Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:52 PM UTC

PDB ID	:	7F9O / pdb_00007f9o
EMDB ID	:	EMD-31498
Title	:	PSI-NDH supercomplex of Barley
Authors	:	Wang, W.D.; Shen, L.; Tang, K.; Han, G.Y.; Shen, J.R.; Zhang, X.
Deposited on	:	2021-07-04
Resolution	:	4.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

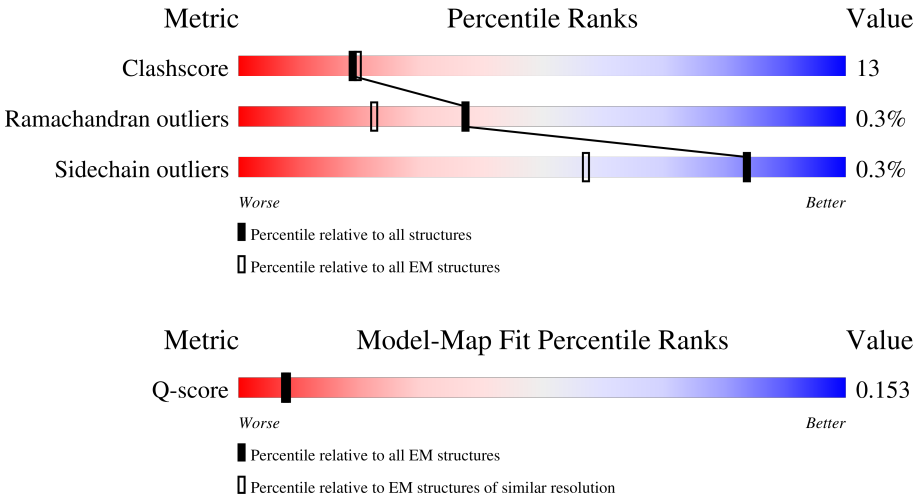
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

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



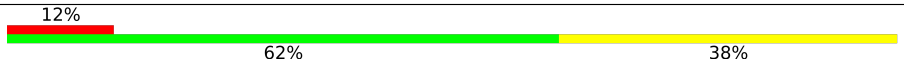
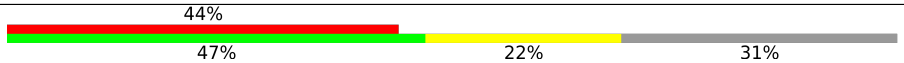
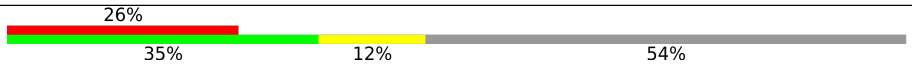
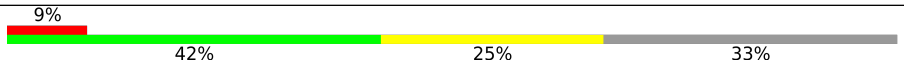
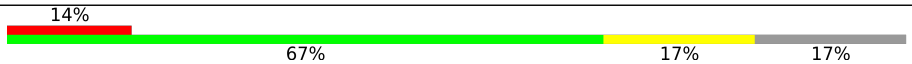
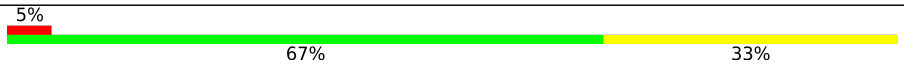
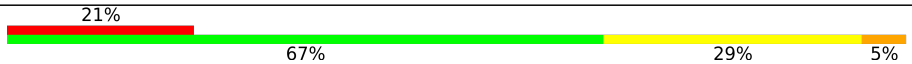
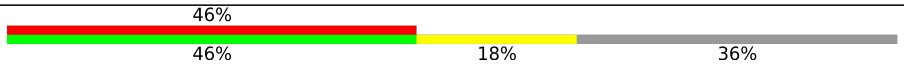
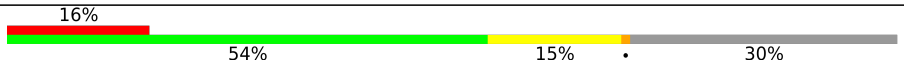
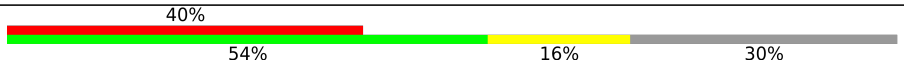
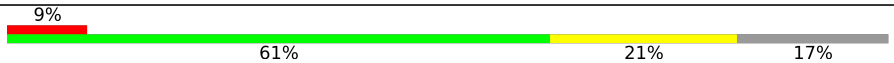
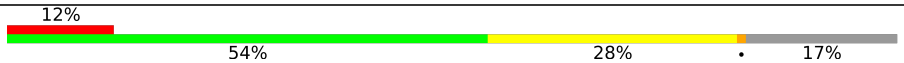
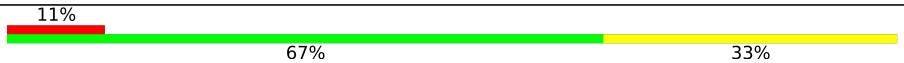
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	750	78% 21%
1	e	750	19% 72% 27%
2	B	734	84% 16%
2	f	734	12% 72% 28%

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Mol	Chain	Length	Quality of chain
3	C	81	
3	g	81	
4	D	205	
4	h	205	
5	E	147	
5	i	147	
6	F	235	
6	j	235	
7	H	143	
7	k	143	
8	I	36	
8	l	36	
9	J	42	
9	m	42	
10	K	131	
10	n	131	
11	L	209	
11	o	209	
12	1	247	
12	p	247	
13	2	255	
14	3	269	
14	q	269	
15	5	257	
16	G	346	

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Mol	Chain	Length	Quality of chain
17	M	483	76% 23%
18	N	117	11% 79% 20%
19	O	499	74% 26%
20	P	100	78% 22%
21	Q	777	65% 21% 14%
22	R	176	80% 20%
23	S	383	63% 60% 40%
24	T	165	52% 76% 23%
25	U	159	58% 64% 36%
26	V	245	27% 51% 28% 21%
27	W	192	22% 17% 18% 64%
28	X	213	28% 37% 15% 47%
29	Y	233	22% 40% 20% 39%
30	Z	61	93% 7%
31	a	154	68% 29%
32	b	216	51% 9% 40%
33	c	227	45% 14% 41%
34	4	130	77% 23%
35	d	243	56% 14% 29%
36	6	469	49% 23% 27%
37	7	361	55% 33% 12%
38	8	119	75% 23%
39	9	83	71% 28%
40	0	155	85% 12%
41	r	197	7% 69% 31%

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Mol	Chain	Length	Quality of chain
42	s	211	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
43	CL0	A	801	X	-	-	-
43	CL0	e	801	X	-	-	-
44	CLA	1	504	X	-	-	-
44	CLA	1	505	X	-	-	-
44	CLA	1	506	X	-	-	-
44	CLA	1	507	X	-	-	-
44	CLA	1	508	X	-	-	-
44	CLA	1	510	X	-	-	-
44	CLA	1	511	X	-	-	-
44	CLA	1	515	X	-	-	-
44	CLA	2	504	X	-	-	-
44	CLA	2	506	X	-	-	-
44	CLA	2	507	X	-	-	-
44	CLA	2	508	X	-	-	-
44	CLA	2	509	X	-	-	-
44	CLA	2	510	X	-	-	-
44	CLA	2	511	X	-	-	-
44	CLA	2	514	X	-	-	-
44	CLA	3	301	X	-	-	-
44	CLA	3	306	X	-	-	-
44	CLA	3	307	X	-	-	-
44	CLA	3	308	X	-	-	-
44	CLA	3	310	X	-	-	-
44	CLA	3	311	X	-	-	-
44	CLA	3	312	X	-	-	-
44	CLA	3	313	X	-	-	-
44	CLA	3	314	X	-	-	-
44	CLA	3	316	X	-	-	-
44	CLA	3	317	X	-	-	-
44	CLA	3	318	X	-	-	-
44	CLA	5	305	X	-	-	-
44	CLA	5	306	X	-	-	-
44	CLA	5	307	X	-	-	-
44	CLA	5	308	X	-	-	-
44	CLA	5	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	CLA	5	310	X	-	-	-
44	CLA	5	311	X	-	-	-
44	CLA	5	312	X	-	-	-
44	CLA	5	313	X	-	-	-
44	CLA	5	316	X	-	-	-
44	CLA	A	802	X	-	-	-
44	CLA	A	803	X	-	-	-
44	CLA	A	804	X	-	-	-
44	CLA	A	805	X	-	-	-
44	CLA	A	806	X	-	-	-
44	CLA	A	807	X	-	-	-
44	CLA	A	808	X	-	-	-
44	CLA	A	809	X	-	-	-
44	CLA	A	810	X	-	-	-
44	CLA	A	811	X	-	-	-
44	CLA	A	812	X	-	-	-
44	CLA	A	813	X	-	-	-
44	CLA	A	814	X	-	-	-
44	CLA	A	815	X	-	-	-
44	CLA	A	816	X	-	-	-
44	CLA	A	817	X	-	-	-
44	CLA	A	818	X	-	-	-
44	CLA	A	819	X	-	-	-
44	CLA	A	820	X	-	-	-
44	CLA	A	821	X	-	-	-
44	CLA	A	822	X	-	-	-
44	CLA	A	823	X	-	-	-
44	CLA	A	824	X	-	-	-
44	CLA	A	825	X	-	-	-
44	CLA	A	826	X	-	-	-
44	CLA	A	827	X	-	-	-
44	CLA	A	828	X	-	-	-
44	CLA	A	829	X	-	-	-
44	CLA	A	830	X	-	-	-
44	CLA	A	831	X	-	-	-
44	CLA	A	832	X	-	-	-
44	CLA	A	833	X	-	-	-
44	CLA	A	834	X	-	-	-
44	CLA	A	835	X	-	-	-
44	CLA	A	836	X	-	-	-
44	CLA	A	837	X	-	-	-
44	CLA	A	838	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	CLA	A	839	X	-	-	-
44	CLA	A	840	X	-	-	-
44	CLA	A	842	X	-	-	-
44	CLA	A	852	X	-	-	-
44	CLA	B	801	X	-	-	-
44	CLA	B	802	X	-	-	-
44	CLA	B	803	X	-	-	-
44	CLA	B	804	X	-	-	-
44	CLA	B	805	X	-	-	-
44	CLA	B	806	X	-	-	-
44	CLA	B	807	X	-	-	-
44	CLA	B	808	X	-	-	-
44	CLA	B	809	X	-	-	-
44	CLA	B	810	X	-	-	-
44	CLA	B	811	X	-	-	-
44	CLA	B	812	X	-	-	-
44	CLA	B	813	X	-	-	-
44	CLA	B	814	X	-	-	-
44	CLA	B	815	X	-	-	-
44	CLA	B	816	X	-	-	-
44	CLA	B	817	X	-	-	-
44	CLA	B	818	X	-	-	-
44	CLA	B	819	X	-	-	-
44	CLA	B	820	X	-	-	-
44	CLA	B	821	X	-	-	-
44	CLA	B	822	X	-	-	-
44	CLA	B	823	X	-	-	-
44	CLA	B	824	X	-	-	-
44	CLA	B	825	X	-	-	-
44	CLA	B	826	X	-	-	-
44	CLA	B	827	X	-	-	-
44	CLA	B	828	X	-	-	-
44	CLA	B	829	X	-	-	-
44	CLA	B	830	X	-	-	-
44	CLA	B	831	X	-	-	-
44	CLA	B	832	X	-	-	-
44	CLA	B	833	X	-	-	-
44	CLA	B	834	X	-	-	-
44	CLA	B	835	X	-	-	-
44	CLA	B	837	X	-	-	-
44	CLA	B	838	X	-	-	-
44	CLA	B	839	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	CLA	B	840	X	-	-	-
44	CLA	B	841	X	-	-	-
44	CLA	B	842	X	-	-	-
44	CLA	F	802	X	-	-	-
44	CLA	F	803	X	-	-	-
44	CLA	J	101	X	-	-	-
44	CLA	K	201	X	-	-	-
44	CLA	K	202	X	-	-	-
44	CLA	K	203	X	-	-	-
44	CLA	K	205	X	-	-	-
44	CLA	L	301	X	-	-	-
44	CLA	L	302	X	-	-	-
44	CLA	L	303	X	-	-	-
44	CLA	L	304	X	-	-	-
44	CLA	e	802	X	-	-	-
44	CLA	e	803	X	-	-	-
44	CLA	e	804	X	-	-	-
44	CLA	e	805	X	-	-	-
44	CLA	e	806	X	-	-	-
44	CLA	e	807	X	-	-	-
44	CLA	e	808	X	-	-	-
44	CLA	e	809	X	-	-	-
44	CLA	e	810	X	-	-	-
44	CLA	e	811	X	-	-	-
44	CLA	e	812	X	-	-	-
44	CLA	e	813	X	-	-	-
44	CLA	e	814	X	-	-	-
44	CLA	e	815	X	-	-	-
44	CLA	e	816	X	-	-	-
44	CLA	e	817	X	-	-	-
44	CLA	e	818	X	-	-	-
44	CLA	e	819	X	-	-	-
44	CLA	e	820	X	-	-	-
44	CLA	e	821	X	-	-	-
44	CLA	e	822	X	-	-	-
44	CLA	e	823	X	-	-	-
44	CLA	e	824	X	-	-	-
44	CLA	e	825	X	-	-	-
44	CLA	e	826	X	-	-	-
44	CLA	e	827	X	-	-	-
44	CLA	e	828	X	-	-	-
44	CLA	e	829	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	CLA	e	830	X	-	-	-
44	CLA	e	831	X	-	-	-
44	CLA	e	832	X	-	-	-
44	CLA	e	833	X	-	-	-
44	CLA	e	834	X	-	-	-
44	CLA	e	835	X	-	-	-
44	CLA	e	836	X	-	-	-
44	CLA	e	837	X	-	-	-
44	CLA	e	838	X	-	-	-
44	CLA	e	839	X	-	-	-
44	CLA	e	840	X	-	-	-
44	CLA	e	841	X	-	-	-
44	CLA	e	843	X	-	-	-
44	CLA	e	852	X	-	-	-
44	CLA	e	853	X	-	-	-
44	CLA	f	801	X	-	-	-
44	CLA	f	803	X	-	-	-
44	CLA	f	804	X	-	-	-
44	CLA	f	805	X	-	-	-
44	CLA	f	806	X	-	-	-
44	CLA	f	807	X	-	-	-
44	CLA	f	808	X	-	-	-
44	CLA	f	809	X	-	-	-
44	CLA	f	810	X	-	-	-
44	CLA	f	811	X	-	-	-
44	CLA	f	812	X	-	-	-
44	CLA	f	813	X	-	-	-
44	CLA	f	814	X	-	-	-
44	CLA	f	815	X	-	-	-
44	CLA	f	816	X	-	-	-
44	CLA	f	817	X	-	-	-
44	CLA	f	818	X	-	-	-
44	CLA	f	819	X	-	-	-
44	CLA	f	820	X	-	-	-
44	CLA	f	821	X	-	-	-
44	CLA	f	822	X	-	-	-
44	CLA	f	823	X	-	-	-
44	CLA	f	824	X	-	-	-
44	CLA	f	825	X	-	-	-
44	CLA	f	826	X	-	-	-
44	CLA	f	827	X	-	-	-
44	CLA	f	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	CLA	f	829	X	-	-	-
44	CLA	f	830	X	-	-	-
44	CLA	f	831	X	-	-	-
44	CLA	f	832	X	-	-	-
44	CLA	f	833	X	-	-	-
44	CLA	f	834	X	-	-	-
44	CLA	f	835	X	-	-	-
44	CLA	f	836	X	-	-	-
44	CLA	f	837	X	-	-	-
44	CLA	f	838	X	-	-	-
44	CLA	f	839	X	-	-	-
44	CLA	f	840	X	-	-	-
44	CLA	f	841	X	-	-	-
44	CLA	f	842	X	-	-	-
44	CLA	f	843	X	-	-	-
44	CLA	j	802	X	-	-	-
44	CLA	m	101	X	-	-	-
44	CLA	m	102	X	-	-	-
44	CLA	n	201	X	-	-	-
44	CLA	n	202	X	-	-	-
44	CLA	n	203	X	-	-	-
44	CLA	n	205	X	-	-	-
44	CLA	o	302	X	-	-	-
44	CLA	o	303	X	-	-	-
44	CLA	o	304	X	-	-	-
44	CLA	p	504	X	-	-	-
44	CLA	p	506	X	-	-	-
44	CLA	p	507	X	-	-	-
44	CLA	p	508	X	-	-	-
44	CLA	p	509	X	-	-	-
44	CLA	p	510	X	-	-	-
44	CLA	p	511	X	-	-	-
44	CLA	p	513	X	-	-	-
44	CLA	p	515	X	-	-	-
44	CLA	q	304	X	-	-	-
44	CLA	q	305	X	-	-	-
44	CLA	q	306	X	-	-	-
44	CLA	q	308	X	-	-	-
44	CLA	q	309	X	-	-	-
44	CLA	q	310	X	-	-	-
44	CLA	q	311	X	-	-	-
44	CLA	q	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	CLA	q	314	X	-	-	-
44	CLA	q	316	X	-	-	-
44	CLA	r	304	X	-	-	-
44	CLA	r	305	X	-	-	-
44	CLA	r	306	X	-	-	-
44	CLA	r	307	X	-	-	-
44	CLA	r	308	X	-	-	-
44	CLA	r	309	X	-	-	-
44	CLA	r	310	X	-	-	-
44	CLA	r	311	X	-	-	-
44	CLA	r	312	X	-	-	-
44	CLA	r	315	X	-	-	-
44	CLA	r	317	X	-	-	-
44	CLA	s	504	X	-	-	-
44	CLA	s	506	X	-	-	-
44	CLA	s	507	X	-	-	-
44	CLA	s	508	X	-	-	-
44	CLA	s	509	X	-	-	-
44	CLA	s	510	X	-	-	-
44	CLA	s	511	X	-	-	-
44	CLA	s	514	X	-	-	-
51	LUT	p	502	X	-	-	-
52	CHL	1	512	X	-	-	-
52	CHL	1	514	X	-	-	-
52	CHL	1	517	X	-	-	-
52	CHL	2	512	X	-	-	-
52	CHL	2	513	X	-	-	-
52	CHL	2	515	X	-	-	-
52	CHL	2	516	X	-	-	-
52	CHL	3	302	X	-	-	-
52	CHL	3	315	X	-	-	-
52	CHL	5	314	X	-	-	-
52	CHL	5	315	X	-	-	-
52	CHL	5	317	X	-	-	-
52	CHL	p	512	X	-	-	-
52	CHL	p	514	X	-	-	-
52	CHL	p	517	X	-	-	-
52	CHL	q	313	X	-	-	-
52	CHL	r	313	X	-	-	-
52	CHL	r	314	X	-	-	-
52	CHL	r	316	X	-	-	-
52	CHL	s	512	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	CHL	s	513	X	-	-	-
52	CHL	s	515	X	-	-	-
52	CHL	s	517	X	-	-	-

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 106329 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	742	Total	C	N	O	S	0	0
			5813	3812	983	1000	18		
1	e	742	Total	C	N	O	S	0	0
			5798	3797	987	996	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5851	3835	995	1007	14		
2	f	733	Total	C	N	O	S	0	0
			5840	3832	991	1003	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	81	Total	C	N	O	S	0	0
			610	376	105	117	12		
3	g	81	Total	C	N	O	S	0	0
			613	377	105	119	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	142	Total	C	N	O	S	0	0
			1113	716	193	201	3		
4	h	142	Total	C	N	O	S	0	0
			1111	714	195	199	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	68	Total	C	N	O	0	0
			538	341	98	99		
5	i	68	Total	C	N	O	0	0
			539	341	99	99		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	158	Total	C	N	O	S	0	0
			1204	774	208	219	3		
6	j	158	Total	C	N	O	S	0	0
			1188	768	203	216	1		

- Molecule 7 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	61	Total	C	N	O	0	0
			454	303	76	75		
7	k	61	Total	C	N	O	0	0
			447	298	73	76		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	30	Total	C	N	O		0	0
			232	161	35	36			
8	l	30	Total	C	N	O	S	0	0
			235	163	35	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	42	Total	C	N	O	S	0	0
			333	228	51	53	1		
9	m	42	Total	C	N	O	S	0	0
			332	225	51	55	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	84	Total	C	N	O	S	0	0
			565	359	94	108	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	n	84	Total	C	N	O	S	0	0
			576	361	101	110	4		

- Molecule 11 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	146	Total	C	N	O	S	0	0
			1088	716	174	197	1		
11	o	146	Total	C	N	O		0	0
			1089	720	174	195			

- Molecule 12 is a protein called Chlorophyll a-b binding protein Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	191	Total	C	N	O	S	0	0
			1422	921	239	258	4		
12	p	193	Total	C	N	O	S	0	0
			1484	965	248	269	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	73	PHE	UNK	conflict	UNP A0A287WC32
1	74	GLU	UNK	conflict	UNP A0A287WC32
1	75	ARG	UNK	conflict	UNP A0A287WC32
p	73	PHE	UNK	conflict	UNP A0A287WC32
p	74	GLU	UNK	conflict	UNP A0A287WC32
p	75	ARG	UNK	conflict	UNP A0A287WC32

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2	203	Total	C	N	O	S	0	0
			1554	1012	257	282	3		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3	222	Total	C	N	O	S	0	0
			1631	1064	271	293	3		
14	q	222	Total	C	N	O	S	0	0
			1672	1097	272	298	5		

- Molecule 15 is a protein called Chlorophyll a-b binding protein Lhca5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5	205	Total	C	N	O	S	0	0
			1486	962	247	270	7		

- Molecule 16 is a protein called NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	346	Total	C	N	O	S	0	0
			2602	1741	390	463	8		

- Molecule 17 is a protein called NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	478	Total	C	N	O	S	0	0
			3646	2400	557	665	24		

- Molecule 18 is a protein called NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	116	Total	C	N	O	S	0	0
			841	575	124	140	2		

- Molecule 19 is a protein called NAD(P)H-quinone oxidoreductase chain 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	499	Total	C	N	O	S	0	0
			3874	2614	598	639	23		

- Molecule 20 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	100	Total	C	N	O	S	0	0
			750	486	127	135	2		

- Molecule 21 is a protein called NADH-plastoquinone oxidoreductase subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	671	Total	C	N	O	S	0	0
			5041	3367	784	870	20		

- Molecule 22 is a protein called NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	176	Total	C	N	O	S	0	0
			1260	841	194	220	5		

- Molecule 23 is a protein called NAD(P)H-quinone oxidoreductase subunit H, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	383	Total	C	N	O	S	0	0
			2991	1944	493	543	11		

- Molecule 24 is a protein called NAD(P)H-quinone oxidoreductase subunit I, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	165	Total	C	N	O	S	0	0
			1229	772	214	231	12		

- Molecule 25 is a protein called NAD(P)H-quinone oxidoreductase subunit J, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	159	Total	C	N	O	S	0	0
			1258	808	213	233	4		

- Molecule 26 is a protein called NAD(P)H-quinone oxidoreductase subunit K, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	194	Total	C	N	O	S	0	0
			1473	931	250	282	10		

- Molecule 27 is a protein called NAD(P)H-quinone oxidoreductase subunit L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	69	Total	C	N	O	S	0	0
			572	399	89	81	3		

- Molecule 28 is a protein called NAD(P)H-quinone oxidoreductase subunit M, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	112	Total	C	N	O	S	0	0
			876	558	150	162	6		

- Molecule 29 is a protein called NAD(P)H-quinone oxidoreductase subunit N, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	142	Total	C	N	O	S	0	0
			1135	741	197	195	2		

- Molecule 30 is a protein called Unidentified stromal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Z	61	Total	C	N	O	0	0
			305	183	61	61		

- Molecule 31 is a protein called Photosynthetic NDH subunit of subcomplex L1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	a	150	Total	C	N	O	0	0
			1185	752	206	227		

- Molecule 32 is a protein called Photosynthetic NDH subunit of subcomplex L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	129	Total	C	N	O	S	0	0
			915	580	156	175	4		

- Molecule 33 is a protein called Photosynthetic NDH subunit of subcomplex L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	134	Total	C	N	O	S	0	0
			989	634	164	187	4		

- Molecule 34 is a protein called Photosynthetic NDH subunit of subcomplex L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	4	130	Total	C	N	O	S	0	0
			878	553	153	163	9		

- Molecule 35 is a protein called Photosynthetic NDH subunit of subcomplex L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	172	Total	C	N	O	S	0	0
			1289	812	229	241	7		

- Molecule 36 is a protein called Photosynthetic NDH subunit of subcomplex B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	6	343	Total	C	N	O	S	0	0
			2541	1617	435	474	15		

- Molecule 37 is a protein called Photosynthetic NDH subunit of subcomplex B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	7	317	Total	C	N	O	S	0	0
			2302	1436	408	448	10		

- Molecule 38 is a protein called Photosynthetic NDH subunit of subcomplex B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	8	119	Total	C	N	O	S	0	0
			828	523	151	147	7		

- Molecule 39 is a protein called Photosynthetic NDH subunit of subcomplex B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	9	82	Total	C	N	O	S	0	0
			617	395	101	118	3		

- Molecule 40 is a protein called Photosynthetic NDH subunit of subcomplex B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	0	149	Total	C	N	O	S	0	0
			1089	704	175	204	6		

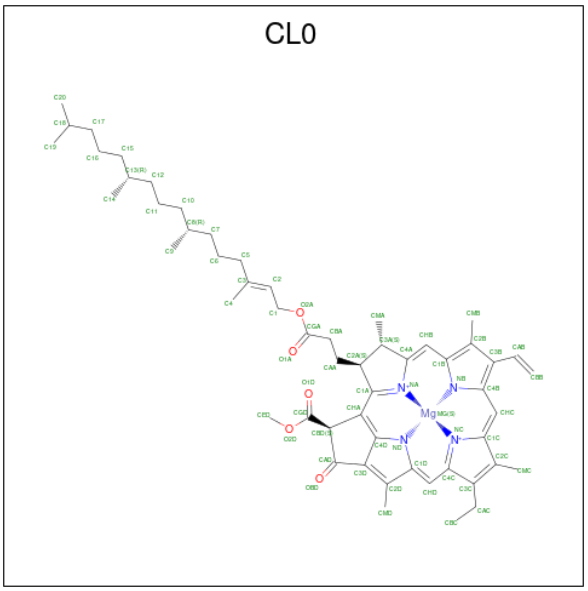
- Molecule 41 is a protein called Chlorophyll a-b binding protein Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	197	Total	C	N	O	S	0	0
			1529	991	253	282	3		

- Molecule 42 is a protein called Chlorophyll a-b binding protein, chloroplastic.

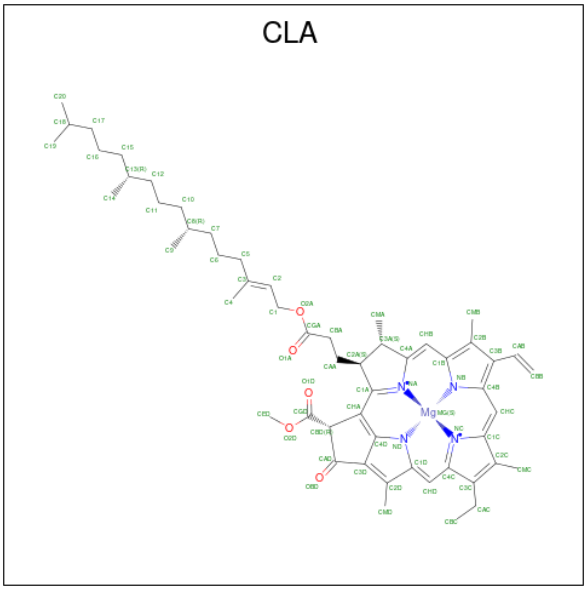
Mol	Chain	Residues	Atoms					AltConf	Trace
42	s	211	Total	C	N	O	S	0	0
			1591	1035	266	283	7		

- Molecule 43 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
43	A	1	Total	C	Mg	N	O	0
			61	52	1	4	4	
43	e	1	Total	C	Mg	N	O	0
			61	52	1	4	4	

- Molecule 44 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
44	A	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
44	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
44	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
44	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
44	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
44	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			45	37	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
44	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
44	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
44	B	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
44	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
44	F	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
44	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
44	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	K	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	K	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
44	L	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
44	L	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	1	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
44	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
44	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
44	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
44	2	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
44	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
44	2	1	Total	C	Mg	N	O	0
			49	41	1	4	3	
44	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
44	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	2	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
44	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	3	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
44	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	5	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
44	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
44	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
44	5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
44	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
44	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			39	32	1	4	2	
44	e	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			45	36	1	4	4	
44	e	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
44	e	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	e	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
44	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
44	f	1	Total	C	Mg	N	O	0
			38	31	1	4	2	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
44	f	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
44	f	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
44	f	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
44	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	f	1	Total	C	Mg	N	O	0
			58	49	1	4	4	
44	f	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	f	1	Total	C	Mg	N	O	0
			38	32	1	4	1	
44	j	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	m	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	m	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	n	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
44	n	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	n	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	n	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
44	o	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	o	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	o	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	p	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	p	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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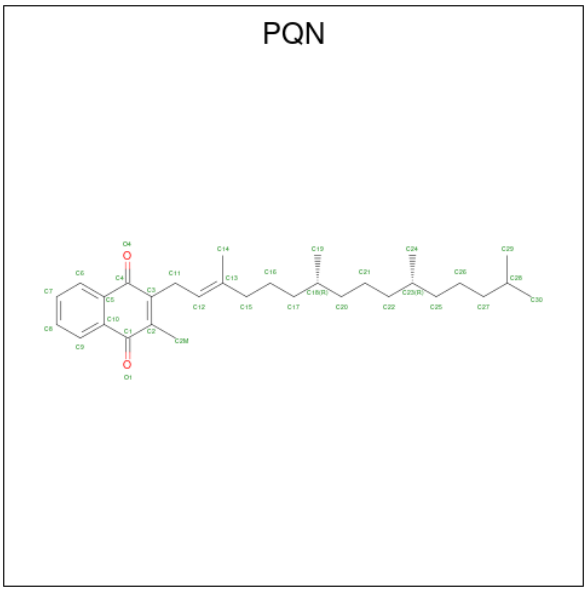
Mol	Chain	Residues	Atoms					AltConf
44	p	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
44	p	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	p	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	p	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	p	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
44	p	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
44	p	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	p	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	q	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
44	q	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
44	q	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	q	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	q	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	q	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	q	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	q	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
44	q	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	q	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	q	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
44	q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
44	r	1	Total	C	Mg	N	O	0
			39	31	1	4	3	

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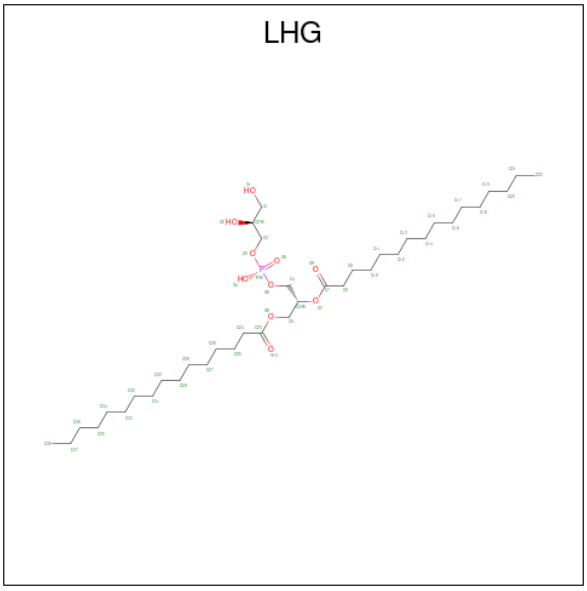
Mol	Chain	Residues	Atoms					AltConf
44	r	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	r	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	r	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	r	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
44	r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
44	r	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	r	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	r	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	s	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
44	s	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
44	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
44	s	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
44	s	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
44	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
44	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
44	s	1	Total	C	Mg	N	O	0
			40	32	1	4	3	

- Molecule 45 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



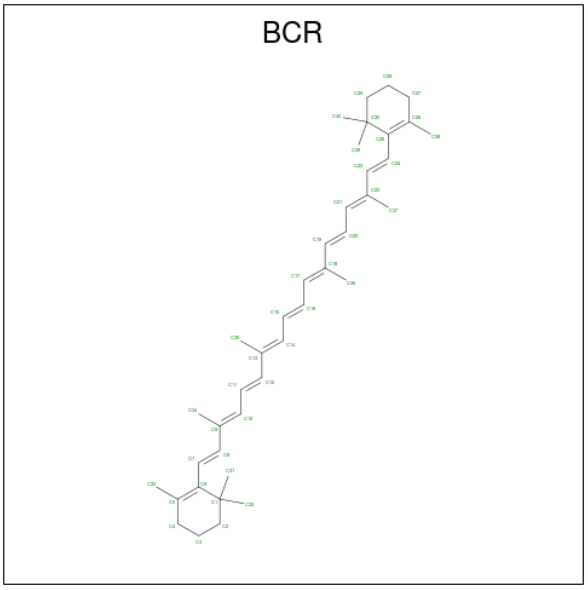
Mol	Chain	Residues	Atoms	AltConf
45	A	1	Total C O 33 31 2	0
45	B	1	Total C O 30 28 2	0
45	e	1	Total C O 14 12 2	0
45	f	1	Total C O 16 14 2	0

- Molecule 46 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
46	A	1	Total	C	O	P	0
			49	38	10	1	
46	A	1	Total	C	O	P	0
			30	19	10	1	
46	B	1	Total	C	O	P	0
			38	27	10	1	
46	1	1	Total	C	O	P	0
			49	38	10	1	
46	2	1	Total	C	O	P	0
			35	24	10	1	
46	O	1	Total	C	O	P	0
			24	15	8	1	
46	e	1	Total	C	O	P	0
			40	29	10	1	
46	e	1	Total	C	O	P	0
			25	15	9	1	
46	f	1	Total	C	O	P	0
			38	27	10	1	
46	p	1	Total	C	O	P	0
			49	38	10	1	
46	s	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 47 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
47	A	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
47	A	1	Total C 40 40	0
47	A	1	Total C 40 40	0
47	A	1	Total C 40 40	0
47	A	1	Total C 39 39	0
47	A	1	Total C 40 40	0
47	A	1	Total C 40 40	0
47	B	1	Total C 40 40	0
47	B	1	Total C 40 40	0
47	B	1	Total C 40 40	0
47	B	1	Total C 40 40	0
47	B	1	Total C 40 40	0
47	B	1	Total C 40 40	0
47	B	1	Total C 40 40	0
47	F	1	Total C 40 40	0
47	F	1	Total C 40 40	0
47	I	1	Total C 40 40	0
47	J	1	Total C 40 40	0
47	K	1	Total C 40 40	0
47	L	1	Total C 40 40	0
47	L	1	Total C 40 40	0
47	1	1	Total C 19 19	0

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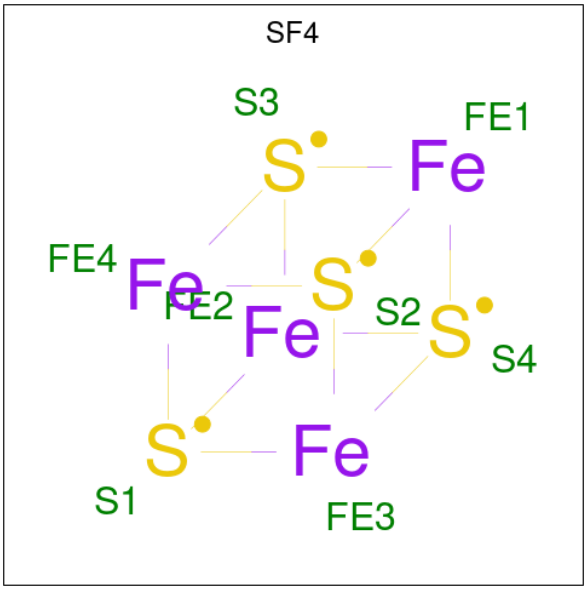
Mol	Chain	Residues	Atoms	AltConf
47	2	1	Total C 40 40	0
47	3	1	Total C 40 40	0
47	5	1	Total C 40 40	0
47	Q	1	Total C 39 39	0
47	e	1	Total C 40 40	0
47	e	1	Total C 40 40	0
47	e	1	Total C 40 40	0
47	e	1	Total C 40 40	0
47	e	1	Total C 40 40	0
47	e	1	Total C 40 40	0
47	e	1	Total C 40 40	0
47	f	1	Total C 40 40	0
47	f	1	Total C 40 40	0
47	f	1	Total C 40 40	0
47	f	1	Total C 40 40	0
47	f	1	Total C 40 40	0
47	f	1	Total C 39 39	0
47	j	1	Total C 40 40	0
47	j	1	Total C 40 40	0
47	l	1	Total C 40 40	0
47	l	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
47	m	1	Total C 40 40	0
47	n	1	Total C 40 40	0
47	o	1	Total C 40 40	0
47	o	1	Total C 40 40	0
47	p	1	Total C 11 11	0
47	q	1	Total C 40 40	0
47	r	1	Total C 40 40	0
47	s	1	Total C 40 40	0

- Molecule 48 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



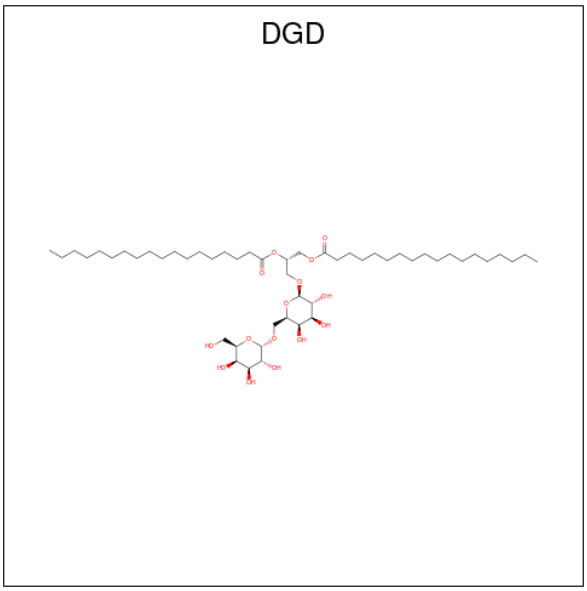
Mol	Chain	Residues	Atoms	AltConf
48	A	1	Total Fe S 8 4 4	0
48	C	1	Total Fe S 8 4 4	0
48	C	1	Total Fe S 8 4 4	0

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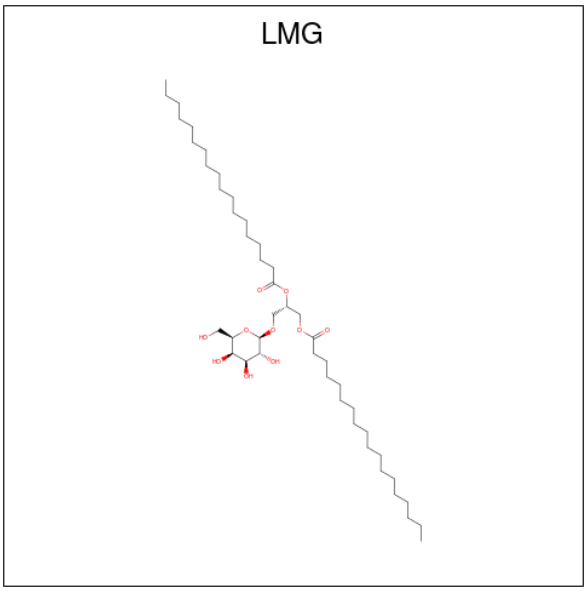
Mol	Chain	Residues	Atoms	AltConf
48	8	1	Total Fe S 8 4 4	0
48	f	1	Total Fe S 8 4 4	0
48	g	1	Total Fe S 8 4 4	0
48	g	1	Total Fe S 8 4 4	0

- Molecule 49 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



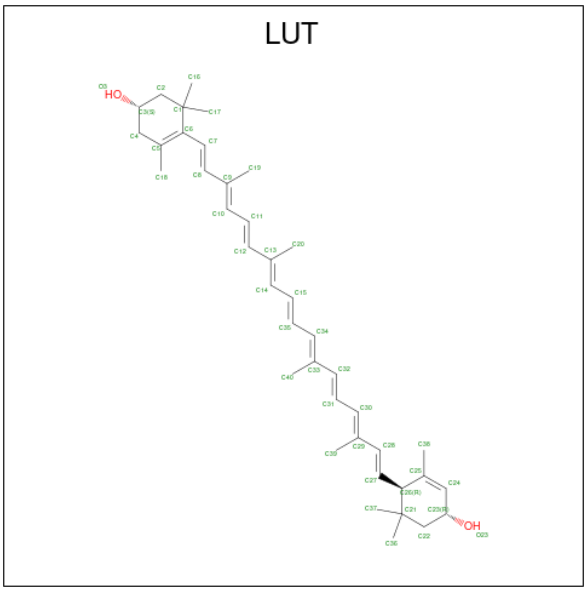
Mol	Chain	Residues	Atoms	AltConf
49	B	1	Total C O 59 44 15	0
49	J	1	Total C O 66 51 15	0
49	f	1	Total C O 52 37 15	0
49	m	1	Total C O 66 51 15	0

- Molecule 50 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



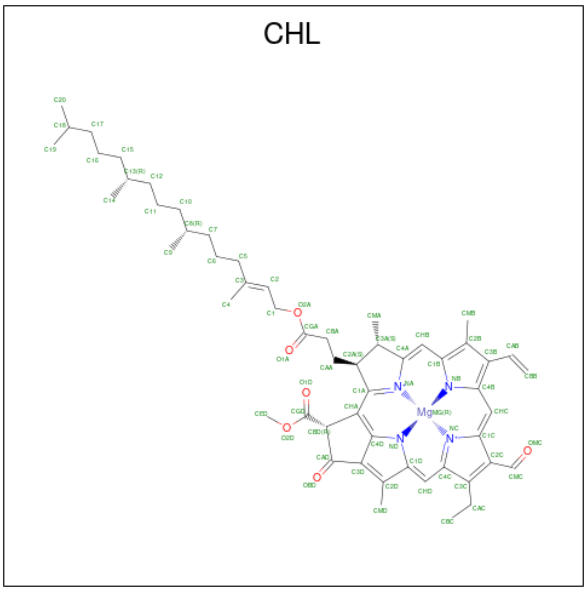
Mol	Chain	Residues	Atoms	AltConf
50	F	1	Total C O 30 20 10	0
50	F	1	Total C O 45 35 10	0
50	2	1	Total C O 16 9 7	0
50	2	1	Total C O 36 26 10	0
50	5	1	Total C O 32 22 10	0
50	m	1	Total C O 30 20 10	0
50	r	1	Total C O 18 10 8	0

- Molecule 51 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms	AltConf
51	1	1	Total C O 42 40 2	0
51	1	1	Total C O 42 40 2	0
51	2	1	Total C O 42 40 2	0
51	3	1	Total C O 42 40 2	0
51	3	1	Total C O 42 40 2	0
51	5	1	Total C O 42 40 2	0
51	p	1	Total C O 42 40 2	0
51	p	1	Total C O 42 40 2	0
51	q	1	Total C O 42 40 2	0
51	q	1	Total C O 42 40 2	0
51	r	1	Total C O 42 40 2	0
51	s	1	Total C O 42 40 2	0

- Molecule 52 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



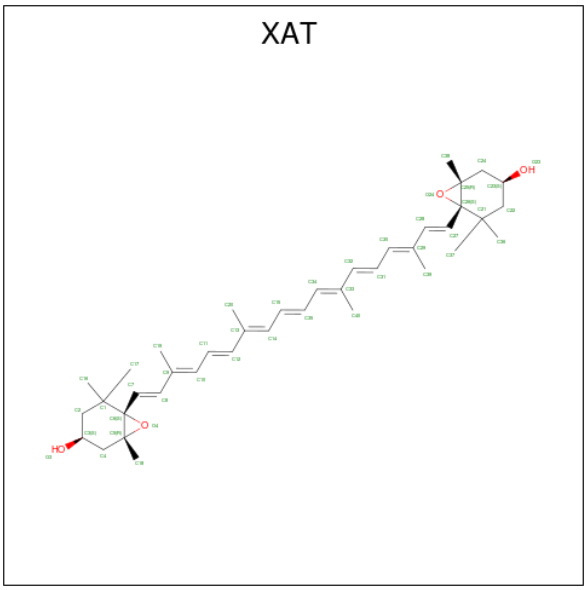
Mol	Chain	Residues	Atoms					AltConf
52	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
52	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
52	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
52	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
52	2	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
52	2	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
52	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
52	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
52	3	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
52	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
52	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
52	5	1	Total	C	Mg	N	O	0
			40	31	1	4	4	
52	p	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
52	p	1	Total	C	Mg	N	O	0
			47	36	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
52	p	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
52	q	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
52	r	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
52	r	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
52	r	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
52	s	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
52	s	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
52	s	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
52	s	1	Total	C	Mg	N	O	0
			47	36	1	4	6	

- Molecule 53 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



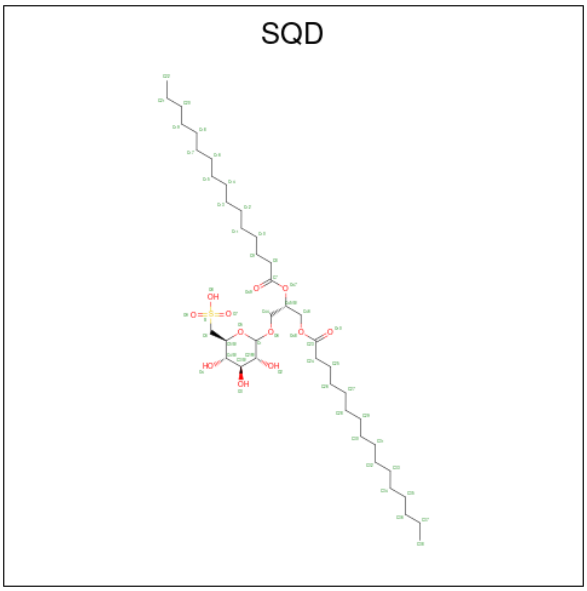
Mol	Chain	Residues	Atoms			AltConf
53	2	1	Total	C	O	0
			44	40	4	
53	5	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
53	r	1	Total 44	C 40	O 4	0
53	s	1	Total 44	C 40	O 4	0

- Molecule 54 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).

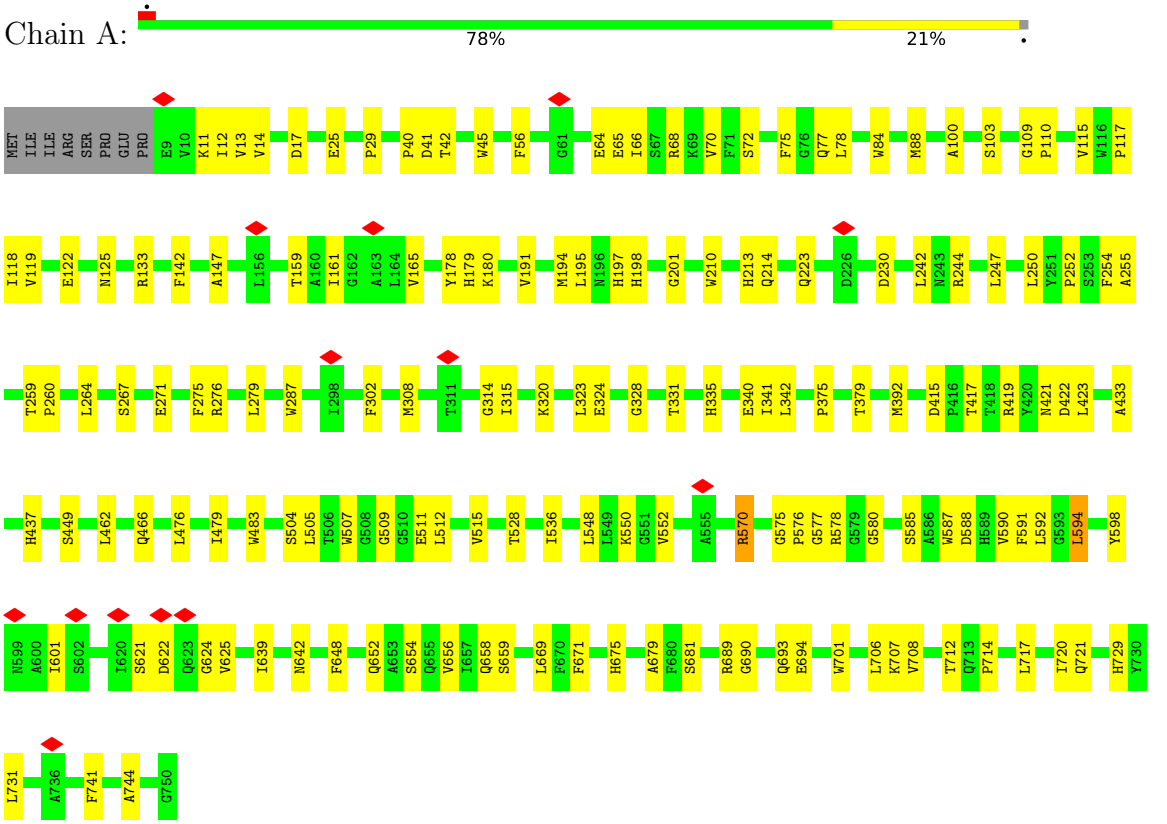


Mol	Chain	Residues	Atoms				AltConf
54	Q	1	Total 54	C 41	O 12	S 1	0
54	Q	1	Total 46	C 33	O 12	S 1	0

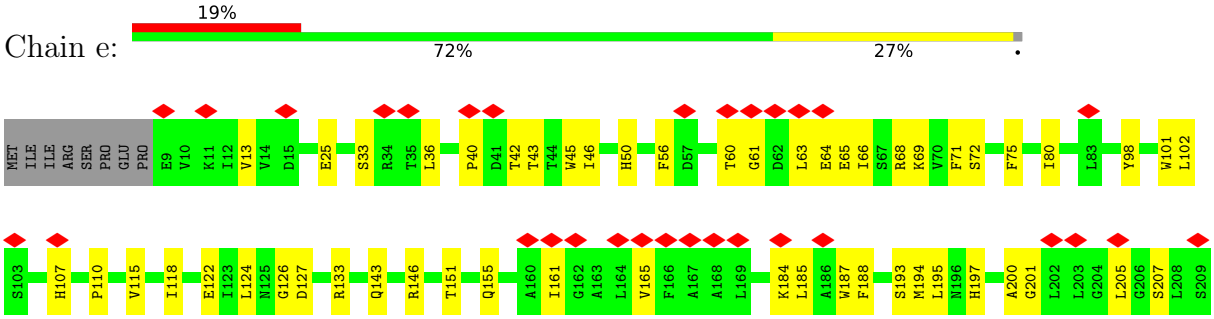
3 Residue-property plots (i)

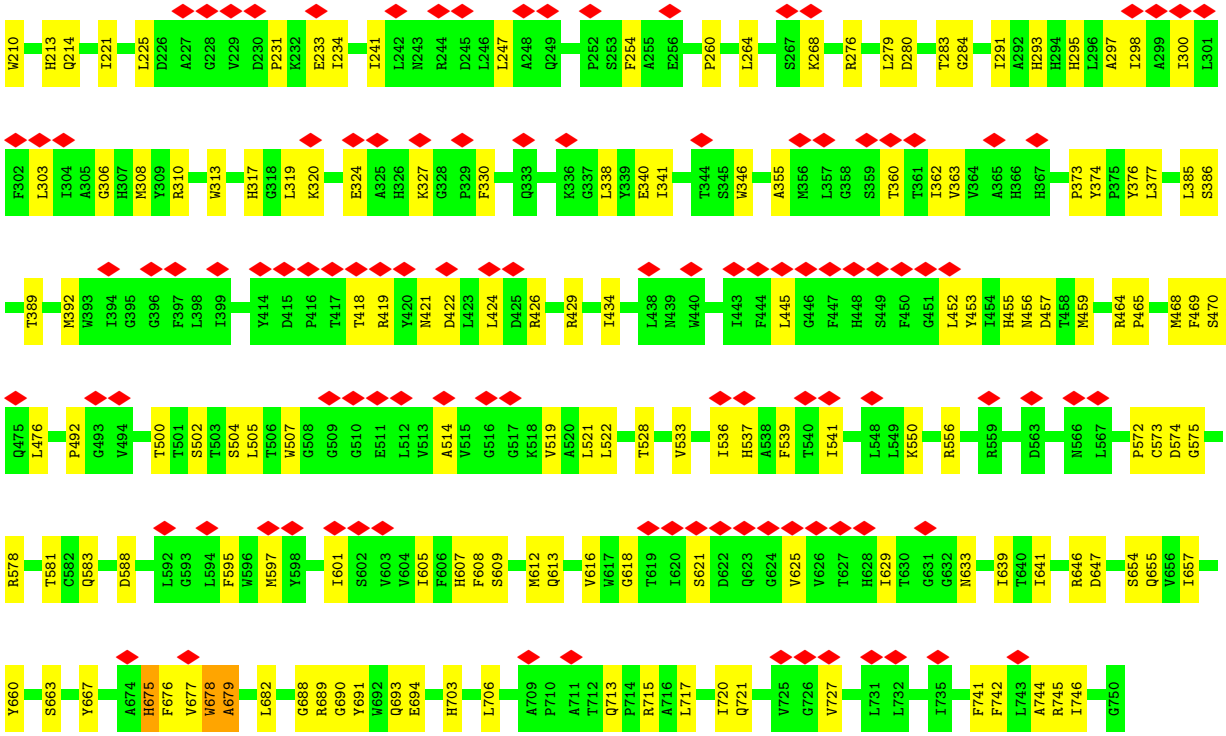
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

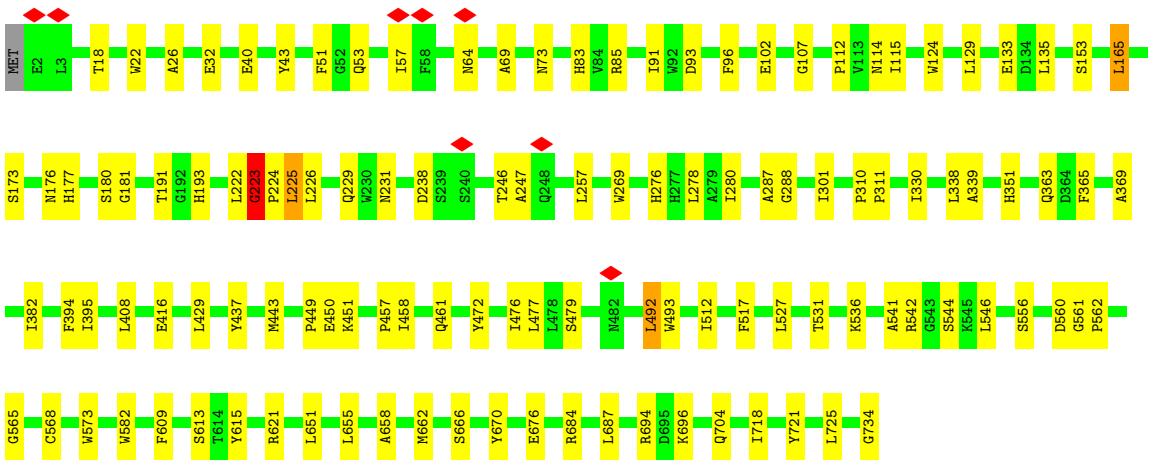




• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

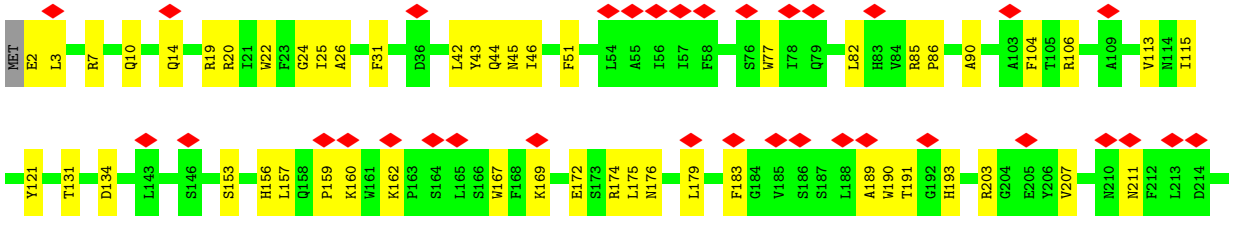


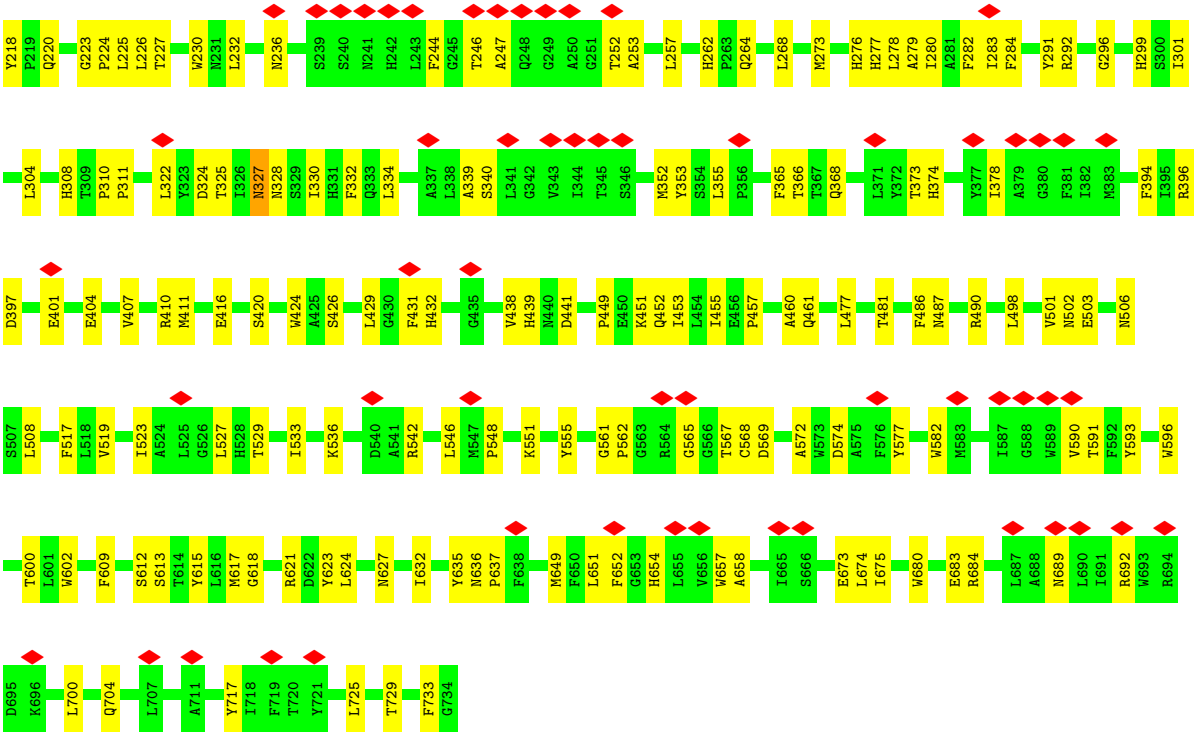


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain f:



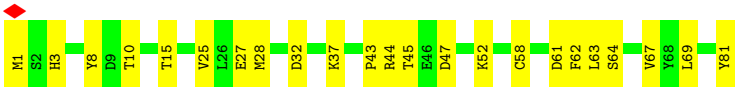




• Molecule 3: Photosystem I iron-sulfur center

Chain C:

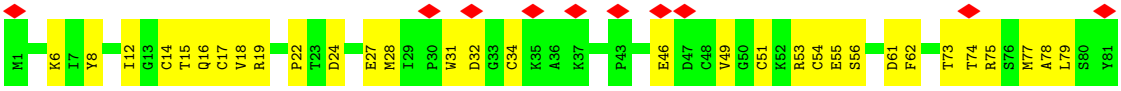




• Molecule 3: Photosystem I iron-sulfur center

Chain g:



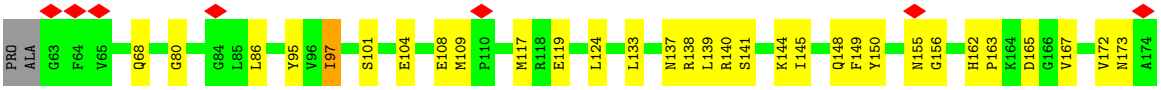


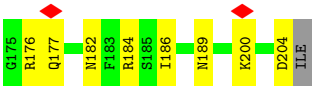
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:



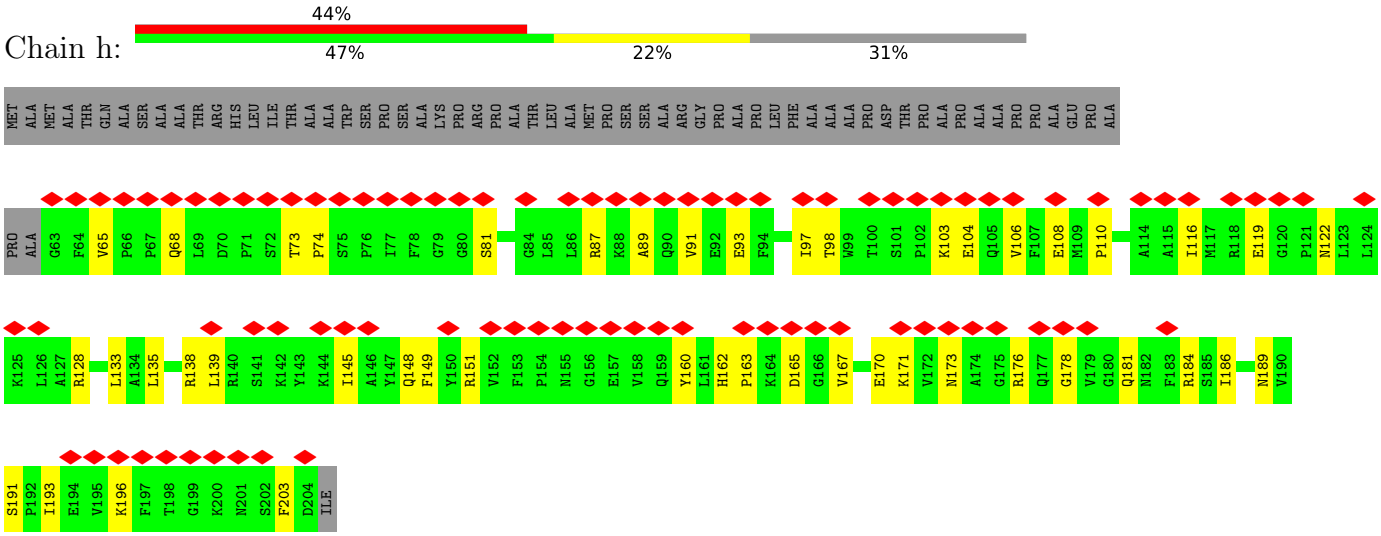






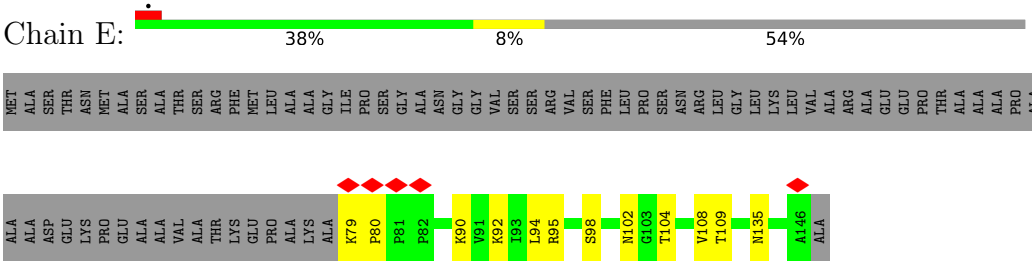
• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain h:



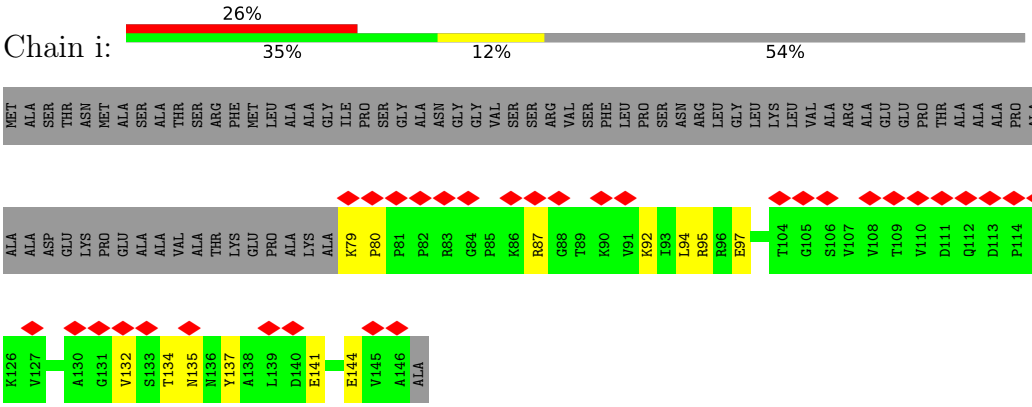
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:



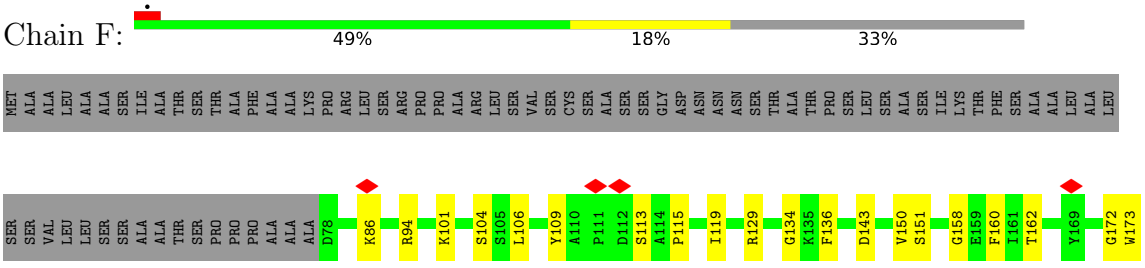
• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain i:



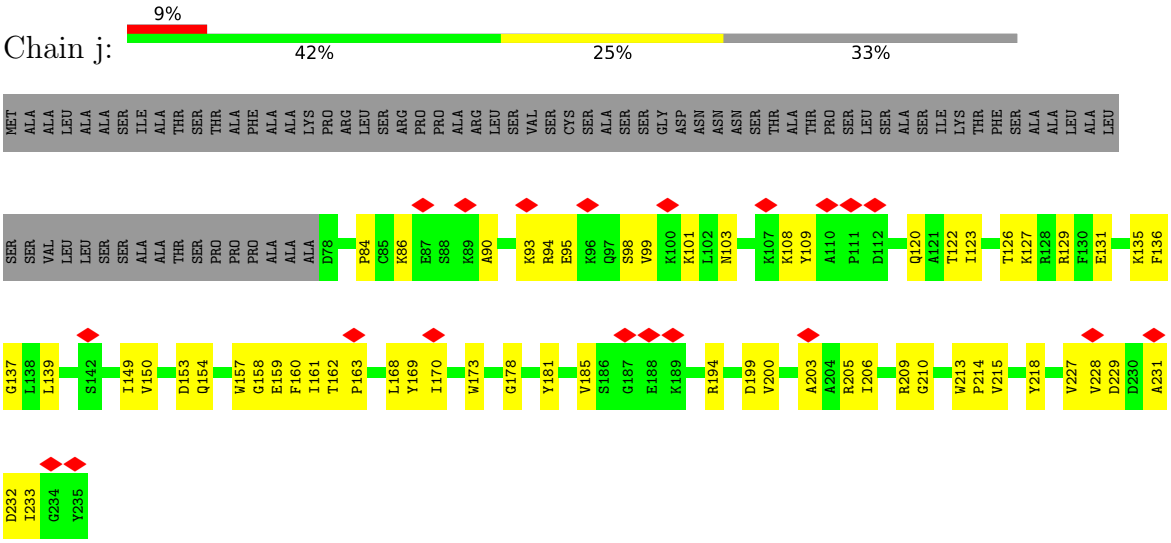
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F:

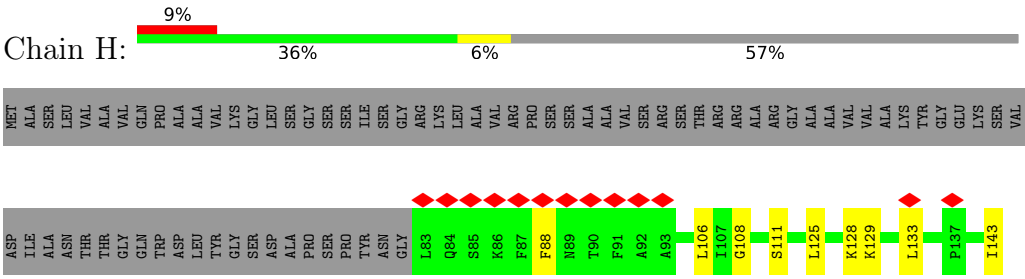




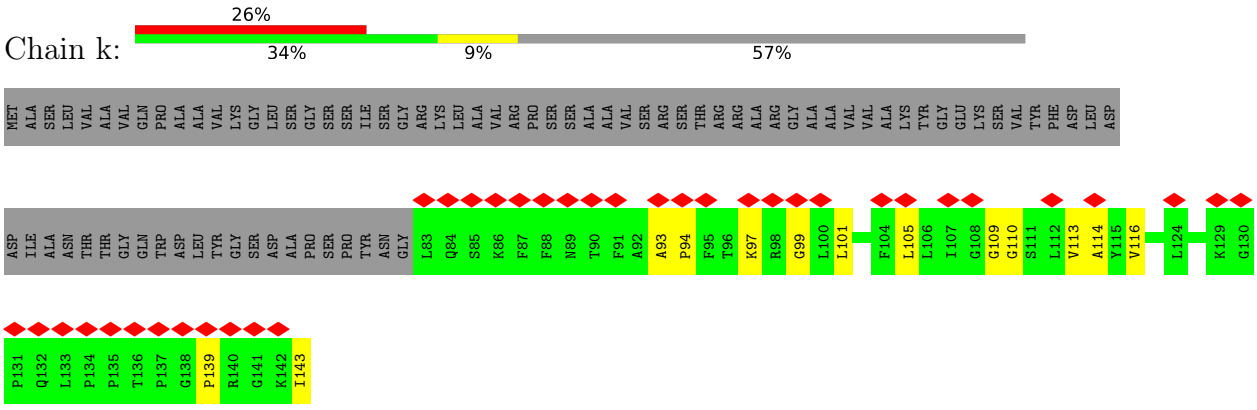
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic



• Molecule 7: Photosystem I reaction center subunit VI, chloroplastic

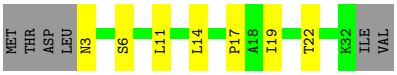


• Molecule 7: Photosystem I reaction center subunit VI, chloroplastic



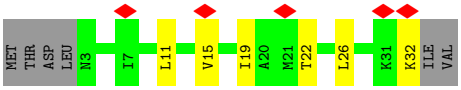
• Molecule 8: Photosystem I reaction center subunit VIII





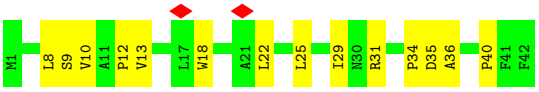
• Molecule 8: Photosystem I reaction center subunit VIII





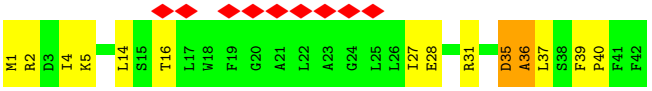
• Molecule 9: Photosystem I reaction center subunit IX





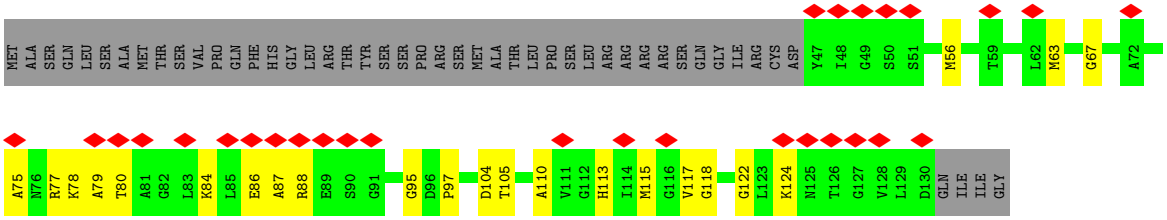
• Molecule 9: Photosystem I reaction center subunit IX





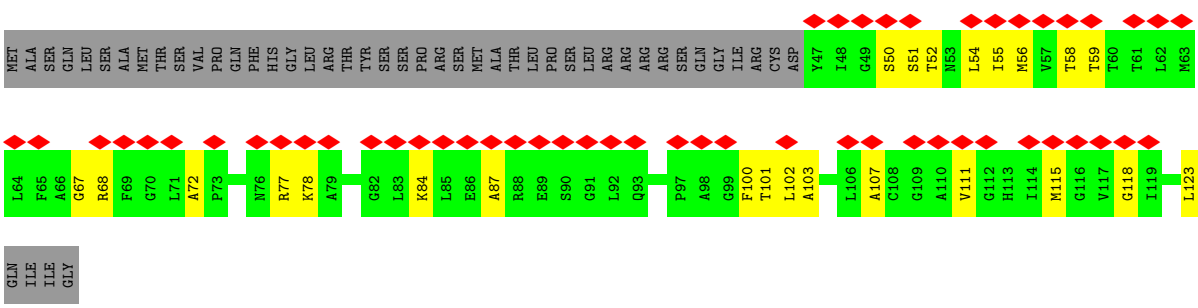
• Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic





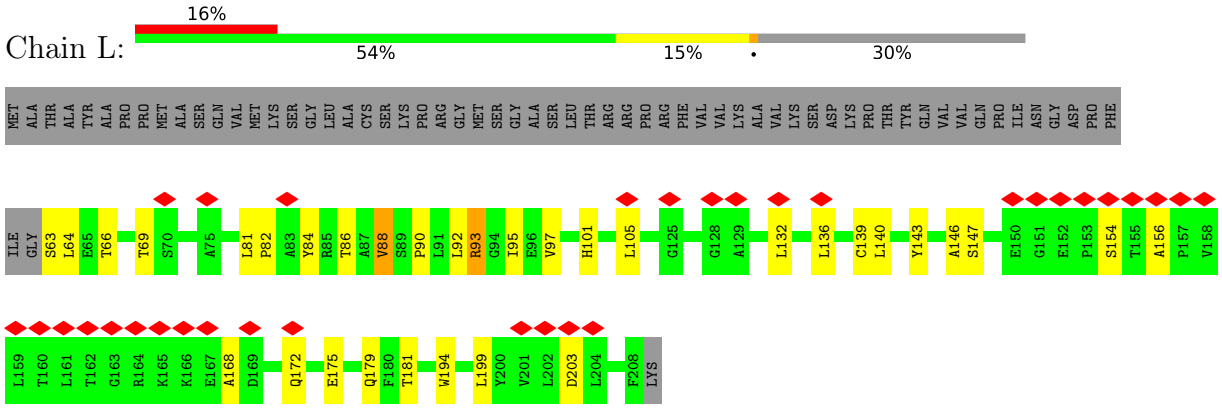
• Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic





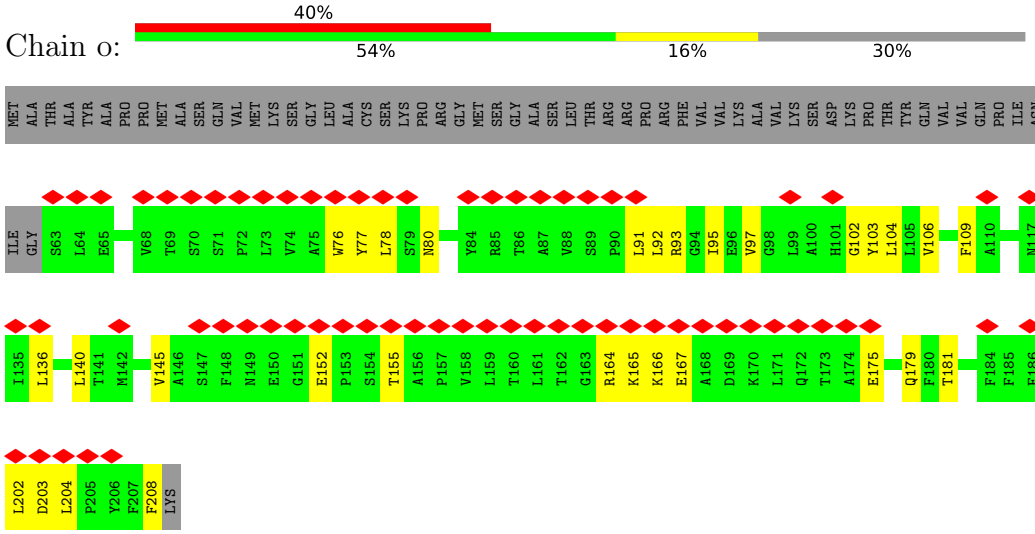
• Molecule 11: Photosystem I reaction center subunit XI, chloroplastic

Chain L:



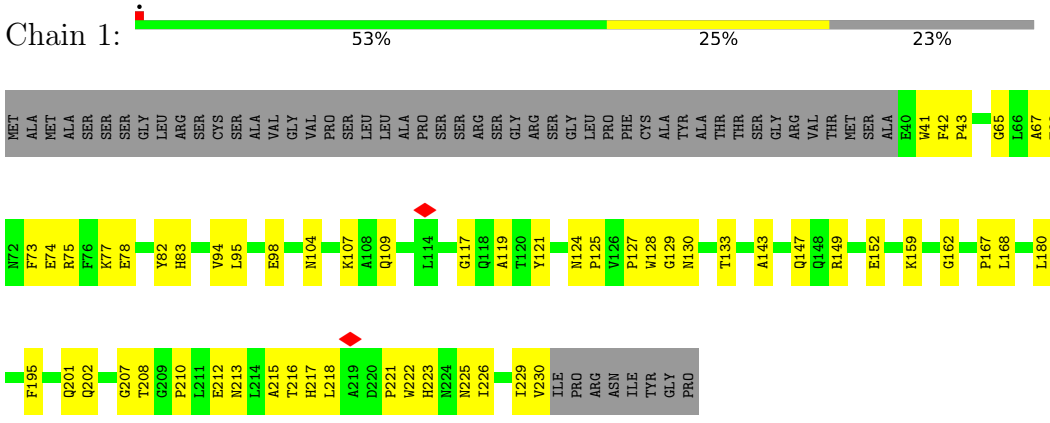
• Molecule 11: Photosystem I reaction center subunit XI, chloroplastic

Chain o:



• Molecule 12: Chlorophyll a-b binding protein Lhca1

Chain 1:



• Molecule 12: Chlorophyll a-b binding protein Lhca1

Chain p:

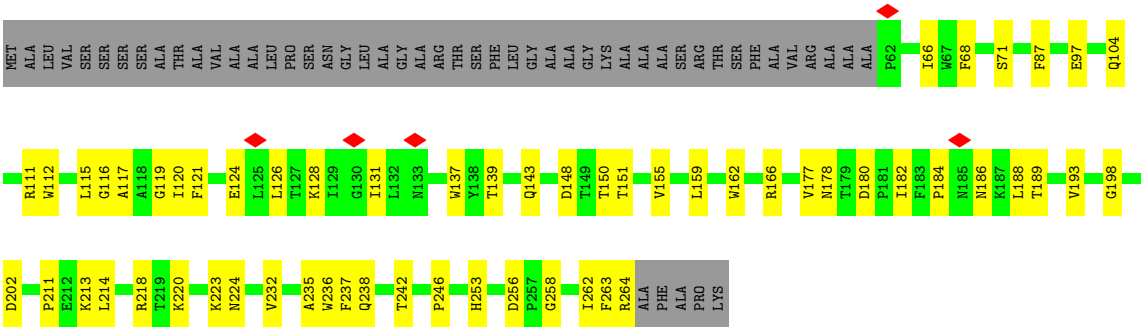




• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 2:

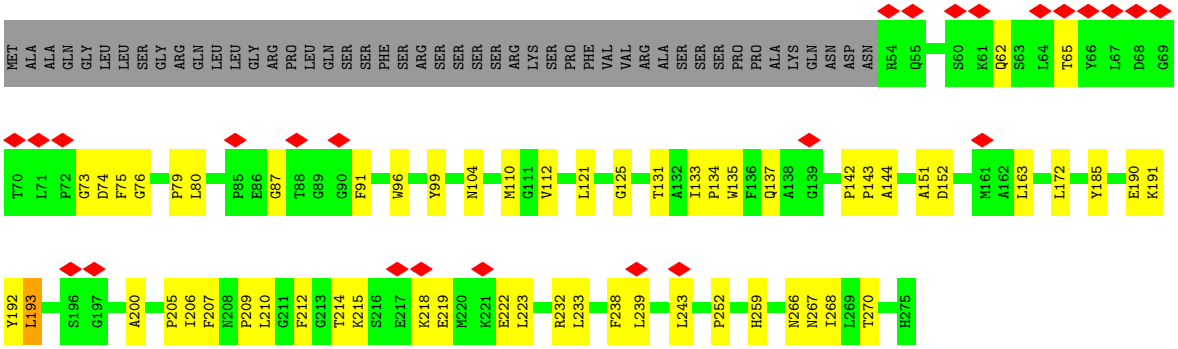




• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 3:

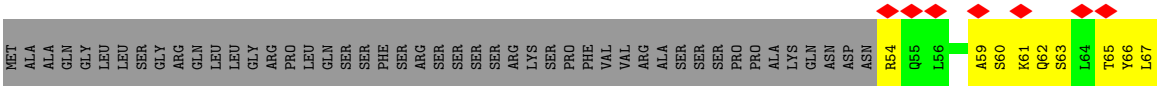


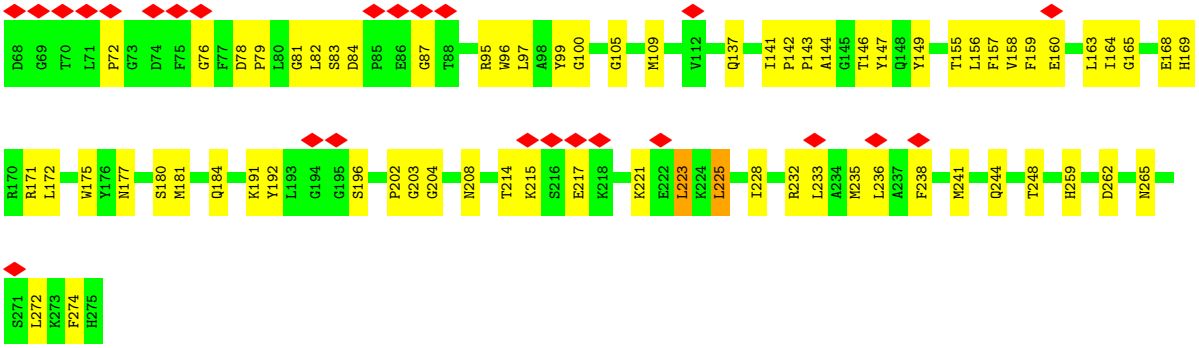


• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain q:

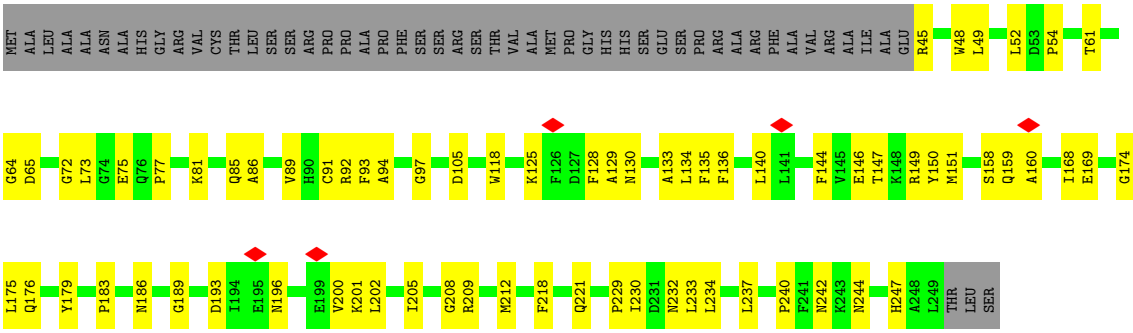






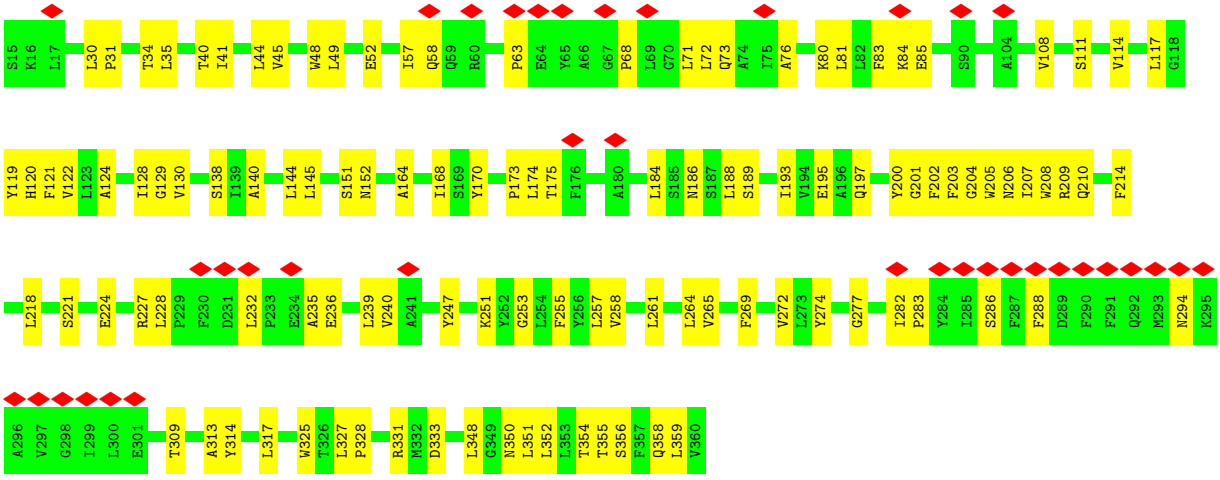
• Molecule 15: Chlorophyll a-b binding protein Lhca5



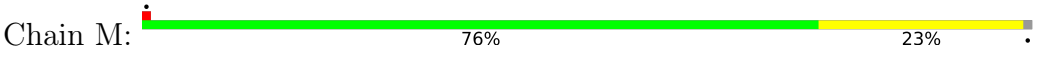


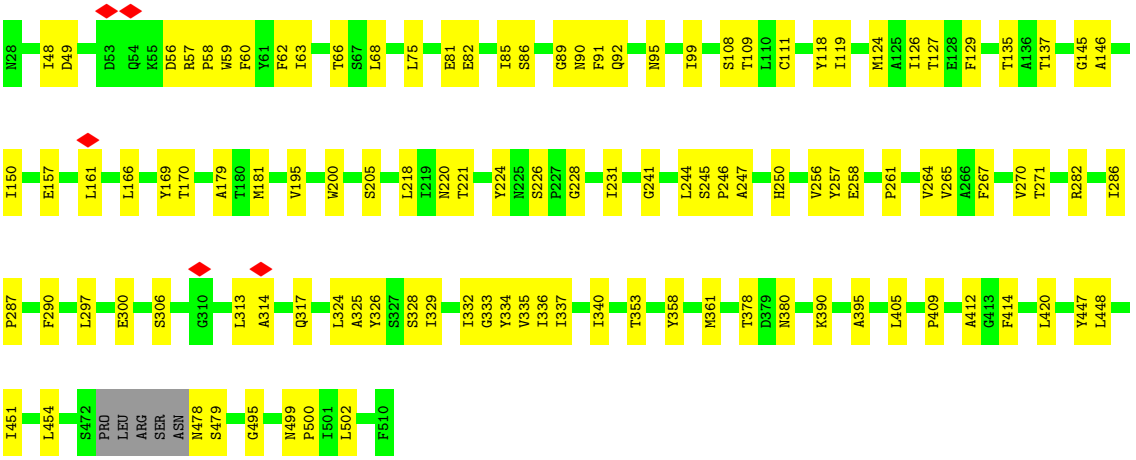
• Molecule 16: NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic



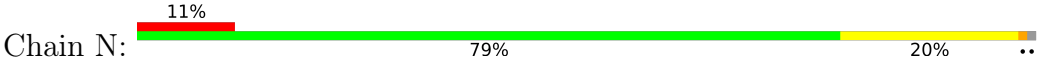


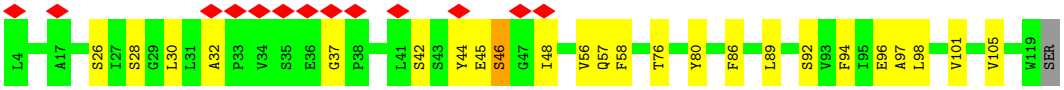
• Molecule 17: NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic





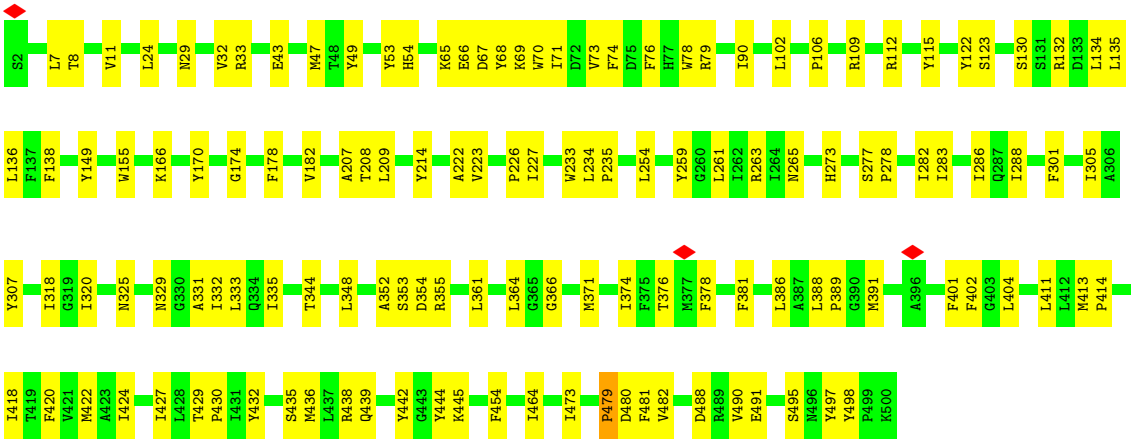
• Molecule 18: NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic



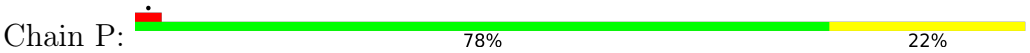


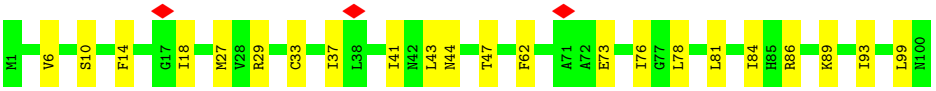
• Molecule 19: NAD(P)H-quinone oxidoreductase chain 4, chloroplastic





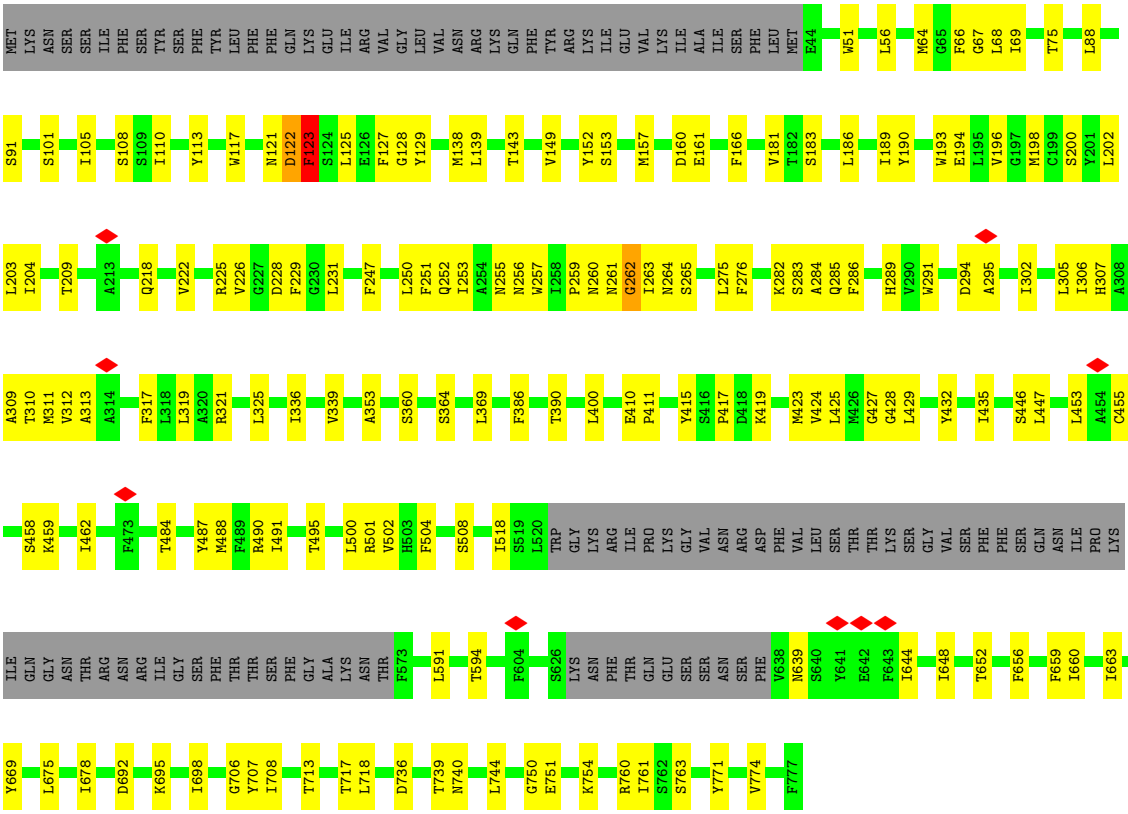
• Molecule 20: NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic





• Molecule 21: NADH-plastoquinone oxidoreductase subunit 5

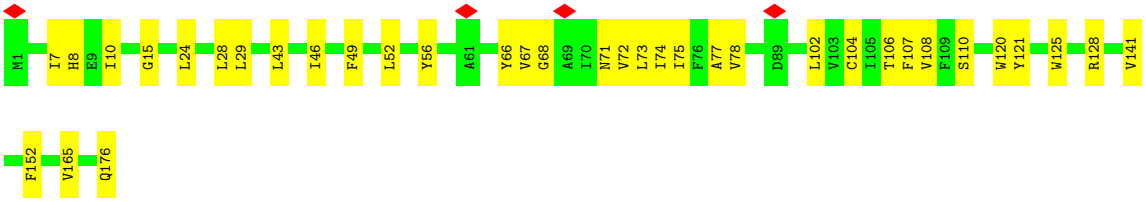




• Molecule 22: NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic

Chain R:

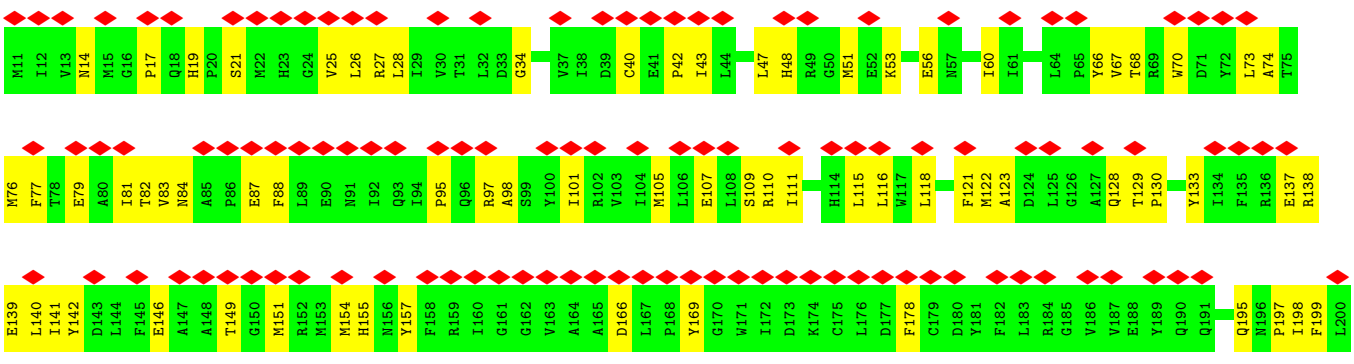


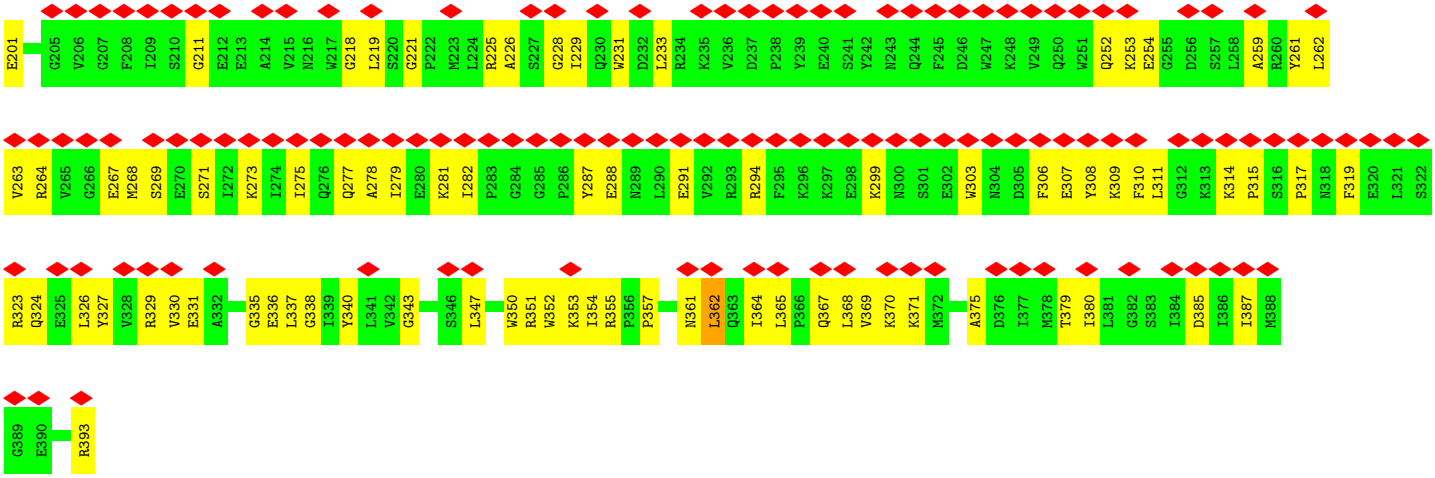


• Molecule 23: NAD(P)H-quinone oxidoreductase subunit H, chloroplastic

Chain S:

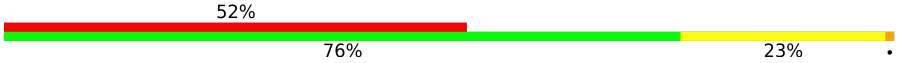


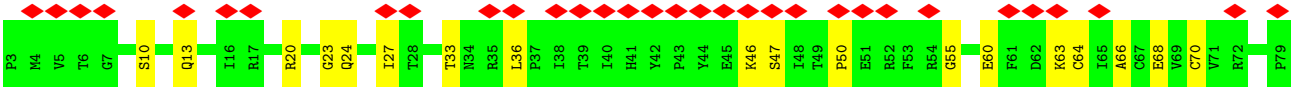




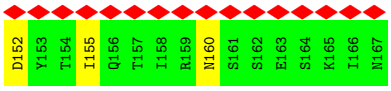
• Molecule 24: NAD(P)H-quinone oxidoreductase subunit I, chloroplastic

Chain T:





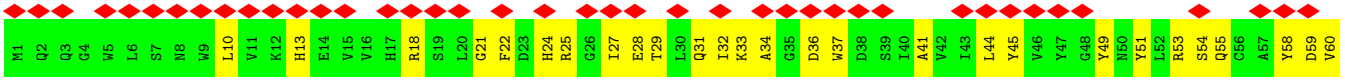


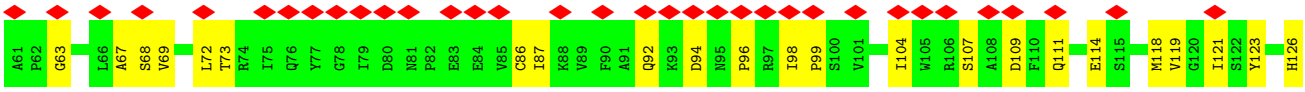


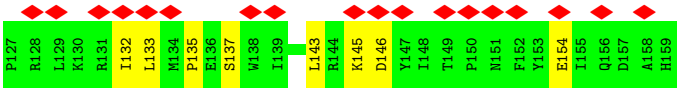
• Molecule 25: NAD(P)H-quinone oxidoreductase subunit J, chloroplastic

Chain U:





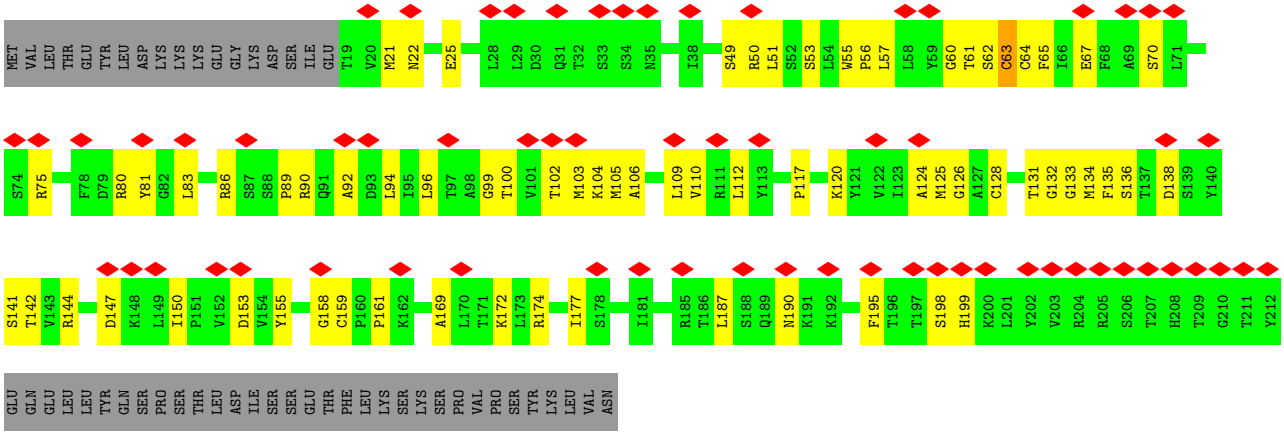




• Molecule 26: NAD(P)H-quinone oxidoreductase subunit K, chloroplastic

Chain V:

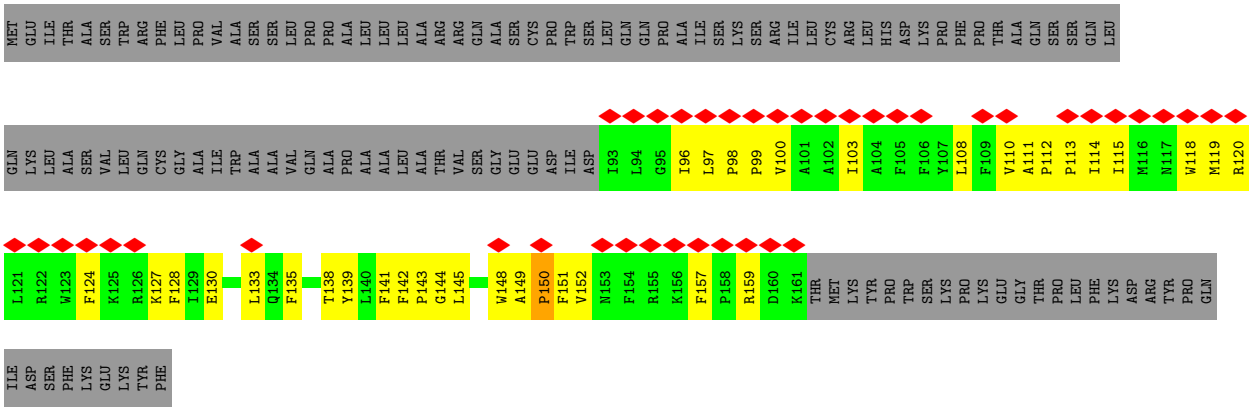




• Molecule 27: NAD(P)H-quinone oxidoreductase subunit L, chloroplastic

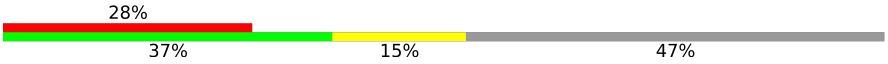
Chain W:

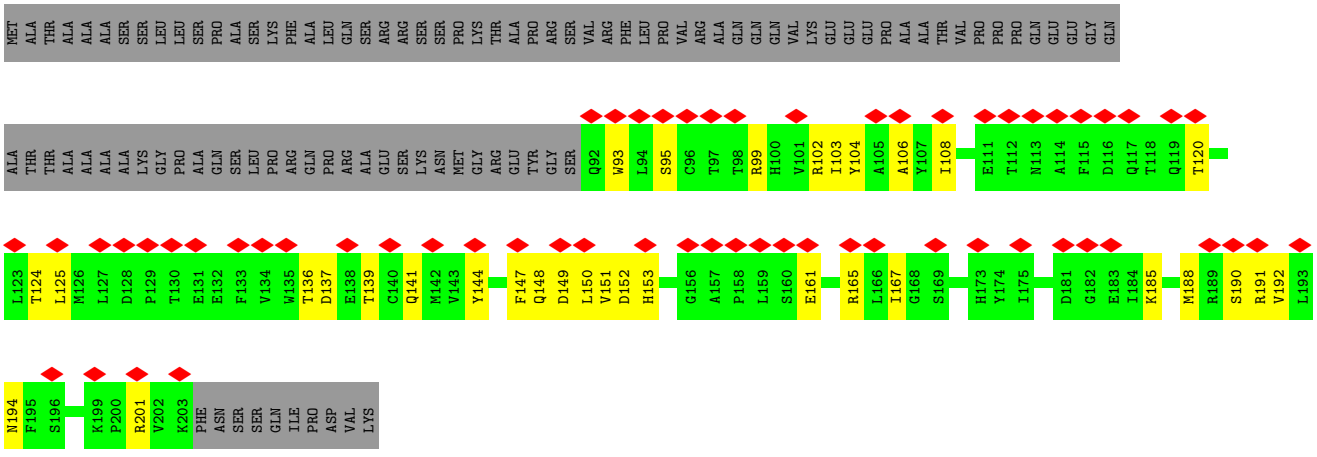




• Molecule 28: NAD(P)H-quinone oxidoreductase subunit M, chloroplastic

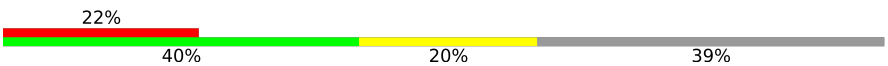
Chain X:

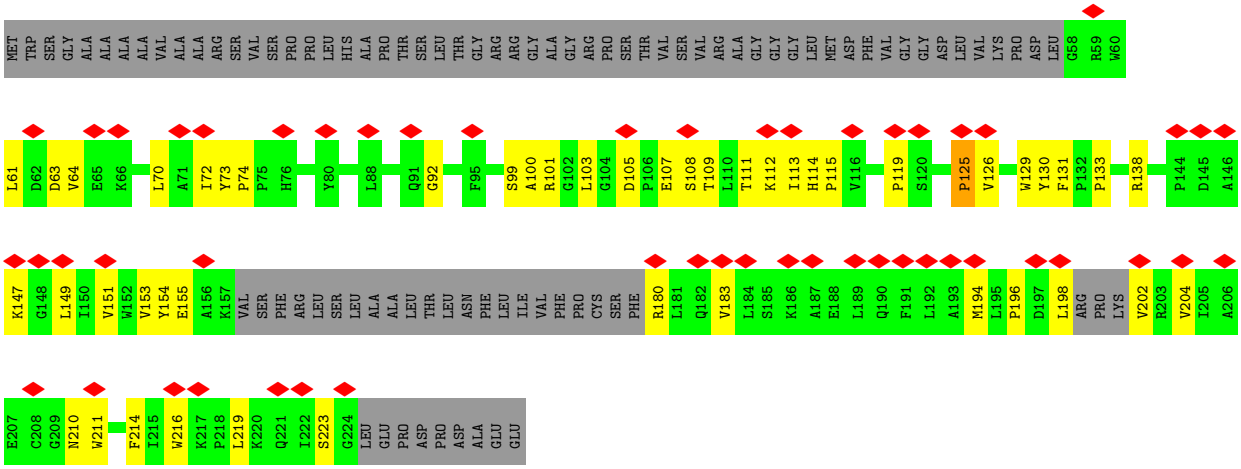




• Molecule 29: NAD(P)H-quinone oxidoreductase subunit N, chloroplastic

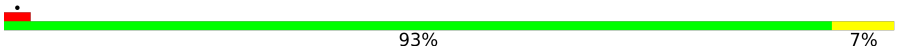
Chain Y:

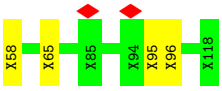




• Molecule 30: Unidentified stromal protein

Chain Z:

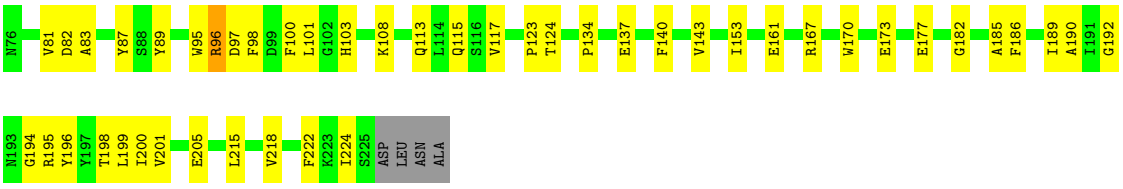




• Molecule 31: Photosynthetic NDH subunit of subcomplex L1

Chain a:

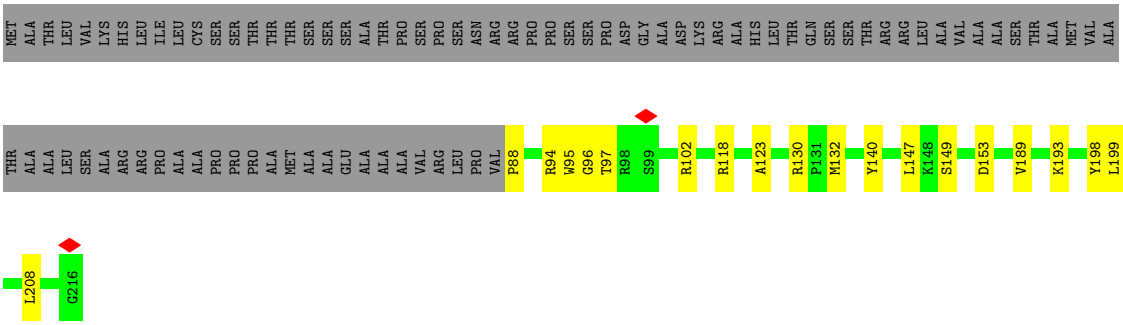




• Molecule 32: Photosynthetic NDH subunit of subcomplex L2

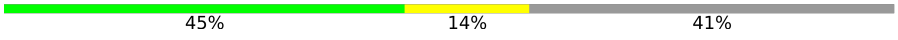
Chain b:

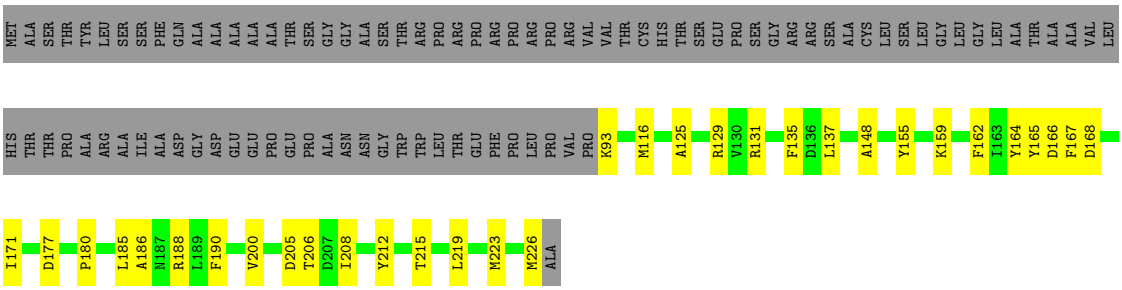




• Molecule 33: Photosynthetic NDH subunit of subcomplex L2

Chain c:





• Molecule 34: Photosynthetic NDH subunit of subcomplex L4

Chain 4:

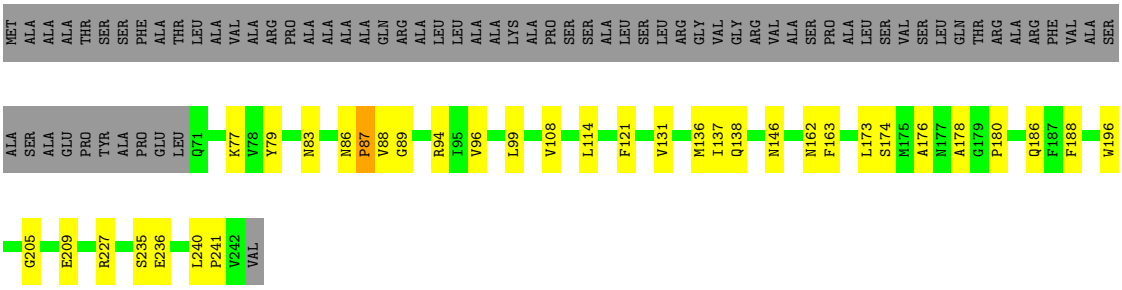




• Molecule 35: Photosynthetic NDH subunit of subcomplex L5

Chain d:

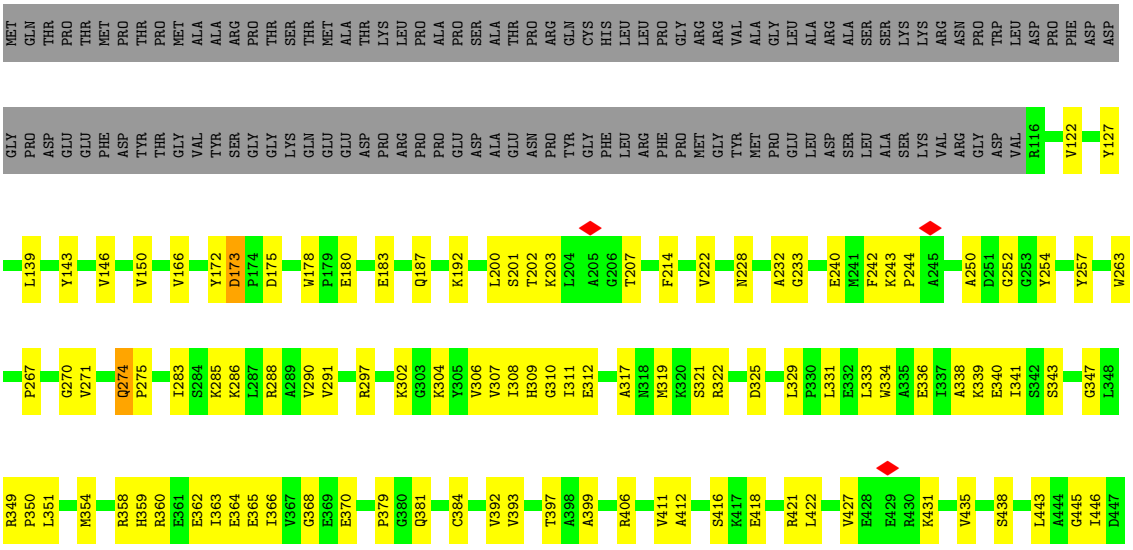




• Molecule 36: Photosynthetic NDH subunit of subcomplex B1

Chain 6:



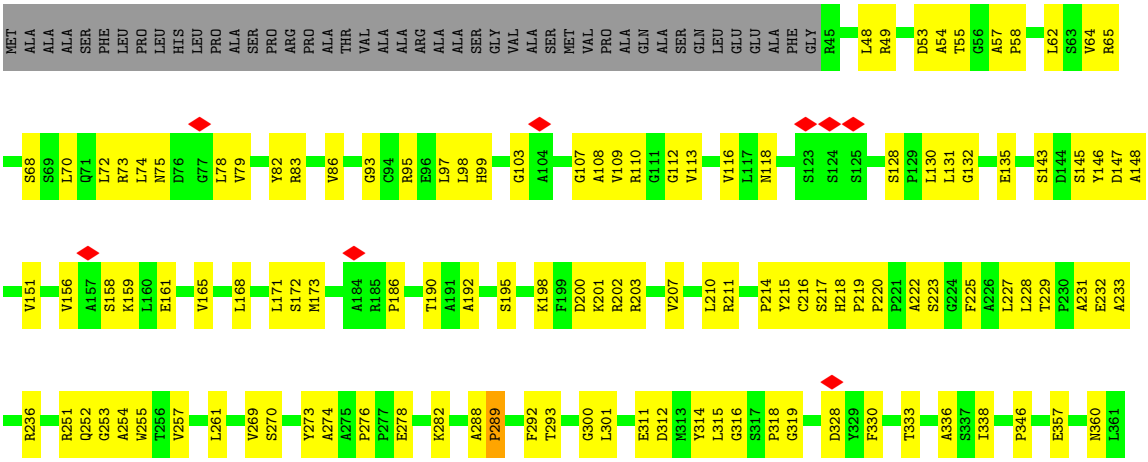




• Molecule 37: Photosynthetic NDH subunit of subcomplex B2

Chain 7:

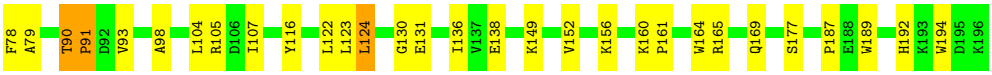




• Molecule 38: Photosynthetic NDH subunit of subcomplex B3

Chain 8:





• Molecule 39: Photosynthetic NDH subunit of subcomplex B4

Chain 9:





• Molecule 40: Photosynthetic NDH subunit of subcomplex B5

Chain 0:

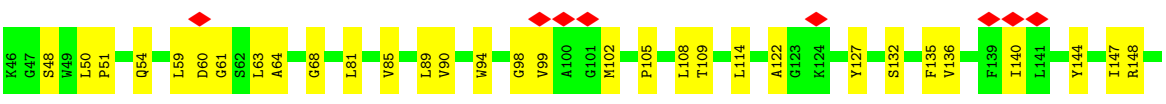


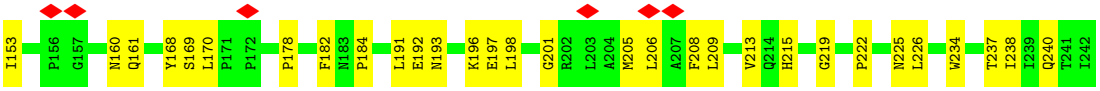


• Molecule 41: Chlorophyll a-b binding protein Lhca4

Chain r:

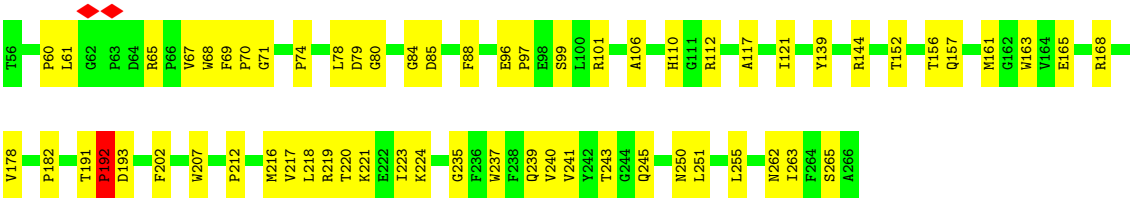






• Molecule 42: Chlorophyll a-b binding protein, chloroplastic





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103844	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	32.847	Depositor
Minimum map value	-13.195	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.3	Depositor
Map size (Å)	575.08, 575.08, 575.08	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XAT, LMG, SF4, BCR, SQD, DGD, LHG, CLA, LUT, PQN, CL0, CHL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.64	0/6010	0.42	0/8202
1	e	0.26	4/5993 (0.1%)	0.39	2/8178 (0.0%)
2	B	0.66	0/6060	0.45	3/8276 (0.0%)
2	f	0.31	5/6052 (0.1%)	0.37	1/8267 (0.0%)
3	C	0.65	0/621	0.49	0/840
3	g	0.20	0/624	0.40	0/844
4	D	0.53	0/1142	0.52	0/1542
4	h	0.15	0/1140	0.43	0/1540
5	E	0.52	0/551	0.44	0/751
5	i	0.17	0/552	0.40	0/751
6	F	0.46	0/1230	0.41	0/1665
6	j	0.15	0/1214	0.40	0/1643
7	H	0.34	0/467	0.38	0/631
7	k	0.13	0/460	0.38	0/623
8	I	0.53	0/238	0.41	0/324
8	l	0.21	0/241	0.40	0/327
9	J	0.58	0/343	0.59	2/467 (0.4%)
9	m	0.13	0/342	0.41	0/465
10	K	0.38	0/571	0.43	0/775
10	n	0.16	0/581	0.46	0/786
11	L	0.51	0/1120	0.42	0/1534
11	o	0.15	0/1121	0.34	0/1537
12	1	0.28	0/1467	0.37	0/2008
12	p	0.20	0/1535	0.45	0/2097
13	2	0.36	0/1608	0.39	0/2204
14	3	0.34	0/1684	0.43	0/2298
14	q	0.29	1/1727 (0.1%)	0.52	1/2353 (0.0%)
15	5	0.40	0/1527	0.49	1/2085 (0.0%)
16	G	0.13	0/2664	0.38	0/3637
17	M	0.15	0/3730	0.39	0/5082
18	N	0.29	0/865	0.48	1/1188 (0.1%)
19	O	0.37	6/3987 (0.2%)	0.49	4/5427 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
20	P	0.14	0/759	0.32	0/1028
21	Q	0.19	0/5180	0.45	3/7068 (0.0%)
22	R	0.15	0/1288	0.45	1/1765 (0.1%)
23	S	0.13	0/3070	0.39	0/4173
24	T	0.22	0/1254	0.54	3/1702 (0.2%)
25	U	0.12	0/1297	0.37	0/1771
26	V	0.13	0/1504	0.40	0/2046
27	W	0.18	0/597	0.46	0/816
28	X	0.12	0/896	0.41	0/1218
29	Y	0.12	0/1170	0.37	0/1592
31	a	0.17	0/1213	0.54	0/1651
32	b	0.13	0/935	0.45	1/1276 (0.1%)
33	c	0.14	0/1006	0.36	0/1365
34	4	0.15	0/894	0.49	0/1216
35	d	0.13	0/1314	0.38	0/1771
36	6	0.19	0/2589	0.58	2/3513 (0.1%)
37	7	0.18	0/2347	0.53	0/3184
38	8	0.19	0/844	0.51	0/1145
39	9	0.14	0/636	0.46	0/868
40	0	0.22	0/1122	0.69	0/1536
41	r	0.16	0/1577	0.38	0/2153
42	s	0.18	0/1650	0.48	3/2255 (0.1%)
All	All	0.34	16/90609 (0.0%)	0.44	28/123459 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
9	m	0	1
12	p	0	1
19	O	0	1
21	Q	0	1
24	T	0	1
29	Y	0	1
31	a	0	1
32	b	0	1
35	d	0	1
36	6	0	4
37	7	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
38	8	0	2
40	0	0	3
All	All	0	20

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	f	657	TRP	C-O	-11.08	1.11	1.24
19	O	479	PRO	CA-C	-9.49	1.39	1.52
2	f	657	TRP	CA-C	-9.13	1.41	1.52
19	O	481	PHE	C-O	-7.58	1.14	1.24
1	e	679	ALA	CA-C	-7.51	1.43	1.52
19	O	481	PHE	N-CA	-6.99	1.36	1.45
19	O	479	PRO	C-O	-6.93	1.15	1.24
1	e	678	TRP	C-O	-6.16	1.16	1.24
2	f	657	TRP	CA-CB	-6.14	1.43	1.53
19	O	481	PHE	CA-CB	-5.93	1.45	1.53
19	O	481	PHE	CA-C	-5.88	1.44	1.52
2	f	657	TRP	CB-CG	-5.88	1.32	1.50
1	e	678	TRP	CA-C	-5.66	1.44	1.52
2	f	657	TRP	C-N	-5.44	1.26	1.33
1	e	679	ALA	N-CA	-5.08	1.40	1.46
14	q	225	LEU	CA-C	-5.04	1.46	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	6	274	GLN	CA-C-N	12.68	135.69	119.84
36	6	274	GLN	C-N-CA	12.68	135.69	119.84
14	q	225	LEU	N-CA-C	-11.77	98.42	111.14
19	O	481	PHE	N-CA-C	-11.69	96.08	113.61
2	B	223	GLY	CA-C-N	8.07	129.93	119.84
2	B	223	GLY	C-N-CA	8.07	129.93	119.84
2	f	657	TRP	CB-CA-C	-7.86	98.55	110.88
22	R	141	VAL	N-CA-C	-7.71	106.39	113.71
1	e	677	VAL	O-C-N	7.21	128.95	121.89
15	5	61	THR	N-CA-C	-7.20	106.42	114.62
42	s	192	PRO	N-CA-C	7.00	126.89	112.47
21	Q	262	GLY	N-CA-C	-6.90	100.81	111.64
21	Q	122	ASP	CA-C-N	6.76	134.44	121.54
21	Q	122	ASP	C-N-CA	6.76	134.44	121.54
18	N	44	TYR	N-CA-C	6.74	120.61	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	s	192	PRO	CA-C-N	-6.70	108.73	121.54
42	s	192	PRO	C-N-CA	-6.70	108.73	121.54
24	T	125	TYR	N-CA-C	6.69	122.57	113.21
24	T	123	GLU	N-CA-C	6.18	123.97	110.80
32	b	189	VAL	N-CA-C	-6.06	107.59	113.53
2	B	223	GLY	N-CA-C	-5.92	100.26	112.34
1	e	679	ALA	N-CA-C	-5.68	103.91	111.24
9	J	34	PRO	O-C-N	-5.63	116.27	123.14
19	O	490	VAL	N-CA-C	-5.50	108.14	113.53
19	O	497	TYR	CA-C-N	-5.25	108.99	121.80
19	O	497	TYR	C-N-CA	-5.25	108.99	121.80
24	T	124	GLU	N-CA-C	5.10	117.39	110.35
9	J	35	ASP	N-CA-CB	5.09	119.10	110.49

