	B	812	CLA	CHB-C1B	3.59	1.47	1.39
20	A	837	CLA	C4C-C3C	-3.59	1.38	1.45
20	2	321	CLA	C4C-C3C	-3.59	1.38	1.45
20	K	103	CLA	C4C-C3C	-3.59	1.38	1.45
20	1	214	CLA	MG-NB	-3.59	1.98	2.05
20	4	307	CLA	CHC-C4B	3.58	1.47	1.39
20	4	307	CLA	CHB-C4A	-3.58	1.28	1.37
20	1	215	CLA	CHC-C4B	3.58	1.49	1.39
20	A	806	CLA	OBD-CAD	3.58	1.28	1.22
20	B	821	CLA	C1B-NB	-3.57	1.33	1.37
20	2	301	CLA	CHB-C1B	3.57	1.47	1.39
20	3	310	CLA	C4C-C3C	-3.56	1.39	1.45
20	A	834	CLA	C4C-C3C	-3.56	1.39	1.45
20	B	827	CLA	C1B-NB	-3.56	1.33	1.37
20	A	831	CLA	C4C-C3C	-3.56	1.39	1.45
20	2	321	CLA	C1D-ND	-3.55	1.33	1.37
20	2	315	CLA	CHB-C1B	3.55	1.49	1.39
20	2	315	CLA	CHD-C4C	3.55	1.52	1.40
20	A	832	CLA	CHB-C1B	3.55	1.47	1.39
20	A	823	CLA	CHB-C1B	3.55	1.47	1.39
20	3	309	CLA	C1D-ND	-3.54	1.33	1.37
20	4	302	CLA	C4C-C3C	-3.54	1.39	1.45
20	A	833	CLA	CHB-C1B	3.54	1.47	1.39
20	A	855	CLA	CHB-C1B	3.53	1.47	1.39
22	3	311	BCR	C20-C19	-3.53	1.25	1.34
20	A	802	CLA	CHB-C1B	3.53	1.47	1.39
20	B	823	CLA	CHB-C1B	3.53	1.47	1.39
20	B	807	CLA	OBD-CAD	3.53	1.28	1.22
20	4	315	CLA	O2D-CGD	3.53	1.41	1.33
20	1	209	CLA	OBD-CAD	3.53	1.28	1.22
20	1	212	CLA	CHB-C1B	3.53	1.47	1.39
20	A	837	CLA	CHB-C1B	3.53	1.47	1.39
20	3	320	CLA	CHB-C1B	3.52	1.47	1.39
20	B	827	CLA	OBD-CAD	3.52	1.28	1.22
20	A	835	CLA	CHB-C1B	3.52	1.47	1.39
20	B	847	CLA	CHB-C1B	3.52	1.47	1.39
20	B	849	CLA	OBD-CAD	3.52	1.28	1.22
20	K	105	CLA	CHB-C1B	3.52	1.47	1.39
20	A	816	CLA	OBD-CAD	3.52	1.28	1.22
20	L	204	CLA	MG-NA	-3.52	1.97	2.06
20	B	818	CLA	CAB-C3B	-3.51	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	825	CLA	C4C-C3C	-3.51	1.39	1.45
20	B	820	CLA	O2A-CGA	3.51	1.43	1.33
20	4	307	CLA	C3A-C2A	-3.51	1.45	1.54
20	B	828	CLA	CHB-C1B	3.51	1.47	1.39
20	1	215	CLA	CHD-C4C	3.51	1.52	1.40
20	F	205	CLA	CHB-C1B	3.51	1.47	1.39
20	A	836	CLA	CHB-C1B	3.51	1.47	1.39
20	A	848	CLA	C1B-NB	-3.51	1.33	1.37
20	3	310	CLA	CHB-C1B	3.51	1.47	1.39
20	1	213	CLA	CHD-C4C	3.50	1.52	1.40
20	K	103	CLA	CHB-C1B	3.50	1.47	1.39
20	2	308	CLA	MG-NA	-3.50	1.98	2.06
20	A	822	CLA	CHB-C1B	3.50	1.47	1.39
20	B	811	CLA	CHB-C1B	3.50	1.47	1.39
20	4	315	CLA	C1C-C2C	-3.50	1.37	1.44
20	H	108	CLA	CHB-C1B	3.50	1.47	1.39
20	3	308	CLA	MG-NA	-3.49	1.98	2.06
20	4	319	CLA	CHB-C1B	3.49	1.47	1.39
20	L	208	CLA	CHB-C1B	3.49	1.47	1.39
20	4	304	CLA	CHC-C4B	3.49	1.47	1.39
20	A	831	CLA	CHB-C1B	3.49	1.47	1.39
20	B	822	CLA	CHB-C1B	3.49	1.47	1.39
20	B	814	CLA	C1B-NB	-3.49	1.33	1.37
20	F	206	CLA	O2A-CGA	3.49	1.43	1.33
20	B	824	CLA	CHB-C1B	3.48	1.47	1.39
20	A	834	CLA	CHB-C1B	3.48	1.47	1.39
20	3	317	CLA	CHB-C1B	3.48	1.49	1.39
20	4	302	CLA	CHB-C1B	3.48	1.47	1.39
20	B	829	CLA	OBD-CAD	3.48	1.28	1.22
22	B	842	BCR	C21-C22	-3.48	1.27	1.35
20	J	102	CLA	CHB-C1B	3.47	1.47	1.39
22	A	841	BCR	C20-C19	-3.47	1.25	1.34
20	4	308	CLA	CHD-C4C	3.47	1.52	1.40
20	4	307	CLA	C4B-NB	-3.46	1.33	1.37
20	A	829	CLA	OBD-CAD	3.46	1.28	1.22
20	2	321	CLA	CHB-C4A	-3.46	1.29	1.37
20	4	303	CLA	C4B-NB	-3.46	1.33	1.37
20	A	828	CLA	C1B-NB	-3.46	1.33	1.37
20	B	830	CLA	C4C-C3C	-3.45	1.39	1.45
21	4	321	LMU	O1'-C1'	3.45	1.45	1.40
20	1	201	CLA	C1D-ND	-3.44	1.33	1.37
20	A	849	CLA	C4C-C3C	-3.44	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	830	CLA	C1B-NB	-3.44	1.33	1.37
20	B	834	CLA	OBD-CAD	3.43	1.28	1.22
20	4	314	CLA	CHB-C1B	3.43	1.49	1.39
20	A	817	CLA	CHB-C1B	3.43	1.47	1.39
20	1	201	CLA	MG-NA	-3.43	1.98	2.06
22	B	844	BCR	C20-C19	-3.42	1.25	1.34
20	K	106	CLA	O2A-CGA	3.41	1.43	1.33
20	A	811	CLA	CHB-C1B	3.41	1.47	1.39
22	G	102	BCR	C20-C19	-3.41	1.25	1.34
20	B	806	CLA	CHB-C1B	3.41	1.47	1.39
20	B	838	CLA	OBD-CAD	3.41	1.28	1.22
20	I	102	CLA	C4C-C3C	-3.40	1.39	1.45
22	I	101	BCR	C26-C25	-3.40	1.28	1.34
20	L	208	CLA	C1B-NB	-3.40	1.33	1.37
22	F	202	BCR	C20-C19	-3.39	1.25	1.34
20	B	820	CLA	MG-NB	-3.38	1.99	2.05
20	3	315	CLA	CHB-C1B	3.38	1.47	1.39
21	H	102	LMU	O3B-C3B	3.38	1.51	1.43
20	B	819	CLA	CHB-C1B	3.37	1.47	1.39
20	A	820	CLA	CHB-C1B	3.37	1.47	1.39
20	4	307	CLA	C1C-NC	-3.36	1.32	1.37
22	A	844	BCR	C20-C19	-3.36	1.25	1.34
22	J	101	BCR	C20-C19	-3.36	1.25	1.34
22	B	841	BCR	C20-C19	-3.36	1.25	1.34
22	B	843	BCR	C20-C19	-3.35	1.25	1.34
20	H	107	CLA	CHB-C1B	3.35	1.46	1.39
20	4	304	CLA	C4B-NB	-3.35	1.33	1.37
22	A	842	BCR	C20-C19	-3.35	1.25	1.34
20	J	103	CLA	MG-NA	-3.35	1.98	2.06
20	3	305	CLA	CHD-C4C	3.35	1.51	1.40
20	3	306	CLA	CHD-C4C	3.35	1.51	1.40
20	A	804	CLA	C1B-NB	-3.35	1.33	1.37
20	4	307	CLA	O2A-CGA	3.35	1.43	1.33
20	B	805	CLA	MG-NA	-3.34	1.98	2.06
20	A	857	CLA	MG-NA	-3.34	1.98	2.06
20	A	809	CLA	C1C-C2C	-3.34	1.37	1.44
22	A	840	BCR	C20-C19	-3.33	1.26	1.34
20	B	820	CLA	C4D-CHA	-3.33	1.27	1.38
20	B	849	CLA	CHB-C1B	3.33	1.46	1.39
20	1	214	CLA	CHC-C4B	3.33	1.46	1.39
22	A	843	BCR	C20-C19	-3.33	1.26	1.34
20	4	307	CLA	C2A-C1A	-3.33	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	804	CLA	CHB-C1B	3.32	1.46	1.39
20	4	315	CLA	C1B-C2B	-3.32	1.35	1.43
20	2	321	CLA	C1B-C2B	-3.32	1.35	1.43
20	1	208	CLA	CHD-C4C	3.32	1.51	1.40
20	3	313	CLA	CHD-C4C	3.32	1.51	1.40
20	A	812	CLA	CHB-C1B	3.32	1.46	1.39
20	4	303	CLA	CHB-C1B	3.31	1.46	1.39
20	A	804	CLA	CHB-C1B	3.31	1.46	1.39
20	B	820	CLA	C1D-C2D	-3.30	1.38	1.45
20	B	804	CLA	C1C-C2C	-3.30	1.37	1.44
20	4	311	CLA	CHD-C4C	3.30	1.51	1.40
20	I	102	CLA	CHB-C1B	3.30	1.46	1.39
20	2	314	CLA	CHC-C4B	3.30	1.48	1.39
20	2	317	CLA	C1B-NB	-3.30	1.33	1.37
20	A	810	CLA	CHB-C1B	3.29	1.46	1.39
20	B	818	CLA	C4C-C3C	-3.29	1.39	1.45
20	B	810	CLA	CHB-C1B	3.28	1.46	1.39
22	B	850	BCR	C39-C30	-3.28	1.47	1.53
20	A	848	CLA	C4C-C3C	-3.28	1.39	1.45
20	A	814	CLA	C1C-C2C	-3.28	1.37	1.44
20	B	816	CLA	C4C-C3C	-3.28	1.39	1.45
20	4	309	CLA	CHB-C1B	3.27	1.48	1.39
20	2	305	CLA	MG-NA	-3.27	1.98	2.06
20	B	803	CLA	C1B-NB	-3.27	1.33	1.37
20	F	205	CLA	C1B-NB	-3.26	1.33	1.37
20	1	211	CLA	C1C-NC	-3.26	1.32	1.37
20	A	847	CLA	CHB-C1B	3.26	1.46	1.39
20	4	312	CLA	MG-NA	-3.26	1.98	2.06
20	4	304	CLA	MG-NA	-3.25	1.98	2.06
20	A	828	CLA	CHB-C1B	3.25	1.46	1.39
20	A	838	CLA	C1B-NB	-3.25	1.33	1.37
22	B	850	BCR	C40-C30	-3.25	1.47	1.53
20	4	304	CLA	OBD-CAD	3.25	1.28	1.22
20	L	208	CLA	C4C-C3C	-3.25	1.39	1.45
20	4	307	CLA	CAA-C2A	-3.25	1.48	1.54
20	3	317	CLA	CHD-C4C	3.25	1.51	1.40
20	4	319	CLA	C1B-NB	-3.24	1.33	1.37
20	K	103	CLA	C1B-NB	-3.24	1.33	1.37
20	1	209	CLA	C1B-C2B	-3.24	1.35	1.43
20	B	821	CLA	C4B-NB	-3.24	1.33	1.37
20	2	305	CLA	C3D-C4D	-3.23	1.36	1.44
20	H	107	CLA	C4C-C3C	-3.23	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	805	CLA	CHB-C1B	3.23	1.46	1.39
20	1	204	CLA	C1B-NB	-3.23	1.33	1.37
20	B	847	CLA	C1D-ND	-3.23	1.33	1.37
20	R	107	CLA	C1B-NB	-3.22	1.33	1.37
20	L	207	CLA	CHB-C1B	3.22	1.46	1.39
20	1	207	CLA	C4C-C3C	-3.22	1.39	1.45
20	3	304	CLA	CHD-C4C	3.21	1.51	1.40
20	B	806	CLA	C1C-C2C	-3.21	1.38	1.44
20	3	307	CLA	CHD-C4C	3.21	1.51	1.40
20	B	835	CLA	C4C-C3C	-3.21	1.39	1.45
20	3	310	CLA	C1B-NB	-3.21	1.33	1.37
20	1	206	CLA	C4C-C3C	-3.20	1.39	1.45
20	A	812	CLA	C1B-NB	-3.20	1.33	1.37
20	1	212	CLA	C1C-C2C	-3.20	1.38	1.44
20	4	311	CLA	MG-NA	-3.20	1.98	2.06
22	I	103	BCR	C20-C19	-3.19	1.26	1.34
20	2	321	CLA	MG-ND	-3.19	1.99	2.05
20	A	847	CLA	OBD-CAD	3.19	1.28	1.22
20	A	822	CLA	C1B-NB	-3.18	1.33	1.37
22	I	101	BCR	C1-C6	-3.18	1.49	1.53
20	B	816	CLA	OBD-CAD	3.18	1.28	1.22
20	4	315	CLA	CBD-CGD	-3.18	1.42	1.52
20	A	837	CLA	C1B-NB	-3.18	1.33	1.37
20	1	207	CLA	C2A-C1A	-3.18	1.45	1.52
20	F	206	CLA	C1D-C2D	-3.18	1.39	1.45
20	3	305	CLA	CHA-C1A	3.18	1.50	1.41
20	3	301	CLA	CHB-C1B	3.18	1.46	1.39
20	H	101	CLA	CHB-C1B	3.17	1.46	1.39
20	4	313	CLA	CHB-C1B	3.17	1.46	1.39
20	A	811	CLA	OBD-CAD	3.17	1.27	1.22
20	A	834	CLA	C1B-NB	-3.16	1.33	1.37
21	B	845	LMU	O1'-C1'	3.16	1.45	1.40
20	A	855	CLA	C1B-NB	-3.16	1.33	1.37
20	B	848	CLA	CHB-C1B	3.16	1.46	1.39
20	3	308	CLA	CHA-C1A	3.15	1.50	1.41
20	A	823	CLA	C1B-NB	-3.15	1.33	1.37
20	A	821	CLA	OBD-CAD	3.15	1.27	1.22
20	B	807	CLA	O2A-CGA	3.15	1.42	1.33
20	A	832	CLA	C1B-NB	-3.15	1.33	1.37
20	A	833	CLA	C1B-NB	-3.14	1.33	1.37
20	1	213	CLA	CHB-C1B	3.14	1.48	1.39
20	B	835	CLA	C1B-NB	-3.14	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	829	CLA	C1C-C2C	-3.14	1.38	1.44
20	4	302	CLA	C1B-NB	-3.14	1.33	1.37
20	2	308	CLA	CHA-C1A	3.13	1.50	1.41
20	B	828	CLA	C4C-C3C	-3.13	1.39	1.45
20	A	836	CLA	C1B-NB	-3.13	1.33	1.37
20	B	832	CLA	C4C-C3C	-3.12	1.39	1.45
20	3	305	CLA	CHB-C1B	3.12	1.48	1.39
20	G	103	CLA	C4C-C3C	-3.12	1.39	1.45
20	4	308	CLA	CHB-C1B	3.12	1.48	1.39
20	K	107	CLA	C4C-C3C	-3.12	1.39	1.45
20	3	306	CLA	CHA-C1A	3.12	1.50	1.41
20	A	831	CLA	C1B-NB	-3.12	1.33	1.37
20	B	847	CLA	C4C-C3C	-3.12	1.39	1.45
20	A	814	CLA	OBD-CAD	3.12	1.27	1.22
20	A	848	CLA	CHB-C1B	3.11	1.46	1.39
20	H	109	CLA	C4C-C3C	-3.11	1.39	1.45
20	4	307	CLA	C1D-ND	-3.11	1.33	1.37
20	A	827	CLA	OBD-CAD	3.11	1.27	1.22
20	3	312	CLA	CHB-C1B	3.11	1.48	1.39
20	3	306	CLA	CHB-C1B	3.11	1.48	1.39
20	2	302	CLA	CHB-C1B	3.11	1.46	1.39
20	A	847	CLA	C1D-C2D	-3.11	1.39	1.45
20	A	835	CLA	C1B-NB	-3.10	1.33	1.37
20	A	809	CLA	CHB-C1B	3.10	1.46	1.39
20	A	806	CLA	C4C-C3C	-3.10	1.39	1.45
20	4	317	CLA	CHD-C4C	3.10	1.50	1.40
20	4	315	CLA	MG-NA	-3.10	1.98	2.06
20	A	828	CLA	C1C-C2C	-3.10	1.38	1.44
20	F	204	CLA	CHB-C1B	3.09	1.46	1.39
20	B	806	CLA	C1B-NB	-3.09	1.33	1.37
22	F	203	BCR	C29-C30	-3.09	1.46	1.54
20	B	823	CLA	C1B-NB	-3.09	1.33	1.37
20	2	301	CLA	C1B-NB	-3.09	1.33	1.37
20	A	847	CLA	C1B-NB	-3.09	1.33	1.37
20	B	813	CLA	C4C-C3C	-3.09	1.39	1.45
20	B	807	CLA	C1B-C2B	-3.08	1.35	1.43
21	R	104	LMU	O1'-C1'	3.08	1.45	1.40
22	F	203	BCR	C39-C30	-3.08	1.47	1.53
20	B	805	CLA	C4C-C3C	-3.08	1.39	1.45
20	A	857	CLA	CHD-C4C	3.08	1.50	1.40
20	4	304	CLA	C1B-C2B	-3.08	1.35	1.43
20	3	316	CLA	CHD-C4C	3.08	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	312	CLA	CHD-C4C	3.08	1.50	1.40
20	B	822	CLA	C1B-NB	-3.07	1.33	1.37
20	B	807	CLA	C4C-C3C	-3.07	1.39	1.45
20	4	315	CLA	C1D-C2D	-3.07	1.39	1.45
20	J	103	CLA	C4B-NB	-3.07	1.33	1.37
20	B	826	CLA	C1B-NB	-3.06	1.33	1.37
20	B	849	CLA	C1C-C2C	-3.06	1.38	1.44
20	3	313	CLA	CHB-C1B	3.06	1.48	1.39
20	3	312	CLA	CHA-C1A	3.06	1.50	1.41
20	4	304	CLA	O2A-CGA	3.06	1.42	1.33
20	A	814	CLA	C4B-NB	-3.06	1.33	1.37
20	A	820	CLA	C1B-NB	-3.06	1.33	1.37
20	1	209	CLA	C1D-ND	-3.06	1.33	1.37
20	K	105	CLA	C1B-NB	-3.06	1.33	1.37
20	4	304	CLA	C1D-C2D	-3.06	1.39	1.45
20	2	308	CLA	CHD-C4C	3.06	1.50	1.40
20	A	857	CLA	CHB-C1B	3.05	1.48	1.39
20	L	204	CLA	MG-NB	-3.05	1.99	2.05
20	L	204	CLA	MG-ND	-3.05	1.99	2.05
20	J	103	CLA	OBD-CAD	3.05	1.27	1.22
20	A	830	CLA	CHB-C1B	3.04	1.46	1.39
20	A	810	CLA	C4C-C3C	-3.04	1.39	1.45
20	4	314	CLA	CHD-C4C	3.04	1.50	1.40
20	2	315	CLA	MG-NA	-3.04	1.99	2.06
21	A	846	LMU	O1'-C1'	3.04	1.45	1.40
22	F	203	BCR	C40-C30	-3.04	1.48	1.53
20	J	102	CLA	C1B-NB	-3.04	1.33	1.37
20	B	836	CLA	OBD-CAD	3.04	1.27	1.22
20	B	817	CLA	OBD-CAD	3.03	1.27	1.22
20	A	801	CLA	C4C-C3C	-3.03	1.39	1.45
20	3	301	CLA	C1C-C2C	-3.03	1.38	1.44
20	3	308	CLA	CHC-C4B	3.03	1.48	1.39
20	A	821	CLA	CHB-C1B	3.03	1.46	1.39
20	4	307	CLA	MG-NC	-3.03	1.99	2.06
22	B	850	BCR	C30-C25	-3.03	1.49	1.53
20	2	321	CLA	C1C-C2C	-3.03	1.38	1.44
20	B	835	CLA	C1C-C2C	-3.03	1.38	1.44
20	4	306	CLA	C1B-NB	-3.02	1.33	1.37
20	B	832	CLA	C1B-NB	-3.02	1.33	1.37
20	L	204	CLA	CHB-C4A	-3.02	1.30	1.37
20	4	311	CLA	CHB-C1B	3.02	1.47	1.39
20	2	309	CLA	CHD-C4C	3.02	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	208	CLA	CHB-C1B	3.02	1.47	1.39
20	H	107	CLA	C1B-NB	-3.02	1.33	1.37
20	B	808	CLA	C1B-NB	-3.01	1.33	1.37
20	4	317	CLA	CHB-C1B	3.01	1.47	1.39
20	B	809	CLA	C1B-NB	-3.01	1.33	1.37
20	4	304	CLA	CHB-C4A	-3.01	1.30	1.37
20	3	301	CLA	OBD-CAD	3.00	1.27	1.22
22	3	311	BCR	C1-C6	-3.00	1.49	1.53
21	R	109	LMU	O2B-C2B	3.00	1.50	1.43
20	1	209	CLA	C3B-C2B	-3.00	1.32	1.44
20	B	829	CLA	C4C-C3C	-3.00	1.39	1.45
20	F	206	CLA	C1B-C2B	-2.99	1.36	1.43
20	B	813	CLA	C1C-C2C	-2.99	1.38	1.44
20	B	807	CLA	CHB-C1B	2.99	1.46	1.39
20	A	850	CLA	CMA-C3A	2.99	1.59	1.53
20	3	307	CLA	MG-NA	-2.99	1.99	2.06
20	1	210	CLA	C1B-NB	-2.99	1.33	1.37
20	4	306	CLA	C4C-C3C	-2.98	1.40	1.45
20	L	204	CLA	OBD-CAD	2.98	1.27	1.22
20	A	849	CLA	C1C-C2C	-2.98	1.38	1.44
22	I	101	BCR	C4-C5	-2.98	1.45	1.51
20	A	825	CLA	C1B-NB	-2.98	1.33	1.37
20	A	814	CLA	MG-NA	-2.97	1.99	2.06
20	L	208	CLA	CBD-CAD	-2.97	1.43	1.56
20	R	106	CLA	C1B-NB	-2.97	1.34	1.37
20	A	849	CLA	MG-NA	-2.96	1.99	2.06
20	2	302	CLA	C1B-NB	-2.96	1.34	1.37
20	A	824	CLA	C1C-C2C	-2.96	1.38	1.44
22	L	209	BCR	C30-C25	-2.96	1.50	1.53
20	3	305	CLA	MG-NA	-2.95	1.99	2.06
20	A	806	CLA	CHB-C1B	2.95	1.46	1.39
20	2	312	CLA	C4C-C3C	-2.95	1.40	1.45
20	B	818	CLA	CHB-C1B	2.95	1.46	1.39
20	L	204	CLA	C1D-ND	-2.95	1.34	1.37
20	F	204	CLA	C3A-C2A	-2.94	1.51	1.54
20	A	818	CLA	C4C-C3C	-2.94	1.40	1.45
20	2	317	CLA	C1B-C2B	-2.94	1.36	1.43
20	B	824	CLA	C4C-C3C	-2.94	1.40	1.45
20	B	837	CLA	CHB-C1B	2.94	1.46	1.39
20	3	316	CLA	C3D-C4D	-2.93	1.36	1.44
20	1	212	CLA	MG-NA	-2.93	1.99	2.06
20	2	314	CLA	C3D-C4D	-2.93	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	804	CLA	C4C-C3C	-2.93	1.40	1.45
20	4	317	CLA	MG-NA	-2.93	1.99	2.06
20	1	202	CLA	CHB-C1B	2.93	1.46	1.39
20	3	306	CLA	MG-NA	-2.93	1.99	2.06
20	4	314	CLA	CHA-C1A	2.93	1.49	1.41
20	B	847	CLA	C1B-NB	-2.92	1.34	1.37
20	A	849	CLA	CHB-C1B	2.92	1.46	1.39
20	4	303	CLA	C1B-NB	-2.92	1.34	1.37
20	H	101	CLA	C1B-NB	-2.91	1.34	1.37
20	B	810	CLA	OBD-CAD	2.91	1.27	1.22
20	2	314	CLA	CHD-C4C	2.91	1.50	1.40
20	A	804	CLA	C1C-C2C	-2.91	1.38	1.44
20	3	308	CLA	C3D-C4D	-2.91	1.36	1.44
20	2	311	CLA	CHB-C1B	2.91	1.45	1.39
20	B	821	CLA	CHB-C1B	2.90	1.45	1.39
20	4	302	CLA	C1C-C2C	-2.90	1.38	1.44
20	4	315	CLA	C1D-ND	-2.90	1.34	1.37
20	2	311	CLA	C4C-C3C	-2.90	1.40	1.45
20	1	208	CLA	CHA-C1A	2.90	1.49	1.41
21	F	201	LMU	C4'-C5'	-2.90	1.45	1.52
20	3	301	CLA	MG-NA	-2.90	1.99	2.06
20	4	319	CLA	C1C-C2C	-2.90	1.38	1.44
20	B	835	CLA	OBD-CAD	2.89	1.27	1.22
22	B	850	BCR	C29-C30	-2.89	1.47	1.54
20	4	312	CLA	CHB-C1B	2.89	1.47	1.39
20	A	809	CLA	C4C-C3C	-2.89	1.40	1.45
20	3	320	CLA	C1B-NB	-2.89	1.34	1.37
21	H	102	LMU	O1'-C1'	2.89	1.45	1.40
20	1	213	CLA	MG-NA	-2.88	1.99	2.06
21	2	318	LMU	O1'-C1'	2.88	1.45	1.40
20	B	823	CLA	C1C-C2C	-2.88	1.38	1.44
20	A	814	CLA	CHB-C1B	2.87	1.45	1.39
20	2	304	CLA	C4C-C3C	-2.87	1.40	1.45
20	B	807	CLA	C1C-C2C	-2.87	1.38	1.44
20	A	850	CLA	C1C-C2C	-2.87	1.38	1.44
22	3	311	BCR	C30-C25	-2.87	1.50	1.53
20	3	312	CLA	MG-NA	-2.87	1.99	2.06
20	2	303	CLA	CHD-C4C	2.86	1.50	1.40
22	B	850	BCR	C31-C1	-2.86	1.48	1.53
20	B	837	CLA	C4C-C3C	-2.86	1.40	1.45
20	4	308	CLA	MG-NA	-2.86	1.99	2.06
20	A	802	CLA	C4C-C3C	-2.86	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	312	CLA	C3D-C4D	-2.86	1.37	1.44
20	A	824	CLA	C4C-C3C	-2.85	1.40	1.45
20	A	803	CLA	C1C-C2C	-2.85	1.38	1.44
20	K	103	CLA	C1C-C2C	-2.85	1.38	1.44
20	2	309	CLA	CHA-C1A	2.85	1.49	1.41
20	A	814	CLA	C1B-C2B	-2.85	1.36	1.43
20	A	829	CLA	C4B-NB	-2.84	1.34	1.37
21	H	102	LMU	O5'-C1'	2.84	1.49	1.41
20	4	318	CLA	C1C-C2C	-2.84	1.38	1.44
20	B	820	CLA	O2D-CGD	2.84	1.40	1.33
20	4	304	CLA	C1D-ND	-2.83	1.34	1.37
20	3	307	CLA	CHA-C1A	2.83	1.49	1.41
20	2	309	CLA	CHB-C1B	2.83	1.47	1.39
20	B	839	CLA	C1B-NB	-2.83	1.34	1.37
20	J	102	CLA	C1C-C2C	-2.82	1.38	1.44
20	A	818	CLA	C1B-NB	-2.82	1.34	1.37
20	L	204	CLA	C4D-CHA	-2.82	1.28	1.38
20	A	815	CLA	C4C-C3C	-2.82	1.40	1.45
20	2	301	CLA	C1C-C2C	-2.82	1.38	1.44
20	A	811	CLA	C1C-C2C	-2.82	1.38	1.44
20	3	315	CLA	C1C-C2C	-2.81	1.38	1.44
20	B	805	CLA	C1B-NB	-2.81	1.34	1.37
20	J	103	CLA	CHB-C1B	2.81	1.45	1.39
20	A	837	CLA	C1C-C2C	-2.81	1.38	1.44
20	A	832	CLA	C1C-C2C	-2.81	1.38	1.44
20	A	855	CLA	C1C-C2C	-2.81	1.38	1.44
20	B	808	CLA	C4C-C3C	-2.81	1.40	1.45
20	B	838	CLA	C1B-NB	-2.81	1.34	1.37
20	A	836	CLA	C1C-C2C	-2.81	1.38	1.44
20	3	304	CLA	C2C-C1C	-2.81	1.36	1.43
20	B	817	CLA	C1B-NB	-2.81	1.34	1.37
20	B	822	CLA	C1C-C2C	-2.81	1.38	1.44
20	A	833	CLA	C1C-C2C	-2.80	1.38	1.44
20	1	213	CLA	CHA-C1A	2.80	1.49	1.41
20	3	317	CLA	CHA-C1A	2.80	1.49	1.41
20	A	824	CLA	C4B-NB	-2.80	1.34	1.37
20	A	831	CLA	C1C-C2C	-2.80	1.38	1.44
20	4	308	CLA	CHA-C1A	2.80	1.49	1.41
20	3	301	CLA	C1D-ND	-2.79	1.34	1.37
20	A	834	CLA	C1C-C2C	-2.79	1.38	1.44
20	A	835	CLA	C1C-C2C	-2.79	1.38	1.44
20	A	807	CLA	C4B-NB	-2.79	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	315	CLA	MG-NA	-2.79	1.99	2.06
20	B	830	CLA	C1C-NC	-2.79	1.33	1.37
20	A	822	CLA	C1C-C2C	-2.79	1.38	1.44
20	3	315	CLA	OBD-CAD	2.79	1.27	1.22
20	4	304	CLA	C1C-NC	-2.79	1.33	1.37
21	B	802	LMU	C4B-C5B	-2.79	1.47	1.53
20	A	823	CLA	C1C-C2C	-2.79	1.38	1.44
20	B	814	CLA	C1C-C2C	-2.78	1.38	1.44
20	3	304	CLA	C3D-C4D	-2.78	1.37	1.44
21	R	109	LMU	O1'-C1'	2.78	1.44	1.40
20	4	305	CLA	C1C-C2C	-2.78	1.38	1.44
20	1	214	CLA	MG-NA	-2.78	1.99	2.06
20	A	838	CLA	CHB-C1B	2.78	1.45	1.39
21	G	101	LMU	O5B-C5B	-2.78	1.37	1.44
20	H	101	CLA	C1C-C2C	-2.77	1.38	1.44
20	3	313	CLA	CHA-C1A	2.77	1.49	1.41
20	2	321	CLA	C1D-C2D	-2.77	1.39	1.45
21	2	313	LMU	O1'-C1'	2.77	1.44	1.40
20	B	809	CLA	C4C-C3C	-2.77	1.40	1.45
20	K	106	CLA	C1D-C2D	-2.77	1.39	1.45
20	B	826	CLA	MG-NA	-2.77	1.99	2.06
20	3	310	CLA	C1C-C2C	-2.76	1.38	1.44
20	L	202	CLA	C4C-C3C	-2.76	1.40	1.45
20	2	305	CLA	CHB-C1B	2.76	1.47	1.39
20	A	826	CLA	C1B-NB	-2.76	1.34	1.37
20	K	105	CLA	C1C-C2C	-2.76	1.38	1.44
20	2	306	CLA	C1B-NB	-2.76	1.34	1.37
20	A	848	CLA	C4B-NB	-2.76	1.34	1.37
20	1	212	CLA	C4B-NB	-2.76	1.34	1.37
20	B	819	CLA	C1C-C2C	-2.76	1.38	1.44
20	B	831	CLA	C1B-NB	-2.76	1.34	1.37
20	B	820	CLA	CHB-C4A	-2.75	1.30	1.37
20	A	819	CLA	C1C-C2C	-2.75	1.38	1.44
20	L	204	CLA	C3D-CAD	-2.75	1.36	1.45
20	2	312	CLA	C1C-C2C	-2.75	1.38	1.44
20	B	826	CLA	C1C-C2C	-2.75	1.38	1.44
20	3	319	CLA	C4C-C3C	-2.75	1.38	1.44
21	F	201	LMU	C3'-C4'	-2.75	1.44	1.52
20	A	804	CLA	C4C-C3C	-2.75	1.40	1.45
20	4	313	CLA	C3A-C2A	-2.74	1.52	1.54
20	A	817	CLA	C1C-C2C	-2.74	1.39	1.44
20	3	309	CLA	OBD-CAD	2.74	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	824	CLA	C1C-C2C	-2.74	1.39	1.44
20	J	103	CLA	C1B-C2B	-2.74	1.36	1.43
20	A	810	CLA	C1C-C2C	-2.73	1.39	1.44
22	I	103	BCR	C38-C26	-2.73	1.46	1.50
20	B	815	CLA	OBD-CAD	2.73	1.27	1.22
20	2	309	CLA	MG-NA	-2.73	1.99	2.06
20	B	825	CLA	C1D-C2D	-2.73	1.39	1.45
20	1	211	CLA	C3B-C4B	-2.72	1.35	1.42
20	3	308	CLA	C2C-C1C	-2.72	1.36	1.43
20	A	808	CLA	C4C-C3C	-2.72	1.40	1.45
20	2	308	CLA	CHB-C1B	2.72	1.47	1.39
20	1	209	CLA	CHB-C4A	-2.71	1.30	1.37
20	1	211	CLA	C3D-C2D	-2.71	1.31	1.39
20	B	820	CLA	MG-ND	-2.71	2.00	2.05
20	B	820	CLA	CHB-C1B	2.71	1.45	1.39
20	F	205	CLA	C1C-C2C	-2.71	1.39	1.44
20	1	215	CLA	C3D-C4D	-2.70	1.37	1.44
20	A	815	CLA	C1B-NB	-2.70	1.34	1.37
20	2	307	CLA	C1B-NB	-2.70	1.34	1.37
20	F	204	CLA	C1C-C2C	-2.70	1.39	1.44
20	3	319	CLA	C1B-NB	-2.70	1.34	1.37
21	R	105	LMU	O1'-C1'	2.69	1.44	1.40
21	4	316	LMU	O1'-C1'	2.69	1.44	1.40
22	B	850	BCR	C2-C1	-2.69	1.47	1.54
22	F	203	BCR	C32-C1	-2.69	1.48	1.53
20	F	206	CLA	C1C-NC	-2.68	1.33	1.37
20	2	305	CLA	CHD-C4C	2.68	1.49	1.40
20	1	214	CLA	CHB-C4A	-2.68	1.31	1.37
20	B	827	CLA	C1B-C2B	-2.68	1.36	1.43
20	A	847	CLA	C1D-ND	-2.68	1.34	1.37
20	1	203	CLA	C1B-NB	-2.68	1.34	1.37
20	4	317	CLA	C3D-C4D	-2.68	1.37	1.44
20	1	204	CLA	C1C-C2C	-2.67	1.39	1.44
20	4	304	CLA	MG-NB	-2.67	2.00	2.05
20	B	817	CLA	C4C-C3C	-2.67	1.40	1.45
20	4	303	CLA	C1B-C2B	-2.66	1.36	1.43
20	B	805	CLA	OBD-CAD	2.66	1.27	1.22
20	1	201	CLA	C3B-C4B	-2.66	1.35	1.42
20	2	317	CLA	CHB-C1B	2.66	1.45	1.39
20	B	824	CLA	C1B-NB	-2.66	1.34	1.37
20	4	309	CLA	MG-NA	-2.66	2.00	2.06
22	L	209	BCR	C1-C6	-2.65	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	202	CLA	C1B-C2B	-2.65	1.36	1.43
20	3	309	CLA	C1D-C2D	-2.65	1.40	1.45
20	2	315	CLA	CHA-C1A	2.65	1.48	1.41
20	2	306	CLA	C4C-C3C	-2.65	1.40	1.45
20	B	803	CLA	C4C-C3C	-2.65	1.40	1.45
22	B	850	BCR	C37-C22	-2.65	1.45	1.50
20	3	319	CLA	C1C-C2C	-2.65	1.39	1.44
20	3	317	CLA	MG-NA	-2.65	2.00	2.06
20	2	303	CLA	C3D-C4D	-2.64	1.37	1.44
20	B	837	CLA	C1C-C2C	-2.64	1.39	1.44
20	B	827	CLA	CHB-C1B	2.64	1.45	1.39
20	B	848	CLA	C4C-C3C	-2.64	1.40	1.45
20	B	806	CLA	C4C-C3C	-2.64	1.40	1.45
20	B	816	CLA	C1B-NB	-2.64	1.34	1.37
20	2	305	CLA	C2C-C1C	-2.63	1.36	1.43
20	B	833	CLA	C1B-NB	-2.63	1.34	1.37
20	1	201	CLA	CHB-C1B	2.63	1.45	1.39
21	L	210	LMU	O1'-C1'	2.63	1.44	1.40
20	B	833	CLA	C4C-C3C	-2.63	1.40	1.45
20	B	837	CLA	C1B-NB	-2.63	1.34	1.37
20	F	206	CLA	C1C-C2C	-2.63	1.39	1.44
20	B	803	CLA	CHB-C1B	2.62	1.45	1.39
21	C	101	LMU	O1'-C1'	2.62	1.44	1.40
20	3	309	CLA	MG-NA	-2.62	2.00	2.06
20	2	305	CLA	C3C-C4C	-2.62	1.36	1.43
20	1	201	CLA	C3D-CAD	-2.62	1.36	1.45
20	1	201	CLA	CHC-C4B	2.62	1.45	1.39
20	3	313	CLA	MG-NA	-2.62	2.00	2.06
20	L	208	CLA	C4B-NB	-2.62	1.34	1.37
20	B	820	CLA	CAC-C3C	-2.61	1.44	1.51
20	A	857	CLA	C3D-C4D	-2.61	1.37	1.44
20	3	309	CLA	C1B-C2B	-2.61	1.37	1.43
20	B	849	CLA	MG-NA	-2.60	2.00	2.06
20	2	302	CLA	C1C-C2C	-2.60	1.39	1.44
20	A	849	CLA	C1C-NC	-2.59	1.33	1.37
20	4	307	CLA	C1D-C2D	-2.59	1.40	1.45
20	2	307	CLA	C1C-C2C	-2.59	1.39	1.44
20	1	205	CLA	C3A-C2A	-2.59	1.52	1.54
20	B	827	CLA	C1D-ND	-2.59	1.34	1.37
20	L	208	CLA	C1B-C2B	-2.58	1.37	1.43
20	K	106	CLA	OBD-CAD	2.58	1.26	1.22
20	A	808	CLA	C1C-C2C	-2.58	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	209	CLA	MG-NB	-2.58	2.00	2.05
20	L	204	CLA	C1C-C2C	-2.58	1.39	1.44
20	A	805	CLA	C4C-C3C	-2.58	1.40	1.45
20	2	310	CLA	C1C-C2C	-2.57	1.39	1.44
20	1	212	CLA	C1D-ND	-2.57	1.34	1.37
20	3	301	CLA	C1B-C2B	-2.57	1.37	1.43
20	B	812	CLA	C4C-C3C	-2.56	1.40	1.45
21	H	104	LMU	O5'-C5'	-2.56	1.38	1.44
20	R	106	CLA	C4C-C3C	-2.56	1.40	1.45
20	2	303	CLA	CHB-C1B	2.55	1.46	1.39
20	1	209	CLA	C4B-C3B	-2.55	1.37	1.43
20	A	828	CLA	MG-NA	-2.55	2.00	2.06
20	B	808	CLA	C1C-C2C	-2.55	1.39	1.44
20	2	314	CLA	CHB-C1B	2.55	1.46	1.39
20	2	317	CLA	C4B-NB	-2.55	1.34	1.37
20	4	318	CLA	C1B-NB	-2.55	1.34	1.37
20	B	836	CLA	C1C-C2C	-2.54	1.39	1.44
20	A	816	CLA	C1B-NB	-2.54	1.34	1.37
20	A	848	CLA	MG-NA	-2.54	2.00	2.06
20	4	311	CLA	C3D-C4D	-2.54	1.37	1.44
20	3	304	CLA	C3C-C4C	-2.54	1.37	1.43
20	A	826	CLA	C4C-C3C	-2.54	1.40	1.45
20	3	314	CLA	C1B-NB	-2.54	1.34	1.37
20	1	205	CLA	C1B-NB	-2.54	1.34	1.37
20	4	305	CLA	C1B-NB	-2.53	1.34	1.37
20	A	817	CLA	C4B-NB	-2.53	1.34	1.37
20	3	304	CLA	CHC-C4B	2.53	1.46	1.39
20	A	848	CLA	C1B-C2B	-2.53	1.37	1.43
22	B	842	BCR	C20-C19	-2.53	1.28	1.34
20	A	811	CLA	C4C-C3C	-2.52	1.40	1.45
20	B	804	CLA	MG-NA	-2.52	2.00	2.06
20	A	803	CLA	OBD-CAD	2.52	1.26	1.22
20	1	203	CLA	C4C-C3C	-2.52	1.40	1.45
20	H	110	CLA	C1B-NB	-2.52	1.34	1.37
20	A	821	CLA	C1B-NB	-2.52	1.34	1.37
20	1	211	CLA	MG-NA	-2.52	2.00	2.06
20	B	827	CLA	C1C-C2C	-2.52	1.39	1.44
20	3	315	CLA	C4B-NB	-2.52	1.34	1.37
20	1	214	CLA	C3A-C2A	-2.51	1.47	1.54
20	1	204	CLA	C4C-C3C	-2.51	1.40	1.45
20	3	308	CLA	CHB-C1B	2.51	1.46	1.39
20	A	801	CLA	C1C-C2C	-2.51	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	850	BCR	C5-C6	-2.51	1.30	1.34
20	3	301	CLA	C4B-NB	-2.50	1.34	1.37
20	4	307	CLA	MG-NB	-2.50	2.00	2.05
20	B	830	CLA	MG-NA	-2.50	2.00	2.06
20	1	210	CLA	C4C-C3C	-2.50	1.39	1.44
20	1	204	CLA	MG-NA	-2.50	2.00	2.06
20	K	106	CLA	C4B-NB	-2.50	1.34	1.37
22	B	850	BCR	C36-C18	-2.50	1.45	1.50
20	B	825	CLA	C1D-ND	-2.50	1.34	1.37
20	3	303	CLA	C4C-C3C	-2.50	1.39	1.44
20	F	206	CLA	C3B-C2B	-2.49	1.32	1.41
21	4	322	LMU	O1'-C1'	2.49	1.44	1.40
21	G	101	LMU	C4B-C3B	2.49	1.58	1.52
20	B	837	CLA	MG-NA	-2.49	2.00	2.06
20	K	105	CLA	MG-NA	-2.49	2.00	2.06
20	L	201	CLA	C4C-C3C	-2.49	1.40	1.45
20	1	206	CLA	C1B-NB	-2.49	1.34	1.37
20	B	820	CLA	C2A-C1A	-2.49	1.46	1.52
20	A	847	CLA	C1B-C2B	-2.48	1.37	1.43
20	A	838	CLA	C1C-C2C	-2.48	1.39	1.44
20	B	820	CLA	C3C-C2C	-2.48	1.31	1.36
20	H	101	CLA	C4C-C3C	-2.48	1.40	1.45
20	4	315	CLA	MG-ND	-2.48	2.00	2.05
20	2	321	CLA	C3A-C2A	-2.48	1.47	1.54
20	J	103	CLA	C1D-ND	-2.47	1.34	1.37
21	E	101	LMU	C4'-C5'	-2.47	1.46	1.52
20	4	311	CLA	CHA-C1A	2.47	1.48	1.41
20	4	307	CLA	C4D-CHA	-2.47	1.30	1.38
20	B	820	CLA	C3D-CAD	-2.46	1.37	1.45
20	1	211	CLA	CBD-CGD	-2.46	1.45	1.52
20	3	310	CLA	MG-NA	-2.46	2.00	2.06
20	4	302	CLA	MG-NA	-2.46	2.00	2.06
20	B	803	CLA	MG-NA	-2.46	2.00	2.06
22	I	101	BCR	C40-C30	-2.46	1.49	1.53
20	K	103	CLA	MG-NA	-2.46	2.00	2.06
20	B	830	CLA	C1D-C2D	-2.45	1.40	1.45
20	3	315	CLA	C1D-ND	-2.45	1.34	1.37
20	A	835	CLA	MG-NA	-2.45	2.00	2.06
20	A	816	CLA	C1C-C2C	-2.45	1.39	1.44
20	A	850	CLA	C2A-C1A	-2.45	1.46	1.52
20	3	315	CLA	C1B-C2B	-2.44	1.37	1.43
20	A	813	CLA	C4C-C3C	-2.44	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	815	CLA	C1C-C2C	-2.44	1.39	1.44
20	B	821	CLA	C1B-C2B	-2.44	1.37	1.43
22	B	850	BCR	C10-C9	-2.44	1.30	1.35
20	4	309	CLA	C3D-C2D	2.44	1.40	1.35
20	B	816	CLA	C1D-C2D	-2.44	1.40	1.45
20	K	106	CLA	CHB-C4A	-2.44	1.31	1.37
21	B	802	LMU	O1'-C1'	2.44	1.44	1.40
20	4	317	CLA	CHA-C1A	2.44	1.48	1.41
20	4	309	CLA	CHA-C1A	2.43	1.48	1.41
20	B	822	CLA	MG-NA	-2.43	2.00	2.06
20	B	831	CLA	C1D-C2D	-2.43	1.40	1.45
20	L	204	CLA	C1D-C2D	-2.43	1.40	1.45
20	A	827	CLA	C1C-C2C	-2.43	1.39	1.44
20	2	301	CLA	MG-NA	-2.43	2.00	2.06
20	A	820	CLA	C1B-C2B	-2.42	1.37	1.43
20	4	319	CLA	MG-NA	-2.42	2.00	2.06
20	1	201	CLA	C1C-NC	-2.42	1.34	1.37
22	L	209	BCR	C40-C30	-2.42	1.49	1.53
20	4	303	CLA	C4C-C3C	-2.42	1.39	1.44
20	1	211	CLA	C3B-C2B	-2.42	1.33	1.41
20	B	803	CLA	C1B-C2B	-2.42	1.37	1.43
20	A	819	CLA	C1B-NB	-2.42	1.34	1.37
20	K	106	CLA	CHB-C1B	2.42	1.44	1.39
20	A	805	CLA	C1B-NB	-2.42	1.34	1.37
20	A	813	CLA	C1B-NB	-2.42	1.34	1.37
20	A	822	CLA	MG-NA	-2.42	2.00	2.06
20	A	833	CLA	MG-NA	-2.42	2.00	2.06
20	B	847	CLA	C1C-C2C	-2.41	1.39	1.44
20	A	834	CLA	MG-NA	-2.41	2.00	2.06
20	A	825	CLA	C4C-C3C	-2.41	1.40	1.45
20	J	102	CLA	MG-NA	-2.41	2.00	2.06
21	1	218	LMU	C4B-C5B	2.41	1.58	1.53
20	3	313	CLA	C3D-C4D	-2.41	1.38	1.44
21	A	852	LMU	O5'-C5'	-2.41	1.38	1.44
20	F	206	CLA	MG-ND	-2.41	2.01	2.05
20	A	820	CLA	C4C-C3C	-2.41	1.40	1.45
20	A	821	CLA	C1B-C2B	-2.41	1.37	1.43
20	2	314	CLA	CHA-C1A	2.41	1.48	1.41
21	L	210	LMU	O5B-C1B	2.40	1.48	1.41
20	3	306	CLA	C3D-C2D	2.40	1.40	1.35
20	A	836	CLA	MG-NA	-2.40	2.00	2.06
20	I	102	CLA	OBD-CAD	2.40	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	848	CLA	C1C-C2C	-2.40	1.39	1.44
20	A	814	CLA	C1D-ND	-2.40	1.34	1.37
20	L	203	CLA	C1B-NB	-2.40	1.34	1.37
20	4	304	CLA	C3A-C2A	-2.40	1.48	1.54
20	A	804	CLA	MG-NA	-2.40	2.00	2.06
22	I	101	BCR	C29-C30	-2.40	1.48	1.54
20	A	831	CLA	MG-NA	-2.40	2.00	2.06
20	A	855	CLA	MG-NA	-2.40	2.00	2.06
20	A	815	CLA	C1C-C2C	-2.39	1.39	1.44
20	A	832	CLA	MG-NA	-2.39	2.00	2.06
20	F	205	CLA	MG-NA	-2.39	2.00	2.06
20	R	107	CLA	C4C-C3C	-2.39	1.41	1.45
20	K	106	CLA	C1C-NC	-2.39	1.34	1.37
20	2	321	CLA	MG-NA	-2.39	2.00	2.06
20	4	315	CLA	C3D-CAD	-2.39	1.37	1.45
20	B	823	CLA	MG-NA	-2.38	2.00	2.06
20	A	823	CLA	MG-NA	-2.38	2.00	2.06
20	A	812	CLA	C1C-C2C	-2.38	1.39	1.44
20	H	109	CLA	C1B-NB	-2.38	1.34	1.37
20	A	837	CLA	MG-NA	-2.38	2.00	2.06
20	B	818	CLA	C1B-C2B	-2.38	1.37	1.43
20	2	310	CLA	C1B-NB	-2.38	1.34	1.37
20	3	312	CLA	C3D-C2D	2.37	1.40	1.35
22	B	850	BCR	C32-C1	-2.37	1.49	1.53
20	A	838	CLA	CHB-C4A	-2.37	1.31	1.37
22	I	101	BCR	C32-C1	-2.37	1.49	1.53
20	F	206	CLA	CAA-C2A	-2.37	1.49	1.54
20	B	811	CLA	C4C-C3C	-2.37	1.41	1.45
20	L	207	CLA	C1B-NB	-2.37	1.34	1.37
20	A	814	CLA	CHB-C4A	-2.36	1.31	1.37
22	B	842	BCR	C12-C13	2.36	1.51	1.46
20	A	830	CLA	MG-NA	-2.36	2.00	2.06
22	L	209	BCR	C17-C18	-2.36	1.30	1.35
20	2	314	CLA	C2C-C1C	-2.36	1.37	1.43
21	H	104	LMU	C1B-C2B	-2.36	1.45	1.52
20	4	307	CLA	C3D-CAD	-2.36	1.37	1.45
20	B	816	CLA	C1D-ND	-2.36	1.34	1.37
20	L	201	CLA	C1B-NB	-2.36	1.34	1.37
20	A	808	CLA	C1B-NB	-2.35	1.34	1.37
20	3	305	CLA	C3D-C2D	2.35	1.40	1.35
20	A	848	CLA	CHB-C4A	-2.35	1.31	1.37
20	B	829	CLA	C1B-C2B	-2.35	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	810	CLA	MG-NA	-2.35	2.00	2.06
20	2	317	CLA	C4C-C3C	-2.35	1.41	1.45
20	2	304	CLA	C1B-NB	-2.35	1.34	1.37
20	4	313	CLA	C1C-C2C	-2.34	1.39	1.44
21	A	853	LMU	C4B-C5B	-2.34	1.48	1.53
20	A	806	CLA	C1D-ND	-2.34	1.34	1.37
20	3	307	CLA	C3D-C4D	-2.34	1.38	1.44
20	3	307	CLA	CHB-C1B	2.34	1.46	1.39
20	A	850	CLA	C1B-NB	-2.34	1.34	1.37
20	1	205	CLA	C4C-C3C	-2.34	1.39	1.44
20	3	316	CLA	CHA-C1A	2.34	1.48	1.41
20	J	103	CLA	CHB-C4A	-2.34	1.31	1.37
20	4	307	CLA	CAC-C3C	-2.34	1.45	1.51
20	B	820	CLA	C3B-C2B	-2.33	1.33	1.41
21	H	103	LMU	C4B-C5B	-2.33	1.48	1.53
20	A	857	CLA	CHA-C1A	2.33	1.47	1.41
22	B	850	BCR	C4-C5	-2.33	1.46	1.51
20	B	821	CLA	C1C-C2C	-2.33	1.39	1.44
20	B	829	CLA	C1C-C2C	-2.33	1.39	1.44
20	B	834	CLA	C4C-C3C	-2.33	1.41	1.45
20	A	816	CLA	C1B-C2B	-2.33	1.37	1.43
20	A	825	CLA	C4B-NB	-2.32	1.34	1.37
21	B	802	LMU	O5B-C5B	-2.32	1.38	1.44
20	3	309	CLA	MG-ND	-2.32	2.01	2.05
20	1	207	CLA	C3A-C2A	-2.32	1.48	1.54
20	3	304	CLA	C1C-NC	-2.32	1.33	1.38
20	2	302	CLA	C4C-C3C	-2.31	1.41	1.45
20	A	813	CLA	C1C-C2C	-2.31	1.39	1.44
20	3	309	CLA	C3D-CAD	-2.31	1.37	1.45
20	B	826	CLA	C3D-CAD	-2.31	1.37	1.45
20	B	831	CLA	C1D-ND	-2.31	1.34	1.37
20	2	310	CLA	C4B-NB	-2.31	1.34	1.37
20	2	302	CLA	MG-NA	-2.30	2.00	2.06
21	L	206	LMU	C4B-C5B	-2.30	1.48	1.53
20	4	304	CLA	CHB-C1B	2.30	1.44	1.39
20	L	208	CLA	CBD-CGD	-2.30	1.45	1.52
22	I	101	BCR	C16-C17	2.29	1.50	1.43
20	A	819	CLA	C4C-C3C	-2.29	1.41	1.45
20	I	102	CLA	C1B-NB	-2.29	1.34	1.37
20	J	103	CLA	C1C-NC	-2.29	1.34	1.37
22	I	101	BCR	C34-C9	-2.29	1.46	1.50
22	B	850	BCR	C34-C9	-2.29	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	810	CLA	C1C-C2C	-2.29	1.39	1.44
20	B	809	CLA	C1D-ND	-2.28	1.34	1.37
20	B	831	CLA	C1C-C2C	-2.28	1.39	1.44
20	L	201	CLA	C1B-C2B	-2.28	1.37	1.43
20	A	811	CLA	C1B-C2B	-2.27	1.37	1.43
22	G	102	BCR	C30-C25	-2.27	1.50	1.53
20	B	809	CLA	C1C-C2C	-2.27	1.39	1.44
20	F	204	CLA	C4C-C3C	-2.27	1.39	1.44
20	3	309	CLA	C3B-C4B	-2.27	1.36	1.42
20	3	320	CLA	C4C-C3C	-2.27	1.41	1.45
20	H	110	CLA	C4C-C3C	-2.27	1.41	1.45
20	1	201	CLA	C1B-C2B	-2.26	1.37	1.43
20	A	806	CLA	C1B-C2B	-2.26	1.37	1.43
20	B	830	CLA	C1D-ND	-2.26	1.34	1.37
20	B	805	CLA	C1C-NC	-2.26	1.34	1.37
20	A	830	CLA	C4B-NB	-2.26	1.34	1.37
20	2	303	CLA	CHA-C1A	2.26	1.47	1.41
20	A	827	CLA	C1B-NB	-2.25	1.34	1.37
20	1	205	CLA	C1B-C2B	-2.25	1.37	1.43
22	B	842	BCR	C19-C18	2.25	1.50	1.46
20	K	106	CLA	O2A-C1	-2.25	1.40	1.46
20	A	806	CLA	C1B-NB	-2.25	1.34	1.37
20	2	305	CLA	C4C-NC	-2.25	1.33	1.37
22	I	101	BCR	C37-C22	-2.25	1.46	1.50
20	1	212	CLA	C1D-C2D	-2.25	1.40	1.45
22	B	850	BCR	C16-C15	-2.25	1.30	1.36
20	1	209	CLA	C3D-CAD	-2.25	1.37	1.45
20	H	108	CLA	C1B-NB	-2.24	1.34	1.37
20	B	838	CLA	C1D-ND	-2.24	1.34	1.37
20	B	849	CLA	C1B-NB	-2.24	1.34	1.37
22	I	101	BCR	C30-C25	-2.24	1.50	1.53
20	3	312	CLA	C3D-C4D	-2.24	1.38	1.44
22	B	841	BCR	C1-C6	-2.24	1.50	1.53
20	J	103	CLA	C3D-CAD	-2.24	1.37	1.45
22	F	203	BCR	C37-C22	-2.24	1.46	1.50
20	B	814	CLA	C4C-C3C	-2.24	1.41	1.45
20	3	316	CLA	CHB-C1B	2.23	1.45	1.39
20	L	208	CLA	C3A-C2A	-2.23	1.48	1.54
20	B	803	CLA	CHB-C4A	-2.23	1.32	1.37
20	1	202	CLA	C4B-NB	-2.23	1.34	1.37
20	A	849	CLA	C4B-NB	-2.23	1.34	1.37
20	B	821	CLA	C2-C3	2.23	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	208	CLA	C3D-C2D	2.23	1.40	1.35
20	3	314	CLA	C1C-C2C	-2.23	1.40	1.44
20	A	811	CLA	C1B-NB	-2.23	1.34	1.37
20	2	309	CLA	C3D-C4D	-2.23	1.38	1.44
20	A	829	CLA	C3A-C2A	-2.23	1.48	1.54
20	2	308	CLA	C3D-C4D	-2.23	1.38	1.44
20	4	310	CLA	C1D-ND	-2.22	1.34	1.37
21	L	205	LMU	O1'-C1'	2.22	1.43	1.40
20	A	802	CLA	C1B-NB	-2.22	1.34	1.37
20	2	314	CLA	C3C-C4C	-2.22	1.37	1.43
20	B	834	CLA	C4B-NB	-2.22	1.34	1.37
21	A	854	LMU	O1'-C1'	2.22	1.43	1.40
20	F	206	CLA	C3B-C4B	-2.22	1.36	1.42
20	A	825	CLA	C1C-C2C	-2.21	1.40	1.44
20	B	823	CLA	C1B-C2B	-2.21	1.37	1.43
22	L	209	BCR	C26-C25	-2.21	1.30	1.34
20	1	211	CLA	OBD-CAD	2.21	1.26	1.22
20	A	821	CLA	C4B-NB	-2.21	1.35	1.37
20	1	201	CLA	MG-NB	-2.21	2.01	2.05
20	B	821	CLA	CHB-C4A	-2.21	1.32	1.37
20	4	303	CLA	C1C-C2C	-2.21	1.40	1.44
22	F	203	BCR	C26-C25	-2.21	1.30	1.34
20	B	839	CLA	C1C-C2C	-2.21	1.40	1.44
22	J	101	BCR	C1-C6	-2.21	1.51	1.53
20	B	847	CLA	MG-NA	-2.20	2.01	2.06
20	3	301	CLA	C3D-CAD	-2.20	1.37	1.45
20	A	802	CLA	C1C-C2C	-2.20	1.40	1.44
20	2	306	CLA	C1C-C2C	-2.20	1.40	1.44
20	I	102	CLA	C1B-C2B	-2.20	1.38	1.43
20	A	822	CLA	C1B-C2B	-2.20	1.38	1.43
20	4	304	CLA	O2A-C1	-2.20	1.40	1.46
20	A	817	CLA	C1B-C2B	-2.20	1.38	1.43
20	1	212	CLA	MG-ND	-2.19	2.01	2.05
20	4	314	CLA	C3D-C4D	-2.19	1.38	1.44
20	3	307	CLA	C3D-C2D	2.19	1.40	1.35
20	B	815	CLA	C1D-C2D	-2.19	1.41	1.45
20	1	206	CLA	C1C-C2C	-2.19	1.40	1.44
20	L	202	CLA	C1D-C2D	-2.18	1.41	1.45
22	A	840	BCR	C1-C6	-2.18	1.51	1.53
23	A	839	PQN	O1-C1	2.18	1.27	1.23
21	L	210	LMU	C4B-C5B	2.18	1.57	1.53
20	2	321	CLA	C1C-NC	-2.18	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	304	CLA	CBD-CGD	-2.18	1.45	1.52
20	A	850	CLA	C3A-C2A	-2.18	1.48	1.54
20	B	809	CLA	C1-C2	2.18	1.55	1.49
20	2	301	CLA	C1B-C2B	-2.18	1.38	1.43
20	1	211	CLA	CBA-CGA	2.18	1.57	1.50
20	B	819	CLA	MG-NA	-2.18	2.01	2.06
20	B	830	CLA	C4B-NB	-2.18	1.35	1.37
20	3	303	CLA	C1C-C2C	-2.18	1.40	1.44
22	B	843	BCR	C1-C6	-2.18	1.51	1.53
22	A	842	BCR	C1-C6	-2.18	1.51	1.53
20	A	816	CLA	C4B-NB	-2.17	1.35	1.37
20	4	314	CLA	C3D-C2D	2.17	1.40	1.35
20	A	838	CLA	C4B-NB	-2.17	1.35	1.37
20	K	105	CLA	C1B-C2B	-2.17	1.38	1.43
20	1	213	CLA	C3D-C2D	2.17	1.40	1.35
20	4	304	CLA	CBD-CHA	-2.17	1.39	1.51
20	A	810	CLA	C1B-NB	-2.17	1.35	1.37
20	A	818	CLA	C1C-C2C	-2.16	1.40	1.44
20	B	831	CLA	C4B-NB	-2.16	1.35	1.37
22	B	841	BCR	C30-C25	-2.16	1.51	1.53
20	4	308	CLA	C3D-C2D	2.16	1.40	1.35
20	B	824	CLA	MG-NA	-2.16	2.01	2.06
20	A	855	CLA	C1B-C2B	-2.15	1.38	1.43
20	H	101	CLA	MG-NA	-2.15	2.01	2.06
20	2	305	CLA	CHA-C1A	2.15	1.47	1.41
22	F	202	BCR	C30-C25	-2.15	1.51	1.53
21	R	104	LMU	O5B-C1B	2.15	1.47	1.41
21	E	101	LMU	C4B-C3B	-2.15	1.46	1.52
20	A	848	CLA	CBD-CGD	-2.15	1.46	1.52
20	B	822	CLA	C1B-C2B	-2.15	1.38	1.43
20	3	316	CLA	C2C-C1C	-2.15	1.38	1.43
20	2	321	CLA	C3A-C4A	-2.14	1.44	1.51
20	B	829	CLA	C1A-CHA	2.14	1.51	1.43
20	B	820	CLA	C3B-C4B	-2.14	1.36	1.42
20	4	307	CLA	C3C-C2C	-2.14	1.32	1.36
20	A	826	CLA	C1B-C2B	-2.14	1.38	1.43
20	A	831	CLA	C1B-C2B	-2.14	1.38	1.43
20	1	214	CLA	C3B-C4B	-2.14	1.36	1.42
20	A	836	CLA	C1B-C2B	-2.14	1.38	1.43
20	B	836	CLA	C1D-C2D	-2.14	1.41	1.45
20	A	826	CLA	C1D-C2D	-2.14	1.41	1.45
20	A	823	CLA	C1B-C2B	-2.14	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	1	214	CLA	MG-NC	-2.13	2.01	2.06
20	A	835	CLA	C1B-C2B	-2.13	1.38	1.43
20	B	827	CLA	C1D-C2D	-2.13	1.41	1.45
22	A	843	BCR	C1-C6	-2.13	1.51	1.53
20	1	212	CLA	C1B-C2B	-2.13	1.38	1.43
20	4	303	CLA	C1D-ND	-2.13	1.35	1.37
20	I	102	CLA	C4B-NB	-2.13	1.35	1.37
20	A	803	CLA	C1A-CHA	2.13	1.51	1.43
20	J	102	CLA	C1B-C2B	-2.13	1.38	1.43
20	3	304	CLA	CHB-C1B	2.13	1.45	1.39
20	A	833	CLA	C1B-C2B	-2.13	1.38	1.43
20	4	302	CLA	C1B-C2B	-2.13	1.38	1.43
20	B	803	CLA	C4B-NB	-2.13	1.35	1.37
21	L	205	LMU	C4B-C5B	-2.13	1.48	1.53
20	2	311	CLA	C3D-CAD	-2.13	1.38	1.45
20	H	107	CLA	C1C-C2C	-2.13	1.40	1.44
22	B	844	BCR	C1-C6	-2.13	1.51	1.53
20	1	206	CLA	MG-NA	-2.13	2.01	2.06
20	1	202	CLA	C1C-C2C	-2.13	1.40	1.44
20	F	205	CLA	C1B-C2B	-2.13	1.38	1.43
20	B	821	CLA	C4C-C3C	-2.13	1.41	1.45
20	2	317	CLA	CHB-C4A	-2.13	1.32	1.37
20	1	215	CLA	CHB-C1B	2.13	1.45	1.39
20	B	819	CLA	C4C-C3C	-2.13	1.41	1.45
20	G	103	CLA	MG-NA	-2.13	2.01	2.06
20	3	309	CLA	C4D-CHA	-2.12	1.31	1.38
20	3	315	CLA	C3D-CAD	-2.12	1.38	1.45
20	B	821	CLA	C1D-C2D	-2.12	1.41	1.45
20	B	820	CLA	O2D-CED	-2.12	1.40	1.45
20	B	832	CLA	C1C-C2C	-2.12	1.40	1.44
22	A	843	BCR	C30-C25	-2.12	1.51	1.53
20	4	304	CLA	C4D-CHA	-2.12	1.31	1.38
20	1	201	CLA	MG-ND	-2.12	2.01	2.05
20	1	207	CLA	CAA-C2A	-2.11	1.50	1.54
20	A	832	CLA	C1B-C2B	-2.11	1.38	1.43
20	2	315	CLA	C3D-C2D	2.11	1.40	1.35
22	I	101	BCR	C33-C5	-2.11	1.47	1.50
22	A	842	BCR	C30-C25	-2.11	1.51	1.53
20	A	834	CLA	C1B-C2B	-2.11	1.38	1.43
20	R	106	CLA	C1C-C2C	-2.11	1.40	1.44
20	1	206	CLA	C1D-ND	-2.11	1.35	1.37
20	A	801	CLA	C1B-NB	-2.11	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	314	CLA	C1C-NC	-2.11	1.33	1.38
20	B	818	CLA	C1B-NB	-2.11	1.35	1.37
20	1	201	CLA	C3D-C2D	-2.11	1.33	1.39
21	H	104	LMU	C3B-C2B	-2.10	1.46	1.52
20	B	836	CLA	C1D-ND	-2.10	1.35	1.37
20	F	204	CLA	CHB-C4A	-2.10	1.32	1.37
20	B	821	CLA	C1A-CHA	2.10	1.51	1.43
20	3	304	CLA	CHA-C1A	2.10	1.47	1.41
22	F	203	BCR	C14-C13	-2.10	1.30	1.35
21	1	218	LMU	O1'-C1'	2.10	1.43	1.40
20	4	304	CLA	C3B-C2B	-2.10	1.34	1.41
20	A	817	CLA	C4C-C3C	-2.10	1.41	1.45
20	F	206	CLA	MG-NB	-2.10	2.01	2.05
20	1	207	CLA	C1B-C2B	-2.10	1.38	1.43
20	2	312	CLA	C1D-C2D	-2.09	1.41	1.45
20	4	313	CLA	MG-NA	-2.09	2.01	2.06
20	1	210	CLA	C3A-C2A	-2.09	1.52	1.54
20	B	829	CLA	C4B-NB	-2.09	1.35	1.37
20	B	848	CLA	C1A-CHA	2.09	1.51	1.43
20	B	825	CLA	C1C-C2C	-2.09	1.40	1.44
20	A	828	CLA	C4B-NB	-2.09	1.35	1.37
22	G	102	BCR	C1-C6	-2.09	1.51	1.53
20	3	313	CLA	C3D-C2D	2.09	1.40	1.35
20	B	827	CLA	CHB-C4A	-2.09	1.32	1.37
20	A	837	CLA	C1B-C2B	-2.09	1.38	1.43
20	A	830	CLA	C1C-C2C	-2.09	1.40	1.44
20	1	211	CLA	C1D-C2D	-2.08	1.41	1.45
20	B	804	CLA	C1B-NB	-2.08	1.35	1.37
20	B	819	CLA	C4B-NB	-2.08	1.35	1.37
20	K	107	CLA	C1B-NB	-2.08	1.35	1.37
20	L	201	CLA	C4B-NB	-2.08	1.35	1.37
20	B	829	CLA	C3D-CAD	-2.08	1.38	1.45
20	A	801	CLA	C4B-NB	-2.08	1.35	1.37
20	3	310	CLA	C1B-C2B	-2.08	1.38	1.43
20	1	210	CLA	C1C-C2C	-2.08	1.40	1.44
20	2	321	CLA	MG-NB	-2.07	2.01	2.05
20	4	307	CLA	CHB-C1B	2.07	1.44	1.39
20	4	319	CLA	C1B-C2B	-2.07	1.38	1.43
22	I	103	BCR	C7-C6	2.07	1.52	1.45
20	2	321	CLA	CHB-C1B	2.07	1.44	1.39
20	1	209	CLA	C1D-C2D	-2.07	1.41	1.45
22	A	844	BCR	C1-C6	-2.07	1.51	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	838	CLA	C3B-C4B	-2.07	1.36	1.42
20	I	102	CLA	C1C-C2C	-2.07	1.40	1.44
20	B	817	CLA	C1C-C2C	-2.07	1.40	1.44
20	H	101	CLA	C3A-C2A	-2.07	1.48	1.54
21	L	206	LMU	O5'-C5'	-2.07	1.39	1.44
20	A	857	CLA	C2C-C1C	-2.06	1.38	1.43
20	A	814	CLA	C1C-NC	-2.06	1.34	1.37
20	B	849	CLA	C1C-NC	-2.06	1.34	1.37
20	B	814	CLA	C1B-C2B	-2.06	1.38	1.43
20	2	311	CLA	C1D-C2D	-2.06	1.41	1.45
20	A	802	CLA	C1-C2	2.06	1.55	1.49
20	A	857	CLA	C3C-C4C	-2.06	1.38	1.43
20	1	212	CLA	C1C-NC	-2.06	1.34	1.37
20	L	202	CLA	C1C-C2C	-2.06	1.40	1.44
20	4	307	CLA	C3A-C4A	-2.06	1.45	1.51
22	B	843	BCR	C30-C25	-2.06	1.51	1.53
20	A	828	CLA	C1B-C2B	-2.05	1.38	1.43
20	B	811	CLA	CHB-C4A	-2.05	1.32	1.37
20	A	820	CLA	C1C-C2C	-2.05	1.40	1.44
20	2	304	CLA	C1A-CHA	2.05	1.51	1.43
20	A	802	CLA	C2-C3	2.05	1.37	1.33
22	I	101	BCR	C2-C1	-2.05	1.49	1.54
20	1	203	CLA	C3D-CAD	-2.05	1.38	1.45
20	1	208	CLA	MG-NA	-2.04	2.01	2.06
20	K	103	CLA	C1B-C2B	-2.04	1.38	1.43
20	A	818	CLA	MG-NA	-2.04	2.01	2.06
20	A	838	CLA	C1B-C2B	-2.04	1.38	1.43
20	1	211	CLA	C1B-C2B	-2.04	1.38	1.43
22	A	844	BCR	C30-C25	-2.04	1.51	1.53
21	F	201	LMU	C4B-C5B	-2.04	1.48	1.53
20	2	321	CLA	C1A-CHA	2.04	1.51	1.43
20	B	808	CLA	C4B-NB	-2.04	1.35	1.37
20	B	839	CLA	MG-NA	-2.04	2.01	2.06
20	B	810	CLA	C1B-C2B	-2.04	1.38	1.43
22	B	844	BCR	C30-C25	-2.04	1.51	1.53
22	J	101	BCR	C30-C25	-2.03	1.51	1.53
20	B	848	CLA	MG-NA	-2.03	2.01	2.06
20	B	815	CLA	MG-NA	-2.03	2.01	2.06
21	1	218	LMU	O1B-C4'	-2.03	1.38	1.43
20	3	305	CLA	C3C-C4C	-2.03	1.38	1.43
20	A	802	CLA	CHB-C4A	-2.03	1.32	1.37
20	H	108	CLA	C1C-C2C	-2.03	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	302	CLA	CHB-C4A	-2.03	1.32	1.37
22	L	209	BCR	C32-C1	-2.03	1.49	1.53
20	3	301	CLA	C4D-CHA	-2.03	1.31	1.38
20	2	303	CLA	C3C-C4C	-2.03	1.38	1.43
20	A	806	CLA	MG-NA	-2.03	2.01	2.06
20	A	828	CLA	C5-C3	2.02	1.55	1.51
20	3	301	CLA	CHB-C4A	-2.02	1.32	1.37
20	L	208	CLA	CHB-C4A	-2.02	1.32	1.37
20	1	207	CLA	C2-C3	2.02	1.37	1.33
20	F	206	CLA	CHB-C4A	-2.02	1.32	1.37
20	A	817	CLA	C1A-CHA	2.02	1.51	1.43
20	A	817	CLA	C1B-NB	-2.02	1.35	1.37
22	F	202	BCR	C1-C6	-2.01	1.51	1.53
20	4	311	CLA	C2D-C1D	-2.01	1.39	1.44
20	B	834	CLA	C3D-CAD	-2.01	1.38	1.45
20	B	820	CLA	C3A-C2A	-2.01	1.49	1.54
20	B	838	CLA	MG-NA	-2.01	2.01	2.06
20	A	826	CLA	C1D-ND	-2.01	1.35	1.37
20	K	105	CLA	C4B-NB	-2.01	1.35	1.37
20	3	306	CLA	C3C-C4C	-2.01	1.38	1.43
20	A	825	CLA	C1B-C2B	-2.01	1.38	1.43
20	K	106	CLA	C4D-CHA	-2.01	1.31	1.38
20	L	207	CLA	C1C-C2C	-2.00	1.40	1.44
22	L	209	BCR	C31-C1	-2.00	1.50	1.53
20	A	823	CLA	C4B-NB	-2.00	1.35	1.37
20	B	816	CLA	C1A-CHA	2.00	1.51	1.43
20	1	212	CLA	C4D-CHA	-2.00	1.31	1.38