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	0	121	PRO	Peptide
40	0	207	GLY	Peptide
40	0	91	GLY	Peptide
36	6	173	ASP	Peptide
36	6	178	TRP	Peptide
36	6	274	GLN	Mainchain
36	6	368	GLY	Peptide
37	7	254	ALA	Peptide
38	8	160	LYS	Peptide
38	8	90	THR	Peptide
2	B	222	LEU	Mainchain
19	O	495	SER	Peptide
21	Q	261	ASN	Peptide
24	T	122	THR	Mainchain
29	Y	125	PRO	Peptide
31	a	115	GLN	Peptide
32	b	96	GLY	Peptide
35	d	86	ASN	Peptide
9	m	35	ASP	Peptide
12	p	231	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5813	0	5633	125	0
1	e	5798	0	5613	169	0
2	B	5851	0	5605	95	0
2	f	5840	0	5580	175	0
3	C	610	0	597	23	0
3	g	613	0	607	30	0
4	D	1113	0	1113	32	0
4	h	1111	0	1113	40	0
5	E	538	0	537	8	0
5	i	539	0	539	12	0
6	F	1204	0	1202	35	0
6	j	1188	0	1178	42	0
7	H	454	0	487	7	0
7	k	447	0	472	9	0
8	I	232	0	254	5	0
8	l	235	0	261	6	0
9	J	333	0	347	11	0
9	m	332	0	335	16	0
10	K	565	0	557	19	0
10	n	576	0	584	18	0
11	L	1088	0	1079	29	0
11	o	1089	0	1075	29	0
12	1	1422	0	1324	52	0
12	p	1484	0	1410	61	0
13	2	1554	0	1478	59	0
14	3	1631	0	1501	44	0
14	q	1672	0	1575	66	0
15	5	1486	0	1389	62	0
16	G	2602	0	2598	82	0
17	M	3646	0	3652	83	0
18	N	841	0	761	19	0
19	O	3874	0	3923	94	0
20	P	750	0	760	20	0
21	Q	5041	0	4852	132	0
22	R	1260	0	1197	28	0
23	S	2991	0	2849	131	0
24	T	1229	0	1109	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	U	1258	0	1151	52	0
26	V	1473	0	1441	56	0
27	W	572	0	559	28	0
28	X	876	0	801	29	0
29	Y	1135	0	1107	31	0
30	Z	305	0	69	3	0
31	a	1185	0	1086	30	0
32	b	915	0	764	14	0
33	c	989	0	927	21	0
34	4	878	0	823	20	0
35	d	1289	0	1247	21	0
36	6	2541	0	2461	75	0
37	7	2302	0	2224	91	0
38	8	828	0	742	21	0
39	9	617	0	520	17	0
40	0	1089	0	901	13	0
41	r	1529	0	1448	49	0
42	s	1591	0	1446	55	0
43	A	61	0	62	2	0
43	e	61	0	62	5	0
44	1	485	0	395	30	0
44	2	454	0	383	20	0
44	3	595	0	452	25	0
44	5	468	0	375	17	0
44	A	2024	0	1724	52	0
44	B	2118	0	1848	66	0
44	F	83	0	60	3	0
44	J	42	0	31	2	0
44	K	157	0	107	6	0
44	L	193	0	152	6	0
44	e	2028	0	1626	68	0
44	f	1921	0	1521	67	0
44	j	41	0	29	1	0
44	m	83	0	59	0	0
44	n	162	0	112	3	0
44	o	145	0	118	6	0
44	p	474	0	373	20	0
44	q	543	0	404	20	0
44	r	525	0	424	21	0
44	s	431	0	349	20	0
45	A	33	0	46	2	0
45	B	30	0	37	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	e	14	0	7	1	0
45	f	16	0	10	6	0
46	1	49	0	74	5	0
46	2	35	0	40	2	0
46	A	79	0	104	7	0
46	B	38	0	46	0	0
46	O	24	0	19	1	0
46	e	65	0	77	2	0
46	f	38	0	46	1	0
46	p	49	0	74	7	0
46	s	35	0	40	1	0
47	1	19	0	26	3	0
47	2	40	0	56	4	0
47	3	40	0	56	4	0
47	5	40	0	56	5	0
47	A	279	0	389	18	0
47	B	280	0	392	19	0
47	F	80	0	112	4	0
47	I	40	0	56	4	0
47	J	40	0	56	1	0
47	K	40	0	56	2	0
47	L	80	0	112	10	0
47	Q	39	0	53	6	0
47	e	280	0	392	23	0
47	f	239	0	333	14	0
47	j	80	0	112	2	0
47	l	80	0	112	5	0
47	m	40	0	56	3	0
47	n	40	0	56	1	0
47	o	80	0	112	4	0
47	p	11	0	16	1	0
47	q	40	0	56	3	0
47	r	40	0	56	5	0
47	s	40	0	56	4	0
48	8	8	0	0	1	0
48	A	8	0	0	0	0
48	C	16	0	0	1	0
48	f	8	0	0	0	0
48	g	16	0	0	1	0
49	B	59	0	79	4	0
49	J	66	0	96	3	0
49	f	52	0	62	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	m	66	0	96	2	0
50	2	52	0	55	3	0
50	5	32	0	34	1	0
50	F	75	0	90	3	0
50	m	30	0	30	1	0
50	r	18	0	12	0	0
51	1	84	0	112	11	0
51	2	42	0	56	8	0
51	3	84	0	112	12	0
51	5	42	0	56	8	0
51	p	84	0	111	11	0
51	q	84	0	112	11	0
51	r	42	0	56	10	0
51	s	42	0	56	5	0
52	1	129	0	83	5	0
52	2	174	0	110	13	0
52	3	90	0	60	1	0
52	5	133	0	80	8	0
52	p	137	0	91	7	0
52	q	46	0	31	1	0
52	r	141	0	97	2	0
52	s	183	0	121	7	0
53	2	44	0	56	7	0
53	5	44	0	56	5	0
53	r	44	0	56	4	0
53	s	44	0	56	8	0
54	Q	100	0	137	6	0
All	All	106329	0	101185	2666	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (2666) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:G:240:VAL:HG11	18:N:45:GLU:CB	2.03	0.88
2:f:700:LEU:HB2	45:f:844:PQN:H6	1.62	0.81
33:c:148:ALA:HB3	39:9:105:PHE:HB2	1.67	0.76
18:N:48:ILE:CB	23:S:14:ASN:ND2	2.50	0.75
37:7:68:SER:HA	37:7:83:ARG:O	1.87	0.75
2:B:124:TRP:CD2	2:B:124:TRP:CZ2	2.75	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:95:GLY:C	44:K:201:CLA:H3A	2.13	0.73
38:8:152:VAL:HG21	38:8:169:GLN:OE1	1.87	0.73
15:5:129:ALA:HB1	15:5:134:LEU:HD11	1.71	0.73
3:g:54:CYS:SG	3:g:55:GLU:N	2.61	0.72
6:j:215:VAL:O	6:j:218:TYR:HB3	1.89	0.72
2:B:26:ALA:HB2	49:B:850:DGD:HA42	1.72	0.71
44:A:821:CLA:HAA2	10:K:79:ALA:HB3	1.73	0.71
9:J:10:VAL:HG13	9:J:12:PRO:HD2	1.72	0.71
12:p:90:CYS:CB	51:p:502:LUT:H392	2.21	0.70
5:E:92:LYS:NZ	5:E:102:ASN:OD1	2.23	0.70
14:3:219:GLU:O	14:3:223:LEU:N	2.24	0.70
12:1:128:TRP:HE1	44:1:515:CLA:CAD	2.06	0.69
42:s:67:VAL:HG22	42:s:69:PHE:H	1.57	0.69
42:s:207:TRP:HA	42:s:212:PRO:HG3	1.75	0.69
21:Q:424:VAL:HG23	38:8:124:LEU:CD2	2.22	0.69
21:Q:669:TYR:HB3	37:7:300:GLY:HA2	1.74	0.69
12:1:83:HIS:HD2	51:1:502:LUT:H35	1.58	0.69
1:e:69:LYS:NZ	44:e:810:CLA:OBD	2.26	0.69
1:e:197:HIS:O	1:e:201:GLY:N	2.24	0.69
19:O:109:ARG:HB3	19:O:155:TRP:HE1	1.58	0.68
13:2:186:ASN:HB3	52:2:516:CHL:C1D	2.23	0.68
42:s:192:PRO:O	42:s:193:ASP:C	2.30	0.68
44:p:509:CLA:H11	44:p:515:CLA:CAD	2.23	0.68
11:L:156:ALA:HB2	11:L:172:GLN:HG3	1.76	0.68
15:5:183:PRO:HG3	36:6:233:GLY:HA2	1.74	0.68
4:D:104:GLU:N	4:D:104:GLU:OE1	2.27	0.68
2:f:700:LEU:HB2	45:f:844:PQN:C6	2.23	0.68
33:c:185:LEU:HA	33:c:188:ARG:HH11	1.57	0.67
19:O:488:ASP:HA	19:O:491:GLU:HB3	1.76	0.67
32:b:94:ARG:O	32:b:118:ARG:NH2	2.27	0.67
2:f:299:HIS:HD2	2:f:304:LEU:HD21	1.59	0.67
15:5:135:PHE:HB2	52:5:314:CHL:HBC1	1.75	0.67
35:d:131:VAL:HG13	35:d:137:ILE:HG22	1.76	0.67
31:a:134:PRO:HG2	31:a:137:GLU:HB2	1.77	0.67
15:5:183:PRO:HG3	36:6:233:GLY:CA	2.25	0.67
14:q:168:GLU:OE2	14:q:171:ARG:NE	2.27	0.67
41:r:51:PRO:HB2	42:s:178:VAL:HG22	1.76	0.67
17:M:247:ALA:O	17:M:250:HIS:ND1	2.28	0.66
36:6:310:GLY:O	36:6:334:TRP:NE1	2.28	0.66
36:6:285:LYS:HA	36:6:288:ARG:HB3	1.77	0.66
2:f:311:PRO:HB2	46:f:852:LHG:HC12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3:112:VAL:HG11	51:3:303:LUT:H12	1.77	0.66
42:s:168:ARG:NH2	44:s:514:CLA:O1D	2.27	0.66
3:g:73:THR:HG22	3:g:74:THR:H	1.59	0.66
44:B:807:CLA:H51	49:B:850:DGD:HB71	1.76	0.66
12:1:67:ALA:HB1	12:1:73:PHE:HD1	1.60	0.66
1:A:570:ARG:NH2	46:A:843:LHG:O10	2.29	0.66
1:A:40:PRO:HG2	6:F:192:ALA:HB1	1.77	0.66
31:a:140:PHE:HA	31:a:143:VAL:HG12	1.78	0.66
1:e:453:TYR:HB3	1:e:641:ILE:HD11	1.78	0.66
1:e:33:SER:HB3	1:e:36:LEU:HB2	1.78	0.66
1:e:210:TRP:NE1	1:e:214:GLN:OE1	2.29	0.66
46:p:516:LHG:H151	46:p:516:LHG:H271	1.78	0.66
12:p:69:VAL:HB	12:p:72:ASN:HB2	1.79	0.65
31:a:82:ASP:HB2	31:a:87:TYR:HE1	1.61	0.65
41:r:144:TYR:OH	41:r:148:ARG:NH1	2.29	0.65
44:B:826:CLA:HMA1	47:B:848:BCR:H14C	1.78	0.65
14:3:209:PRO:HD2	51:3:303:LUT:H23	1.79	0.65
18:N:58:PHE:HB2	23:S:34:GLY:HA3	1.78	0.65
1:e:13:VAL:HG22	1:e:184:LYS:HD3	1.78	0.65
12:p:82:TYR:HB3	52:p:514:CHL:HMD2	1.78	0.65
12:p:152:GLU:O	12:p:158:LYS:NZ	2.29	0.65
41:r:234:TRP:O	41:r:240:GLN:NE2	2.29	0.65
38:8:130:GLY:N	48:8:201:SF4:S3	2.70	0.65
44:r:309:CLA:H3A	52:r:316:CHL:HBC2	1.78	0.65
1:A:264:LEU:HD21	10:K:117:VAL:HG22	1.78	0.65
11:L:88:VAL:HG23	11:L:93:ARG:HD3	1.78	0.65
12:1:98:GLU:HG2	12:1:104:ASN:HA	1.79	0.65
14:q:225:LEU:O	14:q:228:ILE:HG22	1.97	0.65
41:r:98:GLY:O	41:r:102:MET:HG2	1.97	0.65
37:7:58:PRO:HB2	37:7:74:LEU:HB2	1.79	0.65
2:f:90:ALA:HA	2:f:113:VAL:HG12	1.78	0.64
11:o:203:ASP:HB2	11:o:208:PHE:HZ	1.63	0.64
2:f:353:TYR:HA	2:f:368:GLN:HE21	1.62	0.64
14:3:131:THR:OG1	44:3:311:CLA:O1D	2.16	0.64
10:n:72:ALA:HA	10:n:84:LYS:HZ3	1.61	0.64
41:r:226:LEU:HD11	51:r:302:LUT:H163	1.78	0.64
2:B:476:ILE:HG22	2:B:477:LEU:H	1.62	0.64
15:5:48:TRP:CD1	15:5:48:TRP:H	2.15	0.64
15:5:118:TRP:HE1	15:5:229:PRO:HD3	1.63	0.64
3:g:61:ASP:HA	5:i:135:ASN:HD22	1.62	0.64
14:q:232:ARG:HA	14:q:235:MET:HE3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:s:262:ASN:H	42:s:265:SER:HG	1.43	0.64
23:S:324:GLN:H	23:S:343:GLY:HA3	1.62	0.64
2:f:352:MET:O	2:f:368:GLN:NE2	2.30	0.64
2:f:683:GLU:OE2	4:h:87:ARG:N	2.31	0.64
44:B:823:CLA:HAB	44:B:842:CLA:HED1	1.80	0.64
12:1:149:ARG:HA	44:1:513:CLA:HBC3	1.80	0.64
1:e:426:ARG:HG2	1:e:429:ARG:HH21	1.62	0.64
5:i:116:THR:HG22	5:i:118:TYR:H	1.63	0.64
12:p:201:GLN:OE1	12:p:213:ASN:ND2	2.31	0.64
1:A:275:PHE:HE2	44:A:817:CLA:HBB1	1.63	0.64
44:A:806:CLA:H41	46:A:843:LHG:H271	1.80	0.64
52:1:517:CHL:HED1	15:5:147:THR:HB	1.79	0.64
1:e:655:GLN:OE1	1:e:745:ARG:NH1	2.31	0.64
2:f:582:TRP:CH2	44:f:803:CLA:HAB	2.33	0.64
6:F:181:TYR:OH	6:F:194:ARG:O	2.16	0.64
1:e:194:MET:HB2	44:e:812:CLA:HBC2	1.80	0.63
2:B:238:ASP:HB2	2:B:269:TRP:HZ3	1.62	0.63
12:1:229:ILE:HG13	12:1:230:VAL:H	1.63	0.63
36:6:250:ALA:HB3	36:6:422:LEU:HA	1.78	0.63
4:D:167:VAL:HG21	4:D:173:ASN:HD21	1.64	0.63
21:Q:291:TRP:O	21:Q:295:ALA:HB2	1.99	0.63
1:e:264:LEU:HD23	44:n:203:CLA:HMD1	1.80	0.63
2:f:174:ARG:HH21	44:f:826:CLA:HMD2	1.63	0.63
44:f:835:CLA:HBD	44:f:835:CLA:HBA1	1.79	0.63
39:9:93:SER:HG	39:9:95:TRP:CD1	2.17	0.63
2:f:654:HIS:NE2	44:f:804:CLA:NA	2.45	0.63
12:1:119:ALA:H	12:1:129:GLY:HA3	1.63	0.63
13:2:186:ASN:HB3	52:2:516:CHL:C2D	2.29	0.63
16:G:201:GLY:O	16:G:205:TRP:NE1	2.32	0.63
1:A:314:GLY:HA2	10:K:88:ARG:HH22	1.63	0.63
49:J:103:DGD:O5E	49:J:103:DGD:O4E	2.09	0.63
12:1:183:LYS:O	12:1:187:ASN:ND2	2.24	0.63
36:6:397:THR:HG23	36:6:399:ALA:H	1.63	0.63
1:e:193:SER:O	1:e:197:HIS:ND1	2.30	0.63
44:e:809:CLA:O2D	44:e:809:CLA:H2A	1.99	0.63
2:f:397:ASP:OD1	4:h:196:LYS:NZ	2.31	0.63
1:A:341:ILE:HG22	1:A:419:ARG:HB3	1.79	0.63
1:e:42:THR:HG22	1:e:713:GLN:HB2	1.81	0.63
2:f:700:LEU:CB	45:f:844:PQN:H6	2.28	0.63
42:s:112:ARG:NH1	52:s:513:CHL:OBD	2.32	0.63
2:B:339:ALA:HB2	47:B:848:BCR:H372	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:63:MET:HE1	10:K:115:MET:HB2	1.79	0.63
1:e:578:ARG:HH11	1:e:581:THR:HG21	1.64	0.63
44:e:828:CLA:CBA	44:e:828:CLA:O1A	2.46	0.63
2:f:481:THR:O	2:f:487:ASN:ND2	2.31	0.62
2:f:169:LYS:NZ	2:f:327:ASN:O	2.29	0.62
13:2:258:GLY:HA3	14:3:151:ALA:HA	1.81	0.62
26:V:62:SER:OG	26:V:100:THR:N	2.32	0.62
11:o:140:LEU:HB3	11:o:181:THR:HG22	1.80	0.62
1:e:717:LEU:HD23	1:e:721:GLN:HG2	1.82	0.62
14:q:177:ASN:ND2	42:s:71:GLY:O	2.32	0.62
14:q:137:GLN:HG2	14:q:144:ALA:HB1	1.81	0.62
2:f:257:LEU:HD12	44:f:819:CLA:HMB3	1.82	0.62
51:p:502:LUT:H361	51:p:502:LUT:H28	1.82	0.62
14:3:268:ILE:HD11	44:3:308:CLA:H11	1.81	0.62
51:3:303:LUT:O23	44:3:306:CLA:O1A	2.16	0.62
31:a:173:GLU:HA	31:a:185:ALA:O	1.98	0.62
1:A:117:PRO:HB3	1:A:122:GLU:HB3	1.79	0.62
1:A:694:GLU:OE1	2:B:536:LYS:NZ	2.29	0.62
1:e:573:CYS:SG	1:e:575:GLY:N	2.71	0.62
42:s:224:LYS:NZ	46:s:516:LHG:O5	2.33	0.62
44:B:805:CLA:HBC3	44:B:830:CLA:H41	1.82	0.62
15:5:209:ARG:NH1	44:5:308:CLA:O2D	2.33	0.62
2:B:223:GLY:O	2:B:226:LEU:N	2.33	0.61
21:Q:424:VAL:HG23	38:8:124:LEU:HD23	1.82	0.61
9:m:28:GLU:OE1	9:m:31:ARG:NH2	2.32	0.61
12:p:109:GLN:HG2	44:p:515:CLA:HAC2	1.81	0.61
46:p:516:LHG:H342	41:r:140:ILE:HD13	1.81	0.61
18:N:48:ILE:CB	23:S:14:ASN:HD21	2.11	0.61
12:p:180:LEU:HD23	12:p:183:LYS:HD2	1.82	0.61
26:V:110:VAL:HA	26:V:150:ILE:HD11	1.82	0.61
2:B:124:TRP:HB3	2:B:129:LEU:HD12	1.81	0.61
10:n:67:GLY:O	10:n:77:ARG:NH1	2.29	0.61
11:o:126:THR:HG21	11:o:196:TYR:HB2	1.83	0.61
1:A:65:GLU:N	1:A:65:GLU:OE1	2.33	0.61
26:V:103:MET:N	26:V:141:SER:O	2.34	0.61
1:e:706:LEU:HD21	44:f:833:CLA:H3A	1.83	0.61
2:f:529:THR:O	2:f:533:ILE:HG12	2.00	0.61
42:s:157:GLN:HG2	52:s:515:CHL:HMA3	1.82	0.61
19:O:438:ARG:HA	19:O:442:TYR:HD2	1.66	0.61
2:B:330:ILE:HG21	44:B:806:CLA:HAC1	1.83	0.61
15:5:85:GLN:N	15:5:85:GLN:OE1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Q:706:GLY:O	21:Q:708:ILE:N	2.34	0.60
2:f:2:GLU:HB2	2:f:7:ARG:HH11	1.65	0.60
1:e:13:VAL:HA	14:q:87:GLY:HA3	1.83	0.60
44:r:307:CLA:HHD	44:r:312:CLA:HBB2	1.83	0.60
15:5:176:GLN:NE2	15:5:193:ASP:O	2.35	0.60
44:f:832:CLA:HBC1	47:f:848:BCR:H21C	1.83	0.60
3:g:31:TRP:CD1	3:g:32:ASP:H	2.19	0.60
6:F:213:TRP:CD1	6:F:214:PRO:HD3	2.37	0.60
1:e:127:ASP:OD2	6:j:108:LYS:NZ	2.31	0.60
2:f:310:PRO:HG3	44:f:843:CLA:HBD	1.83	0.60
13:2:104:GLN:HE21	13:2:193:VAL:HG12	1.65	0.60
29:Y:194:MET:O	29:Y:198:LEU:N	2.34	0.60
14:q:191:LYS:HE3	14:q:192:TYR:CZ	2.37	0.60
1:A:331:THR:HG21	46:A:844:LHG:HC11	1.82	0.60
21:Q:262:GLY:O	21:Q:264:ASN:N	2.35	0.60
13:2:166:ARG:NH2	13:2:177:VAL:O	2.34	0.60
16:G:57:ILE:HG13	16:G:58:GLN:H	1.66	0.60
1:e:533:VAL:HG11	1:e:607:HIS:CG	2.37	0.60
47:e:851:BCR:H313	9:m:31:ARG:HD3	1.82	0.60
38:8:105:ARG:NE	38:8:116:TYR:OH	2.32	0.60
2:B:133:GLU:OE1	2:B:133:GLU:N	2.34	0.59
41:r:144:TYR:CZ	41:r:148:ARG:HD2	2.37	0.59
6:F:183:ILE:O	6:F:186:SER:OG	2.15	0.59
14:3:112:VAL:HG11	51:3:303:LUT:H10	1.84	0.59
15:5:212:MET:HE1	44:5:308:CLA:HAB	1.84	0.59
1:e:421:ASN:OD1	1:e:422:ASP:N	2.35	0.59
44:A:802:CLA:H3A	44:A:802:CLA:CGA	2.32	0.59
2:B:721:TYR:HB2	44:B:803:CLA:HED3	1.83	0.59
18:N:101:VAL:O	18:N:105:VAL:HG23	2.03	0.59
14:q:214:THR:HG23	14:q:215:LYS:H	1.65	0.59
41:r:206:LEU:HD22	44:r:306:CLA:HAB	1.83	0.59
13:2:220:LYS:O	13:2:224:ASN:ND2	2.31	0.59
17:M:150:ILE:HG12	20:P:62:PHE:CD1	2.38	0.59
21:Q:313:ALA:O	21:Q:317:PHE:HB3	2.03	0.59
1:e:72:SER:OG	44:e:810:CLA:HHD	2.03	0.59
2:f:299:HIS:CD2	2:f:304:LEU:HD21	2.37	0.59
17:M:81:GLU:HG3	17:M:82:GLU:H	1.67	0.59
23:S:275:ILE:O	23:S:279:ILE:HG13	2.03	0.59
35:d:173:LEU:N	35:d:205:GLY:O	2.35	0.59
1:A:244:ARG:NH2	1:A:255:ALA:O	2.36	0.59
20:P:43:LEU:HB2	22:R:46:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:7:99:HIS:NE2	37:7:110:ARG:HD3	2.17	0.59
21:Q:459:LYS:HA	21:Q:462:ILE:HG12	1.85	0.59
52:p:512:CHL:HHC	52:p:512:CHL:HBB1	1.85	0.59
42:s:139:TYR:CG	42:s:240:VAL:HG11	2.38	0.59
42:s:239:GLN:O	42:s:243:THR:N	2.35	0.59
1:e:536:ILE:HD12	43:e:801:CL0:H63	1.84	0.59
42:s:262:ASN:N	42:s:265:SER:OG	2.31	0.59
37:7:217:SER:O	37:7:219:PRO:HD3	2.03	0.58
2:f:174:ARG:HB2	44:f:815:CLA:HBC2	1.84	0.58
2:B:191:THR:HG21	2:B:278:LEU:HB2	1.85	0.58
19:O:68:TYR:O	19:O:69:LYS:NZ	2.36	0.58
1:e:657:ILE:HA	2:f:617:MET:HE1	1.85	0.58
2:B:85:ARG:HB3	2:B:115:ILE:HD12	1.85	0.58
17:M:86:SER:HB2	17:M:90:ASN:H	1.68	0.58
21:Q:88:LEU:O	21:Q:91:SER:HB3	2.02	0.58
25:U:107:SER:O	25:U:111:GLN:NE2	2.36	0.58
31:a:215:LEU:O	31:a:218:VAL:HB	2.03	0.58
1:A:656:VAL:HG21	1:A:741:PHE:HA	1.85	0.58
23:S:67:VAL:HG11	23:S:82:THR:HG21	1.85	0.58
23:S:277:GLN:O	23:S:281:LYS:HB2	2.04	0.58
1:e:155:GLN:N	1:e:155:GLN:OE1	2.36	0.58
2:f:268:LEU:HB2	2:f:273:MET:HE2	1.84	0.58
1:A:656:VAL:HG22	1:A:744:ALA:HB3	1.85	0.58
12:1:229:ILE:HG13	12:1:230:VAL:N	2.18	0.58
21:Q:121:ASN:O	21:Q:122:ASP:CB	2.49	0.58
26:V:21:MET:HE3	26:V:22:ASN:H	1.68	0.58
34:4:152:GLN:NE2	34:4:153:VAL:O	2.36	0.58
36:6:288:ARG:HA	36:6:384:CYS:SG	2.43	0.58
39:9:85:GLN:HG3	39:9:98:SER:HB3	1.85	0.58
1:e:330:PHE:O	1:e:426:ARG:NH2	2.37	0.58
44:s:506:CLA:H11	44:s:511:CLA:HED2	1.85	0.58
1:A:279:LEU:HG	1:A:505:LEU:HD23	1.85	0.58
2:f:654:HIS:NE2	44:f:804:CLA:C1A	2.67	0.58
42:s:237:TRP:O	42:s:241:VAL:HG23	2.04	0.58
44:A:815:CLA:HED2	44:A:815:CLA:H2A	1.85	0.58
2:B:257:LEU:HD21	2:B:493:TRP:HE3	1.67	0.58
17:M:119:ILE:HD11	17:M:126:ILE:HG23	1.85	0.58
28:X:93:TRP:CD1	28:X:95:SER:HG	2.22	0.58
29:Y:108:SER:O	29:Y:114:HIS:ND1	2.37	0.58
2:f:615:TYR:OH	2:f:621:ARG:NH2	2.36	0.58
52:p:514:CHL:HHC	52:p:514:CHL:HBB1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:108:VAL:HG23	5:E:109:THR:HG22	1.86	0.58
8:I:3:ASN:O	8:I:6:SER:OG	2.21	0.58
21:Q:260:ASN:O	21:Q:262:GLY:N	2.34	0.58
1:e:386:SER:OG	44:e:827:CLA:HHB	2.03	0.58
44:f:808:CLA:H12	44:f:831:CLA:H12	1.84	0.58
3:C:62:PHE:O	3:C:63:LEU:HG	2.03	0.58
16:G:288:PHE:HB3	16:G:294:ASN:HD21	1.68	0.58
21:Q:250:LEU:HD21	21:Q:325:LEU:HD11	1.86	0.58
23:S:140:LEU:HD13	23:S:178:PHE:HB2	1.85	0.58
23:S:362:LEU:HG	23:S:365:LEU:HD22	1.86	0.58
25:U:118:MET:HE2	25:U:143:LEU:HD13	1.86	0.58
1:e:60:THR:HG22	1:e:61:GLY:H	1.68	0.58
1:e:522:LEU:HD21	1:e:616:VAL:HA	1.86	0.58
2:f:355:LEU:HB2	44:f:819:CLA:HED1	1.85	0.58
26:V:57:LEU:N	26:V:94:LEU:O	2.36	0.58
37:7:116:VAL:HG13	37:7:192:ALA:HB3	1.86	0.58
44:r:305:CLA:H2A	44:r:305:CLA:HED2	1.85	0.58
1:A:267:SER:O	1:A:267:SER:OG	2.17	0.57
16:G:128:ILE:HD13	22:R:56:TYR:HB3	1.86	0.57
18:N:86:PHE:HE1	18:N:94:PHE:HB2	1.69	0.57
23:S:138:ARG:NH1	23:S:142:TYR:OH	2.37	0.57
24:T:132:ARG:HD2	26:V:131:THR:HG22	1.85	0.57
25:U:31:GLN:HA	25:U:87:ILE:HG23	1.86	0.57
26:V:169:ALA:HA	26:V:172:LYS:HD2	1.86	0.57
31:a:100:PHE:HB2	31:a:108:LYS:NZ	2.17	0.57
6:j:150:VAL:HG12	6:j:160:PHE:HB2	1.85	0.57
44:A:838:CLA:H91	44:F:802:CLA:HBC3	1.85	0.57
3:C:1:MET:N	3:C:45:THR:OG1	2.37	0.57
16:G:49:LEU:HD21	16:G:314:TYR:CE2	2.39	0.57
17:M:378:THR:OG1	17:M:380:ASN:OD1	2.22	0.57
23:S:51:MET:HE1	23:S:66:TYR:HD1	1.68	0.57
35:d:87:PRO:HG2	35:d:88:VAL:HG22	1.86	0.57
38:8:149:LYS:HG2	38:8:165:ARG:HE	1.69	0.57
17:M:62:PHE:O	17:M:66:THR:HG23	2.04	0.57
17:M:361:MET:HE2	17:M:405:LEU:HD23	1.85	0.57
37:7:251:ARG:HG2	37:7:276:PRO:HB3	1.85	0.57
38:8:131:GLU:O	38:8:156:LYS:NZ	2.37	0.57
12:p:154:ASP:HB3	12:p:157:LYS:H	1.69	0.57
6:F:190:LYS:HE2	6:F:193:MET:HG2	1.85	0.57
31:a:186:PHE:HB2	31:a:201:VAL:HG22	1.87	0.57
47:e:850:BCR:H372	2:f:438:VAL:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:10:GLN:NE2	2:f:14:GLN:OE1	2.36	0.57
3:g:61:ASP:OD2	5:i:95:ARG:NH1	2.37	0.57
13:2:139:THR:O	13:2:143:GLN:NE2	2.32	0.57
17:M:195:VAL:HG13	20:P:41:ILE:HG21	1.84	0.57
31:a:100:PHE:HB2	31:a:108:LYS:HZ3	1.69	0.57
37:7:220:PRO:HD2	37:7:225:PHE:CZ	2.40	0.57
1:e:25:GLU:HB2	44:e:810:CLA:HBA1	1.86	0.57
1:e:689:ARG:NH2	2:f:565:GLY:O	2.38	0.57
44:e:821:CLA:HED2	44:e:821:CLA:H2A	1.85	0.57
11:o:77:TYR:HD2	11:o:78:LEU:HD12	1.69	0.57
44:B:818:CLA:H8	44:B:835:CLA:H11	1.85	0.57
15:5:75:GLU:OE1	15:5:75:GLU:N	2.37	0.57
47:A:845:BCR:H383	47:A:853:BCR:H10C	1.86	0.57
15:5:240:PRO:O	15:5:244:ASN:ND2	2.38	0.57
14:q:62:GLN:O	14:q:65:THR:OG1	2.22	0.57
42:s:117:ALA:HB1	53:s:502:XAT:H161	1.87	0.57
1:A:75:PHE:CZ	44:3:301:CLA:HBB1	2.40	0.57
1:A:476:LEU:HB2	1:A:528:THR:HG23	1.87	0.57
23:S:19:HIS:CE1	23:S:26:LEU:HB2	2.40	0.57
36:6:283:ILE:HG12	36:6:406:ARG:HH11	1.68	0.57
2:f:717:TYR:CE1	44:f:804:CLA:HED1	2.39	0.57
1:A:466:GLN:OE1	1:A:466:GLN:N	2.36	0.57
6:F:106:LEU:HB2	6:F:119:ILE:HG21	1.87	0.57
17:M:161:LEU:HD12	20:P:76:ILE:HD12	1.85	0.57
23:S:83:VAL:O	23:S:87:GLU:HG2	2.05	0.57
25:U:118:MET:HA	25:U:118:MET:HE3	1.86	0.57
26:V:50:ARG:HH21	26:V:177:ILE:HG23	1.69	0.57
33:c:131:ARG:HD2	33:c:226:MET:HE3	1.85	0.57
37:7:112:GLY:O	37:7:195:SER:HA	2.03	0.57
9:m:1:MET:HG3	9:m:5:LYS:HE2	1.86	0.57
1:e:717:LEU:N	45:e:842:PQN:O4	2.37	0.57
2:f:51:PHE:HB3	2:f:153:SER:HB2	1.85	0.57
4:D:155:ASN:OD1	4:D:156:GLY:N	2.38	0.56
4:D:162:HIS:HB3	4:D:163:PRO:HD3	1.87	0.56
44:3:308:CLA:HBD	44:3:308:CLA:CGA	2.35	0.56
21:Q:291:TRP:O	21:Q:295:ALA:CB	2.53	0.56
23:S:326:LEU:HA	25:U:25:ARG:HE	1.70	0.56
25:U:10:LEU:HA	25:U:13:HIS:HD2	1.70	0.56
27:W:135:PHE:O	27:W:138:THR:HB	2.05	0.56
37:7:72:LEU:HD12	37:7:79:VAL:HG22	1.87	0.56
44:e:839:CLA:HBB2	6:j:178:GLY:HA3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:q:301:LUT:H30	44:q:304:CLA:HBB1	1.86	0.56
13:2:166:ARG:CZ	52:2:516:CHL:HMC	2.35	0.56
22:R:74:ILE:O	22:R:78:VAL:HG23	2.04	0.56
23:S:354:ILE:O	23:S:393:ARG:NH1	2.39	0.56
2:f:366:THR:HG22	2:f:729:THR:HG23	1.85	0.56
2:f:411:MET:HE2	47:f:848:BCR:H292	1.87	0.56
44:A:840:CLA:HBB2	47:L:305:BCR:H372	1.87	0.56
2:B:83:HIS:HA	7:H:143:ILE:HB	1.86	0.56
44:L:302:CLA:C1B	44:L:303:CLA:HED1	2.35	0.56
17:M:85:ILE:HG22	17:M:89:GLY:HA2	1.86	0.56
20:P:33:CYS:O	20:P:37:ILE:HG13	2.04	0.56
21:Q:203:LEU:HD13	21:Q:302:ILE:HD12	1.86	0.56
26:V:147:ASP:O	28:X:99:ARG:NH1	2.37	0.56
36:6:139:LEU:HD11	36:6:200:LEU:HD21	1.85	0.56
40:0:67:GLU:N	40:0:68:PRO:HD2	2.21	0.56
2:f:19:ARG:HA	2:f:22:TRP:HD1	1.70	0.56
3:g:24:ASP:OD2	4:h:162:HIS:ND1	2.37	0.56
14:q:147:TYR:HB3	14:q:149:TYR:CZ	2.41	0.56
14:q:184:GLN:NE2	42:s:67:VAL:O	2.35	0.56
46:2:517:LHG:HC91	46:2:517:LHG:H281	1.87	0.56
15:5:196:ASN:O	15:5:200:VAL:N	2.30	0.56
19:O:386:LEU:O	21:Q:225:ARG:NH2	2.38	0.56
36:6:338:ALA:HA	36:6:341:ILE:HG12	1.87	0.56
36:6:359:HIS:O	36:6:363:ILE:N	2.30	0.56
36:6:366:ILE:HB	36:6:370:GLU:HG3	1.86	0.56
2:f:279:ALA:O	2:f:283:ILE:HG12	2.06	0.56
19:O:333:LEU:HD13	19:O:482:VAL:HG21	1.88	0.56
21:Q:123:PHE:CD1	21:Q:123:PHE:C	2.82	0.56
23:S:277:GLN:O	23:S:281:LYS:CB	2.53	0.56
4:D:68:GLN:HB3	4:D:150:TYR:OH	2.06	0.56
11:L:82:PRO:O	11:L:93:ARG:NH1	2.38	0.56
51:1:501:LUT:H32	44:1:504:CLA:CAB	2.36	0.56
14:3:79:PRO:HD2	51:3:304:LUT:H23	1.87	0.56
1:A:64:GLU:OE2	1:A:68:ARG:NH2	2.38	0.56
15:5:234:LEU:HD23	15:5:237:LEU:HD21	1.87	0.56
25:U:68:SER:OG	25:U:123:TYR:OH	2.21	0.56
38:8:192:HIS:C	38:8:194:TRP:H	2.14	0.56
1:e:618:GLY:HA2	1:e:629:ILE:HG12	1.88	0.56
44:2:509:CLA:H12	52:2:515:CHL:CAD	2.35	0.56
50:5:301:LMG:O5	50:5:301:LMG:O4	2.23	0.56
25:U:132:ILE:HG13	25:U:133:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:115:LEU:O	13:2:119:GLY:N	2.38	0.56
19:O:376:THR:OG1	54:Q:803:SQD:O47	2.24	0.56
25:U:18:ARG:HB3	25:U:31:GLN:HB3	1.88	0.56
2:f:223:GLY:HA2	2:f:226:LEU:HB2	1.88	0.56
2:f:600:THR:HG21	2:f:609:PHE:HB2	1.86	0.56
11:o:175:GLU:O	11:o:179:GLN:HG2	2.06	0.56
1:A:507:TRP:O	1:A:509:GLY:N	2.38	0.56
15:5:91:CYS:HB2	15:5:208:GLY:HA3	1.88	0.56
15:5:233:LEU:HD23	15:5:237:LEU:HD23	1.88	0.56
16:G:41:ILE:O	16:G:45:VAL:HG23	2.05	0.56
18:N:42:SER:O	26:V:90:ARG:NH2	2.39	0.56
23:S:353:LYS:NZ	23:S:354:ILE:O	2.36	0.56
31:a:100:PHE:O	31:a:101:LEU:HD22	2.06	0.56
1:e:660:TYR:OH	2:f:441:ASP:OD1	2.21	0.56
5:i:97:GLU:N	5:i:97:GLU:OE1	2.36	0.56
1:A:247:LEU:HB3	1:A:254:PHE:HD2	1.70	0.55
1:A:717:LEU:HD23	1:A:721:GLN:HG2	1.88	0.55
6:F:173:TRP:CD1	6:F:210:GLY:HA3	2.41	0.55
12:1:82:TYR:CE1	44:1:513:CLA:HMD1	2.41	0.55
17:M:129:PHE:HD2	17:M:169:TYR:HD2	1.54	0.55
19:O:283:ILE:HD13	19:O:286:ILE:HD11	1.88	0.55
23:S:195:GLN:HE22	24:T:24:GLN:HB3	1.71	0.55
36:6:243:LYS:HB2	36:6:244:PRO:HD2	1.87	0.55
37:7:65:ARG:N	37:7:146:TYR:O	2.37	0.55
42:s:106:ALA:O	42:s:110:HIS:ND1	2.39	0.55
21:Q:251:PHE:O	21:Q:255:ASN:ND2	2.39	0.55
23:S:319:PHE:H	23:S:347:LEU:HD12	1.71	0.55
41:r:206:LEU:HD21	44:r:306:CLA:H101	1.88	0.55
24:T:80:VAL:HG21	24:T:96:ASN:ND2	2.20	0.55
1:e:691:TYR:CE1	2:f:536:LYS:HD2	2.41	0.55
3:g:27:GLU:HG3	4:h:176:ARG:HH11	1.72	0.55
41:r:144:TYR:CE2	47:r:301:BCR:H12C	2.41	0.55
36:6:333:LEU:HD22	36:6:448:ILE:HG21	1.89	0.55
1:e:146:ARG:HH21	1:e:376:TYR:HE2	1.54	0.55
26:V:187:LEU:HD13	28:X:190:SER:HB2	1.88	0.55
49:f:851:DGD:O5D	49:f:851:DGD:O4D	2.22	0.55
4:h:106:VAL:HG12	4:h:116:ILE:HG22	1.87	0.55
47:l:102:BCR:H403	11:o:136:LEU:HD12	1.88	0.55
14:q:54:ARG:NH2	14:q:67:LEU:O	2.39	0.55
46:1:516:LHG:H241	52:1:517:CHL:C1C	2.37	0.55
19:O:32:VAL:HG12	19:O:115:TYR:HD2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:U:135:PRO:HG3	26:V:104:LYS:HD3	1.89	0.55
34:4:155:ASP:O	34:4:220:GLY:HA2	2.06	0.55
1:e:313:TRP:NE1	44:e:819:CLA:O1A	2.39	0.55
1:e:445:LEU:HB3	1:e:539:PHE:HB2	1.87	0.55
1:e:675:HIS:NE2	43:e:801:CL0:NA	2.55	0.55
1:e:741:PHE:CD1	43:e:801:CL0:H26	2.42	0.55
44:B:812:CLA:H2A	44:B:812:CLA:O1D	2.06	0.55
19:O:178:PHE:O	19:O:182:VAL:HG23	2.07	0.55
1:e:340:GLU:HB3	1:e:419:ARG:HH11	1.71	0.55
41:r:160:ASN:HB3	41:r:170:LEU:HD22	1.88	0.55
1:A:585:SER:OG	1:A:588:ASP:OD2	2.25	0.55
15:5:218:PHE:HE1	51:5:303:LUT:H41	1.70	0.55
29:Y:63:ASP:OD2	29:Y:216:TRP:NE1	2.39	0.55
37:7:301:LEU:HA	37:7:360:ASN:ND2	2.21	0.55
2:f:22:TRP:CG	2:f:704:GLN:HE22	2.25	0.55
2:f:85:ARG:HB3	2:f:115:ILE:HD12	1.89	0.55
2:f:582:TRP:HH2	44:f:803:CLA:HAB	1.72	0.55
2:f:733:PHE:HD2	7:k:139:PRO:HG2	1.71	0.55
3:g:14:CYS:O	3:g:16:GLN:NE2	2.40	0.55
41:r:237:THR:N	41:r:240:GLN:OE1	2.39	0.55
6:F:198:ILE:O	9:J:9:SER:OG	2.25	0.55
21:Q:306:ILE:HA	21:Q:310:THR:HG22	1.89	0.55
41:r:213:VAL:HG21	44:r:306:CLA:HAC2	1.89	0.55
42:s:239:GLN:OE1	42:s:250:ASN:ND2	2.39	0.55
44:s:506:CLA:HMA3	44:s:511:CLA:HBC3	1.88	0.55
4:D:137:ASN:OD1	4:D:140:ARG:NH2	2.25	0.55
12:1:217:HIS:HB2	44:1:506:CLA:HAA2	1.90	0.55
15:5:125:LYS:HE3	15:5:129:ALA:H	1.72	0.55
19:O:438:ARG:HH12	40:0:81:ASN:HA	1.71	0.55
21:Q:183:SER:HB2	21:Q:189:ILE:HG22	1.88	0.55
23:S:310:PHE:HD2	23:S:311:LEU:HD13	1.71	0.55
10:n:101:THR:HG23	10:n:103:ALA:H	1.72	0.55
11:L:136:LEU:HD13	47:L:305:BCR:H401	1.88	0.54
16:G:151:SER:OG	16:G:152:ASN:N	2.40	0.54
23:S:268:MET:O	23:S:271:SER:OG	2.24	0.54
26:V:153:ASP:HA	28:X:192:VAL:HG21	1.89	0.54
34:4:133:GLU:HG3	34:4:134:LEU:H	1.72	0.54
41:r:208:PHE:CD2	53:r:303:XAT:H12	2.41	0.54
15:5:169:GLU:OE1	15:5:169:GLU:N	2.39	0.54
23:S:351:ARG:NH1	23:S:352:TRP:O	2.40	0.54
25:U:119:VAL:HG23	25:U:121:ILE:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:177:GLU:HA	31:a:182:GLY:HA2	1.89	0.54
1:e:200:ALA:HB2	1:e:306:GLY:HA3	1.89	0.54
2:f:203:ARG:NH2	2:f:253:ALA:O	2.37	0.54
2:f:207:VAL:HA	2:f:211:ASN:HD21	1.72	0.54
4:h:87:ARG:O	4:h:91:VAL:HG22	2.07	0.54
43:A:801:CL0:H13	44:B:802:CLA:OBD	2.08	0.54
15:5:221:GLN:HB3	15:5:232:ASN:ND2	2.21	0.54
16:G:247:TYR:HD2	16:G:251:LYS:HB3	1.71	0.54
21:Q:252:GLN:OE1	21:Q:256:ASN:ND2	2.38	0.54
23:S:169:TYR:HA	23:S:287:TYR:HB3	1.89	0.54
23:S:365:LEU:HA	23:S:368:LEU:HD12	1.89	0.54
1:e:56:PHE:HB3	1:e:66:ILE:HG22	1.89	0.54
4:h:171:LYS:O	4:h:176:ARG:NH2	2.33	0.54
6:j:213:TRP:CD1	6:j:214:PRO:HD3	2.42	0.54
13:2:121:PHE:CE2	51:2:501:LUT:H28	2.43	0.54
19:O:53:TYR:CE2	40:0:147:GLY:HA3	2.43	0.54
19:O:79:ARG:HG3	19:O:132:ARG:HB3	1.89	0.54
19:O:420:PHE:O	19:O:424:ILE:HG12	2.08	0.54
22:R:43:LEU:HG	22:R:66:TYR:CE1	2.42	0.54
24:T:46:LYS:NZ	24:T:47:SER:O	2.40	0.54
29:Y:72:ILE:HG22	29:Y:74:PRO:HD3	1.90	0.54
33:c:167:PHE:CE2	33:c:186:ALA:HB2	2.42	0.54
36:6:308:ILE:O	36:6:354:MET:HB3	2.07	0.54
14:q:157:PHE:CD2	44:q:312:CLA:HAA2	2.42	0.54
41:r:89:LEU:HD22	41:r:198:LEU:HD21	1.88	0.54
1:A:276:ARG:HD2	1:A:287:TRP:CD1	2.42	0.54
44:3:313:CLA:C1B	44:3:313:CLA:H2	2.38	0.54
25:U:41:ALA:HB1	25:U:104:ILE:HG21	1.87	0.54
33:c:131:ARG:HG3	33:c:223:MET:HG3	1.89	0.54
33:c:137:LEU:HB2	33:c:219:LEU:HD21	1.90	0.54
8:l:26:LEU:HD21	11:o:145:VAL:HG13	1.89	0.54
12:p:134:ILE:HA	12:p:137:ILE:HG22	1.89	0.54
42:s:96:GLU:OE2	42:s:99:SER:N	2.38	0.54
46:1:516:LHG:H162	46:1:516:LHG:H282	1.89	0.54
13:2:214:LEU:O	13:2:218:ARG:N	2.27	0.54
19:O:444:TYR:HB2	21:Q:209:THR:HG22	1.88	0.54
21:Q:68:LEU:HD23	54:Q:803:SQD:H91	1.88	0.54
34:4:162:SER:OG	34:4:163:MET:N	2.41	0.54
36:6:416:SER:OG	36:6:438:SER:O	2.24	0.54
37:7:215:TYR:HE2	37:7:252:GLN:HE21	1.53	0.54
37:7:269:VAL:O	37:7:316:GLY:HA2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:75:PHE:CZ	44:e:809:CLA:HBB1	2.43	0.54
17:M:267:PHE:O	17:M:271:THR:HG22	2.07	0.54
25:U:72:LEU:HD23	25:U:73:THR:N	2.23	0.54
39:9:151:ASP:N	39:9:151:ASP:OD1	2.39	0.54
2:f:426:SER:HB3	44:f:801:CLA:HBA1	1.89	0.54
2:B:18:THR:HG23	2:B:696:LYS:O	2.08	0.54
17:M:261:PRO:O	17:M:265:VAL:HG23	2.08	0.54
17:M:325:ALA:HA	17:M:329:ILE:HD13	1.89	0.54
23:S:76:MET:HG3	23:S:157:TYR:OH	2.08	0.54
37:7:223:SER:HB3	37:7:227:LEU:HD12	1.90	0.54
2:f:176:ASN:ND2	2:f:291:TYR:O	2.41	0.54
2:f:330:ILE:HG21	44:f:807:CLA:HAC1	1.88	0.54
3:g:77:MET:HB3	3:g:79:LEU:HG	1.89	0.54
14:3:267:ASN:OD1	14:3:270:THR:OG1	2.26	0.54
16:G:236:GLU:HG3	16:G:239:LEU:C	2.33	0.54
21:Q:740:ASN:O	21:Q:744:LEU:N	2.41	0.54
28:X:99:ARG:HH22	28:X:194:ASN:HD21	1.55	0.54
47:e:846:BCR:H362	47:e:847:BCR:H21C	1.90	0.54
2:f:612:SER:O	2:f:612:SER:OG	2.25	0.54
44:f:818:CLA:CHD	44:f:819:CLA:HBB2	2.38	0.54
1:A:11:LYS:HG3	1:A:13:VAL:HG23	1.90	0.54
16:G:352:LEU:O	16:G:355:THR:OG1	2.26	0.54
21:Q:423:MET:HB2	21:Q:495:THR:HB	1.89	0.54
26:V:142:THR:O	26:V:144:ARG:NH2	2.41	0.54
36:6:172:TYR:CG	36:6:187:GLN:HG2	2.42	0.54
42:s:144:ARG:HH11	44:s:509:CLA:H2A	1.71	0.54
44:A:831:CLA:H2A	44:A:831:CLA:O1D	2.08	0.53
4:D:108:GLU:OE2	4:D:138:ARG:NH1	2.41	0.53
13:2:180:ASP:HB2	13:2:186:ASN:HB2	1.89	0.53
14:3:73:GLY:O	14:3:232:ARG:NH2	2.38	0.53
23:S:169:TYR:HB2	23:S:288:GLU:HB3	1.90	0.53
28:X:106:ALA:HA	28:X:120:THR:HA	1.91	0.53
36:6:127:TYR:HB3	36:6:319:MET:HA	1.90	0.53
2:f:43:TYR:HE1	2:f:330:ILE:HD11	1.72	0.53
12:p:166:ASP:N	12:p:167:PRO:HD3	2.24	0.53
14:q:66:TYR:OH	14:q:78:ASP:OD2	2.25	0.53
44:L:304:CLA:HBC3	44:L:304:CLA:HHD	1.89	0.53
16:G:31:PRO:O	16:G:35:LEU:HG	2.07	0.53
16:G:184:LEU:HA	16:G:358:GLN:HE21	1.74	0.53
21:Q:675:LEU:HA	21:Q:678:ILE:HB	1.89	0.53
2:B:450:GLU:OE2	6:F:129:ARG:NH2	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:V:51:LEU:HD13	26:V:174:ARG:HG2	1.91	0.53
27:W:149:ALA:O	27:W:152:VAL:HG23	2.08	0.53
29:Y:92:GLY:HA3	29:Y:147:LYS:H	1.73	0.53
36:6:393:VAL:HG22	36:6:411:VAL:HB	1.90	0.53
1:A:133:ARG:NH1	6:F:109:TYR:OH	2.41	0.53
2:B:73:ASN:ND2	2:B:107:GLY:O	2.27	0.53
14:3:135:TRP:CD1	14:3:252:PRO:HG3	2.44	0.53
44:5:308:CLA:HBB1	44:5:308:CLA:HMB3	1.90	0.53
16:G:145:LEU:HD13	22:R:75:ILE:HG21	1.89	0.53
16:G:197:GLN:NE2	16:G:206:ASN:H	2.07	0.53
21:Q:276:PHE:HZ	21:Q:339:VAL:HG11	1.72	0.53
47:Q:801:BCR:H271	54:Q:803:SQD:H121	1.90	0.53
28:X:136:THR:O	28:X:139:THR:OG1	2.26	0.53
2:f:304:LEU:O	2:f:308:HIS:ND1	2.42	0.53
2:f:438:VAL:HG12	44:f:835:CLA:HAC1	1.91	0.53
4:D:80:GLY:C	11:L:64:LEU:HD21	2.34	0.53
21:Q:203:LEU:HB3	21:Q:302:ILE:HG21	1.90	0.53
36:6:427:VAL:HG13	36:6:431:LYS:H	1.72	0.53
2:f:190:TRP:HD1	2:f:277:HIS:CD2	2.26	0.53
2:f:506:ASN:OD1	2:f:508:LEU:N	2.35	0.53
44:f:810:CLA:O1A	44:f:829:CLA:HBD	2.09	0.53
8:l:11:LEU:HA	8:l:15:VAL:HG22	1.90	0.53
11:o:203:ASP:HB2	11:o:208:PHE:CZ	2.44	0.53
1:A:392:MET:HG3	1:A:601:ILE:HD12	1.91	0.53
11:L:199:LEU:HD13	44:L:304:CLA:HED2	1.89	0.53
16:G:164:ALA:O	16:G:168:ILE:HG12	2.09	0.53
19:O:170:TYR:CE2	19:O:223:VAL:HG13	2.44	0.53
37:7:82:TYR:OH	37:7:171:LEU:O	2.27	0.53
37:7:214:PRO:O	37:7:253:GLY:HA3	2.08	0.53
6:j:194:ARG:NH2	50:m:105:LMG:O3	2.40	0.53
1:A:588:ASP:HA	1:A:591:PHE:HB3	1.89	0.53
44:B:816:CLA:HBC3	47:B:844:BCR:H391	1.90	0.53
4:D:141:SER:O	4:D:144:LYS:NZ	2.41	0.53
12:1:167:PRO:HD2	51:1:501:LUT:H23	1.91	0.53
51:5:303:LUT:H3	44:5:307:CLA:HMA2	1.91	0.53
21:Q:692:ASP:O	21:Q:695:LYS:HB2	2.07	0.53
21:Q:760:ARG:O	21:Q:763:SER:N	2.40	0.53
22:R:15:GLY:HA3	22:R:49:PHE:HE1	1.73	0.53
23:S:195:GLN:NE2	24:T:24:GLN:HB3	2.24	0.53
11:o:76:TRP:CD1	11:o:80:ASN:HD21	2.27	0.53
12:p:177:PHE:HE1	44:p:504:CLA:HED1	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:r:226:LEU:HG	51:r:302:LUT:H22	1.90	0.53
42:s:65:ARG:HH12	42:s:85:ASP:CG	2.17	0.53
36:6:362:GLU:O	36:6:365:GLU:HG3	2.08	0.53
1:e:213:HIS:HB2	44:e:813:CLA:CHC	2.39	0.53
41:r:209:LEU:HD13	44:r:308:CLA:HBB2	1.91	0.53
1:A:275:PHE:CE2	44:A:817:CLA:HBB1	2.44	0.53
1:A:504:SER:OG	1:A:505:LEU:N	2.40	0.53
44:B:811:CLA:HHC	44:B:811:CLA:HBB1	1.90	0.53
12:1:43:PRO:HD2	52:1:517:CHL:O1D	2.09	0.53
17:M:409:PRO:HA	17:M:414:PHE:CG	2.44	0.53
31:a:161:GLU:HG2	31:a:170:TRP:CD1	2.44	0.53
1:e:64:GLU:OE2	1:e:68:ARG:NH2	2.42	0.53
1:e:283:THR:OG1	1:e:376:TYR:N	2.41	0.53
44:e:803:CLA:HBA2	44:e:810:CLA:H2	1.90	0.53
44:e:818:CLA:CAC	47:e:847:BCR:H352	2.39	0.53
10:n:67:GLY:HA2	10:n:72:ALA:HB3	1.91	0.53
41:r:60:ASP:OD1	41:r:61:GLY:N	2.41	0.53
3:C:61:ASP:HA	5:E:135:ASN:HD22	1.73	0.53
15:5:92:ARG:NH1	52:5:315:CHL:OBD	2.40	0.53
19:O:388:LEU:HD21	21:Q:198:MET:HE2	1.89	0.53
24:T:160:ASN:HD22	26:V:75:ARG:HH12	1.57	0.53
25:U:37:TRP:HB3	25:U:99:PRO:HB2	1.90	0.53
2:B:527:LEU:O	2:B:531:THR:OG1	2.16	0.52
38:8:161:PRO:HD2	38:8:164:TRP:CZ2	2.44	0.52
14:3:62:GLN:O	14:3:65:THR:OG1	2.27	0.52
16:G:175:THR:HG21	18:N:76:THR:HB	1.90	0.52
17:M:226:SER:HB2	34:4:239:CYS:HB2	1.92	0.52
25:U:22:PHE:HA	25:U:28:GLU:HA	1.91	0.52
27:W:115:ILE:HD13	27:W:145:LEU:HD22	1.90	0.52
29:Y:151:VAL:HB	29:Y:204:VAL:HG12	1.90	0.52
34:4:177:GLY:HA3	35:d:180:PRO:HD2	1.91	0.52
1:e:340:GLU:N	1:e:340:GLU:OE1	2.42	0.52
1:e:572:PRO:HD3	1:e:720:ILE:HD11	1.91	0.52
2:f:700:LEU:HG	45:f:844:PQN:O4	2.09	0.52
44:f:806:CLA:HHC	44:f:808:CLA:OBD	2.09	0.52
6:j:227:VAL:HG12	6:j:228:VAL:H	1.74	0.52
2:B:363:GLN:OE1	2:B:363:GLN:N	2.42	0.52
19:O:438:ARG:NH1	40:0:81:ASN:O	2.41	0.52
21:Q:415:TYR:O	40:0:93:TYR:HB2	2.09	0.52
23:S:151:MET:N	23:S:151:MET:SD	2.82	0.52
1:e:392:MET:HG3	1:e:601:ILE:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:s:504:CLA:H2A	44:s:504:CLA:O1D	2.09	0.52
21:Q:484:THR:HA	21:Q:487:TYR:CE2	2.44	0.52
25:U:55:GLN:HG3	25:U:111:GLN:HB3	1.92	0.52
26:V:132:GLY:O	26:V:136:SER:OG	2.25	0.52
36:6:412:ALA:HB3	36:6:435:VAL:HG22	1.92	0.52
1:e:225:LEU:HD21	1:e:231:PRO:HG3	1.91	0.52
1:e:293:HIS:HB3	44:e:817:CLA:HMB2	1.91	0.52
1:e:373:PRO:HG2	1:e:374:TYR:CD1	2.44	0.52
1:e:455:HIS:HB2	44:e:833:CLA:C1C	2.39	0.52
4:h:178:GLY:CA	4:h:181:GLN:HE22	2.22	0.52
12:p:56:PRO:HG3	12:p:181:LYS:HE2	1.92	0.52
1:A:210:TRP:NE1	1:A:214:GLN:OE1	2.42	0.52
43:A:801:CL0:CMB	44:B:802:CLA:OBD	2.57	0.52
2:B:338:LEU:HD22	2:B:382:ILE:HG23	1.90	0.52
15:5:174:GLY:HA3	15:5:179:TYR:O	2.10	0.52
26:V:100:THR:HG21	26:V:135:PHE:HD2	1.75	0.52
35:d:138:GLN:NE2	35:d:186:GLN:OE1	2.42	0.52
44:f:801:CLA:H3A	44:f:801:CLA:CGA	2.39	0.52
42:s:161:MET:HG2	44:s:514:CLA:HMC3	1.90	0.52
44:A:803:CLA:C4D	9:J:12:PRO:HG3	2.40	0.52
12:1:82:TYR:HE1	44:1:513:CLA:HMD1	1.73	0.52
12:1:202:GLN:OE1	12:1:207:GLY:N	2.41	0.52
16:G:30:LEU:O	16:G:34:THR:HG23	2.08	0.52
19:O:438:ARG:HA	19:O:442:TYR:CD2	2.44	0.52
21:Q:736:ASP:HA	21:Q:739:THR:HG22	1.91	0.52
28:X:149:ASP:O	28:X:153:HIS:HB2	2.09	0.52
39:9:115:TRP:C	39:9:117:VAL:H	2.17	0.52
1:e:470:SER:OG	1:e:471:ASP:N	2.43	0.52
1:e:575:GLY:HA2	2:f:562:PRO:HD3	1.91	0.52
7:k:114:ALA:HB2	8:l:11:LEU:HD11	1.92	0.52
44:5:310:CLA:H12	52:5:317:CHL:C3D	2.40	0.52
16:G:114:VAL:HG11	16:G:129:GLY:HA2	1.92	0.52
19:O:207:ALA:O	19:O:208:THR:HG22	2.09	0.52
21:Q:312:VAL:HG12	21:Q:369:LEU:HD21	1.90	0.52
22:R:102:LEU:O	22:R:106:THR:HG23	2.09	0.52
29:Y:114:HIS:HE1	29:Y:133:PRO:HA	1.75	0.52
14:q:159:PHE:CG	44:s:511:CLA:HBA1	2.45	0.52
13:2:258:GLY:O	14:3:152:ASP:N	2.30	0.52
15:5:158:SER:O	15:5:158:SER:OG	2.22	0.52
17:M:135:THR:HG21	22:R:165:VAL:HG21	1.92	0.52
21:Q:424:VAL:HG23	38:8:124:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:98:PHE:HB2	31:a:108:LYS:HD3	1.91	0.52
1:e:703:HIS:CE1	44:e:852:CLA:HAC1	2.45	0.52
12:p:104:ASN:OD1	12:p:105:TRP:N	2.43	0.52
44:A:810:CLA:HMB3	44:A:810:CLA:HBB1	1.91	0.52
44:B:822:CLA:H11	47:B:844:BCR:HC22	1.92	0.52
16:G:72:LEU:HB2	27:W:150:PRO:HG2	1.92	0.52
22:R:7:ILE:HA	22:R:10:ILE:HD12	1.92	0.52
23:S:291:GLU:HA	23:S:294:ARG:HE	1.74	0.52
26:V:80:ARG:NH2	26:V:81:TYR:OH	2.43	0.52
27:W:130:GLU:HA	27:W:133:LEU:HD13	1.91	0.52
12:p:93:GLY:O	51:p:502:LUT:H24	2.09	0.52
41:r:48:SER:C	41:r:50:LEU:H	2.17	0.52
44:r:306:CLA:NC	44:r:306:CLA:H52	2.25	0.52
2:B:582:TRP:CH2	44:B:802:CLA:HAB	2.45	0.52
13:2:111:ARG:HH11	52:2:513:CHL:CAD	2.23	0.52
16:G:108:VAL:O	16:G:111:SER:OG	2.28	0.52
19:O:49:TYR:HB2	40:0:151:TYR:HD2	1.74	0.52
19:O:388:LEU:HG	19:O:389:PRO:HD2	1.92	0.52
25:U:33:LYS:HB3	25:U:36:ASP:HB2	1.92	0.52
26:V:89:PRO:HG3	26:V:112:LEU:HD22	1.91	0.52
34:4:137:SER:HB2	34:4:173:ARG:HH12	1.75	0.52
36:6:322:ARG:O	36:6:322:ARG:NH2	2.43	0.52
1:e:65:GLU:OE1	1:e:65:GLU:N	2.31	0.52
2:f:658:ALA:HB3	44:f:805:CLA:HBB2	1.92	0.52
14:q:165:GLY:O	14:q:169:HIS:ND1	2.39	0.52
4:D:109:MET:HE1	4:D:124:LEU:HD21	1.91	0.51
6:F:86:LYS:HB3	6:F:134:GLY:O	2.10	0.51
17:M:57:ARG:HB2	17:M:58:PRO:HD3	1.92	0.51
21:Q:193:TRP:CZ2	21:Q:282:LYS:HB2	2.45	0.51
23:S:375:ALA:O	23:S:379:THR:HG23	2.09	0.51
26:V:25:GLU:HG3	28:X:185:LYS:HB2	1.92	0.51
37:7:314:TYR:OH	37:7:336:ALA:HB3	2.10	0.51
47:e:854:BCR:H403	10:n:107:ALA:HB1	1.91	0.51
10:n:50:SER:OG	10:n:51:SER:N	2.42	0.51
12:p:183:LYS:HG2	44:p:510:CLA:OBD	2.10	0.51
46:p:516:LHG:H132	52:p:517:CHL:HBB1	1.92	0.51
42:s:262:ASN:N	42:s:265:SER:HG	2.06	0.51
1:A:25:GLU:HB2	44:A:810:CLA:HAA2	1.91	0.51
52:5:315:CHL:HHC	52:5:315:CHL:HBB1	1.90	0.51
16:G:232:LEU:HB2	16:G:235:ALA:HB3	1.92	0.51
35:d:136:MET:HE1	35:d:138:GLN:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:7:145:SER:OG	37:7:146:TYR:N	2.43	0.51
2:f:339:ALA:HB2	47:f:849:BCR:H372	1.92	0.51
3:g:14:CYS:SG	3:g:16:GLN:HG2	2.50	0.51
11:o:152:GLU:OE1	11:o:152:GLU:N	2.44	0.51
14:q:233:LEU:HD22	44:q:310:CLA:HHD	1.91	0.51
12:1:143:ALA:O	12:1:147:GLN:N	2.41	0.51
25:U:59:ASP:OD1	25:U:60:VAL:N	2.44	0.51
36:6:379:PRO:C	36:6:381:GLN:H	2.18	0.51
12:p:168:LEU:O	12:p:172:LYS:NZ	2.43	0.51
12:p:173:ASP:HB2	12:p:176:LYS:HB3	1.92	0.51
44:B:806:CLA:HBB1	44:B:806:CLA:HMB1	1.91	0.51
51:3:303:LUT:H26	44:3:306:CLA:H12	1.92	0.51
34:4:200:LEU:HD12	34:4:231:ALA:HA	1.92	0.51
37:7:270:SER:HA	37:7:315:LEU:O	2.10	0.51
12:p:87:ALA:O	12:p:91:VAL:HG23	2.09	0.51
14:q:163:LEU:HB3	47:q:303:BCR:H363	1.92	0.51
2:B:449:PRO:HG2	6:F:94:ARG:HH11	1.75	0.51
2:B:658:ALA:HB3	44:B:804:CLA:HBB2	1.93	0.51
44:B:808:CLA:HAA2	44:B:810:CLA:HED1	1.92	0.51
47:I:101:BCR:H382	47:I:101:BCR:H23C	1.93	0.51
11:L:203:ASP:OD1	11:L:203:ASP:N	2.43	0.51
13:2:162:TRP:CH2	47:2:503:BCR:H321	2.46	0.51
44:3:314:CLA:H2A	44:3:314:CLA:O1D	2.11	0.51
16:G:348:LEU:O	16:G:352:LEU:HG	2.10	0.51
23:S:231:TRP:CE2	23:S:233:LEU:HD21	2.46	0.51
23:S:314:LYS:NZ	23:S:315:PRO:O	2.43	0.51
36:6:175:ASP:HB3	36:6:203:LYS:HE3	1.92	0.51
36:6:311:ILE:HG23	36:6:331:LEU:HD13	1.93	0.51
44:f:808:CLA:HED1	44:f:831:CLA:H43	1.92	0.51
46:p:516:LHG:H302	46:p:516:LHG:H162	1.92	0.51
14:q:244:GLN:O	14:q:248:THR:N	2.31	0.51
1:A:340:GLU:OE1	1:A:340:GLU:N	2.42	0.51
44:3:311:CLA:HED2	44:3:311:CLA:H2A	1.93	0.51
16:G:174:LEU:HD11	16:G:224:GLU:HG3	1.92	0.51
21:Q:190:TYR:OH	21:Q:194:GLU:OE2	2.23	0.51
23:S:324:GLN:HG3	25:U:25:ARG:HA	1.92	0.51
29:Y:70:LEU:HD21	29:Y:216:TRP:HB2	1.93	0.51
29:Y:115:PRO:HA	29:Y:130:TYR:HA	1.93	0.51
37:7:278:GLU:HG3	37:7:282:LYS:HB2	1.91	0.51
1:e:279:LEU:HD11	1:e:521:LEU:HD12	1.92	0.51
2:f:432:HIS:HD2	49:m:104:DGD:HAF2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:q:63:SER:HB2	14:q:67:LEU:HD12	1.92	0.51
42:s:70:PRO:HD2	52:s:517:CHL:O1D	2.11	0.51
4:D:184:ARG:NH1	4:D:189:ASN:OD1	2.40	0.51
13:2:104:GLN:NE2	13:2:193:VAL:HG12	2.25	0.51
44:3:314:CLA:H52	44:3:314:CLA:C1B	2.41	0.51
19:O:67:ASP:OD1	19:O:67:ASP:N	2.44	0.51
21:Q:51:TRP:HB3	21:Q:129:TYR:CE1	2.46	0.51
26:V:124:ALA:HB3	26:V:155:TYR:HA	1.93	0.51
37:7:65:ARG:HB3	37:7:146:TYR:CD2	2.45	0.51
1:e:161:ILE:O	1:e:165:VAL:HG23	2.10	0.51
1:e:195:LEU:HD12	1:e:319:LEU:HD11	1.93	0.51
6:j:158:GLY:O	9:m:39:PHE:N	2.44	0.51
47:q:303:BCR:C20	44:q:315:CLA:H3A	2.41	0.51
2:B:394:PHE:O	2:B:542:ARG:NH1	2.44	0.51
2:B:461:GLN:HG2	2:B:472:TYR:CZ	2.46	0.51
2:B:556:SER:HG	2:B:573:TRP:CG	2.29	0.51
12:1:195:PHE:CE2	51:1:502:LUT:H34	2.46	0.51
14:3:214:THR:HG23	14:3:215:LYS:H	1.75	0.51
16:G:283:PRO:O	16:G:286:SER:OG	2.27	0.51
19:O:331:ALA:O	19:O:335:ILE:HG23	2.10	0.51
26:V:67:GLU:O	26:V:70:SER:OG	2.24	0.51
37:7:73:ARG:HH22	37:7:108:ALA:HB1	1.75	0.51
37:7:98:LEU:HD22	37:7:330:PHE:CD1	2.46	0.51
14:q:181:MET:HG3	52:q:313:CHL:HMC	1.93	0.51
16:G:117:LEU:HB2	16:G:121:PHE:HD2	1.75	0.51
18:N:37:GLY:HA3	26:V:190:ASN:HD21	1.75	0.51
22:R:43:LEU:HG	22:R:66:TYR:CD1	2.45	0.51
39:9:136:HIS:ND1	39:9:136:HIS:O	2.44	0.51
1:e:418:THR:HG23	1:e:419:ARG:HG2	1.93	0.51
1:e:445:LEU:HD11	44:e:837:CLA:HMB2	1.93	0.51
1:e:688:GLY:HA3	2:f:569:ASP:HB2	1.93	0.51
44:e:838:CLA:H42	47:e:849:BCR:H363	1.92	0.51
2:f:85:ARG:HG3	7:k:143:ILE:HA	1.93	0.51
2:B:369:ALA:HB1	2:B:725:LEU:HD11	1.92	0.51
2:B:658:ALA:O	44:B:804:CLA:HAB	2.11	0.51
6:F:101:LYS:O	6:F:104:SER:OG	2.20	0.51
52:2:513:CHL:HHC	52:2:513:CHL:HBB1	1.92	0.51
17:M:337:ILE:HD13	17:M:340:ILE:HD12	1.93	0.51
19:O:102:LEU:HG	19:O:464:ILE:HD11	1.93	0.51
21:Q:386:PHE:O	21:Q:390:THR:HG23	2.11	0.51
26:V:103:MET:HG3	26:V:104:LYS:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:452:LEU:HD22	1:e:469:PHE:HE2	1.76	0.51
42:s:243:THR:OG1	42:s:245:GLN:OE1	2.20	0.51
12:1:221:PRO:O	12:1:225:ASN:ND2	2.44	0.50
15:5:105:ASP:HB3	15:5:230:ILE:HD12	1.93	0.50
19:O:43:GLU:HG2	19:O:122:TYR:CE1	2.46	0.50
27:W:114:ILE:HG13	27:W:118:TRP:CD1	2.45	0.50
27:W:149:ALA:HB1	27:W:150:PRO:HD2	1.93	0.50
28:X:137:ASP:O	28:X:141:GLN:HG2	2.09	0.50
2:f:431:PHE:HZ	47:j:801:BCR:H372	1.76	0.50
12:p:85:ARG:HH21	12:p:184:GLU:CD	2.19	0.50
12:p:100:LEU:O	12:p:102:LEU:N	2.44	0.50
1:A:415:ASP:OD1	1:A:417:THR:OG1	2.28	0.50
52:2:515:CHL:HBD	52:2:515:CHL:HBA2	1.92	0.50
15:5:233:LEU:HD12	51:5:303:LUT:H163	1.92	0.50
16:G:277:GLY:O	16:G:309:THR:OG1	2.22	0.50
21:Q:423:MET:HG2	21:Q:423:MET:O	2.10	0.50
23:S:73:LEU:HB2	23:S:387:ILE:HD13	1.92	0.50
23:S:76:MET:SD	23:S:105:MET:HB3	2.52	0.50
37:7:222:ALA:HB2	37:7:236:ARG:HH21	1.75	0.50
14:q:83:SER:HB2	14:q:97:LEU:HD11	1.93	0.50
44:A:827:CLA:C4A	44:A:827:CLA:HBA2	2.41	0.50
4:D:97:ILE:HG13	4:D:148:GLN:O	2.12	0.50
19:O:386:LEU:HD22	19:O:430:PRO:HG3	1.92	0.50
19:O:427:ILE:HD13	21:Q:226:VAL:HG22	1.93	0.50
24:T:60:GLU:HB2	24:T:118:CYS:SG	2.51	0.50
44:f:809:CLA:HHB	44:f:810:CLA:HMB3	1.93	0.50
10:n:118:GLY:HA3	44:n:202:CLA:HBC3	1.93	0.50
47:A:851:BCR:H331	44:J:101:CLA:HBC3	1.93	0.50
44:F:802:CLA:C4B	9:J:22:LEU:HD21	2.41	0.50
44:1:507:CLA:HED2	44:1:507:CLA:H2A	1.94	0.50
46:1:516:LHG:H241	52:1:517:CHL:NC	2.26	0.50
19:O:353:SER:O	19:O:354:ASP:HB3	2.11	0.50
19:O:402:PHE:HD2	21:Q:123:PHE:CZ	2.30	0.50
21:Q:663:ILE:HG23	21:Q:678:ILE:HD11	1.94	0.50
27:W:149:ALA:O	27:W:151:PHE:N	2.45	0.50
29:Y:105:ASP:N	29:Y:105:ASP:OD1	2.44	0.50
31:a:103:HIS:CD2	32:b:193:LYS:HA	2.46	0.50
36:6:302:LYS:HD3	36:6:304:LYS:HE3	1.92	0.50
3:g:61:ASP:OD1	3:g:62:PHE:N	2.40	0.50
6:j:173:TRP:CD2	6:j:210:GLY:HA3	2.46	0.50
12:p:75:ARG:HG3	52:p:514:CHL:HED1	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:VAL:O	1:A:659:SER:OG	2.26	0.50
2:B:32:GLU:OE1	2:B:32:GLU:N	2.44	0.50
15:5:179:TYR:HB3	44:5:305:CLA:O1D	2.11	0.50
17:M:91:PHE:O	17:M:92:GLN:HB2	2.12	0.50
37:7:314:TYR:O	37:7:333:THR:HA	2.11	0.50
3:g:54:CYS:HB3	48:g:101:SF4:S4	2.52	0.50
42:s:163:TRP:HH2	47:s:503:BCR:H321	1.76	0.50
44:B:820:CLA:HMB2	44:B:825:CLA:HMA3	1.93	0.50
13:2:116:GLY:HA2	53:2:502:XAT:H161	1.94	0.50
23:S:111:ILE:O	23:S:115:LEU:HG	2.11	0.50
33:c:215:THR:O	33:c:219:LEU:HB2	2.12	0.50
1:e:133:ARG:NH1	6:j:109:TYR:OH	2.45	0.50
1:e:601:ILE:O	1:e:605:ILE:HG12	2.11	0.50
1:A:56:PHE:CD2	44:A:805:CLA:HMC2	2.47	0.50
15:5:144:PHE:CE2	47:5:302:BCR:H12C	2.47	0.50
25:U:34:ALA:HB1	25:U:98:ILE:HD12	1.94	0.50
27:W:127:LYS:HG2	27:W:128:PHE:H	1.77	0.50
1:e:456:ASN:ND2	1:e:639:ILE:HB	2.26	0.50
44:e:852:CLA:H93	9:m:14:LEU:HD11	1.93	0.50
2:f:225:LEU:HA	2:f:230:TRP:CD1	2.47	0.50
4:h:110:PRO:HD3	4:h:135:LEU:HD12	1.92	0.50
1:A:331:THR:HB	1:A:423:LEU:HD21	1.94	0.50
3:C:52:LYS:HE3	3:C:67:VAL:HB	1.94	0.50
6:F:218:TYR:CZ	6:F:222:ILE:HD11	2.47	0.50
14:3:193:LEU:HD12	52:3:315:CHL:CMC	2.41	0.50
16:G:327:LEU:HD22	23:S:198:ILE:HD12	1.93	0.50
23:S:107:GLU:HA	23:S:110:ARG:HG3	1.92	0.50
27:W:108:LEU:HB2	27:W:144:GLY:HA3	1.93	0.50
34:4:164:VAL:HG22	34:4:165:VAL:H	1.76	0.50
36:6:329:LEU:HB2	36:6:334:TRP:NE1	2.26	0.50
2:f:3:LEU:HA	8:l:32:LYS:HB3	1.93	0.50
6:j:84:PRO:HG3	6:j:139:LEU:HD23	1.93	0.50
14:q:147:TYR:HB3	14:q:149:TYR:CE2	2.47	0.50
14:q:196:SER:N	14:q:202:PRO:O	2.45	0.50
44:A:816:CLA:CHD	44:A:817:CLA:HBB2	2.42	0.50
22:R:125:TRP:HZ2	32:b:147:LEU:HD23	1.77	0.50
26:V:25:GLU:HB2	28:X:188:MET:HG3	1.93	0.50
29:Y:113:ILE:HA	29:Y:133:PRO:HD3	1.94	0.50
33:c:168:ASP:HA	33:c:171:ILE:HG22	1.94	0.50
1:e:392:MET:HG2	1:e:605:ILE:HD11	1.93	0.50
1:e:434:ILE:HG23	44:e:838:CLA:HBB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:A:838:CLA:HAB	44:A:838:CLA:H122	1.93	0.49
13:2:246:PRO:O	51:2:501:LUT:O23	2.26	0.49
14:3:210:LEU:HD23	14:3:212:PHE:HE1	1.77	0.49
19:O:402:PHE:CD2	21:Q:123:PHE:CE2	3.00	0.49
36:6:143:TYR:HB2	36:6:146:VAL:HG21	1.95	0.49
14:q:62:GLN:HB3	14:q:81:GLY:HA3	1.93	0.49
42:s:152:THR:O	42:s:156:THR:HG23	2.11	0.49
1:A:230:ASP:N	1:A:230:ASP:OD1	2.45	0.49
1:A:421:ASN:OD1	1:A:422:ASP:N	2.45	0.49
6:F:172:GLY:O	6:F:176:TRP:N	2.31	0.49
13:2:182:ILE:O	13:2:184:PRO:HD3	2.12	0.49
51:3:303:LUT:C15	44:3:307:CLA:HBB1	2.41	0.49
17:M:335:VAL:HG22	17:M:420:LEU:HD13	1.95	0.49
19:O:318:ILE:HD13	19:O:422:MET:HE2	1.94	0.49
23:S:81:ILE:HD12	23:S:337:LEU:HG	1.94	0.49
25:U:96:PRO:HB2	25:U:121:ILE:HA	1.94	0.49
25:U:137:SER:OG	28:X:161:GLU:OE1	2.26	0.49
38:8:138:GLU:HA	38:8:164:TRP:HB3	1.93	0.49
1:e:595:PHE:CZ	1:e:727:VAL:HG23	2.47	0.49
12:p:142:ILE:HD11	44:p:515:CLA:HMB3	1.94	0.49
2:B:560:ASP:OD1	3:C:52:LYS:NZ	2.45	0.49
4:D:95:TYR:HD2	4:D:150:TYR:O	1.94	0.49
23:S:73:LEU:HG	23:S:387:ILE:HG21	1.93	0.49
26:V:126:GLY:HA2	26:V:161:PRO:HG3	1.95	0.49
2:f:179:LEU:HD21	44:f:821:CLA:HAB	1.94	0.49
2:f:324:ASP:OD1	2:f:328:ASN:ND2	2.45	0.49
2:f:700:LEU:H	45:f:844:PQN:H6	1.77	0.49
6:j:206:ILE:HD13	6:j:209:ARG:HH12	1.77	0.49
14:q:65:THR:OG1	14:q:84:ASP:OD1	2.21	0.49
41:r:108:LEU:HB3	41:r:114:LEU:HD12	1.94	0.49
23:S:329:ARG:HD3	25:U:53:ARG:HH12	1.77	0.49
2:f:449:PRO:O	2:f:452:GLN:NE2	2.45	0.49
2:f:654:HIS:CE1	44:f:804:CLA:ND	2.80	0.49
4:h:108:GLU:O	4:h:138:ARG:NH1	2.45	0.49
12:p:196:VAL:HG12	44:p:506:CLA:HAC1	1.93	0.49
42:s:216:MET:O	42:s:220:THR:OG1	2.24	0.49
2:B:301:ILE:HG23	44:B:820:CLA:HED2	1.95	0.49
6:F:194:ARG:HH21	6:F:199:ASP:HB2	1.77	0.49
16:G:209:ARG:O	16:G:210:GLN:NE2	2.39	0.49
21:Q:257:TRP:CG	33:c:125:ALA:HB2	2.46	0.49
23:S:225:ARG:HH21	23:S:263:VAL:HG22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:V:67:GLU:OE1	26:V:70:SER:OG	2.31	0.49
32:b:95:TRP:O	32:b:118:ARG:NH2	2.44	0.49
1:e:207:SER:OG	1:e:295:HIS:O	2.27	0.49
2:f:25:ILE:HD13	47:l:102:BCR:HC21	1.95	0.49
6:j:228:VAL:HG11	6:j:231:ALA:HB3	1.93	0.49
1:A:320:LYS:NZ	1:A:324:GLU:OE2	2.33	0.49
16:G:269:PHE:HA	16:G:272:VAL:HG12	1.93	0.49
17:M:68:LEU:HB3	17:M:109:THR:HG22	1.95	0.49
19:O:376:THR:HG21	21:Q:69:ILE:HD11	1.95	0.49
19:O:404:LEU:HD22	19:O:422:MET:HE1	1.94	0.49
46:O:601:LHG:H241	39:9:124:LYS:HD3	1.94	0.49
21:Q:435:ILE:HD11	42:s:182:PRO:HB2	1.94	0.49
23:S:19:HIS:NE2	23:S:21:SER:HB2	2.27	0.49
37:7:274:ALA:HB2	37:7:312:ASP:HA	1.95	0.49
1:e:276:ARG:O	1:e:500:THR:OG1	2.22	0.49
12:p:177:PHE:CE2	12:p:181:LYS:HD2	2.47	0.49
14:q:156:LEU:HD21	44:q:315:CLA:C1D	2.42	0.49
14:q:262:ASP:O	14:q:265:ASN:ND2	2.45	0.49
2:B:177:HIS:O	2:B:181:GLY:N	2.43	0.49
7:H:88:PHE:CG	11:L:95:ILE:HD13	2.48	0.49
12:1:78:GLU:HG2	12:1:82:TYR:CE2	2.47	0.49
17:M:205:SER:HA	17:M:218:LEU:HD13	1.93	0.49
21:Q:200:SER:O	21:Q:204:ILE:HG12	2.12	0.49
21:Q:487:TYR:HA	21:Q:490:ARG:HB3	1.95	0.49
23:S:19:HIS:CD2	23:S:21:SER:HB2	2.48	0.49
25:U:49:TYR:HB3	25:U:72:LEU:HD21	1.94	0.49
31:a:153:ILE:HG13	31:a:177:GLU:HB2	1.95	0.49
35:d:176:ALA:HB2	35:d:188:PHE:HD1	1.78	0.49
36:6:290:VAL:HG23	36:6:291:VAL:HG23	1.95	0.49
4:h:108:GLU:HG3	4:h:138:ARG:NH1	2.27	0.49
6:j:232:ASP:OD1	6:j:233:ILE:N	2.46	0.49
41:r:178:PRO:HB2	41:r:182:PHE:CD1	2.48	0.49
13:2:236:TRP:CZ3	52:2:512:CHL:HHB	2.47	0.49
14:3:137:GLN:HG2	14:3:144:ALA:O	2.12	0.49
16:G:83:PHE:O	16:G:85:GLU:N	2.46	0.49
21:Q:446:SER:HB2	21:Q:453:LEU:HD23	1.94	0.49
25:U:44:LEU:HB3	25:U:49:TYR:HB2	1.93	0.49
1:e:310:ARG:N	1:e:317:HIS:O	2.37	0.49
14:q:259:HIS:CD2	14:q:265:ASN:HD22	2.31	0.49
1:A:147:ALA:HB2	1:A:375:PRO:HD2	1.94	0.49
44:A:820:CLA:HMB1	44:A:820:CLA:HBB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.95	0.49
2:B:276:HIS:CE1	2:B:280:ILE:HD13	2.46	0.49
49:B:850:DGD:O1B	49:B:850:DGD:HB42	2.13	0.49
13:2:112:TRP:CD1	44:2:514:CLA:HMD3	2.48	0.49
13:2:202:ASP:OD1	44:2:504:CLA:HBD	2.12	0.49
13:2:263:PHE:C	13:2:264:ARG:HD3	2.38	0.49
18:N:57:GLN:OE1	18:N:57:GLN:N	2.46	0.49
21:Q:247:PHE:CE2	21:Q:321:ARG:HD3	2.47	0.49
37:7:86:VAL:H	37:7:93:GLY:HA3	1.77	0.49
44:e:805:CLA:O1D	44:e:805:CLA:H2A	2.13	0.49
44:e:830:CLA:C4D	46:e:845:LHG:HC92	2.43	0.49
2:f:86:PRO:HB3	2:f:121:TYR:CE2	2.48	0.49
12:p:111:TRP:NE1	12:p:119:ALA:HA	2.27	0.49
14:q:141:ILE:HG22	14:q:143:PRO:HG2	1.95	0.49
2:B:43:TYR:CZ	2:B:330:ILE:HD11	2.47	0.49
2:B:687:LEU:HD23	11:L:84:TYR:HE1	1.77	0.49
47:1:503:BCR:H333	44:1:509:CLA:C1B	2.43	0.49
15:5:97:GLY:HA2	53:5:304:XAT:H181	1.95	0.49
17:M:150:ILE:HD12	22:R:152:PHE:CE1	2.47	0.49
17:M:412:ALA:HA	17:M:495:GLY:HA3	1.94	0.49
19:O:8:THR:HG23	19:O:78:TRP:HE1	1.78	0.49
19:O:371:MET:HE3	19:O:454:PHE:HD1	1.77	0.49
19:O:427:ILE:HD11	21:Q:229:PHE:CD2	2.48	0.49
31:a:182:GLY:O	31:a:205:GLU:HB2	2.12	0.49
34:4:238:GLY:HA2	34:4:242:GLU:HA	1.95	0.49
1:e:504:SER:H	1:e:507:TRP:HE1	1.61	0.49
2:f:2:GLU:HG3	2:f:7:ARG:HA	1.94	0.49
11:o:201:VAL:HG12	11:o:202:LEU:HD12	1.95	0.49
14:q:204:GLY:O	14:q:208:ASN:N	2.46	0.49
1:A:72:SER:OG	1:A:178:TYR:HB2	2.13	0.48
10:K:77:ARG:HA	10:K:87:ALA:HA	1.94	0.48
14:3:266:ASN:HD21	44:3:313:CLA:HED3	1.78	0.48
25:U:111:GLN:O	25:U:114:GLU:HG3	2.13	0.48
35:d:162:ASN:OD1	35:d:163:PHE:N	2.46	0.48
2:f:43:TYR:CE1	2:f:330:ILE:HD11	2.47	0.48
2:f:193:HIS:HB2	44:f:816:CLA:CHC	2.43	0.48
44:f:827:CLA:CAD	44:f:838:CLA:HBB1	2.43	0.48
4:h:149:PHE:CE2	4:h:162:HIS:HB2	2.48	0.48
6:j:126:THR:OG1	6:j:129:ARG:NH2	2.46	0.48
1:A:328:GLY:HA3	46:A:844:LHG:HC32	1.94	0.48
2:B:694:ARG:NH1	11:L:146:ALA:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:29:ARG:NH2	22:R:29:LEU:O	2.46	0.48
21:Q:491:ILE:O	21:Q:495:THR:HG22	2.13	0.48
25:U:58:TYR:HD2	25:U:67:ALA:HB3	1.77	0.48
38:8:136:ILE:HB	38:8:187:PRO:HD2	1.95	0.48
2:f:542:ARG:HH21	2:f:551:LYS:HD2	1.77	0.48
4:h:139:LEU:HD22	4:h:145:ILE:HD11	1.95	0.48
5:i:132:VAL:HG12	5:i:134:THR:H	1.78	0.48
1:A:110:PRO:HB3	1:A:142:PHE:CD2	2.48	0.48
2:B:180:SER:HB3	2:B:288:GLY:HA3	1.95	0.48
3:C:28:MET:HB3	4:D:172:VAL:HG12	1.95	0.48
13:2:66:ILE:HG22	13:2:68:PHE:H	1.77	0.48
13:2:87:PHE:HE2	53:2:502:XAT:H383	1.77	0.48
13:2:112:TRP:HD1	44:2:514:CLA:HMD3	1.78	0.48
16:G:205:TRP:HB2	16:G:208:TRP:CD1	2.48	0.48
17:M:241:GLY:O	17:M:245:SER:N	2.45	0.48
23:S:60:ILE:HD13	23:S:319:PHE:CE1	2.49	0.48
23:S:264:ARG:NE	23:S:385:ASP:OD2	2.45	0.48
23:S:306:PHE:HA	23:S:309:LYS:HE2	1.94	0.48
36:6:350:PRO:O	36:6:351:LEU:HD23	2.13	0.48
37:7:252:GLN:HG3	37:7:253:GLY:H	1.76	0.48
3:g:15:THR:HG22	3:g:28:MET:HE3	1.93	0.48
6:j:90:ALA:O	6:j:94:ARG:HG2	2.14	0.48
12:p:160:TYR:HB3	44:p:504:CLA:HED3	1.95	0.48
2:B:351:HIS:ND1	44:B:818:CLA:OBD	2.47	0.48
23:S:326:LEU:HG	25:U:25:ARG:HE	1.78	0.48
26:V:195:PHE:HB3	28:X:144:TYR:HE1	1.78	0.48
1:e:187:TRP:CZ2	44:e:809:CLA:HMA1	2.48	0.48
1:e:456:ASN:HD22	1:e:639:ILE:HB	1.77	0.48
6:j:86:LYS:HZ1	6:j:136:PHE:N	2.11	0.48
47:A:846:BCR:H11C	47:A:846:BCR:H341	1.73	0.48
2:B:687:LEU:HD21	11:L:81:LEU:HD11	1.95	0.48
13:2:120:ILE:O	13:2:124:GLU:HG2	2.13	0.48
16:G:72:LEU:HD22	27:W:150:PRO:HB2	1.96	0.48
23:S:76:MET:HG3	23:S:157:TYR:HH	1.78	0.48
23:S:299:LYS:HD3	23:S:299:LYS:N	2.29	0.48
1:e:689:ARG:N	2:f:568:CYS:SG	2.87	0.48
2:f:502:ASN:OD1	2:f:503:GLU:N	2.47	0.48
12:p:65:GLY:O	12:p:68:THR:HG23	2.13	0.48
12:p:169:GLY:O	12:p:172:LYS:N	2.45	0.48
42:s:84:GLY:HA3	42:s:223:ILE:HD13	1.95	0.48
44:A:836:CLA:HBB1	44:A:836:CLA:HHC	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:ASP:N	3:C:32:ASP:OD1	2.45	0.48
13:2:117:ALA:HB1	51:2:501:LUT:H32	1.96	0.48
16:G:197:GLN:HE22	16:G:274:TYR:C	2.21	0.48
16:G:218:LEU:O	16:G:221:SER:OG	2.30	0.48
19:O:479:PRO:O	19:O:479:PRO:HG2	2.14	0.48
23:S:48:HIS:HE1	25:U:133:LEU:HD23	1.78	0.48
23:S:133:TYR:O	23:S:137:GLU:HG2	2.14	0.48
23:S:367:GLN:HA	23:S:370:LYS:HD3	1.95	0.48
31:a:124:THR:H	31:a:195:ARG:CB	2.26	0.48
37:7:318:PRO:HG3	37:7:330:PHE:CZ	2.49	0.48
1:e:279:LEU:HG	1:e:505:LEU:HD23	1.94	0.48
44:f:821:CLA:HBB1	44:f:826:CLA:H62	1.95	0.48
12:p:41:TRP:NE1	12:p:60:GLY:O	2.46	0.48
1:A:259:THR:HG23	1:A:260:PRO:HD3	1.94	0.48
1:A:577:GLY:O	1:A:580:GLY:N	2.39	0.48
49:J:103:DGD:HO4E	49:J:103:DGD:HO5E	1.60	0.48
13:2:166:ARG:NH2	13:2:177:VAL:HG12	2.29	0.48
21:Q:518:ILE:HA	37:7:165:VAL:HG11	1.94	0.48
23:S:337:LEU:HD12	23:S:338:GLY:H	1.79	0.48
25:U:96:PRO:HB2	25:U:121:ILE:HG13	1.95	0.48
26:V:64:CYS:H	26:V:99:GLY:HA2	1.79	0.48
28:X:147:PHE:O	28:X:151:VAL:HG12	2.14	0.48
29:Y:107:GLU:O	29:Y:111:THR:HG22	2.14	0.48
31:a:199:LEU:HD22	31:a:222:PHE:HD2	1.78	0.48
33:c:212:TYR:HA	33:c:215:THR:HG22	1.96	0.48
36:6:339:LYS:O	36:6:343:SER:OG	2.32	0.48
37:7:82:TYR:CE1	37:7:173:MET:HB3	2.48	0.48
1:e:197:HIS:CD2	44:e:812:CLA:HAB	2.49	0.48
1:e:429:ARG:O	4:h:81:SER:HB3	2.13	0.48
2:f:20:ARG:O	2:f:24:GLY:N	2.45	0.48
2:f:498:LEU:HA	2:f:501:VAL:HG22	1.95	0.48
41:r:59:LEU:HD12	41:r:68:GLY:HA2	1.96	0.48
2:B:93:ASP:HB3	2:B:96:PHE:CD1	2.49	0.48
12:1:71:GLU:OE1	12:1:71:GLU:N	2.38	0.48
13:2:211:PRO:C	13:2:213:LYS:H	2.20	0.48
19:O:325:ASN:O	19:O:329:ASN:HB2	2.14	0.48
24:T:64:CYS:C	24:T:66:ALA:H	2.22	0.48
37:7:79:VAL:H	37:7:113:VAL:HG12	1.78	0.48
1:e:573:CYS:SG	1:e:574:ASP:N	2.87	0.48
2:f:42:LEU:O	2:f:46:ILE:HG12	2.14	0.48
14:q:67:LEU:HD22	44:q:307:CLA:HED2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:r:308:CLA:HED2	44:r:308:CLA:H2A	1.96	0.48
1:A:575:GLY:HA2	2:B:562:PRO:HD3	1.95	0.48
14:3:218:LYS:O	14:3:222:GLU:N	2.30	0.48
20:P:78:LEU:HD12	22:R:73:LEU:HG	1.96	0.48
35:d:146:ASN:HA	35:d:227:ARG:HH11	1.78	0.48
36:6:306:VAL:N	36:6:350:PRO:HB3	2.29	0.48
40:0:134:PRO:O	40:0:138:ILE:HG22	2.13	0.48
1:e:107:HIS:ND1	1:e:107:HIS:O	2.46	0.48
1:e:280:ASP:O	1:e:284:GLY:N	2.41	0.48
1:e:682:LEU:HB2	44:f:801:CLA:HMC2	1.96	0.48
51:p:501:LUT:H21	44:p:506:CLA:HMB2	1.96	0.48
44:1:507:CLA:CGA	44:1:507:CLA:H3A	2.44	0.48
23:S:42:PRO:HG3	23:S:365:LEU:HD23	1.96	0.48
23:S:149:THR:OG1	23:S:157:TYR:HB3	2.14	0.48
33:c:200:VAL:HG22	33:c:208:ILE:HG23	1.95	0.48
34:4:139:CYS:H	35:d:196:TRP:CD1	2.32	0.48
44:e:809:CLA:HBA1	44:e:811:CLA:HMD3	1.95	0.48
44:f:842:CLA:HBC1	47:f:850:BCR:H24C	1.96	0.48
6:j:129:ARG:HD3	9:m:35:ASP:OD2	2.14	0.48
12:p:179:GLU:O	12:p:183:LYS:HG3	2.14	0.48
47:A:848:BCR:H15C	47:A:848:BCR:H351	1.74	0.47
2:B:457:PRO:HB3	2:B:517:PHE:HB2	1.95	0.47
3:C:43:PRO:HB2	4:D:177:GLN:HE21	1.78	0.47
47:F:801:BCR:C10	44:F:802:CLA:HAB	2.44	0.47
10:K:84:LYS:HB2	44:K:205:CLA:HMD2	1.96	0.47
16:G:40:THR:O	16:G:44:LEU:HG	2.13	0.47
16:G:351:LEU:HA	16:G:354:THR:HG22	1.96	0.47
19:O:413:MET:HB3	19:O:414:PRO:HD3	1.95	0.47
21:Q:659:PHE:CZ	21:Q:663:ILE:HD11	2.49	0.47
23:S:97:ARG:O	23:S:101:ILE:HG13	2.14	0.47
35:d:83:ASN:HB3	35:d:89:GLY:HA3	1.96	0.47
1:e:300:ILE:HD12	47:e:854:BCR:H352	1.96	0.47
42:s:117:ALA:HB2	53:s:502:XAT:H10	1.96	0.47
44:3:306:CLA:H92	44:3:306:CLA:H61	1.74	0.47
17:M:502:LEU:HD13	19:O:73:VAL:HG21	1.96	0.47
19:O:429:THR:HA	19:O:432:TYR:CE2	2.50	0.47
21:Q:305:LEU:O	21:Q:309:ALA:HB3	2.14	0.47
23:S:278:ALA:O	23:S:282:ILE:HG13	2.14	0.47
24:T:133:HIS:ND1	29:Y:119:PRO:HD2	2.29	0.47
35:d:99:LEU:HB3	35:d:108:VAL:HG13	1.95	0.47
37:7:227:LEU:O	37:7:228:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:322:LEU:HA	2:f:325:THR:HG22	1.96	0.47
2:f:675:ILE:HD11	47:f:850:BCR:H282	1.96	0.47
46:p:516:LHG:H242	52:p:517:CHL:C1C	2.44	0.47
41:r:184:PRO:HD2	51:r:302:LUT:H23	1.95	0.47
42:s:202:PHE:O	51:s:501:LUT:H42	2.14	0.47
1:A:118:ILE:HG13	47:A:851:BCR:H322	1.95	0.47
2:B:684:ARG:HE	11:L:63:SER:HB3	1.78	0.47
44:1:510:CLA:H2A	44:1:510:CLA:O2D	2.14	0.47
17:M:247:ALA:HB2	17:M:306:SER:HA	1.95	0.47
19:O:332:ILE:O	19:O:335:ILE:HG12	2.14	0.47
21:Q:692:ASP:HA	21:Q:695:LYS:HD2	1.94	0.47
23:S:226:ALA:HB1	23:S:259:ALA:HB1	1.97	0.47
25:U:21:GLY:O	25:U:29:THR:OG1	2.26	0.47
33:c:116:MET:HE1	33:c:165:TYR:HB2	1.96	0.47
12:p:61:PHE:N	44:p:507:CLA:OBD	2.40	0.47
51:p:501:LUT:H15	51:p:501:LUT:H201	1.69	0.47
51:q:302:LUT:H32	44:q:307:CLA:HAB	1.96	0.47
3:C:32:ASP:O	3:C:37:LYS:NZ	2.47	0.47
51:1:502:LUT:H383	44:1:509:CLA:C3B	2.45	0.47
16:G:140:ALA:O	16:G:144:LEU:HG	2.14	0.47
16:G:227:ARG:HA	16:G:228:LEU:HA	1.59	0.47
23:S:53:LYS:HZ3	25:U:143:LEU:HA	1.79	0.47
23:S:364:ILE:HD12	23:S:367:GLN:HB3	1.96	0.47
36:6:201:SER:OG	36:6:202:THR:N	2.47	0.47
37:7:195:SER:OG	37:7:333:THR:O	2.33	0.47
1:e:418:THR:OG1	1:e:419:ARG:NH2	2.47	0.47
1:e:421:ASN:ND2	1:e:424:LEU:H	2.13	0.47
2:f:352:MET:HE3	44:f:820:CLA:H11	1.96	0.47
2:f:593:TYR:CZ	44:f:838:CLA:HBC3	2.50	0.47
14:q:155:THR:HA	14:q:158:VAL:HG12	1.96	0.47
47:r:301:BCR:H351	47:r:301:BCR:H15C	1.72	0.47
44:A:852:CLA:H101	9:J:18:TRP:CZ3	2.49	0.47
15:5:45:ARG:HH21	15:5:54:PRO:HG3	1.79	0.47
16:G:175:THR:HG23	18:N:80:TYR:OH	2.14	0.47
16:G:257:LEU:O	16:G:261:LEU:HG	2.14	0.47
21:Q:117:TRP:HB3	21:Q:127:PHE:CD2	2.49	0.47
21:Q:508:SER:HB2	38:8:189:TRP:HE3	1.78	0.47
26:V:104:LYS:C	26:V:106:ALA:H	2.22	0.47
29:Y:61:LEU:HA	29:Y:64:VAL:HG12	1.97	0.47
37:7:73:ARG:HH22	37:7:108:ALA:CB	2.27	0.47
2:f:410:ARG:NH1	44:f:832:CLA:O1D	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:j:206:ILE:HA	6:j:209:ARG:HH12	1.79	0.47
47:j:803:BCR:H11C	47:j:803:BCR:H341	1.64	0.47
14:q:76:GLY:N	44:q:307:CLA:OBD	2.47	0.47
51:r:302:LUT:H35	51:r:302:LUT:H401	1.76	0.47
47:A:853:BCR:C12	47:K:204:BCR:H333	2.45	0.47
2:B:365:PHE:CD2	2:B:734:GLY:HA2	2.50	0.47
47:B:844:BCR:H351	47:B:844:BCR:H15C	1.60	0.47
12:1:215:ALA:HA	12:1:218:LEU:HB2	1.97	0.47
21:Q:231:LEU:HD12	21:Q:275:LEU:HD22	1.97	0.47
21:Q:264:ASN:OD1	21:Q:265:SER:N	2.48	0.47
23:S:116:LEU:HD21	23:S:138:ARG:NH1	2.29	0.47
23:S:141:ILE:H	23:S:141:ILE:HD12	1.78	0.47
26:V:62:SER:H	26:V:99:GLY:HA3	1.80	0.47
28:X:151:VAL:HG13	28:X:152:ASP:OD1	2.14	0.47
8:l:19:ILE:HA	8:l:22:THR:HG22	1.97	0.47
1:A:118:ILE:HG22	1:A:119:VAL:HG13	1.97	0.47
44:A:803:CLA:O2D	44:A:803:CLA:H2A	2.15	0.47
13:2:236:TRP:HZ3	52:2:512:CHL:HHB	1.80	0.47
47:2:503:BCR:H21C	47:2:503:BCR:H361	1.95	0.47
14:3:185:TYR:HA	14:3:190:GLU:OE2	2.15	0.47
47:5:302:BCR:H311	47:5:302:BCR:HC8	1.96	0.47
16:G:130:VAL:HG22	16:G:188:LEU:O	2.14	0.47
16:G:200:TYR:HB2	16:G:204:GLY:H	1.79	0.47
16:G:356:SER:HA	16:G:359:LEU:HB2	1.96	0.47
17:M:181:MET:SD	20:P:84:ILE:HD12	2.55	0.47
17:M:317:GLN:HE22	21:Q:754:LYS:HE3	1.80	0.47
21:Q:294:ASP:OD1	21:Q:294:ASP:N	2.44	0.47
26:V:56:PRO:HG3	26:V:83:LEU:HD12	1.96	0.47
37:7:48:LEU:O	37:7:49:ARG:HD2	2.15	0.47
38:8:79:ALA:N	38:8:98:ALA:O	2.47	0.47
1:e:360:THR:HA	1:e:363:VAL:HG22	1.96	0.47
1:e:457:ASP:OD1	2:f:635:TYR:OH	2.27	0.47
44:e:804:CLA:H152	47:e:846:BCR:H323	1.96	0.47
44:e:815:CLA:HBC2	44:q:312:CLA:HBB2	1.96	0.47
44:f:805:CLA:HMB1	44:f:805:CLA:HBB1	1.97	0.47
44:f:810:CLA:CGA	44:f:810:CLA:C1A	2.93	0.47
47:f:850:BCR:H20C	47:f:850:BCR:H361	1.74	0.47
10:n:55:ILE:O	10:n:59:THR:HG23	2.14	0.47
12:p:86:TRP:HB2	51:p:502:LUT:H402	1.95	0.47
42:s:96:GLU:CD	42:s:99:SER:H	2.22	0.47
2:B:229:GLN:C	2:B:231:ASN:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:104:GLU:OE2	4:D:119:GLU:HB2	2.15	0.47
11:L:105:LEU:HD12	11:L:132:LEU:HD23	1.96	0.47
13:2:97:GLU:OE2	50:2:518:LMG:O2	2.28	0.47
15:5:64:GLY:H	15:5:202:LEU:HD13	1.79	0.47
17:M:124:MET:HE2	17:M:170:THR:HA	1.95	0.47
20:P:14:PHE:O	20:P:18:ILE:HG12	2.14	0.47
20:P:27:MET:HG2	20:P:81:LEU:HD13	1.96	0.47
21:Q:639:ASN:HB3	21:Q:644:ILE:HD11	1.96	0.47
22:R:43:LEU:HA	22:R:46:ILE:HG22	1.97	0.47
36:6:359:HIS:HA	36:6:362:GLU:HG3	1.97	0.47
44:e:826:CLA:H12	47:e:849:BCR:H15C	1.96	0.47
44:e:837:CLA:H41	44:e:837:CLA:H62	1.75	0.47
2:f:700:LEU:N	45:f:844:PQN:H6	2.30	0.47
44:f:839:CLA:HMA3	44:f:840:CLA:HED1	1.97	0.47
6:j:86:LYS:HE2	6:j:137:GLY:H	1.79	0.47
11:o:80:ASN:HB3	44:o:302:CLA:HAC1	1.97	0.47
42:s:139:TYR:CZ	52:s:512:CHL:HMA2	2.50	0.47
1:A:223:GLN:HE22	1:A:250:LEU:HD22	1.79	0.47
1:A:340:GLU:HG2	1:A:419:ARG:HH11	1.79	0.47
45:A:841:PQN:H193	45:A:841:PQN:H211	1.70	0.47
2:B:310:PRO:HG3	44:B:842:CLA:HBD	1.97	0.47
2:B:658:ALA:CB	44:B:804:CLA:HBB2	2.44	0.47
4:D:149:PHE:CZ	4:D:162:HIS:HB2	2.50	0.47
6:F:194:ARG:NH2	50:F:805:LMG:O3	2.37	0.47
16:G:80:LYS:HD3	26:V:53:SER:HB2	1.96	0.47
19:O:24:LEU:O	19:O:112:ARG:NH2	2.48	0.47
19:O:444:TYR:O	40:0:85:PRO:HD3	2.14	0.47
21:Q:319:LEU:HD21	21:Q:336:ILE:HD13	1.96	0.47
23:S:233:LEU:HB2	23:S:331:GLU:HB2	1.97	0.47
32:b:123:ALA:HA	32:b:208:LEU:HD23	1.96	0.47
1:e:115:VAL:HG11	1:e:124:LEU:HB2	1.95	0.47
1:e:504:SER:H	1:e:507:TRP:NE1	2.13	0.47
42:s:144:ARG:NH1	44:s:509:CLA:H2A	2.29	0.47
1:A:195:LEU:HG	44:A:824:CLA:HMD2	1.96	0.47
19:O:70:TRP:HD1	19:O:71:ILE:HG12	1.79	0.47
21:Q:750:GLY:O	21:Q:754:LYS:HB2	2.15	0.47
22:R:67:VAL:HA	22:R:71:ASN:HD22	1.80	0.47
23:S:27:ARG:HB3	23:S:43:ILE:HB	1.97	0.47
33:c:164:TYR:HA	33:c:190:PHE:CZ	2.50	0.47
37:7:95:ARG:NH1	37:7:198:LYS:HG2	2.30	0.47
2:f:44:GLN:NE2	2:f:162:LYS:HE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:223:GLY:N	2:f:224:PRO:HD2	2.30	0.47
47:l:101:BCR:H351	47:l:101:BCR:H15C	1.68	0.47
53:r:303:XAT:H35	53:r:303:XAT:H401	1.80	0.47
1:A:689:ARG:NH2	2:B:565:GLY:O	2.48	0.46
44:B:818:CLA:H91	44:B:818:CLA:H111	1.71	0.46
11:L:139:CYS:CB	47:L:305:BCR:H19C	2.45	0.46
13:2:159:LEU:HB3	47:2:503:BCR:C15	2.44	0.46
18:N:94:PHE:O	18:N:98:LEU:HD23	2.15	0.46
1:e:355:ALA:HB1	47:e:849:BCR:H343	1.97	0.46
1:e:362:ILE:HD12	1:e:392:MET:SD	2.54	0.46
44:e:839:CLA:HED2	2:f:420:SER:HB2	1.96	0.46
2:f:555:TYR:HE1	2:f:572:ALA:HB3	1.80	0.46
4:h:149:PHE:CZ	4:h:162:HIS:HB2	2.49	0.46
14:q:165:GLY:C	14:q:169:HIS:HD1	2.23	0.46
51:q:301:LUT:H31	51:q:301:LUT:H391	1.72	0.46
41:r:105:PRO:O	41:r:109:THR:HG23	2.15	0.46
1:A:721:GLN:HB2	46:A:843:LHG:HC42	1.96	0.46
2:B:676:GLU:HG2	3:C:81:TYR:HE1	1.80	0.46
10:K:118:GLY:HA3	44:K:202:CLA:C2C	2.46	0.46
12:1:167:PRO:HG2	44:1:513:CLA:H122	1.97	0.46
13:2:121:PHE:HE1	13:2:235:ALA:HB2	1.79	0.46
17:M:60:PHE:HA	17:M:63:ILE:HB	1.96	0.46
17:M:111:CYS:SG	17:M:267:PHE:HB2	2.55	0.46
19:O:7:LEU:HD22	19:O:130:SER:HB2	1.97	0.46
21:Q:644:ILE:O	21:Q:648:ILE:HG12	2.16	0.46
21:Q:713:THR:HA	21:Q:717:THR:HG22	1.97	0.46
23:S:97:ARG:N	23:S:307:GLU:OE1	2.48	0.46
23:S:211:GLY:HA3	23:S:229:ILE:HD11	1.96	0.46
23:S:226:ALA:O	23:S:254:GLU:N	2.47	0.46
2:f:582:TRP:HE1	44:f:801:CLA:C1D	2.27	0.46
44:p:510:CLA:HED2	44:p:510:CLA:H2A	1.98	0.46
51:q:301:LUT:H35	51:q:301:LUT:H401	1.67	0.46
44:B:817:CLA:HED3	44:B:817:CLA:H2A	1.96	0.46
7:H:106:LEU:HD13	8:I:19:ILE:HG12	1.97	0.46
12:1:78:GLU:HB2	12:1:159:LYS:HE2	1.98	0.46
12:1:117:GLY:O	12:1:130:ASN:HA	2.16	0.46
44:2:506:CLA:H192	44:2:506:CLA:H161	1.74	0.46
46:2:517:LHG:H112	46:2:517:LHG:H301	1.97	0.46
47:3:305:BCR:H11C	47:3:305:BCR:H341	1.79	0.46
15:5:86:ALA:N	44:5:316:CLA:HED2	2.30	0.46
16:G:81:LEU:HD21	26:V:55:TRP:CH2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:46:SER:C	18:N:48:ILE:H	2.23	0.46
19:O:355:ARG:HD2	19:O:371:MET:HE1	1.97	0.46
1:e:550:LYS:NZ	2:f:673:GLU:OE1	2.47	0.46
2:f:77:TRP:CZ3	2:f:121:TYR:HB3	2.50	0.46
6:j:154:GLN:HE22	6:j:161:ILE:HG21	1.80	0.46
41:r:201:GLY:O	41:r:205:MET:HG3	2.14	0.46
4:D:163:PRO:C	4:D:165:ASP:H	2.23	0.46
13:2:112:TRP:CE2	52:2:513:CHL:HED2	2.51	0.46
14:3:74:ASP:OD1	14:3:76:GLY:N	2.41	0.46
47:3:305:BCR:H272	44:3:311:CLA:C1C	2.46	0.46
16:G:80:LYS:HG3	26:V:50:ARG:HA	1.97	0.46
17:M:91:PHE:HB2	17:M:146:ALA:H	1.80	0.46
19:O:47:MET:HE3	19:O:90:ILE:HG22	1.98	0.46
21:Q:458:SER:O	21:Q:462:ILE:HG23	2.15	0.46
23:S:68:THR:OG1	23:S:155:HIS:ND1	2.43	0.46
27:W:96:ILE:O	27:W:100:VAL:HG22	2.14	0.46
37:7:130:LEU:HB2	37:7:132:GLY:H	1.80	0.46
37:7:255:TRP:C	37:7:257:VAL:H	2.23	0.46
44:q:314:CLA:CHB	44:q:316:CLA:HBB1	2.46	0.46
51:s:501:LUT:H15	51:s:501:LUT:H201	1.67	0.46
12:1:223:HIS:HA	15:5:130:ASN:ND2	2.30	0.46
44:2:508:CLA:OBD	44:2:514:CLA:H2	2.15	0.46
17:M:118:TYR:OH	30:Z:65:UNK:O	2.32	0.46
17:M:324:LEU:O	17:M:328:SER:OG	2.23	0.46
20:P:86:ARG:O	20:P:89:LYS:NZ	2.48	0.46
21:Q:101:SER:O	21:Q:105:ILE:HG12	2.15	0.46
21:Q:591:LEU:HA	21:Q:594:THR:HG22	1.96	0.46
36:6:457:ASP:OD1	36:6:458:LEU:N	2.49	0.46
1:e:291:ILE:HD11	44:e:818:CLA:H2A	1.97	0.46
44:e:812:CLA:HMB1	44:e:812:CLA:HBB1	1.98	0.46
2:f:548:PRO:HD2	3:g:62:PHE:CE1	2.50	0.46
47:f:847:BCR:H371	47:f:847:BCR:H24C	1.56	0.46
5:i:144:GLU:OE1	5:i:144:GLU:N	2.45	0.46
9:m:1:MET:O	9:m:4:ILE:HG22	2.15	0.46
42:s:192:PRO:O	42:s:193:ASP:O	2.34	0.46
42:s:219:ARG:O	42:s:223:ILE:HG22	2.16	0.46
1:A:197:HIS:O	1:A:201:GLY:N	2.44	0.46
1:A:247:LEU:HB3	1:A:254:PHE:CD2	2.50	0.46
1:A:335:HIS:CE1	46:A:844:LHG:HC12	2.50	0.46
2:B:64:ASN:ND2	44:B:828:CLA:HED1	2.30	0.46
44:1:506:CLA:HHC	44:1:506:CLA:HBB1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2:501:LUT:H191	51:2:501:LUT:H11	1.73	0.46
44:2:505:CLA:HMD2	44:2:510:CLA:H52	1.97	0.46
19:O:134:LEU:HD21	19:O:182:VAL:HG22	1.98	0.46
19:O:277:SER:N	19:O:278:PRO:HD2	2.31	0.46
21:Q:656:PHE:O	21:Q:660:ILE:HG12	2.16	0.46
24:T:148:SER:O	24:T:151:GLY:N	2.47	0.46
28:X:201:ARG:HD3	29:Y:129:TRP:CG	2.51	0.46
2:f:172:GLU:H	2:f:172:GLU:CD	2.23	0.46
9:m:40:PRO:HG2	49:m:104:DGD:HD61	1.97	0.46
11:o:93:ARG:O	11:o:97:VAL:HG23	2.15	0.46
12:p:155:PRO:O	12:p:159:LYS:NZ	2.49	0.46
44:A:805:CLA:H2	44:A:805:CLA:H62	1.77	0.46
3:C:27:GLU:OE2	4:D:176:ARG:HD3	2.16	0.46
12:1:41:TRP:CD2	12:1:42:PHE:HB2	2.50	0.46
44:3:308:CLA:H12	44:3:313:CLA:CAD	2.46	0.46
23:S:97:ARG:HH12	23:S:166:ASP:CG	2.24	0.46
23:S:326:LEU:HG	25:U:25:ARG:HH11	1.80	0.46
27:W:141:PHE:C	27:W:145:LEU:HG	2.41	0.46
31:a:190:ALA:O	31:a:196:TYR:HA	2.15	0.46
34:4:151:LEU:HD22	34:4:213:VAL:HG22	1.97	0.46
36:6:347:GLY:C	36:6:349:ARG:H	2.23	0.46
1:e:126:GLY:HA3	1:e:663:SER:HB2	1.98	0.46
44:f:835:CLA:HBA2	9:m:36:ALA:HB3	1.98	0.46
47:f:850:BCR:H15C	47:f:850:BCR:H351	1.85	0.46
53:s:502:XAT:H192	52:s:512:CHL:HAB	1.97	0.46
1:A:29:PRO:HA	44:A:803:CLA:HBC1	1.97	0.46
12:1:104:ASN:OD1	12:1:107:LYS:HG2	2.16	0.46
15:5:49:LEU:HD23	15:5:52:LEU:HB2	1.97	0.46
21:Q:186:LEU:O	21:Q:189:ILE:HG12	2.15	0.46
26:V:128:CYS:SG	26:V:134:MET:HG3	2.56	0.46
33:c:129:ARG:HD2	33:c:166:ASP:OD2	2.15	0.46
37:7:156:VAL:HG12	37:7:161:GLU:HA	1.97	0.46
1:e:578:ARG:HB3	3:g:49:VAL:HG13	1.98	0.46
4:h:73:THR:OG1	4:h:74:PRO:HD2	2.16	0.46
47:m:103:BCR:H371	47:m:103:BCR:H24C	1.78	0.46
1:A:714:PRO:HB3	44:A:852:CLA:HMC3	1.98	0.46
44:A:827:CLA:H141	44:A:827:CLA:H161	1.73	0.46
2:B:176:ASN:HB3	44:B:821:CLA:HMD1	1.97	0.46
10:K:63:MET:O	10:K:67:GLY:N	2.42	0.46
44:L:303:CLA:CHA	44:L:303:CLA:HBA1	2.45	0.46
16:G:76:ALA:O	26:V:49:SER:OG	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:259:TYR:OH	19:O:263:ARG:NE	2.48	0.46
21:Q:66:PHE:CZ	47:Q:801:BCR:H21C	2.51	0.46
21:Q:283:SER:OG	21:Q:284:ALA:N	2.49	0.46
26:V:198:SER:OG	26:V:199:HIS:N	2.49	0.46
28:X:108:ILE:H	28:X:124:THR:HG21	1.80	0.46
36:6:358:ARG:O	36:6:360:ARG:N	2.48	0.46
1:e:40:PRO:HB3	1:e:45:TRP:CE3	2.51	0.46
1:e:324:GLU:OE1	1:e:324:GLU:N	2.49	0.46
1:e:385:LEU:O	1:e:389:THR:HG22	2.16	0.46
43:e:801:CL0:H49	43:e:801:CL0:H41	1.78	0.46
2:f:654:HIS:HE1	44:f:804:CLA:ND	2.14	0.46
3:g:51:CYS:SG	3:g:53:ARG:NE	2.88	0.46
4:h:173:ASN:HB3	4:h:176:ARG:HH21	1.81	0.46
11:o:92:LEU:HA	11:o:95:ILE:HG22	1.97	0.46
14:q:157:PHE:O	14:q:160:GLU:HG3	2.15	0.46
47:s:503:BCR:H24C	47:s:503:BCR:H402	1.64	0.46
10:K:80:THR:HG23	10:K:86:GLU:HG3	1.98	0.46
16:G:313:ALA:O	16:G:317:LEU:HG	2.16	0.46
19:O:402:PHE:CD2	21:Q:123:PHE:HE2	2.34	0.46
21:Q:139:LEU:O	21:Q:143:THR:HG22	2.16	0.46
21:Q:695:LYS:HA	21:Q:698:ILE:HG22	1.98	0.46
23:S:28:LEU:HD12	23:S:40:CYS:SG	2.56	0.46
37:7:202:ARG:NH1	37:7:319:GLY:O	2.39	0.46
2:f:636:ASN:HB2	2:f:637:PRO:HD2	1.97	0.46
9:m:2:ARG:HA	9:m:5:LYS:HD2	1.98	0.46
12:p:51:LEU:HD23	12:p:51:LEU:HA	1.79	0.46
1:A:707:LYS:HB2	6:F:179:ARG:HH12	1.81	0.45
3:C:8:TYR:HE1	4:D:182:ASN:HD22	1.64	0.45
12:1:95:LEU:HD11	12:1:210:PRO:HB2	1.97	0.45
20:P:27:MET:HB2	20:P:93:ILE:HD11	1.98	0.45
21:Q:110:ILE:HD11	39:9:95:TRP:CD2	2.51	0.45
21:Q:648:ILE:O	21:Q:652:THR:OG1	2.24	0.45
21:Q:771:TYR:HA	21:Q:774:VAL:HG12	1.98	0.45
37:7:225:PHE:HD2	37:7:338:ILE:HG21	1.81	0.45
44:e:824:CLA:HMA2	44:e:826:CLA:H92	1.99	0.45
14:q:63:SER:HB3	14:q:78:ASP:O	2.16	0.45
2:B:718:ILE:HG23	44:B:828:CLA:HAB	1.97	0.45
12:1:222:TRP:HB3	15:5:128:PHE:O	2.16	0.45
14:3:238:PHE:CD2	51:3:304:LUT:H12	2.52	0.45
15:5:72:GLY:HA2	15:5:75:GLU:OE2	2.16	0.45
16:G:328:PRO:HD3	23:S:199:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:258:GLU:HB3	20:P:99:LEU:HD11	1.98	0.45
21:Q:108:SER:O	39:9:94:ILE:HD12	2.16	0.45
21:Q:306:ILE:O	21:Q:311:MET:HB2	2.17	0.45
24:T:36:LEU:HA	27:W:124:PHE:O	2.16	0.45
33:c:177:ASP:O	33:c:180:PRO:HD2	2.16	0.45
35:d:83:ASN:HB3	35:d:89:GLY:C	2.41	0.45
44:e:839:CLA:H12	44:f:834:CLA:CGD	2.46	0.45
2:f:424:TRP:HZ3	44:f:840:CLA:HAC1	1.82	0.45
2:f:429:LEU:HD11	44:f:839:CLA:HMB2	1.97	0.45
12:p:160:TYR:CE1	12:p:181:LYS:HE3	2.51	0.45
51:r:302:LUT:H3	44:r:306:CLA:HMA1	1.98	0.45
13:2:189:THR:HG1	13:2:198:GLY:H	1.62	0.45
52:2:512:CHL:C4C	50:2:519:LMG:H312	2.45	0.45
14:3:110:MET:O	44:3:311:CLA:HAB	2.15	0.45
47:3:305:BCR:H15C	47:3:305:BCR:H351	1.64	0.45
15:5:183:PRO:HA	36:6:207:THR:HG21	1.98	0.45
21:Q:117:TRP:HE1	21:Q:125:LEU:HB3	1.82	0.45
21:Q:153:SER:HB2	21:Q:166:PHE:HE2	1.81	0.45
21:Q:259:PRO:HG2	21:Q:264:ASN:HD21	1.81	0.45
22:R:128:ARG:HA	32:b:140:TYR:HE2	1.82	0.45
23:S:154:MET:O	23:S:157:TYR:HD1	2.00	0.45
27:W:111:ALA:HA	27:W:114:ILE:HG22	1.98	0.45
28:X:124:THR:C	28:X:125:LEU:HD12	2.42	0.45
29:Y:108:SER:HA	29:Y:112:LYS:HB2	1.97	0.45
36:6:445:GLY:C	36:6:446:ILE:HG13	2.42	0.45
37:7:219:PRO:HA	37:7:225:PHE:CE1	2.52	0.45
1:e:247:LEU:HD13	1:e:254:PHE:CE2	2.51	0.45
1:e:445:LEU:HD23	1:e:445:LEU:HA	1.78	0.45
1:e:654:SER:O	1:e:657:ILE:HG22	2.17	0.45
2:f:365:PHE:HB3	2:f:602:TRP:CH2	2.52	0.45
2:f:373:THR:HG23	2:f:591:THR:HG21	1.98	0.45
6:j:194:ARG:HH21	6:j:199:ASP:HA	1.81	0.45
12:p:104:ASN:HB3	12:p:107:LYS:HG2	1.99	0.45
12:p:145:ALA:HB1	12:p:149:ARG:CZ	2.46	0.45
52:p:514:CHL:HBB1	52:p:514:CHL:CHC	2.46	0.45
41:r:197:GLU:HB2	44:r:304:CLA:C1B	2.46	0.45
2:B:287:ALA:HB2	44:B:820:CLA:HBC2	1.98	0.45
2:B:662:MET:O	2:B:666:SER:OG	2.32	0.45
47:B:846:BCR:H371	47:B:846:BCR:H24C	1.62	0.45
51:2:501:LUT:H401	51:2:501:LUT:H35	1.74	0.45
15:5:221:GLN:HB3	15:5:232:ASN:HD22	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:214:TYR:OH	19:O:273:HIS:ND1	2.37	0.45
20:P:81:LEU:HA	20:P:84:ILE:HG22	1.97	0.45
23:S:228:GLY:N	23:S:252:GLN:O	2.43	0.45
24:T:105:ILE:HG23	26:V:159:CYS:HB3	1.99	0.45
28:X:150:LEU:HD13	28:X:167:ILE:HD12	1.97	0.45
37:7:118:ASN:ND2	37:7:227:LEU:O	2.46	0.45
44:e:803:CLA:HBA2	44:e:810:CLA:H51	1.99	0.45
2:f:131:THR:OG1	2:f:134:ASP:OD2	2.31	0.45
2:f:332:PHE:CE2	47:f:849:BCR:H292	2.52	0.45
3:g:17:CYS:SG	3:g:18:VAL:N	2.89	0.45
4:h:162:HIS:HB3	4:h:163:PRO:HD3	1.98	0.45
4:h:163:PRO:C	4:h:165:ASP:H	2.24	0.45
4:h:184:ARG:HH12	4:h:189:ASN:HA	1.82	0.45
10:n:115:MET:HE1	44:n:205:CLA:HBB2	1.97	0.45
1:A:125:ASN:O	1:A:133:ARG:NH2	2.50	0.45
1:A:594:LEU:HD13	1:A:594:LEU:HA	1.83	0.45
44:B:838:CLA:H142	44:B:838:CLA:H112	1.71	0.45
6:F:213:TRP:CG	6:F:214:PRO:HD3	2.52	0.45
44:2:508:CLA:H2	44:2:508:CLA:HED3	1.98	0.45
15:5:242:ASN:HA	15:5:247:HIS:CE1	2.51	0.45
19:O:344:THR:HG21	19:O:381:PHE:CZ	2.52	0.45
19:O:411:LEU:O	19:O:411:LEU:HD12	2.16	0.45
23:S:254:GLU:HB2	23:S:259:ALA:HB2	1.97	0.45
23:S:371:LYS:HD3	23:S:371:LYS:N	2.32	0.45
24:T:128:SER:O	24:T:128:SER:OG	2.30	0.45
26:V:102:THR:HA	26:V:142:THR:HA	1.98	0.45
1:e:578:ARG:HE	3:g:49:VAL:HG11	1.81	0.45
44:e:808:CLA:H2A	44:e:808:CLA:O1D	2.17	0.45
41:r:54:GLN:CD	41:r:54:GLN:H	2.24	0.45
41:r:102:MET:HE1	53:r:303:XAT:H173	1.98	0.45
1:A:621:SER:OG	1:A:625:VAL:N	2.50	0.45
47:A:851:BCR:H15C	47:A:851:BCR:H351	1.72	0.45
47:1:503:BCR:C10	44:1:515:CLA:H3A	2.47	0.45
13:2:166:ARG:NE	52:2:513:CHL:OMC	2.48	0.45
14:3:74:ASP:HA	44:3:309:CLA:O1D	2.16	0.45
17:M:49:ASP:HB2	17:M:127:THR:HG21	1.99	0.45
19:O:106:PRO:HG3	39:9:132:TYR:CD2	2.52	0.45
21:Q:259:PRO:HG2	21:Q:264:ASN:ND2	2.31	0.45
23:S:81:ILE:HD11	23:S:330:VAL:HB	1.99	0.45
35:d:77:LYS:HB2	35:d:240:LEU:O	2.16	0.45
35:d:174:SER:HB2	35:d:188:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:6:449:GLU:O	36:6:453:LYS:HG2	2.16	0.45
37:7:190:THR:HG22	37:7:338:ILE:HG13	1.99	0.45
44:e:853:CLA:O2D	44:e:853:CLA:H2A	2.16	0.45
4:h:65:VAL:HB	4:h:165:ASP:HA	1.98	0.45
11:o:91:LEU:HB2	11:o:179:GLN:HB3	1.99	0.45
11:o:104:LEU:HG	44:o:304:CLA:HBC2	1.99	0.45
42:s:97:PRO:O	42:s:101:ARG:HG2	2.16	0.45
2:B:676:GLU:HG2	3:C:81:TYR:CE1	2.52	0.45
10:K:78:LYS:O	10:K:86:GLU:HB2	2.16	0.45
17:M:161:LEU:HD11	20:P:73:GLU:HG3	1.97	0.45
17:M:358:TYR:HA	17:M:361:MET:HG2	1.97	0.45
19:O:391:MET:HE3	54:Q:803:SQD:H332	1.99	0.45
21:Q:410:GLU:N	21:Q:411:PRO:HD2	2.32	0.45
21:Q:751:GLU:HB3	36:6:214:PHE:CZ	2.51	0.45
21:Q:761:ILE:HD12	21:Q:761:ILE:H	1.81	0.45
47:Q:801:BCR:HC8	39:9:112:PHE:CE1	2.52	0.45
27:W:142:PHE:N	27:W:143:PRO:HD2	2.32	0.45
28:X:102:ARG:HB3	28:X:104:TYR:CE1	2.52	0.45
28:X:148:GLN:HA	28:X:151:VAL:HG12	1.98	0.45
29:Y:129:TRP:HB2	29:Y:131:PHE:CE1	2.52	0.45
36:6:364:GLU:OE1	36:6:364:GLU:N	2.49	0.45
39:9:90:VAL:HG13	39:9:93:SER:H	1.82	0.45
44:f:807:CLA:H2A	44:f:807:CLA:O1D	2.16	0.45
6:j:168:LEU:HD23	6:j:168:LEU:HA	1.80	0.45
41:r:215:HIS:O	41:r:219:GLY:N	2.49	0.45
51:s:501:LUT:H11	51:s:501:LUT:H191	1.78	0.45
1:A:507:TRP:CH2	44:A:835:CLA:HED1	2.51	0.45
44:A:825:CLA:H141	44:A:835:CLA:H52	1.98	0.45
44:L:301:CLA:HBB1	44:L:301:CLA:HMB3	1.98	0.45
13:2:180:ASP:CB	13:2:186:ASN:HB2	2.46	0.45
44:2:507:CLA:H62	44:2:507:CLA:H93	1.83	0.45
16:G:119:TYR:CE2	16:G:120:HIS:HD2	2.34	0.45
17:M:91:PHE:CG	17:M:92:GLN:N	2.84	0.45
17:M:353:THR:HG21	17:M:502:LEU:HD23	1.98	0.45
19:O:29:ASN:HD21	19:O:33:ARG:HD3	1.82	0.45
19:O:235:PRO:HG3	19:O:307:TYR:CE1	2.52	0.45
28:X:147:PHE:HA	28:X:150:LEU:HG	1.99	0.45
32:b:102:ARG:HD2	32:b:102:ARG:HA	1.75	0.45
36:6:307:VAL:HB	36:6:392:VAL:HG23	1.99	0.45
37:7:62:LEU:HD21	37:7:151:VAL:HG23	1.99	0.45
37:7:216:CYS:O	37:7:218:HIS:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:e:807:CLA:O2D	44:e:807:CLA:H2A	2.15	0.45
47:e:850:BCR:H371	47:e:850:BCR:H24C	1.77	0.45
47:e:851:BCR:H11C	47:e:851:BCR:H341	1.72	0.45
2:f:276:HIS:HB2	44:f:819:CLA:CHB	2.46	0.45
2:f:301:ILE:HG23	44:f:821:CLA:HED2	1.98	0.45
2:f:477:LEU:H	2:f:477:LEU:HD12	1.82	0.45
12:p:50:HIS:CE1	12:p:68:THR:HG22	2.52	0.45
42:s:263:ILE:HD12	44:s:506:CLA:H42	1.99	0.45
51:s:501:LUT:H383	44:s:506:CLA:C2B	2.47	0.45
1:A:12:ILE:O	1:A:14:VAL:HG13	2.16	0.45
2:B:609:PHE:O	2:B:613:SER:OG	2.33	0.45
2:B:615:TYR:OH	2:B:621:ARG:NH2	2.50	0.45
44:B:833:CLA:HBC1	44:B:838:CLA:H192	1.98	0.45
8:I:14:LEU:C	8:I:17:PRO:HD2	2.41	0.45
12:1:162:GLY:N	44:1:504:CLA:OBD	2.33	0.45
13:2:178:ASN:HB2	13:2:188:LEU:HB2	1.99	0.45
16:G:170:TYR:O	16:G:173:PRO:HD2	2.16	0.45
21:Q:276:PHE:CZ	21:Q:339:VAL:HG11	2.50	0.45
1:e:583:GLN:HA	1:e:588:ASP:OD2	2.16	0.45
1:e:621:SER:OG	1:e:625:VAL:N	2.49	0.45
47:e:854:BCR:H351	47:e:854:BCR:H15C	1.70	0.45
4:h:104:GLU:OE1	4:h:104:GLU:N	2.48	0.45
11:o:76:TRP:NE1	11:o:80:ASN:HD21	2.14	0.45
14:q:60:SER:OG	14:q:61:LYS:N	2.49	0.45
51:q:301:LUT:H11	51:q:301:LUT:H191	1.76	0.45
1:A:706:LEU:O	6:F:179:ARG:NH1	2.50	0.45
2:B:91:ILE:HD11	2:B:114:ASN:OD1	2.16	0.45
44:1:511:CLA:HED1	15:5:133:ALA:HB1	1.98	0.45
46:1:516:LHG:H242	46:1:516:LHG:H131	1.99	0.45
44:5:309:CLA:HBB1	44:5:309:CLA:HMB3	1.98	0.45
16:G:57:ILE:HG22	24:T:33:THR:HA	1.99	0.45
16:G:200:TYR:HB3	16:G:203:PHE:HD2	1.82	0.45
17:M:91:PHE:HA	17:M:146:ALA:HA	1.99	0.45
19:O:473:ILE:HD13	47:Q:801:BCR:H372	1.99	0.45
20:P:86:ARG:NH1	22:R:176:GLN:HB3	2.32	0.45
21:Q:113:TYR:O	21:Q:128:GLY:HA3	2.17	0.45
21:Q:225:ARG:HA	21:Q:228:ASP:OD2	2.17	0.45
23:S:303:TRP:HA	23:S:308:TYR:HB2	1.99	0.45
25:U:154:GLU:OE1	28:X:165:ARG:NH2	2.50	0.45
26:V:60:GLY:HA3	26:V:65:PHE:CD1	2.51	0.45
26:V:187:LEU:O	28:X:191:ARG:NH1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Y:100:ALA:HB2	29:Y:153:VAL:HG13	1.98	0.45
33:c:93:LYS:HB2	33:c:93:LYS:HE3	1.83	0.45
37:7:200:ASP:O	37:7:328:ASP:HB3	2.17	0.45
1:e:185:LEU:HD23	1:e:185:LEU:HA	1.78	0.45
44:e:826:CLA:H2	44:e:826:CLA:H62	1.76	0.45
2:f:374:HIS:O	2:f:378:ILE:HG12	2.17	0.45
6:j:181:TYR:O	6:j:185:VAL:HG22	2.17	0.45
12:p:118:GLN:NE2	12:p:126:VAL:O	2.50	0.45
12:p:160:TYR:CZ	12:p:181:LYS:HE3	2.52	0.45
1:A:576:PRO:HD3	2:B:561:GLY:HA2	1.98	0.44
1:A:642:ASN:HB2	2:B:651:LEU:HD11	1.99	0.44
1:A:701:TRP:CE3	2:B:416:GLU:HB3	2.52	0.44
44:A:805:CLA:H162	44:A:805:CLA:H122	1.74	0.44
44:A:829:CLA:H62	44:A:829:CLA:H41	1.72	0.44
47:A:853:BCR:H15C	47:A:853:BCR:H351	1.74	0.44
44:B:824:CLA:HBA2	47:B:847:BCR:H16C	1.97	0.44
11:L:140:LEU:HD23	47:L:305:BCR:H23C	1.98	0.44
12:1:74:GLU:OE2	12:1:75:ARG:HG3	2.17	0.44
12:1:152:GLU:HB3	44:1:513:CLA:HBC1	1.99	0.44
44:1:511:CLA:O2D	44:1:511:CLA:H2A	2.17	0.44
13:2:223:LYS:HD3	44:2:510:CLA:O1D	2.18	0.44
44:2:508:CLA:HBA1	44:2:508:CLA:H3A	1.71	0.44
19:O:11:VAL:O	19:O:123:SER:OG	2.34	0.44
19:O:366:GLY:H	19:O:445:LYS:CB	2.29	0.44
21:Q:67:GLY:HA3	21:Q:75:THR:HG21	1.99	0.44
21:Q:193:TRP:O	21:Q:196:VAL:HG22	2.17	0.44
21:Q:447:LEU:HD23	21:Q:488:MET:HE2	1.98	0.44
23:S:17:PRO:O	23:S:25:VAL:HG23	2.16	0.44
23:S:98:ALA:HA	23:S:101:ILE:HD12	2.00	0.44
23:S:146:GLU:OE1	24:T:50:PRO:HG2	2.16	0.44
36:6:317:ALA:C	36:6:319:MET:H	2.25	0.44
37:7:236:ARG:HA	37:7:236:ARG:NH2	2.31	0.44
1:e:320:LYS:NZ	1:e:340:GLU:OE2	2.48	0.44
1:e:502:SER:HB3	1:e:507:TRP:HD1	1.80	0.44
1:e:641:ILE:H	1:e:641:ILE:HD12	1.81	0.44
1:e:675:HIS:O	1:e:678:TRP:CB	2.66	0.44
44:e:836:CLA:HBA2	44:e:837:CLA:HAA2	1.99	0.44
2:f:498:LEU:HA	2:f:498:LEU:HD12	1.87	0.44
2:f:523:ILE:HD13	2:f:590:VAL:HG22	1.98	0.44
2:f:725:LEU:O	2:f:729:THR:HG22	2.15	0.44
47:f:849:BCR:H351	47:f:849:BCR:H15C	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:r:48:SER:O	41:r:50:LEU:N	2.50	0.44
16:G:138:SER:O	16:G:138:SER:OG	2.28	0.44
16:G:253:GLY:O	16:G:257:LEU:HD23	2.17	0.44
17:M:92:GLN:HG2	17:M:282:ARG:HH12	1.82	0.44
19:O:261:LEU:HD22	19:O:320:ILE:HG21	2.00	0.44
21:Q:66:PHE:CD1	47:Q:801:BCR:H403	2.52	0.44
23:S:118:LEU:O	23:S:122:MET:N	2.44	0.44
29:Y:103:LEU:HD13	29:Y:109:THR:HB	1.99	0.44
1:e:205:LEU:HD23	1:e:303:LEU:HD11	1.99	0.44
1:e:260:PRO:HB3	1:e:268:LYS:HG3	1.99	0.44
1:e:504:SER:OG	1:e:505:LEU:N	2.50	0.44
1:e:667:TYR:HB3	1:e:744:ALA:HB2	1.97	0.44
44:e:834:CLA:H2A	44:e:834:CLA:O1D	2.17	0.44
2:f:276:HIS:O	2:f:280:ILE:HG12	2.17	0.44
2:f:692:ARG:NH1	11:o:155:THR:OG1	2.29	0.44
4:h:178:GLY:HA3	4:h:181:GLN:HE22	1.81	0.44
6:j:169:TYR:HA	6:j:213:TRP:HZ2	1.82	0.44
47:l:102:BCR:H20C	47:l:102:BCR:H361	1.84	0.44
44:r:317:CLA:O2D	44:r:317:CLA:H2A	2.17	0.44
44:B:806:CLA:HBC2	44:B:830:CLA:HMA1	1.99	0.44
4:D:167:VAL:HB	4:D:173:ASN:OD1	2.17	0.44
6:F:212:ILE:HD12	15:5:73:LEU:HD22	2.00	0.44
13:2:162:TRP:HH2	47:2:503:BCR:H321	1.81	0.44
51:5:303:LUT:H15	51:5:303:LUT:H201	1.82	0.44
16:G:255:PHE:HA	16:G:258:VAL:HG12	1.98	0.44
16:G:325:TRP:HE3	23:S:128:GLN:HG3	1.82	0.44
24:T:139:GLN:OE1	29:Y:180:ARG:NH2	2.50	0.44
26:V:128:CYS:HA	26:V:133:GLY:H	1.82	0.44
39:9:87:ASP:HA	39:9:96:HIS:HB2	2.00	0.44
44:e:839:CLA:H202	44:e:852:CLA:H61	1.98	0.44
2:f:82:LEU:HD23	2:f:82:LEU:HA	1.75	0.44
44:f:828:CLA:H2A	44:f:828:CLA:O1D	2.17	0.44
4:h:160:TYR:CE1	4:h:163:PRO:HD2	2.53	0.44
12:p:69:VAL:HG12	12:p:71:GLU:HG3	1.99	0.44
14:q:82:LEU:HD12	14:q:82:LEU:H	1.82	0.44
41:r:81:LEU:O	41:r:85:VAL:HG23	2.17	0.44
44:A:836:CLA:H3A	44:A:836:CLA:HBA2	1.76	0.44
47:A:849:BCR:H24C	47:A:849:BCR:H371	1.75	0.44
10:K:56:MET:HE1	10:K:113:HIS:HA	1.98	0.44
46:1:516:LHG:H262	46:1:516:LHG:H151	1.99	0.44
14:3:267:ASN:HB3	44:3:308:CLA:OBD	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:3:308:CLA:H43	44:3:313:CLA:OBD	2.18	0.44
16:G:207:ILE:HB	16:G:274:TYR:HB3	2.00	0.44
16:G:232:LEU:HD23	23:S:128:GLN:HA	2.00	0.44
17:M:499:ASN:HB3	17:M:500:PRO:HD3	1.99	0.44
18:N:97:ALA:O	18:N:101:VAL:HG22	2.17	0.44
19:O:53:TYR:O	19:O:54:HIS:ND1	2.50	0.44
24:T:68:GLU:C	24:T:70:CYS:H	2.25	0.44
32:b:130:ARG:NE	32:b:198:TYR:OH	2.50	0.44
34:4:128:ALA:N	34:4:241:SER:HB3	2.32	0.44
36:6:270:GLY:O	36:6:271:VAL:C	2.61	0.44
36:6:359:HIS:C	36:6:362:GLU:H	2.24	0.44
37:7:192:ALA:HA	37:7:336:ALA:HB2	1.98	0.44
37:7:255:TRP:NE1	37:7:257:VAL:HB	2.32	0.44
1:e:197:HIS:HB3	44:e:812:CLA:HAB	2.00	0.44
2:f:299:HIS:HE1	44:f:823:CLA:NA	2.15	0.44
7:k:101:LEU:O	7:k:105:LEU:HG	2.17	0.44
10:n:107:ALA:O	10:n:111:VAL:HG23	2.18	0.44
12:p:90:CYS:CB	51:p:502:LUT:C39	2.93	0.44
2:B:173:SER:O	2:B:177:HIS:ND1	2.38	0.44
2:B:655:LEU:HD13	44:B:801:CLA:HAA1	2.00	0.44
45:B:843:PQN:H171	47:B:849:BCR:H382	2.00	0.44
3:C:15:THR:HG22	3:C:28:MET:HE3	1.98	0.44
13:2:256:ASP:N	13:2:256:ASP:OD1	2.50	0.44
44:2:505:CLA:HED2	44:2:510:CLA:H61	1.99	0.44
14:3:99:TYR:HE1	14:3:200:ALA:HA	1.82	0.44
15:5:175:LEU:HD13	15:5:175:LEU:HA	1.89	0.44
47:5:302:BCR:H352	47:5:302:BCR:H10C	2.00	0.44
16:G:350:ASN:OD1	16:G:351:LEU:N	2.50	0.44
17:M:256:VAL:HG13	17:M:257:TYR:HD1	1.83	0.44
19:O:166:LYS:HD3	19:O:233:TRP:HA	2.00	0.44
20:P:18:ILE:HD13	20:P:37:ILE:HD13	1.98	0.44
25:U:114:GLU:HB2	25:U:133:LEU:HD11	2.00	0.44
33:c:215:THR:O	33:c:219:LEU:CB	2.65	0.44
36:6:359:HIS:O	36:6:362:GLU:N	2.41	0.44
2:f:460:ALA:HB2	44:f:839:CLA:HED2	1.99	0.44
10:n:101:THR:OG1	10:n:102:LEU:N	2.49	0.44
41:r:191:LEU:C	41:r:193:ASN:H	2.26	0.44
44:B:833:CLA:H61	47:F:804:BCR:HC32	1.99	0.44
8:I:11:LEU:HD23	8:I:11:LEU:HA	1.83	0.44
12:1:229:ILE:HD13	44:1:506:CLA:HMD2	2.00	0.44
14:3:104:ASN:HA	44:3:316:CLA:HMD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:353:SER:C	19:O:355:ARG:H	2.24	0.44
21:Q:253:ILE:HD13	21:Q:257:TRP:HE3	1.82	0.44
21:Q:317:PHE:HZ	21:Q:321:ARG:HH21	1.66	0.44
23:S:218:GLY:HA2	25:U:51:TYR:HE1	1.83	0.44
23:S:278:ALA:O	23:S:281:LYS:N	2.51	0.44
23:S:335:GLY:HA3	23:S:357:PRO:HB3	1.99	0.44
34:4:172:ALA:HB3	34:4:181:ASP:OD1	2.18	0.44
37:7:86:VAL:HG11	37:7:301:LEU:HD22	1.98	0.44
37:7:131:LEU:O	37:7:159:LYS:NZ	2.36	0.44
37:7:222:ALA:HB2	37:7:236:ARG:NH2	2.33	0.44
1:e:609:SER:OG	1:e:613:GLN:OE1	2.33	0.44
2:f:175:LEU:HD11	44:f:821:CLA:HMA2	1.99	0.44
2:f:191:THR:HG21	2:f:278:LEU:HB2	1.99	0.44
6:j:162:THR:OG1	6:j:163:PRO:HD3	2.17	0.44
1:A:449:SER:HB3	1:A:536:ILE:HD13	1.98	0.44
1:A:570:ARG:HB3	1:A:587:TRP:HB2	1.98	0.44
2:B:193:HIS:HB2	44:B:815:CLA:CHC	2.48	0.44
2:B:225:LEU:HD22	47:B:844:BCR:H292	2.00	0.44
44:B:811:CLA:HHC	44:B:811:CLA:CBB	2.48	0.44
47:B:844:BCR:H24C	47:B:844:BCR:H371	1.72	0.44
4:D:97:ILE:HB	4:D:149:PHE:HB3	2.00	0.44
47:F:804:BCR:H11C	47:F:804:BCR:H341	1.67	0.44
16:G:232:LEU:HD13	23:S:123:ALA:O	2.17	0.44
17:M:63:ILE:O	17:M:66:THR:OG1	2.30	0.44
17:M:314:ALA:HB2	17:M:326:TYR:HB3	1.99	0.44
21:Q:446:SER:O	21:Q:455:CYS:HB3	2.18	0.44
21:Q:501:ARG:HA	21:Q:504:PHE:CD1	2.53	0.44
23:S:323:ARG:O	25:U:24:HIS:HB3	2.18	0.44
25:U:29:THR:HG22	25:U:86:CYS:HB2	2.00	0.44
36:6:254:TYR:O	36:6:257:TYR:N	2.44	0.44
1:e:476:LEU:HB2	1:e:528:THR:HG23	1.99	0.44
2:f:244:PHE:N	2:f:264:GLN:OE1	2.44	0.44
44:f:835:CLA:O1D	9:m:35:ASP:HA	2.18	0.44
3:g:12:ILE:HA	3:g:34:CYS:SG	2.58	0.44
7:k:97:LYS:NZ	7:k:99:GLY:H	2.15	0.44
12:p:157:LYS:HD2	12:p:161:PRO:O	2.17	0.44
41:r:168:TYR:O	41:r:168:TYR:CG	2.70	0.44
47:A:845:BCR:H361	47:A:845:BCR:H20C	1.77	0.44
14:3:191:LYS:HE2	14:3:192:TYR:CZ	2.53	0.44
20:P:78:LEU:HD13	22:R:77:ALA:HB2	2.00	0.44
24:T:23:GLY:O	24:T:27:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:66:ALA:O	24:T:68:GLU:HG2	2.18	0.44
1:e:676:PHE:O	1:e:679:ALA:HB3	2.17	0.44
44:e:830:CLA:HBB2	44:e:838:CLA:HAB	2.00	0.44
2:f:334:LEU:HD13	44:f:807:CLA:C2D	2.48	0.44
2:f:596:TRP:O	2:f:600:THR:HG23	2.18	0.44
3:g:15:THR:HA	3:g:28:MET:HE3	1.99	0.44
4:h:89:ALA:HA	4:h:93:GLU:O	2.18	0.44
7:k:110:GLY:HA2	8:l:15:VAL:HG11	2.00	0.44
51:p:501:LUT:H32	44:p:504:CLA:CHC	2.48	0.44
51:r:302:LUT:H31	51:r:302:LUT:H391	1.71	0.44
52:s:513:CHL:HHC	52:s:513:CHL:HBB1	2.00	0.44
1:A:41:ASP:OD1	1:A:42:THR:N	2.44	0.44
1:A:379:THR:HG21	1:A:515:VAL:HB	1.99	0.44
1:A:693:GLN:HG2	2:B:546:LEU:HD22	1.98	0.44
2:B:40:GLU:HG2	2:B:165:LEU:HD23	2.00	0.44
2:B:477:LEU:C	2:B:479:SER:H	2.26	0.44
47:B:845:BCR:H15C	47:B:845:BCR:H351	1.69	0.44
11:L:97:VAL:HG13	11:L:101:HIS:CE1	2.53	0.44
14:3:91:PHE:HA	14:3:96:TRP:CD1	2.53	0.44
14:3:192:TYR:HD1	14:3:205:PRO:HD2	1.83	0.44
44:5:307:CLA:H12	44:5:307:CLA:NA	2.33	0.44
16:G:186:ASN:O	31:a:113:GLN:NE2	2.51	0.44
17:M:395:ALA:HB1	17:M:454:LEU:HD23	2.00	0.44
21:Q:285:GLN:O	21:Q:289:HIS:HB3	2.18	0.44
22:R:104:CYS:O	22:R:108:VAL:HG23	2.18	0.44
34:4:160:SER:OG	34:4:161:VAL:N	2.50	0.44
37:7:195:SER:OG	37:7:195:SER:O	2.36	0.44
37:7:229:THR:OG1	37:7:233:ALA:N	2.51	0.44
2:f:159:PRO:O	2:f:160:LYS:HB2	2.18	0.44
2:f:167:TRP:CZ2	44:f:813:CLA:HHB	2.53	0.44
4:h:68:GLN:OE1	4:h:148:GLN:NE2	2.51	0.44
11:o:104:LEU:HD11	44:o:303:CLA:HMB3	1.99	0.44
47:o:305:BCR:H24C	47:o:305:BCR:H371	1.72	0.44
12:p:130:ASN:O	12:p:134:ILE:HG12	2.17	0.44
14:q:217:GLU:O	14:q:221:LYS:HG2	2.16	0.44
42:s:60:PRO:O	42:s:65:ARG:HB2	2.17	0.44
44:B:828:CLA:O1D	44:B:828:CLA:H2A	2.18	0.43
47:1:503:BCR:H341	47:1:503:BCR:H11C	1.67	0.43
13:2:232:VAL:HG21	53:2:502:XAT:H12	2.00	0.43
53:5:304:XAT:H183	44:5:310:CLA:C3B	2.48	0.43
17:M:59:TRP:O	17:M:63:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:200:TRP:HZ3	22:R:120:TRP:HH2	1.65	0.43
17:M:270:VAL:HG23	17:M:271:THR:N	2.33	0.43
22:R:67:VAL:HA	22:R:71:ASN:ND2	2.33	0.43
24:T:63:LYS:HB3	24:T:116:THR:O	2.18	0.43
27:W:99:PRO:O	27:W:103:ILE:HG22	2.18	0.43
37:7:210:LEU:HD23	37:7:210:LEU:HA	1.84	0.43
37:7:211:ARG:HA	37:7:255:TRP:HD1	1.83	0.43
1:e:241:ILE:HD11	44:e:814:CLA:HMA2	2.00	0.43
2:f:86:PRO:HB3	2:f:121:TYR:CD2	2.53	0.43
47:f:848:BCR:H15C	47:f:848:BCR:H351	1.68	0.43
2:B:102:GLU:CD	7:H:133:LEU:HD12	2.42	0.43
2:B:124:TRP:CZ2	2:B:124:TRP:NE1	2.86	0.43
44:B:802:CLA:H91	44:B:802:CLA:H111	1.74	0.43
44:B:820:CLA:CMB	44:B:825:CLA:HMA3	2.48	0.43
44:B:824:CLA:HAB	44:B:831:CLA:HMD2	2.00	0.43
11:L:66:THR:H	11:L:69:THR:HG22	1.83	0.43
51:2:501:LUT:H12	44:2:504:CLA:CAB	2.47	0.43
51:3:304:LUT:H35	51:3:304:LUT:H401	1.67	0.43
15:5:234:LEU:O	15:5:237:LEU:HG	2.19	0.43
17:M:48:ILE:HG21	17:M:59:TRP:CZ3	2.53	0.43
17:M:333:GLY:HA2	17:M:336:ILE:HD12	2.01	0.43
19:O:138:PHE:HB2	19:O:178:PHE:HE1	1.82	0.43
21:Q:123:PHE:CD1	21:Q:123:PHE:O	2.70	0.43
23:S:350:TRP:NE1	25:U:145:LYS:HE3	2.33	0.43
24:T:129:THR:OG1	26:V:155:TYR:HB2	2.18	0.43
27:W:112:PRO:HB3	27:W:148:TRP:HB2	2.00	0.43
31:a:81:VAL:HG13	31:a:83:ALA:H	1.83	0.43
32:b:88:PRO:HB2	34:4:175:PRO:HB2	2.01	0.43
37:7:99:HIS:HE2	37:7:110:ARG:HD3	1.83	0.43
10:n:72:ALA:CA	10:n:84:LYS:HZ3	2.30	0.43
44:o:302:CLA:HMB3	47:o:305:BCR:H373	2.00	0.43
44:o:304:CLA:HBB1	44:o:304:CLA:HMB1	2.00	0.43
41:r:122:ALA:O	41:r:127:TYR:OH	2.22	0.43
44:s:510:CLA:H91	44:s:510:CLA:H112	1.83	0.43
1:A:84:TRP:O	1:A:88:MET:HG2	2.18	0.43
1:A:259:THR:CG2	1:A:260:PRO:HD3	2.48	0.43
2:B:246:THR:OG1	2:B:247:ALA:N	2.32	0.43
2:B:443:MET:HG3	2:B:451:LYS:O	2.18	0.43
5:E:79:LYS:N	5:E:80:PRO:HD2	2.33	0.43
5:E:90:LYS:HE3	5:E:104:THR:HG21	2.00	0.43
11:L:194:TRP:CE3	47:L:306:BCR:H333	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:5:304:XAT:H15	53:5:304:XAT:H201	1.85	0.43
16:G:184:LEU:HD13	16:G:358:GLN:NE2	2.34	0.43
17:M:129:PHE:HD2	17:M:169:TYR:CD2	2.34	0.43
18:N:26:SER:O	18:N:30:LEU:HG	2.18	0.43
19:O:371:MET:SD	19:O:374:ILE:HD12	2.58	0.43
23:S:261:TYR:HD2	23:S:262:LEU:HD22	1.84	0.43
24:T:152:ASP:HB3	24:T:155:ILE:HD12	2.00	0.43
27:W:139:TYR:O	27:W:142:PHE:CB	2.66	0.43
29:Y:138:ARG:HD2	29:Y:138:ARG:N	2.33	0.43
37:7:223:SER:HG	37:7:225:PHE:C	2.26	0.43
1:e:646:ARG:HA	2:f:632:ILE:HD12	2.00	0.43
2:f:51:PHE:HE2	2:f:156:HIS:HD2	1.66	0.43
2:f:396:ARG:HB3	4:h:196:LYS:NZ	2.34	0.43
2:f:401:GLU:HA	2:f:404:GLU:HG2	2.00	0.43
11:o:166:LYS:HA	11:o:166:LYS:HD2	1.87	0.43
51:p:501:LUT:H11	51:p:501:LUT:H191	1.74	0.43
47:q:303:BCR:H15C	47:q:303:BCR:H351	1.80	0.43
51:r:302:LUT:H32	44:r:304:CLA:CAB	2.49	0.43
1:A:213:HIS:HB2	44:A:813:CLA:C1C	2.48	0.43
47:B:848:BCR:H11C	47:B:848:BCR:H341	1.86	0.43
7:H:108:GLY:O	7:H:111:SER:OG	2.27	0.43
10:K:105:THR:CB	44:K:201:CLA:HAB	2.48	0.43
47:L:305:BCR:H15C	47:L:305:BCR:H351	1.82	0.43
12:1:128:TRP:HB2	12:1:133:THR:HG21	2.00	0.43
51:1:501:LUT:H15	51:1:501:LUT:H201	1.90	0.43
51:1:501:LUT:H8	51:1:501:LUT:H161	1.99	0.43
16:G:247:TYR:CD2	16:G:251:LYS:HB3	2.53	0.43
18:N:92:SER:O	18:N:96:GLU:HG3	2.19	0.43
20:P:10:SER:OG	20:P:44:ASN:HB2	2.18	0.43
23:S:19:HIS:O	23:S:21:SER:N	2.48	0.43
23:S:116:LEU:HD11	23:S:138:ARG:NH2	2.33	0.43
23:S:329:ARG:HD3	25:U:53:ARG:NH1	2.33	0.43
25:U:63:GLY:H	25:U:146:ASP:HB2	1.83	0.43
36:6:222:VAL:HG12	36:6:240:GLU:HB2	2.01	0.43
2:f:157:LEU:HD23	2:f:157:LEU:HA	1.88	0.43
2:f:561:GLY:O	2:f:567:THR:OG1	2.32	0.43
14:q:241:MET:HA	14:q:244:GLN:OE1	2.18	0.43
42:s:235:GLY:O	42:s:239:GLN:HG3	2.19	0.43
2:B:276:HIS:HB2	44:B:818:CLA:C1B	2.47	0.43
4:D:109:MET:HE3	4:D:109:MET:HB3	1.83	0.43
7:H:125:LEU:HD23	7:H:128:LYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:120:ILE:HG13	53:2:502:XAT:C16	2.48	0.43
44:5:307:CLA:H12	44:5:307:CLA:HBA2	1.80	0.43
16:G:261:LEU:HA	16:G:264:LEU:HD12	2.01	0.43
17:M:166:LEU:HB3	17:M:264:VAL:HG21	2.01	0.43
17:M:290:PHE:HB3	34:4:186:ARG:HD3	1.99	0.43
19:O:226:PRO:HD3	19:O:254:LEU:HD22	1.99	0.43
21:Q:56:LEU:HD12	21:Q:56:LEU:HA	1.87	0.43
23:S:317:PRO:O	23:S:347:LEU:HD11	2.19	0.43
32:b:97:THR:HG23	34:4:240:PHE:HA	1.99	0.43
36:6:122:VAL:HA	36:6:202:THR:OG1	2.17	0.43
37:7:135:GLU:H	37:7:135:GLU:CD	2.25	0.43
4:h:165:ASP:OD2	4:h:167:VAL:HB	2.18	0.43
7:k:93:ALA:HB3	7:k:94:PRO:HD3	2.01	0.43
12:p:226:ILE:HG12	44:p:506:CLA:HBD	1.99	0.43
44:A:805:CLA:H112	44:A:805:CLA:H91	1.70	0.43
44:A:808:CLA:H202	44:A:808:CLA:H161	1.87	0.43
2:B:43:TYR:CE2	2:B:330:ILE:HD11	2.54	0.43
47:B:852:BCR:H15C	47:B:852:BCR:H351	1.65	0.43
6:F:158:GLY:HA2	6:F:162:THR:HB	2.01	0.43
47:I:101:BCR:H15C	47:I:101:BCR:H351	1.79	0.43
12:1:127:PRO:HG2	12:1:128:TRP:CE3	2.54	0.43
17:M:129:PHE:HB2	17:M:169:TYR:HE2	1.83	0.43
18:N:28:SER:O	18:N:32:ALA:HB2	2.18	0.43
21:Q:66:PHE:HZ	47:Q:801:BCR:H21C	1.83	0.43
21:Q:360:SER:OG	21:Q:491:ILE:HD11	2.18	0.43
23:S:74:ALA:HB1	23:S:77:PHE:HD2	1.84	0.43
23:S:118:LEU:HA	23:S:121:PHE:HB3	2.01	0.43
24:T:20:ARG:O	24:T:24:GLN:HB2	2.19	0.43
36:6:242:PHE:HB3	36:6:243:LYS:H	1.69	0.43
37:7:64:VAL:HB	37:7:147:ASP:HA	1.99	0.43
37:7:128:SER:OG	37:7:227:LEU:HB3	2.18	0.43
38:8:104:LEU:HA	38:8:107:ILE:HG22	2.00	0.43
47:e:851:BCR:H15C	47:e:851:BCR:H351	1.75	0.43
42:s:251:LEU:O	42:s:255:LEU:HG	2.18	0.43
1:A:17:ASP:HA	1:A:179:HIS:O	2.18	0.43
1:A:40:PRO:HA	1:A:45:TRP:CG	2.54	0.43
1:A:669:LEU:HB3	44:B:802:CLA:H62	2.01	0.43
1:A:712:THR:OG1	6:F:195:GLU:OE1	2.33	0.43
47:A:853:BCR:H20C	47:A:853:BCR:H361	1.80	0.43
3:C:28:MET:O	4:D:176:ARG:HD2	2.19	0.43
6:F:233:ILE:HG13	6:F:234:GLY:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:64:LEU:HA	11:L:64:LEU:HD23	1.71	0.43
17:M:108:SER:OG	17:M:137:THR:OG1	2.29	0.43
17:M:157:GLU:HB3	17:M:161:LEU:HD23	1.99	0.43
19:O:261:LEU:HD22	19:O:320:ILE:HD13	2.01	0.43
21:Q:218:GLN:O	21:Q:222:VAL:HG23	2.19	0.43
21:Q:432:TYR:HE2	21:Q:500:LEU:HD22	1.83	0.43
23:S:291:GLU:HA	23:S:294:ARG:NE	2.34	0.43
23:S:369:VAL:HG12	23:S:380:ILE:HD12	2.01	0.43
25:U:133:LEU:HD12	25:U:133:LEU:H	1.83	0.43
31:a:95:TRP:O	31:a:97:ASP:N	2.51	0.43
37:7:143:SER:C	37:7:145:SER:H	2.27	0.43
1:e:195:LEU:HD23	1:e:195:LEU:HA	1.89	0.43
1:e:363:VAL:HA	44:e:825:CLA:HED2	2.01	0.43
44:e:825:CLA:CHB	44:e:838:CLA:HAA2	2.49	0.43
47:e:854:BCR:H402	10:n:111:VAL:HG21	2.00	0.43
6:j:170:ILE:O	6:j:173:TRP:HB3	2.19	0.43
14:q:232:ARG:O	14:q:236:LEU:HG	2.18	0.43
41:r:132:SER:O	41:r:136:VAL:HG13	2.19	0.43
1:A:159:THR:HG22	44:A:813:CLA:CGA	2.49	0.43
1:A:654:SER:O	1:A:658:GLN:HG2	2.18	0.43
2:B:53:GLN:O	2:B:53:GLN:NE2	2.50	0.43
2:B:582:TRP:HH2	44:B:802:CLA:HAB	1.81	0.43
4:D:200:LYS:HD2	4:D:204:ASP:C	2.44	0.43
6:F:113:SER:OG	6:F:115:PRO:HD2	2.19	0.43
44:L:301:CLA:H62	44:L:301:CLA:H41	1.75	0.43
12:1:94:VAL:HG12	12:1:95:LEU:HD22	1.99	0.43
15:5:149:ARG:HA	52:5:315:CHL:HAC2	2.00	0.43
15:5:218:PHE:CE1	51:5:303:LUT:H41	2.53	0.43
17:M:145:GLY:HA2	17:M:282:ARG:NH2	2.34	0.43
19:O:361:LEU:HD21	19:O:436:MET:HA	2.00	0.43
21:Q:202:LEU:HD11	54:Q:803:SQD:H291	1.99	0.43
21:Q:500:LEU:O	21:Q:502:VAL:N	2.52	0.43
23:S:67:VAL:HG21	23:S:79:GLU:HG2	2.00	0.43
31:a:89:TYR:HE2	31:a:117:VAL:HG21	1.83	0.43
33:c:116:MET:HE3	33:c:162:PHE:HA	2.01	0.43
37:7:148:ALA:HA	37:7:168:LEU:O	2.19	0.43
2:f:282:PHE:CZ	44:f:818:CLA:HBB2	2.53	0.43
7:k:113:VAL:HA	7:k:116:VAL:HG12	2.00	0.43
11:o:203:ASP:OD1	11:o:203:ASP:N	2.48	0.43
41:r:161:GLN:HA	41:r:169:SER:HB3	2.01	0.43
1:A:100:ALA:O	1:A:103:SER:OG	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PRO:HG2	1:A:271:GLU:OE1	2.18	0.43
44:A:816:CLA:C4A	44:A:816:CLA:HBA2	2.48	0.43
47:A:845:BCR:H11C	47:A:845:BCR:H341	1.87	0.43
44:B:837:CLA:HBC2	44:B:837:CLA:HHD	2.00	0.43
7:H:129:LYS:HE3	7:H:129:LYS:HB2	1.86	0.43
11:L:64:LEU:O	11:L:69:THR:HG21	2.19	0.43
11:L:175:GLU:O	11:L:179:GLN:HG2	2.18	0.43
12:1:42:PHE:CE1	52:1:517:CHL:HED3	2.54	0.43
12:1:82:TYR:CE2	12:1:149:ARG:HD2	2.54	0.43
12:1:201:GLN:HB3	12:1:213:ASN:ND2	2.33	0.43
15:5:159:GLN:HG2	52:5:315:CHL:HMC	2.01	0.43
17:M:56:ASP:HB3	17:M:60:PHE:CD2	2.54	0.43
17:M:297:LEU:O	17:M:300:GLU:HB3	2.19	0.43
19:O:207:ALA:C	19:O:209:LEU:H	2.27	0.43
19:O:301:PHE:O	19:O:305:ILE:HG12	2.18	0.43
26:V:158:GLY:HA3	26:V:161:PRO:HA	2.00	0.43
29:Y:101:ARG:H	29:Y:155:GLU:HB2	1.83	0.43
31:a:123:PRO:HG3	32:b:199:LEU:HA	2.01	0.43
36:6:302:LYS:HB2	36:6:349:ARG:HE	1.83	0.43
37:7:255:TRP:HZ2	37:7:261:LEU:HD22	1.84	0.43
44:e:852:CLA:H62	9:m:14:LEU:HD21	2.00	0.43
47:m:103:BCR:H11C	47:m:103:BCR:H341	1.79	0.43
14:q:78:ASP:HA	51:q:302:LUT:O23	2.19	0.43
14:q:96:TRP:CE2	44:q:314:CLA:HED1	2.54	0.43
14:q:146:THR:OG1	14:q:147:TYR:N	2.52	0.43
44:r:307:CLA:H62	44:r:307:CLA:H41	1.86	0.43
42:s:79:ASP:OD1	42:s:80:GLY:N	2.51	0.43
1:A:88:MET:HE1	44:A:808:CLA:H2A	2.00	0.43
12:1:124:ASN:HA	12:1:125:PRO:HD3	1.94	0.43
12:1:168:LEU:HD23	12:1:168:LEU:O	2.19	0.43
13:2:253:HIS:ND1	44:2:506:CLA:HAA2	2.34	0.43
16:G:122:VAL:HG22	16:G:124:ALA:H	1.84	0.43
19:O:435:SER:O	19:O:439:GLN:HG3	2.18	0.43
21:Q:760:ARG:O	21:Q:763:SER:OG	2.34	0.43
23:S:51:MET:HE2	23:S:70:TRP:CD1	2.54	0.43
23:S:76:MET:HB3	23:S:109:SER:HB3	2.01	0.43
23:S:327:TYR:CD2	23:S:340:TYR:HB2	2.54	0.43
24:T:10:SER:HA	24:T:13:GLN:HG2	1.99	0.43
28:X:108:ILE:H	28:X:124:THR:CG2	2.31	0.43
36:6:150:VAL:HG12	36:6:166:VAL:HG11	2.01	0.43
36:6:339:LYS:HG3	36:6:340:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:7:207:VAL:HG11	37:7:292:PHE:CZ	2.53	0.43
37:7:210:LEU:HD13	37:7:273:TYR:CD2	2.54	0.43
1:e:597:MET:HE3	1:e:597:MET:HB3	1.86	0.43
2:f:609:PHE:O	2:f:613:SER:OG	2.34	0.43
2:f:651:LEU:HD23	2:f:651:LEU:HA	1.82	0.43
6:j:98:SER:O	6:j:101:LYS:HG3	2.19	0.43
12:p:78:GLU:HA	12:p:159:LYS:HG2	2.01	0.43
14:q:105:GLY:O	14:q:109:MET:HG3	2.19	0.43
47:s:503:BCR:H21C	47:s:503:BCR:H361	2.01	0.43
1:A:77:GLN:O	1:A:77:GLN:NE2	2.52	0.42
1:A:109:GLY:HA2	1:A:110:PRO:HD3	1.92	0.42
1:A:598:TYR:HB2	1:A:731:LEU:HD11	2.01	0.42
4:D:86:LEU:HA	4:D:86:LEU:HD23	1.75	0.42
6:F:94:ARG:NH2	6:F:143:ASP:O	2.51	0.42
12:1:149:ARG:HA	44:1:513:CLA:CBC	2.49	0.42
44:2:505:CLA:H12	44:2:505:CLA:O1D	2.19	0.42
15:5:65:ASP:HA	44:5:308:CLA:O1D	2.19	0.42
17:M:328:SER:HA	17:M:332:ILE:HD12	2.01	0.42
19:O:8:THR:OG1	19:O:66:GLU:OE2	2.37	0.42
19:O:352:ALA:O	19:O:355:ARG:HB2	2.19	0.42
21:Q:428:GLY:O	21:Q:429:LEU:HD12	2.18	0.42
23:S:51:MET:HG3	23:S:70:TRP:CD1	2.54	0.42
26:V:86:ARG:HB2	26:V:92:ALA:HB2	2.00	0.42
34:4:133:GLU:O	35:d:178:ALA:HB2	2.18	0.42
36:6:250:ALA:N	36:6:421:ARG:O	2.36	0.42
37:7:49:ARG:HB3	37:7:146:TYR:CE1	2.53	0.42
37:7:216:CYS:C	37:7:218:HIS:H	2.26	0.42
1:e:741:PHE:CD1	43:e:801:CL0:CMD	3.02	0.42
47:e:846:BCR:H20C	47:e:846:BCR:H361	1.78	0.42
2:f:455:ILE:HD12	2:f:517:PHE:CE2	2.54	0.42
2:f:481:THR:HA	2:f:486:PHE:CD2	2.54	0.42
3:g:75:ARG:HH12	4:h:151:ARG:CZ	2.32	0.42
6:j:131:GLU:O	6:j:135:LYS:HG3	2.19	0.42
51:q:301:LUT:H15	51:q:301:LUT:H201	1.91	0.42
53:r:303:XAT:H15	53:r:303:XAT:H201	1.80	0.42
42:s:117:ALA:CB	53:s:502:XAT:H10	2.49	0.42
1:A:17:ASP:OD1	1:A:180:LYS:HD3	2.19	0.42
1:A:78:LEU:HD12	1:A:78:LEU:HA	1.84	0.42
1:A:576:PRO:HD2	3:C:52:LYS:HG2	2.00	0.42
44:A:806:CLA:H112	44:A:806:CLA:H91	1.75	0.42
6:F:208:PRO:HG3	50:F:806:LMG:H111	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:31:ARG:NH2	44:J:101:CLA:O1D	2.53	0.42
12:1:109:GLN:NE2	51:1:502:LUT:H372	2.34	0.42
44:1:509:CLA:HMA2	44:1:515:CLA:C3C	2.48	0.42
13:2:236:TRP:HD1	13:2:237:PHE:CD1	2.38	0.42
13:2:237:PHE:HB2	44:2:506:CLA:HAC2	2.01	0.42
44:2:510:CLA:H12	44:2:510:CLA:HBA1	1.81	0.42
14:3:259:HIS:CG	44:3:308:CLA:HAA2	2.54	0.42
15:5:146:GLU:HG3	44:5:316:CLA:C4B	2.50	0.42
16:G:48:TRP:CE2	16:G:52:GLU:HG3	2.54	0.42
19:O:67:ASP:HB3	19:O:79:ARG:HD2	2.00	0.42
21:Q:64:MET:O	21:Q:68:LEU:N	2.46	0.42
21:Q:427:GLY:HA2	21:Q:495:THR:HA	2.02	0.42
24:T:55:GLY:HA3	24:T:123:GLU:HA	2.01	0.42
27:W:112:PRO:HG3	27:W:145:LEU:HD23	2.00	0.42
28:X:103:ILE:HA	28:X:125:LEU:HG	2.00	0.42
29:Y:115:PRO:HB3	29:Y:130:TYR:CD1	2.54	0.42
36:6:180:GLU:OE2	36:6:183:GLU:N	2.50	0.42
36:6:286:LYS:O	36:6:290:VAL:HG22	2.19	0.42
36:6:297:ARG:HD2	36:6:297:ARG:N	2.34	0.42
37:7:116:VAL:HA	37:7:131:LEU:HD21	2.01	0.42
38:8:78:PHE:N	38:8:177:SER:O	2.52	0.42
1:e:101:TRP:NE1	1:e:110:PRO:HG3	2.34	0.42
1:e:221:ILE:HG13	1:e:234:ILE:HG21	2.00	0.42
1:e:308:MET:HG2	44:e:821:CLA:CAC	2.49	0.42
1:e:327:LYS:H	44:e:843:CLA:HAC1	1.83	0.42
44:e:838:CLA:H2A	44:e:838:CLA:O2D	2.19	0.42
44:f:840:CLA:H2A	44:f:840:CLA:O1D	2.19	0.42
12:p:104:ASN:HD22	12:p:107:LYS:NZ	2.17	0.42
14:q:235:MET:HB3	51:q:302:LUT:H402	2.01	0.42
42:s:221:LYS:HG2	44:s:510:CLA:OBD	2.19	0.42
1:A:191:VAL:HA	1:A:194:MET:HB2	2.00	0.42
1:A:507:TRP:CZ2	44:A:826:CLA:HMC2	2.53	0.42
47:A:848:BCR:H20C	47:A:848:BCR:H361	1.83	0.42
47:L:306:BCR:H15C	47:L:306:BCR:H351	1.70	0.42
12:1:77:LYS:HB2	12:1:159:LYS:NZ	2.34	0.42
13:2:126:LEU:O	13:2:131:ILE:HG22	2.19	0.42
17:M:380:ASN:OD1	17:M:380:ASN:N	2.51	0.42
23:S:331:GLU:HA	23:S:336:GLU:HA	2.00	0.42
25:U:109:ASP:O	25:U:126:HIS:NE2	2.52	0.42
37:7:172:SER:OG	37:7:357:GLU:HA	2.20	0.42
40:0:133:PHE:HB3	40:0:134:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:143:GLN:HB3	1:e:374:TYR:HB3	2.00	0.42
2:f:31:PHE:CE2	2:f:45:ASN:HB3	2.54	0.42
2:f:169:LYS:NZ	2:f:328:ASN:HA	2.34	0.42
2:f:340:SER:OG	44:f:826:CLA:H2	2.19	0.42
2:f:519:VAL:HG11	2:f:593:TYR:HB2	2.00	0.42
2:f:624:LEU:HD22	44:f:804:CLA:HMD3	2.02	0.42
3:g:78:ALA:O	4:h:128:ARG:NH1	2.52	0.42
11:o:103:TYR:OH	44:o:304:CLA:OBD	2.29	0.42
14:q:156:LEU:HD11	44:q:315:CLA:CMD	2.50	0.42
2:B:458:ILE:HG21	6:F:151:SER:HB3	2.00	0.42
47:B:849:BCR:H20C	47:B:849:BCR:H361	1.84	0.42
3:C:25:VAL:HG13	3:C:44:ARG:O	2.18	0.42
6:F:136:PHE:CD2	9:J:40:PRO:HG3	2.53	0.42
9:J:8:LEU:HD23	9:J:13:VAL:HG11	2.01	0.42
12:1:70:PRO:HA	12:1:73:PHE:HB3	2.02	0.42
15:5:77:PRO:O	15:5:81:LYS:HG2	2.19	0.42
15:5:89:VAL:HG21	15:5:149:ARG:NH1	2.35	0.42
15:5:93:PHE:CE2	44:5:316:CLA:HAC2	2.54	0.42
15:5:212:MET:HE1	44:5:308:CLA:CAB	2.49	0.42
16:G:282:ILE:HG22	16:G:286:SER:OG	2.19	0.42
16:G:331:ARG:C	16:G:333:ASP:H	2.27	0.42
19:O:361:LEU:HA	19:O:364:LEU:HD23	2.00	0.42
23:S:53:LYS:O	23:S:56:GLU:HG2	2.19	0.42
23:S:252:GLN:CD	23:S:253:LYS:H	2.26	0.42
1:e:75:PHE:HZ	44:e:809:CLA:HBB1	1.84	0.42
2:f:292:ARG:HD2	2:f:296:GLY:HA2	2.00	0.42
2:f:689:ASN:N	2:f:689:ASN:OD1	2.53	0.42
11:o:204:LEU:HD12	11:o:204:LEU:HA	1.91	0.42
12:p:177:PHE:CE1	44:p:504:CLA:HED1	2.54	0.42
12:p:208:THR:OG1	12:p:209:GLY:N	2.52	0.42
1:A:314:GLY:HA2	10:K:88:ARG:NH2	2.34	0.42
44:A:806:CLA:H161	44:A:828:CLA:HBB2	2.00	0.42
2:B:22:TRP:CG	2:B:704:GLN:HE22	2.36	0.42
2:B:69:ALA:HB2	2:B:135:LEU:HD12	2.01	0.42
44:B:841:CLA:H2A	44:B:841:CLA:O1D	2.19	0.42
11:L:81:LEU:HB2	11:L:82:PRO:HD2	2.01	0.42
52:2:512:CHL:C1A	50:2:519:LMG:H152	2.49	0.42
14:3:233:LEU:CD2	51:3:303:LUT:H11	2.49	0.42
16:G:214:PHE:HB2	16:G:274:TYR:CD2	2.54	0.42
19:O:74:PHE:HE2	19:O:135:LEU:HD22	1.84	0.42
22:R:121:TYR:O	22:R:125:TRP:NE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:S:53:LYS:NZ	25:U:143:LEU:HA	2.33	0.42
23:S:95:PRO:HG2	23:S:309:LYS:O	2.18	0.42
28:X:99:ARG:NH2	28:X:194:ASN:HD21	2.17	0.42
44:f:834:CLA:H2A	44:f:834:CLA:O1D	2.19	0.42
6:j:200:VAL:HA	6:j:203:ALA:HB3	2.01	0.42
14:q:142:PRO:N	14:q:143:PRO:HD2	2.34	0.42
53:s:502:XAT:H391	53:s:502:XAT:H31	1.77	0.42
47:A:846:BCR:H20C	47:A:846:BCR:H361	1.89	0.42
3:C:27:GLU:OE1	3:C:44:ARG:NH2	2.52	0.42
3:C:58:CYS:HA	48:C:102:SF4:S4	2.59	0.42
13:2:148:ASP:OD2	13:2:150:THR:OG1	2.36	0.42
19:O:222:ALA:HB2	19:O:227:ILE:HD12	2.01	0.42
22:R:24:LEU:O	22:R:28:LEU:HB2	2.19	0.42
25:U:54:SER:O	25:U:69:VAL:HG13	2.19	0.42
36:6:443:LEU:HD12	36:6:446:ILE:HD11	2.01	0.42
47:e:846:BCR:H351	47:e:846:BCR:H15C	1.71	0.42
2:f:183:PHE:CE2	44:f:821:CLA:HBB2	2.54	0.42
6:j:228:VAL:HG12	6:j:229:ASP:N	2.35	0.42
12:p:154:ASP:CB	12:p:157:LYS:H	2.33	0.42
14:q:156:LEU:HD11	44:q:315:CLA:C2D	2.50	0.42
42:s:218:LEU:HD23	42:s:218:LEU:HA	1.91	0.42
44:s:510:CLA:HBA1	44:s:510:CLA:H3A	1.90	0.42
1:A:13:VAL:HA	14:3:87:GLY:HA2	2.02	0.42
1:A:161:ILE:O	1:A:165:VAL:HG23	2.20	0.42
1:A:308:MET:HE1	44:A:820:CLA:C1D	2.50	0.42
1:A:511:GLU:OE1	1:A:512:LEU:HG	2.19	0.42
1:A:690:GLY:N	2:B:568:CYS:O	2.52	0.42
47:A:851:BCR:H321	47:A:851:BCR:HC8	2.00	0.42
44:B:824:CLA:H2A	44:B:824:CLA:HED3	2.01	0.42
47:B:847:BCR:H341	47:B:847:BCR:H11C	1.73	0.42
44:1:506:CLA:HHC	44:1:506:CLA:CBB	2.49	0.42
15:5:94:ALA:HB2	53:5:304:XAT:C13	2.50	0.42
15:5:136:PHE:O	15:5:140:LEU:HG	2.19	0.42
16:G:48:TRP:CD2	16:G:52:GLU:HG3	2.54	0.42
17:M:95:ASN:O	17:M:99:ILE:HG13	2.20	0.42
21:Q:183:SER:CB	21:Q:189:ILE:HG22	2.48	0.42
23:S:139:GLU:HA	23:S:142:TYR:CD2	2.55	0.42
31:a:167:ARG:CZ	31:a:224:ILE:HD11	2.50	0.42
31:a:192:GLY:C	31:a:194:GLY:H	2.27	0.42
38:8:124:LEU:HD12	38:8:124:LEU:HA	1.92	0.42
1:e:122:GLU:HG2	6:j:122:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:233:GLU:OE2	1:e:233:GLU:N	2.46	0.42
2:f:220:GLN:O	2:f:224:PRO:HD3	2.20	0.42
7:k:109:GLY:O	7:k:113:VAL:HG12	2.20	0.42
47:p:503:BCR:H381	44:p:509:CLA:H12	2.02	0.42
41:r:51:PRO:HG3	44:r:312:CLA:HMD2	2.02	0.42
1:A:302:PHE:HE1	44:A:820:CLA:HAB	1.85	0.42
1:A:592:LEU:HA	1:A:592:LEU:HD23	1.86	0.42
1:A:671:PHE:CE2	1:A:675:HIS:HE1	2.36	0.42
44:B:832:CLA:HMB1	44:B:832:CLA:HBB1	2.01	0.42
11:L:140:LEU:HB3	11:L:181:THR:HG22	2.02	0.42
12:1:65:GLY:O	12:1:68:THR:HG23	2.19	0.42
14:3:210:LEU:HD23	14:3:212:PHE:CE1	2.55	0.42
16:G:189:SER:O	16:G:193:ILE:HG12	2.20	0.42
17:M:448:LEU:HD12	19:O:149:TYR:CE2	2.55	0.42
26:V:96:LEU:HD12	26:V:125:MET:HB2	2.01	0.42
29:Y:149:LEU:HB2	29:Y:202:VAL:HG12	2.02	0.42
37:7:53:ASP:OD1	37:7:54:ALA:N	2.43	0.42
37:7:97:LEU:HD13	37:7:112:GLY:O	2.20	0.42
38:8:91:PRO:HB2	38:8:93:VAL:HG13	2.01	0.42
2:f:487:ASN:O	2:f:490:ARG:NH2	2.53	0.42
2:f:519:VAL:HG11	2:f:593:TYR:CG	2.55	0.42
44:f:818:CLA:H92	44:f:818:CLA:H62	1.84	0.42
14:q:202:PRO:HG2	44:q:304:CLA:OBD	2.20	0.42
14:q:238:PHE:CE2	51:q:302:LUT:H14	2.54	0.42
1:A:75:PHE:HZ	44:3:301:CLA:HBB1	1.84	0.42
1:A:621:SER:HG	1:A:624:GLY:H	1.65	0.42
1:A:622:ASP:N	1:A:622:ASP:OD1	2.51	0.42
46:A:843:LHG:H272	46:A:843:LHG:H242	1.75	0.42
2:B:64:ASN:HD21	44:B:828:CLA:HED1	1.84	0.42
44:B:813:CLA:HBA1	44:B:813:CLA:H3A	1.72	0.42
10:K:110:ALA:HA	47:K:204:BCR:C11	2.50	0.42
11:L:143:TYR:O	11:L:147:SER:OG	2.35	0.42
44:1:506:CLA:HBA2	44:1:506:CLA:H3A	1.77	0.42
44:2:506:CLA:H51	44:2:506:CLA:C4C	2.50	0.42
53:5:304:XAT:H173	53:5:304:XAT:H3	1.71	0.42
16:G:81:LEU:HD21	26:V:55:TRP:HH2	1.85	0.42
17:M:228:GLY:O	17:M:231:ILE:N	2.44	0.42
19:O:411:LEU:O	19:O:413:MET:N	2.53	0.42
54:Q:802:SQD:H322	54:Q:802:SQD:H291	1.83	0.42
22:R:68:GLY:O	22:R:72:VAL:HG22	2.20	0.42
23:S:314:LYS:HD2	23:S:315:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:S:364:ILE:O	23:S:368:LEU:HG	2.20	0.42
25:U:25:ARG:HH21	25:U:27:ILE:HD13	1.85	0.42
25:U:92:GLN:HG3	25:U:94:ASP:H	1.84	0.42
1:e:98:TYR:CE2	1:e:102:LEU:HD11	2.55	0.42
1:e:102:LEU:HD13	1:e:151:THR:HA	2.02	0.42
1:e:151:THR:HG21	1:e:221:ILE:HD11	2.02	0.42
1:e:197:HIS:HD2	44:e:812:CLA:HAB	1.83	0.42
1:e:338:LEU:HA	1:e:341:ILE:HD13	2.01	0.42
47:e:851:BCR:H24C	47:e:851:BCR:H371	1.87	0.42
2:f:394:PHE:HD1	2:f:394:PHE:HA	1.71	0.42
2:f:674:LEU:HD12	2:f:674:LEU:HA	1.85	0.42
47:f:845:BCR:H15C	47:f:845:BCR:H351	1.88	0.42
4:h:98:THR:HG23	4:h:122:ASN:O	2.19	0.42
47:r:301:BCR:H341	47:r:301:BCR:H11C	1.79	0.42
1:A:323:LEU:O	1:A:335:HIS:HB2	2.20	0.42
1:A:648:PHE:O	1:A:652:GLN:HB2	2.20	0.42
45:A:841:PQN:H222	45:A:841:PQN:H262	1.77	0.42
6:F:136:PHE:CE2	9:J:40:PRO:HG3	2.54	0.42
14:3:163:LEU:O	47:3:305:BCR:H16C	2.20	0.42
16:G:52:GLU:HG2	16:G:63:PRO:HD2	2.02	0.42
16:G:202:PHE:HA	16:G:205:TRP:CD1	2.55	0.42
17:M:286:ILE:HB	17:M:287:PRO:HD3	2.02	0.42
21:Q:157:MET:HG3	21:Q:160:ASP:CB	2.50	0.42
21:Q:425:LEU:O	21:Q:502:VAL:HG23	2.20	0.42
23:S:47:LEU:HD11	26:V:61:THR:HB	2.02	0.42
36:6:263:TRP:O	36:6:263:TRP:CG	2.73	0.42
37:7:215:TYR:O	37:7:216:CYS:C	2.63	0.42
1:e:118:ILE:HD11	9:m:27:ILE:HB	2.02	0.42
1:e:693:GLN:HB3	2:f:546:LEU:HD22	2.02	0.42
44:e:827:CLA:O1D	44:e:828:CLA:HHB	2.20	0.42
44:e:829:CLA:H62	44:e:829:CLA:H41	1.97	0.42
2:f:527:LEU:HD23	2:f:527:LEU:HA	1.88	0.42
44:f:804:CLA:O2D	44:f:804:CLA:HAA2	2.18	0.42
3:g:6:LYS:HE3	4:h:203:PHE:HD1	1.84	0.42
4:h:191:SER:OG	4:h:193:ILE:HG22	2.20	0.42
5:i:92:LYS:HD2	5:i:92:LYS:HA	1.79	0.42
47:A:846:BCR:H351	47:A:846:BCR:H15C	1.78	0.41
44:B:815:CLA:H91	44:B:815:CLA:H112	1.88	0.41
10:K:122:GLY:HA2	10:K:124:LYS:NZ	2.34	0.41
12:1:208:THR:HG21	12:1:213:ASN:HD21	1.85	0.41
12:1:212:GLU:O	12:1:216:THR:OG1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:160:ALA:HB1	15:5:168:ILE:O	2.19	0.41
17:M:179:ALA:HB1	17:M:256:VAL:HA	2.01	0.41
17:M:220:ASN:OD1	17:M:221:THR:N	2.53	0.41
17:M:313:LEU:HD22	21:Q:754:LYS:HG3	2.02	0.41
20:P:6:VAL:HG11	20:P:47:THR:HG21	2.01	0.41
21:Q:138:MET:HB2	21:Q:181:VAL:HG11	2.02	0.41
21:Q:417:PRO:C	21:Q:419:LYS:H	2.28	0.41
21:Q:718:LEU:HD23	21:Q:718:LEU:HA	1.85	0.41
23:S:138:ARG:CZ	23:S:142:TYR:HE1	2.33	0.41
33:c:205:ASP:OD1	33:c:206:THR:N	2.51	0.41
35:d:96:VAL:HB	35:d:209:GLU:HB2	2.02	0.41
38:8:149:LYS:HE2	38:8:165:ARG:HG2	2.02	0.41
40:0:137:VAL:O	40:0:137:VAL:HG12	2.20	0.41
44:e:804:CLA:H202	44:e:804:CLA:H161	1.77	0.41
47:e:848:BCR:H15C	47:e:848:BCR:H351	1.84	0.41
11:o:164:ARG:NH2	11:o:166:LYS:HA	2.35	0.41
12:p:226:ILE:HD11	44:p:506:CLA:H11	2.01	0.41
51:p:501:LUT:H35	51:p:501:LUT:H401	1.75	0.41
14:q:159:PHE:CD1	44:s:511:CLA:HBA1	2.55	0.41
44:q:311:CLA:H3A	44:q:311:CLA:CGA	2.50	0.41
42:s:217:VAL:HG13	44:s:510:CLA:HED1	2.02	0.41
51:s:501:LUT:H383	44:s:506:CLA:C3B	2.50	0.41
52:s:512:CHL:HHC	52:s:512:CHL:HBB1	2.01	0.41
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.82	0.41
1:A:550:LYS:HD3	2:B:670:TYR:HE1	1.85	0.41
1:A:681:SER:HB3	1:A:729:HIS:HB2	2.03	0.41
44:B:822:CLA:C1D	47:B:844:BCR:H323	2.49	0.41
6:F:150:VAL:HG12	6:F:160:PHE:HB2	2.02	0.41
10:K:97:PRO:HD3	44:K:201:CLA:CAA	2.50	0.41
11:L:92:LEU:HA	11:L:95:ILE:HG22	2.01	0.41
51:1:502:LUT:H11	51:1:502:LUT:H191	1.92	0.41
17:M:75:LEU:HD23	17:M:75:LEU:HA	1.85	0.41
17:M:361:MET:HE2	17:M:405:LEU:HA	2.02	0.41
22:R:107:PHE:O	22:R:110:SER:OG	2.35	0.41
29:Y:196:PRO:HG3	29:Y:204:VAL:HG22	2.01	0.41
35:d:240:LEU:HD12	35:d:241:PRO:HD2	2.00	0.41
36:6:416:SER:C	36:6:418:GLU:H	2.27	0.41
1:e:146:ARG:NH1	1:e:225:LEU:HD13	2.34	0.41
1:e:452:LEU:HD22	1:e:469:PHE:CE2	2.53	0.41
1:e:465:PRO:HA	1:e:468:MET:HG3	2.02	0.41
2:f:26:ALA:HB2	49:f:851:DGD:HA22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:189:ALA:HB1	44:f:816:CLA:HAB	2.02	0.41
2:f:236:ASN:O	2:f:252:THR:N	2.54	0.41
2:f:246:THR:OG1	2:f:247:ALA:N	2.53	0.41
2:f:416:GLU:OE1	2:f:416:GLU:N	2.45	0.41
4:h:103:LYS:HD3	4:h:103:LYS:HA	1.82	0.41
5:i:79:LYS:N	5:i:80:PRO:HD2	2.35	0.41
6:j:95:GLU:O	6:j:99:VAL:HG22	2.21	0.41
10:n:54:LEU:O	10:n:58:THR:HG22	2.19	0.41
12:p:230:VAL:HG23	12:p:232:PRO:C	2.45	0.41
41:r:192:GLU:HG2	41:r:196:LYS:HE3	2.01	0.41
41:r:237:THR:OG1	41:r:238:ILE:N	2.53	0.41
1:A:314:GLY:HA3	10:K:75:ALA:HB1	2.02	0.41
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.73	0.41
44:B:822:CLA:CAD	47:B:844:BCR:HC41	2.50	0.41
5:E:94:LEU:HD13	5:E:94:LEU:HA	1.89	0.41
13:2:87:PHE:HB3	44:2:507:CLA:CAD	2.50	0.41
13:2:121:PHE:CD2	51:2:501:LUT:H28	2.55	0.41
51:3:304:LUT:H15	51:3:304:LUT:H201	1.94	0.41
15:5:150:TYR:CD2	15:5:151:MET:HE2	2.55	0.41
15:5:174:GLY:O	15:5:175:LEU:HB2	2.20	0.41
47:5:302:BCR:H351	47:5:302:BCR:H15C	1.73	0.41
17:M:218:LEU:O	17:M:224:TYR:HB3	2.20	0.41
21:Q:353:ALA:HB2	38:8:123:LEU:HB3	2.01	0.41
27:W:157:PHE:O	27:W:159:ARG:HD2	2.20	0.41
35:d:235:SER:OG	35:d:236:GLU:N	2.53	0.41
36:6:336:GLU:HG2	36:6:448:ILE:HD12	2.01	0.41
37:7:288:ALA:HA	37:7:289:PRO:HD3	1.91	0.41
39:9:148:TRP:O	39:9:150:TYR:N	2.53	0.41
2:f:439:HIS:NE2	2:f:453:ILE:HG13	2.35	0.41
47:f:848:BCR:H24C	47:f:848:BCR:H371	1.91	0.41
6:j:139:LEU:HD12	6:j:149:ILE:HG13	2.03	0.41
10:n:78:LYS:HD3	10:n:78:LYS:HA	1.93	0.41
11:o:109:PHE:CE1	11:o:128:GLY:HA3	2.55	0.41
47:o:305:BCR:H351	47:o:305:BCR:H15C	1.75	0.41
14:q:95:ARG:HG3	14:q:175:TRP:HH2	1.84	0.41
1:A:223:GLN:NE2	1:A:250:LEU:HD22	2.35	0.41
1:A:315:ILE:HB	44:A:821:CLA:HMD3	2.02	0.41
2:B:429:LEU:HA	2:B:429:LEU:HD23	1.80	0.41
2:B:492:LEU:HD13	2:B:492:LEU:HA	1.76	0.41
44:B:808:CLA:H2	47:I:101:BCR:HC31	2.03	0.41
44:B:811:CLA:H2A	44:B:811:CLA:O1D	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:B:844:BCR:H11C	47:B:844:BCR:H341	1.71	0.41
14:3:142:PRO:N	14:3:143:PRO:HD2	2.35	0.41
47:5:302:BCR:C37	52:5:317:CHL:HHB	2.50	0.41
16:G:63:PRO:HB3	16:G:73:GLN:HG2	2.02	0.41
17:M:447:TYR:O	17:M:451:ILE:HG12	2.20	0.41
19:O:226:PRO:HG2	19:O:234:LEU:HD22	2.03	0.41
21:Q:286:PHE:O	21:Q:289:HIS:ND1	2.53	0.41
23:S:47:LEU:HD21	26:V:61:THR:HB	2.02	0.41
25:U:32:ILE:HG12	25:U:87:ILE:HD12	2.02	0.41
26:V:63:CYS:SG	26:V:100:THR:OG1	2.76	0.41
29:Y:74:PRO:HB3	29:Y:214:PHE:HD1	1.86	0.41
29:Y:210:ASN:CG	29:Y:211:TRP:H	2.27	0.41
35:d:79:TYR:HB2	35:d:94:ARG:HD2	2.02	0.41
36:6:325:ASP:CG	36:6:443:LEU:H	2.29	0.41
36:6:366:ILE:N	36:6:370:GLU:OE2	2.53	0.41
1:e:43:THR:HG22	1:e:715:ARG:HB2	2.02	0.41
1:e:80:ILE:HD12	47:m:103:BCR:HC31	2.01	0.41
1:e:556:ARG:HD2	1:e:556:ARG:HA	1.83	0.41
2:f:615:TYR:O	2:f:618:GLY:N	2.49	0.41
47:f:849:BCR:H11C	47:f:849:BCR:H341	1.78	0.41
3:g:53:ARG:HA	3:g:56:SER:HB3	2.01	0.41
6:j:90:ALA:HA	6:j:93:LYS:HG2	2.02	0.41
6:j:99:VAL:O	6:j:103:ASN:ND2	2.53	0.41
6:j:206:ILE:HG23	6:j:209:ARG:HH22	1.85	0.41
47:l:102:BCR:H351	47:l:102:BCR:H15C	1.73	0.41
14:q:172:LEU:HD12	44:q:314:CLA:HMA2	2.02	0.41
51:q:302:LUT:H15	51:q:302:LUT:H201	1.87	0.41
47:r:301:BCR:H24C	47:r:301:BCR:H371	1.87	0.41
51:r:302:LUT:H15	51:r:302:LUT:H201	1.72	0.41
44:r:306:CLA:H51	44:r:306:CLA:H11	1.79	0.41
44:r:310:CLA:H2A	44:r:310:CLA:O2D	2.20	0.41
1:A:66:ILE:O	1:A:70:VAL:HG13	2.20	0.41
1:A:194:MET:SD	1:A:198:HIS:CE1	3.13	0.41
1:A:679:ALA:HB3	44:A:802:CLA:HBB2	2.01	0.41
44:A:820:CLA:H92	44:A:820:CLA:H62	1.89	0.41
44:A:827:CLA:H151	47:J:102:BCR:H351	2.02	0.41
2:B:310:PRO:HA	2:B:311:PRO:HD3	1.93	0.41
3:C:27:GLU:OE1	3:C:44:ARG:NH1	2.54	0.41
11:L:154:SER:HB2	11:L:168:ALA:HB1	2.02	0.41
12:1:226:ILE:HB	44:1:506:CLA:H11	2.01	0.41
14:3:239:LEU:HD12	14:3:239:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:5:186:ASN:ND2	15:5:189:GLY:HA2	2.35	0.41
17:M:390:LYS:HD2	17:M:390:LYS:HA	1.90	0.41
19:O:388:LEU:HD11	21:Q:198:MET:HB2	2.02	0.41
23:S:25:VAL:O	23:S:26:LEU:HD23	2.21	0.41
26:V:138:ASP:N	26:V:138:ASP:OD1	2.53	0.41
27:W:112:PRO:CB	27:W:148:TRP:HB2	2.51	0.41
1:e:71:PHE:HD2	1:e:188:PHE:CE1	2.38	0.41
1:e:742:PHE:O	1:e:746:ILE:HG22	2.20	0.41
14:q:203:GLY:N	44:q:304:CLA:OBD	2.54	0.41
44:q:305:CLA:H61	44:q:305:CLA:H41	1.79	0.41
41:r:90:VAL:O	41:r:94:TRP:HD1	2.04	0.41
42:s:165:GLU:OE1	42:s:168:ARG:NE	2.40	0.41
42:s:216:MET:H	42:s:216:MET:HE2	1.85	0.41
1:A:548:LEU:O	1:A:552:VAL:HG23	2.21	0.41
49:B:850:DGD:O6D	49:B:850:DGD:O3D	2.37	0.41
3:C:62:PHE:HD2	4:D:186:ILE:HG21	1.86	0.41
6:F:209:ARG:HH22	15:5:72:GLY:HA3	1.84	0.41
9:J:25:LEU:O	9:J:29:ILE:HG13	2.21	0.41
53:2:502:XAT:H35	53:2:502:XAT:H401	1.81	0.41
44:3:309:CLA:O2D	44:3:309:CLA:H2A	2.21	0.41
44:3:311:CLA:C4A	44:3:311:CLA:HBA2	2.51	0.41
51:5:303:LUT:H11	51:5:303:LUT:H191	1.93	0.41
19:O:29:ASN:ND2	19:O:33:ARG:HD3	2.35	0.41
34:4:128:ALA:N	34:4:239:CYS:SG	2.93	0.41
36:6:250:ALA:C	36:6:252:GLY:H	2.29	0.41
36:6:309:HIS:ND1	36:6:399:ALA:HB2	2.34	0.41
40:0:101:GLU:HG2	40:0:102:GLY:N	2.34	0.41
1:e:537:HIS:CD2	44:e:836:CLA:HAB	2.55	0.41
2:f:190:TRP:HZ2	44:f:820:CLA:HED2	1.86	0.41
2:f:276:HIS:HB2	44:f:819:CLA:C1B	2.51	0.41
2:f:451:LYS:HE3	9:m:35:ASP:HB3	2.02	0.41
4:h:104:GLU:OE2	4:h:119:GLU:N	2.54	0.41
5:i:87:ARG:HD3	5:i:87:ARG:HA	1.76	0.41
46:p:516:LHG:H241	47:r:301:BCR:HC21	2.01	0.41
14:q:272:LEU:HB3	14:q:274:PHE:CE2	2.55	0.41
41:r:48:SER:C	41:r:50:LEU:N	2.79	0.41
44:A:827:CLA:H143	44:A:827:CLA:H111	1.84	0.41
2:B:53:GLN:HE21	2:B:57:ILE:HG13	1.86	0.41
5:E:95:ARG:HD2	5:E:98:SER:HB2	2.02	0.41
12:1:180:LEU:C	44:1:504:CLA:HMA1	2.46	0.41
13:2:120:ILE:HG12	13:2:137:TRP:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:128:LYS:HA	13:2:128:LYS:HD2	1.91	0.41
15:5:200:VAL:HG12	44:5:305:CLA:HMA1	2.02	0.41
17:M:478:ASN:HB3	17:M:479:SER:H	1.61	0.41
19:O:288:ILE:HD12	19:O:422:MET:HG3	2.03	0.41
19:O:401:PHE:HE1	19:O:422:MET:SD	2.43	0.41
22:R:121:TYR:HD2	32:b:147:LEU:HD13	1.86	0.41
23:S:116:LEU:HD21	23:S:138:ARG:CZ	2.51	0.41
23:S:197:PRO:O	23:S:201:GLU:N	2.34	0.41
25:U:44:LEU:HD13	25:U:49:TYR:HD2	1.84	0.41
27:W:110:VAL:O	27:W:113:PRO:HD2	2.21	0.41
37:7:73:ARG:HG3	37:7:75:ASN:H	1.85	0.41
38:8:107:ILE:HD12	38:8:107:ILE:HA	1.88	0.41
1:e:210:TRP:CZ2	44:e:818:CLA:O1D	2.73	0.41
1:e:605:ILE:HG22	1:e:742:PHE:CZ	2.56	0.41
47:e:848:BCR:H11C	47:e:848:BCR:H341	1.73	0.41
2:f:680:TRP:HE1	2:f:684:ARG:NH1	2.18	0.41
6:j:205:ARG:O	6:j:209:ARG:NH1	2.54	0.41
10:n:77:ARG:HA	10:n:87:ALA:HA	2.02	0.41
12:p:97:PRO:HB3	44:p:509:CLA:O1D	2.20	0.41
12:p:174:PRO:O	12:p:177:PHE:HB3	2.20	0.41
12:p:212:GLU:O	12:p:216:THR:HG23	2.20	0.41
14:q:79:PRO:HD2	51:q:302:LUT:O23	2.20	0.41
44:r:306:CLA:H41	44:r:306:CLA:H61	1.80	0.41
53:s:502:XAT:H35	53:s:502:XAT:H401	1.79	0.41
1:A:41:ASP:OD1	1:A:45:TRP:HB2	2.21	0.41
44:B:826:CLA:H102	44:B:838:CLA:H2	2.01	0.41
44:B:838:CLA:H192	44:B:838:CLA:H162	1.76	0.41
44:B:838:CLA:H151	47:F:804:BCR:H402	2.02	0.41
6:F:212:ILE:HD12	15:5:73:LEU:HD13	2.02	0.41
44:1:510:CLA:HBA1	44:1:510:CLA:H3A	1.69	0.41
13:2:68:PHE:HD2	13:2:71:SER:HB3	1.85	0.41
14:3:80:LEU:N	51:3:304:LUT:O23	2.54	0.41
16:G:68:PRO:HA	27:W:120:ARG:HH12	1.85	0.41
23:S:219:LEU:HD23	23:S:219:LEU:HA	1.96	0.41
23:S:221:GLY:O	23:S:225:ARG:HG3	2.21	0.41
24:T:141:ALA:HA	29:Y:183:VAL:HG22	2.03	0.41
30:Z:58:UNK:HA	30:Z:95:UNK:CB	2.51	0.41
36:6:290:VAL:HG23	36:6:291:VAL:N	2.36	0.41
36:6:311:ILE:HG22	36:6:312:GLU:HG2	2.02	0.41
44:e:813:CLA:H3A	47:e:846:BCR:C33	2.50	0.41
44:e:843:CLA:H3A	44:e:843:CLA:HBA1	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:574:ASP:O	2:f:577:TYR:HB3	2.21	0.41
3:g:8:TYR:HE2	4:h:186:ILE:HG13	1.86	0.41
11:o:102:GLY:O	11:o:106:VAL:HG23	2.20	0.41
14:q:59:ALA:HB2	14:q:76:GLY:O	2.20	0.41
42:s:78:LEU:HD13	42:s:78:LEU:HA	1.96	0.41
1:A:694:GLU:OE2	2:B:544:SER:OG	2.28	0.41
47:A:847:BCR:H371	47:A:847:BCR:H24C	1.82	0.41
2:B:193:HIS:HB2	44:B:815:CLA:C1C	2.51	0.41
2:B:395:ILE:HD11	2:B:541:ALA:HB1	2.03	0.41
44:B:806:CLA:HBC2	44:B:830:CLA:CMA	2.51	0.41
44:B:807:CLA:H61	44:B:807:CLA:H93	1.73	0.41
44:B:811:CLA:HBA2	44:B:811:CLA:HBD	2.03	0.41
44:B:815:CLA:H112	44:B:815:CLA:H142	1.85	0.41
47:B:844:BCR:H20C	47:B:844:BCR:H361	1.80	0.41
4:D:101:SER:OG	4:D:117:MET:SD	2.66	0.41
4:D:104:GLU:CD	4:D:119:GLU:HB2	2.46	0.41
4:D:133:LEU:HA	4:D:133:LEU:HD12	1.84	0.41
5:E:135:ASN:OD1	5:E:135:ASN:N	2.52	0.41
47:L:305:BCR:C8	47:L:305:BCR:H331	2.50	0.41
51:1:502:LUT:H201	51:1:502:LUT:H15	1.74	0.41
53:2:502:XAT:H15	53:2:502:XAT:H201	1.83	0.41
44:2:506:CLA:HBB1	44:2:506:CLA:HMB1	2.03	0.41
14:3:121:LEU:O	14:3:125:GLY:N	2.54	0.41
14:3:243:LEU:HD13	14:3:243:LEU:HA	1.95	0.41
52:5:314:CHL:CMC	52:5:317:CHL:HHC	2.50	0.41
16:G:71:LEU:HD12	16:G:71:LEU:H	1.86	0.41
16:G:197:GLN:HE21	16:G:206:ASN:H	1.69	0.41
18:N:56:VAL:HG13	23:S:34:GLY:H	1.86	0.41
18:N:89:LEU:HD23	18:N:89:LEU:HA	1.96	0.41
19:O:65:LYS:HB3	19:O:65:LYS:HE2	1.85	0.41
19:O:174:GLY:HA3	19:O:223:VAL:HG11	2.03	0.41
19:O:282:ILE:HD13	19:O:418:ILE:HD11	2.03	0.41
21:Q:160:ASP:OD1	21:Q:161:GLU:N	2.46	0.41
21:Q:417:PRO:HD2	40:0:93:TYR:CD2	2.55	0.41
23:S:84:ASN:HA	23:S:88:PHE:HB3	2.02	0.41
23:S:101:ILE:O	23:S:105:MET:HG3	2.20	0.41
25:U:137:SER:OG	28:X:161:GLU:HB2	2.20	0.41
26:V:105:MET:O	26:V:109:LEU:HB2	2.21	0.41
26:V:117:PRO:O	26:V:120:LYS:HG2	2.21	0.41
27:W:149:ALA:C	27:W:151:PHE:N	2.78	0.41
31:a:185:ALA:HA	31:a:201:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:d:114:LEU:HD22	35:d:121:PHE:O	2.21	0.41
37:7:55:THR:C	37:7:57:ALA:H	2.28	0.41
37:7:109:VAL:HG12	37:7:231:ALA:O	2.20	0.41
37:7:186:PRO:HG3	37:7:346:PRO:HD3	2.03	0.41
37:7:229:THR:O	37:7:231:ALA:N	2.43	0.41
1:e:346:TRP:HB3	44:e:804:CLA:HAC1	2.02	0.41
1:e:633:ASN:ND2	1:e:647:ASP:OD1	2.54	0.41
1:e:721:GLN:HE21	46:e:844:LHG:HC92	1.85	0.41
44:e:803:CLA:H2	44:e:803:CLA:H61	1.76	0.41
2:f:218:TYR:OH	2:f:232:LEU:O	2.21	0.41
2:f:223:GLY:O	2:f:227:THR:OG1	2.31	0.41
2:f:451:LYS:HB3	2:f:451:LYS:HE2	1.90	0.41
2:f:457:PRO:O	2:f:461:GLN:HG3	2.21	0.41
44:f:813:CLA:HBA1	44:f:813:CLA:H3A	1.79	0.41
5:i:120:VAL:HG12	5:i:137:TYR:O	2.21	0.41
6:j:120:GLN:HA	6:j:123:ILE:HD12	2.02	0.41
10:n:52:THR:O	10:n:56:MET:HG2	2.21	0.41
10:n:68:ARG:HA	10:n:100:PHE:CZ	2.56	0.41
11:o:165:LYS:HA	11:o:165:LYS:HD2	1.82	0.41
11:o:166:LYS:NZ	11:o:167:GLU:HB3	2.36	0.41
12:p:161:PRO:HG2	44:p:504:CLA:OBD	2.21	0.41
46:p:516:LHG:HC82	46:p:516:LHG:H111	1.79	0.41
14:q:72:PRO:HB3	14:q:221:LYS:NZ	2.35	0.41
14:q:159:PHE:HB2	44:s:511:CLA:HAA2	2.03	0.41
14:q:180:SER:OG	42:s:71:GLY:HA2	2.21	0.41
47:s:503:BCR:H23C	47:s:503:BCR:H382	2.03	0.41
1:A:479:ILE:O	1:A:483:TRP:N	2.48	0.41
3:C:3:HIS:ND1	3:C:69:LEU:HA	2.36	0.41
12:1:121:TYR:CE1	44:1:509:CLA:H2	2.56	0.41
16:G:195:GLU:HA	31:a:96:ARG:HH11	1.85	0.41
21:Q:428:GLY:C	21:Q:429:LEU:HD12	2.46	0.41
23:S:225:ARG:NH2	23:S:267:GLU:OE2	2.53	0.41
33:c:155:TYR:CZ	33:c:159:LYS:HG3	2.56	0.41
36:6:192:LYS:HE2	36:6:192:LYS:HB2	1.88	0.41
36:6:416:SER:O	36:6:418:GLU:N	2.54	0.41
37:7:103:GLY:H	37:7:107:GLY:HA2	1.86	0.41
47:e:851:BCR:H403	9:m:16:THR:HG21	2.01	0.41
2:f:104:PHE:O	2:f:106:ARG:HG2	2.21	0.41
2:f:279:ALA:HA	44:f:818:CLA:HMC2	2.02	0.41
5:i:94:LEU:HD22	5:i:141:GLU:HA	2.02	0.41
5:i:116:THR:HG22	5:i:117:ARG:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:p:192:MET:CB	51:p:502:LUT:H202	2.51	0.41
41:r:99:VAL:HG21	51:r:302:LUT:H10	2.03	0.41
53:s:502:XAT:H15	53:s:502:XAT:H201	1.61	0.41
44:A:836:CLA:C1A	44:A:836:CLA:CGA	2.99	0.40
2:B:51:PHE:HB2	2:B:153:SER:HB3	2.03	0.40
44:B:811:CLA:HAC2	47:I:101:BCR:H373	2.03	0.40
10:K:124:LYS:HE3	44:K:202:CLA:HMA3	2.03	0.40
51:1:502:LUT:H12	44:1:507:CLA:CBB	2.50	0.40
13:2:238:GLN:OE1	51:2:501:LUT:H24	2.22	0.40
21:Q:306:ILE:HG13	21:Q:307:HIS:ND1	2.37	0.40
22:R:8:HIS:CD2	22:R:52:LEU:HD11	2.56	0.40
23:S:129:THR:N	23:S:130:PRO:HD3	2.36	0.40
24:T:114:CYS:SG	24:T:118:CYS:HB3	2.61	0.40
26:V:25:GLU:HG3	28:X:185:LYS:CB	2.50	0.40
31:a:189:ILE:HG12	31:a:198:THR:HG22	2.03	0.40
36:6:228:ASN:HA	36:6:232:ALA:HB2	2.03	0.40
37:7:201:LYS:C	37:7:203:ARG:H	2.29	0.40
1:e:492:PRO:HG2	1:e:502:SER:HA	2.03	0.40
47:e:849:BCR:H11C	47:e:849:BCR:H341	1.93	0.40
3:g:19:ARG:NH2	4:h:170:GLU:OE2	2.55	0.40
3:g:46:GLU:H	3:g:46:GLU:CD	2.27	0.40
4:h:97:ILE:HD13	4:h:135:LEU:HD22	2.04	0.40
47:n:204:BCR:H11C	47:n:204:BCR:H341	1.82	0.40
12:p:145:ALA:HB1	12:p:149:ARG:NE	2.36	0.40
12:p:169:GLY:C	12:p:171:SER:N	2.78	0.40
12:p:226:ILE:HG12	44:p:506:CLA:CBD	2.51	0.40
44:p:505:CLA:HMA2	44:p:505:CLA:HBA1	2.03	0.40
41:r:64:ALA:O	44:r:307:CLA:HED1	2.21	0.40
41:r:198:LEU:HD23	41:r:198:LEU:HA	1.92	0.40
1:A:433:ALA:O	1:A:437:HIS:ND1	2.40	0.40
44:A:806:CLA:H193	44:A:806:CLA:HED2	2.02	0.40
44:A:806:CLA:H203	44:A:806:CLA:H162	1.71	0.40
44:A:831:CLA:H12	44:A:831:CLA:H52	1.97	0.40
4:D:139:LEU:HB3	4:D:145:ILE:CG2	2.52	0.40
6:F:189:LYS:HG3	6:F:190:LYS:N	2.36	0.40
8:I:19:ILE:HA	8:I:22:THR:HG22	2.03	0.40
9:J:8:LEU:HD23	9:J:8:LEU:HA	1.93	0.40
49:J:103:DGD:HAG2	49:J:103:DGD:HAN1	1.76	0.40
13:2:238:GLN:O	13:2:242:THR:OG1	2.26	0.40
51:5:303:LUT:H401	51:5:303:LUT:H35	1.61	0.40
17:M:332:ILE:C	17:M:334:TYR:H	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:348:LEU:HD13	19:O:378:PHE:HA	2.03	0.40
21:Q:152:TYR:CD1	21:Q:400:LEU:HD22	2.56	0.40
21:Q:305:LEU:HD12	21:Q:305:LEU:HA	1.93	0.40
23:S:269:SER:O	23:S:273:LYS:HG2	2.20	0.40
25:U:10:LEU:HA	25:U:13:HIS:CD2	2.53	0.40
29:Y:219:LEU:O	29:Y:223:SER:N	2.53	0.40
32:b:149:SER:O	32:b:153:ASP:N	2.54	0.40
33:c:135:PHE:HE1	39:9:84:ASN:HB3	1.85	0.40
36:6:172:TYR:CD2	36:6:173:ASP:HB3	2.56	0.40
36:6:319:MET:HE2	36:6:319:MET:HB2	2.01	0.40
37:7:215:TYR:HA	37:7:273:TYR:HA	2.02	0.40
1:e:46:ILE:HD12	44:e:853:CLA:HBD	2.02	0.40
1:e:297:ALA:HB1	44:e:816:CLA:HBC2	2.03	0.40
1:e:690:GLY:O	1:e:694:GLU:HG3	2.22	0.40
44:e:833:CLA:H2A	44:e:833:CLA:HED3	2.03	0.40
2:f:649:MET:O	2:f:652:PHE:HB3	2.21	0.40
3:g:24:ASP:HB2	4:h:133:LEU:HD22	2.03	0.40
6:j:127:LYS:O	6:j:131:GLU:HG2	2.21	0.40
6:j:153:ASP:HB2	44:j:802:CLA:HMD3	2.04	0.40
47:o:301:BCR:H24C	47:o:301:BCR:H371	1.88	0.40
14:q:223:LEU:HD12	14:q:223:LEU:HA	1.76	0.40
41:r:153:ILE:HD13	41:r:153:ILE:HA	1.93	0.40
1:A:462:LEU:HD22	2:B:96:PHE:HA	2.03	0.40
44:A:804:CLA:H62	44:A:804:CLA:H2	1.80	0.40
44:A:831:CLA:H192	47:L:305:BCR:H10C	2.02	0.40
47:A:845:BCR:H351	47:A:845:BCR:H15C	1.72	0.40
2:B:408:LEU:HD12	2:B:408:LEU:HA	1.81	0.40
3:C:10:THR:HB	3:C:64:SER:OG	2.21	0.40
6:F:209:ARG:NH1	50:F:806:LMG:O5	2.55	0.40
13:2:151:THR:O	13:2:155:VAL:HG23	2.21	0.40
51:5:303:LUT:H183	44:5:307:CLA:C3B	2.51	0.40
16:G:261:LEU:O	16:G:265:VAL:HG13	2.22	0.40
21:Q:364:SER:HB2	21:Q:487:TYR:HE1	1.85	0.40
29:Y:99:SER:HA	29:Y:154:TYR:HB3	2.02	0.40
36:6:319:MET:C	36:6:321:SER:H	2.29	0.40
37:7:78:LEU:HD21	37:7:110:ARG:HG3	2.03	0.40
37:7:158:SER:OG	37:7:159:LYS:N	2.54	0.40
1:e:374:TYR:HB2	1:e:377:LEU:HD22	2.02	0.40
1:e:502:SER:HB3	1:e:507:TRP:CD1	2.55	0.40
1:e:522:LEU:HD23	1:e:616:VAL:HG13	2.02	0.40
2:f:31:PHE:CD2	44:f:807:CLA:HMC2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:g:73:THR:HG22	3:g:74:THR:N	2.33	0.40
9:m:35:ASP:O	9:m:37:LEU:N	2.54	0.40
14:q:164:ILE:HG21	44:q:314:CLA:HMC2	2.03	0.40
41:r:222:PRO:HA	41:r:225:ASN:ND2	2.37	0.40
1:A:115:VAL:HG22	1:A:125:ASN:OD1	2.21	0.40
2:B:472:TYR:OH	2:B:512:ILE:O	2.39	0.40
44:B:804:CLA:CGA	44:B:804:CLA:H3A	2.44	0.40
4:D:139:LEU:O	4:D:145:ILE:HG22	2.20	0.40
11:L:84:TYR:O	11:L:86:THR:HG23	2.22	0.40
11:L:90:PRO:HA	11:L:93:ARG:HG3	2.03	0.40
11:L:136:LEU:HA	11:L:136:LEU:HD23	1.88	0.40
47:L:305:BCR:H11C	47:L:305:BCR:H341	1.74	0.40
12:1:226:ILE:HG21	44:1:506:CLA:H42	2.04	0.40
14:3:74:ASP:OD1	14:3:75:PHE:N	2.53	0.40
14:3:206:ILE:HG23	14:3:207:PHE:CD1	2.57	0.40
15:5:201:LYS:O	15:5:205:ILE:HG12	2.21	0.40
17:M:244:LEU:HD12	17:M:246:PRO:HD3	2.03	0.40
17:M:502:LEU:HD23	17:M:502:LEU:HA	1.88	0.40
19:O:76:PHE:HE1	19:O:136:LEU:HB2	1.87	0.40
23:S:74:ALA:HB1	23:S:77:PHE:CD2	2.56	0.40
23:S:128:GLN:HG2	23:S:129:THR:N	2.37	0.40
25:U:45:TYR:HA	25:U:49:TYR:H	1.87	0.40
37:7:70:LEU:HD23	37:7:168:LEU:HD22	2.03	0.40
37:7:109:VAL:HB	37:7:232:GLU:OE1	2.21	0.40
37:7:311:GLU:N	37:7:336:ALA:O	2.35	0.40
39:9:144:GLY:O	39:9:148:TRP:N	2.54	0.40
1:e:298:ILE:HD11	44:e:817:CLA:C3C	2.52	0.40
1:e:514:ALA:HB2	1:e:519:VAL:HG12	2.04	0.40
1:e:541:ILE:HG21	44:e:838:CLA:HED1	2.03	0.40
1:e:608:PHE:O	1:e:612:MET:HG2	2.21	0.40
2:f:183:PHE:HB3	2:f:284:PHE:CD2	2.56	0.40
3:g:22:PRO:O	4:h:133:LEU:HD23	2.22	0.40
6:j:157:TRP:C	6:j:159:GLU:H	2.30	0.40
14:q:95:ARG:HH12	14:q:99:TYR:HD1	1.67	0.40
14:q:100:GLY:HA2	44:q:314:CLA:HED3	2.03	0.40
41:r:135:PHE:HB2	52:r:313:CHL:HBC1	2.03	0.40
51:r:302:LUT:C14	44:r:305:CLA:HBB1	2.52	0.40
44:r:307:CLA:H3A	44:r:307:CLA:CGA	2.51	0.40
42:s:61:LEU:HD11	42:s:74:PRO:HG2	2.03	0.40
42:s:121:ILE:HG13	53:s:502:XAT:H163	2.02	0.40
44:s:505:CLA:O2A	44:s:505:CLA:H2A	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:B:807:CLA:H152	44:B:807:CLA:H111	1.90	0.40
44:1:506:CLA:H41	44:1:506:CLA:H62	1.83	0.40
13:2:87:PHE:CE2	53:2:502:XAT:H383	2.56	0.40
13:2:120:ILE:HG23	13:2:137:TRP:CD1	2.56	0.40
14:3:133:ILE:HG22	14:3:134:PRO:O	2.22	0.40
14:3:172:LEU:HD12	44:3:316:CLA:HMA2	2.02	0.40
17:M:324:LEU:HD23	17:M:324:LEU:HA	1.88	0.40
19:O:261:LEU:O	19:O:265:ASN:HB2	2.20	0.40
21:Q:149:VAL:HG11	21:Q:305:LEU:HD22	2.03	0.40
23:S:337:LEU:HA	23:S:355:ARG:O	2.22	0.40
23:S:361:ASN:O	23:S:364:ILE:HG22	2.21	0.40
27:W:96:ILE:O	27:W:99:PRO:HD2	2.22	0.40
27:W:97:LEU:HB3	27:W:98:PRO:HD3	2.04	0.40
27:W:119:MET:HE2	27:W:119:MET:HA	2.03	0.40
29:Y:73:TYR:HB3	29:Y:210:ASN:HB3	2.04	0.40
30:Z:95:UNK:O	30:Z:96:UNK:C	2.68	0.40
31:a:117:VAL:HA	31:a:200:ILE:O	2.22	0.40
31:a:173:GLU:HB2	31:a:186:PHE:CE1	2.57	0.40
32:b:132:MET:HE1	32:b:140:TYR:CD2	2.57	0.40
37:7:207:VAL:HG13	37:7:293:THR:O	2.21	0.40
39:9:113:THR:HG22	40:0:141:MET:HE1	2.03	0.40
1:e:45:TRP:HE3	1:e:46:ILE:HG22	1.86	0.40
1:e:46:ILE:O	1:e:50:HIS:ND1	2.54	0.40
1:e:63:LEU:HD23	1:e:63:LEU:H	1.85	0.40
1:e:459:MET:CE	1:e:464:ARG:HH21	2.34	0.40
2:f:262:HIS:CE1	2:f:264:GLN:HB3	2.56	0.40
2:f:310:PRO:HA	2:f:311:PRO:HD3	1.98	0.40
2:f:407:VAL:O	2:f:411:MET:HG2	2.22	0.40
2:f:623:TYR:O	2:f:627:ASN:HB2	2.22	0.40
11:o:164:ARG:HH21	11:o:166:LYS:HA	1.87	0.40
12:p:165:PHE:CE2	44:p:513:CLA:HBA2	2.57	0.40
41:r:63:LEU:HD12	41:r:63:LEU:H	1.85	0.40
41:r:147:ILE:HD12	41:r:147:ILE:HA	1.97	0.40
42:s:68:TRP:CD2	42:s:88:PHE:HD1	2.40	0.40
42:s:239:GLN:HG2	44:s:506:CLA:C4D	2.52	0.40
44:s:511:CLA:H3A	44:s:511:CLA:HBA2	1.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/750 (99%)	690 (93%)	50 (7%)	0	100	100
1	e	740/750 (99%)	684 (92%)	56 (8%)	0	100	100
2	B	731/734 (100%)	688 (94%)	42 (6%)	1 (0%)	48	83
2	f	731/734 (100%)	680 (93%)	51 (7%)	0	100	100
3	C	79/81 (98%)	70 (89%)	9 (11%)	0	100	100
3	g	79/81 (98%)	68 (86%)	11 (14%)	0	100	100
4	D	140/205 (68%)	118 (84%)	22 (16%)	0	100	100
4	h	140/205 (68%)	125 (89%)	15 (11%)	0	100	100
5	E	66/147 (45%)	61 (92%)	5 (8%)	0	100	100
5	i	66/147 (45%)	61 (92%)	5 (8%)	0	100	100
6	F	156/235 (66%)	150 (96%)	6 (4%)	0	100	100
6	j	156/235 (66%)	148 (95%)	8 (5%)	0	100	100
7	H	59/143 (41%)	58 (98%)	1 (2%)	0	100	100
7	k	59/143 (41%)	56 (95%)	3 (5%)	0	100	100
8	I	28/36 (78%)	28 (100%)	0	0	100	100
8	l	28/36 (78%)	28 (100%)	0	0	100	100
9	J	40/42 (95%)	37 (92%)	2 (5%)	1 (2%)	4	26
9	m	40/42 (95%)	38 (95%)	1 (2%)	1 (2%)	4	26
10	K	82/131 (63%)	73 (89%)	9 (11%)	0	100	100
10	n	82/131 (63%)	75 (92%)	7 (8%)	0	100	100
11	L	144/209 (69%)	135 (94%)	9 (6%)	0	100	100
11	o	144/209 (69%)	134 (93%)	10 (7%)	0	100	100
12	1	189/247 (76%)	179 (95%)	10 (5%)	0	100	100
12	p	191/247 (77%)	171 (90%)	18 (9%)	2 (1%)	12	47
13	2	201/255 (79%)	185 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	3	220/269 (82%)	195 (89%)	25 (11%)	0	100	100
14	q	220/269 (82%)	193 (88%)	27 (12%)	0	100	100
15	5	203/257 (79%)	173 (85%)	30 (15%)	0	100	100
16	G	344/346 (99%)	303 (88%)	40 (12%)	1 (0%)	36	71
17	M	474/483 (98%)	424 (90%)	50 (10%)	0	100	100
18	N	114/117 (97%)	96 (84%)	17 (15%)	1 (1%)	14	49
19	O	497/499 (100%)	447 (90%)	48 (10%)	2 (0%)	30	67
20	P	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
21	Q	665/777 (86%)	598 (90%)	64 (10%)	3 (0%)	24	63
22	R	174/176 (99%)	148 (85%)	26 (15%)	0	100	100
23	S	381/383 (100%)	339 (89%)	42 (11%)	0	100	100
24	T	163/165 (99%)	123 (76%)	40 (24%)	0	100	100
25	U	157/159 (99%)	141 (90%)	16 (10%)	0	100	100
26	V	192/245 (78%)	174 (91%)	17 (9%)	1 (0%)	24	63
27	W	67/192 (35%)	59 (88%)	7 (10%)	1 (2%)	8	38
28	X	110/213 (52%)	92 (84%)	18 (16%)	0	100	100
29	Y	136/233 (58%)	114 (84%)	20 (15%)	2 (2%)	8	38
31	a	148/154 (96%)	112 (76%)	35 (24%)	1 (1%)	18	55
32	b	127/216 (59%)	106 (84%)	21 (16%)	0	100	100
33	c	132/227 (58%)	116 (88%)	16 (12%)	0	100	100
34	4	128/130 (98%)	102 (80%)	26 (20%)	0	100	100
35	d	170/243 (70%)	156 (92%)	13 (8%)	1 (1%)	21	58
36	6	341/469 (73%)	249 (73%)	90 (26%)	2 (1%)	21	58
37	7	315/361 (87%)	226 (72%)	88 (28%)	1 (0%)	36	71
38	8	117/119 (98%)	79 (68%)	34 (29%)	4 (3%)	3	21
39	9	80/83 (96%)	65 (81%)	14 (18%)	1 (1%)	9	41
40	0	147/155 (95%)	98 (67%)	48 (33%)	1 (1%)	18	55
41	r	195/197 (99%)	183 (94%)	12 (6%)	0	100	100
42	s	209/211 (99%)	190 (91%)	17 (8%)	2 (1%)	12	47
All	All	11435/13623 (84%)	10134 (89%)	1272 (11%)	29 (0%)	37	71

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	G	84	LYS
19	O	480	ASP
36	6	275	PRO
42	s	191	THR
42	s	192	PRO
21	Q	123	PHE
21	Q	707	TYR
39	9	149	TYR
2	B	223	GLY
19	O	498	TYR
31	a	96	ARG
9	m	36	ALA
12	p	101	GLY
26	V	63	CYS
38	8	90	THR
38	8	124	LEU
40	0	213	THR
9	J	36	ALA
35	d	87	PRO
37	7	289	PRO
18	N	46	SER
36	6	267	PRO
38	8	122	LEU
27	W	150	PRO
21	Q	263	ILE
29	Y	125	PRO
38	8	91	PRO
29	Y	126	VAL
12	p	221	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	592/608 (97%)	585 (99%)	7 (1%)	63 73
1	e	588/608 (97%)	587 (100%)	1 (0%)	87 85
2	B	595/601 (99%)	590 (99%)	5 (1%)	73 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	f	589/601 (98%)	588 (100%)	1 (0%)	87 85
3	C	70/71 (99%)	69 (99%)	1 (1%)	59 71
3	g	71/71 (100%)	71 (100%)	0	100 100
4	D	119/160 (74%)	118 (99%)	1 (1%)	73 77
4	h	118/160 (74%)	118 (100%)	0	100 100
5	E	58/112 (52%)	58 (100%)	0	100 100
5	i	58/112 (52%)	58 (100%)	0	100 100
6	F	121/183 (66%)	121 (100%)	0	100 100
6	j	115/183 (63%)	115 (100%)	0	100 100
7	H	48/110 (44%)	48 (100%)	0	100 100
7	k	47/110 (43%)	47 (100%)	0	100 100
8	I	26/33 (79%)	26 (100%)	0	100 100
8	l	27/33 (82%)	27 (100%)	0	100 100
9	J	35/36 (97%)	35 (100%)	0	100 100
9	m	34/36 (94%)	34 (100%)	0	100 100
10	K	52/102 (51%)	51 (98%)	1 (2%)	50 66
10	n	56/102 (55%)	55 (98%)	1 (2%)	51 67
11	L	112/166 (68%)	110 (98%)	2 (2%)	51 67
11	o	110/166 (66%)	110 (100%)	0	100 100
12	1	134/196 (68%)	134 (100%)	0	100 100
12	p	147/196 (75%)	147 (100%)	0	100 100
13	2	155/194 (80%)	154 (99%)	1 (1%)	78 80
14	3	148/216 (68%)	147 (99%)	1 (1%)	76 79
14	q	159/216 (74%)	158 (99%)	1 (1%)	78 80
15	5	139/202 (69%)	139 (100%)	0	100 100
16	G	270/301 (90%)	270 (100%)	0	100 100
17	M	397/419 (95%)	397 (100%)	0	100 100
18	N	71/100 (71%)	71 (100%)	0	100 100
19	O	399/427 (93%)	399 (100%)	0	100 100
20	P	78/88 (89%)	78 (100%)	0	100 100
21	Q	495/674 (73%)	494 (100%)	1 (0%)	87 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	R	119/154 (77%)	119 (100%)	0	100 100
23	S	298/336 (89%)	297 (100%)	1 (0%)	86 84
24	T	123/155 (79%)	123 (100%)	0	100 100
25	U	126/141 (89%)	126 (100%)	0	100 100
26	V	162/226 (72%)	162 (100%)	0	100 100
27	W	55/167 (33%)	55 (100%)	0	100 100
28	X	86/184 (47%)	86 (100%)	0	100 100
29	Y	115/192 (60%)	115 (100%)	0	100 100
31	a	116/132 (88%)	116 (100%)	0	100 100
32	b	74/181 (41%)	74 (100%)	0	100 100
33	c	92/183 (50%)	92 (100%)	0	100 100
34	4	80/102 (78%)	80 (100%)	0	100 100
35	d	135/191 (71%)	135 (100%)	0	100 100
36	6	250/389 (64%)	250 (100%)	0	100 100
37	7	232/279 (83%)	232 (100%)	0	100 100
38	8	69/102 (68%)	69 (100%)	0	100 100
39	9	55/70 (79%)	54 (98%)	1 (2%)	51 67
40	0	93/137 (68%)	93 (100%)	0	100 100
41	r	156/164 (95%)	156 (100%)	0	100 100
42	s	151/172 (88%)	151 (100%)	0	100 100
All	All	8820/11250 (78%)	8794 (100%)	26 (0%)	84 84

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	570	ARG
1	A	578	ARG
1	A	590	VAL
1	A	594	LEU
1	A	639	ILE
1	A	708	VAL
1	A	720	ILE
2	B	165	LEU
2	B	224	PRO
2	B	225	LEU

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Mol	Chain	Res	Type
2	B	437	TYR
2	B	492	LEU
3	C	47	ASP
4	D	97	ILE
10	K	104	ASP
11	L	88	VAL
11	L	93	ARG
13	2	262	ILE
14	3	193	LEU
21	Q	123	PHE
23	S	362	LEU
39	9	106	TYR
1	e	675	HIS
2	f	327	ASN
10	n	123	LEU
14	q	223	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	HIS
1	A	317	HIS
2	B	193	HIS
2	B	196	HIS
2	B	235	GLN
2	B	308	HIS
2	B	627	ASN
2	B	630	GLN
2	B	633	ASN
4	D	68	GLN
4	D	177	GLN
4	D	182	ASN
9	J	30	ASN
11	L	121	HIS
14	3	266	ASN
15	5	244	ASN
16	G	73	GLN
16	G	120	HIS
16	G	197	GLN
16	G	262	ASN
16	G	294	ASN
16	G	358	GLN

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Mol	Chain	Res	Type
17	M	92	GLN
17	M	147	ASN
17	M	317	GLN
17	M	362	ASN
19	O	26	HIS
19	O	29	ASN
19	O	265	ASN
21	Q	174	ASN
21	Q	391	HIS
21	Q	465	ASN
21	Q	503	HIS
21	Q	646	ASN
21	Q	679	ASN
22	R	71	ASN
23	S	14	ASN
23	S	19	HIS
23	S	48	HIS
23	S	367	GLN
24	T	14	GLN
25	U	13	HIS
25	U	50	ASN
25	U	95	ASN
26	V	91	GLN
28	X	145	ASN
28	X	148	GLN
28	X	194	ASN
29	Y	143	HIS
29	Y	182	GLN
31	a	113	GLN
31	a	141	ASN
35	d	138	GLN
35	d	206	GLN
36	6	381	GLN
37	7	252	GLN
37	7	297	GLN
38	8	184	GLN
39	9	147	HIS
40	0	97	HIS
1	e	317	HIS
1	e	367	HIS
1	e	448	HIS
1	e	535	HIS

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Mol	Chain	Res	Type
1	e	537	HIS
1	e	642	ASN
1	e	693	GLN
2	f	44	GLN
2	f	53	GLN
2	f	132	ASN
2	f	156	HIS
2	f	220	GLN
2	f	235	GLN
2	f	248	GLN
2	f	299	HIS
2	f	368	GLN
2	f	432	HIS
2	f	585	ASN
2	f	598	HIS
2	f	627	ASN
2	f	630	GLN
4	h	68	GLN
4	h	148	GLN
4	h	181	GLN
4	h	201	ASN
5	i	135	ASN
8	l	29	GLN
9	m	30	ASN
11	o	80	ASN
12	p	72	ASN
12	p	187	ASN
14	q	173	GLN
14	q	208	ASN
14	q	255	ASN
14	q	265	ASN
41	r	67	ASN
41	r	151	GLN
41	r	225	ASN
42	s	225	ASN
42	s	250	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

400 ligands 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	$\#\|Z\| > 2$
44	CLA	3	311	-	54,58,73	1.24	7 (12%)	64,95,113	1.57	8 (12%)
50	LMG	2	518	-	16,16,55	0.48	0	22,22,63	0.99	2 (9%)
51	LUT	1	502	-	42,43,43	0.92	2 (4%)	51,60,60	1.81	12 (23%)
44	CLA	e	821	-	46,50,73	1.38	9 (19%)	53,85,113	1.44	5 (9%)
44	CLA	A	825	-	63,67,73	1.25	9 (14%)	74,105,113	1.34	5 (6%)
44	CLA	A	840	-	45,49,73	1.44	10 (22%)	54,84,113	1.51	5 (9%)
44	CLA	A	802	-	62,66,73	1.25	9 (14%)	73,104,113	1.35	5 (6%)
44	CLA	f	818	-	59,63,73	1.24	9 (15%)	70,101,113	1.32	4 (5%)
52	CHL	p	517	-	37,51,74	4.34	18 (48%)	30,86,114	2.50	9 (30%)
44	CLA	f	822	-	45,49,73	1.41	9 (20%)	54,84,113	1.46	5 (9%)
44	CLA	B	818	-	63,67,73	1.19	7 (11%)	74,105,113	1.45	8 (10%)
44	CLA	f	806	-	45,49,73	1.40	9 (20%)	54,84,113	1.43	5 (9%)
48	SF4	C	101	3	0,12,12	-	-	-		
44	CLA	r	308	-	45,49,73	1.41	9 (20%)	54,84,113	1.50	5 (9%)
44	CLA	B	806	-	42,47,73	1.46	9 (21%)	50,80,113	1.56	7 (14%)
52	CHL	r	314	-	45,59,74	3.83	19 (42%)	40,96,114	2.49	15 (37%)
47	BCR	A	846	-	41,41,41	0.99	1 (2%)	56,56,56	2.07	18 (32%)
44	CLA	1	507	12	60,64,73	1.21	8 (13%)	71,102,113	1.42	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	CLA	5	313	15	44,48,73	1.38	7 (15%)	51,82,113	1.53	5 (9%)
47	BCR	A	849	-	40,40,41	1.05	2 (5%)	54,54,56	1.88	13 (24%)
44	CLA	e	839	-	69,73,73	1.17	8 (11%)	82,113,113	1.30	6 (7%)
44	CLA	q	305	-	56,60,73	1.31	7 (12%)	65,97,113	1.34	7 (10%)
51	LUT	3	304	-	42,43,43	0.90	2 (4%)	51,60,60	1.65	10 (19%)
44	CLA	r	315	41	45,49,73	1.41	8 (17%)	54,84,113	1.52	6 (11%)
46	LHG	B	851	-	37,37,48	1.09	2 (5%)	40,43,54	1.19	4 (10%)
52	CHL	5	317	-	34,48,74	3.89	18 (52%)	32,82,114	2.84	13 (40%)
44	CLA	B	820	-	57,61,73	1.30	9 (15%)	67,98,113	1.35	6 (8%)
51	LUT	5	303	-	42,43,43	0.92	2 (4%)	51,60,60	2.12	14 (27%)
44	CLA	f	803	-	43,49,73	1.36	8 (18%)	48,83,113	1.36	4 (8%)
44	CLA	e	832	-	47,51,73	1.38	8 (17%)	55,86,113	1.38	5 (9%)
44	CLA	r	311	-	50,54,73	1.36	8 (16%)	59,90,113	1.35	4 (6%)
48	SF4	A	850	1,2	0,12,12	-	-	-		
44	CLA	B	827	-	45,49,73	1.38	10 (22%)	54,84,113	1.64	10 (18%)
44	CLA	B	826	-	66,70,73	1.17	7 (10%)	78,109,113	1.36	8 (10%)
45	PQN	f	844	-	17,17,34	2.17	2 (11%)	22,24,45	1.34	4 (18%)
44	CLA	J	101	9	46,50,73	1.37	8 (17%)	53,85,113	1.49	4 (7%)
44	CLA	1	504	-	45,49,73	1.40	9 (20%)	52,84,113	1.42	5 (9%)
44	CLA	B	821	-	54,58,73	1.34	8 (14%)	64,95,113	1.49	5 (7%)
44	CLA	1	509	-	54,58,73	1.30	7 (12%)	64,95,113	1.43	7 (10%)
47	BCR	A	847	-	41,41,41	0.94	2 (4%)	56,56,56	2.01	20 (35%)
44	CLA	A	834	1	45,49,73	1.41	9 (20%)	54,84,113	1.47	7 (12%)
44	CLA	e	804	-	69,73,73	1.15	9 (13%)	82,113,113	1.30	6 (7%)
44	CLA	A	839	-	46,50,73	1.39	8 (17%)	53,85,113	1.57	5 (9%)
52	CHL	q	313	-	38,54,74	4.11	17 (44%)	31,89,114	1.95	9 (29%)
44	CLA	e	825	-	45,49,73	1.38	9 (20%)	54,84,113	1.49	7 (12%)
44	CLA	e	840	-	45,49,73	1.39	9 (20%)	54,84,113	1.51	5 (9%)
51	LUT	p	501	-	42,43,43	0.80	0	51,60,60	2.00	13 (25%)
44	CLA	5	307	15	69,73,73	1.16	8 (11%)	82,113,113	1.25	5 (6%)
44	CLA	e	802	-	44,48,73	1.42	9 (20%)	51,82,113	1.49	5 (9%)
44	CLA	e	805	-	50,54,73	1.34	9 (18%)	59,90,113	1.43	4 (6%)
44	CLA	e	822	-	45,49,73	1.39	9 (20%)	54,84,113	1.54	5 (9%)
44	CLA	f	814	-	47,51,73	1.37	9 (19%)	55,86,113	1.43	4 (7%)
44	CLA	f	842	-	45,49,73	1.40	9 (20%)	54,84,113	1.52	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	CLA	K	201	-	41,45,73	1.43	10 (24%)	50,78,113	1.51	6 (12%)
47	BCR	m	103	-	41,41,41	0.76	1 (2%)	56,56,56	2.11	17 (30%)
47	BCR	f	846	-	41,41,41	0.74	0	56,56,56	1.95	14 (25%)
51	LUT	q	302	-	42,43,43	0.71	0	51,60,60	2.02	17 (33%)
44	CLA	e	836	-	55,59,73	1.30	9 (16%)	64,96,113	1.37	6 (9%)
44	CLA	3	307	-	44,48,73	1.51	9 (20%)	51,82,113	1.39	4 (7%)
47	BCR	B	846	-	41,41,41	1.01	2 (4%)	56,56,56	2.29	18 (32%)
46	LHG	A	843	-	48,48,48	0.90	3 (6%)	51,54,54	1.30	5 (9%)
44	CLA	p	505	-	50,54,73	1.32	8 (16%)	59,90,113	1.29	8 (13%)
44	CLA	B	803	-	69,73,73	1.19	7 (10%)	82,113,113	1.30	7 (8%)
46	LHG	p	516	-	48,48,48	0.93	2 (4%)	51,54,54	1.09	4 (7%)
47	BCR	J	102	-	41,41,41	0.98	2 (4%)	56,56,56	2.19	21 (37%)
44	CLA	B	811	-	59,63,73	1.29	9 (15%)	70,101,113	1.39	6 (8%)
44	CLA	B	812	-	58,62,73	1.37	10 (17%)	71,100,113	1.43	8 (11%)
44	CLA	e	823	-	46,50,73	1.47	10 (21%)	56,85,113	1.51	8 (14%)
47	BCR	B	849	-	41,41,41	1.06	2 (4%)	56,56,56	2.01	16 (28%)
44	CLA	e	837	-	59,63,73	1.23	9 (15%)	70,101,113	1.41	8 (11%)
44	CLA	e	810	44	59,63,73	1.27	9 (15%)	70,101,113	1.34	5 (7%)
44	CLA	s	507	-	45,49,73	1.41	8 (17%)	54,84,113	1.46	6 (11%)
44	CLA	f	804	-	42,50,73	1.85	8 (19%)	50,83,113	2.14	8 (16%)
44	CLA	1	511	-	50,54,73	1.36	9 (18%)	59,90,113	1.46	5 (8%)
44	CLA	f	809	-	56,60,73	1.28	9 (16%)	65,97,113	1.35	5 (7%)
44	CLA	f	840	-	45,49,73	1.38	9 (20%)	54,84,113	1.52	7 (12%)
53	XAT	r	303	-	41,47,47	0.87	2 (4%)	54,74,74	2.65	20 (37%)
46	LHG	1	516	44	48,48,48	0.91	2 (4%)	51,54,54	1.18	5 (9%)
44	CLA	B	808	-	56,60,73	1.31	9 (16%)	65,97,113	1.48	7 (10%)
44	CLA	3	308	-	59,63,73	1.18	8 (13%)	70,101,113	1.44	7 (10%)
44	CLA	5	311	-	46,50,73	1.32	8 (17%)	53,85,113	1.56	5 (9%)
44	CLA	f	841	-	45,49,73	1.38	9 (20%)	54,84,113	1.51	5 (9%)
44	CLA	A	824	-	44,48,73	1.39	7 (15%)	51,82,113	1.52	5 (9%)
44	CLA	B	842	-	61,65,73	1.22	10 (16%)	72,103,113	1.34	4 (5%)
44	CLA	s	510	-	64,68,73	1.21	8 (12%)	76,107,113	1.25	5 (6%)
44	CLA	5	310	-	54,58,73	1.29	8 (14%)	64,95,113	1.41	7 (10%)
44	CLA	2	505	-	56,60,73	1.21	9 (16%)	65,97,113	1.45	6 (9%)
47	BCR	e	851	-	41,41,41	0.69	0	56,56,56	2.17	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	CLA	f	827	-	44,48,73	1.41	9 (20%)	50,82,113	1.48	6 (12%)
44	CLA	e	816	-	64,68,73	1.22	9 (14%)	76,107,113	1.30	4 (5%)
44	CLA	B	830	-	60,64,73	1.32	11 (18%)	71,102,113	1.34	5 (7%)
44	CLA	2	508	-	51,55,73	1.38	8 (15%)	60,91,113	1.32	4 (6%)
52	CHL	2	515	-	40,53,74	4.06	18 (45%)	35,89,114	2.69	13 (37%)
47	BCR	j	801	-	41,41,41	0.72	0	56,56,56	2.25	20 (35%)
52	CHL	r	313	-	41,55,74	4.21	19 (46%)	35,91,114	2.24	10 (28%)
44	CLA	A	832	-	47,53,73	1.37	7 (14%)	59,88,113	1.59	5 (8%)
50	LMG	2	519	-	36,36,55	1.10	2 (5%)	44,44,63	1.38	8 (18%)
44	CLA	e	831	-	60,64,73	1.22	9 (15%)	71,102,113	1.32	7 (9%)
52	CHL	s	512	-	41,55,74	4.25	19 (46%)	35,91,114	2.31	10 (28%)
52	CHL	2	516	13	38,51,74	4.01	17 (44%)	32,86,114	2.73	11 (34%)
44	CLA	e	835	1	44,50,73	1.43	9 (20%)	56,85,113	1.36	5 (8%)
44	CLA	3	306	-	56,60,73	1.32	7 (12%)	69,97,113	1.60	7 (10%)
45	PQN	A	841	-	34,34,34	1.41	2 (5%)	43,45,45	1.26	5 (11%)
44	CLA	e	833	-	45,49,73	1.39	8 (17%)	54,84,113	1.47	6 (11%)
48	SF4	g	102	-	0,12,12	-	-	-		
44	CLA	A	820	-	61,65,73	1.21	6 (9%)	72,103,113	1.51	10 (13%)
47	BCR	2	503	-	41,41,41	0.92	1 (2%)	56,56,56	3.71	27 (48%)
47	BCR	5	302	-	41,41,41	0.86	1 (2%)	56,56,56	1.95	12 (21%)
44	CLA	3	312	-	45,49,73	1.41	9 (20%)	54,84,113	1.46	6 (11%)
44	CLA	A	822	-	45,49,73	1.37	8 (17%)	54,84,113	1.61	6 (11%)
49	DGD	m	104	-	67,67,67	0.85	2 (2%)	81,81,81	0.86	3 (3%)
44	CLA	B	815	-	69,73,73	1.21	9 (13%)	82,113,113	1.34	6 (7%)
50	LMG	F	805	-	30,30,55	1.23	2 (6%)	38,38,63	1.20	3 (7%)
44	CLA	r	312	-	45,49,73	1.41	8 (17%)	54,84,113	1.48	5 (9%)
44	CLA	B	833	-	69,73,73	1.15	8 (11%)	82,113,113	1.42	7 (8%)
44	CLA	s	511	-	54,58,73	1.31	8 (14%)	64,95,113	1.37	5 (7%)
44	CLA	f	813	-	58,62,73	1.36	10 (17%)	71,100,113	1.36	7 (9%)
47	BCR	A	853	-	41,41,41	0.99	2 (4%)	56,56,56	2.25	18 (32%)
44	CLA	L	304	-	49,53,73	1.32	9 (18%)	58,89,113	1.67	9 (15%)
46	LHG	s	516	-	34,34,48	1.09	2 (5%)	37,40,54	1.16	3 (8%)
44	CLA	s	509	-	54,58,73	1.32	9 (16%)	64,95,113	1.38	6 (9%)
44	CLA	B	838	-	69,73,73	1.18	9 (13%)	82,113,113	1.36	7 (8%)
47	BCR	l	102	-	41,41,41	0.68	0	56,56,56	2.17	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	CLA	e	819	-	49,53,73	1.36	9 (18%)	58,89,113	1.47	5 (8%)
44	CLA	5	312	-	50,54,73	1.34	9 (18%)	59,90,113	1.34	4 (6%)
44	CLA	f	825	-	46,50,73	1.39	9 (19%)	53,85,113	1.42	4 (7%)
44	CLA	n	201	-	41,45,73	1.47	10 (24%)	50,78,113	1.45	4 (8%)
44	CLA	A	837	-	45,49,73	1.42	11 (24%)	54,84,113	1.65	9 (16%)
47	BCR	o	305	-	41,41,41	0.71	0	56,56,56	2.17	14 (25%)
44	CLA	5	316	-	45,49,73	1.35	8 (17%)	54,84,113	1.56	7 (12%)
52	CHL	5	314	-	41,55,74	4.00	19 (46%)	35,91,114	2.51	13 (37%)
44	CLA	B	829	-	44,48,73	1.40	7 (15%)	51,82,113	1.60	7 (13%)
44	CLA	e	853	-	49,53,73	1.36	9 (18%)	58,89,113	1.46	7 (12%)
47	BCR	n	204	-	41,41,41	0.66	0	56,56,56	2.10	19 (33%)
44	CLA	e	843	-	53,57,73	1.41	9 (16%)	65,94,113	1.44	7 (10%)
44	CLA	f	835	-	49,53,73	1.36	9 (18%)	58,89,113	1.46	6 (10%)
44	CLA	j	802	-	45,49,73	1.40	9 (20%)	54,84,113	1.43	5 (9%)
44	CLA	f	837	-	46,50,73	1.40	8 (17%)	53,85,113	1.42	4 (7%)
49	DGD	f	851	-	53,53,67	0.93	2 (3%)	67,67,81	1.07	3 (4%)
47	BCR	p	503	-	11,11,41	0.68	0	15,16,56	1.99	5 (33%)
44	CLA	3	310	-	49,53,73	1.34	8 (16%)	58,89,113	1.45	6 (10%)
45	PQN	B	843	-	31,31,34	1.38	2 (6%)	39,41,45	1.52	6 (15%)
44	CLA	A	812	-	46,50,73	1.37	8 (17%)	53,85,113	1.57	8 (15%)
46	LHG	e	845	-	24,24,48	0.97	1 (4%)	26,29,54	1.29	3 (11%)
44	CLA	B	813	-	47,51,73	1.41	7 (14%)	55,86,113	1.49	5 (9%)
44	CLA	B	817	-	53,57,73	1.33	9 (16%)	61,93,113	1.47	5 (8%)
47	BCR	e	847	-	41,41,41	0.75	1 (2%)	56,56,56	1.91	17 (30%)
44	CLA	f	823	-	45,49,73	1.41	9 (20%)	54,84,113	1.50	5 (9%)
51	LUT	1	501	-	42,43,43	0.87	2 (4%)	51,60,60	1.77	12 (23%)
44	CLA	1	513	-	69,73,73	1.18	9 (13%)	82,113,113	1.26	6 (7%)
44	CLA	A	808	1	69,73,73	1.15	8 (11%)	82,113,113	1.34	7 (8%)
44	CLA	2	507	13	52,56,73	1.61	9 (17%)	60,91,113	1.68	8 (13%)
47	BCR	B	848	-	41,41,41	1.00	2 (4%)	56,56,56	1.99	16 (28%)
44	CLA	f	819	-	45,49,73	1.39	9 (20%)	54,84,113	1.47	6 (11%)
44	CLA	q	307	14	44,48,73	1.46	8 (18%)	51,82,113	1.49	6 (11%)
51	LUT	r	302	-	42,43,43	0.72	0	51,60,60	2.02	16 (31%)
44	CLA	p	509	-	54,58,73	1.54	8 (14%)	64,95,113	1.91	17 (26%)
44	CLA	B	805	-	45,49,73	1.39	9 (20%)	54,84,113	1.55	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	BCR	f	849	-	41,41,41	0.77	2 (4%)	56,56,56	2.03	16 (28%)
44	CLA	B	841	-	58,62,73	1.27	10 (17%)	68,99,113	1.41	7 (10%)
44	CLA	f	801	-	68,72,73	1.23	10 (14%)	83,112,113	1.32	8 (9%)
44	CLA	f	816	-	42,46,73	1.42	9 (21%)	49,79,113	1.42	5 (10%)
44	CLA	e	820	-	45,49,73	1.39	9 (20%)	54,84,113	1.50	6 (11%)
44	CLA	e	827	-	45,49,73	1.40	9 (20%)	54,84,113	1.43	6 (11%)
53	XAT	2	502	-	41,47,47	1.16	4 (9%)	54,74,74	2.78	19 (35%)
50	LMG	r	318	-	18,18,55	1.57	2 (11%)	22,23,63	1.58	2 (9%)
44	CLA	2	506	-	69,73,73	1.14	7 (10%)	82,113,113	1.39	5 (6%)
44	CLA	B	837	-	54,58,73	1.31	9 (16%)	64,95,113	1.46	8 (12%)
44	CLA	2	514	-	59,63,73	1.23	9 (15%)	70,101,113	1.37	5 (7%)
44	CLA	A	826	-	64,68,73	1.23	8 (12%)	76,107,113	1.41	7 (9%)
47	BCR	e	854	-	41,41,41	0.69	0	56,56,56	2.26	20 (35%)
44	CLA	3	314	14	64,68,73	1.18	9 (14%)	76,107,113	1.38	7 (9%)
47	BCR	B	845	-	41,41,41	1.04	1 (2%)	56,56,56	2.07	16 (28%)
44	CLA	2	504	13	37,44,73	1.52	8 (21%)	48,76,113	1.67	7 (14%)
52	CHL	r	316	-	37,51,74	4.23	18 (48%)	30,86,114	2.34	11 (36%)
44	CLA	5	306	-	43,48,73	1.38	7 (16%)	51,83,113	1.56	5 (9%)
44	CLA	q	309	-	54,58,73	1.30	8 (14%)	64,95,113	1.39	6 (9%)
44	CLA	B	814	-	45,49,73	1.45	10 (22%)	54,84,113	1.58	10 (18%)
44	CLA	A	833	-	44,48,73	1.38	9 (20%)	51,82,113	1.59	6 (11%)
52	CHL	5	315	-	40,54,74	3.94	20 (50%)	34,90,114	2.38	13 (38%)
44	CLA	m	101	-	45,49,73	1.52	9 (20%)	54,84,113	1.42	5 (9%)
44	CLA	B	802	-	68,72,73	1.18	10 (14%)	80,111,113	1.33	8 (10%)
44	CLA	e	806	-	45,49,73	1.40	9 (20%)	54,84,113	1.52	7 (12%)
47	BCR	f	847	-	41,41,41	0.74	0	56,56,56	2.22	17 (30%)
47	BCR	l	101	-	41,41,41	0.77	1 (2%)	56,56,56	2.30	19 (33%)
44	CLA	f	839	-	45,49,73	1.40	8 (17%)	54,84,113	1.54	6 (11%)
44	CLA	A	809	1	40,47,73	1.46	8 (20%)	43,80,113	1.43	3 (6%)
51	LUT	q	301	-	42,43,43	0.75	1 (2%)	51,60,60	2.11	11 (21%)
44	CLA	r	307	-	64,68,73	1.21	9 (14%)	76,107,113	1.33	8 (10%)
44	CLA	A	810	44	58,62,73	1.27	11 (18%)	68,99,113	1.50	6 (8%)
44	CLA	5	305	-	41,46,73	1.52	10 (24%)	50,79,113	1.72	10 (20%)
44	CLA	B	807	2	69,73,73	1.21	9 (13%)	82,113,113	1.30	6 (7%)
44	CLA	r	305	-	54,58,73	1.33	9 (16%)	64,95,113	1.36	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
52	CHL	s	515	-	35,49,74	4.34	17 (48%)	30,83,114	2.28	11 (36%)
44	CLA	B	801	-	69,73,73	1.21	11 (15%)	82,113,113	1.29	7 (8%)
44	CLA	B	816	-	47,51,73	1.37	7 (14%)	55,86,113	1.50	4 (7%)
44	CLA	B	825	-	46,50,73	1.37	8 (17%)	53,85,113	1.46	7 (13%)
44	CLA	f	824	-	46,50,73	1.39	8 (17%)	53,85,113	1.45	4 (7%)
44	CLA	e	803	44	56,60,73	1.28	9 (16%)	65,97,113	1.40	6 (9%)
44	CLA	A	815	-	49,53,73	1.41	9 (18%)	58,89,113	1.42	5 (8%)
44	CLA	e	811	-	45,49,73	1.39	9 (20%)	54,84,113	1.49	6 (11%)
44	CLA	f	817	-	47,51,73	1.37	9 (19%)	55,86,113	1.42	4 (7%)
47	BCR	j	803	-	41,41,41	0.76	1 (2%)	56,56,56	2.16	17 (30%)
44	CLA	r	306	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	6 (7%)
54	SQD	Q	803	-	44,46,54	1.21	3 (6%)	54,57,65	1.13	4 (7%)
44	CLA	p	506	-	59,63,73	1.25	8 (13%)	70,101,113	1.26	6 (8%)
44	CLA	s	514	-	44,48,73	1.43	8 (18%)	51,82,113	1.54	6 (11%)
44	CLA	3	313	-	52,56,73	1.33	7 (13%)	61,92,113	1.51	5 (8%)
44	CLA	B	819	-	45,49,73	1.43	8 (17%)	54,84,113	1.63	7 (12%)
44	CLA	2	511	-	44,48,73	1.40	10 (22%)	51,82,113	1.74	6 (11%)
53	XAT	s	502	-	41,47,47	0.92	2 (4%)	54,74,74	2.78	22 (40%)
44	CLA	p	504	-	45,49,73	1.44	9 (20%)	52,84,113	1.61	7 (13%)
44	CLA	q	304	-	41,46,73	1.65	9 (21%)	50,79,113	1.58	10 (20%)
44	CLA	B	831	-	47,51,73	1.41	8 (17%)	55,86,113	1.46	4 (7%)
44	CLA	A	818	-	44,48,73	1.38	7 (15%)	51,82,113	1.57	7 (13%)
44	CLA	s	504	-	42,47,73	1.58	7 (16%)	53,81,113	1.70	9 (16%)
49	DGD	B	850	-	60,60,67	0.88	2 (3%)	74,74,81	1.40	11 (14%)
44	CLA	3	316	-	41,45,73	1.36	8 (19%)	50,78,113	1.58	6 (12%)
44	CLA	A	806	1	69,73,73	1.19	7 (10%)	82,113,113	1.31	5 (6%)
50	LMG	m	105	-	30,30,55	1.21	2 (6%)	38,38,63	1.21	3 (7%)
44	CLA	B	809	-	44,48,73	1.40	8 (18%)	51,82,113	1.51	5 (9%)
50	LMG	5	301	-	32,32,55	1.18	2 (6%)	40,40,63	1.16	3 (7%)
47	BCR	L	306	-	41,41,41	0.85	1 (2%)	56,56,56	1.97	18 (32%)
52	CHL	3	302	13	41,55,74	4.01	21 (51%)	35,91,114	2.49	12 (34%)
52	CHL	1	512	-	41,55,74	4.09	18 (43%)	35,91,114	2.29	13 (37%)
44	CLA	f	843	46	40,46,73	1.46	9 (22%)	52,80,113	1.48	5 (9%)
47	BCR	B	852	-	41,41,41	1.21	2 (4%)	56,56,56	2.05	17 (30%)
48	SF4	f	802	-	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	CLA	e	830	-	54,58,73	1.31	9 (16%)	64,95,113	1.35	6 (9%)
51	LUT	s	501	-	42,43,43	0.74	0	51,60,60	2.04	15 (29%)
54	SQD	Q	802	-	52,54,54	1.11	3 (5%)	62,65,65	1.01	2 (3%)
44	CLA	f	829	-	54,58,73	1.30	9 (16%)	64,95,113	1.40	8 (12%)
52	CHL	2	513	-	32,48,74	4.05	15 (46%)	27,81,114	2.56	15 (55%)
44	CLA	B	835	-	64,68,73	1.21	9 (14%)	76,107,113	1.38	6 (7%)
44	CLA	A	827	-	69,73,73	1.20	9 (13%)	82,113,113	1.36	8 (9%)
44	CLA	L	301	-	60,64,73	1.24	11 (18%)	71,102,113	1.35	7 (9%)
44	CLA	e	815	-	49,53,73	1.39	8 (16%)	58,89,113	1.39	4 (6%)
44	CLA	f	832	-	44,48,73	1.43	9 (20%)	51,82,113	1.57	6 (11%)
44	CLA	s	506	-	69,73,73	1.18	8 (11%)	82,113,113	1.25	4 (4%)
47	BCR	3	305	-	41,41,41	0.90	2 (4%)	56,56,56	1.99	15 (26%)
47	BCR	r	301	-	41,41,41	0.73	0	56,56,56	1.85	12 (21%)
47	BCR	K	204	-	41,41,41	1.00	2 (4%)	56,56,56	2.02	16 (28%)
49	DGD	J	103	-	67,67,67	0.83	2 (2%)	81,81,81	1.11	4 (4%)
47	BCR	A	851	-	41,41,41	0.90	1 (2%)	56,56,56	2.18	18 (32%)
44	CLA	s	505	-	50,54,73	1.36	9 (18%)	59,90,113	1.43	4 (6%)
46	LHG	f	852	44	37,37,48	1.05	2 (5%)	40,43,54	1.18	3 (7%)
47	BCR	q	303	-	41,41,41	0.74	1 (2%)	56,56,56	2.03	18 (32%)
44	CLA	K	203	-	44,48,73	1.38	8 (18%)	51,82,113	1.51	5 (9%)
44	CLA	f	820	-	54,58,73	1.31	9 (16%)	64,95,113	1.43	5 (7%)
44	CLA	A	842	46	54,58,73	1.30	10 (18%)	64,95,113	1.40	6 (9%)
44	CLA	p	515	-	44,48,73	1.48	9 (20%)	51,82,113	1.52	6 (11%)
44	CLA	f	821	-	59,63,73	1.25	9 (15%)	70,101,113	1.34	6 (8%)
44	CLA	B	834	-	49,53,73	1.35	7 (14%)	58,89,113	1.52	7 (12%)
44	CLA	A	813	-	49,53,73	1.34	9 (18%)	58,89,113	1.48	5 (8%)
44	CLA	o	304	-	49,53,73	1.37	8 (16%)	58,89,113	1.40	5 (8%)
44	CLA	r	310	-	46,50,73	1.41	8 (17%)	53,85,113	1.45	5 (9%)
44	CLA	e	828	-	47,51,73	1.37	9 (19%)	53,85,113	1.44	4 (7%)
46	LHG	e	844	-	39,39,48	1.01	2 (5%)	42,45,54	1.25	4 (9%)
44	CLA	A	821	-	46,50,73	1.38	9 (19%)	53,85,113	1.59	7 (13%)
44	CLA	f	836	-	62,66,73	1.23	8 (12%)	69,103,113	1.28	4 (5%)
44	CLA	f	828	-	45,49,73	1.40	9 (20%)	54,84,113	1.56	5 (9%)
44	CLA	A	803	-	45,49,73	1.40	9 (20%)	54,84,113	1.63	7 (12%)
51	LUT	3	303	-	42,43,43	0.85	1 (2%)	51,60,60	1.66	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	CLA	A	819	-	44,48,73	1.40	7 (15%)	51,82,113	1.54	5 (9%)
44	CLA	e	838	-	56,60,73	1.27	9 (16%)	65,97,113	1.42	7 (10%)
44	CLA	B	832	-	47,51,73	1.31	7 (14%)	55,86,113	1.44	4 (7%)
43	CL0	A	801	-	55,69,73	2.41	6 (10%)	58,107,113	2.27	15 (25%)
44	CLA	A	852	-	61,65,73	1.26	9 (14%)	72,103,113	1.32	6 (8%)
44	CLA	2	510	46	64,68,73	1.18	10 (15%)	76,107,113	1.38	7 (9%)
44	CLA	f	812	-	44,48,73	1.44	10 (22%)	51,82,113	1.58	6 (11%)
44	CLA	A	828	-	45,49,73	1.39	7 (15%)	54,84,113	1.51	6 (11%)
44	CLA	q	306	-	45,49,73	1.42	8 (17%)	54,84,113	1.54	6 (11%)
46	LHG	O	601	-	23,23,48	1.33	2 (8%)	26,28,54	1.34	4 (15%)
47	BCR	I	101	-	41,41,41	1.19	2 (4%)	56,56,56	2.09	16 (28%)
44	CLA	A	804	44	56,60,73	1.27	8 (14%)	65,97,113	1.43	4 (6%)
44	CLA	B	804	-	69,73,73	1.19	9 (13%)	82,113,113	1.32	4 (4%)
47	BCR	B	847	-	41,41,41	1.02	2 (4%)	56,56,56	2.35	20 (35%)
48	SF4	8	201	38	0,12,12	-	-	-		
52	CHL	1	517	12	35,49,74	4.09	19 (54%)	30,83,114	3.11	14 (46%)
44	CLA	e	829	-	62,66,73	1.23	8 (12%)	73,104,113	1.32	6 (8%)
44	CLA	B	839	-	51,55,73	1.32	8 (15%)	60,91,113	1.54	7 (11%)
44	CLA	B	840	-	45,49,73	1.37	8 (17%)	54,84,113	1.62	6 (11%)
44	CLA	q	314	-	44,48,73	1.41	8 (18%)	51,82,113	1.59	7 (13%)
52	CHL	s	513	-	42,56,74	4.12	19 (45%)	36,92,114	2.34	11 (30%)
44	CLA	n	202	-	49,53,73	1.39	8 (16%)	58,89,113	1.44	6 (10%)
44	CLA	f	811	2	55,59,73	1.32	9 (16%)	64,96,113	1.40	7 (10%)
44	CLA	o	303	-	64,68,73	1.20	9 (14%)	76,107,113	1.32	6 (7%)
46	LHG	A	844	44	29,29,48	1.21	3 (10%)	32,35,54	1.21	3 (9%)
44	CLA	q	311	-	52,56,73	1.33	8 (15%)	61,92,113	1.38	5 (8%)
44	CLA	A	811	-	44,48,73	1.39	7 (15%)	51,82,113	1.55	7 (13%)
44	CLA	n	203	-	45,49,73	1.41	8 (17%)	54,84,113	1.51	6 (11%)
52	CHL	3	315	-	37,51,74	3.96	19 (51%)	30,86,114	2.97	11 (36%)
52	CHL	p	514	-	41,55,74	4.22	18 (43%)	35,91,114	2.18	11 (31%)
47	BCR	B	844	-	41,41,41	0.83	1 (2%)	56,56,56	2.60	17 (30%)
44	CLA	r	304	-	43,47,73	1.52	8 (18%)	52,81,113	1.66	10 (19%)
48	SF4	g	101	-	0,12,12	-	-	-		
46	LHG	2	517	44	34,34,48	1.07	2 (5%)	37,40,54	1.23	5 (13%)
44	CLA	s	508	-	44,48,73	1.42	9 (20%)	53,83,113	1.50	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	BCR	e	850	-	41,41,41	0.81	2 (4%)	56,56,56	2.32	20 (35%)
44	CLA	q	310	-	45,49,73	1.42	7 (15%)	54,84,113	1.44	4 (7%)
44	CLA	B	836	-	46,50,73	1.39	9 (19%)	53,85,113	1.39	4 (7%)
44	CLA	e	813	-	46,50,73	1.40	9 (19%)	53,85,113	1.40	5 (9%)
44	CLA	1	506	-	59,63,73	1.26	8 (13%)	70,101,113	1.39	6 (8%)
44	CLA	e	817	-	42,47,73	1.44	9 (21%)	49,81,113	1.51	5 (10%)
44	CLA	B	824	-	49,53,73	1.40	9 (18%)	58,89,113	1.41	5 (8%)
44	CLA	1	508	-	44,48,73	1.38	8 (18%)	51,82,113	1.46	7 (13%)
44	CLA	q	308	-	46,50,73	1.41	8 (17%)	53,85,113	1.47	6 (11%)
47	BCR	e	848	-	41,41,41	0.75	1 (2%)	56,56,56	2.16	21 (37%)
44	CLA	p	511	-	42,47,73	1.46	8 (19%)	50,80,113	1.51	6 (12%)
44	CLA	e	841	-	45,49,73	1.41	9 (20%)	54,84,113	1.51	6 (11%)
44	CLA	n	205	-	42,47,73	1.50	8 (19%)	48,81,113	1.45	5 (10%)
52	CHL	1	514	-	35,49,74	4.49	18 (51%)	30,83,114	2.36	10 (33%)
47	BCR	s	503	-	41,41,41	0.70	0	56,56,56	3.70	30 (53%)
44	CLA	A	831	-	67,71,73	1.29	13 (19%)	81,110,113	1.39	8 (9%)
44	CLA	p	508	-	69,73,73	1.17	9 (13%)	82,113,113	1.21	4 (4%)
44	CLA	f	808	-	58,62,73	1.26	7 (12%)	68,99,113	1.35	7 (10%)
44	CLA	p	513	-	56,60,73	1.32	6 (10%)	65,97,113	1.34	7 (10%)
44	CLA	r	309	-	54,58,73	1.30	9 (16%)	64,95,113	1.30	4 (6%)
44	CLA	B	823	-	46,50,73	1.39	10 (21%)	53,85,113	1.50	4 (7%)
44	CLA	3	317	-	45,49,73	1.40	10 (22%)	54,84,113	1.57	9 (16%)
50	LMG	F	806	-	45,45,55	0.95	2 (4%)	53,53,63	1.08	5 (9%)
43	CL0	e	801	-	55,69,73	2.42	6 (10%)	58,107,113	2.28	15 (25%)
44	CLA	e	852	-	61,65,73	1.24	8 (13%)	72,103,113	1.33	6 (8%)
44	CLA	B	810	2	44,48,73	1.38	9 (20%)	51,82,113	1.63	8 (15%)
44	CLA	3	318	-	49,53,73	1.40	8 (16%)	60,89,113	1.45	7 (11%)
44	CLA	f	805	-	41,46,73	1.44	9 (21%)	47,79,113	1.69	8 (17%)
44	CLA	f	830	-	43,47,73	1.54	10 (23%)	52,81,113	1.58	9 (17%)
52	CHL	p	512	-	41,55,74	4.24	19 (46%)	35,91,114	2.34	11 (31%)
44	CLA	f	831	-	60,64,73	1.26	8 (13%)	71,102,113	1.35	5 (7%)
44	CLA	A	805	-	68,72,73	1.21	10 (14%)	80,111,113	1.46	9 (11%)
53	XAT	5	304	-	41,47,47	1.26	5 (12%)	54,74,74	2.43	19 (35%)
44	CLA	e	826	-	68,72,73	1.24	10 (14%)	83,112,113	1.34	8 (9%)
44	CLA	A	830	-	54,58,73	1.30	7 (12%)	64,95,113	1.50	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	BCR	A	848	-	41,41,41	1.07	2 (4%)	56,56,56	2.00	11 (19%)
44	CLA	f	826	-	69,73,73	1.16	8 (11%)	82,113,113	1.33	8 (9%)
51	LUT	2	501	-	42,43,43	0.89	1 (2%)	51,60,60	2.06	14 (27%)
44	CLA	e	814	-	46,50,73	1.39	9 (19%)	53,85,113	1.45	4 (7%)
44	CLA	m	102	-	46,50,73	1.41	8 (17%)	53,85,113	1.44	4 (7%)
47	BCR	e	849	-	41,41,41	0.73	0	56,56,56	2.07	15 (26%)
44	CLA	o	302	-	44,48,73	1.52	10 (22%)	55,83,113	1.62	7 (12%)
44	CLA	f	834	-	47,51,73	1.36	8 (17%)	55,86,113	1.46	5 (9%)
47	BCR	f	845	-	41,41,41	0.74	1 (2%)	56,56,56	2.15	17 (30%)
44	CLA	1	505	-	46,50,73	1.41	7 (15%)	53,85,113	1.42	4 (7%)
44	CLA	2	509	-	54,58,73	1.27	8 (14%)	64,95,113	1.48	6 (9%)
47	BCR	o	301	-	41,41,41	0.75	1 (2%)	56,56,56	2.04	18 (32%)
44	CLA	e	807	-	46,50,73	1.40	9 (19%)	53,85,113	1.50	5 (9%)
44	CLA	e	812	-	41,47,73	1.44	9 (21%)	50,80,113	1.54	7 (14%)
44	CLA	B	822	-	51,55,73	1.34	11 (21%)	60,91,113	1.57	6 (10%)
47	BCR	F	804	-	41,41,41	1.00	1 (2%)	56,56,56	1.98	17 (30%)
52	CHL	2	512	-	41,54,74	3.89	18 (43%)	36,90,114	2.75	11 (30%)
47	BCR	f	848	-	41,41,41	0.76	1 (2%)	56,56,56	2.05	16 (28%)
48	SF4	C	102	3	0,12,12	-	-	-		
47	BCR	A	845	-	41,41,41	1.12	2 (4%)	56,56,56	2.29	19 (33%)
44	CLA	q	316	-	50,54,73	1.37	9 (18%)	59,90,113	1.35	4 (6%)
47	BCR	Q	801	-	40,40,41	0.76	0	54,54,56	2.99	20 (37%)
44	CLA	A	814	-	46,50,73	1.39	10 (21%)	53,85,113	1.55	5 (9%)
44	CLA	q	312	14	64,68,73	1.21	7 (10%)	76,107,113	1.30	7 (9%)
44	CLA	p	510	-	50,54,73	1.35	9 (18%)	59,90,113	1.35	4 (6%)
44	CLA	5	308	-	64,68,73	1.23	9 (14%)	76,107,113	1.41	7 (9%)
44	CLA	e	808	1	45,49,73	1.41	9 (20%)	54,84,113	1.52	6 (11%)
44	CLA	f	838	-	44,48,73	1.41	9 (20%)	51,82,113	1.52	6 (11%)
44	CLA	q	315	-	49,53,73	1.37	8 (16%)	58,89,113	1.41	6 (10%)
44	CLA	e	834	-	49,53,73	1.36	9 (18%)	58,89,113	1.43	4 (6%)
44	CLA	f	815	-	47,51,73	1.37	8 (17%)	55,86,113	1.33	4 (7%)
44	CLA	1	515	-	48,52,73	1.50	11 (22%)	58,87,113	1.41	5 (8%)
44	CLA	f	833	-	47,51,73	1.37	9 (19%)	55,86,113	1.38	4 (7%)
47	BCR	F	801	-	41,41,41	0.98	2 (4%)	56,56,56	2.11	17 (30%)
44	CLA	A	838	-	69,73,73	1.21	8 (11%)	82,113,113	1.33	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
44	CLA	A	807	-	41,47,73	1.40	9 (21%)	50,80,113	1.58	5 (10%)
44	CLA	3	309	-	43,48,73	1.57	10 (23%)	52,82,113	1.58	6 (11%)
44	CLA	e	818	-	43,47,73	1.71	7 (16%)	49,81,113	1.99	11 (22%)
47	BCR	e	846	-	41,41,41	0.78	2 (4%)	56,56,56	2.20	16 (28%)
44	CLA	A	817	-	42,47,73	1.65	12 (28%)	49,81,113	1.63	5 (10%)
44	CLA	f	810	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	6 (7%)
44	CLA	B	828	-	45,49,73	1.38	9 (20%)	54,84,113	1.59	9 (16%)
44	CLA	A	823	-	58,62,73	1.35	10 (17%)	65,99,113	1.38	7 (10%)
44	CLA	e	809	-	54,58,73	1.30	8 (14%)	64,95,113	1.53	7 (10%)
44	CLA	f	807	-	45,49,73	1.40	9 (20%)	54,84,113	1.47	9 (16%)
45	PQN	e	842	-	15,15,34	1.49	2 (13%)	20,22,45	0.84	0
44	CLA	K	202	-	45,49,73	1.38	9 (20%)	54,84,113	1.53	6 (11%)
44	CLA	p	507	12	44,48,73	1.50	10 (22%)	55,83,113	1.57	8 (14%)
44	CLA	L	302	-	44,48,73	1.40	6 (13%)	50,82,113	1.61	6 (12%)
44	CLA	3	301	-	45,49,73	1.39	9 (20%)	54,84,113	1.58	7 (12%)
44	CLA	K	205	10	42,47,73	1.44	8 (19%)	48,81,113	1.57	5 (10%)
44	CLA	5	309	-	49,53,73	1.39	10 (20%)	58,89,113	1.45	7 (12%)
44	CLA	L	303	-	56,60,73	1.26	9 (16%)	65,97,113	1.59	8 (12%)
47	BCR	f	850	-	40,40,41	0.75	0	54,54,56	2.08	14 (25%)
44	CLA	r	317	-	54,58,73	1.31	8 (14%)	64,95,113	1.37	7 (10%)
44	CLA	A	829	-	59,63,73	1.29	8 (13%)	70,101,113	1.46	8 (11%)
44	CLA	e	824	-	60,64,73	1.23	9 (15%)	71,102,113	1.32	7 (9%)
51	LUT	p	502	-	42,43,43	2.48	1 (2%)	51,60,60	1.66	7 (13%)
44	CLA	1	510	46	50,54,73	1.31	10 (20%)	59,90,113	1.42	5 (8%)
44	CLA	A	816	-	63,67,73	1.21	7 (11%)	74,105,113	1.42	7 (9%)
47	BCR	L	305	-	41,41,41	0.95	1 (2%)	56,56,56	2.15	17 (30%)
52	CHL	s	517	42	41,55,74	4.13	19 (46%)	35,91,114	2.32	13 (37%)
44	CLA	A	835	-	55,59,73	1.33	8 (14%)	64,96,113	1.62	7 (10%)
44	CLA	A	836	-	59,63,73	1.29	9 (15%)	70,101,113	1.50	7 (10%)
47	BCR	1	503	-	19,19,41	0.66	0	26,26,56	2.04	7 (26%)
44	CLA	F	803	-	45,49,73	1.39	9 (20%)	54,84,113	1.48	5 (9%)
44	CLA	F	802	-	46,50,73	1.40	10 (21%)	53,85,113	1.49	4 (7%)