All (5222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	844	BCR	C20-C21-C22	37.59	179.99	127.28
22	J	101	BCR	C20-C21-C22	37.57	179.97	127.28
22	A	842	BCR	C20-C21-C22	37.56	179.95	127.28
22	A	843	BCR	C20-C21-C22	37.56	179.95	127.28
22	A	841	BCR	C20-C21-C22	37.54	179.93	127.28
22	A	844	BCR	C20-C21-C22	37.53	179.91	127.28
22	F	202	BCR	C20-C21-C22	37.52	179.89	127.28
22	A	840	BCR	C20-C21-C22	37.51	179.88	127.28
22	G	102	BCR	C20-C21-C22	37.50	179.88	127.28
22	B	841	BCR	C20-C21-C22	37.48	179.84	127.28
22	B	843	BCR	C20-C21-C22	37.48	179.84	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	3	311	BCR	C20-C21-C22	36.32	178.21	127.28
22	B	850	BCR	C20-C21-C22	35.80	177.48	127.28
22	L	209	BCR	C20-C21-C22	35.67	177.30	127.28
22	F	203	BCR	C20-C21-C22	35.37	176.88	127.28
22	I	103	BCR	C20-C21-C22	34.78	176.05	127.28
22	B	842	BCR	C20-C21-C22	30.64	170.25	127.28
22	I	101	BCR	C20-C21-C22	25.38	162.87	127.28
22	A	842	BCR	C21-C20-C19	19.60	179.98	123.20
22	A	840	BCR	C21-C20-C19	19.59	179.97	123.20
22	A	844	BCR	C21-C20-C19	19.59	179.97	123.20
22	A	843	BCR	C21-C20-C19	19.58	179.95	123.20
22	B	844	BCR	C21-C20-C19	19.58	179.94	123.20
22	B	843	BCR	C21-C20-C19	19.58	179.94	123.20
22	J	101	BCR	C21-C20-C19	19.58	179.93	123.20
22	F	202	BCR	C21-C20-C19	19.58	179.93	123.20
22	G	102	BCR	C21-C20-C19	19.57	179.90	123.20
22	A	841	BCR	C21-C20-C19	19.57	179.90	123.20
22	B	841	BCR	C21-C20-C19	19.57	179.89	123.20
22	3	311	BCR	C21-C20-C19	19.03	178.35	123.20
22	L	209	BCR	C21-C20-C19	18.95	178.12	123.20
22	F	203	BCR	C21-C20-C19	18.64	177.20	123.20
22	I	103	BCR	C21-C20-C19	18.40	176.51	123.20
22	B	850	BCR	C21-C20-C19	18.19	175.92	123.20
22	B	842	BCR	C21-C20-C19	15.97	169.48	123.20
22	I	101	BCR	C21-C20-C19	14.48	165.16	123.20
20	1	209	CLA	CAB-C3B-C4B	-14.22	103.76	125.42
22	I	101	BCR	C24-C23-C22	-14.08	105.41	126.23
20	2	312	CLA	OBD-CAD-C3D	-13.56	96.73	128.42
20	1	211	CLA	OBD-CAD-C3D	-13.56	96.73	128.42
22	B	850	BCR	C7-C8-C9	-13.35	106.49	126.23
22	I	103	BCR	C30-C25-C26	-13.21	104.59	122.64
20	4	303	CLA	CAB-C3B-C4B	-12.97	105.67	125.42
20	3	309	CLA	OBD-CAD-C3D	-12.43	99.36	128.42
20	2	306	CLA	OBD-CAD-C3D	-11.95	100.48	128.42
20	B	839	CLA	CAB-C3B-C4B	-11.91	107.28	125.42
22	B	850	BCR	C15-C16-C17	-11.80	99.38	123.52
20	1	214	CLA	OBD-CAD-C3D	-11.78	100.88	128.42
20	B	834	CLA	OBD-CAD-C3D	-11.74	100.99	128.42
20	A	850	CLA	OBD-CAD-C3D	-11.72	101.03	128.42
20	B	807	CLA	OBD-CAD-C3D	-11.59	101.33	128.42
20	A	850	CLA	CAB-C3B-C4B	-11.48	107.94	125.42
20	B	824	CLA	OBD-CAD-C3D	-11.46	101.63	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	313	CLA	CAB-C3B-C4B	-11.41	108.05	125.42
20	H	107	CLA	OBD-CAD-C3D	-11.28	102.06	128.42
20	1	201	CLA	C4A-NA-C1A	11.15	111.76	106.68
20	A	806	CLA	OBD-CAD-C3D	-11.12	102.42	128.42
20	1	211	CLA	CMD-C2D-C1D	11.09	144.26	124.73
20	I	102	CLA	OBD-CAD-C3D	-11.08	102.53	128.42
22	I	101	BCR	C7-C8-C9	-11.02	109.94	126.23
20	B	818	CLA	OBD-CAD-C3D	-11.01	102.69	128.42
20	L	208	CLA	OBD-CAD-C3D	-10.99	102.72	128.42
20	L	204	CLA	OBD-CAD-C3D	-10.98	102.75	128.42
20	2	311	CLA	OBD-CAD-C3D	-10.89	102.96	128.42
20	L	204	CLA	C1-C2-C3	-10.86	108.40	126.20
20	L	202	CLA	OBD-CAD-C3D	-10.76	103.27	128.42
20	4	307	CLA	OBD-CAD-C3D	-10.74	103.31	128.42
22	I	103	BCR	C24-C23-C22	-10.67	110.45	126.23
20	H	101	CLA	OBD-CAD-C3D	-10.56	103.72	128.42
20	1	205	CLA	OBD-CAD-C3D	-10.55	103.76	128.42
20	1	210	CLA	CAB-C3B-C4B	-10.52	109.39	125.42
20	B	833	CLA	OBD-CAD-C3D	-10.52	103.82	128.42
20	A	836	CLA	CBB-CAB-C3B	10.50	179.99	127.53
20	A	833	CLA	CBB-CAB-C3B	10.50	179.98	127.53
20	1	201	CLA	OBD-CAD-C3D	-10.50	103.89	128.42
20	A	832	CLA	CBB-CAB-C3B	10.49	179.96	127.53
20	A	831	CLA	CBB-CAB-C3B	10.49	179.96	127.53
20	A	837	CLA	CBB-CAB-C3B	10.49	179.96	127.53
20	A	835	CLA	CBB-CAB-C3B	10.49	179.96	127.53
20	A	823	CLA	CBB-CAB-C3B	10.49	179.96	127.53
20	2	301	CLA	CBB-CAB-C3B	10.49	179.96	127.53
20	J	102	CLA	CBB-CAB-C3B	10.49	179.95	127.53
20	4	319	CLA	CBB-CAB-C3B	10.49	179.94	127.53
20	3	310	CLA	CBB-CAB-C3B	10.49	179.93	127.53
20	4	302	CLA	CBB-CAB-C3B	10.49	179.93	127.53
20	A	855	CLA	CBB-CAB-C3B	10.49	179.92	127.53
20	A	834	CLA	CBB-CAB-C3B	10.49	179.92	127.53
20	K	103	CLA	CBB-CAB-C3B	10.49	179.92	127.53
20	B	823	CLA	CBB-CAB-C3B	10.49	179.91	127.53
20	K	105	CLA	CBB-CAB-C3B	10.48	179.90	127.53
20	B	822	CLA	CBB-CAB-C3B	10.48	179.89	127.53
20	F	205	CLA	CBB-CAB-C3B	10.48	179.87	127.53
20	A	822	CLA	CBB-CAB-C3B	10.47	179.84	127.53
20	A	827	CLA	OBD-CAD-C3D	-10.43	104.04	128.42
20	B	820	CLA	OBD-CAD-C3D	-10.42	104.05	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	315	CLA	CBB-CAB-C3B	10.41	179.53	127.53
20	A	824	CLA	OBD-CAD-C3D	-10.39	104.13	128.42
20	A	820	CLA	OBD-CAD-C3D	-10.37	104.18	128.42
20	L	208	CLA	CBB-CAB-C3B	10.29	178.95	127.53
20	J	103	CLA	CBB-CAB-C3B	10.29	178.94	127.53
20	A	849	CLA	OBD-CAD-C3D	-10.25	104.46	128.42
20	3	319	CLA	OBD-CAD-C3D	-10.24	104.47	128.42
20	I	102	CLA	CBB-CAB-C3B	10.24	178.70	127.53
20	2	321	CLA	CBB-CAB-C3B	10.24	178.66	127.53
20	A	849	CLA	CBB-CAB-C3B	10.23	178.66	127.53
20	K	106	CLA	CBB-CAB-C3B	10.22	178.57	127.53
20	A	804	CLA	CBB-CAB-C3B	10.21	178.56	127.53
20	K	107	CLA	CBB-CAB-C3B	10.21	178.53	127.53
20	B	807	CLA	CBB-CAB-C3B	10.19	178.43	127.53
20	B	819	CLA	CBB-CAB-C3B	10.19	178.41	127.53
20	B	832	CLA	CBB-CAB-C3B	10.18	178.41	127.53
20	1	214	CLA	CBB-CAB-C3B	10.16	178.29	127.53
20	3	301	CLA	CBB-CAB-C3B	10.14	178.17	127.53
20	2	317	CLA	CBB-CAB-C3B	10.12	178.09	127.53
20	B	826	CLA	CBB-CAB-C3B	10.11	178.03	127.53
20	B	806	CLA	CBB-CAB-C3B	10.11	178.03	127.53
20	3	320	CLA	CBB-CAB-C3B	10.08	177.89	127.53
20	B	829	CLA	CBB-CAB-C3B	10.06	177.78	127.53
20	B	847	CLA	OBD-CAD-C3D	-10.06	104.91	128.42
20	A	817	CLA	OBD-CAD-C3D	-10.04	104.96	128.42
20	4	304	CLA	OBD-CAD-C3D	-10.02	105.00	128.42
20	H	109	CLA	CBB-CAB-C3B	9.98	177.39	127.53
20	B	830	CLA	OBD-CAD-C3D	-9.94	105.19	128.42
20	1	212	CLA	CBB-CAB-C3B	9.93	177.16	127.53
20	A	826	CLA	OBD-CAD-C3D	-9.92	105.23	128.42
20	A	814	CLA	CBB-CAB-C3B	9.92	177.09	127.53
20	L	201	CLA	CBB-CAB-C3B	9.92	177.07	127.53
20	A	828	CLA	CBB-CAB-C3B	9.88	176.91	127.53
20	B	831	CLA	OBD-CAD-C3D	-9.88	105.32	128.42
20	B	832	CLA	OBD-CAD-C3D	-9.87	105.34	128.42
20	B	828	CLA	CBB-CAB-C3B	9.86	176.78	127.53
20	1	203	CLA	OBD-CAD-C3D	-9.84	105.41	128.42
20	R	106	CLA	CBB-CAB-C3B	9.83	176.62	127.53
20	4	318	CLA	CBB-CAB-C3B	9.83	176.62	127.53
20	4	315	CLA	CBB-CAB-C3B	9.82	176.57	127.53
20	A	847	CLA	CBB-CAB-C3B	9.80	176.49	127.53
20	B	820	CLA	CBB-CAB-C3B	9.80	176.49	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	818	CLA	CBB-CAB-C3B	9.78	176.39	127.53
20	A	828	CLA	OBD-CAD-C3D	-9.75	105.62	128.42
20	4	306	CLA	OBD-CAD-C3D	-9.74	105.64	128.42
22	I	103	BCR	C1-C6-C5	-9.72	109.35	122.64
20	A	848	CLA	CBB-CAB-C3B	9.71	176.05	127.53
20	A	805	CLA	CBB-CAB-C3B	9.71	176.03	127.53
20	A	804	CLA	OBD-CAD-C3D	-9.70	105.73	128.42
20	1	201	CLA	CBB-CAB-C3B	9.69	175.92	127.53
20	B	805	CLA	CBB-CAB-C3B	9.68	175.91	127.53
20	4	310	CLA	CBB-CAB-C3B	9.68	175.91	127.53
20	A	808	CLA	OBD-CAD-C3D	-9.66	105.83	128.42
22	F	203	BCR	C15-C14-C13	-9.65	113.74	127.28
20	A	815	CLA	CBB-CAB-C3B	9.63	175.64	127.53
20	3	319	CLA	CAB-C3B-C4B	-9.61	110.78	125.42
20	B	838	CLA	CBB-CAB-C3B	9.61	175.52	127.53
20	A	815	CLA	OBD-CAD-C3D	-9.60	105.97	128.42
20	A	850	CLA	C4D-C3D-CAD	9.58	118.51	108.11
20	A	814	CLA	OBD-CAD-C3D	-9.56	106.06	128.42
20	H	110	CLA	CBB-CAB-C3B	9.56	175.30	127.53
20	1	211	CLA	CBB-CAB-C3B	9.54	175.20	127.53
20	3	309	CLA	CBB-CAB-C3B	9.54	175.19	127.53
20	A	809	CLA	CBB-CAB-C3B	9.54	175.18	127.53
20	L	208	CLA	O2D-CGD-CBD	9.54	127.90	111.23
20	H	108	CLA	OBD-CAD-C3D	-9.53	106.14	128.42
20	A	820	CLA	CBB-CAB-C3B	9.52	175.10	127.53
20	B	837	CLA	CBB-CAB-C3B	9.51	175.02	127.53
20	3	301	CLA	OBD-CAD-C3D	-9.50	106.22	128.42
20	H	107	CLA	CBB-CAB-C3B	9.49	174.93	127.53
20	A	803	CLA	OBD-CAD-C3D	-9.48	106.26	128.42
20	R	107	CLA	CBB-CAB-C3B	9.47	174.84	127.53
20	B	812	CLA	CBB-CAB-C3B	9.46	174.80	127.53
20	A	838	CLA	CBB-CAB-C3B	9.46	174.78	127.53
20	L	207	CLA	CBB-CAB-C3B	9.45	174.72	127.53
20	L	202	CLA	CBB-CAB-C3B	9.44	174.68	127.53
20	B	834	CLA	CBB-CAB-C3B	9.44	174.68	127.53
20	A	801	CLA	CBB-CAB-C3B	9.41	174.52	127.53
20	3	314	CLA	CBB-CAB-C3B	9.40	174.51	127.53
20	B	821	CLA	CBB-CAB-C3B	9.39	174.46	127.53
20	2	306	CLA	CBB-CAB-C3B	9.38	174.38	127.53
20	1	203	CLA	CBB-CAB-C3B	9.38	174.37	127.53
20	B	829	CLA	CAA-C2A-C3A	-9.37	87.67	113.00
20	H	101	CLA	CBB-CAB-C3B	9.35	174.24	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	829	CLA	CBB-CAB-C3B	9.32	174.10	127.53
20	B	809	CLA	OBD-CAD-C3D	-9.32	106.63	128.42
20	B	849	CLA	CBB-CAB-C3B	9.28	173.90	127.53
20	3	315	CLA	OBD-CAD-C3D	-9.26	106.78	128.42
20	A	818	CLA	OBD-CAD-C3D	-9.24	106.83	128.42
20	B	831	CLA	CBB-CAB-C3B	9.23	173.66	127.53
20	2	310	CLA	OBD-CAD-C3D	-9.23	106.85	128.42
22	I	101	BCR	C23-C22-C21	9.22	133.51	119.01
22	3	311	BCR	C16-C17-C18	-9.22	114.35	127.28
20	A	813	CLA	CBB-CAB-C3B	9.21	173.53	127.53
20	A	801	CLA	OBD-CAD-C3D	-9.20	106.91	128.42
20	B	816	CLA	OBD-CAD-C3D	-9.18	106.96	128.42
20	A	827	CLA	CBB-CAB-C3B	9.16	173.30	127.53
20	R	106	CLA	OBD-CAD-C3D	-9.16	107.01	128.42
20	B	847	CLA	CBB-CAB-C3B	9.12	173.08	127.53
20	B	816	CLA	CBB-CAB-C3B	9.12	173.08	127.53
20	1	202	CLA	CBB-CAB-C3B	9.11	173.05	127.53
20	4	304	CLA	CGD-CBD-CAD	9.10	140.30	110.85
20	4	307	CLA	CBB-CAB-C3B	9.09	172.95	127.53
20	A	801	CLA	O2D-CGD-CBD	9.09	127.12	111.23
20	F	206	CLA	CBB-CAB-C3B	9.09	172.93	127.53
20	1	209	CLA	CAB-C3B-C2B	-9.08	99.40	123.53
20	A	824	CLA	CBB-CAB-C3B	9.08	172.91	127.53
20	B	815	CLA	CBB-CAB-C3B	9.07	172.85	127.53
20	1	204	CLA	CBB-CAB-C3B	9.05	172.75	127.53
20	1	212	CLA	OBD-CAD-C3D	-9.05	107.27	128.42
20	A	806	CLA	CBB-CAB-C3B	9.04	172.71	127.53
20	L	207	CLA	OBD-CAD-C3D	-9.02	107.34	128.42
21	L	205	LMU	C1B-O1B-C4'	-8.99	96.66	117.98
20	A	803	CLA	CBB-CAB-C3B	8.99	172.43	127.53
20	2	307	CLA	CBB-CAB-C3B	8.98	172.40	127.53
20	4	313	CLA	OBD-CAD-C3D	-8.96	107.47	128.42
20	L	203	CLA	CBB-CAB-C3B	8.96	172.28	127.53
20	B	818	CLA	CBB-CAB-C3B	8.94	172.21	127.53
20	K	106	CLA	OBD-CAD-C3D	-8.91	107.59	128.42
20	1	209	CLA	OBD-CAD-C3D	-8.86	107.71	128.42
20	B	835	CLA	CBB-CAB-C3B	8.81	171.53	127.53
20	B	804	CLA	CBB-CAB-C3B	8.81	171.52	127.53
21	1	218	LMU	C1B-O1B-C4'	-8.78	97.17	117.98
20	4	319	CLA	OBD-CAD-C3D	-8.76	107.93	128.42
20	3	310	CLA	OBD-CAD-C3D	-8.76	107.95	128.42
20	B	829	CLA	OBD-CAD-C3D	-8.75	107.95	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	301	CLA	OBD-CAD-C3D	-8.75	107.95	128.42
20	J	102	CLA	OBD-CAD-C3D	-8.75	107.96	128.42
20	A	833	CLA	OBD-CAD-C3D	-8.75	107.96	128.42
20	A	832	CLA	OBD-CAD-C3D	-8.75	107.96	128.42
20	B	822	CLA	OBD-CAD-C3D	-8.74	107.98	128.42
20	A	837	CLA	OBD-CAD-C3D	-8.74	107.98	128.42
20	B	823	CLA	OBD-CAD-C3D	-8.74	107.99	128.42
20	K	105	CLA	OBD-CAD-C3D	-8.74	107.99	128.42
20	A	834	CLA	OBD-CAD-C3D	-8.74	107.99	128.42
20	A	831	CLA	OBD-CAD-C3D	-8.73	108.00	128.42
20	A	836	CLA	OBD-CAD-C3D	-8.73	108.02	128.42
20	A	822	CLA	OBD-CAD-C3D	-8.72	108.03	128.42
20	A	855	CLA	OBD-CAD-C3D	-8.72	108.03	128.42
20	4	302	CLA	OBD-CAD-C3D	-8.72	108.03	128.42
20	H	108	CLA	CBB-CAB-C3B	8.72	171.09	127.53
20	A	823	CLA	OBD-CAD-C3D	-8.72	108.04	128.42
20	A	835	CLA	OBD-CAD-C3D	-8.72	108.04	128.42
20	K	103	CLA	OBD-CAD-C3D	-8.71	108.07	128.42
20	F	205	CLA	OBD-CAD-C3D	-8.70	108.08	128.42
20	A	821	CLA	CBB-CAB-C3B	8.69	170.95	127.53
20	3	303	CLA	OBD-CAD-C3D	-8.67	108.15	128.42
20	4	303	CLA	OBD-CAD-C3D	-8.64	108.21	128.42
20	A	825	CLA	CBB-CAB-C3B	8.64	170.70	127.53
20	4	305	CLA	CBB-CAB-C3B	8.64	170.70	127.53
20	G	103	CLA	CBB-CAB-C3B	8.64	170.67	127.53
20	B	815	CLA	OBD-CAD-C3D	-8.62	108.27	128.42
20	B	813	CLA	CBB-CAB-C3B	8.61	170.56	127.53
20	A	830	CLA	CBB-CAB-C3B	8.60	170.48	127.53
20	B	804	CLA	OBD-CAD-C3D	-8.59	108.34	128.42
20	1	207	CLA	CBB-CAB-C3B	8.59	170.44	127.53
20	B	833	CLA	CBB-CAB-C3B	8.59	170.44	127.53
20	B	808	CLA	CAB-C3B-C4B	-8.57	112.37	125.42
20	B	848	CLA	OBD-CAD-C3D	-8.55	108.42	128.42
20	4	304	CLA	CBB-CAB-C3B	8.52	170.11	127.53
20	B	825	CLA	CBB-CAB-C3B	8.52	170.09	127.53
20	F	206	CLA	OBD-CAD-C3D	-8.51	108.53	128.42
20	B	817	CLA	OBD-CAD-C3D	-8.48	108.60	128.42
20	4	318	CLA	OBD-CAD-C3D	-8.43	108.70	128.42
20	A	817	CLA	CBB-CAB-C3B	8.43	169.63	127.53
22	F	203	BCR	C30-C25-C26	-8.41	111.15	122.64
20	B	811	CLA	CBB-CAB-C3B	8.38	169.41	127.53
20	B	817	CLA	CBB-CAB-C3B	8.38	169.40	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	304	CLA	C4D-CHA-C1A	8.38	131.24	121.24
20	B	810	CLA	CBB-CAB-C3B	8.38	169.39	127.53
20	B	848	CLA	CBB-CAB-C3B	8.36	169.29	127.53
21	H	103	LMU	C3B-C4B-C5B	-8.35	95.09	110.23
20	B	828	CLA	OBD-CAD-C3D	-8.34	108.92	128.42
20	H	110	CLA	OBD-CAD-C3D	-8.33	108.94	128.42
20	B	824	CLA	CBB-CAB-C3B	8.32	169.08	127.53
20	A	808	CLA	CBB-CAB-C3B	8.29	168.97	127.53
20	A	807	CLA	CBB-CAB-C3B	8.28	168.92	127.53
20	4	304	CLA	CMD-C2D-C1D	8.28	139.31	124.73
20	A	813	CLA	OBD-CAD-C3D	-8.28	109.06	128.42
20	B	812	CLA	OBD-CAD-C3D	-8.27	109.08	128.42
20	1	207	CLA	C3A-C2A-C1A	8.26	113.71	101.34
20	B	805	CLA	OBD-CAD-C3D	-8.21	109.22	128.42
20	3	314	CLA	OBD-CAD-C3D	-8.21	109.22	128.42
20	L	204	CLA	CMD-C2D-C1D	8.20	139.16	124.73
20	B	814	CLA	CBB-CAB-C3B	8.19	168.47	127.53
20	A	848	CLA	OBD-CAD-C3D	-8.19	109.27	128.42
20	A	819	CLA	CBB-CAB-C3B	8.18	168.42	127.53
20	3	304	CLA	C4A-NA-C1A	8.17	110.41	106.68
20	L	204	CLA	C1D-CHD-C4C	-8.17	108.66	126.02
20	2	321	CLA	OBD-CAD-C3D	-8.16	109.35	128.42
20	J	103	CLA	OBD-CAD-C3D	-8.16	109.35	128.42
21	H	104	LMU	C1B-C2B-C3B	-8.14	92.88	110.01
20	2	311	CLA	CBB-CAB-C3B	8.12	168.11	127.53
20	4	306	CLA	CBB-CAB-C3B	8.11	168.06	127.53
20	B	806	CLA	O2D-CGD-CBD	8.09	125.38	111.23
20	2	312	CLA	CBB-CAB-C3B	8.09	167.92	127.53
20	2	302	CLA	CBB-CAB-C3B	8.08	167.89	127.53
20	B	834	CLA	CMD-C2D-C1D	8.08	138.95	124.73
20	1	205	CLA	CAB-C3B-C4B	-8.07	113.14	125.42
20	1	209	CLA	CMD-C2D-C1D	8.05	138.90	124.73
22	I	101	BCR	C3-C4-C5	-8.04	99.73	114.06
20	B	819	CLA	OBD-CAD-C3D	-8.04	109.63	128.42
20	B	830	CLA	CBB-CAB-C3B	8.03	167.65	127.53
20	B	825	CLA	O2D-CGD-CBD	8.03	125.27	111.23
20	A	830	CLA	OBD-CAD-C3D	-7.98	109.77	128.42
20	A	850	CLA	CMD-C2D-C1D	7.97	138.76	124.73
20	2	307	CLA	OBD-CAD-C3D	-7.96	109.81	128.42
20	B	809	CLA	CBB-CAB-C3B	7.95	167.24	127.53
20	A	809	CLA	CMD-C2D-C1D	7.92	138.67	124.73
20	A	825	CLA	O2D-CGD-CBD	7.92	125.07	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	837	CLA	CMD-C2D-C1D	7.91	138.67	124.73
20	4	307	CLA	CHD-C4C-NC	7.90	136.48	124.23
22	I	103	BCR	C16-C15-C14	-7.87	107.42	123.52
20	2	304	CLA	CBB-CAB-C3B	7.84	166.68	127.53
21	E	101	LMU	C1B-O5B-C5B	-7.83	98.43	113.72
20	A	805	CLA	OBD-CAD-C3D	-7.83	110.13	128.42
20	1	214	CLA	C1D-CHD-C4C	-7.79	109.46	126.02
20	A	827	CLA	O2D-CGD-CBD	7.78	124.84	111.23
20	B	826	CLA	O2D-CGD-CBD	7.76	124.80	111.23
20	H	110	CLA	CMD-C2D-C1D	7.76	138.39	124.73
20	1	203	CLA	CMD-C2D-C1D	7.73	138.35	124.73
20	4	315	CLA	O2D-CGD-CBD	7.71	124.71	111.23
21	E	101	LMU	C4B-C3B-C2B	-7.68	97.34	110.83
20	A	826	CLA	CBB-CAB-C3B	7.68	165.90	127.53
20	3	315	CLA	CMD-C2D-C1D	7.66	138.21	124.73
22	B	850	BCR	C15-C14-C13	-7.65	116.54	127.28
20	3	320	CLA	OBD-CAD-C3D	-7.64	110.56	128.42
20	2	302	CLA	CMD-C2D-C1D	7.64	138.17	124.73
20	R	107	CLA	CMD-C2D-C1D	7.63	138.17	124.73
20	A	810	CLA	OBD-CAD-C3D	-7.63	110.58	128.42
20	B	813	CLA	OBD-CAD-C3D	-7.63	110.58	128.42
20	1	203	CLA	C4D-C3D-CAD	7.62	116.38	108.11
20	1	211	CLA	C4D-C3D-CAD	7.61	116.37	108.11
20	2	307	CLA	O2D-CGD-CBD	7.59	124.50	111.23
20	A	812	CLA	CBB-CAB-C3B	7.58	165.42	127.53
20	A	825	CLA	OBD-CAD-C3D	-7.58	110.69	128.42
20	2	310	CLA	CBB-CAB-C3B	7.58	165.39	127.53
20	L	207	CLA	CAA-C2A-C3A	-7.57	92.53	113.00
20	1	201	CLA	C4D-C3D-CAD	7.57	116.33	108.11
20	B	803	CLA	O2D-CGD-CBD	7.57	124.46	111.23
20	B	826	CLA	OBD-CAD-C3D	-7.55	110.77	128.42
20	B	836	CLA	OBD-CAD-C3D	-7.55	110.77	128.42
20	G	103	CLA	OBD-CAD-C3D	-7.53	110.82	128.42
20	1	206	CLA	CBB-CAB-C3B	7.53	165.14	127.53
20	3	303	CLA	CAB-C3B-C4B	-7.52	113.96	125.42
20	A	829	CLA	OBD-CAD-C3D	-7.52	110.83	128.42
20	R	106	CLA	CMD-C2D-C1D	7.51	137.96	124.73
20	A	829	CLA	CMD-C2D-C1D	7.51	137.95	124.73
20	B	826	CLA	CMD-C2D-C1D	7.50	137.94	124.73
20	A	838	CLA	CMD-C2D-C1D	7.50	137.93	124.73
20	L	204	CLA	CBB-CAB-C3B	7.49	164.94	127.53
20	H	109	CLA	OBD-CAD-C3D	-7.49	110.91	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	304	CLA	OBD-CAD-C3D	-7.49	110.92	128.42
20	B	825	CLA	OBD-CAD-C3D	-7.48	110.93	128.42
20	F	204	CLA	C1B-C2B-C3B	-7.48	100.00	107.03
20	B	803	CLA	CBB-CAB-C3B	7.47	164.85	127.53
20	1	207	CLA	CMD-C2D-C1D	7.46	137.87	124.73
20	B	816	CLA	O2D-CGD-CBD	7.45	124.26	111.23
21	H	102	LMU	C3B-C4B-C5B	-7.45	96.72	110.23
20	B	827	CLA	OBD-CAD-C3D	-7.44	111.03	128.42
20	B	835	CLA	O2D-CGD-CBD	7.44	124.23	111.23
20	A	819	CLA	OBD-CAD-C3D	-7.43	111.05	128.42
20	4	305	CLA	OBD-CAD-C3D	-7.43	111.05	128.42
21	G	101	LMU	C1B-O5B-C5B	-7.40	99.26	113.72
20	A	810	CLA	CBB-CAB-C3B	7.40	164.48	127.53
20	B	826	CLA	C4D-C3D-CAD	7.39	116.13	108.11
20	B	849	CLA	OBD-CAD-C3D	-7.38	111.16	128.42
20	4	304	CLA	C1D-CHD-C4C	-7.37	110.36	126.02
20	1	211	CLA	CHD-C4C-NC	7.36	135.65	124.23
21	B	802	LMU	O5B-C5B-C4B	-7.36	96.43	109.70
20	A	838	CLA	OBD-CAD-C3D	-7.35	111.22	128.42
20	B	827	CLA	CBB-CAB-C3B	7.35	164.22	127.53
20	3	309	CLA	CHD-C4C-C3C	-7.34	114.08	124.77
20	A	816	CLA	CBB-CAB-C3B	7.33	164.15	127.53
20	B	811	CLA	CMD-C2D-C1D	7.31	137.61	124.73
20	4	303	CLA	C1D-CHD-C4C	-7.31	110.49	126.02
20	4	307	CLA	C1D-CHD-C4C	-7.29	110.53	126.02
22	B	850	BCR	C3-C4-C5	-7.29	101.06	114.06
20	1	209	CLA	C4D-C3D-CAD	7.28	116.02	108.11
20	3	309	CLA	CHD-C4C-NC	7.27	135.50	124.23
20	2	302	CLA	OBD-CAD-C3D	-7.24	111.48	128.42
20	1	201	CLA	CMD-C2D-C1D	7.23	137.47	124.73
21	B	801	LMU	C3'-C4'-C5'	-7.21	94.96	110.93
20	1	204	CLA	O2D-CGD-CBD	7.20	123.81	111.23
20	B	817	CLA	C4D-C3D-CAD	7.19	115.91	108.11
20	R	106	CLA	C4D-C3D-CAD	7.18	115.91	108.11
20	A	830	CLA	CMD-C2D-C1D	7.18	137.37	124.73
20	B	839	CLA	OBD-CAD-C3D	-7.17	111.65	128.42
20	4	305	CLA	O2D-CGD-CBD	7.17	123.76	111.23
20	1	207	CLA	O2D-CGD-CBD	7.15	123.72	111.23
20	B	804	CLA	CAA-C2A-C3A	-7.14	93.69	113.00
20	B	836	CLA	CBB-CAB-C3B	7.14	163.19	127.53
20	A	847	CLA	OBD-CAD-C3D	-7.13	111.76	128.42
20	B	834	CLA	O2D-CGD-CBD	7.12	123.67	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	207	CLA	OBD-CAD-C3D	-7.12	111.78	128.42
22	B	850	BCR	C4-C5-C6	-7.12	113.09	122.70
20	3	309	CLA	O2D-CGD-CBD	7.11	123.66	111.23
20	4	304	CLA	CHD-C4C-NC	7.09	135.23	124.23
20	B	817	CLA	CMD-C2D-C1D	7.09	137.21	124.73
20	A	807	CLA	OBD-CAD-C3D	-7.08	111.86	128.42
20	1	211	CLA	CHD-C4C-C3C	-7.08	114.45	124.77
20	F	204	CLA	CMD-C2D-C1D	7.07	137.19	124.73
20	A	818	CLA	CMD-C2D-C1D	7.05	137.15	124.73
20	A	811	CLA	CBB-CAB-C3B	7.04	162.72	127.53
21	F	201	LMU	C2'-C3'-C4'	-7.04	93.70	109.68
20	4	310	CLA	OBD-CAD-C3D	-7.03	111.98	128.42
20	A	850	CLA	O2D-CGD-CBD	7.02	123.50	111.23
21	E	101	LMU	O2'-C2'-C1'	-7.01	93.37	110.08
20	B	821	CLA	O2D-CGD-CBD	7.00	123.46	111.23
20	H	109	CLA	O2D-CGD-CBD	6.99	123.45	111.23
20	2	317	CLA	OBD-CAD-C3D	-6.98	112.10	128.42
20	B	833	CLA	CMD-C2D-C1D	6.98	137.01	124.73
22	3	311	BCR	C11-C10-C9	-6.97	117.50	127.28
20	B	808	CLA	CMD-C2D-C1D	6.97	137.01	124.73
20	A	826	CLA	O2D-CGD-CBD	6.97	123.42	111.23
20	H	108	CLA	O2D-CGD-CBD	6.97	123.42	111.23
20	1	211	CLA	O2A-CGA-O1A	-6.96	106.22	123.63
20	B	818	CLA	CMD-C2D-C1D	6.96	136.98	124.73
20	1	204	CLA	CMD-C2D-C1D	6.95	136.97	124.73
20	B	831	CLA	C4D-C3D-CAD	6.95	115.65	108.11
20	A	809	CLA	C3B-C2B-C1B	-6.95	98.98	107.17
20	K	106	CLA	O2D-CGD-CBD	6.94	123.37	111.23
20	3	309	CLA	C1D-CHD-C4C	-6.94	111.28	126.02
20	B	825	CLA	C4A-NA-C1A	6.93	109.84	106.68
20	1	211	CLA	C1D-CHD-C4C	-6.93	111.29	126.02
21	H	102	LMU	C1B-C2B-C3B	-6.91	95.47	110.01
21	H	102	LMU	C3'-C4'-C5'	-6.91	95.61	110.93
20	1	207	CLA	C4D-C3D-CAD	6.91	115.61	108.11
20	B	803	CLA	OBD-CAD-C3D	-6.90	112.30	128.42
20	1	206	CLA	OBD-CAD-C3D	-6.89	112.31	128.42
21	R	109	LMU	O1B-C1B-C2B	6.89	125.04	108.09
20	A	829	CLA	O2D-CGD-CBD	6.89	123.27	111.23
20	A	847	CLA	C4D-C3D-CAD	6.88	115.58	108.11
20	A	819	CLA	O2D-CGD-CBD	6.88	123.26	111.23
20	B	824	CLA	O2D-CGD-CBD	6.88	123.25	111.23
20	B	803	CLA	CMD-C2D-C1D	6.86	136.81	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	802	CLA	CBB-CAB-C3B	6.85	161.77	127.53
20	L	201	CLA	OBD-CAD-C3D	-6.83	112.46	128.42
20	1	211	CLA	C4A-NA-C1A	6.82	109.79	106.68
20	A	819	CLA	C4D-C3D-CAD	6.82	115.51	108.11
21	H	104	LMU	C1B-O5B-C5B	6.81	127.03	113.72
20	B	836	CLA	O2D-CGD-CBD	6.80	123.12	111.23
20	B	804	CLA	CMD-C2D-C1D	6.80	136.70	124.73
20	F	206	CLA	C1-C2-C3	-6.79	115.06	126.20
20	2	321	CLA	C1D-CHD-C4C	-6.77	111.64	126.02
20	A	820	CLA	C4D-C3D-CAD	6.76	115.45	108.11
20	A	808	CLA	CMD-C2D-C1D	6.76	136.63	124.73
20	A	802	CLA	C3B-C2B-C1B	-6.75	99.21	107.17
20	2	321	CLA	O2D-CGD-CBD	6.73	122.99	111.23
20	L	204	CLA	O2D-CGD-CBD	6.72	122.97	111.23
20	B	806	CLA	O1D-CGD-CBD	-6.71	111.28	124.52
21	R	109	LMU	C4B-C3B-C2B	-6.71	99.05	110.83
20	A	806	CLA	CMD-C2D-C1D	6.71	136.54	124.73
21	K	104	LMU	C3B-C4B-C5B	-6.71	98.07	110.23
20	J	103	CLA	CMD-C2D-C1D	6.70	136.53	124.73
20	B	835	CLA	CMD-C2D-C1D	6.70	136.52	124.73
20	4	310	CLA	C4D-C3D-CAD	6.69	115.38	108.11
20	A	849	CLA	CMD-C2D-C1D	6.68	136.50	124.73
20	1	202	CLA	CMD-C2D-C1D	6.68	136.49	124.73
20	A	807	CLA	CMD-C2D-C1D	6.68	136.48	124.73
20	L	208	CLA	C1D-CHD-C4C	-6.67	111.84	126.02
20	2	310	CLA	CMD-C2D-C1D	6.67	136.47	124.73
20	B	805	CLA	O2D-CGD-CBD	6.66	122.88	111.23
20	B	837	CLA	OBD-CAD-C3D	-6.66	112.84	128.42
20	2	310	CLA	C4D-C3D-CAD	6.65	115.33	108.11
20	1	212	CLA	C1D-CHD-C4C	-6.64	111.90	126.02
22	B	850	BCR	C8-C9-C10	6.64	129.45	119.01
20	A	815	CLA	CMD-C2D-C1D	6.64	136.41	124.73
20	B	849	CLA	CMD-C2D-C1D	6.62	136.39	124.73
20	A	811	CLA	OBD-CAD-C3D	-6.62	112.94	128.42
20	B	838	CLA	OBD-CAD-C3D	-6.62	112.94	128.42
20	A	824	CLA	CMD-C2D-C1D	6.62	136.39	124.73
20	1	201	CLA	CHC-C4B-NB	6.61	133.97	124.05
20	4	304	CLA	CHC-C1C-NC	6.61	134.27	124.31
20	B	810	CLA	OBD-CAD-C3D	-6.60	112.99	128.42
20	3	315	CLA	C4D-C3D-CAD	6.60	115.27	108.11
20	A	821	CLA	OBD-CAD-C3D	-6.59	113.01	128.42
20	B	808	CLA	O2D-CGD-CBD	6.58	122.73	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	210	CLA	CAB-C3B-C2B	-6.58	106.06	123.53
20	B	830	CLA	C4D-C3D-CAD	6.58	115.25	108.11
20	L	207	CLA	CMD-C2D-C1D	6.57	136.30	124.73
20	B	834	CLA	C4D-C3D-CAD	6.56	115.23	108.11
20	L	203	CLA	O2D-CGD-CBD	6.56	122.69	111.23
20	3	314	CLA	CMD-C2D-C1D	6.56	136.28	124.73
20	1	214	CLA	O2D-CGD-CBD	6.53	122.65	111.23
20	A	808	CLA	O2D-CGD-CBD	6.53	122.65	111.23
20	B	825	CLA	C4D-C3D-CAD	6.52	115.19	108.11
20	2	321	CLA	CAA-C2A-C3A	-6.52	95.37	113.00
20	1	205	CLA	C4D-C3D-CAD	6.52	115.19	108.11
21	R	109	LMU	O2B-C2B-C3B	6.52	125.75	110.38
20	3	319	CLA	CMD-C2D-C1D	6.52	136.21	124.73
20	K	106	CLA	CMD-C2D-C1D	6.52	136.21	124.73
20	A	816	CLA	OBD-CAD-C3D	-6.52	113.18	128.42
20	B	819	CLA	CMD-C2D-C1D	6.52	136.21	124.73
20	B	803	CLA	C4D-C3D-CAD	6.51	115.18	108.11
20	B	835	CLA	OBD-CAD-C3D	-6.51	113.20	128.42
20	4	304	CLA	CAA-C2A-C3A	-6.51	95.41	113.00
20	J	103	CLA	C1D-CHD-C4C	-6.51	112.19	126.02
20	A	819	CLA	CMD-C2D-C1D	6.50	136.18	124.73
20	4	307	CLA	CHC-C1C-NC	6.50	134.10	124.31
20	4	315	CLA	C1D-CHD-C4C	-6.50	112.21	126.02
20	B	803	CLA	C2B-C1B-NB	6.50	117.06	110.33
22	F	203	BCR	C3-C4-C5	-6.49	102.49	114.06
20	B	818	CLA	C1D-CHD-C4C	-6.48	112.24	126.02
20	3	301	CLA	CMD-C2D-C1D	6.48	136.15	124.73
20	4	313	CLA	C4D-C3D-CAD	6.48	115.14	108.11
20	B	824	CLA	CMD-C2D-C1D	6.47	136.12	124.73
20	B	838	CLA	C4D-C3D-CAD	6.46	115.12	108.11
20	3	309	CLA	O1D-CGD-CBD	-6.46	111.79	124.52
20	B	830	CLA	O2D-CGD-CBD	6.45	122.51	111.23
20	4	302	CLA	CMD-C2D-C1D	6.45	136.08	124.73
20	L	203	CLA	OBD-CAD-C3D	-6.44	113.36	128.42
20	B	813	CLA	CMD-C2D-C1D	6.44	136.07	124.73
20	B	818	CLA	CHD-C4C-NC	6.44	134.21	124.23
20	1	203	CLA	O2D-CGD-CBD	6.44	122.48	111.23
20	A	832	CLA	CMD-C2D-C1D	6.43	136.05	124.73
20	A	815	CLA	C4D-C3D-CAD	6.43	115.08	108.11
20	3	310	CLA	CMD-C2D-C1D	6.41	136.03	124.73
20	A	836	CLA	CMD-C2D-C1D	6.41	136.02	124.73
20	F	205	CLA	CMD-C2D-C1D	6.41	136.01	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	823	CLA	CMD-C2D-C1D	6.41	136.01	124.73
20	J	102	CLA	CMD-C2D-C1D	6.41	136.01	124.73
20	K	103	CLA	CMD-C2D-C1D	6.41	136.01	124.73
20	A	855	CLA	CMD-C2D-C1D	6.40	136.01	124.73
20	K	105	CLA	CMD-C2D-C1D	6.40	136.00	124.73
20	A	837	CLA	CMD-C2D-C1D	6.40	136.00	124.73
22	F	203	BCR	C24-C23-C22	-6.40	116.77	126.23
20	A	831	CLA	CMD-C2D-C1D	6.40	136.00	124.73
20	B	822	CLA	CMD-C2D-C1D	6.40	136.00	124.73
20	A	805	CLA	O2D-CGD-CBD	6.40	122.41	111.23
20	3	301	CLA	C4D-C3D-CAD	6.40	115.05	108.11
20	A	835	CLA	CMD-C2D-C1D	6.40	135.99	124.73
20	A	812	CLA	OBD-CAD-C3D	-6.39	113.48	128.42
20	A	834	CLA	CMD-C2D-C1D	6.39	135.98	124.73
20	2	301	CLA	CMD-C2D-C1D	6.39	135.98	124.73
20	A	802	CLA	CMD-C2D-C1D	6.38	135.97	124.73
20	A	833	CLA	CMD-C2D-C1D	6.38	135.97	124.73
20	K	107	CLA	OBD-CAD-C3D	-6.38	113.50	128.42
20	4	303	CLA	C4D-C3D-CAD	6.38	115.03	108.11
20	B	810	CLA	C1D-CHD-C4C	-6.38	112.46	126.02
20	A	809	CLA	C4D-C3D-CAD	6.38	115.03	108.11
20	B	823	CLA	CMD-C2D-C1D	6.37	135.95	124.73
20	4	319	CLA	CMD-C2D-C1D	6.37	135.95	124.73
22	I	103	BCR	C34-C9-C10	-6.37	112.49	122.82
20	B	829	CLA	CMD-C2D-C1D	6.37	135.94	124.73
20	A	822	CLA	CMD-C2D-C1D	6.37	135.94	124.73
20	L	204	CLA	C4D-C3D-CAD	6.37	115.02	108.11
20	2	321	CLA	C4D-C3D-CAD	6.35	115.01	108.11
20	B	818	CLA	CHD-C4C-C3C	-6.35	115.52	124.77
20	4	305	CLA	C4D-C3D-CAD	6.35	115.00	108.11
20	B	828	CLA	O2D-CGD-CBD	6.34	122.32	111.23
20	H	110	CLA	C4D-C3D-CAD	6.34	115.00	108.11
20	B	820	CLA	CHD-C4C-C3C	-6.34	115.53	124.77
20	B	809	CLA	CMD-C2D-C1D	6.33	135.88	124.73
20	1	212	CLA	O2D-CGD-CBD	6.33	122.30	111.23
20	I	102	CLA	C1D-CHD-C4C	-6.33	112.57	126.02
20	L	201	CLA	CMD-C2D-C1D	6.33	135.87	124.73
20	B	832	CLA	CMD-C2D-C1D	6.31	135.84	124.73
20	B	849	CLA	C4D-C3D-CAD	6.31	114.95	108.11
20	B	804	CLA	C4D-C3D-CAD	6.30	114.95	108.11
22	L	209	BCR	C27-C26-C25	-6.30	114.19	122.70
20	A	850	CLA	CAA-C2A-C3A	6.29	130.01	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	H	107	CLA	C3B-C2B-C1B	-6.29	99.75	107.17
20	4	305	CLA	CMD-C2D-C1D	6.29	135.80	124.73
20	3	303	CLA	CMD-C2D-C1D	6.28	135.79	124.73
20	3	320	CLA	O2D-CGD-CBD	6.28	122.21	111.23
20	B	829	CLA	C4D-C3D-CAD	6.28	114.93	108.11
20	2	304	CLA	CMD-C2D-C1D	6.28	135.79	124.73
20	A	828	CLA	C4D-C3D-CAD	6.28	114.92	108.11
20	1	211	CLA	CMD-C2D-C3D	-6.28	113.29	127.69
20	4	310	CLA	CMD-C2D-C1D	6.28	135.78	124.73
20	1	209	CLA	C1D-CHD-C4C	-6.27	112.69	126.02
20	L	203	CLA	CMD-C2D-C1D	6.27	135.77	124.73
20	B	818	CLA	C4D-C3D-CAD	6.27	114.91	108.11
20	B	819	CLA	C4D-C3D-CAD	6.26	114.90	108.11
20	B	848	CLA	C4-C3-C5	6.25	126.08	115.23
20	I	102	CLA	O2D-CGD-CBD	6.25	122.16	111.23
20	B	807	CLA	C1D-CHD-C4C	-6.25	112.74	126.02
20	A	804	CLA	CMD-C2D-C1D	6.24	135.72	124.73
20	B	848	CLA	O2D-CGD-CBD	6.24	122.14	111.23
20	B	832	CLA	C4D-C3D-CAD	6.24	114.88	108.11
20	B	826	CLA	C1D-CHD-C4C	-6.23	112.78	126.02
20	4	310	CLA	C1D-CHD-C4C	-6.23	112.79	126.02
20	A	801	CLA	CMD-C2D-C1D	6.22	135.69	124.73
20	H	107	CLA	CMD-C2D-C1D	6.22	135.69	124.73
20	1	205	CLA	CMD-C2D-C1D	6.22	135.68	124.73
20	G	103	CLA	CMD-C2D-C1D	6.21	135.66	124.73
20	A	850	CLA	CAB-C3B-C2B	-6.21	107.05	123.53
20	4	307	CLA	CMD-C2D-C1D	6.21	135.66	124.73
20	A	847	CLA	CHD-C4C-C3C	-6.19	115.75	124.77
20	B	837	CLA	O2D-CGD-CBD	6.18	122.04	111.23
20	4	318	CLA	C4D-C3D-CAD	6.17	114.81	108.11
20	B	806	CLA	C4D-C3D-CAD	6.17	114.81	108.11
20	B	831	CLA	C1D-CHD-C4C	-6.17	112.91	126.02
20	A	821	CLA	CMD-C2D-C1D	6.17	135.59	124.73
20	1	206	CLA	C1D-CHD-C4C	-6.15	112.95	126.02
20	2	306	CLA	C1D-CHD-C4C	-6.15	112.96	126.02
20	A	809	CLA	C1D-CHD-C4C	-6.15	112.96	126.02
20	1	215	CLA	C4A-NA-C1A	6.13	109.48	106.68
20	2	311	CLA	C4A-NA-C1A	6.13	109.47	106.68
22	I	103	BCR	C11-C10-C9	-6.12	118.70	127.28
20	B	810	CLA	CHD-C4C-NC	6.11	133.71	124.23
20	4	315	CLA	OBD-CAD-C3D	-6.11	114.14	128.42
20	L	201	CLA	O2D-CGD-CBD	6.10	121.90	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	802	LMU	C1B-O1B-C4'	-6.10	103.52	117.98
20	1	210	CLA	CMD-C2D-C1D	6.10	135.47	124.73
20	A	849	CLA	C4D-C3D-CAD	6.09	114.72	108.11
20	L	207	CLA	O2D-CGD-CBD	6.08	121.86	111.23
20	2	311	CLA	C1D-CHD-C4C	-6.08	113.09	126.02
20	3	301	CLA	C1D-CHD-C4C	-6.08	113.10	126.02
20	4	307	CLA	CAA-C2A-C1A	6.08	131.89	111.97
20	1	206	CLA	C4D-C3D-CAD	6.07	114.70	108.11
20	A	848	CLA	C1D-CHD-C4C	-6.07	113.12	126.02
20	B	809	CLA	C4D-C3D-CAD	6.07	114.70	108.11
21	G	101	LMU	O5B-C5B-C6B	-6.07	91.41	106.44
20	1	201	CLA	C1D-CHD-C4C	-6.06	113.14	126.02
22	I	103	BCR	C38-C26-C25	-6.06	117.88	124.48
22	I	103	BCR	C8-C9-C10	6.05	128.53	119.01
20	1	209	CLA	CHD-C4C-NC	6.05	133.62	124.23
20	K	106	CLA	C4D-C3D-CAD	6.05	114.68	108.11
20	3	304	CLA	CHC-C1C-NC	6.05	133.22	124.33
20	2	306	CLA	CMD-C2D-C1D	6.05	135.38	124.73
20	F	204	CLA	C4D-C3D-CAD	6.05	114.67	108.11
20	4	308	CLA	C3A-C4A-CHB	-6.05	116.51	123.91
20	J	103	CLA	CHD-C4C-NC	6.05	133.60	124.23
20	F	206	CLA	C1D-CHD-C4C	-6.04	113.18	126.02
20	A	814	CLA	C1D-CHD-C4C	-6.04	113.18	126.02
20	4	310	CLA	CHD-C4C-NC	6.04	133.59	124.23
20	1	213	CLA	C3A-C4A-CHB	-6.04	116.52	123.91
20	3	320	CLA	C4D-C3D-CAD	6.03	114.66	108.11
20	A	820	CLA	CMD-C2D-C1D	6.03	135.34	124.73
20	B	829	CLA	O2D-CGD-CBD	6.02	121.76	111.23
20	2	302	CLA	O2D-CGD-CBD	6.02	121.76	111.23
20	B	838	CLA	CHC-C4B-NB	6.02	133.08	124.05
20	A	817	CLA	CMD-C2D-C1D	6.02	135.33	124.73
20	B	830	CLA	C1D-CHD-C4C	-6.02	113.23	126.02
20	B	821	CLA	C1D-CHD-C4C	-6.01	113.25	126.02
20	4	310	CLA	CHD-C4C-C3C	-6.01	116.02	124.77
20	1	209	CLA	CBD-CAD-C3D	-6.01	100.23	108.25
20	A	824	CLA	C4D-C3D-CAD	6.00	114.63	108.11
20	2	302	CLA	C4D-C3D-CAD	6.00	114.62	108.11
20	A	849	CLA	O2D-CGD-CBD	6.00	121.72	111.23
21	H	102	LMU	C1'-C2'-C3'	-6.00	97.40	110.01
20	1	202	CLA	C4D-C3D-CAD	5.99	114.62	108.11
20	4	315	CLA	O1D-CGD-CBD	-5.99	112.70	124.52
20	B	830	CLA	CMD-C2D-C1D	5.99	135.27	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	812	CLA	CMD-C2D-C1D	5.98	135.26	124.73
20	B	804	CLA	O2D-CGD-CBD	5.98	121.69	111.23
20	A	814	CLA	CMD-C2D-C1D	5.98	135.26	124.73
22	I	101	BCR	C30-C25-C24	5.98	131.87	115.65
20	1	214	CLA	CHD-C4C-NC	5.98	133.50	124.23
20	B	810	CLA	CHD-C4C-C3C	-5.97	116.06	124.77
20	B	813	CLA	O2D-CGD-CBD	5.96	121.66	111.23
20	A	810	CLA	CMD-C2D-C1D	5.96	135.23	124.73
20	B	847	CLA	C4D-C3D-CAD	5.96	114.58	108.11
22	F	203	BCR	C10-C11-C12	-5.96	105.93	123.20
20	A	809	CLA	OBD-CAD-C3D	-5.95	114.51	128.42
20	R	107	CLA	C4D-C3D-CAD	5.95	114.56	108.11
20	2	304	CLA	C4D-C3D-CAD	5.94	114.56	108.11
20	B	805	CLA	C1D-CHD-C4C	-5.94	113.39	126.02
20	B	828	CLA	CHD-C4C-NC	5.94	133.44	124.23
20	3	319	CLA	C1D-CHD-C4C	-5.93	113.41	126.02
22	I	103	BCR	C29-C30-C25	-5.93	101.82	110.44
20	B	836	CLA	C1D-CHD-C4C	-5.93	113.41	126.02
20	A	812	CLA	C2B-C1B-NB	5.93	116.47	110.33
20	A	807	CLA	CHC-C1C-NC	5.92	133.23	124.31
20	4	318	CLA	CMD-C2D-C1D	5.92	135.16	124.73
20	1	207	CLA	CBA-CAA-C2A	-5.92	96.19	113.79
20	B	831	CLA	CMD-C2D-C1D	5.91	135.13	124.73
20	A	818	CLA	C4D-C3D-CAD	5.91	114.52	108.11
20	A	830	CLA	C4D-C3D-CAD	5.90	114.51	108.11
20	B	816	CLA	C4D-C3D-CAD	5.90	114.51	108.11
20	B	805	CLA	C4A-NA-C1A	5.90	109.37	106.68
20	B	815	CLA	C1D-CHD-C4C	-5.89	113.49	126.02
20	K	103	CLA	C1D-CHD-C4C	-5.89	113.50	126.02
20	3	316	CLA	C3A-C4A-CHB	-5.89	116.70	123.91
20	K	105	CLA	C1D-CHD-C4C	-5.89	113.50	126.02
20	3	319	CLA	C4D-C3D-CAD	5.89	114.50	108.11
20	B	834	CLA	O2D-CGD-O1D	-5.89	112.39	123.85
20	3	314	CLA	C4D-C3D-CAD	5.89	114.50	108.11
20	A	850	CLA	CMD-C2D-C3D	-5.88	114.19	127.69
20	B	820	CLA	CBC-CAC-C3C	-5.88	96.47	112.42
20	A	828	CLA	CMD-C2D-C1D	5.88	135.09	124.73
20	4	304	CLA	C4D-C3D-CAD	5.88	114.49	108.11
20	2	312	CLA	O2D-CGD-CBD	5.88	121.50	111.23
20	4	302	CLA	C1D-CHD-C4C	-5.88	113.53	126.02
20	2	301	CLA	C1D-CHD-C4C	-5.87	113.54	126.02
20	4	306	CLA	CMD-C2D-C1D	5.87	135.07	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	820	CLA	C6-C5-C3	-5.87	99.16	113.47
20	3	303	CLA	C1D-CHD-C4C	-5.87	113.54	126.02
20	4	303	CLA	CBD-CAD-C3D	-5.87	100.41	108.25
20	B	837	CLA	C4D-C3D-CAD	5.87	114.48	108.11
20	A	809	CLA	CMB-C2B-C1B	5.87	134.36	125.42
20	A	837	CLA	C1D-CHD-C4C	-5.87	113.55	126.02
20	3	315	CLA	C1D-CHD-C4C	-5.87	113.55	126.02
20	4	319	CLA	C1D-CHD-C4C	-5.87	113.55	126.02
20	B	808	CLA	OBD-CAD-C3D	-5.87	114.71	128.42
20	J	102	CLA	C1D-CHD-C4C	-5.87	113.55	126.02
20	A	855	CLA	C1D-CHD-C4C	-5.86	113.56	126.02
20	3	308	CLA	C4A-NA-C1A	5.86	109.35	106.68
20	A	831	CLA	C1D-CHD-C4C	-5.86	113.56	126.02
20	2	317	CLA	CMD-C2D-C1D	5.86	135.05	124.73
20	F	205	CLA	C1D-CHD-C4C	-5.86	113.56	126.02
20	B	822	CLA	C1D-CHD-C4C	-5.86	113.56	126.02
20	H	109	CLA	C4D-C3D-CAD	5.86	114.47	108.11
20	3	310	CLA	C1D-CHD-C4C	-5.86	113.57	126.02
20	A	835	CLA	C1D-CHD-C4C	-5.85	113.58	126.02
20	A	834	CLA	C1D-CHD-C4C	-5.85	113.58	126.02
20	1	212	CLA	CMD-C2D-C1D	5.85	135.03	124.73
20	B	823	CLA	C1D-CHD-C4C	-5.84	113.60	126.02
20	A	832	CLA	C1D-CHD-C4C	-5.84	113.60	126.02
20	A	833	CLA	C1D-CHD-C4C	-5.84	113.60	126.02
20	K	107	CLA	O2D-CGD-CBD	5.84	121.44	111.23
20	A	829	CLA	C4D-C3D-CAD	5.84	114.45	108.11
20	2	310	CLA	O2D-CGD-CBD	5.84	121.44	111.23
20	A	823	CLA	C1D-CHD-C4C	-5.84	113.61	126.02
20	A	822	CLA	C1D-CHD-C4C	-5.84	113.61	126.02
20	L	204	CLA	C4-C3-C5	5.84	125.36	115.23
20	4	303	CLA	CMD-C2D-C1D	5.83	135.00	124.73
22	I	101	BCR	C4-C5-C6	-5.83	114.82	122.70
20	A	836	CLA	C1D-CHD-C4C	-5.83	113.62	126.02
20	1	201	CLA	C4B-CHC-C1C	-5.83	112.54	126.25
20	B	832	CLA	O2D-CGD-CBD	5.82	121.41	111.23
20	3	305	CLA	C3A-C4A-CHB	-5.82	116.78	123.91
20	B	811	CLA	C4D-C3D-CAD	5.82	114.42	108.11
20	B	825	CLA	C1D-CHD-C4C	-5.81	113.66	126.02
20	1	211	CLA	CGD-CBD-CAD	-5.81	92.03	110.85
20	1	201	CLA	O2D-CGD-CBD	5.81	121.39	111.23
20	H	101	CLA	C4D-C3D-CAD	5.81	114.41	108.11
20	A	806	CLA	C4D-C3D-CAD	5.80	114.41	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	210	CLA	C4D-C3D-CAD	5.80	114.41	108.11
20	3	306	CLA	C3A-C4A-CHB	-5.80	116.81	123.91
20	A	816	CLA	C4D-C3D-CAD	5.80	114.40	108.11
20	H	107	CLA	C4D-C3D-CAD	5.79	114.39	108.11
20	H	101	CLA	CMD-C2D-C1D	5.79	134.92	124.73
20	A	812	CLA	O2D-CGD-CBD	5.79	121.35	111.23
20	1	215	CLA	C2A-C1A-CHA	-5.79	112.76	122.63
20	2	301	CLA	C4D-C3D-CAD	5.78	114.39	108.11
20	3	309	CLA	CMD-C2D-C1D	5.78	134.91	124.73
20	A	822	CLA	C4D-C3D-CAD	5.78	114.38	108.11
20	4	306	CLA	C1D-CHD-C4C	-5.78	113.74	126.02
20	B	828	CLA	CHD-C4C-C3C	-5.77	116.36	124.77
20	1	210	CLA	C1D-CHD-C4C	-5.77	113.75	126.02
20	B	813	CLA	C4D-C3D-CAD	5.77	114.37	108.11
20	4	313	CLA	C1D-CHD-C4C	-5.77	113.76	126.02
20	F	205	CLA	C4D-C3D-CAD	5.76	114.37	108.11
20	F	204	CLA	C1D-CHD-C4C	-5.76	113.77	126.02
20	B	807	CLA	C4D-C3D-CAD	5.76	114.36	108.11
20	3	320	CLA	C1D-CHD-C4C	-5.76	113.78	126.02
20	A	855	CLA	C4D-C3D-CAD	5.76	114.36	108.11
20	A	836	CLA	C4D-C3D-CAD	5.75	114.36	108.11
20	3	320	CLA	CMD-C2D-C1D	5.75	134.85	124.73
20	A	803	CLA	C1D-CHD-C4C	-5.75	113.80	126.02
20	4	302	CLA	C4D-C3D-CAD	5.75	114.35	108.11
20	H	109	CLA	C1D-CHD-C4C	-5.75	113.81	126.02
20	B	823	CLA	C4D-C3D-CAD	5.74	114.34	108.11
20	4	307	CLA	C3A-C2A-C1A	5.74	109.94	101.34
20	A	831	CLA	C4D-C3D-CAD	5.74	114.34	108.11
20	K	103	CLA	C4D-C3D-CAD	5.74	114.34	108.11
20	A	833	CLA	C4D-C3D-CAD	5.74	114.34	108.11
20	B	805	CLA	C3B-C2B-C1B	-5.74	100.40	107.17
20	B	838	CLA	C3B-C2B-C1B	-5.74	100.41	107.17
20	A	804	CLA	C4D-C3D-CAD	5.74	114.34	108.11
20	B	834	CLA	C1D-CHD-C4C	-5.74	113.83	126.02
20	A	832	CLA	C4D-C3D-CAD	5.74	114.34	108.11
20	B	822	CLA	C4D-C3D-CAD	5.74	114.33	108.11
20	G	103	CLA	O2D-CGD-CBD	5.74	121.26	111.23
20	A	834	CLA	C4D-C3D-CAD	5.73	114.33	108.11
20	L	202	CLA	O2D-CGD-CBD	5.73	121.25	111.23
20	A	811	CLA	C1D-CHD-C4C	-5.73	113.84	126.02
20	A	810	CLA	C1D-CHD-C4C	-5.73	113.84	126.02
20	A	837	CLA	C4D-C3D-CAD	5.73	114.33	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	306	CLA	C4D-C3D-CAD	5.73	114.33	108.11
20	3	310	CLA	C4D-C3D-CAD	5.72	114.32	108.11
21	K	104	LMU	O1'-C1'-C2'	5.72	116.97	108.27
20	1	207	CLA	CGD-CBD-CAD	-5.72	92.32	110.85
20	B	803	CLA	C1D-CHD-C4C	-5.72	113.86	126.02
20	A	835	CLA	C4D-C3D-CAD	5.72	114.32	108.11
20	J	102	CLA	C4D-C3D-CAD	5.72	114.32	108.11
20	A	829	CLA	C1D-CHD-C4C	-5.72	113.87	126.02
20	1	211	CLA	O2A-CGA-CBA	5.71	129.24	111.83
21	B	802	LMU	C3B-C4B-C5B	-5.71	99.88	110.23
20	L	208	CLA	CHD-C4C-NC	5.70	133.07	124.23
20	B	817	CLA	C1D-CHD-C4C	-5.70	113.90	126.02
21	H	102	LMU	C1'-O5'-C5'	5.70	124.84	113.72
21	A	852	LMU	C1'-O5'-C5'	-5.69	102.60	113.72
20	A	824	CLA	C1D-CHD-C4C	-5.69	113.93	126.02
20	3	304	CLA	CHD-C4C-NC	5.69	132.88	124.24
20	A	829	CLA	C3B-C2B-C1B	-5.69	100.47	107.17
20	B	829	CLA	C1D-CHD-C4C	-5.69	113.93	126.02
20	H	110	CLA	C1D-CHD-C4C	-5.69	113.93	126.02
20	G	103	CLA	C1D-CHD-C4C	-5.69	113.93	126.02
20	B	806	CLA	C4A-NA-C1A	5.69	109.27	106.68
22	I	103	BCR	C16-C17-C18	-5.69	119.31	127.28
20	A	847	CLA	CHD-C4C-NC	5.68	133.04	124.23
20	1	205	CLA	C1D-CHD-C4C	-5.68	113.94	126.02
20	F	204	CLA	C2B-C1B-NB	5.68	116.22	110.33
20	B	805	CLA	CMD-C2D-C1D	5.68	134.73	124.73
20	A	816	CLA	C3B-C2B-C1B	-5.68	100.48	107.17
20	B	833	CLA	C4D-C3D-CAD	5.68	114.27	108.11
20	L	203	CLA	C1D-CHD-C4C	-5.67	113.97	126.02
20	3	305	CLA	CHD-C4C-NC	5.67	132.85	124.24
20	4	313	CLA	CBD-CAD-C3D	-5.66	100.69	108.25
20	H	107	CLA	C2B-C1B-NB	5.66	116.20	110.33
20	A	803	CLA	CMD-C2D-C1D	5.66	134.69	124.73
20	3	306	CLA	CHD-C4C-NC	5.65	132.83	124.24
20	A	823	CLA	C4D-C3D-CAD	5.65	114.25	108.11
20	B	808	CLA	C4D-C3D-CAD	5.65	114.24	108.11
20	B	820	CLA	CHD-C4C-NC	5.65	132.99	124.23
22	I	103	BCR	C15-C16-C17	5.65	135.07	123.52
20	A	815	CLA	C1D-CHD-C4C	-5.64	114.02	126.02
20	4	307	CLA	CBA-CAA-C2A	-5.64	97.00	113.79
20	H	108	CLA	C1D-CHD-C4C	-5.64	114.02	126.02
20	L	204	CLA	CMD-C2D-C3D	-5.64	114.75	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	839	CLA	CAB-C3B-C2B	-5.64	108.55	123.53
20	B	819	CLA	C1D-CHD-C4C	-5.64	114.03	126.02
20	1	206	CLA	CHD-C4C-C3C	-5.64	116.55	124.77
22	B	850	BCR	C36-C18-C19	5.63	126.68	118.09
20	K	107	CLA	C4D-C3D-CAD	5.63	114.22	108.11
20	4	303	CLA	CHD-C4C-NC	5.62	132.95	124.23
20	1	214	CLA	CHC-C1C-NC	5.62	132.78	124.31
20	A	826	CLA	C1D-CHD-C4C	-5.62	114.08	126.02
20	I	102	CLA	CMD-C2D-C1D	5.62	134.62	124.73
20	1	212	CLA	CHD-C4C-NC	5.61	132.94	124.23
20	A	816	CLA	C1D-CHD-C4C	-5.61	114.10	126.02
20	A	807	CLA	O2D-CGD-CBD	5.61	121.03	111.23
20	B	824	CLA	C1D-CHD-C4C	-5.61	114.10	126.02
20	3	312	CLA	C3A-C4A-CHB	-5.61	117.05	123.91
20	1	201	CLA	CAC-C3C-C4C	5.61	132.08	124.79
20	B	836	CLA	CMD-C2D-C1D	5.60	134.60	124.73
20	A	847	CLA	C3B-C4B-NB	-5.60	105.53	110.53
20	A	812	CLA	C3B-C2B-C1B	-5.60	100.57	107.17
20	B	849	CLA	C1D-CHD-C4C	-5.60	114.13	126.02
20	K	105	CLA	C4D-C3D-CAD	5.59	114.18	108.11
20	A	821	CLA	C1D-CHD-C4C	-5.59	114.13	126.02
20	4	306	CLA	C4D-C3D-CAD	5.59	114.18	108.11
20	A	801	CLA	C4D-C3D-CAD	5.59	114.18	108.11
22	I	103	BCR	C7-C8-C9	5.59	134.50	126.23
20	1	214	CLA	C4-C3-C5	5.58	122.70	116.13
20	3	304	CLA	C1B-NB-C4B	-5.58	102.40	106.31
21	F	201	LMU	C1B-O1B-C4'	-5.58	104.76	117.98
21	H	104	LMU	C3B-C4B-C5B	-5.58	100.12	110.23
20	A	804	CLA	C3B-C2B-C1B	-5.58	100.60	107.17
20	1	202	CLA	C4A-NA-C1A	5.57	109.22	106.68
20	A	828	CLA	C1D-CHD-C4C	-5.57	114.18	126.02
21	H	105	LMU	O5B-C5B-C4B	5.56	119.72	109.70
20	2	311	CLA	O2D-CGD-CBD	5.56	120.95	111.23
20	B	835	CLA	C4D-C3D-CAD	5.56	114.14	108.11
20	3	301	CLA	CHD-C4C-NC	5.56	132.85	124.23
21	G	101	LMU	O4'-C4B-C3B	5.55	123.47	110.38
20	B	816	CLA	C1D-CHD-C4C	-5.55	114.22	126.02
20	B	808	CLA	C1D-CHD-C4C	-5.55	114.22	126.02
20	B	817	CLA	CHD-C4C-NC	5.55	132.84	124.23
20	B	810	CLA	CMD-C2D-C1D	5.55	134.50	124.73
20	3	303	CLA	CHD-C4C-NC	5.55	132.83	124.23
21	L	205	LMU	O4'-C4B-C5B	-5.54	95.68	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	802	CLA	C2B-C1B-NB	5.54	116.07	110.33
20	2	312	CLA	C1D-CHD-C4C	-5.53	114.26	126.02
20	4	315	CLA	CHD-C4C-C3C	-5.52	116.72	124.77
20	A	815	CLA	O2D-CGD-CBD	5.52	120.88	111.23
20	4	319	CLA	C4D-C3D-CAD	5.52	114.10	108.11
20	L	208	CLA	CHD-C4C-C3C	-5.52	116.73	124.77
20	A	811	CLA	C4D-C3D-CAD	5.51	114.09	108.11
20	B	814	CLA	OBD-CAD-C3D	-5.51	115.55	128.42
20	H	108	CLA	C4D-C3D-CAD	5.50	114.08	108.11
22	L	209	BCR	C30-C25-C26	-5.50	115.12	122.64
20	L	207	CLA	C4D-C3D-CAD	5.48	114.06	108.11
20	K	107	CLA	C1D-CHD-C4C	-5.48	114.37	126.02
20	A	817	CLA	C1D-CHD-C4C	-5.48	114.37	126.02
20	B	804	CLA	C1D-CHD-C4C	-5.48	114.38	126.02
20	B	839	CLA	CMD-C2D-C1D	5.48	134.37	124.73
20	L	208	CLA	CMD-C2D-C1D	5.48	134.37	124.73
20	F	204	CLA	CHD-C4C-NC	5.48	132.72	124.23
20	1	204	CLA	C1D-CHD-C4C	-5.48	114.38	126.02
22	B	850	BCR	C10-C11-C12	-5.47	107.34	123.20
20	B	812	CLA	C1D-CHD-C4C	-5.47	114.39	126.02
22	I	103	BCR	C38-C26-C27	5.47	125.26	113.60
20	A	811	CLA	CMD-C2D-C1D	5.47	134.36	124.73
20	1	201	CLA	CMD-C2D-C3D	-5.47	115.15	127.69
20	B	824	CLA	C2B-C1B-NB	5.47	115.99	110.33
20	A	814	CLA	C1-C2-C3	-5.46	117.25	126.20
21	G	101	LMU	O1B-C1B-C2B	5.46	121.53	108.09
20	A	814	CLA	O2D-CGD-CBD	5.46	120.78	111.23
20	A	803	CLA	CHC-C1C-NC	5.46	132.53	124.31
20	L	203	CLA	C4D-C3D-CAD	5.46	114.03	108.11
20	A	826	CLA	C4D-C3D-CAD	5.46	114.03	108.11
20	L	204	CLA	CHD-C4C-C3C	-5.46	116.82	124.77
20	B	814	CLA	CMD-C2D-C1D	5.45	134.33	124.73
20	A	801	CLA	C1D-CHD-C4C	-5.45	114.43	126.02
20	A	809	CLA	CMD-C2D-C3D	-5.45	115.18	127.69
20	4	304	CLA	CMD-C2D-C3D	-5.45	115.19	127.69
20	A	848	CLA	C2B-C1B-NB	5.45	115.98	110.33
20	A	807	CLA	C4D-C3D-CAD	5.45	114.02	108.11
20	B	814	CLA	O2D-CGD-CBD	5.44	120.74	111.23
20	2	305	CLA	C2A-C1A-CHA	-5.44	113.35	122.63
20	B	839	CLA	C4D-C3D-CAD	5.44	114.01	108.11
21	B	802	LMU	O3B-C3B-C2B	-5.43	97.57	110.38
20	3	315	CLA	CHD-C4C-NC	5.43	132.66	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	847	CLA	C3B-C2B-C1B	-5.43	100.77	107.17
20	A	802	CLA	C1D-CHD-C4C	-5.42	114.50	126.02
20	B	848	CLA	C1D-CHD-C4C	-5.42	114.50	126.02
20	B	837	CLA	C4B-CHC-C1C	-5.42	113.51	126.25
20	A	806	CLA	O2D-CGD-CBD	5.42	120.70	111.23
20	B	805	CLA	CHC-C1C-NC	5.42	132.47	124.31
20	1	211	CLA	CMB-C2B-C1B	5.41	133.66	125.42
20	A	838	CLA	C4D-C3D-CAD	5.41	113.99	108.11
20	H	107	CLA	C1D-CHD-C4C	-5.41	114.52	126.02
20	B	826	CLA	C4A-NA-C1A	5.41	109.15	106.68
20	B	813	CLA	C1D-CHD-C4C	-5.41	114.52	126.02
20	A	803	CLA	CHD-C4C-NC	5.40	132.61	124.23
20	B	821	CLA	CMD-C2D-C1D	5.40	134.24	124.73
20	B	838	CLA	C4A-NA-C1A	5.40	109.14	106.68
20	B	804	CLA	CHC-C1C-NC	5.40	132.45	124.31
20	3	304	CLA	C2A-C1A-CHA	-5.40	113.42	122.63
20	B	810	CLA	C4D-C3D-CAD	5.40	113.97	108.11
20	A	819	CLA	O1D-CGD-CBD	-5.40	113.87	124.52
20	K	107	CLA	CMD-C2D-C1D	5.40	134.23	124.73
20	1	202	CLA	OBD-CAD-C3D	-5.39	115.82	128.42
20	A	802	CLA	CHD-C4C-NC	5.39	132.58	124.23
20	1	212	CLA	C4D-C3D-CAD	5.39	113.95	108.11
20	3	309	CLA	CED-O2D-CGD	5.38	128.13	115.92
20	1	212	CLA	CHD-C4C-C3C	-5.38	116.93	124.77
21	A	854	LMU	O1B-C4'-C3'	5.38	120.90	107.23
20	A	817	CLA	O2D-CGD-CBD	5.38	120.63	111.23
20	A	820	CLA	C1D-CHD-C4C	-5.38	114.59	126.02
20	A	818	CLA	O2D-CGD-CBD	5.38	120.63	111.23
20	1	214	CLA	CAA-C2A-C3A	-5.38	98.47	113.00
20	A	811	CLA	CHC-C1C-NC	5.38	132.41	124.31
20	B	839	CLA	CBD-CAD-C3D	-5.37	101.08	108.25
21	G	101	LMU	O5B-C1B-C2B	-5.37	99.34	110.37
20	L	204	CLA	O2D-CGD-O1D	-5.37	113.40	123.85
20	L	207	CLA	C1D-CHD-C4C	-5.37	114.61	126.02
21	K	101	LMU	C4B-C3B-C2B	-5.36	101.41	110.83
20	A	816	CLA	CMD-C2D-C1D	5.36	134.17	124.73
20	1	206	CLA	CMD-C2D-C1D	5.36	134.17	124.73
20	A	806	CLA	C3B-C2B-C1B	-5.35	100.86	107.17
20	A	814	CLA	C4D-C3D-CAD	5.34	113.91	108.11
20	1	210	CLA	OBD-CAD-C3D	-5.34	115.92	128.42
20	1	209	CLA	CHD-C4C-C3C	-5.34	116.59	125.03
20	4	307	CLA	C4D-C3D-CAD	5.34	113.91	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	825	CLA	C1D-CHD-C4C	-5.34	114.67	126.02
20	A	838	CLA	C1D-CHD-C4C	-5.34	114.67	126.02
20	L	202	CLA	C4D-C3D-CAD	5.34	113.90	108.11
20	B	812	CLA	C3B-C2B-C1B	-5.33	100.88	107.17
20	2	307	CLA	C4D-C3D-CAD	5.33	113.90	108.11
20	A	803	CLA	C4B-CHC-C1C	-5.33	113.70	126.25
20	A	807	CLA	C1D-CHD-C4C	-5.33	114.68	126.02
20	A	817	CLA	C4D-C3D-CAD	5.33	113.90	108.11
20	A	830	CLA	C1D-CHD-C4C	-5.33	114.69	126.02
20	A	810	CLA	C4D-C3D-CAD	5.33	113.89	108.11
20	F	204	CLA	OBD-CAD-C3D	-5.33	115.97	128.42
20	A	827	CLA	CMD-C2D-C1D	5.32	134.10	124.73
20	B	816	CLA	CHD-C4C-C3C	-5.32	117.01	124.77
20	A	816	CLA	C2B-C1B-NB	5.32	115.84	110.33
20	A	826	CLA	CMD-C2D-C1D	5.32	134.10	124.73
20	3	319	CLA	CHD-C4C-NC	5.32	132.48	124.23
20	A	805	CLA	C4D-C3D-CAD	5.32	113.88	108.11
20	G	103	CLA	C4D-C3D-CAD	5.31	113.88	108.11
20	4	318	CLA	C4A-NA-C1A	5.31	109.10	106.68
20	1	203	CLA	CMD-C2D-C3D	-5.31	115.50	127.69
20	1	215	CLA	C3A-C4A-CHB	-5.31	117.41	123.91
20	A	818	CLA	C1D-CHD-C4C	-5.31	114.74	126.02
20	A	803	CLA	C4D-C3D-CAD	5.30	113.87	108.11
20	A	813	CLA	C4D-C3D-CAD	5.30	113.87	108.11
20	3	314	CLA	O2D-CGD-CBD	5.30	120.50	111.23
20	1	209	CLA	CMD-C2D-C3D	-5.30	115.53	127.69
20	2	312	CLA	CMD-C2D-C1D	5.30	134.06	124.73
20	A	809	CLA	CHC-C1C-NC	5.30	132.29	124.31
20	A	809	CLA	C2B-C1B-NB	5.30	115.82	110.33
20	2	311	CLA	C4D-C3D-CAD	5.30	113.86	108.11
20	B	827	CLA	C4D-C3D-CAD	5.29	113.85	108.11
20	F	204	CLA	CBD-CAD-C3D	-5.29	101.19	108.25
22	F	202	BCR	C11-C10-C9	-5.29	119.86	127.28
20	2	305	CLA	CHC-C1C-NC	5.28	132.09	124.33
20	2	307	CLA	CMD-C2D-C1D	5.28	134.03	124.73
21	R	102	LMU	O3B-C3B-C4B	-5.28	97.93	110.38
22	F	202	BCR	C15-C14-C13	-5.28	119.88	127.28
21	R	103	LMU	O1B-C1B-C2B	5.28	121.07	108.09
20	2	302	CLA	C1D-CHD-C4C	-5.27	114.81	126.02
20	J	103	CLA	C4D-C3D-CAD	5.27	113.83	108.11
20	B	815	CLA	C4D-C3D-CAD	5.27	113.83	108.11
20	H	101	CLA	C1D-CHD-C4C	-5.27	114.83	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	841	BCR	C11-C10-C9	-5.26	119.90	127.28
20	4	315	CLA	CHD-C4C-NC	5.26	132.39	124.23
20	2	321	CLA	C2B-C1B-NB	5.26	115.78	110.33
20	1	202	CLA	C1D-CHD-C4C	-5.26	114.84	126.02
20	B	838	CLA	CMD-C2D-C1D	5.26	133.99	124.73
22	A	844	BCR	C16-C17-C18	-5.26	119.91	127.28
20	K	105	CLA	CHD-C4C-NC	5.25	132.38	124.23
20	K	103	CLA	CHD-C4C-NC	5.25	132.37	124.23
20	A	812	CLA	C4D-C3D-CAD	5.25	113.81	108.11
20	4	302	CLA	CHD-C4C-NC	5.25	132.37	124.23
20	A	831	CLA	CHD-C4C-NC	5.25	132.37	124.23
20	3	315	CLA	CMD-C2D-C3D	-5.25	115.65	127.69
20	4	311	CLA	C3A-C4A-CHB	-5.25	117.48	123.91
20	2	317	CLA	C1D-CHD-C4C	-5.25	114.87	126.02
20	B	848	CLA	CMD-C2D-C1D	5.24	133.96	124.73
20	1	203	CLA	C1D-CHD-C4C	-5.24	114.88	126.02
22	A	843	BCR	C15-C14-C13	-5.24	119.93	127.28
20	B	832	CLA	C1D-CHD-C4C	-5.24	114.88	126.02
20	A	837	CLA	CHD-C4C-NC	5.24	132.35	124.23
20	A	816	CLA	CHD-C4C-NC	5.24	132.35	124.23
20	2	312	CLA	C4D-C3D-CAD	5.24	113.79	108.11
20	2	314	CLA	C1B-NB-C4B	-5.23	102.64	106.31
20	B	826	CLA	CHC-C4B-NB	5.23	131.90	124.05
20	F	205	CLA	CHD-C4C-NC	5.23	132.34	124.23
20	R	107	CLA	C1D-CHD-C4C	-5.23	114.90	126.02
20	2	305	CLA	C2D-C3D-C4D	-5.23	101.00	107.35
20	J	102	CLA	CHD-C4C-NC	5.23	132.34	124.23
20	L	203	CLA	CHD-C4C-C3C	-5.23	117.15	124.77
20	2	317	CLA	C2B-C1B-NB	5.23	115.75	110.33
20	4	305	CLA	C4B-CHC-C1C	-5.23	113.96	126.25
20	A	855	CLA	CHD-C4C-NC	5.23	132.33	124.23
20	A	847	CLA	CMD-C2D-C1D	5.23	133.93	124.73
20	B	822	CLA	CHD-C4C-NC	5.22	132.33	124.23
20	3	310	CLA	CHD-C4C-NC	5.22	132.33	124.23
22	B	842	BCR	C24-C23-C22	-5.22	118.51	126.23
22	J	101	BCR	C15-C14-C13	-5.22	119.95	127.28
20	A	835	CLA	CHD-C4C-NC	5.22	132.33	124.23
22	B	844	BCR	C16-C17-C18	-5.22	119.95	127.28
20	B	824	CLA	C4D-C3D-CAD	5.22	113.78	108.11
20	A	834	CLA	CHD-C4C-NC	5.22	132.32	124.23
20	A	819	CLA	C4A-NA-C1A	5.22	109.06	106.68
20	R	106	CLA	C1D-CHD-C4C	-5.22	114.93	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	843	BCR	C11-C10-C9	-5.22	119.96	127.28
20	A	821	CLA	C2B-C1B-NB	5.21	115.73	110.33
20	B	847	CLA	C3B-C2B-C1B	-5.21	101.02	107.17
20	A	808	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
21	R	103	LMU	O3B-C3B-C4B	-5.21	98.09	110.38
20	4	304	CLA	C4B-CHC-C1C	-5.21	114.00	126.25
21	R	102	LMU	O1B-C4'-C3'	5.21	120.47	107.23
20	A	833	CLA	CHD-C4C-NC	5.21	132.30	124.23
21	K	101	LMU	C6B-C5B-C4B	-5.20	100.24	113.02
20	A	836	CLA	CHD-C4C-NC	5.20	132.30	124.23
22	A	840	BCR	C16-C17-C18	-5.20	119.98	127.28
22	B	841	BCR	C15-C14-C13	-5.20	119.98	127.28
20	1	207	CLA	C1D-CHD-C4C	-5.20	114.97	126.02
22	A	840	BCR	C15-C14-C13	-5.20	119.98	127.28
21	G	101	LMU	C1B-C2B-C3B	-5.20	99.08	110.01
20	B	848	CLA	C2B-C1B-NB	5.20	115.72	110.33
20	A	822	CLA	CHD-C4C-NC	5.20	132.29	124.23
20	L	202	CLA	CMD-C2D-C1D	5.20	133.88	124.73
22	A	842	BCR	C11-C10-C9	-5.20	119.99	127.28
22	F	202	BCR	C16-C17-C18	-5.20	119.99	127.28
20	A	832	CLA	CHD-C4C-NC	5.19	132.28	124.23
20	A	823	CLA	CHD-C4C-NC	5.19	132.28	124.23
22	J	101	BCR	C16-C17-C18	-5.19	120.00	127.28
22	B	843	BCR	C15-C14-C13	-5.19	120.00	127.28
20	3	319	CLA	CAB-C3B-C2B	-5.19	109.75	123.53
20	B	823	CLA	CHD-C4C-NC	5.19	132.28	124.23
22	A	841	BCR	C11-C10-C9	-5.19	120.01	127.28
22	B	843	BCR	C11-C10-C9	-5.19	120.01	127.28
20	4	319	CLA	CHD-C4C-NC	5.18	132.27	124.23
22	A	844	BCR	C11-C10-C9	-5.18	120.01	127.28
22	A	841	BCR	C15-C14-C13	-5.18	120.01	127.28
22	A	843	BCR	C16-C17-C18	-5.18	120.01	127.28
20	2	317	CLA	O2D-CGD-CBD	5.18	120.28	111.23
22	A	841	BCR	C16-C17-C18	-5.18	120.02	127.28
22	A	842	BCR	C16-C17-C18	-5.18	120.02	127.28
20	3	301	CLA	O2D-CGD-CBD	5.18	120.28	111.23
20	A	801	CLA	CHD-C4C-NC	5.18	132.25	124.23
20	H	101	CLA	O2D-CGD-CBD	5.18	120.28	111.23
20	B	803	CLA	O2D-CGD-O1D	-5.17	113.78	123.85
20	B	833	CLA	O2D-CGD-CBD	5.17	120.28	111.23
22	B	842	BCR	C27-C26-C25	-5.17	115.71	122.70
20	B	828	CLA	C1D-CHD-C4C	-5.17	115.03	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	301	CLA	CHD-C4C-NC	5.17	132.25	124.23
20	4	313	CLA	C4A-NA-C1A	5.17	109.04	106.68
20	1	210	CLA	CBD-CAD-C3D	-5.17	101.35	108.25
22	B	844	BCR	C15-C14-C13	-5.17	120.03	127.28
20	B	847	CLA	C4B-CHC-C1C	-5.17	114.09	126.25
22	B	844	BCR	C11-C10-C9	-5.17	120.03	127.28
20	B	825	CLA	CHD-C4C-C3C	-5.17	117.24	124.77
20	A	823	CLA	O2D-CGD-CBD	5.16	120.25	111.23
20	4	307	CLA	CBC-CAC-C3C	-5.16	98.43	112.42
20	A	827	CLA	C1D-CHD-C4C	-5.16	115.05	126.02
22	B	843	BCR	C16-C17-C18	-5.16	120.05	127.28
20	A	821	CLA	C4D-C3D-CAD	5.16	113.70	108.11
22	B	841	BCR	C16-C17-C18	-5.15	120.05	127.28
20	A	819	CLA	C1D-CHD-C4C	-5.15	115.07	126.02
22	J	101	BCR	C11-C10-C9	-5.15	120.06	127.28
20	4	306	CLA	O2D-CGD-CBD	5.15	120.23	111.23
20	2	309	CLA	C3A-C4A-CHB	-5.14	117.61	123.91
22	A	842	BCR	C15-C14-C13	-5.14	120.06	127.28
20	A	813	CLA	C1D-CHD-C4C	-5.14	115.09	126.02
20	A	850	CLA	C4A-NA-C1A	5.14	109.03	106.68
20	B	839	CLA	C1D-CHD-C4C	-5.14	115.09	126.02
22	A	844	BCR	C15-C14-C13	-5.14	120.07	127.28
20	H	108	CLA	CMD-C2D-C1D	5.14	133.78	124.73
20	G	103	CLA	CHD-C4C-NC	5.14	132.20	124.23
21	E	101	LMU	C3B-C4B-C5B	-5.14	100.92	110.23
20	L	201	CLA	C1D-CHD-C4C	-5.14	115.10	126.02
22	G	102	BCR	C16-C17-C18	-5.13	120.08	127.28
20	A	807	CLA	CAC-C3C-C4C	5.13	131.47	124.79
22	G	102	BCR	C15-C14-C13	-5.13	120.08	127.28
20	B	815	CLA	CHD-C4C-C3C	-5.13	117.29	124.77
20	B	806	CLA	C1D-CHD-C4C	-5.13	115.12	126.02
20	A	822	CLA	O2D-CGD-CBD	5.13	120.19	111.23
21	E	101	LMU	O4'-C4B-C5B	5.13	121.95	109.32
22	G	102	BCR	C11-C10-C9	-5.12	120.09	127.28
20	A	835	CLA	O2D-CGD-CBD	5.12	120.19	111.23
20	A	813	CLA	CMD-C2D-C1D	5.12	133.75	124.73
20	2	308	CLA	C4A-NA-C1A	5.12	109.02	106.68
20	2	301	CLA	O2D-CGD-CBD	5.12	120.18	111.23
20	A	832	CLA	O2D-CGD-CBD	5.12	120.18	111.23
20	K	103	CLA	O2D-CGD-CBD	5.12	120.18	111.23
20	K	105	CLA	O2D-CGD-CBD	5.12	120.18	111.23
20	A	831	CLA	O2D-CGD-CBD	5.12	120.18	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	833	CLA	O2D-CGD-CBD	5.12	120.18	111.23
20	J	102	CLA	O2D-CGD-CBD	5.12	120.18	111.23
20	4	304	CLA	O2A-CGA-O1A	-5.12	110.83	123.63
20	A	806	CLA	C2B-C1B-NB	5.11	115.63	110.33
20	4	319	CLA	O2D-CGD-CBD	5.11	120.17	111.23
20	A	829	CLA	CMD-C2D-C3D	-5.11	115.96	127.69
22	A	840	BCR	C11-C10-C9	-5.11	120.11	127.28
20	A	804	CLA	C2B-C1B-NB	5.11	115.63	110.33
20	L	201	CLA	C2B-C1B-NB	5.11	115.63	110.33
20	K	106	CLA	C1D-CHD-C4C	-5.11	115.16	126.02
20	F	206	CLA	CHD-C4C-C3C	-5.11	117.32	124.77
20	1	205	CLA	CBD-CAD-C3D	-5.11	101.43	108.25
20	A	855	CLA	O2D-CGD-CBD	5.11	120.16	111.23
20	L	203	CLA	CHD-C4C-NC	5.11	132.15	124.23
20	2	306	CLA	CHD-C4C-NC	5.11	132.15	124.23
20	B	823	CLA	O2D-CGD-CBD	5.11	120.16	111.23
20	4	303	CLA	C1B-C2B-C3B	-5.10	102.23	107.03
20	A	806	CLA	C1D-CHD-C4C	-5.10	115.17	126.02
20	3	310	CLA	O2D-CGD-CBD	5.10	120.15	111.23
20	A	834	CLA	O2D-CGD-CBD	5.10	120.15	111.23
22	I	103	BCR	C15-C14-C13	5.10	134.43	127.28
20	B	813	CLA	C4A-NA-C1A	5.10	109.01	106.68
20	A	804	CLA	O2D-CGD-CBD	5.10	120.14	111.23
20	A	836	CLA	O2D-CGD-CBD	5.10	120.14	111.23
20	A	837	CLA	O2D-CGD-CBD	5.10	120.14	111.23
20	B	833	CLA	C1D-CHD-C4C	-5.09	115.19	126.02
20	A	848	CLA	CHD-C4C-NC	5.09	132.13	124.23
20	A	849	CLA	C2B-C1B-NB	5.09	115.61	110.33
20	B	837	CLA	CMD-C2D-C3D	-5.09	116.02	127.69
20	4	302	CLA	O2D-CGD-CBD	5.09	120.13	111.23
20	B	828	CLA	CMD-C2D-C1D	5.09	133.69	124.73
20	A	808	CLA	C4D-C3D-CAD	5.09	113.63	108.11
20	B	822	CLA	O2D-CGD-CBD	5.09	120.12	111.23
20	B	805	CLA	C2B-C1B-NB	5.09	115.60	110.33
20	F	205	CLA	O2D-CGD-CBD	5.08	120.12	111.23
20	A	827	CLA	O2D-CGD-O1D	-5.08	113.95	123.85
20	R	107	CLA	CMD-C2D-C3D	-5.08	116.03	127.69
20	3	307	CLA	C3A-C4A-CHB	-5.08	117.69	123.91
20	2	310	CLA	C4A-NA-C1A	5.08	109.00	106.68
20	A	848	CLA	CMD-C2D-C1D	5.08	133.67	124.73
20	B	811	CLA	OBD-CAD-C3D	-5.08	116.55	128.42
20	B	836	CLA	CHD-C4C-NC	5.07	132.10	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	850	CLA	C1D-CHD-C4C	-5.07	115.24	126.02
20	1	211	CLA	CHC-C1C-NC	5.07	131.95	124.31
20	B	803	CLA	CHD-C4C-NC	5.07	132.09	124.23
20	2	308	CLA	CHD-C4C-NC	5.07	131.94	124.24
20	4	318	CLA	CHD-C4C-NC	5.06	132.08	124.23
20	G	103	CLA	C2B-C1B-NB	5.06	115.58	110.33
20	4	312	CLA	C2A-C1A-CHA	-5.06	114.00	122.63
22	B	850	BCR	C34-C9-C10	-5.06	114.62	122.82
20	B	820	CLA	C2A-C1A-CHA	-5.06	115.09	123.87
20	B	832	CLA	CHD-C4C-NC	5.06	132.07	124.23
20	A	829	CLA	O1D-CGD-CBD	-5.05	114.55	124.52
20	1	201	CLA	CHB-C4A-NA	5.05	131.69	124.40
20	B	834	CLA	CMD-C2D-C3D	-5.05	116.10	127.69
20	A	838	CLA	CMD-C2D-C3D	-5.05	116.11	127.69
20	2	302	CLA	C2B-C1B-NB	5.05	115.56	110.33
20	B	805	CLA	C6-C5-C3	-5.05	101.17	113.47
20	4	311	CLA	CHD-C4C-NC	5.05	131.91	124.24
20	K	106	CLA	C4B-CHC-C1C	-5.04	114.39	126.25
20	B	812	CLA	CMD-C2D-C1D	5.04	133.61	124.73
20	4	307	CLA	CHD-C4C-C3C	-5.04	117.42	124.77
20	A	821	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
21	L	205	LMU	O5B-C5B-C4B	-5.03	100.63	109.70
21	R	109	LMU	C1'-C2'-C3'	-5.03	99.42	110.01
20	4	318	CLA	C1D-CHD-C4C	-5.03	115.33	126.02
20	B	804	CLA	CHD-C4C-NC	5.03	132.03	124.23
20	1	214	CLA	C4A-NA-C1A	-5.03	104.39	106.68
20	1	202	CLA	CAA-C2A-C1A	5.03	128.45	111.97
21	H	103	LMU	C4B-C3B-C2B	-5.03	102.01	110.83
20	A	802	CLA	C1-O2A-CGA	5.02	128.81	116.65
20	A	804	CLA	C1D-CHD-C4C	-5.02	115.34	126.02
20	B	805	CLA	C4D-C3D-CAD	5.02	113.56	108.11
20	A	802	CLA	C4B-CHC-C1C	-5.02	114.45	126.25
20	3	320	CLA	C2B-C1B-NB	5.02	115.53	110.33
20	4	305	CLA	CHC-C1C-NC	5.01	131.86	124.31
20	B	809	CLA	C1D-CHD-C4C	-5.01	115.36	126.02
20	4	304	CLA	O2D-CGD-CBD	5.01	119.99	111.23
20	3	304	CLA	C1C-CHC-C4B	-5.01	112.83	126.04
20	A	814	CLA	CHD-C4C-NC	5.01	132.00	124.23
20	3	301	CLA	CHD-C4C-C3C	-5.01	117.47	124.77
20	1	206	CLA	CHD-C4C-NC	5.01	132.00	124.23
22	F	203	BCR	C16-C17-C18	-5.00	120.26	127.28
20	B	838	CLA	C1D-CHD-C4C	-5.00	115.38	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	R	102	LMU	C1B-O1B-C4'	5.00	129.83	117.98
20	J	103	CLA	CHD-C4C-C3C	-5.00	117.49	124.77
20	B	828	CLA	C4A-NA-C1A	5.00	108.96	106.68
20	L	208	CLA	C4D-C3D-CAD	4.99	113.53	108.11
20	B	830	CLA	CHD-C4C-C3C	-4.99	117.50	124.77
20	A	805	CLA	CMD-C2D-C1D	4.99	133.51	124.73
20	2	310	CLA	C1D-CHD-C4C	-4.99	115.42	126.02
20	A	812	CLA	C1D-CHD-C4C	-4.99	115.42	126.02
20	1	215	CLA	C1B-NB-C4B	-4.99	102.81	106.31
20	L	202	CLA	C1D-CHD-C4C	-4.99	115.42	126.02
20	A	848	CLA	CHD-C4C-C3C	-4.99	117.50	124.77
20	1	208	CLA	C3A-C4A-CHB	-4.98	117.81	123.91
22	3	311	BCR	C33-C5-C6	-4.98	119.05	124.48
23	B	840	PQN	C11-C12-C13	-4.98	118.25	126.83
20	A	811	CLA	C2B-C1B-NB	4.98	115.49	110.33
20	A	811	CLA	CHD-C4C-NC	4.98	131.95	124.23
21	H	102	LMU	O5B-C5B-C4B	-4.98	100.73	109.70
20	B	812	CLA	C2B-C1B-NB	4.97	115.48	110.33
20	A	809	CLA	C1-C2-C3	-4.97	118.05	126.20
20	B	837	CLA	CHD-C4C-NC	4.97	131.94	124.23
20	B	837	CLA	CHC-C1C-NC	4.97	131.80	124.31
20	A	847	CLA	C1D-CHD-C4C	-4.97	115.46	126.02
21	H	105	LMU	C4B-C3B-C2B	-4.97	102.11	110.83
20	B	804	CLA	C2B-C1B-NB	4.97	115.48	110.33
20	A	811	CLA	O2D-CGD-CBD	4.97	119.91	111.23
20	B	807	CLA	CHD-C4C-NC	4.96	131.93	124.23
20	A	801	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
20	A	826	CLA	C4A-NA-C1A	4.96	108.94	106.68
20	A	807	CLA	C4B-CHC-C1C	-4.96	114.58	126.25
20	L	204	CLA	C4-C3-C2	-4.96	110.89	123.63
20	1	207	CLA	C2A-C3A-C4A	-4.96	93.86	101.87
20	B	816	CLA	CMD-C2D-C1D	4.96	133.46	124.73
20	B	837	CLA	C2B-C1B-NB	4.96	115.47	110.33
20	L	201	CLA	C4-C3-C5	4.96	123.83	115.23
20	B	835	CLA	C1D-CHD-C4C	-4.95	115.49	126.02
20	2	321	CLA	CMD-C2D-C1D	4.95	133.44	124.73
20	2	304	CLA	C1D-CHD-C4C	-4.95	115.50	126.02
20	B	816	CLA	CHD-C4C-NC	4.95	131.90	124.23
20	B	804	CLA	C4B-CHC-C1C	-4.95	114.61	126.25
20	B	826	CLA	CMD-C2D-C3D	-4.95	116.35	127.69
20	B	812	CLA	C4D-C3D-CAD	4.95	113.48	108.11
21	H	105	LMU	O3'-C3'-C4'	-4.94	97.27	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	R	106	CLA	CMD-C2D-C3D	-4.94	116.36	127.69
21	H	105	LMU	C1B-C2B-C3B	4.94	120.40	110.01
20	B	811	CLA	CMD-C2D-C3D	-4.94	116.36	127.69
20	A	810	CLA	CHD-C4C-NC	4.94	131.89	124.23
20	3	315	CLA	O2D-CGD-CBD	4.94	119.86	111.23
21	K	104	LMU	O5B-C5B-C4B	-4.94	100.81	109.70
20	A	850	CLA	CHC-C1C-NC	4.93	131.74	124.31
20	A	847	CLA	C4B-CHC-C1C	-4.93	114.66	126.25
22	3	311	BCR	C7-C8-C9	-4.93	118.95	126.23
20	B	838	CLA	C4B-CHC-C1C	-4.93	114.67	126.25
20	K	106	CLA	CHC-C1C-NC	4.93	131.73	124.31
22	L	209	BCR	C7-C8-C9	-4.92	118.95	126.23
22	L	209	BCR	C36-C18-C19	4.92	125.61	118.09
20	4	309	CLA	C2A-C1A-CHA	-4.92	114.24	122.63
20	B	808	CLA	CMD-C2D-C3D	-4.92	116.41	127.69
20	A	824	CLA	C2B-C1B-NB	4.92	115.43	110.33
20	A	848	CLA	C4D-C3D-CAD	4.92	113.45	108.11
20	H	110	CLA	CMD-C2D-C3D	-4.92	116.42	127.69
20	B	820	CLA	O2D-CGD-O1D	-4.91	114.29	123.85
20	B	817	CLA	O2D-CGD-CBD	4.91	119.82	111.23
20	B	847	CLA	C2B-C1B-NB	4.91	115.42	110.33
20	4	304	CLA	CHD-C4C-C3C	-4.91	117.62	124.77
20	1	214	CLA	C4B-CHC-C1C	-4.90	114.73	126.25
22	L	209	BCR	C33-C5-C6	-4.90	119.14	124.48
20	A	849	CLA	C1D-CHD-C4C	-4.90	115.61	126.02
20	4	307	CLA	CMB-C2B-C1B	-4.90	117.96	125.42
20	3	303	CLA	C4D-C3D-CAD	4.90	113.42	108.11
20	B	813	CLA	CHD-C4C-NC	4.90	131.82	124.23
20	A	809	CLA	C4B-C3B-C2B	4.90	113.39	107.30
20	3	314	CLA	C1D-CHD-C4C	-4.89	115.62	126.02
20	L	204	CLA	C4D-CHA-C1A	4.89	127.08	121.24
20	B	820	CLA	C4B-CHC-C1C	-4.89	114.75	126.25
20	A	824	CLA	C1-C2-C3	-4.89	118.19	126.20
21	2	318	LMU	C1B-O1B-C4'	-4.89	106.39	117.98
20	1	205	CLA	CHD-C4C-NC	4.89	131.81	124.23
20	A	849	CLA	CHD-C4C-NC	4.89	131.81	124.23
20	3	306	CLA	CHC-C1C-NC	4.89	131.51	124.33
20	1	206	CLA	O2D-CGD-CBD	4.89	119.77	111.23
20	2	303	CLA	CHD-C4C-NC	4.88	131.66	124.24
20	I	102	CLA	CHD-C4C-NC	4.88	131.79	124.23
20	2	307	CLA	C2B-C1B-NB	4.88	115.38	110.33
20	3	308	CLA	C1C-CHC-C4B	-4.87	113.19	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	314	CLA	C2A-C1A-CHA	-4.87	114.32	122.63
20	A	803	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
20	3	309	CLA	C4B-CHC-C1C	-4.87	114.80	126.25
20	2	302	CLA	CMD-C2D-C3D	-4.87	116.52	127.69
20	H	109	CLA	CHD-C4C-NC	4.87	131.78	124.23
22	F	203	BCR	C35-C13-C14	-4.87	114.93	122.82
20	B	806	CLA	CMD-C2D-C1D	4.86	133.29	124.73
20	1	202	CLA	C4B-CHC-C1C	-4.86	114.81	126.25
20	B	849	CLA	CHC-C1C-NC	4.86	131.63	124.31
20	2	307	CLA	C1D-CHD-C4C	-4.86	115.69	126.02
20	B	848	CLA	C4A-NA-C1A	4.86	108.90	106.68
20	2	314	CLA	C2D-C3D-C4D	-4.86	101.45	107.35
20	B	827	CLA	C2B-C1B-NB	4.86	115.36	110.33
20	B	832	CLA	CHD-C4C-C3C	-4.86	117.69	124.77
20	B	803	CLA	CMD-C2D-C3D	-4.85	116.56	127.69
20	A	826	CLA	CHD-C4C-NC	4.85	131.75	124.23
20	B	824	CLA	CHD-C4C-NC	4.85	131.75	124.23
20	3	305	CLA	CHC-C1C-NC	4.85	131.46	124.33
20	B	815	CLA	CHD-C4C-NC	4.85	131.75	124.23
20	4	313	CLA	CMD-C2D-C1D	4.85	133.26	124.73
20	A	847	CLA	CHC-C4B-NB	4.85	131.32	124.05
20	2	308	CLA	CHC-C1C-NC	4.84	131.45	124.33
20	A	824	CLA	CHD-C4C-NC	4.84	131.74	124.23
20	B	831	CLA	CHD-C4C-NC	4.84	131.74	124.23
20	B	848	CLA	CHD-C4C-NC	4.84	131.74	124.23
20	B	821	CLA	C4D-C3D-CAD	4.84	113.36	108.11
20	4	305	CLA	C4A-NA-C1A	4.84	108.89	106.68
20	1	211	CLA	CBA-CAA-C2A	4.84	128.19	113.79
20	B	811	CLA	C1D-CHD-C4C	-4.84	115.73	126.02
20	2	305	CLA	CHD-C4C-NC	4.84	131.59	124.24
21	R	109	LMU	O1'-C1'-C2'	4.84	115.62	108.27
20	B	834	CLA	CHD-C4C-NC	4.83	131.73	124.23
20	B	804	CLA	CMD-C2D-C3D	-4.83	116.61	127.69
20	3	308	CLA	C1B-NB-C4B	-4.83	102.92	106.31
21	K	102	LMU	O1B-C4'-C5'	4.83	122.14	109.48
20	B	814	CLA	C1D-CHD-C4C	-4.83	115.76	126.02
20	1	201	CLA	CHD-C4C-NC	4.82	131.71	124.23
20	A	819	CLA	C3B-C2B-C1B	-4.82	101.48	107.17
20	J	103	CLA	C4A-NA-C1A	4.82	108.88	106.68
20	H	109	CLA	CHD-C4C-C3C	-4.81	117.76	124.77
21	2	318	LMU	O1'-C1'-C2'	4.81	115.58	108.27
20	B	804	CLA	C3B-C2B-C1B	-4.81	101.50	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	H	103	LMU	O5'-C1'-C2'	-4.80	100.50	110.37
20	A	838	CLA	C2B-C1B-NB	4.80	115.31	110.33
20	K	106	CLA	C2B-C1B-NB	4.80	115.31	110.33
20	1	207	CLA	CAA-C2A-C3A	4.80	125.97	113.00
20	2	302	CLA	CHD-C4C-NC	4.80	131.67	124.23
20	A	805	CLA	C1D-CHD-C4C	-4.80	115.82	126.02
20	B	805	CLA	CMB-C2B-C1B	4.80	132.72	125.42
20	B	835	CLA	O2D-CGD-O1D	-4.80	114.51	123.85
20	4	307	CLA	C4A-NA-C1A	4.80	108.87	106.68
20	L	201	CLA	CHD-C4C-NC	4.79	131.66	124.23
22	B	842	BCR	C16-C17-C18	-4.79	120.56	127.28
22	I	101	BCR	C30-C25-C26	-4.79	116.09	122.64
20	3	309	CLA	CHC-C4B-NB	4.79	131.24	124.05
22	I	101	BCR	C37-C22-C23	-4.79	110.77	118.09
20	R	107	CLA	CMB-C2B-C1B	4.79	132.71	125.42
20	B	836	CLA	C3B-C2B-C1B	-4.79	101.53	107.17
20	2	314	CLA	C4A-NA-C1A	4.78	108.86	106.68
20	K	106	CLA	CMA-C3A-C4A	-4.78	98.92	111.77
20	B	814	CLA	C4D-C3D-CAD	4.78	113.30	108.11
23	B	840	PQN	C2M-C2-C3	-4.78	116.59	124.45
20	A	830	CLA	O2D-CGD-CBD	4.78	119.58	111.23
20	H	109	CLA	C2B-C1B-NB	4.78	115.28	110.33
22	F	203	BCR	C34-C9-C8	4.77	125.38	118.09
20	3	303	CLA	CHD-C4C-C3C	-4.77	117.50	125.03
20	B	805	CLA	CHD-C4C-NC	4.77	131.63	124.23
20	A	808	CLA	CMD-C2D-C3D	-4.77	116.75	127.69
20	L	204	CLA	CHD-C4C-NC	4.77	131.63	124.23
20	B	831	CLA	C4A-NA-C1A	4.77	108.86	106.68
22	I	101	BCR	C28-C27-C26	-4.77	105.55	114.06
20	B	830	CLA	CHD-C4C-NC	4.77	131.62	124.23
20	B	831	CLA	CHD-C4C-C3C	-4.77	117.82	124.77
20	B	835	CLA	C4B-CHC-C1C	-4.77	115.04	126.25
20	3	308	CLA	CHC-C1C-NC	4.76	131.33	124.33
20	H	109	CLA	CMD-C2D-C1D	4.76	133.11	124.73
20	I	102	CLA	C4D-C3D-CAD	4.75	113.26	108.11
21	H	102	LMU	O4'-C4B-C5B	4.75	121.02	109.32
20	4	313	CLA	C1B-C2B-C3B	-4.75	102.57	107.03
20	3	312	CLA	C4A-NA-C1A	4.75	108.84	106.68
20	1	211	CLA	C4B-CHC-C1C	-4.75	115.09	126.25
20	K	107	CLA	CHD-C4C-NC	4.74	131.59	124.23
20	A	817	CLA	C2B-C1B-NB	4.73	115.24	110.33
20	3	316	CLA	C2A-C1A-CHA	-4.73	114.56	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	827	CLA	C4D-C3D-CAD	4.73	113.25	108.11
20	4	313	CLA	CBD-CHA-C1A	4.73	134.52	127.38
20	A	802	CLA	O2A-CGA-CBA	4.73	126.25	111.83
20	A	809	CLA	CHD-C4C-NC	4.73	131.56	124.23
20	H	110	CLA	C4-C3-C5	4.73	123.44	115.23
20	L	202	CLA	C1-C2-C3	-4.73	118.45	126.20
20	A	802	CLA	C4B-C3B-C2B	4.73	113.18	107.30
20	3	313	CLA	C2A-C1A-CHA	-4.73	114.57	122.63
20	1	215	CLA	CHC-C1C-NC	4.72	131.27	124.33
20	A	829	CLA	CHC-C1C-NC	4.72	131.43	124.31
20	A	857	CLA	C2A-C1A-CHA	-4.72	114.58	122.63
20	R	107	CLA	CHD-C4C-NC	4.72	131.55	124.23
20	B	807	CLA	CMD-C2D-C1D	4.72	133.04	124.73
20	A	849	CLA	C1-C2-C3	4.72	133.93	126.20
22	F	203	BCR	C8-C7-C6	-4.72	114.40	127.00
20	B	837	CLA	C1D-CHD-C4C	-4.71	116.00	126.02
20	B	817	CLA	CHD-C4C-C3C	-4.71	117.91	124.77
20	1	207	CLA	CMD-C2D-C3D	-4.71	116.90	127.69
20	2	305	CLA	C1C-CHC-C4B	-4.71	113.63	126.04
20	3	308	CLA	C2A-C1A-CHA	-4.71	114.61	122.63
20	A	802	CLA	C3B-C4B-NB	-4.70	106.33	110.53
20	B	836	CLA	C4D-C3D-CAD	4.70	113.21	108.11
20	K	107	CLA	CHD-C4C-C3C	-4.70	117.92	124.77
20	1	201	CLA	CAC-C3C-C2C	-4.70	118.92	127.56
21	H	102	LMU	O3B-C3B-C4B	4.70	121.46	110.38
20	2	307	CLA	C4B-CHC-C1C	-4.70	115.20	126.25
20	1	201	CLA	CBC-CAC-C3C	-4.70	99.68	112.42
20	1	215	CLA	C3B-C2B-C1B	-4.70	101.58	106.81
20	A	828	CLA	CHD-C4C-NC	4.70	131.51	124.23
20	3	313	CLA	CHD-C4C-NC	4.69	131.37	124.24
20	A	850	CLA	CAC-C3C-C4C	4.69	130.90	124.79
20	4	315	CLA	C2B-C1B-NB	4.69	115.19	110.33
20	A	801	CLA	CHD-C4C-C3C	-4.69	117.93	124.77
20	A	807	CLA	CMD-C2D-C3D	-4.69	116.93	127.69
20	B	826	CLA	CHD-C4C-NC	4.69	131.50	124.23
20	L	207	CLA	CHD-C4C-NC	4.69	131.50	124.23
20	B	839	CLA	C4A-NA-C1A	4.69	108.82	106.68
20	B	826	CLA	C4B-CHC-C1C	-4.68	115.23	126.25
20	B	833	CLA	C4-C3-C5	4.68	121.64	116.13
20	J	103	CLA	O2D-CGD-CBD	4.68	119.42	111.23
20	F	204	CLA	CMD-C2D-C3D	-4.68	116.95	127.69
20	1	202	CLA	C2B-C1B-NB	4.68	115.18	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	835	CLA	CHD-C4C-NC	4.68	131.49	124.23
20	3	320	CLA	CHD-C4C-NC	4.68	131.49	124.23
20	A	806	CLA	CHD-C4C-NC	4.68	131.49	124.23
20	B	848	CLA	C4D-C3D-CAD	4.68	113.19	108.11
20	B	808	CLA	CAB-C3B-C2B	-4.68	111.11	123.53
20	A	808	CLA	C4B-CHC-C1C	-4.68	115.25	126.25
20	4	307	CLA	O2A-CGA-O1A	-4.67	111.94	123.63
20	2	303	CLA	C3A-C4A-CHB	-4.67	118.19	123.91
20	2	307	CLA	O2D-CGD-O1D	-4.67	114.76	123.85
20	B	849	CLA	CHD-C4C-NC	4.67	131.47	124.23
20	A	808	CLA	C1D-CHD-C4C	-4.66	116.11	126.02
20	B	829	CLA	CHD-C4C-NC	4.66	131.46	124.23
20	B	815	CLA	C2B-C1B-NB	4.66	115.16	110.33
21	G	101	LMU	O3B-C3B-C4B	4.66	121.36	110.38
20	1	210	CLA	CHD-C4C-NC	4.66	131.46	124.23
20	B	827	CLA	C1D-CHD-C4C	-4.65	116.13	126.02
21	L	205	LMU	C1'-O5'-C5'	4.65	122.81	113.72
21	B	801	LMU	O1B-C4'-C3'	4.65	119.05	107.23
20	B	830	CLA	O1D-CGD-CBD	-4.65	115.35	124.52
20	A	807	CLA	CHC-C4B-NB	4.65	131.02	124.05
20	B	804	CLA	C4A-NA-C1A	4.64	108.80	106.68
20	4	309	CLA	CHA-C4D-ND	4.64	131.40	124.84
20	4	311	CLA	C4C-CHD-C1D	-4.64	112.75	125.98
20	2	304	CLA	C2B-C1B-NB	4.64	115.14	110.33
20	B	815	CLA	CHC-C1C-NC	4.64	131.30	124.31
20	2	307	CLA	CHC-C1C-NC	4.64	131.30	124.31
20	4	318	CLA	C4B-CHC-C1C	-4.64	115.34	126.25
20	4	318	CLA	O2D-CGD-CBD	4.64	119.33	111.23
20	H	110	CLA	CHD-C4C-NC	4.63	131.41	124.23
22	3	311	BCR	C16-C15-C14	-4.63	114.05	123.52
20	B	806	CLA	OBD-CAD-C3D	-4.63	117.59	128.42
20	A	828	CLA	C4B-CHC-C1C	-4.63	115.36	126.25
20	K	106	CLA	C1-C2-C3	-4.63	119.28	126.76
20	2	311	CLA	CMD-C2D-C1D	4.62	132.87	124.73
20	4	303	CLA	CHD-C4C-C3C	-4.62	117.73	125.03
20	2	309	CLA	CHD-C4C-NC	4.62	131.26	124.24
20	3	306	CLA	C4C-CHD-C1D	-4.62	112.82	125.98
21	B	801	LMU	O2'-C2'-C3'	4.62	121.26	110.38
20	3	305	CLA	C4C-CHD-C1D	-4.61	112.83	125.98
20	3	317	CLA	CHD-C4C-NC	4.61	131.25	124.24
20	1	202	CLA	CED-O2D-CGD	4.61	126.38	115.92
20	F	204	CLA	CHC-C1C-NC	4.61	131.26	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	F	206	CLA	C4-C3-C5	4.61	123.23	115.23
20	3	320	CLA	CHD-C4C-C3C	-4.61	118.05	124.77
20	B	815	CLA	C3B-C2B-C1B	-4.61	101.73	107.17
20	H	107	CLA	CHD-C4C-NC	4.61	131.38	124.23
20	1	215	CLA	C2D-C3D-C4D	-4.61	101.75	107.35
20	3	312	CLA	CHD-C4C-NC	4.60	131.24	124.24
20	4	318	CLA	CHD-C4C-C3C	-4.60	118.06	124.77
20	4	304	CLA	C1-O2A-CGA	-4.60	105.51	116.65
20	2	314	CLA	C3A-C4A-CHB	-4.60	118.28	123.91
20	3	317	CLA	CHC-C1C-NC	4.60	131.09	124.33
20	A	810	CLA	O2D-CGD-CBD	4.60	119.27	111.23
20	B	839	CLA	CAA-C2A-C3A	-4.60	105.69	116.23
20	3	309	CLA	C4D-C3D-CAD	4.60	113.10	108.11
20	G	103	CLA	CHD-C4C-C3C	-4.59	118.07	124.77
20	4	312	CLA	CHA-C4D-ND	4.59	131.33	124.84
20	1	203	CLA	O2D-CGD-O1D	-4.59	114.91	123.85
20	H	107	CLA	O2D-CGD-CBD	4.59	119.26	111.23
20	B	827	CLA	C1-O2A-CGA	4.59	127.77	116.65
21	H	102	LMU	O3B-C3B-C2B	4.59	121.19	110.38
20	A	830	CLA	CMD-C2D-C3D	-4.59	117.17	127.69
20	A	808	CLA	C2B-C1B-NB	4.58	115.08	110.33
20	A	816	CLA	C4B-CHC-C1C	-4.58	115.47	126.25
20	B	829	CLA	CHD-C4C-C3C	-4.58	118.09	124.77
20	1	207	CLA	C4A-NA-C1A	4.58	108.77	106.68
20	1	214	CLA	CHD-C4C-C3C	-4.58	118.09	124.77
20	L	202	CLA	CHD-C4C-C3C	-4.58	118.09	124.77
20	B	829	CLA	O2D-CGD-O1D	-4.58	114.93	123.85
22	B	850	BCR	C16-C17-C18	-4.58	120.86	127.28
21	B	801	LMU	C6B-C5B-C4B	-4.57	101.79	113.02
20	B	824	CLA	O1D-CGD-CBD	-4.57	115.50	124.52
20	B	847	CLA	C1D-CHD-C4C	-4.57	116.30	126.02
20	4	303	CLA	CAB-C3B-C2B	-4.57	111.39	123.53
20	B	849	CLA	CHB-C4A-NA	4.57	131.00	124.40
22	L	209	BCR	C3-C4-C5	-4.57	105.91	114.06
20	3	306	CLA	C4A-NA-C1A	4.57	108.76	106.68
20	A	829	CLA	CHC-C4B-NB	4.57	130.90	124.05
20	3	319	CLA	CHD-C4C-C3C	-4.56	117.82	125.03
21	B	801	LMU	O5'-C5'-C6'	4.56	117.75	106.44
20	B	838	CLA	CMB-C2B-C1B	4.56	132.37	125.42
20	A	825	CLA	CHD-C4C-NC	4.56	131.30	124.23
21	K	104	LMU	C1B-C2B-C3B	4.56	119.60	110.01
21	1	218	LMU	O1B-C4'-C5'	-4.56	97.52	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	812	CLA	CMB-C2B-C1B	4.55	132.35	125.42
20	L	201	CLA	C3B-C2B-C1B	-4.55	101.80	107.17
20	A	849	CLA	CMD-C2D-C3D	-4.55	117.25	127.69
20	L	203	CLA	C4A-NA-C1A	4.55	108.75	106.68
20	A	804	CLA	CHD-C4C-NC	4.55	131.29	124.23
20	B	811	CLA	CHD-C4C-NC	4.55	131.28	124.23
20	B	836	CLA	CHD-C4C-C3C	-4.55	118.14	124.77
20	4	312	CLA	C3D-C4D-CHA	-4.55	115.04	125.20
21	H	104	LMU	O5B-C5B-C4B	-4.55	101.50	109.70
20	A	811	CLA	C1-C2-C3	-4.55	118.75	126.20
20	2	317	CLA	C4D-C3D-CAD	4.54	113.04	108.11
20	B	825	CLA	CHD-C4C-NC	4.54	131.28	124.23
20	2	310	CLA	CMD-C2D-C3D	-4.54	117.27	127.69
20	R	106	CLA	O2D-CGD-CBD	4.54	119.17	111.23
20	4	309	CLA	CHD-C4C-NC	4.54	131.14	124.24
20	A	850	CLA	O2D-CGD-O1D	-4.54	115.01	123.85
20	2	311	CLA	CHD-C4C-C3C	-4.54	118.16	124.77
20	A	827	CLA	CHC-C1C-NC	4.54	131.15	124.31
20	I	102	CLA	CHD-C4C-C3C	-4.54	118.16	124.77
22	I	103	BCR	C7-C6-C5	4.53	132.00	121.56
20	A	815	CLA	CHD-C4C-C3C	-4.53	118.16	124.77
22	I	103	BCR	C27-C26-C25	-4.53	116.58	122.70
20	3	317	CLA	C3A-C4A-CHB	-4.53	118.36	123.91
20	4	303	CLA	C2B-C1B-NB	4.53	115.03	110.33
20	3	304	CLA	C3A-C4A-CHB	-4.53	118.36	123.91
20	1	201	CLA	CHC-C1C-NC	4.53	131.13	124.31
20	1	202	CLA	CHC-C1C-NC	4.53	131.13	124.31
20	1	215	CLA	CHD-C4C-NC	4.53	131.12	124.24
20	B	835	CLA	CMD-C2D-C3D	-4.53	117.31	127.69
20	K	106	CLA	CMD-C2D-C3D	-4.53	117.31	127.69
20	A	809	CLA	C4B-CHC-C1C	-4.53	115.60	126.25
20	L	202	CLA	CMB-C2B-C1B	4.53	132.31	125.42
20	B	808	CLA	CHD-C4C-NC	4.53	131.25	124.23
20	3	319	CLA	CBD-CAD-C3D	-4.52	102.21	108.25
20	B	838	CLA	O2A-CGA-CBA	4.52	125.62	111.83
21	E	101	LMU	O1'-C1'-C2'	-4.52	101.41	108.27
20	2	305	CLA	C3D-C4D-CHA	-4.52	115.11	125.20
20	A	849	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
20	B	836	CLA	CHC-C1C-NC	4.52	131.11	124.31
20	B	811	CLA	C3B-C2B-C1B	-4.52	101.85	107.17
20	2	304	CLA	O2D-CGD-CBD	4.51	119.12	111.23
20	4	307	CLA	C4B-CHC-C1C	-4.51	115.64	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	R	106	CLA	O2A-CGA-CBA	4.51	125.58	111.83
20	2	308	CLA	C3A-C4A-CHB	-4.51	118.39	123.91
20	B	837	CLA	C3B-C2B-C1B	-4.51	101.86	107.17
20	B	819	CLA	CMD-C2D-C3D	-4.51	117.35	127.69
20	A	808	CLA	C3B-C4B-NB	-4.50	106.51	110.53
20	4	318	CLA	CHC-C1C-NC	4.50	131.09	124.31
20	B	820	CLA	CAA-C2A-C1A	-4.50	97.22	111.97
20	A	857	CLA	CHC-C1C-NC	4.50	130.95	124.33
20	A	802	CLA	CMD-C2D-C3D	-4.50	117.37	127.69
20	1	207	CLA	CHD-C4C-NC	4.50	131.21	124.23
20	R	107	CLA	CHD-C4C-C3C	-4.50	118.22	124.77
20	B	810	CLA	C2B-C1B-NB	4.50	114.99	110.33
21	R	104	LMU	O5B-C1B-C2B	4.50	119.61	110.37
20	A	824	CLA	CMD-C2D-C3D	-4.49	117.38	127.69
20	2	311	CLA	CHC-C4B-NB	4.49	130.79	124.05
20	3	316	CLA	C3B-C2B-C1B	-4.49	101.81	106.81
20	1	203	CLA	CGD-CBD-CAD	-4.49	96.31	110.85
20	1	209	CLA	CMB-C2B-C1B	4.49	132.25	125.42
20	B	803	CLA	C3B-C2B-C1B	-4.49	101.88	107.17
20	L	207	CLA	C2B-C1B-NB	4.49	114.98	110.33
20	B	814	CLA	CHC-C1C-NC	4.48	131.06	124.31
20	B	822	CLA	CHD-C4C-C3C	-4.48	118.24	124.77
20	B	835	CLA	CHC-C1C-NC	4.48	131.06	124.31
20	3	308	CLA	C3B-C2B-C1B	-4.48	101.83	106.81
20	4	302	CLA	CHD-C4C-C3C	-4.48	118.25	124.77
20	F	205	CLA	CHD-C4C-C3C	-4.48	118.25	124.77
20	B	832	CLA	C4B-CHC-C1C	-4.48	115.72	126.25
21	F	201	LMU	C6B-C5B-C4B	-4.47	102.03	113.02
21	C	101	LMU	O1'-C1'-C2'	4.47	115.06	108.27
20	3	316	CLA	C2D-C3D-C4D	-4.47	101.92	107.35
20	A	801	CLA	C4B-CHC-C1C	-4.47	115.75	126.25
20	3	305	CLA	C4A-NA-C1A	4.46	108.72	106.68
20	4	309	CLA	C4A-NA-C1A	4.46	108.72	106.68
21	A	854	LMU	C3'-C4'-C5'	-4.46	101.03	110.93
20	A	825	CLA	C4B-CHC-C1C	-4.46	115.75	126.25
22	B	842	BCR	C30-C25-C26	-4.46	116.54	122.64
20	B	847	CLA	CHC-C1C-NC	4.46	131.03	124.31
20	A	803	CLA	C4A-NA-C1A	4.46	108.71	106.68
20	A	818	CLA	CHD-C4C-NC	4.46	131.15	124.23
20	B	823	CLA	CHD-C4C-C3C	-4.46	118.27	124.77
20	A	813	CLA	C2B-C1B-NB	4.46	114.95	110.33
20	K	103	CLA	CHD-C4C-C3C	-4.46	118.28	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	207	CLA	CHD-C4C-C3C	-4.45	118.28	124.77
20	A	825	CLA	C4D-C3D-CAD	4.45	112.94	108.11
20	B	830	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
20	A	831	CLA	CHD-C4C-C3C	-4.45	118.29	124.77
20	3	308	CLA	C3A-C4A-CHB	-4.45	118.46	123.91
20	B	805	CLA	CHB-C4A-NA	4.45	130.82	124.40
20	A	837	CLA	CHD-C4C-C3C	-4.45	118.29	124.77
20	2	308	CLA	C1B-NB-C4B	-4.45	103.19	106.31
20	B	820	CLA	CMD-C2D-C1D	4.44	132.55	124.73
20	3	301	CLA	C4B-CHC-C1C	-4.44	115.80	126.25
20	B	808	CLA	C2B-C1B-NB	4.44	114.93	110.33
20	B	832	CLA	C2B-C1B-NB	4.44	114.93	110.33
20	2	309	CLA	C3B-C2B-C1B	-4.44	101.87	106.81
20	A	833	CLA	CHD-C4C-C3C	-4.44	118.30	124.77
20	A	819	CLA	C4B-CHC-C1C	-4.44	115.81	126.25
20	B	820	CLA	C1D-CHD-C4C	-4.44	116.59	126.02
21	K	102	LMU	C4B-C3B-C2B	-4.44	103.04	110.83
20	1	203	CLA	CHD-C4C-NC	4.44	131.11	124.23
20	2	307	CLA	C6-C5-C3	-4.44	102.66	113.47
20	3	310	CLA	CHD-C4C-C3C	-4.43	118.31	124.77
20	A	803	CLA	CHC-C4B-NB	4.43	130.70	124.05
20	1	214	CLA	O2A-CGA-O1A	-4.43	112.54	123.63
20	2	315	CLA	CHD-C4C-NC	4.43	130.98	124.24
20	A	815	CLA	CHD-C4C-NC	4.43	131.10	124.23
20	B	814	CLA	C4B-CHC-C1C	-4.43	115.83	126.25
20	A	807	CLA	CHC-C1C-C2C	-4.43	114.36	126.95
20	B	839	CLA	CHD-C4C-NC	4.43	131.10	124.23
20	4	304	CLA	C1-C2-C3	-4.43	118.94	126.20
20	A	834	CLA	CHD-C4C-C3C	-4.43	118.32	124.77
20	2	303	CLA	CHC-C1C-NC	4.43	130.84	124.33
20	4	319	CLA	CHD-C4C-C3C	-4.43	118.32	124.77
20	J	102	CLA	CHD-C4C-C3C	-4.43	118.32	124.77
20	3	313	CLA	CHC-C1C-NC	4.43	130.84	124.33
20	B	824	CLA	C3B-C2B-C1B	-4.43	101.95	107.17
20	B	826	CLA	C3B-C2B-C1B	-4.42	101.95	107.17
21	4	322	LMU	O1'-C1'-C2'	4.42	114.99	108.27
20	A	855	CLA	CHD-C4C-C3C	-4.42	118.32	124.77
20	A	806	CLA	O2D-CGD-O1D	-4.42	115.24	123.85
20	B	833	CLA	C2B-C1B-NB	4.42	114.91	110.33
20	B	824	CLA	O2A-CGA-CBA	4.42	125.32	111.83
20	A	825	CLA	C3B-C2B-C1B	-4.42	101.96	107.17
20	B	849	CLA	C2B-C1B-NB	4.42	114.91	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	835	CLA	CHD-C4C-C3C	-4.42	118.33	124.77
20	B	819	CLA	C4B-CHC-C1C	-4.42	115.85	126.25
20	3	317	CLA	C2A-C1A-CHA	-4.42	115.10	122.63
20	B	807	CLA	C4B-CHC-C1C	-4.42	115.86	126.25
20	B	812	CLA	CHD-C4C-NC	4.42	131.08	124.23
20	A	807	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
20	A	850	CLA	O2A-CGA-CBA	4.41	125.29	111.83
20	B	803	CLA	CHD-C4C-C3C	-4.41	118.34	124.77
20	K	105	CLA	CHD-C4C-C3C	-4.41	118.34	124.77
20	4	315	CLA	C4D-C3D-CAD	4.41	112.90	108.11
22	I	101	BCR	C37-C22-C21	-4.41	115.67	122.82
20	A	802	CLA	CHC-C1C-NC	4.41	130.96	124.31
20	A	820	CLA	C4B-CHC-C1C	-4.41	115.88	126.25
20	3	303	CLA	CBD-CAD-C3D	-4.41	102.36	108.25
20	R	107	CLA	C4B-CHC-C1C	-4.41	115.88	126.25
20	B	826	CLA	CMB-C2B-C1B	4.41	132.13	125.42
20	2	310	CLA	O2D-CGD-O1D	-4.41	115.27	123.85
20	L	202	CLA	C4A-NA-C1A	4.41	108.69	106.68
20	3	303	CLA	C2B-C1B-NB	4.41	114.90	110.33
20	A	830	CLA	C2B-C1B-NB	4.41	114.90	110.33
20	A	822	CLA	CHD-C4C-C3C	-4.41	118.35	124.77
20	A	818	CLA	CMD-C2D-C3D	-4.41	117.58	127.69
20	B	810	CLA	O2D-CGD-CBD	4.41	118.93	111.23
20	A	836	CLA	CHD-C4C-C3C	-4.41	118.35	124.77
20	A	802	CLA	CHD-C4C-C3C	-4.40	118.35	124.77
20	B	826	CLA	CHD-C4C-C3C	-4.40	118.35	124.77
20	B	836	CLA	C2B-C1B-NB	4.40	114.89	110.33
20	A	832	CLA	CHD-C4C-C3C	-4.40	118.35	124.77
20	A	823	CLA	CHD-C4C-C3C	-4.40	118.36	124.77
20	1	212	CLA	C4B-CHC-C1C	-4.40	115.90	126.25
20	4	309	CLA	C4C-CHD-C1D	-4.40	113.45	125.98
21	A	852	LMU	O1'-C1'-C2'	4.40	114.95	108.27
20	2	306	CLA	C4B-CHC-C1C	-4.40	115.91	126.25
20	A	857	CLA	CHD-C4C-NC	4.40	130.92	124.24
20	2	303	CLA	C2A-C1A-CHA	-4.39	115.14	122.63
20	3	315	CLA	CHD-C4C-C3C	-4.39	118.37	124.77
20	2	301	CLA	CHD-C4C-C3C	-4.39	118.37	124.77
21	B	802	LMU	O1'-C1'-C2'	4.39	114.94	108.27
20	A	813	CLA	CHD-C4C-NC	4.39	131.04	124.23
20	R	107	CLA	O2A-CGA-CBA	4.39	125.23	111.83
20	B	810	CLA	CHC-C1C-NC	4.39	130.92	124.31
20	B	806	CLA	CHC-C1C-NC	4.39	130.92	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	312	CLA	C2A-C1A-CHA	-4.39	115.15	122.63
20	4	307	CLA	C4B-C3B-C2B	-4.39	101.85	107.30
20	1	210	CLA	CMD-C2D-C3D	-4.39	117.63	127.69
20	4	310	CLA	C4A-NA-C1A	4.39	108.68	106.68
20	B	830	CLA	C4B-CHC-C1C	-4.38	115.94	126.25
20	H	101	CLA	C2B-C1B-NB	4.38	114.87	110.33
21	K	102	LMU	O1'-C1'-C2'	4.38	114.93	108.27
20	2	311	CLA	C4B-CHC-C1C	-4.38	115.94	126.25
20	B	803	CLA	CHC-C1C-NC	4.38	130.91	124.31
20	A	847	CLA	C4B-C3B-C2B	4.38	112.75	107.30
20	A	804	CLA	C4B-CHC-C1C	-4.38	115.95	126.25
20	2	306	CLA	CHD-C4C-C3C	-4.38	118.39	124.77
20	B	837	CLA	CHD-C4C-C3C	-4.38	118.39	124.77
20	A	828	CLA	CHC-C4B-NB	4.38	130.62	124.05
20	3	308	CLA	C2D-C3D-C4D	-4.37	102.03	107.35
20	H	101	CLA	CED-O2D-CGD	4.37	125.84	115.92
20	B	821	CLA	O2D-CGD-O1D	-4.37	115.34	123.85
20	A	811	CLA	C4A-NA-C1A	4.37	108.67	106.68
20	A	819	CLA	CHC-C1C-NC	4.37	130.90	124.31
20	4	315	CLA	CGD-CBD-CAD	-4.37	96.69	110.85
20	B	817	CLA	CMD-C2D-C3D	-4.37	117.67	127.69
20	A	816	CLA	CHD-C4C-C3C	-4.37	118.40	124.77
20	3	301	CLA	CMD-C2D-C3D	-4.37	117.67	127.69
21	K	102	LMU	C1'-O5'-C5'	-4.37	105.19	113.72
20	A	820	CLA	CHD-C4C-NC	4.37	131.01	124.23
21	B	802	LMU	O3'-C3'-C2'	-4.37	100.08	110.38
20	B	809	CLA	O2D-CGD-CBD	4.37	118.86	111.23
20	B	830	CLA	C2B-C1B-NB	4.37	114.85	110.33
20	2	315	CLA	C3A-C4A-CHB	-4.36	118.57	123.91
20	A	806	CLA	CHD-C4C-C3C	-4.36	118.42	124.77
20	A	829	CLA	C4B-CHC-C1C	-4.36	116.00	126.25
20	A	848	CLA	C3B-C2B-C1B	-4.36	102.03	107.17
20	B	827	CLA	C3B-C2B-C1B	-4.36	102.03	107.17
20	2	308	CLA	C2A-C1A-CHA	-4.36	115.20	122.63
20	4	314	CLA	CHA-C4D-ND	4.36	131.00	124.84
20	2	307	CLA	C3B-C2B-C1B	-4.36	102.03	107.17
20	B	833	CLA	CHD-C4C-NC	4.36	130.98	124.23
20	B	809	CLA	C4A-NA-C1A	4.35	108.66	106.68
20	B	813	CLA	CHD-C4C-C3C	-4.35	118.43	124.77
20	1	208	CLA	CHD-C4C-NC	4.35	130.85	124.24
20	1	203	CLA	CHD-C4C-C3C	-4.35	118.43	124.77
20	A	801	CLA	O2D-CGD-O1D	-4.35	115.39	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	314	CLA	C3B-C2B-C1B	-4.35	101.97	106.81
20	B	824	CLA	CMD-C2D-C3D	-4.35	117.72	127.69
20	A	820	CLA	C2B-C1B-NB	4.35	114.83	110.33
20	B	806	CLA	C4B-CHC-C1C	-4.34	116.04	126.25
20	B	806	CLA	C1-C2-C3	-4.34	119.08	126.20
20	A	808	CLA	CHD-C4C-NC	4.34	130.96	124.23
20	A	829	CLA	C2B-C1B-NB	4.34	114.83	110.33
20	A	809	CLA	CHC-C4B-NB	4.34	130.56	124.05
20	F	204	CLA	C4B-C3B-C2B	4.34	111.12	107.03
21	H	104	LMU	C2'-C3'-C4'	4.34	119.53	109.68
20	A	829	CLA	C4-C3-C5	4.34	122.76	115.23
20	4	307	CLA	O2A-CGA-CBA	4.33	125.05	111.83
20	B	847	CLA	C4A-NA-C1A	4.33	108.66	106.68
21	2	320	LMU	O1'-C1'-C2'	4.33	114.85	108.27
20	4	309	CLA	CHC-C1C-NC	4.33	130.69	124.33
20	1	209	CLA	C4B-CHC-C1C	-4.33	116.07	126.25
22	3	311	BCR	C38-C26-C25	-4.33	119.76	124.48
20	B	821	CLA	C2B-C1B-NB	4.33	114.81	110.33
20	4	305	CLA	CMD-C2D-C3D	-4.33	117.77	127.69
20	B	819	CLA	CHC-C1C-NC	4.32	130.82	124.31
20	A	818	CLA	C2B-C1B-NB	4.32	114.81	110.33
20	1	211	CLA	CHC-C4B-NB	4.32	130.53	124.05
20	R	106	CLA	CHD-C4C-NC	4.32	130.93	124.23
20	H	107	CLA	C4B-CHC-C1C	-4.32	116.09	126.25
21	E	101	LMU	C1B-O1B-C4'	-4.32	107.74	117.98
20	B	818	CLA	C4B-CHC-C1C	-4.32	116.09	126.25
20	B	819	CLA	CHD-C4C-NC	4.32	130.92	124.23
20	1	215	CLA	C3D-C4D-CHA	-4.32	115.56	125.20
20	B	849	CLA	CGD-CBD-CAD	4.31	124.81	110.85
20	L	201	CLA	C4D-C3D-CAD	4.31	112.79	108.11
20	B	809	CLA	C4B-CHC-C1C	-4.31	116.10	126.25
21	L	210	LMU	C3B-C4B-C5B	4.31	118.05	110.23
21	E	101	LMU	O1B-C1B-C2B	4.31	118.70	108.09
20	B	828	CLA	C4D-C3D-CAD	4.31	112.79	108.11
20	1	201	CLA	CED-O2D-CGD	4.31	125.70	115.92
20	3	313	CLA	C4C-CHD-C1D	-4.31	113.70	125.98
20	A	806	CLA	C4B-CHC-C1C	-4.31	116.12	126.25
20	B	811	CLA	C4B-CHC-C1C	-4.31	116.12	126.25
20	A	850	CLA	C4B-CHC-C1C	-4.31	116.12	126.25
20	B	817	CLA	C4B-CHC-C1C	-4.30	116.12	126.25
20	1	210	CLA	CHD-C4C-C3C	-4.30	118.23	125.03
20	4	315	CLA	C3B-C2B-C1B	-4.30	102.10	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	804	CLA	CHB-C4A-NA	4.30	130.61	124.40
20	4	307	CLA	CMD-C2D-C3D	-4.30	117.83	127.69
20	A	808	CLA	CHC-C1C-NC	4.30	130.79	124.31
20	A	848	CLA	CAA-C2A-C1A	4.30	126.06	111.97
20	A	847	CLA	C2B-C1B-NB	4.30	114.78	110.33
20	4	308	CLA	C4A-NA-C1A	4.30	108.64	106.68
21	1	217	LMU	C4B-C3B-C2B	-4.30	103.29	110.83
20	4	308	CLA	C3B-C2B-C1B	-4.29	102.03	106.81
20	3	315	CLA	CHC-C1C-NC	4.29	130.78	124.31
20	1	213	CLA	C3B-C2B-C1B	-4.29	102.03	106.81
20	L	207	CLA	C4B-CHC-C1C	-4.29	116.16	126.25
20	B	829	CLA	C2B-C1B-NB	4.29	114.78	110.33
20	H	110	CLA	C4B-CHC-C1C	-4.29	116.16	126.25
20	3	307	CLA	CHD-C4C-NC	4.29	130.76	124.24
20	A	805	CLA	C4B-CHC-C1C	-4.29	116.16	126.25
20	B	815	CLA	C1-C2-C3	-4.29	119.17	126.20
20	L	208	CLA	O2D-CGD-O1D	-4.29	115.50	123.85
20	A	848	CLA	C4B-CHC-C1C	-4.29	116.17	126.25
20	H	101	CLA	CAA-C2A-C3A	-4.29	101.42	113.00
21	B	801	LMU	C2'-C3'-C4'	-4.28	99.96	109.68
22	A	842	BCR	C7-C8-C9	-4.28	119.90	126.23
22	B	850	BCR	C33-C5-C4	4.28	122.72	113.60
22	A	840	BCR	C24-C23-C22	-4.28	119.90	126.23
21	K	102	LMU	C1B-O1B-C4'	-4.28	107.83	117.98
21	A	846	LMU	C3B-C4B-C5B	-4.28	102.47	110.23
20	F	205	CLA	C4B-CHC-C1C	-4.28	116.18	126.25
20	4	311	CLA	CHC-C1C-NC	4.28	130.62	124.33
22	J	101	BCR	C7-C8-C9	-4.28	119.91	126.23
20	3	316	CLA	C4A-NA-C1A	4.28	108.63	106.68
20	4	305	CLA	CAC-C3C-C4C	4.28	130.35	124.79
20	3	314	CLA	C4B-CHC-C1C	-4.28	116.19	126.25
20	B	822	CLA	C4B-CHC-C1C	-4.28	116.19	126.25
22	A	841	BCR	C7-C8-C9	-4.27	119.91	126.23
20	3	314	CLA	CHC-C1C-NC	4.27	130.75	124.31
20	F	206	CLA	O2D-CGD-O1D	-4.27	115.53	123.85
20	B	807	CLA	CHD-C4C-C3C	-4.27	118.55	124.77
20	1	214	CLA	CGD-CBD-CAD	-4.27	97.03	110.85
20	K	103	CLA	C4B-CHC-C1C	-4.26	116.22	126.25
20	B	809	CLA	CHD-C4C-NC	4.26	130.83	124.23
20	2	306	CLA	C2B-C1B-NB	4.26	114.74	110.33
20	4	319	CLA	C4B-CHC-C1C	-4.26	116.23	126.25
20	B	838	CLA	C4B-C3B-C2B	4.26	112.59	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	823	CLA	C4B-CHC-C1C	-4.26	116.24	126.25
20	1	204	CLA	CMD-C2D-C3D	-4.26	117.93	127.69
20	F	205	CLA	CHC-C1C-NC	4.26	130.72	124.31
20	B	822	CLA	CMD-C2D-C3D	-4.25	117.93	127.69
20	1	201	CLA	CGD-CBD-CAD	-4.25	97.08	110.85
20	A	809	CLA	CAA-C2A-C3A	-4.25	101.51	113.00
20	4	307	CLA	C2B-C1B-NB	4.25	114.74	110.33
20	4	308	CLA	CHD-C4C-NC	4.25	130.70	124.24
20	2	301	CLA	C4B-CHC-C1C	-4.25	116.25	126.25
21	2	320	LMU	O1B-C4'-C5'	4.25	120.62	109.48
20	H	110	CLA	CHD-C4C-C3C	-4.25	118.58	124.77
20	A	822	CLA	CMD-C2D-C3D	-4.25	117.94	127.69
20	J	103	CLA	CHC-C1C-NC	4.25	130.71	124.31
20	4	312	CLA	C3B-C2B-C1B	-4.25	102.08	106.81
20	A	831	CLA	C4B-CHC-C1C	-4.25	116.26	126.25
20	3	308	CLA	CHD-C4C-NC	4.25	130.69	124.24
20	B	836	CLA	C4B-CHC-C1C	-4.25	116.26	126.25
20	K	105	CLA	C4B-CHC-C1C	-4.25	116.26	126.25
20	3	319	CLA	CMD-C2D-C3D	-4.24	117.95	127.69
20	A	833	CLA	C4B-CHC-C1C	-4.24	116.27	126.25
20	A	834	CLA	C4B-CHC-C1C	-4.24	116.27	126.25
20	B	823	CLA	C4B-CHC-C1C	-4.24	116.27	126.25
20	4	302	CLA	C4B-CHC-C1C	-4.24	116.27	126.25
20	B	823	CLA	CMD-C2D-C3D	-4.24	117.96	127.69
22	B	844	BCR	C38-C26-C25	-4.24	119.86	124.48
20	A	835	CLA	C4B-CHC-C1C	-4.24	116.27	126.25
22	G	102	BCR	C7-C8-C9	-4.24	119.96	126.23
20	A	837	CLA	CMD-C2D-C3D	-4.24	117.96	127.69
20	1	212	CLA	C1-C2-C3	-4.24	119.25	126.20
20	A	836	CLA	C4B-CHC-C1C	-4.24	116.28	126.25
20	A	855	CLA	C4B-CHC-C1C	-4.24	116.28	126.25
20	K	105	CLA	CMD-C2D-C3D	-4.24	117.97	127.69
20	A	809	CLA	C4A-NA-C1A	4.24	108.61	106.68
22	B	844	BCR	C24-C23-C22	-4.24	119.96	126.23
20	A	831	CLA	CMD-C2D-C3D	-4.24	117.97	127.69
22	F	202	BCR	C24-C23-C22	-4.24	119.97	126.23
20	B	833	CLA	CMD-C2D-C3D	-4.24	117.97	127.69
20	A	857	CLA	C3A-C4A-CHB	-4.24	118.72	123.91
20	B	838	CLA	CHD-C4C-C3C	-4.24	118.60	124.77
22	B	841	BCR	C24-C23-C22	-4.24	119.97	126.23
20	A	819	CLA	CHD-C4C-NC	4.24	130.80	124.23
20	1	213	CLA	CHD-C4C-NC	4.24	130.68	124.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	205	CLA	CHD-C4C-C3C	-4.24	118.34	125.03
20	3	315	CLA	C2B-C1B-NB	4.24	114.72	110.33
20	A	827	CLA	C4B-CHC-C1C	-4.24	116.29	126.25
20	A	837	CLA	C4B-CHC-C1C	-4.23	116.29	126.25
20	3	310	CLA	C4B-CHC-C1C	-4.23	116.29	126.25
22	B	843	BCR	C7-C8-C9	-4.23	119.97	126.23
22	A	843	BCR	C24-C23-C22	-4.23	119.97	126.23
20	A	836	CLA	CMD-C2D-C3D	-4.23	117.98	127.69
22	A	840	BCR	C7-C8-C9	-4.23	119.97	126.23
20	1	204	CLA	O2D-CGD-O1D	-4.23	115.61	123.85
20	A	832	CLA	C4B-CHC-C1C	-4.23	116.30	126.25
20	4	311	CLA	C2A-C1A-CHA	-4.23	115.42	122.63
20	A	825	CLA	C2B-C1B-NB	4.23	114.71	110.33
20	1	204	CLA	CHD-C4C-C3C	-4.23	118.61	124.77
20	3	310	CLA	CHC-C1C-NC	4.23	130.68	124.31
20	A	833	CLA	CMD-C2D-C3D	-4.23	117.99	127.69
22	A	842	BCR	C24-C23-C22	-4.23	119.98	126.23
20	1	213	CLA	C1B-NB-C4B	-4.23	103.35	106.31
20	A	855	CLA	CMD-C2D-C3D	-4.23	118.00	127.69
20	A	822	CLA	C4B-CHC-C1C	-4.23	116.31	126.25
20	A	817	CLA	CHD-C4C-NC	4.23	130.78	124.23
20	A	832	CLA	CMD-C2D-C3D	-4.23	118.00	127.69
20	A	834	CLA	CMD-C2D-C3D	-4.23	118.00	127.69
20	A	824	CLA	C3B-C2B-C1B	-4.23	102.19	107.17
20	B	816	CLA	C4B-CHC-C1C	-4.23	116.31	126.25
22	B	844	BCR	C7-C8-C9	-4.22	119.98	126.23
20	F	206	CLA	CHD-C4C-NC	4.22	130.78	124.23
20	1	208	CLA	C3B-C2B-C1B	-4.22	102.11	106.81
20	4	302	CLA	CMD-C2D-C3D	-4.22	118.00	127.69
20	A	835	CLA	CMD-C2D-C3D	-4.22	118.00	127.69
20	4	307	CLA	C2A-C3A-C4A	-4.22	95.05	101.87
20	3	301	CLA	CHC-C1C-NC	4.22	130.67	124.31
22	I	101	BCR	C24-C25-C26	-4.22	111.83	121.56
20	2	301	CLA	CMD-C2D-C3D	-4.22	118.01	127.69
20	4	317	CLA	C2A-C1A-CHA	-4.22	115.44	122.63
20	A	806	CLA	CAA-C2A-C1A	-4.22	98.15	111.97
22	3	311	BCR	C11-C12-C13	-4.22	114.80	126.36
20	K	106	CLA	O2D-CGD-O1D	-4.22	115.64	123.85
20	1	204	CLA	CHD-C4C-NC	4.22	130.77	124.23
21	B	802	LMU	O1B-C1B-C2B	4.22	118.46	108.09
20	3	315	CLA	C1-C2-C3	-4.21	119.94	126.76
20	A	806	CLA	C6-C5-C3	-4.21	103.20	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	835	CLA	C3B-C2B-C1B	-4.21	102.20	107.17
20	4	308	CLA	C1B-NB-C4B	-4.21	103.36	106.31
20	4	319	CLA	CMD-C2D-C3D	-4.21	118.03	127.69
22	A	844	BCR	C24-C23-C22	-4.21	120.00	126.23
20	3	315	CLA	C4B-CHC-C1C	-4.21	116.34	126.25
20	1	209	CLA	C2B-C1B-NB	4.21	114.69	110.33
20	4	306	CLA	CHD-C4C-NC	4.21	130.76	124.23
20	4	313	CLA	CHD-C4C-NC	4.21	130.76	124.23
20	B	814	CLA	C2B-C1B-NB	4.21	114.69	110.33
20	A	807	CLA	O2D-CGD-O1D	-4.21	115.66	123.85
20	3	309	CLA	C4A-NA-C1A	4.21	108.60	106.68
20	3	313	CLA	C3A-C4A-CHB	-4.21	118.76	123.91
22	F	202	BCR	C7-C8-C9	-4.21	120.01	126.23
20	J	103	CLA	C4B-CHC-C1C	-4.21	116.36	126.25
20	3	314	CLA	CMD-C2D-C3D	-4.21	118.04	127.69
20	B	815	CLA	C4B-CHC-C1C	-4.21	116.36	126.25
22	L	209	BCR	C38-C26-C27	4.21	122.56	113.60
20	A	802	CLA	C4D-C3D-CAD	4.20	112.67	108.11
20	A	821	CLA	C4-C3-C5	4.20	122.52	115.23
20	B	808	CLA	C1B-C2B-C3B	-4.20	103.08	107.03
20	A	857	CLA	C1C-CHC-C4B	-4.20	114.96	126.04
20	A	823	CLA	CMD-C2D-C3D	-4.20	118.05	127.69
20	J	102	CLA	CMD-C2D-C3D	-4.20	118.05	127.69
20	1	213	CLA	C4C-CHD-C1D	-4.20	114.01	125.98
22	B	841	BCR	C7-C8-C9	-4.20	120.02	126.23
20	B	825	CLA	CMD-C2D-C1D	4.20	132.13	124.73
20	3	310	CLA	CMD-C2D-C3D	-4.20	118.05	127.69
20	B	847	CLA	CHD-C4C-NC	4.20	130.74	124.23
20	B	812	CLA	CHD-C4C-C3C	-4.20	118.65	124.77
20	B	826	CLA	CHC-C1C-NC	4.20	130.63	124.31
20	B	823	CLA	CHC-C1C-NC	4.20	130.63	124.31
20	2	310	CLA	CAC-C3C-C4C	4.19	130.25	124.79
22	A	844	BCR	C33-C5-C6	-4.19	119.91	124.48
20	2	306	CLA	C3B-C2B-C1B	-4.19	102.23	107.17
20	4	303	CLA	CAA-C2A-C3A	-4.19	106.61	116.23
20	K	103	CLA	CMD-C2D-C3D	-4.19	118.07	127.69
20	2	315	CLA	C2A-C1A-CHA	-4.19	115.48	122.63
20	K	105	CLA	CHC-C1C-NC	4.19	130.62	124.31
20	3	307	CLA	CHC-C1C-NC	4.19	130.49	124.33
20	B	822	CLA	CHC-C1C-NC	4.19	130.62	124.31
22	A	840	BCR	C38-C26-C25	-4.19	119.91	124.48
20	F	205	CLA	CMD-C2D-C3D	-4.19	118.08	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	305	CLA	CHC-C4B-NB	4.19	130.34	124.05
20	3	317	CLA	C1C-CHC-C4B	-4.19	114.99	126.04
20	A	828	CLA	C3B-C2B-C1B	-4.19	102.23	107.17
20	2	303	CLA	C4C-CHD-C1D	-4.19	114.05	125.98
20	4	312	CLA	C3A-C4A-CHB	-4.19	118.78	123.91
22	A	844	BCR	C7-C8-C9	-4.19	120.04	126.23
20	2	315	CLA	CHC-C1C-NC	4.19	130.49	124.33
20	4	308	CLA	C4C-CHD-C1D	-4.18	114.06	125.98
21	4	321	LMU	C2'-C3'-C4'	4.18	119.17	109.68
20	L	208	CLA	O1D-CGD-CBD	-4.18	116.27	124.52
20	A	828	CLA	C2B-C1B-NB	4.18	114.66	110.33
20	A	823	CLA	CHC-C1C-NC	4.18	130.61	124.31
20	2	312	CLA	C4B-CHC-C1C	-4.18	116.41	126.25
20	4	303	CLA	CMD-C2D-C3D	-4.18	118.10	127.69
20	1	202	CLA	CMD-C2D-C3D	-4.18	118.11	127.69
22	A	841	BCR	C38-C26-C25	-4.18	119.92	124.48
20	2	308	CLA	C4C-CHD-C1D	-4.18	114.08	125.98
20	B	828	CLA	C4B-CHC-C1C	-4.18	116.42	126.25
20	J	102	CLA	C4B-CHC-C1C	-4.18	116.42	126.25
22	B	843	BCR	C24-C23-C22	-4.18	120.06	126.23
22	A	843	BCR	C7-C8-C9	-4.18	120.06	126.23
20	2	301	CLA	CHC-C1C-NC	4.17	130.60	124.31
20	4	309	CLA	C3D-C4D-CHA	-4.17	115.88	125.20
20	3	316	CLA	CHD-C4C-NC	4.17	130.58	124.24
21	E	101	LMU	O3B-C3B-C2B	4.17	120.21	110.38
20	1	215	CLA	C1C-CHC-C4B	-4.17	115.04	126.04
20	A	855	CLA	CHC-C1C-NC	4.17	130.59	124.31
20	1	214	CLA	O2A-CGA-CBA	4.17	124.55	111.83
20	B	809	CLA	CMD-C2D-C3D	-4.17	118.13	127.69
21	H	105	LMU	C6'-C5'-C4'	-4.17	101.66	113.38
20	L	202	CLA	C4B-CHC-C1C	-4.17	116.45	126.25
20	H	101	CLA	CHC-C1C-NC	4.17	130.59	124.31
20	A	836	CLA	CHC-C1C-NC	4.16	130.58	124.31
22	J	101	BCR	C24-C23-C22	-4.16	120.07	126.23
20	A	834	CLA	CHC-C1C-NC	4.16	130.58	124.31
20	A	835	CLA	CHC-C1C-NC	4.16	130.58	124.31
20	4	305	CLA	C1D-CHD-C4C	-4.16	117.17	126.02
20	A	813	CLA	CHC-C1C-NC	4.16	130.58	124.31
20	1	208	CLA	C4C-CHD-C1D	-4.16	114.12	125.98
20	1	207	CLA	C4B-CHC-C1C	-4.16	116.46	126.25
20	3	312	CLA	C4C-CHD-C1D	-4.16	114.13	125.98
20	A	821	CLA	C4B-CHC-C1C	-4.16	116.47	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	302	CLA	CHC-C1C-NC	4.16	130.57	124.31
22	A	842	BCR	C33-C5-C6	-4.16	119.95	124.48
22	A	843	BCR	C38-C26-C25	-4.16	119.95	124.48
20	A	825	CLA	CHC-C1C-NC	4.16	130.57	124.31
20	A	825	CLA	CMD-C2D-C1D	4.16	132.05	124.73
20	B	804	CLA	CMB-C2B-C1B	4.16	131.75	125.42
20	2	302	CLA	C1-O2A-CGA	4.15	126.71	116.65
20	A	831	CLA	CHC-C1C-NC	4.15	130.57	124.31
20	A	833	CLA	CHC-C1C-NC	4.15	130.57	124.31
22	J	101	BCR	C38-C26-C25	-4.15	119.95	124.48
20	1	201	CLA	CAA-C2A-C3A	-4.15	101.78	113.00
20	I	102	CLA	C2B-C1B-NB	4.15	114.63	110.33
20	A	832	CLA	CHC-C1C-NC	4.15	130.56	124.31
20	A	837	CLA	CHC-C1C-NC	4.15	130.56	124.31
20	4	312	CLA	C4A-NA-C1A	4.15	108.57	106.68
22	A	843	BCR	C33-C5-C6	-4.15	119.96	124.48
22	I	103	BCR	C30-C25-C24	4.15	126.90	115.65
20	B	820	CLA	C4D-C3D-CAD	4.15	112.61	108.11
20	3	320	CLA	C4-C3-C5	4.15	122.43	115.23
20	2	304	CLA	CMD-C2D-C3D	-4.15	118.18	127.69
20	F	204	CLA	C4B-CHC-C1C	-4.15	116.49	126.25
22	B	842	BCR	C8-C9-C10	4.15	125.53	119.01
20	B	830	CLA	CHC-C4B-NB	4.15	130.27	124.05
20	K	103	CLA	CHC-C1C-NC	4.14	130.55	124.31
20	A	815	CLA	CMD-C2D-C3D	-4.14	118.19	127.69
20	1	205	CLA	C4B-CHC-C1C	-4.14	116.50	126.25
20	A	814	CLA	C2B-C1B-NB	4.14	114.62	110.33
20	2	310	CLA	C4B-CHC-C1C	-4.14	116.51	126.25
20	A	830	CLA	CHD-C4C-NC	4.14	130.65	124.23
20	2	309	CLA	C4C-CHD-C1D	-4.14	114.19	125.98
20	L	202	CLA	C3B-C2B-C1B	-4.14	102.29	107.17
20	A	810	CLA	CHD-C4C-C3C	-4.14	118.74	124.77
20	2	303	CLA	C4A-NA-C1A	4.14	108.57	106.68
20	3	319	CLA	C4B-CHC-C1C	-4.14	116.52	126.25
20	B	839	CLA	CMA-C3A-C2A	-4.14	106.75	116.23
20	A	802	CLA	CHC-C4B-NB	4.13	130.25	124.05
22	G	102	BCR	C33-C5-C6	-4.13	119.97	124.48
22	A	841	BCR	C24-C23-C22	-4.13	120.12	126.23
20	A	827	CLA	C2B-C1B-NB	4.13	114.61	110.33
20	B	816	CLA	C2B-C1B-NB	4.13	114.61	110.33
20	A	822	CLA	CHC-C1C-NC	4.13	130.53	124.31
20	2	306	CLA	C4A-NA-C1A	4.13	108.56	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	321	CLA	CAC-C3C-C4C	4.13	130.16	124.79
20	B	811	CLA	O2D-CGD-CBD	4.13	118.45	111.23
20	4	317	CLA	C1C-CHC-C4B	-4.13	115.15	126.04
20	B	825	CLA	O2D-CGD-O1D	-4.13	115.81	123.85
20	2	311	CLA	CHD-C4C-NC	4.13	130.63	124.23
22	G	102	BCR	C24-C23-C22	-4.13	120.13	126.23
21	R	105	LMU	C1B-O1B-C4'	-4.13	108.19	117.98
20	4	310	CLA	CMD-C2D-C3D	-4.13	118.23	127.69
20	G	103	CLA	C4-C3-C5	4.13	120.98	116.13
20	A	819	CLA	CMD-C2D-C3D	-4.12	118.23	127.69
20	B	849	CLA	CMD-C2D-C3D	-4.12	118.23	127.69
20	4	317	CLA	C3A-C4A-CHB	-4.12	118.86	123.91
20	B	848	CLA	CHB-C4A-NA	4.12	130.35	124.40
20	A	806	CLA	CMD-C2D-C3D	-4.12	118.24	127.69
20	B	813	CLA	CHC-C1C-NC	4.12	130.52	124.31
20	2	315	CLA	C1B-NB-C4B	-4.12	103.42	106.31
20	B	827	CLA	O2D-CGD-CBD	4.12	118.43	111.23
20	B	814	CLA	CHD-C4C-NC	4.12	130.61	124.23
20	3	303	CLA	C1B-C2B-C3B	-4.12	103.16	107.03
20	4	319	CLA	CHC-C1C-NC	4.12	130.51	124.31
21	H	104	LMU	O1'-C1'-C2'	-4.11	102.03	108.27
21	R	102	LMU	C1B-O5B-C5B	4.11	121.75	113.72
20	3	319	CLA	C1B-C2B-C3B	-4.11	103.17	107.03
20	A	819	CLA	CAA-C2A-C1A	4.11	121.24	112.14
20	F	206	CLA	C4D-C3D-CAD	4.11	112.57	108.11
20	A	821	CLA	CMD-C2D-C3D	-4.11	118.27	127.69
20	4	315	CLA	C4A-NA-C1A	4.11	108.55	106.68
20	L	202	CLA	CHD-C4C-NC	4.11	130.60	124.23
20	L	207	CLA	CMD-C2D-C3D	-4.11	118.27	127.69
22	A	841	BCR	C33-C5-C6	-4.11	120.00	124.48
20	2	312	CLA	CHD-C4C-NC	4.11	130.60	124.23
20	3	303	CLA	CAB-C3B-C2B	-4.10	112.63	123.53
22	G	102	BCR	C38-C26-C25	-4.10	120.01	124.48
22	F	202	BCR	C33-C5-C6	-4.10	120.01	124.48
20	L	202	CLA	C6-C5-C3	-4.10	103.47	113.47
20	B	818	CLA	C2B-C1B-NB	4.10	114.58	110.33
20	1	212	CLA	CHC-C4B-NB	4.10	130.20	124.05
20	2	321	CLA	C3B-C2B-C1B	-4.10	102.34	107.17
22	B	844	BCR	C33-C5-C6	-4.10	120.01	124.48
20	4	302	CLA	CHC-C1C-NC	4.10	130.48	124.31
20	B	829	CLA	C4B-CHC-C1C	-4.10	116.61	126.25
20	1	213	CLA	C4A-NA-C1A	4.10	108.55	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	843	BCR	C33-C5-C6	-4.10	120.02	124.48
20	B	848	CLA	CHD-C4C-C3C	-4.09	118.80	124.77
20	4	305	CLA	C2B-C1B-NB	4.09	114.57	110.33
20	A	826	CLA	CHD-C4C-C3C	-4.09	118.81	124.77
20	J	102	CLA	CHC-C1C-NC	4.09	130.48	124.31
22	F	202	BCR	C38-C26-C25	-4.09	120.02	124.48
20	A	816	CLA	CHC-C1C-NC	4.09	130.47	124.31
20	2	317	CLA	CHD-C4C-NC	4.09	130.57	124.23
20	A	814	CLA	C4B-CHC-C1C	-4.09	116.63	126.25
21	R	103	LMU	O2'-C2'-C1'	-4.09	100.33	110.08
22	B	841	BCR	C33-C5-C6	-4.09	120.02	124.48
20	2	314	CLA	C3D-C4D-CHA	-4.09	116.07	125.20
20	2	315	CLA	C4C-CHD-C1D	-4.09	114.34	125.98
20	A	804	CLA	CHC-C1C-NC	4.09	130.47	124.31
20	L	203	CLA	O2D-CGD-O1D	-4.09	115.89	123.85
20	2	317	CLA	C3B-C2B-C1B	-4.09	102.35	107.17
20	G	103	CLA	C3B-C2B-C1B	-4.09	102.35	107.17
20	A	828	CLA	O2D-CGD-CBD	4.08	118.37	111.23
20	H	108	CLA	C2B-C1B-NB	4.08	114.56	110.33
20	A	819	CLA	C2B-C1B-NB	4.08	114.56	110.33
20	2	321	CLA	CHD-C4C-NC	4.08	130.56	124.23
20	R	106	CLA	C4B-CHC-C1C	-4.08	116.65	126.25
20	4	313	CLA	C2B-C1B-NB	4.08	114.56	110.33
20	2	312	CLA	CHD-C4C-C3C	-4.08	118.82	124.77
20	L	204	CLA	C3B-C2B-C1B	-4.08	102.36	107.17
20	4	313	CLA	CAC-C3C-C4C	4.08	131.41	125.03
20	1	211	CLA	CAA-C2A-C1A	-4.08	98.60	111.97
20	3	314	CLA	CAC-C3C-C4C	4.08	130.10	124.79
20	B	815	CLA	CMD-C2D-C1D	4.08	131.91	124.73
20	3	307	CLA	C2A-C1A-CHA	-4.08	115.67	122.63
21	B	801	LMU	C1B-O5B-C5B	4.08	121.69	113.72
20	B	837	CLA	CHC-C4B-NB	4.08	130.17	124.05
20	J	103	CLA	CMD-C2D-C3D	-4.08	118.34	127.69
20	4	309	CLA	C3A-C4A-CHB	-4.08	118.92	123.91
20	L	201	CLA	C4B-CHC-C1C	-4.08	116.66	126.25
20	F	204	CLA	C4A-NA-C1A	4.07	108.54	106.68
20	A	838	CLA	C3B-C2B-C1B	-4.07	102.37	107.17
20	K	106	CLA	O2A-CGA-CBA	4.07	124.26	111.83
20	K	107	CLA	O2D-CGD-O1D	-4.07	115.92	123.85
20	3	308	CLA	CHC-C4B-NB	4.07	129.96	124.08
20	B	848	CLA	CAC-C3C-C4C	4.07	130.08	124.79
20	H	101	CLA	CHD-C4C-NC	4.07	130.54	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	809	CLA	CHC-C1C-NC	4.07	130.44	124.31
20	H	101	CLA	CHB-C4A-NA	4.07	130.27	124.40
20	4	313	CLA	CAB-C3B-C2B	-4.07	112.73	123.53
21	A	853	LMU	O3'-C3'-C2'	-4.07	100.79	110.38
20	1	204	CLA	C4B-CHC-C1C	-4.06	116.69	126.25
20	B	817	CLA	C2B-C1B-NB	4.06	114.54	110.33
22	A	842	BCR	C38-C26-C25	-4.06	120.05	124.48
22	B	843	BCR	C38-C26-C25	-4.06	120.05	124.48
21	R	109	LMU	C1B-O1B-C4'	-4.06	108.35	117.98
22	A	844	BCR	C38-C26-C25	-4.06	120.05	124.48
20	L	207	CLA	CHC-C1C-NC	4.06	130.43	124.31
20	3	313	CLA	C4A-NA-C1A	4.06	108.53	106.68
21	L	206	LMU	O5'-C1'-C2'	-4.06	102.03	110.37
20	A	807	CLA	O2A-CGA-CBA	4.06	124.20	111.83
20	1	205	CLA	C1B-C2B-C3B	-4.06	103.22	107.03
20	B	839	CLA	CBD-CHA-C1A	4.06	133.50	127.38
20	B	831	CLA	O2D-CGD-CBD	4.06	118.32	111.23
21	F	201	LMU	O3B-C3B-C4B	-4.06	100.82	110.38
20	B	827	CLA	C4B-CHC-C1C	-4.05	116.71	126.25
20	A	818	CLA	CHD-C4C-C3C	-4.05	118.86	124.77
20	3	316	CLA	C3D-C4D-CHA	-4.05	116.15	125.20
20	2	304	CLA	C4B-CHC-C1C	-4.05	116.72	126.25
20	A	847	CLA	CED-O2D-CGD	4.05	125.11	115.92
20	B	818	CLA	O2D-CGD-CBD	4.05	118.31	111.23
20	3	309	CLA	CHC-C1C-NC	4.05	130.41	124.31
20	A	814	CLA	CHD-C4C-C3C	-4.05	118.87	124.77
20	4	314	CLA	C3A-C4A-CHB	-4.05	118.95	123.91
23	A	839	PQN	C14-C13-C15	4.05	122.25	115.23
20	A	817	CLA	CHC-C1C-NC	4.05	130.41	124.31
25	B	846	LMG	O7-C10-C11	4.05	120.23	111.48
20	A	805	CLA	CHD-C4C-NC	4.04	130.50	124.23
20	K	106	CLA	CHD-C4C-NC	4.04	130.50	124.23
20	A	804	CLA	CHD-C4C-C3C	-4.04	118.88	124.77
20	B	833	CLA	CHD-C4C-C3C	-4.04	118.88	124.77
20	1	214	CLA	CAA-C2A-C1A	4.04	125.22	111.97
21	L	205	LMU	C1B-O5B-C5B	-4.04	105.83	113.72
20	1	215	CLA	C3D-C4D-ND	4.04	115.02	109.50
22	F	203	BCR	C27-C26-C25	-4.04	117.25	122.70
20	A	803	CLA	C2B-C1B-NB	4.04	114.51	110.33
20	B	839	CLA	CHD-C4C-C3C	-4.04	118.66	125.03
20	A	830	CLA	C1-C2-C3	-4.04	120.23	126.76
20	1	207	CLA	C2B-C1B-NB	4.03	114.51	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	L	208	CLA	C2B-C1B-NB	4.03	114.51	110.33
20	B	849	CLA	CHD-C4C-C3C	-4.03	118.89	124.77
20	3	317	CLA	C4C-CHD-C1D	-4.03	114.50	125.98
20	2	306	CLA	CHC-C1C-NC	4.03	130.38	124.31
20	B	806	CLA	CHC-C4B-NB	4.03	130.09	124.05
20	H	108	CLA	C4B-CHC-C1C	-4.03	116.77	126.25
22	A	840	BCR	C33-C5-C6	-4.03	120.09	124.48
22	J	101	BCR	C33-C5-C6	-4.03	120.09	124.48
20	A	812	CLA	CHD-C4C-NC	4.03	130.48	124.23
20	4	306	CLA	CHD-C4C-C3C	-4.03	118.90	124.77
20	H	110	CLA	CHC-C1C-NC	4.03	130.38	124.31
20	R	107	CLA	C1-C2-C3	4.03	132.79	126.20
22	I	101	BCR	C31-C1-C6	4.03	116.56	110.24
20	2	302	CLA	CHD-C4C-C3C	-4.03	118.90	124.77
20	B	825	CLA	C4B-CHC-C1C	-4.02	116.80	126.25
20	1	205	CLA	CBD-CHA-C1A	4.02	133.44	127.38
21	A	853	LMU	C2'-C3'-C4'	4.02	118.80	109.68
20	2	310	CLA	C3B-C2B-C1B	-4.02	102.44	107.17
21	E	101	LMU	O5'-C1'-C2'	-4.01	102.12	110.37
20	H	108	CLA	CHC-C1C-NC	4.01	130.36	124.31
20	1	206	CLA	C4B-CHC-C1C	-4.01	116.82	126.25
21	H	104	LMU	C1'-C2'-C3'	-4.01	101.58	110.01
20	A	807	CLA	C2B-C1B-NB	4.01	114.48	110.33
20	3	316	CLA	CHC-C1C-NC	4.01	130.22	124.33
20	3	313	CLA	CHA-C4D-ND	4.01	130.50	124.84
20	3	303	CLA	CHC-C1C-NC	4.00	130.34	124.31
20	A	815	CLA	C2B-C1B-NB	4.00	114.48	110.33
20	B	825	CLA	CMB-C2B-C1B	4.00	131.52	125.42
20	A	850	CLA	CED-O2D-CGD	4.00	125.00	115.92
20	B	831	CLA	CMD-C2D-C3D	-4.00	118.51	127.69
20	2	308	CLA	C1C-CHC-C4B	-4.00	115.48	126.04
20	4	308	CLA	CHC-C1C-NC	4.00	130.21	124.33
20	3	306	CLA	C1C-CHC-C4B	-4.00	115.49	126.04
20	3	316	CLA	C1C-CHC-C4B	-4.00	115.49	126.04
20	1	209	CLA	CHC-C4B-NB	4.00	130.05	124.05
20	A	814	CLA	CHC-C1C-NC	4.00	130.34	124.31
20	B	849	CLA	C1-O2A-CGA	4.00	126.33	116.65
20	3	307	CLA	C1C-CHC-C4B	-4.00	115.49	126.04
20	A	838	CLA	CHD-C4C-NC	4.00	130.43	124.23
20	A	803	CLA	CHD-C4C-C3C	-4.00	118.95	124.77
20	A	848	CLA	CHC-C1C-NC	3.99	130.33	124.31
20	A	812	CLA	CHC-C1C-NC	3.99	130.33	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	213	CLA	C2A-C1A-CHA	-3.99	115.82	122.63
20	2	310	CLA	C2B-C1B-NB	3.99	114.47	110.33
20	B	834	CLA	CHD-C4C-C3C	-3.99	118.95	124.77
20	H	110	CLA	C4A-NA-C1A	3.99	108.50	106.68
20	1	207	CLA	O2D-CGD-O1D	-3.99	116.08	123.85
20	A	817	CLA	CMD-C2D-C3D	-3.99	118.54	127.69
20	A	803	CLA	CMB-C2B-C1B	3.99	131.49	125.42
20	B	818	CLA	CMD-C2D-C3D	-3.99	118.55	127.69
20	A	815	CLA	O2A-CGA-CBA	3.99	123.99	111.83
20	3	305	CLA	C1C-CHC-C4B	-3.99	115.53	126.04
20	B	820	CLA	CHC-C4B-NB	3.98	130.03	124.05
20	L	207	CLA	CHB-C4A-NA	3.98	130.15	124.40
20	A	807	CLA	CMB-C2B-C1B	3.98	131.49	125.42
21	A	852	LMU	C1-O1'-C1'	-3.98	106.88	113.68
21	4	316	LMU	C1B-O5B-C5B	3.98	121.50	113.72
20	B	827	CLA	CMD-C2D-C1D	3.98	131.74	124.73
20	A	828	CLA	CHC-C1C-NC	3.98	130.31	124.31
20	2	302	CLA	O2D-CGD-O1D	-3.98	116.10	123.85
20	A	810	CLA	C2B-C1B-NB	3.97	114.45	110.33
22	B	841	BCR	C38-C26-C25	-3.97	120.15	124.48
20	A	811	CLA	CHD-C4C-C3C	-3.97	118.98	124.77
20	B	848	CLA	O2D-CGD-O1D	-3.97	116.11	123.85
20	1	211	CLA	C1-C2-C3	-3.97	119.69	126.20
20	B	810	CLA	C4B-CHC-C1C	-3.97	116.91	126.25
20	B	847	CLA	CHC-C4B-NB	3.97	130.01	124.05
20	1	213	CLA	CHC-C1C-NC	3.97	130.17	124.33
21	H	104	LMU	O2B-C2B-C3B	-3.97	101.02	110.38
20	4	304	CLA	C11-C10-C8	-3.97	102.78	115.97
20	1	205	CLA	CMD-C2D-C3D	-3.97	118.59	127.69
20	3	320	CLA	C4A-NA-C1A	3.96	108.49	106.68
20	A	826	CLA	C4B-CHC-C1C	-3.96	116.94	126.25
21	H	104	LMU	C4B-C3B-C2B	-3.96	103.88	110.83
20	B	849	CLA	C4A-NA-C1A	3.96	108.48	106.68
20	B	808	CLA	CHC-C1C-NC	3.96	130.27	124.31
20	4	304	CLA	O2A-CGA-CBA	3.96	123.90	111.83
20	A	813	CLA	O2D-CGD-CBD	3.96	118.14	111.23
20	4	308	CLA	C2A-C1A-CHA	-3.96	115.89	122.63
20	4	311	CLA	C3B-C2B-C1B	-3.95	102.41	106.81
20	2	305	CLA	C3D-C4D-ND	3.95	114.90	109.50
20	A	810	CLA	CHC-C1C-NC	3.95	130.26	124.31
20	A	809	CLA	C11-C12-C13	-3.95	102.83	115.97
20	A	818	CLA	C4B-CHC-C1C	-3.95	116.96	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	821	CLA	CHD-C4C-NC	3.95	130.35	124.23
20	4	317	CLA	CHC-C1C-NC	3.95	130.13	124.33
20	2	303	CLA	C1B-NB-C4B	-3.95	103.54	106.31
21	B	801	LMU	O5B-C5B-C4B	3.95	116.81	109.70
20	A	812	CLA	C4B-CHC-C1C	-3.95	116.97	126.25
20	A	804	CLA	O2D-CGD-O1D	-3.95	116.17	123.85
20	3	314	CLA	C4A-NA-C1A	3.94	108.48	106.68
20	A	819	CLA	CHC-C4B-NB	3.94	129.96	124.05
20	2	306	CLA	CED-O2D-CGD	3.94	124.86	115.92
20	B	805	CLA	O2D-CGD-O1D	-3.94	116.18	123.85
20	4	312	CLA	C2D-C3D-C4D	-3.94	102.56	107.35
20	3	312	CLA	C1B-NB-C4B	-3.94	103.55	106.31
20	A	811	CLA	C4B-CHC-C1C	-3.94	116.98	126.25
20	B	813	CLA	O1D-CGD-CBD	-3.94	116.75	124.52
20	4	309	CLA	C1B-NB-C4B	-3.94	103.55	106.31
20	2	309	CLA	C1C-CHC-C4B	-3.94	115.66	126.04
20	1	201	CLA	C3B-C2B-C1B	-3.94	102.53	107.17
20	H	101	CLA	CMA-C3A-C2A	-3.94	98.77	113.98
21	R	103	LMU	C6B-C5B-C4B	-3.94	103.36	113.02
20	4	309	CLA	C1C-CHC-C4B	-3.93	115.67	126.04
20	4	305	CLA	O2D-CGD-O1D	-3.93	116.19	123.85
20	H	107	CLA	CHD-C4C-C3C	-3.93	119.04	124.77
20	B	813	CLA	C4B-CHC-C1C	-3.93	117.00	126.25
20	4	317	CLA	CHD-C4C-NC	3.93	130.21	124.24
20	2	310	CLA	CHC-C1C-NC	3.93	130.23	124.31
20	B	835	CLA	CHC-C4B-NB	3.92	129.94	124.05
20	A	815	CLA	C4B-CHC-C1C	-3.92	117.02	126.25
20	4	313	CLA	C4B-CHC-C1C	-3.92	117.02	126.25
21	H	102	LMU	O4'-C4B-C3B	3.92	119.62	110.38
20	B	829	CLA	CMD-C2D-C3D	-3.92	118.70	127.69
20	A	849	CLA	C4B-CHC-C1C	-3.92	117.03	126.25
20	B	837	CLA	O2A-CGA-CBA	3.92	123.79	111.83
20	1	207	CLA	C3B-C2B-C1B	-3.92	102.55	107.17
20	B	825	CLA	O2A-CGA-CBA	3.92	123.78	111.83
20	A	821	CLA	CHD-C4C-NC	3.92	130.30	124.23
20	1	215	CLA	C4C-CHD-C1D	-3.92	114.82	125.98
20	A	820	CLA	CMD-C2D-C3D	-3.92	118.71	127.69
20	B	824	CLA	CHD-C4C-C3C	-3.91	119.07	124.77
20	A	829	CLA	CAC-C3C-C4C	3.91	129.88	124.79
20	1	214	CLA	CMD-C2D-C1D	3.91	131.62	124.73
20	B	820	CLA	O2D-CGD-CBD	3.91	118.06	111.23
20	4	307	CLA	CGD-CBD-CAD	3.91	123.49	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	311	CLA	C1C-CHC-C4B	-3.90	115.74	126.04
20	H	110	CLA	CHC-C4B-NB	3.90	129.91	124.05
21	B	802	LMU	O2'-C2'-C3'	-3.90	101.18	110.38
20	2	303	CLA	C1C-CHC-C4B	-3.90	115.75	126.04
21	2	318	LMU	C6B-C5B-C4B	3.90	122.60	113.02
21	F	201	LMU	C3'-C4'-C5'	-3.90	102.28	110.93
20	B	848	CLA	CHC-C1C-NC	3.90	130.19	124.31
20	1	202	CLA	CHD-C4C-C3C	-3.90	119.09	124.77
20	3	303	CLA	CMD-C2D-C3D	-3.90	118.75	127.69
20	3	303	CLA	C4B-CHC-C1C	-3.90	117.09	126.25
20	A	848	CLA	O2A-CGA-CBA	3.89	123.71	111.83
20	B	807	CLA	C2B-C1B-NB	3.89	114.36	110.33
20	B	847	CLA	CAA-C2A-C3A	-3.89	102.48	113.00
20	A	829	CLA	CMA-C3A-C2A	-3.89	98.95	113.98
20	A	817	CLA	CHD-C4C-C3C	-3.89	119.11	124.77
21	K	101	LMU	O6B-C6B-C5B	-3.89	98.10	111.33
20	2	304	CLA	CHC-C1C-NC	3.88	130.16	124.31
20	4	304	CLA	O2D-CGD-O1D	-3.88	116.29	123.85
20	A	815	CLA	CHC-C1C-NC	3.88	130.16	124.31
20	B	819	CLA	C2B-C1B-NB	3.88	114.35	110.33
20	B	848	CLA	C3B-C2B-C1B	-3.88	102.60	107.17
20	A	812	CLA	CMD-C2D-C3D	-3.88	118.80	127.69
20	3	313	CLA	C1B-NB-C4B	-3.88	103.59	106.31
20	1	212	CLA	CHC-C1C-NC	3.87	130.15	124.31
20	R	106	CLA	CHD-C4C-C3C	-3.87	119.12	124.77
20	H	101	CLA	C4B-CHC-C1C	-3.87	117.14	126.25
20	A	828	CLA	CHD-C4C-C3C	-3.87	119.13	124.77
20	3	312	CLA	CHC-C1C-NC	3.87	130.02	124.33
20	B	828	CLA	CMB-C2B-C1B	3.87	131.31	125.42
20	2	321	CLA	C4B-CHC-C1C	-3.87	117.15	126.25
20	1	205	CLA	CAB-C3B-C2B	-3.87	113.26	123.53
20	4	317	CLA	CHA-C4D-ND	3.87	130.31	124.84
20	2	303	CLA	C2D-C3D-C4D	-3.87	102.65	107.35
20	4	314	CLA	CHC-C4B-NB	3.87	129.67	124.08
20	A	801	CLA	CHC-C4B-NB	3.87	129.85	124.05
20	A	825	CLA	CHC-C4B-NB	3.87	129.85	124.05
20	R	106	CLA	C2B-C1B-NB	3.87	114.34	110.33
20	F	204	CLA	CHD-C4C-C3C	-3.87	118.92	125.03
21	B	845	LMU	O1'-C1'-C2'	3.87	114.14	108.27
21	2	319	LMU	O1'-C1'-C2'	3.86	114.14	108.27
20	B	812	CLA	O2D-CGD-CBD	3.86	117.98	111.23
20	B	805	CLA	CMD-C2D-C3D	-3.86	118.83	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	808	CLA	C2A-C1A-CHA	-3.86	117.17	123.87
20	B	821	CLA	CAC-C3C-C4C	3.86	129.81	124.79
21	1	218	LMU	C3B-C4B-C5B	3.86	117.23	110.23
20	2	304	CLA	CHD-C4C-NC	3.86	130.21	124.23
20	K	107	CLA	C2B-C1B-NB	3.86	114.33	110.33
20	B	809	CLA	CHC-C4B-NB	3.86	129.84	124.05
20	A	838	CLA	CHC-C1C-NC	3.86	130.12	124.31
20	2	314	CLA	C3D-C4D-ND	3.85	114.77	109.50
21	F	201	LMU	C4B-C3B-C2B	-3.85	104.06	110.83
20	A	826	CLA	CHC-C1C-NC	3.85	130.12	124.31
20	4	314	CLA	C4C-CHD-C1D	-3.85	115.01	125.98
20	B	821	CLA	CAA-CBA-CGA	-3.85	102.28	113.21
20	B	826	CLA	O2D-CGD-O1D	-3.85	116.36	123.85
20	A	813	CLA	C4B-CHC-C1C	-3.85	117.20	126.25
20	4	317	CLA	CHC-C4B-NB	3.85	129.64	124.08
20	2	311	CLA	CGD-CBD-CAD	-3.85	98.39	110.85
20	3	308	CLA	C3D-C4D-CHA	-3.84	116.61	125.20
20	F	206	CLA	O2D-CGD-CBD	3.84	117.95	111.23
20	B	833	CLA	C4B-CHC-C1C	-3.84	117.21	126.25
20	H	110	CLA	C2B-C1B-NB	3.84	114.31	110.33
22	F	203	BCR	C40-C30-C25	-3.84	104.22	110.24
20	3	307	CLA	C4A-NA-C1A	3.84	108.43	106.68
20	A	804	CLA	CMD-C2D-C3D	-3.84	118.88	127.69
20	2	315	CLA	C1C-CHC-C4B	-3.84	115.91	126.04
20	A	814	CLA	CMD-C2D-C3D	-3.84	118.88	127.69
20	2	314	CLA	CHD-C4C-NC	3.84	130.07	124.24
20	1	205	CLA	CHC-C4B-NB	3.84	129.81	124.05
20	4	312	CLA	C4C-CHD-C1D	-3.84	115.04	125.98
20	A	813	CLA	O2D-CGD-O1D	-3.84	116.38	123.85
20	2	321	CLA	CHC-C1C-NC	3.84	130.09	124.31
20	K	103	CLA	C1-C2-C3	-3.84	120.56	126.76
20	3	316	CLA	C1B-NB-C4B	-3.84	103.62	106.31
20	A	828	CLA	CMD-C2D-C3D	-3.84	118.89	127.69
20	B	825	CLA	CHC-C4B-NB	3.83	129.80	124.05
20	A	830	CLA	C4B-CHC-C1C	-3.83	117.23	126.25
20	A	810	CLA	C4B-CHC-C1C	-3.83	117.23	126.25
20	3	306	CLA	C3B-C2B-C1B	-3.83	102.54	106.81
20	H	110	CLA	CMB-C2B-C1B	3.83	131.25	125.42
20	3	308	CLA	C3D-C4D-ND	3.83	114.74	109.50
21	H	102	LMU	O5B-C5B-C6B	3.83	115.94	106.44
21	R	103	LMU	O2'-C2'-C3'	-3.83	101.35	110.38
20	2	307	CLA	CHD-C4C-NC	3.83	130.17	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	838	CLA	C4B-CHC-C1C	-3.83	117.24	126.25
20	1	202	CLA	CHD-C4C-NC	3.83	130.17	124.23
20	4	314	CLA	C1C-CHC-C4B	-3.83	115.95	126.04
20	3	313	CLA	C1C-CHC-C4B	-3.83	115.95	126.04
20	B	849	CLA	C3B-C2B-C1B	-3.82	102.66	107.17
20	L	202	CLA	CHC-C4B-NB	3.82	129.78	124.05
20	3	319	CLA	C2B-C1B-NB	3.82	114.29	110.33
20	L	207	CLA	CGD-CBD-CAD	-3.82	98.47	110.85
22	L	209	BCR	C11-C10-C9	-3.82	121.92	127.28
20	H	107	CLA	CMD-C2D-C3D	-3.82	118.93	127.69
20	A	849	CLA	O2D-CGD-O1D	-3.82	116.42	123.85
21	K	104	LMU	O3'-C3'-C2'	-3.82	101.38	110.38
20	B	823	CLA	C2B-C1B-NB	3.82	114.28	110.33
20	2	309	CLA	CHC-C4B-NB	3.82	129.59	124.08
20	L	207	CLA	O2D-CGD-O1D	-3.81	116.42	123.85
20	2	305	CLA	C4A-NA-C1A	3.81	108.42	106.68
20	2	317	CLA	C4B-CHC-C1C	-3.81	117.28	126.25
21	K	104	LMU	O5B-C5B-C6B	3.81	115.88	106.44
20	3	307	CLA	C4C-CHD-C1D	-3.81	115.13	125.98
21	1	218	LMU	C3'-C4'-C5'	-3.81	102.50	110.93
20	1	207	CLA	CHC-C1C-NC	3.81	130.04	124.31
20	B	816	CLA	C3B-C2B-C1B	-3.80	102.69	107.17
20	B	824	CLA	C4B-CHC-C1C	-3.80	117.30	126.25
20	A	816	CLA	O2D-CGD-CBD	3.80	117.88	111.23
21	R	102	LMU	C6B-C5B-C4B	-3.80	103.68	113.02
20	4	313	CLA	CHC-C1C-NC	3.80	130.04	124.31
20	A	822	CLA	C2B-C1B-NB	3.80	114.27	110.33
20	L	207	CLA	C3B-C2B-C1B	-3.80	102.69	107.17
20	4	314	CLA	CHD-C4C-NC	3.80	130.01	124.24
20	A	821	CLA	CHC-C1C-NC	3.80	130.03	124.31
20	H	101	CLA	CMD-C2D-C3D	-3.80	118.98	127.69
20	B	821	CLA	CGD-CBD-CAD	-3.80	98.56	110.85
20	F	206	CLA	CHC-C4B-NB	3.79	129.74	124.05
20	B	824	CLA	CHC-C1C-NC	3.79	130.03	124.31
21	R	101	LMU	C3'-C4'-C5'	-3.79	102.52	110.93
20	4	304	CLA	C2B-C1B-NB	3.79	114.26	110.33
20	3	305	CLA	C2A-C1A-CHA	-3.79	116.16	122.63
20	1	210	CLA	C4B-CHC-C1C	-3.79	117.33	126.25
20	A	857	CLA	CHA-C4D-ND	3.79	130.20	124.84
20	B	807	CLA	CHC-C4B-NB	3.79	129.73	124.05
20	A	801	CLA	C2B-C1B-NB	3.79	114.25	110.33
20	B	818	CLA	CHB-C4A-NA	3.79	129.86	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	830	CLA	CHC-C1C-NC	3.79	130.01	124.31
20	B	820	CLA	C2B-C1B-NB	3.78	114.25	110.33
20	B	822	CLA	C2B-C1B-NB	3.78	114.25	110.33
20	A	816	CLA	C1-C2-C3	-3.78	120.00	126.20
20	B	811	CLA	CHC-C4B-NB	3.78	129.72	124.05
20	B	832	CLA	CHC-C1C-NC	3.78	130.00	124.31
20	A	829	CLA	CMB-C2B-C1B	3.78	131.17	125.42
20	B	817	CLA	C4A-NA-C1A	3.78	108.40	106.68
21	R	105	LMU	O3B-C3B-C4B	3.78	119.28	110.38
20	2	302	CLA	C4B-CHC-C1C	-3.78	117.37	126.25
20	4	315	CLA	C4B-CHC-C1C	-3.78	117.37	126.25
20	4	303	CLA	CHC-C1C-NC	3.77	130.00	124.31
20	4	306	CLA	C4B-CHC-C1C	-3.77	117.37	126.25
20	B	813	CLA	CMD-C2D-C3D	-3.77	119.03	127.69
20	2	312	CLA	CHC-C1C-NC	3.77	129.99	124.31
20	A	849	CLA	CHD-C4C-C3C	-3.77	119.27	124.77
22	B	850	BCR	C37-C22-C21	-3.77	116.70	122.82
20	B	807	CLA	CHC-C1C-NC	3.77	129.99	124.31
20	4	306	CLA	CMD-C2D-C3D	-3.77	119.04	127.69
20	3	306	CLA	C2A-C1A-CHA	-3.77	116.20	122.63
20	A	810	CLA	C4A-NA-C1A	3.77	108.40	106.68
20	J	103	CLA	C1-C2-C3	-3.77	120.02	126.20
21	A	845	LMU	O5'-C5'-C4'	3.77	117.52	109.72
20	2	309	CLA	CHC-C1C-NC	3.77	129.87	124.33
20	2	312	CLA	CHC-C4B-NB	3.77	129.70	124.05
20	A	827	CLA	C3B-C2B-C1B	-3.77	102.73	107.17
20	2	301	CLA	C2B-C1B-NB	3.77	114.23	110.33
20	L	201	CLA	CHD-C4C-C3C	-3.77	119.28	124.77
21	R	102	LMU	O2B-C2B-C1B	3.77	119.05	110.08
20	3	313	CLA	C3D-C4D-CHA	-3.77	116.79	125.20
20	B	807	CLA	O2A-CGA-O1A	-3.76	114.21	123.63
20	A	801	CLA	CHC-C1C-NC	3.76	129.98	124.31
20	H	107	CLA	CHC-C1C-NC	3.76	129.98	124.31
20	B	835	CLA	CMB-C2B-C1B	3.76	131.15	125.42
20	A	857	CLA	C4A-NA-C1A	3.76	108.40	106.68
20	1	209	CLA	C1B-C2B-C3B	-3.76	103.49	107.03
20	A	832	CLA	C2B-C1B-NB	3.76	114.23	110.33
20	A	829	CLA	CHC-C1C-C2C	-3.76	116.26	126.95
20	B	830	CLA	CMD-C2D-C3D	-3.76	119.07	127.69
20	A	823	CLA	C2B-C1B-NB	3.76	114.22	110.33
20	B	814	CLA	O2D-CGD-O1D	-3.76	116.53	123.85
21	1	218	LMU	O2B-C2B-C1B	-3.76	101.12	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	202	CLA	O2A-CGA-CBA	3.76	123.29	111.83
20	3	307	CLA	CHA-C4D-ND	3.76	130.15	124.84
20	1	209	CLA	CAA-C2A-C3A	-3.76	107.61	116.23
20	L	204	CLA	O2A-CGA-CBA	3.76	123.29	111.83
20	B	828	CLA	C2B-C1B-NB	3.76	114.22	110.33
20	B	827	CLA	CAC-C3C-C4C	3.76	129.68	124.79
20	B	814	CLA	CMD-C2D-C3D	-3.76	119.08	127.69
20	B	808	CLA	C4B-CHC-C1C	-3.75	117.42	126.25
20	A	831	CLA	C2B-C1B-NB	3.75	114.22	110.33
20	R	106	CLA	CHC-C1C-NC	3.75	129.96	124.31
20	2	308	CLA	C2D-C3D-C4D	-3.75	102.79	107.35
20	B	805	CLA	C4B-CHC-C1C	-3.75	117.43	126.25
20	B	825	CLA	CHC-C1C-NC	3.75	129.96	124.31
20	1	206	CLA	C3B-C2B-C1B	-3.75	102.75	107.17
20	4	318	CLA	CMD-C2D-C3D	-3.75	119.09	127.69
22	I	101	BCR	C38-C26-C27	3.75	121.59	113.60
20	1	203	CLA	C2B-C1B-NB	3.75	114.21	110.33
20	A	803	CLA	CMD-C2D-C3D	-3.75	119.10	127.69
20	R	107	CLA	CMA-C3A-C4A	3.74	121.84	111.77
20	4	302	CLA	C2B-C1B-NB	3.74	114.21	110.33
21	R	103	LMU	O2B-C2B-C1B	3.74	119.00	110.08
21	K	104	LMU	O2'-C2'-C1'	3.74	118.99	110.08
20	A	855	CLA	C2B-C1B-NB	3.74	114.21	110.33
20	3	320	CLA	C3B-C2B-C1B	-3.74	102.76	107.17
20	B	833	CLA	C3B-C2B-C1B	-3.74	102.76	107.17
20	B	828	CLA	C1-C2-C3	-3.74	120.71	126.76
20	B	825	CLA	CHB-C4A-NA	3.74	129.80	124.40
20	1	208	CLA	CHC-C1C-NC	3.74	129.82	124.33
20	A	835	CLA	C2B-C1B-NB	3.74	114.20	110.33
20	A	837	CLA	C2B-C1B-NB	3.74	114.20	110.33
20	B	847	CLA	CMD-C2D-C1D	3.74	131.31	124.73
21	1	218	LMU	O5'-C1'-C2'	3.74	118.05	110.37
20	L	201	CLA	CHC-C1C-NC	3.74	129.94	124.31
20	A	813	CLA	CMD-C2D-C3D	-3.74	119.12	127.69
20	A	803	CLA	O2D-CGD-CBD	3.74	117.76	111.23
20	F	205	CLA	C2B-C1B-NB	3.73	114.20	110.33
20	B	834	CLA	C4B-CHC-C1C	-3.73	117.47	126.25
20	4	312	CLA	CHD-C4C-NC	3.73	129.91	124.24
20	1	203	CLA	C4B-CHC-C1C	-3.73	117.47	126.25
20	4	314	CLA	C2A-C1A-CHA	-3.73	116.27	122.63
20	2	307	CLA	CHC-C4B-NB	3.73	129.65	124.05
20	K	105	CLA	C2B-C1B-NB	3.73	114.20	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	H	107	CLA	C3B-C4B-NB	-3.73	107.20	110.53
20	3	312	CLA	C2D-C3D-C4D	-3.73	102.81	107.35
20	1	214	CLA	C2B-C1B-NB	3.73	114.20	110.33
20	L	203	CLA	CMD-C2D-C3D	-3.73	119.13	127.69
20	2	302	CLA	C3B-C2B-C1B	-3.73	102.77	107.17
20	1	205	CLA	C2B-C1B-NB	3.73	114.19	110.33
20	A	857	CLA	C4C-CHD-C1D	-3.73	115.36	125.98
20	A	825	CLA	C1-O2A-CGA	3.73	125.68	116.65
20	4	313	CLA	CHC-C4B-NB	3.73	129.64	124.05
20	A	826	CLA	O2D-CGD-O1D	-3.73	116.59	123.85
20	A	836	CLA	C2B-C1B-NB	3.73	114.19	110.33
20	A	833	CLA	C2B-C1B-NB	3.73	114.19	110.33
20	3	314	CLA	CHD-C4C-NC	3.73	130.01	124.23
20	2	310	CLA	CHC-C4B-NB	3.72	129.64	124.05
20	H	108	CLA	CHD-C4C-NC	3.72	130.00	124.23
20	4	311	CLA	CHA-C4D-ND	3.72	130.09	124.84
20	4	310	CLA	O2D-CGD-CBD	3.72	117.73	111.23
20	4	317	CLA	C3D-C4D-CHA	-3.72	116.90	125.20
20	3	320	CLA	C4B-CHC-C1C	-3.72	117.51	126.25
23	A	839	PQN	C2M-C2-C3	-3.71	118.34	124.45
20	B	835	CLA	C2B-C1B-NB	3.71	114.18	110.33
22	F	203	BCR	C1-C6-C5	-3.71	117.56	122.64
20	B	817	CLA	CHC-C1C-NC	3.71	129.90	124.31
20	H	108	CLA	C4-C3-C5	3.71	121.67	115.23
20	B	837	CLA	C3B-C4B-NB	-3.71	107.22	110.53
20	A	821	CLA	CHD-C4C-C3C	-3.71	119.36	124.77
20	1	210	CLA	C2B-C1B-NB	3.71	114.17	110.33
20	A	830	CLA	C3B-C2B-C1B	-3.71	102.80	107.17
20	1	204	CLA	CHC-C4B-NB	3.71	129.61	124.05
20	2	304	CLA	C3B-C2B-C1B	-3.71	102.80	107.17
20	1	209	CLA	CHC-C1C-NC	3.71	129.90	124.31
20	3	310	CLA	C2B-C1B-NB	3.71	114.17	110.33
20	3	317	CLA	CHA-C4D-ND	3.71	130.08	124.84
20	B	839	CLA	C4B-CHC-C1C	-3.71	117.53	126.25
20	2	321	CLA	CHD-C4C-C3C	-3.71	119.37	124.77
20	B	827	CLA	CHC-C1C-NC	3.71	129.89	124.31
20	A	821	CLA	CHC-C4B-NB	3.70	129.60	124.05
20	B	805	CLA	O2A-CGA-CBA	3.70	123.11	111.83
20	B	821	CLA	C4B-CHC-C1C	-3.70	117.55	126.25
20	A	804	CLA	CHC-C4B-NB	3.70	129.59	124.05
20	A	816	CLA	C3B-C4B-NB	-3.70	107.23	110.53
20	A	805	CLA	CHC-C4B-NB	3.69	129.59	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	848	CLA	C4B-CHC-C1C	-3.69	117.56	126.25
20	B	806	CLA	O2A-CGA-CBA	3.69	123.10	111.83
20	A	818	CLA	CHC-C1C-NC	3.69	129.87	124.31
20	A	812	CLA	CHD-C4C-C3C	-3.69	119.39	124.77
20	A	834	CLA	C2B-C1B-NB	3.69	114.15	110.33
22	B	850	BCR	C1-C6-C7	3.69	125.66	115.65
20	3	320	CLA	CHC-C1C-NC	3.69	129.87	124.31
20	2	317	CLA	CHB-C4A-NA	3.69	129.72	124.40
20	H	101	CLA	C1-O2A-CGA	3.69	125.58	116.65
20	1	206	CLA	C2B-C1B-NB	3.69	114.15	110.33
20	B	809	CLA	CHD-C4C-C3C	-3.69	119.40	124.77
20	B	816	CLA	C1-C2-C3	-3.68	120.16	126.20
20	4	311	CLA	C1B-NB-C4B	-3.68	103.73	106.31
20	J	102	CLA	C2B-C1B-NB	3.68	114.15	110.33
20	K	107	CLA	C4B-CHC-C1C	-3.68	117.59	126.25
22	I	101	BCR	C38-C26-C25	-3.68	120.47	124.48
20	A	804	CLA	C1-C2-C3	-3.68	120.17	126.20
20	B	828	CLA	C3B-C2B-C1B	-3.68	102.83	107.17
20	2	306	CLA	CHC-C4B-NB	3.68	129.57	124.05
20	B	803	CLA	C4B-CHC-C1C	-3.68	117.59	126.25
20	B	849	CLA	C4B-CHC-C1C	-3.68	117.59	126.25
21	F	201	LMU	O5B-C5B-C6B	3.68	115.56	106.44
20	4	313	CLA	CHB-C4A-NA	3.68	129.71	124.40
20	2	307	CLA	CMD-C2D-C3D	-3.68	119.26	127.69
20	B	811	CLA	C2B-C1B-NB	3.67	114.14	110.33
20	K	103	CLA	C2B-C1B-NB	3.67	114.14	110.33
20	1	202	CLA	CHC-C4B-NB	3.67	129.56	124.05
20	B	806	CLA	C3B-C2B-C1B	-3.67	102.84	107.17
20	4	310	CLA	CMB-C2B-C1B	3.67	131.01	125.42
20	1	209	CLA	CBD-CHA-C1A	3.67	132.92	127.38
20	1	204	CLA	CED-O2D-CGD	3.67	124.25	115.92
20	B	819	CLA	C4-C3-C5	3.67	121.60	115.23
20	A	810	CLA	CMD-C2D-C3D	-3.67	119.27	127.69
20	L	207	CLA	CHD-C4C-C3C	-3.67	119.42	124.77
20	R	107	CLA	O2D-CGD-CBD	3.67	117.65	111.23
20	B	831	CLA	C4B-CHC-C1C	-3.67	117.62	126.25
20	B	815	CLA	C4A-NA-C1A	3.67	108.35	106.68
20	4	312	CLA	C1C-CHC-C4B	-3.67	116.37	126.04
22	B	850	BCR	C7-C6-C5	-3.67	113.11	121.56
20	3	312	CLA	C3B-C2B-C1B	-3.66	102.73	106.81
20	B	816	CLA	CHC-C4B-NB	3.66	129.54	124.05
20	B	847	CLA	CBA-CAA-C2A	-3.66	102.90	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	306	CLA	O2A-CGA-CBA	3.66	123.00	111.83
20	H	109	CLA	CHC-C1C-NC	3.66	129.83	124.31
20	H	109	CLA	CED-O2D-CGD	3.66	124.22	115.92
20	4	314	CLA	C3D-C4D-CHA	-3.66	117.03	125.20
20	B	803	CLA	C4A-NA-C1A	3.66	108.35	106.68
20	B	829	CLA	C3B-C2B-C1B	-3.66	102.86	107.17
20	F	206	CLA	CMD-C2D-C1D	3.66	131.17	124.73
20	4	306	CLA	CHC-C1C-NC	3.66	129.82	124.31
20	B	849	CLA	O2D-CGD-CBD	3.66	117.62	111.23
22	B	842	BCR	C37-C22-C21	-3.66	116.89	122.82
20	3	305	CLA	C1B-NB-C4B	-3.66	103.75	106.31
20	2	311	CLA	CHC-C1C-NC	3.65	129.81	124.31
20	A	824	CLA	CHD-C4C-C3C	-3.65	119.45	124.77
20	4	319	CLA	C2B-C1B-NB	3.65	114.11	110.33
20	B	806	CLA	CHD-C4C-NC	3.65	129.89	124.23
20	4	318	CLA	C1-C2-C3	-3.65	120.22	126.20
21	L	206	LMU	C1B-O1B-C4'	-3.65	109.32	117.98
20	A	805	CLA	C2B-C1B-NB	3.65	114.11	110.33
20	2	317	CLA	CHD-C4C-C3C	-3.65	119.46	124.77
20	2	305	CLA	CHA-C4D-ND	3.65	129.99	124.84
20	B	818	CLA	CHC-C1C-NC	3.64	129.80	124.31
20	B	811	CLA	CHD-C4C-C3C	-3.64	119.46	124.77
20	J	103	CLA	C4-C3-C5	3.64	121.55	115.23
20	A	809	CLA	C3B-C4B-NB	-3.64	107.28	110.53
20	2	317	CLA	CHC-C1C-NC	3.64	129.80	124.31
20	4	312	CLA	CHC-C1C-NC	3.64	129.68	124.33
20	3	305	CLA	C3B-C2B-C1B	-3.64	102.76	106.81
20	2	309	CLA	C2A-C1A-CHA	-3.64	116.43	122.63
20	A	847	CLA	CMC-C2C-C1C	3.64	130.72	125.03
20	4	317	CLA	C4A-NA-C1A	3.64	108.34	106.68
20	2	303	CLA	C3B-C2B-C1B	-3.64	102.76	106.81
20	4	310	CLA	C4-C3-C2	-3.64	114.29	123.63
20	A	829	CLA	CHD-C4C-NC	3.64	129.87	124.23
20	4	305	CLA	C3B-C2B-C1B	-3.63	102.89	107.17
21	A	846	LMU	O5B-C1B-C2B	3.63	117.84	110.37
20	H	109	CLA	C4B-CHC-C1C	-3.63	117.70	126.25
20	3	316	CLA	C4C-CHD-C1D	-3.63	115.63	125.98
21	R	104	LMU	O1'-C1'-C2'	3.63	113.79	108.27
20	4	310	CLA	C4-C3-C5	3.63	121.53	115.23
20	H	108	CLA	CHB-C4A-NA	3.63	129.64	124.40
20	4	310	CLA	C4B-CHC-C1C	-3.63	117.71	126.25
21	H	104	LMU	O5B-C5B-C6B	3.63	115.43	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	838	CLA	C3B-C4B-NB	-3.63	107.29	110.53
21	H	102	LMU	C1B-O5B-C5B	-3.63	106.64	113.72
20	L	201	CLA	CMD-C2D-C3D	-3.63	119.37	127.69
20	2	311	CLA	CAA-C2A-C1A	3.63	123.86	111.97
20	2	306	CLA	CMD-C2D-C3D	-3.63	119.37	127.69
20	2	321	CLA	O2A-CGA-CBA	3.62	122.88	111.83
21	B	801	LMU	O5B-C5B-C6B	3.62	115.42	106.44
20	A	824	CLA	O2D-CGD-CBD	3.62	117.56	111.23
20	B	838	CLA	CHD-C4C-NC	3.62	129.84	124.23
20	B	821	CLA	CMD-C2D-C3D	-3.62	119.40	127.69
20	A	857	CLA	C3D-C4D-CHA	-3.62	117.13	125.20
20	A	857	CLA	C1B-NB-C4B	-3.61	103.78	106.31
20	A	848	CLA	O2D-CGD-CBD	3.61	117.55	111.23
20	3	308	CLA	C4D-ND-C1D	-3.61	103.78	106.31
20	A	807	CLA	C4A-NA-C1A	3.61	108.33	106.68
20	1	204	CLA	CHC-C1C-NC	3.61	129.75	124.31
20	G	103	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
20	B	810	CLA	CMD-C2D-C3D	-3.61	119.42	127.69
20	A	820	CLA	CHC-C4B-NB	3.61	129.46	124.05
20	B	807	CLA	CGD-CBD-CAD	3.61	122.52	110.85
20	B	812	CLA	C4B-CHC-C1C	-3.61	117.77	126.25
20	3	314	CLA	C2B-C1B-NB	3.61	114.06	110.33
20	B	834	CLA	CHC-C4B-NB	3.60	129.46	124.05
20	B	816	CLA	O2D-CGD-O1D	-3.60	116.83	123.85
20	B	811	CLA	CHC-C1C-NC	3.60	129.74	124.31
20	J	103	CLA	CHC-C4B-NB	3.60	129.46	124.05
20	3	320	CLA	CMD-C2D-C3D	-3.60	119.43	127.69
20	2	317	CLA	CMD-C2D-C3D	-3.60	119.43	127.69
20	I	102	CLA	CHC-C1C-NC	3.60	129.73	124.31
20	A	830	CLA	CHC-C1C-NC	3.60	129.73	124.31
20	L	204	CLA	C2D-C1D-ND	-3.60	106.57	110.13
20	A	827	CLA	CMD-C2D-C3D	-3.60	119.44	127.69
20	4	305	CLA	CHC-C1C-C2C	-3.59	116.73	126.95
20	A	849	CLA	CMB-C2B-C1B	3.59	130.89	125.42
20	1	212	CLA	CMD-C2D-C3D	-3.59	119.45	127.69
20	B	829	CLA	CHC-C1C-NC	3.59	129.72	124.31
21	B	801	LMU	C1'-O5'-C5'	3.59	120.73	113.72
20	3	317	CLA	CHC-C4B-NB	3.59	129.27	124.08
22	I	103	BCR	C8-C7-C6	-3.59	117.41	127.00
20	B	825	CLA	C3B-C2B-C1B	-3.59	102.94	107.17
20	3	315	CLA	O2A-CGA-CBA	3.59	122.78	111.83
20	A	848	CLA	O1D-CGD-CBD	-3.59	117.44	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	849	CLA	CHC-C4B-NB	3.59	129.43	124.05
20	R	107	CLA	CHC-C4B-NB	3.59	129.43	124.05
20	2	304	CLA	CHD-C4C-C3C	-3.59	119.55	124.77
20	A	819	CLA	CMB-C2B-C1B	3.59	130.88	125.42
21	R	104	LMU	C3B-C4B-C5B	-3.59	103.73	110.23
20	2	312	CLA	CMD-C2D-C3D	-3.59	119.47	127.69
20	B	806	CLA	C2B-C1B-NB	3.58	114.04	110.33
20	3	304	CLA	C4C-CHD-C1D	-3.58	115.77	125.98
20	3	319	CLA	CHC-C1C-NC	3.58	129.71	124.31
21	A	853	LMU	O2'-C2'-C3'	-3.58	101.94	110.38
20	A	811	CLA	CMD-C2D-C3D	-3.58	119.48	127.69
20	A	814	CLA	C3B-C2B-C1B	-3.58	102.95	107.17
21	C	101	LMU	C1B-C2B-C3B	3.58	117.54	110.01
20	B	832	CLA	CMD-C2D-C3D	-3.57	119.49	127.69
20	B	834	CLA	C1-O2A-CGA	3.57	125.30	116.65
20	B	821	CLA	CHC-C4B-NB	3.57	129.41	124.05
21	2	319	LMU	O1B-C1B-C2B	3.57	116.88	108.09
20	1	201	CLA	CHD-C4C-C3C	-3.57	119.57	124.77
20	A	825	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
20	A	850	CLA	CHC-C1C-C2C	-3.57	116.81	126.95
20	2	303	CLA	C3D-C4D-CHA	-3.56	117.24	125.20
22	I	101	BCR	C19-C18-C17	3.56	124.61	119.01
20	B	829	CLA	C4-C3-C5	3.56	121.41	115.23
20	A	801	CLA	O1D-CGD-CBD	-3.56	117.49	124.52
20	A	805	CLA	CHD-C4C-C3C	-3.56	119.58	124.77
20	H	107	CLA	CHC-C4B-NB	3.56	129.39	124.05
20	F	204	CLA	CMB-C2B-C3B	3.56	132.99	123.53
20	A	801	CLA	CMD-C2D-C3D	-3.56	119.53	127.69
20	3	319	CLA	CHC-C4B-NB	3.56	129.39	124.05
20	R	107	CLA	CHC-C1C-NC	3.56	129.67	124.31
21	A	853	LMU	C3B-C4B-C5B	-3.56	103.78	110.23
20	A	814	CLA	C4-C3-C5	3.56	121.40	115.23
20	I	102	CLA	C4A-NA-C1A	3.56	108.30	106.68
20	F	206	CLA	C4-C3-C2	-3.55	114.50	123.63
20	3	306	CLA	C1B-NB-C4B	-3.55	103.82	106.31
20	3	316	CLA	CHA-C4D-ND	3.55	129.86	124.84
20	2	305	CLA	C3A-C4A-CHB	-3.55	119.56	123.91
20	B	805	CLA	CHB-C1B-NB	-3.55	118.72	124.05
22	F	203	BCR	C28-C29-C30	-3.55	101.86	114.43
20	2	307	CLA	CHC-C1C-C2C	-3.55	116.85	126.95
20	A	820	CLA	CHC-C1C-NC	3.55	129.66	124.31
22	3	311	BCR	C23-C24-C25	-3.55	117.51	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	302	CLA	O2A-CGA-CBA	3.55	122.66	111.83
20	B	831	CLA	C3B-C2B-C1B	-3.55	102.98	107.17
20	B	815	CLA	O2A-CGA-CBA	3.55	122.66	111.83
20	3	306	CLA	CHC-C4B-NB	3.55	129.21	124.08
20	A	826	CLA	C4-C3-C5	3.55	121.38	115.23
20	B	848	CLA	C5-C3-C2	-3.54	113.21	121.17
20	A	813	CLA	CHD-C4C-C3C	-3.54	119.61	124.77
20	3	309	CLA	C2A-C1A-CHA	-3.54	117.72	123.87
20	3	307	CLA	CHC-C4B-NB	3.54	129.20	124.08
20	B	819	CLA	CED-O2D-CGD	3.54	123.95	115.92
20	A	803	CLA	CHC-C1C-C2C	-3.54	116.89	126.95
20	A	806	CLA	CHC-C4B-NB	3.54	129.35	124.05
20	A	816	CLA	C4B-C3B-C2B	3.54	111.70	107.30
20	B	804	CLA	CHC-C4B-NB	3.53	129.35	124.05
20	I	102	CLA	C3B-C2B-C1B	-3.53	103.01	107.17
20	3	305	CLA	CHC-C4B-NB	3.53	129.18	124.08
20	4	312	CLA	CHC-C4B-NB	3.53	129.18	124.08
20	3	317	CLA	C3D-C4D-CHA	-3.53	117.32	125.20
20	A	825	CLA	CHD-C4C-C3C	-3.53	119.63	124.77
20	4	313	CLA	CAA-C2A-C3A	-3.53	108.14	116.23
20	3	307	CLA	C1B-NB-C4B	-3.53	103.84	106.31
22	B	850	BCR	C29-C30-C25	3.53	115.56	110.44
20	A	838	CLA	CHC-C4B-NB	3.53	129.34	124.05
20	B	847	CLA	CHD-C4C-C3C	-3.53	119.63	124.77
22	I	101	BCR	C27-C26-C25	-3.53	117.94	122.70
20	1	210	CLA	CHC-C1C-NC	3.52	129.62	124.31
20	B	806	CLA	CHB-C4A-NA	3.52	129.49	124.40
20	1	206	CLA	CHC-C1C-NC	3.52	129.62	124.31
20	1	208	CLA	CHA-C4D-ND	3.52	129.82	124.84
20	A	828	CLA	O2A-CGA-CBA	3.52	122.58	111.83
21	R	101	LMU	C1B-C2B-C3B	3.52	117.42	110.01
20	1	208	CLA	C2A-C1A-CHA	-3.52	116.63	122.63
20	4	317	CLA	C4C-CHD-C1D	-3.52	115.94	125.98
20	J	102	CLA	C1-C2-C3	-3.52	120.43	126.20
20	L	207	CLA	CHC-C4B-NB	3.52	129.33	124.05
20	3	301	CLA	C2B-C1B-NB	3.52	113.98	110.33
20	A	808	CLA	CMA-C3A-C2A	-3.52	100.38	113.98
22	I	101	BCR	C36-C18-C19	-3.52	112.72	118.09
20	3	314	CLA	CHC-C4B-NB	3.52	129.32	124.05
20	B	805	CLA	CHC-C1C-C2C	-3.51	116.96	126.95
20	4	311	CLA	C3D-C4D-CHA	-3.51	117.35	125.20
20	B	819	CLA	CHC-C4B-NB	3.51	129.32	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	822	CLA	C1-C2-C3	-3.51	120.44	126.20
20	A	813	CLA	C3B-C2B-C1B	-3.51	103.03	107.17
20	K	106	CLA	O2A-CGA-O1A	-3.51	114.85	123.63
20	A	808	CLA	CHC-C4B-NB	3.51	129.31	124.05
20	3	307	CLA	C3B-C2B-C1B	-3.51	102.91	106.81
20	1	201	CLA	CBA-CAA-C2A	-3.51	103.36	113.79
20	A	835	CLA	C1-C2-C3	-3.51	120.45	126.20
20	B	806	CLA	CMD-C2D-C3D	-3.50	119.65	127.69
20	B	836	CLA	CMB-C2B-C1B	3.50	130.75	125.42
20	A	801	CLA	C1-C2-C3	-3.50	121.09	126.76
20	L	204	CLA	C2B-C1B-NB	3.50	113.96	110.33
22	B	842	BCR	C34-C9-C10	-3.50	117.14	122.82
20	1	201	CLA	C4D-CHA-C1A	-3.50	117.06	121.24
20	B	836	CLA	CMD-C2D-C3D	-3.50	119.66	127.69
20	1	208	CLA	C1B-NB-C4B	-3.50	103.85	106.31
20	1	214	CLA	CHC-C1C-C2C	-3.50	117.00	126.95
20	B	821	CLA	C4A-NA-C1A	3.50	108.28	106.68
20	A	817	CLA	C3B-C2B-C1B	-3.50	103.05	107.17
20	B	817	CLA	CHC-C4B-NB	3.50	129.30	124.05
20	B	823	CLA	C1-C2-C3	-3.50	120.47	126.20
20	2	306	CLA	C4-C3-C5	3.50	121.30	115.23
20	A	830	CLA	CMB-C2B-C1B	3.50	130.74	125.42
20	3	317	CLA	C4A-NA-C1A	3.50	108.27	106.68
21	R	101	LMU	O1'-C1'-C2'	3.50	113.58	108.27
20	A	832	CLA	C1-C2-C3	-3.49	120.47	126.20
20	B	826	CLA	CMA-C3A-C2A	-3.49	100.47	113.98
20	A	814	CLA	CAC-C3C-C4C	3.49	129.34	124.79
21	R	101	LMU	C1-O1'-C1'	-3.49	107.71	113.68
21	E	101	LMU	O5'-C5'-C6'	3.49	115.10	106.44
20	2	305	CLA	C4C-CHD-C1D	-3.49	116.03	125.98
20	A	837	CLA	C1-C2-C3	-3.49	120.48	126.20
20	4	309	CLA	C3B-C2B-C1B	-3.49	102.92	106.81
20	A	833	CLA	C1-C2-C3	-3.49	120.48	126.20
20	B	824	CLA	O2A-CGA-O1A	-3.49	114.90	123.63
21	A	852	LMU	C1B-C2B-C3B	3.49	117.35	110.01
20	H	110	CLA	O2D-CGD-CBD	3.49	117.33	111.23
20	2	317	CLA	C1-C2-C3	-3.49	120.48	126.20
21	K	104	LMU	O1B-C4'-C5'	3.49	118.62	109.48
20	2	315	CLA	CHA-C4D-ND	3.49	129.77	124.84
20	4	307	CLA	CMB-C2B-C3B	3.49	134.75	126.55
23	A	839	PQN	C21-C20-C18	-3.49	104.38	115.97
20	F	204	CLA	CHB-C4A-NA	3.48	129.43	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	815	CLA	O2D-CGD-CBD	3.48	117.32	111.23
20	A	821	CLA	O2A-CGA-CBA	3.48	122.45	111.83
20	A	808	CLA	C4B-C3B-C2B	3.48	111.63	107.30
20	A	809	CLA	CHC-C1C-C2C	-3.48	117.06	126.95
20	A	836	CLA	C1-C2-C3	-3.48	120.50	126.20
20	1	201	CLA	CMC-C2C-C1C	3.48	130.47	125.03
21	R	101	LMU	C1'-O5'-C5'	-3.48	106.93	113.72
20	B	838	CLA	CHC-C1C-NC	3.48	129.55	124.31
20	B	827	CLA	CGD-CBD-CAD	3.48	122.10	110.85
20	B	822	CLA	C1-C2-C3	-3.48	120.50	126.20
21	R	103	LMU	C3B-C4B-C5B	-3.48	103.93	110.23
20	3	316	CLA	CHC-C4B-NB	3.48	129.10	124.08
21	R	103	LMU	O1B-C1B-O5B	-3.47	101.55	110.69
21	H	104	LMU	O1B-C1B-C2B	-3.47	99.54	108.09
20	1	201	CLA	CHC-C1C-C2C	-3.47	117.08	126.95
20	2	308	CLA	C3D-C4D-CHA	-3.47	117.45	125.20
20	4	302	CLA	C1-C2-C3	-3.47	120.51	126.20
20	A	802	CLA	OBD-CAD-C3D	-3.47	120.30	128.42
20	A	855	CLA	C1-C2-C3	-3.46	120.52	126.20
20	R	107	CLA	OBD-CAD-C3D	-3.46	120.32	128.42
20	L	203	CLA	C4B-CHC-C1C	-3.46	118.10	126.25
20	B	830	CLA	CED-O2D-CGD	3.46	123.77	115.92
20	A	811	CLA	CHB-C4A-NA	3.46	129.40	124.40
20	A	823	CLA	C1-C2-C3	-3.46	120.53	126.20
20	F	206	CLA	CAA-C2A-C3A	-3.46	103.65	113.00
20	4	304	CLA	C7-C6-C5	-3.46	104.04	113.26
20	A	817	CLA	C4B-CHC-C1C	-3.46	118.11	126.25
20	3	315	CLA	C4A-NA-C1A	3.46	108.26	106.68
20	4	314	CLA	CHC-C1C-NC	3.46	129.41	124.33
20	3	320	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
20	3	310	CLA	C1-C2-C3	-3.46	120.53	126.20
20	B	836	CLA	O1D-CGD-CBD	-3.46	117.70	124.52
20	A	806	CLA	CHC-C1C-NC	3.46	129.51	124.31
20	B	831	CLA	C2B-C1B-NB	3.46	113.91	110.33
20	3	317	CLA	C3B-C2B-C1B	-3.45	102.97	106.81
22	L	209	BCR	C15-C16-C17	-3.45	116.46	123.52
20	2	309	CLA	CHA-C4D-ND	3.45	129.72	124.84
20	2	310	CLA	CHD-C4C-NC	3.45	129.58	124.23
20	B	831	CLA	CED-O2D-CGD	3.44	123.73	115.92
21	L	205	LMU	C4B-C3B-C2B	3.44	116.88	110.83
20	B	848	CLA	C1-O2A-CGA	3.44	124.99	116.65
20	1	214	CLA	CHC-C4B-NB	3.44	129.22	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	848	CLA	CHB-C4A-NA	3.44	129.37	124.40
20	A	827	CLA	CHD-C4C-NC	3.44	129.57	124.23
20	3	307	CLA	C3D-C4D-CHA	-3.44	117.51	125.20
20	4	313	CLA	CHD-C4C-C3C	-3.44	119.60	125.03
20	1	208	CLA	C3D-C4D-CHA	-3.44	117.52	125.20
21	G	101	LMU	O1B-C1B-O5B	3.44	119.74	110.69
20	1	207	CLA	CHC-C4B-NB	3.44	129.20	124.05
20	1	208	CLA	C1C-CHC-C4B	-3.44	116.98	126.04
20	H	107	CLA	C4B-C3B-C2B	3.44	111.57	107.30
20	A	848	CLA	O2A-CGA-O1A	-3.44	115.03	123.63
20	2	309	CLA	C1B-NB-C4B	-3.43	103.90	106.31
20	B	818	CLA	O1D-CGD-CBD	-3.43	117.75	124.52
20	I	102	CLA	C4B-CHC-C1C	-3.43	118.18	126.25
20	4	318	CLA	C2B-C1B-NB	3.43	113.88	110.33
20	1	208	CLA	C2D-C3D-C4D	-3.43	103.18	107.35
20	4	318	CLA	CHC-C4B-NB	3.43	129.19	124.05
20	2	305	CLA	CHC-C4B-NB	3.43	129.03	124.08
21	2	318	LMU	O1B-C1B-C2B	3.43	116.52	108.09
20	H	101	CLA	O2A-CGA-CBA	3.43	122.28	111.83
20	2	309	CLA	C3D-C4D-CHA	-3.42	117.55	125.20
21	E	101	LMU	O1B-C1B-O5B	3.42	119.70	110.69
20	B	809	CLA	C2B-C1B-NB	3.42	113.88	110.33
20	J	103	CLA	CHB-C4A-NA	3.42	129.34	124.40
20	1	212	CLA	O1D-CGD-CBD	-3.42	117.77	124.52
20	1	215	CLA	C4D-ND-C1D	-3.42	103.91	106.31
22	F	203	BCR	C4-C5-C6	-3.42	118.08	122.70
20	1	206	CLA	O2A-CGA-CBA	3.42	122.26	111.83
20	K	106	CLA	CHB-C4A-NA	3.42	129.33	124.40
20	B	831	CLA	CHC-C4B-NB	3.42	129.18	124.05
21	K	101	LMU	O5'-C1'-C2'	-3.42	103.35	110.37
20	B	825	CLA	C16-C15-C13	-3.42	104.61	115.97
20	A	825	CLA	CMB-C2B-C1B	3.41	130.62	125.42
20	4	309	CLA	C2D-C3D-C4D	-3.41	103.20	107.35
21	L	206	LMU	O5B-C5B-C4B	-3.41	103.55	109.70
20	3	301	CLA	CHC-C4B-NB	3.41	129.17	124.05
20	2	302	CLA	C4A-NA-C1A	3.41	108.23	106.68
20	4	311	CLA	CHC-C4B-NB	3.41	129.01	124.08
20	4	317	CLA	C2D-C3D-C4D	-3.41	103.21	107.35
20	2	314	CLA	C4C-CHD-C1D	-3.41	116.27	125.98
20	A	849	CLA	CHB-C4A-NA	3.41	129.32	124.40
20	B	828	CLA	CHC-C4B-NB	3.41	129.16	124.05
20	L	203	CLA	C4-C3-C5	3.41	121.15	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	R	106	CLA	CED-O2D-CGD	3.41	123.65	115.92
20	B	839	CLA	CHC-C4B-NB	3.41	129.16	124.05
20	1	202	CLA	CHC-C1C-C2C	-3.41	117.27	126.95
21	A	846	LMU	O1'-C1'-C2'	3.41	113.44	108.27
20	A	827	CLA	O2A-CGA-CBA	3.40	122.22	111.83
20	A	816	CLA	CHC-C4B-NB	3.40	129.16	124.05
20	2	301	CLA	C1-C2-C3	-3.40	120.62	126.20
20	A	847	CLA	CMD-C2D-C3D	-3.40	119.89	127.69
20	G	103	CLA	CMD-C2D-C3D	-3.40	119.89	127.69
20	2	302	CLA	C1D-ND-C4D	-3.40	103.92	106.31
20	B	828	CLA	CHC-C1C-NC	3.40	129.43	124.31
21	H	102	LMU	O3'-C3'-C4'	3.40	118.65	109.94
21	R	101	LMU	C3B-C4B-C5B	-3.40	104.07	110.23
21	K	104	LMU	O2B-C2B-C1B	-3.40	101.98	110.08
20	2	321	CLA	CHB-C4A-NA	3.40	129.30	124.40
20	B	827	CLA	CHC-C4B-NB	3.39	129.14	124.05
20	L	208	CLA	C4D-CHA-C1A	3.39	125.29	121.24
20	B	835	CLA	C4-C3-C5	3.39	121.12	115.23
20	4	307	CLA	C3C-C4C-NC	-3.39	106.08	110.43
20	2	306	CLA	O2D-CGD-CBD	3.39	117.16	111.23
20	H	110	CLA	CED-O2D-CGD	3.39	123.61	115.92
21	E	101	LMU	C6'-C5'-C4'	-3.39	103.84	113.38
20	A	814	CLA	CHC-C4B-NB	3.39	129.14	124.05
20	2	305	CLA	C3B-C2B-C1B	-3.39	103.04	106.81
20	2	321	CLA	C3A-C2A-C1A	3.38	106.41	101.34
21	L	205	LMU	O5B-C5B-C6B	3.38	114.82	106.44
20	L	202	CLA	CAC-C3C-C4C	3.38	129.19	124.79
20	B	811	CLA	C3B-C4B-NB	-3.38	107.51	110.53
20	F	206	CLA	CMB-C2B-C1B	3.38	130.56	125.42
20	4	305	CLA	CHB-C4A-NA	3.38	129.28	124.40
20	I	102	CLA	O2A-CGA-CBA	3.38	122.13	111.83
20	2	302	CLA	C4-C3-C2	-3.38	114.96	123.63
20	4	315	CLA	CHB-C4A-NA	3.38	129.27	124.40
20	H	110	CLA	C3B-C2B-C1B	-3.37	103.19	107.17
21	R	101	LMU	C1B-O5B-C5B	3.37	120.30	113.72
20	4	315	CLA	CMD-C2D-C1D	3.37	130.66	124.73
20	A	857	CLA	CHC-C4B-NB	3.37	128.95	124.08
20	2	311	CLA	CHB-C4A-NA	3.37	129.26	124.40
20	B	820	CLA	C3A-C2A-C1A	-3.37	96.30	101.34
20	B	832	CLA	O1D-CGD-CBD	-3.37	117.88	124.52
20	A	838	CLA	CAC-C3C-C4C	3.37	129.17	124.79
20	A	847	CLA	CAA-C2A-C3A	-3.37	103.90	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	849	CLA	CMA-C3A-C4A	-3.37	102.73	111.77
20	A	820	CLA	CHD-C4C-C3C	-3.37	119.87	124.77
20	4	308	CLA	C3D-C4D-CHA	-3.36	117.69	125.20
20	A	830	CLA	CHD-C4C-C3C	-3.36	119.87	124.77
20	B	806	CLA	O2A-CGA-O1A	-3.36	115.22	123.63
20	J	103	CLA	CAA-CBA-CGA	-3.36	103.66	113.21
20	J	103	CLA	C2B-C1B-NB	3.36	113.81	110.33
20	1	213	CLA	C3D-C4D-CHA	-3.36	117.70	125.20
20	4	311	CLA	C4A-NA-C1A	3.36	108.21	106.68
20	K	107	CLA	C4A-NA-C1A	3.36	108.21	106.68
20	4	308	CLA	C1C-CHC-C4B	-3.36	117.18	126.04
21	1	217	LMU	O4'-C4B-C5B	3.36	117.59	109.32
20	A	813	CLA	O2A-CGA-CBA	3.36	122.07	111.83
20	A	816	CLA	CMD-C2D-C3D	-3.36	119.99	127.69
20	3	304	CLA	CHB-C4A-NA	3.36	129.20	124.43
22	3	311	BCR	C15-C14-C13	-3.36	122.57	127.28
20	B	805	CLA	CMA-C3A-C2A	-3.35	101.01	113.98
21	H	104	LMU	C1-O1'-C1'	-3.35	107.95	113.68
20	B	835	CLA	CHD-C4C-C3C	-3.35	119.89	124.77
20	B	839	CLA	C1B-C2B-C3B	-3.35	103.88	107.03
20	4	308	CLA	C2D-C3D-C4D	-3.35	103.28	107.35
20	B	829	CLA	C1-C2-C3	-3.35	120.71	126.20
21	A	852	LMU	C2'-C3'-C4'	3.35	117.28	109.68
20	B	836	CLA	C3B-C4B-NB	-3.35	107.54	110.53
20	3	304	CLA	C2C-C1C-CHC	-3.35	117.07	125.84
20	H	101	CLA	CHD-C4C-C3C	-3.35	119.90	124.77
20	3	312	CLA	C1C-CHC-C4B	-3.34	117.22	126.04
20	A	830	CLA	CHC-C4B-NB	3.34	129.06	124.05
21	H	104	LMU	C1'-O5'-C5'	-3.34	107.19	113.72
20	B	812	CLA	CHC-C1C-NC	3.34	129.34	124.31
20	B	812	CLA	O2A-CGA-CBA	3.34	122.02	111.83
20	A	806	CLA	CHB-C4A-NA	3.34	129.22	124.40
20	1	206	CLA	CHC-C4B-NB	3.34	129.06	124.05
20	1	205	CLA	CHC-C1C-NC	3.34	129.34	124.31
20	3	312	CLA	C3D-C4D-CHA	-3.34	117.74	125.20
20	B	827	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
20	B	820	CLA	C3B-C2B-C1B	-3.34	103.23	107.17
20	1	213	CLA	C1C-CHC-C4B	-3.34	117.24	126.04
20	4	319	CLA	CHC-C4B-NB	3.34	129.05	124.05
20	4	304	CLA	CMA-C3A-C4A	3.33	120.73	111.77
21	F	201	LMU	O5'-C1'-C2'	-3.33	103.52	110.37
20	A	850	CLA	C3A-C2A-C1A	3.33	106.33	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	213	CLA	C2D-C3D-C4D	-3.33	103.30	107.35
20	B	848	CLA	CMD-C2D-C3D	-3.33	120.05	127.69
20	B	834	CLA	CHC-C1C-NC	3.33	129.33	124.31
20	3	314	CLA	C3B-C2B-C1B	-3.33	103.25	107.17
21	H	103	LMU	O5B-C5B-C6B	3.33	114.69	106.44
20	K	107	CLA	CMD-C2D-C3D	-3.33	120.06	127.69
21	2	319	LMU	O5'-C1'-O1'	3.33	117.90	110.04
20	A	809	CLA	CHD-C4C-C3C	-3.33	119.92	124.77
20	A	810	CLA	CHC-C4B-NB	3.33	129.04	124.05
20	B	835	CLA	O2A-CGA-CBA	3.32	121.97	111.83
20	B	832	CLA	C3B-C2B-C1B	-3.32	103.25	107.17
20	A	805	CLA	CHC-C1C-NC	3.32	129.32	124.31
20	B	836	CLA	CAA-C2A-C3A	-3.32	104.02	113.00
20	B	830	CLA	O2A-CGA-CBA	3.32	121.97	111.83
21	R	109	LMU	O5'-C1'-O1'	3.32	117.89	110.04
20	A	806	CLA	C4B-C3B-C2B	3.32	111.43	107.30
20	H	108	CLA	CMD-C2D-C3D	-3.32	120.08	127.69
20	A	809	CLA	CAA-C2A-C1A	-3.32	101.11	111.97
20	B	818	CLA	C4A-NA-C1A	3.31	108.19	106.68
20	4	304	CLA	CBC-CAC-C3C	-3.31	103.44	112.42
20	A	835	CLA	C4-C3-C5	3.31	120.03	116.13
21	L	206	LMU	O3'-C3'-C4'	-3.31	101.45	109.94
20	L	204	CLA	C2A-C1A-CHA	-3.31	118.12	123.87
20	3	304	CLA	C3D-C4D-CHA	-3.31	117.81	125.20
20	3	319	CLA	CBD-CHA-C1A	3.31	132.37	127.38
20	B	838	CLA	C2B-C1B-NB	3.31	113.76	110.33
20	4	315	CLA	CHC-C1C-NC	3.30	129.29	124.31
20	B	829	CLA	CHC-C4B-NB	3.30	129.00	124.05
20	B	804	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
20	A	825	CLA	O1D-CGD-CBD	-3.30	118.01	124.52
20	4	307	CLA	CED-O2D-CGD	3.30	123.40	115.92
20	L	202	CLA	C2B-C1B-NB	3.30	113.75	110.33
20	A	819	CLA	CHD-C4C-C3C	-3.30	119.96	124.77
20	1	215	CLA	CHB-C4A-NA	3.30	129.12	124.43
20	4	315	CLA	CHC-C4B-NB	3.30	128.99	124.05
20	B	821	CLA	CHB-C4A-NA	3.29	129.16	124.40
21	E	101	LMU	C1'-C2'-C3'	3.29	116.94	110.01
20	L	204	CLA	CHC-C4B-NB	3.29	128.99	124.05
20	1	205	CLA	C4A-NA-C1A	3.29	108.18	106.68
20	2	301	CLA	C4-C3-C5	3.29	120.00	116.13
20	4	309	CLA	CHC-C4B-NB	3.29	128.84	124.08
20	3	309	CLA	CAC-C3C-C4C	-3.29	120.51	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	F	204	CLA	CAA-C2A-C1A	-3.29	103.68	111.81
20	1	209	CLA	C4A-NA-C1A	3.29	108.18	106.68
20	B	835	CLA	C4A-NA-C1A	3.29	108.18	106.68
21	R	105	LMU	C1'-O5'-C5'	3.29	120.14	113.72
20	B	832	CLA	CHC-C4B-NB	3.29	128.98	124.05
21	L	205	LMU	C1'-C2'-C3'	3.29	116.92	110.01
20	3	316	CLA	C3D-C4D-ND	3.29	113.99	109.50
20	4	310	CLA	C1D-ND-C4D	-3.29	104.01	106.31
20	4	303	CLA	C4B-CHC-C1C	-3.29	118.52	126.25
20	A	850	CLA	CHD-C4C-NC	3.28	129.32	124.23
20	B	827	CLA	CED-O2D-CGD	3.28	123.36	115.92
21	2	318	LMU	C2'-C3'-C4'	3.28	117.13	109.68
20	3	304	CLA	CHC-C4B-NB	3.28	128.82	124.08
20	2	309	CLA	C2D-C3D-C4D	-3.28	103.36	107.35
22	B	850	BCR	C24-C23-C22	-3.28	121.38	126.23
21	1	217	LMU	O5B-C1B-C2B	-3.28	103.63	110.37
20	A	832	CLA	C4-C3-C5	3.28	119.99	116.13
20	A	824	CLA	O2A-CGA-CBA	3.28	121.84	111.83
20	L	201	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
20	A	805	CLA	CMD-C2D-C3D	-3.28	120.17	127.69
21	A	852	LMU	O5'-C1'-O1'	-3.28	102.30	110.04
20	B	822	CLA	CHC-C4B-NB	3.28	128.97	124.05
20	B	821	CLA	C3B-C2B-C1B	-3.28	103.31	107.17
20	B	817	CLA	C3B-C2B-C1B	-3.28	103.31	107.17
20	B	814	CLA	CHD-C4C-C3C	-3.27	120.00	124.77
20	K	103	CLA	CHC-C4B-NB	3.27	128.96	124.05
21	H	103	LMU	C1'-O5'-C5'	-3.27	107.33	113.72
20	H	108	CLA	CED-O2D-CGD	3.27	123.34	115.92
20	2	321	CLA	CBC-CAC-C3C	-3.27	103.56	112.42
21	R	104	LMU	C1'-C2'-C3'	3.27	116.88	110.01
20	F	205	CLA	CHC-C4B-NB	3.27	128.95	124.05
20	B	831	CLA	CHB-C4A-NA	3.27	129.11	124.40
20	A	815	CLA	CED-O2D-CGD	3.26	123.32	115.92
20	2	321	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
20	B	813	CLA	C2B-C1B-NB	3.26	113.71	110.33
20	A	819	CLA	CHC-C1C-C2C	-3.26	117.67	126.95
20	A	826	CLA	CMD-C2D-C3D	-3.26	120.21	127.69
20	B	804	CLA	CHD-C4C-C3C	-3.26	120.02	124.77
20	A	850	CLA	CBA-CAA-C2A	3.26	123.50	113.79
20	3	304	CLA	CHA-C4D-ND	3.26	129.45	124.84
20	B	834	CLA	C3B-C2B-C1B	-3.26	103.33	107.17
20	A	827	CLA	CHC-C4B-NB	3.26	128.94	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	L	203	CLA	O2A-CGA-CBA	3.26	121.77	111.83
21	R	103	LMU	O5B-C1B-C2B	-3.26	103.68	110.37
20	A	804	CLA	C4A-NA-C1A	3.26	108.17	106.68
20	3	320	CLA	C7-C6-C5	-3.26	104.58	113.26
22	B	842	BCR	C16-C15-C14	-3.25	116.86	123.52
20	1	203	CLA	CHC-C4B-NB	3.25	128.93	124.05
20	2	321	CLA	CHC-C4B-NB	3.25	128.93	124.05
21	G	101	LMU	O3'-C3'-C4'	-3.25	101.61	109.94
20	B	839	CLA	C2B-C1B-NB	3.25	113.70	110.33
21	R	102	LMU	O5B-C5B-C4B	3.25	115.56	109.70
20	B	818	CLA	CHC-C4B-NB	3.25	128.92	124.05
22	I	103	BCR	C19-C18-C17	3.25	124.12	119.01
20	3	308	CLA	C2C-C1C-CHC	-3.25	117.33	125.84
20	1	202	CLA	C3A-C2A-C1A	3.25	106.20	101.34
20	B	830	CLA	O2A-CGA-O1A	-3.25	115.51	123.63
20	A	834	CLA	CHC-C4B-NB	3.25	128.92	124.05
20	A	824	CLA	CHC-C1C-NC	3.24	129.20	124.31
20	H	108	CLA	O2D-CGD-O1D	-3.24	117.53	123.85
21	H	102	LMU	O1B-C1B-C2B	3.24	116.06	108.09
20	1	215	CLA	CHA-C4D-ND	3.24	129.42	124.84
20	B	833	CLA	CHC-C1C-NC	3.24	129.19	124.31
20	4	314	CLA	C4A-NA-C1A	3.24	108.16	106.68
20	A	811	CLA	C3B-C2B-C1B	-3.23	103.36	107.17
20	3	314	CLA	CMB-C2B-C1B	3.23	130.34	125.42
20	B	838	CLA	O2A-CGA-O1A	-3.23	115.54	123.63
20	B	834	CLA	CMB-C2B-C1B	3.23	130.34	125.42
20	A	855	CLA	CHC-C4B-NB	3.23	128.90	124.05
20	A	806	CLA	C3B-C4B-NB	-3.23	107.64	110.53
20	A	847	CLA	C4A-NA-C1A	3.23	108.15	106.68
21	A	845	LMU	C1B-O5B-C5B	3.23	120.03	113.72
20	4	304	CLA	CHC-C1C-C2C	-3.23	117.77	126.95
20	A	831	CLA	CHC-C4B-NB	3.23	128.89	124.05
20	A	833	CLA	CHC-C4B-NB	3.23	128.89	124.05
20	3	317	CLA	C1B-NB-C4B	-3.23	104.05	106.31
20	A	820	CLA	C1-C2-C3	-3.23	120.91	126.20
20	B	820	CLA	CMC-C2C-C1C	3.23	130.08	125.03
20	L	208	CLA	C4B-CHC-C1C	-3.23	118.66	126.25
20	A	836	CLA	CHC-C4B-NB	3.23	128.89	124.05
20	A	835	CLA	CHC-C4B-NB	3.23	128.89	124.05
20	2	315	CLA	CHC-C4B-NB	3.23	128.74	124.08
20	A	823	CLA	CHC-C4B-NB	3.22	128.89	124.05
20	B	847	CLA	CBC-CAC-C3C	-3.22	103.69	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	G	103	CLA	C4A-NA-C1A	3.22	108.15	106.68
20	B	821	CLA	O2A-CGA-CBA	3.22	121.65	111.83
20	1	206	CLA	CAC-C3C-C4C	3.22	128.98	124.79
20	F	204	CLA	CHC-C4B-NB	3.22	128.88	124.05
20	A	857	CLA	C3B-C2B-C1B	-3.22	103.23	106.81
20	B	847	CLA	CHB-C4A-NA	3.22	129.04	124.40
20	R	107	CLA	O2A-C1-C2	3.22	120.48	108.11
20	2	301	CLA	CHC-C4B-NB	3.22	128.87	124.05
20	R	106	CLA	O2A-CGA-O1A	-3.21	115.59	123.63
20	K	105	CLA	CHC-C4B-NB	3.21	128.87	124.05
20	G	103	CLA	CHC-C1C-NC	3.21	129.15	124.31
20	I	102	CLA	CMD-C2D-C3D	-3.21	120.32	127.69
22	B	842	BCR	C38-C26-C27	3.21	120.44	113.60
22	B	842	BCR	C23-C22-C21	3.21	124.06	119.01
20	4	302	CLA	CHC-C4B-NB	3.21	128.87	124.05
20	B	808	CLA	CAA-C2A-C3A	-3.21	104.32	113.00
20	B	826	CLA	C2A-C1A-CHA	-3.21	118.30	123.87
20	B	821	CLA	CHD-C4C-C3C	-3.21	120.09	124.77
20	A	837	CLA	CHC-C4B-NB	3.21	128.86	124.05
22	I	103	BCR	C32-C1-C6	-3.21	105.21	110.24
20	A	816	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
20	A	822	CLA	CHC-C4B-NB	3.21	128.86	124.05
20	L	202	CLA	CHC-C1C-NC	3.21	129.14	124.31
20	R	107	CLA	C4A-NA-C1A	3.20	108.14	106.68
22	B	842	BCR	C35-C13-C14	-3.20	117.63	122.82
20	L	207	CLA	C4A-NA-C1A	3.20	108.14	106.68
20	2	317	CLA	CHC-C4B-NB	3.20	128.85	124.05
21	F	201	LMU	O3'-C3'-C2'	3.20	117.92	110.38
20	A	832	CLA	CHC-C4B-NB	3.20	128.85	124.05
20	B	813	CLA	CHC-C4B-NB	3.20	128.85	124.05
20	A	820	CLA	CAC-C3C-C4C	3.20	128.95	124.79
20	A	827	CLA	CHC-C1C-C2C	-3.20	117.86	126.95
20	B	831	CLA	CHC-C1C-NC	3.20	129.13	124.31
20	A	807	CLA	CAC-C3C-C2C	-3.20	121.68	127.56
21	4	321	LMU	O5B-C5B-C6B	3.20	114.36	106.44
20	A	811	CLA	CHC-C1C-C2C	-3.20	117.86	126.95
20	B	807	CLA	C4-C3-C5	3.20	120.77	115.23
20	3	310	CLA	CHC-C4B-NB	3.20	128.84	124.05
20	A	825	CLA	C4A-NA-C1A	3.19	108.14	106.68
20	A	815	CLA	C3B-C2B-C1B	-3.19	103.41	107.17
20	A	815	CLA	O1D-CGD-CBD	-3.19	118.22	124.52
21	L	206	LMU	O5B-C1B-C2B	-3.19	103.81	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	304	CLA	C16-C15-C13	-3.19	105.36	115.97
20	L	207	CLA	CMA-C3A-C4A	-3.19	103.20	111.77
20	B	823	CLA	CHC-C4B-NB	3.19	128.83	124.05
20	3	309	CLA	O2A-CGA-CBA	3.19	121.56	111.83
20	A	821	CLA	O2A-CGA-O1A	-3.19	115.66	123.63
20	4	305	CLA	CAC-C3C-C2C	-3.19	121.70	127.56
20	1	203	CLA	CMB-C2B-C1B	3.19	130.27	125.42
21	H	105	LMU	C1'-C2'-C3'	3.18	116.71	110.01
20	2	310	CLA	CMB-C2B-C1B	3.18	130.27	125.42
20	F	206	CLA	C4B-CHC-C1C	-3.18	118.76	126.25
21	2	313	LMU	O1B-C4'-C3'	3.18	115.32	107.23
20	B	827	CLA	CMD-C2D-C3D	-3.18	120.39	127.69
20	B	849	CLA	O2A-CGA-CBA	3.18	121.54	111.83
20	R	106	CLA	C1-O2A-CGA	3.18	124.35	116.65
20	B	839	CLA	CHC-C1C-NC	3.18	129.10	124.31
20	4	307	CLA	O2D-CGD-CBD	3.18	116.79	111.23
20	2	307	CLA	C4A-NA-C1A	3.18	108.13	106.68
20	A	824	CLA	CHB-C4A-NA	3.18	128.98	124.40
23	B	840	PQN	C2M-C2-C1	3.17	122.52	116.68
20	A	830	CLA	CHB-C4A-NA	3.17	128.98	124.40
20	B	848	CLA	CMB-C2B-C1B	3.17	130.25	125.42
21	1	218	LMU	O1B-C1B-O5B	-3.17	102.34	110.69
20	B	821	CLA	CHC-C1C-NC	3.17	129.09	124.31
20	4	303	CLA	CMB-C2B-C3B	3.17	131.97	123.53
20	F	206	CLA	CMA-C3A-C4A	3.17	120.30	111.77
22	B	842	BCR	C15-C14-C13	-3.17	122.83	127.28
20	1	210	CLA	CBD-CHA-C1A	3.17	132.17	127.38
23	B	840	PQN	C16-C15-C13	-3.17	105.74	113.47
20	K	106	CLA	CHD-C4C-C3C	-3.17	120.15	124.77
20	B	812	CLA	C3B-C4B-NB	-3.17	107.70	110.53
21	K	102	LMU	C1'-C2'-C3'	-3.17	103.35	110.01
21	R	104	LMU	O5'-C5'-C6'	3.17	114.28	106.44
20	B	804	CLA	CHC-C1C-C2C	-3.16	117.95	126.95
20	1	212	CLA	C6-C5-C3	-3.16	105.76	113.47
20	2	314	CLA	C1C-CHC-C4B	-3.16	117.69	126.04
20	2	312	CLA	O2A-CGA-CBA	3.16	121.48	111.83
20	B	809	CLA	C3B-C2B-C1B	-3.16	103.44	107.17
20	2	314	CLA	CHC-C1C-NC	3.16	128.98	124.33
20	A	847	CLA	CHB-C4A-NA	3.16	128.96	124.40
20	B	837	CLA	CAA-C2A-C3A	-3.16	104.45	113.00
20	A	850	CLA	CGD-CBD-CAD	3.16	121.08	110.85
20	B	808	CLA	CHD-C4C-C3C	-3.16	120.17	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	301	CLA	C1-C2-C3	-3.16	121.02	126.20
20	A	807	CLA	C4-C3-C5	3.16	120.71	115.23
21	R	101	LMU	O5B-C1B-C2B	3.16	116.86	110.37
20	1	201	CLA	CMB-C2B-C1B	3.16	130.23	125.42
20	3	320	CLA	CMB-C2B-C1B	3.16	130.23	125.42
20	B	803	CLA	CHB-C4A-NA	3.16	128.96	124.40
20	A	824	CLA	C4A-NA-C1A	3.16	108.12	106.68
20	A	828	CLA	C4A-NA-C1A	3.16	108.12	106.68
20	3	312	CLA	CHB-C4A-NA	3.16	128.92	124.43
21	H	103	LMU	O3'-C3'-C2'	-3.15	102.94	110.38
22	L	209	BCR	C15-C14-C13	3.15	131.70	127.28
20	A	818	CLA	C3B-C2B-C1B	-3.15	103.45	107.17
20	F	206	CLA	C2A-C1A-CHA	-3.15	118.40	123.87
20	2	302	CLA	CMB-C2B-C1B	3.15	130.22	125.42
20	A	817	CLA	CGD-CBD-CAD	3.15	121.05	110.85
20	J	102	CLA	CHC-C4B-NB	3.15	128.78	124.05
20	3	320	CLA	CED-O2D-CGD	3.15	123.06	115.92
22	B	842	BCR	C33-C5-C6	-3.15	121.05	124.48
21	L	206	LMU	O5'-C1'-O1'	-3.15	102.60	110.04
20	B	811	CLA	CHB-C4A-NA	3.15	128.95	124.40
21	R	105	LMU	O1B-C1B-C2B	3.15	115.84	108.09
20	4	308	CLA	CHA-C4D-ND	3.15	129.29	124.84
20	A	857	CLA	C2D-C3D-C4D	-3.15	103.53	107.35
20	3	320	CLA	C1-O2A-CGA	3.15	124.27	116.65
20	B	838	CLA	CHB-C1B-NB	-3.15	119.33	124.05
21	E	101	LMU	O1B-C4'-C3'	3.14	115.22	107.23
21	A	852	LMU	O3'-C3'-C4'	-3.14	101.89	109.94
20	3	312	CLA	CHA-C4D-ND	3.14	129.28	124.84
20	A	850	CLA	C2B-C1B-NB	3.14	113.58	110.33
21	H	103	LMU	O5'-C5'-C4'	-3.14	103.24	109.72
20	B	811	CLA	C4B-C3B-C2B	3.14	111.20	107.30
20	B	830	CLA	C4A-NA-C1A	3.13	108.11	106.68
21	E	101	LMU	C3'-C4'-C5'	-3.13	104.00	110.93
20	G	103	CLA	C4B-CHC-C1C	-3.13	118.89	126.25
20	B	838	CLA	CAA-CBA-CGA	3.13	122.09	113.21
20	4	314	CLA	C1C-NC-C4C	-3.13	105.25	106.68
20	A	850	CLA	CHC-C4B-NB	3.13	128.74	124.05
20	3	309	CLA	C4-C3-C5	3.13	120.65	115.23
20	B	825	CLA	C1-C2-C3	-3.13	121.08	126.20
20	B	806	CLA	CAA-C2A-C3A	-3.13	104.55	113.00
20	A	805	CLA	C3B-C2B-C1B	-3.13	103.48	107.17
20	3	301	CLA	O2A-CGA-CBA	3.12	121.36	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	313	CLA	CMB-C2B-C1B	3.12	130.17	125.42
20	B	838	CLA	CMD-C2D-C3D	-3.12	120.53	127.69
20	3	304	CLA	C2D-C3D-C4D	-3.12	103.56	107.35
20	G	103	CLA	C1D-ND-C4D	-3.12	104.12	106.31
20	B	806	CLA	CMB-C2B-C1B	3.12	130.17	125.42
21	H	103	LMU	C3'-C4'-C5'	-3.12	104.02	110.93
20	A	818	CLA	CHC-C4B-NB	3.12	128.72	124.05
20	L	201	CLA	CHC-C4B-NB	3.12	128.72	124.05
20	1	214	CLA	C1D-ND-C4D	3.12	108.50	106.31
20	A	806	CLA	C1-C2-C3	-3.11	121.10	126.20
20	1	213	CLA	CHA-C4D-ND	3.11	129.24	124.84
20	4	310	CLA	C3B-C2B-C1B	-3.11	103.50	107.17
20	2	309	CLA	C4A-NA-C1A	3.11	108.10	106.68
20	1	208	CLA	CHC-C4B-NB	3.11	128.58	124.08
21	2	319	LMU	O1B-C4'-C3'	3.11	115.14	107.23
20	A	817	CLA	C1-O2A-CGA	3.11	124.18	116.65
20	B	826	CLA	CHB-C1B-NB	-3.11	119.38	124.05
20	A	849	CLA	CHC-C1C-NC	3.11	129.00	124.31
20	3	305	CLA	C2D-C3D-C4D	-3.11	103.57	107.35
20	A	804	CLA	C2A-C1A-CHA	-3.11	118.47	123.87
21	1	217	LMU	O1B-C4'-C3'	3.11	115.13	107.23
21	R	104	LMU	C4B-C3B-C2B	-3.11	105.38	110.83
20	H	109	CLA	C3B-C2B-C1B	-3.11	103.51	107.17
20	A	808	CLA	CHD-C4C-C3C	-3.11	120.25	124.77
20	3	314	CLA	CHC-C1C-C2C	-3.10	118.13	126.95
20	A	829	CLA	O2A-CGA-CBA	3.10	121.30	111.83
20	A	815	CLA	CHC-C4B-NB	3.10	128.71	124.05
22	L	209	BCR	C19-C18-C17	-3.10	114.13	119.01
20	1	215	CLA	CHC-C4B-NB	3.10	128.56	124.08
20	B	839	CLA	CGD-CBD-CAD	-3.10	101.59	114.30
20	L	207	CLA	CHC-C1C-C2C	-3.10	118.14	126.95
20	A	821	CLA	O2D-CGD-CBD	3.10	116.64	111.23
20	B	808	CLA	CAC-C3C-C4C	3.09	128.82	124.79
20	A	802	CLA	CMB-C2B-C1B	3.09	130.13	125.42
20	1	208	CLA	C4A-NA-C1A	3.09	108.09	106.68
20	B	835	CLA	CBC-CAC-C3C	-3.09	104.04	112.42
20	B	835	CLA	CHC-C1C-C2C	-3.09	118.16	126.95
20	A	826	CLA	CAA-C2A-C1A	-3.09	101.84	111.97
22	B	850	BCR	C32-C1-C6	3.09	115.09	110.24
20	3	314	CLA	CHD-C4C-C3C	-3.09	120.27	124.77
20	4	317	CLA	C1B-NB-C4B	-3.09	104.14	106.31
20	4	307	CLA	O1D-CGD-CBD	-3.09	118.42	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	809	CLA	C4-C3-C2	-3.09	115.69	123.63
20	A	826	CLA	CMB-C2B-C1B	3.09	130.12	125.42
20	1	203	CLA	CMC-C2C-C1C	3.09	129.86	125.03
20	A	829	CLA	O2A-CGA-O1A	-3.09	115.91	123.63
20	2	311	CLA	O2A-CGA-CBA	3.09	121.25	111.83
21	R	102	LMU	C1'-O5'-C5'	-3.09	107.69	113.72
20	R	106	CLA	C4-C3-C5	3.09	120.58	115.23
20	2	305	CLA	C1B-NB-C4B	-3.08	104.15	106.31
20	R	106	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
20	A	826	CLA	CHC-C4B-NB	3.08	128.67	124.05
21	H	102	LMU	O5'-C5'-C6'	3.08	114.08	106.44
20	1	201	CLA	C2B-C1B-NB	3.08	113.52	110.33
21	L	206	LMU	O5B-C5B-C6B	3.08	114.08	106.44
20	B	825	CLA	CHB-C1B-NB	-3.08	119.43	124.05
21	H	103	LMU	C1B-O5B-C5B	3.08	119.73	113.72
20	B	848	CLA	C6-C5-C3	3.08	120.97	113.47
21	H	103	LMU	O1B-C4'-C3'	3.07	115.05	107.23
21	2	318	LMU	C1'-C2'-C3'	3.07	116.48	110.01
20	2	303	CLA	CHC-C4B-NB	3.07	128.52	124.08
22	I	101	BCR	C32-C1-C31	-3.07	99.83	108.63
20	2	317	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
20	F	206	CLA	CBA-CAA-C2A	-3.07	104.65	113.79
20	H	101	CLA	CHC-C1C-C2C	-3.07	118.22	126.95
20	1	211	CLA	CHC-C1C-C2C	-3.07	118.23	126.95
20	A	820	CLA	C3B-C2B-C1B	-3.07	103.55	107.17
20	1	206	CLA	C1-C2-C3	-3.07	121.17	126.20
20	A	806	CLA	C4A-NA-C1A	3.07	108.08	106.68
20	1	211	CLA	C1D-ND-C4D	-3.07	104.16	106.31
20	B	830	CLA	CAA-CBA-CGA	-3.07	104.50	113.21
20	B	811	CLA	CMB-C2B-C1B	3.07	130.09	125.42
20	1	209	CLA	C1D-ND-C4D	-3.06	104.16	106.31
20	2	305	CLA	C2C-C1C-CHC	-3.06	117.81	125.84
20	A	824	CLA	C4B-CHC-C1C	-3.06	119.05	126.25
20	B	807	CLA	C4A-NA-C1A	3.06	108.08	106.68
20	A	847	CLA	C6-C7-C8	-3.06	105.79	115.97
20	3	307	CLA	C2D-C3D-C4D	-3.06	103.63	107.35
20	A	816	CLA	C4-C3-C5	3.06	120.54	115.23
20	1	204	CLA	CGD-CBD-CAD	3.06	120.75	110.85
20	3	319	CLA	C4A-NA-C1A	3.06	108.08	106.68
21	E	101	LMU	O3'-C3'-C4'	3.06	117.78	109.94
20	A	818	CLA	O2A-CGA-CBA	3.06	121.16	111.83
20	B	825	CLA	CMA-C3A-C2A	-3.06	102.16	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	806	CLA	CHC-C1C-C2C	-3.06	118.26	126.95
20	2	314	CLA	CHA-C4D-ND	3.06	129.16	124.84
20	A	805	CLA	CAA-C2A-C1A	-3.05	101.96	111.97
20	1	212	CLA	C2B-C1B-NB	3.05	113.49	110.33
21	H	102	LMU	C6B-C5B-C4B	3.05	120.52	113.02
20	B	820	CLA	C1D-ND-C4D	-3.05	104.17	106.31
20	2	312	CLA	CHC-C1C-C2C	-3.05	118.27	126.95
20	4	308	CLA	CHB-C4A-NA	3.05	128.77	124.43
20	4	307	CLA	CMA-C3A-C2A	-3.05	102.19	113.98
20	3	313	CLA	C3B-C2B-C1B	-3.05	103.41	106.81
20	H	109	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
20	2	303	CLA	C3D-C4D-ND	3.05	113.67	109.50
20	A	816	CLA	O2A-CGA-CBA	3.04	121.12	111.83
20	2	308	CLA	C3D-C4D-ND	3.04	113.66	109.50
20	A	849	CLA	C2A-C1A-CHA	-3.04	118.58	123.87
20	2	307	CLA	CGD-CBD-CAD	3.04	120.70	110.85
21	C	101	LMU	C4B-C3B-C2B	3.04	116.17	110.83
20	4	307	CLA	CHB-C1B-C2B	-3.04	118.59	127.43
20	B	812	CLA	CHC-C4B-NB	3.04	128.61	124.05
20	4	310	CLA	CHC-C1C-NC	3.04	128.89	124.31
20	A	821	CLA	CAC-C3C-C4C	3.04	128.75	124.79
20	A	848	CLA	CHC-C4B-NB	3.04	128.61	124.05
20	3	303	CLA	C4A-NA-C1A	3.04	108.07	106.68
20	3	301	CLA	O1D-CGD-CBD	-3.04	118.52	124.52
20	2	310	CLA	CHB-C4A-NA	3.04	128.79	124.40
21	1	217	LMU	C3B-C4B-C5B	-3.04	104.72	110.23
20	B	847	CLA	CHC-C1C-C2C	-3.04	118.31	126.95
21	A	845	LMU	C2'-C3'-C4'	3.04	116.58	109.68
20	H	109	CLA	CMD-C2D-C3D	-3.04	120.72	127.69
20	3	304	CLA	C3B-C2B-C1B	-3.04	103.43	106.81
22	I	103	BCR	C40-C30-C25	-3.04	105.48	110.24
20	4	307	CLA	CHC-C1C-C2C	-3.04	118.32	126.95
20	4	317	CLA	C3B-C2B-C1B	-3.04	103.43	106.81
22	A	842	BCR	C38-C26-C27	3.04	120.07	113.60
20	A	807	CLA	O2A-CGA-O1A	-3.04	116.03	123.63
22	B	842	BCR	C36-C18-C19	3.04	122.72	118.09
22	A	840	BCR	C38-C26-C27	3.03	120.07	113.60
20	B	833	CLA	CHC-C4B-NB	3.03	128.60	124.05
20	B	811	CLA	C4A-NA-C1A	3.03	108.06	106.68
20	3	306	CLA	C2D-C3D-C4D	-3.03	103.66	107.35
21	L	210	LMU	O5'-C5'-C6'	3.03	113.95	106.44
20	2	311	CLA	C1-O2A-CGA	3.03	123.99	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	308	CLA	C4D-ND-C1D	-3.03	104.19	106.31
22	A	844	BCR	C33-C5-C4	3.03	120.06	113.60
20	H	110	CLA	O2A-CGA-CBA	3.03	121.07	111.83
20	1	207	CLA	CAA-CBA-CGA	3.03	121.81	113.21
22	B	843	BCR	C38-C26-C27	3.03	120.05	113.60
20	A	824	CLA	CMA-C3A-C4A	-3.03	103.64	111.77
20	B	819	CLA	CHC-C1C-C2C	-3.03	118.34	126.95
22	F	202	BCR	C38-C26-C27	3.03	120.05	113.60
20	A	805	CLA	C2A-C1A-CHA	-3.03	118.61	123.87
20	A	810	CLA	C3B-C2B-C1B	-3.03	103.60	107.17
22	G	102	BCR	C38-C26-C27	3.03	120.05	113.60
22	A	842	BCR	C33-C5-C4	3.03	120.05	113.60
20	I	102	CLA	O1D-CGD-CBD	-3.03	118.55	124.52
20	B	815	CLA	CGD-CBD-CAD	-3.03	101.05	110.85
20	A	812	CLA	C4B-C3B-C2B	3.02	111.06	107.30
20	A	825	CLA	CMA-C3A-C4A	-3.02	103.65	111.77
20	B	813	CLA	C1D-ND-C4D	-3.02	104.19	106.31
20	B	805	CLA	CAA-C2A-C3A	-3.02	104.83	113.00
20	4	312	CLA	C3D-C4D-ND	3.02	113.63	109.50
20	R	106	CLA	CHC-C4B-NB	3.02	128.58	124.05
20	B	826	CLA	CHC-C1C-C2C	-3.02	118.37	126.95
20	A	809	CLA	CHB-C4A-NA	3.02	128.76	124.40
22	G	102	BCR	C33-C5-C4	3.02	120.03	113.60
22	J	101	BCR	C38-C26-C27	3.02	120.03	113.60
22	B	844	BCR	C38-C26-C27	3.02	120.03	113.60
22	A	841	BCR	C38-C26-C27	3.02	120.03	113.60
20	3	313	CLA	CHC-C4B-NB	3.02	128.44	124.08
21	K	104	LMU	C1B-O5B-C5B	-3.01	107.83	113.72
20	3	315	CLA	C3B-C2B-C1B	-3.01	103.62	107.17
20	L	203	CLA	CHC-C4B-NB	3.01	128.57	124.05
22	B	843	BCR	C33-C5-C4	3.01	120.02	113.60
20	A	838	CLA	O2D-CGD-CBD	3.01	116.49	111.23
22	F	203	BCR	C23-C22-C21	3.01	123.74	119.01
22	A	843	BCR	C38-C26-C27	3.01	120.01	113.60
20	2	303	CLA	CHA-C4D-ND	3.01	129.09	124.84
20	B	824	CLA	CHB-C4A-NA	3.01	128.74	124.40
20	4	318	CLA	CHC-C1C-C2C	-3.01	118.40	126.95
22	I	103	BCR	C24-C25-C26	3.01	128.48	121.56
20	3	316	CLA	CHB-C4A-NA	3.01	128.71	124.43
20	3	303	CLA	CBD-CHA-C1A	3.01	131.92	127.38
22	B	841	BCR	C33-C5-C4	3.01	120.00	113.60
20	K	107	CLA	CAA-CBA-CGA	-3.00	104.68	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	K	106	CLA	CMB-C2B-C3B	3.00	133.61	126.55
20	1	203	CLA	C4A-NA-C1A	3.00	108.05	106.68
20	2	315	CLA	C1C-NC-C4C	-3.00	105.31	106.68
20	B	821	CLA	OBD-CAD-C3D	-3.00	121.40	128.42
20	K	107	CLA	C3B-C2B-C1B	-3.00	103.63	107.17
22	A	843	BCR	C33-C5-C4	3.00	120.00	113.60
20	3	304	CLA	CHB-C1B-NB	-3.00	119.74	124.08
20	4	310	CLA	C2B-C1B-NB	3.00	113.44	110.33
20	1	213	CLA	CHB-C4A-NA	3.00	128.70	124.43
20	2	321	CLA	CMD-C2D-C3D	-3.00	120.81	127.69
22	A	840	BCR	C33-C5-C4	3.00	119.99	113.60
21	H	104	LMU	O1B-C4'-C3'	-3.00	99.62	107.23
20	K	107	CLA	O2A-CGA-CBA	3.00	120.97	111.83
20	H	109	CLA	O1D-CGD-CBD	-2.99	118.61	124.52
22	B	844	BCR	C33-C5-C4	2.99	119.98	113.60
20	A	803	CLA	C4B-C3B-C2B	2.99	111.02	107.30
21	4	316	LMU	O1'-C1'-C2'	2.99	112.82	108.27
20	B	827	CLA	CHD-C4C-NC	2.99	128.87	124.23
21	A	854	LMU	O3'-C3'-C4'	2.99	117.60	109.94
21	R	103	LMU	O1B-C4'-C3'	2.99	114.83	107.23
22	I	101	BCR	C33-C5-C4	2.99	119.97	113.60
20	B	812	CLA	CMD-C2D-C3D	-2.99	120.83	127.69
20	A	803	CLA	O2A-CGA-CBA	2.99	120.95	111.83
20	A	807	CLA	CHD-C4C-NC	2.99	128.87	124.23
22	A	841	BCR	C33-C5-C4	2.99	119.96	113.60
20	A	808	CLA	O1D-CGD-CBD	-2.99	118.63	124.52
20	B	837	CLA	C4-C3-C5	2.99	120.41	115.23
20	1	212	CLA	C4A-NA-C1A	2.99	108.04	106.68
20	A	848	CLA	CMD-C2D-C3D	-2.98	120.84	127.69
20	4	308	CLA	CHC-C4B-NB	2.98	128.39	124.08
20	1	204	CLA	C4D-C3D-CAD	2.98	111.34	108.11
22	A	844	BCR	C38-C26-C27	2.98	119.95	113.60
20	2	315	CLA	C4A-NA-C1A	2.98	108.04	106.68
20	1	215	CLA	CHB-C1B-NB	-2.98	119.77	124.08
22	J	101	BCR	C33-C5-C4	2.98	119.95	113.60
20	K	106	CLA	CHC-C4B-NB	2.98	128.52	124.05
20	1	206	CLA	CMD-C2D-C3D	-2.98	120.86	127.69
20	B	819	CLA	CHD-C4C-C3C	-2.98	120.43	124.77
22	B	841	BCR	C38-C26-C27	2.98	119.95	113.60
21	R	104	LMU	C2'-C3'-C4'	2.98	116.44	109.68
20	B	805	CLA	O2A-CGA-O1A	-2.98	116.18	123.63
20	4	306	CLA	O2D-CGD-O1D	-2.98	118.06	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	812	CLA	O1D-CGD-CBD	-2.98	118.65	124.52
20	4	304	CLA	CHC-C4B-NB	2.98	128.51	124.05
22	3	311	BCR	C38-C26-C27	2.97	119.94	113.60
20	B	836	CLA	CHC-C4B-NB	2.97	128.51	124.05
20	B	837	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
20	A	806	CLA	O2A-CGA-O1A	-2.97	116.19	123.63
20	1	201	CLA	CMA-C3A-C4A	2.97	119.76	111.77
20	3	305	CLA	CHB-C4A-NA	2.97	128.65	124.43
20	1	201	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
20	4	313	CLA	CMD-C2D-C3D	-2.97	120.88	127.69
20	A	801	CLA	C4B-C3B-C2B	2.97	110.99	107.30
20	3	306	CLA	CHB-C4A-NA	2.97	128.65	124.43
20	2	302	CLA	C4-C3-C5	2.96	120.37	115.23
20	H	108	CLA	C3B-C2B-C1B	-2.96	103.67	107.17
20	A	815	CLA	C1-O2A-CGA	2.96	123.82	116.65
20	B	839	CLA	CMD-C2D-C3D	-2.96	120.90	127.69
21	L	210	LMU	O5'-C5'-C4'	-2.96	103.60	109.72
20	B	849	CLA	CHC-C1C-C2C	-2.96	118.53	126.95
20	B	820	CLA	C3D-C4D-ND	2.96	114.80	109.99
20	B	820	CLA	CBA-CAA-C2A	2.96	122.60	113.79
20	A	810	CLA	CHB-C4A-NA	2.96	128.67	124.40
20	B	847	CLA	C7-C6-C5	-2.96	105.38	113.26
22	F	203	BCR	C37-C22-C21	-2.96	118.03	122.82
20	A	849	CLA	C4A-NA-C1A	2.96	108.03	106.68
20	1	206	CLA	C1-O2A-CGA	2.96	123.81	116.65
20	A	823	CLA	C3B-C2B-C1B	-2.95	103.69	107.17
22	F	202	BCR	C33-C5-C4	2.95	119.90	113.60
20	1	204	CLA	C2B-C1B-NB	2.95	113.39	110.33
20	A	850	CLA	CAC-C3C-C2C	-2.95	122.13	127.56
20	2	311	CLA	CHC-C1C-C2C	-2.95	118.56	126.95
20	B	812	CLA	C4-C3-C5	2.95	120.35	115.23
20	B	808	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
20	1	213	CLA	CHC-C4B-NB	2.95	128.34	124.08
20	A	829	CLA	CED-O2D-CGD	2.95	122.60	115.92
20	3	312	CLA	CHC-C4B-NB	2.95	128.34	124.08
20	A	811	CLA	CAA-C2A-C1A	-2.95	102.32	111.97
20	B	809	CLA	CHC-C1C-C2C	-2.94	118.58	126.95
20	B	814	CLA	C4A-NA-C1A	2.94	108.02	106.68
20	B	822	CLA	C3B-C2B-C1B	-2.94	103.70	107.17
20	B	847	CLA	O2A-CGA-CBA	2.94	120.80	111.83
20	A	850	CLA	CMB-C2B-C1B	2.94	129.90	125.42
20	A	850	CLA	CAA-C2A-C1A	2.94	121.61	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	H	108	CLA	O2A-CGA-CBA	2.94	120.80	111.83
20	1	214	CLA	CAC-C3C-C4C	2.94	128.61	124.79
20	A	809	CLA	CAA-CBA-CGA	2.94	121.55	113.21
21	4	321	LMU	O5'-C5'-C4'	2.94	115.80	109.72
20	B	837	CLA	C4A-NA-C1A	2.94	108.02	106.68
20	R	106	CLA	C4A-NA-C1A	2.94	108.02	106.68
20	1	212	CLA	C3B-C2B-C1B	-2.94	103.71	107.17
20	2	315	CLA	C3D-C4D-CHA	-2.94	118.64	125.20
20	B	838	CLA	CHC-C1C-C2C	-2.94	118.60	126.95
20	B	834	CLA	C2B-C1B-NB	2.94	113.37	110.33
21	R	104	LMU	O5B-C5B-C6B	2.94	113.72	106.44
20	A	820	CLA	C4-C3-C5	2.94	120.32	115.23
21	A	846	LMU	C2'-C3'-C4'	2.94	116.34	109.68
21	B	802	LMU	C1'-C2'-C3'	2.94	116.19	110.01
20	A	820	CLA	CHB-C4A-NA	2.94	128.64	124.40
21	H	102	LMU	C1B-O1B-C4'	-2.93	111.02	117.98
20	A	850	CLA	C1B-C2B-C3B	-2.93	104.27	107.03
20	B	813	CLA	C3B-C2B-C1B	-2.93	103.71	107.17
20	B	828	CLA	O2A-C1-C2	2.93	119.39	108.11
21	L	206	LMU	O2'-C2'-C1'	-2.93	103.09	110.08
20	A	818	CLA	CHB-C4A-NA	2.93	128.63	124.40
20	B	847	CLA	O2D-CGD-CBD	2.93	116.35	111.23
20	4	311	CLA	C2D-C3D-C4D	-2.93	103.79	107.35
21	A	846	LMU	O2B-C2B-C1B	-2.93	103.10	110.08
20	4	309	CLA	CHB-C4A-NA	2.93	128.59	124.43
20	1	205	CLA	CHB-C4A-NA	2.93	128.62	124.40
20	A	837	CLA	C3B-C2B-C1B	-2.93	103.72	107.17
21	A	853	LMU	C6B-C5B-C4B	-2.93	105.83	113.02
22	3	311	BCR	C24-C23-C22	-2.93	121.91	126.23
21	A	853	LMU	C1'-O5'-C5'	-2.93	108.01	113.72
20	L	204	CLA	C3B-C4B-NB	-2.92	107.92	110.53
20	K	107	CLA	CHC-C4B-NB	2.92	128.44	124.05
20	B	814	CLA	CHC-C1C-C2C	-2.92	118.64	126.95
20	A	801	CLA	C3B-C4B-NB	-2.92	107.92	110.53
20	K	107	CLA	CHC-C1C-NC	2.92	128.71	124.31
22	F	203	BCR	C38-C26-C27	2.92	119.83	113.60
20	B	816	CLA	CHC-C1C-NC	2.92	128.71	124.31
20	B	828	CLA	C1D-ND-C4D	-2.92	104.26	106.31
20	4	314	CLA	C2D-C3D-C4D	-2.92	103.80	107.35
20	B	830	CLA	CHC-C1C-C2C	-2.92	118.65	126.95
20	A	807	CLA	CHB-C1B-NB	-2.92	119.67	124.05
20	A	827	CLA	CAC-C3C-C4C	2.92	128.59	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	211	CLA	CHB-C1B-NB	-2.92	119.67	124.05
20	K	105	CLA	C3B-C2B-C1B	-2.92	103.73	107.17
20	2	308	CLA	CHC-C4B-NB	2.92	128.29	124.08
20	B	805	CLA	CAC-C3C-C4C	2.92	128.58	124.79
20	2	304	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
21	A	846	LMU	C1B-O5B-C5B	2.91	119.41	113.72
20	4	318	CLA	CHB-C4A-NA	2.91	128.61	124.40
21	A	854	LMU	O5'-C1'-C2'	2.91	116.36	110.37
20	3	310	CLA	C3B-C2B-C1B	-2.91	103.74	107.17
20	1	207	CLA	C1D-ND-C4D	-2.91	104.27	106.31
20	4	312	CLA	C1B-NB-C4B	-2.91	104.27	106.31
20	A	821	CLA	CHB-C4A-NA	2.91	128.60	124.40
20	A	832	CLA	C3B-C2B-C1B	-2.91	103.74	107.17
20	A	802	CLA	CBA-CAA-C2A	2.91	122.45	113.79
20	4	313	CLA	CMC-C2C-C1C	2.91	129.58	125.03
20	I	102	CLA	CHC-C4B-NB	2.91	128.41	124.05
20	2	311	CLA	C2B-C1B-NB	2.91	113.34	110.33
20	3	315	CLA	C2A-C1A-CHA	-2.90	118.83	123.87
20	1	214	CLA	O1D-CGD-CBD	-2.90	118.79	124.52
21	L	205	LMU	C6'-C5'-C4'	-2.90	105.22	113.38
20	B	817	CLA	C1D-ND-C4D	-2.90	104.28	106.31
20	H	108	CLA	CHC-C1C-C2C	-2.90	118.71	126.95
20	A	831	CLA	C3B-C2B-C1B	-2.90	103.75	107.17
20	B	812	CLA	C4-C3-C2	-2.90	116.19	123.63
20	F	206	CLA	O2A-CGA-CBA	2.90	120.67	111.83
20	B	821	CLA	CHC-C1C-C2C	-2.90	118.71	126.95
20	3	314	CLA	CHB-C1B-NB	-2.90	119.70	124.05
20	A	804	CLA	CHC-C1C-C2C	-2.90	118.72	126.95
21	1	218	LMU	O5'-C5'-C4'	-2.89	103.74	109.72
20	2	315	CLA	C3B-C2B-C1B	-2.89	103.59	106.81
20	A	817	CLA	CED-O2D-CGD	2.89	122.48	115.92
20	B	818	CLA	C3B-C2B-C1B	-2.89	103.76	107.17
20	B	811	CLA	O1D-CGD-CBD	-2.89	118.81	124.52
21	E	101	LMU	O3B-C3B-C4B	-2.89	103.56	110.38
20	4	319	CLA	C3B-C2B-C1B	-2.89	103.76	107.17
20	4	305	CLA	CHD-C4C-NC	2.89	128.72	124.23
20	B	805	CLA	C16-C15-C13	-2.89	106.35	115.97
20	B	808	CLA	O2A-CGA-CBA	2.89	120.65	111.83
20	4	304	CLA	CMB-C2B-C1B	2.89	129.82	125.42
21	R	109	LMU	C1B-C2B-C3B	2.89	116.09	110.01
20	B	819	CLA	C3B-C2B-C1B	-2.89	103.76	107.17
21	K	102	LMU	O2'-C2'-C1'	2.89	116.96	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	828	CLA	CHC-C1C-C2C	-2.89	118.73	126.95
20	2	311	CLA	O1D-CGD-CBD	-2.89	118.82	124.52
20	H	107	CLA	CAC-C3C-C4C	2.89	128.54	124.79
20	A	804	CLA	CHB-C4A-NA	2.89	128.56	124.40
20	B	815	CLA	CHB-C4A-NA	2.89	128.56	124.40
20	B	820	CLA	CMA-C3A-C4A	-2.88	104.02	111.77
20	A	834	CLA	C3B-C2B-C1B	-2.88	103.77	107.17
20	A	833	CLA	C3B-C2B-C1B	-2.88	103.77	107.17
20	K	103	CLA	C3B-C2B-C1B	-2.88	103.77	107.17
20	B	834	CLA	CMC-C2C-C1C	2.88	129.54	125.03
20	B	826	CLA	O1D-CGD-CBD	-2.88	118.84	124.52
20	B	823	CLA	C3B-C2B-C1B	-2.88	103.77	107.17
20	B	821	CLA	C1-O2A-CGA	2.88	123.62	116.65
20	H	108	CLA	CHC-C4B-NB	2.88	128.37	124.05
20	A	825	CLA	CHB-C4A-NA	2.88	128.55	124.40
20	B	847	CLA	C16-C17-C18	-2.88	103.09	115.94
21	A	853	LMU	C1B-C2B-C3B	2.88	116.06	110.01
20	L	202	CLA	CMD-C2D-C3D	-2.88	121.09	127.69
21	2	318	LMU	O5B-C5B-C4B	-2.88	104.51	109.70
20	B	848	CLA	CAA-C2A-C1A	2.88	121.40	111.97
22	I	101	BCR	C15-C16-C17	2.88	129.40	123.52
20	1	202	CLA	C3B-C2B-C1B	-2.88	103.78	107.17
20	2	310	CLA	CHC-C1C-C2C	-2.88	118.78	126.95
20	2	301	CLA	C3B-C2B-C1B	-2.87	103.78	107.17
21	A	845	LMU	C3'-C4'-C5'	2.87	117.30	110.93
20	2	308	CLA	C3C-C4C-CHD	-2.87	117.77	125.23
20	B	837	CLA	O2A-CGA-O1A	-2.87	116.44	123.63
21	L	205	LMU	O5'-C1'-C2'	2.87	116.27	110.37
20	B	805	CLA	CHC-C4B-NB	2.87	128.36	124.05
20	A	855	CLA	C3B-C2B-C1B	-2.87	103.78	107.17
20	A	820	CLA	CAA-C2A-C3A	-2.87	105.24	113.00
20	B	825	CLA	C11-C12-C13	-2.87	106.42	115.97
20	A	822	CLA	C3B-C2B-C1B	-2.87	103.78	107.17
20	B	838	CLA	C4-C3-C5	2.87	120.21	115.23
20	B	825	CLA	O1D-CGD-CBD	-2.87	118.86	124.52
20	A	835	CLA	C3B-C2B-C1B	-2.87	103.79	107.17
20	K	106	CLA	CHC-C1C-C2C	-2.87	118.79	126.95
20	A	820	CLA	O2D-CGD-CBD	2.87	116.25	111.23
20	B	819	CLA	CAC-C3C-C4C	2.87	128.52	124.79
20	L	203	CLA	C2A-C1A-CHA	-2.87	118.89	123.87
20	2	308	CLA	CHA-C4D-ND	2.87	128.89	124.84
20	G	103	CLA	CHB-C4A-NA	2.87	128.54	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	805	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
20	3	317	CLA	C2C-C1C-CHC	-2.87	118.33	125.84
20	3	301	CLA	C4A-NA-C1A	2.86	107.99	106.68
20	B	816	CLA	CMC-C2C-C1C	2.86	129.51	125.03
20	A	814	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
20	A	836	CLA	C3B-C2B-C1B	-2.86	103.80	107.17
21	E	101	LMU	O5'-C5'-C4'	-2.86	103.81	109.72
20	B	816	CLA	C4A-NA-C1A	2.86	107.98	106.68
20	2	314	CLA	CHB-C1B-NB	-2.86	119.95	124.08
21	R	105	LMU	C4B-C3B-C2B	-2.86	105.81	110.83
20	A	813	CLA	CGD-CBD-CAD	2.86	120.09	110.85
20	J	102	CLA	C3B-C2B-C1B	-2.86	103.80	107.17
20	L	203	CLA	C1D-ND-C4D	-2.86	104.31	106.31
20	4	306	CLA	C2B-C1B-NB	2.86	113.29	110.33
20	B	829	CLA	CMB-C2B-C1B	2.85	129.77	125.42
20	A	804	CLA	O2A-CGA-CBA	2.85	120.54	111.83
21	F	201	LMU	C1B-O5B-C5B	2.85	119.29	113.72
20	B	816	CLA	O1D-CGD-CBD	-2.85	118.89	124.52
20	A	815	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
20	F	205	CLA	C3B-C2B-C1B	-2.85	103.81	107.17
20	3	309	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
20	4	318	CLA	CAA-C2A-C1A	-2.85	102.63	111.97
20	A	805	CLA	CAC-C3C-C4C	2.85	128.50	124.79
20	A	817	CLA	C4-C3-C5	2.85	120.18	115.23
21	H	104	LMU	C1B-O1B-C4'	-2.85	111.22	117.98
20	L	204	CLA	O2A-CGA-O1A	-2.85	116.50	123.63
20	H	107	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
20	A	813	CLA	CHC-C1C-C2C	-2.84	118.86	126.95
20	B	828	CLA	CHB-C4A-NA	2.84	128.50	124.40
20	H	107	CLA	O2A-CGA-CBA	2.84	120.50	111.83
20	4	313	CLA	CHC-C1C-C2C	-2.84	118.88	126.95
21	H	105	LMU	O3B-C3B-C2B	2.84	117.07	110.38
20	B	817	CLA	O2A-CGA-CBA	2.84	120.49	111.83
20	R	106	CLA	C1D-ND-C4D	-2.84	104.32	106.31
20	L	203	CLA	CHC-C1C-NC	2.84	128.59	124.31
20	B	829	CLA	C1-O2A-CGA	2.84	123.52	116.65
20	B	816	CLA	CMD-C2D-C3D	-2.84	121.18	127.69
20	B	815	CLA	CAC-C3C-C4C	2.84	128.48	124.79
20	2	321	CLA	CHC-C1C-C2C	-2.84	118.89	126.95
20	A	838	CLA	O2A-CGA-O1A	-2.83	116.54	123.63
20	A	826	CLA	CED-O2D-CGD	2.83	122.34	115.92
20	B	815	CLA	CMB-C2B-C1B	2.83	129.73	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	805	CLA	CMC-C2C-C1C	2.83	129.46	125.03
20	4	310	CLA	CHC-C4B-NB	2.83	128.30	124.05
20	B	812	CLA	C4B-C3B-C2B	2.83	110.82	107.30
20	2	317	CLA	CAC-C3C-C4C	2.83	128.47	124.79
20	J	103	CLA	CED-O2D-CGD	2.83	122.34	115.92
20	3	315	CLA	O2A-CGA-O1A	-2.83	116.55	123.63
20	A	812	CLA	CHC-C1C-C2C	-2.83	118.90	126.95
20	4	310	CLA	CED-O2D-CGD	2.83	122.34	115.92
20	A	838	CLA	O1D-CGD-CBD	-2.83	118.94	124.52
20	4	309	CLA	CHD-C1D-ND	2.83	128.84	124.84
20	B	828	CLA	CED-O2D-CGD	2.83	122.33	115.92
20	2	312	CLA	O2A-CGA-O1A	-2.83	116.55	123.63
20	B	815	CLA	O2A-CGA-O1A	-2.83	116.56	123.63
20	1	211	CLA	CMA-C3A-C4A	-2.83	104.18	111.77
21	R	105	LMU	O3B-C3B-C2B	-2.82	103.72	110.38
21	B	845	LMU	O5B-C5B-C4B	2.82	114.79	109.70
21	1	217	LMU	O3'-C3'-C4'	-2.82	102.70	109.94
20	4	302	CLA	C3B-C2B-C1B	-2.82	103.84	107.17
21	L	205	LMU	O5'-C5'-C6'	2.82	113.44	106.44
20	B	817	CLA	C1-O2A-CGA	2.82	123.48	116.65
20	2	314	CLA	CHB-C4A-NA	2.82	128.44	124.43
20	4	307	CLA	C3D-C4D-ND	2.82	114.57	109.99
20	B	805	CLA	CHD-C4C-C3C	-2.82	120.66	124.77
20	1	203	CLA	C3B-C2B-C1B	-2.82	103.84	107.17
20	G	103	CLA	CAA-CBA-CGA	-2.82	105.20	113.21
20	A	803	CLA	CED-O2D-CGD	2.82	122.31	115.92
20	B	809	CLA	CHB-C4A-NA	2.82	128.47	124.40
20	H	108	CLA	CHD-C4C-C3C	-2.82	120.66	124.77
20	B	809	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
20	B	847	CLA	CMD-C2D-C3D	-2.82	121.23	127.69
20	3	305	CLA	C3C-C4C-CHD	-2.82	117.92	125.23
20	A	830	CLA	C4A-NA-C1A	2.81	107.96	106.68
20	A	830	CLA	CHC-C1C-C2C	-2.81	118.95	126.95
20	3	305	CLA	C3D-C4D-CHA	-2.81	118.92	125.20
20	B	819	CLA	C5-C3-C2	-2.81	114.86	121.17
20	B	828	CLA	O1D-CGD-CBD	-2.81	118.98	124.52
21	A	853	LMU	O1B-C1B-C2B	2.81	115.00	108.09
20	B	829	CLA	CHB-C4A-NA	2.81	128.45	124.40
20	R	107	CLA	CGD-CBD-CAD	-2.81	101.76	110.85
20	L	208	CLA	CHC-C1C-NC	2.81	128.54	124.31
21	H	104	LMU	C3'-C4'-C5'	2.81	117.15	110.93
20	A	817	CLA	CHC-C1C-C2C	-2.81	118.98	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	L	210	LMU	O5B-C5B-C4B	2.80	114.75	109.70
21	4	321	LMU	C1'-C2'-C3'	2.80	115.91	110.01
20	A	820	CLA	CMC-C2C-C1C	2.80	129.42	125.03
20	B	819	CLA	O2D-CGD-CBD	2.80	116.13	111.23
20	B	832	CLA	C4A-NA-C1A	2.80	107.96	106.68
21	H	105	LMU	O2'-C2'-C1'	-2.80	103.39	110.08
21	R	109	LMU	O2B-C2B-C1B	2.80	116.75	110.08
20	3	319	CLA	CMB-C2B-C1B	2.80	129.69	125.42
20	A	818	CLA	C4-C3-C5	2.80	119.43	116.13
20	2	307	CLA	CHD-C4C-C3C	-2.80	120.69	124.77
20	2	314	CLA	C4D-ND-C1D	-2.80	104.35	106.31
20	B	836	CLA	C4B-C3B-C2B	2.80	110.78	107.30
20	B	810	CLA	O1D-CGD-CBD	-2.80	119.00	124.52
20	3	306	CLA	C3C-C4C-CHD	-2.80	117.97	125.23
20	B	829	CLA	CAA-CBA-CGA	-2.80	105.27	113.21
20	A	847	CLA	O2A-CGA-CBA	2.79	120.36	111.83
20	L	207	CLA	O2A-CGA-CBA	2.79	120.36	111.83
20	A	804	CLA	C4B-C3B-C2B	2.79	110.78	107.30
20	B	847	CLA	C4B-C3B-C2B	2.79	110.78	107.30
20	A	809	CLA	O2D-CGD-CBD	2.79	116.11	111.23
20	B	806	CLA	CMA-C3A-C4A	-2.79	104.26	111.77
20	B	825	CLA	C4B-C3B-C2B	2.79	110.77	107.30
20	3	301	CLA	C3B-C2B-C1B	-2.79	103.88	107.17
20	B	827	CLA	CHC-C1C-C2C	-2.79	119.02	126.95
20	3	305	CLA	C2C-C1C-CHC	-2.79	118.53	125.84
20	A	826	CLA	C1-C2-C3	-2.79	121.63	126.20
20	A	825	CLA	CHC-C1C-C2C	-2.79	119.02	126.95
21	K	101	LMU	O2B-C2B-C1B	-2.79	103.43	110.08
20	G	103	CLA	C1-C2-C3	-2.79	121.63	126.20
20	1	201	CLA	CHC-C4B-C3B	-2.79	115.28	127.37
20	A	829	CLA	CAC-C3C-C2C	-2.79	122.44	127.56
20	1	206	CLA	C4-C3-C5	2.79	120.06	115.23
22	F	203	BCR	C2-C3-C4	-2.78	105.15	111.28
21	2	318	LMU	C4B-C3B-C2B	-2.78	105.94	110.83
20	K	107	CLA	C4-C3-C5	2.78	120.06	115.23
20	L	203	CLA	CMC-C2C-C1C	2.78	129.38	125.03
20	B	804	CLA	O2A-CGA-CBA	2.78	120.32	111.83
20	A	847	CLA	CMA-C3A-C2A	-2.78	103.23	113.98
20	L	207	CLA	CED-O2D-CGD	2.78	122.22	115.92
20	A	804	CLA	C3B-C4B-NB	-2.78	108.05	110.53
20	A	801	CLA	CAA-C2A-C3A	-2.78	105.49	113.00
20	B	824	CLA	CAA-C2A-C3A	-2.78	105.49	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	315	CLA	CBA-CAA-C2A	-2.78	105.53	113.79
20	B	813	CLA	CHC-C1C-C2C	-2.78	119.05	126.95
20	B	809	CLA	C5-C3-C2	2.78	127.40	121.17
20	1	210	CLA	CHC-C4B-NB	2.78	128.21	124.05
21	1	218	LMU	O1'-C1'-C2'	2.78	112.49	108.27
20	B	822	CLA	C4-C3-C5	2.78	120.05	115.23
20	A	801	CLA	CHC-C1C-C2C	-2.77	119.06	126.95
20	H	108	CLA	O1D-CGD-CBD	-2.77	119.05	124.52
21	E	101	LMU	O6B-C6B-C5B	-2.77	101.89	111.33
20	L	202	CLA	C6-C7-C8	-2.77	106.75	115.97
20	B	838	CLA	CHB-C4A-NA	2.77	128.40	124.40
20	3	306	CLA	C3D-C4D-CHA	-2.77	119.02	125.20
20	3	306	CLA	C2C-C1C-CHC	-2.77	118.58	125.84
20	J	103	CLA	CHC-C1C-C2C	-2.77	119.08	126.95
20	L	201	CLA	O2A-CGA-CBA	2.77	120.28	111.83
20	A	810	CLA	O2A-CGA-CBA	2.77	120.28	111.83
20	B	849	CLA	C1-C2-C3	-2.77	121.66	126.20
20	A	803	CLA	CAC-C3C-C4C	2.77	128.39	124.79
20	A	803	CLA	C1-O2A-CGA	2.77	123.35	116.65
20	B	814	CLA	O2A-CGA-CBA	2.77	120.27	111.83
20	J	102	CLA	C4-C3-C5	2.77	120.03	115.23
20	A	810	CLA	CHC-C1C-C2C	-2.77	119.09	126.95
20	G	103	CLA	CED-O2D-CGD	2.76	122.19	115.92
20	1	202	CLA	CHB-C4A-NA	2.76	128.39	124.40
20	A	823	CLA	C4-C3-C5	2.76	120.03	115.23
20	A	855	CLA	C4-C3-C5	2.76	120.03	115.23
21	K	101	LMU	C1B-O5B-C5B	-2.76	108.32	113.72
20	4	314	CLA	C3B-C2B-C1B	-2.76	103.73	106.81
21	A	852	LMU	O5B-C5B-C4B	-2.76	104.72	109.70
20	3	310	CLA	C4-C3-C5	2.76	120.02	115.23
20	B	813	CLA	CHB-C4A-NA	2.76	128.39	124.40
20	1	203	CLA	O2A-CGA-CBA	2.76	120.26	111.83
20	B	823	CLA	C4-C3-C5	2.76	120.02	115.23
20	B	822	CLA	O2A-CGA-CBA	2.76	120.26	111.83
20	4	302	CLA	C4-C3-C5	2.76	120.02	115.23
20	3	304	CLA	C1C-NC-C4C	2.76	107.94	106.68
21	A	846	LMU	O3B-C3B-C2B	2.76	116.88	110.38
20	A	838	CLA	CHD-C4C-C3C	-2.76	120.75	124.77
21	1	217	LMU	O5'-C5'-C6'	2.76	113.28	106.44
21	K	101	LMU	O2'-C2'-C1'	-2.76	103.50	110.08
20	B	811	CLA	CMC-C2C-C1C	2.76	129.34	125.03
20	A	822	CLA	C4-C3-C5	2.76	120.02	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	833	CLA	C4-C3-C5	2.76	120.01	115.23
20	L	208	CLA	C3B-C2B-C1B	-2.76	103.92	107.17
20	L	208	CLA	CAA-C2A-C1A	2.75	121.00	111.97
20	3	320	CLA	CHB-C4A-NA	2.75	128.38	124.40
20	H	107	CLA	CMC-C2C-C1C	2.75	129.34	125.03
21	B	801	LMU	O3B-C3B-C2B	2.75	116.87	110.38
21	1	218	LMU	C6B-C5B-C4B	2.75	119.78	113.02
20	K	106	CLA	C2D-C1D-ND	-2.75	107.40	110.13
20	1	204	CLA	C4A-NA-C1A	2.75	107.94	106.68
20	B	805	CLA	C11-C12-C13	-2.75	106.81	115.97
20	4	312	CLA	CHD-C1D-ND	2.75	128.73	124.84
20	F	204	CLA	C3B-C4B-NB	-2.75	107.47	110.33
20	K	103	CLA	O2A-CGA-CBA	2.75	120.22	111.83
20	R	107	CLA	CHC-C1C-C2C	-2.75	119.13	126.95
20	A	850	CLA	CHC-C4B-C3B	-2.75	119.44	127.43
20	3	315	CLA	CAA-C2A-C3A	2.75	120.43	113.00
20	B	825	CLA	CHC-C1C-C2C	-2.75	119.13	126.95
20	A	850	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
20	3	315	CLA	CED-O2D-CGD	2.75	122.15	115.92
20	B	816	CLA	CAA-C2A-C1A	2.75	120.99	111.97
20	2	307	CLA	O2A-CGA-CBA	2.75	120.22	111.83
25	B	846	LMG	O8-C28-C29	2.75	120.22	111.83
20	A	836	CLA	C4-C3-C5	2.75	120.00	115.23
20	1	206	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
20	3	313	CLA	C2D-C3D-C4D	-2.75	104.01	107.35
20	1	212	CLA	CHC-C1C-C2C	-2.75	119.14	126.95
22	3	311	BCR	C36-C18-C17	-2.75	118.37	122.82
20	4	302	CLA	O2A-CGA-CBA	2.75	120.21	111.83
20	4	305	CLA	CMB-C2B-C1B	2.75	129.60	125.42
20	B	816	CLA	C4-C3-C5	2.75	119.99	115.23
20	1	210	CLA	C1B-C2B-C3B	-2.75	104.45	107.03
20	2	310	CLA	CHD-C4C-C3C	-2.75	120.77	124.77
21	B	802	LMU	C4B-C3B-C2B	-2.75	106.01	110.83
20	3	320	CLA	CHB-C1B-NB	-2.74	119.93	124.05
20	B	823	CLA	O2A-CGA-CBA	2.74	120.20	111.83
20	B	807	CLA	C4D-CHA-C1A	2.74	124.52	121.24
21	K	102	LMU	O6'-C6'-C5'	2.74	120.67	111.33
20	2	308	CLA	C3B-C2B-C1B	-2.74	103.76	106.81
20	1	214	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
20	2	301	CLA	O2A-CGA-CBA	2.74	120.19	111.83
21	H	105	LMU	O5'-C5'-C6'	2.74	113.23	106.44
20	K	107	CLA	C1-O2A-CGA	2.74	123.28	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	810	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
20	A	849	CLA	CHB-C1B-NB	-2.74	119.94	124.05
20	A	835	CLA	O2A-CGA-CBA	2.74	120.18	111.83
20	B	815	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
20	B	821	CLA	CMB-C2B-C1B	2.74	129.59	125.42
20	A	838	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
20	A	811	CLA	C3D-C4D-ND	2.74	114.43	109.99
21	K	101	LMU	C6'-C5'-C4'	-2.74	105.69	113.38
20	A	813	CLA	C1-O2A-CGA	2.73	123.27	116.65
21	4	322	LMU	C3B-C4B-C5B	2.73	115.19	110.23
20	A	834	CLA	O2A-CGA-CBA	2.73	120.17	111.83
20	A	855	CLA	O2A-CGA-CBA	2.73	120.17	111.83
20	J	102	CLA	O2A-CGA-CBA	2.73	120.17	111.83
20	B	847	CLA	C1D-ND-C4D	-2.73	104.39	106.31
20	H	101	CLA	C4A-NA-C1A	2.73	107.93	106.68
20	3	315	CLA	CHC-C4B-NB	2.73	128.15	124.05
20	A	833	CLA	O2A-CGA-CBA	2.73	120.17	111.83
20	A	837	CLA	C4-C3-C5	2.73	119.97	115.23
20	B	814	CLA	CHC-C4B-NB	2.73	128.15	124.05
20	A	832	CLA	O2A-CGA-CBA	2.73	120.17	111.83
20	A	812	CLA	C3B-C4B-NB	-2.73	108.09	110.53
20	2	306	CLA	CHC-C1C-C2C	-2.73	119.19	126.95
20	B	839	CLA	CMB-C2B-C1B	2.73	129.58	125.42
20	B	847	CLA	CHB-C1B-NB	-2.73	119.95	124.05
20	A	837	CLA	O2A-CGA-CBA	2.73	120.16	111.83
20	B	828	CLA	CMD-C2D-C3D	-2.73	121.43	127.69
20	A	822	CLA	O2A-CGA-CBA	2.73	120.15	111.83
20	4	318	CLA	C3B-C2B-C1B	-2.73	103.95	107.17
20	B	847	CLA	CMB-C2B-C1B	2.73	129.57	125.42
20	A	809	CLA	C3A-C2A-C1A	2.73	105.42	101.34
20	L	208	CLA	CMD-C2D-C3D	-2.73	121.44	127.69
20	A	813	CLA	C1-C2-C3	-2.73	122.35	126.76
20	H	101	CLA	O1D-CGD-CBD	-2.73	119.14	124.52
21	A	853	LMU	O5B-C5B-C6B	2.72	113.19	106.44
20	A	836	CLA	O2A-CGA-CBA	2.72	120.14	111.83
20	A	811	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
20	3	310	CLA	O2A-CGA-CBA	2.72	120.13	111.83
20	A	828	CLA	CHB-C4A-NA	2.72	128.33	124.40
21	R	105	LMU	O5'-C5'-C4'	2.72	115.35	109.72
20	1	203	CLA	CHC-C1C-NC	2.72	128.41	124.31
20	B	826	CLA	C2B-C1B-NB	2.72	113.14	110.33
20	B	808	CLA	O1D-CGD-CBD	-2.72	119.16	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	823	CLA	C4A-NA-C1A	2.72	107.92	106.68
20	A	811	CLA	CAA-CBA-CGA	-2.72	105.50	113.21
22	B	850	BCR	C36-C18-C17	-2.71	118.42	122.82
21	2	318	LMU	O3'-C3'-C4'	-2.71	102.98	109.94
20	1	201	CLA	C2D-C1D-ND	-2.71	107.44	110.13
20	R	107	CLA	CAA-CBA-CGA	2.71	120.91	113.21
20	B	828	CLA	O2A-CGA-CBA	2.71	120.11	111.83
20	F	204	CLA	CBD-CHA-C1A	2.71	131.47	127.38
20	3	308	CLA	CHB-C4A-NA	2.71	128.28	124.43
20	1	204	CLA	OBD-CAD-C3D	-2.71	122.09	128.42
20	2	321	CLA	O2A-CGA-O1A	-2.71	116.86	123.63
20	R	106	CLA	CHC-C1C-C2C	-2.71	119.26	126.95
20	A	817	CLA	CAA-C2A-C3A	-2.71	105.69	113.00
21	R	102	LMU	O1B-C1B-C2B	2.70	114.74	108.09
20	2	312	CLA	O1D-CGD-CBD	-2.70	119.18	124.52
20	B	811	CLA	CAC-C3C-C4C	2.70	128.31	124.79
20	B	838	CLA	CMA-C3A-C2A	-2.70	103.53	113.98
20	4	319	CLA	O2A-CGA-CBA	2.70	120.08	111.83
21	H	105	LMU	O2B-C2B-C3B	-2.70	104.00	110.38
20	L	201	CLA	CMB-C2B-C3B	2.70	132.91	126.55
20	3	313	CLA	CHB-C4A-NA	2.70	128.27	124.43
20	4	305	CLA	C1-O2A-CGA	2.70	123.19	116.65
20	B	809	CLA	CAC-C3C-C4C	2.70	128.30	124.79
20	B	810	CLA	C4A-NA-C1A	2.70	107.91	106.68
20	B	811	CLA	CED-O2D-CGD	2.70	122.04	115.92
20	1	204	CLA	C2A-C1A-CHA	-2.70	119.18	123.87
22	L	209	BCR	C8-C7-C6	-2.70	119.79	127.00
20	R	107	CLA	CHB-C1B-NB	-2.70	120.00	124.05
20	2	302	CLA	C3D-C4D-ND	2.70	114.37	109.99
22	L	209	BCR	C30-C25-C24	2.70	122.97	115.65
20	1	204	CLA	CHC-C1C-C2C	-2.70	119.28	126.95
20	F	204	CLA	CHC-C1C-C2C	-2.70	119.29	126.95
20	2	304	CLA	CHC-C4B-NB	2.70	128.09	124.05
20	J	103	CLA	CGD-CBD-CAD	-2.70	102.12	110.85
20	H	110	CLA	CHC-C1C-C2C	-2.70	119.29	126.95
20	1	214	CLA	CHA-C1A-NA	-2.69	120.29	126.39
20	3	308	CLA	CHA-C4D-ND	2.69	128.65	124.84
20	J	103	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
20	B	804	CLA	CBC-CAC-C3C	-2.69	105.12	112.42
20	1	211	CLA	C2A-C3A-C4A	2.69	106.22	101.87
20	B	821	CLA	CAC-C3C-C2C	-2.69	122.61	127.56
21	H	105	LMU	C1'-O5'-C5'	2.69	118.98	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	H	105	LMU	C1B-O5B-C5B	2.69	118.98	113.72
20	A	823	CLA	O2A-CGA-CBA	2.69	120.04	111.83
20	2	308	CLA	C2C-C1C-CHC	-2.69	118.79	125.84
20	B	803	CLA	C1D-ND-C4D	-2.69	104.42	106.31
20	A	838	CLA	CHB-C4A-NA	2.69	128.28	124.40
20	R	107	CLA	C2B-C1B-NB	2.69	113.11	110.33
20	A	829	CLA	CHB-C4A-NA	2.69	128.28	124.40
20	B	814	CLA	CED-O2D-CGD	2.69	122.01	115.92
20	2	303	CLA	C3C-C4C-CHD	-2.69	118.26	125.23
20	3	310	CLA	CHC-C1C-C2C	-2.69	119.32	126.95
20	1	211	CLA	CHB-C4A-NA	2.69	128.28	124.40
21	1	218	LMU	O2'-C2'-C1'	2.68	116.47	110.08
20	L	204	CLA	CMA-C3A-C4A	2.68	118.99	111.77
20	A	824	CLA	C6-C7-C8	-2.68	107.04	115.97
20	1	210	CLA	C4A-NA-C1A	2.68	107.90	106.68
20	I	102	CLA	CHB-C4A-NA	2.68	128.27	124.40
20	A	816	CLA	CMB-C2B-C1B	2.68	129.50	125.42
20	A	857	CLA	C2C-C1C-CHC	-2.68	118.81	125.84
20	2	308	CLA	CHB-C4A-NA	2.68	128.24	124.43
21	B	845	LMU	C3B-C4B-C5B	2.68	115.09	110.23
20	A	825	CLA	CMD-C2D-C3D	-2.68	121.54	127.69
20	4	315	CLA	C1D-ND-C4D	-2.68	104.43	106.31
20	1	214	CLA	CHA-C4D-ND	2.68	138.07	132.55
20	B	817	CLA	CHC-C1C-C2C	-2.68	119.34	126.95
20	1	203	CLA	CAC-C3C-C4C	2.68	128.27	124.79
22	F	203	BCR	C39-C30-C25	2.68	114.44	110.24
21	L	206	LMU	C1B-C2B-C3B	-2.68	104.38	110.01
20	2	315	CLA	C3C-C4C-CHD	-2.68	118.28	125.23
21	B	802	LMU	O2B-C2B-C1B	2.68	116.45	110.08
21	A	854	LMU	O5'-C5'-C4'	-2.68	104.19	109.72
20	3	301	CLA	C2A-C1A-CHA	-2.68	119.22	123.87
20	3	315	CLA	CHC-C1C-C2C	-2.68	119.34	126.95
20	B	830	CLA	C3A-C2A-C1A	2.67	105.34	101.34
20	L	202	CLA	CHB-C1B-NB	-2.67	120.04	124.05
20	F	205	CLA	CHC-C1C-C2C	-2.67	119.35	126.95
20	K	106	CLA	C5-C3-C4	2.67	120.74	114.59
20	B	827	CLA	C1-C2-C3	-2.67	122.44	126.76
20	B	808	CLA	CHC-C1C-C2C	-2.67	119.35	126.95
20	A	807	CLA	C2D-C1D-ND	-2.67	107.48	110.13
20	H	109	CLA	C1D-ND-C4D	-2.67	104.44	106.31
20	L	202	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
20	3	320	CLA	CHC-C1C-C2C	-2.67	119.36	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	321	CLA	C11-C12-C13	-2.67	107.09	115.97
20	K	103	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
20	B	826	CLA	C7-C6-C5	-2.67	106.15	113.26
20	2	305	CLA	C3C-C4C-CHD	-2.67	118.30	125.23
20	3	309	CLA	CAA-C2A-C1A	-2.67	103.23	111.97
20	4	303	CLA	CHC-C4B-NB	2.67	128.05	124.05
20	3	319	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
20	A	804	CLA	CAA-C2A-C1A	-2.67	103.23	111.97
20	G	103	CLA	C2A-C1A-CHA	-2.67	119.24	123.87
21	H	105	LMU	C3'-C4'-C5'	-2.67	105.02	110.93
20	A	833	CLA	C4A-NA-C1A	2.67	107.90	106.68
20	K	103	CLA	C4A-NA-C1A	2.67	107.90	106.68
21	4	301	LMU	C1B-O1B-C4'	-2.67	111.66	117.98
20	B	822	CLA	CHC-C1C-C2C	-2.67	119.37	126.95
21	1	218	LMU	C4B-C3B-C2B	2.67	115.51	110.83
20	1	211	CLA	C3A-C2A-C1A	-2.67	97.35	101.34
20	B	828	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
20	B	823	CLA	CHC-C1C-C2C	-2.66	119.38	126.95
20	2	302	CLA	CHC-C1C-C2C	-2.66	119.38	126.95
20	2	304	CLA	CHB-C4A-NA	2.66	128.25	124.40
20	B	839	CLA	CHB-C4A-NA	2.66	128.25	124.40
20	A	823	CLA	CHC-C1C-C2C	-2.66	119.38	126.95
20	4	304	CLA	C1D-ND-C4D	-2.66	104.44	106.31
21	1	218	LMU	O5'-C5'-C6'	2.66	113.04	106.44
22	B	844	BCR	C23-C24-C25	-2.66	119.88	127.00
20	3	313	CLA	C3C-C4C-CHD	-2.66	118.31	125.23
20	3	307	CLA	C2C-C1C-CHC	-2.66	118.86	125.84
20	2	307	CLA	CHB-C1B-NB	-2.66	120.06	124.05
20	A	850	CLA	CMA-C3A-C4A	2.66	118.92	111.77
20	K	107	CLA	C6-C7-C8	-2.66	107.12	115.97
22	F	203	BCR	C32-C1-C6	-2.66	106.07	110.24
20	A	828	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
20	A	819	CLA	CHB-C1B-NB	-2.66	120.06	124.05
20	1	215	CLA	C2C-C1C-CHC	-2.66	118.87	125.84
22	B	843	BCR	C3-C4-C5	-2.66	109.32	114.06
20	A	802	CLA	CHC-C1C-C2C	-2.66	119.40	126.95
20	4	304	CLA	CHA-C1A-NA	-2.66	120.38	126.39
20	2	314	CLA	CHC-C4B-NB	2.65	127.92	124.08
20	A	833	CLA	CHC-C1C-C2C	-2.65	119.40	126.95
20	L	202	CLA	CMC-C2C-C1C	2.65	129.18	125.03
20	A	855	CLA	CHC-C1C-C2C	-2.65	119.41	126.95
22	B	842	BCR	C39-C30-C25	-2.65	106.08	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	2	316	LMU	C1B-O1B-C4'	-2.65	111.69	117.98
21	L	206	LMU	O4'-C4B-C5B	-2.65	102.79	109.32
20	1	206	CLA	C1D-ND-C4D	-2.65	104.45	106.31
20	1	206	CLA	C4A-NA-C1A	2.65	107.89	106.68
20	A	822	CLA	C4A-NA-C1A	2.65	107.89	106.68
20	A	805	CLA	O1D-CGD-CBD	-2.65	119.29	124.52
20	A	834	CLA	CHC-C1C-C2C	-2.65	119.41	126.95
20	4	311	CLA	CHB-C4A-NA	2.65	128.20	124.43
20	1	207	CLA	O2A-CGA-CBA	2.65	119.92	111.83
20	3	303	CLA	CHC-C4B-NB	2.65	128.02	124.05
20	A	824	CLA	O2A-CGA-O1A	-2.65	117.00	123.63
20	F	204	CLA	CAB-C3B-C4B	-2.65	121.39	125.42
20	A	847	CLA	CHC-C1C-NC	2.65	128.30	124.31
22	B	841	BCR	C23-C24-C25	-2.65	119.92	127.00
20	K	105	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
20	A	831	CLA	CHC-C1C-C2C	-2.65	119.43	126.95
20	2	302	CLA	CAC-C3C-C4C	2.65	128.23	124.79
20	A	808	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
20	A	849	CLA	CGD-CBD-CAD	2.65	119.41	110.85
20	4	317	CLA	C2C-C1C-CHC	-2.64	118.91	125.84
20	2	302	CLA	CHC-C4B-NB	2.64	128.01	124.05
20	A	832	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
20	B	805	CLA	CBC-CAC-C3C	-2.64	105.25	112.42
21	L	206	LMU	C3B-C4B-C5B	-2.64	105.44	110.23
20	A	835	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
20	A	837	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
21	4	320	LMU	C1B-O1B-C4'	-2.64	111.72	117.98
20	B	817	CLA	C3D-C4D-ND	2.64	114.28	109.99
20	4	318	CLA	C1D-ND-C4D	-2.64	104.46	106.31
21	2	318	LMU	C3'-C4'-C5'	2.64	116.78	110.93
20	3	309	CLA	CAC-C3C-C2C	2.64	132.41	127.56
20	A	812	CLA	CHC-C4B-NB	2.64	128.01	124.05
20	A	818	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
20	B	839	CLA	CMC-C2C-C1C	2.64	129.16	125.03
21	K	102	LMU	C3B-C4B-C5B	-2.64	105.45	110.23
20	2	301	CLA	CHC-C1C-C2C	-2.64	119.45	126.95
20	A	836	CLA	CHC-C1C-C2C	-2.64	119.45	126.95
20	B	848	CLA	CMC-C2C-C1C	2.64	129.16	125.03
20	2	303	CLA	C2C-C1C-CHC	-2.64	118.93	125.84
20	A	822	CLA	CHC-C1C-C2C	-2.64	119.45	126.95
22	G	102	BCR	C8-C7-C6	-2.64	119.95	127.00
20	B	823	CLA	C4A-NA-C1A	2.64	107.88	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	302	CLA	CHC-C1C-C2C	-2.64	119.45	126.95
22	I	101	BCR	C40-C30-C25	2.64	114.38	110.24
20	L	203	CLA	C2B-C1B-NB	2.64	113.06	110.33
20	4	309	CLA	C2C-C1C-CHC	-2.64	118.94	125.84
22	A	842	BCR	C23-C24-C25	-2.63	119.96	127.00
21	B	801	LMU	O1B-C1B-C2B	2.63	114.57	108.09
21	L	210	LMU	O3B-C3B-C2B	-2.63	104.17	110.38
20	2	317	CLA	C4-C3-C5	2.63	119.80	115.23
20	A	811	CLA	C1D-ND-C4D	-2.63	104.46	106.31
20	4	302	CLA	C4A-NA-C1A	2.63	107.88	106.68
20	L	203	CLA	C4-C3-C2	-2.63	116.87	123.63
22	A	842	BCR	C8-C7-C6	-2.63	119.97	127.00
20	A	808	CLA	C3D-C4D-ND	2.63	114.26	109.99
20	3	305	CLA	CHA-C4D-ND	2.63	128.56	124.84
21	B	801	LMU	O3'-C3'-C2'	2.63	116.57	110.38
22	G	102	BCR	C3-C4-C5	-2.63	109.37	114.06
20	4	311	CLA	C2C-C1C-CHC	-2.63	118.95	125.84
20	1	211	CLA	CMB-C2B-C3B	-2.63	120.37	126.55
22	B	844	BCR	C8-C7-C6	-2.63	119.98	127.00
20	A	818	CLA	C4A-NA-C1A	2.63	107.88	106.68
20	B	829	CLA	C4A-NA-C1A	2.63	107.88	106.68
21	A	853	LMU	C8-C7-C6	-2.63	101.09	114.37
20	H	110	CLA	CGD-CBD-CAD	-2.63	102.35	110.85
21	A	851	LMU	C1B-O1B-C4'	-2.63	111.75	117.98
20	3	320	CLA	C1-C2-C3	-2.62	121.90	126.20
20	B	849	CLA	CMB-C2B-C1B	2.62	129.41	125.42
22	A	841	BCR	C8-C7-C6	-2.62	119.99	127.00
20	B	815	CLA	CHC-C4B-NB	2.62	127.98	124.05
20	1	208	CLA	C3C-C4C-CHD	-2.62	118.42	125.23
20	1	201	CLA	CMA-C3A-C2A	2.62	124.12	113.98
20	B	815	CLA	O2A-C1-C2	2.62	118.19	108.11
22	A	840	BCR	C23-C24-C25	-2.62	120.00	127.00
20	3	309	CLA	CMD-C2D-C3D	-2.62	121.68	127.69
20	4	303	CLA	CHB-C4A-NA	2.62	128.18	124.40
22	A	843	BCR	C23-C24-C25	-2.62	120.00	127.00
20	A	814	CLA	CHC-C1C-C2C	-2.62	119.50	126.95
21	A	853	LMU	C4B-C3B-C2B	-2.62	106.23	110.83
21	K	104	LMU	O3B-C3B-C2B	2.62	116.55	110.38
20	B	811	CLA	CHC-C1C-C2C	-2.62	119.51	126.95
20	A	801	CLA	O2A-CGA-CBA	2.62	119.82	111.83
22	B	843	BCR	C23-C24-C25	-2.62	120.00	127.00
20	4	319	CLA	CHC-C1C-C2C	-2.62	119.51	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	3	316	CLA	C2C-C1C-CHC	-2.62	118.98	125.84
21	H	104	LMU	O6'-C6'-C5'	-2.62	102.42	111.33
22	F	203	BCR	C7-C8-C9	2.62	130.11	126.23
20	4	313	CLA	CHB-C1B-NB	-2.62	120.12	124.05
22	F	203	BCR	C24-C25-C26	2.62	127.58	121.56
20	R	106	CLA	C3B-C2B-C1B	-2.62	104.09	107.17
22	F	202	BCR	C23-C24-C25	-2.62	120.01	127.00
22	B	850	BCR	C19-C18-C17	-2.62	114.89	119.01
20	A	821	CLA	CHC-C1C-C2C	-2.62	119.52	126.95
22	J	101	BCR	C8-C7-C6	-2.61	120.01	127.00
20	B	839	CLA	CHC-C4B-C3B	-2.61	119.84	127.43
20	B	812	CLA	CHB-C4A-NA	2.61	128.17	124.40
20	H	108	CLA	C4-C3-C2	-2.61	116.91	123.63
22	B	843	BCR	C8-C7-C6	-2.61	120.02	127.00
22	A	840	BCR	C8-C7-C6	-2.61	120.02	127.00
22	A	844	BCR	C23-C24-C25	-2.61	120.02	127.00
23	A	839	PQN	C2M-C2-C1	2.61	121.48	116.68
20	4	310	CLA	O1D-CGD-CBD	-2.61	119.37	124.52
20	4	305	CLA	O2A-CGA-CBA	2.61	119.80	111.83
20	4	318	CLA	CED-O2D-CGD	2.61	121.84	115.92
22	A	843	BCR	C8-C7-C6	-2.61	120.03	127.00
20	H	108	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
21	1	216	LMU	C1B-O1B-C4'	-2.61	111.79	117.98
20	4	306	CLA	CHC-C4B-NB	2.61	127.96	124.05
20	K	105	CLA	C4A-NA-C1A	2.61	107.87	106.68
20	4	313	CLA	CAC-C3C-C2C	-2.61	121.33	126.75
20	B	811	CLA	O2A-CGA-CBA	2.61	119.79	111.83
20	4	311	CLA	C3C-C4C-CHD	-2.61	118.46	125.23
21	A	853	LMU	O5'-C5'-C6'	-2.61	99.98	106.44
20	B	833	CLA	CMB-C2B-C1B	2.61	129.39	125.42
20	2	305	CLA	C3D-C2D-C1D	2.61	110.51	107.35
20	2	312	CLA	CAC-C3C-C4C	2.61	128.18	124.79
20	2	312	CLA	C2B-C1B-NB	2.61	113.03	110.33
20	A	831	CLA	C4A-NA-C1A	2.61	107.87	106.68
20	1	213	CLA	C3D-C4D-ND	2.60	113.06	109.50
20	B	834	CLA	CHC-C1C-C2C	-2.60	119.55	126.95
20	J	102	CLA	CHC-C1C-C2C	-2.60	119.55	126.95
20	A	808	CLA	CHC-C1C-C2C	-2.60	119.55	126.95
22	F	202	BCR	C28-C27-C26	-2.60	109.41	114.06
20	B	807	CLA	CHC-C1C-C2C	-2.60	119.55	126.95
21	H	102	LMU	C4B-C3B-C2B	-2.60	106.26	110.83
21	H	105	LMU	O1B-C1B-C2B	2.60	114.49	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	R	108	LMU	C1B-O1B-C4'	-2.60	111.81	117.98
20	3	317	CLA	CHB-C4A-NA	2.60	128.13	124.43
22	A	844	BCR	C8-C7-C6	-2.60	120.05	127.00
20	4	306	CLA	CED-O2D-CGD	2.60	121.81	115.92
20	A	830	CLA	O2A-CGA-CBA	2.60	119.76	111.83
20	B	817	CLA	CMA-C3A-C2A	-2.60	103.93	113.98
20	3	314	CLA	CHB-C4A-NA	2.60	128.15	124.40
21	L	210	LMU	C1B-O1B-C4'	-2.60	111.82	117.98
20	A	816	CLA	CHC-C1C-C2C	-2.60	119.56	126.95
22	B	842	BCR	C32-C1-C6	2.60	114.32	110.24
22	F	202	BCR	C3-C4-C5	-2.60	109.42	114.06
20	1	213	CLA	C2C-C1C-CHC	-2.60	119.04	125.84
20	2	315	CLA	C2C-C1C-CHC	-2.60	119.04	125.84
20	A	812	CLA	C1D-ND-C4D	-2.60	104.49	106.31
22	J	101	BCR	C23-C24-C25	-2.59	120.07	127.00
20	4	308	CLA	C2C-C1C-CHC	-2.59	119.05	125.84
21	R	103	LMU	O4'-C4B-C5B	2.59	115.71	109.32
20	3	317	CLA	C3C-C4C-CHD	-2.59	118.50	125.23
20	H	101	CLA	CHC-C4B-NB	2.59	127.93	124.05
20	A	855	CLA	C4A-NA-C1A	2.59	107.86	106.68
20	A	812	CLA	C3D-C4D-ND	2.59	114.19	109.99
20	B	847	CLA	CGD-CBD-CAD	2.59	119.22	110.85
21	L	210	LMU	O3'-C3'-C4'	-2.59	103.31	109.94
22	F	202	BCR	C8-C7-C6	-2.59	120.09	127.00
20	3	304	CLA	C3C-C4C-CHD	-2.59	118.51	125.23
20	B	835	CLA	CHB-C1B-NB	-2.59	120.17	124.05
22	I	103	BCR	C23-C22-C21	2.59	123.08	119.01
22	A	840	BCR	C28-C27-C26	-2.59	109.44	114.06
20	2	301	CLA	C2A-C1A-CHA	-2.59	119.38	123.87
22	A	843	BCR	C3-C4-C5	-2.58	109.45	114.06
20	3	314	CLA	C3D-C4D-ND	2.58	114.19	109.99
20	B	808	CLA	CHC-C4B-NB	2.58	127.92	124.05
21	A	854	LMU	C2'-C3'-C4'	-2.58	103.82	109.68
20	3	308	CLA	C4C-CHD-C1D	-2.58	118.62	125.98
20	B	823	CLA	C2A-C1A-CHA	-2.58	119.39	123.87
20	A	801	CLA	C5-C3-C4	2.58	120.53	114.59
20	2	307	CLA	CHB-C4A-NA	2.58	128.12	124.40
21	3	318	LMU	C1B-O1B-C4'	-2.58	111.86	117.98
22	B	841	BCR	C8-C7-C6	-2.58	120.11	127.00
22	G	102	BCR	C28-C27-C26	-2.58	109.46	114.06
21	H	102	LMU	O3'-C3'-C2'	2.58	116.46	110.38
22	I	101	BCR	C34-C9-C8	-2.58	114.15	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	E	101	LMU	O2B-C2B-C3B	-2.58	104.30	110.38
20	B	812	CLA	CED-O2D-CGD	2.58	121.76	115.92
22	G	102	BCR	C23-C24-C25	-2.58	120.11	127.00
20	A	814	CLA	CHB-C4A-NA	2.58	128.12	124.40
20	L	207	CLA	CAC-C3C-C4C	2.58	128.14	124.79
20	B	837	CLA	C1-C2-C3	-2.58	121.98	126.20
20	4	308	CLA	C3D-C4D-ND	2.58	113.02	109.50
20	2	321	CLA	CED-O2D-CGD	2.58	121.76	115.92
20	1	206	CLA	CHB-C1B-NB	-2.58	120.19	124.05
23	B	840	PQN	C11-C3-C2	-2.57	120.48	124.89
20	A	813	CLA	CAA-C2A-C3A	-2.57	106.04	113.00
22	J	101	BCR	C28-C27-C26	-2.57	109.47	114.06
20	A	832	CLA	C4A-NA-C1A	2.57	107.85	106.68
20	A	823	CLA	C2A-C1A-CHA	-2.57	119.40	123.87
20	L	201	CLA	O2A-CGA-O1A	-2.57	117.19	123.63
20	A	812	CLA	CED-O2D-CGD	2.57	121.75	115.92
20	L	204	CLA	CHC-C1C-NC	2.57	128.18	124.31
20	A	821	CLA	C4A-NA-C1A	2.57	107.85	106.68
20	A	836	CLA	C4A-NA-C1A	2.57	107.85	106.68
20	B	820	CLA	CHB-C1B-NB	-2.57	120.19	124.05
20	B	820	CLA	C3B-C4B-NB	-2.57	108.23	110.53
20	2	309	CLA	C3C-C4C-CHD	-2.57	118.56	125.23
21	L	206	LMU	O5'-C5'-C6'	-2.57	100.07	106.44
20	G	103	CLA	C3D-C4D-ND	2.57	114.16	109.99
20	3	317	CLA	C2D-C3D-C4D	-2.57	104.23	107.35
22	B	850	BCR	C2-C1-C6	2.57	114.17	110.44
22	A	841	BCR	C23-C24-C25	-2.57	120.14	127.00
20	1	209	CLA	CHC-C4B-C3B	-2.57	119.97	127.43
20	2	304	CLA	CHC-C1C-C2C	-2.57	119.65	126.95
20	H	107	CLA	CHC-C1C-C2C	-2.57	119.65	126.95
20	B	825	CLA	C3B-C4B-NB	-2.57	108.24	110.53
21	R	109	LMU	O5B-C5B-C6B	2.57	112.80	106.44
20	A	831	CLA	C2A-C1A-CHA	-2.57	119.41	123.87
20	B	847	CLA	C12-C11-C10	-2.56	101.78	113.28
21	H	103	LMU	O5B-C5B-C4B	-2.56	105.08	109.70
22	I	101	BCR	C20-C19-C18	2.56	133.40	126.36
22	A	841	BCR	C3-C4-C5	-2.56	109.48	114.06
22	B	841	BCR	C28-C27-C26	-2.56	109.48	114.06
20	J	102	CLA	C2A-C1A-CHA	-2.56	119.42	123.87
20	A	833	CLA	C2A-C1A-CHA	-2.56	119.42	123.87
20	4	304	CLA	C3C-C4C-NC	-2.56	107.15	110.43
22	B	841	BCR	C3-C4-C5	-2.56	109.49	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	850	BCR	C11-C10-C9	2.56	130.87	127.28
20	A	805	CLA	C3D-C4D-ND	2.56	114.15	109.99
20	H	101	CLA	CGD-CBD-CAD	2.56	119.13	110.85
20	2	302	CLA	CHB-C4A-NA	2.56	128.09	124.40
22	B	844	BCR	C3-C4-C5	-2.56	109.50	114.06
20	L	208	CLA	O2A-CGA-CBA	2.56	119.63	111.83
20	4	313	CLA	CHC-C4B-C3B	-2.56	120.01	127.43
21	H	103	LMU	O3'-C3'-C4'	-2.56	103.39	109.94
20	H	107	CLA	C1-C2-C3	2.56	130.38	126.20
20	A	850	CLA	CHB-C4A-NA	2.56	128.09	124.40
20	2	321	CLA	O1D-CGD-CBD	-2.56	119.48	124.52
20	B	847	CLA	C3B-C4B-NB	-2.56	108.25	110.53
21	G	101	LMU	O3B-C3B-C2B	-2.55	104.35	110.38
20	B	837	CLA	CHC-C1C-C2C	-2.55	119.69	126.95
20	L	208	CLA	C1-C2-C3	-2.55	122.63	126.76
20	A	836	CLA	C2A-C1A-CHA	-2.55	119.44	123.87
20	K	103	CLA	C2A-C1A-CHA	-2.55	119.44	123.87
20	4	307	CLA	CMA-C3A-C4A	-2.55	104.92	111.77
20	F	205	CLA	C2A-C1A-CHA	-2.55	119.44	123.86
21	A	853	LMU	C1-O1'-C1'	-2.55	109.32	113.68
20	B	807	CLA	CHB-C4A-NA	2.55	128.08	124.40
20	3	310	CLA	C2A-C1A-CHA	-2.55	119.44	123.87
20	A	829	CLA	C2D-C1D-ND	-2.55	107.60	110.13
20	I	102	CLA	CHC-C1C-C2C	-2.55	119.70	126.95
20	G	103	CLA	O2A-CGA-CBA	2.55	119.61	111.83
21	3	302	LMU	C1B-O1B-C4'	-2.55	111.94	117.98
20	K	105	CLA	C2A-C1A-CHA	-2.55	119.44	123.87
20	2	303	CLA	CHB-C4A-NA	2.55	128.05	124.43
20	B	804	CLA	C1-C2-C3	2.55	130.37	126.20
20	B	822	CLA	C2A-C1A-CHA	-2.55	119.45	123.87
20	B	831	CLA	O2A-CGA-CBA	2.55	122.05	114.00
21	A	854	LMU	O5'-C5'-C6'	2.55	112.75	106.44
20	B	839	CLA	CHB-C1B-NB	-2.55	120.23	124.05
20	3	312	CLA	C3D-C4D-ND	2.55	112.98	109.50
20	A	826	CLA	CHC-C1C-C2C	-2.55	119.71	126.95
20	4	314	CLA	C3C-C4C-CHD	-2.55	118.62	125.23
21	B	801	LMU	C4B-C3B-C2B	-2.55	106.36	110.83
20	A	857	CLA	CHB-C1B-NB	-2.54	120.40	124.08
20	2	305	CLA	C4D-ND-C1D	-2.54	104.53	106.31
20	A	837	CLA	C2A-C1A-CHA	-2.54	119.45	123.87
20	A	815	CLA	C3D-C4D-ND	2.54	114.12	109.99
21	2	318	LMU	O5'-C5'-C6'	2.54	112.74	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	L	205	LMU	O2B-C2B-C3B	2.54	116.37	110.38
22	A	844	BCR	C3-C4-C5	-2.54	109.52	114.06
22	A	844	BCR	C28-C27-C26	-2.54	109.52	114.06
22	B	843	BCR	C28-C27-C26	-2.54	109.52	114.06
20	L	208	CLA	CHC-C4B-NB	2.54	127.86	124.05
20	B	833	CLA	O2A-CGA-CBA	2.54	119.58	111.83
20	4	307	CLA	C1D-ND-C4D	-2.54	104.53	106.31
20	A	822	CLA	C2A-C1A-CHA	-2.54	119.46	123.87
21	A	854	LMU	O1B-C4'-C5'	2.54	116.14	109.48
20	A	835	CLA	C2A-C1A-CHA	-2.54	119.46	123.87
20	A	848	CLA	CHC-C1C-C2C	-2.54	119.73	126.95
20	2	307	CLA	C1-O2A-CGA	2.54	122.80	116.65
20	A	855	CLA	C2A-C1A-CHA	-2.54	119.46	123.87
20	L	203	CLA	CMB-C2B-C1B	2.54	129.28	125.42
20	B	821	CLA	CMC-C2C-C1C	2.54	129.00	125.03
20	2	306	CLA	C1-C2-C3	-2.54	122.04	126.20
20	R	107	CLA	CED-O2D-CGD	2.54	121.67	115.92
20	B	812	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
20	H	110	CLA	C1-O2A-CGA	2.54	122.79	116.65
20	F	205	CLA	C4A-NA-C1A	2.54	107.84	106.68
20	A	829	CLA	CAA-C2A-C3A	-2.54	106.15	113.00
25	B	846	LMG	C8-O7-C10	-2.53	111.73	117.80
21	C	101	LMU	O5B-C5B-C4B	-2.53	105.13	109.70
20	4	310	CLA	C3D-C4D-ND	2.53	114.11	109.99
20	2	312	CLA	C4-C3-C5	2.53	119.63	115.23
20	4	310	CLA	C2A-C1A-CHA	-2.53	119.47	123.87
20	3	303	CLA	CHC-C1C-C2C	-2.53	119.75	126.95
20	B	836	CLA	CHC-C1C-C2C	-2.53	119.75	126.95
20	A	814	CLA	C2A-C1A-CHA	-2.53	119.47	123.87
20	A	834	CLA	C2A-C1A-CHA	-2.53	119.47	123.87
20	J	103	CLA	C3B-C2B-C1B	-2.53	104.18	107.17
20	A	837	CLA	C4A-NA-C1A	2.53	107.83	106.68
22	L	209	BCR	C33-C5-C4	2.53	118.99	113.60
20	K	106	CLA	C4D-CHA-C1A	-2.53	118.22	121.24
20	A	832	CLA	C2A-C1A-CHA	-2.53	119.47	123.87
20	3	319	CLA	CHC-C4B-C3B	-2.53	120.08	127.43
22	A	842	BCR	C3-C4-C5	-2.53	109.54	114.06
20	3	314	CLA	CAC-C3C-C2C	-2.53	122.91	127.56
22	F	203	BCR	C33-C5-C4	2.53	118.99	113.60
20	2	321	CLA	CAC-C3C-C2C	-2.53	122.91	127.56
22	3	311	BCR	C8-C7-C6	-2.53	120.25	127.00
20	B	833	CLA	O2D-CGD-O1D	-2.53	118.93	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	1	203	CLA	CHB-C4A-NA	2.53	128.05	124.40
20	K	107	CLA	CMC-C2C-C1C	2.53	128.98	125.03
20	3	312	CLA	C2C-C1C-CHC	-2.53	119.22	125.84
20	1	201	CLA	CHB-C1B-NB	-2.53	120.26	124.05
20	B	813	CLA	CAC-C3C-C4C	2.53	128.08	124.79
20	1	211	CLA	C6-C5-C3	-2.53	101.72	113.70
22	A	843	BCR	C28-C27-C26	-2.52	109.55	114.06
20	B	810	CLA	CBA-CAA-C2A	-2.52	106.28	113.79
22	F	203	BCR	C35-C13-C12	2.52	121.94	118.09
20	B	803	CLA	C3D-C4D-ND	2.52	114.09	109.99
20	A	815	CLA	CMB-C2B-C1B	2.52	129.26	125.42
20	A	826	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
20	L	201	CLA	CHC-C1C-C2C	-2.52	119.78	126.95
20	3	306	CLA	CHA-C4D-ND	2.52	128.40	124.84
21	4	322	LMU	O2B-C2B-C3B	-2.52	104.43	110.38
20	H	101	CLA	C3B-C2B-C1B	-2.52	104.20	107.17
20	A	815	CLA	CHB-C4A-NA	2.52	128.03	124.40
22	B	850	BCR	C32-C1-C31	-2.52	101.42	108.63
20	B	815	CLA	CHB-C1B-NB	-2.52	120.27	124.05
20	4	319	CLA	C4A-NA-C1A	2.52	107.83	106.68
22	B	842	BCR	C1-C6-C7	2.52	122.47	115.65
20	A	803	CLA	C6-C7-C8	-2.52	107.61	115.97
20	B	829	CLA	C3A-C2A-C1A	2.51	105.11	101.34
20	3	309	CLA	C3B-C2B-C1B	-2.51	104.21	107.17
20	B	831	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
22	A	841	BCR	C28-C27-C26	-2.51	109.57	114.06
20	B	834	CLA	O2A-CGA-CBA	2.51	119.50	111.83
22	A	842	BCR	C28-C27-C26	-2.51	109.58	114.06
20	B	815	CLA	CMD-C2D-C3D	-2.51	121.93	127.69
20	A	821	CLA	C4-C3-C2	-2.51	117.18	123.63
20	4	314	CLA	C1B-NB-C4B	-2.51	104.55	106.31
22	F	203	BCR	C12-C13-C14	2.51	122.96	119.01
20	A	825	CLA	O2A-CGA-CBA	2.51	119.49	111.83
20	B	832	CLA	C1D-ND-C4D	-2.51	104.55	106.31
20	L	204	CLA	C4A-NA-C1A	-2.51	105.53	106.68
22	A	840	BCR	C3-C4-C5	-2.51	109.58	114.06
20	1	208	CLA	C2C-C1C-CHC	-2.51	119.27	125.84
20	A	848	CLA	O2A-C1-C2	2.51	117.76	108.11
21	K	102	LMU	C1-O1'-C1'	-2.51	109.39	113.68
20	B	809	CLA	CMB-C2B-C1B	2.51	129.24	125.42
20	K	107	CLA	C4-C3-C2	-2.51	117.19	123.63
22	I	101	BCR	C8-C9-C10	2.51	122.95	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	806	CLA	CAA-CBA-CGA	2.51	120.33	113.21
22	B	844	BCR	C28-C27-C26	-2.51	109.59	114.06
20	3	314	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
20	4	315	CLA	CHB-C1B-NB	-2.51	120.29	124.05
20	B	804	CLA	CHB-C1B-NB	-2.51	120.29	124.05
20	A	815	CLA	C1D-ND-C4D	-2.51	104.55	106.31
20	K	106	CLA	C3B-C2B-C1B	-2.51	104.22	107.17
20	A	825	CLA	CGD-CBD-CAD	2.50	118.95	110.85
20	4	303	CLA	C4A-NA-C1A	2.50	107.82	106.68
20	J	102	CLA	C4A-NA-C1A	2.50	107.82	106.68
20	4	319	CLA	C2A-C1A-CHA	-2.50	119.52	123.87
20	B	832	CLA	CHC-C1C-C2C	-2.50	119.83	126.95
20	A	802	CLA	C1D-ND-C4D	-2.50	104.56	106.31
20	B	837	CLA	CHB-C4A-NA	2.50	128.01	124.40
20	A	806	CLA	CAA-C2A-C3A	-2.50	106.24	113.00
20	B	847	CLA	CAC-C3C-C4C	2.50	128.04	124.79
20	A	802	CLA	O2A-CGA-O1A	-2.50	117.37	123.63
20	A	857	CLA	C3C-C4C-CHD	-2.50	118.74	125.23
20	4	302	CLA	C2A-C1A-CHA	-2.50	119.53	123.87
20	B	806	CLA	CAC-C3C-C4C	2.50	128.04	124.79
20	3	319	CLA	CHB-C4A-NA	2.50	128.01	124.40
20	3	314	CLA	CED-O2D-CGD	2.50	121.58	115.92
20	B	810	CLA	C3B-C2B-C1B	-2.50	104.22	107.17
20	1	205	CLA	CMA-C3A-C2A	-2.50	110.50	116.23
20	4	306	CLA	CAC-C3C-C4C	2.50	128.04	124.79
20	A	849	CLA	O2A-CGA-CBA	2.50	119.45	111.83
20	3	301	CLA	C3D-C4D-ND	2.50	114.04	109.99
20	A	805	CLA	CBC-CAC-C3C	-2.50	105.66	112.42
20	B	810	CLA	C11-C10-C8	-2.50	107.67	115.97
20	H	109	CLA	C1-O2A-CGA	2.49	122.69	116.65
20	3	313	CLA	C2C-C1C-CHC	-2.49	119.31	125.84
20	1	212	CLA	C6-C7-C8	-2.49	107.68	115.97
21	G	101	LMU	C1'-O5'-C5'	2.49	118.59	113.72
20	3	303	CLA	CHB-C4A-NA	2.49	128.00	124.40
20	A	824	CLA	C11-C10-C8	-2.49	107.68	115.97
20	B	827	CLA	CHD-C4C-C3C	-2.49	121.14	124.77
21	B	845	LMU	O1B-C4'-C3'	2.49	113.56	107.23
20	A	806	CLA	CHC-C1C-C2C	-2.49	119.87	126.95
20	2	311	CLA	CMD-C2D-C3D	-2.49	121.98	127.69
20	2	302	CLA	CAA-C2A-C1A	-2.49	103.81	111.97
20	B	822	CLA	C4A-NA-C1A	2.49	107.81	106.68
20	A	819	CLA	CHB-C4A-NA	2.49	127.99	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	J	101	BCR	C3-C4-C5	-2.49	109.62	114.06
20	L	208	CLA	CAA-CBA-CGA	-2.49	106.15	113.21
22	3	311	BCR	C35-C13-C12	2.49	121.89	118.09
20	L	203	CLA	CHB-C1B-NB	-2.48	120.32	124.05
20	1	211	CLA	C3D-C2D-C1D	-2.48	102.44	105.83
20	1	209	CLA	C3D-C4D-ND	2.48	114.02	109.99
20	A	816	CLA	C1-O2A-CGA	2.48	122.66	116.65
20	B	827	CLA	C2D-C1D-ND	-2.48	107.67	110.13
20	A	847	CLA	C2A-C1A-CHA	-2.48	119.56	123.87
20	2	305	CLA	CHB-C4A-NA	2.48	127.96	124.43
20	A	834	CLA	C4A-NA-C1A	2.48	107.81	106.68
20	R	106	CLA	C4-C3-C2	-2.48	117.25	123.63
20	4	312	CLA	CHB-C4A-NA	2.48	127.96	124.43
21	K	104	LMU	O2'-C2'-C3'	-2.48	104.53	110.38
21	R	103	LMU	O5'-C5'-C4'	2.48	114.85	109.72
20	A	814	CLA	CBC-CAC-C3C	-2.48	105.70	112.42
20	1	214	CLA	C3B-C2B-C1B	-2.48	104.25	107.17
20	K	107	CLA	CHB-C4A-NA	2.48	127.98	124.40
20	B	830	CLA	C1D-ND-C4D	-2.48	104.57	106.31
20	B	847	CLA	C11-C10-C8	-2.48	107.73	115.97
20	B	816	CLA	O2A-CGA-CBA	2.48	119.38	111.83
20	B	818	CLA	CHC-C1C-C2C	-2.48	119.91	126.95
21	K	102	LMU	O5B-C5B-C6B	2.47	112.57	106.44
20	4	310	CLA	O2A-CGA-CBA	2.47	119.38	111.83
20	1	209	CLA	CHC-C1C-C2C	-2.47	119.92	126.95
20	B	824	CLA	CHC-C1C-C2C	-2.47	119.92	126.95
20	B	839	CLA	CHC-C1C-C2C	-2.47	119.92	126.95
20	B	849	CLA	CAA-C2A-C3A	-2.47	106.32	113.00
20	A	835	CLA	C4A-NA-C1A	2.47	107.81	106.68
20	A	816	CLA	CAA-CBA-CGA	-2.47	106.19	113.21
20	B	831	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
20	1	207	CLA	CHC-C1C-C2C	-2.47	119.93	126.95
20	B	833	CLA	C1-C2-C3	-2.47	122.15	126.20
21	R	103	LMU	C1B-O1B-C4'	2.47	123.83	117.98
20	4	307	CLA	CHB-C4A-NA	2.47	127.96	124.40
21	2	319	LMU	C1-O1'-C1'	2.47	117.90	113.68
20	4	303	CLA	C2D-C1D-ND	-2.47	107.68	110.13
20	1	210	CLA	C3D-C4D-ND	2.47	114.00	109.99
20	3	303	CLA	CMB-C2B-C3B	2.47	130.09	123.53
20	3	320	CLA	CHC-C4B-NB	2.47	127.75	124.05
20	1	212	CLA	C2A-C1A-CHA	-2.47	119.59	123.87
20	I	102	CLA	CMB-C2B-C1B	2.47	129.18	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	315	CLA	CHB-C1B-NB	-2.47	120.52	124.08
20	A	849	CLA	CHC-C1C-C2C	-2.47	119.94	126.95
20	B	810	CLA	O2A-CGA-CBA	2.47	119.36	111.83
20	R	106	CLA	C3D-C4D-ND	2.47	113.99	109.99
20	4	305	CLA	C4-C3-C5	2.46	119.50	115.23
20	B	810	CLA	C16-C15-C13	-2.46	107.78	115.97
21	G	101	LMU	O5'-C1'-C2'	-2.46	105.31	110.37
20	K	103	CLA	CHB-C4A-NA	2.46	127.95	124.40
20	4	311	CLA	CHD-C1D-ND	2.46	128.32	124.84
20	B	805	CLA	C1-C2-C3	-2.46	122.17	126.20
20	4	314	CLA	CHD-C1D-ND	2.46	128.32	124.84
20	H	101	CLA	CMA-C3A-C4A	-2.46	105.16	111.77
20	2	311	CLA	C3B-C2B-C1B	-2.46	104.27	107.17
20	4	306	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
20	2	317	CLA	C4A-NA-C1A	2.46	107.80	106.68
20	B	830	CLA	CAA-C2A-C1A	-2.45	103.93	111.97
20	B	807	CLA	O2A-CGA-CBA	2.45	119.32	111.83
20	B	804	CLA	C6-C7-C8	-2.45	107.81	115.97
20	2	314	CLA	C2C-C1C-CHC	-2.45	119.41	125.84
20	1	206	CLA	O1D-CGD-CBD	-2.45	119.68	124.52
20	A	821	CLA	C14-C13-C12	2.45	120.02	111.27
20	B	820	CLA	C7-C6-C5	-2.45	106.72	113.26
20	B	803	CLA	CHC-C1C-C2C	-2.45	119.98	126.95
20	B	824	CLA	CAA-C2A-C1A	-2.45	103.94	111.97
20	B	825	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
20	B	809	CLA	CHB-C1B-NB	-2.45	120.37	124.05
20	K	105	CLA	CHB-C4A-NA	2.45	127.93	124.40
20	B	804	CLA	CAA-C2A-C1A	-2.45	103.95	111.97
21	H	105	LMU	O4'-C4B-C5B	2.45	115.35	109.32
20	3	301	CLA	CHC-C1C-C2C	-2.45	119.99	126.95
21	R	109	LMU	C1'-O5'-C5'	-2.45	108.94	113.72
20	B	833	CLA	CED-O2D-CGD	2.45	121.47	115.92
20	A	817	CLA	O2D-CGD-O1D	-2.45	119.09	123.85
20	1	208	CLA	C1C-NC-C4C	-2.44	105.56	106.68
20	A	838	CLA	C5-C3-C4	2.44	120.21	114.59
20	L	203	CLA	CMA-C3A-C4A	2.44	118.34	111.77
20	3	310	CLA	C4A-NA-C1A	2.44	107.79	106.68
20	2	310	CLA	C5-C3-C4	2.44	120.21	114.59
20	1	214	CLA	CED-O2D-CGD	2.44	121.45	115.92
22	I	101	BCR	C16-C15-C14	-2.44	118.52	123.52
20	H	110	CLA	CHB-C1B-NB	-2.44	120.39	124.05
20	4	319	CLA	O2D-CGD-O1D	-2.44	119.10	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	316	LMU	C4B-C3B-C2B	-2.44	106.55	110.83
20	A	828	CLA	C4-C3-C5	2.44	119.46	115.23
20	A	803	CLA	O1A-CGA-CBA	-2.44	114.25	123.78
21	A	853	LMU	O4'-C4B-C5B	-2.44	103.33	109.32
20	B	829	CLA	CHC-C1C-C2C	-2.43	120.03	126.95
20	B	849	CLA	CHB-C1B-NB	-2.43	120.40	124.05
21	K	101	LMU	O1'-C1-C2	-2.43	101.11	109.37
20	2	304	CLA	C4A-NA-C1A	2.43	107.79	106.68
20	A	836	CLA	CHB-C4A-NA	2.43	127.91	124.40
20	L	203	CLA	C3B-C2B-C1B	-2.43	104.30	107.17
21	1	217	LMU	O1B-C4'-C5'	2.43	115.86	109.48
20	B	807	CLA	O2D-CGD-CBD	2.43	115.48	111.23
20	A	823	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
20	K	103	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
20	2	317	CLA	CHC-C1C-C2C	-2.43	120.04	126.95
20	A	823	CLA	CHB-C4A-NA	2.43	127.91	124.40
20	A	833	CLA	CHB-C4A-NA	2.43	127.91	124.40
20	B	836	CLA	CHB-C1B-NB	-2.43	120.40	124.05
21	A	853	LMU	O1'-C1'-C2'	2.43	111.96	108.27
20	H	110	CLA	CAC-C3C-C4C	2.43	127.95	124.79
20	B	836	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
20	B	848	CLA	CHC-C4B-NB	2.43	127.69	124.05
20	A	824	CLA	C4-C3-C2	-2.43	117.39	123.63
20	B	849	CLA	CMA-C3A-C2A	-2.43	104.60	113.98
20	K	105	CLA	O2D-CGD-O1D	-2.43	119.13	123.85
20	B	808	CLA	C1-O2A-CGA	2.42	122.52	116.65
20	A	816	CLA	CED-O2D-CGD	2.42	121.42	115.92
20	B	812	CLA	O2A-CGA-O1A	-2.42	117.56	123.63
20	2	304	CLA	CED-O2D-CGD	2.42	121.41	115.92
20	J	102	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
20	B	817	CLA	O1D-CGD-CBD	-2.42	119.74	124.52
20	B	828	CLA	CMC-C2C-C1C	2.42	128.82	125.03
20	A	855	CLA	CHB-C4A-NA	2.42	127.89	124.40
20	4	305	CLA	CHB-C1B-NB	-2.42	120.42	124.05
20	A	848	CLA	CED-O2D-CGD	2.42	121.40	115.92
20	A	822	CLA	CHB-C4A-NA	2.42	127.89	124.40
20	A	833	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
20	B	828	CLA	C2A-C1A-CHA	-2.42	119.67	123.87
22	L	209	BCR	C28-C27-C26	-2.42	109.75	114.06
20	B	812	CLA	C3D-C4D-ND	2.41	113.91	109.99
20	B	807	CLA	CMD-C2D-C3D	-2.41	122.15	127.69
20	L	202	CLA	C1D-ND-C4D	-2.41	104.62	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	832	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
20	A	803	CLA	CHB-C1B-NB	-2.41	120.43	124.05
20	B	847	CLA	C3D-C4D-ND	2.41	113.91	109.99
20	B	849	CLA	C3D-C4D-ND	2.41	113.91	109.99
20	A	829	CLA	C4B-C3B-C2B	2.41	110.30	107.30
20	A	835	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
20	3	301	CLA	CHB-C4A-NA	2.41	127.88	124.40
20	4	302	CLA	CHB-C4A-NA	2.41	127.88	124.40
20	A	834	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
20	J	103	CLA	O2A-CGA-CBA	2.41	119.19	111.83
20	2	303	CLA	C4D-ND-C1D	-2.41	104.62	106.31
20	H	109	CLA	C3D-C4D-ND	2.41	113.90	109.99
20	3	310	CLA	CHB-C4A-NA	2.41	127.88	124.40
20	B	804	CLA	C4-C3-C5	2.41	119.41	115.23
20	B	827	CLA	C3D-C4D-ND	2.41	113.90	109.99
20	J	102	CLA	CHB-C4A-NA	2.41	127.88	124.40
20	4	317	CLA	C3D-C4D-ND	2.41	112.79	109.50
20	B	806	CLA	CHD-C4C-C3C	-2.41	121.26	124.77
20	2	309	CLA	C2C-C1C-CHC	-2.41	119.54	125.84
20	3	315	CLA	C3D-C4D-ND	2.40	113.89	109.99
20	4	305	CLA	C4D-CHA-C1A	-2.40	118.38	121.24
20	A	837	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
20	A	817	CLA	CHB-C4A-NA	2.40	127.87	124.40
20	A	835	CLA	CHB-C4A-NA	2.40	127.87	124.40
20	I	102	CLA	C1-O2A-CGA	2.40	122.47	116.65
20	R	107	CLA	C4-C3-C2	-2.40	117.46	123.63
20	A	807	CLA	CHC-C4B-C3B	-2.40	116.94	127.37
20	A	836	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
20	A	849	CLA	C3D-C4D-ND	2.40	113.89	109.99
20	2	301	CLA	C4A-NA-C1A	2.40	107.78	106.68
20	A	802	CLA	O2D-CGD-CBD	2.40	115.43	111.23
21	R	103	LMU	O5B-C5B-C4B	2.40	114.03	109.70
20	F	205	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
20	F	204	CLA	C3D-C4D-ND	2.40	113.89	109.99
20	A	832	CLA	CHB-C4A-NA	2.40	127.86	124.40
20	3	304	CLA	C3B-C4B-CHC	-2.40	118.26	126.76
20	A	831	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
22	B	842	BCR	C2-C1-C6	2.40	113.92	110.44
22	B	842	BCR	C35-C13-C12	2.40	121.75	118.09
20	B	813	CLA	CED-O2D-CGD	2.40	121.35	115.92
20	A	855	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
20	2	301	CLA	O2D-CGD-O1D	-2.40	119.19	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	306	CLA	CHC-C1C-C2C	-2.40	120.14	126.95
21	L	206	LMU	O4'-C4B-C3B	2.39	116.02	110.38
21	L	205	LMU	O5'-C5'-C4'	2.39	114.67	109.72
20	3	316	CLA	CHB-C1B-NB	-2.39	120.62	124.08
20	B	823	CLA	CHB-C4A-NA	2.39	127.85	124.40
20	A	810	CLA	CHB-C1B-NB	-2.39	120.46	124.05
20	A	803	CLA	C4-C3-C5	2.39	119.38	115.23
20	A	827	CLA	CHB-C4A-NA	2.39	127.85	124.40
20	A	828	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
20	A	838	CLA	C2D-C1D-ND	-2.39	107.76	110.13
20	A	806	CLA	CMB-C2B-C1B	2.39	129.06	125.42
20	L	204	CLA	C4B-CHC-C1C	-2.39	120.63	126.25
20	2	303	CLA	CHB-C1B-NB	-2.39	120.63	124.08
20	A	837	CLA	CHB-C4A-NA	2.39	127.85	124.40
20	A	830	CLA	CHB-C1B-NB	-2.39	120.47	124.05
20	2	312	CLA	CED-O2D-CGD	2.39	121.33	115.92
20	F	205	CLA	CHB-C4A-NA	2.39	127.84	124.40
20	4	302	CLA	C3D-C4D-ND	2.39	113.87	109.99
20	B	818	CLA	O2A-CGA-CBA	2.39	121.15	112.14
20	2	321	CLA	CHB-C1B-C2B	-2.39	120.50	127.43
21	4	321	LMU	C3'-C4'-C5'	2.39	116.22	110.93
20	A	831	CLA	CHB-C4A-NA	2.39	127.84	124.40
20	3	310	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
20	1	214	CLA	C4D-CHA-C1A	2.38	124.09	121.24
20	B	827	CLA	CHB-C4A-NA	2.38	127.84	124.40
20	A	827	CLA	C1-O2A-CGA	2.38	122.42	116.65
20	4	302	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
20	A	826	CLA	CAA-CBA-CGA	2.38	119.97	113.21
20	B	822	CLA	C3D-C4D-ND	2.38	113.86	109.99
20	2	306	CLA	CMB-C2B-C1B	2.38	129.04	125.42
20	H	107	CLA	CHB-C4A-NA	2.38	127.83	124.40
20	A	838	CLA	CMB-C2B-C1B	2.38	129.04	125.42
20	L	201	CLA	C4A-NA-C1A	2.38	107.76	106.68
20	2	302	CLA	C3A-C2A-C1A	2.38	104.90	101.34
22	A	840	BCR	C11-C12-C13	-2.37	119.85	126.36
21	A	852	LMU	C4B-C3B-C2B	2.37	115.00	110.83
20	A	807	CLA	O2A-C1-C2	2.37	117.25	108.11
20	K	106	CLA	CED-O2D-CGD	2.37	121.30	115.92
20	L	204	CLA	CMC-C2C-C1C	-2.37	121.33	125.03
20	H	107	CLA	CMB-C2B-C1B	2.37	129.03	125.42
20	1	212	CLA	C11-C12-C13	-2.37	108.08	115.97
20	B	829	CLA	C9-C8-C10	2.37	119.73	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	825	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
20	B	816	CLA	CHC-C1C-C2C	-2.37	120.21	126.95
20	B	838	CLA	CAC-C3C-C4C	2.37	127.88	124.79
20	3	304	CLA	C3D-C4D-ND	2.37	112.74	109.50
22	B	850	BCR	C23-C22-C21	2.37	122.74	119.01
20	2	321	CLA	C6-C5-C3	-2.37	107.70	113.47
20	A	809	CLA	CHB-C1B-NB	-2.37	120.50	124.05
20	A	822	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
20	A	809	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
21	2	318	LMU	C1'-O5'-C5'	2.37	118.34	113.72
20	3	315	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
21	F	201	LMU	C6'-C5'-C4'	-2.37	106.72	113.38
20	B	824	CLA	C1-C2-C3	-2.37	122.32	126.20
20	B	823	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
22	B	844	BCR	C11-C12-C13	-2.36	119.88	126.36
20	2	309	CLA	C3D-C4D-ND	2.36	112.73	109.50
22	3	311	BCR	C34-C9-C10	-2.36	118.99	122.82
20	4	319	CLA	CHB-C4A-NA	2.36	127.81	124.40
20	A	815	CLA	C4A-NA-C1A	2.36	107.76	106.68
20	B	837	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
20	B	820	CLA	CMB-C2B-C1B	2.36	129.01	125.42
21	H	102	LMU	O5'-C5'-C4'	2.36	114.60	109.72
20	1	206	CLA	CHC-C1C-C2C	-2.36	120.24	126.95
20	A	811	CLA	CAC-C3C-C4C	2.36	127.86	124.79
20	L	203	CLA	CED-O2D-CGD	2.36	121.27	115.92
20	4	312	CLA	CHB-C1B-NB	-2.36	120.67	124.08
20	1	201	CLA	CHA-C4D-ND	2.36	137.41	132.55
20	3	315	CLA	CHB-C4A-NA	2.36	127.80	124.40
20	2	307	CLA	CAA-CBA-CGA	-2.36	106.52	113.21
20	A	822	CLA	C3D-C4D-ND	2.36	113.82	109.99
20	A	828	CLA	C3D-C4D-ND	2.36	113.82	109.99
20	B	810	CLA	C4-C3-C5	2.36	119.32	115.23
20	4	309	CLA	C3D-C4D-ND	2.36	112.72	109.50
20	B	810	CLA	C3D-C4D-ND	2.36	113.82	109.99
22	A	841	BCR	C11-C12-C13	-2.36	119.90	126.36
20	A	847	CLA	CMB-C2B-C1B	2.36	129.01	125.42
21	R	102	LMU	C3B-C4B-C5B	-2.36	105.96	110.23
21	B	845	LMU	O5'-C5'-C4'	2.35	114.59	109.72
20	B	849	CLA	CED-O2D-CGD	2.35	121.26	115.92
20	B	814	CLA	C1-C2-C3	-2.35	122.34	126.20
20	A	847	CLA	CBC-CAC-C3C	-2.35	106.04	112.42
20	4	304	CLA	C3B-C2B-C1B	-2.35	104.39	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	808	CLA	C2D-C1D-ND	-2.35	107.80	110.13
20	B	804	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
20	3	307	CLA	C3C-C4C-CHD	-2.35	119.12	125.23
20	4	304	CLA	CAC-C3C-C4C	2.35	127.85	124.79
20	4	304	CLA	C3D-C4D-ND	2.35	113.81	109.99
22	B	843	BCR	C11-C12-C13	-2.35	119.92	126.36
22	A	844	BCR	C20-C19-C18	-2.35	119.92	126.36
20	B	828	CLA	CHC-C1C-C2C	-2.35	120.27	126.95
20	B	824	CLA	CHC-C4B-NB	2.35	127.57	124.05
20	A	834	CLA	CHB-C4A-NA	2.35	127.79	124.40
22	3	311	BCR	C28-C27-C26	-2.35	109.87	114.06
20	B	819	CLA	C2A-C1A-CHA	-2.35	119.79	123.87
20	H	109	CLA	CHC-C1C-C2C	-2.35	120.28	126.95
21	K	101	LMU	O5'-C5'-C4'	2.35	114.58	109.72
20	A	814	CLA	CAC-C3C-C2C	-2.35	123.25	127.56
20	B	822	CLA	CHB-C4A-NA	2.35	127.79	124.40
20	B	832	CLA	O2A-CGA-CBA	2.35	121.41	114.00
20	3	313	CLA	C3D-C4D-ND	2.35	112.71	109.50
21	A	845	LMU	O6'-C6'-C5'	-2.34	103.35	111.33
20	A	815	CLA	CHB-C1B-NB	-2.34	120.53	124.05
20	I	102	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
20	A	814	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
20	A	827	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
21	R	102	LMU	O1'-C1'-C2'	2.34	111.83	108.27
20	2	301	CLA	CHB-C4A-NA	2.34	127.78	124.40
20	A	847	CLA	CHB-C1B-NB	-2.34	120.54	124.05
20	A	803	CLA	CHB-C4A-NA	2.34	127.78	124.40
20	A	808	CLA	CED-O2D-CGD	2.34	121.22	115.92
20	B	806	CLA	C11-C12-C13	-2.34	108.19	115.97
22	A	842	BCR	C20-C19-C18	-2.34	119.95	126.36
20	A	824	CLA	C1-O2A-CGA	2.34	122.31	116.65
20	A	830	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
20	B	834	CLA	CAC-C3C-C4C	2.34	127.83	124.79
20	B	810	CLA	CHC-C1C-C2C	-2.34	120.31	126.95
21	F	201	LMU	O3'-C3'-C4'	-2.34	103.95	109.94
20	A	806	CLA	C1-O2A-CGA	2.34	122.31	116.65
21	H	102	LMU	O5B-C1B-C2B	2.34	115.17	110.37
20	B	827	CLA	CMB-C2B-C1B	2.34	128.98	125.42
20	2	321	CLA	C2A-C3A-C4A	-2.34	98.10	101.87
20	A	805	CLA	CGD-CBD-CAD	-2.34	103.28	110.85
20	A	805	CLA	CHC-C1C-C2C	-2.34	120.31	126.95
20	A	820	CLA	CHC-C1C-C2C	-2.34	120.31	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	807	CLA	C3D-C4D-ND	2.33	113.78	109.99
20	B	815	CLA	CAA-C2A-C3A	-2.33	106.69	113.00
20	4	304	CLA	C1C-C2C-C3C	2.33	109.43	106.98
20	B	805	CLA	C2A-C1A-CHA	-2.33	119.82	123.87
20	K	106	CLA	CHA-C4D-ND	2.33	137.36	132.55
20	B	833	CLA	C1D-ND-C4D	-2.33	104.68	106.31
22	G	102	BCR	C11-C12-C13	-2.33	119.97	126.36
22	J	101	BCR	C20-C19-C18	-2.33	119.97	126.36
20	2	312	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
20	A	829	CLA	CHB-C1B-NB	-2.33	120.55	124.05
20	B	835	CLA	C3D-C4D-ND	2.33	113.78	109.99
20	B	815	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
20	A	857	CLA	CHB-C4A-NA	2.33	127.74	124.43
20	A	811	CLA	CBC-CAC-C3C	-2.33	106.10	112.42
22	F	202	BCR	C11-C12-C13	-2.33	119.97	126.36
21	4	322	LMU	C1B-C2B-C3B	2.33	114.91	110.01
20	2	304	CLA	CAA-C2A-C3A	-2.33	106.71	113.00
20	B	829	CLA	CAA-C2A-C1A	-2.33	104.35	111.97
20	4	307	CLA	C4C-C3C-C2C	2.33	110.28	106.89
22	A	844	BCR	C11-C12-C13	-2.33	119.98	126.36
20	B	825	CLA	C12-C11-C10	-2.33	102.85	113.28
20	K	107	CLA	C2A-C1A-CHA	-2.33	119.83	123.87
20	1	201	CLA	CAA-C2A-C1A	2.33	119.60	111.97
20	A	827	CLA	CMB-C2B-C1B	2.33	128.96	125.42
21	R	103	LMU	C1'-C2'-C3'	2.33	114.90	110.01
20	H	107	CLA	C1-O2A-CGA	2.32	122.28	116.65
20	1	212	CLA	O2A-CGA-CBA	2.32	118.92	111.83
20	K	103	CLA	C3D-C4D-ND	2.32	113.77	109.99
20	A	857	CLA	C3D-C4D-ND	2.32	112.68	109.50
20	B	804	CLA	C3D-C4D-ND	2.32	113.76	109.99
21	H	103	LMU	O2'-C2'-C1'	-2.32	104.54	110.08
22	G	102	BCR	C20-C19-C18	-2.32	120.00	126.36
20	A	818	CLA	C1-C2-C3	-2.32	122.40	126.20
20	1	214	CLA	CMA-C3A-C2A	-2.32	105.02	113.98
21	B	845	LMU	C2'-C3'-C4'	2.32	114.94	109.68
20	K	103	CLA	C5-C3-C4	2.32	119.92	114.59
20	2	310	CLA	CHB-C1B-NB	-2.32	120.57	124.05
20	L	201	CLA	CBA-CAA-C2A	2.31	120.68	113.79
20	A	801	CLA	C4A-NA-C1A	2.31	107.73	106.68
20	B	849	CLA	C6-C7-C8	-2.31	108.27	115.97
22	J	101	BCR	C11-C12-C13	-2.31	120.02	126.36
23	A	839	PQN	C8-C7-C6	2.31	123.09	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	806	CLA	C1D-ND-C4D	-2.31	104.69	106.31
20	2	301	CLA	C3D-C4D-ND	2.31	113.75	109.99
21	2	313	LMU	O5'-C5'-C6'	2.31	112.17	106.44
20	A	807	CLA	C1-C2-C3	2.31	129.98	126.20
21	K	102	LMU	O4'-C4B-C5B	2.31	115.02	109.32
22	A	843	BCR	C11-C12-C13	-2.31	120.03	126.36
20	A	814	CLA	O2A-CGA-CBA	2.31	118.88	111.83
20	2	307	CLA	CMB-C2B-C1B	2.31	128.94	125.42
20	1	208	CLA	C3D-C4D-ND	2.31	112.66	109.50
20	F	204	CLA	CGD-CBD-CAD	-2.31	104.83	114.30
21	R	104	LMU	C1B-O5B-C5B	2.31	118.23	113.72
22	B	844	BCR	C20-C19-C18	-2.31	120.03	126.36
20	B	822	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
20	B	848	CLA	O2A-CGA-CBA	2.31	118.87	111.83
20	A	810	CLA	CMB-C2B-C1B	2.31	128.93	125.42
20	3	301	CLA	CED-O2D-CGD	2.31	121.15	115.92
20	L	202	CLA	CHC-C1C-C2C	-2.31	120.39	126.95
20	A	826	CLA	C2A-C1A-CHA	-2.31	119.86	123.87
20	1	204	CLA	C3B-C2B-C1B	-2.31	104.45	107.17
20	A	814	CLA	C4A-NA-C1A	2.31	107.73	106.68
22	I	101	BCR	C10-C11-C12	-2.30	116.52	123.20
22	I	103	BCR	C4-C5-C6	-2.30	119.59	122.70
20	A	817	CLA	CHC-C4B-NB	2.30	127.50	124.05
22	A	843	BCR	C20-C19-C18	-2.30	120.05	126.36
20	A	807	CLA	C2C-C1C-NC	2.30	112.40	109.98
20	4	315	CLA	C3A-C2A-C1A	2.30	104.79	101.34
21	L	205	LMU	O1B-C1B-C2B	2.30	113.75	108.09
20	B	814	CLA	C3B-C2B-C1B	-2.30	104.46	107.17
21	2	318	LMU	O5'-C1'-C2'	2.30	115.10	110.37
20	B	812	CLA	CHC-C1C-C2C	-2.30	120.41	126.95
20	3	310	CLA	C3D-C4D-ND	2.30	113.72	109.99
21	F	201	LMU	O5'-C5'-C4'	-2.30	104.97	109.72
20	A	830	CLA	C1-O2A-CGA	2.30	122.22	116.65
22	A	841	BCR	C20-C19-C18	-2.30	120.06	126.36
22	A	840	BCR	C20-C19-C18	-2.30	120.06	126.36
22	B	841	BCR	C11-C12-C13	-2.30	120.06	126.36
21	1	217	LMU	O5'-C1'-C2'	-2.30	105.65	110.37
20	B	814	CLA	C1-O2A-CGA	2.30	122.21	116.65
20	A	826	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
22	B	843	BCR	C20-C19-C18	-2.30	120.07	126.36
22	F	202	BCR	C20-C19-C18	-2.30	120.07	126.36
20	3	309	CLA	C1-O2A-CGA	2.30	122.21	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	807	CLA	C3B-C2B-C1B	-2.29	104.46	107.17
20	3	312	CLA	C3C-C4C-CHD	-2.29	119.27	125.23
20	B	828	CLA	CHB-C1B-NB	-2.29	120.61	124.05
20	A	833	CLA	C3D-C4D-ND	2.29	113.72	109.99
20	A	827	CLA	CHD-C4C-C3C	-2.29	121.43	124.77
22	F	203	BCR	C34-C9-C10	-2.29	119.10	122.82
20	F	204	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
21	2	319	LMU	O5'-C5'-C6'	2.29	112.12	106.44
20	A	806	CLA	O2A-CGA-CBA	2.29	118.83	111.83
20	3	316	CLA	C3D-C2D-C1D	2.29	110.13	107.35
22	B	841	BCR	C20-C19-C18	-2.29	120.08	126.36
20	H	108	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
20	A	836	CLA	C3D-C4D-ND	2.29	113.71	109.99
20	A	825	CLA	C4-C3-C5	2.29	119.21	115.23
20	A	855	CLA	C3D-C4D-ND	2.29	113.71	109.99
20	A	831	CLA	C3D-C4D-ND	2.29	113.71	109.99
20	1	215	CLA	C3C-C4C-CHD	-2.29	119.28	125.23
20	R	107	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
20	F	205	CLA	C3D-C4D-ND	2.29	113.71	109.99
20	4	307	CLA	C2C-C1C-NC	-2.29	107.58	109.98
20	A	806	CLA	C2A-C1A-CHA	-2.29	119.90	123.87
20	A	849	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
20	1	203	CLA	C2A-C1A-CHA	-2.28	119.90	123.87
21	L	206	LMU	O3'-C3'-C2'	2.28	115.76	110.38
20	2	314	CLA	C3D-C2D-C1D	2.28	110.12	107.35
20	A	832	CLA	C3D-C4D-ND	2.28	113.69	109.99
20	A	820	CLA	CAC-C3C-C2C	-2.28	123.37	127.56
20	H	101	CLA	CHB-C1B-NB	-2.28	120.63	124.05
20	A	835	CLA	C3D-C4D-ND	2.28	113.69	109.99
20	2	321	CLA	CMA-C3A-C4A	-2.28	105.65	111.77
22	F	203	BCR	C15-C16-C17	-2.28	118.86	123.52
20	L	204	CLA	CHB-C4A-NA	2.28	127.69	124.40
20	B	809	CLA	C2A-C1A-CHA	-2.28	119.91	123.87
20	B	813	CLA	C3D-C4D-ND	2.28	113.69	109.99
20	A	804	CLA	CED-O2D-CGD	2.28	121.08	115.92
21	R	105	LMU	O4'-C4B-C3B	2.28	115.74	110.38
20	3	314	CLA	C1D-ND-C4D	-2.27	104.72	106.31
20	2	302	CLA	C2A-C1A-CHA	-2.27	119.92	123.87
20	2	307	CLA	C11-C10-C8	-2.27	108.41	115.97
20	A	818	CLA	CHC-C1C-C2C	-2.27	120.49	126.95
20	2	312	CLA	C3B-C2B-C1B	-2.27	104.49	107.17
20	A	828	CLA	C1-O2A-CGA	2.27	122.15	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	4	305	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
20	A	837	CLA	C3D-C4D-ND	2.27	113.68	109.99
20	1	211	CLA	CHC-C4B-C3B	-2.27	117.50	127.37
20	B	833	CLA	CHB-C4A-NA	2.27	127.68	124.40
20	A	827	CLA	C2D-C1D-ND	-2.27	107.88	110.13
21	A	845	LMU	C3B-C4B-C5B	2.27	114.35	110.23
20	B	825	CLA	C2B-C1B-NB	2.27	112.68	110.33
20	L	202	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
20	4	312	CLA	C3C-C4C-CHD	-2.27	119.33	125.23
20	3	317	CLA	C3D-C4D-ND	2.27	112.60	109.50
22	A	842	BCR	C11-C12-C13	-2.27	120.14	126.36
21	C	101	LMU	C6B-C5B-C4B	2.27	118.59	113.02
20	H	101	CLA	C1-C2-C3	2.27	129.91	126.20
20	1	209	CLA	CHB-C1B-NB	-2.27	120.64	124.05
20	3	312	CLA	C3D-C2D-C1D	2.27	110.10	107.35
20	B	803	CLA	CHB-C1B-C2B	-2.27	120.85	127.43
20	4	315	CLA	CMA-C3A-C4A	-2.26	105.69	111.77
21	A	846	LMU	C1B-C2B-C3B	2.26	114.77	110.01
20	L	208	CLA	CMC-C2C-C1C	2.26	128.57	125.03
20	1	202	CLA	C1-O2A-CGA	2.26	123.10	116.67
20	A	834	CLA	C3D-C4D-ND	2.26	113.67	109.99
20	R	106	CLA	CGD-CBD-CAD	-2.26	103.52	110.85
20	B	847	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
20	1	210	CLA	CHC-C1C-C2C	-2.26	120.52	126.95
20	A	838	CLA	O2A-CGA-CBA	2.26	118.73	111.83
20	4	319	CLA	C3D-C4D-ND	2.26	113.66	109.99
20	B	816	CLA	C4-C3-C2	-2.26	117.82	123.63
20	B	804	CLA	C11-C12-C13	-2.26	108.46	115.97
20	L	204	CLA	CHB-C1B-C2B	-2.26	120.87	127.43
20	B	838	CLA	CED-O2D-CGD	2.26	121.04	115.92
20	A	826	CLA	CMC-C2C-C1C	2.26	128.56	125.03
20	B	817	CLA	CMC-C2C-C1C	2.26	128.56	125.03
20	A	803	CLA	O1D-CGD-CBD	-2.26	120.07	124.52
20	A	802	CLA	C3D-C4D-ND	2.26	113.65	109.99
20	B	832	CLA	CED-O2D-CGD	2.26	121.03	115.92
21	L	206	LMU	O1B-C4'-C5'	2.26	115.39	109.48
20	A	821	CLA	C3B-C4B-NB	-2.25	108.52	110.53
20	J	102	CLA	C3D-C4D-ND	2.25	113.65	109.99
20	B	826	CLA	CHB-C4A-NA	2.25	127.65	124.40
21	C	101	LMU	O1B-C1B-C2B	2.25	113.63	108.09
20	A	818	CLA	CED-O2D-CGD	2.25	121.02	115.92
20	4	318	CLA	CAA-CBA-CGA	-2.25	106.81	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	R	103	LMU	C6'-C5'-C4'	-2.25	107.05	113.38
20	A	803	CLA	C1D-ND-C4D	-2.25	104.73	106.31
20	1	207	CLA	O1D-CGD-CBD	-2.25	120.08	124.52
20	3	306	CLA	C3D-C4D-ND	2.25	112.58	109.50
20	B	836	CLA	O2A-CGA-CBA	2.25	118.69	111.83
21	A	846	LMU	C4B-C3B-C2B	-2.25	106.88	110.83
20	L	201	CLA	CHB-C4A-NA	2.25	127.64	124.40
20	F	206	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
22	F	203	BCR	C20-C19-C18	-2.25	120.20	126.36
22	F	203	BCR	C8-C9-C10	-2.25	115.48	119.01
20	B	848	CLA	CHB-C1B-NB	-2.25	120.68	124.05
20	A	813	CLA	CHC-C4B-NB	2.24	127.42	124.05
20	A	827	CLA	CAA-C2A-C3A	-2.24	106.94	113.00
20	1	202	CLA	O2D-CGD-CBD	2.24	115.15	111.23
21	R	109	LMU	O5B-C5B-C4B	2.24	113.74	109.70
21	L	206	LMU	O2B-C2B-C1B	-2.24	104.73	110.08
21	K	101	LMU	O5B-C1B-C2B	-2.24	105.77	110.37
20	2	307	CLA	C6-C7-C8	-2.24	108.52	115.97
21	A	852	LMU	C4-C3-C2	-2.24	103.05	114.37
20	B	827	CLA	CAA-CBA-CGA	-2.24	106.85	113.21
22	L	209	BCR	C37-C22-C21	-2.24	119.19	122.82
20	4	309	CLA	C3C-C4C-CHD	-2.24	119.42	125.23
21	K	102	LMU	O1B-C1B-C2B	-2.24	102.58	108.09
20	B	830	CLA	CHB-C1B-NB	-2.24	120.69	124.05
20	2	310	CLA	CAC-C3C-C2C	-2.24	123.45	127.56
20	B	836	CLA	CED-O2D-CGD	2.24	120.99	115.92
20	1	205	CLA	CHC-C1C-C2C	-2.24	120.59	126.95
20	4	311	CLA	C3D-C4D-ND	2.24	112.56	109.50
22	I	101	BCR	C29-C30-C25	-2.24	107.19	110.44
20	3	301	CLA	C4-C3-C5	2.24	119.11	115.23
20	R	107	CLA	C1D-ND-C4D	-2.23	104.74	106.31
20	B	830	CLA	CAC-C3C-C4C	2.23	127.70	124.79
20	A	819	CLA	CED-O2D-CGD	2.23	120.98	115.92
21	K	102	LMU	C5-C4-C3	-2.23	103.08	114.37
20	A	823	CLA	C3D-C4D-ND	2.23	113.62	109.99
20	2	321	CLA	CHD-C1D-ND	2.23	127.95	124.80
20	B	805	CLA	C3D-C4D-ND	2.23	113.61	109.99
20	A	819	CLA	C4B-C3B-C2B	2.23	110.08	107.30
22	L	209	BCR	C23-C24-C25	-2.23	121.04	127.00
20	B	823	CLA	C3D-C4D-ND	2.23	113.61	109.99
20	B	833	CLA	CHC-C1C-C2C	-2.23	120.61	126.95
20	B	821	CLA	CAA-C2A-C1A	2.23	119.28	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	832	CLA	O2A-CGA-O1A	-2.23	117.61	123.33
20	B	848	CLA	CAC-C3C-C2C	-2.23	123.47	127.56
20	B	805	CLA	C4B-C3B-C2B	2.23	110.07	107.30
20	4	312	CLA	C3D-C2D-C1D	2.23	110.05	107.35
20	3	301	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
20	B	809	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
20	B	808	CLA	CHB-C4A-NA	2.22	127.61	124.40
20	A	829	CLA	C2C-C1C-NC	2.22	112.32	109.98
20	1	207	CLA	C4D-CHA-C1A	-2.22	118.59	121.24
20	4	303	CLA	CHC-C1C-C2C	-2.22	120.63	126.95
22	B	842	BCR	C8-C7-C6	-2.22	121.06	127.00
20	B	839	CLA	CAC-C3C-C4C	2.22	128.50	125.03
20	L	202	CLA	O2A-CGA-CBA	2.22	118.60	111.83
20	B	837	CLA	C2A-C1A-CHA	-2.22	120.02	123.87
20	A	810	CLA	C3D-C4D-ND	2.22	113.59	109.99
20	B	824	CLA	C2A-C1A-CHA	-2.22	120.02	123.87
21	R	102	LMU	O5'-C5'-C6'	-2.22	100.94	106.44
20	4	314	CLA	C2C-C1C-CHC	-2.22	120.03	125.84
20	A	809	CLA	CAC-C3C-C4C	2.22	127.67	124.79
21	4	321	LMU	O2'-C2'-C3'	-2.22	105.15	110.38
20	A	827	CLA	CGD-CBD-CAD	2.22	118.02	110.85
20	F	204	CLA	CAA-C2A-C3A	-2.22	111.15	116.23
20	2	309	CLA	CHB-C4A-NA	2.21	127.58	124.43
21	H	103	LMU	O1'-C1'-C2'	2.21	111.63	108.27
20	3	315	CLA	C1D-ND-C4D	-2.21	104.76	106.31
20	1	207	CLA	C3B-C4B-NB	-2.21	108.56	110.53
20	L	201	CLA	C4-C3-C2	-2.21	117.95	123.63
20	A	803	CLA	C3B-C4B-NB	-2.21	108.56	110.53
20	B	807	CLA	C1-C2-C3	-2.21	122.58	126.20
21	R	101	LMU	C8-C7-C6	-2.21	103.20	114.37
20	3	305	CLA	C3D-C4D-ND	2.21	112.52	109.50
21	A	846	LMU	C1'-C2'-C3'	2.21	114.66	110.01
20	L	208	CLA	CMA-C3A-C4A	2.21	117.70	111.77
20	1	206	CLA	CBC-CAC-C3C	2.21	118.40	112.42
22	3	311	BCR	C37-C22-C21	-2.21	119.24	122.82
20	A	801	CLA	CHB-C4A-NA	2.21	127.58	124.40
20	B	803	CLA	CMB-C2B-C1B	2.21	128.78	125.42
20	1	208	CLA	CHD-C1D-ND	2.21	127.96	124.84
22	I	101	BCR	C15-C14-C13	2.21	130.37	127.28
20	L	202	CLA	CHB-C4A-NA	2.20	127.58	124.40
20	3	319	CLA	CHB-C1B-NB	-2.20	120.75	124.05
20	4	307	CLA	C4-C3-C2	-2.20	117.97	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	827	CLA	C2A-C1A-CHA	-2.20	120.05	123.87
20	2	312	CLA	C4A-NA-C1A	2.20	107.68	106.68
20	A	824	CLA	CHC-C1C-C2C	-2.20	120.70	126.95
20	2	304	CLA	C4D-CHA-C1A	-2.20	118.62	121.24
20	B	809	CLA	C1D-ND-C4D	-2.20	104.77	106.31
21	B	801	LMU	O5'-C1'-C2'	2.20	114.89	110.37
20	A	849	CLA	C16-C15-C13	-2.20	108.66	115.97
20	B	848	CLA	CBA-CAA-C2A	-2.20	107.26	113.79
20	3	307	CLA	CHB-C4A-NA	2.20	127.55	124.43
20	4	310	CLA	CHB-C4A-NA	2.19	127.57	124.40
21	H	104	LMU	O3'-C3'-C4'	-2.19	104.31	109.94
20	A	802	CLA	C1-C2-C3	2.19	129.79	126.20
20	3	301	CLA	C1D-ND-C4D	-2.19	104.77	106.31
20	2	306	CLA	CHB-C4A-NA	2.19	127.56	124.40
20	1	204	CLA	CAA-C2A-C3A	-2.19	107.07	113.00
20	1	201	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
20	A	812	CLA	CHB-C1B-NB	-2.19	120.76	124.05
20	4	306	CLA	C2A-C1A-CHA	-2.19	120.07	123.87
20	H	109	CLA	C4A-NA-C1A	2.19	107.68	106.68
20	4	308	CLA	C3C-C4C-CHD	-2.19	119.55	125.23
20	B	835	CLA	C2A-C1A-CHA	-2.19	120.07	123.87
21	A	853	LMU	C1'-C2'-C3'	2.19	114.61	110.01
20	A	816	CLA	C3D-C4D-ND	2.19	113.54	109.99
21	R	102	LMU	C1-O1'-C1'	-2.19	109.95	113.68
20	A	829	CLA	C4A-NA-C1A	2.19	107.68	106.68
20	B	815	CLA	CED-O2D-CGD	2.18	120.87	115.92
20	1	210	CLA	CHC-C4B-C3B	-2.18	121.08	127.43
20	B	826	CLA	C4B-C3B-C2B	2.18	110.02	107.30
22	L	209	BCR	C24-C23-C22	-2.18	123.01	126.23
20	2	317	CLA	CED-O2D-CGD	2.18	120.87	115.92
20	F	204	CLA	CHB-C1B-C2B	-2.18	121.09	127.43
21	B	802	LMU	O5'-C5'-C4'	-2.18	105.21	109.72
20	A	802	CLA	CHB-C4A-NA	2.18	127.55	124.40
20	1	203	CLA	CHC-C1C-C2C	-2.18	120.75	126.95
20	B	832	CLA	CHB-C4A-NA	2.18	127.55	124.40
20	B	819	CLA	C3D-C4D-ND	2.18	113.53	109.99
21	A	853	LMU	O5B-C5B-C4B	-2.18	105.77	109.70
21	C	101	LMU	O4'-C4B-C5B	2.18	114.69	109.32
20	L	207	CLA	CBC-CAC-C3C	-2.18	106.51	112.42
20	K	105	CLA	C3D-C4D-ND	2.18	113.53	109.99
20	2	310	CLA	CAA-C2A-C3A	-2.18	107.11	113.00
20	A	815	CLA	C4-C3-C5	2.18	119.01	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	813	CLA	C3D-C4D-ND	2.18	113.53	109.99
20	F	206	CLA	CHC-C1C-C2C	-2.18	120.76	126.95
20	1	213	CLA	C3C-C4C-CHD	-2.18	119.58	125.23
20	B	820	CLA	CHC-C1C-NC	2.18	127.59	124.31
20	3	313	CLA	CHB-C1B-NB	-2.18	120.94	124.08
20	R	107	CLA	O1D-CGD-CBD	-2.18	120.23	124.52
20	4	310	CLA	CBC-CAC-C3C	-2.17	106.52	112.42
21	H	104	LMU	O1'-C1-C2	2.17	116.74	109.37
20	B	826	CLA	C3D-C4D-ND	2.17	113.52	109.99
20	2	311	CLA	CHC-C4B-C3B	-2.17	117.94	127.37
20	A	808	CLA	CMB-C2B-C3B	2.17	131.66	126.55
21	K	101	LMU	C1'-O5'-C5'	2.17	117.96	113.72
20	4	311	CLA	CHB-C1B-NB	-2.17	120.94	124.08
21	E	101	LMU	C6-C5-C4	-2.17	103.39	114.37
20	K	107	CLA	C3D-C4D-ND	2.17	113.51	109.99
22	I	103	BCR	C3-C2-C1	-2.17	106.75	114.43
20	B	819	CLA	CHB-C4A-NA	2.17	127.53	124.40
20	B	827	CLA	C3B-C4B-NB	-2.17	108.59	110.53
20	3	319	CLA	C2A-C1A-CHA	-2.17	120.11	123.86
20	A	813	CLA	CED-O2D-CGD	2.17	120.83	115.92
20	A	817	CLA	O1D-CGD-CBD	-2.17	120.25	124.52
20	1	202	CLA	CMB-C2B-C3B	2.16	131.64	126.55
21	R	105	LMU	O2B-C2B-C1B	2.16	115.23	110.08
20	4	318	CLA	C3D-C4D-ND	2.16	113.50	109.99
21	L	210	LMU	C1'-C2'-C3'	-2.16	105.46	110.01
20	A	821	CLA	C1-C2-C3	-2.16	122.66	126.20
20	A	801	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
20	2	310	CLA	O2A-CGA-CBA	2.16	118.42	111.83
20	2	305	CLA	CHB-C1B-NB	-2.16	120.96	124.08
23	A	839	PQN	C12-C11-C3	-2.16	106.76	112.08
20	B	806	CLA	C3A-C2A-C1A	2.16	104.57	101.34
20	A	827	CLA	CBA-CAA-C2A	2.16	120.21	113.79
20	1	206	CLA	C3D-C4D-ND	2.16	113.49	109.99
20	1	207	CLA	C3D-C4D-ND	2.16	113.49	109.99
20	H	107	CLA	C4-C3-C5	2.16	118.97	115.23
20	B	803	CLA	C3A-C2A-C1A	2.16	104.57	101.34
20	J	103	CLA	CAA-C2A-C1A	-2.15	104.91	111.97
20	F	206	CLA	C2C-C1C-NC	2.15	112.24	109.98
20	J	103	CLA	CMB-C2B-C1B	2.15	128.70	125.42
20	B	848	CLA	CHC-C1C-C2C	-2.15	120.83	126.95
20	B	847	CLA	CMA-C3A-C2A	-2.15	105.66	113.98
20	A	824	CLA	O2D-CGD-O1D	-2.15	119.66	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	848	CLA	CMA-C3A-C4A	-2.15	105.99	111.77
20	B	816	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
20	2	304	CLA	O2A-CGA-CBA	2.15	118.40	111.83
20	K	106	CLA	C2A-C1A-CHA	-2.15	120.13	123.87
20	L	204	CLA	C4C-C3C-C2C	-2.15	103.76	106.89
20	F	206	CLA	CMC-C2C-C1C	2.15	128.39	125.03
21	R	102	LMU	O5B-C5B-C6B	2.15	111.77	106.44
20	B	838	CLA	C2A-C1A-CHA	-2.15	120.14	123.87
20	4	303	CLA	CAC-C3C-C4C	2.15	128.39	125.03
20	B	824	CLA	C7-C6-C5	-2.15	107.54	113.26
20	1	210	CLA	C1D-ND-C4D	-2.15	104.81	106.31
20	B	810	CLA	C1D-ND-C4D	-2.15	104.81	106.31
20	3	313	CLA	CHD-C1D-ND	2.15	127.88	124.84
20	B	808	CLA	CMB-C2B-C1B	2.15	128.69	125.42
20	B	817	CLA	CHB-C1B-NB	-2.15	120.83	124.05
20	4	318	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
20	A	804	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
22	I	101	BCR	C2-C1-C6	-2.15	107.32	110.44
20	B	826	CLA	O2A-CGA-CBA	2.14	118.38	111.83
20	A	814	CLA	C3D-C4D-ND	2.14	113.47	109.99
20	4	312	CLA	C2C-C1C-CHC	-2.14	120.22	125.84
20	1	212	CLA	CGD-CBD-CAD	-2.14	103.91	110.85
20	1	210	CLA	CMB-C2B-C1B	2.14	128.68	125.42
20	A	819	CLA	C3D-C4D-ND	2.14	113.47	109.99
20	A	810	CLA	C2A-C1A-CHA	-2.14	120.15	123.87
20	4	315	CLA	C1-O2A-CGA	2.14	122.92	116.07
22	B	850	BCR	C27-C26-C25	-2.14	119.81	122.70
20	B	837	CLA	C4B-C3B-C2B	2.14	109.96	107.30
20	3	303	CLA	CAA-C2A-C3A	-2.14	111.33	116.23
20	K	106	CLA	CMB-C2B-C1B	-2.14	122.17	125.42
20	2	312	CLA	C4-C3-C2	-2.14	118.14	123.63
21	H	102	LMU	O1B-C1B-O5B	2.13	116.31	110.69
20	2	306	CLA	O2A-CGA-CBA	2.13	118.34	111.83
20	1	212	CLA	CHB-C4A-NA	2.13	127.48	124.40
21	K	101	LMU	O4'-C4B-C3B	2.13	115.41	110.38
21	R	109	LMU	O1B-C4'-C3'	2.13	112.65	107.23
20	B	807	CLA	CMB-C2B-C3B	2.13	131.57	126.55
20	L	201	CLA	C1-O2A-CGA	2.13	121.81	116.65
21	2	318	LMU	C3B-C4B-C5B	2.13	114.10	110.23
20	B	837	CLA	CMA-C3A-C2A	-2.13	105.75	113.98
20	1	214	CLA	C2D-C1D-ND	-2.13	108.02	110.13
20	A	809	CLA	O2A-CGA-CBA	2.13	118.33	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	824	CLA	C4-C3-C5	2.13	118.92	115.23
20	B	808	CLA	CAC-C3C-C2C	-2.13	123.65	127.56
23	B	840	PQN	C14-C13-C12	-2.13	118.16	123.63
20	B	813	CLA	CHB-C1B-NB	-2.13	120.86	124.05
20	L	203	CLA	C3D-C4D-ND	2.13	113.44	109.99
20	B	805	CLA	C3C-C4C-NC	-2.12	107.71	110.43
20	B	811	CLA	CAC-C3C-C2C	-2.12	123.66	127.56
20	B	816	CLA	CHB-C1B-NB	-2.12	120.86	124.05
20	3	301	CLA	CGD-CBD-CAD	-2.12	103.97	110.85
20	4	315	CLA	CHC-C1C-C2C	-2.12	120.92	126.95
20	1	214	CLA	C2A-C1A-CHA	-2.12	120.19	123.87
22	3	311	BCR	C33-C5-C4	2.12	118.12	113.60
20	1	213	CLA	CHD-C1D-ND	2.12	127.84	124.84
20	B	848	CLA	C1D-ND-C4D	-2.12	104.82	106.31
21	L	205	LMU	C3B-C4B-C5B	2.12	114.08	110.23
20	2	302	CLA	CED-O2D-CGD	2.12	120.72	115.92
20	1	211	CLA	O2A-C1-C2	2.12	116.27	108.11
21	A	852	LMU	C6B-C5B-C4B	-2.12	107.81	113.02
21	K	102	LMU	C6B-C5B-C4B	-2.12	107.81	113.02
20	B	804	CLA	C2A-C1A-CHA	-2.12	120.19	123.87
20	A	826	CLA	CHB-C4A-NA	2.12	127.46	124.40
21	R	101	LMU	O2B-C2B-C3B	-2.12	105.38	110.38
20	B	811	CLA	CAA-C2A-C3A	-2.12	107.27	113.00
21	R	104	LMU	C1'-O5'-C5'	-2.12	109.58	113.72
20	B	804	CLA	CMA-C3A-C2A	-2.12	105.80	113.98
20	A	804	CLA	CHB-C1B-NB	-2.12	120.87	124.05
20	1	205	CLA	CHC-C4B-C3B	-2.12	121.28	127.43
20	B	804	CLA	C4D-CHA-C1A	-2.12	118.72	121.24
20	B	817	CLA	CHB-C4A-NA	2.12	127.45	124.40
20	B	813	CLA	O2A-CGA-CBA	2.11	120.13	112.14
20	4	308	CLA	CHD-C1D-ND	2.11	127.83	124.84
20	3	309	CLA	C3A-C2A-C1A	-2.11	98.17	101.34
20	B	808	CLA	CHC-C4B-C3B	-2.11	121.29	127.43
20	3	309	CLA	CHC-C4B-C3B	-2.11	118.20	127.37
20	A	812	CLA	CHB-C4A-NA	2.11	127.45	124.40
20	1	207	CLA	CAC-C3C-C4C	2.11	127.54	124.79
20	3	308	CLA	C3B-C4B-CHC	-2.11	119.28	126.76
20	1	212	CLA	CBA-CAA-C2A	-2.11	107.51	113.79
20	1	212	CLA	CED-O2D-CGD	2.11	120.70	115.92
21	H	103	LMU	O2B-C2B-C3B	-2.11	105.40	110.38
20	B	808	CLA	C3D-C4D-ND	2.11	113.42	109.99
20	1	209	CLA	CHB-C4A-NA	2.11	127.44	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	B	802	LMU	O4'-C4B-C3B	2.11	115.35	110.38
20	A	824	CLA	C3A-C2A-C1A	2.11	104.50	101.34
20	A	850	CLA	CHD-C4C-C3C	-2.11	121.70	124.77
20	1	208	CLA	CHB-C4A-NA	2.11	127.43	124.43
22	3	311	BCR	C39-C30-C25	-2.11	106.94	110.24
21	L	210	LMU	O1B-C1B-O5B	2.11	116.23	110.69
20	3	314	CLA	C2A-C1A-CHA	-2.11	120.21	123.87
20	B	821	CLA	C2C-C1C-NC	2.11	112.19	109.98
20	L	204	CLA	C3D-C4D-ND	2.10	113.41	109.99
21	R	101	LMU	O6B-C6B-C5B	-2.10	104.17	111.33
20	A	824	CLA	CHC-C4B-NB	2.10	127.20	124.05
20	G	103	CLA	CHC-C1C-C2C	-2.10	120.98	126.95
20	A	824	CLA	CMB-C2B-C1B	2.10	128.62	125.42
20	A	850	CLA	CMA-C3A-C2A	2.10	122.10	113.98
21	R	105	LMU	C3'-C4'-C5'	2.10	115.59	110.93
21	F	201	LMU	O5'-C1'-O1'	-2.10	105.08	110.04
20	A	816	CLA	CAA-C2A-C1A	-2.10	105.10	111.97
20	A	807	CLA	C5-C3-C2	-2.10	116.46	121.17
20	B	806	CLA	CHB-C1B-NB	-2.10	120.90	124.05
20	A	826	CLA	C3A-C2A-C1A	2.10	104.48	101.34
20	L	208	CLA	CHB-C4A-NA	2.10	127.43	124.40
20	A	814	CLA	C6-C7-C8	-2.10	109.00	115.97
20	4	304	CLA	CHB-C1B-C2B	-2.10	121.34	127.43
20	A	848	CLA	CMB-C2B-C1B	2.10	128.61	125.42
20	B	837	CLA	C3D-C4D-ND	2.10	113.39	109.99
20	4	303	CLA	CAA-C2A-C1A	-2.10	106.63	111.81
20	2	315	CLA	CHB-C4A-NA	2.10	127.41	124.43
20	3	320	CLA	C4-C3-C2	-2.10	118.25	123.63
20	4	307	CLA	C3B-C4B-NB	2.09	112.40	110.53
20	K	107	CLA	C1D-ND-C4D	-2.09	104.84	106.31
20	H	107	CLA	CHB-C1B-C2B	-2.09	121.35	127.43
20	A	816	CLA	C4-C3-C2	-2.09	118.25	123.63
20	B	839	CLA	C3D-C4D-ND	2.09	113.39	109.99
20	I	102	CLA	C4-C3-C5	2.09	118.86	115.23
21	F	201	LMU	O1B-C4'-C3'	-2.09	101.92	107.23
20	3	316	CLA	C3C-C4C-CHD	-2.09	119.80	125.23
20	L	207	CLA	CMA-C3A-C2A	-2.09	105.90	113.98
20	B	830	CLA	C1-O2A-CGA	2.09	121.71	116.65
22	A	842	BCR	C27-C26-C25	-2.09	119.88	122.70
22	I	103	BCR	C36-C18-C19	-2.09	114.90	118.09
20	4	304	CLA	C9-C8-C10	-2.09	103.83	111.27
20	B	814	CLA	CHB-C4A-NA	2.09	127.41	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	4	321	LMU	O5B-C5B-C4B	-2.09	105.94	109.70
20	4	317	CLA	C1C-NC-C4C	-2.08	105.73	106.68
20	1	204	CLA	CHB-C4A-NA	2.08	127.41	124.40
20	1	209	CLA	CMA-C3A-C2A	-2.08	111.45	116.23
21	R	109	LMU	O5'-C1'-C2'	-2.08	106.09	110.37
20	2	306	CLA	CBC-CAC-C3C	-2.08	106.77	112.42
21	H	105	LMU	O3'-C3'-C2'	2.08	115.28	110.38
20	2	314	CLA	C3C-C4C-CHD	-2.08	119.83	125.23
20	R	106	CLA	CAC-C3C-C4C	2.08	127.50	124.79
20	B	812	CLA	CMB-C2B-C1B	2.08	128.59	125.42
23	A	839	PQN	O1-C1-C2	2.08	123.19	120.45
20	F	206	CLA	CGD-CBD-CAD	-2.08	104.12	110.85
20	R	107	CLA	CAA-C2A-C1A	2.08	118.79	111.97
20	L	203	CLA	CHB-C4A-NA	2.08	127.40	124.40
20	2	311	CLA	CMB-C2B-C1B	2.08	128.58	125.42
22	3	311	BCR	C20-C19-C18	-2.08	120.67	126.36
21	R	101	LMU	O5B-C5B-C4B	2.08	113.44	109.70
20	A	820	CLA	O2D-CGD-O1D	-2.08	119.81	123.85
20	A	829	CLA	C3D-C4D-ND	2.08	113.36	109.99
20	A	813	CLA	C2D-C1D-ND	-2.08	108.07	110.13
20	3	312	CLA	CHD-C1D-ND	2.08	127.78	124.84
20	B	814	CLA	CAC-C3C-C4C	2.08	127.49	124.79
22	B	843	BCR	C27-C26-C25	-2.08	119.90	122.70
20	B	836	CLA	C4A-NA-C1A	2.08	107.63	106.68
20	3	307	CLA	C3D-C4D-ND	2.08	112.34	109.50
20	3	309	CLA	CHB-C1B-NB	-2.08	120.94	124.05
20	J	103	CLA	CAA-C2A-C3A	-2.07	107.39	113.00
20	2	304	CLA	CGD-CBD-CAD	-2.07	104.13	110.85
20	A	820	CLA	CGD-CBD-CAD	2.07	117.56	110.85
20	B	833	CLA	C4A-NA-C1A	2.07	107.62	106.68
20	L	207	CLA	CMC-C2C-C1C	2.07	128.27	125.03
21	2	320	LMU	C1B-O1B-C4'	2.07	122.89	117.98
20	2	307	CLA	C3D-C4D-ND	2.07	113.36	109.99
21	A	846	LMU	O1'-C1-C2	2.07	116.39	109.37
22	B	841	BCR	C27-C26-C25	-2.07	119.91	122.70
20	B	827	CLA	CAA-C2A-C3A	-2.07	107.40	113.00
20	1	204	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
20	F	206	CLA	C3B-C2B-C1B	-2.07	104.73	107.17
20	H	101	CLA	C3B-C4B-NB	2.07	112.38	110.53
20	3	309	CLA	C1-C2-C3	-2.07	122.81	126.20
20	4	317	CLA	C3C-C4C-CHD	-2.07	119.87	125.23
20	B	832	CLA	C3D-C4D-ND	2.06	113.34	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	2	304	CLA	C3D-C4D-ND	2.06	113.34	109.99
20	1	214	CLA	CMD-C2D-C3D	-2.06	122.96	127.69
20	A	805	CLA	O2A-CGA-CBA	2.06	119.94	112.14
20	A	825	CLA	C4B-C3B-C2B	2.06	109.87	107.30
20	3	309	CLA	C4-C3-C2	-2.06	118.33	123.63
20	2	306	CLA	CHB-C1B-NB	-2.06	120.95	124.05
20	B	822	CLA	C1D-ND-C4D	-2.06	104.86	106.31
20	B	828	CLA	C3D-C4D-ND	2.06	113.34	109.99
22	F	203	BCR	C30-C25-C24	2.06	121.24	115.65
20	A	813	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
20	4	305	CLA	CMA-C3A-C4A	-2.06	106.24	111.77
20	3	317	CLA	C4D-ND-C1D	-2.06	104.87	106.31
20	1	205	CLA	C1D-ND-C4D	-2.06	104.87	106.31
22	A	840	BCR	C4-C5-C6	-2.06	119.92	122.70
20	B	839	CLA	C1D-ND-C4D	-2.06	104.87	106.31
20	1	206	CLA	C2A-C1A-CHA	-2.06	120.30	123.87
20	A	804	CLA	C3D-C4D-ND	2.05	113.33	109.99
21	R	104	LMU	C3'-C4'-C5'	2.05	115.48	110.93
20	A	817	CLA	O2A-CGA-CBA	2.05	118.10	111.83
20	4	304	CLA	C9-C8-C7	2.05	118.59	111.27
20	4	310	CLA	C6-C5-C3	-2.05	108.47	113.47
20	2	306	CLA	CAC-C3C-C4C	2.05	127.46	124.79
22	F	202	BCR	C27-C26-C25	-2.05	119.93	122.70
21	4	321	LMU	C4B-C3B-C2B	2.05	114.43	110.83
20	1	212	CLA	CMB-C2B-C1B	2.05	128.54	125.42
20	B	838	CLA	O2D-CGD-CBD	2.05	114.81	111.23
20	A	826	CLA	C5-C3-C2	-2.05	116.57	121.17
20	4	303	CLA	CMA-C3A-C2A	-2.05	111.53	116.23
20	A	850	CLA	C3D-C4D-ND	2.05	113.31	109.99
20	A	809	CLA	C2D-C1D-ND	-2.05	108.10	110.13
22	B	850	BCR	C23-C24-C25	-2.05	121.53	127.00
20	L	201	CLA	C3D-C4D-ND	2.05	113.31	109.99
20	L	201	CLA	CHB-C1B-C2B	-2.04	121.49	127.43
20	A	830	CLA	CED-O2D-CGD	2.04	120.55	115.92
20	B	824	CLA	C4-C3-C5	2.04	118.78	115.23
20	G	103	CLA	C1-O2A-CGA	2.04	121.60	116.65
20	1	205	CLA	C3D-C4D-ND	2.04	113.31	109.99
22	B	842	BCR	C33-C5-C4	2.04	117.95	113.60
20	B	837	CLA	CBA-CAA-C2A	2.04	119.87	113.79
20	B	838	CLA	CMA-C3A-C4A	-2.04	106.28	111.77
20	2	309	CLA	CHD-C1D-ND	2.04	127.73	124.84
20	B	811	CLA	C3D-C4D-ND	2.04	113.31	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	809	CLA	O2A-CGA-CBA	2.04	118.06	111.83
20	1	210	CLA	C2A-C1A-CHA	-2.04	120.32	123.86
22	G	102	BCR	C27-C26-C25	-2.04	119.95	122.70
20	B	824	CLA	C1-O2A-CGA	-2.04	111.71	116.65
20	4	305	CLA	CHC-C4B-C3B	-2.04	118.52	127.37
21	H	103	LMU	C1B-O1B-C4'	-2.04	113.14	117.98
20	H	109	CLA	CAA-CBA-CGA	-2.04	107.42	113.21
20	B	806	CLA	C3D-C4D-ND	2.04	113.30	109.99
20	A	829	CLA	CGD-CBD-CAD	-2.04	104.25	110.85
20	A	811	CLA	C4-C3-C5	2.04	118.77	115.23
20	B	809	CLA	CAA-CBA-CGA	2.04	118.99	113.21
20	A	830	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
20	B	849	CLA	CHC-C4B-NB	2.04	127.10	124.05
20	H	101	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
20	A	813	CLA	CHB-C4A-NA	2.04	127.34	124.40
20	A	801	CLA	CMA-C3A-C2A	-2.03	106.11	113.98
20	L	203	CLA	C1-O2A-CGA	2.03	121.58	116.65
20	1	212	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
20	2	315	CLA	C4D-ND-C1D	-2.03	104.89	106.31
20	3	315	CLA	C5-C3-C4	2.03	119.27	114.59
21	K	102	LMU	O3'-C3'-C2'	-2.03	105.58	110.38
20	B	814	CLA	C4-C3-C5	2.03	118.75	115.23
20	A	827	CLA	C4A-NA-C1A	2.03	107.61	106.68
20	B	847	CLA	C2A-C1A-CHA	-2.03	120.34	123.87
20	A	821	CLA	C4B-C3B-C2B	2.03	109.83	107.30
20	B	818	CLA	CGD-CBD-CAD	2.03	117.42	110.85
20	A	826	CLA	C6-C7-C8	-2.03	109.22	115.97
20	B	810	CLA	CHC-C4B-NB	2.03	127.09	124.05
22	J	101	BCR	C4-C5-C6	-2.03	119.97	122.70
20	B	822	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
20	B	816	CLA	C11-C10-C8	-2.03	109.23	115.97
21	R	109	LMU	O5B-C1B-C2B	-2.03	106.21	110.37
20	3	314	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
20	B	835	CLA	C1-O2A-CGA	2.03	121.55	116.65
20	I	102	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
22	I	103	BCR	C31-C1-C6	-2.02	107.07	110.24
20	B	833	CLA	C3D-C4D-ND	2.02	113.28	109.99
22	B	843	BCR	C4-C5-C6	-2.02	119.97	122.70
20	A	825	CLA	C2A-C1A-CHA	-2.02	120.36	123.87
20	B	829	CLA	C1D-ND-C4D	-2.02	104.89	106.31
20	4	306	CLA	CGD-CBD-CAD	-2.02	104.30	110.85
20	2	312	CLA	C2A-C1A-CHA	-2.02	120.36	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	839	PQN	C17-C16-C15	-2.02	107.88	113.26
22	B	841	BCR	C4-C5-C6	-2.02	119.97	122.70
20	A	830	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
20	H	110	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
20	A	813	CLA	C2A-C1A-CHA	-2.02	120.36	123.87
21	L	206	LMU	C1-O1'-C1'	-2.02	110.23	113.68
20	B	849	CLA	C2A-C1A-CHA	-2.02	120.37	123.87
20	4	302	CLA	C1D-ND-C4D	-2.02	104.90	106.31
20	3	312	CLA	CHB-C1B-NB	-2.01	121.17	124.08
21	R	103	LMU	C1-O1'-C1'	2.01	117.12	113.68
20	B	808	CLA	O2A-C1-C2	2.01	115.85	108.11
21	G	101	LMU	O5B-C5B-C4B	-2.01	106.07	109.70
20	2	314	CLA	C1C-NC-C4C	-2.01	105.76	106.68
20	B	808	CLA	CHB-C1B-NB	-2.01	121.03	124.05
20	2	302	CLA	C1-C2-C3	2.01	129.49	126.20
20	A	817	CLA	C1-C2-C3	2.01	129.49	126.20
20	A	806	CLA	O2A-C1-C2	2.01	115.85	108.11
20	A	818	CLA	C2A-C1A-CHA	-2.01	120.38	123.87
20	A	850	CLA	CHB-C1B-NB	-2.01	121.03	124.05
20	A	801	CLA	CGD-CBD-CAD	2.01	117.35	110.85
20	A	804	CLA	CMB-C2B-C3B	2.01	131.28	126.55
20	A	817	CLA	C3A-C2A-C1A	2.01	104.35	101.34
21	2	320	LMU	O5B-C5B-C6B	2.01	111.42	106.44
20	R	107	CLA	CBA-CAA-C2A	2.01	119.77	113.79
20	L	204	CLA	CAA-CBA-CGA	-2.01	107.51	113.21
20	L	202	CLA	CED-O2D-CGD	2.01	120.47	115.92
22	G	102	BCR	C4-C5-C6	-2.01	119.99	122.70
20	A	816	CLA	CHB-C4A-NA	2.01	127.30	124.40
20	B	836	CLA	CHB-C4A-NA	2.01	127.30	124.40
20	K	106	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
20	2	308	CLA	CHB-C1B-NB	-2.01	121.18	124.08
20	L	208	CLA	CHA-C1A-NA	-2.01	121.85	126.39
21	K	101	LMU	C3-C2-C1	-2.00	104.75	113.47
20	B	827	CLA	CMA-C3A-C2A	-2.00	106.23	113.98
20	4	315	CLA	O2A-CGA-CBA	2.00	119.71	112.14
22	A	844	BCR	C27-C26-C25	-2.00	120.00	122.70
20	A	815	CLA	O1A-CGA-CBA	-2.00	115.95	123.78
20	A	822	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
20	A	816	CLA	C2A-C1A-CHA	-2.00	120.39	123.87
20	A	824	CLA	C3D-C4D-ND	2.00	113.24	109.99
20	4	310	CLA	C1-O2A-CGA	2.00	121.50	116.65
23	A	839	PQN	O1-C1-C10	-2.00	118.37	121.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	A	826	CLA	CAC-C3C-C4C	2.00	127.39	124.79
20	3	319	CLA	C3D-C4D-ND	2.00	113.24	109.99
21	H	104	LMU	O5'-C5'-C4'	-2.00	105.59	109.72

All (271) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	1	201	CLA	ND
20	1	202	CLA	ND
20	1	203	CLA	ND
20	1	204	CLA	ND
20	1	205	CLA	ND
20	1	206	CLA	ND
20	1	206	CLA	C8
20	1	207	CLA	ND
20	1	207	CLA	C2A
20	1	208	CLA	ND
20	1	209	CLA	ND
20	1	210	CLA	ND
20	1	211	CLA	ND
20	1	211	CLA	CBD
20	1	212	CLA	ND
20	1	212	CLA	C8
20	1	213	CLA	ND
20	1	214	CLA	C3A
20	1	214	CLA	ND
20	1	214	CLA	C2A
20	1	215	CLA	ND
20	2	301	CLA	ND
20	2	302	CLA	ND
20	2	302	CLA	C8
20	2	303	CLA	ND
20	2	304	CLA	ND
20	2	305	CLA	ND
20	2	306	CLA	ND
20	2	306	CLA	C8
20	2	307	CLA	ND
20	2	307	CLA	C8
20	2	308	CLA	ND
20	2	309	CLA	ND
20	2	310	CLA	ND
20	2	311	CLA	ND

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Mol	Chain	Res	Type	Atom
20	2	312	CLA	ND
20	2	312	CLA	C8
20	2	314	CLA	ND
20	2	315	CLA	ND
20	2	317	CLA	ND
20	2	317	CLA	C8
20	2	321	CLA	ND
20	2	321	CLA	C8
20	3	301	CLA	ND
20	3	301	CLA	C8
20	3	303	CLA	ND
20	3	304	CLA	ND
20	3	305	CLA	ND
20	3	306	CLA	ND
20	3	307	CLA	ND
20	3	308	CLA	ND
20	3	309	CLA	ND
20	3	309	CLA	C8
20	3	310	CLA	ND
20	3	310	CLA	C8
20	3	312	CLA	ND
20	3	313	CLA	ND
20	3	314	CLA	ND
20	3	315	CLA	ND
20	3	316	CLA	ND
20	3	317	CLA	ND
20	3	319	CLA	ND
20	3	320	CLA	ND
20	3	320	CLA	C8
20	4	302	CLA	ND
20	4	302	CLA	C8
20	4	303	CLA	ND
20	4	304	CLA	ND
20	4	304	CLA	C8
20	4	304	CLA	CBD
20	4	305	CLA	ND
20	4	305	CLA	C8
20	4	306	CLA	ND
20	4	307	CLA	ND
20	4	307	CLA	C2A
20	4	308	CLA	ND
20	4	309	CLA	ND

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Mol	Chain	Res	Type	Atom
20	4	310	CLA	ND
20	4	310	CLA	C8
20	4	311	CLA	ND
20	4	312	CLA	ND
20	4	313	CLA	ND
20	4	314	CLA	ND
20	4	315	CLA	ND
20	4	317	CLA	ND
20	4	318	CLA	ND
20	4	319	CLA	ND
20	A	801	CLA	ND
20	A	802	CLA	ND
20	A	802	CLA	C8
20	A	803	CLA	ND
20	A	803	CLA	C8
20	A	804	CLA	ND
20	A	804	CLA	C8
20	A	805	CLA	ND
20	A	806	CLA	ND
20	A	806	CLA	C8
20	A	807	CLA	ND
20	A	807	CLA	C8
20	A	808	CLA	ND
20	A	809	CLA	ND
20	A	809	CLA	C8
20	A	810	CLA	ND
20	A	811	CLA	ND
20	A	812	CLA	ND
20	A	813	CLA	ND
20	A	814	CLA	ND
20	A	814	CLA	C8
20	A	815	CLA	ND
20	A	816	CLA	ND
20	A	816	CLA	C8
20	A	817	CLA	ND
20	A	817	CLA	C8
20	A	818	CLA	ND
20	A	819	CLA	ND
20	A	820	CLA	ND
20	A	820	CLA	C8
20	A	821	CLA	ND
20	A	821	CLA	C8

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Mol	Chain	Res	Type	Atom
20	A	822	CLA	ND
20	A	822	CLA	C8
20	A	823	CLA	ND
20	A	823	CLA	C8
20	A	824	CLA	ND
20	A	824	CLA	C8
20	A	825	CLA	ND
20	A	825	CLA	C8
20	A	826	CLA	ND
20	A	826	CLA	C8
20	A	827	CLA	ND
20	A	828	CLA	ND
20	A	828	CLA	C8
20	A	829	CLA	ND
20	A	829	CLA	C8
20	A	830	CLA	ND
20	A	831	CLA	ND
20	A	832	CLA	ND
20	A	833	CLA	ND
20	A	833	CLA	C8
20	A	834	CLA	ND
20	A	835	CLA	ND
20	A	836	CLA	ND
20	A	836	CLA	C8
20	A	837	CLA	ND
20	A	837	CLA	C8
20	A	838	CLA	ND
20	A	847	CLA	ND
20	A	847	CLA	C8
20	A	848	CLA	ND
20	A	848	CLA	C8
20	A	849	CLA	ND
20	A	849	CLA	C8
20	A	850	CLA	ND
20	A	850	CLA	CBD
20	A	850	CLA	C2A
20	A	855	CLA	ND
20	A	855	CLA	C8
20	A	857	CLA	ND
20	B	803	CLA	ND
20	B	804	CLA	ND
20	B	804	CLA	C8

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Mol	Chain	Res	Type	Atom
20	B	805	CLA	ND
20	B	805	CLA	C8
20	B	806	CLA	ND
20	B	806	CLA	C8
20	B	807	CLA	ND
20	B	807	CLA	C8
20	B	808	CLA	ND
20	B	808	CLA	C8
20	B	809	CLA	ND
20	B	809	CLA	C8
20	B	810	CLA	ND
20	B	810	CLA	C8
20	B	811	CLA	ND
20	B	811	CLA	C8
20	B	812	CLA	ND
20	B	812	CLA	C8
20	B	813	CLA	ND
20	B	814	CLA	ND
20	B	814	CLA	C8
20	B	815	CLA	ND
20	B	815	CLA	C8
20	B	816	CLA	ND
20	B	816	CLA	C8
20	B	817	CLA	ND
20	B	818	CLA	ND
20	B	819	CLA	ND
20	B	819	CLA	C8
20	B	820	CLA	ND
20	B	821	CLA	ND
20	B	822	CLA	ND
20	B	822	CLA	C8
20	B	823	CLA	ND
20	B	823	CLA	C8
20	B	824	CLA	ND
20	B	824	CLA	C8
20	B	825	CLA	ND
20	B	825	CLA	C8
20	B	826	CLA	ND
20	B	826	CLA	C8
20	B	827	CLA	ND
20	B	828	CLA	ND
20	B	829	CLA	ND

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Mol	Chain	Res	Type	Atom
20	B	829	CLA	C8
20	B	830	CLA	ND
20	B	831	CLA	ND
20	B	832	CLA	ND
20	B	833	CLA	ND
20	B	834	CLA	ND
20	B	834	CLA	C8
20	B	835	CLA	ND
20	B	835	CLA	C8
20	B	836	CLA	ND
20	B	837	CLA	ND
20	B	837	CLA	C8
20	B	838	CLA	ND
20	B	838	CLA	C8
20	B	839	CLA	ND
20	B	847	CLA	ND
20	B	847	CLA	C8
20	B	848	CLA	ND
20	B	848	CLA	C8
20	B	849	CLA	ND
20	B	849	CLA	C8
20	F	204	CLA	ND
20	F	205	CLA	ND
20	F	206	CLA	C3A
20	F	206	CLA	ND
20	F	206	CLA	CBD
20	F	206	CLA	C2A
20	G	103	CLA	ND
20	H	101	CLA	ND
20	H	101	CLA	C8
20	H	101	CLA	CBD
20	H	107	CLA	ND
20	H	107	CLA	C8
20	H	108	CLA	ND
20	H	108	CLA	C8
20	H	109	CLA	ND
20	H	110	CLA	ND
20	H	110	CLA	C8
20	I	102	CLA	ND
20	I	102	CLA	C8
20	J	102	CLA	ND
20	J	102	CLA	C8

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Mol	Chain	Res	Type	Atom
20	J	103	CLA	ND
20	J	103	CLA	C8
20	K	103	CLA	ND
20	K	105	CLA	ND
20	K	106	CLA	ND
20	K	107	CLA	ND
20	K	107	CLA	C8
20	L	201	CLA	ND
20	L	201	CLA	C8
20	L	202	CLA	ND
20	L	202	CLA	C8
20	L	203	CLA	ND
20	L	203	CLA	C8
20	L	204	CLA	C3A
20	L	204	CLA	ND
20	L	204	CLA	C2A
20	L	207	CLA	ND
20	L	208	CLA	ND
20	L	208	CLA	CBD
20	R	106	CLA	ND
20	R	106	CLA	C8
20	R	107	CLA	ND
20	R	107	CLA	C8
21	R	109	LMU	C2B
23	A	839	PQN	C23
23	B	840	PQN	C23

All (2714) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	1	201	CLA	C1A-C2A-CAA-CBA
20	1	201	CLA	C3A-C2A-CAA-CBA
20	1	201	CLA	CBA-CGA-O2A-C1
20	1	201	CLA	C4B-C3B-CAB-CBB
20	1	201	CLA	CHA-CBD-CGD-O1D
20	1	201	CLA	CHA-CBD-CGD-O2D
20	1	202	CLA	C3A-C2A-CAA-CBA
20	1	202	CLA	CBD-CGD-O2D-CED
20	1	203	CLA	C4B-C3B-CAB-CBB
20	1	204	CLA	C1A-C2A-CAA-CBA
20	1	204	CLA	CBD-CGD-O2D-CED
20	1	204	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	1	206	CLA	C1A-C2A-CAA-CBA
20	1	206	CLA	C2C-C3C-CAC-CBC
20	1	206	CLA	C4C-C3C-CAC-CBC
20	1	206	CLA	CHA-CBD-CGD-O1D
20	1	206	CLA	CHA-CBD-CGD-O2D
20	1	207	CLA	C2B-C3B-CAB-CBB
20	1	207	CLA	C2-C3-C5-C6
20	1	207	CLA	C4-C3-C5-C6
20	1	211	CLA	C2B-C3B-CAB-CBB
20	1	211	CLA	CBD-CGD-O2D-CED
20	1	211	CLA	C2-C3-C5-C6
20	1	211	CLA	C4-C3-C5-C6
20	1	212	CLA	C4-C3-C5-C6
20	1	214	CLA	C3A-C2A-CAA-CBA
20	1	214	CLA	CBD-CGD-O2D-CED
20	1	214	CLA	C2-C3-C5-C6
20	2	301	CLA	C1A-C2A-CAA-CBA
20	2	301	CLA	C3A-C2A-CAA-CBA
20	2	301	CLA	O2A-C1-C2-C3
20	2	302	CLA	C1A-C2A-CAA-CBA
20	2	302	CLA	C3A-C2A-CAA-CBA
20	2	302	CLA	C4B-C3B-CAB-CBB
20	2	302	CLA	CAD-CBD-CGD-O1D
20	2	302	CLA	CAD-CBD-CGD-O2D
20	2	304	CLA	C2-C1-O2A-CGA
20	2	306	CLA	C1A-C2A-CAA-CBA
20	2	306	CLA	CBD-CGD-O2D-CED
20	2	307	CLA	CBA-CGA-O2A-C1
20	2	307	CLA	O1A-CGA-O2A-C1
20	2	311	CLA	CBA-CGA-O2A-C1
20	2	311	CLA	O1A-CGA-O2A-C1
20	2	311	CLA	C2B-C3B-CAB-CBB
20	2	312	CLA	C2-C1-O2A-CGA
20	2	312	CLA	C4B-C3B-CAB-CBB
20	2	312	CLA	CHA-CBD-CGD-O1D
20	2	312	CLA	CHA-CBD-CGD-O2D
20	2	312	CLA	CBD-CGD-O2D-CED
20	2	312	CLA	C14-C13-C15-C16
20	2	317	CLA	C4B-C3B-CAB-CBB
20	2	317	CLA	CHA-CBD-CGD-O1D
20	2	317	CLA	CHA-CBD-CGD-O2D
20	2	321	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	2	321	CLA	C3A-C2A-CAA-CBA
20	2	321	CLA	CAD-CBD-CGD-O1D
20	2	321	CLA	CAD-CBD-CGD-O2D
20	2	321	CLA	CBD-CGD-O2D-CED
20	3	301	CLA	C1A-C2A-CAA-CBA
20	3	301	CLA	C4B-C3B-CAB-CBB
20	3	309	CLA	C1A-C2A-CAA-CBA
20	3	309	CLA	C3A-C2A-CAA-CBA
20	3	309	CLA	CAD-CBD-CGD-O1D
20	3	309	CLA	CAD-CBD-CGD-O2D
20	3	310	CLA	CHA-CBD-CGD-O1D
20	3	310	CLA	CHA-CBD-CGD-O2D
20	3	314	CLA	C1A-C2A-CAA-CBA
20	3	314	CLA	C4B-C3B-CAB-CBB
20	3	315	CLA	C1A-C2A-CAA-CBA
20	3	320	CLA	C3A-C2A-CAA-CBA
20	3	320	CLA	CBD-CGD-O2D-CED
20	3	320	CLA	O1D-CGD-O2D-CED
20	4	302	CLA	C2C-C3C-CAC-CBC
20	4	302	CLA	C4C-C3C-CAC-CBC
20	4	302	CLA	C4-C3-C5-C6
20	4	304	CLA	C1A-C2A-CAA-CBA
20	4	304	CLA	C3A-C2A-CAA-CBA
20	4	305	CLA	CHA-CBD-CGD-O1D
20	4	305	CLA	CHA-CBD-CGD-O2D
20	4	310	CLA	C2B-C3B-CAB-CBB
20	4	310	CLA	CBD-CGD-O2D-CED
20	4	315	CLA	C1A-C2A-CAA-CBA
20	4	315	CLA	C4B-C3B-CAB-CBB
20	4	319	CLA	CHA-CBD-CGD-O1D
20	4	319	CLA	CHA-CBD-CGD-O2D
20	4	319	CLA	CBD-CGD-O2D-CED
20	A	802	CLA	C3A-C2A-CAA-CBA
20	A	802	CLA	CBA-CGA-O2A-C1
20	A	802	CLA	O1A-CGA-O2A-C1
20	A	803	CLA	C1A-C2A-CAA-CBA
20	A	803	CLA	C3A-C2A-CAA-CBA
20	A	803	CLA	C4B-C3B-CAB-CBB
20	A	804	CLA	CBA-CGA-O2A-C1
20	A	804	CLA	O1A-CGA-O2A-C1
20	A	804	CLA	CBD-CGD-O2D-CED
20	A	805	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	805	CLA	C3A-C2A-CAA-CBA
20	A	805	CLA	CBA-CGA-O2A-C1
20	A	806	CLA	C1A-C2A-CAA-CBA
20	A	806	CLA	C3A-C2A-CAA-CBA
20	A	806	CLA	CHA-CBD-CGD-O1D
20	A	806	CLA	CHA-CBD-CGD-O2D
20	A	807	CLA	C1A-C2A-CAA-CBA
20	A	808	CLA	CBD-CGD-O2D-CED
20	A	809	CLA	CBD-CGD-O2D-CED
20	A	811	CLA	C1A-C2A-CAA-CBA
20	A	811	CLA	C3A-C2A-CAA-CBA
20	A	811	CLA	C2B-C3B-CAB-CBB
20	A	811	CLA	CBD-CGD-O2D-CED
20	A	812	CLA	C1A-C2A-CAA-CBA
20	A	812	CLA	C2B-C3B-CAB-CBB
20	A	813	CLA	C1A-C2A-CAA-CBA
20	A	813	CLA	CBA-CGA-O2A-C1
20	A	813	CLA	O1A-CGA-O2A-C1
20	A	813	CLA	C2B-C3B-CAB-CBB
20	A	813	CLA	CBD-CGD-O2D-CED
20	A	814	CLA	CBA-CGA-O2A-C1
20	A	814	CLA	O1A-CGA-O2A-C1
20	A	815	CLA	C1A-C2A-CAA-CBA
20	A	815	CLA	C3A-C2A-CAA-CBA
20	A	815	CLA	O1A-CGA-O2A-C1
20	A	815	CLA	C2B-C3B-CAB-CBB
20	A	815	CLA	CBD-CGD-O2D-CED
20	A	816	CLA	C1A-C2A-CAA-CBA
20	A	816	CLA	C3A-C2A-CAA-CBA
20	A	816	CLA	CBA-CGA-O2A-C1
20	A	816	CLA	O1A-CGA-O2A-C1
20	A	816	CLA	CAD-CBD-CGD-O1D
20	A	816	CLA	CAD-CBD-CGD-O2D
20	A	816	CLA	CBD-CGD-O2D-CED
20	A	818	CLA	C1A-C2A-CAA-CBA
20	A	818	CLA	CAD-CBD-CGD-O1D
20	A	818	CLA	CAD-CBD-CGD-O2D
20	A	819	CLA	C1A-C2A-CAA-CBA
20	A	819	CLA	C3A-C2A-CAA-CBA
20	A	819	CLA	C4B-C3B-CAB-CBB
20	A	820	CLA	C1A-C2A-CAA-CBA
20	A	822	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
20	A	822	CLA	C4B-C3B-CAB-CBB
20	A	822	CLA	C2C-C3C-CAC-CBC
20	A	822	CLA	C4C-C3C-CAC-CBC
20	A	822	CLA	CBD-CGD-O2D-CED
20	A	823	CLA	C1A-C2A-CAA-CBA
20	A	823	CLA	O2A-C1-C2-C3
20	A	826	CLA	C1A-C2A-CAA-CBA
20	A	826	CLA	C3A-C2A-CAA-CBA
20	A	826	CLA	CHA-CBD-CGD-O1D
20	A	826	CLA	CHA-CBD-CGD-O2D
20	A	826	CLA	CBD-CGD-O2D-CED
20	A	828	CLA	C4B-C3B-CAB-CBB
20	A	828	CLA	CBD-CGD-O2D-CED
20	A	829	CLA	CHA-CBD-CGD-O1D
20	A	829	CLA	CHA-CBD-CGD-O2D
20	A	829	CLA	C14-C13-C15-C16
20	A	830	CLA	C1A-C2A-CAA-CBA
20	A	830	CLA	C3A-C2A-CAA-CBA
20	A	830	CLA	C4B-C3B-CAB-CBB
20	A	830	CLA	CAD-CBD-CGD-O1D
20	A	830	CLA	CAD-CBD-CGD-O2D
20	A	831	CLA	C1A-C2A-CAA-CBA
20	A	831	CLA	C4B-C3B-CAB-CBB
20	A	832	CLA	C1A-C2A-CAA-CBA
20	A	833	CLA	C4B-C3B-CAB-CBB
20	A	833	CLA	CAD-CBD-CGD-O1D
20	A	833	CLA	CAD-CBD-CGD-O2D
20	A	834	CLA	C1A-C2A-CAA-CBA
20	A	835	CLA	C1A-C2A-CAA-CBA
20	A	835	CLA	CBD-CGD-O2D-CED
20	A	836	CLA	C1A-C2A-CAA-CBA
20	A	836	CLA	C3A-C2A-CAA-CBA
20	A	838	CLA	C3A-C2A-CAA-CBA
20	A	838	CLA	C2B-C3B-CAB-CBB
20	A	838	CLA	CBD-CGD-O2D-CED
20	A	838	CLA	O1D-CGD-O2D-CED
20	A	847	CLA	C3A-C2A-CAA-CBA
20	A	847	CLA	CBA-CGA-O2A-C1
20	A	848	CLA	CBD-CGD-O2D-CED
20	A	848	CLA	O1D-CGD-O2D-CED
20	A	848	CLA	C6-C7-C8-C9
20	A	850	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	A	850	CLA	CAD-CBD-CGD-O2D
20	A	850	CLA	CBD-CGD-O2D-CED
20	A	855	CLA	C14-C13-C15-C16
20	B	803	CLA	C1A-C2A-CAA-CBA
20	B	803	CLA	C3A-C2A-CAA-CBA
20	B	803	CLA	C2B-C3B-CAB-CBB
20	B	804	CLA	C1A-C2A-CAA-CBA
20	B	804	CLA	C2-C1-O2A-CGA
20	B	804	CLA	CAD-CBD-CGD-O1D
20	B	804	CLA	CAD-CBD-CGD-O2D
20	B	805	CLA	C4B-C3B-CAB-CBB
20	B	805	CLA	CBD-CGD-O2D-CED
20	B	806	CLA	CHA-CBD-CGD-O2D
20	B	806	CLA	C11-C10-C8-C9
20	B	806	CLA	C12-C13-C15-C16
20	B	807	CLA	C1A-C2A-CAA-CBA
20	B	807	CLA	C2B-C3B-CAB-CBB
20	B	808	CLA	C1A-C2A-CAA-CBA
20	B	808	CLA	C3A-C2A-CAA-CBA
20	B	808	CLA	CBA-CGA-O2A-C1
20	B	808	CLA	O1A-CGA-O2A-C1
20	B	810	CLA	C1A-C2A-CAA-CBA
20	B	810	CLA	C4B-C3B-CAB-CBB
20	B	810	CLA	CAD-CBD-CGD-O1D
20	B	810	CLA	CAD-CBD-CGD-O2D
20	B	811	CLA	C1A-C2A-CAA-CBA
20	B	811	CLA	C3A-C2A-CAA-CBA
20	B	811	CLA	C2B-C3B-CAB-CBB
20	B	812	CLA	C1A-C2A-CAA-CBA
20	B	812	CLA	C4B-C3B-CAB-CBB
20	B	812	CLA	CAD-CBD-CGD-O1D
20	B	812	CLA	CAD-CBD-CGD-O2D
20	B	813	CLA	C3A-C2A-CAA-CBA
20	B	813	CLA	C2C-C3C-CAC-CBC
20	B	813	CLA	C4C-C3C-CAC-CBC
20	B	813	CLA	CBD-CGD-O2D-CED
20	B	814	CLA	C1A-C2A-CAA-CBA
20	B	814	CLA	C3A-C2A-CAA-CBA
20	B	814	CLA	CBD-CGD-O2D-CED
20	B	815	CLA	C1A-C2A-CAA-CBA
20	B	815	CLA	C3A-C2A-CAA-CBA
20	B	815	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	B	816	CLA	C1A-C2A-CAA-CBA
20	B	816	CLA	C3A-C2A-CAA-CBA
20	B	816	CLA	CHA-CBD-CGD-O1D
20	B	816	CLA	CHA-CBD-CGD-O2D
20	B	816	CLA	CBD-CGD-O2D-CED
20	B	817	CLA	C4B-C3B-CAB-CBB
20	B	817	CLA	CBD-CGD-O2D-CED
20	B	817	CLA	O1D-CGD-O2D-CED
20	B	818	CLA	C4B-C3B-CAB-CBB
20	B	818	CLA	CHA-CBD-CGD-O1D
20	B	818	CLA	CHA-CBD-CGD-O2D
20	B	818	CLA	CBD-CGD-O2D-CED
20	B	819	CLA	C1A-C2A-CAA-CBA
20	B	819	CLA	C3A-C2A-CAA-CBA
20	B	820	CLA	CBA-CGA-O2A-C1
20	B	820	CLA	O1A-CGA-O2A-C1
20	B	820	CLA	CBD-CGD-O2D-CED
20	B	820	CLA	C6-C7-C8-C9
20	B	821	CLA	C2B-C3B-CAB-CBB
20	B	822	CLA	C1A-C2A-CAA-CBA
20	B	822	CLA	C3A-C2A-CAA-CBA
20	B	822	CLA	C2C-C3C-CAC-CBC
20	B	822	CLA	C4C-C3C-CAC-CBC
20	B	822	CLA	CBD-CGD-O2D-CED
20	B	822	CLA	C11-C10-C8-C9
20	B	823	CLA	C1A-C2A-CAA-CBA
20	B	823	CLA	C3A-C2A-CAA-CBA
20	B	824	CLA	C3A-C2A-CAA-CBA
20	B	824	CLA	C2B-C3B-CAB-CBB
20	B	824	CLA	CBD-CGD-O2D-CED
20	B	825	CLA	C3A-C2A-CAA-CBA
20	B	826	CLA	CAD-CBD-CGD-O1D
20	B	826	CLA	CAD-CBD-CGD-O2D
20	B	827	CLA	C1A-C2A-CAA-CBA
20	B	827	CLA	C3A-C2A-CAA-CBA
20	B	827	CLA	C2B-C3B-CAB-CBB
20	B	827	CLA	CBD-CGD-O2D-CED
20	B	827	CLA	O1D-CGD-O2D-CED
20	B	828	CLA	C1A-C2A-CAA-CBA
20	B	828	CLA	C2B-C3B-CAB-CBB
20	B	828	CLA	C2C-C3C-CAC-CBC
20	B	828	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
20	B	828	CLA	CHA-CBD-CGD-O1D
20	B	828	CLA	CHA-CBD-CGD-O2D
20	B	829	CLA	C1A-C2A-CAA-CBA
20	B	830	CLA	C1A-C2A-CAA-CBA
20	B	830	CLA	C3A-C2A-CAA-CBA
20	B	830	CLA	CBD-CGD-O2D-CED
20	B	831	CLA	C1A-C2A-CAA-CBA
20	B	831	CLA	C3A-C2A-CAA-CBA
20	B	831	CLA	CAD-CBD-CGD-O1D
20	B	831	CLA	CAD-CBD-CGD-O2D
20	B	831	CLA	CBD-CGD-O2D-CED
20	B	832	CLA	CBD-CGD-O2D-CED
20	B	833	CLA	C3A-C2A-CAA-CBA
20	B	833	CLA	C2-C3-C5-C6
20	B	833	CLA	C4-C3-C5-C6
20	B	834	CLA	C4B-C3B-CAB-CBB
20	B	838	CLA	C3A-C2A-CAA-CBA
20	B	848	CLA	C4-C3-C5-C6
20	B	849	CLA	C2B-C3B-CAB-CBB
20	F	205	CLA	C2B-C3B-CAB-CBB
20	F	205	CLA	CBD-CGD-O2D-CED
20	F	206	CLA	C1A-C2A-CAA-CBA
20	F	206	CLA	C3A-C2A-CAA-CBA
20	F	206	CLA	C4B-C3B-CAB-CBB
20	F	206	CLA	CBD-CGD-O2D-CED
20	F	206	CLA	O1D-CGD-O2D-CED
20	G	103	CLA	CAD-CBD-CGD-O1D
20	G	103	CLA	CAD-CBD-CGD-O2D
20	G	103	CLA	CBD-CGD-O2D-CED
20	G	103	CLA	C2-C3-C5-C6
20	G	103	CLA	C4-C3-C5-C6
20	H	101	CLA	C1A-C2A-CAA-CBA
20	H	101	CLA	C3A-C2A-CAA-CBA
20	H	101	CLA	CAD-CBD-CGD-O1D
20	H	101	CLA	CAD-CBD-CGD-O2D
20	H	101	CLA	CBD-CGD-O2D-CED
20	H	107	CLA	C2B-C3B-CAB-CBB
20	H	107	CLA	C4B-C3B-CAB-CBB
20	H	107	CLA	O2A-C1-C2-C3
20	H	108	CLA	CAD-CBD-CGD-O1D
20	H	108	CLA	CAD-CBD-CGD-O2D
20	H	108	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	H	109	CLA	C1A-C2A-CAA-CBA
20	H	109	CLA	C3A-C2A-CAA-CBA
20	H	109	CLA	CBD-CGD-O2D-CED
20	H	110	CLA	C2B-C3B-CAB-CBB
20	H	110	CLA	C2-C3-C5-C6
20	H	110	CLA	C4-C3-C5-C6
20	I	102	CLA	C2B-C3B-CAB-CBB
20	J	102	CLA	C3A-C2A-CAA-CBA
20	J	102	CLA	CHA-CBD-CGD-O1D
20	J	102	CLA	CHA-CBD-CGD-O2D
20	J	102	CLA	CBD-CGD-O2D-CED
20	J	103	CLA	C2C-C3C-CAC-CBC
20	J	103	CLA	C4C-C3C-CAC-CBC
20	J	103	CLA	CAD-CBD-CGD-O1D
20	J	103	CLA	CAD-CBD-CGD-O2D
20	J	103	CLA	CBD-CGD-O2D-CED
20	K	103	CLA	O2A-C1-C2-C3
20	K	105	CLA	C4B-C3B-CAB-CBB
20	K	107	CLA	C1A-C2A-CAA-CBA
20	K	107	CLA	C3A-C2A-CAA-CBA
20	K	107	CLA	C2-C1-O2A-CGA
20	L	201	CLA	C1A-C2A-CAA-CBA
20	L	201	CLA	C4B-C3B-CAB-CBB
20	L	201	CLA	CBD-CGD-O2D-CED
20	L	203	CLA	C2B-C3B-CAB-CBB
20	L	203	CLA	CBD-CGD-O2D-CED
20	L	204	CLA	C1A-C2A-CAA-CBA
20	L	204	CLA	C3A-C2A-CAA-CBA
20	L	204	CLA	C2-C1-O2A-CGA
20	L	204	CLA	C2C-C3C-CAC-CBC
20	L	204	CLA	C4C-C3C-CAC-CBC
20	L	207	CLA	CHA-CBD-CGD-O1D
20	L	207	CLA	CHA-CBD-CGD-O2D
20	L	207	CLA	CBD-CGD-O2D-CED
20	L	208	CLA	C1A-C2A-CAA-CBA
20	L	208	CLA	C3A-C2A-CAA-CBA
20	L	208	CLA	C2C-C3C-CAC-CBC
20	L	208	CLA	C4C-C3C-CAC-CBC
20	R	106	CLA	C1A-C2A-CAA-CBA
20	R	106	CLA	CHA-CBD-CGD-O1D
20	R	106	CLA	CHA-CBD-CGD-O2D
20	R	106	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	R	107	CLA	C1A-C2A-CAA-CBA
20	R	107	CLA	C4B-C3B-CAB-CBB
20	R	107	CLA	CAD-CBD-CGD-O1D
20	R	107	CLA	CAD-CBD-CGD-O2D
20	R	107	CLA	O2A-C1-C2-C3
21	1	216	LMU	C2'-C1'-O1'-C1
21	1	217	LMU	C2-C1-O1'-C1'
21	2	313	LMU	C2-C1-O1'-C1'
21	2	316	LMU	O5'-C1'-O1'-C1
21	2	318	LMU	C2'-C1'-O1'-C1
21	2	318	LMU	O5'-C1'-O1'-C1
21	2	319	LMU	C2B-C1B-O1B-C4'
21	2	320	LMU	O5'-C1'-O1'-C1
21	2	320	LMU	C2-C1-O1'-C1'
21	3	302	LMU	C2'-C1'-O1'-C1
21	3	302	LMU	O5'-C1'-O1'-C1
21	3	318	LMU	O5'-C1'-O1'-C1
21	4	301	LMU	C5'-C4'-O1B-C1B
21	4	301	LMU	O5'-C1'-O1'-C1
21	4	320	LMU	O5'-C1'-O1'-C1
21	4	321	LMU	O5'-C1'-O1'-C1
21	4	322	LMU	C2'-C1'-O1'-C1
21	4	322	LMU	O5'-C1'-O1'-C1
21	A	846	LMU	C2-C1-O1'-C1'
21	A	851	LMU	O5'-C1'-O1'-C1
21	B	802	LMU	O5'-C1'-O1'-C1
21	E	101	LMU	C2'-C1'-O1'-C1
21	E	101	LMU	O5'-C1'-O1'-C1
21	F	201	LMU	C2'-C1'-O1'-C1
21	F	201	LMU	O5'-C1'-O1'-C1
21	H	102	LMU	C2'-C1'-O1'-C1
21	H	102	LMU	O5'-C1'-O1'-C1
21	H	103	LMU	C2-C1-O1'-C1'
21	H	104	LMU	O5'-C1'-O1'-C1
21	H	105	LMU	O5'-C1'-O1'-C1
21	K	101	LMU	C2B-C1B-O1B-C4'
21	K	102	LMU	C3'-C4'-O1B-C1B
21	K	102	LMU	C2'-C1'-O1'-C1
21	K	102	LMU	O5'-C1'-O1'-C1
21	L	210	LMU	C2-C1-O1'-C1'
21	R	101	LMU	C2-C1-O1'-C1'
21	R	103	LMU	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
21	R	103	LMU	C2-C1-O1'-C1'
21	R	105	LMU	C2-C1-O1'-C1'
21	R	108	LMU	O5B-C1B-O1B-C4'
21	R	108	LMU	O5'-C1'-O1'-C1
21	R	108	LMU	C2-C1-O1'-C1'
22	3	311	BCR	C18-C19-C20-C21
22	3	311	BCR	C20-C21-C22-C23
22	3	311	BCR	C20-C21-C22-C37
22	3	311	BCR	C21-C22-C23-C24
22	3	311	BCR	C37-C22-C23-C24
22	A	840	BCR	C18-C19-C20-C21
22	A	840	BCR	C20-C21-C22-C23
22	A	840	BCR	C20-C21-C22-C37
22	A	840	BCR	C21-C22-C23-C24
22	A	840	BCR	C37-C22-C23-C24
22	A	841	BCR	C1-C6-C7-C8
22	A	841	BCR	C5-C6-C7-C8
22	A	841	BCR	C7-C8-C9-C10
22	A	841	BCR	C7-C8-C9-C34
22	A	841	BCR	C11-C12-C13-C14
22	A	841	BCR	C11-C12-C13-C35
22	A	841	BCR	C20-C21-C22-C23
22	A	841	BCR	C20-C21-C22-C37
22	A	841	BCR	C21-C22-C23-C24
22	A	841	BCR	C37-C22-C23-C24
22	A	842	BCR	C5-C6-C7-C8
22	A	842	BCR	C11-C12-C13-C14
22	A	842	BCR	C36-C18-C19-C20
22	A	842	BCR	C20-C21-C22-C23
22	A	842	BCR	C20-C21-C22-C37
22	A	842	BCR	C21-C22-C23-C24
22	A	842	BCR	C37-C22-C23-C24
22	A	843	BCR	C1-C6-C7-C8
22	A	843	BCR	C5-C6-C7-C8
22	A	843	BCR	C7-C8-C9-C10
22	A	843	BCR	C7-C8-C9-C34
22	A	843	BCR	C18-C19-C20-C21
22	A	843	BCR	C37-C22-C23-C24
22	A	844	BCR	C17-C18-C19-C20
22	A	844	BCR	C18-C19-C20-C21
22	A	844	BCR	C19-C20-C21-C22
22	A	844	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
22	A	844	BCR	C20-C21-C22-C37
22	A	844	BCR	C23-C24-C25-C26
22	A	844	BCR	C23-C24-C25-C30
22	B	841	BCR	C1-C6-C7-C8
22	B	841	BCR	C5-C6-C7-C8
22	B	841	BCR	C18-C19-C20-C21
22	B	841	BCR	C20-C21-C22-C23
22	B	841	BCR	C20-C21-C22-C37
22	B	842	BCR	C20-C21-C22-C23
22	B	842	BCR	C20-C21-C22-C37
22	B	842	BCR	C37-C22-C23-C24
22	B	842	BCR	C23-C24-C25-C26
22	B	842	BCR	C23-C24-C25-C30
22	B	843	BCR	C9-C10-C11-C12
22	B	843	BCR	C17-C18-C19-C20
22	B	843	BCR	C36-C18-C19-C20
22	B	843	BCR	C21-C22-C23-C24
22	B	844	BCR	C1-C6-C7-C8
22	B	844	BCR	C5-C6-C7-C8
22	B	844	BCR	C7-C8-C9-C34
22	B	844	BCR	C18-C19-C20-C21
22	B	844	BCR	C19-C20-C21-C22
22	B	844	BCR	C20-C21-C22-C23
22	B	844	BCR	C20-C21-C22-C37
22	B	844	BCR	C21-C22-C23-C24
22	B	844	BCR	C37-C22-C23-C24
22	B	850	BCR	C11-C12-C13-C14
22	B	850	BCR	C11-C12-C13-C35
22	B	850	BCR	C20-C21-C22-C23
22	B	850	BCR	C20-C21-C22-C37
22	B	850	BCR	C21-C22-C23-C24
22	B	850	BCR	C37-C22-C23-C24
22	F	202	BCR	C5-C6-C7-C8
22	F	202	BCR	C18-C19-C20-C21
22	F	203	BCR	C7-C8-C9-C10
22	F	203	BCR	C15-C16-C17-C18
22	F	203	BCR	C18-C19-C20-C21
22	F	203	BCR	C20-C21-C22-C23
22	F	203	BCR	C20-C21-C22-C37
22	G	102	BCR	C7-C8-C9-C10
22	G	102	BCR	C7-C8-C9-C34
22	G	102	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
22	G	102	BCR	C18-C19-C20-C21
22	I	101	BCR	C1-C6-C7-C8
22	I	101	BCR	C5-C6-C7-C8
22	I	101	BCR	C17-C18-C19-C20
22	I	101	BCR	C19-C20-C21-C22
22	I	103	BCR	C11-C12-C13-C14
22	I	103	BCR	C11-C12-C13-C35
22	I	103	BCR	C17-C18-C19-C20
22	I	103	BCR	C36-C18-C19-C20
22	I	103	BCR	C18-C19-C20-C21
22	I	103	BCR	C19-C20-C21-C22
22	I	103	BCR	C20-C21-C22-C23
22	I	103	BCR	C20-C21-C22-C37
22	J	101	BCR	C5-C6-C7-C8
22	J	101	BCR	C7-C8-C9-C10
22	J	101	BCR	C7-C8-C9-C34
22	J	101	BCR	C18-C19-C20-C21
22	J	101	BCR	C20-C21-C22-C23
22	J	101	BCR	C20-C21-C22-C37
22	L	209	BCR	C7-C8-C9-C10
22	L	209	BCR	C7-C8-C9-C34
22	L	209	BCR	C20-C21-C22-C23
22	L	209	BCR	C20-C21-C22-C37
22	L	209	BCR	C21-C22-C23-C24
25	B	846	LMG	O6-C1-O1-C7
25	B	846	LMG	C11-C10-O7-C8
21	2	316	LMU	C5'-C4'-O1B-C1B
21	H	105	LMU	C3'-C4'-O1B-C1B
20	1	202	CLA	C4C-C3C-CAC-CBC
20	K	106	CLA	C4C-C3C-CAC-CBC
20	1	202	CLA	O1D-CGD-O2D-CED
20	1	214	CLA	O1D-CGD-O2D-CED
20	2	306	CLA	O1D-CGD-O2D-CED
20	3	314	CLA	O1D-CGD-O2D-CED
20	4	318	CLA	O1D-CGD-O2D-CED
20	4	319	CLA	O1D-CGD-O2D-CED
20	A	804	CLA	O1D-CGD-O2D-CED
20	A	814	CLA	O1D-CGD-O2D-CED
20	A	821	CLA	O1D-CGD-O2D-CED
20	A	850	CLA	O1D-CGD-O2D-CED
20	B	808	CLA	O1D-CGD-O2D-CED
20	B	813	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	B	814	CLA	O1D-CGD-O2D-CED
20	F	205	CLA	O1D-CGD-O2D-CED
20	G	103	CLA	O1D-CGD-O2D-CED
20	H	101	CLA	O1D-CGD-O2D-CED
20	H	109	CLA	O1D-CGD-O2D-CED
20	H	110	CLA	O1D-CGD-O2D-CED
20	L	201	CLA	O1D-CGD-O2D-CED
21	B	801	LMU	O5B-C1B-O1B-C4'
21	E	101	LMU	O5B-C1B-O1B-C4'
21	K	102	LMU	O5B-C1B-O1B-C4'
21	1	217	LMU	C3'-C4'-O1B-C1B
21	4	322	LMU	C5'-C4'-O1B-C1B
21	B	845	LMU	C3'-C4'-O1B-C1B
21	R	102	LMU	C3'-C4'-O1B-C1B
21	R	109	LMU	C3'-C4'-O1B-C1B
20	1	201	CLA	C4C-C3C-CAC-CBC
20	A	813	CLA	C4C-C3C-CAC-CBC
20	A	850	CLA	C4C-C3C-CAC-CBC
20	B	824	CLA	C4C-C3C-CAC-CBC
20	B	838	CLA	C4C-C3C-CAC-CBC
20	1	202	CLA	C2C-C3C-CAC-CBC
20	1	212	CLA	C2C-C3C-CAC-CBC
20	4	305	CLA	C2C-C3C-CAC-CBC
20	4	319	CLA	C2C-C3C-CAC-CBC
20	1	203	CLA	O1D-CGD-O2D-CED
20	1	206	CLA	O1D-CGD-O2D-CED
20	2	321	CLA	O1D-CGD-O2D-CED
20	4	315	CLA	O1D-CGD-O2D-CED
20	A	805	CLA	O1D-CGD-O2D-CED
20	A	809	CLA	O1D-CGD-O2D-CED
20	A	813	CLA	O1D-CGD-O2D-CED
20	A	815	CLA	O1D-CGD-O2D-CED
20	A	816	CLA	O1D-CGD-O2D-CED
20	A	828	CLA	O1D-CGD-O2D-CED
20	A	835	CLA	O1D-CGD-O2D-CED
20	B	818	CLA	O1D-CGD-O2D-CED
20	B	822	CLA	O1D-CGD-O2D-CED
20	B	830	CLA	O1D-CGD-O2D-CED
20	L	203	CLA	O1D-CGD-O2D-CED
20	L	207	CLA	O1D-CGD-O2D-CED
20	R	106	CLA	O1D-CGD-O2D-CED
20	1	201	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	1	203	CLA	CBD-CGD-O2D-CED
20	1	206	CLA	CBD-CGD-O2D-CED
20	1	207	CLA	CBD-CGD-O2D-CED
20	2	311	CLA	CBD-CGD-O2D-CED
20	3	314	CLA	CBD-CGD-O2D-CED
20	4	306	CLA	CBD-CGD-O2D-CED
20	4	315	CLA	CBD-CGD-O2D-CED
20	4	318	CLA	CBD-CGD-O2D-CED
20	A	802	CLA	CBD-CGD-O2D-CED
20	A	805	CLA	CBD-CGD-O2D-CED
20	A	807	CLA	CBD-CGD-O2D-CED
20	A	812	CLA	CBD-CGD-O2D-CED
20	A	814	CLA	CBD-CGD-O2D-CED
20	A	820	CLA	CBD-CGD-O2D-CED
20	A	821	CLA	CBD-CGD-O2D-CED
20	A	823	CLA	CBD-CGD-O2D-CED
20	A	824	CLA	CBD-CGD-O2D-CED
20	A	832	CLA	CBD-CGD-O2D-CED
20	A	836	CLA	CBD-CGD-O2D-CED
20	A	855	CLA	CBD-CGD-O2D-CED
20	B	804	CLA	CBD-CGD-O2D-CED
20	B	808	CLA	CBD-CGD-O2D-CED
20	B	812	CLA	CBD-CGD-O2D-CED
20	B	826	CLA	CBD-CGD-O2D-CED
20	B	829	CLA	CBD-CGD-O2D-CED
20	B	834	CLA	CBD-CGD-O2D-CED
20	B	847	CLA	CBD-CGD-O2D-CED
20	B	848	CLA	CBD-CGD-O2D-CED
20	B	849	CLA	CBD-CGD-O2D-CED
20	H	107	CLA	CBD-CGD-O2D-CED
20	H	110	CLA	CBD-CGD-O2D-CED
20	K	107	CLA	CBD-CGD-O2D-CED
20	L	208	CLA	CBD-CGD-O2D-CED
21	B	801	LMU	C2B-C1B-O1B-C4'
21	E	101	LMU	C2B-C1B-O1B-C4'
21	K	102	LMU	C2B-C1B-O1B-C4'
20	2	317	CLA	O1A-CGA-O2A-C1
20	3	310	CLA	O1A-CGA-O2A-C1
20	A	830	CLA	O1A-CGA-O2A-C1
20	A	847	CLA	O1A-CGA-O2A-C1
20	B	807	CLA	O1A-CGA-O2A-C1
20	B	814	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	B	836	CLA	O1A-CGA-O2A-C1
20	H	110	CLA	O1A-CGA-O2A-C1
20	R	106	CLA	O1A-CGA-O2A-C1
20	4	315	CLA	O1A-CGA-O2A-C1
20	A	805	CLA	O1A-CGA-O2A-C1
20	1	203	CLA	C2-C1-O2A-CGA
21	2	320	LMU	C5'-C4'-O1B-C1B
20	1	214	CLA	C4C-C3C-CAC-CBC
20	3	310	CLA	C4C-C3C-CAC-CBC
20	3	315	CLA	C4C-C3C-CAC-CBC
20	4	305	CLA	C4C-C3C-CAC-CBC
20	4	319	CLA	C4C-C3C-CAC-CBC
20	A	809	CLA	C4C-C3C-CAC-CBC
20	A	814	CLA	C4C-C3C-CAC-CBC
20	A	834	CLA	C4C-C3C-CAC-CBC
20	B	820	CLA	C4C-C3C-CAC-CBC
20	H	101	CLA	C4C-C3C-CAC-CBC
20	1	201	CLA	C2C-C3C-CAC-CBC
20	1	214	CLA	C2C-C3C-CAC-CBC
20	2	302	CLA	C2C-C3C-CAC-CBC
20	3	310	CLA	C2C-C3C-CAC-CBC
20	3	315	CLA	C2C-C3C-CAC-CBC
20	A	813	CLA	C2C-C3C-CAC-CBC
20	A	814	CLA	C2C-C3C-CAC-CBC
20	A	850	CLA	C2C-C3C-CAC-CBC
20	B	818	CLA	C2C-C3C-CAC-CBC
20	B	824	CLA	C2C-C3C-CAC-CBC
20	B	838	CLA	C2C-C3C-CAC-CBC
20	H	101	CLA	C2C-C3C-CAC-CBC
20	K	106	CLA	C2C-C3C-CAC-CBC
20	1	211	CLA	O1D-CGD-O2D-CED
20	B	805	CLA	O1D-CGD-O2D-CED
20	B	824	CLA	O1D-CGD-O2D-CED
20	J	102	CLA	O1D-CGD-O2D-CED
20	J	103	CLA	O1D-CGD-O2D-CED
21	1	216	LMU	O5B-C1B-O1B-C4'
21	2	313	LMU	O5B-C1B-O1B-C4'
21	A	846	LMU	O5B-C1B-O1B-C4'
21	G	101	LMU	O5B-C1B-O1B-C4'
21	L	210	LMU	O5B-C1B-O1B-C4'
21	R	101	LMU	O5B-C1B-O1B-C4'
21	R	104	LMU	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
20	4	315	CLA	CBA-CGA-O2A-C1
20	B	818	CLA	CBA-CGA-O2A-C1
21	A	845	LMU	C4B-C5B-C6B-O6B
21	A	846	LMU	C5'-C4'-O1B-C1B
21	K	104	LMU	C5'-C4'-O1B-C1B
25	B	846	LMG	C8-C9-O8-C28
20	1	204	CLA	C4C-C3C-CAC-CBC
20	1	212	CLA	C4C-C3C-CAC-CBC
20	A	817	CLA	C4C-C3C-CAC-CBC
20	B	834	CLA	C4C-C3C-CAC-CBC
20	1	204	CLA	C2C-C3C-CAC-CBC
20	B	820	CLA	C2C-C3C-CAC-CBC
20	1	207	CLA	O1D-CGD-O2D-CED
20	4	306	CLA	O1D-CGD-O2D-CED
20	A	807	CLA	O1D-CGD-O2D-CED
20	A	822	CLA	O1D-CGD-O2D-CED
20	A	824	CLA	O1D-CGD-O2D-CED
20	A	855	CLA	O1D-CGD-O2D-CED
20	B	804	CLA	O1D-CGD-O2D-CED
20	B	812	CLA	O1D-CGD-O2D-CED
20	K	107	CLA	O1D-CGD-O2D-CED
20	2	317	CLA	CBA-CGA-O2A-C1
20	3	310	CLA	CBA-CGA-O2A-C1
20	A	830	CLA	CBA-CGA-O2A-C1
20	B	821	CLA	CBA-CGA-O2A-C1
20	B	833	CLA	CBA-CGA-O2A-C1
20	B	836	CLA	CBA-CGA-O2A-C1
20	H	110	CLA	CBA-CGA-O2A-C1
20	R	106	CLA	CBA-CGA-O2A-C1
20	I	102	CLA	CBD-CGD-O2D-CED
20	1	206	CLA	O1A-CGA-O2A-C1
20	1	207	CLA	O1A-CGA-O2A-C1
20	2	312	CLA	O1A-CGA-O2A-C1
20	A	824	CLA	O1A-CGA-O2A-C1
20	A	838	CLA	O1A-CGA-O2A-C1
20	A	849	CLA	O1A-CGA-O2A-C1
20	B	817	CLA	O1A-CGA-O2A-C1
20	B	821	CLA	O1A-CGA-O2A-C1
20	B	828	CLA	O1A-CGA-O2A-C1
20	B	833	CLA	O1A-CGA-O2A-C1
20	B	847	CLA	O1A-CGA-O2A-C1
20	J	102	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	K	103	CLA	O1A-CGA-O2A-C1
20	L	202	CLA	O1A-CGA-O2A-C1
20	R	107	CLA	O1A-CGA-O2A-C1
20	1	201	CLA	O1A-CGA-O2A-C1
20	2	301	CLA	C4C-C3C-CAC-CBC
20	2	302	CLA	C4C-C3C-CAC-CBC
20	A	815	CLA	C4C-C3C-CAC-CBC
20	A	830	CLA	C4C-C3C-CAC-CBC
20	B	849	CLA	C4C-C3C-CAC-CBC
20	4	310	CLA	O1D-CGD-O2D-CED
20	A	812	CLA	O1D-CGD-O2D-CED
20	A	832	CLA	O1D-CGD-O2D-CED
20	B	831	CLA	O1D-CGD-O2D-CED
21	B	802	LMU	C3'-C4'-O1B-C1B
20	2	311	CLA	C4C-C3C-CAC-CBC
20	B	818	CLA	C4C-C3C-CAC-CBC
20	2	301	CLA	C2C-C3C-CAC-CBC
20	2	311	CLA	C2C-C3C-CAC-CBC
20	A	809	CLA	C2C-C3C-CAC-CBC
20	A	817	CLA	C2C-C3C-CAC-CBC
20	A	830	CLA	C2C-C3C-CAC-CBC
20	A	834	CLA	C2C-C3C-CAC-CBC
20	B	849	CLA	C2C-C3C-CAC-CBC
20	A	808	CLA	O1D-CGD-O2D-CED
20	A	811	CLA	O1D-CGD-O2D-CED
20	A	826	CLA	O1D-CGD-O2D-CED
20	B	820	CLA	O1D-CGD-O2D-CED
20	B	832	CLA	O1D-CGD-O2D-CED
20	H	108	CLA	O1D-CGD-O2D-CED
21	4	316	LMU	O5'-C5'-C6'-O6'
20	2	306	CLA	C15-C16-C17-C18
20	1	212	CLA	CBD-CGD-O2D-CED
21	1	218	LMU	C3'-C4'-O1B-C1B
20	A	823	CLA	C4C-C3C-CAC-CBC
20	B	826	CLA	C4C-C3C-CAC-CBC
20	B	834	CLA	C2C-C3C-CAC-CBC
25	B	846	LMG	O9-C10-O7-C8
20	B	813	CLA	CBA-CGA-O2A-C1
20	B	813	CLA	O1A-CGA-O2A-C1
20	4	302	CLA	C3-C5-C6-C7
20	4	305	CLA	C3-C5-C6-C7
20	A	803	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	A	817	CLA	C3-C5-C6-C7
20	A	824	CLA	C3-C5-C6-C7
20	A	826	CLA	C3-C5-C6-C7
20	A	828	CLA	C3-C5-C6-C7
20	B	804	CLA	C3-C5-C6-C7
20	B	808	CLA	C3-C5-C6-C7
20	B	834	CLA	C3-C5-C6-C7
20	B	837	CLA	C3-C5-C6-C7
20	B	838	CLA	C3-C5-C6-C7
21	A	851	LMU	C3'-C4'-O1B-C1B
21	A	854	LMU	C3'-C4'-O1B-C1B
20	A	815	CLA	C2C-C3C-CAC-CBC
20	A	823	CLA	C2C-C3C-CAC-CBC
20	B	826	CLA	C2C-C3C-CAC-CBC
20	1	206	CLA	CBA-CGA-O2A-C1
20	A	815	CLA	CBA-CGA-O2A-C1
20	A	849	CLA	CBA-CGA-O2A-C1
20	A	850	CLA	CBA-CGA-O2A-C1
20	B	807	CLA	CBA-CGA-O2A-C1
20	B	814	CLA	CBA-CGA-O2A-C1
20	B	828	CLA	CBA-CGA-O2A-C1
20	B	847	CLA	CBA-CGA-O2A-C1
20	F	206	CLA	CBA-CGA-O2A-C1
20	K	103	CLA	CBA-CGA-O2A-C1
20	L	202	CLA	CBA-CGA-O2A-C1
20	R	107	CLA	CBA-CGA-O2A-C1
21	R	103	LMU	O5B-C5B-C6B-O6B
20	2	317	CLA	CBD-CGD-O2D-CED
20	3	301	CLA	CBD-CGD-O2D-CED
20	3	310	CLA	CBD-CGD-O2D-CED
20	4	305	CLA	CBD-CGD-O2D-CED
20	A	810	CLA	CBD-CGD-O2D-CED
20	A	829	CLA	CBD-CGD-O2D-CED
20	A	831	CLA	CBD-CGD-O2D-CED
20	A	833	CLA	CBD-CGD-O2D-CED
20	B	815	CLA	CBD-CGD-O2D-CED
20	A	837	CLA	C2C-C3C-CAC-CBC
20	2	312	CLA	O1D-CGD-O2D-CED
20	B	816	CLA	O1D-CGD-O2D-CED
20	4	318	CLA	O1A-CGA-O2A-C1
20	1	207	CLA	C2C-C3C-CAC-CBC
21	R	109	LMU	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
20	2	302	CLA	C4-C3-C5-C6
20	2	317	CLA	C4-C3-C5-C6
20	3	301	CLA	C4-C3-C5-C6
20	A	803	CLA	C4-C3-C5-C6
20	A	814	CLA	C4-C3-C5-C6
20	A	837	CLA	C4-C3-C5-C6
20	B	816	CLA	C4-C3-C5-C6
20	B	822	CLA	C4-C3-C5-C6
20	L	201	CLA	C4-C3-C5-C6
20	L	203	CLA	C4-C3-C5-C6
20	R	106	CLA	C4-C3-C5-C6
23	A	839	PQN	C14-C13-C15-C16
23	B	840	PQN	C14-C13-C15-C16
20	1	212	CLA	C2-C3-C5-C6
20	2	317	CLA	C2-C3-C5-C6
20	3	301	CLA	C2-C3-C5-C6
20	4	302	CLA	C2-C3-C5-C6
20	A	803	CLA	C2-C3-C5-C6
20	A	814	CLA	C2-C3-C5-C6
20	B	822	CLA	C2-C3-C5-C6
20	B	848	CLA	C2-C3-C5-C6
20	L	203	CLA	C2-C3-C5-C6
20	R	106	CLA	C2-C3-C5-C6
23	A	839	PQN	C12-C13-C15-C16
23	B	840	PQN	C12-C13-C15-C16
20	2	311	CLA	O1D-CGD-O2D-CED
20	A	837	CLA	C2A-CAA-CBA-CGA
20	B	814	CLA	C2A-CAA-CBA-CGA
20	H	107	CLA	C2A-CAA-CBA-CGA
20	J	102	CLA	C2A-CAA-CBA-CGA
20	K	106	CLA	C2A-CAA-CBA-CGA
20	R	106	CLA	C2A-CAA-CBA-CGA
20	3	301	CLA	O1A-CGA-O2A-C1
20	A	807	CLA	O1A-CGA-O2A-C1
20	2	312	CLA	C3-C5-C6-C7
20	A	825	CLA	C3-C5-C6-C7
20	A	836	CLA	C3-C5-C6-C7
20	B	819	CLA	C3-C5-C6-C7
20	B	848	CLA	C3-C5-C6-C7
20	J	103	CLA	C3-C5-C6-C7
20	1	207	CLA	CBA-CGA-O2A-C1
20	2	312	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	824	CLA	CBA-CGA-O2A-C1
20	A	838	CLA	CBA-CGA-O2A-C1
20	B	809	CLA	CBA-CGA-O2A-C1
20	B	816	CLA	CBA-CGA-O2A-C1
20	B	817	CLA	CBA-CGA-O2A-C1
20	H	108	CLA	CBA-CGA-O2A-C1
20	J	102	CLA	CBA-CGA-O2A-C1
20	L	208	CLA	CBA-CGA-O2A-C1
21	B	845	LMU	O5'-C5'-C6'-O6'
21	K	102	LMU	C4B-C5B-C6B-O6B
21	R	102	LMU	C4B-C5B-C6B-O6B
21	R	105	LMU	O5B-C5B-C6B-O6B
21	H	102	LMU	C2B-C1B-O1B-C4'
21	4	320	LMU	C4'-C5'-C6'-O6'
22	3	311	BCR	C19-C20-C21-C22
22	A	840	BCR	C9-C10-C11-C12
22	A	842	BCR	C19-C20-C21-C22
22	B	842	BCR	C19-C20-C21-C22
22	B	850	BCR	C19-C20-C21-C22
22	F	203	BCR	C13-C14-C15-C16
22	F	203	BCR	C19-C20-C21-C22
20	4	319	CLA	O1A-CGA-O2A-C1
20	A	850	CLA	O1A-CGA-O2A-C1
20	B	816	CLA	O1A-CGA-O2A-C1
20	F	206	CLA	O1A-CGA-O2A-C1
20	H	108	CLA	O1A-CGA-O2A-C1
20	B	826	CLA	O1D-CGD-O2D-CED
20	B	829	CLA	O1D-CGD-O2D-CED
20	3	301	CLA	C5-C6-C7-C8
21	R	103	LMU	C3'-C4'-O1B-C1B
20	B	818	CLA	O1A-CGA-O2A-C1
21	G	101	LMU	O5'-C5'-C6'-O6'
20	A	837	CLA	C4C-C3C-CAC-CBC
20	J	102	CLA	C2C-C3C-CAC-CBC
21	B	801	LMU	C4B-C5B-C6B-O6B
21	K	101	LMU	C4'-C5'-C6'-O6'
20	A	802	CLA	O1D-CGD-O2D-CED
20	3	310	CLA	C3-C5-C6-C7
20	A	820	CLA	C3-C5-C6-C7
20	H	110	CLA	C3-C5-C6-C7
20	4	307	CLA	CBD-CGD-O2D-CED
20	A	830	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	4	321	LMU	C2B-C1B-O1B-C4'
20	A	820	CLA	O1D-CGD-O2D-CED
20	A	823	CLA	O1D-CGD-O2D-CED
20	2	304	CLA	CBA-CGA-O2A-C1
20	4	310	CLA	CBA-CGA-O2A-C1
20	4	318	CLA	CBA-CGA-O2A-C1
20	A	807	CLA	CBA-CGA-O2A-C1
20	A	826	CLA	CBA-CGA-O2A-C1
20	A	855	CLA	CBA-CGA-O2A-C1
20	H	107	CLA	CBA-CGA-O2A-C1
21	2	313	LMU	O5'-C5'-C6'-O6'
21	3	318	LMU	O5'-C5'-C6'-O6'
21	4	321	LMU	O5B-C5B-C6B-O6B
21	F	201	LMU	O5B-C5B-C6B-O6B
21	R	103	LMU	O5'-C5'-C6'-O6'
21	R	104	LMU	O5B-C5B-C6B-O6B
20	L	208	CLA	O1A-CGA-O2A-C1
21	H	103	LMU	C3-C4-C5-C6
21	1	218	LMU	O5'-C5'-C6'-O6'
21	R	102	LMU	O5'-C5'-C6'-O6'
21	1	216	LMU	C4'-C5'-C6'-O6'
21	4	316	LMU	C4'-C5'-C6'-O6'
20	B	828	CLA	CBD-CGD-O2D-CED
20	1	207	CLA	C4C-C3C-CAC-CBC
20	K	103	CLA	C2C-C3C-CAC-CBC
21	A	845	LMU	C3'-C4'-O1B-C1B
20	A	855	CLA	O1A-CGA-O2A-C1
21	F	201	LMU	O5'-C5'-C6'-O6'
21	L	205	LMU	O5'-C5'-C6'-O6'
21	4	321	LMU	O5B-C1B-O1B-C4'
20	K	107	CLA	C3-C5-C6-C7
20	L	203	CLA	C3-C5-C6-C7
23	A	839	PQN	C13-C15-C16-C17
21	A	852	LMU	C2-C3-C4-C5
21	G	101	LMU	C11-C10-C9-C8
21	E	101	LMU	C1-C2-C3-C4
20	4	319	CLA	C2-C1-O2A-CGA
20	A	818	CLA	CBD-CGD-O2D-CED
20	A	834	CLA	CBD-CGD-O2D-CED
20	B	811	CLA	CBD-CGD-O2D-CED
20	B	836	CLA	CBD-CGD-O2D-CED
21	2	318	LMU	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
21	R	104	LMU	O5'-C5'-C6'-O6'
21	4	322	LMU	C4B-C5B-C6B-O6B
21	G	101	LMU	C4'-C5'-C6'-O6'
21	R	103	LMU	C4B-C5B-C6B-O6B
21	R	105	LMU	C4B-C5B-C6B-O6B
20	B	834	CLA	O1D-CGD-O2D-CED
20	B	848	CLA	O1D-CGD-O2D-CED
20	I	102	CLA	O1D-CGD-O2D-CED
20	3	301	CLA	CBA-CGA-O2A-C1
20	4	319	CLA	CBA-CGA-O2A-C1
20	1	206	CLA	C4-C3-C5-C6
20	A	829	CLA	C4-C3-C5-C6
20	A	848	CLA	C4-C3-C5-C6
20	A	829	CLA	C2-C3-C5-C6
20	A	837	CLA	C2-C3-C5-C6
20	A	848	CLA	C2-C3-C5-C6
20	L	201	CLA	C2-C3-C5-C6
20	2	304	CLA	O1A-CGA-O2A-C1
20	A	826	CLA	O1A-CGA-O2A-C1
20	B	809	CLA	O1A-CGA-O2A-C1
21	1	218	LMU	C4'-C5'-C6'-O6'
21	3	318	LMU	C4'-C5'-C6'-O6'
21	R	102	LMU	C4'-C5'-C6'-O6'
21	R	104	LMU	C4B-C5B-C6B-O6B
20	A	849	CLA	C2C-C3C-CAC-CBC
20	B	808	CLA	C5-C6-C7-C8
21	1	216	LMU	O5'-C5'-C6'-O6'
21	4	321	LMU	O5'-C5'-C6'-O6'
21	A	854	LMU	O5'-C5'-C6'-O6'
21	2	316	LMU	C4'-C5'-C6'-O6'
21	L	206	LMU	C4B-C5B-C6B-O6B
20	4	318	CLA	C3-C5-C6-C7
20	A	803	CLA	C2A-CAA-CBA-CGA
20	B	837	CLA	C2A-CAA-CBA-CGA
20	H	110	CLA	C2A-CAA-CBA-CGA
20	A	836	CLA	O1D-CGD-O2D-CED
20	4	310	CLA	O1A-CGA-O2A-C1
21	1	216	LMU	O5'-C1'-O1'-C1
21	4	316	LMU	O5'-C1'-O1'-C1
21	A	853	LMU	O5'-C1'-O1'-C1
21	C	101	LMU	O5'-C1'-O1'-C1
21	H	103	LMU	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
21	K	101	LMU	O5'-C1'-O1'-C1
21	L	206	LMU	O5'-C1'-O1'-C1
21	L	210	LMU	O5'-C1'-O1'-C1
21	R	104	LMU	O5'-C1'-O1'-C1
21	R	105	LMU	O5'-C1'-O1'-C1
21	R	109	LMU	O5'-C1'-O1'-C1
21	4	320	LMU	O5'-C5'-C6'-O6'
21	A	851	LMU	O5'-C5'-C6'-O6'
21	A	853	LMU	O5B-C5B-C6B-O6B
21	R	109	LMU	O5'-C5'-C6'-O6'
21	H	104	LMU	O1'-C1-C2-C3
20	A	835	CLA	CBA-CGA-O2A-C1
21	R	103	LMU	C11-C10-C9-C8
20	A	825	CLA	CBD-CGD-O2D-CED
21	3	302	LMU	O5'-C5'-C6'-O6'
21	B	801	LMU	O5B-C5B-C6B-O6B
21	H	103	LMU	O5'-C5'-C6'-O6'
21	K	104	LMU	O5'-C5'-C6'-O6'
20	2	304	CLA	C2C-C3C-CAC-CBC
21	1	217	LMU	C1-C2-C3-C4
21	2	313	LMU	C5'-C4'-O1B-C1B
20	H	107	CLA	O1A-CGA-O2A-C1
21	1	218	LMU	C7-C8-C9-C10
21	R	101	LMU	C6-C7-C8-C9
21	R	101	LMU	C11-C10-C9-C8
20	L	207	CLA	C2C-C3C-CAC-CBC
21	2	316	LMU	O5B-C1B-O1B-C4'
21	3	318	LMU	O5B-C5B-C6B-O6B
21	A	845	LMU	O5B-C5B-C6B-O6B
21	K	101	LMU	O5'-C5'-C6'-O6'
21	K	102	LMU	O5B-C5B-C6B-O6B
21	L	205	LMU	O5B-C5B-C6B-O6B
21	L	206	LMU	O5B-C5B-C6B-O6B
21	R	102	LMU	O5B-C5B-C6B-O6B
20	H	107	CLA	O1D-CGD-O2D-CED
21	F	201	LMU	C4'-C5'-C6'-O6'
21	K	104	LMU	C5-C6-C7-C8
20	A	849	CLA	CBD-CGD-O2D-CED
20	B	837	CLA	C2C-C3C-CAC-CBC
21	A	851	LMU	O5B-C1B-O1B-C4'
21	F	201	LMU	C4B-C5B-C6B-O6B
21	R	109	LMU	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
21	4	321	LMU	C7-C8-C9-C10
22	A	840	BCR	C19-C20-C21-C22
22	A	841	BCR	C19-C20-C21-C22
20	1	211	CLA	CBA-CGA-O2A-C1
20	2	301	CLA	CBA-CGA-O2A-C1
20	2	310	CLA	CBA-CGA-O2A-C1
20	4	305	CLA	CBA-CGA-O2A-C1
20	A	810	CLA	CBA-CGA-O2A-C1
20	A	834	CLA	CBA-CGA-O2A-C1
20	A	836	CLA	CBA-CGA-O2A-C1
20	H	109	CLA	CBA-CGA-O2A-C1
20	K	106	CLA	CBA-CGA-O2A-C1
25	B	846	LMG	C29-C28-O8-C9
21	E	101	LMU	C3-C4-C5-C6
20	2	310	CLA	CBD-CGD-O2D-CED
21	L	205	LMU	C4'-C5'-C6'-O6'
21	A	845	LMU	C2-C3-C4-C5
21	A	851	LMU	C2-C3-C4-C5
21	A	852	LMU	C4-C5-C6-C7
21	F	201	LMU	C7-C8-C9-C10
21	H	105	LMU	C7-C8-C9-C10
21	R	105	LMU	C2-C3-C4-C5
20	4	307	CLA	O1D-CGD-O2D-CED
20	B	815	CLA	O1D-CGD-O2D-CED
20	B	847	CLA	O1D-CGD-O2D-CED
21	H	103	LMU	C6-C7-C8-C9
21	H	104	LMU	C5-C6-C7-C8
21	A	845	LMU	C4'-C5'-C6'-O6'
21	A	853	LMU	C4B-C5B-C6B-O6B
21	L	210	LMU	C5-C6-C7-C8
21	H	102	LMU	C1-C2-C3-C4
20	3	310	CLA	C4-C3-C5-C6
20	B	823	CLA	C4-C3-C5-C6
20	2	302	CLA	C2-C3-C5-C6
20	3	310	CLA	C2-C3-C5-C6
20	B	816	CLA	C2-C3-C5-C6
20	B	823	CLA	C2-C3-C5-C6
20	A	810	CLA	C3-C5-C6-C7
20	1	212	CLA	C11-C12-C13-C14
20	3	301	CLA	C6-C7-C8-C9
20	4	304	CLA	C6-C7-C8-C9
20	A	814	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	A	816	CLA	C6-C7-C8-C9
20	A	821	CLA	C11-C10-C8-C9
20	A	821	CLA	C14-C13-C15-C16
20	A	823	CLA	C11-C10-C8-C9
20	A	823	CLA	C14-C13-C15-C16
20	A	849	CLA	C11-C10-C8-C9
20	A	855	CLA	C11-C10-C8-C9
20	B	807	CLA	C11-C10-C8-C9
20	B	811	CLA	C14-C13-C15-C16
20	B	820	CLA	C14-C13-C15-C16
20	B	823	CLA	C11-C12-C13-C14
20	B	824	CLA	C6-C7-C8-C9
20	B	826	CLA	C11-C10-C8-C9
20	B	829	CLA	C11-C10-C8-C9
20	B	835	CLA	C11-C12-C13-C14
20	B	847	CLA	C11-C12-C13-C14
20	B	849	CLA	C14-C13-C15-C16
20	J	102	CLA	C11-C12-C13-C14
20	R	107	CLA	C11-C10-C8-C9
20	R	107	CLA	C11-C12-C13-C14
23	A	839	PQN	C21-C22-C23-C24
21	A	845	LMU	C5'-C4'-O1B-C1B
21	2	313	LMU	C4'-C5'-C6'-O6'
21	3	302	LMU	C4'-C5'-C6'-O6'
21	A	854	LMU	C4'-C5'-C6'-O6'
21	B	845	LMU	C4'-C5'-C6'-O6'
21	H	103	LMU	C4'-C5'-C6'-O6'
21	H	105	LMU	C4B-C5B-C6B-O6B
21	L	205	LMU	C4B-C5B-C6B-O6B
21	R	103	LMU	C4'-C5'-C6'-O6'
21	R	104	LMU	C4'-C5'-C6'-O6'
20	A	829	CLA	O1D-CGD-O2D-CED
20	L	208	CLA	O1D-CGD-O2D-CED
21	K	101	LMU	O5B-C1B-O1B-C4'
21	4	316	LMU	C2'-C1'-O1'-C1
21	4	321	LMU	C2'-C1'-O1'-C1
21	A	851	LMU	C2'-C1'-O1'-C1
21	A	853	LMU	C2'-C1'-O1'-C1
21	C	101	LMU	C2'-C1'-O1'-C1
21	K	101	LMU	C2'-C1'-O1'-C1
21	L	210	LMU	C2'-C1'-O1'-C1
21	R	104	LMU	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
21	R	105	LMU	C2'-C1'-O1'-C1
21	R	108	LMU	C2'-C1'-O1'-C1
21	R	109	LMU	C2'-C1'-O1'-C1
21	R	105	LMU	C6-C7-C8-C9
21	R	108	LMU	C5'-C4'-O1B-C1B
20	1	201	CLA	O1D-CGD-O2D-CED
20	1	212	CLA	O1D-CGD-O2D-CED
20	B	849	CLA	O1D-CGD-O2D-CED
25	B	846	LMG	O10-C28-O8-C9
22	3	311	BCR	C36-C18-C19-C20
22	A	840	BCR	C7-C8-C9-C34
22	A	842	BCR	C11-C12-C13-C35
22	A	843	BCR	C11-C12-C13-C35
22	A	844	BCR	C36-C18-C19-C20
22	B	843	BCR	C37-C22-C23-C24
22	F	202	BCR	C37-C22-C23-C24
22	F	203	BCR	C7-C8-C9-C34
22	G	102	BCR	C36-C18-C19-C20
22	I	101	BCR	C36-C18-C19-C20
22	I	103	BCR	C37-C22-C23-C24
22	L	209	BCR	C37-C22-C23-C24
21	2	316	LMU	O5'-C5'-C6'-O6'
21	4	322	LMU	O5B-C5B-C6B-O6B
22	3	311	BCR	C17-C18-C19-C20
22	A	842	BCR	C7-C8-C9-C10
22	A	842	BCR	C17-C18-C19-C20
22	A	843	BCR	C21-C22-C23-C24
22	B	842	BCR	C21-C22-C23-C24
22	B	844	BCR	C7-C8-C9-C10
22	F	202	BCR	C21-C22-C23-C24
22	I	103	BCR	C21-C22-C23-C24
21	3	318	LMU	C4B-C5B-C6B-O6B
21	K	102	LMU	C3-C4-C5-C6
20	A	815	CLA	C3-C5-C6-C7
20	A	847	CLA	C2A-CAA-CBA-CGA
20	B	811	CLA	C2A-CAA-CBA-CGA
20	A	829	CLA	C2C-C3C-CAC-CBC
21	R	108	LMU	C7-C8-C9-C10
20	2	310	CLA	O1A-CGA-O2A-C1
20	A	836	CLA	O1A-CGA-O2A-C1
20	A	816	CLA	C3-C5-C6-C7
21	A	851	LMU	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
20	3	310	CLA	O1D-CGD-O2D-CED
20	2	306	CLA	CBA-CGA-O2A-C1
20	A	855	CLA	C13-C15-C16-C17
20	B	829	CLA	C13-C15-C16-C17
20	1	206	CLA	C2-C1-O2A-CGA
20	4	307	CLA	C2-C1-O2A-CGA
20	A	803	CLA	C2-C1-O2A-CGA
20	A	821	CLA	C2-C1-O2A-CGA
20	A	835	CLA	C2-C1-O2A-CGA
21	B	802	LMU	O5B-C5B-C6B-O6B
21	H	103	LMU	C4B-C5B-C6B-O6B
20	2	301	CLA	CBD-CGD-O2D-CED
20	B	837	CLA	CBD-CGD-O2D-CED
21	2	318	LMU	C3-C4-C5-C6
20	4	315	CLA	C2C-C3C-CAC-CBC
20	A	806	CLA	C5-C6-C7-C8
20	A	817	CLA	C10-C11-C12-C13
20	A	824	CLA	C15-C16-C17-C18
20	A	837	CLA	C5-C6-C7-C8
20	B	824	CLA	C8-C10-C11-C12
20	L	202	CLA	C15-C16-C17-C18
21	L	210	LMU	O5B-C5B-C6B-O6B
20	A	809	CLA	C3-C5-C6-C7
20	A	837	CLA	C3-C5-C6-C7
21	R	108	LMU	C3'-C4'-O1B-C1B
20	1	212	CLA	C10-C11-C12-C13
20	L	202	CLA	C8-C10-C11-C12
20	4	302	CLA	CBD-CGD-O2D-CED
20	A	817	CLA	CBD-CGD-O2D-CED
20	B	809	CLA	CBD-CGD-O2D-CED
21	1	217	LMU	O5'-C5'-C6'-O6'
20	1	212	CLA	C6-C7-C8-C10
20	2	306	CLA	C11-C10-C8-C7
20	2	317	CLA	C11-C10-C8-C7
20	2	321	CLA	C11-C12-C13-C15
20	4	304	CLA	C12-C13-C15-C16
20	A	806	CLA	C12-C13-C15-C16
20	A	847	CLA	C12-C13-C15-C16
20	B	820	CLA	C11-C12-C13-C15
20	L	201	CLA	C12-C13-C15-C16
20	L	202	CLA	C11-C10-C8-C7
20	2	317	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	2	319	LMU	C2-C3-C4-C5
21	K	101	LMU	C11-C10-C9-C8
21	A	851	LMU	O1'-C1-C2-C3
21	C	101	LMU	O5'-C5'-C6'-O6'
21	R	109	LMU	C1-C2-C3-C4
22	A	843	BCR	C19-C20-C21-C22
22	F	203	BCR	C9-C10-C11-C12
22	I	103	BCR	C9-C10-C11-C12
22	L	209	BCR	C19-C20-C21-C22
20	J	102	CLA	C4C-C3C-CAC-CBC
21	A	851	LMU	C4B-C5B-C6B-O6B
21	K	104	LMU	C4'-C5'-C6'-O6'
21	F	201	LMU	O1'-C1-C2-C3
21	L	206	LMU	O1'-C1-C2-C3
21	A	853	LMU	C5-C6-C7-C8
20	A	809	CLA	C5-C6-C7-C8
21	B	801	LMU	C6-C7-C8-C9
21	A	851	LMU	C2B-C1B-O1B-C4'
21	R	109	LMU	O5B-C5B-C6B-O6B
21	H	104	LMU	C3'-C4'-O1B-C1B
20	A	807	CLA	C2C-C3C-CAC-CBC
20	A	834	CLA	O1A-CGA-O2A-C1
20	H	109	CLA	O1A-CGA-O2A-C1
20	A	810	CLA	O1D-CGD-O2D-CED
20	A	831	CLA	O1D-CGD-O2D-CED
20	A	847	CLA	C10-C11-C12-C13
20	B	829	CLA	C10-C11-C12-C13
20	B	838	CLA	C15-C16-C17-C18
20	B	849	CLA	C13-C15-C16-C17
20	L	201	CLA	C13-C15-C16-C17
23	B	840	PQN	C15-C16-C17-C18
21	4	316	LMU	O5B-C5B-C6B-O6B
20	2	306	CLA	C2A-CAA-CBA-CGA
20	3	301	CLA	C2A-CAA-CBA-CGA
20	A	805	CLA	C2A-CAA-CBA-CGA
20	A	812	CLA	C2A-CAA-CBA-CGA
20	A	814	CLA	C2A-CAA-CBA-CGA
20	A	815	CLA	C2A-CAA-CBA-CGA
20	A	821	CLA	C2A-CAA-CBA-CGA
20	A	822	CLA	C2A-CAA-CBA-CGA
20	A	830	CLA	C2A-CAA-CBA-CGA
20	A	835	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	A	855	CLA	C2A-CAA-CBA-CGA
20	B	810	CLA	C2A-CAA-CBA-CGA
20	B	819	CLA	C2A-CAA-CBA-CGA
20	B	826	CLA	C2A-CAA-CBA-CGA
20	B	827	CLA	C2A-CAA-CBA-CGA
20	L	201	CLA	C2A-CAA-CBA-CGA
20	A	807	CLA	C5-C6-C7-C8
20	A	816	CLA	C10-C11-C12-C13
20	A	829	CLA	C5-C6-C7-C8
20	A	836	CLA	C13-C15-C16-C17
20	B	804	CLA	C15-C16-C17-C18
20	B	806	CLA	C8-C10-C11-C12
20	B	811	CLA	C13-C15-C16-C17
20	B	826	CLA	C15-C16-C17-C18
20	B	849	CLA	C10-C11-C12-C13
20	L	201	CLA	C5-C6-C7-C8
20	R	107	CLA	C8-C10-C11-C12
21	4	321	LMU	C4B-C5B-C6B-O6B
20	2	301	CLA	O1A-CGA-O2A-C1
20	A	810	CLA	O1A-CGA-O2A-C1
20	A	811	CLA	C3-C5-C6-C7
20	B	820	CLA	C3-C5-C6-C7
20	B	826	CLA	C3-C5-C6-C7
20	R	107	CLA	CBD-CGD-O2D-CED
21	A	852	LMU	O5'-C1'-O1'-C1
21	1	218	LMU	C3-C4-C5-C6
21	4	320	LMU	C7-C8-C9-C10
20	A	833	CLA	O1D-CGD-O2D-CED
20	B	836	CLA	O1D-CGD-O2D-CED
20	1	206	CLA	C8-C10-C11-C12
20	4	310	CLA	C5-C6-C7-C8
20	A	825	CLA	C5-C6-C7-C8
20	A	836	CLA	C5-C6-C7-C8
20	A	836	CLA	C10-C11-C12-C13
20	A	849	CLA	C8-C10-C11-C12
20	A	855	CLA	C15-C16-C17-C18
20	B	806	CLA	C15-C16-C17-C18
20	B	807	CLA	C5-C6-C7-C8
20	B	807	CLA	C10-C11-C12-C13
20	B	809	CLA	C5-C6-C7-C8
20	B	816	CLA	C10-C11-C12-C13
20	B	819	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	B	837	CLA	C10-C11-C12-C13
20	H	110	CLA	C5-C6-C7-C8
20	J	103	CLA	C5-C6-C7-C8
21	R	102	LMU	C7-C8-C9-C10
21	1	217	LMU	O1'-C1-C2-C3
20	1	203	CLA	CBA-CGA-O2A-C1
20	4	305	CLA	O1A-CGA-O2A-C1
20	A	835	CLA	O1A-CGA-O2A-C1
20	K	106	CLA	O1A-CGA-O2A-C1
20	A	809	CLA	C10-C11-C12-C13
20	A	847	CLA	C5-C6-C7-C8
20	B	815	CLA	C10-C11-C12-C13
20	B	823	CLA	C15-C16-C17-C18
20	B	835	CLA	C8-C10-C11-C12
23	A	839	PQN	C25-C26-C27-C28
21	2	313	LMU	O1'-C1-C2-C3
21	B	801	LMU	O1'-C1-C2-C3
21	L	206	LMU	O5'-C5'-C6'-O6'
20	A	849	CLA	C4C-C3C-CAC-CBC
21	B	801	LMU	C7-C8-C9-C10
21	2	316	LMU	O1'-C1-C2-C3
21	A	853	LMU	O1'-C1-C2-C3
21	2	318	LMU	C1-C2-C3-C4
20	3	301	CLA	O1D-CGD-O2D-CED
20	4	305	CLA	O1D-CGD-O2D-CED
20	A	830	CLA	O1D-CGD-O2D-CED
20	B	828	CLA	O1D-CGD-O2D-CED
20	3	310	CLA	C13-C15-C16-C17
20	B	805	CLA	C13-C15-C16-C17
20	I	102	CLA	C5-C6-C7-C8
20	J	102	CLA	C8-C10-C11-C12
23	A	839	PQN	C20-C21-C22-C23
23	B	840	PQN	C18-C20-C21-C22
21	H	103	LMU	O5B-C5B-C6B-O6B
21	3	318	LMU	O1'-C1-C2-C3
21	L	206	LMU	C4'-C5'-C6'-O6'
21	A	853	LMU	O5'-C5'-C6'-O6'
21	R	108	LMU	O5B-C5B-C6B-O6B
20	3	309	CLA	C5-C6-C7-C8
20	A	833	CLA	C5-C6-C7-C8
20	H	107	CLA	C8-C10-C11-C12
20	B	837	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	H	102	LMU	C4-C5-C6-C7
20	2	306	CLA	O1A-CGA-O2A-C1
20	B	815	CLA	O1A-CGA-O2A-C1
20	A	814	CLA	C3-C5-C6-C7
20	B	811	CLA	C3-C5-C6-C7
20	B	815	CLA	C3-C5-C6-C7
20	R	106	CLA	C8-C10-C11-C12
21	R	108	LMU	C4B-C5B-C6B-O6B
22	B	841	BCR	C19-C20-C21-C22
22	I	101	BCR	C9-C10-C11-C12
20	A	817	CLA	C5-C6-C7-C8
20	B	811	CLA	C5-C6-C7-C8
20	B	811	CLA	C10-C11-C12-C13
20	H	101	CLA	C5-C6-C7-C8
20	B	803	CLA	C2C-C3C-CAC-CBC
21	R	108	LMU	C9-C10-C11-C12
20	A	831	CLA	C2A-CAA-CBA-CGA
20	B	818	CLA	C2A-CAA-CBA-CGA
20	B	815	CLA	CBA-CGA-O2A-C1
20	B	823	CLA	CBA-CGA-O2A-C1
20	G	103	CLA	CBA-CGA-O2A-C1
20	L	204	CLA	CBA-CGA-O2A-C1
20	B	837	CLA	C4C-C3C-CAC-CBC
21	1	218	LMU	C1-C2-C3-C4
20	2	312	CLA	C8-C10-C11-C12
20	A	804	CLA	C5-C6-C7-C8
20	A	829	CLA	C8-C10-C11-C12
20	B	814	CLA	C8-C10-C11-C12
20	B	826	CLA	C5-C6-C7-C8
20	B	847	CLA	C10-C11-C12-C13
21	4	320	LMU	C3'-C4'-O1B-C1B
20	B	811	CLA	O1D-CGD-O2D-CED
20	4	304	CLA	C8-C10-C11-C12
20	A	847	CLA	C8-C10-C11-C12
20	A	849	CLA	C15-C16-C17-C18
20	B	835	CLA	C13-C15-C16-C17
20	B	848	CLA	C13-C15-C16-C17
21	4	301	LMU	C4'-C5'-C6'-O6'
21	R	105	LMU	O1'-C1-C2-C3
20	K	103	CLA	C4C-C3C-CAC-CBC
21	2	318	LMU	C4B-C5B-C6B-O6B
21	4	320	LMU	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
20	3	309	CLA	C10-C11-C12-C13
20	3	310	CLA	C5-C6-C7-C8
20	A	803	CLA	C13-C15-C16-C17
20	A	816	CLA	C5-C6-C7-C8
20	A	816	CLA	C15-C16-C17-C18
20	A	821	CLA	C15-C16-C17-C18
20	B	820	CLA	C13-C15-C16-C17
20	B	823	CLA	C8-C10-C11-C12
20	B	834	CLA	C5-C6-C7-C8
20	K	107	CLA	C13-C15-C16-C17
23	B	840	PQN	C20-C21-C22-C23
21	3	302	LMU	O1'-C1-C2-C3
20	A	823	CLA	C8-C10-C11-C12
21	E	101	LMU	O5'-C5'-C6'-O6'
21	2	316	LMU	C2'-C1'-O1'-C1
21	3	318	LMU	C2'-C1'-O1'-C1
21	4	320	LMU	C2'-C1'-O1'-C1
21	A	854	LMU	C2'-C1'-O1'-C1
21	B	802	LMU	C2'-C1'-O1'-C1
21	H	103	LMU	C2'-C1'-O1'-C1
21	H	105	LMU	C2'-C1'-O1'-C1
25	B	846	LMG	C2-C1-O1-C7
20	A	834	CLA	O1D-CGD-O2D-CED
20	A	809	CLA	C16-C17-C18-C19
20	A	833	CLA	C16-C17-C18-C19
20	B	837	CLA	C16-C17-C18-C19
20	2	317	CLA	C8-C10-C11-C12
20	B	810	CLA	C15-C16-C17-C18
22	F	202	BCR	C20-C21-C22-C37
20	A	829	CLA	C3-C5-C6-C7
21	A	851	LMU	O5B-C5B-C6B-O6B
20	B	807	CLA	C15-C16-C17-C18
22	A	842	BCR	C7-C8-C9-C34
22	A	843	BCR	C36-C18-C19-C20
22	B	842	BCR	C11-C12-C13-C35
22	G	102	BCR	C37-C22-C23-C24
22	J	101	BCR	C37-C22-C23-C24
21	H	102	LMU	C2-C3-C4-C5
22	A	840	BCR	C7-C8-C9-C10
22	A	843	BCR	C11-C12-C13-C14
22	G	102	BCR	C21-C22-C23-C24
22	J	101	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
20	1	211	CLA	O1A-CGA-O2A-C1
20	B	837	CLA	O1A-CGA-O2A-C1
20	3	320	CLA	C2A-CAA-CBA-CGA
20	4	302	CLA	C2A-CAA-CBA-CGA
20	A	806	CLA	C2A-CAA-CBA-CGA
20	A	810	CLA	C2A-CAA-CBA-CGA
20	A	820	CLA	C2A-CAA-CBA-CGA
20	A	827	CLA	C2A-CAA-CBA-CGA
20	A	828	CLA	C2A-CAA-CBA-CGA
20	B	823	CLA	C2A-CAA-CBA-CGA
20	H	101	CLA	C2A-CAA-CBA-CGA
20	F	205	CLA	C2C-C3C-CAC-CBC
20	B	825	CLA	C10-C11-C12-C13
20	A	807	CLA	O2A-C1-C2-C3
20	A	835	CLA	O2A-C1-C2-C3
20	2	317	CLA	C16-C17-C18-C19
20	4	310	CLA	C6-C7-C8-C9
20	A	826	CLA	C16-C17-C18-C19
20	B	835	CLA	C16-C17-C18-C19
20	L	202	CLA	C16-C17-C18-C20
20	B	814	CLA	C10-C11-C12-C13
20	A	847	CLA	C3-C5-C6-C7
20	B	849	CLA	C15-C16-C17-C18
22	F	202	BCR	C20-C21-C22-C23
21	2	313	LMU	O5'-C1'-O1'-C1
21	R	103	LMU	O1'-C1-C2-C3
21	K	102	LMU	C5-C6-C7-C8
20	R	107	CLA	C10-C11-C12-C13
20	1	206	CLA	C2-C3-C5-C6
21	R	104	LMU	O1'-C1-C2-C3
20	A	818	CLA	O1D-CGD-O2D-CED
20	A	821	CLA	CBA-CGA-O2A-C1
21	3	318	LMU	C1-C2-C3-C4
20	A	828	CLA	C15-C16-C17-C18
20	B	810	CLA	C5-C6-C7-C8
20	B	838	CLA	CBD-CGD-O2D-CED
20	2	307	CLA	C3-C5-C6-C7
21	2	319	LMU	C4B-C5B-C6B-O6B
20	3	309	CLA	C2-C1-O2A-CGA
20	A	832	CLA	C2-C1-O2A-CGA
20	B	829	CLA	C2-C1-O2A-CGA
20	3	310	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
20	A	825	CLA	C6-C7-C8-C9
20	A	826	CLA	C16-C17-C18-C20
20	A	848	CLA	C16-C17-C18-C20
20	B	834	CLA	C11-C12-C13-C14
23	A	839	PQN	C26-C27-C28-C30
21	R	102	LMU	C1-C2-C3-C4
21	R	108	LMU	C1-C2-C3-C4
20	1	203	CLA	O1A-CGA-O2A-C1
20	B	807	CLA	C8-C10-C11-C12
21	A	852	LMU	O5'-C5'-C6'-O6'
20	2	304	CLA	C4C-C3C-CAC-CBC
25	B	846	LMG	C33-C34-C35-C36
21	A	852	LMU	C1-C2-C3-C4
21	4	301	LMU	C3-C4-C5-C6
21	A	851	LMU	C7-C8-C9-C10
21	C	101	LMU	C11-C10-C9-C8
21	L	210	LMU	C6-C7-C8-C9
21	R	105	LMU	C3-C4-C5-C6
21	2	313	LMU	C6-C7-C8-C9
21	A	854	LMU	C6-C7-C8-C9
21	B	802	LMU	C4-C5-C6-C7
21	2	319	LMU	C3-C4-C5-C6
21	4	316	LMU	C2-C3-C4-C5
21	4	322	LMU	C4-C5-C6-C7
21	B	801	LMU	C11-C10-C9-C8
21	C	101	LMU	C7-C8-C9-C10
21	H	102	LMU	C3-C4-C5-C6
21	K	102	LMU	C11-C10-C9-C8
21	R	108	LMU	C11-C10-C9-C8
25	B	846	LMG	C32-C33-C34-C35
21	A	845	LMU	C2-C1-O1'-C1'
21	H	102	LMU	C2-C1-O1'-C1'
21	L	205	LMU	C2-C1-O1'-C1'
21	L	206	LMU	C2-C1-O1'-C1'
21	1	217	LMU	C5-C6-C7-C8
21	3	302	LMU	C4-C5-C6-C7
21	A	846	LMU	C5-C6-C7-C8
21	L	206	LMU	C6-C7-C8-C9
20	2	306	CLA	C4B-C3B-CAB-CBB
20	2	310	CLA	C4B-C3B-CAB-CBB
20	3	315	CLA	C4B-C3B-CAB-CBB
20	3	320	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	A	814	CLA	C4B-C3B-CAB-CBB
20	A	823	CLA	C4B-C3B-CAB-CBB
20	A	829	CLA	C4B-C3B-CAB-CBB
20	B	806	CLA	C4B-C3B-CAB-CBB
20	B	811	CLA	C4B-C3B-CAB-CBB
20	B	831	CLA	C4B-C3B-CAB-CBB
20	H	101	CLA	C4B-C3B-CAB-CBB
20	3	310	CLA	C16-C17-C18-C20
20	4	305	CLA	C6-C7-C8-C10
20	4	310	CLA	C6-C7-C8-C10
20	A	806	CLA	C16-C17-C18-C19
20	B	811	CLA	C16-C17-C18-C19
20	B	837	CLA	C16-C17-C18-C20
20	H	107	CLA	C16-C17-C18-C19
20	H	107	CLA	C16-C17-C18-C20
20	L	202	CLA	C16-C17-C18-C19
20	A	832	CLA	C2A-CAA-CBA-CGA
20	B	831	CLA	C2A-CAA-CBA-CGA
20	G	103	CLA	C2A-CAA-CBA-CGA
21	L	210	LMU	C11-C10-C9-C8
20	2	312	CLA	C10-C11-C12-C13
20	4	304	CLA	C5-C6-C7-C8
21	A	845	LMU	C11-C10-C9-C8
21	A	852	LMU	C11-C10-C9-C8
21	L	210	LMU	C4B-C5B-C6B-O6B
20	A	821	CLA	C11-C10-C8-C7
20	B	811	CLA	C11-C10-C8-C7
20	R	107	CLA	C6-C7-C8-C10
21	A	846	LMU	C6-C7-C8-C9
21	L	205	LMU	C6-C7-C8-C9
20	A	848	CLA	C13-C15-C16-C17
21	4	301	LMU	C1-C2-C3-C4
21	4	320	LMU	C4-C5-C6-C7
20	4	310	CLA	C3-C5-C6-C7
20	1	203	CLA	C3A-C2A-CAA-CBA
20	1	206	CLA	C3A-C2A-CAA-CBA
20	2	306	CLA	C3A-C2A-CAA-CBA
20	2	312	CLA	C3A-C2A-CAA-CBA
20	3	301	CLA	C3A-C2A-CAA-CBA
20	4	310	CLA	C3A-C2A-CAA-CBA
20	A	801	CLA	C3A-C2A-CAA-CBA
20	A	804	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	807	CLA	C3A-C2A-CAA-CBA
20	A	812	CLA	C3A-C2A-CAA-CBA
20	A	823	CLA	C3A-C2A-CAA-CBA
20	A	835	CLA	C3A-C2A-CAA-CBA
20	B	807	CLA	C3A-C2A-CAA-CBA
20	B	810	CLA	C3A-C2A-CAA-CBA
20	B	812	CLA	C3A-C2A-CAA-CBA
20	B	828	CLA	C3A-C2A-CAA-CBA
20	L	201	CLA	C3A-C2A-CAA-CBA
20	L	207	CLA	C3A-C2A-CAA-CBA
20	R	106	CLA	C3A-C2A-CAA-CBA
21	A	853	LMU	C3-C4-C5-C6
21	R	104	LMU	C2-C3-C4-C5
20	B	838	CLA	C10-C11-C12-C13
20	L	201	CLA	C10-C11-C12-C13
21	1	218	LMU	C5'-C4'-O1B-C1B
21	R	102	LMU	O1'-C1-C2-C3
20	2	307	CLA	C16-C17-C18-C20
20	A	809	CLA	C16-C17-C18-C20
20	A	822	CLA	C16-C17-C18-C19
20	A	848	CLA	C16-C17-C18-C19
20	B	848	CLA	C16-C17-C18-C19
21	A	851	LMU	C1-C2-C3-C4
20	B	823	CLA	O1A-CGA-O2A-C1
21	4	316	LMU	C7-C8-C9-C10
21	4	321	LMU	C6-C7-C8-C9
20	B	821	CLA	C5-C6-C7-C8
21	3	318	LMU	C5-C6-C7-C8
21	G	101	LMU	C2-C3-C4-C5
20	B	826	CLA	CBA-CGA-O2A-C1
21	L	210	LMU	C1-C2-C3-C4
21	A	852	LMU	O1'-C1-C2-C3
21	A	854	LMU	C7-C8-C9-C10
21	C	101	LMU	C6-C7-C8-C9
21	E	101	LMU	C11-C10-C9-C8
21	K	102	LMU	C6-C7-C8-C9
20	A	811	CLA	C5-C6-C7-C8
21	3	302	LMU	C2-C3-C4-C5
21	4	321	LMU	C3-C4-C5-C6
21	4	322	LMU	C2-C3-C4-C5
25	B	846	LMG	C37-C38-C39-C40
20	G	103	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	H	103	LMU	C1-C2-C3-C4
21	H	104	LMU	C5'-C4'-O1B-C1B
21	2	313	LMU	C11-C10-C9-C8
21	H	104	LMU	O5'-C5'-C6'-O6'
21	R	104	LMU	C1-C2-C3-C4
21	2	316	LMU	C7-C8-C9-C10
21	2	319	LMU	C5-C6-C7-C8
21	K	102	LMU	C4-C5-C6-C7
20	B	829	CLA	C16-C17-C18-C20
21	G	101	LMU	O1'-C1-C2-C3
21	R	105	LMU	C9-C10-C11-C12
20	A	820	CLA	C2B-C3B-CAB-CBB
20	A	827	CLA	C2B-C3B-CAB-CBB
20	A	837	CLA	C2B-C3B-CAB-CBB
20	B	812	CLA	C2B-C3B-CAB-CBB
20	B	820	CLA	C2B-C3B-CAB-CBB
20	B	823	CLA	C2B-C3B-CAB-CBB
20	G	103	CLA	C2B-C3B-CAB-CBB
20	K	106	CLA	C2B-C3B-CAB-CBB
20	L	202	CLA	C2B-C3B-CAB-CBB
22	A	842	BCR	C1-C6-C7-C8
22	A	842	BCR	C23-C24-C25-C26
22	A	842	BCR	C23-C24-C25-C30
22	B	844	BCR	C23-C24-C25-C26
22	F	202	BCR	C1-C6-C7-C8
22	F	202	BCR	C23-C24-C25-C26
22	F	202	BCR	C23-C24-C25-C30
22	J	101	BCR	C1-C6-C7-C8
21	A	851	LMU	C11-C10-C9-C8
25	B	846	LMG	C35-C36-C37-C38
20	B	810	CLA	CBA-CGA-O2A-C1
20	A	822	CLA	C10-C11-C12-C13
20	B	816	CLA	C5-C6-C7-C8
21	R	105	LMU	C1-C2-C3-C4
20	1	206	CLA	C3-C5-C6-C7
20	B	821	CLA	C3-C5-C6-C7
21	K	101	LMU	C4-C5-C6-C7
20	B	825	CLA	C2A-CAA-CBA-CGA
20	K	105	CLA	C2A-CAA-CBA-CGA
20	B	835	CLA	C15-C16-C17-C18
21	K	104	LMU	C9-C10-C11-C12
21	1	217	LMU	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
21	A	845	LMU	C3-C4-C5-C6
21	K	102	LMU	C2-C3-C4-C5
21	L	205	LMU	C7-C8-C9-C10
21	R	103	LMU	C5-C6-C7-C8
20	A	821	CLA	O1A-CGA-O2A-C1
21	3	302	LMU	C11-C10-C9-C8
21	2	316	LMU	C4-C5-C6-C7
22	A	841	BCR	C18-C19-C20-C21
22	A	842	BCR	C18-C19-C20-C21
22	B	843	BCR	C18-C19-C20-C21
20	A	847	CLA	C13-C15-C16-C17
20	B	810	CLA	C10-C11-C12-C13
21	4	316	LMU	C4-C5-C6-C7
21	L	210	LMU	C3-C4-C5-C6
20	L	201	CLA	C11-C10-C8-C9
21	4	301	LMU	C4-C5-C6-C7
21	L	206	LMU	C2-C3-C4-C5
21	K	102	LMU	O5'-C5'-C6'-O6'
20	3	309	CLA	C13-C15-C16-C17
20	4	305	CLA	C5-C6-C7-C8
20	A	826	CLA	C8-C10-C11-C12
21	A	846	LMU	C2-C3-C4-C5
21	L	205	LMU	C1-C2-C3-C4
21	2	320	LMU	C7-C8-C9-C10
21	L	206	LMU	C5-C6-C7-C8
21	B	802	LMU	O5'-C5'-C6'-O6'
21	2	319	LMU	C2'-C1'-O1'-C1
20	A	848	CLA	C15-C16-C17-C18
20	I	102	CLA	C8-C10-C11-C12
20	L	204	CLA	O1A-CGA-O2A-C1
21	A	851	LMU	C5-C6-C7-C8
21	R	104	LMU	C7-C8-C9-C10
20	A	825	CLA	O1D-CGD-O2D-CED
21	R	101	LMU	O5'-C5'-C6'-O6'
20	A	810	CLA	C5-C6-C7-C8
21	4	316	LMU	C11-C10-C9-C8
25	B	846	LMG	C15-C16-C17-C18
25	B	846	LMG	C40-C41-C42-C43
21	H	104	LMU	C7-C8-C9-C10
21	R	109	LMU	C11-C10-C9-C8
21	K	104	LMU	C1-C2-C3-C4
22	I	101	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
20	A	825	CLA	C6-C7-C8-C10
20	I	102	CLA	C11-C12-C13-C14
20	I	102	CLA	C11-C12-C13-C15
21	H	104	LMU	C9-C10-C11-C12
21	R	102	LMU	C9-C10-C11-C12
21	A	854	LMU	C4-C5-C6-C7
20	B	804	CLA	C10-C11-C12-C13
20	B	805	CLA	C10-C11-C12-C13
20	L	207	CLA	C4C-C3C-CAC-CBC
21	L	205	LMU	C4-C5-C6-C7
22	J	101	BCR	C36-C18-C19-C20
21	2	320	LMU	C2-C3-C4-C5
21	R	102	LMU	C4-C5-C6-C7
22	3	311	BCR	C11-C12-C13-C14
21	1	217	LMU	C6-C7-C8-C9
21	2	313	LMU	C2-C3-C4-C5
21	H	103	LMU	C4-C5-C6-C7
20	2	317	CLA	C16-C17-C18-C20
20	B	825	CLA	C16-C17-C18-C20
21	4	322	LMU	C3-C4-C5-C6
21	1	218	LMU	C6-C7-C8-C9
21	2	318	LMU	C2-C3-C4-C5
21	E	101	LMU	C4-C5-C6-C7
20	A	821	CLA	C2C-C3C-CAC-CBC
20	2	312	CLA	C5-C6-C7-C8
21	R	109	LMU	C2-C3-C4-C5
21	2	313	LMU	C1-C2-C3-C4
21	B	802	LMU	C5-C6-C7-C8
20	B	826	CLA	O1A-CGA-O2A-C1
20	B	807	CLA	C3-C5-C6-C7
20	A	821	CLA	C10-C11-C12-C13
20	A	829	CLA	C13-C15-C16-C17
21	3	318	LMU	C3-C4-C5-C6
21	R	101	LMU	C1-C2-C3-C4
20	B	849	CLA	CBA-CGA-O2A-C1
21	2	313	LMU	C7-C8-C9-C10
21	2	318	LMU	C4-C5-C6-C7
21	G	101	LMU	C1-C2-C3-C4
21	A	846	LMU	O1'-C1-C2-C3
20	A	816	CLA	C16-C17-C18-C19
20	B	834	CLA	C11-C12-C13-C15
20	B	835	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
21	1	216	LMU	C5'-C4'-O1B-C1B
21	F	201	LMU	C5-C6-C7-C8
25	B	846	LMG	C13-C14-C15-C16
21	A	853	LMU	C4'-C5'-C6'-O6'
20	B	847	CLA	C5-C6-C7-C8
21	A	845	LMU	C5-C6-C7-C8
20	2	306	CLA	C3-C5-C6-C7
21	H	104	LMU	C4-C5-C6-C7
20	A	828	CLA	CBA-CGA-O2A-C1
21	K	104	LMU	C7-C8-C9-C10
20	B	816	CLA	C8-C10-C11-C12
21	4	301	LMU	O5'-C5'-C6'-O6'
21	1	216	LMU	C3'-C4'-O1B-C1B
21	K	101	LMU	C6-C7-C8-C9
20	H	101	CLA	C2-C1-O2A-CGA
20	A	849	CLA	O1D-CGD-O2D-CED
20	2	307	CLA	C16-C17-C18-C19
20	A	816	CLA	C16-C17-C18-C20
20	A	833	CLA	C16-C17-C18-C20
20	B	811	CLA	C16-C17-C18-C20
20	B	825	CLA	C5-C6-C7-C8
21	H	103	LMU	C2B-C1B-O1B-C4'
21	K	101	LMU	O1'-C1-C2-C3
20	B	806	CLA	C4-C3-C5-C6
20	B	829	CLA	C3-C5-C6-C7
20	A	823	CLA	C2-C3-C5-C6
20	A	836	CLA	C2A-CAA-CBA-CGA
20	A	838	CLA	C2A-CAA-CBA-CGA
20	B	803	CLA	C2A-CAA-CBA-CGA
20	B	828	CLA	C2A-CAA-CBA-CGA
20	K	105	CLA	CBD-CGD-O2D-CED
20	A	823	CLA	CBA-CGA-O2A-C1
20	A	829	CLA	CBA-CGA-O2A-C1
21	4	301	LMU	C2-C3-C4-C5
21	A	846	LMU	C11-C10-C9-C8
21	R	101	LMU	C2-C3-C4-C5
20	A	829	CLA	C4C-C3C-CAC-CBC
20	B	810	CLA	O1A-CGA-O2A-C1
21	2	313	LMU	C4-C5-C6-C7
20	A	821	CLA	C5-C6-C7-C8
20	A	849	CLA	C13-C15-C16-C17
20	B	826	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	4	301	LMU	C5-C6-C7-C8
21	C	101	LMU	C5-C6-C7-C8
20	2	310	CLA	O1D-CGD-O2D-CED
21	L	206	LMU	C1-C2-C3-C4
20	A	822	CLA	C16-C17-C18-C20
20	1	203	CLA	C1A-C2A-CAA-CBA
20	1	214	CLA	C1A-C2A-CAA-CBA
20	3	320	CLA	C1A-C2A-CAA-CBA
20	4	310	CLA	C1A-C2A-CAA-CBA
20	A	801	CLA	C1A-C2A-CAA-CBA
20	A	802	CLA	C1A-C2A-CAA-CBA
20	A	838	CLA	C1A-C2A-CAA-CBA
20	A	847	CLA	C1A-C2A-CAA-CBA
20	A	850	CLA	C1A-C2A-CAA-CBA
20	B	813	CLA	C1A-C2A-CAA-CBA
20	B	824	CLA	C1A-C2A-CAA-CBA
20	B	825	CLA	C1A-C2A-CAA-CBA
20	B	833	CLA	C1A-C2A-CAA-CBA
20	B	836	CLA	C1A-C2A-CAA-CBA
20	B	838	CLA	C1A-C2A-CAA-CBA
20	J	102	CLA	C1A-C2A-CAA-CBA
20	J	103	CLA	C1A-C2A-CAA-CBA
20	L	207	CLA	C1A-C2A-CAA-CBA
20	2	321	CLA	C8-C10-C11-C12
20	A	803	CLA	C15-C16-C17-C18
20	B	837	CLA	C8-C10-C11-C12
21	2	318	LMU	C5-C6-C7-C8
20	A	826	CLA	C13-C15-C16-C17
20	A	828	CLA	C13-C15-C16-C17
21	2	320	LMU	O5B-C5B-C6B-O6B
21	K	104	LMU	C11-C10-C9-C8
20	R	107	CLA	C3-C5-C6-C7
20	2	321	CLA	C11-C10-C8-C7
20	A	803	CLA	C11-C10-C8-C7
20	A	814	CLA	C12-C13-C15-C16
20	A	821	CLA	C11-C12-C13-C15
20	A	829	CLA	C11-C12-C13-C15
20	A	837	CLA	C11-C10-C8-C7
20	A	847	CLA	C11-C10-C8-C7
20	A	848	CLA	C6-C7-C8-C10
20	A	849	CLA	C12-C13-C15-C16
20	B	804	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
20	B	805	CLA	C12-C13-C15-C16
20	B	807	CLA	C11-C10-C8-C7
20	B	807	CLA	C12-C13-C15-C16
20	B	811	CLA	C6-C7-C8-C10
20	B	816	CLA	C11-C12-C13-C15
20	B	824	CLA	C11-C10-C8-C7
20	B	825	CLA	C11-C12-C13-C15
20	B	834	CLA	C6-C7-C8-C10
20	B	837	CLA	C11-C10-C8-C7
20	H	107	CLA	C12-C13-C15-C16
20	K	107	CLA	C11-C10-C8-C7
20	K	107	CLA	C12-C13-C15-C16
21	2	318	LMU	C7-C8-C9-C10
20	3	309	CLA	C16-C17-C18-C20
20	L	204	CLA	C6-C7-C8-C10
21	R	104	LMU	C5'-C4'-O1B-C1B
20	B	824	CLA	C5-C6-C7-C8
20	3	314	CLA	C3A-C2A-CAA-CBA
20	A	832	CLA	CBA-CGA-O2A-C1
21	L	210	LMU	C2-C3-C4-C5
20	A	803	CLA	C5-C6-C7-C8
21	1	218	LMU	C11-C10-C9-C8
21	B	801	LMU	C5-C6-C7-C8
20	A	828	CLA	C4-C3-C5-C6
20	A	828	CLA	C2-C3-C5-C6
20	B	806	CLA	C2-C3-C5-C6
20	B	849	CLA	O1A-CGA-O2A-C1
21	R	108	LMU	C5-C6-C7-C8
20	A	822	CLA	C5-C6-C7-C8
20	A	849	CLA	C10-C11-C12-C13
20	R	107	CLA	C5-C6-C7-C8
20	1	211	CLA	C2A-CAA-CBA-CGA
20	L	208	CLA	C2A-CAA-CBA-CGA
20	2	306	CLA	C11-C12-C13-C14
20	2	317	CLA	C11-C10-C8-C9
20	2	321	CLA	C11-C10-C8-C9
20	4	304	CLA	C11-C12-C13-C14
20	4	304	CLA	C14-C13-C15-C16
20	A	803	CLA	C11-C10-C8-C9
20	A	824	CLA	C6-C7-C8-C9
20	B	804	CLA	C6-C7-C8-C9
20	B	805	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	B	807	CLA	C14-C13-C15-C16
20	B	814	CLA	C11-C10-C8-C9
20	B	834	CLA	C6-C7-C8-C9
20	B	837	CLA	C11-C10-C8-C9
20	K	107	CLA	C11-C12-C13-C14
21	A	845	LMU	C6-C7-C8-C9
21	B	802	LMU	C11-C10-C9-C8
21	R	108	LMU	C2-C3-C4-C5
21	K	104	LMU	O5B-C5B-C6B-O6B
21	A	854	LMU	C11-C10-C9-C8
21	H	105	LMU	C11-C10-C9-C8
20	2	321	CLA	CBA-CGA-O2A-C1
20	A	809	CLA	C8-C10-C11-C12
21	B	801	LMU	O5'-C5'-C6'-O6'
21	K	101	LMU	C3-C4-C5-C6
21	4	301	LMU	C2'-C1'-O1'-C1
21	L	206	LMU	C2'-C1'-O1'-C1
21	R	103	LMU	C2'-C1'-O1'-C1
20	R	107	CLA	O1D-CGD-O2D-CED
20	2	321	CLA	C14-C13-C15-C16
21	R	105	LMU	C4-C5-C6-C7
21	H	102	LMU	O5'-C5'-C6'-O6'
20	B	805	CLA	C15-C16-C17-C18
20	B	848	CLA	C15-C16-C17-C18
21	B	845	LMU	C4B-C5B-C6B-O6B
20	2	301	CLA	O1D-CGD-O2D-CED
20	B	819	CLA	CBA-CGA-O2A-C1
21	2	319	LMU	O5'-C5'-C6'-O6'
21	R	105	LMU	O5'-C5'-C6'-O6'
20	3	309	CLA	C16-C17-C18-C19
21	1	216	LMU	C2-C3-C4-C5
21	H	104	LMU	C4'-C5'-C6'-O6'
21	K	102	LMU	C4'-C5'-C6'-O6'
21	G	101	LMU	C4-C5-C6-C7
20	4	315	CLA	C4C-C3C-CAC-CBC
21	E	101	LMU	O5B-C5B-C6B-O6B
25	B	846	LMG	C17-C18-C19-C20
20	B	838	CLA	O1D-CGD-O2D-CED
21	4	320	LMU	O5B-C5B-C6B-O6B
21	2	318	LMU	O5B-C1B-O1B-C4'
20	A	823	CLA	C4-C3-C5-C6
20	B	803	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
20	B	809	CLA	C2-C3-C5-C6
20	L	204	CLA	C2-C3-C5-C6
21	3	318	LMU	C7-C8-C9-C10
22	I	103	BCR	C7-C8-C9-C34
21	A	854	LMU	C5-C6-C7-C8
22	I	103	BCR	C7-C8-C9-C10
20	2	321	CLA	O1A-CGA-O2A-C1
20	A	823	CLA	O1A-CGA-O2A-C1
20	B	837	CLA	C5-C6-C7-C8
20	A	825	CLA	C2A-CAA-CBA-CGA
20	2	307	CLA	C2C-C3C-CAC-CBC
21	A	852	LMU	C4'-C5'-C6'-O6'
20	A	817	CLA	C8-C10-C11-C12
21	K	104	LMU	C2-C3-C4-C5
21	H	102	LMU	C5'-C4'-O1B-C1B
20	A	829	CLA	O1A-CGA-O2A-C1
20	A	832	CLA	O1A-CGA-O2A-C1
20	4	306	CLA	O2A-C1-C2-C3
20	A	849	CLA	O2A-C1-C2-C3
20	B	807	CLA	O2A-C1-C2-C3
20	B	830	CLA	O2A-C1-C2-C3
20	L	202	CLA	O2A-C1-C2-C3
25	B	846	LMG	C9-C8-O7-C10
21	A	846	LMU	C3-C4-C5-C6
22	L	209	BCR	C18-C19-C20-C21
20	B	809	CLA	C6-C7-C8-C9
25	B	846	LMG	C11-C12-C13-C14
20	4	302	CLA	O1D-CGD-O2D-CED
20	B	809	CLA	O1D-CGD-O2D-CED
21	2	316	LMU	O5B-C5B-C6B-O6B
20	A	806	CLA	C15-C16-C17-C18
20	A	837	CLA	C13-C15-C16-C17
21	H	105	LMU	C6-C7-C8-C9
20	A	820	CLA	CBA-CGA-O2A-C1
20	A	827	CLA	CBA-CGA-O2A-C1
20	B	804	CLA	CBA-CGA-O2A-C1
20	A	828	CLA	O1A-CGA-O2A-C1
21	F	201	LMU	C3'-C4'-O1B-C1B
21	4	316	LMU	C1-C2-C3-C4
21	A	846	LMU	C9-C10-C11-C12
21	2	316	LMU	C5-C6-C7-C8
20	L	204	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
20	A	810	CLA	C2-C3-C5-C6
21	1	218	LMU	C9-C10-C11-C12
21	A	851	LMU	C4-C5-C6-C7
21	L	206	LMU	C11-C10-C9-C8
21	2	319	LMU	C9-C10-C11-C12
21	H	105	LMU	C9-C10-C11-C12
21	L	205	LMU	C11-C10-C9-C8
20	A	802	CLA	C2C-C3C-CAC-CBC
21	2	320	LMU	C9-C10-C11-C12
21	G	101	LMU	C5-C6-C7-C8
21	R	104	LMU	C3'-C4'-O1B-C1B
21	2	316	LMU	C9-C10-C11-C12
21	F	201	LMU	C11-C10-C9-C8
21	R	109	LMU	C9-C10-C11-C12
21	L	210	LMU	C7-C8-C9-C10
21	R	103	LMU	C9-C10-C11-C12
21	H	104	LMU	C2-C3-C4-C5
21	H	102	LMU	C9-C10-C11-C12
21	2	313	LMU	C3'-C4'-O1B-C1B
21	A	845	LMU	C9-C10-C11-C12
25	B	846	LMG	C10-C11-C12-C13
21	H	102	LMU	C6-C7-C8-C9
20	A	809	CLA	CBA-CGA-O2A-C1
20	B	838	CLA	CBA-CGA-O2A-C1
20	L	203	CLA	CBA-CGA-O2A-C1
20	A	811	CLA	C6-C7-C8-C9
21	R	104	LMU	C5-C6-C7-C8
20	A	837	CLA	C15-C16-C17-C18
22	J	101	BCR	C19-C20-C21-C22
20	B	809	CLA	C6-C7-C8-C10
21	4	322	LMU	C5-C6-C7-C8
20	B	809	CLA	C4-C3-C5-C6
20	B	815	CLA	C4-C3-C5-C6
20	B	826	CLA	C4-C3-C5-C6
20	B	847	CLA	C4-C3-C5-C6
20	A	818	CLA	CBA-CGA-O2A-C1
20	K	107	CLA	CBA-CGA-O2A-C1
25	B	846	LMG	C39-C40-C41-C42
21	B	802	LMU	C3-C4-C5-C6
21	2	316	LMU	C2-C1-O1'-C1'
21	A	851	LMU	C2-C1-O1'-C1'
21	E	101	LMU	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
21	G	101	LMU	C2-C1-O1'-C1'
21	K	102	LMU	C2-C1-O1'-C1'
21	R	102	LMU	C2-C1-O1'-C1'
21	A	854	LMU	C1-C2-C3-C4
20	2	306	CLA	C6-C7-C8-C9
20	2	321	CLA	C11-C12-C13-C14
20	3	309	CLA	C11-C12-C13-C14
20	A	806	CLA	C11-C10-C8-C9
20	A	809	CLA	C6-C7-C8-C9
20	A	821	CLA	C11-C12-C13-C14
20	A	826	CLA	C11-C10-C8-C9
20	A	833	CLA	C14-C13-C15-C16
20	A	849	CLA	C6-C7-C8-C9
20	A	849	CLA	C14-C13-C15-C16
20	B	805	CLA	C6-C7-C8-C9
20	B	811	CLA	C6-C7-C8-C9
20	B	816	CLA	C11-C10-C8-C9
20	B	824	CLA	C11-C10-C8-C9
20	B	825	CLA	C6-C7-C8-C9
20	B	825	CLA	C11-C12-C13-C14
20	H	107	CLA	C14-C13-C15-C16
20	K	107	CLA	C11-C10-C8-C9
20	K	107	CLA	C14-C13-C15-C16
20	L	202	CLA	C11-C10-C8-C9
20	A	829	CLA	C10-C11-C12-C13
20	3	310	CLA	C4B-C3B-CAB-CBB
20	4	307	CLA	C4B-C3B-CAB-CBB
20	A	812	CLA	C4B-C3B-CAB-CBB
20	A	824	CLA	C4B-C3B-CAB-CBB
20	A	832	CLA	C4B-C3B-CAB-CBB
20	A	835	CLA	C4B-C3B-CAB-CBB
20	A	848	CLA	C4B-C3B-CAB-CBB
20	B	815	CLA	C4B-C3B-CAB-CBB
20	B	820	CLA	C4B-C3B-CAB-CBB
20	B	829	CLA	C4B-C3B-CAB-CBB
20	H	109	CLA	C4B-C3B-CAB-CBB
21	A	852	LMU	C5-C6-C7-C8
21	G	101	LMU	C6-C7-C8-C9
20	B	808	CLA	C6-C7-C8-C10
21	4	320	LMU	O5B-C1B-O1B-C4'
20	B	848	CLA	C2A-CAA-CBA-CGA
21	H	104	LMU	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
20	1	212	CLA	C11-C12-C13-C15
20	2	306	CLA	C11-C12-C13-C15
20	2	307	CLA	C11-C10-C8-C7
20	3	309	CLA	C11-C12-C13-C15
20	4	304	CLA	C11-C12-C13-C15
20	A	824	CLA	C6-C7-C8-C10
20	A	829	CLA	C12-C13-C15-C16
20	A	833	CLA	C12-C13-C15-C16
20	A	849	CLA	C11-C10-C8-C7
20	A	855	CLA	C12-C13-C15-C16
20	B	805	CLA	C6-C7-C8-C10
20	B	806	CLA	C11-C10-C8-C7
20	B	816	CLA	C11-C10-C8-C7
20	B	820	CLA	C6-C7-C8-C10
20	B	822	CLA	C6-C7-C8-C10
20	B	822	CLA	C11-C10-C8-C7
20	B	825	CLA	C6-C7-C8-C10
20	B	835	CLA	C11-C10-C8-C7
20	B	849	CLA	C12-C13-C15-C16
20	J	102	CLA	C11-C12-C13-C15
20	K	107	CLA	C11-C12-C13-C15
20	R	107	CLA	C11-C10-C8-C7
21	A	851	LMU	C5'-C4'-O1B-C1B
20	A	855	CLA	C5-C6-C7-C8
20	B	819	CLA	O1A-CGA-O2A-C1
21	4	301	LMU	O1'-C1-C2-C3
21	4	320	LMU	C5-C6-C7-C8
21	L	205	LMU	C9-C10-C11-C12
20	A	810	CLA	C4-C3-C5-C6
20	A	818	CLA	C3A-C2A-CAA-CBA
20	A	829	CLA	C3A-C2A-CAA-CBA
20	A	831	CLA	C3A-C2A-CAA-CBA
20	A	832	CLA	C3A-C2A-CAA-CBA
20	B	804	CLA	C3A-C2A-CAA-CBA
20	J	102	CLA	C4-C3-C5-C6
20	A	801	CLA	CAA-CBA-CGA-O2A
20	B	815	CLA	C2-C3-C5-C6
21	L	205	LMU	C5-C6-C7-C8
20	B	834	CLA	C10-C11-C12-C13
20	1	214	CLA	CBA-CGA-O2A-C1
20	A	811	CLA	CBA-CGA-O2A-C1
21	R	101	LMU	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
22	B	843	BCR	C19-C20-C21-C22
22	B	850	BCR	C13-C14-C15-C16
22	B	850	BCR	C15-C16-C17-C18
20	B	824	CLA	C10-C11-C12-C13
20	A	807	CLA	C4C-C3C-CAC-CBC
22	3	311	BCR	C11-C12-C13-C35
21	3	318	LMU	C3'-C4'-O1B-C1B
20	B	821	CLA	C6-C7-C8-C9
20	1	214	CLA	C4-C3-C5-C6
20	2	301	CLA	C4-C3-C5-C6
20	A	827	CLA	O1A-CGA-O2A-C1
20	K	107	CLA	O1A-CGA-O2A-C1
21	1	218	LMU	O1'-C1-C2-C3
22	A	843	BCR	C17-C18-C19-C20
21	1	218	LMU	C5-C6-C7-C8
21	3	318	LMU	C6-C7-C8-C9
21	K	104	LMU	O1'-C1-C2-C3
20	1	212	CLA	C2A-CAA-CBA-CGA
20	A	817	CLA	C13-C15-C16-C17
21	1	217	LMU	C4'-C5'-C6'-O6'
21	K	102	LMU	C9-C10-C11-C12
21	3	302	LMU	C5-C6-C7-C8
20	A	828	CLA	C16-C17-C18-C19
20	A	855	CLA	C16-C17-C18-C19
20	B	822	CLA	C5-C6-C7-C8
21	L	205	LMU	C2-C3-C4-C5
21	R	101	LMU	C3-C4-C5-C6
21	A	854	LMU	C2-C3-C4-C5
20	B	811	CLA	C2-C3-C5-C6
20	B	826	CLA	C2-C3-C5-C6
20	B	847	CLA	C2-C3-C5-C6
20	F	206	CLA	C2-C3-C5-C6
20	J	102	CLA	C2-C3-C5-C6
20	A	820	CLA	O1A-CGA-O2A-C1
20	2	304	CLA	O1D-CGD-O2D-CED
20	A	806	CLA	C16-C17-C18-C20
20	B	848	CLA	C16-C17-C18-C20
23	B	840	PQN	C26-C27-C28-C30
21	3	318	LMU	C5'-C4'-O1B-C1B
21	C	101	LMU	C3'-C4'-O1B-C1B
20	A	814	CLA	C2B-C3B-CAB-CBB
20	B	806	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	A	840	BCR	C23-C24-C25-C26
22	A	843	BCR	C23-C24-C25-C30
22	B	841	BCR	C23-C24-C25-C30
22	B	844	BCR	C23-C24-C25-C30
22	G	102	BCR	C23-C24-C25-C30
22	L	209	BCR	C1-C6-C7-C8
20	B	847	CLA	CAA-CBA-CGA-O2A
20	B	847	CLA	C8-C10-C11-C12
21	L	206	LMU	C7-C8-C9-C10
20	J	102	CLA	C14-C13-C15-C16
20	B	848	CLA	C5-C6-C7-C8
20	A	833	CLA	C2C-C3C-CAC-CBC
21	R	103	LMU	O5B-C1B-O1B-C4'
22	3	311	BCR	C15-C16-C17-C18
22	A	843	BCR	C13-C14-C15-C16
20	4	305	CLA	C6-C7-C8-C9
20	2	312	CLA	C13-C15-C16-C17
20	2	317	CLA	C5-C6-C7-C8
20	A	823	CLA	C5-C6-C7-C8
21	1	216	LMU	C11-C10-C9-C8
21	A	845	LMU	O5'-C5'-C6'-O6'
20	B	826	CLA	C13-C15-C16-C17
21	R	101	LMU	C5-C6-C7-C8
20	J	102	CLA	C12-C13-C15-C16
21	B	802	LMU	C5'-C4'-O1B-C1B
21	B	801	LMU	C9-C10-C11-C12
20	B	807	CLA	C4-C3-C5-C6
20	B	811	CLA	C4-C3-C5-C6
20	F	206	CLA	C4-C3-C5-C6
20	H	107	CLA	C4-C3-C5-C6
20	A	817	CLA	O1D-CGD-O2D-CED
20	2	307	CLA	C13-C15-C16-C17
21	H	105	LMU	O5B-C5B-C6B-O6B
20	A	836	CLA	C16-C17-C18-C20
23	A	839	PQN	C26-C27-C28-C29
20	4	304	CLA	C2C-C3C-CAC-CBC
20	B	837	CLA	O1D-CGD-O2D-CED
20	1	202	CLA	CBA-CGA-O2A-C1
20	1	212	CLA	CBA-CGA-O2A-C1
21	3	302	LMU	C7-C8-C9-C10
20	A	829	CLA	C11-C12-C13-C14
20	A	847	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	B	816	CLA	C11-C12-C13-C14
20	B	826	CLA	C6-C7-C8-C9
20	B	829	CLA	C11-C12-C13-C14
21	A	852	LMU	C6-C7-C8-C9
21	4	322	LMU	C1-C2-C3-C4
21	F	201	LMU	C2-C3-C4-C5
20	A	803	CLA	C16-C17-C18-C20
20	B	820	CLA	C16-C17-C18-C20
20	J	103	CLA	C6-C7-C8-C9
20	L	204	CLA	C6-C7-C8-C9
21	2	320	LMU	C6-C7-C8-C9
20	B	805	CLA	C8-C10-C11-C12
21	K	101	LMU	C9-C10-C11-C12
21	A	845	LMU	O1'-C1-C2-C3
20	B	824	CLA	C3-C5-C6-C7
22	B	850	BCR	C9-C10-C11-C12
22	F	202	BCR	C9-C10-C11-C12
20	4	304	CLA	C16-C17-C18-C20
20	B	808	CLA	C6-C7-C8-C9
20	B	829	CLA	C16-C17-C18-C19
25	B	846	LMG	C41-C42-C43-C44
23	B	840	PQN	C23-C25-C26-C27
21	H	102	LMU	O5B-C1B-O1B-C4'
20	4	304	CLA	CBA-CGA-O2A-C1
20	4	302	CLA	C6-C7-C8-C10
20	A	814	CLA	C16-C17-C18-C19
21	C	101	LMU	C5'-C4'-O1B-C1B
21	1	217	LMU	C7-C8-C9-C10
20	1	212	CLA	O1A-CGA-O2A-C1
20	A	809	CLA	C13-C15-C16-C17
22	B	844	BCR	C36-C18-C19-C20
20	2	306	CLA	C6-C7-C8-C10
20	2	312	CLA	C12-C13-C15-C16
20	2	317	CLA	C11-C12-C13-C15
20	3	310	CLA	C11-C10-C8-C7
20	A	803	CLA	C11-C12-C13-C15
20	A	806	CLA	C11-C10-C8-C7
20	A	816	CLA	C12-C13-C15-C16
20	A	849	CLA	C11-C12-C13-C15
20	A	855	CLA	C11-C10-C8-C7
20	B	814	CLA	C11-C10-C8-C7
20	B	823	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
20	B	826	CLA	C11-C12-C13-C15
20	B	838	CLA	C11-C12-C13-C15
20	B	838	CLA	C12-C13-C15-C16
20	B	847	CLA	C11-C10-C8-C7
21	B	801	LMU	C3-C4-C5-C6
22	B	842	BCR	C11-C12-C13-C14
22	J	101	BCR	C17-C18-C19-C20
20	A	837	CLA	CBA-CGA-O2A-C1
20	A	818	CLA	O1A-CGA-O2A-C1
20	B	804	CLA	O1A-CGA-O2A-C1
20	3	309	CLA	C15-C16-C17-C18
20	A	806	CLA	C13-C15-C16-C17
20	L	207	CLA	C2A-CAA-CBA-CGA
20	1	206	CLA	C14-C13-C15-C16
20	A	803	CLA	C16-C17-C18-C19
20	B	825	CLA	C16-C17-C18-C19
20	B	823	CLA	CBD-CGD-O2D-CED
21	H	102	LMU	C4B-C5B-C6B-O6B
20	1	202	CLA	O1A-CGA-O2A-C1
20	B	807	CLA	C2-C3-C5-C6
20	B	825	CLA	C3-C5-C6-C7
20	B	848	CLA	C10-C11-C12-C13
20	F	205	CLA	C4C-C3C-CAC-CBC
20	L	203	CLA	O1A-CGA-O2A-C1
21	2	313	LMU	C5-C6-C7-C8
20	B	823	CLA	C5-C6-C7-C8
21	2	319	LMU	C11-C10-C9-C8
20	A	821	CLA	C4C-C3C-CAC-CBC
20	3	310	CLA	C10-C11-C12-C13
20	A	822	CLA	C3-C5-C6-C7
20	A	848	CLA	C2A-CAA-CBA-CGA
21	K	104	LMU	C3'-C4'-O1B-C1B
20	H	107	CLA	C2-C3-C5-C6
20	A	806	CLA	C3-C5-C6-C7
20	A	803	CLA	C11-C12-C13-C14
20	A	806	CLA	C14-C13-C15-C16
20	A	809	CLA	C14-C13-C15-C16
20	A	828	CLA	C6-C7-C8-C9
20	B	804	CLA	C11-C10-C8-C9
20	B	829	CLA	C14-C13-C15-C16
20	L	201	CLA	C14-C13-C15-C16
25	B	846	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
20	A	811	CLA	O1A-CGA-O2A-C1
20	G	103	CLA	C2C-C3C-CAC-CBC
21	4	321	LMU	C2-C3-C4-C5
21	B	801	LMU	C4-C5-C6-C7
20	B	809	CLA	C3-C5-C6-C7
21	R	103	LMU	C5'-C4'-O1B-C1B
20	A	802	CLA	C6-C7-C8-C10
21	1	216	LMU	C4-C5-C6-C7
20	H	101	CLA	C3-C5-C6-C7
20	B	822	CLA	C2A-CAA-CBA-CGA
20	A	855	CLA	C16-C17-C18-C20
20	J	103	CLA	C6-C7-C8-C10
20	K	105	CLA	O1D-CGD-O2D-CED
21	2	319	LMU	O5B-C5B-C6B-O6B
20	A	809	CLA	O1A-CGA-O2A-C1
20	B	812	CLA	C10-C11-C12-C13
21	L	205	LMU	C3'-C4'-O1B-C1B
21	4	320	LMU	C11-C10-C9-C8
21	A	853	LMU	O5B-C1B-O1B-C4'
21	H	103	LMU	O5B-C1B-O1B-C4'
20	A	828	CLA	C16-C17-C18-C20
20	A	850	CLA	CAA-CBA-CGA-O2A
21	B	801	LMU	C3'-C4'-O1B-C1B
21	A	852	LMU	C2-C1-O1'-C1'
21	C	101	LMU	C2-C1-O1'-C1'
21	4	320	LMU	C2-C3-C4-C5
20	1	204	CLA	C4B-C3B-CAB-CBB
20	1	206	CLA	C4B-C3B-CAB-CBB
20	2	312	CLA	C1A-C2A-CAA-CBA
20	3	309	CLA	C4B-C3B-CAB-CBB
20	4	305	CLA	C4B-C3B-CAB-CBB
20	A	807	CLA	C4B-C3B-CAB-CBB
20	A	829	CLA	C1A-C2A-CAA-CBA
20	B	834	CLA	C1A-C2A-CAA-CBA
20	B	848	CLA	C1A-C2A-CAA-CBA
20	R	106	CLA	C4B-C3B-CAB-CBB
20	4	302	CLA	C6-C7-C8-C9
20	B	838	CLA	O1A-CGA-O2A-C1
20	A	837	CLA	O1A-CGA-O2A-C1
20	2	301	CLA	C2-C3-C5-C6
20	A	832	CLA	C2-C3-C5-C6
20	A	812	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
20	B	806	CLA	C3-C5-C6-C7
20	3	309	CLA	C11-C10-C8-C7
20	A	823	CLA	C11-C10-C8-C7
20	A	826	CLA	C6-C7-C8-C10
20	A	828	CLA	C11-C10-C8-C7
20	A	847	CLA	C6-C7-C8-C10
20	B	804	CLA	C11-C12-C13-C15
20	B	810	CLA	C11-C10-C8-C7
20	B	811	CLA	C11-C12-C13-C15
20	B	826	CLA	C12-C13-C15-C16
20	B	829	CLA	C11-C10-C8-C7
20	B	847	CLA	C11-C12-C13-C15
20	I	102	CLA	C11-C10-C8-C7
20	K	107	CLA	C6-C7-C8-C10
23	A	839	PQN	C22-C23-C25-C26
20	4	304	CLA	C16-C17-C18-C19
20	B	812	CLA	C11-C12-C13-C14
20	B	849	CLA	C16-C17-C18-C20
21	H	103	LMU	C7-C8-C9-C10
20	J	103	CLA	CAA-CBA-CGA-O2A
20	4	307	CLA	C3A-C2A-CAA-CBA
20	B	834	CLA	C3A-C2A-CAA-CBA
20	B	819	CLA	C6-C7-C8-C9
20	H	110	CLA	C6-C7-C8-C9
20	3	310	CLA	C11-C10-C8-C9
20	A	816	CLA	C14-C13-C15-C16
20	A	849	CLA	C11-C12-C13-C14
20	B	835	CLA	C11-C10-C8-C9
20	1	214	CLA	O1A-CGA-O2A-C1
22	L	209	BCR	C15-C16-C17-C18
21	4	316	LMU	C3-C4-C5-C6
21	C	101	LMU	O1'-C1-C2-C3
20	L	202	CLA	C4-C3-C5-C6
20	2	317	CLA	C10-C11-C12-C13
20	A	836	CLA	C15-C16-C17-C18
21	4	316	LMU	O1'-C1-C2-C3
20	2	307	CLA	CAD-CBD-CGD-O2D
20	4	302	CLA	CAD-CBD-CGD-O2D
20	A	824	CLA	CAD-CBD-CGD-O2D
20	B	805	CLA	CAD-CBD-CGD-O2D
20	B	832	CLA	CAD-CBD-CGD-O2D
20	B	834	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	B	848	CLA	CAD-CBD-CGD-O2D
20	4	304	CLA	O1A-CGA-O2A-C1
20	A	822	CLA	C13-C15-C16-C17
20	B	815	CLA	C11-C12-C13-C15
20	B	822	CLA	C3-C5-C6-C7
20	2	306	CLA	C10-C11-C12-C13
20	A	824	CLA	C13-C15-C16-C17
21	A	854	LMU	C5'-C4'-O1B-C1B
21	A	853	LMU	C2-C3-C4-C5
20	2	307	CLA	CAD-CBD-CGD-O1D
20	4	302	CLA	CAD-CBD-CGD-O1D
20	4	310	CLA	CHA-CBD-CGD-O1D
20	4	310	CLA	CHA-CBD-CGD-O2D
20	A	812	CLA	CHA-CBD-CGD-O1D
20	A	812	CLA	CHA-CBD-CGD-O2D
20	A	824	CLA	CAD-CBD-CGD-O1D
20	B	805	CLA	CAD-CBD-CGD-O1D
20	B	806	CLA	CHA-CBD-CGD-O1D
20	B	830	CLA	CHA-CBD-CGD-O1D
20	B	830	CLA	CHA-CBD-CGD-O2D
20	B	832	CLA	CAD-CBD-CGD-O1D
20	B	834	CLA	CAD-CBD-CGD-O1D
20	B	848	CLA	CAD-CBD-CGD-O1D
22	A	842	BCR	C13-C14-C15-C16
20	B	805	CLA	C5-C6-C7-C8
20	A	836	CLA	C16-C17-C18-C19
20	2	321	CLA	C2B-C3B-CAB-CBB
20	A	810	CLA	C2B-C3B-CAB-CBB
20	A	821	CLA	C2B-C3B-CAB-CBB
20	A	828	CLA	C2B-C3B-CAB-CBB
20	B	819	CLA	C2B-C3B-CAB-CBB
20	B	831	CLA	C2B-C3B-CAB-CBB
20	L	207	CLA	C2B-C3B-CAB-CBB
20	L	208	CLA	C2B-C3B-CAB-CBB
22	B	843	BCR	C23-C24-C25-C26
20	3	315	CLA	CAA-CBA-CGA-O2A
21	G	101	LMU	C9-C10-C11-C12
20	A	833	CLA	C13-C15-C16-C17
20	3	309	CLA	C2C-C3C-CAC-CBC
21	H	105	LMU	C5-C6-C7-C8
21	B	801	LMU	C2-C3-C4-C5
20	2	317	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
21	A	846	LMU	C7-C8-C9-C10
20	2	307	CLA	C4C-C3C-CAC-CBC
20	B	823	CLA	O1D-CGD-O2D-CED
22	B	843	BCR	C13-C14-C15-C16
21	3	318	LMU	C9-C10-C11-C12
20	B	820	CLA	C16-C17-C18-C19
23	B	840	PQN	C26-C27-C28-C29
20	2	307	CLA	C11-C10-C8-C9
20	A	823	CLA	C6-C7-C8-C9
20	B	810	CLA	C11-C10-C8-C9
20	B	811	CLA	C11-C10-C8-C9
20	B	822	CLA	C6-C7-C8-C9
20	B	838	CLA	C11-C12-C13-C14
23	B	840	PQN	C21-C22-C23-C24
20	A	823	CLA	C6-C7-C8-C10
20	B	811	CLA	C12-C13-C15-C16
20	B	820	CLA	C12-C13-C15-C16
20	B	826	CLA	C6-C7-C8-C10
20	B	829	CLA	C11-C12-C13-C15
20	R	107	CLA	C11-C12-C13-C15
21	4	322	LMU	C11-C10-C9-C8
21	4	322	LMU	C6-C7-C8-C9
21	R	108	LMU	C3-C4-C5-C6
21	1	218	LMU	C4-C5-C6-C7
20	A	847	CLA	C4-C3-C5-C6
21	A	846	LMU	C1-C2-C3-C4
20	3	309	CLA	C8-C10-C11-C12
21	R	101	LMU	C5'-C4'-O1B-C1B
21	E	101	LMU	C9-C10-C11-C12
22	A	840	BCR	C13-C14-C15-C16
21	4	301	LMU	C6-C7-C8-C9
21	F	201	LMU	C6-C7-C8-C9
21	2	318	LMU	O1'-C1-C2-C3
21	4	322	LMU	O1'-C1-C2-C3
20	A	810	CLA	C6-C7-C8-C9
20	J	102	CLA	C2-C1-O2A-CGA
21	B	801	LMU	C1-C2-C3-C4
20	B	810	CLA	CAA-CBA-CGA-O2A
20	B	813	CLA	CAA-CBA-CGA-O2A
21	1	216	LMU	C7-C8-C9-C10
21	4	321	LMU	C4-C5-C6-C7
22	B	844	BCR	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
20	B	830	CLA	C2A-CAA-CBA-CGA
20	B	836	CLA	C2A-CAA-CBA-CGA
20	H	109	CLA	C2A-CAA-CBA-CGA
22	F	202	BCR	C13-C14-C15-C16
20	A	829	CLA	C16-C17-C18-C19
20	2	321	CLA	C4-C3-C5-C6
20	A	809	CLA	C4-C3-C5-C6
21	R	104	LMU	C9-C10-C11-C12
20	A	847	CLA	C2-C3-C5-C6
21	1	216	LMU	C5-C6-C7-C8
21	A	845	LMU	C4-C5-C6-C7
21	3	302	LMU	C2-C1-O1'-C1'
21	4	321	LMU	C2-C1-O1'-C1'
20	B	807	CLA	O1D-CGD-O2D-CED
20	A	828	CLA	C11-C10-C8-C9
20	A	847	CLA	C6-C7-C8-C9
20	B	810	CLA	C14-C13-C15-C16
20	B	826	CLA	C11-C12-C13-C14
20	K	107	CLA	C6-C7-C8-C9
20	3	301	CLA	C2C-C3C-CAC-CBC
21	4	320	LMU	C6-C7-C8-C9
20	B	823	CLA	C13-C15-C16-C17
20	H	110	CLA	C6-C7-C8-C10
20	A	817	CLA	CBA-CGA-O2A-C1
20	A	833	CLA	C4C-C3C-CAC-CBC
20	H	108	CLA	C5-C6-C7-C8
20	L	204	CLA	C5-C6-C7-C8
20	A	817	CLA	O1A-CGA-O2A-C1
21	C	101	LMU	C9-C10-C11-C12
20	B	810	CLA	C4-C3-C5-C6
21	4	320	LMU	C2B-C1B-O1B-C4'
20	A	816	CLA	C6-C7-C8-C10
20	B	826	CLA	C11-C10-C8-C7
20	B	834	CLA	C11-C10-C8-C7
20	J	102	CLA	C6-C7-C8-C10
20	A	825	CLA	O1A-CGA-O2A-C1
21	A	846	LMU	C4-C5-C6-C7
20	B	829	CLA	O1A-CGA-O2A-C1
20	B	829	CLA	CBA-CGA-O2A-C1
20	B	810	CLA	C13-C15-C16-C17
20	B	824	CLA	CAA-CBA-CGA-O2A
21	R	103	LMU	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
21	2	313	LMU	C9-C10-C11-C12
20	3	310	CLA	C3A-C2A-CAA-CBA
20	3	315	CLA	C3A-C2A-CAA-CBA
20	4	302	CLA	C3A-C2A-CAA-CBA
20	4	315	CLA	C3A-C2A-CAA-CBA
20	4	318	CLA	C4-C3-C5-C6
20	A	810	CLA	C3A-C2A-CAA-CBA
20	A	813	CLA	C3A-C2A-CAA-CBA
20	A	855	CLA	C3A-C2A-CAA-CBA
20	L	202	CLA	C2-C3-C5-C6
20	A	812	CLA	C4C-C3C-CAC-CBC
20	1	206	CLA	C2A-CAA-CBA-CGA
21	4	321	LMU	C1-C2-C3-C4
22	A	844	BCR	C35-C13-C14-C15
22	B	842	BCR	C11-C10-C9-C34
22	B	843	BCR	C20-C21-C22-C37
22	B	850	BCR	C11-C10-C9-C34
22	F	203	BCR	C16-C17-C18-C36
20	B	811	CLA	C8-C10-C11-C12
21	F	201	LMU	C4-C5-C6-C7
20	A	855	CLA	C2-C1-O2A-CGA
22	A	841	BCR	C13-C14-C15-C16
20	R	107	CLA	CAA-CBA-CGA-O2A
20	B	814	CLA	C11-C12-C13-C14
20	A	832	CLA	C4-C3-C5-C6
20	A	824	CLA	C4-C3-C5-C6
20	B	829	CLA	C4-C3-C5-C6
20	B	823	CLA	C16-C17-C18-C20
21	A	853	LMU	C2B-C1B-O1B-C4'
20	3	309	CLA	C2A-CAA-CBA-CGA
20	A	825	CLA	CBA-CGA-O2A-C1
20	A	821	CLA	C3-C5-C6-C7
20	2	307	CLA	C14-C13-C15-C16
20	A	803	CLA	C14-C13-C15-C16
20	A	809	CLA	C11-C12-C13-C14
20	A	848	CLA	C11-C12-C13-C14
20	B	805	CLA	C11-C10-C8-C9
20	B	820	CLA	C11-C12-C13-C14
20	B	849	CLA	C6-C7-C8-C9
20	J	102	CLA	C6-C7-C8-C9
20	L	202	CLA	C11-C12-C13-C14
21	3	318	LMU	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	2	321	CLA	C3-C5-C6-C7
20	A	814	CLA	C16-C17-C18-C20
20	4	318	CLA	C2-C3-C5-C6
20	K	105	CLA	C2C-C3C-CAC-CBC
20	3	310	CLA	C1A-C2A-CAA-CBA
20	4	307	CLA	C1A-C2A-CAA-CBA
20	B	832	CLA	C1A-C2A-CAA-CBA
22	A	844	BCR	C12-C13-C14-C15
22	B	842	BCR	C11-C10-C9-C8
22	B	843	BCR	C20-C21-C22-C23
22	B	850	BCR	C11-C10-C9-C8
22	F	203	BCR	C16-C17-C18-C19
20	A	820	CLA	C6-C7-C8-C10
21	A	851	LMU	C6-C7-C8-C9
21	A	845	LMU	C1-C2-C3-C4
21	R	103	LMU	C2-C3-C4-C5
20	1	201	CLA	C2B-C3B-CAB-CBB
20	2	306	CLA	C2B-C3B-CAB-CBB
20	3	320	CLA	C2B-C3B-CAB-CBB
20	A	804	CLA	C2B-C3B-CAB-CBB
20	A	835	CLA	C2B-C3B-CAB-CBB
20	B	822	CLA	C2B-C3B-CAB-CBB
20	B	836	CLA	C2B-C3B-CAB-CBB
20	H	109	CLA	C2B-C3B-CAB-CBB
20	J	102	CLA	C2B-C3B-CAB-CBB
20	L	204	CLA	C2B-C3B-CAB-CBB
22	3	311	BCR	C1-C6-C7-C8
22	A	840	BCR	C23-C24-C25-C30
22	A	843	BCR	C23-C24-C25-C26
22	B	841	BCR	C23-C24-C25-C26
22	G	102	BCR	C23-C24-C25-C26
20	A	828	CLA	C8-C10-C11-C12
20	2	312	CLA	C11-C10-C8-C7
20	4	304	CLA	C6-C7-C8-C10
20	A	821	CLA	C12-C13-C15-C16
20	B	805	CLA	C11-C10-C8-C7
20	B	824	CLA	C6-C7-C8-C10
20	B	847	CLA	C6-C7-C8-C10
23	B	840	PQN	C21-C22-C23-C25
20	B	824	CLA	C2A-CAA-CBA-CGA
20	B	807	CLA	C13-C15-C16-C17
20	A	831	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
20	A	828	CLA	C10-C11-C12-C13
20	A	812	CLA	CAA-CBA-CGA-O1A
20	A	848	CLA	C8-C10-C11-C12
20	A	849	CLA	C16-C17-C18-C20
20	1	206	CLA	C12-C13-C15-C16
20	2	321	CLA	C12-C13-C15-C16
22	F	203	BCR	C11-C12-C13-C35
21	H	105	LMU	C2-C3-C4-C5
20	A	822	CLA	C4-C3-C5-C6
21	K	102	LMU	O1'-C1-C2-C3
21	C	101	LMU	C4'-C5'-C6'-O6'
20	B	826	CLA	C8-C10-C11-C12
20	A	809	CLA	C2-C3-C5-C6
20	A	822	CLA	C2-C3-C5-C6
20	A	824	CLA	C2-C3-C5-C6
20	B	810	CLA	C2-C3-C5-C6
20	B	829	CLA	C2-C3-C5-C6
20	L	207	CLA	C2-C1-O2A-CGA
21	H	104	LMU	C2B-C1B-O1B-C4'
20	A	808	CLA	CAA-CBA-CGA-O2A
21	2	319	LMU	O5B-C1B-O1B-C4'
22	F	202	BCR	C15-C16-C17-C18
20	B	811	CLA	C15-C16-C17-C18
25	B	846	LMG	C31-C32-C33-C34
21	2	318	LMU	C2B-C1B-O1B-C4'
20	B	825	CLA	C4-C3-C5-C6
20	A	831	CLA	CAA-CBA-CGA-O2A
21	B	802	LMU	C1-C2-C3-C4
20	3	309	CLA	CAA-CBA-CGA-O2A
20	H	107	CLA	C13-C15-C16-C17
20	A	808	CLA	CAA-CBA-CGA-O1A
20	A	812	CLA	CAA-CBA-CGA-O2A
20	B	838	CLA	CAA-CBA-CGA-O2A
20	A	855	CLA	C2C-C3C-CAC-CBC
20	J	103	CLA	C2A-CAA-CBA-CGA
21	2	316	LMU	C3-C4-C5-C6
21	2	319	LMU	C1-C2-C3-C4
21	G	101	LMU	C5'-C4'-O1B-C1B
20	A	802	CLA	C4-C3-C5-C6
20	A	849	CLA	C16-C17-C18-C19
20	B	815	CLA	C5-C6-C7-C8
20	B	827	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	L	204	CLA	C4B-C3B-CAB-CBB
20	H	107	CLA	C3-C5-C6-C7
20	B	804	CLA	CAA-CBA-CGA-O2A
20	A	824	CLA	C16-C17-C18-C19
20	B	827	CLA	CAA-CBA-CGA-O2A
20	A	822	CLA	C8-C10-C11-C12
20	B	832	CLA	CAA-CBA-CGA-O2A
20	B	847	CLA	CAA-CBA-CGA-O1A
20	B	825	CLA	C2-C3-C5-C6
20	3	310	CLA	C8-C10-C11-C12
20	2	307	CLA	C12-C13-C15-C16
20	1	212	CLA	C8-C10-C11-C12
21	C	101	LMU	C3-C4-C5-C6
20	A	801	CLA	CAA-CBA-CGA-O1A
20	A	814	CLA	C6-C7-C8-C9
20	A	822	CLA	C11-C12-C13-C14
20	A	824	CLA	C11-C12-C13-C14
20	A	828	CLA	C11-C12-C13-C14
20	B	805	CLA	C11-C12-C13-C14
20	B	815	CLA	C6-C7-C8-C9
20	B	847	CLA	C11-C10-C8-C9
20	J	102	CLA	C11-C10-C8-C9
23	A	839	PQN	C24-C23-C25-C26
20	4	307	CLA	C2A-CAA-CBA-CGA
20	2	321	CLA	C2-C1-O2A-CGA
20	4	306	CLA	C2-C1-O2A-CGA
20	A	802	CLA	C2-C1-O2A-CGA
20	A	830	CLA	C2-C1-O2A-CGA
20	B	823	CLA	C2-C1-O2A-CGA
21	2	319	LMU	C7-C8-C9-C10
20	2	304	CLA	C3A-C2A-CAA-CBA
20	A	809	CLA	C3A-C2A-CAA-CBA
20	A	834	CLA	C3A-C2A-CAA-CBA
20	B	818	CLA	C3A-C2A-CAA-CBA
20	K	106	CLA	C3A-C2A-CAA-CBA
20	2	306	CLA	CAA-CBA-CGA-O2A
20	A	824	CLA	C10-C11-C12-C13
20	B	832	CLA	CAA-CBA-CGA-O1A
20	A	823	CLA	C10-C11-C12-C13
21	4	316	LMU	C4B-C5B-C6B-O6B
21	A	854	LMU	O5'-C1'-O1'-C1
20	B	837	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
21	R	108	LMU	O1'-C1-C2-C3
20	B	821	CLA	C4-C3-C5-C6
20	A	855	CLA	CAA-CBA-CGA-O2A
20	B	817	CLA	CAA-CBA-CGA-O2A
20	B	804	CLA	C14-C13-C15-C16
20	B	838	CLA	C14-C13-C15-C16
20	I	102	CLA	C11-C10-C8-C9
20	R	107	CLA	C14-C13-C15-C16
20	A	847	CLA	C16-C17-C18-C19
20	B	818	CLA	CAA-CBA-CGA-O2A
20	B	831	CLA	CAA-CBA-CGA-O1A
21	A	854	LMU	C9-C10-C11-C12
20	B	829	CLA	C5-C6-C7-C8
21	4	322	LMU	C4'-C5'-C6'-O6'
20	A	847	CLA	CAA-CBA-CGA-O2A
20	B	807	CLA	C2A-CAA-CBA-CGA
20	I	102	CLA	C2A-CAA-CBA-CGA
20	3	301	CLA	C6-C7-C8-C10
20	A	806	CLA	C6-C7-C8-C10
20	A	809	CLA	C6-C7-C8-C10
20	A	809	CLA	C11-C10-C8-C7
20	A	822	CLA	C11-C12-C13-C15
20	A	848	CLA	C11-C12-C13-C15
20	A	849	CLA	C6-C7-C8-C10
20	B	835	CLA	C6-C7-C8-C10
20	H	107	CLA	C11-C10-C8-C7
20	J	102	CLA	C11-C10-C8-C7
23	A	839	PQN	C21-C22-C23-C25
20	J	102	CLA	C3-C5-C6-C7
20	1	204	CLA	C2B-C3B-CAB-CBB
20	1	214	CLA	C2B-C3B-CAB-CBB
20	H	101	CLA	C2B-C3B-CAB-CBB
20	H	108	CLA	C2B-C3B-CAB-CBB
20	R	106	CLA	C2B-C3B-CAB-CBB
22	3	311	BCR	C5-C6-C7-C8
22	B	843	BCR	C1-C6-C7-C8
22	B	843	BCR	C5-C6-C7-C8
22	L	209	BCR	C5-C6-C7-C8
20	A	807	CLA	C2-C1-O2A-CGA
20	A	838	CLA	C2-C1-O2A-CGA
20	F	206	CLA	C2-C1-O2A-CGA
20	H	107	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
20	A	817	CLA	C16-C17-C18-C20
20	A	821	CLA	C8-C10-C11-C12
20	R	107	CLA	C13-C15-C16-C17
20	A	803	CLA	CAA-CBA-CGA-O2A
20	H	110	CLA	CAA-CBA-CGA-O2A
20	A	855	CLA	C10-C11-C12-C13
20	2	311	CLA	CAA-CBA-CGA-O2A
20	B	823	CLA	CAA-CBA-CGA-O2A
20	I	102	CLA	CAA-CBA-CGA-O2A
20	B	805	CLA	C2C-C3C-CAC-CBC
20	3	320	CLA	C3-C5-C6-C7
20	A	803	CLA	C2C-C3C-CAC-CBC
21	E	101	LMU	O1'-C1-C2-C3
20	B	808	CLA	C2C-C3C-CAC-CBC
20	A	828	CLA	C5-C6-C7-C8
21	4	321	LMU	C9-C10-C11-C12
20	4	304	CLA	CAA-CBA-CGA-O2A
20	A	835	CLA	CAA-CBA-CGA-O2A
20	B	833	CLA	CAA-CBA-CGA-O2A
20	2	321	CLA	C2-C3-C5-C6
21	H	103	LMU	C3'-C4'-O1B-C1B
21	R	103	LMU	C2B-C1B-O1B-C4'
21	G	101	LMU	C3-C4-C5-C6
20	1	211	CLA	CAA-CBA-CGA-O2A
20	2	304	CLA	CBD-CGD-O2D-CED
20	3	309	CLA	C11-C10-C8-C9
20	A	823	CLA	CAA-CBA-CGA-O2A
20	2	304	CLA	C1A-C2A-CAA-CBA
20	A	804	CLA	C1A-C2A-CAA-CBA
20	A	810	CLA	C1A-C2A-CAA-CBA
20	A	837	CLA	C1A-C2A-CAA-CBA
20	B	818	CLA	C1A-C2A-CAA-CBA
20	B	825	CLA	C4B-C3B-CAB-CBB
20	K	106	CLA	C1A-C2A-CAA-CBA
20	B	849	CLA	C4-C3-C5-C6
20	4	304	CLA	C4C-C3C-CAC-CBC
20	1	206	CLA	CAA-CBA-CGA-O2A
20	A	802	CLA	C2-C3-C5-C6
22	G	102	BCR	C15-C16-C17-C18
20	1	214	CLA	CAA-CBA-CGA-O2A
20	A	809	CLA	CAA-CBA-CGA-O2A
20	A	836	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	1	216	LMU	C9-C10-C11-C12
20	A	849	CLA	C2A-CAA-CBA-CGA
21	3	318	LMU	C11-C10-C9-C8
20	H	109	CLA	C2C-C3C-CAC-CBC
20	A	818	CLA	C2-C3-C5-C6
20	4	310	CLA	C2-C1-O2A-CGA
20	A	806	CLA	C2-C1-O2A-CGA
20	B	826	CLA	C2-C1-O2A-CGA
20	B	848	CLA	C2-C1-O2A-CGA
20	R	106	CLA	C2-C1-O2A-CGA
20	A	806	CLA	C11-C12-C13-C15
20	A	809	CLA	C12-C13-C15-C16
20	A	824	CLA	C11-C12-C13-C15
20	B	805	CLA	C11-C12-C13-C15
20	B	810	CLA	C12-C13-C15-C16
20	B	812	CLA	C11-C10-C8-C7
20	B	835	CLA	C11-C12-C13-C15
20	B	837	CLA	C6-C7-C8-C10
20	B	849	CLA	C6-C7-C8-C10
20	B	831	CLA	CAA-CBA-CGA-O2A
20	A	837	CLA	C16-C17-C18-C20
20	A	850	CLA	C2-C1-O2A-CGA
21	H	103	LMU	O1'-C1-C2-C3
21	L	205	LMU	C5'-C4'-O1B-C1B
20	K	107	CLA	CAA-CBA-CGA-O2A
20	4	306	CLA	C2A-CAA-CBA-CGA
20	A	817	CLA	C2A-CAA-CBA-CGA
20	1	204	CLA	C3A-C2A-CAA-CBA
20	A	820	CLA	C3A-C2A-CAA-CBA
20	A	837	CLA	C3A-C2A-CAA-CBA
20	I	102	CLA	CAA-CBA-CGA-O1A
20	A	833	CLA	C2-C3-C5-C6
21	L	210	LMU	C4'-C5'-C6'-O6'
20	H	108	CLA	CAA-CBA-CGA-O2A
20	A	847	CLA	C2C-C3C-CAC-CBC
21	E	101	LMU	C6-C7-C8-C9
20	B	833	CLA	CAA-CBA-CGA-O1A
20	2	317	CLA	C11-C12-C13-C14
20	A	826	CLA	C6-C7-C8-C9
20	B	810	CLA	C6-C7-C8-C9
20	B	811	CLA	C11-C12-C13-C14
20	A	837	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	4	304	CLA	CAA-CBA-CGA-O1A
20	A	835	CLA	CAA-CBA-CGA-O1A
20	B	818	CLA	CAA-CBA-CGA-O1A
20	B	823	CLA	CAA-CBA-CGA-O1A
21	R	102	LMU	C2-C3-C4-C5
22	L	209	BCR	C36-C18-C19-C20
20	A	833	CLA	C4-C3-C5-C6
21	4	301	LMU	C7-C8-C9-C10
25	B	846	LMG	C28-C29-C30-C31
21	R	102	LMU	C5-C6-C7-C8
20	A	826	CLA	C10-C11-C12-C13
20	B	823	CLA	C10-C11-C12-C13
20	1	214	CLA	CAA-CBA-CGA-O1A
20	A	803	CLA	CAA-CBA-CGA-O1A
20	A	809	CLA	CAA-CBA-CGA-O1A
20	A	855	CLA	CAA-CBA-CGA-O1A
20	B	817	CLA	CAA-CBA-CGA-O1A
20	H	110	CLA	CAA-CBA-CGA-O1A
20	2	302	CLA	O1A-CGA-O2A-C1
20	A	847	CLA	CAA-CBA-CGA-O1A
20	K	107	CLA	CAA-CBA-CGA-O1A
20	2	310	CLA	CAA-CBA-CGA-O2A
20	B	849	CLA	CAA-CBA-CGA-O2A
20	2	302	CLA	CBA-CGA-O2A-C1
21	H	103	LMU	C5-C6-C7-C8
20	A	850	CLA	CAA-CBA-CGA-O1A
20	H	108	CLA	CAA-CBA-CGA-O1A
20	2	317	CLA	C15-C16-C17-C18
20	A	816	CLA	C8-C10-C11-C12
20	2	311	CLA	CAA-CBA-CGA-O1A
20	1	212	CLA	CAD-CBD-CGD-O2D
20	B	835	CLA	CAA-CBA-CGA-O2A
20	A	838	CLA	C2C-C3C-CAC-CBC
20	4	302	CLA	C2-C1-O2A-CGA
20	A	848	CLA	C2-C1-O2A-CGA
20	B	828	CLA	C2-C1-O2A-CGA
20	B	835	CLA	C2-C1-O2A-CGA
20	K	106	CLA	C2-C1-O2A-CGA
20	L	202	CLA	C2-C1-O2A-CGA
21	A	853	LMU	C1-C2-C3-C4
21	A	853	LMU	C9-C10-C11-C12
20	A	823	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
20	1	202	CLA	CAA-CBA-CGA-O2A
20	A	813	CLA	CAA-CBA-CGA-O2A
20	A	806	CLA	C2C-C3C-CAC-CBC
20	B	809	CLA	C2A-CAA-CBA-CGA
20	B	829	CLA	C8-C10-C11-C12
20	4	318	CLA	CAA-CBA-CGA-O2A
20	2	302	CLA	C5-C6-C7-C8
20	A	803	CLA	C10-C11-C12-C13
20	4	306	CLA	C2C-C3C-CAC-CBC
20	4	315	CLA	CAA-CBA-CGA-O2A
20	F	206	CLA	CAA-CBA-CGA-O2A
20	1	206	CLA	CAA-CBA-CGA-O1A
20	B	849	CLA	CAA-CBA-CGA-O1A
20	1	202	CLA	C2-C1-O2A-CGA

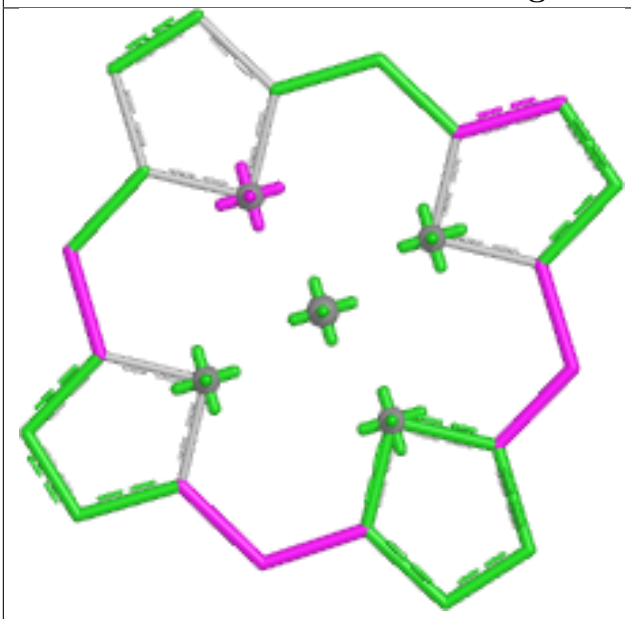
There are no ring outliers.

4 monomers are involved in 3 short contacts:

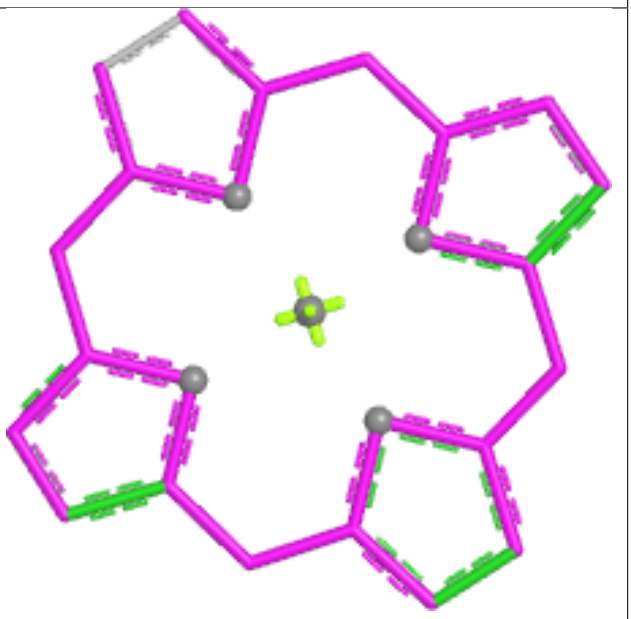
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	313	LMU	0	1
20	1	207	CLA	0	2
20	K	105	CLA	0	2
20	A	831	CLA	0	1

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.

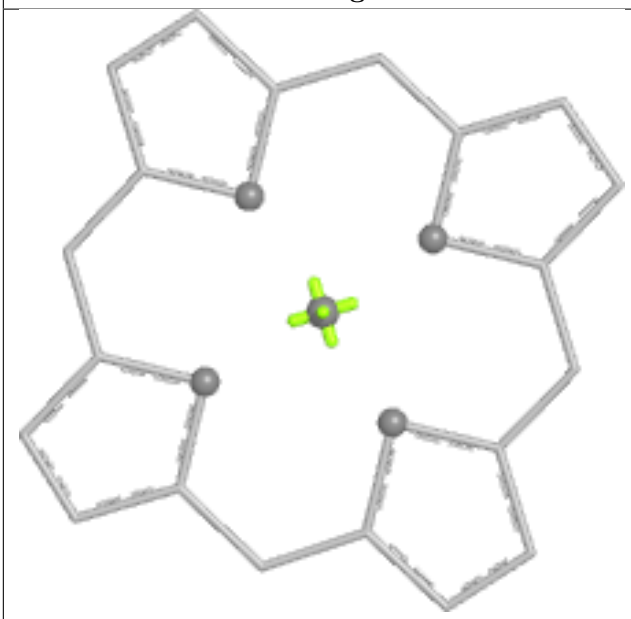
Ligand CLA 1 215



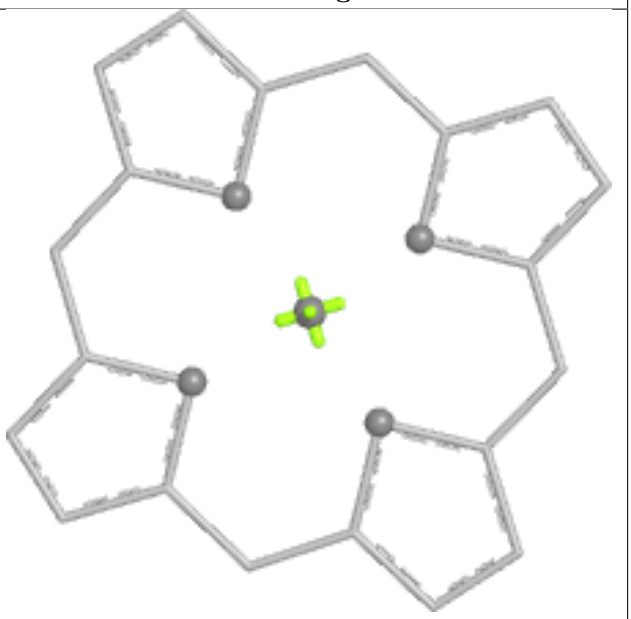
Bond lengths



Bond angles

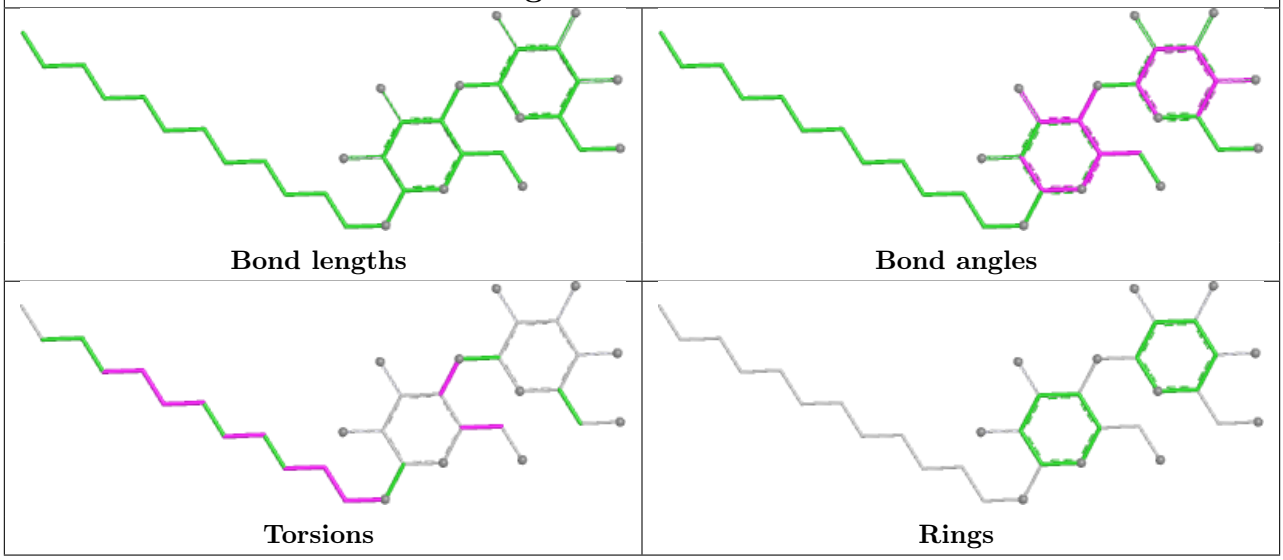


Torsions

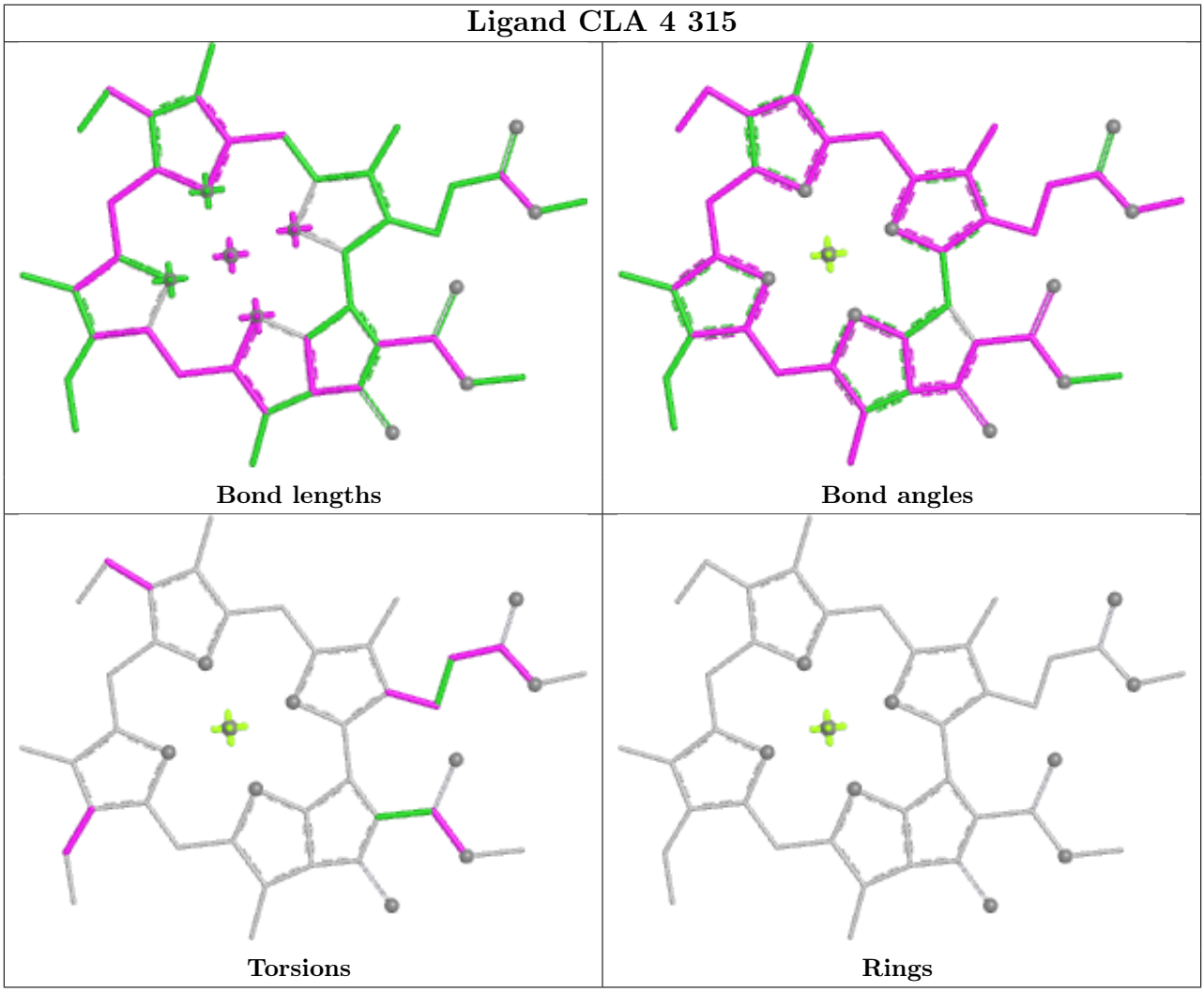


Rings

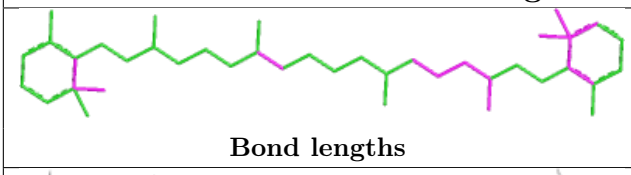
Ligand LMU 1 217



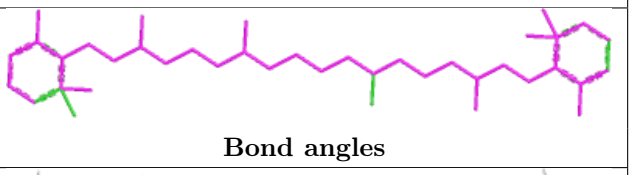
Ligand CLA 4 315



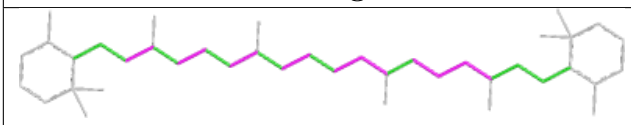
Ligand BCR F 203



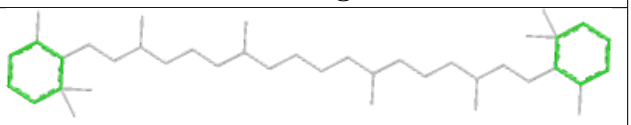
Bond lengths



Bond angles

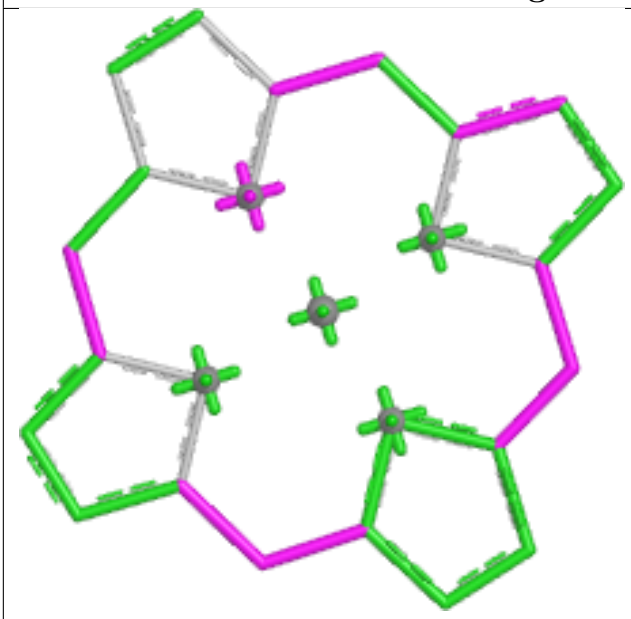


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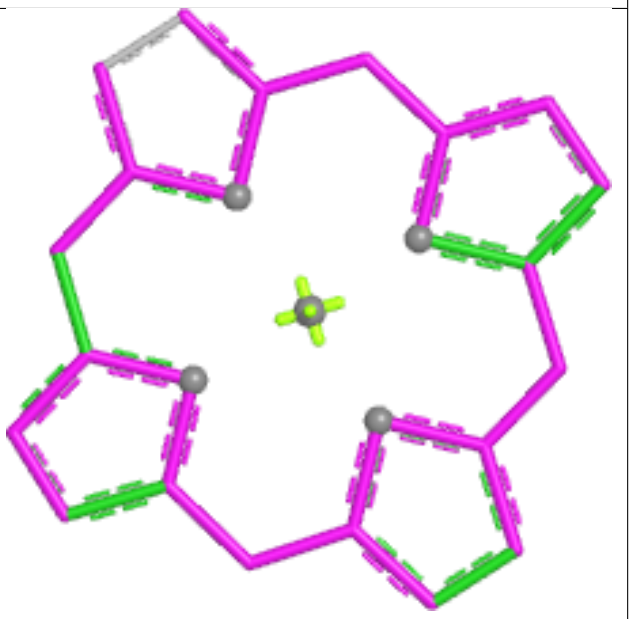


Rings

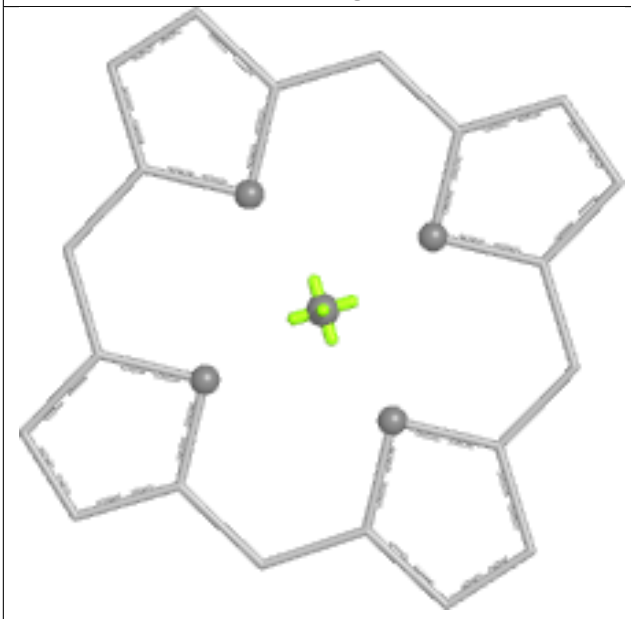
Ligand CLA 4 317



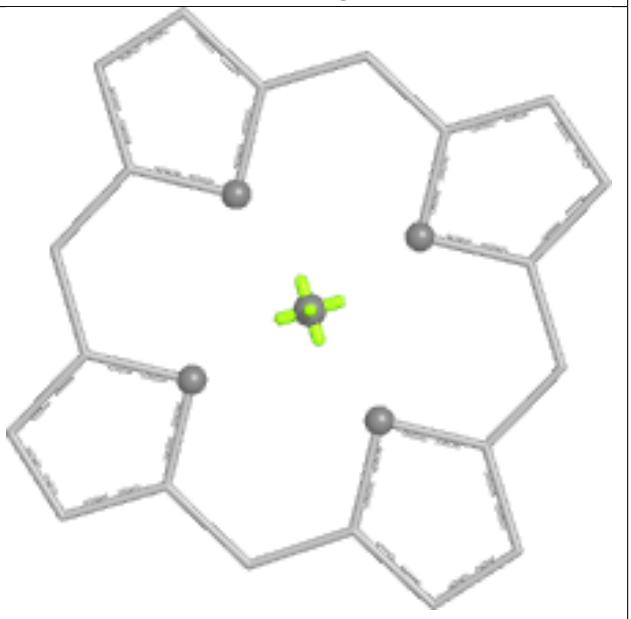
Bond lengths



Bond angles

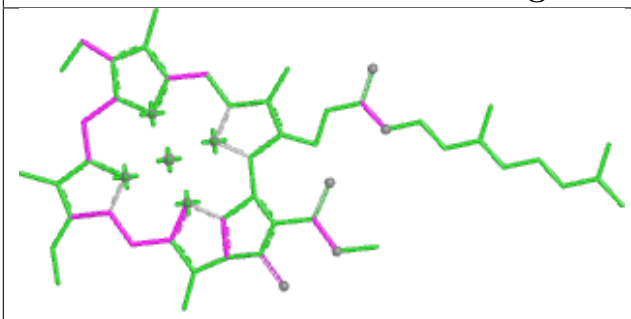


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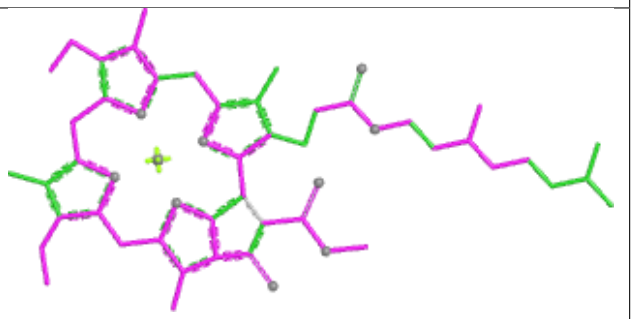


Rings

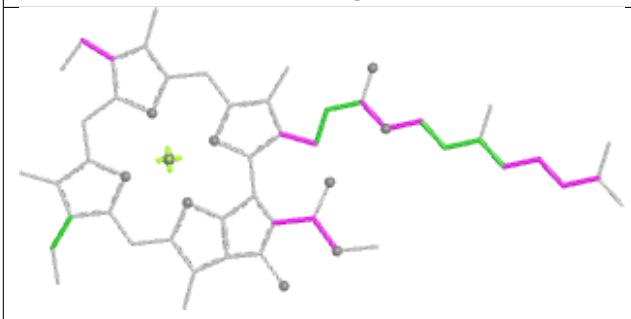
Ligand CLA 4 310



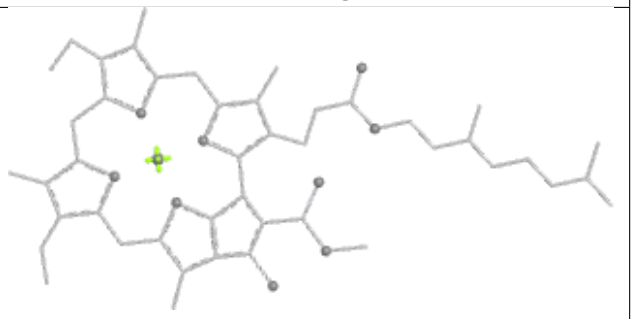
Bond lengths



Bond angles

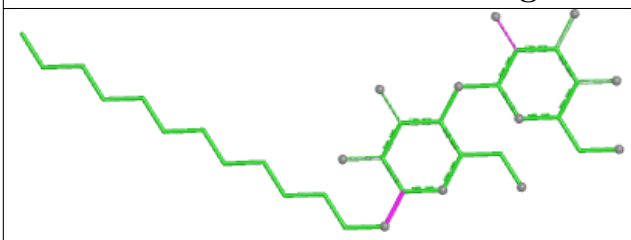


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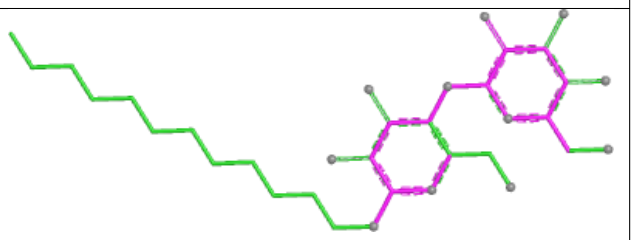


Rings

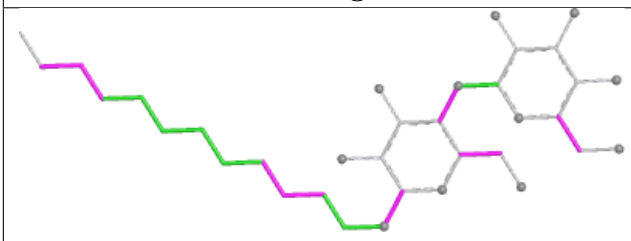
Ligand LMU R 109



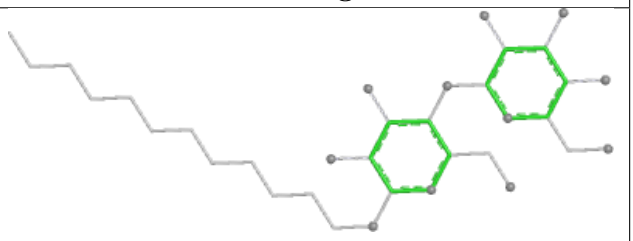
Bond lengths



Bond angles

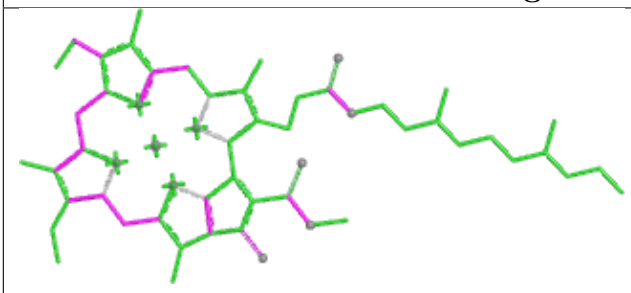


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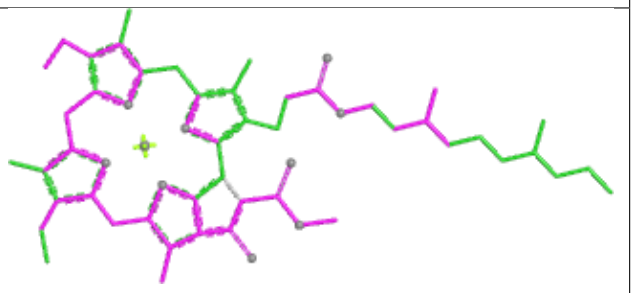


Rings

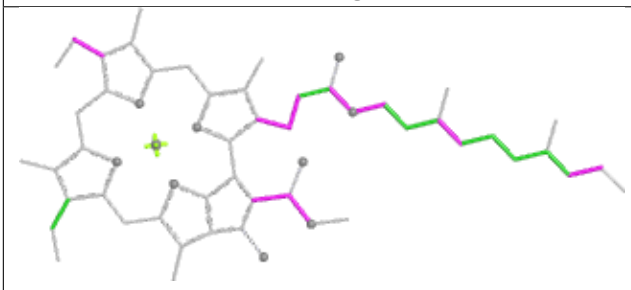
Ligand CLA R 106



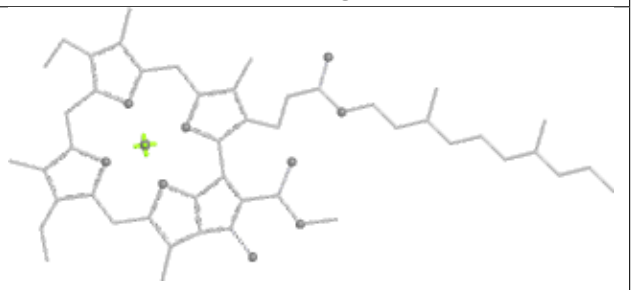
Bond lengths



Bond angles

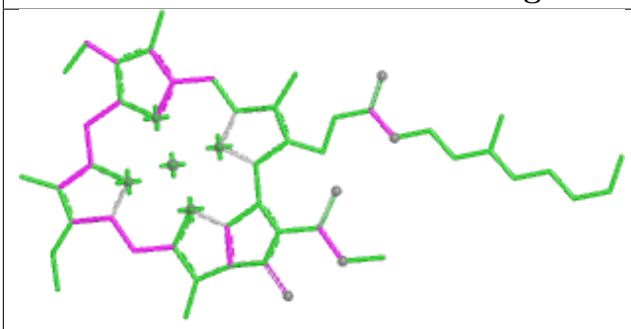


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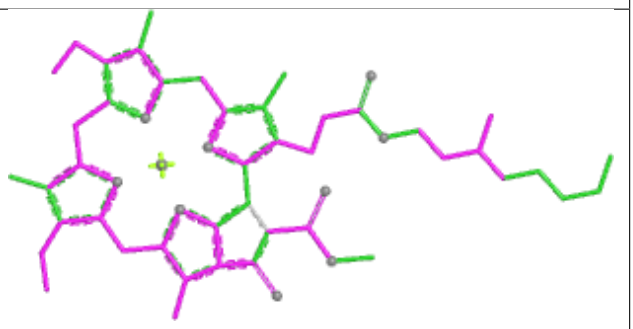


Rings

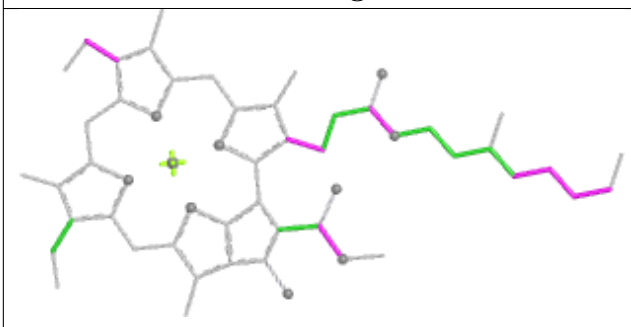
Ligand CLA A 811



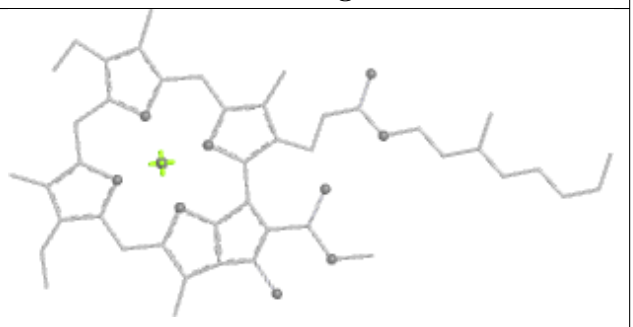
Bond lengths



Bond angles

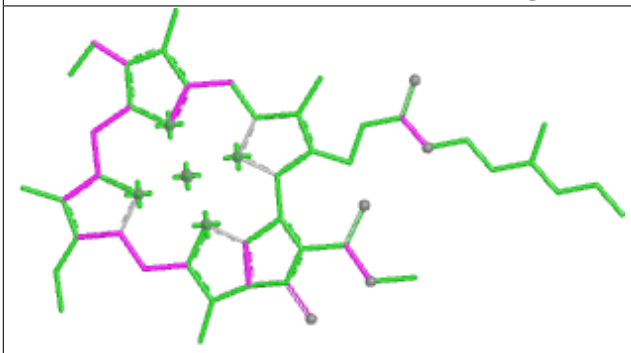


Torsions

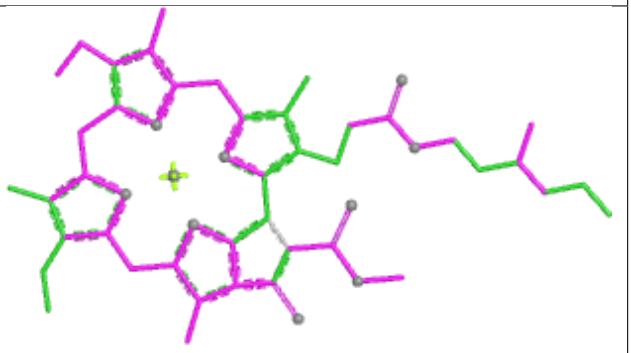


Rings

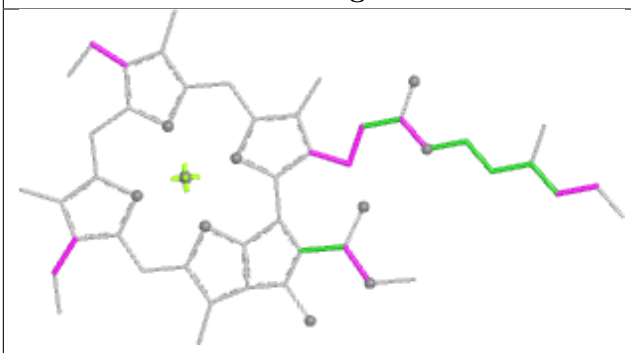
Ligand CLA A 815



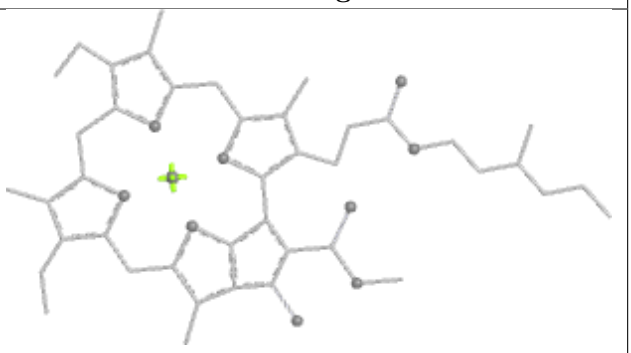
Bond lengths



Bond angles

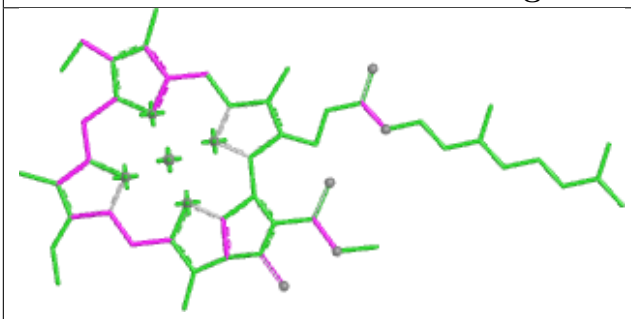


Torsions

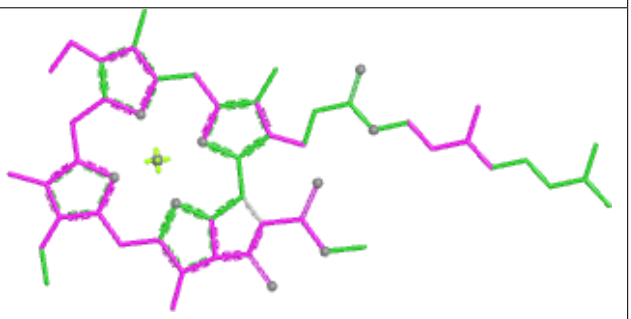


Rings

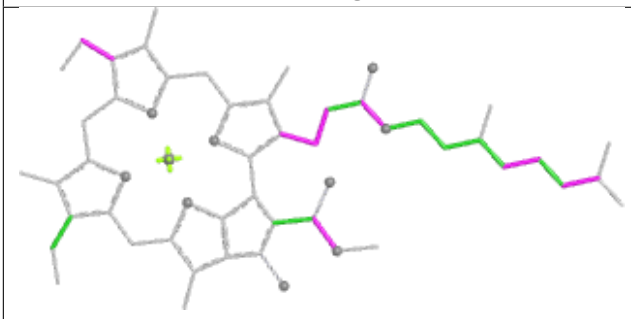
Ligand CLA A 820



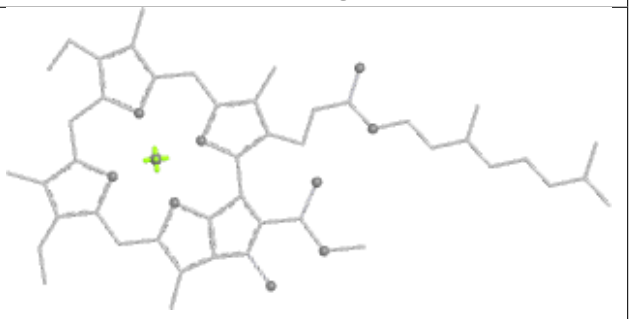
Bond lengths



Bond angles

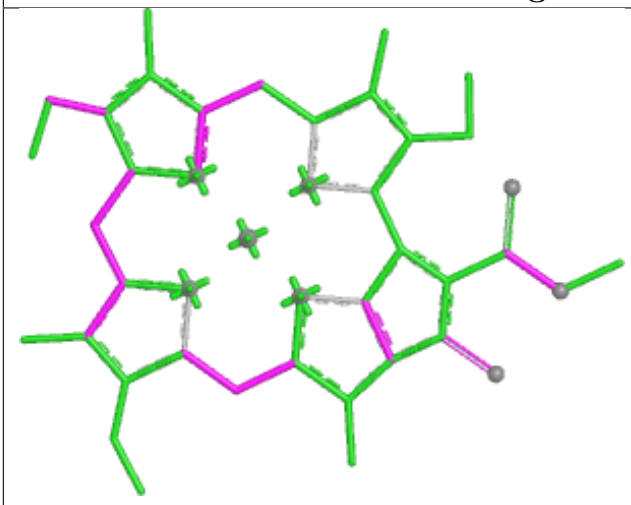


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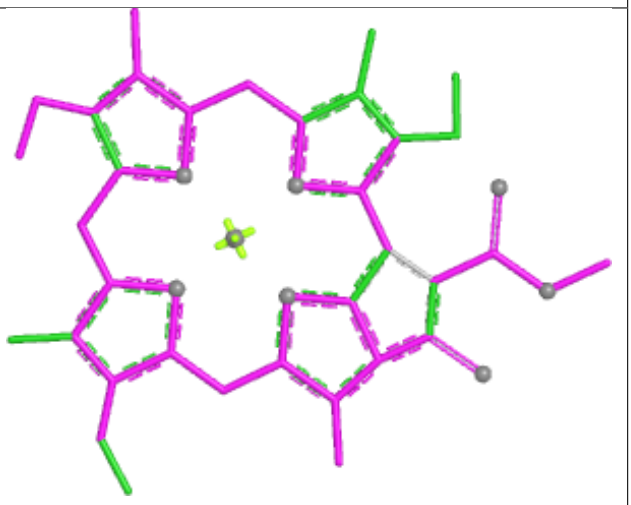


Rings

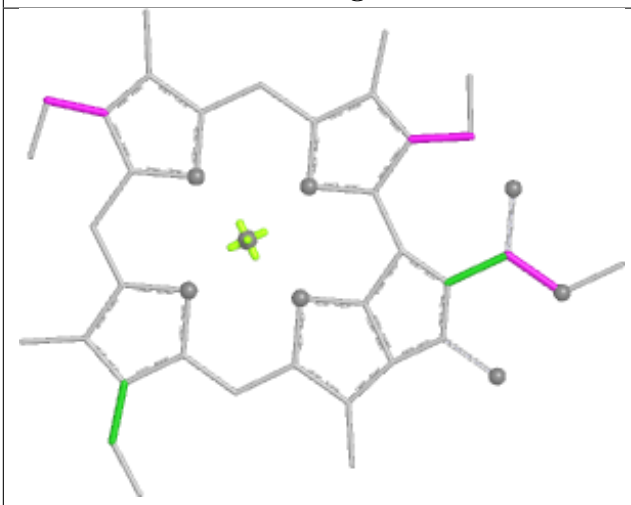
Ligand CLA 3 314



Bond lengths



Bond angles

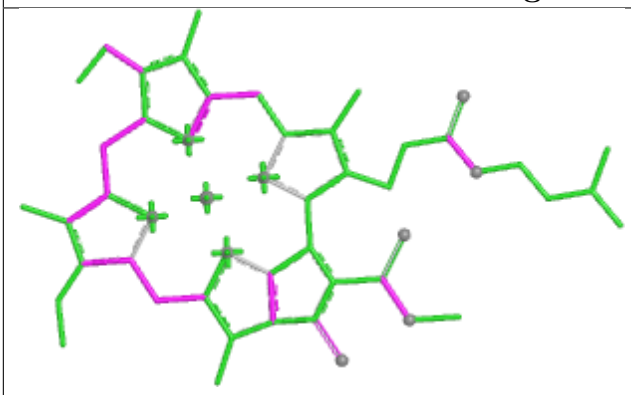


Torsions

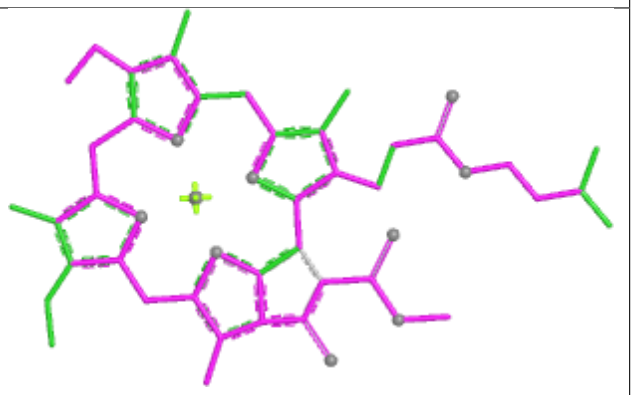


Rings

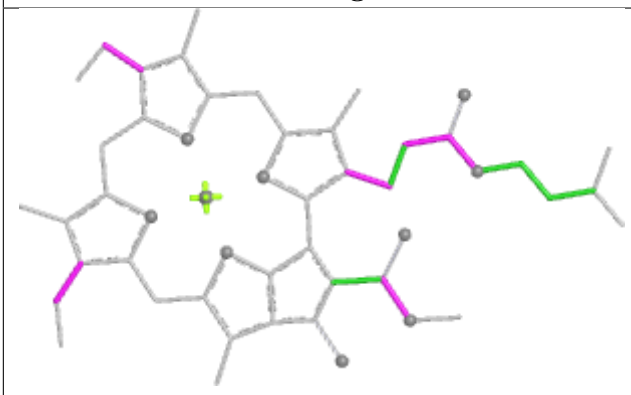
Ligand CLA A 813



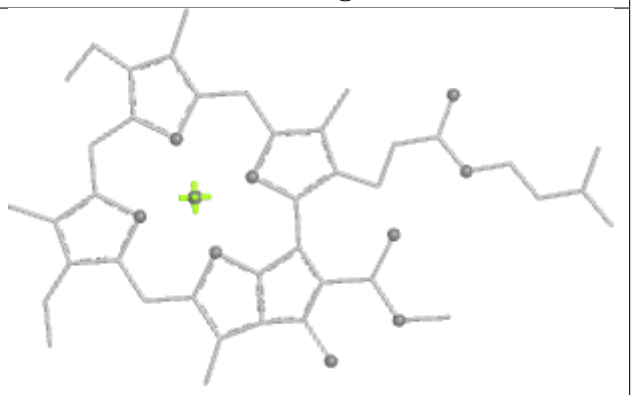
Bond lengths



Bond angles

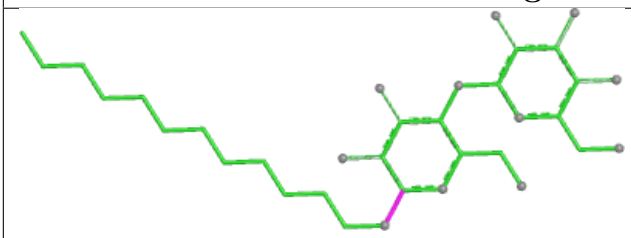


Torsions

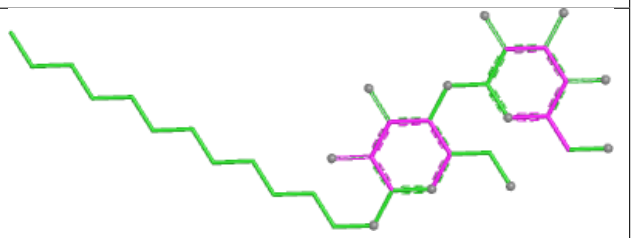


Rings

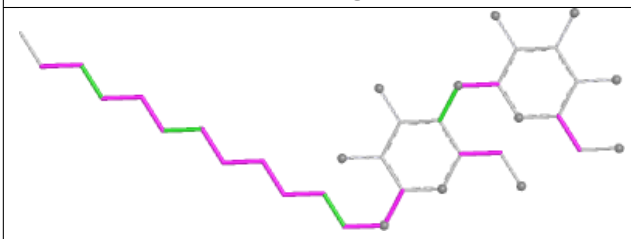
Ligand LMU 4 321



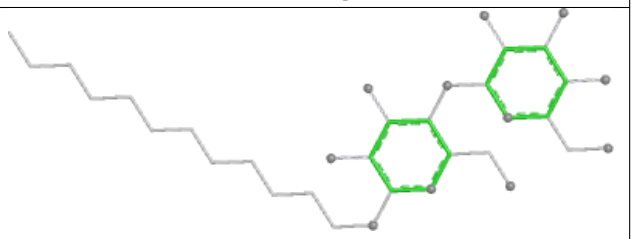
Bond lengths



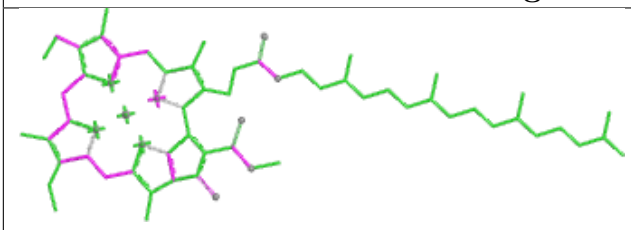
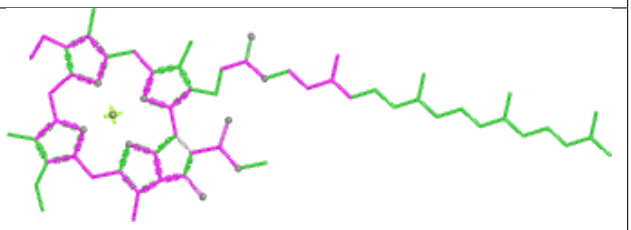
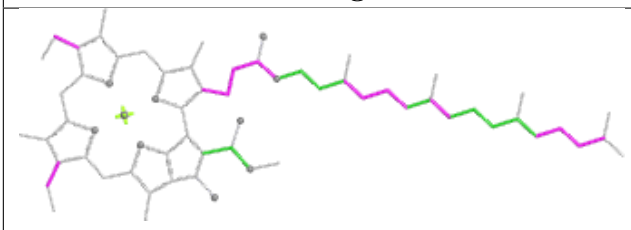
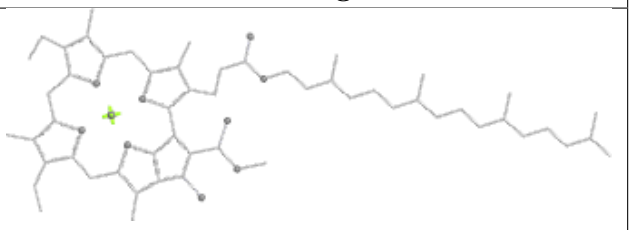
Bond angles

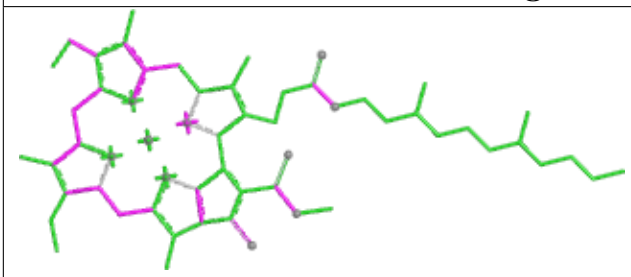
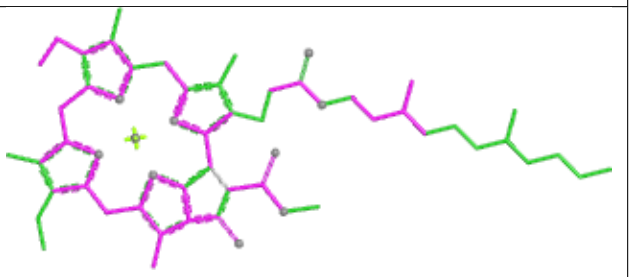
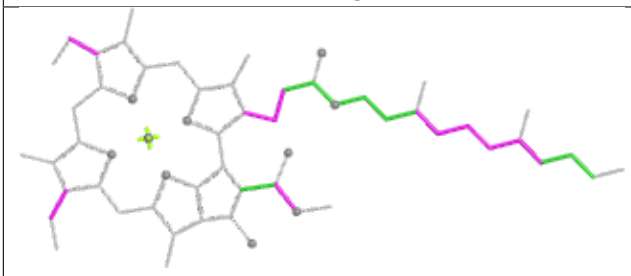
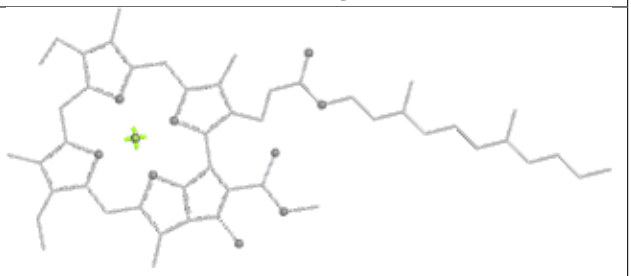


Torsions

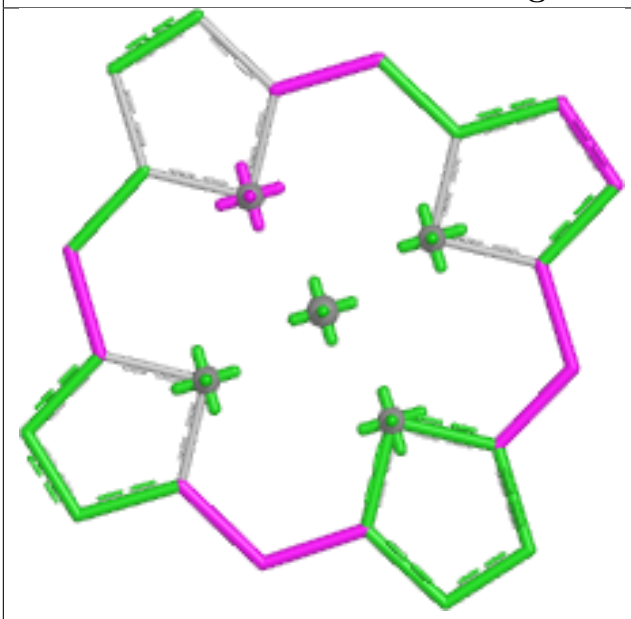


Rings

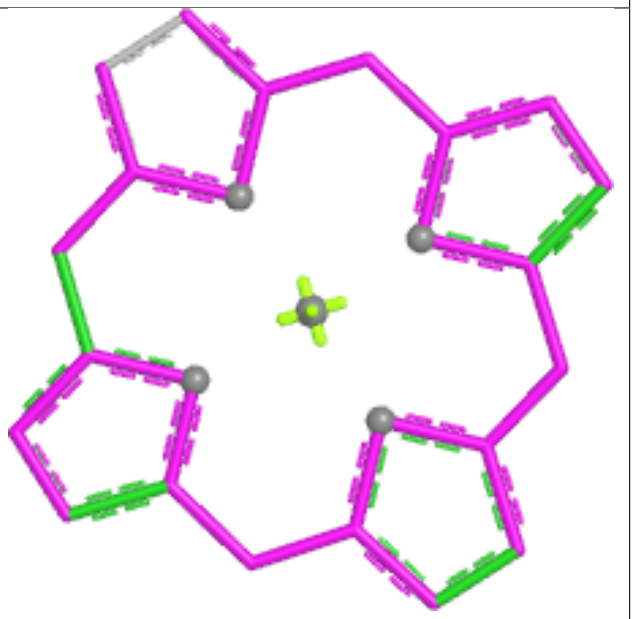
Ligand CLA A 837	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 822	
 Bond lengths	 Bond angles
 Torsions	 Rings