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
44	CLA	3	311	-	1/1/12/20	9/21/97/115	-
50	LMG	2	518	-	-	3/7/27/70	0/1/1/1
51	LUT	1	502	-	-	3/29/67/67	0/2/2/2
44	CLA	e	821	-	1/1/10/20	4/12/88/115	-
44	CLA	A	825	-	1/1/13/20	8/32/108/115	-
44	CLA	A	840	-	1/1/10/20	4/10/86/115	-
44	CLA	A	802	-	1/1/13/20	10/31/107/115	-
44	CLA	f	818	-	1/1/13/20	6/27/103/115	-
52	CHL	p	517	-	3/3/15/26	4/12/110/137	-
44	CLA	f	822	-	1/1/10/20	3/10/86/115	-
44	CLA	B	818	-	1/1/13/20	14/32/108/115	-
44	CLA	f	806	-	1/1/10/20	0/10/86/115	-
48	SF4	C	101	3	-	-	0/6/5/5
44	CLA	r	308	-	1/1/10/20	4/10/86/115	-
44	CLA	B	806	-	1/1/8/20	2/10/79/115	-
52	CHL	r	314	-	3/3/17/26	3/21/119/137	-
47	BCR	A	846	-	-	7/29/63/63	0/2/2/2
44	CLA	1	507	12	1/1/13/20	5/29/105/115	-
44	CLA	5	313	15	1/1/9/20	4/10/82/115	-
47	BCR	A	849	-	-	2/27/61/63	0/2/2/2
44	CLA	e	839	-	1/1/15/20	14/39/115/115	-
44	CLA	q	305	-	1/1/12/20	8/24/100/115	-
51	LUT	3	304	-	-	2/29/67/67	0/2/2/2
44	CLA	r	315	41	1/1/10/20	2/10/86/115	-
46	LHG	B	851	-	-	17/42/42/53	-
52	CHL	5	317	-	3/3/14/26	4/8/102/137	-
44	CLA	B	820	-	1/1/12/20	7/25/101/115	-
51	LUT	5	303	-	-	2/29/67/67	0/2/2/2
44	CLA	f	803	-	1/1/10/20	2/12/88/115	-
44	CLA	e	832	-	1/1/10/20	7/13/89/115	-
44	CLA	r	311	-	1/1/11/20	6/17/93/115	-
48	SF4	A	850	1,2	-	-	0/6/5/5
44	CLA	B	827	-	1/1/10/20	2/10/86/115	-
44	CLA	B	826	-	1/1/14/20	8/36/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	PQN	f	844	-	-	0/3/23/43	0/2/2/2
44	CLA	J	101	9	1/1/10/20	7/12/88/115	-
44	CLA	1	504	-	1/1/10/20	3/10/86/115	-
44	CLA	B	821	-	1/1/12/20	4/21/97/115	-
44	CLA	1	509	-	-	4/21/97/115	-
47	BCR	A	847	-	-	2/29/63/63	0/2/2/2
44	CLA	A	834	1	1/1/10/20	3/10/86/115	-
44	CLA	e	804	-	1/1/15/20	17/39/115/115	-
44	CLA	A	839	-	1/1/10/20	4/12/88/115	-
52	CHL	q	313	-	3/3/15/26	11/17/111/137	-
44	CLA	e	825	-	1/1/10/20	0/10/86/115	-
44	CLA	e	840	-	1/1/10/20	0/10/86/115	-
51	LUT	p	501	-	-	2/29/67/67	0/2/2/2
44	CLA	5	307	15	1/1/15/20	17/39/115/115	-
44	CLA	e	802	-	1/1/9/20	4/10/82/115	-
44	CLA	e	805	-	1/1/11/20	5/17/93/115	-
44	CLA	e	822	-	1/1/10/20	2/10/86/115	-
44	CLA	f	814	-	1/1/10/20	2/13/89/115	-
44	CLA	f	842	-	1/1/10/20	2/10/86/115	-
44	CLA	K	201	-	1/1/8/20	2/4/76/115	-
47	BCR	m	103	-	-	2/29/63/63	0/2/2/2
47	BCR	f	846	-	-	4/29/63/63	0/2/2/2
51	LUT	q	302	-	-	5/29/67/67	0/2/2/2
44	CLA	e	836	-	1/1/12/20	4/23/99/115	-
44	CLA	3	307	-	1/1/9/20	4/10/82/115	-
47	BCR	B	846	-	-	5/29/63/63	0/2/2/2
46	LHG	A	843	-	-	12/53/53/53	-
44	CLA	p	505	-	-	3/17/93/115	-
44	CLA	B	803	-	1/1/15/20	16/39/115/115	-
46	LHG	p	516	-	-	11/53/53/53	-
47	BCR	J	102	-	-	2/29/63/63	0/2/2/2
44	CLA	B	811	-	1/1/13/20	9/27/103/115	-
44	CLA	B	812	-	1/1/13/20	7/25/101/115	-
44	CLA	e	823	-	1/1/10/20	2/11/87/115	-
47	BCR	B	849	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	e	837	-	1/1/13/20	9/27/103/115	-
44	CLA	e	810	44	1/1/13/20	12/27/103/115	-
44	CLA	s	507	-	1/1/10/20	2/10/86/115	-
44	CLA	f	804	-	1/1/9/20	3/11/84/115	-
44	CLA	1	511	-	1/1/11/20	6/17/93/115	-
44	CLA	f	809	-	1/1/12/20	3/24/100/115	-
44	CLA	f	840	-	1/1/10/20	4/10/86/115	-
53	XAT	r	303	-	-	2/31/93/93	0/4/4/4
46	LHG	1	516	44	-	23/53/53/53	-
44	CLA	B	808	-	1/1/12/20	5/24/100/115	-
44	CLA	3	308	-	1/1/13/20	12/27/103/115	-
44	CLA	5	311	-	1/1/10/20	3/12/88/115	-
44	CLA	f	841	-	1/1/10/20	2/10/86/115	-
44	CLA	A	824	-	1/1/9/20	4/10/82/115	-
44	CLA	B	842	-	1/1/13/20	14/30/106/115	-
44	CLA	s	510	-	1/1/14/20	10/33/109/115	-
44	CLA	5	310	-	1/1/12/20	8/21/97/115	-
44	CLA	2	505	-	-	13/24/100/115	-
47	BCR	e	851	-	-	4/29/63/63	0/2/2/2
44	CLA	f	827	-	1/1/9/20	0/10/82/115	-
44	CLA	e	816	-	1/1/14/20	11/33/109/115	-
44	CLA	B	830	-	1/1/13/20	10/29/105/115	-
44	CLA	2	508	-	1/1/11/20	3/17/93/115	-
52	CHL	2	515	-	3/3/16/26	5/15/111/137	-
47	BCR	j	801	-	-	2/29/63/63	0/2/2/2
52	CHL	r	313	-	3/3/16/26	7/17/115/137	-
44	CLA	A	832	-	1/1/10/20	5/13/89/115	-
50	LMG	2	519	-	-	14/31/51/70	0/1/1/1
44	CLA	e	831	-	1/1/13/20	5/29/105/115	-
52	CHL	s	512	-	3/3/16/26	5/17/115/137	-
52	CHL	2	516	13	3/3/15/26	8/13/109/137	-
44	CLA	e	835	1	1/1/10/20	4/9/85/115	-
44	CLA	3	306	-	1/1/13/20	12/23/99/115	-
45	PQN	A	841	-	-	13/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	e	833	-	1/1/10/20	4/10/86/115	-
48	SF4	g	102	-	-	-	0/6/5/5
44	CLA	A	820	-	1/1/13/20	10/30/106/115	-
47	BCR	2	503	-	-	8/29/63/63	0/2/2/2
47	BCR	5	302	-	-	7/29/63/63	0/2/2/2
44	CLA	3	312	-	1/1/10/20	6/10/86/115	-
44	CLA	A	822	-	1/1/10/20	4/10/86/115	-
49	DGD	m	104	-	-	14/55/95/95	0/2/2/2
44	CLA	B	815	-	1/1/15/20	10/39/115/115	-
50	LMG	F	805	-	-	4/25/45/70	0/1/1/1
44	CLA	r	312	-	1/1/10/20	4/10/86/115	-
44	CLA	B	833	-	1/1/15/20	3/39/115/115	-
44	CLA	s	511	-	1/1/12/20	9/21/97/115	-
44	CLA	f	813	-	1/1/13/20	10/25/101/115	-
47	BCR	A	853	-	-	2/29/63/63	0/2/2/2
44	CLA	L	304	-	1/1/11/20	6/15/91/115	-
46	LHG	s	516	-	-	5/39/39/53	-
44	CLA	s	509	-	1/1/12/20	7/21/97/115	-
44	CLA	B	838	-	1/1/15/20	2/39/115/115	-
47	BCR	l	102	-	-	8/29/63/63	0/2/2/2
44	CLA	e	819	-	1/1/11/20	5/15/91/115	-
44	CLA	5	312	-	1/1/11/20	7/17/93/115	-
44	CLA	f	825	-	1/1/10/20	2/12/88/115	-
44	CLA	n	201	-	1/1/8/20	2/4/76/115	-
44	CLA	A	837	-	1/1/10/20	2/10/86/115	-
47	BCR	o	305	-	-	2/29/63/63	0/2/2/2
44	CLA	5	316	-	1/1/10/20	2/10/86/115	-
52	CHL	5	314	-	3/3/16/26	9/17/115/137	-
44	CLA	B	829	-	1/1/9/20	2/10/82/115	-
44	CLA	e	853	-	1/1/11/20	6/15/91/115	-
47	BCR	n	204	-	-	9/29/63/63	0/2/2/2
44	CLA	e	843	-	1/1/12/20	7/19/95/115	-
44	CLA	f	835	-	1/1/11/20	7/15/91/115	-
44	CLA	j	802	-	1/1/10/20	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	f	837	-	1/1/10/20	4/12/88/115	-
49	DGD	f	851	-	-	10/41/81/95	0/2/2/2
47	BCR	p	503	-	-	1/1/19/63	0/1/1/2
44	CLA	3	310	-	1/1/11/20	4/15/91/115	-
45	PQN	B	843	-	-	8/20/40/43	0/2/2/2
44	CLA	A	812	-	1/1/10/20	2/12/88/115	-
46	LHG	e	845	-	-	8/28/28/53	-
44	CLA	B	813	-	1/1/10/20	2/13/89/115	-
44	CLA	B	817	-	1/1/11/20	7/20/96/115	-
47	BCR	e	847	-	-	0/29/63/63	0/2/2/2
44	CLA	f	823	-	1/1/10/20	4/10/86/115	-
51	LUT	1	501	-	-	2/29/67/67	0/2/2/2
44	CLA	1	513	-	-	18/39/115/115	-
44	CLA	A	808	1	1/1/15/20	8/39/115/115	-
44	CLA	2	507	13	2/2/11/20	3/16/88/115	-
47	BCR	B	848	-	-	2/29/63/63	0/2/2/2
44	CLA	f	819	-	1/1/10/20	4/10/86/115	-
44	CLA	q	307	14	-	2/10/82/115	-
51	LUT	r	302	-	-	2/29/67/67	0/2/2/2
44	CLA	p	509	-	1/1/12/20	6/21/97/115	-
44	CLA	B	805	-	1/1/10/20	4/10/86/115	-
47	BCR	f	849	-	-	0/29/63/63	0/2/2/2
44	CLA	B	841	-	1/1/12/20	11/26/102/115	-
44	CLA	f	801	-	1/1/15/20	10/37/113/115	-
44	CLA	f	816	-	1/1/8/20	1/6/78/115	-
44	CLA	e	820	-	1/1/10/20	3/10/86/115	-
44	CLA	e	827	-	1/1/10/20	1/10/86/115	-
53	XAT	2	502	-	-	6/31/93/93	0/4/4/4
50	LMG	r	318	-	-	11/11/28/70	0/1/1/1
44	CLA	2	506	-	1/1/15/20	13/39/115/115	-
44	CLA	B	837	-	1/1/12/20	4/21/97/115	-
44	CLA	2	514	-	1/1/13/20	9/27/103/115	-
44	CLA	A	826	-	1/1/14/20	12/33/109/115	-
47	BCR	e	854	-	-	4/29/63/63	0/2/2/2
44	CLA	3	314	14	1/1/14/20	15/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	BCR	B	845	-	-	6/29/63/63	0/2/2/2
52	CHL	r	316	-	3/3/15/26	4/12/110/137	-
44	CLA	2	504	13	1/1/7/20	2/4/73/115	-
44	CLA	5	306	-	1/1/10/20	4/8/84/115	-
44	CLA	q	309	-	1/1/12/20	5/21/97/115	-
44	CLA	B	814	-	1/1/10/20	4/10/86/115	-
44	CLA	A	833	-	1/1/9/20	1/10/82/115	-
52	CHL	5	315	-	3/3/16/26	6/15/113/137	-
44	CLA	m	101	-	1/1/10/20	6/10/86/115	-
44	CLA	B	802	-	1/1/14/20	6/37/113/115	-
44	CLA	e	806	-	1/1/10/20	2/10/86/115	-
47	BCR	f	847	-	-	6/29/63/63	0/2/2/2
47	BCR	l	101	-	-	5/29/63/63	0/2/2/2
44	CLA	f	839	-	1/1/10/20	2/10/86/115	-
44	CLA	A	809	1	1/1/9/20	3/6/84/115	-
51	LUT	q	301	-	-	6/29/67/67	0/2/2/2
44	CLA	r	307	-	1/1/14/20	9/33/109/115	-
44	CLA	A	810	44	1/1/12/20	5/26/102/115	-
44	CLA	5	305	-	1/1/9/20	0/8/80/115	-
44	CLA	B	807	2	1/1/15/20	7/39/115/115	-
44	CLA	r	305	-	1/1/12/20	8/21/97/115	-
52	CHL	s	515	-	3/3/14/26	3/10/104/137	-
44	CLA	B	801	-	1/1/15/20	8/39/115/115	-
44	CLA	B	816	-	1/1/10/20	4/13/89/115	-
44	CLA	B	825	-	1/1/10/20	2/12/88/115	-
44	CLA	f	824	-	1/1/10/20	5/12/88/115	-
44	CLA	e	803	44	1/1/12/20	4/24/100/115	-
44	CLA	A	815	-	1/1/11/20	4/15/91/115	-
44	CLA	e	811	-	1/1/10/20	4/10/86/115	-
44	CLA	f	817	-	1/1/10/20	7/13/89/115	-
47	BCR	j	803	-	-	2/29/63/63	0/2/2/2
44	CLA	r	306	-	1/1/15/20	15/39/115/115	-
54	SQD	Q	803	-	-	9/41/61/69	0/1/1/1
44	CLA	p	506	-	1/1/13/20	12/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	s	514	-	1/1/9/20	2/10/82/115	-
44	CLA	3	313	-	1/1/11/20	7/19/95/115	-
44	CLA	B	819	-	1/1/10/20	0/10/86/115	-
44	CLA	2	511	-	1/1/9/20	2/10/82/115	-
53	XAT	s	502	-	-	6/31/93/93	0/4/4/4
44	CLA	p	504	-	1/1/10/20	6/10/86/115	-
44	CLA	q	304	-	1/1/10/20	1/7/84/115	-
44	CLA	B	831	-	1/1/10/20	2/13/89/115	-
44	CLA	A	818	-	1/1/9/20	2/10/82/115	-
44	CLA	s	504	-	1/1/10/20	4/8/84/115	-
49	DGD	B	850	-	-	20/48/88/95	0/2/2/2
44	CLA	3	316	-	1/1/8/20	0/4/76/115	-
44	CLA	A	806	1	1/1/15/20	19/39/115/115	-
50	LMG	m	105	-	-	5/25/45/70	0/1/1/1
44	CLA	B	809	-	1/1/9/20	4/10/82/115	-
50	LMG	5	301	-	-	7/27/47/70	0/1/1/1
47	BCR	L	306	-	-	6/29/63/63	0/2/2/2
52	CHL	3	302	13	3/3/16/26	2/17/115/137	-
52	CHL	1	512	-	3/3/16/26	8/17/115/137	-
44	CLA	f	843	46	1/1/9/20	0/4/80/115	-
47	BCR	B	852	-	-	4/29/63/63	0/2/2/2
48	SF4	f	802	-	-	-	0/6/5/5
44	CLA	e	830	-	1/1/12/20	7/21/97/115	-
51	LUT	s	501	-	-	3/29/67/67	0/2/2/2
54	SQD	Q	802	-	-	10/49/69/69	0/1/1/1
44	CLA	f	829	-	1/1/12/20	7/21/97/115	-
52	CHL	2	513	-	3/3/13/26	7/10/100/137	-
44	CLA	B	835	-	1/1/14/20	6/33/109/115	-
44	CLA	A	827	-	1/1/15/20	16/39/115/115	-
44	CLA	L	301	-	1/1/13/20	4/29/105/115	-
44	CLA	e	815	-	1/1/11/20	8/15/91/115	-
44	CLA	f	832	-	1/1/9/20	3/10/82/115	-
44	CLA	s	506	-	1/1/15/20	16/39/115/115	-
47	BCR	3	305	-	-	7/29/63/63	0/2/2/2
47	BCR	r	301	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	BCR	K	204	-	-	8/29/63/63	0/2/2/2
49	DGD	J	103	-	-	26/55/95/95	0/2/2/2
47	BCR	A	851	-	-	6/29/63/63	0/2/2/2
44	CLA	s	505	-	-	12/17/93/115	-
46	LHG	f	852	44	-	13/42/42/53	-
47	BCR	q	303	-	-	6/29/63/63	0/2/2/2
44	CLA	K	203	-	1/1/9/20	5/10/82/115	-
44	CLA	f	820	-	1/1/12/20	11/21/97/115	-
44	CLA	A	842	46	1/1/12/20	10/21/97/115	-
44	CLA	p	515	-	1/1/9/20	2/10/82/115	-
44	CLA	f	821	-	1/1/13/20	7/27/103/115	-
44	CLA	B	834	-	1/1/11/20	8/15/91/115	-
44	CLA	A	813	-	1/1/11/20	8/15/91/115	-
44	CLA	o	304	-	1/1/11/20	6/15/91/115	-
44	CLA	r	310	-	1/1/10/20	6/12/88/115	-
44	CLA	e	828	-	1/1/10/20	3/12/88/115	-
46	LHG	e	844	-	-	8/44/44/53	-
44	CLA	A	821	-	1/1/10/20	2/12/88/115	-
44	CLA	f	836	-	1/1/12/20	11/31/103/115	-
44	CLA	f	828	-	1/1/10/20	6/10/86/115	-
44	CLA	A	803	-	1/1/10/20	3/10/86/115	-
51	LUT	3	303	-	-	2/29/67/67	0/2/2/2
44	CLA	A	819	-	1/1/9/20	4/10/82/115	-
44	CLA	e	838	-	1/1/12/20	5/24/100/115	-
44	CLA	B	832	-	1/1/10/20	3/13/89/115	-
43	CL0	A	801	-	3/3/18/25	6/33/125/135	-
44	CLA	A	852	-	1/1/13/20	10/30/106/115	-
44	CLA	2	510	46	1/1/14/20	14/33/109/115	-
44	CLA	f	812	-	1/1/9/20	4/10/82/115	-
44	CLA	A	828	-	1/1/10/20	2/10/86/115	-
44	CLA	q	306	-	1/1/10/20	5/10/86/115	-
46	LHG	O	601	-	-	2/27/27/53	-
47	BCR	I	101	-	-	4/29/63/63	0/2/2/2
44	CLA	A	804	44	1/1/12/20	4/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	B	804	-	1/1/15/20	14/39/115/115	-
47	BCR	B	847	-	-	5/29/63/63	0/2/2/2
52	CHL	1	517	12	3/3/14/26	5/10/104/137	-
52	CHL	s	513	-	3/3/16/26	4/18/116/137	-
44	CLA	e	829	-	1/1/13/20	13/31/107/115	-
44	CLA	B	839	-	1/1/11/20	5/18/94/115	-
44	CLA	B	840	-	1/1/10/20	3/10/86/115	-
44	CLA	q	314	-	1/1/9/20	2/10/82/115	-
48	SF4	8	201	38	-	-	0/6/5/5
44	CLA	n	202	-	1/1/11/20	10/15/91/115	-
44	CLA	f	811	2	1/1/12/20	6/23/99/115	-
44	CLA	o	303	-	1/1/14/20	9/33/109/115	-
46	LHG	A	844	44	-	11/34/34/53	-
44	CLA	q	311	-	1/1/11/20	10/19/95/115	-
44	CLA	A	811	-	1/1/9/20	2/10/82/115	-
44	CLA	n	203	-	1/1/10/20	4/10/86/115	-
52	CHL	3	315	-	3/3/15/26	3/12/110/137	-
52	CHL	p	514	-	3/3/16/26	7/17/115/137	-
47	BCR	B	844	-	-	4/29/63/63	0/2/2/2
44	CLA	r	304	-	1/1/9/20	2/8/80/115	-
48	SF4	g	101	-	-	-	0/6/5/5
46	LHG	2	517	44	-	3/39/39/53	-
44	CLA	s	508	-	1/1/10/20	2/8/84/115	-
47	BCR	e	850	-	-	6/29/63/63	0/2/2/2
44	CLA	q	310	-	1/1/10/20	4/10/86/115	-
44	CLA	B	836	-	-	5/12/88/115	-
44	CLA	e	813	-	1/1/10/20	2/12/88/115	-
44	CLA	1	506	-	1/1/13/20	9/27/103/115	-
44	CLA	e	817	-	1/1/9/20	0/4/82/115	-
44	CLA	B	824	-	1/1/11/20	6/15/91/115	-
44	CLA	1	508	-	1/1/9/20	2/10/82/115	-
44	CLA	q	308	-	1/1/10/20	4/12/88/115	-
47	BCR	e	848	-	-	6/29/63/63	0/2/2/2
44	CLA	p	511	-	1/1/8/20	4/10/79/115	-
44	CLA	e	841	-	1/1/10/20	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	n	205	-	1/1/9/20	2/8/80/115	-
52	CHL	1	514	-	3/3/14/26	4/10/104/137	-
47	BCR	s	503	-	-	5/29/63/63	0/2/2/2
44	CLA	A	831	-	1/1/14/20	14/35/111/115	-
44	CLA	p	508	-	1/1/15/20	16/39/115/115	-
44	CLA	f	808	-	1/1/12/20	6/25/101/115	-
44	CLA	p	513	-	1/1/12/20	5/24/100/115	-
44	CLA	r	309	-	1/1/12/20	7/21/97/115	-
44	CLA	B	823	-	1/1/10/20	4/12/88/115	-
44	CLA	3	317	-	1/1/10/20	2/10/86/115	-
50	LMG	F	806	-	-	18/40/60/70	0/1/1/1
43	CL0	e	801	-	3/3/18/25	6/33/125/135	-
44	CLA	e	852	-	1/1/13/20	10/30/106/115	-
44	CLA	B	810	2	1/1/9/20	0/10/82/115	-
44	CLA	3	318	-	1/1/11/20	6/15/91/115	-
44	CLA	f	805	-	1/1/8/20	0/4/78/115	-
44	CLA	f	830	-	1/1/9/20	2/8/80/115	-
52	CHL	p	512	-	3/3/16/26	3/17/115/137	-
44	CLA	f	831	-	1/1/13/20	4/29/105/115	-
44	CLA	A	805	-	1/1/14/20	17/38/114/115	-
53	XAT	5	304	-	-	2/31/93/93	0/4/4/4
44	CLA	e	826	-	1/1/15/20	16/37/113/115	-
44	CLA	A	830	-	1/1/12/20	1/21/97/115	-
47	BCR	A	848	-	-	6/29/63/63	0/2/2/2
44	CLA	f	826	-	1/1/15/20	11/39/115/115	-
51	LUT	2	501	-	-	0/29/67/67	0/2/2/2
44	CLA	e	814	-	1/1/10/20	5/12/88/115	-
44	CLA	m	102	-	1/1/10/20	6/12/88/115	-
47	BCR	e	849	-	-	7/29/63/63	0/2/2/2
44	CLA	o	302	-	1/1/10/20	2/8/84/115	-
44	CLA	f	834	-	1/1/10/20	4/13/89/115	-
47	BCR	f	845	-	-	7/29/63/63	0/2/2/2
44	CLA	1	505	-	1/1/10/20	4/12/88/115	-
44	CLA	2	509	-	1/1/12/20	7/21/97/115	-
47	BCR	o	301	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	e	807	-	1/1/10/20	6/12/88/115	-
44	CLA	e	812	-	1/1/8/20	3/7/79/115	-
44	CLA	B	822	-	1/1/11/20	4/18/94/115	-
47	BCR	F	804	-	-	2/29/63/63	0/2/2/2
52	CHL	2	512	-	3/3/16/26	5/17/113/137	-
47	BCR	f	848	-	-	0/29/63/63	0/2/2/2
48	SF4	C	102	3	-	-	0/6/5/5
47	BCR	A	845	-	-	4/29/63/63	0/2/2/2
44	CLA	q	316	-	1/1/11/20	9/17/93/115	-
47	BCR	Q	801	-	-	10/27/61/63	0/2/2/2
44	CLA	A	814	-	1/1/10/20	2/12/88/115	-
44	CLA	q	312	14	1/1/14/20	11/33/109/115	-
44	CLA	p	510	-	1/1/11/20	9/17/93/115	-
44	CLA	5	308	-	1/1/14/20	14/33/109/115	-
44	CLA	e	808	1	1/1/10/20	6/10/86/115	-
44	CLA	f	838	-	1/1/9/20	3/10/82/115	-
44	CLA	q	315	-	-	8/15/91/115	-
44	CLA	e	834	-	1/1/11/20	4/15/91/115	-
44	CLA	f	815	-	1/1/10/20	5/13/89/115	-
44	CLA	1	515	-	1/1/10/20	5/15/87/115	-
44	CLA	f	833	-	1/1/10/20	3/13/89/115	-
47	BCR	F	801	-	-	6/29/63/63	0/2/2/2
44	CLA	A	838	-	1/1/15/20	13/39/115/115	-
44	CLA	A	807	-	1/1/8/20	3/7/79/115	-
44	CLA	3	309	-	-	2/10/86/115	-
44	CLA	e	818	-	1/1/9/20	2/8/80/115	-
47	BCR	e	846	-	-	5/29/63/63	0/2/2/2
44	CLA	A	817	-	1/1/9/20	2/4/82/115	-
44	CLA	f	810	-	1/1/15/20	14/39/115/115	-
44	CLA	B	828	-	1/1/10/20	2/10/86/115	-
44	CLA	A	823	-	1/1/12/20	14/27/99/115	-
44	CLA	e	809	-	1/1/12/20	6/21/97/115	-
44	CLA	f	807	-	1/1/10/20	2/10/86/115	-
45	PQN	e	842	-	-	-	0/2/2/2
44	CLA	K	202	-	1/1/10/20	5/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	CLA	p	507	12	1/1/10/20	2/8/84/115	-
44	CLA	L	302	-	1/1/9/20	2/10/82/115	-
44	CLA	3	301	-	1/1/10/20	4/10/86/115	-
44	CLA	K	205	10	1/1/9/20	2/8/80/115	-
44	CLA	5	309	-	1/1/11/20	6/15/91/115	-
44	CLA	L	303	-	1/1/12/20	10/24/100/115	-
47	BCR	f	850	-	-	2/27/61/63	0/2/2/2
44	CLA	r	317	-	1/1/12/20	7/21/97/115	-
44	CLA	A	829	-	1/1/13/20	5/27/103/115	-
44	CLA	e	824	-	1/1/13/20	8/29/105/115	-
51	LUT	p	502	-	1/1/12/27	8/29/67/67	0/2/2/2
44	CLA	1	510	46	1/1/11/20	8/17/93/115	-
44	CLA	A	816	-	1/1/13/20	12/31/107/115	-
47	BCR	L	305	-	-	8/29/63/63	0/2/2/2
52	CHL	s	517	42	3/3/16/26	2/17/115/137	-
44	CLA	A	835	-	1/1/12/20	10/23/99/115	-
44	CLA	A	836	-	1/1/13/20	10/27/103/115	-
47	BCR	1	503	-	-	4/11/28/63	0/1/1/2
44	CLA	F	803	-	1/1/10/20	4/10/86/115	-
44	CLA	F	802	-	1/1/10/20	4/12/88/115	-

All (2928) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	p	502	LUT	C24-C25	15.30	1.51	1.33
52	p	512	CHL	C2C-C3C	11.22	1.47	1.36
52	s	512	CHL	C2C-C3C	11.20	1.47	1.36
52	1	514	CHL	C2C-C3C	11.16	1.47	1.36
52	p	514	CHL	C2C-C3C	10.96	1.47	1.36
52	p	517	CHL	C2C-C3C	10.90	1.46	1.36
52	r	313	CHL	C2C-C3C	10.87	1.46	1.36
52	s	512	CHL	C1D-C2D	10.71	1.51	1.39
52	s	515	CHL	C2C-C3C	10.64	1.46	1.36
52	s	513	CHL	C2C-C3C	10.53	1.46	1.36
52	q	313	CHL	C2C-C3C	10.52	1.46	1.36
52	s	517	CHL	C2C-C3C	10.50	1.46	1.36
52	p	512	CHL	C1D-C2D	10.45	1.51	1.39
52	r	313	CHL	C1D-C2D	10.41	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	s	513	CHL	C1D-C2D	10.37	1.51	1.39
52	r	316	CHL	C2C-C3C	10.37	1.46	1.36
52	p	517	CHL	C1D-C2D	10.35	1.51	1.39
52	q	313	CHL	C1D-C2D	10.34	1.51	1.39
52	2	516	CHL	C1D-C2D	10.32	1.51	1.39
52	p	514	CHL	C1D-C2D	10.26	1.51	1.39
52	1	512	CHL	C2C-C3C	10.25	1.46	1.36
52	1	512	CHL	C1D-C2D	10.22	1.51	1.39
52	s	517	CHL	C1D-C2D	10.20	1.51	1.39
52	s	515	CHL	C1D-C2D	10.16	1.51	1.39
52	1	517	CHL	C1D-C2D	10.13	1.51	1.39
52	1	514	CHL	C1D-C2D	10.12	1.51	1.39
52	r	314	CHL	C1D-C2D	10.09	1.51	1.39
52	2	515	CHL	C2C-C3C	10.07	1.46	1.36
52	r	316	CHL	C1D-C2D	10.07	1.51	1.39
52	5	314	CHL	C1D-C2D	10.04	1.51	1.39
52	2	512	CHL	C1D-C2D	10.03	1.51	1.39
52	2	513	CHL	C2C-C3C	10.01	1.46	1.36
52	5	317	CHL	C1D-C2D	10.00	1.50	1.39
52	r	314	CHL	C2C-C3C	9.95	1.46	1.36
52	5	314	CHL	C2C-C3C	9.89	1.45	1.36
52	2	515	CHL	C1D-C2D	9.81	1.50	1.39
52	3	302	CHL	C2C-C3C	9.72	1.45	1.36
43	e	801	CL0	C1A-CHA	9.69	1.51	1.40
52	2	513	CHL	C1D-C2D	9.69	1.50	1.39
43	A	801	CL0	C1A-CHA	9.66	1.51	1.40
52	5	315	CHL	C1D-C2D	9.57	1.50	1.39
52	1	517	CHL	C2C-C3C	9.45	1.45	1.36
52	3	315	CHL	C1D-C2D	9.40	1.50	1.39
52	3	315	CHL	C2C-C3C	9.39	1.45	1.36
52	2	516	CHL	C2C-C3C	9.32	1.45	1.36
43	A	801	CL0	C1D-C2D	9.25	1.50	1.39
52	2	512	CHL	C2C-C3C	9.22	1.45	1.36
43	e	801	CL0	C1D-C2D	9.20	1.50	1.39
52	3	302	CHL	C1D-C2D	9.12	1.49	1.39
52	5	315	CHL	C2C-C3C	9.04	1.45	1.36
43	e	801	CL0	C1B-C2B	8.76	1.49	1.39
43	A	801	CL0	C1B-C2B	8.74	1.49	1.39
52	r	314	CHL	C1B-C2B	8.58	1.49	1.39
52	r	316	CHL	C1B-C2B	8.53	1.49	1.39
52	p	517	CHL	C1B-C2B	8.53	1.49	1.39
52	p	514	CHL	C1B-C2B	8.47	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	r	313	CHL	C1B-C2B	8.39	1.49	1.39
52	q	313	CHL	C1B-C2B	8.38	1.49	1.39
52	s	517	CHL	C1B-C2B	8.37	1.49	1.39
52	s	513	CHL	C1B-C2B	8.33	1.49	1.39
52	1	512	CHL	C1B-C2B	8.32	1.49	1.39
52	s	515	CHL	C1B-C2B	8.29	1.49	1.39
52	s	512	CHL	C1B-C2B	8.28	1.49	1.39
52	5	314	CHL	C1B-C2B	8.25	1.48	1.39
52	1	514	CHL	C1B-C2B	8.24	1.48	1.39
52	2	515	CHL	C1B-C2B	8.22	1.48	1.39
52	p	512	CHL	C1B-C2B	8.17	1.48	1.39
52	3	302	CHL	C1B-C2B	8.15	1.48	1.39
52	5	315	CHL	C1B-C2B	8.01	1.48	1.39
52	p	512	CHL	C3B-C4B	8.01	1.49	1.41
52	2	512	CHL	C1B-C2B	8.00	1.48	1.39
52	p	514	CHL	C3B-C4B	7.99	1.49	1.41
52	s	513	CHL	C3B-C4B	7.98	1.49	1.41
52	r	313	CHL	C3B-C4B	7.78	1.49	1.41
52	s	512	CHL	C3B-C4B	7.77	1.49	1.41
52	s	517	CHL	C3B-C4B	7.70	1.48	1.41
52	1	514	CHL	C3B-C4B	7.70	1.48	1.41
52	s	517	CHL	C1A-CHA	7.69	1.48	1.40
52	q	313	CHL	C3B-C4B	7.62	1.48	1.41
52	1	517	CHL	C1B-C2B	7.58	1.48	1.39
52	s	515	CHL	C3B-C4B	7.53	1.48	1.41
52	2	515	CHL	C4B-C3B	7.52	1.48	1.39
52	q	313	CHL	C1A-CHA	7.48	1.48	1.40
52	p	517	CHL	C3B-C4B	7.45	1.48	1.41
52	s	513	CHL	C1A-CHA	7.44	1.48	1.40
52	1	512	CHL	C3B-C4B	7.41	1.48	1.41
52	p	517	CHL	C1A-CHA	7.40	1.48	1.40
52	5	317	CHL	C3B-C4B	7.36	1.48	1.41
52	2	516	CHL	C1B-C2B	7.36	1.47	1.39
52	3	315	CHL	C1B-C2B	7.35	1.47	1.39
52	s	515	CHL	C1A-CHA	7.34	1.48	1.39
45	f	844	PQN	C3-C2	7.33	1.48	1.35
52	r	316	CHL	C1A-CHA	7.31	1.48	1.40
52	r	316	CHL	C3B-C4B	7.25	1.48	1.41
52	p	514	CHL	C1A-CHA	7.24	1.48	1.40
52	5	314	CHL	C3B-C4B	7.22	1.48	1.41
52	2	513	CHL	C1B-C2B	7.17	1.47	1.39
52	5	317	CHL	C1B-C2B	7.15	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	3	302	CHL	C3B-C4B	7.07	1.48	1.41
52	1	512	CHL	C1A-CHA	7.06	1.48	1.40
52	r	313	CHL	C1A-CHA	7.04	1.48	1.40
52	r	314	CHL	C3B-C4B	7.04	1.48	1.41
52	3	302	CHL	C1A-CHA	7.04	1.48	1.40
52	5	314	CHL	C1A-CHA	7.01	1.48	1.40
52	2	513	CHL	C3B-C4B	7.00	1.48	1.41
52	r	314	CHL	C1A-CHA	6.94	1.47	1.40
52	p	512	CHL	C1A-CHA	6.91	1.47	1.40
45	A	841	PQN	C3-C2	6.86	1.47	1.35
52	1	514	CHL	C1A-CHA	6.84	1.48	1.39
52	3	315	CHL	C3B-C4B	6.84	1.48	1.41
52	s	512	CHL	C1A-CHA	6.79	1.47	1.40
52	2	512	CHL	C4B-C3B	6.77	1.47	1.39
52	1	517	CHL	C3B-C4B	6.72	1.47	1.41
52	2	516	CHL	C3A-C2A	-6.68	1.48	1.54
52	2	512	CHL	C1A-CHA	6.66	1.47	1.40
52	5	315	CHL	C1A-CHA	6.65	1.47	1.40
52	2	516	CHL	C1A-CHA	6.61	1.47	1.40
44	2	507	CLA	C2-C3	6.59	1.52	1.33
52	5	315	CHL	C3B-C4B	6.57	1.47	1.41
44	p	509	CLA	MG-NA	6.47	2.21	2.06
52	5	317	CHL	C1A-CHA	6.46	1.47	1.40
52	5	315	CHL	C3D-C4D	-6.44	1.31	1.41
52	2	515	CHL	C3A-C2A	-6.43	1.49	1.54
44	e	818	CLA	MG-NA	6.33	2.21	2.06
45	B	843	PQN	C3-C2	6.32	1.46	1.35
52	2	516	CHL	C4B-C3B	6.20	1.46	1.39
44	f	804	CLA	MG-NA	6.18	2.21	2.06
52	2	513	CHL	C1A-CHA	6.18	1.47	1.39
52	1	517	CHL	C1A-CHA	6.01	1.47	1.39
52	2	515	CHL	C1A-CHA	5.93	1.46	1.40
52	2	516	CHL	C3D-C4D	-5.72	1.32	1.41
52	1	514	CHL	C3D-C4D	-5.72	1.32	1.41
52	1	517	CHL	C3D-C4D	-5.72	1.32	1.41
52	2	515	CHL	C3D-C4D	-5.69	1.32	1.41
52	3	302	CHL	C3D-C4D	-5.63	1.32	1.41
52	2	512	CHL	C3A-C2A	-5.57	1.49	1.54
50	r	318	LMG	O7-C10	5.57	1.45	1.33
52	3	315	CHL	C3D-C4D	-5.55	1.33	1.41
52	5	317	CHL	C3D-C4D	-5.52	1.33	1.41
52	p	514	CHL	C3B-C2B	5.51	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	2	512	CHL	C3D-C4D	-5.50	1.33	1.41
52	p	514	CHL	C3D-C4D	-5.48	1.33	1.41
52	3	302	CHL	C3A-C2A	-5.46	1.50	1.54
52	p	512	CHL	C3B-C2B	5.46	1.47	1.40
52	1	514	CHL	CHC-C4B	5.44	1.48	1.39
52	p	512	CHL	CHC-C4B	5.42	1.48	1.39
52	5	314	CHL	C3D-C4D	-5.41	1.33	1.41
52	3	315	CHL	C1A-CHA	5.40	1.46	1.40
52	s	512	CHL	C3D-C4D	-5.39	1.33	1.41
52	p	512	CHL	C3D-C4D	-5.38	1.33	1.41
52	2	516	CHL	CHB-C4A	-5.36	1.32	1.38
52	3	302	CHL	CHB-C4A	-5.36	1.32	1.38
52	r	313	CHL	C3B-C2B	5.35	1.47	1.40
52	p	517	CHL	C3D-C4D	-5.33	1.33	1.41
52	1	512	CHL	C3D-C4D	-5.31	1.33	1.41
52	r	313	CHL	CHC-C4B	5.30	1.48	1.39
52	s	512	CHL	C3B-C2B	5.30	1.47	1.40
52	r	313	CHL	C3D-C4D	-5.29	1.33	1.41
52	s	513	CHL	C3D-C4D	-5.28	1.33	1.41
52	1	514	CHL	CHD-C4C	5.28	1.49	1.39
52	r	316	CHL	O2D-CGD	5.22	1.46	1.33
52	2	513	CHL	CHB-C4A	-5.21	1.32	1.38
52	1	514	CHL	C3B-C2B	5.21	1.47	1.40
52	r	316	CHL	C3D-C4D	-5.20	1.33	1.41
52	1	514	CHL	OBD-CAD	5.20	1.29	1.22
52	2	512	CHL	O2D-CGD	5.20	1.46	1.33
52	s	512	CHL	CHD-C1D	5.19	1.48	1.39
52	r	314	CHL	C3D-C4D	-5.18	1.33	1.41
52	p	514	CHL	CHC-C4B	5.17	1.48	1.39
52	s	512	CHL	CHC-C4B	5.17	1.48	1.39
52	5	314	CHL	CHB-C4A	-5.16	1.32	1.38
52	1	514	CHL	CHD-C1D	5.16	1.48	1.39
52	s	517	CHL	C3D-C4D	-5.16	1.33	1.41
52	s	512	CHL	CHD-C4C	5.16	1.49	1.39
52	s	515	CHL	C3D-C4D	-5.15	1.33	1.41
52	1	512	CHL	O2D-CGD	5.13	1.45	1.33
52	p	514	CHL	CHD-C1D	5.12	1.47	1.39
52	p	512	CHL	O2D-CGD	5.08	1.45	1.33
52	p	512	CHL	CHD-C4C	5.07	1.49	1.39
52	s	515	CHL	O2D-CGD	5.07	1.45	1.33
52	p	512	CHL	CHD-C1D	5.06	1.47	1.39
52	p	514	CHL	CHD-C4C	5.06	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	s	512	CHL	O2D-CGD	5.06	1.45	1.33
52	r	314	CHL	O2D-CGD	5.06	1.45	1.33
52	p	514	CHL	O2D-CGD	5.05	1.45	1.33
52	r	313	CHL	O2D-CGD	5.05	1.45	1.33
52	p	512	CHL	CHB-C1B	5.04	1.47	1.39
52	p	517	CHL	CHC-C4B	5.04	1.47	1.39
52	p	512	CHL	OBD-CAD	5.04	1.28	1.22
52	5	315	CHL	C3A-C2A	-5.04	1.50	1.54
52	1	514	CHL	C3D-C2D	5.04	1.48	1.39
52	q	313	CHL	O2D-CGD	5.04	1.45	1.33
52	s	513	CHL	C3B-C2B	5.03	1.47	1.40
52	1	512	CHL	OBD-CAD	5.01	1.28	1.22
52	r	313	CHL	OBD-CAD	5.01	1.28	1.22
52	2	515	CHL	CHB-C4A	-5.00	1.32	1.38
52	s	513	CHL	O2D-CGD	5.00	1.45	1.33
52	2	513	CHL	O2D-CGD	5.00	1.45	1.33
52	5	317	CHL	O2D-CGD	4.99	1.45	1.33
52	2	515	CHL	O2D-CGD	4.98	1.45	1.33
52	p	514	CHL	CHB-C1B	4.98	1.47	1.39
52	1	517	CHL	O2D-CGD	4.97	1.45	1.33
52	3	315	CHL	O2D-CGD	4.97	1.45	1.33
52	s	513	CHL	CHC-C4B	4.97	1.47	1.39
52	p	517	CHL	CHD-C4C	4.97	1.48	1.39
52	s	515	CHL	C3B-C2B	4.96	1.47	1.40
52	s	515	CHL	OBD-CAD	4.96	1.28	1.22
52	5	314	CHL	O2D-CGD	4.95	1.45	1.33
52	r	313	CHL	CHB-C1B	4.95	1.47	1.39
52	r	314	CHL	C3A-C2A	-4.94	1.50	1.54
52	1	512	CHL	C3B-C2B	4.94	1.47	1.40
52	1	514	CHL	CHB-C1B	4.93	1.47	1.39
52	p	517	CHL	CHB-C1B	4.93	1.47	1.39
52	s	512	CHL	CHB-C1B	4.92	1.47	1.39
52	q	313	CHL	CHC-C4B	4.92	1.47	1.39
52	p	517	CHL	O2D-CGD	4.91	1.45	1.33
52	3	315	CHL	CHC-C4B	4.90	1.47	1.39
52	r	316	CHL	OBD-CAD	4.90	1.28	1.22
52	r	313	CHL	CHD-C4C	4.89	1.48	1.39
52	s	513	CHL	OBD-CAD	4.89	1.28	1.22
52	q	313	CHL	C3B-C2B	4.89	1.47	1.40
52	r	314	CHL	OBD-CAD	4.88	1.28	1.22
52	2	516	CHL	O2D-CGD	4.87	1.45	1.33
52	3	315	CHL	OBD-CAD	4.86	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	1	517	CHL	CHC-C4B	4.86	1.47	1.39
52	p	517	CHL	OBD-CAD	4.86	1.28	1.22
52	p	512	CHL	C3D-C2D	4.85	1.47	1.39
52	5	317	CHL	CHC-C4B	4.84	1.47	1.39
52	s	517	CHL	CHB-C4A	-4.84	1.32	1.38
52	p	514	CHL	OBD-CAD	4.84	1.28	1.22
52	3	315	CHL	CHB-C4A	-4.83	1.32	1.38
52	s	517	CHL	OBD-CAD	4.83	1.28	1.22
52	r	313	CHL	C3D-C2D	4.82	1.47	1.39
52	s	512	CHL	OBD-CAD	4.82	1.28	1.22
52	p	517	CHL	C3B-C2B	4.82	1.46	1.40
52	s	515	CHL	CHD-C4C	4.82	1.48	1.39
52	1	512	CHL	CHC-C4B	4.81	1.47	1.39
52	s	517	CHL	CHC-C4B	4.80	1.47	1.39
52	1	514	CHL	O2D-CGD	4.80	1.45	1.33
52	s	517	CHL	O2D-CGD	4.80	1.45	1.33
52	p	517	CHL	CHD-C1D	4.79	1.47	1.39
52	s	512	CHL	C3D-C2D	4.78	1.47	1.39
52	r	313	CHL	CHD-C1D	4.77	1.47	1.39
52	p	512	CHL	CHC-C1C	4.76	1.48	1.39
52	s	512	CHL	CHC-C1C	4.75	1.48	1.39
52	s	517	CHL	CHD-C4C	4.75	1.48	1.39
52	s	517	CHL	C3B-C2B	4.75	1.46	1.40
52	p	514	CHL	C3D-C2D	4.75	1.47	1.39
52	1	512	CHL	CHB-C1B	4.74	1.47	1.39
52	s	513	CHL	CHB-C1B	4.74	1.47	1.39
52	1	512	CHL	CHD-C1D	4.73	1.47	1.39
52	3	302	CHL	OBD-CAD	4.73	1.28	1.22
52	s	515	CHL	CHC-C4B	4.73	1.47	1.39
52	s	515	CHL	CHD-C1D	4.72	1.47	1.39
52	s	513	CHL	CHD-C4C	4.72	1.48	1.39
52	2	515	CHL	CHD-C4C	4.72	1.48	1.39
52	1	512	CHL	CHD-C4C	4.72	1.48	1.39
52	r	316	CHL	CHD-C4C	4.72	1.48	1.39
52	r	313	CHL	CHC-C1C	4.71	1.48	1.39
45	e	842	PQN	C10-C5	4.71	1.48	1.40
52	s	513	CHL	CHD-C1D	4.71	1.47	1.39
52	2	515	CHL	CHC-C4B	4.70	1.47	1.39
52	1	514	CHL	CHC-C1C	4.69	1.48	1.39
52	r	316	CHL	C3B-C2B	4.69	1.46	1.40
52	r	316	CHL	CHD-C1D	4.67	1.47	1.39
44	s	504	CLA	C3B-C4B	4.66	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	r	314	CHL	CHD-C4C	4.66	1.48	1.39
52	5	314	CHL	CHC-C4B	4.66	1.47	1.39
52	p	517	CHL	C3D-C2D	4.66	1.47	1.39
45	f	844	PQN	C10-C5	4.64	1.48	1.40
52	2	512	CHL	CHB-C4A	-4.63	1.33	1.38
52	3	302	CHL	O2D-CGD	4.62	1.44	1.33
52	5	314	CHL	OBD-CAD	4.62	1.28	1.22
52	q	313	CHL	CHD-C4C	4.61	1.48	1.39
52	r	316	CHL	CHB-C1B	4.61	1.47	1.39
44	q	304	CLA	C2B-C1B	4.61	1.49	1.39
52	q	313	CHL	CHB-C1B	4.61	1.47	1.39
52	2	516	CHL	OBD-CAD	4.61	1.28	1.22
52	s	513	CHL	C3D-C2D	4.61	1.47	1.39
52	5	317	CHL	CHD-C4C	4.61	1.48	1.39
52	2	515	CHL	CHD-C1D	4.60	1.47	1.39
52	5	314	CHL	C3B-C2B	4.60	1.46	1.40
52	p	514	CHL	CHC-C1C	4.60	1.48	1.39
52	5	315	CHL	O2D-CGD	4.59	1.44	1.33
44	s	504	CLA	C1B-C2B	4.59	1.49	1.41
52	r	314	CHL	CHB-C4A	-4.58	1.33	1.38
52	5	315	CHL	CHB-C4A	-4.57	1.33	1.38
52	q	313	CHL	CHD-C1D	4.57	1.47	1.39
52	s	517	CHL	CHD-C1D	4.55	1.47	1.39
52	s	515	CHL	CHB-C1B	4.55	1.47	1.39
52	2	516	CHL	CHD-C4C	4.54	1.48	1.39
52	3	302	CHL	C3B-C2B	4.54	1.46	1.40
52	s	515	CHL	CHB-C4A	-4.54	1.33	1.38
52	5	314	CHL	CHD-C4C	4.53	1.48	1.39
52	2	515	CHL	O2A-CGA	4.53	1.45	1.30
52	5	315	CHL	CHB-C1B	4.52	1.46	1.39
52	p	517	CHL	CHC-C1C	4.52	1.48	1.39
52	r	316	CHL	CHC-C4B	4.52	1.46	1.39
52	3	315	CHL	C3A-C2A	-4.52	1.50	1.54
52	q	313	CHL	CHB-C4A	-4.50	1.33	1.38
52	1	512	CHL	CHB-C4A	-4.50	1.33	1.38
52	s	513	CHL	CHB-C4A	-4.50	1.33	1.38
52	2	512	CHL	CHD-C4C	4.50	1.48	1.39
52	2	512	CHL	CHC-C4B	4.50	1.46	1.39
52	2	512	CHL	OBD-CAD	4.50	1.28	1.22
52	r	314	CHL	CHB-C1B	4.49	1.46	1.39
52	2	516	CHL	CHD-C1D	4.49	1.46	1.39
52	1	517	CHL	CHD-C1D	4.49	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	5	315	CHL	O2A-CGA	4.48	1.45	1.30
52	s	517	CHL	C3D-C2D	4.48	1.47	1.39
52	2	512	CHL	CHD-C1D	4.47	1.46	1.39
52	2	513	CHL	CHC-C4B	4.46	1.46	1.39
52	3	302	CHL	CHD-C1D	4.46	1.46	1.39
52	5	317	CHL	CHD-C1D	4.46	1.46	1.39
52	r	314	CHL	CHD-C1D	4.46	1.46	1.39
52	1	512	CHL	C3D-C2D	4.45	1.47	1.39
52	q	313	CHL	CHC-C1C	4.44	1.47	1.39
52	r	316	CHL	C3D-C2D	4.44	1.47	1.39
52	5	317	CHL	C2C-C3C	4.44	1.46	1.37
52	5	317	CHL	OBD-CAD	4.44	1.28	1.22
52	r	316	CHL	CHB-C4A	-4.43	1.33	1.38
54	Q	802	SQD	O8-S	4.43	1.63	1.47
54	Q	803	SQD	O8-S	4.42	1.63	1.47
52	5	317	CHL	C3B-C2B	4.42	1.46	1.40
52	5	315	CHL	OBD-CAD	4.42	1.28	1.22
52	1	517	CHL	OBD-CAD	4.42	1.28	1.22
52	1	517	CHL	CHB-C4A	-4.42	1.33	1.38
44	p	509	CLA	CBB-CAB	4.42	1.51	1.30
52	5	317	CHL	C3D-C2D	4.41	1.47	1.39
52	3	302	CHL	CHD-C4C	4.41	1.47	1.39
52	s	517	CHL	CHC-C1C	4.41	1.47	1.39
44	e	818	CLA	CBB-CAB	4.40	1.51	1.30
52	s	513	CHL	CHC-C1C	4.40	1.47	1.39
43	e	801	CL0	C3A-C4A	-4.40	1.47	1.50
52	r	314	CHL	C3B-C2B	4.39	1.46	1.40
43	A	801	CL0	C3A-C4A	-4.38	1.47	1.50
52	3	315	CHL	CHB-C1B	4.38	1.46	1.39
52	2	513	CHL	CHB-C1B	4.37	1.46	1.39
52	3	302	CHL	CHC-C4B	4.37	1.46	1.39
44	3	309	CLA	C1B-C2B	4.37	1.48	1.41
52	s	517	CHL	CHB-C1B	4.37	1.46	1.39
50	F	805	LMG	O8-C28	4.36	1.46	1.33
52	1	517	CHL	C3B-C2B	4.36	1.46	1.40
52	r	314	CHL	CHC-C4B	4.36	1.46	1.39
52	2	512	CHL	CHB-C1B	4.35	1.46	1.39
52	3	315	CHL	CHC-C1C	4.35	1.47	1.39
52	s	515	CHL	C3D-C2D	4.34	1.47	1.39
50	5	301	LMG	O8-C28	4.34	1.46	1.33
52	5	315	CHL	CHD-C1D	4.34	1.46	1.39
52	2	515	CHL	OBD-CAD	4.33	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f	804	CLA	CBB-CAB	4.32	1.51	1.30
46	A	844	LHG	O8-C23	4.32	1.45	1.33
52	1	517	CHL	CHC-C1C	4.32	1.47	1.39
52	2	512	CHL	O2A-CGA	4.31	1.46	1.33
52	5	315	CHL	CHD-C4C	4.31	1.47	1.39
52	2	513	CHL	CHD-C1D	4.31	1.46	1.39
44	3	309	CLA	C3B-C4B	4.30	1.48	1.39
52	1	517	CHL	CHD-C4C	4.30	1.47	1.39
52	1	512	CHL	CHC-C1C	4.29	1.47	1.39
52	r	316	CHL	C3A-C2A	-4.29	1.51	1.54
52	s	513	CHL	O2A-CGA	4.29	1.45	1.33
52	1	517	CHL	CHB-C1B	4.29	1.46	1.39
52	s	515	CHL	CHC-C1C	4.28	1.47	1.39
54	Q	803	SQD	O47-C7	4.28	1.46	1.34
52	3	302	CHL	CHC-C1C	4.28	1.47	1.39
52	3	302	CHL	C3D-C2D	4.28	1.46	1.39
52	2	516	CHL	CHC-C4B	4.28	1.46	1.39
52	5	314	CHL	CHD-C1D	4.28	1.46	1.39
52	2	513	CHL	CHD-C4C	4.27	1.47	1.39
49	m	104	DGD	O2G-C1B	4.26	1.46	1.34
52	p	517	CHL	CHB-C4A	-4.26	1.33	1.38
50	m	105	LMG	O8-C28	4.26	1.45	1.33
52	5	314	CHL	C3D-C2D	4.25	1.46	1.39
54	Q	802	SQD	O48-C23	4.25	1.45	1.33
46	B	851	LHG	O8-C23	4.25	1.45	1.33
52	5	314	CHL	CHB-C1B	4.25	1.46	1.39
46	B	851	LHG	O7-C7	4.25	1.46	1.34
54	Q	803	SQD	O48-C23	4.25	1.45	1.33
52	5	314	CHL	O2A-CGA	4.24	1.46	1.33
44	A	817	CLA	O1D-CGD	4.23	1.36	1.20
52	s	512	CHL	CHB-C4A	-4.22	1.33	1.38
52	1	512	CHL	C3A-C2A	-4.22	1.51	1.54
52	2	515	CHL	CHB-C1B	4.20	1.46	1.39
52	2	512	CHL	CHC-C1C	4.19	1.47	1.39
46	s	516	LHG	O8-C23	4.19	1.45	1.33
52	r	314	CHL	O2A-CGA	4.19	1.45	1.33
49	f	851	DGD	O1G-C1A	4.19	1.45	1.33
52	p	512	CHL	CHB-C4A	-4.17	1.33	1.38
52	s	517	CHL	C3A-C2A	-4.17	1.51	1.54
52	1	512	CHL	O2A-CGA	4.16	1.45	1.33
52	r	313	CHL	CHB-C4A	-4.16	1.33	1.38
52	3	302	CHL	CHB-C1B	4.16	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	2	519	LMG	O8-C28	4.16	1.45	1.33
52	q	313	CHL	C3A-C2A	-4.16	1.51	1.54
46	1	516	LHG	O8-C23	4.15	1.45	1.33
46	O	601	LHG	O8-C23	4.15	1.45	1.33
52	s	512	CHL	O2A-CGA	4.15	1.45	1.33
49	B	850	DGD	O1G-C1A	4.15	1.45	1.33
46	p	516	LHG	O8-C23	4.15	1.45	1.33
46	f	852	LHG	O8-C23	4.15	1.45	1.33
49	m	104	DGD	O1G-C1A	4.15	1.45	1.33
52	r	314	CHL	C3D-C2D	4.14	1.46	1.39
52	r	313	CHL	O2A-CGA	4.14	1.45	1.33
52	3	315	CHL	C3D-C2D	4.14	1.46	1.39
49	J	103	DGD	O1G-C1A	4.13	1.45	1.33
52	q	313	CHL	O2A-CGA	4.13	1.45	1.33
46	O	601	LHG	O7-C7	4.12	1.45	1.34
52	p	514	CHL	O2A-CGA	4.12	1.45	1.33
46	e	844	LHG	O8-C23	4.12	1.45	1.33
52	r	316	CHL	CHC-C1C	4.11	1.47	1.39
46	f	852	LHG	O7-C7	4.10	1.45	1.34
52	5	314	CHL	C3A-C2A	-4.09	1.51	1.54
52	p	512	CHL	O2A-CGA	4.09	1.45	1.33
52	s	517	CHL	O2A-CGA	4.09	1.45	1.33
54	Q	802	SQD	O47-C7	4.08	1.45	1.34
46	p	516	LHG	O7-C7	4.08	1.45	1.34
52	5	315	CHL	C3B-C2B	4.08	1.45	1.40
50	2	519	LMG	O7-C10	4.05	1.45	1.34
52	5	314	CHL	CHC-C1C	4.05	1.47	1.39
50	5	301	LMG	O7-C10	4.04	1.45	1.34
52	5	317	CHL	CHB-C1B	4.03	1.46	1.39
50	F	805	LMG	O7-C10	4.03	1.45	1.34
52	2	515	CHL	C3D-C2D	4.02	1.46	1.39
50	m	105	LMG	O7-C10	4.01	1.45	1.34
52	3	302	CHL	O2A-CGA	4.01	1.45	1.33
52	2	516	CHL	CHC-C1C	4.01	1.47	1.39
49	J	103	DGD	O2G-C1B	4.01	1.45	1.34
44	5	305	CLA	C3B-C4B	4.01	1.48	1.39
46	e	845	LHG	O7-C7	4.00	1.45	1.34
46	A	843	LHG	O8-C23	4.00	1.45	1.33
52	2	516	CHL	CHB-C1B	4.00	1.46	1.39
47	I	101	BCR	C30-C25	-3.99	1.48	1.53
52	5	315	CHL	CHC-C4B	3.99	1.46	1.39
49	f	851	DGD	O2G-C1B	3.98	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	p	514	CHL	CHB-C4A	-3.97	1.33	1.38
52	1	514	CHL	CHB-C4A	-3.97	1.33	1.38
52	3	315	CHL	CHD-C4C	3.94	1.46	1.39
46	e	844	LHG	O7-C7	3.93	1.45	1.34
46	2	517	LHG	O8-C23	3.93	1.44	1.33
52	2	516	CHL	C3D-C2D	3.93	1.46	1.39
52	2	513	CHL	C3B-C2B	3.93	1.45	1.40
46	s	516	LHG	O7-C7	3.93	1.45	1.34
50	F	806	LMG	O8-C28	3.92	1.44	1.33
52	2	515	CHL	CHC-C1C	3.91	1.46	1.39
50	F	806	LMG	O7-C10	3.91	1.45	1.34
52	2	513	CHL	CHC-C1C	3.90	1.46	1.39
46	2	517	LHG	O7-C7	3.89	1.45	1.34
52	r	314	CHL	CHC-C1C	3.87	1.46	1.39
47	I	101	BCR	C1-C6	-3.84	1.48	1.53
46	1	516	LHG	O7-C7	3.83	1.45	1.34
52	5	317	CHL	CHC-C1C	3.83	1.46	1.39
52	s	513	CHL	C3A-C2A	-3.82	1.51	1.54
47	B	852	BCR	C30-C25	-3.80	1.48	1.53
52	3	315	CHL	C3B-C2B	3.80	1.45	1.40
52	1	517	CHL	C3D-C2D	3.79	1.46	1.39
52	2	512	CHL	C3D-C2D	3.77	1.46	1.39
52	p	517	CHL	C3A-C2A	-3.77	1.51	1.54
44	B	812	CLA	CAB-C3B	-3.76	1.43	1.50
46	A	844	LHG	O7-C7	3.75	1.44	1.34
47	B	845	BCR	C30-C25	-3.73	1.49	1.53
44	q	307	CLA	C1D-ND	3.73	1.42	1.37
52	s	512	CHL	C3A-C2A	-3.71	1.51	1.54
44	o	302	CLA	C1D-ND	3.71	1.42	1.37
44	5	305	CLA	C1B-C2B	3.70	1.47	1.41
52	r	313	CHL	C3A-C2A	-3.70	1.51	1.54
45	A	841	PQN	C10-C5	3.70	1.46	1.40
44	1	511	CLA	C1D-ND	3.70	1.42	1.37
44	n	205	CLA	C1D-ND	3.70	1.42	1.37
44	m	101	CLA	C1D-ND	3.69	1.42	1.37
52	3	315	CHL	CHD-C1D	3.68	1.45	1.39
46	A	843	LHG	O7-C7	3.68	1.44	1.34
44	p	513	CLA	C1D-ND	3.67	1.42	1.37
44	r	310	CLA	C1D-ND	3.66	1.42	1.37
52	5	315	CHL	CBD-CGD	-3.66	1.47	1.52
49	B	850	DGD	O2G-C1B	3.65	1.44	1.34
43	e	801	CL0	C4B-C3B	3.65	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	q	308	CLA	C1D-ND	3.63	1.42	1.37
43	A	801	CL0	C4B-C3B	3.62	1.43	1.39
44	n	201	CLA	C1D-ND	3.62	1.42	1.37
44	1	515	CLA	CAD-C3D	-3.62	1.45	1.50
52	5	315	CHL	CHC-C1C	3.62	1.46	1.39
44	m	102	CLA	C1D-ND	3.61	1.42	1.37
47	F	804	BCR	C1-C6	-3.61	1.49	1.53
44	n	202	CLA	C1D-ND	3.61	1.42	1.37
44	q	305	CLA	C1D-ND	3.60	1.42	1.37
44	3	307	CLA	C4B-NB	3.59	1.42	1.37
44	f	804	CLA	MG-ND	-3.58	1.98	2.05
44	r	308	CLA	C1D-ND	3.58	1.42	1.37
44	q	316	CLA	C1D-ND	3.57	1.42	1.37
44	s	506	CLA	C1D-ND	3.57	1.42	1.37
44	f	804	CLA	C2A-C1A	-3.57	1.50	1.53
44	e	817	CLA	C1D-ND	3.56	1.42	1.37
44	e	843	CLA	C1D-ND	3.56	1.42	1.37
44	q	309	CLA	C1D-ND	3.56	1.42	1.37
44	p	515	CLA	C1D-ND	3.56	1.42	1.37
47	A	845	BCR	C1-C6	-3.56	1.49	1.53
44	q	312	CLA	C1D-ND	3.55	1.42	1.37
44	A	829	CLA	CMB-C2B	-3.55	1.43	1.50
44	e	836	CLA	C1D-ND	3.53	1.42	1.37
44	q	310	CLA	C1D-ND	3.53	1.42	1.37
44	q	306	CLA	C1D-ND	3.52	1.42	1.37
44	s	510	CLA	C1D-ND	3.52	1.42	1.37
44	s	509	CLA	C1D-ND	3.51	1.42	1.37
44	f	843	CLA	C1D-ND	3.50	1.42	1.37
44	q	311	CLA	C1D-ND	3.50	1.42	1.37
44	r	312	CLA	C1D-ND	3.49	1.42	1.37
44	f	839	CLA	C1D-ND	3.49	1.42	1.37
44	n	203	CLA	C1D-ND	3.49	1.42	1.37
47	A	845	BCR	C30-C25	-3.49	1.49	1.53
44	q	304	CLA	C1D-ND	3.49	1.42	1.37
44	q	315	CLA	C1D-ND	3.49	1.42	1.37
44	r	315	CLA	C1D-ND	3.48	1.42	1.37
44	e	809	CLA	C1D-ND	3.47	1.42	1.37
44	p	511	CLA	C1D-ND	3.47	1.42	1.37
44	f	813	CLA	C1D-ND	3.47	1.42	1.37
44	r	305	CLA	C1D-ND	3.47	1.42	1.37
44	e	835	CLA	C1D-ND	3.46	1.42	1.37
44	f	823	CLA	C1D-ND	3.46	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	513	CLA	C1D-ND	3.45	1.42	1.37
44	s	511	CLA	C1D-ND	3.45	1.42	1.37
44	e	818	CLA	MG-ND	-3.45	1.98	2.05
44	s	514	CLA	C1D-ND	3.45	1.42	1.37
44	r	309	CLA	C1D-ND	3.44	1.42	1.37
44	e	807	CLA	C1D-ND	3.44	1.42	1.37
44	r	317	CLA	C1D-ND	3.44	1.42	1.37
44	2	508	CLA	C1D-ND	3.44	1.42	1.37
44	f	815	CLA	C1D-ND	3.44	1.42	1.37
44	o	304	CLA	C1D-ND	3.43	1.42	1.37
44	s	508	CLA	C1D-ND	3.43	1.42	1.37
44	e	808	CLA	C1D-ND	3.43	1.42	1.37
44	e	806	CLA	C1D-ND	3.43	1.42	1.37
44	3	307	CLA	C1D-ND	3.42	1.42	1.37
44	j	802	CLA	C1D-ND	3.42	1.42	1.37
44	f	811	CLA	C1D-ND	3.42	1.42	1.37
44	f	807	CLA	C1D-ND	3.42	1.42	1.37
44	e	839	CLA	C1D-ND	3.42	1.42	1.37
52	5	315	CHL	C3D-C2D	3.42	1.45	1.39
44	f	808	CLA	C1D-ND	3.42	1.42	1.37
44	f	822	CLA	C1D-ND	3.41	1.42	1.37
44	e	802	CLA	C1D-ND	3.41	1.42	1.37
47	B	847	BCR	C30-C25	-3.41	1.49	1.53
44	A	831	CLA	CAB-C3B	-3.41	1.43	1.50
44	r	311	CLA	C1D-ND	3.41	1.42	1.37
44	e	841	CLA	C1D-ND	3.40	1.42	1.37
44	e	815	CLA	C1D-ND	3.40	1.42	1.37
44	p	506	CLA	C1D-ND	3.40	1.42	1.37
44	r	304	CLA	C1D-ND	3.40	1.42	1.37
44	f	824	CLA	C1D-ND	3.40	1.42	1.37
44	e	804	CLA	C1D-ND	3.40	1.42	1.37
44	p	507	CLA	CAB-C3B	-3.39	1.43	1.50
44	e	813	CLA	C1D-ND	3.39	1.42	1.37
44	r	306	CLA	C1D-ND	3.39	1.42	1.37
44	f	803	CLA	C2D-C1D	3.39	1.48	1.42
44	f	836	CLA	C1D-ND	3.39	1.42	1.37
44	f	819	CLA	C1D-ND	3.39	1.42	1.37
44	p	508	CLA	C1D-ND	3.38	1.42	1.37
44	f	835	CLA	C1D-ND	3.38	1.42	1.37
44	3	312	CLA	C1D-ND	3.38	1.42	1.37
44	e	816	CLA	C1D-ND	3.38	1.42	1.37
44	r	307	CLA	C1D-ND	3.38	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f	806	CLA	C1D-ND	3.37	1.42	1.37
44	e	821	CLA	C1D-ND	3.37	1.42	1.37
44	p	505	CLA	C1D-ND	3.37	1.42	1.37
44	f	830	CLA	C1D-ND	3.36	1.42	1.37
44	e	832	CLA	C1D-ND	3.36	1.42	1.37
44	f	837	CLA	C1D-ND	3.36	1.42	1.37
44	e	829	CLA	C1D-ND	3.36	1.42	1.37
44	e	814	CLA	C1D-ND	3.36	1.42	1.37
44	p	509	CLA	MG-ND	-3.36	1.99	2.05
44	e	811	CLA	C1D-ND	3.36	1.42	1.37
44	1	504	CLA	C1D-ND	3.36	1.42	1.37
44	e	828	CLA	C1D-ND	3.35	1.42	1.37
44	f	832	CLA	C1D-ND	3.35	1.42	1.37
45	B	843	PQN	C10-C5	3.35	1.46	1.40
44	f	840	CLA	C1D-ND	3.35	1.42	1.37
44	A	823	CLA	C2A-C1A	-3.35	1.50	1.53
44	f	810	CLA	C1D-ND	3.34	1.42	1.37
44	q	314	CLA	C1D-ND	3.34	1.42	1.37
44	f	828	CLA	C1D-ND	3.34	1.42	1.37
44	e	823	CLA	C1D-ND	3.34	1.42	1.37
44	f	812	CLA	C1D-ND	3.33	1.42	1.37
44	1	513	CLA	C4B-NB	3.33	1.42	1.37
44	e	853	CLA	C1D-ND	3.33	1.42	1.37
44	e	810	CLA	C1D-ND	3.33	1.42	1.37
44	e	826	CLA	C1D-ND	3.33	1.42	1.37
44	o	303	CLA	C1D-ND	3.33	1.42	1.37
44	f	801	CLA	C1D-ND	3.33	1.42	1.37
44	e	840	CLA	C1D-ND	3.32	1.42	1.37
44	e	852	CLA	C1D-ND	3.32	1.42	1.37
44	s	507	CLA	C1D-ND	3.32	1.42	1.37
44	e	838	CLA	C1D-ND	3.32	1.42	1.37
44	e	803	CLA	C1D-ND	3.32	1.42	1.37
44	s	505	CLA	C1D-ND	3.32	1.42	1.37
44	m	101	CLA	C4B-NB	3.32	1.42	1.37
44	f	830	CLA	CAB-C3B	-3.32	1.44	1.50
44	e	826	CLA	CAB-C3B	-3.31	1.44	1.50
44	f	809	CLA	C1D-ND	3.31	1.42	1.37
47	B	852	BCR	C1-C6	-3.31	1.49	1.53
44	f	814	CLA	C1D-ND	3.31	1.42	1.37
44	B	813	CLA	C1D-ND	3.30	1.42	1.37
44	2	504	CLA	C1D-ND	3.30	1.42	1.37
52	p	514	CHL	C3A-C2A	-3.30	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f	817	CLA	C1D-ND	3.30	1.42	1.37
52	5	317	CHL	CHB-C4A	-3.30	1.33	1.38
44	3	313	CLA	C1D-ND	3.30	1.42	1.37
44	f	818	CLA	C1D-ND	3.29	1.42	1.37
44	1	509	CLA	C1D-ND	3.29	1.42	1.37
53	5	304	XAT	O24-C25	-3.29	1.42	1.46
44	f	825	CLA	C1D-ND	3.29	1.42	1.37
44	f	833	CLA	C1D-ND	3.29	1.42	1.37
44	f	820	CLA	C1D-ND	3.28	1.42	1.37
44	e	837	CLA	C1D-ND	3.28	1.42	1.37
44	f	826	CLA	C1D-ND	3.28	1.42	1.37
44	e	825	CLA	C1D-ND	3.27	1.42	1.37
44	f	842	CLA	C1D-ND	3.27	1.42	1.37
44	K	202	CLA	C1D-ND	3.27	1.42	1.37
44	e	824	CLA	C1D-ND	3.26	1.42	1.37
44	p	507	CLA	C1D-ND	3.26	1.42	1.37
44	e	820	CLA	C1D-ND	3.26	1.42	1.37
47	A	846	BCR	C1-C6	-3.25	1.49	1.53
44	f	821	CLA	C1D-ND	3.25	1.42	1.37
44	p	510	CLA	C1D-ND	3.25	1.42	1.37
44	e	805	CLA	C1D-ND	3.25	1.42	1.37
44	A	838	CLA	C1D-ND	3.24	1.42	1.37
44	f	831	CLA	C1D-ND	3.24	1.42	1.37
52	q	313	CHL	C3D-C2D	3.24	1.47	1.37
44	s	504	CLA	C1D-ND	3.24	1.42	1.37
44	f	841	CLA	C1D-ND	3.24	1.42	1.37
44	e	834	CLA	C1D-ND	3.24	1.42	1.37
44	L	302	CLA	C1D-ND	3.23	1.42	1.37
44	e	819	CLA	C1D-ND	3.23	1.42	1.37
44	3	306	CLA	C1D-ND	3.23	1.42	1.37
53	5	304	XAT	C22-C21	-3.23	1.49	1.54
52	3	302	CHL	CBD-CGD	-3.23	1.48	1.52
44	p	504	CLA	C1D-ND	3.22	1.42	1.37
44	f	801	CLA	CAB-C3B	-3.22	1.44	1.50
44	1	515	CLA	C1D-ND	3.22	1.42	1.37
44	e	830	CLA	C1D-ND	3.22	1.42	1.37
44	f	827	CLA	C1D-ND	3.22	1.42	1.37
44	e	822	CLA	C1D-ND	3.21	1.42	1.37
44	q	310	CLA	C4B-NB	3.21	1.42	1.37
44	f	813	CLA	CAB-C3B	-3.21	1.44	1.50
44	p	515	CLA	C4B-NB	3.21	1.42	1.37
44	s	509	CLA	C4B-NB	3.20	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f	838	CLA	C1D-ND	3.20	1.42	1.37
44	B	830	CLA	CMB-C2B	-3.20	1.44	1.50
44	B	821	CLA	C1D-ND	3.20	1.42	1.37
44	F	802	CLA	C1D-ND	3.20	1.42	1.37
44	B	829	CLA	CMB-C2B	-3.19	1.44	1.50
44	e	833	CLA	C1D-ND	3.18	1.42	1.37
44	A	815	CLA	C1D-ND	3.18	1.42	1.37
44	3	307	CLA	C1B-C2B	3.18	1.50	1.43
44	f	834	CLA	C1D-ND	3.18	1.42	1.37
44	J	101	CLA	C1D-ND	3.17	1.42	1.37
44	e	829	CLA	C4B-NB	3.17	1.42	1.37
44	2	509	CLA	C1D-ND	3.17	1.42	1.37
44	r	305	CLA	C4B-NB	3.16	1.42	1.37
44	A	836	CLA	CMB-C2B	-3.16	1.44	1.50
44	r	311	CLA	C4B-NB	3.16	1.42	1.37
44	e	812	CLA	C1D-ND	3.16	1.42	1.37
44	p	510	CLA	C4B-NB	3.15	1.42	1.37
44	3	313	CLA	C4B-NB	3.14	1.42	1.37
44	e	835	CLA	C4B-NB	3.14	1.42	1.37
44	e	831	CLA	C1D-ND	3.14	1.42	1.37
44	3	318	CLA	CAB-C3B	-3.14	1.44	1.50
44	f	829	CLA	C1D-ND	3.14	1.42	1.37
44	2	507	CLA	C1D-ND	3.13	1.42	1.37
44	q	304	CLA	C3B-C4B	3.13	1.49	1.40
44	1	505	CLA	C4B-NB	3.12	1.42	1.37
44	3	310	CLA	C4B-NB	3.12	1.42	1.37
44	5	312	CLA	C1D-ND	3.12	1.42	1.37
44	B	814	CLA	C1B-NB	-3.12	1.33	1.37
44	n	205	CLA	C4B-NB	3.11	1.42	1.37
44	K	205	CLA	C4B-NB	3.11	1.42	1.37
44	j	802	CLA	C4B-NB	3.11	1.41	1.37
44	f	816	CLA	C1D-ND	3.11	1.41	1.37
44	f	805	CLA	C1D-ND	3.11	1.41	1.37
52	3	315	CHL	CBD-CGD	-3.10	1.48	1.52
44	r	310	CLA	C4B-NB	3.10	1.41	1.37
44	p	513	CLA	C4B-NB	3.10	1.41	1.37
47	B	844	BCR	C30-C25	-3.10	1.49	1.53
44	s	511	CLA	C4B-NB	3.10	1.41	1.37
44	r	304	CLA	CAB-C3B	-3.09	1.44	1.50
44	o	302	CLA	CAB-C3B	-3.09	1.44	1.50
44	m	102	CLA	C4B-NB	3.09	1.41	1.37
44	f	837	CLA	C4B-NB	3.09	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	e	815	CLA	C4B-NB	3.09	1.41	1.37
47	B	848	BCR	C30-C25	-3.09	1.49	1.53
44	q	306	CLA	C4B-NB	3.08	1.41	1.37
47	K	204	BCR	C30-C25	-3.08	1.49	1.53
44	f	822	CLA	C4B-NB	3.07	1.41	1.37
44	m	101	CLA	C4B-C3B	3.06	1.50	1.43
44	2	511	CLA	C1D-ND	3.06	1.41	1.37
44	A	823	CLA	C1D-ND	3.06	1.41	1.37
44	o	302	CLA	C4B-NB	3.06	1.41	1.37
50	r	318	LMG	O7-C8	-3.05	1.42	1.46
44	A	826	CLA	C1B-NB	-3.05	1.33	1.37
44	5	310	CLA	C1D-ND	3.05	1.41	1.37
44	e	813	CLA	C4B-NB	3.04	1.41	1.37
44	5	307	CLA	C1D-ND	3.04	1.41	1.37
44	e	823	CLA	CAB-C3B	-3.04	1.44	1.50
44	q	305	CLA	C4B-NB	3.04	1.41	1.37
47	A	849	BCR	C30-C25	-3.04	1.49	1.53
44	s	505	CLA	C4B-NB	3.03	1.41	1.37
44	1	506	CLA	C1D-ND	3.03	1.41	1.37
52	2	513	CHL	C3D-C2D	3.02	1.46	1.37
44	f	813	CLA	C4B-NB	3.02	1.41	1.37
44	1	505	CLA	C1D-ND	3.02	1.41	1.37
44	r	315	CLA	C4B-NB	3.02	1.41	1.37
52	p	512	CHL	C3A-C2A	-3.01	1.52	1.54
44	A	818	CLA	CMB-C2B	-3.01	1.44	1.50
44	e	816	CLA	C4B-NB	3.00	1.41	1.37
44	F	803	CLA	C1D-ND	3.00	1.41	1.37
44	n	201	CLA	C4B-NB	3.00	1.41	1.37
44	e	843	CLA	C4B-NB	3.00	1.41	1.37
44	B	815	CLA	CMB-C2B	-3.00	1.44	1.50
44	q	308	CLA	C4B-NB	3.00	1.41	1.37
47	L	306	BCR	C1-C6	-3.00	1.49	1.53
44	1	508	CLA	C1D-ND	2.99	1.41	1.37
44	1	510	CLA	C4B-NB	2.99	1.41	1.37
44	3	310	CLA	C1D-ND	2.99	1.41	1.37
44	3	308	CLA	C1D-ND	2.99	1.41	1.37
44	A	809	CLA	C2D-C1D	2.99	1.47	1.42
44	q	307	CLA	C4B-NB	2.99	1.41	1.37
44	e	827	CLA	C1D-ND	2.99	1.41	1.37
44	e	808	CLA	C4B-NB	2.98	1.41	1.37
44	e	822	CLA	C4B-NB	2.98	1.41	1.37
44	f	804	CLA	C1C-NC	-2.98	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	e	843	CLA	CAB-C3B	-2.97	1.44	1.50
44	K	205	CLA	C1D-ND	2.97	1.41	1.37
44	B	820	CLA	CMB-C2B	-2.97	1.44	1.50
44	A	803	CLA	C1D-ND	2.97	1.41	1.37
44	B	815	CLA	CMC-C2C	-2.97	1.44	1.50
44	e	811	CLA	C4B-NB	2.97	1.41	1.37
44	A	835	CLA	C1B-NB	-2.97	1.34	1.37
44	n	202	CLA	C4B-NB	2.97	1.41	1.37
44	e	817	CLA	C4B-NB	2.96	1.41	1.37
44	f	811	CLA	C4B-NB	2.96	1.41	1.37
44	p	504	CLA	C4B-NB	2.96	1.41	1.37
44	A	835	CLA	CMC-C2C	-2.96	1.44	1.50
44	e	807	CLA	C4B-NB	2.96	1.41	1.37
44	2	506	CLA	C1D-ND	2.96	1.41	1.37
44	p	511	CLA	C4B-NB	2.96	1.41	1.37
44	3	314	CLA	C4B-NB	2.96	1.41	1.37
44	o	304	CLA	C4B-NB	2.95	1.41	1.37
44	q	311	CLA	C4B-NB	2.95	1.41	1.37
44	e	832	CLA	C4B-NB	2.95	1.41	1.37
44	q	316	CLA	C4B-NB	2.95	1.41	1.37
44	f	823	CLA	C4B-NB	2.95	1.41	1.37
44	e	802	CLA	C4B-NB	2.95	1.41	1.37
44	q	315	CLA	C4B-NB	2.95	1.41	1.37
44	B	826	CLA	C1B-NB	-2.95	1.34	1.37
44	p	506	CLA	C4B-NB	2.95	1.41	1.37
44	q	312	CLA	C4B-NB	2.94	1.41	1.37
44	A	825	CLA	C1D-ND	2.93	1.41	1.37
44	f	826	CLA	C4B-NB	2.93	1.41	1.37
44	B	830	CLA	C4B-NB	2.93	1.41	1.37
44	f	824	CLA	C4B-NB	2.93	1.41	1.37
44	e	803	CLA	C4B-NB	2.93	1.41	1.37
44	f	836	CLA	C4B-NB	2.93	1.41	1.37
44	B	813	CLA	CMD-C2D	-2.92	1.44	1.50
47	3	305	BCR	C30-C25	-2.92	1.50	1.53
44	B	838	CLA	C1D-ND	2.92	1.41	1.37
44	1	506	CLA	C4B-NB	2.92	1.41	1.37
44	r	317	CLA	C4B-NB	2.92	1.41	1.37
44	r	306	CLA	C4B-NB	2.92	1.41	1.37
44	A	812	CLA	C1B-NB	-2.91	1.34	1.37
44	e	810	CLA	C4B-NB	2.91	1.41	1.37
44	e	814	CLA	C4B-NB	2.91	1.41	1.37
44	f	814	CLA	C4B-NB	2.91	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	p	508	CLA	C4B-NB	2.91	1.41	1.37
44	A	830	CLA	C1B-NB	-2.91	1.34	1.37
44	s	510	CLA	C4B-NB	2.91	1.41	1.37
44	A	842	CLA	C1D-ND	2.91	1.41	1.37
44	f	834	CLA	C4B-NB	2.90	1.41	1.37
44	A	817	CLA	C3A-C2A	-2.90	1.52	1.54
44	q	309	CLA	C4B-NB	2.90	1.41	1.37
44	q	304	CLA	C4B-NB	2.90	1.41	1.37
44	e	830	CLA	C4B-NB	2.90	1.41	1.37
44	p	515	CLA	C1B-C2B	2.89	1.49	1.43
44	e	839	CLA	C4B-NB	2.89	1.41	1.37
44	r	308	CLA	C4B-NB	2.89	1.41	1.37
44	e	809	CLA	C4B-NB	2.89	1.41	1.37
44	e	841	CLA	C4B-NB	2.89	1.41	1.37
44	f	809	CLA	C4B-NB	2.89	1.41	1.37
47	B	846	BCR	C30-C25	-2.89	1.50	1.53
44	e	826	CLA	C4B-NB	2.88	1.41	1.37
44	e	819	CLA	C4B-NB	2.88	1.41	1.37
44	r	312	CLA	C4B-NB	2.88	1.41	1.37
44	e	805	CLA	C4B-NB	2.88	1.41	1.37
44	f	843	CLA	C4B-NB	2.88	1.41	1.37
44	m	101	CLA	CAB-C3B	-2.87	1.44	1.50
47	L	305	BCR	C30-C25	-2.87	1.50	1.53
44	3	312	CLA	C4B-NB	2.87	1.41	1.37
44	5	309	CLA	C1D-ND	2.87	1.41	1.37
44	s	507	CLA	C4B-NB	2.87	1.41	1.37
47	A	848	BCR	C1-C6	-2.87	1.50	1.53
44	f	825	CLA	C4B-NB	2.87	1.41	1.37
44	s	508	CLA	C4B-NB	2.87	1.41	1.37
44	B	806	CLA	C1D-ND	2.86	1.41	1.37
44	f	815	CLA	C4B-NB	2.86	1.41	1.37
44	r	307	CLA	C4B-NB	2.86	1.41	1.37
44	B	831	CLA	C1D-ND	2.86	1.41	1.37
44	s	506	CLA	C4B-NB	2.86	1.41	1.37
44	3	317	CLA	C1D-ND	2.85	1.41	1.37
47	A	849	BCR	C1-C6	-2.85	1.50	1.53
44	f	819	CLA	C4B-NB	2.85	1.41	1.37
44	e	823	CLA	C4B-NB	2.85	1.41	1.37
44	A	824	CLA	CMB-C2B	-2.85	1.44	1.50
44	3	306	CLA	CAB-C3B	-2.85	1.44	1.50
44	2	510	CLA	C4B-NB	2.85	1.41	1.37
51	1	501	LUT	C22-C21	-2.85	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f	831	CLA	C4B-NB	2.85	1.41	1.37
44	3	301	CLA	CMB-C2B	-2.84	1.44	1.50
44	B	837	CLA	MG-NB	-2.84	2.00	2.05
44	p	509	CLA	C1C-NC	-2.84	1.33	1.37
52	1	514	CHL	CBD-CGD	-2.83	1.48	1.52
44	e	828	CLA	C4B-NB	2.83	1.41	1.37
47	J	102	BCR	C1-C6	-2.83	1.50	1.53
44	A	834	CLA	C1D-ND	2.83	1.41	1.37
44	e	806	CLA	C4B-NB	2.83	1.41	1.37
44	e	852	CLA	C1B-C2B	2.83	1.49	1.43
44	e	840	CLA	C4B-NB	2.83	1.41	1.37
44	f	821	CLA	C4B-NB	2.83	1.41	1.37
44	f	842	CLA	C4B-NB	2.83	1.41	1.37
44	A	833	CLA	CMB-C2B	-2.83	1.45	1.50
44	A	826	CLA	CMC-C2C	-2.83	1.45	1.50
44	A	821	CLA	C4B-NB	2.83	1.41	1.37
44	f	827	CLA	C4B-NB	2.83	1.41	1.37
44	A	817	CLA	CMB-C2B	-2.83	1.45	1.50
44	f	816	CLA	C4B-NB	2.82	1.41	1.37
44	f	840	CLA	C4B-NB	2.82	1.41	1.37
44	B	820	CLA	CMC-C2C	-2.82	1.45	1.50
44	f	839	CLA	C4B-NB	2.82	1.41	1.37
44	A	805	CLA	MG-NB	-2.82	2.00	2.05
44	3	318	CLA	C1D-ND	2.82	1.41	1.37
44	f	817	CLA	C4B-NB	2.82	1.41	1.37
44	B	809	CLA	C1D-ND	2.82	1.41	1.37
44	B	836	CLA	C1D-ND	2.81	1.41	1.37
44	1	508	CLA	C4B-NB	2.81	1.41	1.37
44	f	832	CLA	C4B-NB	2.81	1.41	1.37
44	B	810	CLA	CMC-C2C	-2.81	1.45	1.50
44	f	830	CLA	C4B-NB	2.81	1.41	1.37
44	B	833	CLA	C1D-ND	2.81	1.41	1.37
44	e	833	CLA	C4B-NB	2.81	1.41	1.37
44	e	818	CLA	C1C-NC	-2.81	1.33	1.37
44	f	804	CLA	C2B-C1B	2.81	1.45	1.39
44	e	853	CLA	C4B-NB	2.81	1.41	1.37
44	f	833	CLA	C4B-NB	2.81	1.41	1.37
44	q	314	CLA	C4B-NB	2.80	1.41	1.37
44	B	830	CLA	CMC-C2C	-2.80	1.45	1.50
44	e	831	CLA	C4B-NB	2.80	1.41	1.37
44	e	852	CLA	C4B-NB	2.80	1.41	1.37
44	L	303	CLA	CMB-C2B	-2.80	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	q	305	CLA	C1B-C2B	2.80	1.49	1.43
44	f	806	CLA	C4B-NB	2.80	1.41	1.37
44	f	810	CLA	C4B-NB	2.80	1.41	1.37
44	f	812	CLA	C4B-NB	2.79	1.41	1.37
44	B	809	CLA	CMD-C2D	-2.79	1.45	1.50
44	f	818	CLA	C4B-NB	2.79	1.41	1.37
44	5	308	CLA	C1D-ND	2.79	1.41	1.37
44	5	313	CLA	C1D-ND	2.79	1.41	1.37
47	K	204	BCR	C1-C6	-2.79	1.50	1.53
44	f	807	CLA	C4B-NB	2.79	1.41	1.37
44	A	819	CLA	CMB-C2B	-2.78	1.45	1.50
44	A	802	CLA	C1D-ND	2.78	1.41	1.37
51	5	303	LUT	C1-C6	-2.78	1.50	1.53
44	3	310	CLA	C1B-C2B	2.78	1.49	1.43
44	A	819	CLA	C1B-NB	-2.78	1.34	1.37
44	B	816	CLA	CMD-C2D	-2.78	1.45	1.50
44	n	203	CLA	C4B-NB	2.78	1.41	1.37
47	A	853	BCR	C1-C6	-2.78	1.50	1.53
44	3	316	CLA	C4B-NB	2.78	1.41	1.37
44	B	821	CLA	CMD-C2D	-2.77	1.45	1.50
44	f	841	CLA	C4B-NB	2.77	1.41	1.37
44	B	838	CLA	CMB-C2B	-2.77	1.45	1.50
44	2	507	CLA	C4B-NB	2.77	1.41	1.37
44	B	836	CLA	C4B-NB	2.77	1.41	1.37
44	A	820	CLA	CMB-C2B	-2.77	1.45	1.50
44	B	816	CLA	C1D-ND	2.77	1.41	1.37
44	B	803	CLA	CMC-C2C	-2.77	1.45	1.50
47	A	848	BCR	C30-C25	-2.77	1.50	1.53
44	A	816	CLA	C1D-ND	2.77	1.41	1.37
44	o	303	CLA	C4B-NB	2.77	1.41	1.37
44	p	507	CLA	C4B-NB	2.77	1.41	1.37
44	s	505	CLA	C1B-C2B	2.77	1.49	1.43
44	B	801	CLA	CMC-C2C	-2.77	1.45	1.50
44	A	811	CLA	MG-NB	-2.77	2.00	2.05
44	n	205	CLA	C1B-C2B	2.76	1.49	1.43
44	f	801	CLA	C4B-NB	2.76	1.41	1.37
44	A	811	CLA	CMD-C2D	-2.76	1.45	1.50
44	A	810	CLA	CMB-C2B	-2.76	1.45	1.50
44	K	203	CLA	MG-NB	-2.76	2.00	2.05
44	5	310	CLA	C4B-NB	2.76	1.41	1.37
44	q	310	CLA	C1B-C2B	2.76	1.49	1.43
44	B	827	CLA	CMD-C2D	-2.76	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	B	821	CLA	C4B-NB	2.76	1.41	1.37
44	5	306	CLA	C1D-ND	2.75	1.41	1.37
44	B	812	CLA	CMB-C2B	-2.75	1.45	1.50
44	f	813	CLA	C1B-C2B	2.75	1.49	1.43
44	e	836	CLA	C4B-NB	2.75	1.41	1.37
44	A	812	CLA	CMC-C2C	-2.75	1.45	1.50
44	e	823	CLA	C4B-C3B	2.75	1.49	1.43
44	e	812	CLA	C4B-NB	2.75	1.41	1.37
44	J	101	CLA	C4B-NB	2.75	1.41	1.37
44	B	813	CLA	C1B-NB	-2.74	1.34	1.37
44	o	304	CLA	C1B-C2B	2.74	1.49	1.43
44	e	834	CLA	C4B-NB	2.74	1.41	1.37
44	e	837	CLA	C4B-NB	2.74	1.41	1.37
44	r	304	CLA	C4B-NB	2.74	1.41	1.37
44	A	832	CLA	CMB-C2B	-2.74	1.45	1.50
44	r	304	CLA	C4B-C3B	2.74	1.49	1.43
44	q	304	CLA	C3C-C4C	2.74	1.46	1.40
44	B	842	CLA	C1D-ND	2.74	1.41	1.37
44	1	515	CLA	C4B-NB	2.74	1.41	1.37
44	B	802	CLA	C1D-ND	2.74	1.41	1.37
44	B	835	CLA	C1D-ND	2.74	1.41	1.37
44	f	836	CLA	C1B-C2B	2.74	1.49	1.43
53	5	304	XAT	O4-C5	-2.74	1.42	1.46
44	f	830	CLA	C1B-C2B	2.74	1.49	1.43
44	A	838	CLA	CMD-C2D	-2.74	1.45	1.50
44	A	831	CLA	C1B-NB	-2.74	1.34	1.37
44	3	317	CLA	C4B-NB	2.73	1.41	1.37
44	r	309	CLA	C4B-NB	2.73	1.41	1.37
44	e	825	CLA	C4B-NB	2.73	1.41	1.37
44	A	816	CLA	MG-NB	-2.73	2.00	2.05
44	1	509	CLA	C4B-NB	2.73	1.41	1.37
44	e	838	CLA	C4B-NB	2.73	1.41	1.37
44	o	303	CLA	C1B-C2B	2.73	1.49	1.43
44	e	824	CLA	C4B-NB	2.72	1.41	1.37
44	f	807	CLA	C1B-C2B	2.72	1.49	1.43
44	B	834	CLA	CMB-C2B	-2.72	1.45	1.50
44	f	825	CLA	C1B-C2B	2.72	1.49	1.43
44	e	822	CLA	C1B-C2B	2.72	1.49	1.43
44	B	814	CLA	CMD-C2D	-2.71	1.45	1.50
53	2	502	XAT	O4-C5	-2.71	1.42	1.46
44	s	514	CLA	C1B-C2B	2.71	1.49	1.43
44	A	816	CLA	CMD-C2D	-2.71	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	B	824	CLA	CMD-C2D	-2.71	1.45	1.50
44	f	820	CLA	C4B-NB	2.71	1.41	1.37
44	p	508	CLA	C1B-C2B	2.71	1.49	1.43
44	A	852	CLA	C1D-ND	2.71	1.41	1.37
44	B	824	CLA	CMB-C2B	-2.71	1.45	1.50
44	A	829	CLA	C1B-NB	-2.71	1.34	1.37
44	1	505	CLA	C1B-C2B	2.71	1.49	1.43
44	B	810	CLA	MG-NB	-2.71	2.00	2.05
44	e	814	CLA	C1B-C2B	2.71	1.49	1.43
44	f	822	CLA	C1B-C2B	2.70	1.49	1.43
44	B	817	CLA	C1D-ND	2.70	1.41	1.37
44	F	803	CLA	MG-NB	-2.70	2.00	2.05
44	B	811	CLA	CMB-C2B	-2.70	1.45	1.50
44	B	820	CLA	C4B-NB	2.70	1.41	1.37
44	p	513	CLA	C1B-C2B	2.70	1.49	1.43
44	A	829	CLA	MG-NB	-2.70	2.00	2.05
44	3	309	CLA	C1D-ND	2.70	1.41	1.37
44	5	310	CLA	C1B-C2B	2.70	1.49	1.43
44	f	839	CLA	C1B-C2B	2.70	1.49	1.43
44	B	809	CLA	CMB-C2B	-2.70	1.45	1.50
44	B	839	CLA	C1D-ND	2.70	1.41	1.37
44	j	802	CLA	C1B-C2B	2.70	1.49	1.43
44	5	316	CLA	C1D-ND	2.70	1.41	1.37
44	f	837	CLA	C1B-C2B	2.70	1.49	1.43
44	B	819	CLA	CMD-C2D	-2.70	1.45	1.50
44	B	823	CLA	C1D-ND	2.70	1.41	1.37
44	r	312	CLA	C1B-C2B	2.70	1.49	1.43
44	f	835	CLA	C4B-NB	2.70	1.41	1.37
45	e	842	PQN	C3-C2	2.70	1.48	1.35
44	m	102	CLA	C1B-C2B	2.69	1.49	1.43
44	A	814	CLA	CMD-C2D	-2.69	1.45	1.50
44	B	806	CLA	CMD-C2D	-2.69	1.45	1.50
44	e	840	CLA	C1B-C2B	2.69	1.49	1.43
44	f	809	CLA	C1B-C2B	2.69	1.49	1.43
44	q	311	CLA	C1B-C2B	2.69	1.49	1.43
44	r	308	CLA	C1B-C2B	2.69	1.49	1.43
44	1	511	CLA	MG-NB	-2.69	2.00	2.05
44	s	514	CLA	C4B-NB	2.69	1.41	1.37
44	A	852	CLA	CMB-C2B	-2.69	1.45	1.50
44	o	302	CLA	C1B-C2B	2.69	1.49	1.43
44	e	827	CLA	C4B-NB	2.69	1.41	1.37
44	B	834	CLA	C1D-ND	2.69	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	A	835	CLA	CMB-C2B	-2.69	1.45	1.50
44	s	511	CLA	C1B-C2B	2.69	1.49	1.43
52	3	315	CHL	CHA-CBD	-2.69	1.48	1.51
44	A	815	CLA	MG-NB	-2.69	2.00	2.05
44	2	510	CLA	C1D-ND	2.69	1.41	1.37
44	L	304	CLA	CMD-C2D	-2.68	1.45	1.50
44	n	202	CLA	C1B-C2B	2.68	1.49	1.43
44	n	203	CLA	C1B-C2B	2.68	1.49	1.43
44	e	820	CLA	C4B-NB	2.68	1.41	1.37
44	B	819	CLA	CMB-C2B	-2.68	1.45	1.50
44	f	826	CLA	C1B-C2B	2.68	1.49	1.43
44	A	809	CLA	CMC-C2C	-2.68	1.45	1.50
44	K	201	CLA	C4B-NB	2.68	1.41	1.37
44	f	808	CLA	C1B-C2B	2.68	1.49	1.43
44	q	306	CLA	C1B-C2B	2.68	1.49	1.43
44	B	831	CLA	CMB-C2B	-2.68	1.45	1.50
44	f	838	CLA	C4B-NB	2.68	1.41	1.37
44	f	829	CLA	C4B-NB	2.68	1.41	1.37
44	B	822	CLA	C4B-NB	2.68	1.41	1.37
44	p	510	CLA	C1B-C2B	2.67	1.49	1.43
44	A	817	CLA	MG-NB	-2.67	2.00	2.05
47	A	847	BCR	C30-C25	-2.67	1.50	1.53
44	r	311	CLA	C1B-C2B	2.67	1.49	1.43
44	A	831	CLA	CMC-C2C	-2.67	1.45	1.50
44	s	507	CLA	C1B-C2B	2.67	1.49	1.43
44	B	803	CLA	MG-NB	-2.67	2.00	2.05
44	e	806	CLA	C1B-C2B	2.67	1.49	1.43
44	q	307	CLA	C1B-C2B	2.67	1.49	1.43
44	B	806	CLA	MG-NB	-2.67	2.00	2.05
44	f	811	CLA	C1B-C2B	2.67	1.49	1.43
44	B	823	CLA	MG-NB	-2.67	2.00	2.05
44	A	830	CLA	CMB-C2B	-2.67	1.45	1.50
44	q	308	CLA	C1B-C2B	2.66	1.49	1.43
44	B	831	CLA	CMD-C2D	-2.66	1.45	1.50
44	2	506	CLA	CMB-C2B	-2.66	1.45	1.50
44	B	813	CLA	CMB-C2B	-2.66	1.45	1.50
44	A	828	CLA	CMD-C2D	-2.66	1.45	1.50
44	B	816	CLA	CMC-C2C	-2.66	1.45	1.50
44	A	838	CLA	CMB-C2B	-2.66	1.45	1.50
44	1	510	CLA	C3B-C4B	2.66	1.50	1.42
44	A	818	CLA	MG-NB	-2.66	2.00	2.05
44	f	808	CLA	C4B-NB	2.66	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f	812	CLA	C1B-C2B	2.66	1.49	1.43
44	B	839	CLA	MG-NB	-2.66	2.00	2.05
44	B	801	CLA	MG-NB	-2.66	2.00	2.05
44	A	834	CLA	CMB-C2B	-2.65	1.45	1.50
44	A	836	CLA	CMD-C2D	-2.65	1.45	1.50
44	B	808	CLA	MG-NB	-2.65	2.00	2.05
44	A	840	CLA	MG-NB	-2.65	2.00	2.05
44	e	823	CLA	C1B-C2B	2.65	1.49	1.43
44	A	822	CLA	C1D-ND	2.65	1.41	1.37
44	f	828	CLA	C4B-NB	2.65	1.41	1.37
44	r	304	CLA	C1B-C2B	2.65	1.49	1.43
44	e	821	CLA	C4B-NB	2.65	1.41	1.37
44	3	306	CLA	C4B-C3B	2.65	1.49	1.43
44	r	310	CLA	C1B-C2B	2.65	1.49	1.43
44	B	805	CLA	CMB-C2B	-2.65	1.45	1.50
44	e	843	CLA	C4B-C3B	2.65	1.49	1.43
44	A	826	CLA	MG-NB	-2.65	2.00	2.05
44	e	824	CLA	C1B-C2B	2.65	1.49	1.43
44	A	806	CLA	CMC-C2C	-2.65	1.45	1.50
44	r	315	CLA	C1B-C2B	2.65	1.49	1.43
44	B	838	CLA	CMD-C2D	-2.65	1.45	1.50
44	B	842	CLA	C4B-NB	2.65	1.41	1.37
44	1	504	CLA	MG-NB	-2.65	2.00	2.05
44	A	806	CLA	CMB-C2B	-2.65	1.45	1.50
44	B	826	CLA	CMD-C2D	-2.65	1.45	1.50
44	1	510	CLA	C1D-ND	2.65	1.41	1.37
44	e	841	CLA	C1B-C2B	2.65	1.49	1.43
44	B	813	CLA	CMC-C2C	-2.64	1.45	1.50
44	B	807	CLA	CMC-C2C	-2.64	1.45	1.50
44	q	315	CLA	C1B-C2B	2.64	1.49	1.43
44	r	306	CLA	C1B-C2B	2.64	1.49	1.43
44	r	307	CLA	C1B-C2B	2.64	1.49	1.43
44	3	314	CLA	C1D-ND	2.64	1.41	1.37
44	f	814	CLA	C1B-C2B	2.64	1.49	1.43
44	B	808	CLA	CMD-C2D	-2.64	1.45	1.50
44	A	805	CLA	C1D-ND	2.64	1.41	1.37
44	1	515	CLA	CMD-C2D	-2.64	1.45	1.50
44	B	829	CLA	MG-NB	-2.64	2.00	2.05
44	B	814	CLA	CMC-C2C	-2.64	1.45	1.50
44	s	510	CLA	C1B-C2B	2.64	1.49	1.43
44	A	804	CLA	CMD-C2D	-2.64	1.45	1.50
44	5	305	CLA	CMC-C2C	-2.64	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f	815	CLA	C1B-C2B	2.64	1.49	1.43
44	f	840	CLA	C1B-C2B	2.64	1.49	1.43
44	A	832	CLA	CMD-C2D	-2.64	1.45	1.50
44	A	824	CLA	MG-NB	-2.64	2.00	2.05
44	f	824	CLA	C1B-C2B	2.64	1.49	1.43
44	f	833	CLA	C1B-C2B	2.64	1.49	1.43
44	B	803	CLA	CMD-C2D	-2.63	1.45	1.50
44	5	312	CLA	C4B-NB	2.63	1.41	1.37
44	B	806	CLA	CMC-C2C	-2.63	1.45	1.50
44	s	506	CLA	C1B-C2B	2.63	1.49	1.43
44	A	807	CLA	CMB-C2B	-2.63	1.45	1.50
44	B	830	CLA	MG-NB	-2.63	2.00	2.05
44	f	819	CLA	C1B-C2B	2.63	1.49	1.43
47	l	101	BCR	C30-C25	-2.63	1.50	1.53
44	B	827	CLA	CMB-C2B	-2.63	1.45	1.50
44	f	817	CLA	C1B-C2B	2.63	1.49	1.43
44	A	806	CLA	C1B-NB	-2.63	1.34	1.37
44	A	831	CLA	MG-NB	-2.63	2.00	2.05
44	A	823	CLA	CMB-C2B	-2.63	1.45	1.50
44	s	508	CLA	C1B-C2B	2.63	1.49	1.43
44	A	837	CLA	CMD-C2D	-2.63	1.45	1.50
44	f	835	CLA	C1B-C2B	2.63	1.49	1.43
44	r	317	CLA	C1B-C2B	2.63	1.49	1.43
44	f	818	CLA	C1B-C2B	2.63	1.49	1.43
44	r	309	CLA	C1B-C2B	2.63	1.49	1.43
44	B	807	CLA	CMB-C2B	-2.63	1.45	1.50
44	f	841	CLA	C1B-C2B	2.63	1.49	1.43
44	f	829	CLA	C1B-C2B	2.63	1.49	1.43
44	A	825	CLA	CMD-C2D	-2.63	1.45	1.50
44	A	828	CLA	C1D-ND	2.63	1.41	1.37
44	e	820	CLA	C1B-C2B	2.62	1.49	1.43
44	f	801	CLA	C1B-C2B	2.62	1.49	1.43
44	f	806	CLA	C1B-C2B	2.62	1.49	1.43
44	A	842	CLA	C4B-NB	2.62	1.41	1.37
44	K	203	CLA	C1B-C2B	2.62	1.49	1.43
44	e	838	CLA	C1B-C2B	2.62	1.49	1.43
44	2	507	CLA	MG-NB	-2.62	2.00	2.05
44	e	817	CLA	C1B-C2B	2.62	1.49	1.43
44	e	809	CLA	C1B-C2B	2.62	1.49	1.43
44	A	830	CLA	CMD-C2D	-2.62	1.45	1.50
44	e	807	CLA	C1B-C2B	2.62	1.49	1.43
44	r	305	CLA	C1B-C2B	2.62	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	q	309	CLA	C1B-C2B	2.62	1.49	1.43
44	A	825	CLA	MG-NB	-2.62	2.00	2.05
44	B	811	CLA	CMC-C2C	-2.62	1.45	1.50
44	e	805	CLA	C1B-C2B	2.62	1.49	1.43
44	e	839	CLA	C1B-C2B	2.62	1.49	1.43
44	A	822	CLA	MG-NB	-2.62	2.00	2.05
44	A	824	CLA	CMD-C2D	-2.61	1.45	1.50
44	e	833	CLA	C1B-C2B	2.61	1.49	1.43
44	K	203	CLA	CMD-C2D	-2.61	1.45	1.50
44	A	819	CLA	C1D-ND	2.61	1.41	1.37
44	q	316	CLA	C1B-C2B	2.61	1.49	1.43
44	e	828	CLA	C1B-C2B	2.61	1.49	1.43
44	A	803	CLA	CMB-C2B	-2.61	1.45	1.50
44	B	803	CLA	CMB-C2B	-2.61	1.45	1.50
44	B	804	CLA	CMD-C2D	-2.61	1.45	1.50
44	A	833	CLA	CMD-C2D	-2.61	1.45	1.50
47	A	853	BCR	C30-C25	-2.61	1.50	1.53
44	f	820	CLA	C1B-C2B	2.61	1.49	1.43
44	A	802	CLA	CMB-C2B	-2.61	1.45	1.50
44	A	823	CLA	CMC-C2C	-2.61	1.45	1.50
44	e	843	CLA	C1B-C2B	2.61	1.49	1.43
44	e	853	CLA	C1B-C2B	2.60	1.49	1.43
47	F	801	BCR	C30-C25	-2.60	1.50	1.53
44	e	821	CLA	C1B-C2B	2.60	1.49	1.43
44	B	824	CLA	MG-NB	-2.60	2.00	2.05
52	1	517	CHL	CBD-CGD	-2.60	1.49	1.52
44	1	509	CLA	C1B-C2B	2.60	1.49	1.43
44	5	308	CLA	MG-NB	-2.60	2.00	2.05
44	A	839	CLA	C4B-NB	2.60	1.41	1.37
44	B	816	CLA	CMB-C2B	-2.60	1.45	1.50
44	f	838	CLA	C1B-C2B	2.60	1.49	1.43
44	1	507	CLA	C1D-ND	2.60	1.41	1.37
44	B	826	CLA	MG-NB	-2.59	2.00	2.05
44	2	514	CLA	C1D-ND	2.59	1.41	1.37
44	B	842	CLA	MG-NB	-2.59	2.00	2.05
44	B	802	CLA	MG-NB	-2.59	2.00	2.05
44	1	513	CLA	C1B-C2B	2.59	1.49	1.43
44	A	826	CLA	CMD-C2D	-2.59	1.45	1.50
44	B	840	CLA	CMD-C2D	-2.59	1.45	1.50
44	A	807	CLA	C1D-ND	2.59	1.41	1.37
44	1	508	CLA	C1B-C2B	2.59	1.49	1.43
44	B	833	CLA	MG-NB	-2.59	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f	832	CLA	C1B-C2B	2.59	1.49	1.43
44	e	810	CLA	C1B-C2B	2.59	1.49	1.43
44	A	827	CLA	MG-NB	-2.59	2.00	2.05
44	A	823	CLA	CMD-C2D	-2.59	1.45	1.50
44	3	313	CLA	C1B-C2B	2.59	1.49	1.43
44	2	504	CLA	MG-NB	-2.59	2.00	2.05
44	e	812	CLA	C1B-C2B	2.59	1.49	1.43
44	A	840	CLA	CMB-C2B	-2.59	1.45	1.50
44	3	311	CLA	C1D-ND	2.59	1.41	1.37
44	5	311	CLA	C4B-NB	2.59	1.41	1.37
44	A	811	CLA	CMC-C2C	-2.59	1.45	1.50
44	B	807	CLA	CMD-C2D	-2.59	1.45	1.50
44	A	833	CLA	CMC-C2C	-2.58	1.45	1.50
44	B	825	CLA	CMD-C2D	-2.58	1.45	1.50
44	B	830	CLA	CMD-C2D	-2.58	1.45	1.50
44	e	802	CLA	C1B-C2B	2.58	1.49	1.43
44	A	803	CLA	CMD-C2D	-2.58	1.45	1.50
44	f	843	CLA	C1B-C2B	2.58	1.49	1.43
44	f	828	CLA	C1B-C2B	2.58	1.49	1.43
44	A	827	CLA	CMD-C2D	-2.58	1.45	1.50
44	1	510	CLA	C1B-C2B	2.58	1.49	1.43
44	A	820	CLA	C1D-ND	2.58	1.41	1.37
44	2	507	CLA	C1B-C2B	2.58	1.49	1.43
44	e	808	CLA	C1B-C2B	2.58	1.49	1.43
44	e	815	CLA	C1B-C2B	2.58	1.49	1.43
44	B	834	CLA	MG-NB	-2.58	2.00	2.05
44	e	825	CLA	C1B-C2B	2.58	1.49	1.43
44	A	821	CLA	CMD-C2D	-2.58	1.45	1.50
44	B	840	CLA	CMB-C2B	-2.58	1.45	1.50
44	e	811	CLA	C1B-C2B	2.58	1.49	1.43
44	f	816	CLA	C1B-C2B	2.57	1.49	1.43
44	3	318	CLA	C1B-C2B	2.57	1.49	1.43
44	3	318	CLA	MG-NB	-2.57	2.00	2.05
44	5	308	CLA	CMC-C2C	-2.57	1.45	1.50
44	A	829	CLA	CMC-C2C	-2.57	1.45	1.50
44	5	307	CLA	C1B-C2B	2.57	1.49	1.43
44	A	803	CLA	MG-NB	-2.57	2.00	2.05
44	B	824	CLA	C1D-ND	2.57	1.41	1.37
44	e	804	CLA	C4B-NB	2.57	1.41	1.37
44	A	828	CLA	MG-NB	-2.57	2.00	2.05
44	B	819	CLA	MG-NB	-2.57	2.00	2.05
47	A	851	BCR	C1-C6	-2.57	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	A	824	CLA	C1B-NB	-2.57	1.34	1.37
44	B	834	CLA	CMC-C2C	-2.57	1.45	1.50
44	L	301	CLA	CMB-C2B	-2.57	1.45	1.50
44	B	813	CLA	MG-NB	-2.57	2.00	2.05
44	A	822	CLA	C4B-NB	2.56	1.41	1.37
44	A	837	CLA	C4B-NB	2.56	1.41	1.37
52	5	317	CHL	C3A-C4A	-2.56	1.49	1.50
44	B	814	CLA	C1D-ND	2.56	1.41	1.37
44	p	506	CLA	C1B-C2B	2.56	1.49	1.43
47	B	849	BCR	C30-C25	-2.56	1.50	1.53
44	3	301	CLA	C1D-ND	2.56	1.41	1.37
44	f	805	CLA	C4B-NB	2.56	1.41	1.37
44	A	831	CLA	CMD-C2D	-2.56	1.45	1.50
44	L	304	CLA	C1D-ND	2.56	1.41	1.37
44	A	839	CLA	CMD-C2D	-2.56	1.45	1.50
47	A	847	BCR	C1-C6	-2.56	1.50	1.53
44	A	806	CLA	MG-NB	-2.56	2.00	2.05
44	2	508	CLA	CMD-C2D	-2.56	1.45	1.50
44	5	305	CLA	CMD-C2D	-2.56	1.45	1.50
44	p	507	CLA	C1B-C2B	2.56	1.49	1.43
44	3	311	CLA	MG-NB	-2.56	2.00	2.05
44	A	810	CLA	C1D-ND	2.56	1.41	1.37
44	A	852	CLA	CMC-C2C	-2.56	1.45	1.50
44	B	817	CLA	CMC-C2C	-2.56	1.45	1.50
44	e	834	CLA	C1B-C2B	2.56	1.49	1.43
44	e	803	CLA	C1B-C2B	2.56	1.49	1.43
44	A	835	CLA	MG-NB	-2.55	2.00	2.05
44	f	803	CLA	C1B-C2B	2.55	1.49	1.43
44	B	822	CLA	CMD-C2D	-2.55	1.45	1.50
44	2	505	CLA	C1D-ND	2.55	1.41	1.37
44	e	816	CLA	C1B-C2B	2.55	1.49	1.43
44	A	809	CLA	C1B-C2B	2.55	1.49	1.43
44	f	810	CLA	C1B-C2B	2.55	1.49	1.43
44	B	802	CLA	CMB-C2B	-2.55	1.45	1.50
44	B	804	CLA	MG-NB	-2.55	2.00	2.05
44	p	513	CLA	C3B-C4B	2.55	1.50	1.42
44	3	312	CLA	C1B-C2B	2.55	1.49	1.43
44	e	804	CLA	C1B-C2B	2.55	1.49	1.43
44	B	819	CLA	C1D-ND	2.55	1.41	1.37
44	f	834	CLA	C1B-C2B	2.55	1.49	1.43
44	B	816	CLA	MG-NB	-2.55	2.00	2.05
44	2	504	CLA	CMB-C2B	-2.55	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	5	307	CLA	C4B-NB	2.55	1.41	1.37
44	A	852	CLA	CMD-C2D	-2.54	1.45	1.50
44	e	835	CLA	C1B-C2B	2.54	1.49	1.43
44	A	807	CLA	MG-NB	-2.54	2.00	2.05
44	B	826	CLA	CMC-C2C	-2.54	1.45	1.50
44	A	815	CLA	C1B-C2B	2.54	1.49	1.43
44	m	101	CLA	C1B-C2B	2.54	1.49	1.43
52	2	513	CHL	CAD-C3D	-2.54	1.48	1.51
53	2	502	XAT	O24-C25	-2.54	1.42	1.46
44	e	826	CLA	C4B-C3B	2.54	1.49	1.43
44	B	835	CLA	CMB-C2B	-2.54	1.45	1.50
44	B	817	CLA	MG-NB	-2.54	2.00	2.05
44	e	832	CLA	C1B-C2B	2.54	1.49	1.43
44	B	815	CLA	CMD-C2D	-2.54	1.45	1.50
44	A	828	CLA	CMB-C2B	-2.54	1.45	1.50
44	B	809	CLA	C1B-NB	-2.54	1.34	1.37
44	B	825	CLA	MG-NB	-2.54	2.00	2.05
44	e	826	CLA	C1B-C2B	2.54	1.49	1.43
44	f	823	CLA	C1B-C2B	2.53	1.49	1.43
44	K	201	CLA	MG-NB	-2.53	2.00	2.05
44	3	314	CLA	C1B-C2B	2.53	1.49	1.43
44	e	813	CLA	C1B-C2B	2.53	1.49	1.43
44	p	511	CLA	C1B-C2B	2.53	1.49	1.43
44	A	811	CLA	C1B-NB	-2.53	1.34	1.37
44	A	816	CLA	CMC-C2C	-2.53	1.45	1.50
44	f	803	CLA	C4B-NB	2.53	1.41	1.37
44	B	814	CLA	MG-NB	-2.53	2.00	2.05
44	B	801	CLA	CMB-C2B	-2.53	1.45	1.50
44	A	825	CLA	C1B-NB	-2.53	1.34	1.37
44	B	825	CLA	CMC-C2C	-2.53	1.45	1.50
44	B	805	CLA	C1B-NB	-2.52	1.34	1.37
44	n	201	CLA	C1B-C2B	2.52	1.49	1.43
44	B	810	CLA	C1B-C2B	2.52	1.49	1.43
44	s	509	CLA	C1B-C2B	2.52	1.49	1.43
44	5	309	CLA	MG-NB	-2.52	2.00	2.05
44	A	840	CLA	C1B-C2B	2.52	1.49	1.43
44	B	810	CLA	CMB-C2B	-2.52	1.45	1.50
44	B	832	CLA	CMB-C2B	-2.52	1.45	1.50
47	B	847	BCR	C1-C6	-2.52	1.50	1.53
44	f	813	CLA	C4B-C3B	2.52	1.49	1.43
44	B	811	CLA	MG-NB	-2.52	2.00	2.05
44	B	815	CLA	MG-NB	-2.52	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f	842	CLA	C1B-C2B	2.52	1.49	1.43
44	2	504	CLA	C1B-C2B	2.52	1.49	1.43
44	A	838	CLA	MG-NB	-2.51	2.00	2.05
44	5	312	CLA	MG-NB	-2.51	2.00	2.05
44	A	821	CLA	CMB-C2B	-2.51	1.45	1.50
44	A	813	CLA	MG-NB	-2.51	2.00	2.05
44	A	813	CLA	CMD-C2D	-2.51	1.45	1.50
44	A	839	CLA	CMC-C2C	-2.51	1.45	1.50
44	B	823	CLA	CMD-C2D	-2.51	1.45	1.50
44	A	840	CLA	CMD-C2D	-2.51	1.45	1.50
52	q	313	CHL	CAD-C3D	-2.51	1.48	1.51
44	3	301	CLA	CMC-C2C	-2.51	1.45	1.50
44	B	830	CLA	C1D-ND	2.51	1.41	1.37
44	B	836	CLA	CMB-C2B	-2.51	1.45	1.50
44	e	836	CLA	C1B-C2B	2.51	1.49	1.43
44	3	317	CLA	C1B-C2B	2.51	1.49	1.43
44	A	812	CLA	MG-NB	-2.51	2.00	2.05
44	f	801	CLA	C4B-C3B	2.51	1.49	1.43
44	B	802	CLA	CMC-C2C	-2.51	1.45	1.50
44	p	507	CLA	C4B-C3B	2.51	1.49	1.43
44	2	511	CLA	C1B-C2B	2.50	1.49	1.43
44	A	835	CLA	CMD-C2D	-2.50	1.45	1.50
44	A	808	CLA	C1D-ND	2.50	1.41	1.37
44	B	822	CLA	CMB-C2B	-2.50	1.45	1.50
47	e	850	BCR	C1-C6	-2.50	1.50	1.53
44	A	808	CLA	MG-NB	-2.50	2.00	2.05
44	o	302	CLA	C4B-C3B	2.50	1.49	1.43
44	B	837	CLA	CMC-C2C	-2.50	1.45	1.50
44	1	507	CLA	MG-NB	-2.50	2.00	2.05
44	L	301	CLA	MG-NB	-2.50	2.00	2.05
44	A	827	CLA	CMC-C2C	-2.50	1.45	1.50
44	B	837	CLA	CMB-C2B	-2.50	1.45	1.50
52	s	517	CHL	CBD-CGD	-2.50	1.49	1.52
44	q	314	CLA	C1B-C2B	2.50	1.49	1.43
44	A	808	CLA	CMB-C2B	-2.50	1.45	1.50
44	f	805	CLA	C1B-C2B	2.50	1.49	1.43
44	1	504	CLA	CMC-C2C	-2.49	1.45	1.50
44	A	802	CLA	C1B-NB	-2.49	1.34	1.37
44	A	815	CLA	CMB-C2B	-2.49	1.45	1.50
44	B	837	CLA	CMD-C2D	-2.49	1.45	1.50
44	3	311	CLA	CMB-C2B	-2.49	1.45	1.50
44	B	827	CLA	CMC-C2C	-2.49	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	2	508	CLA	C4B-NB	2.49	1.41	1.37
44	e	819	CLA	C1B-C2B	2.49	1.49	1.43
44	A	808	CLA	CMC-C2C	-2.49	1.45	1.50
44	B	804	CLA	CMB-C2B	-2.49	1.45	1.50
44	p	513	CLA	CHC-C1C	2.49	1.43	1.38
44	2	511	CLA	C4B-NB	2.49	1.41	1.37
44	B	841	CLA	MG-NB	-2.49	2.00	2.05
44	f	827	CLA	C1B-C2B	2.49	1.49	1.43
44	B	804	CLA	CMC-C2C	-2.49	1.45	1.50
44	A	821	CLA	CMC-C2C	-2.48	1.45	1.50
44	L	301	CLA	C1D-ND	2.48	1.41	1.37
44	e	829	CLA	C1B-C2B	2.48	1.49	1.43
44	F	802	CLA	CMD-C2D	-2.48	1.45	1.50
44	3	307	CLA	C3B-C4B	2.48	1.50	1.42
44	B	823	CLA	C1B-NB	-2.48	1.34	1.37
44	p	504	CLA	C1B-C2B	2.48	1.49	1.43
44	e	837	CLA	C1B-C2B	2.48	1.49	1.43
44	A	805	CLA	CMB-C2B	-2.48	1.45	1.50
44	A	832	CLA	C1D-ND	2.48	1.41	1.37
44	A	830	CLA	MG-NB	-2.48	2.00	2.05
44	A	810	CLA	CMD-C2D	-2.48	1.45	1.50
44	5	306	CLA	MG-NB	-2.48	2.00	2.05
44	B	831	CLA	C4B-NB	2.48	1.41	1.37
44	B	840	CLA	C1B-NB	-2.48	1.34	1.37
44	B	804	CLA	C1D-ND	2.48	1.41	1.37
44	e	830	CLA	C1B-C2B	2.48	1.48	1.43
44	A	818	CLA	C1D-ND	2.47	1.41	1.37
44	A	839	CLA	C1D-ND	2.47	1.41	1.37
44	B	808	CLA	C4B-NB	2.47	1.41	1.37
44	B	806	CLA	CMB-C2B	-2.47	1.45	1.50
44	3	306	CLA	CMD-C2D	-2.47	1.45	1.50
44	B	835	CLA	CMC-C2C	-2.47	1.45	1.50
44	B	838	CLA	CMC-C2C	-2.47	1.45	1.50
44	B	833	CLA	C1B-NB	-2.47	1.34	1.37
44	B	829	CLA	C1D-ND	2.47	1.41	1.37
44	B	811	CLA	CMD-C2D	-2.47	1.45	1.50
44	e	831	CLA	C1B-C2B	2.47	1.48	1.43
44	B	841	CLA	CMD-C2D	-2.47	1.45	1.50
44	1	511	CLA	C1B-C2B	2.47	1.48	1.43
44	5	308	CLA	CMD-C2D	-2.47	1.45	1.50
44	f	831	CLA	CMB-C2B	-2.47	1.45	1.50
44	A	829	CLA	CMD-C2D	-2.47	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	B	822	CLA	C1D-ND	2.47	1.41	1.37
44	K	202	CLA	C1B-C2B	2.47	1.48	1.43
44	B	801	CLA	CMD-C2D	-2.47	1.45	1.50
44	B	808	CLA	C1D-ND	2.47	1.41	1.37
44	B	817	CLA	CMB-C2B	-2.46	1.45	1.50
44	B	812	CLA	MG-NB	-2.46	2.00	2.05
44	q	312	CLA	C3B-C4B	2.46	1.49	1.42
44	A	837	CLA	MG-NB	-2.46	2.00	2.05
44	2	514	CLA	C4B-NB	2.46	1.41	1.37
44	A	833	CLA	MG-NB	-2.46	2.00	2.05
44	B	835	CLA	C1B-C2B	2.46	1.48	1.43
44	B	808	CLA	CMB-C2B	-2.46	1.45	1.50
44	B	818	CLA	CMB-C2B	-2.46	1.45	1.50
53	2	502	XAT	C2-C1	-2.46	1.50	1.54
44	B	841	CLA	CMB-C2B	-2.46	1.45	1.50
44	5	306	CLA	C4B-NB	2.46	1.41	1.37
44	A	821	CLA	MG-ND	-2.46	2.00	2.05
44	3	314	CLA	MG-NB	-2.46	2.00	2.05
44	A	822	CLA	CMD-C2D	-2.46	1.45	1.50
44	A	809	CLA	CMB-C2B	-2.45	1.45	1.50
44	F	802	CLA	C4B-NB	2.45	1.41	1.37
44	2	507	CLA	CMB-C2B	-2.45	1.45	1.50
44	B	827	CLA	C1D-ND	2.45	1.41	1.37
44	A	816	CLA	C1B-C2B	2.45	1.48	1.43
44	A	813	CLA	CMC-C2C	-2.45	1.45	1.50
44	2	514	CLA	C1B-C2B	2.45	1.48	1.43
44	f	831	CLA	C1B-C2B	2.45	1.48	1.43
44	B	812	CLA	CMD-C2D	-2.45	1.45	1.50
44	e	827	CLA	C1B-C2B	2.45	1.48	1.43
44	s	509	CLA	C3B-C4B	2.45	1.49	1.42
44	B	835	CLA	MG-NB	-2.45	2.00	2.05
44	A	831	CLA	CMB-C2B	-2.45	1.45	1.50
44	A	802	CLA	CMC-C2C	-2.45	1.45	1.50
44	A	837	CLA	CMC-C2C	-2.45	1.45	1.50
44	B	820	CLA	MG-NB	-2.45	2.00	2.05
44	L	301	CLA	CMD-C2D	-2.44	1.45	1.50
44	3	313	CLA	CMD-C2D	-2.44	1.45	1.50
44	A	840	CLA	C1D-ND	2.44	1.41	1.37
44	B	801	CLA	C1B-NB	-2.44	1.34	1.37
44	A	812	CLA	CMD-C2D	-2.44	1.45	1.50
44	A	839	CLA	MG-NB	-2.44	2.00	2.05
44	A	820	CLA	CMD-C2D	-2.44	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	q	312	CLA	CHC-C1C	2.44	1.43	1.38
44	1	515	CLA	MG-NB	-2.44	2.00	2.05
44	A	821	CLA	C1B-C2B	2.44	1.48	1.43
47	B	849	BCR	C1-C6	-2.44	1.50	1.53
44	B	807	CLA	C1B-NB	-2.44	1.34	1.37
44	B	802	CLA	CMD-C2D	-2.44	1.45	1.50
44	r	305	CLA	C3B-C4B	2.44	1.49	1.42
44	K	201	CLA	C1D-ND	2.44	1.41	1.37
44	J	101	CLA	C1B-C2B	2.44	1.48	1.43
44	5	310	CLA	CMC-C2C	-2.44	1.45	1.50
44	B	821	CLA	CMB-C2B	-2.44	1.45	1.50
44	2	508	CLA	CMB-C2B	-2.44	1.45	1.50
44	f	831	CLA	CMD-C2D	-2.44	1.45	1.50
44	3	306	CLA	C4B-NB	2.44	1.41	1.37
44	5	311	CLA	C1D-ND	2.44	1.41	1.37
44	A	805	CLA	CMC-C2C	-2.44	1.45	1.50
44	A	811	CLA	C1B-C2B	2.44	1.48	1.43
44	B	812	CLA	CMC-C2C	-2.44	1.45	1.50
44	A	834	CLA	C4B-NB	2.44	1.41	1.37
44	1	504	CLA	C4B-NB	2.44	1.41	1.37
44	f	830	CLA	C4B-C3B	2.44	1.48	1.43
44	2	508	CLA	MG-NB	-2.44	2.01	2.05
44	A	842	CLA	C1B-C2B	2.44	1.48	1.43
44	1	506	CLA	C1B-C2B	2.44	1.48	1.43
44	A	834	CLA	MG-NB	-2.44	2.01	2.05
44	B	815	CLA	C1D-ND	2.44	1.41	1.37
44	A	837	CLA	C1D-ND	2.43	1.41	1.37
44	2	505	CLA	C4B-NB	2.43	1.41	1.37
44	A	819	CLA	MG-NB	-2.43	2.01	2.05
44	f	821	CLA	C1B-C2B	2.43	1.48	1.43
44	B	832	CLA	MG-NB	-2.43	2.01	2.05
44	B	817	CLA	CMD-C2D	-2.43	1.45	1.50
44	1	506	CLA	CMB-C2B	-2.43	1.45	1.50
44	B	819	CLA	C1B-NB	-2.43	1.34	1.37
44	B	821	CLA	C1B-C2B	2.43	1.48	1.43
44	2	514	CLA	MG-NB	-2.43	2.01	2.05
44	B	837	CLA	C1B-NB	-2.43	1.34	1.37
44	B	821	CLA	C3B-C4B	2.43	1.49	1.42
44	A	819	CLA	CMC-C2C	-2.43	1.45	1.50
44	L	301	CLA	CMC-C2C	-2.43	1.45	1.50
44	B	822	CLA	C1B-C2B	2.43	1.48	1.43
44	q	312	CLA	C1B-C2B	2.43	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	B	812	CLA	C1B-NB	-2.43	1.34	1.37
44	A	804	CLA	C1B-C2B	2.43	1.48	1.43
44	A	806	CLA	C1D-ND	2.43	1.41	1.37
44	3	318	CLA	C4B-C3B	2.42	1.48	1.43
51	1	502	LUT	C1-C6	-2.42	1.50	1.53
44	1	515	CLA	C1B-C2B	2.42	1.48	1.43
44	F	802	CLA	CMC-C2C	-2.42	1.45	1.50
44	A	814	CLA	CMC-C2C	-2.42	1.45	1.50
44	A	805	CLA	CMD-C2D	-2.42	1.45	1.50
44	B	839	CLA	CMC-C2C	-2.42	1.45	1.50
44	A	842	CLA	CHC-C1C	2.42	1.43	1.38
53	5	304	XAT	C2-C1	-2.42	1.50	1.54
44	A	804	CLA	MG-NB	-2.42	2.01	2.05
44	A	832	CLA	MG-NB	-2.42	2.01	2.05
44	5	306	CLA	C1B-C2B	2.42	1.48	1.43
44	A	825	CLA	CMC-C2C	-2.42	1.45	1.50
44	A	814	CLA	CMB-C2B	-2.42	1.45	1.50
44	B	811	CLA	C1D-ND	2.42	1.41	1.37
44	B	817	CLA	C1B-C2B	2.42	1.48	1.43
44	A	820	CLA	CMC-C2C	-2.41	1.45	1.50
44	A	826	CLA	CMB-C2B	-2.41	1.45	1.50
44	B	823	CLA	CMB-C2B	-2.41	1.45	1.50
44	A	810	CLA	CMC-C2C	-2.41	1.45	1.50
44	B	808	CLA	CMC-C2C	-2.41	1.45	1.50
44	B	802	CLA	C1B-C2B	2.41	1.48	1.43
44	5	311	CLA	C3B-C4B	2.41	1.49	1.42
44	B	818	CLA	MG-NB	-2.41	2.01	2.05
44	A	831	CLA	C1D-ND	2.41	1.41	1.37
44	B	819	CLA	CMC-C2C	-2.41	1.45	1.50
44	A	840	CLA	CMC-C2C	-2.41	1.45	1.50
44	p	505	CLA	C1B-C2B	2.41	1.48	1.43
44	5	313	CLA	CMB-C2B	-2.41	1.45	1.50
44	B	840	CLA	MG-NB	-2.41	2.01	2.05
44	K	203	CLA	CMC-C2C	-2.41	1.45	1.50
44	2	509	CLA	CMB-C2B	-2.41	1.45	1.50
44	B	807	CLA	MG-NB	-2.41	2.01	2.05
44	B	829	CLA	CMD-C2D	-2.41	1.45	1.50
44	2	507	CLA	CMD-C2D	-2.41	1.45	1.50
44	A	812	CLA	CMB-C2B	-2.40	1.45	1.50
44	5	309	CLA	CMD-C2D	-2.40	1.45	1.50
44	F	802	CLA	MG-NB	-2.40	2.01	2.05
44	B	838	CLA	MG-NB	-2.40	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	L	302	CLA	C1B-C2B	2.40	1.48	1.43
44	A	827	CLA	CMB-C2B	-2.40	1.45	1.50
44	B	831	CLA	CMC-C2C	-2.40	1.45	1.50
44	2	511	CLA	MG-NB	-2.40	2.01	2.05
44	A	817	CLA	CHC-C1C	2.40	1.43	1.38
44	B	812	CLA	C1D-ND	2.40	1.41	1.37
44	B	837	CLA	C1D-ND	2.40	1.41	1.37
44	5	311	CLA	CMB-C2B	-2.40	1.45	1.50
44	5	316	CLA	CMD-C2D	-2.40	1.45	1.50
44	3	316	CLA	C1B-C2B	2.40	1.48	1.43
44	A	806	CLA	CMD-C2D	-2.40	1.45	1.50
44	5	313	CLA	C1B-C2B	2.40	1.48	1.43
44	B	820	CLA	CMD-C2D	-2.40	1.45	1.50
44	B	842	CLA	CMC-C2C	-2.40	1.45	1.50
51	3	304	LUT	C22-C21	-2.40	1.51	1.54
44	A	813	CLA	C1B-C2B	2.40	1.48	1.43
44	2	508	CLA	C1B-C2B	2.40	1.48	1.43
44	B	828	CLA	CMC-C2C	-2.39	1.45	1.50
44	A	852	CLA	MG-NB	-2.39	2.01	2.05
44	B	831	CLA	MG-NB	-2.39	2.01	2.05
44	A	802	CLA	CMD-C2D	-2.39	1.45	1.50
44	B	839	CLA	CMD-C2D	-2.39	1.45	1.50
44	A	807	CLA	CMC-C2C	-2.39	1.45	1.50
44	B	840	CLA	CMC-C2C	-2.39	1.45	1.50
47	3	305	BCR	C1-C6	-2.39	1.50	1.53
44	A	811	CLA	CMB-C2B	-2.39	1.45	1.50
44	3	311	CLA	C1B-NB	-2.39	1.34	1.37
44	A	803	CLA	CMC-C2C	-2.39	1.45	1.50
44	B	805	CLA	CMC-C2C	-2.39	1.45	1.50
44	B	804	CLA	C1B-C2B	2.39	1.48	1.43
51	3	303	LUT	C22-C21	-2.39	1.51	1.54
44	r	306	CLA	CHC-C1C	2.39	1.43	1.38
44	n	203	CLA	CMD-C2D	-2.39	1.45	1.50
44	A	821	CLA	MG-NB	-2.39	2.01	2.05
44	A	823	CLA	MG-NB	-2.39	2.01	2.05
44	3	317	CLA	MG-NB	-2.39	2.01	2.05
44	B	839	CLA	C1B-NB	-2.39	1.34	1.37
52	1	517	CHL	CHA-CBD	-2.39	1.48	1.51
44	B	818	CLA	CMD-C2D	-2.38	1.45	1.50
44	f	828	CLA	CMC-C2C	-2.38	1.45	1.50
44	A	840	CLA	C1B-NB	-2.38	1.34	1.37
44	2	510	CLA	C1B-C2B	2.38	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	K	202	CLA	CHC-C1C	2.38	1.43	1.38
44	A	809	CLA	MG-NB	-2.38	2.01	2.05
47	F	801	BCR	C1-C6	-2.38	1.50	1.53
44	1	509	CLA	CMD-C2D	-2.38	1.45	1.50
44	f	821	CLA	C3B-C4B	2.38	1.49	1.42
44	L	302	CLA	CMB-C2B	-2.38	1.45	1.50
44	B	842	CLA	C1B-C2B	2.38	1.48	1.43
51	2	501	LUT	C1-C6	-2.38	1.50	1.53
44	B	818	CLA	CMC-C2C	-2.38	1.45	1.50
44	m	102	CLA	C3B-C4B	2.38	1.49	1.42
44	3	307	CLA	CHC-C1C	2.38	1.43	1.38
44	A	804	CLA	CMB-C2B	-2.38	1.45	1.50
44	e	829	CLA	CMB-C2B	-2.38	1.45	1.50
44	A	836	CLA	C1D-ND	2.38	1.41	1.37
44	5	309	CLA	CMB-C2B	-2.38	1.45	1.50
44	3	311	CLA	CMD-C2D	-2.38	1.45	1.50
44	B	828	CLA	C1B-NB	-2.38	1.34	1.37
44	A	814	CLA	C1B-C2B	2.38	1.48	1.43
44	A	839	CLA	C1B-C2B	2.38	1.48	1.43
44	A	819	CLA	CMD-C2D	-2.38	1.45	1.50
44	B	803	CLA	C1D-ND	2.38	1.41	1.37
44	B	820	CLA	C1D-ND	2.38	1.41	1.37
44	p	504	CLA	CHC-C1C	2.38	1.43	1.38
44	L	304	CLA	CMC-C2C	-2.37	1.45	1.50
52	2	515	CHL	CBD-CGD	-2.37	1.49	1.52
44	B	824	CLA	C1B-C2B	2.37	1.48	1.43
44	f	831	CLA	MG-NB	-2.37	2.01	2.05
44	A	816	CLA	C1B-NB	-2.37	1.34	1.37
44	B	824	CLA	CMC-C2C	-2.37	1.45	1.50
44	F	803	CLA	C4B-NB	2.37	1.41	1.37
44	B	823	CLA	CMC-C2C	-2.37	1.45	1.50
44	A	818	CLA	CMC-C2C	-2.37	1.45	1.50
44	2	510	CLA	MG-NB	-2.37	2.01	2.05
44	B	828	CLA	MG-NB	-2.37	2.01	2.05
44	1	505	CLA	CMB-C2B	-2.37	1.45	1.50
44	A	820	CLA	MG-NB	-2.37	2.01	2.05
44	A	812	CLA	C1D-ND	2.37	1.41	1.37
44	1	513	CLA	MG-NB	-2.36	2.01	2.05
44	B	828	CLA	C1B-C2B	2.36	1.48	1.43
44	1	509	CLA	MG-NB	-2.36	2.01	2.05
44	K	205	CLA	CHC-C1C	2.36	1.43	1.38
44	A	814	CLA	C1D-ND	2.36	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	L	302	CLA	C4B-NB	2.36	1.41	1.37
44	B	814	CLA	CMB-C2B	-2.36	1.45	1.50
51	5	303	LUT	C22-C21	-2.36	1.51	1.54
44	2	505	CLA	CMC-C2C	-2.36	1.45	1.50
44	f	835	CLA	MG-NB	-2.36	2.01	2.05
44	K	201	CLA	CMC-C2C	-2.36	1.45	1.50
44	5	316	CLA	CMB-C2B	-2.36	1.45	1.50
44	A	838	CLA	CMC-C2C	-2.36	1.45	1.50
44	B	816	CLA	C1B-NB	-2.36	1.34	1.37
44	5	316	CLA	MG-NB	-2.36	2.01	2.05
44	A	842	CLA	CMC-C2C	-2.36	1.45	1.50
44	5	309	CLA	C1B-C2B	2.36	1.48	1.43
44	5	316	CLA	C1B-C2B	2.36	1.48	1.43
44	p	510	CLA	CMD-C2D	-2.36	1.45	1.50
43	A	801	CL0	O2A-CGA	-2.36	1.31	1.42
44	e	823	CLA	CHC-C1C	2.36	1.43	1.38
44	A	833	CLA	C1D-ND	2.35	1.41	1.37
44	f	834	CLA	C3B-C4B	2.35	1.49	1.42
44	A	818	CLA	C1B-NB	-2.35	1.34	1.37
44	B	836	CLA	CMC-C2C	-2.35	1.45	1.50
44	5	308	CLA	CMB-C2B	-2.35	1.45	1.50
44	K	202	CLA	C4B-NB	2.35	1.41	1.37
43	e	801	CL0	O2A-CGA	-2.35	1.31	1.42
44	A	825	CLA	CMB-C2B	-2.35	1.45	1.50
44	r	311	CLA	CMD-C2D	-2.35	1.46	1.50
44	1	504	CLA	MG-ND	-2.35	2.01	2.05
44	e	803	CLA	C3B-C4B	2.35	1.49	1.42
44	e	813	CLA	C3B-C4B	2.35	1.49	1.42
44	A	810	CLA	MG-NB	-2.35	2.01	2.05
44	B	828	CLA	C3A-C2A	-2.35	1.52	1.54
44	A	828	CLA	C1B-C2B	2.35	1.48	1.43
44	e	813	CLA	CHC-C1C	2.35	1.43	1.38
44	n	202	CLA	C3B-C4B	2.35	1.49	1.42
44	B	826	CLA	C1D-ND	2.35	1.40	1.37
44	A	827	CLA	C1B-NB	-2.35	1.34	1.37
44	A	824	CLA	C1D-ND	2.35	1.40	1.37
44	2	506	CLA	C4B-NB	2.35	1.40	1.37
44	p	506	CLA	C3B-C4B	2.35	1.49	1.42
44	B	823	CLA	C1B-C2B	2.35	1.48	1.43
44	1	511	CLA	C4B-NB	2.34	1.40	1.37
44	3	301	CLA	C4B-NB	2.34	1.40	1.37
44	B	822	CLA	CMC-C2C	-2.34	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f	820	CLA	MG-NB	-2.34	2.01	2.05
44	p	504	CLA	MG-NB	-2.34	2.01	2.05
44	L	304	CLA	MG-NB	-2.34	2.01	2.05
44	e	822	CLA	C3B-C4B	2.34	1.49	1.42
44	B	829	CLA	CMC-C2C	-2.34	1.46	1.50
44	5	310	CLA	MG-NB	-2.34	2.01	2.05
44	3	307	CLA	CMD-C2D	-2.34	1.46	1.50
44	5	307	CLA	MG-NB	-2.34	2.01	2.05
44	A	832	CLA	C1B-NB	-2.34	1.34	1.37
44	5	309	CLA	C1B-NB	-2.34	1.34	1.37
44	p	504	CLA	C3B-C4B	2.34	1.49	1.42
44	B	842	CLA	CMD-C2D	-2.34	1.46	1.50
44	2	514	CLA	CMB-C2B	-2.34	1.46	1.50
44	F	802	CLA	CMB-C2B	-2.34	1.46	1.50
44	q	316	CLA	C3B-C4B	2.34	1.49	1.42
44	3	316	CLA	CMB-C2B	-2.34	1.46	1.50
44	A	817	CLA	C1B-NB	-2.34	1.34	1.37
52	s	513	CHL	CBD-CGD	-2.34	1.49	1.52
44	p	509	CLA	C1B-NB	-2.34	1.34	1.37
44	B	841	CLA	C1D-ND	2.33	1.40	1.37
44	p	505	CLA	MG-NB	-2.33	2.01	2.05
44	B	833	CLA	CMD-C2D	-2.33	1.46	1.50
44	A	831	CLA	C4B-C3B	2.33	1.48	1.43
44	F	803	CLA	CMC-C2C	-2.33	1.46	1.50
44	3	308	CLA	C1B-C2B	2.33	1.48	1.43
44	B	801	CLA	C1D-ND	2.33	1.40	1.37
44	B	836	CLA	CMD-C2D	-2.33	1.46	1.50
44	A	808	CLA	CMD-C2D	-2.33	1.46	1.50
44	K	205	CLA	CMB-C2B	-2.33	1.46	1.50
44	3	309	CLA	MG-NB	-2.33	2.01	2.05
44	A	830	CLA	C1D-ND	2.33	1.40	1.37
44	A	813	CLA	CMB-C2B	-2.33	1.46	1.50
44	A	852	CLA	C4B-NB	2.33	1.40	1.37
44	e	825	CLA	C3B-C4B	2.33	1.49	1.42
44	B	810	CLA	C1B-NB	-2.33	1.34	1.37
44	B	817	CLA	MG-ND	-2.33	2.01	2.05
44	B	811	CLA	C1B-NB	-2.33	1.34	1.37
44	f	821	CLA	CHC-C1C	2.33	1.43	1.38
44	A	832	CLA	CMC-C2C	-2.33	1.46	1.50
44	A	839	CLA	CMB-C2B	-2.33	1.46	1.50
44	q	308	CLA	C3B-C4B	2.33	1.49	1.42
44	5	313	CLA	MG-NB	-2.33	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f	805	CLA	MG-NB	-2.33	2.01	2.05
44	A	836	CLA	C1B-NB	-2.32	1.34	1.37
44	q	306	CLA	C3B-C4B	2.32	1.49	1.42
44	f	827	CLA	CHC-C1C	2.32	1.43	1.38
44	B	833	CLA	C1B-C2B	2.32	1.48	1.43
44	A	815	CLA	CMD-C2D	-2.32	1.46	1.50
44	B	805	CLA	MG-NB	-2.32	2.01	2.05
44	2	508	CLA	CHC-C1C	2.32	1.43	1.38
44	B	812	CLA	C4B-C3B	2.32	1.48	1.43
44	p	510	CLA	C3B-C4B	2.32	1.49	1.42
44	L	303	CLA	C4B-NB	2.32	1.40	1.37
44	f	816	CLA	MG-NB	-2.32	2.01	2.05
44	A	842	CLA	CMB-C2B	-2.32	1.46	1.50
44	B	832	CLA	CMC-C2C	-2.32	1.46	1.50
44	2	514	CLA	CMD-C2D	-2.32	1.46	1.50
44	5	313	CLA	CMD-C2D	-2.32	1.46	1.50
44	q	305	CLA	C3B-C4B	2.32	1.49	1.42
44	s	505	CLA	C3B-C4B	2.32	1.49	1.42
44	e	839	CLA	CHC-C1C	2.32	1.43	1.38
44	f	834	CLA	CHC-C1C	2.32	1.43	1.38
44	f	837	CLA	C3B-C4B	2.32	1.49	1.42
44	2	506	CLA	CMD-C2D	-2.32	1.46	1.50
51	3	304	LUT	C1-C6	-2.32	1.50	1.53
52	5	314	CHL	CBD-CGD	-2.32	1.49	1.52
44	r	307	CLA	CHC-C1C	2.32	1.43	1.38
44	1	506	CLA	CMC-C2C	-2.31	1.46	1.50
44	3	301	CLA	CMD-C2D	-2.31	1.46	1.50
44	p	505	CLA	C3B-C4B	2.31	1.49	1.42
44	2	511	CLA	CMB-C2B	-2.31	1.46	1.50
44	F	803	CLA	C1B-C2B	2.31	1.48	1.43
44	5	311	CLA	C1B-C2B	2.31	1.48	1.43
44	e	804	CLA	MG-NB	-2.31	2.01	2.05
44	e	838	CLA	MG-NB	-2.31	2.01	2.05
44	A	815	CLA	C1B-NB	-2.31	1.34	1.37
44	A	822	CLA	C1B-C2B	2.31	1.48	1.43
44	3	306	CLA	C2C-C1C	2.31	1.45	1.40
44	f	814	CLA	CHC-C1C	2.31	1.43	1.38
44	B	831	CLA	C1B-C2B	2.31	1.48	1.43
44	f	828	CLA	MG-NB	-2.31	2.01	2.05
44	p	505	CLA	C4B-NB	2.31	1.40	1.37
44	p	515	CLA	C3B-C4B	2.31	1.49	1.42
44	A	852	CLA	C1B-C2B	2.31	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	J	102	BCR	C30-C25	-2.31	1.50	1.53
44	e	821	CLA	MG-NB	-2.31	2.01	2.05
44	q	311	CLA	C3B-C4B	2.31	1.49	1.42
44	e	812	CLA	MG-NB	-2.31	2.01	2.05
44	e	830	CLA	MG-NB	-2.31	2.01	2.05
44	e	803	CLA	CHC-C1C	2.31	1.43	1.38
44	e	836	CLA	MG-NB	-2.31	2.01	2.05
44	r	304	CLA	CHC-C1C	2.31	1.43	1.38
44	A	830	CLA	CMC-C2C	-2.31	1.46	1.50
44	B	821	CLA	MG-NB	-2.31	2.01	2.05
44	e	819	CLA	C3B-C4B	2.31	1.49	1.42
44	e	808	CLA	C3B-C4B	2.31	1.49	1.42
44	3	301	CLA	C1B-NB	-2.31	1.34	1.37
44	n	201	CLA	C3B-C4B	2.30	1.49	1.42
44	B	824	CLA	C4B-NB	2.30	1.40	1.37
44	1	513	CLA	CMD-C2D	-2.30	1.46	1.50
44	5	312	CLA	C1B-C2B	2.30	1.48	1.43
44	3	314	CLA	C3B-C4B	2.30	1.49	1.42
44	A	837	CLA	C3A-C2A	-2.30	1.52	1.54
44	B	841	CLA	CMC-C2C	-2.30	1.46	1.50
44	K	205	CLA	C3B-C4B	2.30	1.49	1.42
44	r	306	CLA	C3B-C4B	2.30	1.49	1.42
44	r	311	CLA	C3B-C4B	2.30	1.49	1.42
44	A	818	CLA	CMD-C2D	-2.30	1.46	1.50
44	A	837	CLA	CMB-C2B	-2.30	1.46	1.50
44	s	511	CLA	C3B-C4B	2.30	1.49	1.42
44	A	802	CLA	MG-NB	-2.30	2.01	2.05
44	K	202	CLA	MG-NB	-2.30	2.01	2.05
44	K	205	CLA	C1B-C2B	2.30	1.48	1.43
44	f	810	CLA	C3B-C4B	2.30	1.49	1.42
44	B	832	CLA	CMD-C2D	-2.30	1.46	1.50
44	A	817	CLA	CMC-C2C	-2.30	1.46	1.50
47	B	848	BCR	C1-C6	-2.30	1.50	1.53
44	B	804	CLA	C1B-NB	-2.30	1.34	1.37
44	A	815	CLA	MG-ND	-2.30	2.01	2.05
44	r	317	CLA	MG-NB	-2.30	2.01	2.05
44	5	311	CLA	MG-NB	-2.30	2.01	2.05
44	A	822	CLA	CMB-C2B	-2.30	1.46	1.50
44	B	833	CLA	CMB-C2B	-2.30	1.46	1.50
44	B	835	CLA	CMD-C2D	-2.30	1.46	1.50
44	J	101	CLA	CHC-C1C	2.30	1.43	1.38
44	e	816	CLA	C3B-C4B	2.30	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	5	313	CLA	C4B-NB	2.29	1.40	1.37
44	e	832	CLA	C3B-C4B	2.29	1.49	1.42
44	q	307	CLA	C3B-C4B	2.29	1.49	1.42
44	3	313	CLA	C3B-C4B	2.29	1.49	1.42
44	f	826	CLA	C3B-C4B	2.29	1.49	1.42
44	2	511	CLA	CMD-C2D	-2.29	1.46	1.50
44	L	302	CLA	MG-NB	-2.29	2.01	2.05
44	5	312	CLA	CMB-C2B	-2.29	1.46	1.50
44	F	803	CLA	CMD-C2D	-2.29	1.46	1.50
44	K	202	CLA	CMD-C2D	-2.29	1.46	1.50
44	f	816	CLA	CMD-C2D	-2.29	1.46	1.50
44	A	803	CLA	C4B-NB	2.29	1.40	1.37
44	f	842	CLA	CMB-C2B	-2.29	1.46	1.50
44	f	806	CLA	C3B-C4B	2.29	1.49	1.42
44	1	510	CLA	CMB-C2B	-2.29	1.46	1.50
44	1	507	CLA	C4B-NB	2.29	1.40	1.37
44	2	504	CLA	CMC-C2C	-2.29	1.46	1.50
44	e	824	CLA	MG-NB	-2.29	2.01	2.05
44	1	507	CLA	CMB-C2B	-2.29	1.46	1.50
44	e	820	CLA	MG-NB	-2.29	2.01	2.05
44	q	314	CLA	MG-NB	-2.29	2.01	2.05
44	A	814	CLA	C4B-NB	2.29	1.40	1.37
44	B	809	CLA	MG-NB	-2.29	2.01	2.05
44	B	827	CLA	MG-NB	-2.29	2.01	2.05
44	f	832	CLA	MG-NB	-2.29	2.01	2.05
44	f	843	CLA	MG-NB	-2.29	2.01	2.05
44	3	317	CLA	CMC-C2C	-2.29	1.46	1.50
44	e	834	CLA	MG-NB	-2.29	2.01	2.05
44	f	805	CLA	CMC-C2C	-2.28	1.46	1.50
44	A	836	CLA	CMC-C2C	-2.28	1.46	1.50
44	e	827	CLA	MG-NB	-2.28	2.01	2.05
44	A	817	CLA	MG-ND	-2.28	2.01	2.05
44	3	301	CLA	MG-NB	-2.28	2.01	2.05
44	3	312	CLA	C3B-C4B	2.28	1.49	1.42
44	r	312	CLA	C3B-C4B	2.28	1.49	1.42
44	B	808	CLA	C1B-C2B	2.28	1.48	1.43
44	e	805	CLA	MG-NB	-2.28	2.01	2.05
44	A	805	CLA	C1B-NB	-2.28	1.34	1.37
44	B	802	CLA	C4B-NB	2.28	1.40	1.37
44	1	507	CLA	C1B-C2B	2.28	1.48	1.43
44	A	833	CLA	C3B-C4B	2.28	1.49	1.42
44	B	812	CLA	C1B-C2B	2.28	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	L	303	CLA	C1D-ND	2.28	1.40	1.37
44	e	818	CLA	C1B-NB	-2.28	1.34	1.37
44	q	309	CLA	C3B-C4B	2.28	1.49	1.42
44	1	508	CLA	MG-NB	-2.28	2.01	2.05
44	q	314	CLA	C3B-C4B	2.28	1.49	1.42
44	B	841	CLA	C1B-NB	-2.28	1.34	1.37
44	1	508	CLA	CMD-C2D	-2.28	1.46	1.50
44	e	816	CLA	CMD-C2D	-2.28	1.46	1.50
47	B	846	BCR	C1-C6	-2.28	1.50	1.53
44	r	310	CLA	C3B-C4B	2.28	1.49	1.42
44	q	315	CLA	C3B-C4B	2.27	1.49	1.42
44	A	828	CLA	CMC-C2C	-2.27	1.46	1.50
44	3	307	CLA	CMC-C2C	-2.27	1.46	1.50
44	f	825	CLA	MG-NB	-2.27	2.01	2.05
44	e	843	CLA	CHC-C1C	2.27	1.43	1.38
44	e	837	CLA	MG-NB	-2.27	2.01	2.05
44	5	316	CLA	CMC-C2C	-2.27	1.46	1.50
44	3	308	CLA	MG-NB	-2.27	2.01	2.05
44	B	836	CLA	MG-NB	-2.27	2.01	2.05
44	B	832	CLA	C1B-C2B	2.27	1.48	1.43
44	f	814	CLA	C3B-C4B	2.27	1.49	1.42
44	B	822	CLA	MG-NB	-2.27	2.01	2.05
44	f	803	CLA	C3B-C4B	2.27	1.49	1.42
44	A	815	CLA	CMC-C2C	-2.27	1.46	1.50
44	e	830	CLA	CMD-C2D	-2.27	1.46	1.50
44	q	316	CLA	CHC-C1C	2.27	1.43	1.38
44	A	824	CLA	CMC-C2C	-2.27	1.46	1.50
44	e	853	CLA	MG-NB	-2.27	2.01	2.05
44	5	307	CLA	CMB-C2B	-2.27	1.46	1.50
44	r	307	CLA	C3B-C4B	2.27	1.49	1.42
44	e	841	CLA	C3B-C4B	2.27	1.49	1.42
44	B	821	CLA	CMC-C2C	-2.27	1.46	1.50
44	f	822	CLA	C3B-C4B	2.27	1.49	1.42
44	j	802	CLA	C3B-C4B	2.27	1.49	1.42
44	e	826	CLA	CHC-C1C	2.26	1.43	1.38
44	f	823	CLA	MG-NB	-2.26	2.01	2.05
44	f	817	CLA	MG-NB	-2.26	2.01	2.05
44	L	303	CLA	MG-NB	-2.26	2.01	2.05
44	A	831	CLA	C1B-C2B	2.26	1.48	1.43
44	B	810	CLA	CMD-C2D	-2.26	1.46	1.50
44	B	825	CLA	C1B-C2B	2.26	1.48	1.43
44	e	806	CLA	CHC-C1C	2.26	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	f	849	BCR	C30-C25	-2.26	1.50	1.53
44	1	504	CLA	C1B-C2B	2.26	1.48	1.43
44	f	833	CLA	MG-NB	-2.26	2.01	2.05
44	A	834	CLA	CMD-C2D	-2.26	1.46	1.50
44	e	839	CLA	C3B-C4B	2.26	1.49	1.42
44	3	306	CLA	C1B-C2B	2.26	1.48	1.43
44	f	815	CLA	C3B-C4B	2.26	1.49	1.42
44	p	504	CLA	CMD-C2D	-2.26	1.46	1.50
44	B	805	CLA	CHC-C1C	2.26	1.43	1.38
44	s	514	CLA	MG-NB	-2.26	2.01	2.05
44	e	810	CLA	MG-NB	-2.26	2.01	2.05
44	B	834	CLA	C4B-NB	2.26	1.40	1.37
44	J	101	CLA	MG-NB	-2.26	2.01	2.05
44	e	828	CLA	C3B-C4B	2.26	1.49	1.42
44	A	825	CLA	MG-ND	-2.26	2.01	2.05
44	B	839	CLA	C4B-NB	2.26	1.40	1.37
44	B	834	CLA	CMD-C2D	-2.26	1.46	1.50
44	1	510	CLA	MG-NB	-2.26	2.01	2.05
44	A	809	CLA	CBD-CGD	-2.26	1.49	1.51
44	A	804	CLA	C1D-ND	2.26	1.40	1.37
44	e	807	CLA	C3B-C4B	2.26	1.49	1.42
44	f	827	CLA	MG-NB	-2.26	2.01	2.05
44	A	807	CLA	CMD-C2D	-2.25	1.46	1.50
44	f	817	CLA	C3B-C4B	2.25	1.49	1.42
44	f	811	CLA	MG-NB	-2.25	2.01	2.05
44	r	306	CLA	MG-NB	-2.25	2.01	2.05
44	B	837	CLA	CHC-C1C	2.25	1.43	1.38
44	3	310	CLA	CMB-C2B	-2.25	1.46	1.50
44	e	817	CLA	CMB-C2B	-2.25	1.46	1.50
44	e	830	CLA	C3B-C4B	2.25	1.49	1.42
44	K	201	CLA	MG-ND	-2.25	2.01	2.05
44	f	830	CLA	CMD-C2D	-2.25	1.46	1.50
44	5	305	CLA	C1D-ND	2.25	1.40	1.37
44	A	810	CLA	C1B-NB	-2.25	1.34	1.37
44	B	806	CLA	C1B-C2B	2.25	1.48	1.43
44	q	307	CLA	MG-NB	-2.25	2.01	2.05
44	e	825	CLA	MG-NB	-2.25	2.01	2.05
44	n	203	CLA	MG-NB	-2.25	2.01	2.05
44	B	823	CLA	C4B-NB	2.25	1.40	1.37
44	3	314	CLA	CMD-C2D	-2.25	1.46	1.50
44	K	201	CLA	CHC-C1C	2.25	1.43	1.38
44	B	840	CLA	C1D-ND	2.25	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	K	203	CLA	C1D-ND	2.25	1.40	1.37
44	A	817	CLA	CMD-C2D	-2.25	1.46	1.50
44	e	831	CLA	MG-NB	-2.25	2.01	2.05
44	B	822	CLA	CHC-C1C	2.25	1.43	1.38
44	q	305	CLA	CHC-C1C	2.25	1.43	1.38
44	B	815	CLA	CHC-C1C	2.25	1.43	1.38
44	e	831	CLA	CHC-C1C	2.25	1.43	1.38
44	n	201	CLA	CHC-C1C	2.25	1.43	1.38
44	s	504	CLA	CHC-C1C	2.25	1.43	1.38
44	e	833	CLA	CMD-C2D	-2.25	1.46	1.50
44	f	827	CLA	C3B-C4B	2.25	1.49	1.42
47	e	848	BCR	C30-C25	-2.25	1.50	1.53
44	e	837	CLA	CHC-C1C	2.25	1.43	1.38
44	1	507	CLA	CMC-C2C	-2.25	1.46	1.50
44	s	507	CLA	C3B-C4B	2.24	1.49	1.42
44	F	802	CLA	C1B-C2B	2.24	1.48	1.43
44	f	818	CLA	CHC-C1C	2.24	1.43	1.38
44	f	838	CLA	CHC-C1C	2.24	1.43	1.38
44	f	838	CLA	MG-NB	-2.24	2.01	2.05
44	1	505	CLA	CHC-C1C	2.24	1.43	1.38
44	3	311	CLA	CMC-C2C	-2.24	1.46	1.50
44	A	826	CLA	C1D-ND	2.24	1.40	1.37
44	s	508	CLA	C3B-C4B	2.24	1.49	1.42
44	3	307	CLA	MG-NB	-2.24	2.01	2.05
44	2	509	CLA	C3B-C4B	2.24	1.49	1.42
44	2	507	CLA	CHC-C1C	2.24	1.43	1.38
44	r	317	CLA	CHC-C1C	2.24	1.43	1.38
44	2	510	CLA	CMD-C2D	-2.24	1.46	1.50
44	f	803	CLA	MG-NB	-2.24	2.01	2.05
44	f	841	CLA	CHC-C1C	2.24	1.43	1.38
44	B	825	CLA	C1D-ND	2.24	1.40	1.37
44	f	807	CLA	CHC-C1C	2.24	1.43	1.38
44	B	803	CLA	C1B-C2B	2.24	1.48	1.43
44	2	509	CLA	MG-NB	-2.24	2.01	2.05
44	1	510	CLA	CMC-C2C	-2.24	1.46	1.50
44	e	837	CLA	C3B-C4B	2.24	1.49	1.42
44	f	843	CLA	C3B-C4B	2.24	1.49	1.42
44	f	808	CLA	CHC-C1C	2.24	1.43	1.38
44	K	202	CLA	CMB-C2B	-2.24	1.46	1.50
44	e	814	CLA	CHC-C1C	2.24	1.43	1.38
44	n	202	CLA	CHC-C1C	2.24	1.43	1.38
44	1	505	CLA	C3B-C4B	2.24	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	e	813	CLA	MG-NB	-2.24	2.01	2.05
44	s	514	CLA	C3B-C4B	2.24	1.49	1.42
44	f	818	CLA	MG-NB	-2.24	2.01	2.05
44	B	828	CLA	CMB-C2B	-2.23	1.46	1.50
44	f	818	CLA	C3B-C4B	2.23	1.49	1.42
44	2	505	CLA	CMB-C2B	-2.23	1.46	1.50
44	5	305	CLA	C1B-NB	-2.23	1.34	1.37
44	B	826	CLA	CMB-C2B	-2.23	1.46	1.50
44	B	805	CLA	C4B-NB	2.23	1.40	1.37
44	f	816	CLA	CHC-C1C	2.23	1.43	1.38
44	f	808	CLA	MG-NB	-2.23	2.01	2.05
44	2	504	CLA	CMD-C2D	-2.23	1.46	1.50
44	A	813	CLA	C1D-ND	2.23	1.40	1.37
44	A	826	CLA	CHC-C1C	2.23	1.43	1.38
44	f	837	CLA	CHC-C1C	2.23	1.43	1.38
44	e	811	CLA	MG-NB	-2.23	2.01	2.05
44	B	825	CLA	CMB-C2B	-2.23	1.46	1.50
44	f	838	CLA	C3B-C4B	2.23	1.49	1.42
44	q	304	CLA	CHC-C1C	2.23	1.43	1.38
44	F	803	CLA	CMB-C2B	-2.23	1.46	1.50
44	f	815	CLA	MG-NB	-2.23	2.01	2.05
44	5	312	CLA	CMD-C2D	-2.23	1.46	1.50
44	B	837	CLA	C1B-C2B	2.23	1.48	1.43
44	B	839	CLA	C1B-C2B	2.23	1.48	1.43
44	B	809	CLA	CMC-C2C	-2.23	1.46	1.50
44	1	506	CLA	MG-NB	-2.23	2.01	2.05
44	B	832	CLA	MG-ND	-2.23	2.01	2.05
44	q	310	CLA	C3B-C4B	2.23	1.49	1.42
44	B	839	CLA	CMB-C2B	-2.23	1.46	1.50
44	f	824	CLA	MG-NB	-2.23	2.01	2.05
44	s	507	CLA	MG-NB	-2.23	2.01	2.05
44	f	807	CLA	CMD-C2D	-2.23	1.46	1.50
44	e	853	CLA	C3B-C4B	2.23	1.49	1.42
44	K	201	CLA	CMB-C2B	-2.22	1.46	1.50
44	e	830	CLA	CMB-C2B	-2.22	1.46	1.50
44	f	831	CLA	C3B-C4B	2.22	1.49	1.42
44	f	801	CLA	MG-NB	-2.22	2.01	2.05
44	p	508	CLA	CHC-C1C	2.22	1.42	1.38
44	f	819	CLA	C3B-C4B	2.22	1.49	1.42
44	r	315	CLA	C3B-C4B	2.22	1.49	1.42
44	A	836	CLA	CHC-C1C	2.22	1.42	1.38
44	s	509	CLA	CHC-C1C	2.22	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	r	304	CLA	CMD-C2D	-2.22	1.46	1.50
44	2	510	CLA	MG-ND	-2.22	2.01	2.05
44	3	317	CLA	CMB-C2B	-2.22	1.46	1.50
44	f	823	CLA	C3B-C4B	2.22	1.49	1.42
44	e	810	CLA	C3B-C4B	2.22	1.49	1.42
44	e	805	CLA	C3B-C4B	2.22	1.49	1.42
44	L	303	CLA	CMC-C2C	-2.22	1.46	1.50
44	e	833	CLA	CMB-C2B	-2.22	1.46	1.50
44	s	506	CLA	C3B-C4B	2.22	1.49	1.42
44	p	507	CLA	MG-NB	-2.22	2.01	2.05
44	e	841	CLA	CMB-C2B	-2.22	1.46	1.50
44	e	822	CLA	MG-NB	-2.22	2.01	2.05
44	f	829	CLA	MG-NB	-2.22	2.01	2.05
44	e	817	CLA	C3B-C4B	2.22	1.49	1.42
44	e	819	CLA	CMB-C2B	-2.22	1.46	1.50
44	e	810	CLA	CHC-C1C	2.22	1.42	1.38
44	5	309	CLA	CMC-C2C	-2.22	1.46	1.50
44	f	828	CLA	CMB-C2B	-2.22	1.46	1.50
44	q	314	CLA	CMB-C2B	-2.22	1.46	1.50
44	B	810	CLA	C4B-NB	2.22	1.40	1.37
44	f	808	CLA	C3B-C4B	2.22	1.49	1.42
44	K	201	CLA	C3B-C4B	2.22	1.49	1.42
44	f	819	CLA	MG-NB	-2.22	2.01	2.05
44	A	807	CLA	C1B-NB	-2.22	1.34	1.37
44	2	506	CLA	MG-NB	-2.22	2.01	2.05
44	s	505	CLA	CMD-C2D	-2.22	1.46	1.50
44	q	307	CLA	CHC-C1C	2.22	1.42	1.38
44	1	504	CLA	C3B-C4B	2.22	1.49	1.42
44	3	309	CLA	CMC-C2C	-2.22	1.46	1.50
44	e	828	CLA	CHC-C1C	2.22	1.42	1.38
44	e	833	CLA	CHC-C1C	2.22	1.42	1.38
44	q	308	CLA	CHC-C1C	2.22	1.42	1.38
44	e	814	CLA	C3B-C4B	2.22	1.49	1.42
44	r	312	CLA	MG-NB	-2.22	2.01	2.05
44	e	836	CLA	C3B-C4B	2.21	1.49	1.42
44	A	825	CLA	C4B-NB	2.21	1.40	1.37
47	o	301	BCR	C1-C6	-2.21	1.50	1.53
44	f	832	CLA	CMB-C2B	-2.21	1.46	1.50
44	B	838	CLA	C4B-NB	2.21	1.40	1.37
44	p	508	CLA	C3B-C4B	2.21	1.49	1.42
44	B	836	CLA	CHC-C1C	2.21	1.42	1.38
44	s	511	CLA	CHC-C1C	2.21	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	e	850	BCR	C30-C25	-2.21	1.50	1.53
44	e	806	CLA	C3B-C4B	2.21	1.49	1.42
44	L	303	CLA	CMD-C2D	-2.21	1.46	1.50
44	e	808	CLA	CHC-C1C	2.21	1.42	1.38
44	f	839	CLA	CHC-C1C	2.21	1.42	1.38
44	e	852	CLA	CMC-C2C	-2.21	1.46	1.50
44	q	310	CLA	CMD-C2D	-2.21	1.46	1.50
44	r	317	CLA	C3B-C4B	2.21	1.49	1.42
44	5	306	CLA	CMB-C2B	-2.21	1.46	1.50
44	e	833	CLA	MG-NB	-2.21	2.01	2.05
44	e	811	CLA	C3B-C4B	2.21	1.49	1.42
44	f	825	CLA	CHC-C1C	2.21	1.42	1.38
44	m	102	CLA	CHC-C1C	2.21	1.42	1.38
44	e	802	CLA	C3B-C4B	2.21	1.49	1.42
44	A	822	CLA	CMC-C2C	-2.21	1.46	1.50
44	f	826	CLA	MG-NB	-2.21	2.01	2.05
44	e	815	CLA	CHC-C1C	2.21	1.42	1.38
44	p	511	CLA	CHC-C1C	2.21	1.42	1.38
44	e	810	CLA	CMD-C2D	-2.21	1.46	1.50
44	o	304	CLA	C3B-C4B	2.21	1.49	1.42
44	f	842	CLA	CMD-C2D	-2.21	1.46	1.50
44	e	838	CLA	C3B-C4B	2.21	1.49	1.42
44	e	826	CLA	MG-NB	-2.21	2.01	2.05
44	e	807	CLA	CHC-C1C	2.21	1.42	1.38
44	e	810	CLA	CMB-C2B	-2.21	1.46	1.50
44	e	831	CLA	C3B-C4B	2.21	1.49	1.42
44	B	817	CLA	C4B-NB	2.21	1.40	1.37
44	A	802	CLA	C1B-C2B	2.21	1.48	1.43
44	1	507	CLA	CMD-C2D	-2.20	1.46	1.50
44	K	202	CLA	C3B-C4B	2.20	1.49	1.42
44	f	839	CLA	C3B-C4B	2.20	1.49	1.42
44	5	308	CLA	C1B-C2B	2.20	1.48	1.43
52	2	516	CHL	CBD-CGD	-2.20	1.49	1.52
44	3	310	CLA	C3B-C4B	2.20	1.49	1.42
44	B	802	CLA	C3B-C4B	2.20	1.49	1.42
44	B	824	CLA	C1B-NB	-2.20	1.35	1.37
44	2	514	CLA	CMC-C2C	-2.20	1.46	1.50
44	e	815	CLA	C3B-C4B	2.20	1.49	1.42
44	r	308	CLA	C3B-C4B	2.20	1.49	1.42
44	B	841	CLA	C1B-C2B	2.20	1.48	1.43
44	2	508	CLA	C3B-C4B	2.20	1.49	1.42
44	s	510	CLA	C3B-C4B	2.20	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	L	303	CLA	C3B-C4B	2.20	1.49	1.42
44	2	509	CLA	C1B-C2B	2.20	1.48	1.43
44	e	819	CLA	CHC-C1C	2.20	1.42	1.38
44	p	510	CLA	MG-NB	-2.20	2.01	2.05
44	A	814	CLA	CAC-C3C	-2.20	1.45	1.51
44	f	835	CLA	C3B-C4B	2.20	1.49	1.42
44	3	317	CLA	C3B-C4B	2.20	1.49	1.42
44	f	805	CLA	C3B-C4B	2.20	1.49	1.42
44	f	811	CLA	CMB-C2B	-2.20	1.46	1.50
44	A	827	CLA	MG-ND	-2.20	2.01	2.05
44	3	317	CLA	CMD-C2D	-2.20	1.46	1.50
44	e	804	CLA	CMD-C2D	-2.20	1.46	1.50
44	e	852	CLA	CMB-C2B	-2.20	1.46	1.50
44	A	814	CLA	MG-NB	-2.20	2.01	2.05
44	o	303	CLA	MG-NB	-2.20	2.01	2.05
44	B	819	CLA	C3A-C2A	-2.20	1.52	1.54
44	B	822	CLA	C3B-C4B	2.20	1.49	1.42
44	1	508	CLA	CHC-C1C	2.20	1.42	1.38
44	r	311	CLA	CHC-C1C	2.20	1.42	1.38
44	f	806	CLA	MG-NB	-2.20	2.01	2.05
44	p	506	CLA	CHC-C1C	2.20	1.42	1.38
44	A	833	CLA	C1B-C2B	2.20	1.48	1.43
44	B	829	CLA	C1B-NB	-2.20	1.35	1.37
44	2	514	CLA	MG-ND	-2.20	2.01	2.05
44	f	809	CLA	C3B-C4B	2.20	1.49	1.42
44	s	511	CLA	CMD-C2D	-2.20	1.46	1.50
44	f	842	CLA	MG-NB	-2.20	2.01	2.05
44	s	510	CLA	MG-NB	-2.20	2.01	2.05
44	3	312	CLA	MG-NB	-2.19	2.01	2.05
47	e	846	BCR	C1-C6	-2.19	1.51	1.53
44	f	803	CLA	CHC-C1C	2.19	1.42	1.38
44	q	314	CLA	CHC-C1C	2.19	1.42	1.38
44	f	841	CLA	C3B-C4B	2.19	1.49	1.42
44	s	507	CLA	CHC-C1C	2.19	1.42	1.38
44	A	829	CLA	MG-ND	-2.19	2.01	2.05
44	s	507	CLA	CMD-C2D	-2.19	1.46	1.50
44	f	815	CLA	CHC-C1C	2.19	1.42	1.38
44	e	814	CLA	MG-NB	-2.19	2.01	2.05
52	5	315	CHL	CHA-CBD	-2.19	1.49	1.51
44	e	808	CLA	CMB-C2B	-2.19	1.46	1.50
44	f	824	CLA	CMB-C2B	-2.19	1.46	1.50
44	f	819	CLA	CHC-C1C	2.19	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f	833	CLA	CHC-C1C	2.19	1.42	1.38
44	s	508	CLA	MG-NB	-2.19	2.01	2.05
44	e	830	CLA	CHC-C1C	2.19	1.42	1.38
52	r	314	CHL	CBD-CGD	-2.19	1.49	1.52
44	e	835	CLA	C3B-C4B	2.19	1.49	1.42
44	f	836	CLA	C3B-C4B	2.19	1.49	1.42
52	3	302	CHL	CHA-CBD	-2.19	1.49	1.51
52	5	317	CHL	CBD-CGD	-2.19	1.49	1.52
44	1	515	CLA	C3B-C4B	2.19	1.49	1.42
44	e	832	CLA	CHC-C1C	2.19	1.42	1.38
44	s	506	CLA	MG-NB	-2.19	2.01	2.05
44	e	802	CLA	CMD-C2D	-2.19	1.46	1.50
44	f	829	CLA	CMB-C2B	-2.19	1.46	1.50
44	e	839	CLA	MG-NB	-2.19	2.01	2.05
44	A	820	CLA	C3B-C4B	2.19	1.49	1.42
44	e	840	CLA	CMD-C2D	-2.19	1.46	1.50
44	B	801	CLA	C1B-C2B	2.19	1.48	1.43
44	p	505	CLA	CHC-C1C	2.19	1.42	1.38
44	A	836	CLA	CAA-C2A	-2.19	1.50	1.54
46	A	844	LHG	O7-C5	-2.19	1.41	1.46
44	r	305	CLA	CHC-C1C	2.19	1.42	1.38
44	B	829	CLA	MG-ND	-2.19	2.01	2.05
44	f	814	CLA	MG-NB	-2.19	2.01	2.05
44	o	304	CLA	CHC-C1C	2.19	1.42	1.38
44	5	305	CLA	CMB-C2B	-2.19	1.45	1.50
44	2	511	CLA	CMC-C2C	-2.19	1.46	1.50
44	f	830	CLA	CHC-C1C	2.19	1.42	1.38
44	f	834	CLA	MG-NB	-2.19	2.01	2.05
44	r	307	CLA	MG-NB	-2.19	2.01	2.05
47	m	103	BCR	C1-C6	-2.19	1.51	1.53
44	e	809	CLA	C3B-C4B	2.19	1.49	1.42
44	s	504	CLA	MG-NB	-2.19	2.01	2.05
44	A	810	CLA	C1B-C2B	2.19	1.48	1.43
44	B	820	CLA	CHC-C1C	2.19	1.42	1.38
44	e	805	CLA	CHC-C1C	2.19	1.42	1.38
44	B	807	CLA	MG-ND	-2.19	2.01	2.05
44	2	510	CLA	C3B-C4B	2.19	1.49	1.42
44	f	828	CLA	C3B-C4B	2.19	1.49	1.42
47	f	848	BCR	C30-C25	-2.19	1.51	1.53
47	q	303	BCR	C30-C25	-2.19	1.51	1.53
44	2	504	CLA	C4B-NB	2.19	1.40	1.37
44	f	804	CLA	C4B-NB	-2.19	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f	824	CLA	C3B-C4B	2.19	1.49	1.42
44	e	833	CLA	C3B-C4B	2.19	1.49	1.42
44	f	825	CLA	C3B-C4B	2.19	1.49	1.42
44	1	511	CLA	CMD-C2D	-2.18	1.46	1.50
44	F	802	CLA	C3B-C4B	2.18	1.49	1.42
44	p	507	CLA	CMB-C2B	-2.18	1.46	1.50
44	p	508	CLA	CMD-C2D	-2.18	1.46	1.50
44	1	509	CLA	C3B-C4B	2.18	1.49	1.42
44	3	316	CLA	C3B-C4B	2.18	1.49	1.42
44	f	806	CLA	CHC-C1C	2.18	1.42	1.38
44	f	830	CLA	CMB-C2B	-2.18	1.46	1.50
44	5	308	CLA	C3B-C4B	2.18	1.49	1.42
44	A	840	CLA	C4B-NB	2.18	1.40	1.37
44	f	813	CLA	CMB-C2B	-2.18	1.46	1.50
44	f	825	CLA	CMD-C2D	-2.18	1.46	1.50
44	f	816	CLA	C3B-C4B	2.18	1.49	1.42
51	1	502	LUT	C22-C21	-2.18	1.52	1.54
44	e	822	CLA	CHC-C1C	2.18	1.42	1.38
44	p	511	CLA	MG-NB	-2.18	2.01	2.05
44	B	827	CLA	CHC-C1C	2.18	1.42	1.38
44	e	825	CLA	CHC-C1C	2.18	1.42	1.38
44	q	314	CLA	CMD-C2D	-2.18	1.46	1.50
44	f	836	CLA	CHC-C1C	2.18	1.42	1.38
44	f	817	CLA	CMD-C2D	-2.18	1.46	1.50
44	B	825	CLA	MG-ND	-2.18	2.01	2.05
52	s	512	CHL	CBD-CGD	-2.18	1.49	1.52
44	A	839	CLA	MG-ND	-2.18	2.01	2.05
44	3	311	CLA	C3B-C4B	2.18	1.49	1.42
44	B	815	CLA	C1B-C2B	2.18	1.48	1.43
44	B	812	CLA	C3B-C2B	-2.18	1.35	1.44
44	5	309	CLA	C4B-NB	2.18	1.40	1.37
44	B	832	CLA	C1B-NB	-2.18	1.35	1.37
44	e	812	CLA	CMD-C2D	-2.18	1.46	1.50
44	q	304	CLA	MG-NB	-2.18	2.01	2.05
44	J	101	CLA	CMD-C2D	-2.18	1.46	1.50
44	q	309	CLA	CHC-C1C	2.18	1.42	1.38
44	A	837	CLA	MG-ND	-2.18	2.01	2.05
44	e	832	CLA	MG-NB	-2.18	2.01	2.05
44	B	831	CLA	C1B-NB	-2.18	1.35	1.37
44	L	304	CLA	C1B-C2B	2.18	1.48	1.43
52	s	515	CHL	CBD-CGD	-2.18	1.49	1.52
44	B	818	CLA	C4B-NB	2.18	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f	812	CLA	CMD-C2D	-2.18	1.46	1.50
44	e	816	CLA	MG-NB	-2.18	2.01	2.05
44	5	308	CLA	C4B-NB	2.18	1.40	1.37
44	f	819	CLA	CMB-C2B	-2.18	1.46	1.50
44	f	830	CLA	MG-NB	-2.18	2.01	2.05
44	f	841	CLA	MG-NB	-2.18	2.01	2.05
44	p	509	CLA	C4B-NB	-2.18	1.35	1.37
44	r	304	CLA	MG-NB	-2.18	2.01	2.05
44	e	803	CLA	CMD-C2D	-2.18	1.46	1.50
44	2	505	CLA	MG-NB	-2.18	2.01	2.05
44	2	506	CLA	C1B-C2B	2.18	1.48	1.43
44	1	506	CLA	C3B-C4B	2.17	1.49	1.42
44	J	101	CLA	CMB-C2B	-2.17	1.46	1.50
44	e	819	CLA	MG-NB	-2.17	2.01	2.05
44	B	824	CLA	C3B-C4B	2.17	1.49	1.42
44	f	807	CLA	MG-NB	-2.17	2.01	2.05
44	f	838	CLA	CMB-C2B	-2.17	1.46	1.50
44	f	833	CLA	C3B-C4B	2.17	1.49	1.42
44	s	505	CLA	CHC-C1C	2.17	1.42	1.38
44	s	506	CLA	CHC-C1C	2.17	1.42	1.38
44	A	852	CLA	C3B-C4B	2.17	1.49	1.42
44	e	828	CLA	MG-NB	-2.17	2.01	2.05
44	e	826	CLA	CMD-C2D	-2.17	1.46	1.50
44	A	808	CLA	C1B-NB	-2.17	1.35	1.37
52	r	313	CHL	CBD-CGD	-2.17	1.49	1.52
44	A	803	CLA	C1B-C2B	2.17	1.48	1.43
44	e	829	CLA	MG-NB	-2.17	2.01	2.05
44	5	312	CLA	CMC-C2C	-2.17	1.46	1.50
44	e	816	CLA	CMB-C2B	-2.17	1.46	1.50
44	f	805	CLA	CMD-C2D	-2.17	1.46	1.50
44	e	841	CLA	MG-NB	-2.17	2.01	2.05
44	A	836	CLA	C4B-NB	2.17	1.40	1.37
44	B	842	CLA	CMB-C2B	-2.17	1.46	1.50
44	f	810	CLA	MG-NB	-2.17	2.01	2.05
44	e	838	CLA	CMD-C2D	-2.17	1.46	1.50
44	f	826	CLA	CMD-C2D	-2.17	1.46	1.50
44	3	314	CLA	CHC-C1C	2.17	1.42	1.38
44	5	310	CLA	CMD-C2D	-2.17	1.46	1.50
44	f	810	CLA	CMD-C2D	-2.17	1.46	1.50
44	f	822	CLA	MG-NB	-2.17	2.01	2.05
44	r	309	CLA	C3B-C4B	2.17	1.49	1.42
44	2	505	CLA	C1B-C2B	2.17	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	s	510	CLA	CHC-C1C	2.17	1.42	1.38
44	L	301	CLA	CAC-C3C	-2.17	1.45	1.51
44	e	821	CLA	CMD-C2D	-2.17	1.46	1.50
44	f	840	CLA	C3B-C4B	2.17	1.49	1.42
44	B	836	CLA	C1B-C2B	2.17	1.48	1.43
44	B	801	CLA	CAC-C3C	-2.17	1.45	1.51
44	A	834	CLA	C1B-C2B	2.17	1.48	1.43
44	e	834	CLA	CHC-C1C	2.17	1.42	1.38
44	n	205	CLA	C3B-C4B	2.17	1.49	1.42
44	e	825	CLA	CMD-C2D	-2.17	1.46	1.50
44	f	827	CLA	CMD-C2D	-2.17	1.46	1.50
44	5	305	CLA	MG-NB	-2.17	2.01	2.05
44	B	835	CLA	C3B-C4B	2.16	1.49	1.42
44	n	203	CLA	C3B-C4B	2.16	1.49	1.42
44	2	510	CLA	CHC-C1C	2.16	1.42	1.38
44	3	317	CLA	CHC-C1C	2.16	1.42	1.38
44	s	508	CLA	CHC-C1C	2.16	1.42	1.38
44	e	832	CLA	CMD-C2D	-2.16	1.46	1.50
44	e	807	CLA	MG-NB	-2.16	2.01	2.05
44	f	838	CLA	CMD-C2D	-2.16	1.46	1.50
44	e	834	CLA	C3B-C4B	2.16	1.49	1.42
44	q	311	CLA	CHC-C1C	2.16	1.42	1.38
44	5	312	CLA	C3B-C4B	2.16	1.49	1.42
44	e	841	CLA	CMD-C2D	-2.16	1.46	1.50
44	B	842	CLA	C3B-C4B	2.16	1.49	1.42
44	e	816	CLA	CHC-C1C	2.16	1.42	1.38
44	p	511	CLA	CMB-C2B	-2.16	1.46	1.50
44	B	830	CLA	CAC-C3C	-2.16	1.45	1.51
44	B	811	CLA	CAA-C2A	-2.16	1.50	1.54
44	f	821	CLA	MG-NB	-2.16	2.01	2.05
44	e	824	CLA	C3B-C4B	2.16	1.49	1.42
44	5	311	CLA	CMD-C2D	-2.16	1.46	1.50
44	f	833	CLA	CMB-C2B	-2.16	1.46	1.50
44	A	813	CLA	C3B-C4B	2.16	1.49	1.42
47	2	503	BCR	C1-C6	-2.16	1.51	1.53
44	f	812	CLA	MG-NB	-2.16	2.01	2.05
44	r	312	CLA	CHC-C1C	2.16	1.42	1.38
44	e	832	CLA	CMB-C2B	-2.16	1.46	1.50
44	q	311	CLA	CMD-C2D	-2.16	1.46	1.50
44	3	316	CLA	MG-NB	-2.16	2.01	2.05
44	e	807	CLA	CMB-C2B	-2.16	1.46	1.50
44	f	829	CLA	CMD-C2D	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	r	315	CLA	CMD-C2D	-2.16	1.46	1.50
44	e	820	CLA	C3B-C4B	2.16	1.49	1.42
44	2	507	CLA	CMC-C2C	-2.16	1.46	1.50
44	f	818	CLA	CMD-C2D	-2.16	1.46	1.50
44	A	810	CLA	C4B-NB	2.16	1.40	1.37
44	f	807	CLA	C3B-C4B	2.16	1.49	1.42
44	B	828	CLA	CHC-C1C	2.16	1.42	1.38
52	2	512	CHL	CBD-CGD	-2.16	1.49	1.52
44	f	821	CLA	CMB-C2B	-2.16	1.46	1.50
44	f	833	CLA	CMD-C2D	-2.16	1.46	1.50
44	f	809	CLA	CMB-C2B	-2.16	1.46	1.50
44	f	837	CLA	CMB-C2B	-2.16	1.46	1.50
44	o	303	CLA	CMD-C2D	-2.16	1.46	1.50
44	B	808	CLA	CAB-C3B	-2.16	1.41	1.47
44	B	838	CLA	MG-ND	-2.16	2.01	2.05
44	f	806	CLA	CMD-C2D	-2.16	1.46	1.50
44	B	840	CLA	C1B-C2B	2.16	1.48	1.43
44	e	840	CLA	C3B-C4B	2.16	1.49	1.42
44	r	308	CLA	CHC-C1C	2.16	1.42	1.38
44	f	832	CLA	C3B-C4B	2.16	1.49	1.42
44	f	828	CLA	CMD-C2D	-2.16	1.46	1.50
44	q	306	CLA	CHC-C1C	2.16	1.42	1.38
44	B	811	CLA	CMA-C3A	-2.16	1.48	1.53
44	B	833	CLA	C4B-NB	2.16	1.40	1.37
44	5	313	CLA	CMC-C2C	-2.15	1.46	1.50
44	m	101	CLA	CHC-C1C	2.15	1.42	1.38
44	B	805	CLA	CMD-C2D	-2.15	1.46	1.50
44	e	828	CLA	CMC-C2C	-2.15	1.46	1.50
44	f	812	CLA	CMC-C2C	-2.15	1.46	1.50
44	n	203	CLA	CHC-C1C	2.15	1.42	1.38
44	e	802	CLA	CHC-C1C	2.15	1.42	1.38
44	A	809	CLA	C4B-NB	2.15	1.40	1.37
44	f	841	CLA	CMC-C2C	-2.15	1.46	1.50
44	2	505	CLA	CHC-C1C	2.15	1.42	1.38
44	e	836	CLA	CHC-C1C	2.15	1.42	1.38
44	f	812	CLA	C2A-C1A	2.15	1.53	1.51
44	L	304	CLA	CMB-C2B	-2.15	1.46	1.50
44	f	841	CLA	CMB-C2B	-2.15	1.46	1.50
44	3	318	CLA	CMD-C2D	-2.15	1.46	1.50
44	e	820	CLA	CMB-C2B	-2.15	1.46	1.50
44	e	817	CLA	MG-NB	-2.15	2.01	2.05
44	A	823	CLA	C4B-NB	2.15	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	L	301	CLA	C1B-C2B	2.15	1.48	1.43
44	A	819	CLA	CHC-C1C	2.15	1.42	1.38
44	A	802	CLA	CHC-C1C	2.15	1.42	1.38
46	A	843	LHG	O7-C5	-2.15	1.41	1.46
44	1	515	CLA	CMC-C2C	-2.15	1.46	1.50
44	e	828	CLA	CMD-C2D	-2.15	1.46	1.50
44	n	202	CLA	MG-NB	-2.15	2.01	2.05
44	e	824	CLA	CMB-C2B	-2.15	1.46	1.50
44	f	835	CLA	CMD-C2D	-2.15	1.46	1.50
44	s	514	CLA	CMD-C2D	-2.15	1.46	1.50
44	A	810	CLA	C3B-C4B	2.15	1.49	1.42
44	e	827	CLA	CMD-C2D	-2.15	1.46	1.50
44	p	511	CLA	CMD-C2D	-2.15	1.46	1.50
44	B	828	CLA	MG-ND	-2.15	2.01	2.05
44	e	829	CLA	CMC-C2C	-2.15	1.46	1.50
44	f	834	CLA	CMD-C2D	-2.15	1.46	1.50
44	A	840	CLA	CHC-C1C	2.15	1.42	1.38
44	B	823	CLA	CHC-C1C	2.15	1.42	1.38
44	n	201	CLA	MG-NB	-2.15	2.01	2.05
44	f	840	CLA	CMD-C2D	-2.15	1.46	1.50
44	f	812	CLA	C3B-C4B	2.15	1.49	1.42
44	e	834	CLA	CMB-C2B	-2.15	1.46	1.50
44	p	507	CLA	CHC-C1C	2.15	1.42	1.38
44	f	811	CLA	C3B-C4B	2.15	1.49	1.42
44	e	802	CLA	MG-NB	-2.15	2.01	2.05
44	e	823	CLA	CMD-C2D	-2.15	1.46	1.50
44	A	837	CLA	C1B-NB	-2.15	1.35	1.37
44	B	814	CLA	CHC-C1C	2.15	1.42	1.38
44	f	809	CLA	MG-NB	-2.15	2.01	2.05
44	e	827	CLA	C3B-C4B	2.15	1.49	1.42
44	p	510	CLA	CHC-C1C	2.15	1.42	1.38
44	e	806	CLA	MG-NB	-2.15	2.01	2.05
47	j	803	BCR	C30-C25	-2.15	1.51	1.53
52	p	517	CHL	CBD-CGD	-2.15	1.49	1.52
44	A	804	CLA	CMC-C2C	-2.15	1.46	1.50
44	p	505	CLA	CMD-C2D	-2.15	1.46	1.50
44	r	315	CLA	CHC-C1C	2.14	1.42	1.38
44	K	203	CLA	CMB-C2B	-2.14	1.46	1.50
44	f	810	CLA	CMC-C2C	-2.14	1.46	1.50
44	3	312	CLA	CMB-C2B	-2.14	1.46	1.50
44	e	829	CLA	CMD-C2D	-2.14	1.46	1.50
44	3	309	CLA	CAA-C2A	-2.14	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f	823	CLA	CHC-C1C	2.14	1.42	1.38
44	e	808	CLA	MG-NB	-2.14	2.01	2.05
44	e	822	CLA	CMD-C2D	-2.14	1.46	1.50
44	B	841	CLA	CHC-C1C	2.14	1.42	1.38
44	f	840	CLA	CHC-C1C	2.14	1.42	1.38
44	e	839	CLA	CMD-C2D	-2.14	1.46	1.50
44	K	203	CLA	MG-ND	-2.14	2.01	2.05
44	e	808	CLA	CMD-C2D	-2.14	1.46	1.50
44	f	801	CLA	CMC-C2C	-2.14	1.46	1.50
44	f	801	CLA	CMD-C2D	-2.14	1.46	1.50
44	e	827	CLA	CHC-C1C	2.14	1.42	1.38
44	f	820	CLA	CHC-C1C	2.14	1.42	1.38
44	q	316	CLA	MG-NB	-2.14	2.01	2.05
44	e	815	CLA	CMB-C2B	-2.14	1.46	1.50
44	f	817	CLA	CMC-C2C	-2.14	1.46	1.50
44	B	838	CLA	C1B-C2B	2.14	1.48	1.43
44	f	841	CLA	CMD-C2D	-2.14	1.46	1.50
44	1	504	CLA	CHC-C1C	2.14	1.42	1.38
44	e	835	CLA	CMB-C2B	-2.14	1.46	1.50
44	f	817	CLA	CHC-C1C	2.14	1.42	1.38
44	B	815	CLA	MG-ND	-2.14	2.01	2.05
44	2	509	CLA	CMD-C2D	-2.14	1.46	1.50
44	e	809	CLA	MG-NB	-2.14	2.01	2.05
44	e	840	CLA	MG-NB	-2.14	2.01	2.05
44	A	815	CLA	C4B-NB	2.14	1.40	1.37
44	L	304	CLA	C1B-NB	-2.14	1.35	1.37
44	5	310	CLA	CHC-C1C	2.14	1.42	1.38
44	e	807	CLA	CMD-C2D	-2.14	1.46	1.50
44	e	812	CLA	C3B-C4B	2.14	1.49	1.42
44	A	833	CLA	MG-ND	-2.14	2.01	2.05
44	A	821	CLA	C1B-NB	-2.14	1.35	1.37
44	e	824	CLA	CMD-C2D	-2.14	1.46	1.50
44	f	836	CLA	MG-NB	-2.14	2.01	2.05
44	3	313	CLA	CHC-C1C	2.14	1.42	1.38
44	A	822	CLA	C1B-NB	-2.14	1.35	1.37
44	B	840	CLA	C4B-NB	2.14	1.40	1.37
44	B	833	CLA	CMC-C2C	-2.14	1.46	1.50
44	5	307	CLA	CMD-C2D	-2.14	1.46	1.50
44	p	507	CLA	CMD-C2D	-2.14	1.46	1.50
44	L	301	CLA	MG-ND	-2.14	2.01	2.05
44	f	840	CLA	MG-NB	-2.14	2.01	2.05
47	e	846	BCR	C30-C25	-2.14	1.51	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	r	308	CLA	CMC-C2C	-2.14	1.46	1.50
44	A	824	CLA	C3B-C4B	2.14	1.49	1.42
44	f	837	CLA	CMD-C2D	-2.14	1.46	1.50
44	f	813	CLA	CHC-C1C	2.14	1.42	1.38
44	B	827	CLA	C1B-C2B	2.14	1.48	1.43
44	e	836	CLA	CMD-C2D	-2.13	1.46	1.50
44	e	853	CLA	CHC-C1C	2.13	1.42	1.38
44	3	309	CLA	CMD-C2D	-2.13	1.46	1.50
44	3	312	CLA	CMC-C2C	-2.13	1.46	1.50
53	2	502	XAT	C22-C21	-2.13	1.51	1.54
44	r	307	CLA	CMD-C2D	-2.13	1.46	1.50
44	n	205	CLA	CHC-C1C	2.13	1.42	1.38
44	o	303	CLA	C3B-C4B	2.13	1.48	1.42
44	e	806	CLA	CMD-C2D	-2.13	1.46	1.50
44	e	826	CLA	CMC-C2C	-2.13	1.46	1.50
44	f	821	CLA	CMD-C2D	-2.13	1.46	1.50
44	F	803	CLA	C3B-C4B	2.13	1.48	1.42
44	1	511	CLA	C3B-C4B	2.13	1.48	1.42
44	B	807	CLA	C1D-ND	2.13	1.40	1.37
44	j	802	CLA	CHC-C1C	2.13	1.42	1.38
44	f	827	CLA	CMB-C2B	-2.13	1.46	1.50
44	3	301	CLA	C3B-C4B	2.13	1.48	1.42
44	A	817	CLA	C1D-ND	2.13	1.40	1.37
44	f	820	CLA	C3B-C4B	2.13	1.48	1.42
44	e	852	CLA	CMD-C2D	-2.13	1.46	1.50
44	n	201	CLA	CBD-CAD	2.13	1.56	1.51
44	q	309	CLA	MG-NB	-2.13	2.01	2.05
44	r	308	CLA	MG-NB	-2.13	2.01	2.05
44	A	837	CLA	CHC-C1C	2.13	1.42	1.38
44	r	315	CLA	MG-NB	-2.13	2.01	2.05
44	1	510	CLA	CMD-C2D	-2.13	1.46	1.50
44	e	804	CLA	CMB-C2B	-2.13	1.46	1.50
44	f	820	CLA	CMD-C2D	-2.13	1.46	1.50
44	q	306	CLA	CMB-C2B	-2.13	1.46	1.50
44	f	843	CLA	CHC-C1C	2.13	1.42	1.38
44	r	310	CLA	MG-NB	-2.13	2.01	2.05
44	e	829	CLA	C3B-C4B	2.13	1.48	1.42
44	r	305	CLA	CMD-C2D	-2.13	1.46	1.50
44	B	814	CLA	MG-ND	-2.13	2.01	2.05
44	e	852	CLA	C3B-C4B	2.12	1.48	1.42
44	3	314	CLA	CMB-C2B	-2.12	1.46	1.50
44	A	842	CLA	C3B-C4B	2.12	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	B	807	CLA	CAC-C3C	-2.12	1.45	1.51
44	L	301	CLA	CHC-C1C	2.12	1.42	1.38
44	e	811	CLA	CHC-C1C	2.12	1.42	1.38
44	f	819	CLA	CMD-C2D	-2.12	1.46	1.50
44	B	801	CLA	MG-ND	-2.12	2.01	2.05
44	p	515	CLA	C2A-C1A	2.12	1.53	1.51
44	e	804	CLA	C3B-C4B	2.12	1.48	1.42
44	f	803	CLA	CMC-C2C	-2.12	1.46	1.50
44	f	820	CLA	CMB-C2B	-2.12	1.46	1.50
44	A	817	CLA	CAB-C3B	-2.12	1.41	1.47
44	e	835	CLA	MG-NB	-2.12	2.01	2.05
44	B	835	CLA	CHC-C1C	2.12	1.42	1.38
44	e	837	CLA	CMD-C2D	-2.12	1.46	1.50
44	p	510	CLA	CMC-C2C	-2.12	1.46	1.50
44	A	811	CLA	C1D-ND	2.12	1.40	1.37
44	2	505	CLA	C1B-NB	-2.12	1.35	1.37
44	K	205	CLA	CMD-C2D	-2.12	1.46	1.50
44	A	842	CLA	MG-NB	-2.12	2.01	2.05
44	1	505	CLA	CMC-C2C	-2.12	1.46	1.50
44	A	828	CLA	MG-ND	-2.12	2.01	2.05
44	p	515	CLA	MG-NB	-2.12	2.01	2.05
44	e	817	CLA	CHC-C1C	2.12	1.42	1.38
44	5	316	CLA	C4B-NB	2.12	1.40	1.37
44	1	504	CLA	CMB-C2B	-2.12	1.46	1.50
44	3	313	CLA	CMB-C2B	-2.12	1.46	1.50
44	f	835	CLA	CHC-C1C	2.12	1.42	1.38
44	e	805	CLA	CMD-C2D	-2.12	1.46	1.50
44	e	836	CLA	CMB-C2B	-2.12	1.46	1.50
44	A	852	CLA	C1B-NB	-2.12	1.35	1.37
44	e	818	CLA	C4B-NB	-2.12	1.35	1.37
44	A	827	CLA	C1B-C2B	2.12	1.48	1.43
44	e	828	CLA	CMB-C2B	-2.12	1.46	1.50
44	5	305	CLA	CHC-C1C	2.12	1.42	1.38
44	f	829	CLA	C3B-C4B	2.12	1.48	1.42
44	f	842	CLA	C3B-C4B	2.12	1.48	1.42
44	p	508	CLA	MG-NB	-2.12	2.01	2.05
44	e	831	CLA	CMD-C2D	-2.11	1.46	1.50
44	f	810	CLA	CHC-C1C	2.11	1.42	1.38
44	f	826	CLA	CHC-C1C	2.11	1.42	1.38
53	5	304	XAT	C22-C23	-2.11	1.49	1.52
44	K	205	CLA	MG-NB	-2.11	2.01	2.05
53	r	303	XAT	O4-C5	-2.11	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	s	510	CLA	CMD-C2D	-2.11	1.46	1.50
44	5	309	CLA	CHC-C1C	2.11	1.42	1.38
44	n	201	CLA	CMB-C2B	-2.11	1.46	1.50
44	B	814	CLA	C1B-C2B	2.11	1.48	1.43
44	B	818	CLA	C1D-ND	2.11	1.40	1.37
44	B	835	CLA	C4B-NB	2.11	1.40	1.37
44	e	815	CLA	CMD-C2D	-2.11	1.46	1.50
44	f	822	CLA	CHC-C1C	2.11	1.42	1.38
44	1	513	CLA	CMB-C2B	-2.11	1.46	1.50
44	e	819	CLA	CMD-C2D	-2.11	1.46	1.50
44	f	824	CLA	CMD-C2D	-2.11	1.46	1.50
44	J	101	CLA	C3B-C4B	2.11	1.48	1.42
44	e	810	CLA	CMC-C2C	-2.11	1.46	1.50
44	f	839	CLA	CMB-C2B	-2.11	1.46	1.50
44	m	101	CLA	CMD-C2D	-2.11	1.46	1.50
44	A	826	CLA	C1B-C2B	2.11	1.48	1.43
44	A	818	CLA	MG-ND	-2.11	2.01	2.05
44	A	810	CLA	CHC-C1C	2.11	1.42	1.38
44	e	824	CLA	CHC-C1C	2.11	1.42	1.38
44	f	828	CLA	CHC-C1C	2.11	1.42	1.38
44	e	811	CLA	CMB-C2B	-2.11	1.46	1.50
44	e	813	CLA	CMC-C2C	-2.11	1.46	1.50
44	e	820	CLA	CMD-C2D	-2.11	1.46	1.50
44	f	820	CLA	CMC-C2C	-2.11	1.46	1.50
44	B	837	CLA	MG-ND	-2.11	2.01	2.05
44	2	510	CLA	CMB-C2B	-2.11	1.46	1.50
44	3	308	CLA	CMC-C2C	-2.11	1.46	1.50
44	s	506	CLA	CMB-C2B	-2.11	1.46	1.50
44	e	804	CLA	CMC-C2C	-2.11	1.46	1.50
44	1	506	CLA	CHC-C1C	2.11	1.42	1.38
44	o	304	CLA	MG-NB	-2.11	2.01	2.05
44	f	836	CLA	CMB-C2B	-2.11	1.46	1.50
44	f	837	CLA	MG-NB	-2.11	2.01	2.05
44	f	839	CLA	MG-NB	-2.11	2.01	2.05
44	q	312	CLA	MG-NB	-2.11	2.01	2.05
44	5	308	CLA	CHC-C1C	2.11	1.42	1.38
44	e	834	CLA	CMC-C2C	-2.11	1.46	1.50
44	f	812	CLA	CMB-C2B	-2.11	1.46	1.50
44	f	825	CLA	CMB-C2B	-2.11	1.46	1.50
44	e	817	CLA	CMD-C2D	-2.11	1.46	1.50
44	e	841	CLA	CMC-C2C	-2.11	1.46	1.50
44	f	810	CLA	CMB-C2B	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	511	CLA	CMB-C2B	-2.11	1.46	1.50
44	e	803	CLA	CMB-C2B	-2.10	1.46	1.50
44	q	315	CLA	CMD-C2D	-2.10	1.46	1.50
44	e	812	CLA	CHC-C1C	2.10	1.42	1.38
44	s	505	CLA	CMC-C2C	-2.10	1.46	1.50
44	1	515	CLA	CHC-C1C	2.10	1.42	1.38
44	B	806	CLA	C1B-NB	-2.10	1.35	1.37
44	o	303	CLA	CHC-C1C	2.10	1.42	1.38
44	e	826	CLA	CMB-C2B	-2.10	1.46	1.50
44	f	809	CLA	CMD-C2D	-2.10	1.46	1.50
44	e	821	CLA	CMC-C2C	-2.10	1.46	1.50
44	r	310	CLA	CMD-C2D	-2.10	1.46	1.50
44	L	302	CLA	CMC-C2C	-2.10	1.46	1.50
44	f	823	CLA	CMB-C2B	-2.10	1.46	1.50
44	A	834	CLA	CMC-C2C	-2.10	1.46	1.50
44	r	317	CLA	CMD-C2D	-2.10	1.46	1.50
44	3	308	CLA	CMD-C2D	-2.10	1.46	1.50
44	A	827	CLA	C1D-ND	2.10	1.40	1.37
44	e	814	CLA	CMD-C2D	-2.10	1.46	1.50
44	e	823	CLA	MG-NB	-2.10	2.01	2.05
44	m	101	CLA	CMB-C2B	-2.10	1.46	1.50
44	e	853	CLA	CMD-C2D	-2.10	1.46	1.50
44	n	205	CLA	MG-NB	-2.10	2.01	2.05
44	p	511	CLA	C3B-C4B	2.10	1.48	1.42
44	B	804	CLA	CAC-C3C	-2.10	1.45	1.51
44	r	306	CLA	CMD-C2D	-2.10	1.46	1.50
44	e	852	CLA	MG-NB	-2.10	2.01	2.05
44	e	802	CLA	CMC-C2C	-2.10	1.46	1.50
44	f	816	CLA	CMC-C2C	-2.10	1.46	1.50
44	f	829	CLA	CHC-C1C	2.10	1.42	1.38
44	1	508	CLA	CMB-C2B	-2.10	1.46	1.50
44	e	814	CLA	CMB-C2B	-2.10	1.46	1.50
44	f	814	CLA	CMD-C2D	-2.10	1.46	1.50
44	2	505	CLA	MG-ND	-2.10	2.01	2.05
44	B	836	CLA	C3B-C4B	2.10	1.48	1.42
44	B	827	CLA	C1B-NB	-2.10	1.35	1.37
44	e	824	CLA	CMC-C2C	-2.10	1.46	1.50
44	f	811	CLA	CMD-C2D	-2.10	1.46	1.50
44	B	806	CLA	CAC-C3C	-2.10	1.45	1.51
44	F	802	CLA	C1B-NB	-2.10	1.35	1.37
44	e	806	CLA	CMC-C2C	-2.09	1.46	1.50
44	f	807	CLA	CMB-C2B	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	K	201	CLA	C1B-C2B	2.09	1.48	1.43
44	f	815	CLA	CMD-C2D	-2.09	1.46	1.50
44	s	507	CLA	CMC-C2C	-2.09	1.46	1.50
44	1	513	CLA	CHC-C1C	2.09	1.42	1.38
44	s	514	CLA	CHC-C1C	2.09	1.42	1.38
44	e	811	CLA	CMC-C2C	-2.09	1.46	1.50
44	f	813	CLA	MG-NB	-2.09	2.01	2.05
44	f	840	CLA	CMC-C2C	-2.09	1.46	1.50
44	q	316	CLA	CMD-C2D	-2.09	1.46	1.50
44	B	842	CLA	C1B-NB	-2.09	1.35	1.37
44	f	832	CLA	CMD-C2D	-2.09	1.46	1.50
44	q	304	CLA	C1C-C2C	2.09	1.46	1.42
44	f	842	CLA	CHC-C1C	2.09	1.42	1.38
44	A	813	CLA	C4B-NB	2.09	1.40	1.37
44	2	511	CLA	CHC-C1C	2.09	1.42	1.38
44	e	820	CLA	CHC-C1C	2.09	1.42	1.38
44	A	832	CLA	C1B-C2B	2.09	1.48	1.43
52	p	512	CHL	CBD-CGD	-2.09	1.49	1.52
44	A	842	CLA	CMD-C2D	-2.09	1.46	1.50
44	e	821	CLA	CMB-C2B	-2.09	1.46	1.50
44	e	804	CLA	CHC-C1C	2.09	1.42	1.38
44	5	306	CLA	CMD-C2D	-2.09	1.46	1.50
44	o	304	CLA	CMD-C2D	-2.09	1.46	1.50
44	j	802	CLA	CMD-C2D	-2.09	1.46	1.50
44	r	305	CLA	MG-NB	-2.09	2.01	2.05
44	e	813	CLA	CMD-C2D	-2.09	1.46	1.50
44	f	804	CLA	C3B-C4B	2.09	1.46	1.40
44	p	504	CLA	CMB-C2B	-2.09	1.46	1.50
44	e	835	CLA	CHC-C1C	2.09	1.42	1.38
44	A	812	CLA	MG-ND	-2.09	2.01	2.05
44	A	821	CLA	CHC-C1C	2.09	1.42	1.38
44	r	309	CLA	CMD-C2D	-2.09	1.46	1.50
44	1	508	CLA	C3B-C4B	2.09	1.48	1.42
44	B	818	CLA	C1B-C2B	2.09	1.48	1.43
44	f	822	CLA	CMB-C2B	-2.09	1.46	1.50
44	e	815	CLA	MG-NB	-2.09	2.01	2.05
44	q	312	CLA	CMD-C2D	-2.09	1.46	1.50
44	B	809	CLA	CAC-C3C	-2.09	1.45	1.51
44	1	511	CLA	CMC-C2C	-2.09	1.46	1.50
44	s	509	CLA	MG-NB	-2.08	2.01	2.05
44	L	303	CLA	C1B-C2B	2.08	1.48	1.43
44	q	310	CLA	CHC-C1C	2.08	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	e	809	CLA	CMD-C2D	-2.08	1.46	1.50
44	e	839	CLA	CMB-C2B	-2.08	1.46	1.50
44	f	831	CLA	CMC-C2C	-2.08	1.46	1.50
44	A	806	CLA	MG-ND	-2.08	2.01	2.05
44	q	315	CLA	CHC-C1C	2.08	1.42	1.38
44	A	833	CLA	C1B-NB	-2.08	1.35	1.37
44	1	507	CLA	C1B-NB	-2.08	1.35	1.37
44	s	505	CLA	MG-NB	-2.08	2.01	2.05
44	1	510	CLA	CHC-C1C	2.08	1.42	1.38
44	1	511	CLA	CHC-C1C	2.08	1.42	1.38
44	e	827	CLA	CMB-C2B	-2.08	1.46	1.50
44	A	838	CLA	CHC-C1C	2.08	1.42	1.38
44	A	803	CLA	C1B-NB	-2.08	1.35	1.37
44	3	310	CLA	CMC-C2C	-2.08	1.46	1.50
44	e	840	CLA	CHC-C1C	2.08	1.42	1.38
44	e	806	CLA	CMB-C2B	-2.08	1.46	1.50
44	f	803	CLA	CMB-C2B	-2.08	1.46	1.50
44	r	309	CLA	CMB-C2B	-2.08	1.46	1.50
44	s	506	CLA	CMD-C2D	-2.08	1.46	1.50
44	B	830	CLA	CAB-C3B	-2.08	1.41	1.47
44	f	801	CLA	CHC-C1C	2.08	1.42	1.38
44	e	809	CLA	CMB-C2B	-2.08	1.46	1.50
44	f	808	CLA	CMD-C2D	-2.08	1.46	1.50
44	f	818	CLA	CMB-C2B	-2.08	1.46	1.50
44	B	819	CLA	C1B-C2B	2.08	1.48	1.43
44	A	802	CLA	C3B-C4B	2.08	1.48	1.42
44	1	513	CLA	CMC-C2C	-2.08	1.46	1.50
44	A	840	CLA	C3B-C4B	2.08	1.48	1.42
44	s	508	CLA	CMD-C2D	-2.08	1.46	1.50
44	e	811	CLA	CMD-C2D	-2.08	1.46	1.50
44	p	505	CLA	CMB-C2B	-2.08	1.46	1.50
44	3	310	CLA	CMD-C2D	-2.08	1.46	1.50
44	e	822	CLA	CMC-C2C	-2.08	1.46	1.50
44	e	830	CLA	CMC-C2C	-2.08	1.46	1.50
44	o	302	CLA	CMB-C2B	-2.08	1.46	1.50
44	r	310	CLA	CMB-C2B	-2.08	1.46	1.50
44	3	316	CLA	CHC-C1C	2.08	1.42	1.38
44	r	308	CLA	CMB-C2B	-2.08	1.46	1.50
44	2	511	CLA	CAC-C3C	-2.08	1.45	1.51
44	f	821	CLA	CMC-C2C	-2.08	1.46	1.50
44	f	822	CLA	CMD-C2D	-2.08	1.46	1.50
44	A	838	CLA	C1B-NB	-2.08	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	f	823	CLA	CMC-C2C	-2.07	1.46	1.50
44	e	805	CLA	CMB-C2B	-2.07	1.46	1.50
44	q	315	CLA	CMC-C2C	-2.07	1.46	1.50
44	r	312	CLA	CMD-C2D	-2.07	1.46	1.50
44	A	810	CLA	CAC-C3C	-2.07	1.45	1.51
44	n	205	CLA	CMB-C2B	-2.07	1.46	1.50
44	2	511	CLA	C1B-NB	-2.07	1.35	1.37
44	p	506	CLA	CMB-C2B	-2.07	1.46	1.50
44	q	304	CLA	CMD-C2D	-2.07	1.46	1.50
44	5	312	CLA	C1B-NB	-2.07	1.35	1.37
44	B	822	CLA	CAC-C3C	-2.07	1.45	1.51
44	f	825	CLA	CMC-C2C	-2.07	1.46	1.50
53	s	502	XAT	O4-C5	-2.07	1.43	1.46
44	e	834	CLA	CMD-C2D	-2.07	1.46	1.50
44	B	827	CLA	MG-ND	-2.07	2.01	2.05
47	5	302	BCR	C1-C6	-2.07	1.51	1.53
44	B	804	CLA	MG-ND	-2.07	2.01	2.05
44	e	812	CLA	CMC-C2C	-2.07	1.46	1.50
44	p	510	CLA	CMB-C2B	-2.07	1.46	1.50
44	q	310	CLA	CMB-C2B	-2.07	1.46	1.50
44	q	306	CLA	MG-NB	-2.07	2.01	2.05
44	e	835	CLA	CMD-C2D	-2.07	1.46	1.50
44	f	830	CLA	CMC-C2C	-2.07	1.46	1.50
44	B	841	CLA	CAA-C2A	-2.07	1.50	1.54
44	A	805	CLA	CAA-C2A	-2.07	1.50	1.54
44	r	311	CLA	CMB-C2B	-2.07	1.46	1.50
44	5	307	CLA	CHC-C1C	2.07	1.42	1.38
44	2	506	CLA	CMC-C2C	-2.07	1.46	1.50
44	f	814	CLA	CMB-C2B	-2.07	1.46	1.50
44	A	830	CLA	C1B-C2B	2.07	1.48	1.43
44	A	805	CLA	CMA-C3A	-2.07	1.48	1.53
44	2	509	CLA	CHC-C1C	2.07	1.42	1.38
44	A	808	CLA	C4B-NB	2.07	1.40	1.37
44	B	808	CLA	C1B-NB	-2.07	1.35	1.37
44	r	317	CLA	CMB-C2B	-2.07	1.46	1.50
44	n	205	CLA	CMD-C2D	-2.07	1.46	1.50
44	r	306	CLA	CMC-C2C	-2.07	1.46	1.50
44	B	813	CLA	CAC-C3C	-2.07	1.45	1.51
44	5	311	CLA	CMC-C2C	-2.07	1.46	1.50
44	f	838	CLA	CMC-C2C	-2.07	1.46	1.50
44	p	513	CLA	CMD-C2D	-2.07	1.46	1.50
44	A	838	CLA	MG-ND	-2.07	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	q	301	LUT	C1-C6	-2.06	1.51	1.53
44	e	853	CLA	CMC-C2C	-2.06	1.46	1.50
44	f	823	CLA	CMD-C2D	-2.06	1.46	1.50
53	r	303	XAT	O24-C25	-2.06	1.43	1.46
44	A	812	CLA	CHC-C1C	2.06	1.42	1.38
44	1	513	CLA	C3B-C4B	2.06	1.48	1.42
44	5	307	CLA	C3B-C4B	2.06	1.48	1.42
44	A	805	CLA	C1B-C2B	2.06	1.48	1.43
44	p	515	CLA	CMC-C2C	-2.06	1.46	1.50
44	f	809	CLA	CMC-C2C	-2.06	1.46	1.50
44	p	506	CLA	CMD-C2D	-2.06	1.46	1.50
44	e	803	CLA	MG-NB	-2.06	2.01	2.05
44	A	804	CLA	C3B-C4B	2.06	1.48	1.42
44	j	802	CLA	CMB-C2B	-2.06	1.46	1.50
44	B	830	CLA	C1B-NB	-2.06	1.35	1.37
44	L	301	CLA	C1B-NB	-2.06	1.35	1.37
44	e	837	CLA	CMB-C2B	-2.06	1.46	1.50
44	r	309	CLA	MG-NB	-2.06	2.01	2.05
44	f	832	CLA	CHC-C1C	2.06	1.42	1.38
44	f	827	CLA	CMC-C2C	-2.06	1.46	1.50
44	f	832	CLA	CMC-C2C	-2.06	1.46	1.50
44	n	201	CLA	CMD-C2D	-2.06	1.46	1.50
44	3	309	CLA	C1B-NB	-2.06	1.35	1.37
44	e	814	CLA	CMC-C2C	-2.06	1.46	1.50
44	B	801	CLA	C4B-NB	2.06	1.40	1.37
44	A	809	CLA	C1B-NB	-2.06	1.35	1.37
44	e	818	CLA	C1A-CHA	2.06	1.51	1.43
44	f	835	CLA	CMC-C2C	-2.06	1.46	1.50
44	f	842	CLA	CMC-C2C	-2.06	1.46	1.50
44	A	835	CLA	MG-ND	-2.06	2.01	2.05
44	A	827	CLA	CAA-C2A	-2.06	1.50	1.54
44	A	807	CLA	C1B-C2B	2.06	1.48	1.43
44	r	315	CLA	CMB-C2B	-2.06	1.46	1.50
44	e	821	CLA	C3B-C4B	2.06	1.48	1.42
44	f	806	CLA	CMB-C2B	-2.06	1.46	1.50
44	s	504	CLA	CMD-C2D	-2.06	1.46	1.50
44	f	805	CLA	CHC-C1C	2.06	1.42	1.38
44	f	814	CLA	CMC-C2C	-2.06	1.46	1.50
44	q	308	CLA	MG-NB	-2.06	2.01	2.05
44	B	809	CLA	CHC-C1C	2.06	1.42	1.38
44	e	838	CLA	CMC-C2C	-2.06	1.46	1.50
44	A	836	CLA	MG-NB	-2.06	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	j	802	CLA	MG-NB	-2.06	2.01	2.05
44	3	308	CLA	MG-ND	-2.06	2.01	2.05
44	e	817	CLA	CMC-C2C	-2.06	1.46	1.50
44	p	515	CLA	CMD-C2D	-2.06	1.46	1.50
44	A	816	CLA	C4B-NB	2.06	1.40	1.37
44	3	318	CLA	C4B-NB	2.06	1.40	1.37
44	e	838	CLA	CHC-C1C	2.06	1.42	1.38
44	p	515	CLA	CHC-C1C	2.06	1.42	1.38
44	q	311	CLA	MG-NB	-2.06	2.01	2.05
44	A	829	CLA	C3B-C4B	2.06	1.48	1.42
44	B	803	CLA	C1B-NB	-2.06	1.35	1.37
44	2	504	CLA	C3B-C4B	2.06	1.48	1.42
44	1	509	CLA	CMC-C2C	-2.05	1.46	1.50
44	q	308	CLA	CMB-C2B	-2.05	1.46	1.50
44	f	812	CLA	CHC-C1C	2.05	1.42	1.38
44	2	510	CLA	CMC-C2C	-2.05	1.46	1.50
44	e	843	CLA	MG-NB	-2.05	2.01	2.05
44	e	822	CLA	CMB-C2B	-2.05	1.46	1.50
44	B	811	CLA	C3B-C4B	2.05	1.48	1.42
44	B	834	CLA	C1B-C2B	2.05	1.47	1.43
44	B	830	CLA	MG-ND	-2.05	2.01	2.05
47	f	849	BCR	C1-C6	-2.05	1.51	1.53
44	f	818	CLA	CMC-C2C	-2.05	1.46	1.50
44	q	316	CLA	CMB-C2B	-2.05	1.46	1.50
44	f	824	CLA	CHC-C1C	2.05	1.42	1.38
44	K	201	CLA	CMD-C2D	-2.05	1.46	1.50
44	f	826	CLA	CMC-C2C	-2.05	1.46	1.50
44	B	842	CLA	MG-ND	-2.05	2.01	2.05
44	e	835	CLA	CMC-C2C	-2.05	1.46	1.50
44	5	310	CLA	C3B-C4B	2.05	1.48	1.42
44	f	817	CLA	CMB-C2B	-2.05	1.46	1.50
52	1	517	CHL	C2A-C3A	-2.05	1.49	1.55
44	B	814	CLA	CAC-C3C	-2.05	1.45	1.51
44	B	802	CLA	MG-ND	-2.05	2.01	2.05
44	5	305	CLA	MG-ND	-2.05	2.01	2.05
44	3	312	CLA	CMD-C2D	-2.05	1.46	1.50
44	f	813	CLA	CMD-C2D	-2.05	1.46	1.50
44	f	836	CLA	CMD-C2D	-2.05	1.46	1.50
44	m	102	CLA	CMB-C2B	-2.05	1.46	1.50
44	A	831	CLA	C3B-C2B	-2.05	1.36	1.44
44	A	831	CLA	CAA-C2A	-2.05	1.50	1.54
44	e	812	CLA	CMB-C2B	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	e	843	CLA	CMD-C2D	-2.05	1.46	1.50
44	f	801	CLA	CMB-C2B	-2.05	1.46	1.50
44	A	829	CLA	C4B-NB	2.05	1.40	1.37
44	B	805	CLA	C1D-ND	2.05	1.40	1.37
44	e	813	CLA	CMB-C2B	-2.05	1.46	1.50
44	n	201	CLA	CMC-C2C	-2.05	1.46	1.50
44	e	840	CLA	CMC-C2C	-2.05	1.46	1.50
44	B	807	CLA	C1B-C2B	2.05	1.47	1.43
44	r	309	CLA	CHC-C1C	2.05	1.42	1.38
44	A	834	CLA	C1B-NB	-2.04	1.35	1.37
44	B	816	CLA	C1B-C2B	2.04	1.47	1.43
44	A	803	CLA	MG-ND	-2.04	2.01	2.05
44	r	311	CLA	MG-NB	-2.04	2.01	2.05
44	5	309	CLA	C3B-C4B	2.04	1.48	1.42
44	s	509	CLA	CMB-C2B	-2.04	1.46	1.50
44	B	823	CLA	C3B-C4B	2.04	1.48	1.42
44	A	814	CLA	C1B-NB	-2.04	1.35	1.37
44	1	515	CLA	MG-ND	-2.04	2.01	2.05
47	e	847	BCR	C1-C6	-2.04	1.51	1.53
44	r	312	CLA	CMB-C2B	-2.04	1.46	1.50
44	e	807	CLA	CMC-C2C	-2.04	1.46	1.50
44	r	309	CLA	CMC-C2C	-2.04	1.46	1.50
44	B	820	CLA	MG-ND	-2.04	2.01	2.05
44	1	510	CLA	MG-ND	-2.04	2.01	2.05
44	3	316	CLA	CMC-C2C	-2.04	1.46	1.50
44	e	837	CLA	CMC-C2C	-2.04	1.46	1.50
44	f	843	CLA	CMD-C2D	-2.04	1.46	1.50
44	e	803	CLA	CMC-C2C	-2.04	1.46	1.50
44	f	843	CLA	CMC-C2C	-2.04	1.46	1.50
44	f	843	CLA	CMB-C2B	-2.04	1.46	1.50
44	q	309	CLA	CMB-C2B	-2.04	1.46	1.50
44	e	853	CLA	CMB-C2B	-2.04	1.46	1.50
44	o	302	CLA	CHC-C1C	2.04	1.42	1.38
44	B	817	CLA	CAB-C3B	-2.04	1.41	1.47
44	L	304	CLA	MG-ND	-2.04	2.01	2.05
44	3	318	CLA	CMB-C2B	-2.04	1.46	1.50
44	f	839	CLA	CMD-C2D	-2.04	1.46	1.50
44	m	101	CLA	CMC-C2C	-2.04	1.46	1.50
44	e	841	CLA	CHC-C1C	2.04	1.42	1.38
44	5	306	CLA	CMC-C2C	-2.04	1.46	1.50
44	e	823	CLA	CMB-C2B	-2.04	1.46	1.50
44	e	831	CLA	CMC-C2C	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	s	510	CLA	CMB-C2B	-2.04	1.46	1.50
44	s	511	CLA	CMB-C2B	-2.04	1.46	1.50
44	3	308	CLA	C3B-C4B	2.04	1.48	1.42
44	e	802	CLA	CMB-C2B	-2.04	1.46	1.50
44	f	807	CLA	CMC-C2C	-2.04	1.46	1.50
44	p	508	CLA	CMB-C2B	-2.04	1.46	1.50
44	A	813	CLA	CHC-C1C	2.04	1.42	1.38
44	e	823	CLA	CMC-C2C	-2.04	1.46	1.50
44	f	805	CLA	CMB-C2B	-2.04	1.46	1.50
44	f	809	CLA	CHC-C1C	2.04	1.42	1.38
44	f	834	CLA	CMC-C2C	-2.04	1.46	1.50
44	r	305	CLA	CMB-C2B	-2.04	1.46	1.50
44	e	825	CLA	CMB-C2B	-2.04	1.46	1.50
44	r	306	CLA	CMB-C2B	-2.04	1.46	1.50
44	e	831	CLA	CMB-C2B	-2.04	1.46	1.50
44	q	315	CLA	MG-NB	-2.04	2.01	2.05
44	s	504	CLA	CMC-C2C	-2.04	1.46	1.50
44	A	825	CLA	C3B-C4B	2.04	1.48	1.42
44	2	514	CLA	C1B-NB	-2.03	1.35	1.37
44	A	823	CLA	CHC-C1C	2.03	1.42	1.38
44	e	809	CLA	CHC-C1C	2.03	1.42	1.38
44	3	316	CLA	C1D-ND	2.03	1.40	1.37
44	B	802	CLA	CHC-C1C	2.03	1.42	1.38
44	e	820	CLA	CMC-C2C	-2.03	1.46	1.50
44	f	822	CLA	CMC-C2C	-2.03	1.46	1.50
44	B	830	CLA	C1B-C2B	2.03	1.47	1.43
44	e	838	CLA	CMB-C2B	-2.03	1.46	1.50
44	o	303	CLA	CMC-C2C	-2.03	1.46	1.50
44	K	202	CLA	CMC-C2C	-2.03	1.46	1.50
44	m	102	CLA	CMD-C2D	-2.03	1.46	1.50
44	n	202	CLA	CMB-C2B	-2.03	1.46	1.50
44	s	508	CLA	CMB-C2B	-2.03	1.46	1.50
44	r	310	CLA	CHC-C1C	2.03	1.42	1.38
44	e	805	CLA	CMC-C2C	-2.03	1.46	1.50
44	e	843	CLA	CMC-C2C	-2.03	1.46	1.50
44	s	511	CLA	MG-NB	-2.03	2.01	2.05
44	s	514	CLA	CMB-C2B	-2.03	1.46	1.50
52	3	302	CHL	CMC-C2C	2.03	1.49	1.44
44	m	102	CLA	MG-NB	-2.03	2.01	2.05
44	3	314	CLA	CMC-C2C	-2.03	1.46	1.50
44	e	836	CLA	CMC-C2C	-2.03	1.46	1.50
44	f	835	CLA	CMB-C2B	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1	515	CLA	CMB-C2B	-2.03	1.46	1.50
44	s	505	CLA	CMB-C2B	-2.03	1.46	1.50
44	A	842	CLA	MG-ND	-2.03	2.01	2.05
44	p	509	CLA	MG-NC	2.03	2.11	2.06
44	3	301	CLA	C1B-C2B	2.03	1.47	1.43
44	p	506	CLA	MG-NB	-2.03	2.01	2.05
44	e	808	CLA	CMC-C2C	-2.03	1.46	1.50
44	B	805	CLA	C1B-C2B	2.03	1.47	1.43
44	B	841	CLA	C3B-C4B	2.03	1.48	1.42
44	p	508	CLA	CMC-C2C	-2.03	1.46	1.50
44	A	808	CLA	CAC-C3C	-2.03	1.45	1.51
44	f	811	CLA	CMC-C2C	-2.03	1.46	1.50
44	e	825	CLA	CMC-C2C	-2.02	1.46	1.50
44	r	308	CLA	CMD-C2D	-2.02	1.46	1.50
44	A	807	CLA	MG-ND	-2.02	2.01	2.05
44	f	816	CLA	CMB-C2B	-2.02	1.46	1.50
44	q	307	CLA	CMB-C2B	-2.02	1.46	1.50
44	B	827	CLA	C3B-C4B	2.02	1.48	1.42
44	A	817	CLA	CBD-CGD	-2.02	1.49	1.51
44	q	309	CLA	CMD-C2D	-2.02	1.46	1.50
44	L	301	CLA	C4B-NB	2.02	1.40	1.37
44	A	807	CLA	C4B-NB	2.02	1.40	1.37
44	B	838	CLA	C1B-NB	-2.02	1.35	1.37
44	2	509	CLA	CMC-C2C	-2.02	1.46	1.50
44	B	815	CLA	CAC-C3C	-2.02	1.45	1.51
44	n	202	CLA	CMD-C2D	-2.02	1.46	1.50
44	A	804	CLA	CHC-C1C	2.02	1.42	1.38
44	e	821	CLA	CHC-C1C	2.02	1.42	1.38
44	B	810	CLA	C1D-ND	2.02	1.40	1.37
44	A	835	CLA	C1B-C2B	2.02	1.47	1.43
44	s	509	CLA	CMC-C2C	-2.02	1.46	1.50
44	f	829	CLA	CMC-C2C	-2.02	1.46	1.50
44	q	306	CLA	CMD-C2D	-2.02	1.46	1.50
44	B	825	CLA	C4B-NB	2.02	1.40	1.37
44	q	308	CLA	CMD-C2D	-2.02	1.46	1.50
44	o	302	CLA	CMC-C2C	-2.02	1.46	1.50
44	n	203	CLA	CMC-C2C	-2.02	1.46	1.50
44	B	801	CLA	CHC-C1C	2.02	1.42	1.38
44	o	304	CLA	CMC-C2C	-2.02	1.46	1.50
44	q	305	CLA	CMB-C2B	-2.02	1.46	1.50
44	B	806	CLA	C4B-NB	2.02	1.40	1.37
44	K	203	CLA	C1B-NB	-2.02	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	q	307	CLA	CMD-C2D	-2.02	1.46	1.50
44	o	302	CLA	CMD-C2D	-2.02	1.46	1.50
44	q	305	CLA	CMD-C2D	-2.02	1.46	1.50
44	q	311	CLA	CMB-C2B	-2.02	1.46	1.50
44	3	317	CLA	MG-ND	-2.01	2.01	2.05
44	3	312	CLA	MG-ND	-2.01	2.01	2.05
44	F	802	CLA	CHC-C1C	2.01	1.42	1.38
44	A	823	CLA	C3B-C4B	2.01	1.48	1.42
44	o	302	CLA	MG-NB	-2.01	2.01	2.05
44	B	810	CLA	CAC-C3C	-2.01	1.45	1.51
44	e	819	CLA	CMC-C2C	-2.01	1.46	1.50
44	A	831	CLA	C4B-NB	2.01	1.40	1.37
44	B	820	CLA	C3B-C4B	2.01	1.48	1.42
44	A	837	CLA	C1B-C2B	2.01	1.47	1.43
44	A	814	CLA	CAB-C3B	-2.01	1.42	1.47
44	3	307	CLA	CMB-C2B	-2.01	1.46	1.50
44	f	806	CLA	CMC-C2C	-2.01	1.46	1.50
44	f	819	CLA	CMC-C2C	-2.01	1.46	1.50
44	A	805	CLA	CAC-C3C	-2.01	1.45	1.51
53	s	502	XAT	O24-C25	-2.01	1.43	1.46
52	r	316	CHL	CBD-CGD	-2.01	1.50	1.52
44	A	823	CLA	C1B-C2B	2.01	1.47	1.43
44	5	316	CLA	CHC-C1C	2.01	1.42	1.38
44	f	833	CLA	CMC-C2C	-2.01	1.46	1.50
44	r	307	CLA	CMC-C2C	-2.01	1.46	1.50
44	3	308	CLA	CHC-C1C	2.01	1.42	1.38
51	1	501	LUT	C1-C6	-2.01	1.51	1.53
44	p	507	CLA	CMC-C2C	-2.01	1.46	1.50
44	L	303	CLA	CHC-C1C	2.01	1.42	1.38
44	A	834	CLA	CHC-C1C	2.01	1.42	1.38
44	f	811	CLA	CHC-C1C	2.01	1.42	1.38
44	f	815	CLA	CMB-C2B	-2.01	1.46	1.50
44	r	307	CLA	CMB-C2B	-2.01	1.46	1.50
44	e	816	CLA	CMC-C2C	-2.01	1.46	1.50
44	e	827	CLA	CMC-C2C	-2.01	1.46	1.50
44	A	831	CLA	CAC-C3C	-2.01	1.46	1.51
44	s	508	CLA	CMC-C2C	-2.01	1.46	1.50
44	s	509	CLA	CMD-C2D	-2.01	1.46	1.50
44	A	835	CLA	CHC-C1C	2.01	1.42	1.38
44	f	813	CLA	CMC-C2C	-2.01	1.46	1.50
44	q	316	CLA	CMC-C2C	-2.01	1.46	1.50
44	j	802	CLA	CMC-C2C	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	o	303	CLA	CMB-C2B	-2.01	1.46	1.50
44	B	826	CLA	CAC-C3C	-2.00	1.46	1.51
52	1	514	CHL	CHA-CBD	-2.00	1.49	1.51
47	f	845	BCR	C30-C25	-2.00	1.51	1.53
44	F	803	CLA	MG-ND	-2.00	2.01	2.05
44	L	304	CLA	CHC-C1C	2.00	1.42	1.38
44	f	840	CLA	CMB-C2B	-2.00	1.46	1.50
44	3	310	CLA	MG-NB	-2.00	2.01	2.05
44	3	309	CLA	CHC-C1C	2.00	1.42	1.38
44	B	822	CLA	C1B-NB	-2.00	1.35	1.37
44	p	504	CLA	MG-ND	-2.00	2.01	2.05
44	r	305	CLA	CMC-C2C	-2.00	1.46	1.50
44	3	309	CLA	MG-ND	-2.00	2.01	2.05
44	p	509	CLA	C3D-C4D	-2.00	1.39	1.44
44	B	828	CLA	CMD-C2D	-2.00	1.46	1.50
44	e	840	CLA	CMB-C2B	-2.00	1.46	1.50

All (3171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	503	BCR	C40-C30-C25	-13.10	89.71	110.24
47	s	503	BCR	C40-C30-C25	-12.78	90.20	110.24
43	A	801	CL0	C1B-CHB-C4A	10.79	130.77	120.23
43	e	801	CL0	C1B-CHB-C4A	10.77	130.76	120.23
47	Q	801	BCR	C11-C10-C9	-10.75	112.21	127.28
52	3	302	CHL	O2D-CGD-CBD	9.95	121.88	110.95
44	f	804	CLA	C4A-NA-C1A	9.90	111.20	106.68
52	p	517	CHL	O2D-CGD-CBD	9.73	121.63	110.95
47	s	503	BCR	C20-C21-C22	-9.61	113.80	127.28
52	1	517	CHL	C1B-CHB-C4A	9.43	127.39	121.32
52	2	512	CHL	C1B-CHB-C4A	9.38	127.36	121.32
52	2	515	CHL	O2D-CGD-CBD	9.27	121.13	110.95
52	1	517	CHL	O2D-CGD-CBD	9.27	121.13	110.95
52	5	317	CHL	CHA-C1A-C2A	-9.12	120.36	133.83
52	p	512	CHL	O2D-CGD-CBD	9.09	120.94	110.95
47	2	503	BCR	C40-C30-C39	-9.08	82.63	108.63
47	2	503	BCR	C20-C21-C22	-9.01	114.64	127.28
52	s	517	CHL	O2D-CGD-CBD	8.93	120.75	110.95
47	s	503	BCR	C40-C30-C39	-8.91	83.12	108.63
47	Q	801	BCR	C7-C8-C9	-8.91	113.06	126.23
52	3	315	CHL	O2D-CGD-CBD	8.89	120.72	110.95
52	s	513	CHL	O2D-CGD-CBD	8.80	120.62	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	s	512	CHL	O2D-CGD-CBD	8.64	120.44	110.95
52	1	514	CHL	O2D-CGD-CBD	8.61	120.41	110.95
44	p	509	CLA	C4A-NA-C1A	8.56	110.58	106.68
52	2	516	CHL	C1B-CHB-C4A	8.54	126.81	121.32
52	r	313	CHL	O2D-CGD-CBD	8.50	120.29	110.95
44	e	818	CLA	C4A-NA-C1A	8.48	110.55	106.68
52	r	314	CHL	C1B-CHB-C4A	8.27	126.64	121.32
52	5	314	CHL	O2D-CGD-CBD	8.23	120.00	110.95
44	3	308	CLA	C4A-NA-C1A	8.17	110.41	106.68
52	s	515	CHL	O2D-CGD-CBD	8.12	119.87	110.95
47	B	847	BCR	C15-C14-C13	-8.11	115.90	127.28
44	A	810	CLA	C4A-NA-C1A	8.08	110.37	106.68
52	p	514	CHL	O2D-CGD-CBD	8.00	119.74	110.95
52	2	512	CHL	O2D-CGD-CBD	7.97	119.70	110.95
44	A	835	CLA	C4A-NA-C1A	7.94	110.30	106.68
52	5	317	CHL	O2D-CGD-CBD	7.94	119.67	110.95
52	1	512	CHL	O2D-CGD-CBD	7.88	119.61	110.95
47	e	850	BCR	C7-C8-C9	-7.88	114.58	126.23
44	2	511	CLA	C4A-NA-C1A	7.83	110.25	106.68
44	A	832	CLA	C4A-NA-C1A	7.80	110.24	106.68
47	s	503	BCR	C24-C23-C22	-7.73	114.80	126.23
52	5	315	CHL	O2D-CGD-CBD	7.73	119.44	110.95
52	r	316	CHL	O2D-CGD-CBD	7.72	119.43	110.95
51	p	502	LUT	C21-C26-C27	7.71	121.69	112.83
44	B	804	CLA	C4A-NA-C1A	7.69	110.19	106.68
44	L	303	CLA	C4A-NA-C1A	7.66	110.17	106.68
44	A	820	CLA	C4A-NA-C1A	7.63	110.16	106.68
44	3	306	CLA	C4A-NA-C1A	7.63	110.16	106.68
52	3	315	CHL	C1B-CHB-C4A	7.57	126.19	121.32
44	B	839	CLA	C4A-NA-C1A	7.55	110.12	106.68
44	2	506	CLA	C4A-NA-C1A	7.52	110.11	106.68
44	2	509	CLA	C4A-NA-C1A	7.50	110.10	106.68
44	A	821	CLA	C4A-NA-C1A	7.48	110.09	106.68
47	B	844	BCR	C7-C8-C9	-7.47	115.18	126.23
44	A	830	CLA	C4A-NA-C1A	7.46	110.08	106.68
44	3	313	CLA	C4A-NA-C1A	7.46	110.08	106.68
51	5	303	LUT	C26-C27-C28	-7.44	113.00	124.58
44	B	822	CLA	C4A-NA-C1A	7.42	110.06	106.68
44	A	839	CLA	C4A-NA-C1A	7.42	110.06	106.68
44	5	311	CLA	C4A-NA-C1A	7.40	110.06	106.68
47	e	854	BCR	C16-C17-C18	-7.40	116.89	127.28
44	L	302	CLA	C4A-NA-C1A	7.40	110.06	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	2	516	CHL	O2D-CGD-CBD	7.38	119.05	110.95
44	2	504	CLA	C4A-NA-C1A	7.36	110.04	106.68
44	3	311	CLA	C4A-NA-C1A	7.32	110.02	106.68
44	A	836	CLA	C4A-NA-C1A	7.25	109.99	106.68
47	n	204	BCR	C16-C17-C18	-7.24	117.12	127.28
44	B	816	CLA	C4A-NA-C1A	7.22	109.97	106.68
53	r	303	XAT	C18-C5-C6	-7.22	110.42	122.30
44	B	821	CLA	C4A-NA-C1A	7.20	109.96	106.68
44	B	840	CLA	C4A-NA-C1A	7.19	109.96	106.68
44	3	301	CLA	C4A-NA-C1A	7.19	109.96	106.68
47	A	853	BCR	C24-C23-C22	-7.18	115.61	126.23
44	A	816	CLA	C4A-NA-C1A	7.18	109.95	106.68
44	B	838	CLA	C4A-NA-C1A	7.15	109.94	106.68
53	2	502	XAT	C38-C25-C26	-7.15	110.54	122.30
44	A	822	CLA	C4A-NA-C1A	7.13	109.93	106.68
44	A	808	CLA	C4A-NA-C1A	7.13	109.93	106.68
44	B	818	CLA	C4A-NA-C1A	7.12	109.93	106.68
47	B	844	BCR	C20-C21-C22	-7.07	117.36	127.28
47	B	846	BCR	C7-C8-C9	-7.05	115.80	126.23
44	A	802	CLA	C4A-NA-C1A	7.04	109.89	106.68
44	3	310	CLA	C4A-NA-C1A	7.03	109.89	106.68
47	F	801	BCR	C24-C23-C22	-7.01	115.86	126.23
52	2	513	CHL	C1B-CHB-C4A	7.00	125.83	121.32
44	e	807	CLA	C4A-NA-C1A	7.00	109.87	106.68
53	2	502	XAT	C18-C5-C6	-6.99	110.80	122.30
44	f	830	CLA	C4A-NA-C1A	6.99	109.87	106.68
53	s	502	XAT	C18-C5-C6	-6.98	110.81	122.30
44	3	316	CLA	C4A-NA-C1A	6.97	109.86	106.68
44	f	828	CLA	C4A-NA-C1A	6.97	109.86	106.68
44	f	839	CLA	C4A-NA-C1A	6.97	109.86	106.68
44	5	306	CLA	C4A-NA-C1A	6.95	109.85	106.68
44	s	504	CLA	C4A-NA-C1A	6.95	109.85	106.68
44	s	505	CLA	C4A-NA-C1A	6.94	109.85	106.68
44	A	828	CLA	C4A-NA-C1A	6.94	109.85	106.68
44	e	809	CLA	C4A-NA-C1A	6.94	109.84	106.68
53	s	502	XAT	C38-C25-C26	-6.93	110.89	122.30
44	B	832	CLA	C4A-NA-C1A	6.91	109.83	106.68
44	B	817	CLA	C4A-NA-C1A	6.91	109.83	106.68
44	f	810	CLA	C4A-NA-C1A	6.91	109.83	106.68
44	5	316	CLA	C4A-NA-C1A	6.90	109.83	106.68
44	1	507	CLA	C4A-NA-C1A	6.85	109.81	106.68
44	q	306	CLA	C4A-NA-C1A	6.85	109.81	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	q	314	CLA	C4A-NA-C1A	6.84	109.80	106.68
53	r	303	XAT	C38-C25-C26	-6.84	111.04	122.30
47	B	844	BCR	C15-C14-C13	-6.84	117.69	127.28
44	2	510	CLA	C4A-NA-C1A	6.84	109.80	106.68
44	2	505	CLA	C4A-NA-C1A	6.83	109.80	106.68
44	f	805	CLA	C4A-NA-C1A	6.82	109.79	106.68
44	p	515	CLA	C4A-NA-C1A	6.82	109.79	106.68
44	3	318	CLA	C4A-NA-C1A	6.81	109.79	106.68
44	B	833	CLA	C4A-NA-C1A	6.79	109.78	106.68
47	l	101	BCR	C11-C10-C9	-6.78	117.77	127.28
44	f	832	CLA	C4A-NA-C1A	6.76	109.77	106.68
44	1	506	CLA	C4A-NA-C1A	6.76	109.76	106.68
44	B	812	CLA	C4A-NA-C1A	6.76	109.76	106.68
44	e	822	CLA	C4A-NA-C1A	6.76	109.76	106.68
44	f	826	CLA	C4A-NA-C1A	6.76	109.76	106.68
53	2	502	XAT	C11-C10-C9	-6.74	117.82	127.28
44	e	814	CLA	C4A-NA-C1A	6.74	109.75	106.68
52	r	314	CHL	O2D-CGD-CBD	6.74	118.35	110.95
44	e	852	CLA	C4A-NA-C1A	6.73	109.75	106.68
44	B	835	CLA	C4A-NA-C1A	6.73	109.75	106.68
44	f	814	CLA	C4A-NA-C1A	6.73	109.75	106.68
44	o	303	CLA	C4A-NA-C1A	6.73	109.75	106.68
44	A	805	CLA	C4A-NA-C1A	6.72	109.74	106.68
44	f	841	CLA	C4A-NA-C1A	6.72	109.74	106.68
44	B	814	CLA	C4A-NA-C1A	6.71	109.74	106.68
44	3	314	CLA	C4A-NA-C1A	6.71	109.74	106.68
44	e	840	CLA	C4A-NA-C1A	6.69	109.73	106.68
44	A	803	CLA	C4A-NA-C1A	6.69	109.73	106.68
44	r	310	CLA	C4A-NA-C1A	6.69	109.73	106.68
44	B	829	CLA	C4A-NA-C1A	6.67	109.72	106.68
44	e	810	CLA	C4A-NA-C1A	6.67	109.72	106.68
44	e	816	CLA	C4A-NA-C1A	6.66	109.72	106.68
53	5	304	XAT	C38-C25-C26	-6.66	111.34	122.30
44	A	807	CLA	C4A-NA-C1A	6.66	109.72	106.68
44	o	302	CLA	C4A-NA-C1A	6.65	109.72	106.68
44	A	809	CLA	C4A-NA-C1A	6.65	109.71	106.68
44	e	808	CLA	C4A-NA-C1A	6.63	109.70	106.68
44	p	504	CLA	C4A-NA-C1A	6.62	109.70	106.68
44	s	511	CLA	C4A-NA-C1A	6.62	109.70	106.68
44	f	824	CLA	C4A-NA-C1A	6.62	109.70	106.68
44	f	822	CLA	C4A-NA-C1A	6.61	109.70	106.68
47	B	845	BCR	C7-C8-C9	-6.61	116.46	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	A	814	CLA	C4A-NA-C1A	6.61	109.69	106.68
44	3	317	CLA	C4A-NA-C1A	6.60	109.69	106.68
47	f	847	BCR	C7-C8-C9	-6.60	116.47	126.23
44	B	808	CLA	C4A-NA-C1A	6.60	109.69	106.68
44	f	809	CLA	C4A-NA-C1A	6.60	109.69	106.68
44	f	813	CLA	C4A-NA-C1A	6.60	109.69	106.68
44	f	840	CLA	C4A-NA-C1A	6.60	109.69	106.68
44	1	511	CLA	C4A-NA-C1A	6.59	109.69	106.68
44	B	841	CLA	C4A-NA-C1A	6.59	109.69	106.68
44	5	310	CLA	C4A-NA-C1A	6.59	109.68	106.68
44	f	820	CLA	C4A-NA-C1A	6.59	109.68	106.68
44	q	309	CLA	C4A-NA-C1A	6.59	109.68	106.68
44	A	840	CLA	C4A-NA-C1A	6.58	109.68	106.68
44	e	829	CLA	C4A-NA-C1A	6.58	109.68	106.68
44	F	803	CLA	C4A-NA-C1A	6.57	109.68	106.68
52	2	515	CHL	C1B-CHB-C4A	6.56	125.54	121.32
44	e	821	CLA	C4A-NA-C1A	6.55	109.67	106.68
44	f	812	CLA	C4A-NA-C1A	6.55	109.67	106.68
44	f	816	CLA	C4A-NA-C1A	6.54	109.66	106.68
44	1	505	CLA	C4A-NA-C1A	6.54	109.66	106.68
44	m	102	CLA	C4A-NA-C1A	6.54	109.66	106.68
44	e	820	CLA	C4A-NA-C1A	6.53	109.66	106.68
47	f	847	BCR	C24-C23-C22	-6.53	116.57	126.23
44	A	827	CLA	C4A-NA-C1A	6.53	109.66	106.68
44	e	838	CLA	C4A-NA-C1A	6.53	109.66	106.68
44	2	514	CLA	C4A-NA-C1A	6.53	109.66	106.68
44	f	823	CLA	C4A-NA-C1A	6.53	109.66	106.68
44	F	802	CLA	C4A-NA-C1A	6.52	109.65	106.68
44	q	311	CLA	C4A-NA-C1A	6.51	109.65	106.68
47	2	503	BCR	C24-C23-C22	-6.51	116.60	126.23
44	A	804	CLA	C4A-NA-C1A	6.51	109.65	106.68
44	B	823	CLA	C4A-NA-C1A	6.51	109.65	106.68
44	e	841	CLA	C4A-NA-C1A	6.51	109.65	106.68
44	A	842	CLA	C4A-NA-C1A	6.50	109.64	106.68
44	B	807	CLA	C4A-NA-C1A	6.50	109.64	106.68
44	B	831	CLA	C4A-NA-C1A	6.50	109.64	106.68
44	e	824	CLA	C4A-NA-C1A	6.50	109.64	106.68
51	5	303	LUT	C35-C34-C33	-6.49	118.17	127.28
47	o	301	BCR	C7-C8-C9	-6.49	116.63	126.23
44	f	808	CLA	C4A-NA-C1A	6.49	109.64	106.68
44	f	837	CLA	C4A-NA-C1A	6.49	109.64	106.68
44	q	310	CLA	C4A-NA-C1A	6.49	109.64	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	e	817	CLA	C4A-NA-C1A	6.49	109.64	106.68
44	n	201	CLA	C4A-NA-C1A	6.48	109.64	106.68
44	e	839	CLA	C4A-NA-C1A	6.47	109.63	106.68
44	B	809	CLA	C4A-NA-C1A	6.47	109.63	106.68
44	f	838	CLA	C4A-NA-C1A	6.47	109.63	106.68
44	A	806	CLA	C4A-NA-C1A	6.47	109.63	106.68
44	5	308	CLA	C4A-NA-C1A	6.47	109.63	106.68
44	p	507	CLA	C4A-NA-C1A	6.46	109.62	106.68
44	o	304	CLA	C4A-NA-C1A	6.45	109.62	106.68
53	s	502	XAT	O4-C5-C4	6.45	119.53	113.49
44	e	811	CLA	C4A-NA-C1A	6.44	109.62	106.68
44	L	304	CLA	C4A-NA-C1A	6.44	109.61	106.68
44	s	514	CLA	C4A-NA-C1A	6.43	109.61	106.68
44	q	308	CLA	C4A-NA-C1A	6.42	109.61	106.68
44	3	309	CLA	C4A-NA-C1A	6.42	109.61	106.68
44	e	828	CLA	C4A-NA-C1A	6.41	109.61	106.68
44	1	510	CLA	C4A-NA-C1A	6.41	109.60	106.68
44	q	315	CLA	C4A-NA-C1A	6.41	109.60	106.68
44	5	307	CLA	C4A-NA-C1A	6.40	109.60	106.68
44	f	842	CLA	C4A-NA-C1A	6.40	109.60	106.68
44	p	510	CLA	C4A-NA-C1A	6.40	109.60	106.68
44	A	811	CLA	C4A-NA-C1A	6.40	109.60	106.68
44	e	853	CLA	C4A-NA-C1A	6.40	109.60	106.68
44	1	509	CLA	C4A-NA-C1A	6.39	109.59	106.68
44	e	802	CLA	C4A-NA-C1A	6.39	109.59	106.68
44	f	817	CLA	C4A-NA-C1A	6.38	109.59	106.68
44	B	819	CLA	C4A-NA-C1A	6.38	109.59	106.68
44	f	825	CLA	C4A-NA-C1A	6.38	109.59	106.68
44	e	803	CLA	C4A-NA-C1A	6.37	109.58	106.68
44	B	803	CLA	C4A-NA-C1A	6.37	109.58	106.68
44	e	819	CLA	C4A-NA-C1A	6.37	109.58	106.68
44	n	202	CLA	C4A-NA-C1A	6.36	109.58	106.68
44	r	317	CLA	C4A-NA-C1A	6.36	109.58	106.68
47	e	854	BCR	C15-C14-C13	-6.36	118.36	127.28
44	A	826	CLA	C4A-NA-C1A	6.35	109.58	106.68
44	B	813	CLA	C4A-NA-C1A	6.35	109.58	106.68
44	e	833	CLA	C4A-NA-C1A	6.35	109.58	106.68
44	e	804	CLA	C4A-NA-C1A	6.35	109.58	106.68
44	e	805	CLA	C4A-NA-C1A	6.35	109.58	106.68
53	s	502	XAT	C15-C14-C13	-6.35	118.37	127.28
44	n	203	CLA	C4A-NA-C1A	6.35	109.58	106.68
44	A	813	CLA	C4A-NA-C1A	6.34	109.57	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	f	834	CLA	C4A-NA-C1A	6.34	109.57	106.68
44	e	806	CLA	C4A-NA-C1A	6.33	109.57	106.68
44	A	837	CLA	C4A-NA-C1A	6.33	109.57	106.68
44	f	835	CLA	C4A-NA-C1A	6.33	109.57	106.68
44	f	801	CLA	C4A-NA-C1A	6.32	109.56	106.68
44	A	817	CLA	C4A-NA-C1A	6.32	109.56	106.68
44	A	831	CLA	C4A-NA-C1A	6.31	109.56	106.68
44	A	852	CLA	C4A-NA-C1A	6.31	109.56	106.68
44	q	304	CLA	C4A-NA-C1A	6.31	109.56	106.68
44	q	307	CLA	C4A-NA-C1A	6.30	109.56	106.68
44	f	818	CLA	C4A-NA-C1A	6.30	109.55	106.68
44	r	312	CLA	C4A-NA-C1A	6.30	109.55	106.68
44	B	810	CLA	C4A-NA-C1A	6.29	109.55	106.68
44	B	827	CLA	C4A-NA-C1A	6.29	109.55	106.68
44	e	815	CLA	C4A-NA-C1A	6.29	109.55	106.68
44	j	802	CLA	C4A-NA-C1A	6.28	109.55	106.68
44	r	304	CLA	C4A-NA-C1A	6.28	109.55	106.68
44	r	308	CLA	C4A-NA-C1A	6.28	109.54	106.68
44	K	201	CLA	C4A-NA-C1A	6.28	109.54	106.68
44	f	811	CLA	C4A-NA-C1A	6.27	109.54	106.68
44	r	305	CLA	C4A-NA-C1A	6.27	109.54	106.68
44	e	825	CLA	C4A-NA-C1A	6.26	109.53	106.68
44	B	802	CLA	C4A-NA-C1A	6.26	109.53	106.68
47	2	503	BCR	C15-C14-C13	6.26	136.05	127.28
44	s	510	CLA	C4A-NA-C1A	6.25	109.53	106.68
47	s	503	BCR	C15-C16-C17	-6.25	110.73	123.52
44	f	843	CLA	C4A-NA-C1A	6.24	109.53	106.68
44	m	101	CLA	C4A-NA-C1A	6.24	109.53	106.68
44	B	825	CLA	C4A-NA-C1A	6.23	109.52	106.68
44	A	833	CLA	C4A-NA-C1A	6.22	109.52	106.68
44	1	513	CLA	C4A-NA-C1A	6.22	109.52	106.68
52	2	516	CHL	CHA-C1A-C2A	-6.22	118.70	133.31
44	f	833	CLA	C4A-NA-C1A	6.22	109.52	106.68
44	r	311	CLA	C4A-NA-C1A	6.21	109.51	106.68
44	s	506	CLA	C4A-NA-C1A	6.21	109.51	106.68
44	A	834	CLA	C4A-NA-C1A	6.21	109.51	106.68
44	B	842	CLA	C4A-NA-C1A	6.21	109.51	106.68
44	f	819	CLA	C4A-NA-C1A	6.21	109.51	106.68
44	s	508	CLA	C4A-NA-C1A	6.21	109.51	106.68
47	j	803	BCR	C11-C10-C9	-6.21	118.57	127.28
44	f	836	CLA	C4A-NA-C1A	6.20	109.51	106.68
44	s	509	CLA	C4A-NA-C1A	6.18	109.50	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	q	312	CLA	C4A-NA-C1A	6.18	109.50	106.68
44	B	834	CLA	C4A-NA-C1A	6.17	109.50	106.68
47	e	846	BCR	C16-C17-C18	-6.17	118.63	127.28
47	s	503	BCR	C40-C30-C29	-6.16	85.30	108.95
44	2	507	CLA	C4A-NA-C1A	6.16	109.49	106.68
44	p	511	CLA	C4A-NA-C1A	6.15	109.48	106.68
44	1	508	CLA	C4A-NA-C1A	6.15	109.48	106.68
44	A	825	CLA	C4A-NA-C1A	6.14	109.48	106.68
44	e	834	CLA	C4A-NA-C1A	6.14	109.48	106.68
52	3	315	CHL	CHA-C1A-C2A	-6.13	118.91	133.31
47	2	503	BCR	C40-C30-C29	-6.12	85.44	108.95
44	e	826	CLA	C4A-NA-C1A	6.12	109.47	106.68
47	A	848	BCR	C28-C27-C26	-6.12	103.14	114.06
53	5	304	XAT	C18-C5-C6	-6.12	112.24	122.30
47	j	801	BCR	C16-C17-C18	-6.12	118.70	127.28
44	p	508	CLA	C4A-NA-C1A	6.12	109.47	106.68
44	f	831	CLA	C4A-NA-C1A	6.11	109.47	106.68
44	5	312	CLA	C4A-NA-C1A	6.11	109.47	106.68
47	Q	801	BCR	C24-C23-C22	-6.11	117.20	126.23
44	B	811	CLA	C4A-NA-C1A	6.11	109.47	106.68
44	e	823	CLA	C4A-NA-C1A	6.10	109.46	106.68
44	e	836	CLA	C4A-NA-C1A	6.09	109.46	106.68
44	A	838	CLA	C4A-NA-C1A	6.09	109.46	106.68
44	B	837	CLA	C4A-NA-C1A	6.09	109.46	106.68
47	B	846	BCR	C24-C23-C22	-6.09	117.23	126.23
44	r	307	CLA	C4A-NA-C1A	6.09	109.46	106.68
44	K	202	CLA	C4A-NA-C1A	6.08	109.45	106.68
44	L	301	CLA	C4A-NA-C1A	6.08	109.45	106.68
44	e	832	CLA	C4A-NA-C1A	6.08	109.45	106.68
44	5	313	CLA	C4A-NA-C1A	6.06	109.44	106.68
44	e	835	CLA	C4A-NA-C1A	6.06	109.44	106.68
47	l	101	BCR	C7-C8-C9	-6.06	117.27	126.23
44	A	812	CLA	C4A-NA-C1A	6.05	109.44	106.68
44	B	806	CLA	C4A-NA-C1A	6.05	109.44	106.68
44	B	828	CLA	C4A-NA-C1A	6.05	109.44	106.68
44	e	843	CLA	C4A-NA-C1A	6.04	109.43	106.68
44	n	205	CLA	C4A-NA-C1A	6.03	109.43	106.68
47	J	102	BCR	C28-C27-C26	-6.03	103.30	114.06
47	f	846	BCR	C7-C8-C9	-6.03	117.31	126.23
44	A	829	CLA	C4A-NA-C1A	6.03	109.43	106.68
44	J	101	CLA	C4A-NA-C1A	6.03	109.43	106.68
44	A	815	CLA	C4A-NA-C1A	6.02	109.43	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	K	205	CLA	C4A-NA-C1A	6.02	109.42	106.68
47	o	305	BCR	C20-C21-C22	-6.02	118.84	127.28
47	j	801	BCR	C24-C23-C22	-6.02	117.33	126.23
44	e	837	CLA	C4A-NA-C1A	6.01	109.42	106.68
44	f	829	CLA	C4A-NA-C1A	6.01	109.42	106.68
44	B	805	CLA	C4A-NA-C1A	6.01	109.42	106.68
44	r	315	CLA	C4A-NA-C1A	6.01	109.42	106.68
47	f	850	BCR	C16-C17-C18	-6.01	118.85	127.28
44	e	831	CLA	C4A-NA-C1A	6.00	109.42	106.68
52	2	512	CHL	CHA-C1A-C2A	-5.99	119.23	133.31
44	f	806	CLA	C4A-NA-C1A	5.99	109.41	106.68
44	B	815	CLA	C4A-NA-C1A	5.99	109.41	106.68
44	3	307	CLA	C4A-NA-C1A	5.99	109.41	106.68
47	L	305	BCR	C28-C27-C26	-5.98	103.39	114.06
52	r	314	CHL	CHA-C1A-C2A	-5.98	119.27	133.31
44	e	812	CLA	C4A-NA-C1A	5.98	109.41	106.68
44	e	830	CLA	C4A-NA-C1A	5.98	109.41	106.68
44	f	807	CLA	C4A-NA-C1A	5.97	109.40	106.68
44	p	513	CLA	C4A-NA-C1A	5.97	109.40	106.68
44	f	821	CLA	C4A-NA-C1A	5.95	109.39	106.68
44	3	312	CLA	C4A-NA-C1A	5.95	109.39	106.68
44	r	306	CLA	C4A-NA-C1A	5.94	109.39	106.68
44	1	504	CLA	C4A-NA-C1A	5.93	109.39	106.68
44	q	316	CLA	C4A-NA-C1A	5.92	109.38	106.68
44	A	824	CLA	C4A-NA-C1A	5.92	109.38	106.68
44	B	830	CLA	C4A-NA-C1A	5.92	109.38	106.68
52	2	515	CHL	CHA-C1A-C2A	-5.91	119.43	133.31
47	3	305	BCR	C15-C14-C13	-5.91	118.99	127.28
47	B	846	BCR	C15-C14-C13	-5.91	118.99	127.28
44	B	836	CLA	C4A-NA-C1A	5.90	109.37	106.68
44	s	507	CLA	C4A-NA-C1A	5.90	109.37	106.68
44	K	203	CLA	C4A-NA-C1A	5.86	109.35	106.68
44	5	309	CLA	C4A-NA-C1A	5.86	109.35	106.68
47	1	503	BCR	C11-C10-C9	-5.86	119.06	127.28
47	e	850	BCR	C20-C21-C22	-5.84	119.09	127.28
47	B	844	BCR	C11-C10-C9	-5.83	119.10	127.28
53	5	304	XAT	O4-C5-C4	5.83	118.95	113.49
51	q	301	LUT	C35-C34-C33	-5.82	119.11	127.28
44	A	818	CLA	C4A-NA-C1A	5.82	109.33	106.68
44	q	305	CLA	C4A-NA-C1A	5.81	109.33	106.68
44	p	506	CLA	C4A-NA-C1A	5.80	109.33	106.68
47	l	101	BCR	C15-C14-C13	-5.80	119.14	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	A	848	BCR	C24-C23-C22	-5.79	117.67	126.23
44	A	819	CLA	C4A-NA-C1A	5.79	109.32	106.68
44	B	826	CLA	C4A-NA-C1A	5.79	109.32	106.68
53	2	502	XAT	O24-C25-C38	5.78	121.51	115.05
52	5	314	CHL	CHA-C1A-C2A	-5.78	119.74	133.31
44	B	820	CLA	C4A-NA-C1A	5.78	109.31	106.68
44	2	508	CLA	C4A-NA-C1A	5.78	109.31	106.68
47	f	848	BCR	C15-C14-C13	-5.77	119.19	127.28
47	2	503	BCR	C39-C30-C25	5.77	119.29	110.24
47	A	845	BCR	C15-C14-C13	-5.76	119.19	127.28
47	B	852	BCR	C7-C8-C9	-5.76	117.71	126.23
51	1	502	LUT	C15-C14-C13	-5.75	119.21	127.28
44	f	815	CLA	C4A-NA-C1A	5.73	109.29	106.68
44	e	813	CLA	C4A-NA-C1A	5.70	109.28	106.68
51	s	501	LUT	C15-C14-C13	-5.70	119.29	127.28
44	5	305	CLA	C4A-NA-C1A	5.68	109.27	106.68
47	l	102	BCR	C7-C8-C9	-5.68	117.83	126.23
47	B	844	BCR	C24-C23-C22	-5.68	117.83	126.23
44	f	827	CLA	C4A-NA-C1A	5.67	109.27	106.68
47	B	844	BCR	C16-C17-C18	-5.67	119.33	127.28
44	A	823	CLA	C4A-NA-C1A	5.66	109.26	106.68
47	A	849	BCR	C7-C8-C9	-5.65	117.87	126.23
47	s	503	BCR	C39-C30-C25	5.64	119.09	110.24
47	2	503	BCR	C15-C16-C17	-5.64	111.98	123.52
44	r	309	CLA	C4A-NA-C1A	5.62	109.24	106.68
44	B	824	CLA	C4A-NA-C1A	5.62	109.24	106.68
53	r	303	XAT	O4-C5-C18	5.61	121.32	115.05
47	A	845	BCR	C16-C17-C18	-5.61	119.41	127.28
47	A	851	BCR	C15-C14-C13	-5.58	119.45	127.28
53	2	502	XAT	O4-C5-C18	5.58	121.28	115.05
47	e	846	BCR	C20-C21-C22	-5.57	119.46	127.28
47	o	305	BCR	C16-C17-C18	-5.57	119.47	127.28
47	s	503	BCR	C30-C25-C26	-5.55	115.05	122.64
50	r	318	LMG	O7-C10-O9	-5.53	118.61	125.70
44	p	509	CLA	CMD-C2D-C1D	5.52	134.45	124.73
47	I	101	BCR	C24-C23-C22	-5.51	118.08	126.23
44	f	803	CLA	C4A-NA-C1A	5.51	109.19	106.68
47	B	852	BCR	C15-C14-C13	-5.50	119.56	127.28
44	e	827	CLA	C4A-NA-C1A	5.50	109.19	106.68
47	L	305	BCR	C16-C17-C18	-5.48	119.59	127.28
47	F	801	BCR	C28-C27-C26	-5.47	104.30	114.06
47	F	804	BCR	C11-C10-C9	-5.46	119.63	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	e	818	CLA	CMD-C2D-C1D	5.45	134.33	124.73
51	p	501	LUT	C11-C10-C9	-5.45	119.64	127.28
47	o	301	BCR	C15-C14-C13	-5.44	119.65	127.28
51	2	501	LUT	C26-C27-C28	-5.44	116.11	124.58
44	B	801	CLA	C4A-NA-C1A	5.44	109.16	106.68
52	1	512	CHL	CHA-C1A-C2A	-5.42	120.58	133.31
47	Q	801	BCR	C13-C12-C11	-5.42	112.19	124.72
47	K	204	BCR	C16-C17-C18	-5.40	119.70	127.28
51	q	301	LUT	C31-C30-C29	-5.40	119.71	127.28
47	e	846	BCR	C15-C14-C13	-5.39	119.72	127.28
47	e	846	BCR	C38-C26-C25	-5.37	118.62	124.48
47	B	849	BCR	C20-C21-C22	-5.37	119.75	127.28
51	r	302	LUT	C31-C30-C29	-5.35	119.77	127.28
53	5	304	XAT	O24-C25-C24	5.35	118.50	113.49
53	r	303	XAT	O24-C25-C24	5.35	118.50	113.49
44	1	515	CLA	C4A-NA-C1A	5.35	109.12	106.68
52	5	315	CHL	CHA-C1A-C2A	-5.34	120.77	133.31
47	m	103	BCR	C28-C27-C26	-5.30	104.60	114.06
47	f	845	BCR	C20-C21-C22	-5.27	119.89	127.28
47	5	302	BCR	C33-C5-C6	-5.24	118.76	124.48
47	F	801	BCR	C20-C21-C22	-5.24	119.93	127.28
47	A	847	BCR	C15-C14-C13	-5.23	119.94	127.28
47	q	303	BCR	C7-C8-C9	-5.22	118.52	126.23
47	q	303	BCR	C15-C14-C13	-5.22	119.96	127.28
47	A	853	BCR	C28-C27-C26	-5.21	104.76	114.06
51	q	302	LUT	C35-C34-C33	-5.20	119.98	127.28
51	p	501	LUT	C15-C14-C13	-5.20	119.98	127.28
52	2	513	CHL	O2D-CGD-CBD	5.20	119.93	111.43
47	f	850	BCR	C20-C21-C22	-5.19	119.99	127.28
44	f	804	CLA	C3B-C2B-C1B	-5.19	104.92	108.37
47	e	849	BCR	C16-C17-C18	-5.18	120.01	127.28
47	f	845	BCR	C24-C23-C22	-5.18	118.57	126.23
47	e	849	BCR	C20-C21-C22	-5.17	120.03	127.28
47	A	845	BCR	C33-C5-C6	-5.16	118.85	124.48
53	s	502	XAT	O24-C25-C24	5.16	118.32	113.49
47	e	848	BCR	C11-C10-C9	-5.16	120.05	127.28
47	2	503	BCR	C16-C15-C14	5.15	134.06	123.52
53	2	502	XAT	O4-C5-C4	5.14	118.31	113.49
53	s	502	XAT	O24-C25-C38	5.14	120.79	115.05
43	e	801	CL0	CHA-C1A-C2A	-5.12	126.26	133.83
47	f	847	BCR	C16-C17-C18	-5.12	120.09	127.28
47	e	851	BCR	C7-C8-C9	-5.12	118.67	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	j	803	BCR	C7-C8-C9	-5.11	118.68	126.23
43	A	801	CL0	CHA-C1A-C2A	-5.11	126.28	133.83
52	r	316	CHL	CHA-C1A-C2A	-5.09	121.35	133.31
47	A	845	BCR	C20-C21-C22	-5.09	120.14	127.28
52	5	314	CHL	C1B-CHB-C4A	5.09	124.60	121.32
51	r	302	LUT	C15-C14-C13	-5.09	120.14	127.28
47	A	846	BCR	C16-C17-C18	-5.07	120.17	127.28
47	e	851	BCR	C11-C10-C9	-5.05	120.20	127.28
47	f	849	BCR	C24-C23-C22	-5.04	118.77	126.23
47	e	854	BCR	C11-C10-C9	-5.04	120.21	127.28
47	Q	801	BCR	C15-C16-C17	-5.04	113.22	123.52
51	1	502	LUT	C26-C27-C28	-5.03	116.75	124.58
47	B	847	BCR	C7-C8-C9	-5.01	118.82	126.23
47	Q	801	BCR	C20-C21-C22	-5.01	120.25	127.28
51	q	302	LUT	C26-C27-C28	-5.00	116.79	124.58
52	q	313	CHL	O2D-CGD-CBD	5.00	119.61	111.43
52	s	513	CHL	CHA-C1A-C2A	-5.00	121.57	133.31
47	f	845	BCR	C16-C17-C18	-4.99	120.27	127.28
51	r	302	LUT	C35-C34-C33	-4.99	120.27	127.28
47	l	102	BCR	C15-C14-C13	-4.99	120.28	127.28
52	3	302	CHL	CHA-C1A-C2A	-4.98	121.61	133.31
47	I	101	BCR	C20-C21-C22	-4.98	120.29	127.28
51	3	304	LUT	C35-C34-C33	-4.96	120.32	127.28
52	s	517	CHL	CHA-C1A-C2A	-4.94	121.70	133.31
47	f	849	BCR	C15-C14-C13	-4.90	120.41	127.28
47	L	306	BCR	C15-C14-C13	-4.89	120.43	127.28
51	2	501	LUT	C7-C8-C9	-4.89	119.01	126.23
47	r	301	BCR	C15-C14-C13	-4.86	120.46	127.28
47	e	850	BCR	C16-C17-C18	-4.86	120.46	127.28
51	1	501	LUT	C18-C5-C6	-4.86	119.19	124.48
46	A	843	LHG	O7-C7-C8	4.85	121.96	111.48
47	B	849	BCR	C24-C23-C22	-4.84	119.07	126.23
50	2	519	LMG	O7-C10-C11	4.84	121.95	111.48
47	5	302	BCR	C7-C8-C9	-4.84	119.08	126.23
52	q	313	CHL	CHA-C1A-C2A	-4.84	121.95	133.31
47	A	846	BCR	C11-C10-C9	-4.83	120.50	127.28
45	B	843	PQN	C11-C12-C13	-4.82	118.53	126.83
44	2	507	CLA	C4-C3-C2	-4.81	110.14	122.23
52	r	313	CHL	CHA-C1A-C2A	-4.81	122.02	133.31
47	j	801	BCR	C28-C27-C26	-4.80	105.49	114.06
47	B	847	BCR	C15-C16-C17	-4.79	113.72	123.52
52	s	512	CHL	CHA-C1A-C2A	-4.78	122.09	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	A	846	BCR	C24-C23-C22	-4.77	119.17	126.23
51	p	501	LUT	C7-C8-C9	-4.77	119.17	126.23
51	q	301	LUT	C11-C10-C9	-4.77	120.59	127.28
47	e	849	BCR	C24-C23-C22	-4.76	119.19	126.23
47	J	102	BCR	C16-C17-C18	-4.72	120.66	127.28
51	3	303	LUT	C26-C27-C28	-4.71	117.25	124.58
51	2	501	LUT	C15-C14-C13	-4.71	120.68	127.28
47	j	803	BCR	C15-C14-C13	-4.70	120.69	127.28
51	q	301	LUT	C26-C27-C28	-4.69	117.29	124.58
53	r	303	XAT	O24-C25-C38	4.68	120.28	115.05
47	3	305	BCR	C24-C23-C22	-4.68	119.31	126.23
51	q	301	LUT	C7-C8-C9	-4.68	119.31	126.23
52	p	517	CHL	CHA-C1A-C2A	-4.68	122.33	133.31
44	2	507	CLA	C5-C3-C2	-4.67	110.69	123.13
47	o	305	BCR	C24-C23-C22	-4.66	119.34	126.23
47	A	851	BCR	C28-C27-C26	-4.65	105.76	114.06
47	e	854	BCR	C28-C27-C26	-4.65	105.76	114.06
47	p	503	BCR	C38-C26-C25	-4.65	119.41	124.48
47	B	845	BCR	C15-C14-C13	-4.64	120.77	127.28
47	e	851	BCR	C15-C14-C13	-4.63	120.78	127.28
53	r	303	XAT	C26-C27-C28	-4.63	116.21	125.99
47	e	846	BCR	C33-C5-C6	-4.62	119.45	124.48
47	A	848	BCR	C20-C21-C22	-4.61	120.81	127.28
47	K	204	BCR	C28-C27-C26	-4.61	105.84	114.06
47	r	301	BCR	C33-C5-C6	-4.60	119.46	124.48
47	A	851	BCR	C38-C26-C25	-4.60	119.46	124.48
44	A	805	CLA	CAA-C2A-C3A	-4.60	100.58	113.00
47	e	848	BCR	C16-C17-C18	-4.58	120.85	127.28
47	B	846	BCR	C16-C17-C18	-4.58	120.85	127.28
47	j	801	BCR	C20-C21-C22	-4.57	120.87	127.28
47	o	305	BCR	C33-C5-C6	-4.57	119.50	124.48
52	p	514	CHL	CHA-C1A-C2A	-4.57	122.59	133.31
47	Q	801	BCR	C15-C14-C13	-4.56	114.18	124.72
44	f	804	CLA	CMD-C2D-C1D	4.56	132.75	124.73
47	e	849	BCR	C15-C14-C13	-4.56	120.89	127.28
47	o	301	BCR	C33-C5-C6	-4.56	119.51	124.48
47	f	847	BCR	C15-C14-C13	-4.56	120.89	127.28
47	B	848	BCR	C15-C14-C13	-4.55	120.90	127.28
47	L	305	BCR	C11-C10-C9	-4.54	120.91	127.28
52	p	512	CHL	CHA-C1A-C2A	-4.53	122.66	133.31
53	s	502	XAT	C31-C30-C29	-4.53	120.92	127.28
47	l	102	BCR	C28-C27-C26	-4.53	105.97	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	F	804	BCR	C15-C14-C13	-4.53	120.92	127.28
47	B	848	BCR	C24-C23-C22	-4.53	119.53	126.23
53	5	304	XAT	C26-C27-C28	-4.53	116.41	125.99
47	f	845	BCR	C11-C10-C9	-4.53	120.93	127.28
47	B	849	BCR	C16-C17-C18	-4.52	120.93	127.28
51	s	501	LUT	C26-C27-C28	-4.51	117.56	124.58
47	A	849	BCR	C20-C21-C22	-4.50	120.96	127.28
47	e	848	BCR	C24-C23-C22	-4.50	119.58	126.23
44	p	505	CLA	C4A-NA-C1A	4.48	108.72	106.68
46	e	844	LHG	O7-C7-C8	4.48	121.16	111.48
47	K	204	BCR	C20-C21-C22	-4.48	121.00	127.28
47	A	845	BCR	C38-C26-C25	-4.48	119.60	124.48
47	B	845	BCR	C30-C25-C26	-4.47	116.53	122.64
47	f	845	BCR	C15-C14-C13	-4.47	121.01	127.28
43	A	801	CL0	C1C-CHC-C4B	4.47	132.06	116.07
47	B	847	BCR	C11-C10-C9	-4.47	121.01	127.28
43	e	801	CL0	C1C-CHC-C4B	4.47	132.05	116.07
47	B	848	BCR	C38-C26-C25	-4.46	119.61	124.48
52	5	317	CHL	CHB-C4A-NA	4.46	126.47	121.83
47	o	305	BCR	C15-C14-C13	-4.45	121.04	127.28
47	e	847	BCR	C16-C17-C18	-4.44	121.05	127.28
47	m	103	BCR	C24-C23-C22	-4.44	119.67	126.23
47	2	503	BCR	C33-C5-C6	-4.43	119.65	124.48
47	o	305	BCR	C11-C10-C9	-4.43	121.07	127.28
47	J	102	BCR	C3-C4-C5	-4.42	106.18	114.06
47	A	851	BCR	C3-C4-C5	-4.42	106.18	114.06
47	A	848	BCR	C15-C14-C13	-4.42	121.08	127.28
44	A	817	CLA	CAA-C2A-C3A	-4.41	106.11	116.23
47	K	204	BCR	C38-C26-C25	-4.41	119.67	124.48
47	m	103	BCR	C20-C21-C22	-4.41	121.09	127.28
47	I	101	BCR	C7-C8-C9	-4.39	119.74	126.23
47	s	503	BCR	C36-C18-C19	4.38	124.78	118.09
51	1	501	LUT	C35-C34-C33	-4.38	121.14	127.28
47	f	846	BCR	C33-C5-C6	-4.37	119.71	124.48
44	L	304	CLA	CAC-C3C-C4C	4.37	130.48	124.79
51	3	304	LUT	C21-C26-C27	-4.36	107.81	112.83
47	A	846	BCR	C15-C14-C13	-4.36	121.17	127.28
52	1	517	CHL	CHA-C1A-NA	4.35	126.04	122.15
51	p	501	LUT	C35-C34-C33	-4.35	121.18	127.28
50	5	301	LMG	O7-C10-C11	4.35	120.89	111.48
47	e	848	BCR	C20-C21-C22	-4.35	121.18	127.28
53	s	502	XAT	O4-C5-C18	4.35	119.91	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	B	851	LHG	O7-C7-C8	4.34	120.88	111.48
47	J	102	BCR	C15-C14-C13	-4.34	121.19	127.28
47	e	851	BCR	C3-C4-C5	-4.33	106.33	114.06
47	f	849	BCR	C11-C10-C9	-4.32	121.22	127.28
51	1	501	LUT	C26-C27-C28	-4.32	117.85	124.58
47	l	102	BCR	C16-C17-C18	-4.32	121.22	127.28
47	f	850	BCR	C24-C23-C22	-4.32	119.85	126.23
47	3	305	BCR	C38-C26-C25	-4.31	119.78	124.48
47	j	803	BCR	C16-C17-C18	-4.31	121.24	127.28
47	B	845	BCR	C33-C5-C6	-4.29	119.80	124.48
51	2	501	LUT	C11-C10-C9	-4.29	121.27	127.28
47	L	306	BCR	C24-C23-C22	-4.28	119.90	126.23
47	r	301	BCR	C11-C10-C9	-4.28	121.27	127.28
51	5	303	LUT	C18-C5-C6	-4.28	119.81	124.48
47	1	503	BCR	C33-C5-C6	-4.28	119.81	124.48
53	s	502	XAT	C35-C34-C33	-4.27	121.30	127.28
47	m	103	BCR	C11-C10-C9	-4.26	121.30	127.28
53	r	303	XAT	C35-C34-C33	-4.24	121.34	127.28
51	s	501	LUT	C11-C10-C9	-4.23	121.34	127.28
47	f	845	BCR	C33-C5-C6	-4.23	119.87	124.48
47	l	102	BCR	C20-C21-C22	-4.23	121.35	127.28
46	f	852	LHG	O7-C7-C8	4.22	120.62	111.48
47	e	848	BCR	C15-C14-C13	-4.22	121.36	127.28
49	B	850	DGD	O2G-C1B-C2B	4.20	120.57	111.48
52	s	515	CHL	C2A-C3A-C4A	-4.20	100.79	103.53
47	A	853	BCR	C16-C17-C18	-4.20	121.39	127.28
47	e	850	BCR	C24-C23-C22	-4.20	120.02	126.23
49	f	851	DGD	O2G-C1B-C2B	4.19	120.55	111.48
44	A	829	CLA	O2D-CGD-O1D	-4.18	115.70	123.85
47	B	852	BCR	C33-C5-C6	-4.18	119.92	124.48
52	5	315	CHL	C1B-CHB-C4A	4.17	124.00	121.32
46	e	845	LHG	O7-C7-C8	4.17	120.49	111.48
47	L	305	BCR	C7-C8-C9	-4.16	120.08	126.23
47	A	845	BCR	C24-C23-C22	-4.15	120.09	126.23
46	O	601	LHG	O7-C7-C8	4.15	120.46	111.48
47	2	503	BCR	C30-C25-C26	-4.15	116.97	122.64
47	f	849	BCR	C38-C26-C25	-4.14	119.97	124.48
53	r	303	XAT	C15-C14-C13	-4.14	121.48	127.28
46	p	516	LHG	O7-C7-C8	4.13	120.42	111.48
53	2	502	XAT	C31-C30-C29	-4.13	121.49	127.28
47	A	851	BCR	C16-C17-C18	-4.12	121.50	127.28
51	2	501	LUT	C35-C34-C33	-4.12	121.50	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	2	502	XAT	C26-C27-C28	-4.10	117.31	125.99
51	p	501	LUT	C26-C27-C28	-4.10	118.20	124.58
51	5	303	LUT	C15-C14-C13	-4.09	121.54	127.28
46	1	516	LHG	O7-C7-C8	4.08	120.30	111.48
47	B	852	BCR	C38-C26-C25	-4.07	120.04	124.48
53	r	303	XAT	O4-C5-C4	4.07	117.31	113.49
47	3	305	BCR	C11-C10-C9	-4.07	121.57	127.28
47	A	853	BCR	C20-C21-C22	-4.07	121.58	127.28
47	s	503	BCR	C29-C30-C25	4.06	116.33	110.44
47	A	853	BCR	C27-C26-C25	-4.06	117.22	122.70
44	f	804	CLA	C4B-NB-C1B	4.05	109.15	106.31
53	r	303	XAT	C6-C7-C8	-4.04	117.44	125.99
47	n	204	BCR	C16-C15-C14	-4.04	115.25	123.52
44	A	836	CLA	O2D-CGD-O1D	-4.04	115.98	123.85
50	F	805	LMG	O7-C10-C11	4.04	120.22	111.48
43	e	801	CL0	CHB-C4A-NA	4.04	126.03	121.83
47	F	801	BCR	C16-C17-C18	-4.04	121.62	127.28
51	3	304	LUT	C26-C27-C28	-4.02	118.32	124.58
47	e	848	BCR	C28-C27-C26	-4.02	106.88	114.06
47	s	503	BCR	C3-C4-C5	-4.02	106.88	114.06
43	A	801	CL0	CHB-C4A-NA	4.02	126.02	121.83
53	s	502	XAT	C6-C7-C8	-4.02	117.50	125.99
47	L	306	BCR	C1-C6-C5	-4.01	117.16	122.64
47	e	847	BCR	C11-C10-C9	-4.01	121.66	127.28
50	m	105	LMG	O7-C10-C11	3.99	120.11	111.48
46	A	844	LHG	O7-C7-C8	3.99	120.10	111.48
47	B	844	BCR	C3-C4-C5	-3.98	106.95	114.06
51	q	302	LUT	C10-C11-C12	-3.97	111.69	123.20
47	A	849	BCR	C24-C23-C22	-3.96	120.37	126.23
46	2	517	LHG	O7-C7-C8	3.96	120.06	111.48
47	A	846	BCR	C20-C21-C22	-3.96	121.72	127.28
47	e	851	BCR	C16-C17-C18	-3.96	121.73	127.28
43	A	801	CL0	C1-C2-C3	-3.95	119.73	126.20
47	I	101	BCR	C15-C14-C13	-3.94	121.75	127.28
47	f	845	BCR	C7-C8-C9	-3.94	120.41	126.23
43	e	801	CL0	C1-C2-C3	-3.93	119.75	126.20
47	5	302	BCR	C15-C14-C13	-3.93	121.77	127.28
47	l	102	BCR	C3-C4-C5	-3.91	107.08	114.06
47	j	801	BCR	C33-C5-C6	-3.91	120.21	124.48
44	A	833	CLA	O2D-CGD-O1D	-3.90	116.25	123.85
47	K	204	BCR	C33-C5-C6	-3.90	120.23	124.48
47	e	851	BCR	C28-C27-C26	-3.89	107.11	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	f	850	BCR	C8-C7-C6	-3.89	121.03	126.28
47	F	804	BCR	C7-C8-C9	-3.88	120.50	126.23
47	l	101	BCR	C24-C23-C22	-3.88	120.50	126.23
47	2	503	BCR	C29-C30-C25	3.87	116.07	110.44
47	A	853	BCR	C2-C1-C6	3.87	116.06	110.44
47	L	305	BCR	C38-C26-C25	-3.86	120.27	124.48
47	e	850	BCR	C15-C14-C13	-3.85	121.87	127.28
47	e	848	BCR	C7-C8-C9	-3.85	120.54	126.23
47	B	849	BCR	C3-C4-C5	-3.84	107.20	114.06
47	e	849	BCR	C33-C5-C6	-3.84	120.29	124.48
52	r	316	CHL	CBC-CAC-C3C	-3.84	107.38	112.87
44	3	306	CLA	C1-C2-C3	-3.83	119.92	126.20
47	B	852	BCR	C28-C27-C26	-3.83	107.23	114.06
46	s	516	LHG	O7-C7-C8	3.83	119.76	111.48
44	e	809	CLA	O2D-CGD-O1D	-3.82	116.40	123.85
53	5	304	XAT	C10-C11-C12	-3.82	112.12	123.20
47	A	853	BCR	C15-C14-C13	-3.82	121.92	127.28
47	B	848	BCR	C15-C16-C17	-3.82	115.71	123.52
47	B	847	BCR	C33-C5-C6	-3.82	120.32	124.48
47	A	851	BCR	C33-C5-C6	-3.82	120.32	124.48
47	l	102	BCR	C38-C26-C25	-3.82	120.32	124.48
44	p	509	CLA	O2A-C1-C2	3.82	122.79	108.11
47	n	204	BCR	C11-C10-C9	-3.81	121.94	127.28
44	B	828	CLA	O2D-CGD-O1D	-3.80	116.45	123.85
51	3	303	LUT	C31-C30-C29	-3.80	121.95	127.28
47	n	204	BCR	C33-C5-C6	-3.80	120.34	124.48
47	f	850	BCR	C33-C5-C6	-3.79	120.34	124.48
47	e	854	BCR	C29-C30-C25	3.79	115.95	110.44
47	B	848	BCR	C7-C8-C9	-3.79	120.62	126.23
47	Q	801	BCR	C8-C9-C10	3.79	124.97	119.01
47	f	849	BCR	C20-C21-C22	-3.79	121.97	127.28
47	I	101	BCR	C16-C17-C18	-3.78	121.97	127.28
44	2	504	CLA	CBD-CHA-C1A	3.78	132.04	128.03
44	B	829	CLA	C3A-C2A-C1A	-3.78	102.43	106.30
47	2	503	BCR	C23-C22-C21	3.77	124.94	119.01
44	e	837	CLA	O2D-CGD-O1D	-3.77	116.50	123.85
53	2	502	XAT	C24-C23-C22	-3.77	103.73	110.79
47	Q	801	BCR	C3-C4-C5	-3.77	107.33	114.06
47	f	846	BCR	C24-C23-C22	-3.77	120.66	126.23
44	A	819	CLA	O2D-CGD-O1D	-3.77	116.51	123.85
47	A	847	BCR	C16-C17-C18	-3.75	122.02	127.28
47	j	803	BCR	C33-C5-C6	-3.74	120.40	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	e	849	BCR	C28-C27-C26	-3.74	107.38	114.06
47	J	102	BCR	C20-C21-C22	-3.74	122.03	127.28
47	f	848	BCR	C33-C5-C6	-3.74	120.40	124.48
49	J	103	DGD	O2G-C1B-C2B	3.74	119.57	111.48
47	A	845	BCR	C28-C27-C26	-3.73	107.40	114.06
47	B	849	BCR	C33-C5-C6	-3.73	120.41	124.48
53	2	502	XAT	C35-C34-C33	-3.73	122.05	127.28
44	A	837	CLA	CAA-C2A-C3A	-3.73	107.68	116.23
47	e	851	BCR	C33-C5-C6	-3.72	120.42	124.48
47	L	305	BCR	C3-C4-C5	-3.72	107.42	114.06
53	s	502	XAT	C26-C27-C28	-3.72	118.13	125.99
47	s	503	BCR	C19-C18-C17	-3.72	113.16	119.01
54	Q	803	SQD	O47-C7-C8	3.71	119.52	111.48
44	K	202	CLA	CAA-C2A-C3A	-3.71	107.72	116.23
47	s	503	BCR	C39-C30-C29	3.71	123.21	108.95
49	B	850	DGD	C4D-C3D-C2D	-3.71	104.31	110.83
47	A	847	BCR	C8-C7-C6	-3.71	117.09	127.00
47	l	101	BCR	C3-C4-C5	-3.71	107.44	114.06
47	F	804	BCR	C28-C27-C26	-3.71	107.44	114.06
44	q	305	CLA	C2A-C1A-CHA	3.71	130.30	123.87
47	A	848	BCR	C38-C26-C25	-3.70	120.44	124.48
53	2	502	XAT	O24-C25-C24	3.70	116.96	113.49
51	s	501	LUT	C21-C26-C27	-3.70	108.58	112.83
47	A	845	BCR	C30-C25-C26	-3.69	117.59	122.64
44	f	805	CLA	CBD-CHA-C1A	3.69	132.29	128.66
47	3	305	BCR	C33-C5-C6	-3.69	120.46	124.48
53	5	304	XAT	O24-C25-C38	3.68	119.17	115.05
44	K	202	CLA	O2D-CGD-O1D	-3.68	116.68	123.85
47	1	503	BCR	C7-C8-C9	-3.68	120.79	126.23
47	2	503	BCR	C39-C30-C29	3.68	123.08	108.95
47	e	851	BCR	C20-C21-C22	-3.67	122.13	127.28
47	o	305	BCR	C7-C8-C9	-3.67	120.81	126.23
47	f	849	BCR	C7-C8-C9	-3.67	120.81	126.23
45	B	843	PQN	C2M-C2-C3	-3.67	118.42	124.45
51	s	501	LUT	C35-C34-C33	-3.66	122.15	127.28
47	q	303	BCR	C33-C5-C6	-3.66	120.49	124.48
44	3	314	CLA	O2D-CGD-O1D	-3.66	116.73	123.85
52	2	513	CHL	C2A-C3A-C4A	-3.66	101.14	103.53
51	r	302	LUT	C27-C28-C29	-3.65	118.48	126.32
47	B	848	BCR	C33-C5-C6	-3.65	120.50	124.48
47	5	302	BCR	C38-C26-C25	-3.64	120.51	124.48
49	f	851	DGD	C2G-O2G-C1B	-3.64	109.08	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	A	838	CLA	O2D-CGD-O1D	-3.64	116.76	123.85
44	B	819	CLA	CAA-C2A-C3A	-3.64	107.89	116.23
47	A	853	BCR	C29-C30-C25	3.64	115.72	110.44
47	j	801	BCR	C27-C26-C25	-3.63	117.79	122.70
44	B	810	CLA	C3A-C2A-C1A	-3.63	102.59	106.30
47	q	303	BCR	C11-C10-C9	-3.63	122.19	127.28
47	B	847	BCR	C38-C26-C25	-3.63	120.53	124.48
53	5	304	XAT	O4-C5-C18	3.62	119.10	115.05
47	I	101	BCR	C11-C10-C9	-3.61	122.21	127.28
47	q	303	BCR	C16-C17-C18	-3.61	122.21	127.28
45	A	841	PQN	C11-C12-C13	-3.61	120.62	126.83
47	e	847	BCR	C33-C5-C6	-3.60	120.55	124.48
47	j	801	BCR	C3-C4-C5	-3.60	107.64	114.06
44	B	822	CLA	O2D-CGD-O1D	-3.60	116.85	123.85
52	p	512	CHL	C1B-CHB-C4A	-3.59	119.01	121.32
44	K	205	CLA	C3B-C4B-NB	-3.59	107.32	110.53
44	r	308	CLA	CAA-C2A-C3A	-3.59	108.01	116.23
44	L	304	CLA	O2D-CGD-O1D	-3.59	116.87	123.85
47	A	848	BCR	C33-C5-C6	-3.58	120.57	124.48
47	n	204	BCR	C3-C4-C5	-3.57	107.68	114.06
44	A	839	CLA	O2D-CGD-O1D	-3.57	116.89	123.85
47	L	305	BCR	C15-C14-C13	-3.57	122.27	127.28
53	2	502	XAT	C4-C3-C2	-3.57	104.12	110.79
44	A	814	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
52	3	315	CHL	CBC-CAC-C3C	-3.57	107.77	112.87
51	r	302	LUT	C18-C5-C6	-3.57	120.59	124.48
47	l	101	BCR	C30-C25-C26	-3.56	117.77	122.64
44	L	303	CLA	O2D-CGD-O1D	-3.55	116.93	123.85
47	B	845	BCR	C28-C27-C26	-3.55	107.73	114.06
46	1	516	LHG	O8-C23-C24	3.55	122.66	111.83
47	e	846	BCR	C24-C23-C22	-3.55	120.99	126.23
44	B	834	CLA	C3B-C4B-NB	-3.54	107.37	110.53
44	2	505	CLA	C3B-C4B-NB	-3.54	107.37	110.53
50	F	806	LMG	O7-C10-C11	3.54	119.14	111.48
47	J	102	BCR	C24-C23-C22	-3.54	121.00	126.23
49	B	850	DGD	C2G-O2G-C1B	-3.54	109.33	117.80
44	B	808	CLA	C3B-C4B-NB	-3.54	107.37	110.53
47	f	848	BCR	C38-C26-C25	-3.53	120.63	124.48
47	q	303	BCR	C21-C20-C19	-3.53	112.97	123.20
53	2	502	XAT	C8-C9-C10	3.53	124.56	119.01
52	5	314	CHL	CBC-CAC-C3C	-3.53	107.82	112.87
44	p	507	CLA	CAA-C2A-C3A	-3.53	108.14	116.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	5	302	BCR	C16-C17-C18	-3.53	122.33	127.28
44	A	830	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
44	B	815	CLA	O2D-CGD-O1D	-3.53	116.98	123.85
47	e	849	BCR	C38-C26-C25	-3.52	120.64	124.48
47	f	850	BCR	C10-C11-C12	-3.52	116.32	124.65
47	f	848	BCR	C20-C21-C22	-3.52	122.34	127.28
44	e	812	CLA	CBD-CHA-C1A	3.52	131.76	128.03
44	A	803	CLA	O2D-CGD-O1D	-3.51	117.01	123.85
44	B	826	CLA	O2D-CGD-O1D	-3.51	117.01	123.85
44	B	820	CLA	C3B-C4B-NB	-3.51	107.40	110.53
51	p	502	LUT	C7-C8-C9	-3.51	121.04	126.23
47	B	847	BCR	C3-C4-C5	-3.51	107.80	114.06
44	A	835	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
47	f	849	BCR	C33-C5-C6	-3.51	120.66	124.48
44	A	813	CLA	C3B-C4B-NB	-3.50	107.41	110.53
44	K	203	CLA	C3A-C2A-C1A	-3.50	102.72	106.30
47	A	847	BCR	C33-C5-C6	-3.49	120.67	124.48
44	5	305	CLA	CMB-C2B-C1B	-3.49	122.47	125.94
49	J	103	DGD	C1E-O6E-C5E	3.49	120.53	113.72
47	r	301	BCR	C28-C27-C26	-3.48	107.85	114.06
52	1	514	CHL	C2A-C3A-C4A	-3.48	101.26	103.53
47	L	306	BCR	C28-C27-C26	-3.48	107.85	114.06
44	A	818	CLA	O2D-CGD-O1D	-3.48	117.07	123.85
44	f	805	CLA	C3A-C2A-C1A	-3.48	102.74	106.30
47	j	801	BCR	C29-C30-C25	3.48	115.49	110.44
47	2	503	BCR	C7-C8-C9	-3.48	121.09	126.23
44	s	508	CLA	CAA-C2A-C3A	-3.48	108.26	116.23
44	A	812	CLA	C3B-C4B-NB	-3.47	107.43	110.53
53	5	304	XAT	C38-C25-C24	3.47	118.14	114.24
47	F	804	BCR	C11-C12-C13	-3.47	116.85	126.36
51	s	501	LUT	C15-C35-C34	-3.47	116.42	123.52
44	A	836	CLA	O2D-CGD-CBD	3.47	117.29	111.23
51	r	302	LUT	C26-C27-C28	-3.47	119.18	124.58
51	5	303	LUT	C7-C8-C9	-3.47	121.11	126.23
47	2	503	BCR	C38-C26-C25	-3.47	120.70	124.48
47	n	204	BCR	C7-C8-C9	-3.47	121.11	126.23
44	5	305	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
47	2	503	BCR	C12-C13-C14	-3.46	113.57	119.01
44	q	306	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
47	B	844	BCR	C28-C27-C26	-3.46	107.89	114.06
51	q	301	LUT	C18-C5-C6	-3.46	120.71	124.48
47	m	103	BCR	C16-C17-C18	-3.46	122.43	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	A	853	BCR	C3-C4-C5	-3.46	107.89	114.06
52	s	512	CHL	CMA-C3A-C4A	-3.46	107.16	114.61
47	f	848	BCR	C23-C24-C25	-3.45	117.77	127.00
52	3	315	CHL	O1D-CGD-CBD	-3.45	119.49	124.72
44	f	810	CLA	C1-C2-C3	-3.45	120.55	126.20
44	p	509	CLA	O2D-CGD-CBD	3.45	117.26	111.23
47	B	844	BCR	C11-C12-C13	-3.44	116.92	126.36
44	A	812	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
47	J	102	BCR	C38-C26-C25	-3.44	120.73	124.48
44	A	824	CLA	C3A-C2A-C1A	-3.44	102.78	106.30
47	m	103	BCR	C15-C14-C13	-3.43	122.47	127.28
47	f	848	BCR	C8-C7-C6	-3.43	117.84	127.00
47	A	848	BCR	C16-C17-C18	-3.43	122.47	127.28
47	l	102	BCR	C33-C5-C6	-3.42	120.75	124.48
47	s	503	BCR	C23-C22-C21	3.42	124.39	119.01
44	A	826	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
47	K	204	BCR	C3-C4-C5	-3.42	107.96	114.06
44	B	802	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
44	e	819	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
44	A	833	CLA	C3A-C2A-C1A	-3.41	102.81	106.30
47	j	803	BCR	C38-C26-C25	-3.41	120.76	124.48
47	A	847	BCR	C20-C21-C22	-3.41	122.50	127.28
47	I	101	BCR	C30-C25-C26	-3.41	117.98	122.64
44	s	504	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
44	B	801	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
47	j	801	BCR	C16-C15-C14	-3.41	116.55	123.52
47	F	801	BCR	C33-C5-C6	-3.41	120.77	124.48
47	B	847	BCR	C23-C24-C25	-3.41	117.90	127.00
47	5	302	BCR	C11-C10-C9	-3.40	122.50	127.28
47	e	851	BCR	C38-C26-C25	-3.40	120.77	124.48
47	B	849	BCR	C10-C11-C12	-3.40	113.35	123.20
47	o	301	BCR	C38-C26-C25	-3.40	120.78	124.48
44	e	808	CLA	O2D-CGD-O1D	-3.40	117.24	123.85
47	s	503	BCR	C16-C15-C14	3.39	130.47	123.52
54	Q	802	SQD	O47-C7-C8	3.39	118.82	111.48
47	B	848	BCR	C3-C4-C5	-3.39	108.00	114.06
44	A	831	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
44	e	818	CLA	O2D-CGD-CBD	3.39	117.16	111.23
47	L	306	BCR	C33-C5-C6	-3.39	120.79	124.48
44	A	827	CLA	C1-C2-C3	-3.38	120.65	126.20
44	A	804	CLA	O2D-CGD-O1D	-3.38	117.26	123.85
44	B	815	CLA	C3B-C4B-NB	-3.38	107.51	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	s	504	CLA	CHB-C1B-C2B	-3.38	123.36	130.51
44	5	305	CLA	CHB-C1B-C2B	-3.38	123.36	130.51
47	A	846	BCR	C33-C5-C6	-3.38	120.80	124.48
44	B	808	CLA	O2D-CGD-O1D	-3.38	117.28	123.85
47	B	846	BCR	C8-C9-C10	3.38	124.32	119.01
44	5	313	CLA	C3B-C4B-NB	-3.37	107.52	110.53
44	1	506	CLA	O2D-CGD-O1D	-3.37	117.28	123.85
44	B	816	CLA	C3B-C4B-NB	-3.37	107.53	110.53
44	K	201	CLA	C3B-C4B-NB	-3.37	107.53	110.53
44	A	825	CLA	O2D-CGD-O1D	-3.37	117.30	123.85
47	3	305	BCR	C16-C17-C18	-3.37	122.56	127.28
47	A	849	BCR	C3-C4-C5	-3.37	108.06	114.06
44	f	840	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
44	p	511	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
47	f	850	BCR	C3-C4-C5	-3.35	108.07	114.06
46	e	844	LHG	C5-O7-C7	-3.35	109.77	117.80
53	5	304	XAT	C15-C14-C13	-3.35	122.58	127.28
51	q	302	LUT	C21-C26-C27	-3.35	108.97	112.83
47	m	103	BCR	C7-C8-C9	-3.35	121.28	126.23
44	A	823	CLA	O2D-CGD-O1D	-3.35	117.34	123.85
47	e	847	BCR	C38-C26-C25	-3.34	120.84	124.48
44	K	205	CLA	C3A-C2A-C1A	-3.34	102.89	106.30
51	q	302	LUT	C15-C14-C13	-3.34	122.60	127.28
45	f	844	PQN	C11-C3-C2	-3.34	119.17	124.89
46	1	516	LHG	C5-O7-C7	-3.34	109.81	117.80
47	L	305	BCR	C20-C21-C22	-3.33	122.60	127.28
44	e	809	CLA	O2D-CGD-CBD	3.33	117.05	111.23
53	s	502	XAT	C24-C23-C22	-3.33	104.56	110.79
47	n	204	BCR	C38-C26-C25	-3.33	120.85	124.48
44	n	202	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
47	f	846	BCR	C16-C17-C18	-3.33	122.61	127.28
47	B	847	BCR	C12-C13-C14	3.33	124.24	119.01
44	A	827	CLA	O2D-CGD-O1D	-3.33	117.38	123.85
47	f	846	BCR	C15-C14-C13	-3.32	122.62	127.28
47	f	848	BCR	C16-C17-C18	-3.32	122.62	127.28
44	A	819	CLA	C3A-C2A-C1A	-3.32	102.90	106.30
47	f	848	BCR	C28-C27-C26	-3.32	108.13	114.06
44	A	832	CLA	CBD-CHA-C1A	3.32	132.39	127.38
47	f	847	BCR	C33-C5-C6	-3.32	120.86	124.48
44	5	313	CLA	C3A-C2A-C1A	-3.32	102.91	106.30
47	j	803	BCR	C23-C24-C25	-3.31	118.15	127.00
44	A	806	CLA	C1-C2-C3	-3.31	120.77	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	2	503	BCR	C10-C11-C12	-3.31	113.61	123.20
44	B	810	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
44	B	827	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
44	B	841	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
47	A	847	BCR	C3-C4-C5	-3.30	108.17	114.06
49	m	104	DGD	O2G-C1B-C2B	3.30	118.62	111.48
44	f	812	CLA	C3A-C2A-C1A	-3.30	102.93	106.30
53	r	303	XAT	C18-C5-C4	3.29	117.94	114.24
44	1	510	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
51	3	304	LUT	C7-C8-C9	-3.29	121.36	126.23
47	l	101	BCR	C16-C17-C18	-3.29	122.66	127.28
44	A	826	CLA	C1-C2-C3	-3.29	120.80	126.20
47	m	103	BCR	C33-C5-C6	-3.29	120.89	124.48
47	f	850	BCR	C15-C14-C13	-3.29	122.66	127.28
49	B	850	DGD	O1G-C1A-C2A	3.29	121.87	111.83
47	5	302	BCR	C34-C9-C10	-3.29	117.49	122.82
44	e	822	CLA	CAA-C2A-C3A	-3.29	108.69	116.23
44	e	813	CLA	C3B-C4B-NB	-3.29	107.59	110.53
44	1	507	CLA	C3B-C4B-NB	-3.29	107.60	110.53
44	B	838	CLA	O2D-CGD-O1D	-3.28	117.45	123.85
47	Q	801	BCR	C27-C26-C25	-3.28	118.27	122.70
47	e	848	BCR	C33-C5-C6	-3.28	120.90	124.48
52	1	517	CHL	CBC-CAC-C3C	-3.28	108.18	112.87
47	e	846	BCR	C20-C19-C18	-3.28	117.38	126.36
47	2	503	BCR	C21-C20-C19	3.28	132.69	123.20
44	A	811	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
47	B	845	BCR	C16-C17-C18	-3.27	122.69	127.28
44	e	838	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
44	A	817	CLA	C3B-C4B-NB	-3.27	107.61	110.53
47	o	305	BCR	C28-C27-C26	-3.27	108.23	114.06
47	m	103	BCR	C38-C26-C25	-3.27	120.92	124.48
47	f	847	BCR	C38-C26-C25	-3.27	120.92	124.48
47	e	847	BCR	C7-C8-C9	-3.26	121.41	126.23
47	n	204	BCR	C24-C23-C22	-3.26	121.42	126.23
47	l	101	BCR	C20-C21-C22	-3.26	122.71	127.28
47	f	849	BCR	C3-C4-C5	-3.26	108.25	114.06
52	s	513	CHL	CBC-CAC-C3C	-3.26	108.21	112.87
52	5	314	CHL	OMC-CMC-C2C	-3.25	119.47	125.12
47	B	849	BCR	C28-C27-C26	-3.25	108.25	114.06
47	e	850	BCR	C20-C19-C18	-3.25	117.44	126.36
44	2	511	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
47	Q	801	BCR	C4-C5-C6	-3.25	118.31	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	F	801	BCR	C20-C19-C18	-3.25	117.45	126.36
44	p	504	CLA	C3B-C4B-NB	-3.25	107.63	110.53
44	J	101	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
44	A	836	CLA	C3B-C4B-NB	-3.24	107.63	110.53
47	f	845	BCR	C28-C27-C26	-3.24	108.27	114.06
44	f	821	CLA	C3B-C4B-NB	-3.24	107.64	110.53
51	3	303	LUT	C10-C11-C12	-3.24	113.81	123.20
44	A	837	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
47	e	854	BCR	C11-C12-C13	-3.24	117.48	126.36
51	p	501	LUT	C18-C5-C6	-3.23	120.96	124.48
44	A	806	CLA	C3B-C4B-NB	-3.23	107.65	110.53
44	B	803	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
51	q	301	LUT	C35-C15-C14	-3.23	116.92	123.52
44	B	812	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
44	A	817	CLA	CMA-C3A-C2A	-3.22	108.83	116.23
44	f	828	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
44	r	311	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
44	5	311	CLA	C3B-C4B-NB	-3.22	107.65	110.53
44	B	817	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
47	A	851	BCR	C2-C1-C6	3.22	115.11	110.44
51	q	302	LUT	C18-C5-C6	-3.21	120.98	124.48
44	2	505	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
47	f	848	BCR	C3-C4-C5	-3.21	108.33	114.06
47	q	303	BCR	C15-C16-C17	-3.21	116.96	123.52
44	f	807	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
44	3	309	CLA	CHB-C1B-C2B	-3.20	123.73	130.51
47	B	846	BCR	C1-C6-C5	-3.20	118.26	122.64
47	r	301	BCR	C16-C17-C18	-3.20	122.78	127.28
44	f	827	CLA	C2A-C3A-C4A	-3.20	102.84	106.24
51	1	502	LUT	C18-C5-C6	-3.20	120.99	124.48
51	r	302	LUT	C21-C26-C27	-3.20	109.15	112.83
47	A	847	BCR	C33-C5-C4	3.20	120.41	113.60
44	e	805	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
44	K	202	CLA	C3B-C4B-NB	-3.19	107.68	110.53
47	m	103	BCR	C3-C4-C5	-3.19	108.36	114.06
47	B	844	BCR	C38-C26-C25	-3.19	121.00	124.48
44	f	826	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
44	e	806	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
47	o	305	BCR	C38-C26-C25	-3.19	121.00	124.48
47	f	848	BCR	C11-C10-C9	-3.19	122.81	127.28
44	3	317	CLA	C3B-C4B-NB	-3.19	107.69	110.53
44	B	833	CLA	C1-C2-C3	-3.19	120.98	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	B	840	CLA	CAA-C2A-C3A	-3.18	108.94	116.23
47	5	302	BCR	C8-C9-C10	3.18	124.01	119.01
44	e	809	CLA	C1-C2-C3	-3.18	121.62	126.76
44	3	301	CLA	C3B-C4B-NB	-3.17	107.70	110.53
44	o	302	CLA	CAA-C2A-C3A	-3.17	108.95	116.23
44	2	509	CLA	C3B-C4B-NB	-3.17	107.70	110.53
44	r	310	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
47	o	301	BCR	C28-C27-C26	-3.17	108.41	114.06
47	A	851	BCR	C20-C21-C22	-3.17	122.84	127.28
44	A	803	CLA	CAA-C2A-C3A	-3.16	108.98	116.23
44	A	842	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
44	j	802	CLA	CAA-C2A-C3A	-3.16	108.98	116.23
51	s	501	LUT	C7-C8-C9	-3.16	121.56	126.23
47	Q	801	BCR	C28-C27-C26	-3.16	108.42	114.06
52	2	515	CHL	CBC-CAC-C3C	-3.16	108.35	112.87
44	3	301	CLA	CAA-C2A-C3A	-3.16	108.99	116.23
47	f	848	BCR	C15-C16-C17	-3.16	117.06	123.52
44	p	504	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
44	B	821	CLA	C3B-C4B-NB	-3.15	107.71	110.53
44	A	818	CLA	C3A-C2A-C1A	-3.15	103.07	106.30
44	B	805	CLA	CAA-C2A-C3A	-3.15	109.00	116.23
44	A	842	CLA	C3B-C4B-NB	-3.15	107.72	110.53
47	K	204	BCR	C15-C14-C13	-3.15	122.86	127.28
44	e	810	CLA	C3B-C4B-NB	-3.15	107.72	110.53
47	I	101	BCR	C33-C5-C6	-3.15	121.05	124.48
44	3	306	CLA	C1C-NC-C4C	3.15	108.12	106.68
44	e	843	CLA	CAB-C3B-C2B	3.15	131.90	123.53
44	A	823	CLA	C3B-C4B-NB	-3.15	107.72	110.53
44	B	842	CLA	C3B-C4B-NB	-3.15	107.72	110.53
47	j	803	BCR	C28-C27-C26	-3.15	108.44	114.06
44	B	819	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
51	2	501	LUT	C18-C5-C6	-3.14	121.05	124.48
44	3	316	CLA	CAA-C2A-C3A	-3.14	109.02	116.23
44	A	803	CLA	C3B-C4B-NB	-3.14	107.73	110.53
44	3	308	CLA	C3B-C4B-NB	-3.14	107.73	110.53
47	A	845	BCR	C38-C26-C27	3.14	120.29	113.60
44	e	808	CLA	C3B-C4B-NB	-3.14	107.73	110.53
44	e	814	CLA	C3B-C4B-NB	-3.14	107.73	110.53
47	B	846	BCR	C33-C5-C6	-3.14	121.06	124.48
44	o	302	CLA	CAB-C3B-C2B	3.14	131.87	123.53
44	e	827	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
46	A	843	LHG	O8-C23-C24	3.13	121.39	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	B	832	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
47	f	846	BCR	C20-C21-C22	-3.13	122.89	127.28
52	2	515	CHL	O1D-CGD-CBD	-3.13	119.98	124.72
44	A	807	CLA	CBD-CHA-C1A	3.13	131.34	128.03
47	n	204	BCR	C28-C27-C26	-3.13	108.48	114.06
44	A	808	CLA	C3B-C4B-NB	-3.12	107.74	110.53
44	f	842	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
44	A	813	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
44	B	824	CLA	C3B-C4B-NB	-3.12	107.75	110.53
44	B	818	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
52	2	513	CHL	C3D-C4D-ND	3.11	116.58	110.42
44	A	822	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
44	5	305	CLA	C3A-C2A-C1A	-3.11	103.12	106.30
44	5	306	CLA	C3B-C4B-NB	-3.11	107.75	110.53
47	e	854	BCR	C3-C4-C5	-3.11	108.51	114.06
44	1	515	CLA	C3B-C4B-NB	-3.11	107.76	110.53
44	r	304	CLA	CAB-C3B-C2B	3.10	131.78	123.53
44	q	310	CLA	CAA-C2A-C3A	-3.10	109.11	116.23
52	1	514	CHL	C1B-CHB-C4A	-3.10	119.33	121.32
52	3	315	CHL	C1C-CHC-C4B	3.10	127.16	116.07
44	A	852	CLA	C3B-C4B-NB	-3.10	107.77	110.53
47	q	303	BCR	C28-C27-C26	-3.10	108.53	114.06
45	A	841	PQN	C2M-C2-C3	-3.09	119.36	124.45
44	e	818	CLA	C2A-C3A-C4A	-3.09	102.95	106.24
44	A	822	CLA	CAA-C2A-C3A	-3.09	109.13	116.23
44	A	835	CLA	C1-C2-C3	-3.09	121.13	126.20
47	l	101	BCR	C15-C16-C17	-3.09	117.19	123.52
44	r	307	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
45	f	844	PQN	C2M-C2-C3	-3.09	119.36	124.45
44	n	205	CLA	C3A-C2A-C1A	-3.09	103.14	106.30
44	B	805	CLA	C3B-C4B-NB	-3.09	107.77	110.53
44	n	202	CLA	C3B-C4B-NB	-3.09	107.77	110.53
45	B	843	PQN	C11-C3-C2	-3.09	119.59	124.89
44	B	814	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
47	f	849	BCR	C15-C16-C17	-3.09	117.20	123.52
44	e	853	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
52	p	517	CHL	O2D-CGD-O1D	-3.09	117.83	123.85
44	B	837	CLA	CAC-C3C-C4C	3.09	128.81	124.79
46	2	517	LHG	O8-C23-C24	3.09	121.25	111.83
47	A	846	BCR	C7-C8-C9	-3.09	121.67	126.23
52	1	512	CHL	OMC-CMC-C2C	-3.09	119.76	125.12
44	e	804	CLA	O2D-CGD-O1D	-3.09	117.84	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	B	827	CLA	CAA-C2A-C3A	-3.08	109.16	116.23
44	A	825	CLA	C3B-C4B-NB	-3.08	107.78	110.53
52	5	317	CHL	C4C-C3C-C2C	-3.08	101.32	108.42
47	L	306	BCR	C16-C17-C18	-3.08	122.96	127.28
44	e	817	CLA	CAA-C2A-C3A	-3.08	109.17	116.23
44	1	510	CLA	C3B-C4B-NB	-3.08	107.78	110.53
44	q	312	CLA	C3B-C4B-NB	-3.08	107.78	110.53
47	l	101	BCR	C27-C26-C25	-3.07	118.56	122.70
44	s	504	CLA	CMB-C2B-C1B	-3.07	122.88	125.94
52	2	513	CHL	C1C-CHC-C4B	3.07	127.05	116.07
44	f	834	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
44	A	838	CLA	C3B-C4B-NB	-3.07	107.79	110.53
52	p	512	CHL	O1D-CGD-CBD	-3.07	120.07	124.72
44	1	513	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
44	A	829	CLA	C3B-C4B-NB	-3.06	107.79	110.53
47	2	503	BCR	C37-C22-C21	-3.06	117.86	122.82
44	B	823	CLA	C3B-C4B-NB	-3.06	107.80	110.53
44	B	842	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
51	q	302	LUT	C8-C7-C6	-3.06	118.82	127.00
47	5	302	BCR	C35-C13-C12	3.06	122.76	118.09
52	2	513	CHL	CHA-C1A-NA	3.06	124.89	122.15
44	e	803	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
47	f	846	BCR	C28-C27-C26	-3.06	108.61	114.06
46	e	845	LHG	C5-O7-C7	-3.05	110.49	117.80
44	2	507	CLA	C3B-C4B-NB	-3.05	107.81	110.53
44	r	306	CLA	C3B-C4B-NB	-3.05	107.81	110.53
44	B	811	CLA	C3B-C4B-NB	-3.05	107.81	110.53
44	e	834	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
47	r	301	BCR	C38-C26-C25	-3.05	121.16	124.48
44	f	839	CLA	CAA-C2A-C3A	-3.05	109.24	116.23
44	e	828	CLA	C3B-C4B-NB	-3.05	107.81	110.53
44	p	505	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
47	j	803	BCR	C20-C21-C22	-3.05	123.00	127.28
52	3	302	CHL	O1D-CGD-CBD	-3.05	120.10	124.72
51	q	302	LUT	C35-C15-C14	-3.05	117.29	123.52
44	f	833	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
43	e	801	CL0	CBC-CAC-C3C	-3.05	108.51	112.87
44	f	831	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
44	p	505	CLA	C2A-C1A-CHA	3.04	129.15	123.87
47	e	847	BCR	C23-C24-C25	-3.04	118.87	127.00
44	e	807	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
52	2	516	CHL	C1C-CHC-C4B	3.04	126.95	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	A	807	CLA	C3A-C2A-C1A	-3.04	103.19	106.30
47	s	503	BCR	C27-C26-C25	-3.04	118.59	122.70
47	A	845	BCR	C11-C10-C9	-3.04	123.01	127.28
44	B	809	CLA	C3B-C4B-NB	-3.04	107.82	110.53
44	s	504	CLA	CAA-C2A-C3A	-3.04	109.26	116.23
47	e	850	BCR	C38-C26-C25	-3.04	121.17	124.48
47	e	850	BCR	C8-C9-C10	3.04	123.79	119.01
44	e	841	CLA	C3B-C4B-NB	-3.04	107.82	110.53
52	r	314	CHL	C1C-CHC-C4B	3.04	126.94	116.07
51	s	501	LUT	C18-C5-C6	-3.04	121.17	124.48
44	2	504	CLA	C3A-C4A-CHB	-3.04	120.19	123.91
47	f	847	BCR	C8-C9-C10	3.04	123.78	119.01
44	B	811	CLA	CAA-C2A-C3A	-3.03	104.80	113.00
47	B	846	BCR	C3-C4-C5	-3.03	108.65	114.06
44	B	830	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
47	Q	801	BCR	C33-C5-C4	3.03	120.06	113.60
44	A	819	CLA	C3B-C4B-NB	-3.03	107.82	110.53
44	f	817	CLA	C3B-C4B-NB	-3.03	107.83	110.53
44	B	839	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
47	f	847	BCR	C34-C9-C10	-3.03	117.91	122.82
44	e	819	CLA	C3B-C4B-NB	-3.02	107.83	110.53
47	B	852	BCR	C3-C4-C5	-3.02	108.66	114.06
44	f	819	CLA	C3B-C4B-NB	-3.02	107.83	110.53
47	e	850	BCR	C1-C6-C5	-3.02	118.51	122.64
43	A	801	CL0	CBC-CAC-C3C	-3.02	108.55	112.87
47	e	847	BCR	C28-C27-C26	-3.02	108.67	114.06
44	r	304	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
53	5	304	XAT	C24-C23-C22	-3.02	105.15	110.79
44	3	311	CLA	C1-C2-C3	-3.02	121.88	126.76
47	f	847	BCR	C23-C22-C21	3.02	123.75	119.01
44	f	816	CLA	C3B-C4B-NB	-3.02	107.84	110.53
47	B	849	BCR	C15-C14-C13	-3.01	123.05	127.28
47	A	851	BCR	C38-C26-C27	3.01	120.02	113.60
44	L	301	CLA	C3B-C4B-NB	-3.01	107.84	110.53
44	L	301	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
52	3	302	CHL	O2D-CGD-O1D	-3.01	117.99	123.85
44	m	102	CLA	C3B-C4B-NB	-3.01	107.84	110.53
44	f	812	CLA	C2A-C1A-CHA	3.01	127.37	122.71
44	r	317	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
53	5	304	XAT	C18-C5-C4	3.01	117.62	114.24
47	J	102	BCR	C33-C5-C6	-3.01	121.20	124.48
44	e	811	CLA	O2D-CGD-O1D	-3.00	118.00	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	5	317	CHL	C1B-CHB-C4A	3.00	123.17	120.23
54	Q	803	SQD	O48-C23-C24	3.00	120.99	111.83
44	e	837	CLA	C3B-C4B-NB	-3.00	107.85	110.53
44	3	317	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
47	e	847	BCR	C15-C14-C13	-3.00	123.07	127.28
47	f	850	BCR	C28-C27-C26	-3.00	108.71	114.06
44	B	836	CLA	C3B-C4B-NB	-3.00	107.85	110.53
47	J	102	BCR	C38-C26-C27	3.00	119.98	113.60
46	A	843	LHG	C5-O7-C7	-3.00	110.63	117.80
44	e	833	CLA	C3B-C4B-NB	-3.00	107.86	110.53
44	q	314	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
44	q	311	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
44	f	801	CLA	CAB-C3B-C2B	2.99	131.47	123.53
44	5	305	CLA	C1B-NB-C4B	2.99	108.41	106.31
47	Q	801	BCR	C34-C9-C10	-2.99	117.97	122.82
44	B	804	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
44	B	833	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
44	f	827	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
44	L	303	CLA	CHB-C4A-NA	2.99	128.71	124.40
44	r	304	CLA	CMB-C2B-C3B	2.99	131.47	123.53
44	B	802	CLA	O2D-CGD-CBD	2.99	116.45	111.23
47	3	305	BCR	C3-C4-C5	-2.99	108.73	114.06
44	f	843	CLA	CBD-CHA-C1A	2.98	131.88	127.38
44	f	823	CLA	CAA-C2A-C3A	-2.98	109.39	116.23
47	B	844	BCR	C33-C5-C6	-2.98	121.23	124.48
44	3	317	CLA	CAA-C2A-C3A	-2.98	109.39	116.23
47	f	846	BCR	C8-C9-C10	2.98	123.70	119.01
44	B	809	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
44	1	505	CLA	C3B-C4B-NB	-2.98	107.87	110.53
44	A	832	CLA	CHB-C4A-NA	2.98	128.69	124.40
47	A	847	BCR	C38-C26-C25	-2.98	121.24	124.48
47	B	852	BCR	C16-C17-C18	-2.98	123.11	127.28
44	e	831	CLA	C3B-C4B-NB	-2.98	107.87	110.53
47	e	851	BCR	C24-C23-C22	-2.97	121.83	126.23
44	2	514	CLA	C3B-C4B-NB	-2.97	107.88	110.53
52	5	315	CHL	OMC-CMC-C2C	-2.97	119.96	125.12
47	L	306	BCR	C33-C5-C4	2.97	119.93	113.60
44	B	807	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
47	B	848	BCR	C20-C21-C22	-2.97	123.11	127.28
47	e	850	BCR	C34-C9-C10	-2.97	118.00	122.82
44	e	822	CLA	C3B-C4B-NB	-2.97	107.88	110.53
51	3	303	LUT	C18-C5-C6	-2.97	121.24	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	A	840	CLA	C3B-C4B-NB	-2.97	107.88	110.53
53	s	502	XAT	C11-C10-C9	-2.97	123.12	127.28
44	e	805	CLA	C3B-C4B-NB	-2.97	107.88	110.53
52	s	512	CHL	O1D-CGD-CBD	-2.96	120.23	124.72
52	1	517	CHL	C1C-CHC-C4B	2.96	126.68	116.07
52	3	315	CHL	OMC-CMC-C2C	-2.96	119.97	125.12
44	A	820	CLA	C3B-C4B-NB	-2.96	107.89	110.53
44	f	839	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
44	B	813	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
44	A	839	CLA	C3B-C4B-NB	-2.96	107.89	110.53
43	e	801	CL0	C4C-CHD-C1D	2.96	126.66	116.07
51	q	302	LUT	C7-C8-C9	-2.96	121.86	126.23
52	5	317	CHL	C1C-CHC-C4B	2.96	126.66	116.07
44	1	506	CLA	C3B-C4B-NB	-2.96	107.89	110.53
44	f	812	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
47	o	301	BCR	C24-C23-C22	-2.96	121.86	126.23
44	f	841	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
43	A	801	CL0	C4C-CHD-C1D	2.96	126.64	116.07
47	f	846	BCR	C3-C4-C5	-2.96	108.79	114.06
51	5	303	LUT	C16-C1-C6	-2.95	105.61	110.24
44	A	816	CLA	C3B-C4B-NB	-2.95	107.90	110.53
44	r	312	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
44	e	807	CLA	C3B-C4B-NB	-2.95	107.90	110.53
47	f	847	BCR	C28-C27-C26	-2.95	108.80	114.06
47	B	848	BCR	C11-C10-C9	-2.95	123.14	127.28
47	3	305	BCR	C7-C8-C9	-2.95	121.88	126.23
44	A	814	CLA	C3B-C4B-NB	-2.95	107.90	110.53
44	e	843	CLA	CMB-C2B-C3B	2.94	131.36	123.53
47	Q	801	BCR	C38-C26-C27	2.94	119.88	113.60
47	2	503	BCR	C36-C18-C19	2.94	122.58	118.09
44	e	835	CLA	CBD-CHA-C1A	2.94	131.82	127.38
44	5	313	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
44	f	843	CLA	C3B-C4B-NB	-2.94	107.90	110.53
44	B	835	CLA	C3B-C4B-NB	-2.94	107.91	110.53
47	q	303	BCR	C23-C24-C25	-2.94	119.15	127.00
44	A	820	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
44	B	836	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
44	f	809	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
44	r	305	CLA	C3B-C4B-NB	-2.93	107.91	110.53
53	r	303	XAT	C10-C11-C12	-2.93	114.70	123.20
47	p	503	BCR	C40-C30-C25	-2.93	105.64	110.24
52	5	314	CHL	C1C-CHC-C4B	2.93	126.56	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	1	502	LUT	C3-C4-C5	-2.93	104.88	112.18
44	3	318	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
44	f	817	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
47	B	852	BCR	C24-C23-C22	-2.93	121.90	126.23
44	e	811	CLA	C3B-C4B-NB	-2.93	107.92	110.53
51	2	501	LUT	C30-C31-C32	-2.93	114.71	123.20
53	5	304	XAT	C6-C7-C8	-2.93	119.80	125.99
44	q	314	CLA	C3A-C2A-C1A	-2.93	103.31	106.30
44	F	803	CLA	CAA-C2A-C3A	-2.93	109.52	116.23
44	e	839	CLA	C3B-C4B-NB	-2.92	107.92	110.53
52	5	315	CHL	O1D-CGD-CBD	-2.92	120.29	124.72
52	s	513	CHL	O1D-CGD-CBD	-2.92	120.29	124.72
44	1	506	CLA	C1-C2-C3	-2.92	121.41	126.20
52	3	302	CHL	C1C-CHC-C4B	2.92	126.53	116.07
44	f	813	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
44	f	834	CLA	C3B-C4B-NB	-2.92	107.92	110.53
44	e	830	CLA	C1-C2-C3	-2.92	122.04	126.76
44	A	805	CLA	C3B-C4B-NB	-2.92	107.92	110.53
44	B	827	CLA	C3B-C4B-NB	-2.92	107.92	110.53
44	n	201	CLA	C3B-C4B-NB	-2.92	107.92	110.53
47	j	801	BCR	C10-C11-C12	-2.92	114.74	123.20
44	f	840	CLA	CAA-C2A-C3A	-2.92	109.54	116.23
50	F	806	LMG	O8-C28-C29	2.92	120.73	111.83
44	e	839	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
44	1	504	CLA	C3B-C4B-NB	-2.92	107.92	110.53
44	f	838	CLA	C3B-C4B-NB	-2.92	107.92	110.53
44	e	822	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
44	5	310	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
44	e	823	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
44	e	834	CLA	C3B-C4B-NB	-2.92	107.93	110.53
47	o	301	BCR	C15-C16-C17	-2.92	117.55	123.52
44	3	309	CLA	CMB-C2B-C1B	-2.92	123.04	125.94
47	f	846	BCR	C34-C9-C10	-2.92	118.09	122.82
44	K	201	CLA	CHB-C4A-NA	2.92	128.61	124.40
44	m	102	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
49	B	850	DGD	O6D-C1D-O3G	-2.91	103.16	110.04
44	B	835	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
44	f	823	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
44	r	304	CLA	C3A-C2A-C1A	-2.91	103.32	106.30
44	e	823	CLA	CMB-C2B-C3B	2.91	131.27	123.53
53	5	304	XAT	C4-C3-C2	-2.91	105.34	110.79
44	f	832	CLA	O2D-CGD-O1D	-2.91	118.18	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	s	503	BCR	C10-C11-C12	-2.91	114.77	123.20
44	5	307	CLA	C3B-C4B-NB	-2.91	107.93	110.53
44	q	316	CLA	C3B-C4B-NB	-2.91	107.93	110.53
47	B	846	BCR	C38-C26-C25	-2.91	121.31	124.48
44	F	802	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
44	3	314	CLA	C3B-C4B-NB	-2.91	107.94	110.53
44	A	840	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
47	A	849	BCR	C15-C14-C13	-2.90	123.20	127.28
44	B	821	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
47	f	847	BCR	C37-C22-C21	-2.90	118.11	122.82
44	A	816	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
52	1	514	CHL	O1D-CGD-CBD	-2.90	120.32	124.72
47	e	848	BCR	C3-C4-C5	-2.90	108.88	114.06
44	e	823	CLA	CAB-C3B-C2B	2.90	131.24	123.53
44	f	823	CLA	C3B-C4B-NB	-2.90	107.94	110.53
52	2	512	CHL	C1C-CHC-C4B	2.90	126.45	116.07
47	3	305	BCR	C20-C21-C22	-2.90	123.21	127.28
47	m	103	BCR	C38-C26-C27	2.90	119.78	113.60
47	s	503	BCR	C21-C20-C19	2.90	131.60	123.20
44	s	514	CLA	C3A-C2A-C1A	-2.90	103.34	106.30
44	s	507	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
44	B	804	CLA	C3B-C4B-NB	-2.90	107.94	110.53
44	p	504	CLA	CHB-C4A-NA	2.90	128.58	124.40
52	2	515	CHL	C1C-CHC-C4B	2.90	126.43	116.07
44	r	306	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
44	r	308	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
51	5	303	LUT	C35-C15-C14	-2.89	117.60	123.52
47	s	503	BCR	C37-C22-C21	-2.89	118.13	122.82
44	r	312	CLA	C3B-C4B-NB	-2.89	107.95	110.53
47	e	847	BCR	C8-C7-C6	-2.89	119.28	127.00
46	A	844	LHG	C5-O7-C7	-2.89	110.88	117.80
44	p	511	CLA	C3A-C4A-CHB	-2.89	120.37	123.91
51	q	302	LUT	C19-C9-C8	2.89	122.50	118.09
44	3	313	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
44	o	304	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
51	1	502	LUT	C8-C7-C6	-2.89	119.28	127.00
44	q	306	CLA	C3B-C4B-NB	-2.89	107.95	110.53
44	q	316	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
44	e	809	CLA	C3B-C4B-NB	-2.89	107.95	110.53
44	f	820	CLA	C3B-C4B-NB	-2.89	107.95	110.53
47	s	503	BCR	C7-C8-C9	-2.88	121.97	126.23
44	B	807	CLA	C3B-C4B-NB	-2.88	107.95	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	f	835	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
47	K	204	BCR	C7-C8-C9	-2.88	121.97	126.23
44	2	511	CLA	CHB-C4A-NA	2.88	128.56	124.40
44	B	841	CLA	C3B-C4B-NB	-2.88	107.96	110.53
53	2	502	XAT	C38-C25-C24	2.88	117.48	114.24
44	B	818	CLA	C3B-C4B-NB	-2.88	107.96	110.53
44	m	101	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
44	r	315	CLA	CAA-C2A-C3A	-2.88	109.64	116.23
44	2	510	CLA	C3B-C4B-NB	-2.88	107.96	110.53
44	1	511	CLA	C3B-C4B-NB	-2.87	107.97	110.53
44	B	835	CLA	C1-C2-C3	-2.87	121.49	126.20
44	j	802	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
44	s	509	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
52	2	515	CHL	OMC-CMC-C2C	-2.87	120.14	125.12
47	B	845	BCR	C27-C26-C25	-2.87	118.83	122.70
44	A	821	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
44	e	826	CLA	CAB-C3B-C2B	2.87	131.15	123.53
44	f	818	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
51	1	501	LUT	C7-C8-C9	-2.87	122.00	126.23
47	L	305	BCR	C29-C30-C25	2.87	114.60	110.44
51	3	303	LUT	C15-C35-C34	-2.87	117.66	123.52
47	n	204	BCR	C15-C14-C13	-2.87	123.26	127.28
47	e	846	BCR	C8-C7-C6	-2.86	119.35	127.00
49	B	850	DGD	C1D-O6D-C5D	2.86	119.31	113.72
44	B	822	CLA	C3B-C4B-NB	-2.86	107.97	110.53
44	3	309	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
44	r	309	CLA	C1-C2-C3	-2.86	122.13	126.76
44	s	508	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
47	A	846	BCR	C38-C26-C25	-2.86	121.36	124.48
44	J	101	CLA	C3B-C4B-NB	-2.86	107.98	110.53
44	A	834	CLA	C3B-C4B-NB	-2.86	107.98	110.53
44	q	309	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
44	B	828	CLA	CAA-C2A-C3A	-2.86	109.68	116.23
44	e	833	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
44	f	810	CLA	C3B-C4B-NB	-2.86	107.98	110.53
44	q	307	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
44	f	824	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
44	o	302	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
44	e	840	CLA	C3B-C4B-NB	-2.85	107.98	110.53
53	r	303	XAT	C31-C30-C29	-2.85	123.28	127.28
44	B	824	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
44	e	832	CLA	O2D-CGD-O1D	-2.85	118.30	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	p	508	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
44	f	814	CLA	C3B-C4B-NB	-2.85	107.98	110.53
49	B	850	DGD	O2G-C1B-O1B	-2.85	117.04	123.70
47	s	503	BCR	C4-C5-C6	-2.85	118.85	122.70
44	q	305	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
44	5	308	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
44	f	837	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
44	q	312	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
44	p	507	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
44	e	840	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
47	F	801	BCR	C10-C11-C12	-2.85	114.95	123.20
44	A	810	CLA	C3B-C4B-NB	-2.85	107.99	110.53
44	f	818	CLA	C3B-C4B-NB	-2.85	107.99	110.53
47	f	850	BCR	C16-C15-C14	-2.85	117.70	123.52
47	e	850	BCR	C4-C5-C6	-2.84	118.86	122.70
47	e	850	BCR	C28-C27-C26	-2.84	108.98	114.06
44	1	509	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
44	q	308	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
47	B	852	BCR	C38-C26-C27	2.84	119.66	113.60
44	B	806	CLA	C3B-C4B-NB	-2.84	107.99	110.53
44	B	819	CLA	C3B-C4B-NB	-2.84	107.99	110.53
44	B	831	CLA	C3B-C4B-NB	-2.84	107.99	110.53
44	2	508	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
47	l	102	BCR	C10-C11-C12	-2.84	114.96	123.20
44	e	852	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
47	F	804	BCR	C16-C17-C18	-2.84	123.29	127.28
44	2	511	CLA	C3A-C2A-C1A	-2.84	103.39	106.30
51	2	501	LUT	C3-C4-C5	-2.84	105.11	112.18
44	A	820	CLA	CHB-C4A-NA	2.84	128.50	124.40
44	F	802	CLA	C3B-C4B-NB	-2.84	108.00	110.53
44	e	814	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
47	e	854	BCR	C27-C26-C25	-2.84	118.87	122.70
53	2	502	XAT	C15-C14-C13	-2.84	123.30	127.28
44	A	834	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
44	2	511	CLA	O2D-CGD-CBD	2.84	116.19	111.23
44	A	811	CLA	C3A-C2A-C1A	-2.84	103.40	106.30
44	B	840	CLA	C3B-C4B-NB	-2.84	108.00	110.53
44	o	302	CLA	CMB-C2B-C3B	2.84	131.07	123.53
47	K	204	BCR	C10-C11-C12	-2.83	114.99	123.20
52	3	315	CHL	CMA-C3A-C4A	-2.83	108.51	114.61
44	e	828	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
51	q	302	LUT	C30-C31-C32	-2.83	115.00	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	l	102	BCR	C29-C30-C25	2.83	114.55	110.44
47	Q	801	BCR	C30-C25-C26	-2.83	118.77	122.64
44	f	836	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
44	e	802	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
44	f	827	CLA	C3B-C4B-NB	-2.83	108.00	110.53
52	s	513	CHL	C1C-CHC-C4B	2.83	126.19	116.07
44	2	507	CLA	C3A-C2A-C1A	-2.83	103.41	106.30
47	Q	801	BCR	C12-C11-C10	2.83	129.30	123.52
44	5	312	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
44	e	806	CLA	C3B-C4B-NB	-2.83	108.01	110.53
44	B	834	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
44	L	302	CLA	C2A-C3A-C4A	-2.82	103.24	106.24
47	B	847	BCR	C28-C27-C26	-2.82	109.02	114.06
44	e	843	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
47	J	102	BCR	C11-C10-C9	-2.82	123.32	127.28
47	A	851	BCR	C7-C8-C9	-2.82	122.06	126.23
44	3	306	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
47	r	301	BCR	C24-C23-C22	-2.82	122.06	126.23
44	e	833	CLA	CAA-C2A-C3A	-2.82	109.77	116.23
44	f	822	CLA	C3B-C4B-NB	-2.82	108.02	110.53
52	s	517	CHL	C1C-CHC-C4B	2.82	126.15	116.07
44	e	812	CLA	C3A-C2A-C1A	-2.82	103.42	106.30
44	f	820	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
52	5	315	CHL	C1C-CHC-C4B	2.82	126.14	116.07
52	1	517	CHL	O1D-CGD-CBD	-2.82	120.45	124.72
52	s	513	CHL	O2A-CGA-CBA	2.81	120.42	111.83
44	r	315	CLA	C3B-C4B-NB	-2.81	108.02	110.53
44	e	841	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
47	L	305	BCR	C38-C26-C27	2.81	119.59	113.60
53	r	303	XAT	C4-C3-C2	-2.81	105.53	110.79
44	1	511	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
44	e	831	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
44	B	817	CLA	C3B-C4B-NB	-2.81	108.02	110.53
44	f	825	CLA	C3B-C4B-NB	-2.81	108.02	110.53
44	q	306	CLA	CAA-C2A-C3A	-2.81	109.78	116.23
44	A	829	CLA	O2D-CGD-CBD	2.81	116.15	111.23
47	F	804	BCR	C38-C26-C25	-2.81	121.42	124.48
44	A	839	CLA	CHB-C4A-NA	2.81	128.46	124.40
47	L	306	BCR	C21-C20-C19	-2.81	115.06	123.20
44	p	510	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
44	s	514	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
44	B	829	CLA	C3B-C4B-NB	-2.81	108.02	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	A	847	BCR	C4-C5-C6	-2.81	118.91	122.70
53	r	303	XAT	C24-C23-C22	-2.81	105.54	110.79
44	f	841	CLA	C3B-C4B-NB	-2.81	108.03	110.53
44	A	803	CLA	O2D-CGD-CBD	2.80	116.13	111.23
44	o	303	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
44	e	806	CLA	CAA-C2A-C3A	-2.80	109.80	116.23
51	r	302	LUT	C31-C32-C33	-2.80	118.68	126.36
44	A	835	CLA	CHB-C4A-NA	2.80	128.44	124.40
44	B	822	CLA	CHB-C4A-NA	2.80	128.44	124.40
47	B	845	BCR	C8-C9-C10	2.80	123.41	119.01
52	s	517	CHL	O2D-CGD-O1D	-2.80	118.40	123.85
44	r	307	CLA	C3B-C4B-NB	-2.80	108.03	110.53
44	e	826	CLA	CMB-C2B-C3B	2.80	130.97	123.53
44	f	826	CLA	CHB-C4A-NA	2.80	128.44	124.40
44	e	837	CLA	O2D-CGD-CBD	2.80	116.12	111.23
44	B	831	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
44	f	819	CLA	CAA-C2A-C3A	-2.80	109.82	116.23
51	3	303	LUT	C22-C23-C24	2.80	115.34	111.18
44	A	840	CLA	CAA-C2A-C3A	-2.80	109.82	116.23
44	B	838	CLA	O2D-CGD-CBD	2.80	116.12	111.23
44	s	504	CLA	CHB-C4A-NA	2.80	128.44	124.40
44	3	311	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
44	A	807	CLA	C3B-C4B-NB	-2.79	108.04	110.53
44	f	820	CLA	C1-C2-C3	-2.79	122.24	126.76
44	f	819	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
44	A	830	CLA	C3B-C4B-NB	-2.79	108.04	110.53
47	L	306	BCR	C38-C26-C25	-2.79	121.44	124.48
46	2	517	LHG	C5-O7-C7	-2.79	111.12	117.80
47	A	848	BCR	C38-C26-C27	2.79	119.54	113.60
52	1	517	CHL	O2D-CGD-O1D	-2.79	118.42	123.85
47	j	803	BCR	C24-C23-C22	-2.79	122.11	126.23
44	5	316	CLA	CAA-C2A-C3A	-2.79	109.84	116.23
47	F	804	BCR	C21-C20-C19	-2.79	115.12	123.20
44	B	837	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
43	e	801	CL0	O2D-CGD-CBD	2.79	120.73	113.90
47	A	847	BCR	C7-C8-C9	-2.78	122.12	126.23
52	1	514	CHL	OMC-CMC-C2C	-2.78	120.29	125.12
44	r	304	CLA	CAB-C3B-C4B	-2.78	121.18	125.42
44	3	306	CLA	CHB-C4A-NA	2.78	128.41	124.40
52	1	512	CHL	CBC-CAC-C3C	-2.78	108.89	112.87
44	e	825	CLA	C3B-C4B-NB	-2.78	108.05	110.53
43	A	801	CL0	C6-C5-C3	-2.78	106.69	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	B	846	BCR	C34-C9-C10	-2.78	118.31	122.82
44	B	823	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
44	3	301	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
44	e	804	CLA	C3B-C4B-NB	-2.78	108.05	110.53
47	o	301	BCR	C20-C21-C22	-2.78	123.38	127.28
51	q	301	LUT	C18-C5-C4	2.78	119.53	114.42
44	B	814	CLA	CAA-C2A-C3A	-2.78	109.86	116.23
44	f	801	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
47	q	303	BCR	C36-C18-C19	2.78	122.33	118.09
44	B	829	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
44	1	515	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
44	e	841	CLA	CAA-C2A-C3A	-2.78	109.86	116.23
43	e	801	CL0	C6-C5-C3	-2.78	106.70	113.47
43	A	801	CL0	O2D-CGD-CBD	2.78	120.71	113.90
44	f	832	CLA	C3B-C4B-NB	-2.78	108.05	110.53
53	r	303	XAT	C38-C25-C24	2.78	117.36	114.24
44	1	511	CLA	CHB-C4A-NA	2.78	128.41	124.40
47	e	854	BCR	C7-C8-C9	-2.78	122.13	126.23
44	s	505	CLA	C3B-C4B-NB	-2.78	108.05	110.53
47	m	103	BCR	C8-C7-C6	-2.78	119.58	127.00
44	A	834	CLA	CAA-C2A-C3A	-2.78	109.87	116.23
47	j	803	BCR	C38-C26-C27	2.78	119.51	113.60
47	f	846	BCR	C10-C11-C12	-2.78	115.16	123.20
44	e	816	CLA	C3B-C4B-NB	-2.77	108.05	110.53
44	B	826	CLA	C3B-C4B-NB	-2.77	108.05	110.53
47	B	847	BCR	C33-C5-C4	2.77	119.51	113.60
47	e	848	BCR	C8-C7-C6	-2.77	119.59	127.00
44	L	303	CLA	C3B-C4B-NB	-2.77	108.06	110.53
44	f	829	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
44	r	307	CLA	C1-C2-C3	-2.77	121.66	126.20
50	F	805	LMG	O8-C28-C29	2.77	119.56	111.15
47	o	305	BCR	C20-C19-C18	-2.77	118.77	126.36
44	e	825	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
47	f	850	BCR	C8-C9-C10	-2.77	118.32	124.72
44	1	508	CLA	C3A-C2A-C1A	-2.77	103.47	106.30
44	f	806	CLA	C3B-C4B-NB	-2.77	108.06	110.53
52	p	517	CHL	O1D-CGD-CBD	-2.77	120.53	124.72
44	3	308	CLA	CHB-C4A-NA	2.77	128.39	124.40
44	q	314	CLA	CHB-C4A-NA	2.76	128.39	124.40
44	f	811	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
44	2	506	CLA	C3B-C4B-NB	-2.76	108.06	110.53
44	f	837	CLA	C3B-C4B-NB	-2.76	108.06	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	J	102	BCR	C29-C30-C25	2.76	114.45	110.44
50	m	105	LMG	O8-C28-C29	2.76	119.53	111.15
52	1	514	CHL	CBC-CAC-C3C	-2.76	108.92	112.87
52	5	317	CHL	CAC-C3C-C4C	2.76	129.70	124.73
49	B	850	DGD	O3G-C3G-C2G	-2.76	104.11	110.82
44	e	810	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
47	A	851	BCR	C29-C30-C25	2.76	114.44	110.44
44	s	506	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
44	1	504	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
47	e	848	BCR	C33-C5-C4	2.76	119.47	113.60
44	f	832	CLA	C3A-C2A-C1A	-2.76	103.48	106.30
47	A	847	BCR	C24-C23-C22	-2.76	122.16	126.23
47	f	849	BCR	C8-C7-C6	-2.75	119.64	127.00
44	A	837	CLA	CMB-C2B-C1B	-2.75	121.23	125.42
47	f	848	BCR	C33-C5-C4	2.75	119.47	113.60
44	A	831	CLA	C1-C2-C3	-2.75	121.69	126.20
46	p	516	LHG	C5-O7-C7	-2.75	111.21	117.80
44	3	312	CLA	C3B-C4B-NB	-2.75	108.07	110.53
44	A	828	CLA	C3B-C4B-NB	-2.75	108.08	110.53
44	r	315	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
51	2	501	LUT	C18-C5-C4	2.75	119.47	114.42
44	A	837	CLA	C3B-C4B-NB	-2.75	108.08	110.53
44	B	806	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
44	B	830	CLA	C3B-C4B-NB	-2.75	108.08	110.53
44	5	308	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
47	q	303	BCR	C24-C23-C22	-2.75	122.17	126.23
44	2	509	CLA	CHB-C4A-NA	2.74	128.36	124.40
47	B	846	BCR	C33-C5-C4	2.74	119.44	113.60
47	B	847	BCR	C36-C18-C19	2.74	122.28	118.09
44	e	820	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
52	q	313	CHL	OMC-CMC-C2C	-2.74	120.36	125.12
44	f	815	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
52	2	516	CHL	CMB-C2B-C3B	2.74	130.43	124.69
47	e	850	BCR	C10-C11-C12	-2.74	115.26	123.20
44	1	507	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
44	f	808	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
44	A	802	CLA	C3B-C4B-NB	-2.74	108.09	110.53
44	3	313	CLA	CHB-C4A-NA	2.74	128.35	124.40
47	l	101	BCR	C38-C26-C27	2.74	119.43	113.60
44	e	819	CLA	CHB-C4A-NA	2.74	128.35	124.40
47	I	101	BCR	C28-C27-C26	-2.74	109.17	114.06
47	B	847	BCR	C1-C6-C5	-2.74	118.90	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	f	810	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
44	p	509	CLA	C1D-ND-C4D	-2.74	104.39	106.31
47	e	847	BCR	C3-C4-C5	-2.73	109.18	114.06
44	f	830	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
52	3	302	CHL	CBC-CAC-C3C	-2.73	108.96	112.87
44	F	803	CLA	C3B-C4B-NB	-2.73	108.09	110.53
44	f	803	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
44	A	842	CLA	C1-C2-C3	-2.73	122.34	126.76
47	A	847	BCR	C11-C10-C9	-2.73	123.45	127.28
52	1	512	CHL	C1C-CHC-C4B	2.73	125.84	116.07
44	B	833	CLA	CHB-C4A-NA	2.73	128.34	124.40
44	p	506	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
47	s	503	BCR	C2-C1-C6	2.73	114.40	110.44
47	I	101	BCR	C15-C16-C17	-2.73	117.93	123.52
47	B	846	BCR	C35-C13-C14	-2.73	118.39	122.82
44	f	805	CLA	CHB-C4A-NA	2.73	128.34	124.40
47	B	847	BCR	C35-C13-C14	-2.73	118.40	122.82
44	1	505	CLA	O2D-CGD-O1D	-2.72	118.54	123.85
44	f	841	CLA	CAA-C2A-C3A	-2.72	109.98	116.23
44	f	801	CLA	CMB-C2B-C3B	2.72	130.77	123.53
44	e	825	CLA	CAA-C2A-C3A	-2.72	109.98	116.23
47	f	847	BCR	C33-C5-C4	2.72	119.40	113.60
47	A	853	BCR	C32-C1-C6	-2.72	105.97	110.24
44	A	811	CLA	O2D-CGD-CBD	2.72	115.99	111.23
44	r	305	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
47	B	847	BCR	C1-C6-C7	2.72	123.04	115.65
50	2	519	LMG	C7-O1-C1	-2.72	107.96	113.80
46	A	843	LHG	C6-C5-C4	-2.72	105.44	111.78
52	r	313	CHL	CBC-CAC-C3C	-2.72	108.98	112.87
44	3	316	CLA	C3B-C4B-NB	-2.72	108.10	110.53
51	1	502	LUT	C15-C35-C34	-2.72	117.95	123.52
47	j	803	BCR	C3-C4-C5	-2.72	109.20	114.06
44	s	506	CLA	C3B-C4B-NB	-2.72	108.10	110.53
47	F	804	BCR	C29-C30-C25	2.72	114.39	110.44
47	B	847	BCR	C21-C20-C19	-2.72	115.33	123.20
44	L	304	CLA	CHB-C4A-NA	2.72	128.32	124.40
46	p	516	LHG	O8-C23-C24	2.72	120.11	111.83
44	q	304	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
46	O	601	LHG	C5-O7-C7	-2.71	111.30	117.80
44	B	825	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
44	f	814	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
51	r	302	LUT	C7-C8-C9	-2.71	122.22	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	B	849	BCR	C37-C22-C21	-2.71	118.42	122.82
47	L	306	BCR	C3-C4-C5	-2.71	109.22	114.06
44	A	815	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
52	r	313	CHL	O1D-CGD-CBD	-2.71	120.61	124.72
52	r	314	CHL	C1-C2-C3	-2.71	122.38	126.76
44	n	203	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
44	B	825	CLA	CHB-C4A-NA	2.71	128.31	124.40
44	p	515	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
51	3	303	LUT	C20-C13-C12	2.71	122.23	118.09
47	B	844	BCR	C15-C16-C17	-2.71	117.98	123.52
44	A	818	CLA	C3B-C4B-NB	-2.71	108.11	110.53
44	e	826	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
44	e	840	CLA	CAA-C2A-C3A	-2.71	110.02	116.23
46	e	844	LHG	O8-C23-C24	2.71	120.09	111.83
44	s	505	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
44	B	819	CLA	CMA-C3A-C2A	-2.71	110.02	116.23
52	r	314	CHL	O2A-CGA-CBA	2.71	120.08	111.83
54	Q	802	SQD	O48-C23-C24	2.70	120.08	111.83
44	f	825	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
44	e	830	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
44	B	811	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
44	A	822	CLA	C3B-C4B-NB	-2.70	108.12	110.53
44	B	803	CLA	C3B-C4B-NB	-2.70	108.12	110.53
44	A	810	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
47	A	846	BCR	C30-C25-C26	-2.70	118.95	122.64
52	s	515	CHL	C1C-CHC-C4B	2.70	125.73	116.07
44	s	511	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
47	A	851	BCR	C23-C24-C25	-2.70	119.79	127.00
44	r	308	CLA	C3B-C4B-NB	-2.70	108.12	110.53
47	e	847	BCR	C20-C21-C22	-2.70	123.50	127.28
44	f	805	CLA	C3B-C4B-NB	-2.70	108.12	110.53
47	B	852	BCR	C34-C9-C10	-2.69	118.45	122.82
44	B	805	CLA	CHB-C4A-NA	2.69	128.29	124.40
52	s	512	CHL	CMB-C2B-C3B	2.69	130.06	124.68
51	s	501	LUT	C30-C31-C32	-2.69	115.40	123.20
44	3	312	CLA	CAA-C2A-C3A	-2.69	110.06	116.23
47	A	846	BCR	C28-C27-C26	-2.69	109.26	114.06
46	B	851	LHG	O8-C23-C24	2.69	120.04	111.83
47	A	853	BCR	C38-C26-C27	2.69	119.33	113.60
44	q	306	CLA	O2D-CGD-CBD	2.69	115.93	111.23
52	q	313	CHL	C1C-CHC-C4B	2.69	125.69	116.07
47	B	848	BCR	C21-C20-C19	-2.69	115.41	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	B	821	CLA	CHB-C4A-NA	2.69	128.28	124.40
43	e	801	CL0	O2D-CGD-O1D	-2.69	117.98	124.08
44	f	835	CLA	C3B-C4B-NB	-2.69	108.13	110.53
44	e	807	CLA	CHB-C4A-NA	2.69	128.28	124.40
52	p	514	CHL	C1C-CHC-C4B	2.69	125.68	116.07
47	A	849	BCR	C28-C27-C26	-2.69	109.27	114.06
44	q	315	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
44	5	310	CLA	C1-C2-C3	-2.69	122.42	126.76
47	f	847	BCR	C10-C11-C12	-2.69	115.42	123.20
44	f	821	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
44	K	203	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
44	B	835	CLA	CHB-C4A-NA	2.68	128.27	124.40
44	f	835	CLA	CAA-C2A-C3A	-2.68	105.75	113.00
44	e	818	CLA	CHD-C1D-ND	-2.68	121.03	124.80
52	s	515	CHL	O1D-CGD-CBD	-2.68	120.66	124.72
47	m	103	BCR	C33-C5-C4	2.68	119.31	113.60
44	e	809	CLA	CHB-C4A-NA	2.68	128.27	124.40
44	f	810	CLA	O2A-CGA-O1A	-2.68	116.92	123.63
52	p	512	CHL	CMB-C2B-C3B	2.68	130.04	124.68
44	s	507	CLA	C3B-C4B-NB	-2.68	108.14	110.53
47	f	847	BCR	C3-C4-C5	-2.68	109.28	114.06
51	q	301	LUT	C15-C14-C13	-2.67	123.53	127.28
44	f	842	CLA	C3B-C4B-NB	-2.67	108.14	110.53
47	I	101	BCR	C10-C11-C12	-2.67	115.45	123.20
44	A	803	CLA	CHB-C4A-NA	2.67	128.26	124.40
44	B	805	CLA	CMA-C3A-C2A	-2.67	110.10	116.23
47	K	204	BCR	C38-C26-C27	2.67	119.29	113.60
44	f	830	CLA	CAB-C3B-C2B	2.67	130.63	123.53
44	p	504	CLA	O2D-CGD-CBD	2.67	115.90	111.23
47	F	804	BCR	C3-C4-C5	-2.67	109.29	114.06
47	e	850	BCR	C3-C4-C5	-2.67	109.29	114.06
44	q	312	CLA	CHB-C4A-NA	2.67	128.25	124.40
47	5	302	BCR	C21-C20-C19	-2.67	115.46	123.20
44	1	510	CLA	CHB-C4A-NA	2.67	128.25	124.40
44	e	815	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
47	A	849	BCR	C38-C26-C25	-2.67	121.57	124.48
44	A	804	CLA	C3B-C4B-NB	-2.67	108.15	110.53
47	F	801	BCR	C15-C14-C13	-2.67	123.54	127.28
44	3	306	CLA	CMB-C2B-C3B	2.67	130.62	123.53
51	s	501	LUT	C27-C28-C29	-2.67	120.59	126.32
51	s	501	LUT	C8-C7-C6	-2.67	119.88	127.00
47	B	849	BCR	C29-C30-C25	2.67	114.31	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	B	845	BCR	C3-C4-C5	-2.67	109.30	114.06
46	f	852	LHG	C5-O7-C7	-2.66	111.42	117.80
43	A	801	CL0	O2D-CGD-O1D	-2.66	118.03	124.08
44	e	843	CLA	CAB-C3B-C4B	-2.66	121.37	125.42
53	2	502	XAT	C19-C9-C10	-2.66	118.51	122.82
44	p	506	CLA	C1-C2-C3	-2.66	121.84	126.20
44	B	840	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
44	2	510	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
44	f	838	CLA	C3A-C2A-C1A	-2.66	103.58	106.30
52	p	512	CHL	C1C-CHC-C4B	2.66	125.58	116.07
44	3	316	CLA	CHB-C4A-NA	2.66	128.24	124.40
44	3	317	CLA	CHB-C4A-NA	2.66	128.24	124.40
44	p	513	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
44	A	828	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
47	j	801	BCR	C8-C7-C6	-2.66	119.90	127.00
44	q	309	CLA	CHB-C4A-NA	2.66	128.23	124.40
47	f	846	BCR	C38-C26-C25	-2.66	121.59	124.48
51	3	304	LUT	C18-C5-C6	-2.66	121.59	124.48
47	B	846	BCR	C23-C22-C21	2.66	123.19	119.01
44	3	313	CLA	C3B-C4B-NB	-2.65	108.16	110.53
44	e	853	CLA	C3B-C4B-NB	-2.65	108.16	110.53
44	2	507	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
44	e	830	CLA	C3B-C4B-NB	-2.65	108.16	110.53
47	F	801	BCR	C29-C30-C25	2.65	114.29	110.44
44	B	837	CLA	O2A-CGA-O1A	-2.65	116.99	123.63
44	e	836	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
47	j	803	BCR	C11-C12-C13	-2.65	119.09	126.36
44	A	805	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
44	A	833	CLA	O2D-CGD-CBD	2.65	115.86	111.23
47	e	849	BCR	C38-C26-C27	2.65	119.25	113.60
47	l	102	BCR	C38-C26-C27	2.65	119.25	113.60
44	f	838	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
44	1	513	CLA	C3B-C4B-NB	-2.65	108.17	110.53
44	o	303	CLA	C3B-C4B-NB	-2.65	108.17	110.53
44	A	805	CLA	CHB-C4A-NA	2.65	128.22	124.40
44	L	302	CLA	C3B-C4B-NB	-2.65	108.17	110.53
44	f	824	CLA	C3B-C4B-NB	-2.65	108.17	110.53
47	A	846	BCR	C8-C7-C6	-2.65	119.92	127.00
44	f	812	CLA	CHB-C4A-NA	2.65	128.22	124.40
47	B	848	BCR	C33-C5-C4	2.65	119.24	113.60
44	f	806	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
44	f	834	CLA	CHB-C4A-NA	2.65	128.22	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	e	812	CLA	C3B-C4B-NB	-2.64	108.17	110.53
44	f	811	CLA	C3B-C4B-NB	-2.64	108.17	110.53
53	s	502	XAT	C15-C35-C34	-2.64	118.11	123.52
51	p	502	LUT	C31-C32-C33	-2.64	119.12	126.36
47	L	306	BCR	C31-C1-C6	-2.64	106.10	110.24
44	B	839	CLA	O2A-CGA-O1A	-2.64	117.02	123.63
47	e	847	BCR	C33-C5-C4	2.64	119.23	113.60
44	A	829	CLA	CMB-C2B-C1B	-2.64	121.40	125.42
51	3	304	LUT	C10-C11-C12	-2.64	115.55	123.20
44	e	820	CLA	C3B-C4B-NB	-2.64	108.17	110.53
52	5	317	CHL	CMB-C2B-C3B	2.64	129.96	124.68
44	B	812	CLA	C1-C2-C3	-2.64	121.87	126.20
44	p	510	CLA	C3B-C4B-NB	-2.64	108.17	110.53
51	s	501	LUT	C18-C5-C4	2.64	119.28	114.42
47	I	101	BCR	C36-C18-C19	2.64	122.12	118.09
44	s	514	CLA	CHB-C4A-NA	2.64	128.21	124.40
52	s	512	CHL	OMC-CMC-C2C	-2.64	120.54	125.12
44	3	311	CLA	CHB-C4A-NA	2.64	128.21	124.40
44	f	839	CLA	C3B-C4B-NB	-2.64	108.18	110.53
52	1	517	CHL	C4D-ND-C1D	-2.64	103.22	105.22
44	B	803	CLA	C1-C2-C3	-2.64	121.88	126.20
44	B	818	CLA	CHB-C4A-NA	2.64	128.20	124.40
47	r	301	BCR	C7-C8-C9	-2.63	122.34	126.23
44	e	853	CLA	CHB-C4A-NA	2.63	128.20	124.40
44	f	839	CLA	CHB-C4A-NA	2.63	128.20	124.40
44	A	836	CLA	O2A-CGA-O1A	-2.63	117.04	123.63
44	e	816	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
51	3	303	LUT	C27-C28-C29	-2.63	120.67	126.32
52	1	512	CHL	O1D-CGD-CBD	-2.63	120.73	124.72
44	e	811	CLA	CAA-C2A-C3A	-2.63	110.20	116.23
44	e	839	CLA	C1-C2-C3	-2.63	121.89	126.20
44	B	837	CLA	C3B-C4B-NB	-2.63	108.18	110.53
44	e	824	CLA	C3B-C4B-NB	-2.63	108.18	110.53
44	5	306	CLA	CAA-C2A-C3A	-2.63	110.20	116.23
47	l	101	BCR	C28-C27-C26	-2.63	109.37	114.06
44	3	311	CLA	CAC-C3C-C4C	2.63	128.21	124.79
44	3	310	CLA	CHB-C4A-NA	2.63	128.19	124.40
44	f	826	CLA	C3B-C4B-NB	-2.63	108.19	110.53
44	f	806	CLA	CAA-C2A-C3A	-2.63	110.21	116.23
44	f	831	CLA	C3B-C4B-NB	-2.62	108.19	110.53
47	e	850	BCR	C33-C5-C4	2.62	119.19	113.60
44	e	803	CLA	C1-C2-C3	-2.62	121.90	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	5	317	CHL	OMC-CMC-C2C	-2.62	120.56	125.12
44	B	820	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
44	1	508	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
47	f	849	BCR	C16-C17-C18	-2.62	123.60	127.28
44	f	808	CLA	C3B-C4B-NB	-2.62	108.19	110.53
47	B	844	BCR	C36-C18-C17	-2.62	118.57	122.82
47	Q	801	BCR	C33-C5-C6	-2.62	121.63	124.48
51	q	302	LUT	C8-C9-C10	-2.62	114.89	119.01
51	q	302	LUT	C18-C5-C4	2.62	119.23	114.42
44	f	815	CLA	C3B-C4B-NB	-2.62	108.19	110.53
47	A	846	BCR	C33-C5-C4	2.62	119.18	113.60
47	F	804	BCR	C24-C23-C22	-2.62	122.36	126.23
44	s	504	CLA	C1B-NB-C4B	2.62	108.15	106.31
47	s	503	BCR	C11-C10-C9	-2.61	123.61	127.28
52	p	517	CHL	C1C-CHC-C4B	2.61	125.42	116.07
47	f	848	BCR	C38-C26-C27	2.61	119.17	113.60
44	p	505	CLA	O2D-CGD-CBD	2.61	115.80	111.23
44	f	836	CLA	C3B-C4B-NB	-2.61	108.20	110.53
44	f	801	CLA	CAB-C3B-C4B	-2.61	121.44	125.42
44	3	307	CLA	C3A-C2A-C1A	-2.61	103.63	106.30
44	B	833	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
44	f	828	CLA	C3B-C4B-NB	-2.61	108.20	110.53
47	l	102	BCR	C23-C24-C25	-2.61	120.02	127.00
47	L	306	BCR	C7-C8-C9	-2.61	122.37	126.23
47	L	306	BCR	C4-C5-C6	-2.61	119.18	122.70
44	e	832	CLA	C3B-C4B-NB	-2.61	108.20	110.53
44	n	203	CLA	C3B-C4B-NB	-2.61	108.20	110.53
44	f	828	CLA	CAA-C2A-C3A	-2.61	110.25	116.23
44	e	805	CLA	CHB-C4A-NA	2.61	128.16	124.40
44	p	513	CLA	CHB-C4A-NA	2.61	128.16	124.40
51	2	501	LUT	C39-C29-C28	2.61	122.07	118.09
44	A	824	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
44	2	506	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
47	o	301	BCR	C34-C9-C10	-2.61	118.59	122.82
44	3	317	CLA	CMA-C3A-C2A	-2.60	110.26	116.23
44	B	825	CLA	C3B-C4B-NB	-2.60	108.20	110.53
47	e	848	BCR	C27-C26-C25	-2.60	119.19	122.70
44	o	302	CLA	CAB-C3B-C4B	-2.60	121.45	125.42
44	L	303	CLA	O2D-CGD-CBD	2.60	115.78	111.23
52	r	316	CHL	C1C-CHC-C4B	2.60	125.38	116.07
44	e	816	CLA	CHB-C4A-NA	2.60	128.15	124.40
45	A	841	PQN	C11-C3-C2	-2.60	120.43	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	A	852	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
44	5	309	CLA	CMB-C2B-C1B	-2.60	121.46	125.42
47	3	305	BCR	C8-C7-C6	-2.60	120.06	127.00
52	2	512	CHL	O1D-CGD-CBD	-2.60	120.78	124.72
47	J	102	BCR	C2-C1-C6	2.60	114.21	110.44
44	5	309	CLA	CAA-CBA-CGA	-2.60	105.56	112.49
47	f	848	BCR	C24-C23-C22	-2.60	122.39	126.23
47	f	849	BCR	C33-C5-C4	2.60	119.13	113.60
44	q	304	CLA	C3B-C2B-C1B	-2.60	106.65	108.37
44	B	827	CLA	CMB-C2B-C1B	-2.59	121.47	125.42
44	e	820	CLA	CAA-C2A-C3A	-2.59	110.28	116.23
44	e	826	CLA	CAB-C3B-C4B	-2.59	121.47	125.42
44	A	802	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
44	s	510	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
44	3	314	CLA	CHB-C4A-NA	2.59	128.14	124.40
44	A	821	CLA	CMB-C2B-C1B	-2.59	121.47	125.42
47	f	845	BCR	C38-C26-C25	-2.59	121.66	124.48
47	r	301	BCR	C20-C21-C22	-2.59	123.64	127.28
50	2	519	LMG	O7-C10-O9	-2.59	117.65	123.70
47	e	847	BCR	C24-C23-C22	-2.59	122.40	126.23
51	3	303	LUT	C8-C7-C6	-2.59	120.08	127.00
44	B	807	CLA	CHB-C4A-NA	2.59	128.14	124.40
44	e	808	CLA	CHB-C4A-NA	2.59	128.14	124.40
47	F	804	BCR	C33-C5-C6	-2.59	121.66	124.48
44	f	828	CLA	CHB-C4A-NA	2.59	128.14	124.40
44	q	310	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
44	2	509	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
50	F	806	LMG	C8-O7-C10	-2.59	111.61	117.80
44	e	836	CLA	C3B-C4B-NB	-2.59	108.22	110.53
47	q	303	BCR	C10-C11-C12	-2.58	115.71	123.20
44	5	310	CLA	CHB-C4A-NA	2.58	128.13	124.40
44	J	101	CLA	CHB-C4A-NA	2.58	128.13	124.40
52	s	512	CHL	C1C-CHC-C4B	2.58	125.31	116.07
44	e	821	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
47	o	301	BCR	C16-C17-C18	-2.58	123.66	127.28
44	f	837	CLA	CHB-C4A-NA	2.58	128.12	124.40
44	e	840	CLA	CHB-C4A-NA	2.58	128.12	124.40
52	5	315	CHL	CBC-CAC-C3C	-2.58	109.18	112.87
44	B	808	CLA	O2A-CGA-O1A	-2.58	117.18	123.63
46	B	851	LHG	C5-O7-C7	-2.58	111.63	117.80
44	1	504	CLA	CHB-C4A-NA	2.58	128.12	124.40
47	e	851	BCR	C2-C1-C6	2.58	114.18	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	3	307	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
44	A	820	CLA	CMB-C2B-C1B	-2.58	121.50	125.42
44	e	803	CLA	CHB-C4A-NA	2.57	128.12	124.40
47	f	845	BCR	C38-C26-C27	2.57	119.08	113.60
44	B	809	CLA	C2A-C1A-CHA	2.57	126.70	122.71
44	r	309	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
44	e	838	CLA	C3B-C4B-NB	-2.57	108.23	110.53
46	f	852	LHG	O8-C23-C24	2.57	119.68	111.83
44	B	825	CLA	CMB-C2B-C1B	-2.57	121.50	125.42
44	A	838	CLA	C1-C2-C3	-2.57	121.98	126.20
47	e	849	BCR	C8-C7-C6	-2.57	120.13	127.00
52	p	514	CHL	O1D-CGD-CBD	-2.57	120.82	124.72
44	e	802	CLA	C2A-C1A-CHA	2.57	126.70	122.71
44	A	809	CLA	C3B-C4B-NB	-2.57	108.23	110.53
44	f	833	CLA	C3B-C4B-NB	-2.57	108.24	110.53
45	B	843	PQN	C14-C13-C15	2.57	119.69	115.23
44	5	316	CLA	CHB-C4A-NA	2.57	128.10	124.40
47	e	849	BCR	C11-C10-C9	-2.57	123.68	127.28
47	B	845	BCR	C24-C23-C22	-2.57	122.44	126.23
52	5	315	CHL	CMA-C3A-C4A	-2.57	109.08	114.61
47	e	846	BCR	C7-C8-C9	-2.57	122.44	126.23
44	e	824	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
52	5	314	CHL	O2D-CGD-O1D	-2.56	118.86	123.85
44	r	317	CLA	C3B-C4B-NB	-2.56	108.24	110.53
52	1	517	CHL	OMC-CMC-C2C	-2.56	120.67	125.12
44	o	303	CLA	CHB-C4A-NA	2.56	128.10	124.40
44	q	304	CLA	CHC-C1C-C2C	-2.56	124.33	129.94
44	e	825	CLA	CHB-C4A-NA	2.56	128.10	124.40
53	s	502	XAT	C27-C28-C29	-2.56	121.55	125.53
44	r	306	CLA	C1-C2-C3	-2.56	122.00	126.20
47	f	845	BCR	C27-C26-C25	-2.56	119.24	122.70
44	e	803	CLA	C3B-C4B-NB	-2.56	108.24	110.53
44	s	509	CLA	C3B-C4B-NB	-2.56	108.24	110.53
47	L	305	BCR	C36-C18-C17	-2.56	118.67	122.82
44	B	827	CLA	CHB-C4A-NA	2.56	128.09	124.40
52	1	517	CHL	CMB-C2B-C3B	2.56	129.80	124.68
51	r	302	LUT	C22-C23-C24	2.56	114.99	111.18
52	s	517	CHL	O1D-CGD-CBD	-2.56	120.84	124.72
44	r	310	CLA	C3B-C4B-NB	-2.56	108.25	110.53
51	2	501	LUT	C40-C33-C32	2.56	122.00	118.09
47	J	102	BCR	C27-C26-C25	-2.56	119.25	122.70
47	A	847	BCR	C28-C27-C26	-2.56	109.49	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	f	829	CLA	CMB-C2B-C1B	-2.56	121.52	125.42
47	e	854	BCR	C33-C5-C6	-2.56	121.69	124.48
47	o	301	BCR	C11-C10-C9	-2.56	123.69	127.28
47	o	301	BCR	C8-C9-C10	2.56	123.03	119.01
44	f	809	CLA	C3B-C4B-NB	-2.56	108.25	110.53
52	2	513	CHL	CMA-C3A-C4A	-2.56	106.54	114.81
52	r	313	CHL	C1C-CHC-C4B	2.56	125.22	116.07
47	2	503	BCR	C35-C13-C12	2.56	121.99	118.09
44	B	816	CLA	CHB-C4A-NA	2.56	128.09	124.40
44	p	509	CLA	O2A-CGA-CBA	2.56	119.63	111.83
47	e	847	BCR	C38-C26-C27	2.55	119.04	113.60
52	5	315	CHL	CMD-C2D-C3D	-2.55	119.58	124.68
44	L	303	CLA	CAA-C2A-C3A	-2.55	106.10	113.00
47	l	102	BCR	C24-C23-C22	-2.55	122.46	126.23
47	e	846	BCR	C38-C26-C27	2.55	119.04	113.60
51	1	502	LUT	C18-C5-C4	2.55	119.11	114.42
44	3	311	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
44	A	818	CLA	O2D-CGD-CBD	2.55	115.69	111.23
52	1	512	CHL	C1B-CHB-C4A	2.55	122.96	121.32
44	B	802	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
49	f	851	DGD	O1G-C1A-C2A	2.55	119.61	111.83
49	m	104	DGD	O1G-C1A-C2A	2.55	119.61	111.83
52	2	515	CHL	O2D-CGD-O1D	-2.55	118.89	123.85
52	1	514	CHL	CHA-C1A-NA	2.55	124.43	122.15
44	B	806	CLA	C3A-C4A-CHB	-2.55	120.79	123.91
47	l	101	BCR	C33-C5-C6	-2.55	121.70	124.48
46	s	516	LHG	O8-C23-C24	2.55	119.60	111.83
44	e	852	CLA	C3B-C4B-NB	-2.55	108.26	110.53
44	B	805	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
47	J	102	BCR	C10-C11-C12	-2.55	115.83	123.20
49	J	103	DGD	O1G-C1A-C2A	2.54	119.59	111.83
50	m	105	LMG	C8-O7-C10	-2.54	111.71	117.80
44	e	834	CLA	CHB-C4A-NA	2.54	128.07	124.40
44	q	308	CLA	CHB-C4A-NA	2.54	128.07	124.40
47	I	101	BCR	C27-C26-C25	-2.54	119.27	122.70
47	J	102	BCR	C31-C1-C6	-2.54	106.26	110.24
44	s	510	CLA	C3B-C4B-NB	-2.54	108.26	110.53
44	A	812	CLA	CMB-C2B-C1B	-2.54	121.55	125.42
47	L	306	BCR	C38-C26-C27	2.54	119.02	113.60
44	f	822	CLA	CAA-C2A-C3A	-2.54	110.40	116.23
47	e	849	BCR	C20-C19-C18	-2.54	119.39	126.36
44	2	514	CLA	O2D-CGD-O1D	-2.54	118.90	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	A	846	BCR	C3-C4-C5	-2.54	109.53	114.06
44	1	505	CLA	CHB-C4A-NA	2.54	128.06	124.40
44	3	308	CLA	C1-C2-C3	-2.54	122.04	126.20
44	p	509	CLA	C3B-C4B-NB	-2.54	108.27	110.53
47	f	846	BCR	C33-C5-C4	2.54	119.00	113.60
47	f	845	BCR	C30-C25-C26	-2.53	119.17	122.64
47	m	103	BCR	C27-C26-C25	-2.53	119.28	122.70
47	e	849	BCR	C3-C4-C5	-2.53	109.54	114.06
44	r	315	CLA	CHB-C4A-NA	2.53	128.06	124.40
44	e	813	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
44	2	514	CLA	CHB-C4A-NA	2.53	128.06	124.40
47	p	503	BCR	C40-C30-C29	2.53	118.68	108.95
44	f	842	CLA	CAA-C2A-C3A	-2.53	110.42	116.23
44	f	830	CLA	CHB-C4A-NA	2.53	128.06	124.40
44	r	305	CLA	CHB-C4A-NA	2.53	128.06	124.40
50	2	518	LMG	O6-C1-C2	-2.53	105.17	110.37
44	1	508	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
44	e	810	CLA	CHB-C4A-NA	2.53	128.05	124.40
47	e	849	BCR	C7-C8-C9	-2.53	122.49	126.23
44	B	822	CLA	O2D-CGD-CBD	2.53	115.66	111.23
47	B	852	BCR	C30-C25-C26	-2.53	119.18	122.64
52	s	515	CHL	CHA-C1A-NA	2.53	124.42	122.15
47	J	102	BCR	C34-C9-C8	2.53	121.95	118.09
44	f	824	CLA	CHB-C4A-NA	2.53	128.05	124.40
52	5	317	CHL	O1D-CGD-CBD	-2.53	120.89	124.72
44	B	821	CLA	C1-C2-C3	-2.53	122.67	126.76
50	2	519	LMG	O8-C28-C29	2.53	119.54	111.83
44	B	834	CLA	CHB-C4A-NA	2.53	128.05	124.40
44	f	805	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
44	A	832	CLA	C3B-C4B-NB	-2.53	108.28	110.53
44	e	827	CLA	C3B-C4B-NB	-2.53	108.28	110.53
44	r	304	CLA	CHB-C4A-NA	2.53	128.04	124.40
44	1	510	CLA	O2D-CGD-CBD	2.53	115.64	111.23
44	p	513	CLA	C3B-C4B-NB	-2.52	108.28	110.53
52	r	313	CHL	OMC-CMC-C2C	-2.52	120.74	125.12
51	5	303	LUT	C39-C29-C28	2.52	121.94	118.09
52	3	315	CHL	CMB-C2B-C3B	2.52	129.73	124.68
44	n	203	CLA	CAA-C2A-C3A	-2.52	110.44	116.23
52	p	517	CHL	OMC-CMC-C2C	-2.52	120.74	125.12
44	f	822	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
44	5	305	CLA	C2A-C1A-CHA	2.52	126.62	122.71
44	e	829	CLA	O2D-CGD-O1D	-2.52	118.94	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	r	312	CLA	CAA-C2A-C3A	-2.52	110.45	116.23
47	A	849	BCR	C16-C15-C14	-2.52	118.36	123.52
44	f	814	CLA	CHB-C4A-NA	2.52	128.03	124.40
44	e	833	CLA	CHB-C4A-NA	2.52	128.03	124.40
47	e	851	BCR	C33-C5-C4	2.52	118.96	113.60
46	s	516	LHG	C5-O7-C7	-2.52	111.77	117.80
44	B	829	CLA	O2D-CGD-CBD	2.52	115.63	111.23
44	A	833	CLA	C3B-C4B-NB	-2.51	108.28	110.53
44	5	308	CLA	C3B-C4B-NB	-2.51	108.28	110.53
44	q	306	CLA	CHB-C4A-NA	2.51	128.03	124.40
44	3	310	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
52	s	517	CHL	CBC-CAC-C3C	-2.51	109.27	112.87
44	3	306	CLA	CAB-C3B-C2B	2.51	130.21	123.53
44	s	505	CLA	CHB-C4A-NA	2.51	128.03	124.40
53	s	502	XAT	C38-C25-C24	2.51	117.06	114.24
47	e	850	BCR	C16-C15-C14	-2.51	118.38	123.52
44	5	307	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
44	2	514	CLA	O2A-CGA-O1A	-2.51	117.35	123.63
44	f	819	CLA	CHB-C4A-NA	2.51	128.02	124.40
44	s	514	CLA	C3B-C4B-NB	-2.51	108.29	110.53
44	K	205	CLA	O2D-CGD-O1D	-2.51	118.39	124.08
44	f	838	CLA	CHB-C4A-NA	2.51	128.02	124.40
47	B	852	BCR	C23-C24-C25	-2.51	120.30	127.00
44	B	838	CLA	CHB-C4A-NA	2.51	128.02	124.40
44	e	839	CLA	CHB-C4A-NA	2.50	128.01	124.40
44	A	837	CLA	CMA-C3A-C2A	-2.50	110.49	116.23
44	n	205	CLA	O2D-CGD-O1D	-2.50	118.40	124.08
45	B	843	PQN	C2M-C2-C1	2.50	121.28	116.68
44	f	810	CLA	CHB-C4A-NA	2.50	128.01	124.40
47	A	849	BCR	C10-C11-C12	-2.50	115.95	123.20
44	p	505	CLA	CHA-C1A-NA	-2.50	120.73	126.39
47	B	846	BCR	C28-C27-C26	-2.50	109.60	114.06
44	n	202	CLA	CHB-C4A-NA	2.50	128.01	124.40
47	B	844	BCR	C20-C19-C18	-2.50	119.51	126.36
52	r	313	CHL	CMB-C2B-C3B	2.50	129.68	124.68
44	s	504	CLA	CMB-C2B-C3B	2.50	130.62	124.63
44	e	822	CLA	CHB-C4A-NA	2.50	128.01	124.40
52	p	512	CHL	O2D-CGD-O1D	-2.50	118.98	123.85
44	e	836	CLA	CHB-C4A-NA	2.50	128.00	124.40
44	f	820	CLA	CHB-C4A-NA	2.50	128.00	124.40
44	B	823	CLA	CHB-C4A-NA	2.50	128.00	124.40
44	f	808	CLA	CHB-C4A-NA	2.50	128.00	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	B	801	CLA	C1-C2-C3	-2.50	122.11	126.20
44	q	307	CLA	C3A-C2A-C1A	-2.50	103.75	106.30
44	f	840	CLA	CHB-C4A-NA	2.49	128.00	124.40
44	5	316	CLA	O2D-CGD-O1D	-2.49	118.99	123.85
52	p	514	CHL	CBC-CAC-C3C	-2.49	109.30	112.87
47	e	847	BCR	C16-C15-C14	-2.49	118.42	123.52
52	2	512	CHL	OMC-CMC-C2C	-2.49	120.79	125.12
52	q	313	CHL	C3D-C4D-ND	2.49	115.35	110.42
44	A	833	CLA	CHB-C4A-NA	2.49	128.00	124.40
47	f	848	BCR	C21-C20-C19	-2.49	115.98	123.20
44	5	309	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
52	3	302	CHL	CMB-C2B-C3B	2.49	129.66	124.68
44	B	813	CLA	C3B-C4B-NB	-2.49	108.31	110.53
44	A	810	CLA	CMB-C2B-C1B	-2.49	121.62	125.42
44	5	311	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
47	A	851	BCR	C21-C20-C19	-2.49	115.98	123.20
47	F	801	BCR	C2-C1-C6	2.49	114.06	110.44
44	A	814	CLA	CHB-C4A-NA	2.49	127.99	124.40
44	A	822	CLA	CHB-C4A-NA	2.49	127.99	124.40
44	3	301	CLA	CHB-C4A-NA	2.49	127.99	124.40
44	r	312	CLA	CHB-C4A-NA	2.49	127.99	124.40
44	e	841	CLA	CHB-C4A-NA	2.49	127.99	124.40
44	e	828	CLA	CHB-C4A-NA	2.49	127.99	124.40
44	f	829	CLA	C1-C2-C3	-2.49	122.74	126.76
44	B	832	CLA	C3B-C4B-NB	-2.49	108.31	110.53
44	2	510	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
50	2	519	LMG	O1-C1-C2	2.49	112.05	108.27
47	A	849	BCR	C34-C9-C10	-2.48	118.79	122.82
44	f	817	CLA	CHB-C4A-NA	2.48	127.98	124.40
44	s	511	CLA	CHB-C4A-NA	2.48	127.98	124.40
44	e	818	CLA	C3B-C4B-NB	-2.48	108.31	110.53
44	B	814	CLA	CAC-C3C-C4C	2.48	128.02	124.79
44	B	835	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
47	2	503	BCR	C20-C19-C18	2.48	133.17	126.36
47	e	848	BCR	C11-C12-C13	-2.48	119.56	126.36
52	s	515	CHL	CMB-C2B-C3B	2.48	129.64	124.68
47	1	503	BCR	C8-C7-C6	-2.48	120.37	127.00
47	j	801	BCR	C38-C26-C27	2.48	118.89	113.60
44	p	506	CLA	C3B-C4B-NB	-2.48	108.32	110.53
44	5	306	CLA	CMA-C3A-C2A	-2.48	110.54	116.23
44	f	813	CLA	CAB-C3B-C2B	2.48	130.12	123.53
44	5	308	CLA	CHB-C4A-NA	2.48	127.98	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	e	852	CLA	CHB-C4A-NA	2.48	127.98	124.40
47	A	847	BCR	C1-C6-C5	-2.48	119.25	122.64
44	A	816	CLA	CHB-C4A-NA	2.48	127.97	124.40
44	f	841	CLA	CHB-C4A-NA	2.48	127.97	124.40
51	1	501	LUT	C21-C26-C27	-2.48	109.98	112.83
44	A	827	CLA	CMB-C2B-C1B	-2.47	121.65	125.42
44	2	504	CLA	CAC-C3C-C4C	2.47	128.01	124.79
44	1	507	CLA	CHB-C4A-NA	2.47	127.97	124.40
52	2	512	CHL	CMB-C2B-C3B	2.47	129.87	124.69
44	e	826	CLA	CHB-C4A-NA	2.47	127.97	124.40
44	e	806	CLA	CMA-C3A-C2A	-2.47	110.56	116.23
47	l	101	BCR	C21-C20-C19	-2.47	116.04	123.20
44	2	510	CLA	CHB-C4A-NA	2.47	127.97	124.40
44	5	308	CLA	CMB-C2B-C3B	2.47	132.36	126.55
47	L	306	BCR	C30-C25-C26	-2.47	119.26	122.64
44	e	817	CLA	C3B-C4B-NB	-2.47	108.33	110.53
47	e	854	BCR	C20-C21-C22	-2.47	123.81	127.28
44	B	834	CLA	O2A-CGA-O1A	-2.47	116.98	123.33
44	2	510	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
47	s	503	BCR	C35-C13-C12	2.47	121.86	118.09
44	B	828	CLA	C3B-C4B-NB	-2.47	108.33	110.53
44	B	817	CLA	CHB-C4A-NA	2.47	127.96	124.40
44	A	831	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
44	p	504	CLA	CBA-CAA-C2A	2.47	118.65	113.41
47	5	302	BCR	C35-C13-C14	-2.47	118.82	122.82
44	f	818	CLA	CHB-C4A-NA	2.46	127.96	124.40
44	L	302	CLA	CHB-C4A-NA	2.46	127.93	124.43
43	A	801	CL0	CMB-C2B-C3B	2.46	129.85	124.69
44	5	307	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
44	f	835	CLA	CHB-C4A-NA	2.46	127.95	124.40
44	p	508	CLA	C3B-C4B-NB	-2.46	108.33	110.53
43	e	801	CL0	CMB-C2B-C3B	2.46	129.85	124.69
47	F	801	BCR	C27-C26-C25	-2.46	119.38	122.70
44	f	807	CLA	C3B-C4B-NB	-2.46	108.33	110.53
44	r	317	CLA	C1-C2-C3	-2.46	122.78	126.76
44	p	507	CLA	CHB-C4A-NA	2.46	127.95	124.40
44	s	506	CLA	CHB-C4A-NA	2.46	127.95	124.40
44	3	311	CLA	O1D-CGD-CBD	2.46	129.36	124.52
44	A	824	CLA	C2A-C1A-CHA	2.46	126.52	122.71
44	A	808	CLA	O2D-CGD-O1D	-2.46	119.07	123.85
44	s	509	CLA	C1-C2-C3	-2.46	122.79	126.76
52	2	513	CHL	O2D-CGD-O1D	-2.46	119.07	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	A	853	BCR	C35-C13-C14	-2.45	118.84	122.82
44	3	318	CLA	CAB-C3B-C2B	2.45	130.05	123.53
44	f	823	CLA	CHB-C4A-NA	2.45	127.94	124.40
47	s	503	BCR	C20-C19-C18	2.45	133.09	126.36
47	J	102	BCR	C36-C18-C19	2.45	121.83	118.09
47	e	848	BCR	C38-C26-C27	2.45	118.82	113.60
47	e	850	BCR	C30-C25-C26	-2.45	119.29	122.64
52	r	316	CHL	O1D-CGD-CBD	-2.45	121.01	124.72
47	e	846	BCR	C23-C24-C25	-2.45	120.45	127.00
50	F	805	LMG	C8-O7-C10	-2.45	111.93	117.80
52	s	513	CHL	O2D-CGD-O1D	-2.45	119.08	123.85
44	f	842	CLA	CHB-C4A-NA	2.45	127.93	124.40
52	p	514	CHL	CMB-C2B-C3B	2.45	129.57	124.68
44	f	843	CLA	CHB-C4A-NA	2.45	127.93	124.40
44	A	827	CLA	C3B-C4B-NB	-2.45	108.35	110.53
44	K	203	CLA	C3B-C4B-NB	-2.45	108.35	110.53
44	p	515	CLA	C3B-C4B-NB	-2.45	108.35	110.53
44	K	201	CLA	CHB-C1B-NB	2.45	127.72	124.05
44	p	505	CLA	CMB-C2B-C1B	-2.45	121.69	125.42
51	1	501	LUT	C30-C31-C32	-2.45	116.11	123.20
51	3	304	LUT	C16-C1-C6	-2.44	106.41	110.24
44	B	820	CLA	O2A-CGA-O1A	-2.44	117.51	123.63
44	A	806	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
44	q	307	CLA	C3B-C4B-NB	-2.44	108.35	110.53
44	q	311	CLA	C3B-C4B-NB	-2.44	108.35	110.53
44	f	826	CLA	O2D-CGD-CBD	2.44	115.50	111.23
44	B	841	CLA	CHB-C4A-NA	2.44	127.93	124.40
52	p	514	CHL	OMC-CMC-C2C	-2.44	120.88	125.12
44	A	828	CLA	CHB-C4A-NA	2.44	127.93	124.40
44	e	818	CLA	C1D-ND-C4D	-2.44	104.60	106.31
44	e	823	CLA	CHB-C4A-NA	2.44	127.92	124.40
44	f	821	CLA	CHB-C4A-NA	2.44	127.92	124.40
44	q	314	CLA	CMB-C2B-C1B	-2.44	121.70	125.42
44	q	308	CLA	CMB-C2B-C1B	-2.44	121.70	125.42
47	A	851	BCR	C31-C1-C6	-2.44	106.42	110.24
47	B	848	BCR	C36-C18-C19	2.44	121.82	118.09
52	r	313	CHL	O2D-CGD-O1D	-2.44	119.10	123.85
44	f	816	CLA	CHB-C4A-NA	2.44	127.92	124.40
44	A	831	CLA	CAB-C3B-C2B	2.44	130.02	123.53
47	e	846	BCR	C15-C16-C17	-2.44	118.53	123.52
44	A	825	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
44	f	830	CLA	C3A-C2A-C1A	-2.44	103.81	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	A	830	CLA	O1D-CGD-CBD	2.44	129.32	124.52
52	1	514	CHL	C1C-CHC-C4B	2.44	124.79	116.07
47	A	845	BCR	C8-C7-C6	-2.44	120.49	127.00
44	f	832	CLA	CHB-C4A-NA	2.44	127.92	124.40
44	q	304	CLA	C4B-NB-C1B	2.44	108.02	106.31
44	m	102	CLA	CHB-C4A-NA	2.44	127.92	124.40
44	r	307	CLA	CHB-C4A-NA	2.44	127.92	124.40
47	e	846	BCR	C10-C11-C12	-2.44	116.14	123.20
44	B	837	CLA	CHB-C4A-NA	2.43	127.91	124.40
52	2	513	CHL	CMD-C2D-C3D	-2.43	120.36	124.94
44	A	810	CLA	CHB-C4A-NA	2.43	127.91	124.40
44	r	315	CLA	CMA-C3A-C2A	-2.43	110.65	116.23
47	3	305	BCR	C15-C16-C17	-2.43	118.54	123.52
52	5	314	CHL	CMB-C2B-C3B	2.43	129.54	124.68
44	A	828	CLA	CAA-C2A-C3A	-2.43	110.65	116.23
44	1	506	CLA	CHB-C4A-NA	2.43	127.91	124.40
47	e	850	BCR	C38-C26-C27	2.43	118.77	113.60
52	s	513	CHL	CMB-C2B-C3B	2.43	129.53	124.68
44	n	201	CLA	CAA-C2A-C3A	-2.43	110.67	116.23
44	B	826	CLA	CHB-C4A-NA	2.43	127.90	124.40
44	B	810	CLA	O2D-CGD-CBD	2.43	115.47	111.23
44	f	804	CLA	CHA-C4D-ND	2.43	137.55	132.55
47	e	849	BCR	C10-C11-C12	-2.43	116.17	123.20
44	A	806	CLA	CHB-C4A-NA	2.43	127.90	124.40
44	s	509	CLA	CHB-C4A-NA	2.42	127.90	124.40
47	j	801	BCR	C39-C30-C25	-2.42	106.44	110.24
46	1	516	LHG	O8-C23-O10	-2.42	117.57	123.63
51	p	501	LUT	C37-C21-C26	-2.42	105.87	109.55
47	L	305	BCR	C39-C30-C25	-2.42	106.44	110.24
44	e	826	CLA	C3B-C4B-NB	-2.42	107.81	110.33
44	3	312	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
47	A	847	BCR	C21-C20-C19	-2.42	116.19	123.20
44	B	828	CLA	CMA-C3A-C2A	-2.42	110.68	116.23
44	A	811	CLA	C3B-C4B-NB	-2.42	108.37	110.53
44	e	820	CLA	CHB-C4A-NA	2.42	127.89	124.40
44	e	821	CLA	C3B-C4B-NB	-2.42	108.37	110.53
52	s	515	CHL	OMC-CMC-C2C	-2.42	120.92	125.12
47	A	845	BCR	C10-C11-C12	-2.42	116.20	123.20
44	A	807	CLA	CHB-C4A-NA	2.42	127.89	124.40
47	A	853	BCR	C39-C30-C25	-2.42	106.45	110.24
44	A	831	CLA	CMB-C2B-C3B	2.42	129.95	123.53
44	3	308	CLA	O2D-CGD-O1D	-2.42	119.15	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	F	803	CLA	CHB-C4A-NA	2.42	127.89	124.40
44	2	504	CLA	CHB-C4A-NA	2.42	127.86	124.43
52	s	515	CHL	CBC-CAC-C3C	-2.41	109.42	112.87
44	2	505	CLA	CHB-C4A-NA	2.41	127.88	124.40
44	e	806	CLA	CHB-C4A-NA	2.41	127.88	124.40
44	e	814	CLA	CHB-C4A-NA	2.41	127.88	124.40
44	n	203	CLA	CHB-C4A-NA	2.41	127.88	124.40
47	j	801	BCR	C33-C5-C4	2.41	118.74	113.60
44	A	821	CLA	O1D-CGD-CBD	2.41	129.28	124.52
47	j	801	BCR	C35-C13-C12	2.41	121.78	118.09
47	e	846	BCR	C11-C10-C9	-2.41	123.89	127.28
44	e	811	CLA	CHB-C4A-NA	2.41	127.88	124.40
44	p	515	CLA	C2A-C1A-CHA	2.41	126.45	122.71
44	e	838	CLA	CHB-C4A-NA	2.41	127.88	124.40
51	1	501	LUT	C20-C13-C12	2.41	121.77	118.09
52	3	302	CHL	C1B-CHB-C4A	2.41	122.87	121.32
44	A	832	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
47	f	850	BCR	C20-C19-C18	-2.41	119.76	126.36
47	A	847	BCR	C34-C9-C8	2.41	121.77	118.09
47	Q	801	BCR	C38-C26-C25	-2.41	121.86	124.48
53	s	502	XAT	C4-C3-C2	-2.41	106.29	110.79
44	B	812	CLA	CHB-C4A-NA	2.41	127.88	124.40
44	B	839	CLA	CHB-C4A-NA	2.41	127.88	124.40
52	1	512	CHL	CMB-C2B-C3B	2.41	129.49	124.68
47	f	845	BCR	C33-C5-C4	2.41	118.73	113.60
44	F	802	CLA	CHB-C4A-NA	2.41	127.87	124.40
47	l	102	BCR	C15-C16-C17	-2.40	118.60	123.52
44	A	838	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
51	r	302	LUT	C10-C11-C12	-2.40	116.24	123.20
44	L	301	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
44	e	802	CLA	C3A-C2A-C1A	-2.40	103.84	106.30
44	B	840	CLA	CHB-C4A-NA	2.40	127.86	124.40
44	2	508	CLA	C3B-C4B-NB	-2.40	108.39	110.53
44	B	830	CLA	O1D-CGD-CBD	2.40	129.25	124.52
44	e	817	CLA	CHB-C4A-NA	2.40	127.86	124.40
44	q	304	CLA	O2D-CGD-CBD	2.40	115.42	111.23
47	B	849	BCR	C38-C26-C25	-2.40	121.87	124.48
47	A	846	BCR	C38-C26-C27	2.40	118.71	113.60
44	3	316	CLA	CMB-C2B-C1B	-2.40	121.77	125.42
47	A	848	BCR	C8-C7-C6	-2.40	120.60	127.00
44	e	831	CLA	CHB-C4A-NA	2.40	127.86	124.40
47	f	845	BCR	C8-C7-C6	-2.40	120.60	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	f	836	CLA	CHB-C4A-NA	2.39	127.83	124.43
44	o	302	CLA	CHB-C4A-NA	2.39	127.86	124.40
44	e	838	CLA	O2D-CGD-CBD	2.39	115.42	111.23
44	B	833	CLA	C3B-C4B-NB	-2.39	108.39	110.53
47	A	847	BCR	C15-C16-C17	-2.39	118.62	123.52
44	A	826	CLA	C3B-C4B-NB	-2.39	108.39	110.53
44	n	201	CLA	CHB-C4A-NA	2.39	127.85	124.40
44	r	306	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
44	1	509	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
44	A	820	CLA	O2D-CGD-CBD	2.39	115.41	111.23
47	f	845	BCR	C3-C4-C5	-2.39	109.79	114.06
44	f	843	CLA	CAA-C2A-C3A	-2.39	110.75	116.23
52	5	314	CHL	CMA-C3A-C4A	-2.39	109.46	114.61
44	1	507	CLA	C1-C2-C3	-2.39	122.28	126.20
47	f	848	BCR	C7-C8-C9	-2.39	122.70	126.23
47	e	848	BCR	C16-C15-C14	-2.39	118.63	123.52
44	e	821	CLA	CHB-C4A-NA	2.39	127.85	124.40
52	1	512	CHL	CAC-C3C-C4C	2.39	130.16	124.03
44	A	821	CLA	C3B-C4B-NB	-2.39	108.40	110.53
44	f	822	CLA	CHB-C4A-NA	2.39	127.84	124.40
44	A	820	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
44	2	511	CLA	C3B-C4B-NB	-2.38	108.40	110.53
47	A	845	BCR	C20-C19-C18	-2.38	119.82	126.36
44	5	311	CLA	CHB-C4A-NA	2.38	127.84	124.40
44	e	824	CLA	CHB-C4A-NA	2.38	127.84	124.40
47	e	850	BCR	C33-C5-C6	-2.38	121.89	124.48
47	B	846	BCR	C4-C5-C6	-2.38	119.49	122.70
44	3	310	CLA	O2A-CGA-O1A	-2.38	117.21	123.33
44	f	805	CLA	C2A-C1A-CHA	2.38	126.40	122.71
44	f	831	CLA	CHB-C4A-NA	2.38	127.83	124.40
44	B	827	CLA	CMA-C3A-C2A	-2.38	110.78	116.23
44	B	833	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
47	I	101	BCR	C35-C13-C12	2.38	121.72	118.09
53	s	502	XAT	C11-C12-C13	-2.38	119.84	126.36
44	L	301	CLA	C1-C2-C3	-2.38	122.30	126.20
44	A	819	CLA	O1D-CGD-CBD	2.38	129.21	124.52
44	3	318	CLA	CHB-C4A-NA	2.38	127.83	124.40
44	A	823	CLA	O1D-CGD-CBD	2.38	129.21	124.52
44	A	802	CLA	CHB-C4A-NA	2.38	127.83	124.40
44	3	301	CLA	O1D-CGD-CBD	2.37	129.20	124.52
50	2	519	LMG	O6-C5-C4	2.37	113.98	109.70
44	e	823	CLA	CAB-C3B-C4B	-2.37	121.81	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	1	517	CHL	C2A-C3A-C4A	-2.37	101.98	103.53
47	B	852	BCR	C8-C9-C10	2.37	122.74	119.01
44	A	822	CLA	CMA-C3A-C2A	-2.37	110.79	116.23
51	q	301	LUT	C31-C32-C33	-2.37	119.86	126.36
44	e	837	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
44	p	515	CLA	C3A-C2A-C1A	-2.37	103.88	106.30
44	e	852	CLA	C1-C2-C3	-2.37	122.31	126.20
44	e	837	CLA	C1-C2-C3	-2.37	122.31	126.20
47	B	849	BCR	C40-C30-C25	-2.37	106.53	110.24
52	3	302	CHL	CMA-C3A-C4A	-2.37	109.51	114.61
44	L	301	CLA	CHB-C4A-NA	2.37	127.82	124.40
44	f	813	CLA	CHB-C4A-NA	2.37	127.82	124.40
47	l	101	BCR	C11-C12-C13	-2.37	119.87	126.36
45	B	843	PQN	C11-C3-C4	2.37	121.07	118.58
52	s	517	CHL	CMB-C2B-C3B	2.37	129.41	124.68
44	s	511	CLA	C3B-C4B-NB	-2.37	108.42	110.53
52	5	315	CHL	CAC-C3C-C4C	2.37	130.11	124.03
44	1	509	CLA	CHB-C4A-NA	2.37	127.81	124.40
44	A	835	CLA	C3B-C4B-NB	-2.36	108.42	110.53
44	A	802	CLA	CMB-C2B-C1B	-2.36	121.82	125.42
44	r	311	CLA	O2D-CGD-CBD	2.36	115.36	111.23
44	A	817	CLA	CHB-C4A-NA	2.36	127.81	124.40
44	B	842	CLA	CHB-C4A-NA	2.36	127.81	124.40
44	f	806	CLA	CHB-C4A-NA	2.36	127.81	124.40
44	f	809	CLA	CHB-C4A-NA	2.36	127.81	124.40
44	B	815	CLA	O2D-CGD-CBD	2.36	115.36	111.23
44	p	511	CLA	O2D-CGD-CBD	2.36	115.36	111.23
44	e	803	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
44	q	315	CLA	CHB-C4A-NA	2.36	127.81	124.40
47	B	846	BCR	C37-C22-C21	-2.36	118.99	122.82
51	1	502	LUT	C30-C31-C32	-2.36	116.36	123.20
44	e	808	CLA	CAA-C2A-C3A	-2.36	110.81	116.23
47	r	301	BCR	C8-C7-C6	-2.36	120.69	127.00
51	3	304	LUT	C40-C33-C34	-2.36	118.99	122.82
51	1	501	LUT	C10-C11-C12	-2.36	116.36	123.20
44	q	314	CLA	C3B-C4B-NB	-2.36	108.42	110.53
47	l	101	BCR	C2-C1-C6	2.36	113.86	110.44
44	p	507	CLA	CAB-C3B-C2B	2.36	129.80	123.53
47	B	845	BCR	C29-C28-C27	-2.36	106.09	111.28
52	3	302	CHL	CAC-C3C-C4C	2.36	130.09	124.03
52	5	314	CHL	O1D-CGD-CBD	-2.36	121.15	124.72
51	1	501	LUT	C15-C14-C13	-2.36	123.97	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	s	513	CHL	OMC-CMC-C2C	-2.36	121.03	125.12
52	1	514	CHL	O2D-CGD-O1D	-2.36	119.26	123.85
44	A	824	CLA	C3B-C4B-NB	-2.36	108.43	110.53
44	s	511	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
44	3	308	CLA	O2D-CGD-CBD	2.35	115.34	111.23
47	e	854	BCR	C24-C23-C22	-2.35	122.75	126.23
44	1	509	CLA	C3B-C4B-NB	-2.35	108.43	110.53
52	p	517	CHL	CBC-CAC-C3C	-2.35	109.50	112.87
47	o	301	BCR	C23-C24-C25	-2.35	120.72	127.00
44	B	813	CLA	CHB-C4A-NA	2.35	127.79	124.40
52	2	513	CHL	CMB-C2B-C3B	2.35	129.38	124.68
44	p	515	CLA	CHB-C4A-NA	2.35	127.79	124.40
47	n	204	BCR	C20-C21-C22	-2.35	123.98	127.28
44	A	829	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
44	f	801	CLA	CHB-C4A-NA	2.35	127.79	124.40
44	B	804	CLA	CHB-C4A-NA	2.35	127.79	124.40
44	f	833	CLA	CHB-C4A-NA	2.35	127.79	124.40
47	q	303	BCR	C38-C26-C25	-2.35	121.92	124.48
44	f	840	CLA	C3B-C4B-NB	-2.35	108.44	110.53
44	A	837	CLA	CHB-C4A-NA	2.35	127.78	124.40
44	f	811	CLA	CHB-C4A-NA	2.35	127.78	124.40
44	f	825	CLA	CHB-C4A-NA	2.34	127.78	124.40
52	p	512	CHL	OMC-CMC-C2C	-2.34	121.05	125.12
51	2	501	LUT	C21-C26-C27	-2.34	110.13	112.83
47	e	854	BCR	C36-C18-C17	-2.34	119.02	122.82
44	B	808	CLA	O2D-CGD-CBD	2.34	115.33	111.23
44	5	309	CLA	C3B-C4B-NB	-2.34	108.44	110.53
44	r	310	CLA	CHB-C4A-NA	2.34	127.78	124.40
52	5	315	CHL	O2A-CGA-CBA	2.34	121.40	114.00
44	r	305	CLA	C1-C2-C3	-2.34	122.97	126.76
44	A	814	CLA	O2D-CGD-CBD	2.34	115.32	111.23
44	A	818	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
44	p	509	CLA	CHA-C4D-ND	2.34	137.38	132.55
52	r	314	CHL	O1D-CGD-CBD	-2.34	121.18	124.72
47	B	849	BCR	C8-C7-C6	-2.34	120.75	127.00
47	B	847	BCR	C34-C9-C10	-2.34	119.03	122.82
52	1	517	CHL	C2A-C1A-CHA	-2.34	117.96	121.84
52	s	517	CHL	OMC-CMC-C2C	-2.34	121.06	125.12
44	A	804	CLA	CHB-C4A-NA	2.34	127.77	124.40
44	B	810	CLA	C2D-C1D-ND	-2.34	107.81	110.13
47	L	306	BCR	C27-C26-C25	-2.34	119.55	122.70
44	B	812	CLA	CAA-CBA-CGA	-2.34	106.57	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	F	801	BCR	C8-C7-C6	-2.34	120.76	127.00
47	J	102	BCR	C8-C7-C6	-2.34	120.76	127.00
47	B	849	BCR	C16-C15-C14	-2.34	118.74	123.52
47	q	303	BCR	C37-C22-C23	2.34	121.66	118.09
44	A	809	CLA	CHB-C4A-NA	2.33	127.77	124.40
44	B	814	CLA	CHB-C4A-NA	2.33	127.77	124.40
44	3	312	CLA	CHB-C4A-NA	2.33	127.76	124.40
47	l	101	BCR	C38-C26-C25	-2.33	121.94	124.48
52	1	514	CHL	CMB-C2B-C3B	2.33	129.34	124.68
51	p	502	LUT	C38-C25-C24	-2.33	117.85	123.36
44	A	835	CLA	O2D-CGD-CBD	2.33	115.30	111.23
47	A	851	BCR	C33-C5-C4	2.33	118.56	113.60
47	j	803	BCR	C33-C5-C4	2.33	118.56	113.60
44	e	813	CLA	CHB-C4A-NA	2.33	127.76	124.40
44	e	815	CLA	CHB-C4A-NA	2.33	127.76	124.40
44	e	802	CLA	CHB-C4A-NA	2.33	127.76	124.40
44	e	826	CLA	C1-C2-C3	-2.32	122.39	126.20
44	B	839	CLA	C3B-C4B-NB	-2.32	108.45	110.53
47	e	848	BCR	C21-C20-C19	-2.32	116.47	123.20
44	B	818	CLA	O2D-CGD-CBD	2.32	115.29	111.23
47	l	102	BCR	C34-C9-C8	2.32	121.64	118.09
44	B	841	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
50	2	519	LMG	C3-C4-C5	2.32	114.44	110.23
47	A	849	BCR	C8-C9-C10	2.32	122.66	119.01
46	A	843	LHG	O7-C7-O9	-2.32	118.28	123.70
44	B	836	CLA	CHB-C4A-NA	2.32	127.75	124.40
44	e	835	CLA	C3B-C4B-NB	-2.32	108.46	110.53
44	B	826	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
52	s	512	CHL	O2D-CGD-O1D	-2.32	119.33	123.85
51	s	501	LUT	C31-C30-C29	-2.32	124.03	127.28
44	r	308	CLA	CHB-C4A-NA	2.32	127.75	124.40
44	B	801	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
47	Q	801	BCR	C36-C18-C19	2.32	121.63	118.09
52	q	313	CHL	CMD-C2D-C3D	-2.32	120.57	124.94
44	p	511	CLA	CHB-C4A-NA	2.32	127.72	124.43
44	2	506	CLA	CHB-C4A-NA	2.32	127.74	124.40
43	e	801	CL0	CAB-C3B-C2B	2.32	129.54	124.69
47	r	301	BCR	C15-C16-C17	-2.31	118.78	123.52
44	o	304	CLA	CHB-C4A-NA	2.31	127.74	124.40
47	f	849	BCR	C21-C20-C19	-2.31	116.50	123.20
44	A	837	CLA	CMB-C2B-C3B	2.31	131.99	126.55
44	p	507	CLA	C3B-C4B-NB	-2.31	107.93	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	3	314	CLA	O2D-CGD-CBD	2.31	115.27	111.23
44	p	508	CLA	CHB-C4A-NA	2.31	127.74	124.40
51	3	303	LUT	C1-C6-C5	-2.31	119.48	122.64
44	r	304	CLA	C2A-C1A-CHA	2.31	126.30	122.71
44	r	317	CLA	CHB-C4A-NA	2.31	127.73	124.40
47	o	305	BCR	C33-C5-C4	2.31	118.52	113.60
44	m	101	CLA	CHB-C4A-NA	2.31	127.73	124.40
44	5	312	CLA	C3B-C4B-NB	-2.31	108.47	110.53
44	B	820	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
44	B	834	CLA	CAA-C2A-C3A	-2.31	106.76	113.00
44	e	853	CLA	CMB-C2B-C1B	-2.31	121.91	125.42
44	A	827	CLA	CMB-C2B-C3B	2.31	131.98	126.55
44	1	509	CLA	CMB-C2B-C1B	-2.31	121.91	125.42
47	j	801	BCR	C20-C19-C18	-2.31	120.04	126.36
44	e	837	CLA	CHB-C4A-NA	2.30	127.73	124.40
44	p	509	CLA	C4B-CHC-C1C	2.30	131.67	126.25
47	K	204	BCR	C2-C1-C6	2.30	113.79	110.44
52	q	313	CHL	CMB-C2B-C3B	2.30	129.29	124.68
47	A	846	BCR	C16-C15-C14	-2.30	118.81	123.52
44	f	838	CLA	C2A-C1A-CHA	2.30	126.28	122.71
47	A	853	BCR	C33-C5-C6	-2.30	121.97	124.48
44	A	808	CLA	CHB-C4A-NA	2.30	127.72	124.40
44	K	205	CLA	CHB-C4A-NA	2.30	127.72	124.40
47	A	853	BCR	C37-C22-C21	-2.30	119.09	122.82
44	q	305	CLA	CHA-C1A-NA	-2.30	121.18	126.39
44	f	807	CLA	CMA-C3A-C2A	-2.30	110.95	116.23
44	f	829	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
44	f	839	CLA	CMA-C3A-C2A	-2.30	110.96	116.23
44	5	310	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
47	j	801	BCR	C7-C8-C9	-2.30	122.83	126.23
47	1	503	BCR	C34-C9-C10	-2.30	119.09	122.82
43	A	801	CL0	CAB-C3B-C2B	2.30	129.50	124.69
44	A	812	CLA	CHB-C4A-NA	2.30	127.71	124.40
44	f	807	CLA	CHB-C4A-NA	2.30	127.71	124.40
52	p	514	CHL	C1B-CHB-C4A	-2.30	119.85	121.32
44	q	307	CLA	C2A-C1A-CHA	2.30	126.27	122.71
52	5	315	CHL	C4C-CHD-C1D	2.30	124.28	116.07
52	r	314	CHL	CBC-CAC-C3C	-2.30	109.59	112.87
47	s	503	BCR	C38-C26-C27	2.29	118.49	113.60
44	e	832	CLA	CBA-CAA-C2A	-2.29	109.30	114.05
44	B	838	CLA	C3B-C4B-NB	-2.29	108.48	110.53
44	s	508	CLA	CHB-C4A-NA	2.29	127.71	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	p	504	CLA	CAA-C2A-C1A	2.29	117.22	112.14
52	r	316	CHL	CAC-C3C-C4C	2.29	129.92	124.03
44	r	304	CLA	CMB-C2B-C1B	-2.29	121.93	125.42
51	3	304	LUT	C15-C14-C13	-2.29	124.06	127.28
47	A	845	BCR	C16-C15-C14	-2.29	118.83	123.52
47	m	103	BCR	C29-C30-C25	2.29	113.77	110.44
51	r	302	LUT	C16-C1-C6	-2.29	106.65	110.24
44	A	842	CLA	CHB-C4A-NA	2.29	127.70	124.40
44	f	830	CLA	CMB-C2B-C3B	2.29	129.62	123.53
44	f	803	CLA	C3B-C4B-NB	-2.29	108.49	110.53
44	f	812	CLA	C3B-C4B-NB	-2.29	108.49	110.53
51	p	501	LUT	C11-C12-C13	-2.29	120.08	126.36
44	e	804	CLA	CHB-C4A-NA	2.29	127.70	124.40
47	e	854	BCR	C8-C7-C6	-2.29	120.89	127.00
44	f	830	CLA	C3B-C4B-NB	-2.29	107.95	110.33
44	e	839	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
44	f	813	CLA	C1-C2-C3	-2.29	122.45	126.20
44	m	101	CLA	CMB-C2B-C3B	2.29	129.61	123.53
47	B	845	BCR	C21-C20-C19	-2.29	116.58	123.20
47	e	851	BCR	C23-C24-C25	-2.29	120.89	127.00
44	q	308	CLA	C3B-C4B-NB	-2.29	108.49	110.53
53	5	304	XAT	C30-C31-C32	-2.29	116.58	123.20
44	q	316	CLA	CHB-C4A-NA	2.28	127.70	124.40
47	e	851	BCR	C29-C30-C25	2.28	113.76	110.44
47	e	848	BCR	C38-C26-C25	-2.28	121.99	124.48
44	A	808	CLA	C1-C2-C3	-2.28	122.46	126.20
44	B	810	CLA	C3B-C4B-NB	-2.28	108.49	110.53
44	B	819	CLA	O2D-CGD-CBD	2.28	115.22	111.23
47	L	305	BCR	C33-C5-C6	-2.28	121.99	124.48
44	A	825	CLA	CHB-C4A-NA	2.28	127.69	124.40
47	e	848	BCR	C4-C5-C6	-2.28	119.62	122.70
47	J	102	BCR	C23-C24-C25	-2.28	120.90	127.00
44	e	838	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
47	q	303	BCR	C27-C26-C25	-2.28	119.62	122.70
44	A	852	CLA	C1-C2-C3	-2.28	122.46	126.20
47	B	845	BCR	C34-C9-C10	-2.28	119.12	122.82
47	j	803	BCR	C21-C20-C19	-2.28	116.59	123.20
52	r	314	CHL	CAC-C3C-C4C	2.28	129.89	124.03
45	f	844	PQN	C11-C3-C4	2.28	120.98	118.58
47	m	103	BCR	C23-C24-C25	-2.28	120.91	127.00
44	B	824	CLA	O2A-CGA-O1A	-2.28	117.47	123.33
47	f	849	BCR	C36-C18-C19	2.28	121.57	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	s	517	CHL	O2A-CGA-CBA	2.28	120.74	112.14
47	q	303	BCR	C38-C26-C27	2.28	118.45	113.60
44	B	828	CLA	CAC-C3C-C4C	2.28	127.75	124.79
44	A	840	CLA	CHB-C4A-NA	2.28	127.69	124.40
44	3	309	CLA	C1B-NB-C4B	2.28	107.91	106.31
47	B	845	BCR	C10-C11-C12	-2.28	116.61	123.20
44	A	852	CLA	CHB-C4A-NA	2.27	127.68	124.40
44	n	202	CLA	O2D-CGD-CBD	2.27	115.20	111.23
44	e	825	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
44	p	509	CLA	CMA-C3A-C4A	2.27	117.88	111.77
44	B	814	CLA	CMA-C3A-C2A	-2.27	111.02	116.23
52	3	315	CHL	C4D-ND-C1D	-2.27	103.49	105.22
44	f	803	CLA	CHB-C4A-NA	2.27	127.68	124.40
44	1	515	CLA	CBD-CHA-C1A	2.27	131.79	127.58
44	f	801	CLA	C3B-C4B-NB	-2.27	107.97	110.33
44	f	804	CLA	C1D-ND-C4D	-2.27	104.72	106.31
44	A	852	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
52	p	514	CHL	O2D-CGD-O1D	-2.27	119.43	123.85
47	L	305	BCR	C23-C24-C25	-2.27	120.94	127.00
51	s	501	LUT	C10-C11-C12	-2.27	116.63	123.20
52	5	317	CHL	O2D-CGD-O1D	-2.27	119.43	123.85
47	o	301	BCR	C33-C5-C4	2.27	118.43	113.60
44	f	830	CLA	C2A-C1A-CHA	2.27	126.23	122.71
44	B	809	CLA	C3A-C2A-C1A	-2.27	103.98	106.30
47	e	851	BCR	C38-C26-C27	2.27	118.43	113.60
51	p	501	LUT	C31-C30-C29	-2.27	124.10	127.28
44	A	834	CLA	C2A-C3A-C4A	2.27	104.25	101.59
47	1	503	BCR	C33-C5-C4	2.27	118.43	113.60
44	r	310	CLA	O2D-CGD-CBD	2.27	115.19	111.23
47	p	503	BCR	C39-C30-C25	-2.27	106.69	110.24
47	2	503	BCR	C34-C9-C10	-2.27	119.15	122.82
44	B	838	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
44	s	509	CLA	O2A-CGA-O1A	-2.26	117.96	123.63
44	p	513	CLA	O2A-CGA-O1A	-2.26	117.96	123.63
47	e	848	BCR	C23-C24-C25	-2.26	120.95	127.00
44	q	305	CLA	CHB-C4A-NA	2.26	127.66	124.40
44	e	815	CLA	C3B-C4B-NB	-2.26	108.51	110.53
44	2	506	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
44	5	316	CLA	C3B-C4B-NB	-2.26	108.51	110.53
44	f	804	CLA	C4B-CHC-C1C	2.26	131.56	126.25
44	r	317	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
44	q	309	CLA	CMB-C2B-C1B	-2.26	121.98	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	o	305	BCR	C3-C4-C5	-2.26	110.03	114.06
44	q	307	CLA	CHB-C4A-NA	2.26	127.66	124.40
44	A	821	CLA	CHB-C4A-NA	2.26	127.66	124.40
44	s	514	CLA	C2A-C1A-CHA	2.26	126.21	122.71
44	B	819	CLA	CHB-C4A-NA	2.26	127.66	124.40
47	3	305	BCR	C35-C13-C14	-2.26	119.16	122.82
47	F	804	BCR	C15-C16-C17	-2.25	118.91	123.52
44	L	304	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
43	A	801	CL0	C1-O2A-CGA	2.25	121.57	112.40
44	5	305	CLA	CMB-C2B-C3B	2.25	130.02	124.63
44	r	307	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
44	e	827	CLA	O2D-CGD-CBD	2.25	115.17	111.23
44	f	829	CLA	C3B-C4B-NB	-2.25	108.52	110.53
52	r	314	CHL	C5-C3-C4	2.25	119.77	114.59
51	1	502	LUT	C38-C25-C24	-2.25	118.03	123.36
44	f	811	CLA	C1-C2-C3	-2.25	122.51	126.20
44	F	803	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
44	5	310	CLA	CMB-C2B-C1B	-2.25	121.99	125.42
47	A	853	BCR	C31-C1-C6	-2.25	106.71	110.24
44	L	304	CLA	C3B-C4B-NB	-2.25	108.52	110.53
51	q	302	LUT	C39-C29-C28	2.25	121.52	118.09
44	e	829	CLA	CHB-C4A-NA	2.25	127.64	124.40
52	2	513	CHL	CED-O2D-CGD	2.25	121.02	115.92
44	2	507	CLA	O1D-CGD-CBD	2.25	128.95	124.52
47	j	801	BCR	C15-C14-C13	-2.25	124.13	127.28
52	s	515	CHL	O2D-CGD-O1D	-2.25	119.47	123.85
44	B	820	CLA	CHB-C4A-NA	2.25	127.64	124.40
44	e	807	CLA	O2D-CGD-CBD	2.25	115.16	111.23
43	e	801	CL0	C1-O2A-CGA	2.25	121.54	112.40
52	2	516	CHL	C4C-CHD-C1D	2.25	124.10	116.07
52	r	314	CHL	CMA-C3A-C4A	-2.25	109.77	114.61
53	r	303	XAT	C19-C9-C8	2.24	121.52	118.09
44	B	802	CLA	C7-C6-C5	-2.24	109.61	114.47
51	1	501	LUT	C18-C5-C4	2.24	118.55	114.42
44	p	505	CLA	CMB-C2B-C3B	2.24	131.83	126.55
44	e	830	CLA	CHB-C4A-NA	2.24	127.64	124.40
44	B	802	CLA	C3B-C4B-NB	-2.24	108.53	110.53
47	A	851	BCR	C10-C11-C12	-2.24	116.70	123.20
44	1	513	CLA	CHB-C4A-NA	2.24	127.63	124.40
49	B	850	DGD	C3G-C2G-C1G	-2.24	106.56	111.78
44	q	304	CLA	CMA-C3A-C2A	-2.24	111.09	116.23
44	1	508	CLA	C3B-C4B-NB	-2.24	108.53	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	B	848	BCR	C39-C30-C25	-2.24	106.73	110.24
44	e	818	CLA	C4B-CHC-C1C	2.24	131.51	126.25
44	e	820	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
44	j	802	CLA	CHB-C4A-NA	2.24	127.63	124.40
47	e	847	BCR	C21-C20-C19	-2.24	116.72	123.20
44	5	307	CLA	CHB-C4A-NA	2.24	127.63	124.40
44	B	829	CLA	CHB-C4A-NA	2.24	127.63	124.40
44	r	311	CLA	CHB-C4A-NA	2.24	127.63	124.40
44	L	302	CLA	O2D-CGD-O1D	-2.24	119.50	123.85
44	A	803	CLA	CMA-C3A-C2A	-2.24	111.10	116.23
44	p	509	CLA	CHD-C1D-ND	-2.24	121.66	124.80
44	A	826	CLA	CHB-C4A-NA	2.23	127.62	124.40
44	p	509	CLA	CMD-C2D-C3D	-2.23	122.56	127.69
44	B	830	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
44	B	802	CLA	CHB-C4A-NA	2.23	127.62	124.40
44	B	811	CLA	CHB-C4A-NA	2.23	127.62	124.40
44	p	507	CLA	CMB-C2B-C3B	2.23	129.47	123.53
44	L	303	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
44	s	507	CLA	CHB-C4A-NA	2.23	127.62	124.40
44	2	504	CLA	C3B-C4B-NB	-2.23	108.54	110.53
47	o	301	BCR	C21-C20-C19	-2.23	116.74	123.20
52	r	314	CHL	OMC-CMC-C2C	-2.23	121.25	125.12
44	e	818	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
52	r	314	CHL	CMB-C2B-C3B	2.23	129.14	124.68
52	3	302	CHL	O2A-CGA-CBA	2.23	120.56	112.14
47	A	847	BCR	C11-C12-C13	-2.23	120.25	126.36
44	f	826	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
52	r	316	CHL	C4C-CHD-C1D	2.23	124.05	116.07
47	B	844	BCR	C40-C30-C25	-2.23	106.75	110.24
44	1	507	CLA	O1D-CGD-CBD	2.23	128.91	124.52
44	e	812	CLA	CHB-C4A-NA	2.23	127.62	124.40
50	5	301	LMG	O7-C10-O9	-2.23	118.50	123.70
52	2	512	CHL	O2D-CGD-O1D	-2.23	119.51	123.85
52	p	514	CHL	CAC-C3C-C4C	2.23	129.76	124.03
52	5	317	CHL	C4C-CHD-C1D	2.23	124.04	116.07
47	n	204	BCR	C20-C19-C18	-2.23	120.25	126.36
47	A	845	BCR	C7-C8-C9	-2.23	122.94	126.23
47	o	301	BCR	C38-C26-C27	2.23	118.34	113.60
52	2	512	CHL	CAC-C3C-C4C	2.23	129.75	124.03
44	q	311	CLA	CHB-C4A-NA	2.23	127.61	124.40
44	3	312	CLA	CAC-C3C-C4C	2.23	127.69	124.79
44	5	310	CLA	C3B-C4B-NB	-2.22	108.54	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	A	823	CLA	CHB-C4A-NA	2.22	127.59	124.43
47	I	101	BCR	C16-C15-C14	-2.22	118.97	123.52
47	B	846	BCR	C36-C18-C17	-2.22	119.21	122.82
44	f	811	CLA	CAC-C3C-C4C	2.22	127.68	124.79
47	B	852	BCR	C21-C20-C19	-2.22	116.76	123.20
51	q	301	LUT	C8-C7-C6	-2.22	121.06	127.00
44	3	318	CLA	CMB-C2B-C3B	2.22	129.44	123.53
44	f	807	CLA	CAA-C2A-C3A	-2.22	111.14	116.23
44	3	314	CLA	C1-C2-C3	-2.22	122.56	126.20
52	2	516	CHL	O1D-CGD-CBD	-2.22	121.36	124.72
47	B	845	BCR	C35-C13-C14	-2.22	119.22	122.82
53	s	502	XAT	O4-C5-C6	-2.22	57.17	58.93
47	e	851	BCR	C31-C1-C6	-2.22	106.76	110.24
47	e	847	BCR	C10-C11-C12	-2.22	116.77	123.20
44	B	816	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
44	e	843	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
44	B	818	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
49	J	103	DGD	C6D-O5D-C1E	-2.22	109.04	113.80
44	e	818	CLA	CHA-C4D-ND	2.22	137.12	132.55
46	2	517	LHG	O8-C23-O10	-2.22	118.08	123.63
44	3	310	CLA	C3B-C4B-NB	-2.22	108.55	110.53
47	n	204	BCR	C37-C22-C23	2.22	121.47	118.09
47	f	846	BCR	C29-C30-C25	2.21	113.66	110.44
44	j	802	CLA	C3B-C4B-NB	-2.21	108.55	110.53
44	r	306	CLA	CHB-C4A-NA	2.21	127.59	124.40
44	3	318	CLA	C3B-C4B-NB	-2.21	108.03	110.33
47	I	101	BCR	C3-C4-C5	-2.21	110.11	114.06
44	5	312	CLA	CHB-C4A-NA	2.21	127.59	124.40
51	r	302	LUT	C11-C10-C9	-2.21	124.18	127.28
47	A	845	BCR	C23-C24-C25	-2.21	121.10	127.00
52	r	314	CHL	C4D-ND-C1D	-2.21	103.54	105.22
51	5	303	LUT	C30-C31-C32	-2.21	116.80	123.20
45	A	841	PQN	C14-C13-C15	2.21	119.06	115.23
51	2	501	LUT	C35-C15-C14	-2.21	119.00	123.52
44	B	818	CLA	CMB-C2B-C1B	-2.21	122.06	125.42
47	f	847	BCR	C1-C6-C5	-2.21	119.62	122.64
47	j	803	BCR	C27-C26-C25	-2.21	119.72	122.70
51	3	303	LUT	C19-C9-C8	2.21	121.46	118.09
44	o	304	CLA	C3B-C4B-NB	-2.21	108.56	110.53
47	f	847	BCR	C4-C5-C6	-2.21	119.72	122.70
52	s	513	CHL	CAC-C3C-C4C	2.21	129.70	124.03
47	F	804	BCR	C31-C1-C6	-2.21	106.78	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	r	316	CHL	O2D-CGD-O1D	-2.20	119.56	123.85
44	A	813	CLA	CHB-C4A-NA	2.20	127.58	124.40
46	O	601	LHG	O8-C23-C24	2.20	118.56	111.83
50	5	301	LMG	O8-C28-C29	2.20	118.56	111.83
44	p	513	CLA	C1-C2-C3	-2.20	122.59	126.20
44	B	812	CLA	CAB-C3B-C2B	2.20	129.39	123.53
47	l	101	BCR	C34-C9-C10	-2.20	119.25	122.82
53	s	502	XAT	C31-C32-C33	-2.20	120.33	126.36
44	f	809	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
47	K	204	BCR	C36-C18-C17	-2.20	119.25	122.82
53	5	304	XAT	C31-C30-C29	-2.20	124.19	127.28
52	r	313	CHL	O2A-CGA-CBA	2.20	120.45	112.14
47	B	848	BCR	C23-C24-C25	-2.20	121.12	127.00
47	f	849	BCR	C38-C26-C27	2.20	118.28	113.60
52	2	513	CHL	CAD-C3D-C4D	2.20	113.65	110.21
52	2	512	CHL	C4C-CHD-C1D	2.20	123.94	116.07
44	A	838	CLA	CHB-C4A-NA	2.20	127.57	124.40
44	A	835	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
52	2	513	CHL	CAC-C3C-C4C	2.20	129.68	124.03
44	s	504	CLA	O1D-CGD-CBD	2.20	128.85	124.52
52	r	316	CHL	CED-O2D-CGD	2.20	120.89	115.92
52	s	513	CHL	CMA-C3A-C4A	-2.20	109.88	114.61
47	F	801	BCR	C35-C13-C12	2.19	121.44	118.09
44	5	316	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
47	J	102	BCR	C21-C20-C19	-2.19	116.84	123.20
44	q	310	CLA	CHB-C4A-NA	2.19	127.57	124.40
49	B	850	DGD	O3G-C1D-C2D	-2.19	104.94	108.27
44	e	817	CLA	CMA-C3A-C2A	-2.19	111.20	116.23
52	p	512	CHL	CBC-CAC-C3C	-2.19	109.73	112.87
47	K	204	BCR	C24-C23-C22	-2.19	122.99	126.23
44	A	830	CLA	CHB-C4A-NA	2.19	127.56	124.40
44	f	815	CLA	CHB-C4A-NA	2.19	127.56	124.40
44	2	509	CLA	C1-C2-C3	-2.19	123.22	126.76
44	q	315	CLA	C3B-C4B-NB	-2.19	108.57	110.53
44	e	841	CLA	CMA-C3A-C2A	-2.19	111.20	116.23
44	B	812	CLA	CMB-C2B-C3B	2.19	129.35	123.53
44	e	823	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
44	p	509	CLA	C1-O2A-CGA	2.19	121.95	116.65
44	L	303	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
52	s	517	CHL	CMA-C3A-C4A	-2.19	109.89	114.61
44	2	510	CLA	O2D-CGD-CBD	2.19	115.06	111.23
44	3	317	CLA	O2D-CGD-CBD	2.19	115.06	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	s	517	CHL	C1B-CHB-C4A	2.19	122.73	121.32
47	e	848	BCR	C15-C16-C17	-2.19	119.04	123.52
52	2	516	CHL	O2D-CGD-O1D	-2.19	119.59	123.85
44	A	823	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
47	B	849	BCR	C2-C1-C6	2.19	113.61	110.44
44	1	506	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
44	r	304	CLA	C3B-C4B-NB	-2.19	108.06	110.33
44	1	508	CLA	CHB-C4A-NA	2.18	127.55	124.40
44	e	811	CLA	CMA-C3A-C2A	-2.18	111.22	116.23
44	1	513	CLA	C1-C2-C3	-2.18	122.62	126.20
44	A	818	CLA	C2A-C1A-CHA	2.18	126.10	122.71
52	p	514	CHL	O2A-CGA-CBA	2.18	120.38	112.14
52	5	317	CHL	C4A-C3A-C2A	-2.18	99.67	103.96
51	q	302	LUT	C31-C30-C29	-2.18	124.22	127.28
44	f	821	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
47	B	847	BCR	C19-C18-C17	-2.18	115.58	119.01
44	B	826	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
44	1	508	CLA	CMB-C2B-C3B	2.18	131.68	126.55
44	m	101	CLA	C3B-C4B-NB	-2.18	108.06	110.33
51	r	302	LUT	C8-C7-C6	-2.18	121.17	127.00
44	5	309	CLA	CHB-C4A-NA	2.18	127.55	124.40
47	e	854	BCR	C19-C18-C17	2.18	122.44	119.01
44	f	829	CLA	CHB-C4A-NA	2.18	127.54	124.40
52	r	316	CHL	OMC-CMC-C2C	-2.18	121.34	125.12
47	s	503	BCR	C33-C5-C4	2.18	118.24	113.60
44	q	308	CLA	CMB-C2B-C3B	2.18	131.67	126.55
44	p	506	CLA	CHB-C4A-NA	2.18	127.54	124.40
52	s	515	CHL	CAC-C3C-C4C	2.18	129.62	124.03
47	s	503	BCR	C12-C13-C14	-2.18	115.59	119.01
47	B	844	BCR	C35-C13-C14	-2.18	119.29	122.82
44	f	832	CLA	C2A-C1A-CHA	2.17	126.08	122.71
44	1	511	CLA	CAA-C2A-C3A	-2.17	107.13	113.00
47	A	849	BCR	C35-C13-C12	2.17	121.41	118.09
47	F	801	BCR	C34-C9-C8	2.17	121.41	118.09
47	o	301	BCR	C3-C4-C5	-2.17	110.18	114.06
44	B	831	CLA	CHB-C4A-NA	2.17	127.53	124.40
47	f	847	BCR	C38-C26-C27	2.17	118.22	113.60
44	A	838	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
44	A	827	CLA	CHB-C4A-NA	2.17	127.53	124.40
44	f	830	CLA	CAB-C3B-C4B	-2.17	122.12	125.42
44	p	510	CLA	CHB-C4A-NA	2.17	127.53	124.40
44	f	816	CLA	CMB-C2B-C1B	-2.17	122.12	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	s	501	LUT	C22-C23-C24	2.17	114.40	111.18
47	A	853	BCR	C30-C25-C26	-2.17	119.67	122.64
44	B	822	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
43	A	801	CL0	C4C-C3C-C2C	-2.17	104.81	113.37
47	f	850	BCR	C33-C5-C4	2.17	118.22	113.60
44	q	312	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
47	e	846	BCR	C34-C9-C8	2.16	121.39	118.09
47	j	801	BCR	C11-C10-C9	-2.16	124.24	127.28
44	B	803	CLA	O1D-CGD-CBD	2.16	128.78	124.52
44	f	827	CLA	CHB-C4A-NA	2.16	127.50	124.43
44	e	827	CLA	CHB-C4A-NA	2.16	127.52	124.40
44	3	311	CLA	C3B-C4B-NB	-2.16	108.60	110.53
44	f	805	CLA	CMB-C2B-C3B	2.16	131.63	126.55
47	F	804	BCR	C33-C5-C4	2.16	118.20	113.60
47	m	103	BCR	C4-C5-C6	-2.16	119.78	122.70
44	e	835	CLA	CHB-C4A-NA	2.16	127.52	124.40
44	B	801	CLA	O2D-CGD-CBD	2.16	115.01	111.23
44	1	504	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
43	e	801	CL0	C4C-C3C-C2C	-2.16	104.84	113.37
52	5	314	CHL	O2A-CGA-CBA	2.16	120.30	112.14
44	p	509	CLA	CAC-C3C-C4C	2.16	127.60	124.79
51	1	502	LUT	C16-C1-C6	-2.16	106.86	110.24
47	1	503	BCR	C11-C12-C13	-2.16	120.44	126.36
44	B	827	CLA	O2D-CGD-CBD	2.16	115.00	111.23
44	1	509	CLA	CMB-C2B-C3B	2.16	131.62	126.55
44	e	843	CLA	CHB-C4A-NA	2.16	127.51	124.40
44	A	836	CLA	C3A-C2A-C1A	2.16	104.57	101.34
47	A	851	BCR	C11-C10-C9	-2.16	124.25	127.28
44	e	824	CLA	O1D-CGD-CBD	2.16	128.77	124.52
44	B	811	CLA	CMB-C2B-C1B	-2.16	122.14	125.42
52	q	313	CHL	O2A-CGA-CBA	2.16	120.29	112.14
47	L	306	BCR	C20-C21-C22	-2.16	124.25	127.28
44	e	837	CLA	CMB-C2B-C1B	-2.16	122.14	125.42
51	p	501	LUT	C19-C9-C10	-2.16	119.32	122.82
44	L	304	CLA	O2A-CGA-O1A	-2.16	117.79	123.33
53	5	304	XAT	C19-C9-C8	2.16	121.38	118.09
47	s	503	BCR	C24-C25-C26	2.16	126.52	121.56
44	f	819	CLA	CMA-C3A-C2A	-2.16	111.29	116.23
47	f	845	BCR	C20-C19-C18	-2.16	120.45	126.36
52	s	512	CHL	CAC-C3C-C4C	2.15	129.57	124.03
47	q	303	BCR	C8-C7-C6	-2.15	121.25	127.00
52	r	316	CHL	CMA-C3A-C4A	-2.15	109.97	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	e	812	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
44	A	805	CLA	C1-C2-C3	-2.15	122.67	126.20
52	2	516	CHL	CMD-C2D-C3D	-2.15	120.38	124.68
52	1	512	CHL	O2D-CGD-O1D	-2.15	119.66	123.85
44	5	316	CLA	CMA-C3A-C2A	-2.15	111.29	116.23
44	B	825	CLA	CMB-C2B-C3B	2.15	131.61	126.55
51	5	303	LUT	C10-C11-C12	-2.15	116.97	123.20
47	L	306	BCR	C34-C9-C8	2.15	121.37	118.09
52	1	512	CHL	O2A-CGA-CBA	2.15	120.27	112.14
47	3	305	BCR	C23-C24-C25	-2.15	121.25	127.00
51	q	302	LUT	C20-C13-C12	2.15	121.37	118.09
44	A	820	CLA	CHD-C1D-ND	-2.15	121.78	124.80
44	5	313	CLA	CHB-C4A-NA	2.15	127.50	124.40
44	B	803	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
44	B	824	CLA	CHB-C4A-NA	2.15	127.50	124.40
47	B	848	BCR	C35-C13-C12	2.15	121.37	118.09
47	e	851	BCR	C11-C12-C13	-2.15	120.48	126.36
47	K	204	BCR	C33-C5-C4	2.15	118.17	113.60
51	p	501	LUT	C39-C29-C28	2.15	121.37	118.09
52	q	313	CHL	CBC-CAC-C3C	-2.15	109.80	112.87
44	5	306	CLA	CHB-C4A-NA	2.15	127.50	124.40
44	B	827	CLA	CMB-C2B-C3B	2.15	131.60	126.55
51	p	502	LUT	C11-C12-C13	-2.15	120.48	126.36
44	A	837	CLA	O2D-CGD-CBD	2.15	114.98	111.23
44	e	833	CLA	CMA-C3A-C2A	-2.14	111.31	116.23
47	o	305	BCR	C8-C7-C6	-2.14	121.27	127.00
47	l	101	BCR	C36-C18-C19	2.14	121.36	118.09
47	L	305	BCR	C34-C9-C10	-2.14	119.34	122.82
44	e	831	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
52	2	516	CHL	CMA-C3A-C4A	-2.14	110.00	114.61
52	2	513	CHL	OMC-CMC-C2C	-2.14	121.40	125.12
53	r	303	XAT	C35-C15-C14	-2.14	119.14	123.52
44	B	810	CLA	C2A-C1A-CHA	2.14	126.03	122.71
52	2	513	CHL	C4C-CHD-C1D	2.14	123.73	116.07
47	K	204	BCR	C23-C24-C25	-2.14	121.28	127.00
44	f	807	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
47	A	847	BCR	C36-C18-C19	2.14	121.36	118.09
44	B	826	CLA	CMB-C2B-C3B	2.14	131.58	126.55
44	L	304	CLA	CAC-C3C-C2C	-2.14	123.63	127.56
44	e	829	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
44	3	313	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
44	e	853	CLA	O2D-CGD-CBD	2.14	114.97	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	B	834	CLA	CAA-C2A-C1A	-2.14	104.97	111.97
47	2	503	BCR	C3-C2-C1	-2.14	106.87	114.43
44	f	829	CLA	CMB-C2B-C3B	2.14	131.57	126.55
44	A	831	CLA	CHB-C4A-NA	2.14	127.48	124.40
44	5	305	CLA	O1D-CGD-CBD	2.13	128.73	124.52
44	e	827	CLA	CMA-C3A-C2A	-2.13	111.33	116.23
44	3	309	CLA	CMB-C2B-C3B	2.13	129.74	124.63
47	e	851	BCR	C15-C16-C17	-2.13	119.15	123.52
44	1	513	CLA	O2D-CGD-CBD	2.13	114.96	111.23
44	f	831	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
47	n	204	BCR	C23-C24-C25	-2.13	121.30	127.00
44	3	301	CLA	CMA-C3A-C2A	-2.13	111.34	116.23
53	5	304	XAT	C35-C34-C33	-2.13	124.29	127.28
44	e	838	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
52	3	302	CHL	C4C-CHD-C1D	2.13	123.70	116.07
44	3	316	CLA	CMA-C3A-C2A	-2.13	111.34	116.23
44	B	806	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
44	B	815	CLA	CHB-C4A-NA	2.13	127.48	124.40
46	e	844	LHG	O7-C7-O9	-2.13	118.72	123.70
52	r	314	CHL	C4C-CHD-C1D	2.13	123.69	116.07
44	e	829	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
44	K	201	CLA	C2A-C1A-CHA	2.13	127.55	123.86
47	n	204	BCR	C35-C13-C12	2.13	121.34	118.09
44	B	815	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
47	A	845	BCR	C39-C30-C25	-2.13	106.91	110.24
44	B	828	CLA	CHB-C4A-NA	2.13	127.47	124.40
44	K	203	CLA	CHB-C4A-NA	2.13	127.47	124.40
44	L	301	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
44	A	827	CLA	O1D-CGD-CBD	2.13	128.71	124.52
52	1	512	CHL	C4C-CHD-C1D	2.13	123.67	116.07
44	p	509	CLA	CHA-C1A-NA	-2.13	121.58	126.39
44	n	205	CLA	CHB-C4A-NA	2.12	127.47	124.40
46	A	844	LHG	O8-C23-C24	2.12	118.31	111.83
44	A	839	CLA	O2D-CGD-CBD	2.12	114.94	111.23
44	f	826	CLA	C1-C2-C3	-2.12	122.72	126.20
52	p	517	CHL	CAA-C2A-C1A	-2.12	109.15	113.35
44	B	839	CLA	O1D-CGD-CBD	2.12	128.71	124.52
44	e	832	CLA	CHB-C4A-NA	2.12	127.46	124.40
47	L	305	BCR	C16-C15-C14	-2.12	119.18	123.52
44	q	305	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
44	f	804	CLA	CHA-C1A-NA	-2.12	121.59	126.39
47	j	801	BCR	C34-C9-C8	2.12	121.33	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	q	312	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
52	p	512	CHL	O2A-CGA-CBA	2.12	120.15	112.14
44	A	826	CLA	C2D-C1D-ND	-2.12	108.03	110.13
44	q	304	CLA	CHB-C4A-NA	2.12	127.46	124.40
44	f	840	CLA	O2D-CGD-CBD	2.12	114.93	111.23
47	F	801	BCR	C16-C15-C14	-2.12	119.19	123.52
44	B	827	CLA	C2A-C3A-C4A	2.12	104.07	101.59
52	5	315	CHL	CMB-C2B-C3B	2.12	128.91	124.68
44	A	826	CLA	O1D-CGD-CBD	2.12	128.69	124.52
53	s	502	XAT	C20-C13-C14	-2.12	119.39	122.82
44	B	828	CLA	O2D-CGD-CBD	2.12	114.93	111.23
44	p	505	CLA	C3B-C4B-NB	-2.12	108.64	110.53
44	2	508	CLA	CHB-C4A-NA	2.12	127.45	124.40
44	p	506	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
47	e	849	BCR	C23-C24-C25	-2.12	121.35	127.00
47	A	848	BCR	C3-C4-C5	-2.11	110.28	114.06
44	e	823	CLA	C3B-C4B-NB	-2.11	108.13	110.33
44	A	813	CLA	O2A-CGA-O1A	-2.11	117.89	123.33
44	e	824	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
44	A	815	CLA	CHB-C4A-NA	2.11	127.45	124.40
54	Q	803	SQD	O48-C23-O10	-2.11	118.34	123.63
44	e	804	CLA	C1-C2-C3	-2.11	122.74	126.20
44	B	803	CLA	CHB-C4A-NA	2.11	127.45	124.40
52	s	512	CHL	O2A-CGA-CBA	2.11	120.11	112.14
44	A	815	CLA	O2A-CGA-O1A	-2.11	117.90	123.33
44	f	808	CLA	CBA-CAA-C2A	-2.11	110.56	114.28
51	1	501	LUT	C35-C15-C14	-2.11	119.20	123.52
44	1	515	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
47	f	849	BCR	C11-C12-C13	-2.11	120.58	126.36
44	A	808	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
47	e	854	BCR	C37-C22-C23	2.11	121.31	118.09
44	r	307	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
44	A	816	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
44	A	834	CLA	CHB-C4A-NA	2.11	127.44	124.40
51	1	502	LUT	C39-C29-C28	2.11	121.31	118.09
44	e	824	CLA	C1-C2-C3	-2.11	122.75	126.20
44	q	311	CLA	O2D-CGD-CBD	2.11	114.91	111.23
44	s	510	CLA	CHB-C4A-NA	2.11	127.44	124.40
44	f	808	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
44	n	205	CLA	C3B-C4B-NB	-2.10	108.65	110.53
46	p	516	LHG	O7-C7-O9	-2.10	118.78	123.70
53	2	502	XAT	C40-C33-C34	-2.10	119.41	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	A	838	CLA	O1D-CGD-CBD	2.10	128.67	124.52
44	o	304	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
52	1	517	CHL	C4C-CHD-C1D	2.10	123.59	116.07
44	A	820	CLA	C1-C2-C3	-2.10	122.75	126.20
44	K	202	CLA	CHB-C4A-NA	2.10	127.43	124.40
51	p	501	LUT	C20-C13-C14	-2.10	119.41	122.82
44	s	507	CLA	CMA-C3A-C2A	-2.10	111.41	116.23
47	e	846	BCR	C33-C5-C4	2.10	118.08	113.60
50	r	318	LMG	C7-O1-C1	-2.10	109.29	113.80
44	e	825	CLA	CMB-C2B-C3B	2.10	131.49	126.55
47	j	803	BCR	C34-C9-C10	-2.10	119.42	122.82
47	K	204	BCR	C31-C1-C6	-2.10	106.95	110.24
44	e	809	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
44	B	807	CLA	C1-C2-C3	-2.10	122.76	126.20
44	A	808	CLA	CAA-C2A-C3A	-2.10	107.33	113.00
53	2	502	XAT	O4-C5-C6	-2.10	57.27	58.93
52	s	515	CHL	C4C-CHD-C1D	2.10	123.57	116.07
44	B	807	CLA	CMB-C2B-C1B	-2.10	122.23	125.42
52	2	516	CHL	C4D-ND-C1D	-2.10	103.63	105.22
44	B	814	CLA	C3B-C4B-NB	-2.09	108.66	110.53
44	B	814	CLA	C2A-C3A-C4A	2.09	104.05	101.59
47	A	846	BCR	C27-C26-C25	-2.09	119.87	122.70
44	e	819	CLA	O2D-CGD-CBD	2.09	114.89	111.23
44	B	806	CLA	C2A-C1A-CHA	2.09	125.96	122.71
44	A	834	CLA	CMA-C3A-C2A	-2.09	111.43	116.23
44	A	810	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
47	e	854	BCR	C33-C5-C4	2.09	118.06	113.60
44	A	811	CLA	CHB-C4A-NA	2.09	127.42	124.40
44	A	820	CLA	CMB-C2B-C3B	2.09	131.47	126.55
44	B	837	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
47	q	303	BCR	C34-C9-C8	2.09	121.28	118.09
51	3	304	LUT	C38-C25-C24	-2.09	118.41	123.36
44	A	812	CLA	CMB-C2B-C3B	2.09	131.47	126.55
47	A	845	BCR	C37-C22-C21	-2.09	119.43	122.82
44	q	315	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
51	r	302	LUT	C15-C35-C34	-2.09	119.25	123.52
44	e	829	CLA	C1-C2-C3	-2.09	122.78	126.20
47	J	102	BCR	C15-C16-C17	-2.09	119.25	123.52
47	F	804	BCR	C1-C6-C5	-2.09	119.78	122.64
44	f	813	CLA	CMB-C2B-C3B	2.09	129.08	123.53
46	e	845	LHG	O7-C7-O9	-2.09	118.82	123.70
44	p	509	CLA	C3D-C2D-C1D	-2.09	102.98	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	2	518	LMG	O6-C5-C4	2.09	113.31	109.55
44	f	842	CLA	CMA-C3A-C2A	-2.09	111.44	116.23
52	3	315	CHL	O2D-CGD-O1D	-2.09	119.79	123.85
45	A	841	PQN	C2M-C2-C1	2.09	120.52	116.68
52	5	314	CHL	C4C-CHD-C1D	2.09	123.53	116.07
53	r	303	XAT	C11-C10-C9	-2.09	124.35	127.28
44	B	825	CLA	C2A-C1A-CHA	2.09	127.49	123.87
44	A	838	CLA	CMB-C2B-C3B	2.09	131.46	126.55
44	B	839	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
51	3	303	LUT	C12-C13-C14	-2.08	115.73	119.01
44	r	309	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
47	B	847	BCR	C10-C11-C12	-2.08	117.17	123.20
50	2	519	LMG	C8-O7-C10	-2.08	112.81	117.80
52	s	517	CHL	C4C-CHD-C1D	2.08	123.52	116.07
44	B	817	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
52	2	515	CHL	CMD-C2D-C3D	-2.08	120.53	124.68
44	e	821	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
44	A	812	CLA	O2D-CGD-CBD	2.08	114.87	111.23
44	A	816	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
44	K	201	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
44	f	821	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
44	f	826	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
44	K	202	CLA	O2D-CGD-CBD	2.08	114.86	111.23
51	5	303	LUT	C21-C26-C27	-2.08	110.44	112.83
47	n	204	BCR	C10-C11-C12	-2.08	117.19	123.20
44	2	507	CLA	C4-C3-C5	-2.08	109.25	114.96
47	s	503	BCR	C28-C29-C30	-2.07	107.08	114.43
47	B	846	BCR	C36-C18-C19	2.07	121.26	118.09
47	2	503	BCR	C38-C26-C27	2.07	118.02	113.60
51	5	303	LUT	C11-C10-C9	-2.07	124.37	127.28
44	f	827	CLA	CMB-C2B-C1B	-2.07	122.26	125.42
44	B	837	CLA	CHA-C1A-NA	-2.07	121.70	126.39
44	A	821	CLA	CAA-C2A-C1A	-2.07	107.56	112.14
44	A	829	CLA	CHB-C1B-NB	2.07	127.16	124.05
47	B	848	BCR	C8-C7-C6	-2.07	121.47	127.00
44	3	314	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
44	B	828	CLA	O1D-CGD-CBD	2.07	128.60	124.52
46	B	851	LHG	O7-C7-O9	-2.07	118.87	123.70
47	n	204	BCR	C2-C1-C6	2.07	113.44	110.44
44	B	832	CLA	CHB-C4A-NA	2.07	127.38	124.40
44	e	810	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
44	L	302	CLA	CMB-C2B-C1B	-2.07	122.27	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	n	204	BCR	C38-C26-C27	2.07	118.00	113.60
44	A	823	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
44	B	841	CLA	C1-C2-C3	-2.07	122.81	126.20
44	B	841	CLA	O1D-CGD-CBD	2.07	128.59	124.52
51	5	303	LUT	C8-C7-C6	-2.07	121.48	127.00
47	l	102	BCR	C2-C1-C6	2.07	113.44	110.44
44	f	835	CLA	O2A-CGA-O1A	-2.07	118.02	123.33
44	e	836	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
47	A	853	BCR	C21-C20-C19	-2.06	117.22	123.20
44	s	507	CLA	CAA-C2A-C3A	-2.06	111.50	116.23
52	2	515	CHL	C4C-CHD-C1D	2.06	123.45	116.07
44	q	309	CLA	CMB-C2B-C3B	2.06	131.40	126.55
47	5	302	BCR	C24-C23-C22	-2.06	123.18	126.23
44	e	830	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
44	q	304	CLA	CAA-C2A-C3A	-2.06	111.50	116.23
44	e	853	CLA	CMB-C2B-C3B	2.06	131.40	126.55
44	B	802	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
47	p	503	BCR	C30-C25-C24	2.06	121.24	115.65
47	B	845	BCR	C33-C5-C4	2.06	117.99	113.60
44	r	317	CLA	O2D-CGD-CBD	2.06	114.83	111.23
44	p	509	CLA	C2D-C1D-ND	2.06	112.16	110.13
47	F	801	BCR	C3-C4-C5	-2.06	110.39	114.06
52	p	517	CHL	C4C-CHD-C1D	2.06	123.43	116.07
44	B	806	CLA	CMB-C2B-C3B	2.06	131.39	126.55
44	e	806	CLA	O2D-CGD-CBD	2.06	114.82	111.23
44	B	814	CLA	CHA-C1A-NA	-2.06	121.74	126.39
47	A	849	BCR	C33-C5-C6	-2.06	122.24	124.48
47	e	854	BCR	C35-C13-C14	-2.06	119.49	122.82
44	A	836	CLA	CHB-C4A-NA	2.06	127.37	124.40
47	A	851	BCR	C30-C25-C24	2.06	121.22	115.65
44	A	812	CLA	CHB-C1B-NB	2.06	127.13	124.05
44	p	511	CLA	C2A-C1A-CHA	2.05	125.90	122.71
44	2	509	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
47	B	844	BCR	C23-C24-C25	-2.05	121.51	127.00
44	3	318	CLA	O1D-CGD-CBD	2.05	128.57	124.52
44	q	304	CLA	C1C-NC-C4C	2.05	107.61	106.68
52	1	517	CHL	C3D-C4D-ND	2.05	116.23	112.94
44	r	307	CLA	CMB-C2B-C3B	2.05	131.38	126.55
44	r	305	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
44	f	808	CLA	C1-C2-C3	-2.05	122.84	126.20
44	A	811	CLA	C2A-C1A-CHA	2.05	125.89	122.71
44	q	314	CLA	CMB-C2B-C3B	2.05	131.37	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	3	307	CLA	C2A-C1A-CHA	2.05	125.89	122.71
47	l	102	BCR	C33-C5-C4	2.05	117.97	113.60
44	q	312	CLA	CMB-C2B-C3B	2.05	131.37	126.55
49	m	104	DGD	C6D-O5D-C1E	-2.05	109.41	113.80
52	5	314	CHL	CAC-C3C-C4C	2.05	129.29	124.03
47	A	847	BCR	C23-C24-C25	-2.05	121.53	127.00
47	B	849	BCR	C23-C22-C21	2.05	122.23	119.01
44	A	805	CLA	O1D-CGD-CBD	2.05	128.55	124.52
52	2	512	CHL	CMD-C2D-C3D	-2.05	120.60	124.68
43	A	801	CL0	C4-C3-C5	2.05	118.78	115.23
47	f	850	BCR	C37-C22-C21	-2.04	119.50	122.82
52	s	517	CHL	CAC-C3C-C4C	2.04	129.29	124.03
44	B	838	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
47	B	852	BCR	C20-C21-C22	-2.04	124.41	127.28
47	B	852	BCR	C10-C11-C12	-2.04	117.28	123.20
44	B	810	CLA	C1D-ND-C4D	2.04	107.75	106.31
44	p	507	CLA	O1D-CGD-CBD	2.04	128.55	124.52
53	s	502	XAT	C18-C5-C4	2.04	116.53	114.24
44	B	801	CLA	CMB-C2B-C3B	2.04	131.35	126.55
47	n	204	BCR	C33-C5-C4	2.04	117.95	113.60
44	3	317	CLA	C2A-C3A-C4A	2.04	103.98	101.59
49	B	850	DGD	C6D-O5D-C1E	-2.04	109.42	113.80
47	A	845	BCR	C36-C18-C17	-2.04	119.51	122.82
44	o	303	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
51	2	501	LUT	C19-C9-C10	-2.04	119.51	122.82
44	e	831	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
44	e	835	CLA	O2A-CGA-O1A	-2.04	118.09	123.33
45	f	844	PQN	C2M-C2-C1	2.04	120.42	116.68
44	3	317	CLA	CHD-C1D-ND	-2.04	121.94	124.80
50	F	806	LMG	C9-C8-C7	-2.04	107.04	111.78
52	2	515	CHL	CMB-C2B-C3B	2.04	128.95	124.69
44	B	812	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
44	B	818	CLA	CMB-C2B-C3B	2.04	131.34	126.55
52	2	515	CHL	CMA-C3A-C4A	-2.03	110.23	114.61
44	p	513	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
51	p	502	LUT	C40-C33-C32	2.03	121.20	118.09
53	r	303	XAT	C20-C13-C12	2.03	121.20	118.09
43	e	801	CL0	C4-C3-C5	2.03	118.76	115.23
51	p	501	LUT	C22-C23-C24	-2.03	108.16	111.18
44	e	812	CLA	C2A-C1A-CHA	2.03	125.86	122.71
47	e	848	BCR	C35-C13-C12	2.03	121.19	118.09
44	B	814	CLA	C2A-C1A-CHA	2.03	127.39	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	1	507	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
51	5	303	LUT	C28-C29-C30	-2.03	115.81	119.01
44	5	305	CLA	CHB-C1B-NB	2.03	127.10	124.05
44	e	831	CLA	CMB-C2B-C3B	2.03	131.33	126.55
44	q	315	CLA	O2D-CGD-CBD	2.03	114.78	111.23
44	q	305	CLA	CAA-C2A-C1A	2.03	118.63	111.97
44	3	308	CLA	C3A-C2A-C1A	2.03	104.38	101.34
47	e	854	BCR	C16-C15-C14	-2.03	119.36	123.52
44	f	801	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
53	2	502	XAT	C40-C33-C32	2.03	121.19	118.09
44	f	807	CLA	O2D-CGD-CBD	2.03	114.78	111.23
47	o	301	BCR	C10-C11-C12	-2.03	117.32	123.20
44	3	310	CLA	O1A-CGA-CBA	2.03	129.53	123.09
44	f	834	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
51	1	502	LUT	C35-C34-C33	-2.03	124.43	127.28
44	2	504	CLA	C2A-C1A-CHA	2.03	125.86	122.71
44	B	801	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
46	O	601	LHG	O7-C7-O9	-2.03	118.96	123.70
44	s	510	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
50	F	806	LMG	O8-C28-O10	-2.03	118.56	123.63
52	r	313	CHL	CMA-C3A-C4A	-2.03	110.25	114.61
44	5	309	CLA	CMB-C2B-C3B	2.03	131.31	126.55
44	5	311	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
44	A	805	CLA	CAA-C2A-C1A	-2.03	105.34	111.97
44	B	808	CLA	CHB-C4A-NA	2.02	127.32	124.40
47	A	846	BCR	C21-C20-C19	-2.02	117.33	123.20
47	f	845	BCR	C11-C12-C13	-2.02	120.81	126.36
44	B	808	CLA	CHD-C1D-ND	-2.02	121.96	124.80
44	B	813	CLA	C2D-C1D-ND	-2.02	108.12	110.13
44	A	829	CLA	CHB-C4A-NA	2.02	127.32	124.40
52	p	512	CHL	CAC-C3C-C4C	2.02	129.23	124.03
44	2	505	CLA	C1-C2-C3	-2.02	122.89	126.20
47	r	301	BCR	C3-C4-C5	-2.02	110.45	114.06
47	L	305	BCR	C37-C22-C21	-2.02	119.54	122.82
54	Q	803	SQD	C9-C8-C7	-2.02	106.29	113.69
52	2	515	CHL	O2A-CGA-CBA	2.02	120.38	114.00
44	o	303	CLA	C1-C2-C3	-2.02	122.89	126.20
44	f	807	CLA	CMB-C2B-C3B	2.02	131.29	126.55
44	f	816	CLA	CMB-C2B-C3B	2.02	131.29	126.55
47	A	848	BCR	C27-C26-C25	-2.02	119.98	122.70
51	q	302	LUT	C16-C1-C6	-2.02	107.08	110.24
44	A	805	CLA	O2A-CGA-O1A	-2.02	118.59	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	5	308	CLA	CAC-C3C-C4C	2.01	127.41	124.79
52	1	512	CHL	CED-O2D-CGD	2.01	120.48	115.92
47	e	850	BCR	C35-C13-C12	2.01	121.16	118.09
46	1	516	LHG	O7-C7-O9	-2.01	119.00	123.70
47	B	847	BCR	C30-C25-C26	-2.01	119.89	122.64
47	2	503	BCR	C28-C29-C30	-2.01	107.31	114.43
47	o	305	BCR	C16-C15-C14	-2.01	119.40	123.52
47	A	846	BCR	C37-C22-C21	-2.01	119.56	122.82
44	B	829	CLA	C2A-C1A-CHA	2.01	125.83	122.71
44	e	852	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
44	n	202	CLA	O2A-CGA-O1A	-2.01	118.16	123.33
44	e	808	CLA	CMA-C3A-C2A	-2.01	111.62	116.23
44	2	505	CLA	CHB-C1B-NB	2.01	127.06	124.05
44	A	842	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
51	p	502	LUT	C19-C9-C8	2.01	121.16	118.09
44	n	203	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
44	e	813	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
44	A	828	CLA	CMA-C3A-C2A	-2.01	111.63	116.23
44	B	840	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
44	A	816	CLA	CMB-C2B-C3B	2.01	131.27	126.55
44	q	309	CLA	C1-C2-C3	-2.01	123.52	126.76
44	A	815	CLA	CMB-C2B-C1B	-2.01	122.37	125.42
44	f	811	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
47	3	305	BCR	C40-C30-C25	-2.00	107.10	110.24
44	A	831	CLA	C3B-C4B-NB	-2.00	108.25	110.33
47	F	804	BCR	C37-C22-C23	2.00	121.15	118.09
44	f	840	CLA	CMA-C3A-C2A	-2.00	111.64	116.23
51	1	501	LUT	C8-C7-C6	-2.00	121.65	127.00
44	e	818	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
44	B	826	CLA	O2D-CGD-CBD	2.00	114.73	111.23
44	e	804	CLA	O2D-CGD-CBD	2.00	114.73	111.23
44	e	836	CLA	C1-C2-C3	-2.00	122.92	126.20
47	3	305	BCR	C36-C18-C19	2.00	121.15	118.09
44	f	813	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
44	L	304	CLA	O1D-CGD-CBD	2.00	128.47	124.52
51	r	302	LUT	C20-C13-C12	2.00	121.15	118.09
47	F	801	BCR	C37-C22-C21	-2.00	119.57	122.82
53	5	304	XAT	C35-C15-C14	-2.00	119.42	123.52
46	2	517	LHG	O7-C7-O9	-2.00	119.03	123.70
47	e	854	BCR	C39-C30-C25	-2.00	107.11	110.24
47	B	852	BCR	C35-C13-C14	-2.00	119.58	122.82