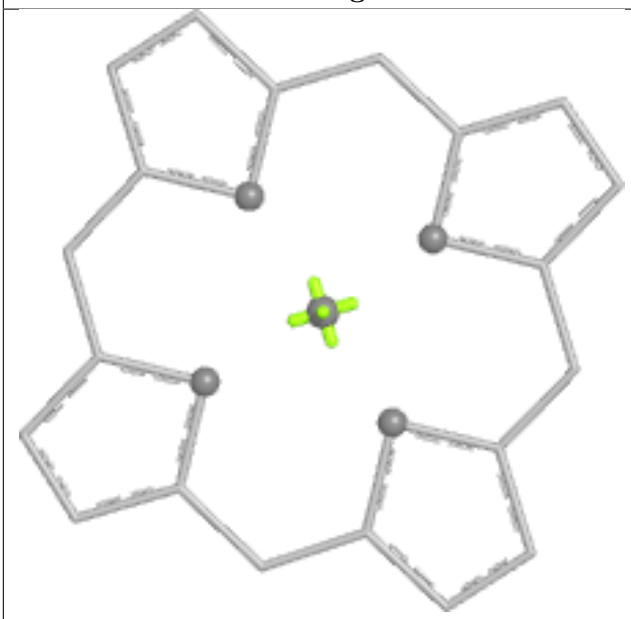
Ligand CLA 1 213



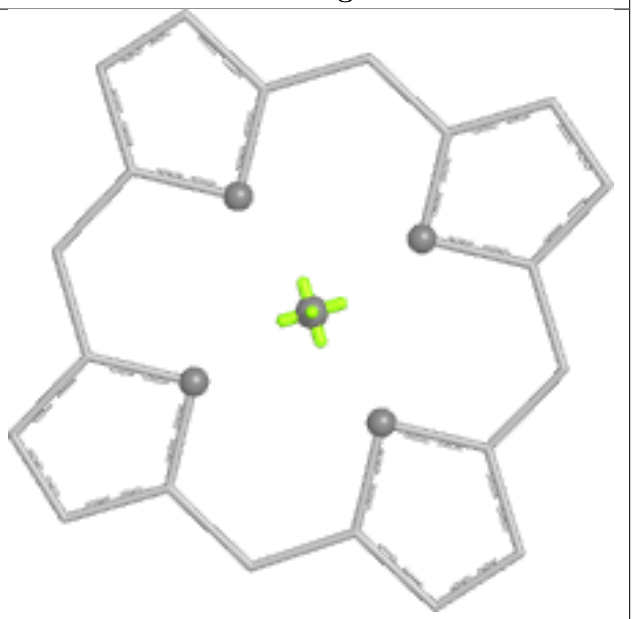
Bond lengths



Bond angles

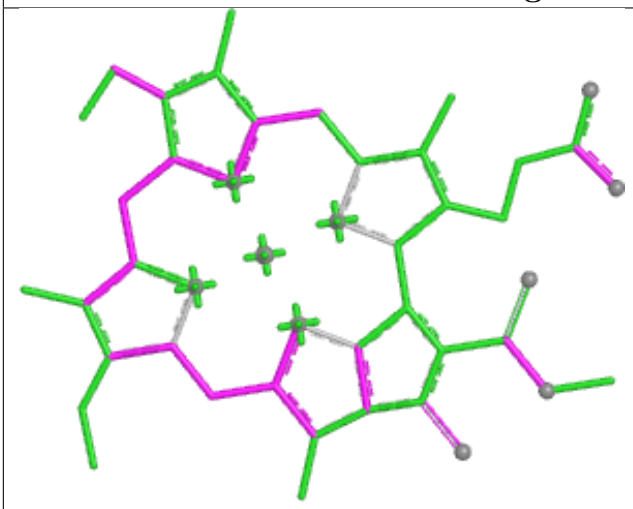


Torsions

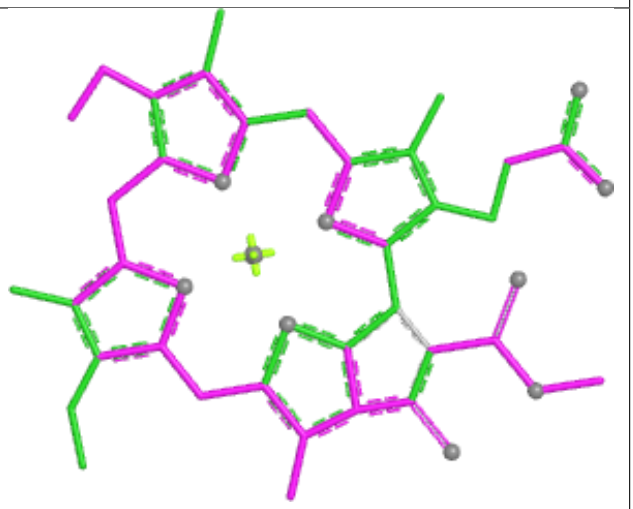


Rings

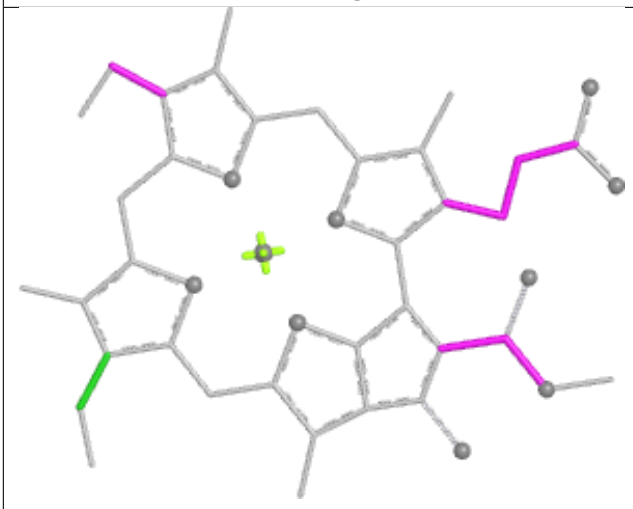
Ligand CLA B 831



Bond lengths



Bond angles

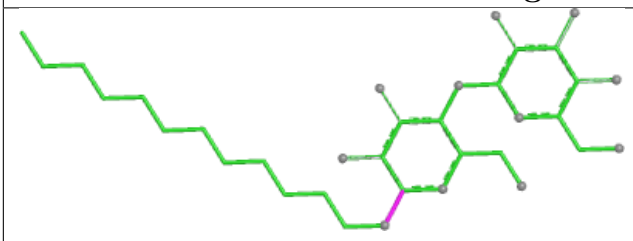


Torsions

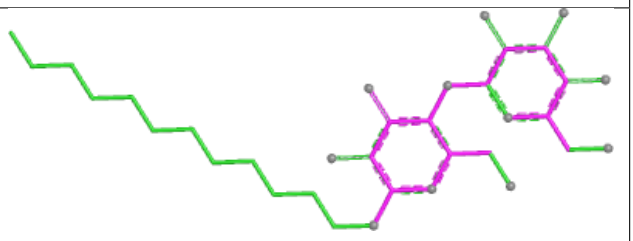


Rings

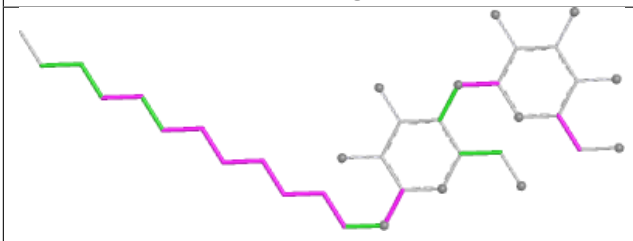
Ligand LMU 2 318



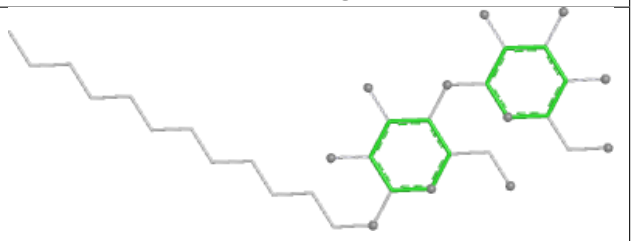
Bond lengths



Bond angles

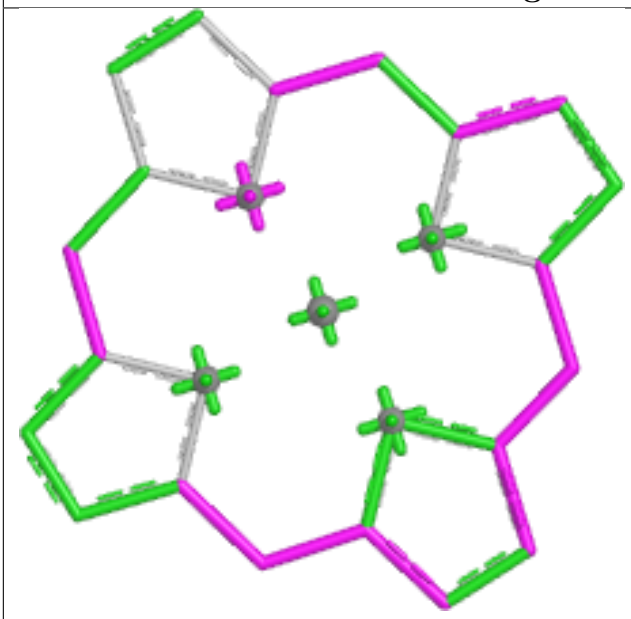


Torsions

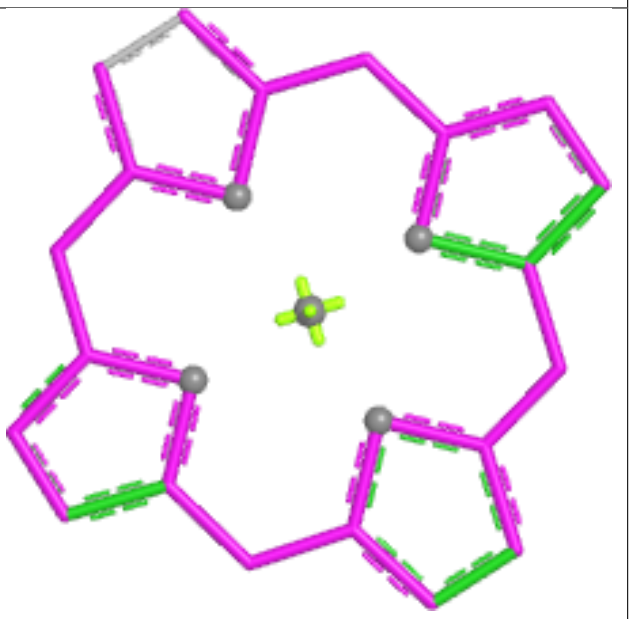


Rings

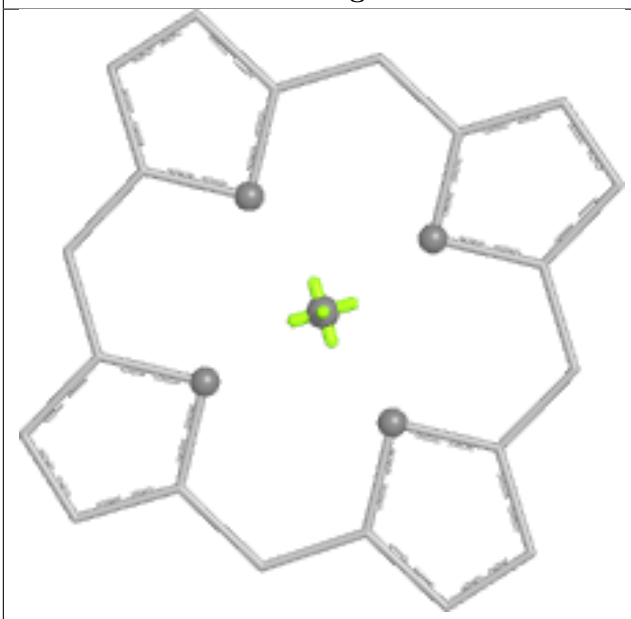
Ligand CLA A 857



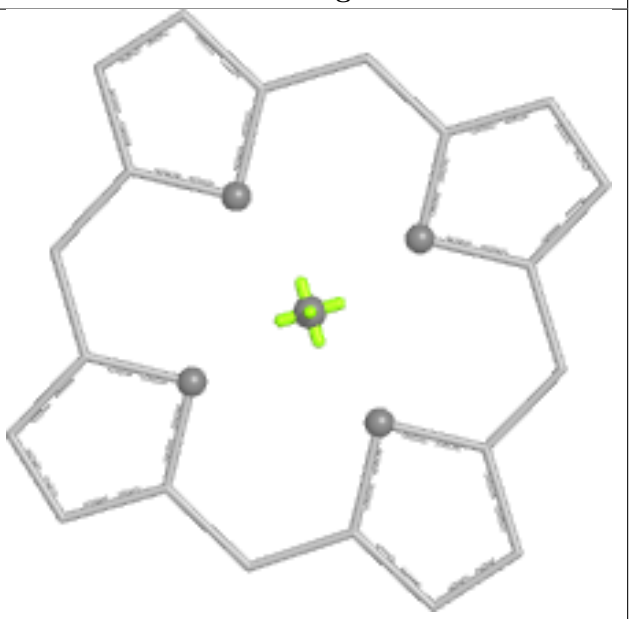
Bond lengths



Bond angles

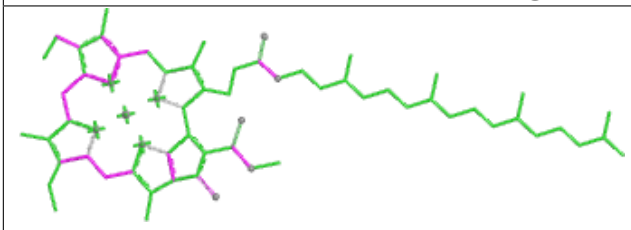


Torsions

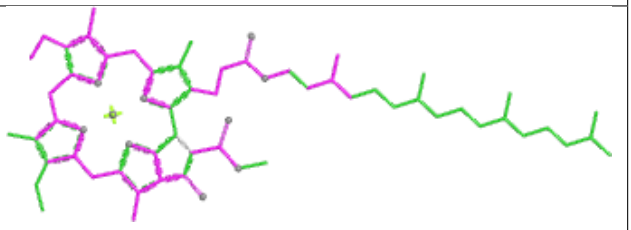


Rings

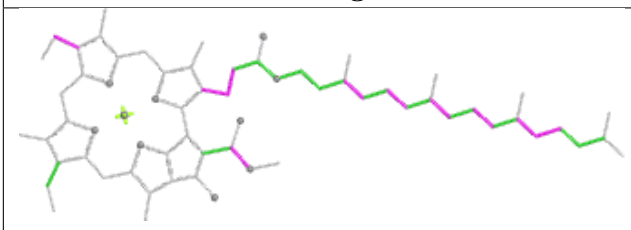
Ligand CLA L 201



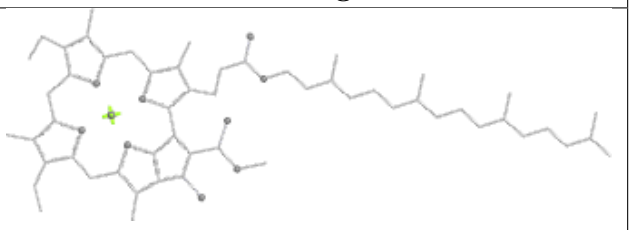
Bond lengths



Bond angles



Torsions

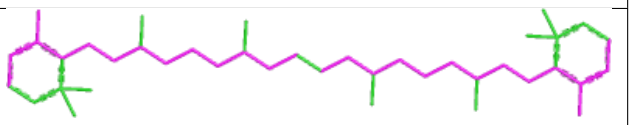


Rings

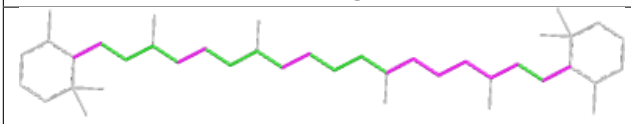
Ligand BCR B 843



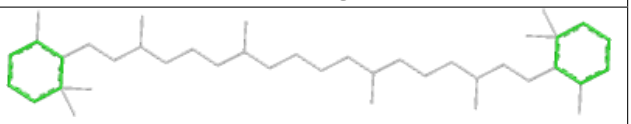
Bond lengths



Bond angles

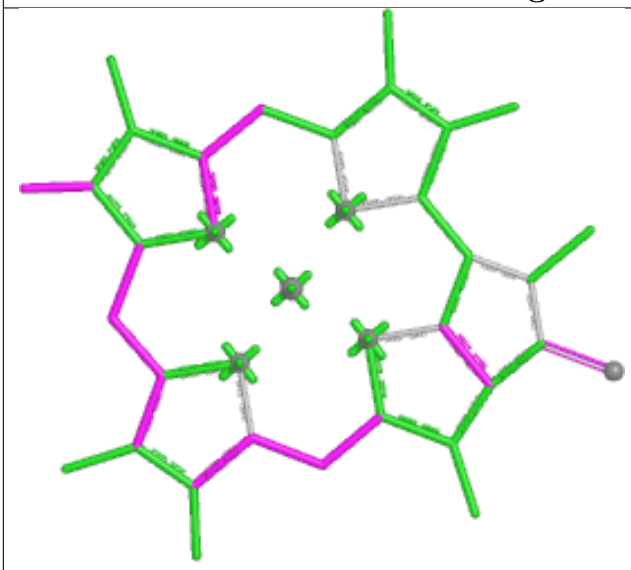


Torsions

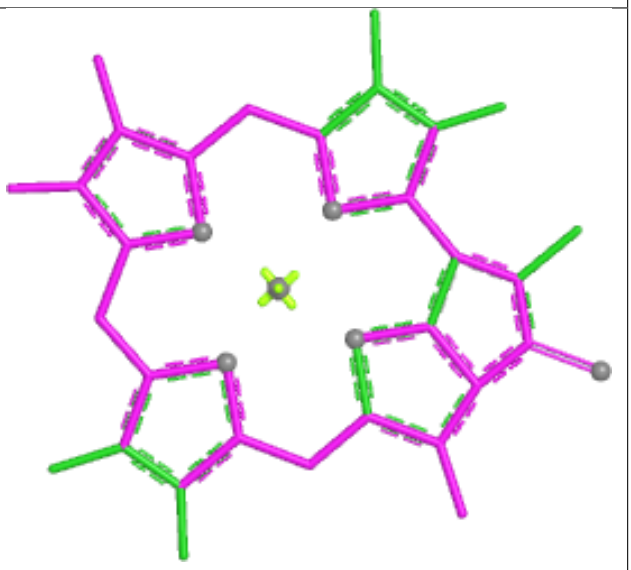


Rings

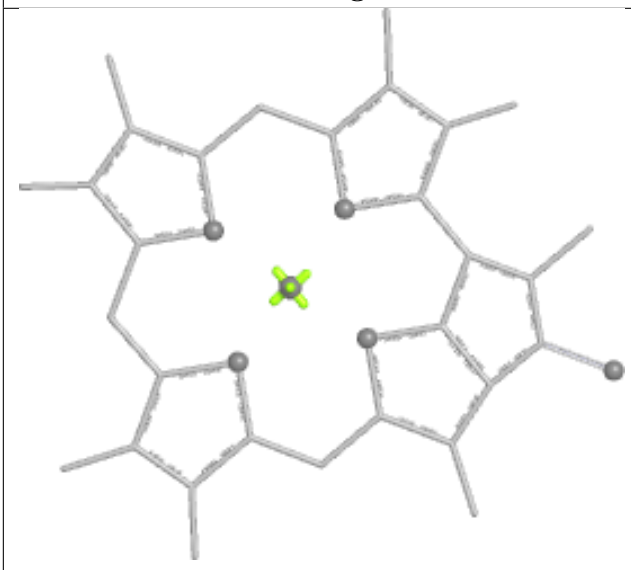
Ligand CLA 3 319



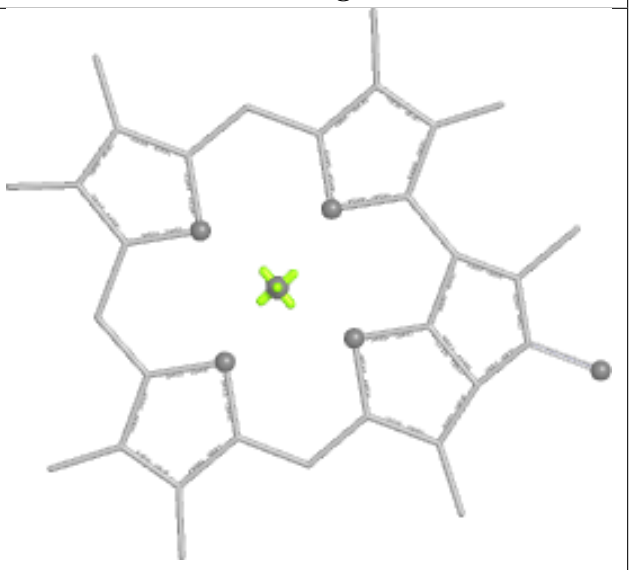
Bond lengths



Bond angles

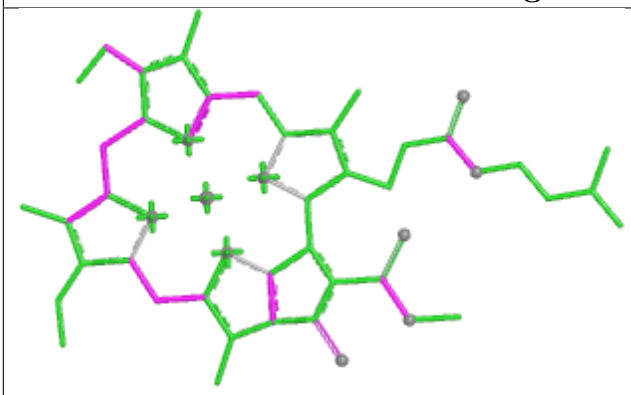


Torsions

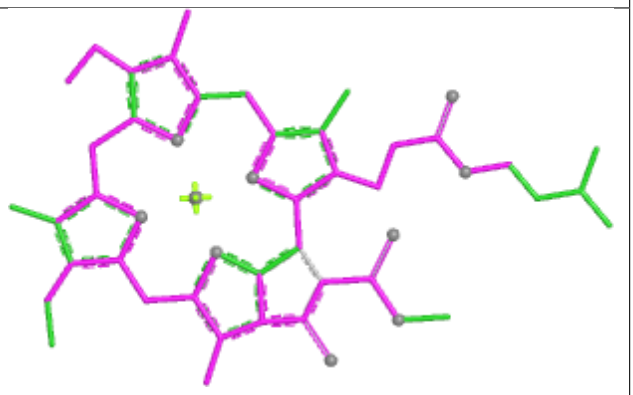


Rings

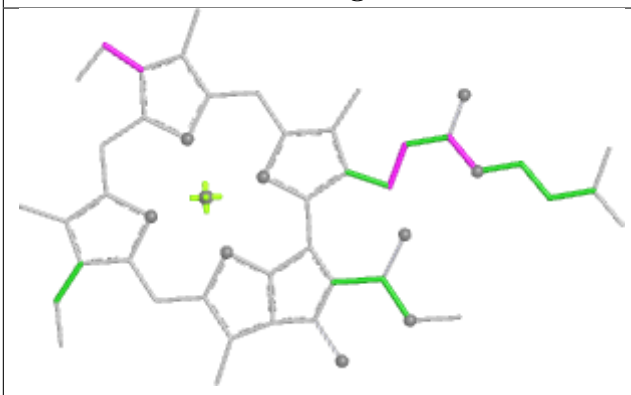
Ligand CLA A 827



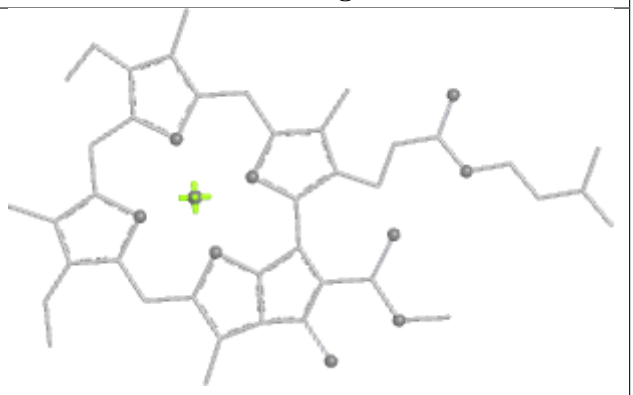
Bond lengths



Bond angles



Torsions

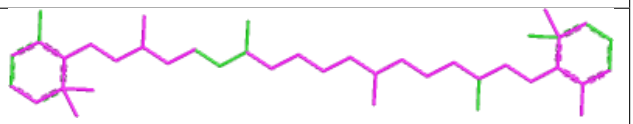


Rings

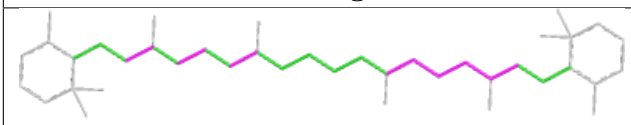
Ligand BCR I 103



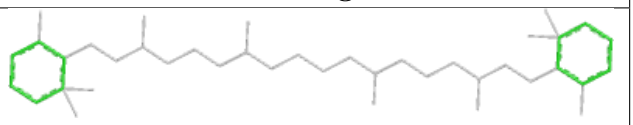
Bond lengths



Bond angles

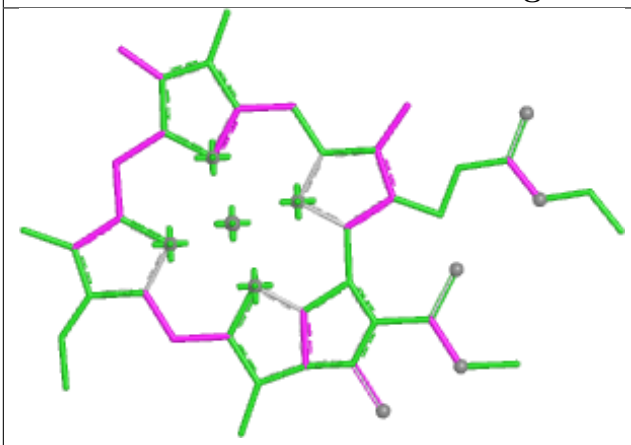


Torsions

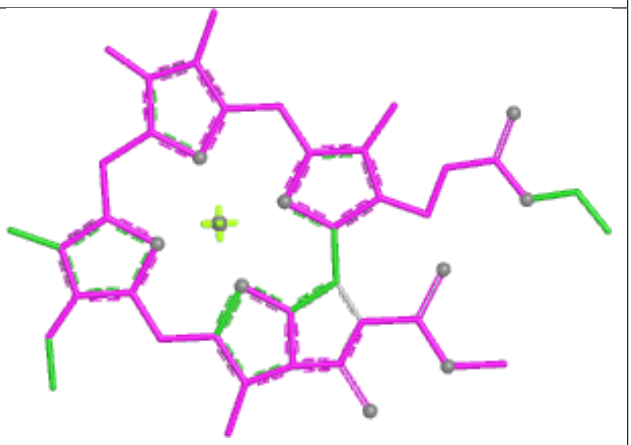


Rings

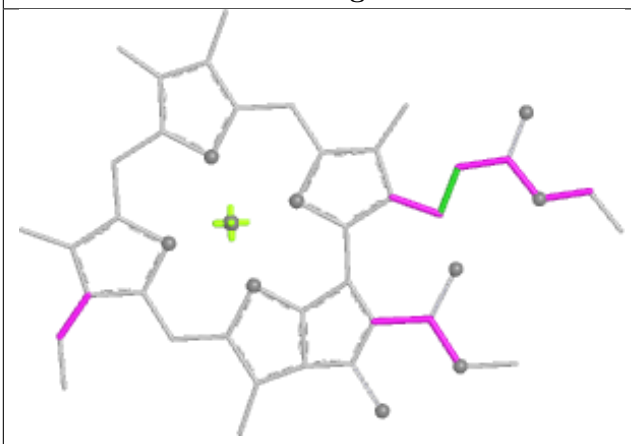
Ligand CLA A 850



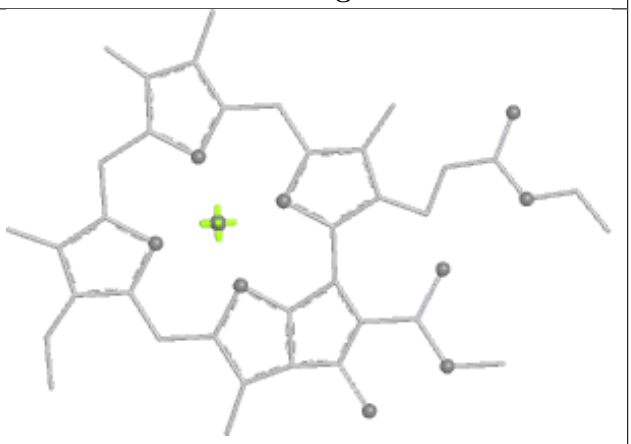
Bond lengths



Bond angles

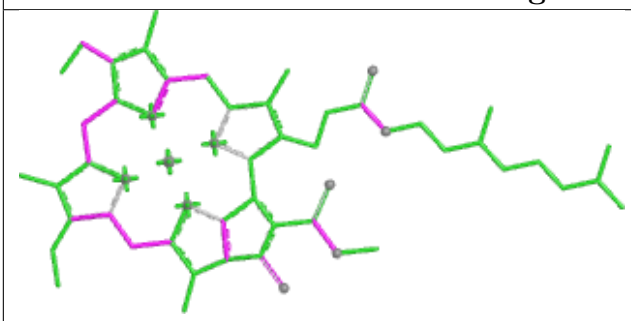


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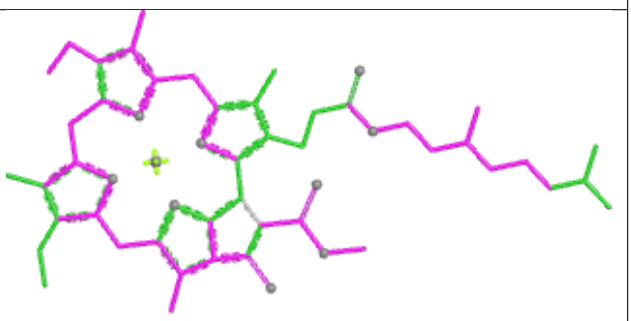


Rings

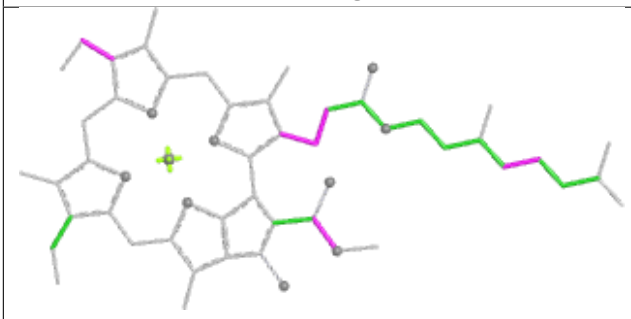
Ligand CLA 3 320



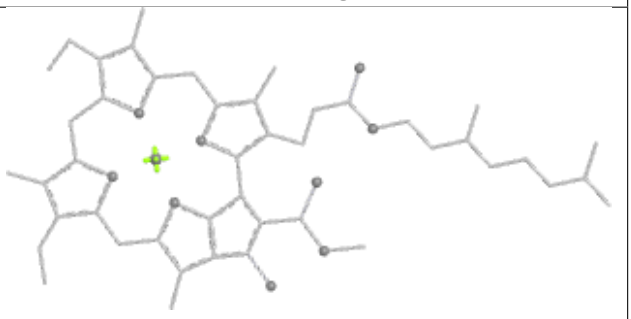
Bond lengths



Bond angles

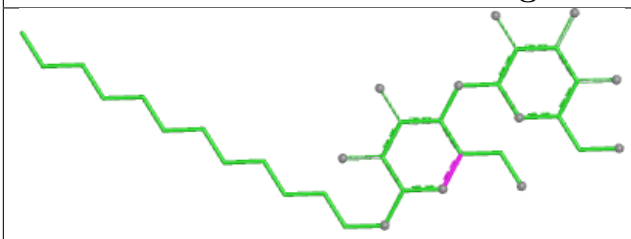


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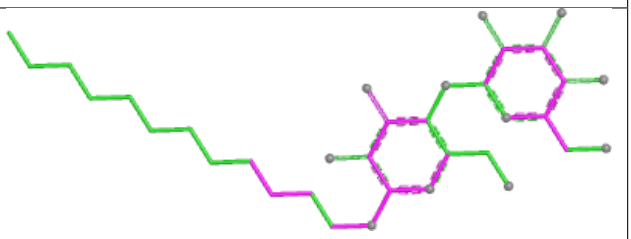


Rings

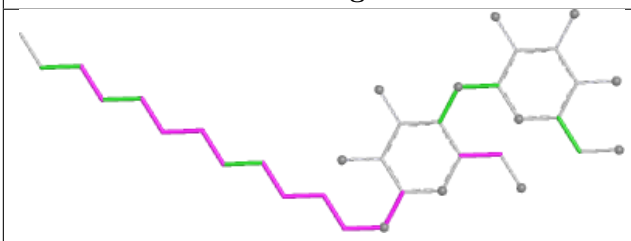
Ligand LMU A 852



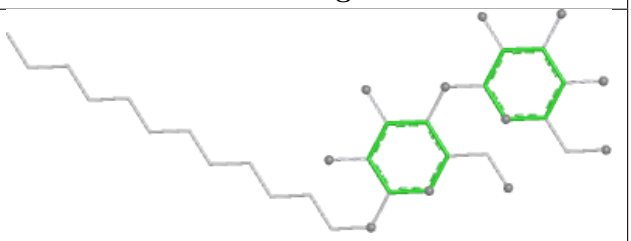
Bond lengths



Bond angles

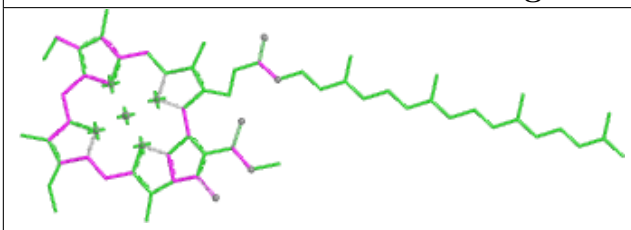


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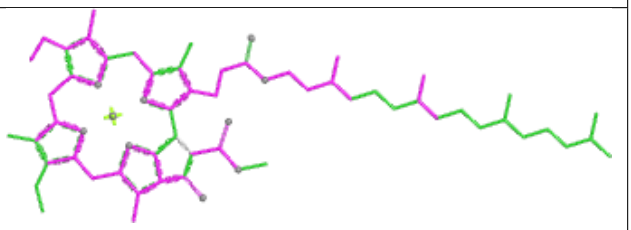


Rings

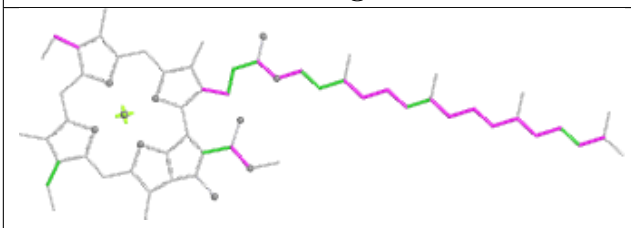
Ligand CLA B 829



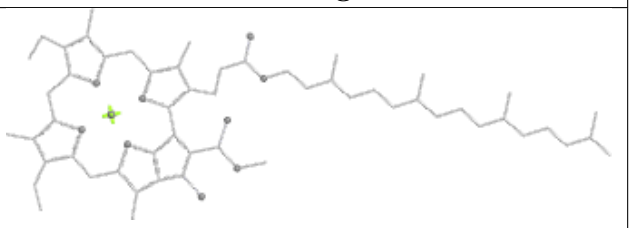
Bond lengths



Bond angles

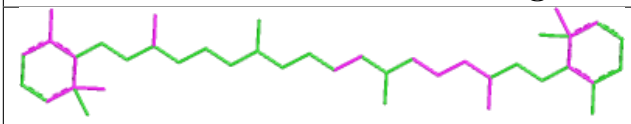


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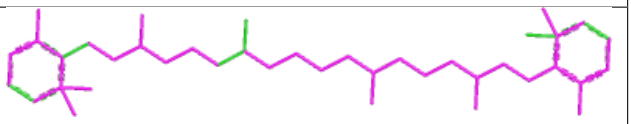


Rings

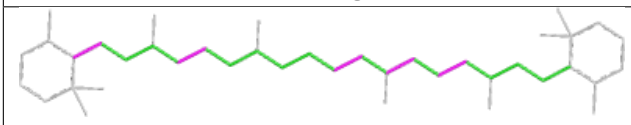
Ligand BCR I 101



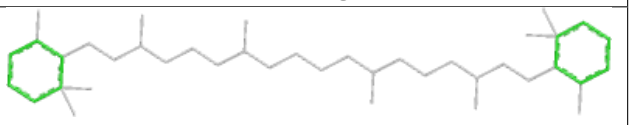
Bond lengths



Bond angles

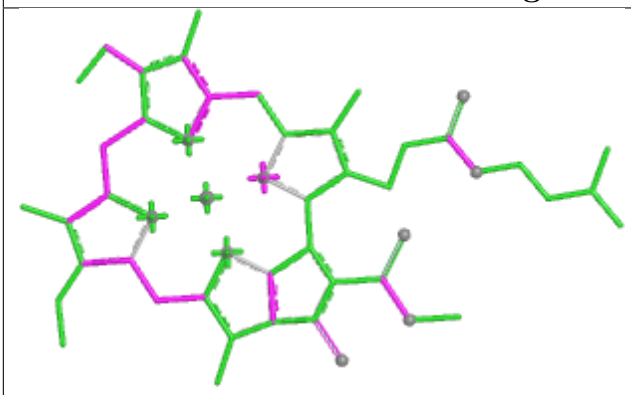


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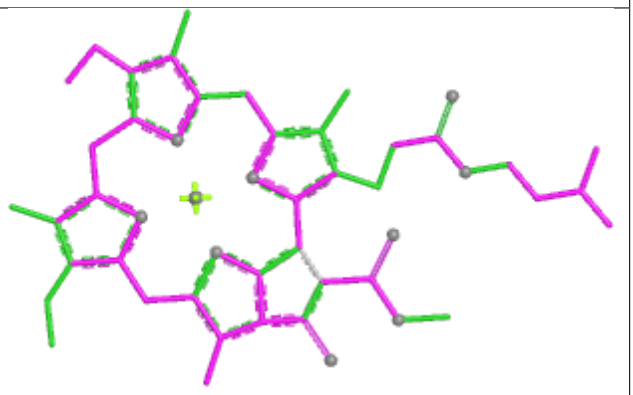


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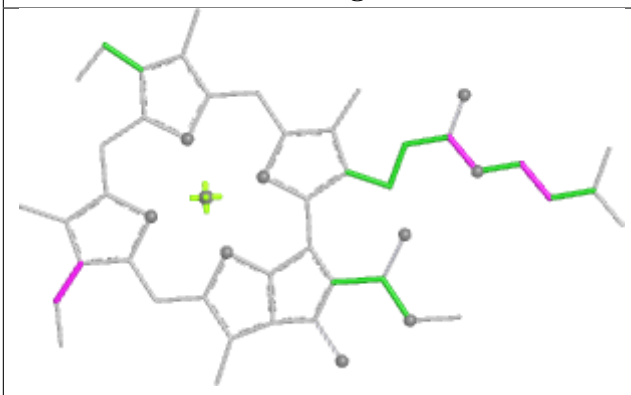
Ligand CLA K 103



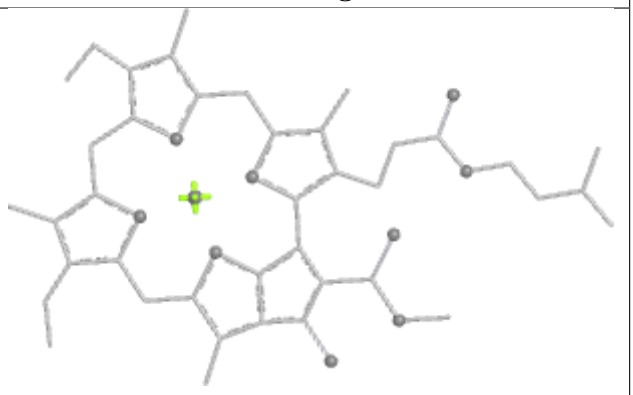
Bond lengths



Bond angles

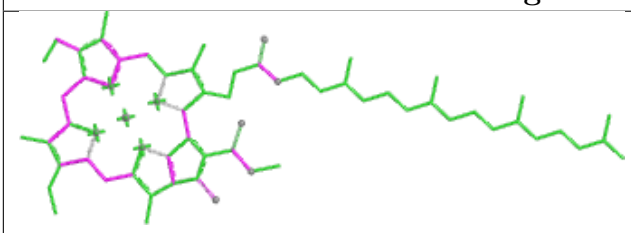


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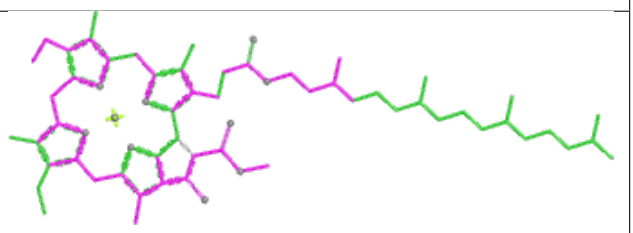


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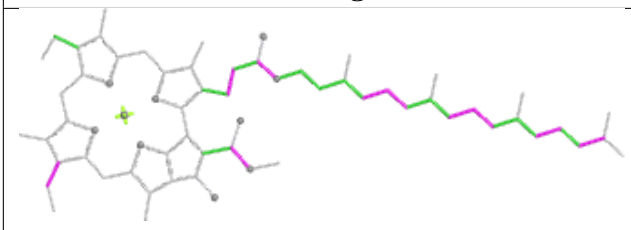
Ligand CLA A 817



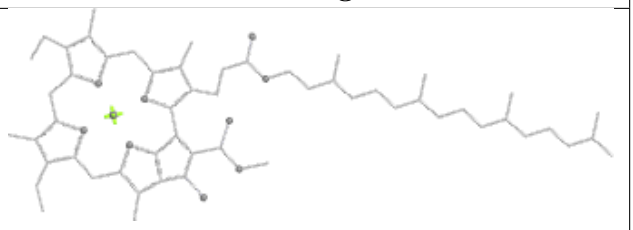
Bond lengths



Bond angles

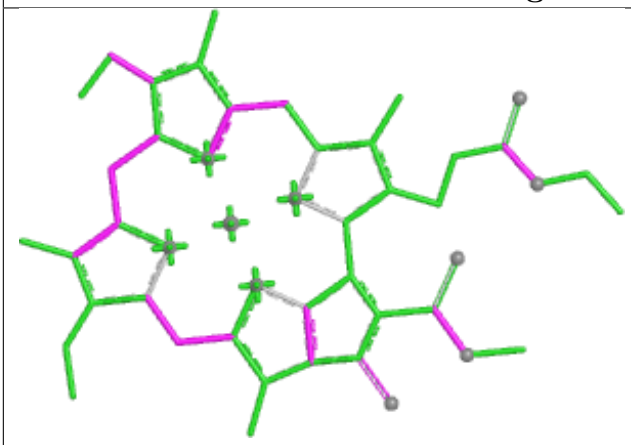


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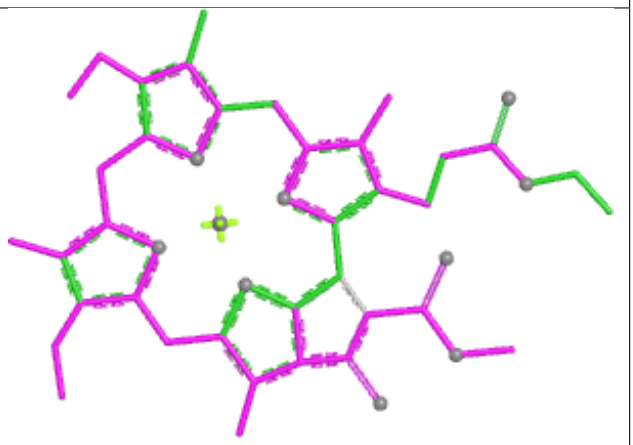


Rings

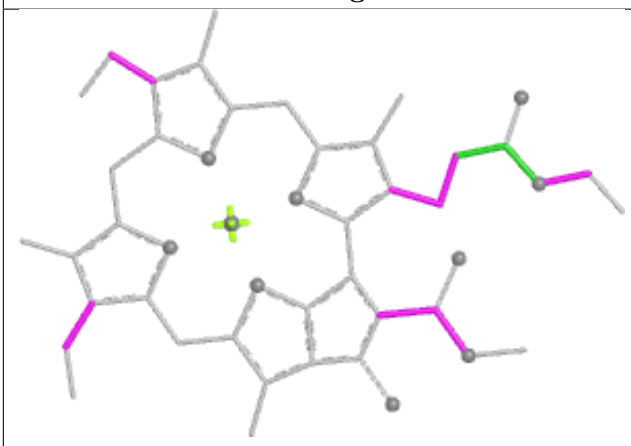
Ligand CLA L 207



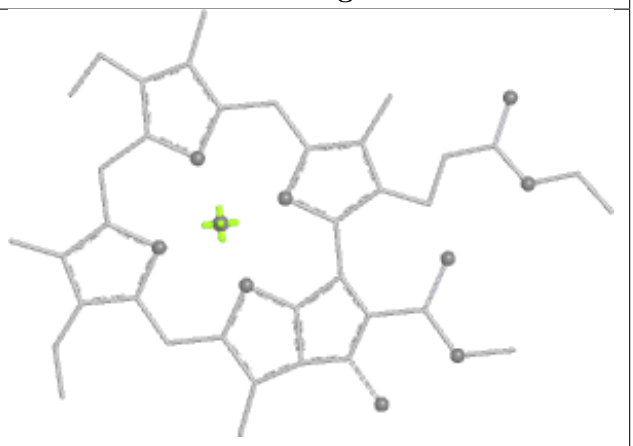
Bond lengths



Bond angles

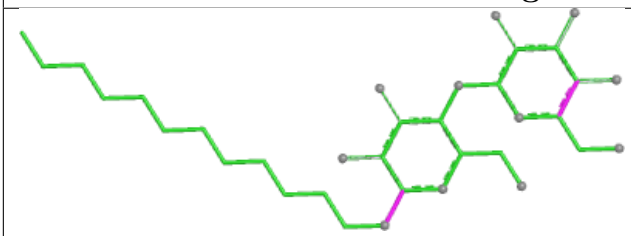


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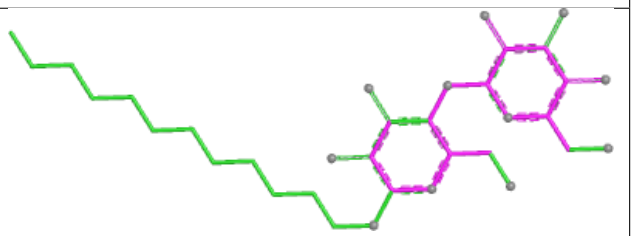


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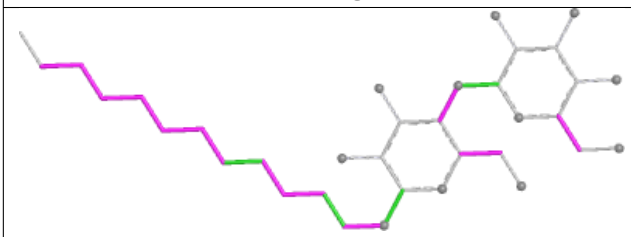
Ligand LMU L 205



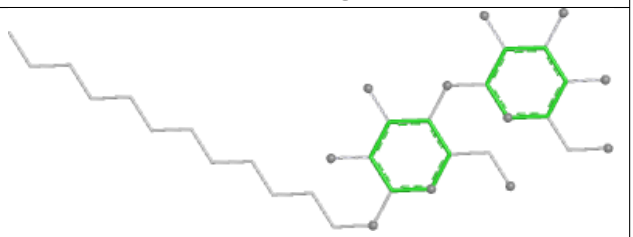
Bond lengths



Bond angles

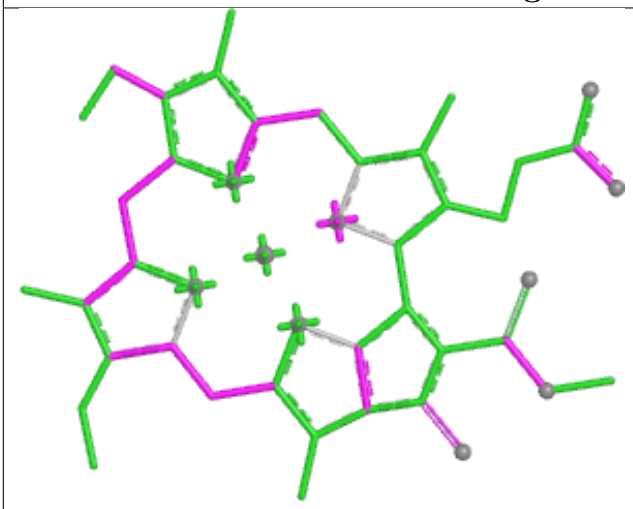


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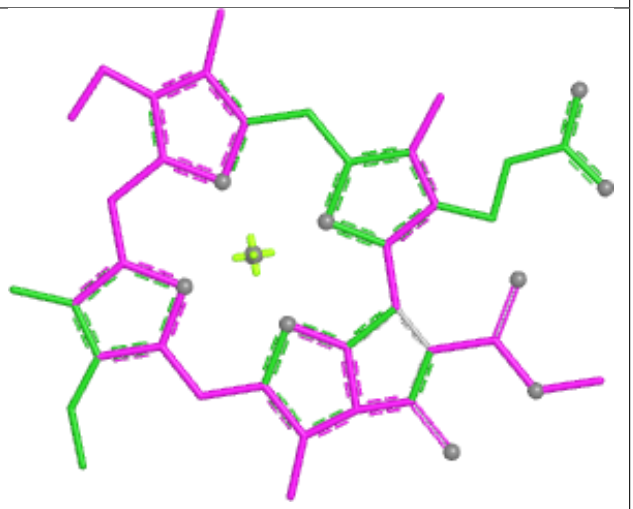


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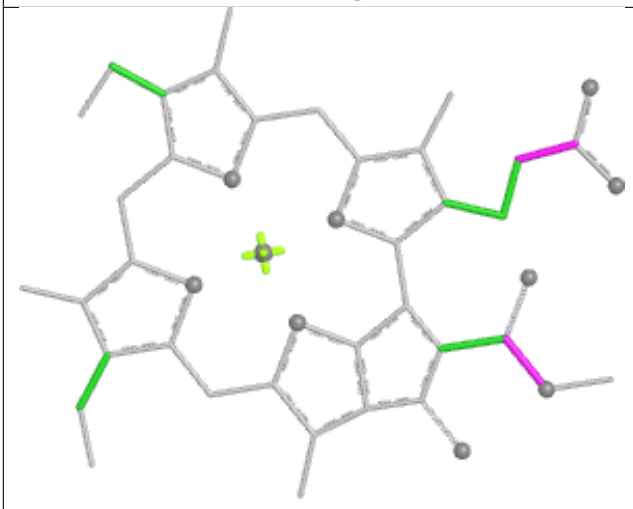
Ligand CLA A 808



Bond lengths



Bond angles

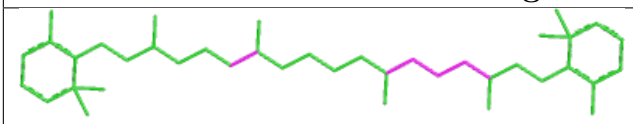


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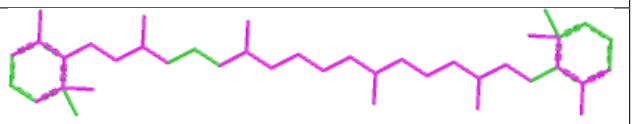


Rings

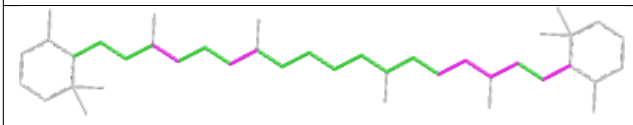
Ligand BCR B 842



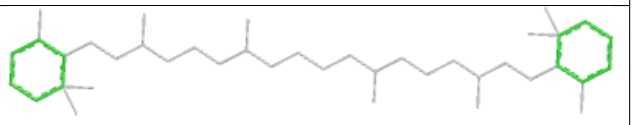
Bond lengths



Bond angles

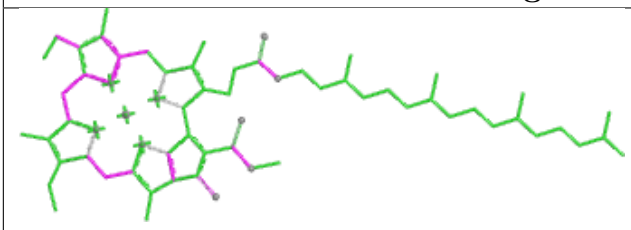


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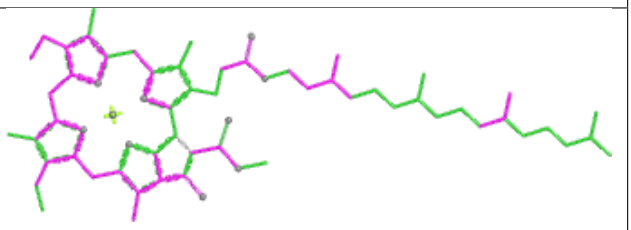


Rings

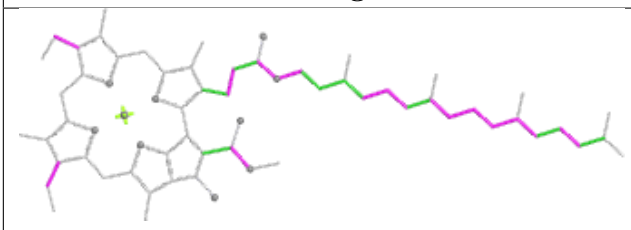
Ligand CLA A 821



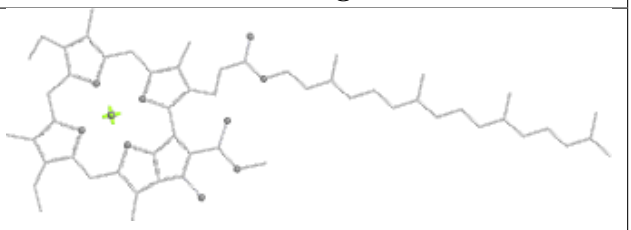
Bond lengths



Bond angles

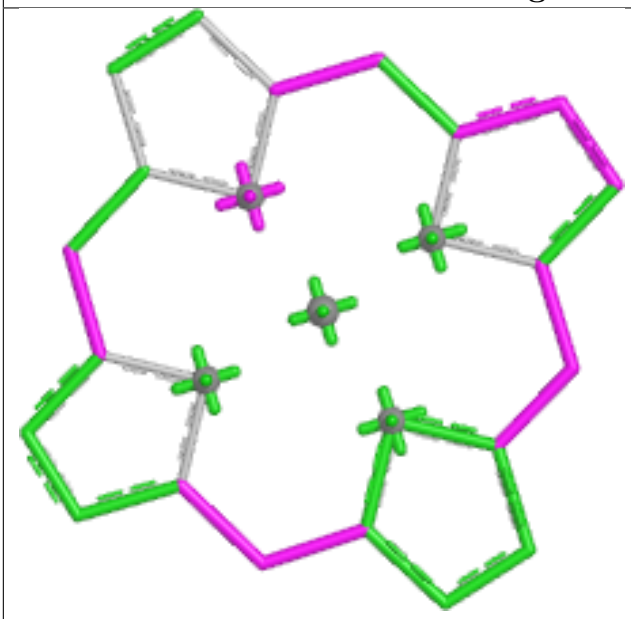


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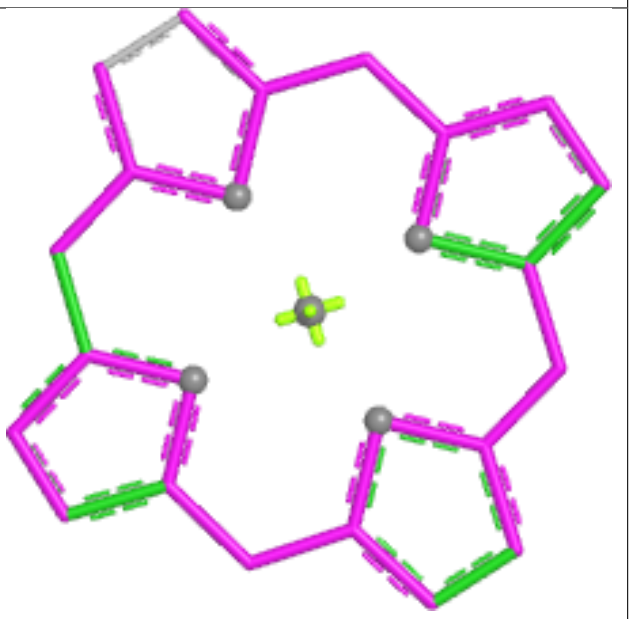


Rings

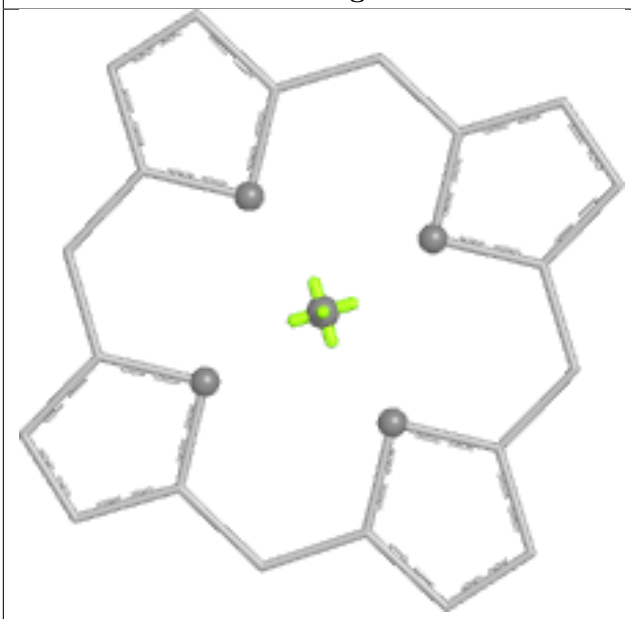
Ligand CLA 3 307



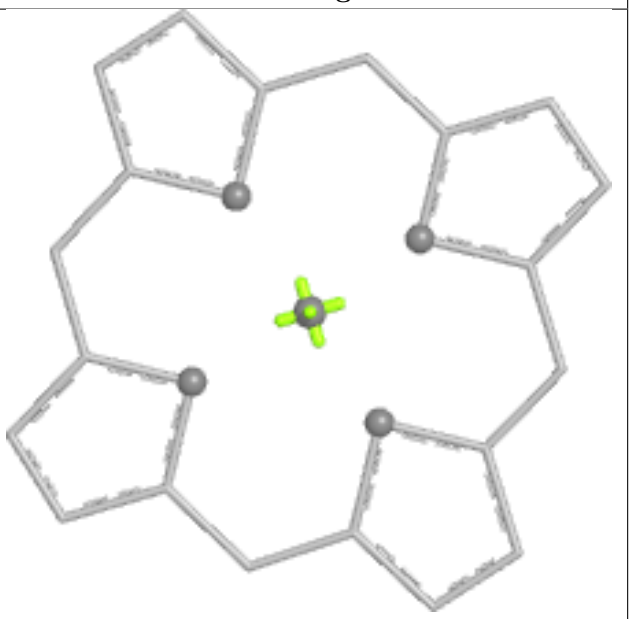
Bond lengths



Bond angles

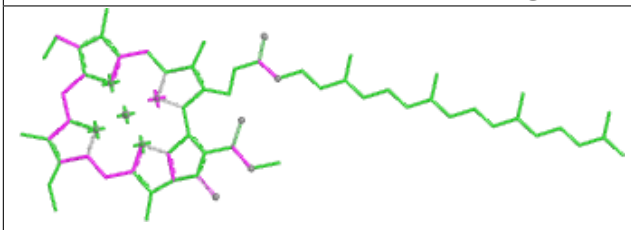


Torsions

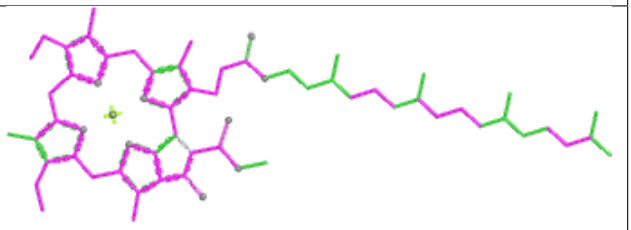


Rings

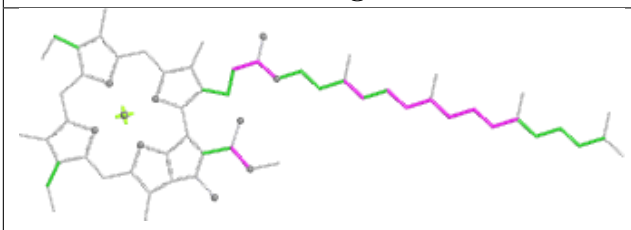
Ligand CLA B 847



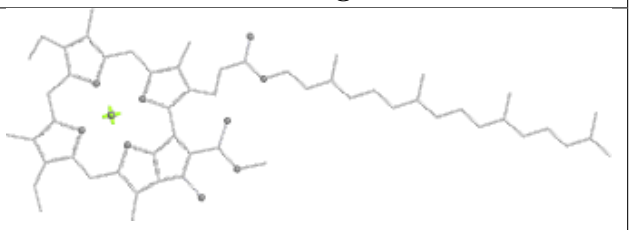
Bond lengths



Bond angles

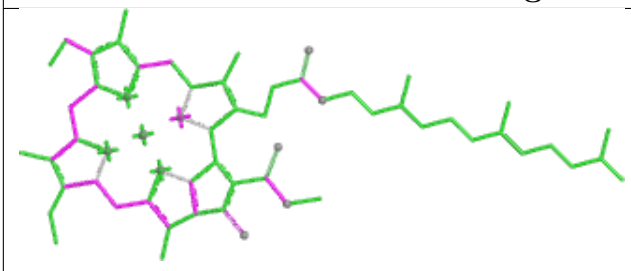


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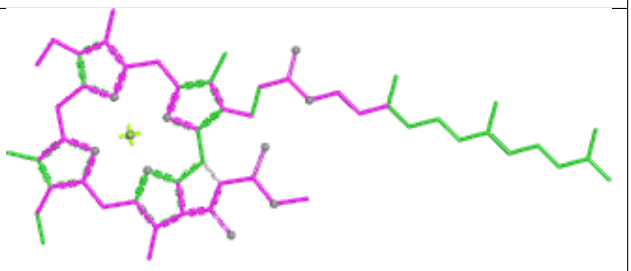


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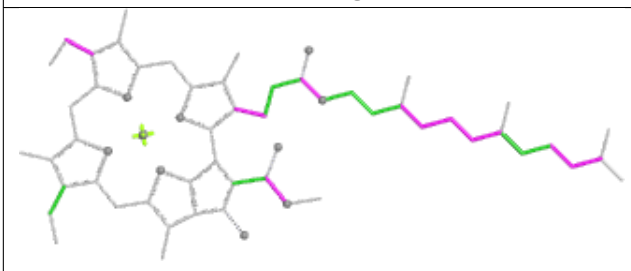
Ligand CLA B 815



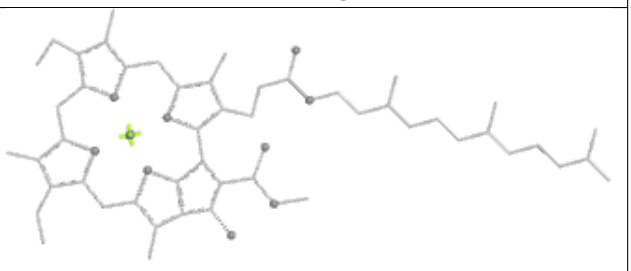
Bond lengths



Bond angles

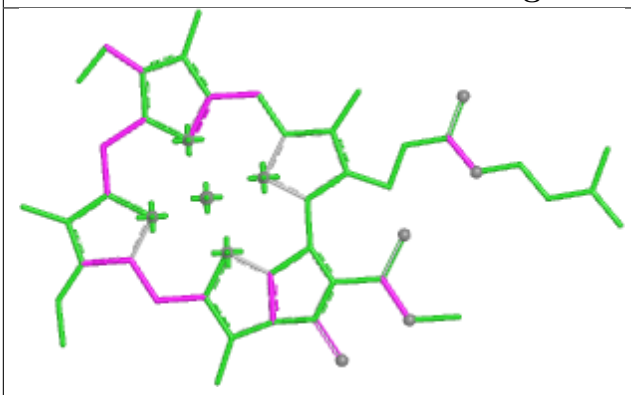


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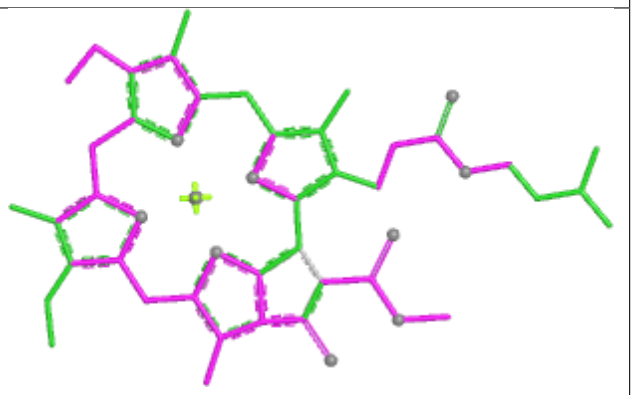


Rings

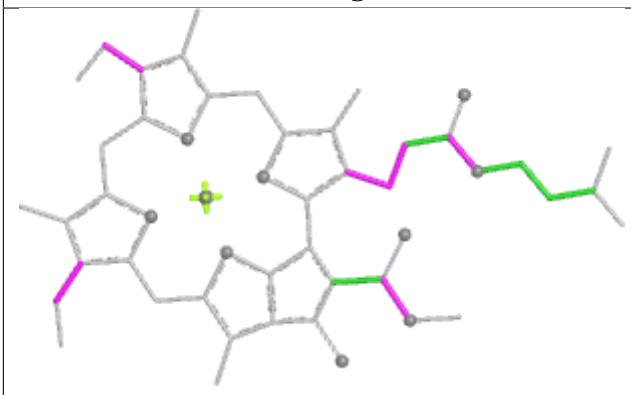
Ligand CLA H 109



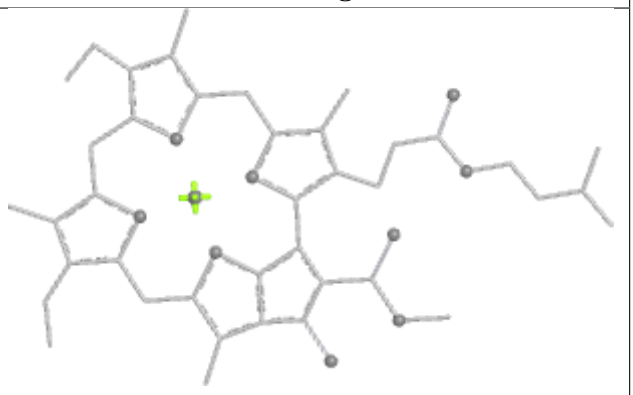
Bond lengths



Bond angles

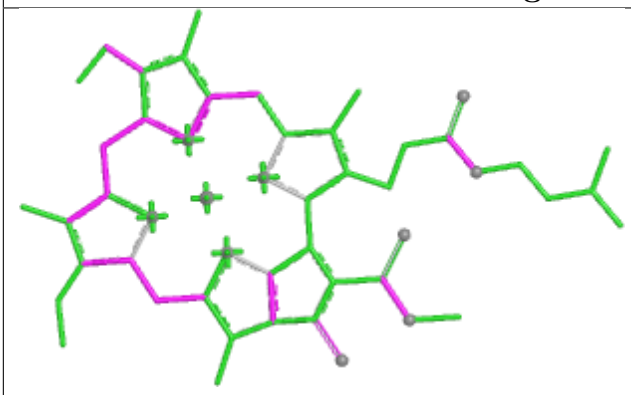


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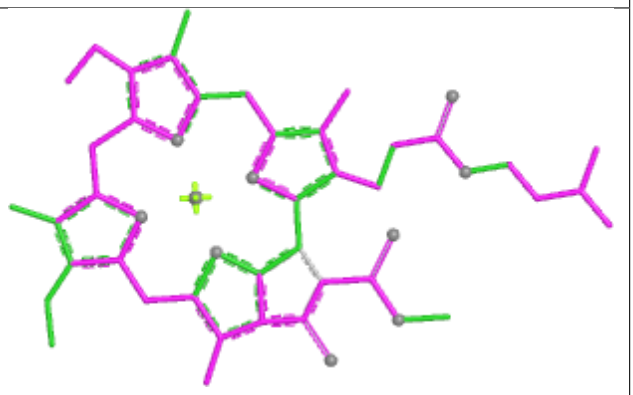


Rings

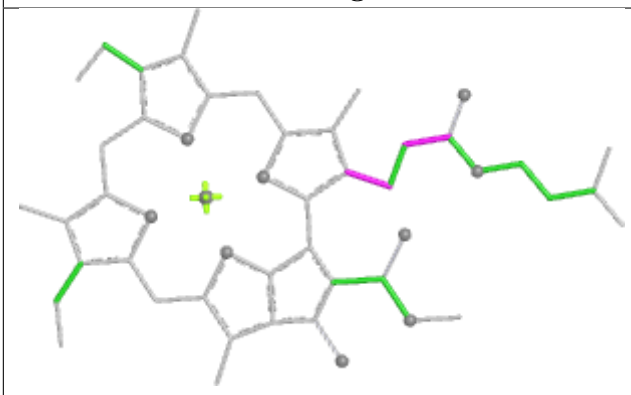
Ligand CLA A 801



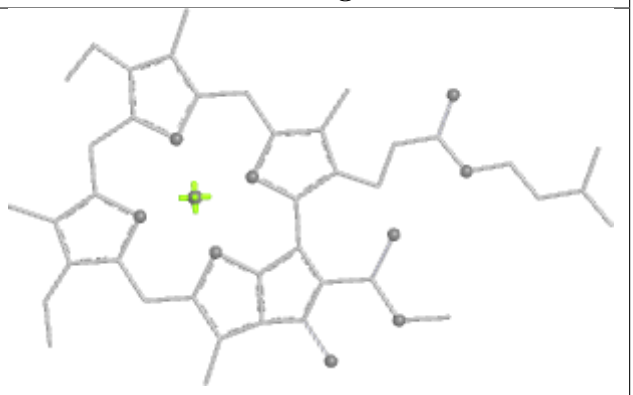
Bond lengths



Bond angles

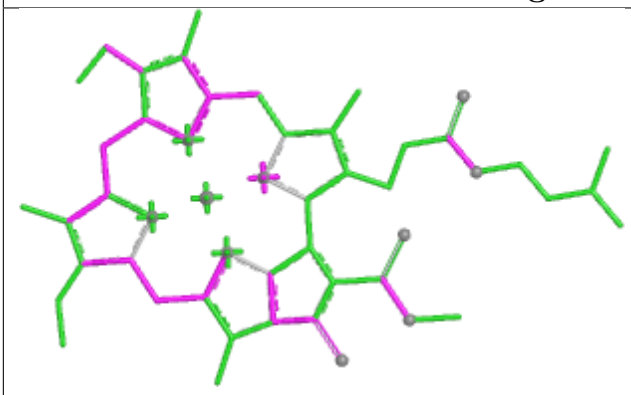


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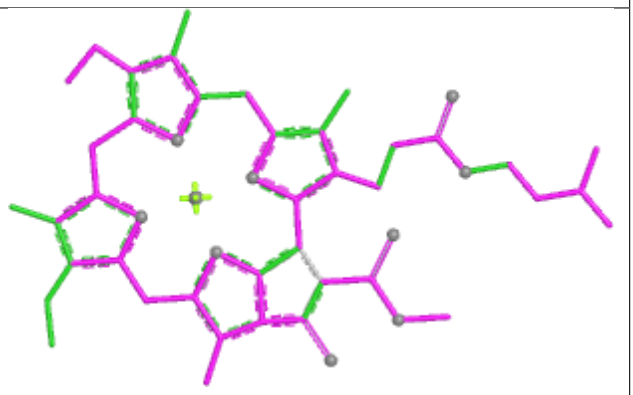


Rings

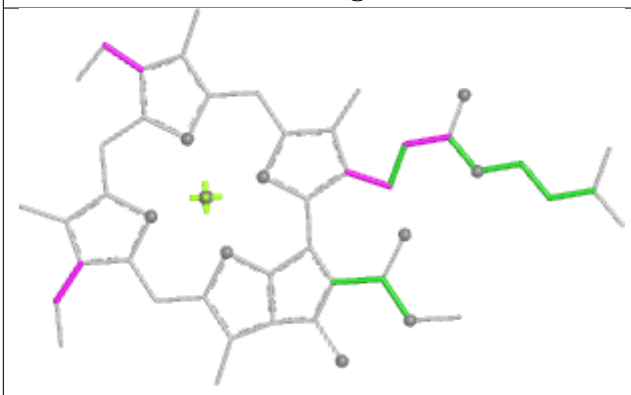
Ligand CLA 3 315



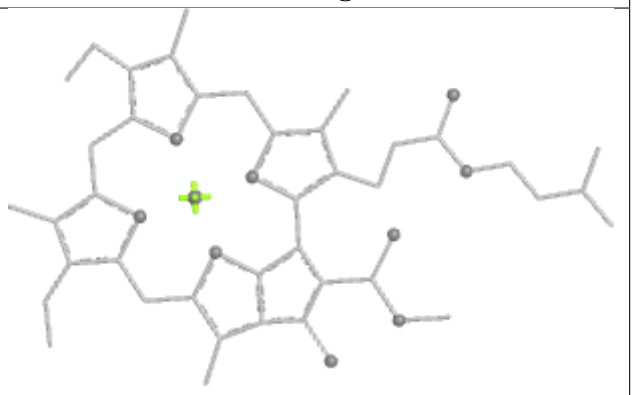
Bond lengths



Bond angles

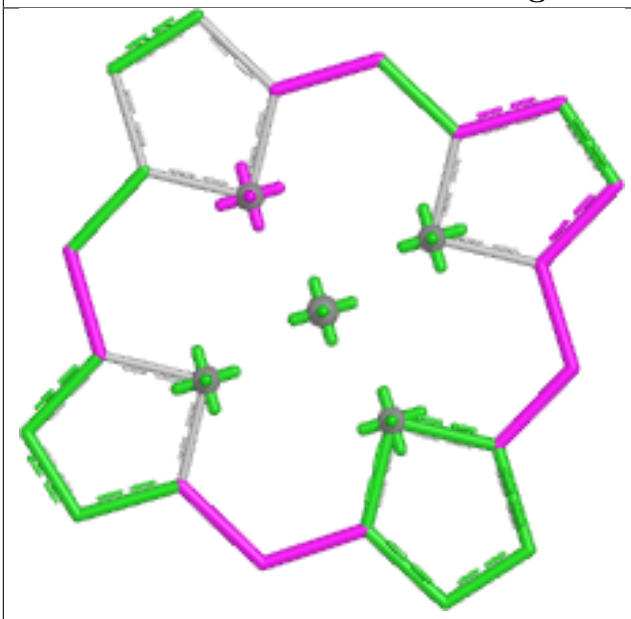


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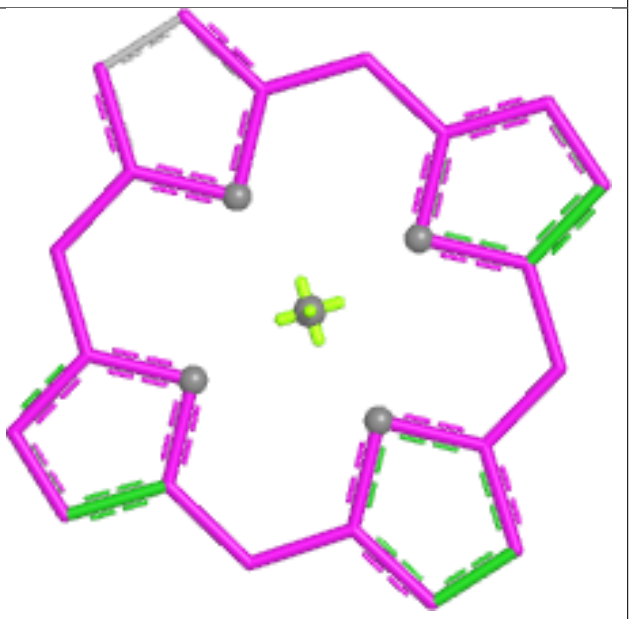


Rings

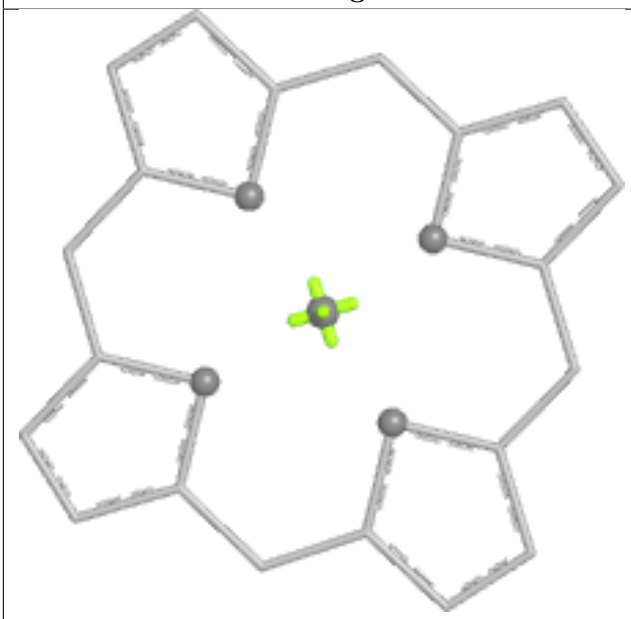
Ligand CLA 4 311



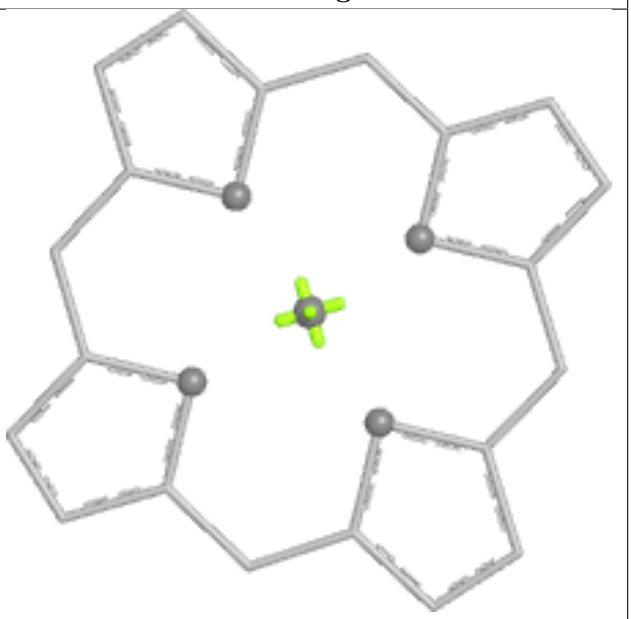
Bond lengths



Bond angles

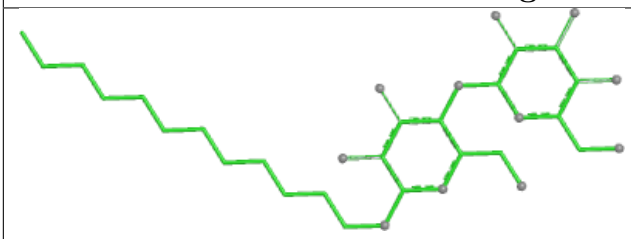


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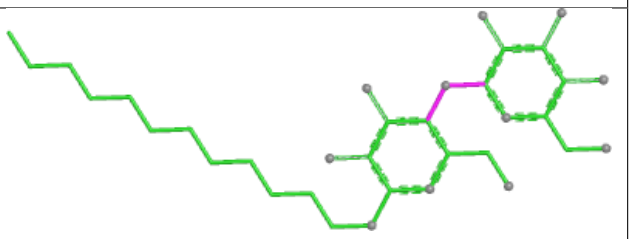


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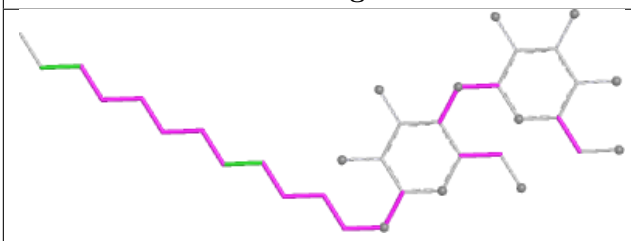
Ligand LMU A 851



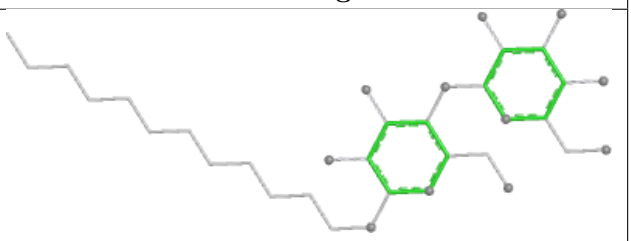
Bond lengths



Bond angles

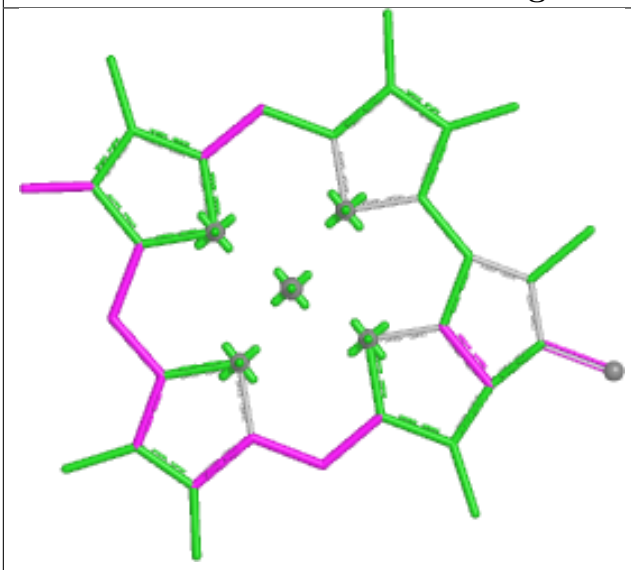


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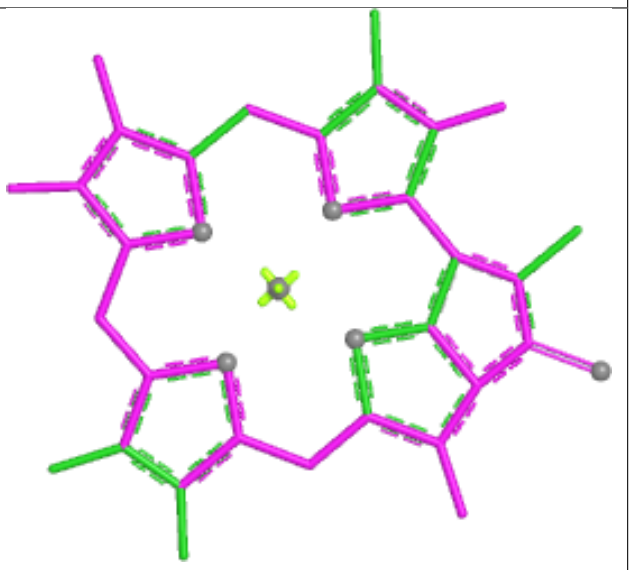


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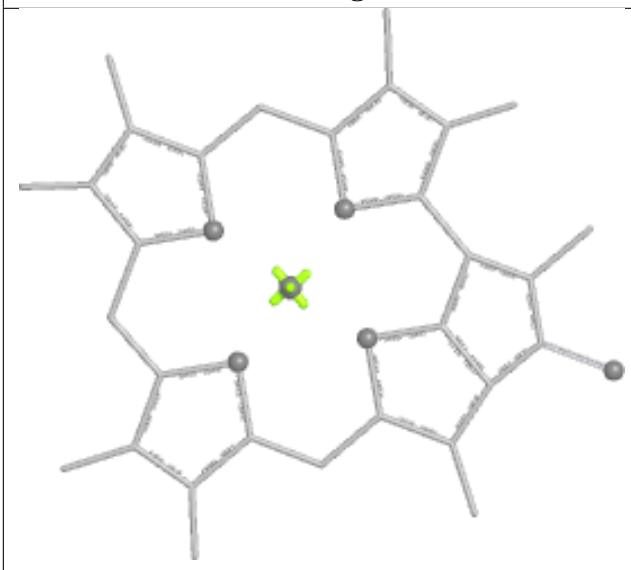
Ligand CLA 3 303



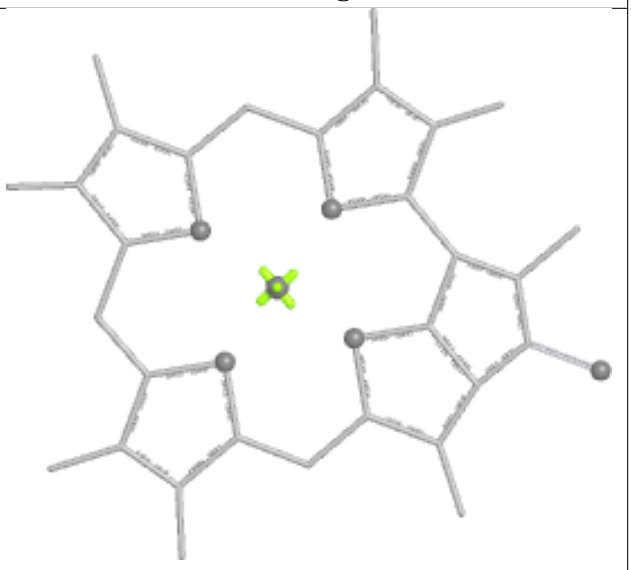
Bond lengths



Bond angles

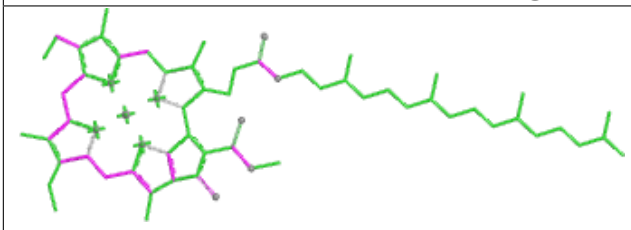


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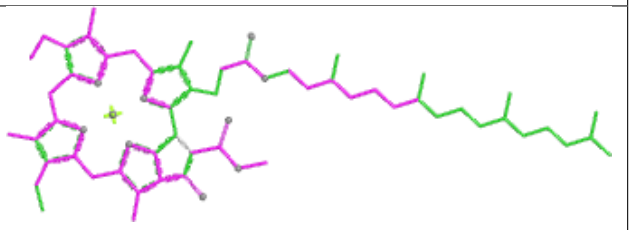


Rings

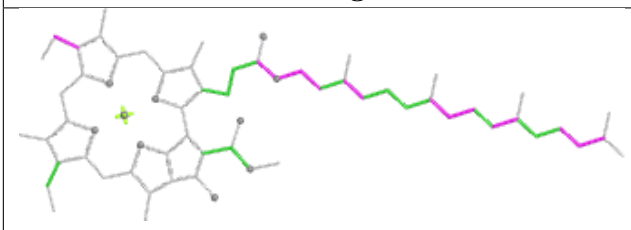
Ligand CLA L 202



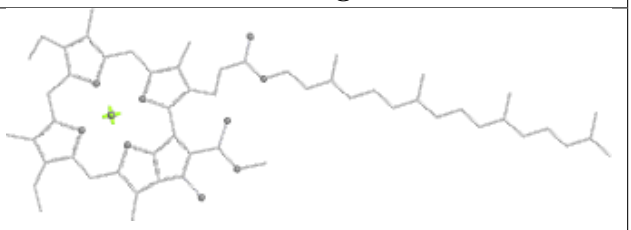
Bond lengths



Bond angles

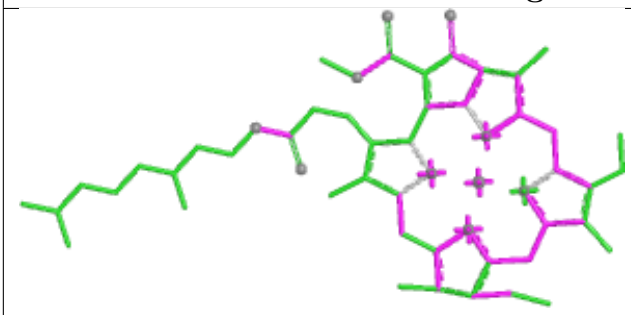


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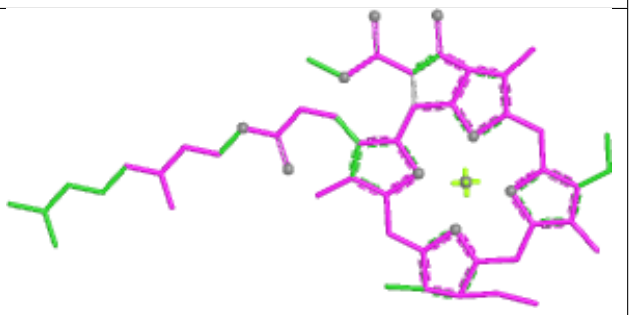


Rings

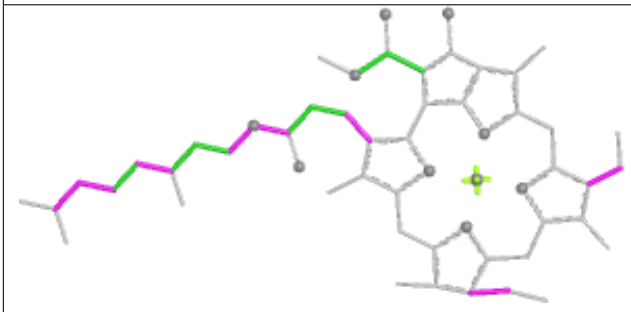
Ligand CLA L 204



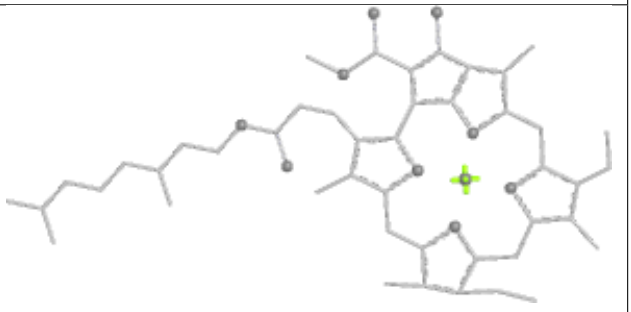
Bond lengths



Bond angles

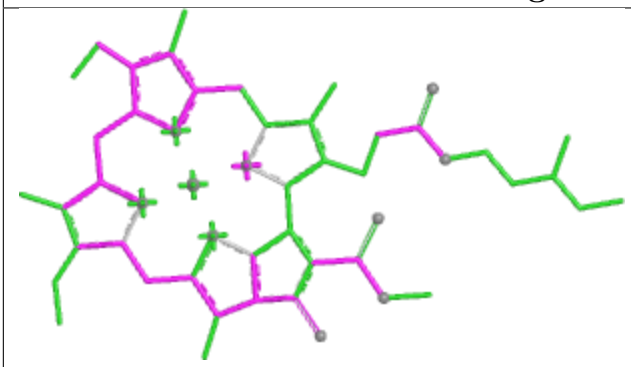


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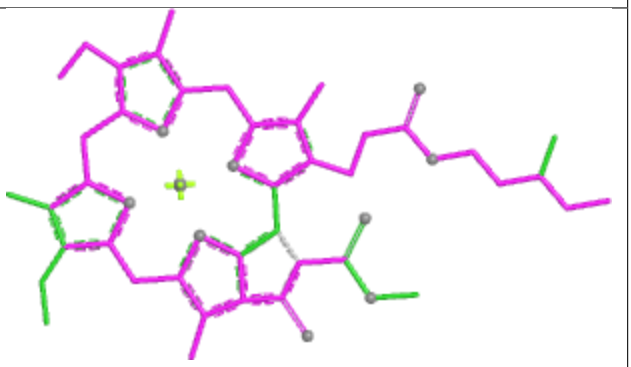


Rings

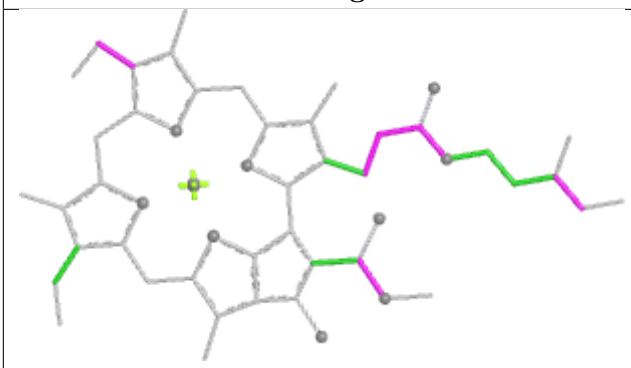
Ligand CLA 1 211



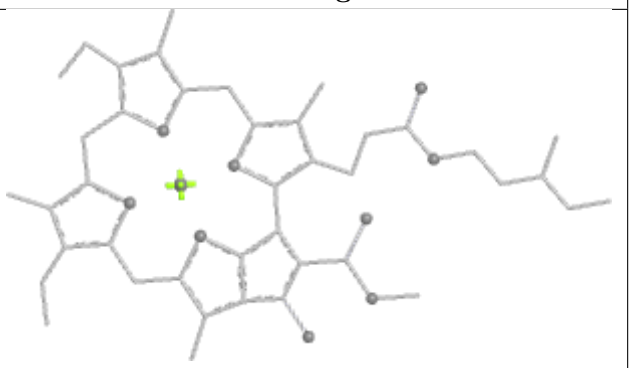
Bond lengths



Bond angles

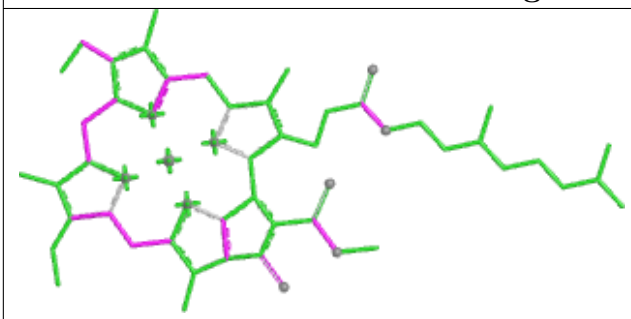


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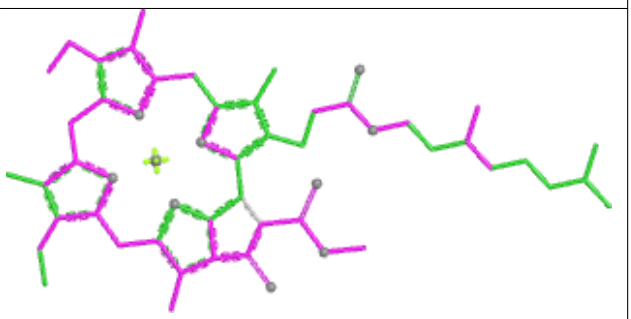


Rings

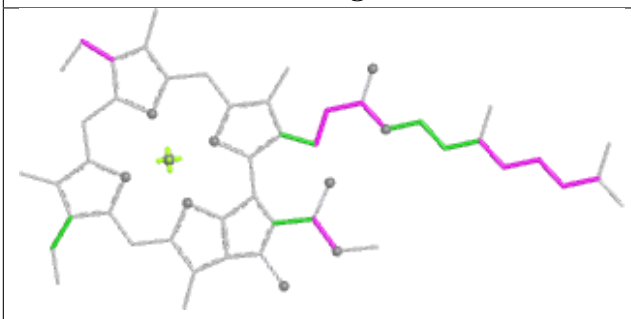
Ligand CLA H 110



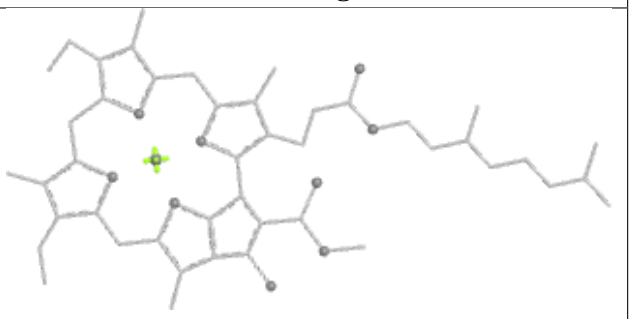
Bond lengths



Bond angles

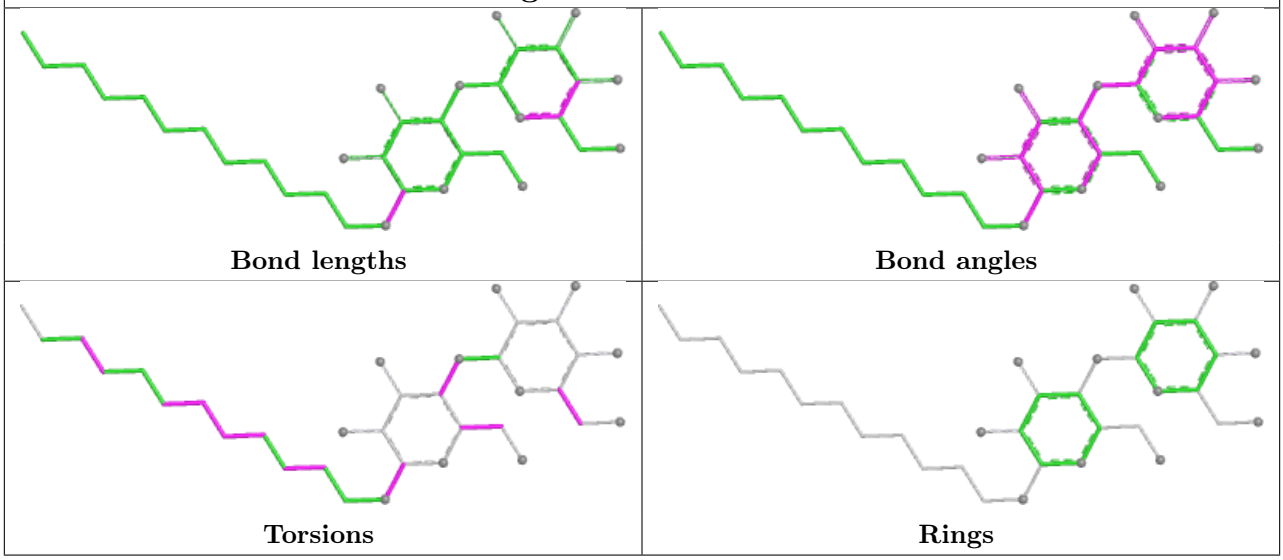


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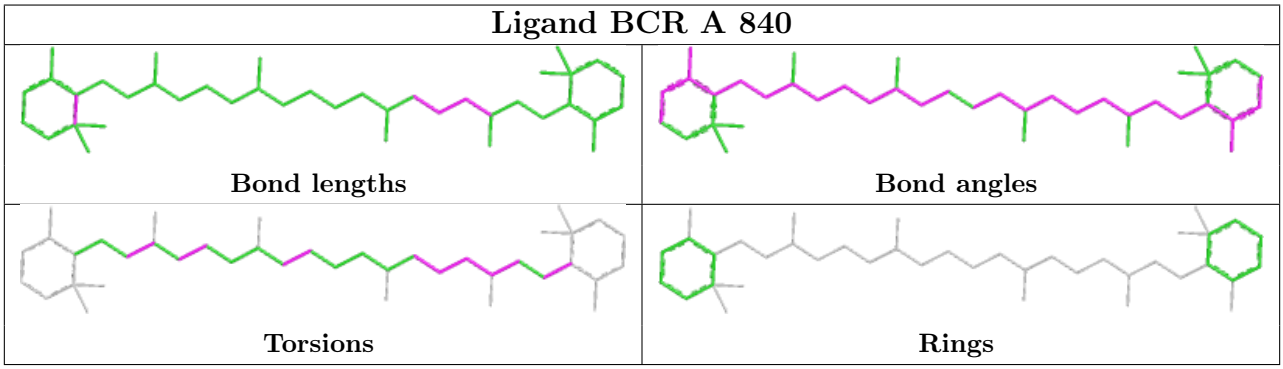


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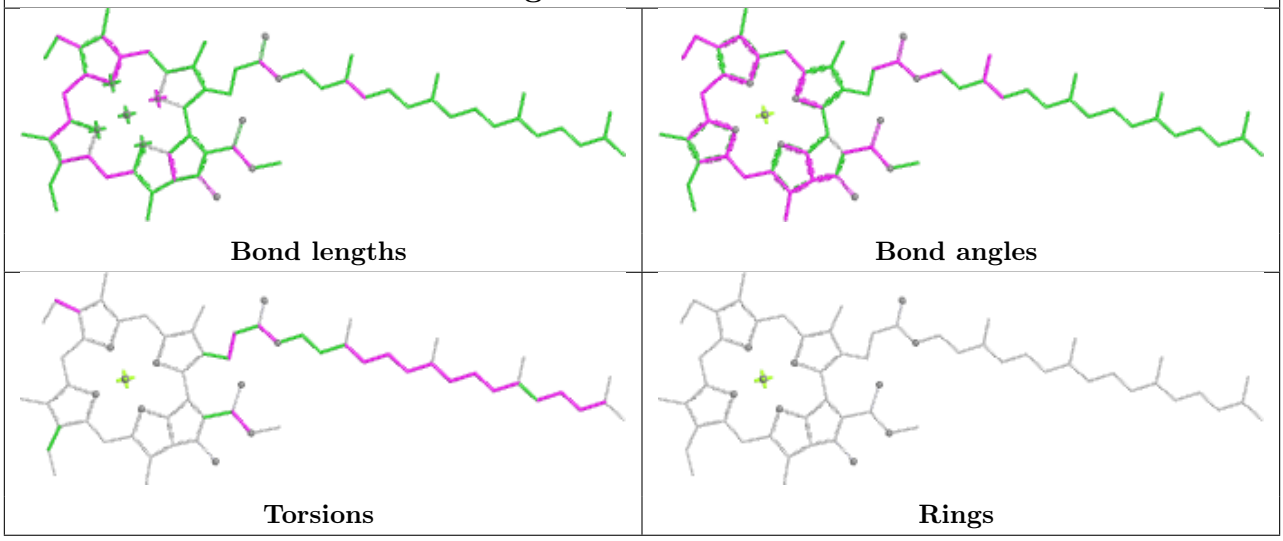
Ligand LMU B 802



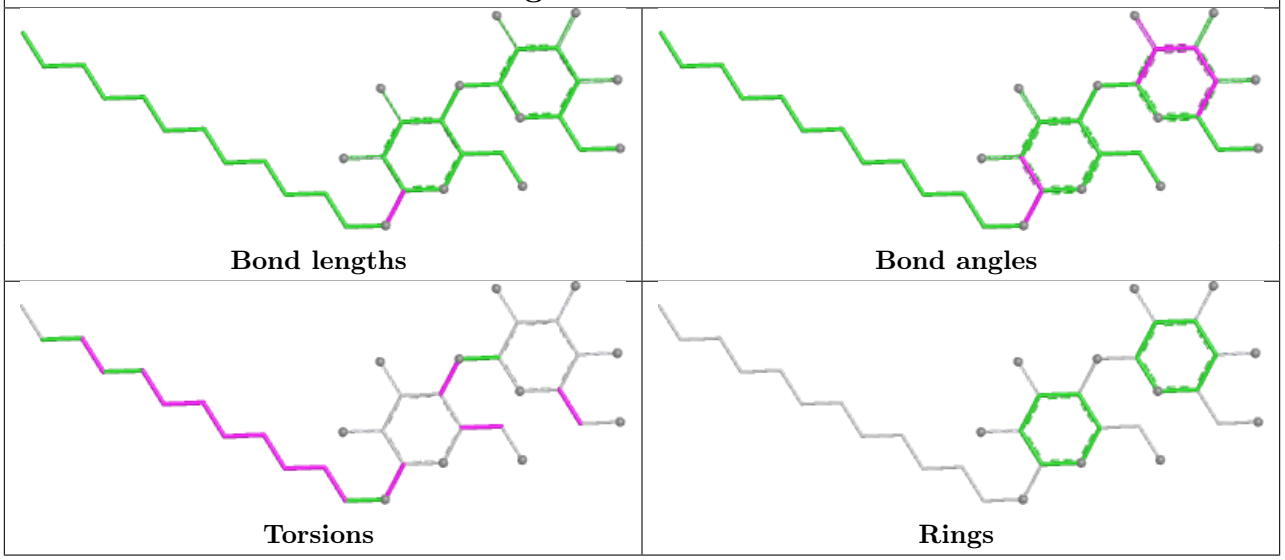
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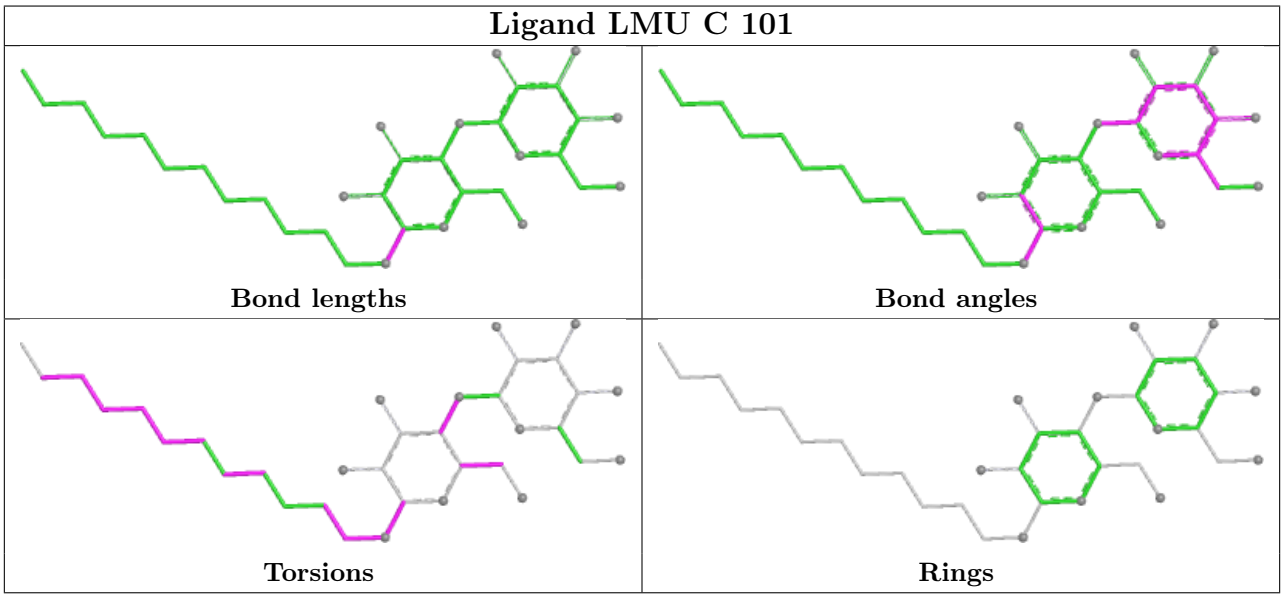
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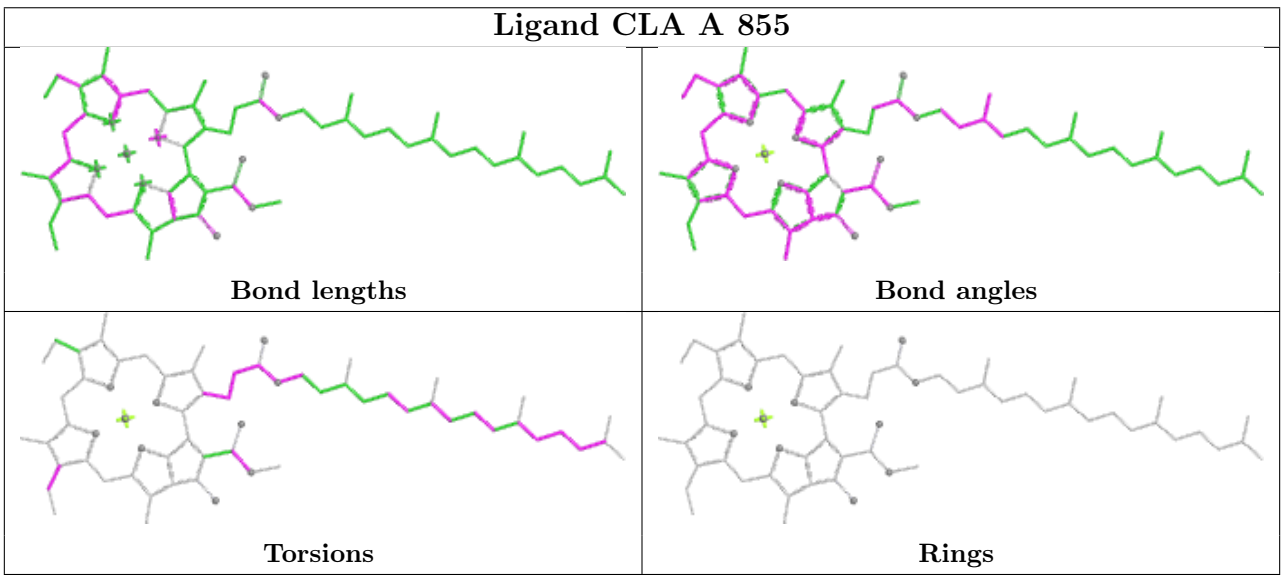
Ligand LMU 4 322



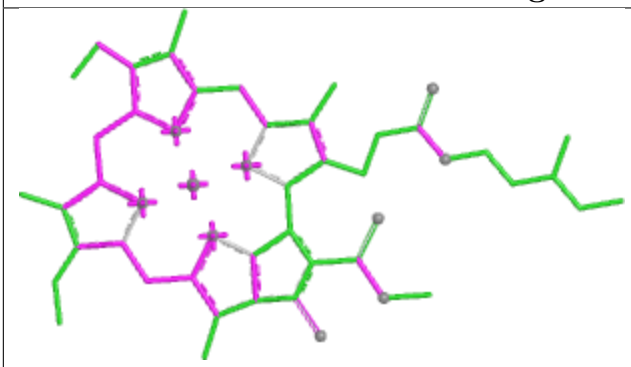
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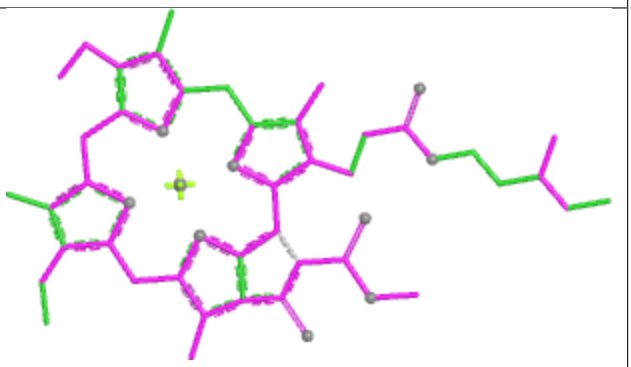
Ligand CLA A 855



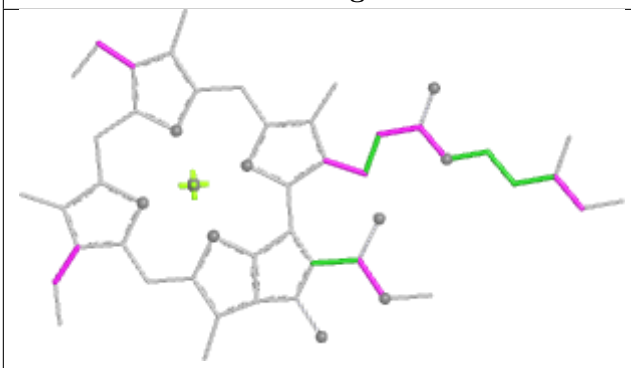
Ligand CLA 1 214



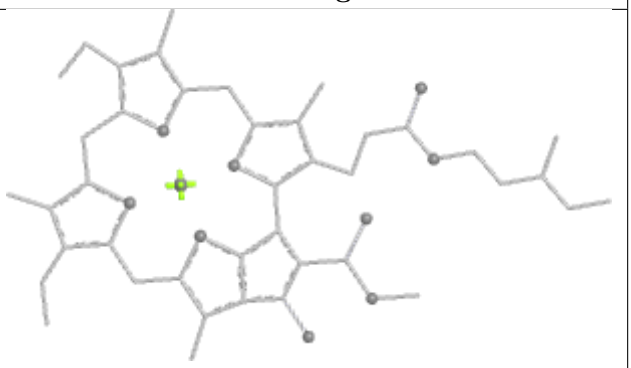
Bond lengths



Bond angles

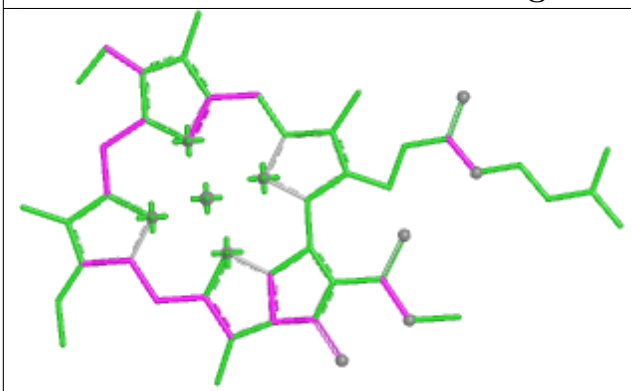


Torsions

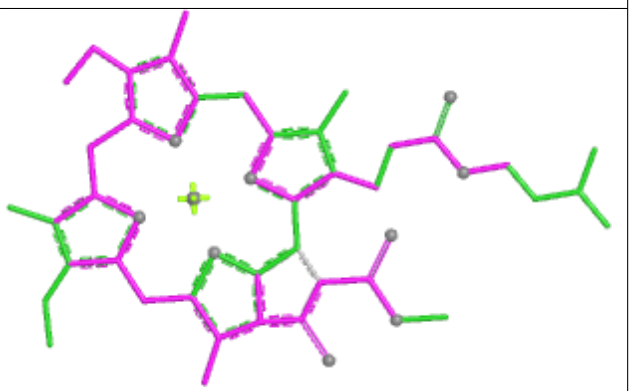


Rings

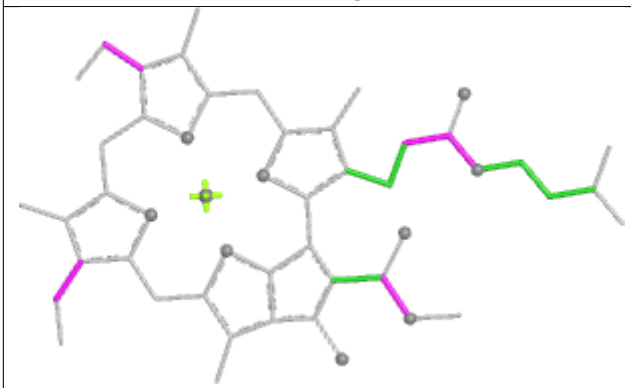
Ligand CLA 2 311



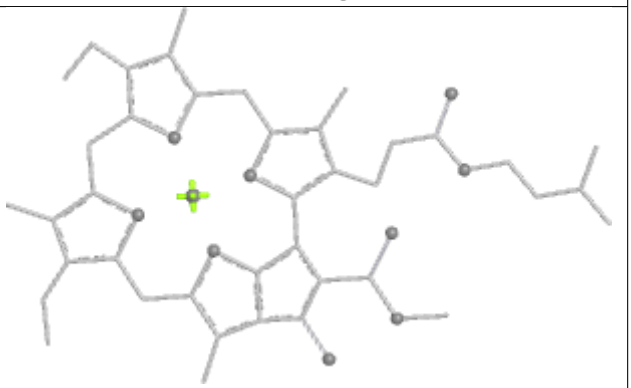
Bond lengths



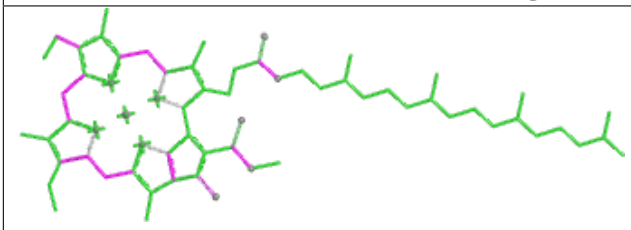
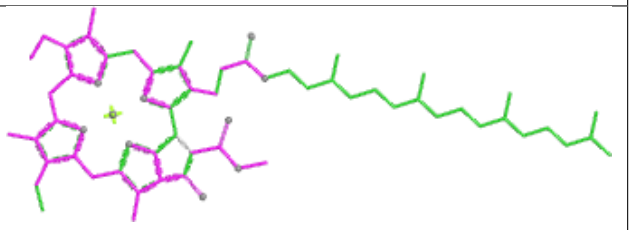
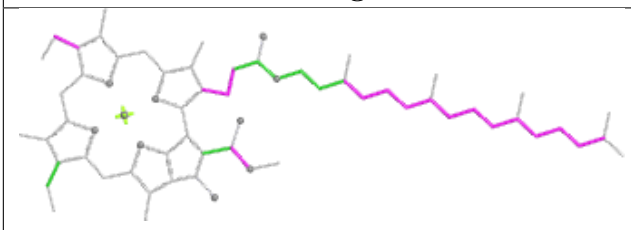
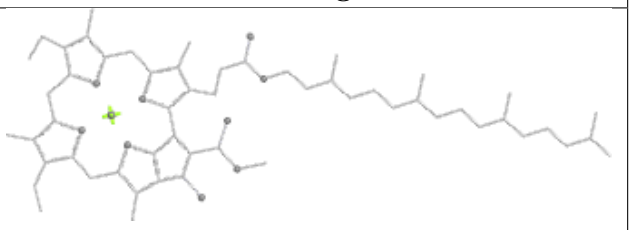
Bond angles



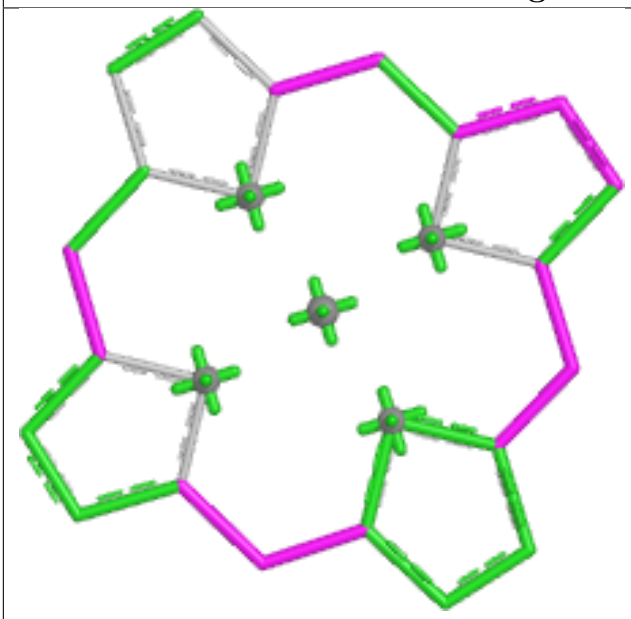
Torsions



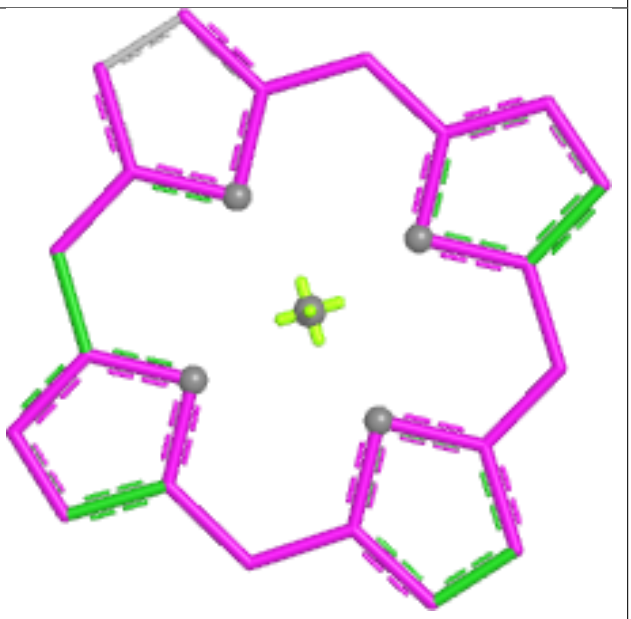
Rings

Ligand CLA B 811	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

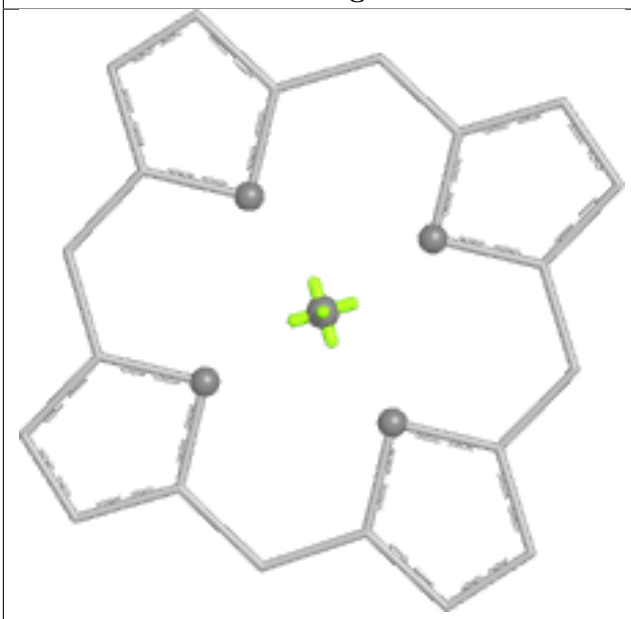
Ligand CLA 4 314



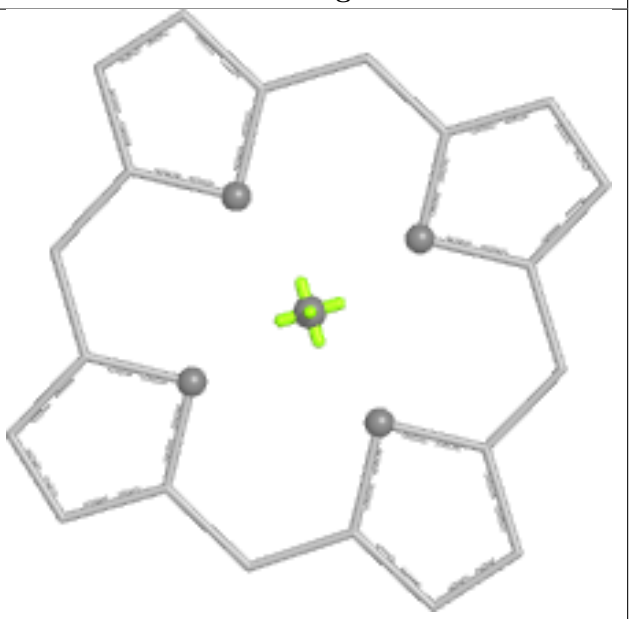
Bond lengths



Bond angles

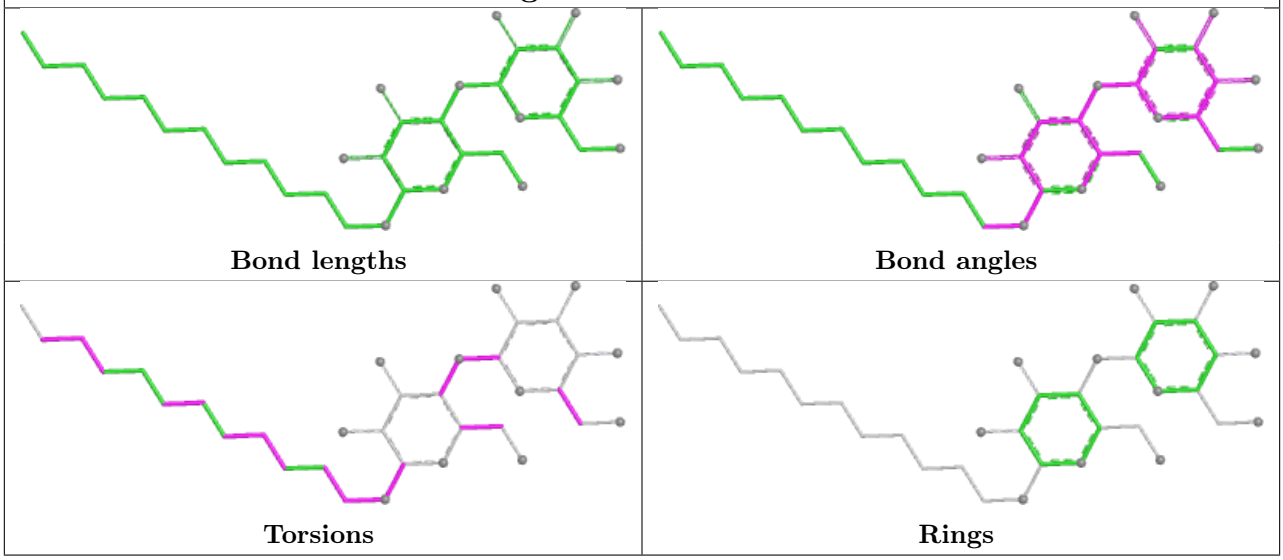


Torsions

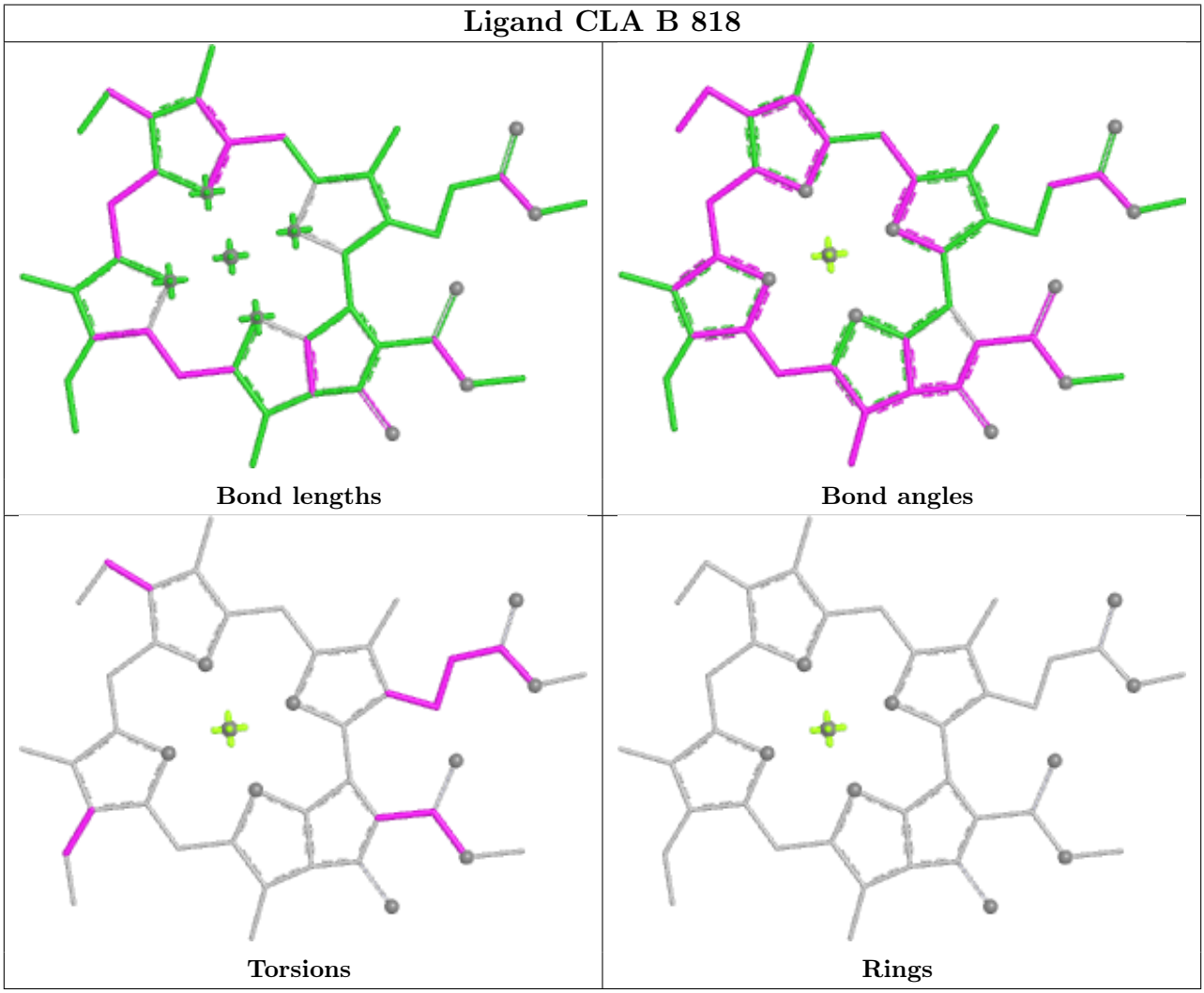


Rings

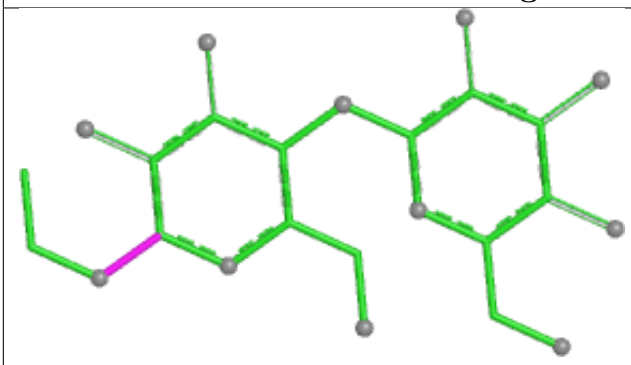
Ligand LMU R 103



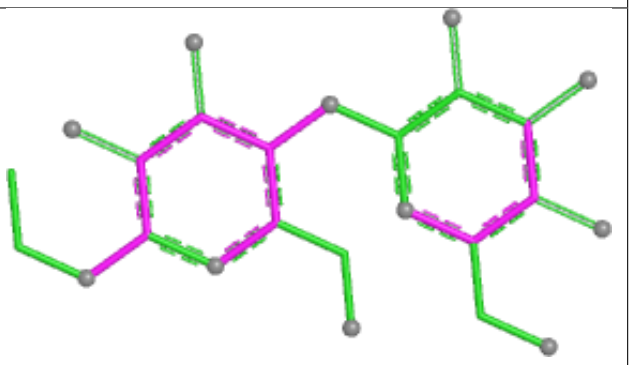
Ligand CLA B 818



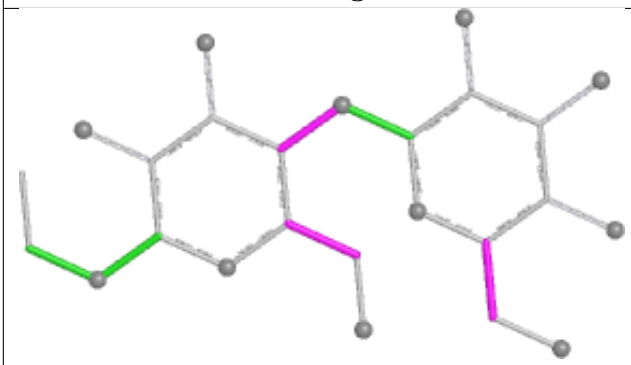
Ligand LMU B 845



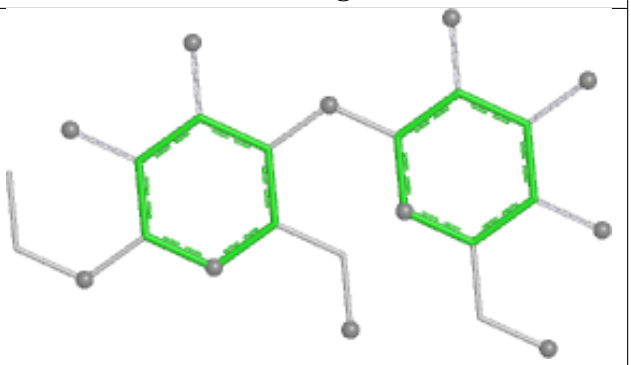
Bond lengths



Bond angles

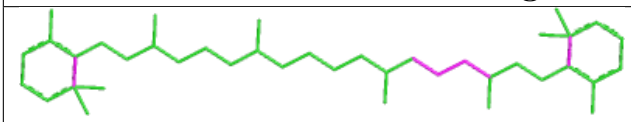


Torsions

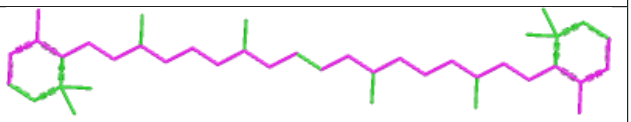


Rings

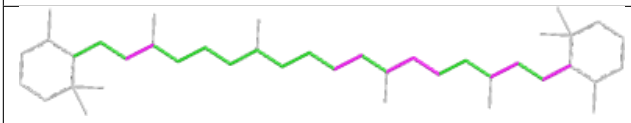
Ligand BCR G 102



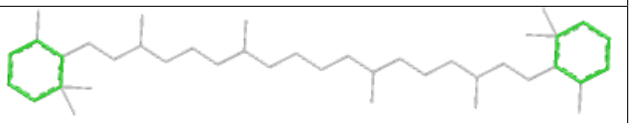
Bond lengths



Bond angles

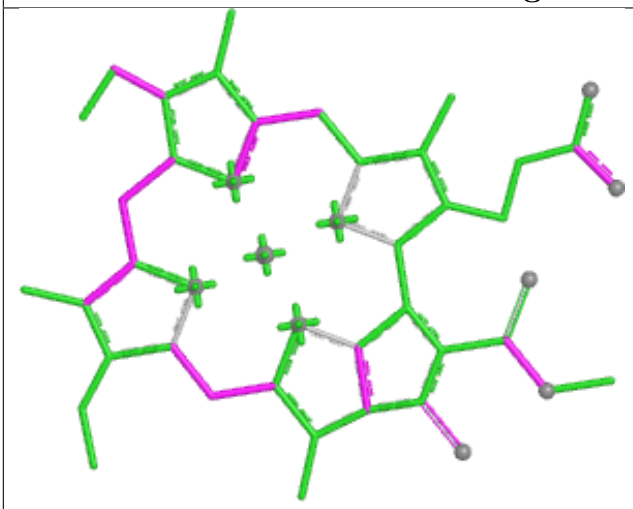


Torsions

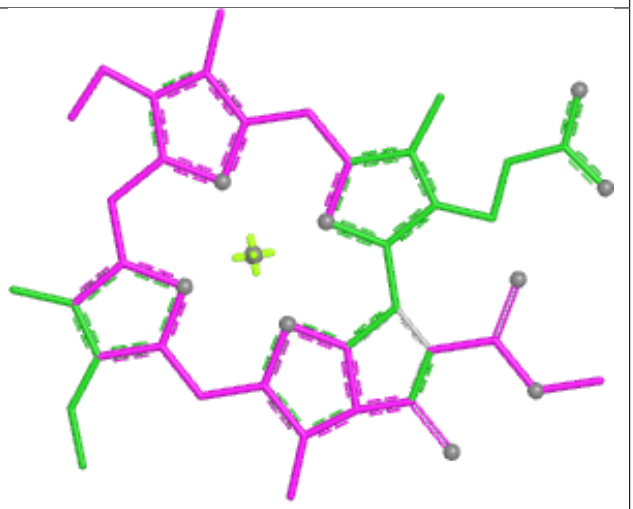


Rings

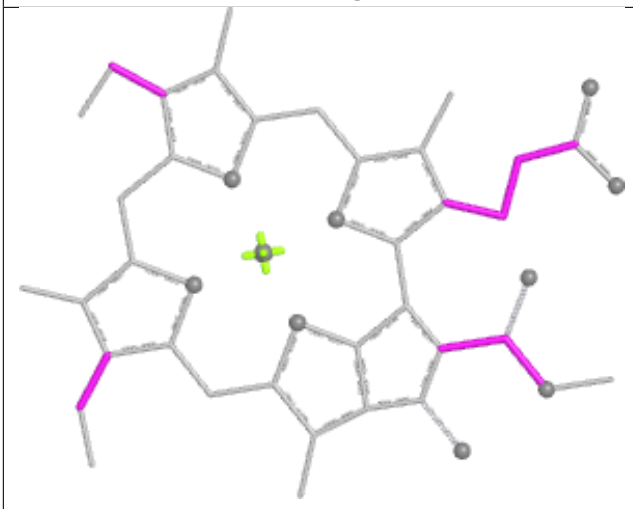
Ligand CLA A 812



Bond lengths



Bond angles

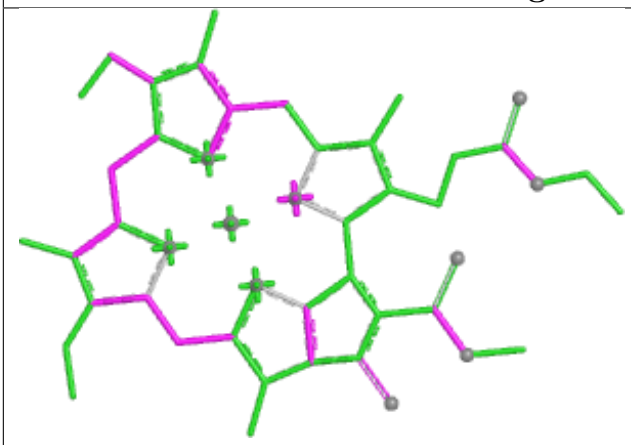


Torsions

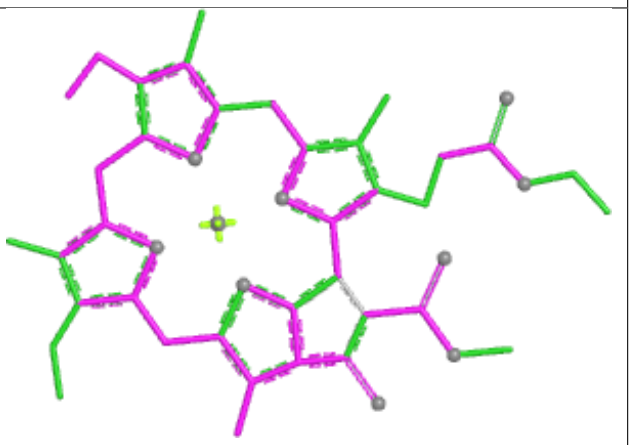


Rings

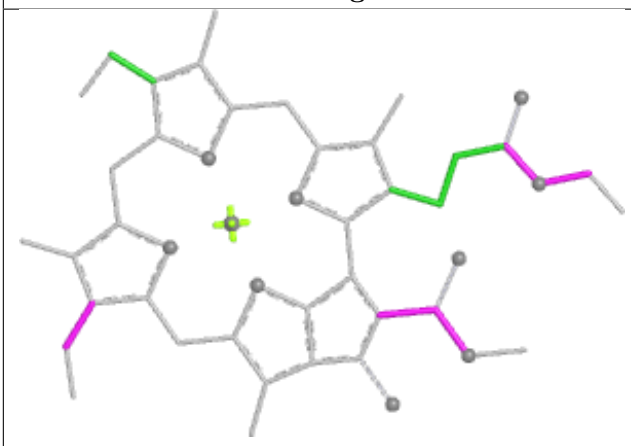
Ligand CLA 4 319



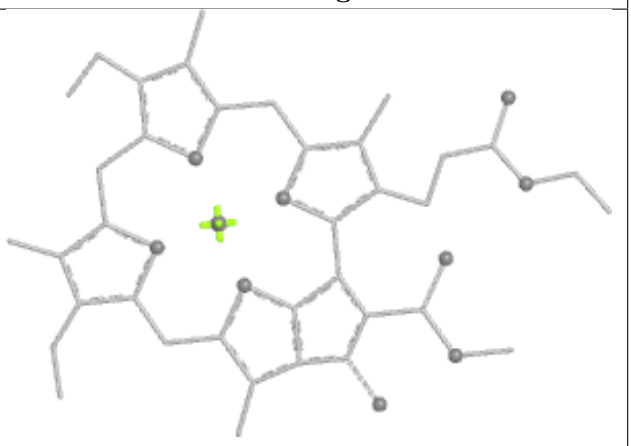
Bond lengths



Bond angles

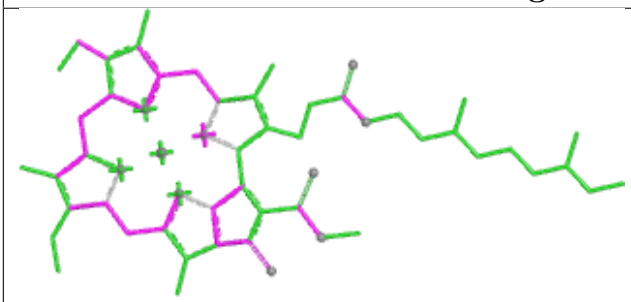


Torsions

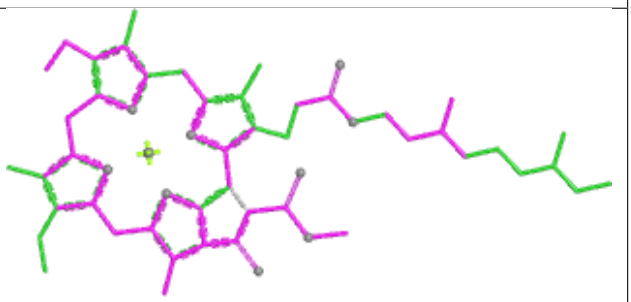


Rings

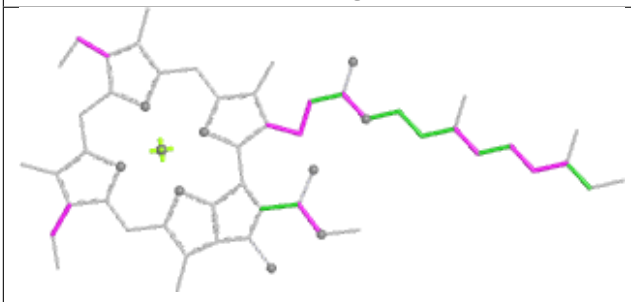
Ligand CLA 3 301



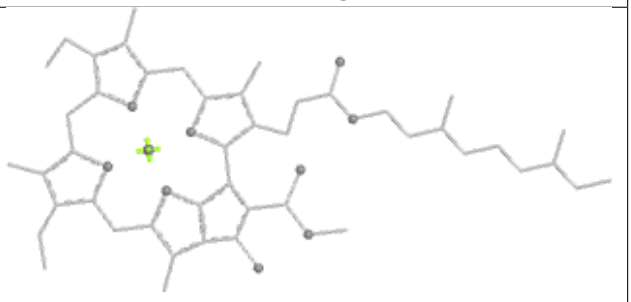
Bond lengths



Bond angles

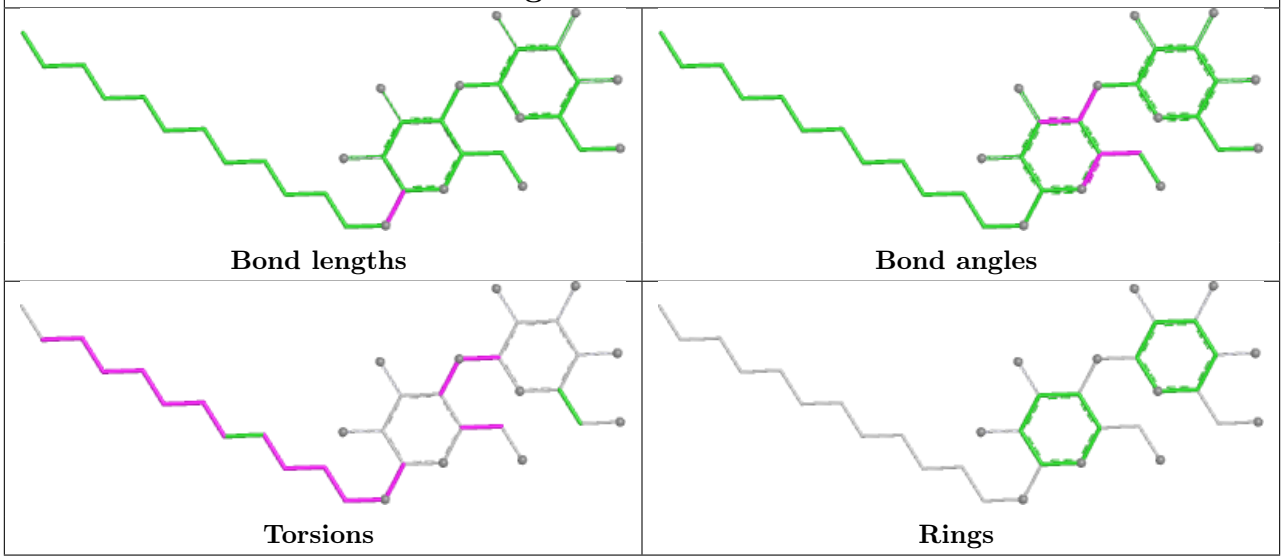


Torsions

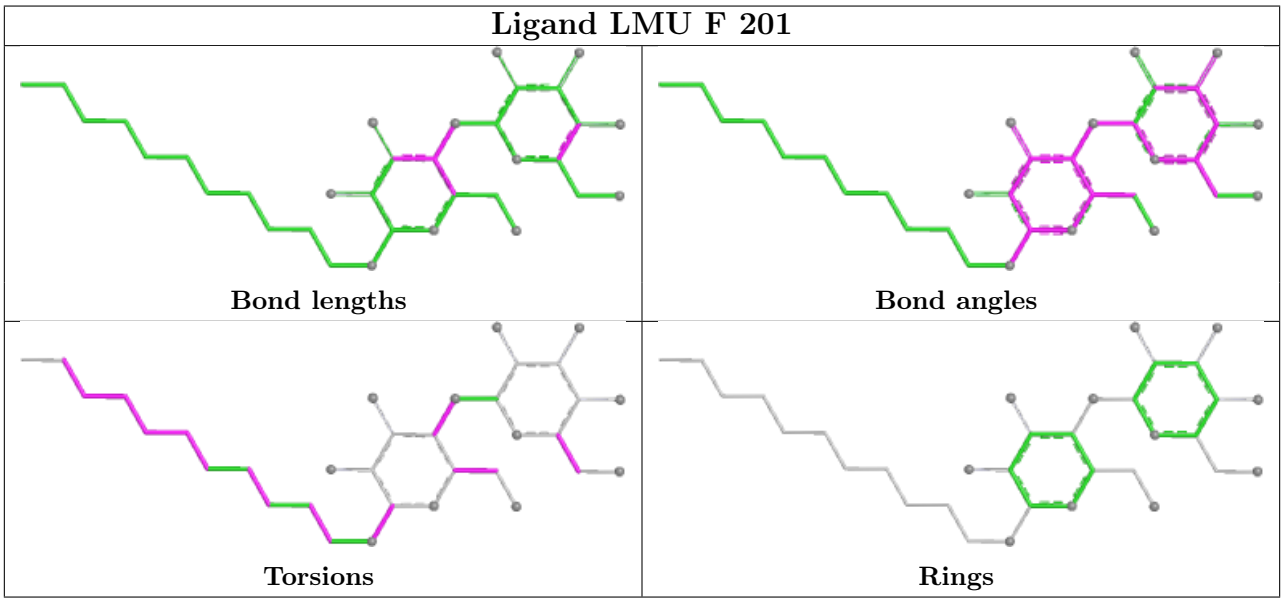


Rings

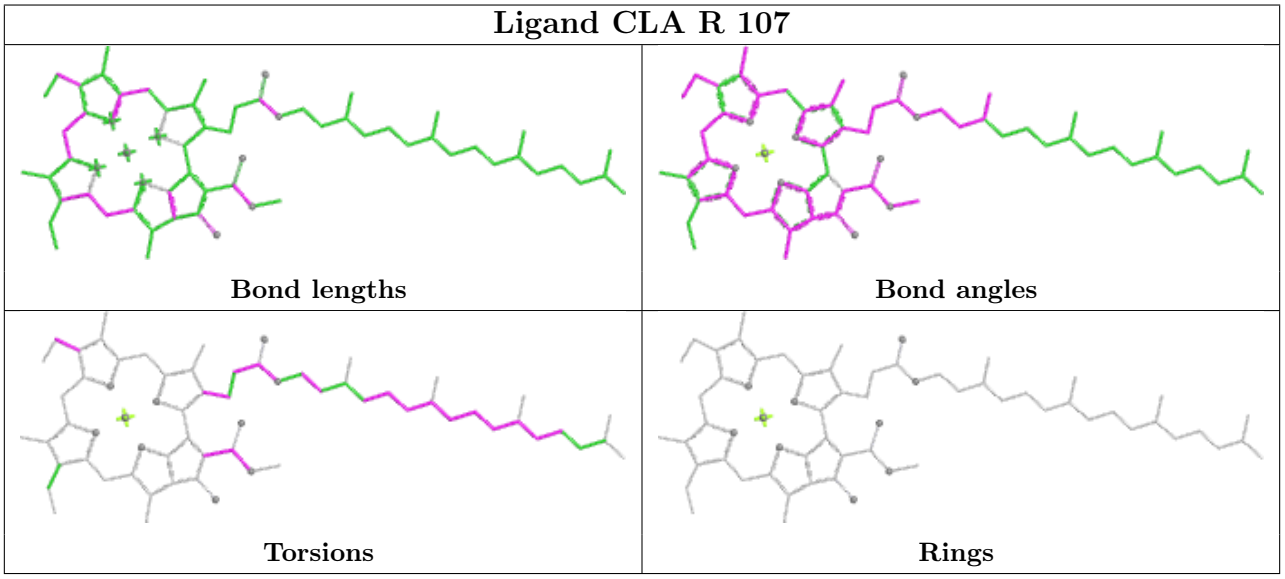
Ligand LMU 2 313



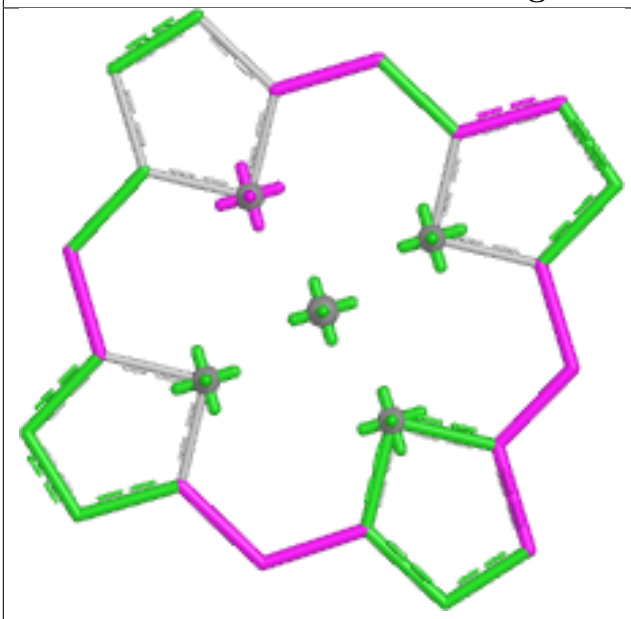
Ligand LMU F 201



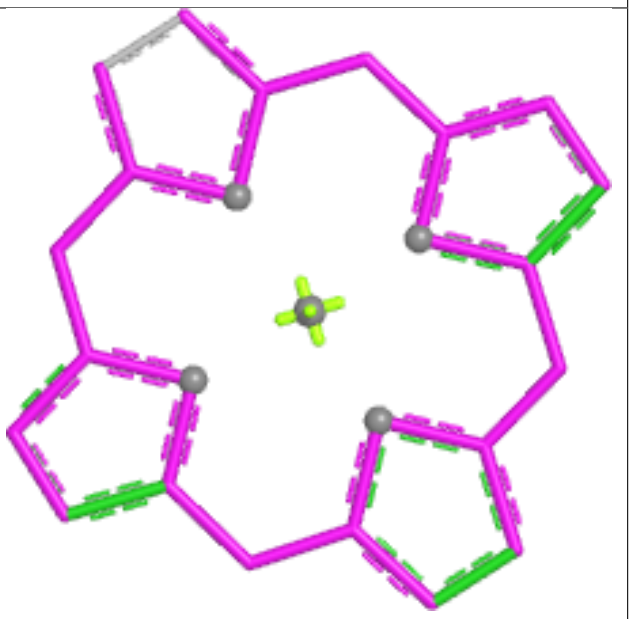
Ligand CLA R 107



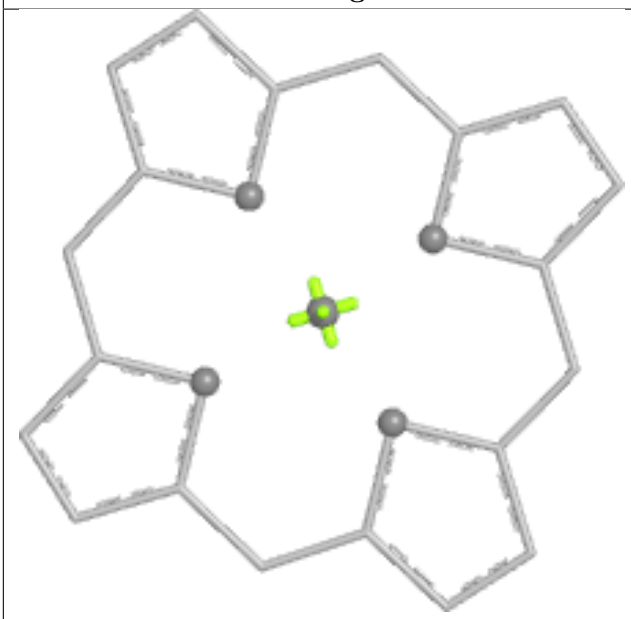
Ligand CLA 2 303



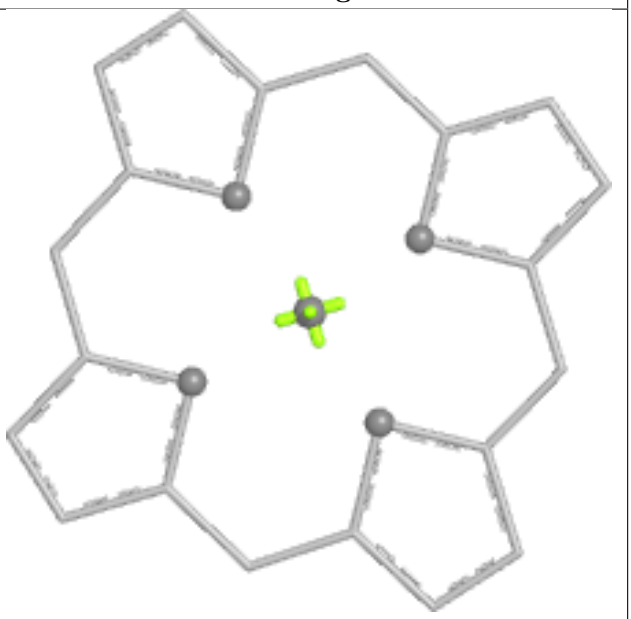
Bond lengths



Bond angles

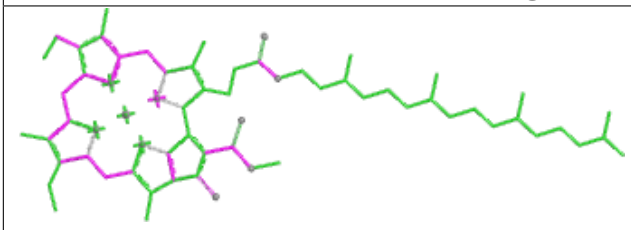


Torsions

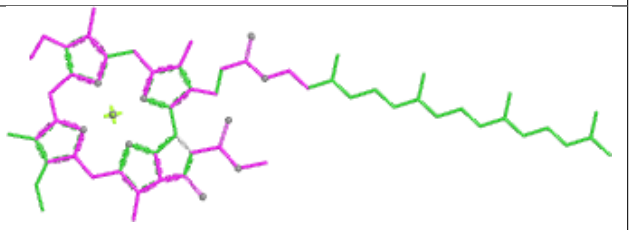


Rings

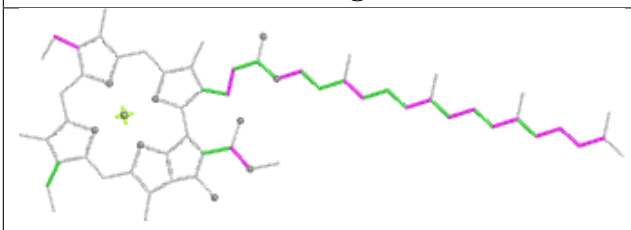
Ligand CLA A 848



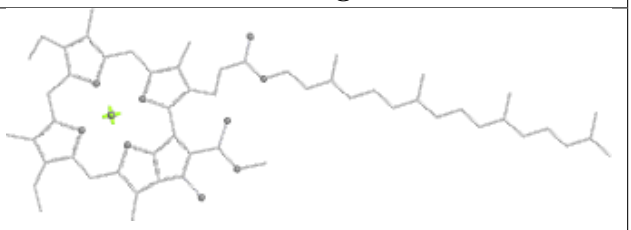
Bond lengths



Bond angles

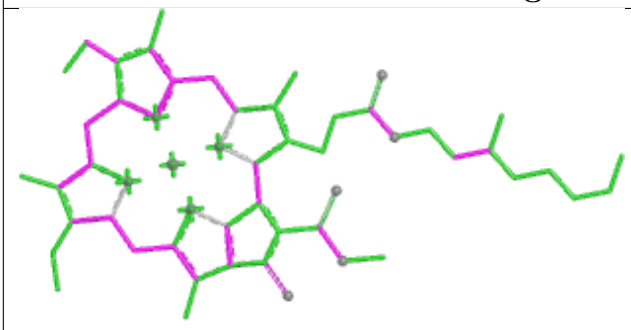


Torsions

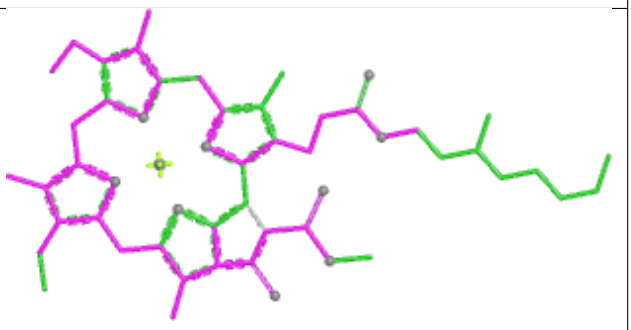


Rings

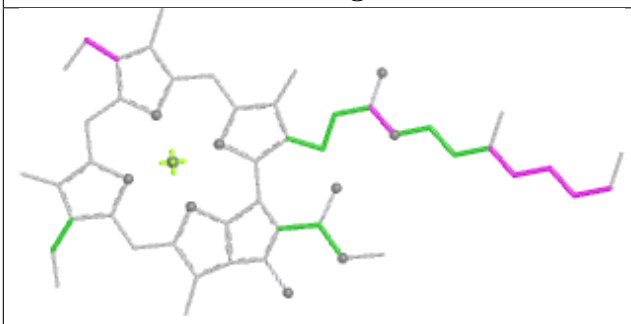
Ligand CLA B 821



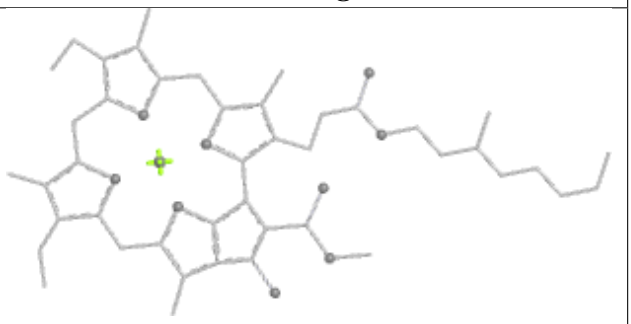
Bond lengths



Bond angles

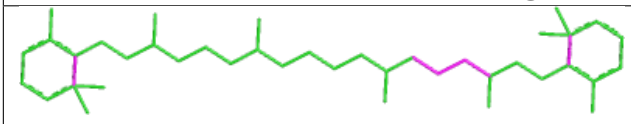


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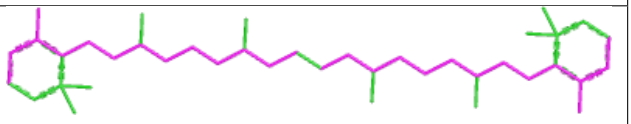


Rings

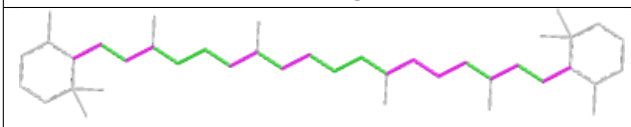
Ligand BCR A 843



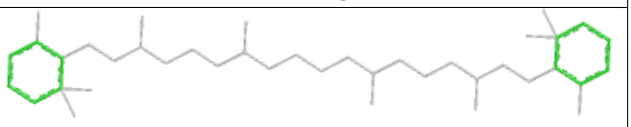
Bond lengths



Bond angles

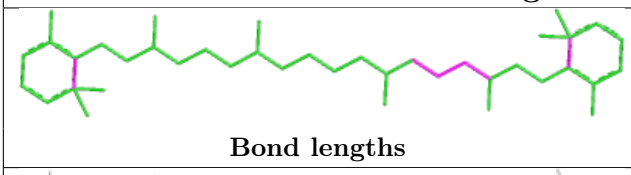


Torsions

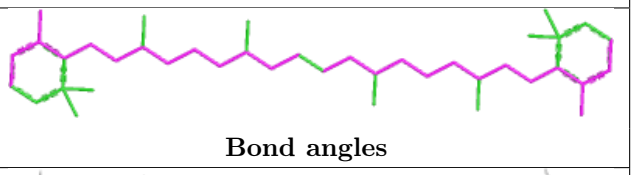


Rings

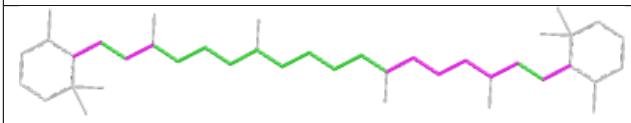
Ligand BCR B 844



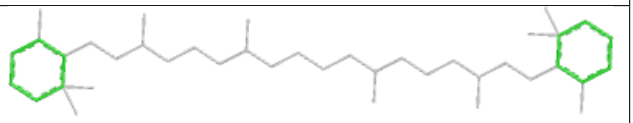
Bond lengths



Bond angles

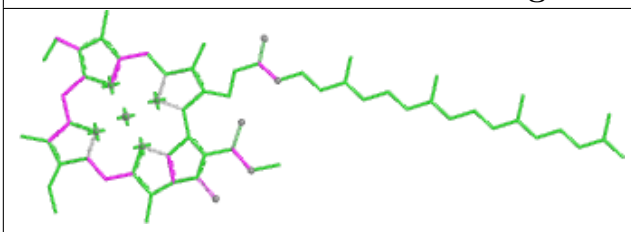


Torsions

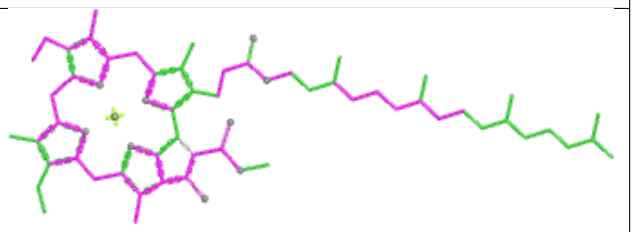


Rings

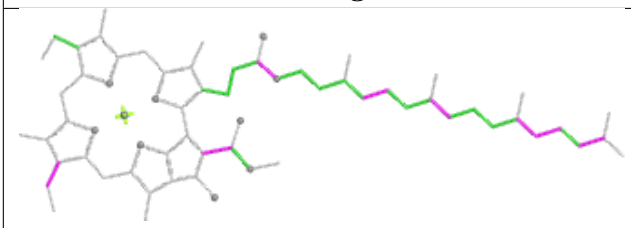
Ligand CLA 2 307



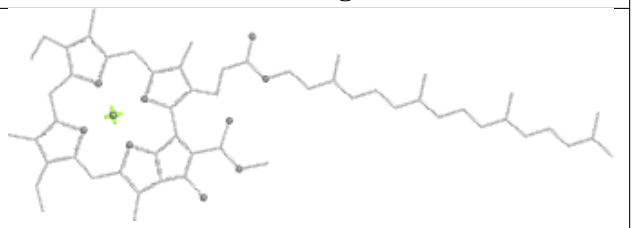
Bond lengths



Bond angles

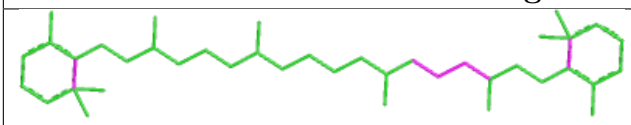


Torsions

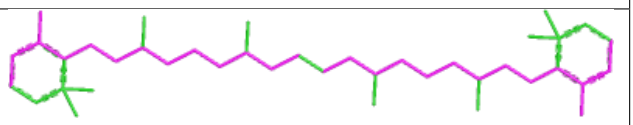


Rings

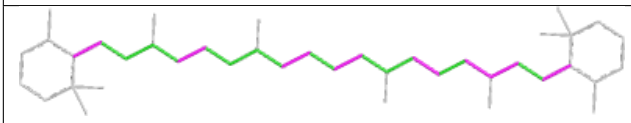
Ligand BCR F 202



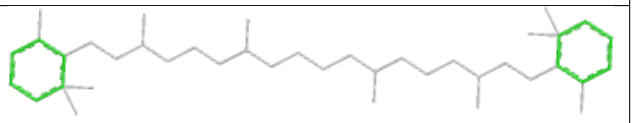
Bond lengths



Bond angles

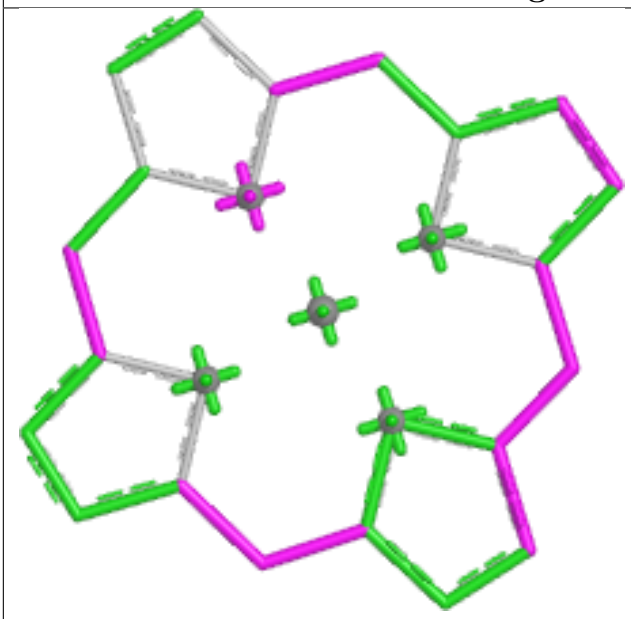


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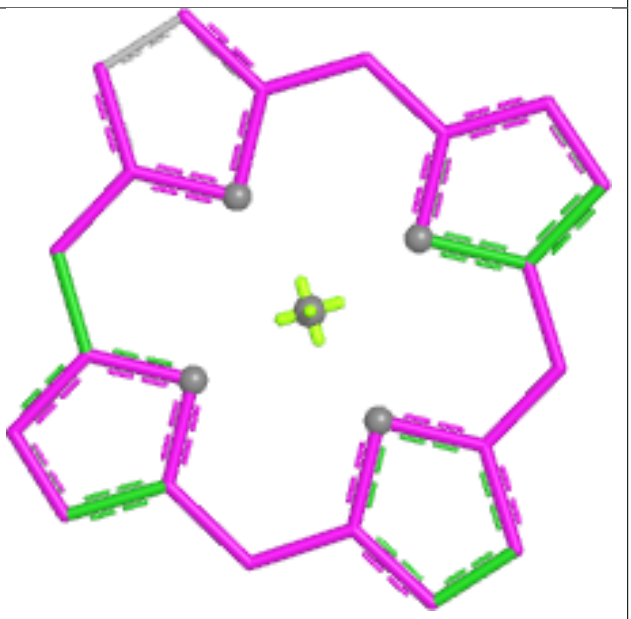


Rings

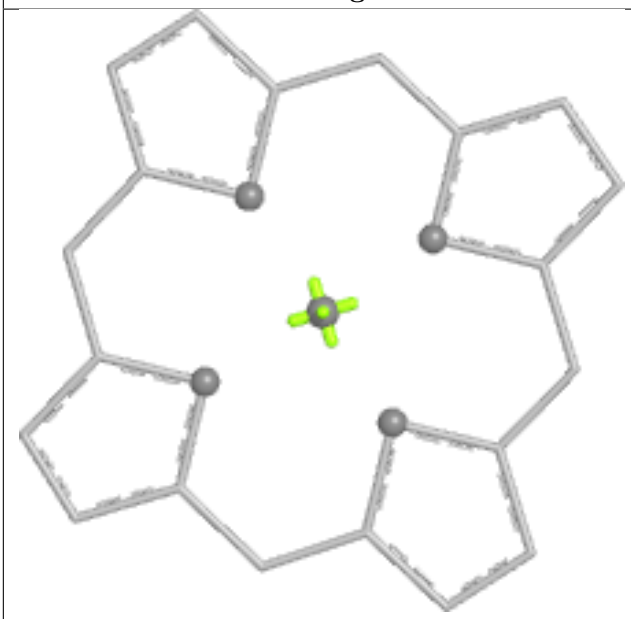
Ligand CLA 3 306



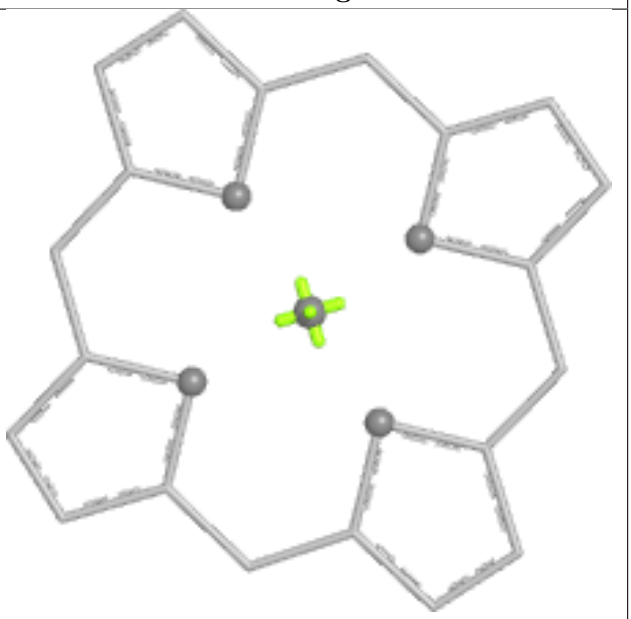
Bond lengths



Bond angles

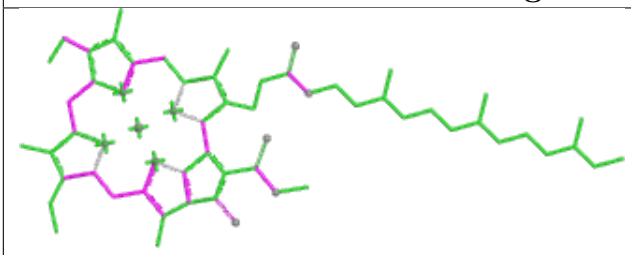


Torsions

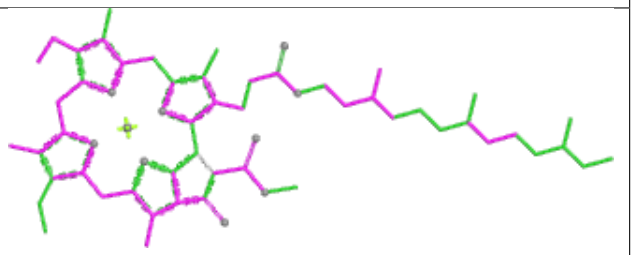


Rings

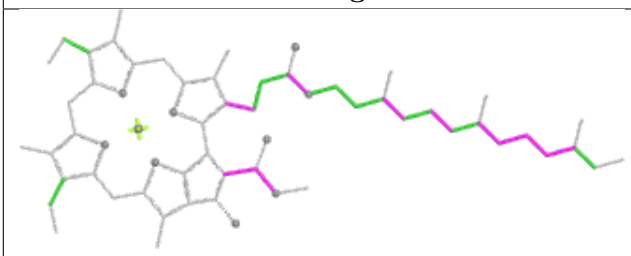
Ligand CLA B 816



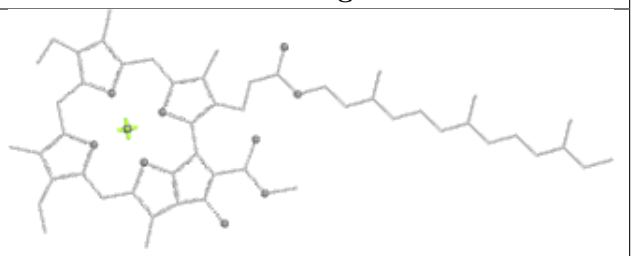
Bond lengths



Bond angles

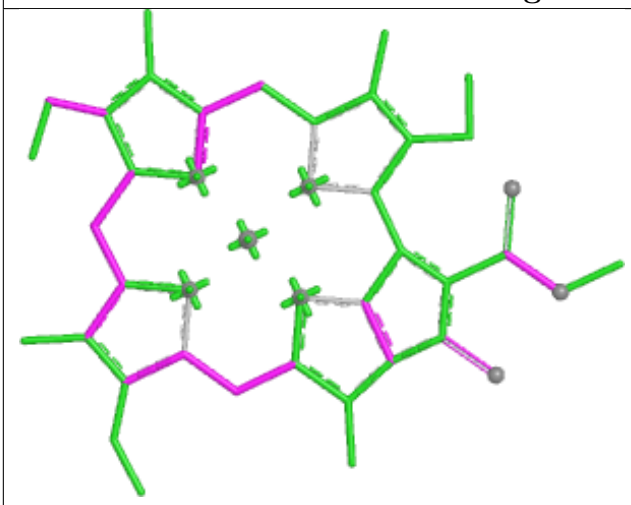


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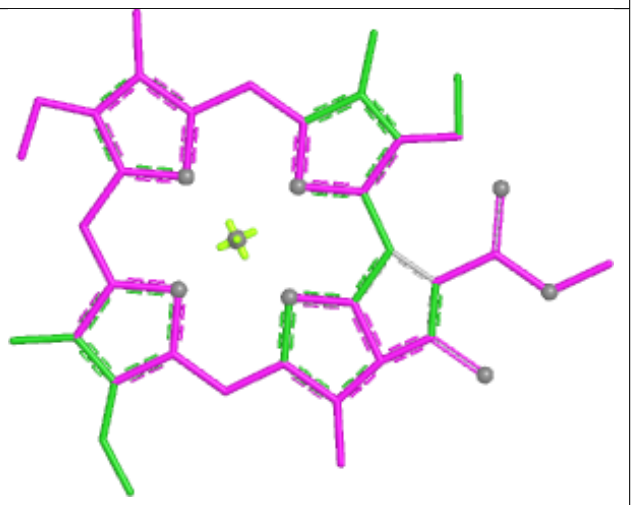


Rings

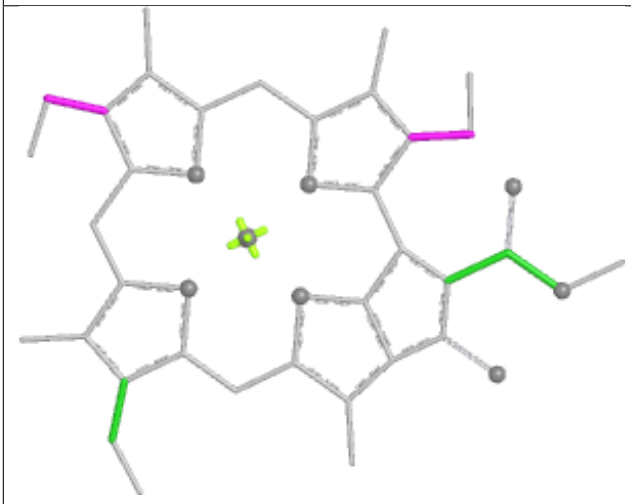
Ligand CLA A 819



Bond lengths



Bond angles

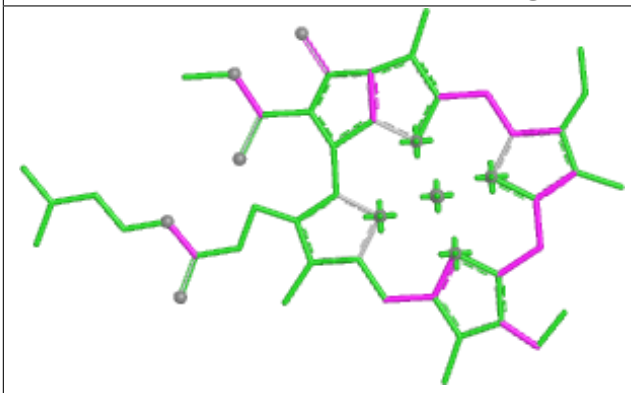


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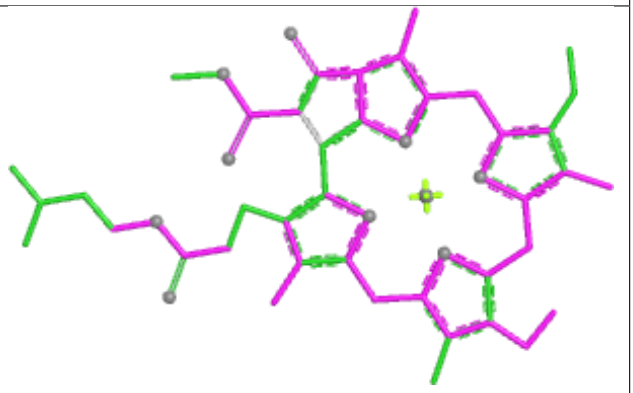


Rings

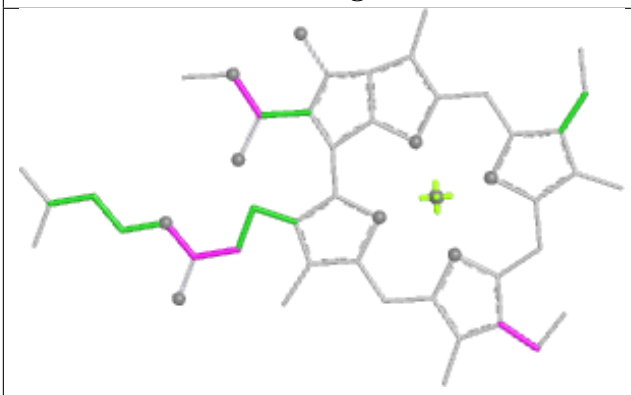
Ligand CLA B 817



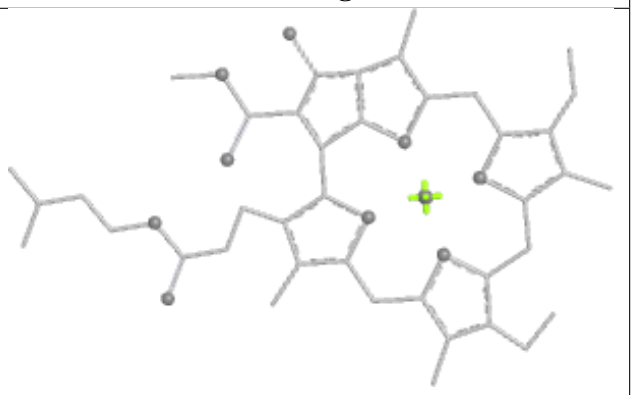
Bond lengths



Bond angles

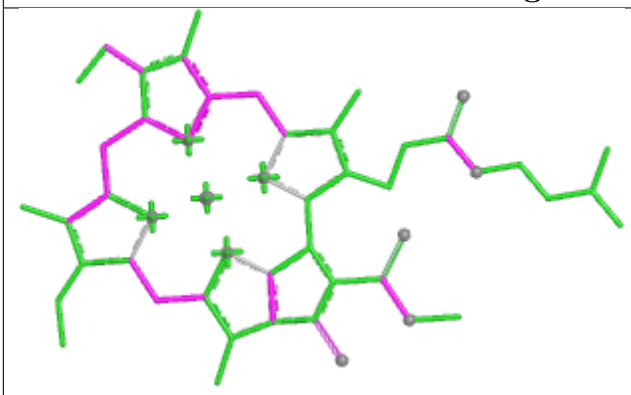


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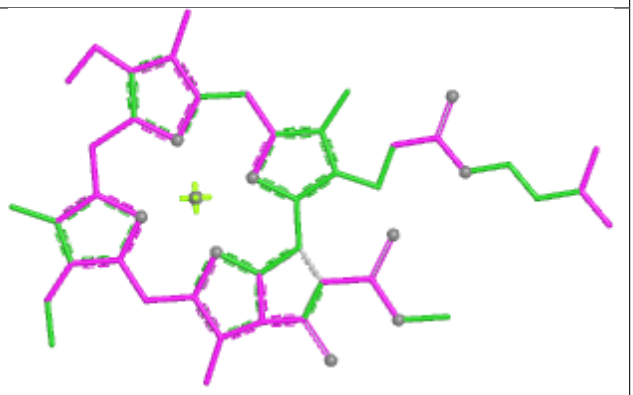


Rings

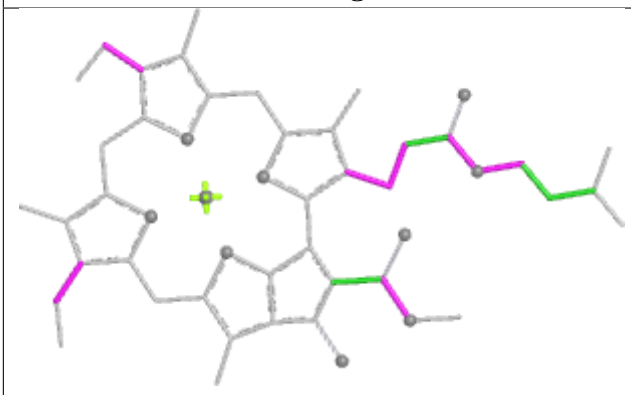
Ligand CLA A 838



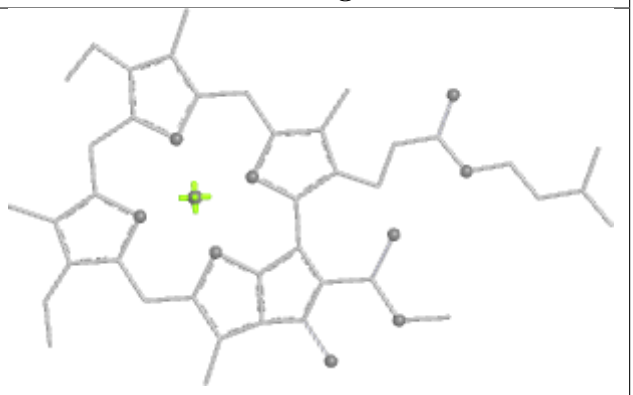
Bond lengths



Bond angles



Torsions

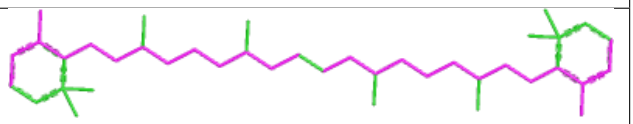


Rings

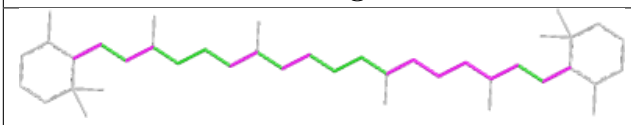
Ligand BCR A 842



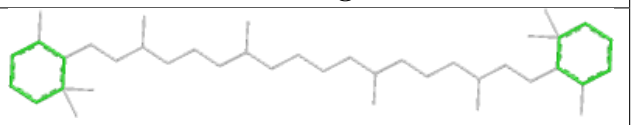
Bond lengths



Bond angles

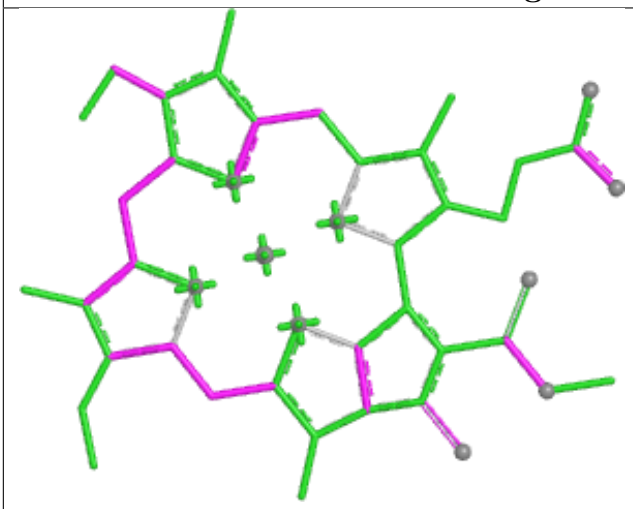


Torsions

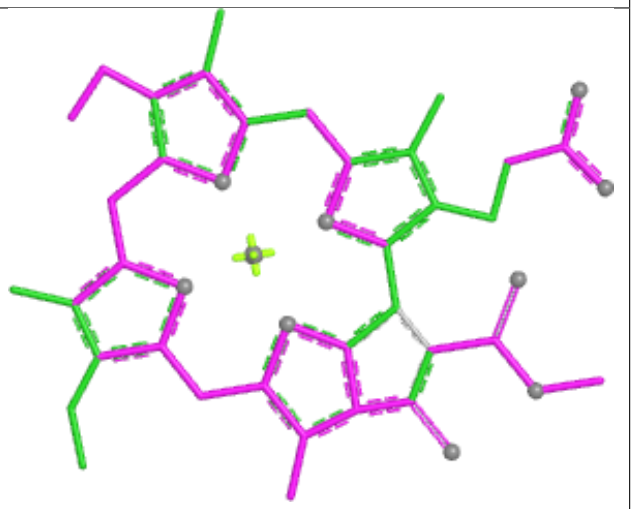


Rings

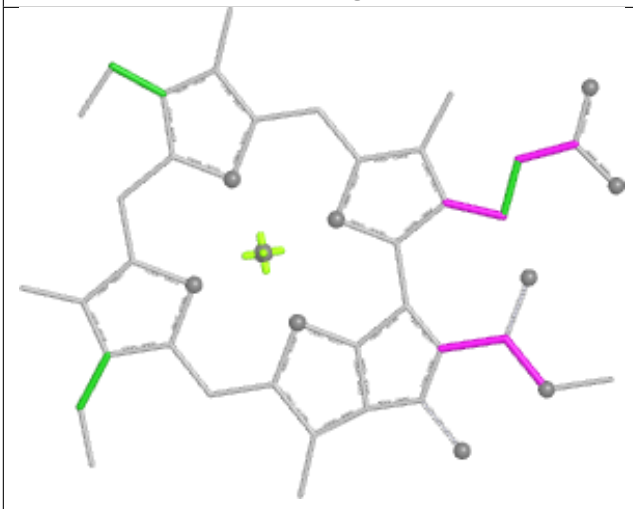
Ligand CLA B 832



Bond lengths



Bond angles

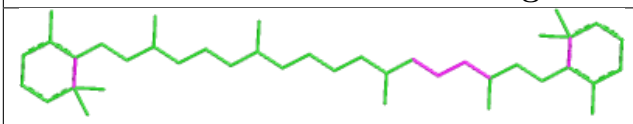


Torsions

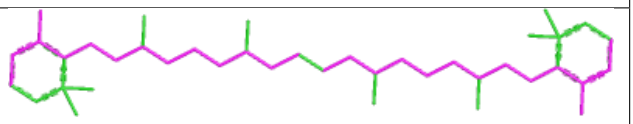


Rings

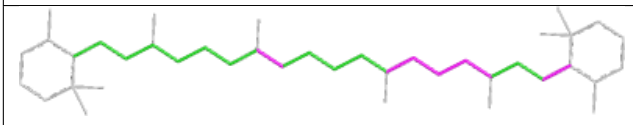
Ligand BCR A 844



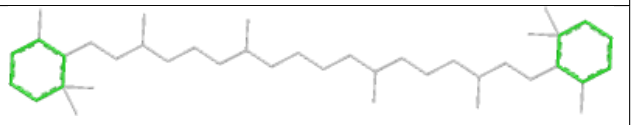
Bond lengths



Bond angles

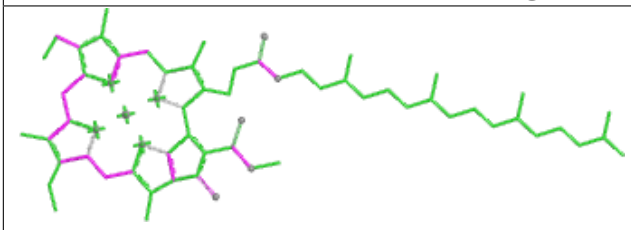


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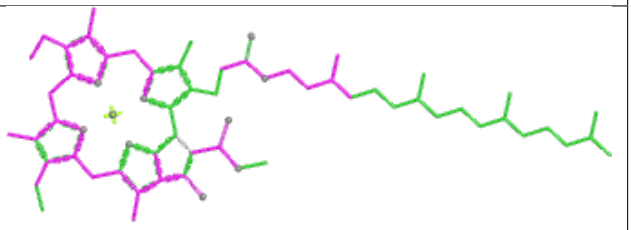


Rings

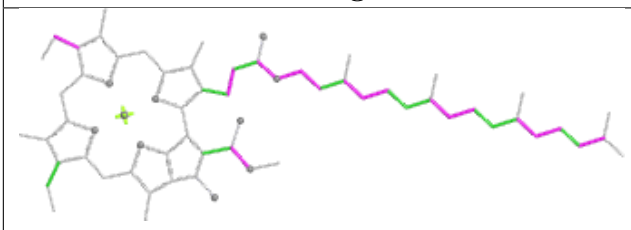
Ligand CLA H 107



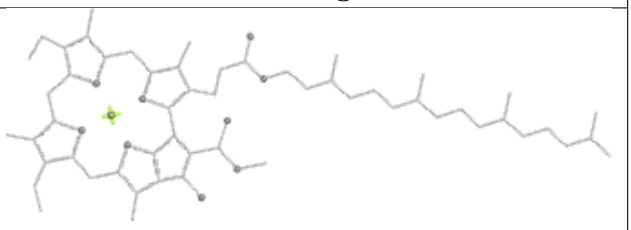
Bond lengths



Bond angles

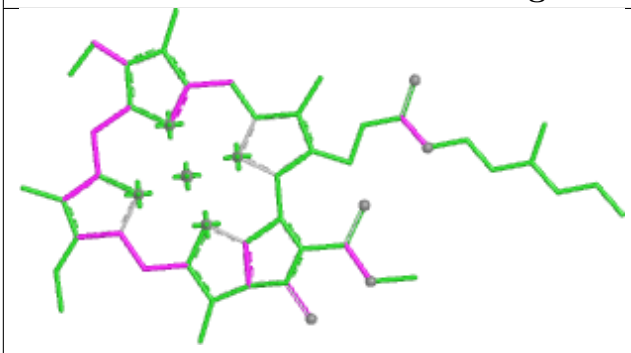


Torsions

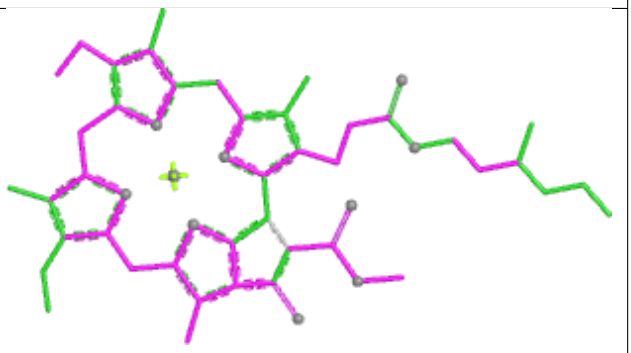


Rings

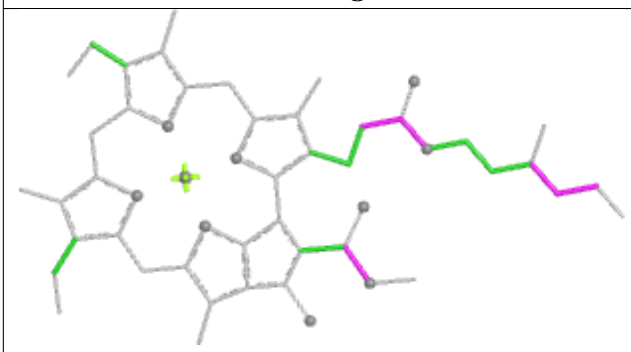
Ligand CLA 4 318



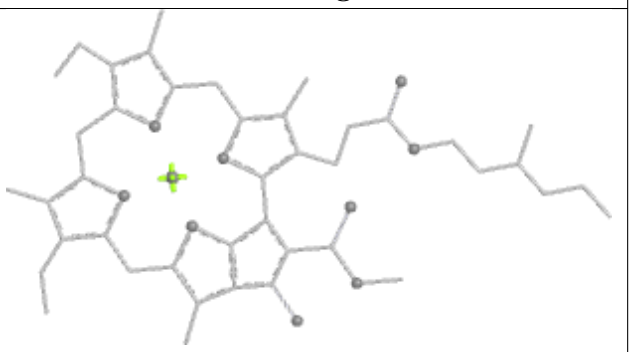
Bond lengths



Bond angles

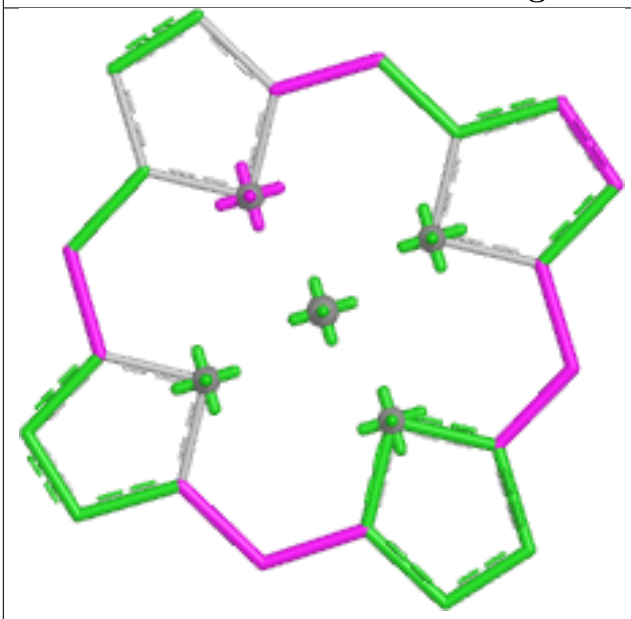


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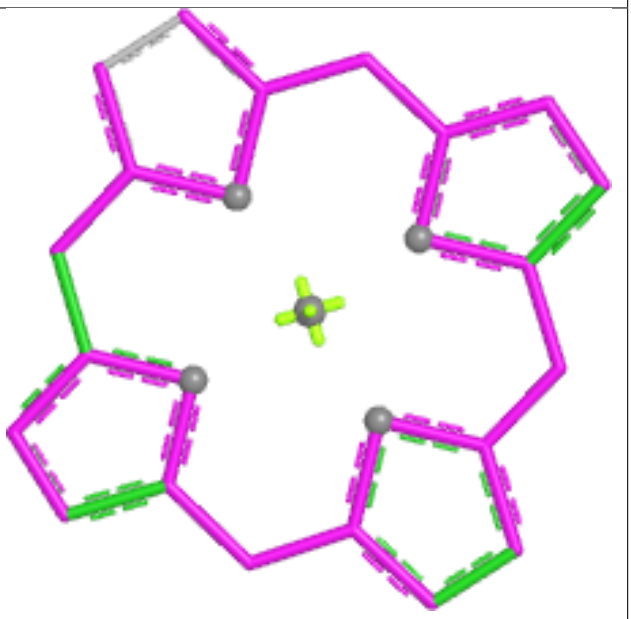


Rings

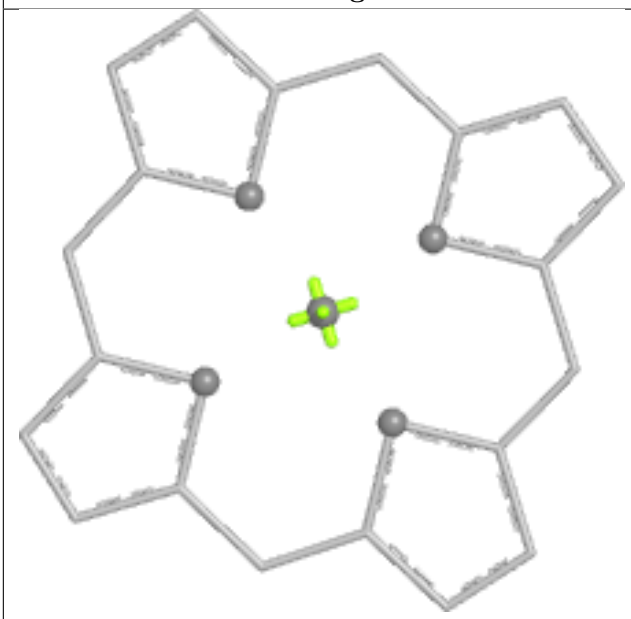
Ligand CLA 4 309



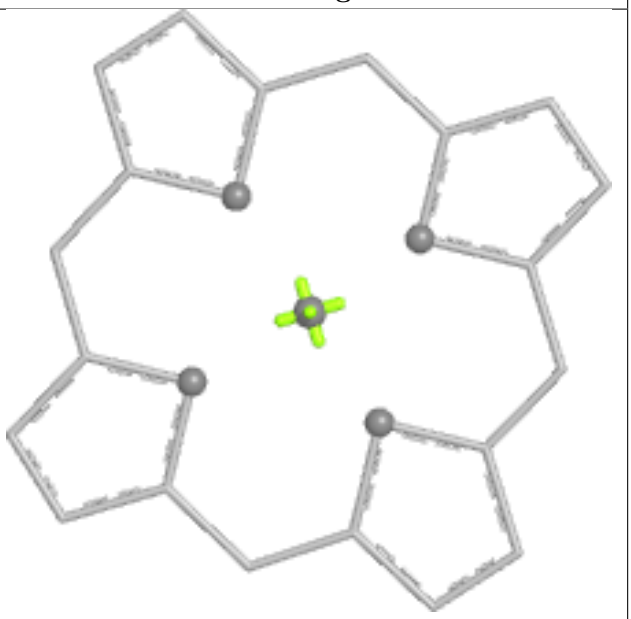
Bond lengths



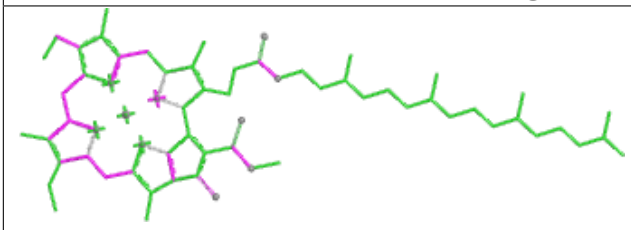
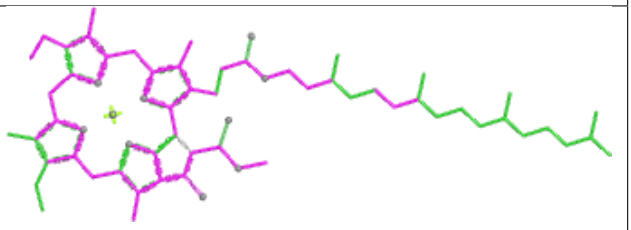
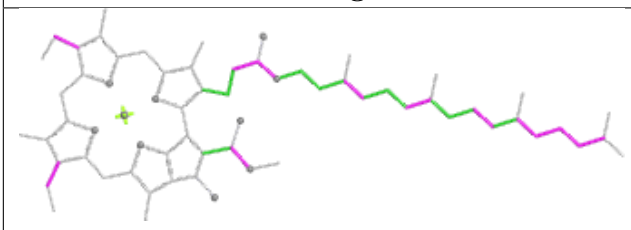
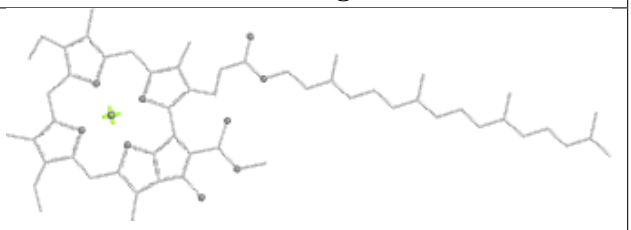
Bond angles



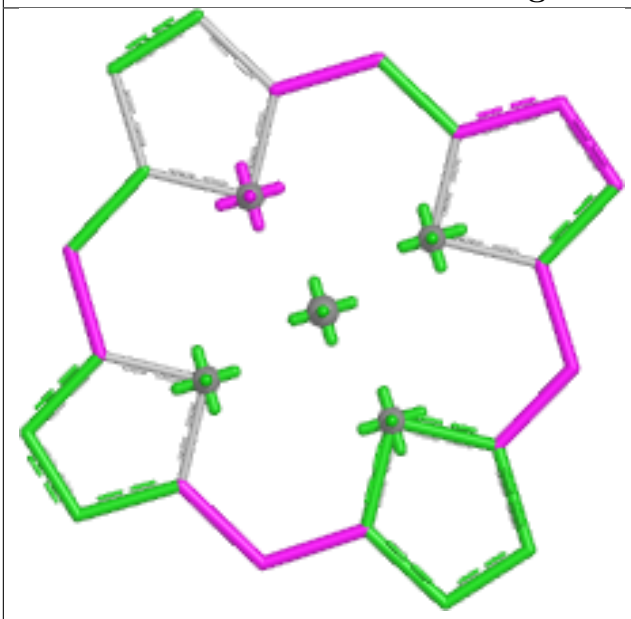
Torsions



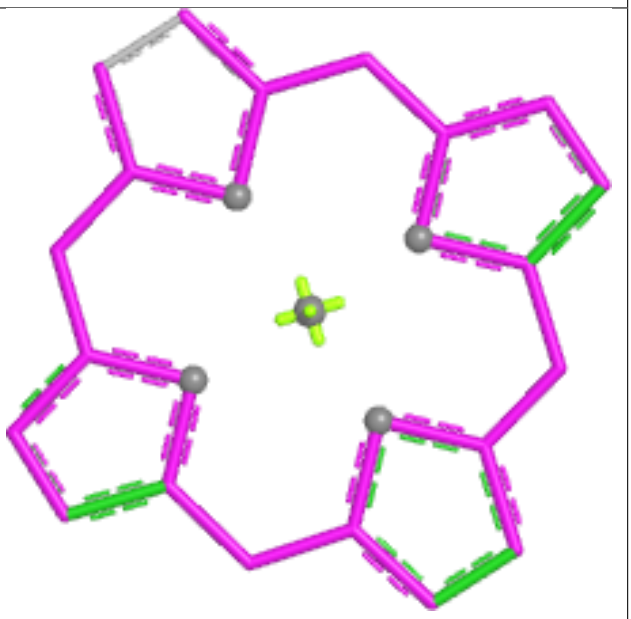
Rings

Ligand CLA B 849	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

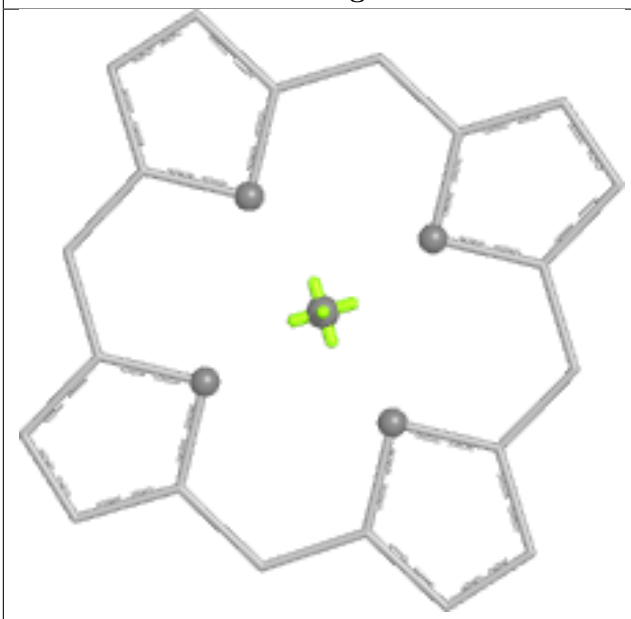
Ligand CLA 3 313



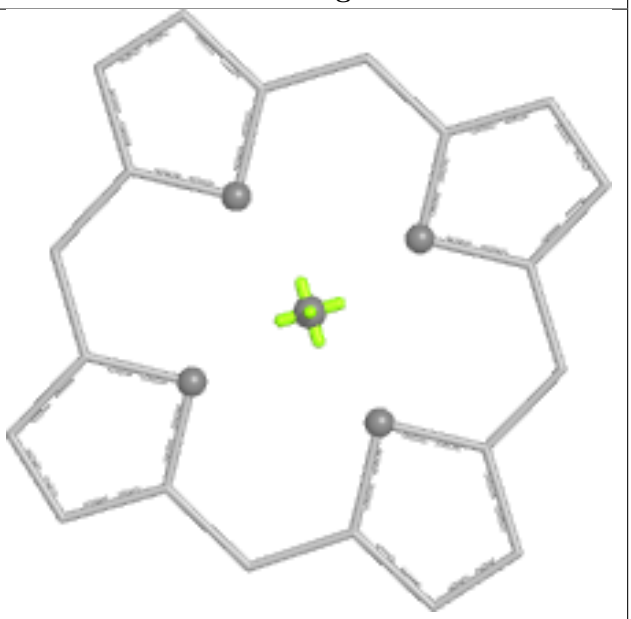
Bond lengths



Bond angles

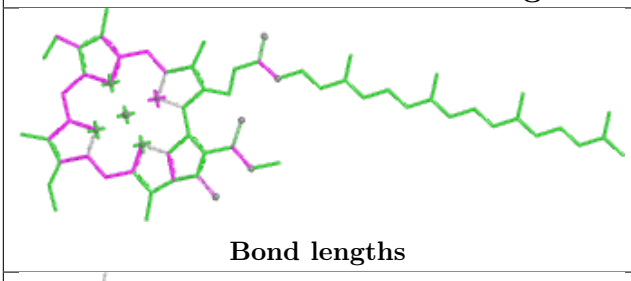


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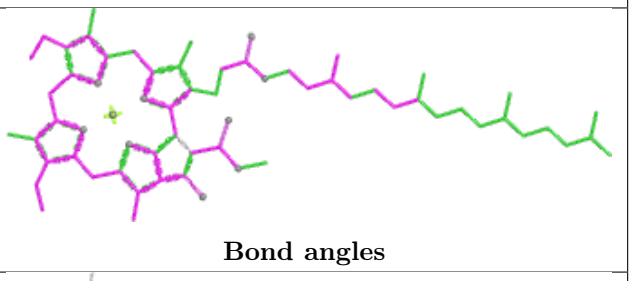


Rings

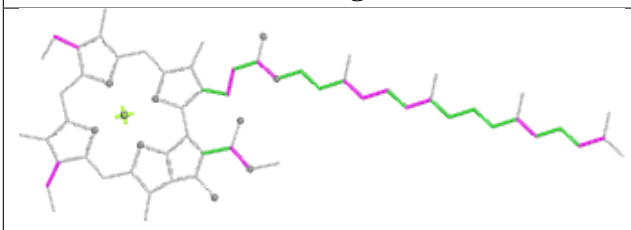
Ligand CLA A 814



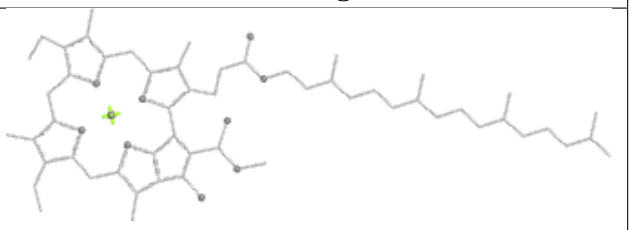
Bond lengths



Bond angles

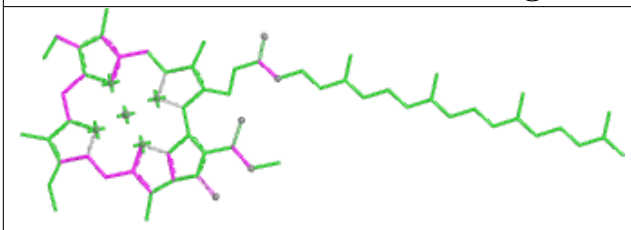


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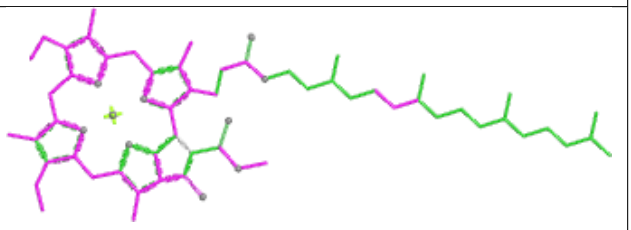


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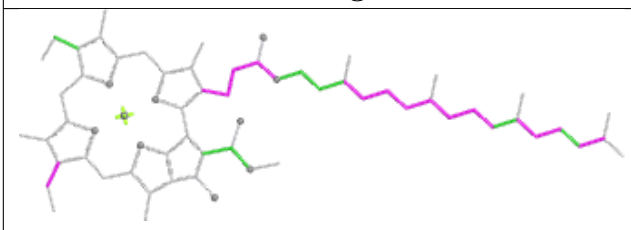
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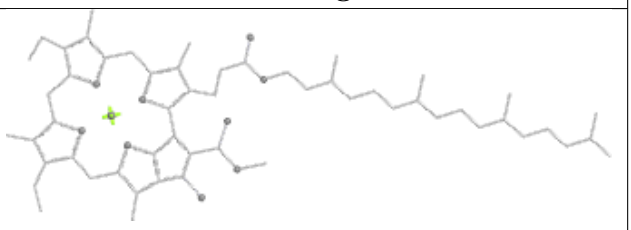
Bond lengths



Bond angles

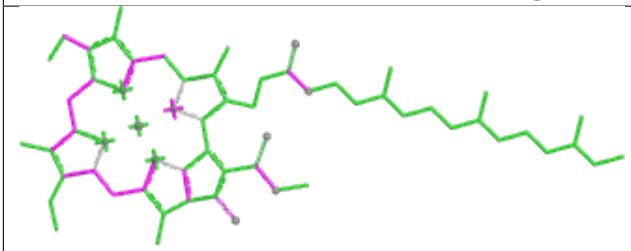


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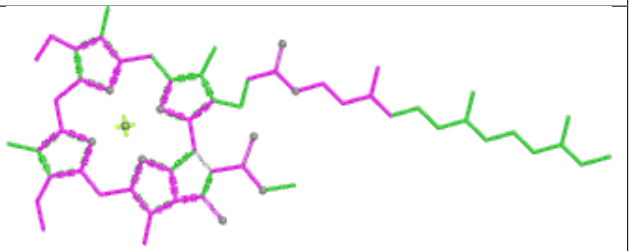


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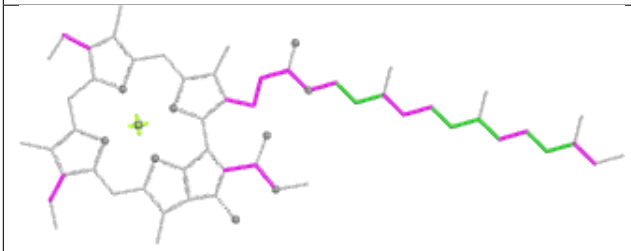
Ligand CLA 1 206



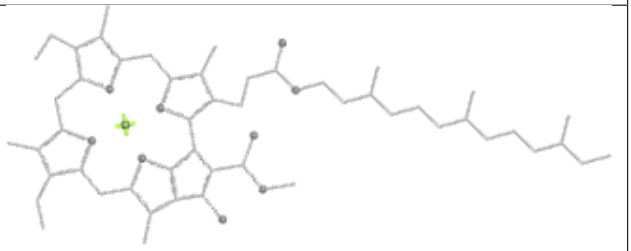
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Bond angles

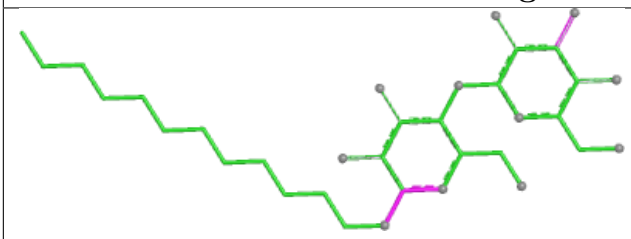


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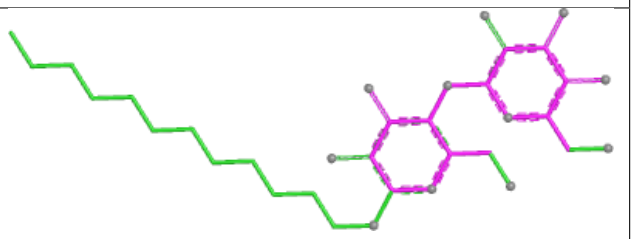


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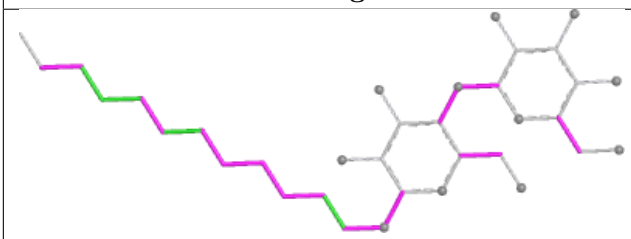
Ligand LMU H 102



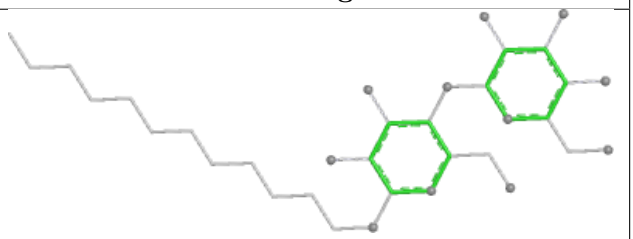
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Bond angles

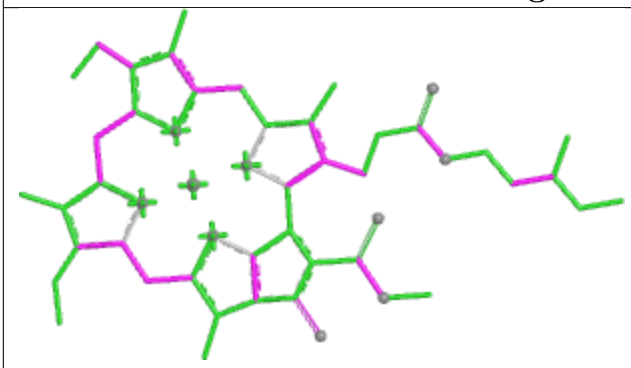


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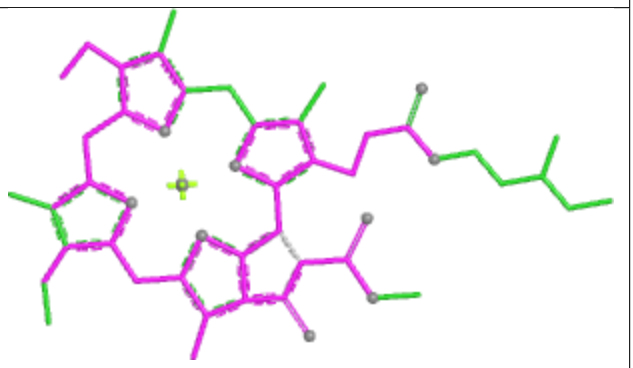


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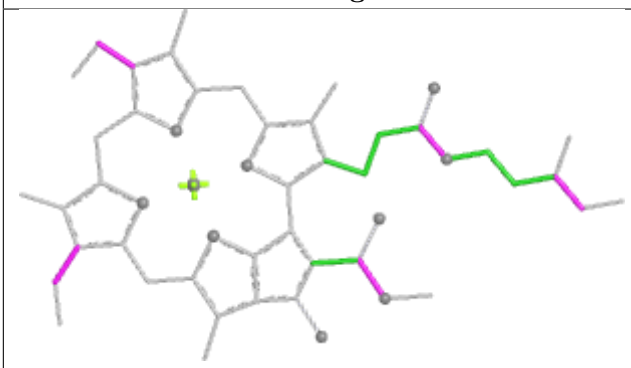
Ligand CLA 1 207



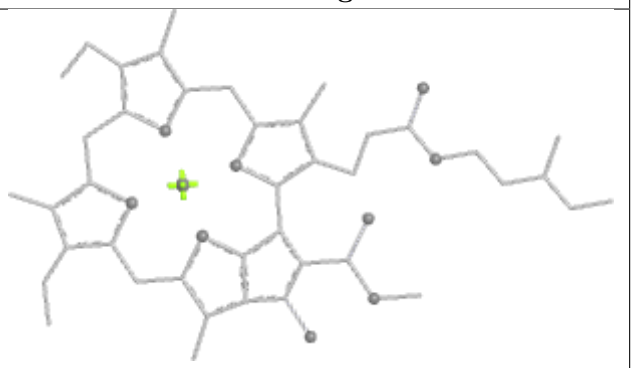
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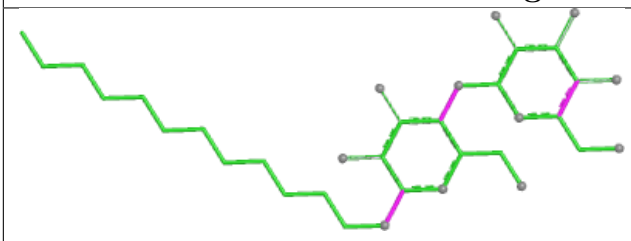


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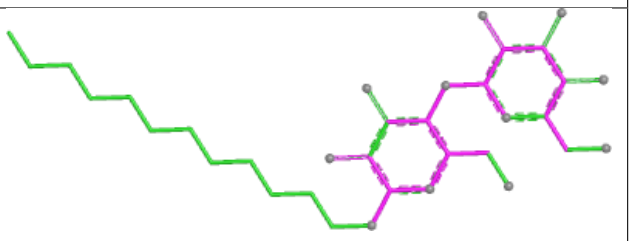


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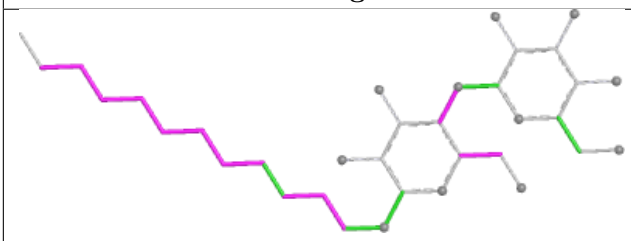
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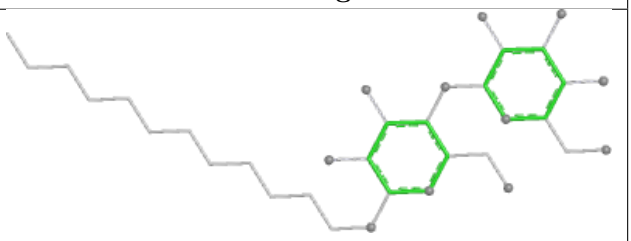
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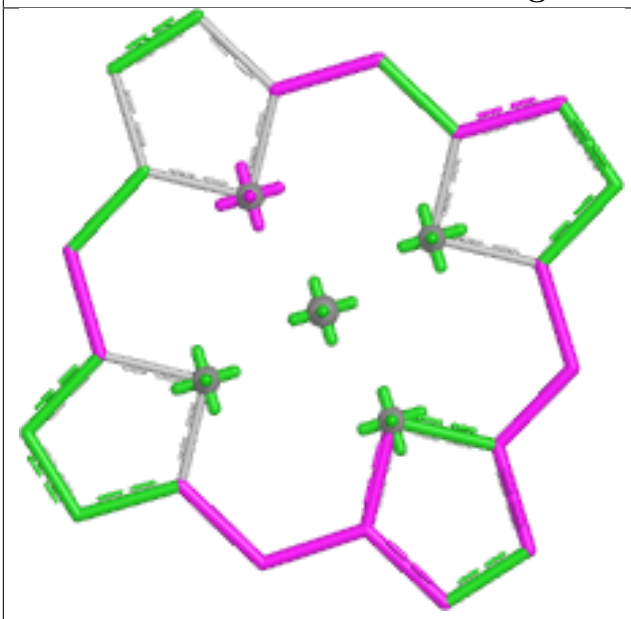


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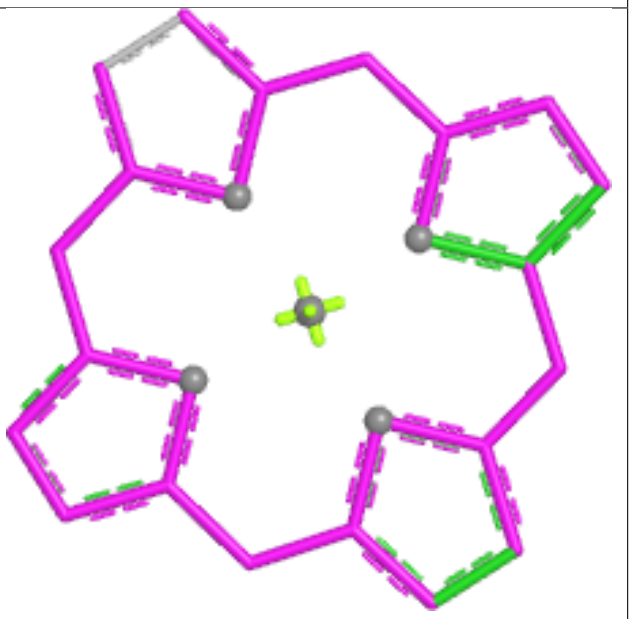


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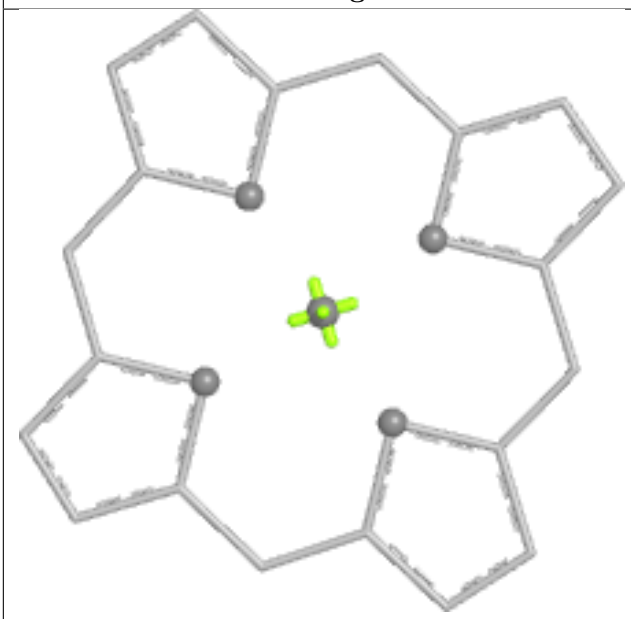
Ligand CLA 3 304



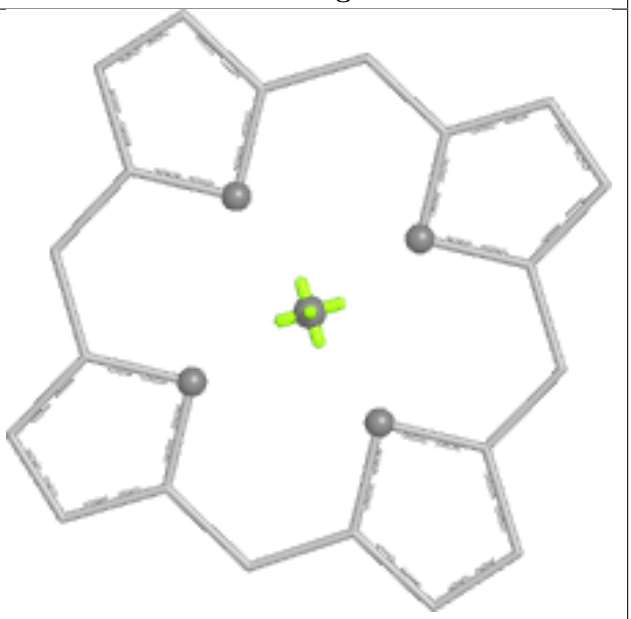
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Bond angles

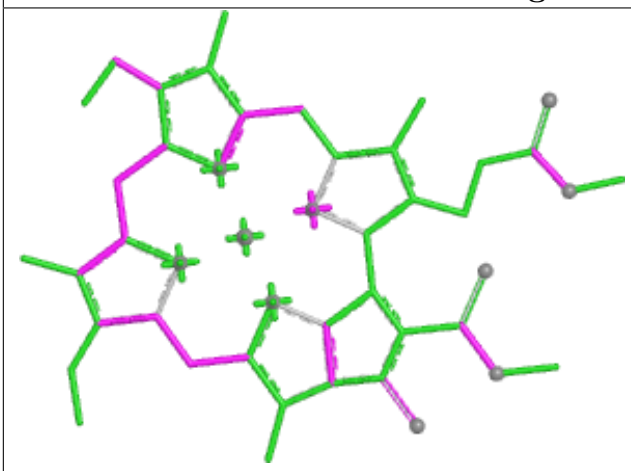


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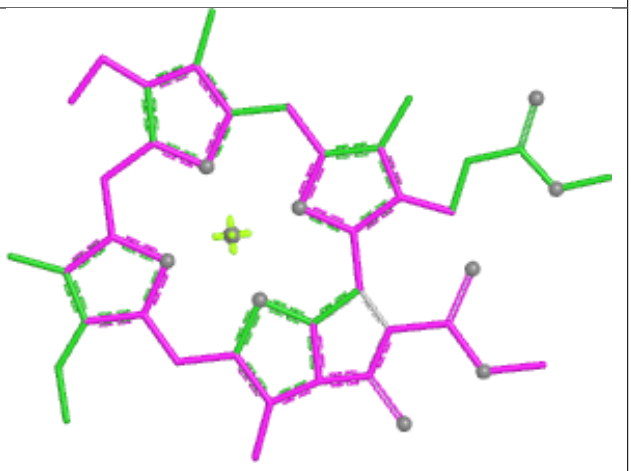


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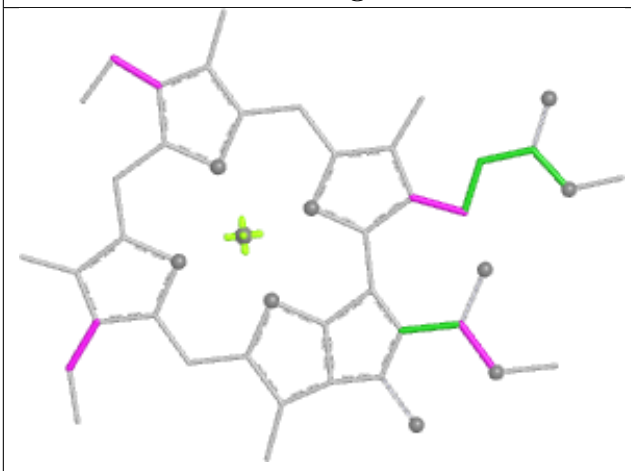
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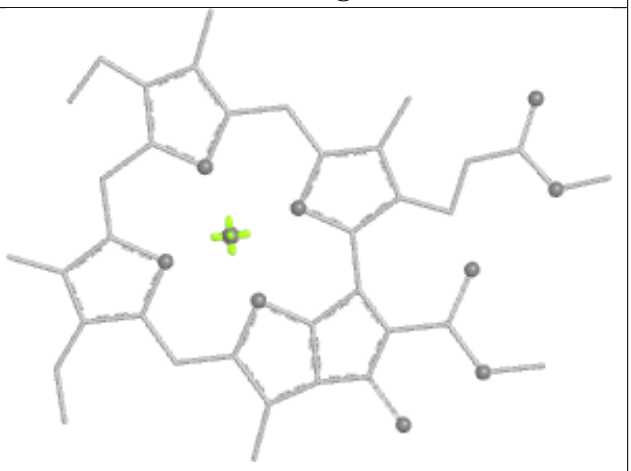
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Bond angles

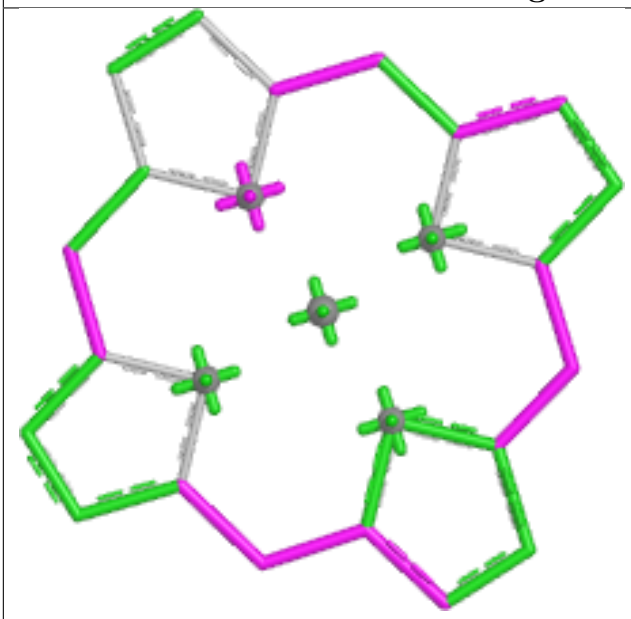


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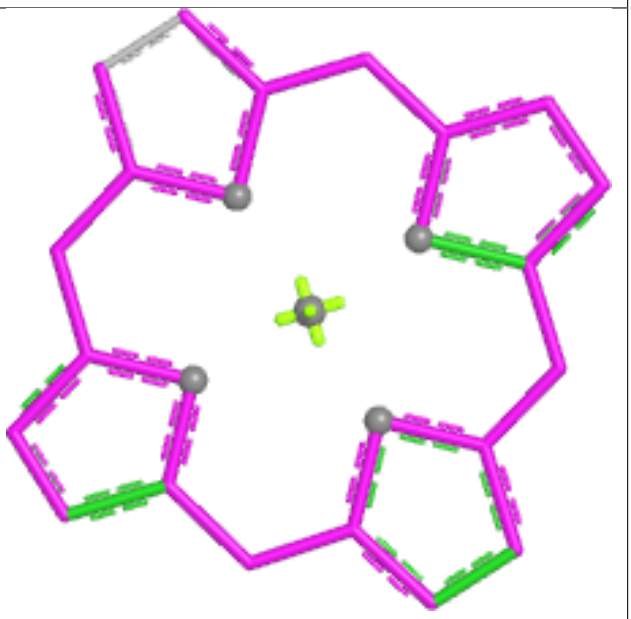


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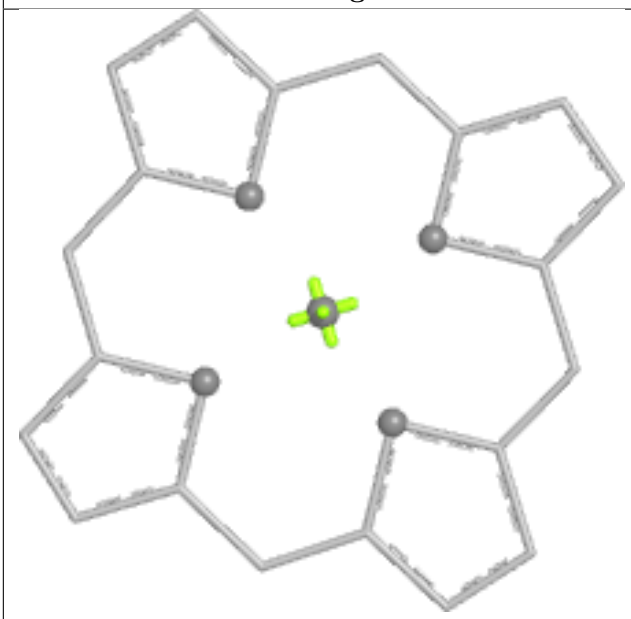
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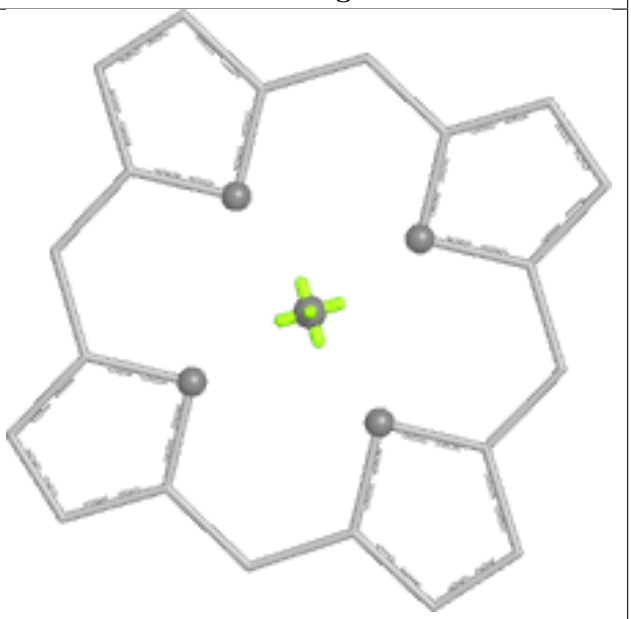
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Bond angles