All (341) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
43	A	801	CL0	ND
43	A	801	CL0	NC
43	A	801	CL0	NA
43	e	801	CL0	ND
43	e	801	CL0	NC
43	e	801	CL0	NA
44	A	802	CLA	ND
44	A	803	CLA	ND
44	A	804	CLA	ND
44	A	805	CLA	ND
44	A	806	CLA	ND
44	A	807	CLA	ND
44	A	808	CLA	ND
44	A	809	CLA	ND
44	A	810	CLA	ND
44	A	811	CLA	ND
44	A	812	CLA	ND
44	A	813	CLA	ND
44	A	814	CLA	ND
44	A	815	CLA	ND
44	A	816	CLA	ND
44	A	817	CLA	ND
44	A	818	CLA	ND
44	A	819	CLA	ND
44	A	820	CLA	ND
44	A	821	CLA	ND
44	A	822	CLA	ND
44	A	823	CLA	ND
44	A	824	CLA	ND
44	A	825	CLA	ND
44	A	826	CLA	ND
44	A	827	CLA	ND
44	A	828	CLA	ND
44	A	829	CLA	ND
44	A	830	CLA	ND
44	A	831	CLA	ND
44	A	832	CLA	ND
44	A	833	CLA	ND
44	A	834	CLA	ND
44	A	835	CLA	ND
44	A	836	CLA	ND
44	A	837	CLA	ND
44	A	838	CLA	ND

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Mol	Chain	Res	Type	Atom
44	A	839	CLA	ND
44	A	840	CLA	ND
44	A	842	CLA	ND
44	A	852	CLA	ND
44	B	801	CLA	ND
44	B	802	CLA	ND
44	B	803	CLA	ND
44	B	804	CLA	ND
44	B	805	CLA	ND
44	B	806	CLA	ND
44	B	807	CLA	ND
44	B	808	CLA	ND
44	B	809	CLA	ND
44	B	810	CLA	ND
44	B	811	CLA	ND
44	B	812	CLA	ND
44	B	813	CLA	ND
44	B	814	CLA	ND
44	B	815	CLA	ND
44	B	816	CLA	ND
44	B	817	CLA	ND
44	B	818	CLA	ND
44	B	819	CLA	ND
44	B	820	CLA	ND
44	B	821	CLA	ND
44	B	822	CLA	ND
44	B	823	CLA	ND
44	B	824	CLA	ND
44	B	825	CLA	ND
44	B	826	CLA	ND
44	B	827	CLA	ND
44	B	828	CLA	ND
44	B	829	CLA	ND
44	B	830	CLA	ND
44	B	831	CLA	ND
44	B	832	CLA	ND
44	B	833	CLA	ND
44	B	834	CLA	ND
44	B	835	CLA	ND
44	B	837	CLA	ND
44	B	838	CLA	ND
44	B	839	CLA	ND

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Mol	Chain	Res	Type	Atom
44	B	840	CLA	ND
44	B	841	CLA	ND
44	B	842	CLA	ND
44	F	802	CLA	ND
44	F	803	CLA	ND
44	J	101	CLA	ND
44	K	201	CLA	ND
44	K	202	CLA	ND
44	K	203	CLA	ND
44	K	205	CLA	ND
44	L	301	CLA	ND
44	L	302	CLA	ND
44	L	303	CLA	ND
44	L	304	CLA	ND
44	1	504	CLA	ND
44	1	505	CLA	ND
44	1	506	CLA	ND
44	1	507	CLA	ND
44	1	508	CLA	ND
44	1	510	CLA	ND
44	1	511	CLA	ND
44	1	515	CLA	ND
44	2	504	CLA	ND
44	2	506	CLA	ND
44	2	507	CLA	ND
44	2	507	CLA	C8
44	2	508	CLA	ND
44	2	509	CLA	ND
44	2	510	CLA	ND
44	2	511	CLA	ND
44	2	514	CLA	ND
44	3	301	CLA	ND
44	3	306	CLA	ND
44	3	307	CLA	ND
44	3	308	CLA	ND
44	3	310	CLA	ND
44	3	311	CLA	ND
44	3	312	CLA	ND
44	3	313	CLA	ND
44	3	314	CLA	ND
44	3	316	CLA	ND
44	3	317	CLA	ND

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Mol	Chain	Res	Type	Atom
44	3	318	CLA	ND
44	5	305	CLA	ND
44	5	306	CLA	ND
44	5	307	CLA	ND
44	5	308	CLA	ND
44	5	309	CLA	ND
44	5	310	CLA	ND
44	5	311	CLA	ND
44	5	312	CLA	ND
44	5	313	CLA	ND
44	5	316	CLA	ND
44	e	802	CLA	ND
44	e	803	CLA	ND
44	e	804	CLA	ND
44	e	805	CLA	ND
44	e	806	CLA	ND
44	e	807	CLA	ND
44	e	808	CLA	ND
44	e	809	CLA	ND
44	e	810	CLA	ND
44	e	811	CLA	ND
44	e	812	CLA	ND
44	e	813	CLA	ND
44	e	814	CLA	ND
44	e	815	CLA	ND
44	e	816	CLA	ND
44	e	817	CLA	ND
44	e	818	CLA	ND
44	e	819	CLA	ND
44	e	820	CLA	ND
44	e	821	CLA	ND
44	e	822	CLA	ND
44	e	823	CLA	ND
44	e	824	CLA	ND
44	e	825	CLA	ND
44	e	826	CLA	ND
44	e	827	CLA	ND
44	e	828	CLA	ND
44	e	829	CLA	ND
44	e	830	CLA	ND
44	e	831	CLA	ND
44	e	832	CLA	ND

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Mol	Chain	Res	Type	Atom
44	e	833	CLA	ND
44	e	834	CLA	ND
44	e	835	CLA	ND
44	e	836	CLA	ND
44	e	837	CLA	ND
44	e	838	CLA	ND
44	e	839	CLA	ND
44	e	840	CLA	ND
44	e	841	CLA	ND
44	e	843	CLA	ND
44	e	852	CLA	ND
44	e	853	CLA	ND
44	f	801	CLA	ND
44	f	803	CLA	ND
44	f	804	CLA	ND
44	f	805	CLA	ND
44	f	806	CLA	ND
44	f	807	CLA	ND
44	f	808	CLA	ND
44	f	809	CLA	ND
44	f	810	CLA	ND
44	f	811	CLA	ND
44	f	812	CLA	ND
44	f	813	CLA	ND
44	f	814	CLA	ND
44	f	815	CLA	ND
44	f	816	CLA	ND
44	f	817	CLA	ND
44	f	818	CLA	ND
44	f	819	CLA	ND
44	f	820	CLA	ND
44	f	821	CLA	ND
44	f	822	CLA	ND
44	f	823	CLA	ND
44	f	824	CLA	ND
44	f	825	CLA	ND
44	f	826	CLA	ND
44	f	827	CLA	ND
44	f	828	CLA	ND
44	f	829	CLA	ND
44	f	830	CLA	ND
44	f	831	CLA	ND

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Mol	Chain	Res	Type	Atom
44	f	832	CLA	ND
44	f	833	CLA	ND
44	f	834	CLA	ND
44	f	835	CLA	ND
44	f	836	CLA	ND
44	f	837	CLA	ND
44	f	838	CLA	ND
44	f	839	CLA	ND
44	f	840	CLA	ND
44	f	841	CLA	ND
44	f	842	CLA	ND
44	f	843	CLA	ND
44	j	802	CLA	ND
44	m	101	CLA	ND
44	m	102	CLA	ND
44	n	201	CLA	ND
44	n	202	CLA	ND
44	n	203	CLA	ND
44	n	205	CLA	ND
44	o	302	CLA	ND
44	o	303	CLA	ND
44	o	304	CLA	ND
44	p	504	CLA	ND
44	p	506	CLA	ND
44	p	507	CLA	ND
44	p	508	CLA	ND
44	p	509	CLA	ND
44	p	510	CLA	ND
44	p	511	CLA	ND
44	p	513	CLA	ND
44	p	515	CLA	ND
44	q	304	CLA	ND
44	q	305	CLA	ND
44	q	306	CLA	ND
44	q	308	CLA	ND
44	q	309	CLA	ND
44	q	310	CLA	ND
44	q	311	CLA	ND
44	q	312	CLA	ND
44	q	314	CLA	ND
44	q	316	CLA	ND
44	r	304	CLA	ND

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Mol	Chain	Res	Type	Atom
44	r	305	CLA	ND
44	r	306	CLA	ND
44	r	307	CLA	ND
44	r	308	CLA	ND
44	r	309	CLA	ND
44	r	310	CLA	ND
44	r	311	CLA	ND
44	r	312	CLA	ND
44	r	315	CLA	ND
44	r	317	CLA	ND
44	s	504	CLA	ND
44	s	506	CLA	ND
44	s	507	CLA	ND
44	s	508	CLA	ND
44	s	509	CLA	ND
44	s	510	CLA	ND
44	s	511	CLA	ND
44	s	514	CLA	ND
51	p	502	LUT	C26
52	1	512	CHL	ND
52	1	512	CHL	NC
52	1	512	CHL	NA
52	1	514	CHL	ND
52	1	514	CHL	NC
52	1	514	CHL	NA
52	1	517	CHL	ND
52	1	517	CHL	NC
52	1	517	CHL	NA
52	2	512	CHL	ND
52	2	512	CHL	NC
52	2	512	CHL	NA
52	2	513	CHL	ND
52	2	513	CHL	NC
52	2	513	CHL	NA
52	2	515	CHL	ND
52	2	515	CHL	NC
52	2	515	CHL	NA
52	2	516	CHL	ND
52	2	516	CHL	NC
52	2	516	CHL	NA
52	3	302	CHL	ND
52	3	302	CHL	NC

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Mol	Chain	Res	Type	Atom
52	3	302	CHL	NA
52	3	315	CHL	ND
52	3	315	CHL	NC
52	3	315	CHL	NA
52	5	314	CHL	ND
52	5	314	CHL	NC
52	5	314	CHL	NA
52	5	315	CHL	ND
52	5	315	CHL	NC
52	5	315	CHL	NA
52	5	317	CHL	ND
52	5	317	CHL	NC
52	5	317	CHL	NA
52	p	512	CHL	ND
52	p	512	CHL	NC
52	p	512	CHL	NA
52	p	514	CHL	ND
52	p	514	CHL	NC
52	p	514	CHL	NA
52	p	517	CHL	ND
52	p	517	CHL	NC
52	p	517	CHL	NA
52	q	313	CHL	ND
52	q	313	CHL	NC
52	q	313	CHL	NA
52	r	313	CHL	ND
52	r	313	CHL	NC
52	r	313	CHL	NA
52	r	314	CHL	ND
52	r	314	CHL	NC
52	r	314	CHL	NA
52	r	316	CHL	ND
52	r	316	CHL	NC
52	r	316	CHL	NA
52	s	512	CHL	ND
52	s	512	CHL	NC
52	s	512	CHL	NA
52	s	513	CHL	ND
52	s	513	CHL	NC
52	s	513	CHL	NA
52	s	515	CHL	ND
52	s	515	CHL	NC

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Mol	Chain	Res	Type	Atom
52	s	515	CHL	NA
52	s	517	CHL	ND
52	s	517	CHL	NC
52	s	517	CHL	NA

All (2297) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	A	801	CL0	CHA-CBD-CGD-O2D
43	e	801	CL0	CHA-CBD-CGD-O2D
44	A	802	CLA	C6-C7-C8-C9
44	A	803	CLA	CHA-CBD-CGD-O2D
44	A	804	CLA	C1A-C2A-CAA-CBA
44	A	804	CLA	C3A-C2A-CAA-CBA
44	A	805	CLA	C1A-C2A-CAA-CBA
44	A	805	CLA	CAD-CBD-CGD-O2D
44	A	806	CLA	CAD-CBD-CGD-O2D
44	A	807	CLA	CAD-CBD-CGD-O2D
44	A	808	CLA	CHA-CBD-CGD-O1D
44	A	808	CLA	CHA-CBD-CGD-O2D
44	A	809	CLA	C1A-C2A-CAA-CBA
44	A	809	CLA	C2B-C3B-CAB-CBB
44	A	809	CLA	C4B-C3B-CAB-CBB
44	A	815	CLA	CHA-CBD-CGD-O1D
44	A	815	CLA	CHA-CBD-CGD-O2D
44	A	816	CLA	CBD-CGD-O2D-CED
44	A	821	CLA	C1A-C2A-CAA-CBA
44	A	821	CLA	C3A-C2A-CAA-CBA
44	A	822	CLA	CBD-CGD-O2D-CED
44	A	823	CLA	C1A-C2A-CAA-CBA
44	A	823	CLA	C2B-C3B-CAB-CBB
44	A	823	CLA	C4B-C3B-CAB-CBB
44	A	827	CLA	CBD-CGD-O2D-CED
44	A	831	CLA	CAD-CBD-CGD-O1D
44	A	831	CLA	CAD-CBD-CGD-O2D
44	A	831	CLA	CBD-CGD-O2D-CED
44	A	835	CLA	CAD-CBD-CGD-O1D
44	A	835	CLA	CAD-CBD-CGD-O2D
44	A	835	CLA	C2-C3-C5-C6
44	A	840	CLA	C2B-C3B-CAB-CBB
44	A	840	CLA	C4B-C3B-CAB-CBB
44	A	842	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
44	A	842	CLA	C3A-C2A-CAA-CBA
44	A	842	CLA	C2B-C3B-CAB-CBB
44	A	842	CLA	C4B-C3B-CAB-CBB
44	A	842	CLA	CHA-CBD-CGD-O1D
44	A	842	CLA	CHA-CBD-CGD-O2D
44	A	842	CLA	CBD-CGD-O2D-CED
44	A	852	CLA	CBD-CGD-O2D-CED
44	B	804	CLA	C3A-C2A-CAA-CBA
44	B	804	CLA	CBD-CGD-O2D-CED
44	B	805	CLA	CBD-CGD-O2D-CED
44	B	806	CLA	CAD-CBD-CGD-O1D
44	B	806	CLA	CAD-CBD-CGD-O2D
44	B	808	CLA	C2B-C3B-CAB-CBB
44	B	808	CLA	C4B-C3B-CAB-CBB
44	B	809	CLA	CHA-CBD-CGD-O1D
44	B	809	CLA	CHA-CBD-CGD-O2D
44	B	811	CLA	C1A-C2A-CAA-CBA
44	B	811	CLA	CAD-CBD-CGD-O1D
44	B	811	CLA	CAD-CBD-CGD-O2D
44	B	812	CLA	CBD-CGD-O2D-CED
44	B	815	CLA	CBD-CGD-O2D-CED
44	B	816	CLA	CHA-CBD-CGD-O1D
44	B	816	CLA	CHA-CBD-CGD-O2D
44	B	817	CLA	CBD-CGD-O2D-CED
44	B	818	CLA	C1A-C2A-CAA-CBA
44	B	818	CLA	C3A-C2A-CAA-CBA
44	B	822	CLA	CHA-CBD-CGD-O1D
44	B	822	CLA	CHA-CBD-CGD-O2D
44	B	823	CLA	C1A-C2A-CAA-CBA
44	B	823	CLA	C3A-C2A-CAA-CBA
44	B	824	CLA	C1A-C2A-CAA-CBA
44	B	824	CLA	C3A-C2A-CAA-CBA
44	B	825	CLA	CHA-CBD-CGD-O1D
44	B	825	CLA	CHA-CBD-CGD-O2D
44	B	826	CLA	C11-C12-C13-C14
44	B	832	CLA	CBD-CGD-O2D-CED
44	B	834	CLA	C1A-C2A-CAA-CBA
44	B	834	CLA	C2B-C3B-CAB-CBB
44	B	834	CLA	C4B-C3B-CAB-CBB
44	B	834	CLA	CHA-CBD-CGD-O1D
44	B	834	CLA	CHA-CBD-CGD-O2D
44	B	835	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
44	B	836	CLA	C3A-C2A-CAA-CBA
44	B	839	CLA	CHA-CBD-CGD-O1D
44	B	839	CLA	CHA-CBD-CGD-O2D
44	B	842	CLA	C1A-C2A-CAA-CBA
44	B	842	CLA	C3A-C2A-CAA-CBA
44	J	101	CLA	C4B-C3B-CAB-CBB
44	K	201	CLA	C2B-C3B-CAB-CBB
44	K	201	CLA	C4B-C3B-CAB-CBB
44	K	202	CLA	C2B-C3B-CAB-CBB
44	K	202	CLA	C4B-C3B-CAB-CBB
44	K	203	CLA	CHA-CBD-CGD-O1D
44	K	203	CLA	CHA-CBD-CGD-O2D
44	K	203	CLA	CBD-CGD-O2D-CED
44	K	205	CLA	C2B-C3B-CAB-CBB
44	K	205	CLA	C4B-C3B-CAB-CBB
44	L	303	CLA	C1A-C2A-CAA-CBA
44	L	303	CLA	C3-C5-C6-C7
44	L	304	CLA	CHA-CBD-CGD-O1D
44	L	304	CLA	CHA-CBD-CGD-O2D
44	1	505	CLA	C1A-C2A-CAA-CBA
44	1	505	CLA	C3A-C2A-CAA-CBA
44	1	506	CLA	C1A-C2A-CAA-CBA
44	1	506	CLA	C3A-C2A-CAA-CBA
44	1	507	CLA	CBD-CGD-O2D-CED
44	1	508	CLA	CBD-CGD-O2D-CED
44	1	510	CLA	C1A-C2A-CAA-CBA
44	1	510	CLA	C3A-C2A-CAA-CBA
44	1	510	CLA	CBD-CGD-O2D-CED
44	1	511	CLA	CBA-CGA-O2A-C1
44	1	511	CLA	CBD-CGD-O2D-CED
44	1	513	CLA	C4B-C3B-CAB-CBB
44	2	505	CLA	CBD-CGD-O2D-CED
44	2	505	CLA	C3-C5-C6-C7
44	2	509	CLA	C1A-C2A-CAA-CBA
44	2	510	CLA	CBA-CGA-O2A-C1
44	2	511	CLA	C2B-C3B-CAB-CBB
44	2	511	CLA	C4B-C3B-CAB-CBB
44	3	306	CLA	C1A-C2A-CAA-CBA
44	3	306	CLA	C3A-C2A-CAA-CBA
44	3	306	CLA	C2-C1-O2A-CGA
44	3	306	CLA	CBD-CGD-O2D-CED
44	3	308	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
44	3	309	CLA	CBD-CGD-O2D-CED
44	3	311	CLA	CBD-CGD-O2D-CED
44	3	312	CLA	CBD-CGD-O2D-CED
44	3	313	CLA	CBD-CGD-O2D-CED
44	5	307	CLA	CBA-CGA-O2A-C1
44	5	307	CLA	O1A-CGA-O2A-C1
44	5	308	CLA	CHA-CBD-CGD-O1D
44	5	308	CLA	CHA-CBD-CGD-O2D
44	5	312	CLA	CBD-CGD-O2D-CED
44	5	313	CLA	CAD-CBD-CGD-O1D
44	5	313	CLA	CAD-CBD-CGD-O2D
44	e	804	CLA	C1A-C2A-CAA-CBA
44	e	805	CLA	CBD-CGD-O2D-CED
44	e	807	CLA	CHA-CBD-CGD-O2D
44	e	807	CLA	CBD-CGD-O2D-CED
44	e	808	CLA	CAD-CBD-CGD-O1D
44	e	808	CLA	CAD-CBD-CGD-O2D
44	e	809	CLA	CBD-CGD-O2D-CED
44	e	810	CLA	C1A-C2A-CAA-CBA
44	e	810	CLA	C3A-C2A-CAA-CBA
44	e	810	CLA	C2B-C3B-CAB-CBB
44	e	810	CLA	C4B-C3B-CAB-CBB
44	e	811	CLA	CAD-CBD-CGD-O1D
44	e	811	CLA	CAD-CBD-CGD-O2D
44	e	812	CLA	CHA-CBD-CGD-O2D
44	e	812	CLA	CAD-CBD-CGD-O2D
44	e	813	CLA	C3A-C2A-CAA-CBA
44	e	815	CLA	CBD-CGD-O2D-CED
44	e	816	CLA	CBD-CGD-O2D-CED
44	e	819	CLA	CAD-CBD-CGD-O1D
44	e	819	CLA	CAD-CBD-CGD-O2D
44	e	820	CLA	CBD-CGD-O2D-CED
44	e	821	CLA	C1A-C2A-CAA-CBA
44	e	821	CLA	C3A-C2A-CAA-CBA
44	e	826	CLA	C1A-C2A-CAA-CBA
44	e	826	CLA	CAD-CBD-CGD-O1D
44	e	826	CLA	CAD-CBD-CGD-O2D
44	e	831	CLA	O1A-CGA-O2A-C1
44	e	832	CLA	CAD-CBD-CGD-O1D
44	e	832	CLA	CAD-CBD-CGD-O2D
44	e	832	CLA	CBD-CGD-O2D-CED
44	e	833	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
44	e	834	CLA	CAD-CBD-CGD-O1D
44	e	834	CLA	CAD-CBD-CGD-O2D
44	e	839	CLA	C11-C12-C13-C14
44	e	843	CLA	CHA-CBD-CGD-O1D
44	e	843	CLA	CHA-CBD-CGD-O2D
44	e	843	CLA	CBD-CGD-O2D-CED
44	e	852	CLA	CBD-CGD-O2D-CED
44	e	853	CLA	C1A-C2A-CAA-CBA
44	f	804	CLA	CHA-CBD-CGD-O2D
44	f	807	CLA	CAD-CBD-CGD-O1D
44	f	807	CLA	CAD-CBD-CGD-O2D
44	f	810	CLA	CHA-CBD-CGD-O2D
44	f	811	CLA	C4-C3-C5-C6
44	f	812	CLA	CAD-CBD-CGD-O1D
44	f	812	CLA	CAD-CBD-CGD-O2D
44	f	813	CLA	CBD-CGD-O2D-CED
44	f	813	CLA	O1D-CGD-O2D-CED
44	f	813	CLA	C4-C3-C5-C6
44	f	814	CLA	CAD-CBD-CGD-O1D
44	f	814	CLA	CAD-CBD-CGD-O2D
44	f	817	CLA	CHA-CBD-CGD-O1D
44	f	817	CLA	CHA-CBD-CGD-O2D
44	f	819	CLA	C4B-C3B-CAB-CBB
44	f	820	CLA	C3A-C2A-CAA-CBA
44	f	823	CLA	CHA-CBD-CGD-O1D
44	f	823	CLA	CHA-CBD-CGD-O2D
44	f	824	CLA	CBD-CGD-O2D-CED
44	f	826	CLA	CHA-CBD-CGD-O1D
44	f	826	CLA	CHA-CBD-CGD-O2D
44	f	828	CLA	CAD-CBD-CGD-O1D
44	f	828	CLA	CAD-CBD-CGD-O2D
44	f	829	CLA	C3A-C2A-CAA-CBA
44	f	832	CLA	CHA-CBD-CGD-O1D
44	f	832	CLA	CHA-CBD-CGD-O2D
44	f	835	CLA	C1A-C2A-CAA-CBA
44	f	835	CLA	CHA-CBD-CGD-O1D
44	f	835	CLA	CHA-CBD-CGD-O2D
44	f	836	CLA	C1A-C2A-CAA-CBA
44	f	836	CLA	C4B-C3B-CAB-CBB
44	f	836	CLA	CBD-CGD-O2D-CED
44	f	836	CLA	O1D-CGD-O2D-CED
44	f	837	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
44	f	838	CLA	CAD-CBD-CGD-O1D
44	f	838	CLA	CAD-CBD-CGD-O2D
44	f	840	CLA	CAD-CBD-CGD-O1D
44	f	840	CLA	CAD-CBD-CGD-O2D
44	f	842	CLA	C4B-C3B-CAB-CBB
44	j	802	CLA	CBD-CGD-O2D-CED
44	m	101	CLA	C1A-C2A-CAA-CBA
44	m	101	CLA	CAD-CBD-CGD-O1D
44	m	101	CLA	CAD-CBD-CGD-O2D
44	m	102	CLA	C1A-C2A-CAA-CBA
44	m	102	CLA	C3A-C2A-CAA-CBA
44	n	202	CLA	CHA-CBD-CGD-O1D
44	n	202	CLA	CHA-CBD-CGD-O2D
44	n	203	CLA	CHA-CBD-CGD-O1D
44	n	203	CLA	CHA-CBD-CGD-O2D
44	n	203	CLA	CBD-CGD-O2D-CED
44	n	205	CLA	C2B-C3B-CAB-CBB
44	n	205	CLA	C4B-C3B-CAB-CBB
44	o	302	CLA	CBD-CGD-O2D-CED
44	o	304	CLA	CHA-CBD-CGD-O1D
44	o	304	CLA	CHA-CBD-CGD-O2D
44	p	504	CLA	C3A-C2A-CAA-CBA
44	p	504	CLA	C2B-C3B-CAB-CBB
44	p	504	CLA	C4B-C3B-CAB-CBB
44	p	506	CLA	C1A-C2A-CAA-CBA
44	p	507	CLA	CBD-CGD-O2D-CED
44	p	508	CLA	CHA-CBD-CGD-O1D
44	p	508	CLA	CHA-CBD-CGD-O2D
44	p	510	CLA	CHA-CBD-CGD-O1D
44	p	510	CLA	CHA-CBD-CGD-O2D
44	p	510	CLA	CBD-CGD-O2D-CED
44	p	511	CLA	C2B-C3B-CAB-CBB
44	p	511	CLA	C4B-C3B-CAB-CBB
44	p	513	CLA	CBD-CGD-O2D-CED
44	q	305	CLA	C2B-C3B-CAB-CBB
44	q	305	CLA	C4B-C3B-CAB-CBB
44	q	305	CLA	CBD-CGD-O2D-CED
44	q	308	CLA	C1A-C2A-CAA-CBA
44	q	308	CLA	C3A-C2A-CAA-CBA
44	q	308	CLA	CBD-CGD-O2D-CED
44	q	310	CLA	C4B-C3B-CAB-CBB
44	q	311	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
44	q	312	CLA	C1A-C2A-CAA-CBA
44	q	312	CLA	C3A-C2A-CAA-CBA
44	q	312	CLA	CBD-CGD-O2D-CED
44	q	312	CLA	O1D-CGD-O2D-CED
44	q	314	CLA	CBD-CGD-O2D-CED
44	q	316	CLA	CBD-CGD-O2D-CED
44	r	304	CLA	CBD-CGD-O2D-CED
44	r	305	CLA	CHA-CBD-CGD-O2D
44	r	306	CLA	CBD-CGD-O2D-CED
44	r	308	CLA	CHA-CBD-CGD-O1D
44	r	308	CLA	CHA-CBD-CGD-O2D
44	r	309	CLA	C1A-C2A-CAA-CBA
44	r	309	CLA	CBD-CGD-O2D-CED
44	r	311	CLA	CBD-CGD-O2D-CED
44	r	315	CLA	CBD-CGD-O2D-CED
44	r	317	CLA	C1A-C2A-CAA-CBA
44	r	317	CLA	C3A-C2A-CAA-CBA
44	s	505	CLA	C1A-C2A-CAA-CBA
44	s	506	CLA	C11-C12-C13-C14
44	s	507	CLA	CBD-CGD-O2D-CED
44	s	508	CLA	CBD-CGD-O2D-CED
44	s	509	CLA	CBD-CGD-O2D-CED
44	s	510	CLA	C1A-C2A-CAA-CBA
44	s	510	CLA	C3A-C2A-CAA-CBA
44	s	510	CLA	CBD-CGD-O2D-CED
44	s	511	CLA	C1A-C2A-CAA-CBA
44	s	511	CLA	C3A-C2A-CAA-CBA
44	s	511	CLA	CBD-CGD-O2D-CED
44	s	514	CLA	CBD-CGD-O2D-CED
46	A	843	LHG	C3-O3-P-O4
46	A	843	LHG	C3-O3-P-O6
46	A	844	LHG	C3-O3-P-O6
46	A	844	LHG	C4-O6-P-O3
46	A	844	LHG	C4-O6-P-O4
46	A	844	LHG	C4-O6-P-O5
46	B	851	LHG	C4-O6-P-O3
46	B	851	LHG	C4-O6-P-O4
46	1	516	LHG	C3-O3-P-O6
46	1	516	LHG	C4-O6-P-O3
46	1	516	LHG	C4-O6-P-O5
46	2	517	LHG	C4-O6-P-O5
46	e	844	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
46	e	844	LHG	C3-O3-P-O6
46	e	844	LHG	C4-O6-P-O3
46	e	844	LHG	C4-O6-P-O4
46	e	845	LHG	C3-O3-P-O6
46	e	845	LHG	C4-O6-P-O3
46	e	845	LHG	C4-O6-P-O4
46	f	852	LHG	C3-O3-P-O4
46	f	852	LHG	C3-O3-P-O5
46	f	852	LHG	C3-O3-P-O6
46	f	852	LHG	C4-O6-P-O3
46	f	852	LHG	C4-O6-P-O4
46	f	852	LHG	C4-O6-P-O5
46	p	516	LHG	C4-O6-P-O3
46	p	516	LHG	C4-O6-P-O5
46	s	516	LHG	C4-O6-P-O3
46	s	516	LHG	C4-O6-P-O5
47	A	845	BCR	C21-C22-C23-C24
47	A	848	BCR	C23-C24-C25-C26
47	A	851	BCR	C5-C6-C7-C8
47	B	845	BCR	C21-C22-C23-C24
47	B	845	BCR	C37-C22-C23-C24
47	B	847	BCR	C1-C6-C7-C8
47	B	847	BCR	C5-C6-C7-C8
47	B	849	BCR	C21-C22-C23-C24
47	B	849	BCR	C37-C22-C23-C24
47	F	801	BCR	C17-C18-C19-C20
47	F	801	BCR	C37-C22-C23-C24
47	I	101	BCR	C21-C22-C23-C24
47	I	101	BCR	C37-C22-C23-C24
47	I	101	BCR	C23-C24-C25-C26
47	I	101	BCR	C23-C24-C25-C30
47	K	204	BCR	C23-C24-C25-C26
47	L	305	BCR	C17-C18-C19-C20
47	L	305	BCR	C36-C18-C19-C20
47	L	305	BCR	C21-C22-C23-C24
47	L	305	BCR	C37-C22-C23-C24
47	2	503	BCR	C21-C22-C23-C24
47	5	302	BCR	C1-C6-C7-C8
47	5	302	BCR	C5-C6-C7-C8
47	5	302	BCR	C11-C12-C13-C14
47	Q	801	BCR	C37-C22-C23-C24
47	e	849	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
47	e	849	BCR	C37-C22-C23-C24
47	e	850	BCR	C1-C6-C7-C8
47	e	850	BCR	C5-C6-C7-C8
47	e	854	BCR	C17-C18-C19-C20
47	f	845	BCR	C7-C8-C9-C10
47	f	845	BCR	C7-C8-C9-C34
47	f	846	BCR	C21-C22-C23-C24
47	f	846	BCR	C37-C22-C23-C24
47	f	850	BCR	C21-C22-C23-C24
47	l	102	BCR	C21-C22-C23-C24
47	q	303	BCR	C7-C8-C9-C10
47	q	303	BCR	C7-C8-C9-C34
47	r	301	BCR	C7-C8-C9-C10
47	r	301	BCR	C7-C8-C9-C34
47	s	503	BCR	C13-C14-C15-C16
47	s	503	BCR	C23-C24-C25-C26
47	s	503	BCR	C23-C24-C25-C30
49	B	850	DGD	C2B-C1B-O2G-C2G
49	B	850	DGD	O1B-C1B-O2G-C2G
49	J	103	DGD	C2E-C1E-O5D-C6D
49	J	103	DGD	O6E-C1E-O5D-C6D
50	2	519	LMG	O9-C10-O7-C8
50	r	318	LMG	O6-C1-O1-C7
50	r	318	LMG	C7-C8-O7-C10
50	r	318	LMG	O9-C10-O7-C8
51	1	501	LUT	C1-C6-C7-C8
51	1	501	LUT	C5-C6-C7-C8
51	p	502	LUT	C21-C26-C27-C28
51	p	502	LUT	C27-C28-C29-C30
51	p	502	LUT	C27-C28-C29-C39
51	q	302	LUT	C7-C8-C9-C10
51	q	302	LUT	C7-C8-C9-C19
51	q	302	LUT	C11-C12-C13-C14
51	q	302	LUT	C11-C12-C13-C20
52	1	512	CHL	C1C-C2C-CMC-OMC
52	1	512	CHL	C3C-C2C-CMC-OMC
52	1	517	CHL	C1C-C2C-CMC-OMC
52	1	517	CHL	C3C-C2C-CMC-OMC
52	2	513	CHL	C4C-C3C-CAC-CBC
52	2	513	CHL	CHA-CBD-CGD-O1D
52	2	515	CHL	C3C-C2C-CMC-OMC
52	2	516	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
52	2	516	CHL	CAD-CBD-CGD-O1D
52	2	516	CHL	CAD-CBD-CGD-O2D
52	5	314	CHL	C1C-C2C-CMC-OMC
52	5	314	CHL	C3C-C2C-CMC-OMC
52	5	315	CHL	C1C-C2C-CMC-OMC
52	5	315	CHL	C3C-C2C-CMC-OMC
52	5	315	CHL	CHA-CBD-CGD-O2D
52	5	317	CHL	C1C-C2C-CMC-OMC
52	5	317	CHL	C3C-C2C-CMC-OMC
52	p	517	CHL	C1A-C2A-CAA-CBA
52	p	517	CHL	C3A-C2A-CAA-CBA
52	r	313	CHL	CHA-CBD-CGD-O1D
52	r	313	CHL	CHA-CBD-CGD-O2D
52	r	314	CHL	CBD-CGD-O2D-CED
53	2	502	XAT	C5-C6-C7-C8
53	2	502	XAT	O4-C6-C7-C8
53	2	502	XAT	C7-C8-C9-C10
53	2	502	XAT	C7-C8-C9-C19
53	2	502	XAT	C27-C28-C29-C30
53	s	502	XAT	O4-C6-C7-C8
53	s	502	XAT	C7-C8-C9-C10
53	s	502	XAT	C7-C8-C9-C19
53	s	502	XAT	C11-C12-C13-C14
54	Q	802	SQD	O5-C1-O6-C44
44	B	836	CLA	O1D-CGD-O2D-CED
44	2	509	CLA	O1D-CGD-O2D-CED
44	e	810	CLA	O1D-CGD-O2D-CED
44	e	852	CLA	O1D-CGD-O2D-CED
44	j	802	CLA	O1D-CGD-O2D-CED
44	m	101	CLA	O1D-CGD-O2D-CED
44	n	203	CLA	O1D-CGD-O2D-CED
44	q	307	CLA	O1D-CGD-O2D-CED
44	q	310	CLA	O1D-CGD-O2D-CED
44	q	311	CLA	O1D-CGD-O2D-CED
44	q	314	CLA	O1D-CGD-O2D-CED
44	r	317	CLA	O1D-CGD-O2D-CED
44	s	514	CLA	O1D-CGD-O2D-CED
44	A	806	CLA	O1D-CGD-O2D-CED
44	A	852	CLA	O1D-CGD-O2D-CED
44	B	803	CLA	O1D-CGD-O2D-CED
44	B	804	CLA	O1D-CGD-O2D-CED
44	B	812	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
44	B	832	CLA	O1D-CGD-O2D-CED
44	3	301	CLA	O1D-CGD-O2D-CED
44	3	306	CLA	O1D-CGD-O2D-CED
44	3	308	CLA	O1D-CGD-O2D-CED
44	3	312	CLA	O1D-CGD-O2D-CED
44	3	317	CLA	O1D-CGD-O2D-CED
44	5	307	CLA	O1D-CGD-O2D-CED
44	e	816	CLA	O1D-CGD-O2D-CED
44	f	812	CLA	O1D-CGD-O2D-CED
44	f	815	CLA	O1D-CGD-O2D-CED
44	o	302	CLA	O1D-CGD-O2D-CED
44	p	506	CLA	O1D-CGD-O2D-CED
44	p	509	CLA	O1D-CGD-O2D-CED
44	p	513	CLA	O1D-CGD-O2D-CED
44	q	305	CLA	O1D-CGD-O2D-CED
44	r	309	CLA	O1D-CGD-O2D-CED
44	s	505	CLA	O1D-CGD-O2D-CED
44	s	509	CLA	O1D-CGD-O2D-CED
44	s	510	CLA	O1D-CGD-O2D-CED
52	r	314	CHL	O1D-CGD-O2D-CED
44	A	806	CLA	CBD-CGD-O2D-CED
44	A	813	CLA	CBD-CGD-O2D-CED
44	A	815	CLA	CBD-CGD-O2D-CED
44	A	820	CLA	CBD-CGD-O2D-CED
44	B	803	CLA	CBD-CGD-O2D-CED
44	B	811	CLA	CBD-CGD-O2D-CED
44	B	814	CLA	CBD-CGD-O2D-CED
44	B	816	CLA	CBD-CGD-O2D-CED
44	B	820	CLA	CBD-CGD-O2D-CED
44	B	823	CLA	CBD-CGD-O2D-CED
44	B	836	CLA	CBD-CGD-O2D-CED
44	F	802	CLA	CBD-CGD-O2D-CED
44	1	506	CLA	CBD-CGD-O2D-CED
44	1	509	CLA	CBD-CGD-O2D-CED
44	1	513	CLA	CBD-CGD-O2D-CED
44	1	515	CLA	CBD-CGD-O2D-CED
44	2	509	CLA	CBD-CGD-O2D-CED
44	3	301	CLA	CBD-CGD-O2D-CED
44	3	307	CLA	CBD-CGD-O2D-CED
44	3	317	CLA	CBD-CGD-O2D-CED
44	5	307	CLA	CBD-CGD-O2D-CED
44	5	309	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
44	e	802	CLA	CBD-CGD-O2D-CED
44	e	810	CLA	CBD-CGD-O2D-CED
44	e	821	CLA	CBD-CGD-O2D-CED
44	e	834	CLA	CBD-CGD-O2D-CED
44	f	803	CLA	CBD-CGD-O2D-CED
44	f	808	CLA	CBD-CGD-O2D-CED
44	f	812	CLA	CBD-CGD-O2D-CED
44	f	815	CLA	CBD-CGD-O2D-CED
44	f	819	CLA	CBD-CGD-O2D-CED
44	f	820	CLA	CBD-CGD-O2D-CED
44	f	821	CLA	CBD-CGD-O2D-CED
44	f	830	CLA	CBD-CGD-O2D-CED
44	f	835	CLA	CBD-CGD-O2D-CED
44	f	839	CLA	CBD-CGD-O2D-CED
44	m	101	CLA	CBD-CGD-O2D-CED
44	m	102	CLA	CBD-CGD-O2D-CED
44	p	504	CLA	CBD-CGD-O2D-CED
44	p	506	CLA	CBD-CGD-O2D-CED
44	p	509	CLA	CBD-CGD-O2D-CED
44	p	511	CLA	CBD-CGD-O2D-CED
44	p	515	CLA	CBD-CGD-O2D-CED
44	q	307	CLA	CBD-CGD-O2D-CED
44	q	309	CLA	CBD-CGD-O2D-CED
44	q	310	CLA	CBD-CGD-O2D-CED
44	q	315	CLA	CBD-CGD-O2D-CED
44	r	305	CLA	CBD-CGD-O2D-CED
44	r	308	CLA	CBD-CGD-O2D-CED
44	r	310	CLA	CBD-CGD-O2D-CED
44	r	317	CLA	CBD-CGD-O2D-CED
44	s	504	CLA	CBD-CGD-O2D-CED
44	s	505	CLA	CBD-CGD-O2D-CED
44	s	506	CLA	CBD-CGD-O2D-CED
52	2	513	CHL	CBD-CGD-O2D-CED
52	5	315	CHL	CBD-CGD-O2D-CED
52	q	313	CHL	CBD-CGD-O2D-CED
52	s	513	CHL	CBD-CGD-O2D-CED
44	L	303	CLA	O1A-CGA-O2A-C1
44	1	509	CLA	O1A-CGA-O2A-C1
44	2	510	CLA	O1A-CGA-O2A-C1
44	e	804	CLA	O1A-CGA-O2A-C1
44	p	509	CLA	O1A-CGA-O2A-C1
44	p	513	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
44	r	306	CLA	O1A-CGA-O2A-C1
44	A	816	CLA	O1D-CGD-O2D-CED
44	B	815	CLA	O1D-CGD-O2D-CED
44	q	315	CLA	CBA-CGA-O2A-C1
44	A	820	CLA	O1D-CGD-O2D-CED
44	1	513	CLA	O1D-CGD-O2D-CED
44	3	307	CLA	O1D-CGD-O2D-CED
44	5	309	CLA	O1D-CGD-O2D-CED
44	f	819	CLA	O1D-CGD-O2D-CED
44	f	839	CLA	O1D-CGD-O2D-CED
44	p	511	CLA	O1D-CGD-O2D-CED
44	q	309	CLA	O1D-CGD-O2D-CED
44	q	315	CLA	O1D-CGD-O2D-CED
44	s	506	CLA	O1D-CGD-O2D-CED
44	1	509	CLA	CBA-CGA-O2A-C1
44	e	804	CLA	CBA-CGA-O2A-C1
44	e	831	CLA	CBA-CGA-O2A-C1
44	p	509	CLA	CBA-CGA-O2A-C1
44	2	514	CLA	CBD-CGD-O2D-CED
44	f	833	CLA	CBD-CGD-O2D-CED
44	A	831	CLA	O1A-CGA-O2A-C1
44	3	308	CLA	O1A-CGA-O2A-C1
44	5	310	CLA	O1A-CGA-O2A-C1
44	s	506	CLA	O1A-CGA-O2A-C1
50	F	806	LMG	O10-C28-O8-C9
44	1	511	CLA	O1A-CGA-O2A-C1
44	A	831	CLA	O1D-CGD-O2D-CED
44	e	805	CLA	O1D-CGD-O2D-CED
44	e	820	CLA	O1D-CGD-O2D-CED
44	e	832	CLA	O1D-CGD-O2D-CED
44	f	837	CLA	O1D-CGD-O2D-CED
44	r	304	CLA	O1D-CGD-O2D-CED
44	r	306	CLA	O1D-CGD-O2D-CED
44	A	827	CLA	O1D-CGD-O2D-CED
44	B	817	CLA	O1D-CGD-O2D-CED
44	B	835	CLA	O1D-CGD-O2D-CED
44	1	507	CLA	O1D-CGD-O2D-CED
44	1	508	CLA	O1D-CGD-O2D-CED
44	1	511	CLA	O1D-CGD-O2D-CED
44	2	505	CLA	O1D-CGD-O2D-CED
44	e	807	CLA	O1D-CGD-O2D-CED
44	e	809	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
44	e	815	CLA	O1D-CGD-O2D-CED
44	e	843	CLA	O1D-CGD-O2D-CED
44	s	508	CLA	O1D-CGD-O2D-CED
44	A	810	CLA	CBD-CGD-O2D-CED
44	A	828	CLA	CBD-CGD-O2D-CED
52	p	514	CHL	CBD-CGD-O2D-CED
44	1	510	CLA	O1D-CGD-O2D-CED
44	3	318	CLA	CBA-CGA-O2A-C1
44	3	318	CLA	O1A-CGA-O2A-C1
44	q	316	CLA	O1A-CGA-O2A-C1
44	B	807	CLA	C3-C5-C6-C7
44	B	811	CLA	C3-C5-C6-C7
44	B	841	CLA	C3-C5-C6-C7
44	3	306	CLA	C3-C5-C6-C7
44	e	852	CLA	C3-C5-C6-C7
44	f	818	CLA	C3-C5-C6-C7
44	p	508	CLA	C3-C5-C6-C7
44	q	312	CLA	C3-C5-C6-C7
45	A	841	PQN	C13-C15-C16-C17
44	A	831	CLA	CBA-CGA-O2A-C1
44	A	835	CLA	CBA-CGA-O2A-C1
44	L	303	CLA	CBA-CGA-O2A-C1
44	3	308	CLA	CBA-CGA-O2A-C1
44	e	816	CLA	CBA-CGA-O2A-C1
44	p	513	CLA	CBA-CGA-O2A-C1
44	q	312	CLA	CBA-CGA-O2A-C1
44	r	306	CLA	CBA-CGA-O2A-C1
49	J	103	DGD	C2A-C1A-O1G-C1G
50	F	806	LMG	C29-C28-O8-C9
44	L	304	CLA	CBD-CGD-O2D-CED
44	2	507	CLA	CBD-CGD-O2D-CED
44	5	316	CLA	CBD-CGD-O2D-CED
44	e	808	CLA	CBD-CGD-O2D-CED
44	e	818	CLA	CBD-CGD-O2D-CED
44	e	833	CLA	CBD-CGD-O2D-CED
44	e	836	CLA	CBD-CGD-O2D-CED
44	e	853	CLA	CBD-CGD-O2D-CED
44	f	825	CLA	CBD-CGD-O2D-CED
44	f	829	CLA	CBD-CGD-O2D-CED
44	n	202	CLA	CBD-CGD-O2D-CED
52	2	516	CHL	CBD-CGD-O2D-CED
52	3	315	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
52	r	313	CHL	CBD-CGD-O2D-CED
50	2	519	LMG	C11-C10-O7-C8
44	L	304	CLA	C2C-C3C-CAC-CBC
44	A	822	CLA	O1D-CGD-O2D-CED
44	A	842	CLA	O1D-CGD-O2D-CED
44	B	805	CLA	O1D-CGD-O2D-CED
44	B	823	CLA	O1D-CGD-O2D-CED
44	K	203	CLA	O1D-CGD-O2D-CED
44	1	515	CLA	O1D-CGD-O2D-CED
44	3	309	CLA	O1D-CGD-O2D-CED
44	3	311	CLA	O1D-CGD-O2D-CED
44	5	312	CLA	O1D-CGD-O2D-CED
44	f	824	CLA	O1D-CGD-O2D-CED
44	f	830	CLA	O1D-CGD-O2D-CED
44	p	507	CLA	O1D-CGD-O2D-CED
44	q	308	CLA	O1D-CGD-O2D-CED
44	r	305	CLA	O1D-CGD-O2D-CED
44	r	310	CLA	O1D-CGD-O2D-CED
44	r	311	CLA	O1D-CGD-O2D-CED
44	r	315	CLA	O1D-CGD-O2D-CED
44	s	507	CLA	O1D-CGD-O2D-CED
44	s	511	CLA	O1D-CGD-O2D-CED
44	2	514	CLA	O1A-CGA-O2A-C1
44	o	303	CLA	O1A-CGA-O2A-C1
44	q	315	CLA	O1A-CGA-O2A-C1
44	3	313	CLA	O1D-CGD-O2D-CED
44	p	510	CLA	O1D-CGD-O2D-CED
44	q	316	CLA	O1D-CGD-O2D-CED
44	A	836	CLA	C4-C3-C5-C6
44	B	818	CLA	C4-C3-C5-C6
44	B	841	CLA	C4-C3-C5-C6
44	5	307	CLA	C4-C3-C5-C6
44	e	810	CLA	C4-C3-C5-C6
44	q	305	CLA	C4-C3-C5-C6
44	B	818	CLA	C2-C3-C5-C6
44	5	307	CLA	C2-C3-C5-C6
44	f	813	CLA	C2-C3-C5-C6
44	q	316	CLA	CBA-CGA-O2A-C1
52	p	514	CHL	CBA-CGA-O2A-C1
44	5	308	CLA	CBD-CGD-O2D-CED
44	B	816	CLA	O1D-CGD-O2D-CED
44	p	515	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
52	q	313	CHL	O1D-CGD-O2D-CED
44	A	831	CLA	C2A-CAA-CBA-CGA
44	q	309	CLA	C2A-CAA-CBA-CGA
44	f	820	CLA	O1A-CGA-O2A-C1
44	A	836	CLA	C3-C5-C6-C7
44	B	835	CLA	C3-C5-C6-C7
44	3	314	CLA	C3-C5-C6-C7
44	e	816	CLA	C3-C5-C6-C7
44	e	839	CLA	C3-C5-C6-C7
44	f	801	CLA	C3-C5-C6-C7
44	o	303	CLA	C3-C5-C6-C7
44	A	816	CLA	CBA-CGA-O2A-C1
44	B	822	CLA	CBA-CGA-O2A-C1
44	B	830	CLA	CBA-CGA-O2A-C1
44	5	310	CLA	CBA-CGA-O2A-C1
44	s	506	CLA	CBA-CGA-O2A-C1
47	2	503	BCR	C13-C14-C15-C16
51	p	502	LUT	C29-C30-C31-C32
44	B	818	CLA	O1A-CGA-O2A-C1
44	2	506	CLA	O1A-CGA-O2A-C1
44	e	816	CLA	O1A-CGA-O2A-C1
49	J	103	DGD	O1A-C1A-O1G-C1G
44	B	820	CLA	O1D-CGD-O2D-CED
44	1	509	CLA	O1D-CGD-O2D-CED
52	5	315	CHL	O1D-CGD-O2D-CED
44	f	813	CLA	C3-C5-C6-C7
44	f	841	CLA	CBD-CGD-O2D-CED
52	1	512	CHL	CBD-CGD-O2D-CED
49	B	850	DGD	C5B-C6B-C7B-C8B
44	J	101	CLA	C2C-C3C-CAC-CBC
46	1	516	LHG	O2-C2-C3-O3
44	A	813	CLA	O1D-CGD-O2D-CED
44	B	811	CLA	O1D-CGD-O2D-CED
44	1	506	CLA	O1D-CGD-O2D-CED
44	e	821	CLA	O1D-CGD-O2D-CED
44	e	834	CLA	O1D-CGD-O2D-CED
44	f	803	CLA	O1D-CGD-O2D-CED
44	f	808	CLA	O1D-CGD-O2D-CED
44	m	102	CLA	O1D-CGD-O2D-CED
44	p	504	CLA	O1D-CGD-O2D-CED
44	r	308	CLA	O1D-CGD-O2D-CED
52	2	513	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
44	B	818	CLA	CBA-CGA-O2A-C1
44	2	506	CLA	CBA-CGA-O2A-C1
44	2	514	CLA	CBA-CGA-O2A-C1
44	f	820	CLA	CBA-CGA-O2A-C1
44	o	303	CLA	CBA-CGA-O2A-C1
44	s	511	CLA	CBA-CGA-O2A-C1
44	A	816	CLA	O1A-CGA-O2A-C1
44	A	835	CLA	O1A-CGA-O2A-C1
44	q	312	CLA	O1A-CGA-O2A-C1
44	F	802	CLA	O1D-CGD-O2D-CED
44	3	318	CLA	CBD-CGD-O2D-CED
52	s	512	CHL	CBD-CGD-O2D-CED
44	f	821	CLA	O1D-CGD-O2D-CED
44	f	835	CLA	O1D-CGD-O2D-CED
44	A	815	CLA	O1D-CGD-O2D-CED
44	f	820	CLA	O1D-CGD-O2D-CED
44	2	506	CLA	CBD-CGD-O2D-CED
44	2	510	CLA	CBD-CGD-O2D-CED
44	5	310	CLA	CBD-CGD-O2D-CED
44	f	828	CLA	CBD-CGD-O2D-CED
50	2	519	LMG	O6-C5-C6-O5
44	e	802	CLA	O1D-CGD-O2D-CED
44	A	820	CLA	CBA-CGA-O2A-C1
44	L	303	CLA	C4-C3-C5-C6
44	3	308	CLA	C4-C3-C5-C6
44	r	306	CLA	C4-C3-C5-C6
44	B	841	CLA	C2-C3-C5-C6
44	q	305	CLA	C2-C3-C5-C6
44	B	830	CLA	O1A-CGA-O2A-C1
44	s	504	CLA	O1D-CGD-O2D-CED
44	B	824	CLA	CBD-CGD-O2D-CED
44	F	803	CLA	CBD-CGD-O2D-CED
44	e	841	CLA	CBD-CGD-O2D-CED
44	f	817	CLA	CBD-CGD-O2D-CED
44	e	838	CLA	C3-C5-C6-C7
44	p	513	CLA	C3-C5-C6-C7
52	2	512	CHL	C2A-CAA-CBA-CGA
44	L	304	CLA	C4C-C3C-CAC-CBC
44	A	828	CLA	O1D-CGD-O2D-CED
52	s	513	CHL	O1D-CGD-O2D-CED
44	B	822	CLA	O1A-CGA-O2A-C1
49	J	103	DGD	O6D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
49	m	104	DGD	O6E-C1E-O5D-C6D
50	F	806	LMG	O6-C1-O1-C7
54	Q	803	SQD	O5-C1-O6-C44
44	B	814	CLA	O1D-CGD-O2D-CED
44	3	314	CLA	CBA-CGA-O2A-C1
44	e	837	CLA	CBA-CGA-O2A-C1
46	B	851	LHG	C24-C23-O8-C6
44	A	802	CLA	CBD-CGD-O2D-CED
44	A	824	CLA	CBD-CGD-O2D-CED
44	A	826	CLA	CBD-CGD-O2D-CED
44	B	834	CLA	CBD-CGD-O2D-CED
44	1	504	CLA	CBD-CGD-O2D-CED
44	e	828	CLA	CBD-CGD-O2D-CED
44	f	810	CLA	CBD-CGD-O2D-CED
44	p	505	CLA	CBD-CGD-O2D-CED
52	p	517	CHL	CBD-CGD-O2D-CED
52	p	514	CHL	O1A-CGA-O2A-C1
44	J	101	CLA	C4C-C3C-CAC-CBC
44	s	511	CLA	O1A-CGA-O2A-C1
44	2	514	CLA	O1D-CGD-O2D-CED
44	A	811	CLA	CBD-CGD-O2D-CED
44	A	825	CLA	CBD-CGD-O2D-CED
44	f	834	CLA	CBD-CGD-O2D-CED
50	m	105	LMG	C11-C10-O7-C8
44	f	833	CLA	O1D-CGD-O2D-CED
44	A	820	CLA	O1A-CGA-O2A-C1
44	e	837	CLA	O1A-CGA-O2A-C1
46	B	851	LHG	O10-C23-O8-C6
44	A	810	CLA	CBA-CGA-O2A-C1
44	A	836	CLA	CBA-CGA-O2A-C1
44	B	812	CLA	CBA-CGA-O2A-C1
44	B	842	CLA	CBA-CGA-O2A-C1
44	L	301	CLA	CBA-CGA-O2A-C1
44	5	308	CLA	CBA-CGA-O2A-C1
44	e	829	CLA	CBA-CGA-O2A-C1
44	f	831	CLA	CBA-CGA-O2A-C1
44	p	506	CLA	CBA-CGA-O2A-C1
44	q	309	CLA	CBA-CGA-O2A-C1
44	s	509	CLA	CBA-CGA-O2A-C1
44	3	310	CLA	CBD-CGD-O2D-CED
44	A	810	CLA	O1D-CGD-O2D-CED
44	L	304	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
44	e	808	CLA	O1D-CGD-O2D-CED
44	e	818	CLA	O1D-CGD-O2D-CED
44	e	836	CLA	O1D-CGD-O2D-CED
52	p	514	CHL	O1D-CGD-O2D-CED
44	A	836	CLA	C2-C3-C5-C6
44	L	303	CLA	C2-C3-C5-C6
44	3	308	CLA	C2-C3-C5-C6
44	e	810	CLA	C2-C3-C5-C6
44	A	852	CLA	C3-C5-C6-C7
44	B	830	CLA	CBD-CGD-O2D-CED
44	A	826	CLA	C6-C7-C8-C9
44	A	827	CLA	C14-C13-C15-C16
44	A	838	CLA	C11-C12-C13-C14
44	B	818	CLA	C11-C10-C8-C9
44	2	506	CLA	C11-C12-C13-C14
44	3	314	CLA	C11-C10-C8-C9
44	e	824	CLA	C6-C7-C8-C9
44	e	829	CLA	C6-C7-C8-C9
44	p	508	CLA	C11-C10-C8-C9
44	s	506	CLA	C11-C10-C8-C9
45	A	841	PQN	C19-C18-C20-C21
45	B	843	PQN	C19-C18-C20-C21
52	3	315	CHL	O1D-CGD-O2D-CED
49	m	104	DGD	C2E-C1E-O5D-C6D
50	F	806	LMG	C2-C1-O1-C7
54	Q	803	SQD	C2-C1-O6-C44
44	e	826	CLA	CBA-CGA-O2A-C1
44	L	301	CLA	O1A-CGA-O2A-C1
44	f	831	CLA	O1A-CGA-O2A-C1
44	J	101	CLA	CBD-CGD-O2D-CED
47	A	845	BCR	C37-C22-C23-C24
47	A	847	BCR	C7-C8-C9-C34
47	A	853	BCR	C37-C22-C23-C24
47	B	844	BCR	C7-C8-C9-C34
47	F	801	BCR	C36-C18-C19-C20
47	L	305	BCR	C7-C8-C9-C34
47	2	503	BCR	C37-C22-C23-C24
47	3	305	BCR	C7-C8-C9-C34
47	5	302	BCR	C11-C12-C13-C35
47	e	846	BCR	C37-C22-C23-C24
47	e	848	BCR	C7-C8-C9-C34
47	e	854	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
47	f	847	BCR	C7-C8-C9-C34
47	f	850	BCR	C37-C22-C23-C24
47	j	801	BCR	C37-C22-C23-C24
47	l	101	BCR	C7-C8-C9-C34
47	l	102	BCR	C7-C8-C9-C34
47	l	102	BCR	C37-C22-C23-C24
47	n	204	BCR	C7-C8-C9-C34
47	n	204	BCR	C37-C22-C23-C24
51	p	501	LUT	C7-C8-C9-C19
51	p	502	LUT	C31-C32-C33-C40
53	2	502	XAT	C27-C28-C29-C39
53	s	502	XAT	C11-C12-C13-C20
47	A	847	BCR	C7-C8-C9-C10
47	A	853	BCR	C21-C22-C23-C24
47	B	844	BCR	C7-C8-C9-C10
47	F	801	BCR	C21-C22-C23-C24
47	L	305	BCR	C7-C8-C9-C10
47	Q	801	BCR	C21-C22-C23-C24
47	e	846	BCR	C21-C22-C23-C24
47	e	848	BCR	C7-C8-C9-C10
47	j	801	BCR	C21-C22-C23-C24
47	l	101	BCR	C7-C8-C9-C10
47	l	102	BCR	C7-C8-C9-C10
47	n	204	BCR	C21-C22-C23-C24
51	p	501	LUT	C7-C8-C9-C10
50	2	519	LMG	C4-C5-C6-O5
44	e	810	CLA	C2A-CAA-CBA-CGA
44	f	811	CLA	C2A-CAA-CBA-CGA
44	q	305	CLA	C2A-CAA-CBA-CGA
52	5	314	CHL	C2A-CAA-CBA-CGA
44	e	829	CLA	O1A-CGA-O2A-C1
44	p	506	CLA	O1A-CGA-O2A-C1
44	1	510	CLA	CBA-CGA-O2A-C1
52	s	517	CHL	CBA-CGA-O2A-C1
43	A	801	CL0	CAA-CBA-CGA-O2A
43	e	801	CL0	CAA-CBA-CGA-O2A
44	3	306	CLA	CBA-CGA-O2A-C1
44	f	829	CLA	CBA-CGA-O2A-C1
44	2	514	CLA	C2-C1-O2A-CGA
44	2	507	CLA	O1D-CGD-O2D-CED
44	e	853	CLA	O1D-CGD-O2D-CED
44	n	202	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
49	J	103	DGD	O6E-C5E-C6E-O5E
44	A	805	CLA	C10-C11-C12-C13
44	2	506	CLA	C15-C16-C17-C18
44	2	510	CLA	C5-C6-C7-C8
44	r	306	CLA	C8-C10-C11-C12
44	e	833	CLA	O1D-CGD-O2D-CED
44	f	829	CLA	O1D-CGD-O2D-CED
44	e	814	CLA	CBD-CGD-O2D-CED
44	q	306	CLA	CBD-CGD-O2D-CED
44	A	806	CLA	C6-C7-C8-C10
44	e	815	CLA	C2C-C3C-CAC-CBC
44	f	825	CLA	O1D-CGD-O2D-CED
46	p	516	LHG	C7-C8-C9-C10
47	l	101	BCR	C9-C10-C11-C12
50	m	105	LMG	O9-C10-O7-C8
44	f	808	CLA	C3-C5-C6-C7
45	A	841	PQN	C18-C20-C21-C22
45	B	843	PQN	C15-C16-C17-C18
50	2	519	LMG	C28-C29-C30-C31
44	A	810	CLA	O1A-CGA-O2A-C1
44	3	306	CLA	O1A-CGA-O2A-C1
44	5	308	CLA	O1A-CGA-O2A-C1
44	f	840	CLA	CBD-CGD-O2D-CED
44	A	805	CLA	C8-C10-C11-C12
44	B	802	CLA	C10-C11-C12-C13
44	B	802	CLA	C15-C16-C17-C18
44	2	514	CLA	C5-C6-C7-C8
44	e	804	CLA	C15-C16-C17-C18
44	e	839	CLA	C5-C6-C7-C8
44	A	808	CLA	C2A-CAA-CBA-CGA
44	A	823	CLA	C2A-CAA-CBA-CGA
44	B	801	CLA	C2A-CAA-CBA-CGA
44	3	308	CLA	C2A-CAA-CBA-CGA
44	3	314	CLA	C2A-CAA-CBA-CGA
44	e	824	CLA	C2A-CAA-CBA-CGA
44	q	315	CLA	C2A-CAA-CBA-CGA
44	s	509	CLA	C2A-CAA-CBA-CGA
52	p	514	CHL	C2A-CAA-CBA-CGA
52	s	512	CHL	C2A-CAA-CBA-CGA
52	2	516	CHL	O1D-CGD-O2D-CED
44	2	507	CLA	C5-C6-C7-C8
44	5	308	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
44	e	804	CLA	C5-C6-C7-C8
44	e	804	CLA	C8-C10-C11-C12
44	e	804	CLA	C13-C15-C16-C17
44	o	303	CLA	C8-C10-C11-C12
44	p	508	CLA	C13-C15-C16-C17
52	r	313	CHL	O1D-CGD-O2D-CED
44	A	836	CLA	O1A-CGA-O2A-C1
44	B	842	CLA	O1A-CGA-O2A-C1
44	q	309	CLA	O1A-CGA-O2A-C1
44	s	509	CLA	O1A-CGA-O2A-C1
44	B	842	CLA	C3-C5-C6-C7
44	3	308	CLA	C3-C5-C6-C7
44	f	831	CLA	C3-C5-C6-C7
50	2	518	LMG	O6-C1-O1-C7
44	A	838	CLA	C5-C6-C7-C8
44	B	838	CLA	C5-C6-C7-C8
44	3	308	CLA	C5-C6-C7-C8
44	5	308	CLA	C5-C6-C7-C8
44	e	810	CLA	C5-C6-C7-C8
44	f	826	CLA	C5-C6-C7-C8
44	r	307	CLA	C8-C10-C11-C12
46	B	851	LHG	O2-C2-C3-O3
44	B	812	CLA	O1A-CGA-O2A-C1
44	f	833	CLA	C2A-CAA-CBA-CGA
44	B	835	CLA	C5-C6-C7-C8
44	5	316	CLA	O1D-CGD-O2D-CED
44	A	823	CLA	C5-C6-C7-C8
44	5	307	CLA	C10-C11-C12-C13
44	o	303	CLA	C5-C6-C7-C8
44	K	202	CLA	CBD-CGD-O2D-CED
52	r	316	CHL	CBD-CGD-O2D-CED
44	3	314	CLA	O1A-CGA-O2A-C1
44	e	826	CLA	O1A-CGA-O2A-C1
44	f	829	CLA	O1A-CGA-O2A-C1
44	r	306	CLA	C2-C3-C5-C6
49	B	850	DGD	O6D-C5D-C6D-O5D
44	5	308	CLA	O1D-CGD-O2D-CED
52	1	512	CHL	O1D-CGD-O2D-CED
44	A	827	CLA	C10-C11-C12-C13
44	B	818	CLA	C5-C6-C7-C8
44	B	826	CLA	C8-C10-C11-C12
44	3	306	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
44	A	804	CLA	CBA-CGA-O2A-C1
44	A	825	CLA	CBA-CGA-O2A-C1
44	e	810	CLA	CBA-CGA-O2A-C1
44	A	838	CLA	CBD-CGD-O2D-CED
44	2	510	CLA	C3-C5-C6-C7
44	3	318	CLA	O1D-CGD-O2D-CED
44	f	841	CLA	O1D-CGD-O2D-CED
52	s	515	CHL	CBD-CGD-O2D-CED
44	A	827	CLA	C8-C10-C11-C12
44	s	506	CLA	C8-C10-C11-C12
44	B	837	CLA	C2C-C3C-CAC-CBC
50	F	806	LMG	C14-C15-C16-C17
50	F	805	LMG	O9-C10-O7-C8
44	A	827	CLA	C2A-CAA-CBA-CGA
44	f	829	CLA	C2A-CAA-CBA-CGA
44	q	316	CLA	C2A-CAA-CBA-CGA
44	r	309	CLA	C2A-CAA-CBA-CGA
52	q	313	CHL	C2A-CAA-CBA-CGA
44	f	813	CLA	CBA-CGA-O2A-C1
44	p	508	CLA	CBA-CGA-O2A-C1
44	A	805	CLA	C5-C6-C7-C8
44	e	839	CLA	C13-C15-C16-C17
44	A	802	CLA	C5-C6-C7-C8
44	A	806	CLA	C13-C15-C16-C17
44	B	803	CLA	C10-C11-C12-C13
44	f	826	CLA	C10-C11-C12-C13
44	s	506	CLA	C10-C11-C12-C13
44	e	832	CLA	C2A-CAA-CBA-CGA
52	2	516	CHL	C2A-CAA-CBA-CGA
44	A	829	CLA	C4-C3-C5-C6
49	B	850	DGD	C4D-C5D-C6D-O5D
50	F	805	LMG	C11-C10-O7-C8
50	F	806	LMG	C11-C10-O7-C8
52	s	512	CHL	O1D-CGD-O2D-CED
50	F	806	LMG	O9-C10-O7-C8
46	1	516	LHG	C23-C24-C25-C26
46	f	852	LHG	O2-C2-C3-O3
44	1	506	CLA	C6-C7-C8-C9
44	5	307	CLA	C16-C17-C18-C20
44	f	810	CLA	C16-C17-C18-C20
44	f	836	CLA	C3-C5-C6-C7
44	s	510	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
47	A	848	BCR	C37-C22-C23-C24
47	A	851	BCR	C37-C22-C23-C24
47	K	204	BCR	C37-C22-C23-C24
47	L	306	BCR	C11-C12-C13-C35
47	1	503	BCR	C7-C8-C9-C34
47	3	305	BCR	C37-C22-C23-C24
47	f	845	BCR	C37-C22-C23-C24
53	5	304	XAT	C27-C28-C29-C39
53	r	303	XAT	C7-C8-C9-C19
47	A	848	BCR	C21-C22-C23-C24
47	K	204	BCR	C21-C22-C23-C24
47	1	503	BCR	C7-C8-C9-C10
47	3	305	BCR	C7-C8-C9-C10
47	3	305	BCR	C21-C22-C23-C24
47	f	845	BCR	C21-C22-C23-C24
51	p	502	LUT	C31-C32-C33-C34
44	e	810	CLA	O1A-CGA-O2A-C1
44	B	802	CLA	C2A-CAA-CBA-CGA
44	B	821	CLA	C2A-CAA-CBA-CGA
44	2	509	CLA	C2A-CAA-CBA-CGA
44	5	308	CLA	C2A-CAA-CBA-CGA
44	q	312	CLA	C2A-CAA-CBA-CGA
44	r	305	CLA	C2A-CAA-CBA-CGA
52	3	302	CHL	CBA-CGA-O2A-C1
44	A	829	CLA	C5-C6-C7-C8
46	A	844	LHG	O1-C1-C2-C3
44	B	824	CLA	O1D-CGD-O2D-CED
44	5	310	CLA	O1D-CGD-O2D-CED
44	f	828	CLA	O1D-CGD-O2D-CED
44	A	823	CLA	C6-C7-C8-C9
44	2	510	CLA	C11-C12-C13-C14
44	3	308	CLA	C6-C7-C8-C9
44	5	308	CLA	C11-C12-C13-C14
44	o	303	CLA	C11-C12-C13-C14
44	B	834	CLA	O1D-CGD-O2D-CED
44	2	510	CLA	O1D-CGD-O2D-CED
44	f	826	CLA	C3-C5-C6-C7
44	F	803	CLA	O1D-CGD-O2D-CED
49	J	103	DGD	C2B-C1B-O2G-C2G
44	e	841	CLA	O1D-CGD-O2D-CED
44	2	506	CLA	O1D-CGD-O2D-CED
44	f	817	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
44	2	505	CLA	CBA-CGA-O2A-C1
44	A	831	CLA	C15-C16-C17-C18
44	p	508	CLA	C8-C10-C11-C12
44	B	842	CLA	CBD-CGD-O2D-CED
46	f	852	LHG	C7-C8-C9-C10
44	e	812	CLA	CBD-CGD-O2D-CED
44	e	815	CLA	C4C-C3C-CAC-CBC
44	3	314	CLA	C2-C1-O2A-CGA
44	5	310	CLA	C2-C1-O2A-CGA
44	2	510	CLA	C11-C12-C13-C15
44	o	303	CLA	C11-C12-C13-C15
44	p	506	CLA	C6-C7-C8-C9
50	5	301	LMG	C11-C12-C13-C14
52	1	512	CHL	CBA-CGA-O2A-C1
52	2	512	CHL	CBA-CGA-O2A-C1
49	m	104	DGD	CBB-CCB-CDB-CEB
44	1	504	CLA	O1D-CGD-O2D-CED
44	A	804	CLA	O1A-CGA-O2A-C1
44	A	825	CLA	O1A-CGA-O2A-C1
49	J	103	DGD	O1B-C1B-O2G-C2G
44	f	810	CLA	C15-C16-C17-C18
44	A	817	CLA	C4B-C3B-CAB-CBB
44	A	822	CLA	C4B-C3B-CAB-CBB
44	A	834	CLA	C4B-C3B-CAB-CBB
44	B	803	CLA	C4B-C3B-CAB-CBB
44	B	815	CLA	C4B-C3B-CAB-CBB
44	B	836	CLA	C4B-C3B-CAB-CBB
44	B	841	CLA	C4B-C3B-CAB-CBB
44	F	802	CLA	C4B-C3B-CAB-CBB
44	2	508	CLA	C4B-C3B-CAB-CBB
44	2	514	CLA	C4B-C3B-CAB-CBB
44	5	313	CLA	C4B-C3B-CAB-CBB
44	e	814	CLA	C4B-C3B-CAB-CBB
44	e	835	CLA	C4B-C3B-CAB-CBB
44	f	809	CLA	C4B-C3B-CAB-CBB
44	f	824	CLA	C4B-C3B-CAB-CBB
44	q	316	CLA	C4B-C3B-CAB-CBB
44	r	311	CLA	C4B-C3B-CAB-CBB
49	J	103	DGD	C1A-C2A-C3A-C4A
44	p	510	CLA	CBA-CGA-O2A-C1
52	5	314	CHL	CBA-CGA-O2A-C1
52	s	512	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
44	3	308	CLA	C6-C7-C8-C10
44	5	308	CLA	C11-C12-C13-C15
44	e	837	CLA	C6-C7-C8-C9
44	A	824	CLA	O1D-CGD-O2D-CED
44	5	307	CLA	C2A-CAA-CBA-CGA
52	r	313	CHL	C2A-CAA-CBA-CGA
49	m	104	DGD	C7B-C8B-C9B-CAB
44	B	842	CLA	C8-C10-C11-C12
49	m	104	DGD	C2B-C1B-O2G-C2G
44	3	314	CLA	C6-C7-C8-C10
46	A	843	LHG	C27-C28-C29-C30
46	A	844	LHG	C7-C8-C9-C10
49	J	103	DGD	C7B-C8B-C9B-CAB
50	2	519	LMG	C11-C12-C13-C14
44	f	813	CLA	O1A-CGA-O2A-C1
44	A	805	CLA	C3A-C2A-CAA-CBA
44	A	852	CLA	C3A-C2A-CAA-CBA
44	B	834	CLA	C3A-C2A-CAA-CBA
44	L	303	CLA	C3A-C2A-CAA-CBA
44	3	310	CLA	C3A-C2A-CAA-CBA
44	3	318	CLA	C3A-C2A-CAA-CBA
44	5	309	CLA	C3A-C2A-CAA-CBA
44	e	804	CLA	C3A-C2A-CAA-CBA
44	e	826	CLA	C3A-C2A-CAA-CBA
44	e	853	CLA	C3A-C2A-CAA-CBA
44	p	506	CLA	C3A-C2A-CAA-CBA
44	q	315	CLA	C3A-C2A-CAA-CBA
44	q	316	CLA	C3A-C2A-CAA-CBA
44	s	505	CLA	C3A-C2A-CAA-CBA
52	2	516	CHL	C3A-C2A-CAA-CBA
52	5	314	CHL	C3A-C2A-CAA-CBA
44	A	802	CLA	O1D-CGD-O2D-CED
44	o	304	CLA	CBD-CGD-O2D-CED
44	A	806	CLA	C5-C6-C7-C8
44	A	806	CLA	C15-C16-C17-C18
50	F	806	LMG	C28-C29-C30-C31
44	A	823	CLA	C6-C7-C8-C10
44	e	826	CLA	C16-C17-C18-C19
44	e	839	CLA	C16-C17-C18-C20
44	f	821	CLA	C6-C7-C8-C10
44	p	508	CLA	O1A-CGA-O2A-C1
50	F	806	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
44	B	821	CLA	CBD-CGD-O2D-CED
44	r	312	CLA	CBD-CGD-O2D-CED
44	f	836	CLA	CAA-CBA-CGA-O2A
46	1	516	LHG	C1-C2-C3-O3
44	A	842	CLA	CBA-CGA-O2A-C1
44	3	311	CLA	CBA-CGA-O2A-C1
44	A	826	CLA	C3-C5-C6-C7
44	A	831	CLA	C13-C15-C16-C17
46	1	516	LHG	C34-C35-C36-C37
52	p	517	CHL	O1D-CGD-O2D-CED
44	e	828	CLA	O1D-CGD-O2D-CED
49	B	850	DGD	CDB-CEB-CFB-CGB
44	2	505	CLA	O1A-CGA-O2A-C1
44	A	822	CLA	C2B-C3B-CAB-CBB
44	A	834	CLA	C2B-C3B-CAB-CBB
44	B	836	CLA	C2B-C3B-CAB-CBB
44	B	841	CLA	C2B-C3B-CAB-CBB
44	F	802	CLA	C2B-C3B-CAB-CBB
44	J	101	CLA	C2B-C3B-CAB-CBB
44	1	511	CLA	C2B-C3B-CAB-CBB
44	1	513	CLA	C2B-C3B-CAB-CBB
44	5	313	CLA	C2B-C3B-CAB-CBB
44	e	814	CLA	C2B-C3B-CAB-CBB
44	e	833	CLA	C2B-C3B-CAB-CBB
44	e	835	CLA	C2B-C3B-CAB-CBB
44	f	809	CLA	C2B-C3B-CAB-CBB
44	f	819	CLA	C2B-C3B-CAB-CBB
44	f	823	CLA	C2B-C3B-CAB-CBB
44	f	824	CLA	C2B-C3B-CAB-CBB
44	f	836	CLA	C2B-C3B-CAB-CBB
44	f	842	CLA	C2B-C3B-CAB-CBB
44	q	310	CLA	C2B-C3B-CAB-CBB
44	q	316	CLA	C2B-C3B-CAB-CBB
44	r	311	CLA	C2B-C3B-CAB-CBB
47	A	848	BCR	C23-C24-C25-C30
47	A	851	BCR	C1-C6-C7-C8
47	A	851	BCR	C23-C24-C25-C26
47	A	851	BCR	C23-C24-C25-C30
47	K	204	BCR	C23-C24-C25-C30
47	L	306	BCR	C23-C24-C25-C26
47	L	306	BCR	C23-C24-C25-C30
47	1	503	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
47	1	503	BCR	C5-C6-C7-C8
47	2	503	BCR	C1-C6-C7-C8
47	2	503	BCR	C5-C6-C7-C8
47	3	305	BCR	C1-C6-C7-C8
47	3	305	BCR	C5-C6-C7-C8
47	Q	801	BCR	C1-C6-C7-C8
47	e	849	BCR	C1-C6-C7-C8
47	e	849	BCR	C23-C24-C25-C26
47	e	849	BCR	C23-C24-C25-C30
47	e	851	BCR	C1-C6-C7-C8
47	l	101	BCR	C23-C24-C25-C26
47	r	301	BCR	C1-C6-C7-C8
47	r	301	BCR	C5-C6-C7-C8
51	q	301	LUT	C1-C6-C7-C8
51	q	301	LUT	C5-C6-C7-C8
46	B	851	LHG	C29-C30-C31-C32
52	1	514	CHL	CBD-CGD-O2D-CED
52	s	517	CHL	O1A-CGA-O2A-C1
50	5	301	LMG	C29-C28-O8-C9
49	J	103	DGD	C6B-C7B-C8B-C9B
44	A	826	CLA	O1D-CGD-O2D-CED
44	f	810	CLA	O1D-CGD-O2D-CED
44	A	816	CLA	C2A-CAA-CBA-CGA
44	5	312	CLA	C2A-CAA-CBA-CGA
44	e	804	CLA	C2A-CAA-CBA-CGA
44	f	820	CLA	C2A-CAA-CBA-CGA
52	p	512	CHL	C2A-CAA-CBA-CGA
44	B	841	CLA	C5-C6-C7-C8
46	A	843	LHG	C14-C15-C16-C17
49	m	104	DGD	O1B-C1B-O2G-C2G
44	A	805	CLA	C13-C15-C16-C17
44	A	831	CLA	C5-C6-C7-C8
44	A	829	CLA	C2-C3-C5-C6
44	e	809	CLA	CBA-CGA-O2A-C1
44	3	311	CLA	O1A-CGA-O2A-C1
44	B	807	CLA	C6-C7-C8-C9
44	e	826	CLA	C14-C13-C15-C16
46	A	843	LHG	C31-C32-C33-C34
50	2	518	LMG	C2-C1-O1-C7
50	r	318	LMG	C2-C1-O1-C7
44	A	842	CLA	O1A-CGA-O2A-C1
44	s	506	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
44	f	810	CLA	C16-C17-C18-C19
44	p	508	CLA	C16-C17-C18-C20
44	A	818	CLA	CBD-CGD-O2D-CED
46	A	844	LHG	C8-C7-O7-C5
46	1	516	LHG	C8-C7-O7-C5
54	Q	803	SQD	C8-C7-O47-C45
44	A	806	CLA	C10-C11-C12-C13
54	Q	803	SQD	O49-C7-O47-C45
44	1	510	CLA	O1A-CGA-O2A-C1
46	1	516	LHG	C9-C10-C11-C12
45	A	841	PQN	C25-C26-C27-C28
47	e	854	BCR	C7-C8-C9-C34
47	q	303	BCR	C37-C22-C23-C24
46	1	516	LHG	C7-C8-C9-C10
47	n	204	BCR	C7-C8-C9-C10
49	J	103	DGD	C5D-C6D-O5D-C1E
44	A	820	CLA	C2A-CAA-CBA-CGA
44	e	824	CLA	C11-C10-C8-C9
44	1	506	CLA	C6-C7-C8-C10
44	5	307	CLA	C16-C17-C18-C19
44	p	508	CLA	C16-C17-C18-C19
45	A	841	PQN	C26-C27-C28-C30
44	L	303	CLA	CBD-CGD-O2D-CED
52	5	317	CHL	CBD-CGD-O2D-CED
46	1	516	LHG	C14-C15-C16-C17
44	e	826	CLA	C4-C3-C5-C6
44	5	308	CLA	C8-C10-C11-C12
46	B	851	LHG	C9-C10-C11-C12
46	A	844	LHG	O9-C7-O7-C5
44	f	834	CLA	O1D-CGD-O2D-CED
44	A	836	CLA	C6-C7-C8-C9
44	f	821	CLA	C6-C7-C8-C9
44	p	506	CLA	C6-C7-C8-C10
49	B	850	DGD	C2B-C3B-C4B-C5B
49	J	103	DGD	CEA-CFA-CGA-CHA
44	A	827	CLA	C5-C6-C7-C8
44	B	807	CLA	C15-C16-C17-C18
46	A	843	LHG	C29-C30-C31-C32
44	p	509	CLA	C2-C1-O2A-CGA
44	A	811	CLA	O1D-CGD-O2D-CED
44	A	825	CLA	O1D-CGD-O2D-CED
44	B	833	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
44	L	301	CLA	C4-C3-C5-C6
44	B	817	CLA	C2A-CAA-CBA-CGA
44	5	310	CLA	C2A-CAA-CBA-CGA
44	e	816	CLA	C2A-CAA-CBA-CGA
44	r	306	CLA	C2A-CAA-CBA-CGA
44	B	829	CLA	CBD-CGD-O2D-CED
44	e	830	CLA	CBA-CGA-O2A-C1
44	3	310	CLA	O1D-CGD-O2D-CED
44	s	506	CLA	C5-C6-C7-C8
44	B	830	CLA	O1D-CGD-O2D-CED
46	A	843	LHG	C10-C11-C12-C13
44	A	836	CLA	C6-C7-C8-C10
44	e	809	CLA	O1A-CGA-O2A-C1
50	5	301	LMG	O10-C28-O8-C9
44	A	852	CLA	C1A-C2A-CAA-CBA
44	B	804	CLA	C1A-C2A-CAA-CBA
44	B	820	CLA	C1A-C2A-CAA-CBA
44	B	821	CLA	C1A-C2A-CAA-CBA
44	3	308	CLA	C1A-C2A-CAA-CBA
44	3	310	CLA	C1A-C2A-CAA-CBA
44	3	313	CLA	C1A-C2A-CAA-CBA
44	3	314	CLA	C1A-C2A-CAA-CBA
44	5	309	CLA	C1A-C2A-CAA-CBA
44	e	830	CLA	C1A-C2A-CAA-CBA
44	e	831	CLA	C1A-C2A-CAA-CBA
44	f	817	CLA	C1A-C2A-CAA-CBA
44	f	820	CLA	C1A-C2A-CAA-CBA
44	f	821	CLA	C1A-C2A-CAA-CBA
44	f	829	CLA	C1A-C2A-CAA-CBA
44	o	303	CLA	C1A-C2A-CAA-CBA
44	q	315	CLA	C1A-C2A-CAA-CBA
44	q	316	CLA	C1A-C2A-CAA-CBA
44	s	509	CLA	C1A-C2A-CAA-CBA
49	m	104	DGD	O6E-C5E-C6E-O5E
49	m	104	DGD	O6D-C1D-O3G-C3G
49	m	104	DGD	O6D-C5D-C6D-O5D
54	Q	802	SQD	C28-C29-C30-C31
44	p	505	CLA	O1D-CGD-O2D-CED
46	1	516	LHG	O9-C7-O7-C5
44	A	805	CLA	C6-C7-C8-C10
44	B	803	CLA	C12-C13-C15-C16
44	B	807	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
44	B	826	CLA	C11-C12-C13-C15
44	B	830	CLA	C6-C7-C8-C10
44	5	307	CLA	C12-C13-C15-C16
44	e	826	CLA	C11-C10-C8-C7
44	e	831	CLA	C6-C7-C8-C10
44	f	801	CLA	C12-C13-C15-C16
44	f	810	CLA	C6-C7-C8-C10
44	f	826	CLA	C12-C13-C15-C16
44	s	506	CLA	C12-C13-C15-C16
44	m	101	CLA	C3A-C2A-CAA-CBA
44	A	805	CLA	C2-C3-C5-C6
44	A	835	CLA	CBD-CGD-O2D-CED
44	B	808	CLA	C2A-CAA-CBA-CGA
44	2	506	CLA	C2A-CAA-CBA-CGA
44	3	306	CLA	C2A-CAA-CBA-CGA
44	s	506	CLA	C2A-CAA-CBA-CGA
44	A	805	CLA	C6-C7-C8-C9
44	A	808	CLA	C11-C12-C13-C14
44	A	816	CLA	C6-C7-C8-C9
44	B	807	CLA	C14-C13-C15-C16
44	B	830	CLA	C6-C7-C8-C9
44	r	306	CLA	C14-C13-C15-C16
44	s	510	CLA	C6-C7-C8-C9
44	q	311	CLA	CBA-CGA-O2A-C1
44	A	825	CLA	C5-C6-C7-C8
50	5	301	LMG	O6-C5-C6-O5
44	A	839	CLA	CBD-CGD-O2D-CED
52	r	316	CHL	O1D-CGD-O2D-CED
49	B	850	DGD	C4A-C5A-C6A-C7A
50	F	805	LMG	C13-C14-C15-C16
46	e	844	LHG	C7-C8-C9-C10
44	J	101	CLA	O1D-CGD-O2D-CED
49	J	103	DGD	O1G-C1G-C2G-C3G
49	J	103	DGD	C1G-C2G-C3G-O3G
46	p	516	LHG	C28-C29-C30-C31
50	F	806	LMG	C11-C12-C13-C14
44	q	306	CLA	O1D-CGD-O2D-CED
44	A	806	CLA	CBA-CGA-O2A-C1
50	2	519	LMG	C29-C28-O8-C9
54	Q	802	SQD	C7-C8-C9-C10
44	r	307	CLA	C11-C12-C13-C15
45	A	841	PQN	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
52	5	314	CHL	CHA-CBD-CGD-O1D
52	5	314	CHL	CHA-CBD-CGD-O2D
49	f	851	DGD	C5A-C6A-C7A-C8A
44	e	826	CLA	C2-C3-C5-C6
47	B	847	BCR	C11-C12-C13-C35
44	B	841	CLA	C6-C7-C8-C9
46	f	852	LHG	C23-C24-C25-C26
47	B	847	BCR	C11-C12-C13-C14
44	e	830	CLA	O1A-CGA-O2A-C1
44	p	508	CLA	C5-C6-C7-C8
46	p	516	LHG	C16-C17-C18-C19
50	F	806	LMG	C38-C39-C40-C41
44	A	832	CLA	CBA-CGA-O2A-C1
44	B	804	CLA	CBA-CGA-O2A-C1
44	3	313	CLA	O2A-C1-C2-C3
54	Q	803	SQD	C44-C45-O47-C7
44	A	816	CLA	C3-C5-C6-C7
52	1	514	CHL	C3C-C2C-CMC-OMC
52	q	313	CHL	C3C-C2C-CMC-OMC
52	s	515	CHL	C3C-C2C-CMC-OMC
44	q	311	CLA	O1A-CGA-O2A-C1
44	A	838	CLA	O1D-CGD-O2D-CED
44	e	814	CLA	O1D-CGD-O2D-CED
44	A	827	CLA	C13-C15-C16-C17
46	p	516	LHG	C24-C23-O8-C6
44	A	823	CLA	CBD-CGD-O2D-CED
54	Q	802	SQD	C8-C7-O47-C45
44	f	840	CLA	O1D-CGD-O2D-CED
44	A	805	CLA	C4-C3-C5-C6
44	r	307	CLA	C4-C3-C5-C6
49	J	103	DGD	C6A-C7A-C8A-C9A
54	Q	803	SQD	O47-C45-C46-O48
49	B	850	DGD	CCB-CDB-CEB-CFB
44	A	829	CLA	CBA-CGA-O2A-C1
49	B	850	DGD	C3B-C4B-C5B-C6B
49	m	104	DGD	CFA-CGA-CHA-CIA
49	f	851	DGD	C4B-C5B-C6B-C7B
44	e	803	CLA	C3-C5-C6-C7
43	A	801	CL0	C3-C5-C6-C7
43	e	801	CL0	C3-C5-C6-C7
44	B	818	CLA	C8-C10-C11-C12
44	A	825	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
44	A	805	CLA	C16-C17-C18-C19
44	B	808	CLA	CBA-CGA-O2A-C1
44	1	506	CLA	CBA-CGA-O2A-C1
52	2	515	CHL	C1C-C2C-CMC-OMC
52	q	313	CHL	C1C-C2C-CMC-OMC
44	A	837	CLA	CBD-CGD-O2D-CED
46	2	517	LHG	C7-C8-C9-C10
44	5	307	CLA	C8-C10-C11-C12
44	f	836	CLA	C8-C10-C11-C12
52	3	302	CHL	O1A-CGA-O2A-C1
44	A	806	CLA	C4-C3-C5-C6
44	A	827	CLA	C4-C3-C5-C6
44	A	852	CLA	C4-C3-C5-C6
44	2	506	CLA	C4-C3-C5-C6
44	q	304	CLA	C4B-C3B-CAB-CBB
44	p	508	CLA	C15-C16-C17-C18
44	A	838	CLA	C11-C10-C8-C9
44	2	510	CLA	C11-C10-C8-C9
44	3	314	CLA	C6-C7-C8-C9
44	5	307	CLA	C14-C13-C15-C16
44	e	826	CLA	C11-C10-C8-C9
44	e	831	CLA	C6-C7-C8-C9
44	f	801	CLA	C14-C13-C15-C16
44	f	810	CLA	C6-C7-C8-C9
44	f	826	CLA	C14-C13-C15-C16
44	s	506	CLA	C14-C13-C15-C16
52	1	514	CHL	O1D-CGD-O2D-CED
44	A	806	CLA	O1A-CGA-O2A-C1
44	A	814	CLA	C4B-C3B-CAB-CBB
44	A	852	CLA	C4B-C3B-CAB-CBB
44	B	805	CLA	C4B-C3B-CAB-CBB
44	1	511	CLA	C4B-C3B-CAB-CBB
44	3	301	CLA	C4B-C3B-CAB-CBB
44	5	307	CLA	C4B-C3B-CAB-CBB
44	5	312	CLA	C4B-C3B-CAB-CBB
44	e	822	CLA	C4B-C3B-CAB-CBB
44	e	830	CLA	C4B-C3B-CAB-CBB
44	f	820	CLA	C4B-C3B-CAB-CBB
44	f	822	CLA	C4B-C3B-CAB-CBB
44	f	823	CLA	C4B-C3B-CAB-CBB
44	j	802	CLA	C4B-C3B-CAB-CBB
44	n	201	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
44	r	312	CLA	C4B-C3B-CAB-CBB
49	B	850	DGD	C4B-C5B-C6B-C7B
52	s	515	CHL	O1D-CGD-O2D-CED
49	J	103	DGD	CFA-CGA-CHA-CIA
44	A	802	CLA	C6-C7-C8-C10
44	A	808	CLA	C11-C12-C13-C15
44	A	816	CLA	C6-C7-C8-C10
44	B	818	CLA	C11-C10-C8-C7
44	1	513	CLA	C12-C13-C15-C16
44	2	510	CLA	C11-C10-C8-C7
44	e	824	CLA	C6-C7-C8-C10
44	e	829	CLA	C6-C7-C8-C10
44	e	839	CLA	C11-C12-C13-C15
44	e	839	CLA	C12-C13-C15-C16
44	p	508	CLA	C11-C10-C8-C7
44	r	306	CLA	C12-C13-C15-C16
44	s	510	CLA	C6-C7-C8-C10
45	B	843	PQN	C17-C18-C20-C21
45	A	841	PQN	C15-C16-C17-C18
44	r	307	CLA	C11-C12-C13-C14
44	K	202	CLA	O1D-CGD-O2D-CED
44	A	813	CLA	C3A-C2A-CAA-CBA
44	A	826	CLA	C3A-C2A-CAA-CBA
44	B	813	CLA	C3A-C2A-CAA-CBA
44	B	830	CLA	C4-C3-C5-C6
44	f	821	CLA	C3A-C2A-CAA-CBA
52	2	515	CHL	C3A-C2A-CAA-CBA
44	1	513	CLA	C5-C6-C7-C8
44	2	506	CLA	C2-C3-C5-C6
52	r	313	CHL	CBA-CGA-O2A-C1
44	A	831	CLA	C10-C11-C12-C13
44	1	506	CLA	O1A-CGA-O2A-C1
44	A	838	CLA	CBA-CGA-O2A-C1
53	s	502	XAT	C9-C10-C11-C12
44	B	833	CLA	C3-C5-C6-C7
44	A	806	CLA	C16-C17-C18-C19
44	A	827	CLA	C16-C17-C18-C19
44	B	803	CLA	C15-C16-C17-C18
51	1	502	LUT	C7-C8-C9-C19
51	q	301	LUT	C27-C28-C29-C39
44	A	835	CLA	C4-C3-C5-C6
44	A	832	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
44	B	804	CLA	O1A-CGA-O2A-C1
52	1	512	CHL	O1A-CGA-O2A-C1
52	q	313	CHL	CBA-CGA-O2A-C1
44	e	839	CLA	CBA-CGA-O2A-C1
44	e	843	CLA	CBA-CGA-O2A-C1
49	f	851	DGD	O1G-C1G-C2G-C3G
50	r	318	LMG	O1-C7-C8-C9
54	Q	803	SQD	C44-C45-C46-O48
52	q	313	CHL	C1A-C2A-CAA-CBA
52	r	314	CHL	C1A-C2A-CAA-CBA
44	A	802	CLA	C8-C10-C11-C12
44	B	803	CLA	C4-C3-C5-C6
44	e	824	CLA	C4-C3-C5-C6
44	e	824	CLA	C2-C3-C5-C6
44	e	826	CLA	C3-C5-C6-C7
52	2	513	CHL	C2C-C3C-CAC-CBC
52	2	513	CHL	CHA-CBD-CGD-O2D
46	B	851	LHG	O6-C4-C5-O7
46	e	845	LHG	O6-C4-C5-O7
44	3	301	CLA	C2B-C3B-CAB-CBB
44	5	307	CLA	C2B-C3B-CAB-CBB
44	e	830	CLA	C2B-C3B-CAB-CBB
44	f	822	CLA	C2B-C3B-CAB-CBB
44	n	202	CLA	C2B-C3B-CAB-CBB
47	A	845	BCR	C1-C6-C7-C8
47	B	844	BCR	C1-C6-C7-C8
47	K	204	BCR	C1-C6-C7-C8
47	e	848	BCR	C23-C24-C25-C30
47	e	851	BCR	C23-C24-C25-C30
47	l	102	BCR	C23-C24-C25-C30
47	n	204	BCR	C1-C6-C7-C8
47	n	204	BCR	C23-C24-C25-C30
47	o	305	BCR	C23-C24-C25-C30
47	q	303	BCR	C23-C24-C25-C30
47	r	301	BCR	C23-C24-C25-C30
51	3	303	LUT	C1-C6-C7-C8
51	s	501	LUT	C1-C6-C7-C8
46	1	516	LHG	C11-C10-C9-C8
44	1	507	CLA	C11-C10-C8-C9
44	B	830	CLA	C3-C5-C6-C7
49	J	103	DGD	C4B-C5B-C6B-C7B
44	2	506	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
52	5	317	CHL	O1D-CGD-O2D-CED
44	e	839	CLA	C16-C17-C18-C19
50	2	519	LMG	O1-C7-C8-O7
50	5	301	LMG	O1-C7-C8-O7
50	r	318	LMG	C8-C9-O8-C28
44	o	304	CLA	O1D-CGD-O2D-CED
46	A	843	LHG	C23-C24-C25-C26
50	F	806	LMG	C10-C11-C12-C13
44	2	510	CLA	C10-C11-C12-C13
45	A	841	PQN	C20-C21-C22-C23
44	A	806	CLA	C2-C3-C5-C6
44	A	852	CLA	C2-C3-C5-C6
44	B	830	CLA	C2-C3-C5-C6
52	2	512	CHL	O1A-CGA-O2A-C1
49	B	850	DGD	C6A-C7A-C8A-C9A
44	1	513	CLA	C14-C13-C15-C16
44	e	816	CLA	C11-C10-C8-C9
44	B	842	CLA	O1D-CGD-O2D-CED
44	r	312	CLA	O1D-CGD-O2D-CED
54	Q	802	SQD	O47-C7-C8-C9
50	2	519	LMG	O10-C28-O8-C9
44	B	829	CLA	O1D-CGD-O2D-CED
44	s	505	CLA	CBA-CGA-O2A-C1
44	e	826	CLA	C16-C17-C18-C20
49	B	850	DGD	CEB-CFB-CGB-CHB
44	J	101	CLA	C1A-C2A-CAA-CBA
44	1	504	CLA	C1A-C2A-CAA-CBA
44	e	828	CLA	C1A-C2A-CAA-CBA
44	f	816	CLA	C1A-C2A-CAA-CBA
44	p	504	CLA	C1A-C2A-CAA-CBA
44	B	815	CLA	C2A-CAA-CBA-CGA
44	f	808	CLA	C2-C1-O2A-CGA
44	B	815	CLA	CBA-CGA-O2A-C1
44	r	309	CLA	CBA-CGA-O2A-C1
44	B	803	CLA	C2-C3-C5-C6
44	5	311	CLA	CBD-CGD-O2D-CED
44	f	838	CLA	C2C-C3C-CAC-CBC
52	s	512	CHL	O1A-CGA-O2A-C1
44	f	808	CLA	CAA-CBA-CGA-O2A
44	B	839	CLA	CBA-CGA-O2A-C1
44	3	306	CLA	C6-C7-C8-C9
44	e	837	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
46	A	843	LHG	C35-C36-C37-C38
44	B	818	CLA	CBD-CGD-O2D-CED
52	1	517	CHL	CBD-CGD-O2D-CED
47	B	852	BCR	C37-C22-C23-C24
47	K	204	BCR	C11-C12-C13-C35
47	2	503	BCR	C7-C8-C9-C34
47	Q	801	BCR	C36-C18-C19-C20
44	A	806	CLA	C12-C13-C15-C16
44	A	838	CLA	C11-C10-C8-C7
44	B	803	CLA	C6-C7-C8-C10
44	e	816	CLA	C11-C10-C8-C7
44	e	829	CLA	C11-C10-C8-C7
44	f	826	CLA	C6-C7-C8-C10
44	p	508	CLA	C6-C7-C8-C10
44	s	506	CLA	C11-C10-C8-C7
44	2	508	CLA	O2A-C1-C2-C3
47	L	306	BCR	C11-C12-C13-C14
47	Q	801	BCR	C17-C18-C19-C20
47	f	847	BCR	C7-C8-C9-C10
53	5	304	XAT	C27-C28-C29-C30
53	r	303	XAT	C7-C8-C9-C10
52	5	314	CHL	O1A-CGA-O2A-C1
46	1	516	LHG	C28-C29-C30-C31
50	r	318	LMG	C8-C7-O1-C1
52	p	512	CHL	CBA-CGA-O2A-C1
46	p	516	LHG	O10-C23-O8-C6
44	B	804	CLA	O2A-C1-C2-C3
49	J	103	DGD	C1G-C2G-O2G-C1B
49	m	104	DGD	C1G-C2G-O2G-C1B
44	A	829	CLA	O1A-CGA-O2A-C1
44	e	839	CLA	O1A-CGA-O2A-C1
44	A	827	CLA	C16-C17-C18-C20
44	B	808	CLA	O1A-CGA-O2A-C1
44	e	843	CLA	O1A-CGA-O2A-C1
44	f	804	CLA	CAD-CBD-CGD-O2D
44	B	803	CLA	CAA-CBA-CGA-O2A
46	p	516	LHG	O6-C4-C5-O7
44	q	311	CLA	O2A-C1-C2-C3
46	1	516	LHG	C4-C5-C6-O8
50	r	318	LMG	C7-C8-C9-O8
44	B	828	CLA	CBD-CGD-O2D-CED
44	A	806	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
44	e	803	CLA	C4-C3-C5-C6
44	e	829	CLA	C2A-CAA-CBA-CGA
44	r	307	CLA	C5-C6-C7-C8
49	J	103	DGD	O1G-C1G-C2G-O2G
49	f	851	DGD	O1G-C1G-C2G-O2G
44	A	806	CLA	C14-C13-C15-C16
44	A	831	CLA	C11-C10-C8-C9
44	B	802	CLA	C6-C7-C8-C9
44	B	803	CLA	C6-C7-C8-C9
44	e	839	CLA	C14-C13-C15-C16
52	p	514	CHL	CAA-CBA-CGA-O2A
44	3	313	CLA	CBA-CGA-O2A-C1
44	r	309	CLA	O1A-CGA-O2A-C1
44	A	823	CLA	C3A-C2A-CAA-CBA
44	f	836	CLA	C3A-C2A-CAA-CBA
49	J	103	DGD	C4E-C5E-C6E-O5E
44	A	838	CLA	O1A-CGA-O2A-C1
44	B	815	CLA	O1A-CGA-O2A-C1
44	1	513	CLA	C2-C1-O2A-CGA
44	e	843	CLA	C2-C1-O2A-CGA
44	A	808	CLA	C15-C16-C17-C18
44	A	835	CLA	O1D-CGD-O2D-CED
45	B	843	PQN	C14-C13-C15-C16
49	J	103	DGD	C3A-C4A-C5A-C6A
44	B	839	CLA	O1A-CGA-O2A-C1
44	B	837	CLA	C4C-C3C-CAC-CBC
52	2	516	CHL	C4C-C3C-CAC-CBC
52	r	316	CHL	C4C-C3C-CAC-CBC
52	s	513	CHL	C4C-C3C-CAC-CBC
44	A	839	CLA	O1D-CGD-O2D-CED
46	A	843	LHG	C30-C31-C32-C33
49	J	103	DGD	C9B-CAB-CBB-CCB
44	p	510	CLA	O1A-CGA-O2A-C1
43	A	801	CL0	C2-C1-O2A-CGA
43	e	801	CL0	C2-C1-O2A-CGA
47	A	846	BCR	C7-C8-C9-C34
47	F	801	BCR	C7-C8-C9-C34
51	3	304	LUT	C7-C8-C9-C19
51	s	501	LUT	C11-C12-C13-C20
44	A	819	CLA	C4B-C3B-CAB-CBB
44	A	826	CLA	C1A-C2A-CAA-CBA
44	A	835	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
44	A	839	CLA	C4B-C3B-CAB-CBB
44	B	820	CLA	C4B-C3B-CAB-CBB
44	F	803	CLA	C4B-C3B-CAB-CBB
44	2	505	CLA	C1A-C2A-CAA-CBA
44	2	505	CLA	C4B-C3B-CAB-CBB
44	3	307	CLA	C4B-C3B-CAB-CBB
44	3	312	CLA	C4B-C3B-CAB-CBB
44	3	318	CLA	C1A-C2A-CAA-CBA
44	5	306	CLA	C4B-C3B-CAB-CBB
44	e	803	CLA	C1A-C2A-CAA-CBA
44	e	809	CLA	C4B-C3B-CAB-CBB
44	e	811	CLA	C4B-C3B-CAB-CBB
44	e	815	CLA	C4B-C3B-CAB-CBB
44	e	816	CLA	C4B-C3B-CAB-CBB
44	e	819	CLA	C4B-C3B-CAB-CBB
44	e	832	CLA	C4B-C3B-CAB-CBB
44	e	852	CLA	C1A-C2A-CAA-CBA
44	f	810	CLA	C4B-C3B-CAB-CBB
44	f	811	CLA	C4B-C3B-CAB-CBB
44	f	817	CLA	C4B-C3B-CAB-CBB
44	f	837	CLA	C4B-C3B-CAB-CBB
44	m	102	CLA	C4B-C3B-CAB-CBB
44	n	202	CLA	C4B-C3B-CAB-CBB
44	p	509	CLA	C1A-C2A-CAA-CBA
44	p	510	CLA	C4B-C3B-CAB-CBB
44	q	311	CLA	C1A-C2A-CAA-CBA
44	q	311	CLA	C4B-C3B-CAB-CBB
44	r	310	CLA	C4B-C3B-CAB-CBB
44	s	505	CLA	C4B-C3B-CAB-CBB
44	B	821	CLA	O1D-CGD-O2D-CED
44	e	829	CLA	C4-C3-C5-C6
44	5	312	CLA	CAA-CBA-CGA-O2A
47	q	303	BCR	C21-C22-C23-C24
51	3	304	LUT	C7-C8-C9-C10
47	n	204	BCR	C19-C20-C21-C22
44	s	510	CLA	C11-C12-C13-C15
44	p	510	CLA	C2A-CAA-CBA-CGA
52	1	512	CHL	C2A-CAA-CBA-CGA
44	1	513	CLA	C13-C15-C16-C17
46	B	851	LHG	O6-C4-C5-C6
46	e	845	LHG	O6-C4-C5-C6
46	p	516	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
54	Q	802	SQD	O49-C7-O47-C45
44	B	826	CLA	C6-C7-C8-C10
44	3	314	CLA	C11-C10-C8-C7
44	e	804	CLA	C6-C7-C8-C10
44	e	839	CLA	C11-C10-C8-C7
44	f	826	CLA	C11-C10-C8-C7
44	r	307	CLA	C6-C7-C8-C10
45	A	841	PQN	C17-C18-C20-C21
44	1	513	CLA	C16-C17-C18-C20
44	3	306	CLA	C6-C7-C8-C10
52	s	513	CHL	CAA-CBA-CGA-O2A
44	e	829	CLA	C10-C11-C12-C13
44	f	824	CLA	C3A-C2A-CAA-CBA
46	f	852	LHG	C24-C23-O8-C6
44	A	840	CLA	CBD-CGD-O2D-CED
44	3	313	CLA	O1A-CGA-O2A-C1
44	f	815	CLA	C2A-CAA-CBA-CGA
44	A	835	CLA	C3A-C2A-CAA-CBA
44	B	811	CLA	C3A-C2A-CAA-CBA
44	2	505	CLA	C3A-C2A-CAA-CBA
44	e	837	CLA	C4-C3-C5-C6
44	L	303	CLA	O1D-CGD-O2D-CED
44	A	838	CLA	C2A-CAA-CBA-CGA
44	B	820	CLA	C2C-C3C-CAC-CBC
44	f	826	CLA	C6-C7-C8-C9
44	p	508	CLA	C6-C7-C8-C9
44	f	808	CLA	CBA-CGA-O2A-C1
44	A	837	CLA	O1D-CGD-O2D-CED
44	B	818	CLA	O1D-CGD-O2D-CED
44	B	817	CLA	C1-C2-C3-C4
51	q	301	LUT	C21-C26-C27-C28
46	2	517	LHG	C23-C24-C25-C26
50	m	105	LMG	C13-C14-C15-C16
49	J	103	DGD	O2G-C2G-C3G-O3G
50	r	318	LMG	O1-C7-C8-O7
50	r	318	LMG	O7-C8-C9-O8
44	A	832	CLA	O2A-C1-C2-C3
44	5	311	CLA	O1D-CGD-O2D-CED
50	2	519	LMG	O1-C7-C8-C9
50	2	519	LMG	C7-C8-C9-O8
50	5	301	LMG	O1-C7-C8-C9
45	A	841	PQN	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
44	e	803	CLA	C2-C3-C5-C6
45	B	843	PQN	C12-C13-C15-C16
44	A	812	CLA	CAD-CBD-CGD-O2D
44	A	813	CLA	CAD-CBD-CGD-O2D
44	A	819	CLA	CAD-CBD-CGD-O2D
44	A	823	CLA	CAD-CBD-CGD-O2D
44	A	824	CLA	CAD-CBD-CGD-O2D
44	B	812	CLA	CAD-CBD-CGD-O2D
44	B	814	CLA	CAD-CBD-CGD-O2D
44	B	827	CLA	CAD-CBD-CGD-O2D
44	B	837	CLA	CAD-CBD-CGD-O2D
44	B	841	CLA	CAD-CBD-CGD-O2D
44	2	505	CLA	CAD-CBD-CGD-O2D
44	3	312	CLA	CAD-CBD-CGD-O2D
44	e	804	CLA	CAD-CBD-CGD-O2D
44	e	805	CLA	CAD-CBD-CGD-O2D
44	e	806	CLA	CAD-CBD-CGD-O2D
44	e	823	CLA	CAD-CBD-CGD-O2D
44	e	830	CLA	CAD-CBD-CGD-O2D
44	f	834	CLA	CAD-CBD-CGD-O2D
44	s	504	CLA	CAD-CBD-CGD-O2D
44	s	505	CLA	CAD-CBD-CGD-O2D
52	3	315	CHL	C1A-C2A-CAA-CBA
44	A	823	CLA	O1D-CGD-O2D-CED
46	1	516	LHG	C24-C23-O8-C6
44	B	803	CLA	C8-C10-C11-C12
43	A	801	CL0	CAD-CBD-CGD-O2D
43	e	801	CL0	CAD-CBD-CGD-O2D
44	A	803	CLA	CHA-CBD-CGD-O1D
44	A	805	CLA	CAD-CBD-CGD-O1D
44	A	806	CLA	CAD-CBD-CGD-O1D
44	A	810	CLA	CHA-CBD-CGD-O1D
44	A	812	CLA	CAD-CBD-CGD-O1D
44	A	813	CLA	CAD-CBD-CGD-O1D
44	A	819	CLA	CAD-CBD-CGD-O1D
44	A	823	CLA	CAD-CBD-CGD-O1D
44	A	824	CLA	CAD-CBD-CGD-O1D
44	B	812	CLA	CAD-CBD-CGD-O1D
44	B	814	CLA	CAD-CBD-CGD-O1D
44	B	827	CLA	CAD-CBD-CGD-O1D
44	B	831	CLA	CHA-CBD-CGD-O1D
44	B	831	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
44	B	837	CLA	CAD-CBD-CGD-O1D
44	B	841	CLA	CAD-CBD-CGD-O1D
44	K	202	CLA	CHA-CBD-CGD-O2D
44	2	505	CLA	CAD-CBD-CGD-O1D
44	3	311	CLA	CHA-CBD-CGD-O1D
44	3	311	CLA	CHA-CBD-CGD-O2D
44	3	312	CLA	CAD-CBD-CGD-O1D
44	5	306	CLA	CHA-CBD-CGD-O2D
44	e	802	CLA	CAD-CBD-CGD-O1D
44	e	804	CLA	CAD-CBD-CGD-O1D
44	e	805	CLA	CAD-CBD-CGD-O1D
44	e	806	CLA	CAD-CBD-CGD-O1D
44	e	807	CLA	CHA-CBD-CGD-O1D
44	e	823	CLA	CAD-CBD-CGD-O1D
44	e	830	CLA	CAD-CBD-CGD-O1D
44	e	838	CLA	CHA-CBD-CGD-O1D
44	e	838	CLA	CHA-CBD-CGD-O2D
44	e	841	CLA	CHA-CBD-CGD-O1D
44	f	810	CLA	CHA-CBD-CGD-O1D
44	f	822	CLA	CHA-CBD-CGD-O2D
44	f	834	CLA	CAD-CBD-CGD-O1D
44	q	306	CLA	CHA-CBD-CGD-O1D
44	q	306	CLA	CHA-CBD-CGD-O2D
44	r	305	CLA	CHA-CBD-CGD-O1D
44	r	310	CLA	CHA-CBD-CGD-O1D
44	r	310	CLA	CHA-CBD-CGD-O2D
44	r	311	CLA	CHA-CBD-CGD-O1D
44	r	311	CLA	CHA-CBD-CGD-O2D
44	s	504	CLA	CAD-CBD-CGD-O1D
44	s	505	CLA	CAD-CBD-CGD-O1D
46	A	843	LHG	C3-O3-P-O5
46	A	844	LHG	C3-O3-P-O5
46	B	851	LHG	C3-O3-P-O4
46	B	851	LHG	C3-O3-P-O5
46	B	851	LHG	C3-O3-P-O6
46	1	516	LHG	C3-O3-P-O5
46	O	601	LHG	C4-O6-P-O5
46	e	845	LHG	C3-O3-P-O5
46	e	845	LHG	C4-O6-P-O5
46	p	516	LHG	C4-O6-P-O4
46	s	516	LHG	C3-O3-P-O5
47	B	847	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
47	f	845	BCR	C9-C10-C11-C12
47	f	845	BCR	C13-C14-C15-C16
47	p	503	BCR	C23-C24-C25-C26
51	q	301	LUT	C25-C26-C27-C28
52	2	512	CHL	CHA-CBD-CGD-O1D
52	2	512	CHL	CHA-CBD-CGD-O2D
52	5	315	CHL	CHA-CBD-CGD-O1D
44	A	808	CLA	C3-C5-C6-C7
49	B	850	DGD	C3A-C4A-C5A-C6A
44	f	821	CLA	C2C-C3C-CAC-CBC
44	3	314	CLA	C4-C3-C5-C6
44	e	852	CLA	C4-C3-C5-C6
44	A	817	CLA	C2B-C3B-CAB-CBB
44	A	839	CLA	C2B-C3B-CAB-CBB
44	A	852	CLA	C2B-C3B-CAB-CBB
44	B	803	CLA	C2B-C3B-CAB-CBB
44	B	815	CLA	C2B-C3B-CAB-CBB
44	2	508	CLA	C2B-C3B-CAB-CBB
44	2	514	CLA	C2B-C3B-CAB-CBB
44	3	307	CLA	C2B-C3B-CAB-CBB
44	5	312	CLA	C2B-C3B-CAB-CBB
44	e	815	CLA	C2B-C3B-CAB-CBB
44	e	816	CLA	C2B-C3B-CAB-CBB
44	e	822	CLA	C2B-C3B-CAB-CBB
44	e	832	CLA	C2B-C3B-CAB-CBB
44	f	811	CLA	C2B-C3B-CAB-CBB
44	f	817	CLA	C2B-C3B-CAB-CBB
44	j	802	CLA	C2B-C3B-CAB-CBB
44	m	102	CLA	C2B-C3B-CAB-CBB
44	n	201	CLA	C2B-C3B-CAB-CBB
44	p	506	CLA	C2B-C3B-CAB-CBB
44	p	510	CLA	C2B-C3B-CAB-CBB
47	A	846	BCR	C23-C24-C25-C26
47	l	101	BCR	C23-C24-C25-C30
52	2	513	CHL	CAD-CBD-CGD-O2D
52	q	313	CHL	CAD-CBD-CGD-O2D
46	B	851	LHG	C2-C3-O3-P
46	1	516	LHG	C2-C3-O3-P
47	A	846	BCR	C37-C22-C23-C24
47	B	846	BCR	C7-C8-C9-C34
44	1	513	CLA	C15-C16-C17-C18
44	1	513	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
46	1	516	LHG	O10-C23-O8-C6
49	B	850	DGD	C1A-C2A-C3A-C4A
50	F	806	LMG	C9-C8-O7-C10
47	2	503	BCR	C18-C19-C20-C21
47	5	302	BCR	C10-C11-C12-C13
47	s	503	BCR	C18-C19-C20-C21
47	Q	801	BCR	C19-C20-C21-C22
44	f	801	CLA	CBA-CGA-O2A-C1
44	A	805	CLA	C11-C10-C8-C9
44	B	807	CLA	C11-C10-C8-C9
44	e	804	CLA	C6-C7-C8-C9
44	e	804	CLA	C14-C13-C15-C16
44	e	839	CLA	C11-C10-C8-C9
44	A	838	CLA	C12-C13-C15-C16
50	2	519	LMG	C14-C15-C16-C17
44	f	801	CLA	O1A-CGA-O2A-C1
44	B	820	CLA	C5-C6-C7-C8
44	r	307	CLA	C2-C3-C5-C6
52	1	517	CHL	O1D-CGD-O2D-CED
46	s	516	LHG	O9-C7-O7-C5
54	Q	803	SQD	O6-C44-C45-O47
44	f	801	CLA	C16-C17-C18-C19
46	s	516	LHG	C8-C7-O7-C5
44	e	839	CLA	C2A-CAA-CBA-CGA
45	B	843	PQN	C13-C15-C16-C17
52	q	313	CHL	O1A-CGA-O2A-C1
44	A	840	CLA	O1D-CGD-O2D-CED
44	r	307	CLA	C10-C11-C12-C13
47	B	848	BCR	C36-C18-C19-C20
50	F	806	LMG	C8-C7-O1-C1
44	B	802	CLA	C8-C10-C11-C12
44	B	804	CLA	C13-C15-C16-C17
44	f	818	CLA	C2A-CAA-CBA-CGA
47	L	306	BCR	C19-C20-C21-C22
44	s	510	CLA	C11-C12-C13-C14
44	r	307	CLA	C6-C7-C8-C9
46	1	516	LHG	C11-C12-C13-C14
46	f	852	LHG	C2-C3-O3-P
44	B	840	CLA	C4B-C3B-CAB-CBB
44	2	504	CLA	C4B-C3B-CAB-CBB
44	e	807	CLA	C4B-C3B-CAB-CBB
44	e	808	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
44	f	828	CLA	C4B-C3B-CAB-CBB
44	B	801	CLA	C16-C17-C18-C19
46	B	851	LHG	C7-C8-C9-C10
44	p	506	CLA	C5-C6-C7-C8
44	e	838	CLA	O1D-CGD-O2D-CED
44	B	811	CLA	C4-C3-C5-C6
44	1	513	CLA	C4-C3-C5-C6
44	B	801	CLA	C8-C10-C11-C12
49	f	851	DGD	O6D-C5D-C6D-O5D
46	f	852	LHG	O10-C23-O8-C6
47	e	849	BCR	C19-C20-C21-C22
44	A	805	CLA	C12-C13-C15-C16
44	B	804	CLA	C11-C10-C8-C7
44	5	307	CLA	C11-C10-C8-C7
44	r	306	CLA	C11-C12-C13-C15
44	f	810	CLA	C4-C3-C5-C6
44	f	813	CLA	C3A-C2A-CAA-CBA
44	f	835	CLA	C3A-C2A-CAA-CBA
44	q	312	CLA	C4-C3-C5-C6
44	3	314	CLA	C2-C3-C5-C6
44	e	852	CLA	C2-C3-C5-C6
47	A	849	BCR	C11-C10-C9-C34
47	B	845	BCR	C11-C10-C9-C34
47	B	846	BCR	C11-C10-C9-C34
47	B	846	BCR	C20-C21-C22-C37
47	B	852	BCR	C11-C10-C9-C34
47	F	804	BCR	C35-C13-C14-C15
47	5	302	BCR	C11-C10-C9-C34
47	e	850	BCR	C11-C10-C9-C34
47	e	850	BCR	C16-C17-C18-C36
47	f	846	BCR	C11-C10-C9-C34
47	f	847	BCR	C11-C10-C9-C34
47	f	847	BCR	C20-C21-C22-C37
47	j	803	BCR	C35-C13-C14-C15
47	o	301	BCR	C11-C10-C9-C34
49	B	850	DGD	C2G-C1G-O1G-C1A
44	A	826	CLA	C2-C1-O2A-CGA
47	s	503	BCR	C15-C16-C17-C18
46	A	843	LHG	C11-C12-C13-C14
49	J	103	DGD	CDA-CEA-CFA-CGA
47	e	848	BCR	C11-C12-C13-C35
52	r	313	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
46	e	844	LHG	C24-C25-C26-C27
44	r	306	CLA	C10-C11-C12-C13
47	B	848	BCR	C17-C18-C19-C20
47	e	854	BCR	C7-C8-C9-C10
51	1	502	LUT	C7-C8-C9-C10
45	A	841	PQN	C12-C13-C15-C16
44	3	311	CLA	C2A-CAA-CBA-CGA
44	s	511	CLA	C2A-CAA-CBA-CGA
49	m	104	DGD	O1G-C1G-C2G-C3G
44	A	820	CLA	C6-C7-C8-C9
44	A	827	CLA	C11-C10-C8-C9
44	B	804	CLA	C14-C13-C15-C16
44	B	826	CLA	C11-C10-C8-C9
44	1	513	CLA	C6-C7-C8-C9
44	r	306	CLA	C11-C12-C13-C14
49	m	104	DGD	CCA-CDA-CEA-CFA
44	e	853	CLA	CAA-CBA-CGA-O1A
50	2	519	LMG	C7-C8-O7-C10
50	2	519	LMG	C9-C8-O7-C10
44	A	818	CLA	O1D-CGD-O2D-CED
44	f	818	CLA	C5-C6-C7-C8
44	A	838	CLA	C3-C5-C6-C7
44	e	837	CLA	C3-C5-C6-C7
44	1	515	CLA	CAA-CBA-CGA-O2A
44	A	831	CLA	C11-C12-C13-C15
46	f	852	LHG	C25-C26-C27-C28
44	e	838	CLA	CBD-CGD-O2D-CED
46	e	844	LHG	C26-C27-C28-C29
52	1	512	CHL	CAA-CBA-CGA-O2A
44	A	808	CLA	C1A-C2A-CAA-CBA
44	A	813	CLA	C1A-C2A-CAA-CBA
44	B	801	CLA	C1A-C2A-CAA-CBA
44	B	813	CLA	C1A-C2A-CAA-CBA
44	B	832	CLA	C1A-C2A-CAA-CBA
44	B	839	CLA	C1A-C2A-CAA-CBA
44	2	510	CLA	C1A-C2A-CAA-CBA
44	f	813	CLA	C1A-C2A-CAA-CBA
47	A	849	BCR	C11-C10-C9-C8
47	B	845	BCR	C11-C10-C9-C8
47	B	846	BCR	C11-C10-C9-C8
47	B	846	BCR	C20-C21-C22-C23
47	B	852	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
47	F	804	BCR	C12-C13-C14-C15
47	5	302	BCR	C11-C10-C9-C8
47	e	850	BCR	C11-C10-C9-C8
47	e	850	BCR	C16-C17-C18-C19
47	f	846	BCR	C11-C10-C9-C8
47	f	847	BCR	C11-C10-C9-C8
47	f	847	BCR	C20-C21-C22-C23
47	j	803	BCR	C12-C13-C14-C15
47	o	301	BCR	C11-C10-C9-C8
44	n	202	CLA	C4C-C3C-CAC-CBC
44	e	853	CLA	CAA-CBA-CGA-O2A
44	A	807	CLA	C2B-C3B-CAB-CBB
44	A	814	CLA	C2B-C3B-CAB-CBB
44	A	819	CLA	C2B-C3B-CAB-CBB
44	B	809	CLA	C2B-C3B-CAB-CBB
44	B	820	CLA	C2B-C3B-CAB-CBB
44	B	824	CLA	C2B-C3B-CAB-CBB
44	F	803	CLA	C2B-C3B-CAB-CBB
44	L	302	CLA	C2B-C3B-CAB-CBB
44	2	504	CLA	C2B-C3B-CAB-CBB
44	2	505	CLA	C2B-C3B-CAB-CBB
44	3	312	CLA	C2B-C3B-CAB-CBB
44	5	306	CLA	C2B-C3B-CAB-CBB
44	e	807	CLA	C2B-C3B-CAB-CBB
44	e	808	CLA	C2B-C3B-CAB-CBB
44	e	809	CLA	C2B-C3B-CAB-CBB
44	e	811	CLA	C2B-C3B-CAB-CBB
44	e	819	CLA	C2B-C3B-CAB-CBB
44	f	810	CLA	C2B-C3B-CAB-CBB
44	f	820	CLA	C2B-C3B-CAB-CBB
44	f	828	CLA	C2B-C3B-CAB-CBB
44	f	837	CLA	C2B-C3B-CAB-CBB
44	q	311	CLA	C2B-C3B-CAB-CBB
44	r	310	CLA	C2B-C3B-CAB-CBB
44	s	505	CLA	C2B-C3B-CAB-CBB
47	A	845	BCR	C5-C6-C7-C8
47	B	844	BCR	C5-C6-C7-C8
47	J	102	BCR	C23-C24-C25-C30
47	K	204	BCR	C5-C6-C7-C8
47	L	305	BCR	C23-C24-C25-C30
47	Q	801	BCR	C5-C6-C7-C8
47	Q	801	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
47	e	846	BCR	C23-C24-C25-C30
47	e	848	BCR	C23-C24-C25-C26
47	e	849	BCR	C5-C6-C7-C8
47	e	851	BCR	C5-C6-C7-C8
47	e	851	BCR	C23-C24-C25-C26
47	l	102	BCR	C1-C6-C7-C8
47	l	102	BCR	C23-C24-C25-C26
47	m	103	BCR	C23-C24-C25-C30
47	n	204	BCR	C5-C6-C7-C8
47	n	204	BCR	C23-C24-C25-C26
47	o	305	BCR	C23-C24-C25-C26
47	q	303	BCR	C23-C24-C25-C26
47	r	301	BCR	C23-C24-C25-C26
51	3	303	LUT	C5-C6-C7-C8
51	r	302	LUT	C1-C6-C7-C8
51	s	501	LUT	C5-C6-C7-C8
46	p	516	LHG	C13-C14-C15-C16
44	B	830	CLA	C11-C10-C8-C9
44	B	842	CLA	C4-C3-C5-C6
44	A	827	CLA	C2-C3-C5-C6
44	L	301	CLA	C2-C3-C5-C6
44	1	513	CLA	C2-C3-C5-C6
44	q	312	CLA	C2-C3-C5-C6
50	F	806	LMG	C29-C30-C31-C32
49	J	103	DGD	C1B-C2B-C3B-C4B
44	1	515	CLA	CAA-CBA-CGA-O1A
44	e	815	CLA	CAA-CBA-CGA-O2A
44	A	825	CLA	C11-C10-C8-C7
44	A	826	CLA	C6-C7-C8-C10
44	A	838	CLA	C11-C12-C13-C15
44	B	804	CLA	C6-C7-C8-C10
44	B	842	CLA	C11-C10-C8-C7
44	e	804	CLA	C12-C13-C15-C16
44	f	801	CLA	C16-C17-C18-C20
44	e	837	CLA	C2A-CAA-CBA-CGA
44	f	836	CLA	CBA-CGA-O2A-C1
46	1	516	LHG	O7-C5-C6-O8
46	e	845	LHG	C5-C6-O8-C23
44	1	507	CLA	C11-C10-C8-C7
44	e	824	CLA	C11-C10-C8-C7
44	s	505	CLA	O1A-CGA-O2A-C1
44	A	826	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
44	B	815	CLA	C4-C3-C5-C6
44	f	831	CLA	C4-C3-C5-C6
44	s	510	CLA	C4-C3-C5-C6
44	B	811	CLA	C2-C3-C5-C6
44	A	836	CLA	CBD-CGD-O2D-CED
44	A	825	CLA	C11-C10-C8-C9
47	A	846	BCR	C19-C20-C21-C22
44	5	307	CLA	C5-C6-C7-C8
50	2	518	LMG	O1-C7-C8-O7
44	r	305	CLA	O1A-CGA-O2A-C1
44	f	818	CLA	C4-C3-C5-C6
44	e	829	CLA	C2-C3-C5-C6
44	e	837	CLA	C2-C3-C5-C6
44	f	810	CLA	C2-C3-C5-C6
44	f	818	CLA	C2-C3-C5-C6
44	B	801	CLA	C13-C15-C16-C17
52	p	512	CHL	O1A-CGA-O2A-C1
44	B	826	CLA	CBA-CGA-O2A-C1
44	r	305	CLA	CBA-CGA-O2A-C1
46	A	844	LHG	C24-C23-O8-C6
44	e	815	CLA	CAA-CBA-CGA-O1A
44	5	311	CLA	C1A-C2A-CAA-CBA
44	e	813	CLA	C1A-C2A-CAA-CBA
44	e	814	CLA	C1A-C2A-CAA-CBA
44	B	826	CLA	O1A-CGA-O2A-C1
44	p	505	CLA	C2A-CAA-CBA-CGA
44	1	510	CLA	CAA-CBA-CGA-O2A
44	1	506	CLA	C4-C3-C5-C6
47	Q	801	BCR	C15-C16-C17-C18
54	Q	802	SQD	O49-C7-C8-C9
44	A	805	CLA	CAA-CBA-CGA-O2A
49	m	104	DGD	C4D-C5D-C6D-O5D
44	A	807	CLA	C4B-C3B-CAB-CBB
44	B	809	CLA	C4B-C3B-CAB-CBB
44	B	824	CLA	C4B-C3B-CAB-CBB
44	L	302	CLA	C4B-C3B-CAB-CBB
44	1	510	CLA	C4B-C3B-CAB-CBB
44	e	852	CLA	C4B-C3B-CAB-CBB
44	f	815	CLA	C4B-C3B-CAB-CBB
44	f	832	CLA	C4B-C3B-CAB-CBB
44	B	801	CLA	C16-C17-C18-C20
52	1	517	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
44	2	505	CLA	C2A-CAA-CBA-CGA
44	A	813	CLA	CAA-CBA-CGA-O2A
52	2	515	CHL	CAA-CBA-CGA-O2A
44	B	801	CLA	C4-C3-C5-C6
44	f	809	CLA	C4-C3-C5-C6
50	F	806	LMG	O1-C7-C8-O7
44	e	835	CLA	CAA-CBA-CGA-O2A
44	A	826	CLA	C2-C3-C5-C6
44	A	823	CLA	C3-C5-C6-C7
44	5	308	CLA	C11-C10-C8-C7
50	F	806	LMG	C31-C32-C33-C34
44	f	810	CLA	C8-C10-C11-C12
44	B	826	CLA	C6-C7-C8-C9
44	1	513	CLA	C11-C12-C13-C14
44	5	308	CLA	C11-C10-C8-C9
44	B	841	CLA	O1A-CGA-O2A-C1
44	1	515	CLA	CHA-CBD-CGD-O2D
49	f	851	DGD	C2G-C3G-O3G-C1D
50	r	318	LMG	C9-C8-O7-C10
44	B	817	CLA	C2-C1-O2A-CGA
44	f	818	CLA	C2-C1-O2A-CGA
44	p	506	CLA	C2-C1-O2A-CGA
44	A	836	CLA	C3A-C2A-CAA-CBA
44	2	514	CLA	C3A-C2A-CAA-CBA
44	e	837	CLA	C3A-C2A-CAA-CBA
44	e	852	CLA	C3A-C2A-CAA-CBA
44	r	309	CLA	C3A-C2A-CAA-CBA
44	A	831	CLA	C3-C5-C6-C7
44	f	813	CLA	C6-C7-C8-C10
44	B	841	CLA	CBA-CGA-O2A-C1
44	o	304	CLA	CAA-CBA-CGA-O2A
46	e	844	LHG	C25-C26-C27-C28
44	B	835	CLA	C4-C3-C5-C6
44	A	816	CLA	C2-C3-C5-C6
44	B	828	CLA	O1D-CGD-O2D-CED
45	B	843	PQN	C20-C21-C22-C23
54	Q	802	SQD	C29-C30-C31-C32
50	F	806	LMG	C7-C8-C9-O8
44	A	802	CLA	O1A-CGA-O2A-C1
44	o	304	CLA	CAA-CBA-CGA-O1A
49	f	851	DGD	C2B-C3B-C4B-C5B
44	2	510	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
44	p	508	CLA	C4-C3-C5-C6
44	e	805	CLA	CBA-CGA-O2A-C1
44	3	311	CLA	CAA-CBA-CGA-O2A
44	A	813	CLA	CAA-CBA-CGA-O1A
44	e	829	CLA	C11-C10-C8-C9
44	f	826	CLA	C11-C10-C8-C9
44	r	306	CLA	C6-C7-C8-C9
44	n	202	CLA	C2C-C3C-CAC-CBC
47	A	846	BCR	C21-C22-C23-C24
47	B	852	BCR	C21-C22-C23-C24
47	F	801	BCR	C7-C8-C9-C10
44	2	506	CLA	C3-C5-C6-C7
44	B	807	CLA	C5-C6-C7-C8
44	B	842	CLA	CAA-CBA-CGA-O2A
44	B	842	CLA	C2-C3-C5-C6
44	e	835	CLA	CAA-CBA-CGA-O1A
44	e	829	CLA	O1D-CGD-O2D-CED
44	A	827	CLA	C12-C13-C15-C16
44	1	513	CLA	C6-C7-C8-C10
45	A	841	PQN	C16-C17-C18-C20
46	A	844	LHG	O10-C23-O8-C6
52	2	515	CHL	CAA-CBA-CGA-O1A
44	A	803	CLA	C2B-C3B-CAB-CBB
44	B	805	CLA	C2B-C3B-CAB-CBB
44	B	840	CLA	C2B-C3B-CAB-CBB
44	5	309	CLA	C2B-C3B-CAB-CBB
44	e	852	CLA	C2B-C3B-CAB-CBB
44	f	815	CLA	C2B-C3B-CAB-CBB
44	r	312	CLA	C2B-C3B-CAB-CBB
44	s	511	CLA	C2B-C3B-CAB-CBB
47	A	846	BCR	C23-C24-C25-C30
47	A	848	BCR	C1-C6-C7-C8
47	A	848	BCR	C5-C6-C7-C8
47	B	845	BCR	C1-C6-C7-C8
47	B	845	BCR	C5-C6-C7-C8
47	J	102	BCR	C23-C24-C25-C26
47	L	305	BCR	C23-C24-C25-C26
47	3	305	BCR	C23-C24-C25-C30
47	Q	801	BCR	C23-C24-C25-C26
47	e	846	BCR	C23-C24-C25-C26
47	l	102	BCR	C5-C6-C7-C8
47	m	103	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
51	1	502	LUT	C1-C6-C7-C8
51	5	303	LUT	C1-C6-C7-C8
51	5	303	LUT	C5-C6-C7-C8
51	p	502	LUT	C1-C6-C7-C8
51	q	302	LUT	C1-C6-C7-C8
51	r	302	LUT	C5-C6-C7-C8
44	B	833	CLA	CAA-CBA-CGA-O2A
44	B	802	CLA	C2-C3-C5-C6
44	A	816	CLA	C2-C1-O2A-CGA
44	B	812	CLA	C2-C1-O2A-CGA
44	e	826	CLA	C2-C1-O2A-CGA
47	f	845	BCR	C15-C16-C17-C18
44	B	817	CLA	CAA-CBA-CGA-O2A
44	f	820	CLA	CAA-CBA-CGA-O2A
44	K	203	CLA	C4C-C3C-CAC-CBC
44	e	829	CLA	CBD-CGD-O2D-CED
44	B	804	CLA	C15-C16-C17-C18
44	A	820	CLA	C4-C3-C5-C6
44	A	820	CLA	C2-C3-C5-C6
44	B	835	CLA	C2-C3-C5-C6
46	B	851	LHG	C1-C2-C3-O3
52	1	514	CHL	C1C-C2C-CMC-OMC
44	e	819	CLA	C2A-CAA-CBA-CGA
44	2	509	CLA	CBA-CGA-O2A-C1
44	r	306	CLA	C15-C16-C17-C18
44	s	505	CLA	CAA-CBA-CGA-O2A
49	B	850	DGD	C8A-C9A-CAA-CBA
44	q	312	CLA	C8-C10-C11-C12
44	f	801	CLA	C2A-CAA-CBA-CGA
44	A	838	CLA	C14-C13-C15-C16
44	B	804	CLA	C6-C7-C8-C9
44	B	818	CLA	C6-C7-C8-C9
44	f	836	CLA	C11-C10-C8-C9
44	e	826	CLA	C8-C10-C11-C12
44	B	818	CLA	CAA-CBA-CGA-O2A
44	q	311	CLA	CAA-CBA-CGA-O2A
44	1	505	CLA	C4B-C3B-CAB-CBB
44	e	841	CLA	C4B-C3B-CAB-CBB
44	p	506	CLA	C4B-C3B-CAB-CBB
44	q	305	CLA	C1A-C2A-CAA-CBA
44	q	306	CLA	C4B-C3B-CAB-CBB
44	r	305	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
44	r	317	CLA	C4B-C3B-CAB-CBB
44	s	509	CLA	C4B-C3B-CAB-CBB
44	s	511	CLA	C4B-C3B-CAB-CBB
44	e	804	CLA	CAA-CBA-CGA-O2A
44	f	811	CLA	CAA-CBA-CGA-O2A
52	q	313	CHL	CAA-CBA-CGA-O2A
49	f	851	DGD	O2G-C2G-C3G-O3G
47	A	846	BCR	C7-C8-C9-C10
47	A	851	BCR	C21-C22-C23-C24
47	K	204	BCR	C11-C12-C13-C14
47	L	306	BCR	C21-C22-C23-C24
47	2	503	BCR	C7-C8-C9-C10
47	e	848	BCR	C11-C12-C13-C14
51	p	502	LUT	C7-C8-C9-C10
51	q	301	LUT	C27-C28-C29-C30
44	A	826	CLA	C11-C12-C13-C15
44	A	816	CLA	CAA-CBA-CGA-O2A
44	A	832	CLA	CAA-CBA-CGA-O2A
46	1	516	LHG	O8-C23-C24-C25
44	A	834	CLA	CBD-CGD-O2D-CED
44	L	303	CLA	C2A-CAA-CBA-CGA
44	e	836	CLA	C2A-CAA-CBA-CGA
44	o	303	CLA	C2A-CAA-CBA-CGA
44	2	510	CLA	C8-C10-C11-C12
46	B	851	LHG	C26-C27-C28-C29
49	B	850	DGD	C7B-C8B-C9B-CAB
44	A	805	CLA	O1D-CGD-O2D-CED
44	e	836	CLA	C2-C3-C5-C6
44	B	815	CLA	C2-C1-O2A-CGA
44	1	513	CLA	C11-C12-C13-C15
44	2	506	CLA	C11-C12-C13-C15
44	s	506	CLA	C11-C12-C13-C15
45	B	843	PQN	C21-C22-C23-C25
44	5	310	CLA	CAA-CBA-CGA-O2A
44	B	803	CLA	CAA-CBA-CGA-O1A
44	A	802	CLA	C2A-CAA-CBA-CGA
44	A	836	CLA	C2A-CAA-CBA-CGA
44	1	507	CLA	C2A-CAA-CBA-CGA
44	2	509	CLA	O1A-CGA-O2A-C1
44	B	801	CLA	C3A-C2A-CAA-CBA
44	2	509	CLA	C3A-C2A-CAA-CBA
44	3	313	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
44	5	306	CLA	CHA-CBD-CGD-O1D
44	2	506	CLA	C16-C17-C18-C19
44	B	815	CLA	C2-C3-C5-C6
49	f	851	DGD	C2A-C3A-C4A-C5A
44	B	842	CLA	CAA-CBA-CGA-O1A
44	f	820	CLA	CAA-CBA-CGA-O1A
44	s	505	CLA	CAA-CBA-CGA-O1A
44	A	827	CLA	O1A-CGA-O2A-C1
44	A	802	CLA	CBA-CGA-O2A-C1
44	B	817	CLA	CAA-CBA-CGA-O1A
52	p	514	CHL	CAA-CBA-CGA-O1A
46	O	601	LHG	C7-C8-C9-C10
44	A	806	CLA	C2A-CAA-CBA-CGA
44	A	806	CLA	C6-C7-C8-C9
44	A	852	CLA	C6-C7-C8-C9
44	B	803	CLA	C14-C13-C15-C16
44	B	842	CLA	C11-C10-C8-C9
44	f	801	CLA	C6-C7-C8-C9
45	A	841	PQN	C16-C17-C18-C19
44	A	802	CLA	CAA-CBA-CGA-O2A
44	A	832	CLA	CAA-CBA-CGA-O1A
47	e	846	BCR	C9-C10-C11-C12
44	B	838	CLA	C10-C11-C12-C13
44	A	820	CLA	CAA-CBA-CGA-O2A
44	s	506	CLA	CAA-CBA-CGA-O2A
50	m	105	LMG	O7-C10-C11-C12
44	A	827	CLA	CBA-CGA-O2A-C1
44	f	811	CLA	CAA-CBA-CGA-O1A
49	B	850	DGD	C2G-C3G-O3G-C1D
54	Q	802	SQD	C45-C44-O6-C1
44	A	826	CLA	O1A-CGA-O2A-C1
44	n	202	CLA	CAA-CBA-CGA-O2A
44	3	311	CLA	CAA-CBA-CGA-O1A
44	f	801	CLA	CAA-CBA-CGA-O2A
44	B	803	CLA	O1A-CGA-O2A-C1
44	3	314	CLA	CBD-CGD-O2D-CED
54	Q	802	SQD	C11-C10-C9-C8
44	e	804	CLA	CAA-CBA-CGA-O1A
54	Q	803	SQD	C7-C8-C9-C10
44	e	827	CLA	C2C-C3C-CAC-CBC
50	F	805	LMG	O7-C10-C11-C12
44	f	804	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
46	1	516	LHG	O10-C23-C24-C25
44	A	830	CLA	CAD-CBD-CGD-O2D
44	A	833	CLA	CAD-CBD-CGD-O2D
44	B	804	CLA	CAD-CBD-CGD-O2D
44	B	840	CLA	CAD-CBD-CGD-O2D
44	1	505	CLA	CAD-CBD-CGD-O2D
44	3	314	CLA	CAD-CBD-CGD-O2D
44	5	309	CLA	CAD-CBD-CGD-O2D
44	e	802	CLA	CAD-CBD-CGD-O2D
44	e	820	CLA	CAD-CBD-CGD-O2D
44	e	829	CLA	CAD-CBD-CGD-O2D
44	r	317	CLA	CAD-CBD-CGD-O2D
52	r	316	CHL	CAD-CBD-CGD-O2D
44	5	312	CLA	CAA-CBA-CGA-O1A
44	A	823	CLA	C2-C1-O2A-CGA
44	e	824	CLA	C2-C1-O2A-CGA
44	r	317	CLA	C2-C1-O2A-CGA
44	n	202	CLA	CAA-CBA-CGA-O1A
44	A	816	CLA	CAA-CBA-CGA-O1A
43	A	801	CL0	C1A-C2A-CAA-CBA
43	e	801	CL0	C1A-C2A-CAA-CBA
52	5	314	CHL	C1A-C2A-CAA-CBA
46	B	851	LHG	C10-C11-C12-C13
44	A	820	CLA	CAA-CBA-CGA-O1A
44	2	505	CLA	CAA-CBA-CGA-O2A
49	f	851	DGD	O2G-C1B-C2B-C3B
44	f	835	CLA	CAA-CBA-CGA-O2A
44	5	310	CLA	CAA-CBA-CGA-O1A
50	m	105	LMG	O9-C10-C11-C12
50	5	301	LMG	C28-C29-C30-C31
44	e	816	CLA	CAA-CBA-CGA-O2A
44	e	852	CLA	CAA-CBA-CGA-O2A
44	q	315	CLA	CAA-CBA-CGA-O2A
44	3	314	CLA	O1D-CGD-O2D-CED
44	q	311	CLA	CAA-CBA-CGA-O1A
52	q	313	CHL	CAA-CBA-CGA-O1A
49	B	850	DGD	C5A-C6A-C7A-C8A

There are no ring outliers.