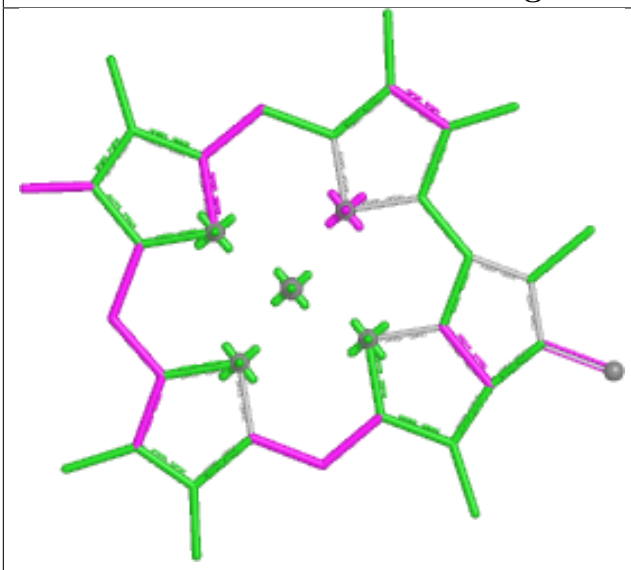


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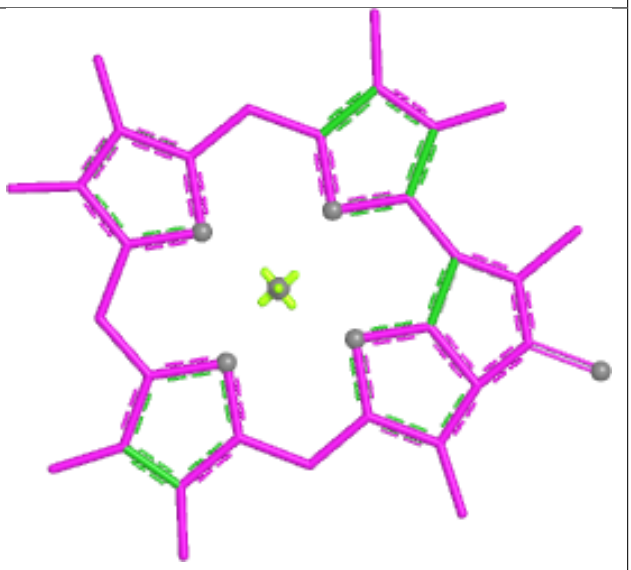


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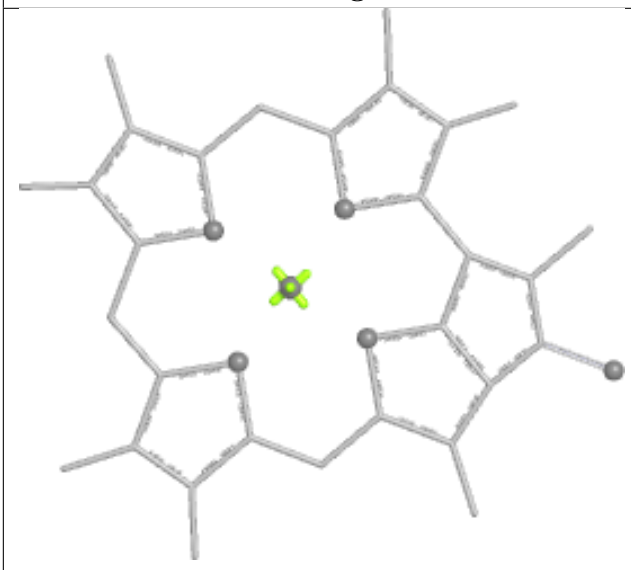
Ligand CLA B 839



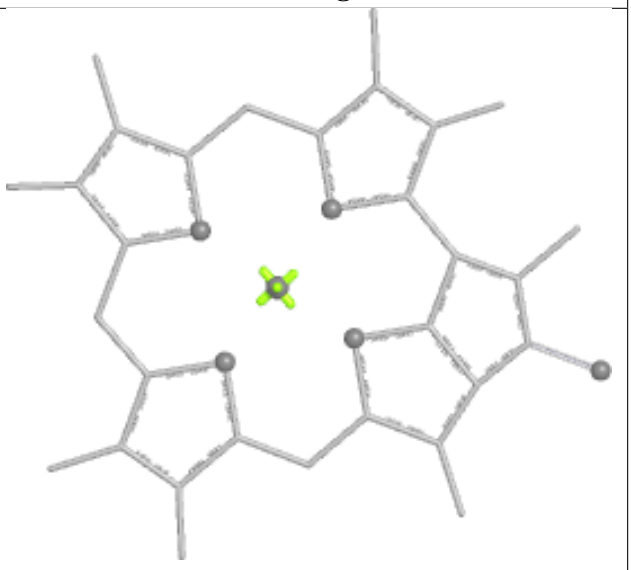
Bond lengths



Bond angles

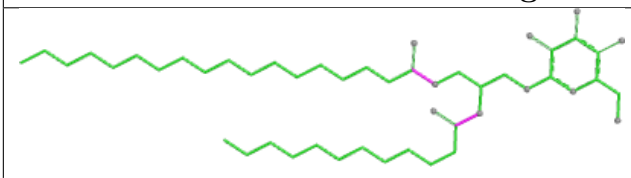


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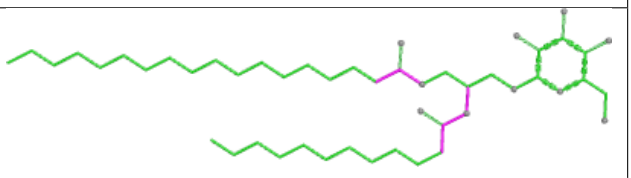


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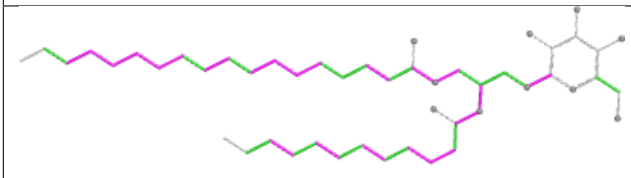
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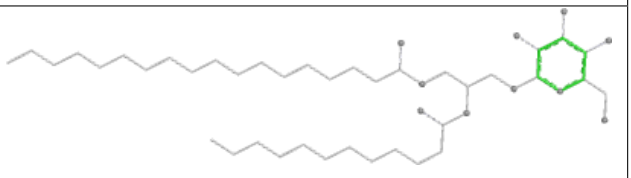
Bond lengths



Bond angles

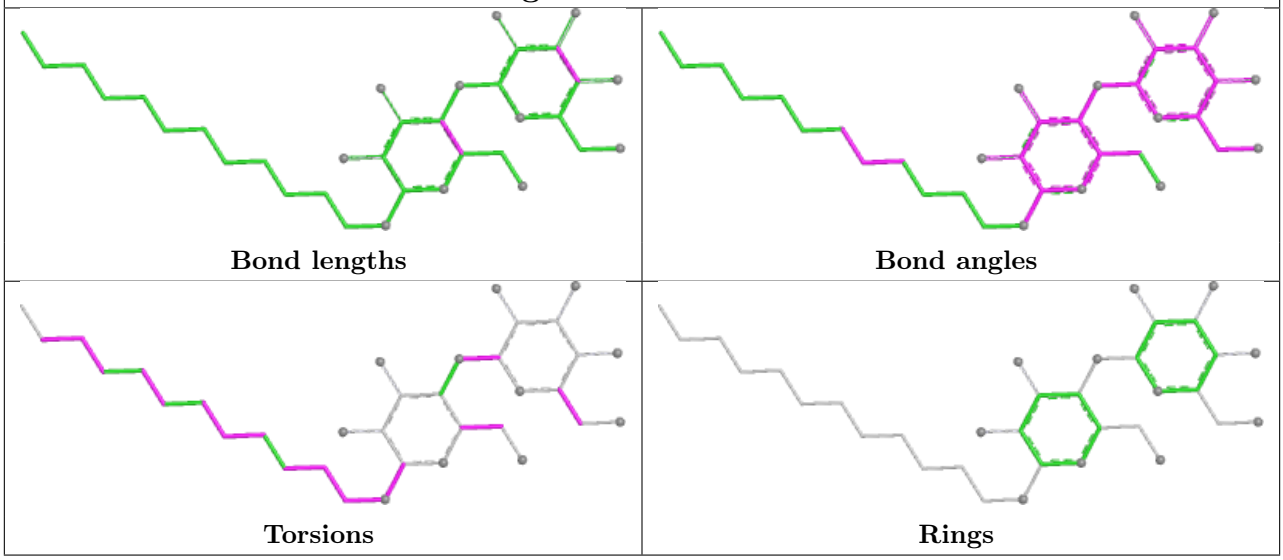


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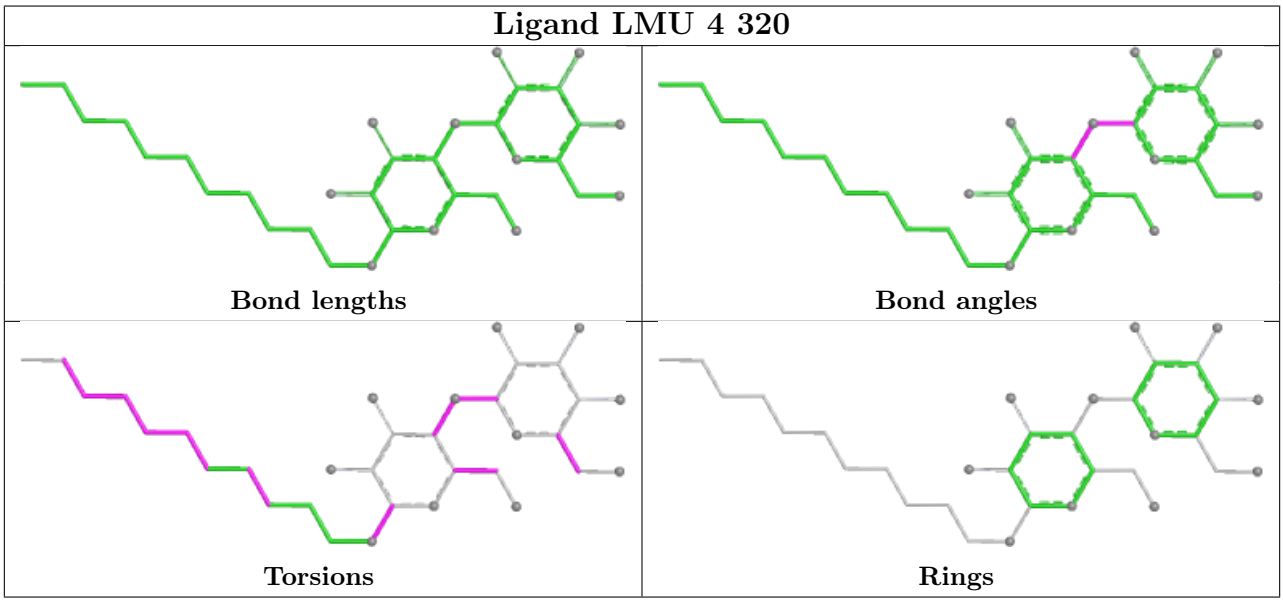


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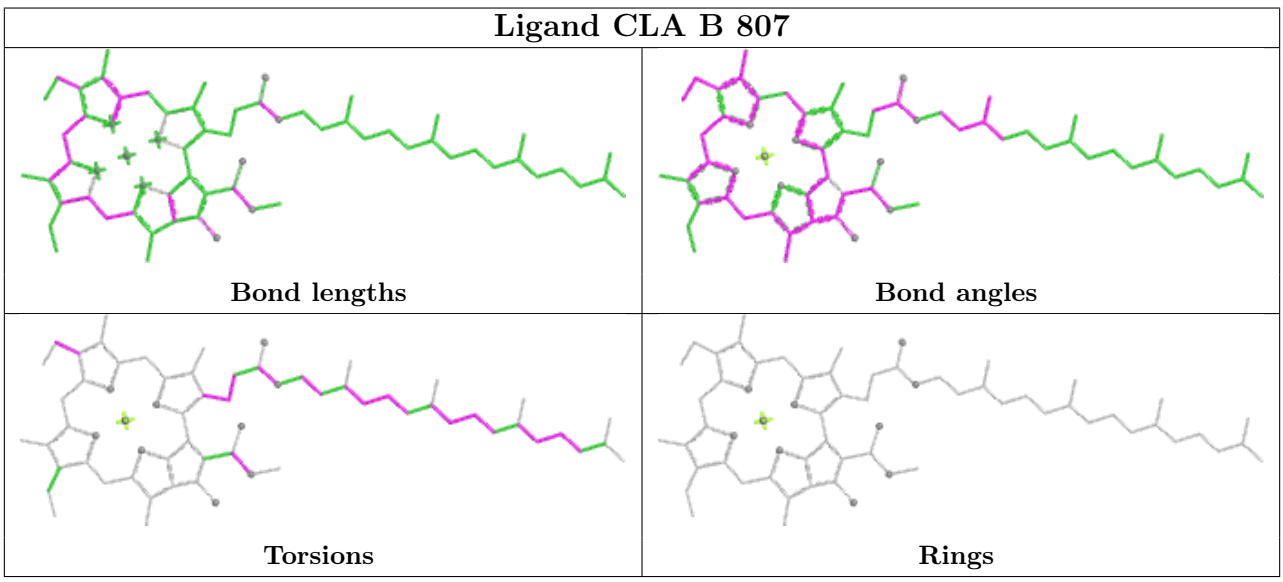
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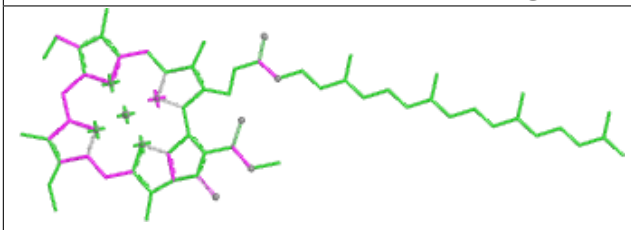
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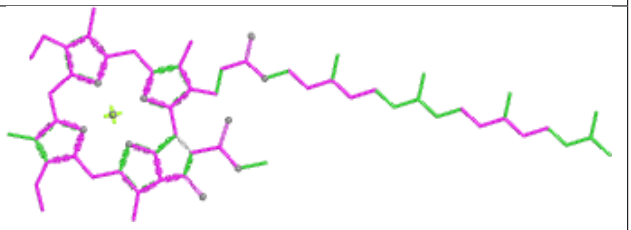
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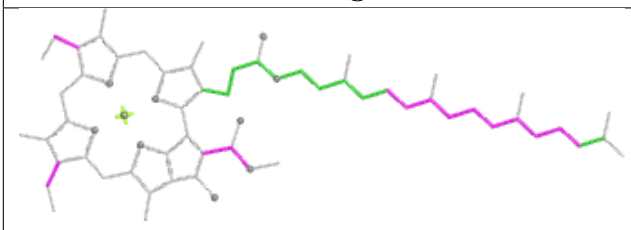
Ligand CLA B 805



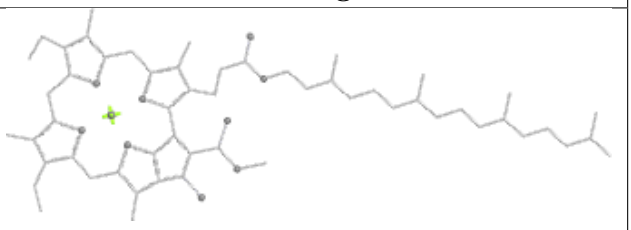
Bond lengths



Bond angles

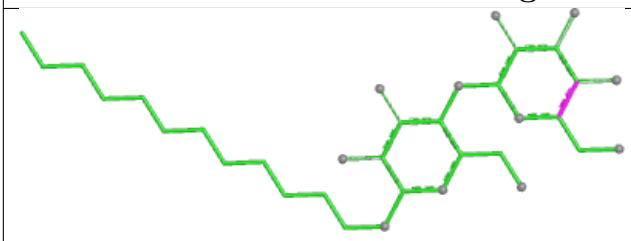


Torsions

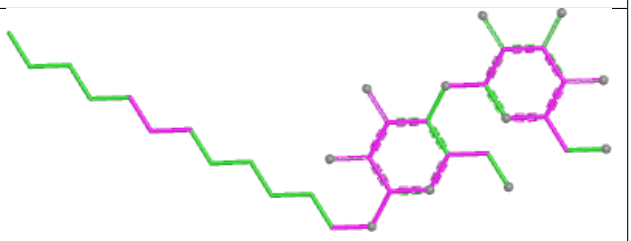


Rings

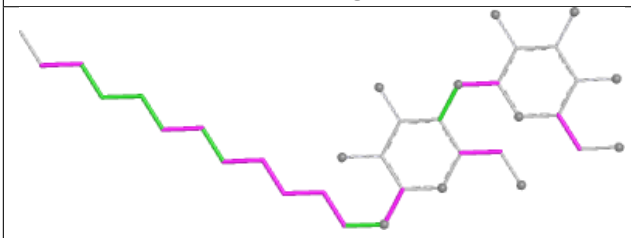
Ligand LMU A 853



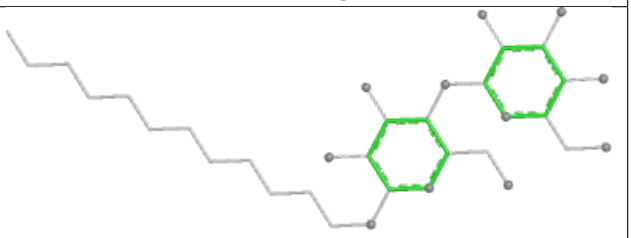
Bond lengths



Bond angles

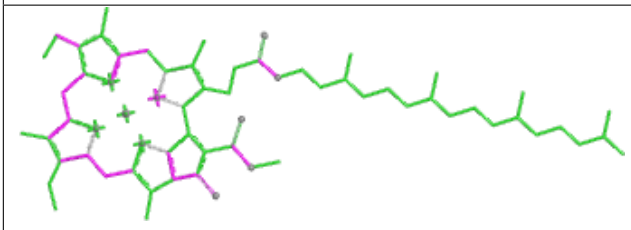


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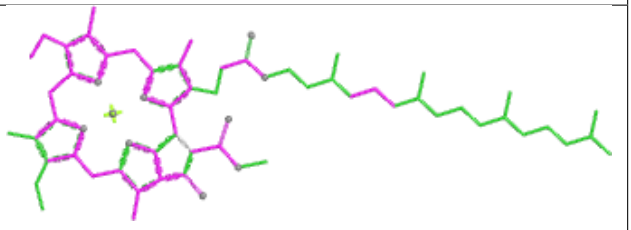


Rings

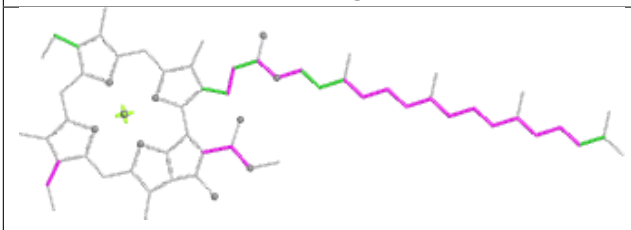
Ligand CLA B 826



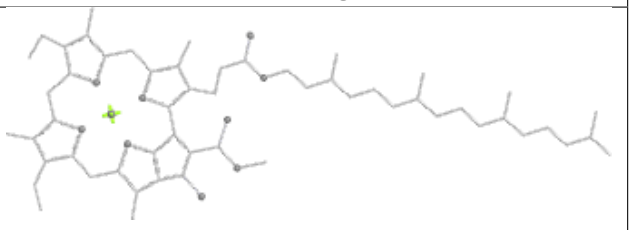
Bond lengths



Bond angles

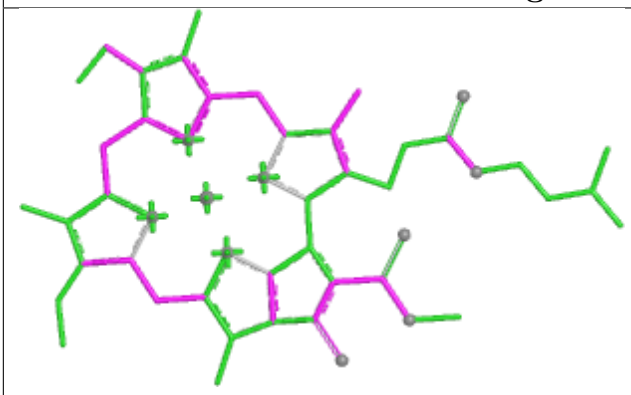


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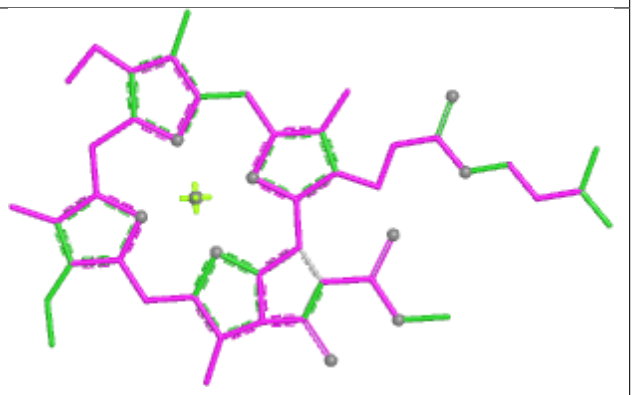


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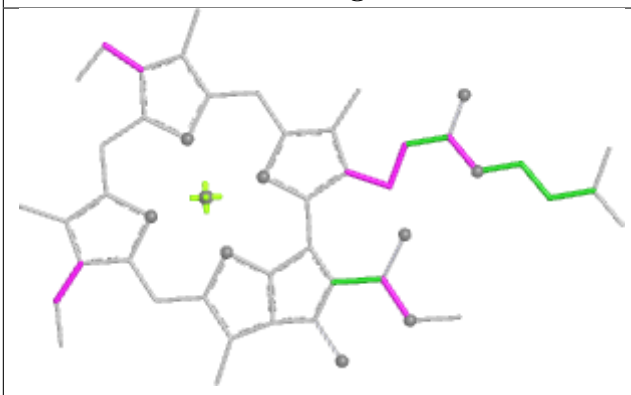
Ligand CLA L 208



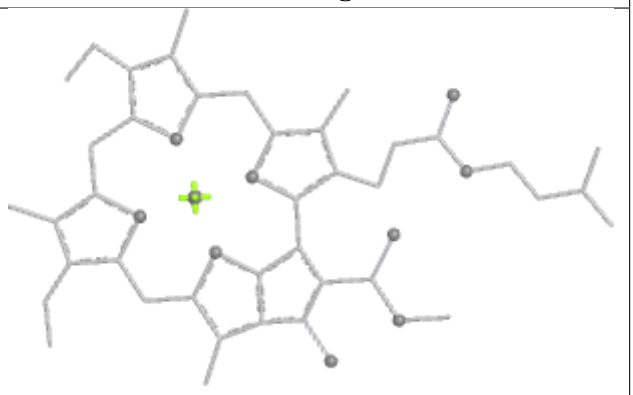
Bond lengths



Bond angles

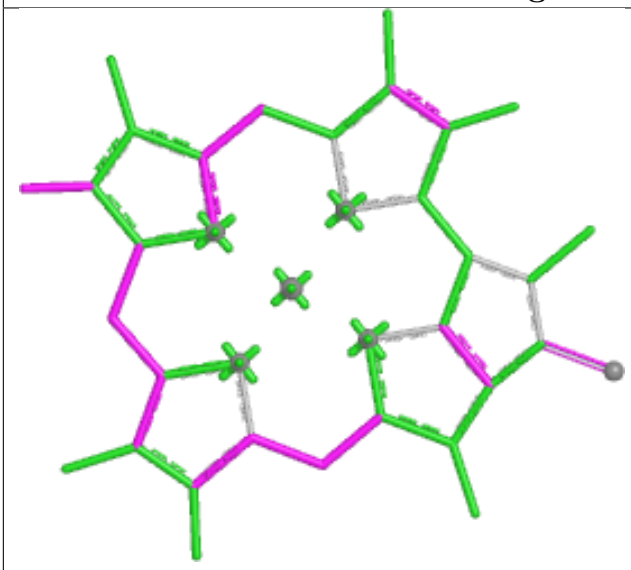


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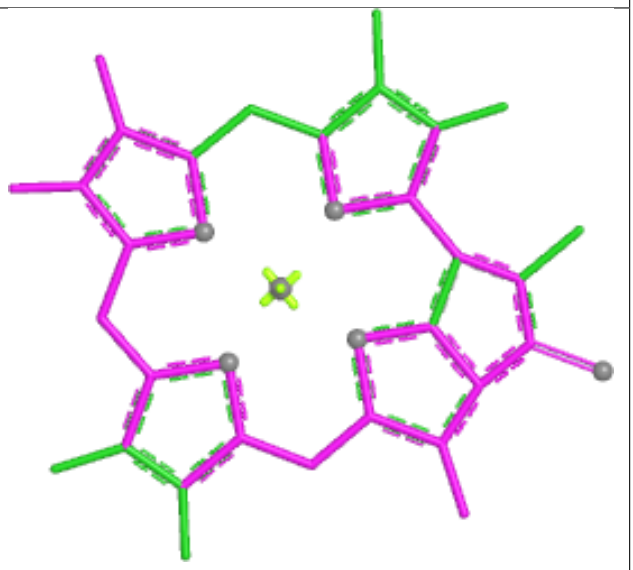


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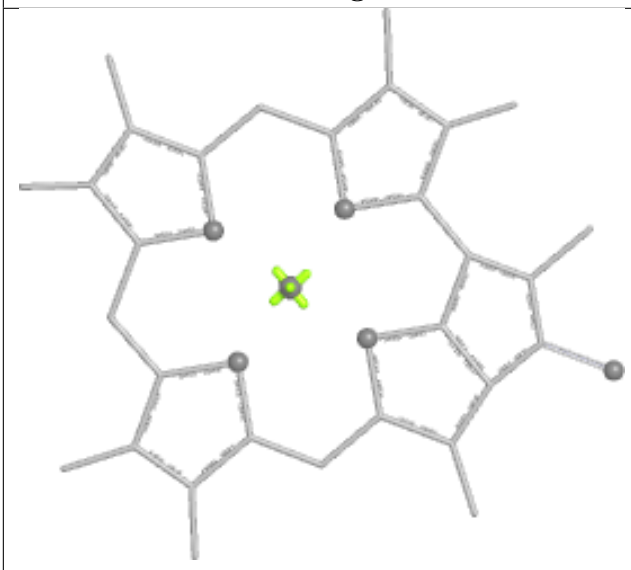
Ligand CLA 1 210



Bond lengths



Bond angles

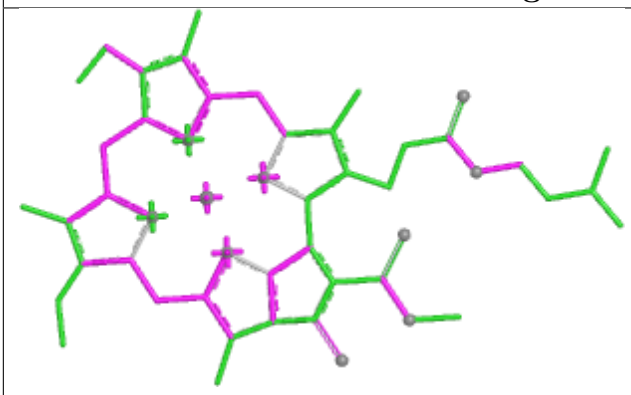


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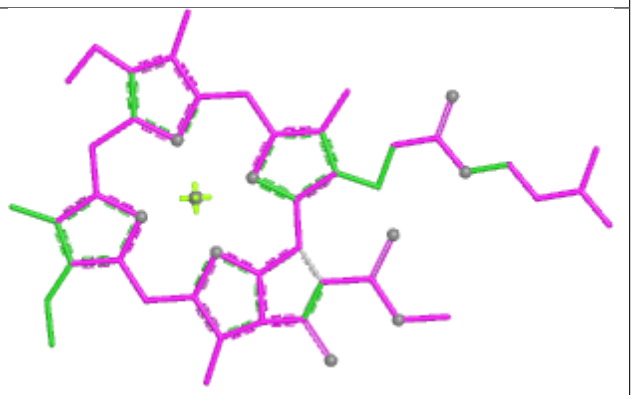


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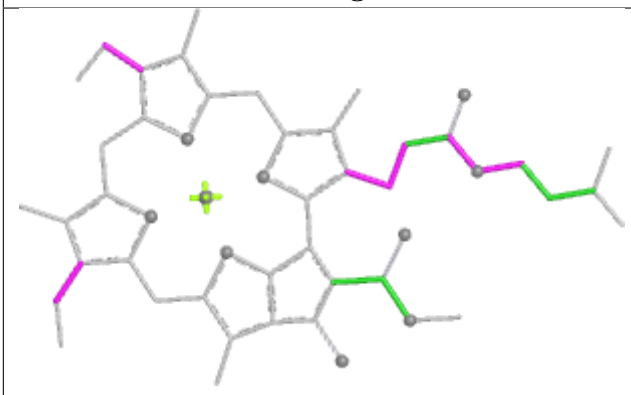
Ligand CLA K 106



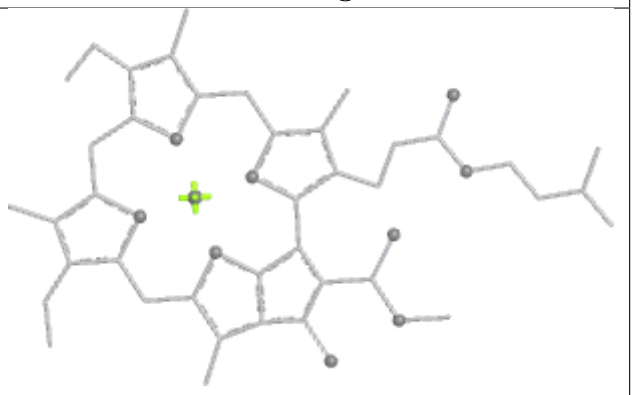
Bond lengths



Bond angles

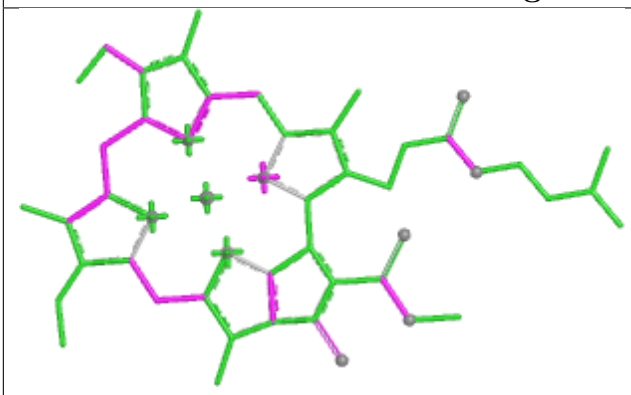


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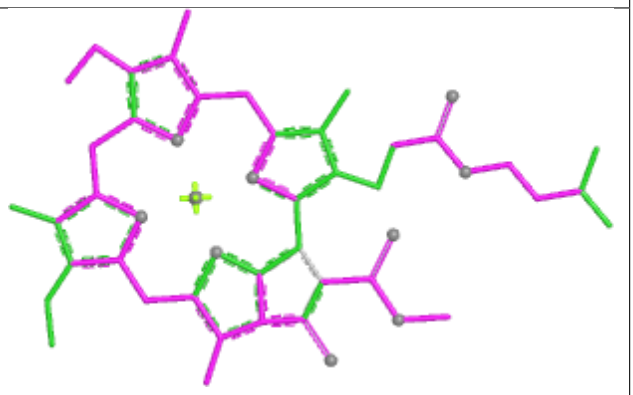


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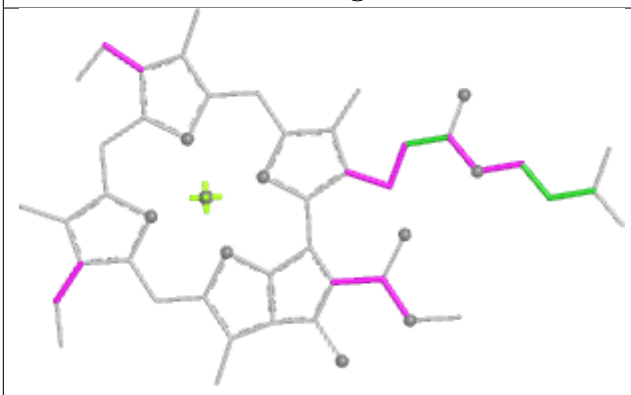
Ligand CLA A 830



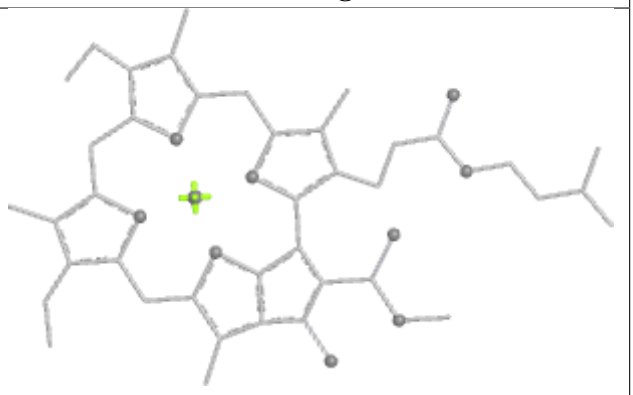
Bond lengths



Bond angles

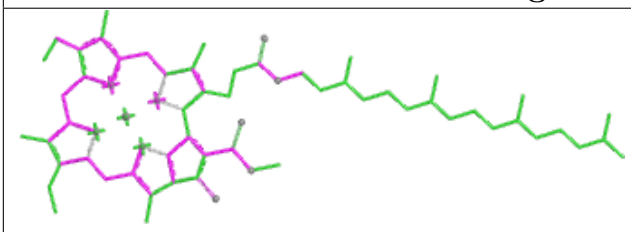


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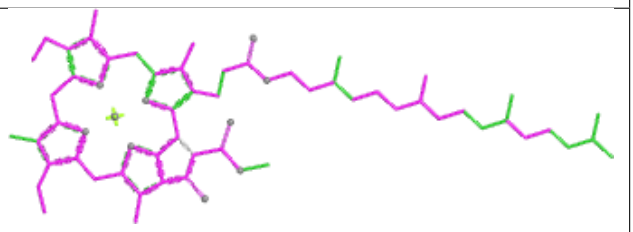


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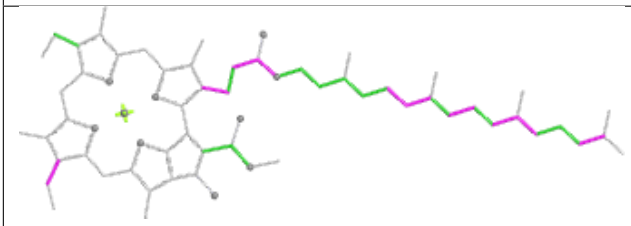
Ligand CLA 4 304



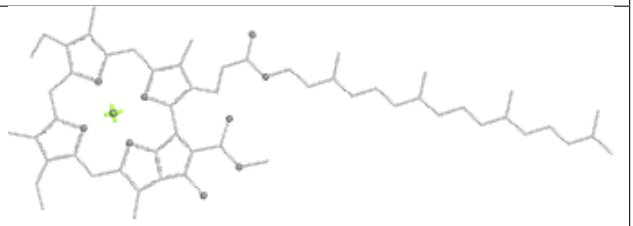
Bond lengths



Bond angles

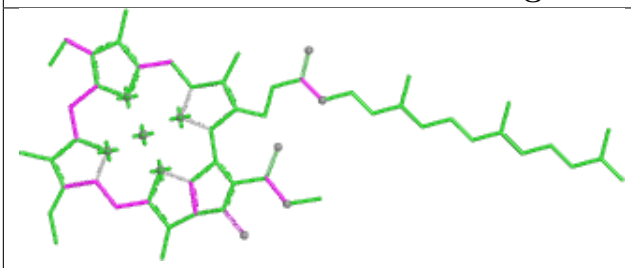


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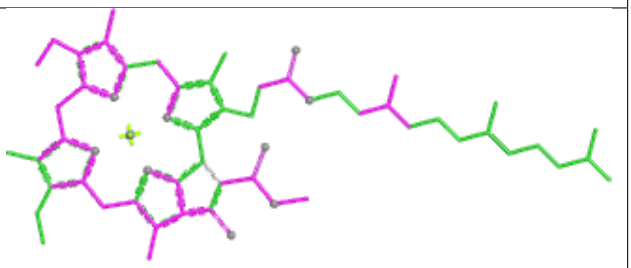


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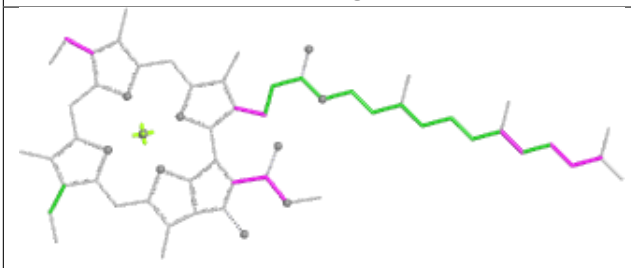
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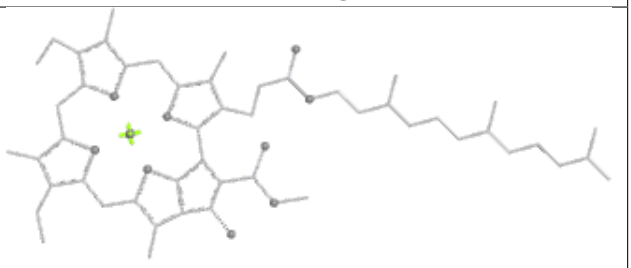
Bond lengths



Bond angles

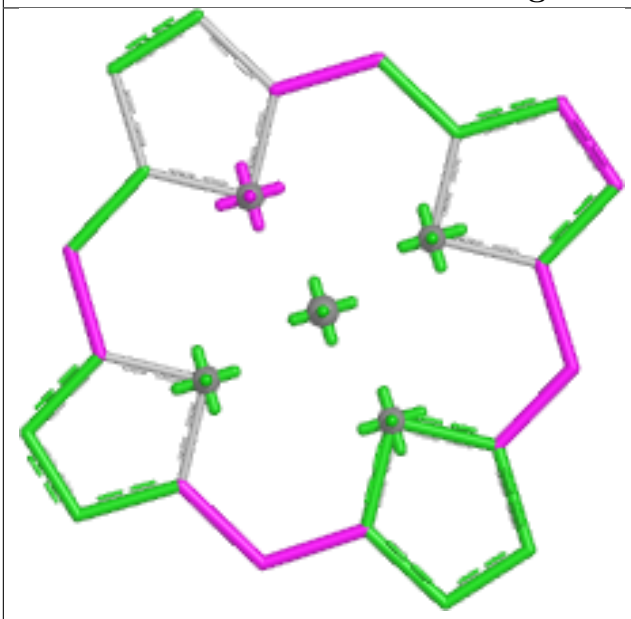


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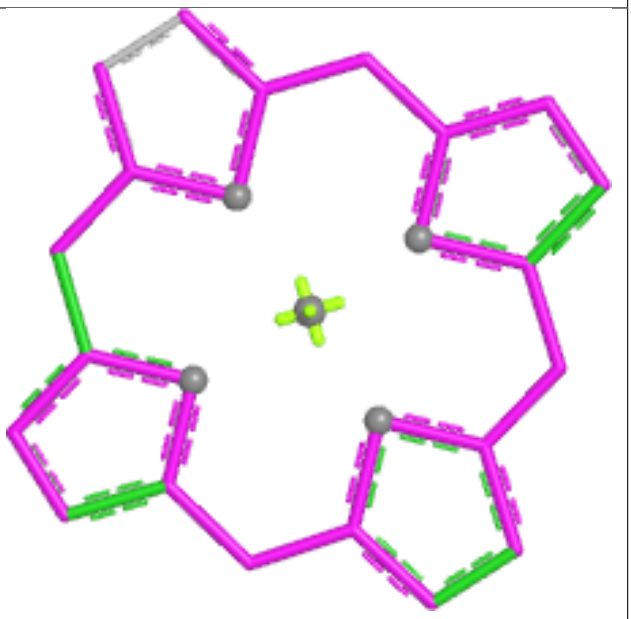


Rings

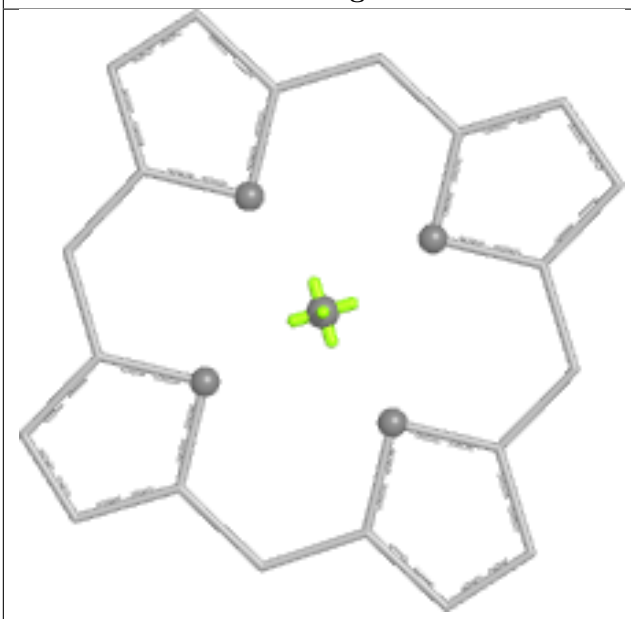
Ligand CLA 4 308



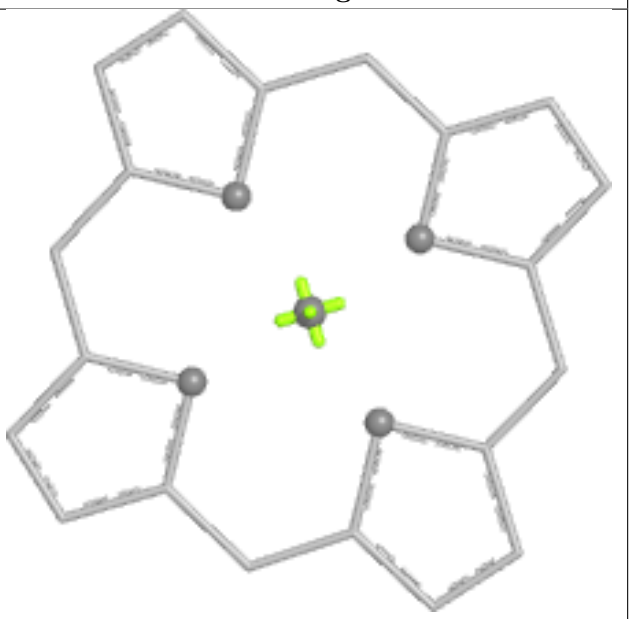
Bond lengths



Bond angles

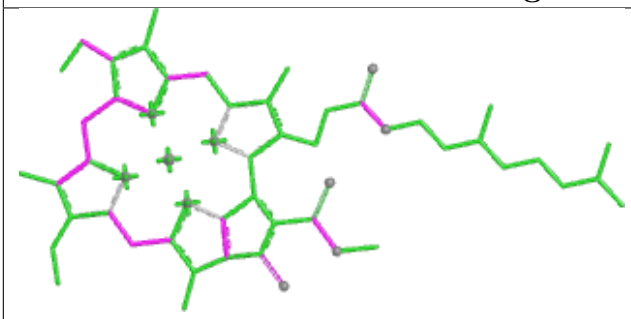


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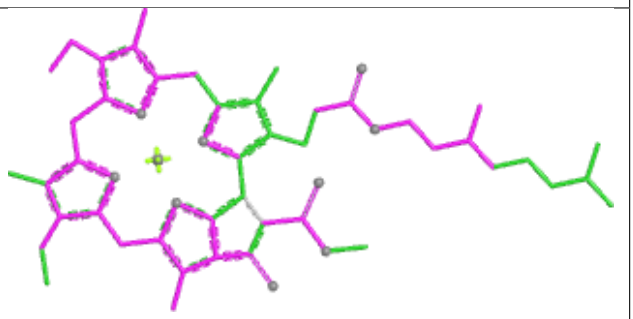


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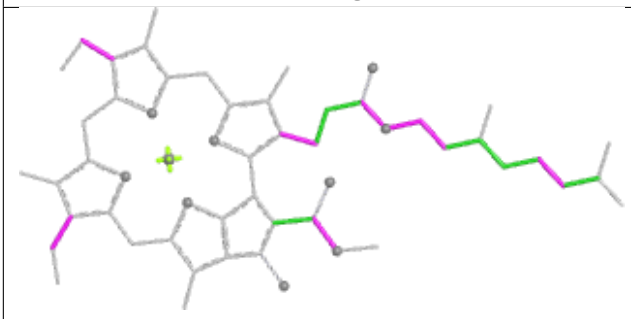
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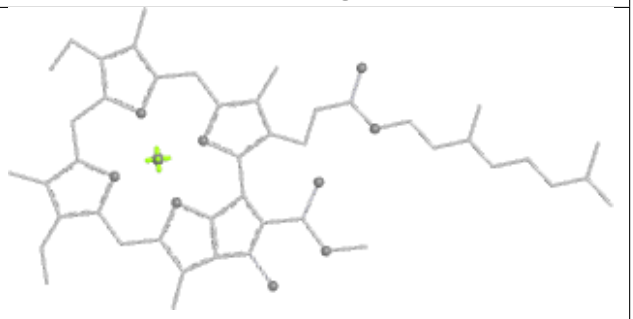
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Bond angles

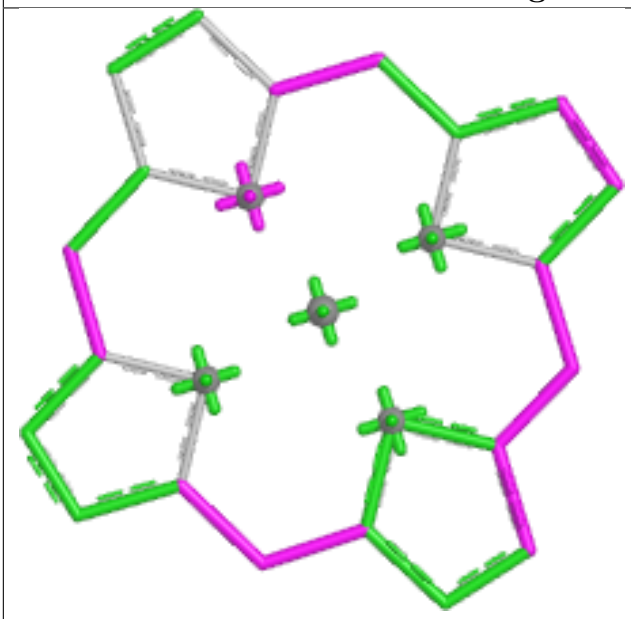


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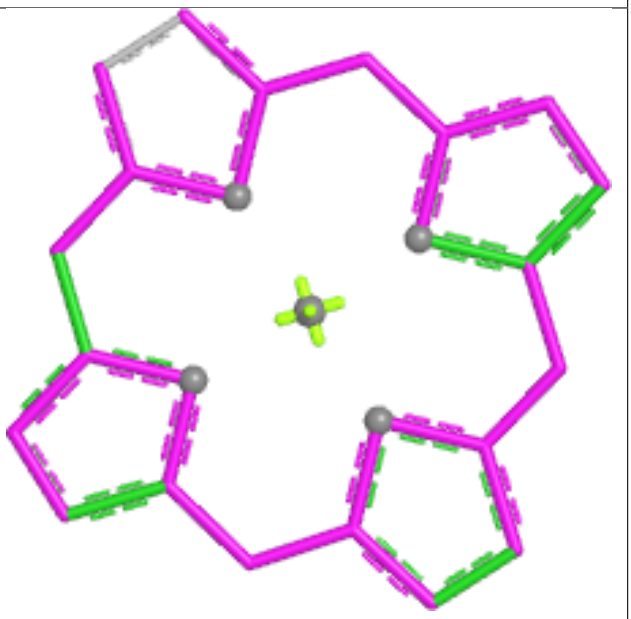


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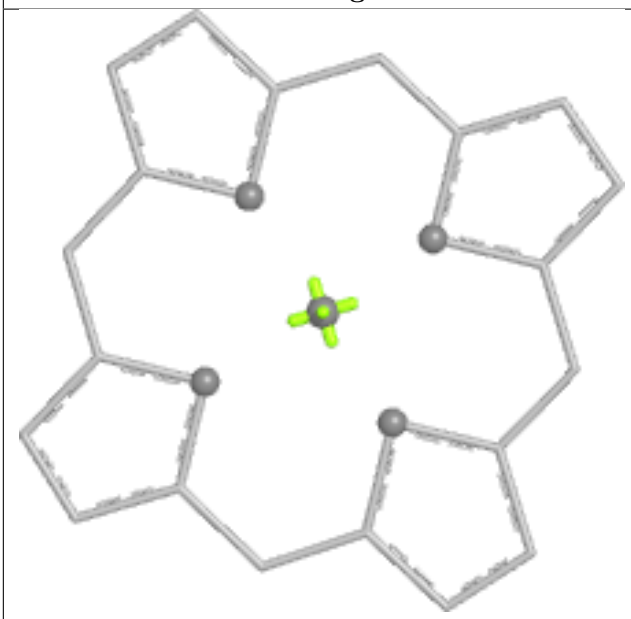
Ligand CLA 3 305



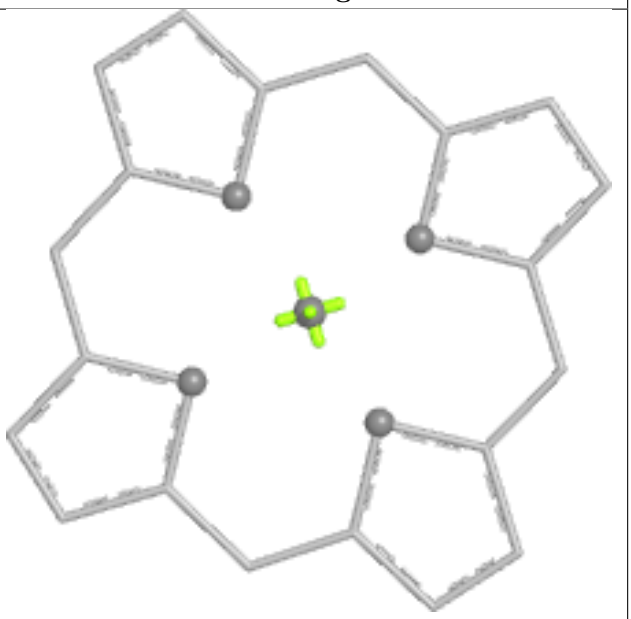
Bond lengths



Bond angles

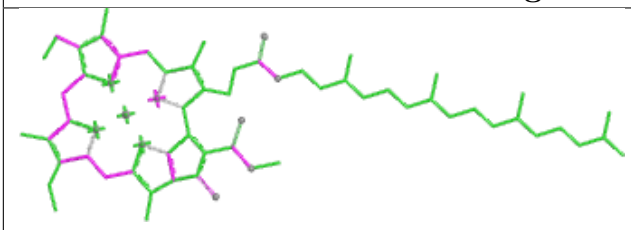


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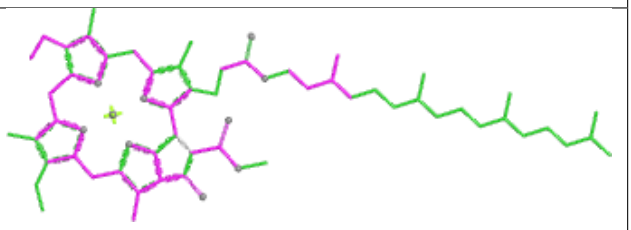


Rings

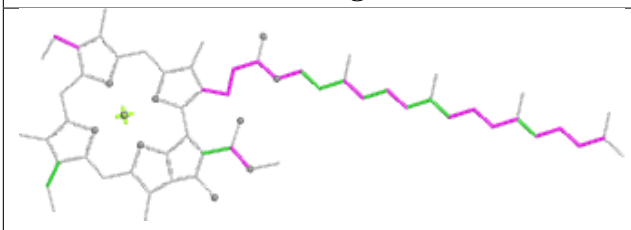
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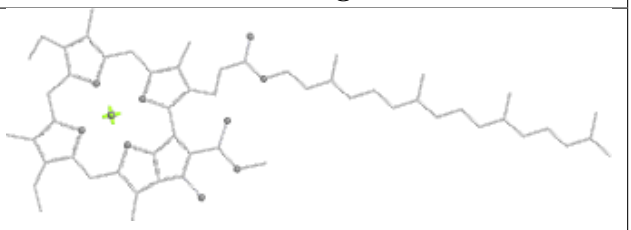
Bond lengths



Bond angles

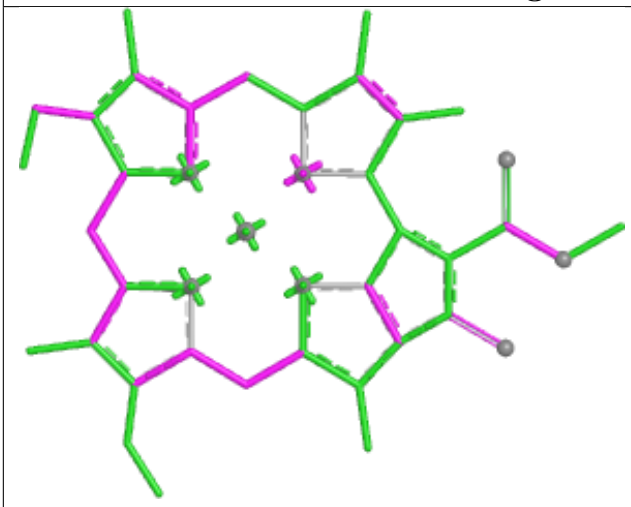


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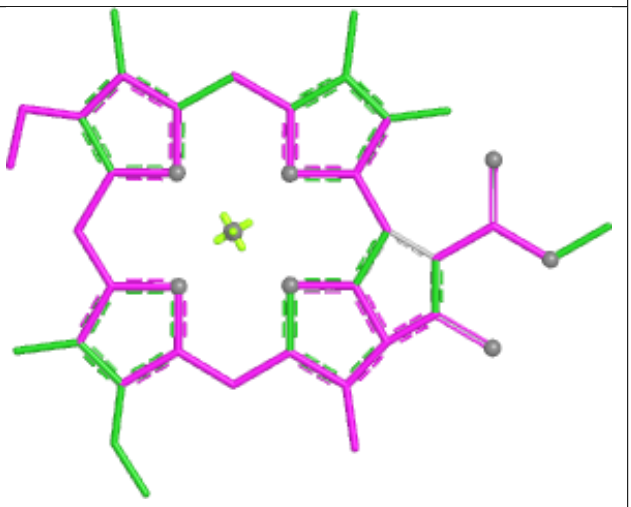


Rings

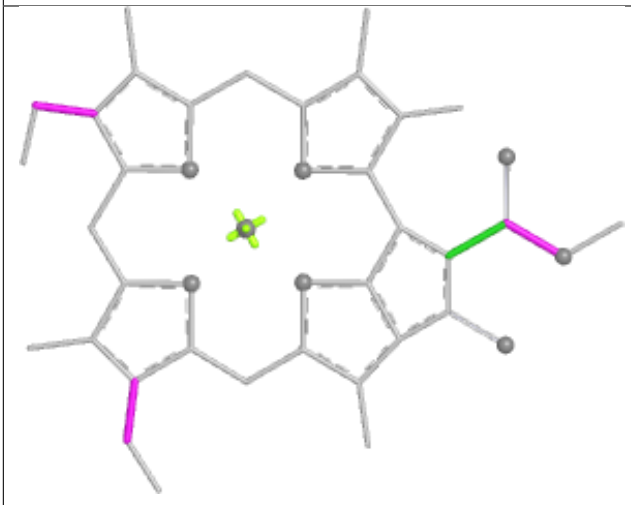
Ligand CLA F 205



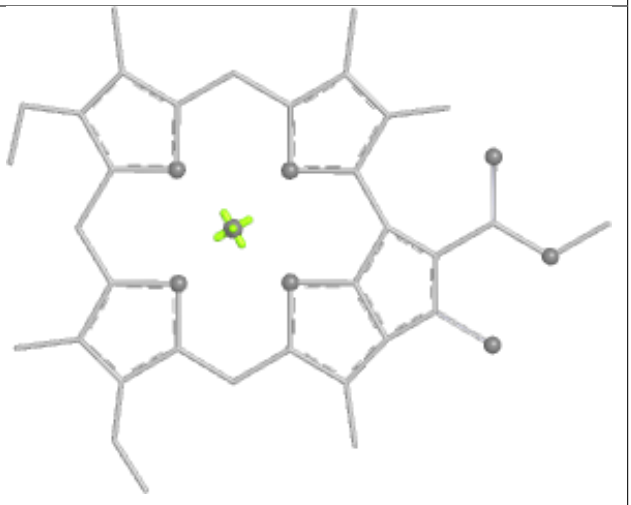
Bond lengths



Bond angles

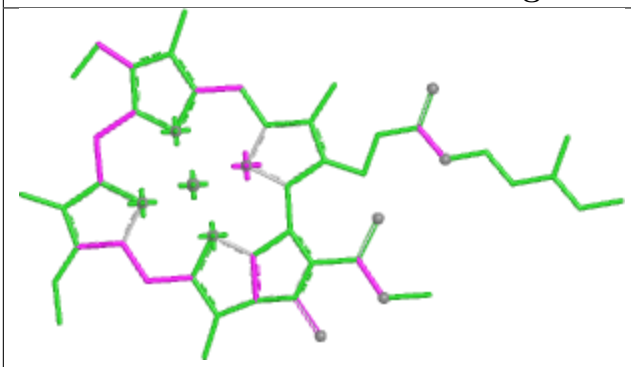


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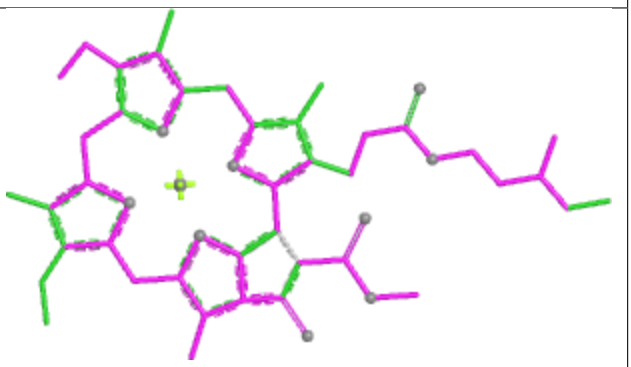


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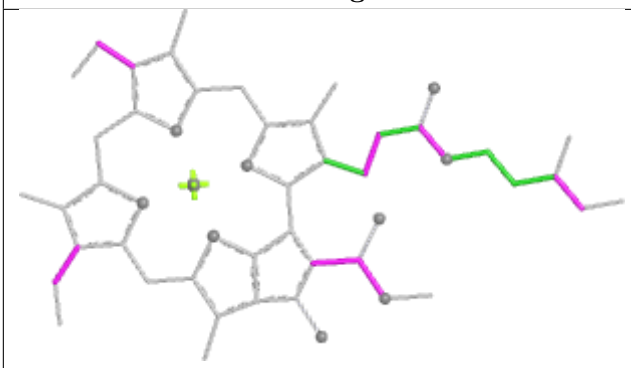
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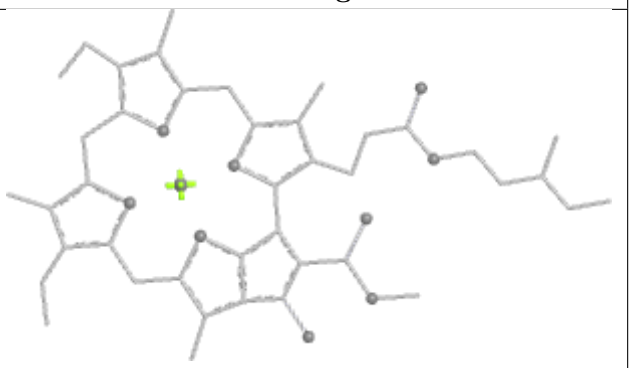
Bond lengths



Bond angles

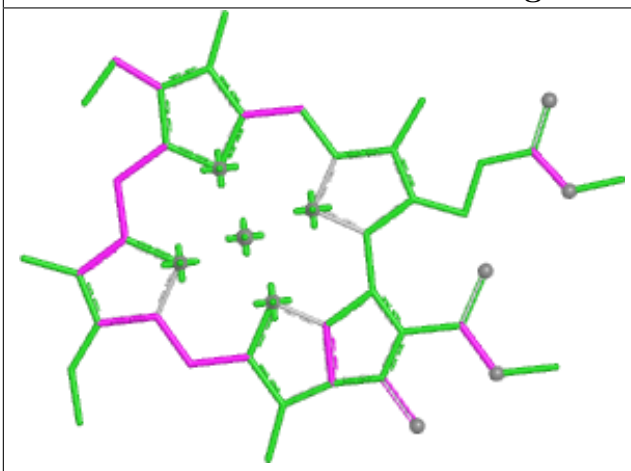


Torsions

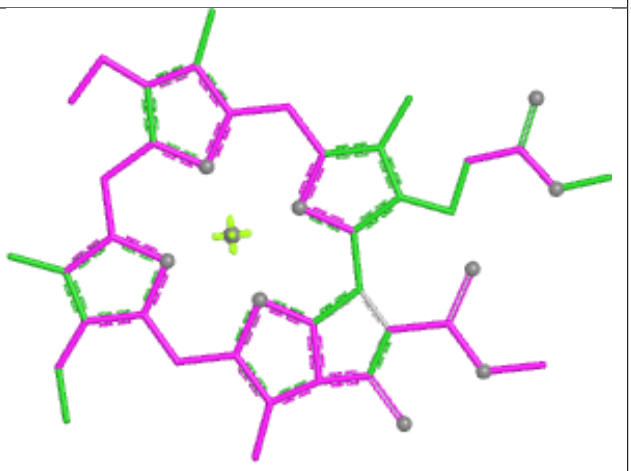


Rings

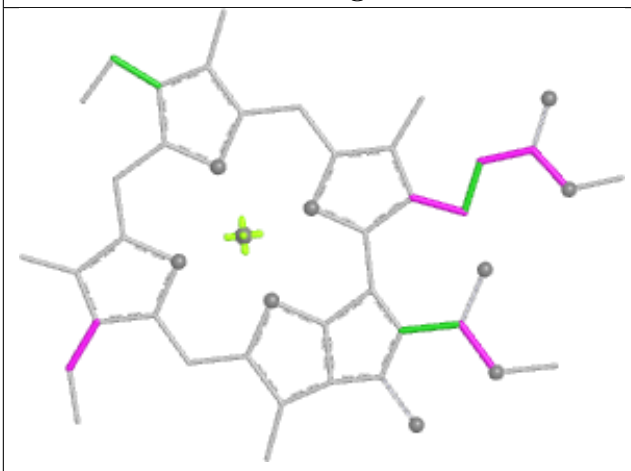
Ligand CLA B 813



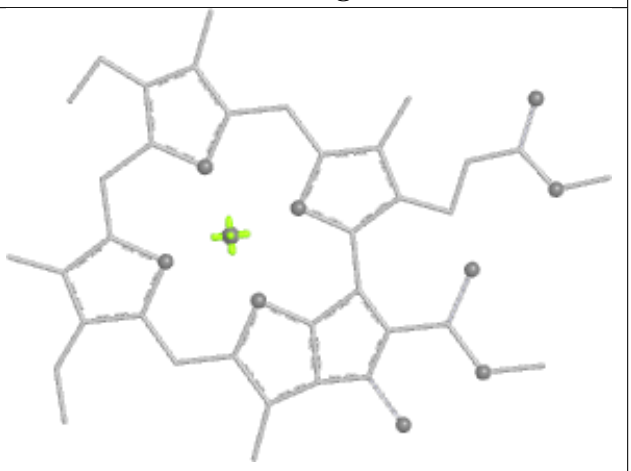
Bond lengths



Bond angles

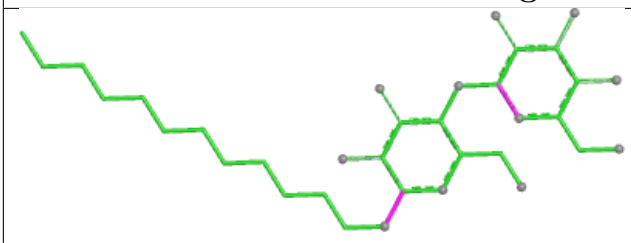


Torsions

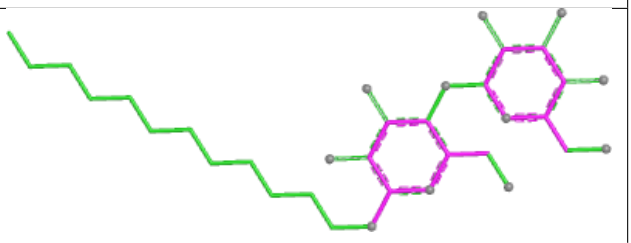


Rings

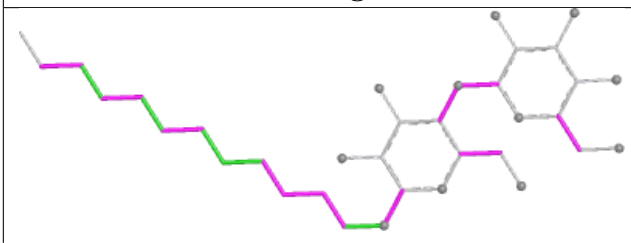
Ligand LMU R 104



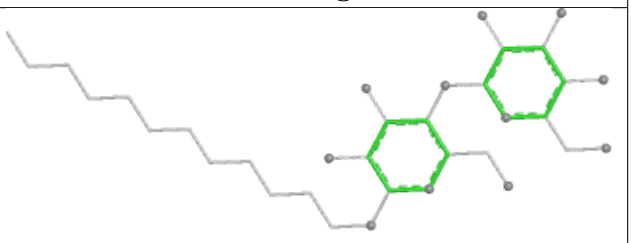
Bond lengths



Bond angles

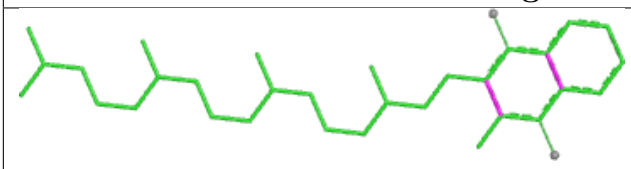


Torsions

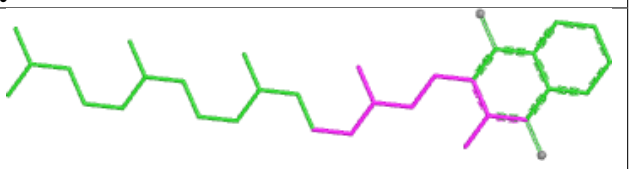


Rings

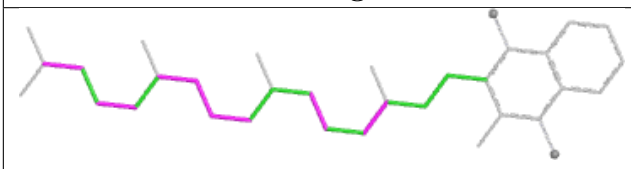
Ligand PQN B 840



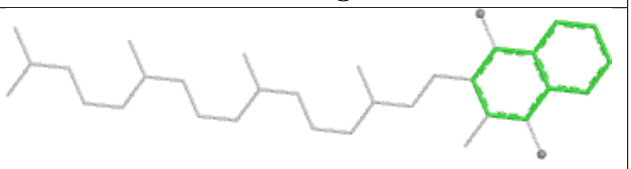
Bond lengths



Bond angles

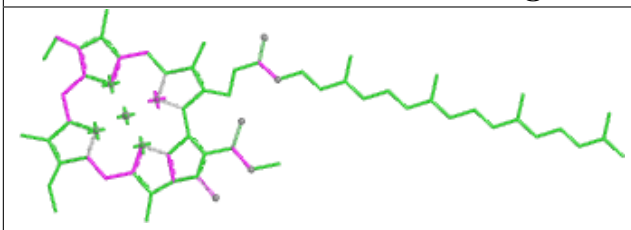


Torsions

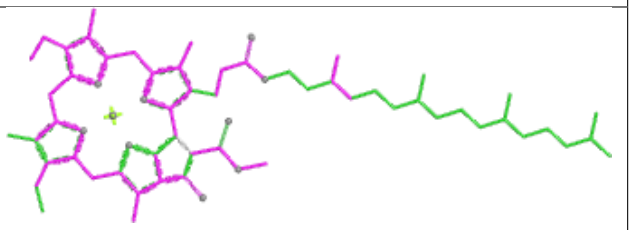


Rings

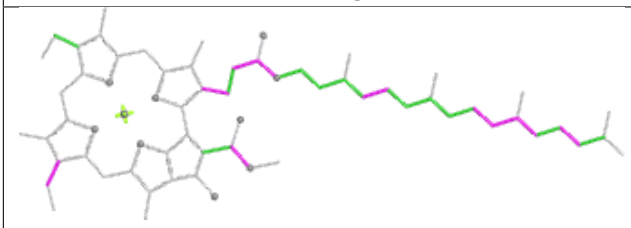
Ligand CLA B 838



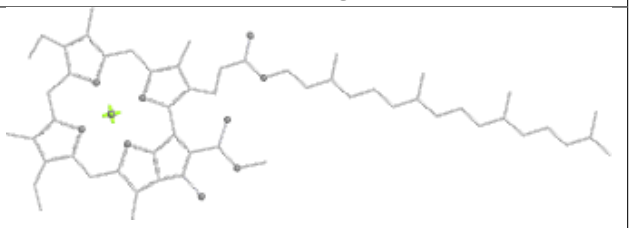
Bond lengths



Bond angles

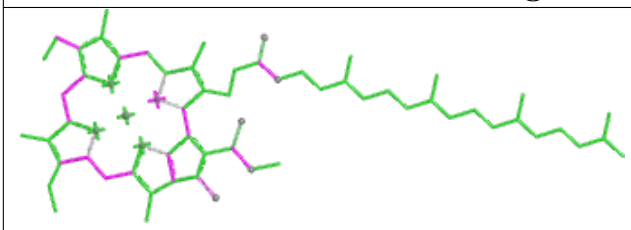


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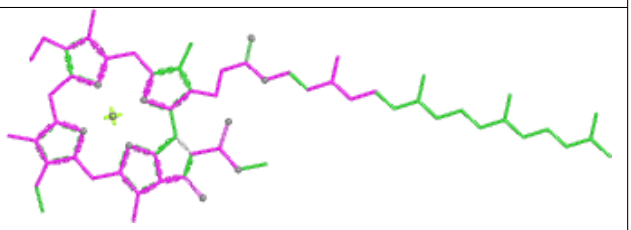


Rings

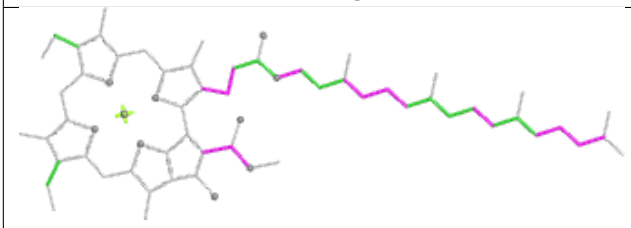
Ligand CLA B 848



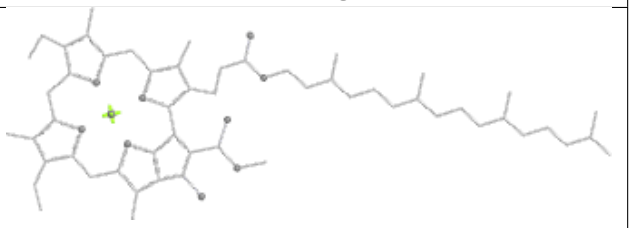
Bond lengths



Bond angles

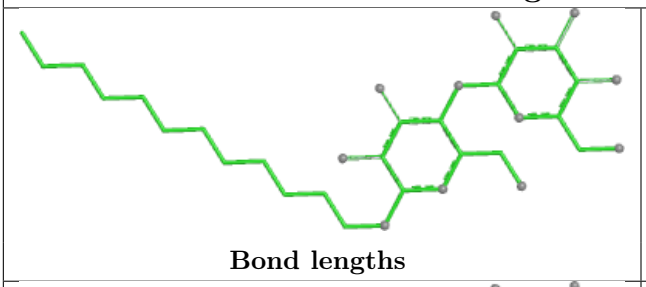


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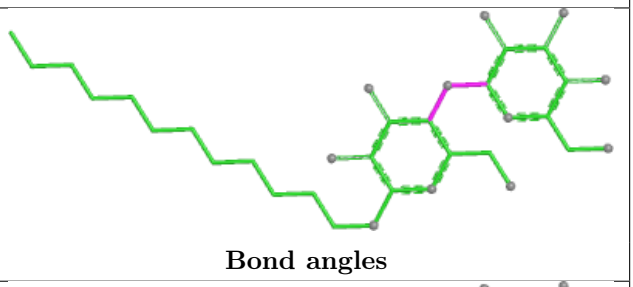


Rings

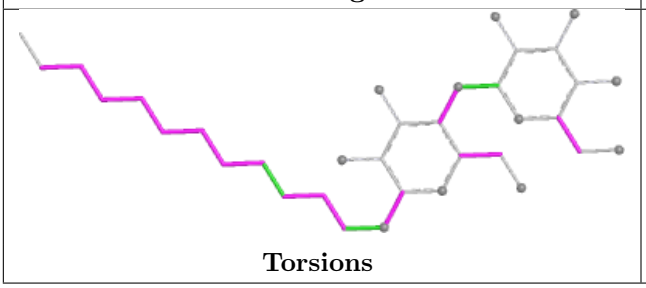
Ligand LMU 3 318



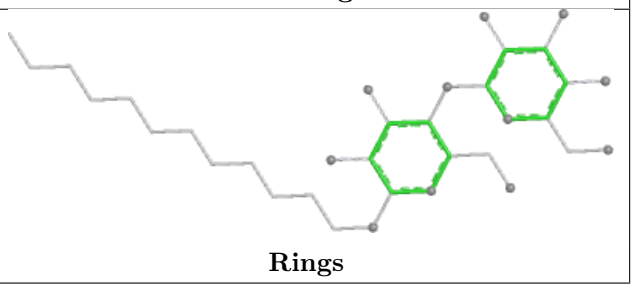
Bond lengths



Bond angles

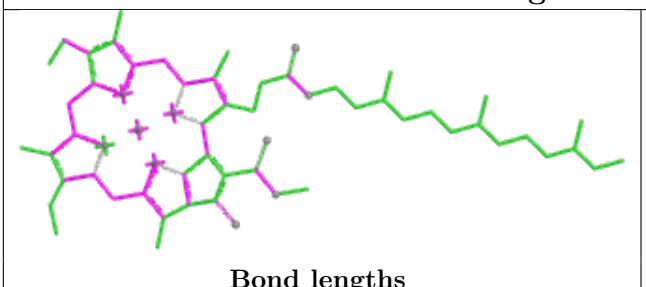


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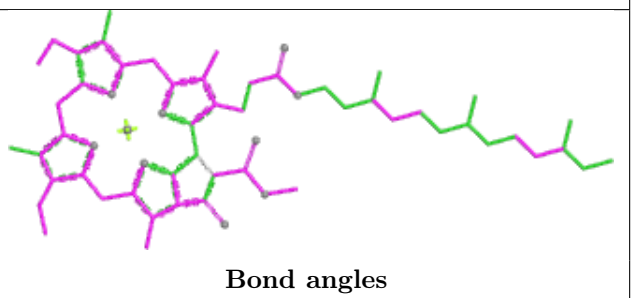


Rings

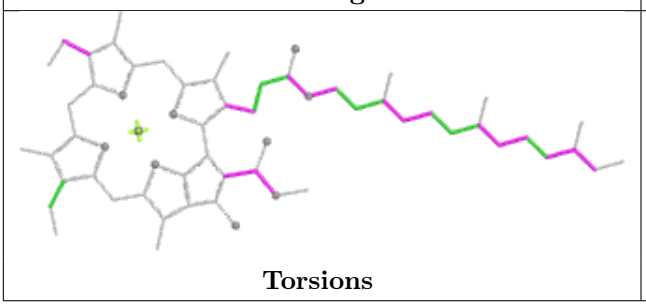
Ligand CLA 2 321



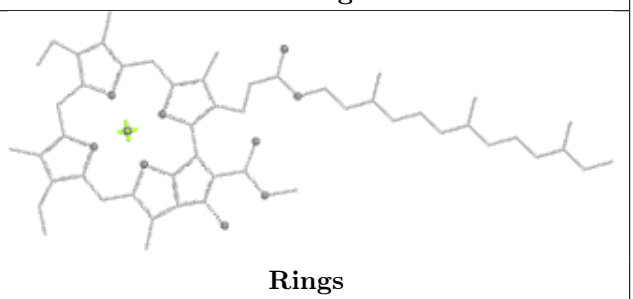
Bond lengths



Bond angles

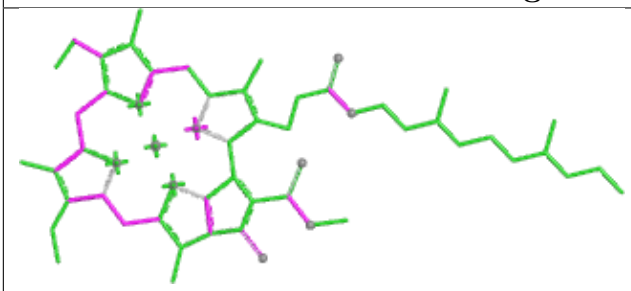


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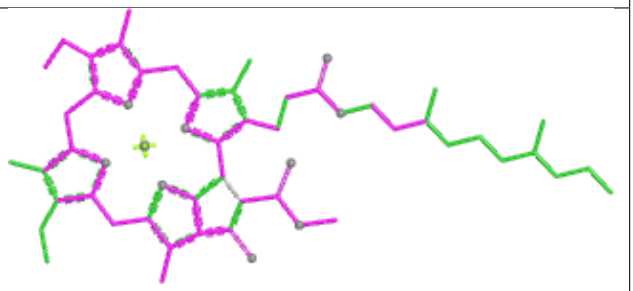


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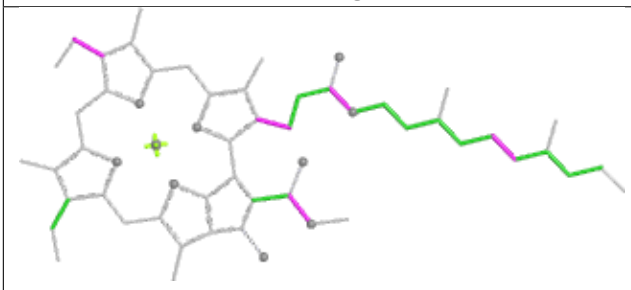
Ligand CLA A 804



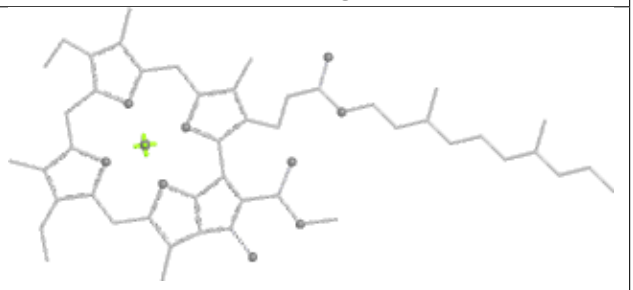
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Bond angles

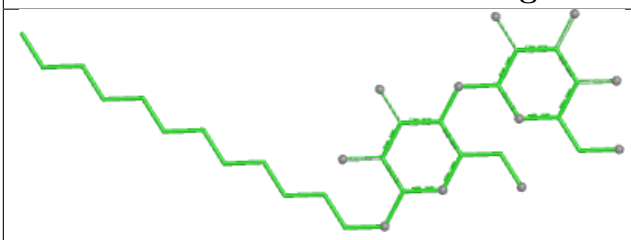


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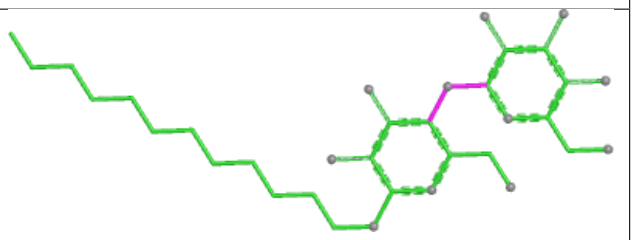


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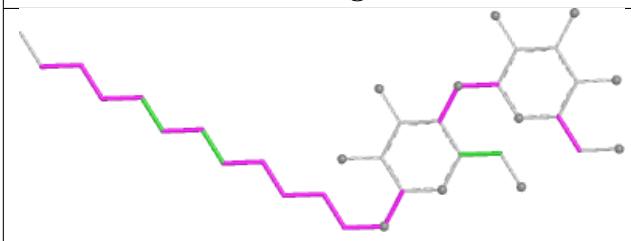
Ligand LMU R 108



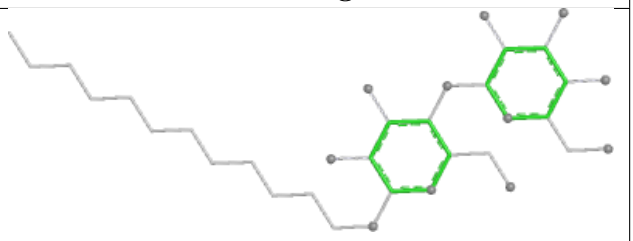
Bond lengths



Bond angles

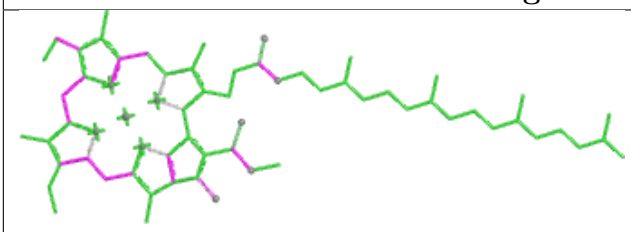


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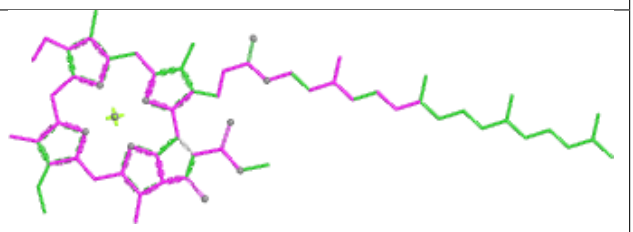


Rings

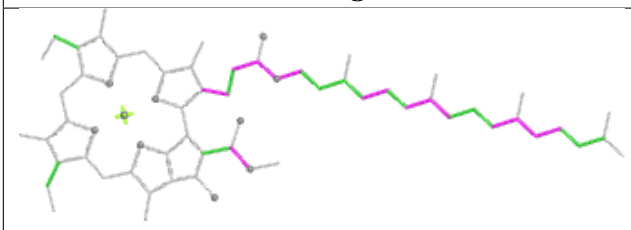
Ligand CLA K 107



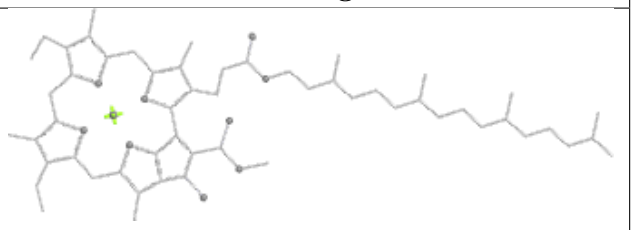
Bond lengths



Bond angles

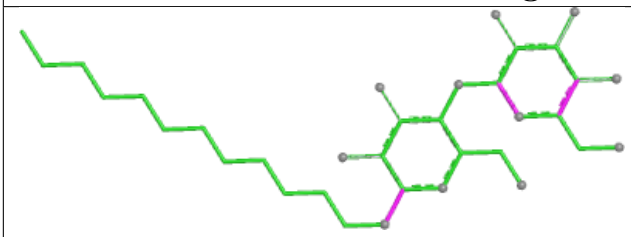


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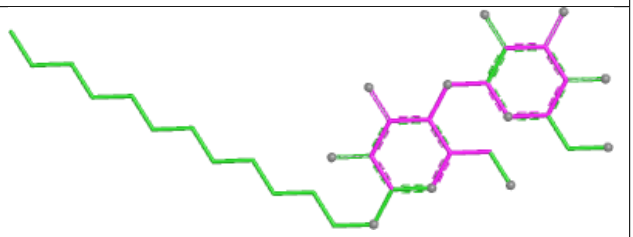


Rings

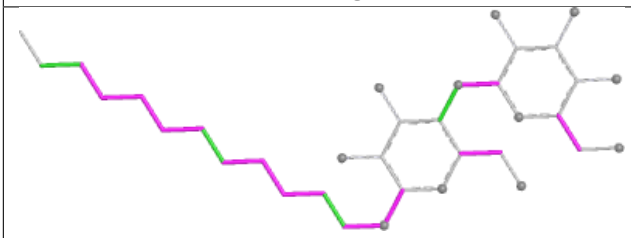
Ligand LMU L 210



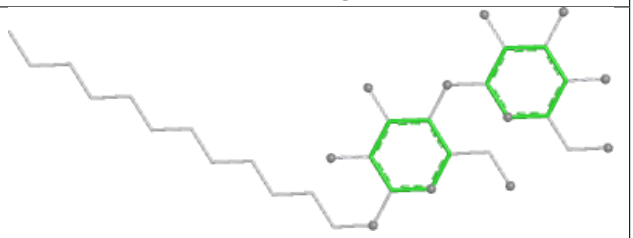
Bond lengths



Bond angles

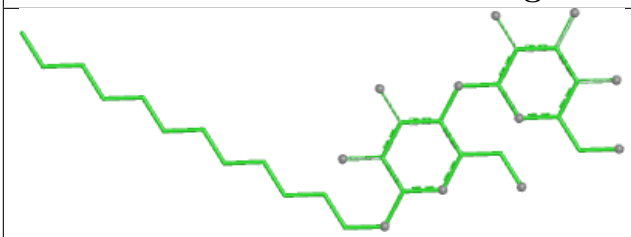


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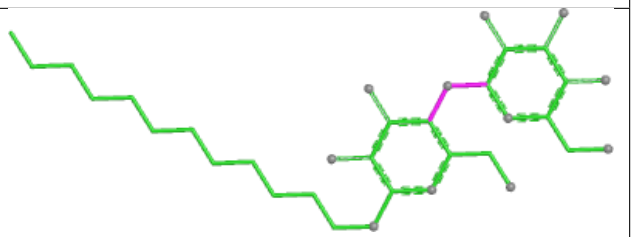


Rings

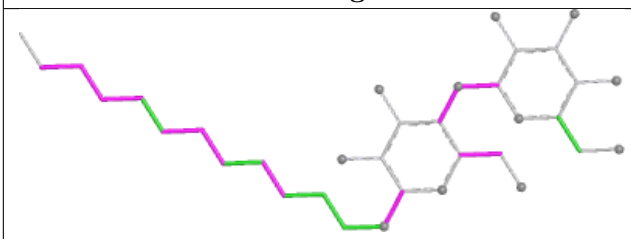
Ligand LMU 1 216



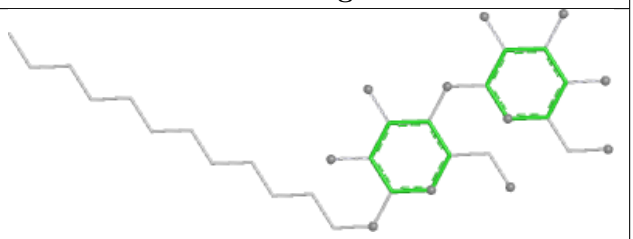
Bond lengths



Bond angles

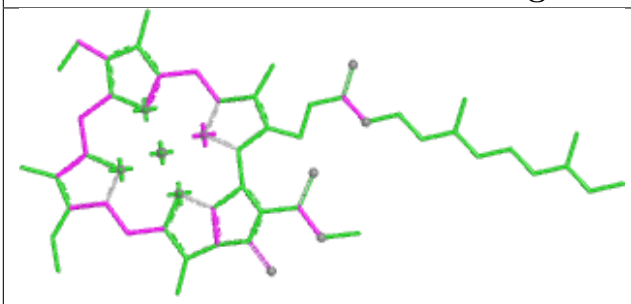


Torsions

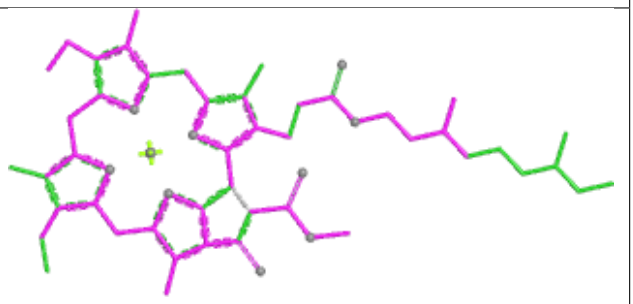


Rings

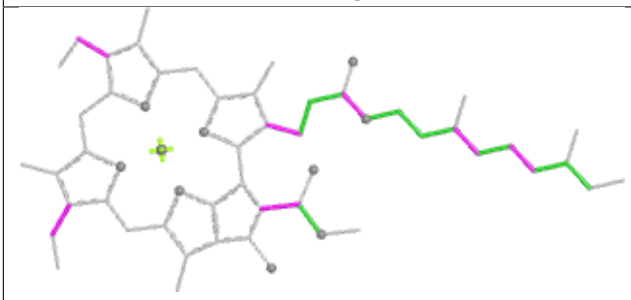
Ligand CLA 2 302



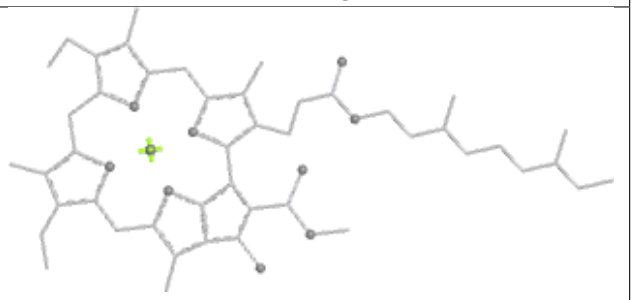
Bond lengths



Bond angles

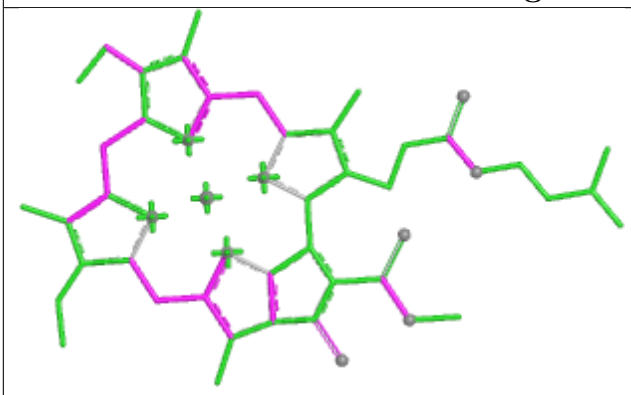


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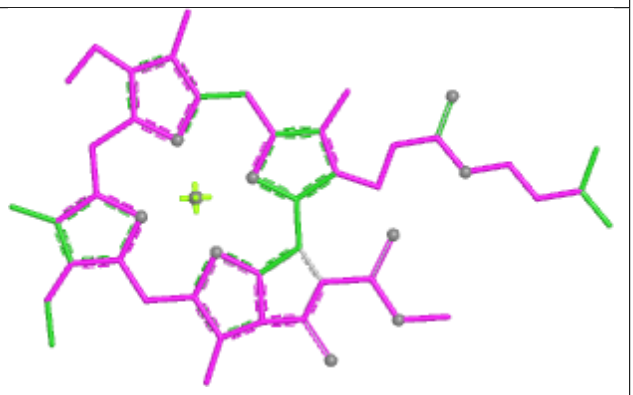


Rings

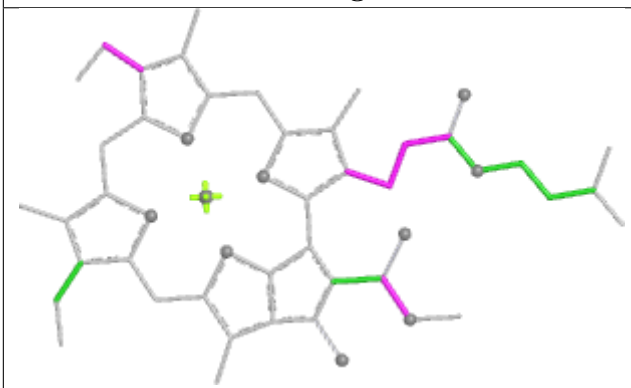
Ligand CLA B 827



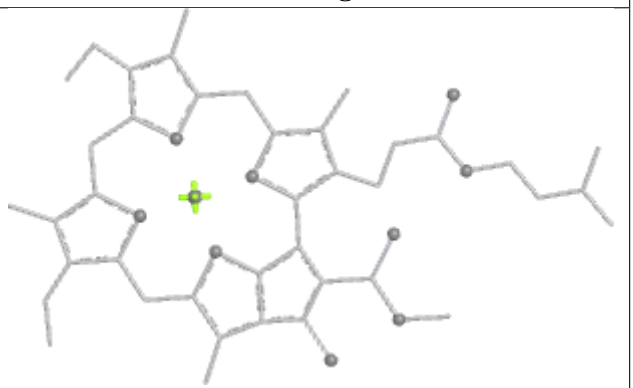
Bond lengths



Bond angles

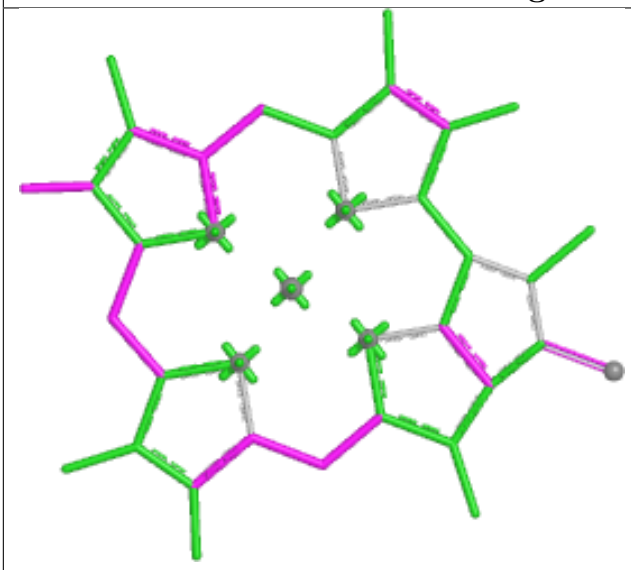


Torsions

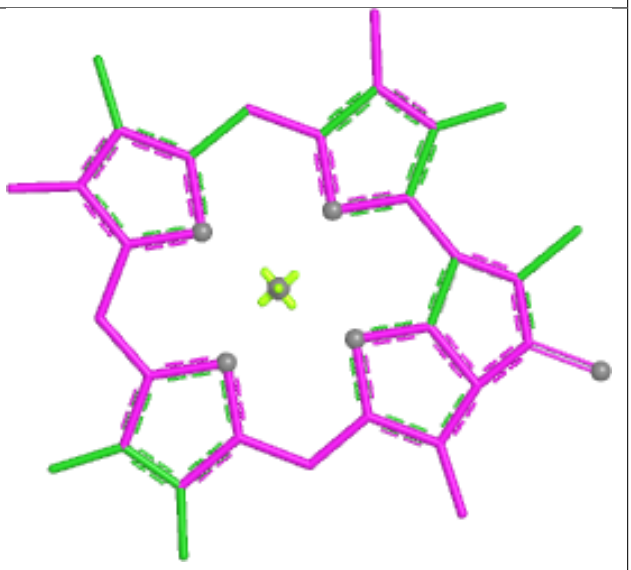


Rings

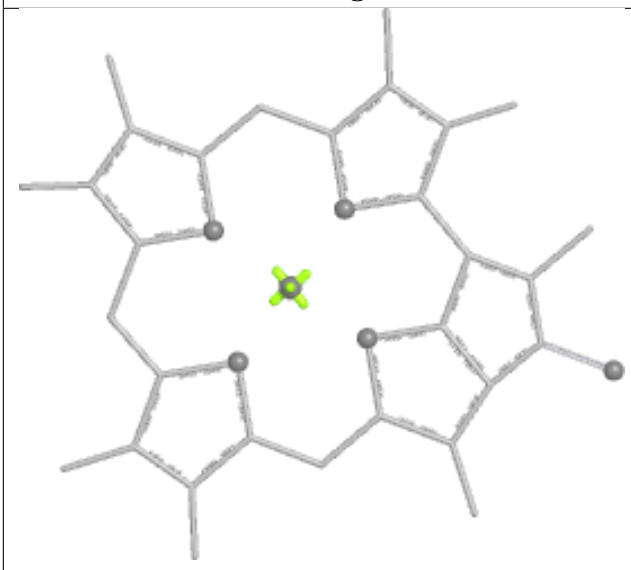
Ligand CLA 1 205



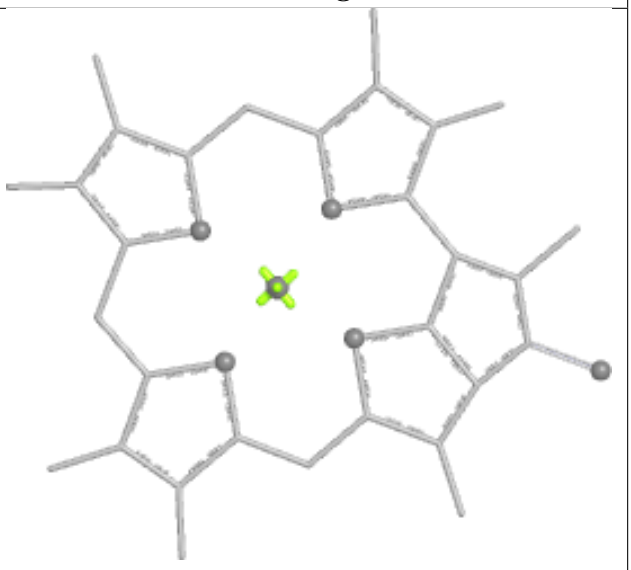
Bond lengths



Bond angles

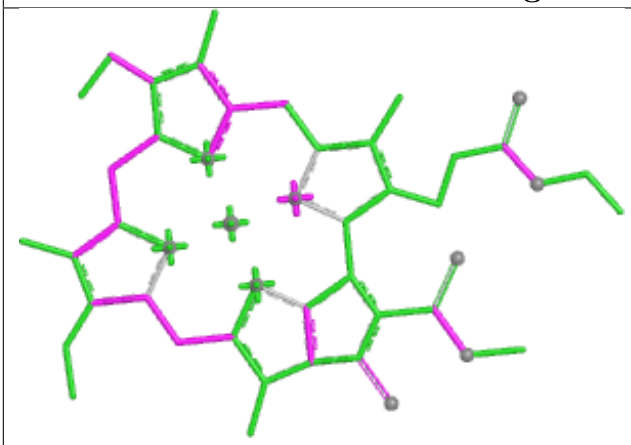


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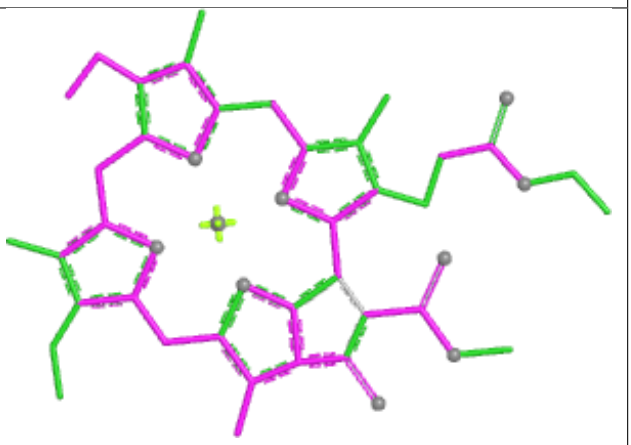


Rings

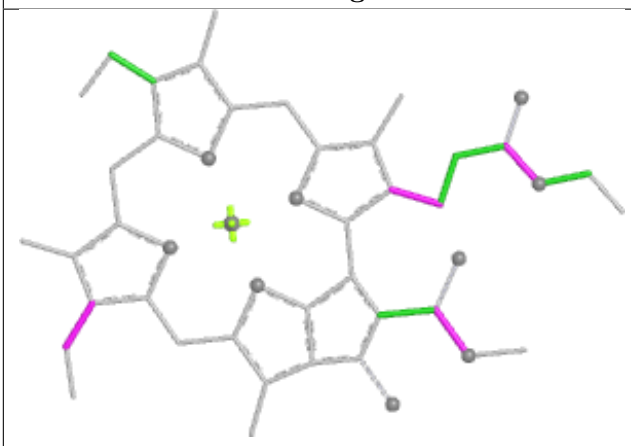
Ligand CLA A 834



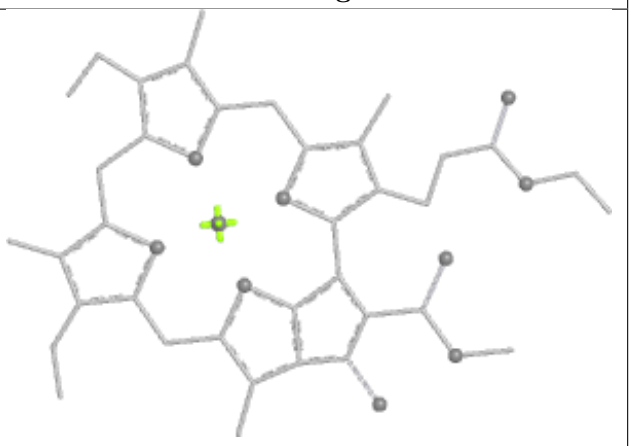
Bond lengths



Bond angles

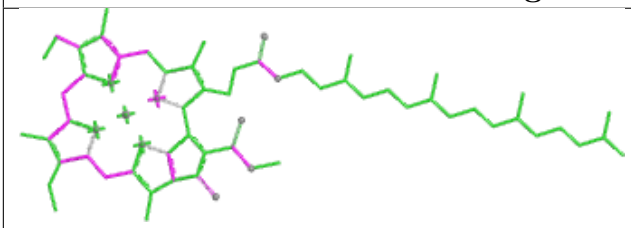


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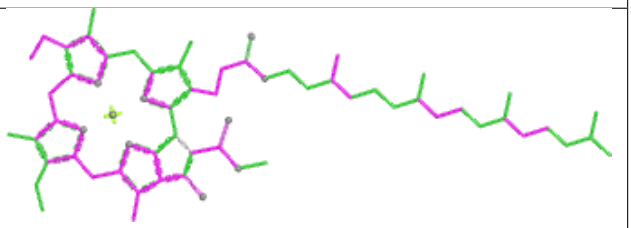


Rings

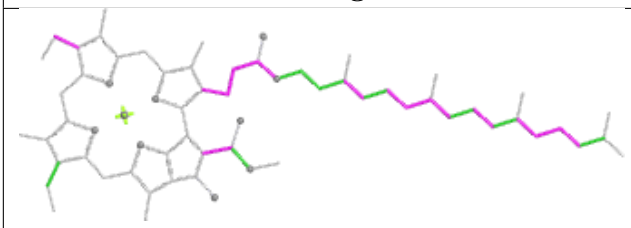
Ligand CLA B 810



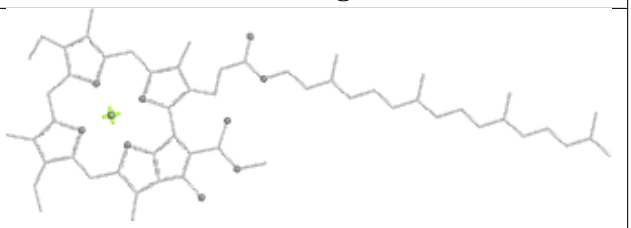
Bond lengths



Bond angles

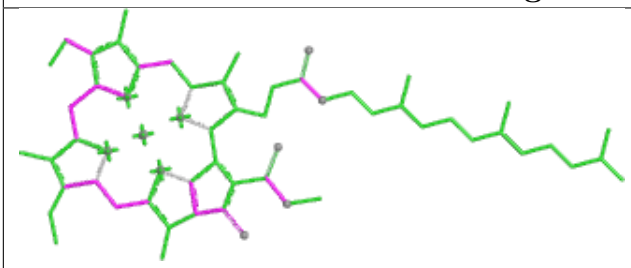


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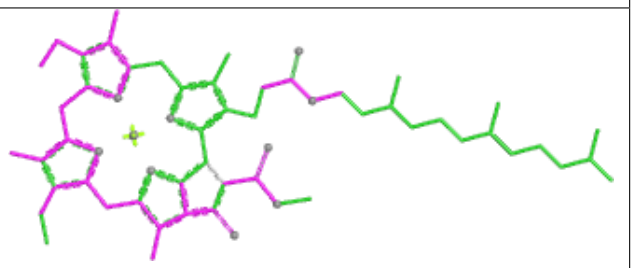


Rings

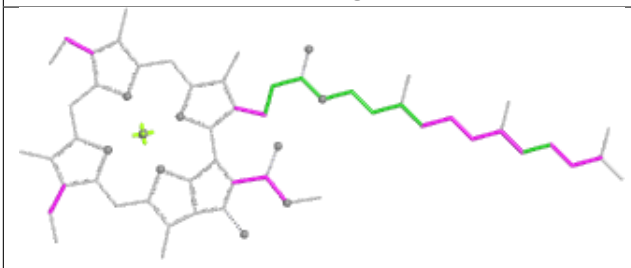
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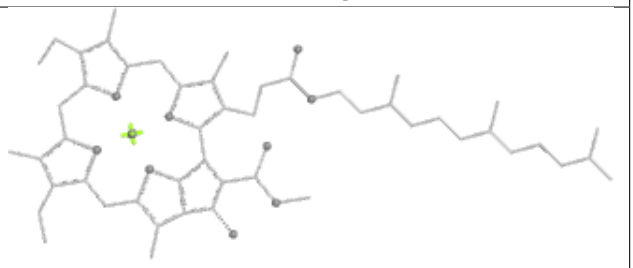
Bond lengths



Bond angles

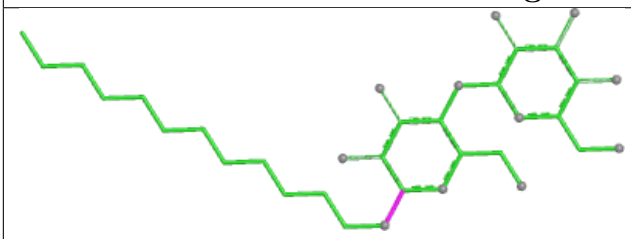


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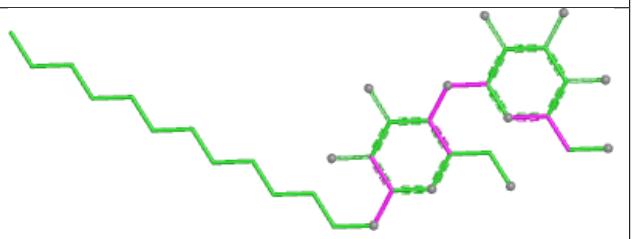


Rings

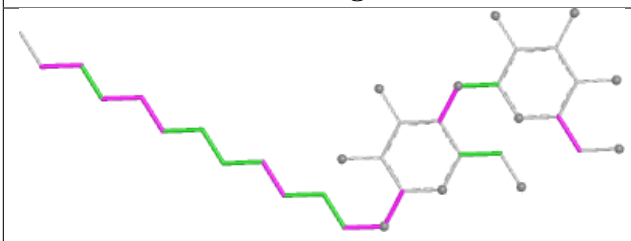
Ligand LMU 2 320



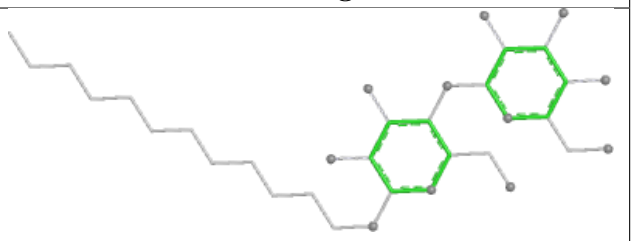
Bond lengths



Bond angles

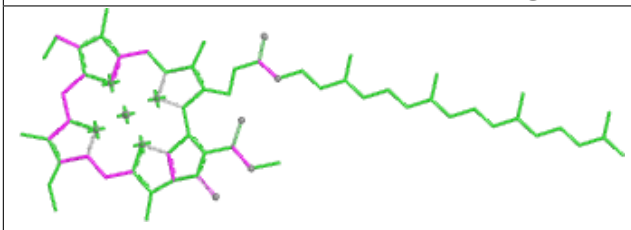


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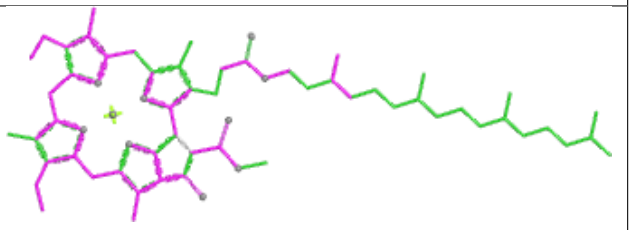


Rings

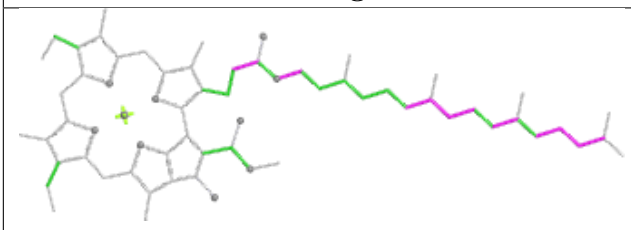
Ligand CLA B 835



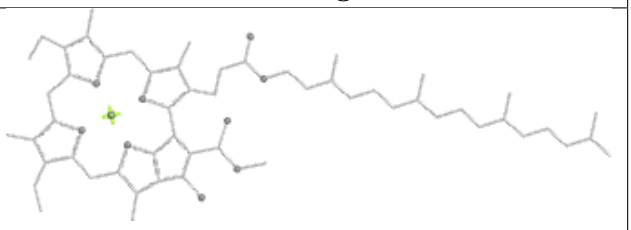
Bond lengths



Bond angles

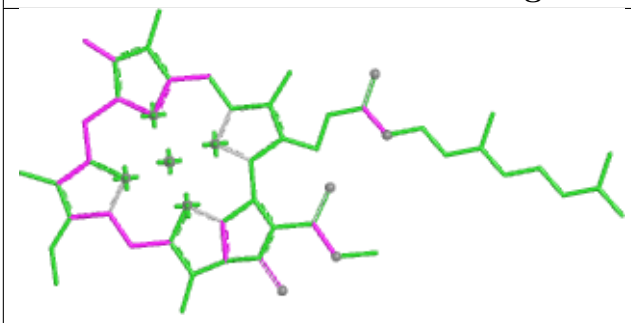


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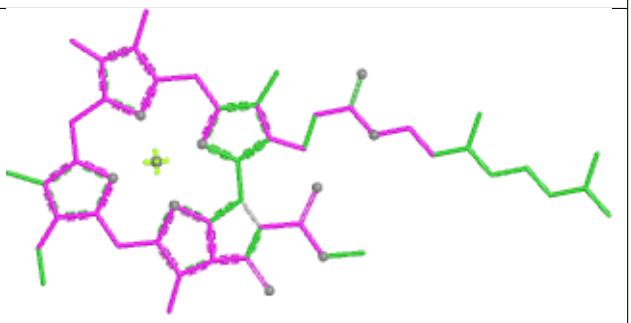


Rings

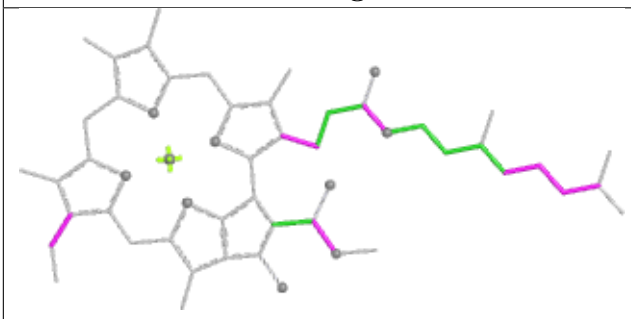
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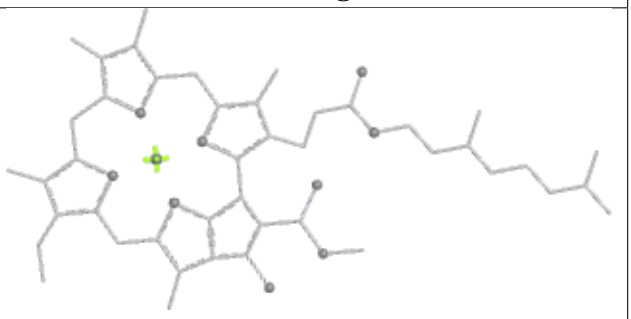
Bond lengths



Bond angles

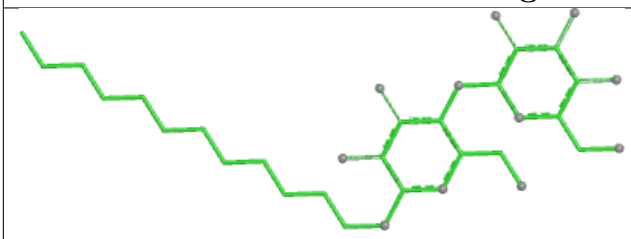


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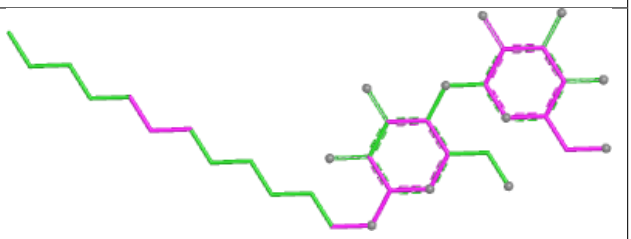


Rings

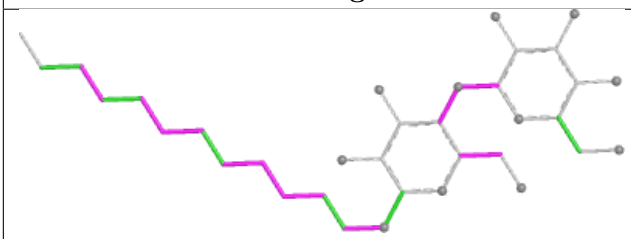
Ligand LMU R 101



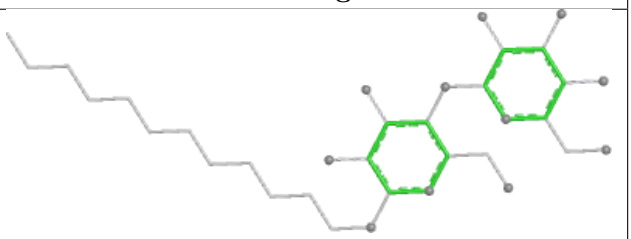
Bond lengths



Bond angles

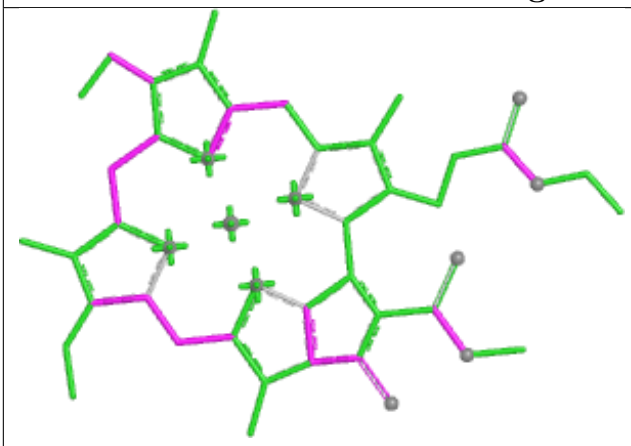


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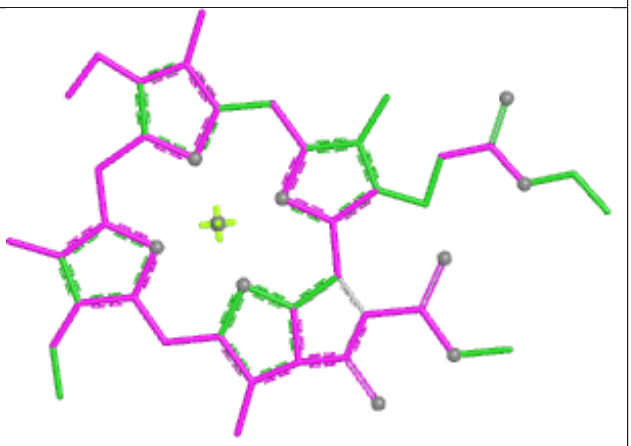


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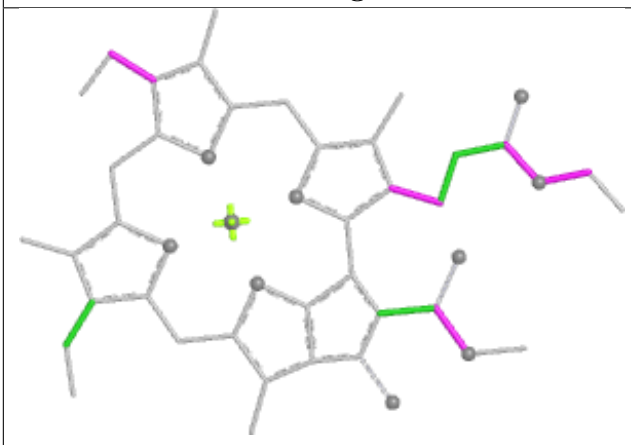
Ligand CLA 1 203



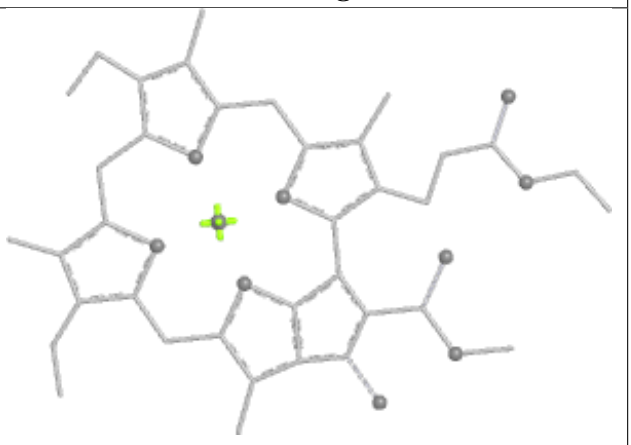
Bond lengths



Bond angles

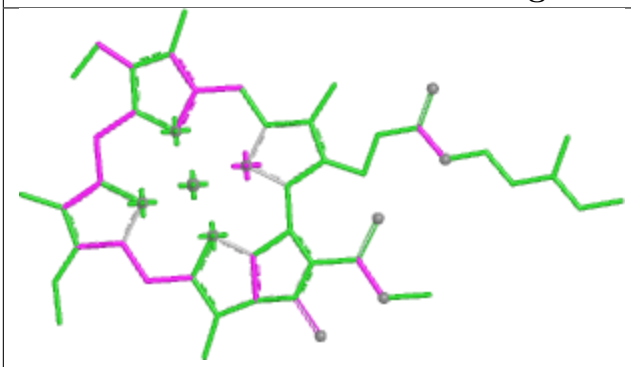


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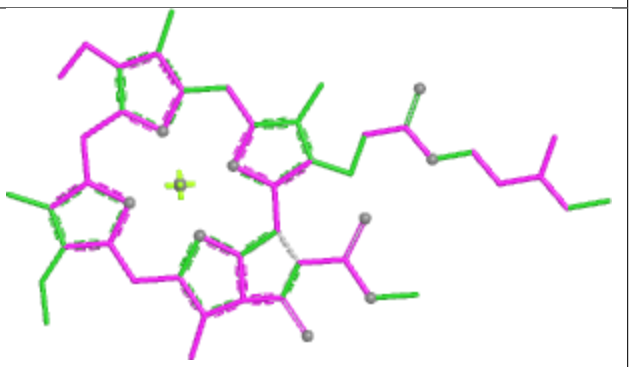


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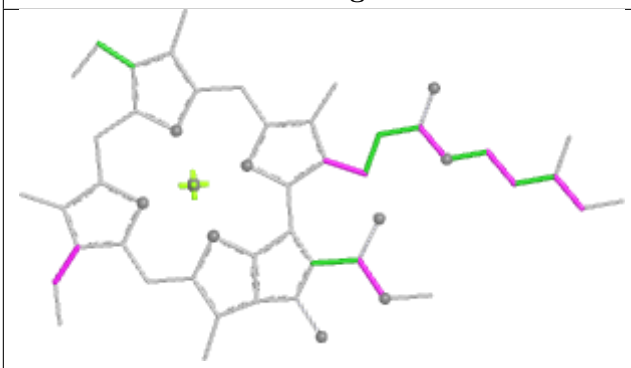
Ligand CLA 2 301



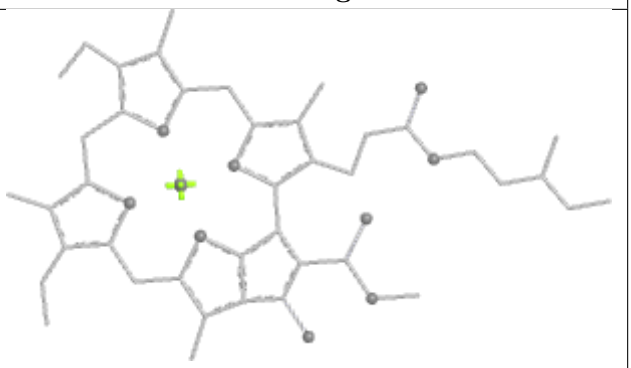
Bond lengths



Bond angles

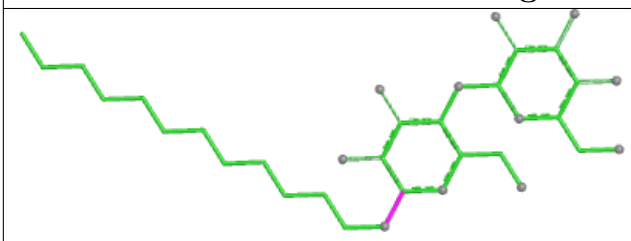


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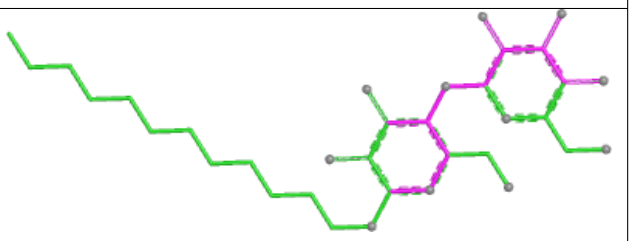


Rings

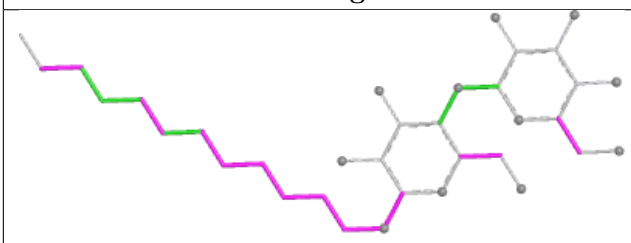
Ligand LMU R 105



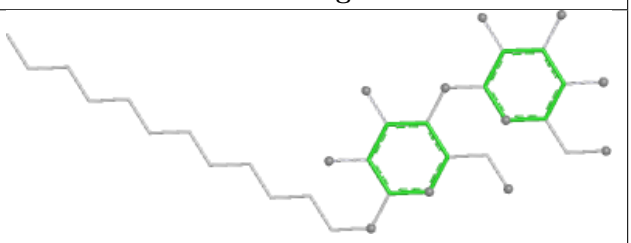
Bond lengths



Bond angles

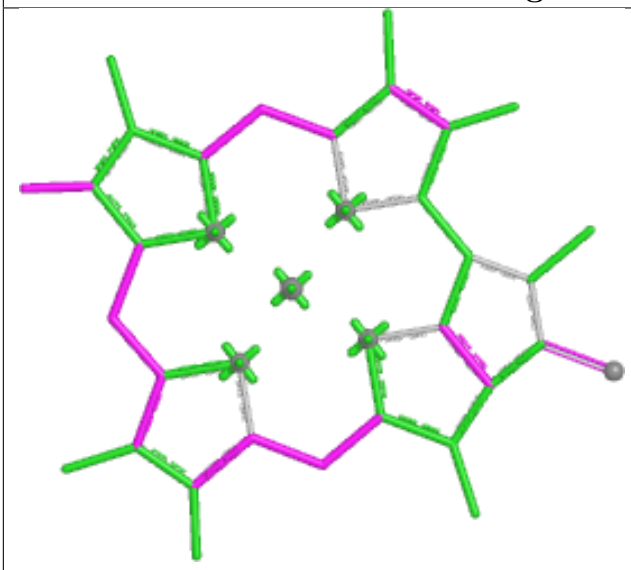


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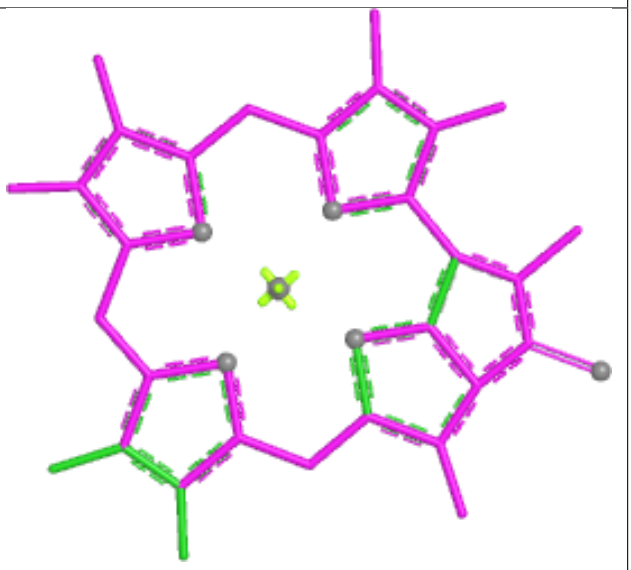


Rings

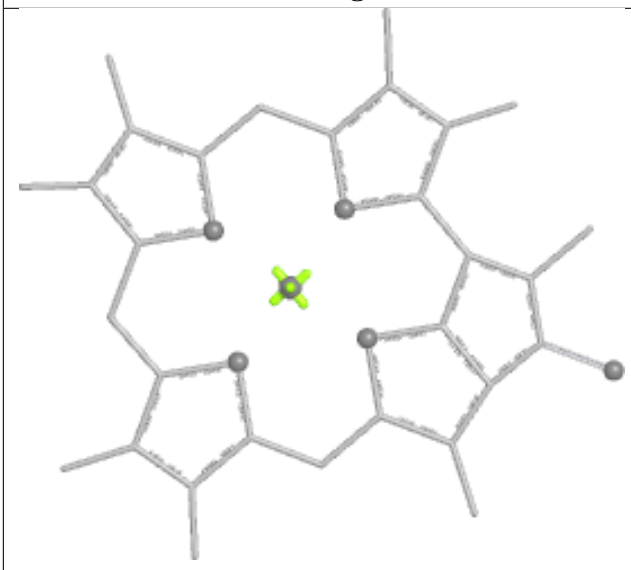
Ligand CLA F 204



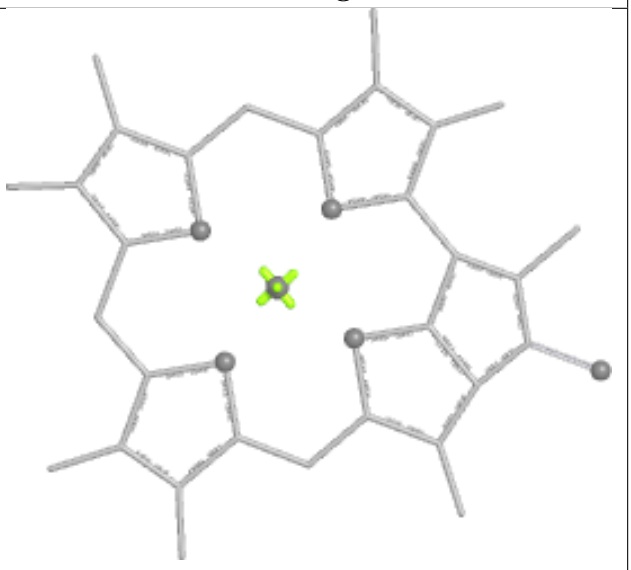
Bond lengths



Bond angles

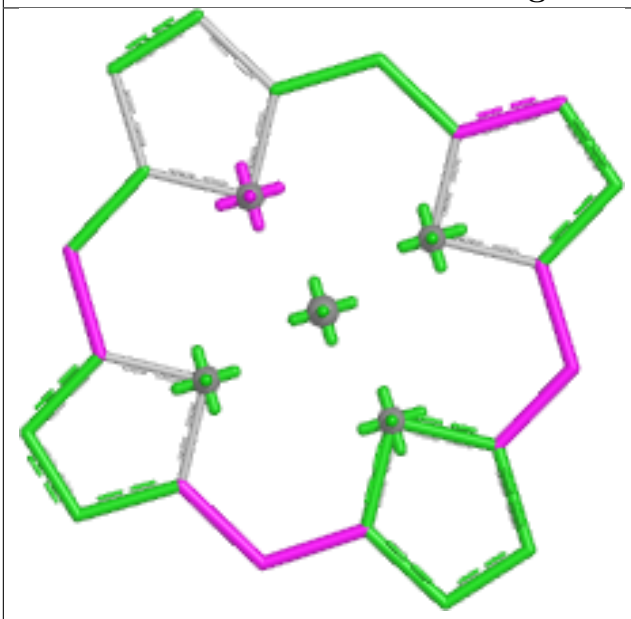


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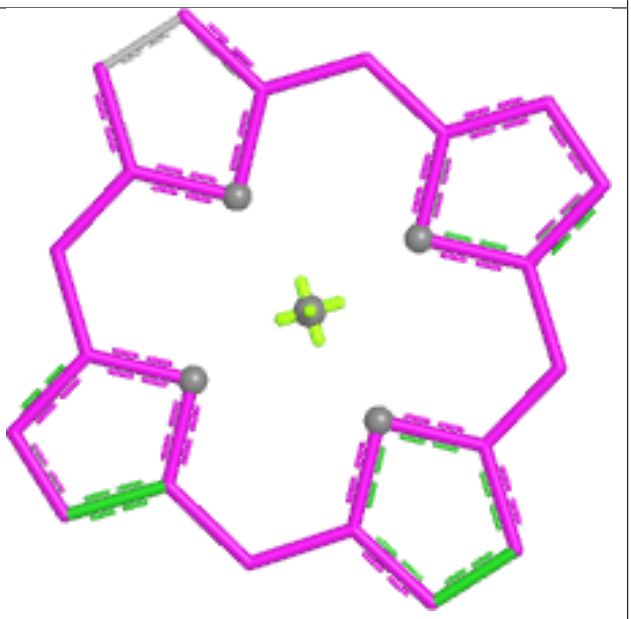


Rings

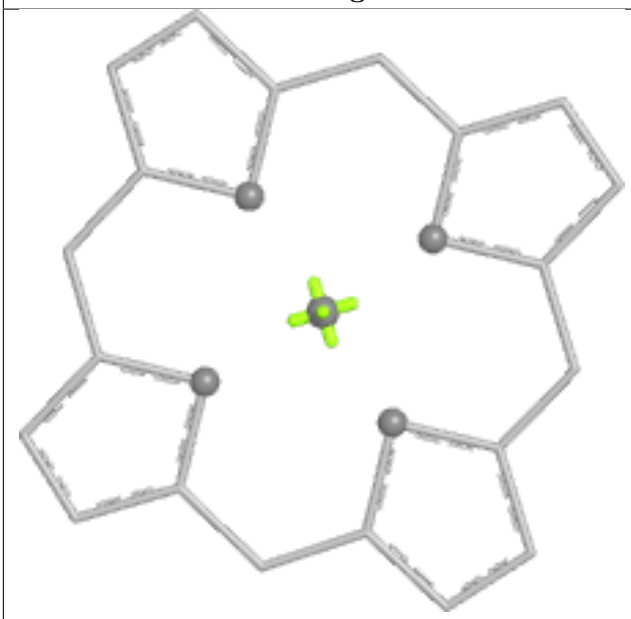
Ligand CLA 4 312



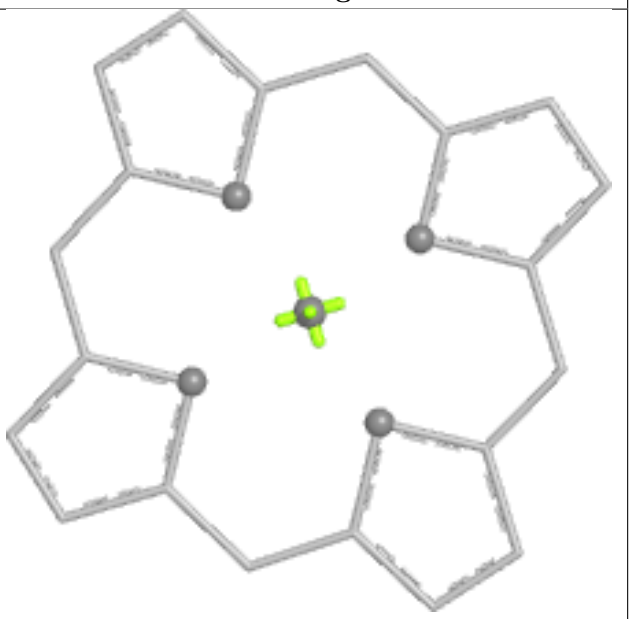
Bond lengths



Bond angles

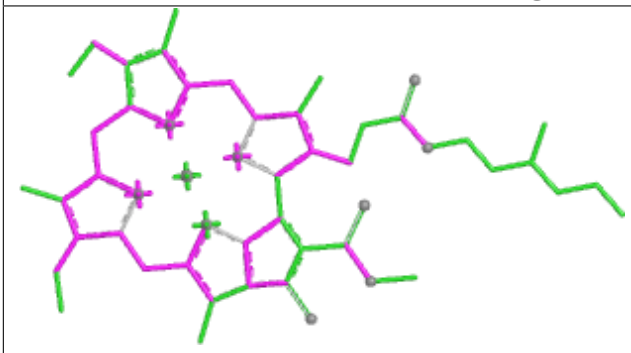


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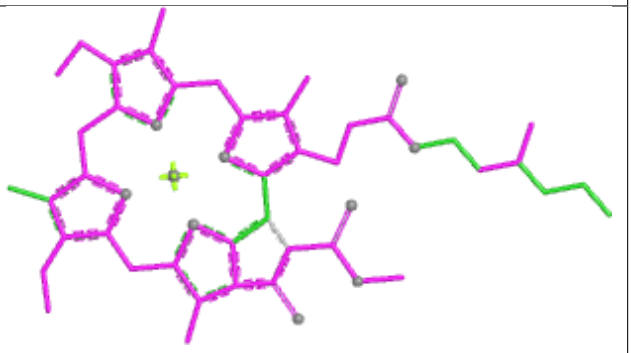


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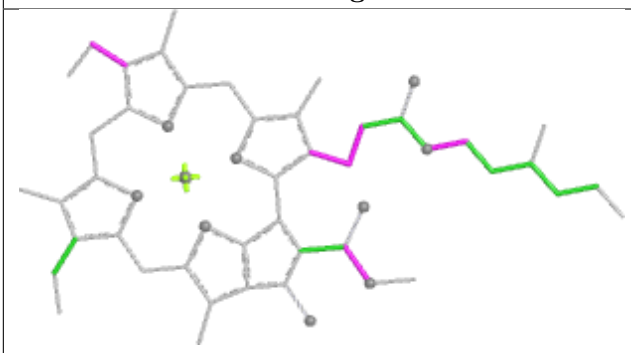
Ligand CLA 4 307



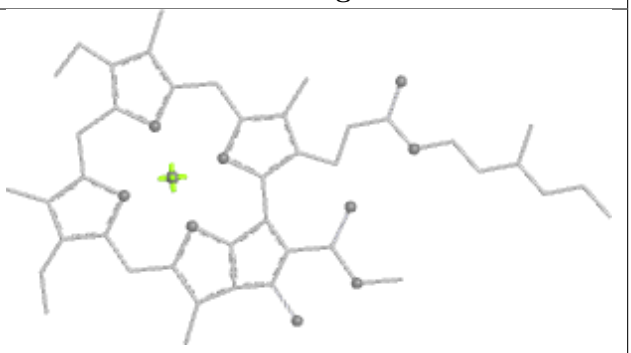
Bond lengths



Bond angles

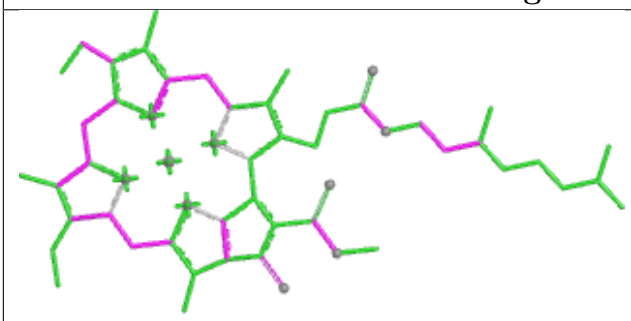


Torsions

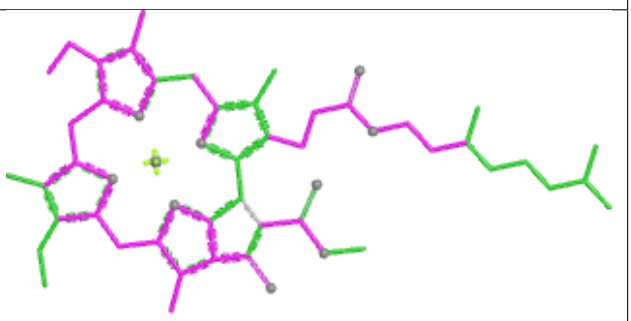


Rings

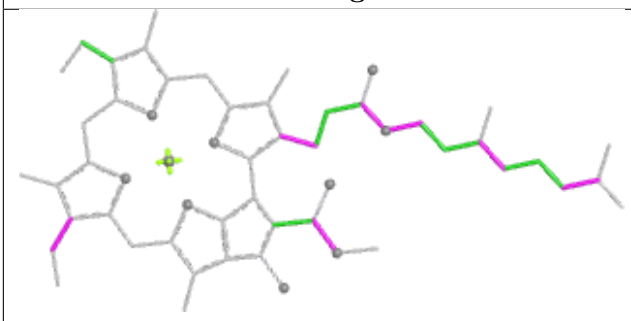
Ligand CLA A 802



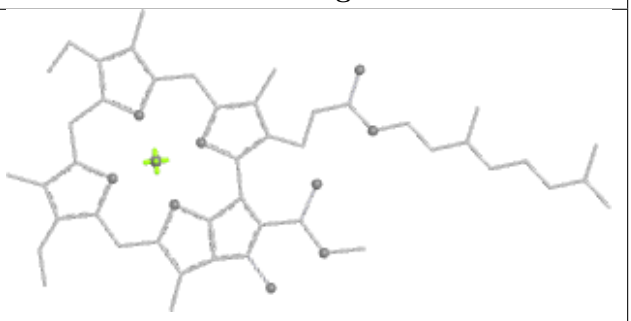
Bond lengths



Bond angles

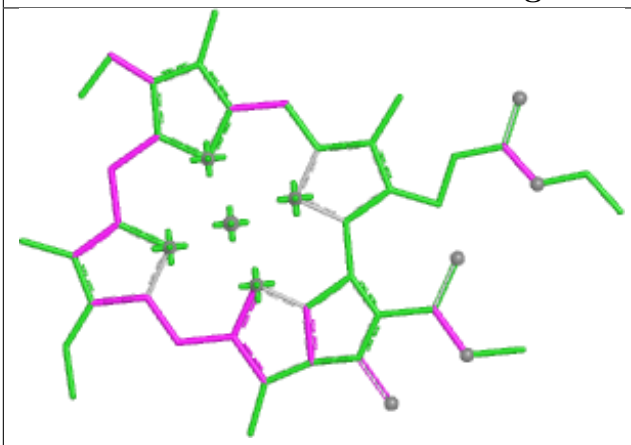


Torsions

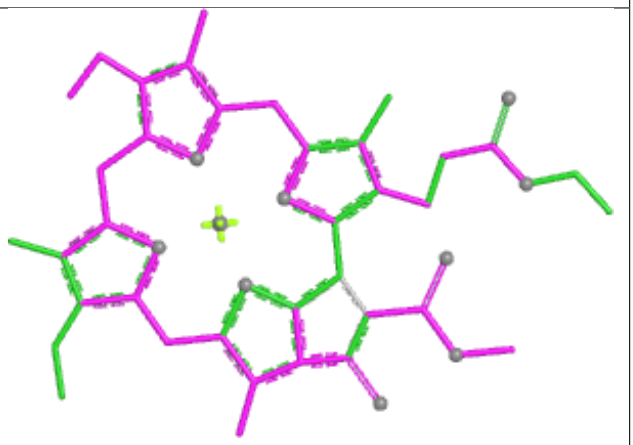


Rings

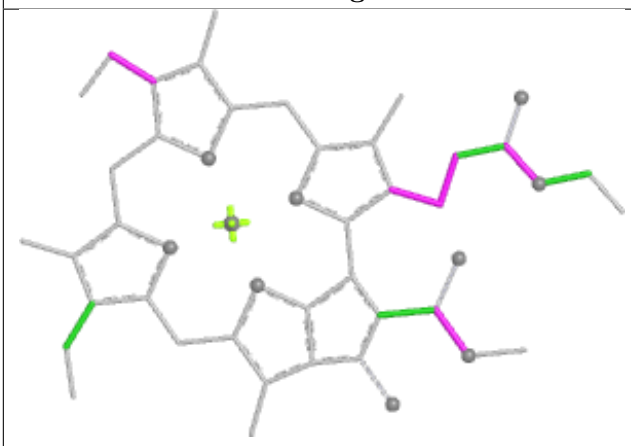
Ligand CLA B 836



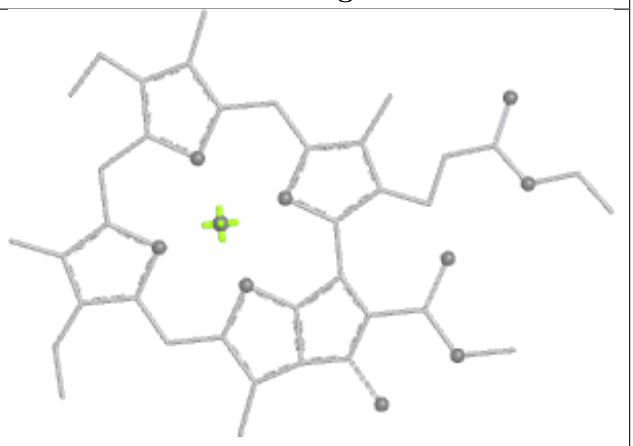
Bond lengths



Bond angles

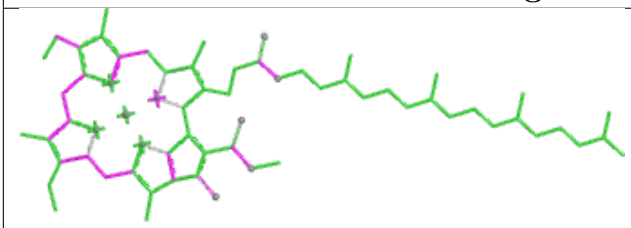


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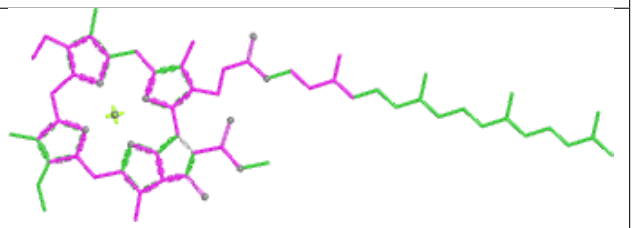


Rings

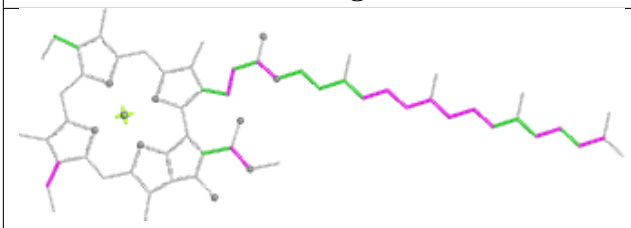
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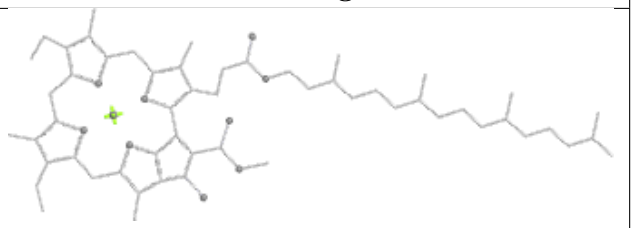
Bond lengths



Bond angles

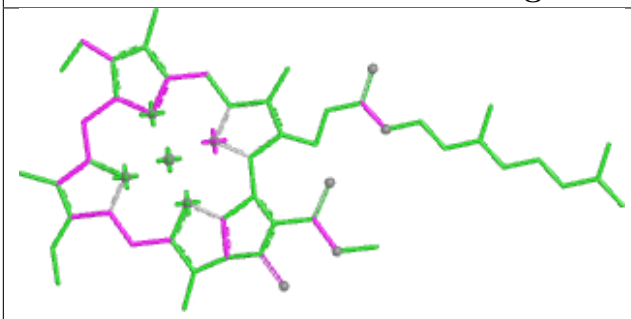


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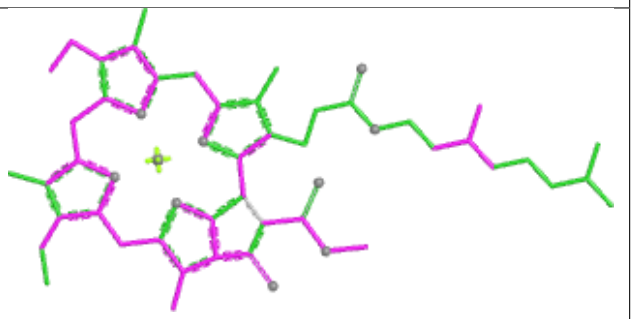


Rings

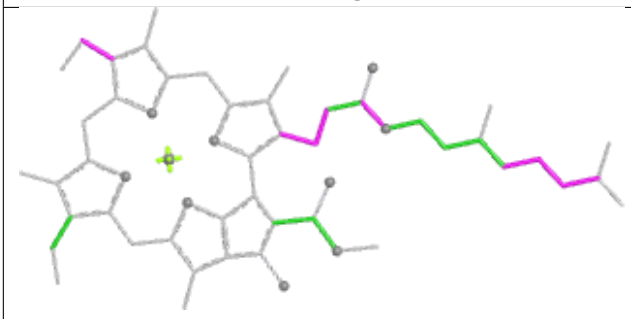
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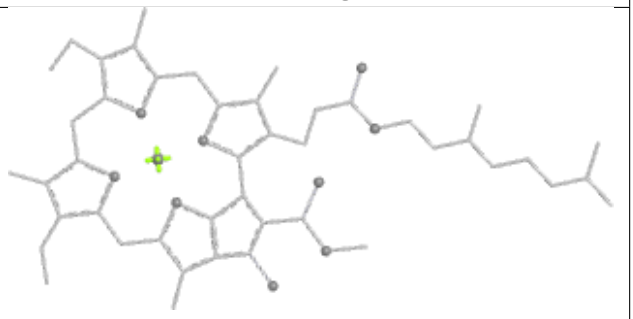
Bond lengths



Bond angles

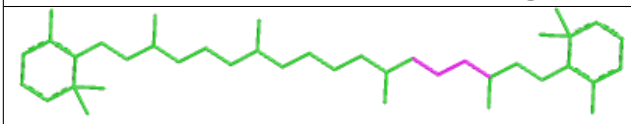


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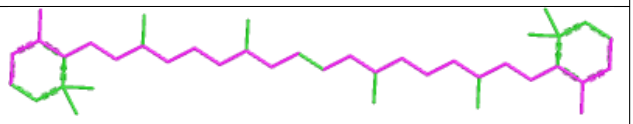


Rings

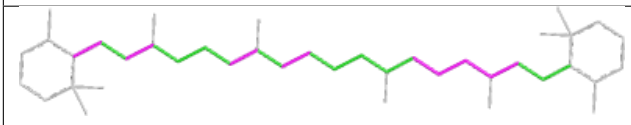
Ligand BCR A 841



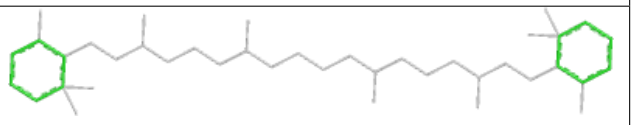
Bond lengths



Bond angles

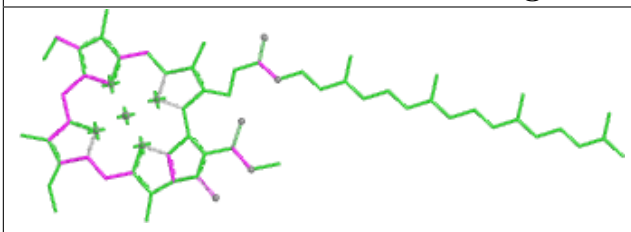


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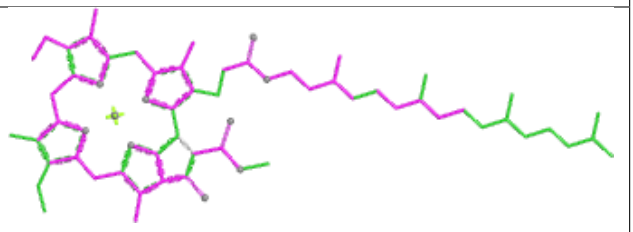


Rings

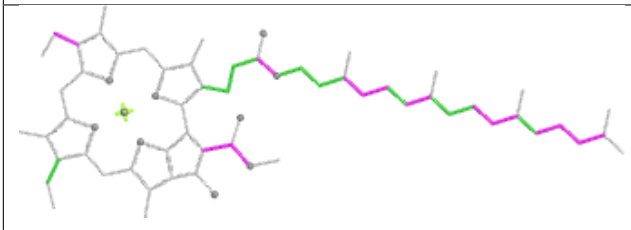
Ligand CLA A 824



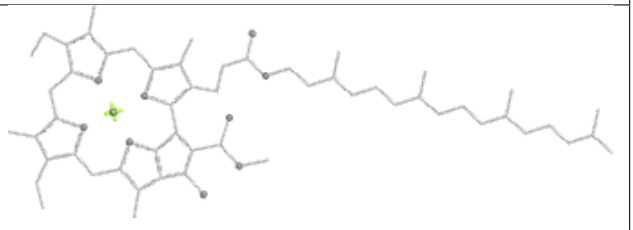
Bond lengths



Bond angles

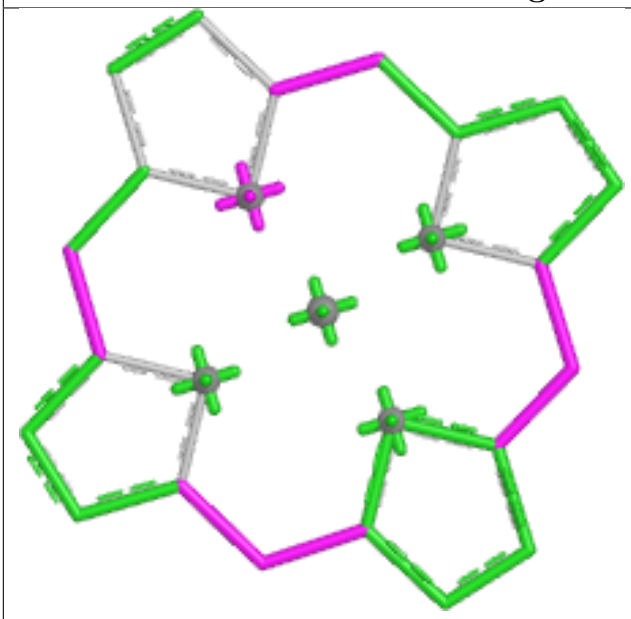


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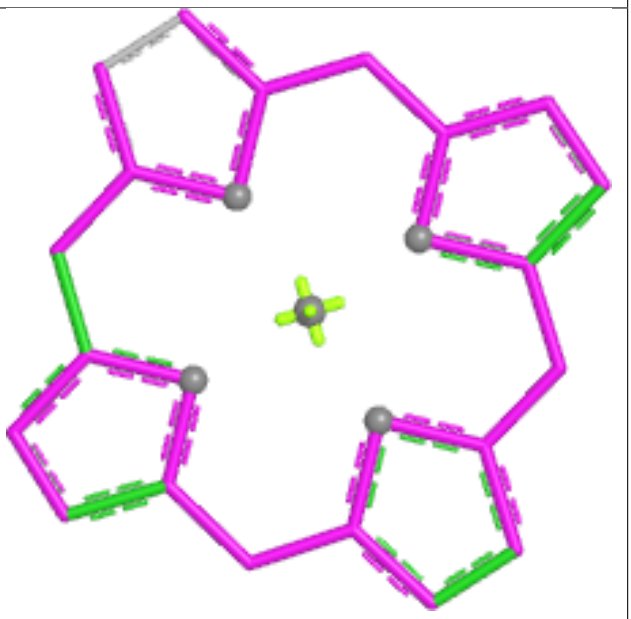


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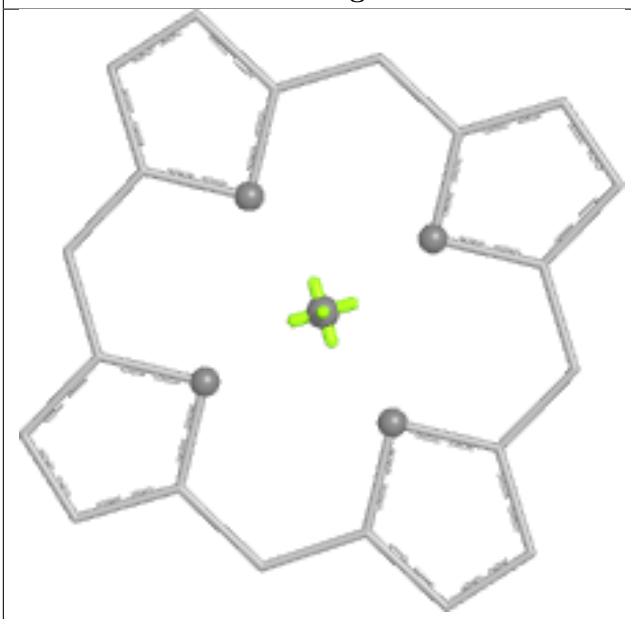
Ligand CLA 3 317



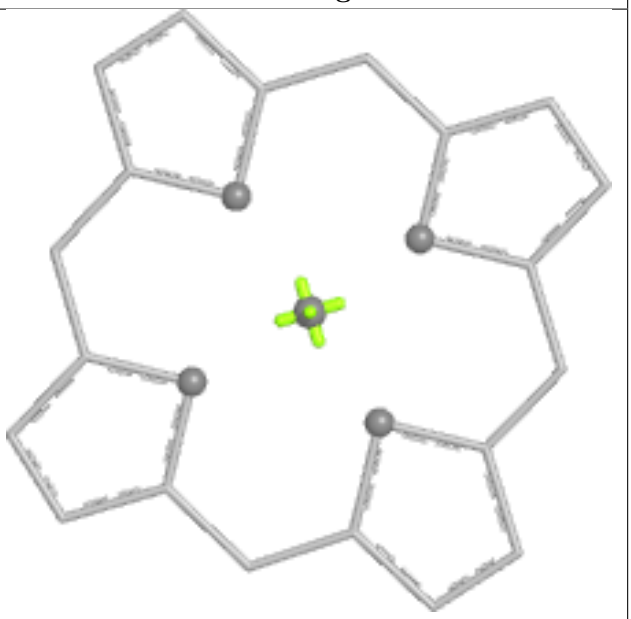
Bond lengths



Bond angles

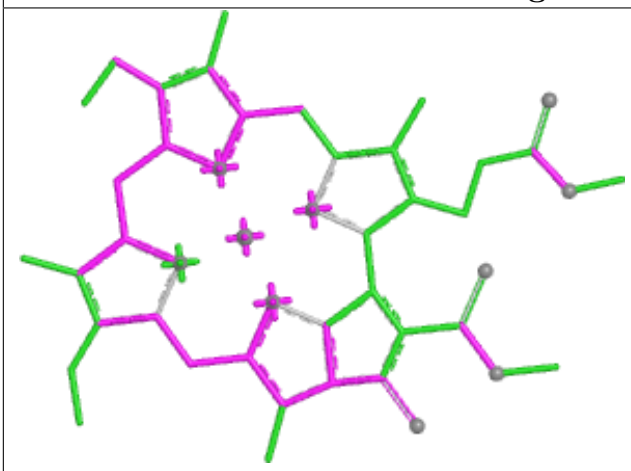


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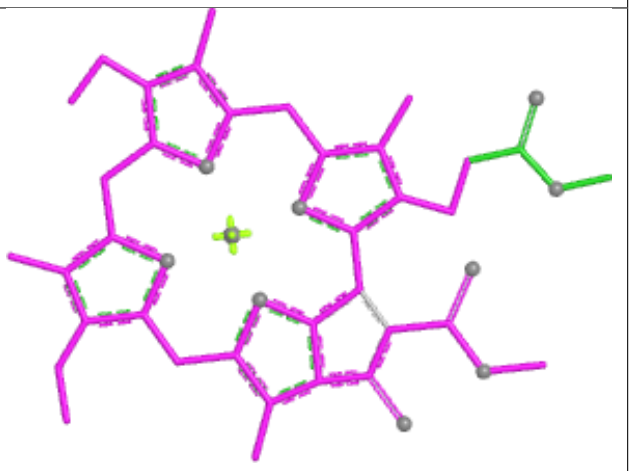


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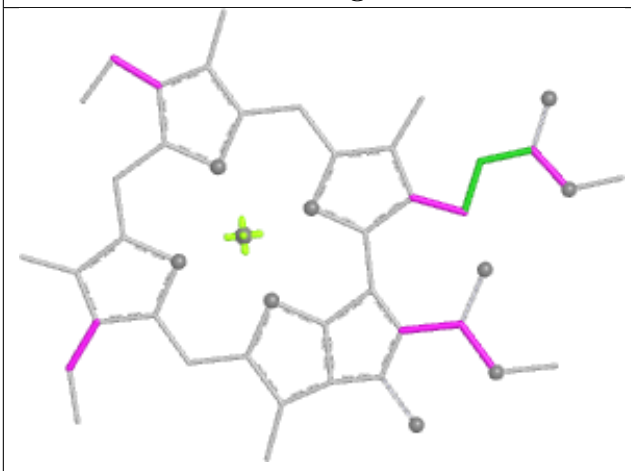
Ligand CLA 1 201



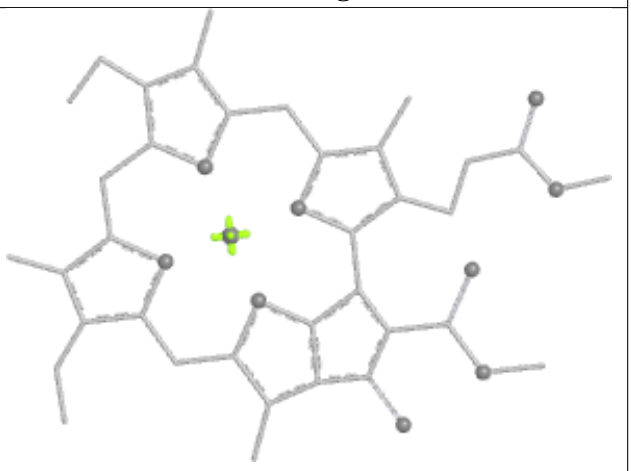
Bond lengths



Bond angles

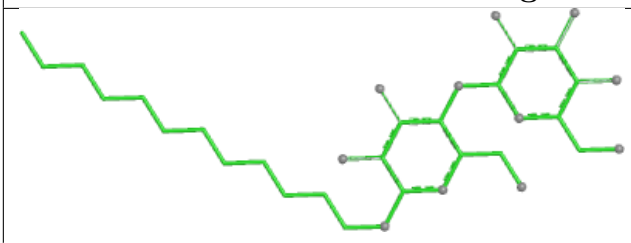


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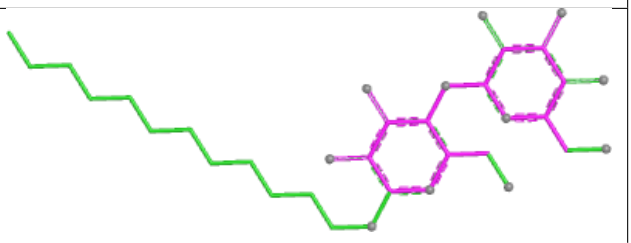


Rings

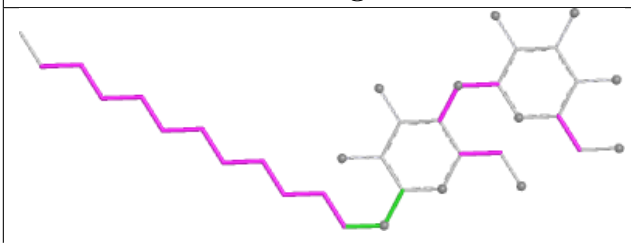
Ligand LMU B 801



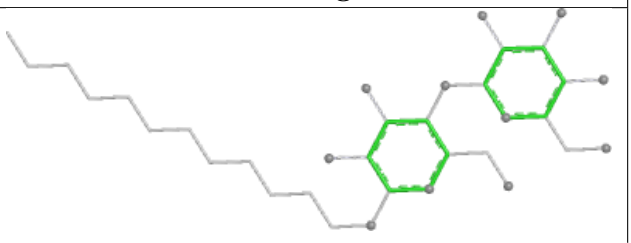
Bond lengths



Bond angles

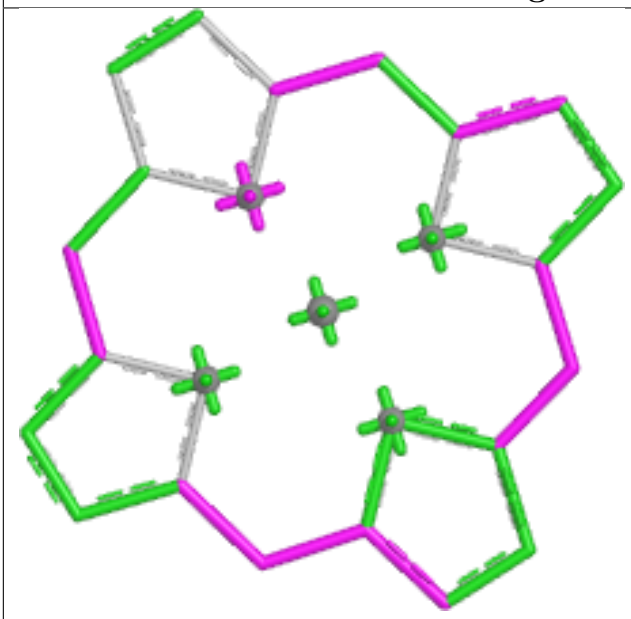


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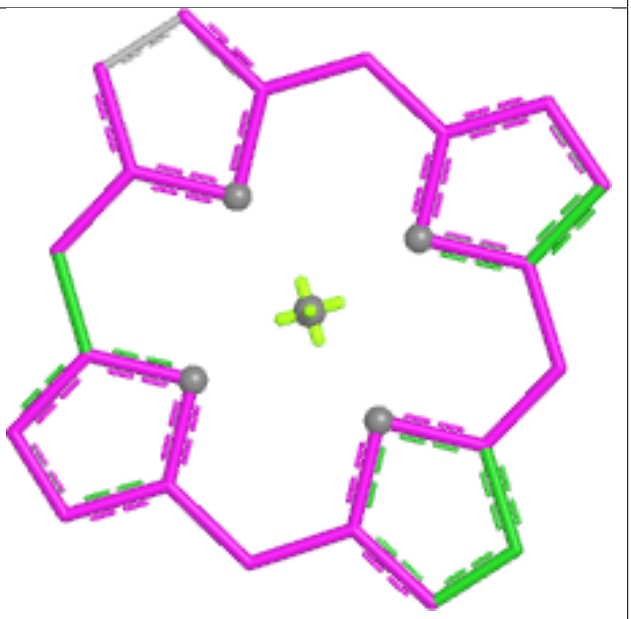


Rings

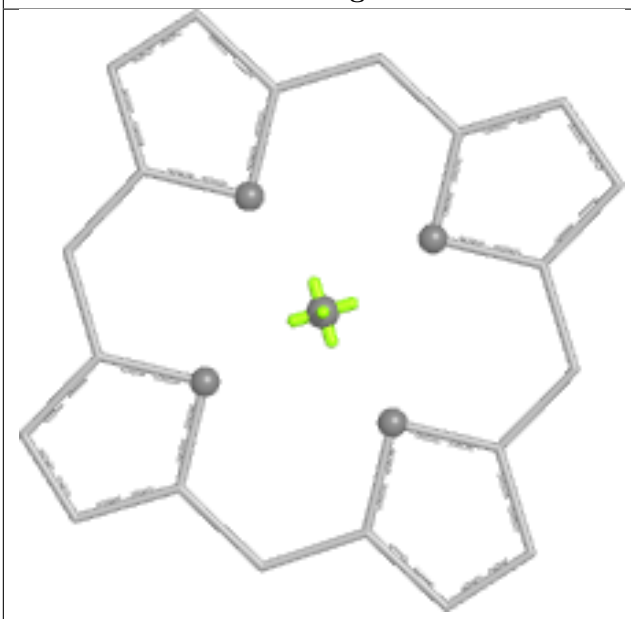
Ligand CLA 3 308



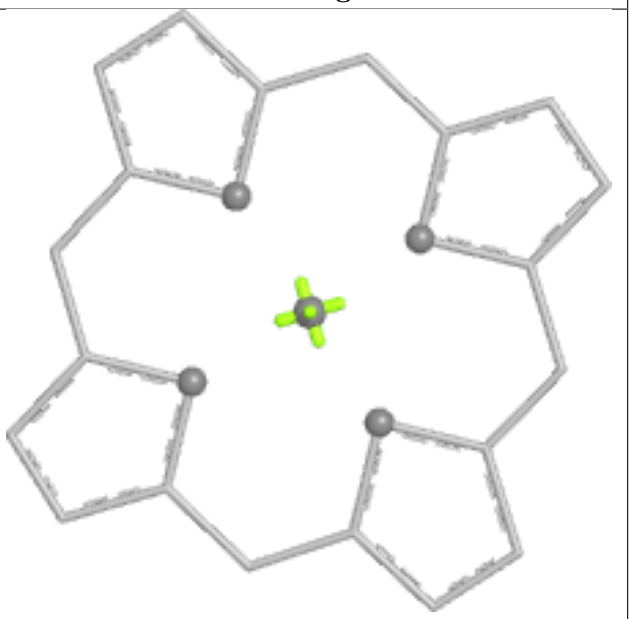
Bond lengths



Bond angles

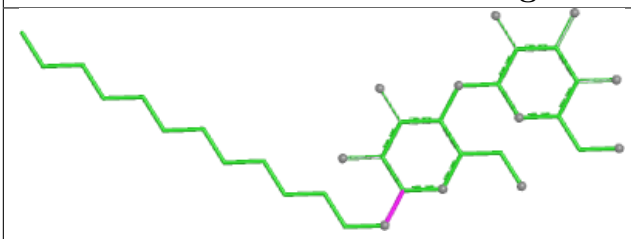


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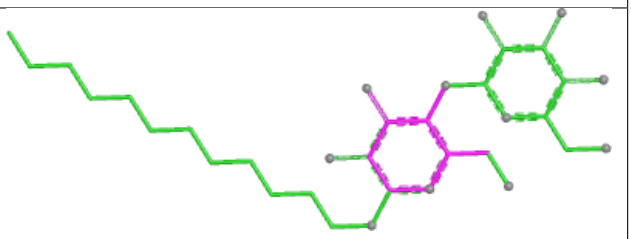


Rings

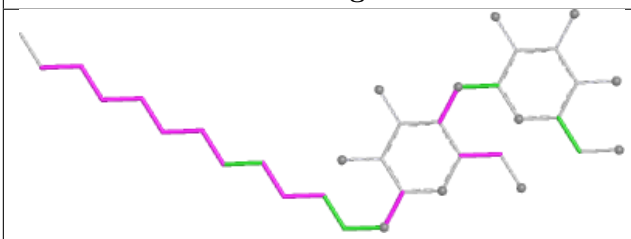
Ligand LMU A 854



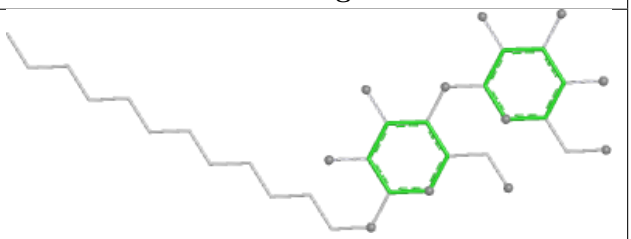
Bond lengths



Bond angles

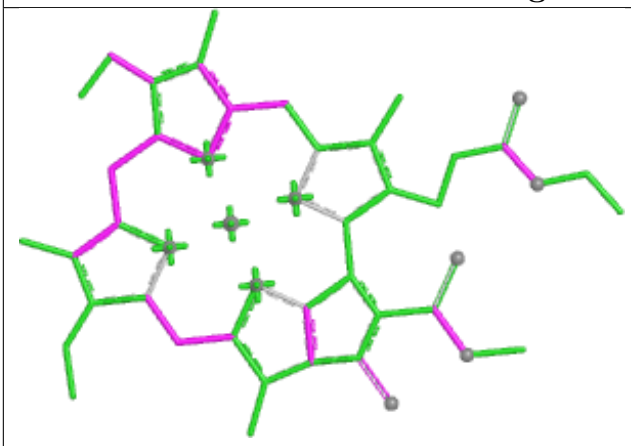


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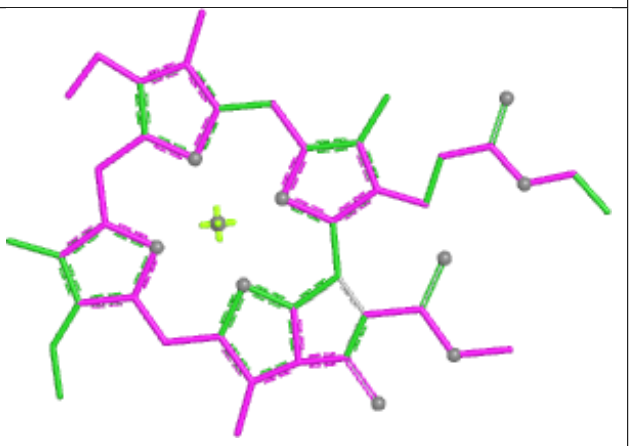


Rings

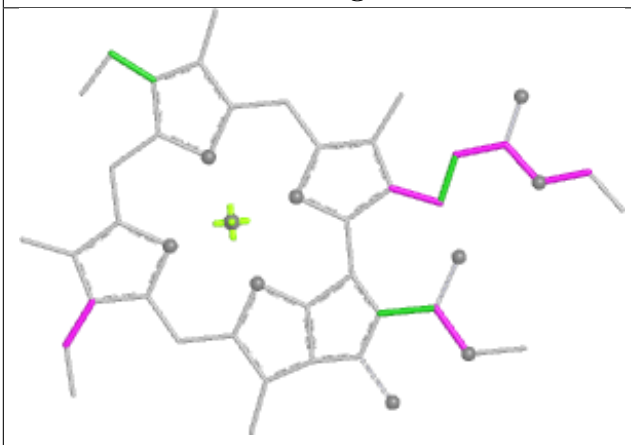
Ligand CLA 1 202



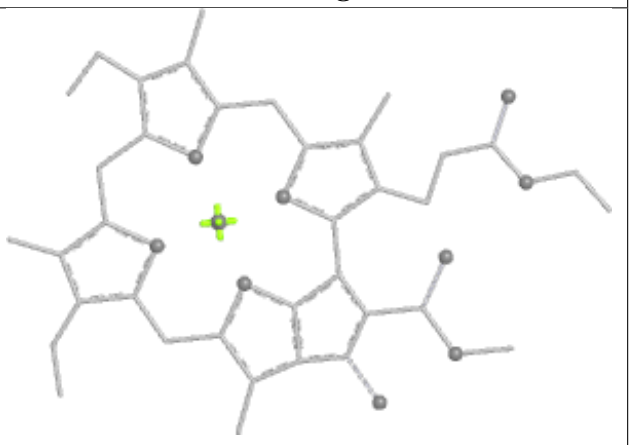
Bond lengths



Bond angles

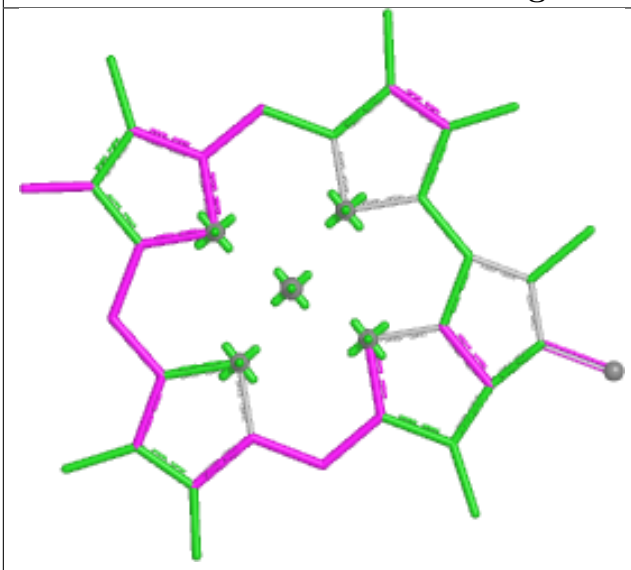


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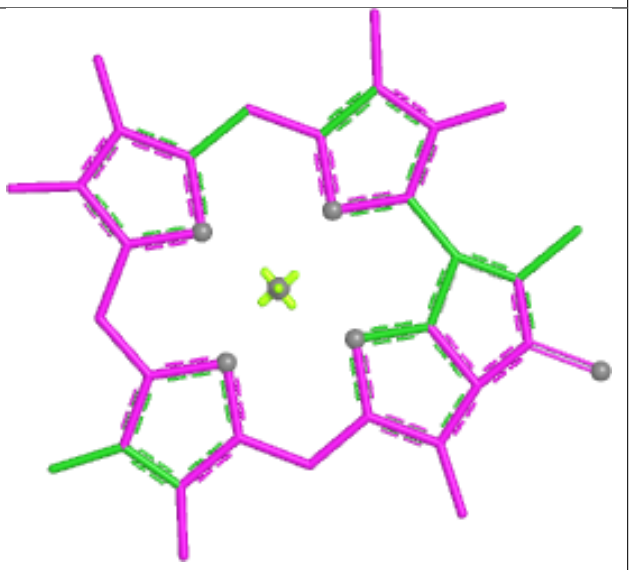


Rings

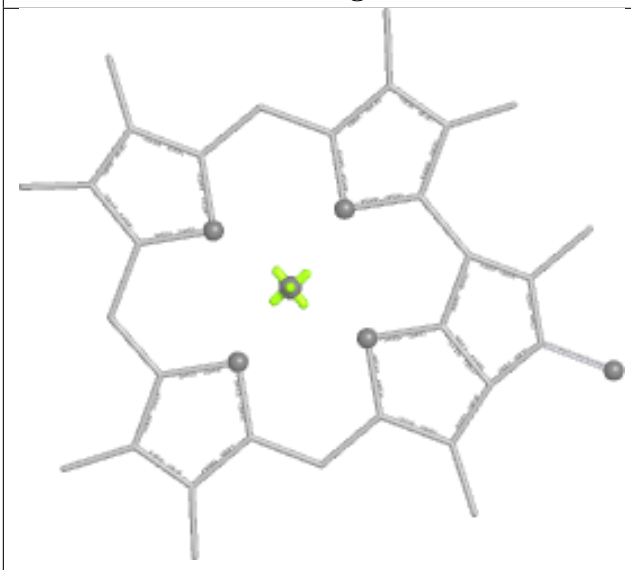
Ligand CLA 4 303



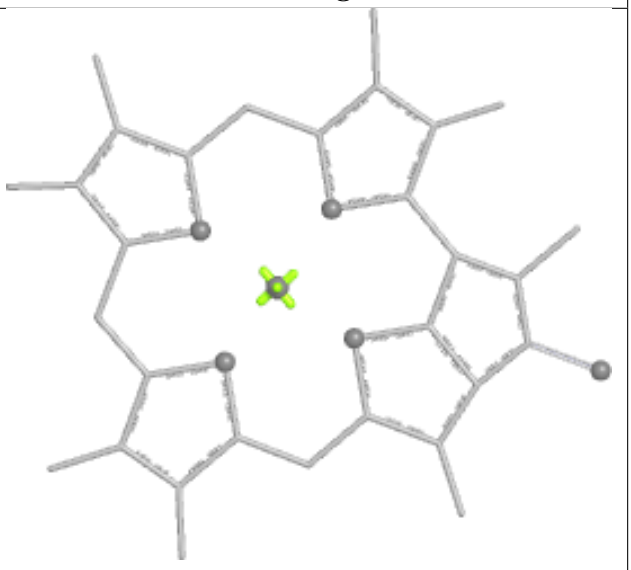
Bond lengths



Bond angles

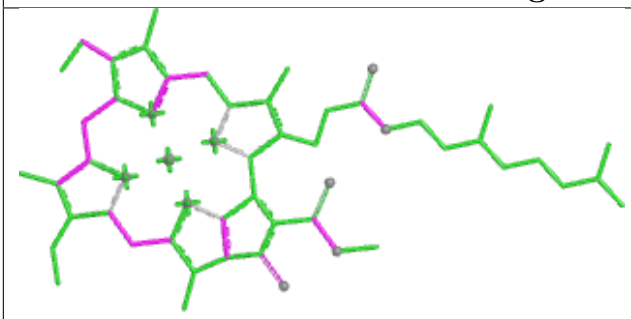


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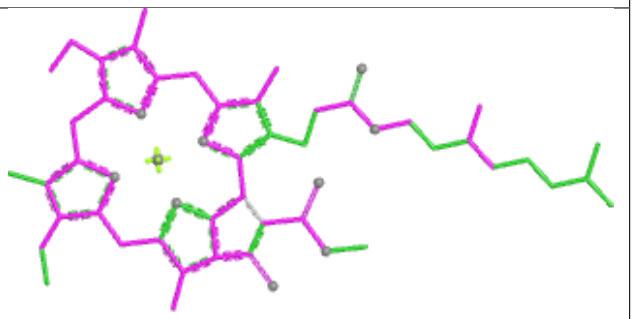


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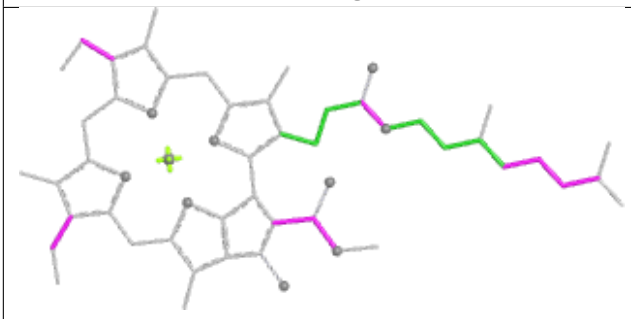
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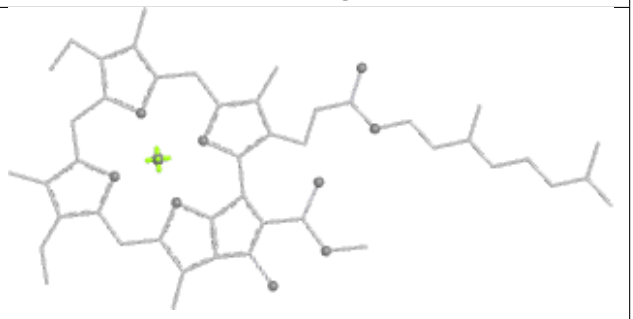
Bond lengths



Bond angles

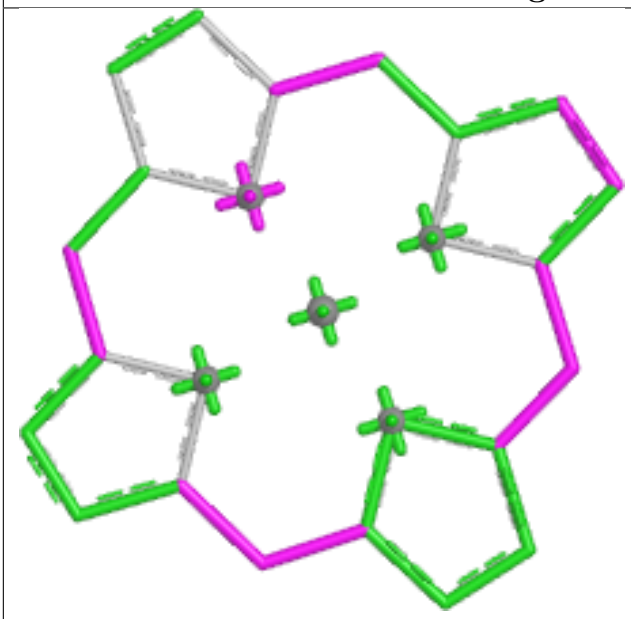


Torsions

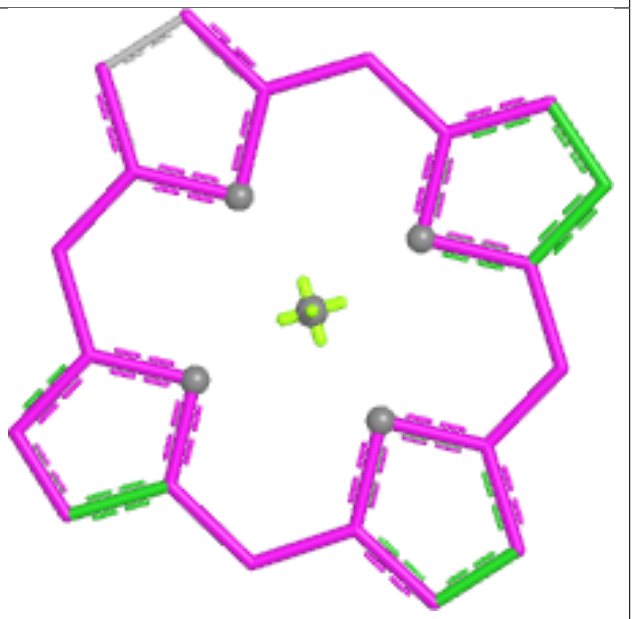


Rings

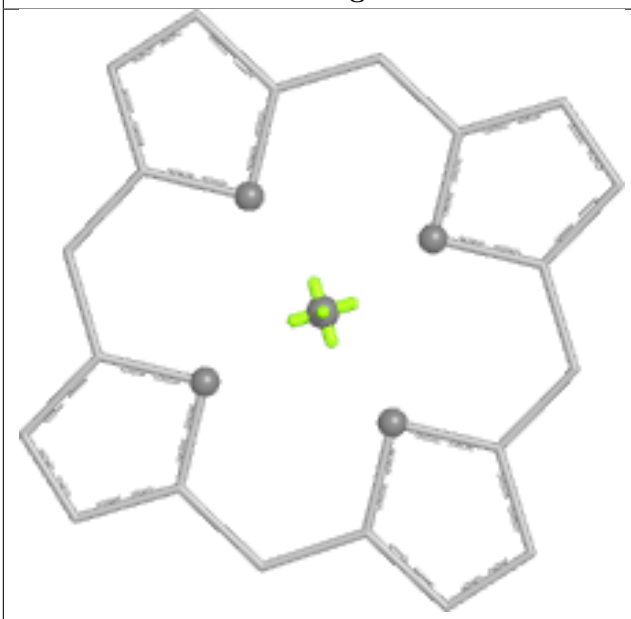
Ligand CLA 2 315



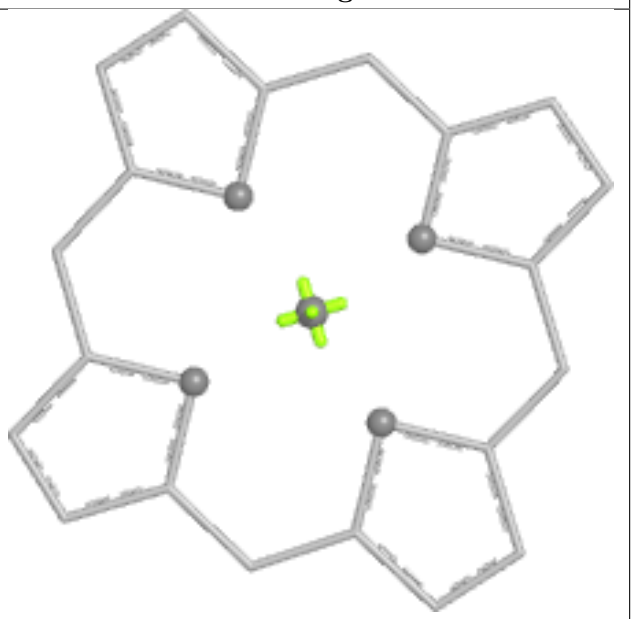
Bond lengths



Bond angles

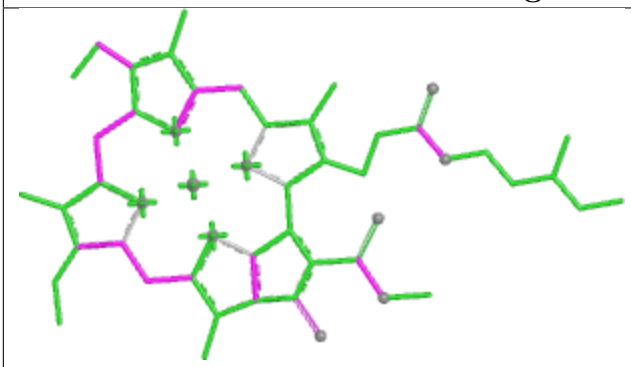


Torsions

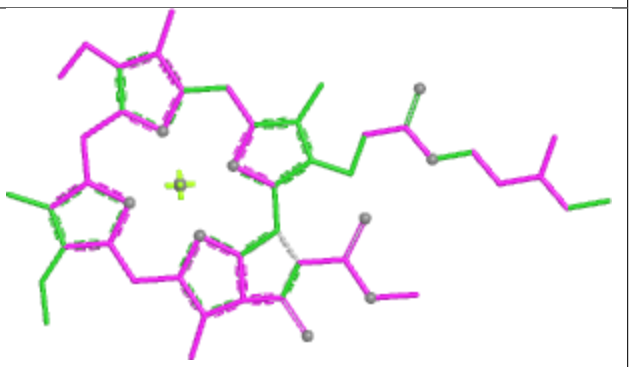


Rings

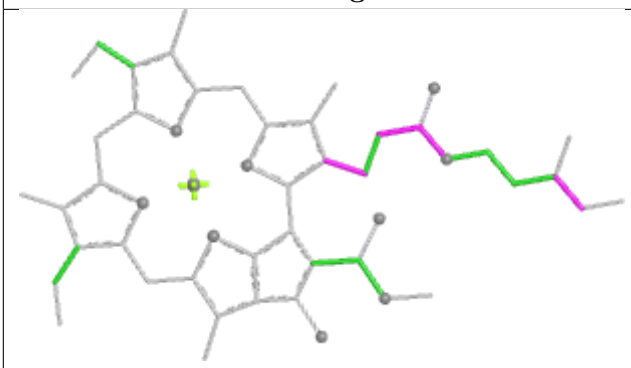
Ligand CLA B 833



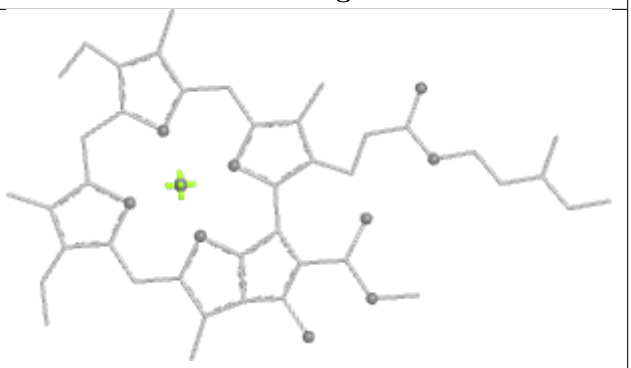
Bond lengths



Bond angles

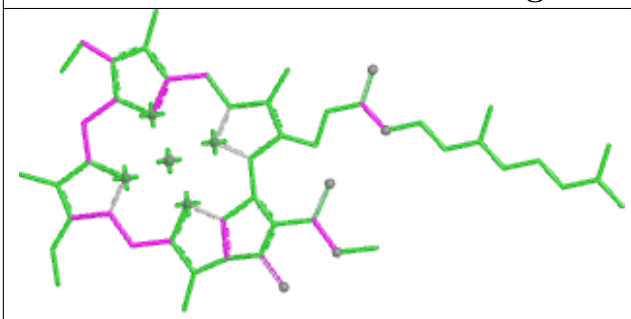


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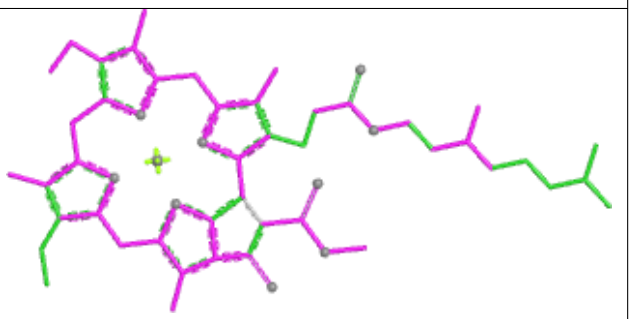


Rings

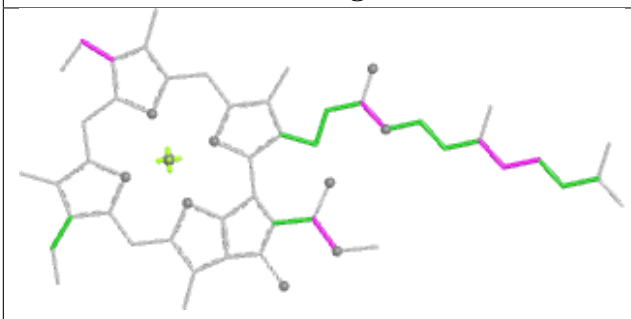
Ligand CLA L 203



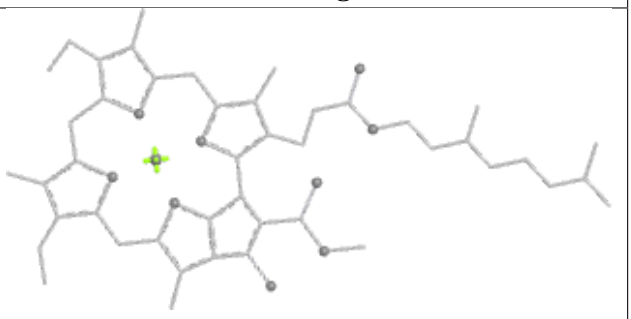
Bond lengths



Bond angles

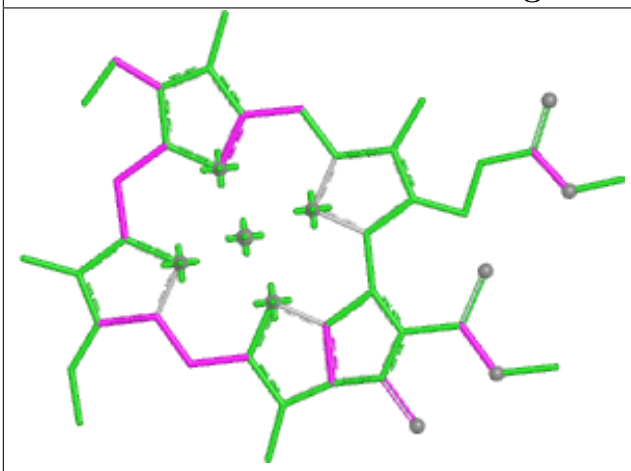


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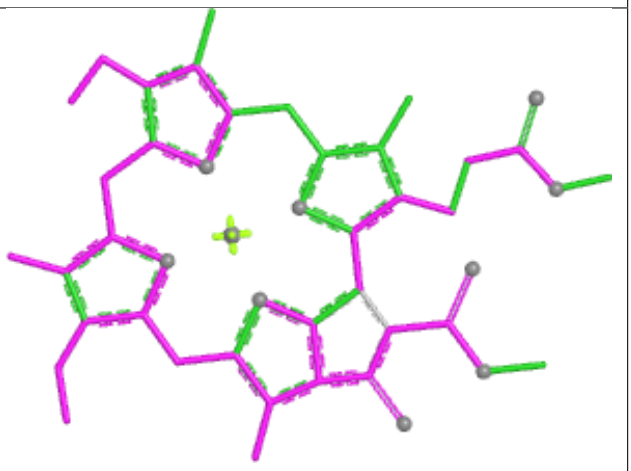


Rings

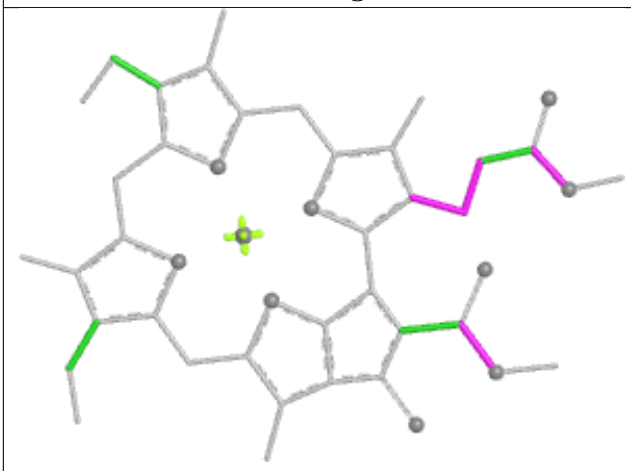
Ligand CLA A 805



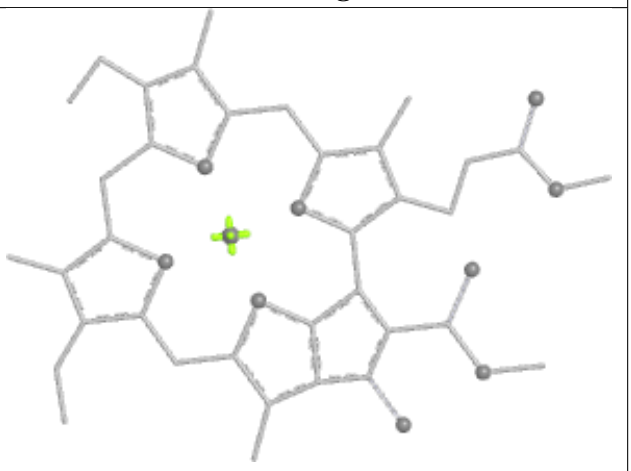
Bond lengths



Bond angles

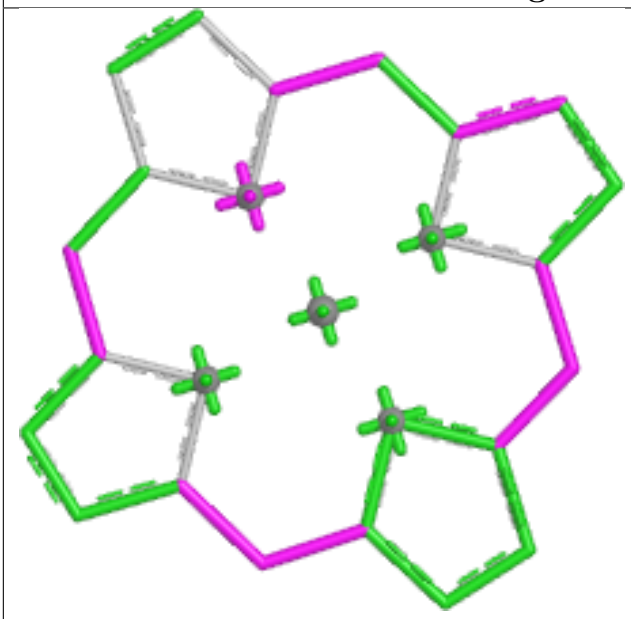


Torsions

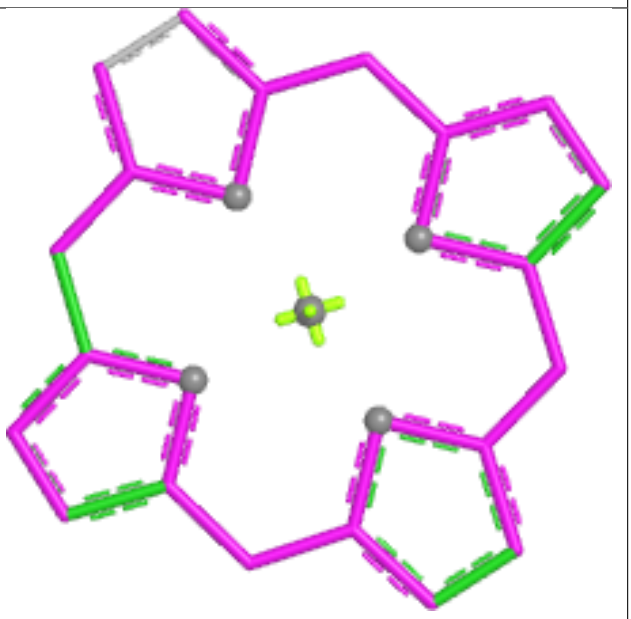


Rings

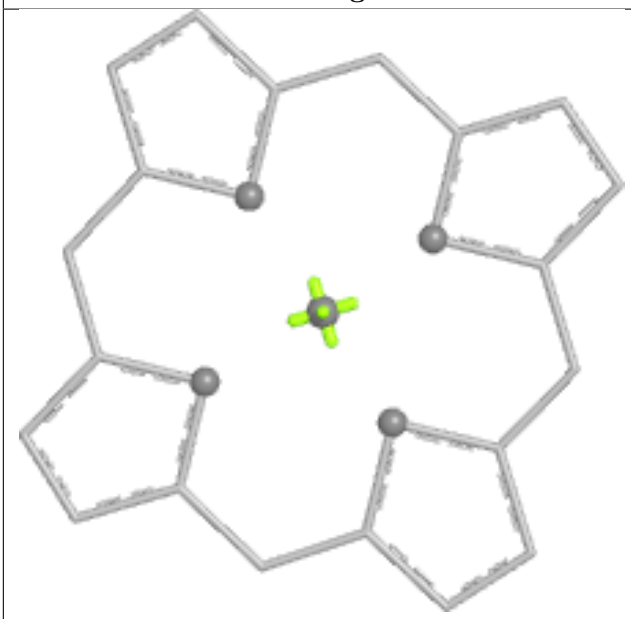
Ligand CLA 2 309



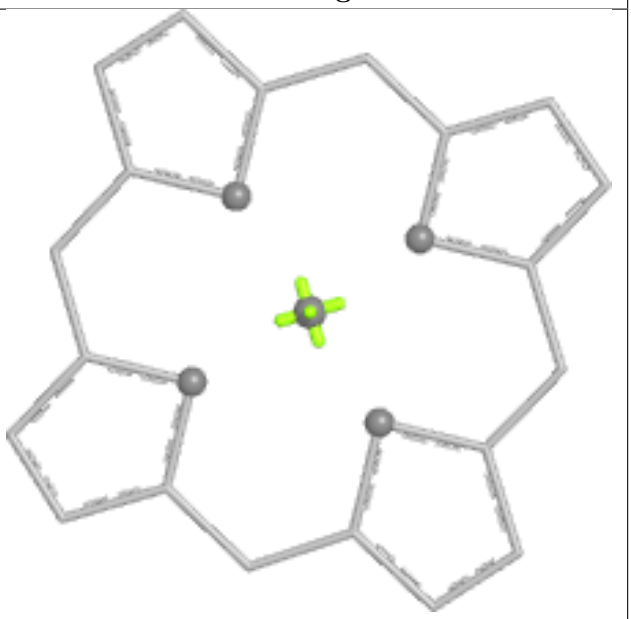
Bond lengths



Bond angles

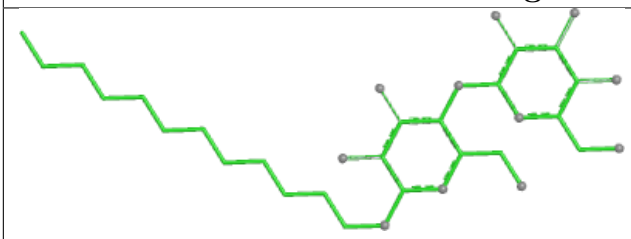


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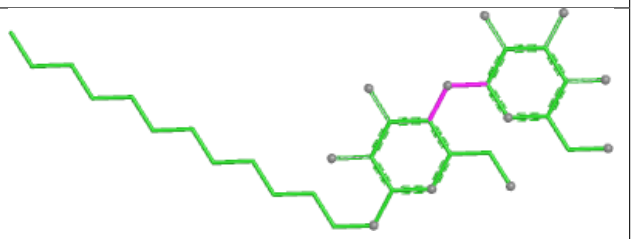


Rings

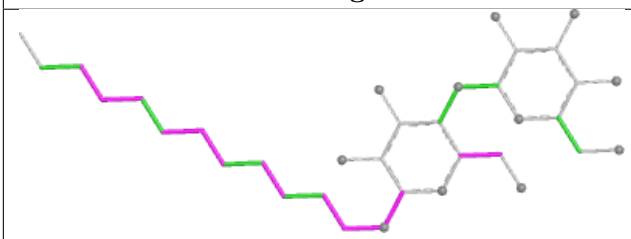
Ligand LMU 3 302



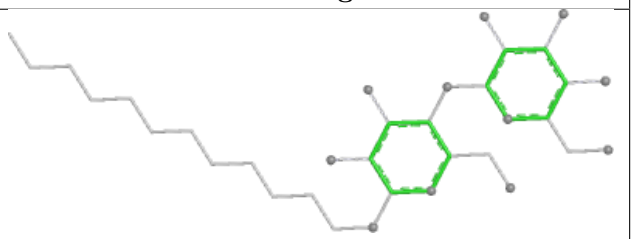
Bond lengths



Bond angles

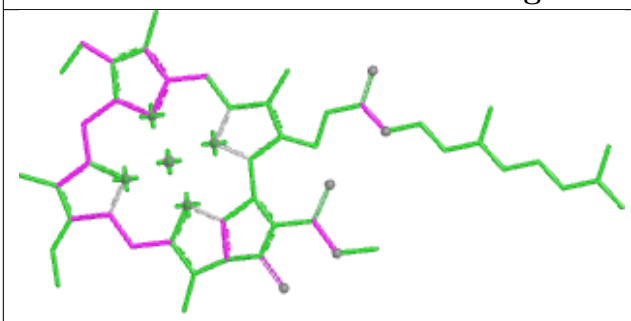


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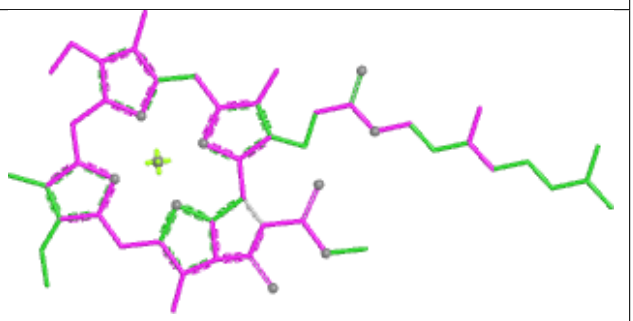


Rings

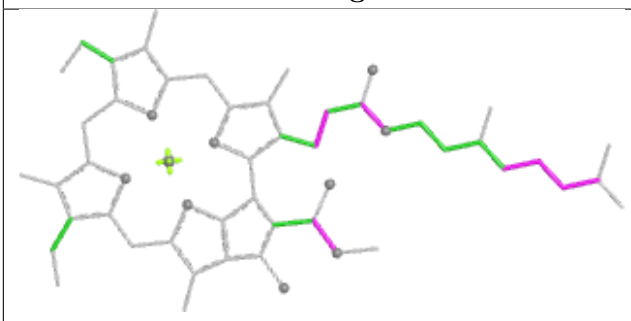
Ligand CLA A 825



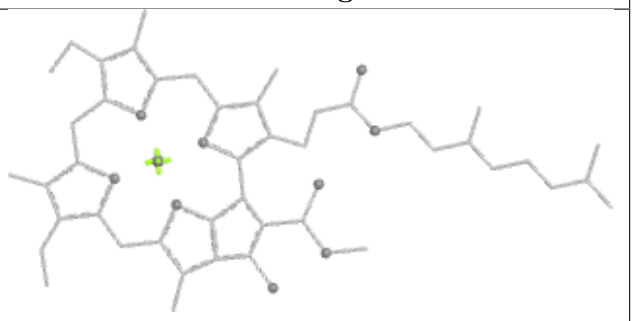
Bond lengths



Bond angles

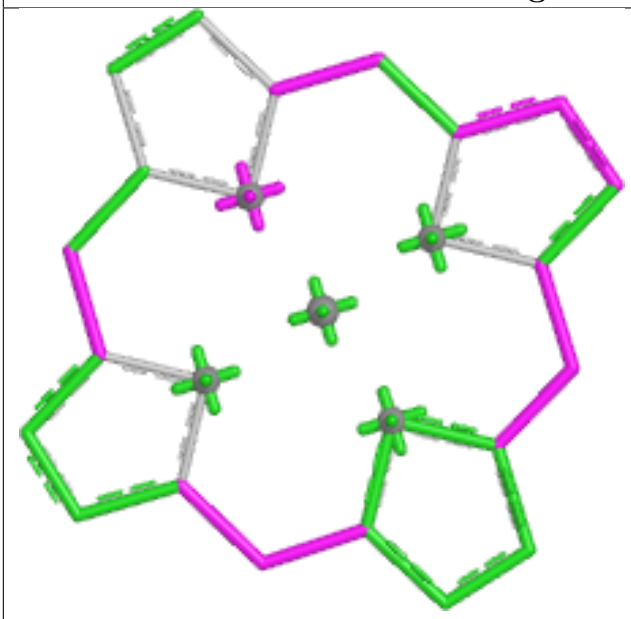


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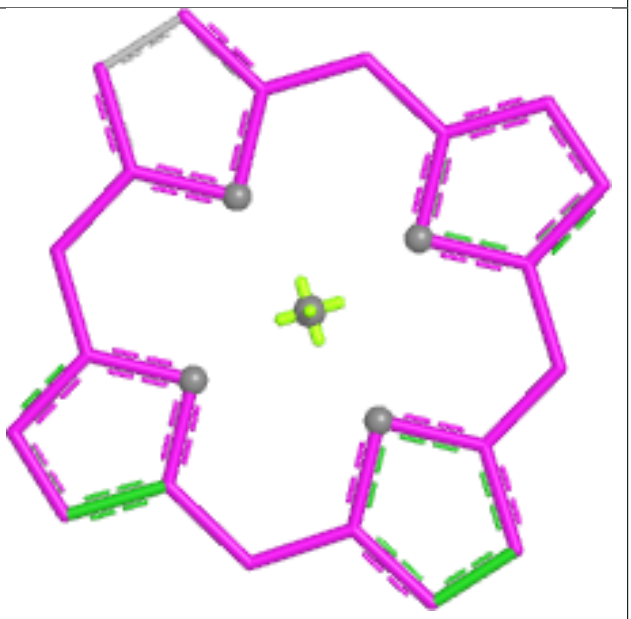


Rings

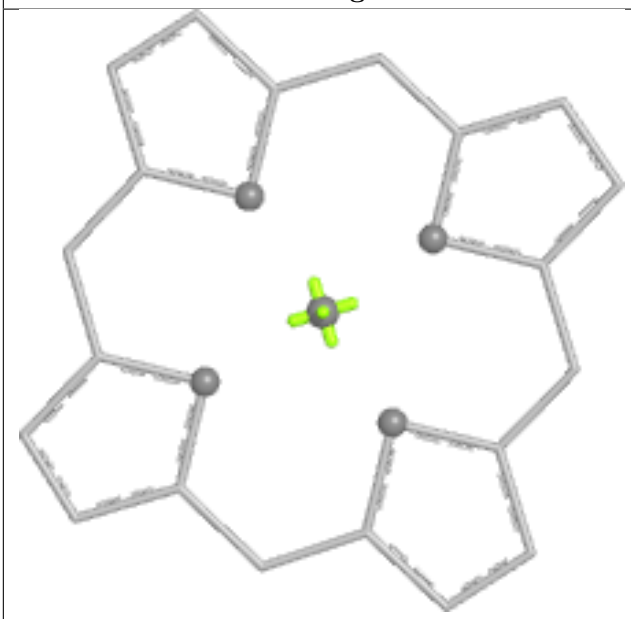
Ligand CLA 3 312



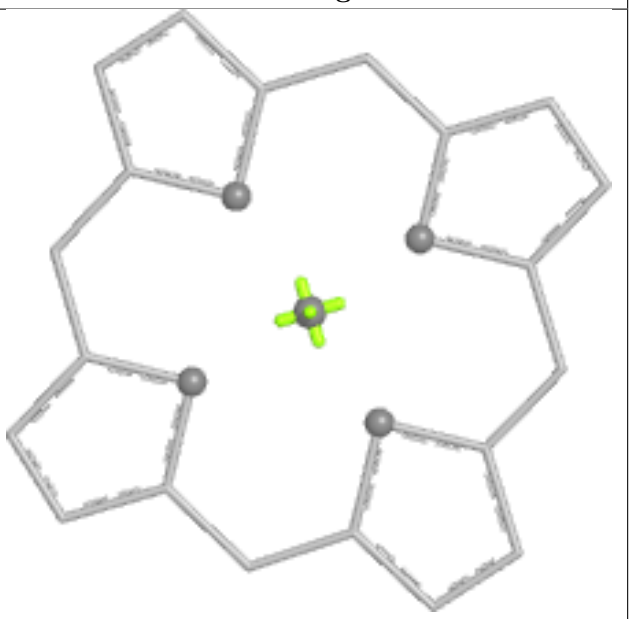
Bond lengths



Bond angles

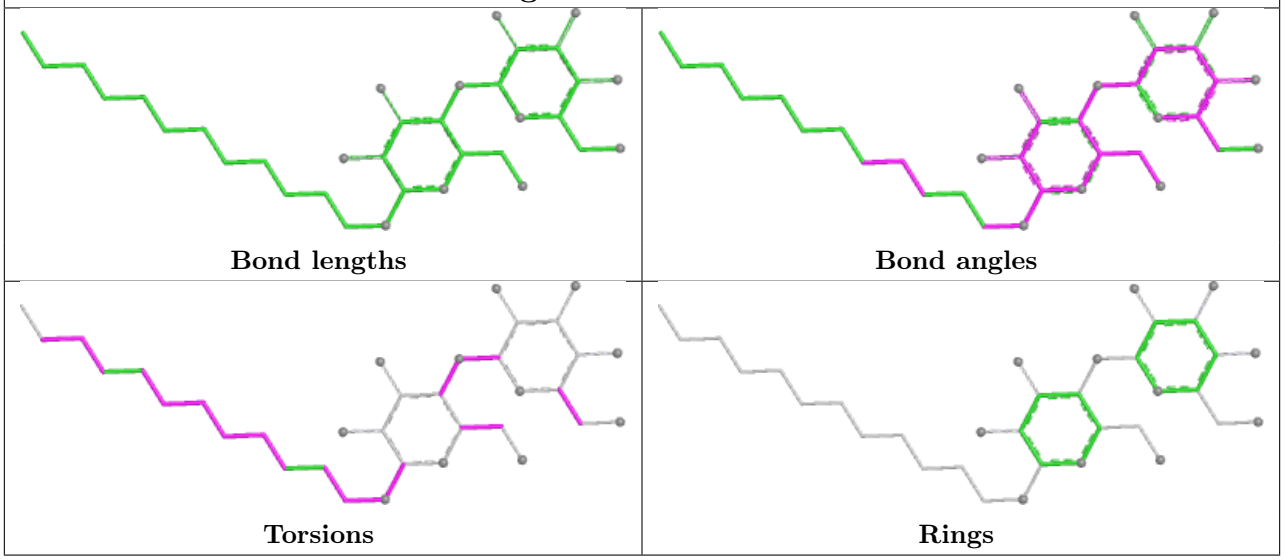


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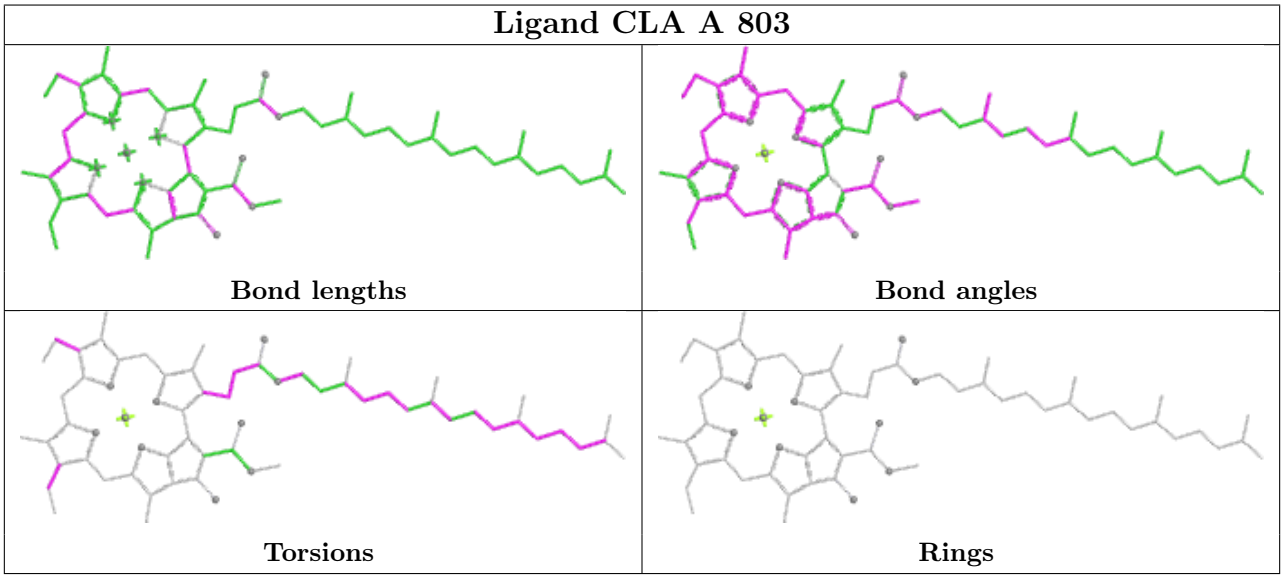


Rings

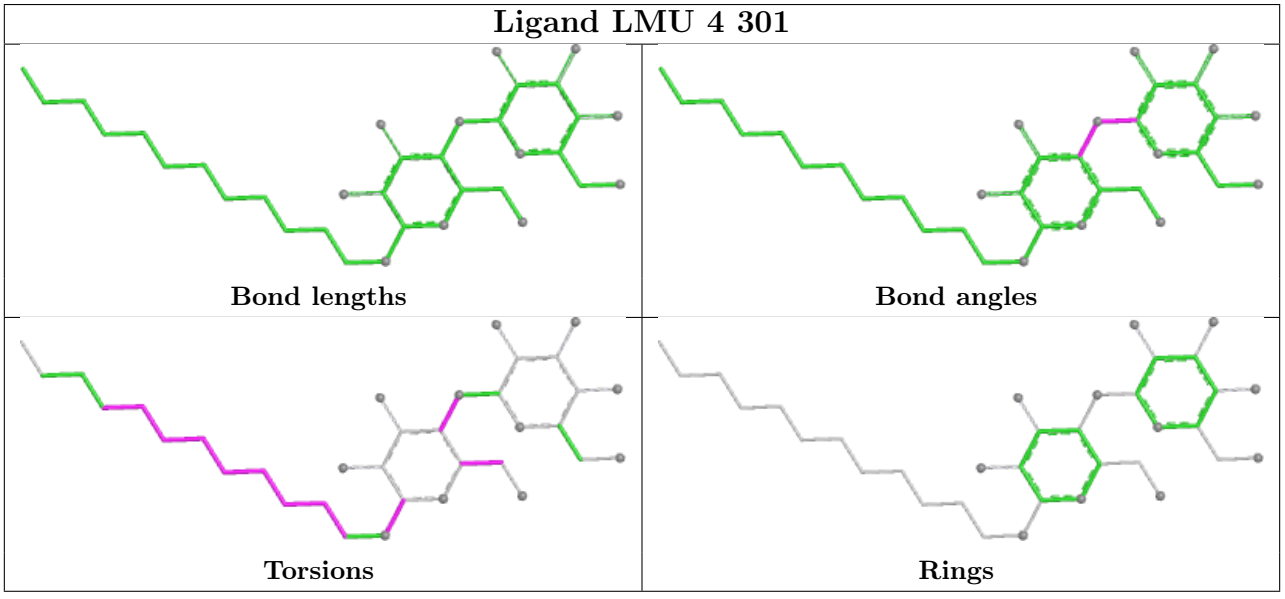
Ligand LMU K 102



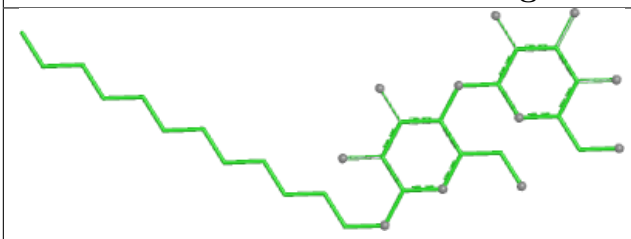
Ligand CLA A 803



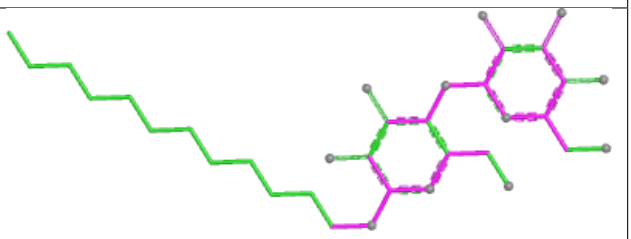
Ligand LMU 4 301



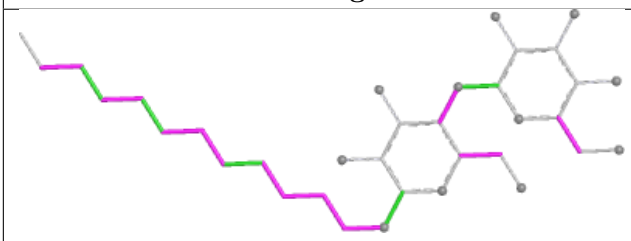
Ligand LMU R 102



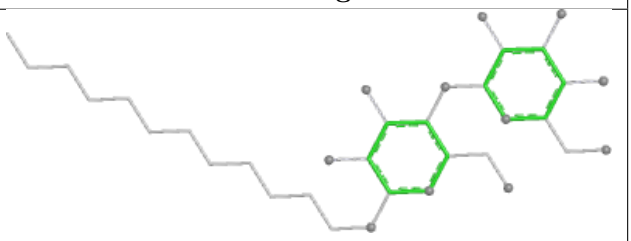
Bond lengths



Bond angles

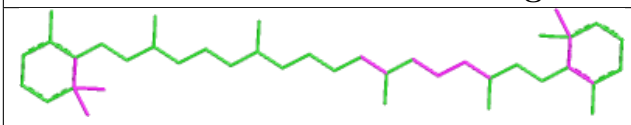


Torsions

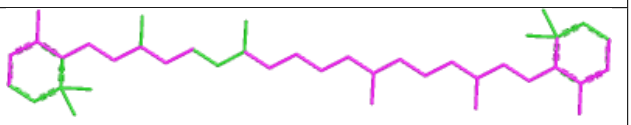


Rings

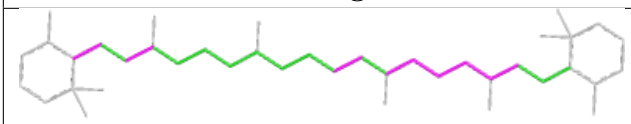
Ligand BCR L 209



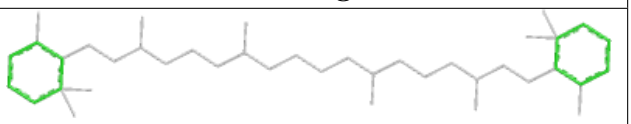
Bond lengths



Bond angles

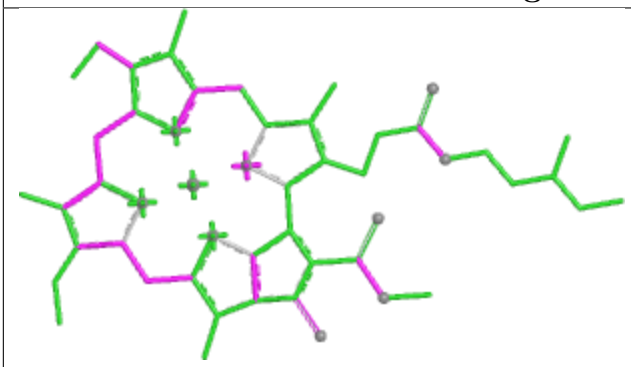


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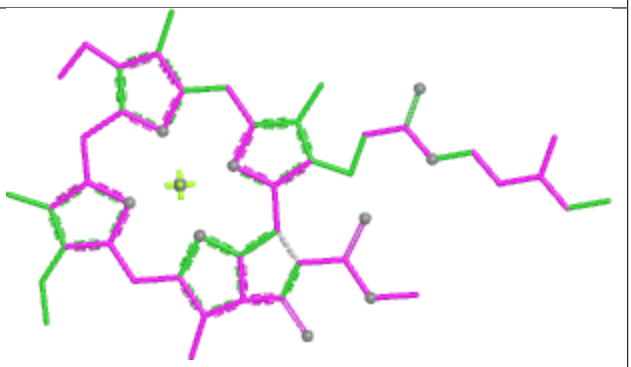


Rings

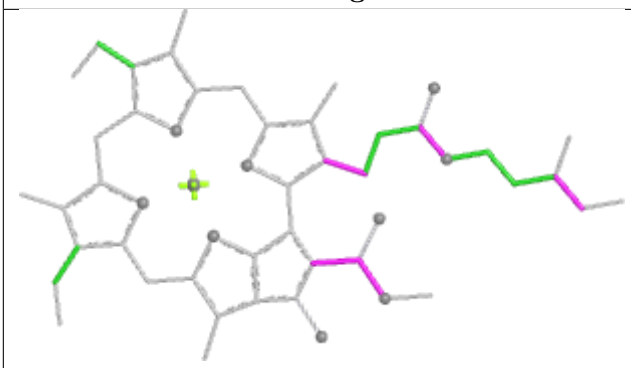
Ligand CLA A 818



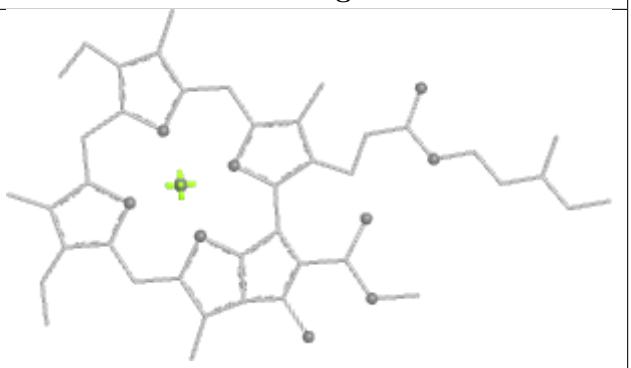
Bond lengths



Bond angles

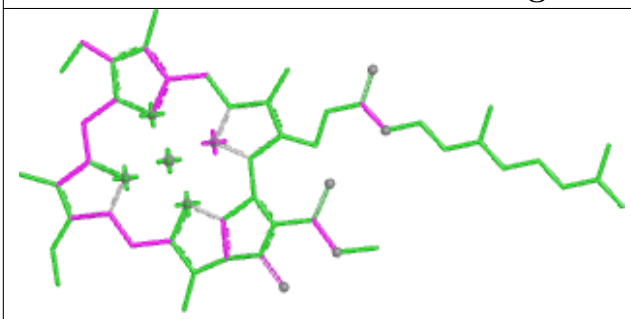


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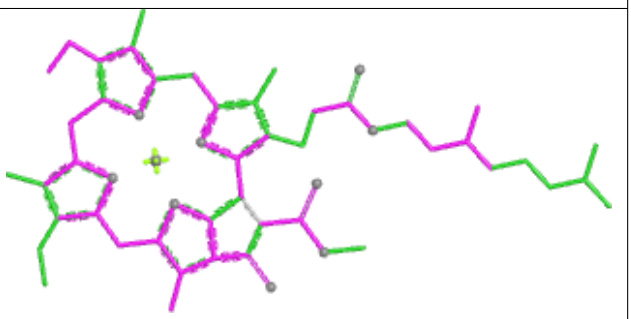


Rings

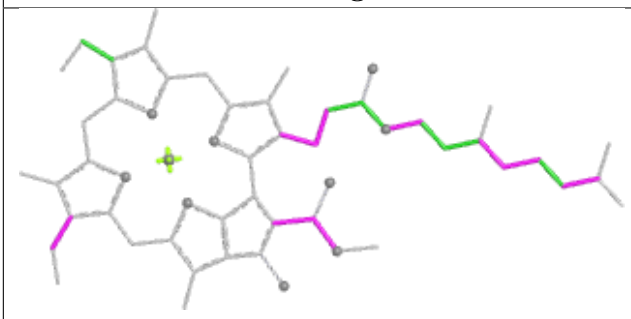
Ligand CLA 4 302



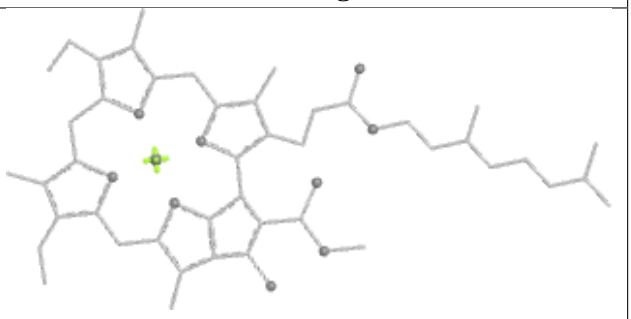
Bond lengths



Bond angles

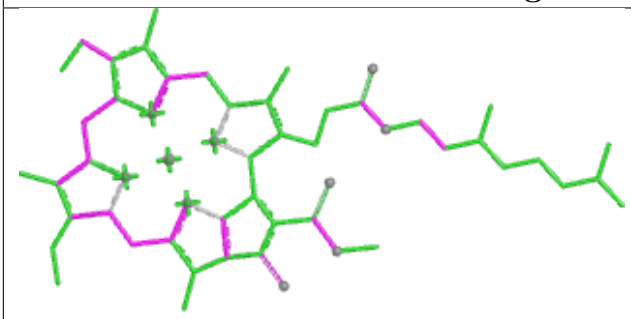


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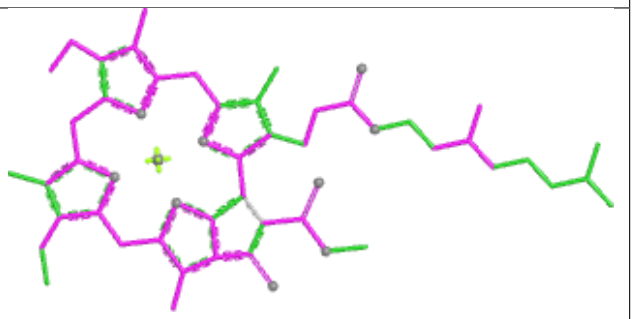


Rings

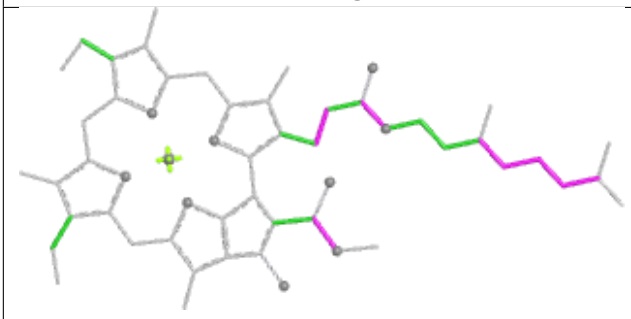
Ligand CLA B 809



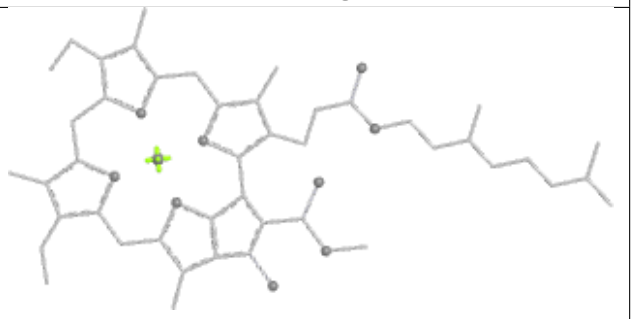
Bond lengths



Bond angles

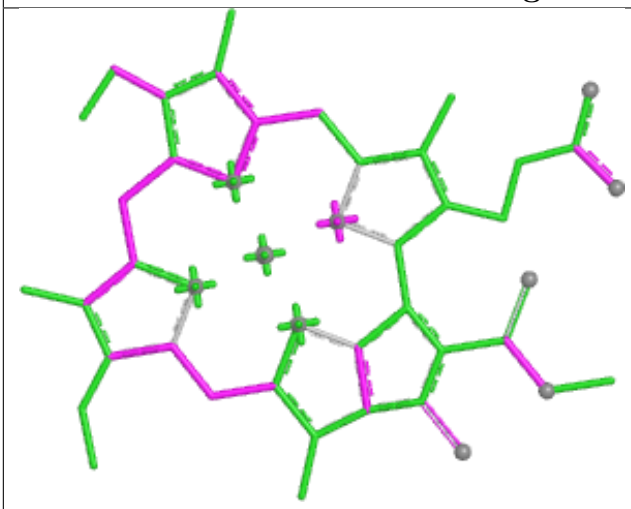


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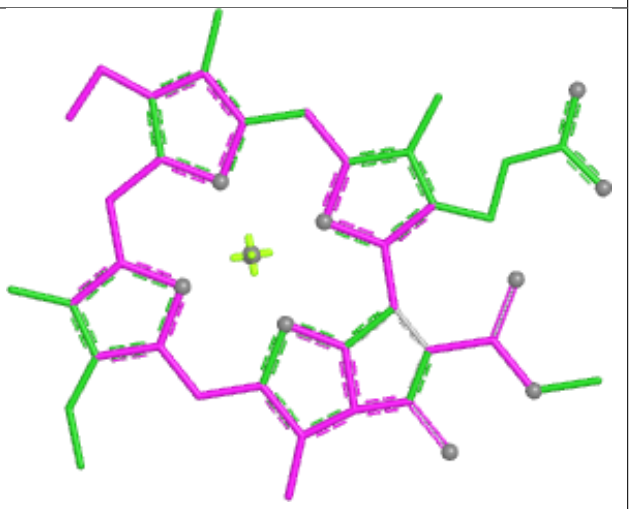