318 monomers are involved in 743 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	3	311	CLA	5	0
50	2	518	LMG	1	0
51	1	502	LUT	7	0
44	e	821	CLA	2	0
44	A	825	CLA	1	0
44	A	840	CLA	1	0
44	A	802	CLA	2	0
44	f	818	CLA	4	0
52	p	517	CHL	2	0
44	B	818	CLA	4	0
44	f	806	CLA	1	0
44	r	308	CLA	2	0
44	B	806	CLA	4	0
47	A	846	BCR	3	0
44	1	507	CLA	3	0
47	A	849	BCR	1	0
44	e	839	CLA	4	0
44	q	305	CLA	1	0
51	3	304	LUT	5	0
52	5	317	CHL	3	0
44	B	820	CLA	4	0
51	5	303	LUT	8	0
44	f	803	CLA	2	0
44	B	826	CLA	2	0
45	f	844	PQN	6	0
44	J	101	CLA	2	0
44	1	504	CLA	3	0
44	B	821	CLA	1	0
44	1	509	CLA	4	0
47	A	847	BCR	1	0
44	e	804	CLA	3	0
52	q	313	CHL	1	0
44	e	825	CLA	2	0
51	p	501	LUT	5	0
44	5	307	CLA	4	0
44	e	805	CLA	1	0
44	f	842	CLA	1	0
44	K	201	CLA	3	0
47	m	103	BCR	3	0
51	q	302	LUT	6	0
44	e	836	CLA	2	0
44	3	307	CLA	1	0
47	B	846	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	A	843	LHG	4	0
44	p	505	CLA	1	0
44	B	803	CLA	1	0
46	p	516	LHG	7	0
47	J	102	BCR	1	0
44	B	811	CLA	5	0
44	B	812	CLA	1	0
47	B	849	BCR	2	0
44	e	837	CLA	3	0
44	e	810	CLA	5	0
44	f	804	CLA	7	0
44	1	511	CLA	2	0
44	f	809	CLA	1	0
44	f	840	CLA	3	0
53	r	303	XAT	4	0
46	1	516	LHG	5	0
44	B	808	CLA	2	0
44	3	308	CLA	6	0
44	A	824	CLA	1	0
44	B	842	CLA	2	0
44	s	510	CLA	4	0
44	5	310	CLA	2	0
44	2	505	CLA	3	0
47	e	851	BCR	5	0
44	f	827	CLA	1	0
44	e	816	CLA	1	0
44	B	830	CLA	3	0
44	2	508	CLA	3	0
52	2	515	CHL	2	0
47	j	801	BCR	1	0
52	r	313	CHL	1	0
50	2	519	LMG	2	0
52	s	512	CHL	3	0
52	2	516	CHL	3	0
44	3	306	CLA	3	0
45	A	841	PQN	2	0
44	e	833	CLA	2	0
44	A	820	CLA	4	0
47	2	503	BCR	4	0
47	5	302	BCR	5	0
49	m	104	DGD	2	0
44	B	815	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	F	805	LMG	1	0
44	r	312	CLA	2	0
44	B	833	CLA	2	0
44	s	511	CLA	6	0
44	f	813	CLA	2	0
47	A	853	BCR	4	0
44	L	304	CLA	2	0
46	s	516	LHG	1	0
44	s	509	CLA	2	0
44	B	838	CLA	5	0
47	l	102	BCR	4	0
44	e	819	CLA	1	0
47	o	305	BCR	3	0
44	5	316	CLA	3	0
52	5	314	CHL	2	0
44	e	853	CLA	2	0
47	n	204	BCR	1	0
44	e	843	CLA	2	0
44	f	835	CLA	4	0
44	j	802	CLA	1	0
49	f	851	DGD	2	0
47	p	503	BCR	1	0
45	B	843	PQN	1	0
46	e	845	LHG	1	0
44	B	813	CLA	1	0
44	B	817	CLA	1	0
47	e	847	BCR	2	0
44	f	823	CLA	1	0
51	1	501	LUT	4	0
44	1	513	CLA	6	0
44	A	808	CLA	2	0
44	2	507	CLA	2	0
47	B	848	BCR	3	0
44	f	819	CLA	5	0
44	q	307	CLA	3	0
51	r	302	LUT	10	0
44	p	509	CLA	3	0
44	B	805	CLA	1	0
47	f	849	BCR	4	0
44	B	841	CLA	1	0
44	f	801	CLA	4	0
44	f	816	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	e	827	CLA	2	0
53	2	502	XAT	7	0
44	2	506	CLA	5	0
44	B	837	CLA	1	0
44	2	514	CLA	3	0
44	A	826	CLA	1	0
47	e	854	BCR	4	0
44	3	314	CLA	2	0
47	B	845	BCR	1	0
44	2	504	CLA	2	0
52	r	316	CHL	1	0
52	5	315	CHL	4	0
44	B	802	CLA	6	0
47	f	847	BCR	1	0
47	l	101	BCR	1	0
44	f	839	CLA	3	0
51	q	301	LUT	5	0
44	r	307	CLA	4	0
44	A	810	CLA	2	0
44	5	305	CLA	2	0
44	B	807	CLA	3	0
44	r	305	CLA	2	0
52	s	515	CHL	1	0
44	B	801	CLA	1	0
44	B	816	CLA	1	0
44	B	825	CLA	2	0
44	e	803	CLA	3	0
44	A	815	CLA	1	0
44	e	811	CLA	1	0
47	j	803	BCR	1	0
44	r	306	CLA	7	0
54	Q	803	SQD	5	0
44	p	506	CLA	5	0
44	s	514	CLA	2	0
44	3	313	CLA	4	0
53	s	502	XAT	8	0
44	p	504	CLA	5	0
44	q	304	CLA	3	0
44	B	831	CLA	1	0
44	s	504	CLA	1	0
49	B	850	DGD	4	0
44	3	316	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	A	806	CLA	5	0
50	m	105	LMG	1	0
50	5	301	LMG	1	0
47	L	306	BCR	2	0
44	f	843	CLA	1	0
47	B	852	BCR	1	0
44	e	830	CLA	2	0
51	s	501	LUT	5	0
54	Q	802	SQD	1	0
44	f	829	CLA	1	0
52	2	513	CHL	4	0
44	B	835	CLA	1	0
44	A	827	CLA	4	0
44	L	301	CLA	2	0
44	e	815	CLA	1	0
44	f	832	CLA	2	0
44	s	506	CLA	6	0
47	3	305	BCR	4	0
47	r	301	BCR	5	0
47	K	204	BCR	2	0
49	J	103	DGD	3	0
47	A	851	BCR	4	0
44	s	505	CLA	1	0
46	f	852	LHG	1	0
47	q	303	BCR	3	0
44	f	820	CLA	2	0
44	p	515	CLA	3	0
44	f	821	CLA	5	0
44	A	813	CLA	2	0
44	o	304	CLA	3	0
44	r	310	CLA	1	0
44	e	828	CLA	2	0
46	e	844	LHG	1	0
44	A	821	CLA	2	0
44	f	828	CLA	1	0
44	A	803	CLA	3	0
51	3	303	LUT	7	0
44	e	838	CLA	6	0
44	B	832	CLA	1	0
43	A	801	CL0	2	0
44	A	852	CLA	2	0
44	2	510	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	A	828	CLA	1	0
46	O	601	LHG	1	0
47	I	101	BCR	4	0
44	A	804	CLA	1	0
44	B	804	CLA	4	0
47	B	847	BCR	2	0
48	8	201	SF4	1	0
52	1	517	CHL	5	0
44	e	829	CLA	1	0
44	q	314	CLA	5	0
52	s	513	CHL	2	0
44	n	202	CLA	1	0
44	o	303	CLA	1	0
46	A	844	LHG	3	0
44	q	311	CLA	1	0
44	n	203	CLA	1	0
52	3	315	CHL	1	0
52	p	514	CHL	4	0
47	B	844	BCR	9	0
44	r	304	CLA	2	0
48	g	101	SF4	1	0
46	2	517	LHG	2	0
47	e	850	BCR	2	0
44	q	310	CLA	1	0
44	e	813	CLA	2	0
44	1	506	CLA	8	0
44	e	817	CLA	2	0
44	B	824	CLA	3	0
47	e	848	BCR	2	0
44	n	205	CLA	1	0
47	s	503	BCR	4	0
44	A	831	CLA	3	0
44	f	808	CLA	3	0
44	p	513	CLA	1	0
44	r	309	CLA	1	0
44	B	823	CLA	1	0
50	F	806	LMG	2	0
43	e	801	CL0	5	0
44	e	852	CLA	4	0
44	B	810	CLA	1	0
44	f	805	CLA	2	0
52	p	512	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	f	831	CLA	2	0
44	A	805	CLA	4	0
53	5	304	XAT	5	0
44	e	826	CLA	3	0
47	A	848	BCR	2	0
44	f	826	CLA	3	0
51	2	501	LUT	8	0
44	e	814	CLA	1	0
47	e	849	BCR	4	0
44	o	302	CLA	2	0
44	f	834	CLA	2	0
47	f	845	BCR	1	0
44	2	509	CLA	1	0
47	o	301	BCR	1	0
44	e	807	CLA	1	0
44	e	812	CLA	5	0
44	B	822	CLA	3	0
47	F	804	BCR	3	0
52	2	512	CHL	4	0
47	f	848	BCR	4	0
48	C	102	SF4	1	0
47	A	845	BCR	4	0
44	q	316	CLA	1	0
47	Q	801	BCR	6	0
44	q	312	CLA	2	0
44	p	510	CLA	2	0
44	5	308	CLA	5	0
44	e	808	CLA	1	0
44	f	838	CLA	2	0
44	q	315	CLA	4	0
44	e	834	CLA	1	0
44	f	815	CLA	1	0
44	1	515	CLA	3	0
44	f	833	CLA	1	0
47	F	801	BCR	1	0
44	A	838	CLA	2	0
44	3	309	CLA	2	0
44	e	818	CLA	3	0
47	e	846	BCR	5	0
44	A	817	CLA	3	0
44	f	810	CLA	3	0
44	B	828	CLA	4	0

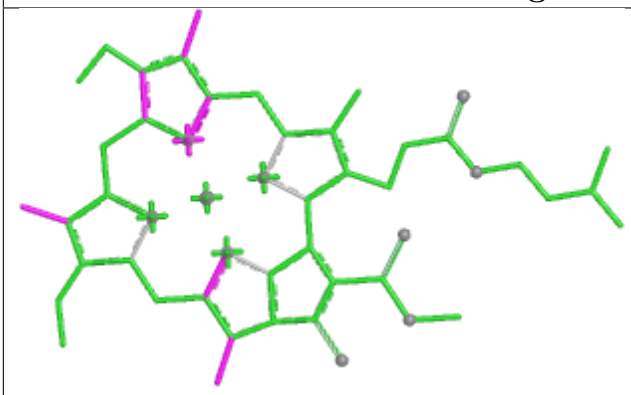
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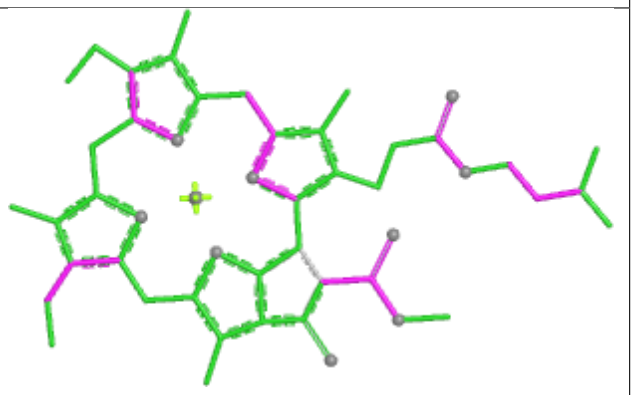
Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	e	809	CLA	5	0
44	f	807	CLA	4	0
45	e	842	PQN	1	0
44	K	202	CLA	2	0
44	p	507	CLA	1	0
44	L	302	CLA	1	0
44	3	301	CLA	2	0
44	K	205	CLA	1	0
44	5	309	CLA	1	0
44	L	303	CLA	2	0
47	f	850	BCR	4	0
44	r	317	CLA	1	0
44	A	829	CLA	1	0
44	e	824	CLA	1	0
51	p	502	LUT	6	0
44	1	510	CLA	2	0
44	A	816	CLA	2	0
47	L	305	BCR	8	0
52	s	517	CHL	1	0
44	A	835	CLA	2	0
44	A	836	CLA	3	0
47	1	503	BCR	3	0
44	F	802	CLA	3	0

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

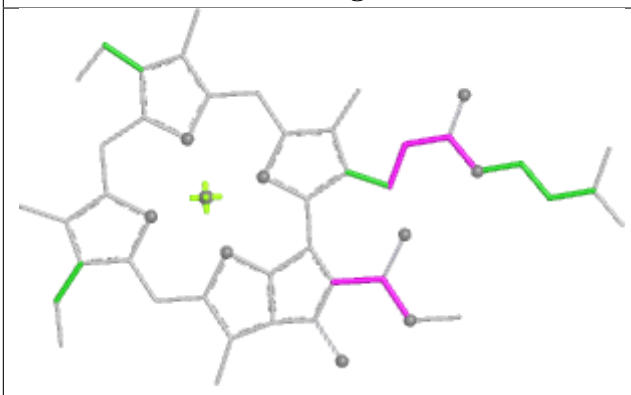
Ligand CLA 3 311



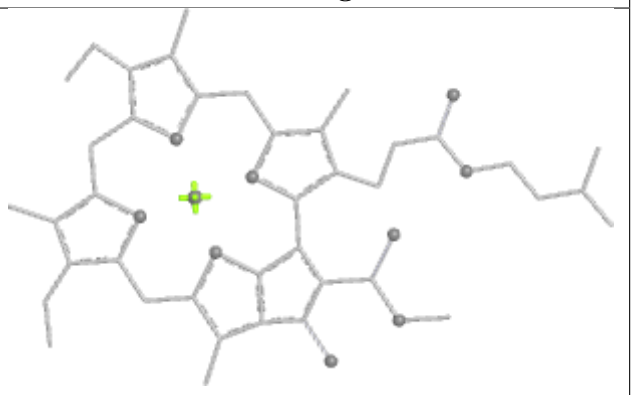
Bond lengths



Bond angles

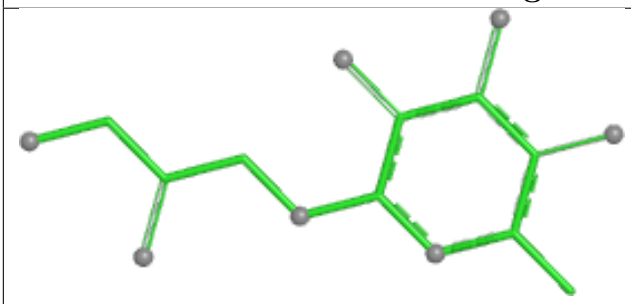


Torsions

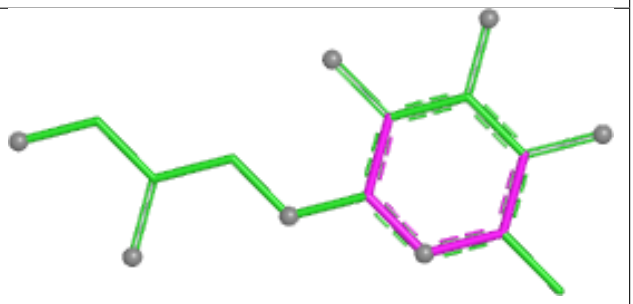


Rings

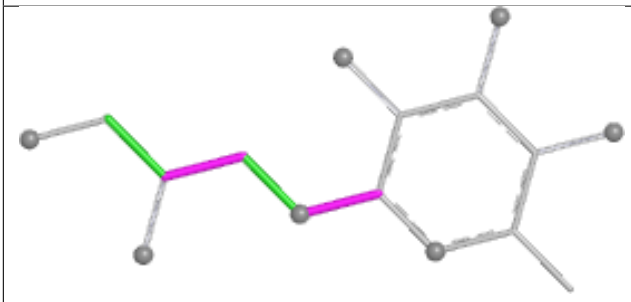
Ligand LMG 2 518



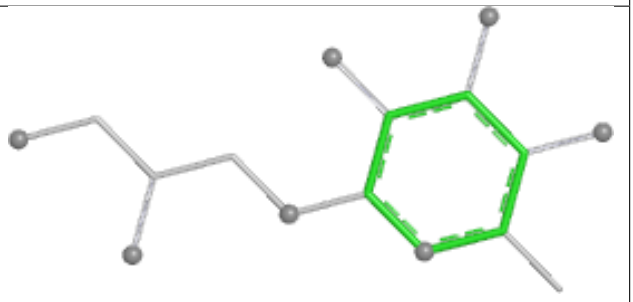
Bond lengths



Bond angles

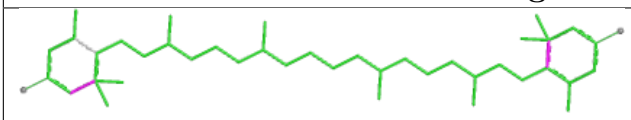


Torsions

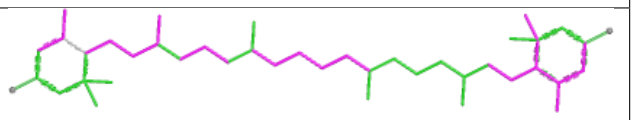


Rings

Ligand LUT 1 502



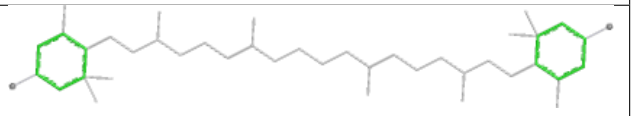
Bond lengths



Bond angles

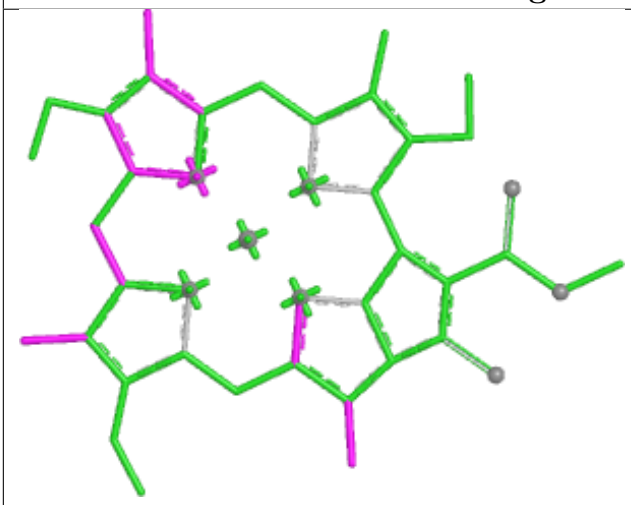


Torsions

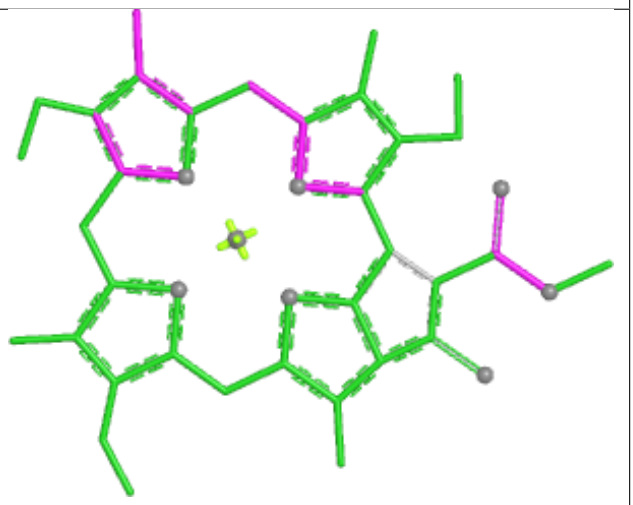


Rings

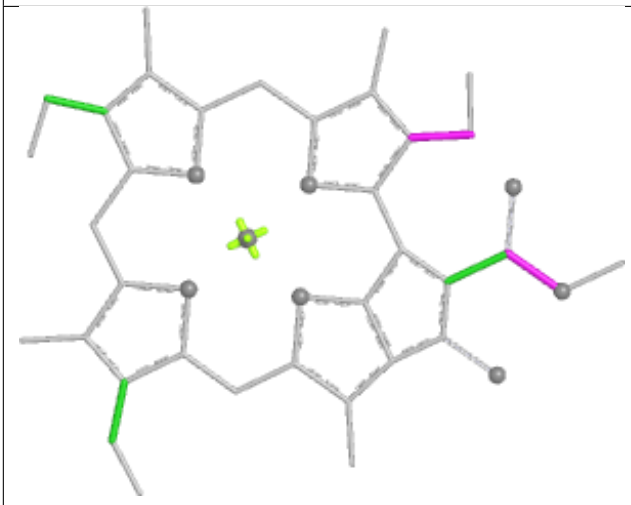
Ligand CLA e 821



Bond lengths



Bond angles

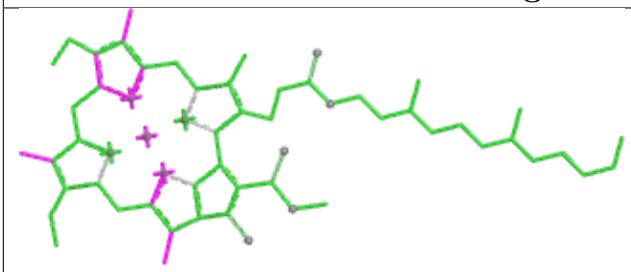


Torsions

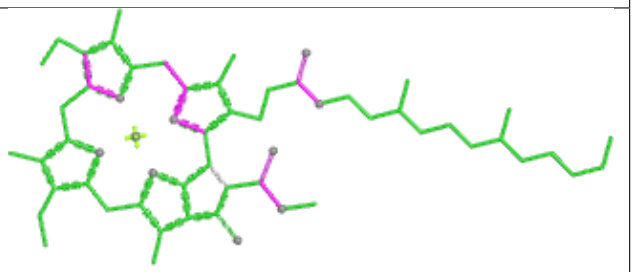


Rings

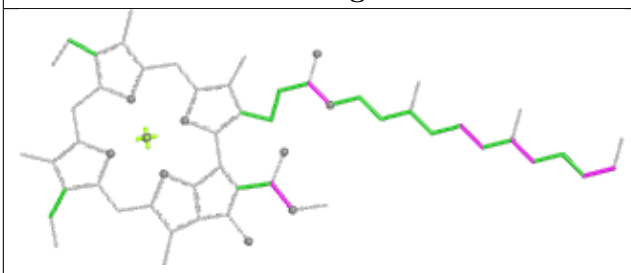
Ligand CLA A 825



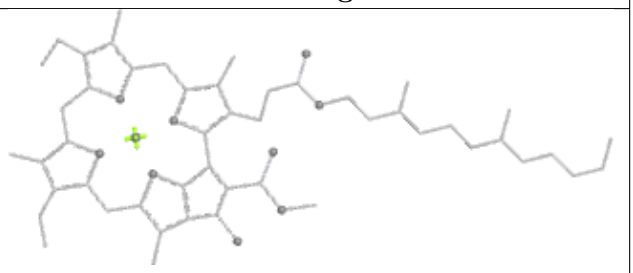
Bond lengths



Bond angles

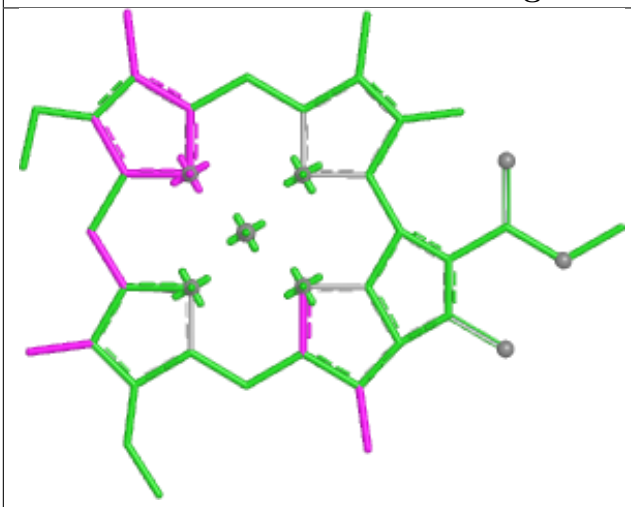


Torsions

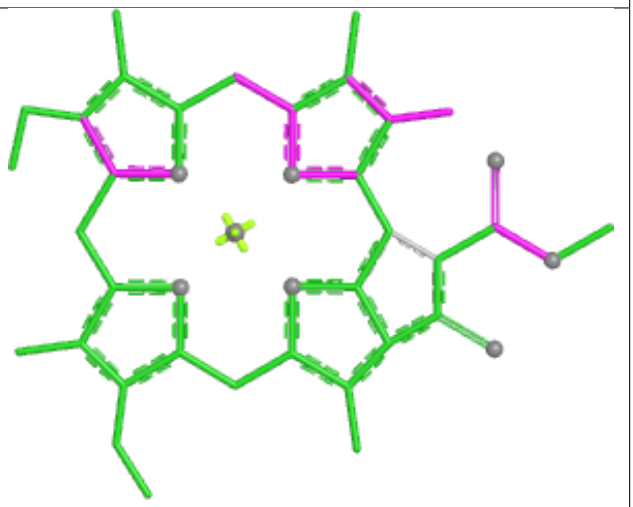


Rings

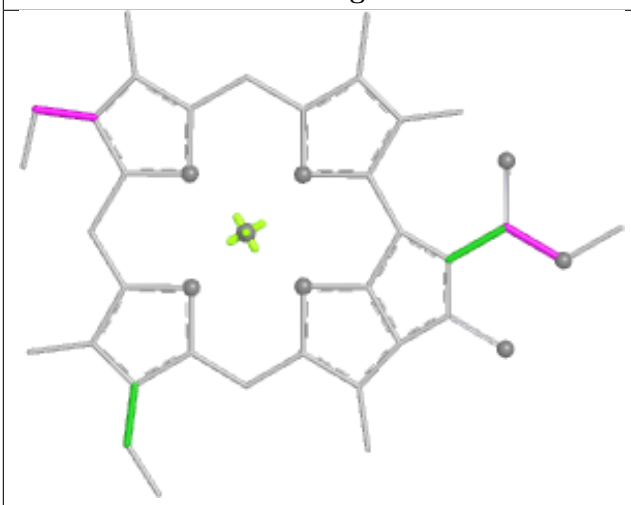
Ligand CLA A 840



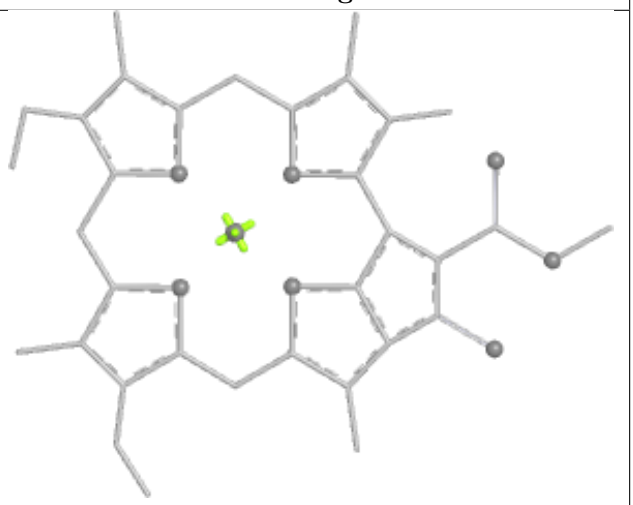
Bond lengths



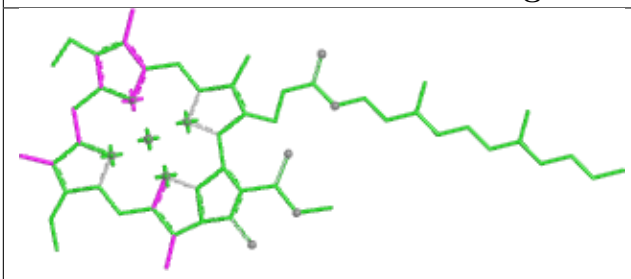
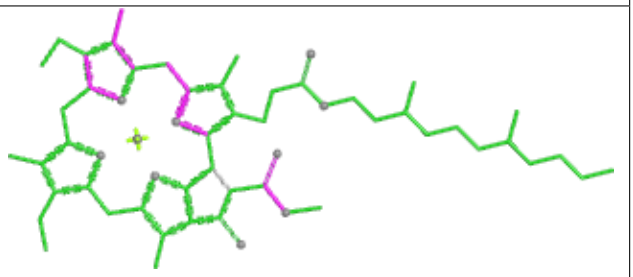
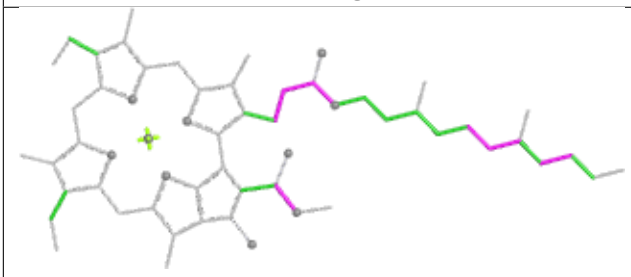
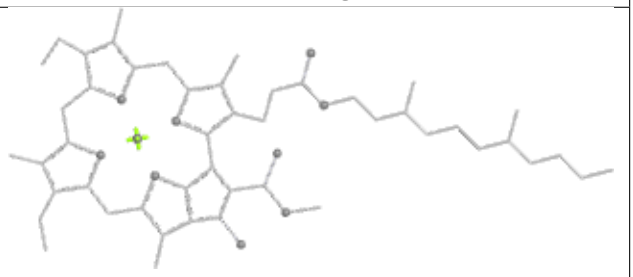
Bond angles

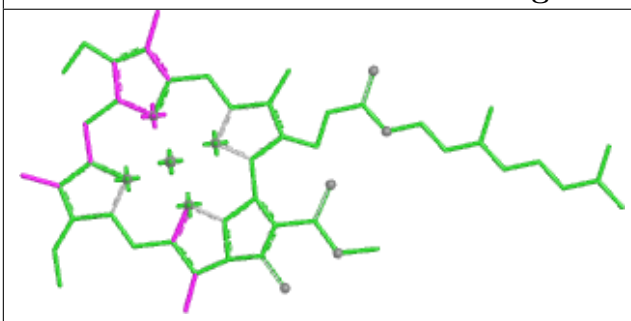
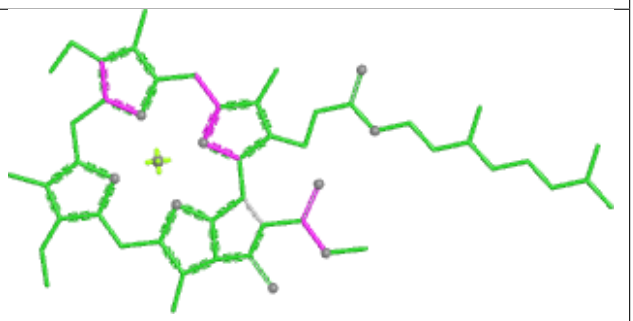
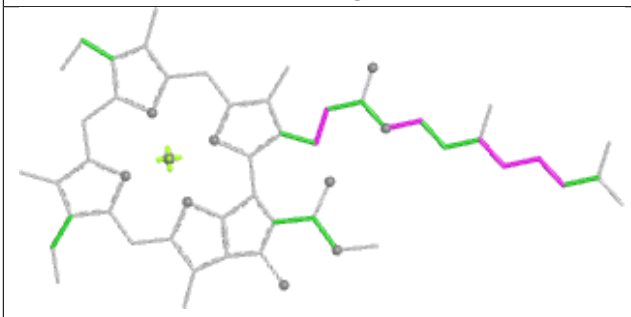
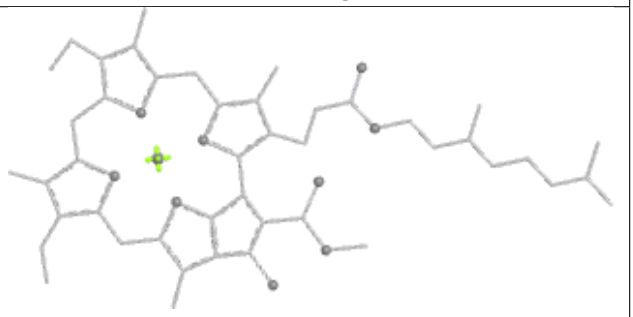


Torsions

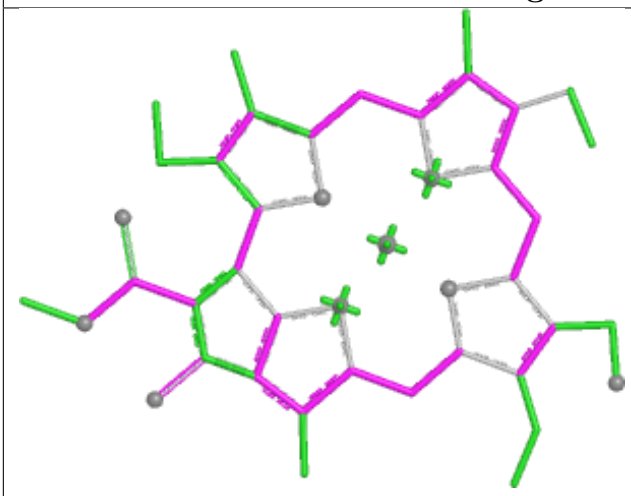


Rings

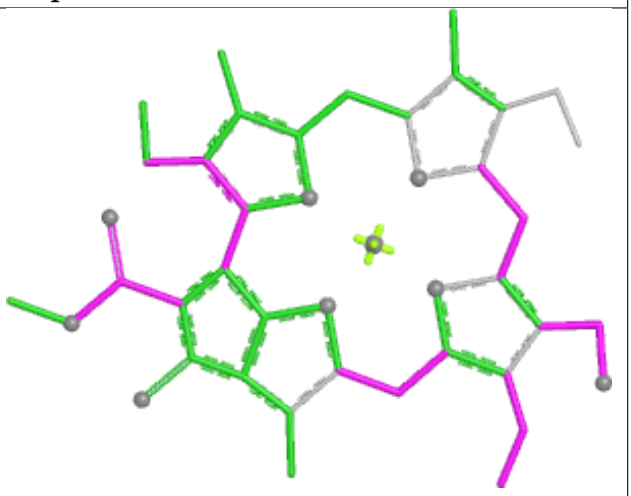
Ligand CLA A 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA f 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

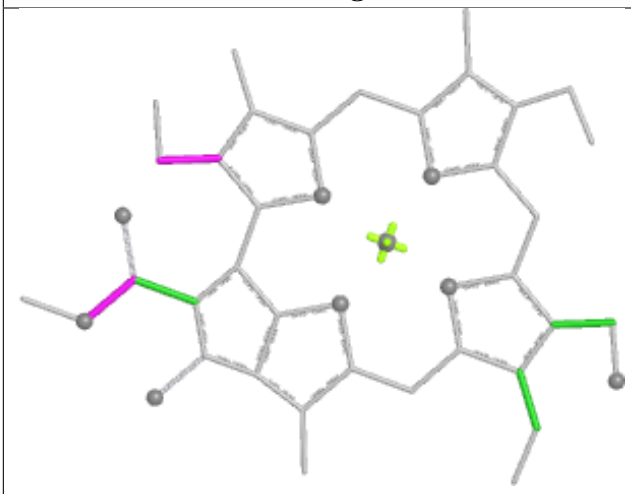
Ligand CHL p 517



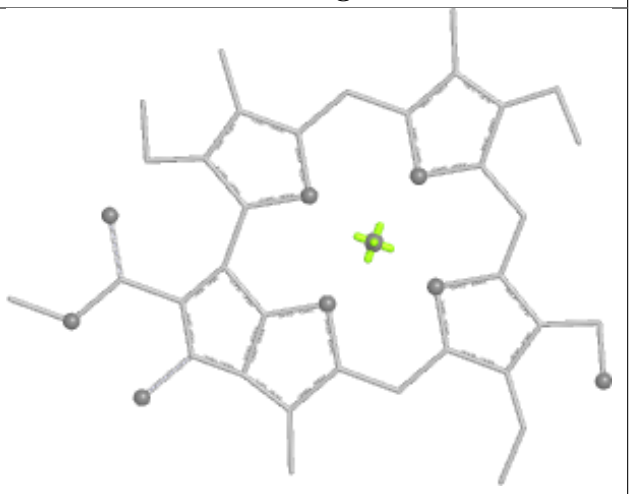
Bond lengths



Bond angles

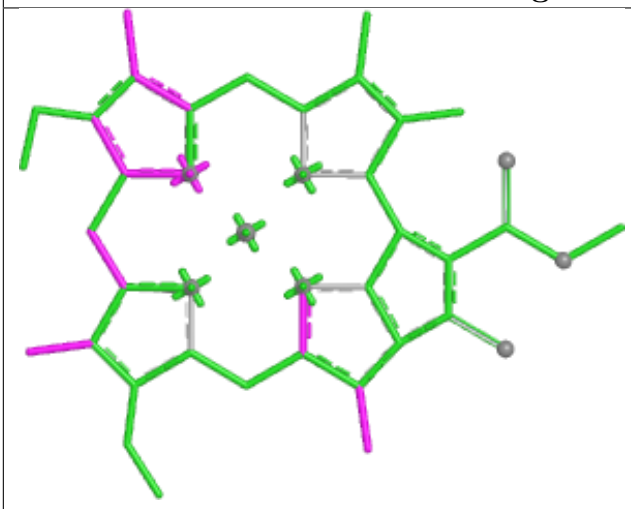


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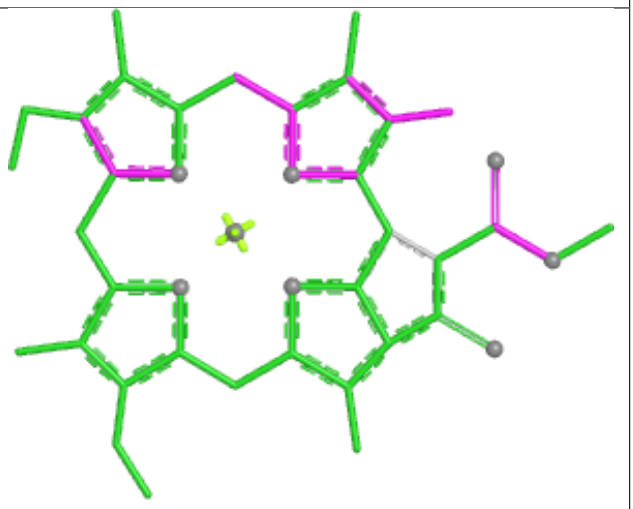


Rings

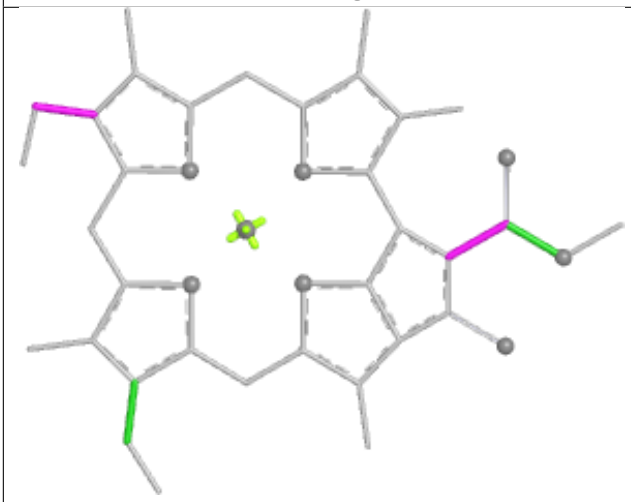
Ligand CLA f 822



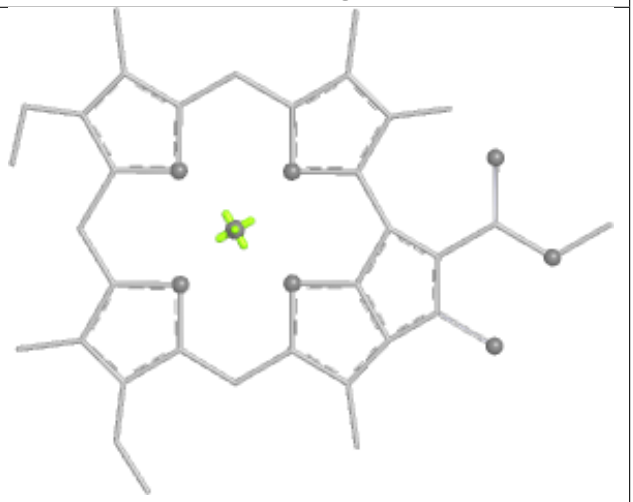
Bond lengths



Bond angles

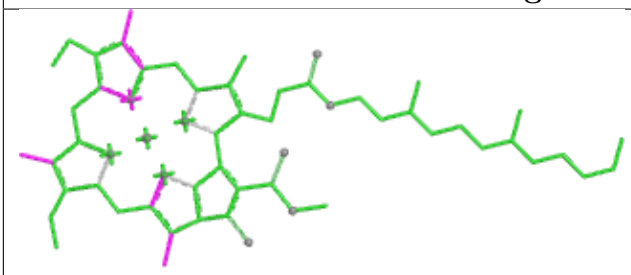


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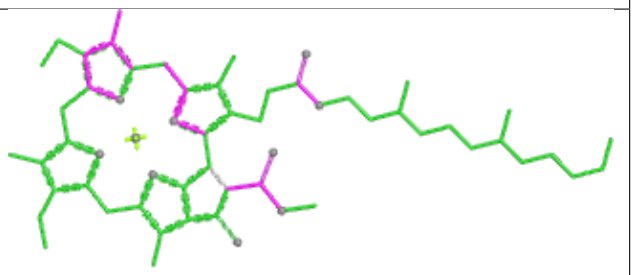


Rings

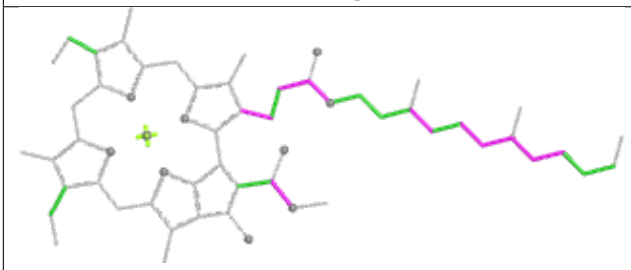
Ligand CLA B 818



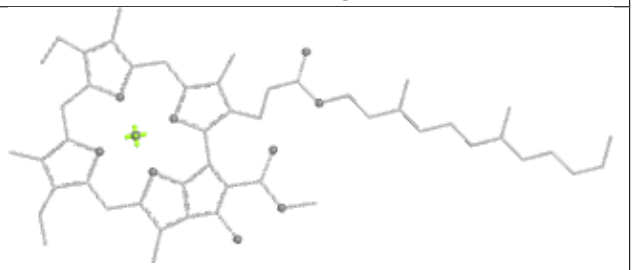
Bond lengths



Bond angles

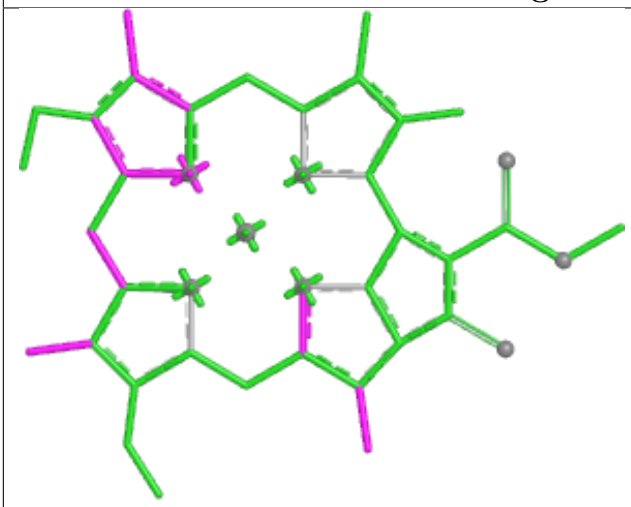


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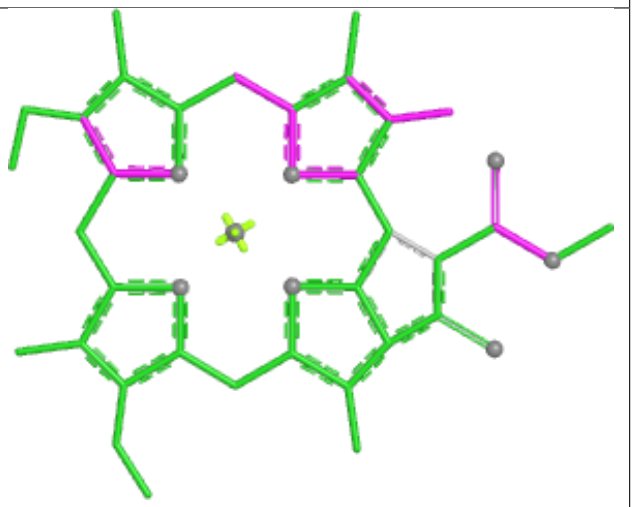


Rings

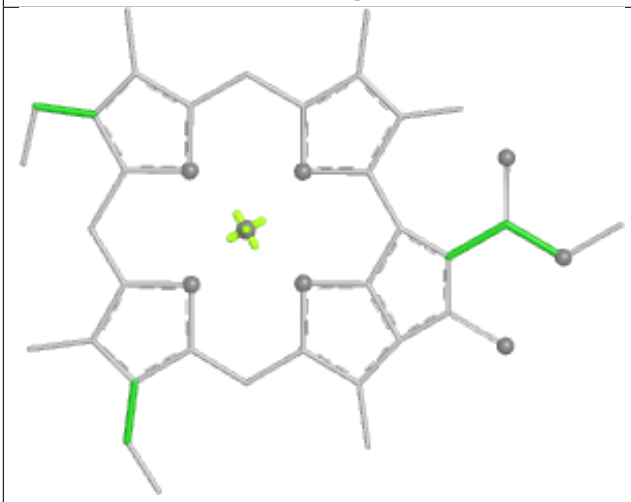
Ligand CLA f 806



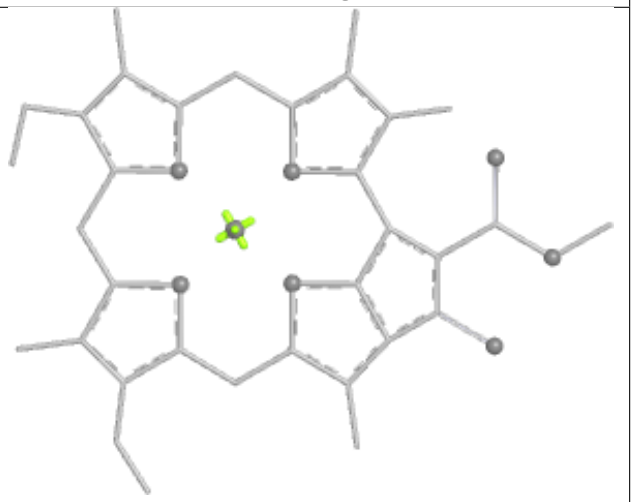
Bond lengths



Bond angles

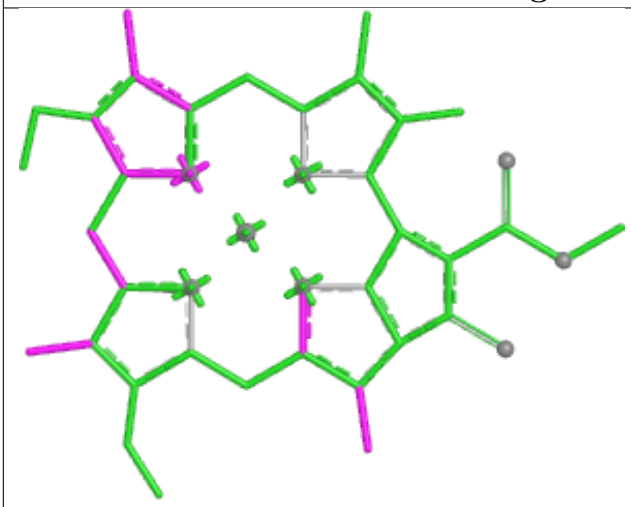


Torsions

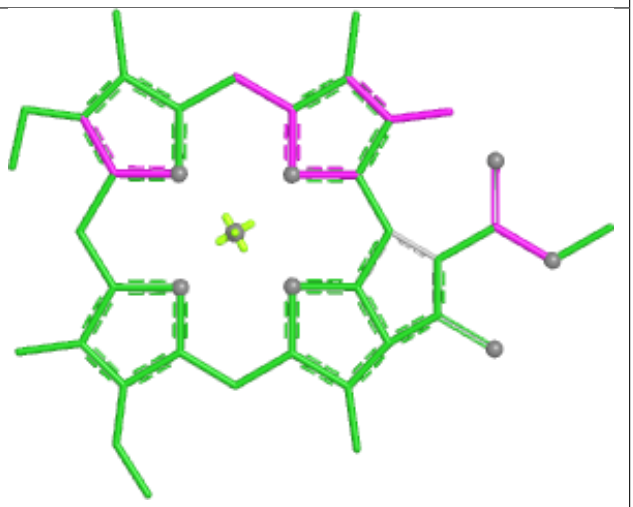


Rings

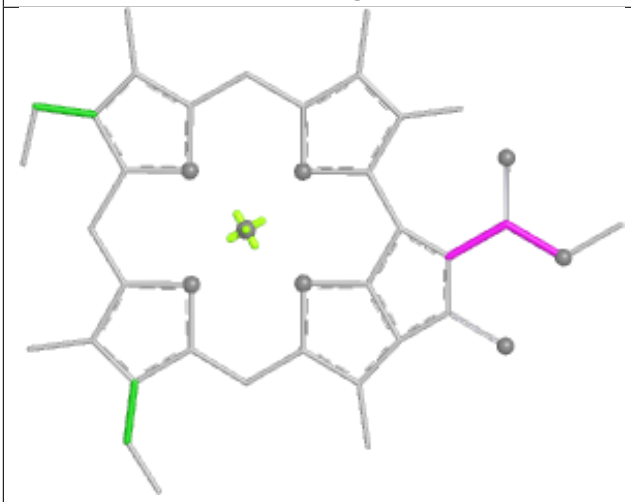
Ligand CLA r 308



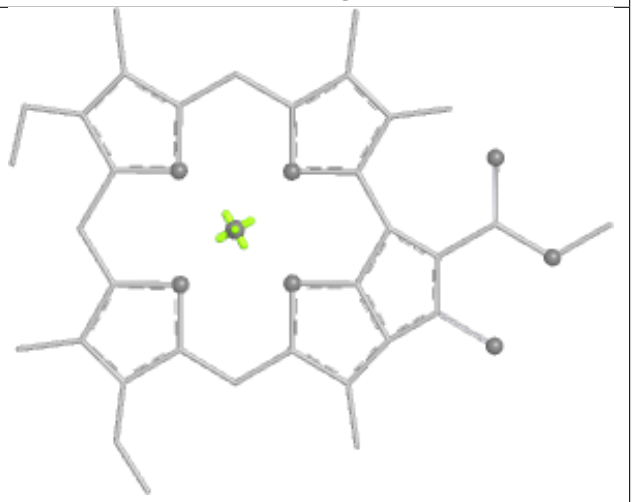
Bond lengths



Bond angles

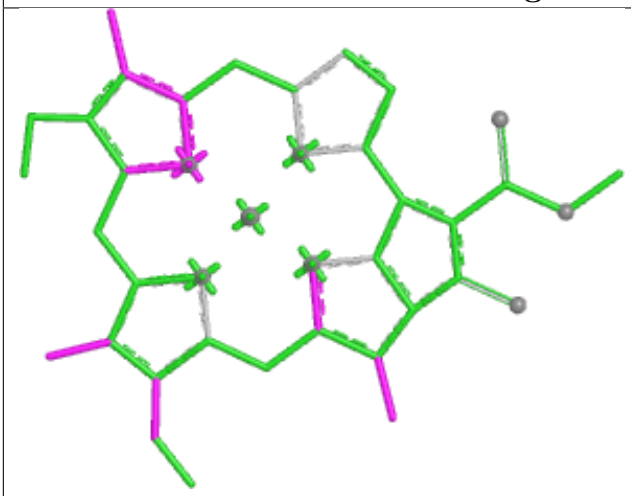


Torsions

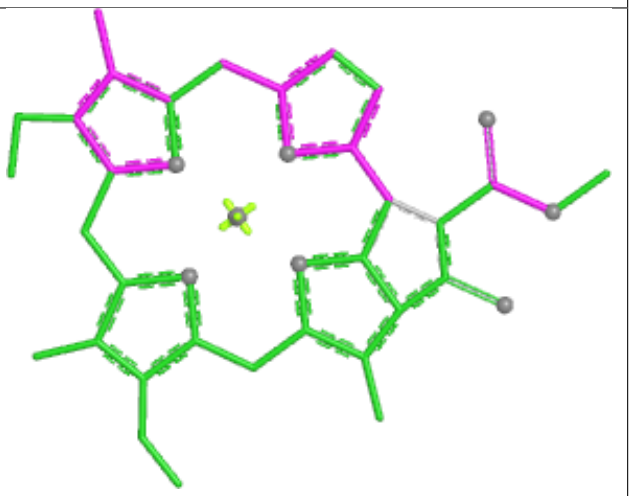


Rings

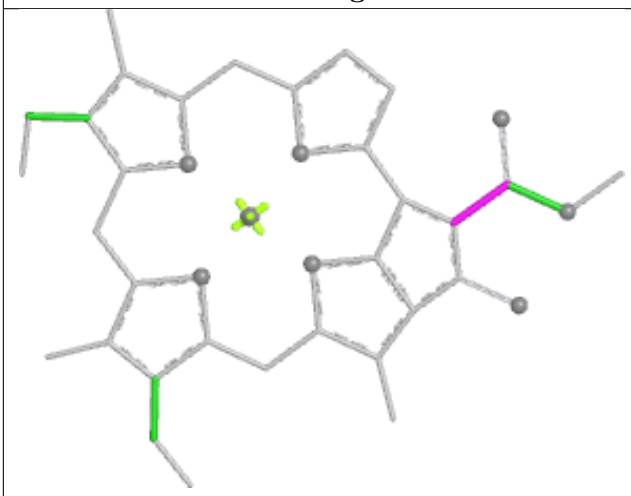
Ligand CLA B 806



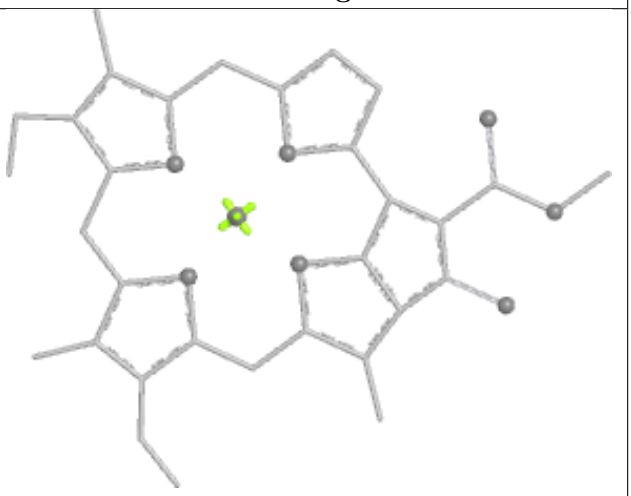
Bond lengths



Bond angles

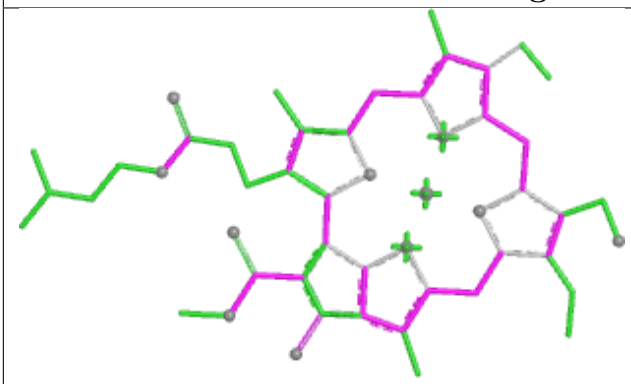


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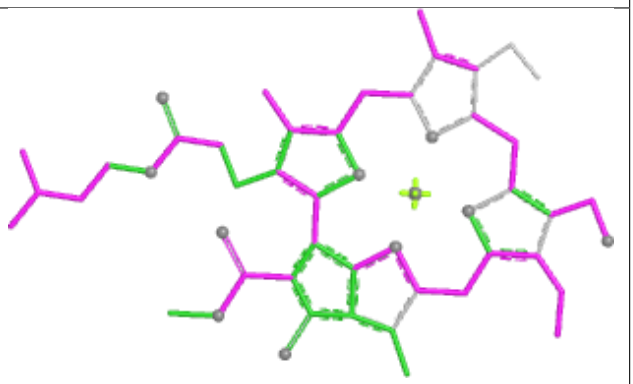


Rings

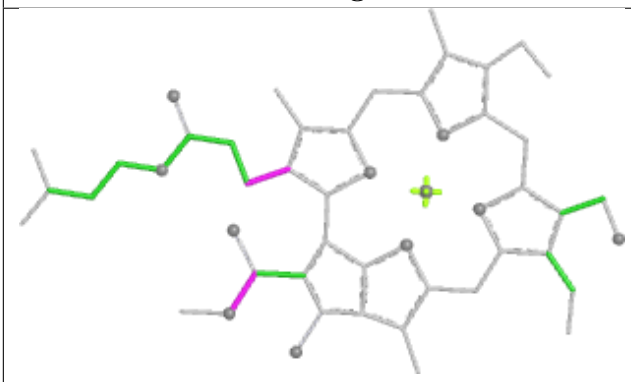
Ligand CHL r 314



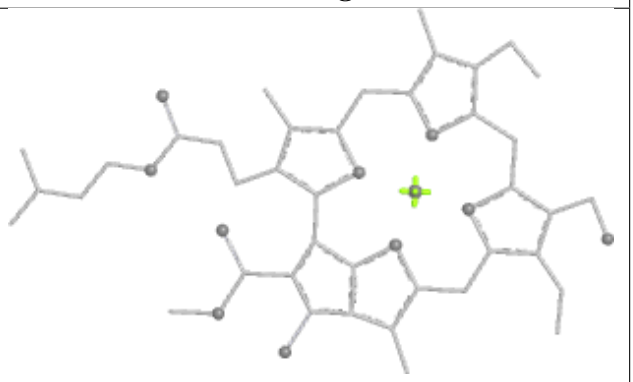
Bond lengths



Bond angles



Torsions

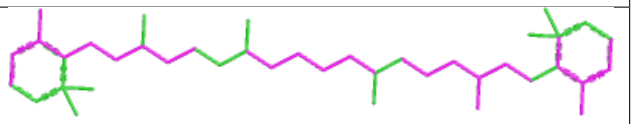


Rings

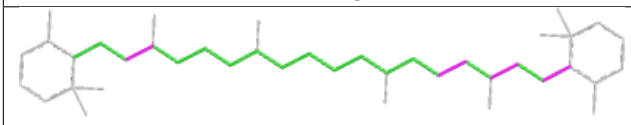
Ligand BCR A 846



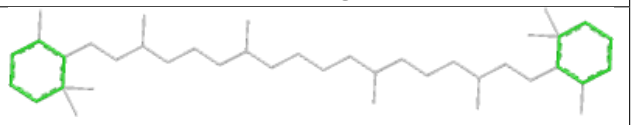
Bond lengths



Bond angles

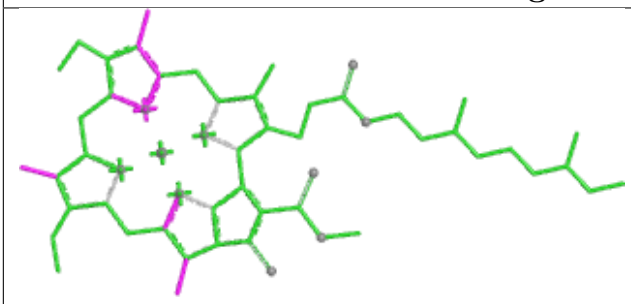


Torsions

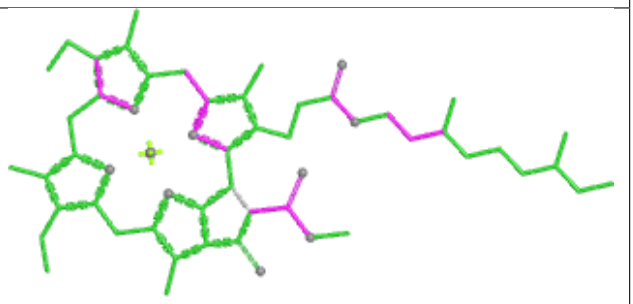


Rings

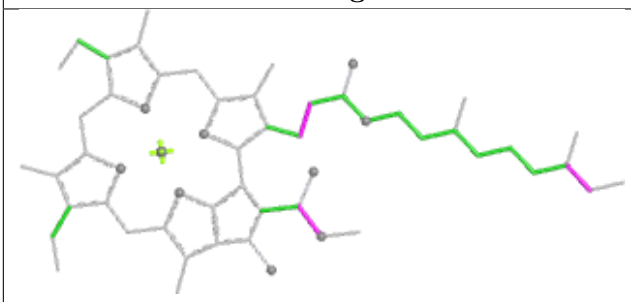
Ligand CLA 1 507



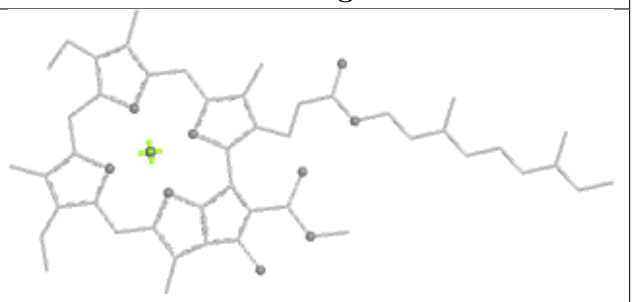
Bond lengths



Bond angles

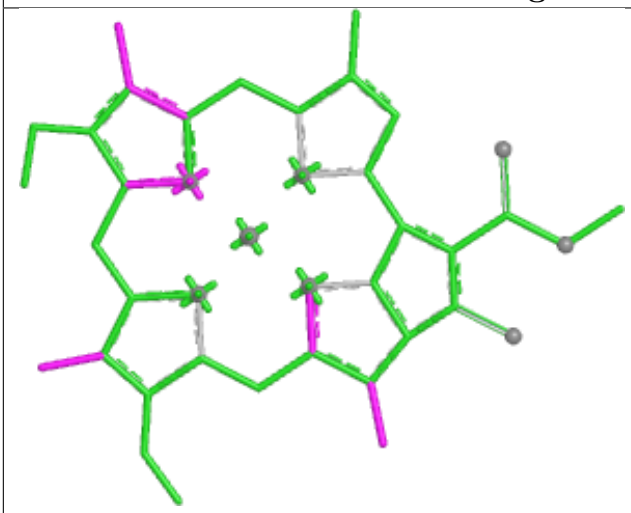


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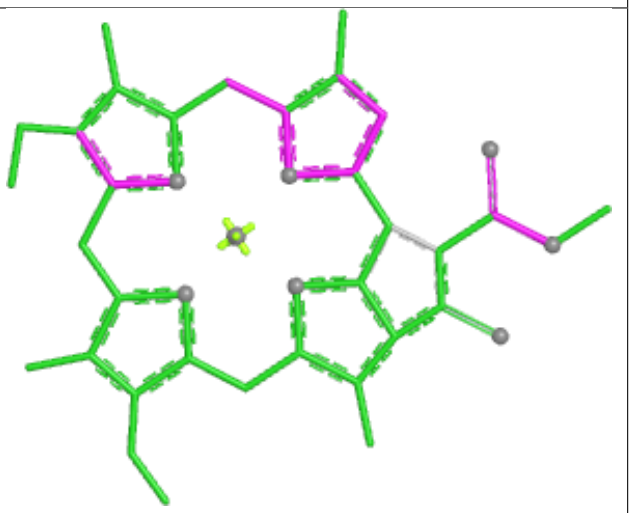


Rings

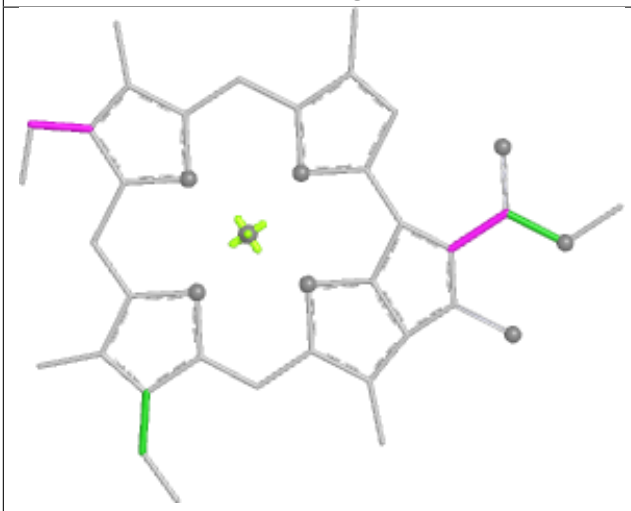
Ligand CLA 5 313



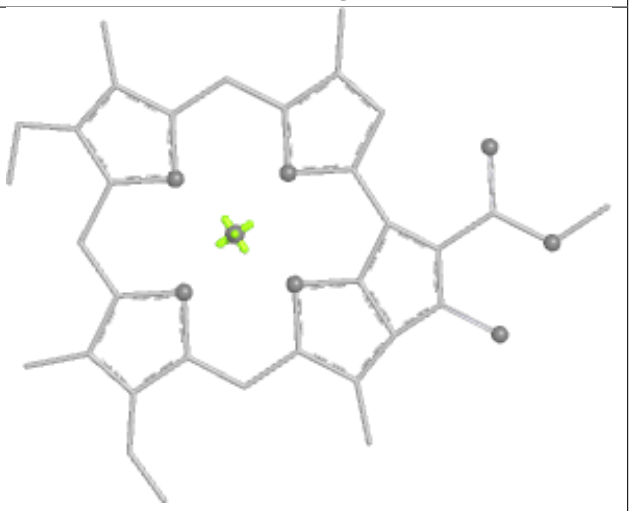
Bond lengths



Bond angles



Torsions



Rings

Ligand BCR A 849



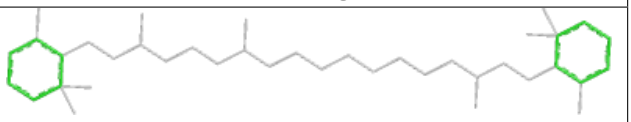
Bond lengths



Bond angles

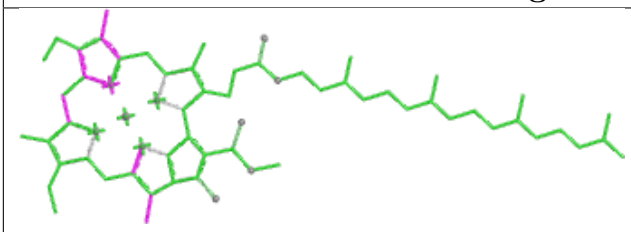


Torsions

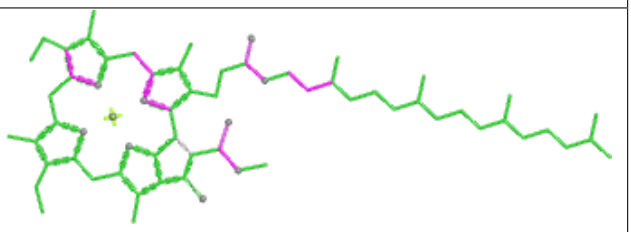


Rings

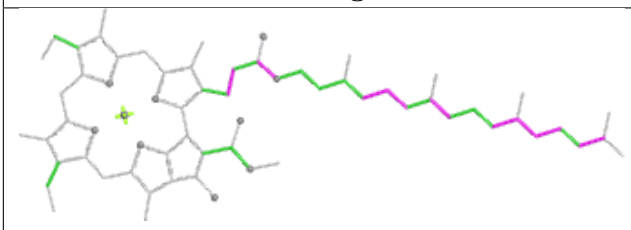
Ligand CLA e 839



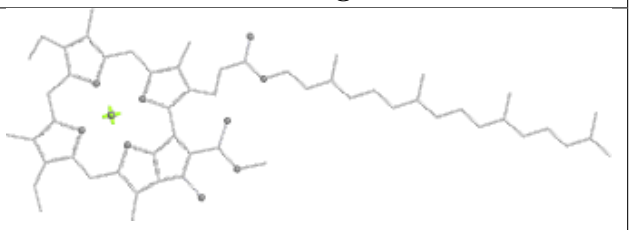
Bond lengths



Bond angles

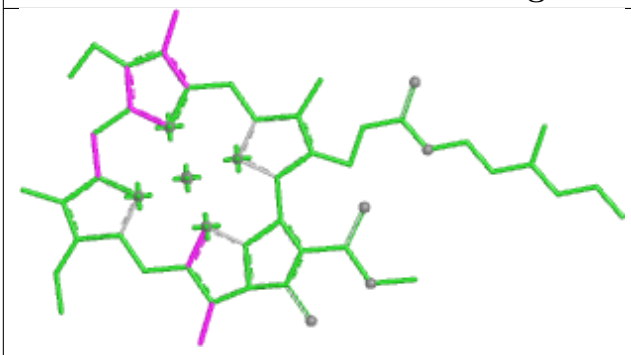


Torsions

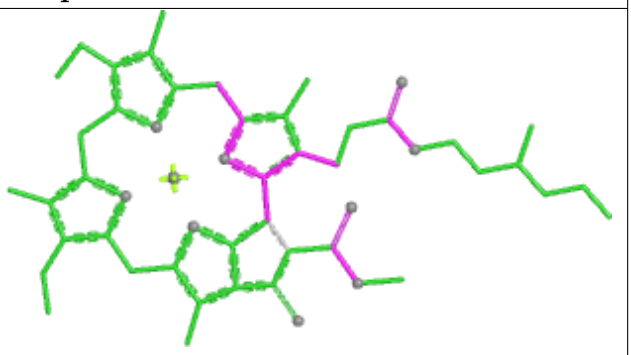


Rings

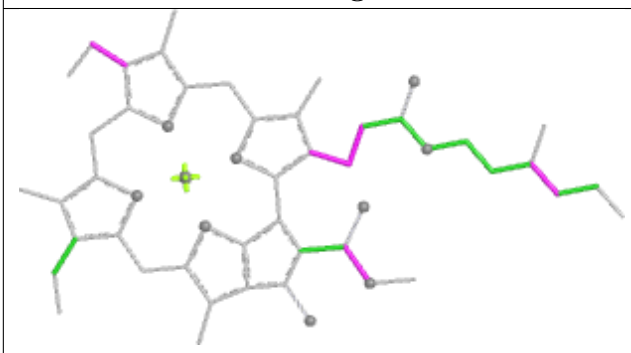
Ligand CLA q 305



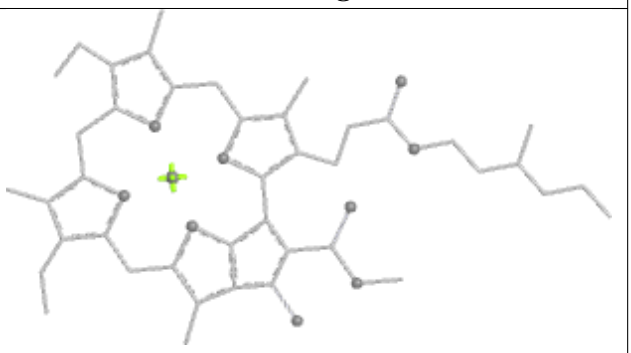
Bond lengths



Bond angles



Torsions

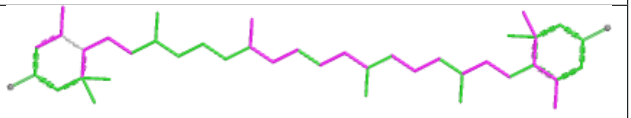


Rings

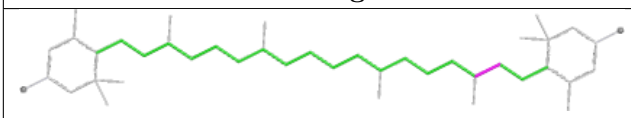
Ligand LUT 3 304



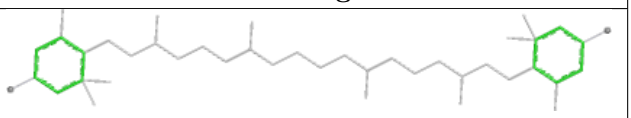
Bond lengths



Bond angles

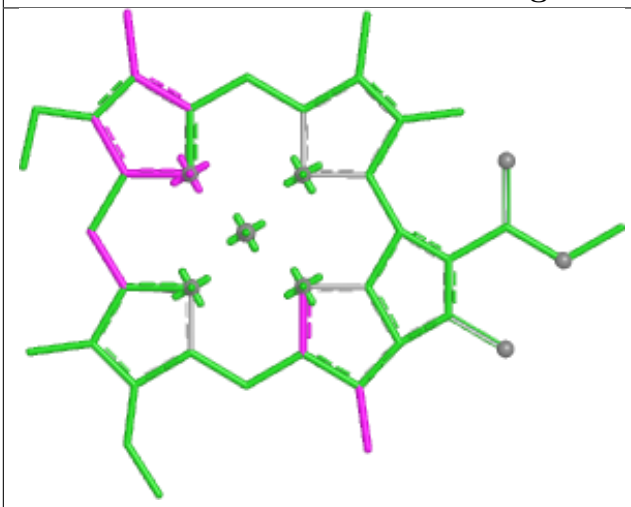


Torsions

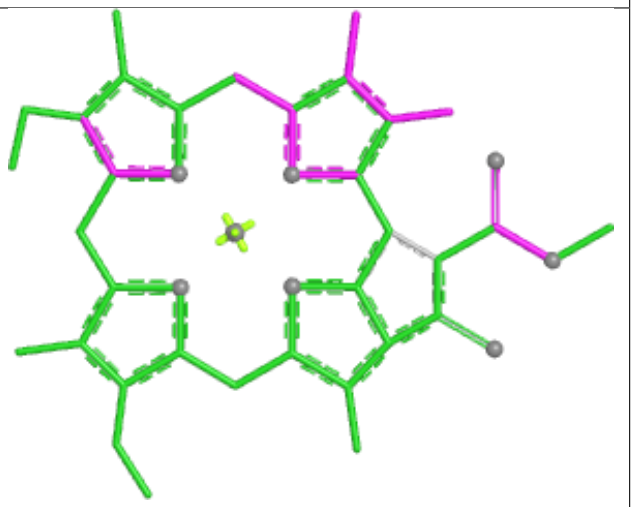


Rings

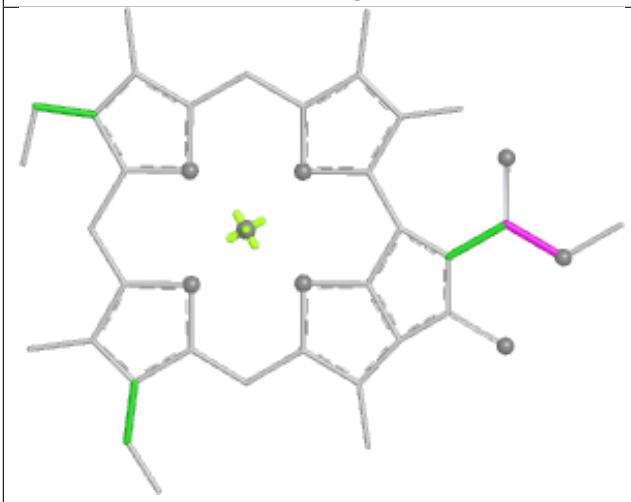
Ligand CLA r 315



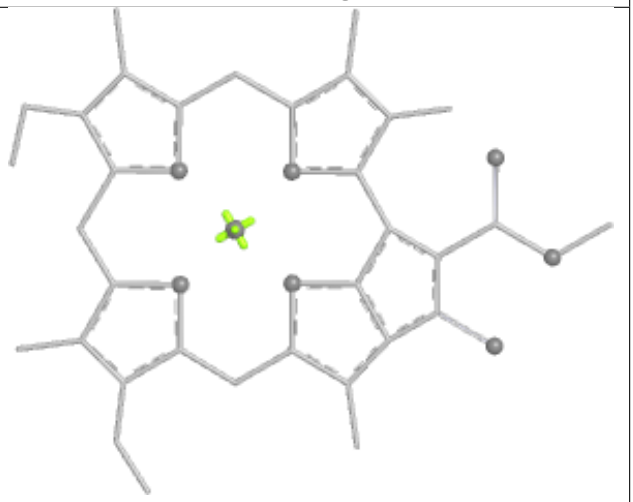
Bond lengths



Bond angles

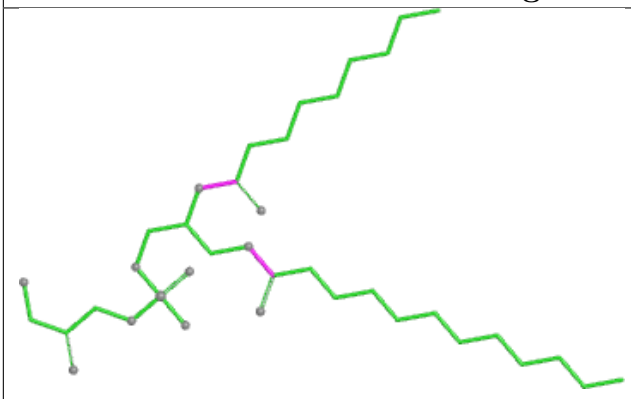


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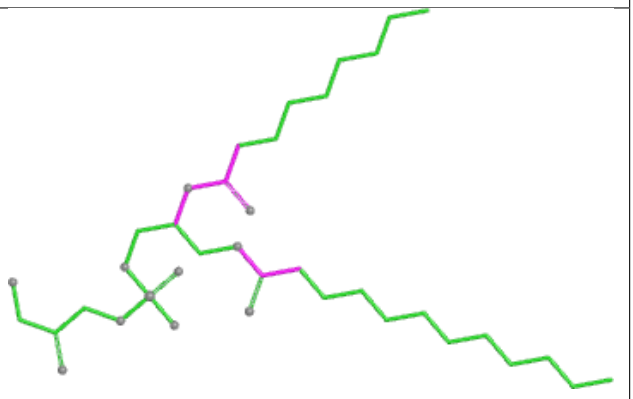


Rings

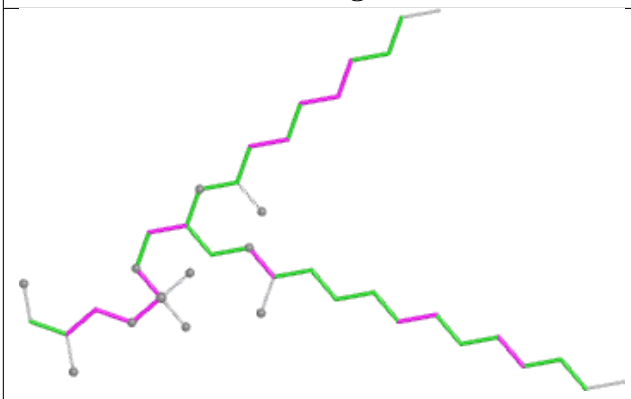
Ligand LHG B 851



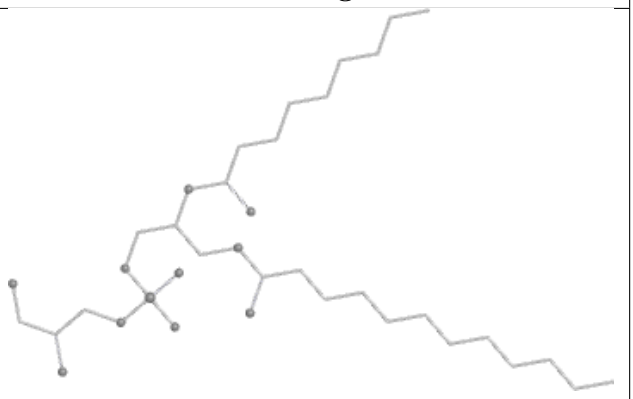
Bond lengths



Bond angles

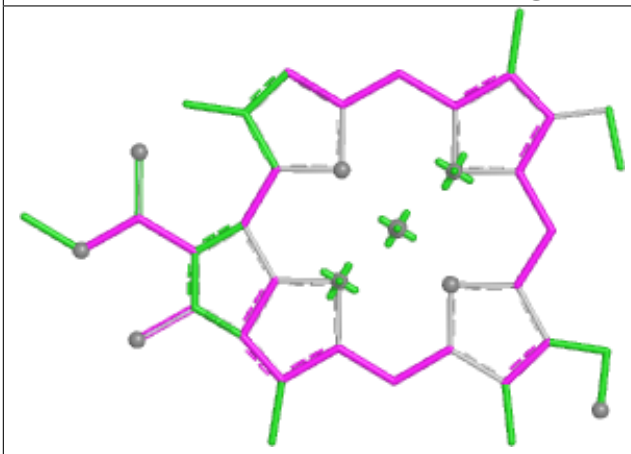


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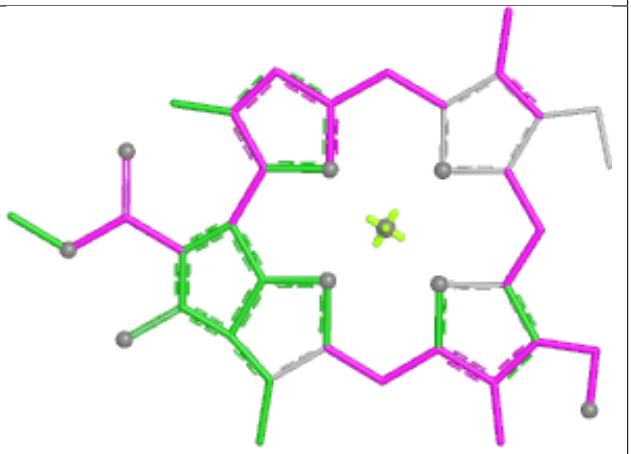


Rings

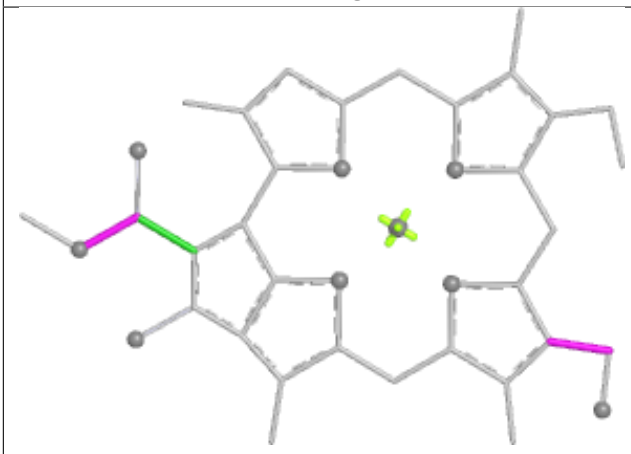
Ligand CHL 5 317



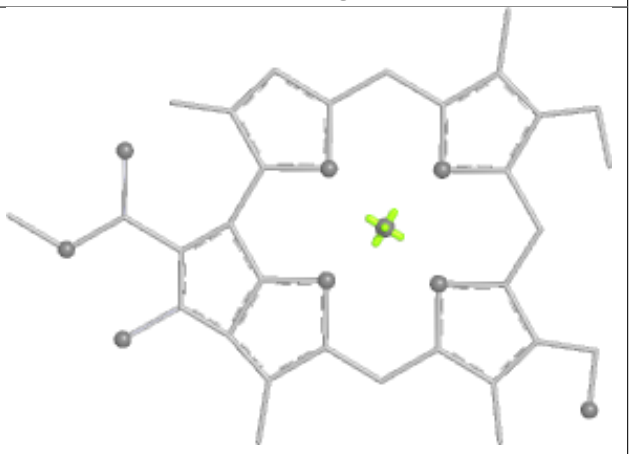
Bond lengths



Bond angles

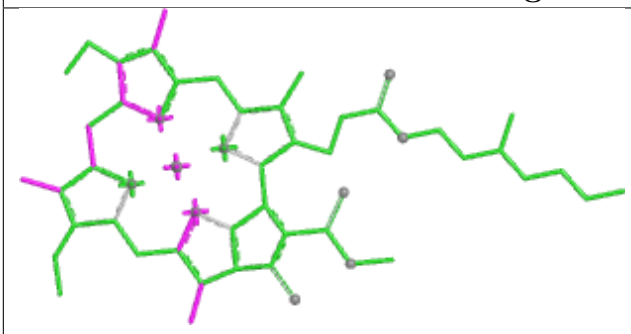


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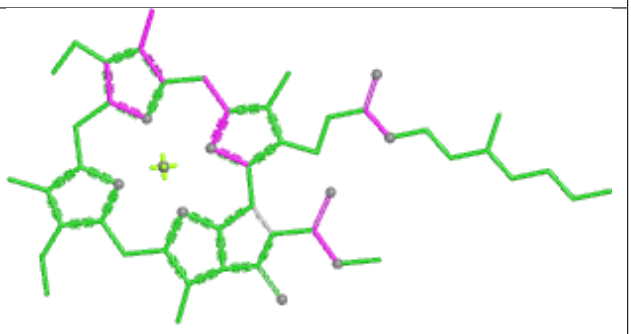


Rings

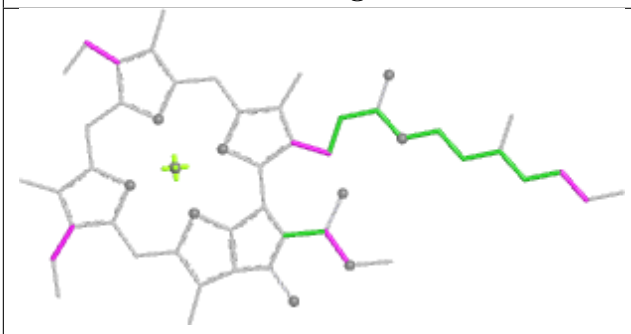
Ligand CLA B 820



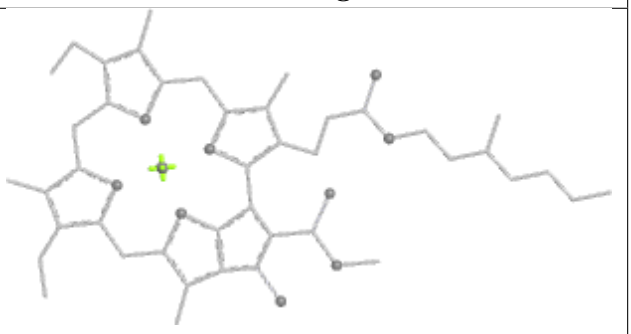
Bond lengths



Bond angles



Torsions

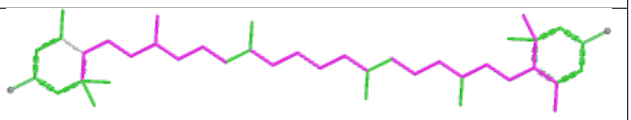


Rings

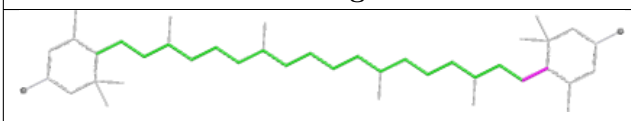
Ligand LUT 5 303



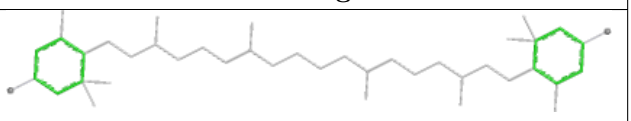
Bond lengths



Bond angles

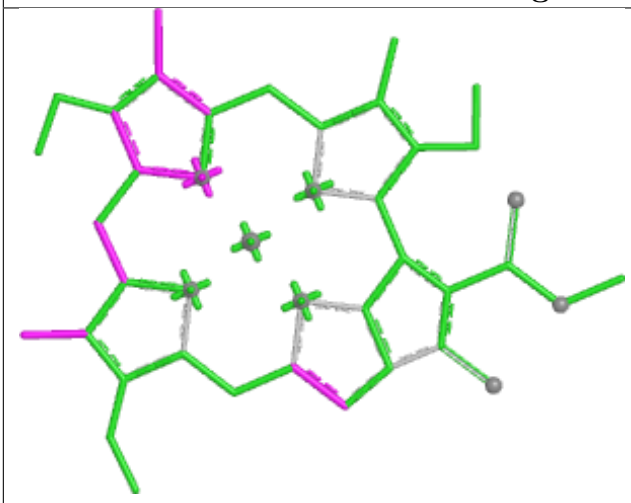


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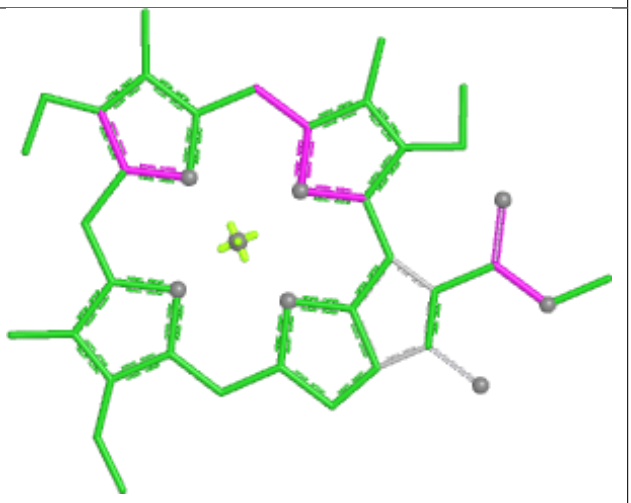


Rings

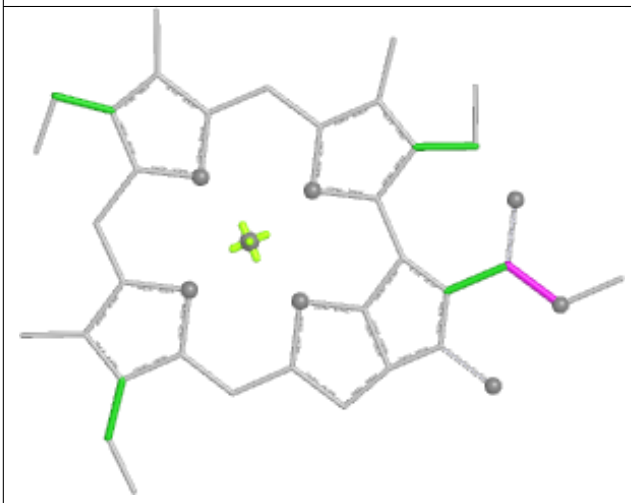
Ligand CLA f 803



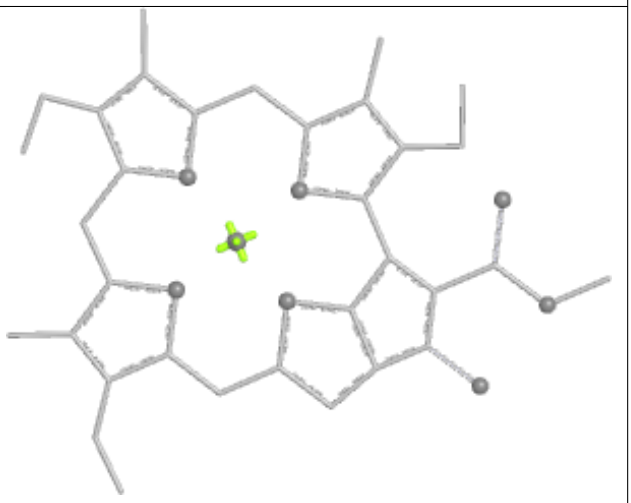
Bond lengths



Bond angles

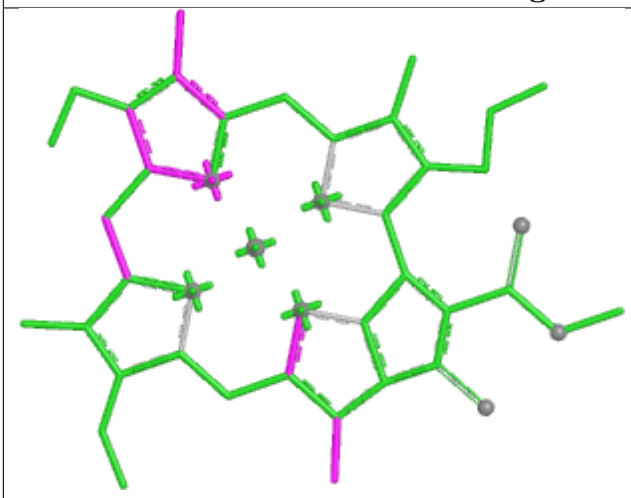


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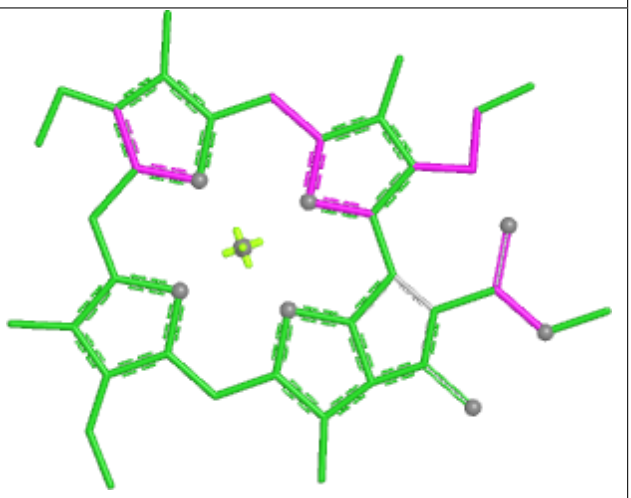


Rings

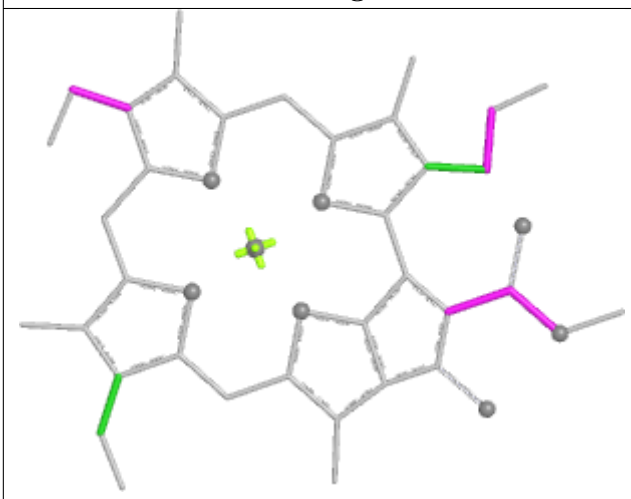
Ligand CLA e 832



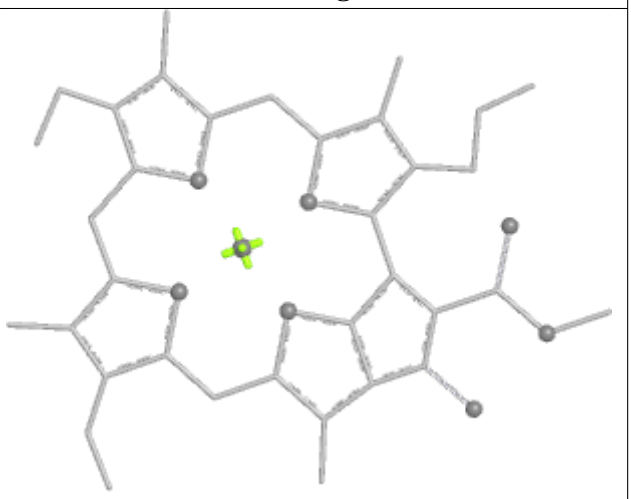
Bond lengths



Bond angles

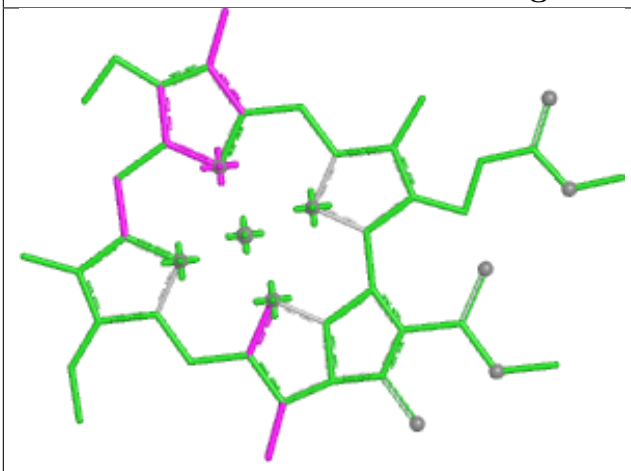


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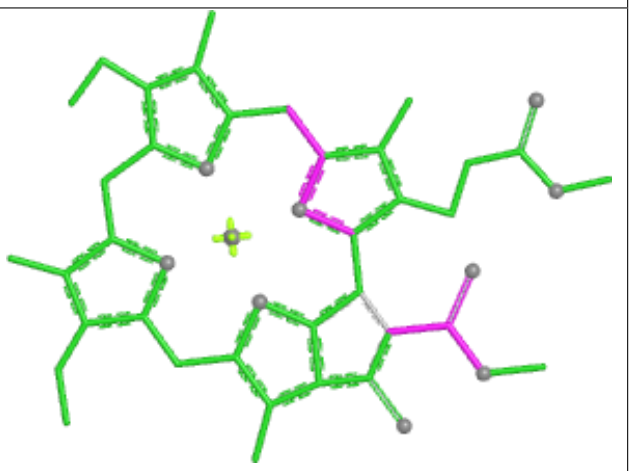


Rings

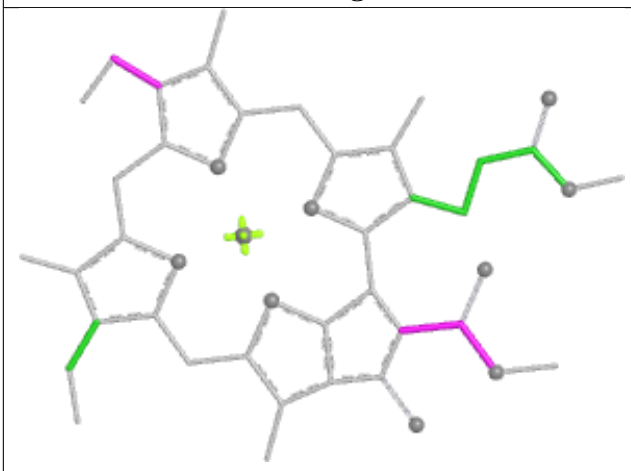
Ligand CLA r 311



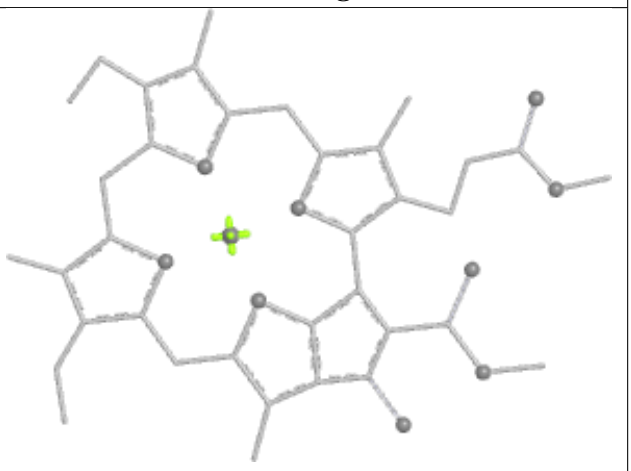
Bond lengths



Bond angles

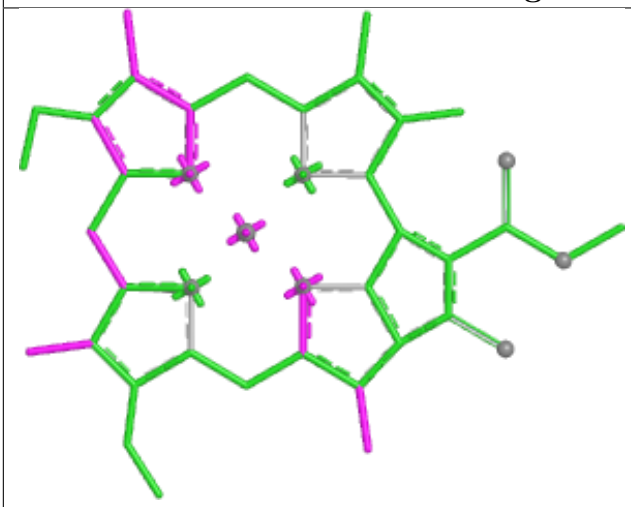


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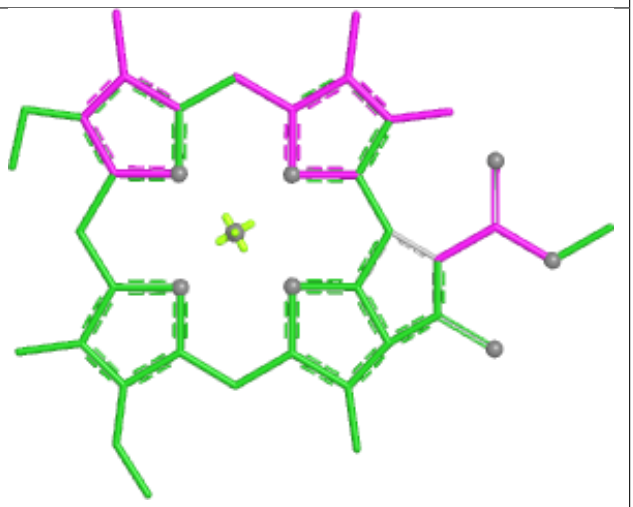


Rings

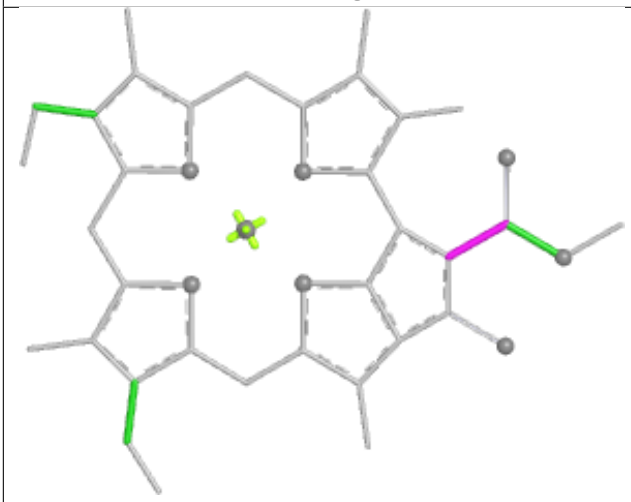
Ligand CLA B 827



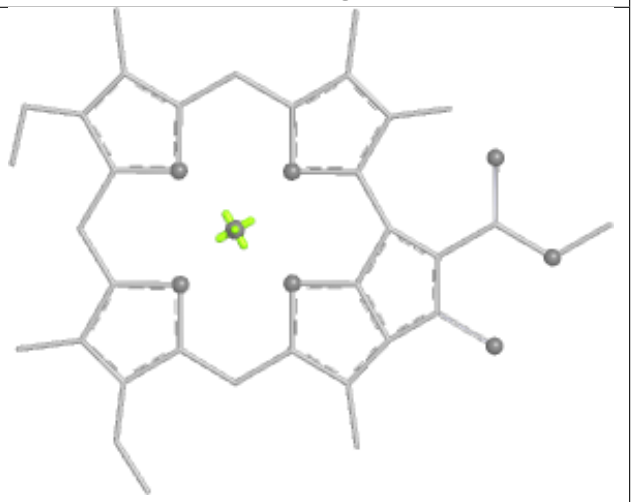
Bond lengths



Bond angles

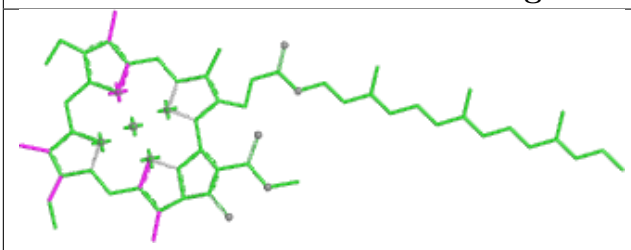


Torsions

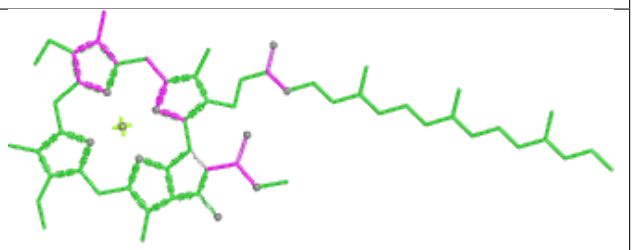


Rings

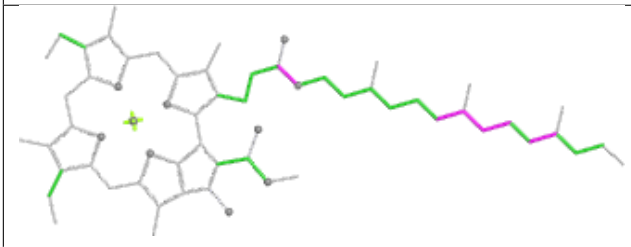
Ligand CLA B 826



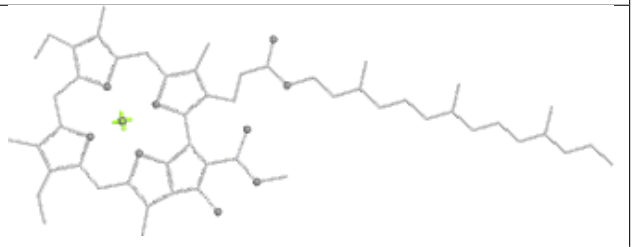
Bond lengths



Bond angles

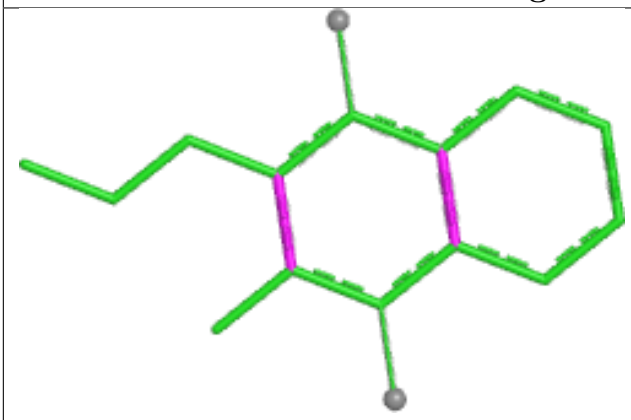


Torsions

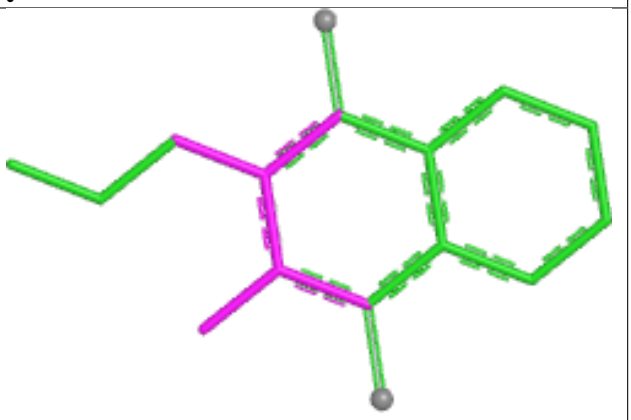


Rings

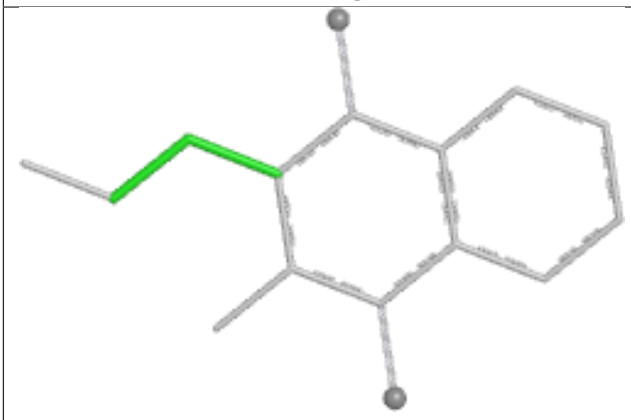
Ligand PQN f 844



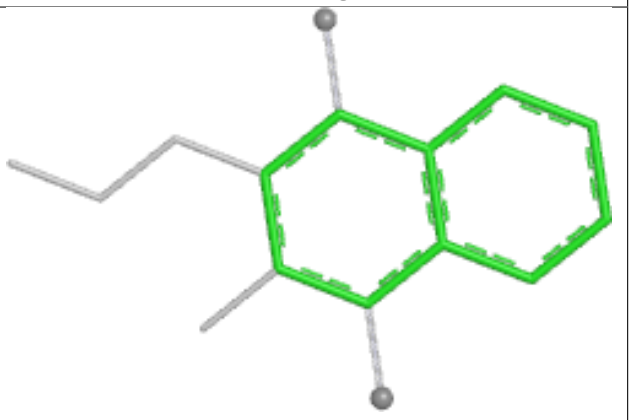
Bond lengths



Bond angles

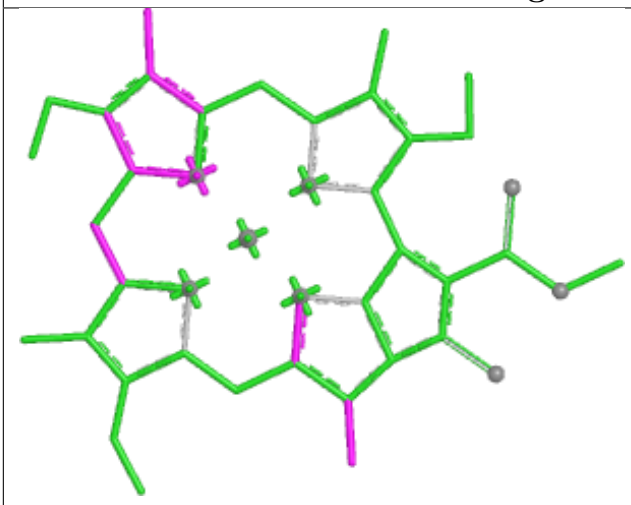


Torsions

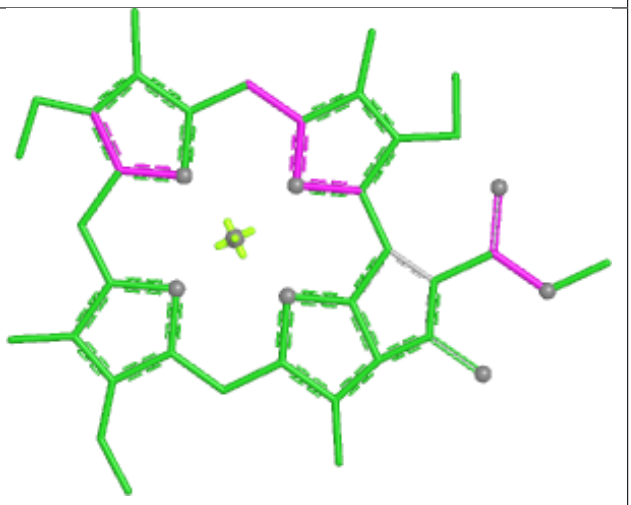


Rings

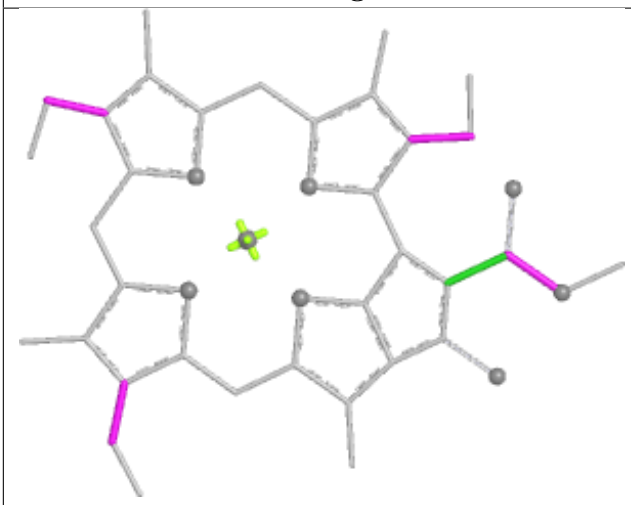
Ligand CLA J 101



Bond lengths



Bond angles

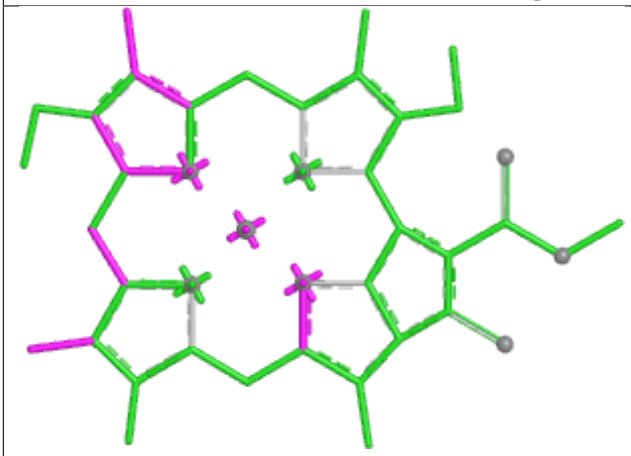


Torsions

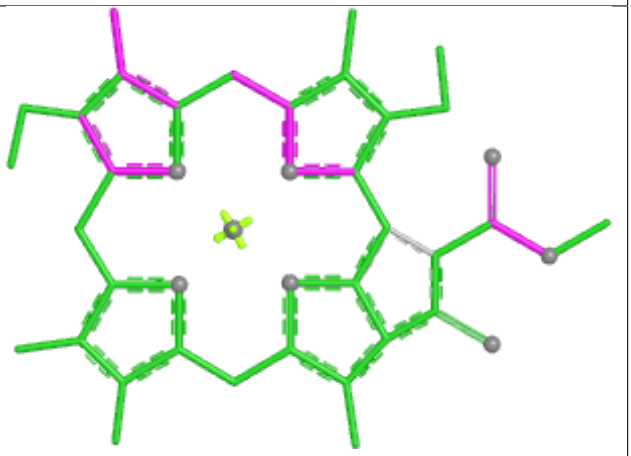


Rings

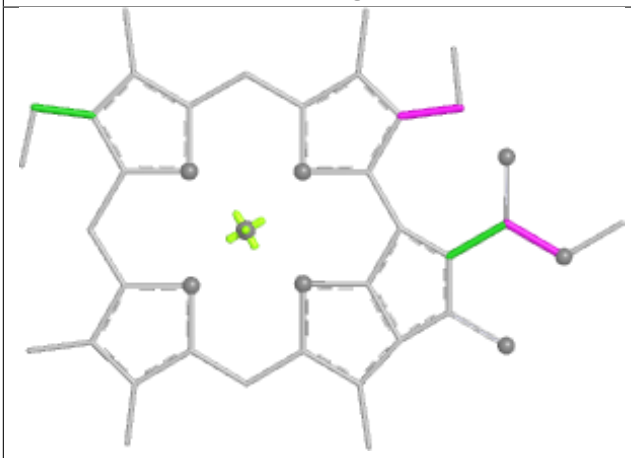
Ligand CLA 1 504



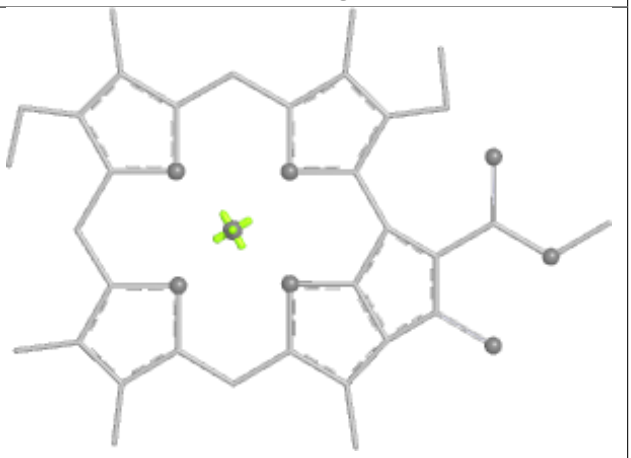
Bond lengths



Bond angles

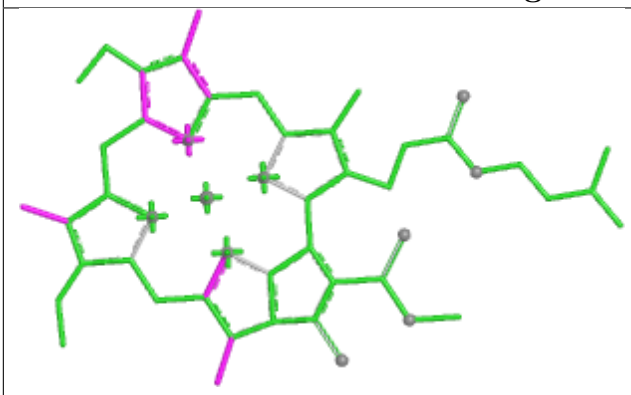


Torsions

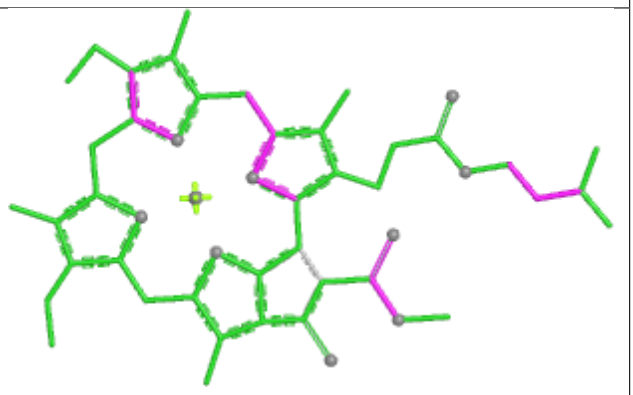


Rings

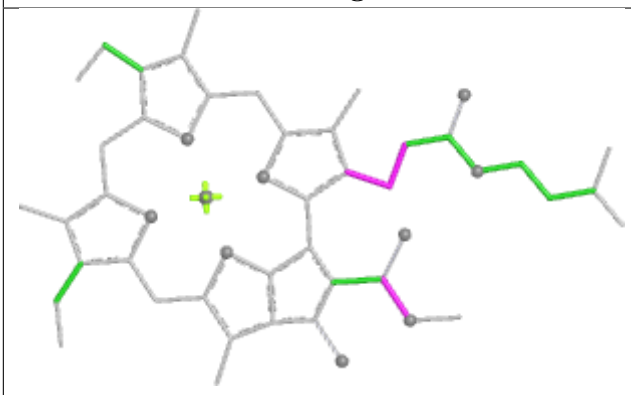
Ligand CLA B 821



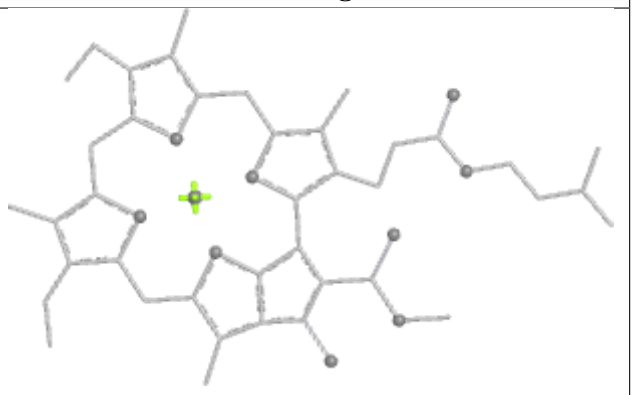
Bond lengths



Bond angles

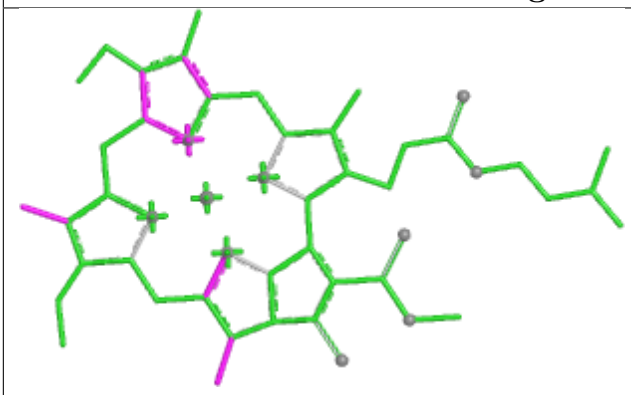


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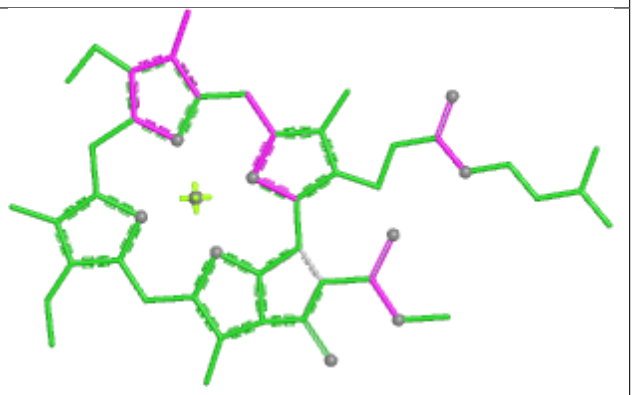


Rings

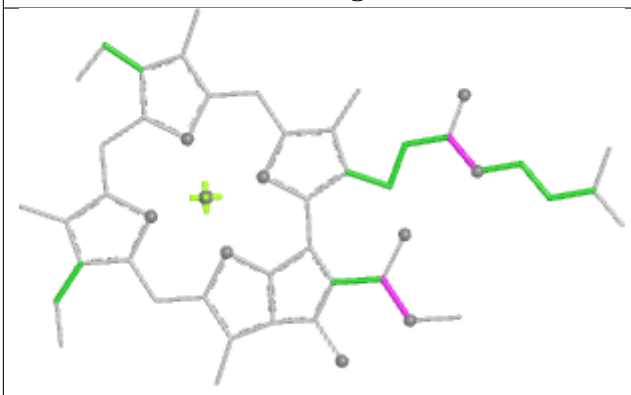
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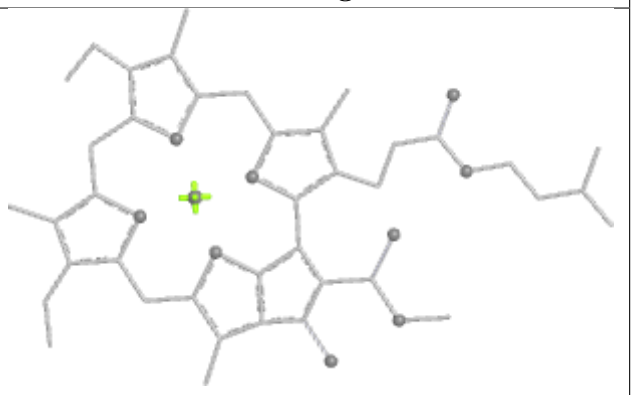
Bond lengths



Bond angles



Torsions

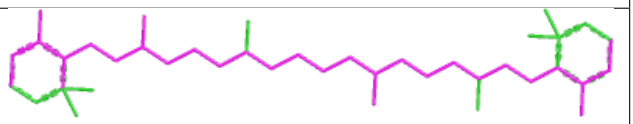


Rings

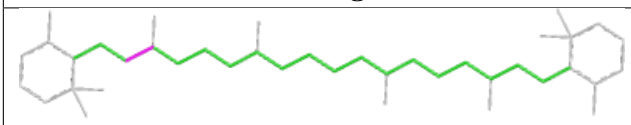
Ligand BCR A 847



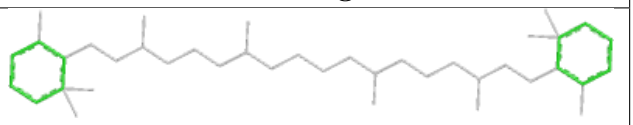
Bond lengths



Bond angles

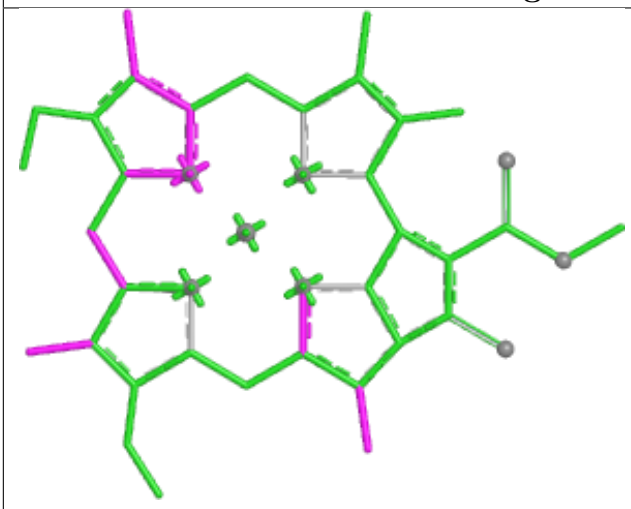


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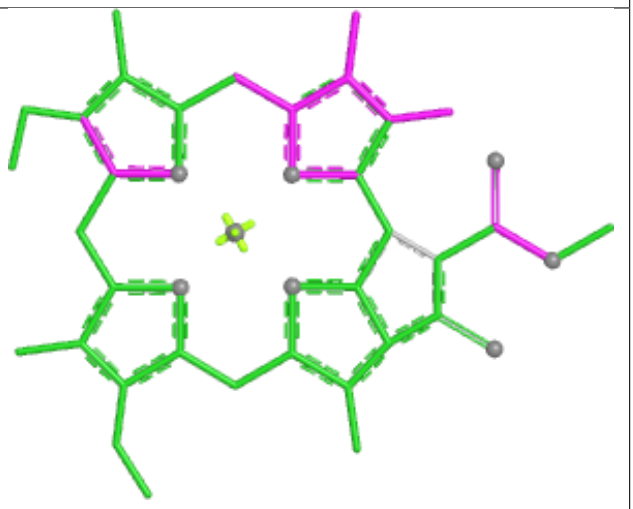


Rings

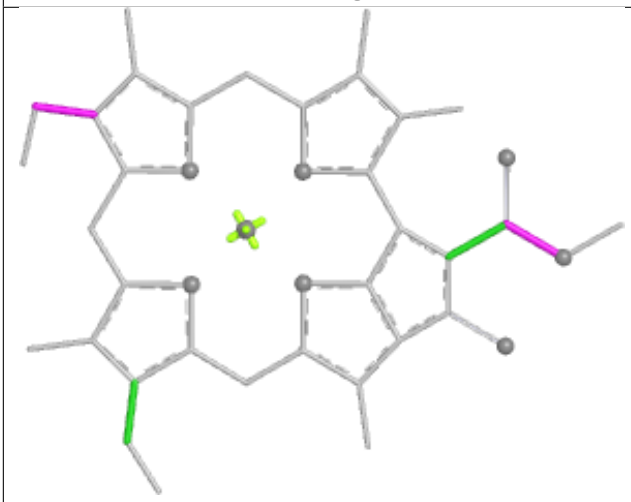
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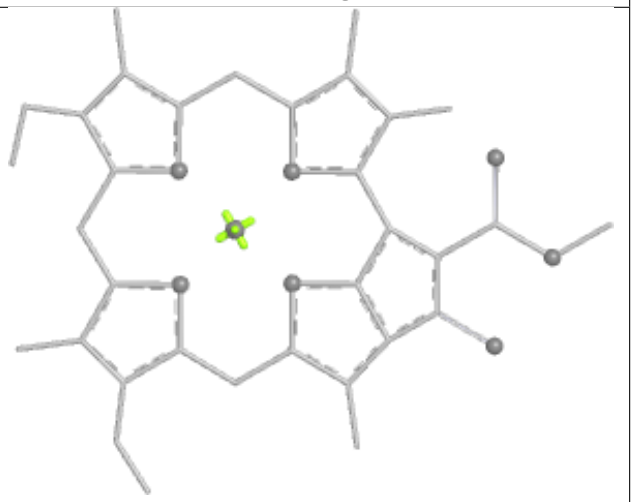
Bond lengths



Bond angles

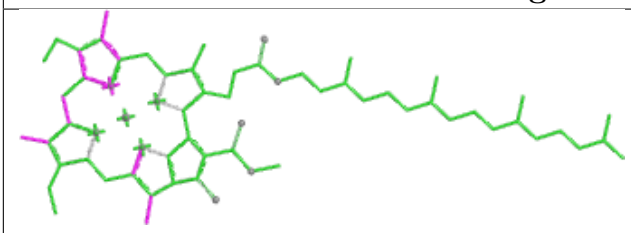


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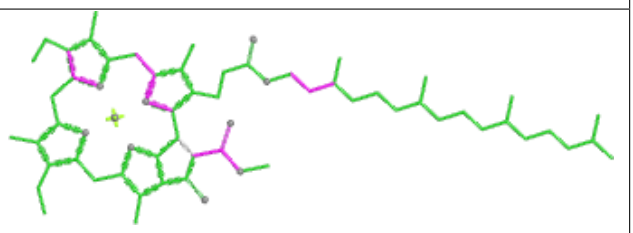


Rings

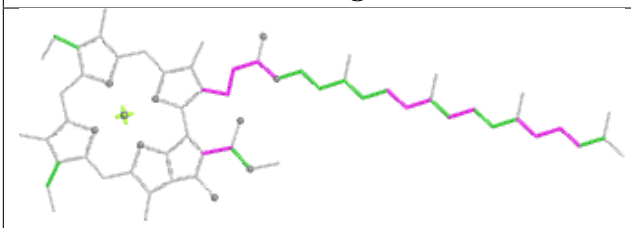
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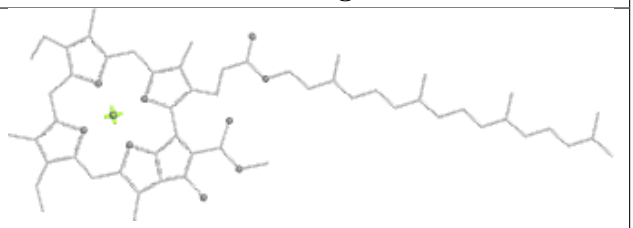
Bond lengths



Bond angles

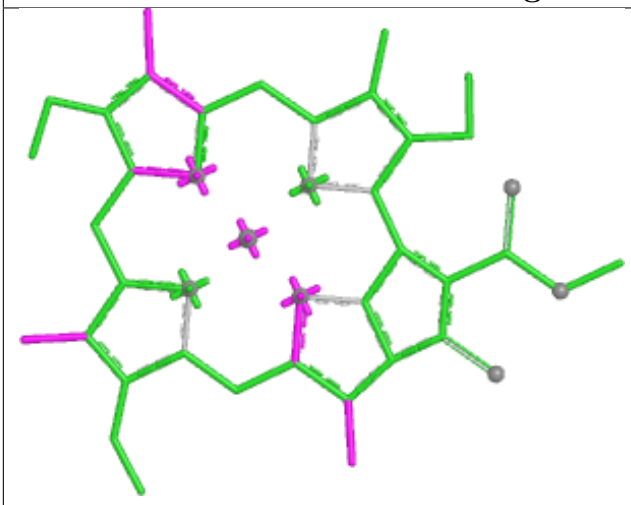


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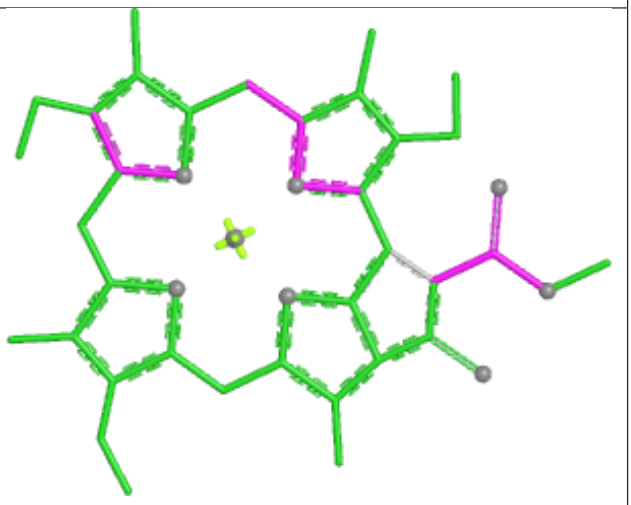


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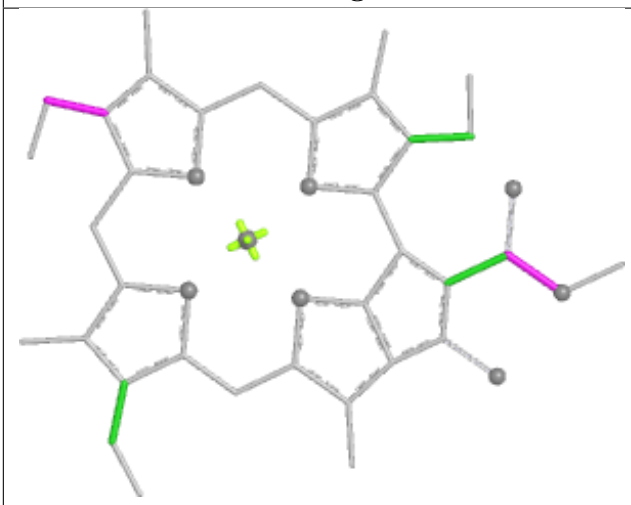
Ligand CLA A 839



Bond lengths



Bond angles

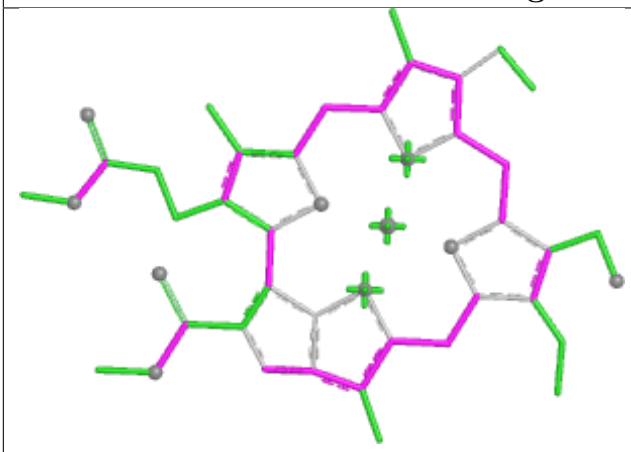


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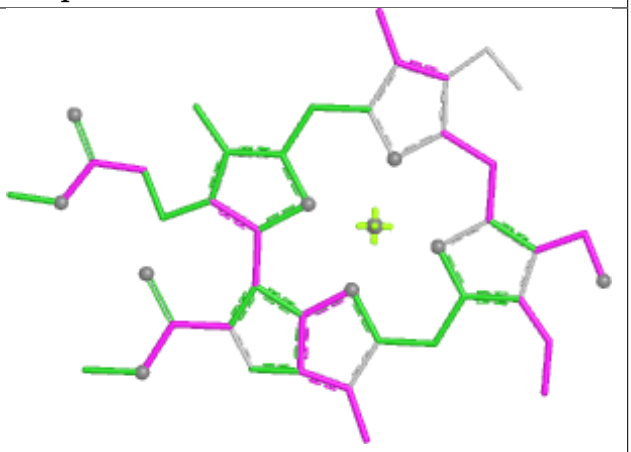


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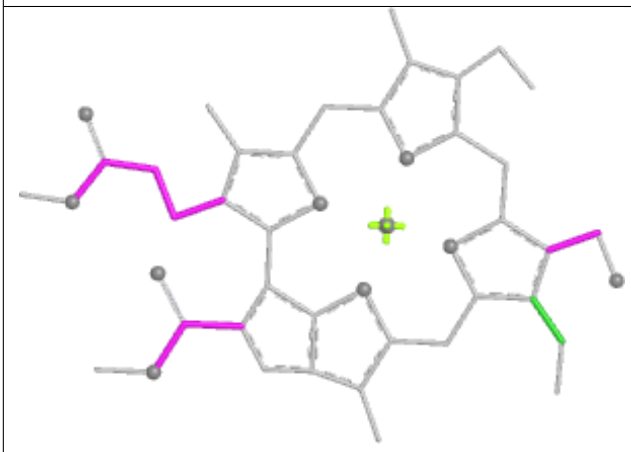
Ligand CHL q 313



Bond lengths



Bond angles

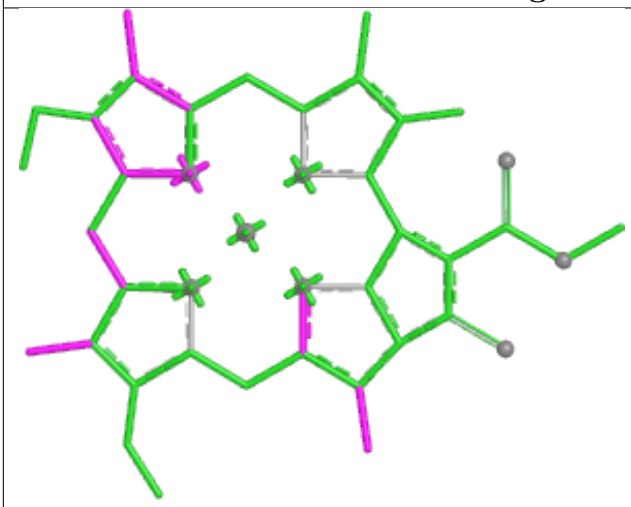


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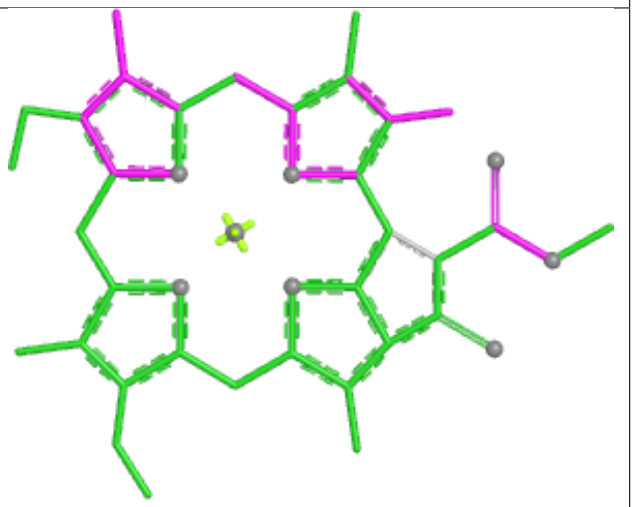


Rings

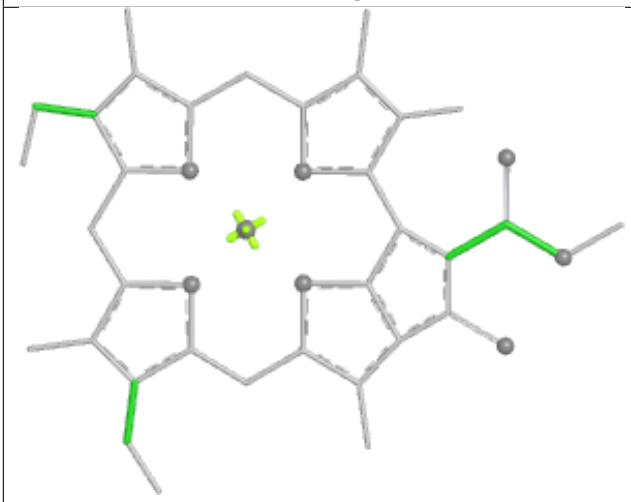
Ligand CLA e 825



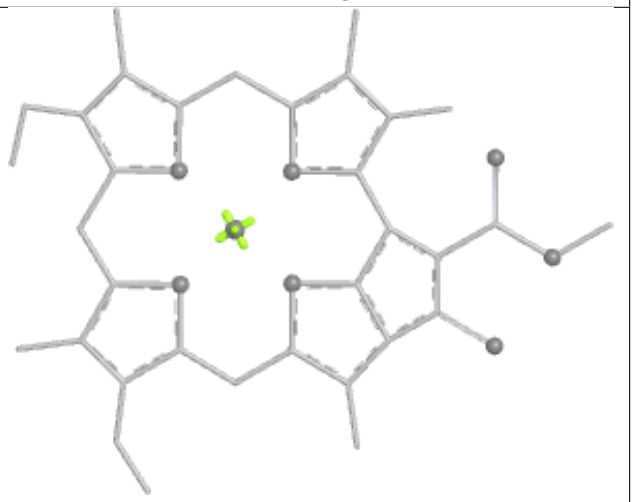
Bond lengths



Bond angles

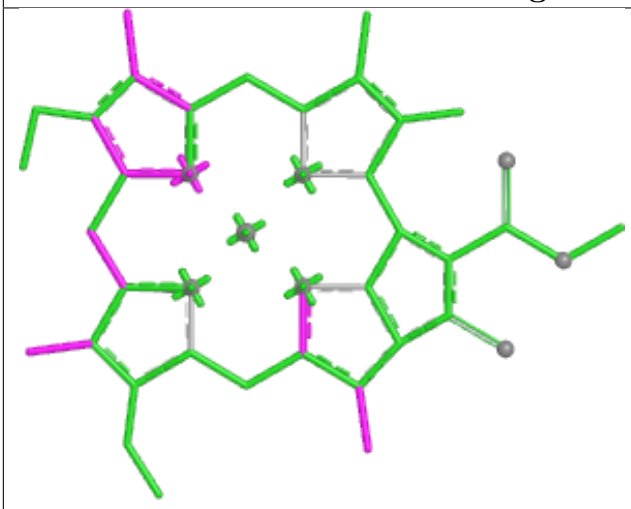


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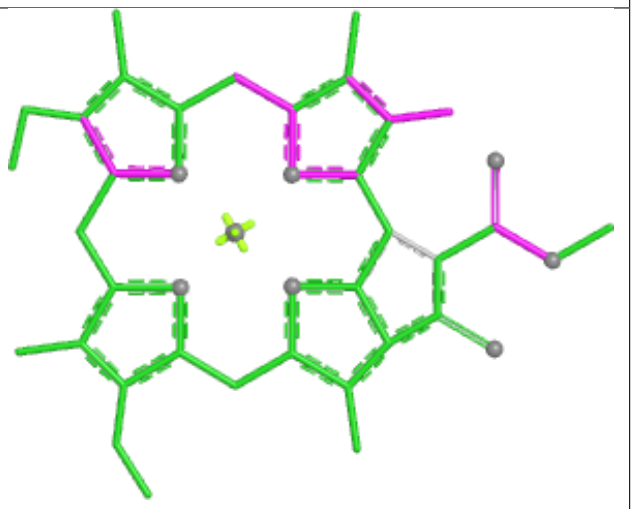


Rings

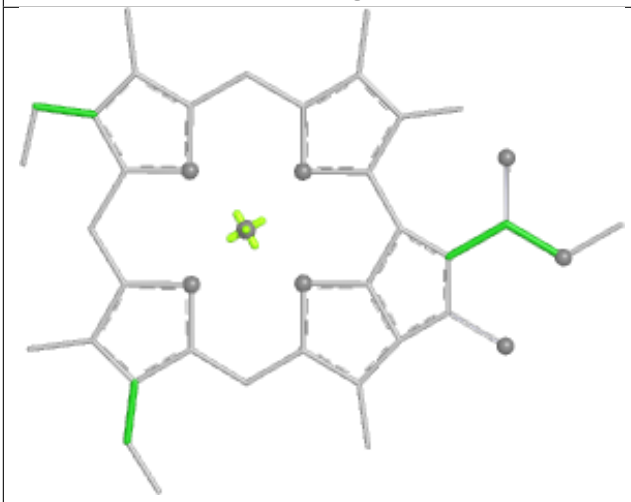
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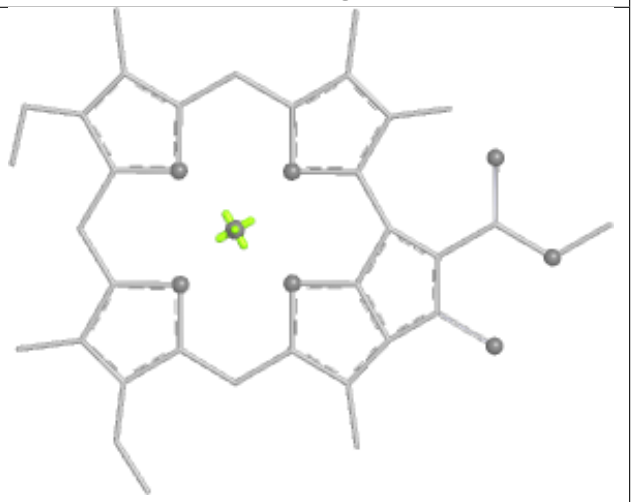
Bond lengths



Bond angles

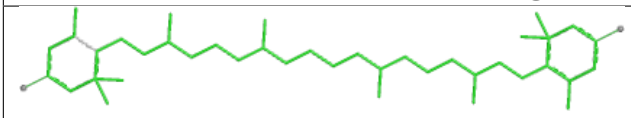


Torsions

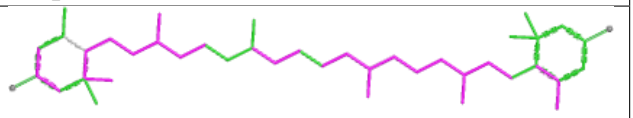


Rings

Ligand LUT p 501



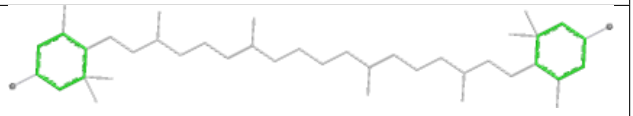
Bond lengths



Bond angles

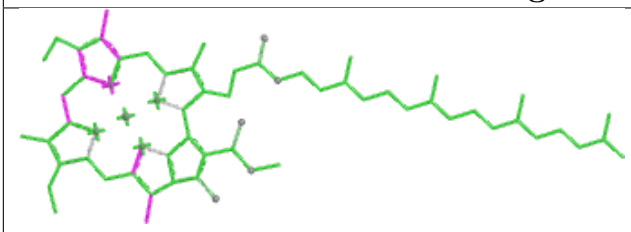


Torsions

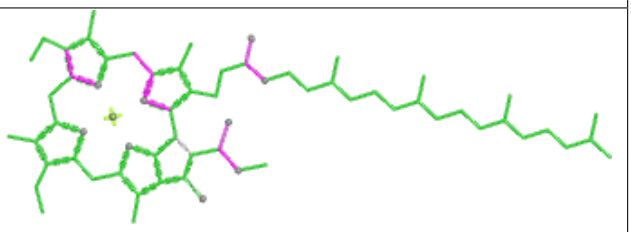


Rings

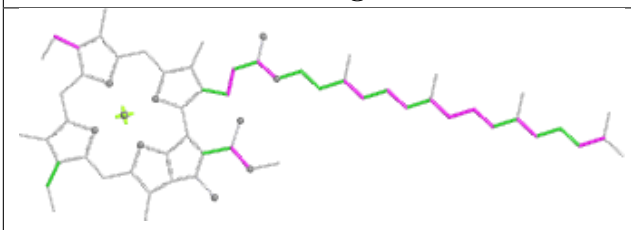
Ligand CLA 5 307



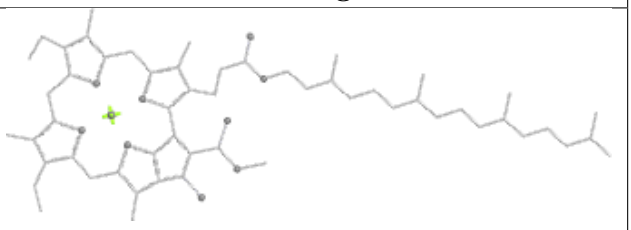
Bond lengths



Bond angles

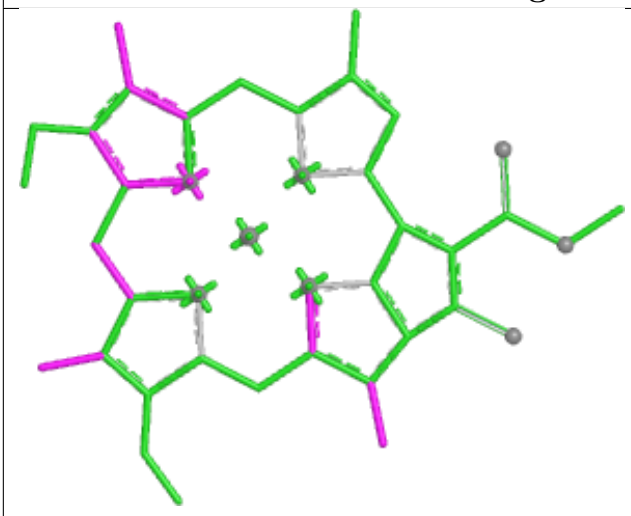


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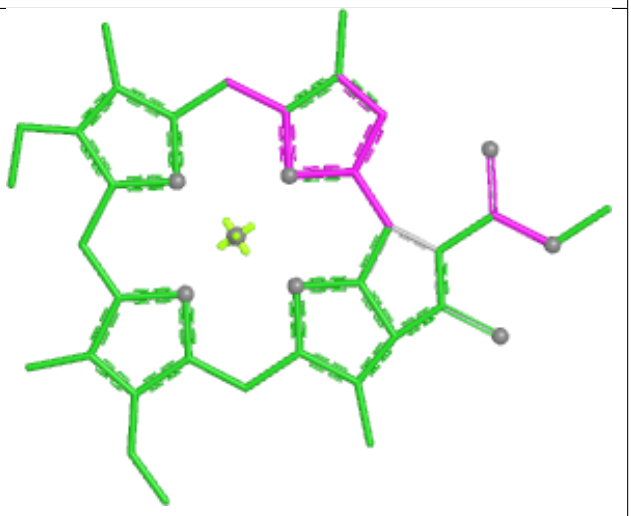


Rings

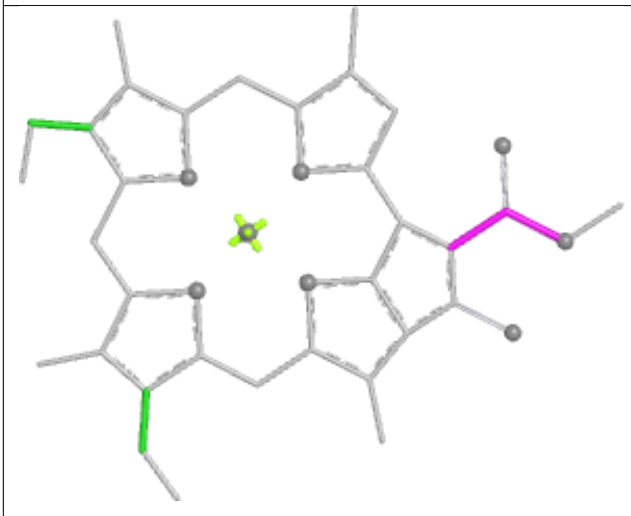
Ligand CLA e 802



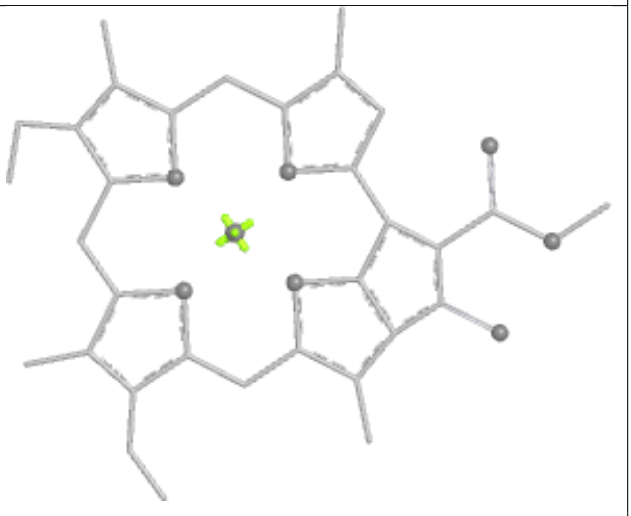
Bond lengths



Bond angles

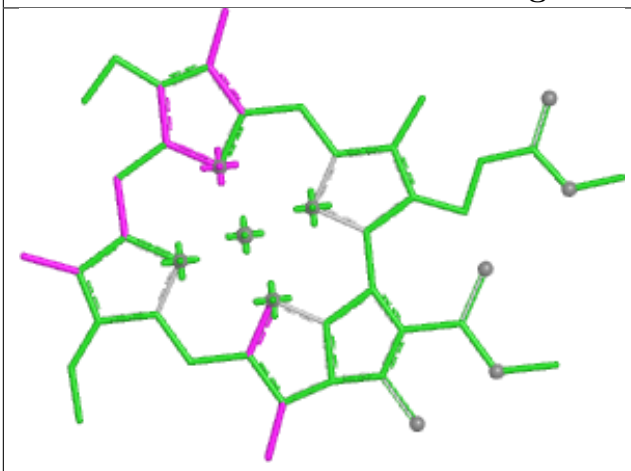


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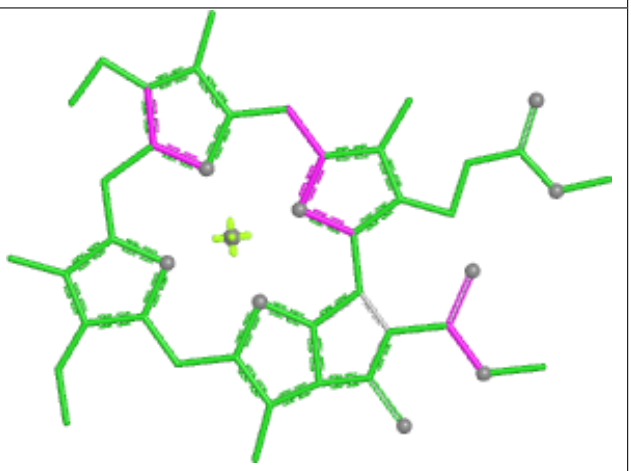


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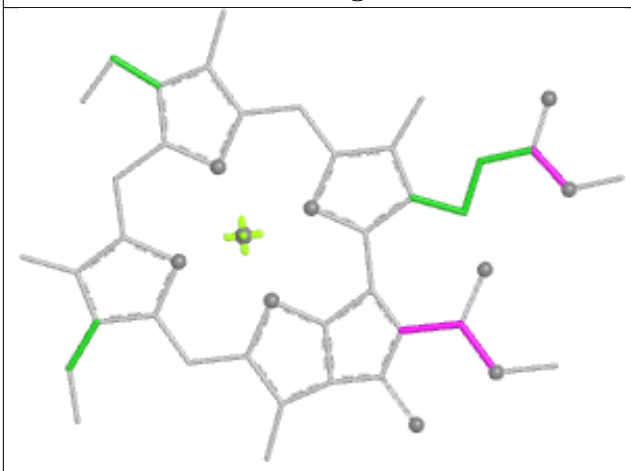
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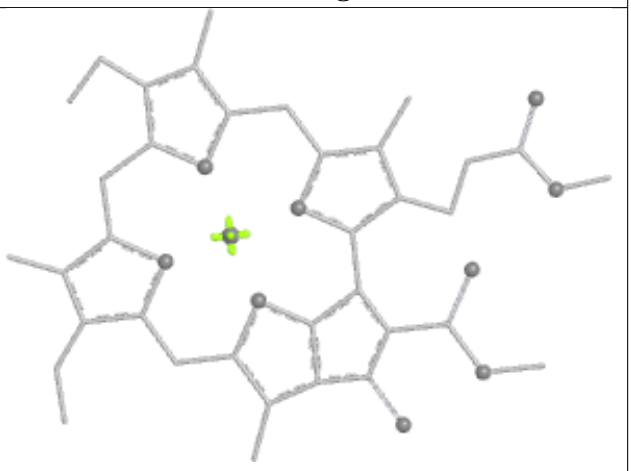
Bond lengths



Bond angles

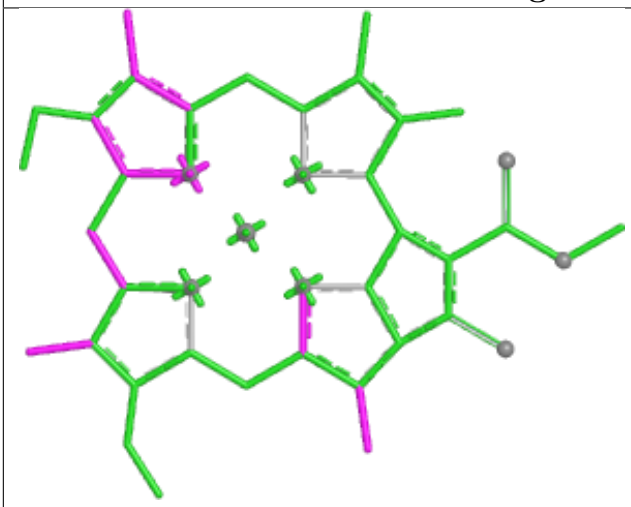


Torsions

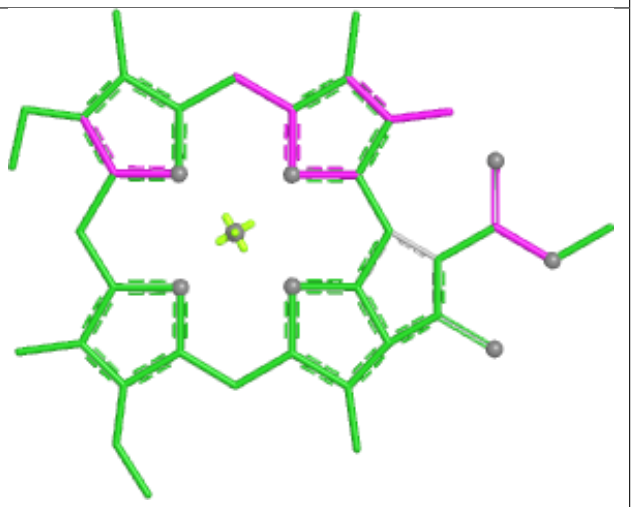


Rings

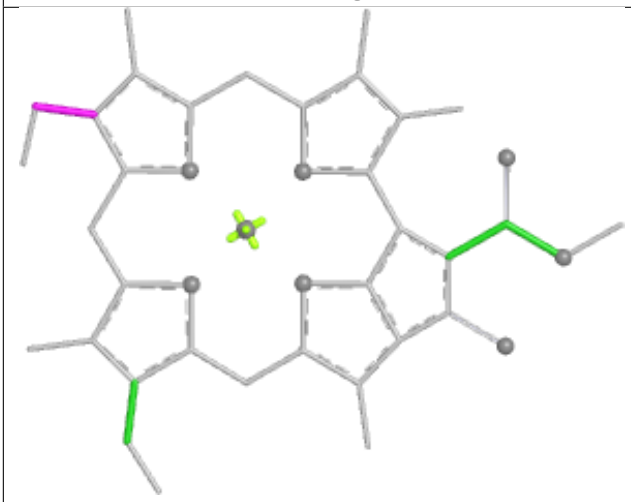
Ligand CLA e 822



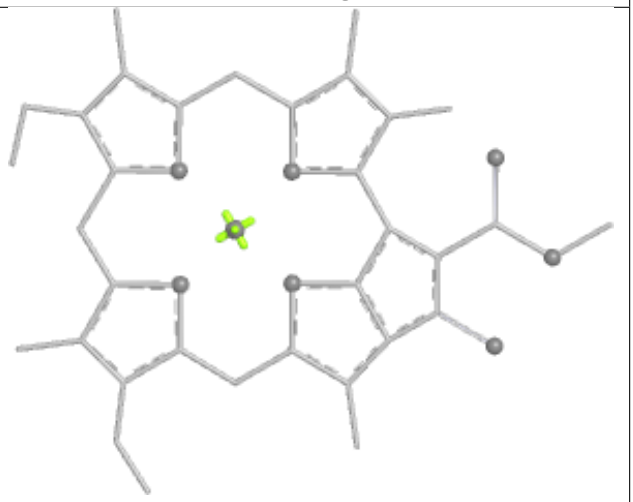
Bond lengths



Bond angles

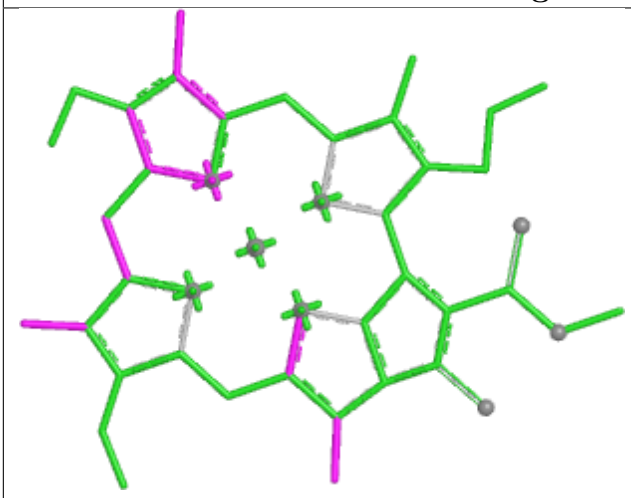


Torsions

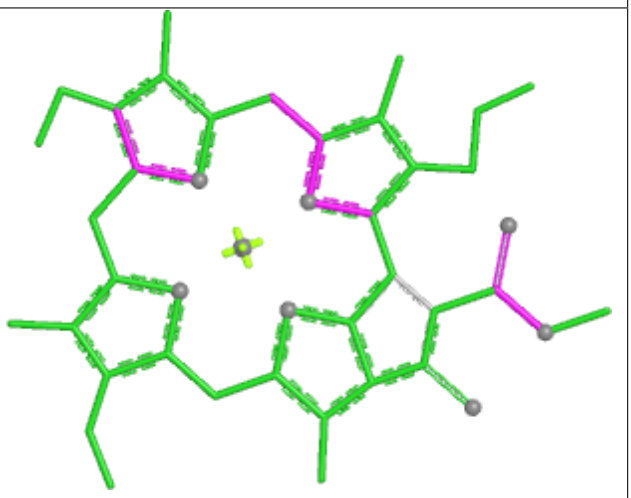


Rings

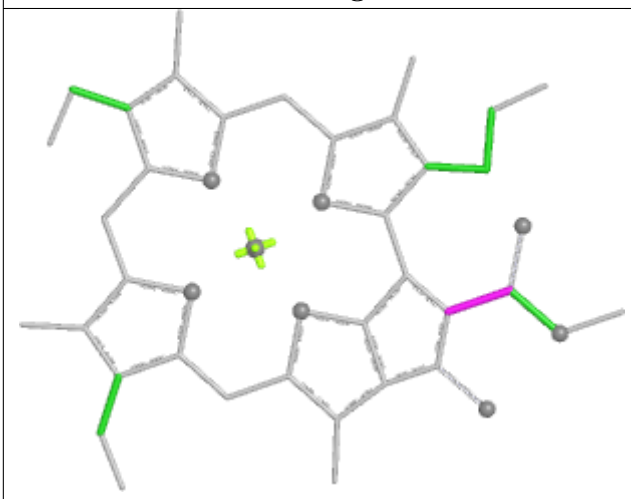
Ligand CLA f 814



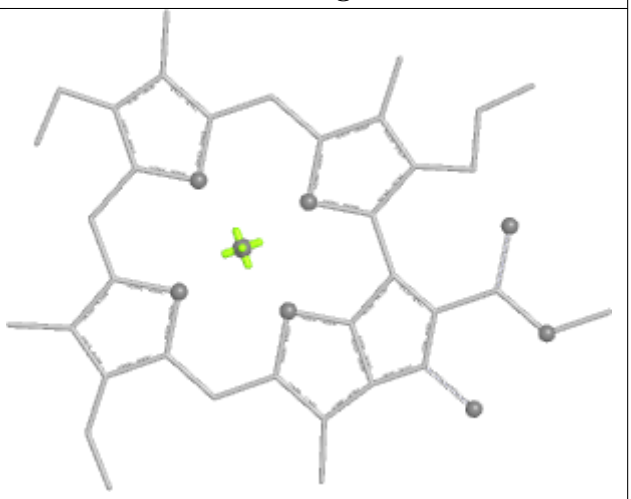
Bond lengths



Bond angles

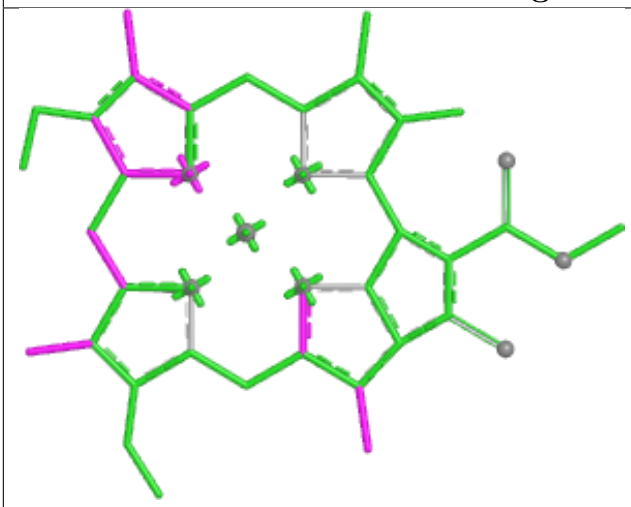


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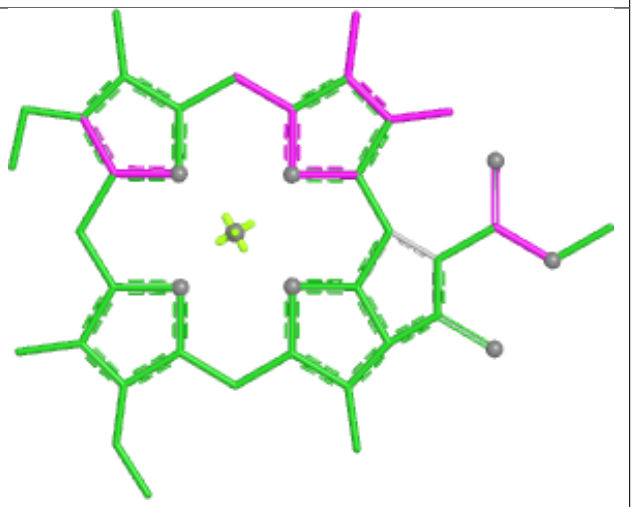


Rings

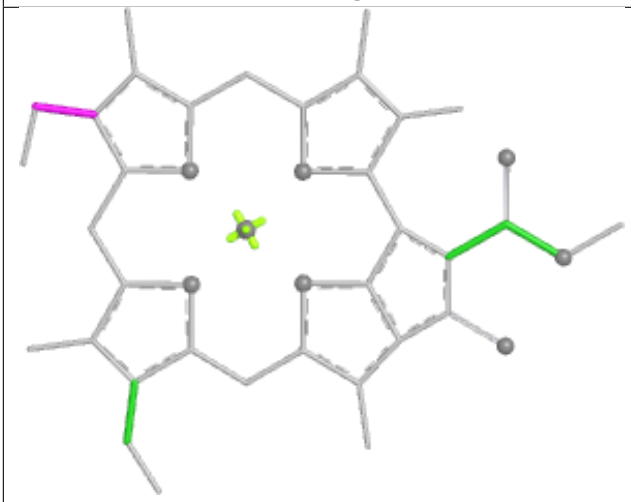
Ligand CLA f 842



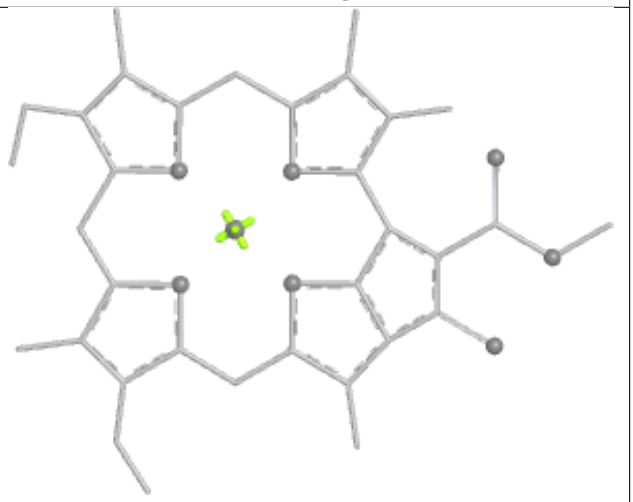
Bond lengths



Bond angles

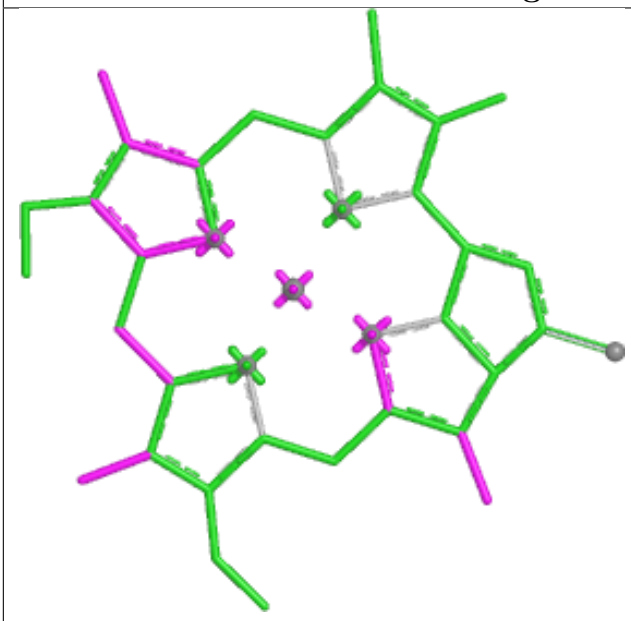


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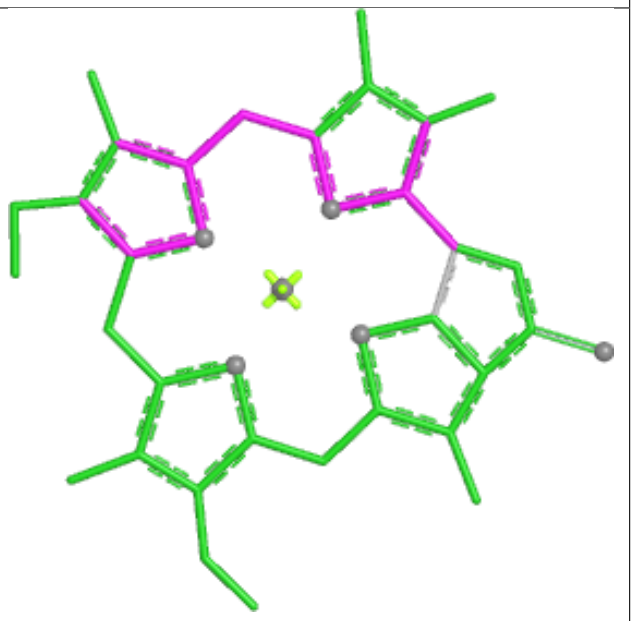


Rings

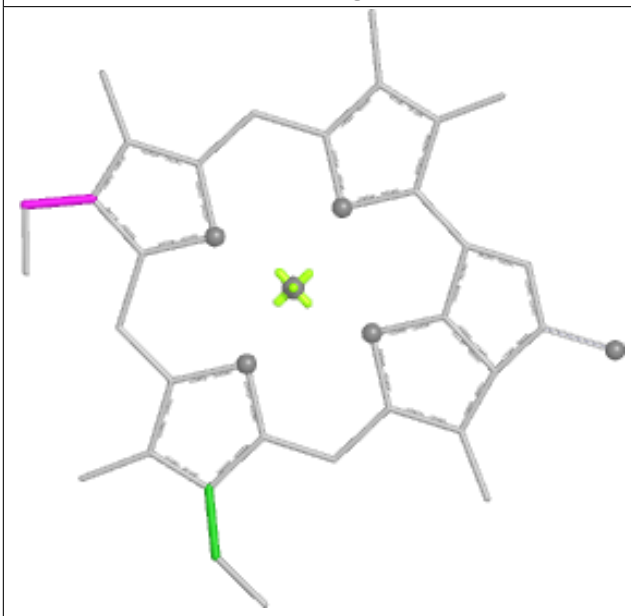
Ligand CLA K 201



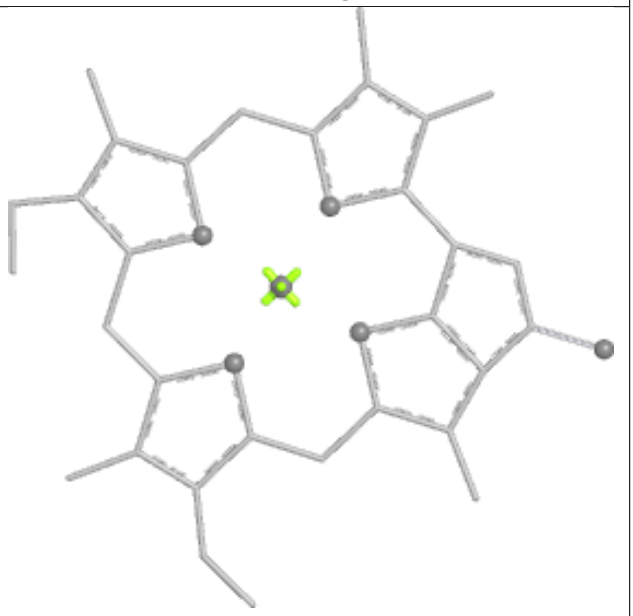
Bond lengths



Bond angles

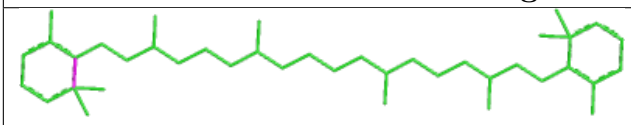


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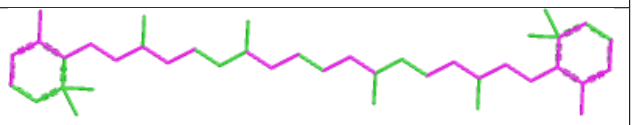


Rings

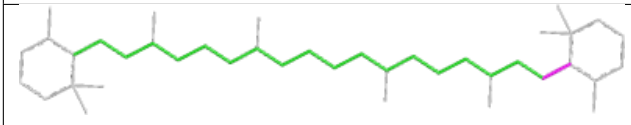
Ligand BCR m 103



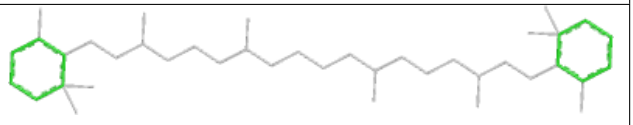
Bond lengths



Bond angles

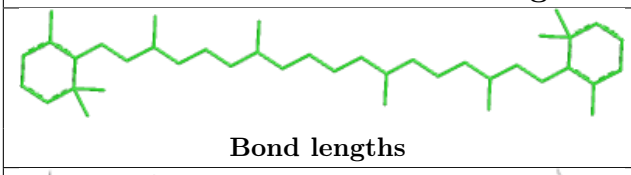


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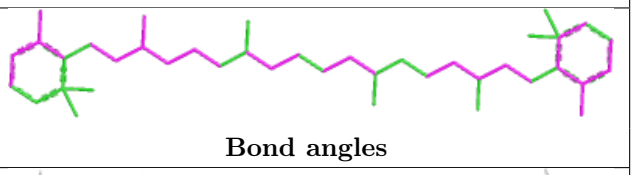


Rings

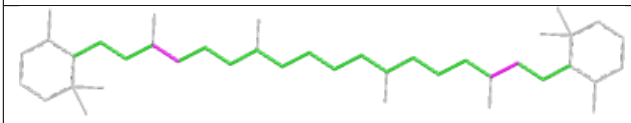
Ligand BCR f 846



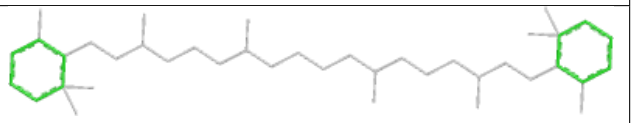
Bond lengths



Bond angles



Torsions

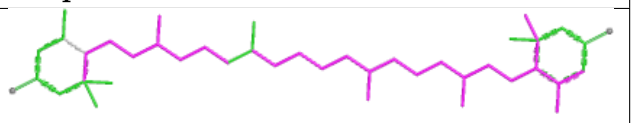


Rings

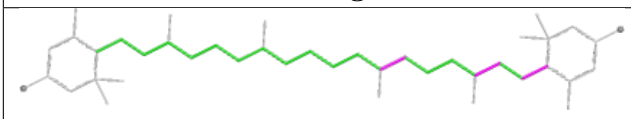
Ligand LUT q 302



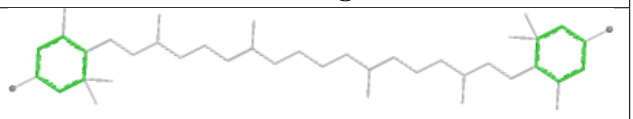
Bond lengths



Bond angles

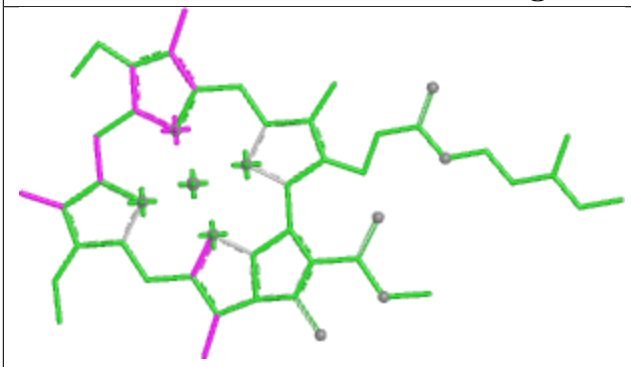


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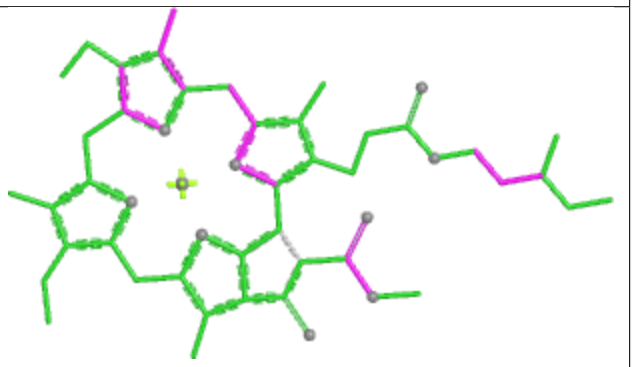


Rings

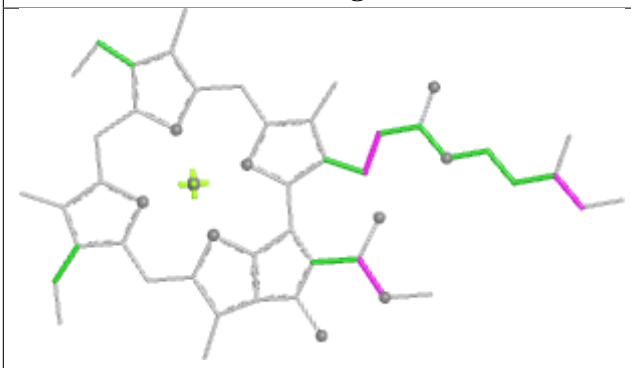
Ligand CLA e 836



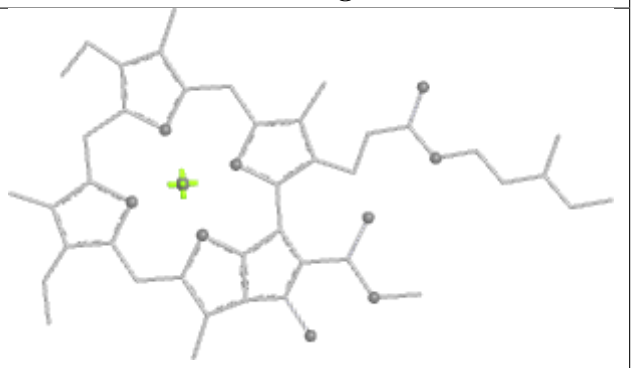
Bond lengths



Bond angles

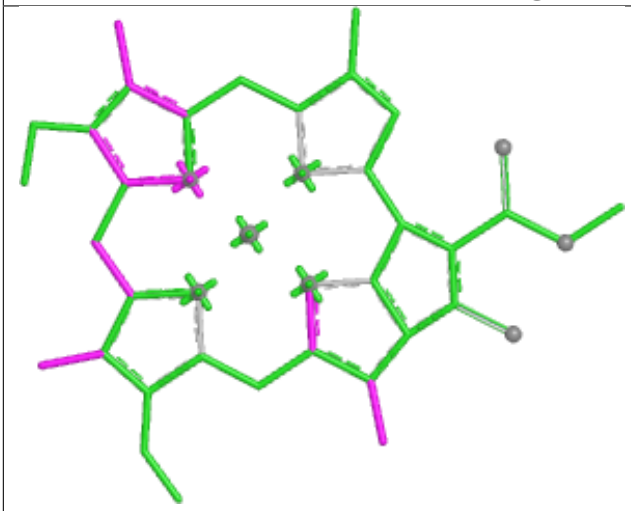


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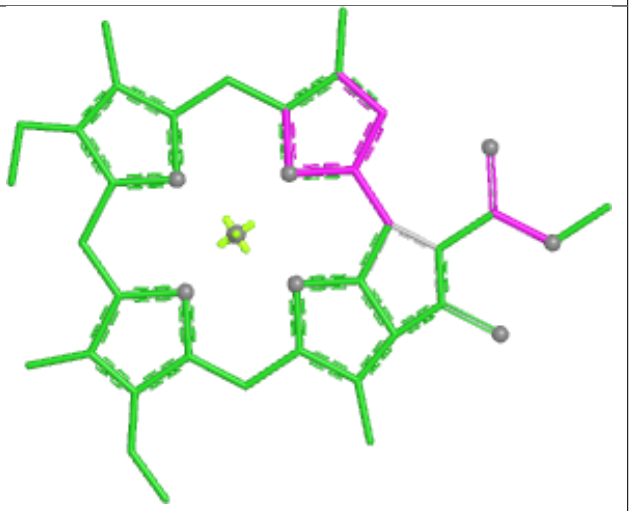


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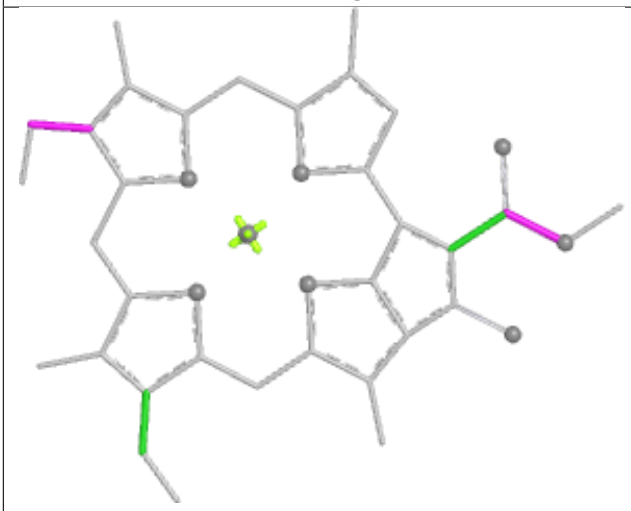
Ligand CLA 3 307



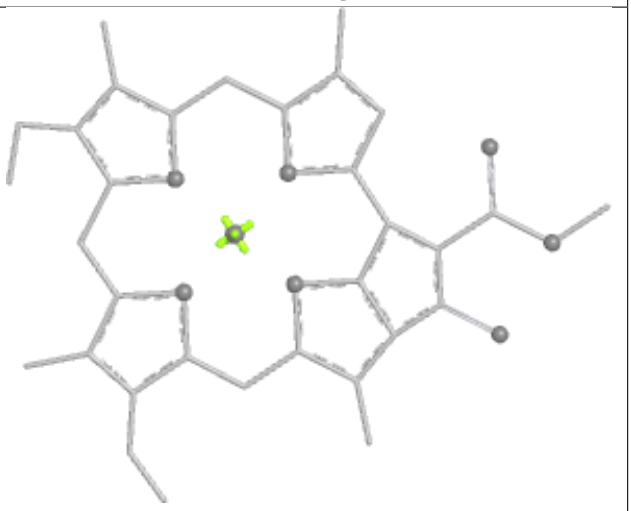
Bond lengths



Bond angles



Torsions

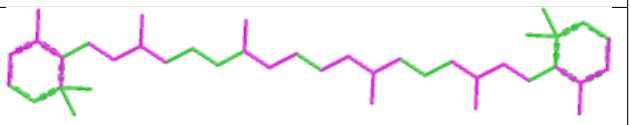


Rings

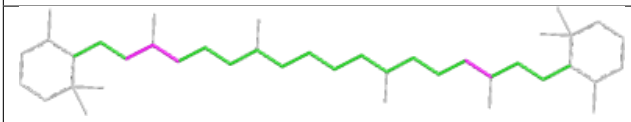
Ligand BCR B 846



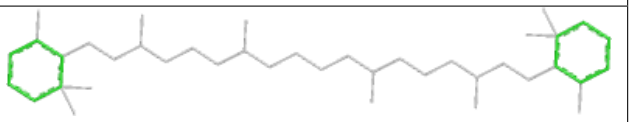
Bond lengths



Bond angles

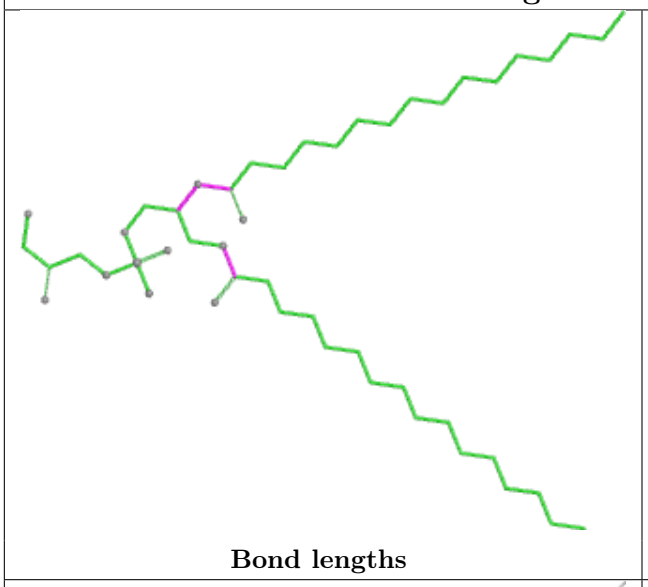


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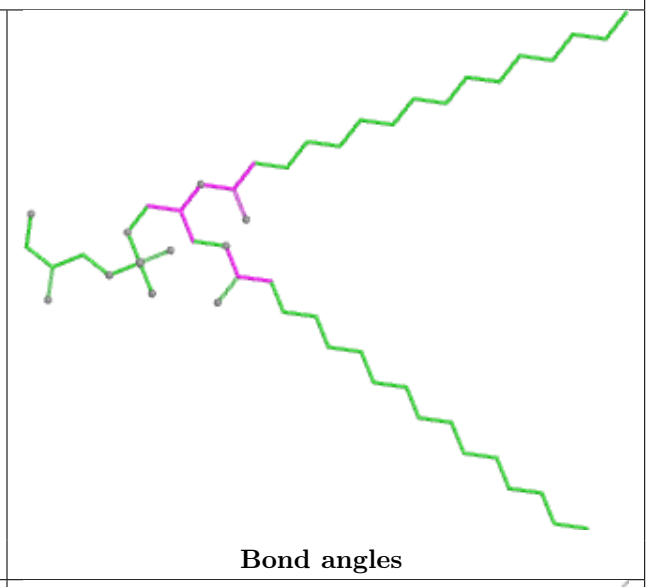


Rings

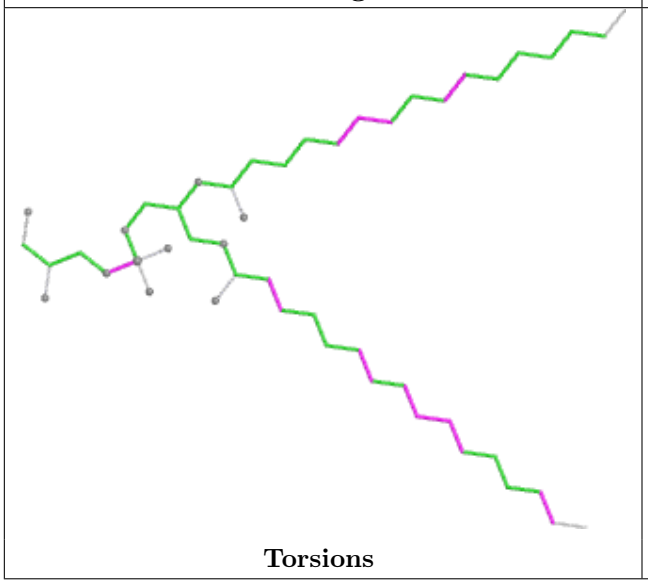
Ligand LHG A 843



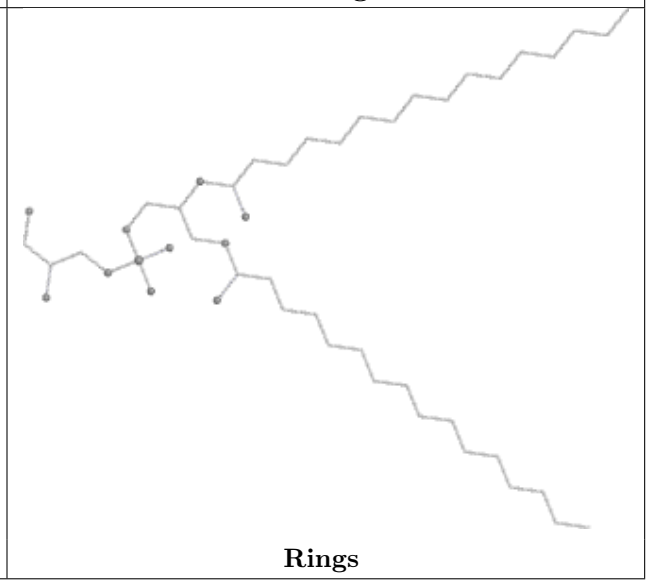
Bond lengths



Bond angles

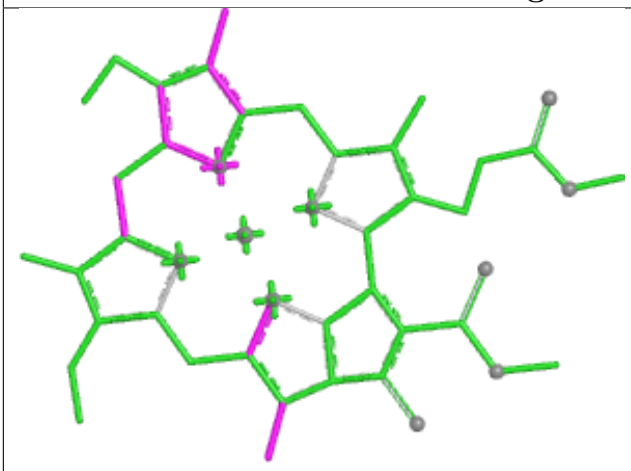


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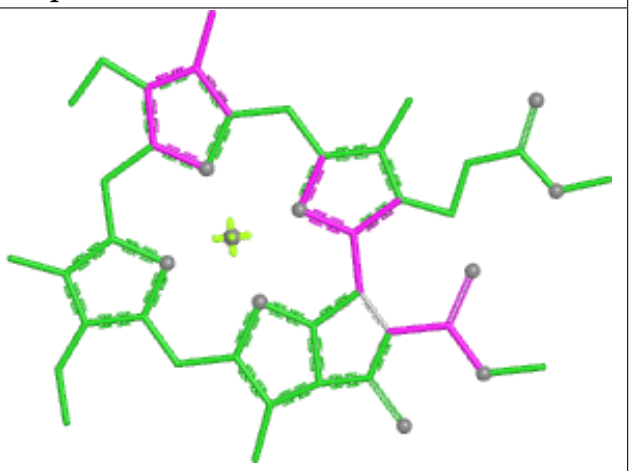


Rings

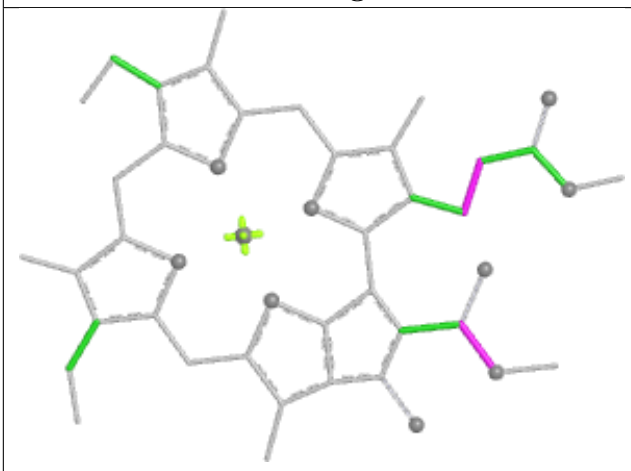
Ligand CLA p 505



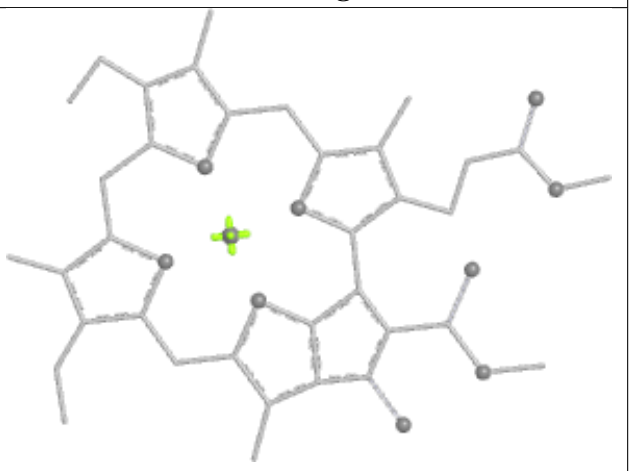
Bond lengths



Bond angles

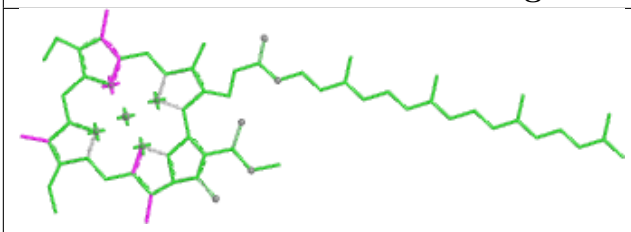


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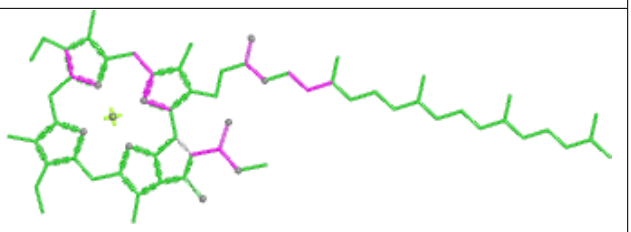


Rings

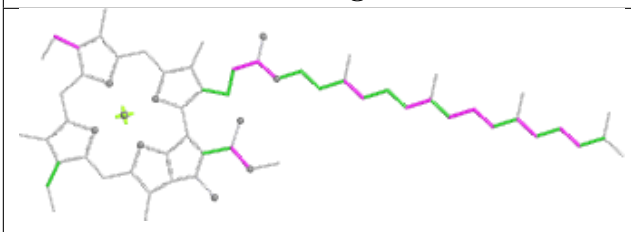
Ligand CLA B 803



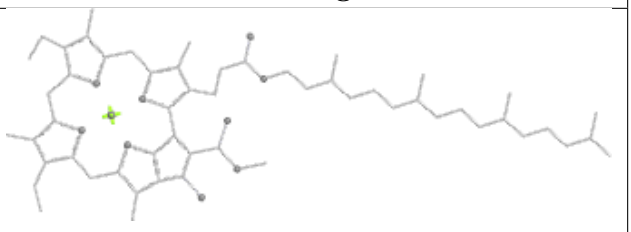
Bond lengths



Bond angles

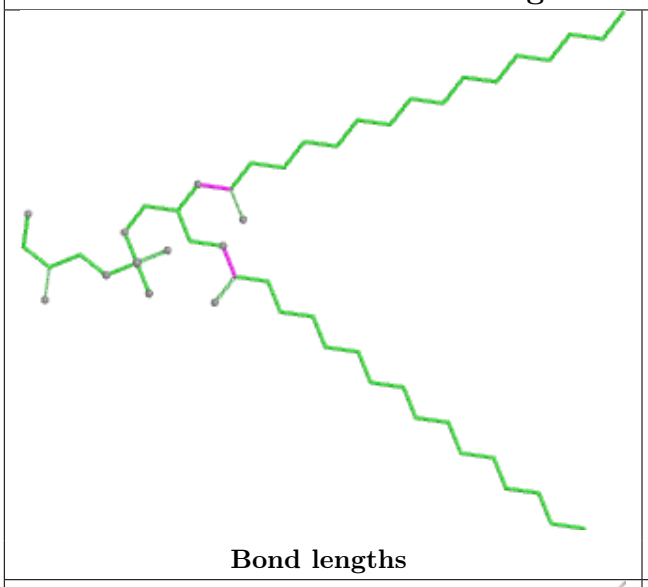


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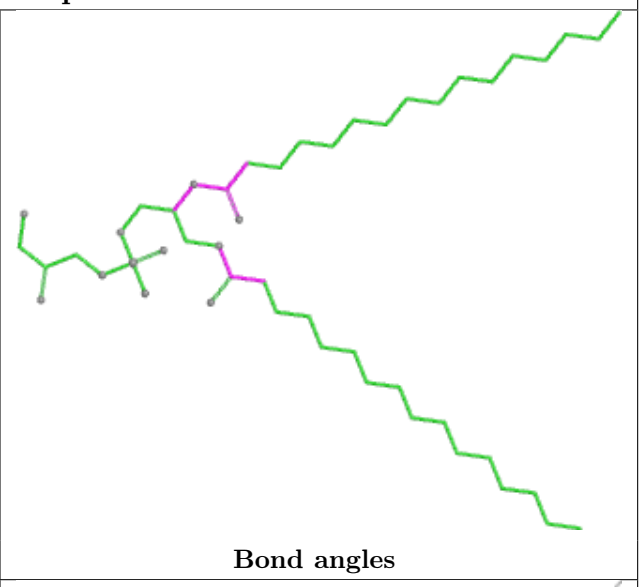


Rings

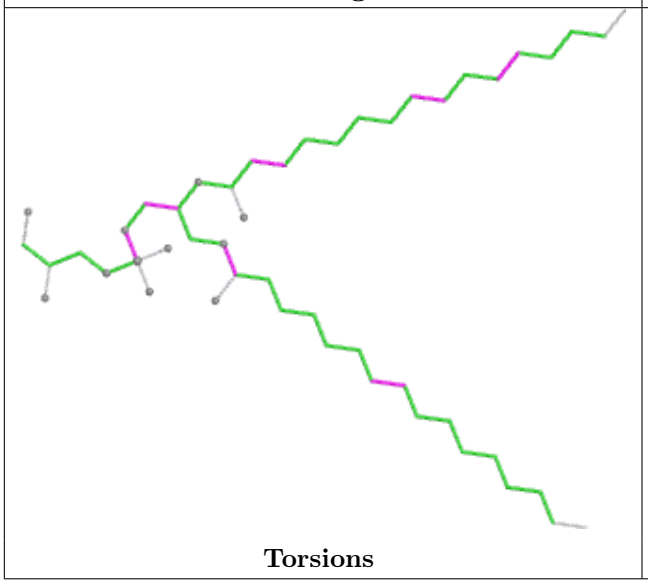
Ligand LHG p 516



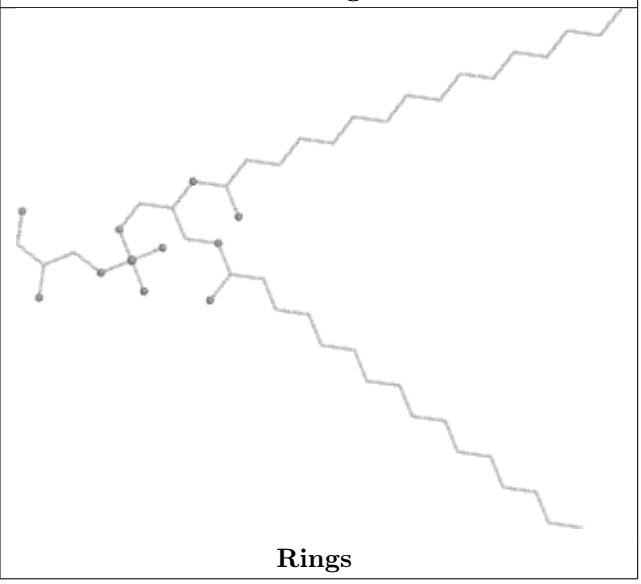
Bond lengths



Bond angles



Torsions



Rings

Ligand BCR J 102



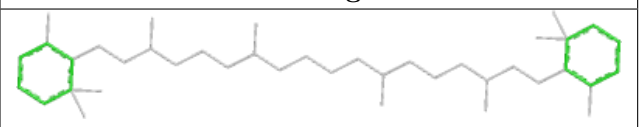
Bond lengths



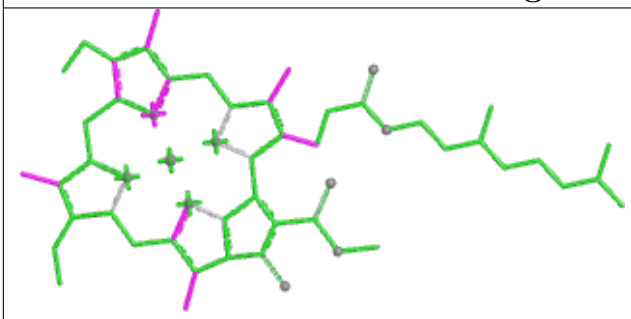
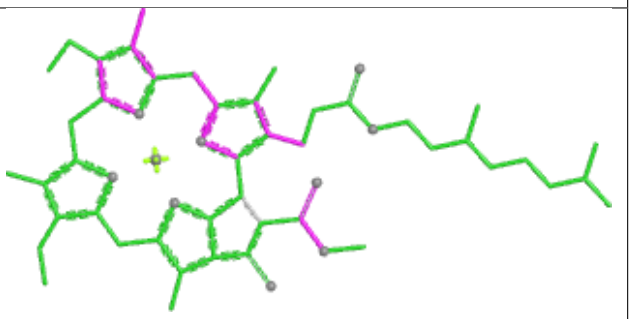
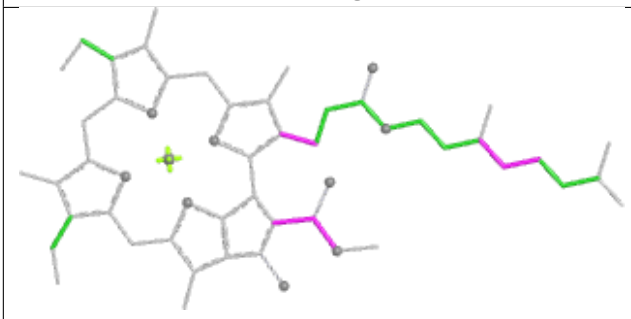
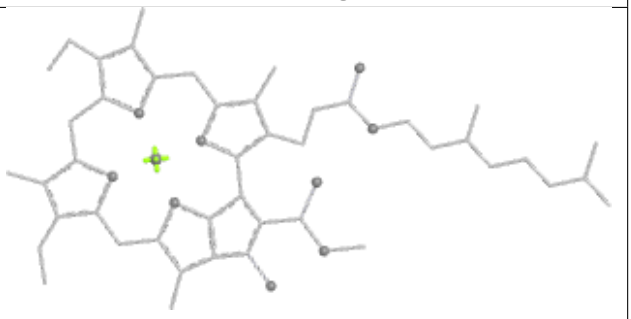
Bond angles

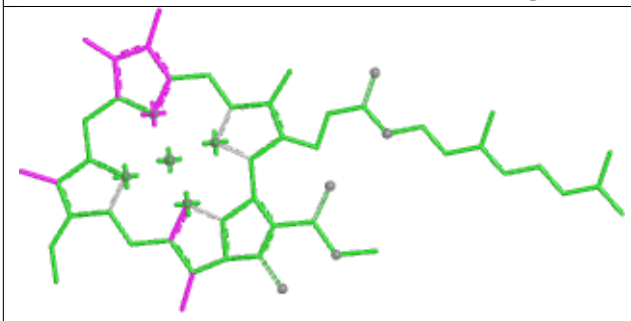
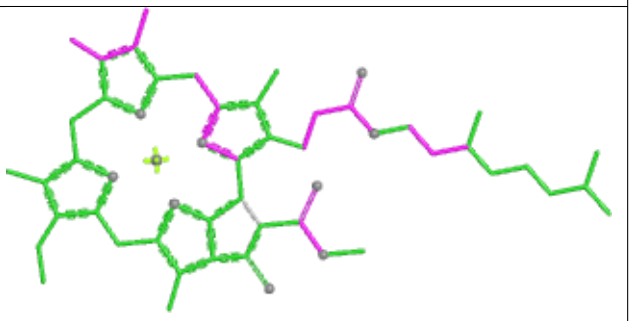
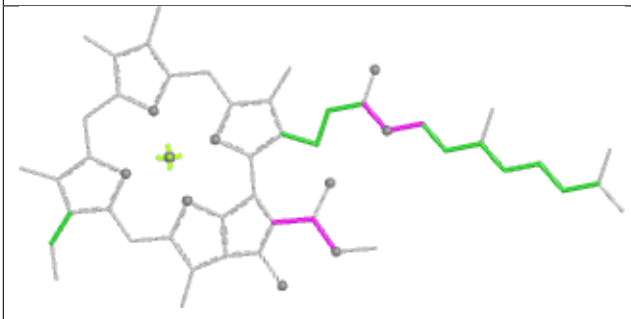
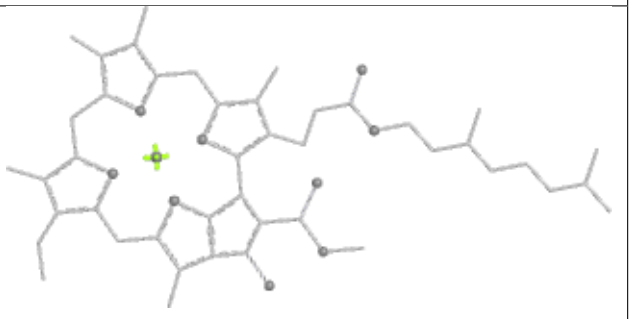


Torsions

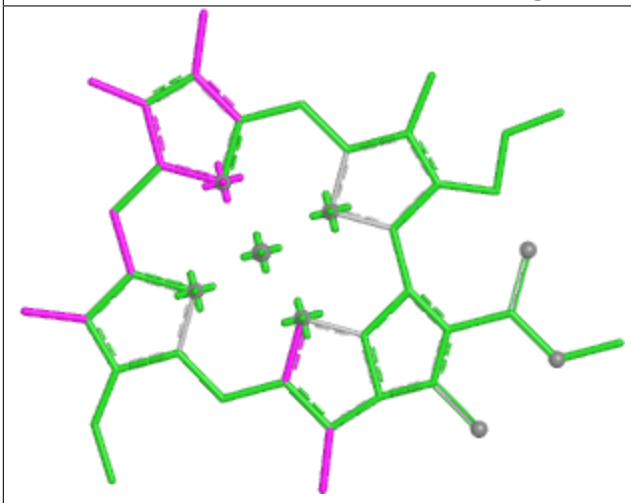


Rings

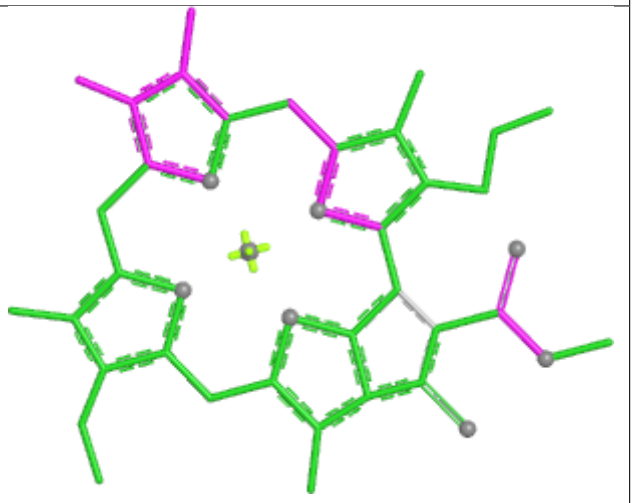
Ligand CLA B 811	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

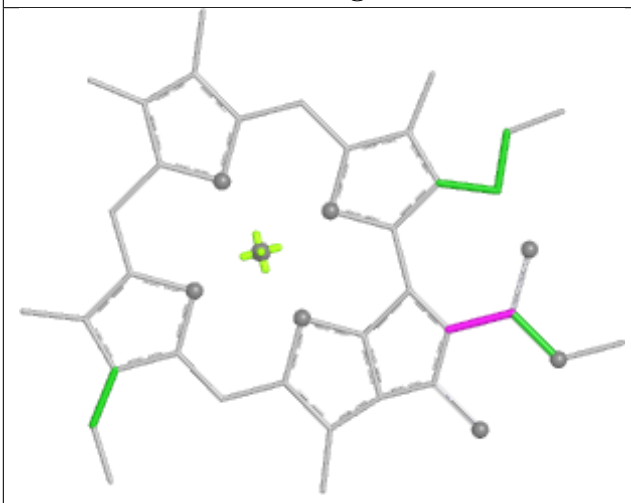
Ligand CLA e 823



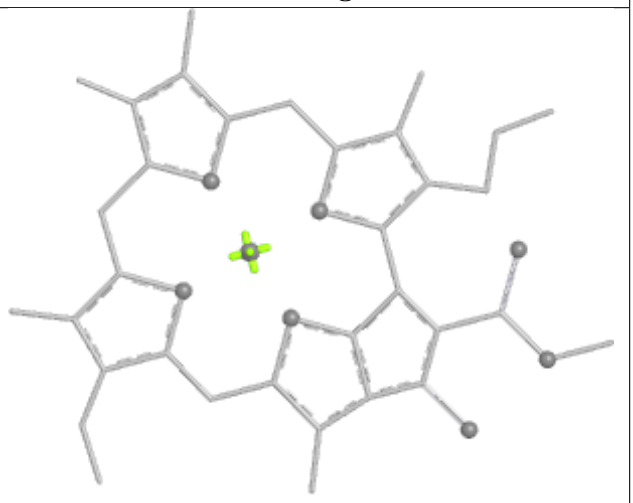
Bond lengths



Bond angles

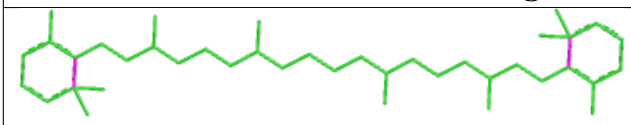


Torsions

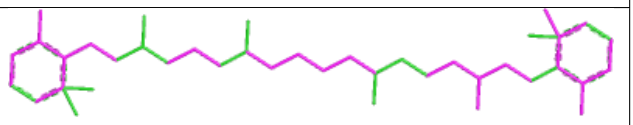


Rings

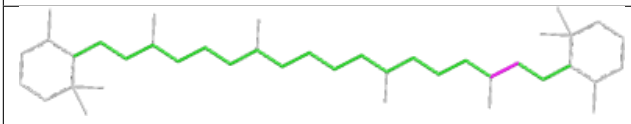
Ligand BCR B 849



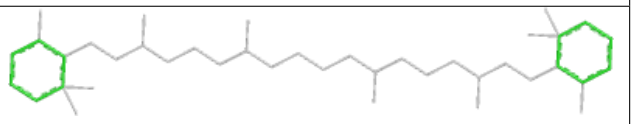
Bond lengths



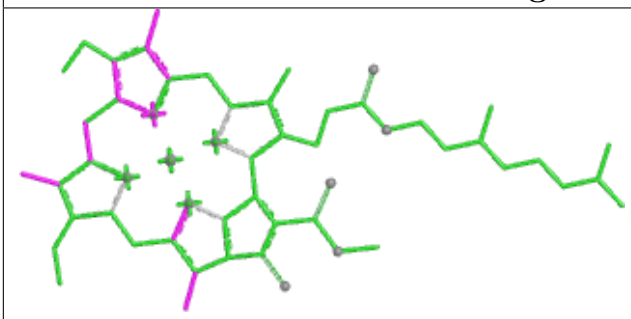
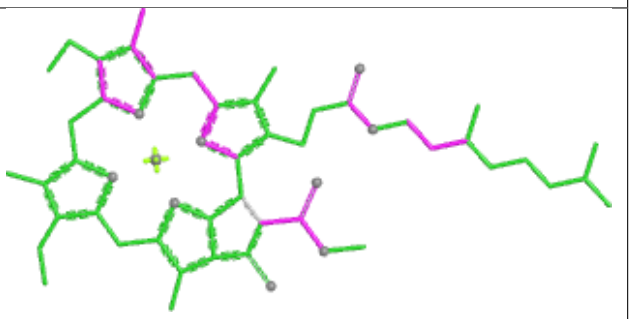
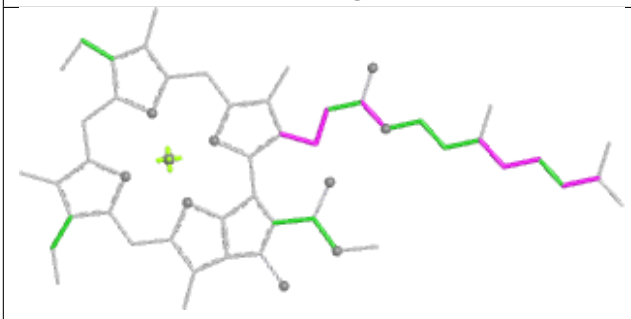
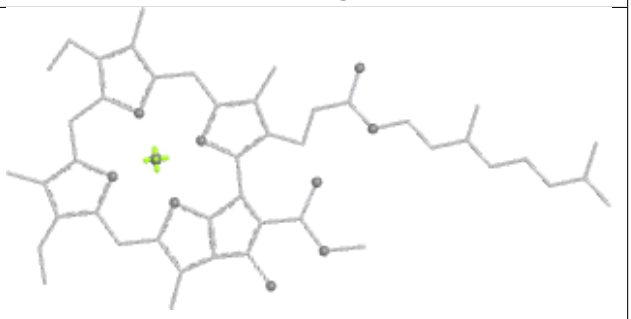
Bond angles

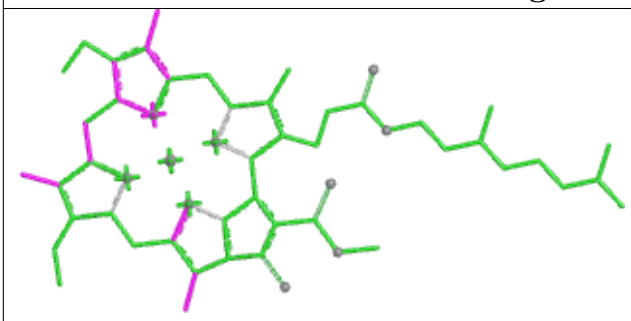
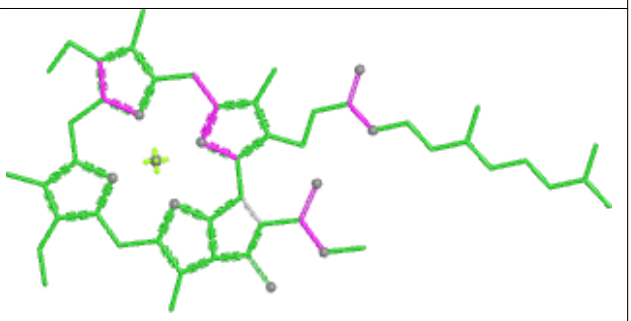
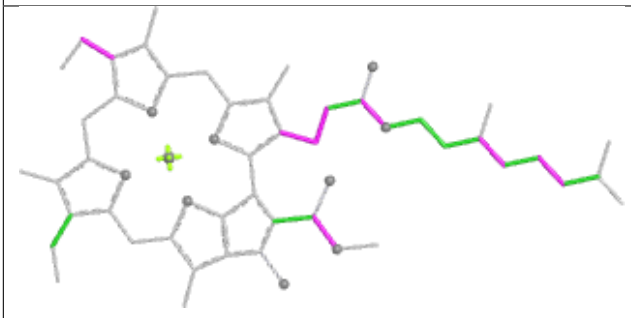
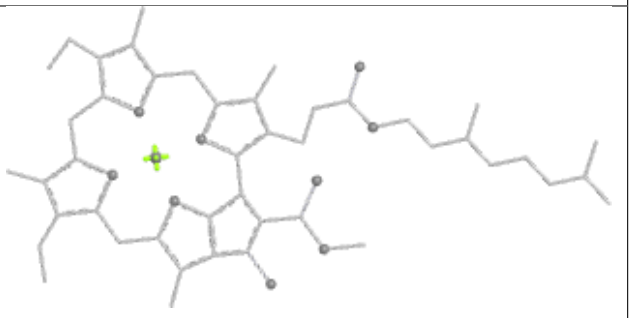


Torsions

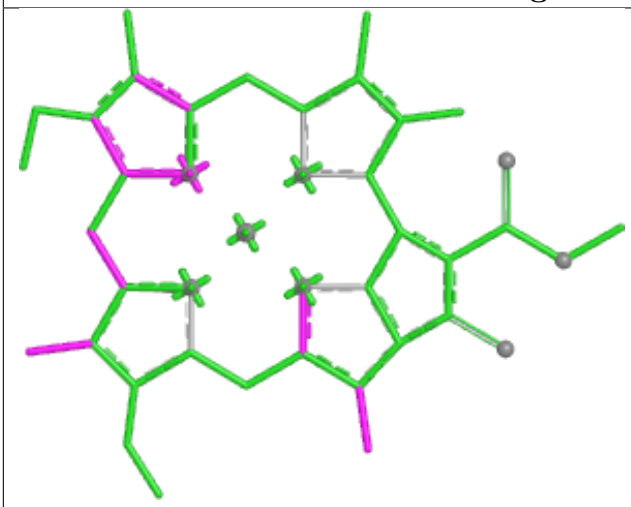


Rings

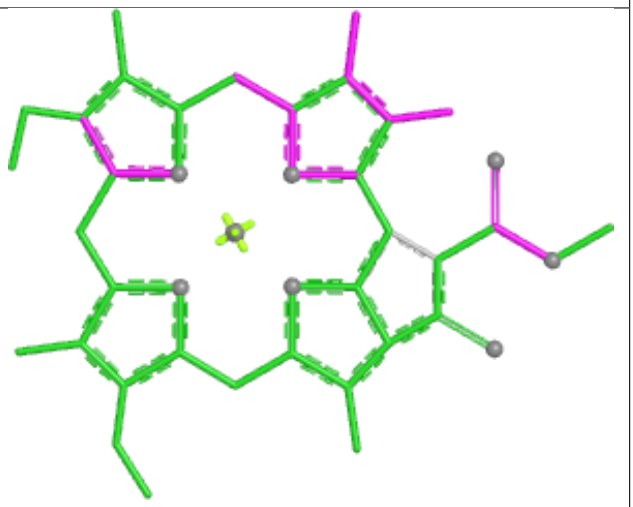
Ligand CLA e 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA e 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

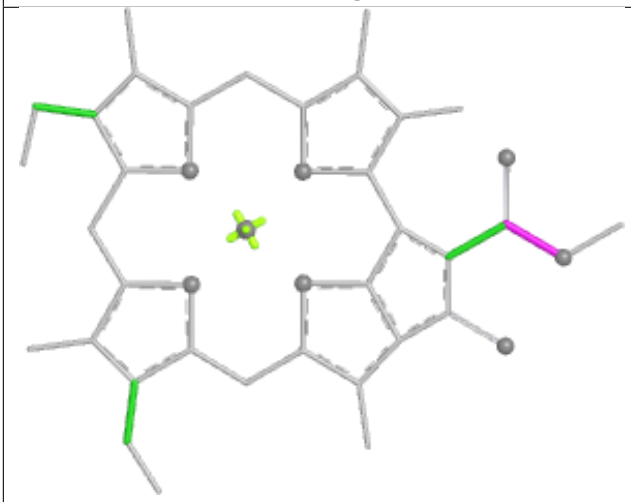
Ligand CLA s 507



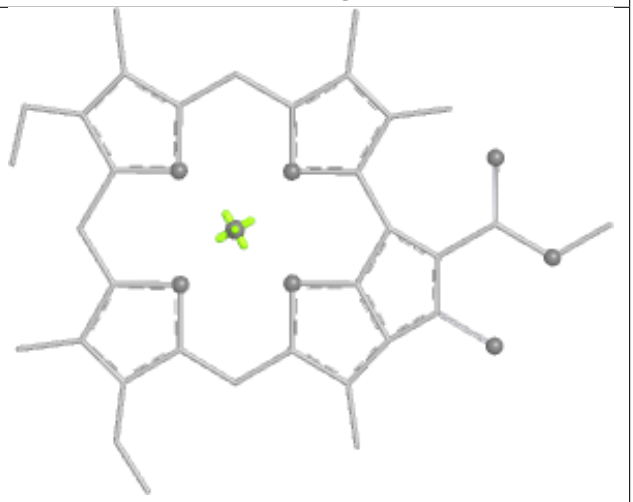
Bond lengths



Bond angles

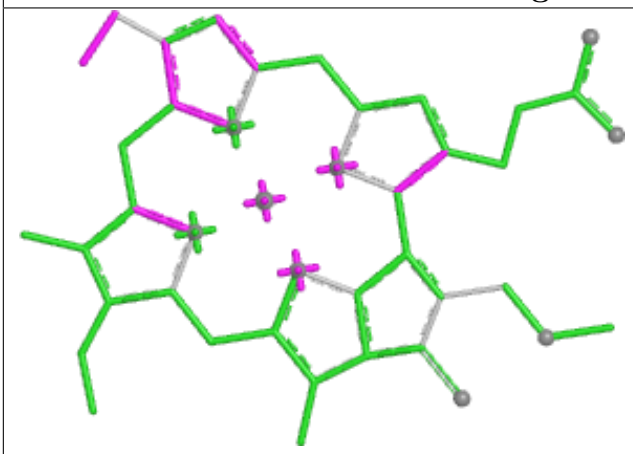


Torsions

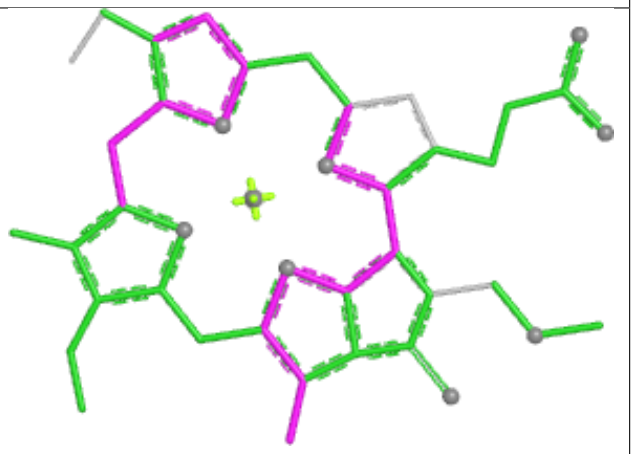


Rings

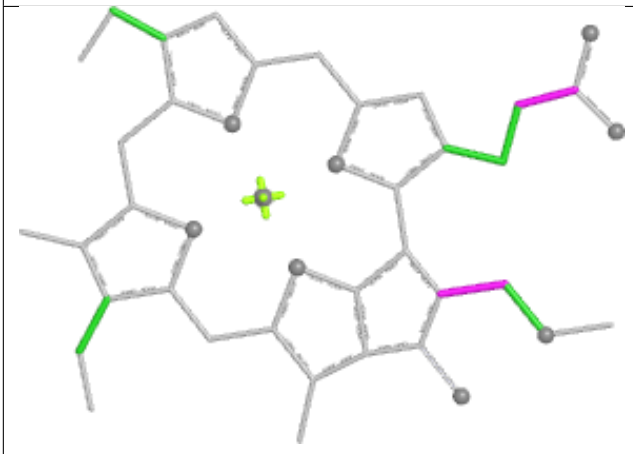
Ligand CLA f 804



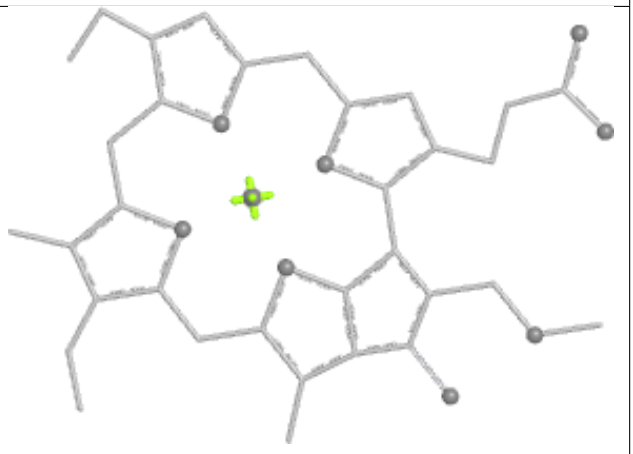
Bond lengths



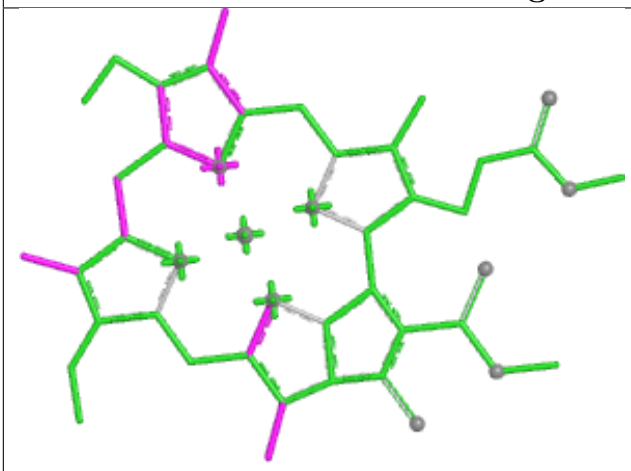
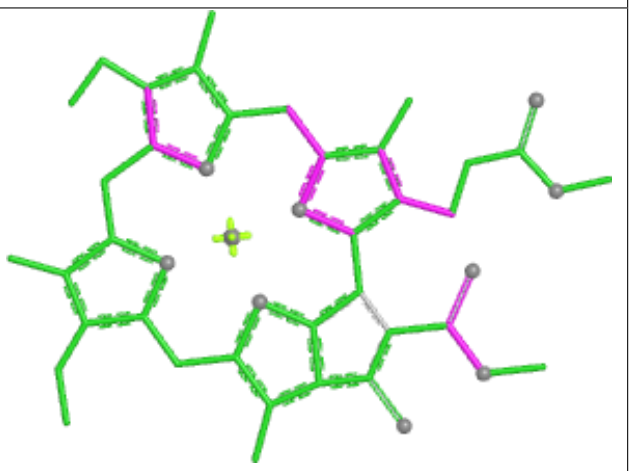
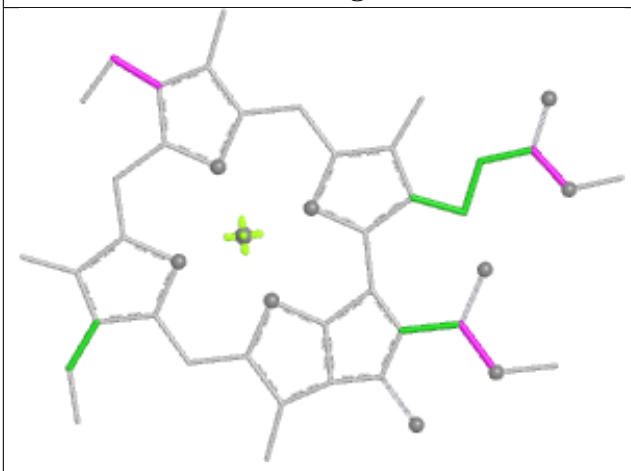
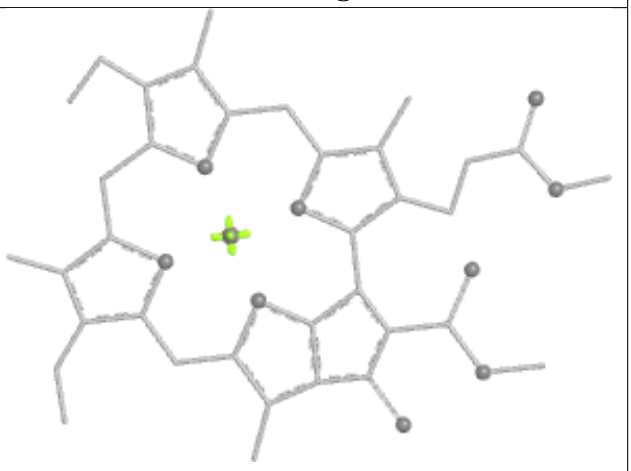
Bond angles