Rings

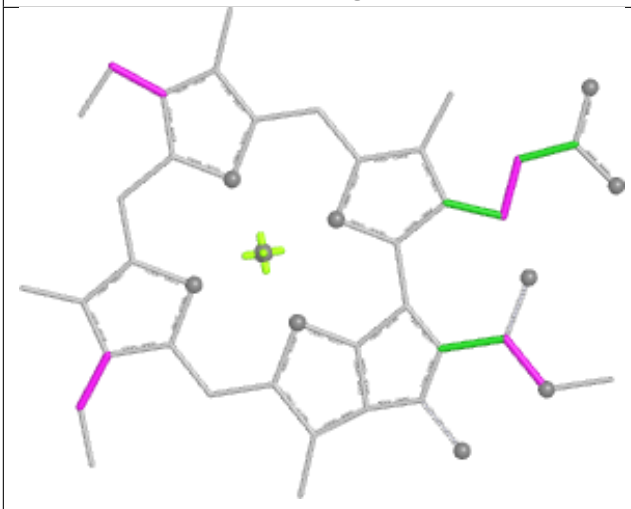
Ligand CLA K 105



Bond lengths



Bond angles

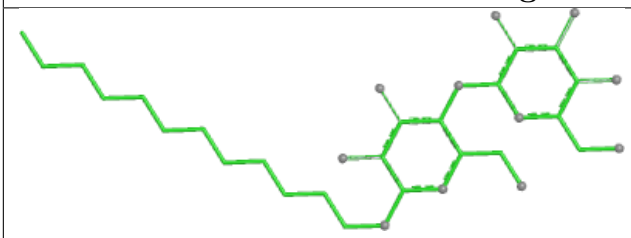


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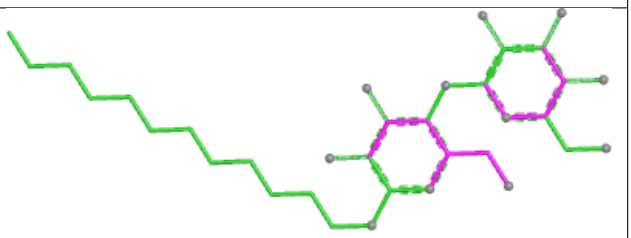


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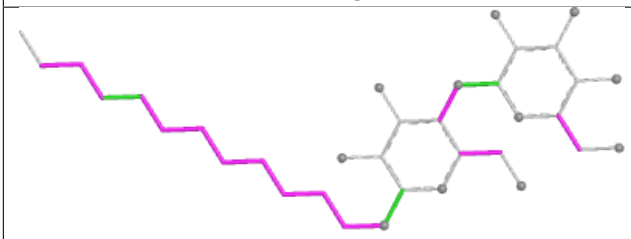
Ligand LMU A 845



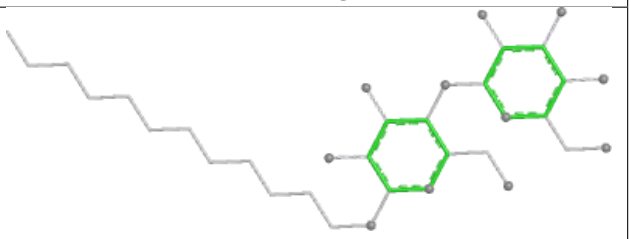
Bond lengths



Bond angles

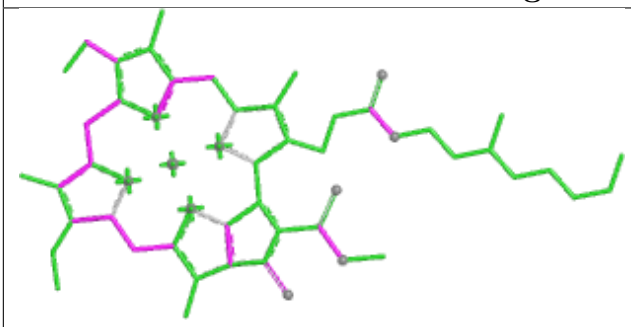


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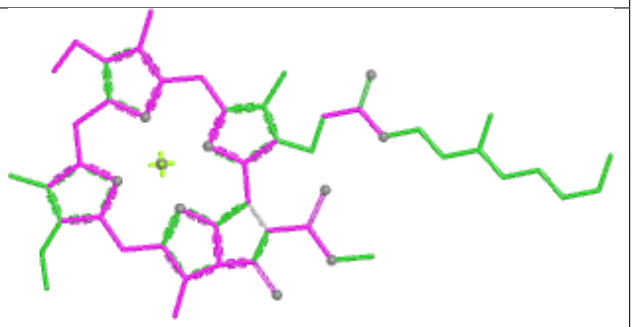


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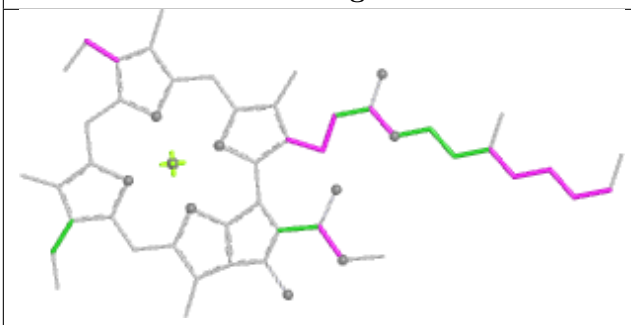
Ligand CLA A 810



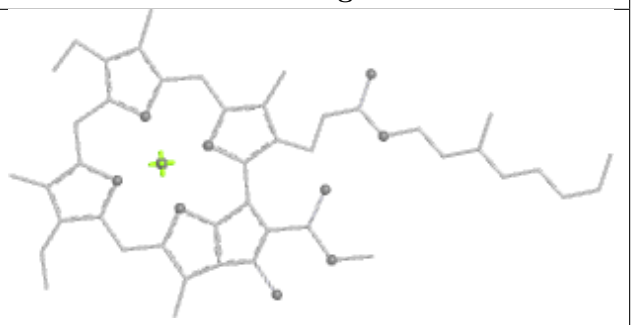
Bond lengths



Bond angles

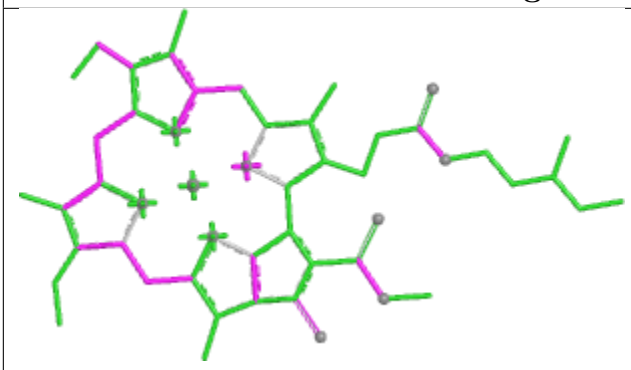


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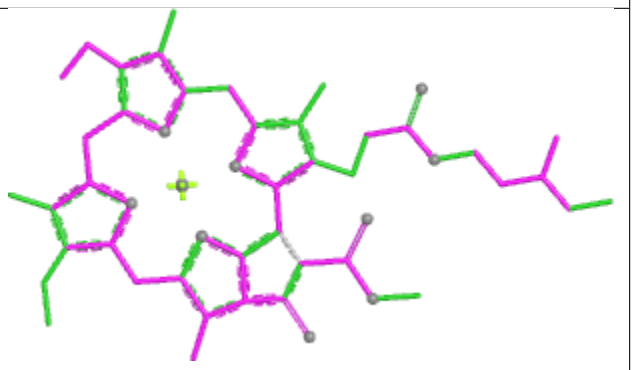


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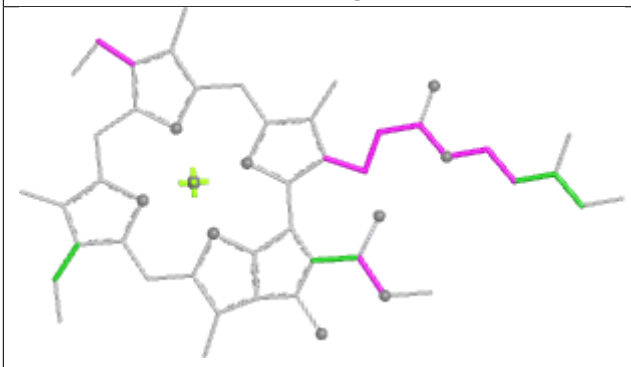
Ligand CLA A 835



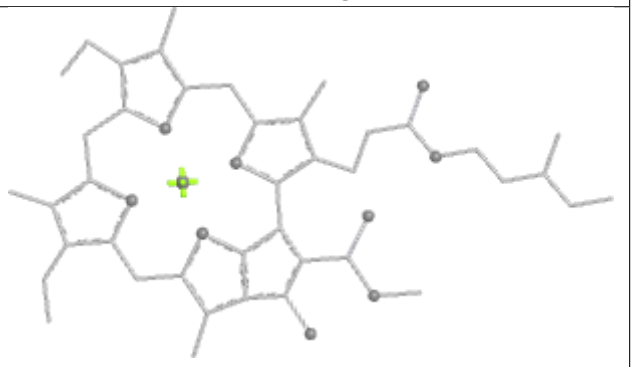
Bond lengths



Bond angles

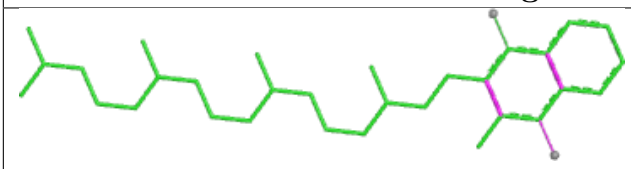


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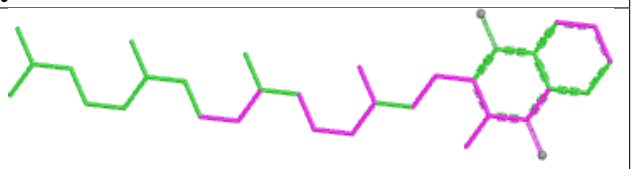


Rings

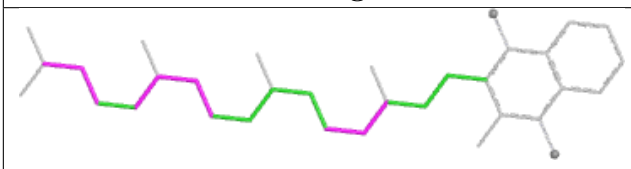
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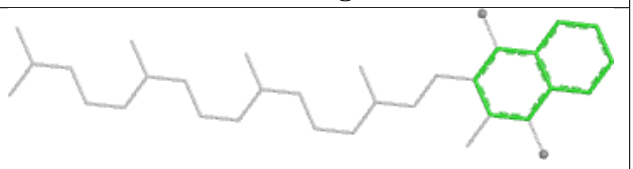
Bond lengths



Bond angles

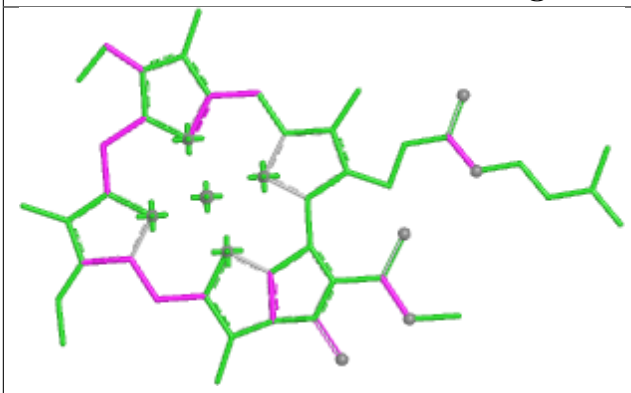


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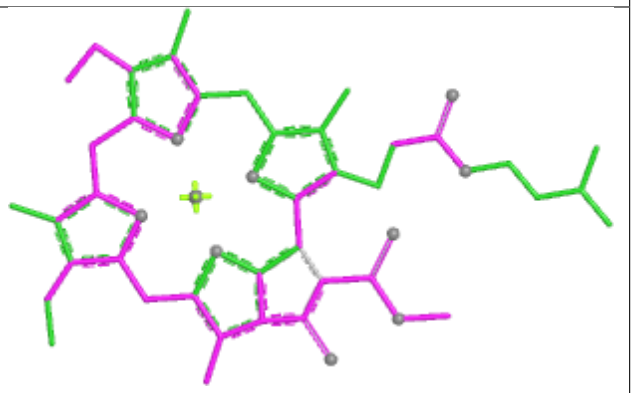


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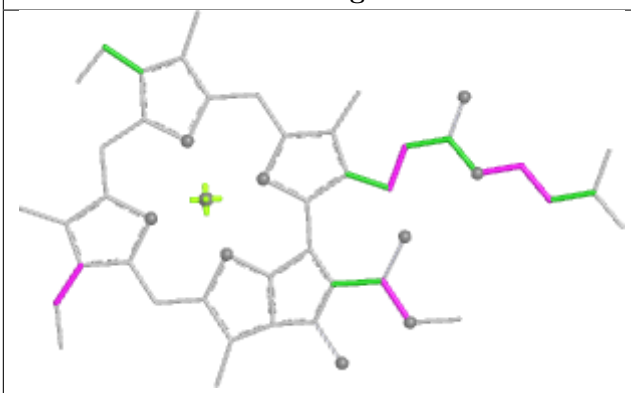
Ligand CLA 4 306



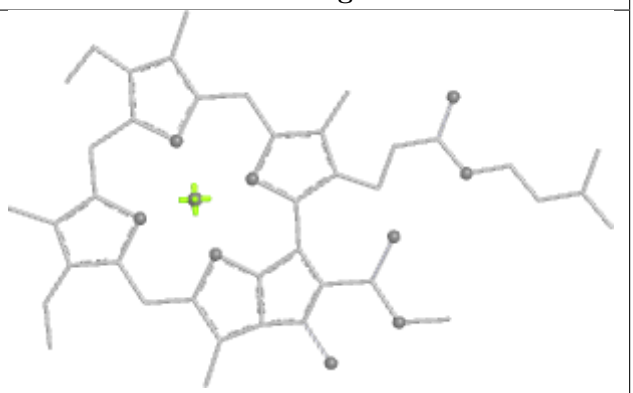
Bond lengths



Bond angles

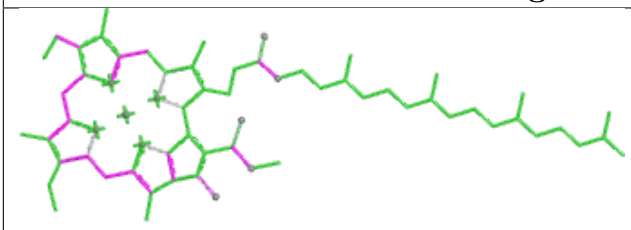


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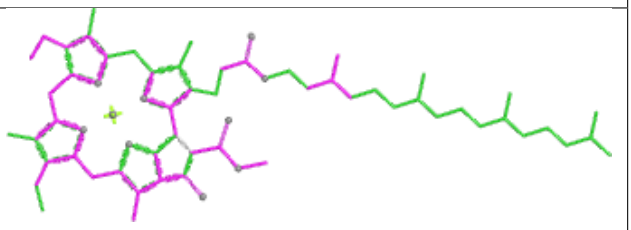


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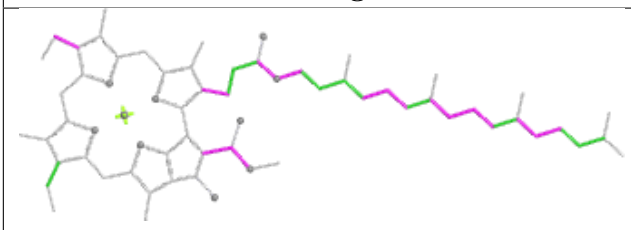
Ligand CLA 2 312



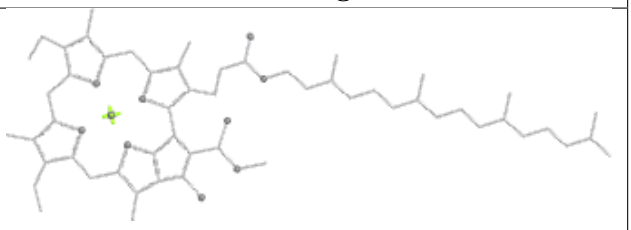
Bond lengths



Bond angles

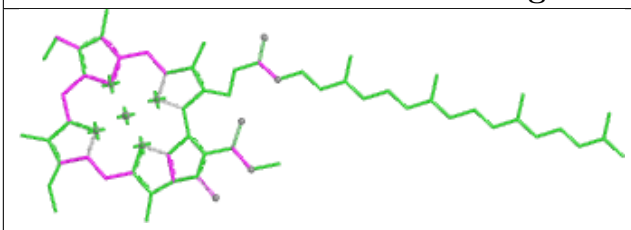


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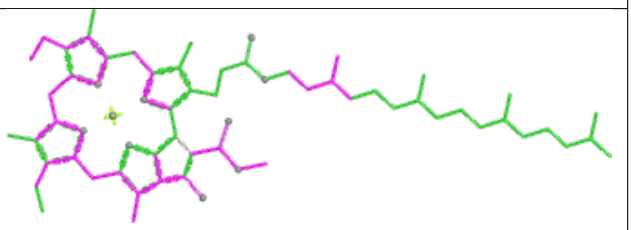


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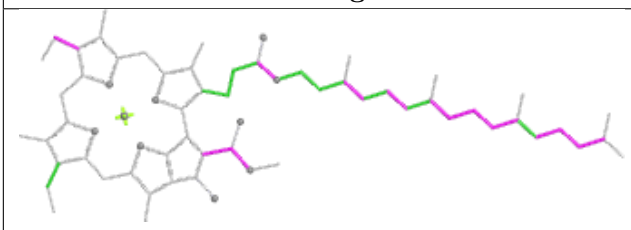
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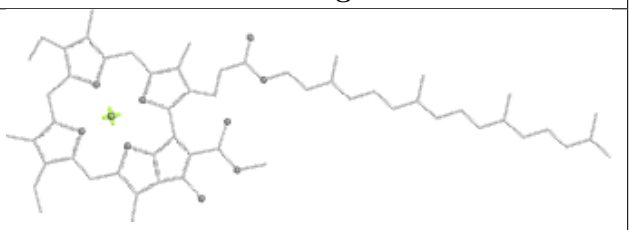
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Bond angles

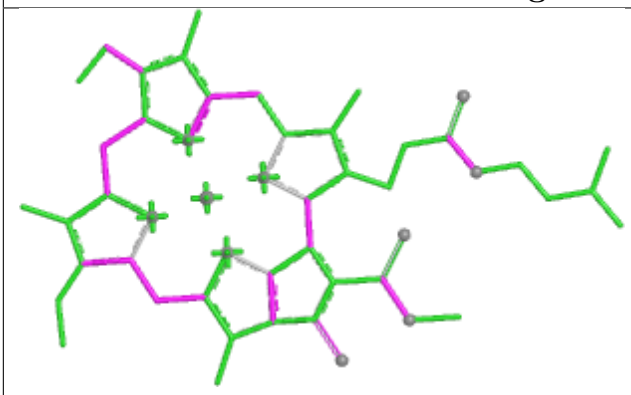


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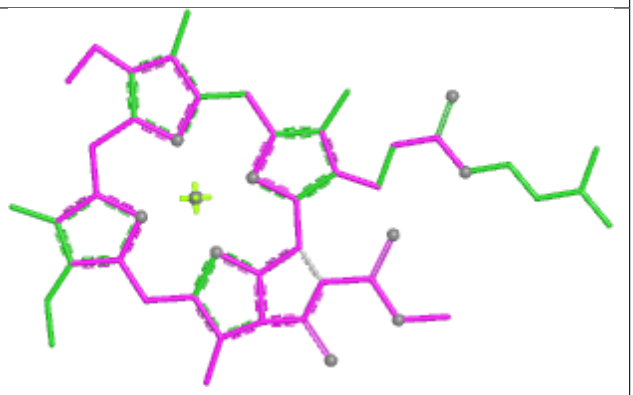


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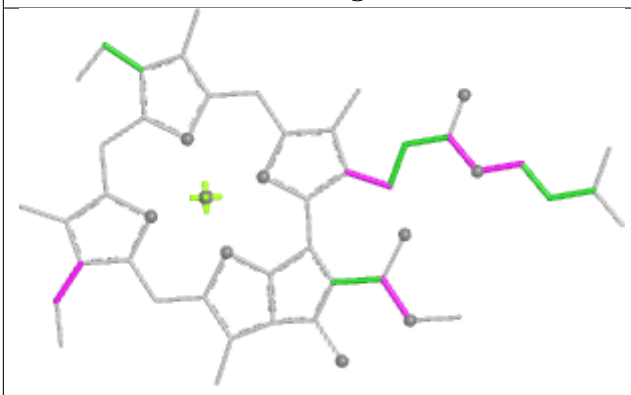
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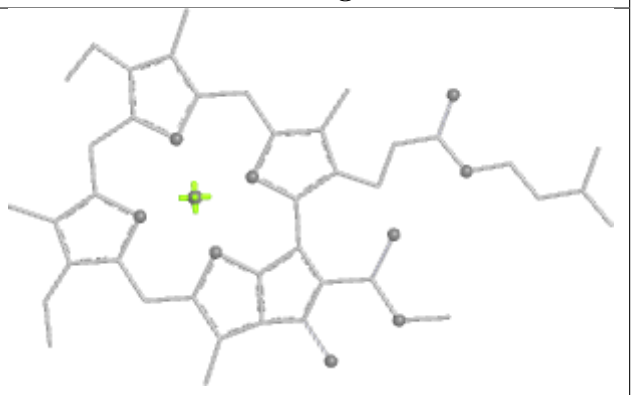
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Bond angles

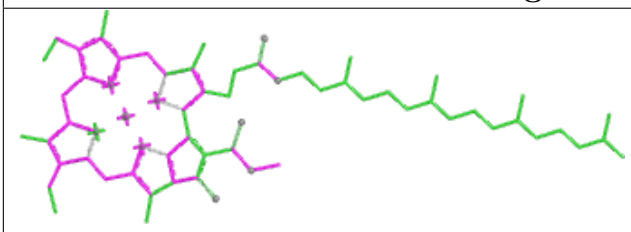


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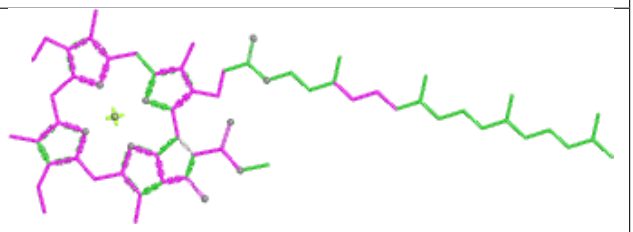


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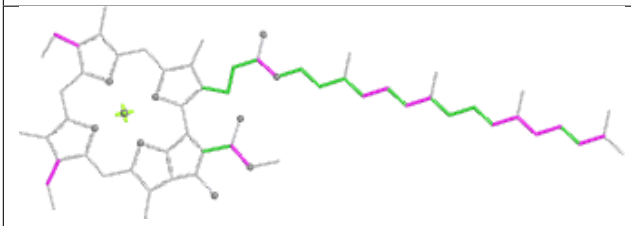
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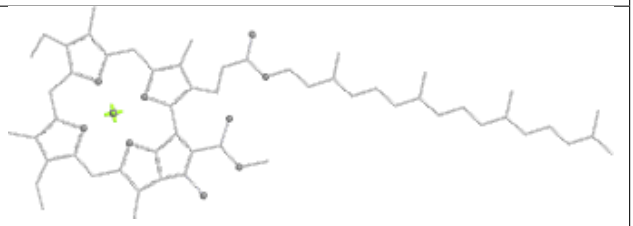
Bond lengths



Bond angles

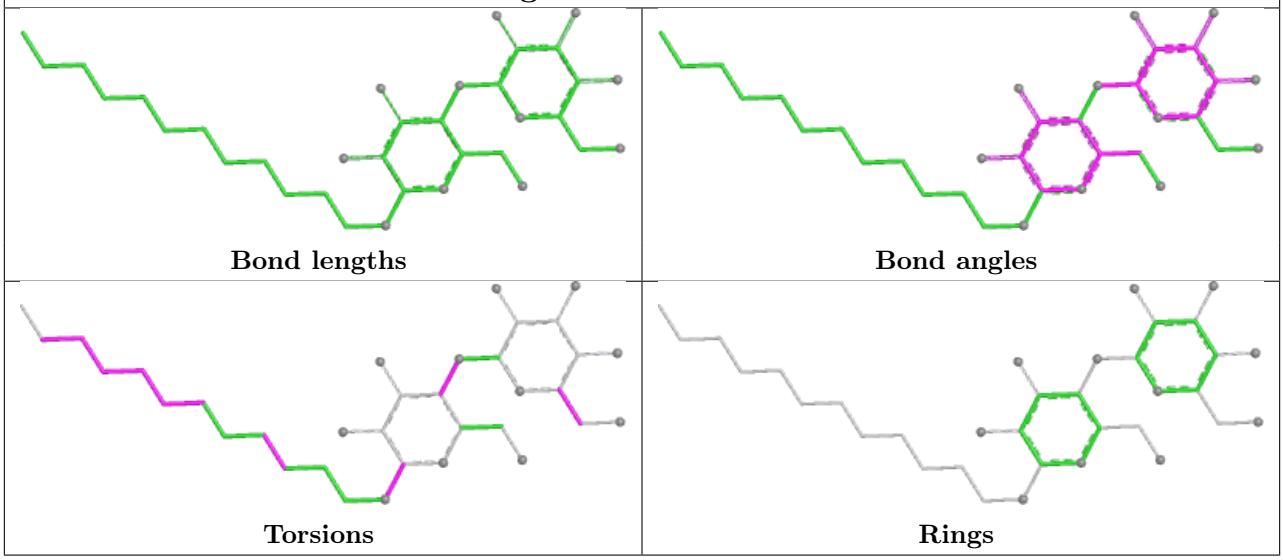


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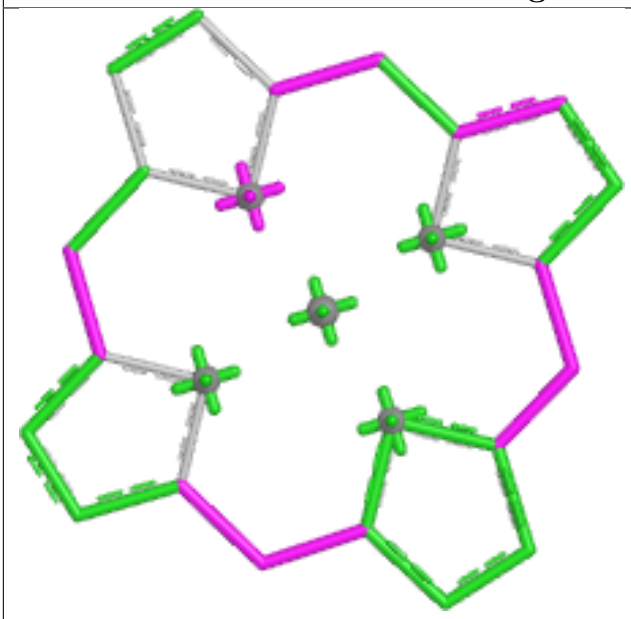


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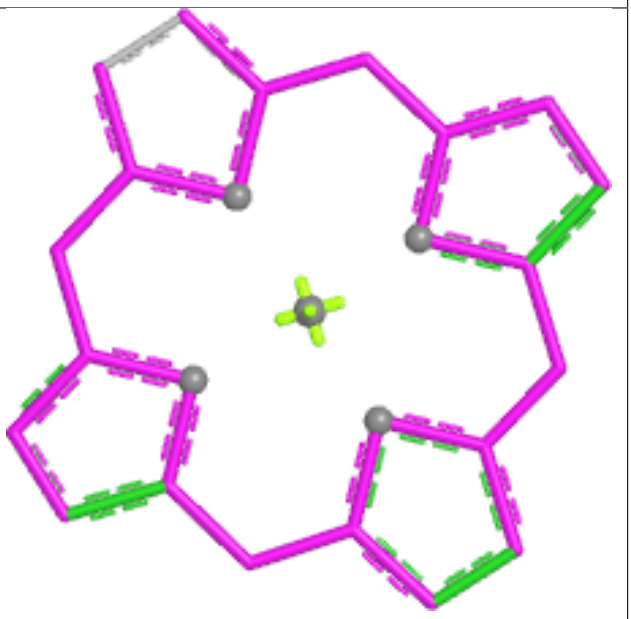
Ligand LMU H 105



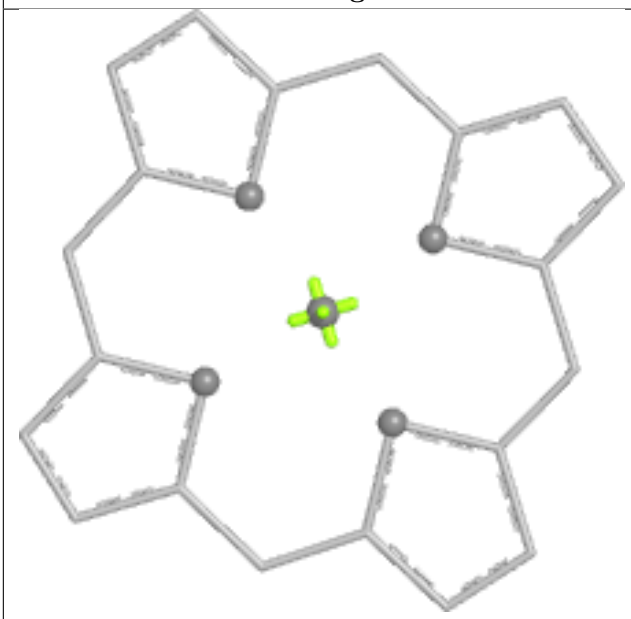
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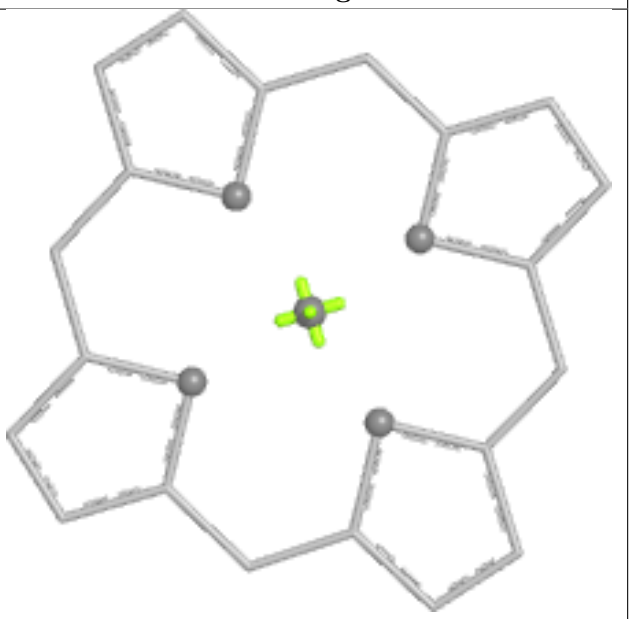
Bond lengths



Bond angles

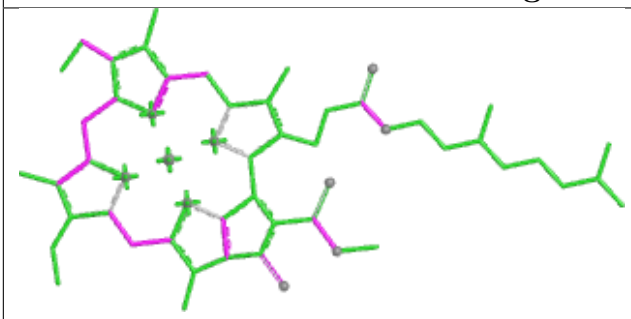


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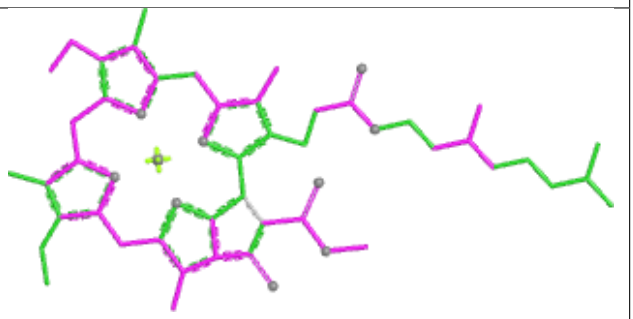


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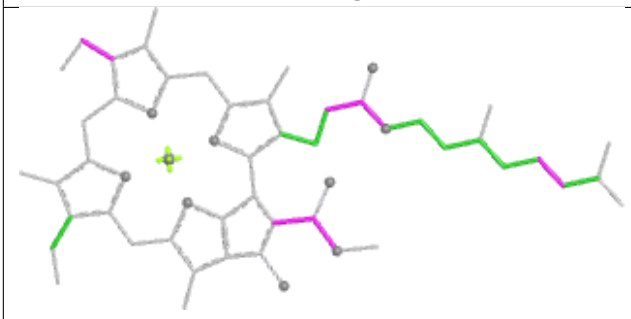
Ligand CLA H 108



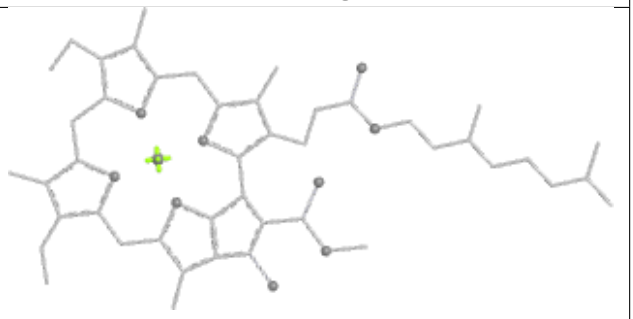
Bond lengths



Bond angles

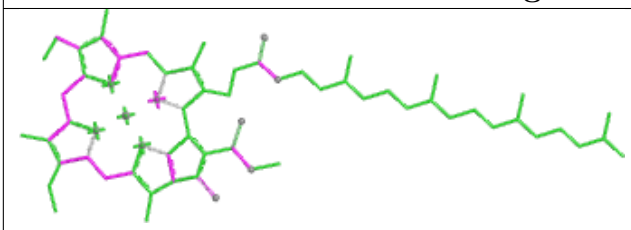


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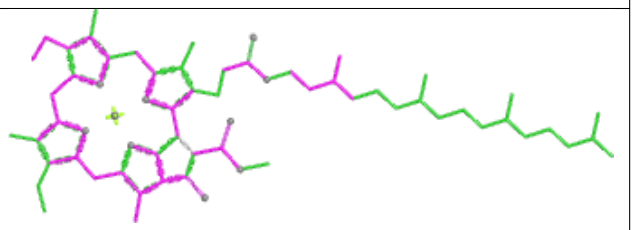


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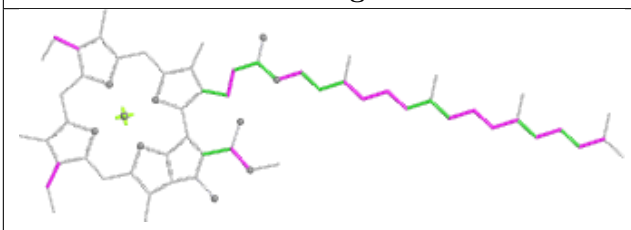
Ligand CLA A 822



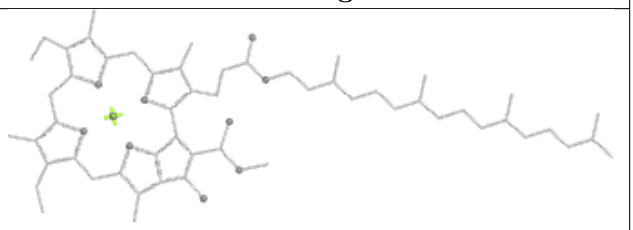
Bond lengths



Bond angles

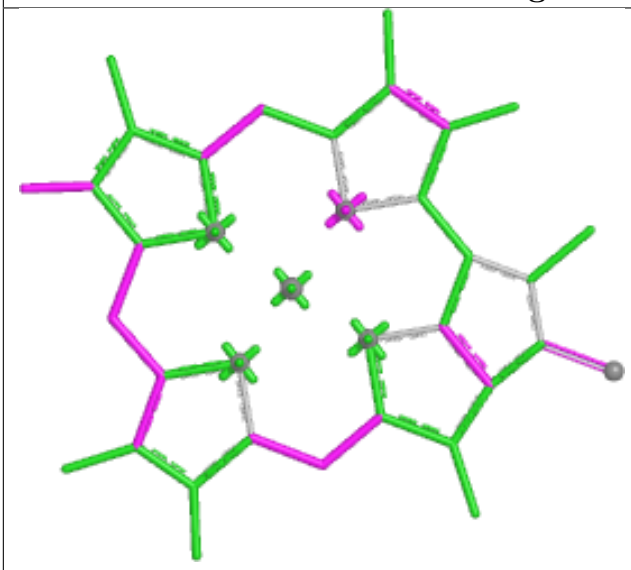


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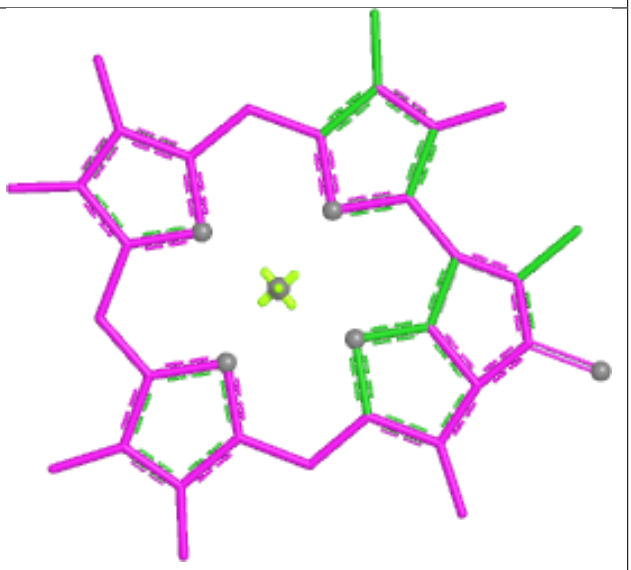


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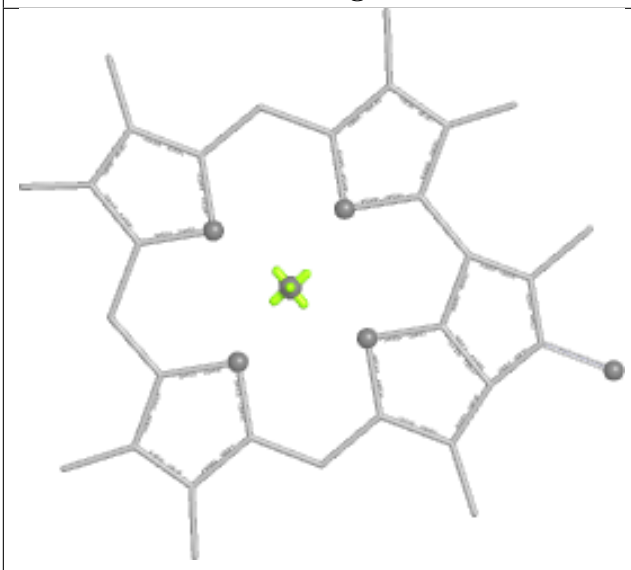
Ligand CLA 4 313



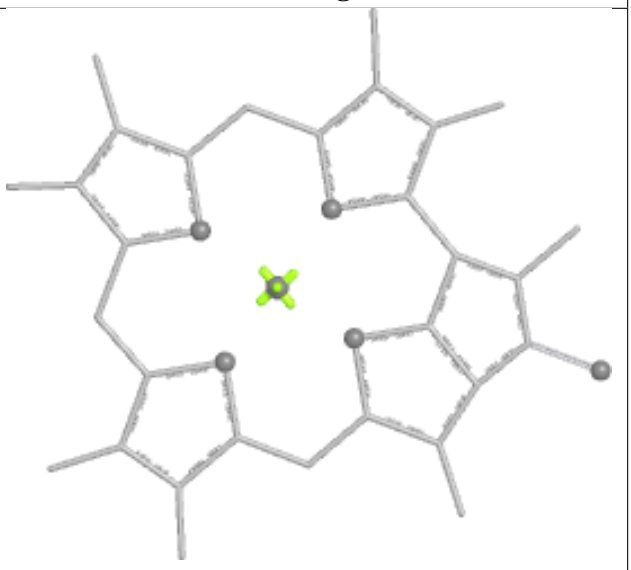
Bond lengths



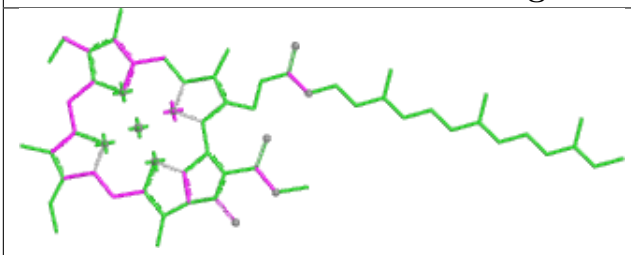
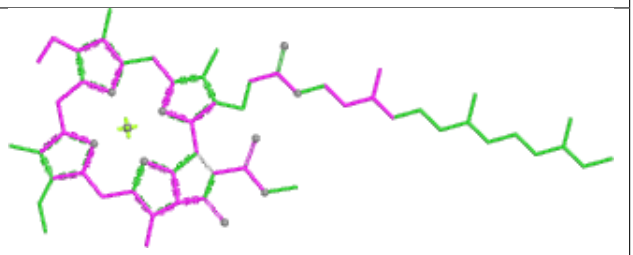
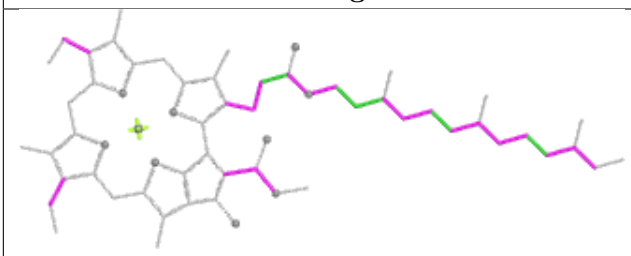
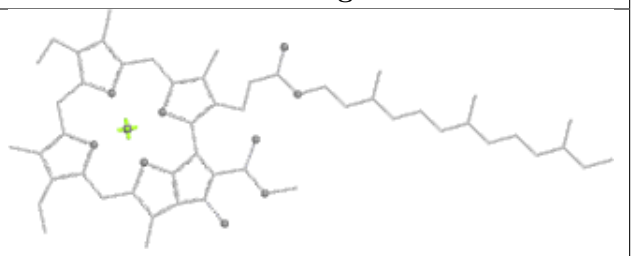
Bond angles

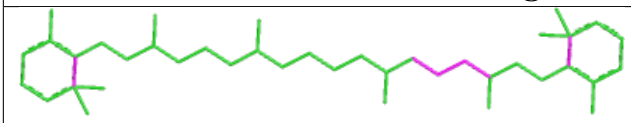
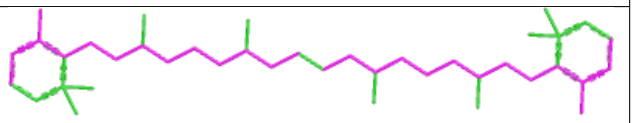
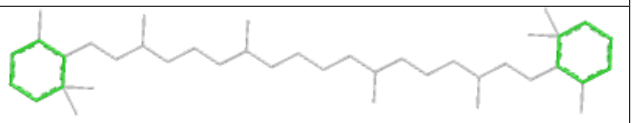


Torsions

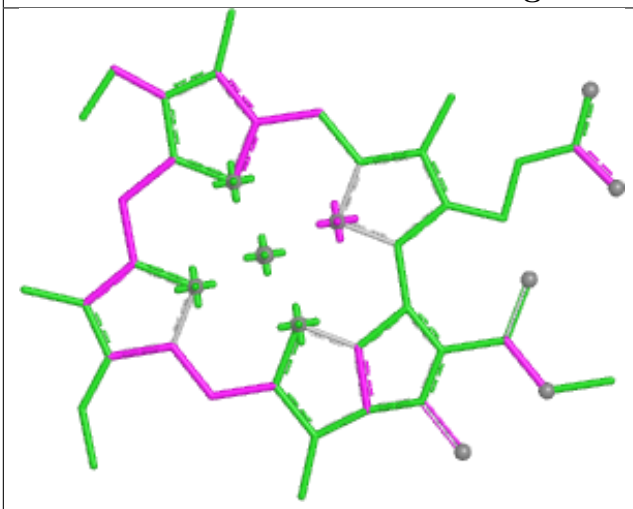


Rings

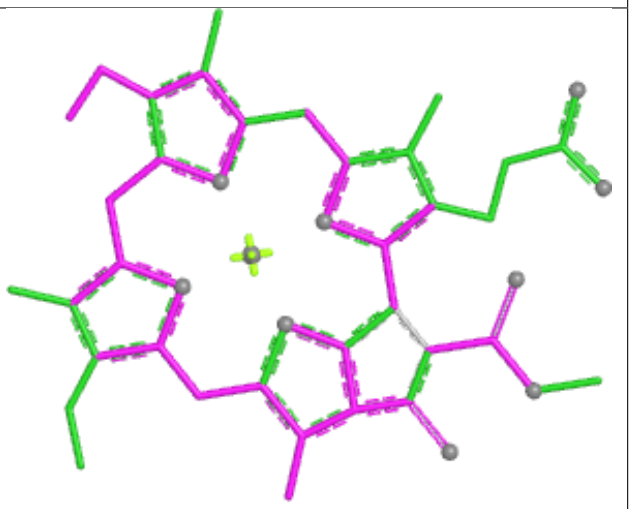
Ligand CLA J 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 841	
 Bond lengths	 Bond angles
 Torsions	 Rings

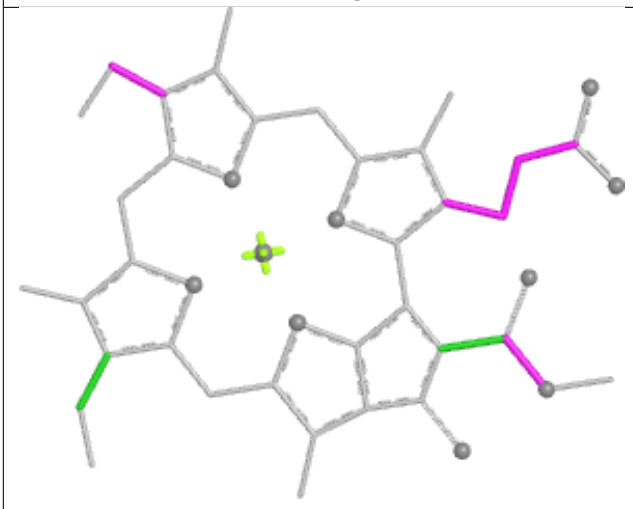
Ligand CLA A 831



Bond lengths



Bond angles

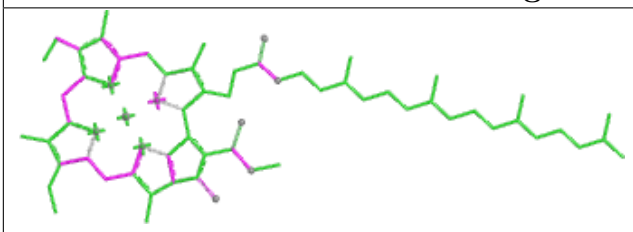


Torsions

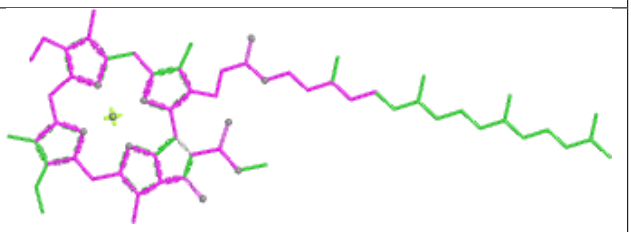


Rings

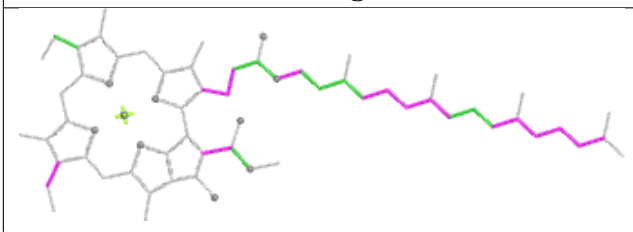
Ligand CLA A 806



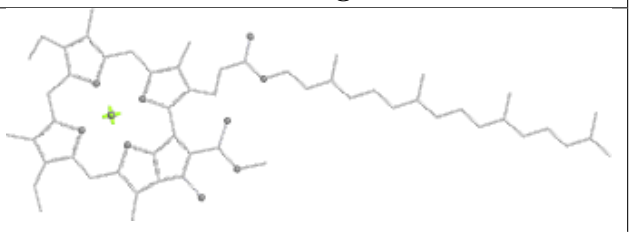
Bond lengths



Bond angles

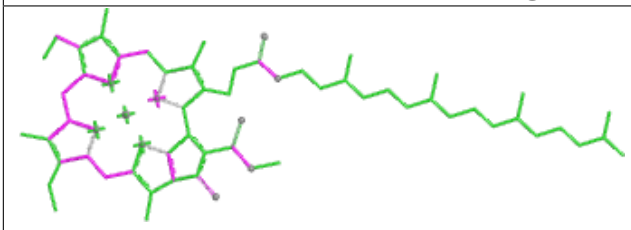


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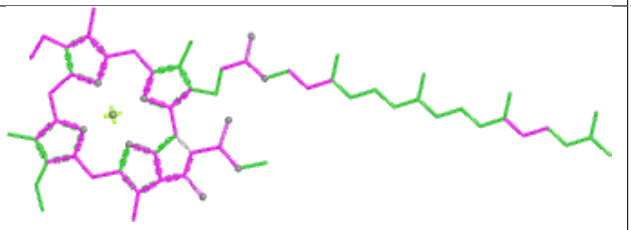


Rings

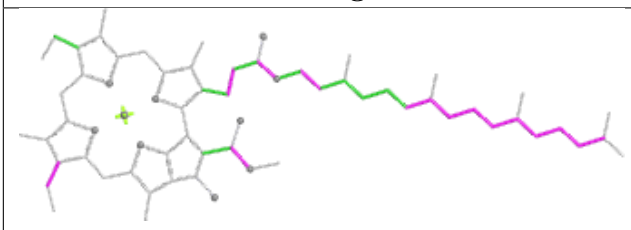
Ligand CLA A 849



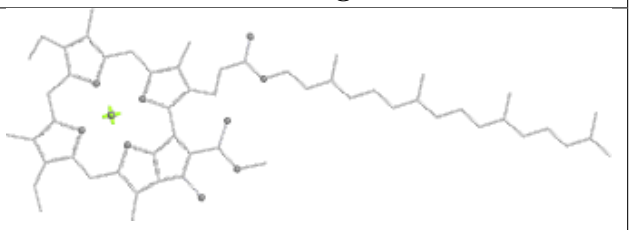
Bond lengths



Bond angles

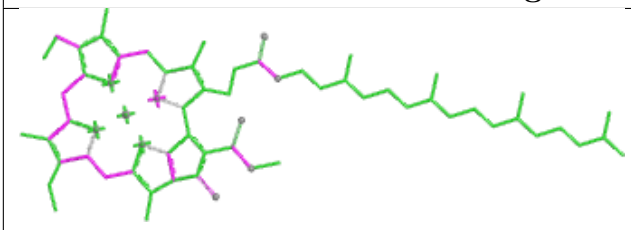


Torsions

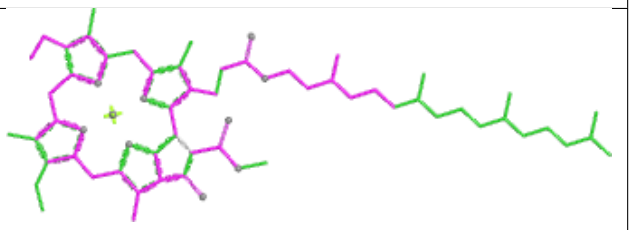


Rings

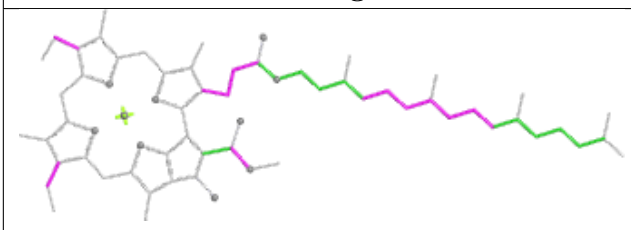
Ligand CLA B 824



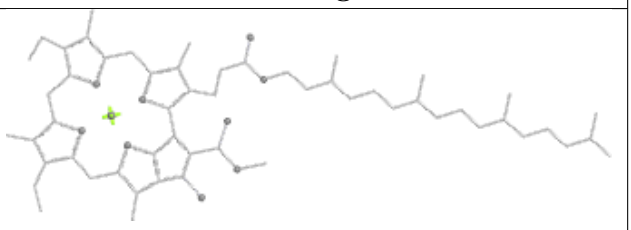
Bond lengths



Bond angles

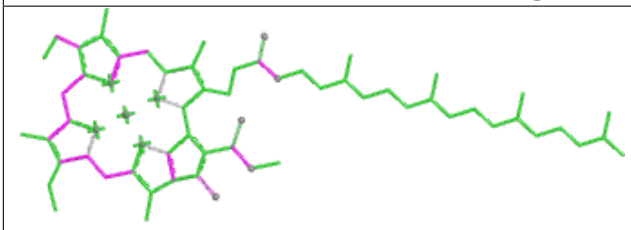


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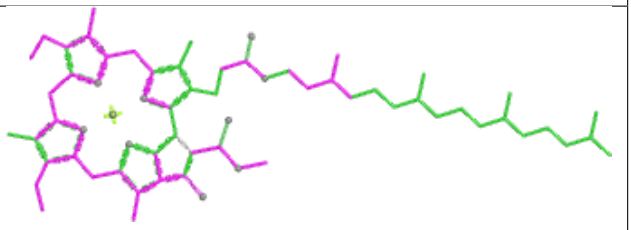


Rings

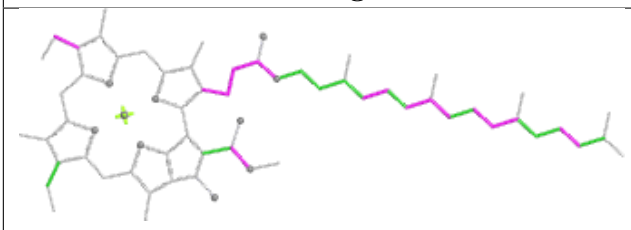
Ligand CLA 2 306



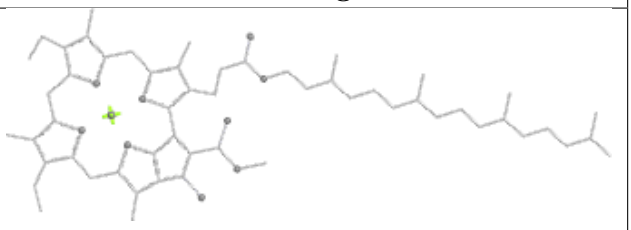
Bond lengths



Bond angles

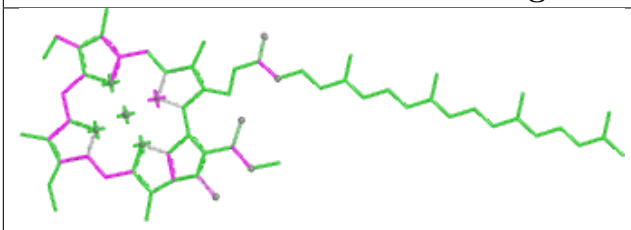


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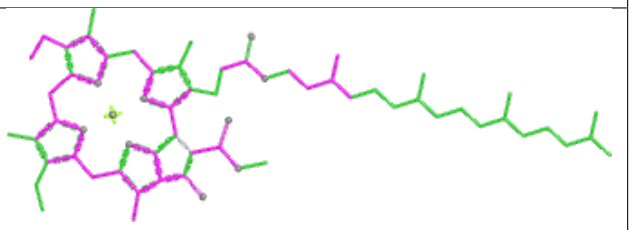


Rings

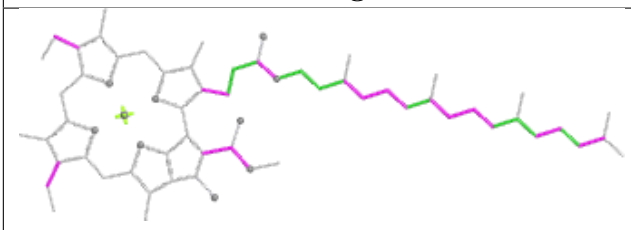
Ligand CLA 3 310



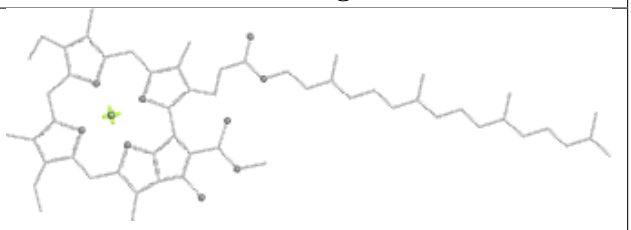
Bond lengths



Bond angles

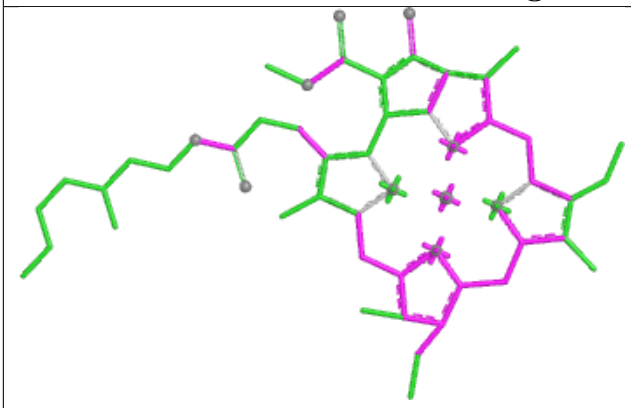


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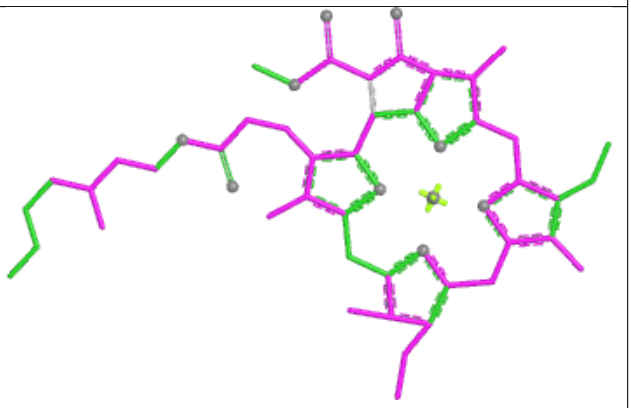


Rings

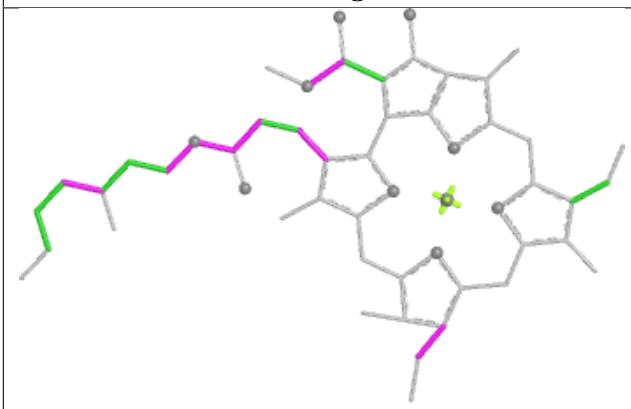
Ligand CLA F 206



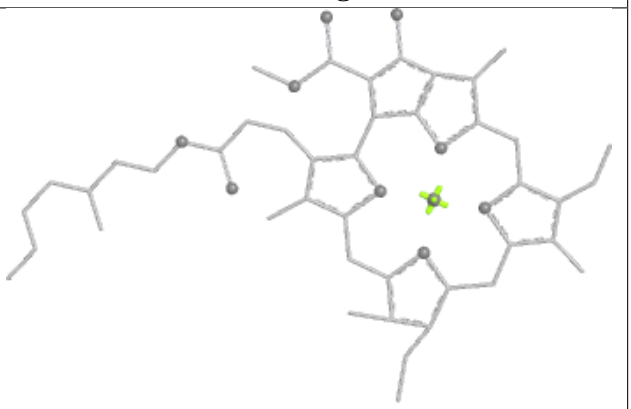
Bond lengths



Bond angles

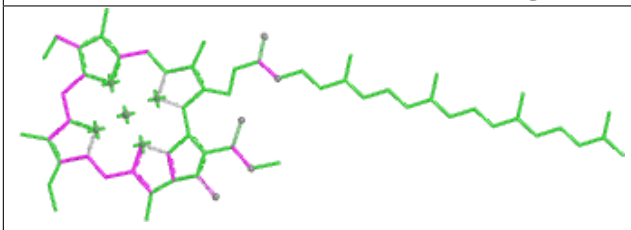


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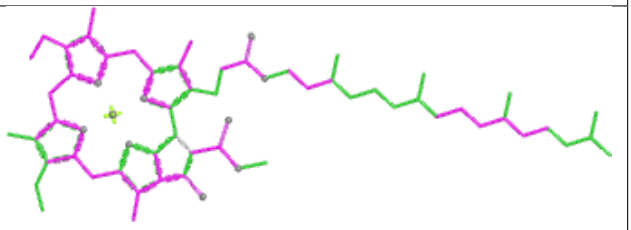


Rings

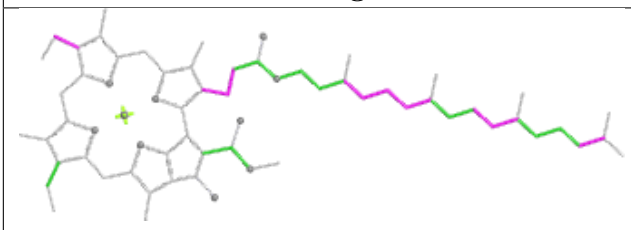
Ligand CLA B 825



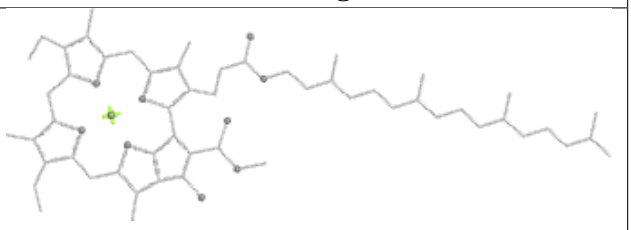
Bond lengths



Bond angles

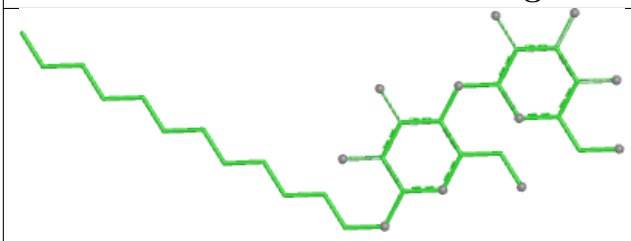


Torsions

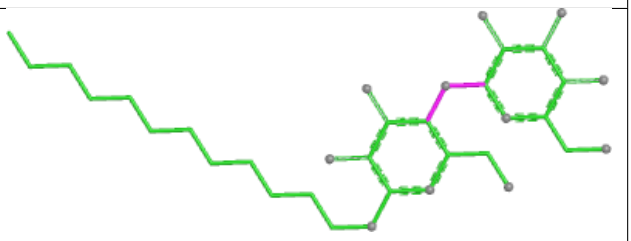


Rings

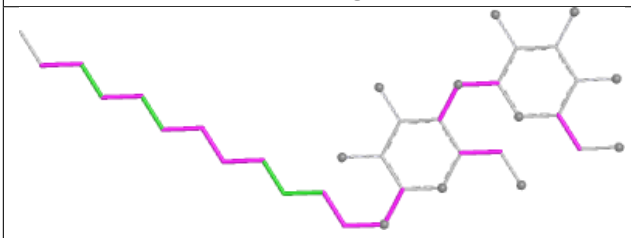
Ligand LMU 2 316



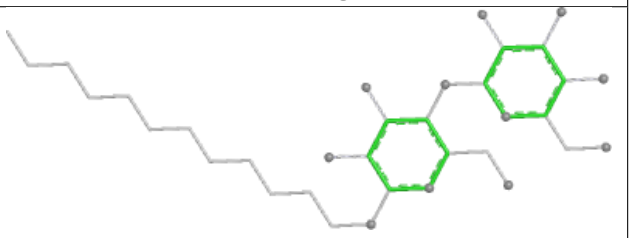
Bond lengths



Bond angles

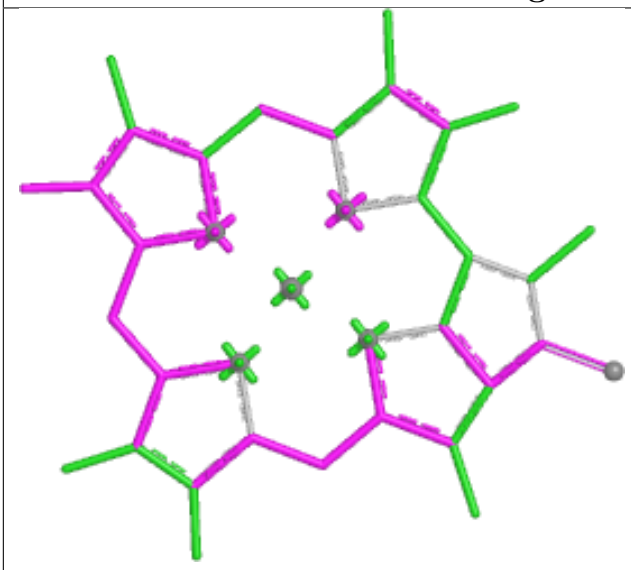


Torsions



Rings

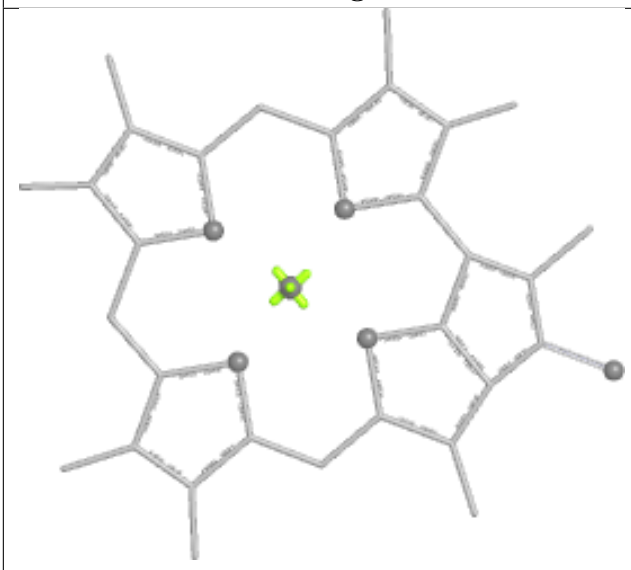
Ligand CLA 1 209



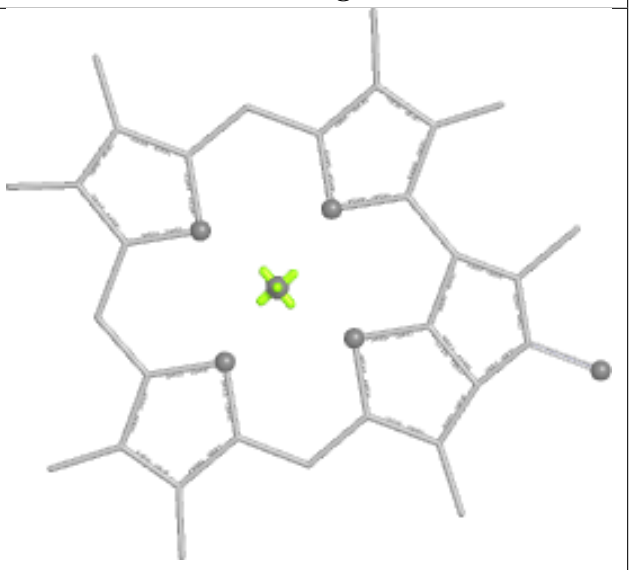
Bond lengths



Bond angles

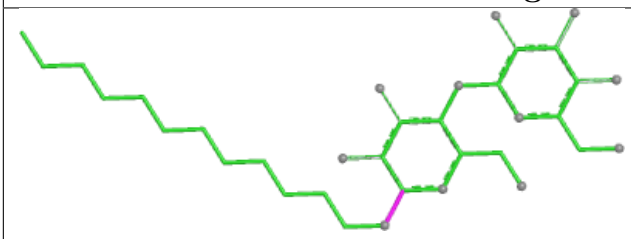


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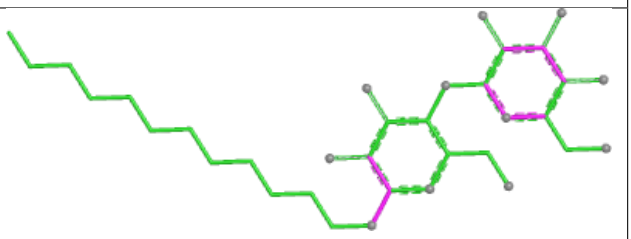


Rings

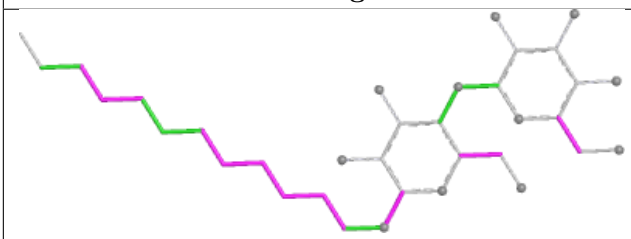
Ligand LMU 4 316



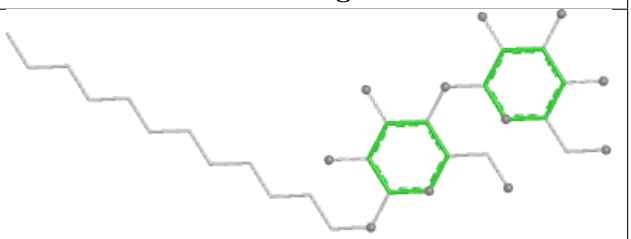
Bond lengths



Bond angles

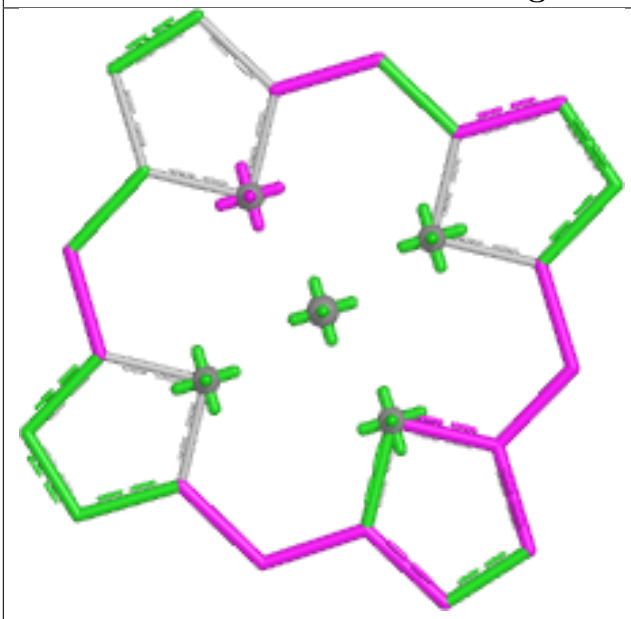


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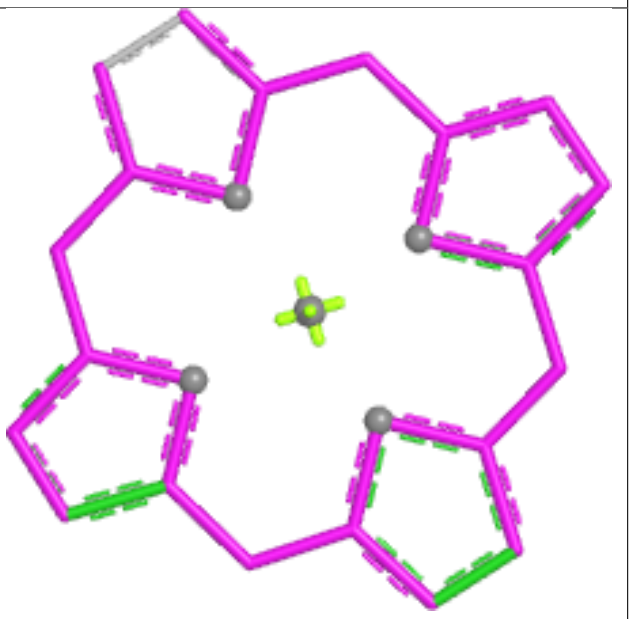


Rings

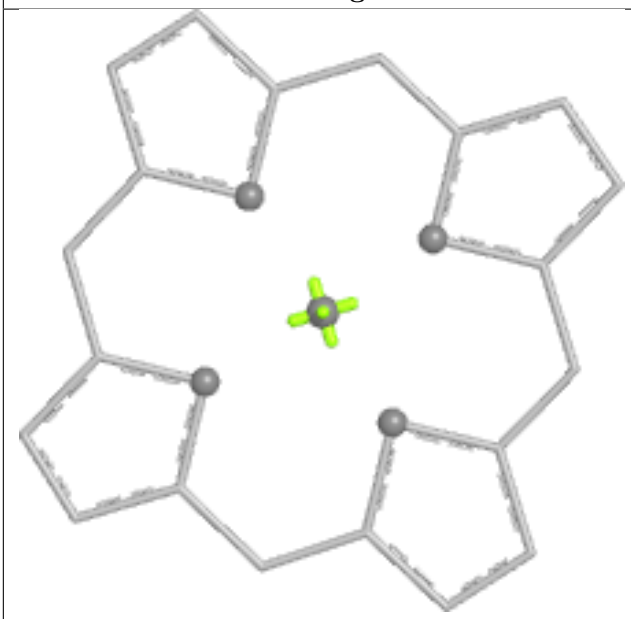
Ligand CLA 2 305



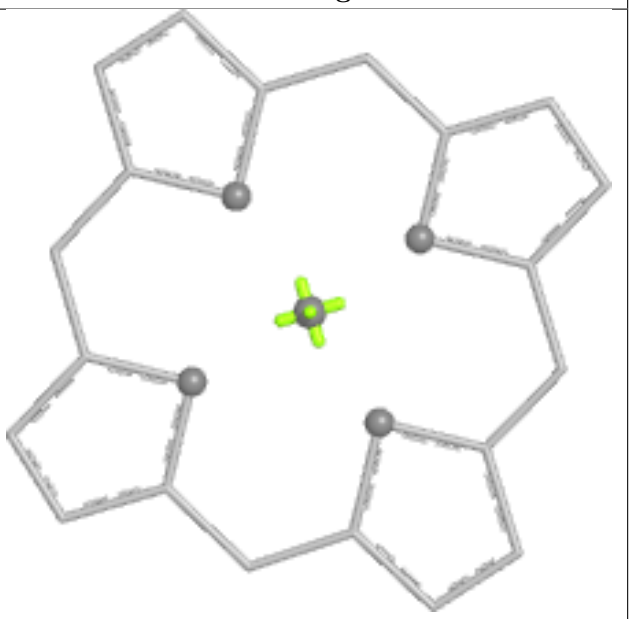
Bond lengths



Bond angles

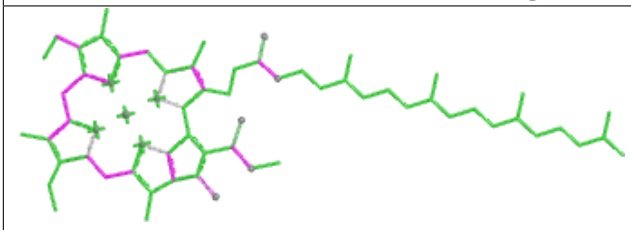


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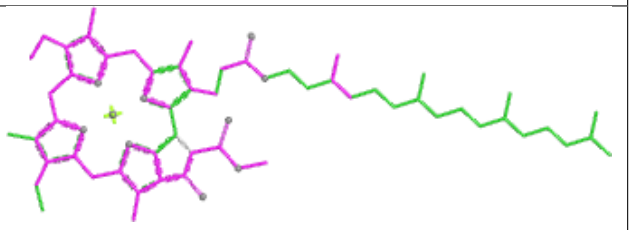


Rings

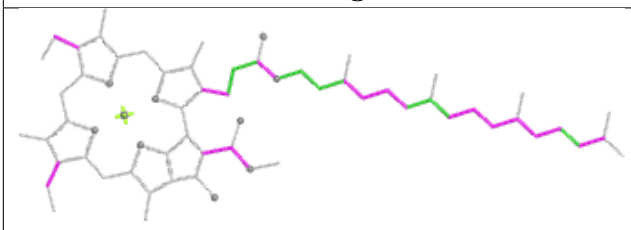
Ligand CLA A 829



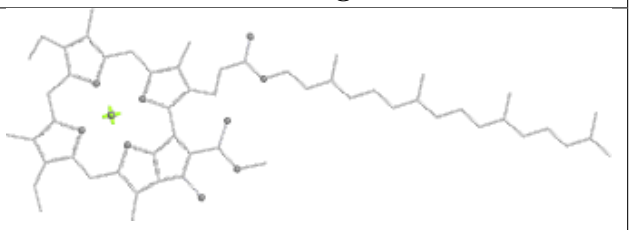
Bond lengths



Bond angles

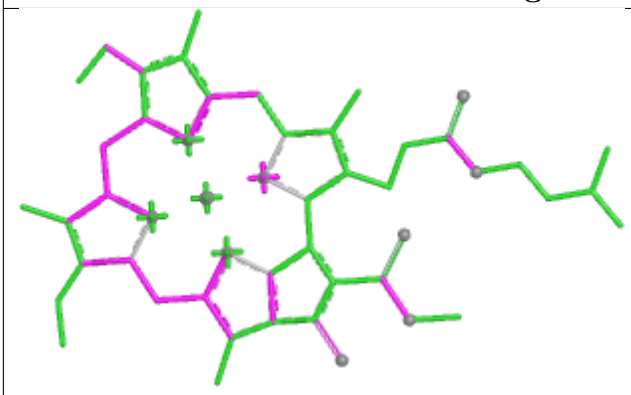


Torsions

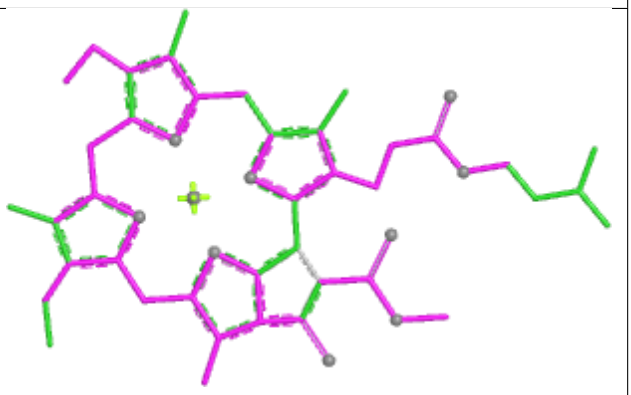


Rings

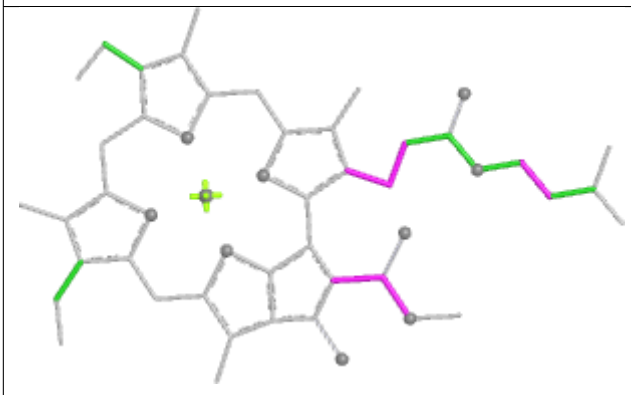
Ligand CLA B 830



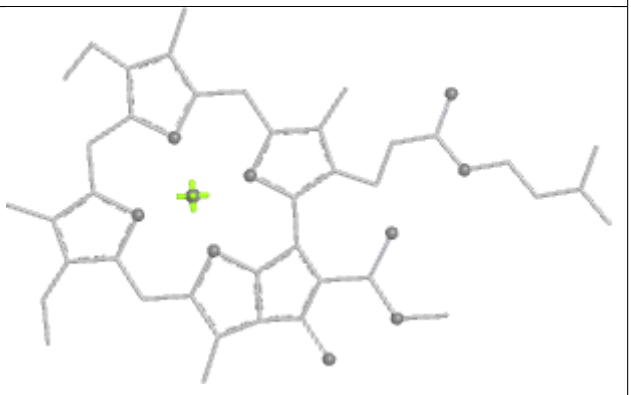
Bond lengths



Bond angles

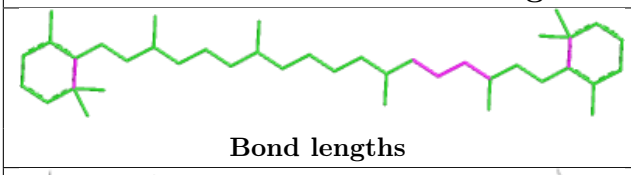


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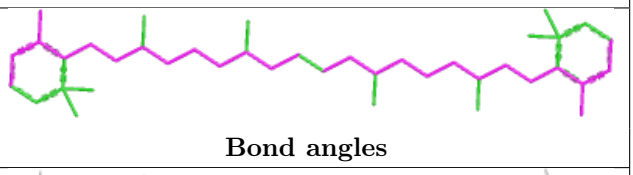


Rings

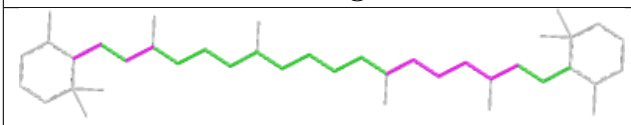
Ligand BCR J 101



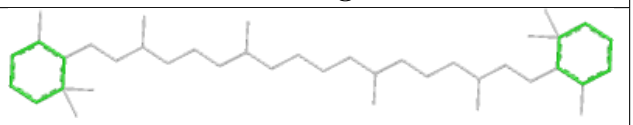
Bond lengths



Bond angles

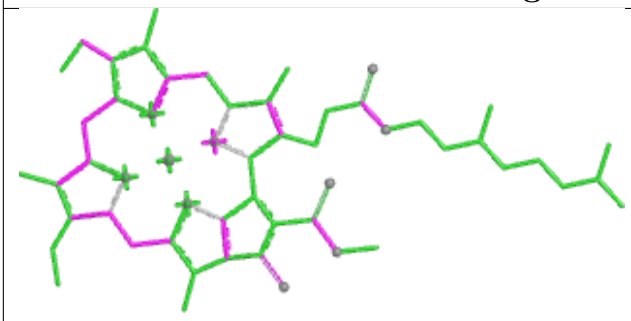


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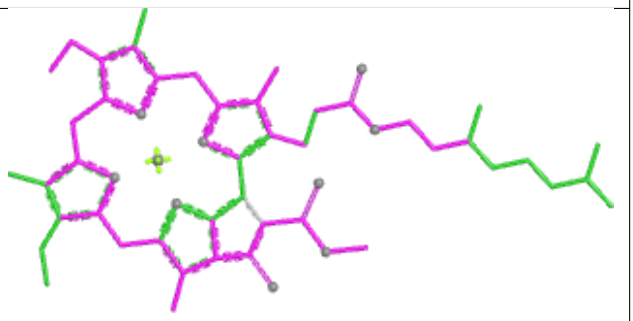


Rings

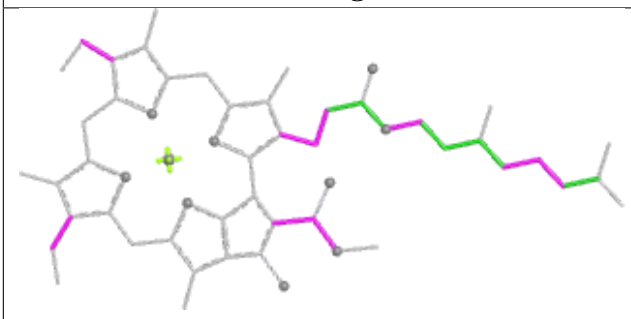
Ligand CLA H 101



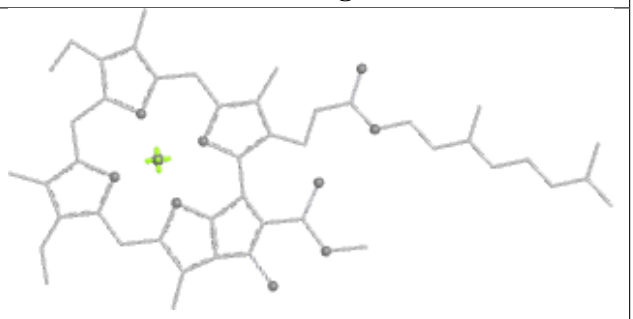
Bond lengths



Bond angles

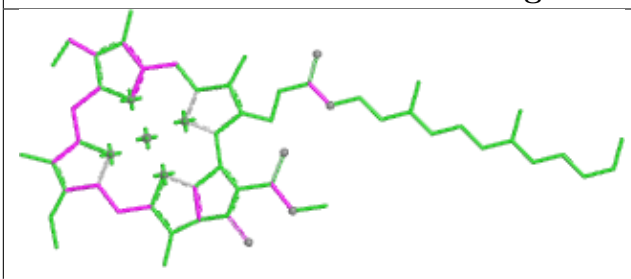


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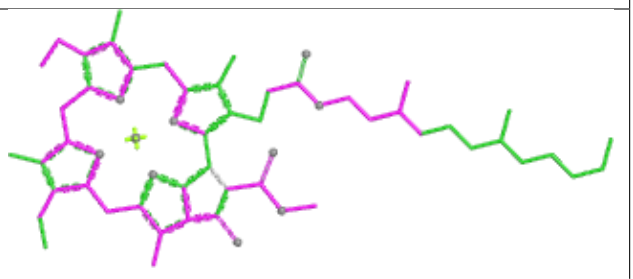


Rings

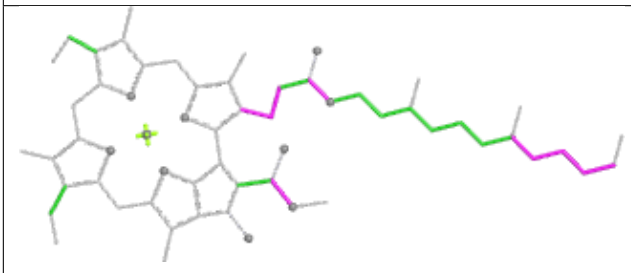
Ligand CLA B 814



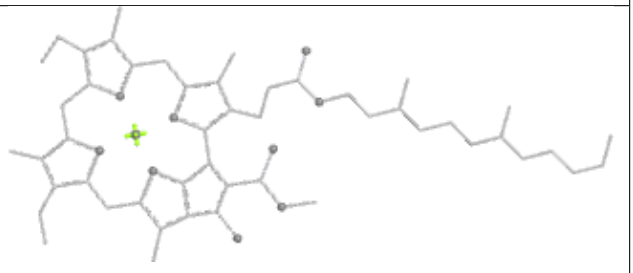
Bond lengths



Bond angles

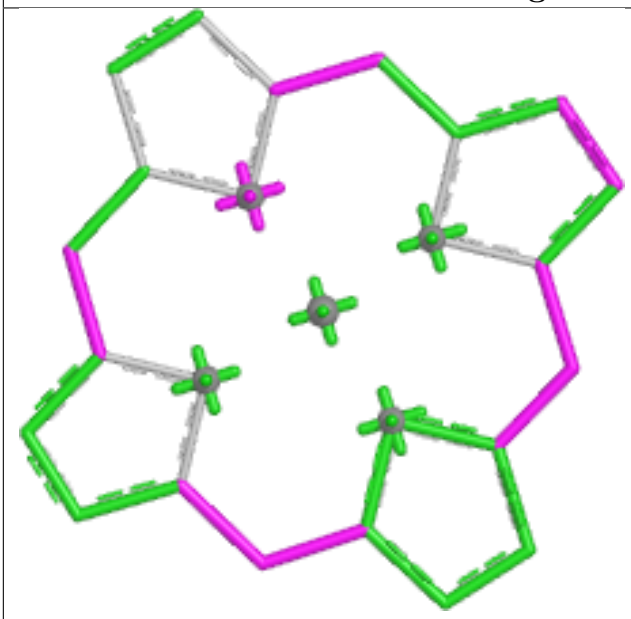


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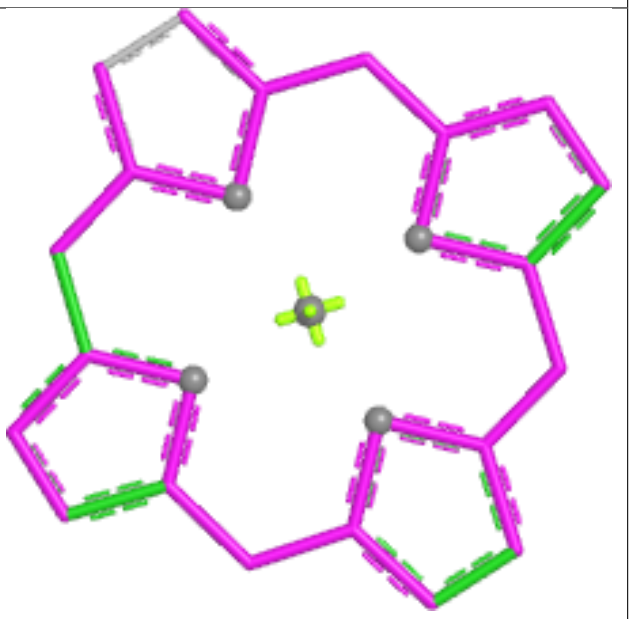


Rings

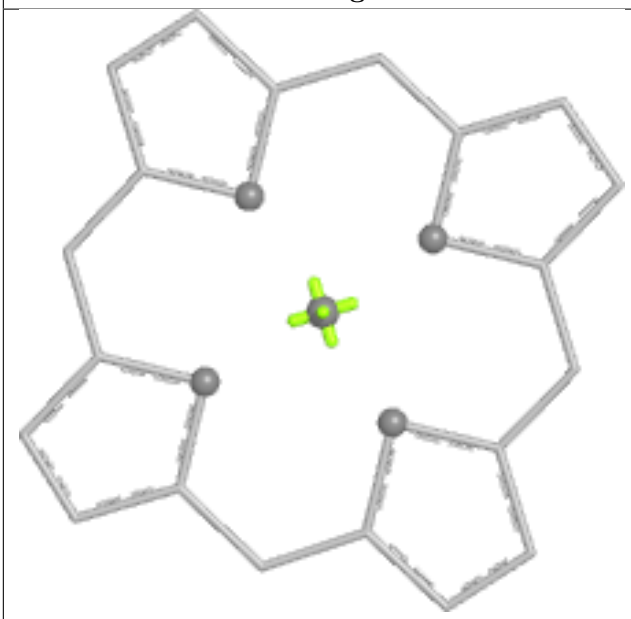
Ligand CLA 1 208



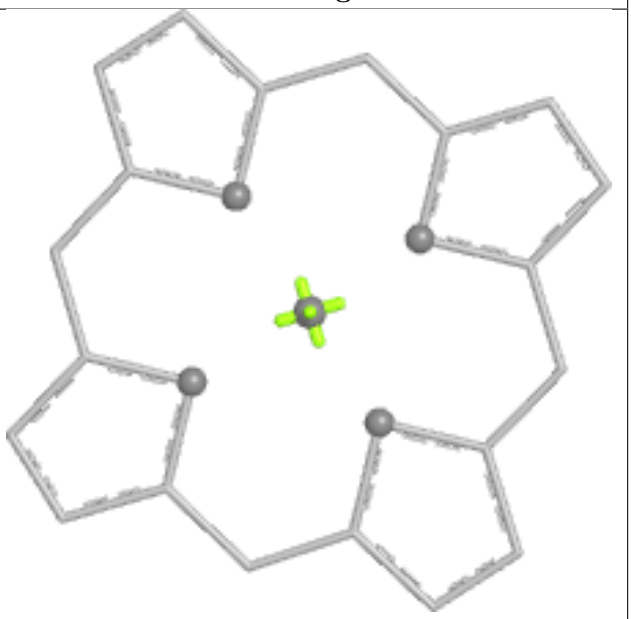
Bond lengths



Bond angles

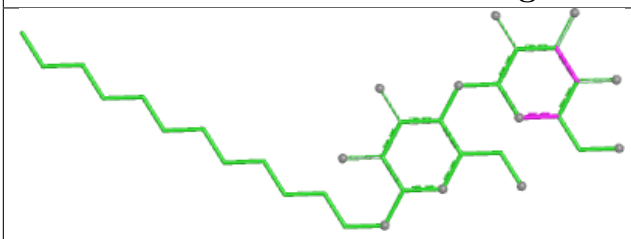


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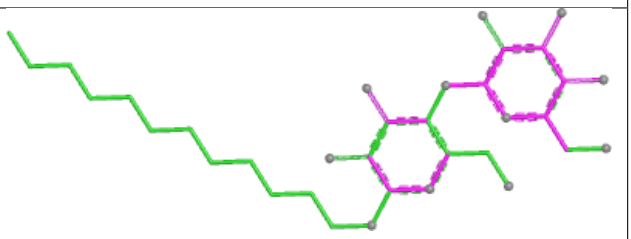


Rings

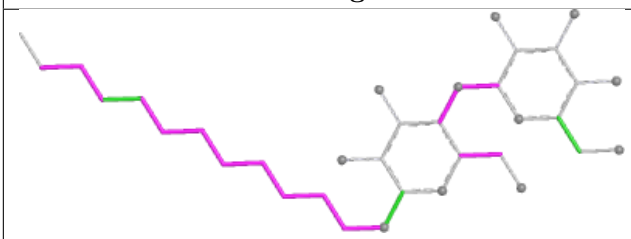
Ligand LMU G 101



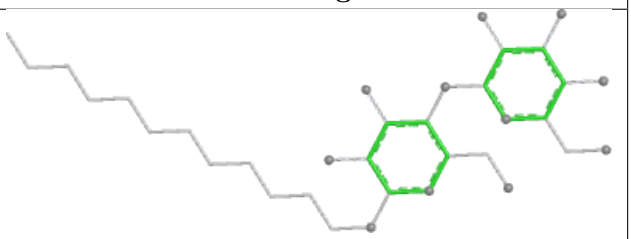
Bond lengths



Bond angles

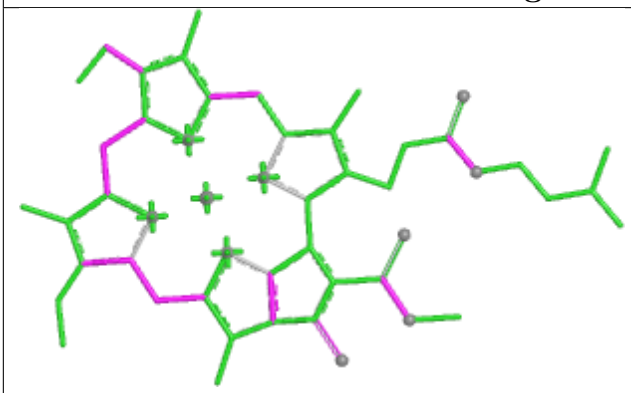


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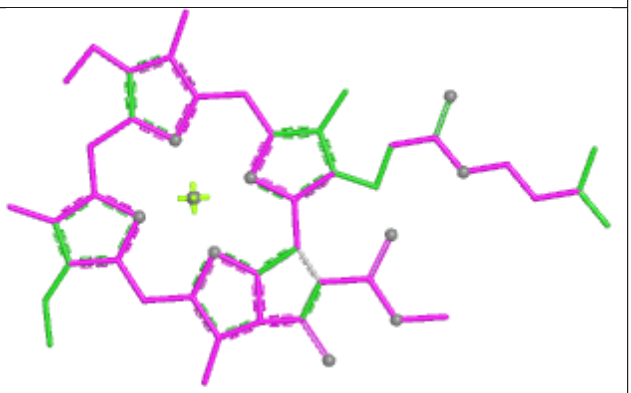


Rings

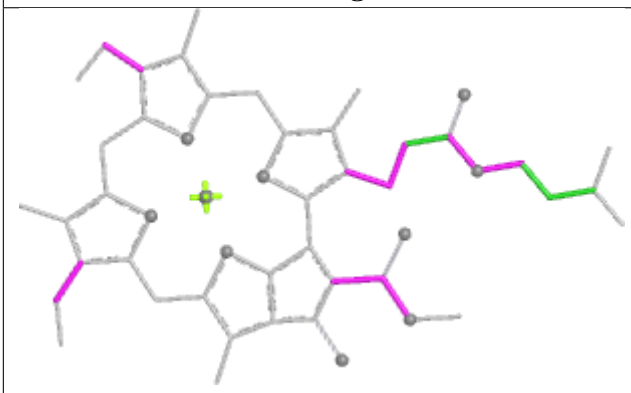
Ligand CLA B 828



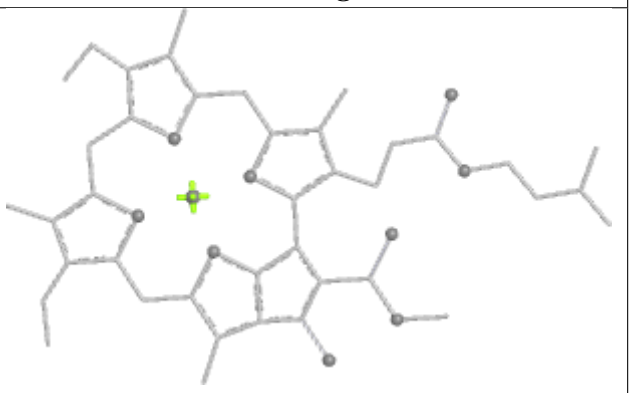
Bond lengths



Bond angles

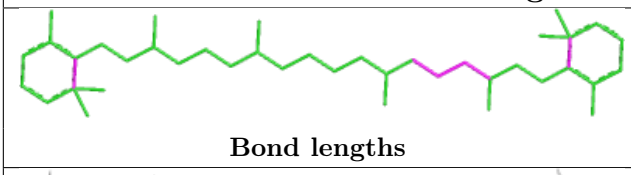


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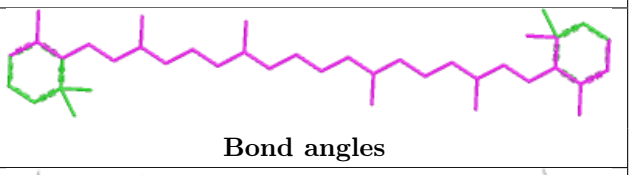


Rings

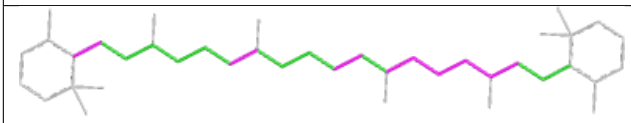
Ligand BCR 3 311



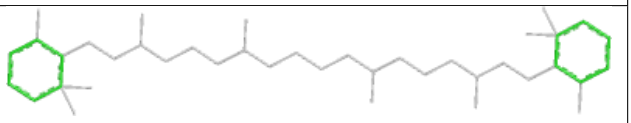
Bond lengths



Bond angles

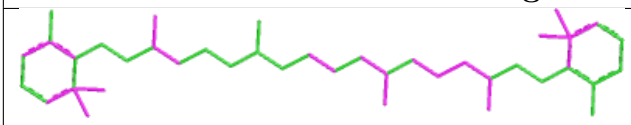


Torsions



Rings

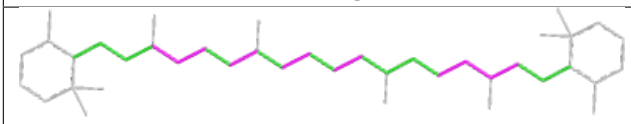
Ligand BCR B 850



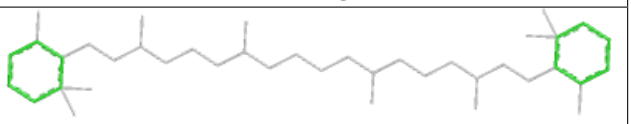
Bond lengths



Bond angles

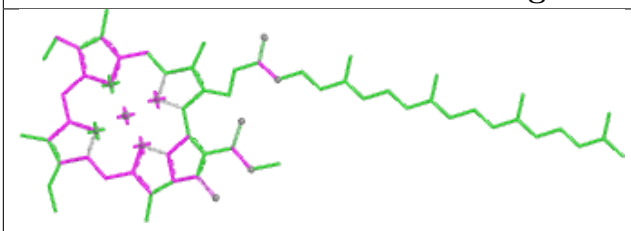


Torsions

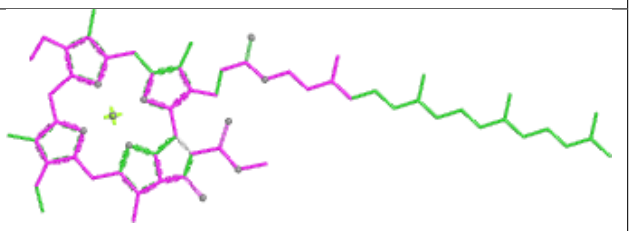


Rings

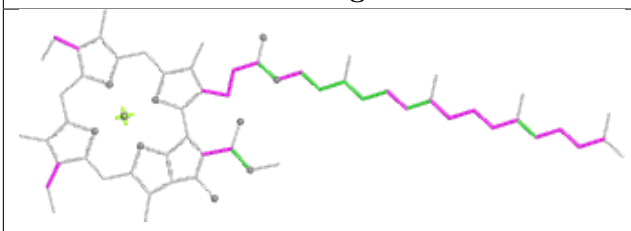
Ligand CLA 3 309



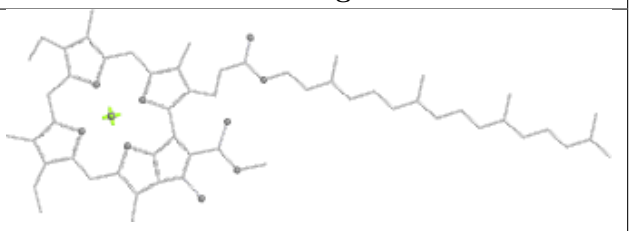
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Bond angles

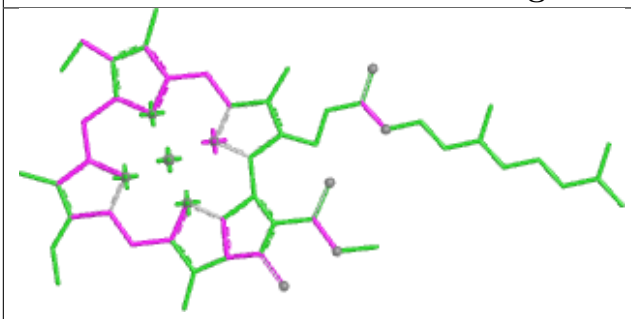


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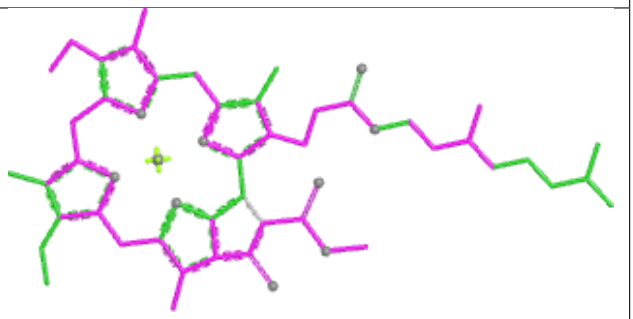


Rings

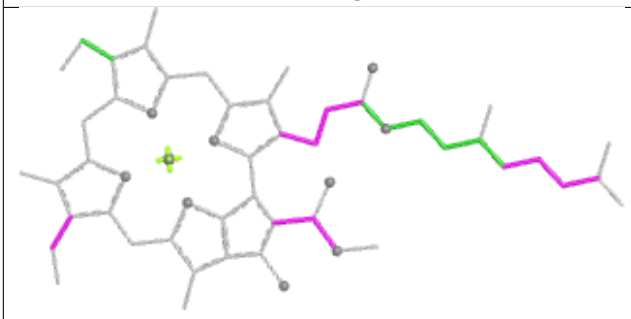
Ligand CLA J 103



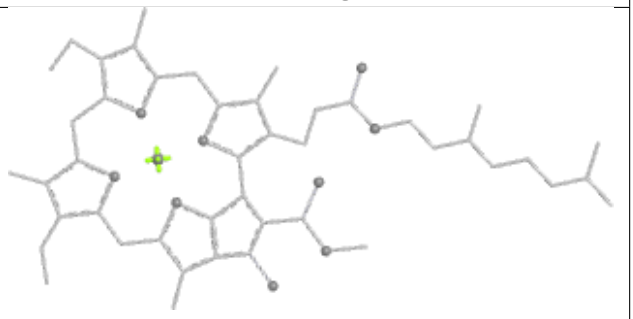
Bond lengths



Bond angles

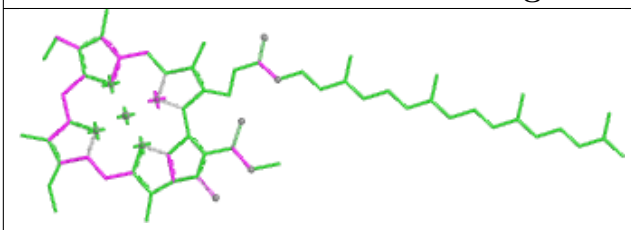


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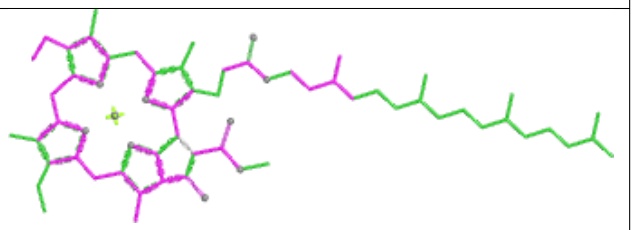


Rings

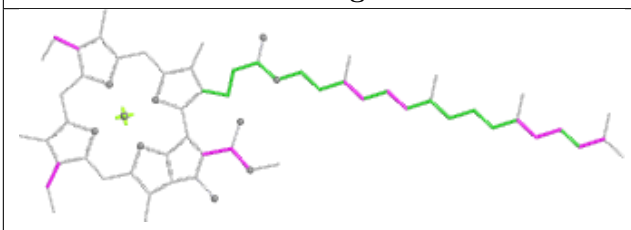
Ligand CLA A 833



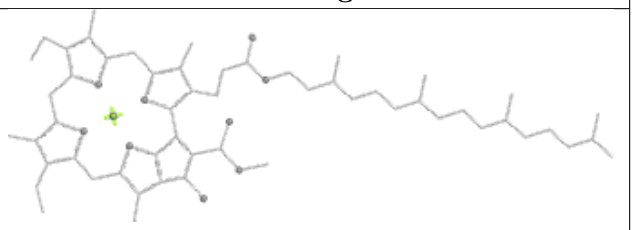
Bond lengths



Bond angles

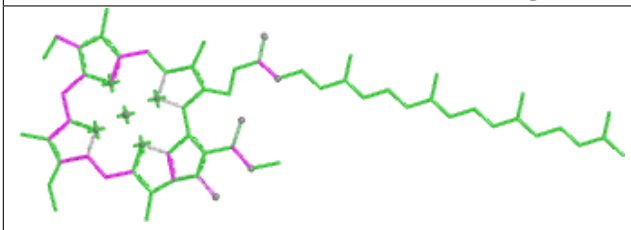


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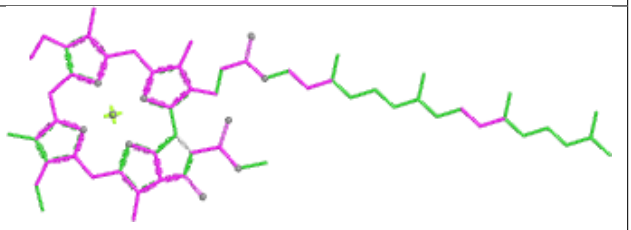


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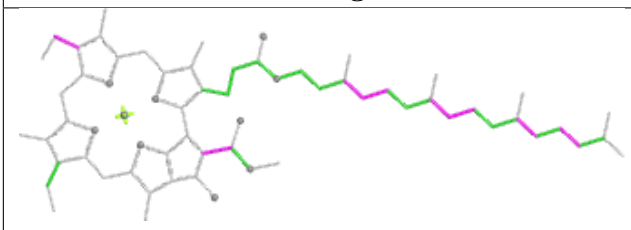
Ligand CLA B 806



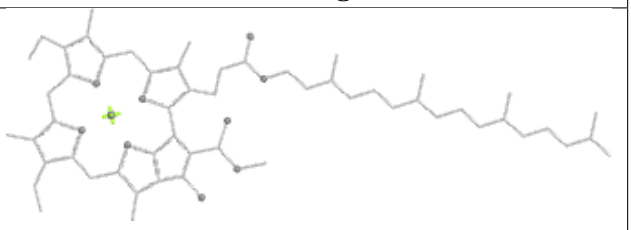
Bond lengths



Bond angles

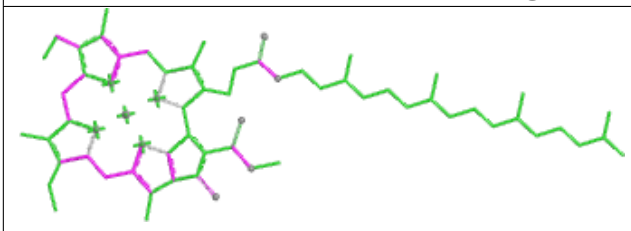


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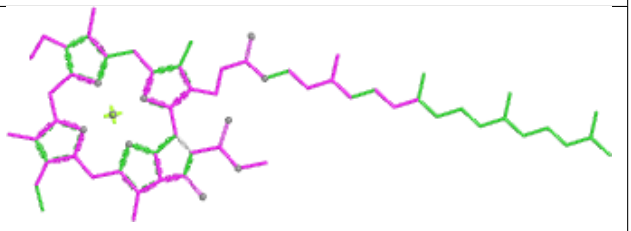


Rings

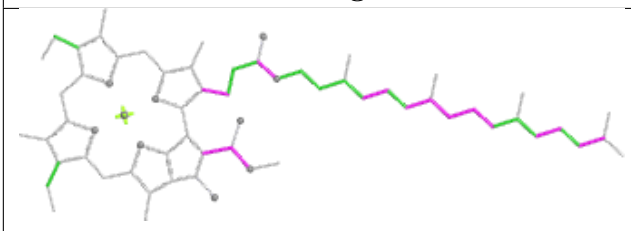
Ligand CLA A 826



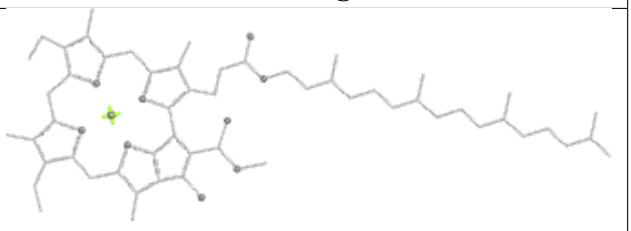
Bond lengths



Bond angles

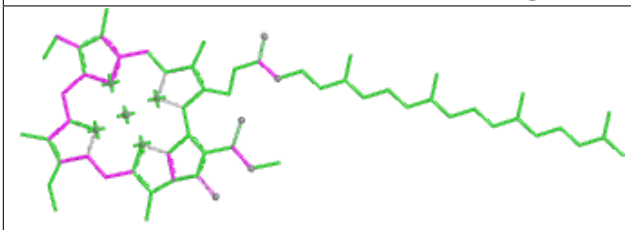


Torsions

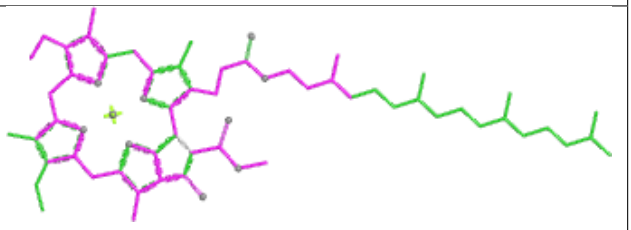


Rings

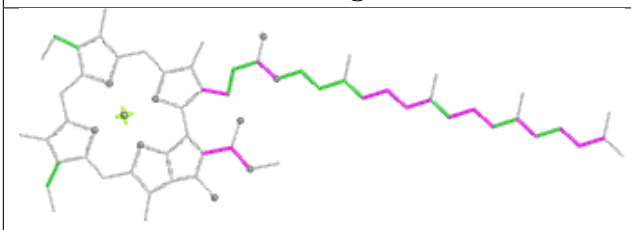
Ligand CLA A 816



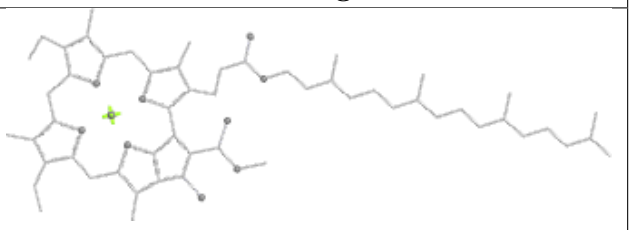
Bond lengths



Bond angles

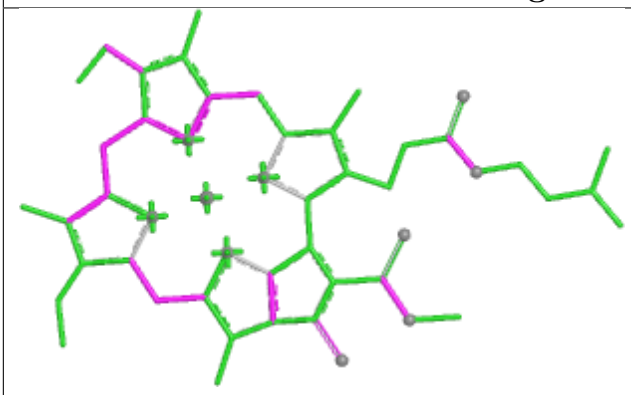


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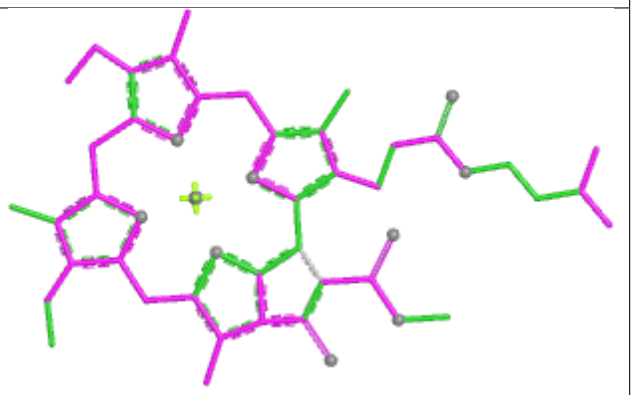


Rings

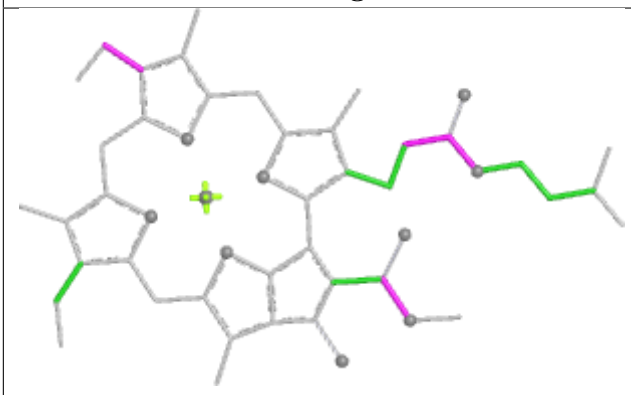
Ligand CLA 2 310



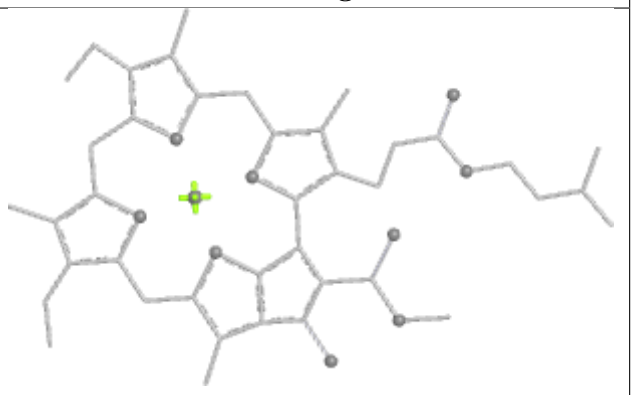
Bond lengths



Bond angles

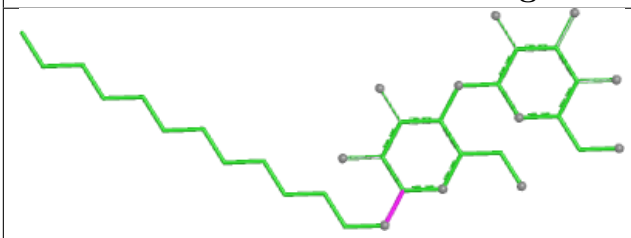


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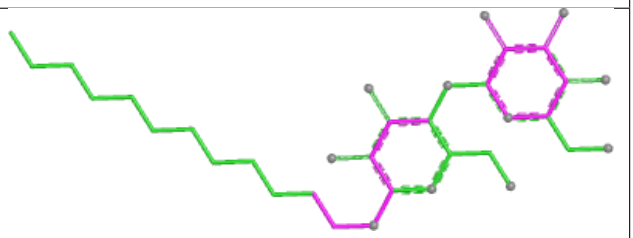


Rings

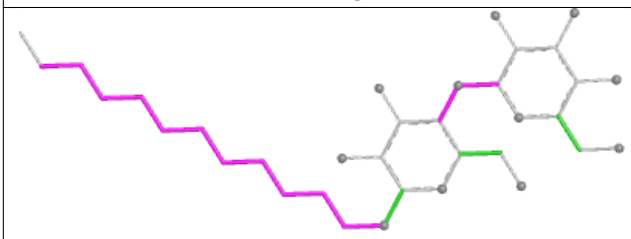
Ligand LMU A 846



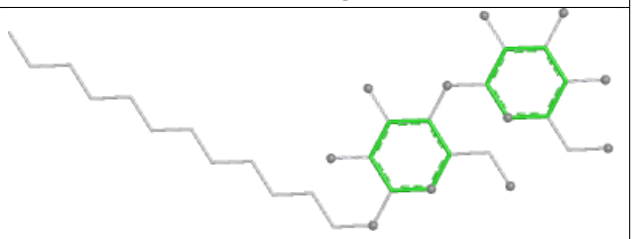
Bond lengths



Bond angles

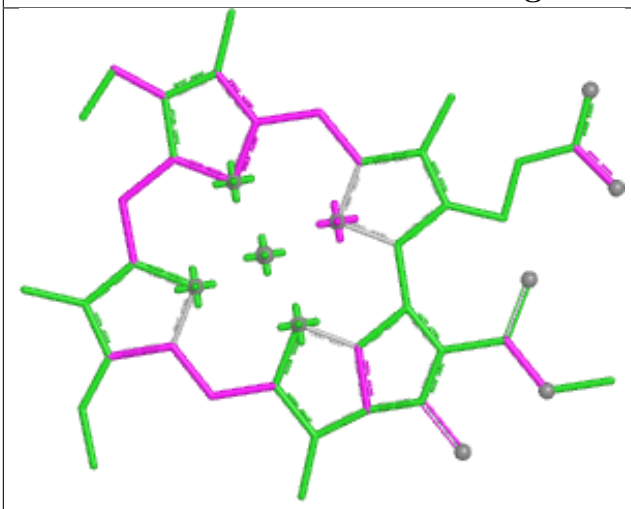


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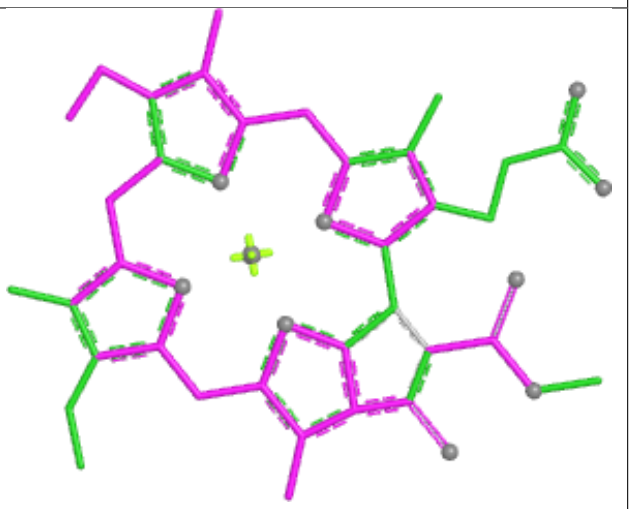


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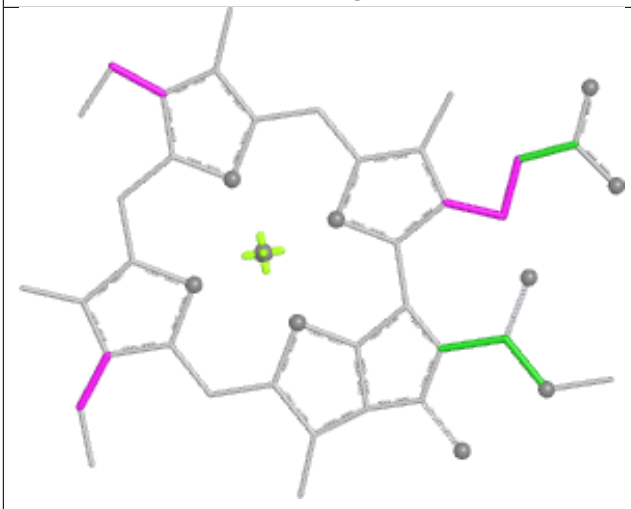
Ligand CLA B 803



Bond lengths



Bond angles

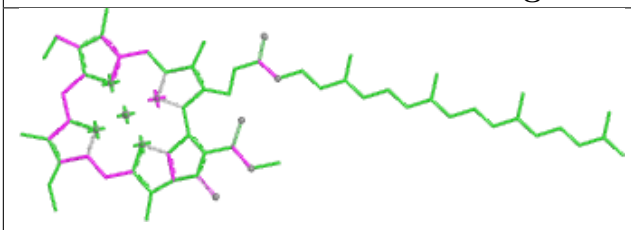


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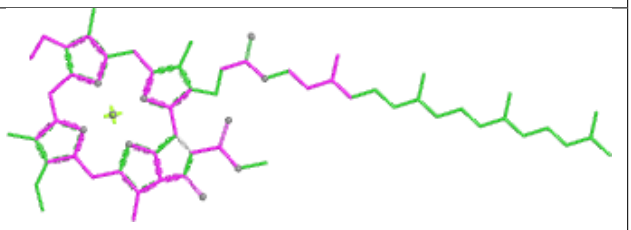


Rings

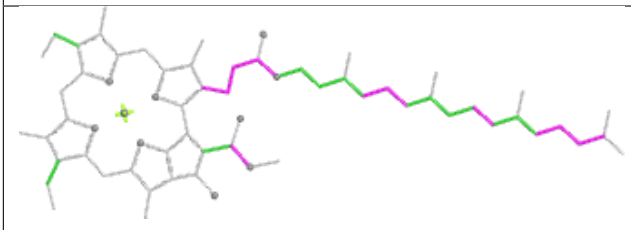
Ligand CLA A 836



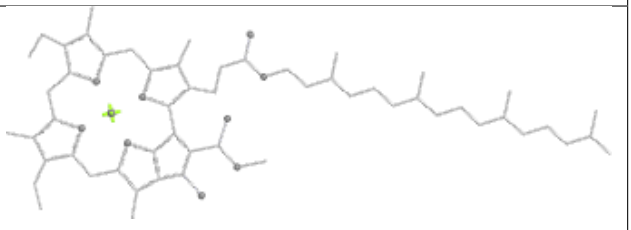
Bond lengths



Bond angles

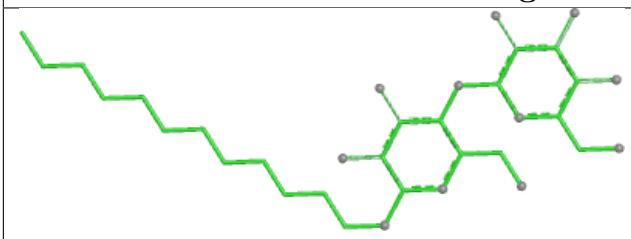


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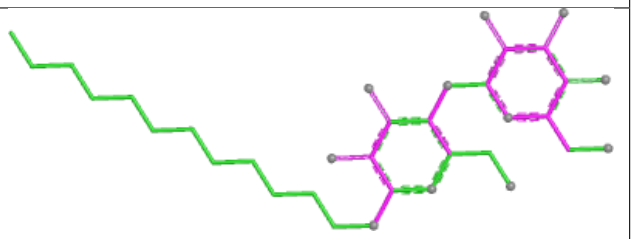


Rings

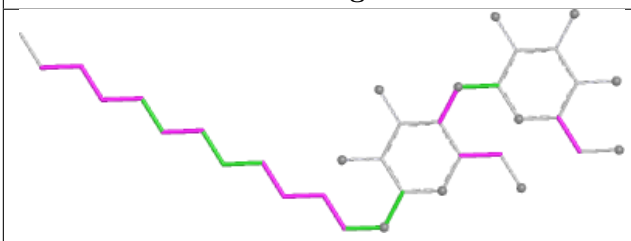
Ligand LMU K 104



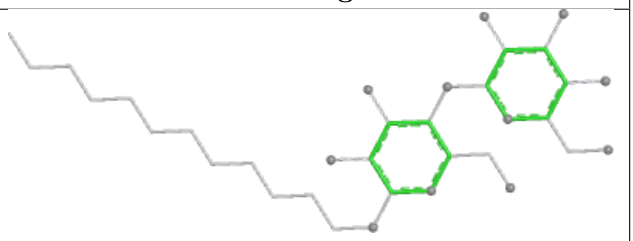
Bond lengths



Bond angles

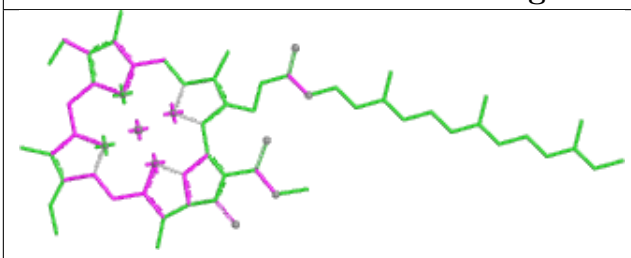


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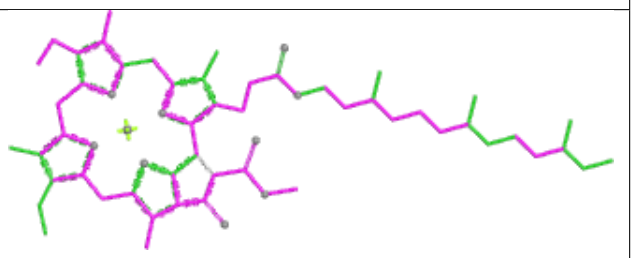


Rings

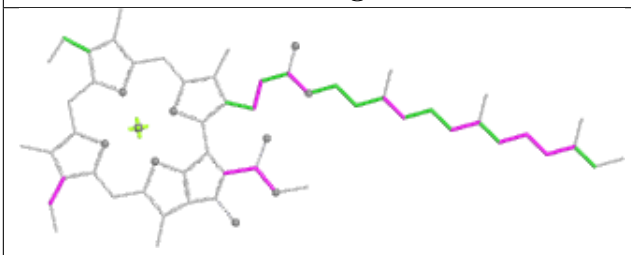
Ligand CLA 1 212



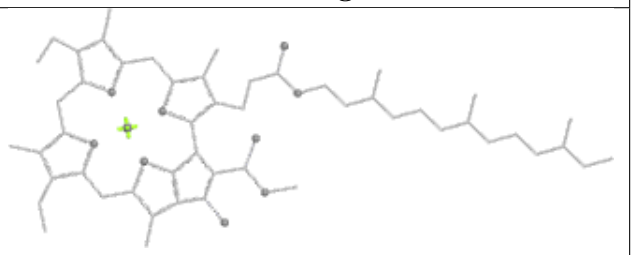
Bond lengths



Bond angles

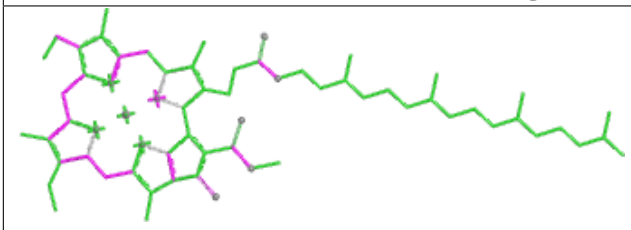


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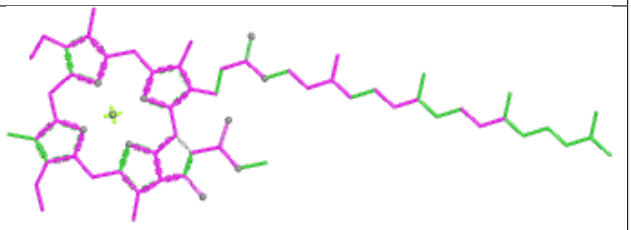


Rings

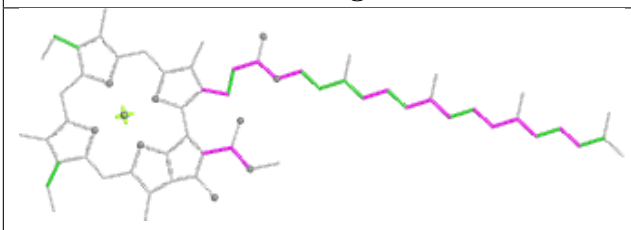
Ligand CLA B 804



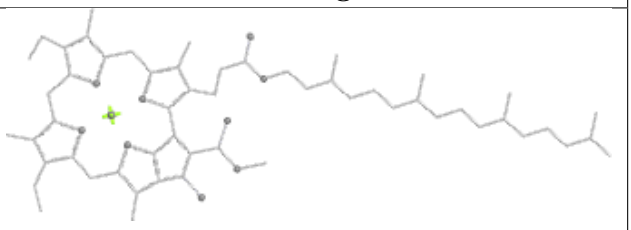
Bond lengths



Bond angles

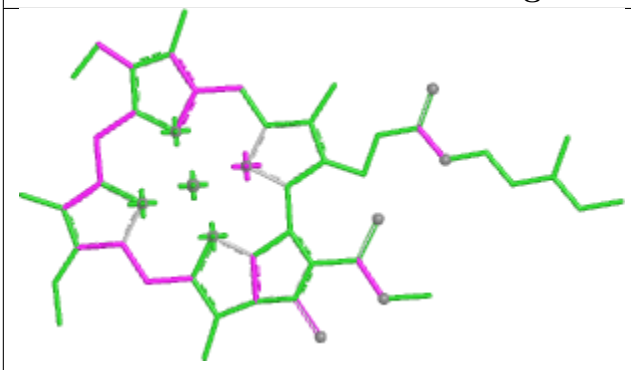


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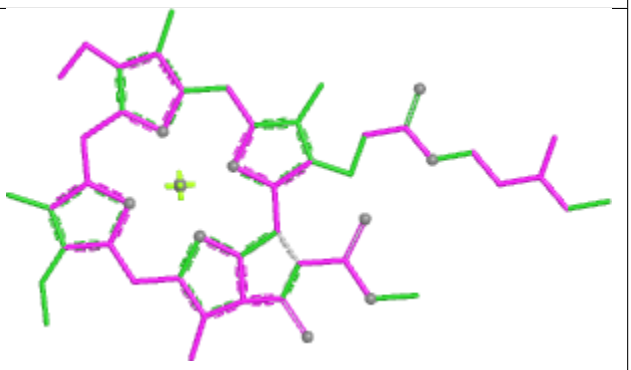


Rings

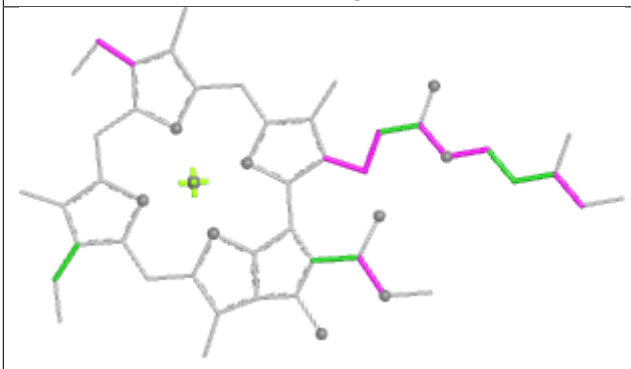
Ligand CLA A 832



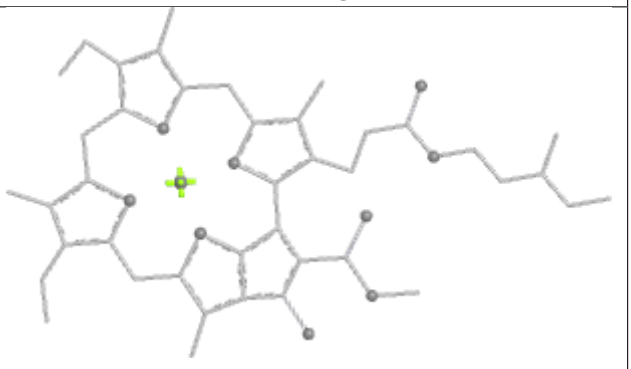
Bond lengths



Bond angles

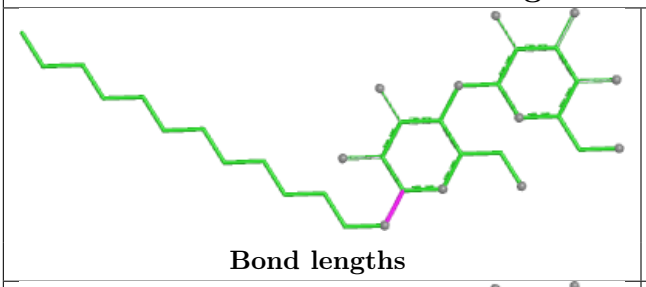


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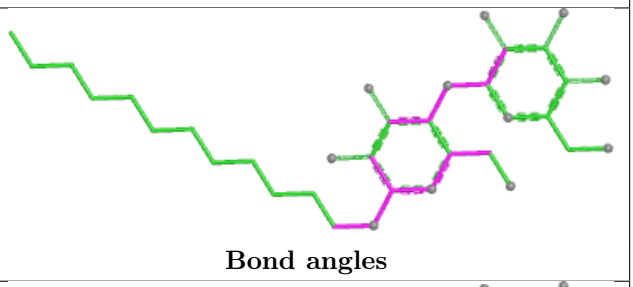


Rings

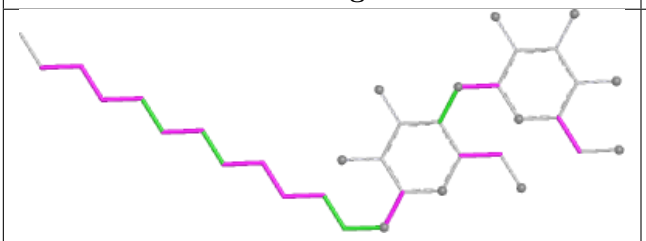
Ligand LMU 2 319



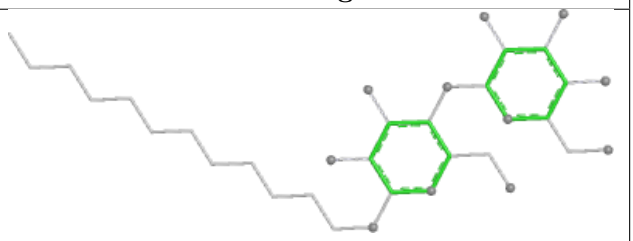
Bond lengths



Bond angles

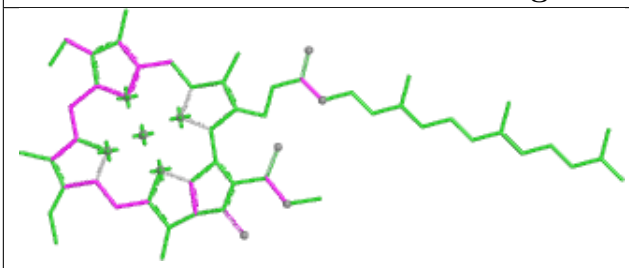


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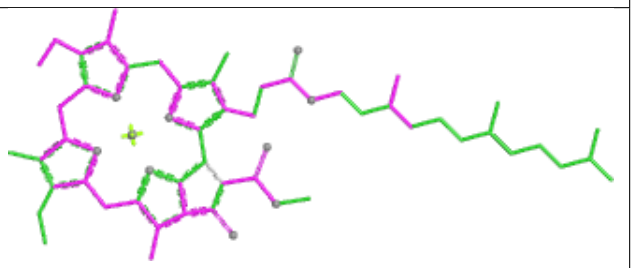


Rings

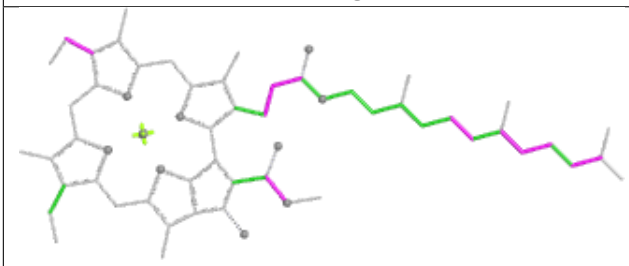
Ligand CLA I 102



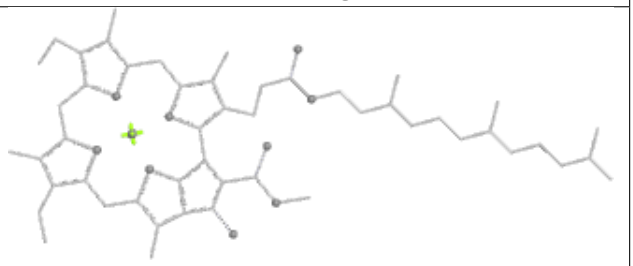
Bond lengths



Bond angles

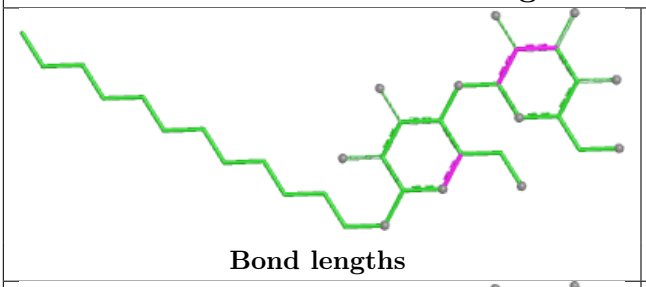


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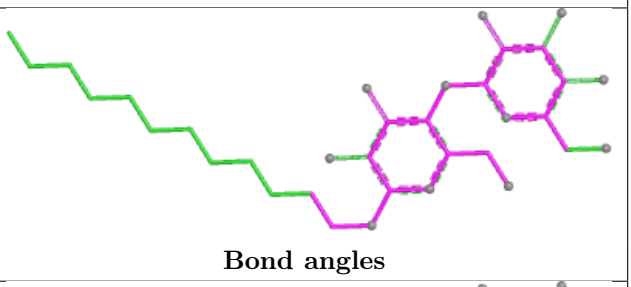


Rings

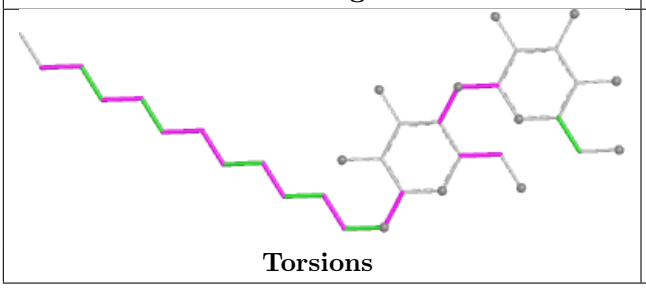
Ligand LMU H 104



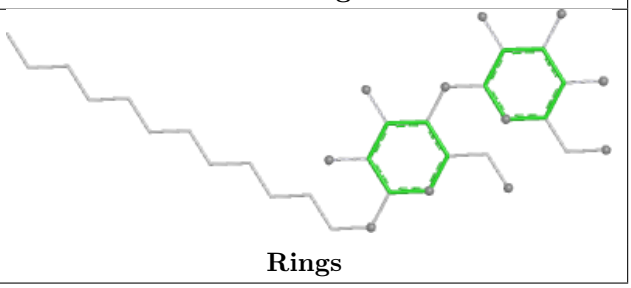
Bond lengths



Bond angles

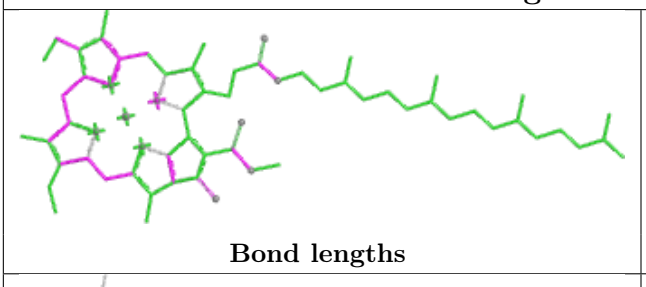


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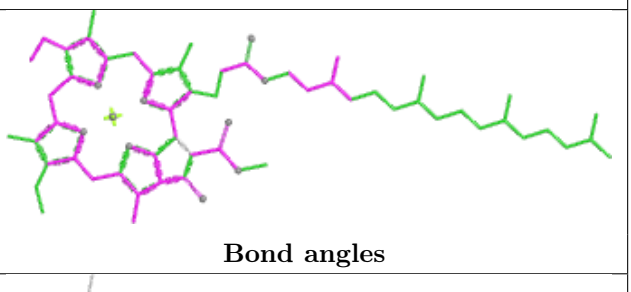


Rings

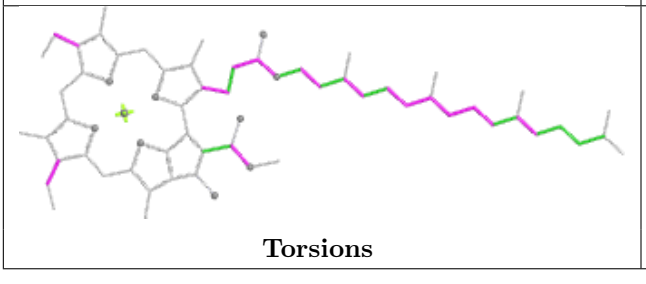
Ligand CLA A 823



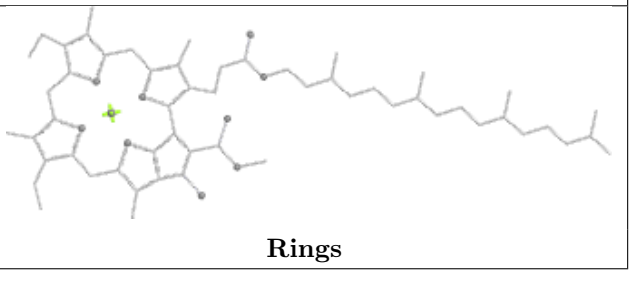
Bond lengths



Bond angles

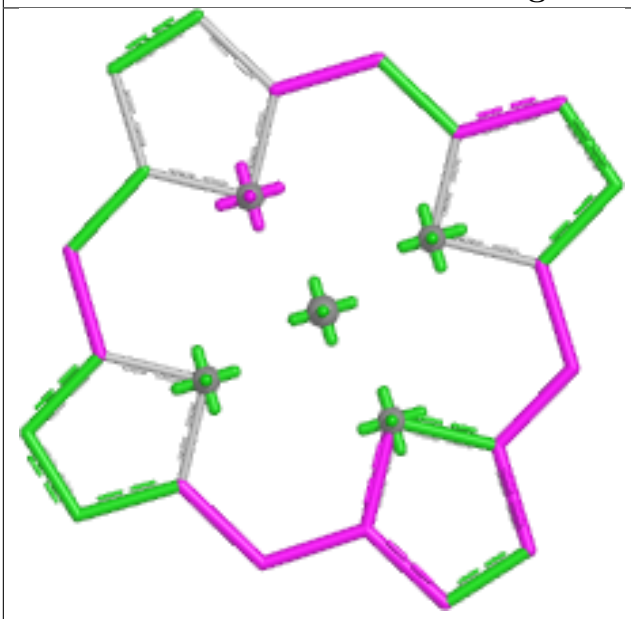


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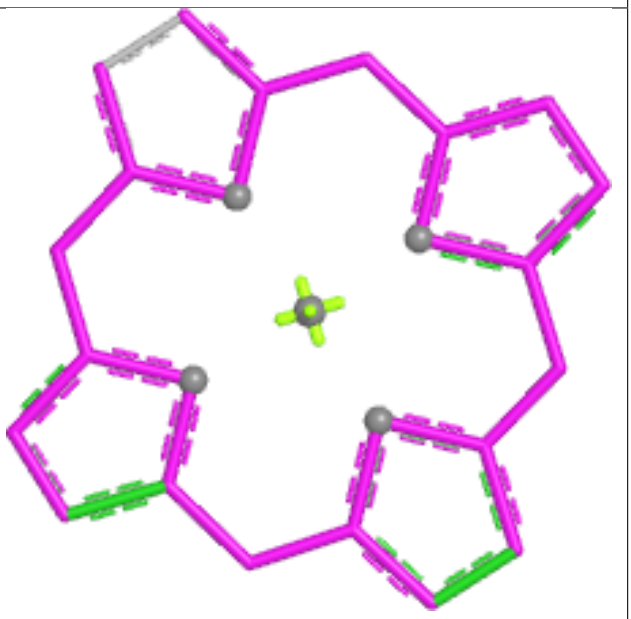


Rings

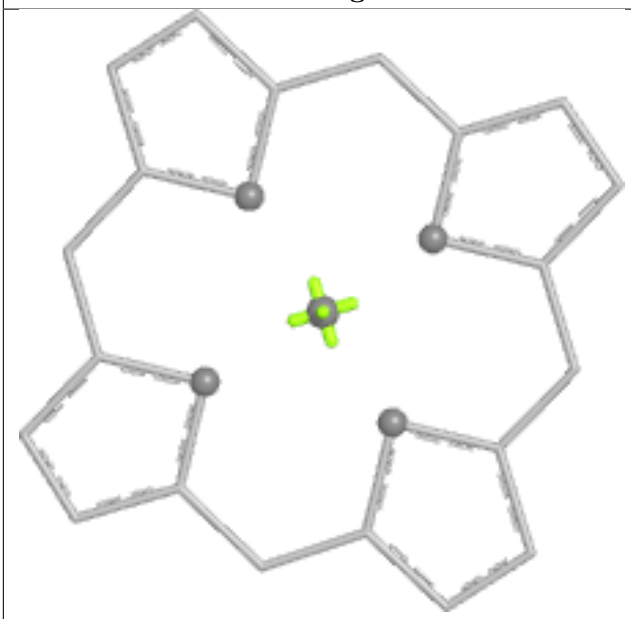
Ligand CLA 2 314



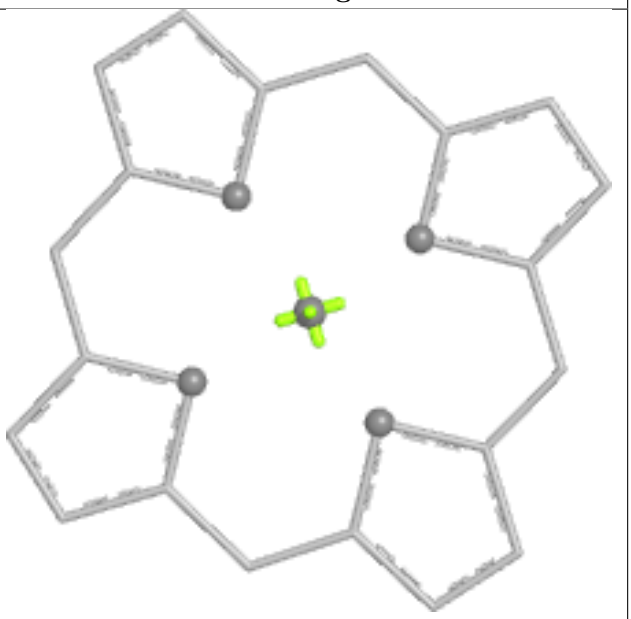
Bond lengths



Bond angles

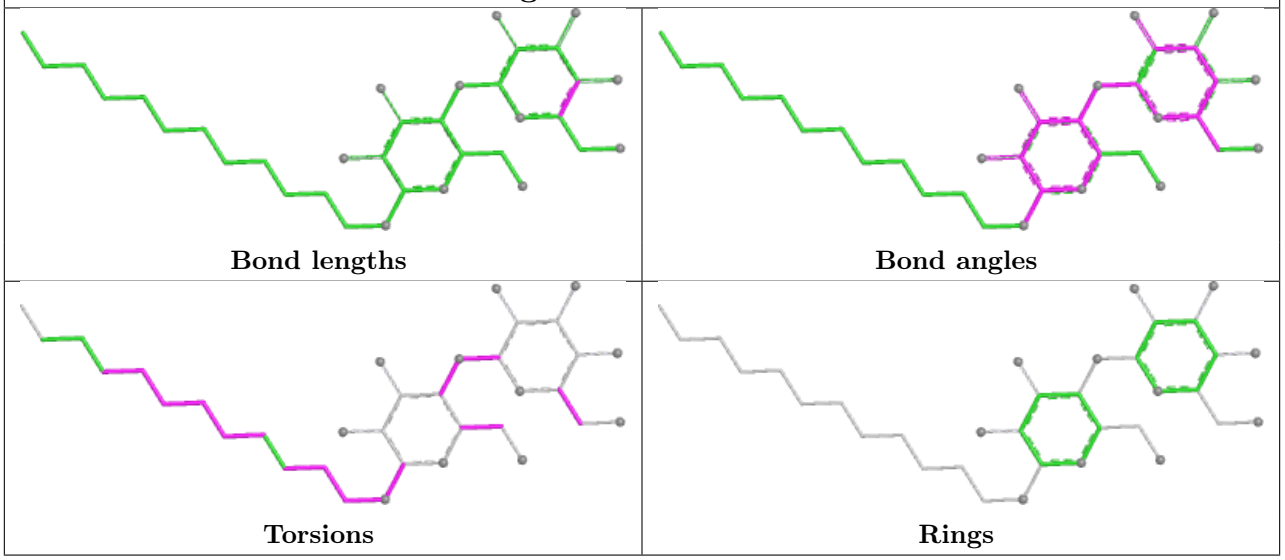


Torsions

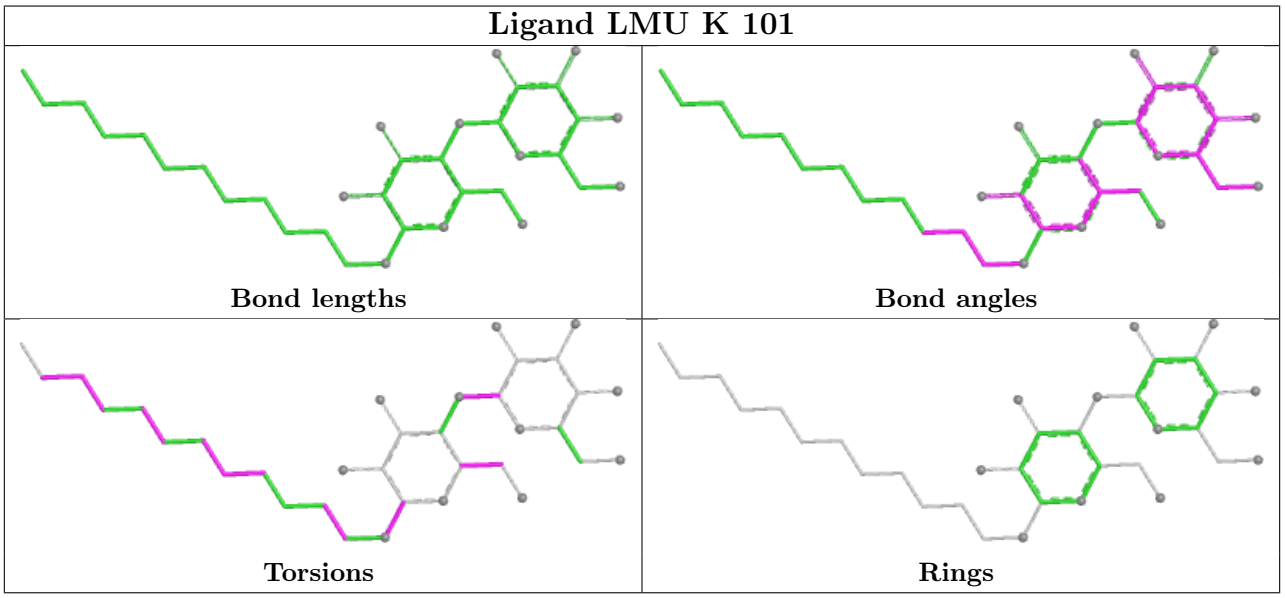


Rings

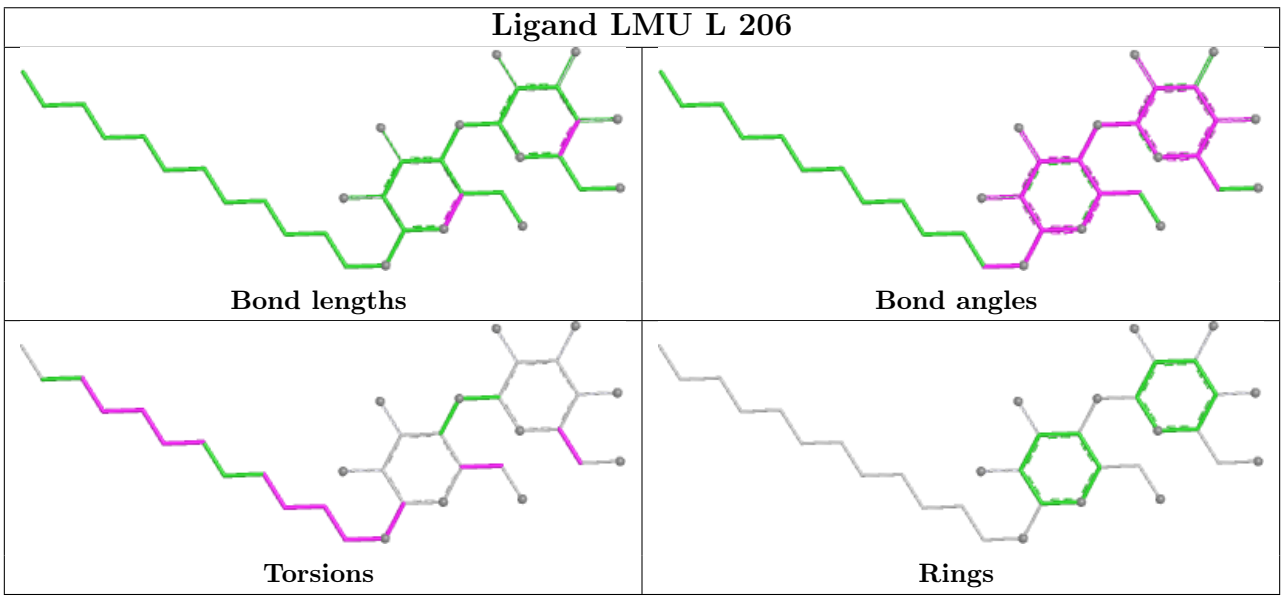
Ligand LMU H 103



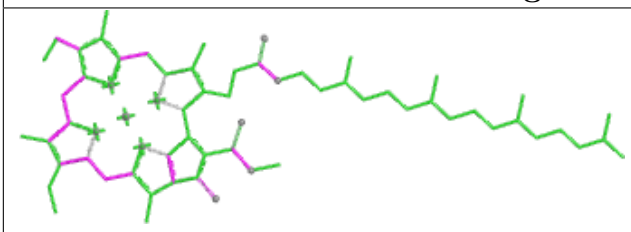
Ligand LMU K 101



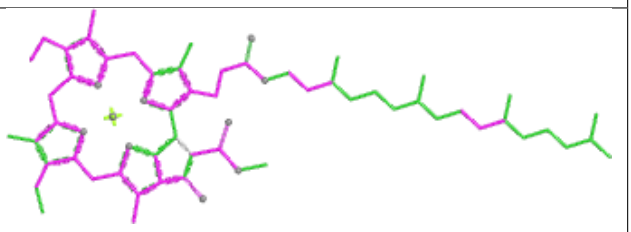
Ligand LMU L 206



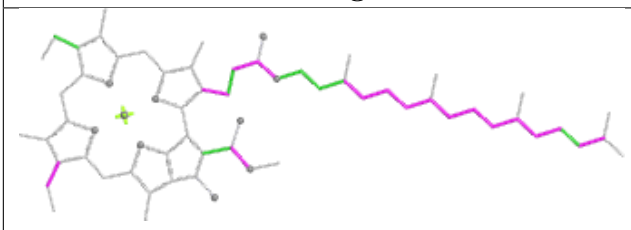
Ligand CLA A 809



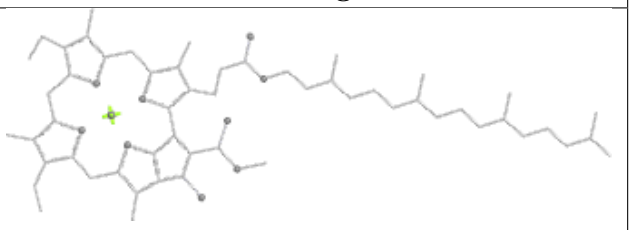
Bond lengths



Bond angles



Torsions



Rings

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	317:TYR	C	318:ARG	N	1.17

5 Fit of model and data

5.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1	165/241 (68%)	2.47	91 (55%) 0 0	31, 61, 71, 72	0
2	2	176/269 (65%)	1.97	66 (37%) 1 1	33, 52, 64, 68	0
3	3	162/276 (58%)	2.41	90 (55%) 0 0	49, 79, 110, 112	0
4	4	166/251 (66%)	1.96	68 (40%) 0 0	21, 44, 57, 58	0
5	A	730/758 (96%)	1.44	170 (23%) 2 2	20, 20, 20, 20	0
6	B	733/734 (99%)	1.51	186 (25%) 1 1	20, 20, 20, 20	0
7	C	81/81 (100%)	1.87	31 (38%) 1 1	20, 20, 20, 20	0
8	D	138/212 (65%)	1.15	19 (13%) 6 5	20, 20, 20, 20	0
9	E	65/143 (45%)	1.13	10 (15%) 5 4	20, 20, 20, 20	0
10	F	154/231 (66%)	1.16	31 (20%) 3 2	20, 20, 20, 20	0
11	G	95/167 (56%)	0.91	8 (8%) 17 13	20, 20, 20, 20	0
12	H	69/144 (47%)	1.03	9 (13%) 7 6	20, 20, 20, 20	0
13	I	30/40 (75%)	0.57	0 100 100	20, 20, 20, 20	0
14	J	42/44 (95%)	0.95	4 (9%) 14 11	20, 20, 20, 20	0
15	K	84/131 (64%)	1.08	12 (14%) 6 5	20, 20, 20, 20	0
16	L	161/216 (74%)	1.16	29 (18%) 3 3	20, 20, 20, 20	0
17	N	85/170 (50%)	0.50	3 (3%) 47 31	20, 20, 20, 20	0
18	R	0/53	-	-	-	-
All	All	3136/4161 (75%)	1.51	827 (26%) 1 1	20, 20, 65, 112	0

All (827) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	B	491	ASN	11.2
2	2	123	PRO	10.9
1	1	92	GLY	9.8

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Mol	Chain	Res	Type	RSRZ
1	1	113	SER	8.7
1	1	75	ALA	8.7
5	A	266	ALA	8.6
5	A	220	ARG	8.4
1	1	42	SER	8.3
5	A	344	LYS	8.2
5	A	388	ASP	8.0
6	B	562	PRO	7.9
3	3	72	ALA	7.9
4	4	114	SER	7.8
5	A	505	PRO	7.8
5	A	617	SER	7.6
4	4	68	GLY	7.3
3	3	58	GLU	7.2
4	4	67	ILE	7.2
6	B	558	PRO	7.2
6	B	170	ASN	6.9
6	B	223	GLY	6.9
2	2	110	TRP	6.7
2	2	173	ALA	6.5
15	K	16	THR	6.3
5	A	126	ILE	6.3
5	A	610	SER	6.3
16	L	117	ALA	6.2
1	1	28	GLY	6.1
5	A	33	GLN	6.1
3	3	55	ALA	6.1
6	B	676	GLU	6.1
6	B	563	GLY	6.1
5	A	724	ALA	6.0
3	3	122	GLY	5.9
3	3	42	PRO	5.9
5	A	381	PRO	5.9
6	B	561	GLY	5.8
6	B	517	PHE	5.8
5	A	487	VAL	5.8
1	1	34	ALA	5.7
7	C	80	ALA	5.7
5	A	272	LEU	5.7
5	A	514	THR	5.6
3	3	40	SER	5.6
1	1	33	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
1	1	32	VAL	5.5
6	B	584	LEU	5.5
4	4	73	PRO	5.5
5	A	191	PRO	5.5
5	A	659	ALA	5.5
5	A	752	ALA	5.4
5	A	470	LEU	5.4
5	A	518	GLY	5.4
6	B	258	LEU	5.4
6	B	527	LEU	5.3
4	4	125	SER	5.3
1	1	41	GLU	5.3
6	B	484	PRO	5.3
2	2	92	THR	5.2
1	1	46	HIS	5.2
3	3	180	LYS	5.2
3	3	75	PRO	5.2
16	L	80	ALA	5.1
1	1	19	PRO	5.1
3	3	91	PRO	5.1
3	3	54	LEU	5.1
6	B	292	ARG	5.1
3	3	83	LEU	5.1
2	2	43	TRP	5.0
2	2	119	VAL	5.0
2	2	53	ARG	4.9
3	3	80	LYS	4.9
7	C	9	ASP	4.9
3	3	67	LEU	4.9
5	A	185	HIS	4.9
2	2	169	LEU	4.9
5	A	484	LEU	4.9
5	A	485	GLN	4.8
2	2	117	GLY	4.8
6	B	470	THR	4.8
6	B	679	ALA	4.8
2	2	125	PHE	4.7
4	4	147	LEU	4.7
5	A	751	LEU	4.7
3	3	71	GLY	4.7
2	2	122	ASP	4.7
6	B	252	THR	4.7

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Mol	Chain	Res	Type	RSRZ
2	2	165	LYS	4.7
1	1	87	ASN	4.7
6	B	69	ALA	4.7
3	3	92	TRP	4.6
6	B	271	THR	4.6
5	A	124	TRP	4.6
5	A	340	GLY	4.6
4	4	69	ILE	4.6
5	A	385	LEU	4.5
1	1	24	PHE	4.5
1	1	172	GLY	4.5
2	2	140	GLY	4.5
4	4	132	GLY	4.5
6	B	260	GLY	4.5
3	3	196	GLY	4.5
3	3	73	ILE	4.5
2	2	116	PRO	4.5
5	A	750	PHE	4.5
10	F	152	ASN	4.4
3	3	84	ILE	4.4
1	1	88	PRO	4.4
1	1	78	PRO	4.4
5	A	130	GLU	4.3
1	1	39	TYR	4.3
1	1	44	LEU	4.3
6	B	93	ASP	4.3
5	A	745	THR	4.3
5	A	329	ASP	4.3
2	2	141	LEU	4.3
3	3	78	LEU	4.3
1	1	38	ARG	4.3
6	B	171	ALA	4.3
1	1	43	GLU	4.3
5	A	391	THR	4.2
6	B	300	SER	4.2
1	1	117	ASP	4.2
6	B	486	LEU	4.2
6	B	212	PHE	4.2
5	A	433	ASP	4.2
6	B	272	ASP	4.2
3	3	187	GLY	4.2
7	C	41	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	1	95	PRO	4.1
2	2	58	GLY	4.1
6	B	233	TYR	4.1
1	1	37	GLU	4.1
1	1	152	ARG	4.1
3	3	79	GLY	4.1
6	B	205	GLU	4.1
3	3	65	ALA	4.1
1	1	164	GLN	4.1
4	4	86	SER	4.0
3	3	190	ALA	4.0
6	B	667	TRP	4.0
1	1	129	ASP	4.0
4	4	135	GLY	4.0
8	D	141	VAL	4.0
3	3	68	GLY	4.0
5	A	32	GLU	4.0
4	4	63	VAL	3.9
1	1	94	LEU	3.9
4	4	93	ILE	3.9
6	B	682	HIS	3.9
6	B	147	PHE	3.9
3	3	82	GLY	3.9
6	B	702	ILE	3.9
2	2	78	SER	3.9
5	A	160	SER	3.9
3	3	181	LEU	3.9
6	B	367	THR	3.9
1	1	26	PRO	3.8
3	3	77	ILE	3.8
5	A	359	SER	3.8
5	A	376	MET	3.8
3	3	114	PHE	3.8
4	4	97	LEU	3.8
3	3	64	TYR	3.8
6	B	458	ILE	3.8
4	4	34	PRO	3.8
4	4	115	VAL	3.8
3	3	107	TRP	3.8
4	4	145	PRO	3.8
5	A	500	PRO	3.8
1	1	148	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
5	A	247	GLU	3.7
3	3	66	MET	3.7
4	4	118	ASP	3.7
5	A	265	GLY	3.7
1	1	169	PRO	3.7
3	3	199	VAL	3.7
8	D	99	GLN	3.7
6	B	502	ASN	3.7
6	B	40	GLY	3.7
1	1	173	PRO	3.7
3	3	184	VAL	3.7
6	B	255	LEU	3.7
8	D	71	GLY	3.7
6	B	346	SER	3.6
7	C	4	SER	3.6
2	2	170	ALA	3.6
3	3	60	ILE	3.6
5	A	471	GLY	3.6
8	D	108	GLU	3.6
6	B	560	ASP	3.6
1	1	79	GLY	3.6
2	2	55	ALA	3.6
16	L	159	TYR	3.6
5	A	707	ILE	3.6
12	H	47	PHE	3.6
7	C	6	LYS	3.6
4	4	89	THR	3.6
6	B	574	ASP	3.6
1	1	55	PRO	3.6
5	A	203	LEU	3.6
1	1	93	THR	3.6
5	A	657	LEU	3.5
6	B	350	GLN	3.5
10	F	64	GLY	3.5
5	A	584	PRO	3.5
5	A	662	SER	3.5
5	A	527	VAL	3.5
10	F	76	ASP	3.5
16	L	81	GLY	3.5
6	B	610	ASN	3.5
4	4	117	GLN	3.5
6	B	513	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
6	B	566	GLY	3.5
6	B	645	VAL	3.5
5	A	181	ALA	3.5
10	F	111	GLU	3.5
7	C	54	CYS	3.5
3	3	81	ALA	3.5
6	B	556	SER	3.5
4	4	104	ARG	3.5
2	2	163	GLU	3.4
6	B	132	ASN	3.4
1	1	27	LEU	3.4
5	A	568	LEU	3.4
5	A	510	SER	3.4
1	1	74	TRP	3.4
10	F	110	ASP	3.4
5	A	635	THR	3.4
15	K	53	ALA	3.4
5	A	299	ILE	3.4
6	B	492	ILE	3.4
4	4	39	TRP	3.4
4	4	126	LEU	3.4
5	A	494	ASN	3.4
8	D	137	ILE	3.4
6	B	457	PRO	3.4
6	B	183	PHE	3.4
10	F	107	ALA	3.4
4	4	109	ILE	3.4
1	1	47	CYS	3.4
9	E	84	LEU	3.4
3	3	191	MET	3.4
7	C	78	GLY	3.4
6	B	319	HIS	3.4
5	A	440	ASP	3.3
1	1	51	MET	3.3
2	2	138	PRO	3.3
3	3	53	TRP	3.3
5	A	34	TRP	3.3
6	B	690	LEU	3.3
16	L	69	VAL	3.3
1	1	134	SER	3.3
2	2	139	GLY	3.3
6	B	453	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
2	2	166	ASN	3.3
2	2	157	LYS	3.3
1	1	84	TYR	3.3
6	B	263	PRO	3.3
6	B	262	HIS	3.3
6	B	113	VAL	3.3
5	A	157	GLY	3.3
5	A	517	GLY	3.3
1	1	21	ASP	3.3
1	1	105	ILE	3.3
1	1	175	GLU	3.3
5	A	249	ILE	3.3
1	1	35	ASN	3.2
5	A	128	GLY	3.2
5	A	345	GLY	3.2
1	1	130	PRO	3.2
16	L	65	VAL	3.2
6	B	570	ILE	3.2
6	B	274	ALA	3.2
3	3	113	LEU	3.2
7	C	8	TYR	3.2
8	D	86	LEU	3.2
14	J	4	PHE	3.2
1	1	82	ALA	3.2
5	A	293	GLY	3.2
1	1	111	GLN	3.2
1	1	76	ALA	3.2
4	4	157	GLY	3.2
5	A	182	GLY	3.2
16	L	96	SER	3.2
5	A	71	LEU	3.1
3	3	76	GLU	3.1
1	1	150	ASN	3.1
2	2	191	ASN	3.1
4	4	83	TYR	3.1
4	4	133	TYR	3.1
2	2	182	ILE	3.1
8	D	116	ASP	3.1
8	D	151	LYS	3.1
5	A	643	ALA	3.1
6	B	321	GLY	3.1
3	3	89	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
16	L	115	ALA	3.1
6	B	734	GLY	3.1
7	C	56	SER	3.1
6	B	208	ARG	3.1
12	H	76	VAL	3.1
10	F	124	PRO	3.1
11	G	27	GLN	3.1
4	4	66	SER	3.1
7	C	67	VAL	3.1
16	L	116	PRO	3.1
7	C	11	CYS	3.1
3	3	90	LEU	3.0
2	2	179	PHE	3.0
4	4	50	TRP	3.0
6	B	217	PRO	3.0
1	1	36	LEU	3.0
3	3	173	GLU	3.0
2	2	210	PRO	3.0
5	A	497	ALA	3.0
1	1	40	LYS	3.0
4	4	142	ASN	3.0
3	3	115	VAL	3.0
1	1	96	THR	3.0
2	2	113	ILE	3.0
6	B	493	TRP	3.0
2	2	152	SER	3.0
5	A	100	GLY	3.0
1	1	145	VAL	3.0
4	4	101	VAL	3.0
4	4	131	VAL	3.0
3	3	95	THR	3.0
5	A	486	PRO	3.0
5	A	551	VAL	3.0
6	B	181	GLY	3.0
7	C	5	VAL	3.0
3	3	116	PHE	3.0
10	F	63	CYS	3.0
17	N	77	CYS	3.0
5	A	693	LEU	2.9
2	2	181	HIS	2.9
2	2	205	PHE	2.9
5	A	341	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
5	A	532	ILE	2.9
1	1	112	ARG	2.9
5	A	362	LEU	2.9
6	B	131	THR	2.9
6	B	135	LEU	2.9
7	C	10	THR	2.9
16	L	86	LEU	2.9
15	K	44	GLU	2.9
6	B	337	ALA	2.9
5	A	106	TYR	2.9
5	A	588	GLY	2.9
9	E	56	ASP	2.9
16	L	134	ASP	2.9
5	A	360	ILE	2.9
1	1	140	LEU	2.9
2	2	114	LEU	2.9
5	A	304	LEU	2.9
5	A	586	ARG	2.9
6	B	620	LEU	2.9
6	B	366	THR	2.9
7	C	17	CYS	2.9
5	A	264	GLU	2.9
6	B	555	TYR	2.9
10	F	98	GLY	2.9
10	F	135	SER	2.9
12	H	30	SER	2.9
7	C	60	THR	2.9
3	3	125	GLU	2.9
4	4	134	PRO	2.9
6	B	568	CYS	2.9
6	B	582	TRP	2.9
5	A	248	PHE	2.9
2	2	207	ALA	2.9
5	A	386	ALA	2.9
3	3	104	TYR	2.9
3	3	202	LEU	2.9
5	A	263	ALA	2.8
5	A	509	ALA	2.8
15	K	49	THR	2.8
11	G	74	TRP	2.8
16	L	93	VAL	2.8
3	3	93	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
5	A	196	PHE	2.8
9	E	74	TYR	2.8
5	A	744	ALA	2.8
6	B	197	VAL	2.8
5	A	407	ILE	2.8
6	B	427	LEU	2.8
10	F	32	TYR	2.8
1	1	186	HIS	2.8
3	3	69	ALA	2.8
3	3	74	ALA	2.8
6	B	642	SER	2.8
12	H	26	SER	2.8
3	3	117	GLU	2.8
6	B	397	ASP	2.8
7	C	37	LYS	2.8
5	A	749	PHE	2.8
6	B	251	GLY	2.8
1	1	146	LYS	2.8
6	B	732	LYS	2.8
7	C	55	GLU	2.8
1	1	45	ILE	2.8
4	4	36	ASN	2.8
6	B	210	ASN	2.8
1	1	81	GLN	2.8
16	L	82	ALA	2.8
6	B	448	THR	2.8
5	A	153	TRP	2.7
6	B	67	HIS	2.7
4	4	51	ALA	2.7
1	1	159	VAL	2.7
4	4	161	LEU	2.7
5	A	607	ASN	2.7
6	B	358	TYR	2.7
2	2	206	ALA	2.7
3	3	126	HIS	2.7
5	A	685	VAL	2.7
9	E	66	VAL	2.7
2	2	175	MET	2.7
10	F	143	GLU	2.7
1	1	64	GLY	2.7
4	4	192	THR	2.7
8	D	63	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
16	L	84	GLY	2.7
5	A	354	TRP	2.7
7	C	52	LYS	2.7
6	B	291	TYR	2.7
1	1	18	ALA	2.7
6	B	114	ASN	2.7
3	3	166	PRO	2.7
2	2	164	ILE	2.7
6	B	632	ILE	2.7
6	B	724	PHE	2.7
1	1	115	GLU	2.7
3	3	43	GLU	2.7
6	B	221	GLY	2.7
1	1	83	THR	2.7
2	2	133	THR	2.7
3	3	112	THR	2.7
4	4	110	LYS	2.7
6	B	511	THR	2.7
6	B	619	TRP	2.7
8	D	50	TRP	2.7
6	B	569	ASP	2.7
4	4	47	ASN	2.7
6	B	487	ASN	2.7
6	B	498	LEU	2.7
5	A	270	PHE	2.7
6	B	340	SER	2.7
7	C	25	VAL	2.7
2	2	62	ILE	2.6
5	A	245	PRO	2.6
7	C	12	ILE	2.6
4	4	174	GLY	2.6
6	B	259	GLY	2.6
6	B	209	TRP	2.6
3	3	120	LEU	2.6
6	B	118	SER	2.6
6	B	479	SER	2.6
16	L	88	ALA	2.6
17	N	2	VAL	2.6
4	4	124	TYR	2.6
5	A	384	TYR	2.6
6	B	303	TYR	2.6
4	4	70	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
5	A	49	ASP	2.6
6	B	12	ILE	2.6
3	3	123	PHE	2.6
5	A	77	LYS	2.6
5	A	45	ALA	2.6
6	B	454	LEU	2.6
10	F	62	LEU	2.6
2	2	87	TYR	2.6
5	A	198	ASP	2.6
6	B	98	GLN	2.6
1	1	80	GLY	2.6
1	1	181	LEU	2.6
1	1	50	ALA	2.6
2	2	121	THR	2.6
3	3	70	VAL	2.6
3	3	108	ALA	2.6
4	4	144	ALA	2.6
4	4	172	VAL	2.6
6	B	27	THR	2.6
6	B	670	TYR	2.6
16	L	102	TYR	2.6
3	3	198	PHE	2.6
1	1	72	GLN	2.6
3	3	41	ASP	2.6
5	A	506	GLY	2.6
6	B	268	LEU	2.6
5	A	122	VAL	2.6
6	B	438	VAL	2.6
9	E	65	VAL	2.6
6	B	123	TRP	2.6
3	3	194	ILE	2.6
5	A	98	PHE	2.6
6	B	31	PHE	2.6
6	B	595	HIS	2.6
3	3	47	GLY	2.6
8	D	34	GLY	2.6
5	A	368	LEU	2.6
2	2	66	GLU	2.6
6	B	195	VAL	2.6
4	4	122	LYS	2.6
17	N	56	LYS	2.6
4	4	173	THR	2.6

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Mol	Chain	Res	Type	RSRZ
5	A	195	TRP	2.5
2	2	63	PHE	2.5
6	B	29	HIS	2.5
9	E	82	TYR	2.5
6	B	613	SER	2.5
5	A	696	GLY	2.5
1	1	177	LEU	2.5
3	3	189	LEU	2.5
4	4	181	LEU	2.5
5	A	127	VAL	2.5
1	1	106	ALA	2.5
2	2	54	TRP	2.5
5	A	743	ILE	2.5
6	B	559	CYS	2.5
5	A	660	GLN	2.5
6	B	608	GLN	2.5
10	F	4	GLY	2.5
2	2	50	VAL	2.5
6	B	343	VAL	2.5
1	1	178	ALA	2.5
2	2	59	ALA	2.5
16	L	140	THR	2.5
6	B	697	PRO	2.5
6	B	347	LEU	2.5
6	B	204	GLY	2.5
4	4	87	SER	2.5
5	A	161	GLU	2.5
1	1	49	TRP	2.5
4	4	106	TRP	2.5
5	A	548	THR	2.5
3	3	111	TYR	2.5
10	F	101	GLY	2.5
16	L	9	GLN	2.5
5	A	512	SER	2.5
1	1	31	GLU	2.5
6	B	533	ILE	2.5
16	L	78	GLU	2.5
10	F	6	THR	2.5
1	1	58	LEU	2.5
6	B	341	LEU	2.5
6	B	478	LEU	2.5
7	C	69	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	2	176	GLY	2.5
3	3	151	GLY	2.5
5	A	682	ALA	2.4
16	L	34	ALA	2.4
6	B	423	SER	2.4
4	4	62	GLU	2.4
6	B	8	PHE	2.4
1	1	25	ASP	2.4
6	B	124	TRP	2.4
2	2	126	PRO	2.4
5	A	123	VAL	2.4
10	F	73	VAL	2.4
12	H	25	GLY	2.4
1	1	165	GLN	2.4
3	3	98	ILE	2.4
6	B	354	SER	2.4
6	B	261	PHE	2.4
15	K	63	CYS	2.4
5	A	567	ARG	2.4
6	B	469	LYS	2.4
2	2	161	THR	2.4
5	A	699	TYR	2.4
6	B	473	GLY	2.4
3	3	201	ALA	2.4
5	A	616	PHE	2.4
6	B	227	THR	2.4
6	B	646	TRP	2.4
4	4	112	PRO	2.4
9	E	79	THR	2.4
3	3	62	GLY	2.4
5	A	461	TYR	2.4
1	1	53	ALA	2.4
15	K	65	ALA	2.4
6	B	713	PHE	2.4
5	A	705	GLU	2.4
10	F	71	LEU	2.4
1	1	54	VAL	2.4
3	3	88	THR	2.4
7	C	49	VAL	2.4
5	A	516	GLY	2.4
3	3	119	ALA	2.4
5	A	186	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	1	109	GLU	2.4
5	A	686	TRP	2.4
16	L	49	PRO	2.4
2	2	103	GLY	2.3
5	A	117	GLY	2.3
5	A	589	THR	2.3
6	B	117	TYR	2.3
6	B	214	ASP	2.3
6	B	437	TYR	2.3
1	1	85	LEU	2.3
5	A	296	LEU	2.3
6	B	175	LEU	2.3
6	B	334	LEU	2.3
5	A	80	SER	2.3
6	B	420	SER	2.3
10	F	38	PRO	2.3
10	F	137	PRO	2.3
11	G	9	SER	2.3
1	1	20	GLY	2.3
2	2	60	ALA	2.3
5	A	82	HIS	2.3
11	G	51	ALA	2.3
10	F	66	ASP	2.3
5	A	493	GLN	2.3
16	L	145	PHE	2.3
11	G	22	VAL	2.3
4	4	105	ARG	2.3
6	B	694	ARG	2.3
3	3	57	GLY	2.3
5	A	236	GLY	2.3
5	A	415	ALA	2.3
5	A	608	SER	2.3
6	B	571	SER	2.3
6	B	701	SER	2.3
7	C	2	SER	2.3
8	D	33	THR	2.3
16	L	106	SER	2.3
2	2	183	TYR	2.3
2	2	159	LEU	2.3
4	4	59	LEU	2.3
4	4	40	PHE	2.3
6	B	446	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
5	A	733	VAL	2.3
2	2	77	PRO	2.3
5	A	613	ILE	2.3
6	B	309	ILE	2.3
3	3	110	SER	2.3
4	4	121	PHE	2.3
5	A	105	ASN	2.3
3	3	188	ARG	2.3
1	1	99	ALA	2.3
7	C	40	ALA	2.3
16	L	141	GLY	2.3
6	B	567	THR	2.3
8	D	90	LEU	2.3
5	A	353	SER	2.3
8	D	32	SER	2.3
10	F	11	SER	2.3
3	3	105	ASN	2.3
2	2	180	GLN	2.3
8	D	115	LYS	2.3
5	A	76	ARG	2.3
6	B	441	ASP	2.3
1	1	141	GLU	2.2
1	1	147	GLU	2.2
5	A	742	GLY	2.2
6	B	237	PRO	2.2
6	B	618	GLY	2.2
1	1	174	LEU	2.2
4	4	37	LEU	2.2
16	L	118	LEU	2.2
6	B	573	TRP	2.2
6	B	657	TRP	2.2
3	3	169	PHE	2.2
11	G	5	SER	2.2
7	C	66	ARG	2.2
1	1	89	VAL	2.2
5	A	143	ILE	2.2
16	L	33	ILE	2.2
2	2	171	MET	2.2
3	3	167	LEU	2.2
5	A	219	ALA	2.2
6	B	250	ALA	2.2
6	B	616	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
6	B	658	ALA	2.2
16	L	101	MET	2.2
6	B	625	TRP	2.2
3	3	140	LYS	2.2
6	B	332	PHE	2.2
4	4	146	THR	2.2
6	B	712	HIS	2.2
4	4	38	ARG	2.2
5	A	753	ARG	2.2
6	B	372	TYR	2.2
5	A	94	SER	2.2
5	A	217	SER	2.2
10	F	128	SER	2.2
9	E	36	VAL	2.2
5	A	197	GLN	2.2
4	4	180	ASN	2.2
5	A	594	ALA	2.2
6	B	655	LEU	2.2
10	F	35	ASP	2.2
6	B	671	TRP	2.2
2	2	137	TYR	2.2
3	3	106	TYR	2.2
7	C	68	TYR	2.2
10	F	138	VAL	2.2
11	G	11	SER	2.2
10	F	116	GLN	2.2
2	2	198	ALA	2.2
6	B	362	ALA	2.2
7	C	42	ALA	2.2
3	3	182	LYS	2.2
12	H	22	ASP	2.2
3	3	94	ARG	2.2
4	4	138	PHE	2.2
5	A	280	PHE	2.2
2	2	89	THR	2.2
1	1	168	TYR	2.2
5	A	165	TYR	2.2
5	A	371	VAL	2.2
5	A	66	SER	2.2
5	A	444	SER	2.2
6	B	455	ILE	2.2
15	K	5	SER	2.2

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Mol	Chain	Res	Type	RSRZ
6	B	116	ALA	2.2
6	B	723	ALA	2.2
15	K	27	ALA	2.2
5	A	570	PRO	2.2
14	J	12	PRO	2.2
4	4	143	PHE	2.2
8	D	62	THR	2.1
8	D	149	THR	2.1
15	K	17	LEU	2.1
2	2	109	ARG	2.1
3	3	51	PRO	2.1
6	B	219	PRO	2.1
6	B	621	ARG	2.1
10	F	153	ASN	2.1
5	A	655	ASP	2.1
5	A	53	TRP	2.1
8	D	49	THR	2.1
5	A	451	ILE	2.1
6	B	472	TYR	2.1
5	A	93	LEU	2.1
5	A	346	LEU	2.1
5	A	395	LEU	2.1
6	B	338	LEU	2.1
2	2	167	GLY	2.1
5	A	734	GLY	2.1
4	4	64	PHE	2.1
4	4	156	ASN	2.1
6	B	474	PHE	2.1
5	A	658	TRP	2.1
7	C	70	TRP	2.1
5	A	271	THR	2.1
3	3	56	TYR	2.1
6	B	129	LEU	2.1
3	3	63	ARG	2.1
5	A	374	GLN	2.1
2	2	72	GLY	2.1
2	2	200	PRO	2.1
6	B	94	PRO	2.1
9	E	30	PRO	2.1
3	3	48	PHE	2.1
5	A	75	SER	2.1
7	C	64	SER	2.1

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Mol	Chain	Res	Type	RSRZ
5	A	574	ASN	2.1
10	F	146	ASN	2.1
6	B	157	LEU	2.1
6	B	419	ILE	2.1
6	B	622	ASP	2.1
6	B	626	LEU	2.1
6	B	490	ARG	2.1
7	C	57	ALA	2.1
15	K	46	GLY	2.1
15	K	64	GLY	2.1
10	F	83	PHE	2.1
1	1	97	ILE	2.1
4	4	49	ARG	2.1
4	4	103	ILE	2.1
5	A	211	LEU	2.1
5	A	187	HIS	2.1
5	A	303	HIS	2.1
6	B	516	ASP	2.1
5	A	511	THR	2.1
16	L	77	THR	2.1
7	C	36	ALA	2.1
9	E	70	ALA	2.1
6	B	264	GLN	2.1
11	G	47	GLY	2.1
1	1	137	PRO	2.1
2	2	84	GLU	2.1
5	A	73	GLU	2.1
5	A	424	PRO	2.1
6	B	133	GLU	2.1
10	F	100	VAL	2.0
14	J	10	VAL	2.0
5	A	119	SER	2.0
6	B	33	SER	2.0
6	B	91	ILE	2.0
6	B	145	LEU	2.0
8	D	36	LEU	2.0
12	H	54	LEU	2.0
5	A	438	HIS	2.0
6	B	242	HIS	2.0
14	J	1	MET	2.0
2	2	184	THR	2.0
4	4	31	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
6	B	43	TYR	2.0
12	H	28	ALA	2.0
6	B	663	PHE	2.0
12	H	46	PRO	2.0
1	1	139	LYS	2.0
2	2	174	VAL	2.0
4	4	98	SER	2.0
6	B	666	SER	2.0
1	1	114	MET	2.0
3	3	118	MET	2.0
6	B	627	ASN	2.0
6	B	641	ASN	2.0
5	A	221	HIS	2.0
5	A	300	ALA	2.0
5	A	717	ALA	2.0
6	B	2	ALA	2.0
16	L	83	ALA	2.0
3	3	44	GLY	2.0
3	3	136	GLY	2.0
5	A	694	PHE	2.0
15	K	50	GLY	2.0
4	4	107	GLN	2.0
4	4	140	PRO	2.0
3	3	195	LEU	2.0
6	B	37	ILE	2.0
10	F	120	ILE	2.0

5.2 Non-standard residues in protein, DNA, RNA chains (i)

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

5.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	GLC	M	1	10/12	-	-	20,20,20,20	0
19	FRU	M	2	12/12	-	-	20,20,20,20	0

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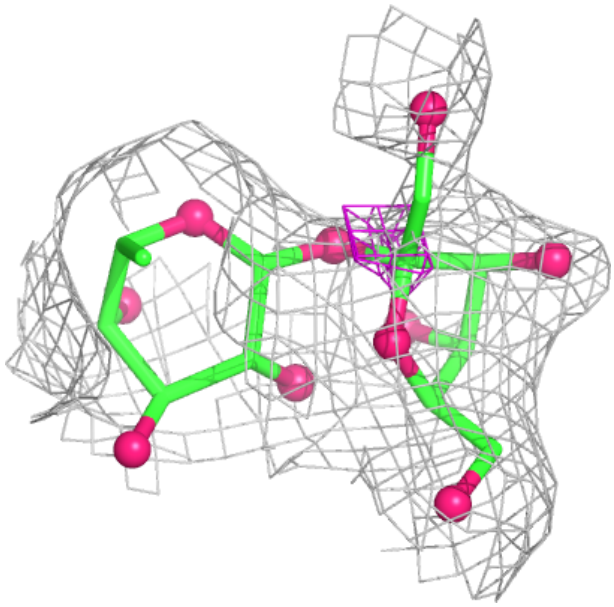
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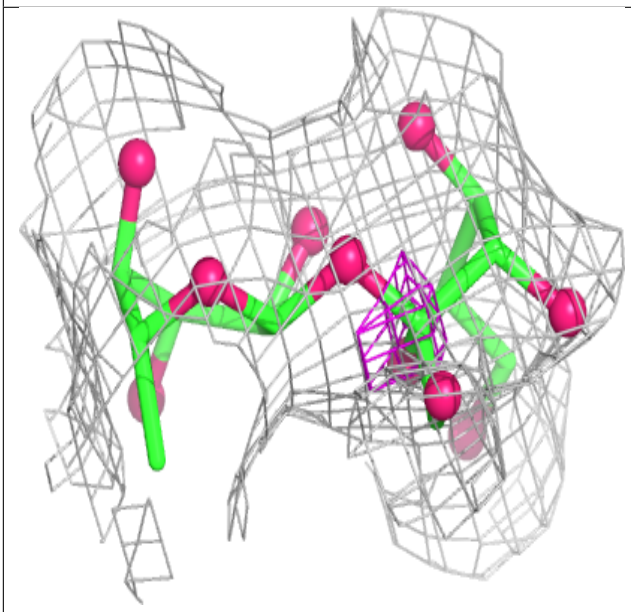
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	GLC	O	1	11/12	-	-	20,20,20,20	0
19	FRU	O	2	12/12	-	-	20,20,20,20	0
19	GLC	P	1	11/12	-	-	20,20,20,20	0
19	FRU	P	2	12/12	-	-	20,20,20,20	0
19	GLC	Q	1	11/12	-	-	20,20,20,20	0
19	FRU	Q	2	12/12	-	-	20,20,20,20	0
19	FRU	W	2	12/12	0.58	0.16	20,20,20,20	0
19	GLC	T	1	11/12	0.65	0.15	20,20,20,20	0
19	GLC	W	1	11/12	0.66	0.12	20,20,20,20	0
19	GLC	X	1	11/12	0.72	0.17	20,20,20,20	0
19	GLC	S	1	11/12	0.73	0.14	4,31,60,60	0
19	GLC	U	1	11/12	0.74	0.12	20,20,20,20	0
19	FRU	S	2	12/12	0.75	0.20	3,43,60,60	0
19	FRU	V	2	12/12	0.76	0.13	20,20,20,20	0
19	GLC	Z	1	11/12	0.76	0.12	20,20,20,20	0
19	GLC	V	1	11/12	0.78	0.11	20,20,20,20	0
19	FRU	Y	2	12/12	0.81	0.11	20,20,20,20	0
19	FRU	X	2	12/12	0.83	0.10	20,20,20,20	0
19	FRU	Z	2	12/12	0.84	0.10	20,20,20,20	0
19	FRU	U	2	12/12	0.86	0.10	20,20,20,20	0
19	FRU	T	2	12/12	0.88	0.09	20,20,20,20	0
19	GLC	Y	1	11/12	0.89	0.08	20,20,20,20	0
19	GLC	a	1	11/12	-	-	20,20,20,20	0
19	FRU	a	2	12/12	-	-	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain M:

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

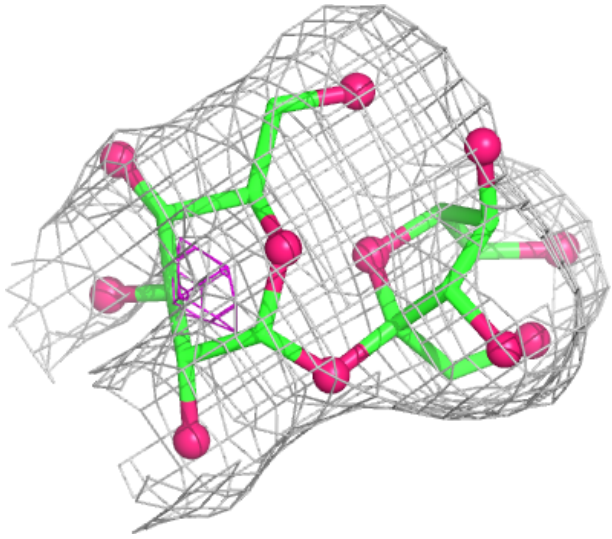


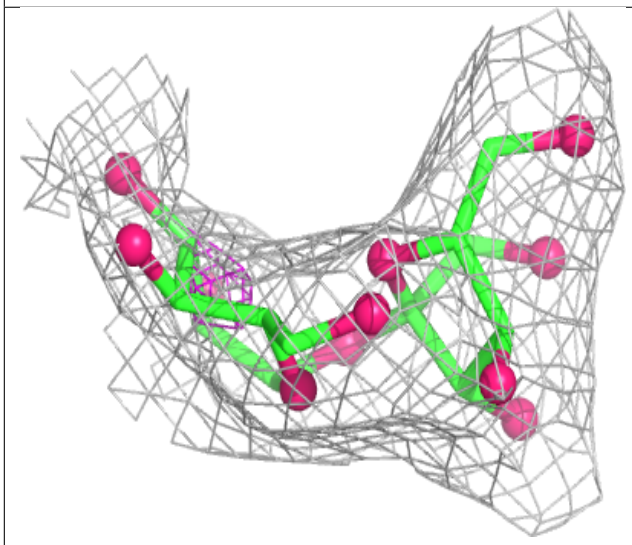


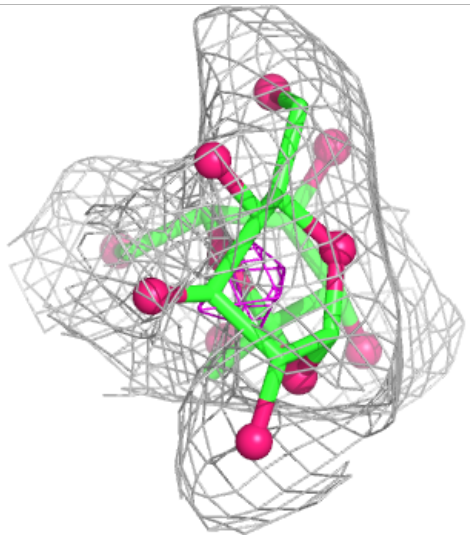


Electron density around Chain O:

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

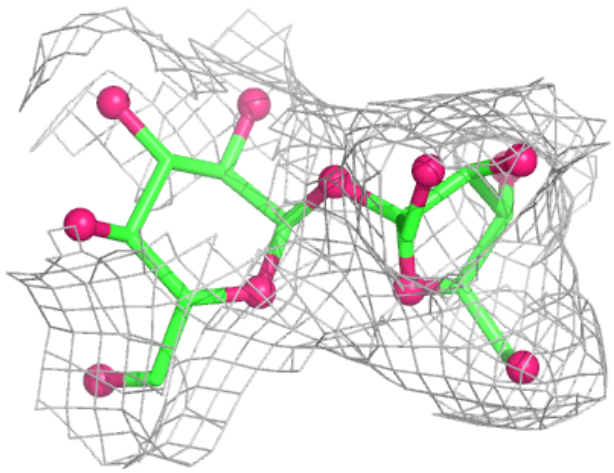


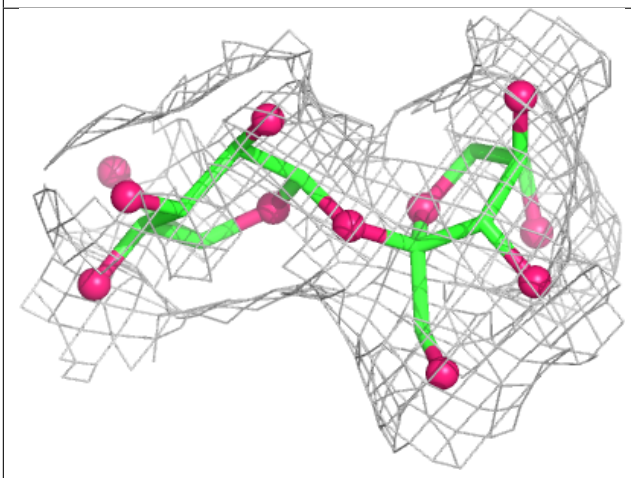


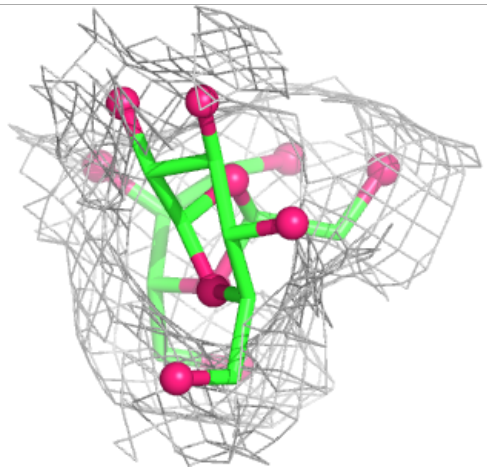


Electron density around Chain P:

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

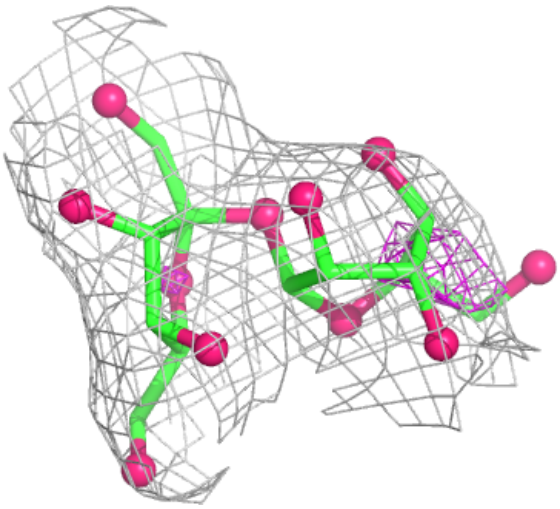


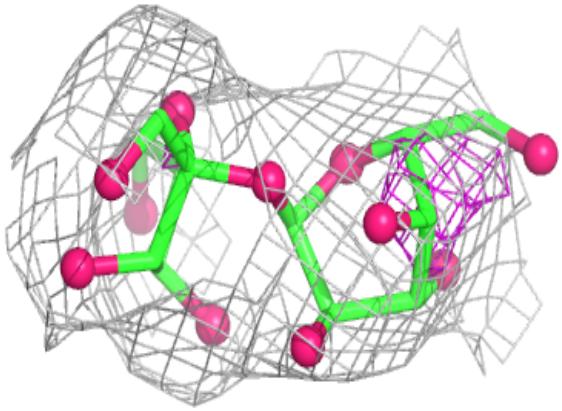


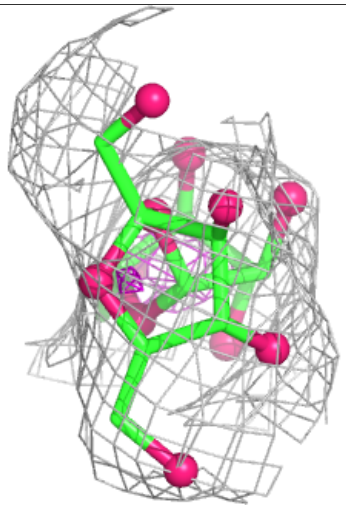


Electron density around Chain Q:

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

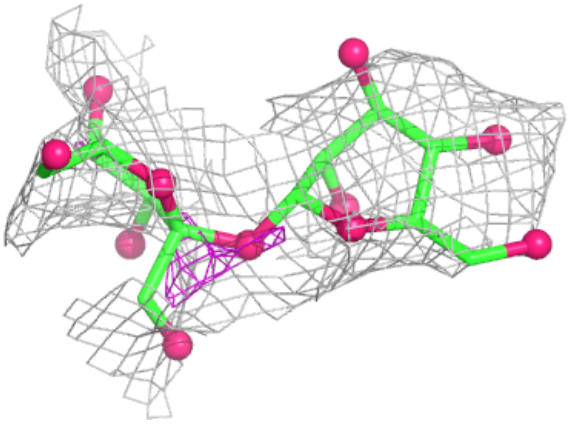


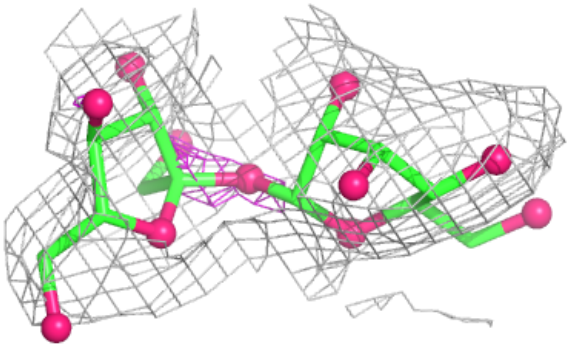


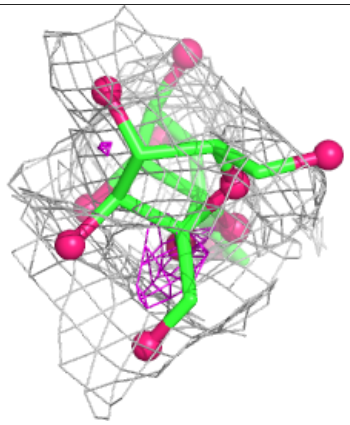


Electron density around Chain S:

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

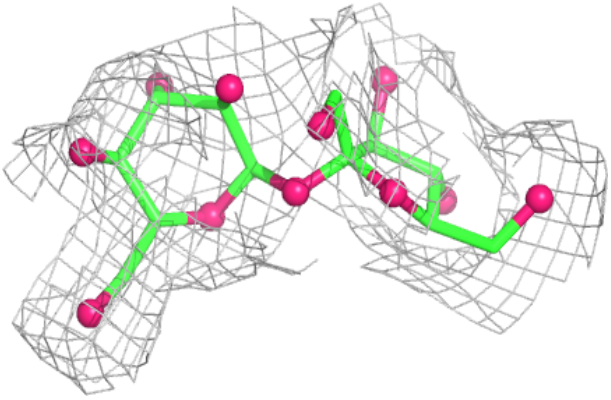


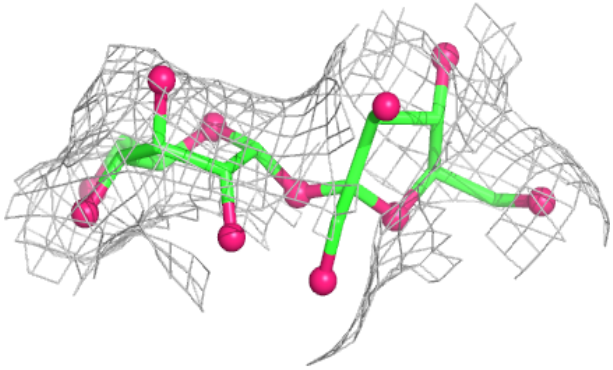


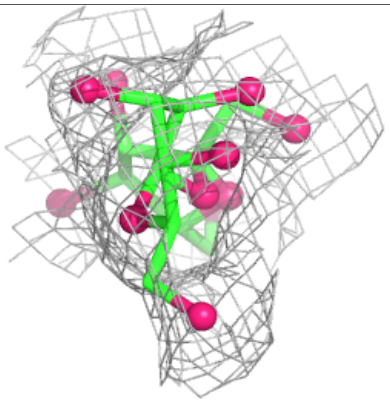


Electron density around Chain T:

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

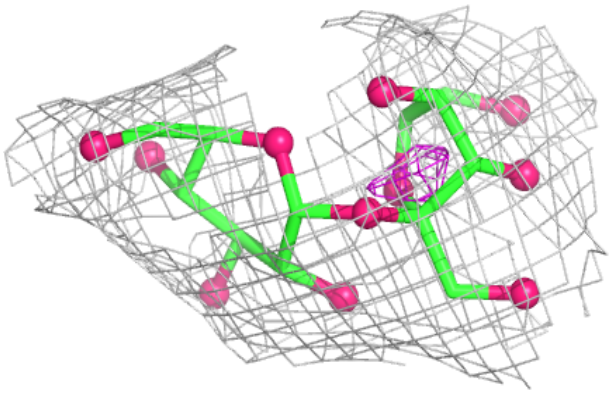


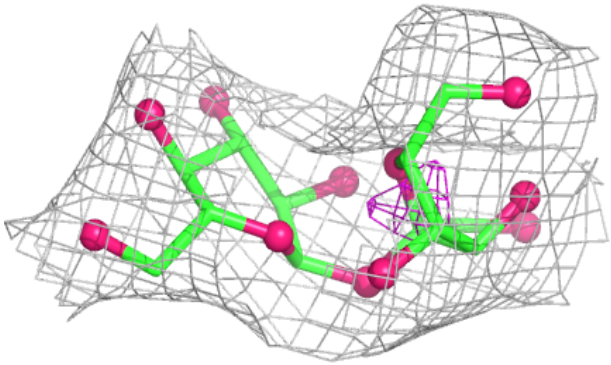


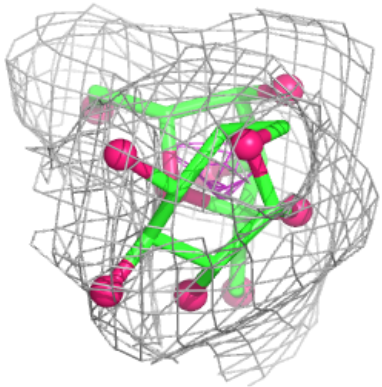


Electron density around Chain U:

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

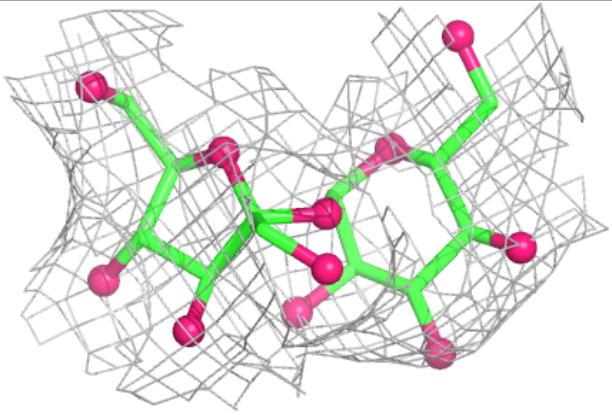


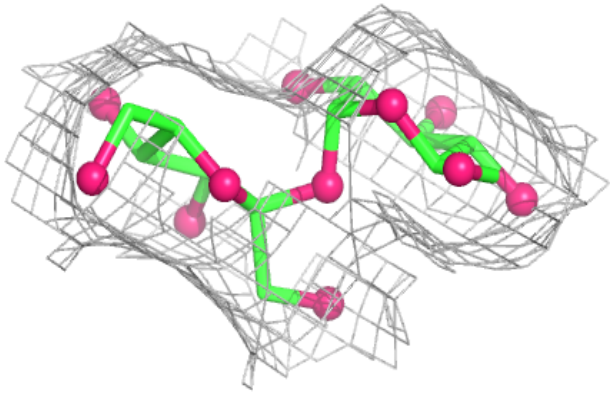


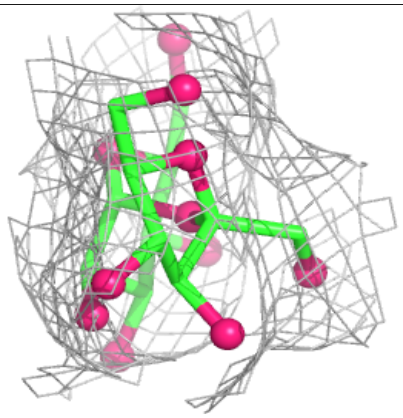


Electron density around Chain V:

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

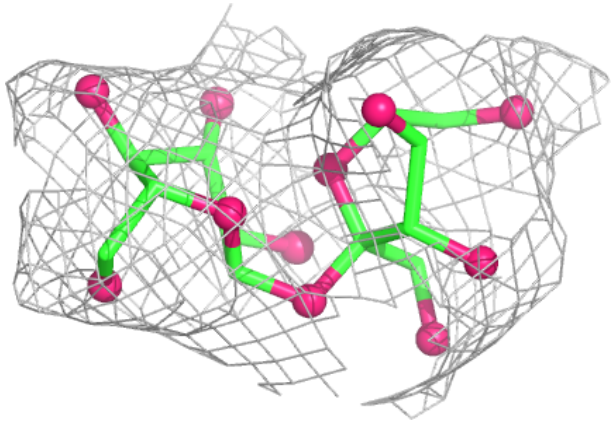


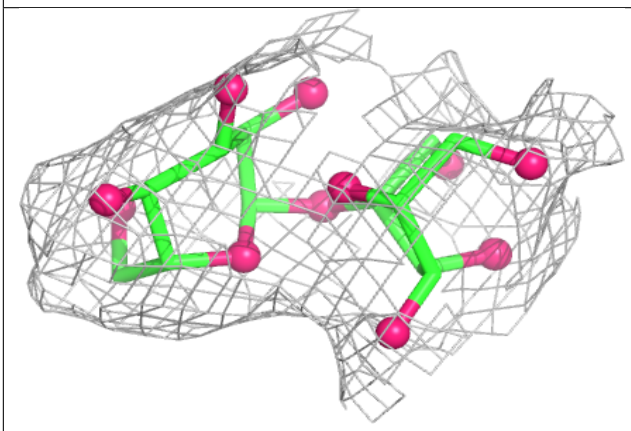


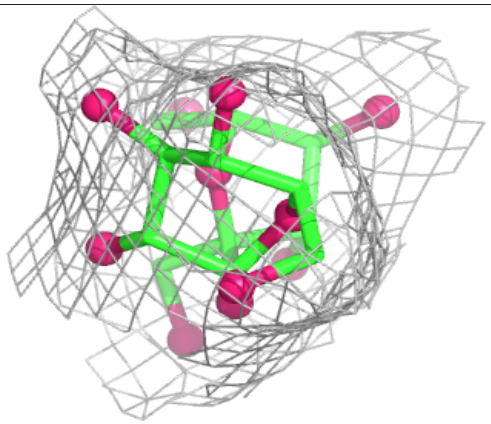


Electron density around Chain W:

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

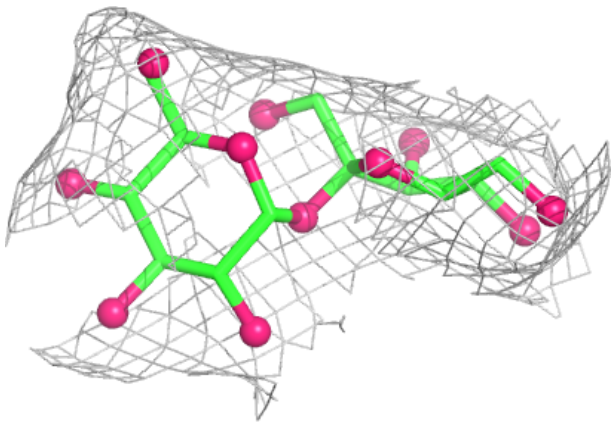


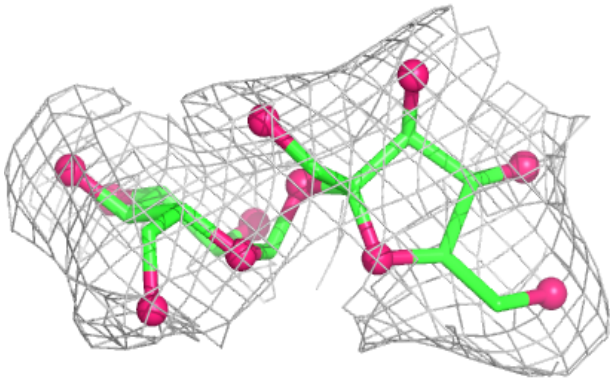


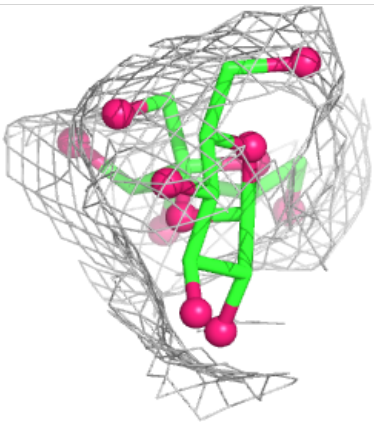


Electron density around Chain X:

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

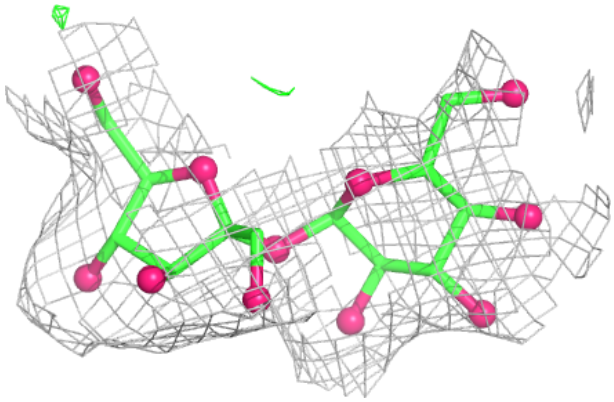


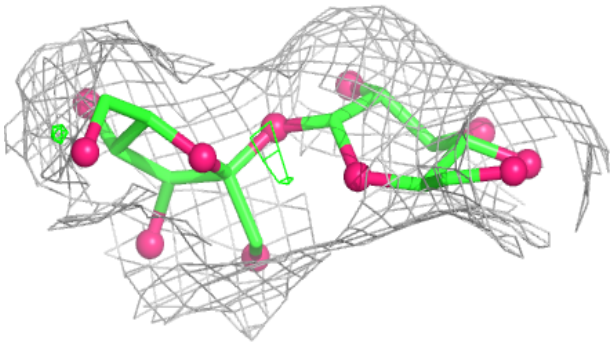


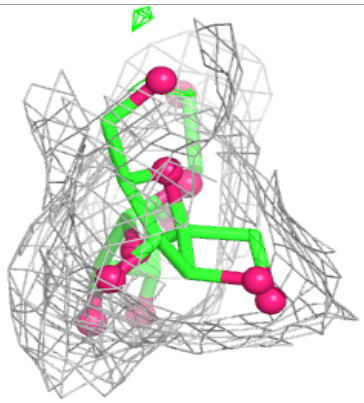


Electron density around Chain Y:

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

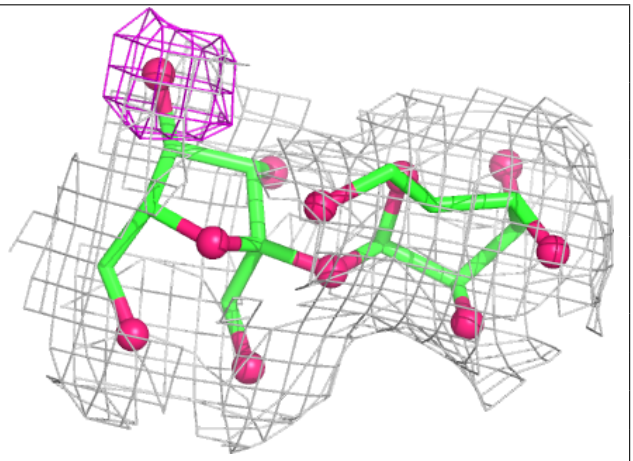


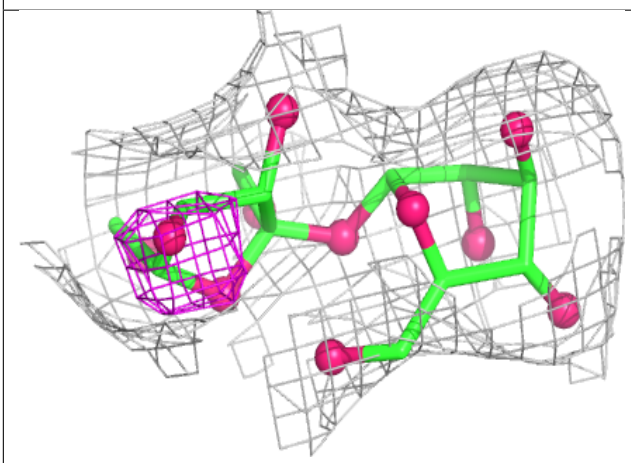


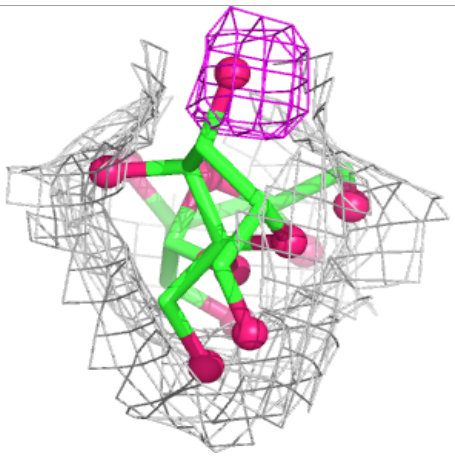


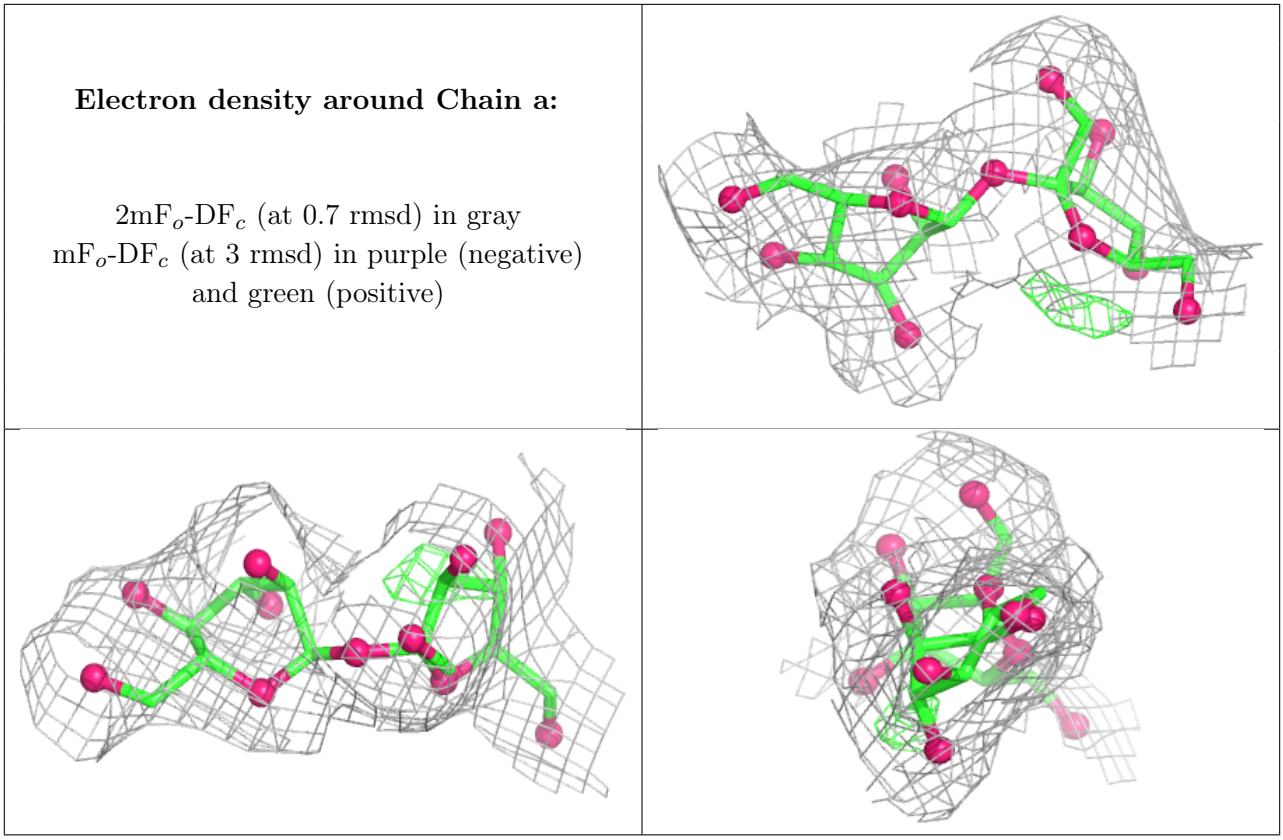
Electron density around Chain Z:

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









5.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	A	857	25/65	0.43	0.17	5,42,60,60	0
22	BCR	A	840	40/40	0.50	0.24	20,20,20,20	0
21	LMU	1	217	35/35	0.57	0.16	20,20,20,20	0
20	CLA	H	110	55/65	0.58	0.17	20,20,20,20	0
20	CLA	3	308	25/65	0.58	0.19	20,20,20,20	0
20	CLA	1	213	25/65	0.58	0.22	20,20,20,20	0
20	CLA	2	307	65/65	0.59	0.18	20,20,20,20	0
22	BCR	J	101	40/40	0.59	0.22	20,20,20,20	0
21	LMU	E	101	35/35	0.60	0.18	20,20,20,20	0
20	CLA	H	108	55/65	0.61	0.16	20,20,20,20	0
22	BCR	3	311	40/40	0.61	0.19	20,20,20,20	0
20	CLA	4	317	25/65	0.61	0.17	20,20,20,20	0
20	CLA	2	301	51/65	0.61	0.20	20,20,20,20	0
20	CLA	A	837	65/65	0.62	0.17	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	LMU	2	313	35/35	0.62	0.16	20,20,20,20	0
20	CLA	B	813	46/65	0.63	0.21	20,20,20,20	0
20	CLA	B	833	51/65	0.63	0.17	20,20,20,20	0
20	CLA	3	310	65/65	0.63	0.17	20,20,20,20	0
21	LMU	K	101	35/35	0.63	0.16	20,20,20,20	0
20	CLA	3	305	25/65	0.63	0.19	20,20,20,20	0
20	CLA	K	105	45/65	0.63	0.16	20,20,20,20	0
20	CLA	L	203	55/65	0.63	0.19	20,20,20,20	0
20	CLA	B	812	60/65	0.64	0.18	20,20,20,20	0
21	LMU	1	216	35/35	0.65	0.15	20,20,20,20	0
20	CLA	2	321	61/65	0.65	0.17	20,20,20,20	0
20	CLA	4	306	50/65	0.65	0.19	20,20,20,20	0
20	CLA	3	301	56/65	0.65	0.16	2,36,60,60	0
20	CLA	4	318	52/65	0.65	0.16	20,20,20,20	0
20	CLA	2	305	25/65	0.65	0.17	20,20,20,20	0
20	CLA	A	838	50/65	0.65	0.15	20,20,20,20	0
20	CLA	1	205	36/65	0.65	0.15	20,20,20,20	0
20	CLA	3	314	42/65	0.66	0.16	20,20,20,20	0
20	CLA	K	107	65/65	0.67	0.17	20,20,20,20	0
20	CLA	4	319	47/65	0.67	0.17	20,20,20,20	0
21	LMU	A	851	35/35	0.67	0.15	20,20,20,20	0
20	CLA	3	309	65/65	0.67	0.17	20,20,20,20	0
20	CLA	4	302	55/65	0.68	0.17	20,20,20,20	0
20	CLA	1	212	61/65	0.68	0.15	2,35,60,60	0
21	LMU	L	205	35/35	0.68	0.13	20,20,20,20	0
20	CLA	B	822	58/65	0.68	0.23	20,20,20,20	0
21	LMU	4	320	34/35	0.68	0.15	20,20,20,20	0
22	BCR	A	842	40/40	0.68	0.21	20,20,20,20	0
20	CLA	L	204	55/65	0.68	0.14	20,20,20,20	0
20	CLA	R	106	57/65	0.69	0.16	20,20,20,20	0
20	CLA	1	211	51/65	0.69	0.15	20,20,20,20	0
21	LMU	C	101	35/35	0.69	0.14	20,20,20,20	0
20	CLA	F	205	41/65	0.69	0.17	20,20,20,20	0
20	CLA	H	101	55/65	0.69	0.14	20,20,20,20	0
21	LMU	H	105	35/35	0.70	0.13	20,20,20,20	0
20	CLA	4	304	65/65	0.70	0.17	20,20,20,20	0
20	CLA	4	305	55/65	0.70	0.16	20,20,20,20	0
21	LMU	4	322	35/35	0.70	0.15	20,20,20,20	0
20	CLA	J	102	61/65	0.70	0.15	20,20,20,20	0
20	CLA	G	103	51/65	0.70	0.14	20,20,20,20	0
20	CLA	B	832	45/65	0.70	0.15	20,20,20,20	0
20	CLA	1	207	51/65	0.71	0.14	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	LMU	H	103	35/35	0.71	0.12	20,20,20,20	0
20	CLA	A	808	45/65	0.71	0.16	20,20,20,20	0
20	CLA	A	812	45/65	0.71	0.19	20,20,20,20	0
21	LMU	A	845	35/35	0.71	0.14	20,20,20,20	0
21	LMU	A	846	35/35	0.71	0.14	20,20,20,20	0
20	CLA	A	831	45/65	0.71	0.16	20,20,20,20	0
21	LMU	B	801	35/35	0.71	0.13	20,20,20,20	0
20	CLA	1	214	51/65	0.71	0.15	20,20,20,20	0
20	CLA	K	103	50/65	0.72	0.15	20,20,20,20	0
20	CLA	3	304	25/65	0.72	0.15	20,20,20,20	0
20	CLA	K	106	50/65	0.72	0.14	20,20,20,20	0
20	CLA	2	304	50/65	0.72	0.17	20,20,20,20	0
20	CLA	3	312	25/65	0.72	0.15	20,20,20,20	0
20	CLA	2	311	50/65	0.72	0.20	20,20,20,20	0
20	CLA	F	206	53/65	0.72	0.14	20,20,20,20	0
20	CLA	3	316	25/65	0.72	0.15	20,20,20,20	0
20	CLA	3	319	36/65	0.72	0.15	20,20,20,20	0
20	CLA	3	320	55/65	0.72	0.17	20,20,20,20	0
21	LMU	R	105	35/35	0.72	0.15	20,20,20,20	0
21	LMU	2	318	35/35	0.72	0.13	20,20,20,20	0
21	LMU	2	319	35/35	0.72	0.13	20,20,20,20	0
20	CLA	A	805	46/65	0.72	0.17	20,20,20,20	0
22	BCR	I	103	40/40	0.72	0.15	20,20,20,20	0
20	CLA	B	818	46/65	0.72	0.19	20,20,20,20	0
20	CLA	2	302	56/65	0.73	0.16	20,20,20,20	0
20	CLA	2	314	25/65	0.73	0.13	20,20,20,20	0
21	LMU	L	206	35/35	0.73	0.13	20,20,20,20	0
21	LMU	R	101	35/35	0.73	0.13	20,20,20,20	0
20	CLA	1	201	46/65	0.73	0.14	20,20,20,20	0
20	CLA	3	306	25/65	0.73	0.15	20,20,20,20	0
21	LMU	2	320	35/35	0.73	0.13	20,20,20,20	0
21	LMU	3	318	35/35	0.73	0.14	20,20,20,20	0
22	BCR	B	842	40/40	0.73	0.18	20,20,20,20	0
22	BCR	B	844	40/40	0.73	0.27	20,20,20,20	0
20	CLA	A	821	65/65	0.73	0.24	20,20,20,20	0
20	CLA	3	313	25/65	0.73	0.14	20,20,20,20	0
21	LMU	4	301	35/35	0.74	0.12	20,20,20,20	0
20	CLA	4	314	25/65	0.74	0.14	20,20,20,20	0
20	CLA	2	306	65/65	0.74	0.15	20,20,20,20	0
20	CLA	1	208	25/65	0.74	0.15	20,20,20,20	0
20	CLA	A	819	42/65	0.74	0.14	20,20,20,20	0
21	LMU	K	102	35/35	0.74	0.14	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	LMU	K	104	35/35	0.74	0.12	20,20,20,20	0
20	CLA	R	107	65/65	0.74	0.14	20,20,20,20	0
20	CLA	4	310	55/65	0.74	0.17	20,20,20,20	0
20	CLA	1	206	61/65	0.75	0.14	20,20,20,20	0
21	LMU	3	302	35/35	0.75	0.13	20,20,20,20	0
21	LMU	F	201	34/35	0.75	0.13	20,20,20,20	0
22	BCR	A	843	40/40	0.75	0.20	20,20,20,20	0
21	LMU	2	316	35/35	0.75	0.13	20,20,20,20	0
20	CLA	L	208	50/65	0.75	0.18	20,20,20,20	0
20	CLA	H	107	65/65	0.75	0.20	20,20,20,20	0
21	LMU	R	109	35/35	0.75	0.12	20,20,20,20	0
21	LMU	4	321	35/35	0.76	0.12	20,20,20,20	0
20	CLA	A	850	46/65	0.76	0.13	20,20,20,20	0
20	CLA	3	303	36/65	0.76	0.13	20,20,20,20	0
20	CLA	1	202	47/65	0.76	0.15	20,20,20,20	0
21	LMU	4	316	35/35	0.76	0.12	20,20,20,20	0
20	CLA	1	203	47/65	0.76	0.14	20,20,20,20	0
21	LMU	B	845	25/35	0.76	0.12	20,20,20,20	0
25	LMG	B	846	49/55	0.76	0.22	20,20,20,20	0
20	CLA	4	315	46/65	0.77	0.13	20,20,20,20	0
20	CLA	A	809	65/65	0.77	0.18	20,20,20,20	0
20	CLA	B	831	45/65	0.77	0.17	20,20,20,20	0
20	CLA	4	308	25/65	0.77	0.15	20,20,20,20	0
22	BCR	A	841	40/40	0.77	0.18	20,20,20,20	0
20	CLA	H	109	50/65	0.77	0.16	20,20,20,20	0
20	CLA	4	309	25/65	0.77	0.15	20,20,20,20	0
22	BCR	A	844	40/40	0.77	0.22	20,20,20,20	0
22	BCR	B	841	40/40	0.77	0.20	20,20,20,20	0
21	LMU	A	853	35/35	0.77	0.12	20,20,20,20	0
20	CLA	B	839	36/65	0.77	0.13	20,20,20,20	0
22	BCR	G	102	40/40	0.77	0.20	20,20,20,20	0
20	CLA	3	315	50/65	0.77	0.13	20,20,20,20	0
20	CLA	2	312	65/65	0.77	0.15	20,20,20,20	0
21	LMU	R	102	35/35	0.77	0.12	20,20,20,20	0
20	CLA	1	209	36/65	0.78	0.14	20,20,20,20	0
20	CLA	L	201	65/65	0.78	0.18	20,20,20,20	0
21	LMU	1	218	35/35	0.78	0.12	20,20,20,20	0
20	CLA	A	813	50/65	0.78	0.15	20,20,20,20	0
22	BCR	F	203	40/40	0.78	0.18	20,20,20,20	0
20	CLA	J	103	55/65	0.78	0.13	2,33,60,60	0
20	CLA	A	814	65/65	0.78	0.17	2,35,60,60	0
20	CLA	B	829	65/65	0.78	0.20	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	BCR	L	209	40/40	0.78	0.18	20,20,20,20	0
20	CLA	A	817	65/65	0.78	0.18	20,20,20,20	0
20	CLA	3	317	25/65	0.79	0.13	20,20,20,20	0
20	CLA	1	204	46/65	0.79	0.14	20,20,20,20	0
20	CLA	1	210	36/65	0.79	0.16	20,20,20,20	0
20	CLA	1	215	25/65	0.79	0.13	20,20,20,20	0
20	CLA	2	315	25/65	0.79	0.15	20,20,20,20	0
20	CLA	B	808	54/65	0.79	0.17	20,20,20,20	0
21	LMU	B	802	35/35	0.79	0.12	20,20,20,20	0
20	CLA	B	809	55/65	0.79	0.18	20,20,20,20	0
20	CLA	2	317	65/65	0.79	0.13	20,20,20,20	0
21	LMU	R	103	35/35	0.79	0.13	20,20,20,20	0
20	CLA	3	307	25/65	0.79	0.12	20,20,20,20	0
21	LMU	R	108	35/35	0.79	0.12	20,20,20,20	0
20	CLA	2	308	25/65	0.79	0.14	20,20,20,20	0
21	LMU	H	102	35/35	0.79	0.12	20,20,20,20	0
20	CLA	B	823	65/65	0.80	0.18	20,20,20,20	0
20	CLA	A	855	65/65	0.80	0.22	20,20,20,20	0
20	CLA	A	803	65/65	0.80	0.21	20,20,20,20	0
20	CLA	A	822	65/65	0.80	0.17	20,20,20,20	0
20	CLA	A	823	65/65	0.80	0.16	20,20,20,20	0
20	CLA	B	811	65/65	0.80	0.17	20,20,20,20	0
20	CLA	4	311	25/65	0.80	0.18	20,20,20,20	0
20	CLA	2	309	25/65	0.80	0.15	20,20,20,20	0
20	CLA	4	303	36/65	0.80	0.17	20,20,20,20	0
20	CLA	A	811	54/65	0.80	0.17	20,20,20,20	0
20	CLA	A	818	51/65	0.81	0.14	20,20,20,20	0
20	CLA	B	803	45/65	0.81	0.17	20,20,20,20	0
21	LMU	L	210	35/35	0.81	0.11	20,20,20,20	0
20	CLA	B	807	65/65	0.81	0.19	20,20,20,20	0
20	CLA	B	828	50/65	0.81	0.16	20,20,20,20	0
22	BCR	B	843	40/40	0.81	0.22	20,20,20,20	0
20	CLA	A	810	54/65	0.81	0.13	20,20,20,20	0
22	BCR	F	202	40/40	0.81	0.22	20,20,20,20	0
20	CLA	B	830	50/65	0.81	0.20	20,20,20,20	0
20	CLA	4	313	36/65	0.81	0.17	20,20,20,20	0
20	CLA	A	849	65/65	0.81	0.19	20,20,20,20	0
20	CLA	A	816	65/65	0.81	0.21	20,20,20,20	0
21	LMU	A	854	35/35	0.81	0.13	20,20,20,20	0
20	CLA	A	802	55/65	0.81	0.17	20,20,20,20	0
20	CLA	2	303	25/65	0.82	0.12	20,20,20,20	0
20	CLA	I	102	60/65	0.82	0.17	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
20	CLA	2	310	50/65	0.82	0.15	20,20,20,20	0
20	CLA	4	307	52/65	0.82	0.12	20,20,20,20	0
20	CLA	B	820	65/65	0.82	0.16	20,20,20,20	0
20	CLA	A	827	50/65	0.82	0.15	20,20,20,20	0
20	CLA	A	807	55/65	0.83	0.18	20,20,20,20	0
20	CLA	F	204	36/65	0.83	0.15	20,20,20,20	0
20	CLA	B	814	59/65	0.83	0.16	20,20,20,20	0
20	CLA	A	832	51/65	0.83	0.17	20,20,20,20	0
21	LMU	A	852	35/35	0.83	0.10	20,20,20,20	0
20	CLA	A	815	52/65	0.83	0.17	20,20,20,20	0
20	CLA	A	829	65/65	0.83	0.18	20,20,20,20	0
20	CLA	L	207	47/65	0.83	0.16	20,20,20,20	0
23	PQN	A	839	33/33	0.83	0.23	20,20,20,20	0
20	CLA	A	848	65/65	0.83	0.20	20,20,20,20	0
20	CLA	4	312	25/65	0.84	0.15	20,20,20,20	0
20	CLA	A	833	65/65	0.84	0.18	20,20,20,20	0
20	CLA	A	835	51/65	0.84	0.20	20,20,20,20	0
21	LMU	G	101	35/35	0.84	0.10	20,20,20,20	0
21	LMU	R	104	35/35	0.84	0.10	20,20,20,20	0
20	CLA	B	810	65/65	0.84	0.17	20,20,20,20	0
20	CLA	B	834	60/65	0.84	0.19	20,20,20,20	0
20	CLA	B	836	47/65	0.84	0.20	20,20,20,20	0
20	CLA	B	837	65/65	0.84	0.18	20,20,20,20	0
20	CLA	A	836	65/65	0.84	0.16	20,20,20,20	0
20	CLA	B	826	65/65	0.84	0.19	20,20,20,20	0
20	CLA	A	825	55/65	0.84	0.18	20,20,20,20	0
20	CLA	A	826	65/65	0.84	0.18	20,20,20,20	0
21	LMU	H	104	35/35	0.85	0.10	20,20,20,20	0
20	CLA	B	819	55/65	0.85	0.14	20,20,20,20	0
20	CLA	A	828	65/65	0.85	0.15	20,20,20,20	0
20	CLA	A	801	50/65	0.85	0.14	20,20,20,20	0
20	CLA	A	830	50/65	0.85	0.15	20,20,20,20	0
20	CLA	A	806	65/65	0.85	0.22	20,20,20,20	0
22	BCR	I	101	40/40	0.85	0.16	20,20,20,20	0
20	CLA	B	815	60/65	0.85	0.21	20,20,20,20	0
20	CLA	B	849	65/65	0.85	0.20	20,20,20,20	0
20	CLA	B	816	61/65	0.85	0.17	20,20,20,20	0
20	CLA	B	817	50/65	0.85	0.16	20,20,20,20	0
20	CLA	A	804	57/65	0.85	0.16	20,20,20,20	0
20	CLA	L	202	65/65	0.86	0.15	20,20,20,20	0
20	CLA	B	825	65/65	0.86	0.21	20,20,20,20	0
22	BCR	B	850	40/40	0.86	0.18	20,20,20,20	0