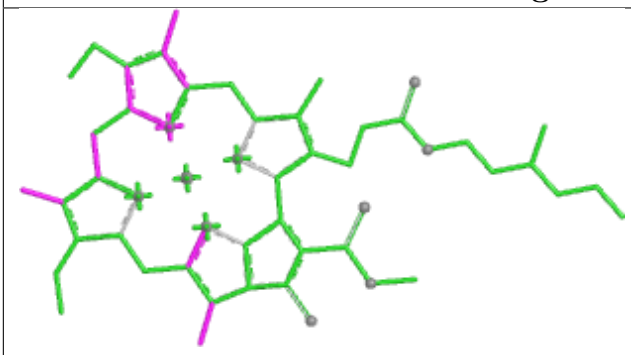
Torsions



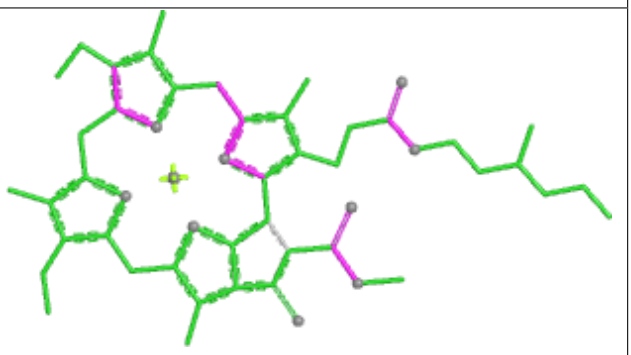
Rings

Ligand CLA 1 511	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

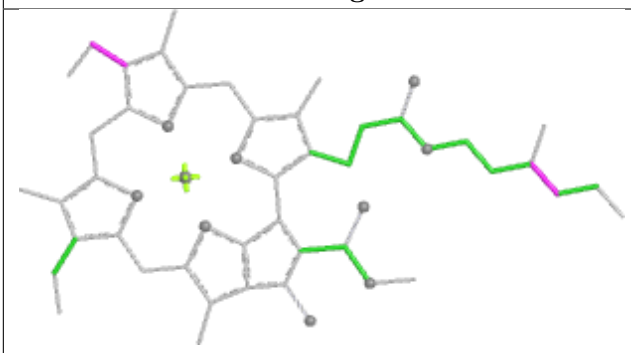
Ligand CLA f 809



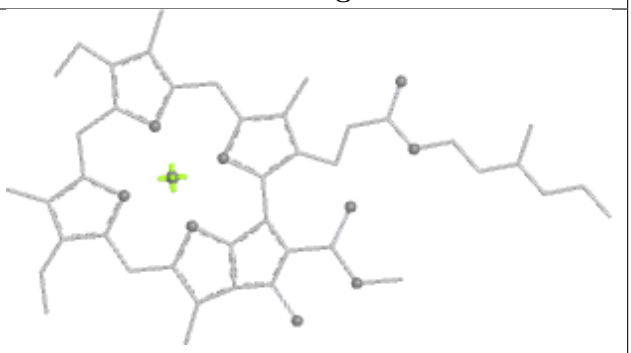
Bond lengths



Bond angles

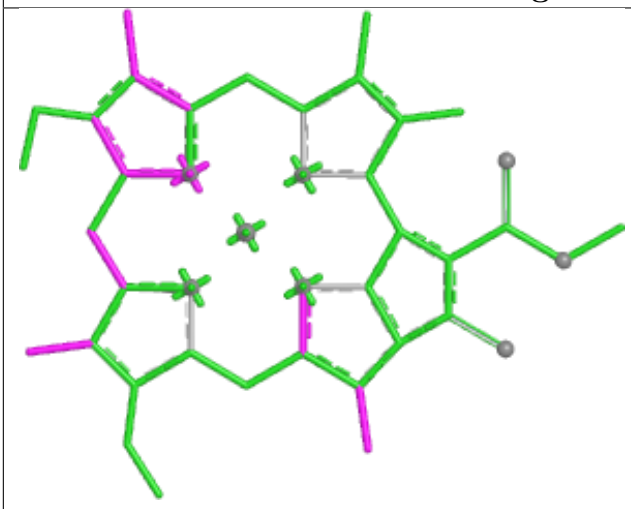


Torsions

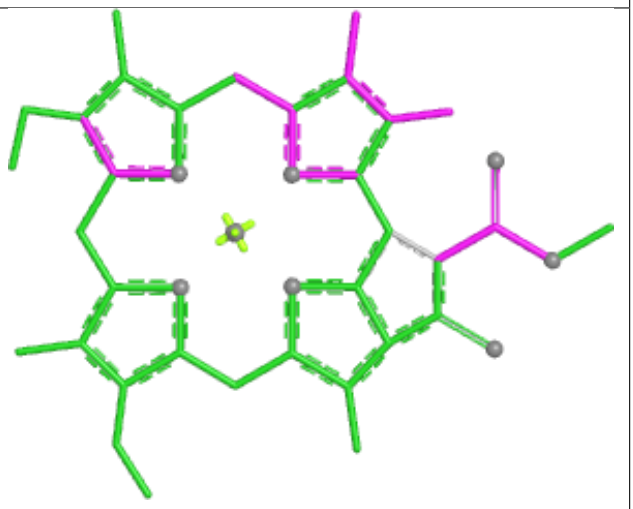


Rings

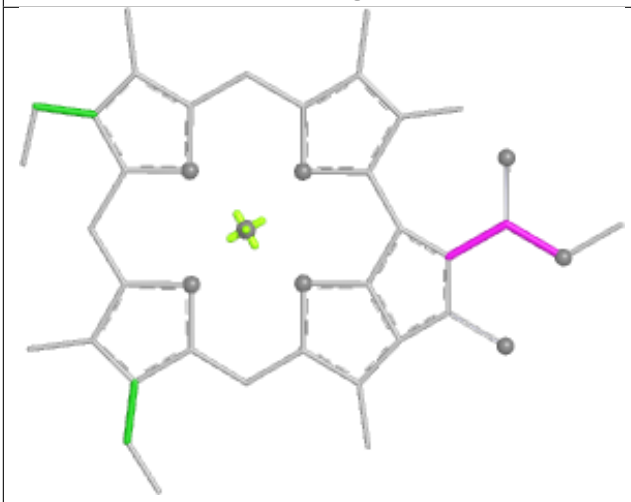
Ligand CLA f 840



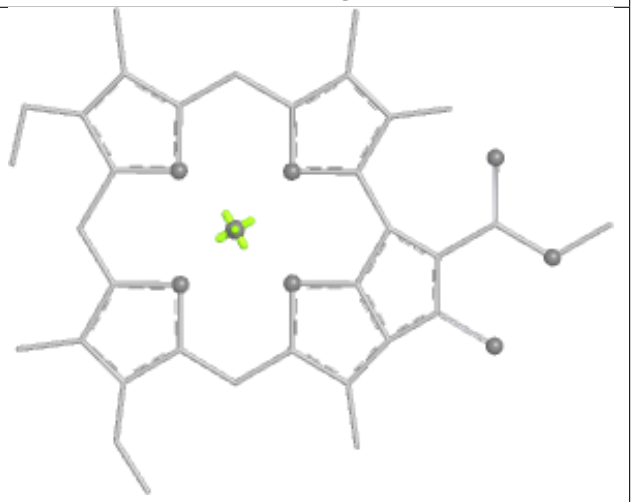
Bond lengths



Bond angles

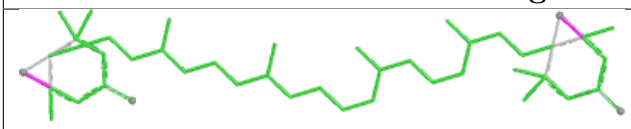


Torsions

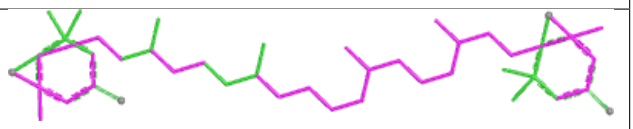


Rings

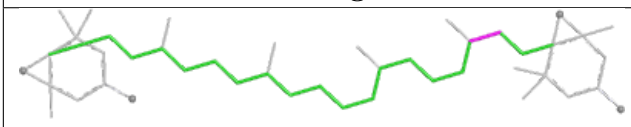
Ligand XAT r 303



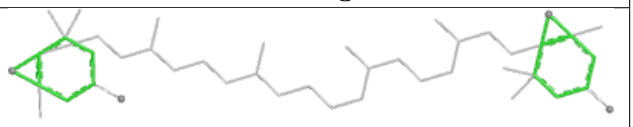
Bond lengths



Bond angles

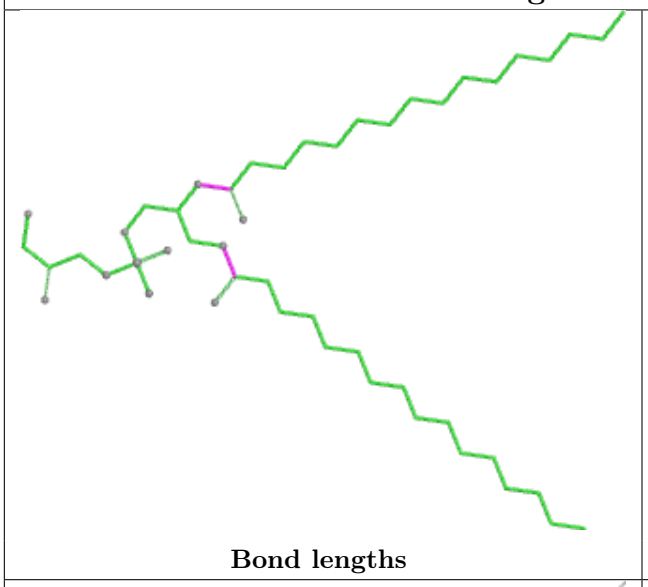


Torsions

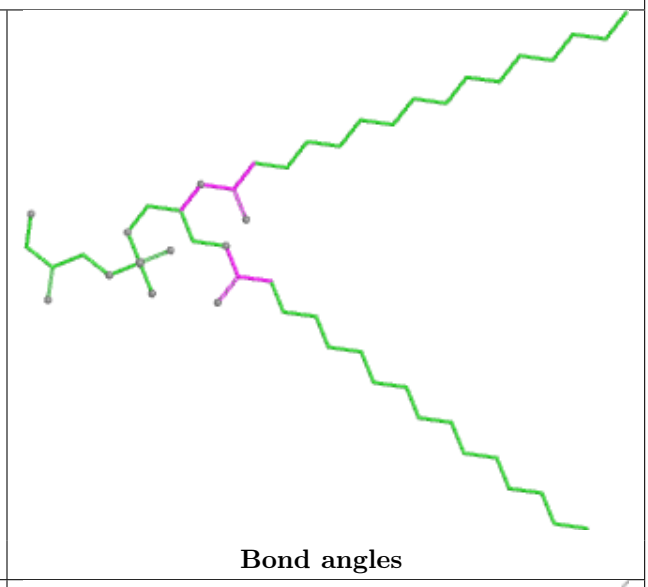


Rings

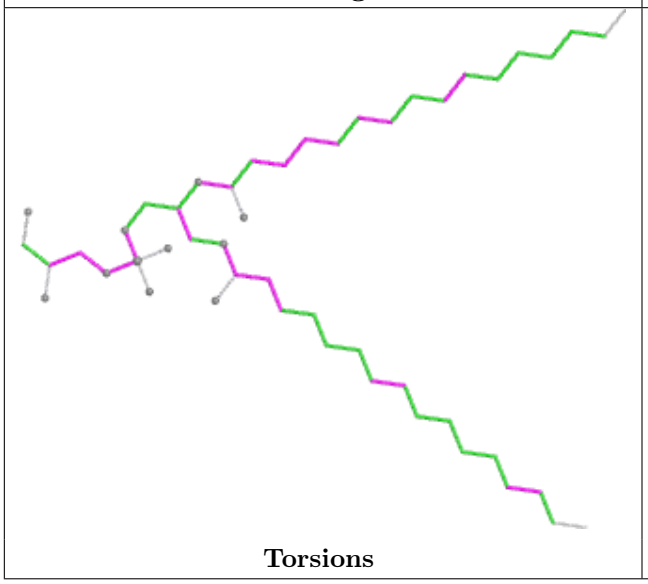
Ligand LHG 1 516



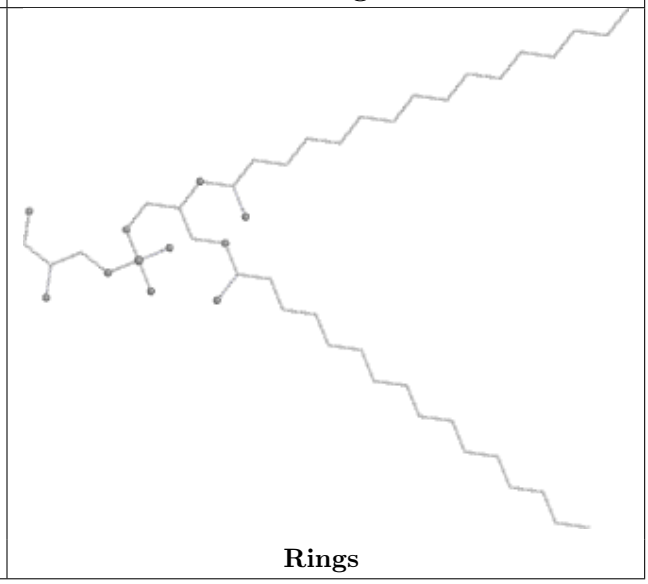
Bond lengths



Bond angles

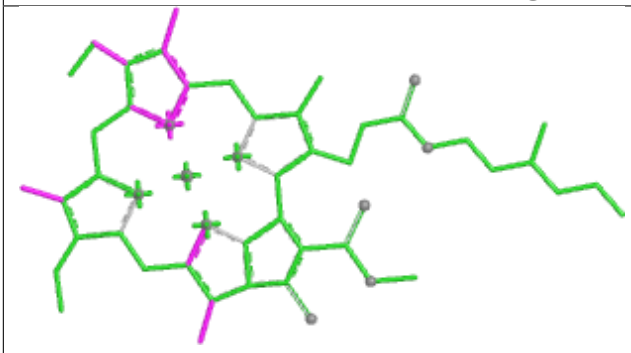


Torsions

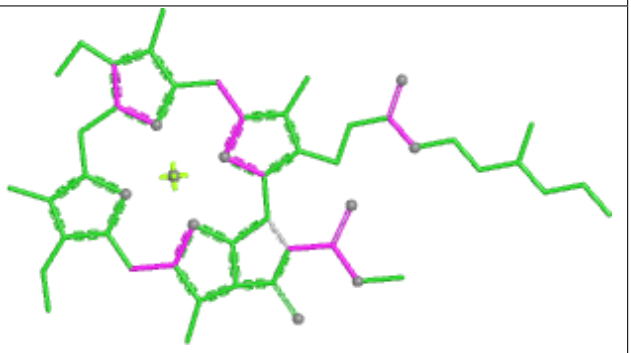


Rings

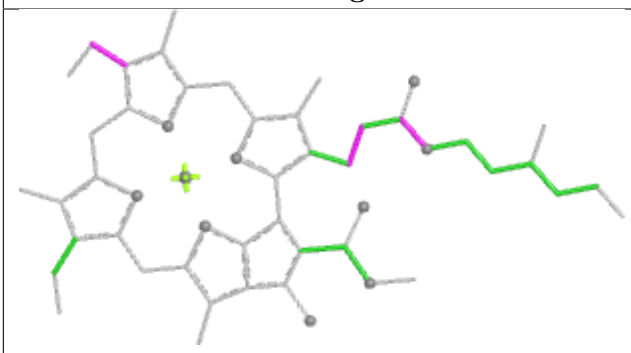
Ligand CLA B 808



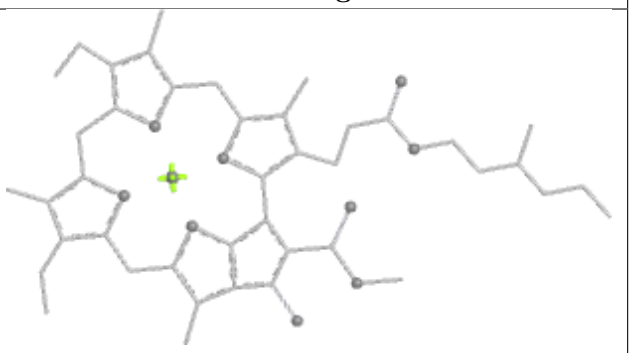
Bond lengths



Bond angles

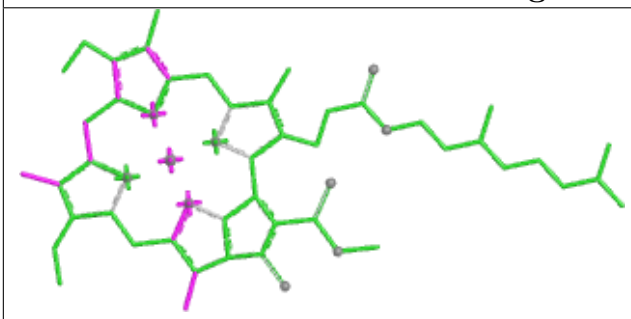


Torsions

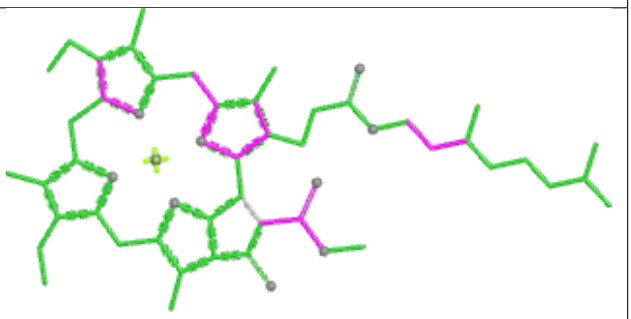


Rings

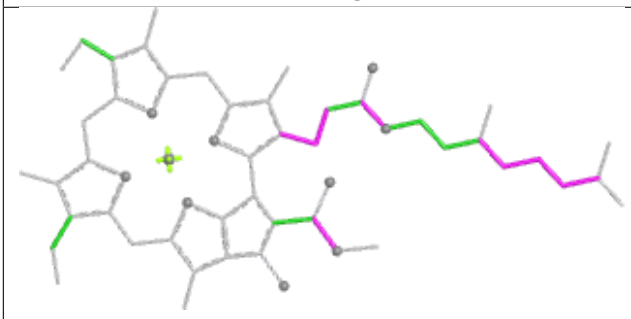
Ligand CLA 3 308



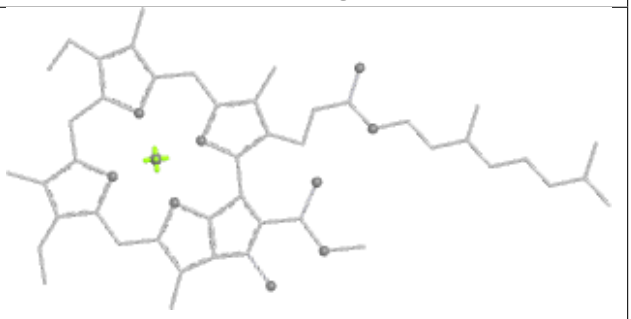
Bond lengths



Bond angles

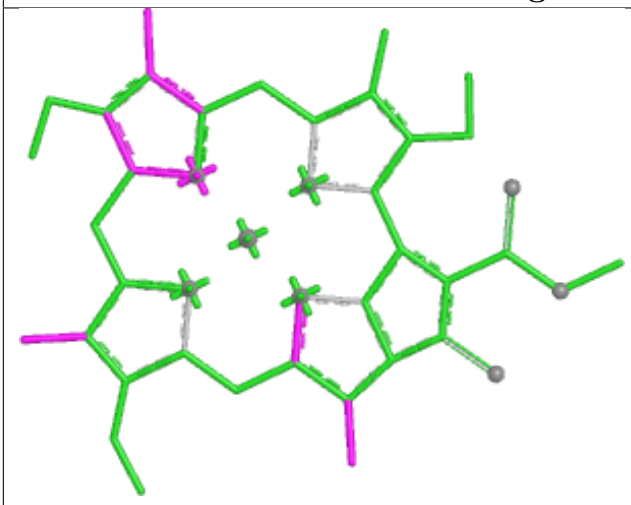


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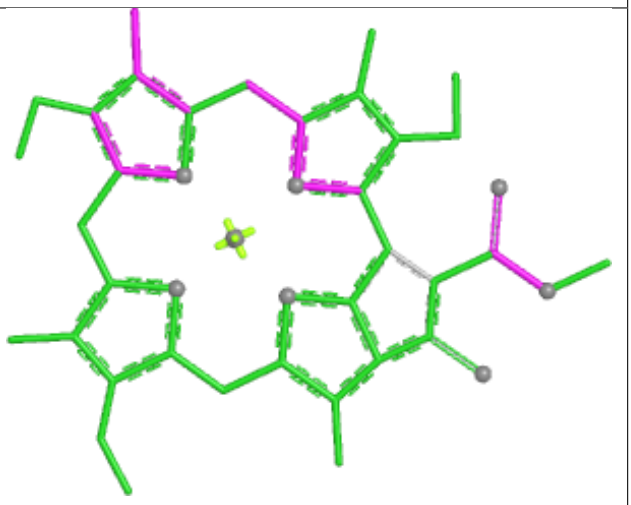


Rings

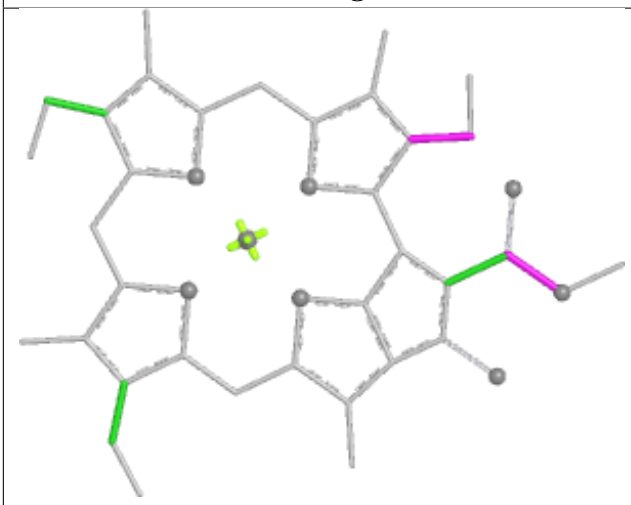
Ligand CLA 5 311



Bond lengths



Bond angles

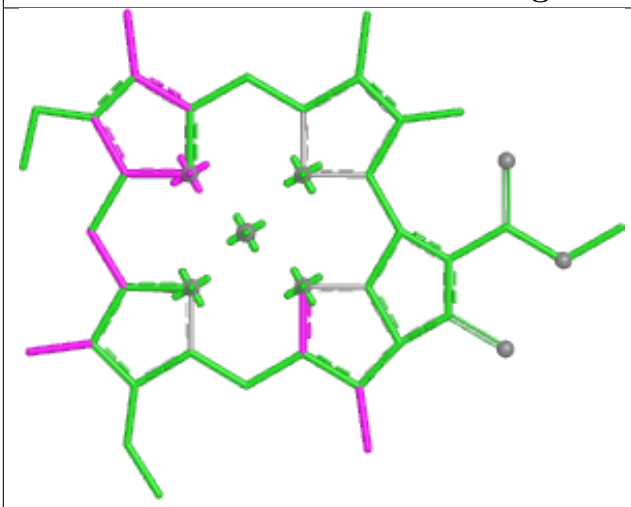


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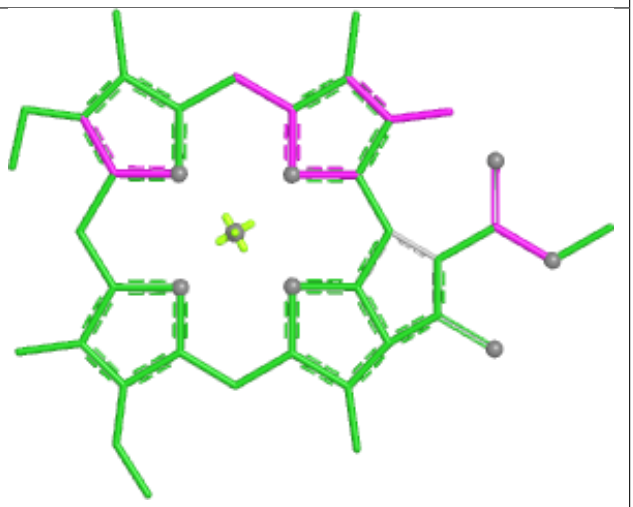


Rings

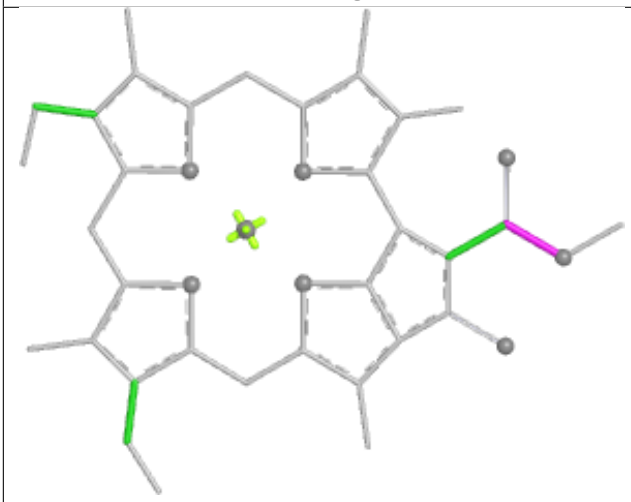
Ligand CLA f 841



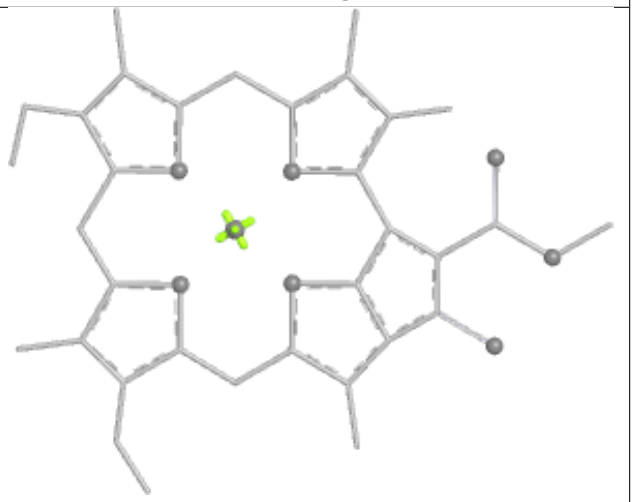
Bond lengths



Bond angles

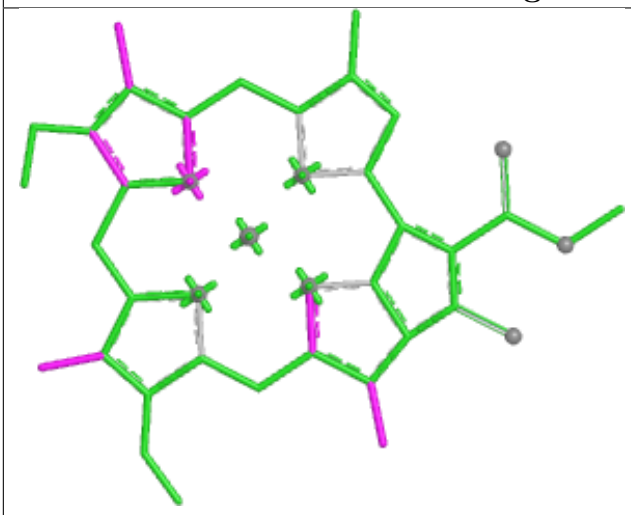


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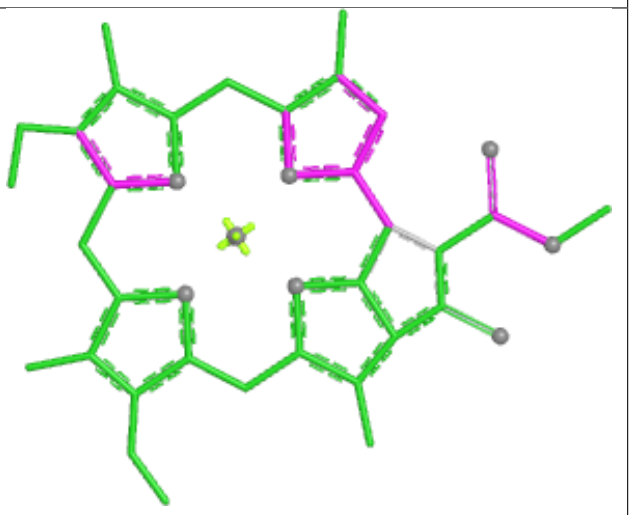


Rings

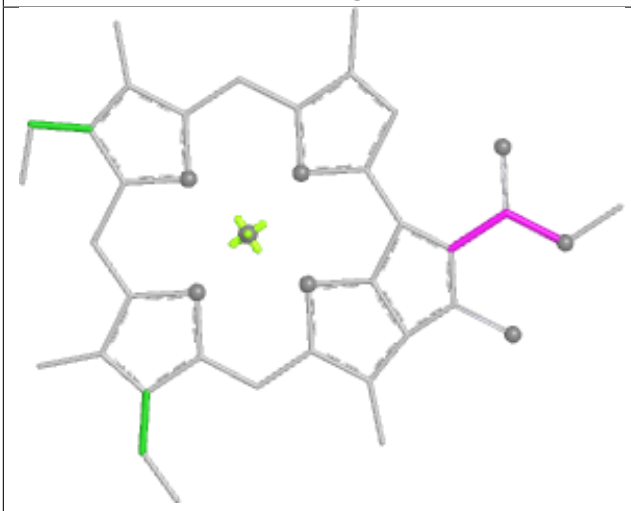
Ligand CLA A 824



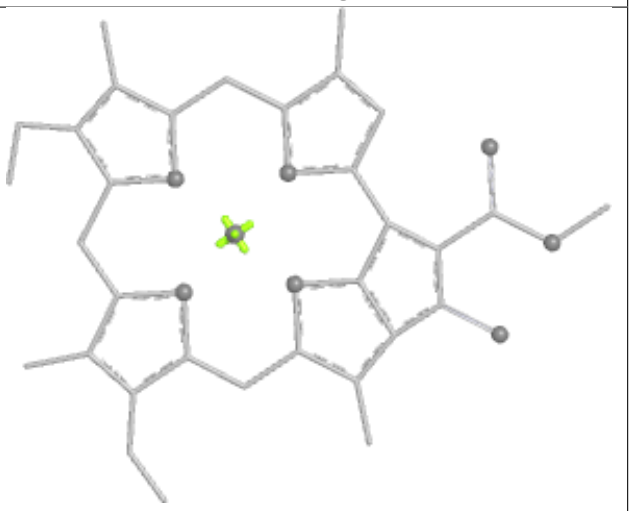
Bond lengths



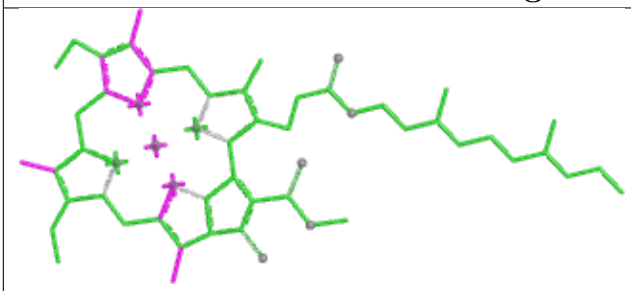
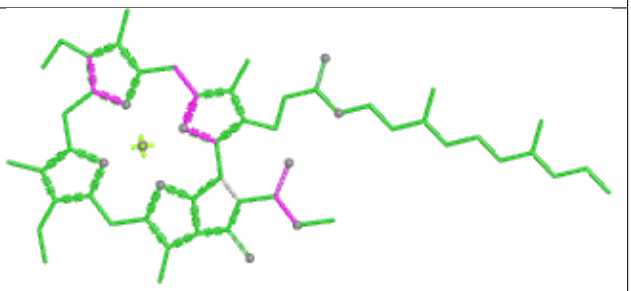
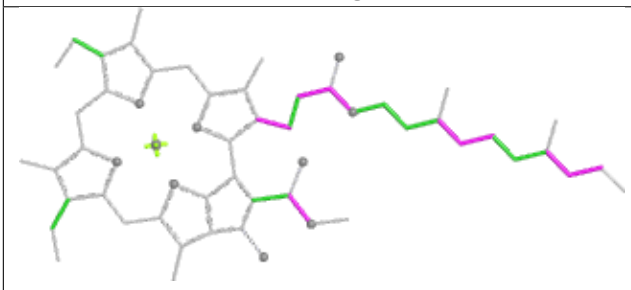
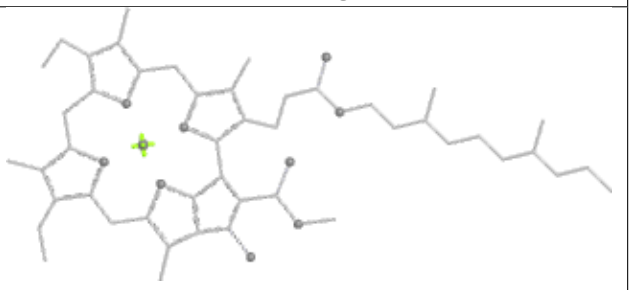
Bond angles

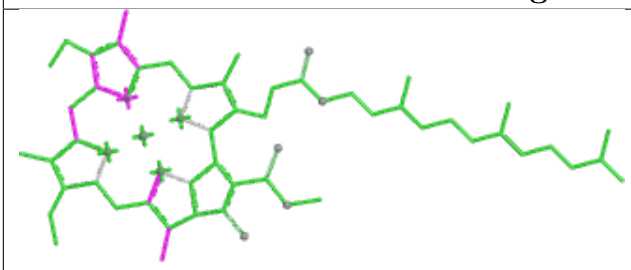
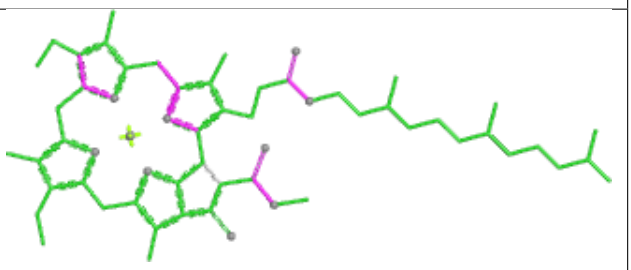
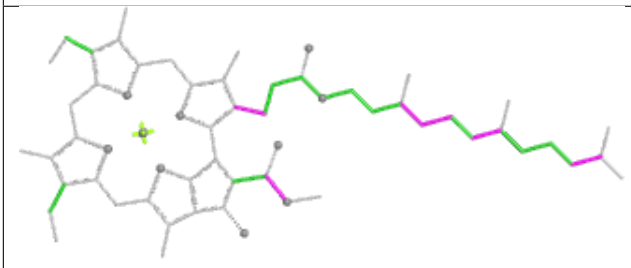
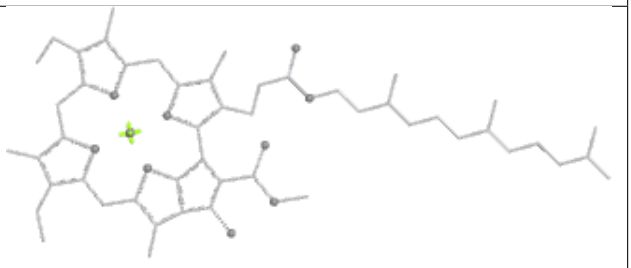


Torsions

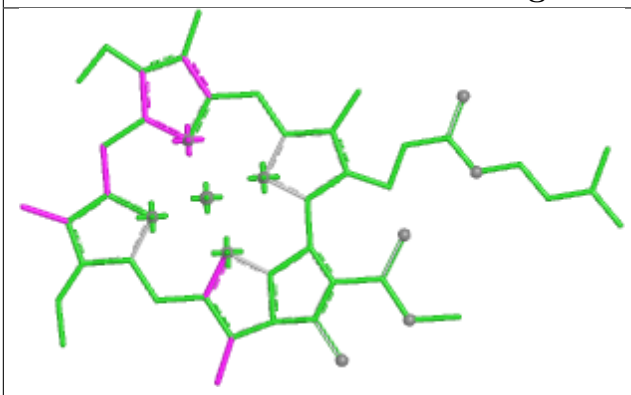


Rings

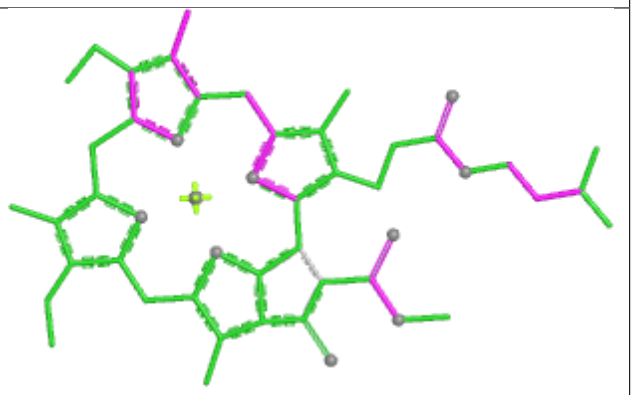
Ligand CLA B 842	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA s 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

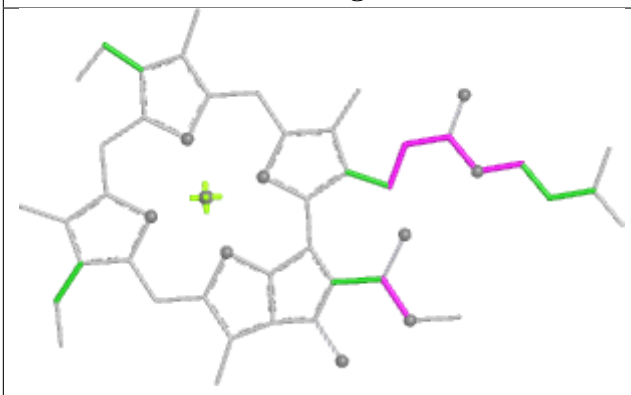
Ligand CLA 5 310



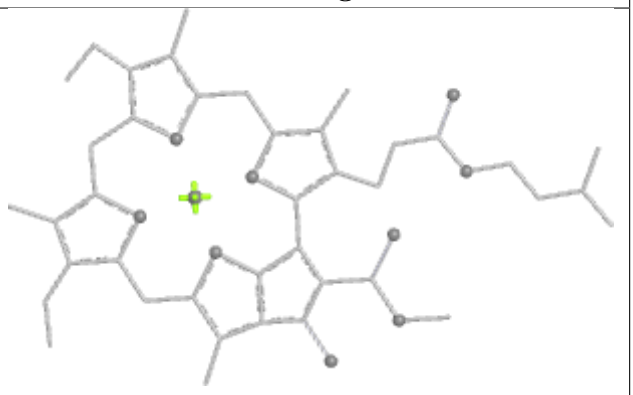
Bond lengths



Bond angles

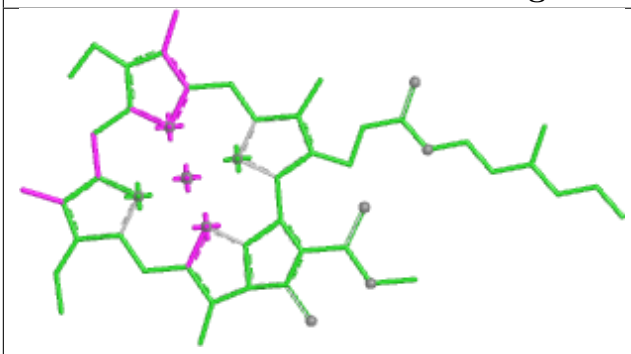


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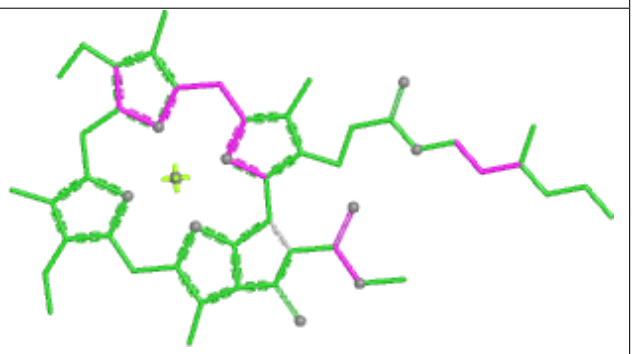


Rings

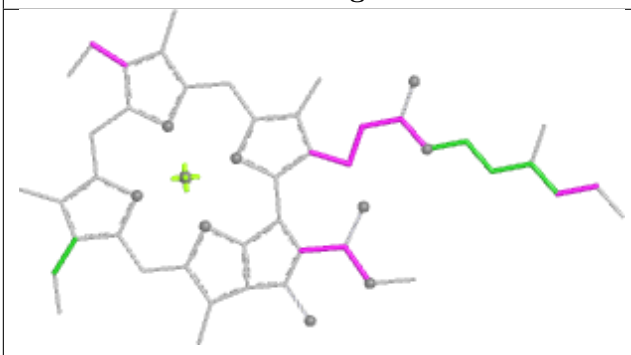
Ligand CLA 2 505



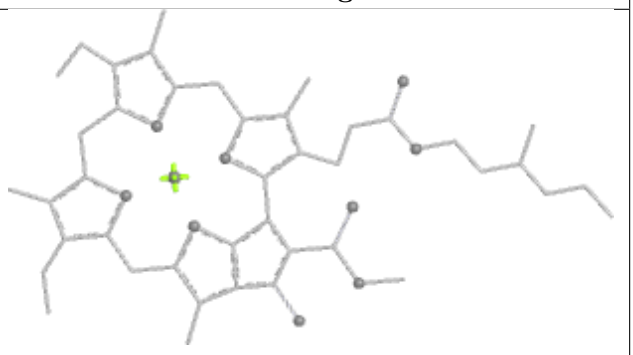
Bond lengths



Bond angles

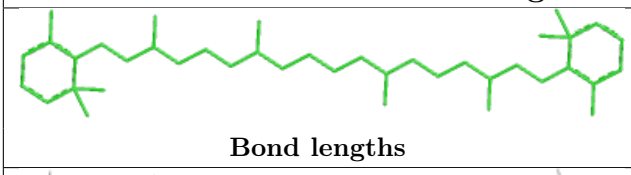


Torsions

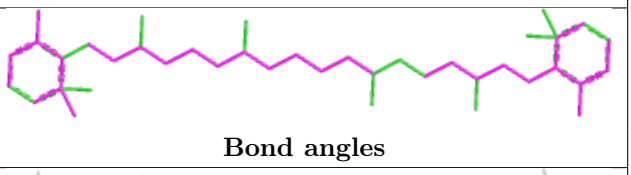


Rings

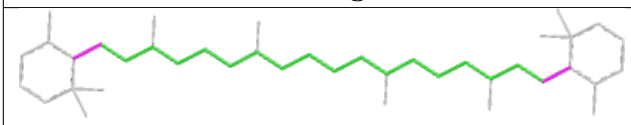
Ligand BCR e 851



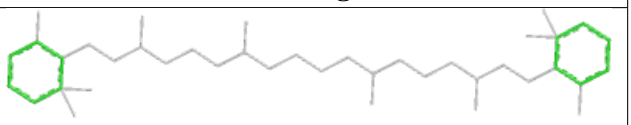
Bond lengths



Bond angles

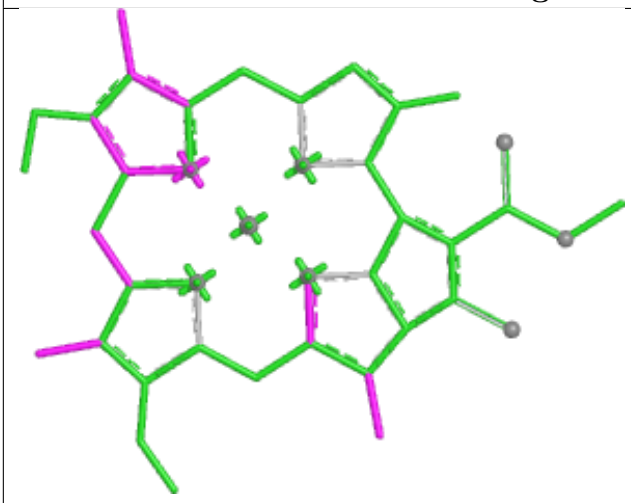


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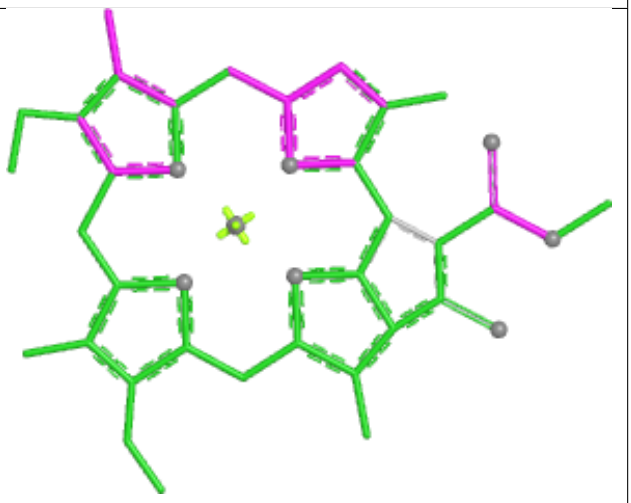


Rings

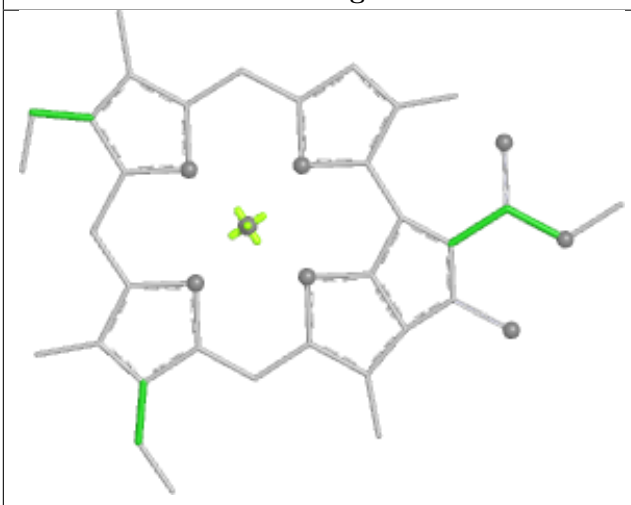
Ligand CLA f 827



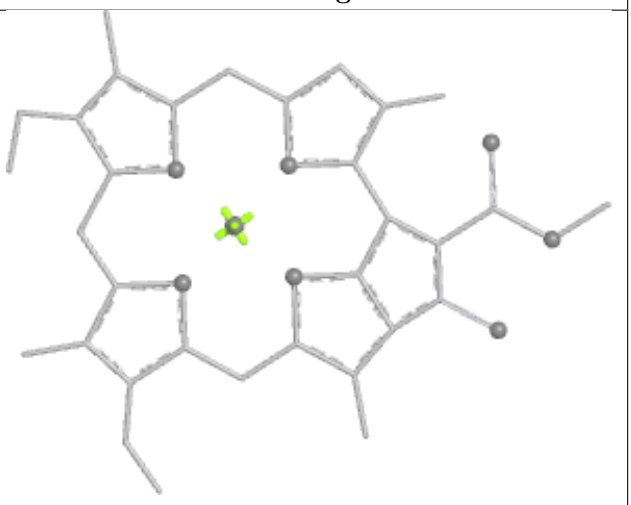
Bond lengths



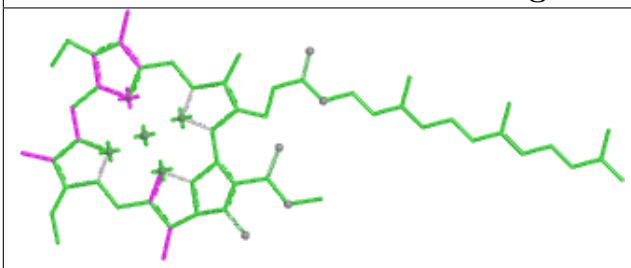
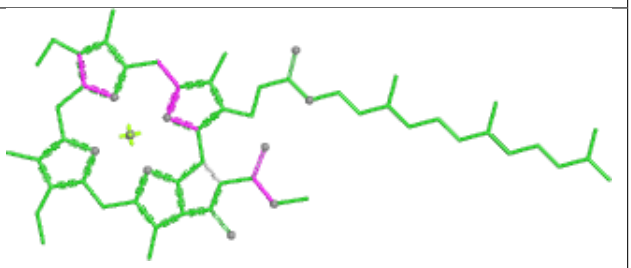
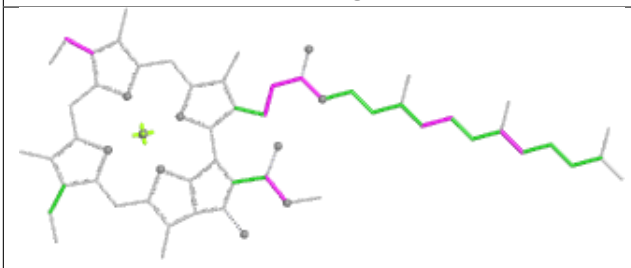
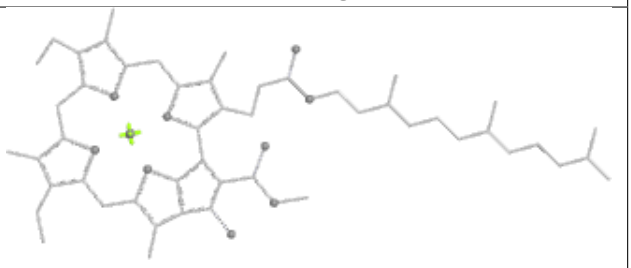
Bond angles

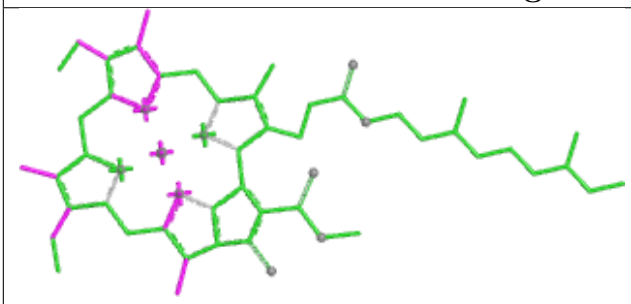
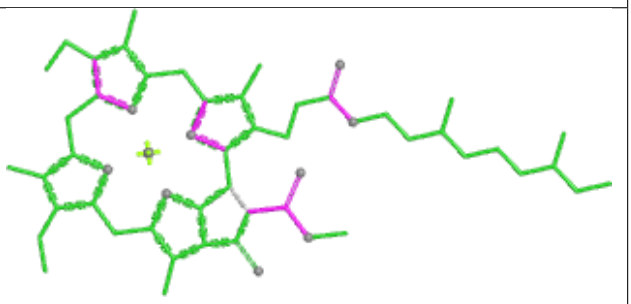
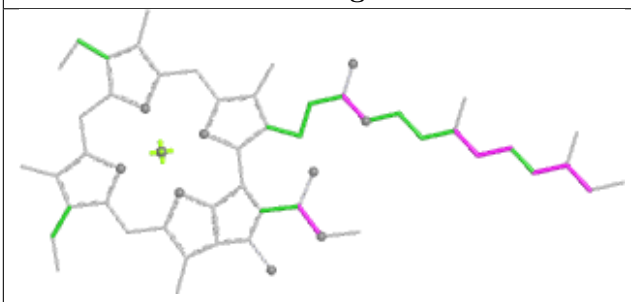
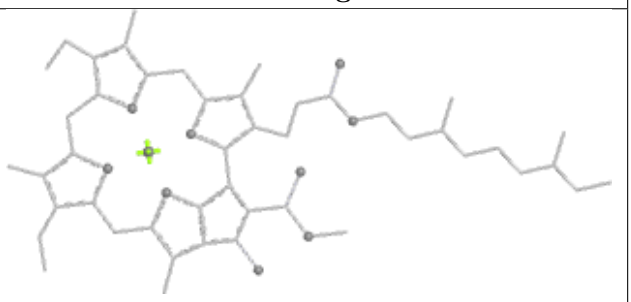


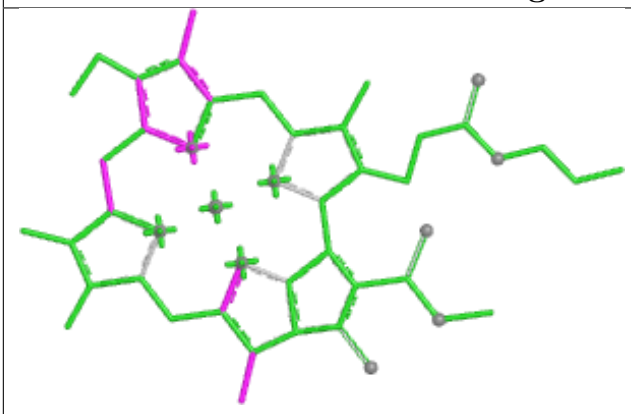
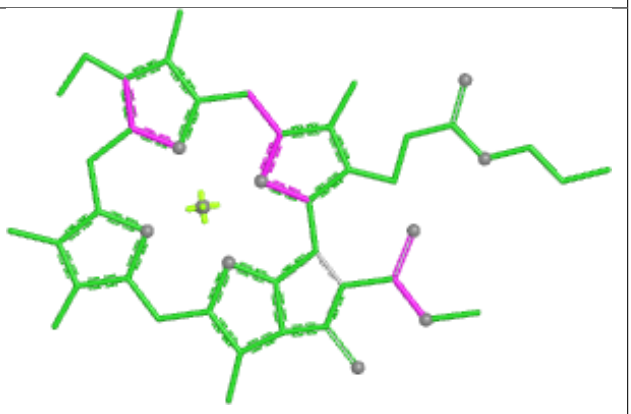
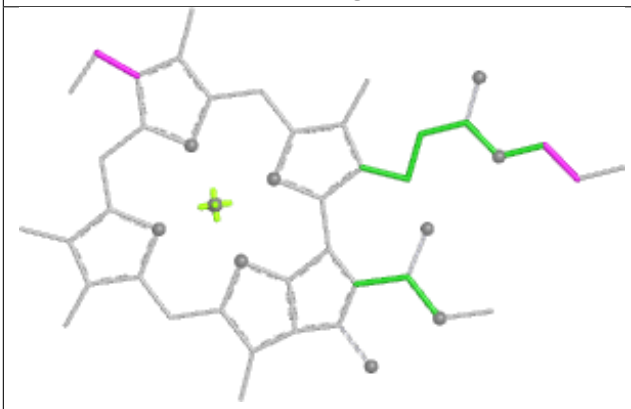
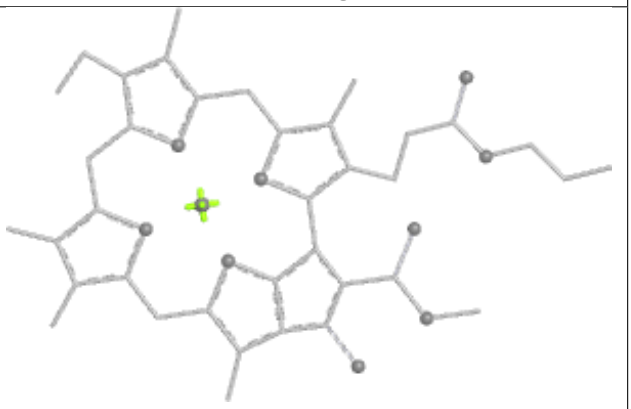
Torsions



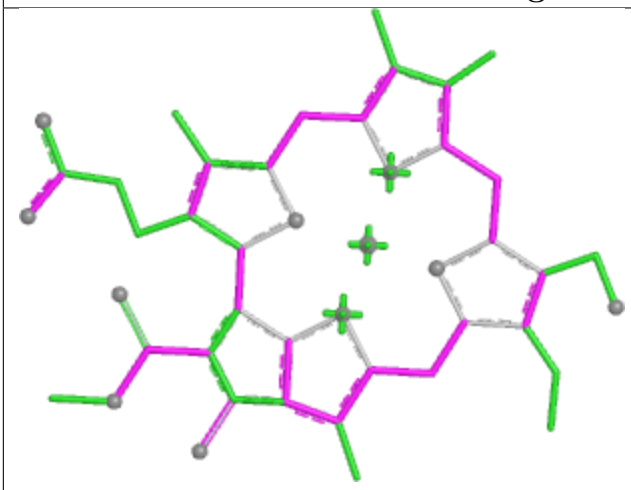
Rings

Ligand CLA e 816	
	
Bond lengths	Bond angles
	
Torsions	Rings

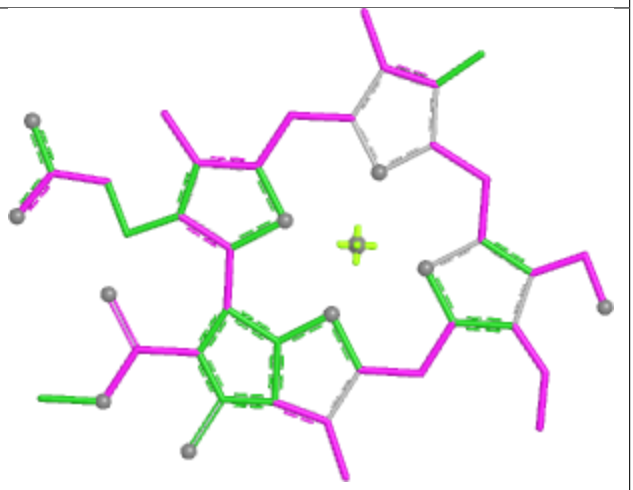
Ligand CLA B 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 2 508	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

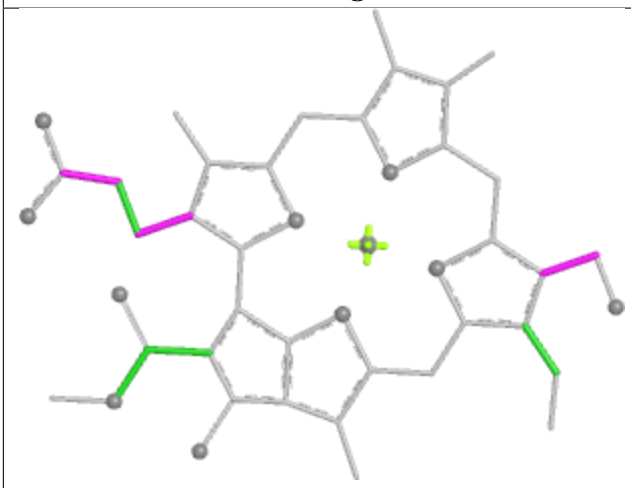
Ligand CHL 2 515



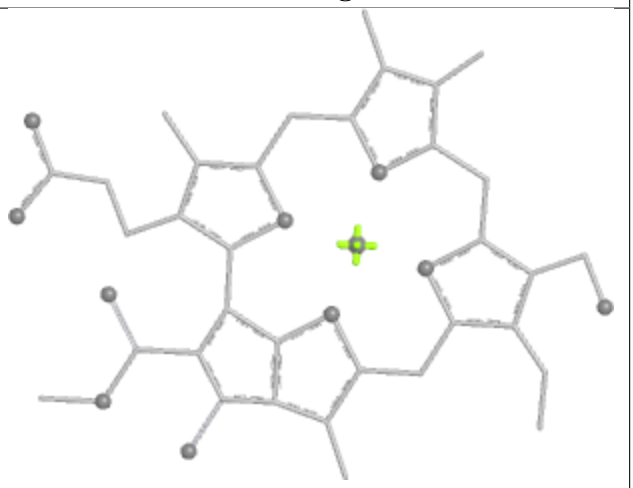
Bond lengths



Bond angles

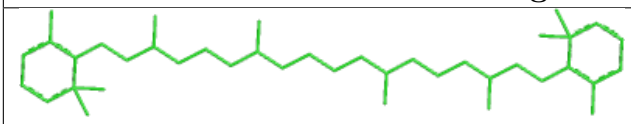


Torsions

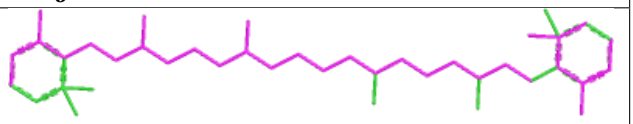


Rings

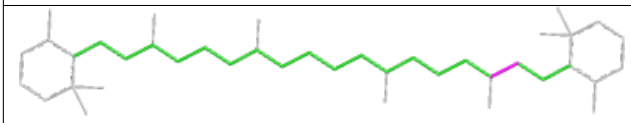
Ligand BCR j 801



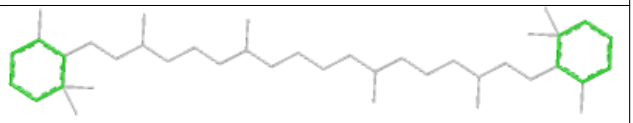
Bond lengths



Bond angles

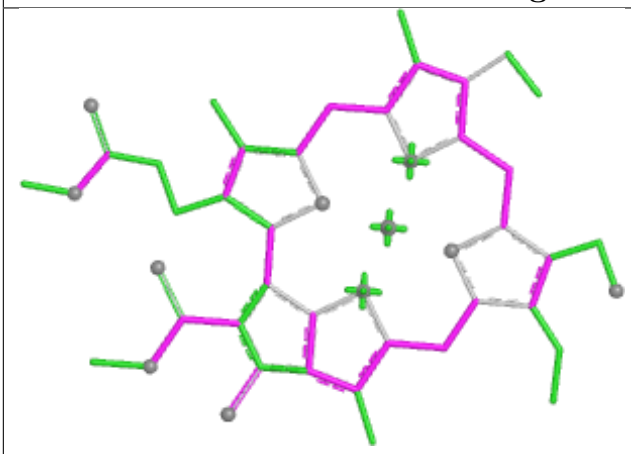


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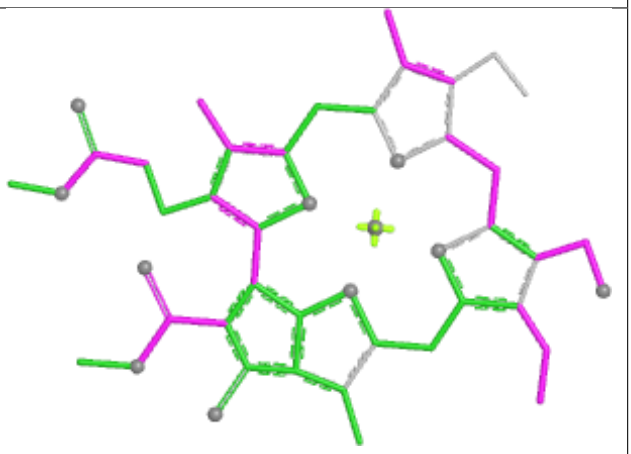


Rings

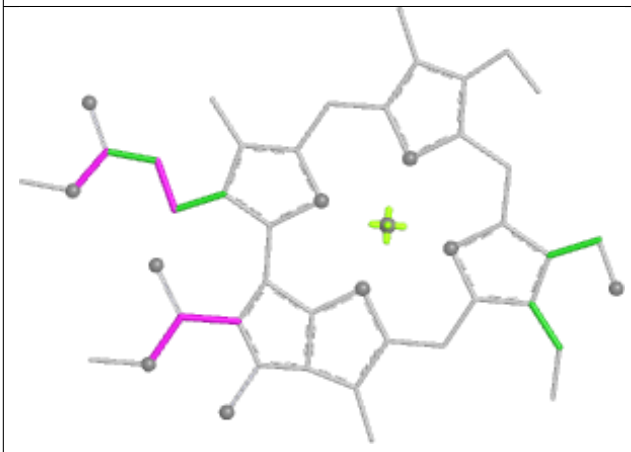
Ligand CHL r 313



Bond lengths



Bond angles

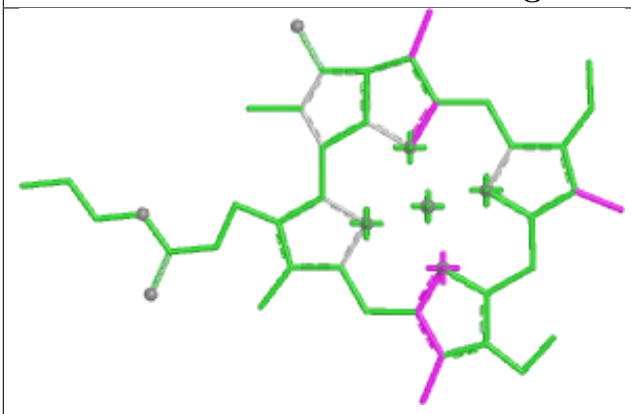


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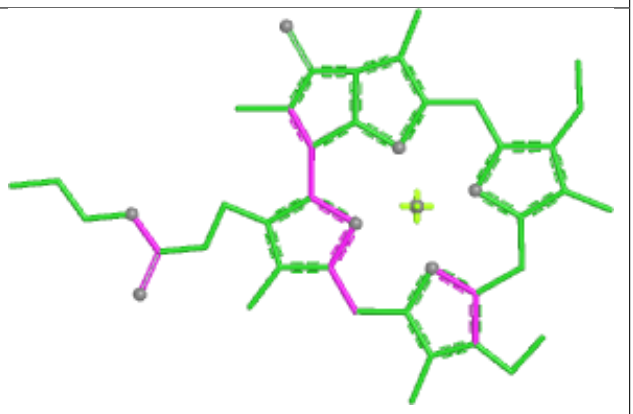


Rings

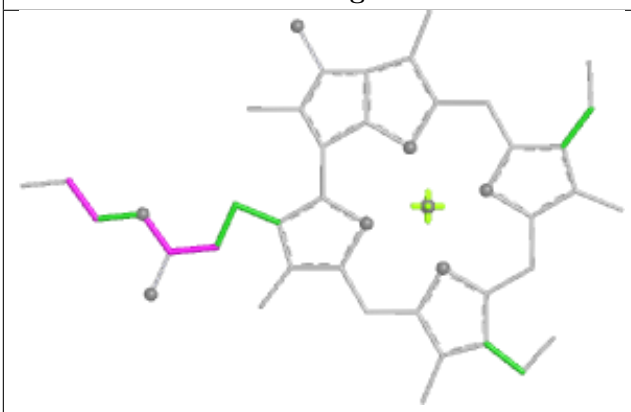
Ligand CLA A 832



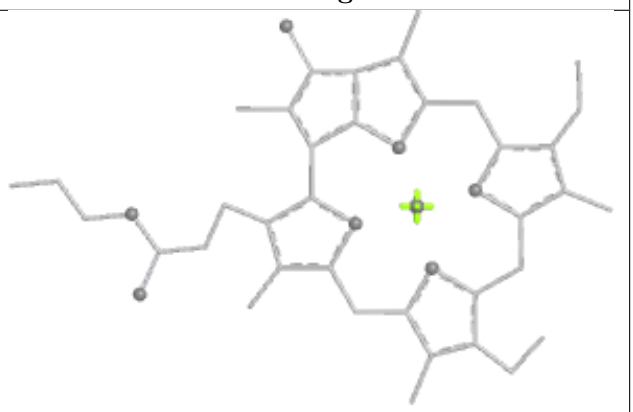
Bond lengths



Bond angles

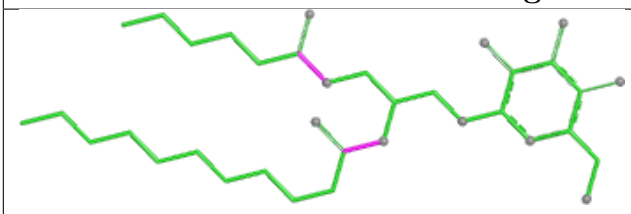


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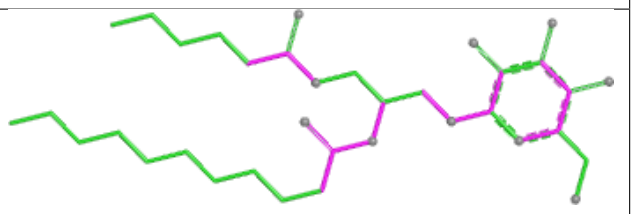


Rings

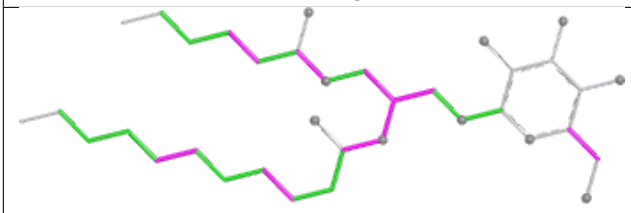
Ligand LMG 2 519



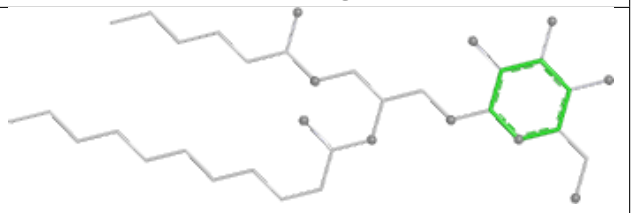
Bond lengths



Bond angles

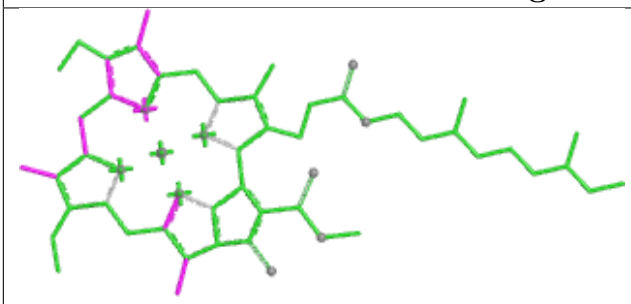


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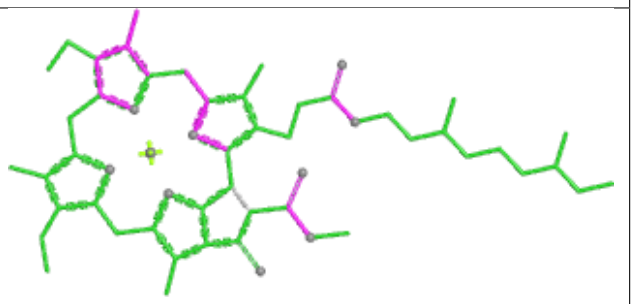


Rings

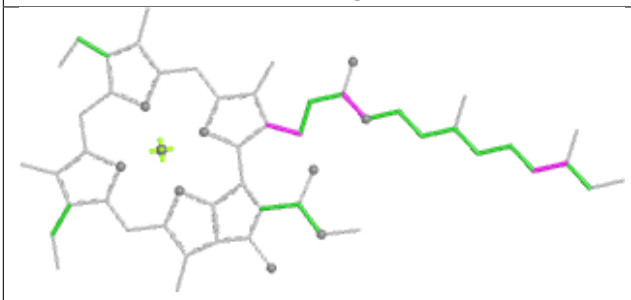
Ligand CLA e 831



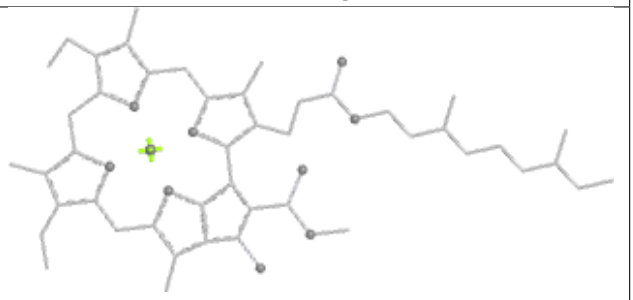
Bond lengths



Bond angles

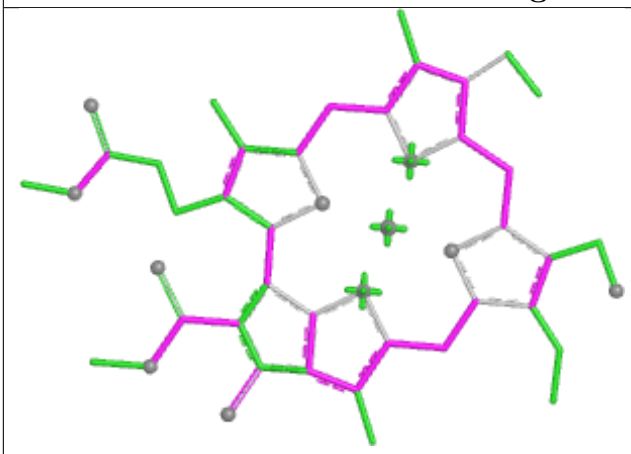


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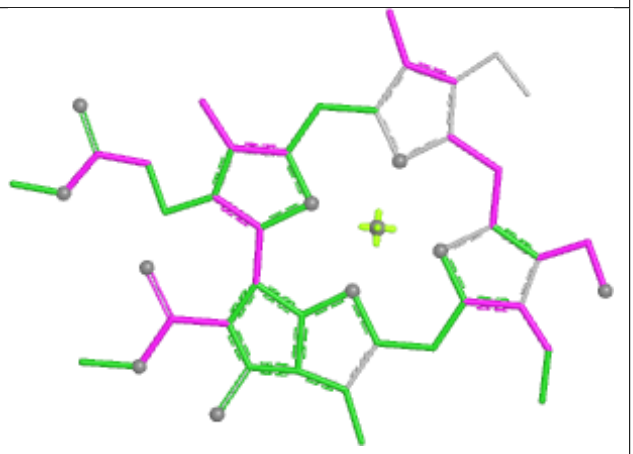


Rings

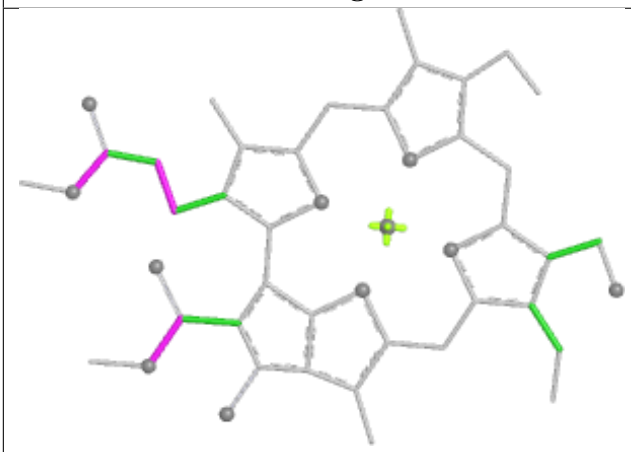
Ligand CHL s 512



Bond lengths



Bond angles

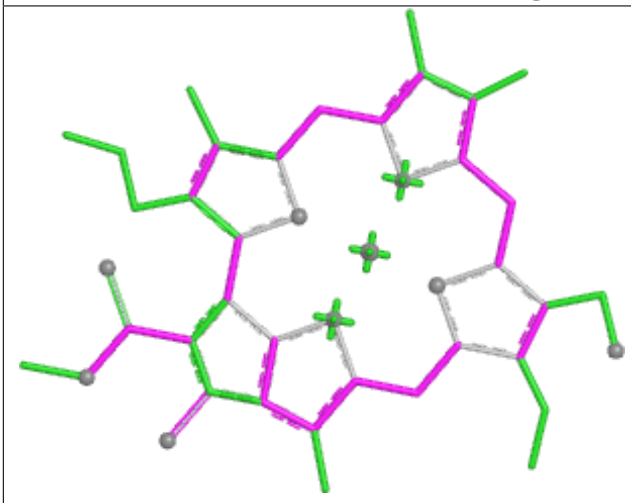


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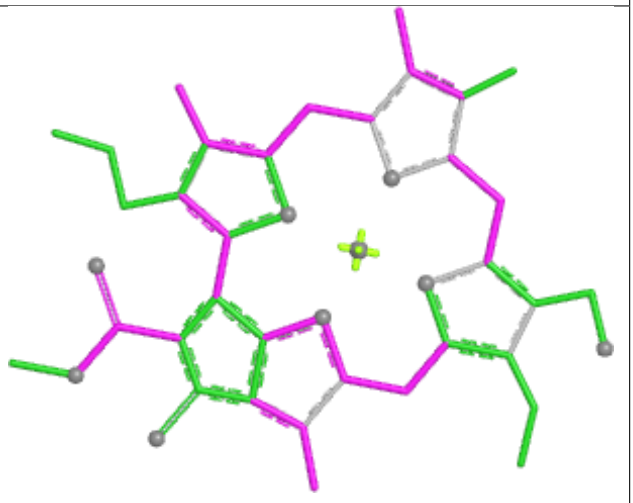


Rings

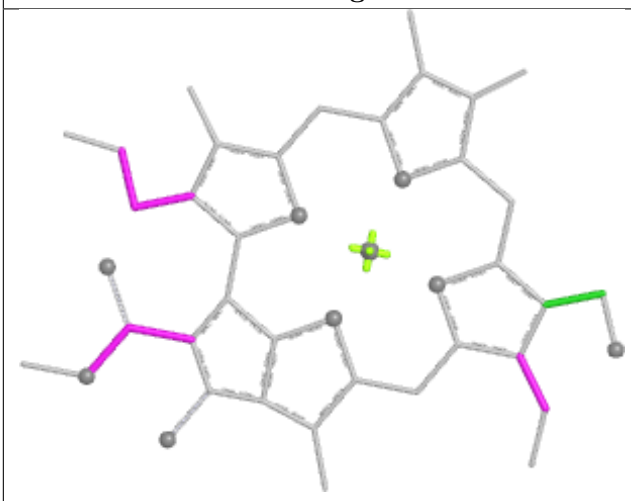
Ligand CHL 2 516



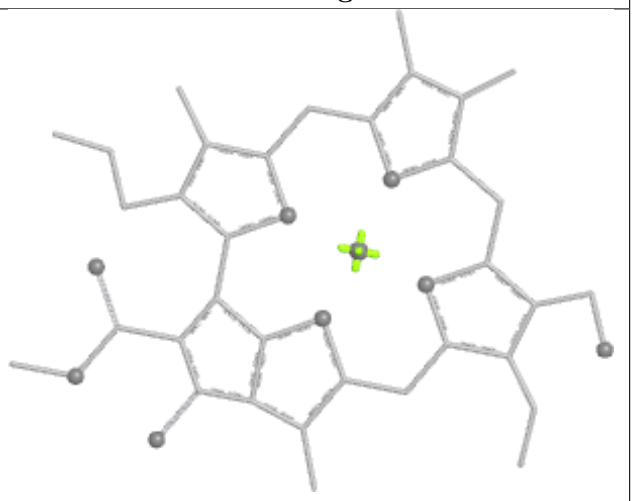
Bond lengths



Bond angles

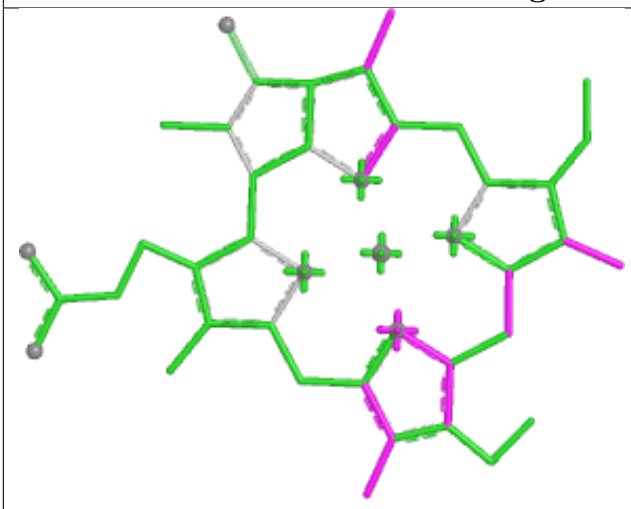


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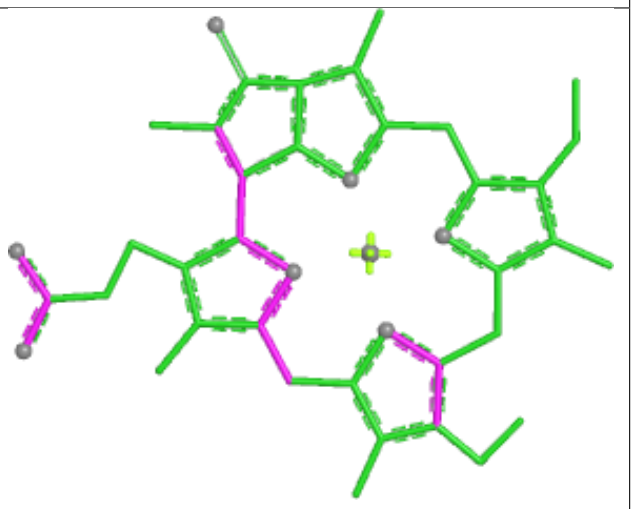


Rings

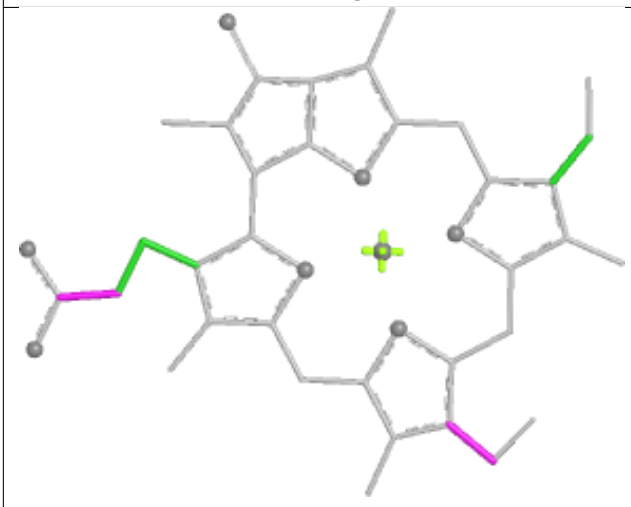
Ligand CLA e 835



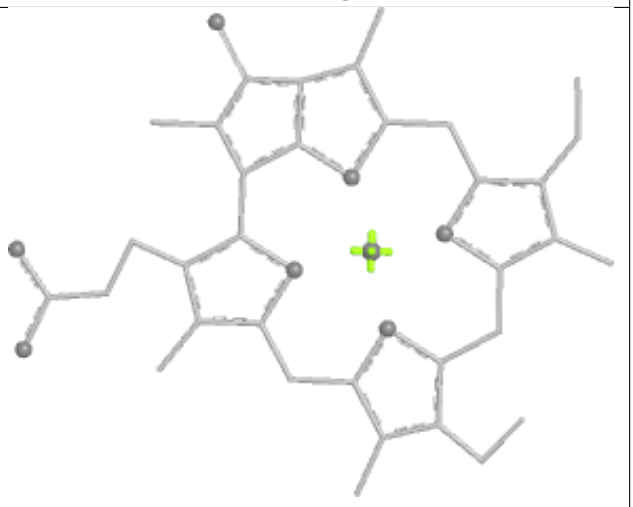
Bond lengths



Bond angles

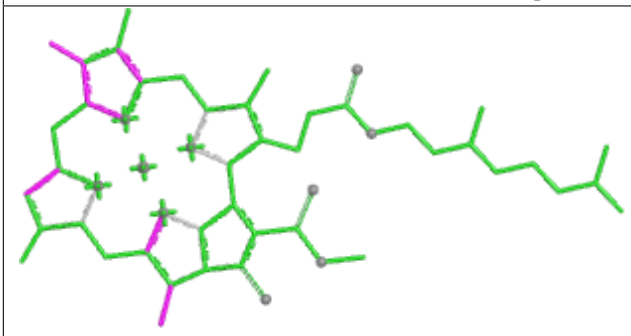


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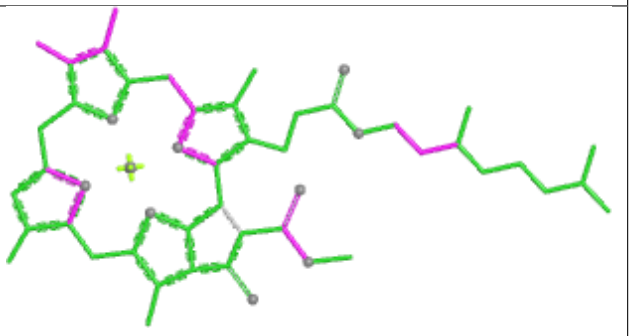


Rings

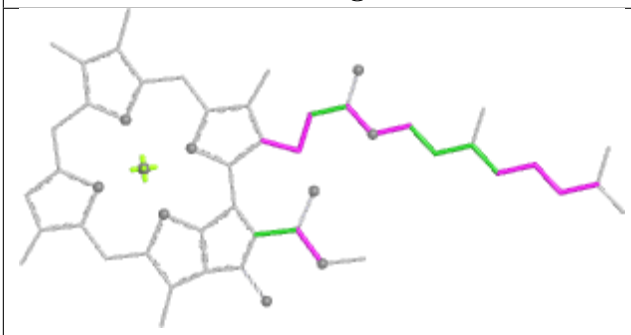
Ligand CLA 3 306



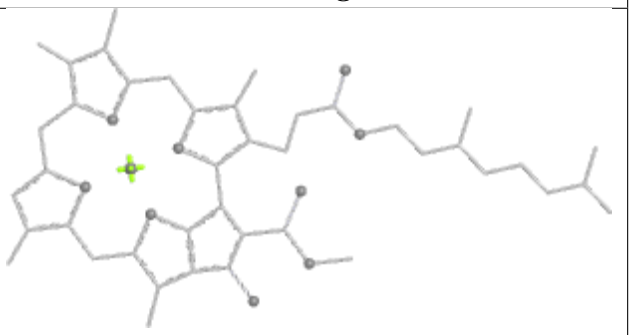
Bond lengths



Bond angles

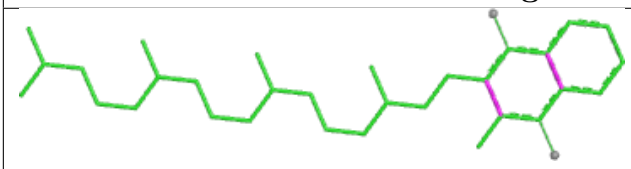


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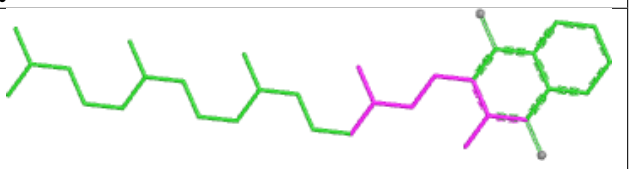


Rings

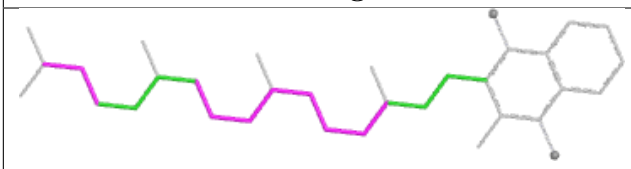
Ligand PQN A 841



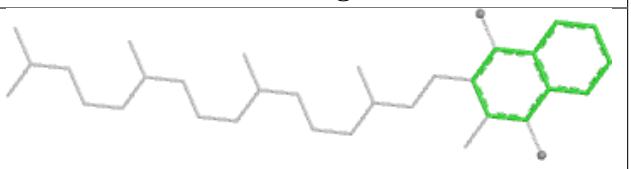
Bond lengths



Bond angles

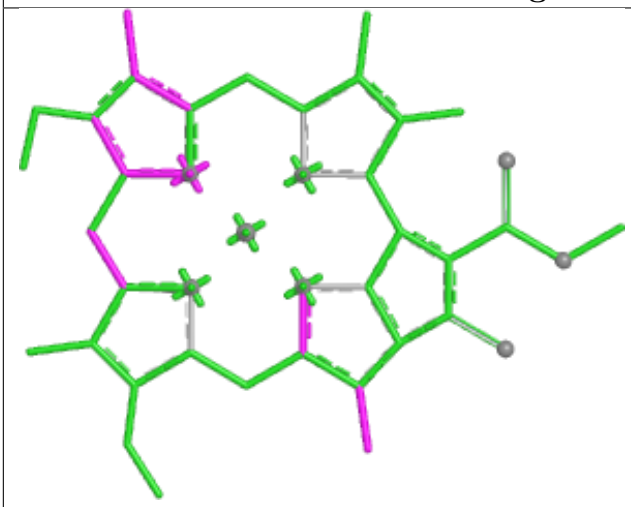


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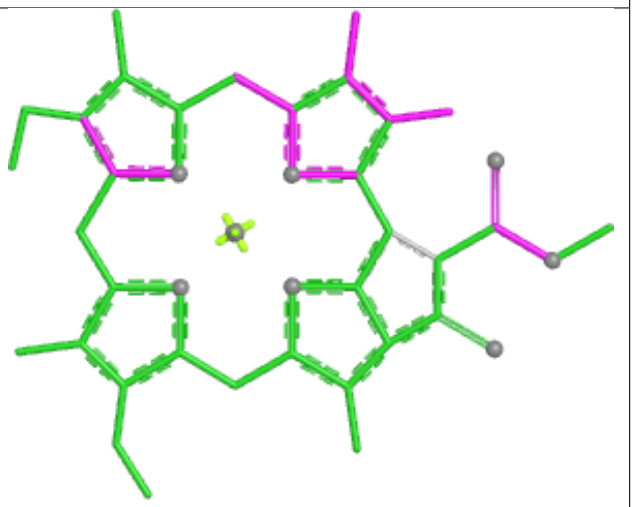


Rings

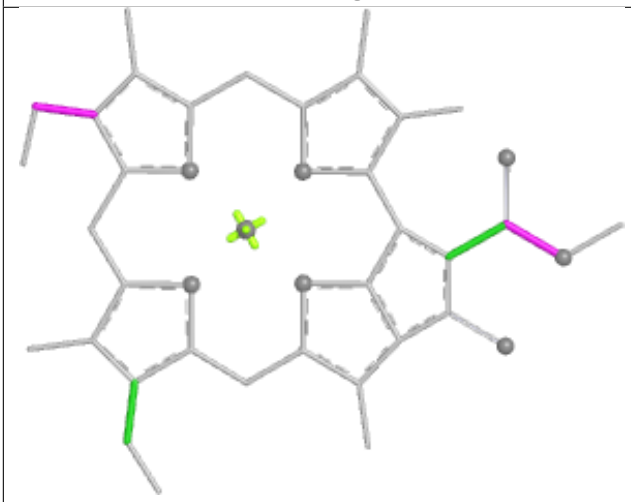
Ligand CLA e 833



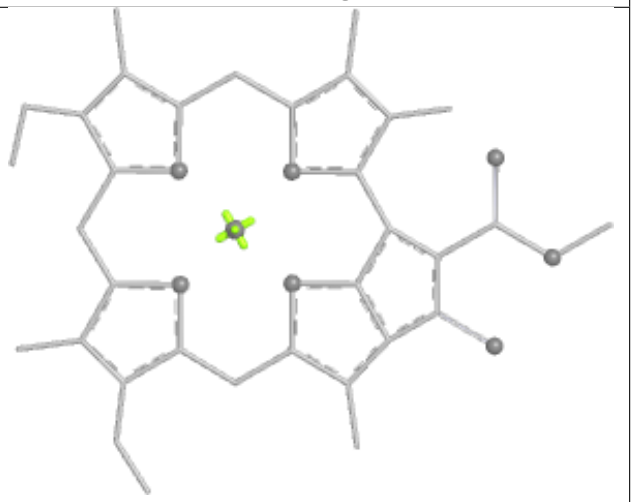
Bond lengths



Bond angles

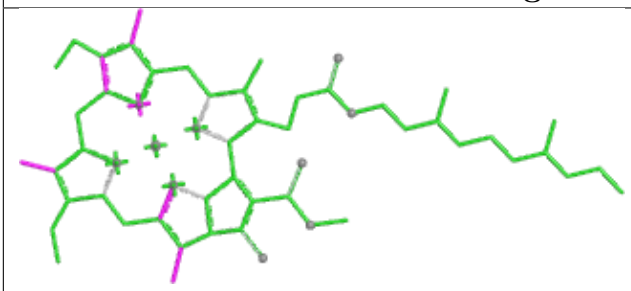


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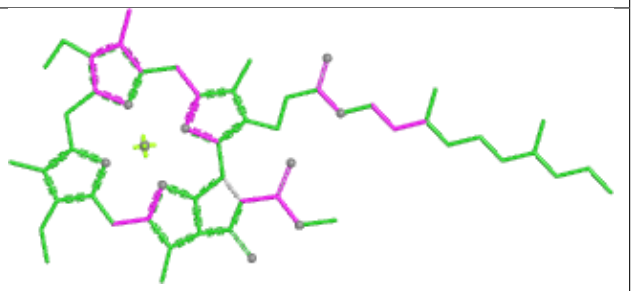


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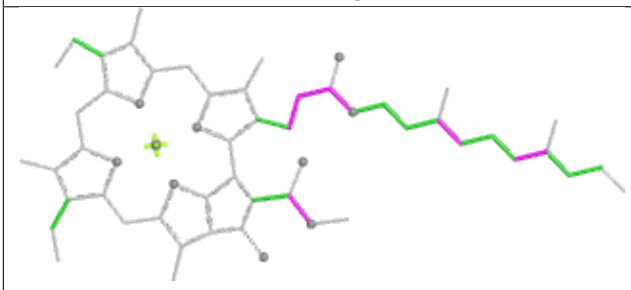
Ligand CLA A 820



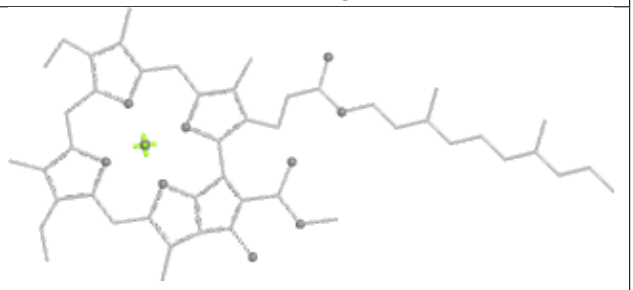
Bond lengths



Bond angles



Torsions

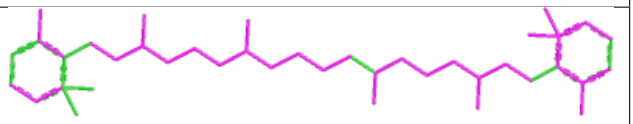


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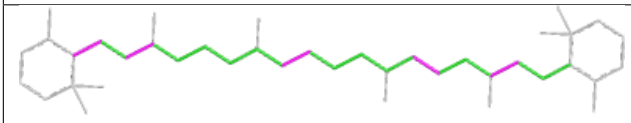
Ligand BCR 2 503



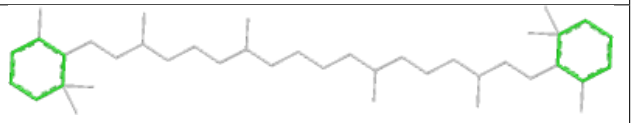
Bond lengths



Bond angles

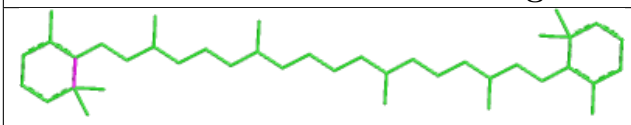


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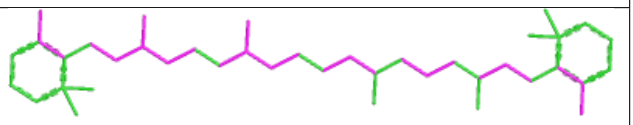


Rings

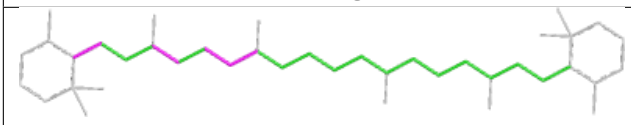
Ligand BCR 5 302



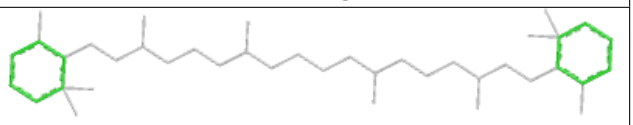
Bond lengths



Bond angles

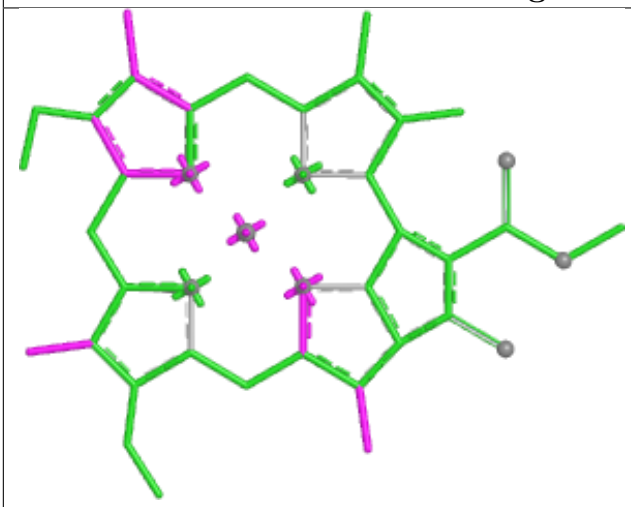


Torsions

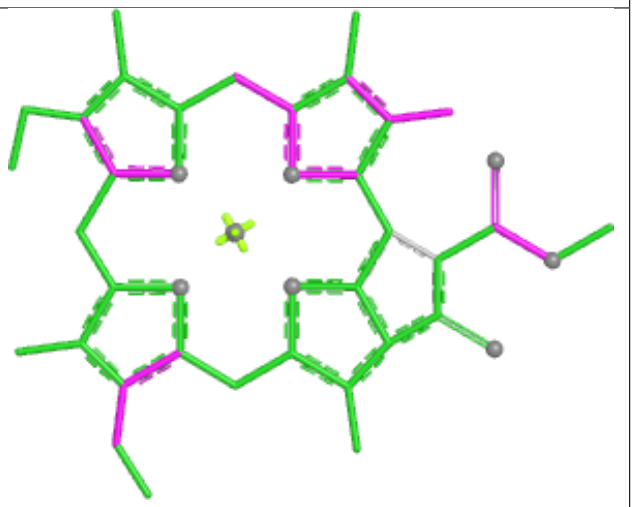


Rings

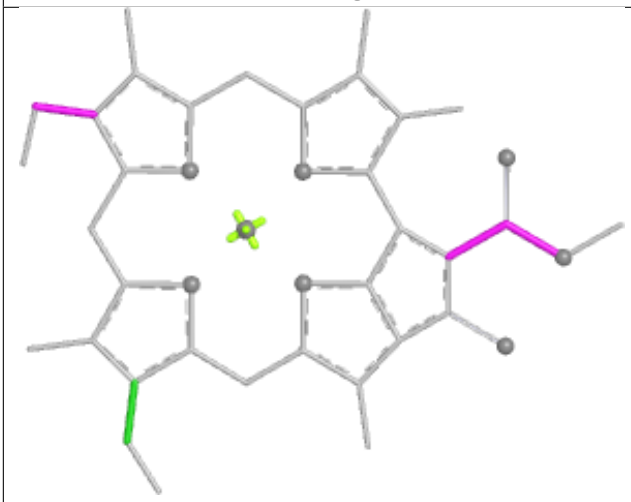
Ligand CLA 3 312



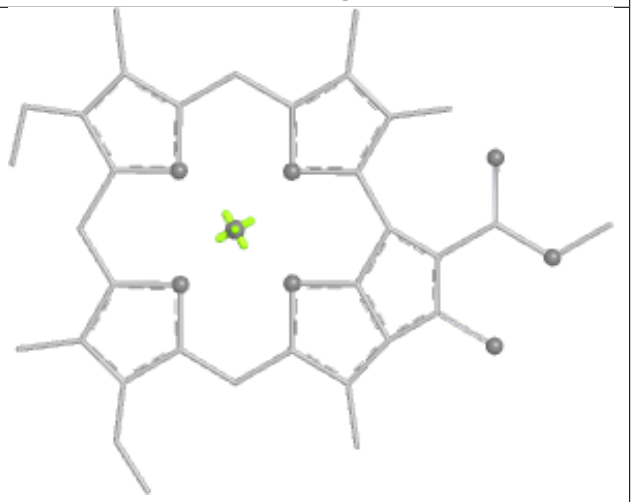
Bond lengths



Bond angles

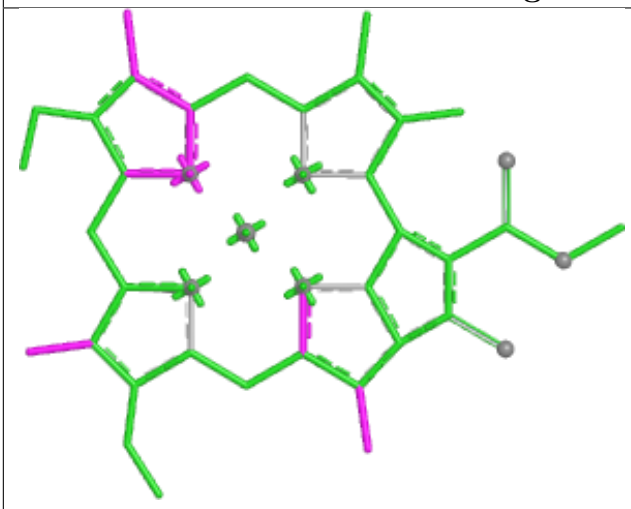


Torsions

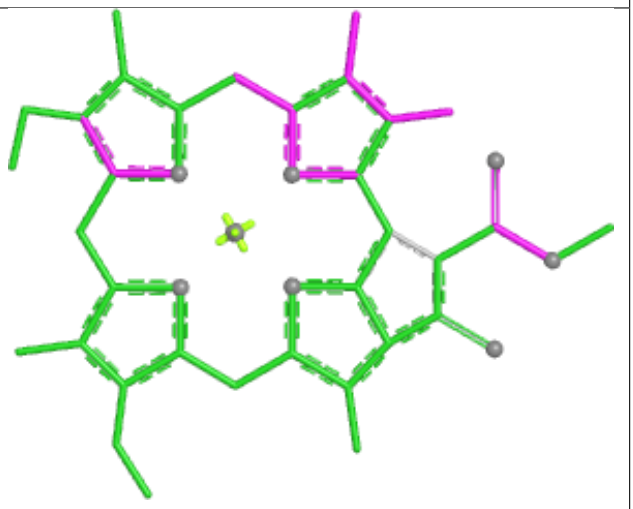


Rings

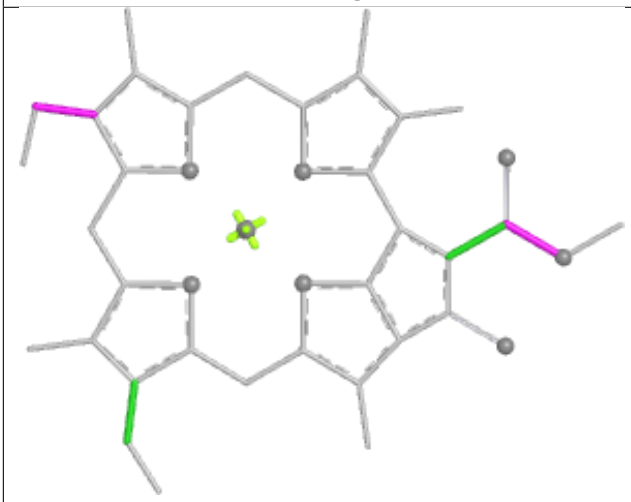
Ligand CLA A 822



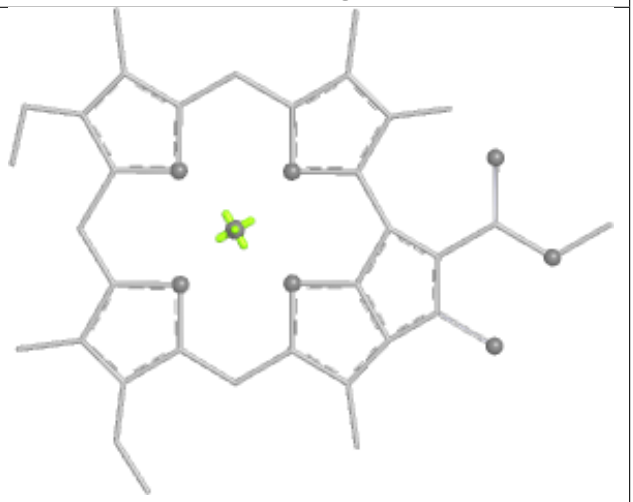
Bond lengths



Bond angles

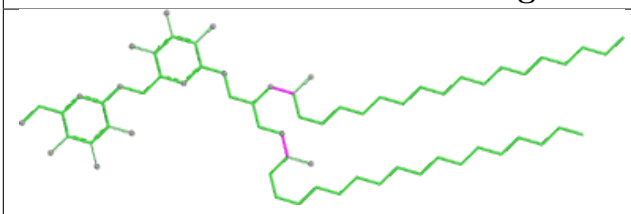


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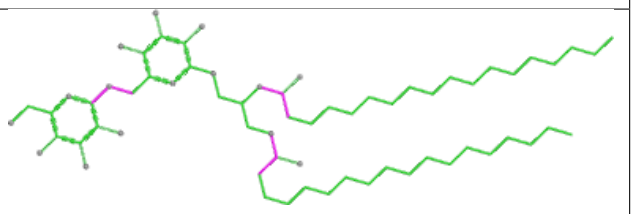


Rings

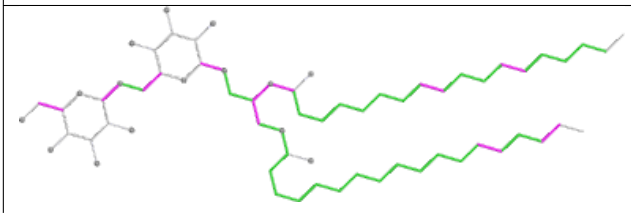
Ligand DGD m 104



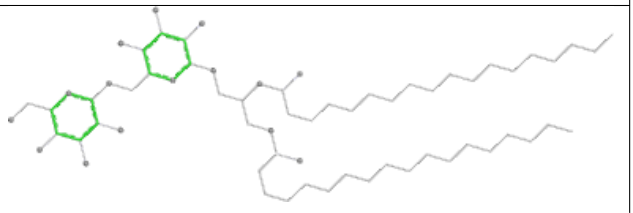
Bond lengths



Bond angles

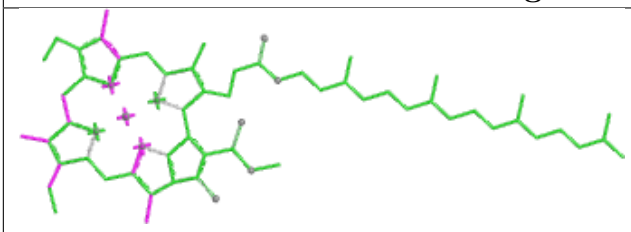


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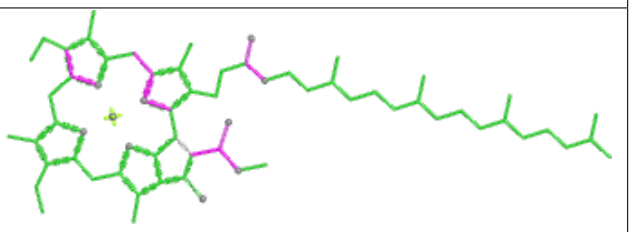


Rings

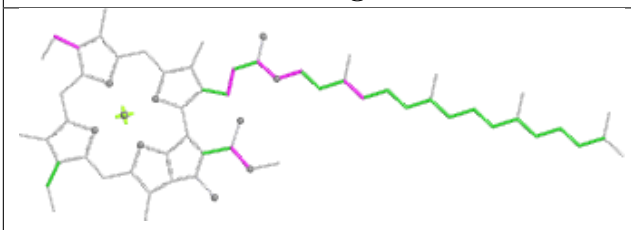
Ligand CLA B 815



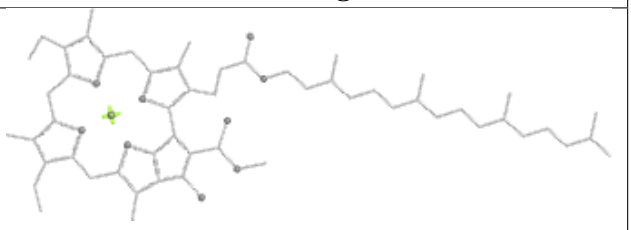
Bond lengths



Bond angles

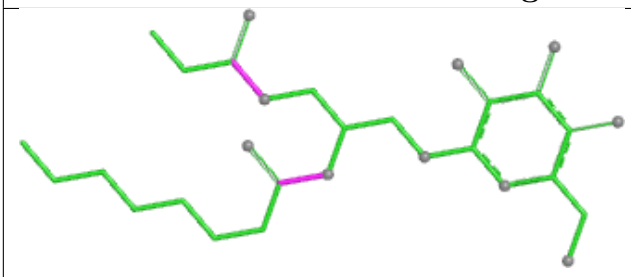


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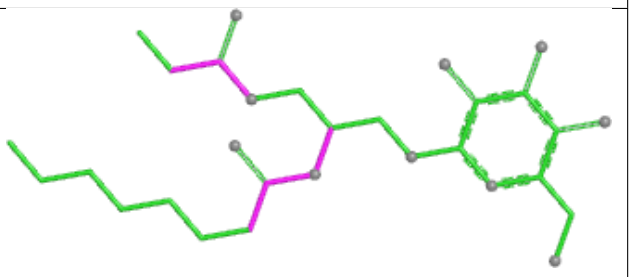


Rings

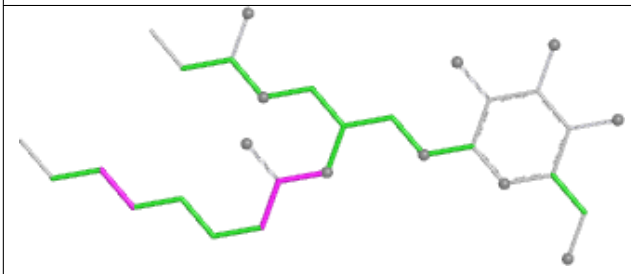
Ligand LMG F 805



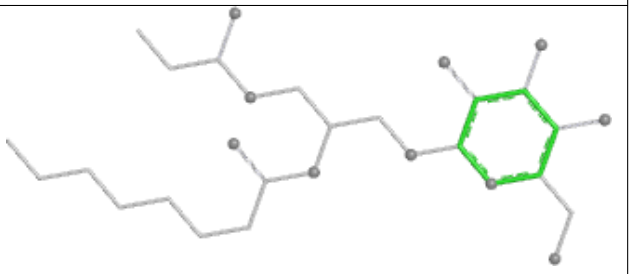
Bond lengths



Bond angles

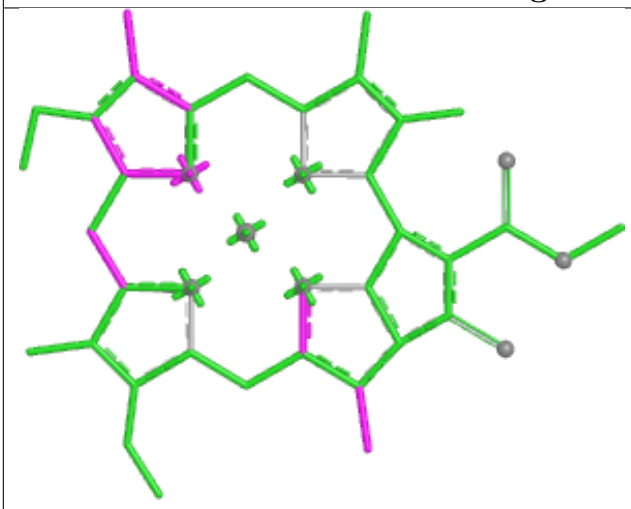


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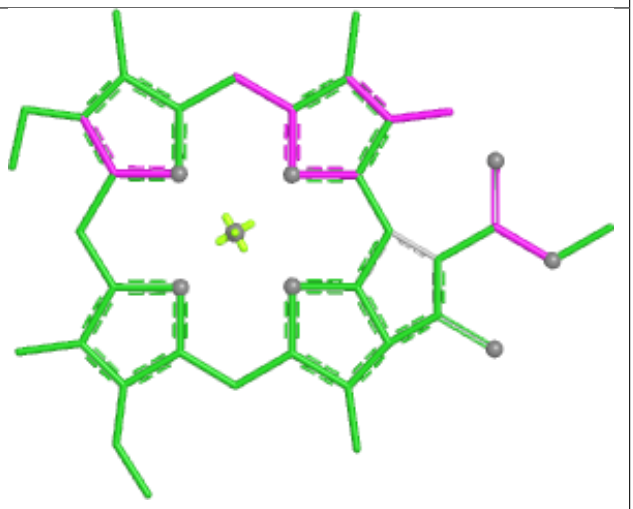


Rings

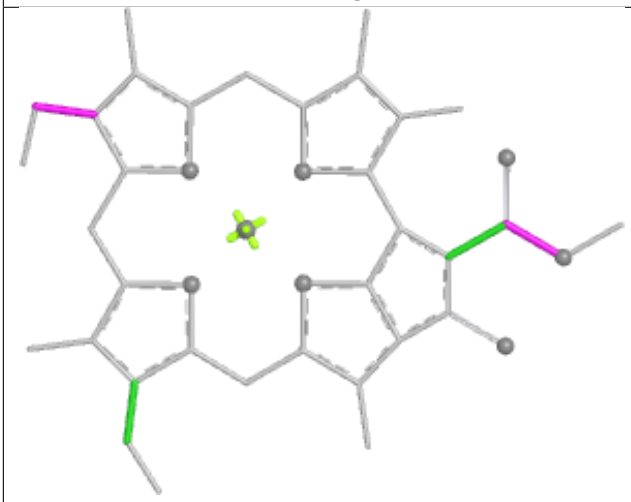
Ligand CLA r 312



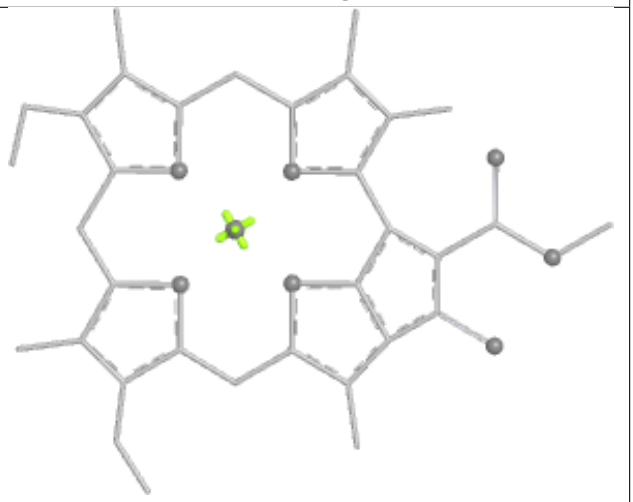
Bond lengths



Bond angles

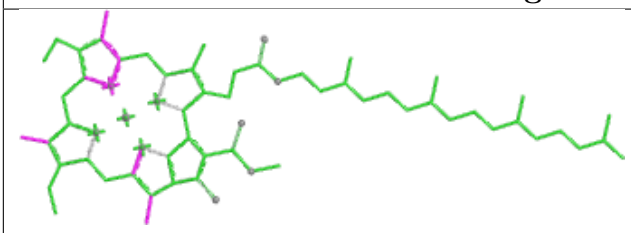


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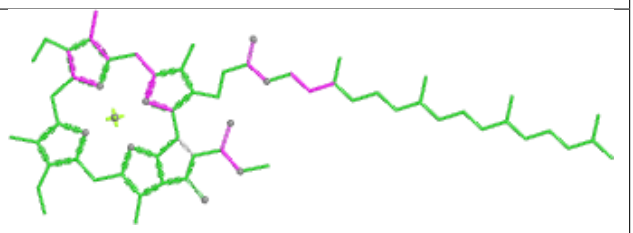


Rings

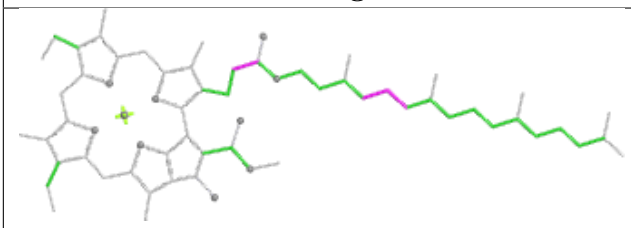
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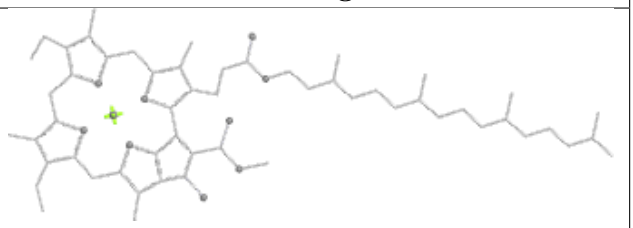
Bond lengths



Bond angles

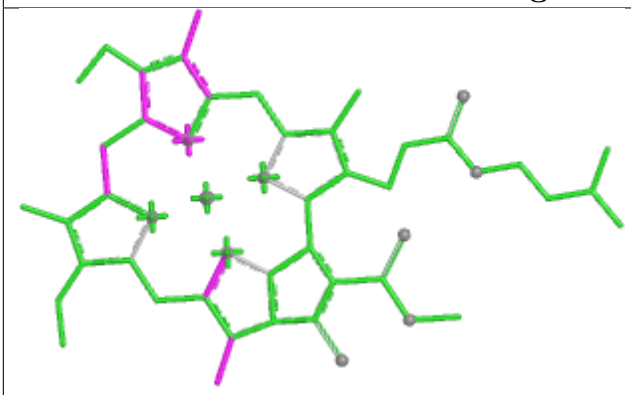


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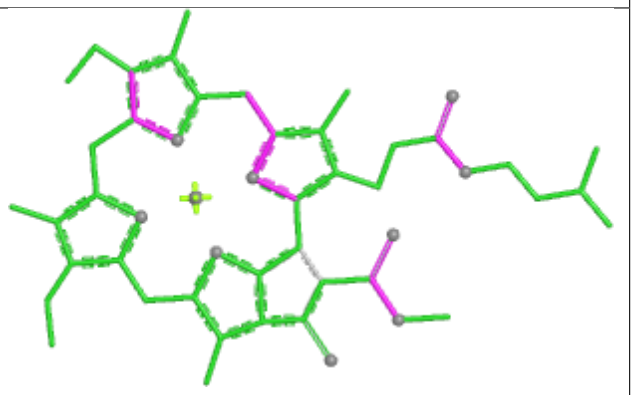


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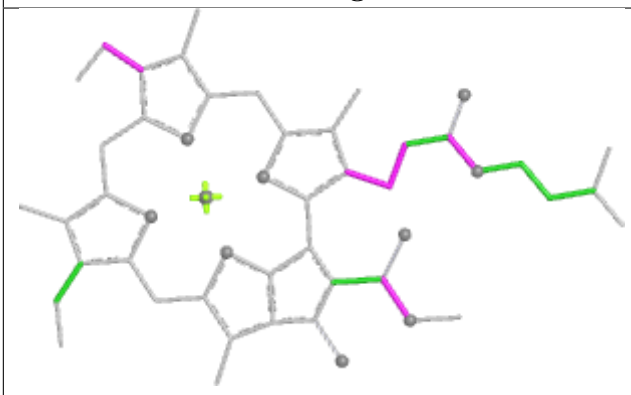
Ligand CLA s 511



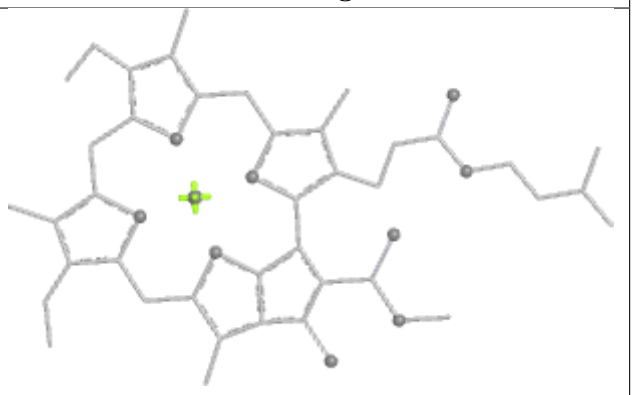
Bond lengths



Bond angles

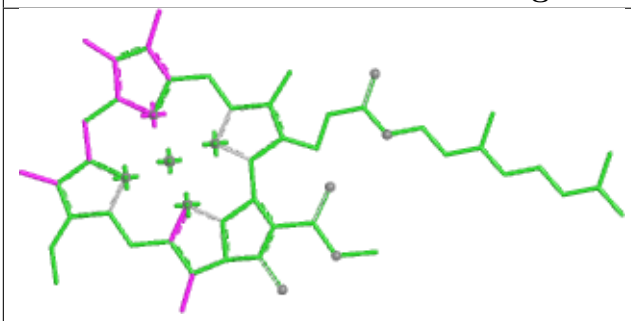


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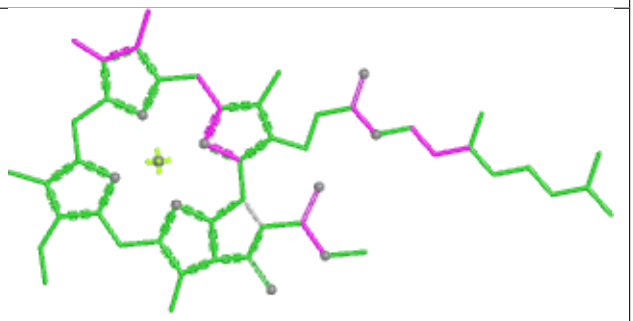


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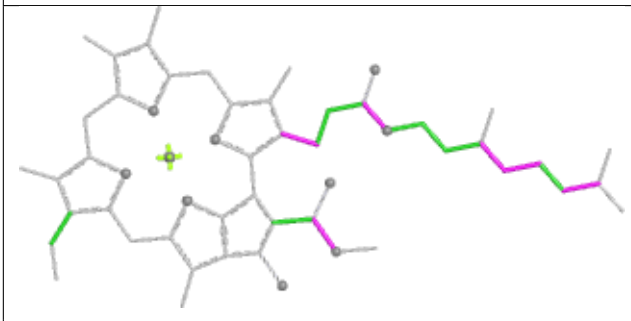
Ligand CLA f 813



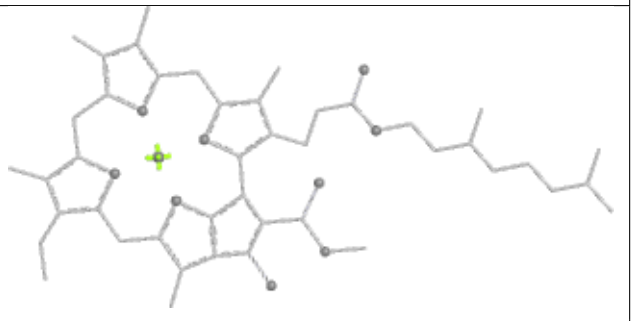
Bond lengths



Bond angles

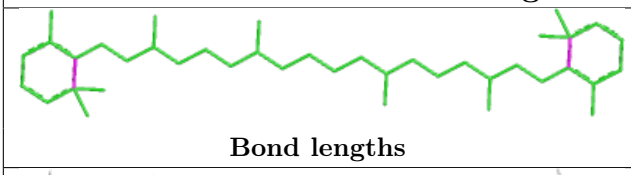


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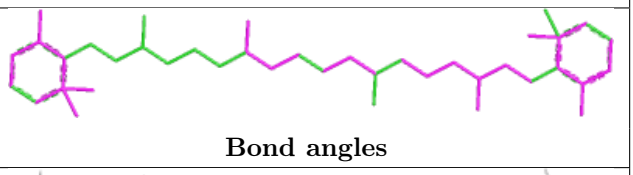


Rings

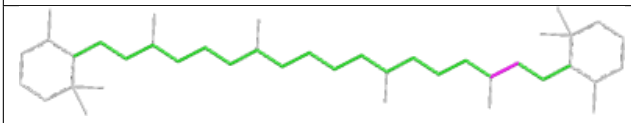
Ligand BCR A 853



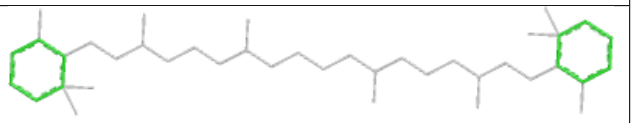
Bond lengths



Bond angles

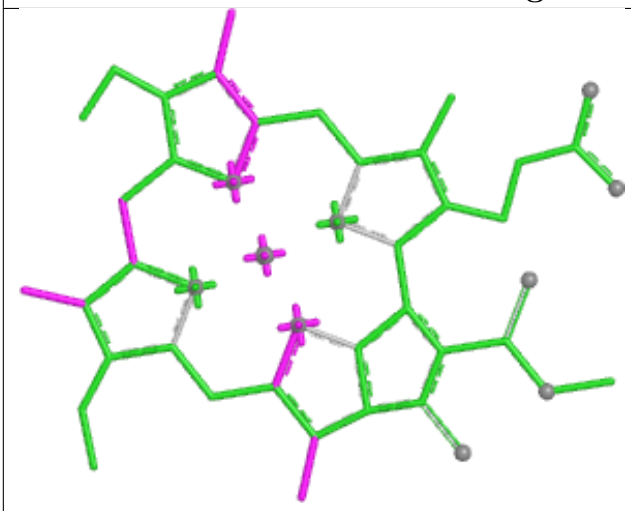


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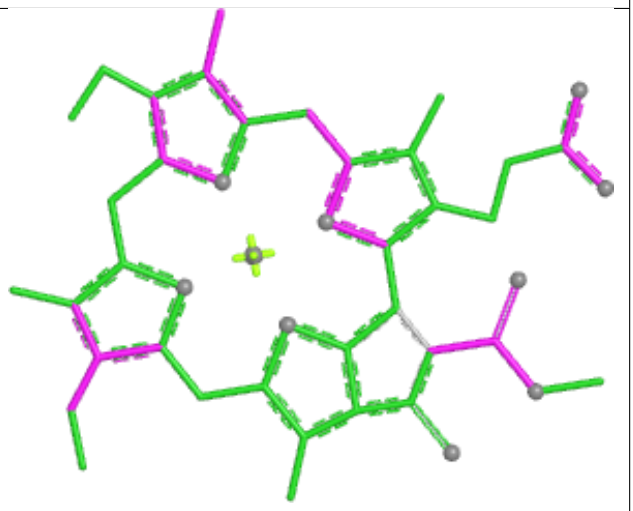


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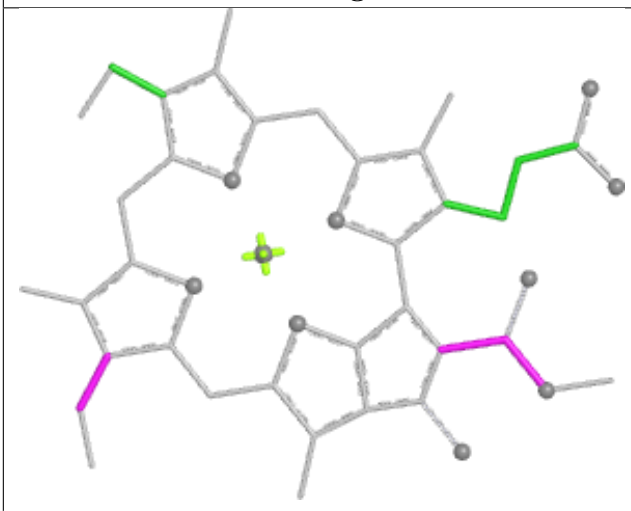
Ligand CLA L 304



Bond lengths



Bond angles

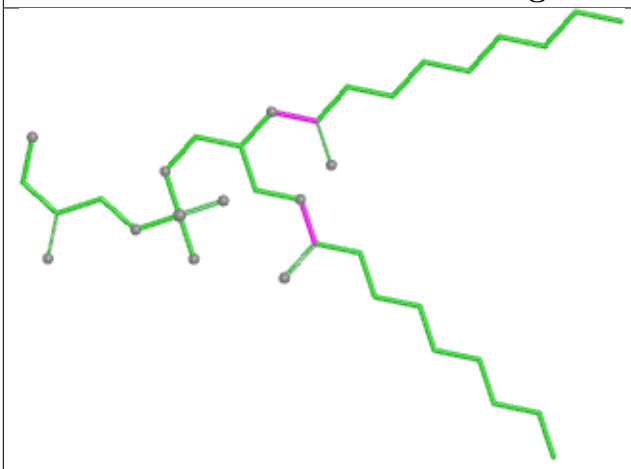


Torsions

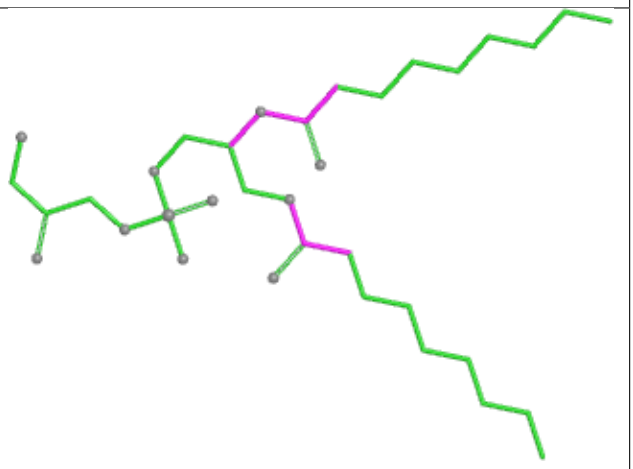


Rings

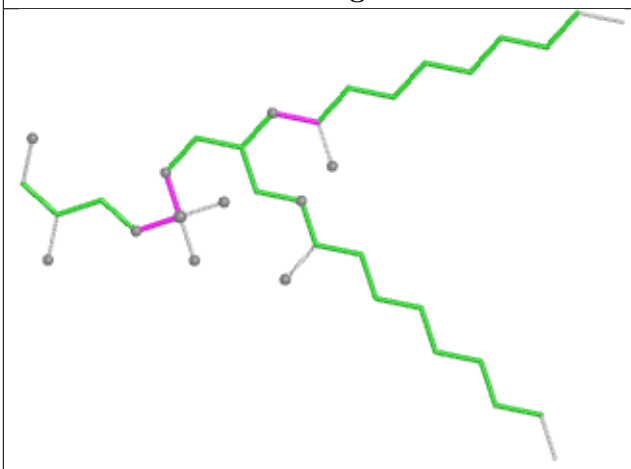
Ligand LHG s 516



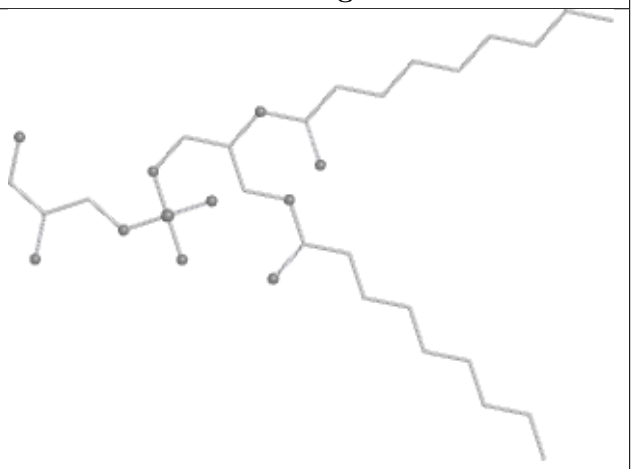
Bond lengths



Bond angles

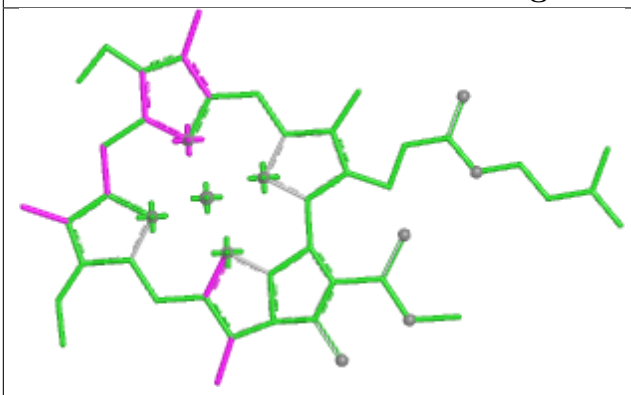


Torsions

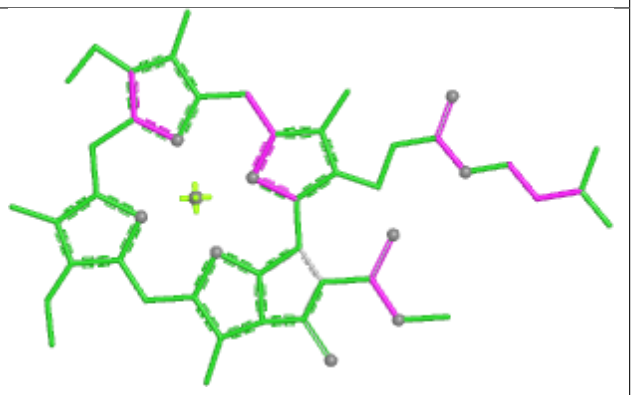


Rings

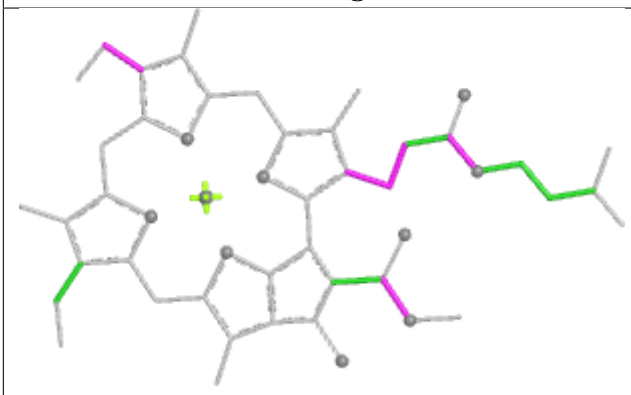
Ligand CLA s 509



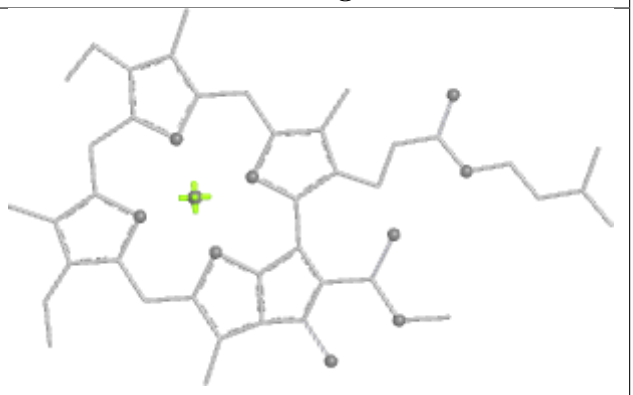
Bond lengths



Bond angles

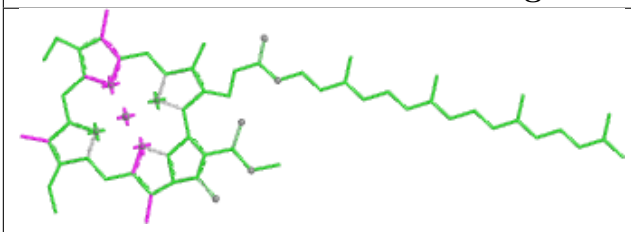


Torsions

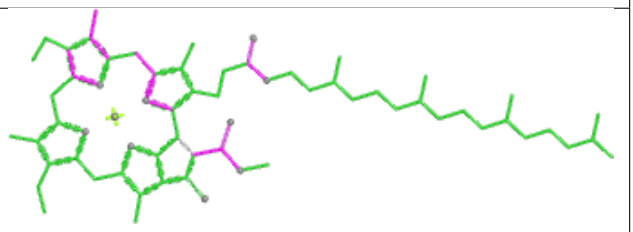


Rings

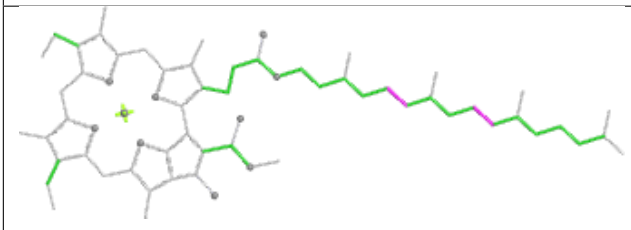
Ligand CLA B 838



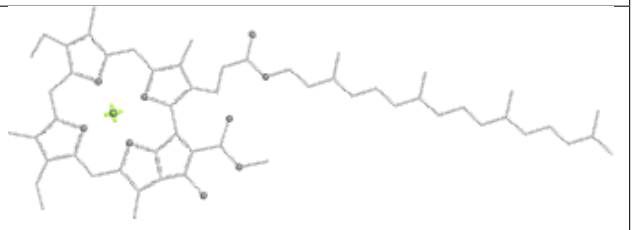
Bond lengths



Bond angles

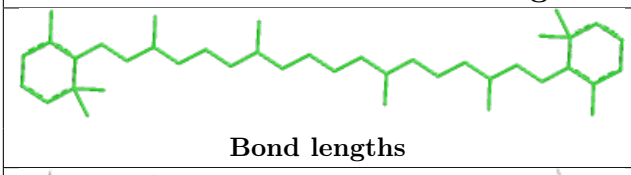


Torsions

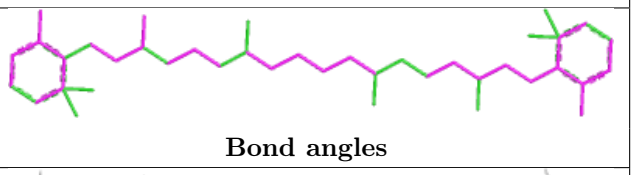


Rings

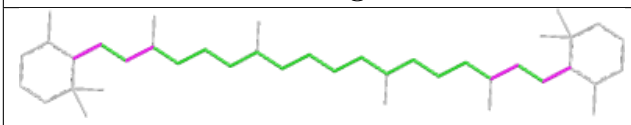
Ligand BCR l 102



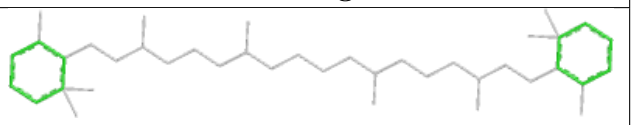
Bond lengths



Bond angles

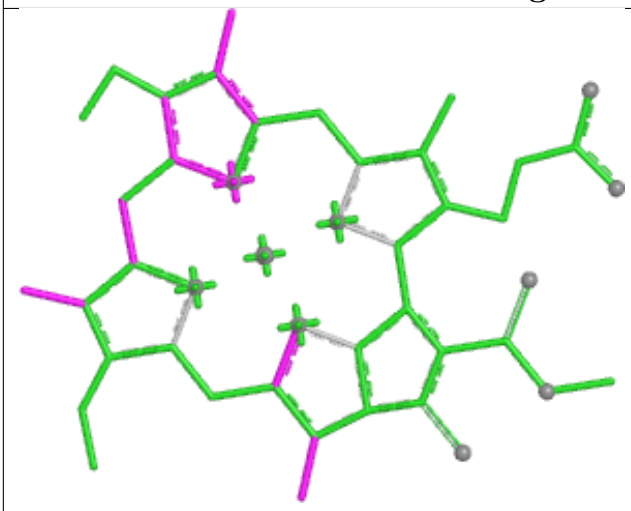


Torsions

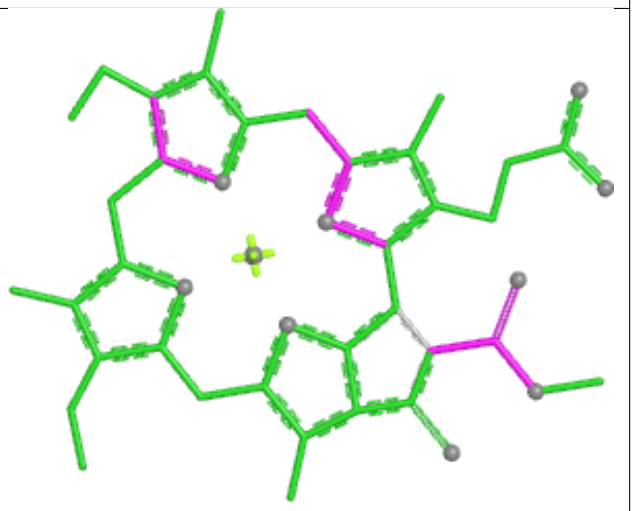


Rings

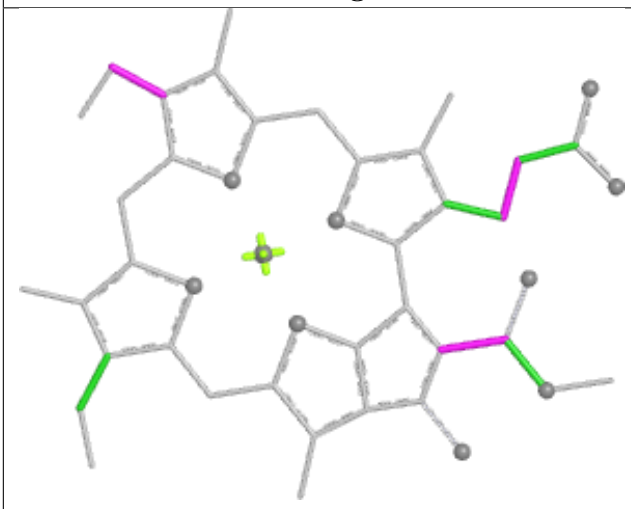
Ligand CLA e 819



Bond lengths



Bond angles

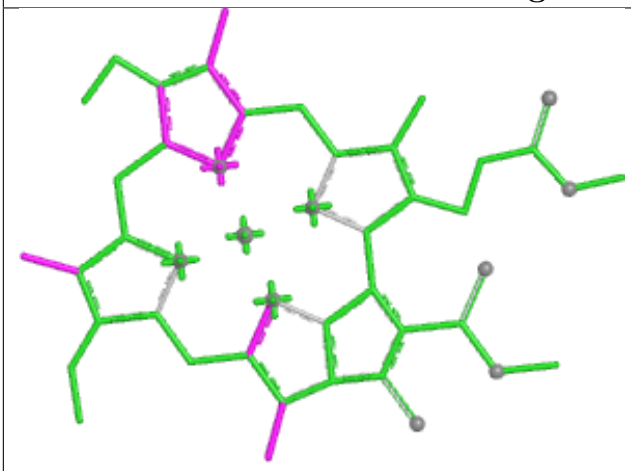


Torsions

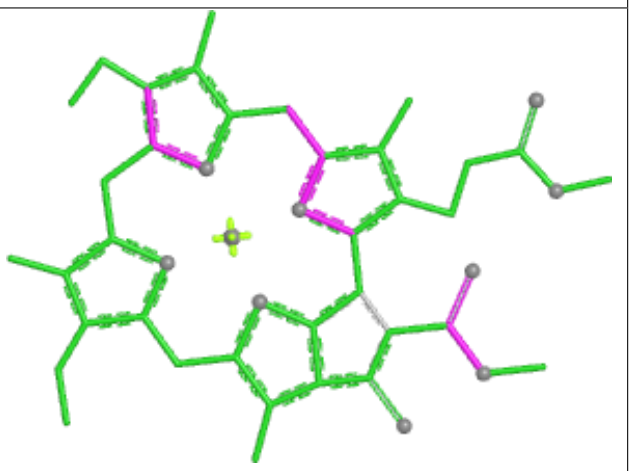


Rings

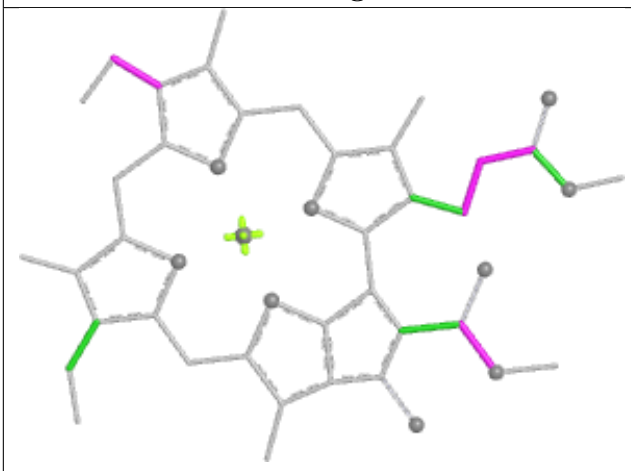
Ligand CLA 5 312



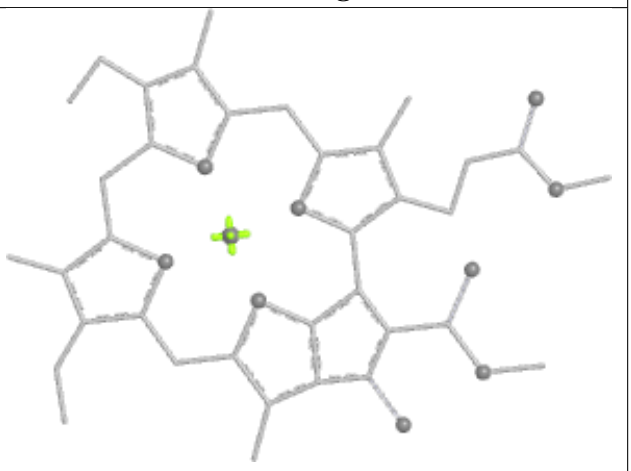
Bond lengths



Bond angles

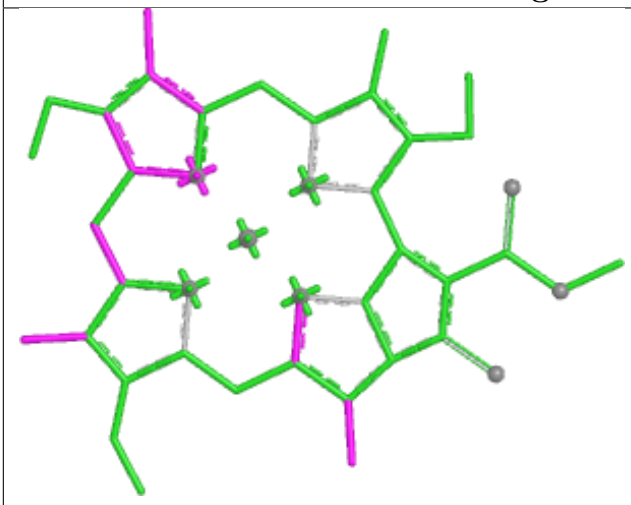


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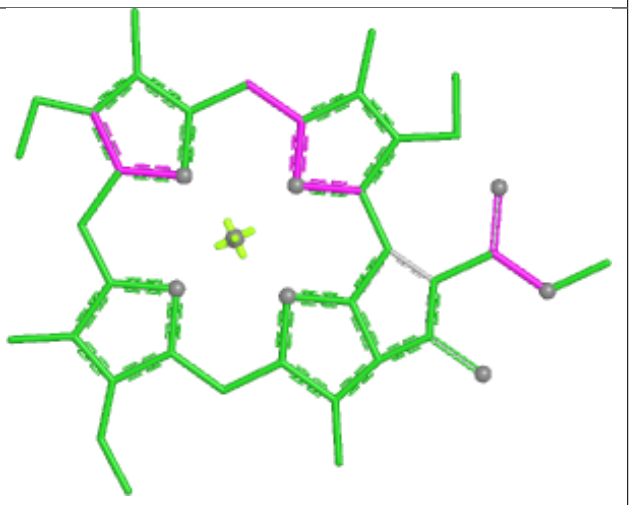


Rings

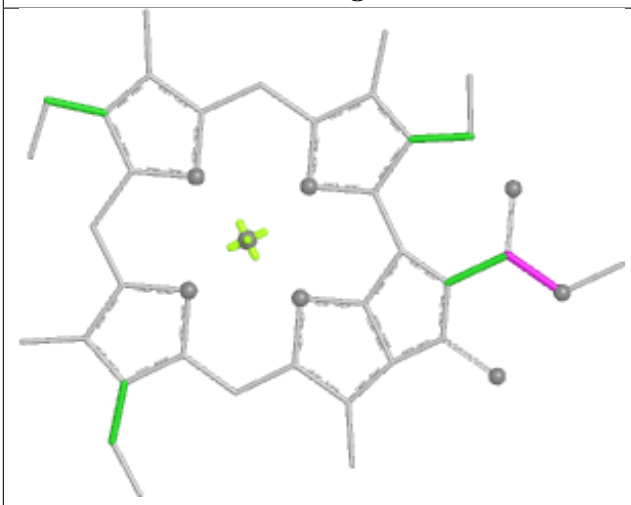
Ligand CLA f 825



Bond lengths



Bond angles

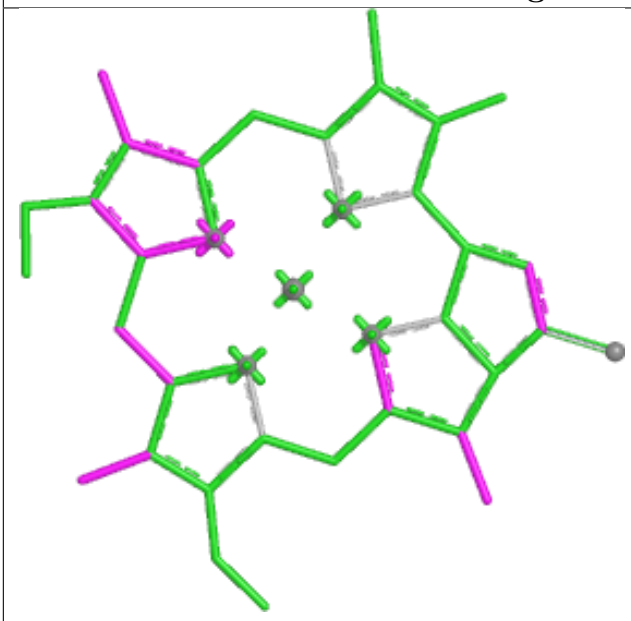


Torsions

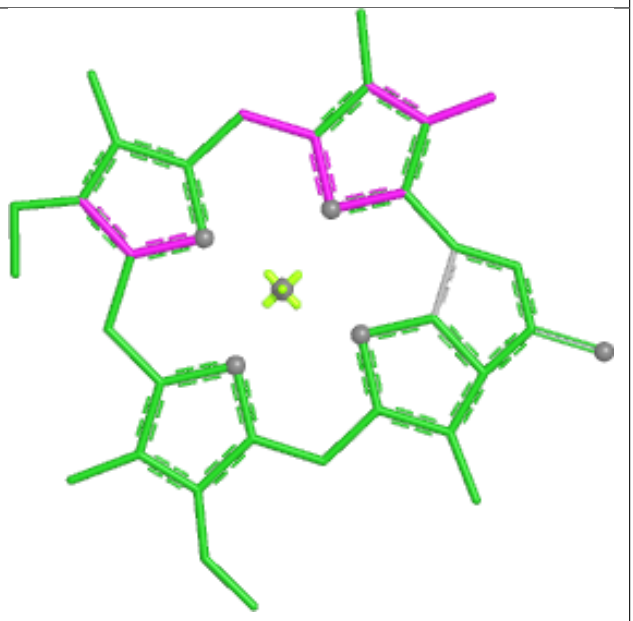


Rings

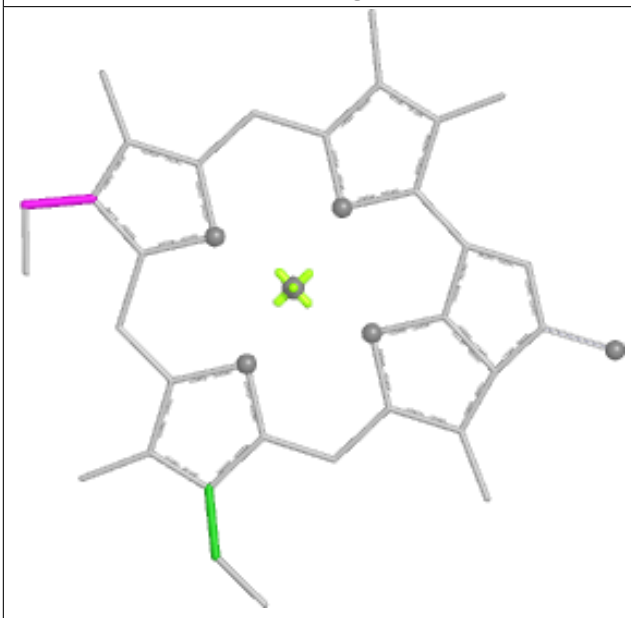
Ligand CLA n 201



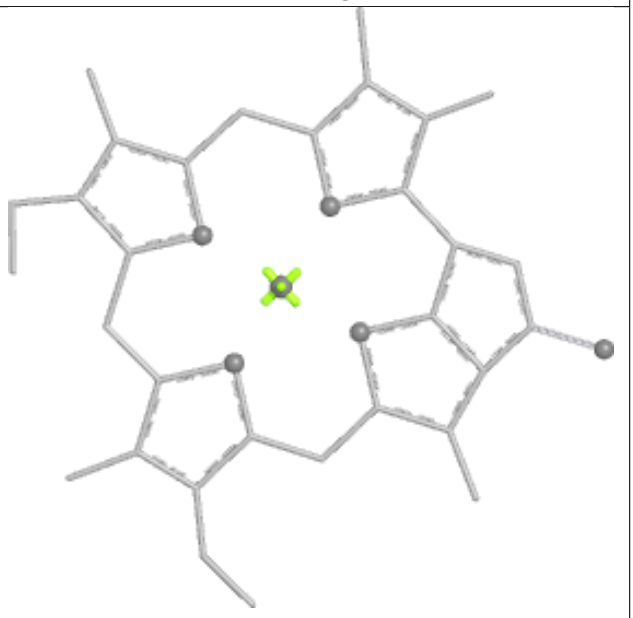
Bond lengths



Bond angles

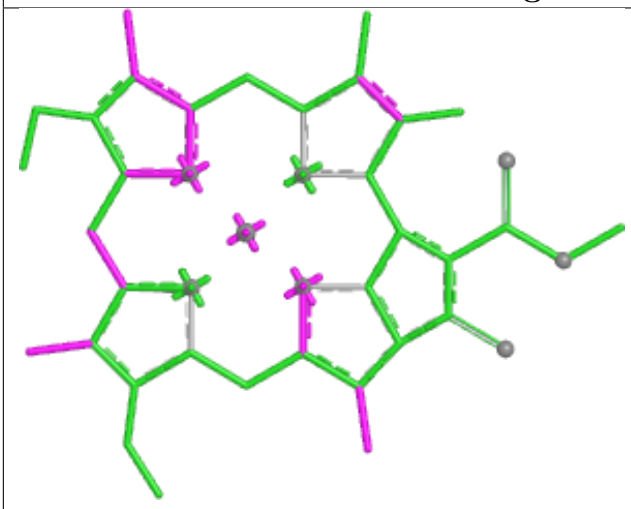


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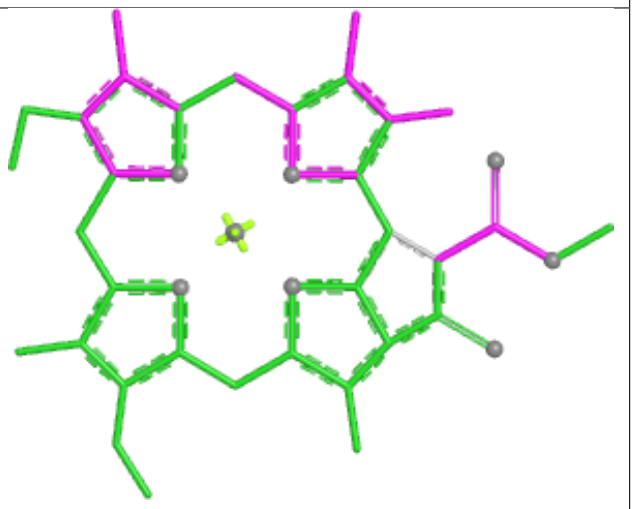


Rings

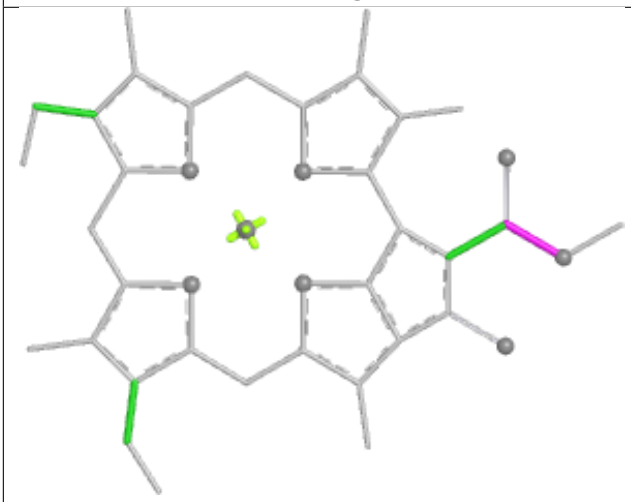
Ligand CLA A 837



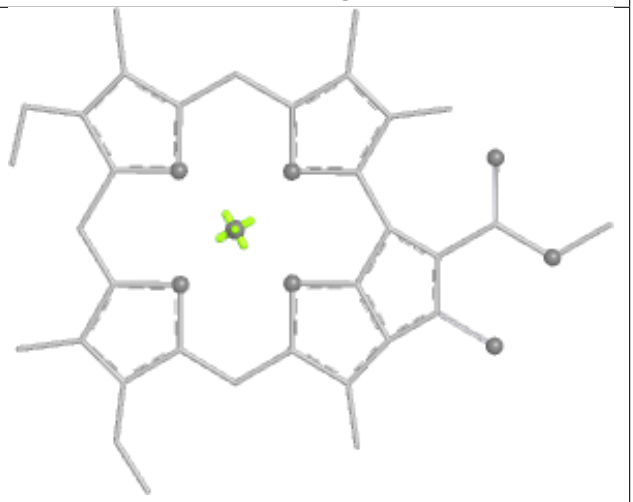
Bond lengths



Bond angles



Torsions

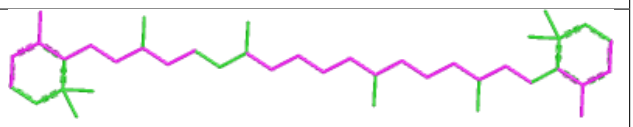


Rings

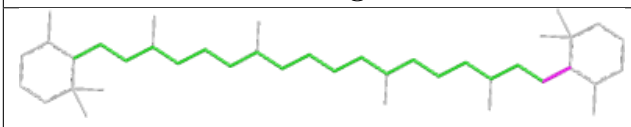
Ligand BCR o 305



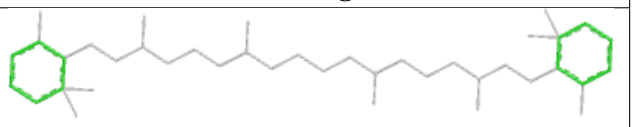
Bond lengths



Bond angles

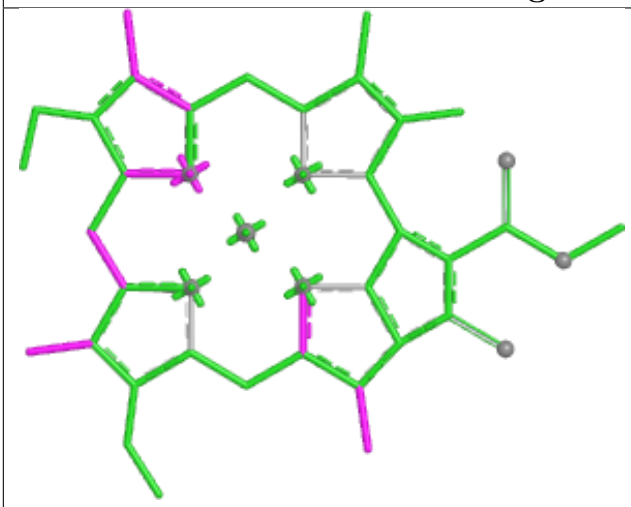


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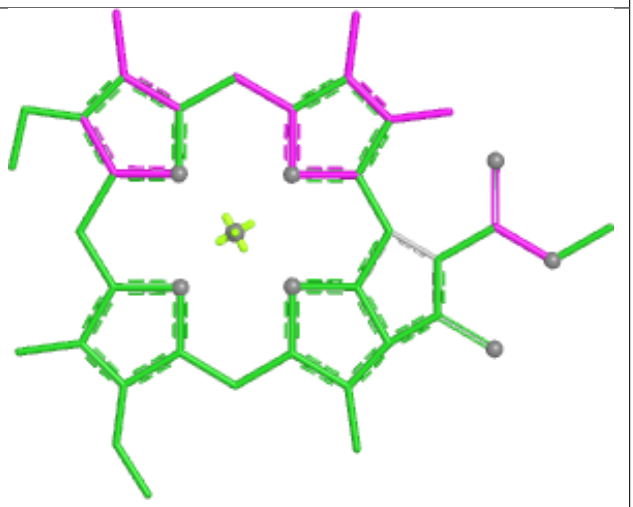


Rings

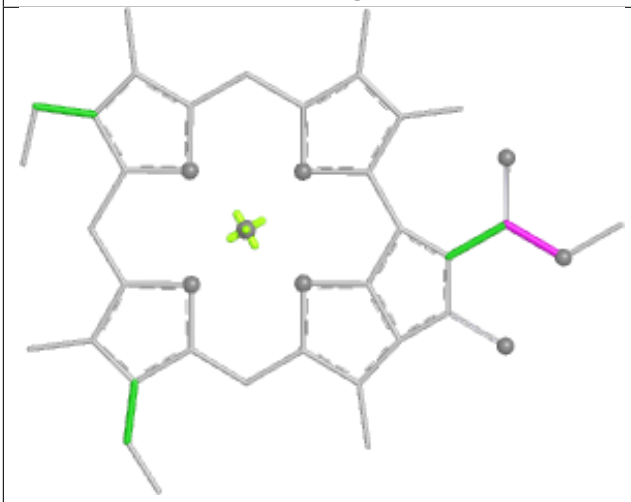
Ligand CLA 5 316



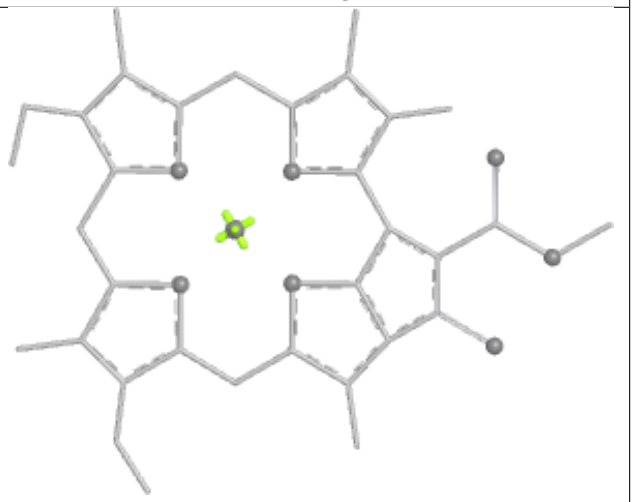
Bond lengths



Bond angles

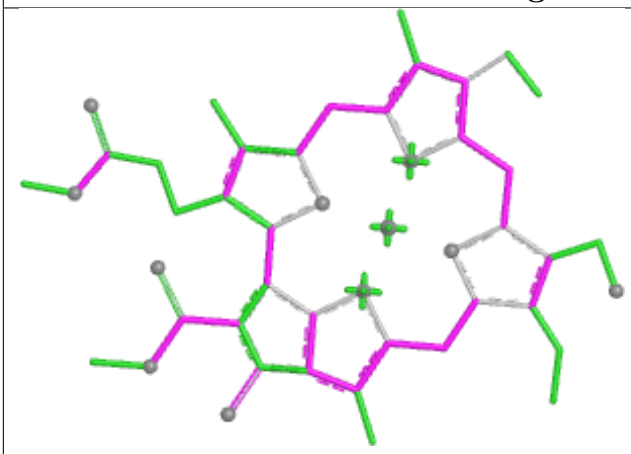


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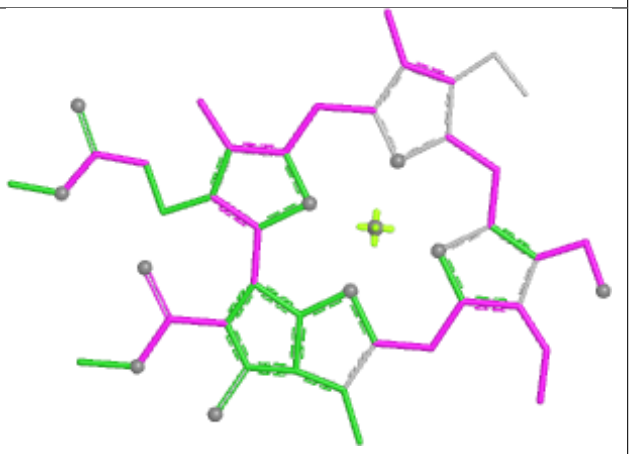


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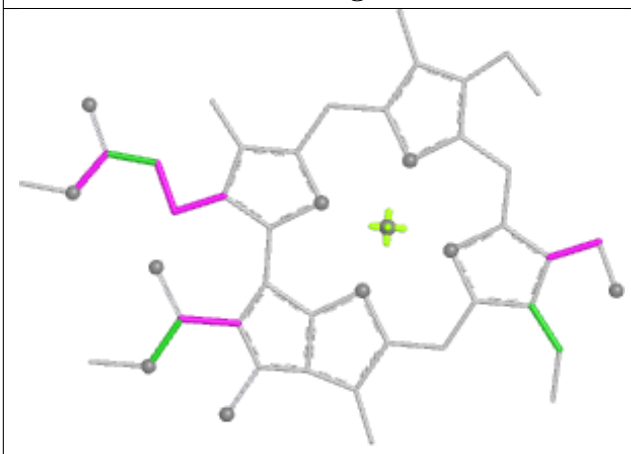
Ligand CHL 5 314



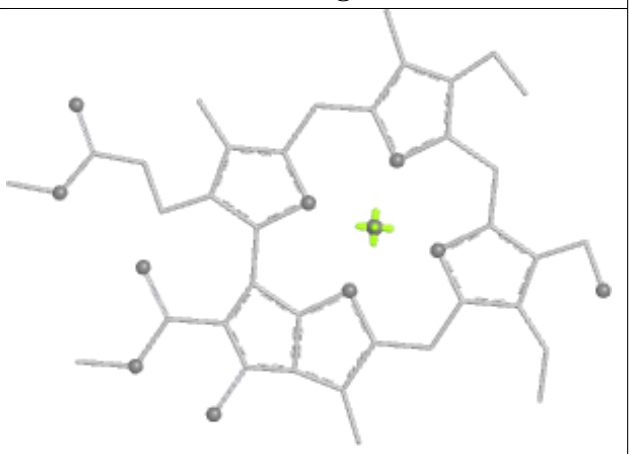
Bond lengths



Bond angles

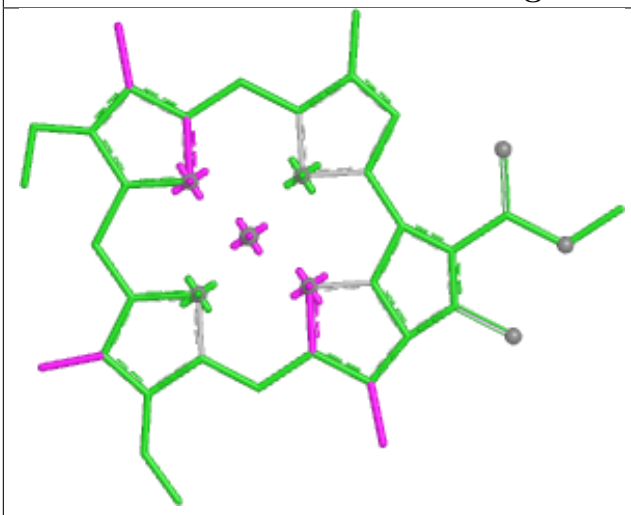


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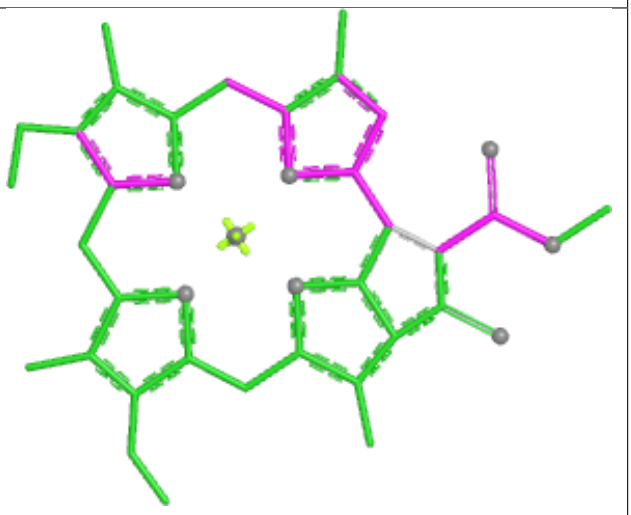


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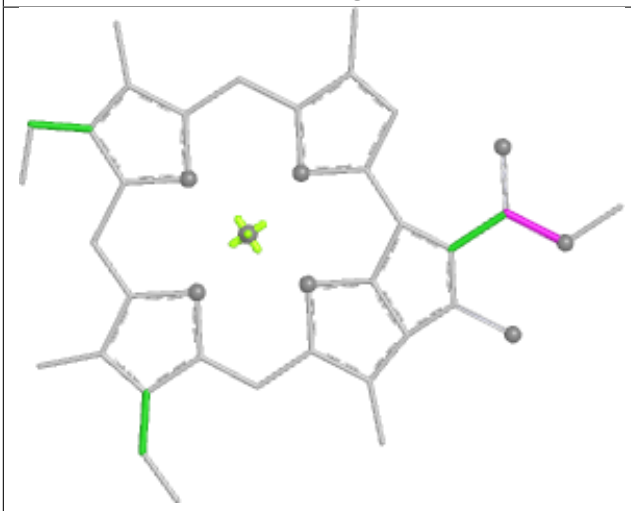
Ligand CLA B 829



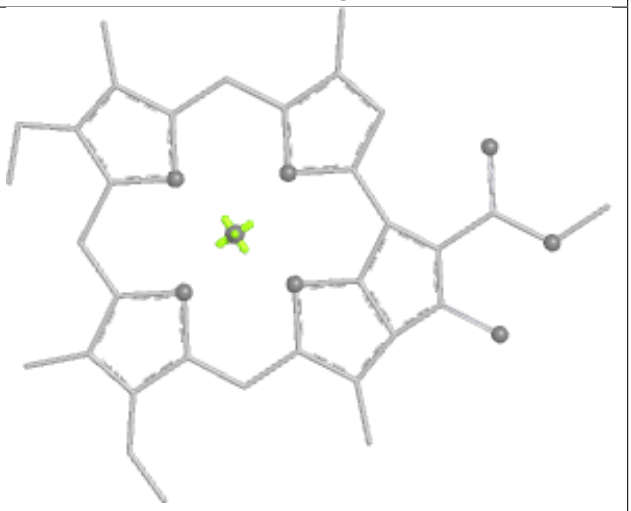
Bond lengths



Bond angles

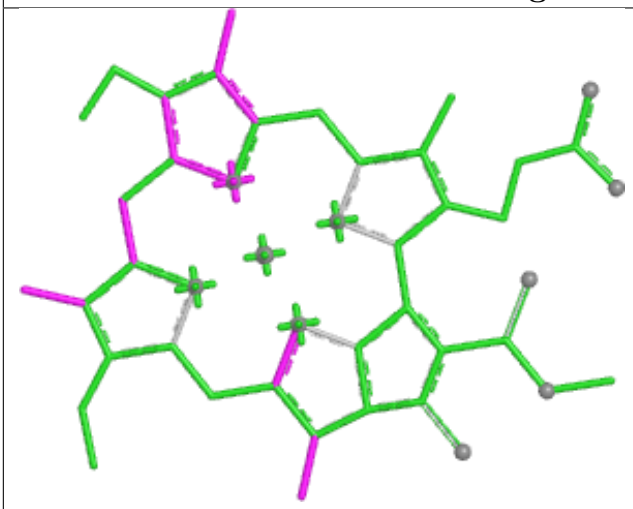


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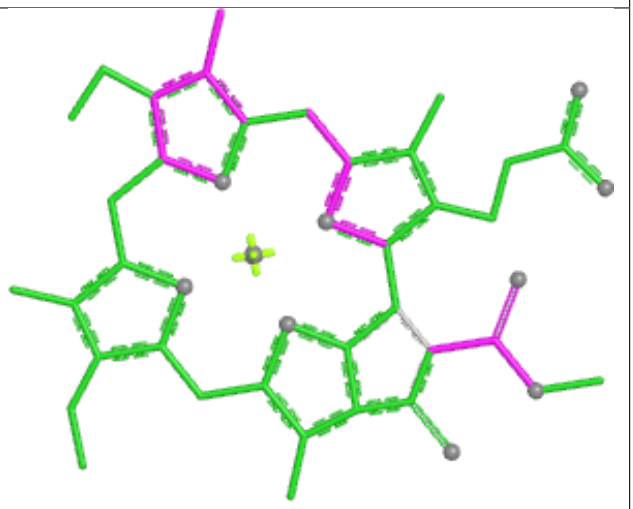


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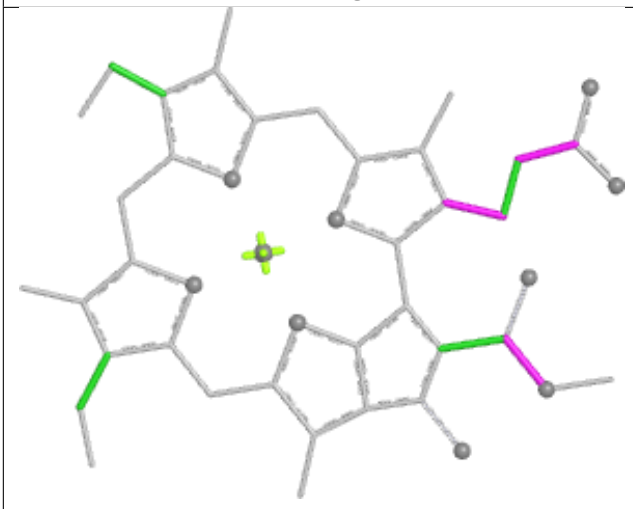
Ligand CLA e 853



Bond lengths



Bond angles

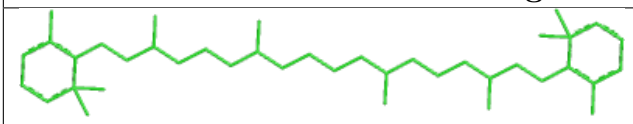


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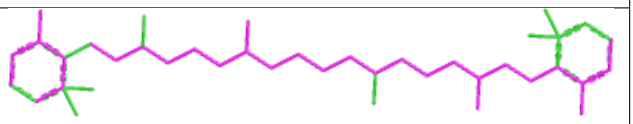


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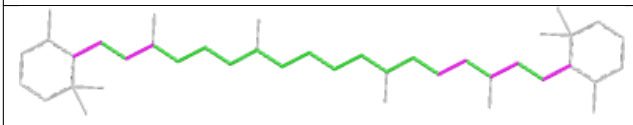
Ligand BCR n 204



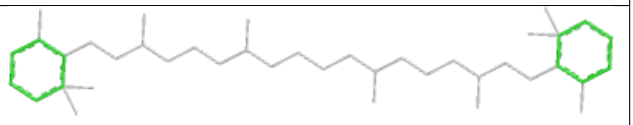
Bond lengths



Bond angles

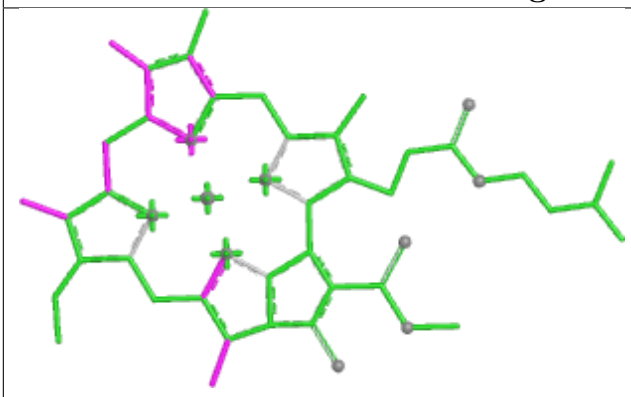


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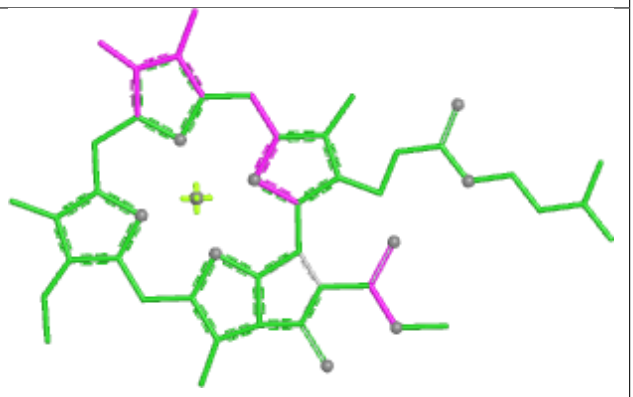


Rings

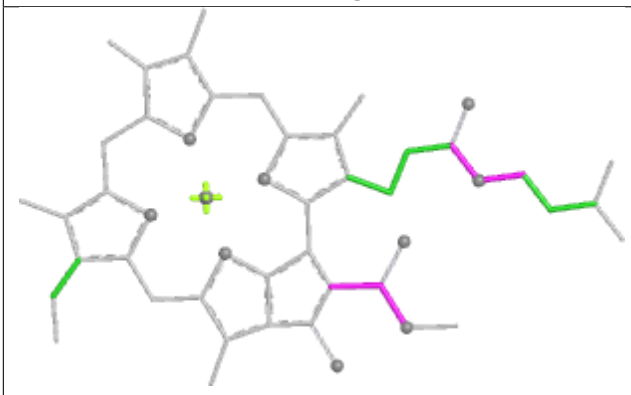
Ligand CLA e 843



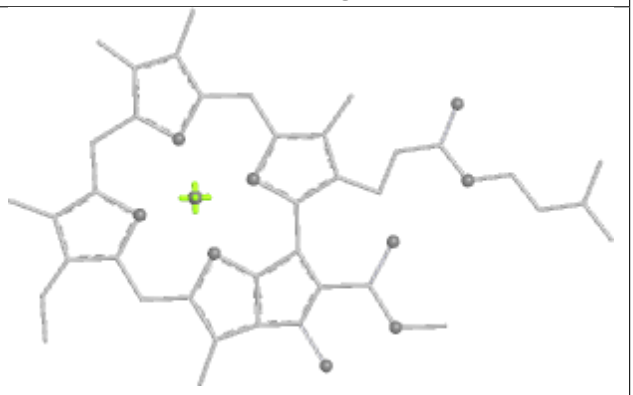
Bond lengths



Bond angles

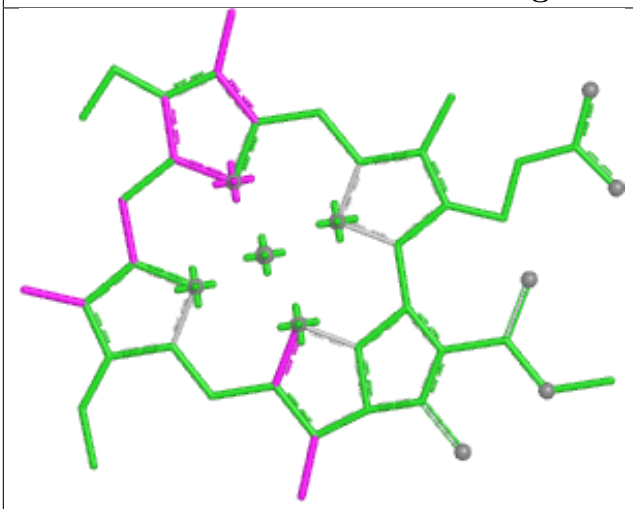


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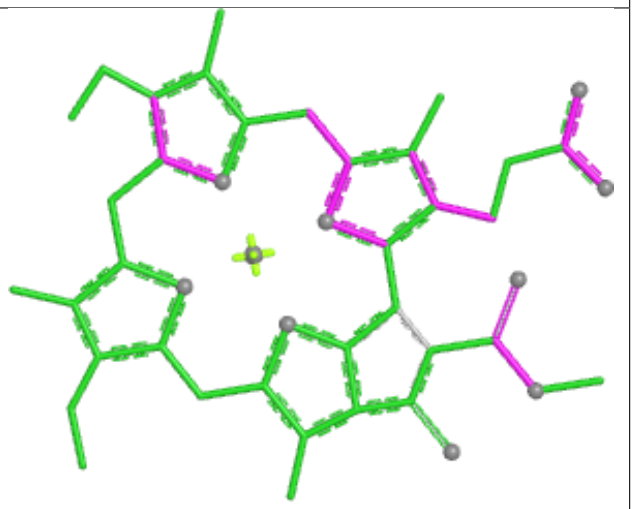


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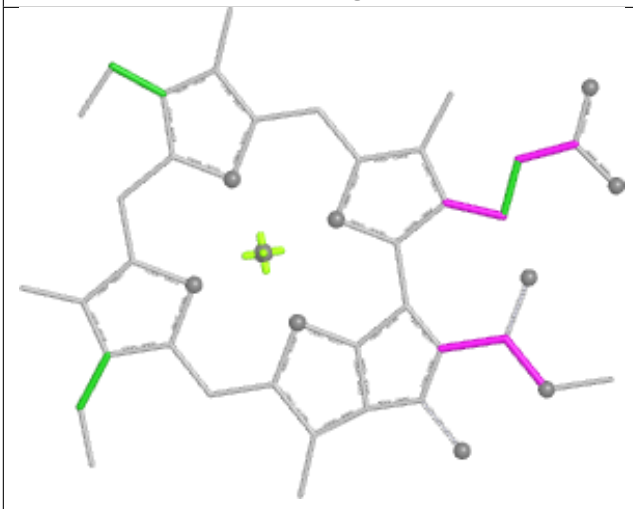
Ligand CLA f 835



Bond lengths



Bond angles

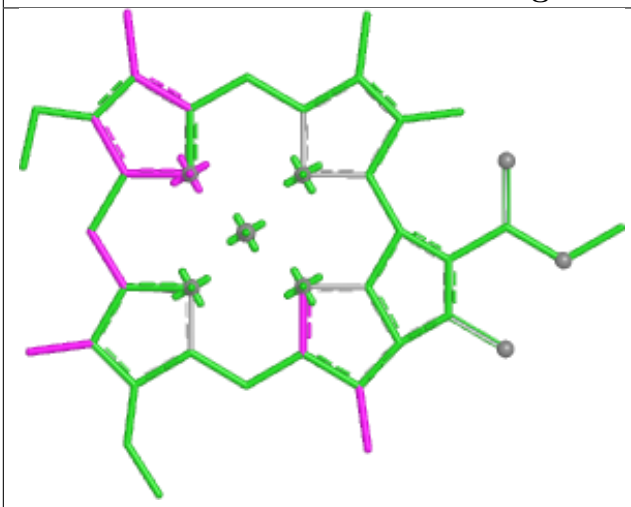


Torsions

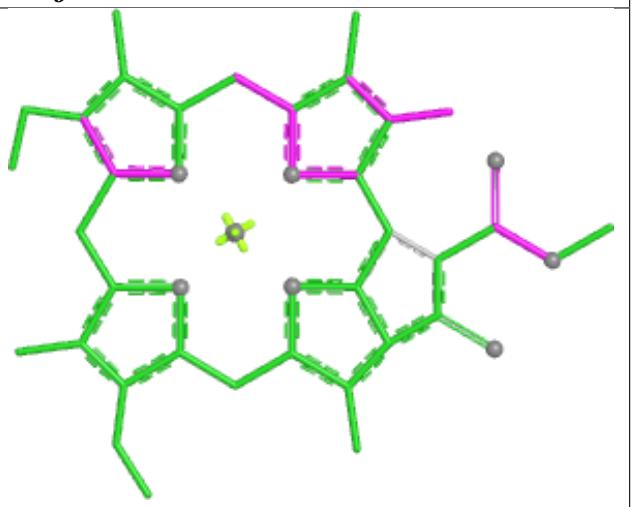


Rings

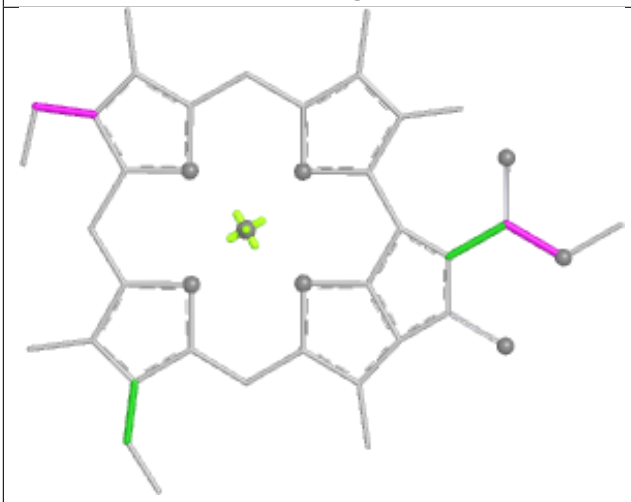
Ligand CLA j 802



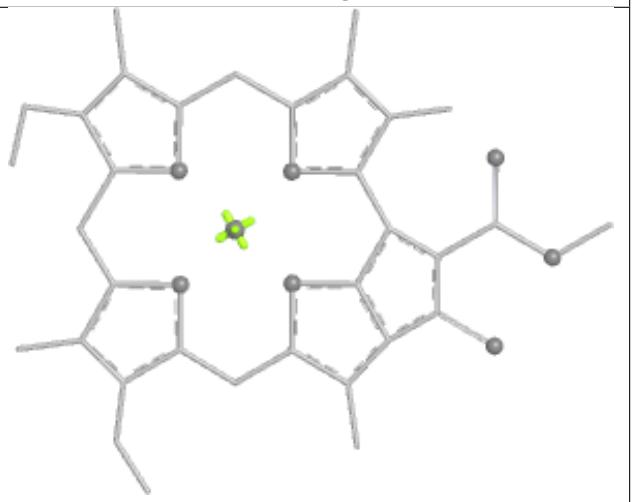
Bond lengths



Bond angles

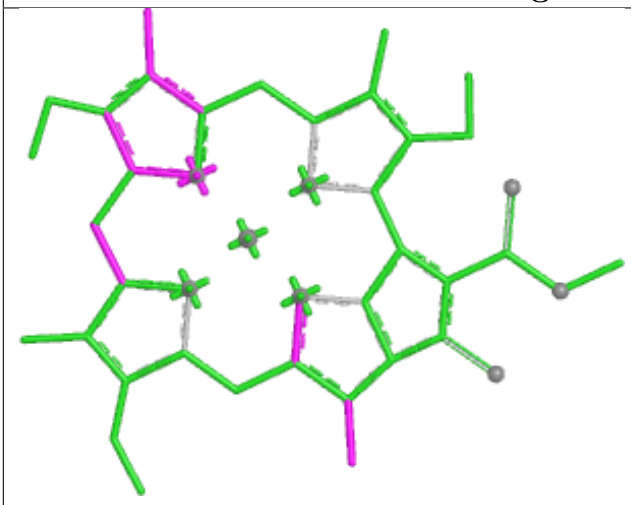


Torsions

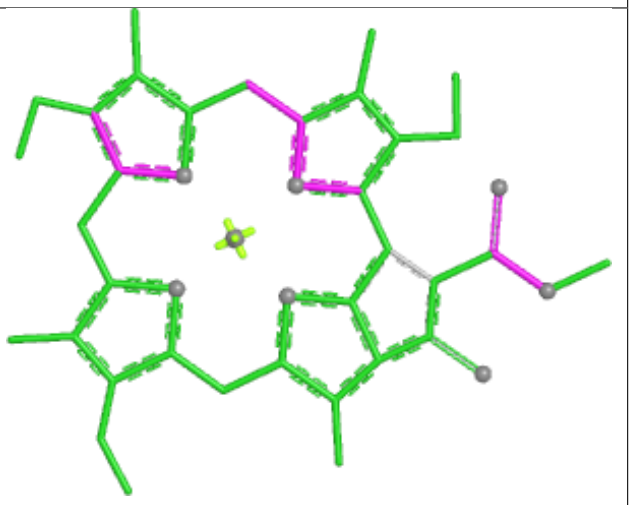


Rings

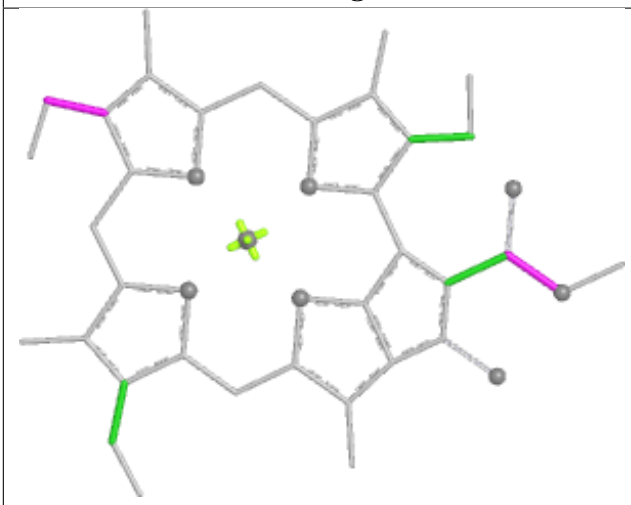
Ligand CLA f 837



Bond lengths



Bond angles

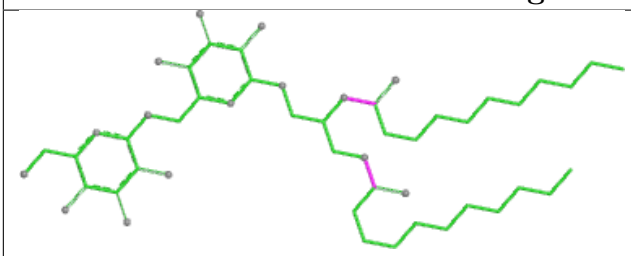


Torsions

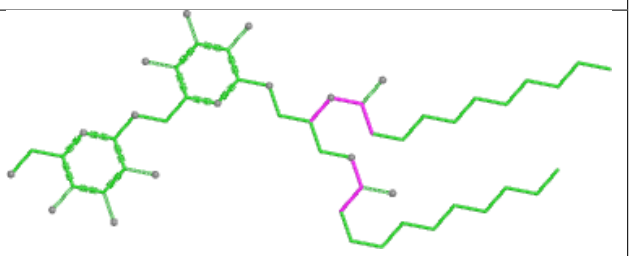


Rings

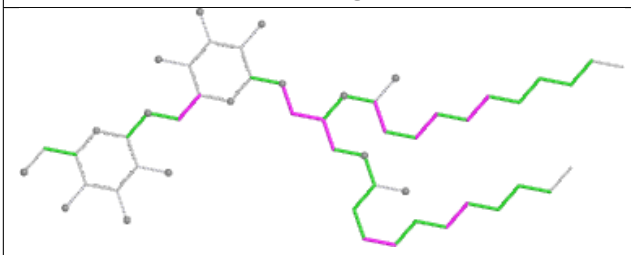
Ligand DGD f 851



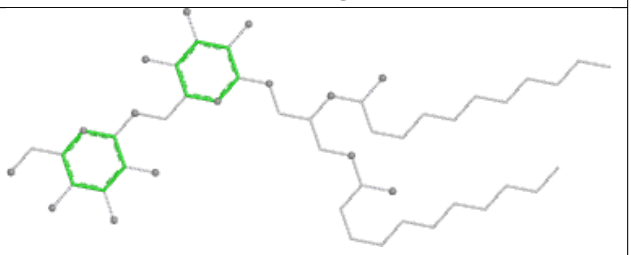
Bond lengths



Bond angles

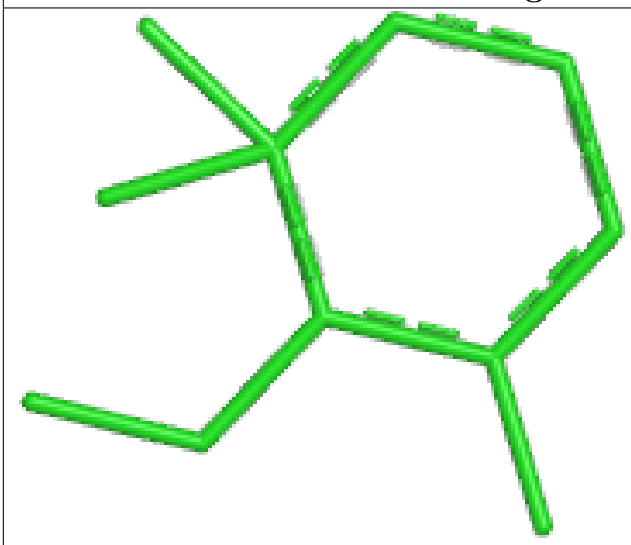


Torsions



Rings

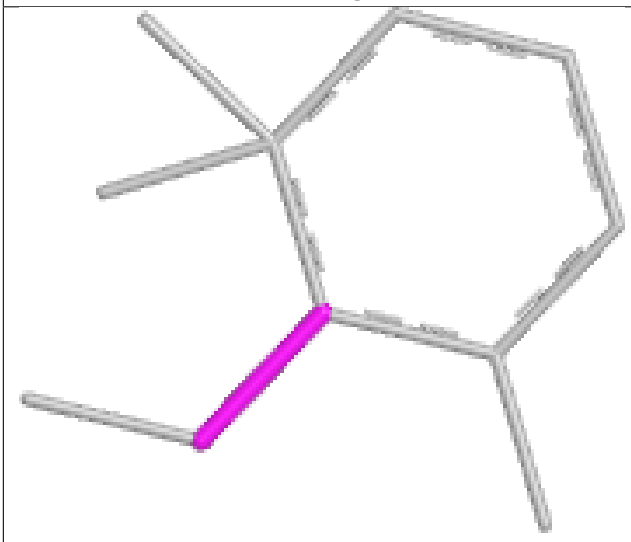
Ligand BCR p 503



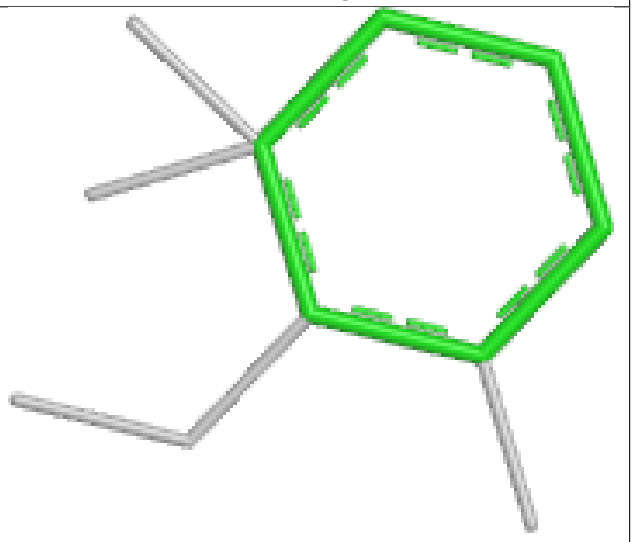
Bond lengths



Bond angles

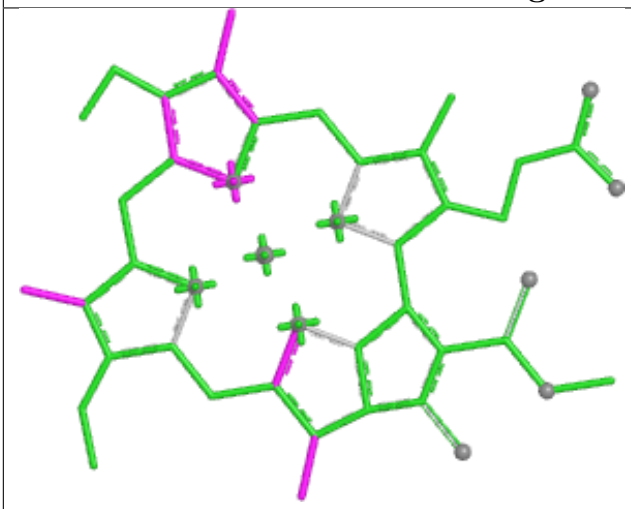


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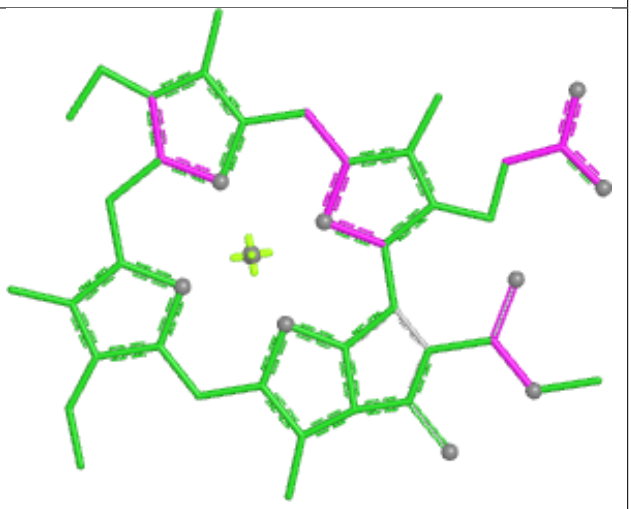


Rings

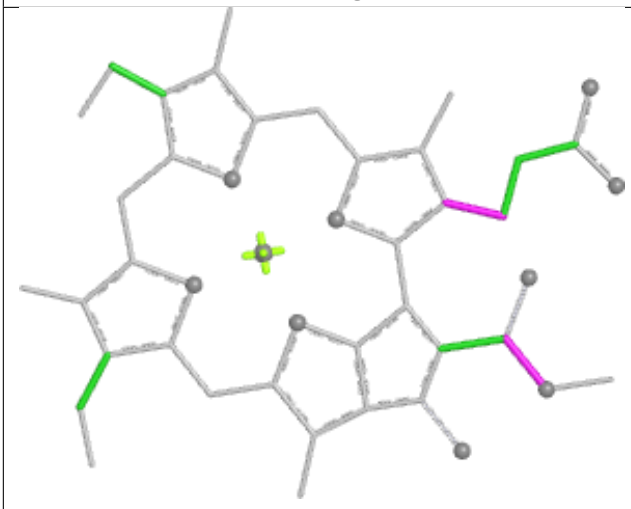
Ligand CLA 3 310



Bond lengths



Bond angles

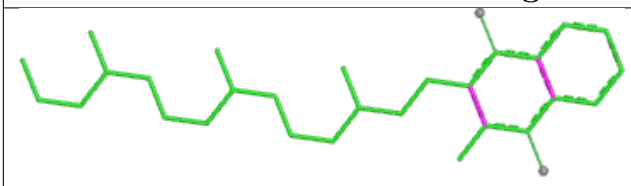


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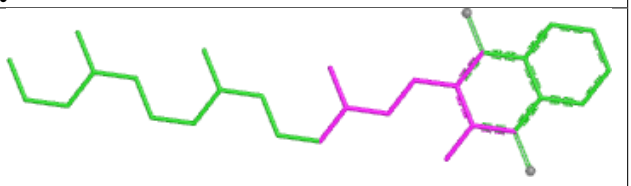


Rings

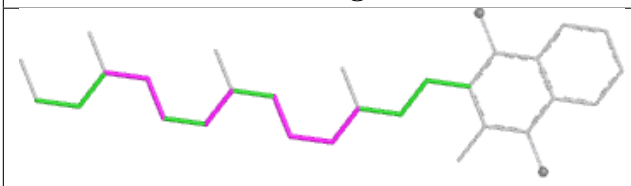
Ligand PQN B 843



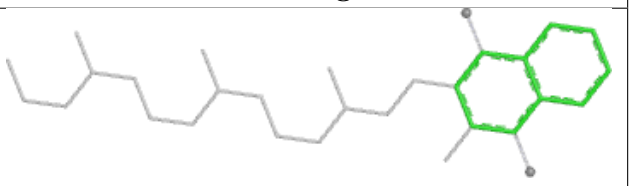
Bond lengths



Bond angles

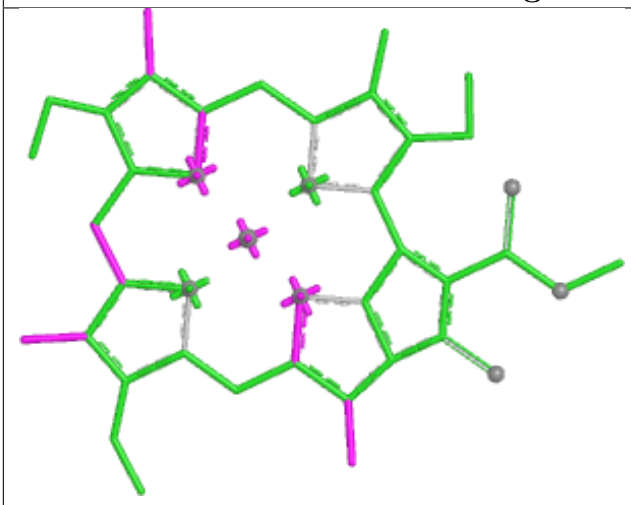


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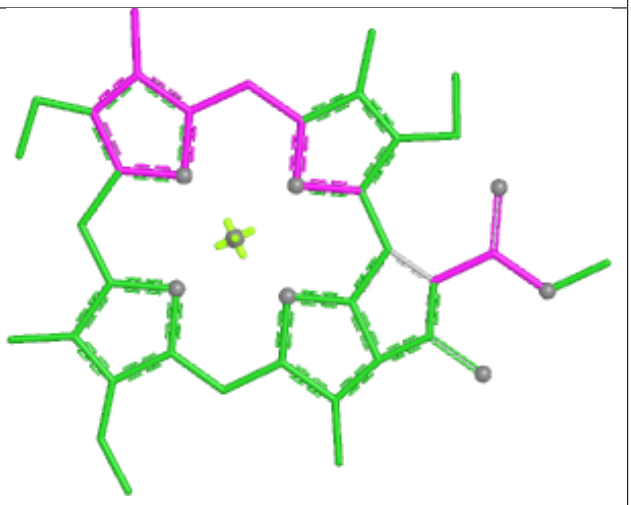


Rings

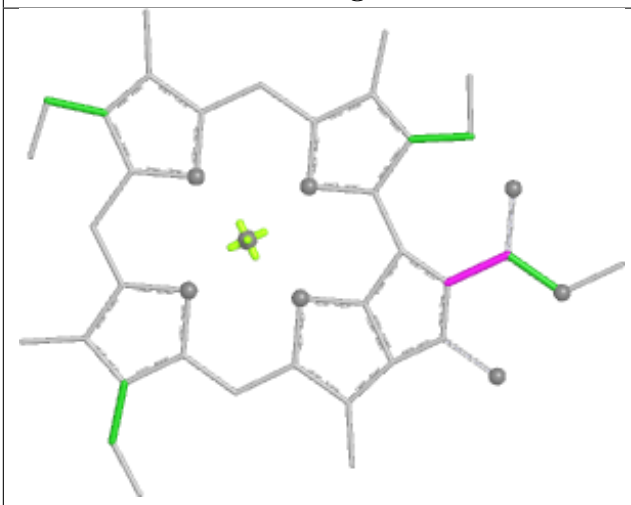
Ligand CLA A 812



Bond lengths



Bond angles

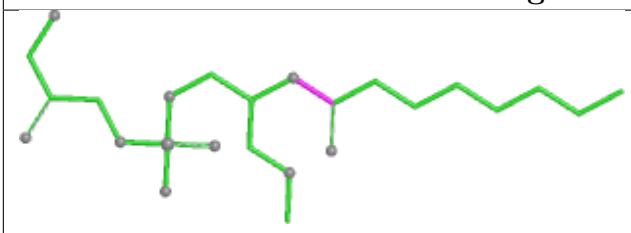


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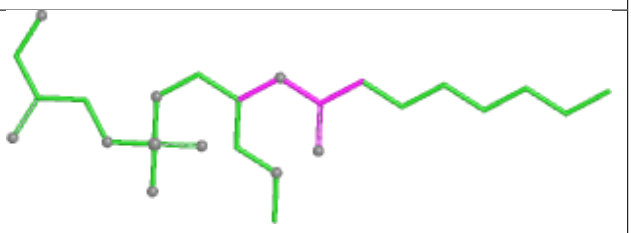


Rings

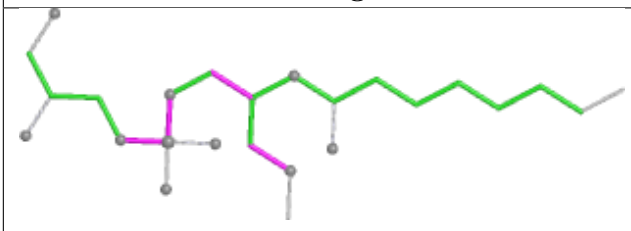
Ligand LHG e 845



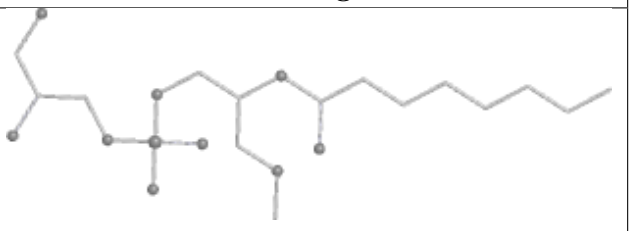
Bond lengths



Bond angles

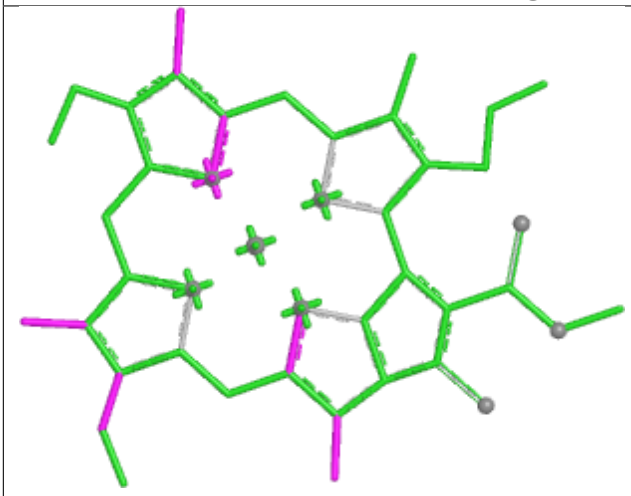


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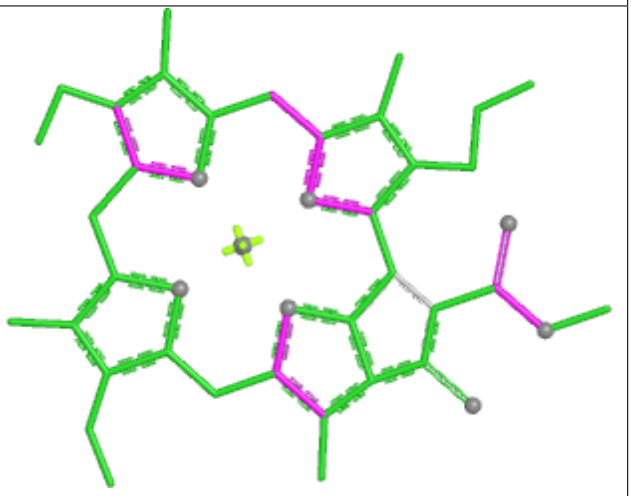


Rings

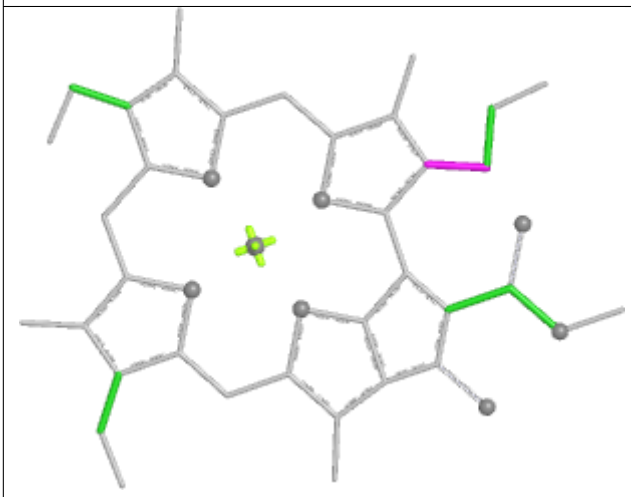
Ligand CLA B 813



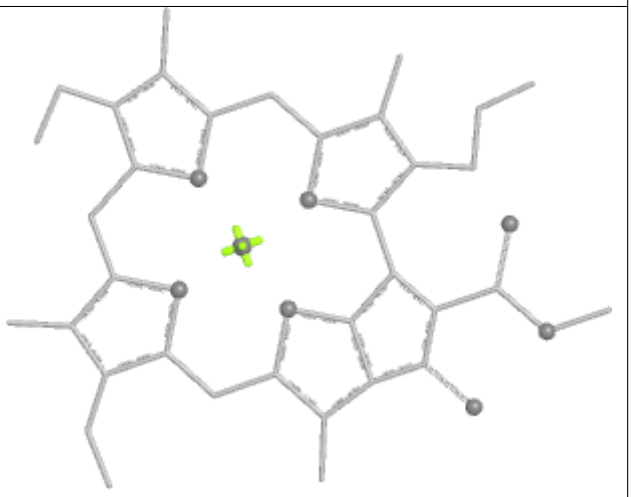
Bond lengths



Bond angles

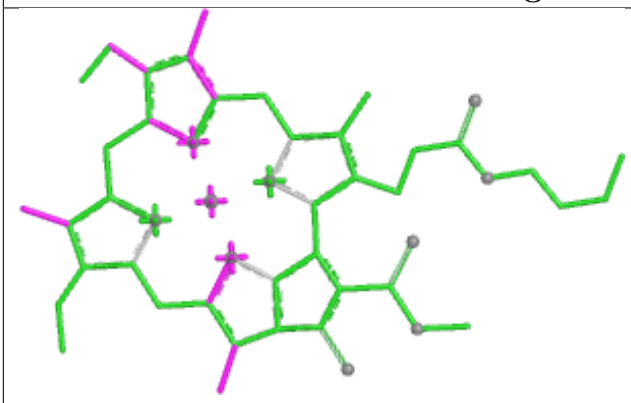


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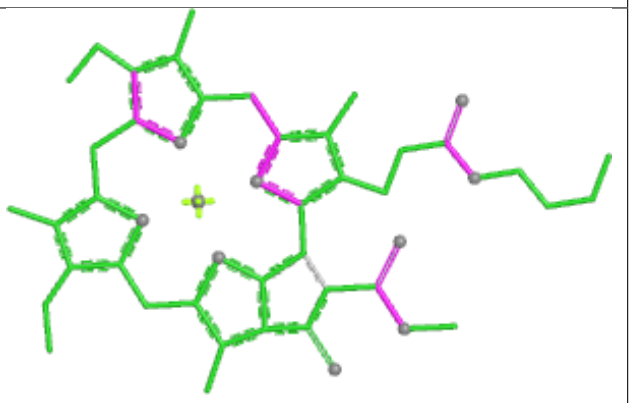