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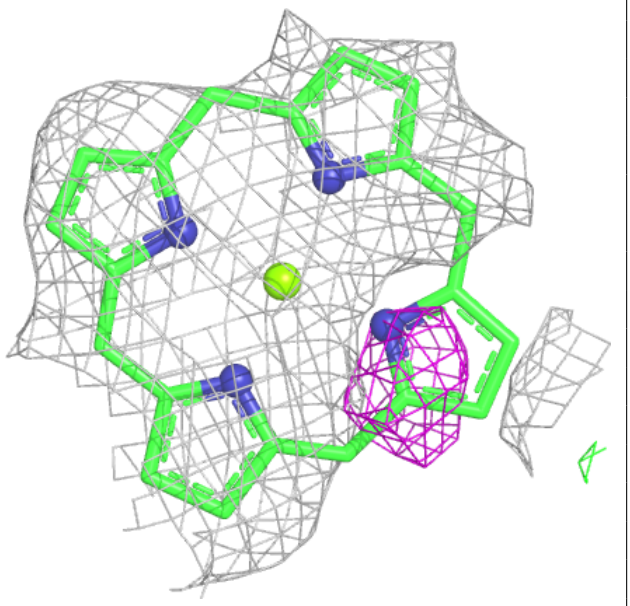
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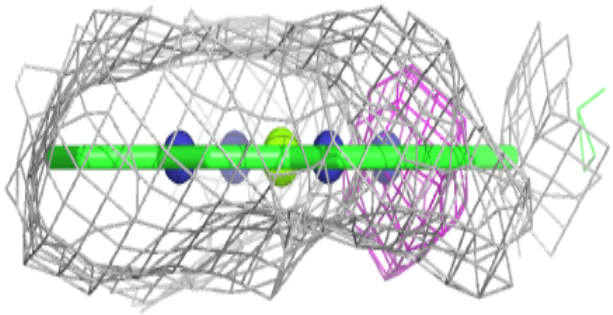
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	UNL	H	106	23/-	0.86	0.09	20,20,20,20	0
20	CLA	B	824	65/65	0.87	0.18	20,20,20,20	0
20	CLA	A	834	47/65	0.87	0.17	20,20,20,20	0
20	CLA	B	838	65/65	0.87	0.17	20,20,20,20	0
20	CLA	B	821	54/65	0.87	0.18	20,20,20,20	0
20	CLA	B	847	65/65	0.87	0.20	20,20,20,20	0
20	CLA	B	804	65/65	0.87	0.18	20,20,20,20	0
20	CLA	A	820	55/65	0.87	0.16	20,20,20,20	0
20	CLA	B	835	65/65	0.87	0.18	20,20,20,20	0
23	PQN	B	840	33/33	0.88	0.18	20,20,20,20	0
20	CLA	B	848	65/65	0.88	0.18	20,20,20,20	0
20	CLA	B	805	65/65	0.88	0.17	20,20,20,20	0
20	CLA	A	847	65/65	0.89	0.23	20,20,20,20	0
20	CLA	B	827	50/65	0.89	0.14	20,20,20,20	0
20	CLA	B	806	65/65	0.89	0.20	20,20,20,20	0
20	CLA	A	824	65/65	0.89	0.18	20,20,20,20	0
24	SF4	C	102	8/8	0.98	0.06	20,20,20,20	0
24	SF4	A	856	8/8	0.99	0.05	20,20,20,20	0
24	SF4	C	103	8/8	0.99	0.05	20,20,20,20	0

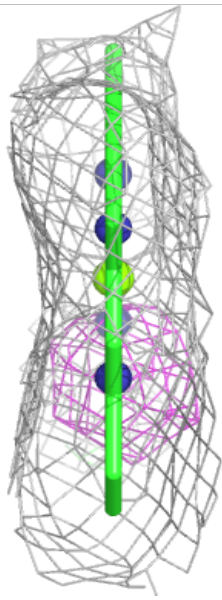
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CLA A 857:

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

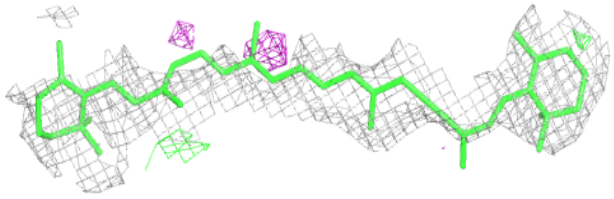


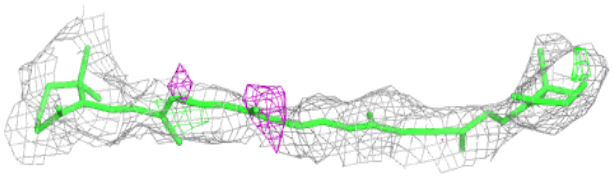


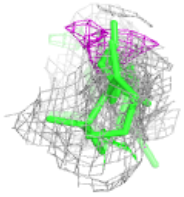


Electron density around BCR A 840:

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

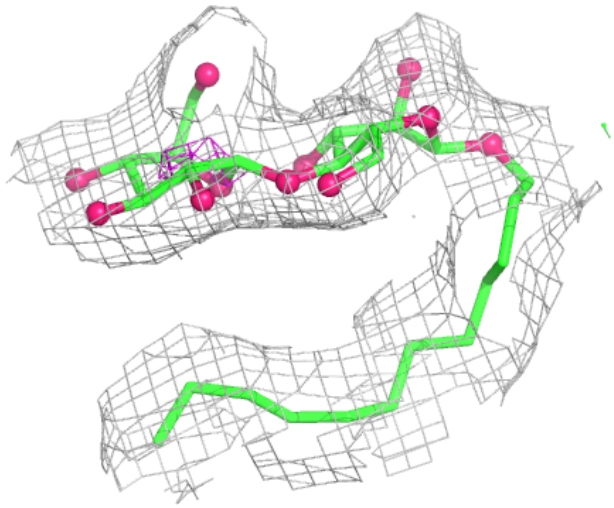


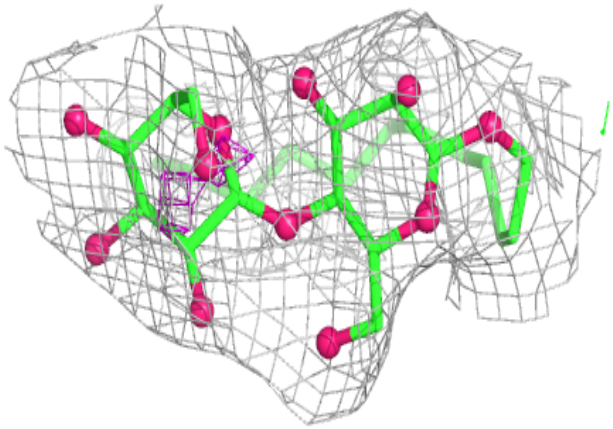




Electron density around LMU 1 217:

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

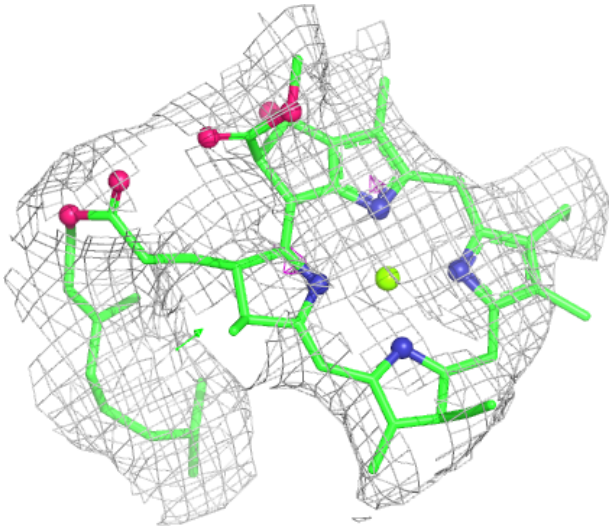


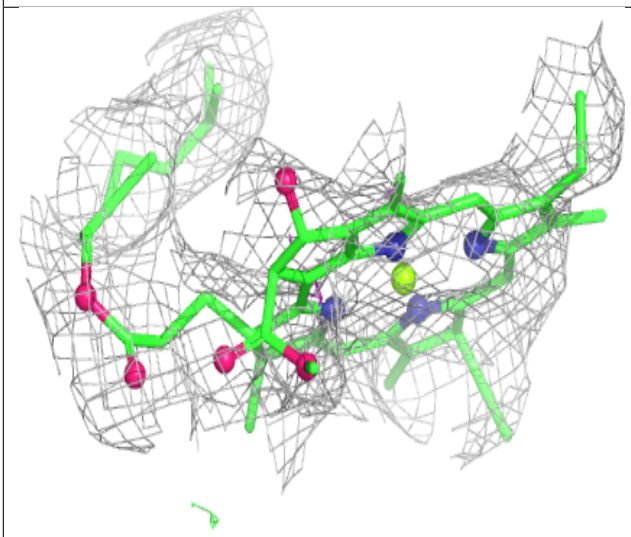




Electron density around CLA H 110:

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

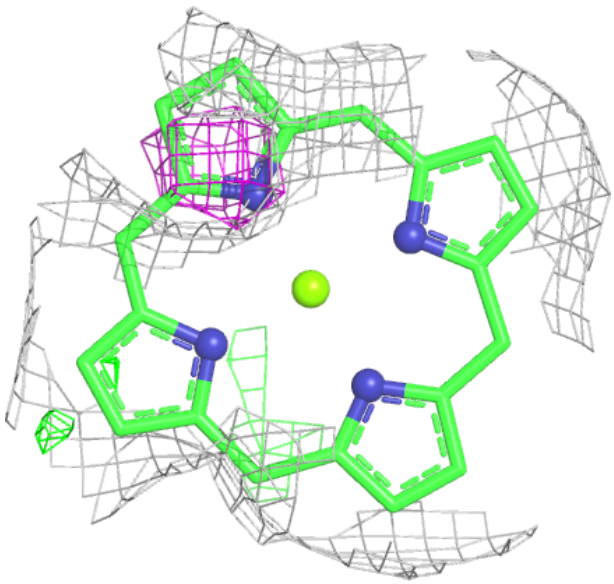


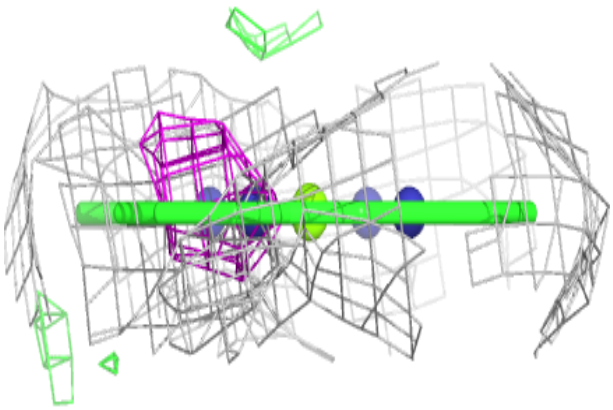


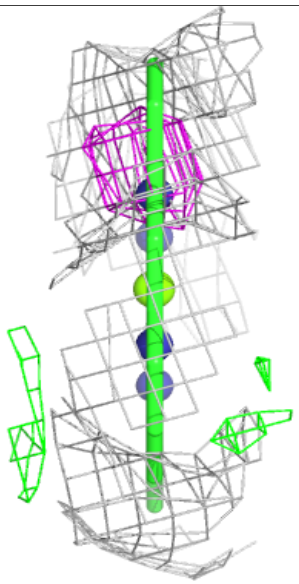


Electron density around CLA 3 308:

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

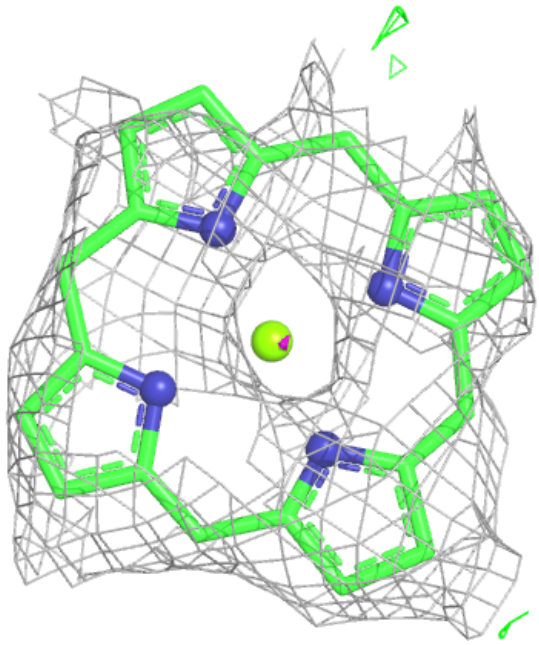


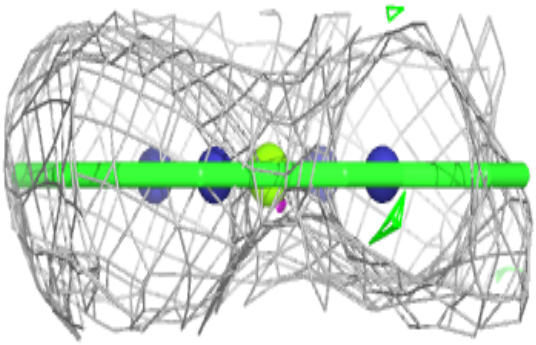


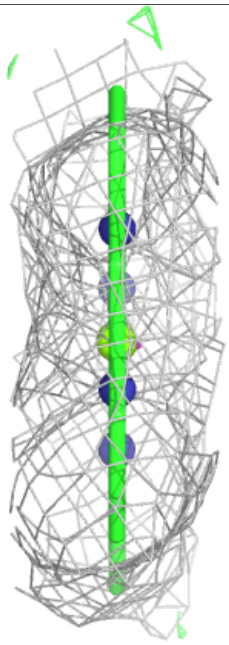


Electron density around CLA 1 213:

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

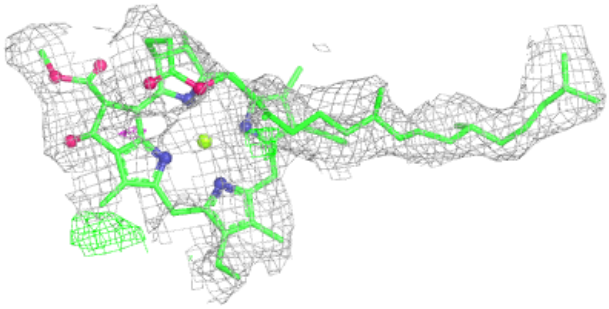


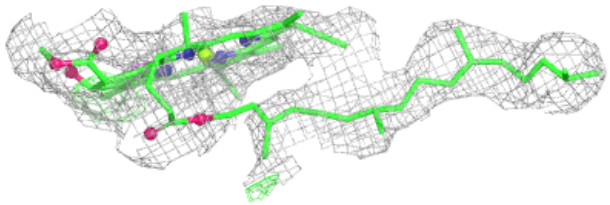


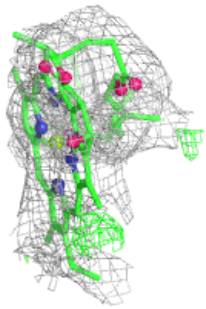


Electron density around CLA 2 307:

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

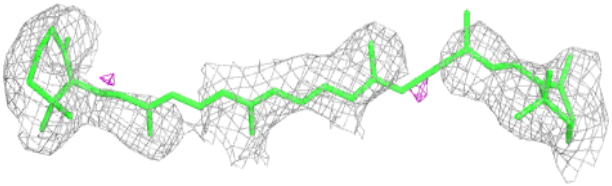


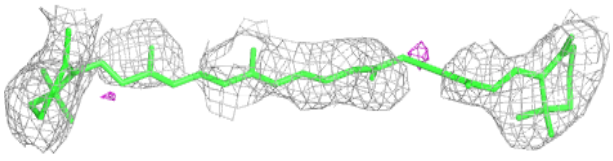


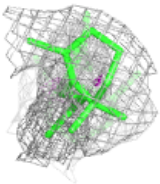


Electron density around BCR J 101:

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

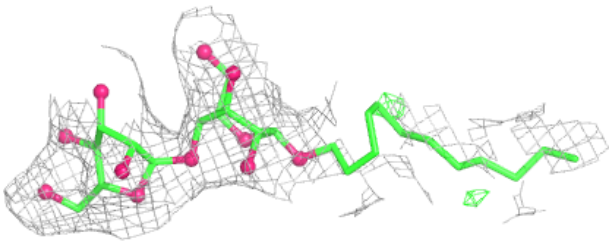


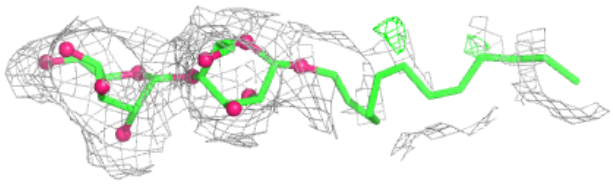


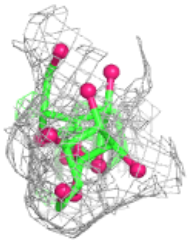


Electron density around LMU E 101:

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

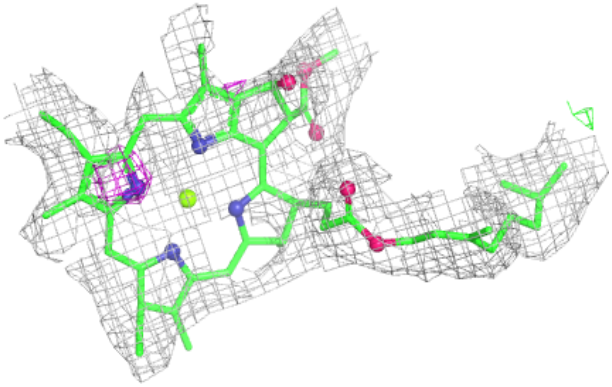


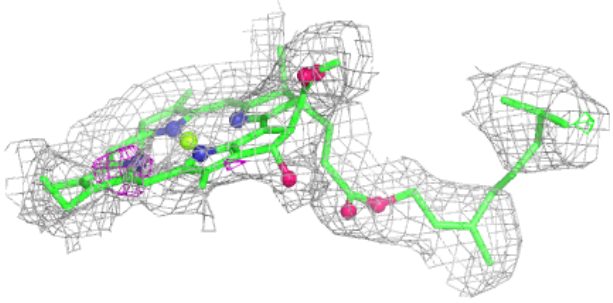


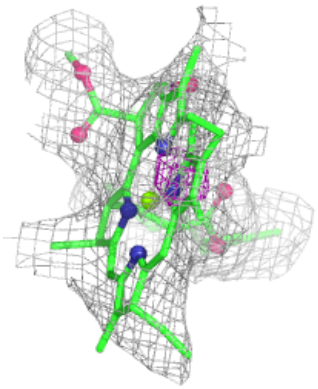


Electron density around CLA H 108:

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

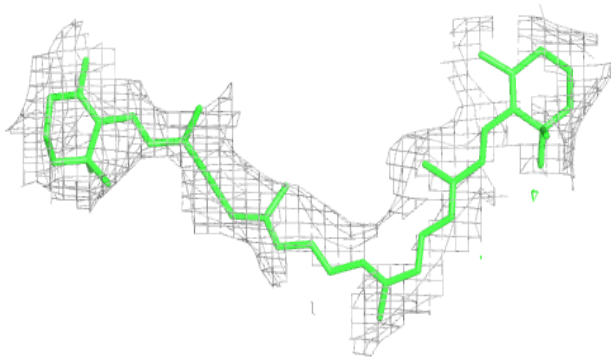


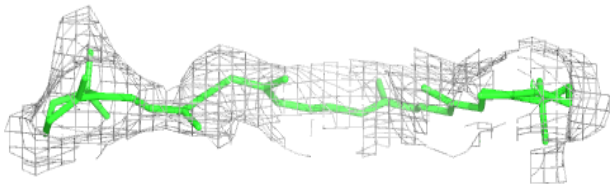




Electron density around BCR 3 311:

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

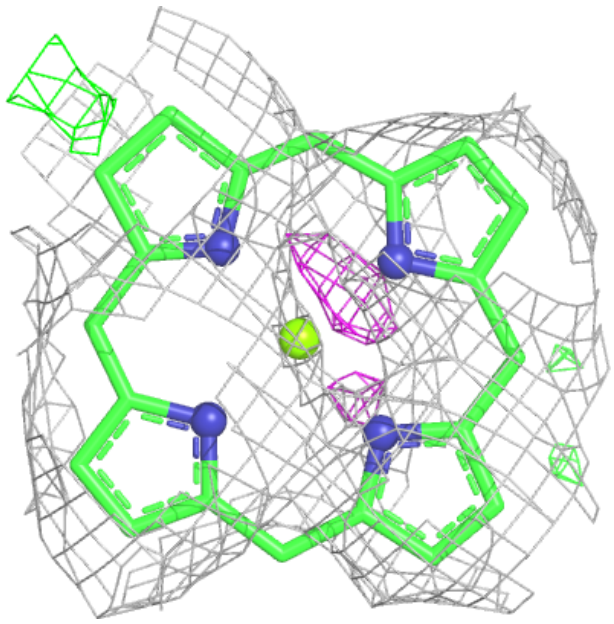


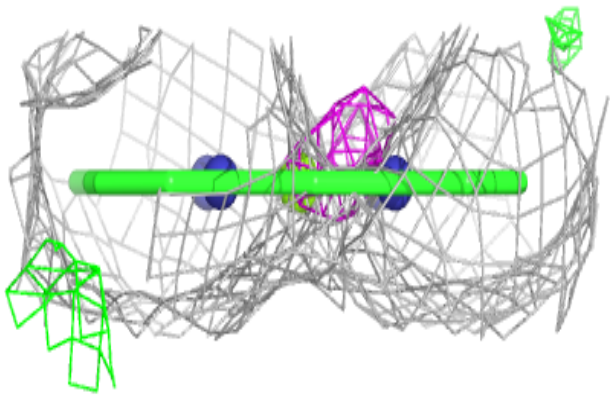


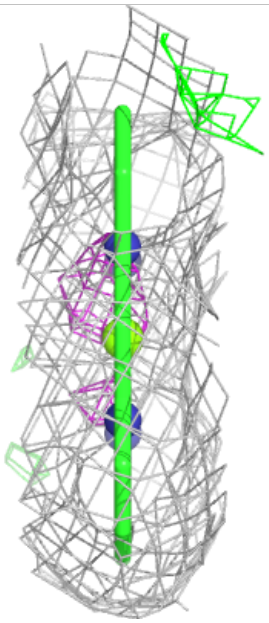


Electron density around CLA 4 317:

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

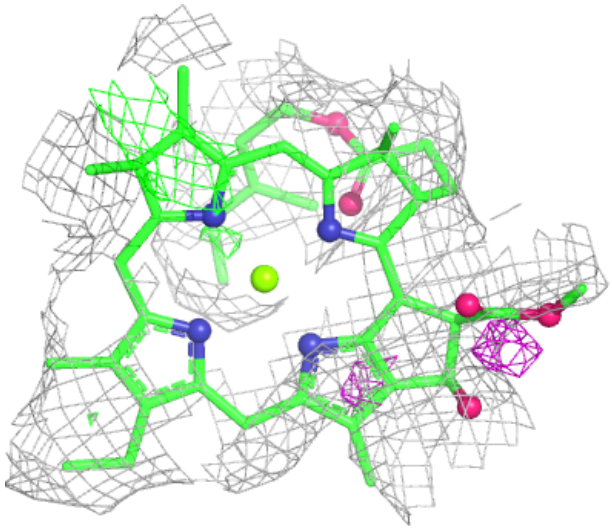


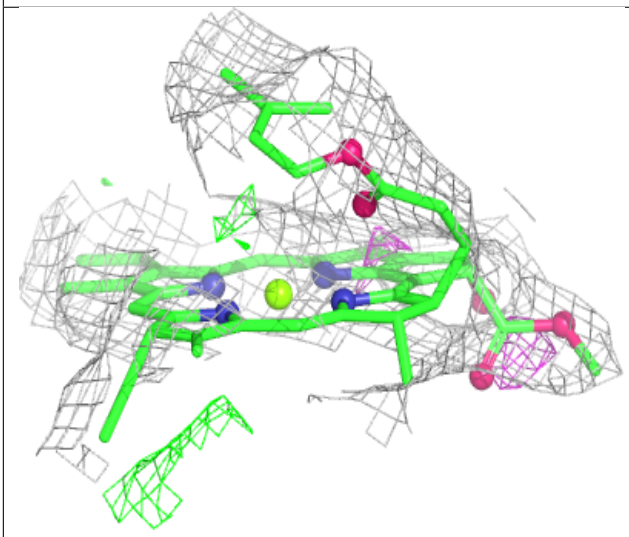


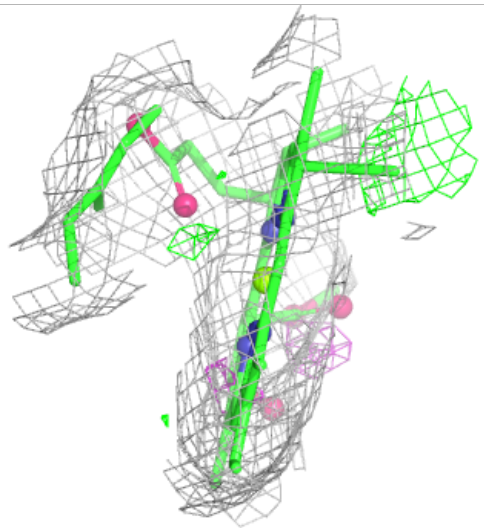


Electron density around CLA 2 301:

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

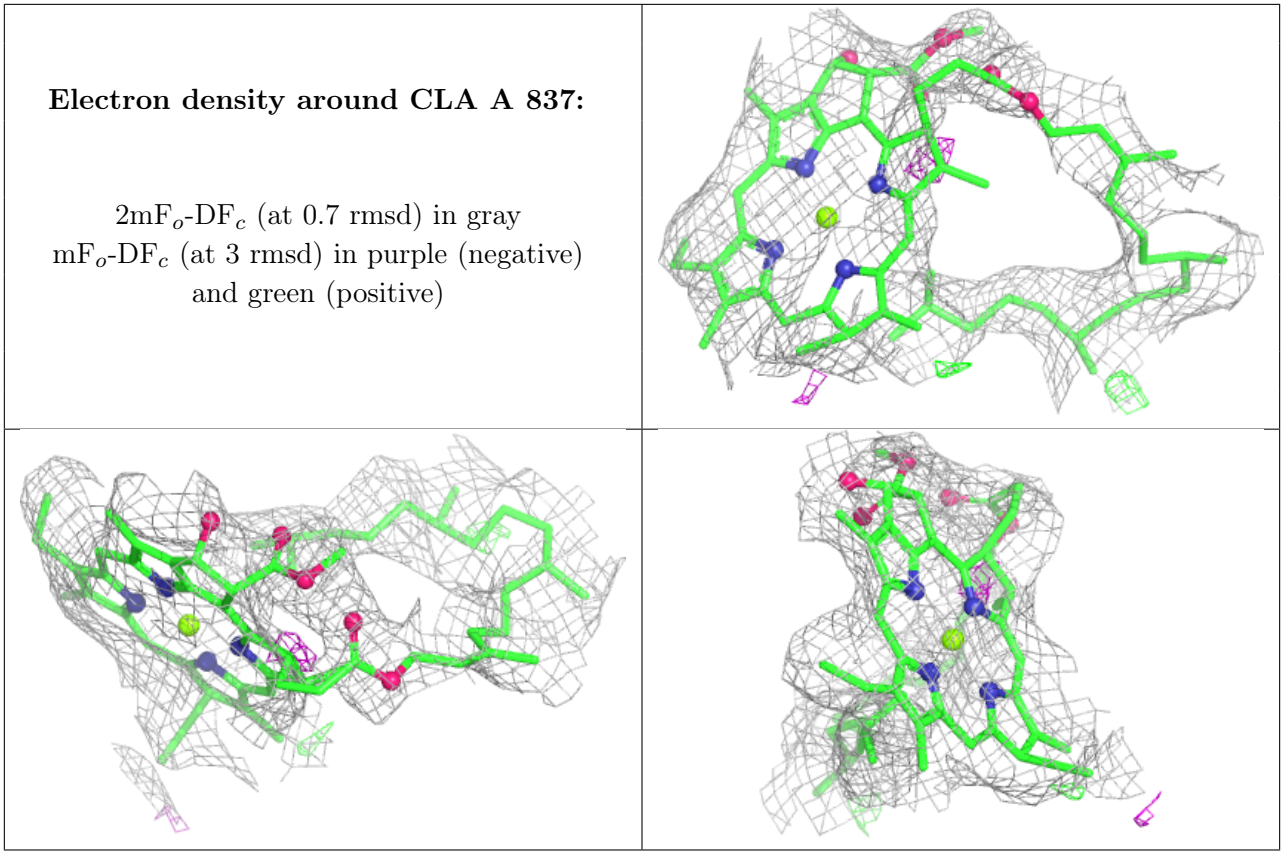






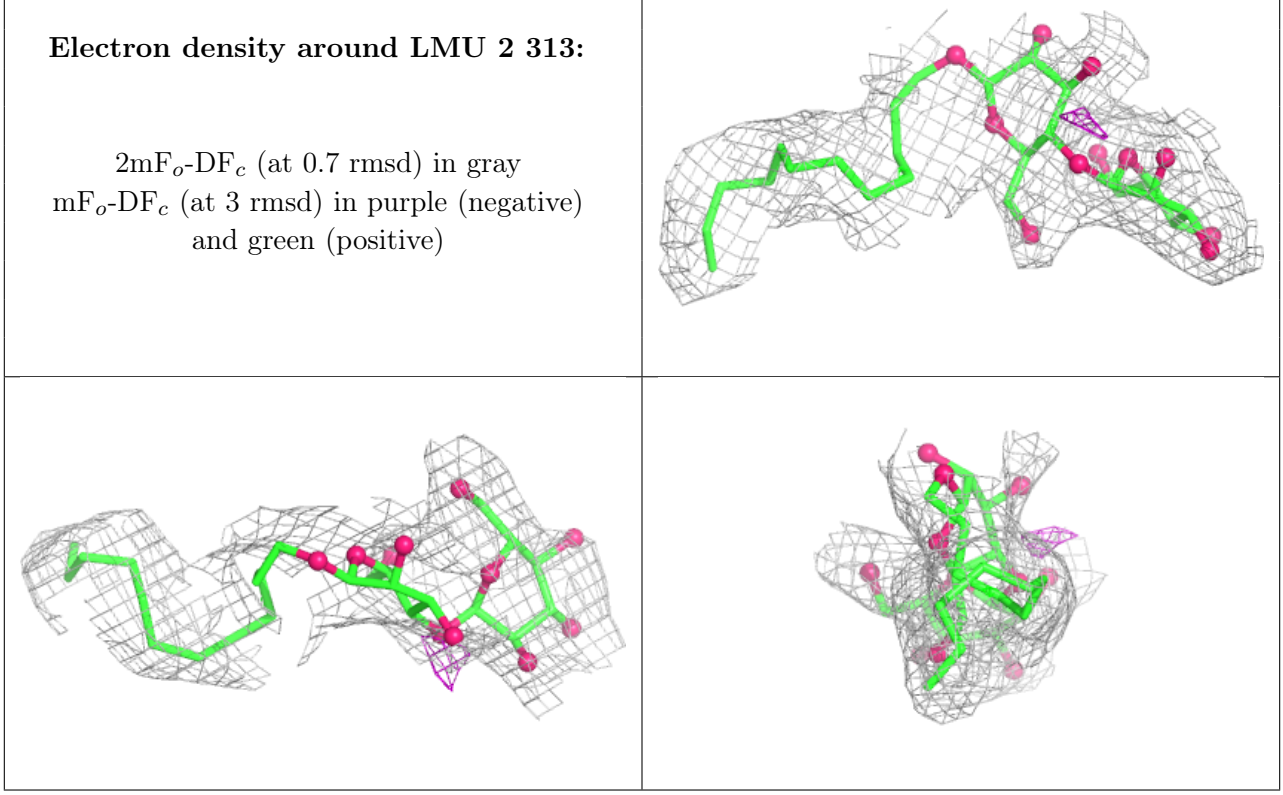
Electron density around CLA A 837:

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



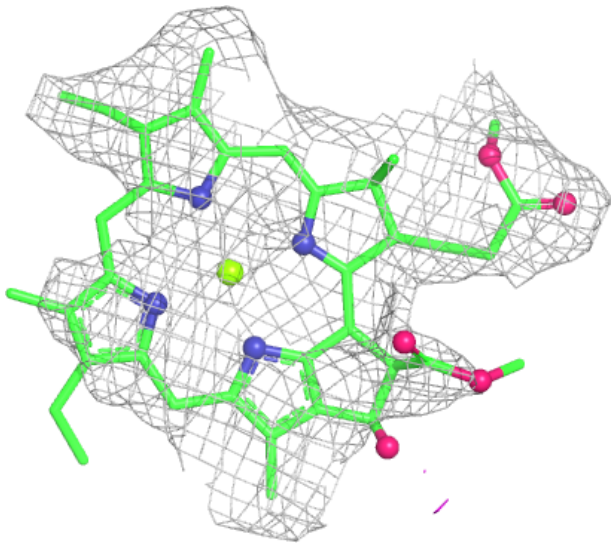
Electron density around LMU 2 313:

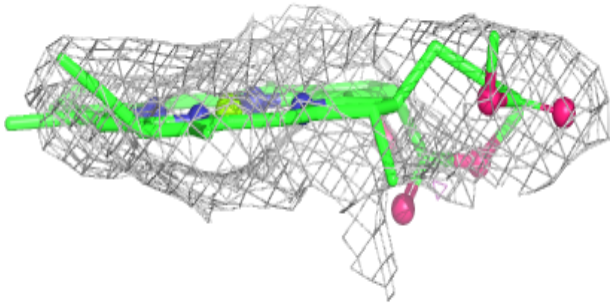
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

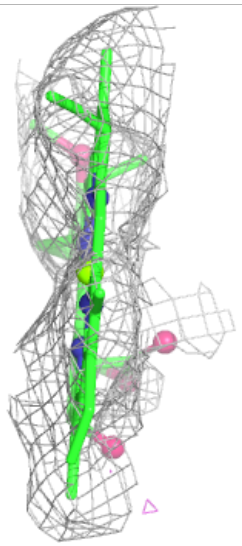


Electron density around CLA B 813:

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

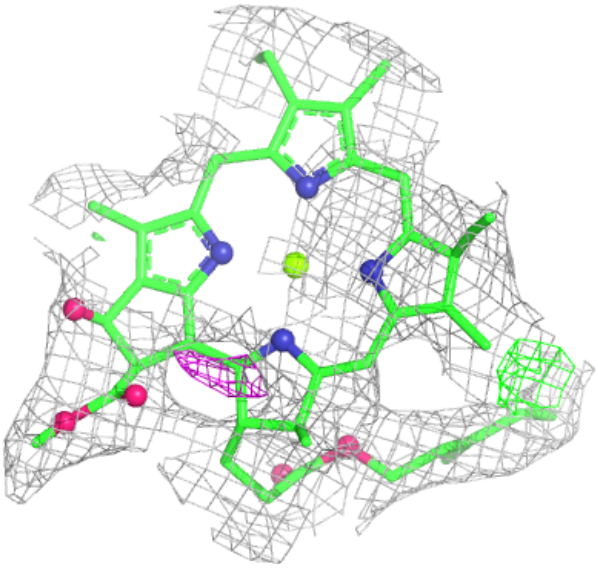


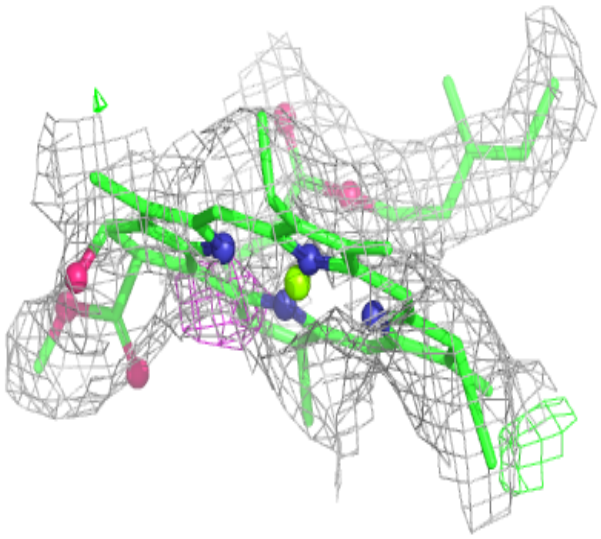


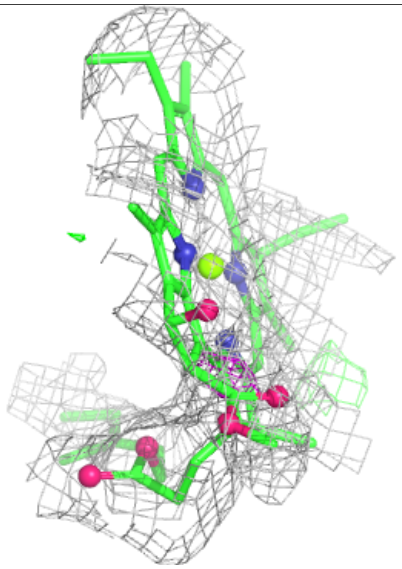


Electron density around CLA B 833:

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

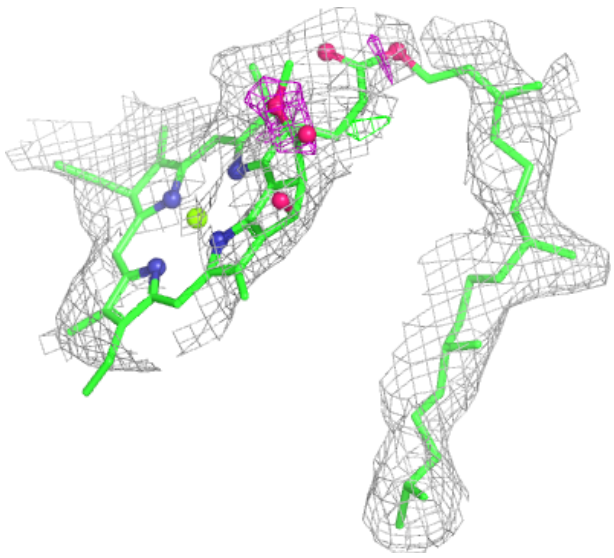


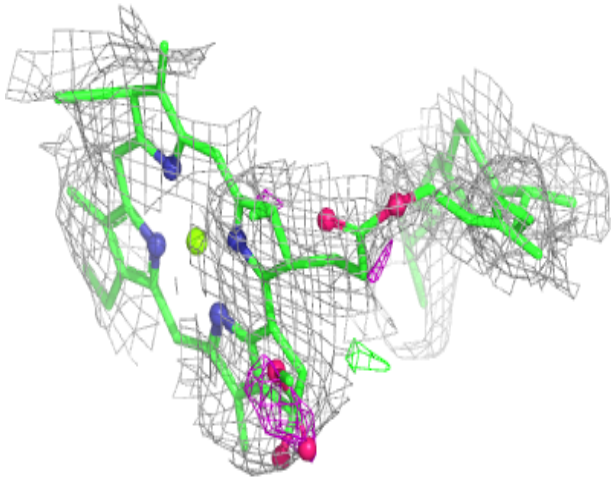


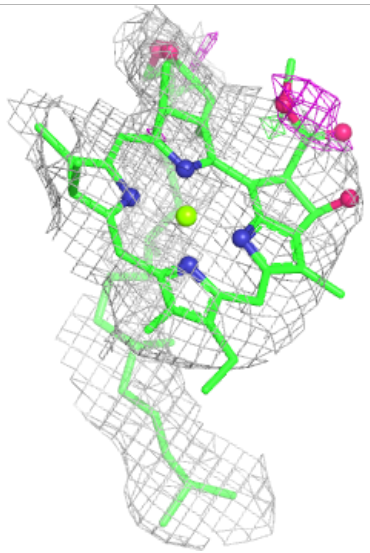


Electron density around CLA 3 310:

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

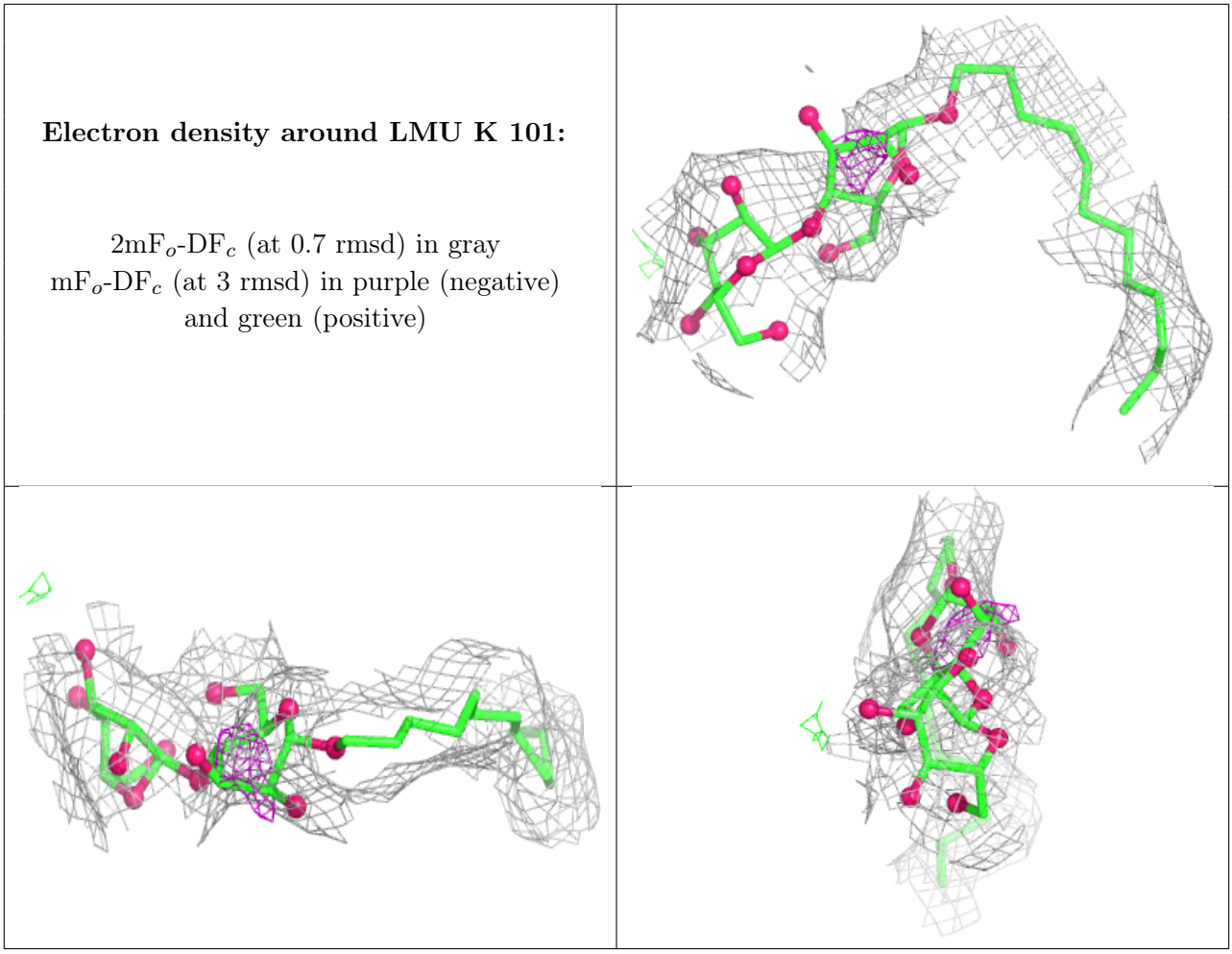






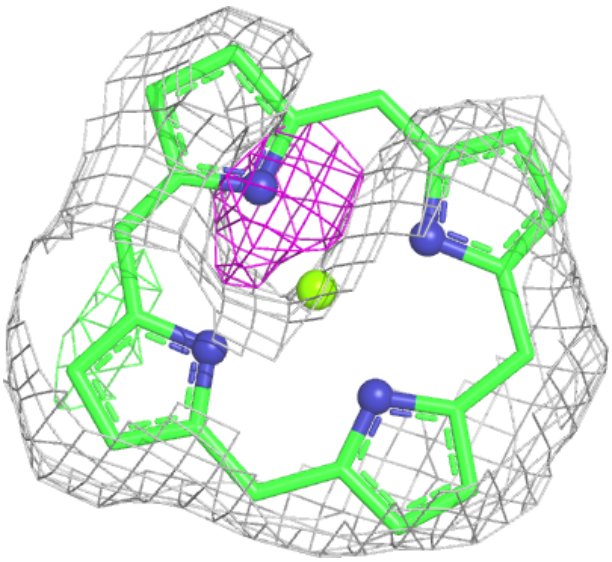
Electron density around LMU K 101:

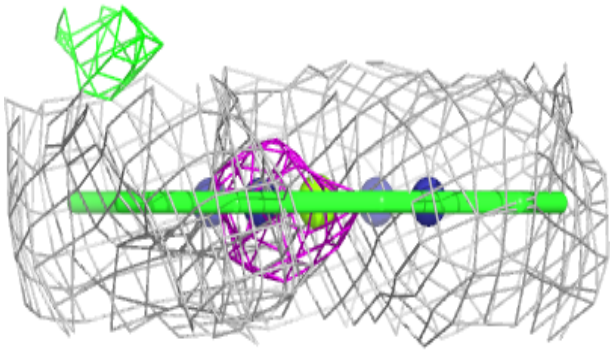
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

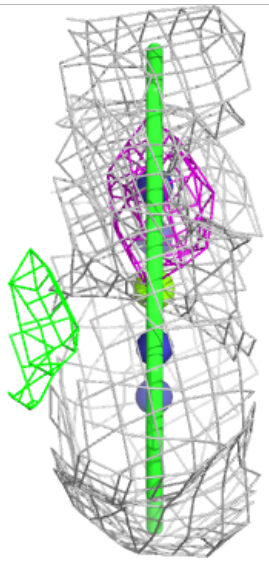


Electron density around CLA 3 305:

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

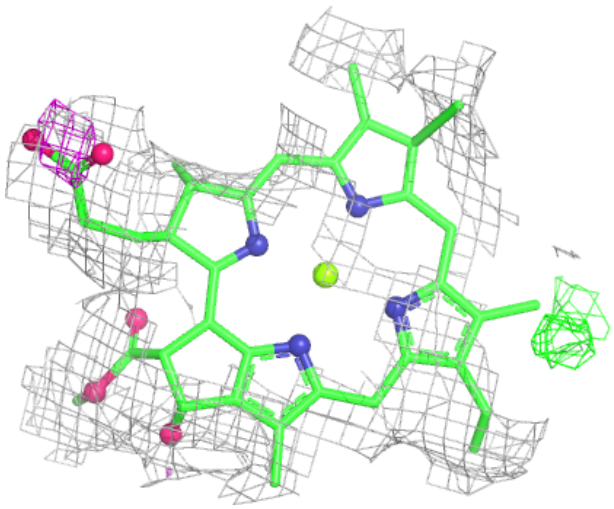


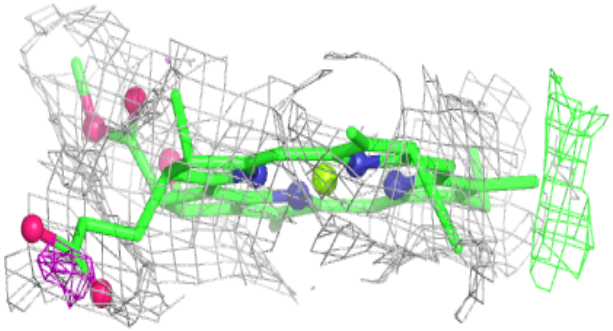




Electron density around CLA K 105:

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

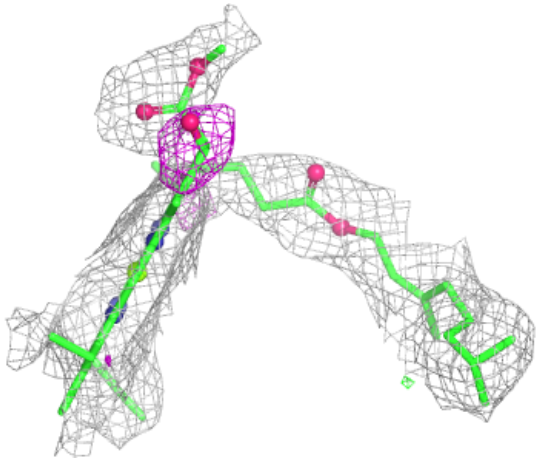


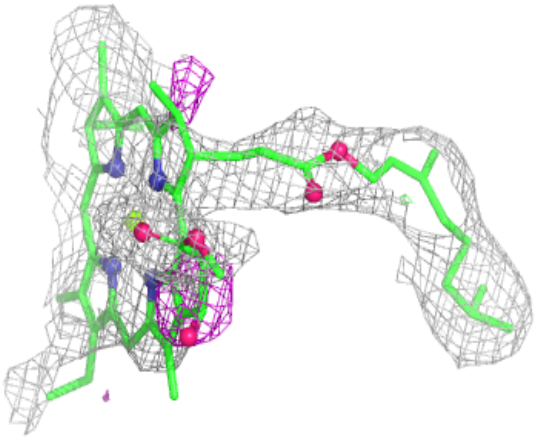


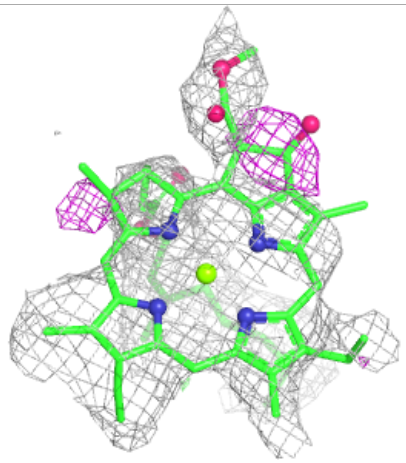


Electron density around CLA L 203:

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

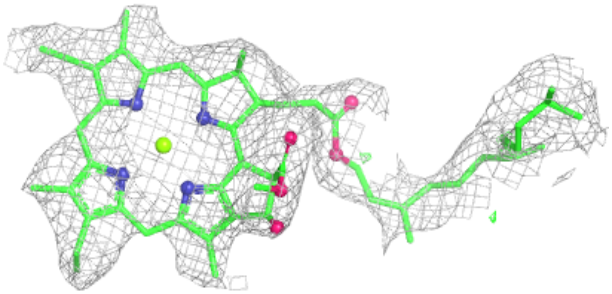


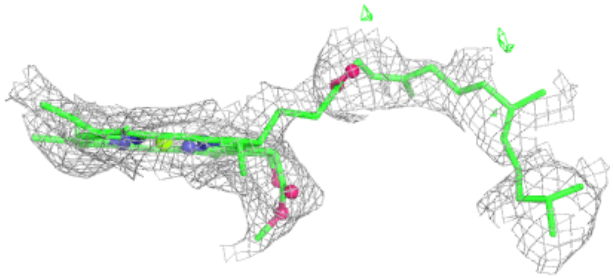


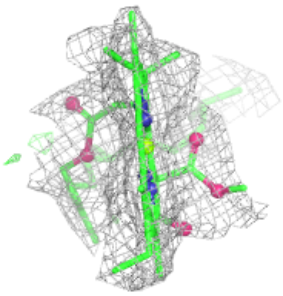


Electron density around CLA B 812:

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

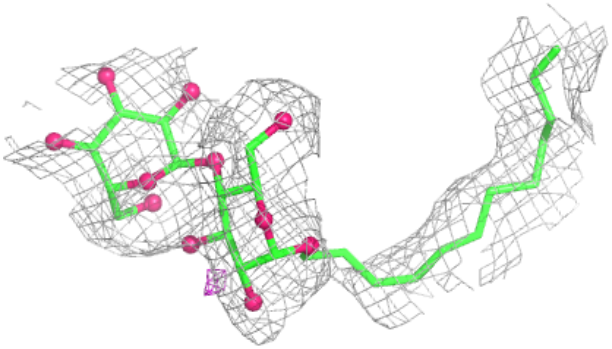


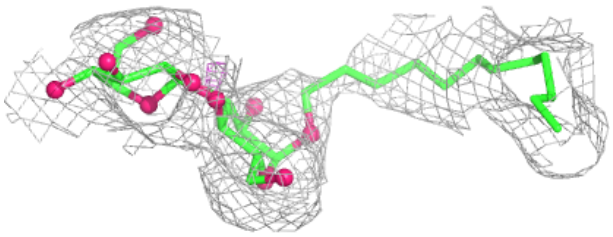


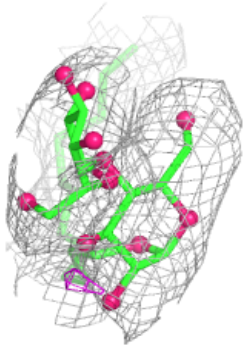


Electron density around LMU 1 216:

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

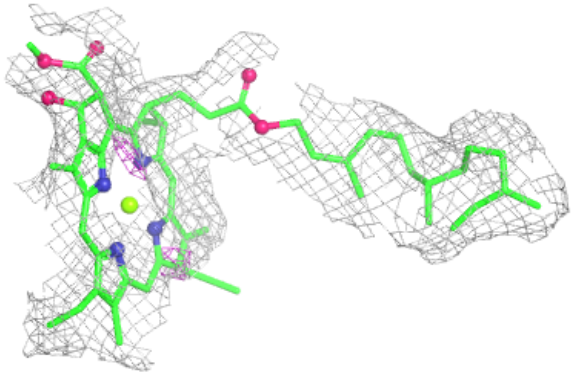


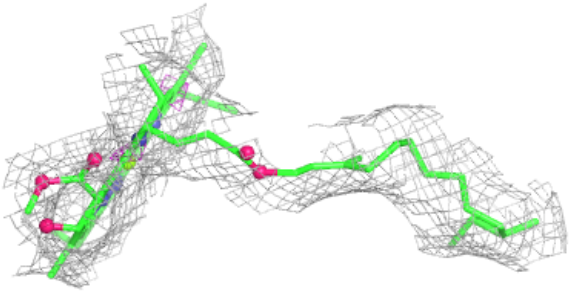


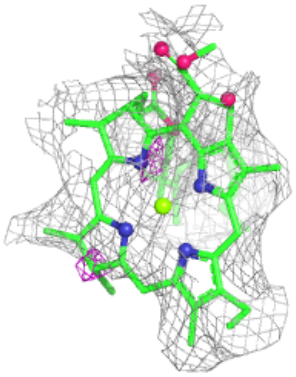


Electron density around CLA 2 321:

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

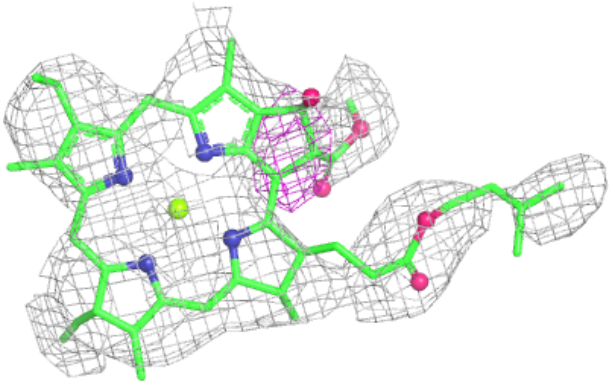


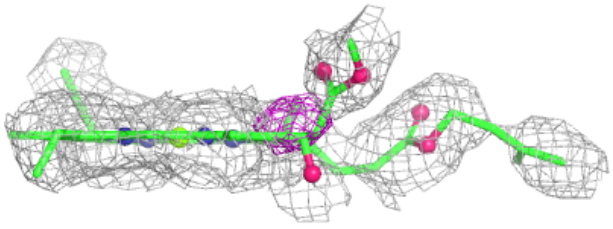


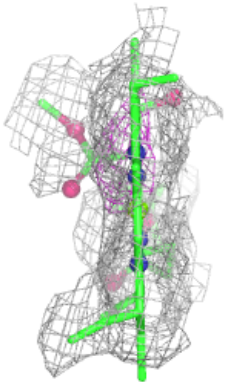


Electron density around CLA 4 306:

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

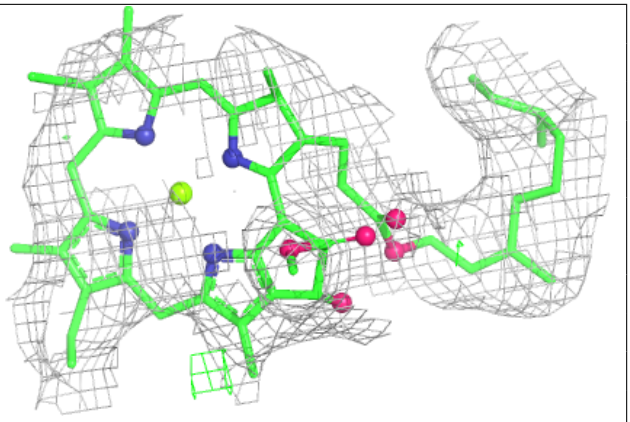


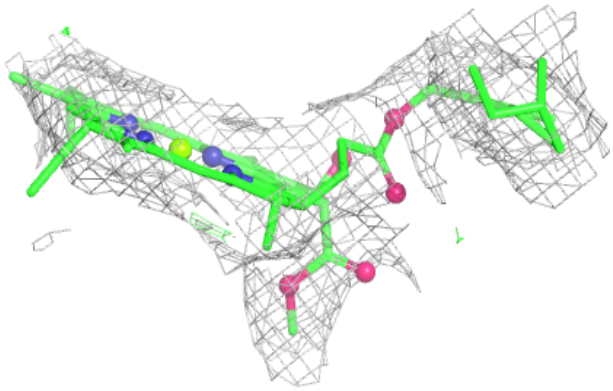


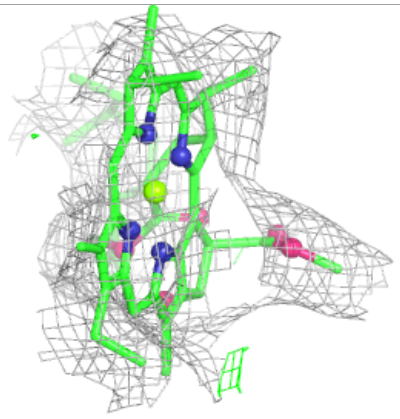


Electron density around CLA 3 301:

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

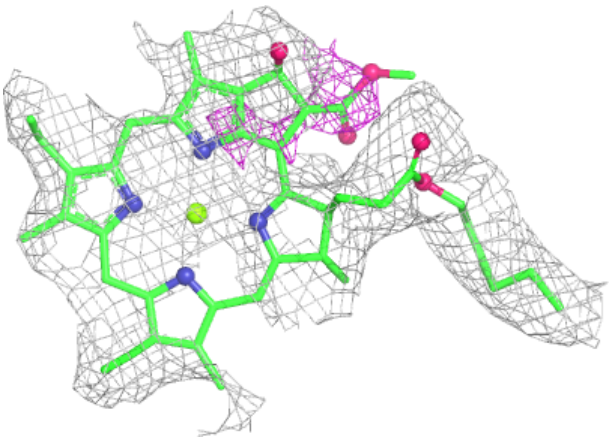


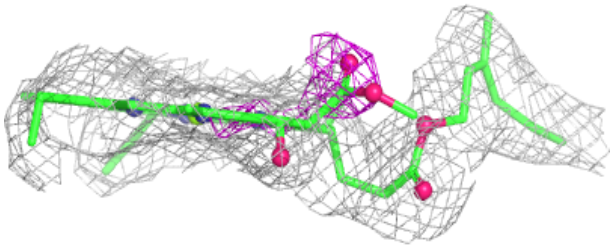


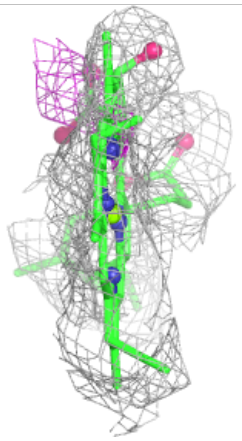


Electron density around CLA 4 318:

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

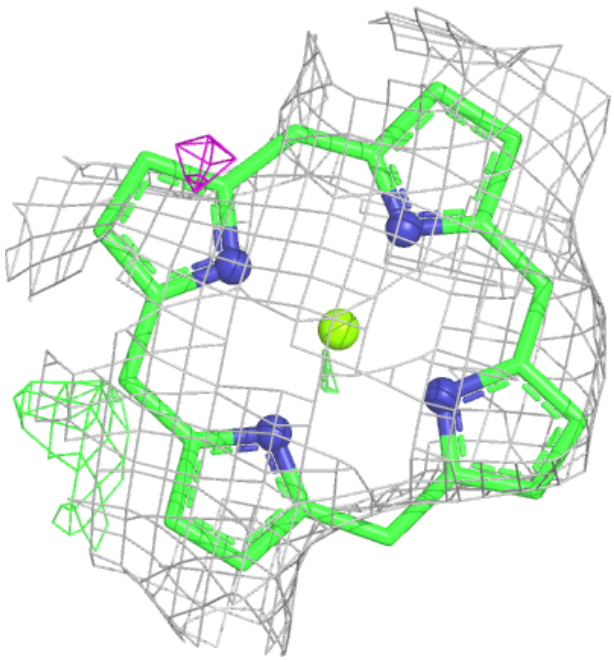


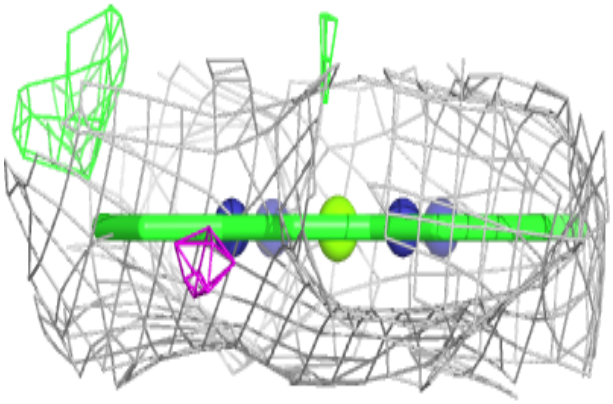


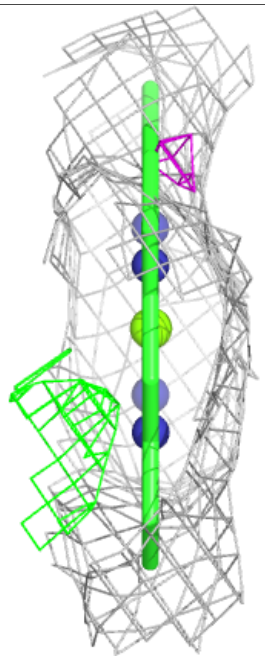


Electron density around CLA 2 305:

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

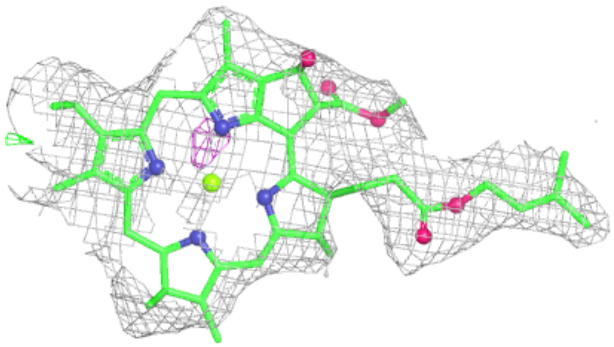


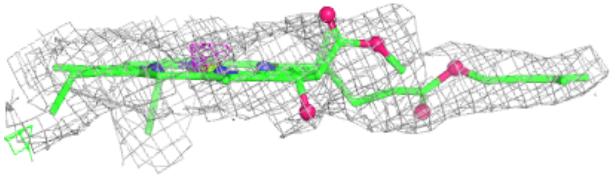


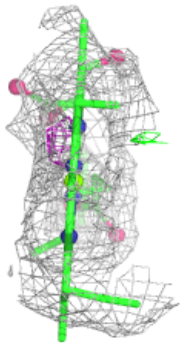


Electron density around CLA A 838:

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

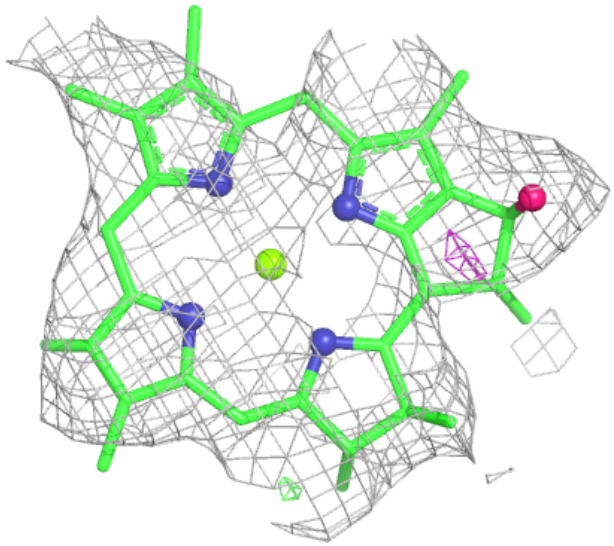


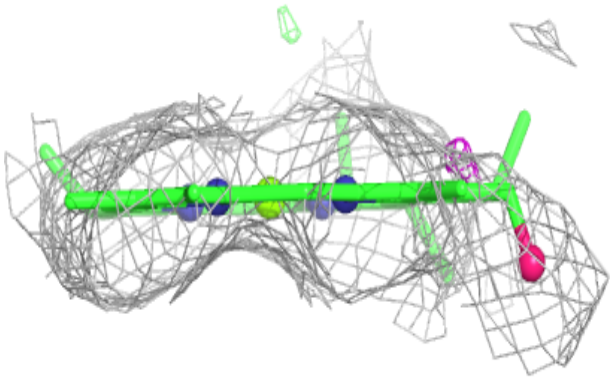


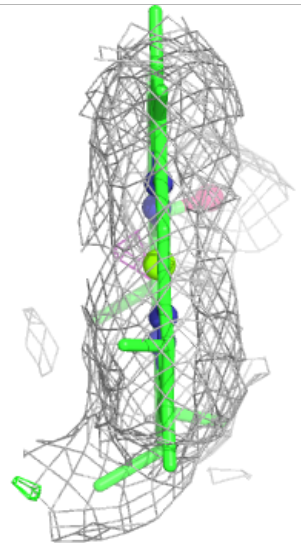


Electron density around CLA 1 205:

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

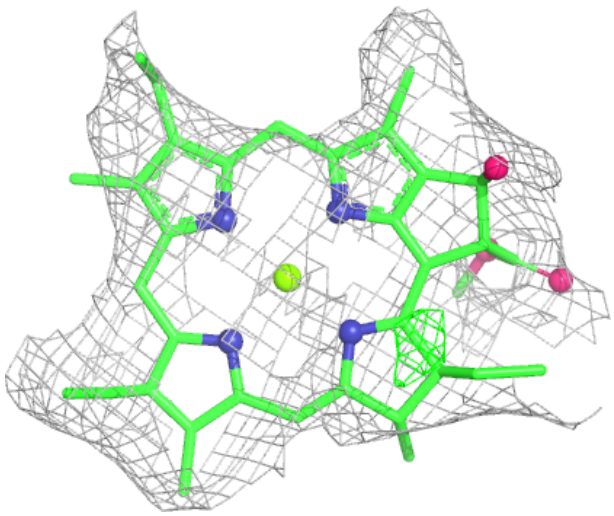


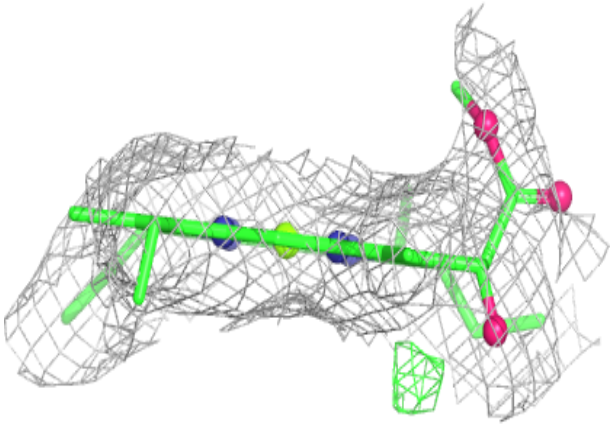


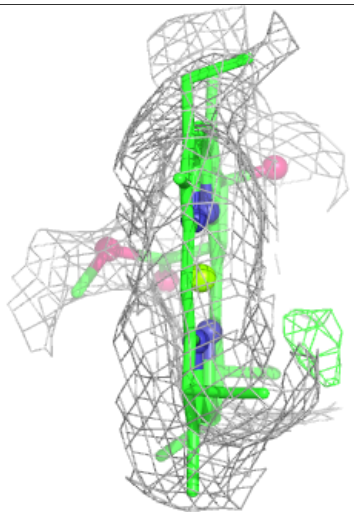


Electron density around CLA 3 314:

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

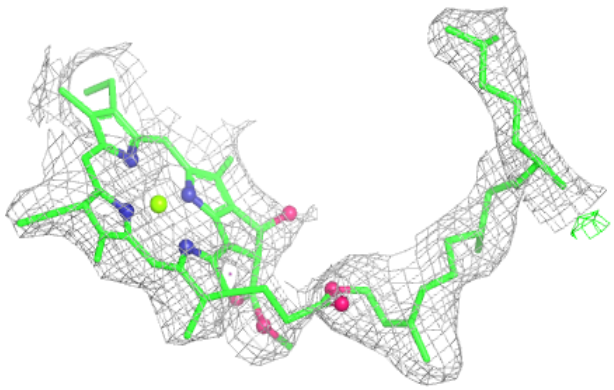


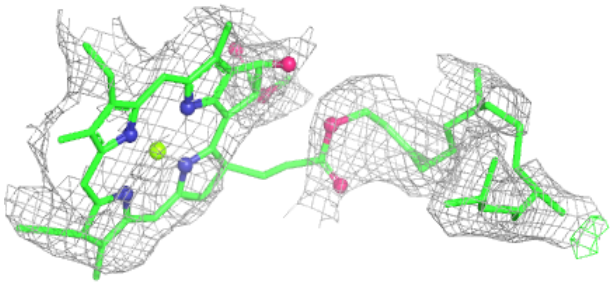


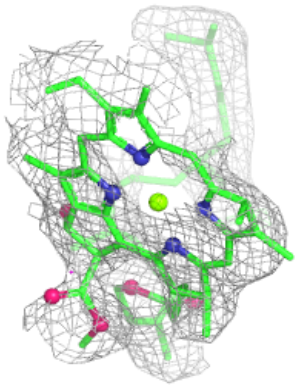


Electron density around CLA K 107:

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

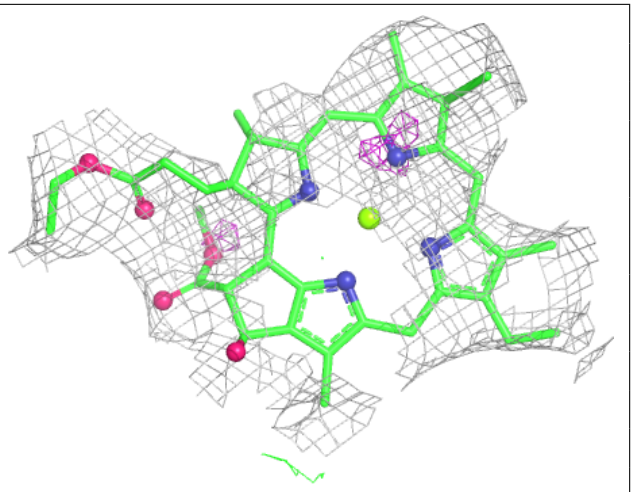


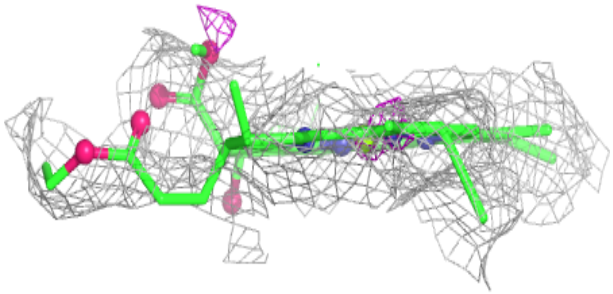




Electron density around CLA 4 319:

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

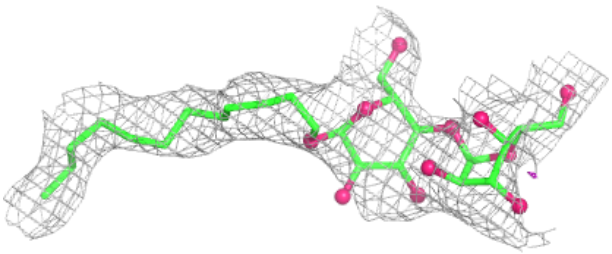


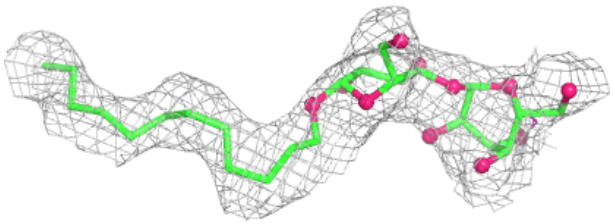


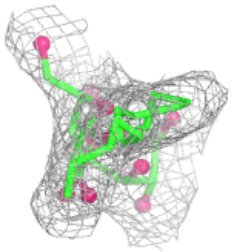


Electron density around LMU A 851:

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

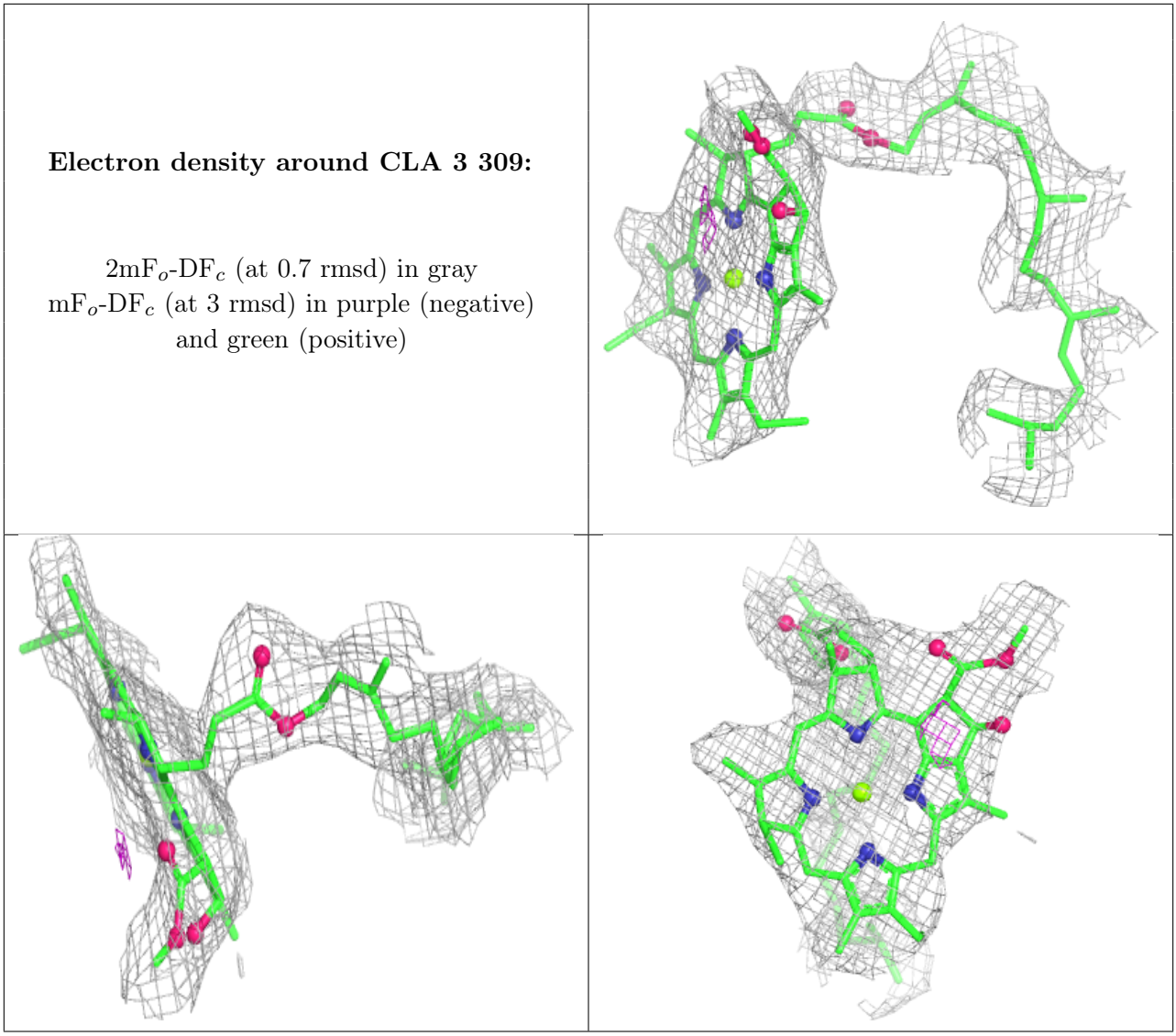






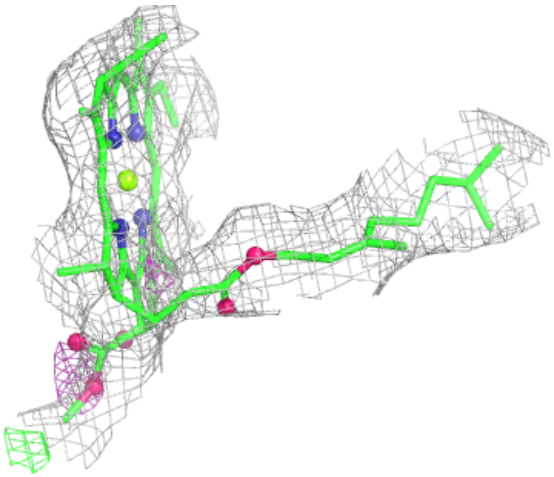
Electron density around CLA 3 309:

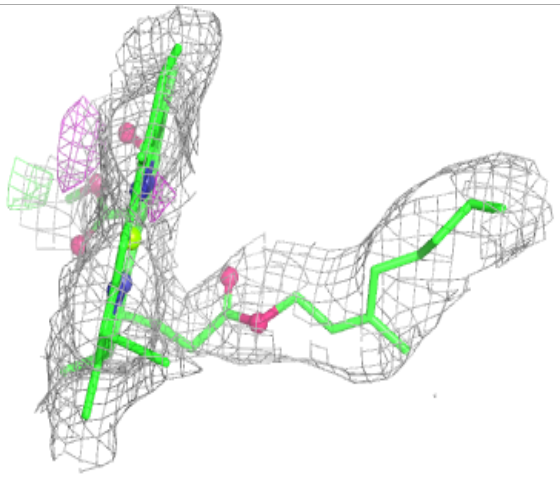
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

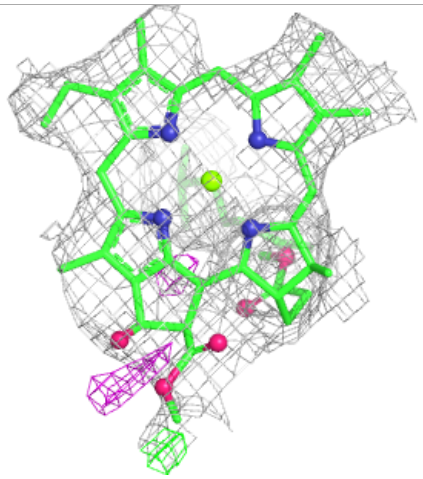


Electron density around CLA 4 302:

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

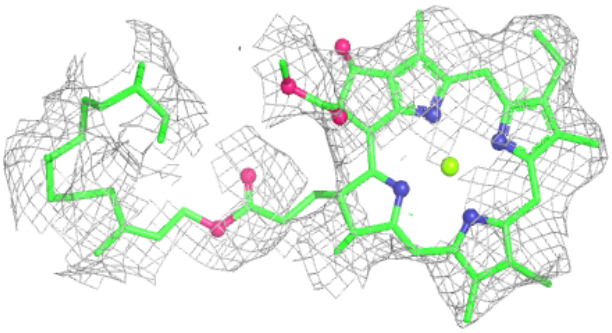


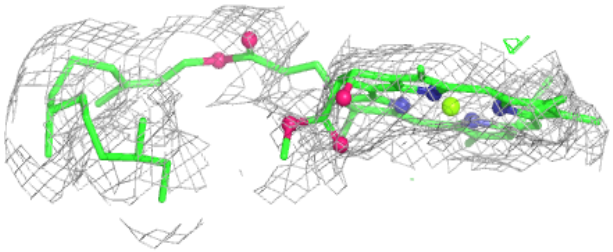


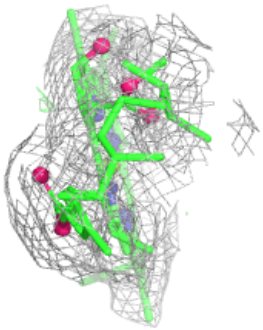


Electron density around CLA 1 212:

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

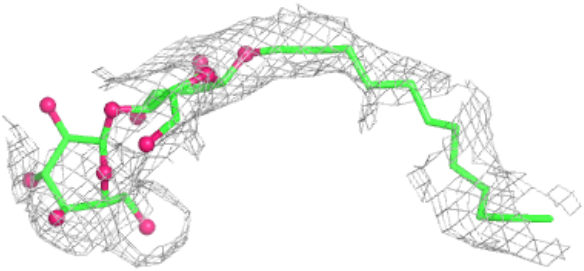


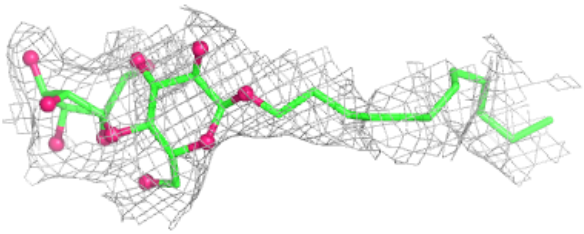


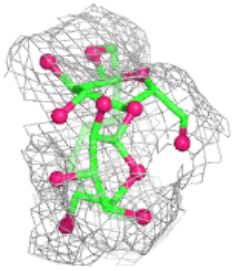


Electron density around LMU L 205:

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

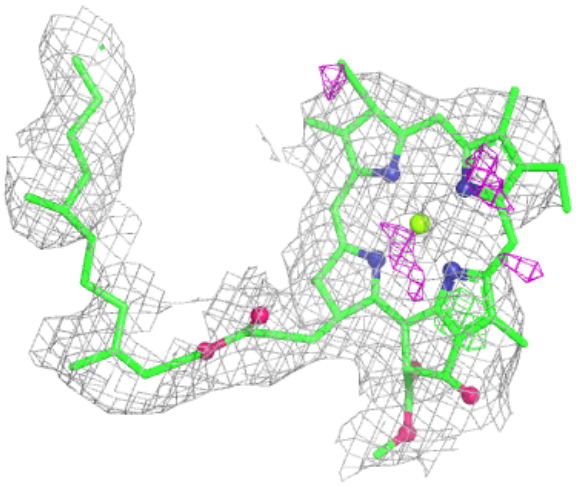


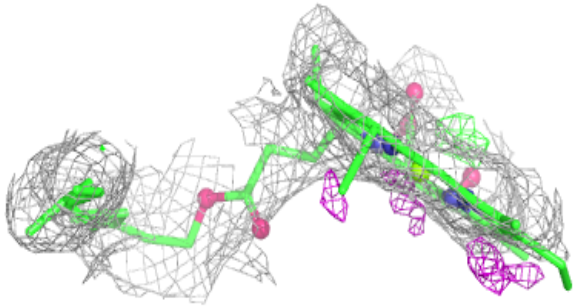


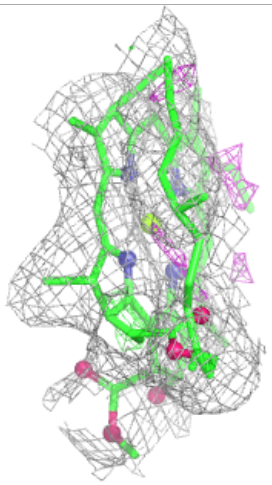


Electron density around CLA B 822:

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

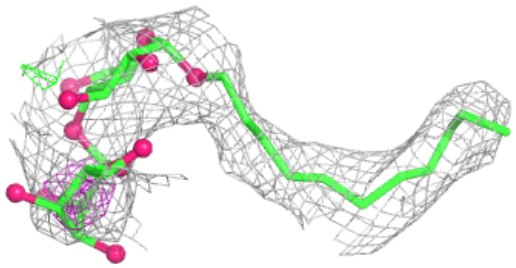


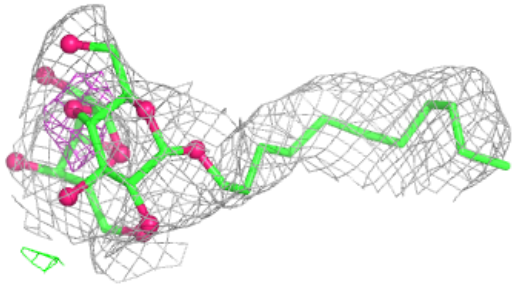


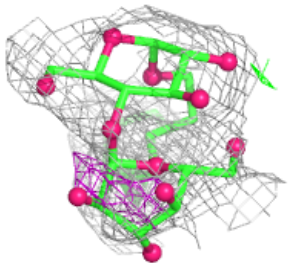


Electron density around LMU 4 320:

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

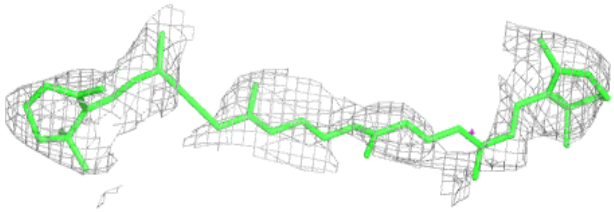


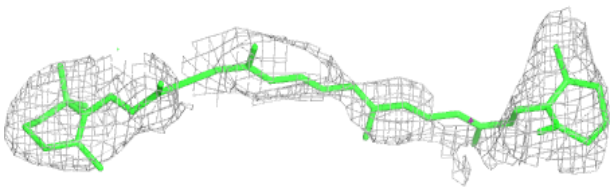


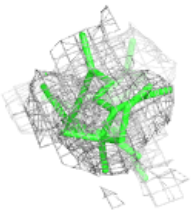


Electron density around BCR A 842:

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

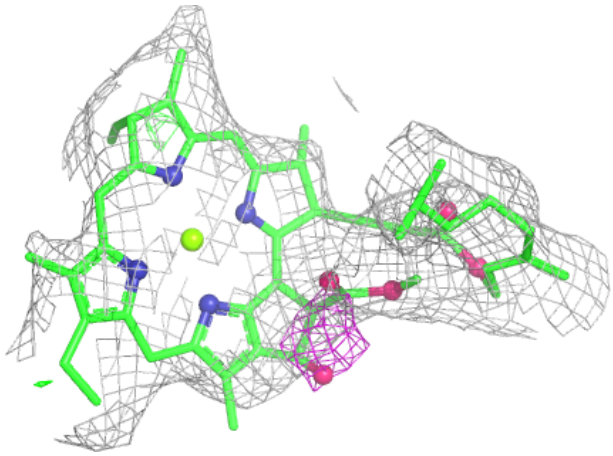


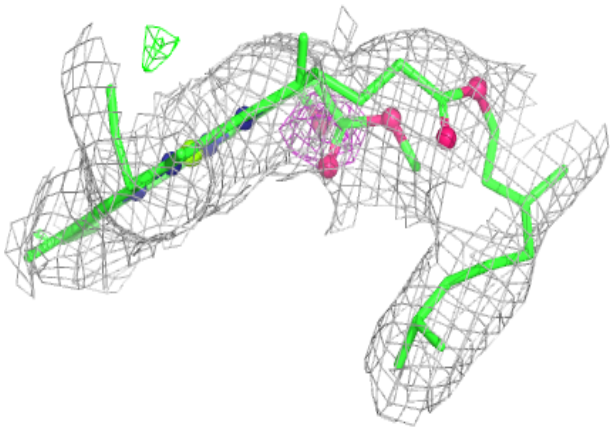


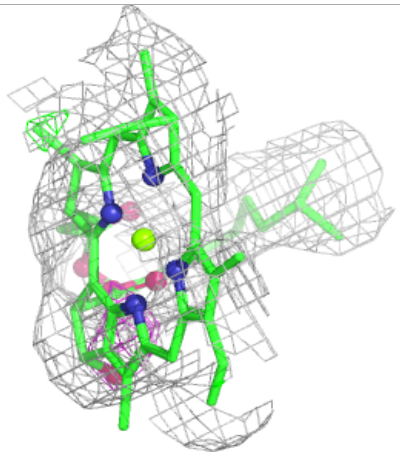


Electron density around CLA L 204:

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

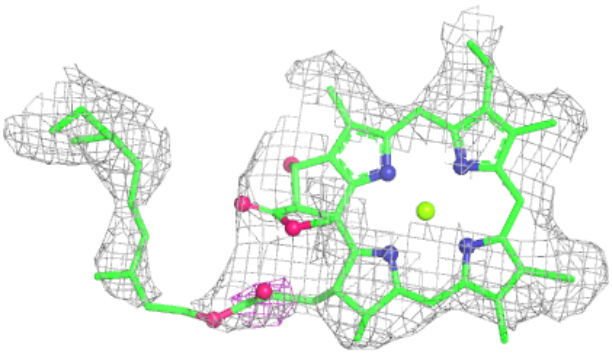


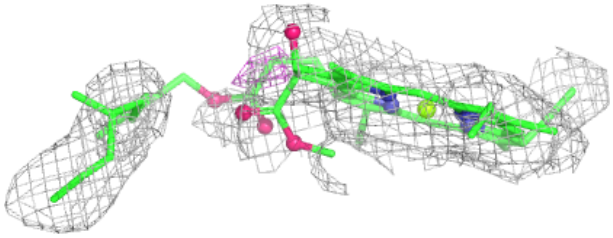


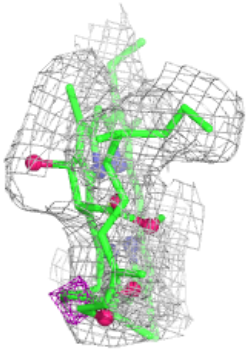


Electron density around CLA R 106:

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

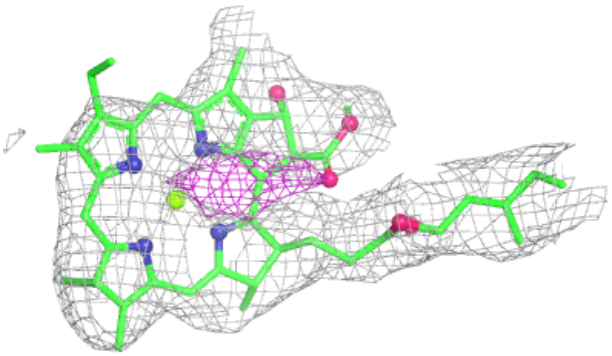


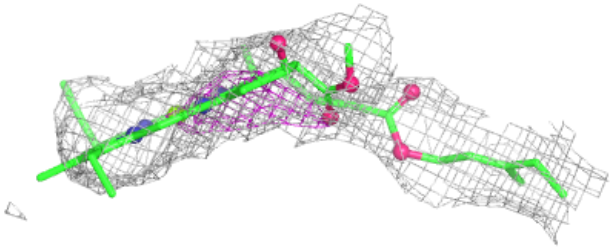


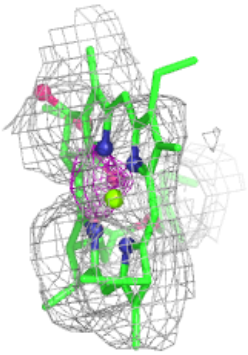


Electron density around CLA 1 211:

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

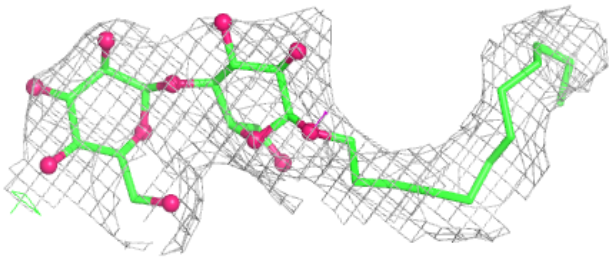


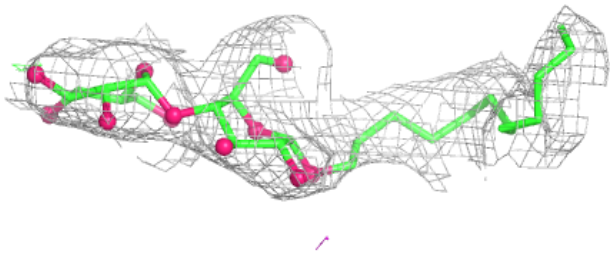


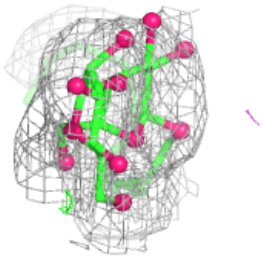


Electron density around LMU C 101:

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

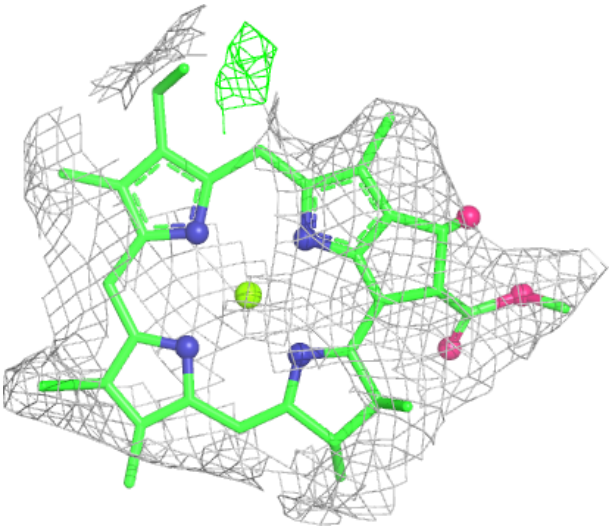


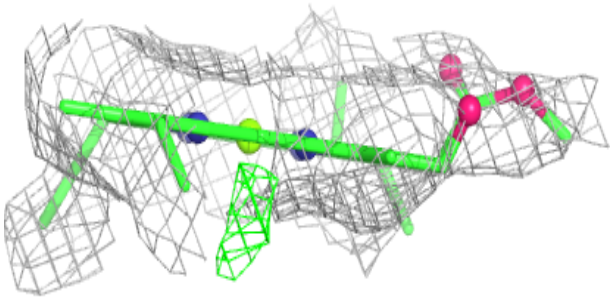


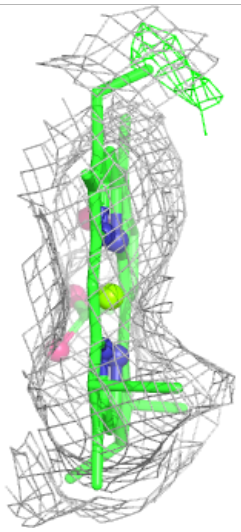


Electron density around CLA F 205:

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

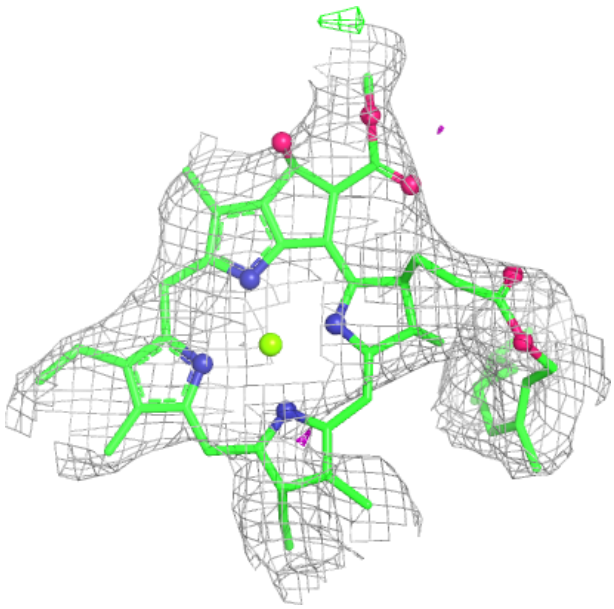


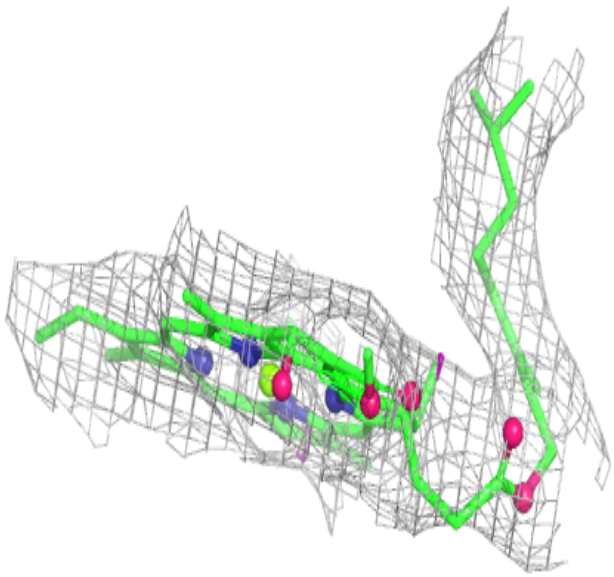


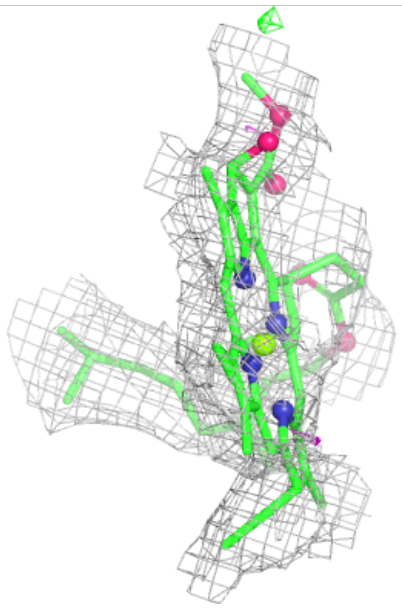


Electron density around CLA H 101:

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

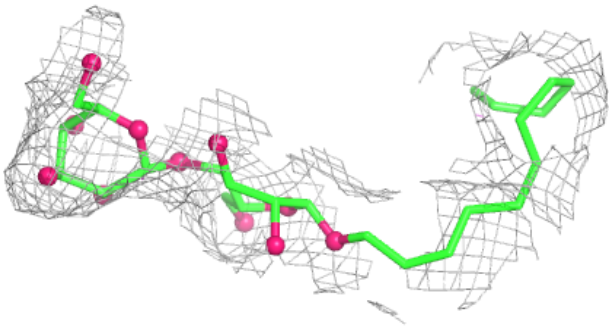


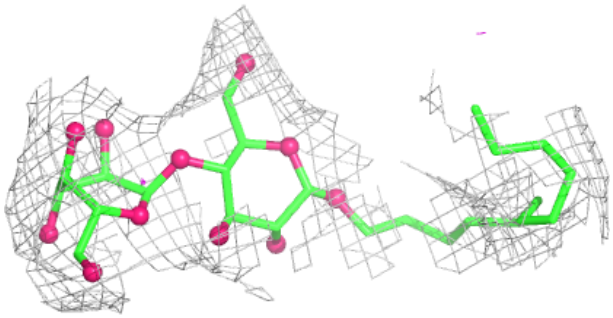


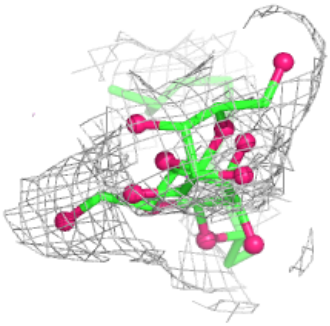


Electron density around LMU H 105:

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

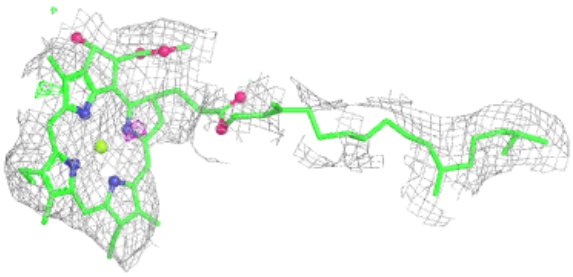


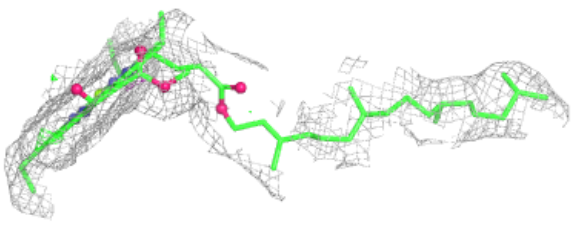




Electron density around CLA 4 304:

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

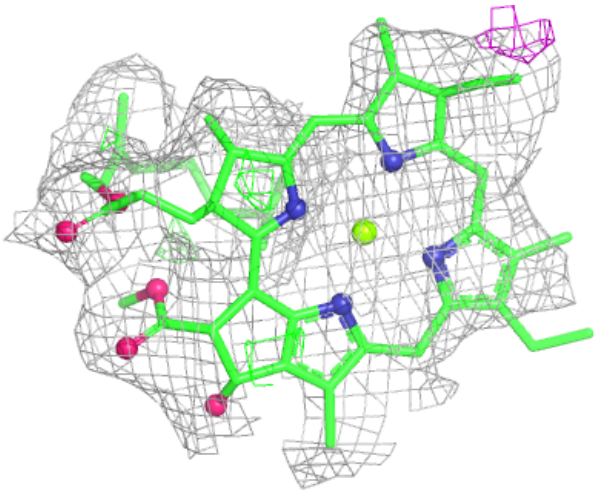


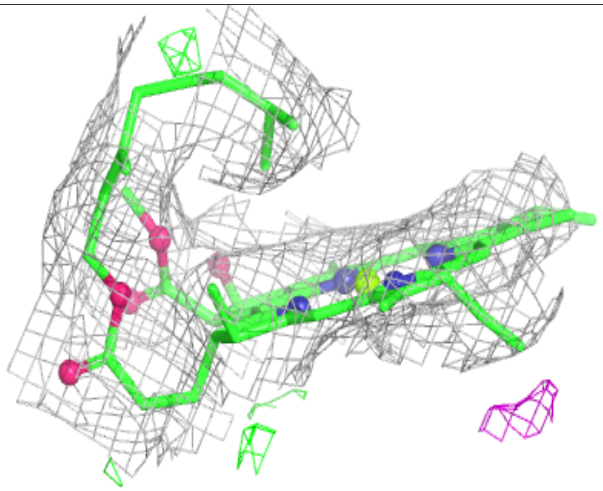


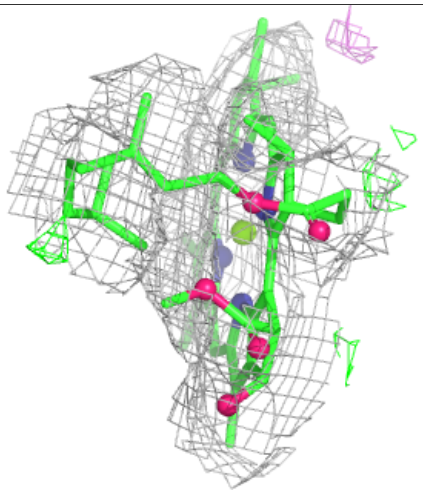


Electron density around CLA 4 305:

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

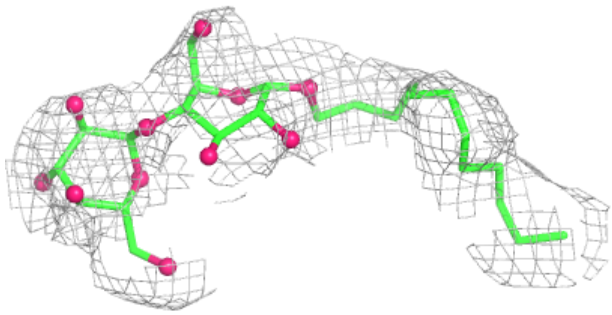


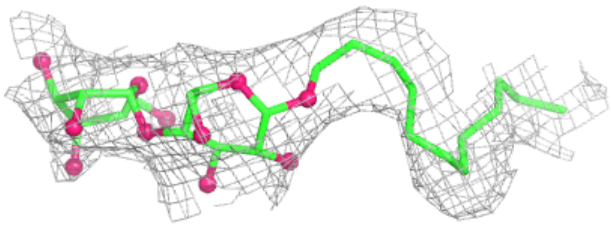


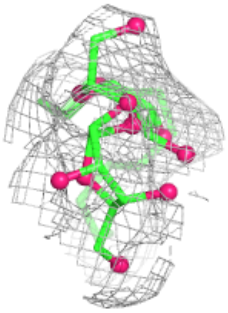


Electron density around LMU 4 322:

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

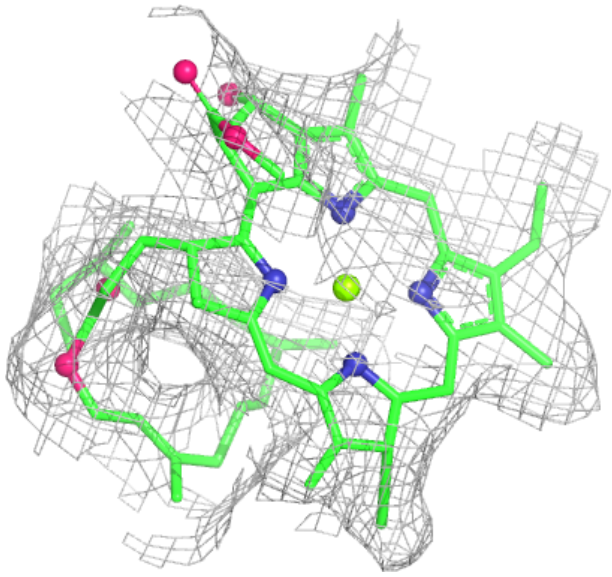


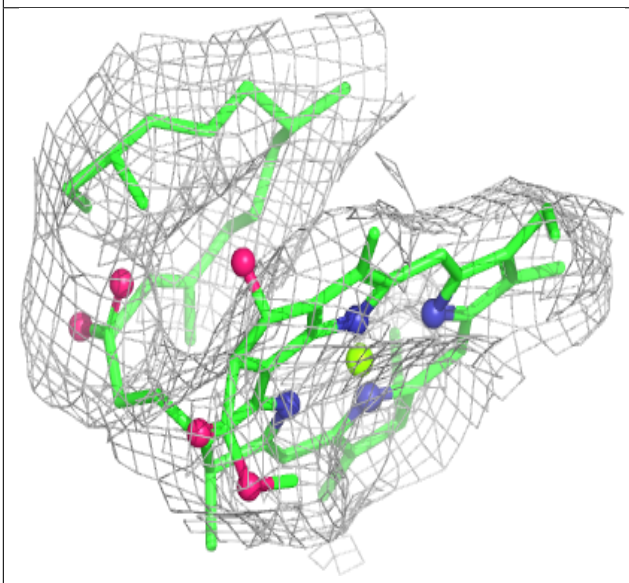


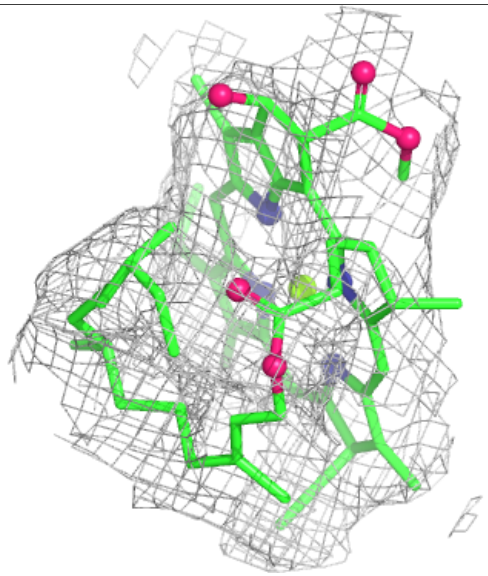


Electron density around CLA J 102:

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

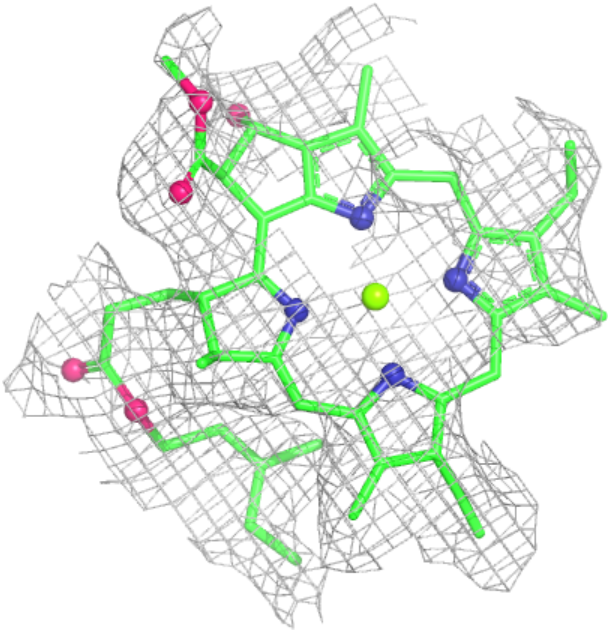


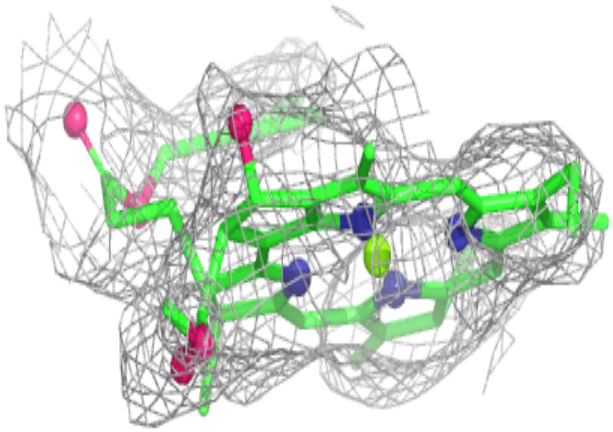


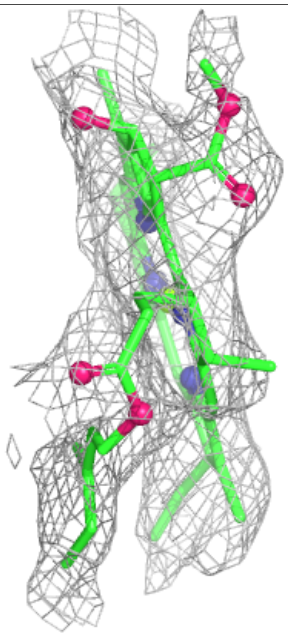


Electron density around CLA G 103:

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

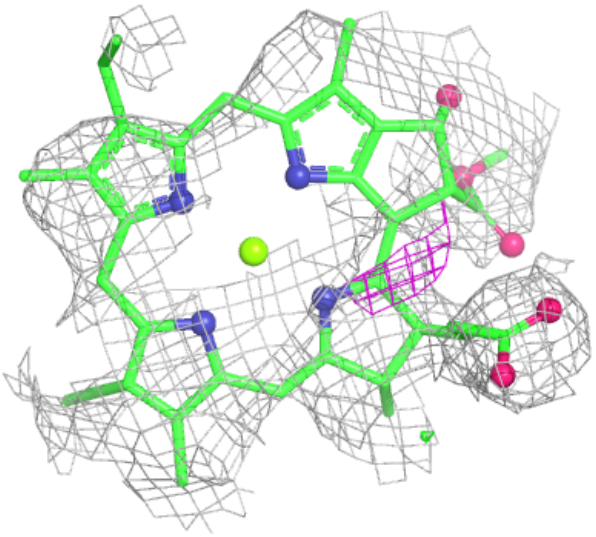


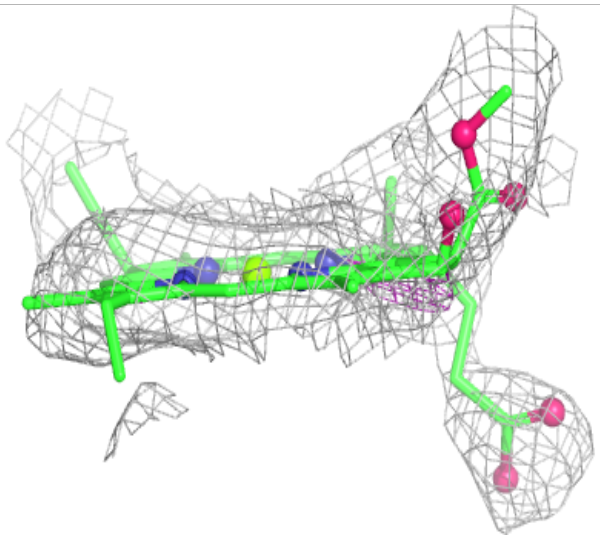


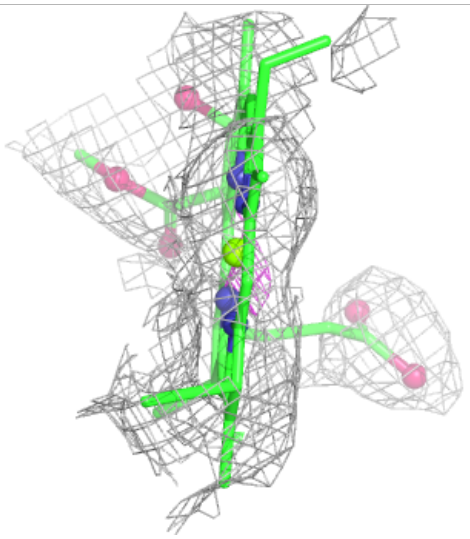


Electron density around CLA B 832:

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

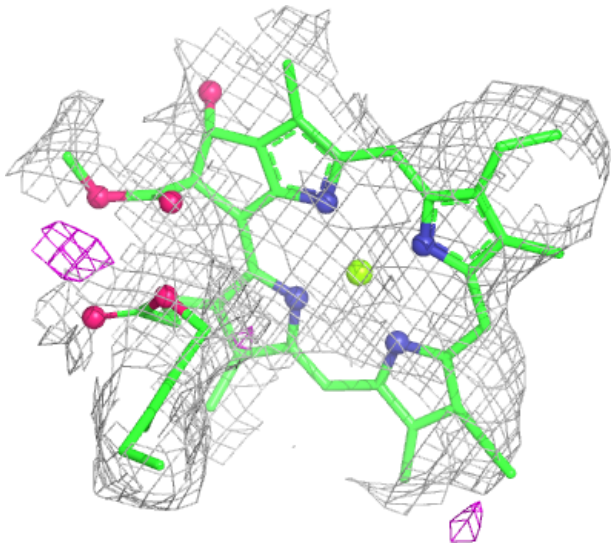


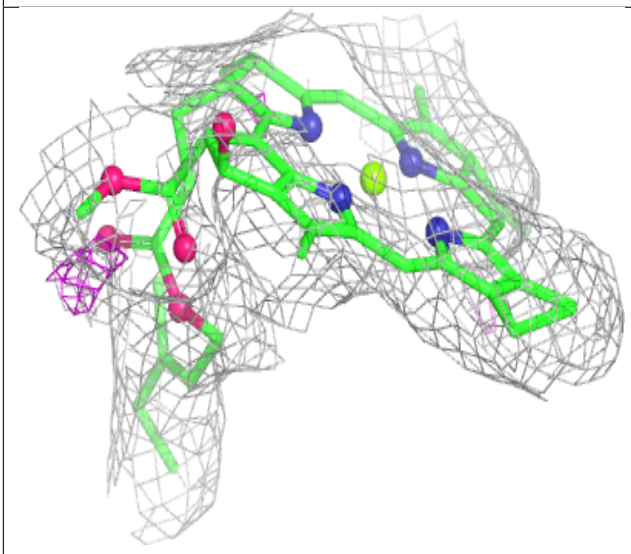




Electron density around CLA 1 207:

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

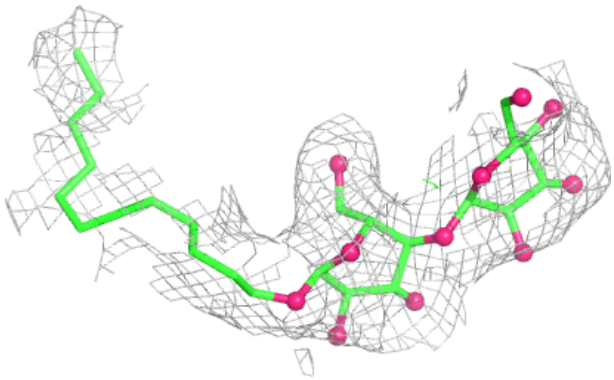


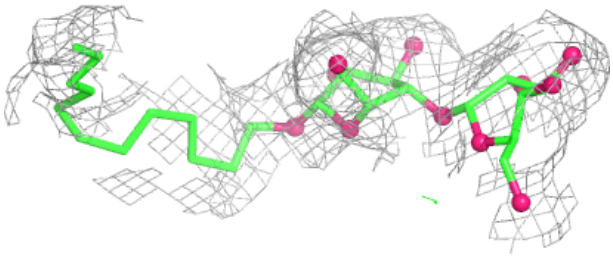




Electron density around LMU H 103:

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

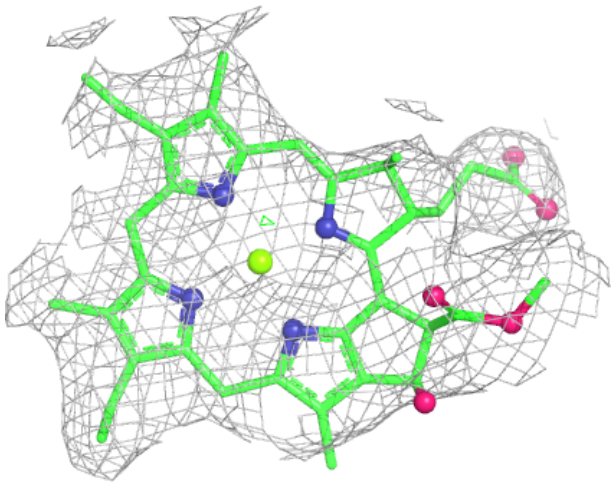


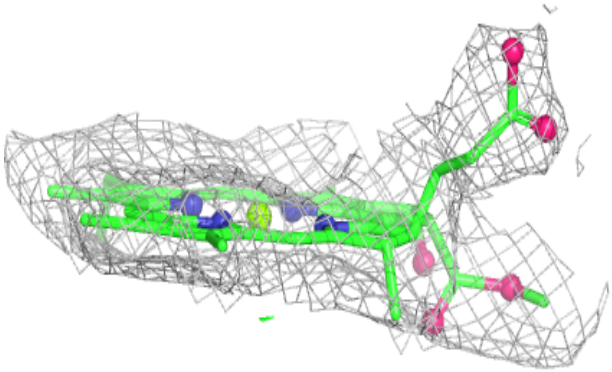


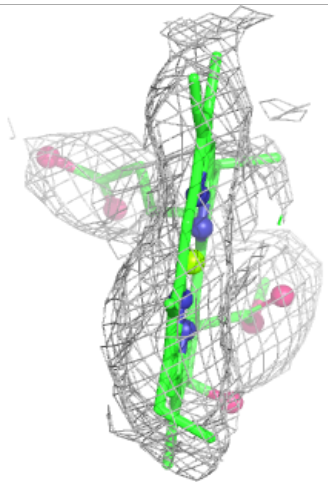


Electron density around CLA A 808:

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

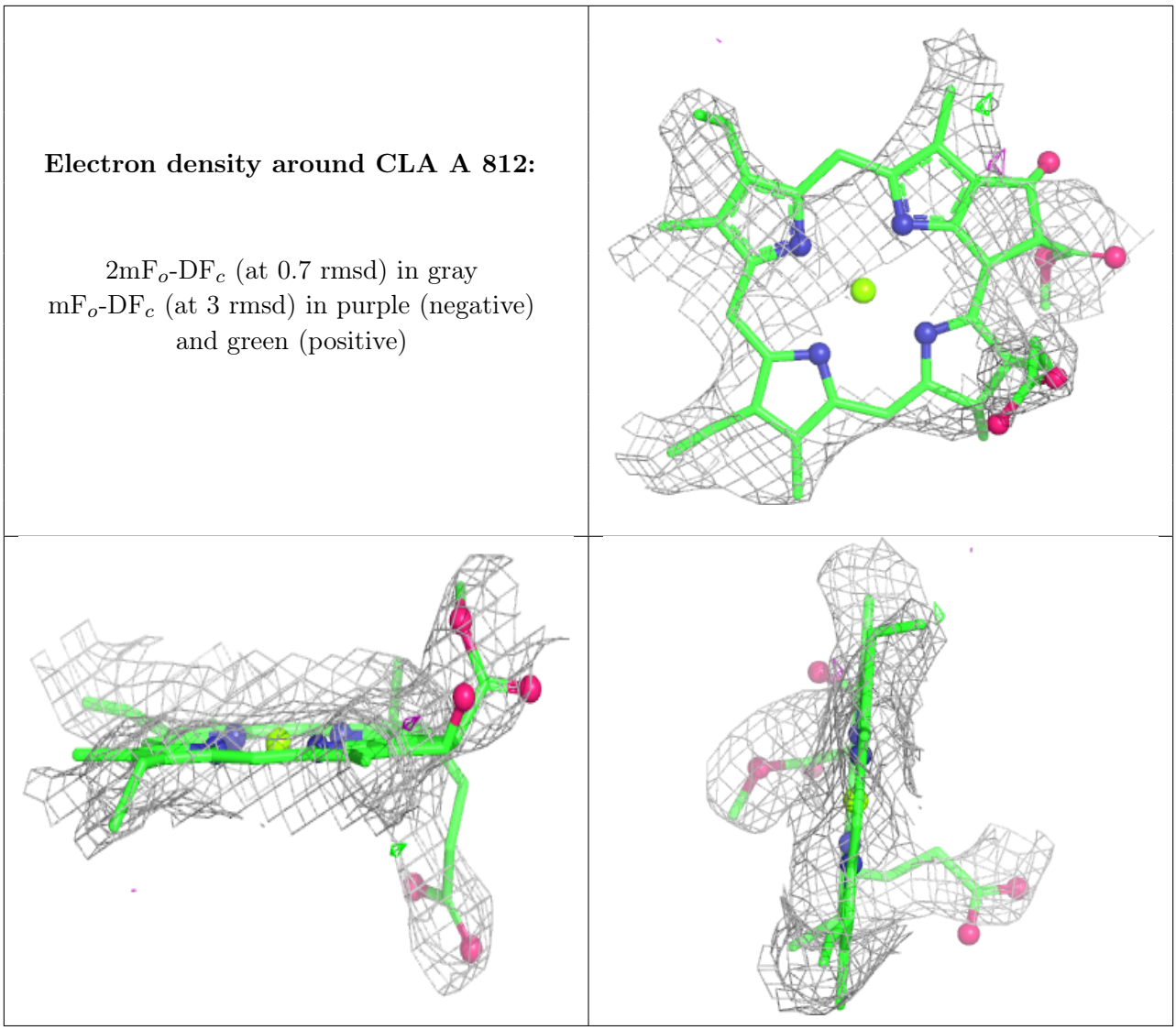






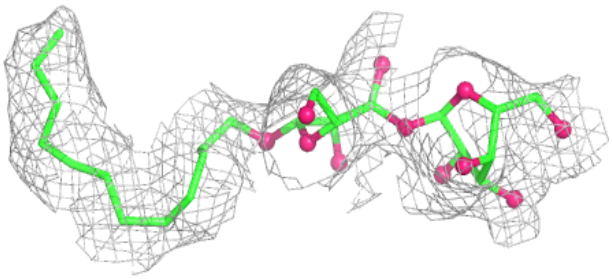
Electron density around CLA A 812:

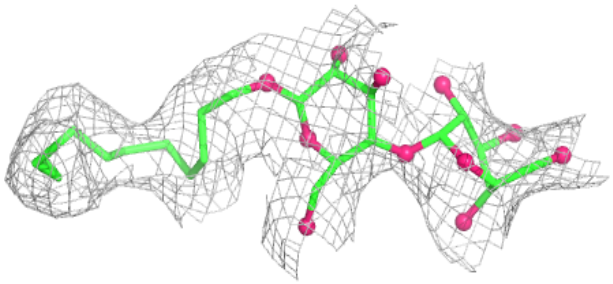
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

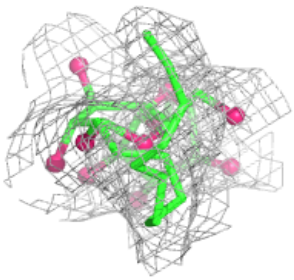


Electron density around LMU A 845:

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



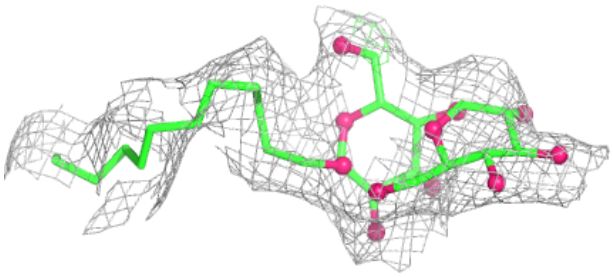


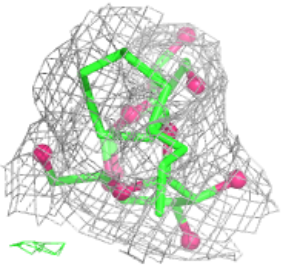


Electron density around LMU A 846:

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

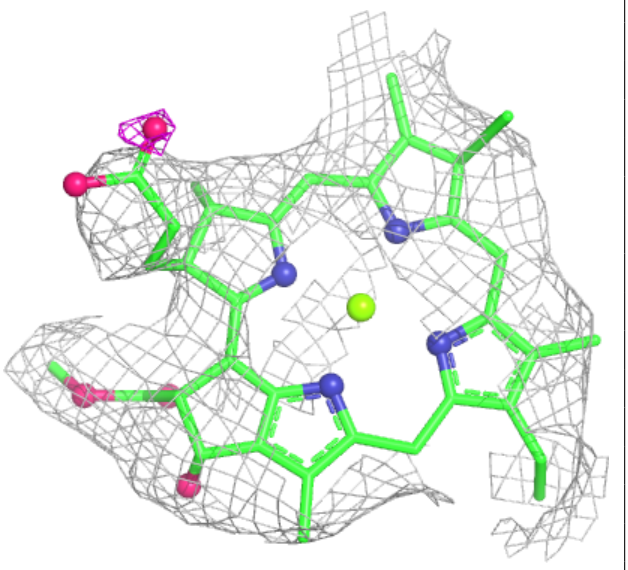


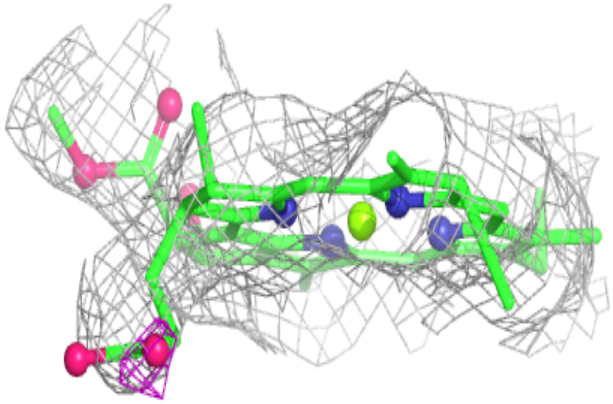


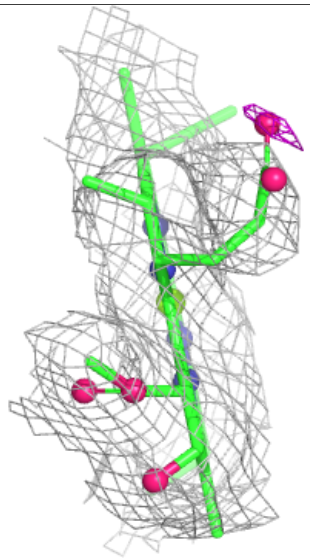


Electron density around CLA A 831:

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

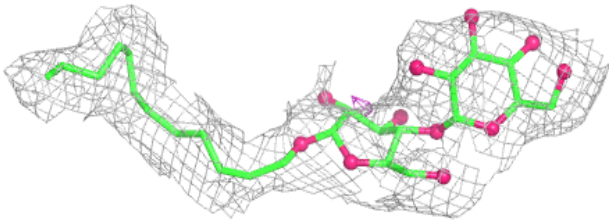


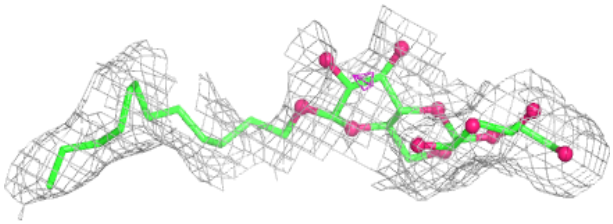


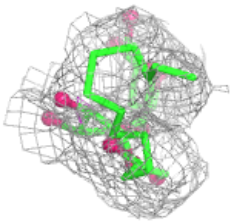


Electron density around LMU B 801:

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

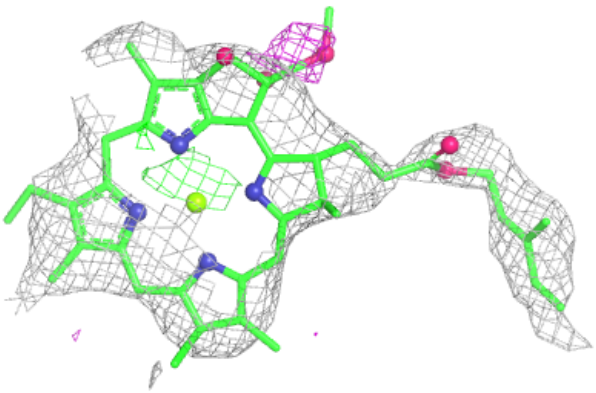


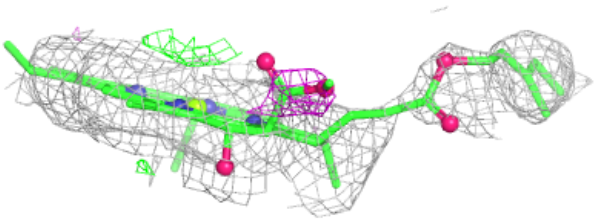


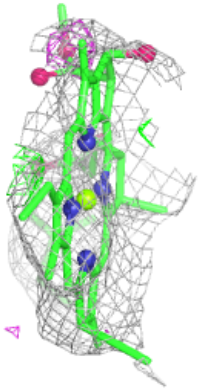


Electron density around CLA 1 214:

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

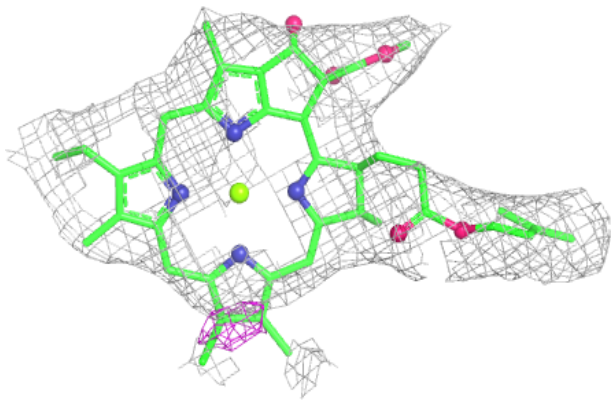


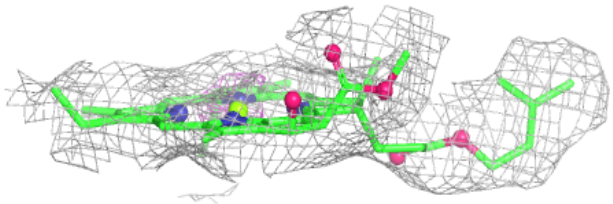


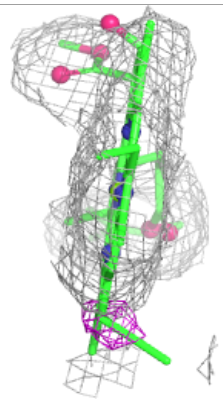


Electron density around CLA K 103:

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

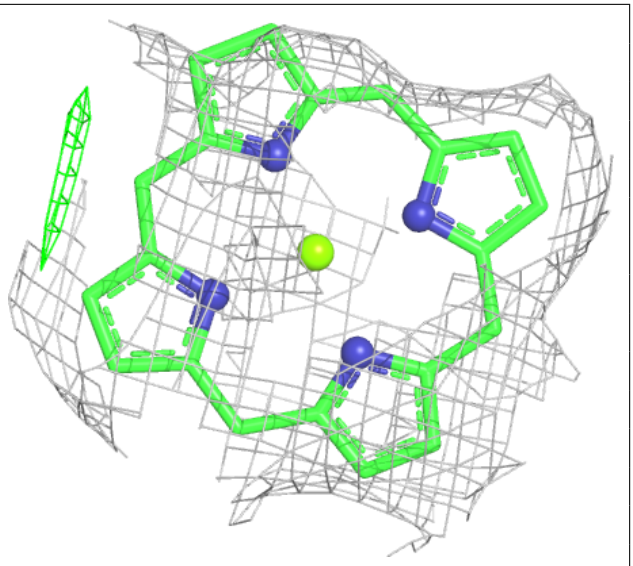


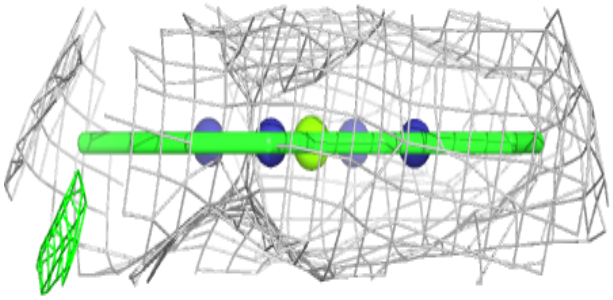


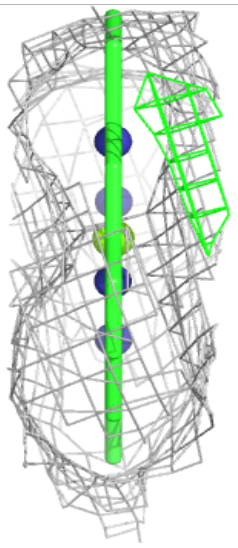


Electron density around CLA 3 304:

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

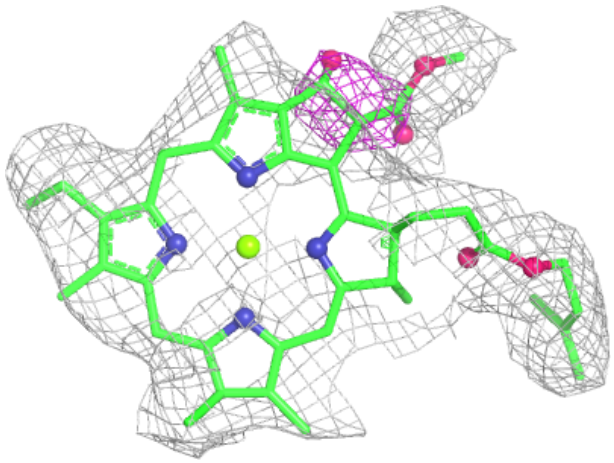


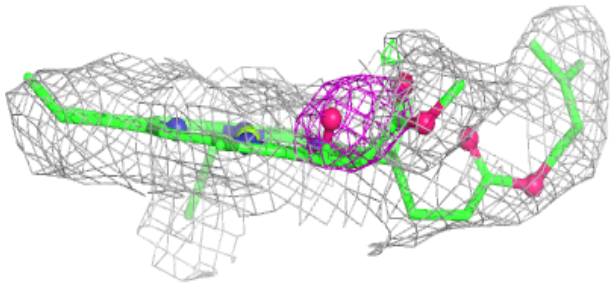


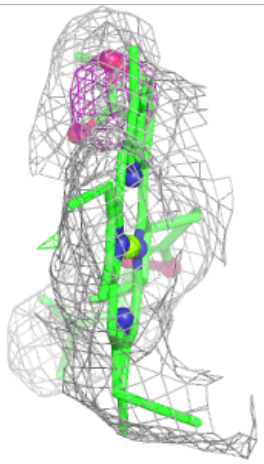


Electron density around CLA K 106:

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

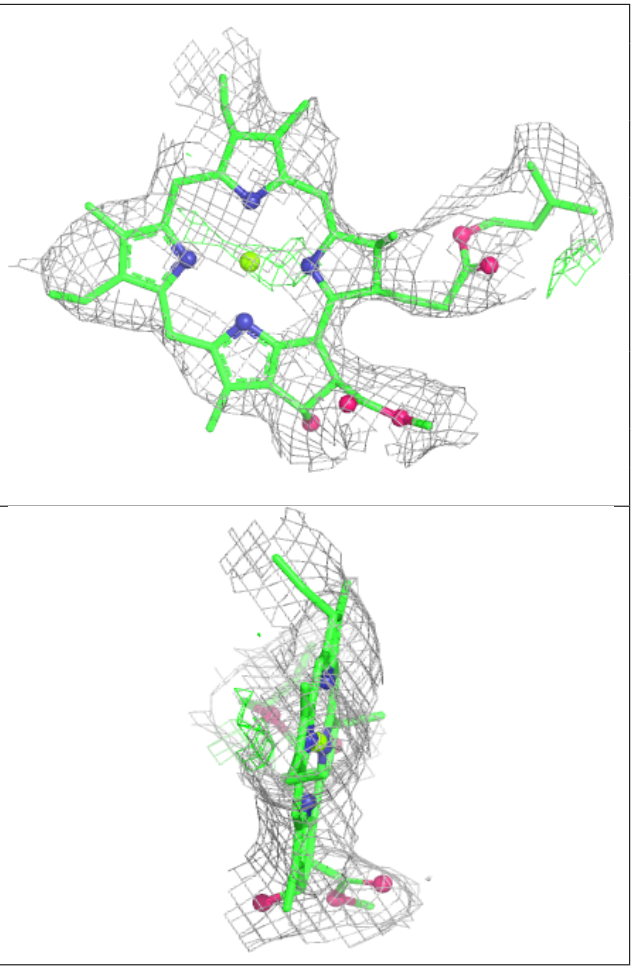






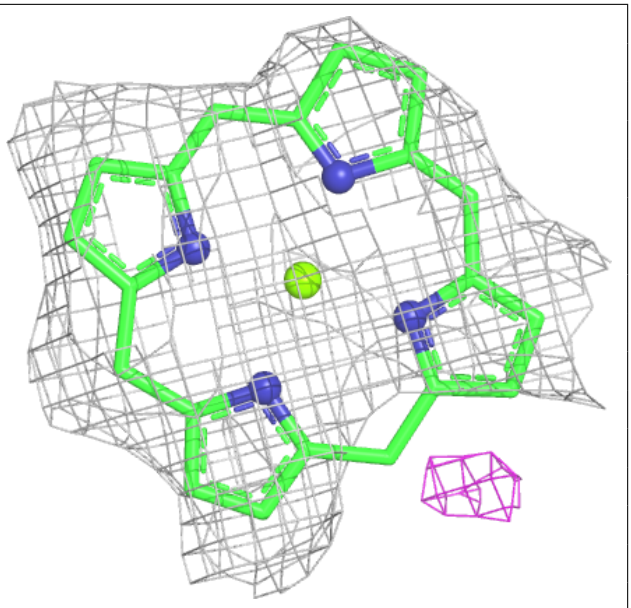
Electron density around CLA 2 304:

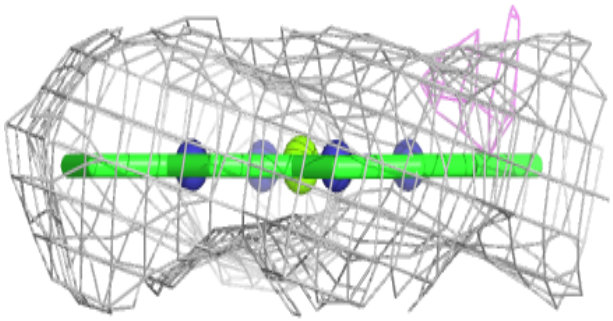
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

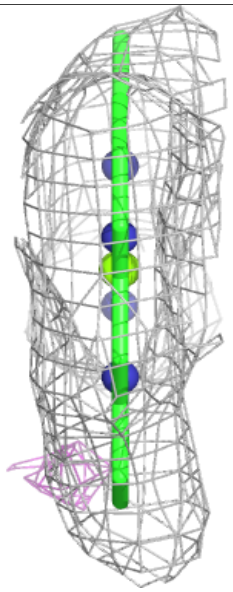


Electron density around CLA 3 312:

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

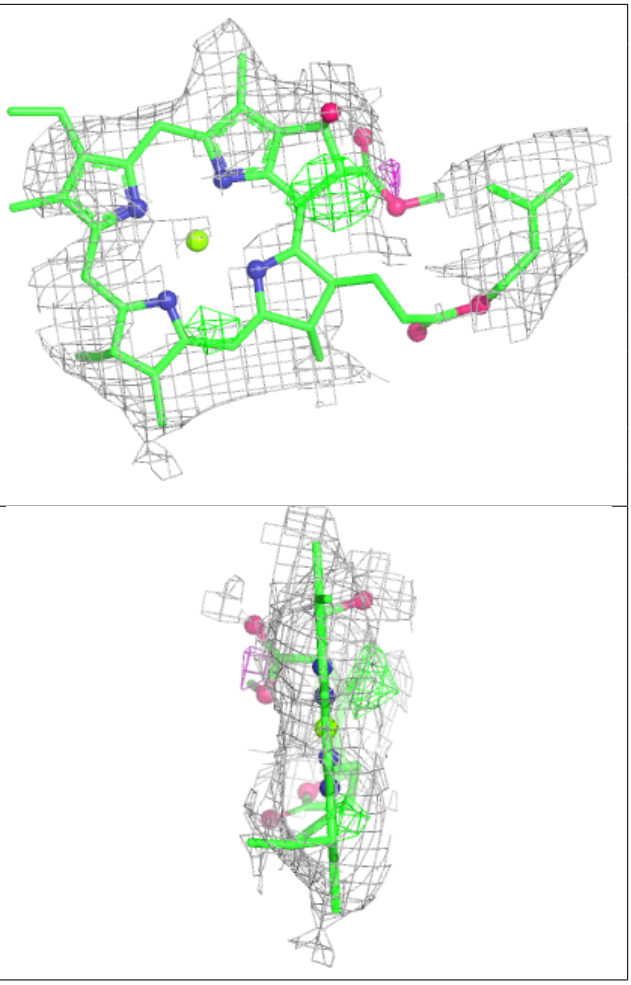


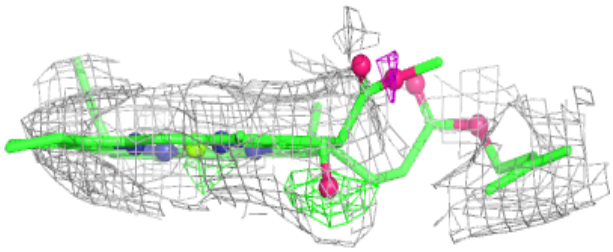




Electron density around CLA 2 311:

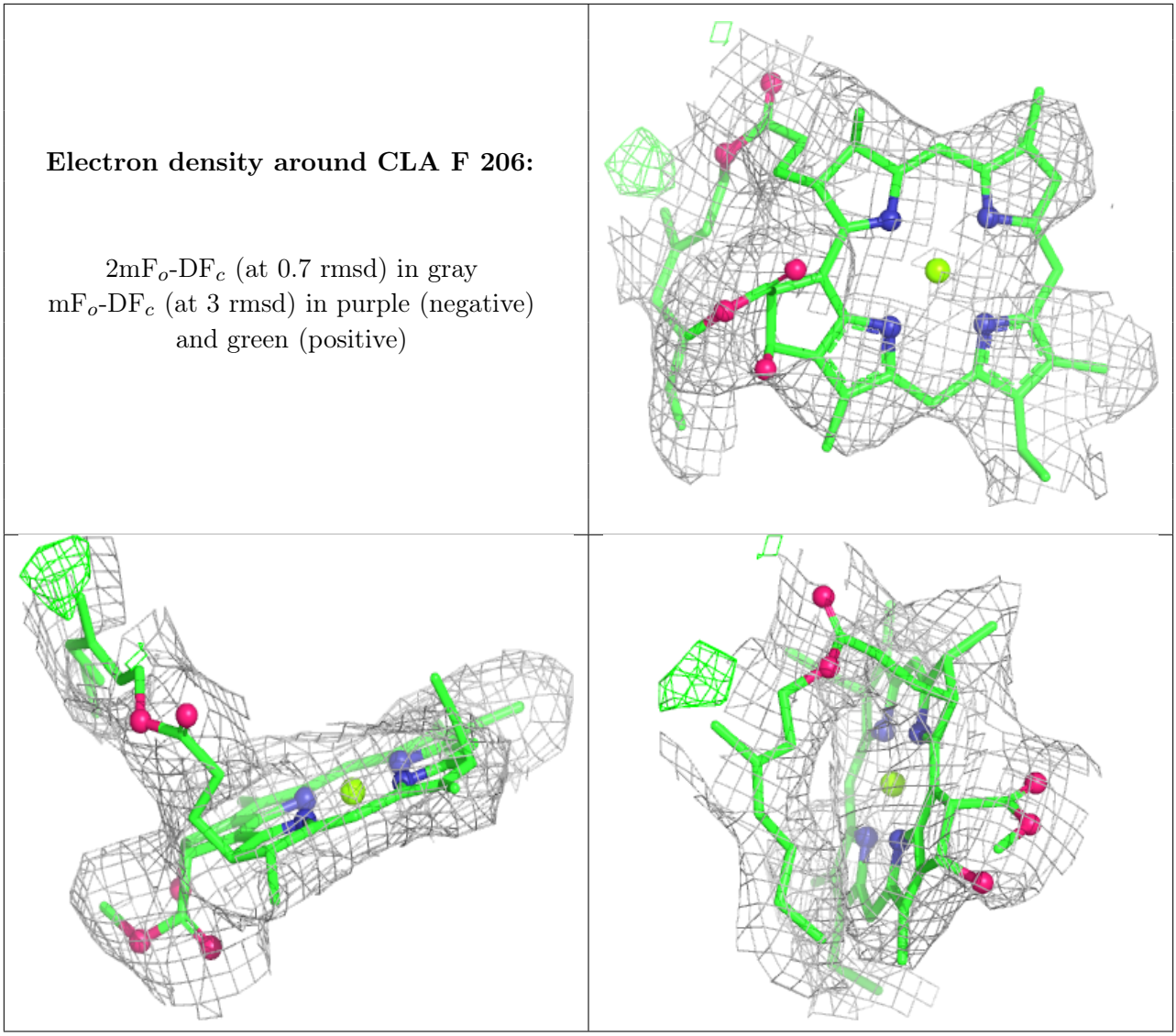
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





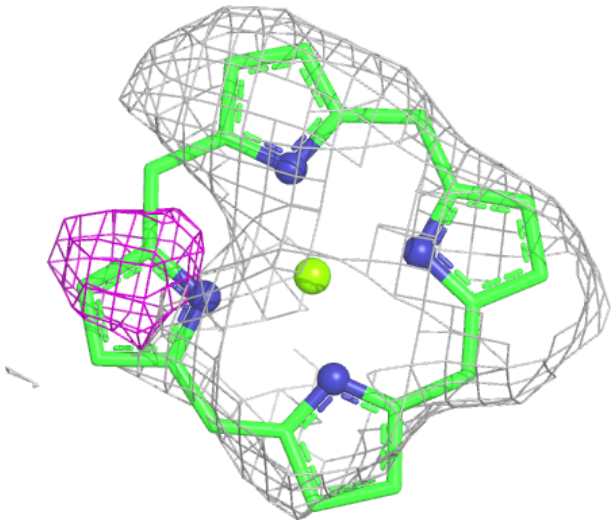
Electron density around CLA F 206:

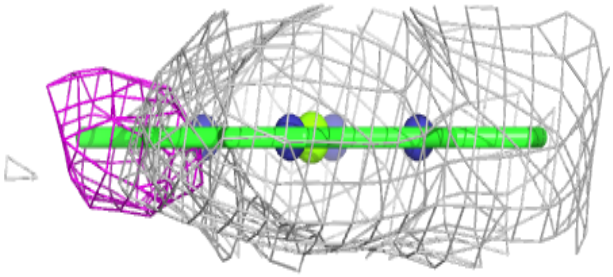
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

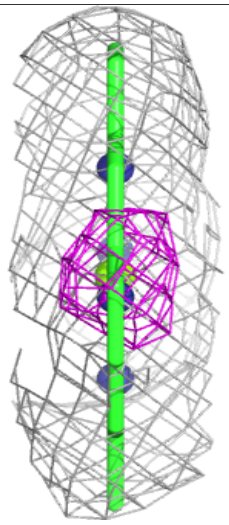


Electron density around CLA 3 316:

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

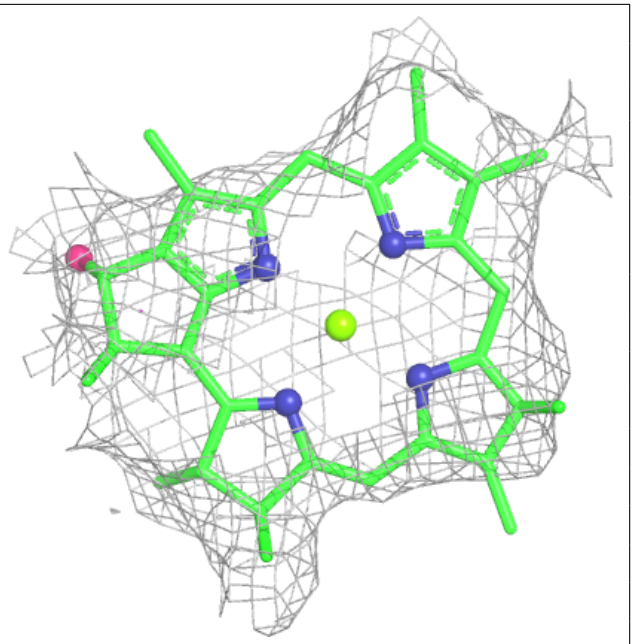


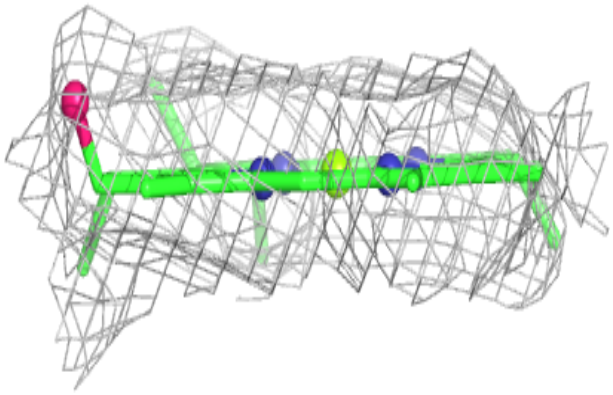


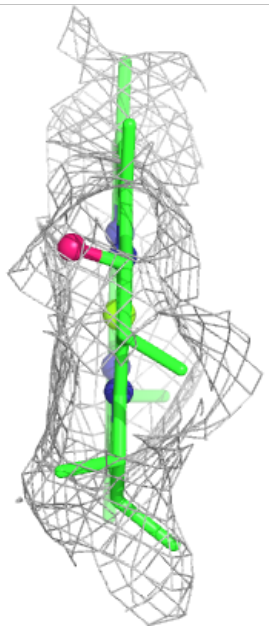


Electron density around CLA 3 319:

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

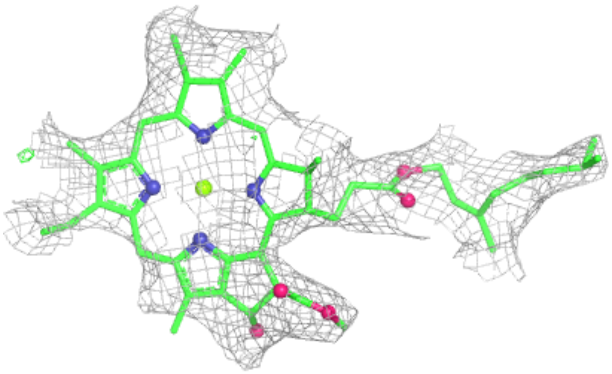


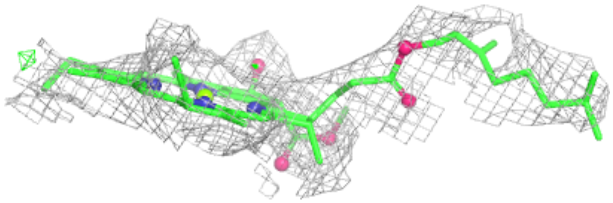


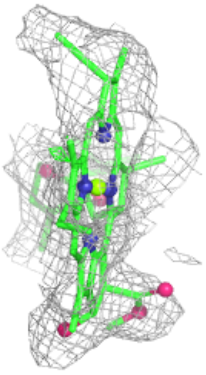


Electron density around CLA 3 320:

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

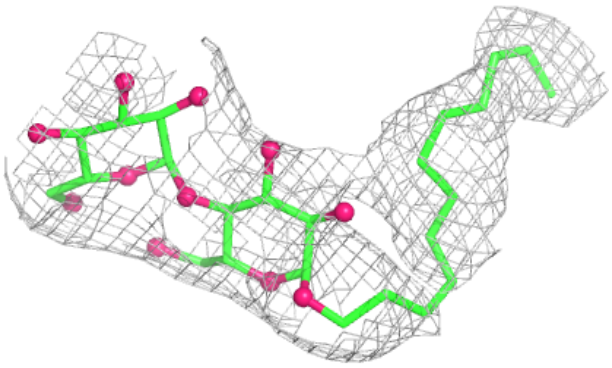


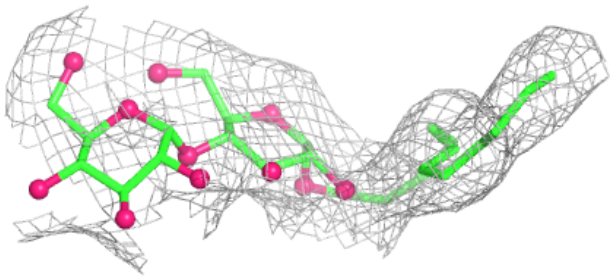


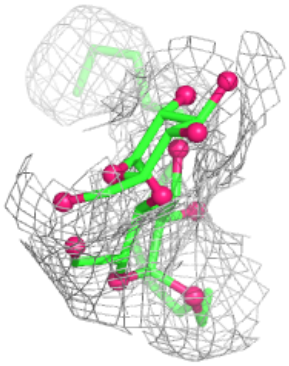


Electron density around LMU R 105:

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

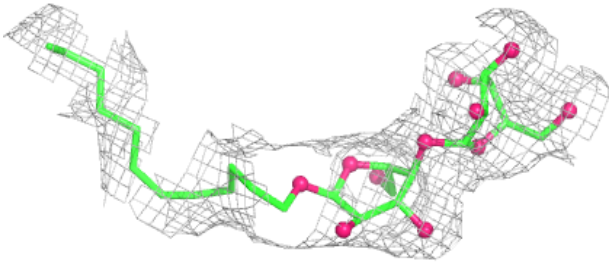


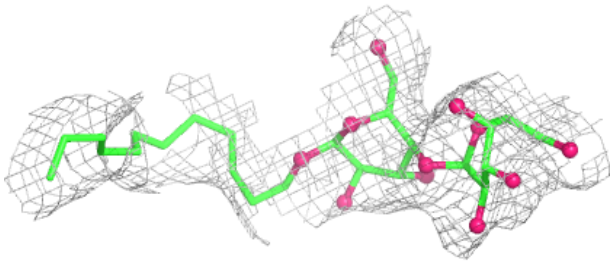




Electron density around LMU 2 318:

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

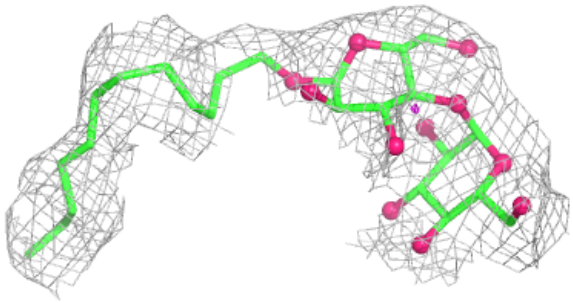


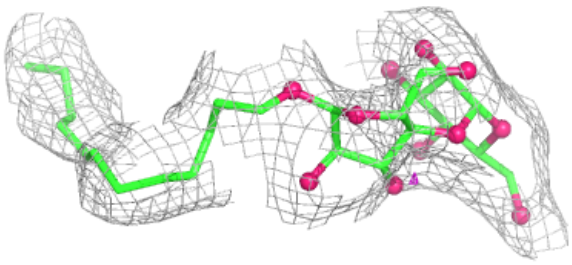


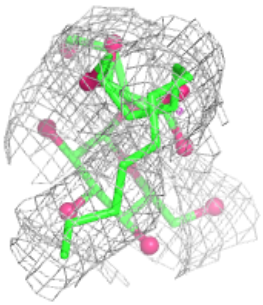


Electron density around LMU 2 319:

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

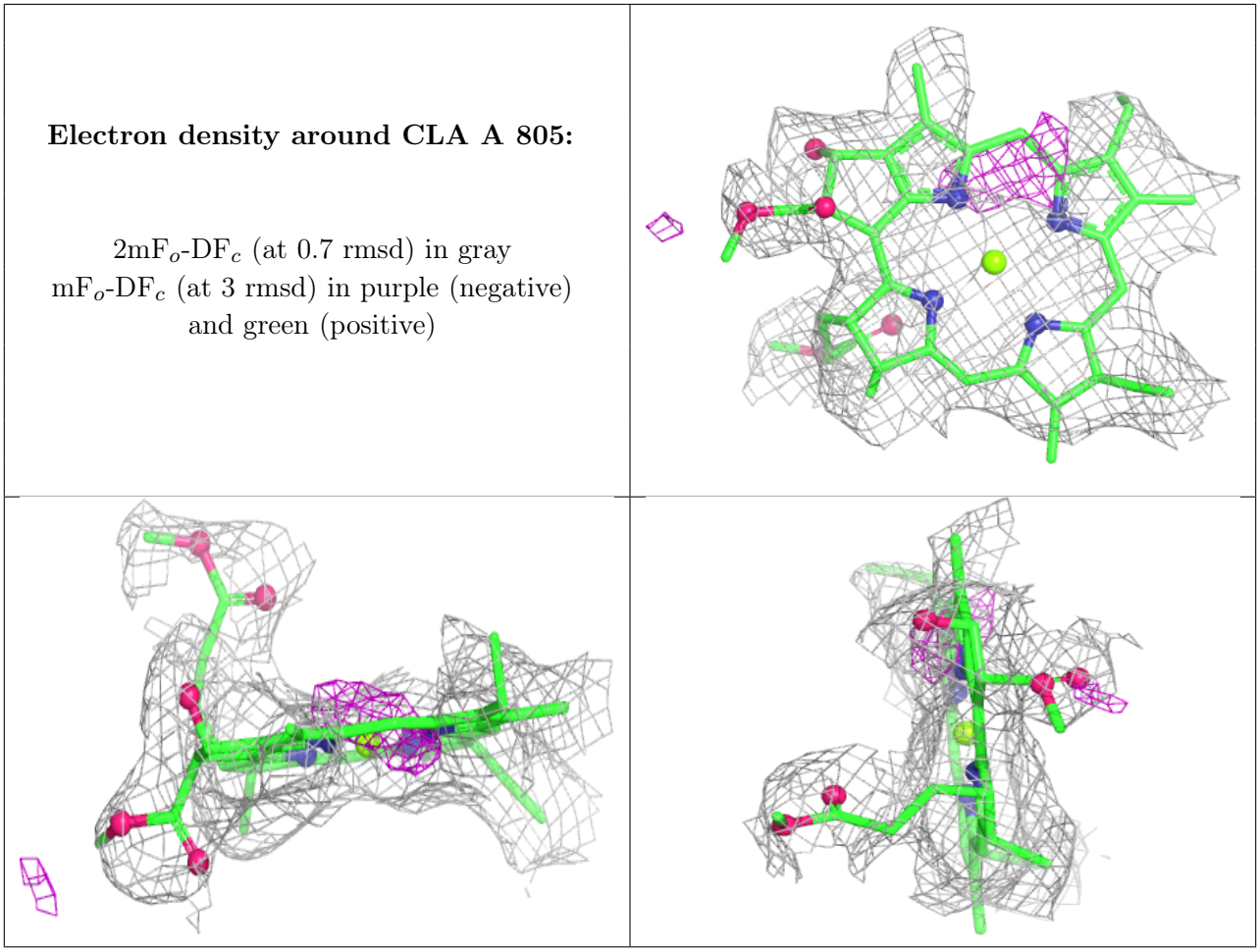






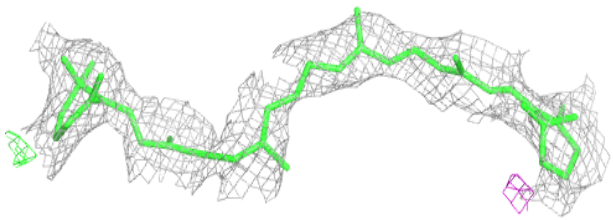
Electron density around CLA A 805:

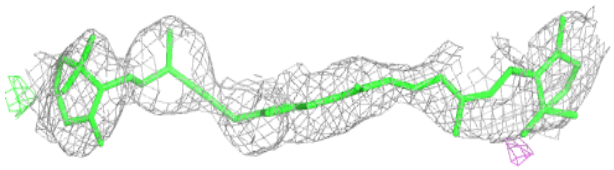
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

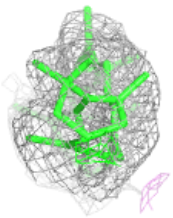


Electron density around BCR I 103:

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

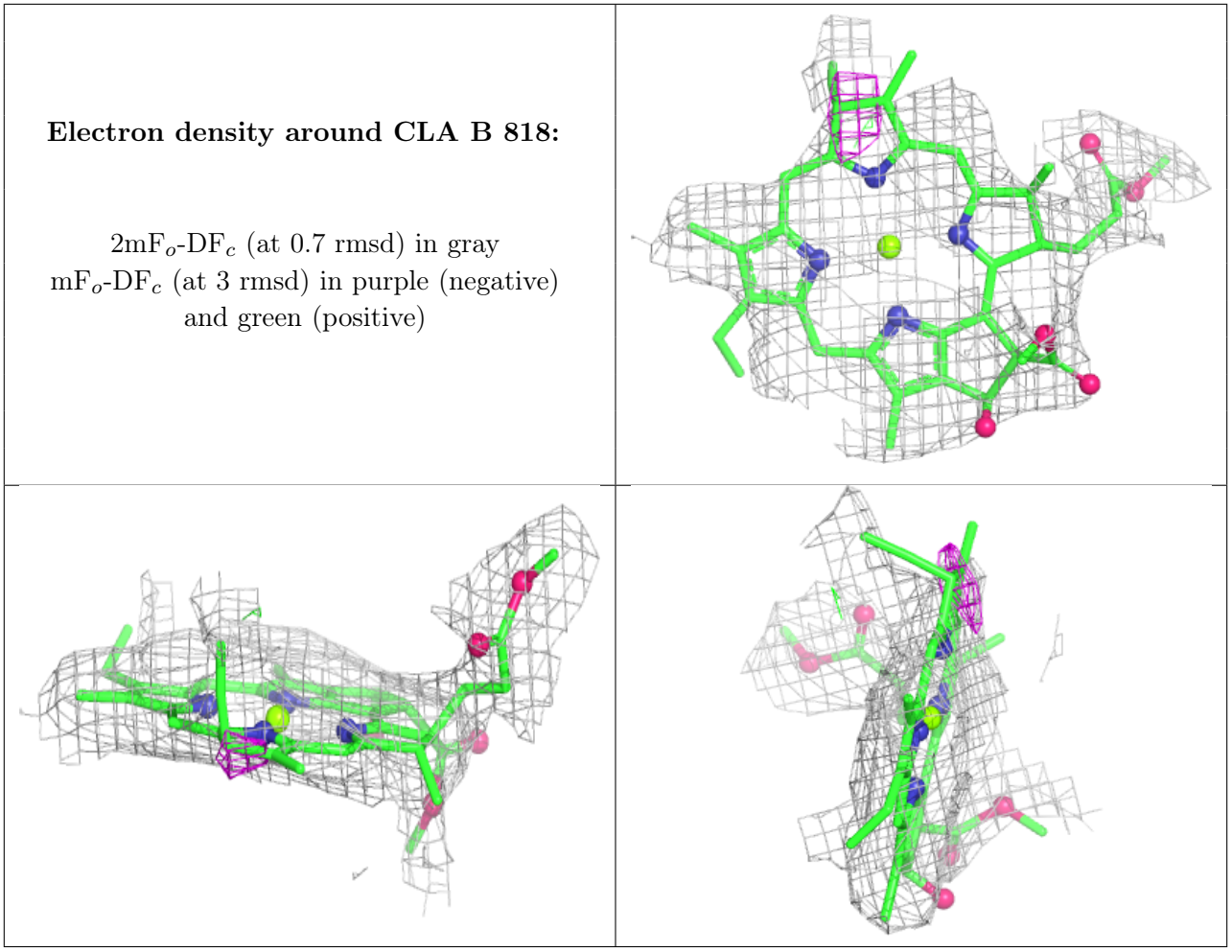






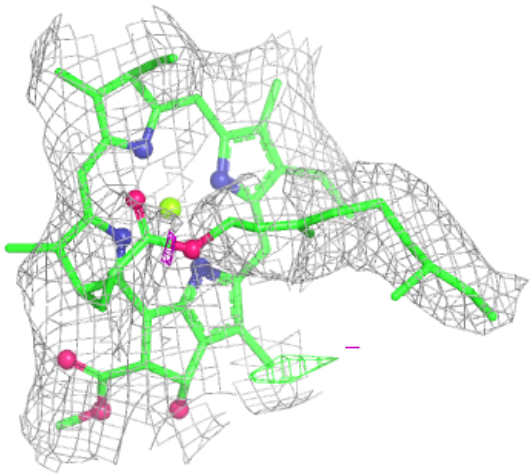
Electron density around CLA B 818:

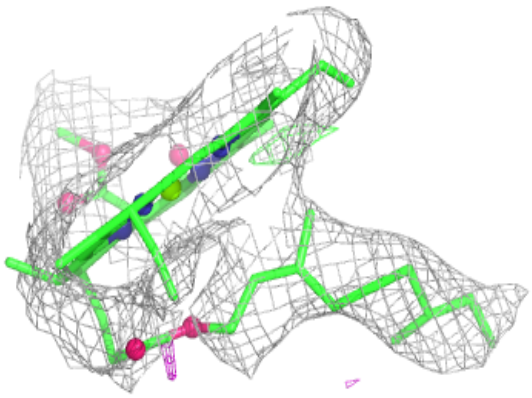
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

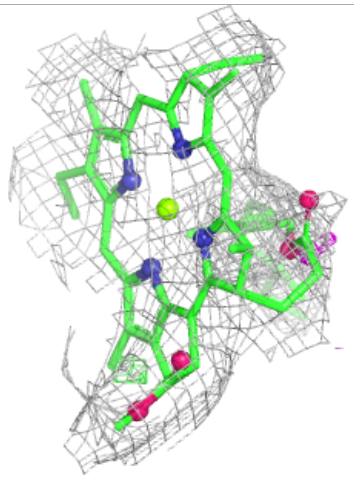


Electron density around CLA 2 302:

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

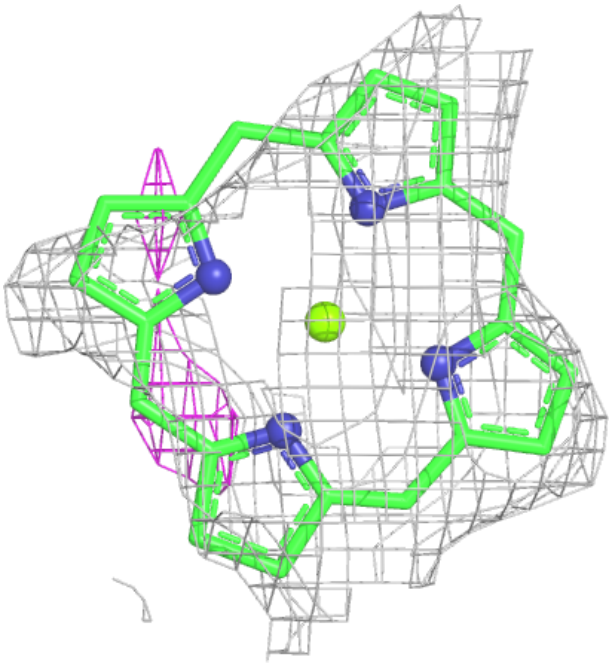


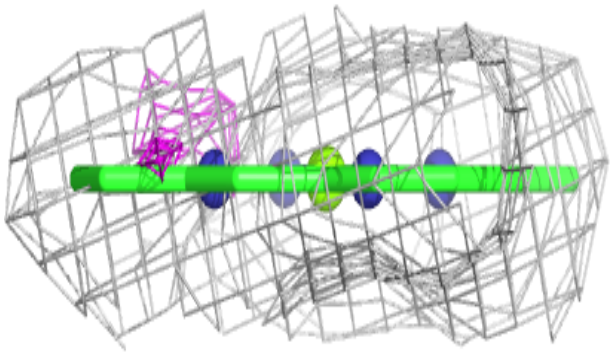


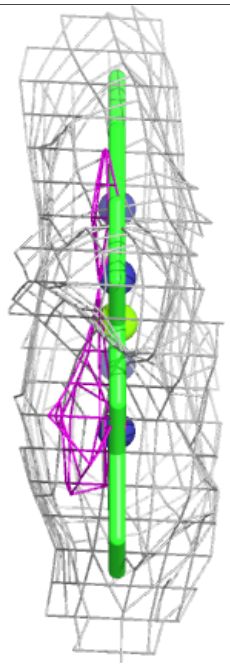


Electron density around CLA 2 314:

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

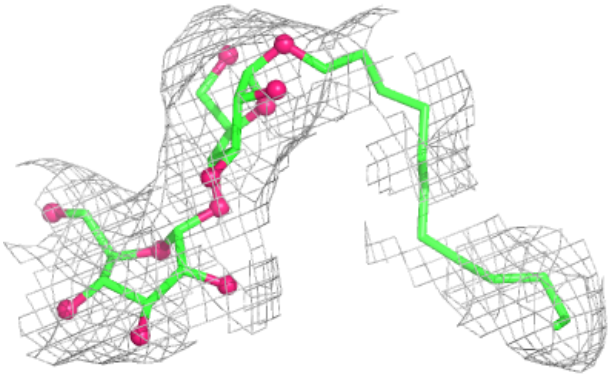


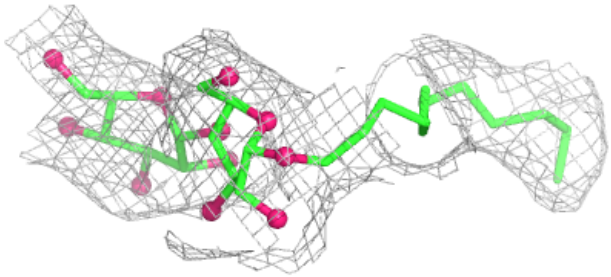


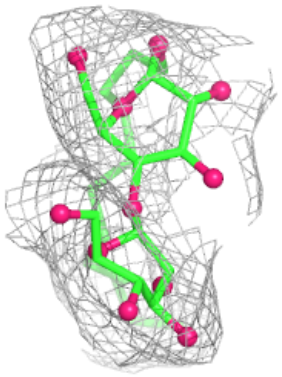


Electron density around LMU L 206:

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

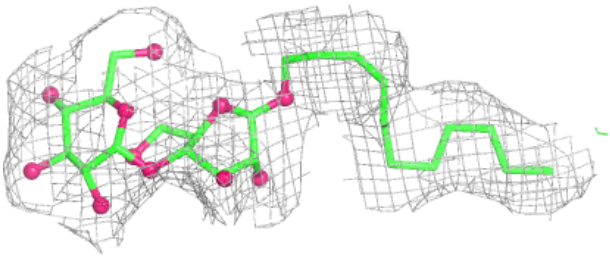


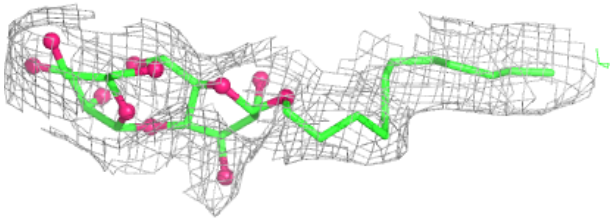


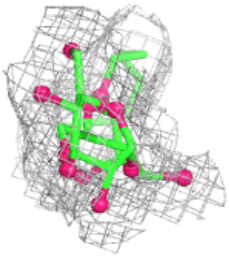


Electron density around LMU R 101:

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

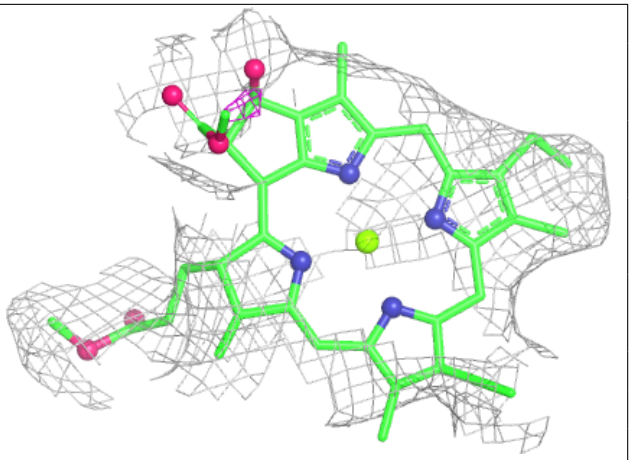


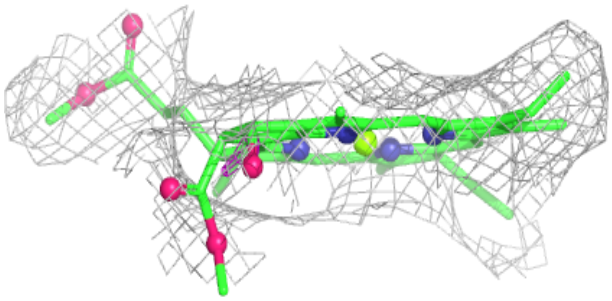




Electron density around CLA 1 201:

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

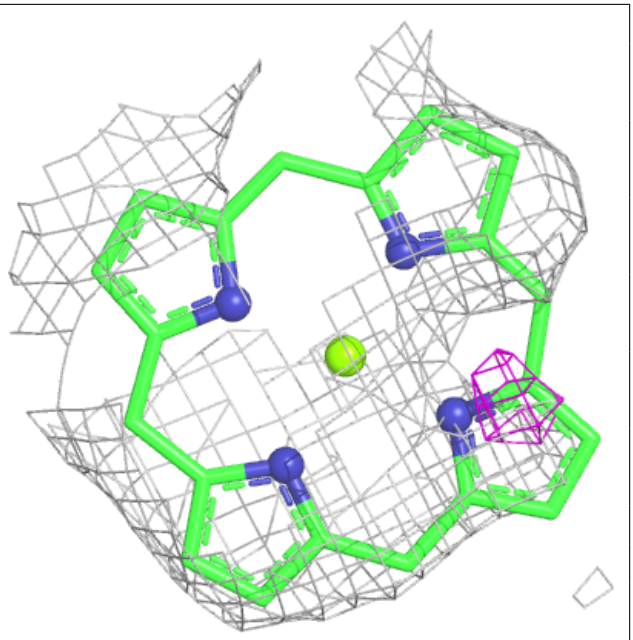


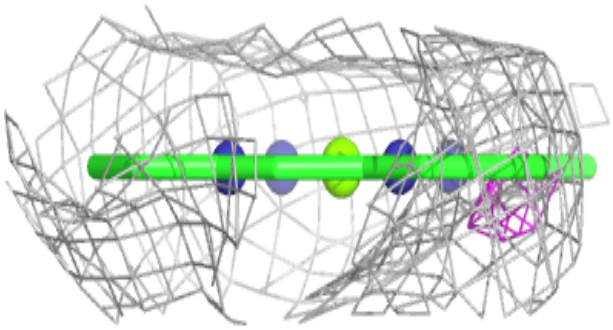


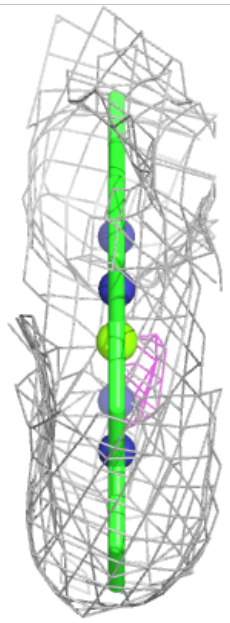


Electron density around CLA 3 306:

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

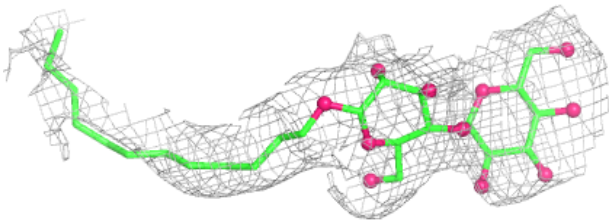


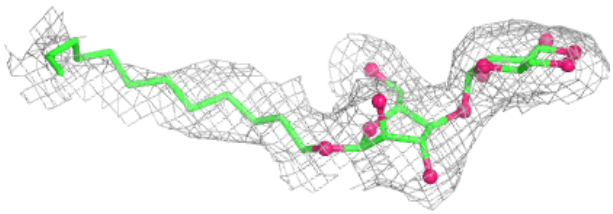


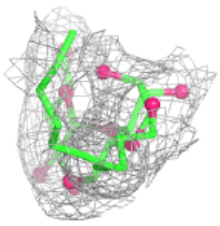


Electron density around LMU 2 320:

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



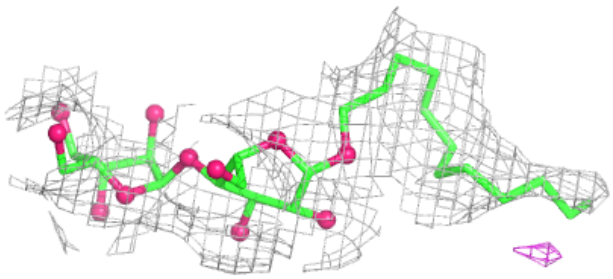


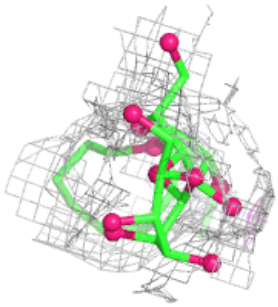


Electron density around LMU 3 318:

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

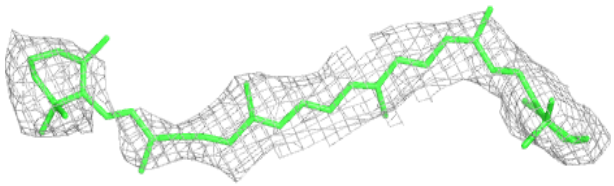


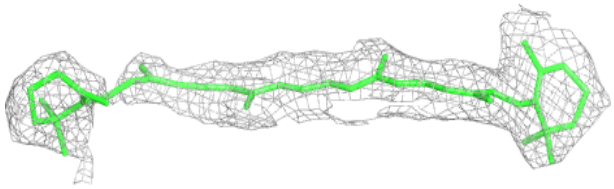


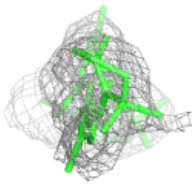


Electron density around BCR B 842:

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

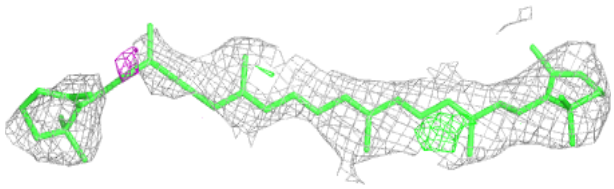


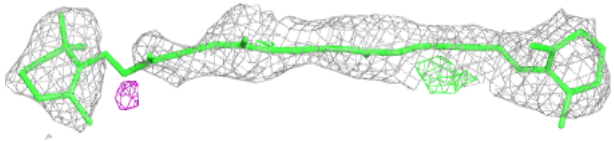


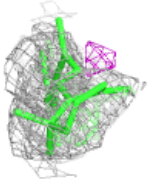


Electron density around BCR B 844:

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

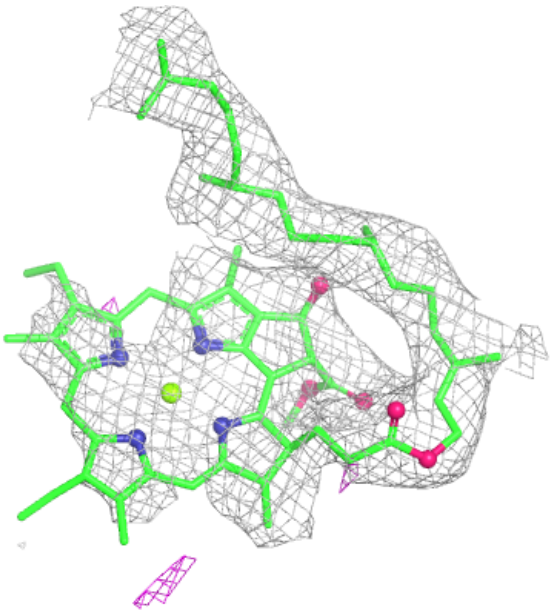


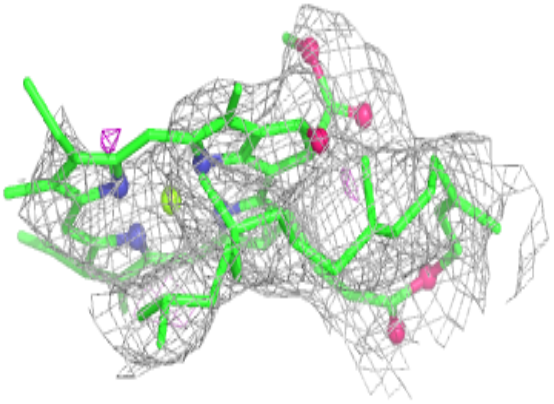


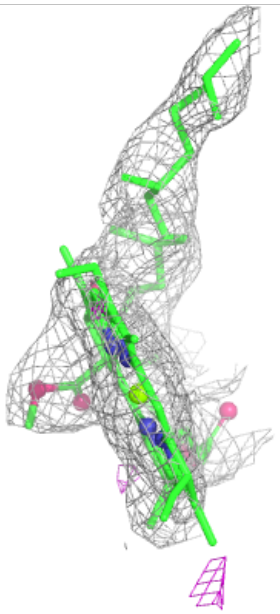


Electron density around CLA A 821:

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

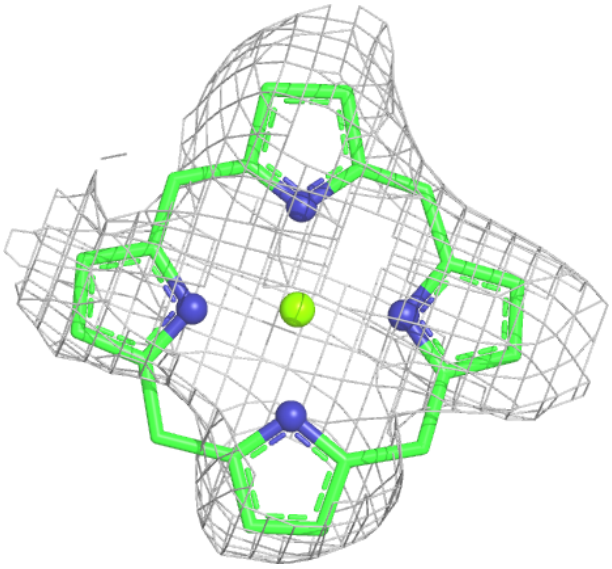


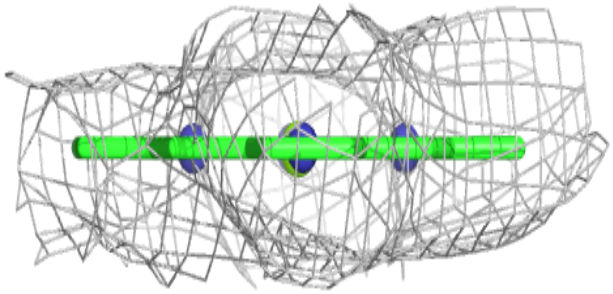


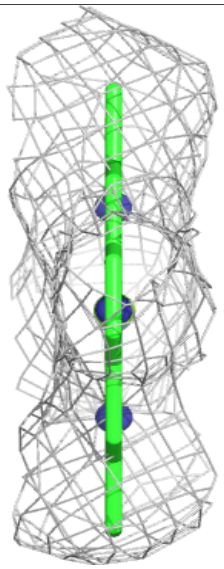


Electron density around CLA 3 313:

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



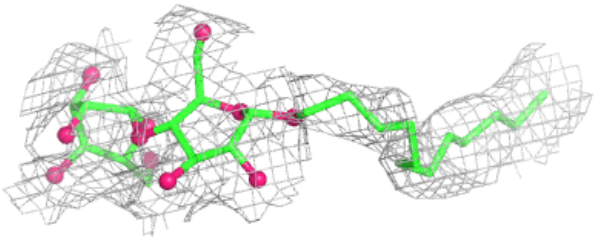




Electron density around LMU 4 301:

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

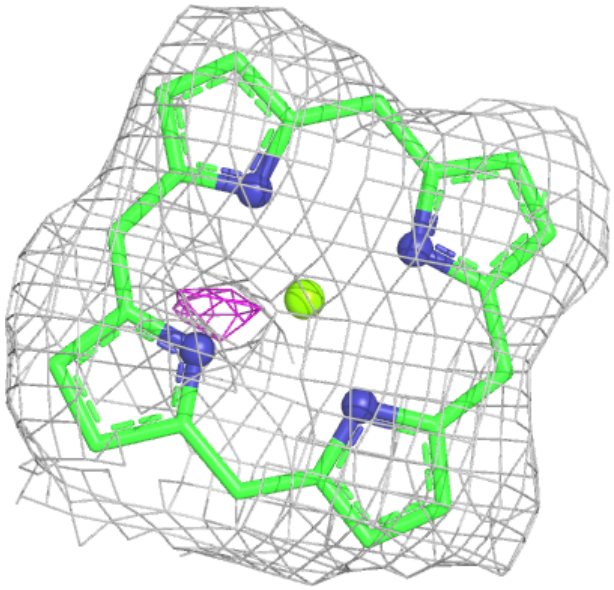


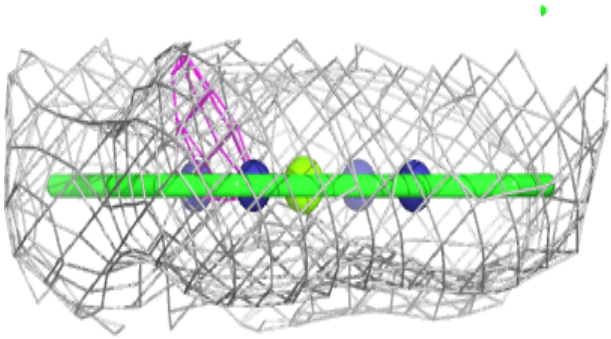


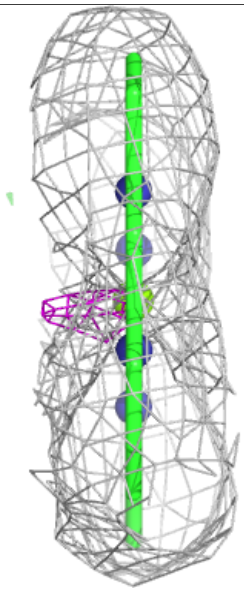


Electron density around CLA 4 314:

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

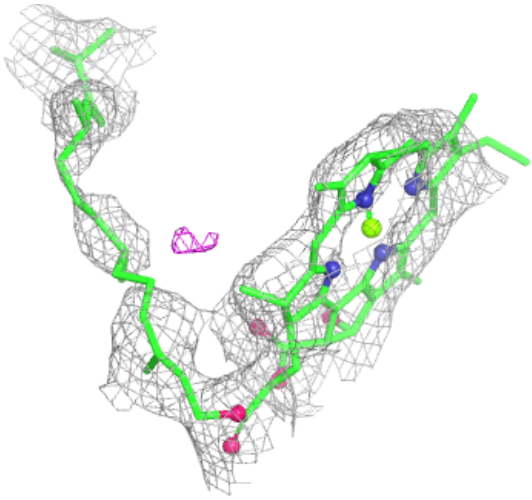


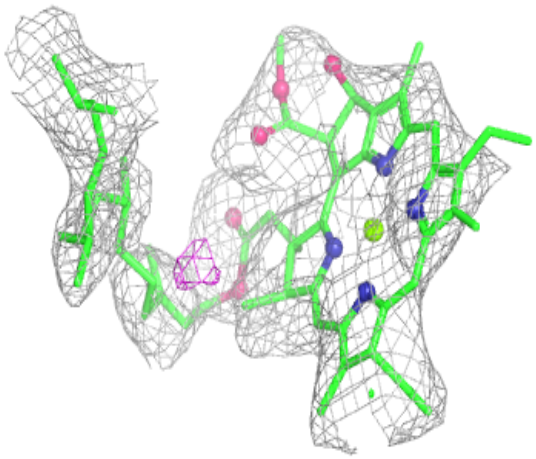


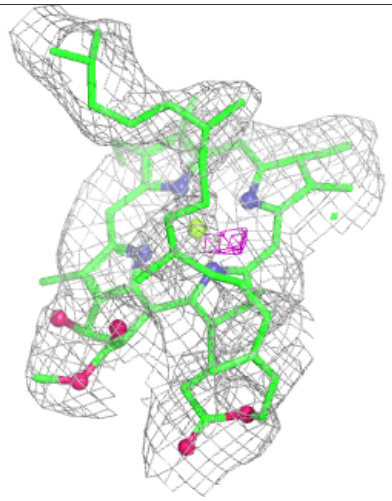


Electron density around CLA 2 306:

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

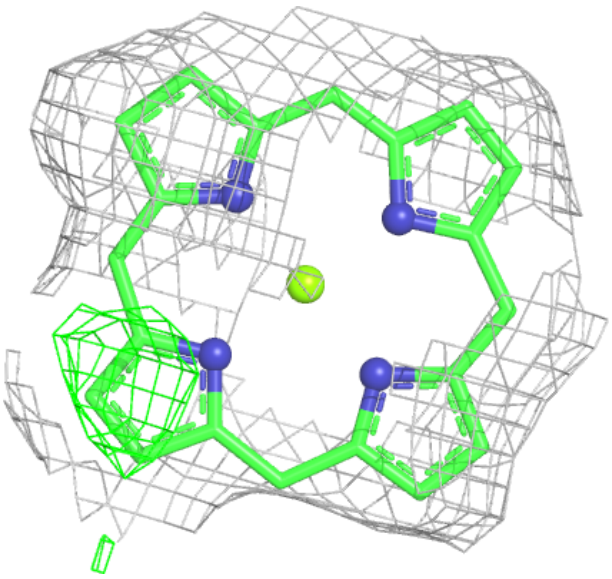


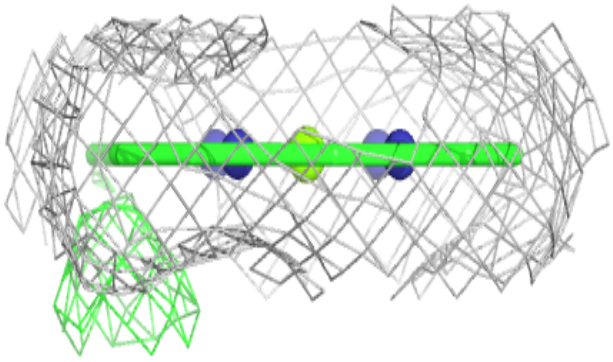


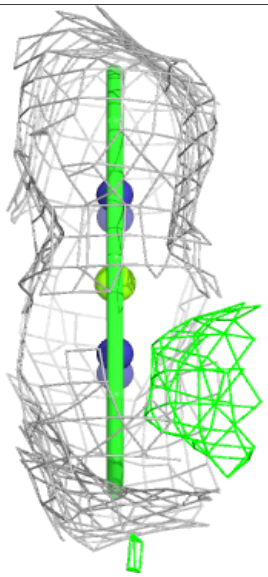


Electron density around CLA 1 208:

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

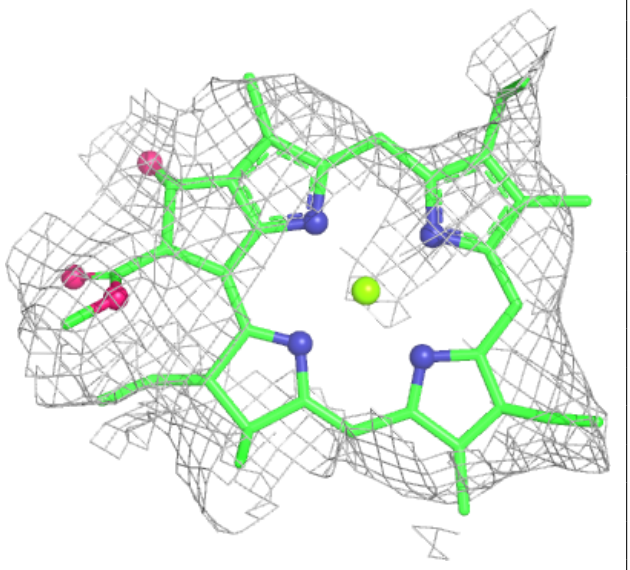


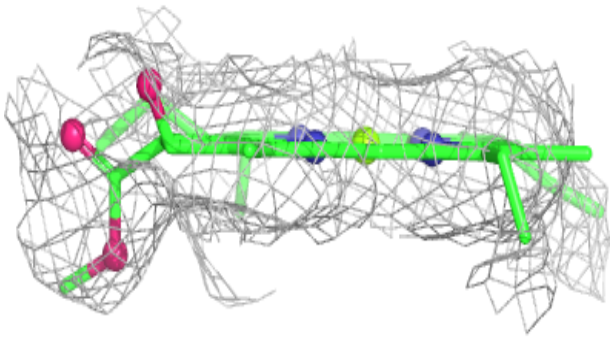


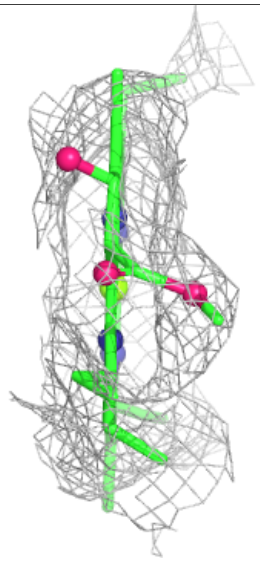


Electron density around CLA A 819:

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



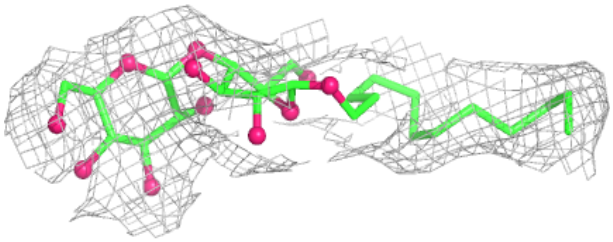


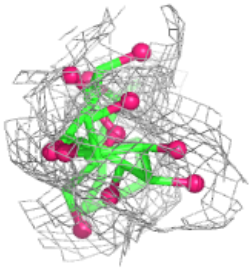


Electron density around LMU K 102:

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

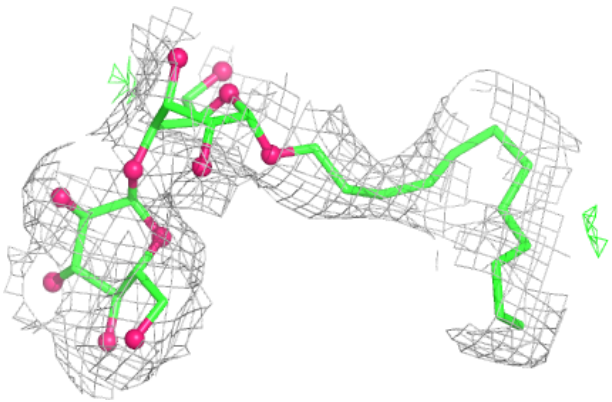


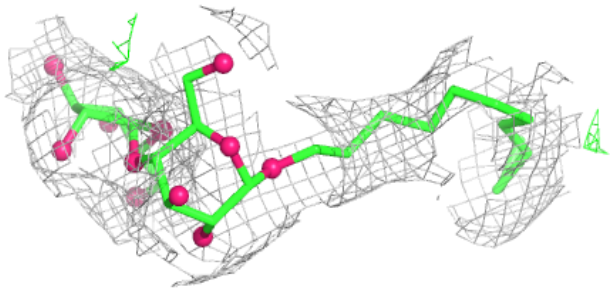


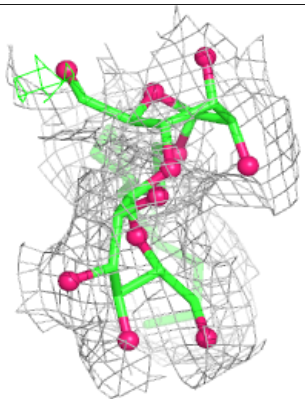


Electron density around LMU K 104:

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

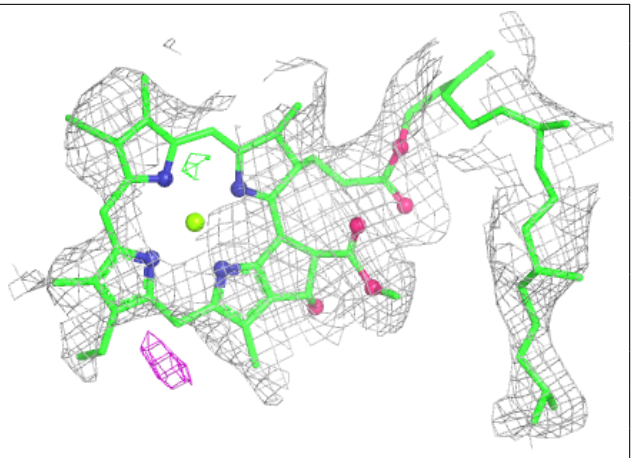


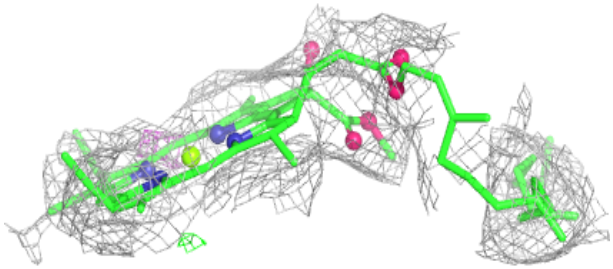


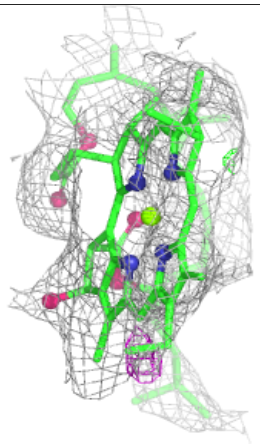


Electron density around CLA R 107:

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

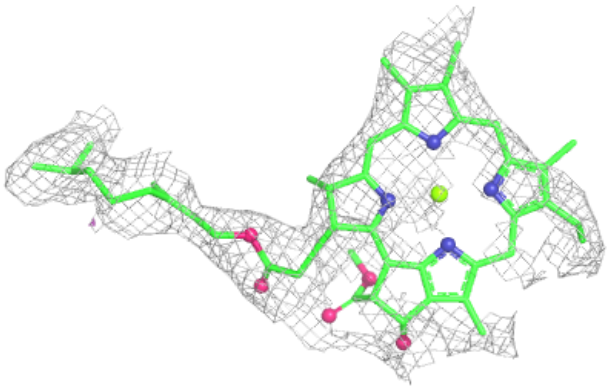


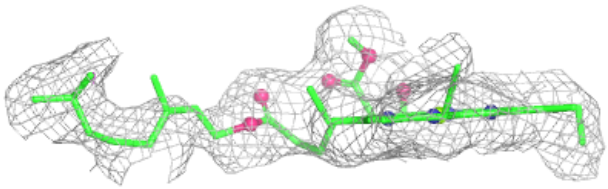


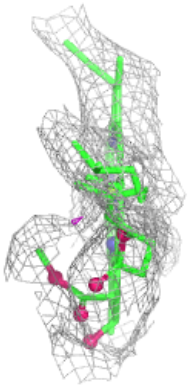


Electron density around CLA 4 310:

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

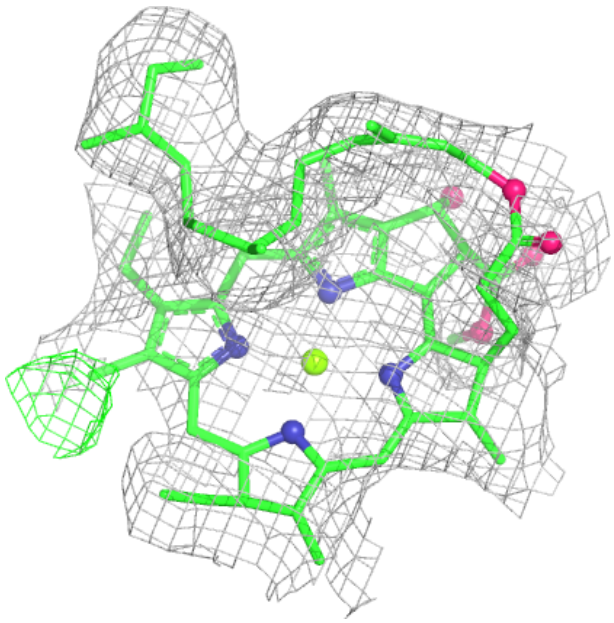


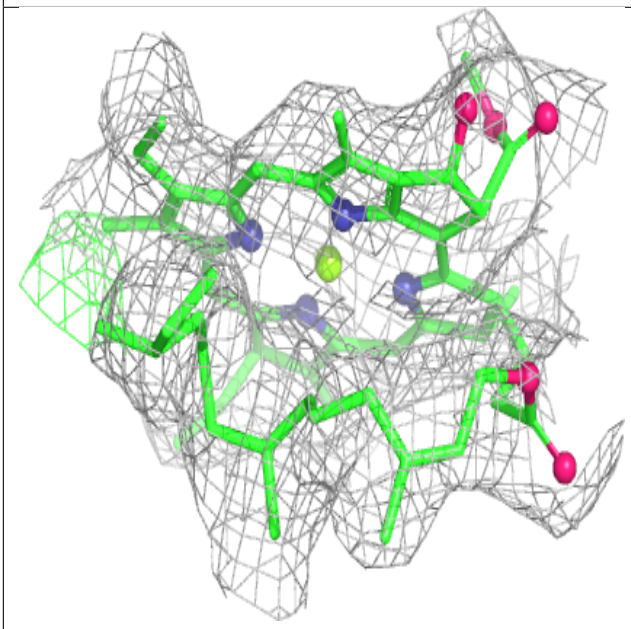


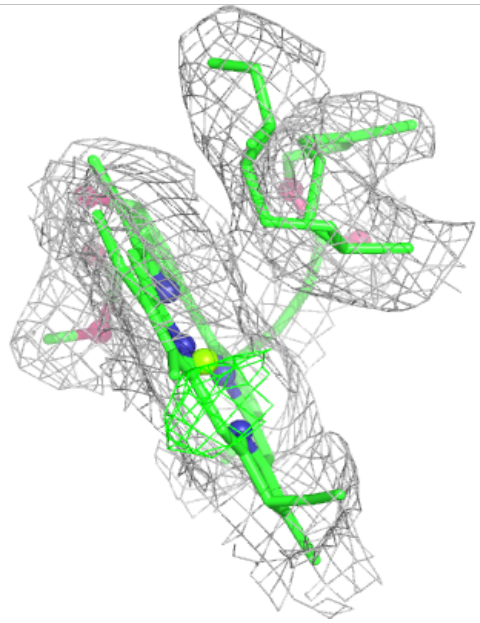


Electron density around CLA 1 206:

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

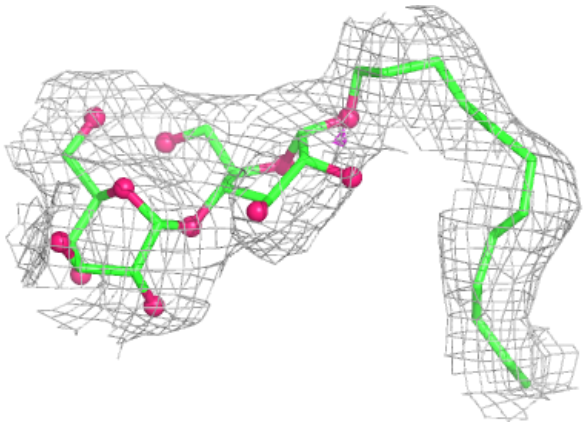


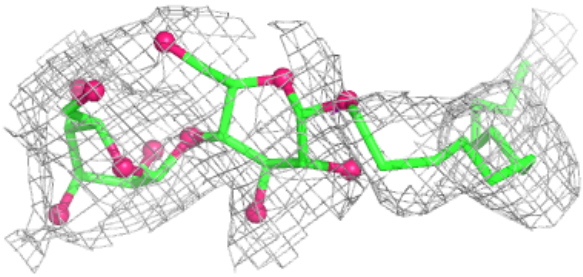


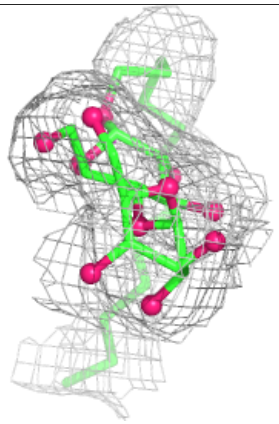


Electron density around LMU 3 302:

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

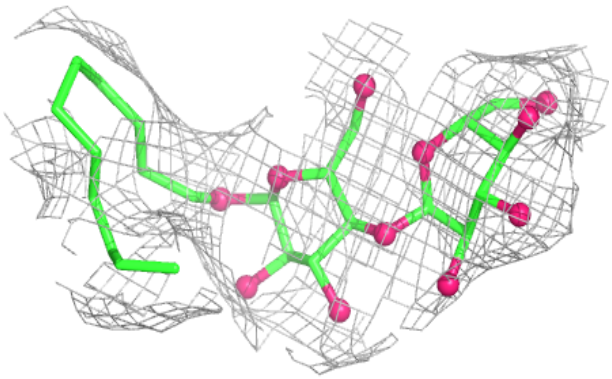


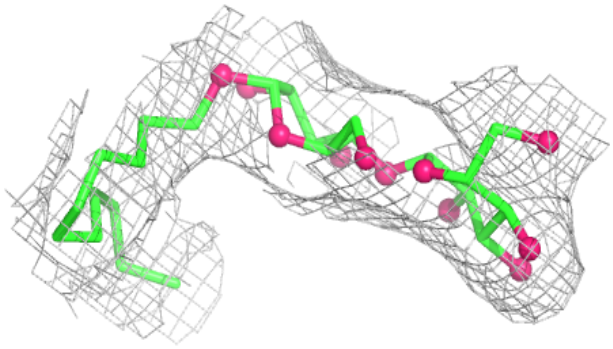


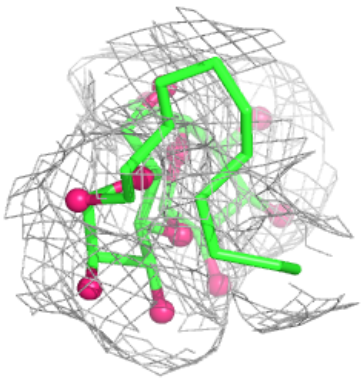


Electron density around LMU F 201:

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

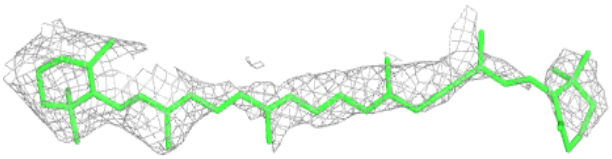


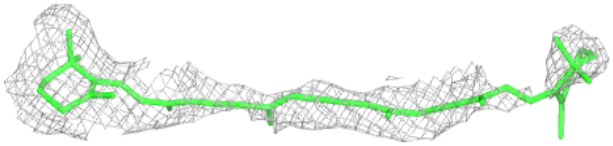


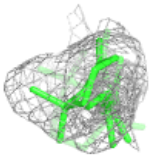


Electron density around BCR A 843:

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

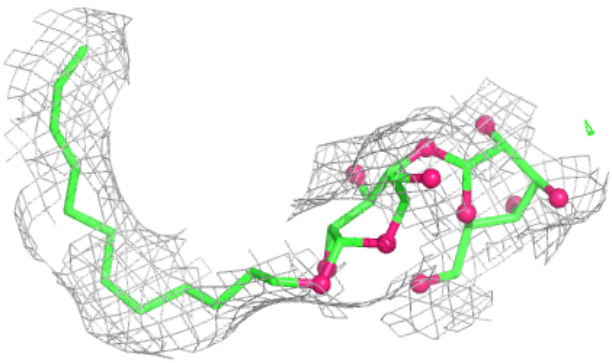


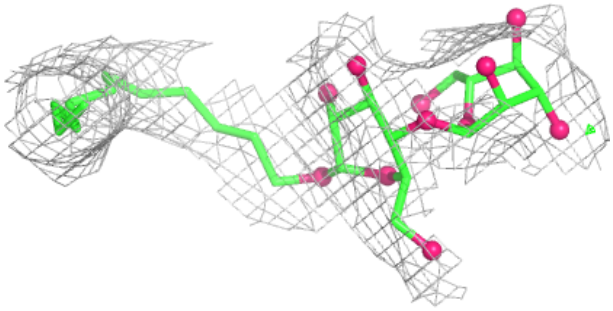


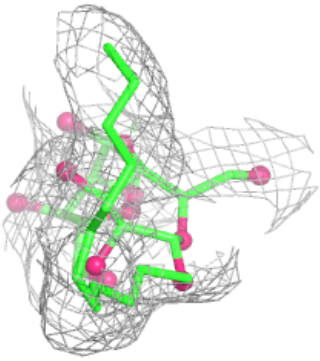


Electron density around LMU 2 316:

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

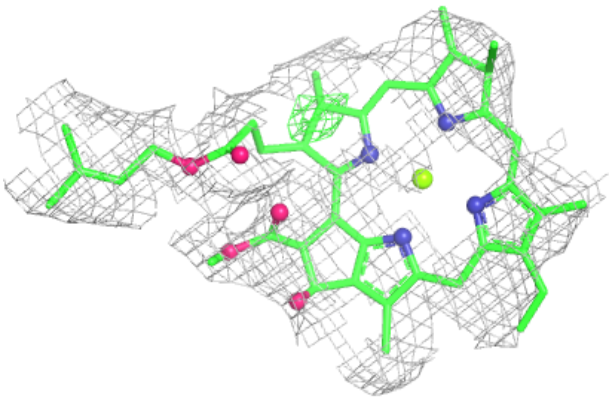


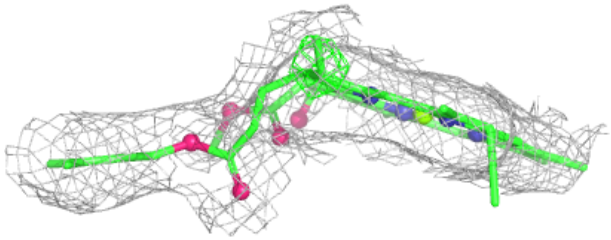


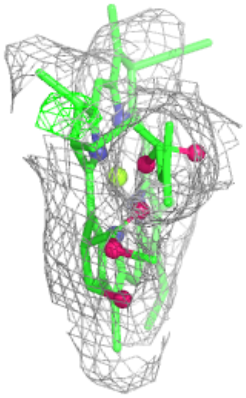


Electron density around CLA L 208:

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

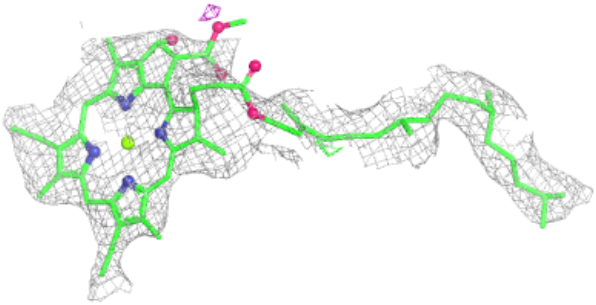


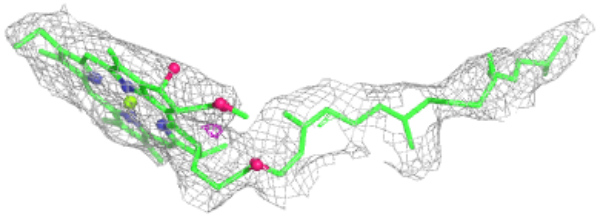


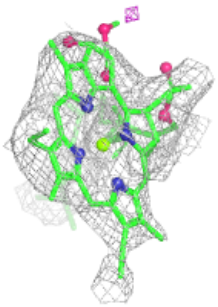


Electron density around CLA H 107:

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

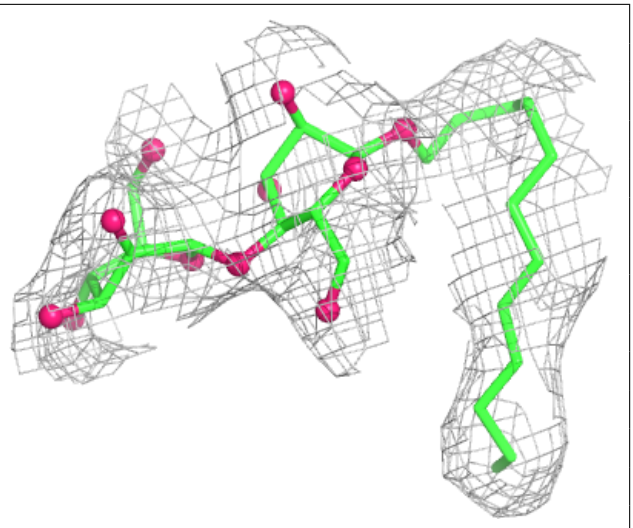


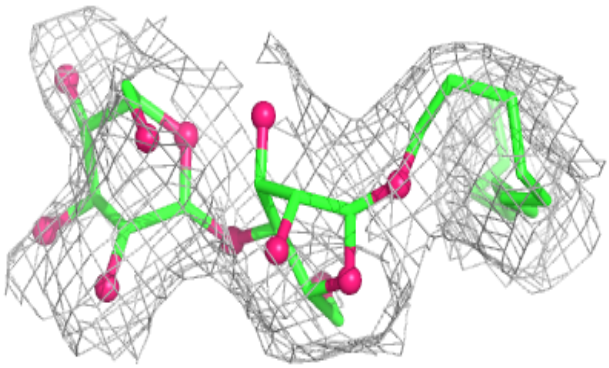


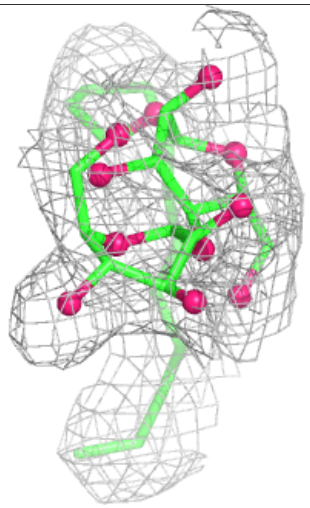


Electron density around LMU R 109:

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

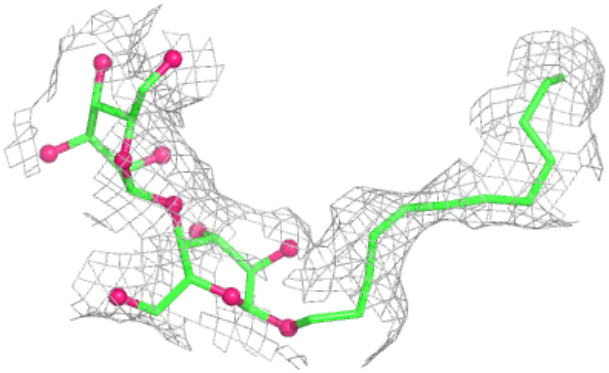


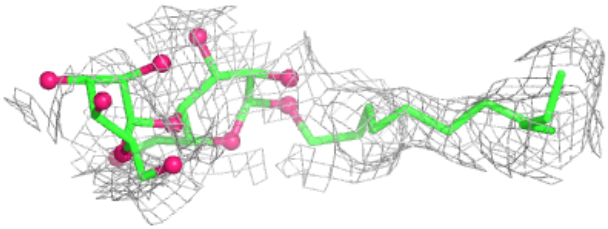


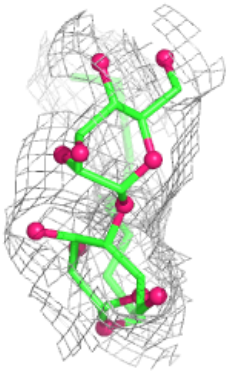


Electron density around LMU 4 321:

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

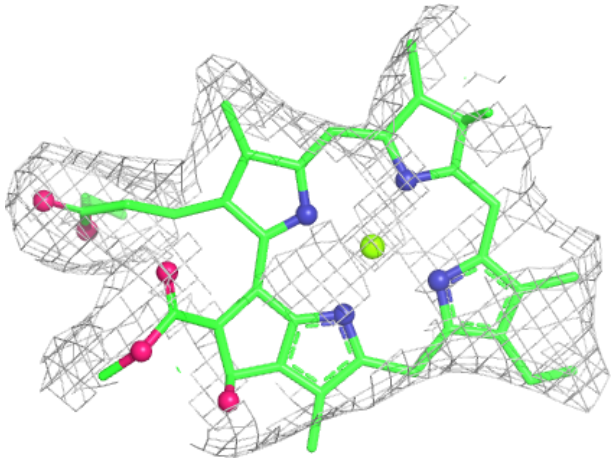


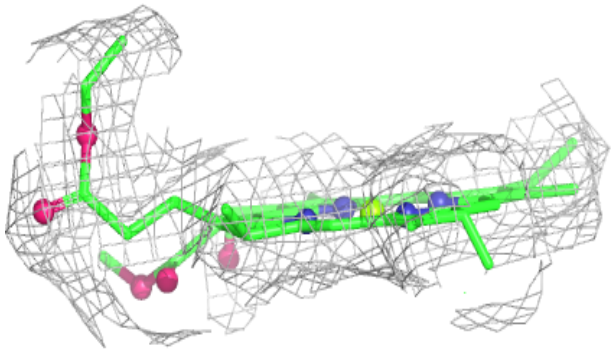




Electron density around CLA A 850:

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

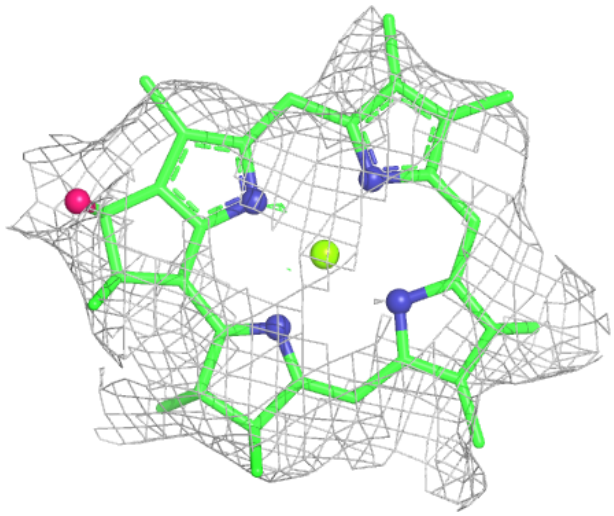


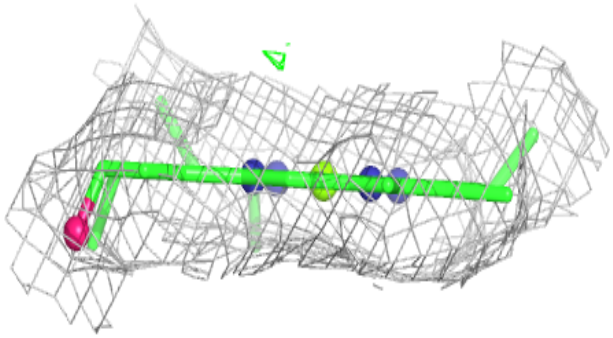


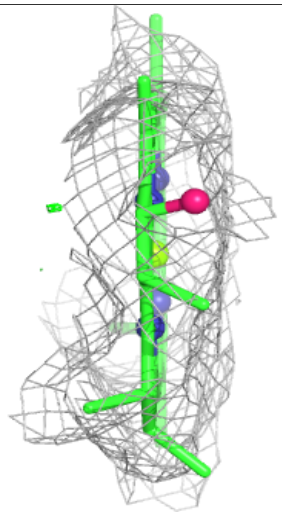


Electron density around CLA 3 303:

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

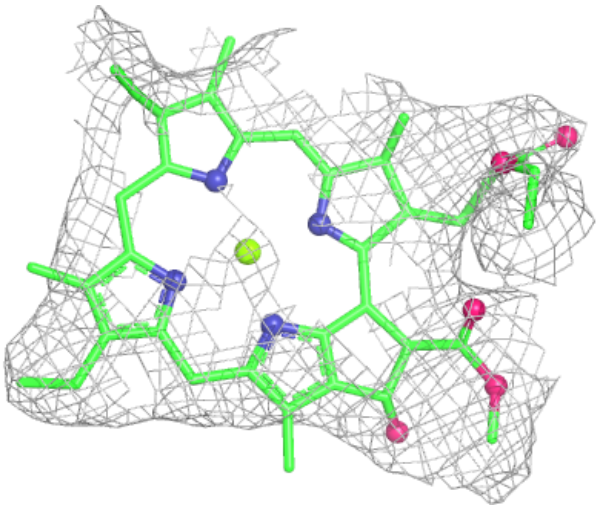


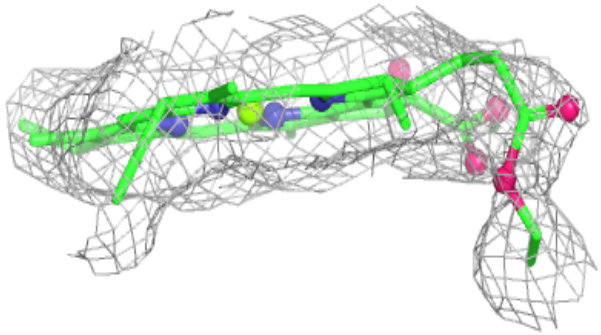


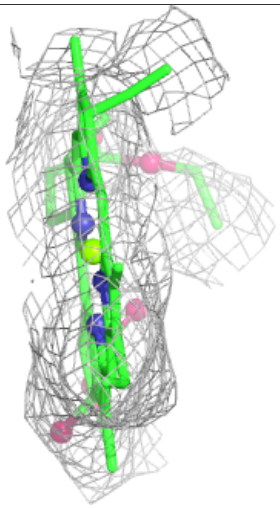


Electron density around CLA 1 202:

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

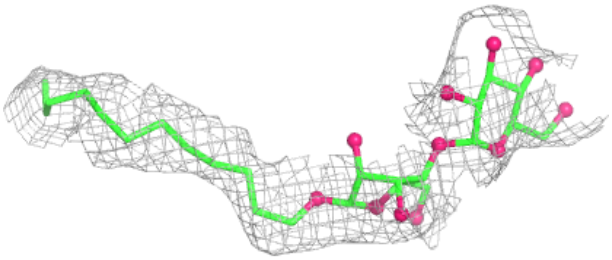


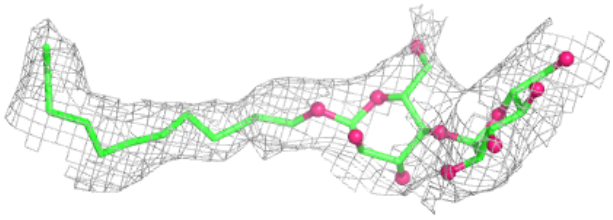


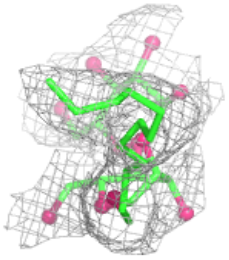


Electron density around LMU 4 316:

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

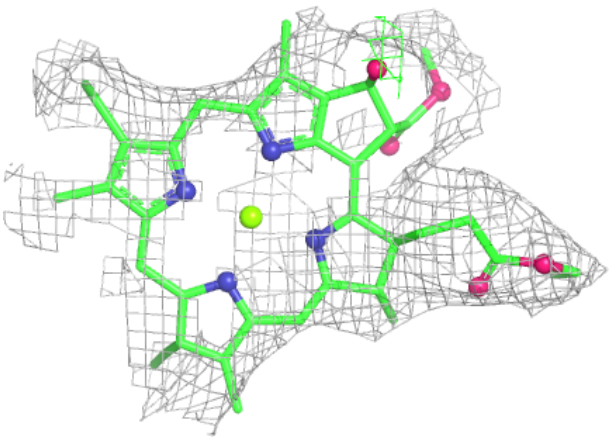


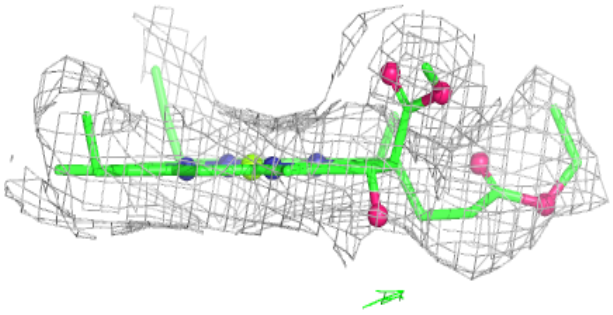


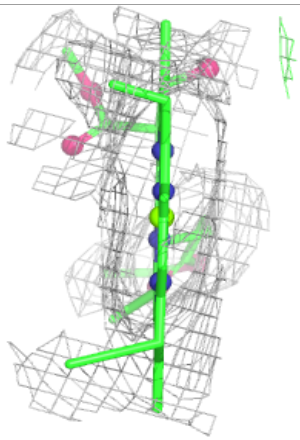


Electron density around CLA 1 203:

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

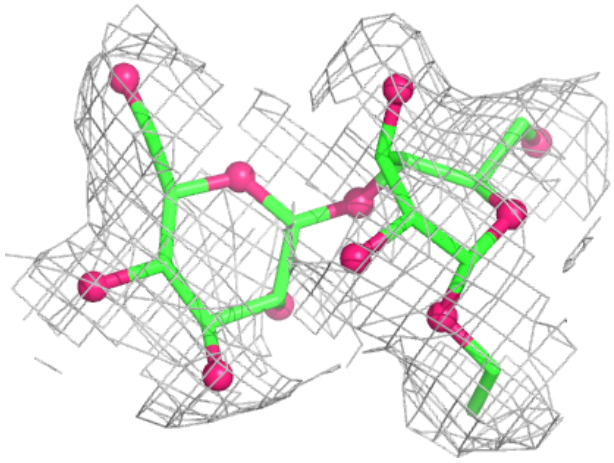


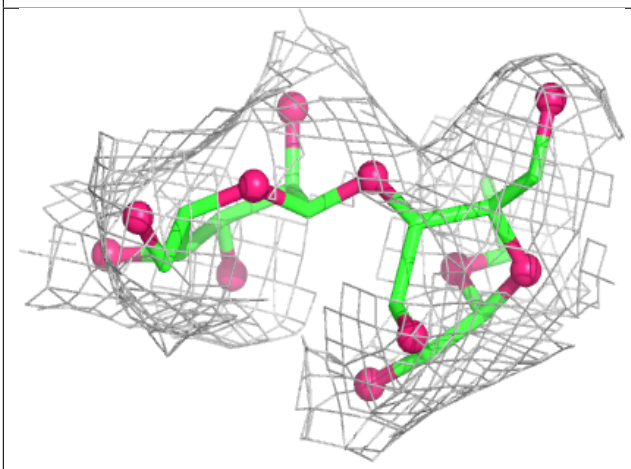


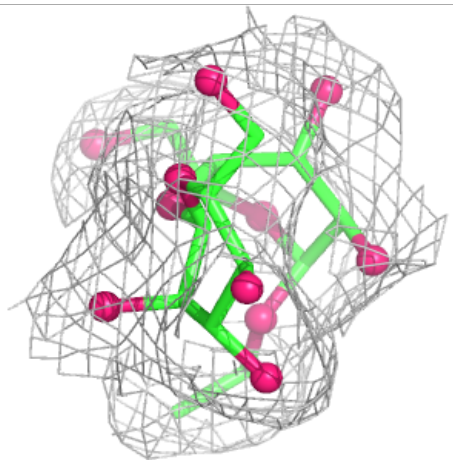


Electron density around LMU B 845:

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

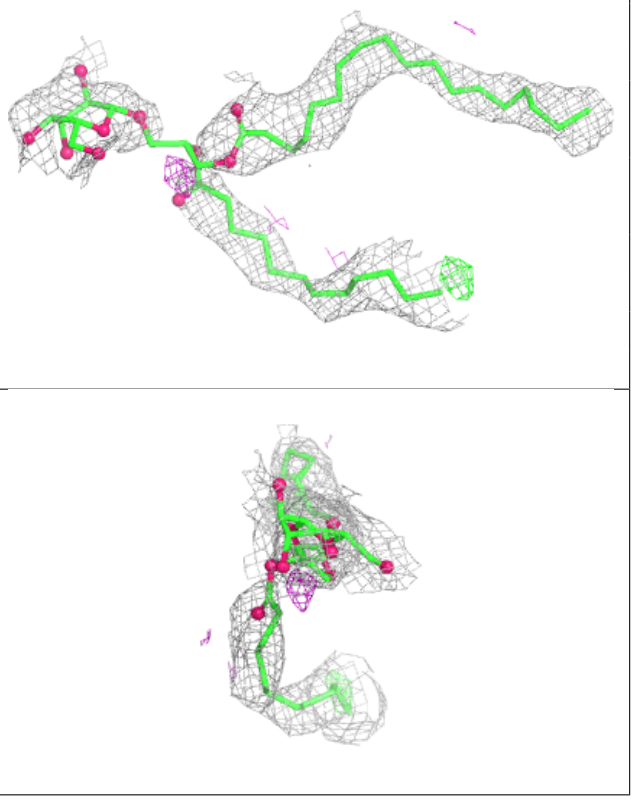


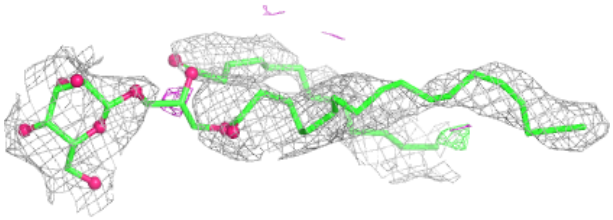




Electron density around LMG B 846:

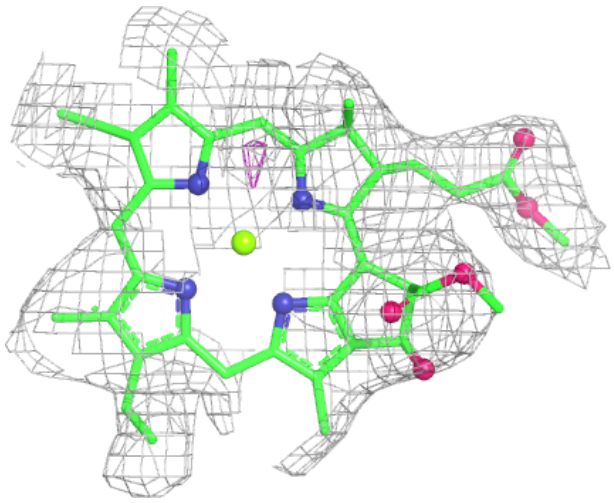
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

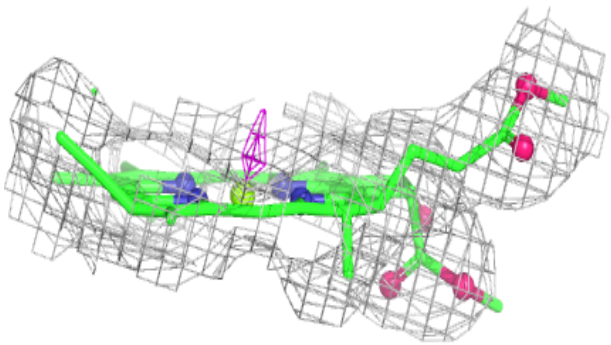


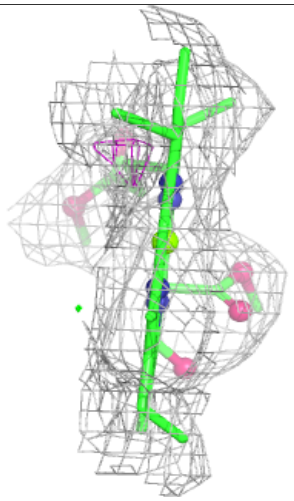


Electron density around CLA 4 315:

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

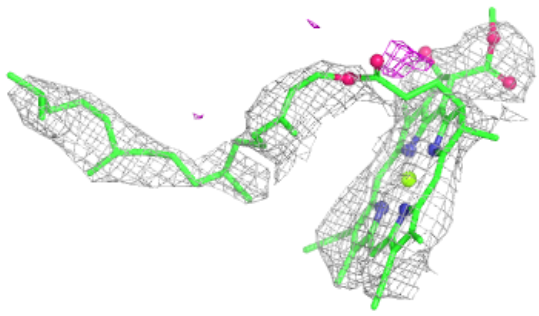


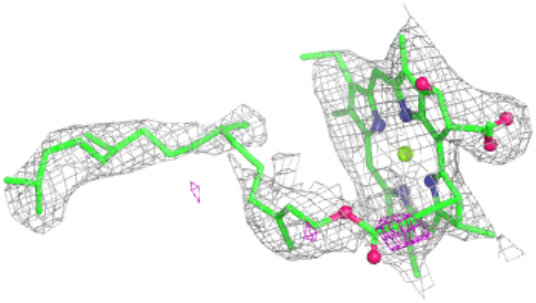


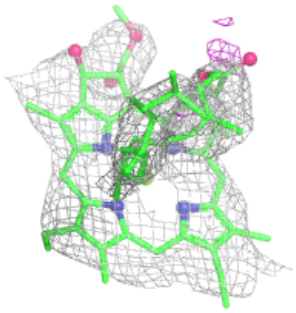


Electron density around CLA A 809:

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

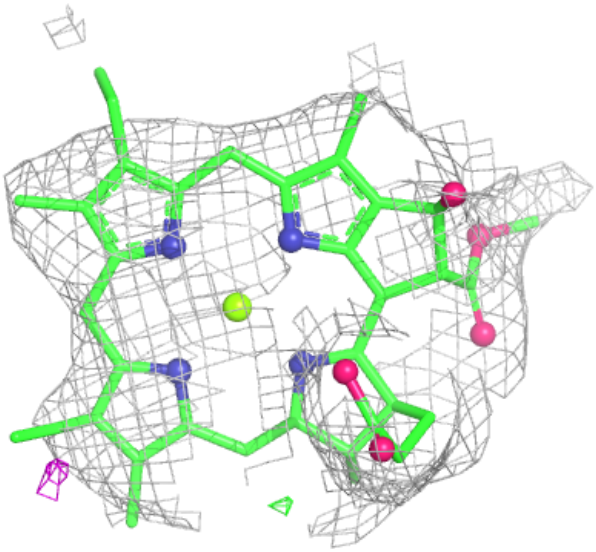


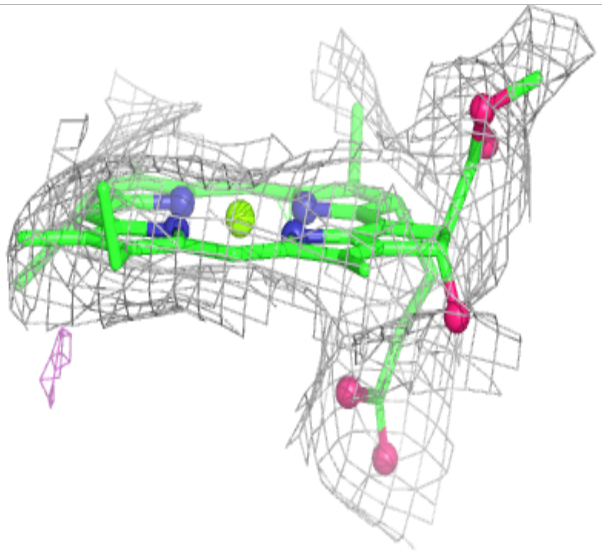


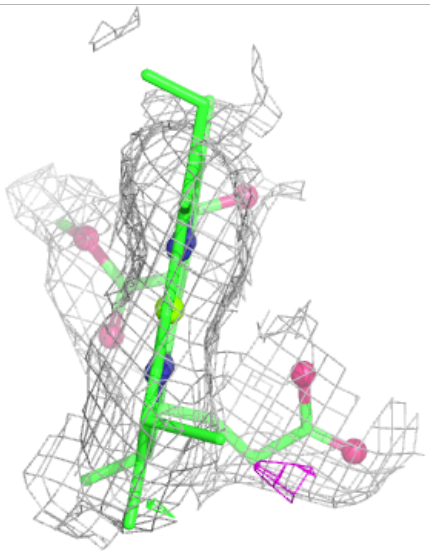


Electron density around CLA B 831:

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

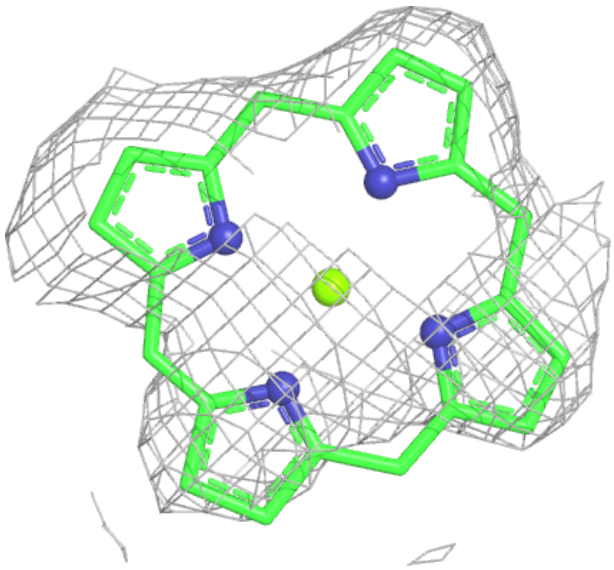


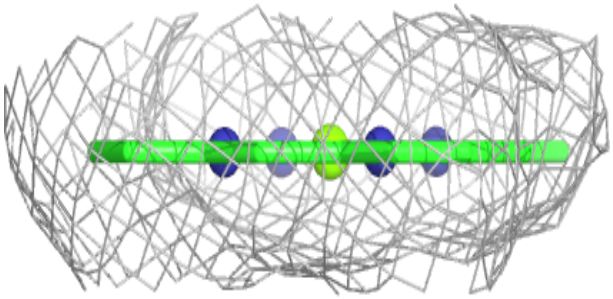


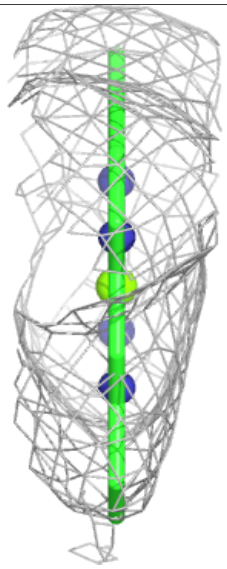


Electron density around CLA 4 308:

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

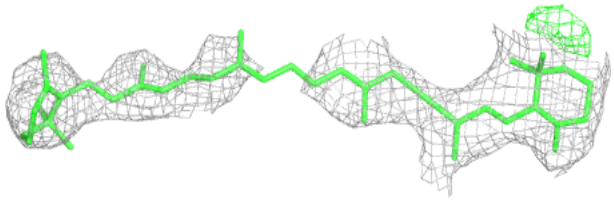


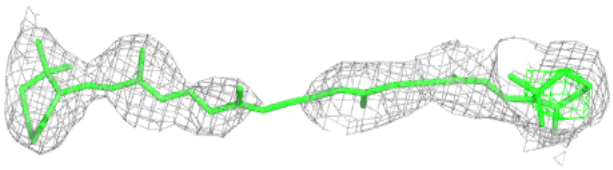




Electron density around BCR A 841:

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

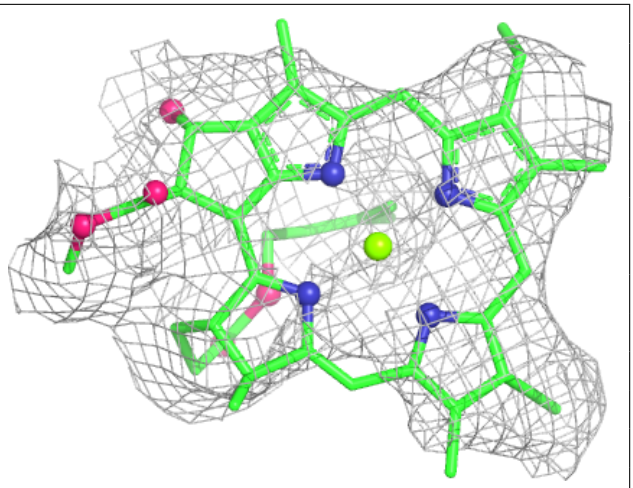


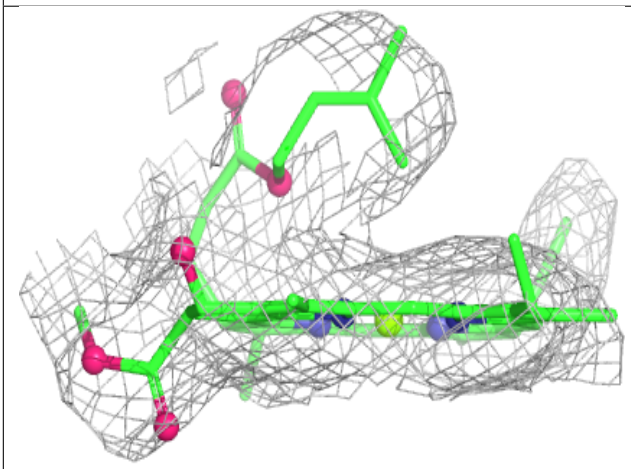


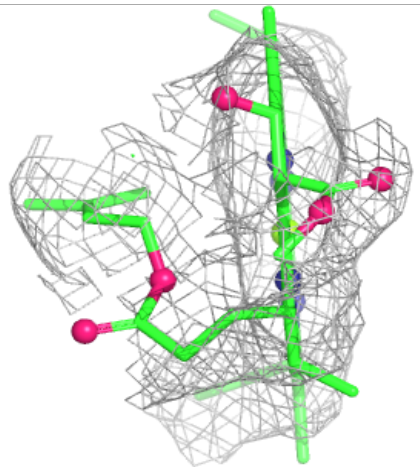


Electron density around CLA H 109:

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

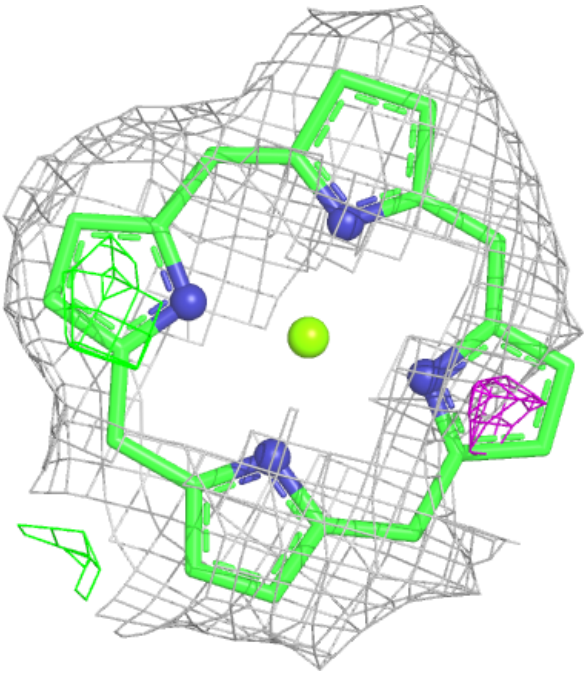


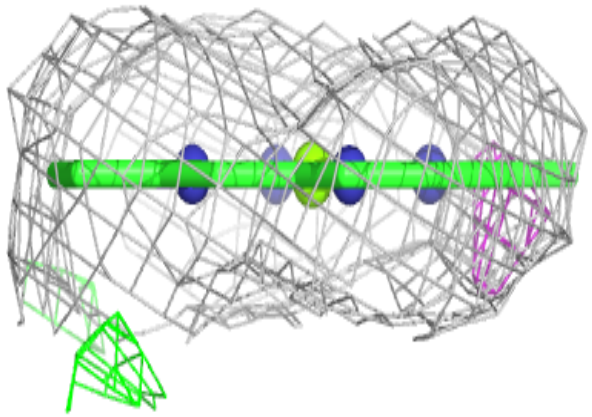


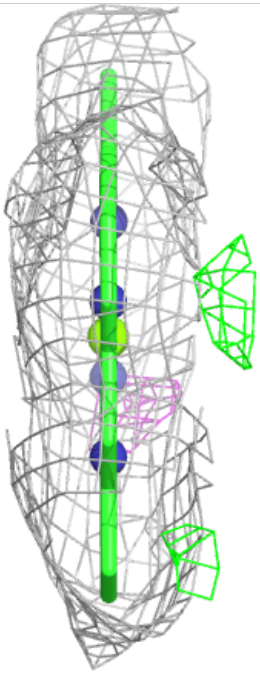


Electron density around CLA 4 309:

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

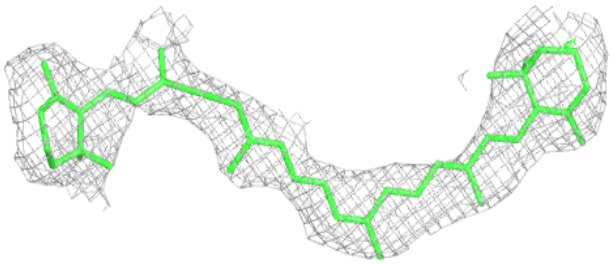


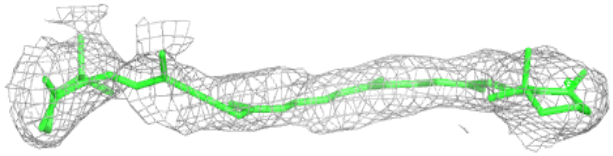


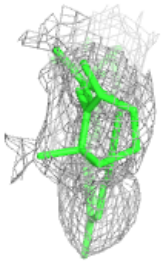


Electron density around BCR A 844:

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

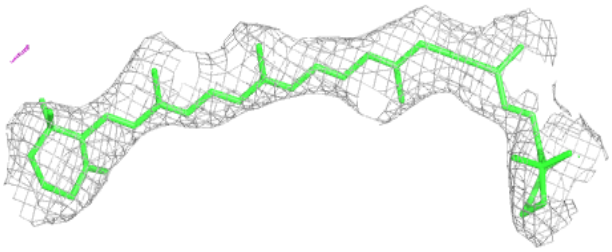


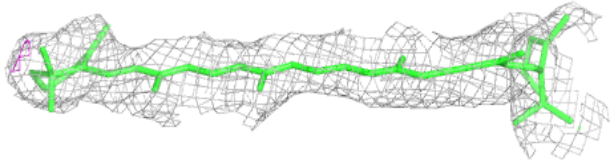


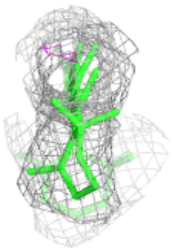


Electron density around BCR B 841:

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

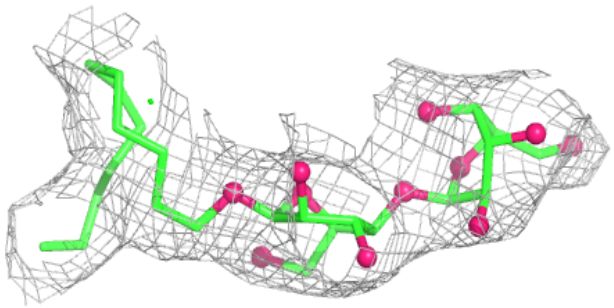


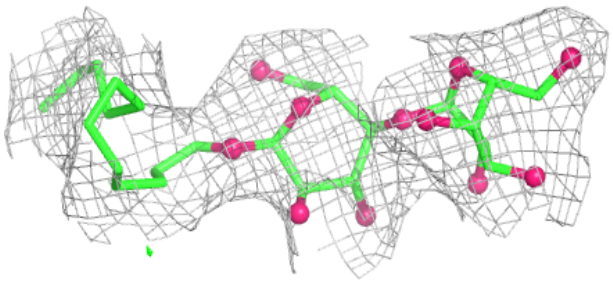


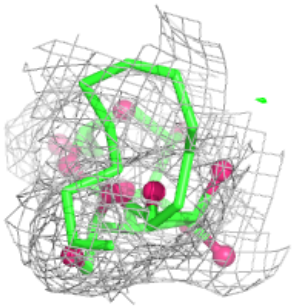


Electron density around LMU A 853:

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

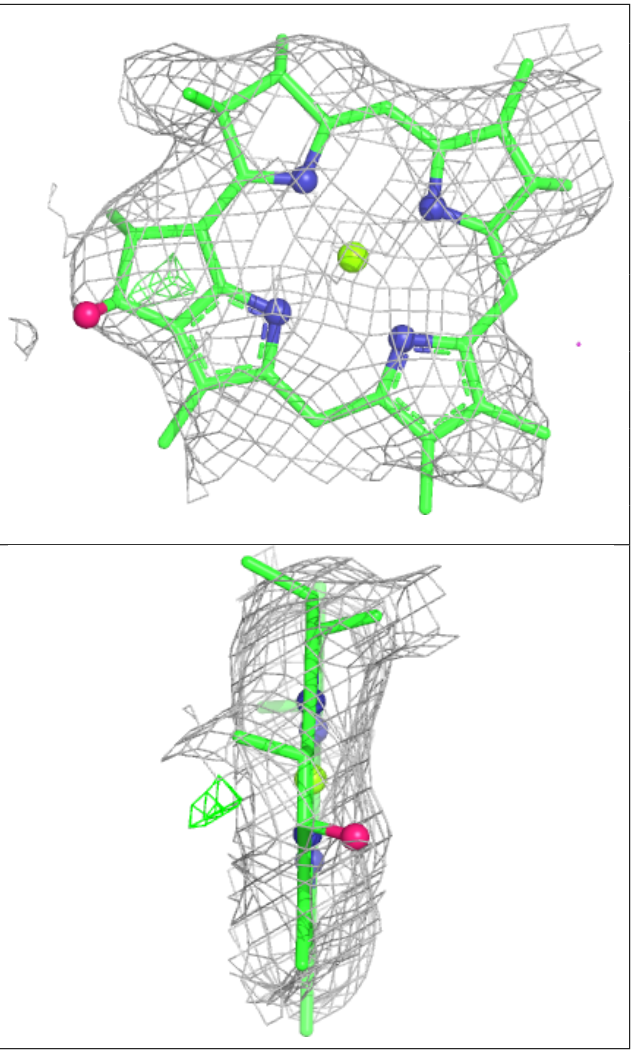






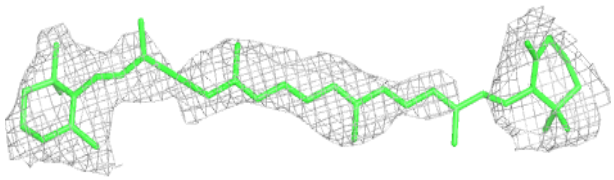
Electron density around CLA B 839:

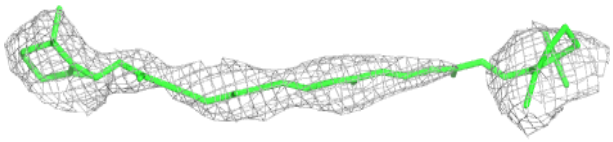
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

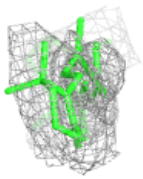


Electron density around BCR G 102:

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

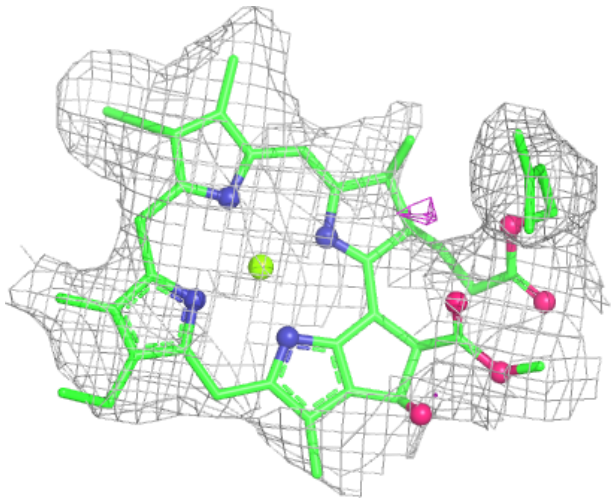


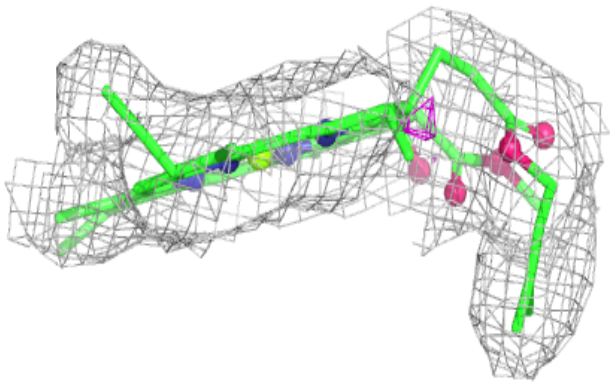




Electron density around CLA 3 315:

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

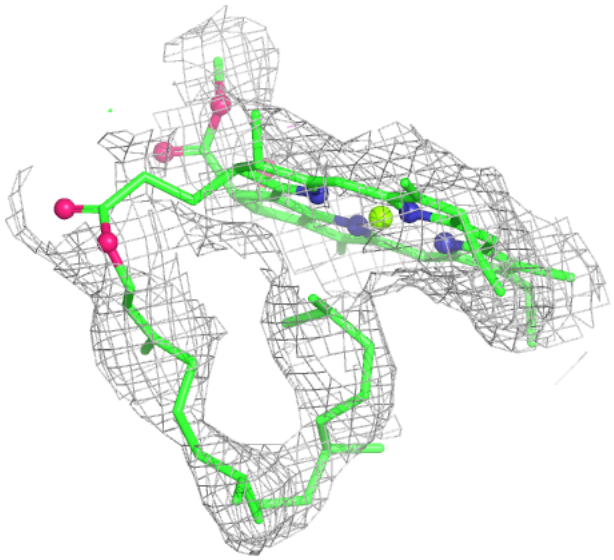


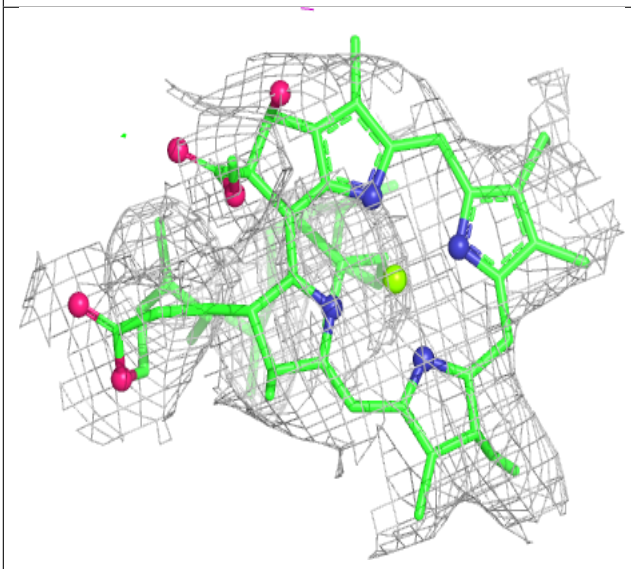


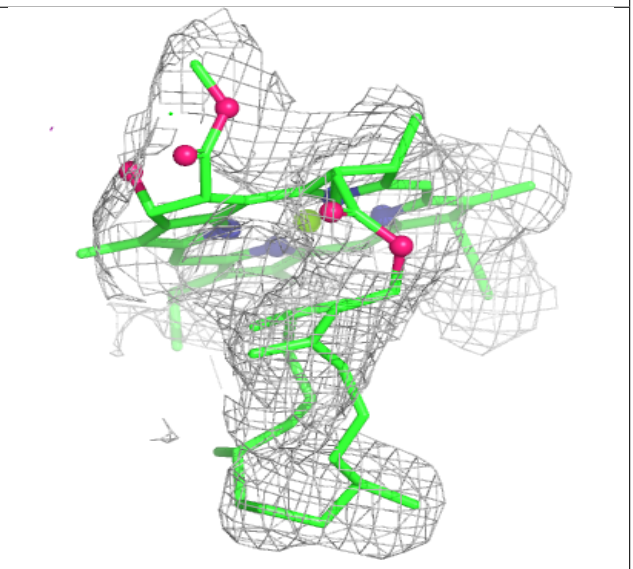


Electron density around CLA 2 312:

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

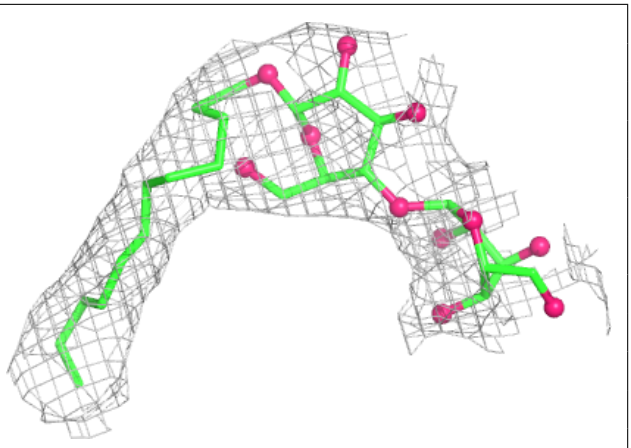


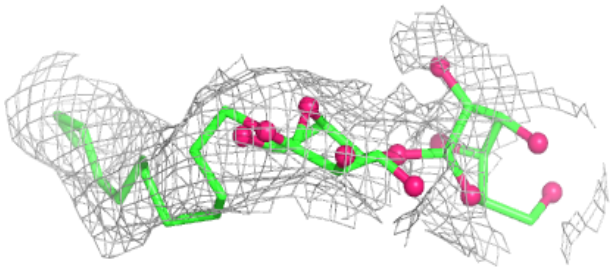


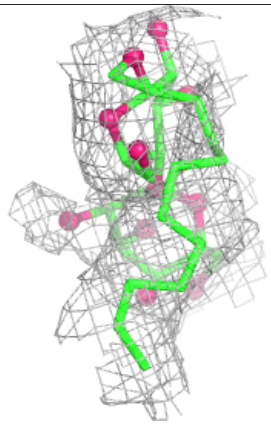


Electron density around LMU R 102:

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

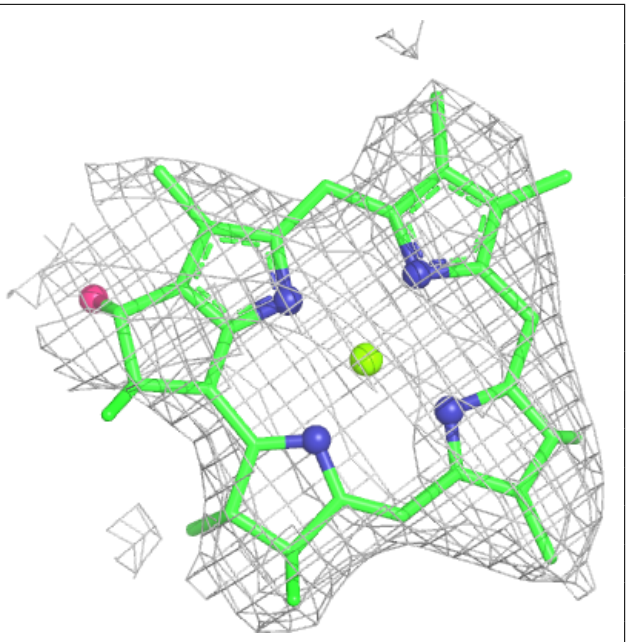


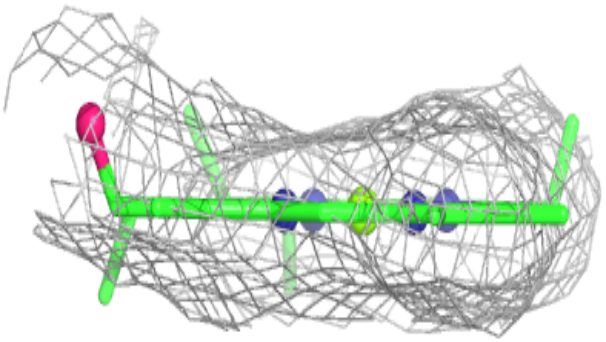


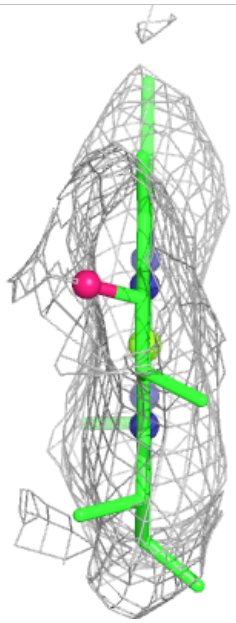


Electron density around CLA 1 209:

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

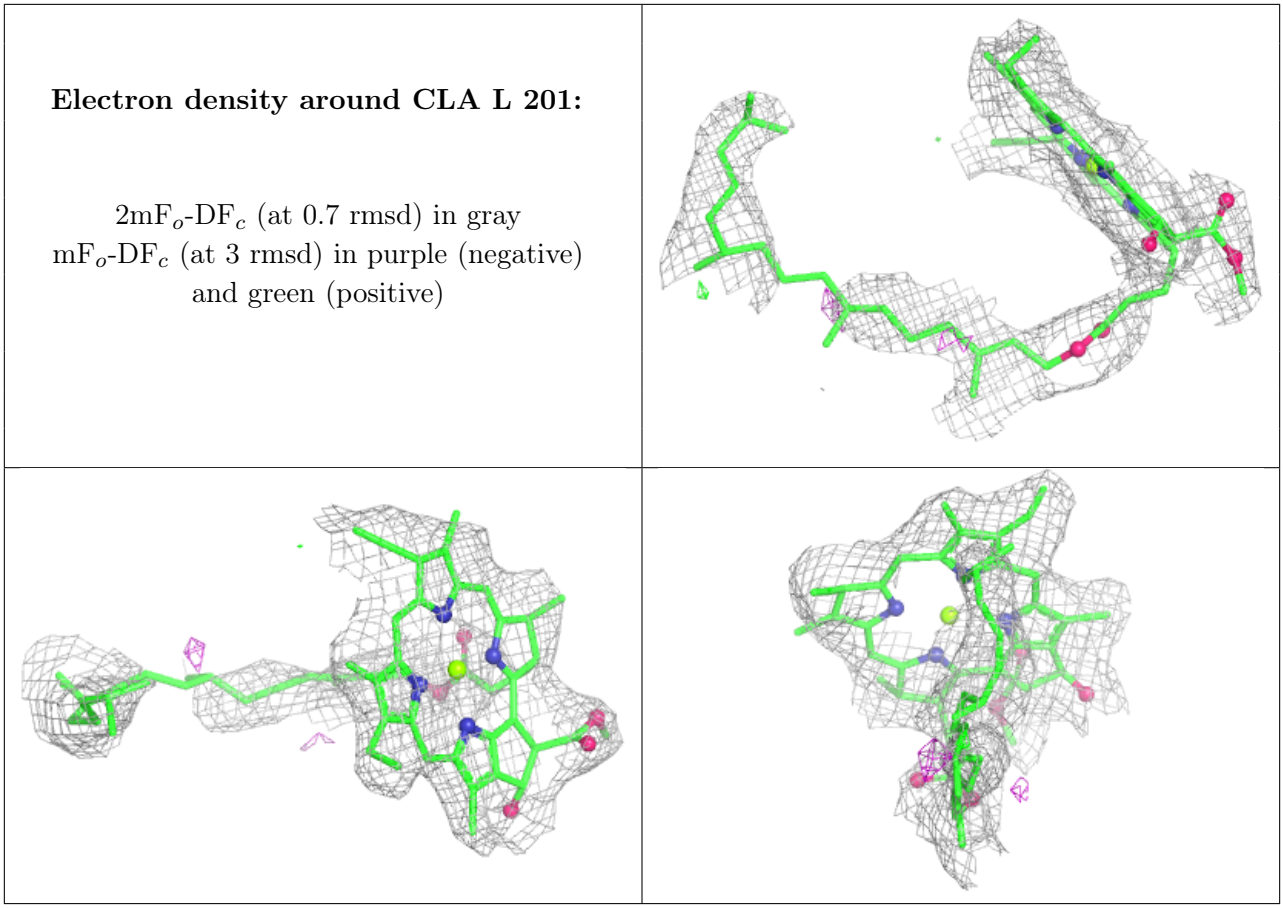






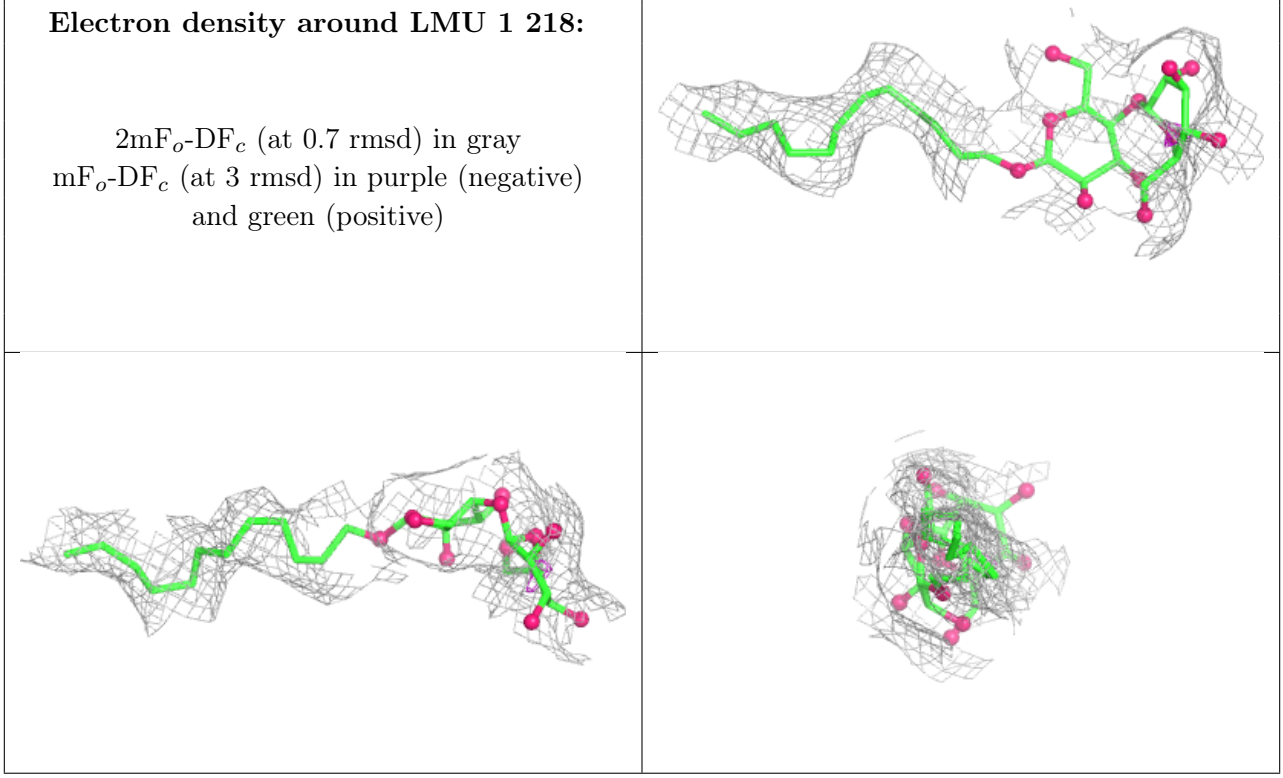
Electron density around CLA L 201:

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



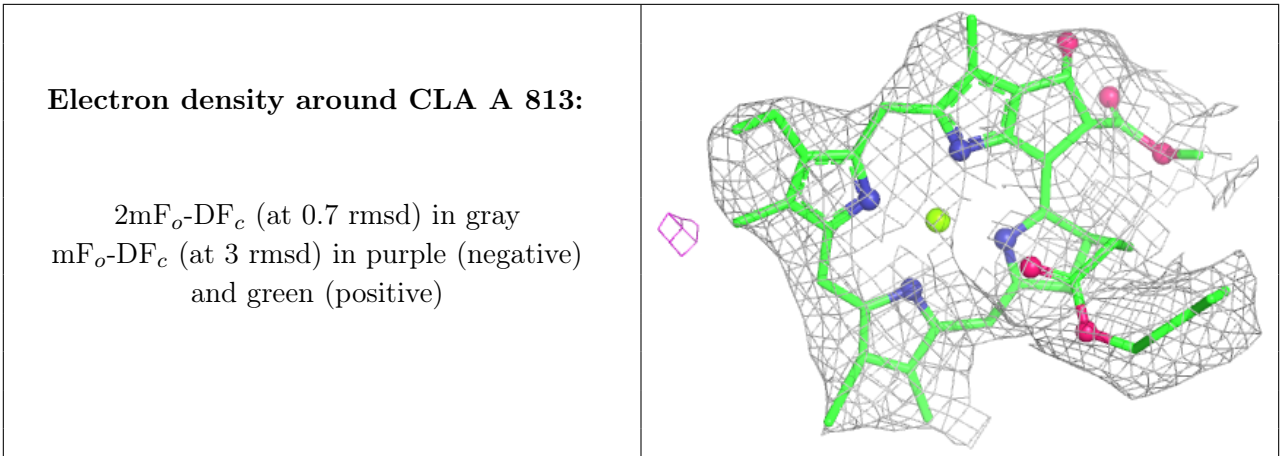
Electron density around LMU 1 218:

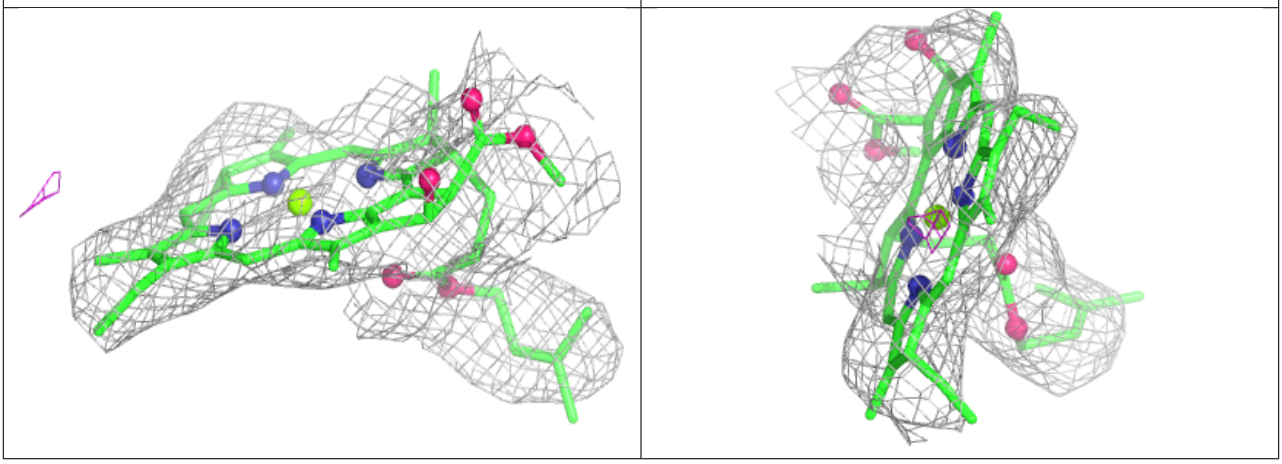
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA A 813:

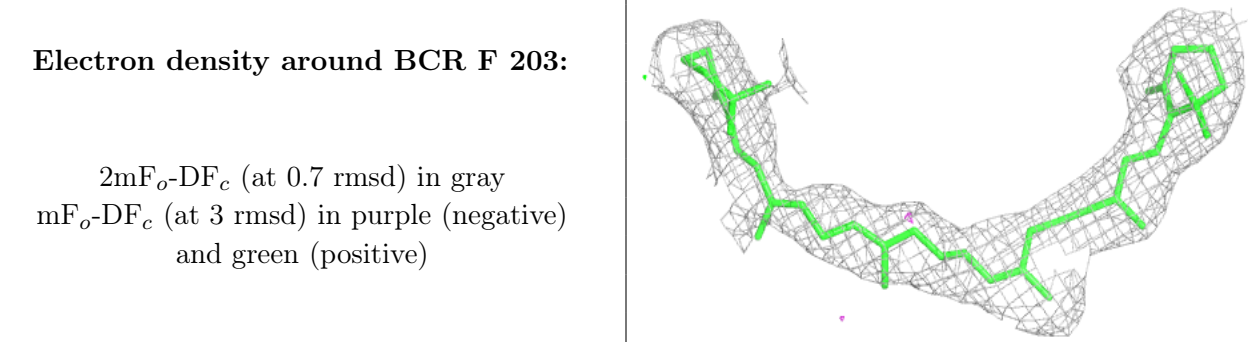
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

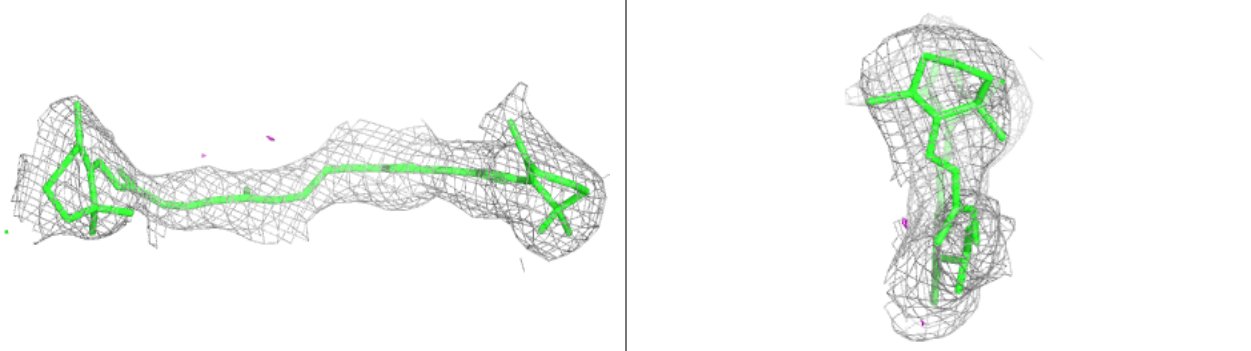




Electron density around BCR F 203:

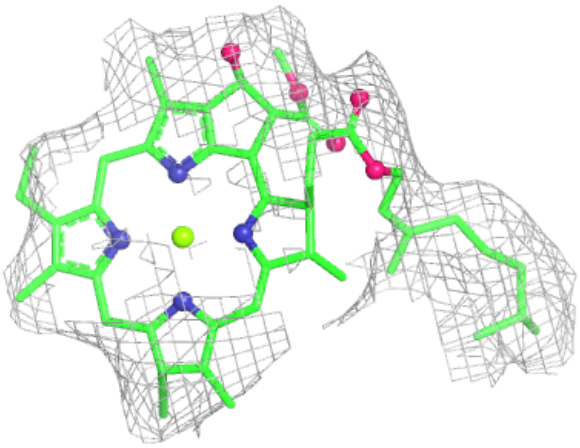
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

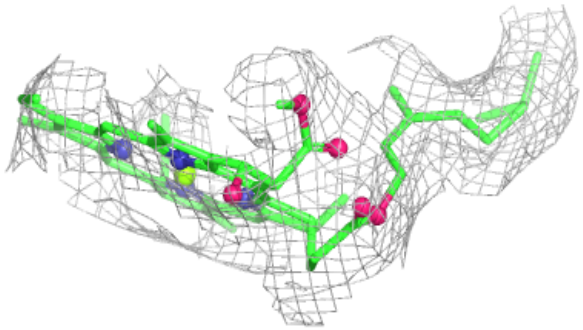


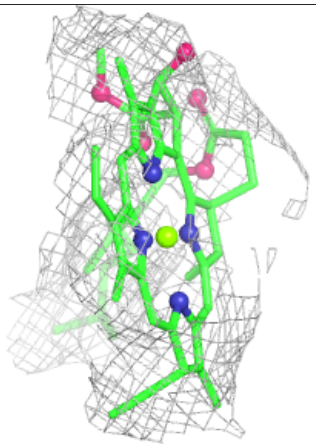


Electron density around CLA J 103:

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

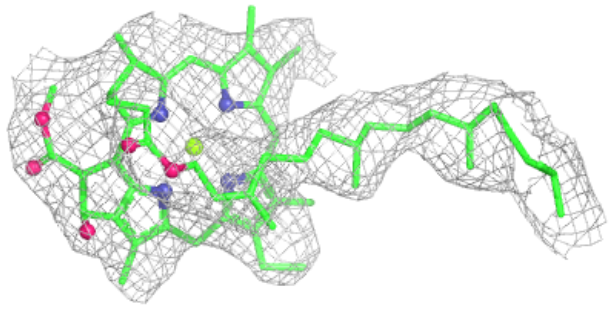


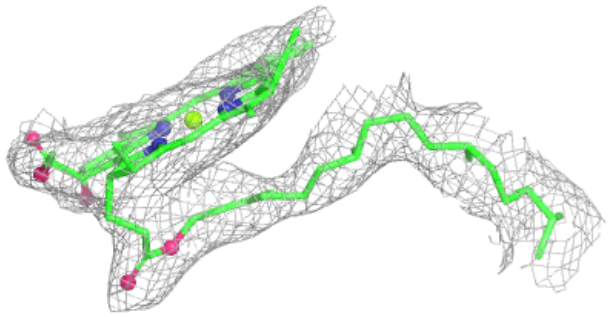


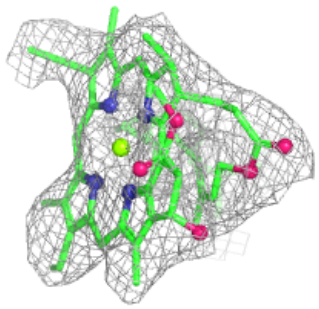


Electron density around CLA A 814:

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

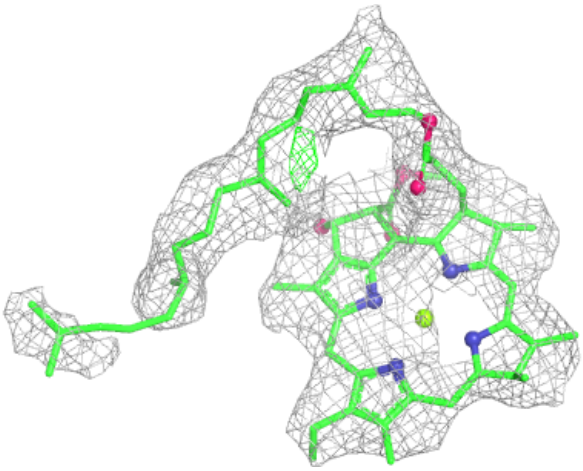


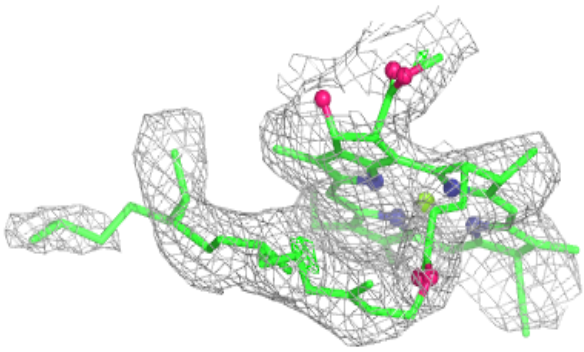




Electron density around CLA B 829:

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

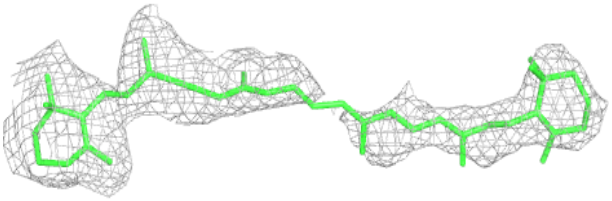


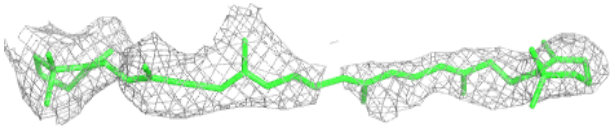


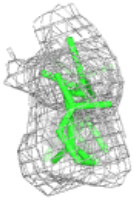


Electron density around BCR L 209:

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

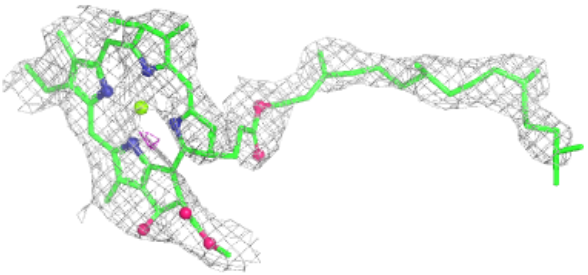


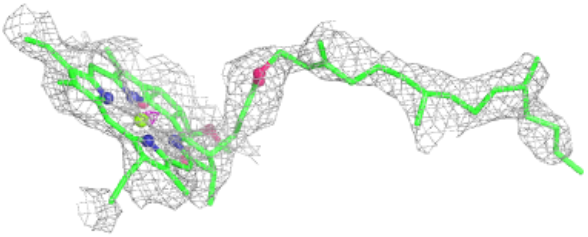


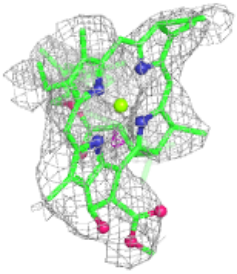


Electron density around CLA A 817:

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

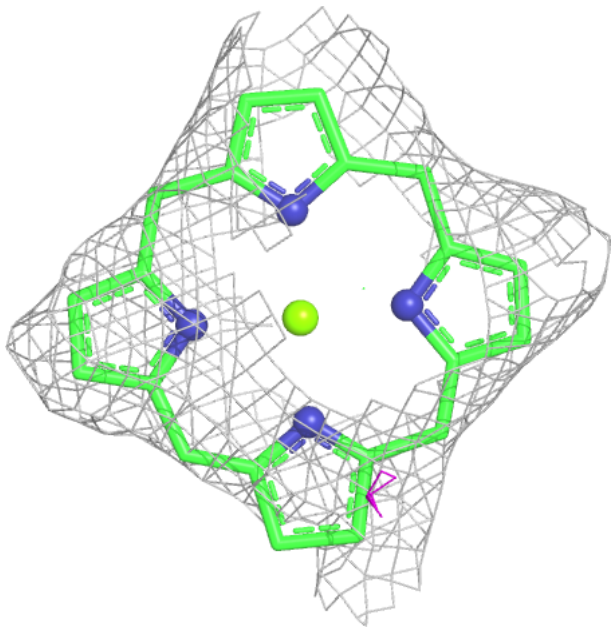


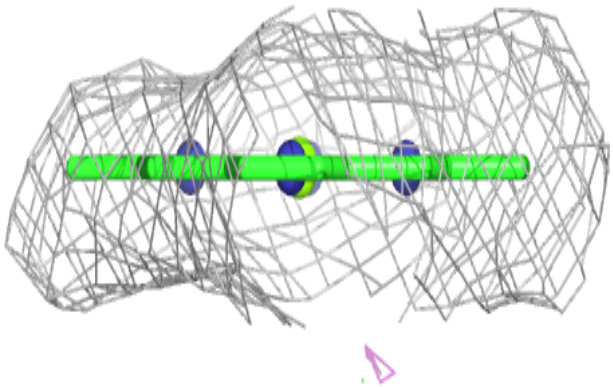


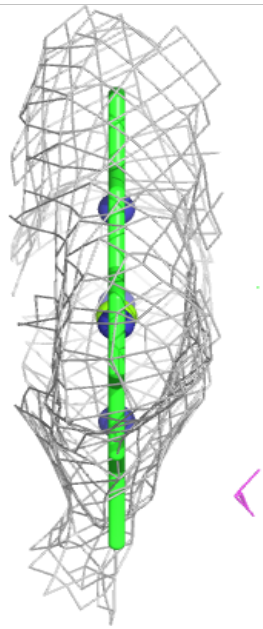


Electron density around CLA 3 317:

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

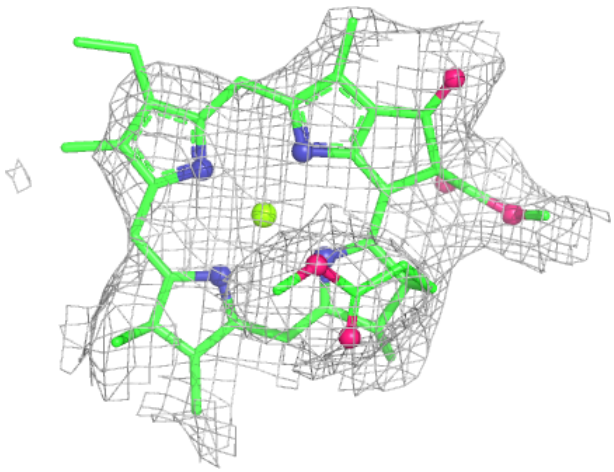


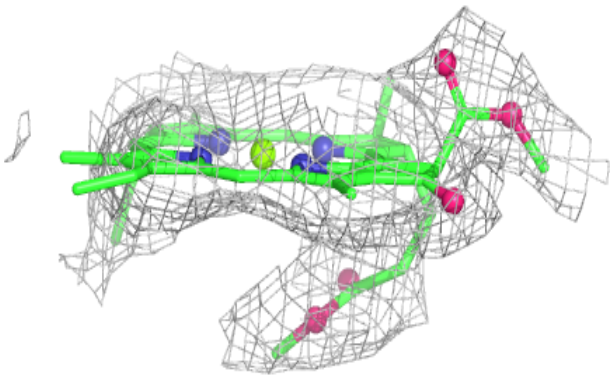


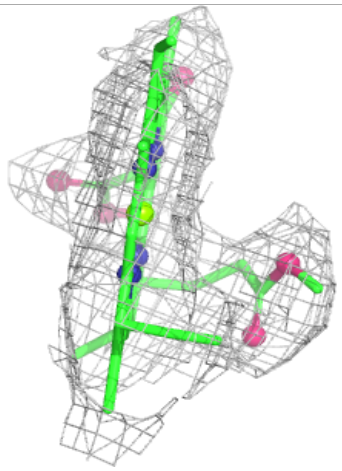


Electron density around CLA 1 204:

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

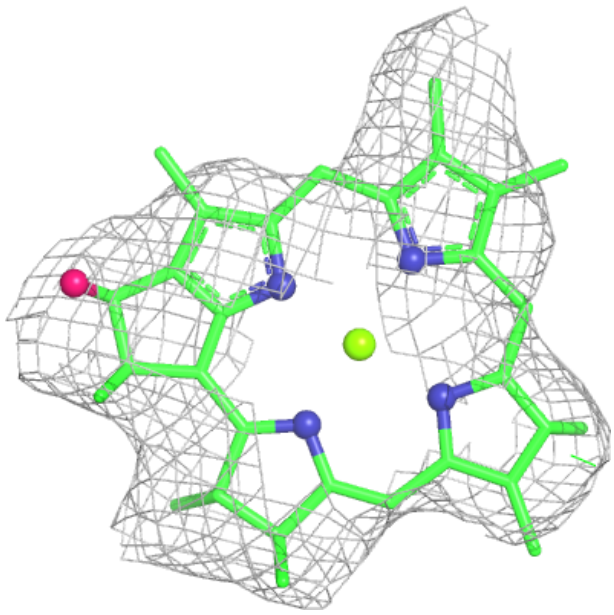


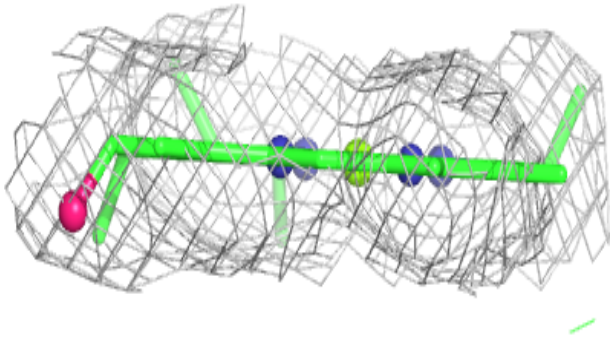


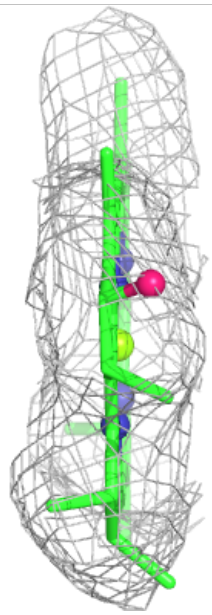


Electron density around CLA 1 210:

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

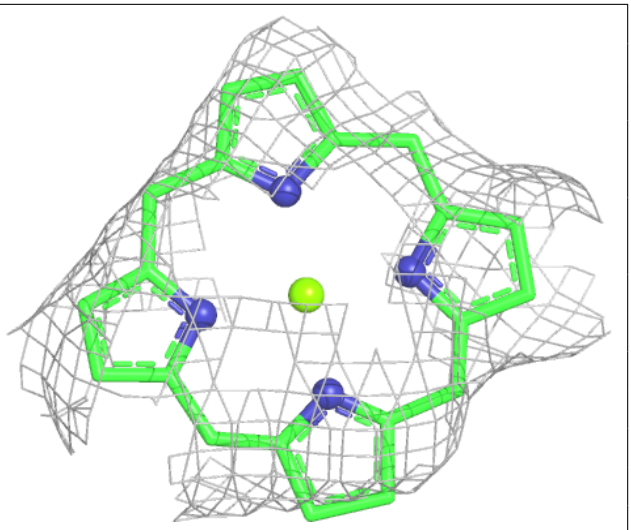


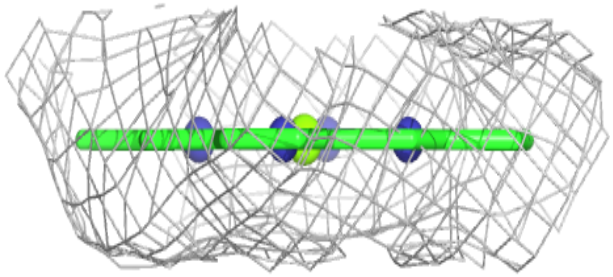


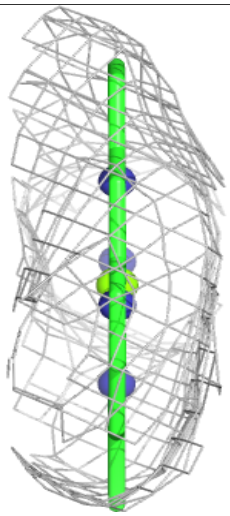


Electron density around CLA 1 215:

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

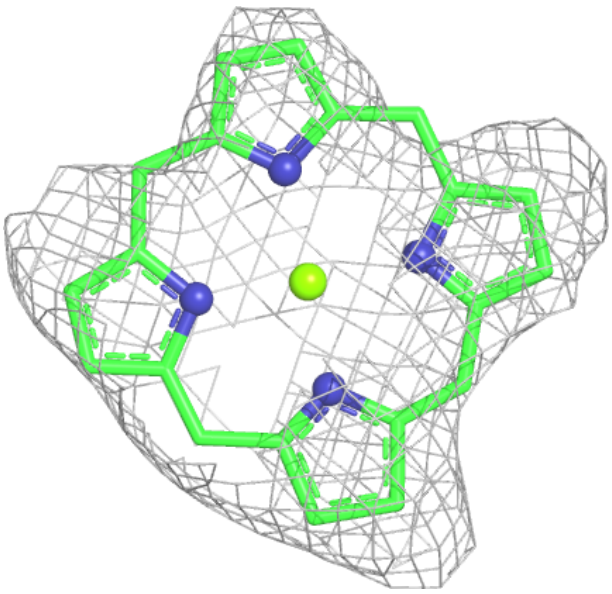


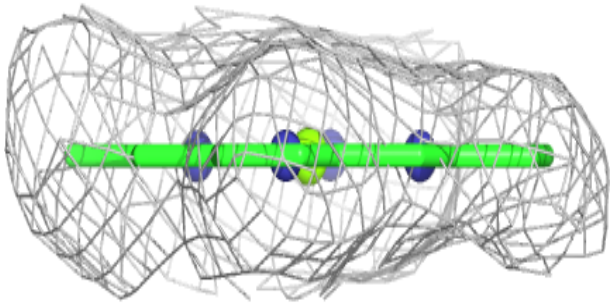


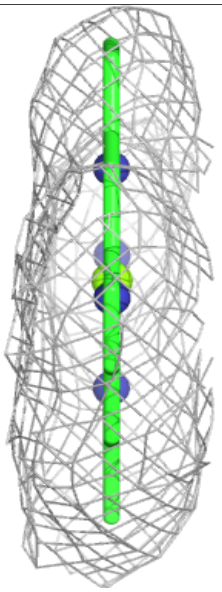


Electron density around CLA 2 315:

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

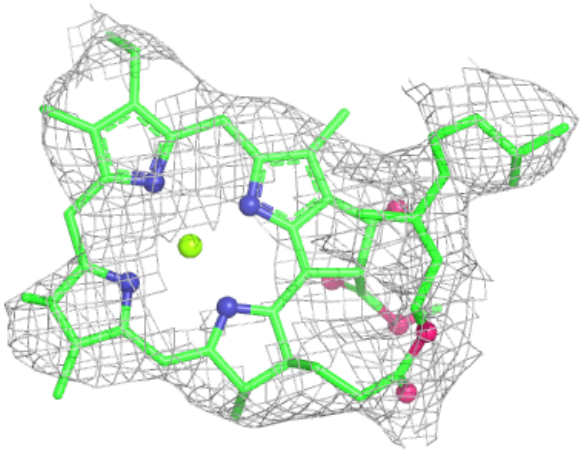


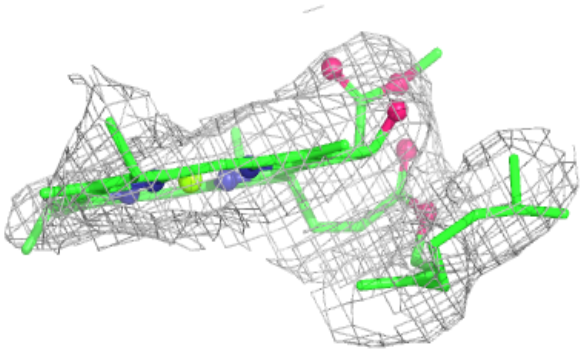


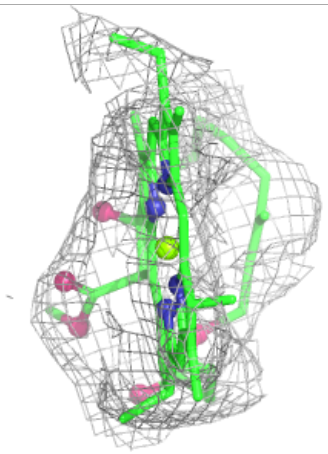


Electron density around CLA B 808:

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

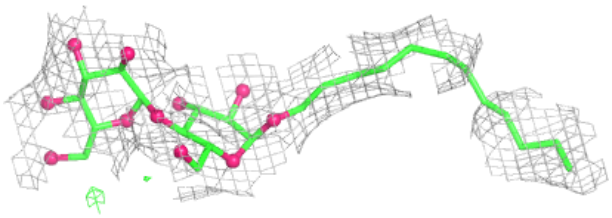


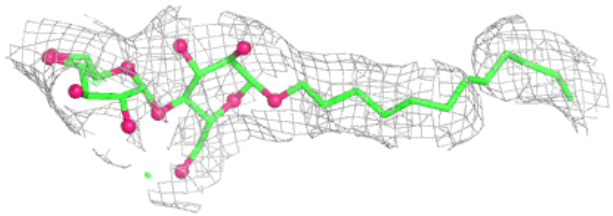


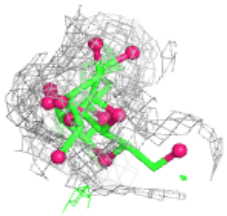


Electron density around LMU B 802:

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

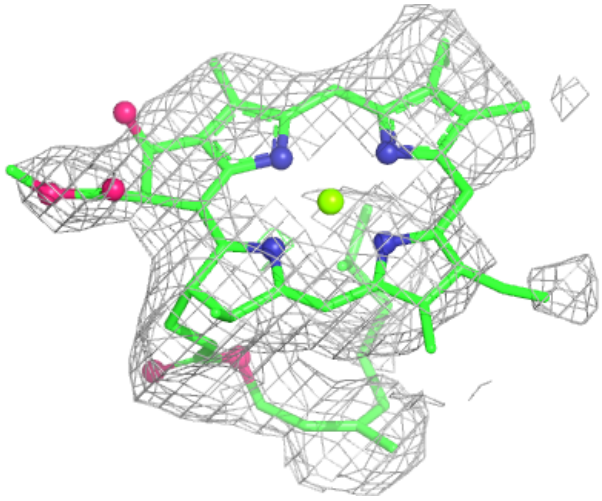


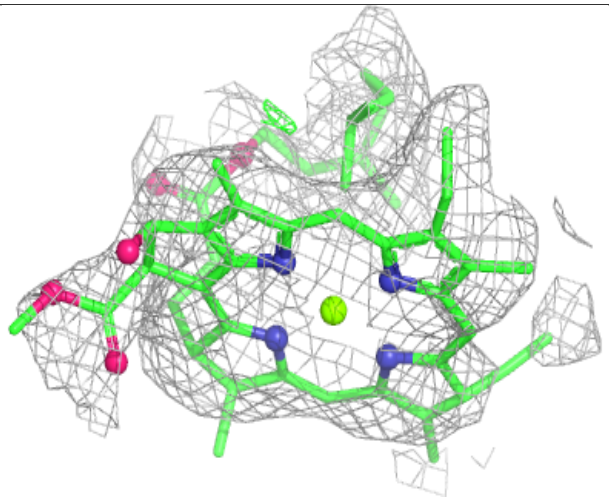


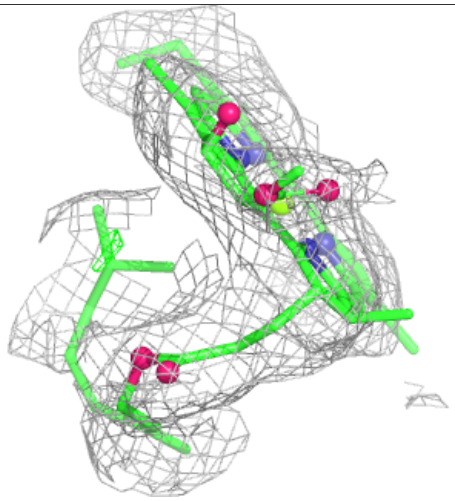


Electron density around CLA B 809:

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

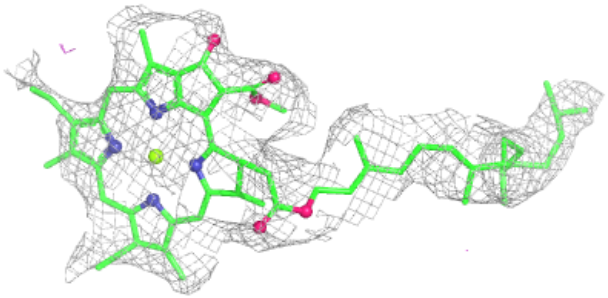


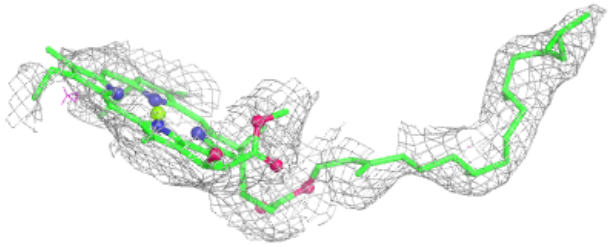


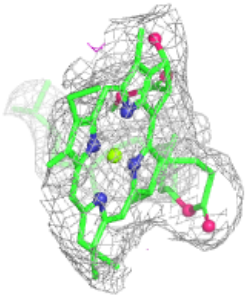


Electron density around CLA 2 317:

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

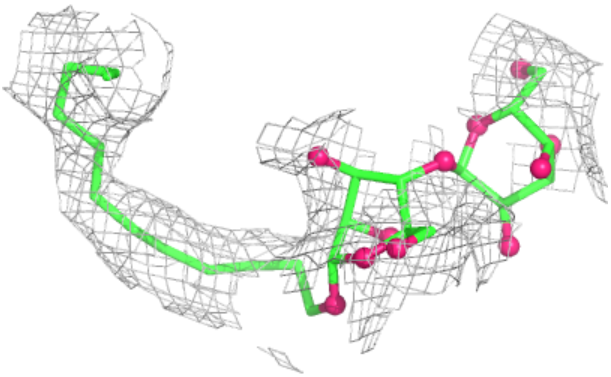


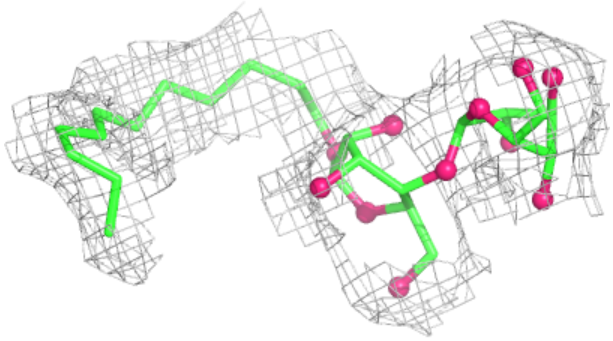


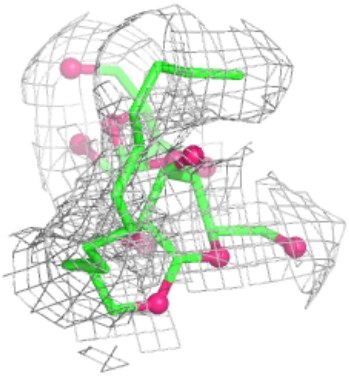


Electron density around LMU R 103:

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

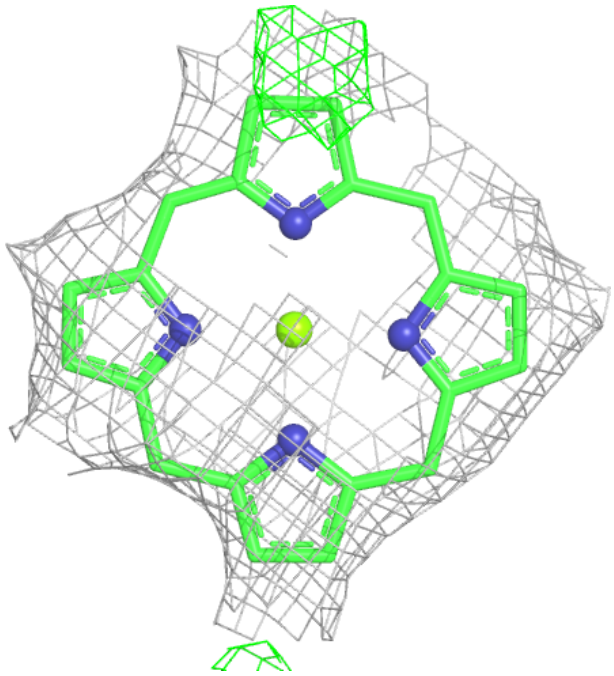


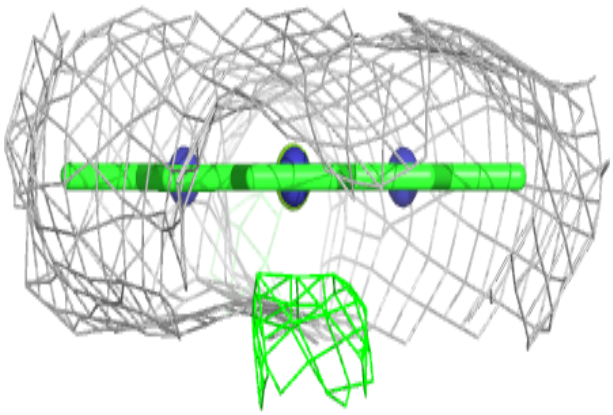


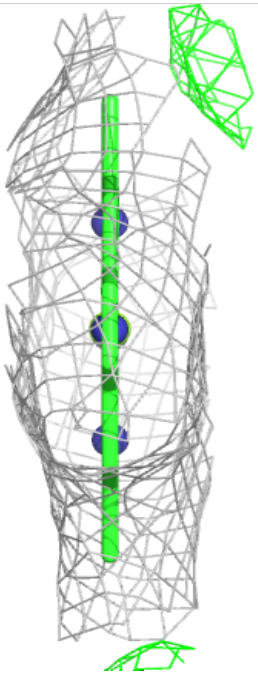


Electron density around CLA 3 307:

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

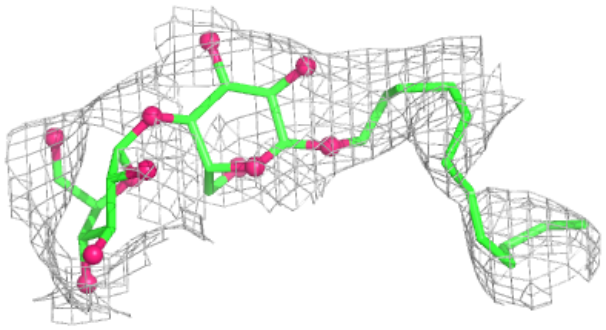


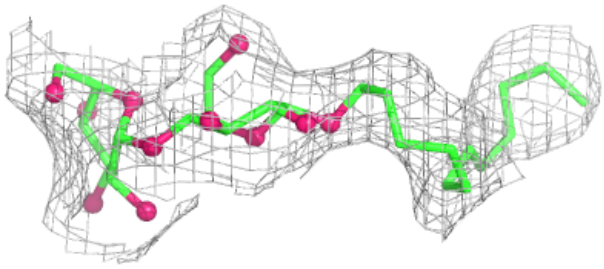


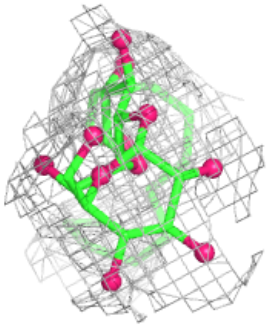


Electron density around LMU R 108:

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

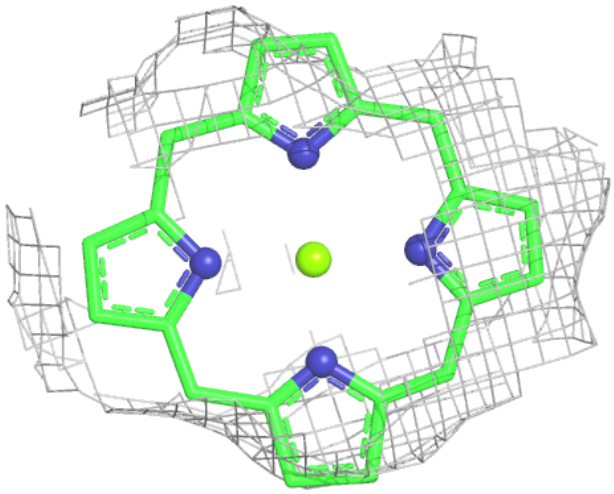


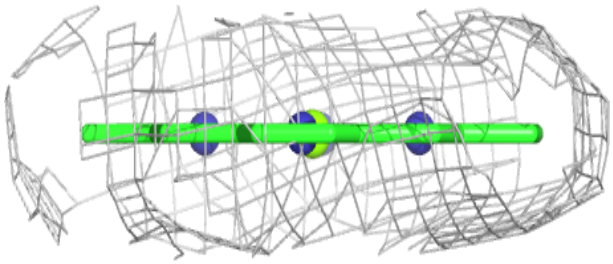


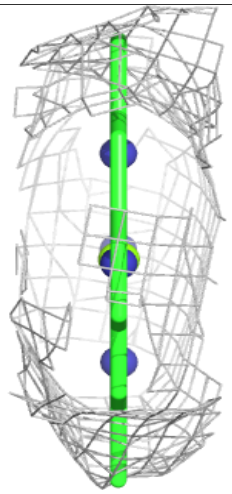


Electron density around CLA 2 308:

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

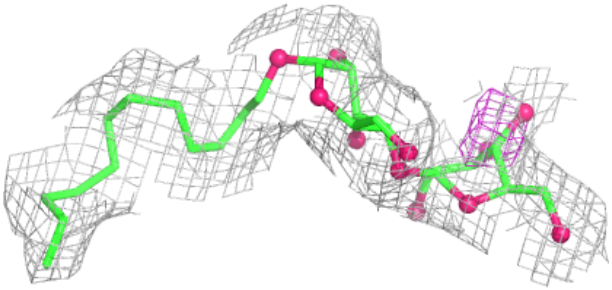


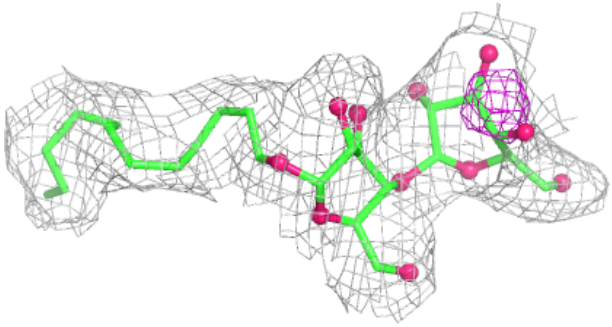


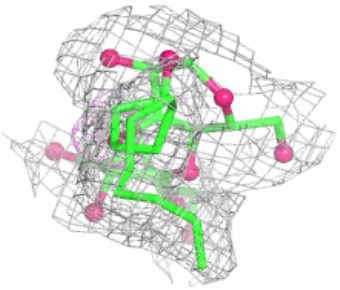


Electron density around LMU H 102:

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

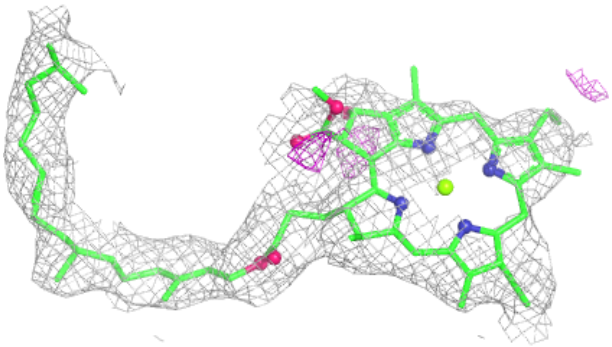


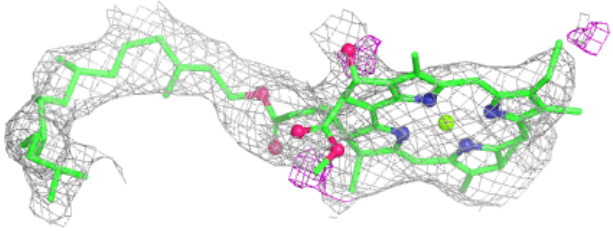




Electron density around CLA B 823:

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

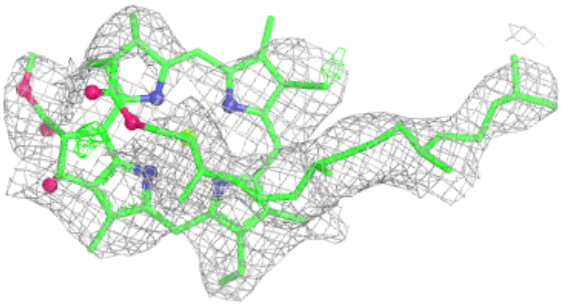


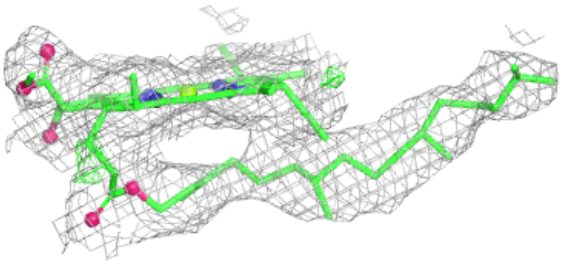


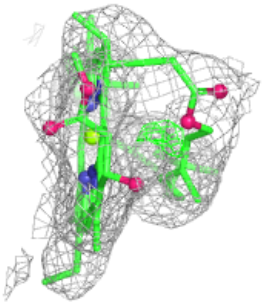


Electron density around CLA A 855:

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



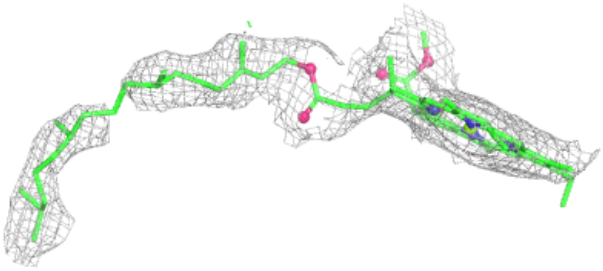




Electron density around CLA A 803:

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

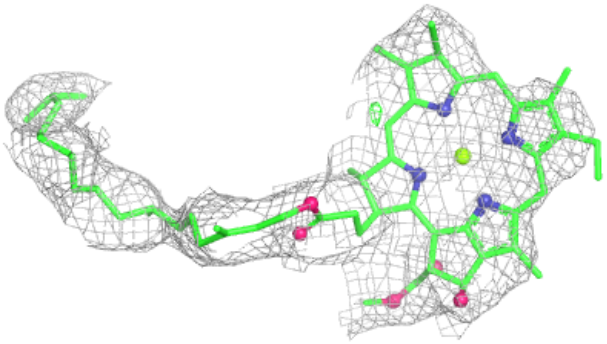




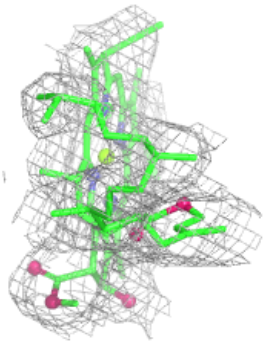


Electron density around CLA A 822:

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

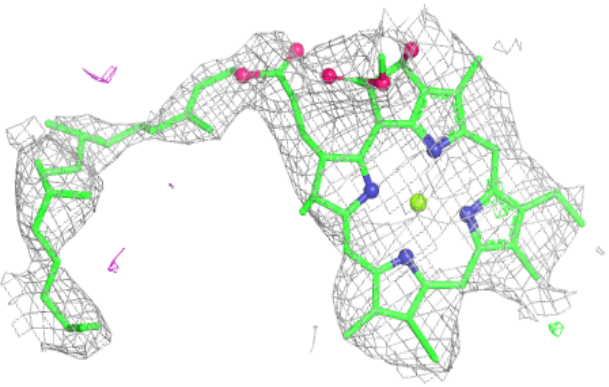


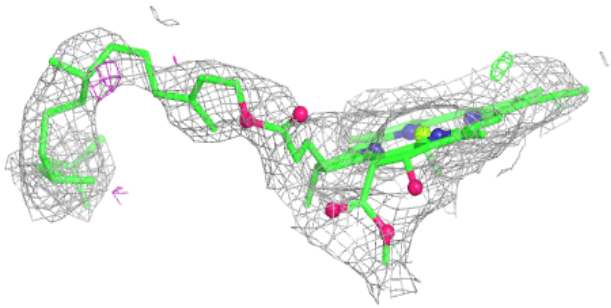


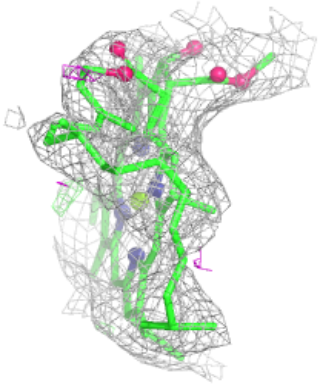


Electron density around CLA A 823:

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

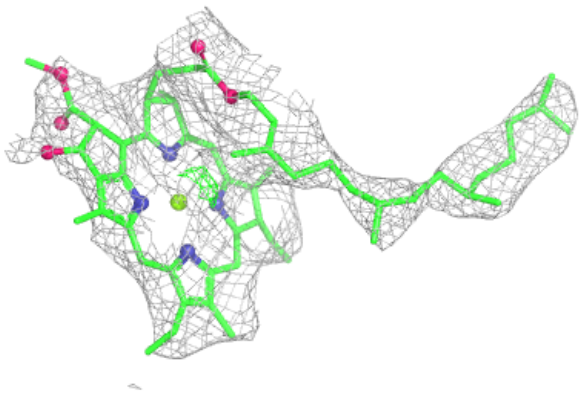


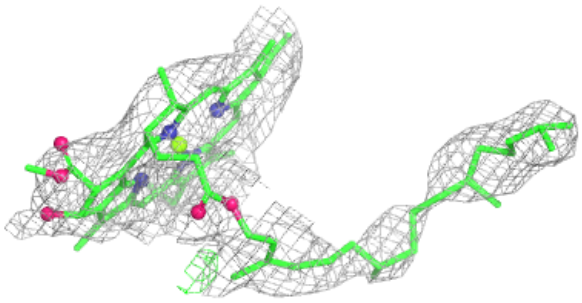


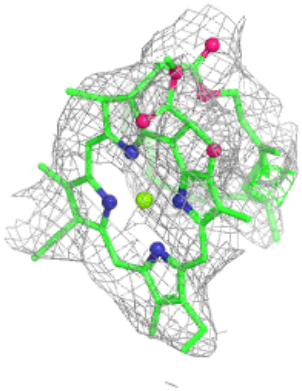


Electron density around CLA B 811:

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

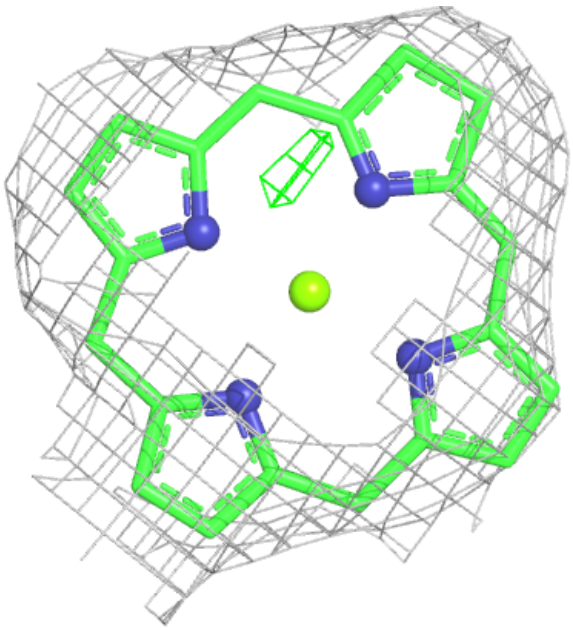


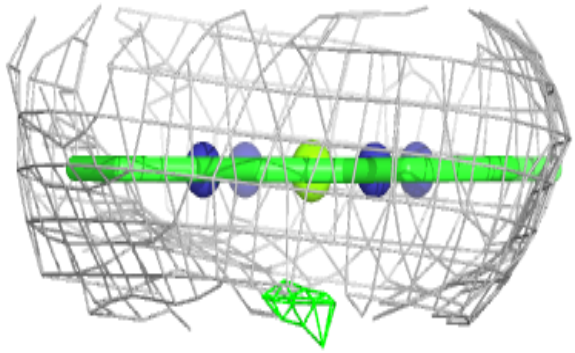


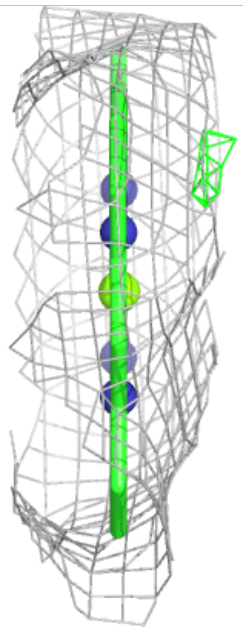


Electron density around CLA 4 311:

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

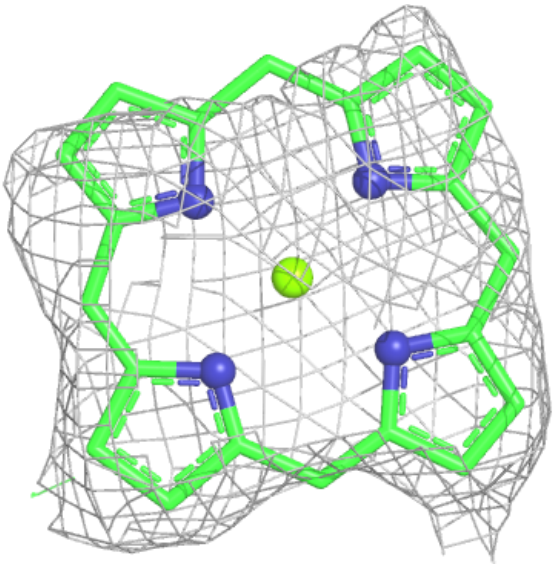


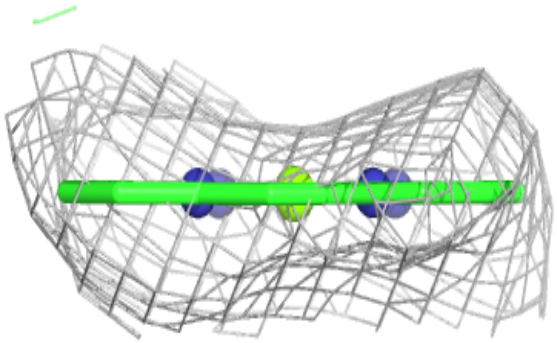


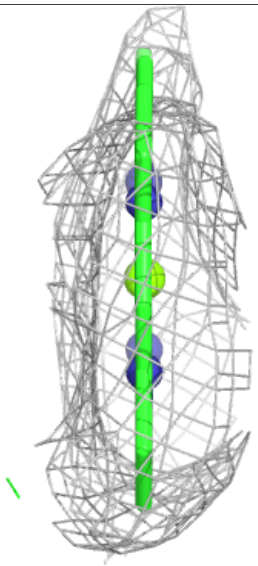


Electron density around CLA 2 309:

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

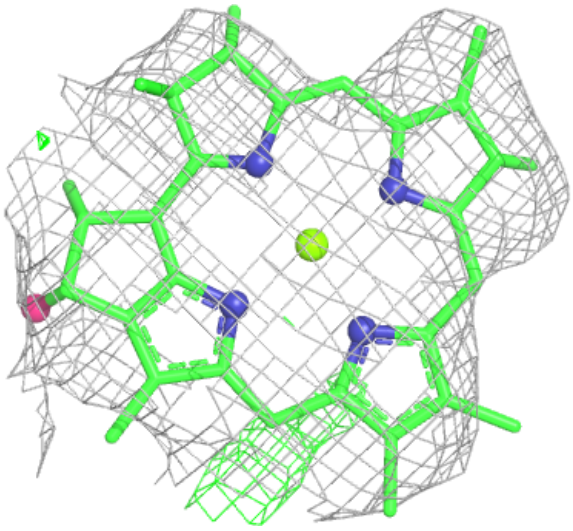


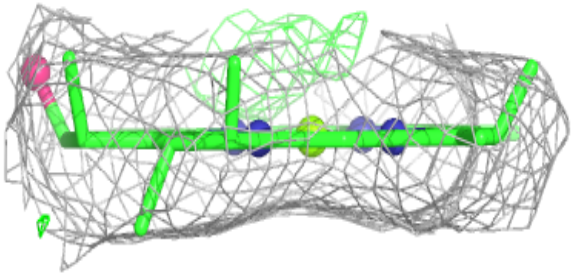


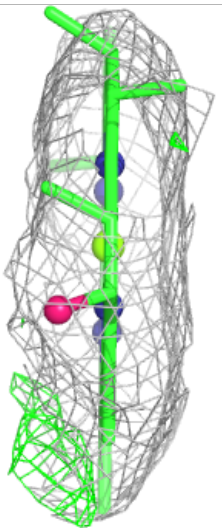


Electron density around CLA 4 303:

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

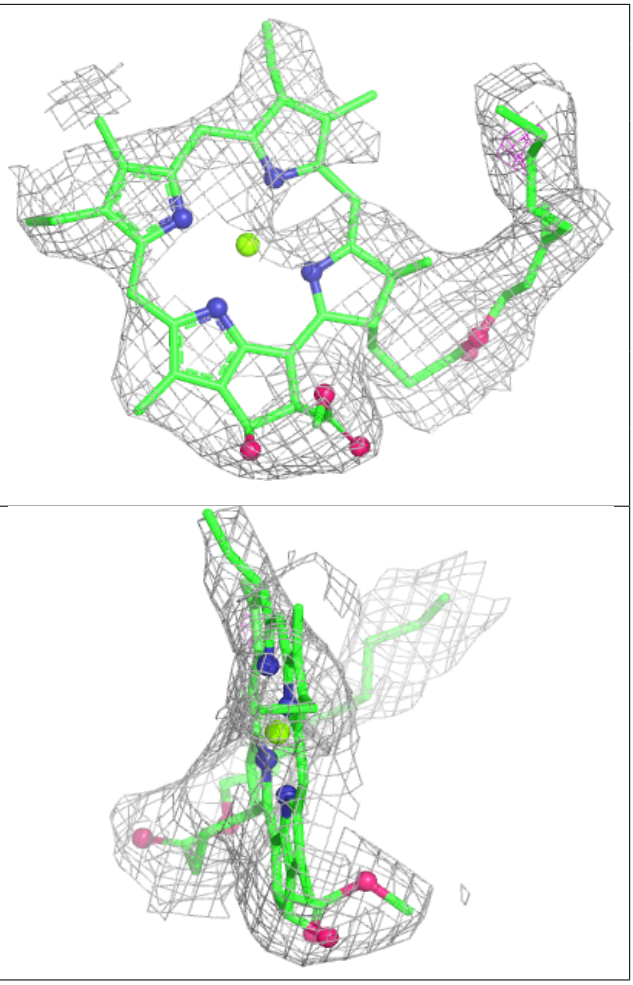






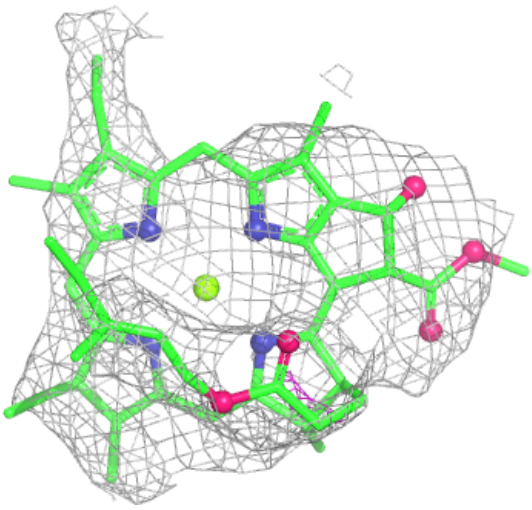
Electron density around CLA A 811:

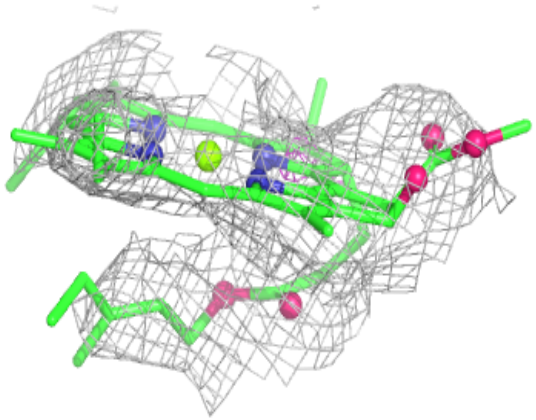
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

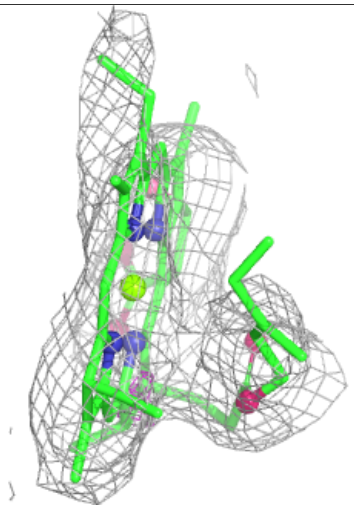


Electron density around CLA A 818:

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

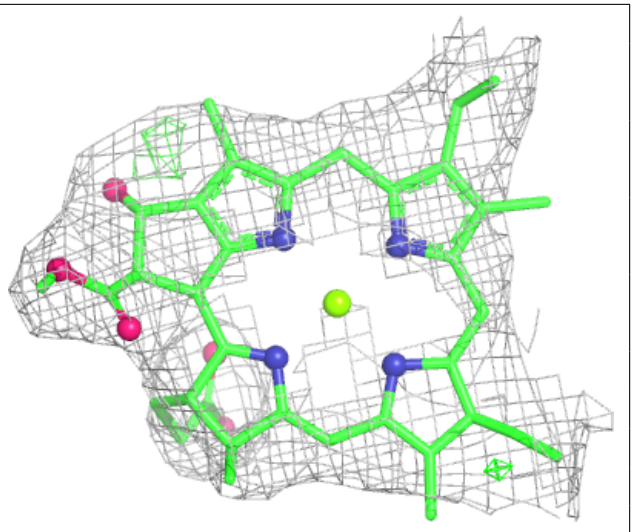


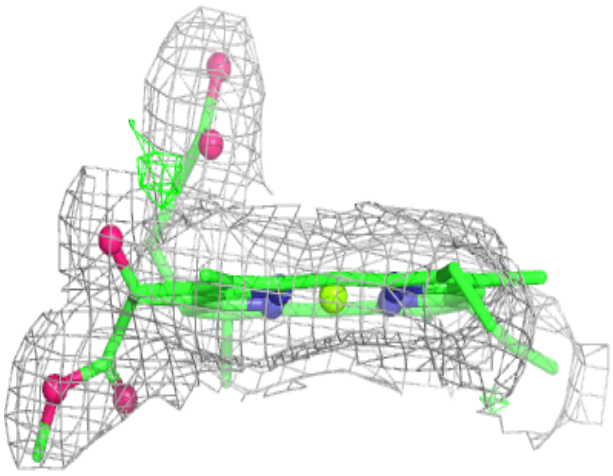


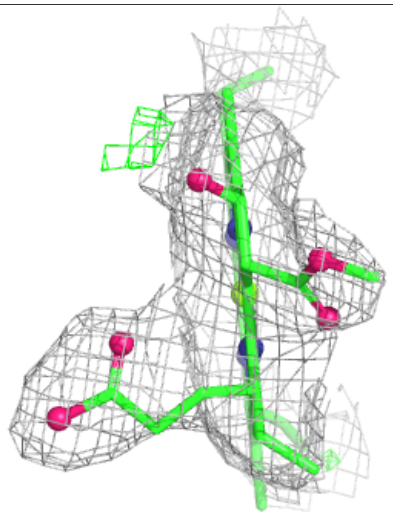


Electron density around CLA B 803:

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

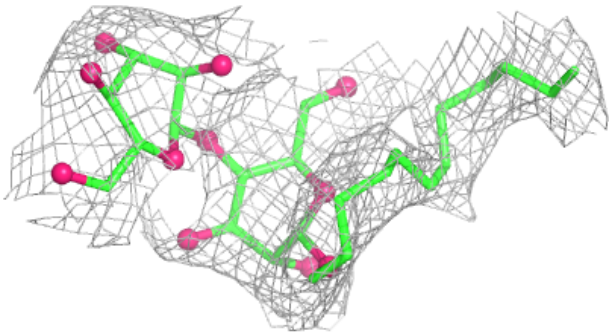


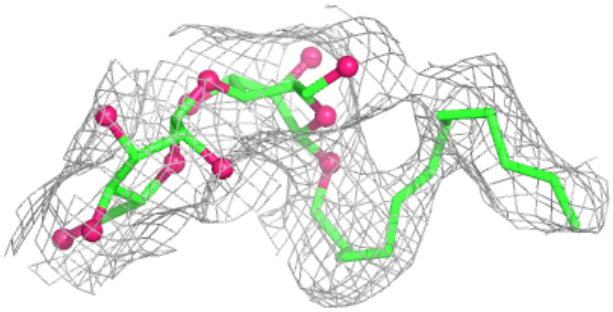


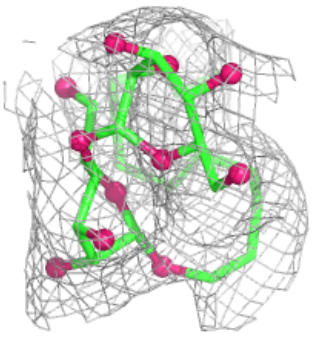


Electron density around LMU L 210:

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

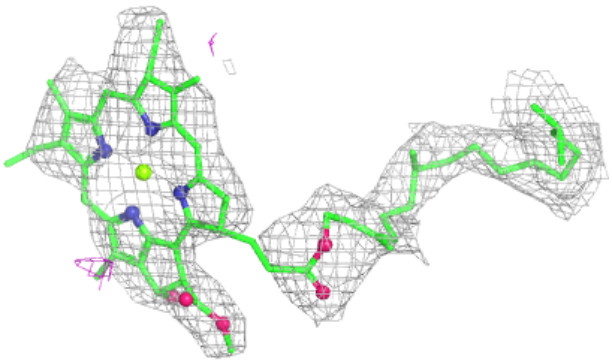


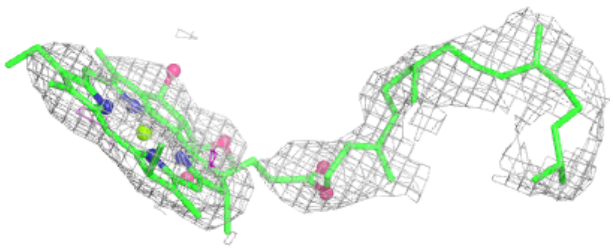


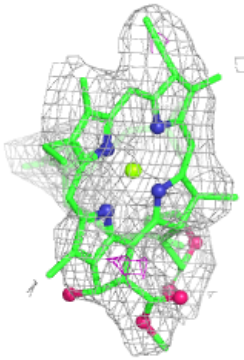


Electron density around CLA B 807:

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

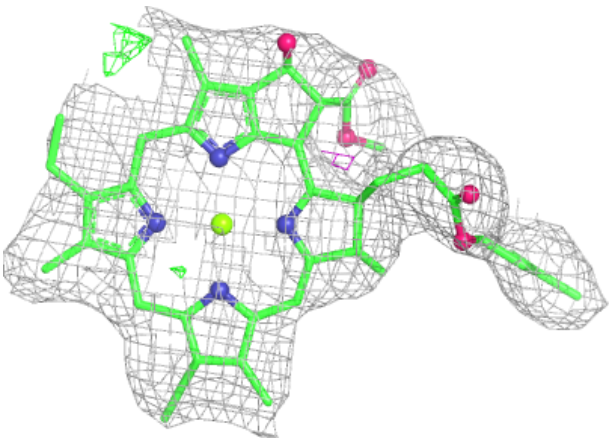


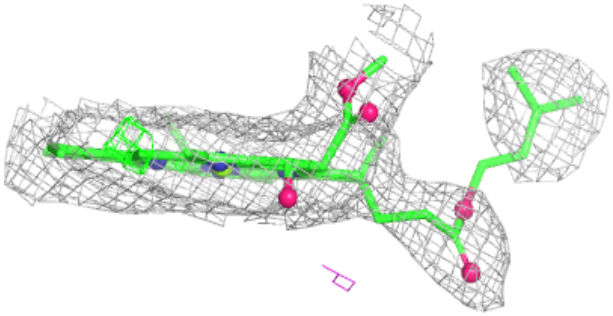




Electron density around CLA B 828:

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

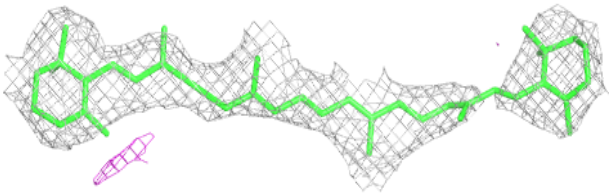


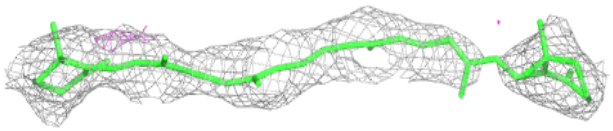


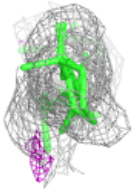


Electron density around BCR B 843:

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

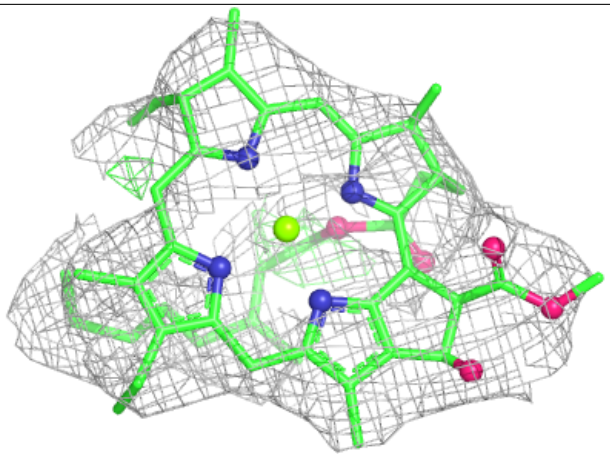


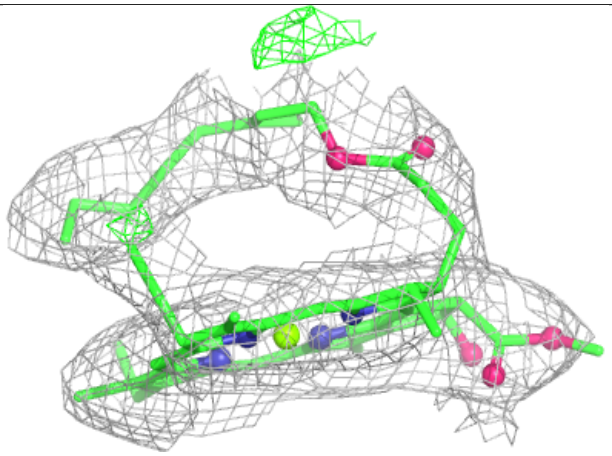


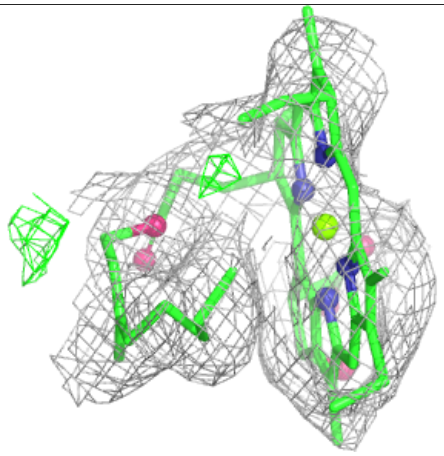


Electron density around CLA A 810:

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

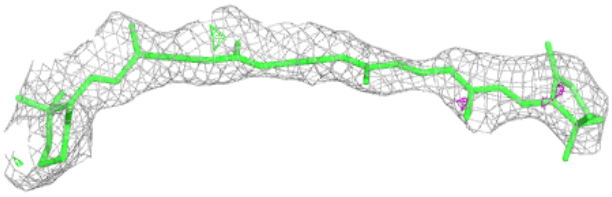


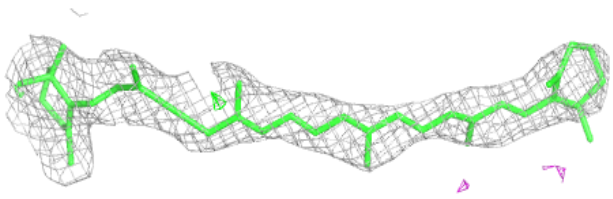


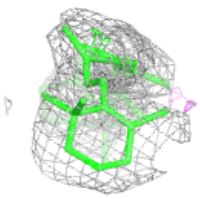


Electron density around BCR F 202:

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

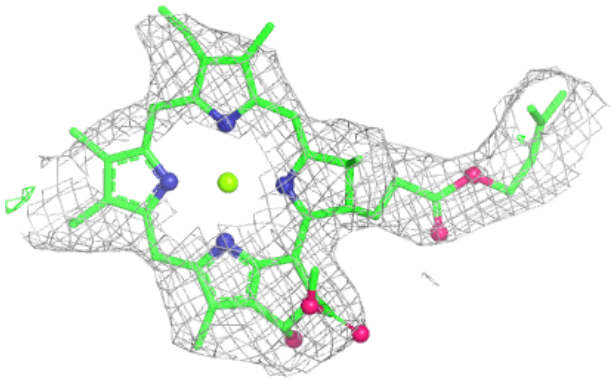


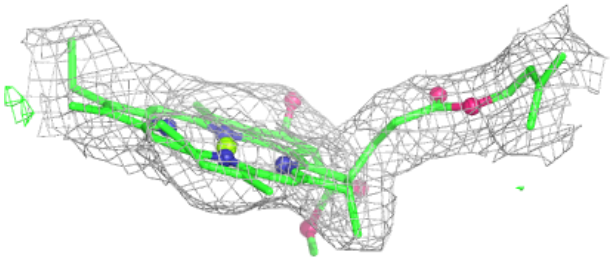


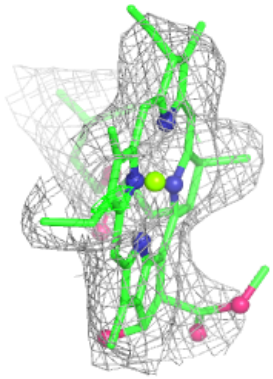


Electron density around CLA B 830:

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

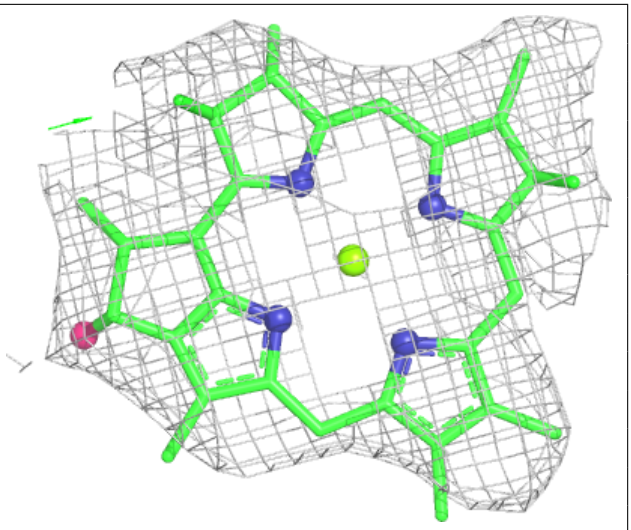


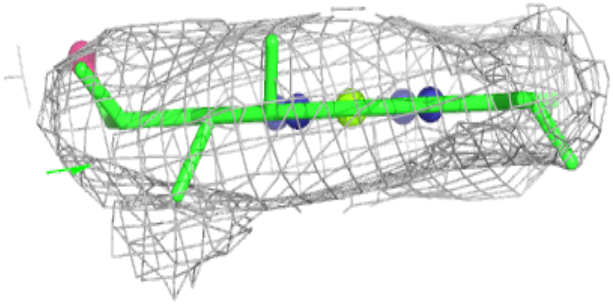


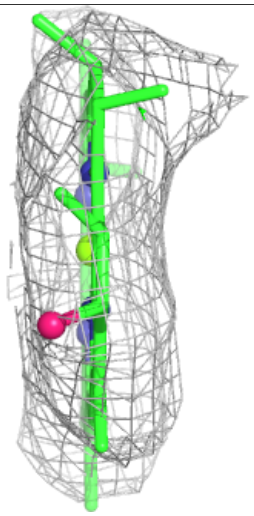


Electron density around CLA 4 313:

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

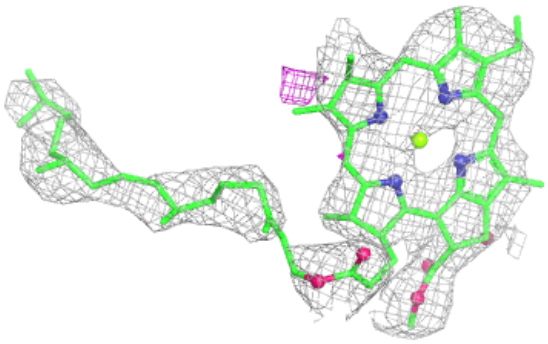


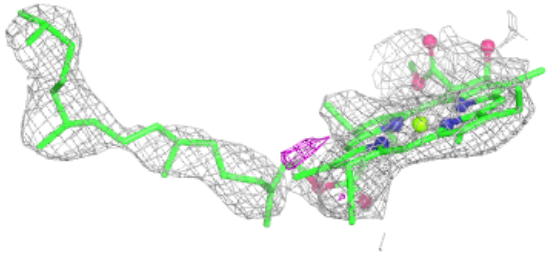


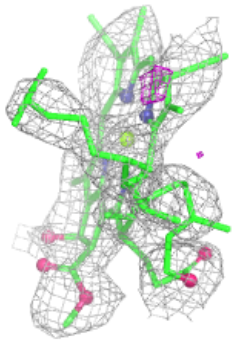


Electron density around CLA A 849:

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

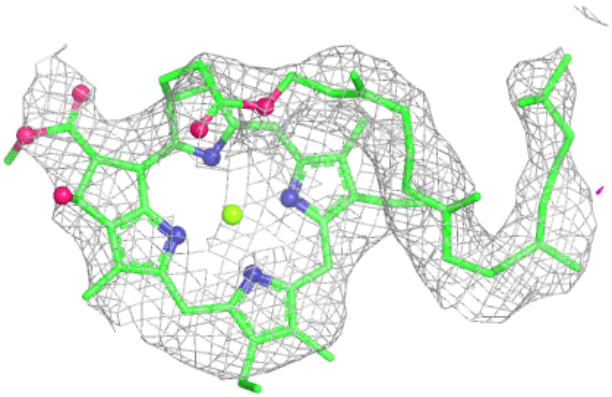


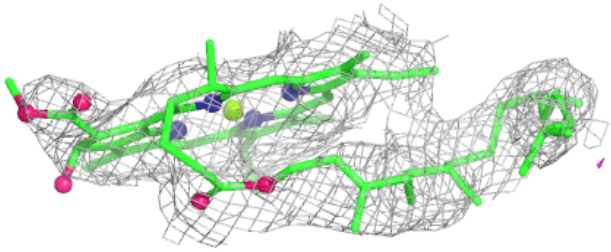


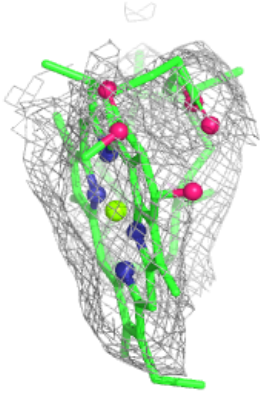


Electron density around CLA A 816:

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

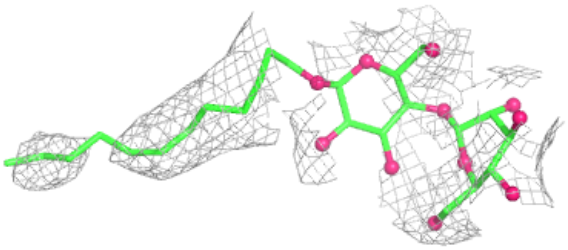


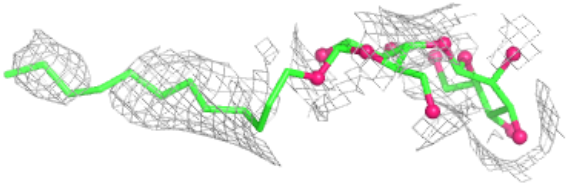


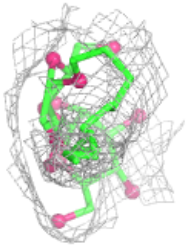


Electron density around LMU A 854:

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

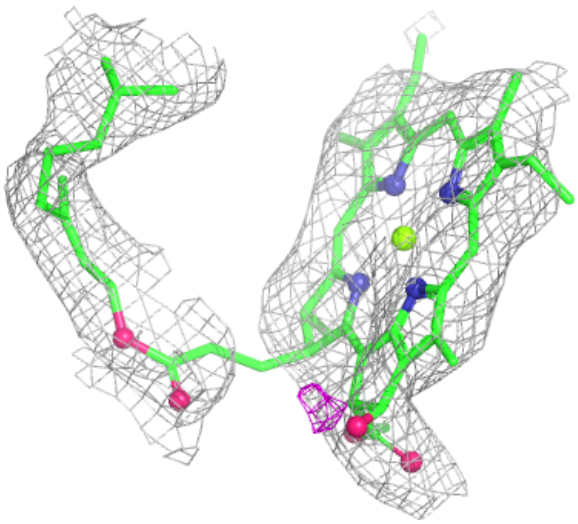


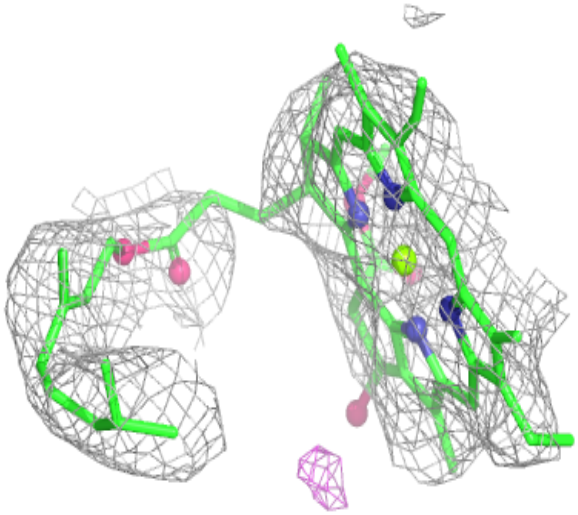


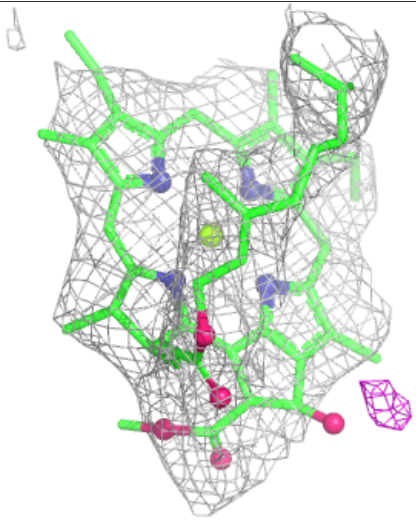


Electron density around CLA A 802:

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

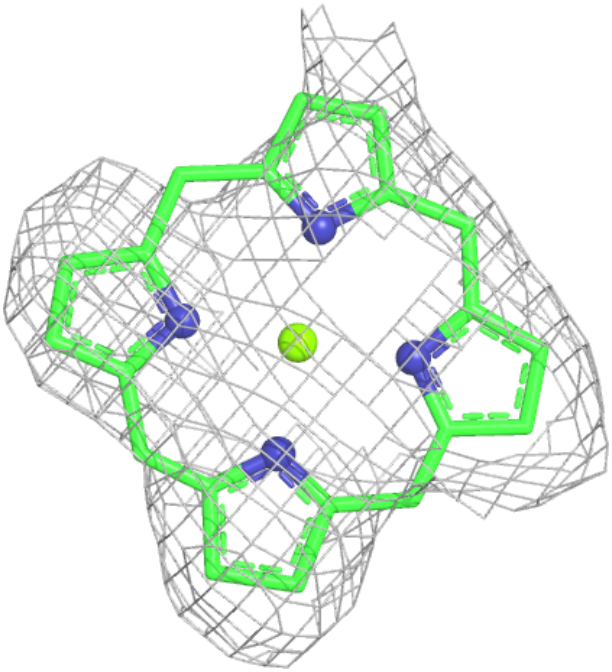


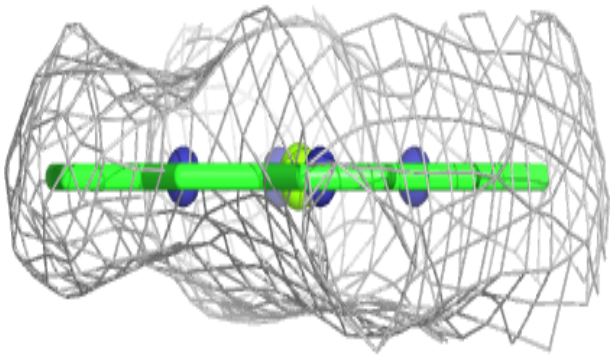


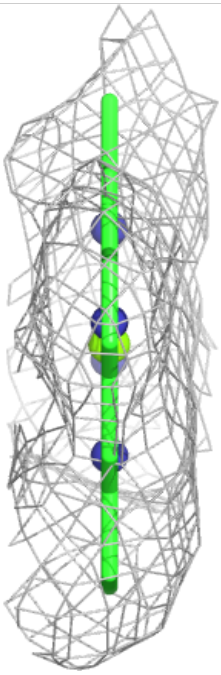


Electron density around CLA 2 303:

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

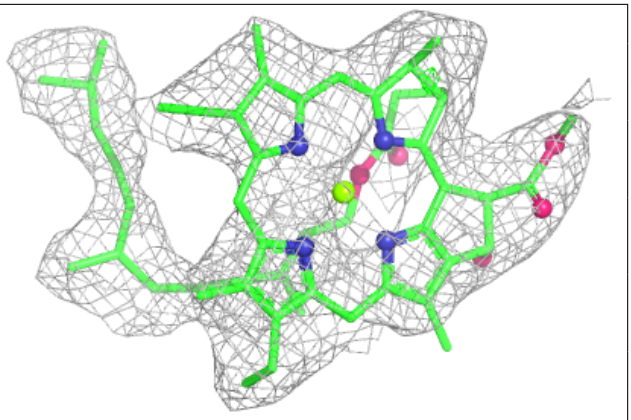


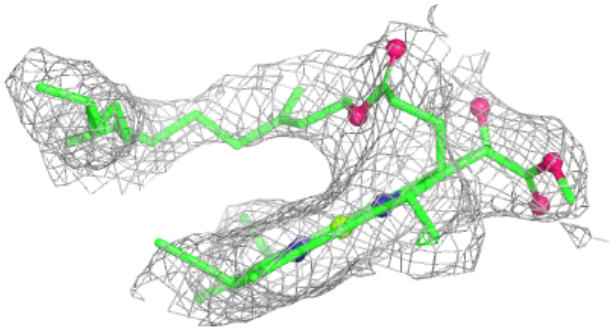




Electron density around CLA I 102:

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

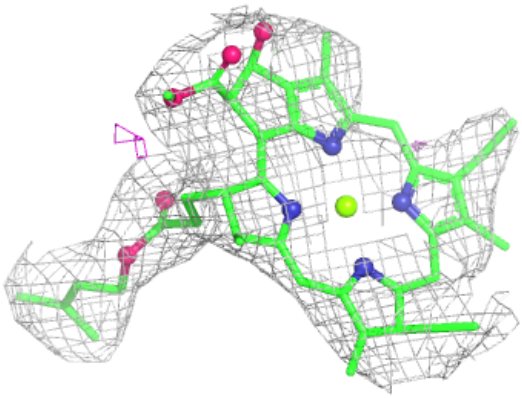


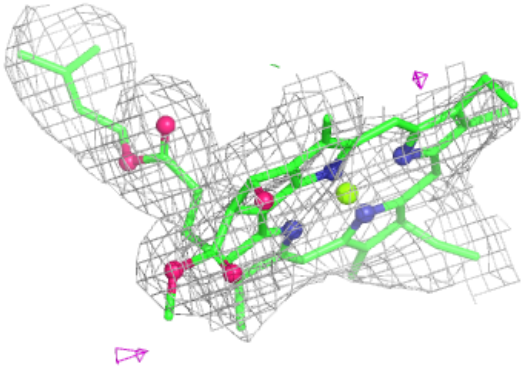


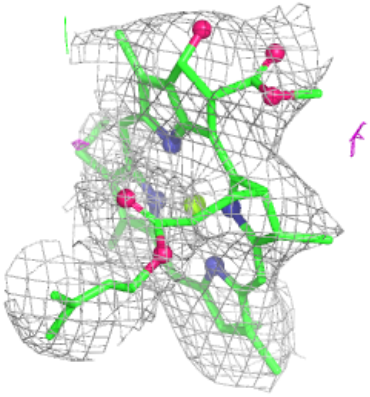


Electron density around CLA 2 310:

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

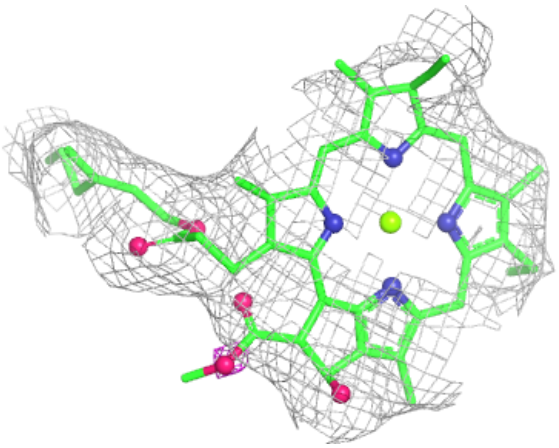


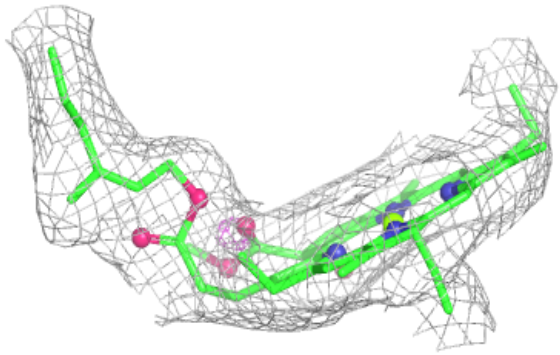


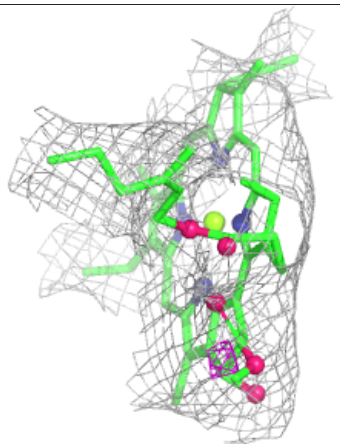


Electron density around CLA 4 307:

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

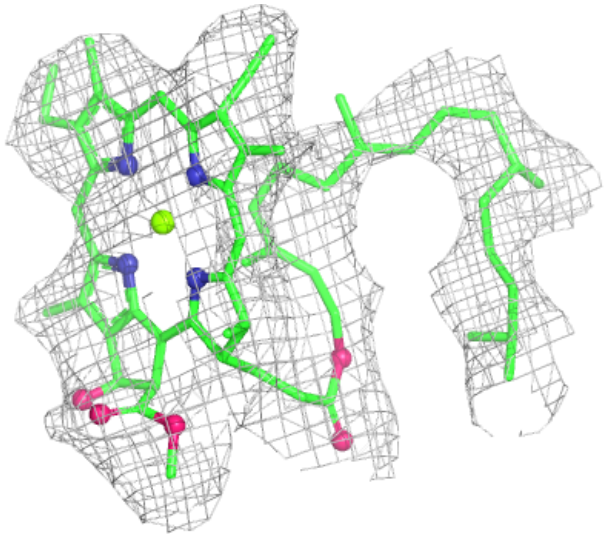


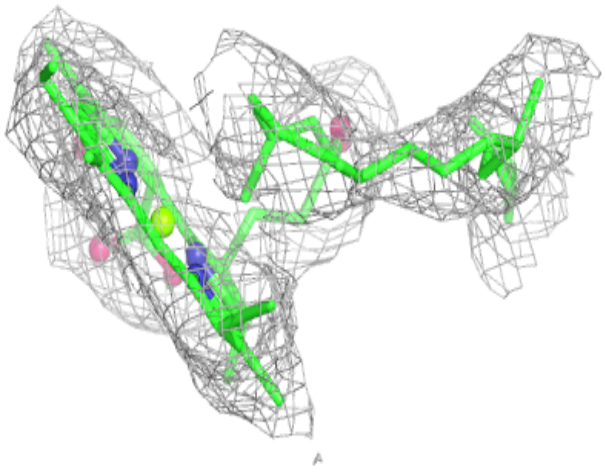


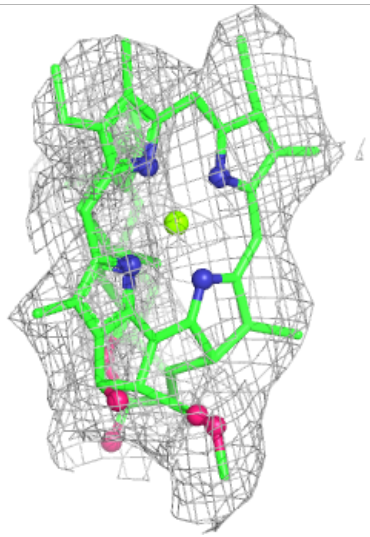


Electron density around CLA B 820:

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

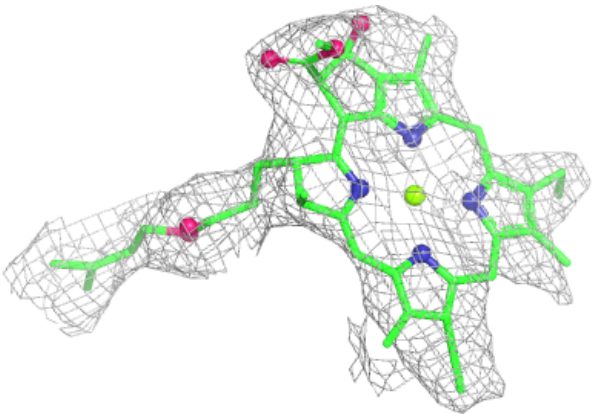


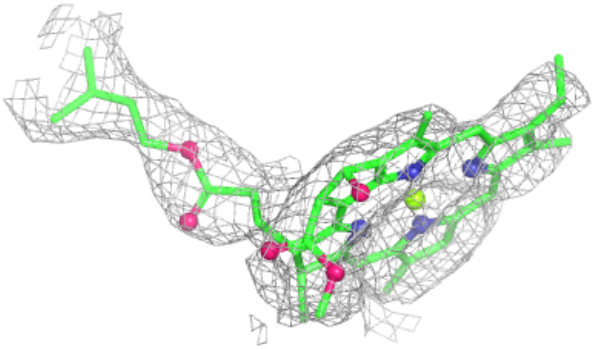




Electron density around CLA A 827:

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

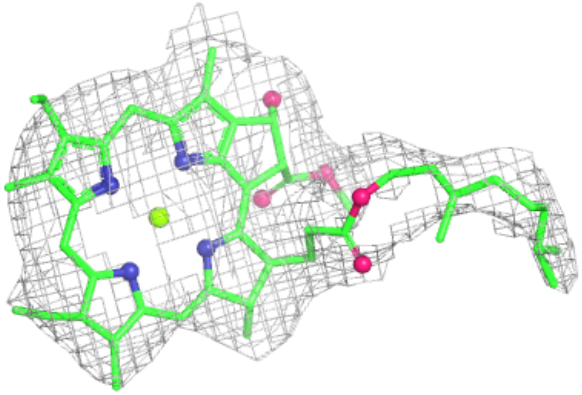


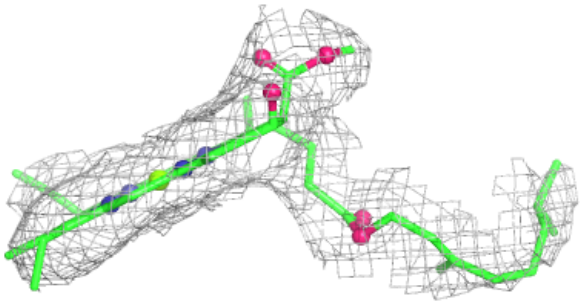


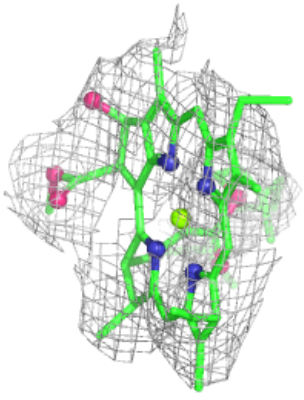


Electron density around CLA A 807:

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

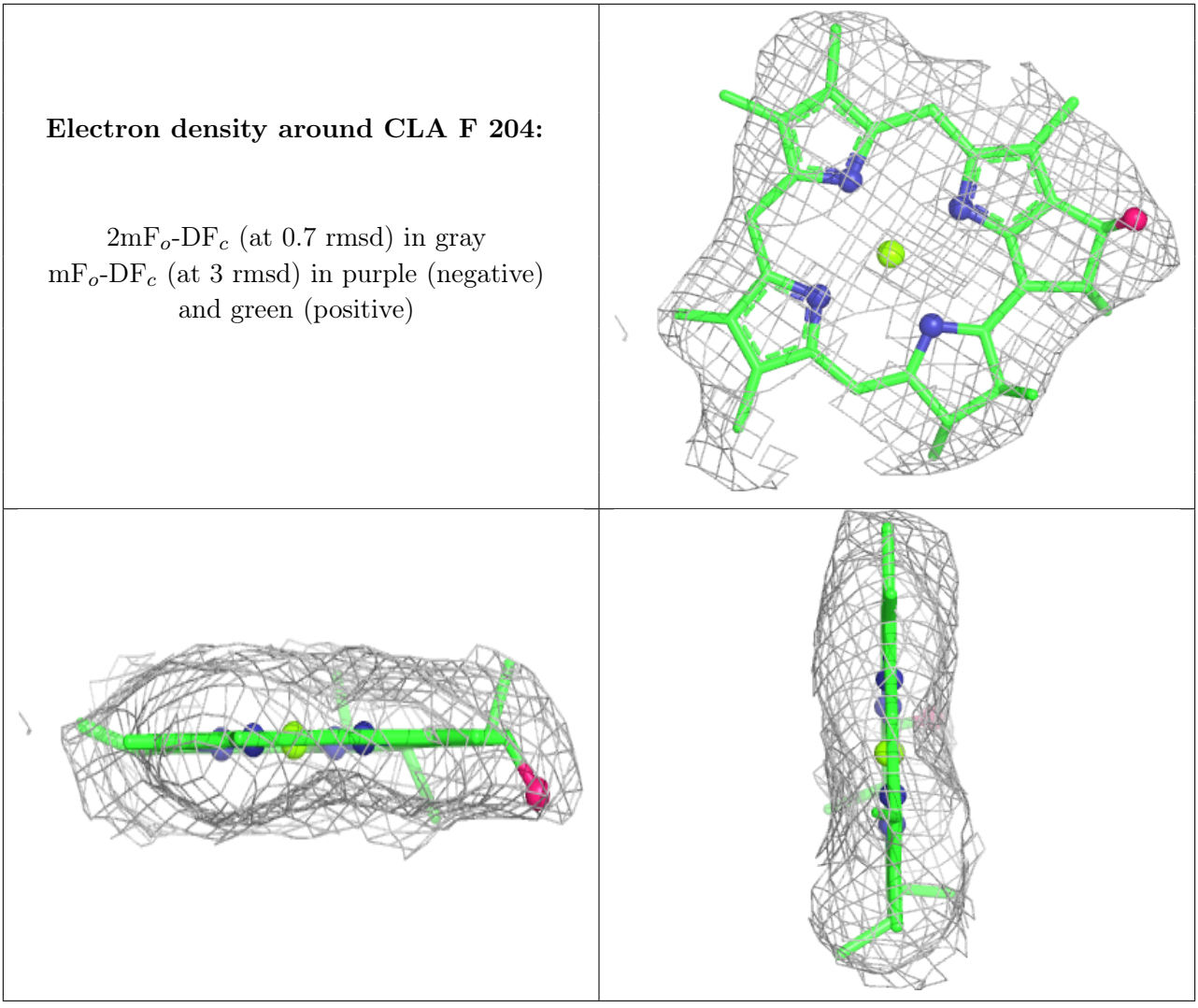






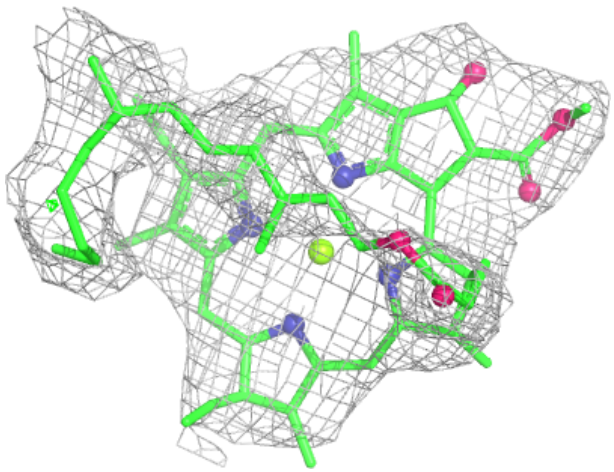
Electron density around CLA F 204:

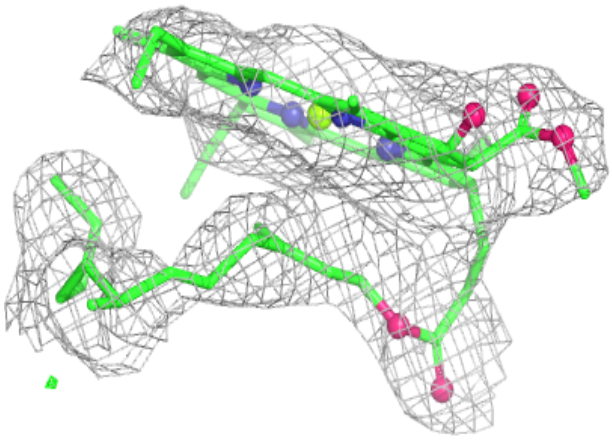
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

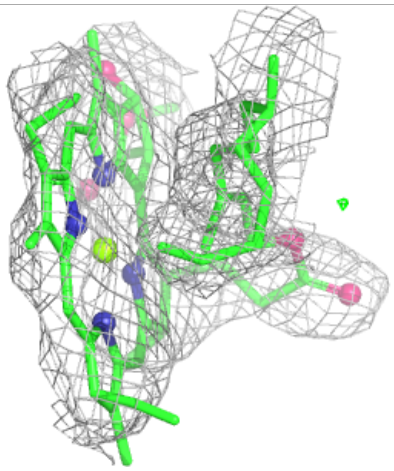


Electron density around CLA B 814:

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

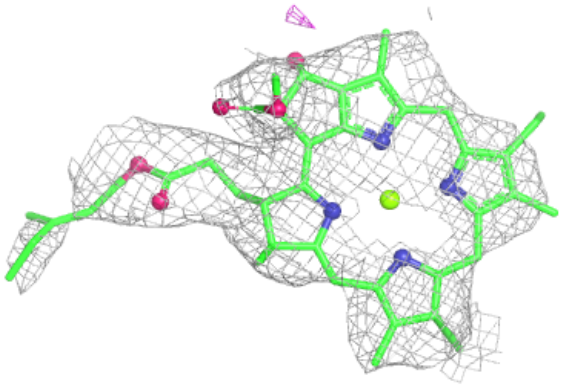


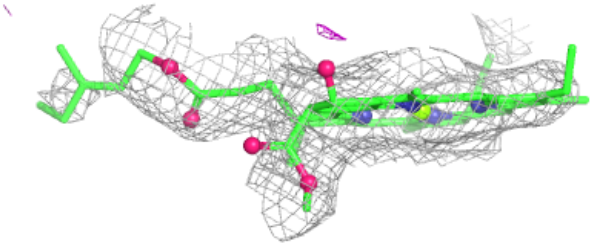




Electron density around CLA A 832:

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

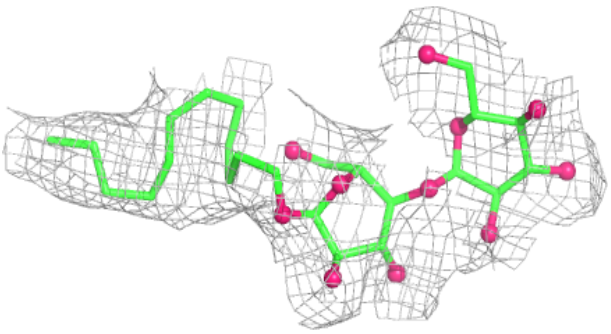


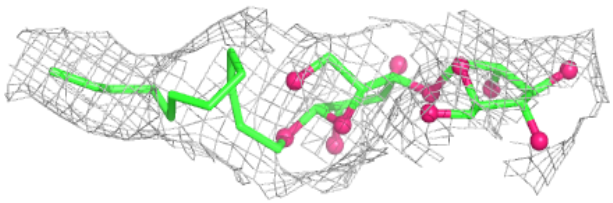


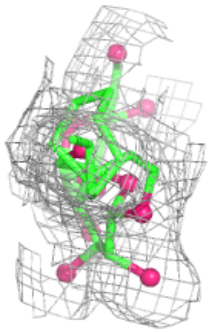


Electron density around LMU A 852:

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

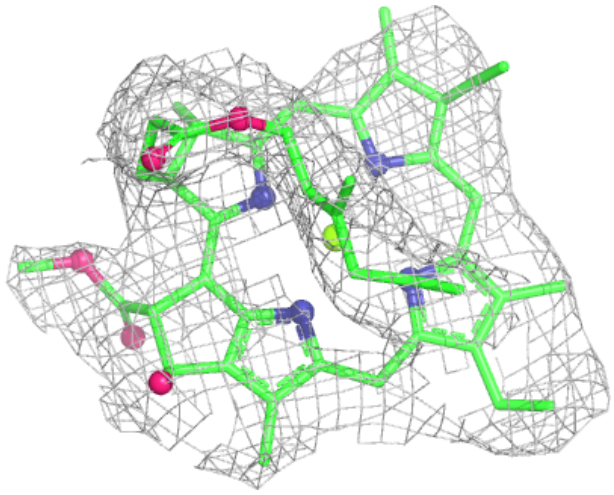


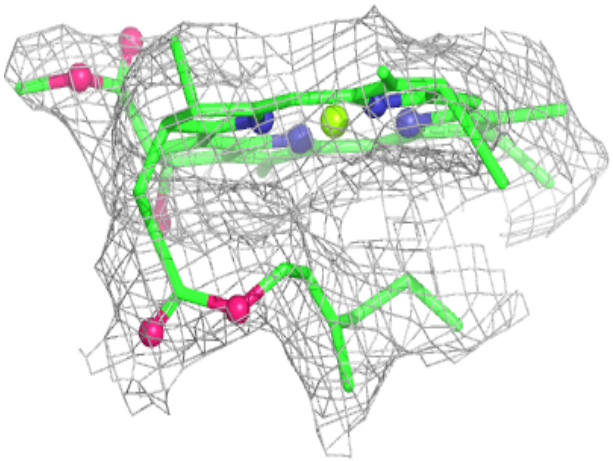




Electron density around CLA A 815:

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

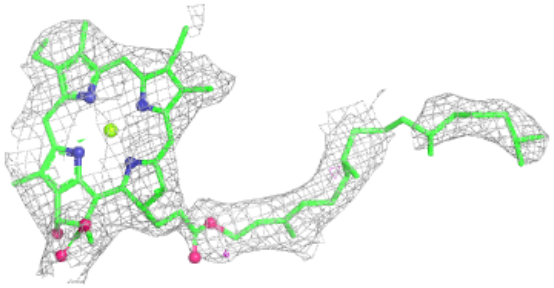


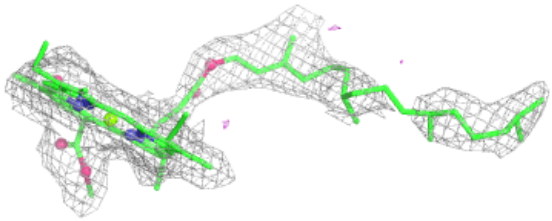


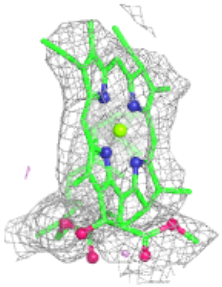


Electron density around CLA A 829:

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

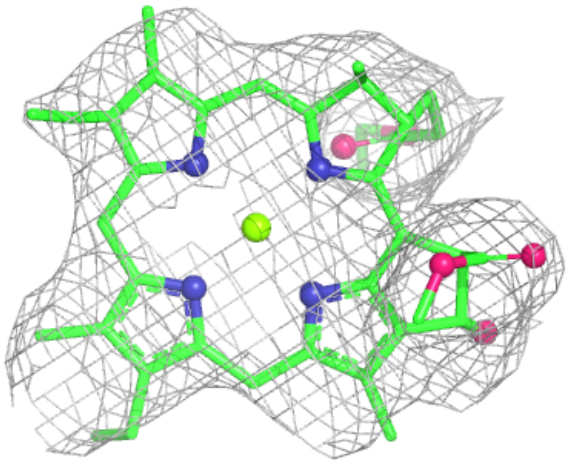


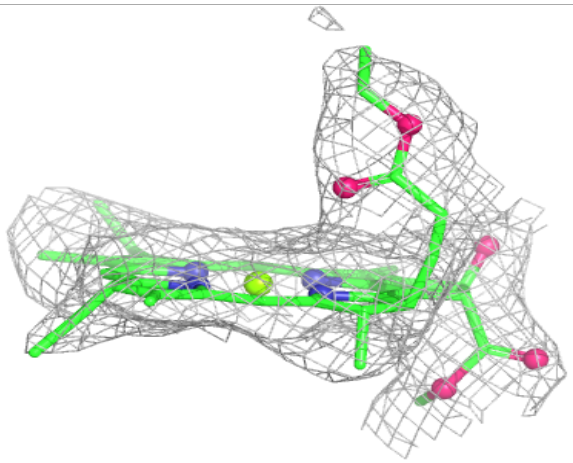


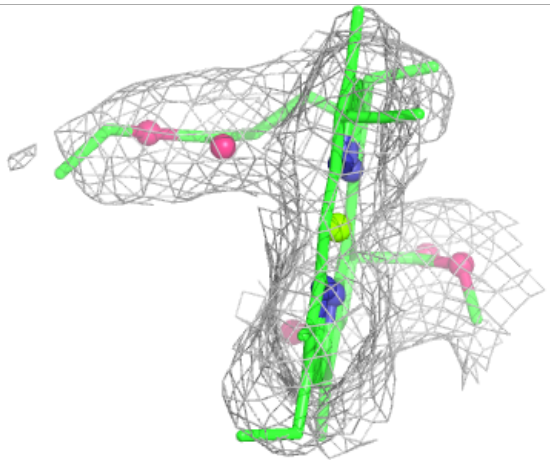


Electron density around CLA L 207:

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

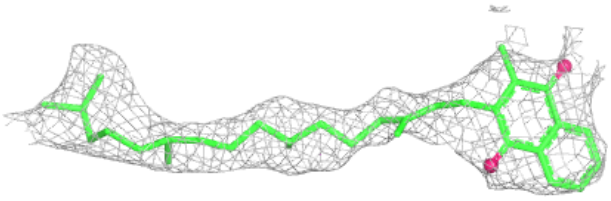


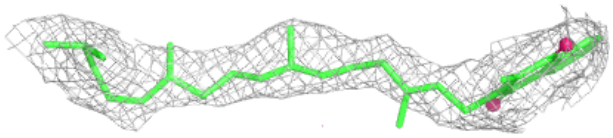


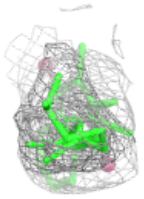


Electron density around PQN A 839:

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

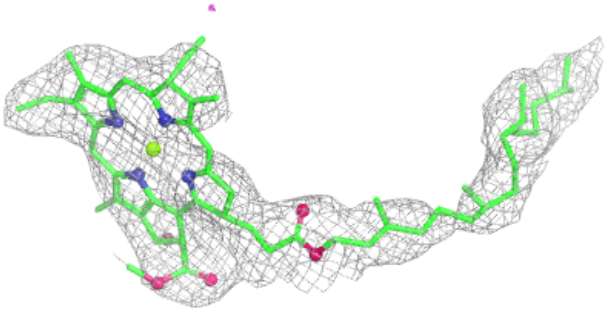


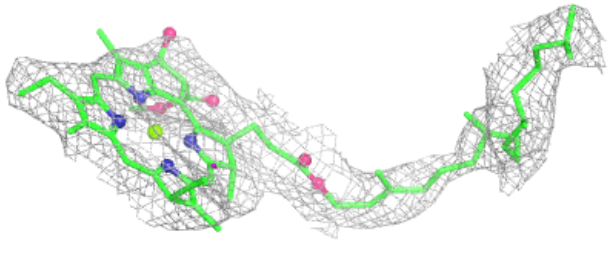


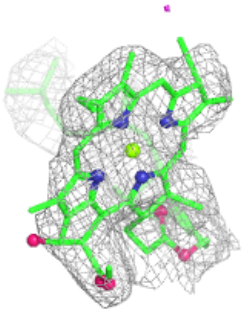


Electron density around CLA A 848:

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

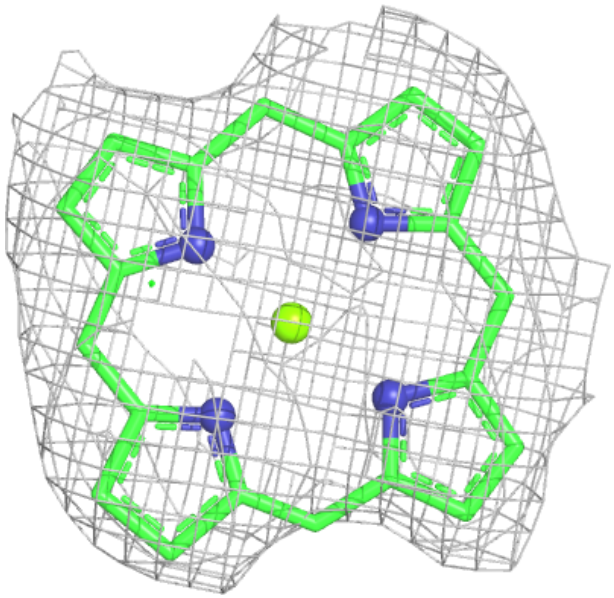


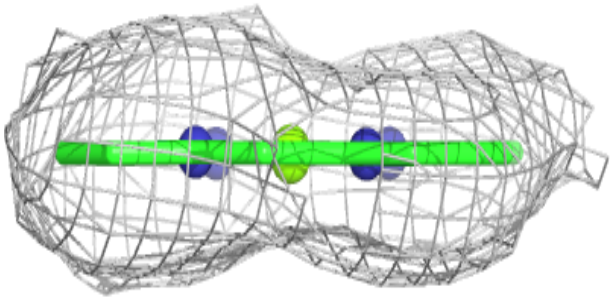


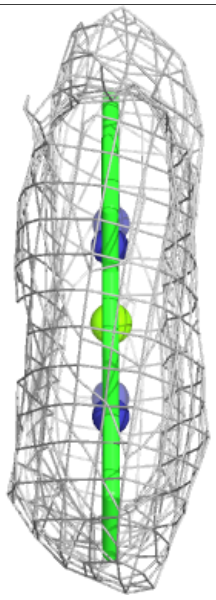


Electron density around CLA 4 312:

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

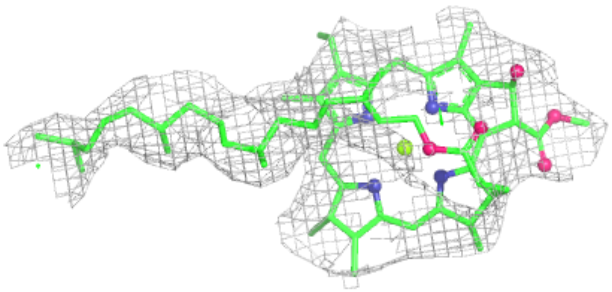


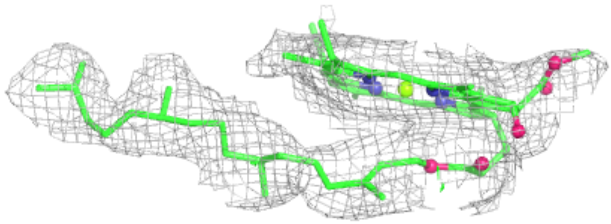


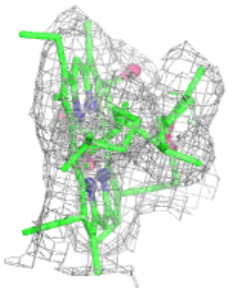


Electron density around CLA A 833:

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

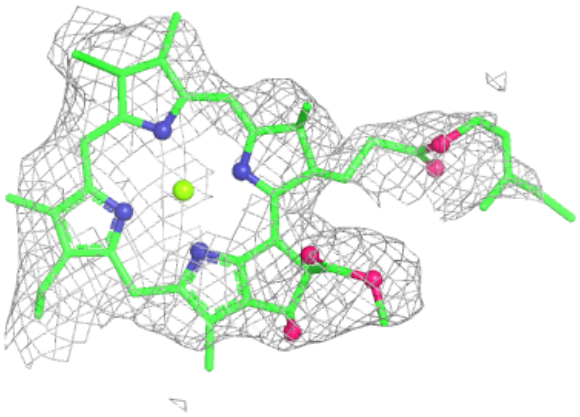


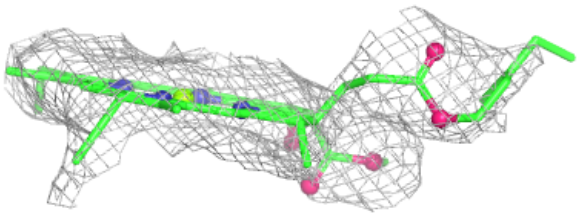


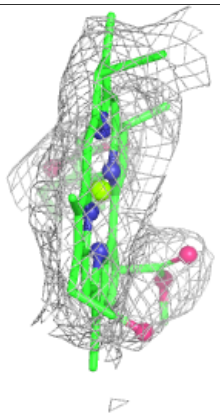


Electron density around CLA A 835:

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



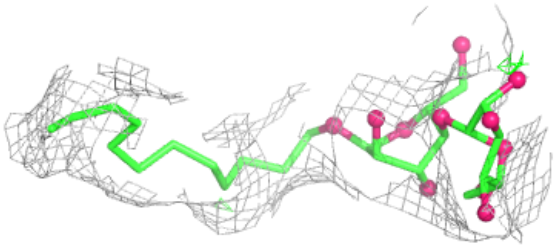


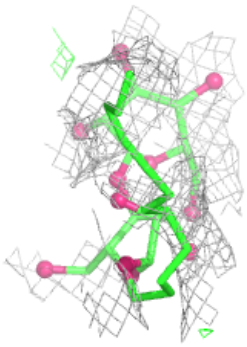


Electron density around LMU G 101:

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

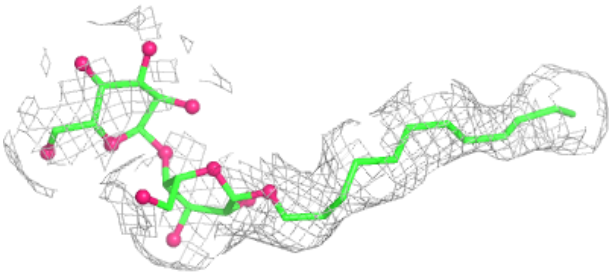


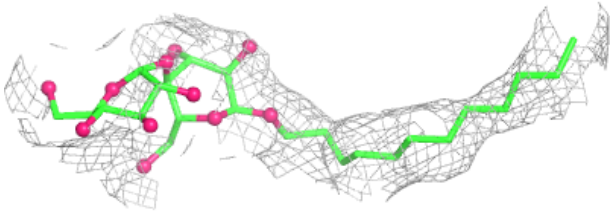


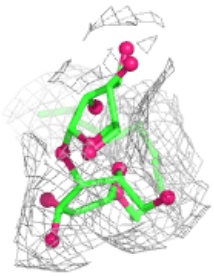


Electron density around LMU R 104:

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

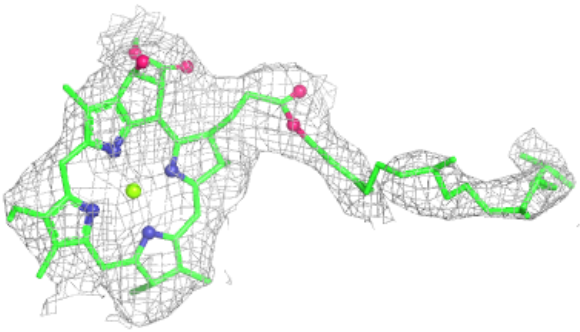


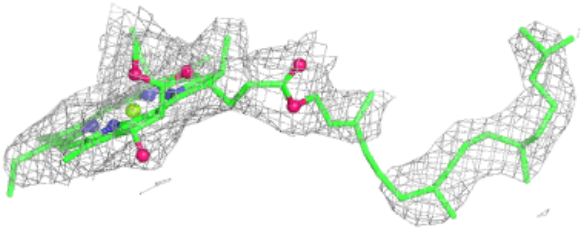




Electron density around CLA B 810:

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

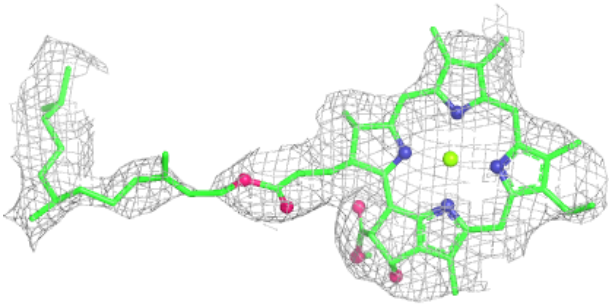


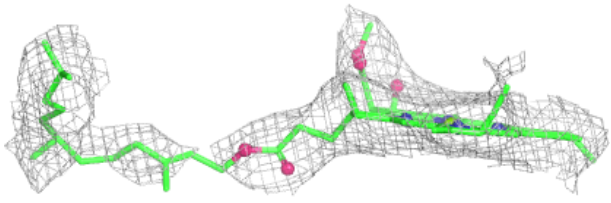


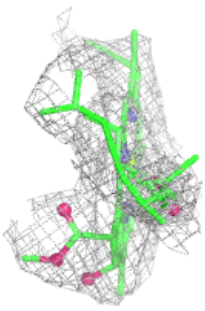


Electron density around CLA B 834:

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

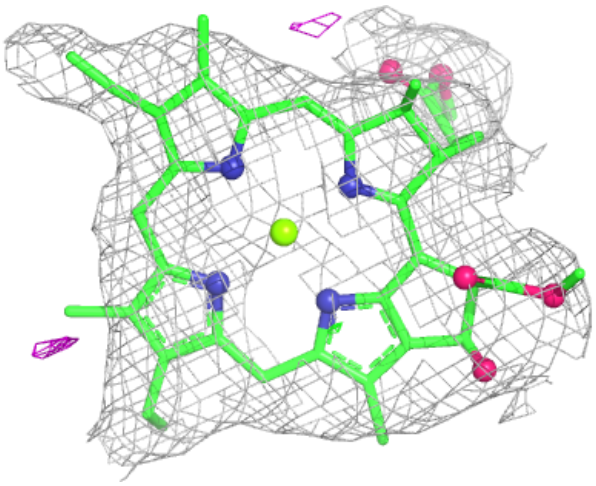


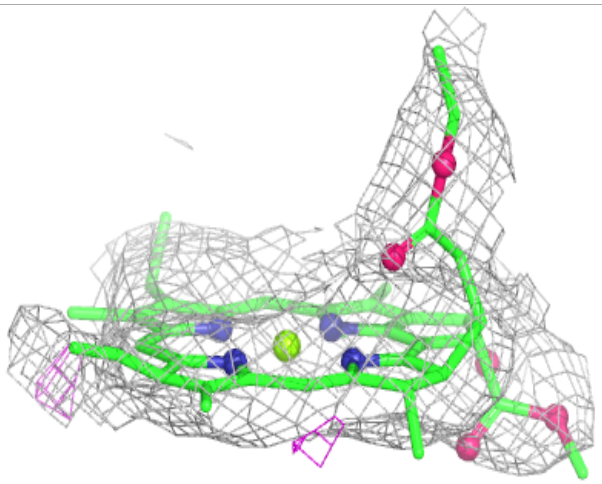


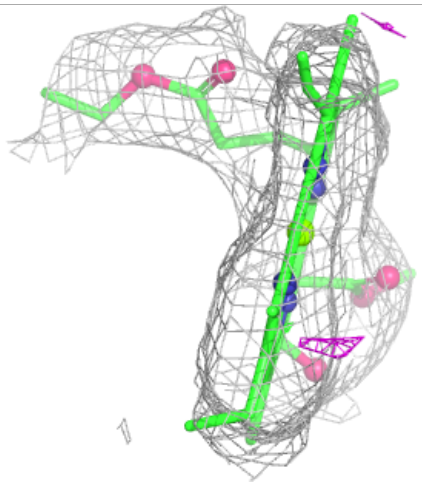


Electron density around CLA B 836:

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

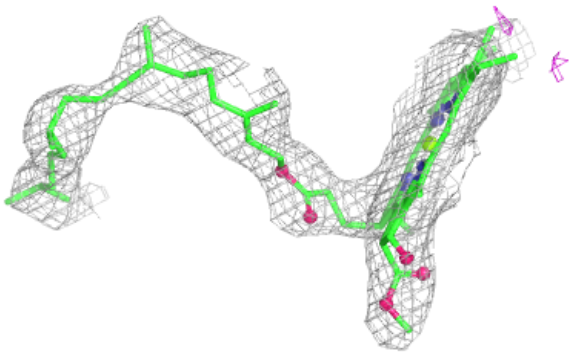


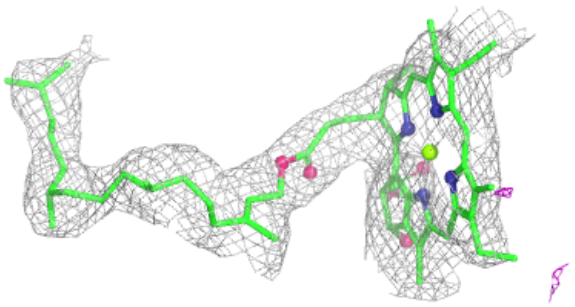


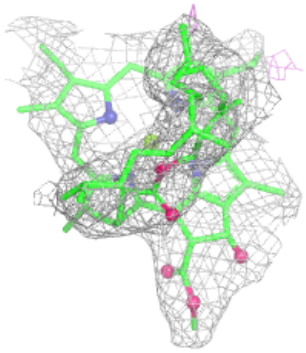


Electron density around CLA B 837:

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

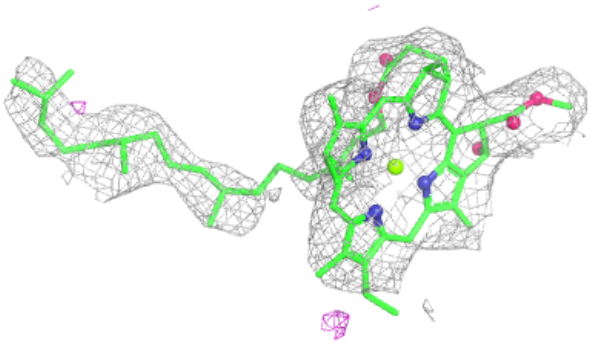


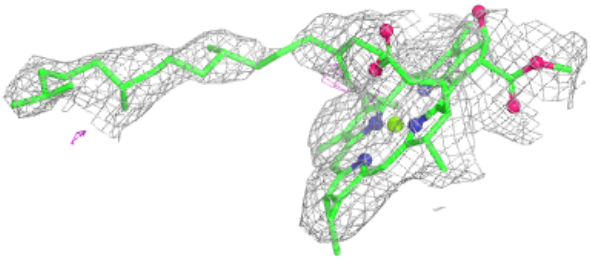


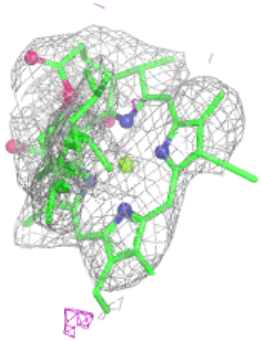


Electron density around CLA A 836:

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

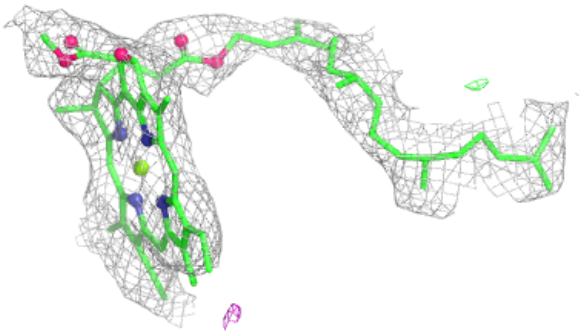


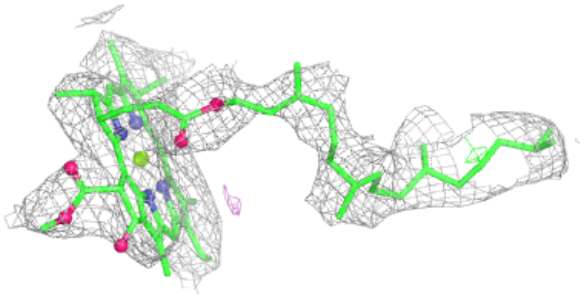


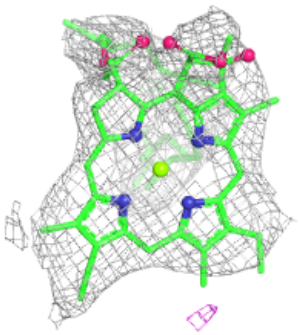


Electron density around CLA B 826:

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

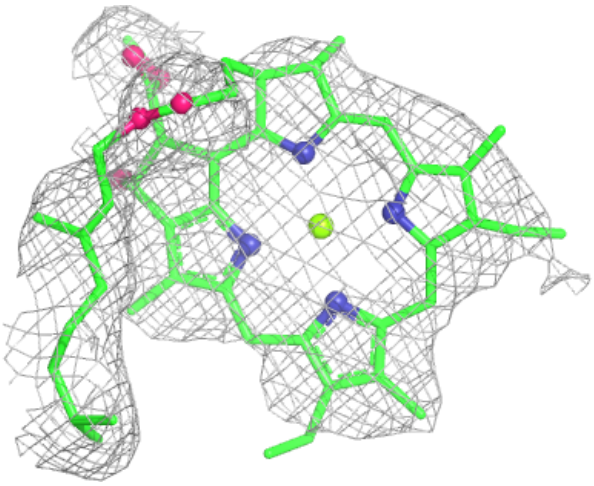


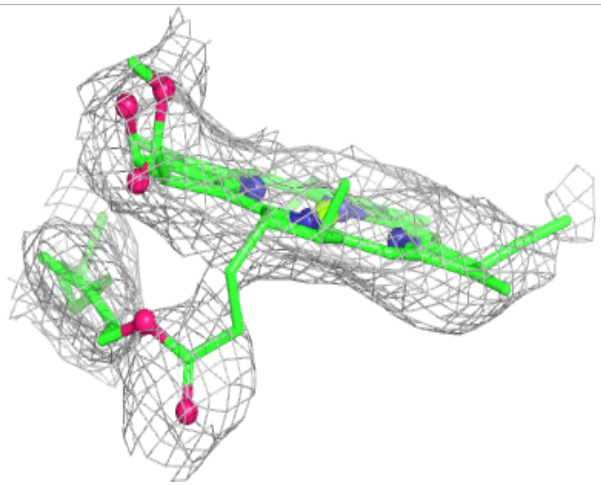


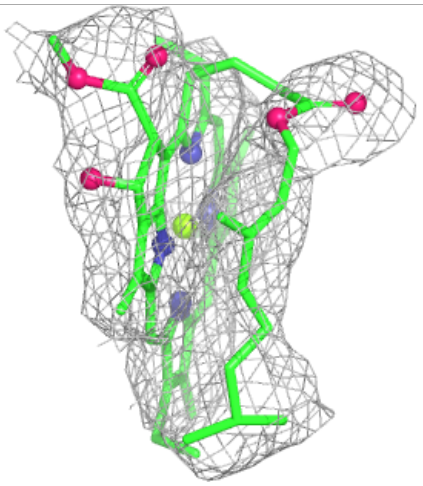


Electron density around CLA A 825:

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

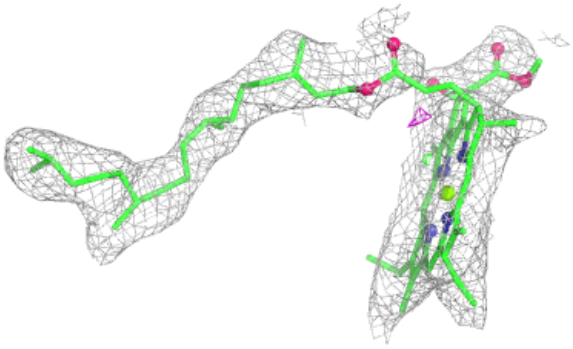


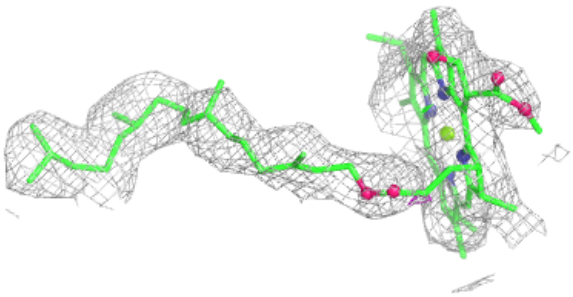


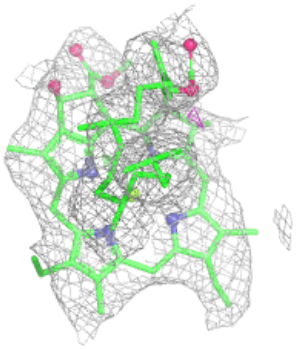


Electron density around CLA A 826:

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

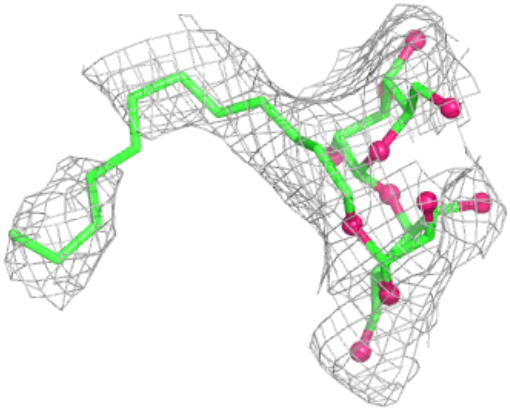


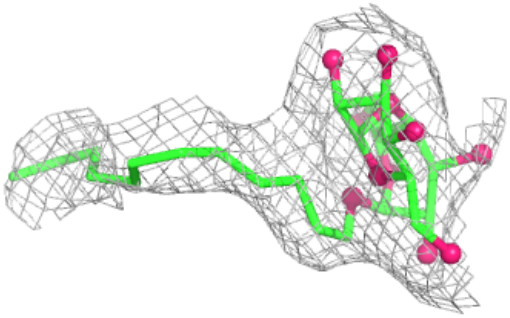


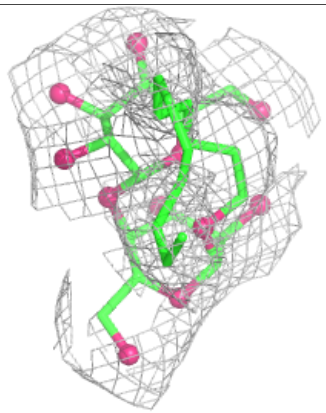


Electron density around LMU H 104:

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

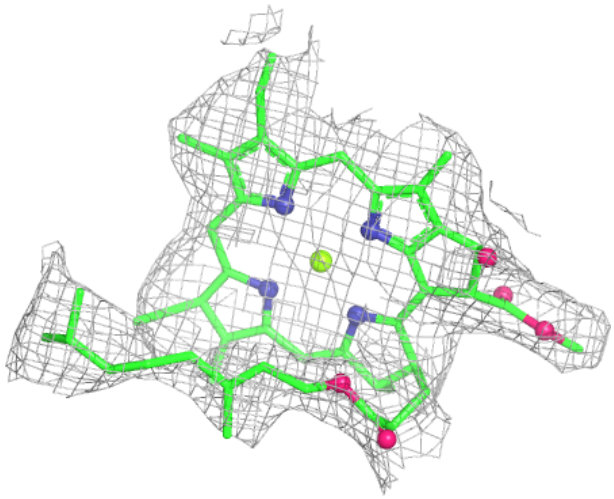


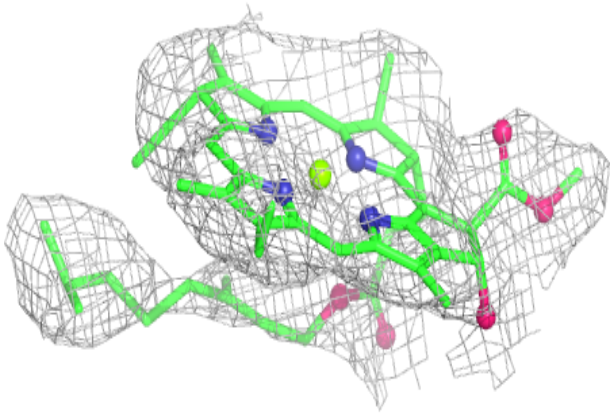




Electron density around CLA B 819:

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

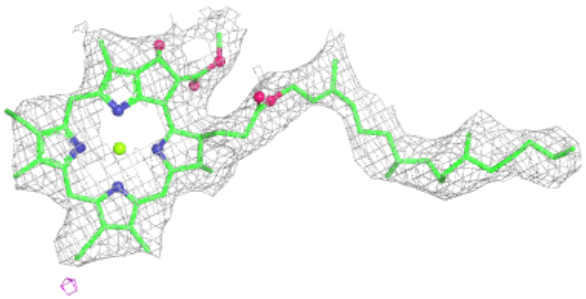


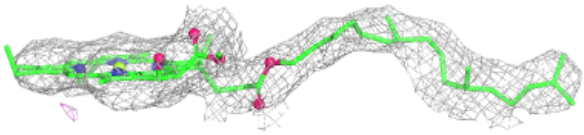


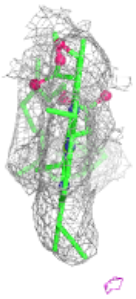


Electron density around CLA A 828:

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

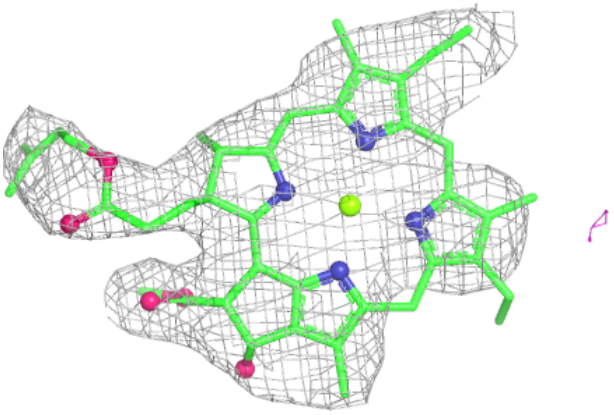


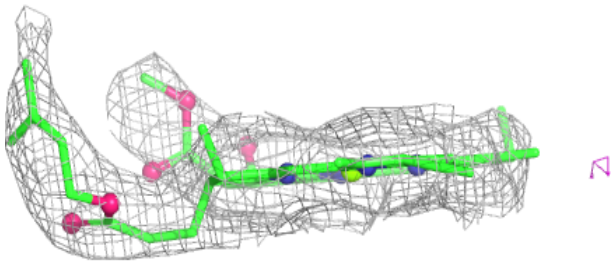


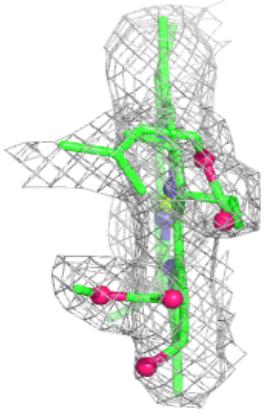


Electron density around CLA A 801:

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

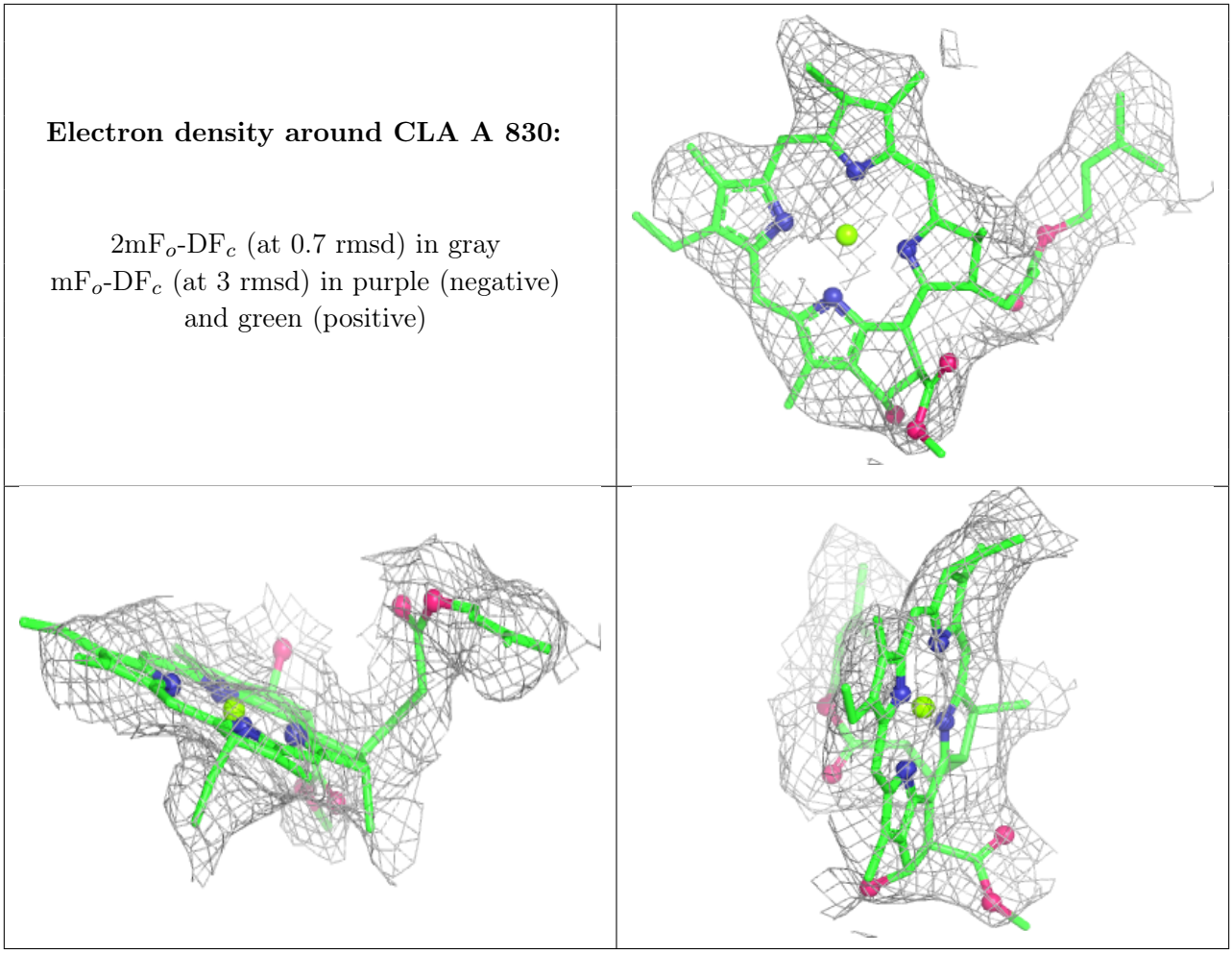






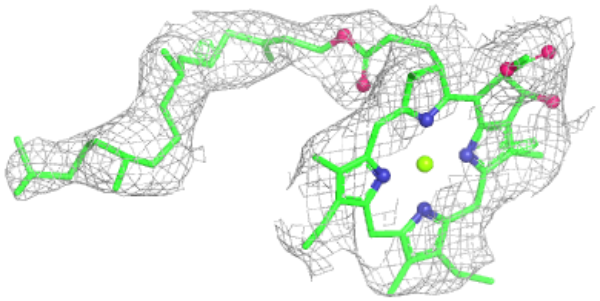
Electron density around CLA A 830:

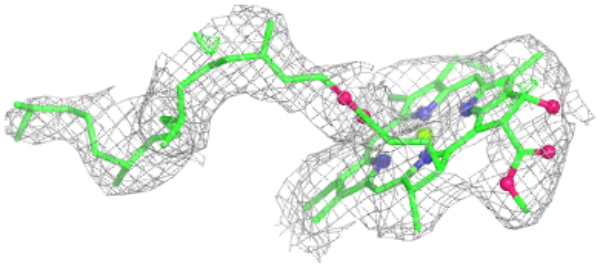
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

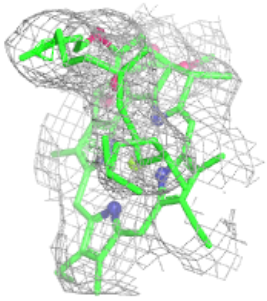


Electron density around CLA A 806:

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

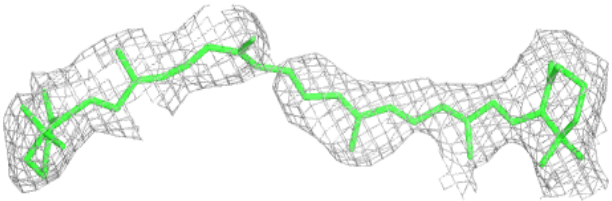


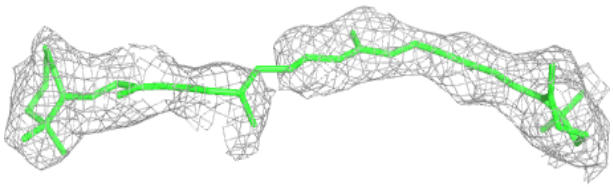


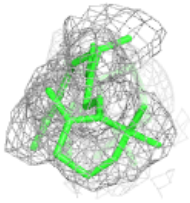


Electron density around BCR I 101:

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

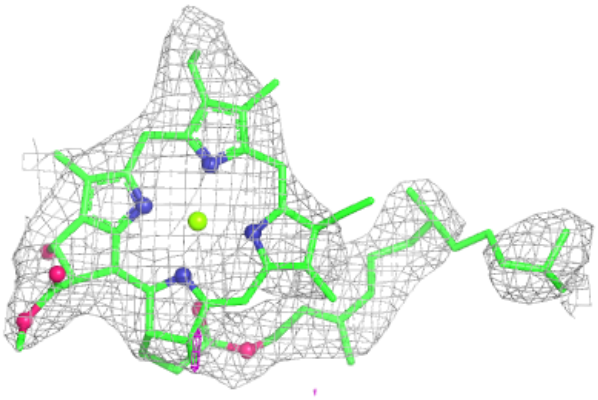


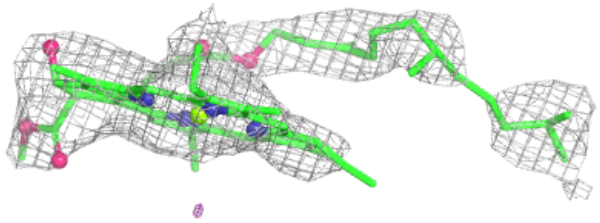


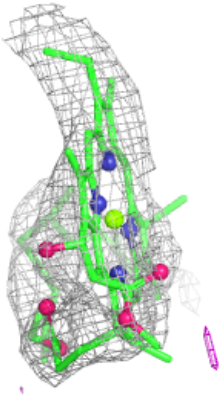


Electron density around CLA B 815:

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

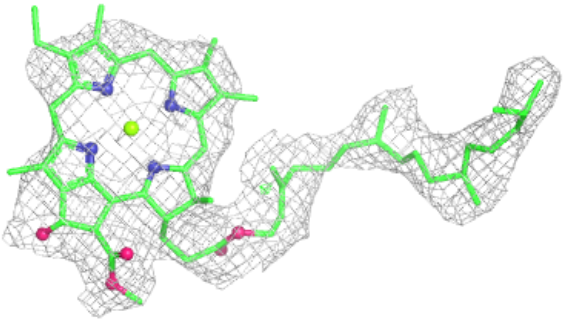


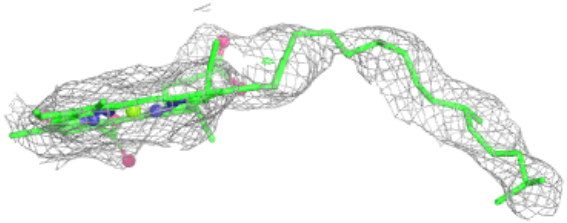


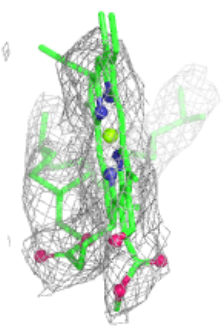


Electron density around CLA B 849:

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

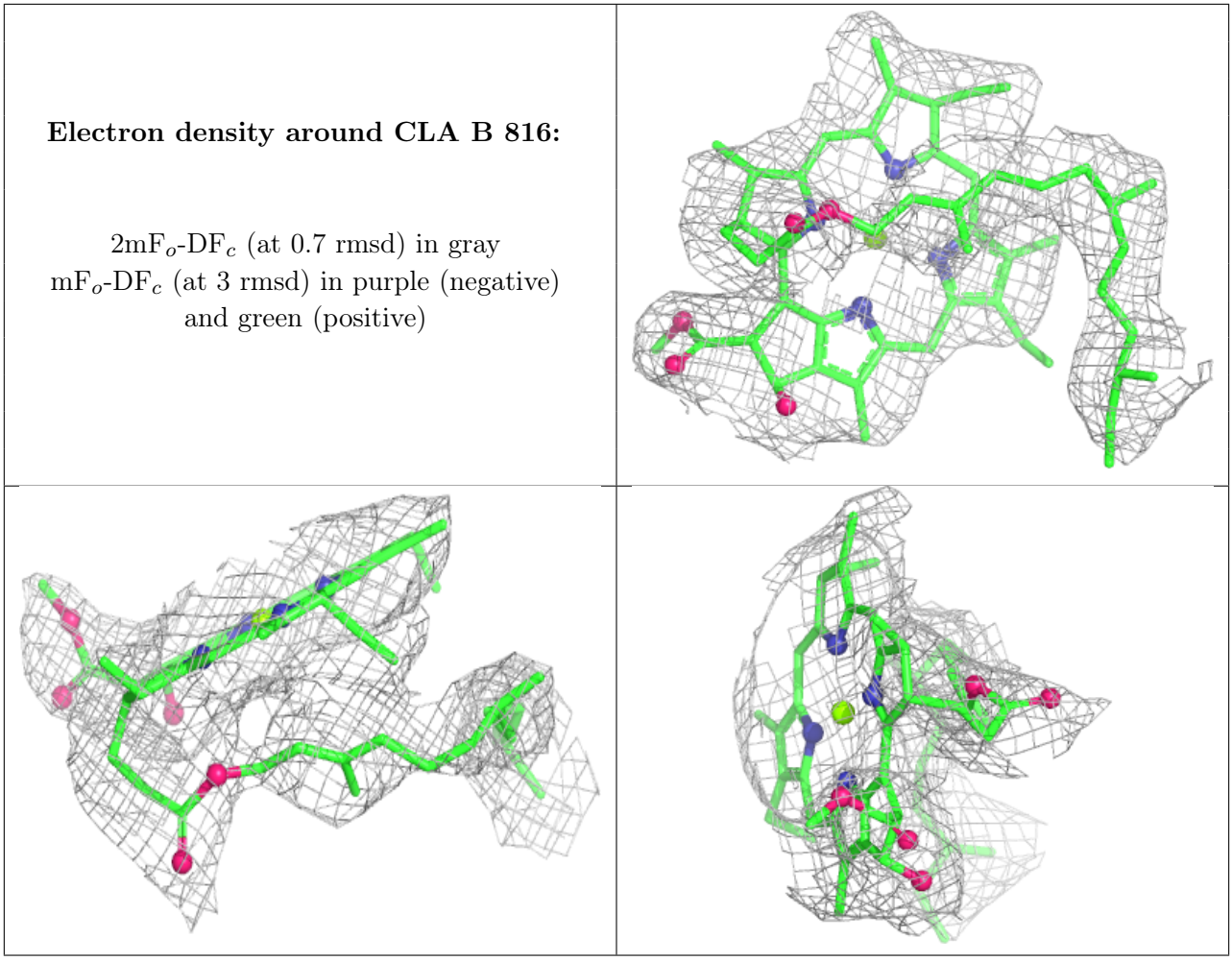






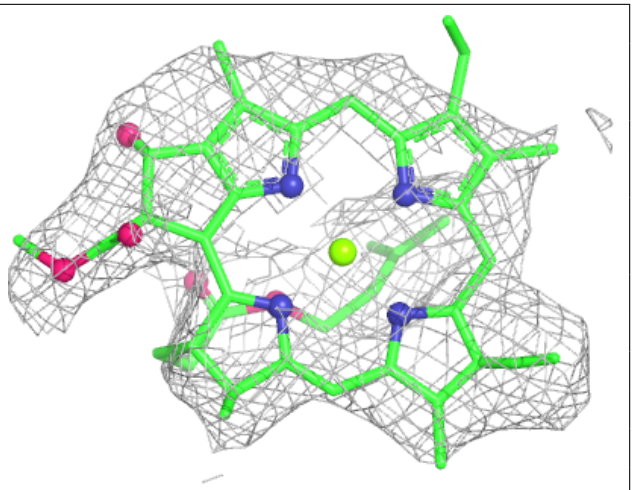
Electron density around CLA B 816:

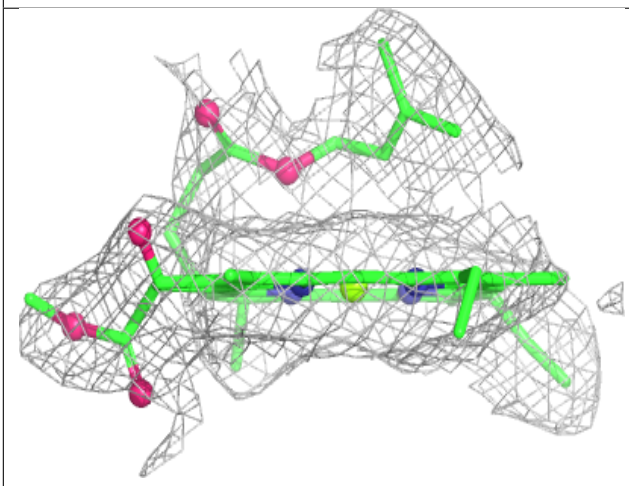
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

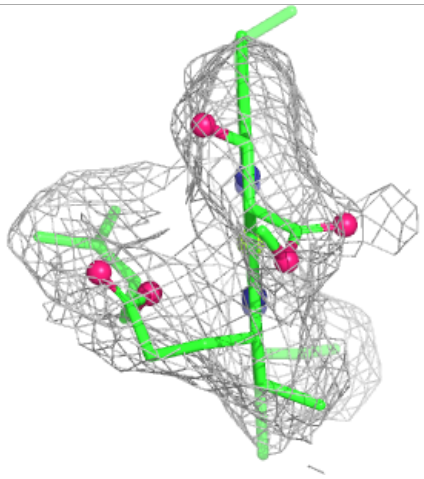


Electron density around CLA B 817:

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

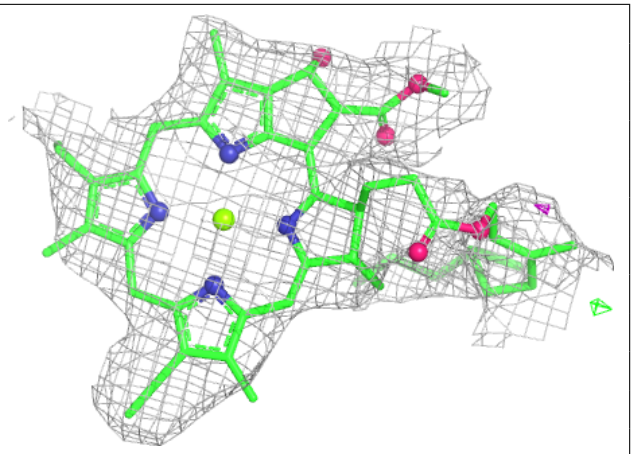


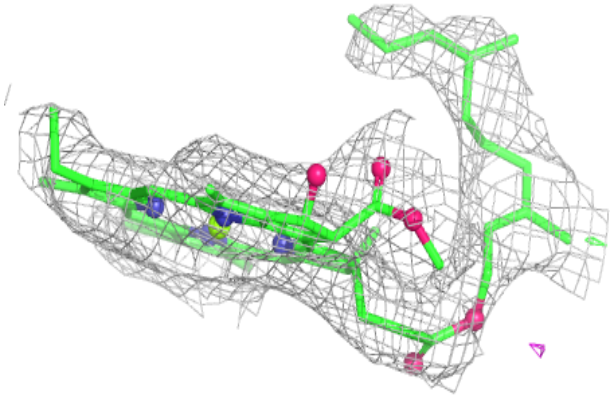


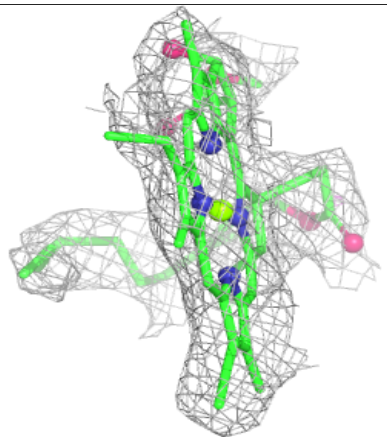


Electron density around CLA A 804:

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

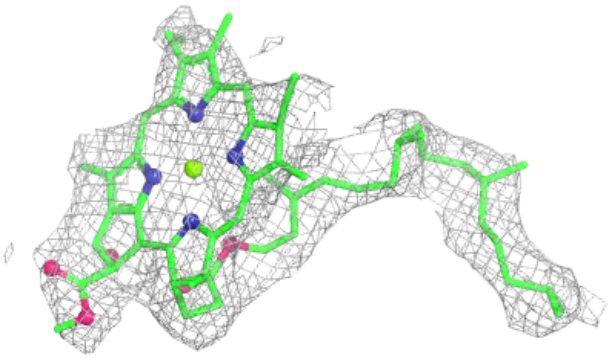


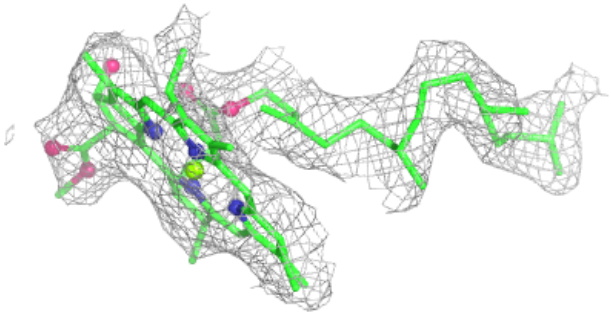


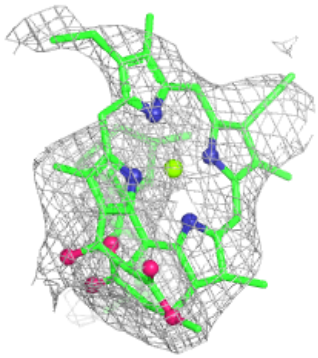


Electron density around CLA L 202:

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

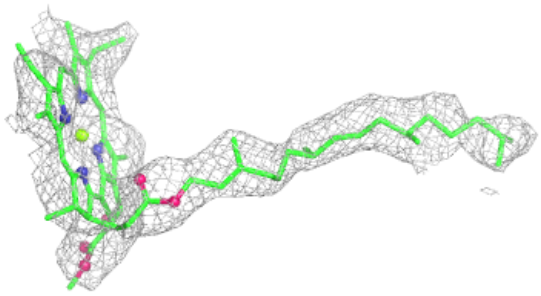


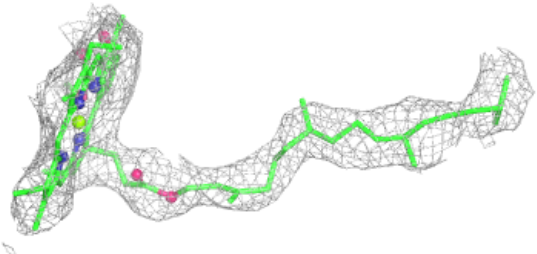


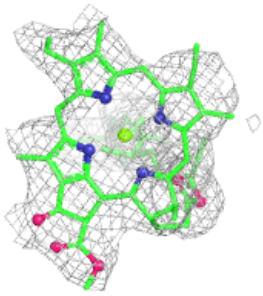


Electron density around CLA B 825:

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

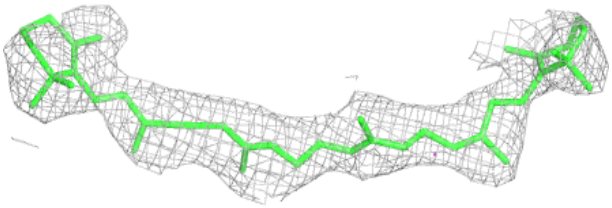


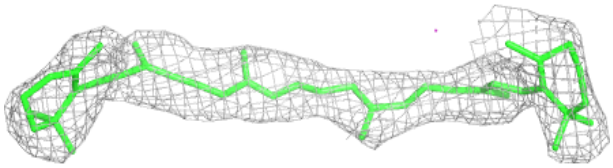


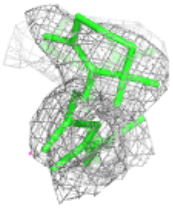


Electron density around BCR B 850:

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

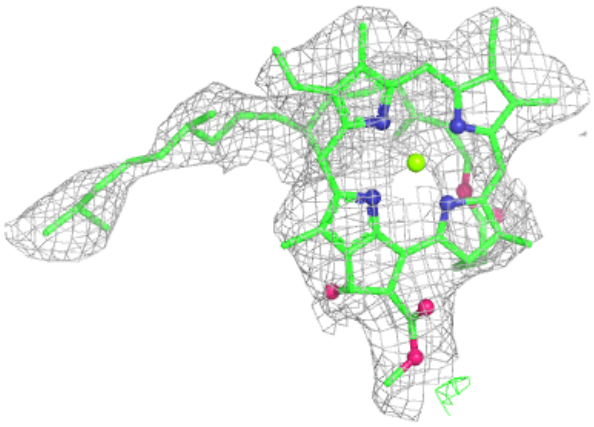


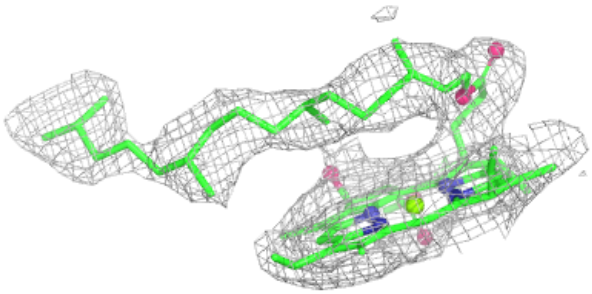




Electron density around CLA B 824:

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

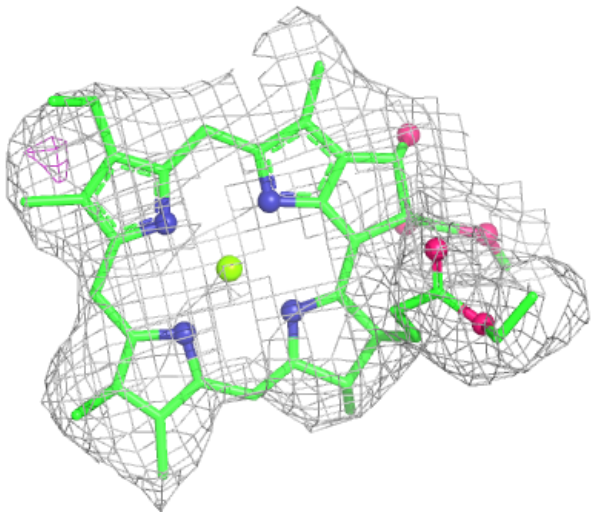


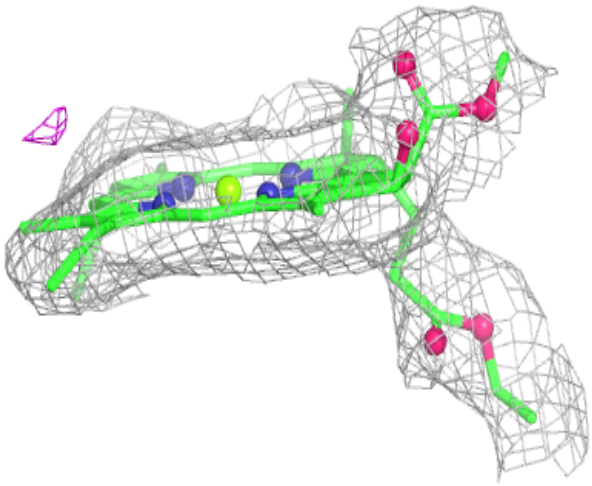


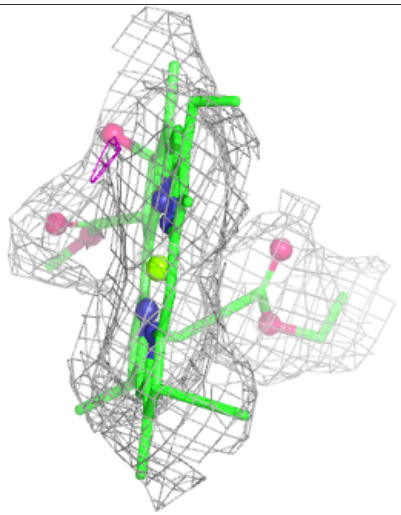


Electron density around CLA A 834:

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

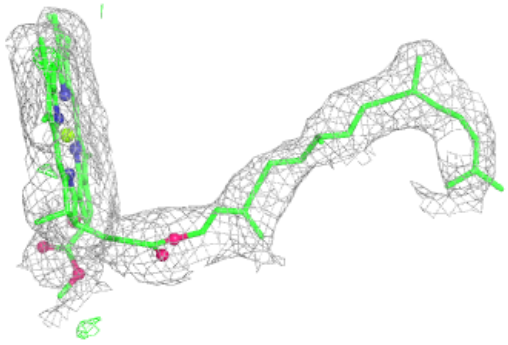


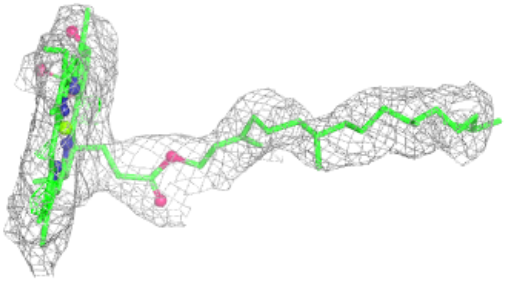


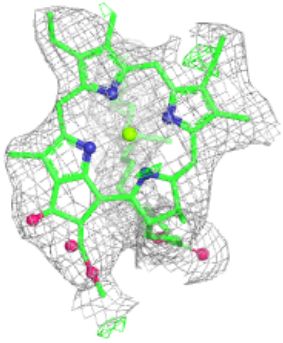


Electron density around CLA B 838:

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

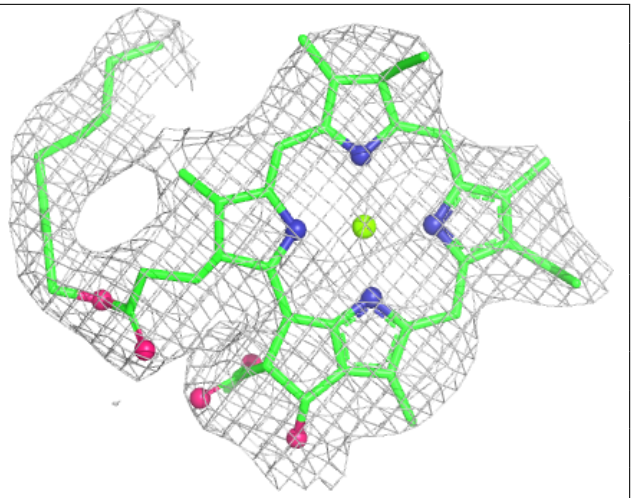


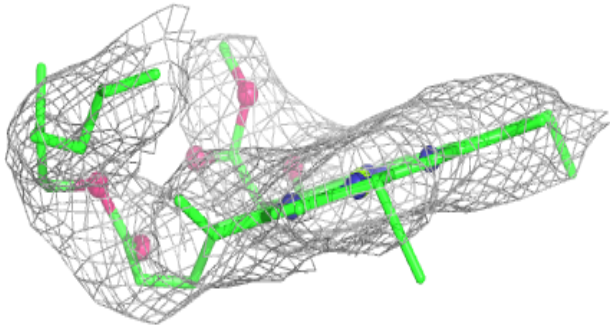


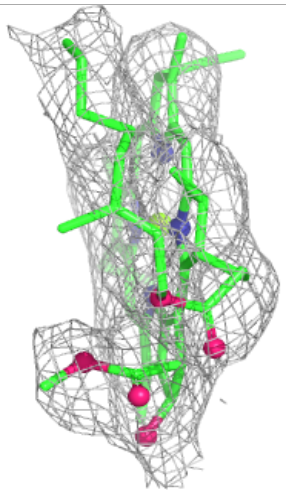


Electron density around CLA B 821:

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

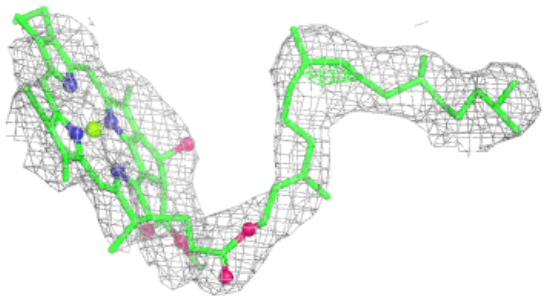


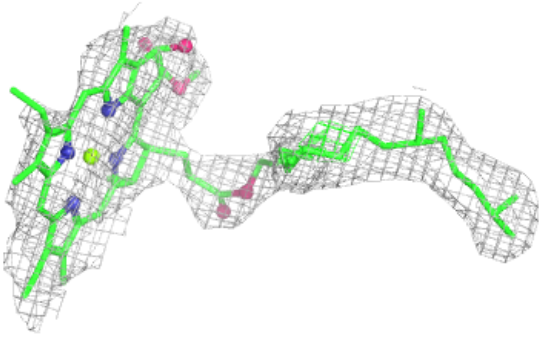


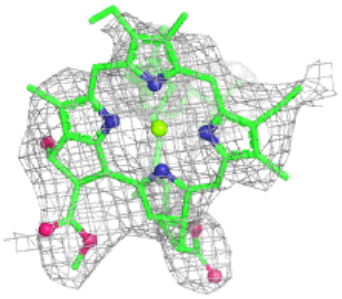


Electron density around CLA B 847:

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

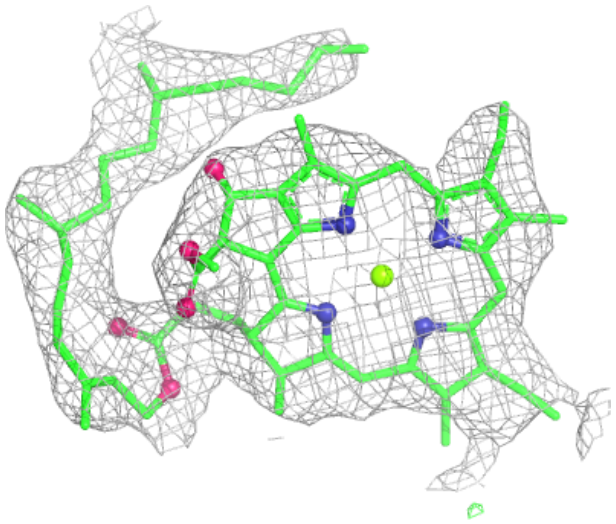


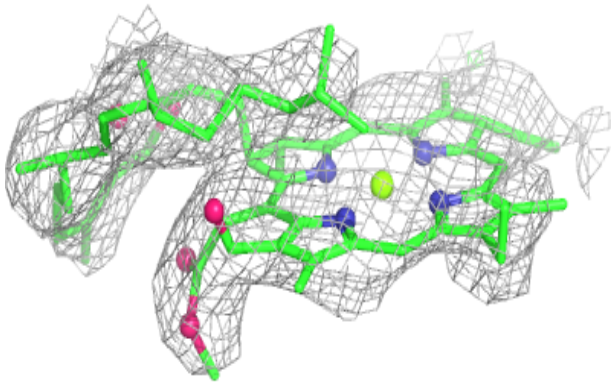


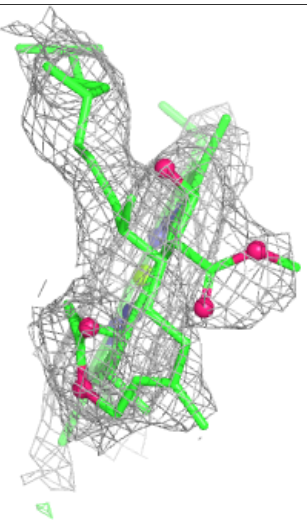


Electron density around CLA B 804:

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

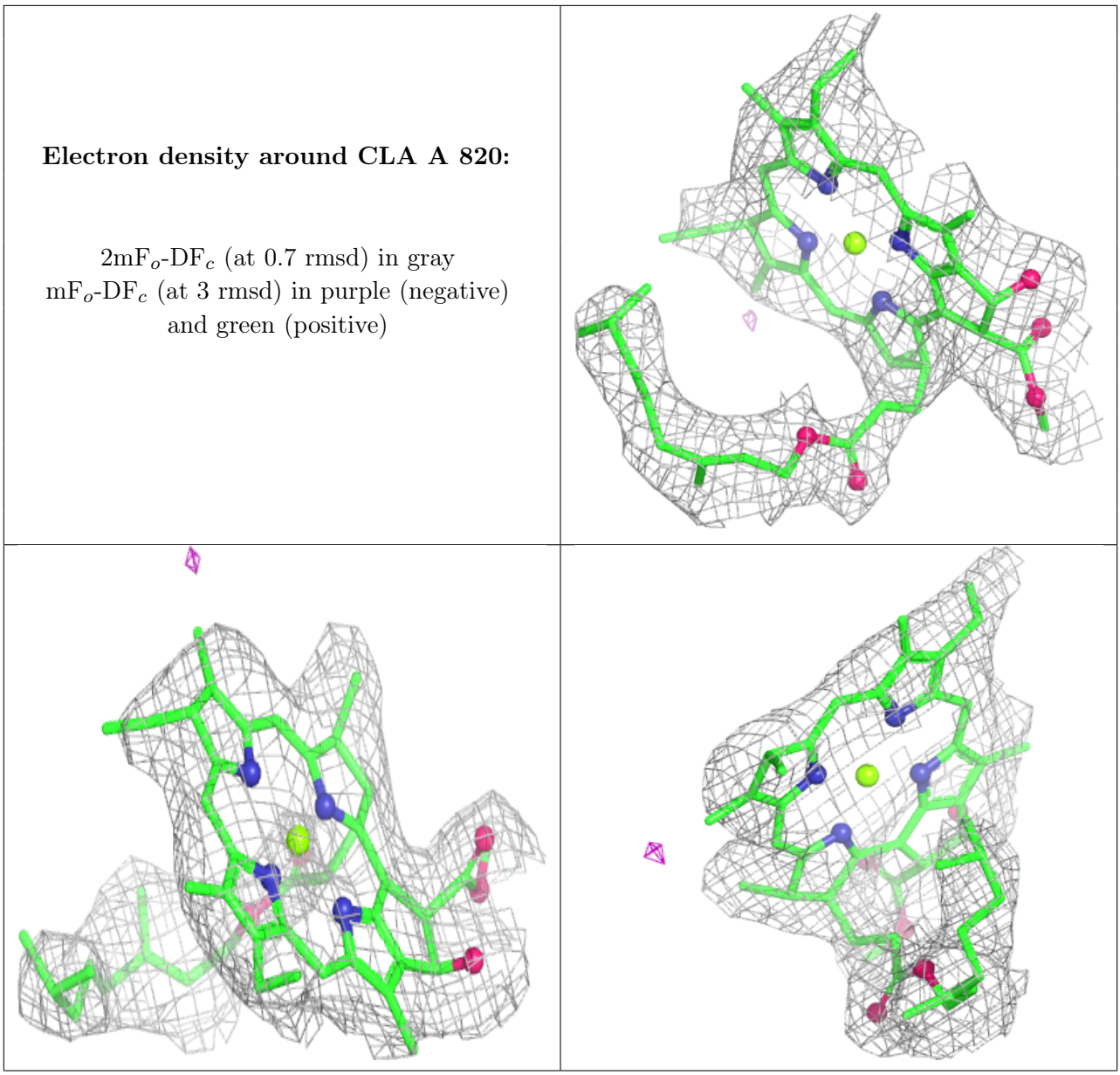






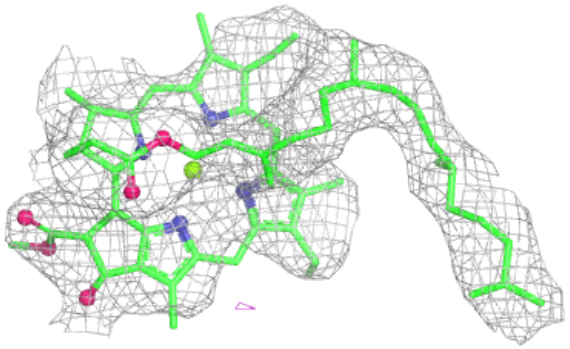
Electron density around CLA A 820:

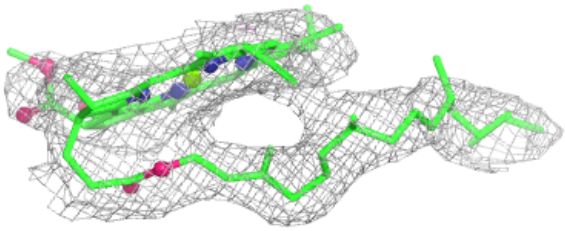
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

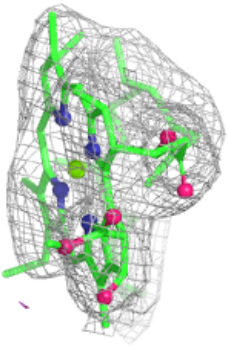


Electron density around CLA B 835:

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

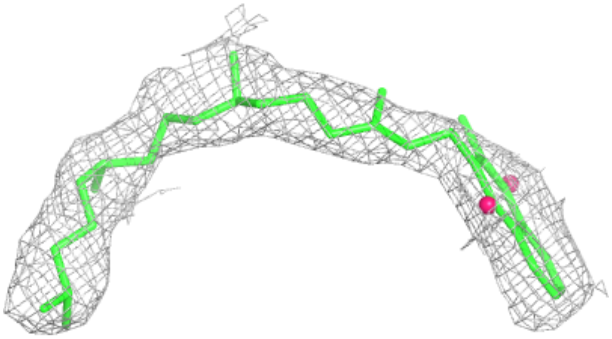


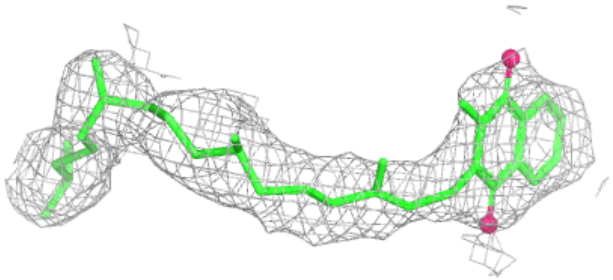




Electron density around PQN B 840:

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

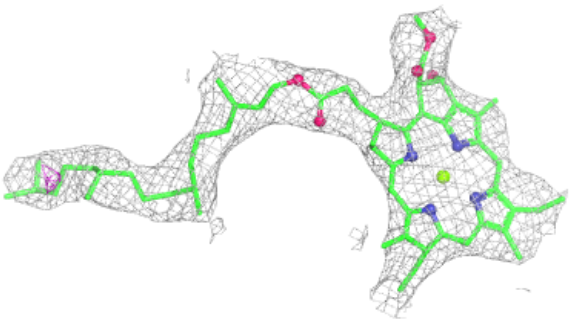


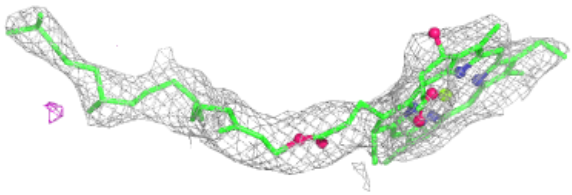


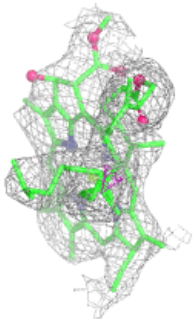


Electron density around CLA B 848:

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

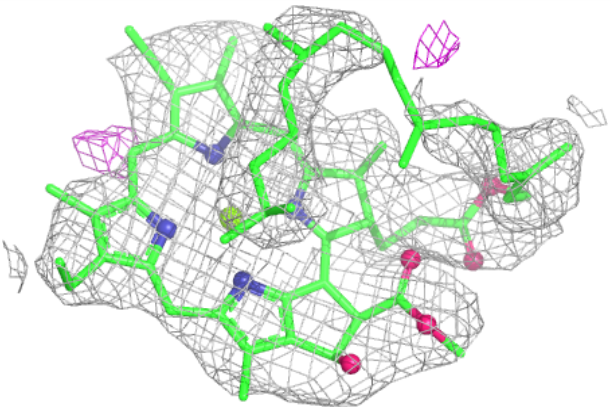


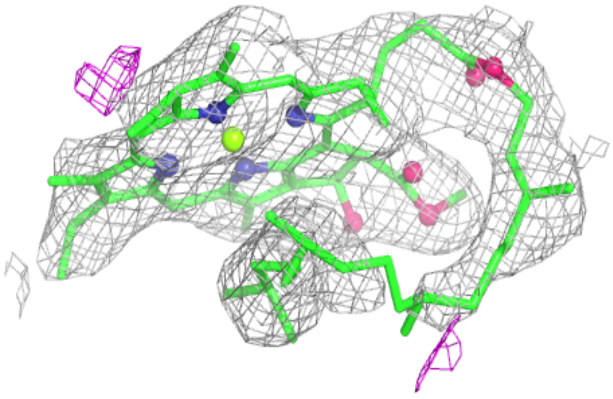


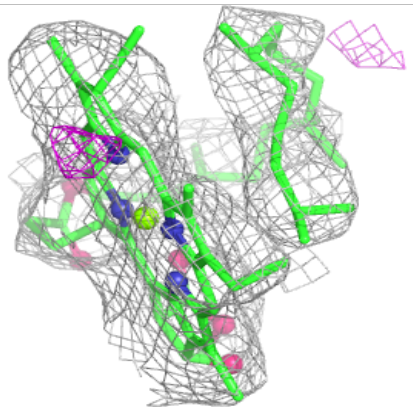


Electron density around CLA B 805:

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

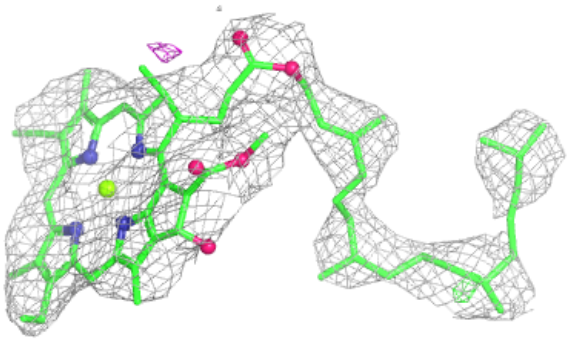


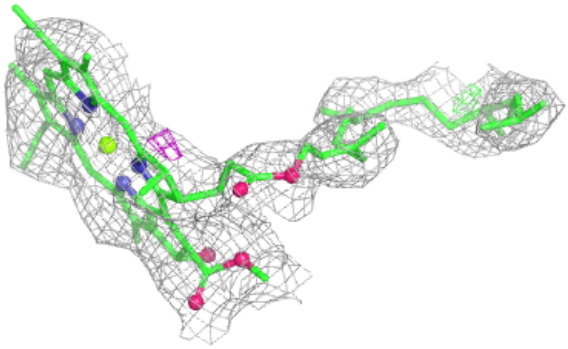


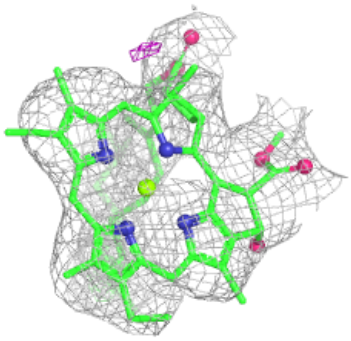


Electron density around CLA A 847:

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

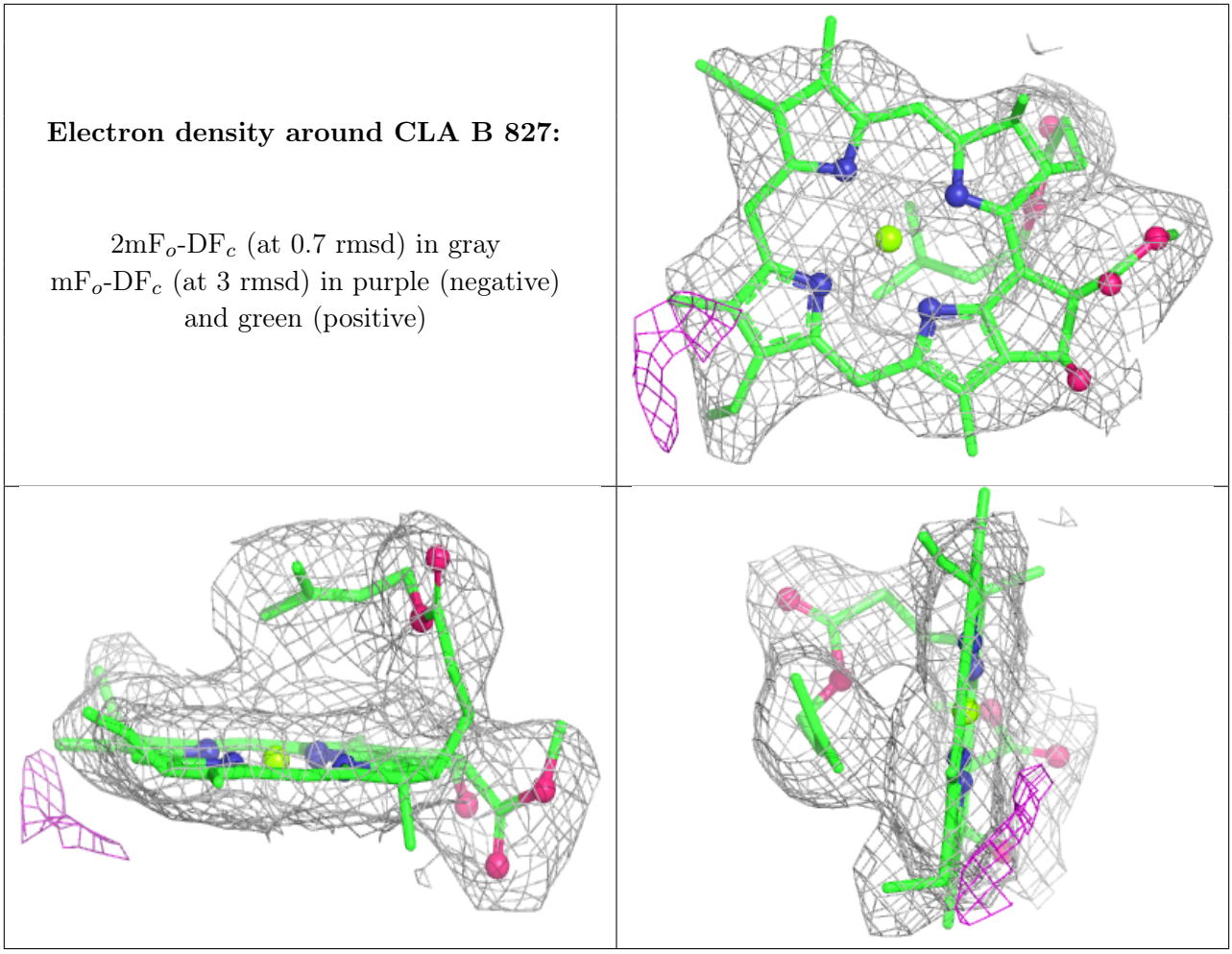






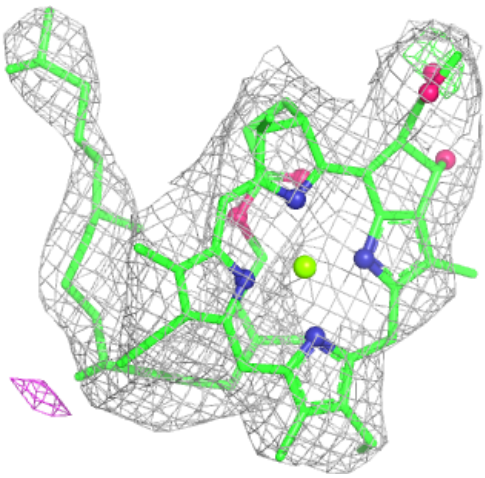
Electron density around CLA B 827:

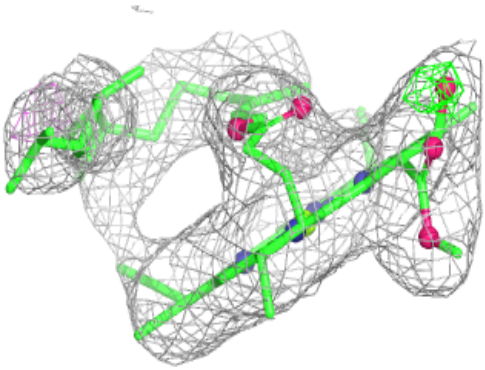
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

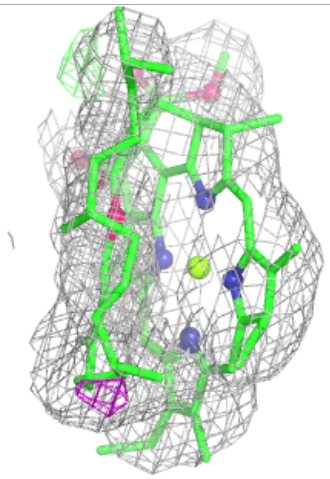


Electron density around CLA B 806:

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

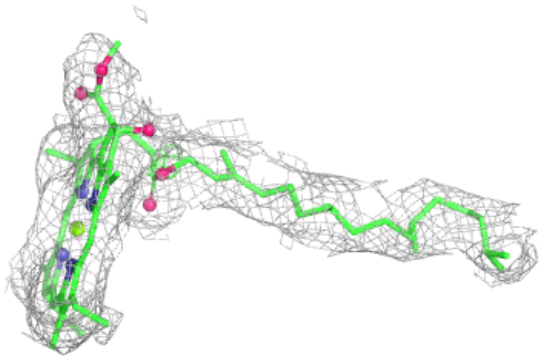


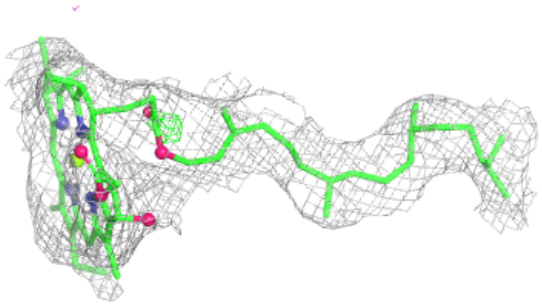


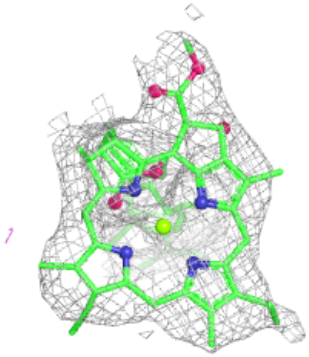


Electron density around CLA A 824:

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







5.5 Other polymers

There are no such residues in this entry.