Rings

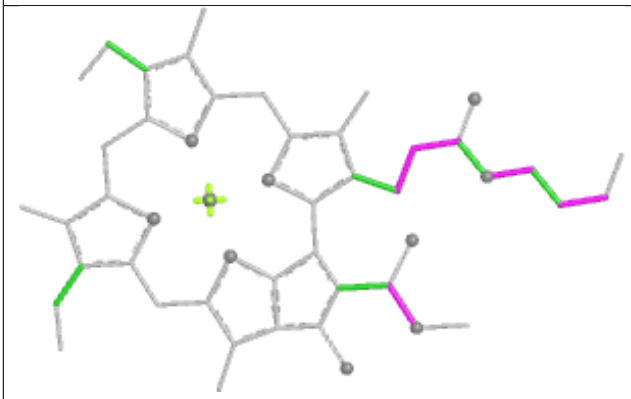
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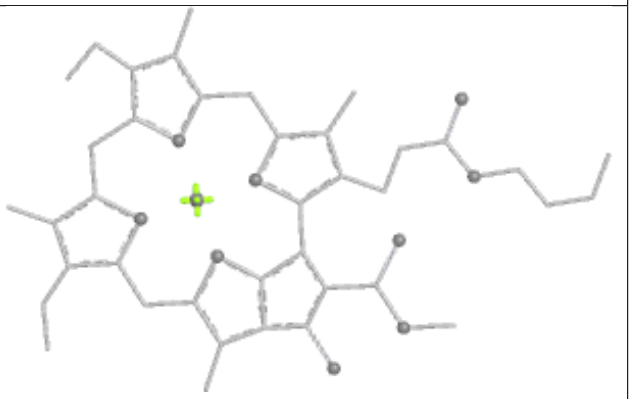
Bond lengths



Bond angles



Torsions

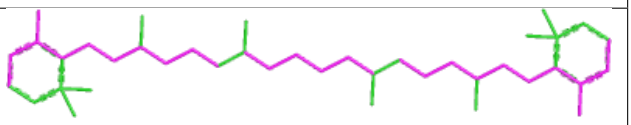


Rings

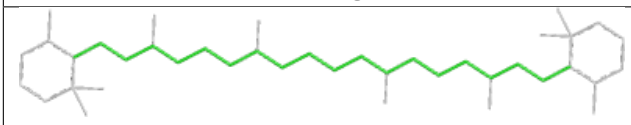
Ligand BCR e 847



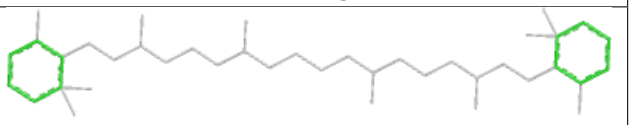
Bond lengths



Bond angles

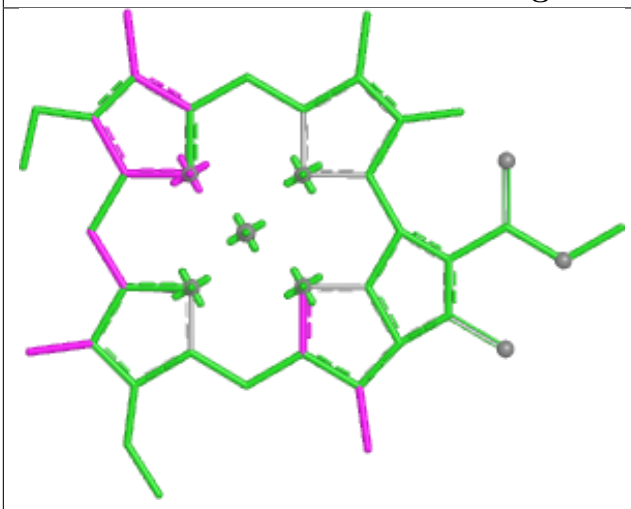


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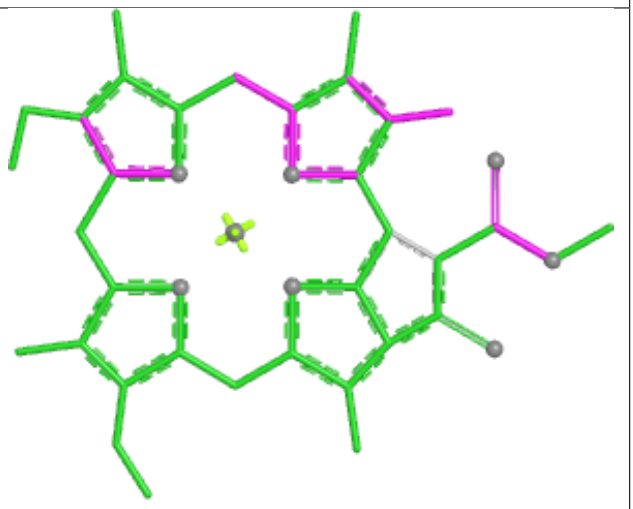


Rings

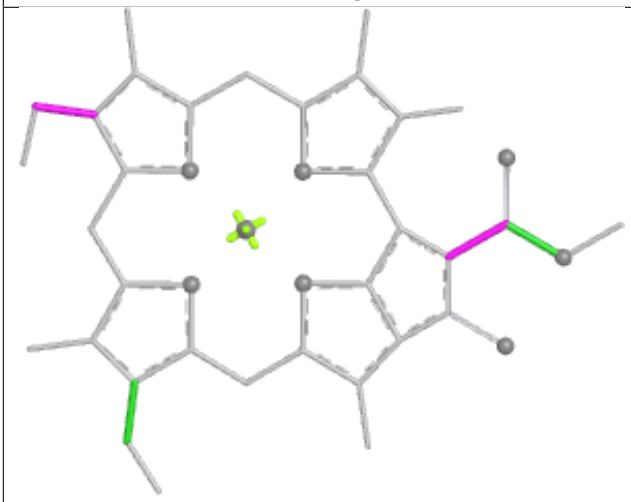
Ligand CLA f 823



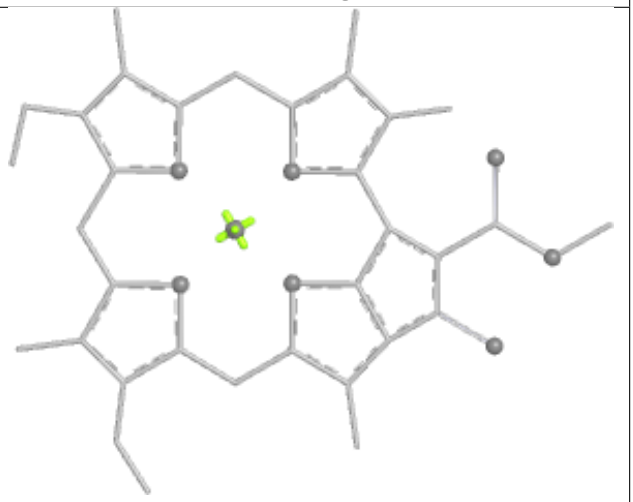
Bond lengths



Bond angles

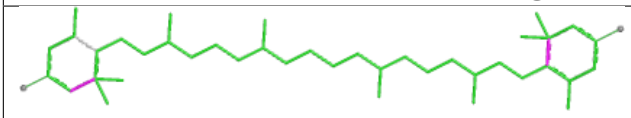


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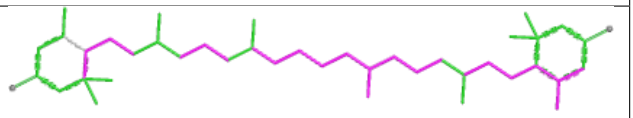


Rings

Ligand LUT 1 501



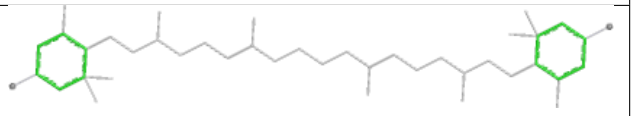
Bond lengths



Bond angles

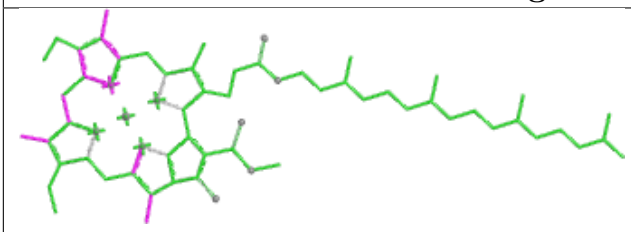


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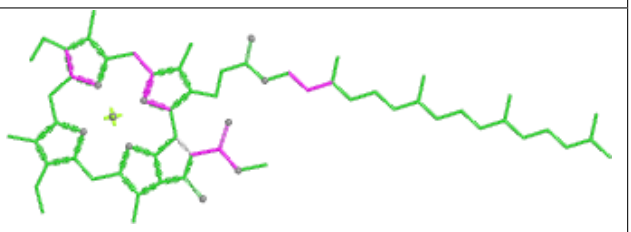


Rings

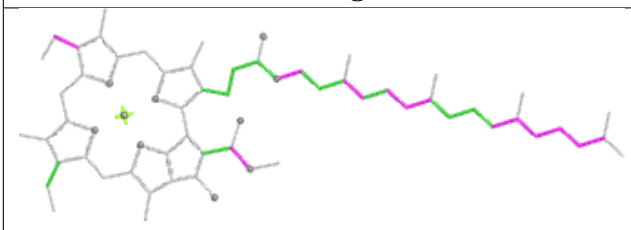
Ligand CLA 1 513



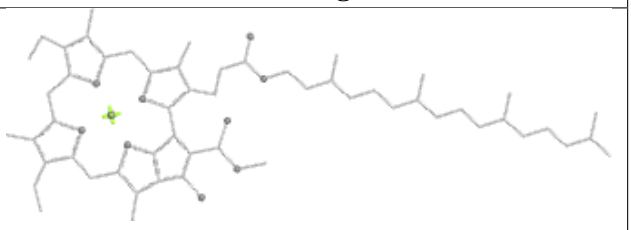
Bond lengths



Bond angles

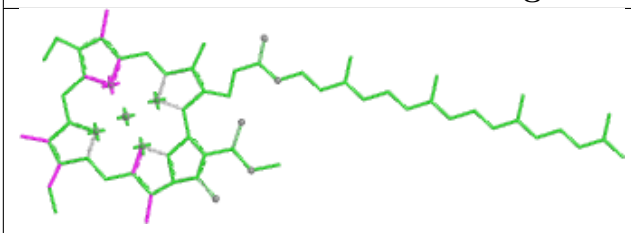


Torsions

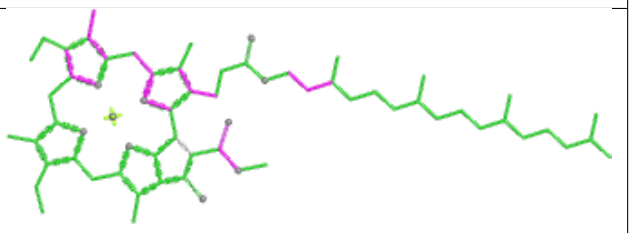


Rings

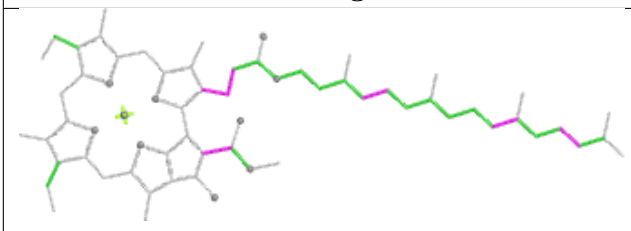
Ligand CLA A 808



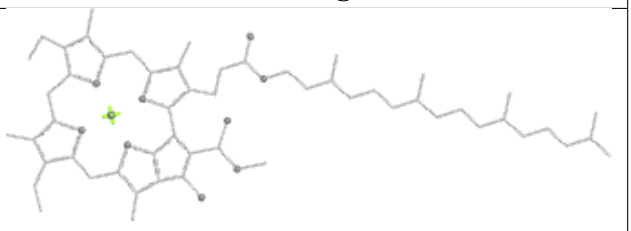
Bond lengths



Bond angles

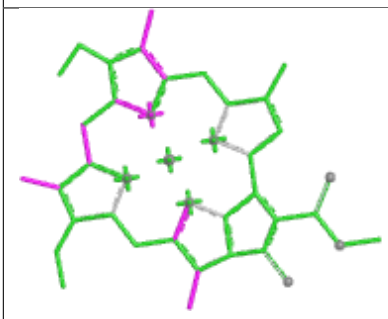


Torsions

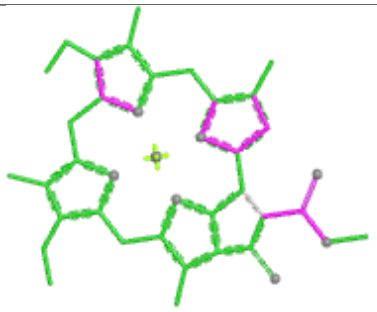


Rings

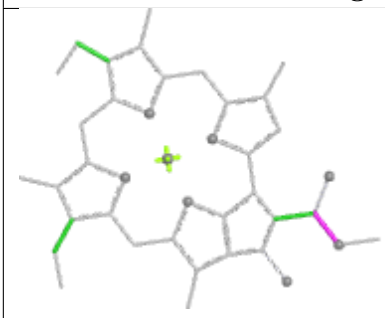
Ligand CLA 2 507



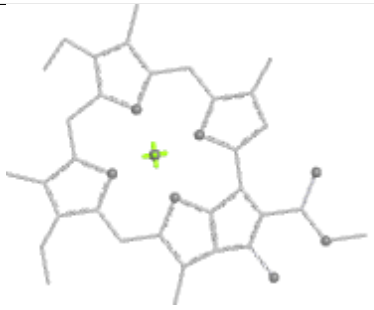
Bond lengths



Bond angles

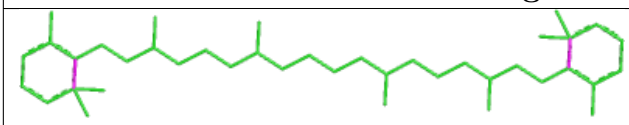


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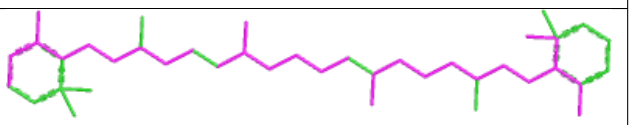


Rings

Ligand BCR B 848



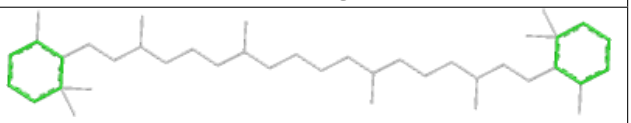
Bond lengths



Bond angles

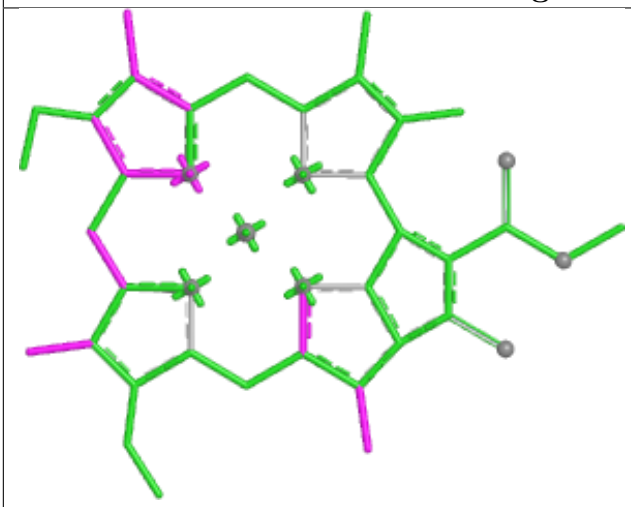


Torsions

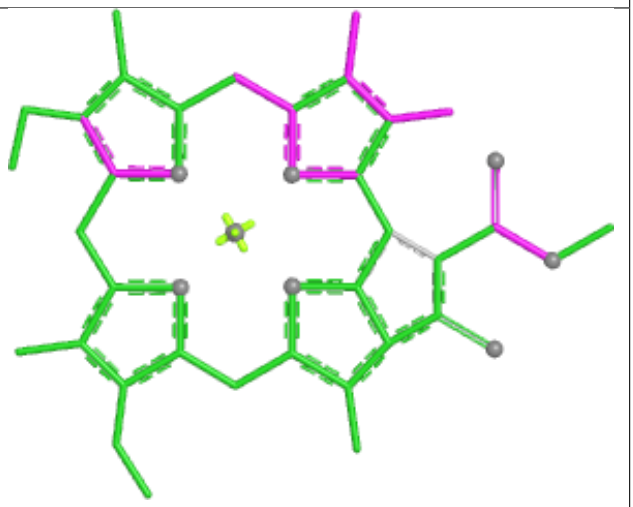


Rings

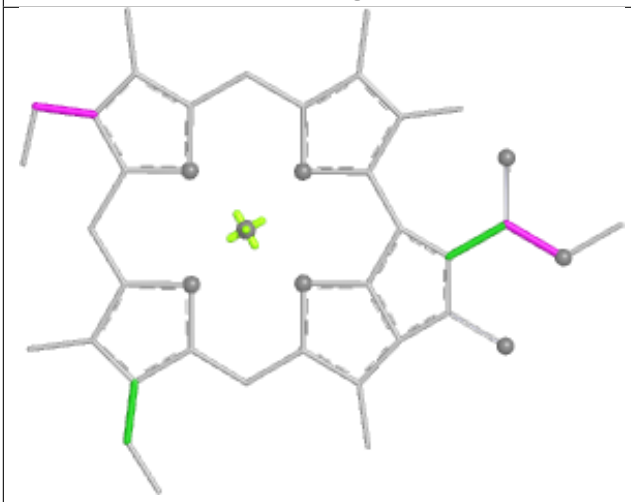
Ligand CLA f 819



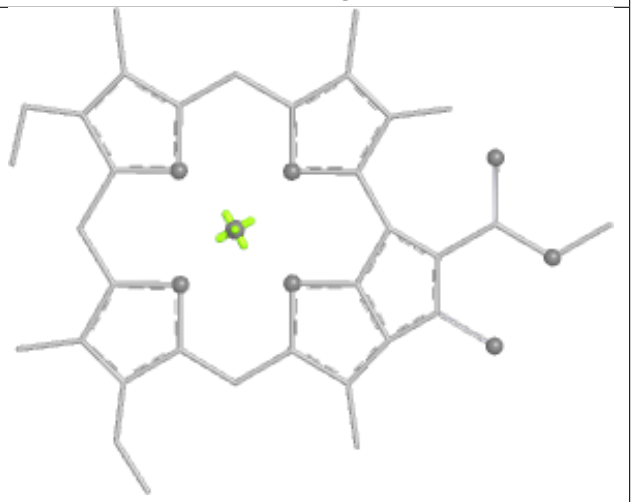
Bond lengths



Bond angles

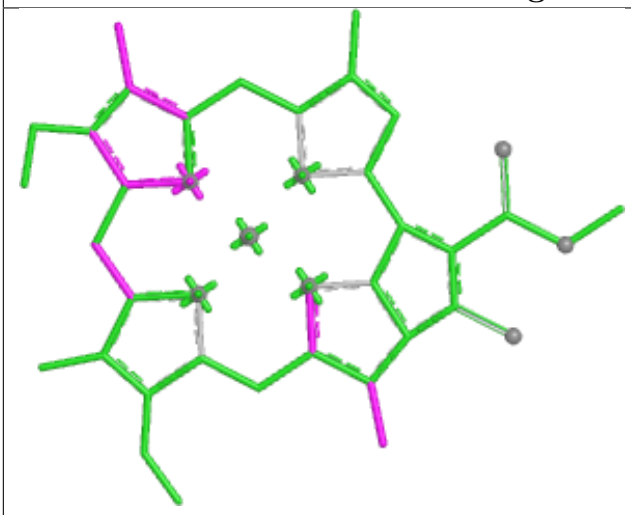


Torsions

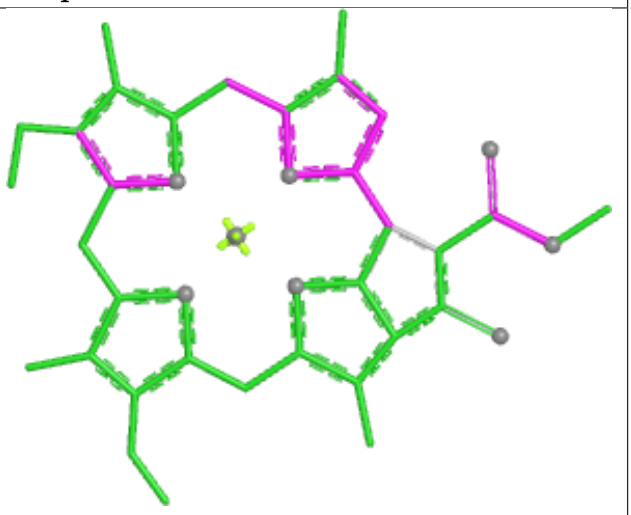


Rings

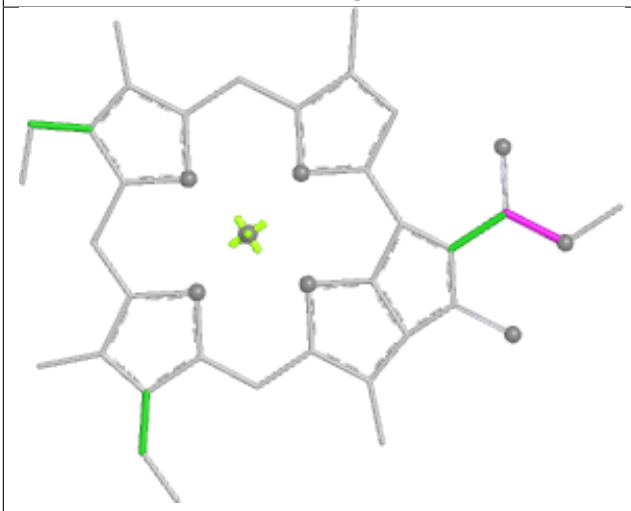
Ligand CLA q 307



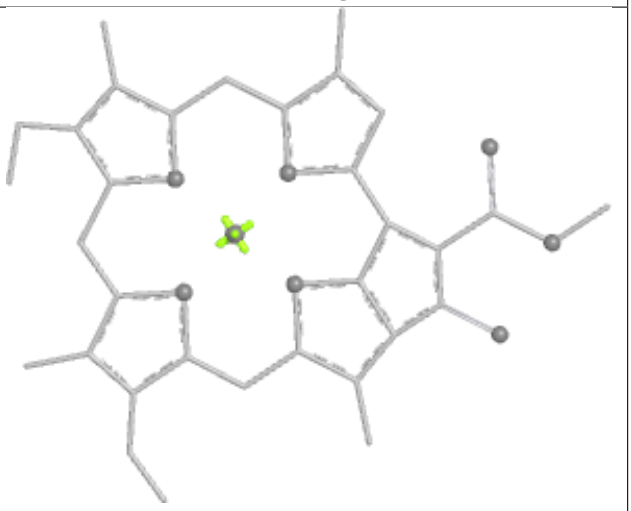
Bond lengths



Bond angles



Torsions



Rings

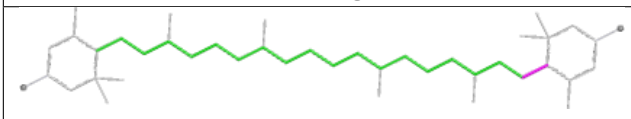
Ligand LUT r 302



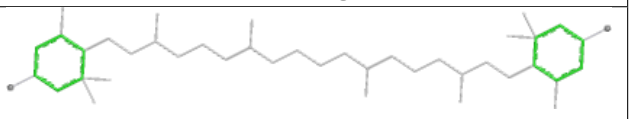
Bond lengths



Bond angles

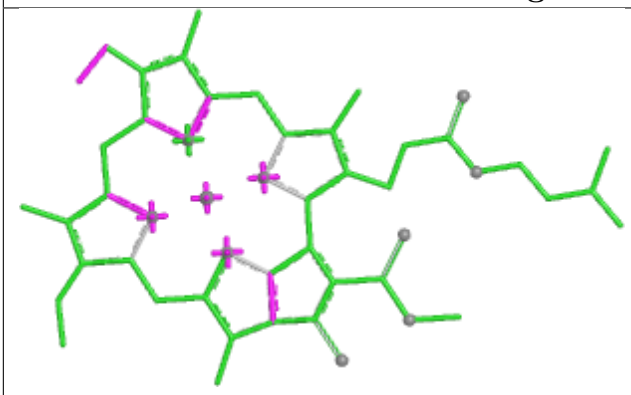


Torsions

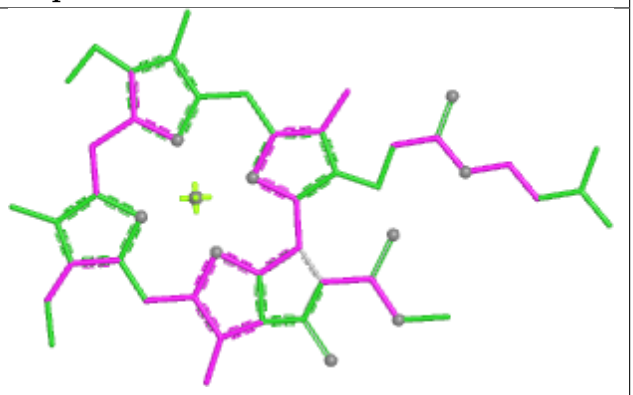


Rings

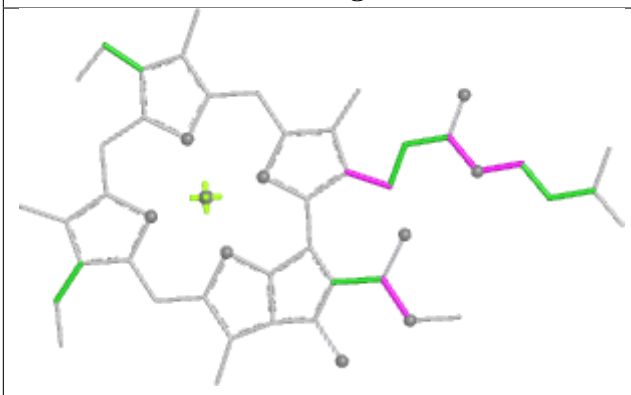
Ligand CLA p 509



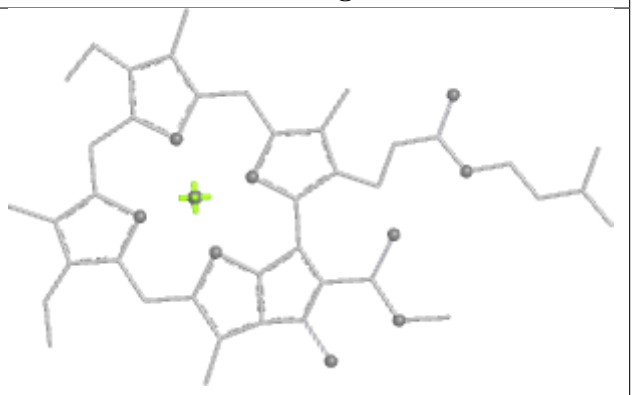
Bond lengths



Bond angles

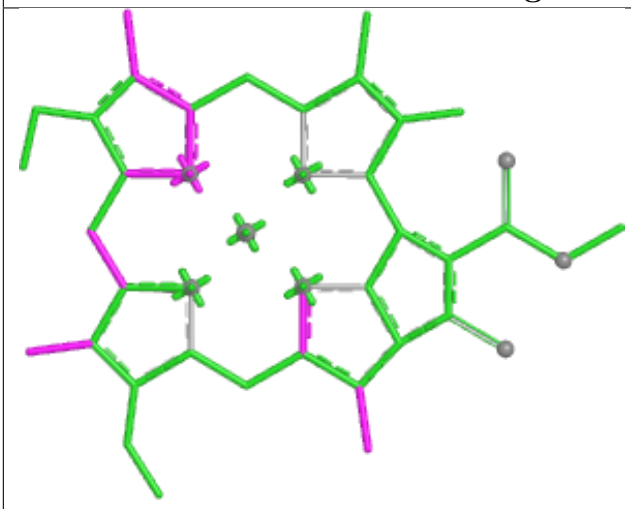


Torsions

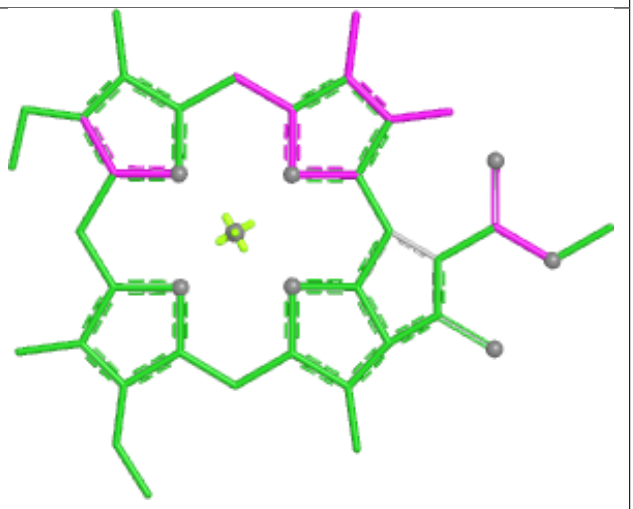


Rings

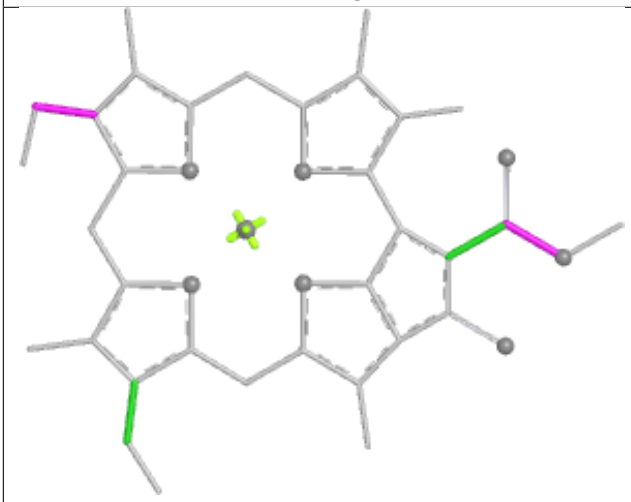
Ligand CLA B 805



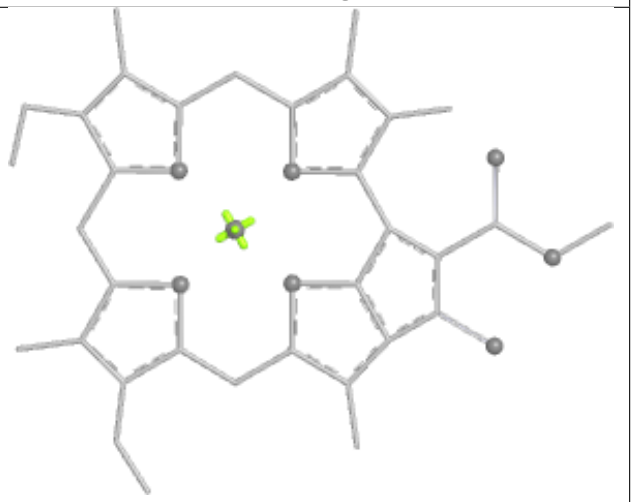
Bond lengths



Bond angles



Torsions

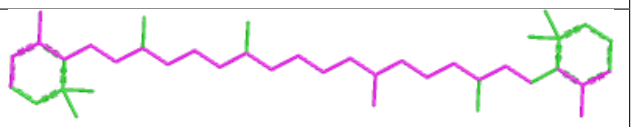


Rings

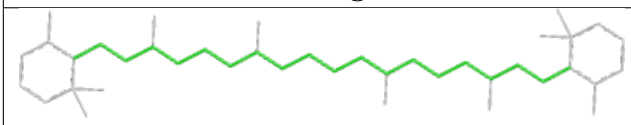
Ligand BCR f 849



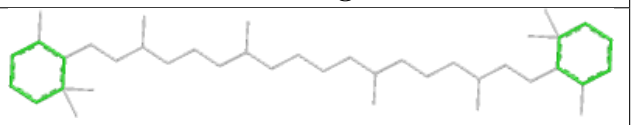
Bond lengths



Bond angles

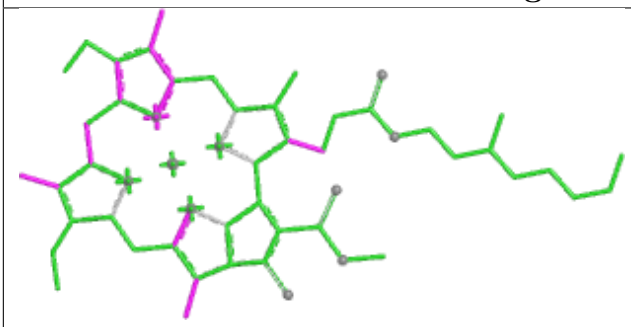


Torsions

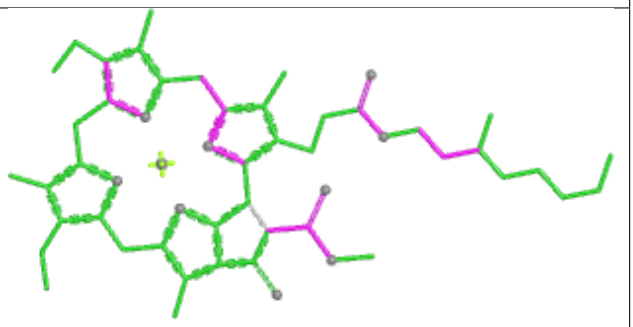


Rings

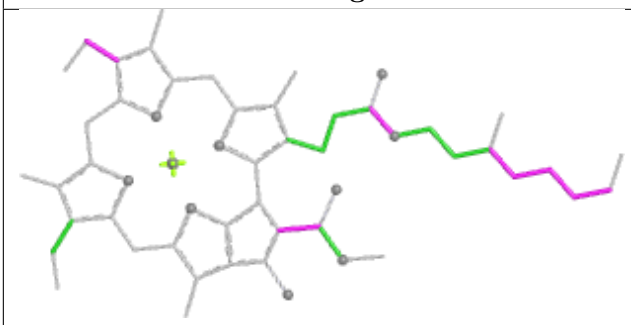
Ligand CLA B 841



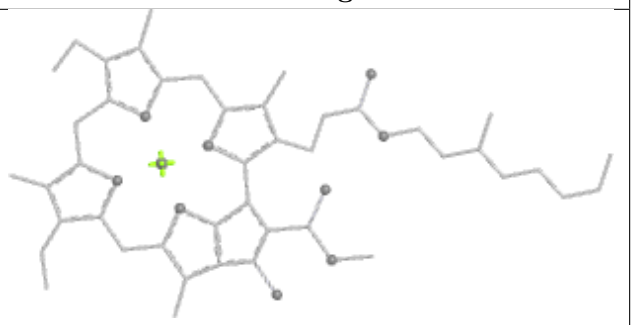
Bond lengths



Bond angles

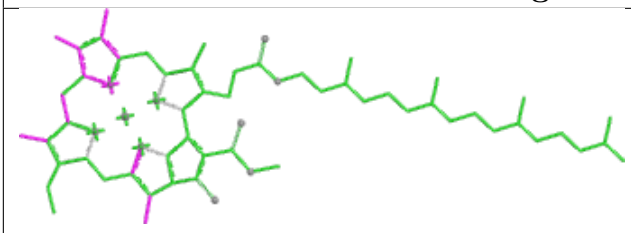


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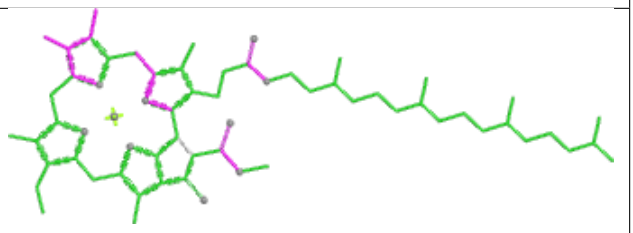


Rings

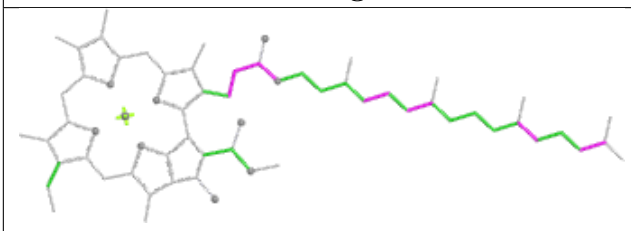
Ligand CLA f 801



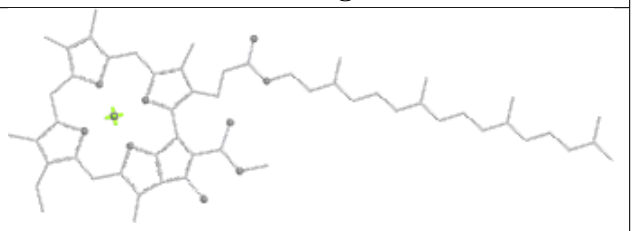
Bond lengths



Bond angles

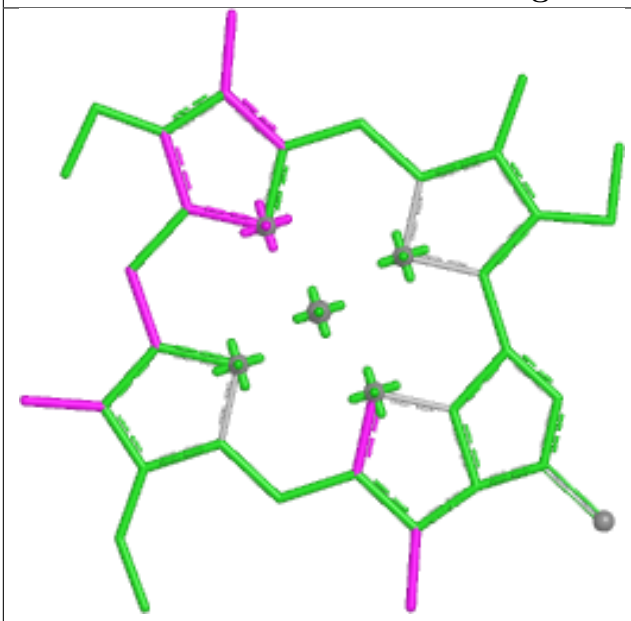


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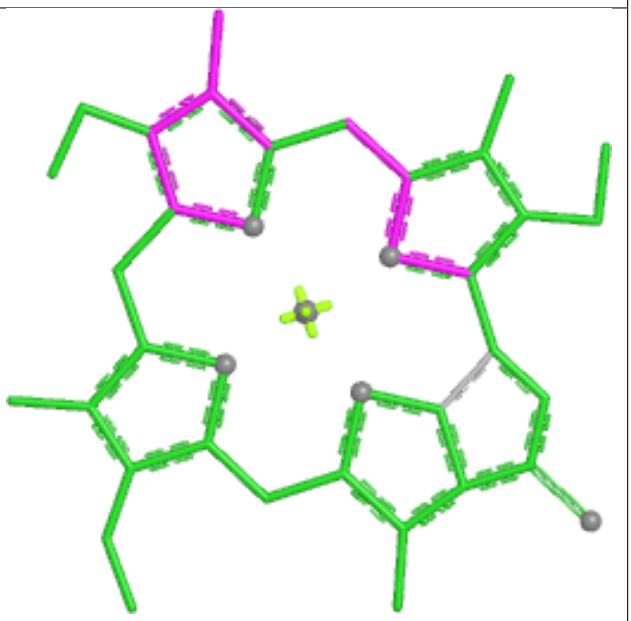


Rings

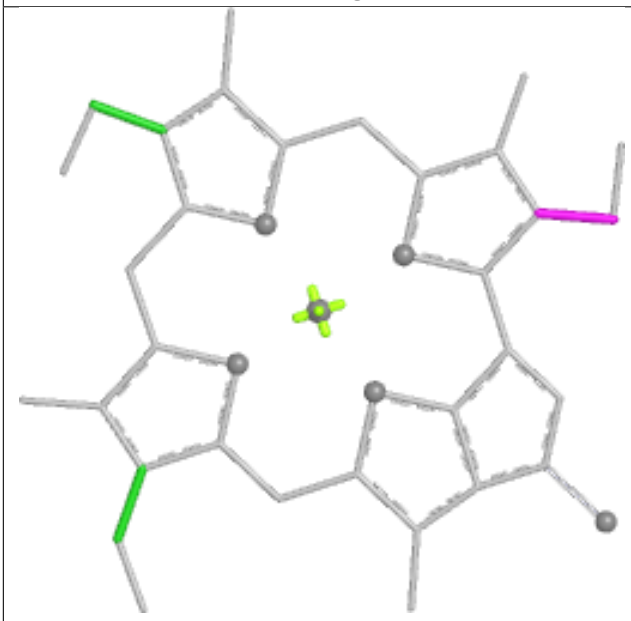
Ligand CLA f 816



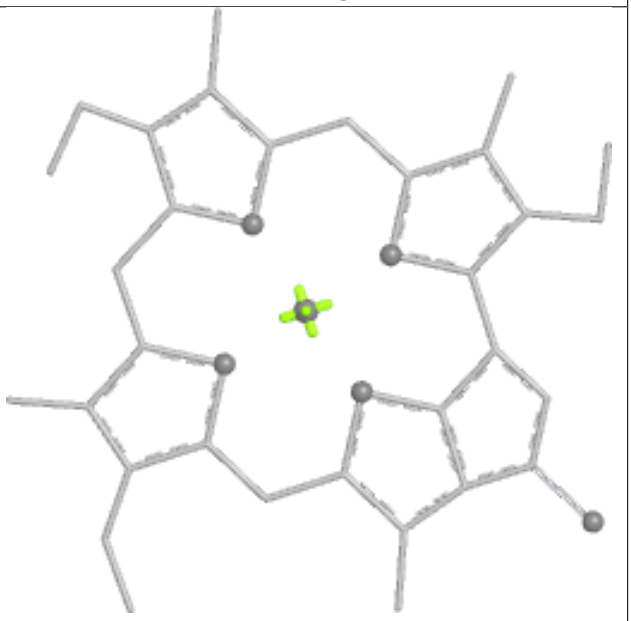
Bond lengths



Bond angles

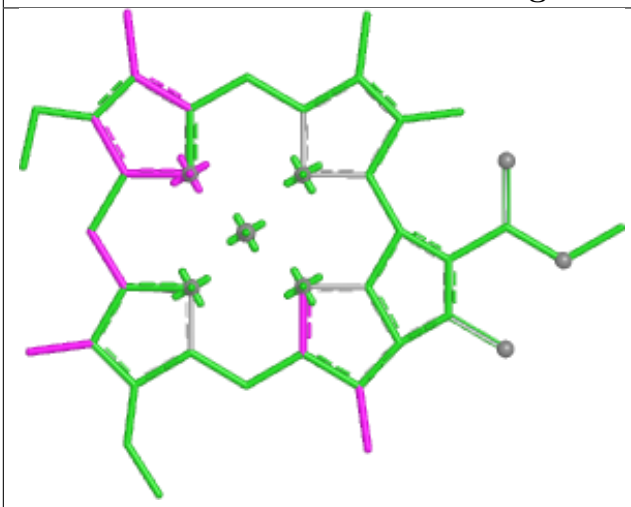


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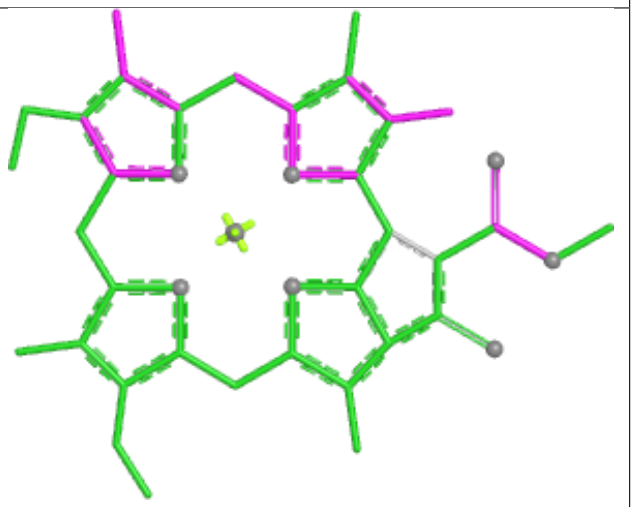


Rings

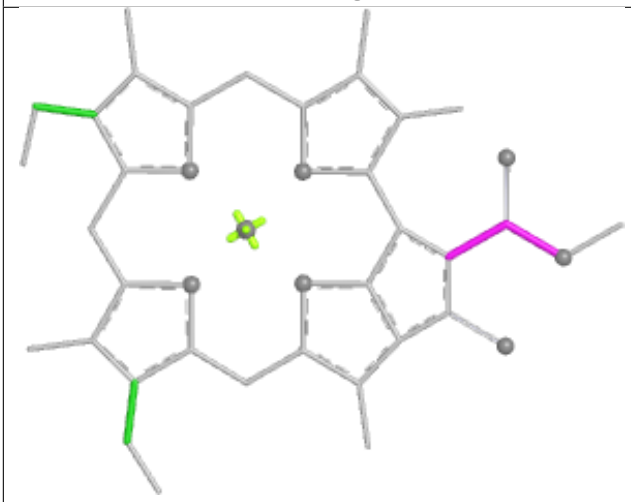
Ligand CLA e 820



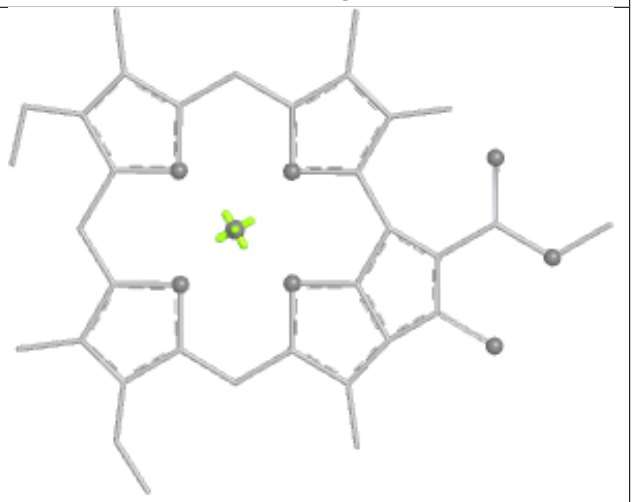
Bond lengths



Bond angles

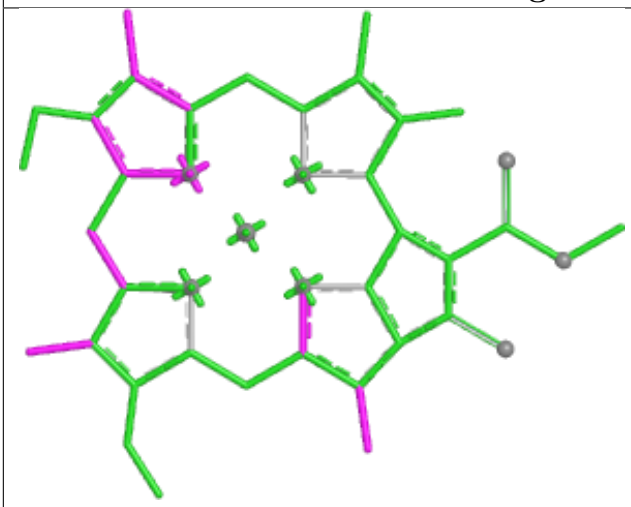


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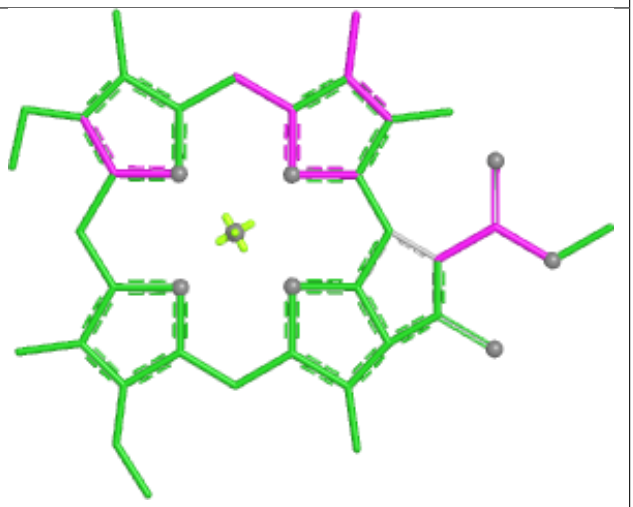


Rings

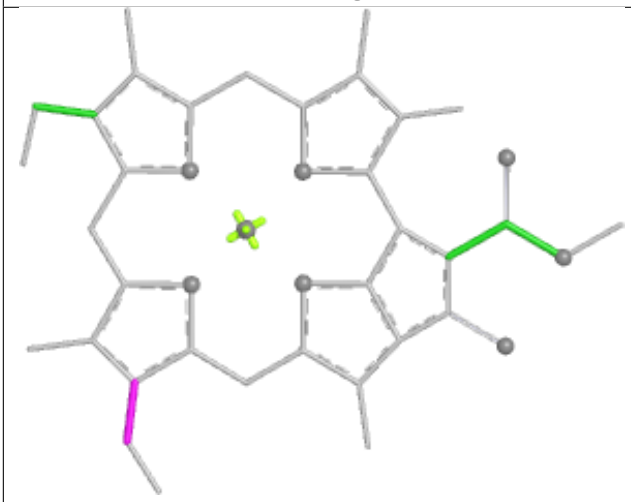
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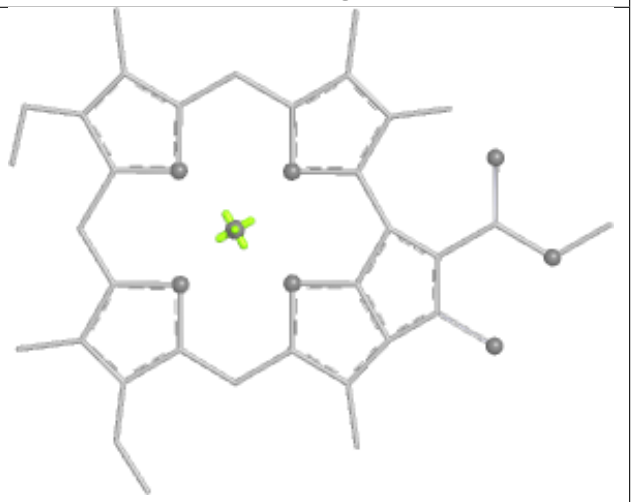
Bond lengths



Bond angles

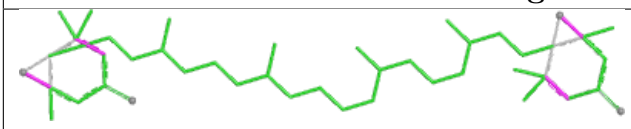


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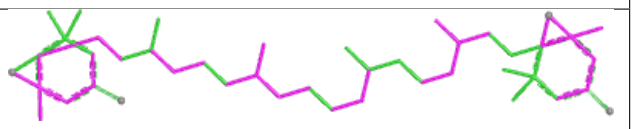


Rings

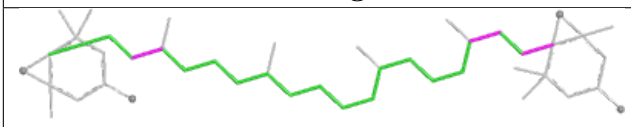
Ligand XAT 2 502



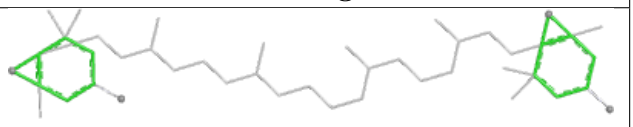
Bond lengths



Bond angles

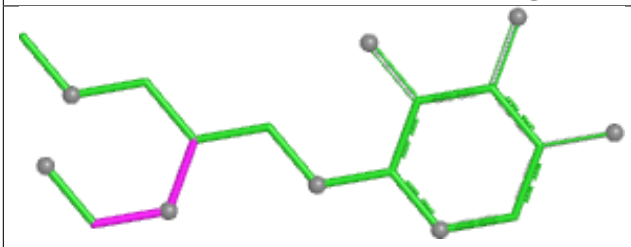


Torsions

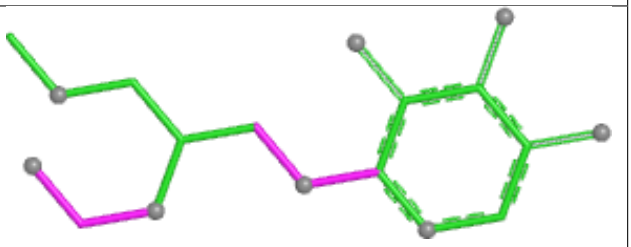


Rings

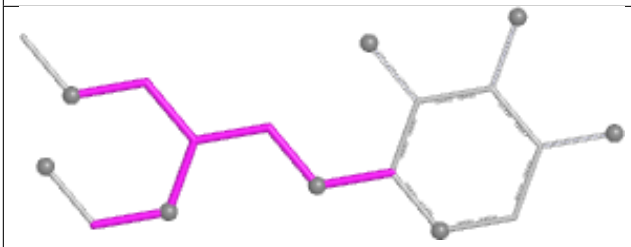
Ligand LMG r 318



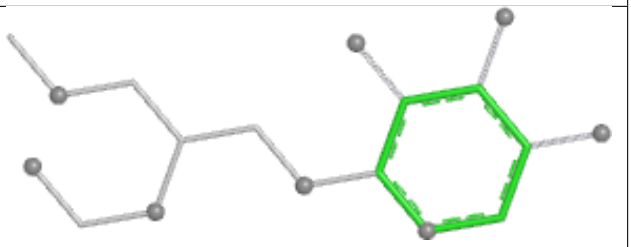
Bond lengths



Bond angles

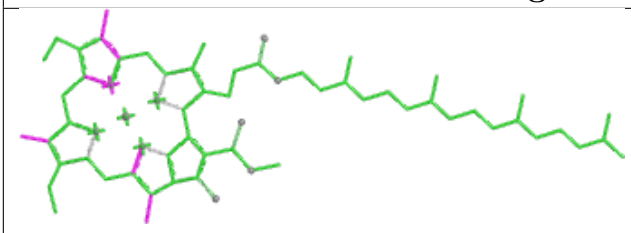


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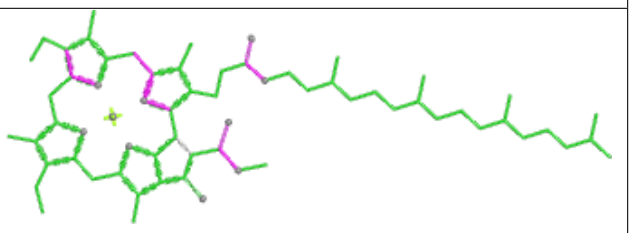


Rings

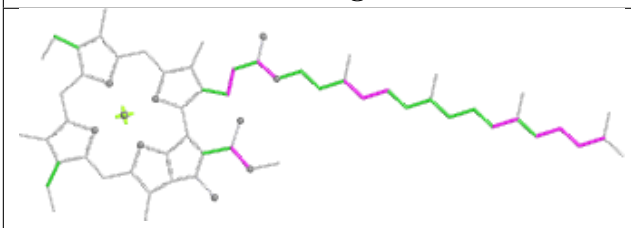
Ligand CLA 2 506



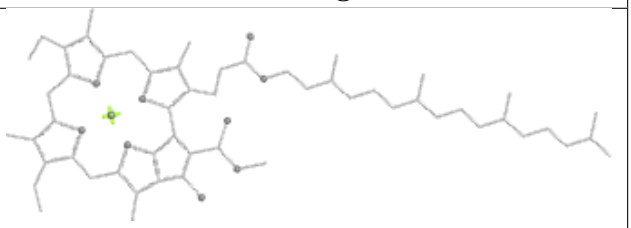
Bond lengths



Bond angles

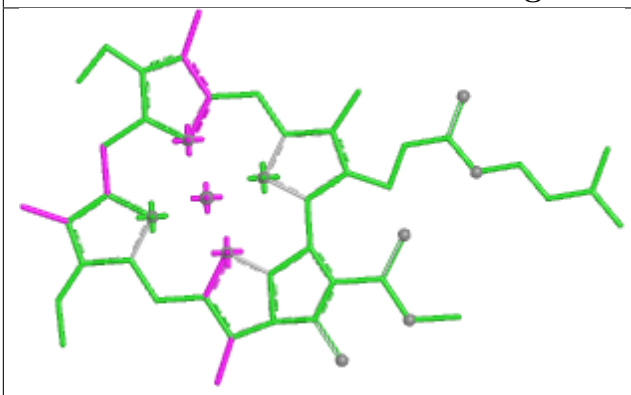


Torsions

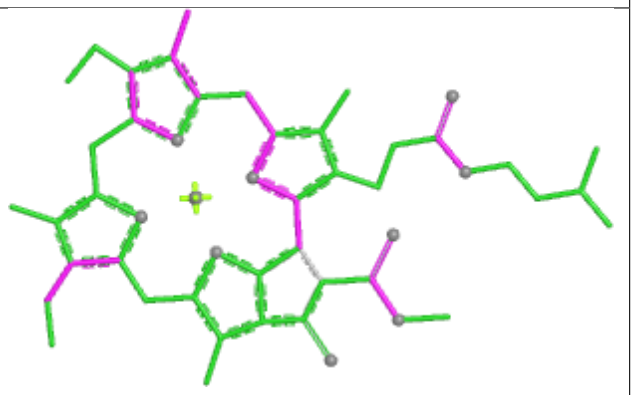


Rings

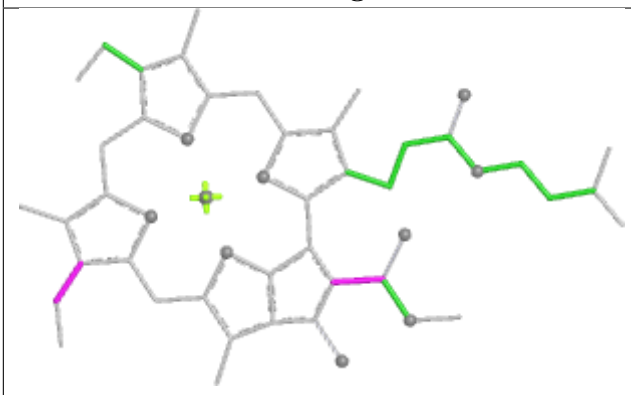
Ligand CLA B 837



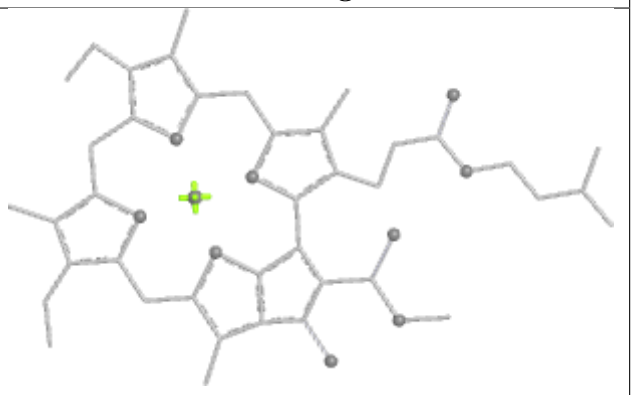
Bond lengths



Bond angles

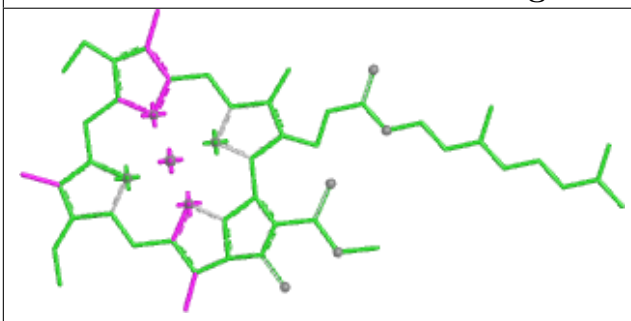


Torsions

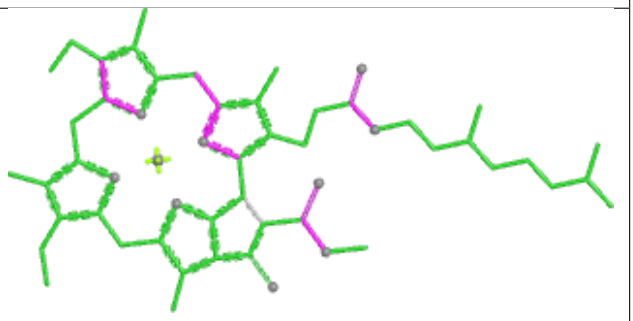


Rings

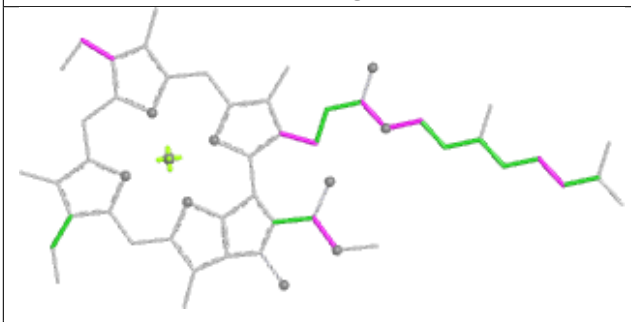
Ligand CLA 2 514



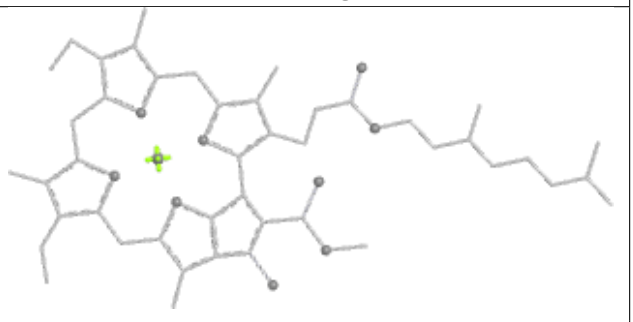
Bond lengths



Bond angles

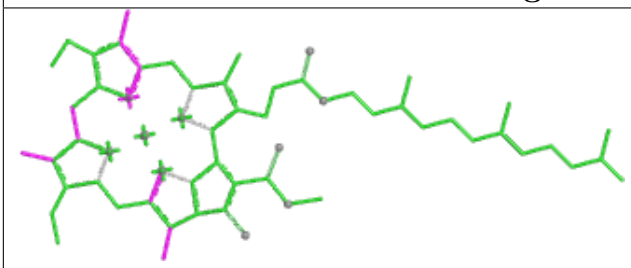


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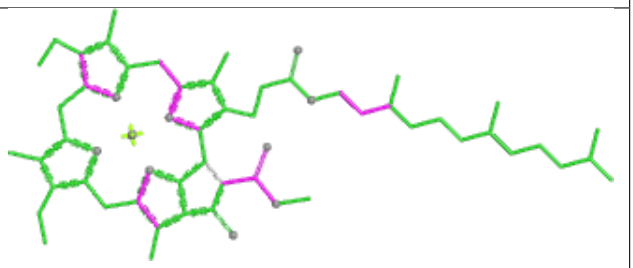


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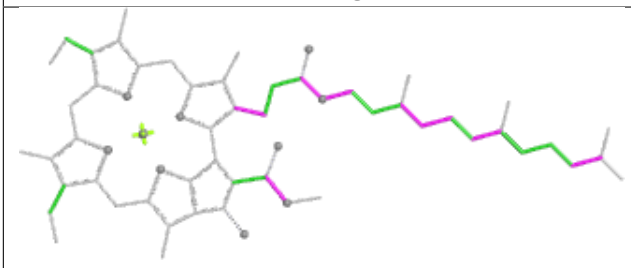
Ligand CLA A 826



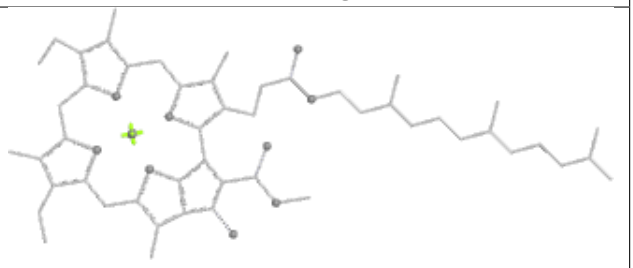
Bond lengths



Bond angles

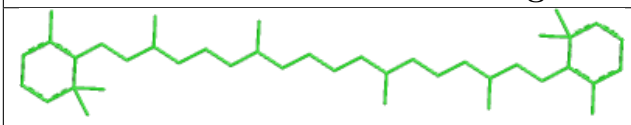


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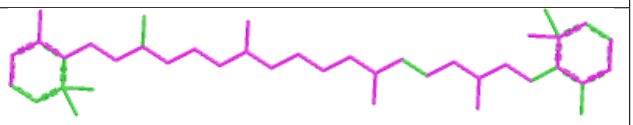


Rings

Ligand BCR e 854



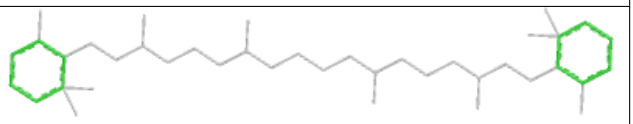
Bond lengths



Bond angles

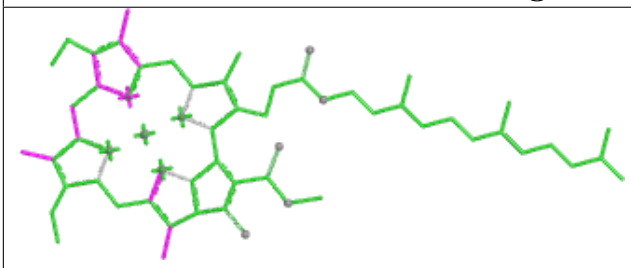


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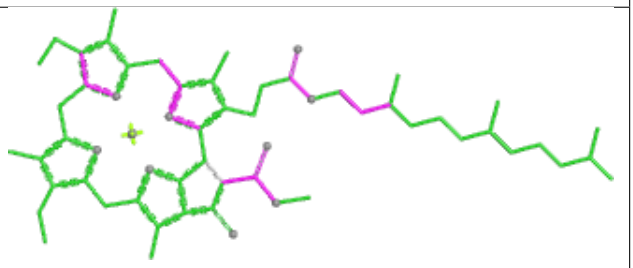


Rings

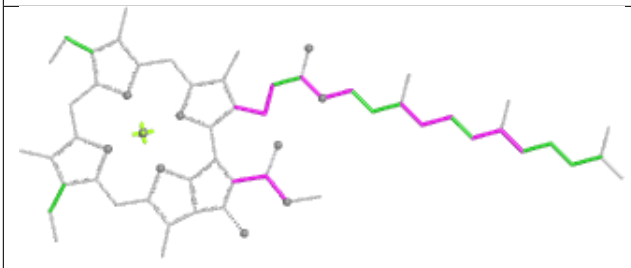
Ligand CLA 3 314



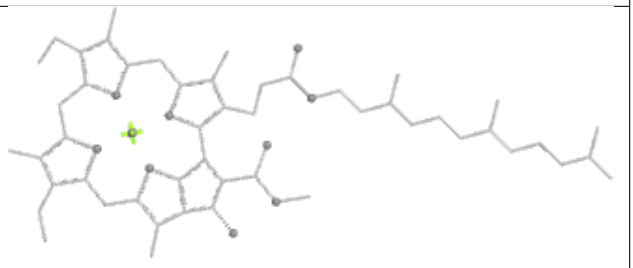
Bond lengths



Bond angles

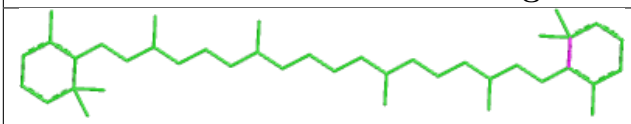


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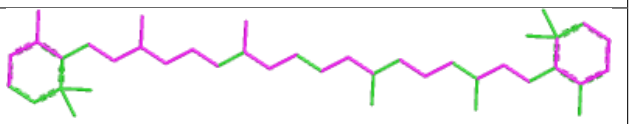


Rings

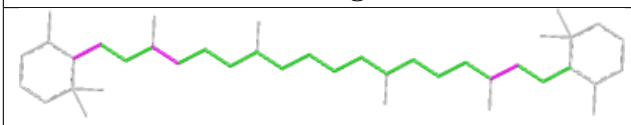
Ligand BCR B 845



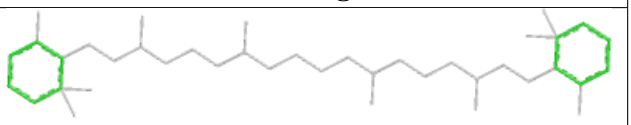
Bond lengths



Bond angles

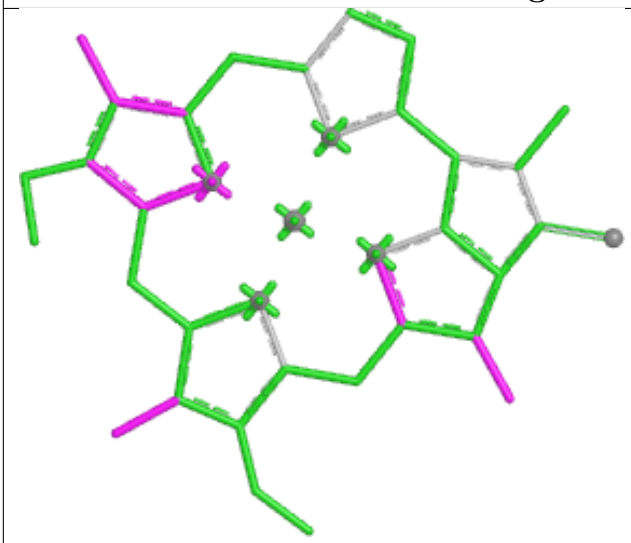


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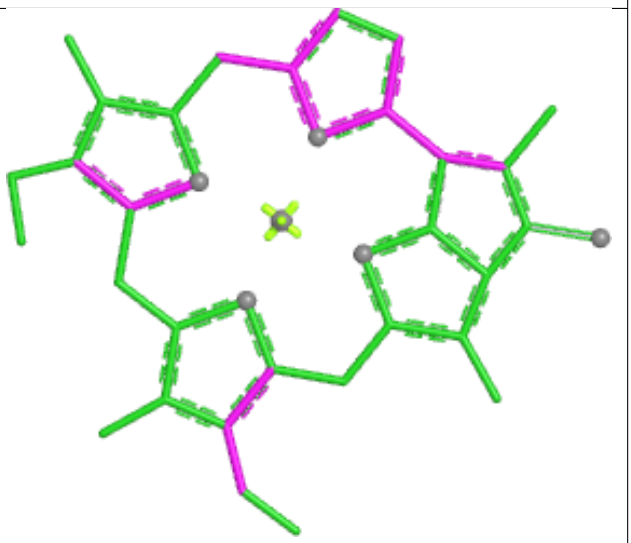


Rings

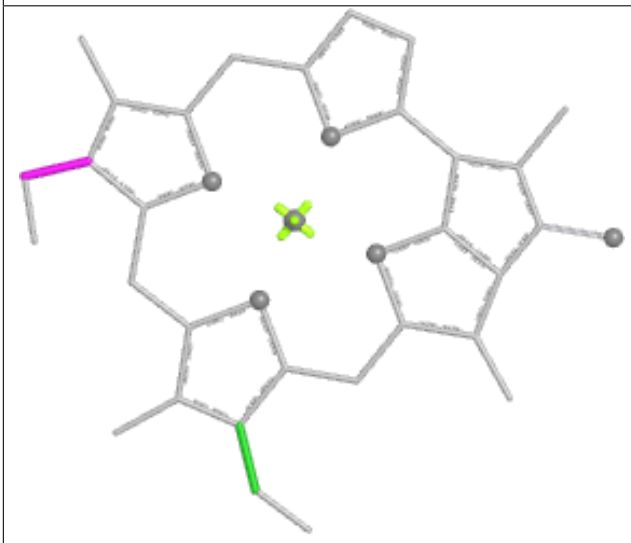
Ligand CLA 2 504



Bond lengths



Bond angles

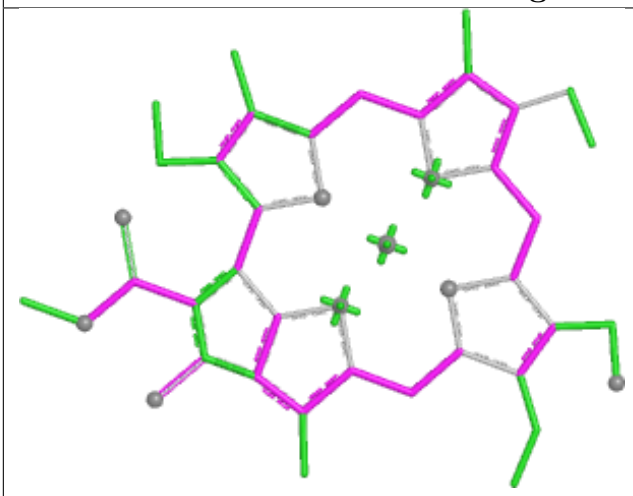


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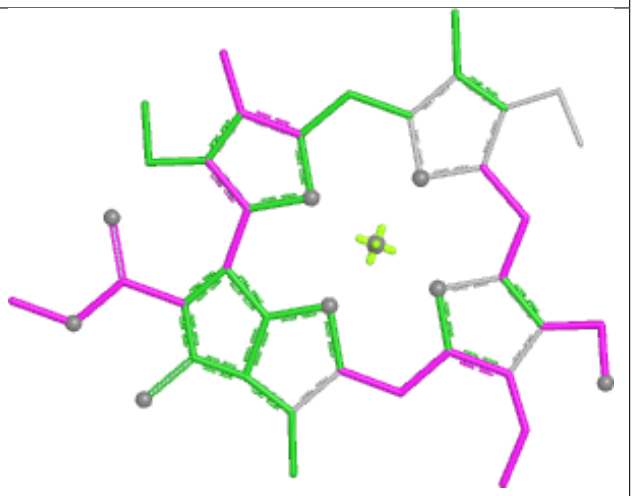


Rings

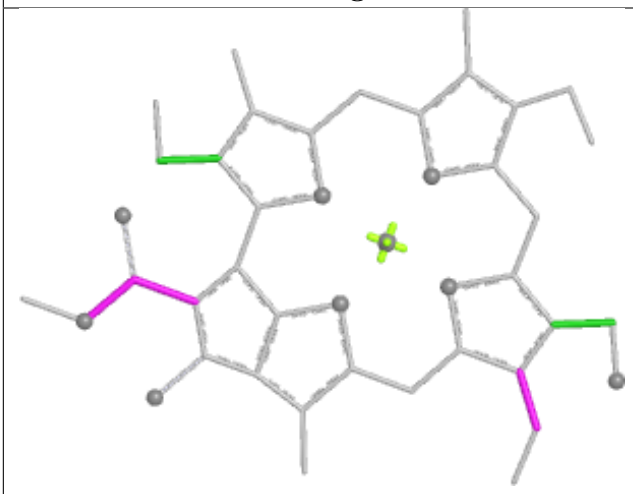
Ligand CHL r 316



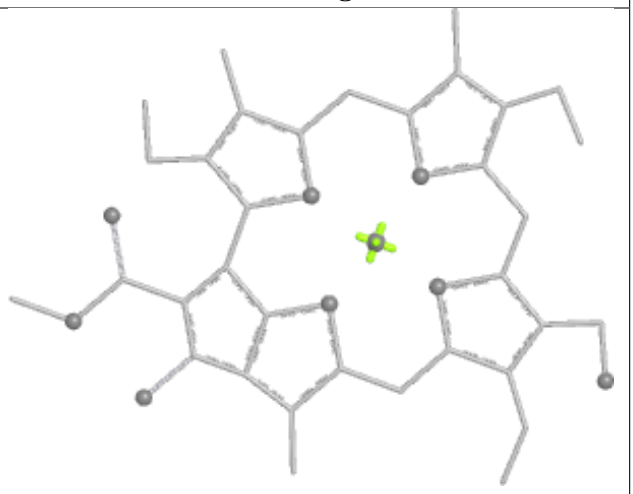
Bond lengths



Bond angles

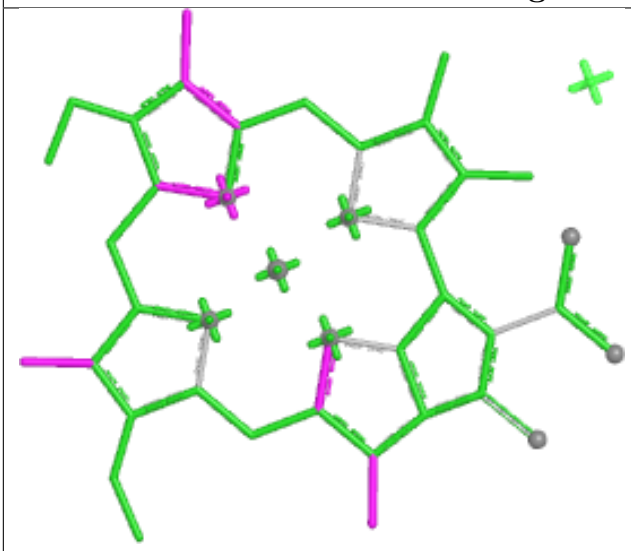


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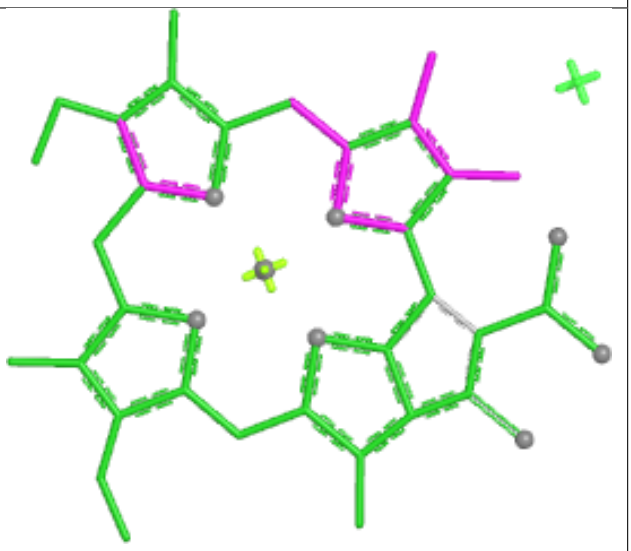


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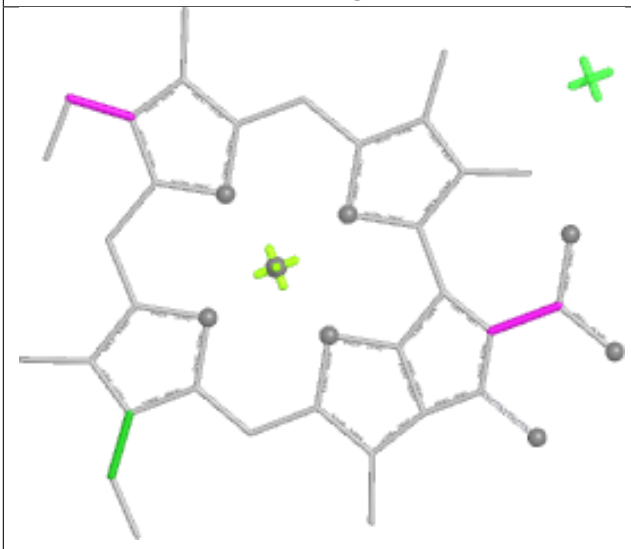
Ligand CLA 5 306



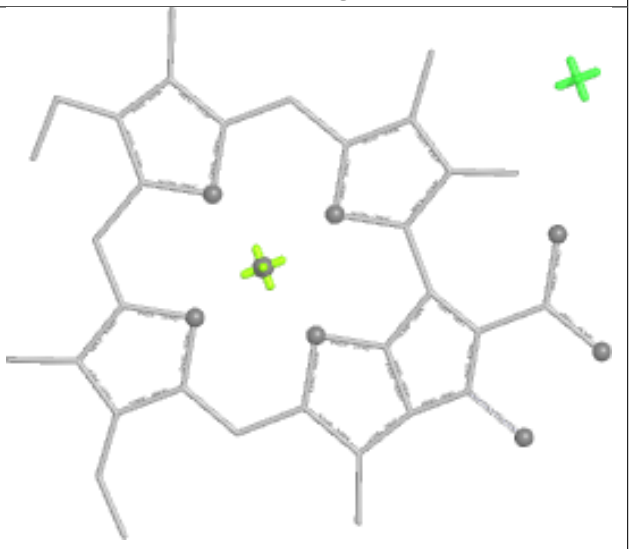
Bond lengths



Bond angles

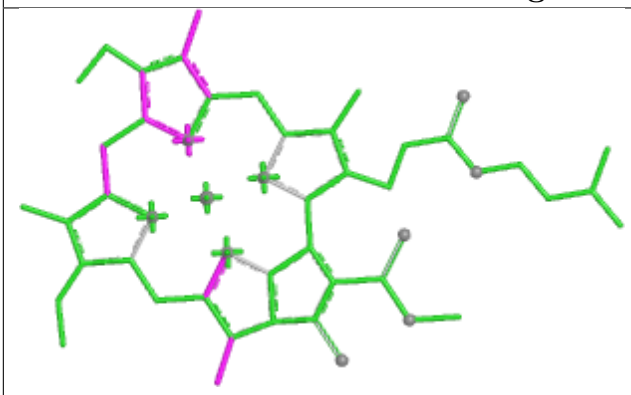


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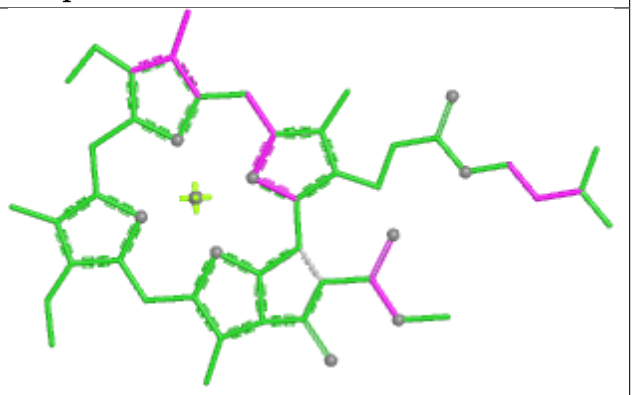


Rings

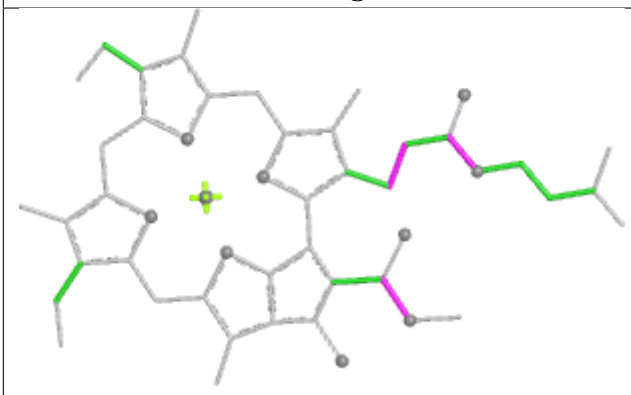
Ligand CLA q 309



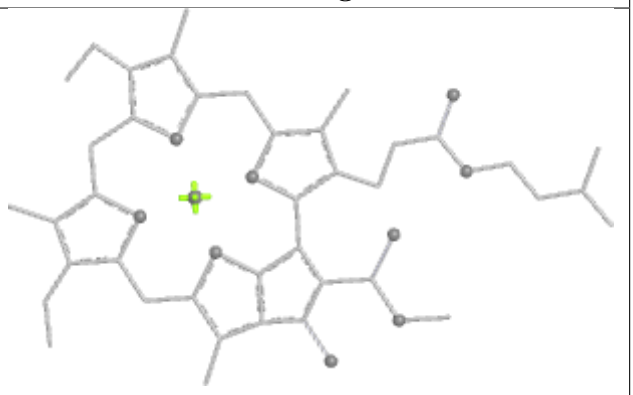
Bond lengths



Bond angles

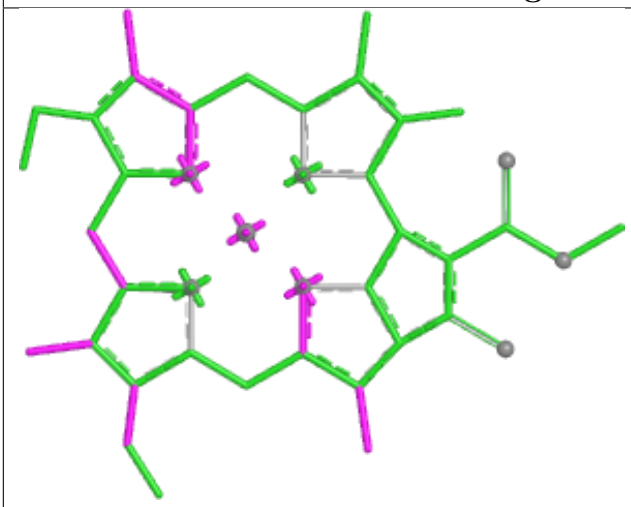


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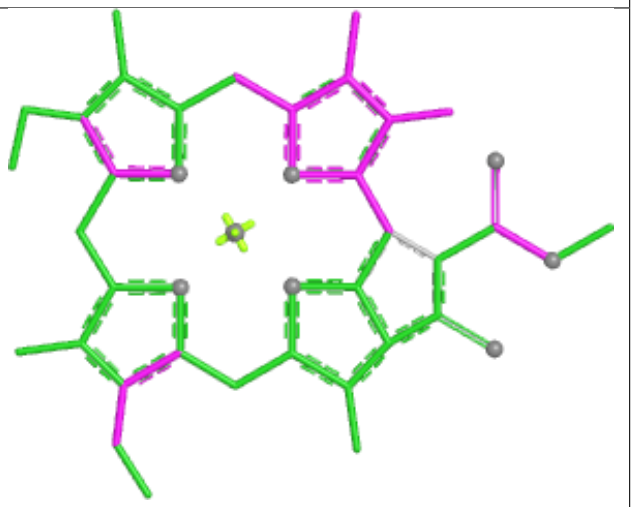


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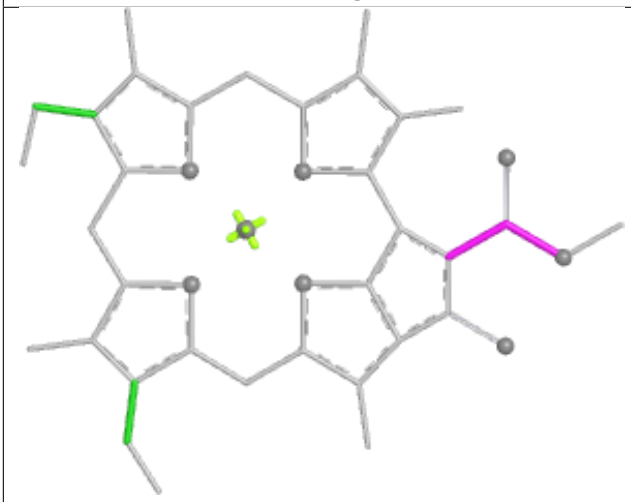
Ligand CLA B 814



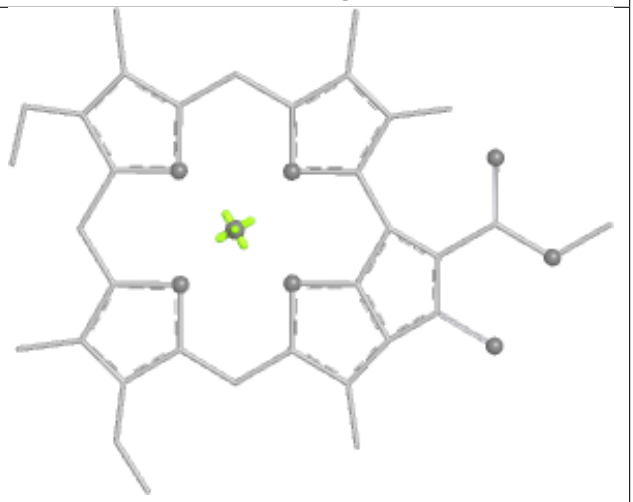
Bond lengths



Bond angles

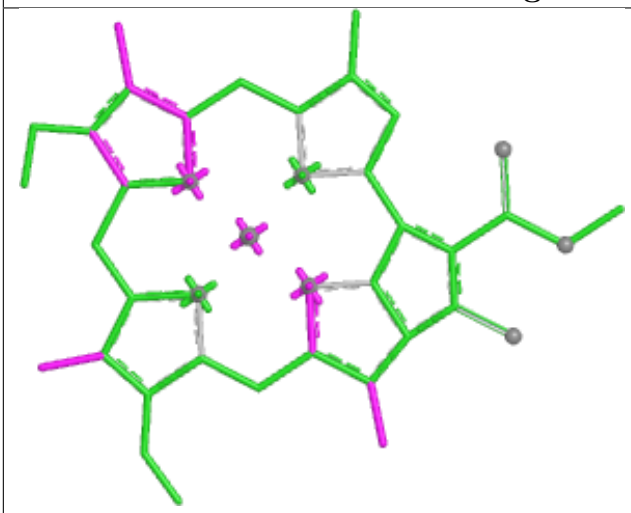


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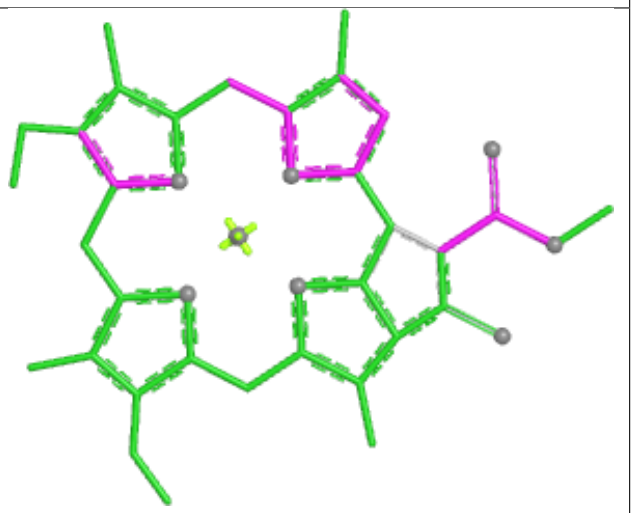


Rings

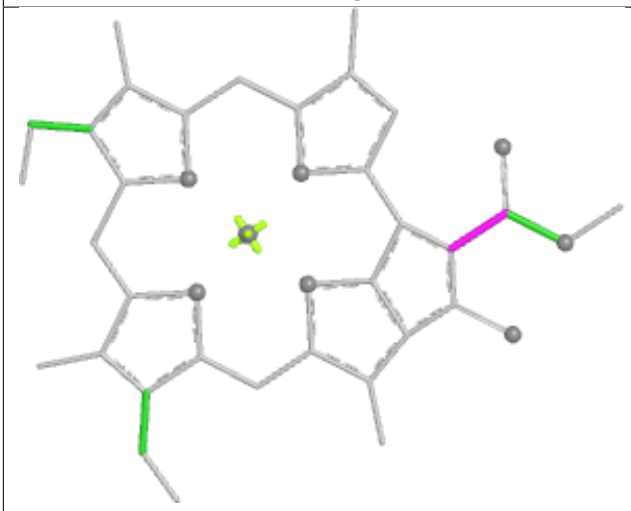
Ligand CLA A 833



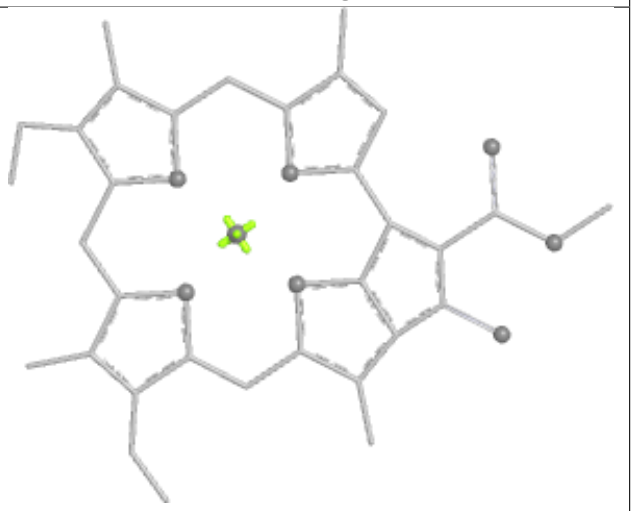
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Bond angles

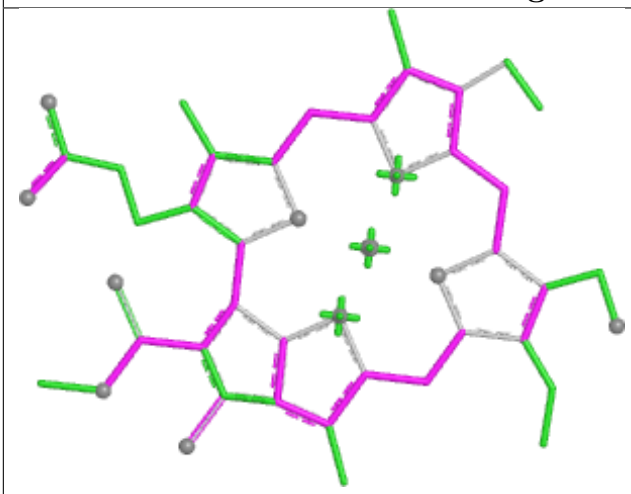


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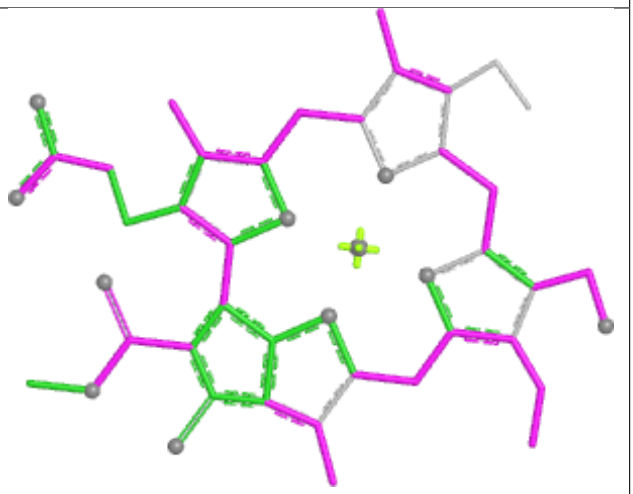


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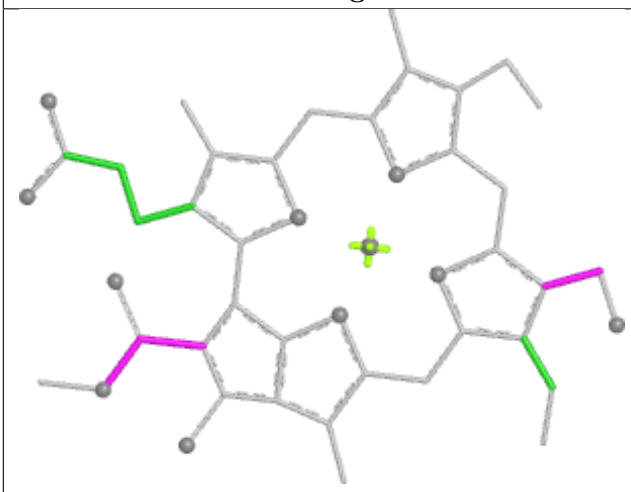
Ligand CHL 5 315



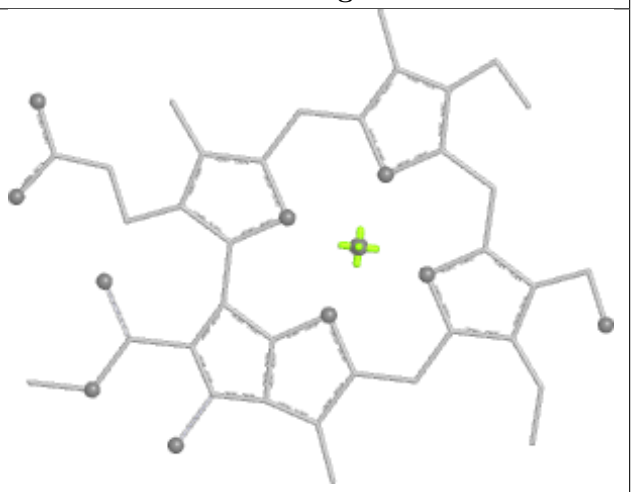
Bond lengths



Bond angles

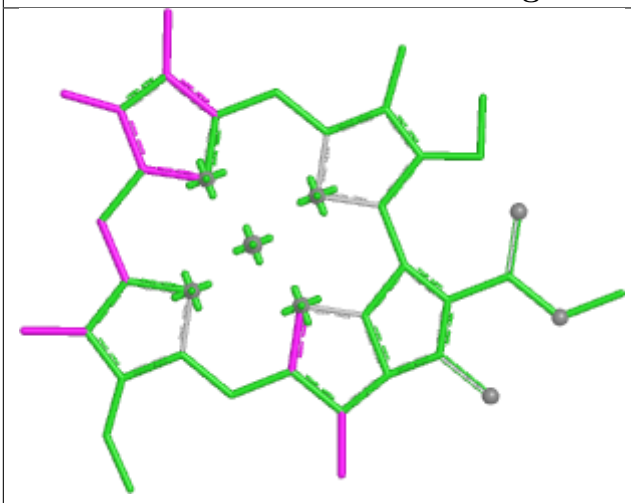


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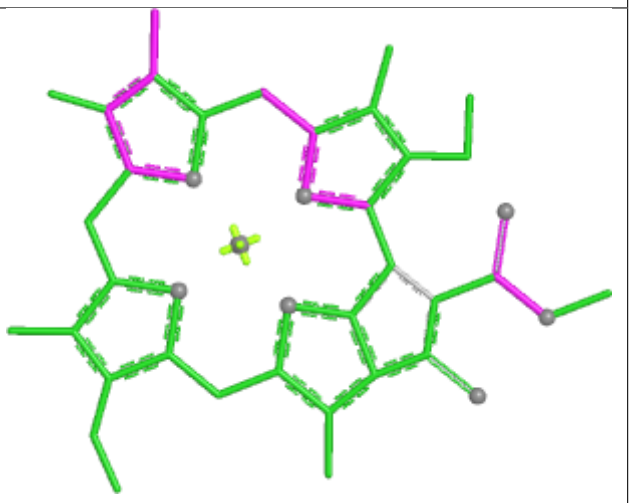


Rings

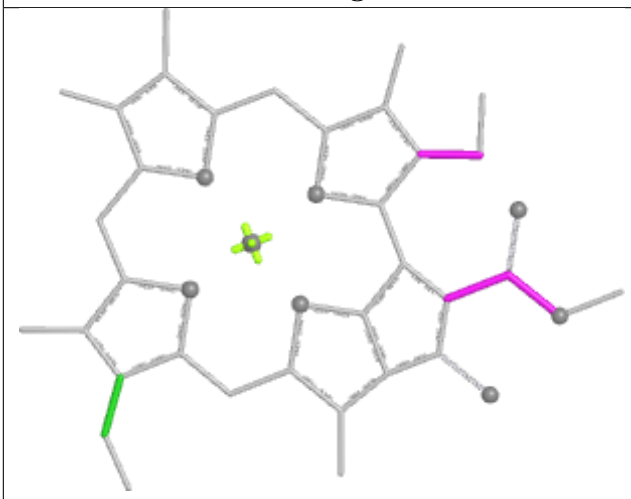
Ligand CLA m 101



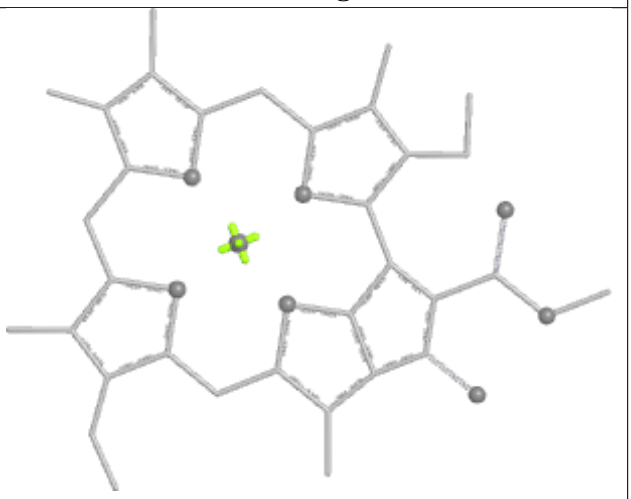
Bond lengths



Bond angles

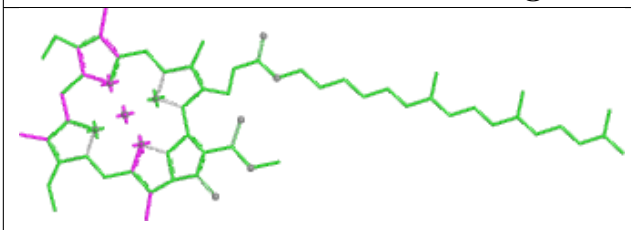


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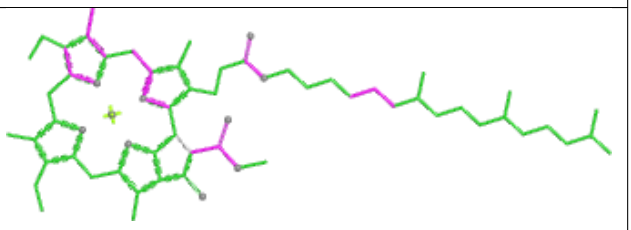


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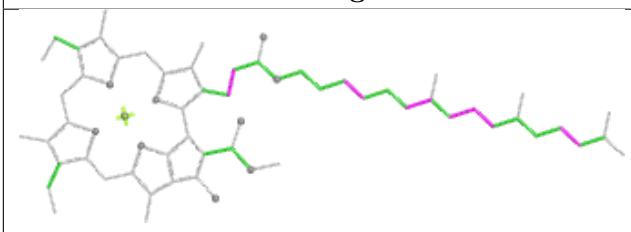
Ligand CLA B 802



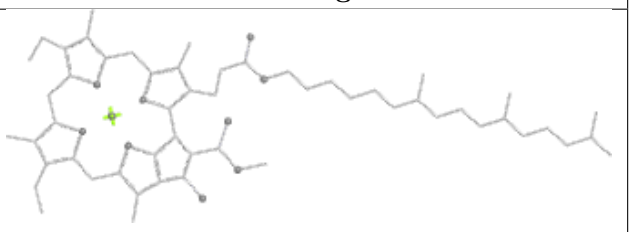
Bond lengths



Bond angles

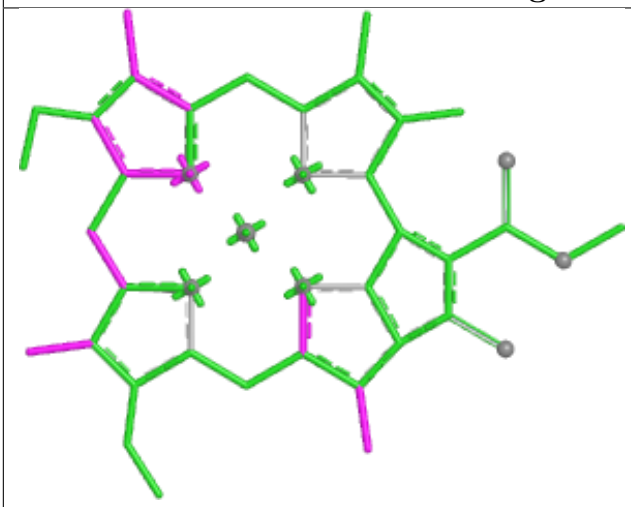


Torsions

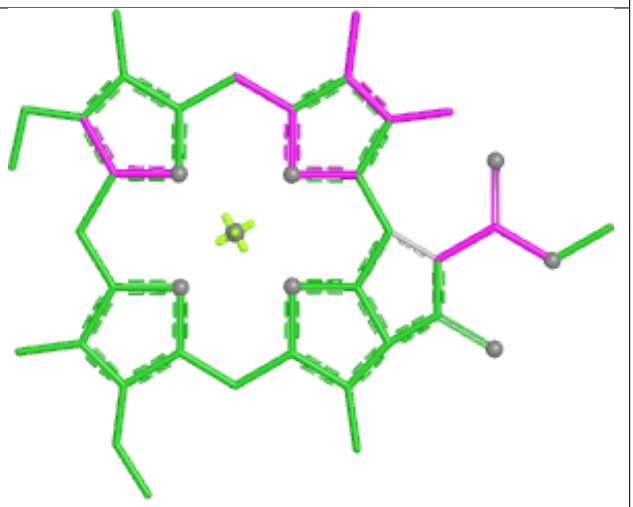


Rings

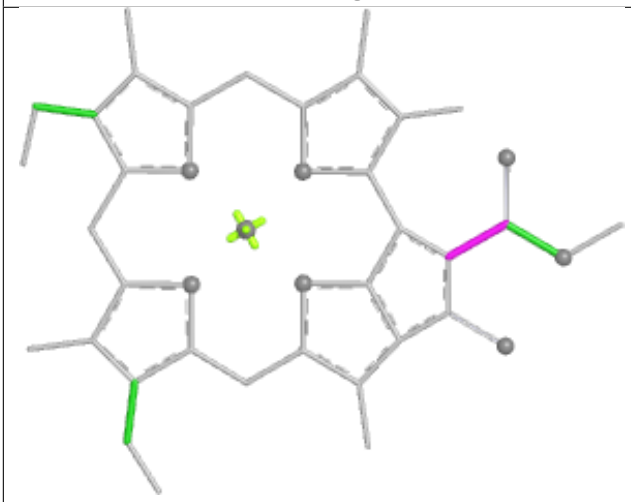
Ligand CLA e 806



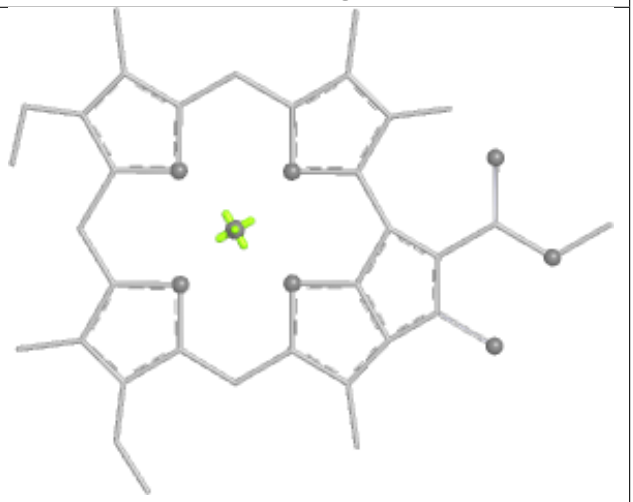
Bond lengths



Bond angles



Torsions

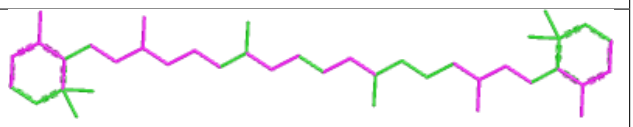


Rings

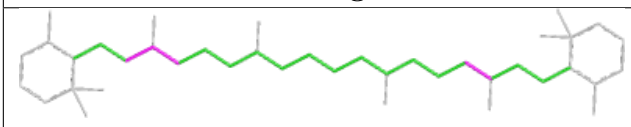
Ligand BCR f 847



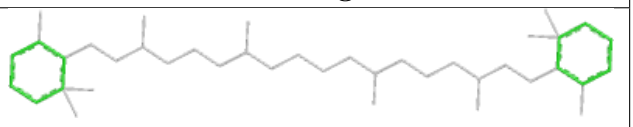
Bond lengths



Bond angles

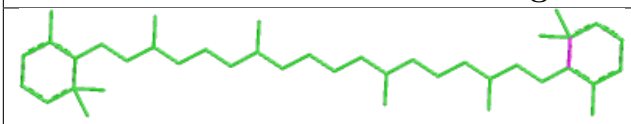


Torsions

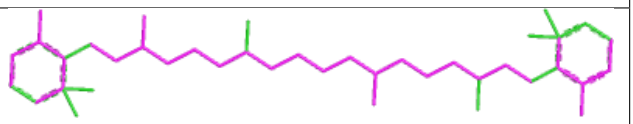


Rings

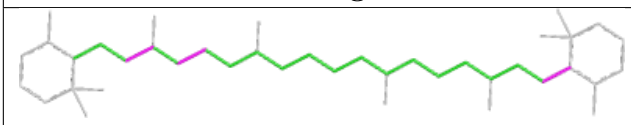
Ligand BCR l 101



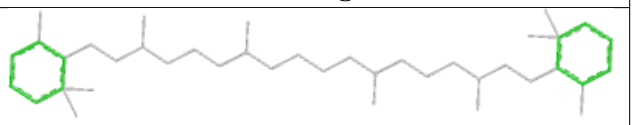
Bond lengths



Bond angles

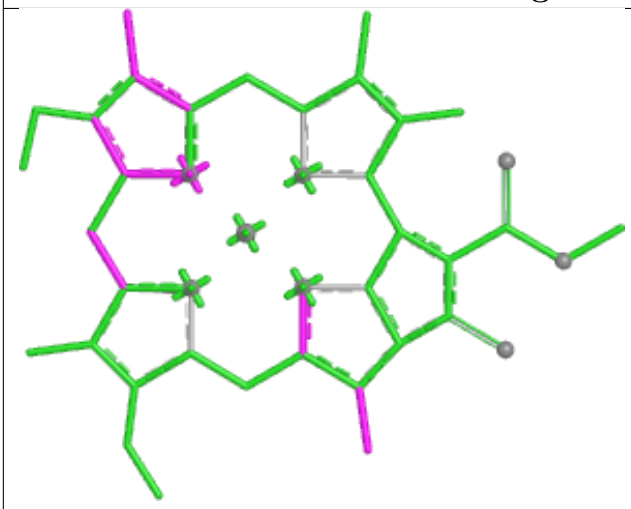


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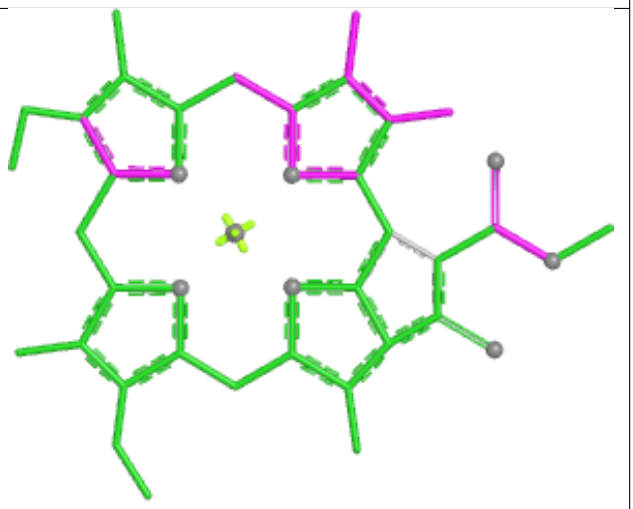


Rings

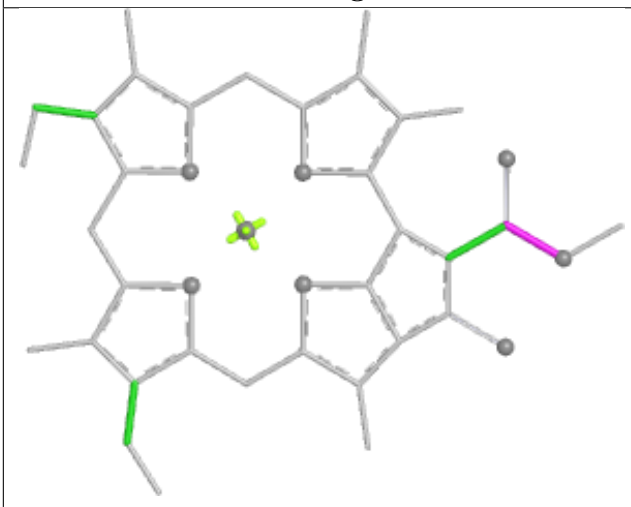
Ligand CLA f 839



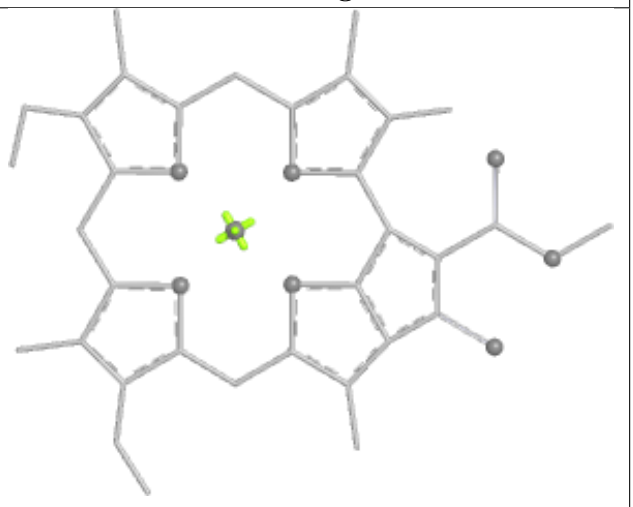
Bond lengths



Bond angles

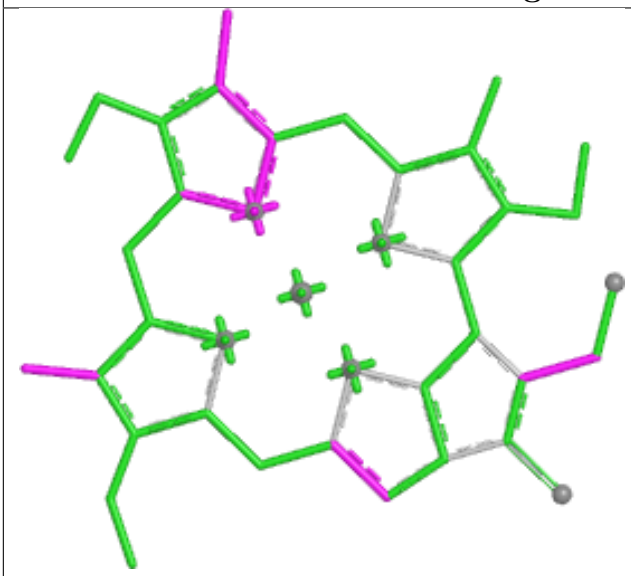


Torsions

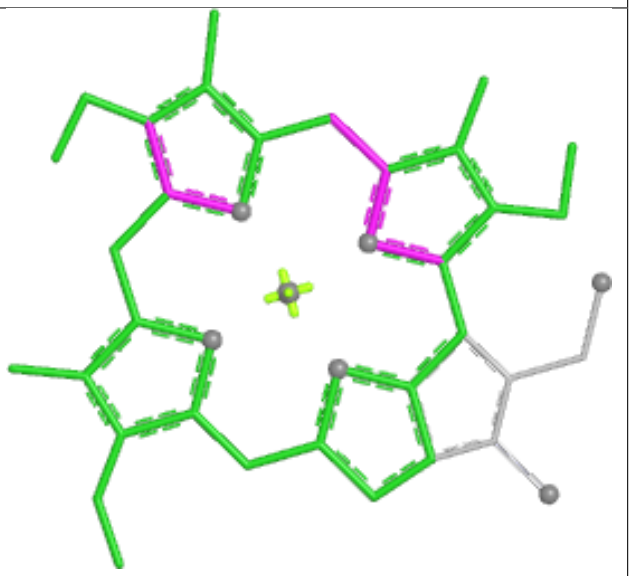


Rings

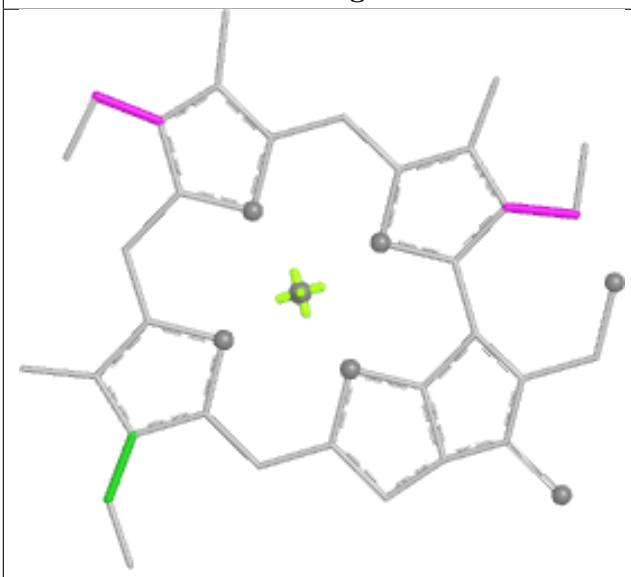
Ligand CLA A 809



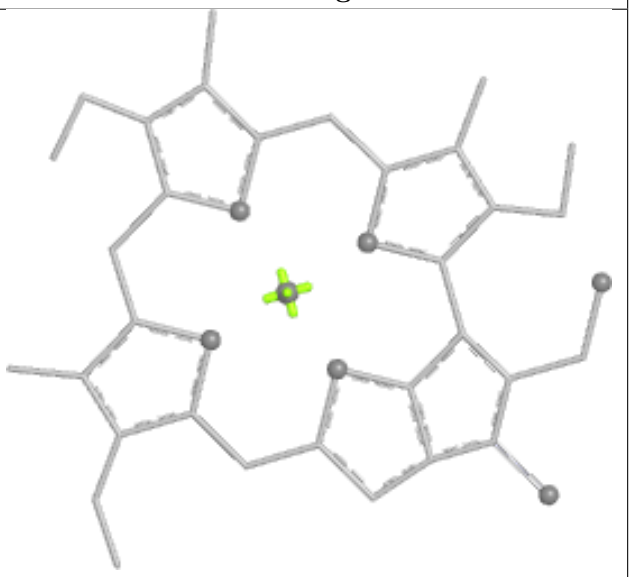
Bond lengths



Bond angles

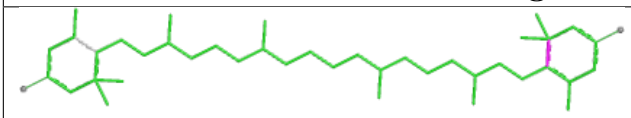


Torsions

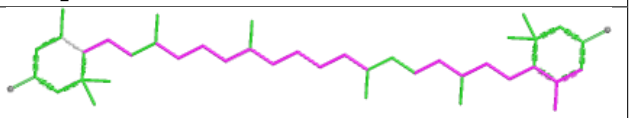


Rings

Ligand LUT q 301



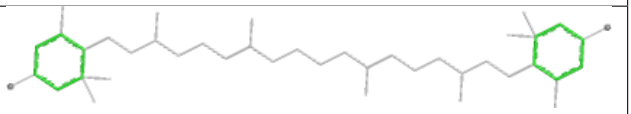
Bond lengths



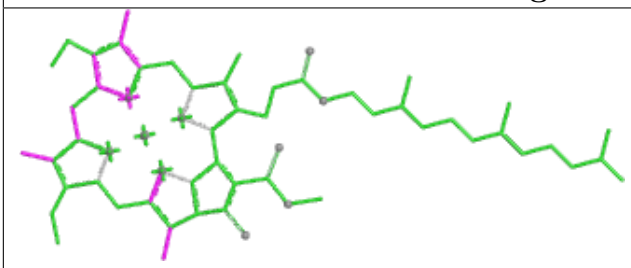
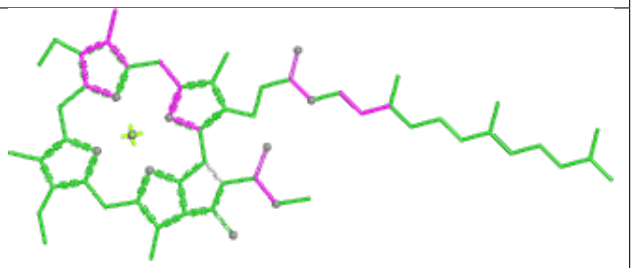
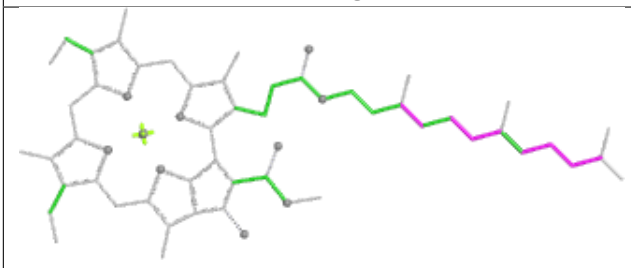
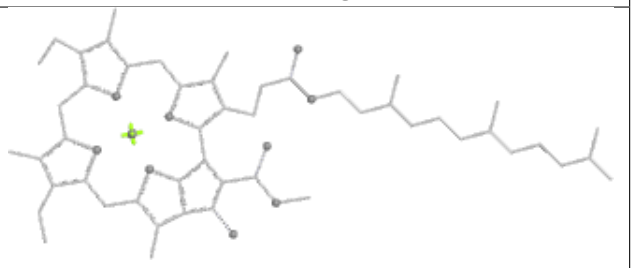
Bond angles

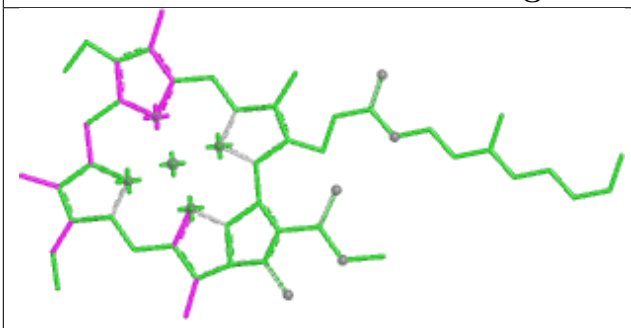
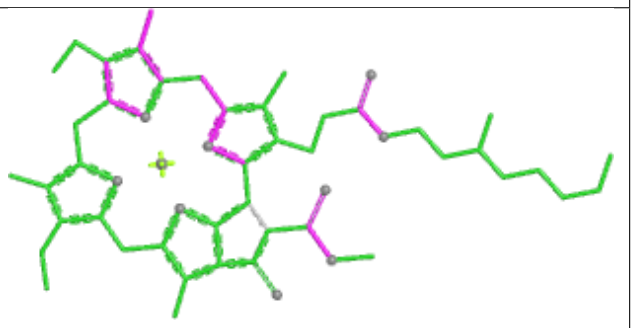
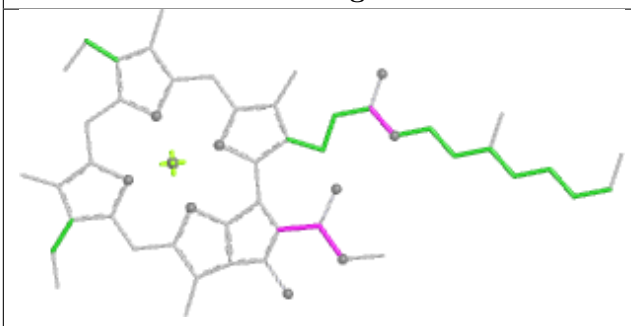
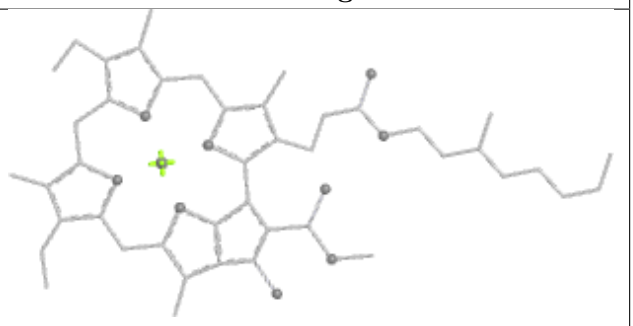


Torsions

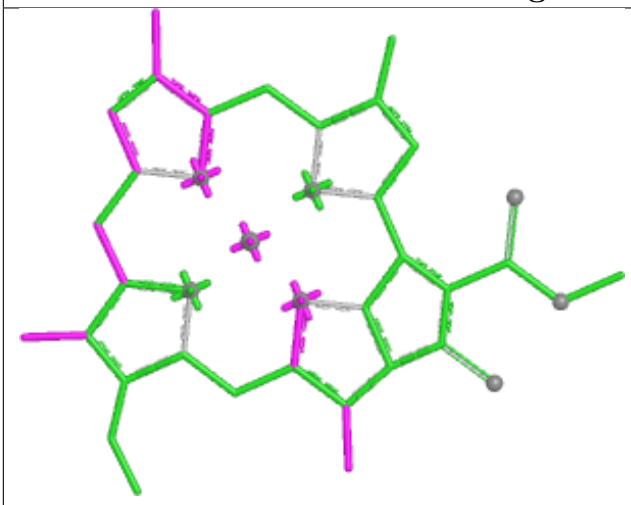


Rings

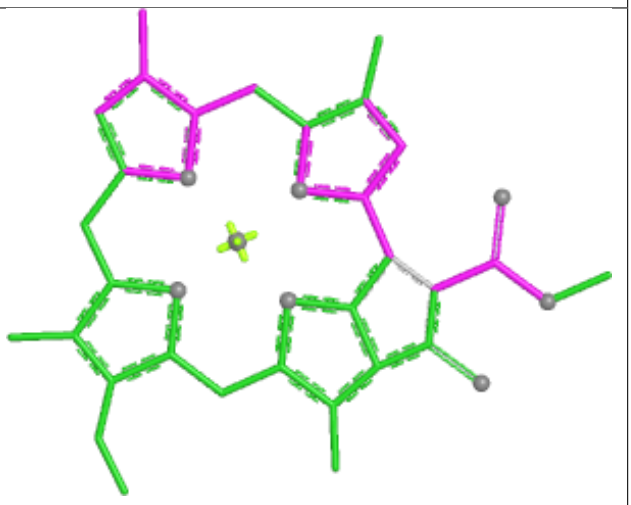
Ligand CLA r 307	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

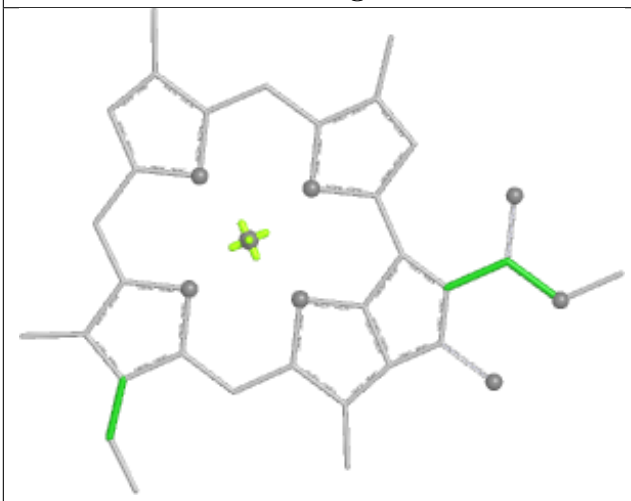
Ligand CLA 5 305



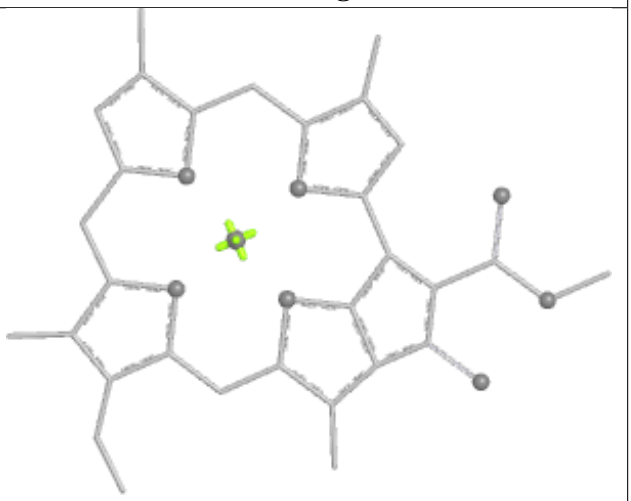
Bond lengths



Bond angles

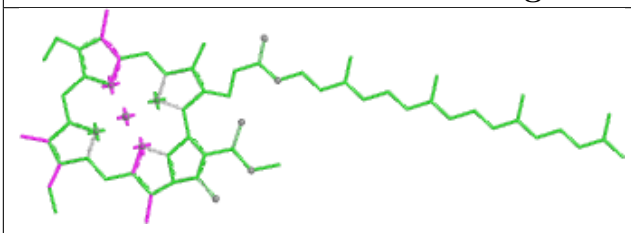


Torsions

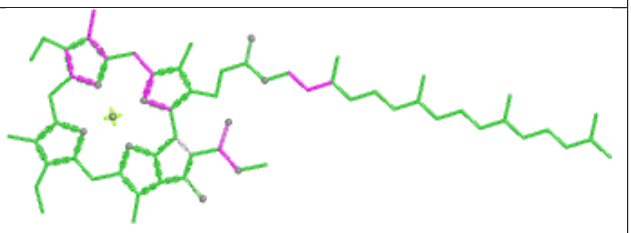


Rings

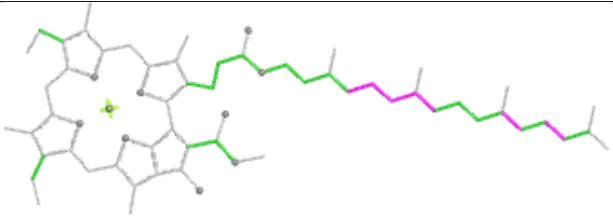
Ligand CLA B 807



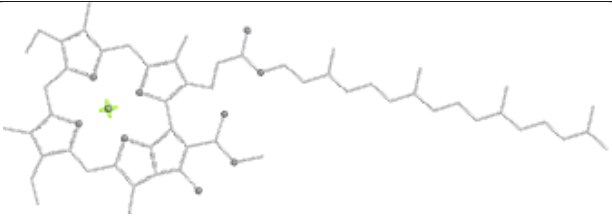
Bond lengths



Bond angles

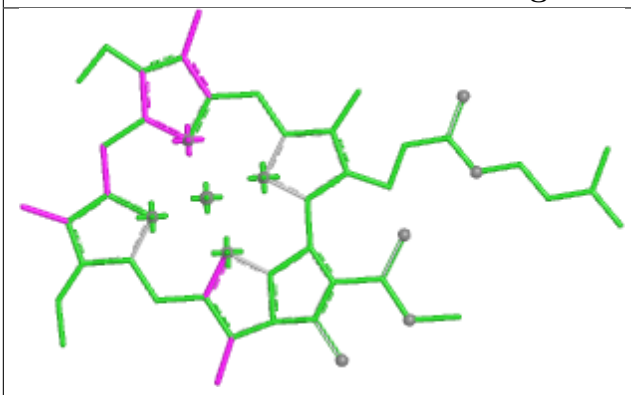


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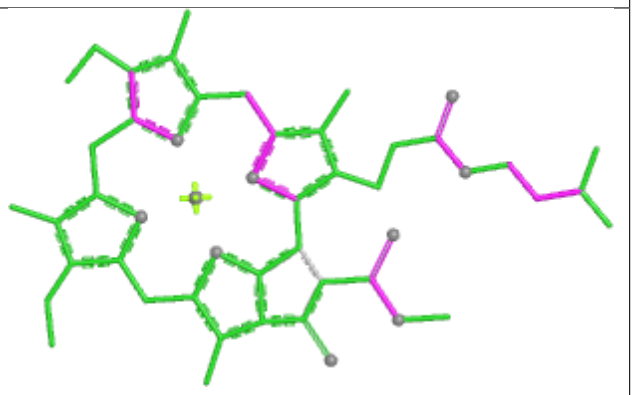


Rings

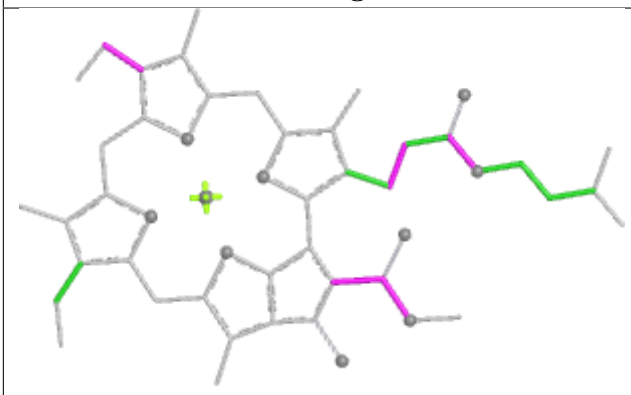
Ligand CLA r 305



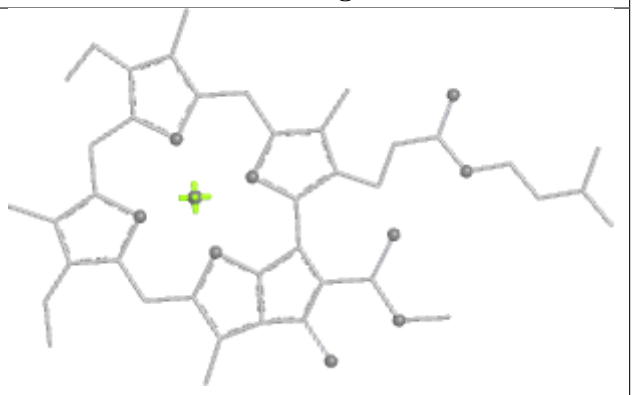
Bond lengths



Bond angles

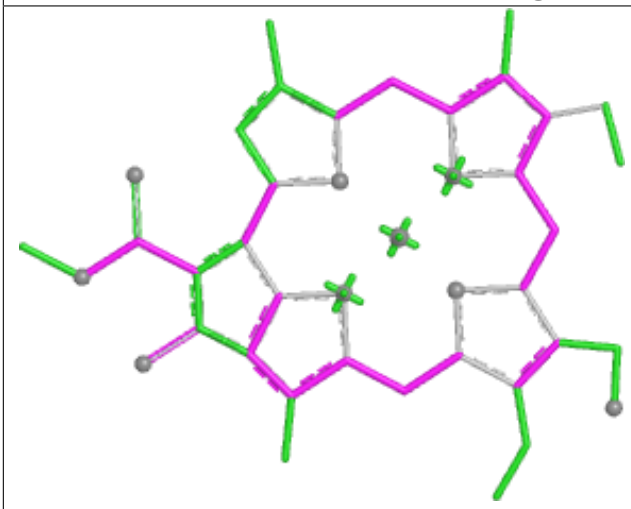


Torsions

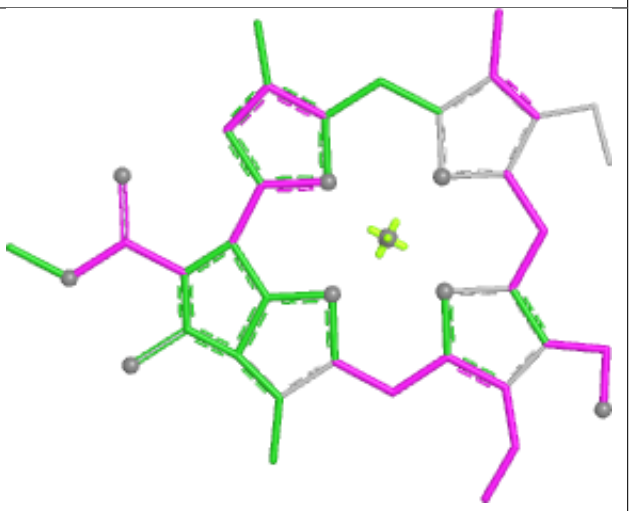


Rings

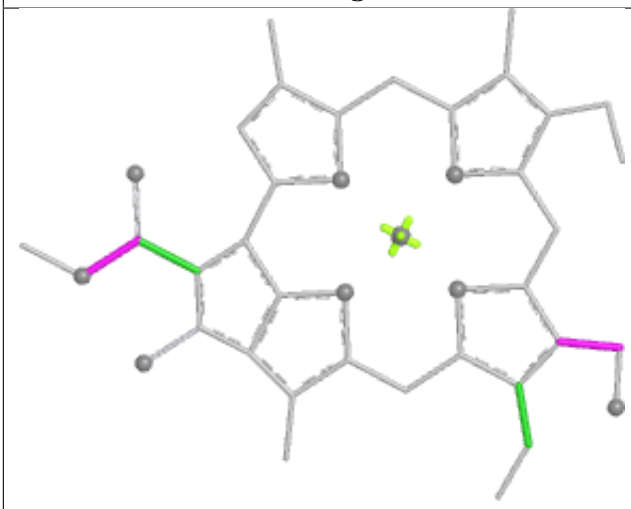
Ligand CHL s 515



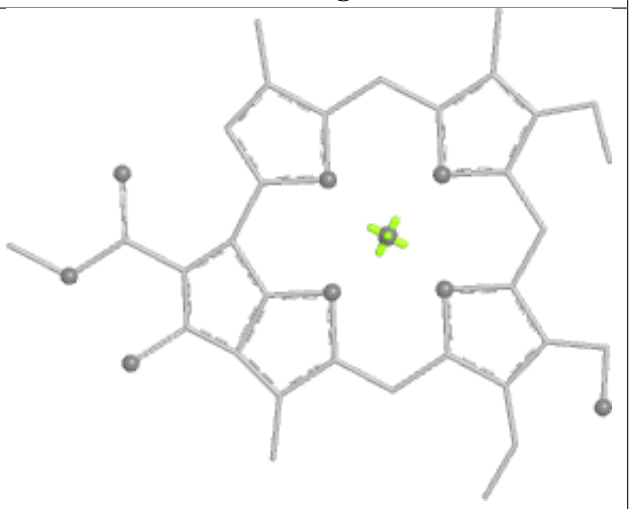
Bond lengths



Bond angles

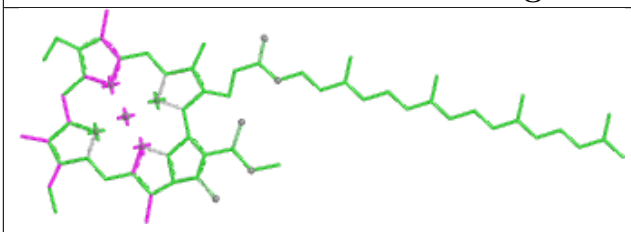


Torsions

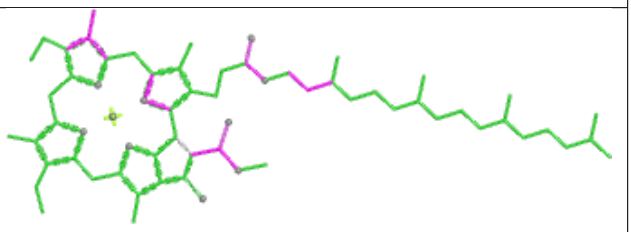


Rings

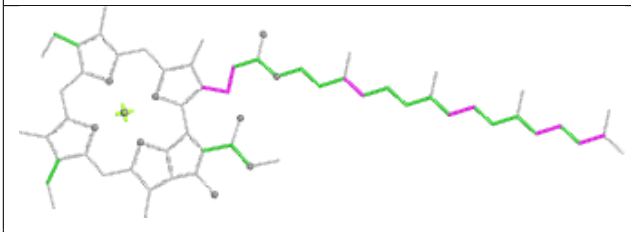
Ligand CLA B 801



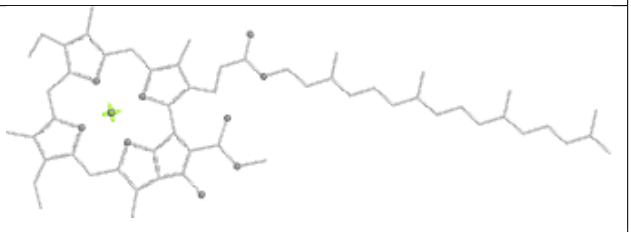
Bond lengths



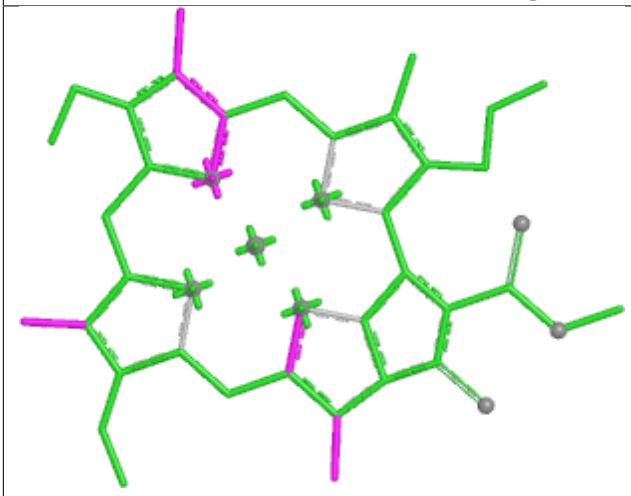
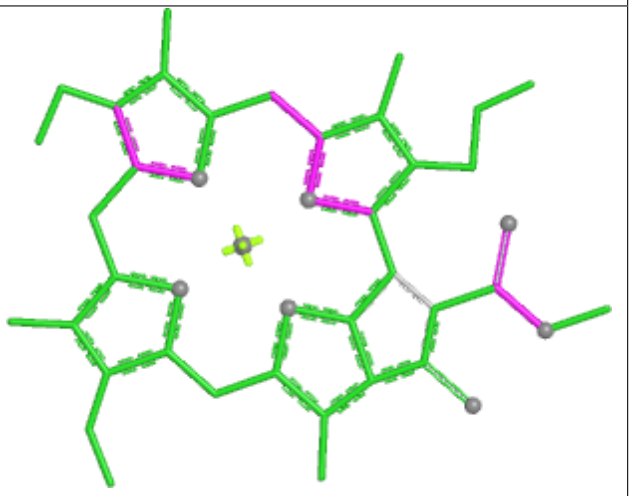
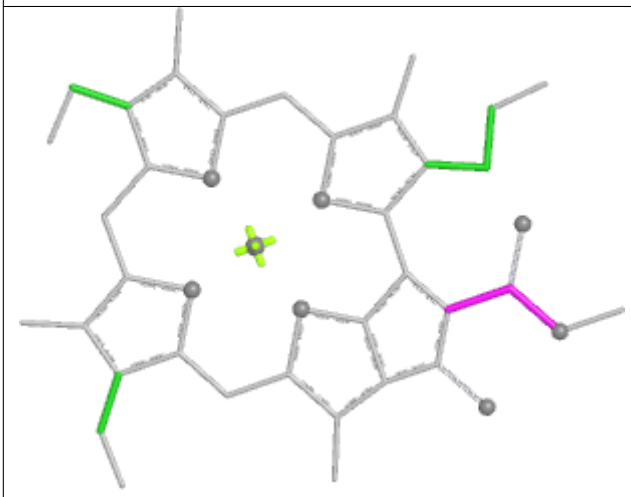
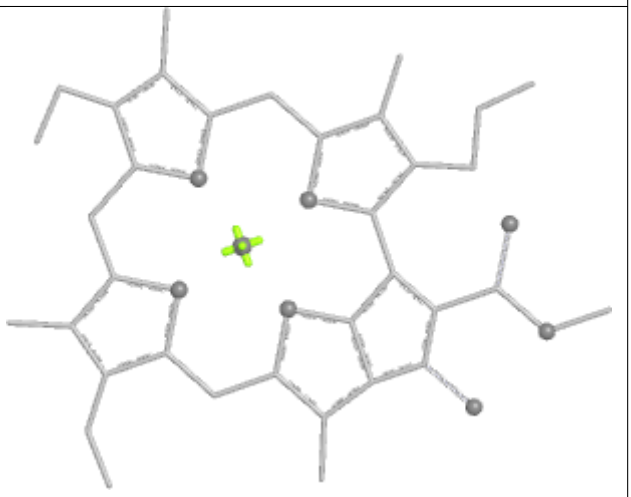
Bond angles



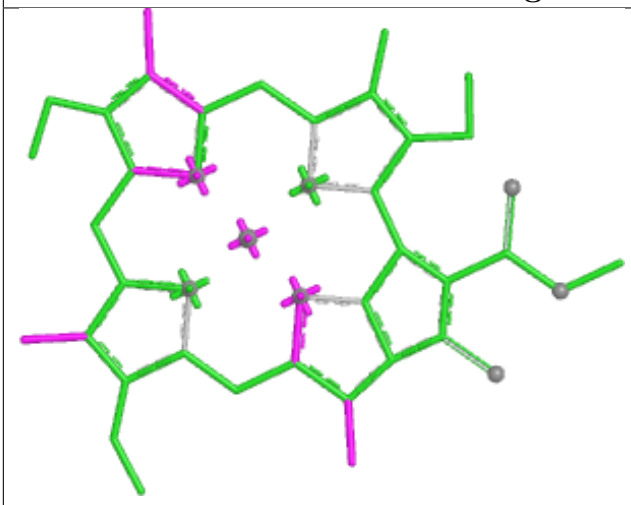
Torsions



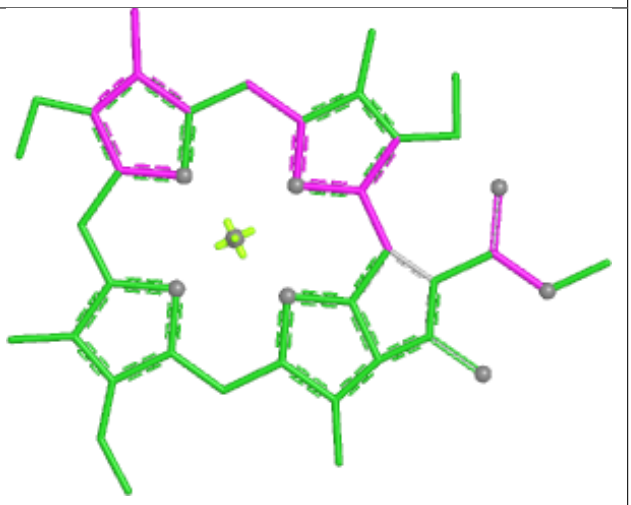
Rings

Ligand CLA B 816	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

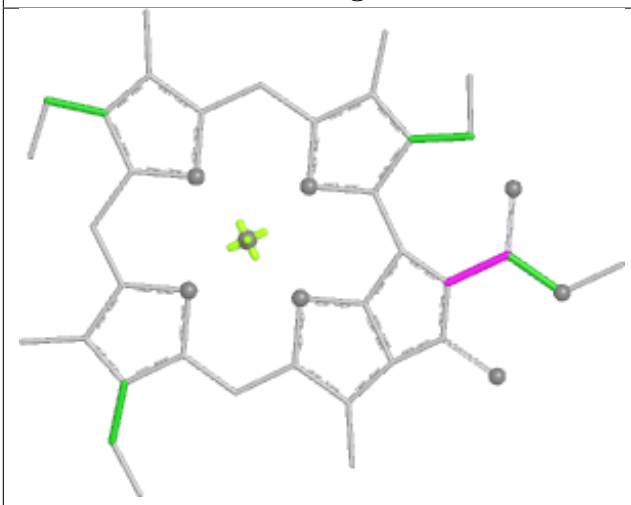
Ligand CLA B 825



Bond lengths



Bond angles

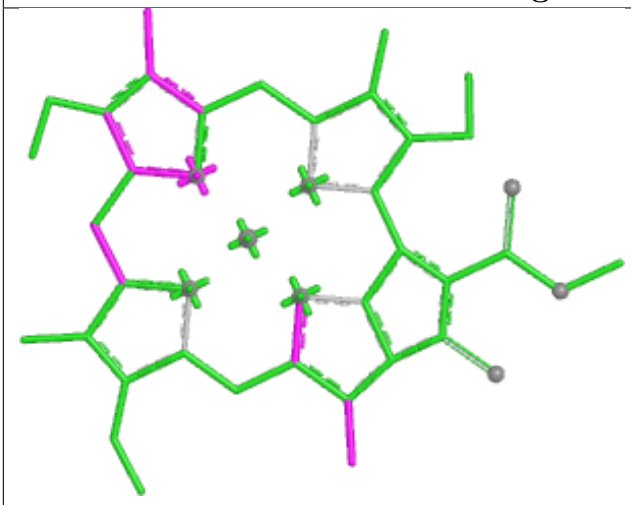


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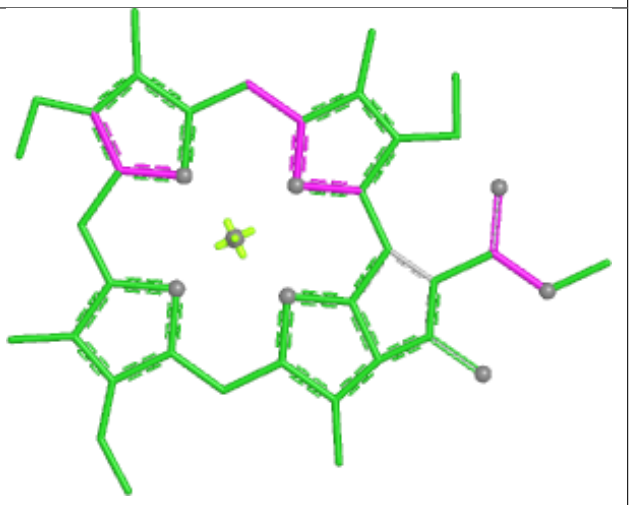


Rings

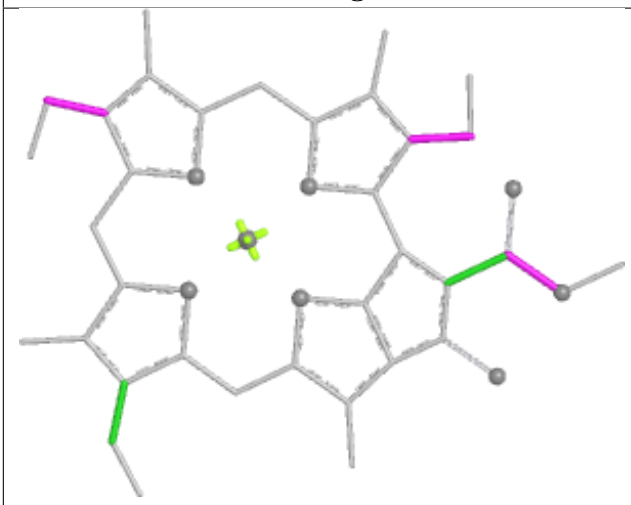
Ligand CLA f 824



Bond lengths



Bond angles

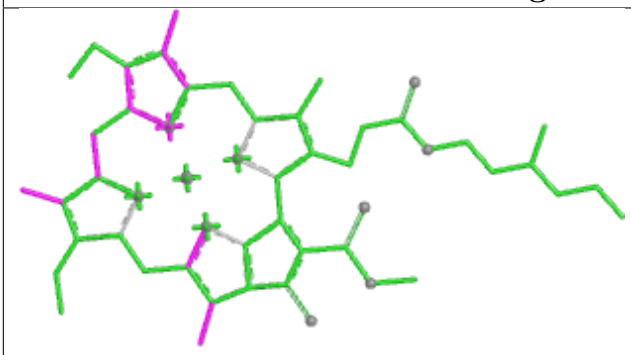


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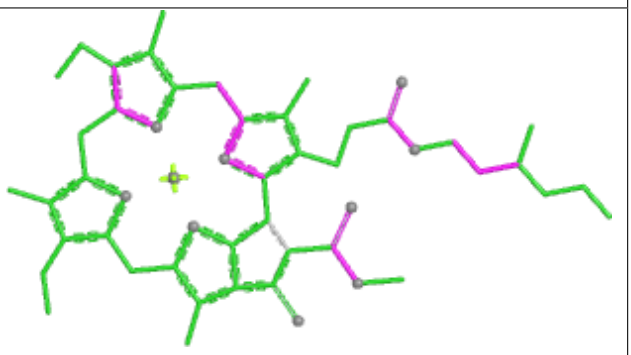


Rings

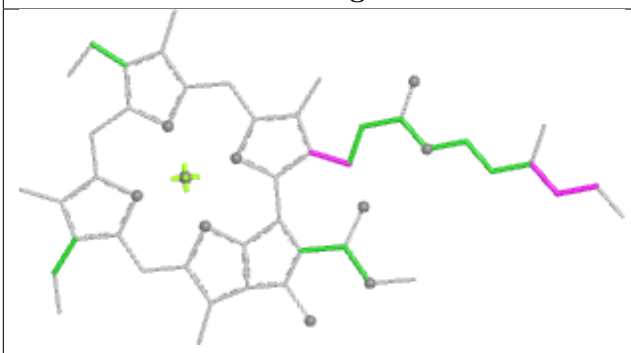
Ligand CLA e 803



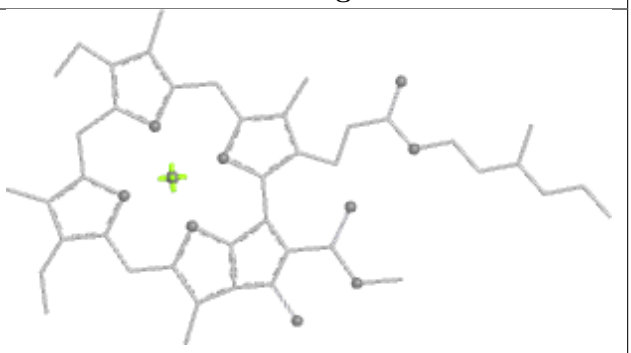
Bond lengths



Bond angles

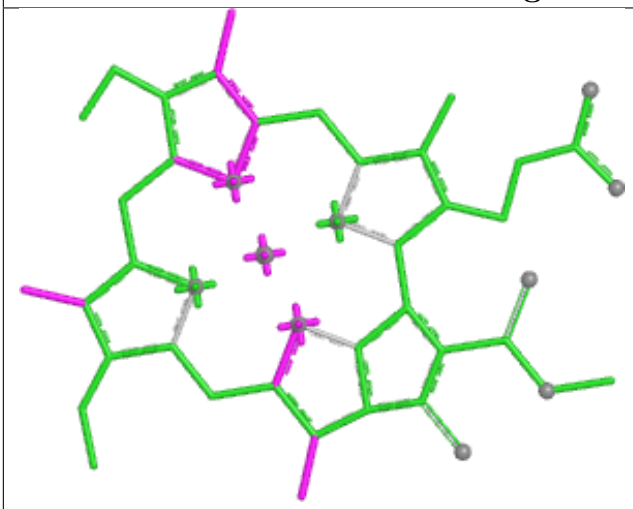


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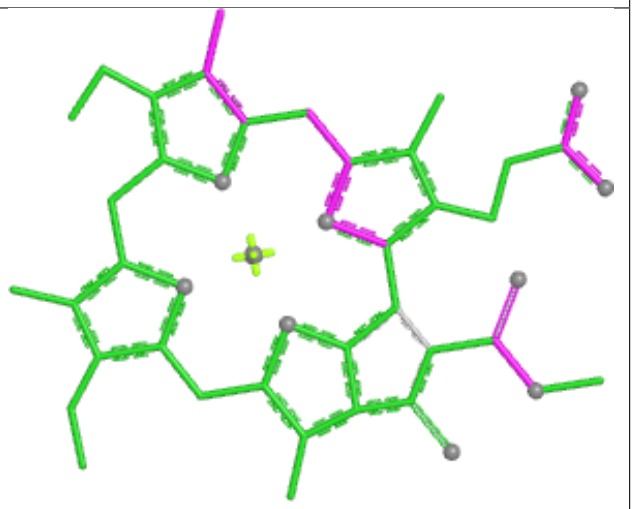


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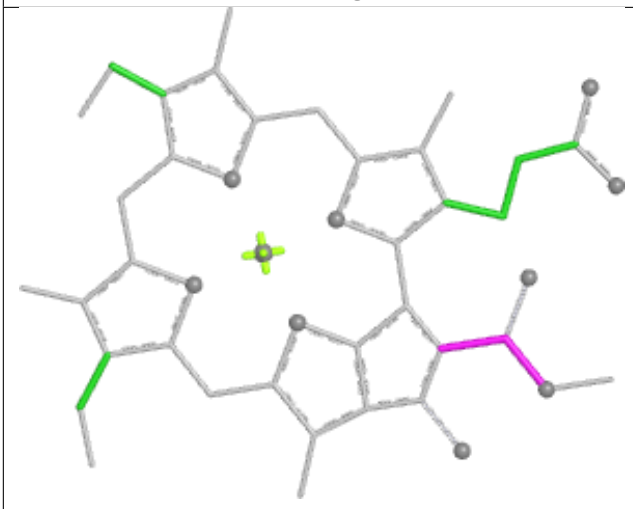
Ligand CLA A 815



Bond lengths



Bond angles

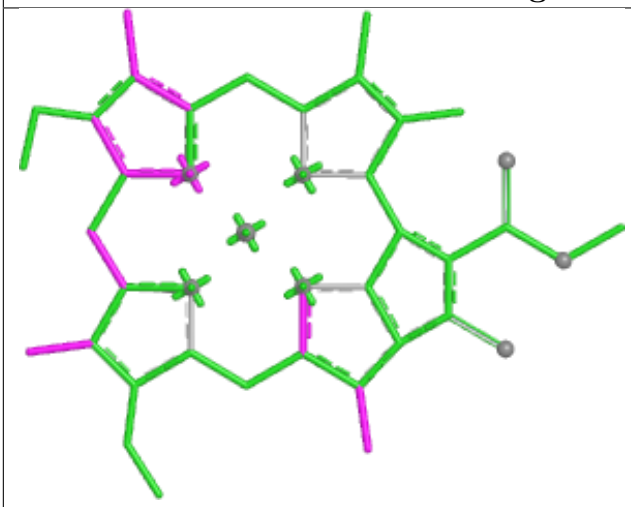


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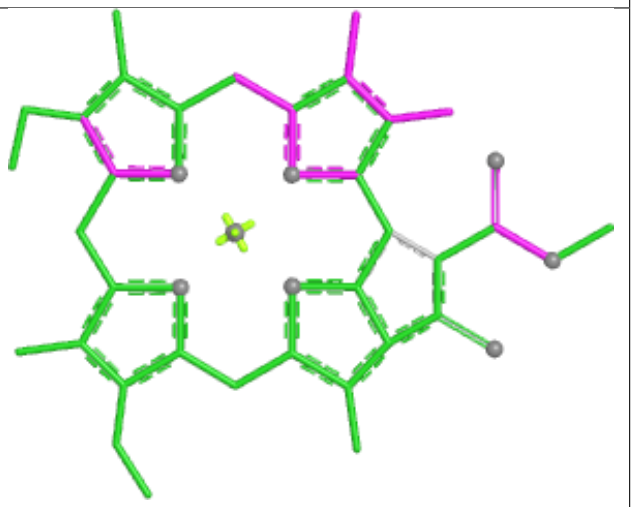


Rings

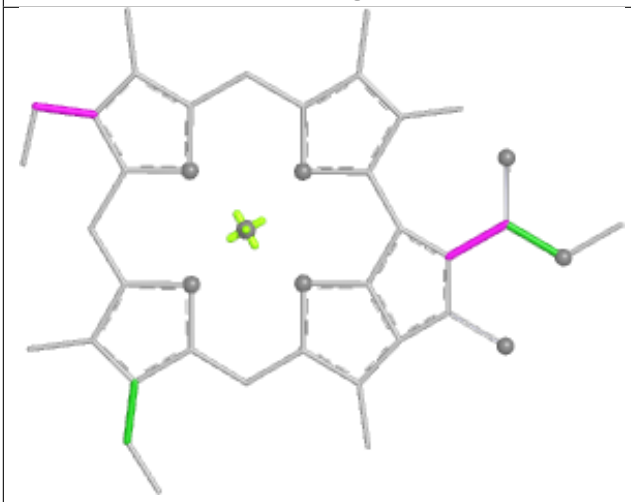
Ligand CLA e 811



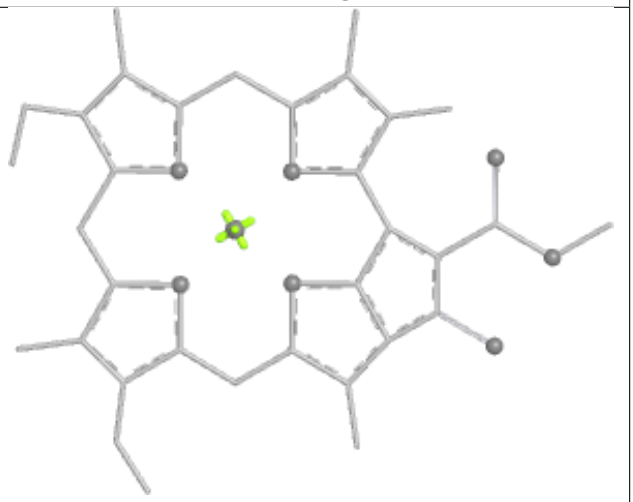
Bond lengths



Bond angles

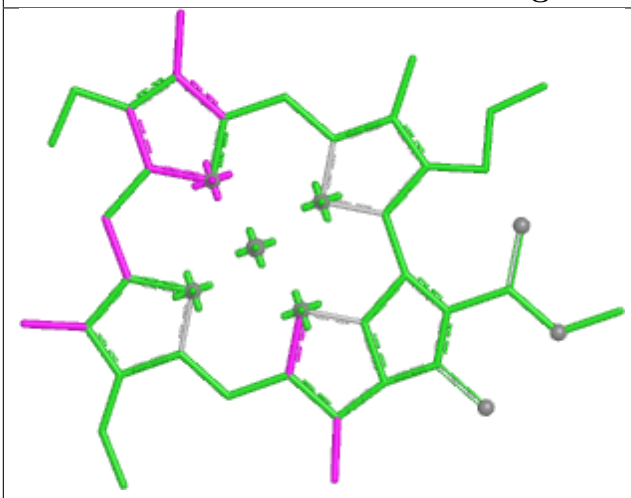


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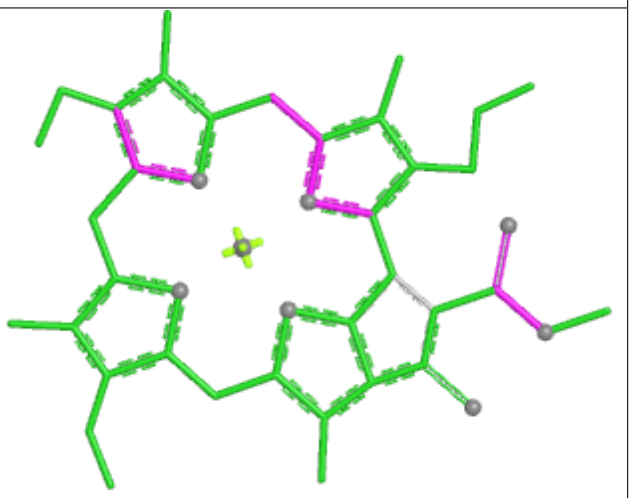


Rings

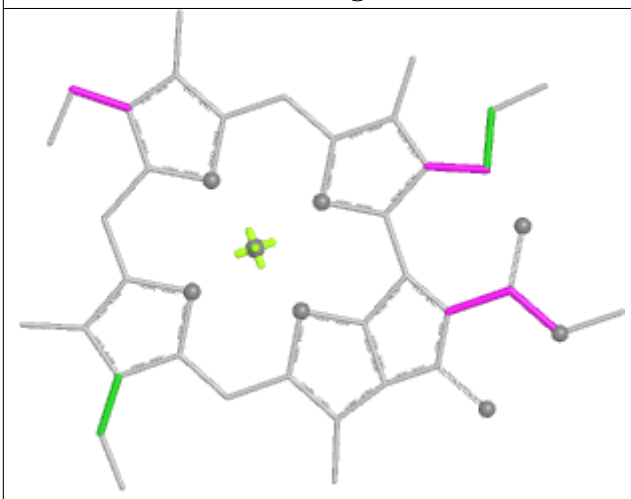
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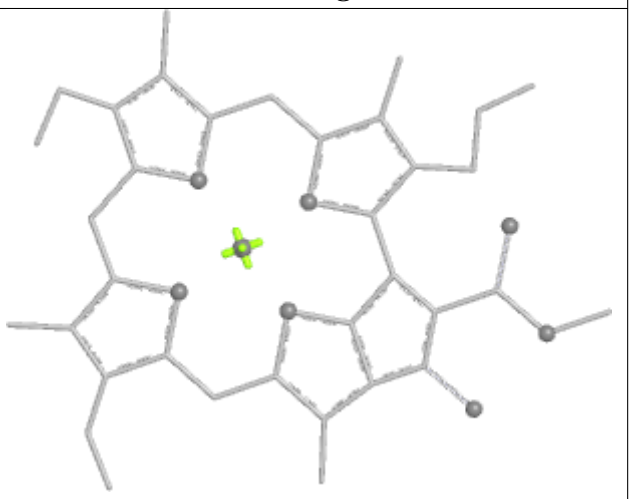
Bond lengths



Bond angles

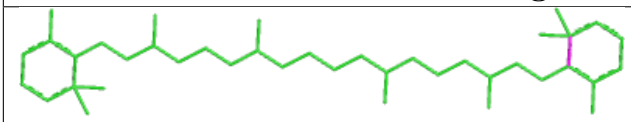


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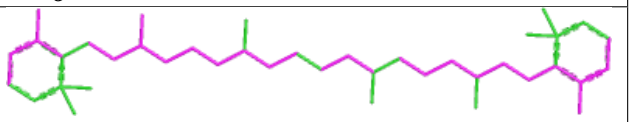


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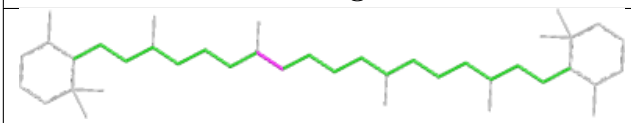
Ligand BCR j 803



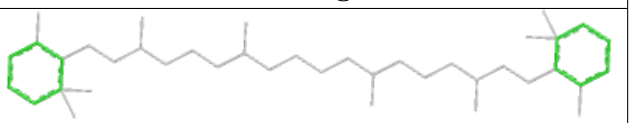
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Bond angles

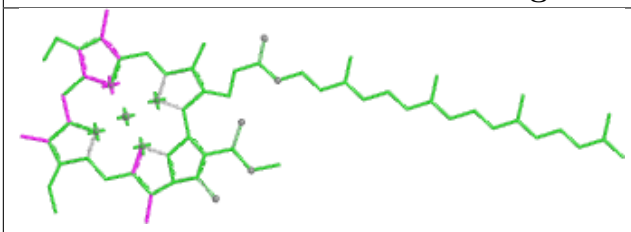


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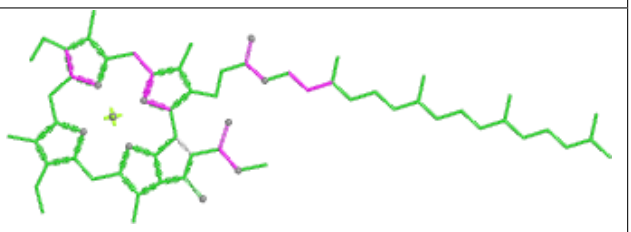


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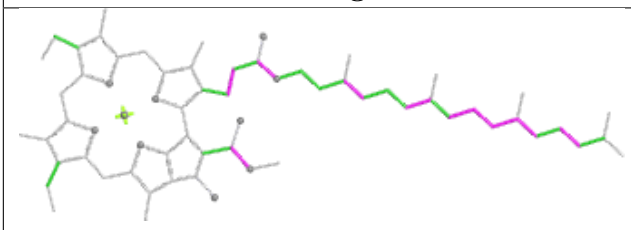
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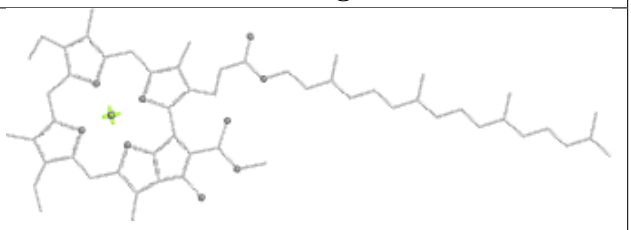
Bond lengths



Bond angles

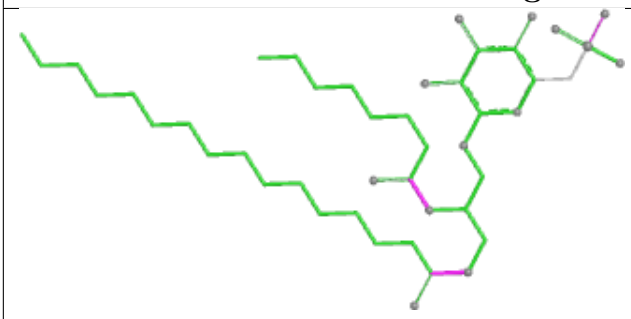


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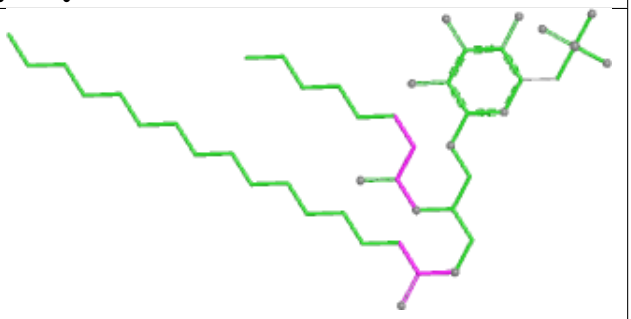


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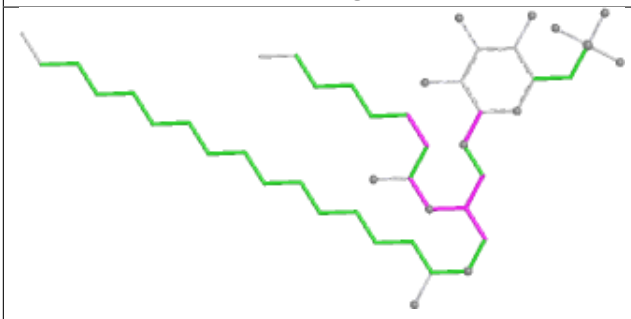
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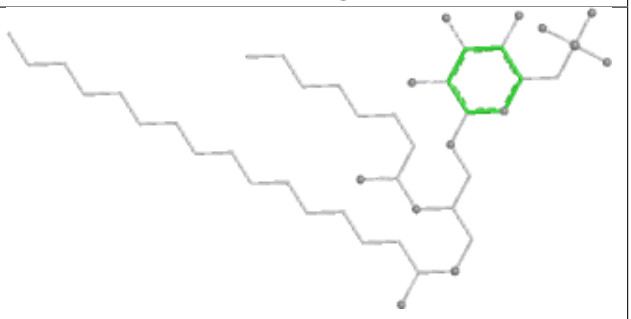
Bond lengths



Bond angles

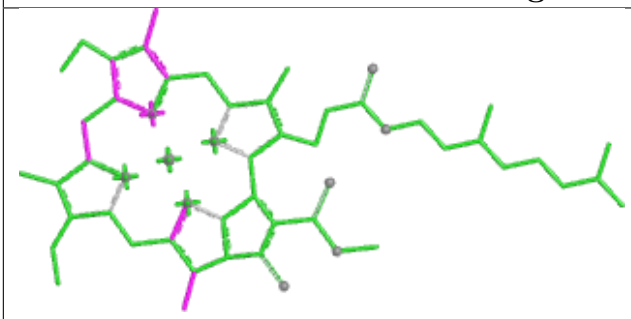


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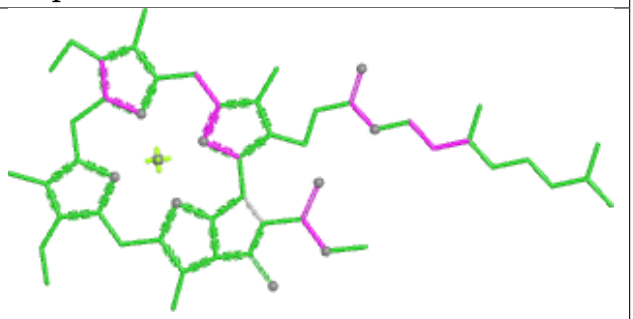


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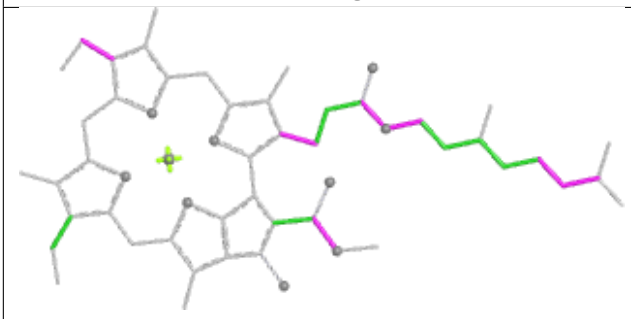
Ligand CLA p 506



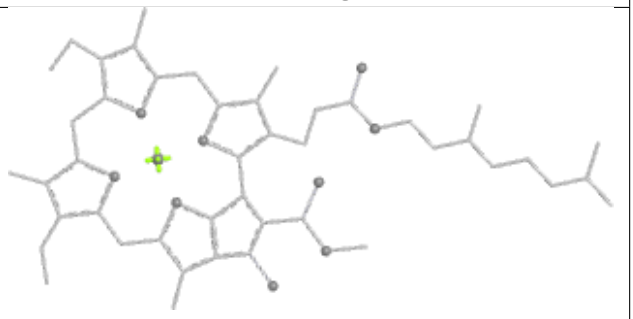
Bond lengths



Bond angles

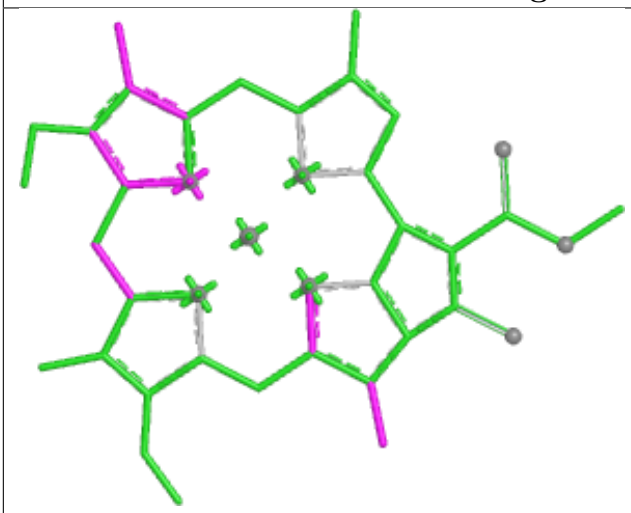


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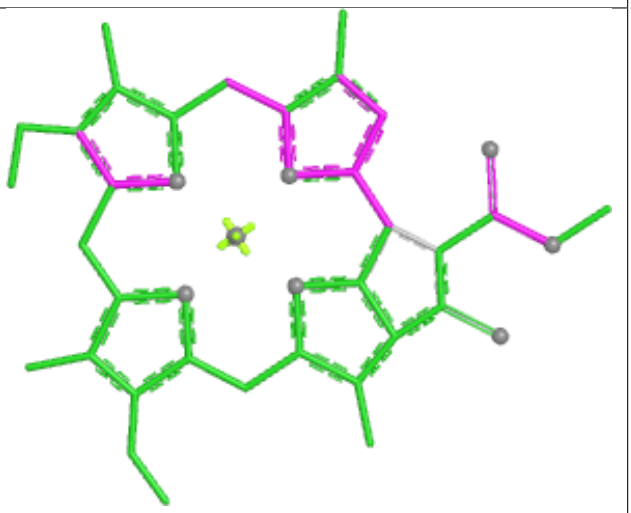


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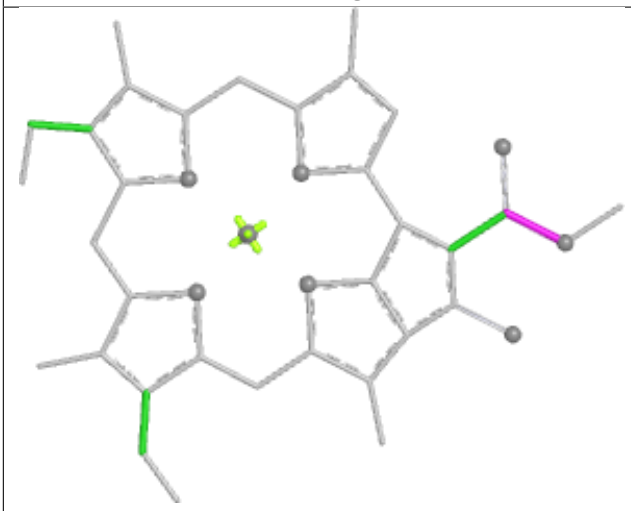
Ligand CLA s 514



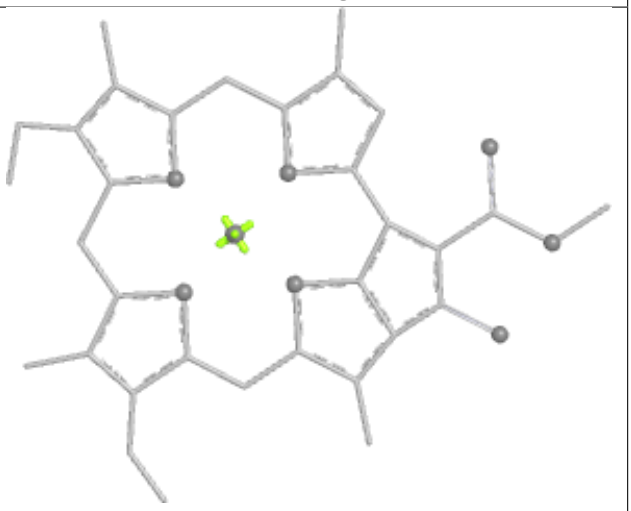
Bond lengths



Bond angles

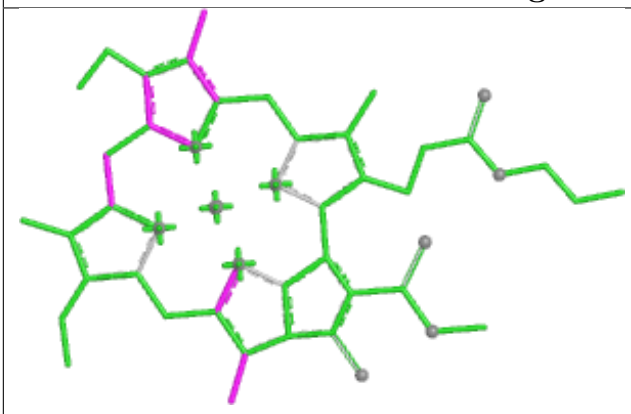


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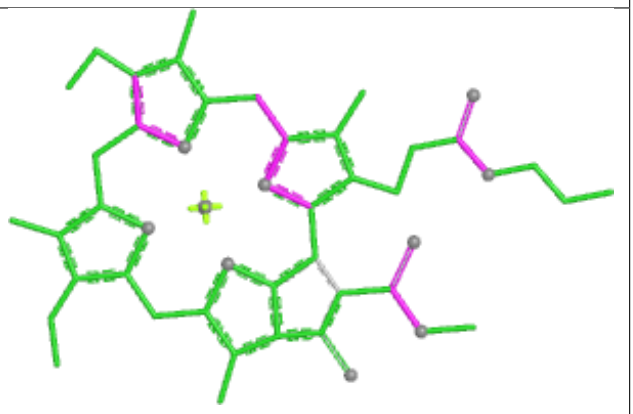


Rings

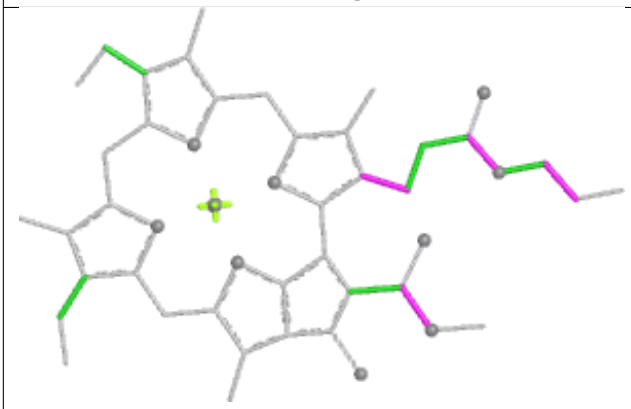
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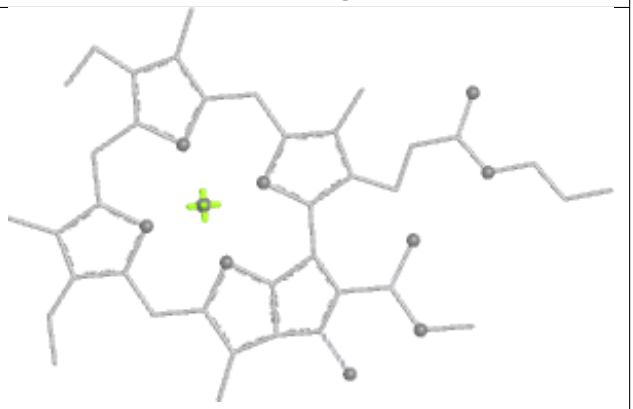
Bond lengths



Bond angles

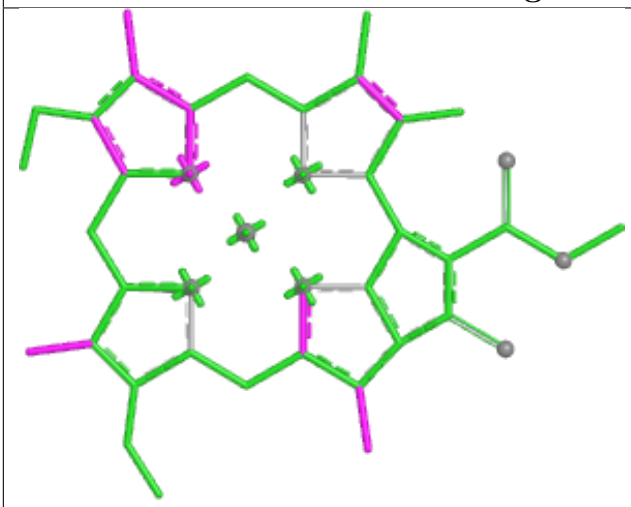


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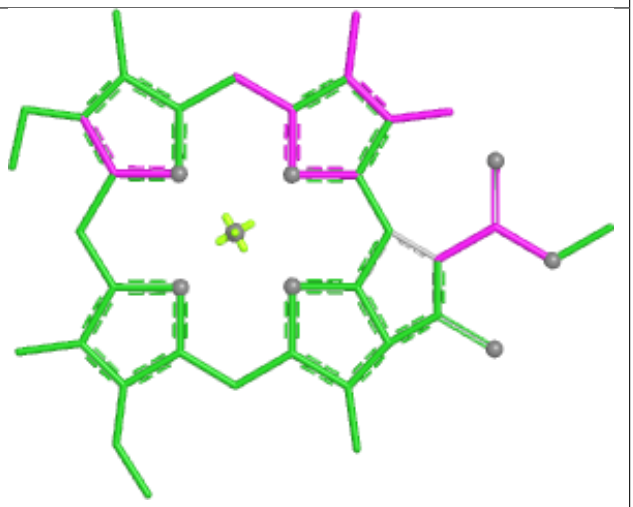


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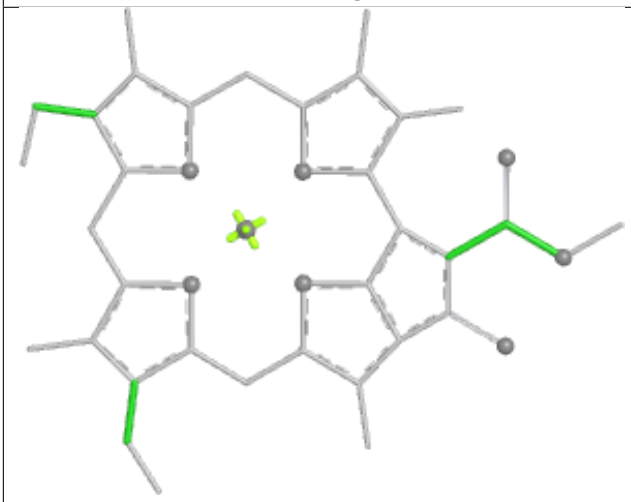
Ligand CLA B 819



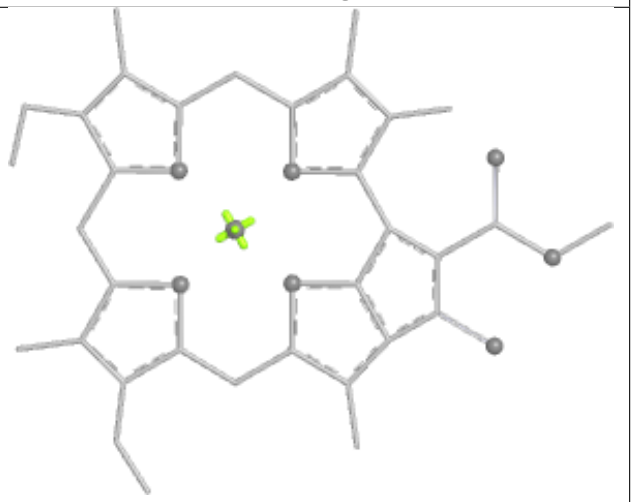
Bond lengths



Bond angles

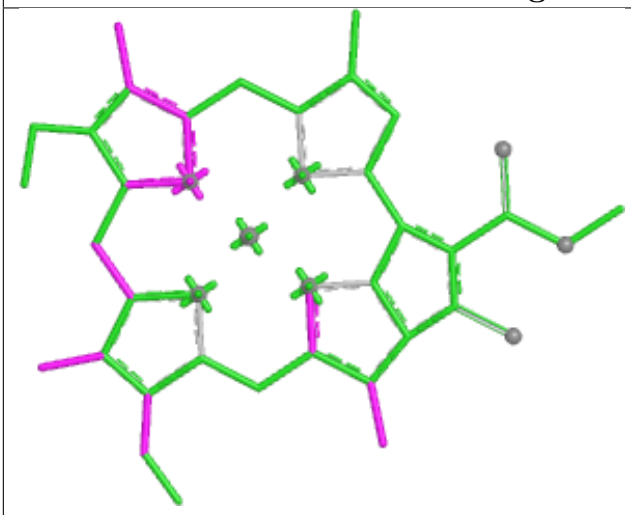


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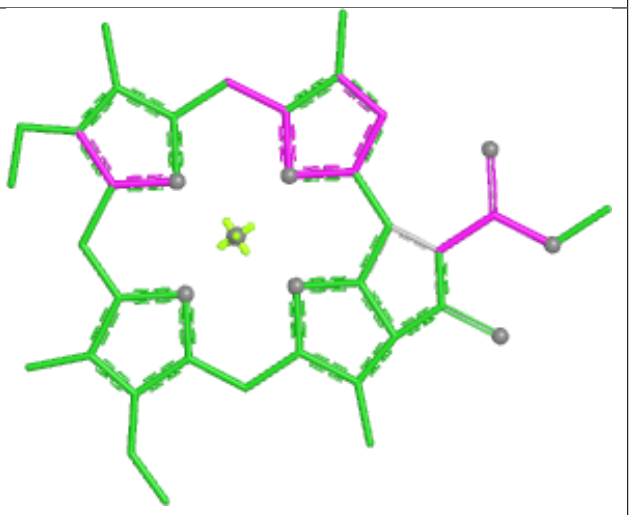


Rings

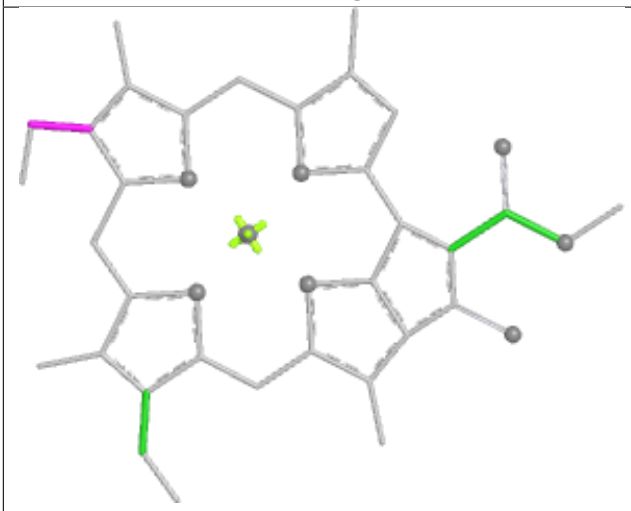
Ligand CLA 2 511



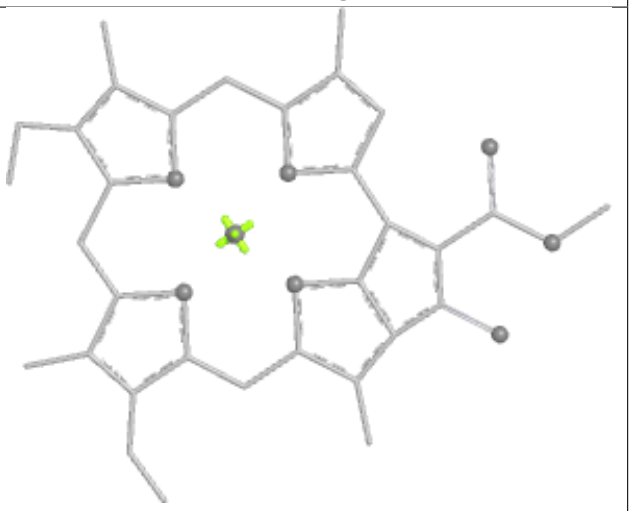
Bond lengths



Bond angles

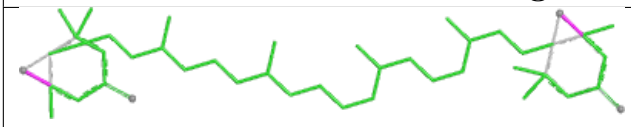


Torsions

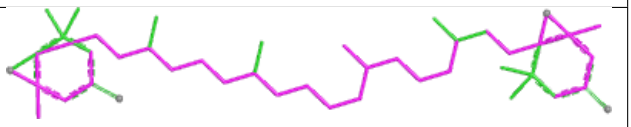


Rings

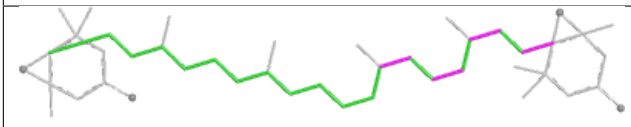
Ligand XAT s 502



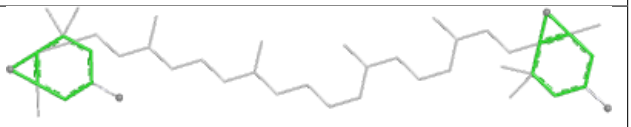
Bond lengths



Bond angles

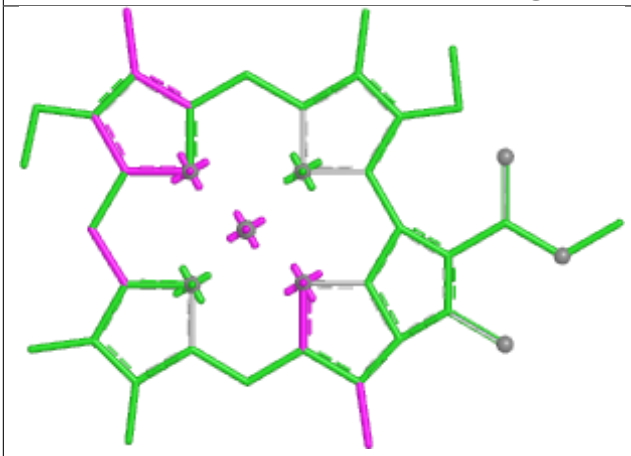


Torsions

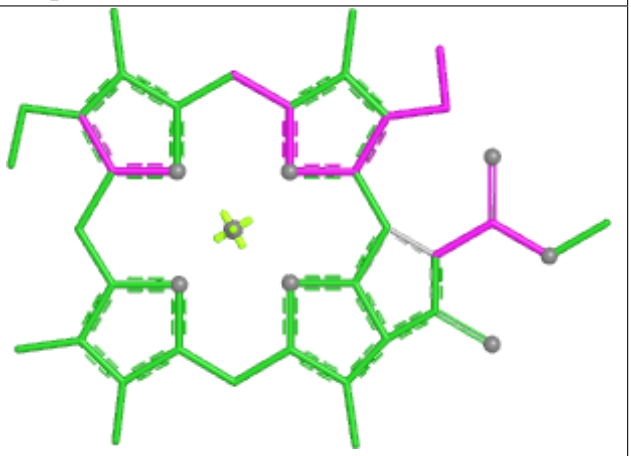


Rings

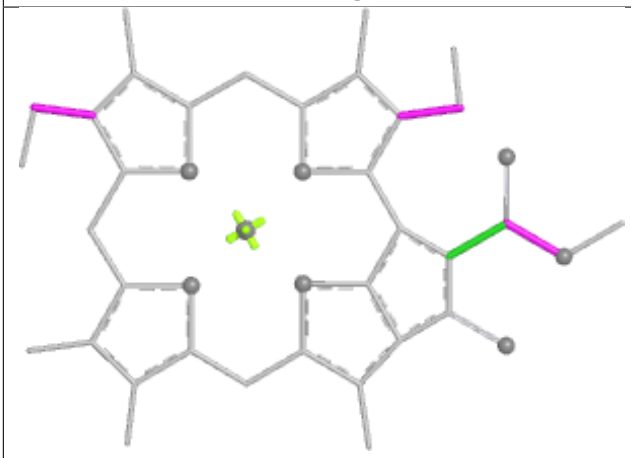
Ligand CLA p 504



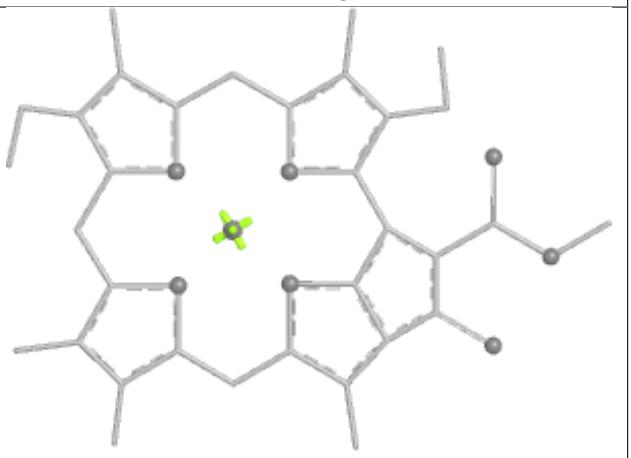
Bond lengths



Bond angles

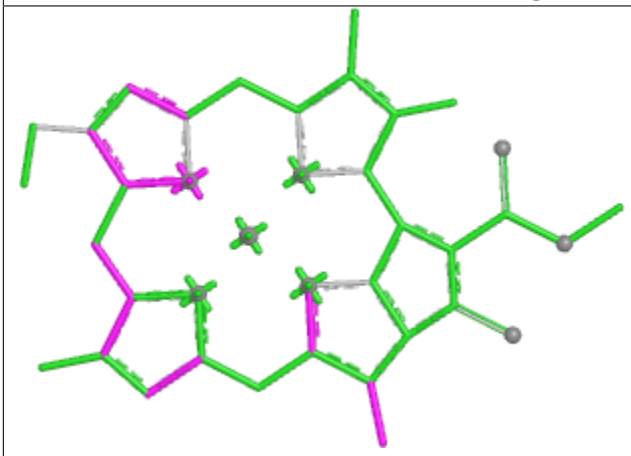


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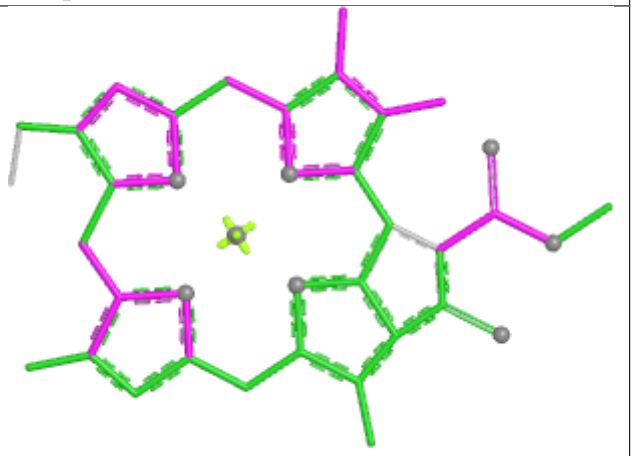


Rings

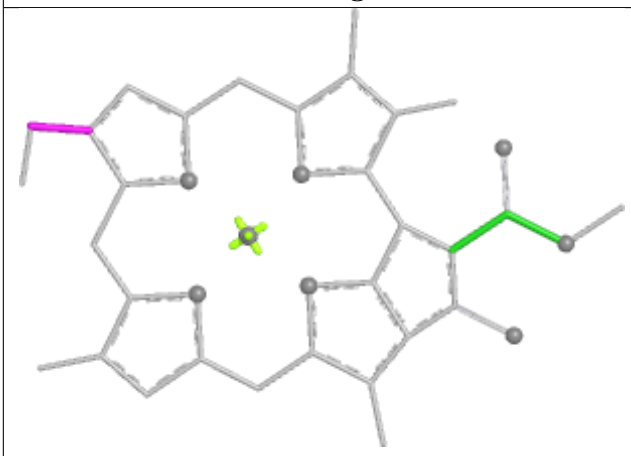
Ligand CLA q 304



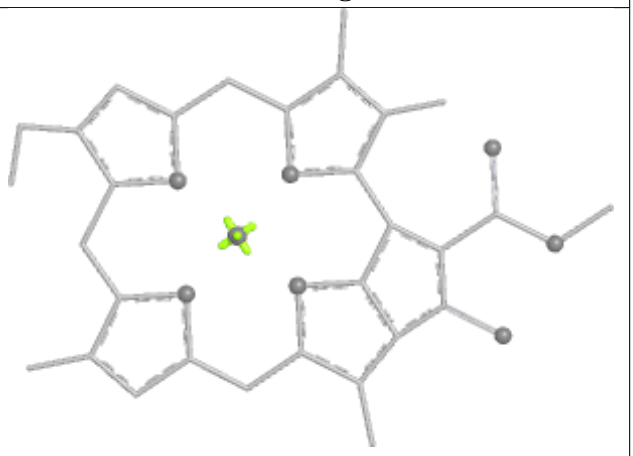
Bond lengths



Bond angles

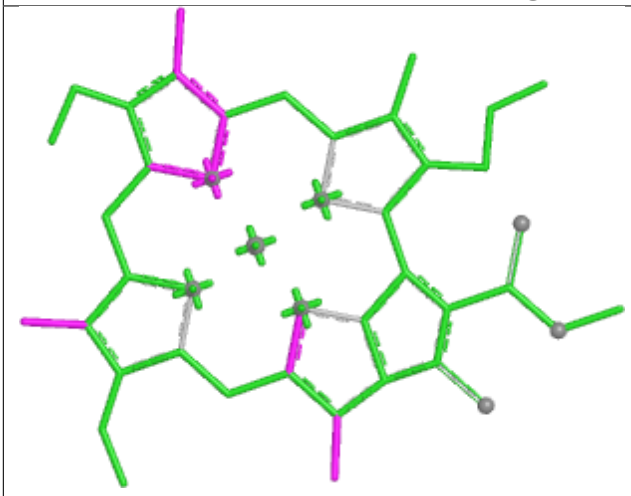


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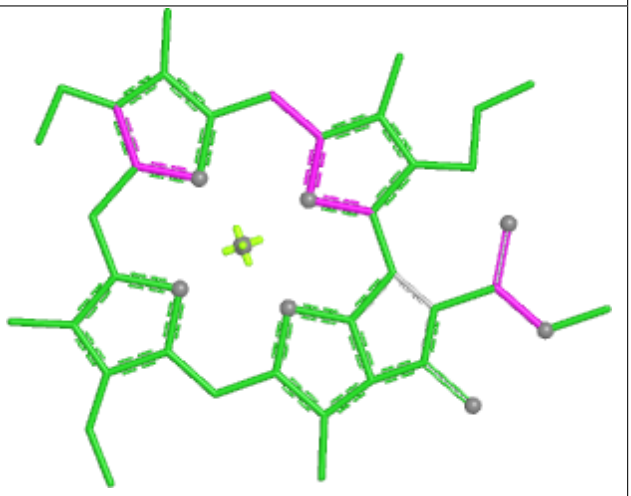


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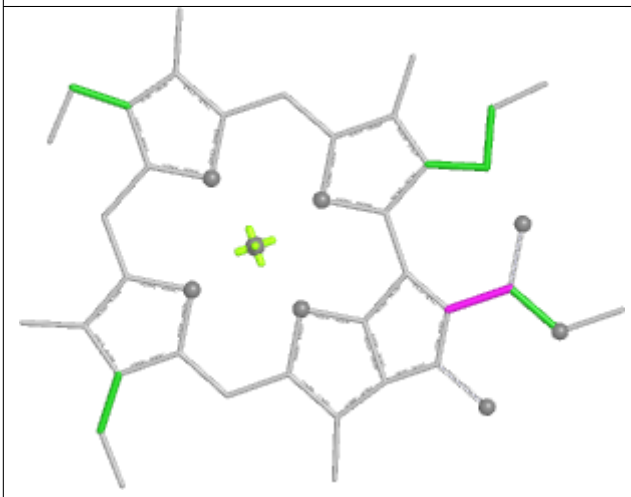
Ligand CLA B 831



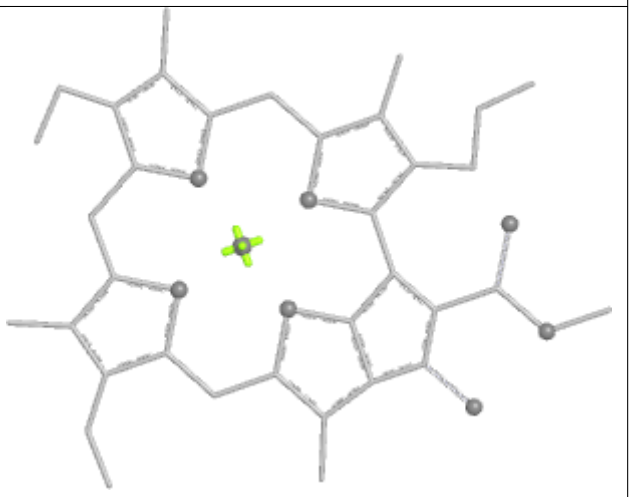
Bond lengths



Bond angles

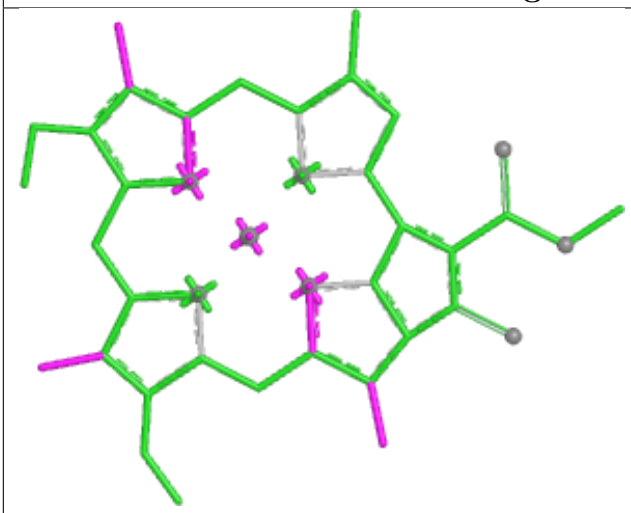


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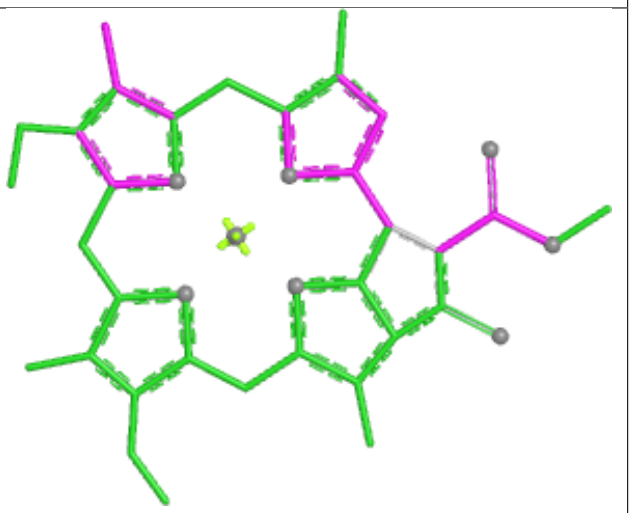


Rings

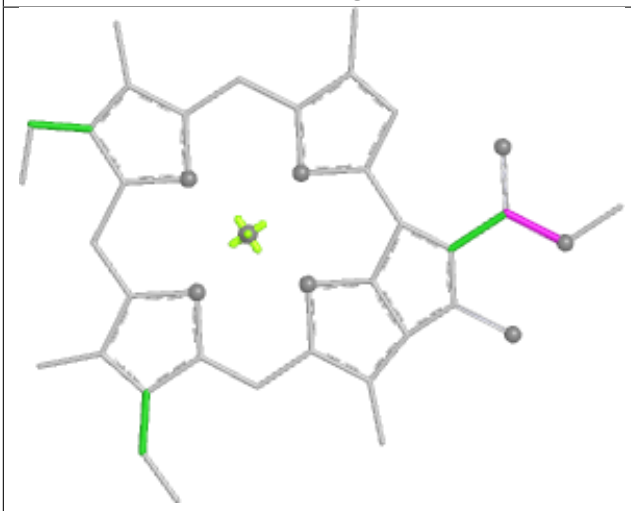
Ligand CLA A 818



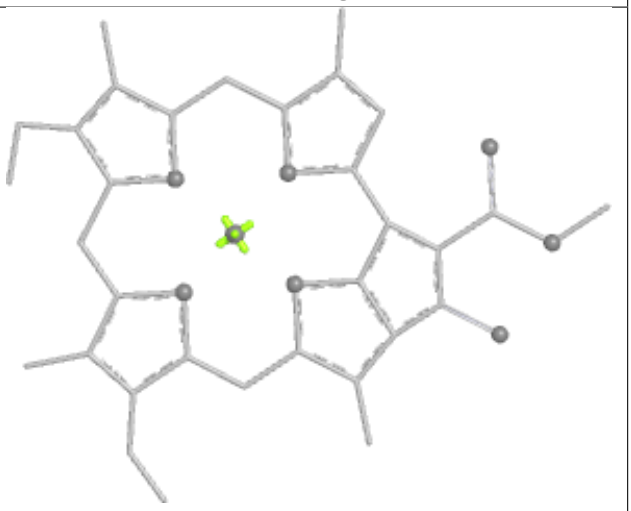
Bond lengths



Bond angles

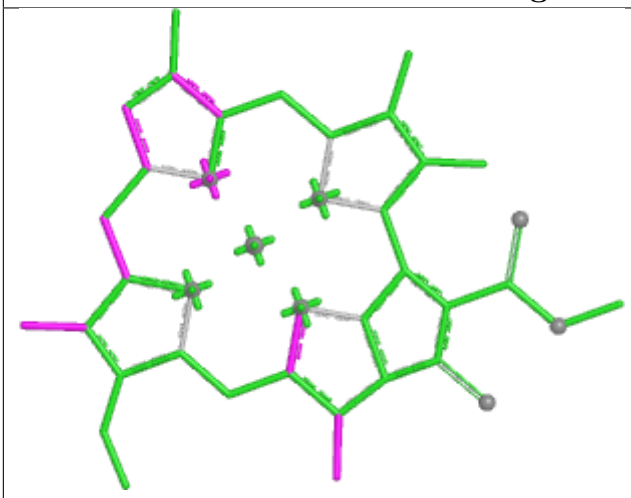


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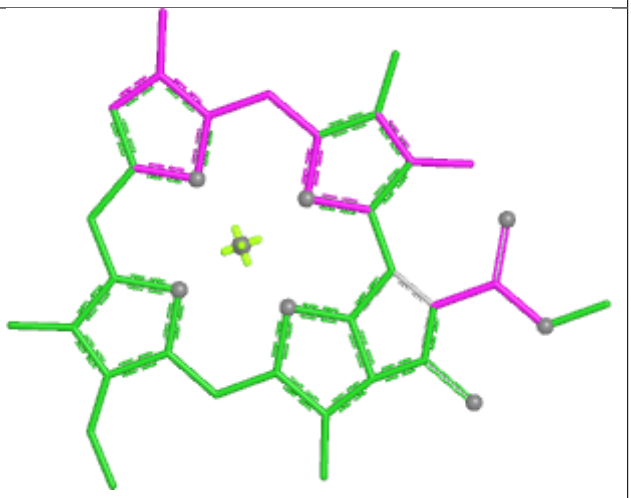


Rings

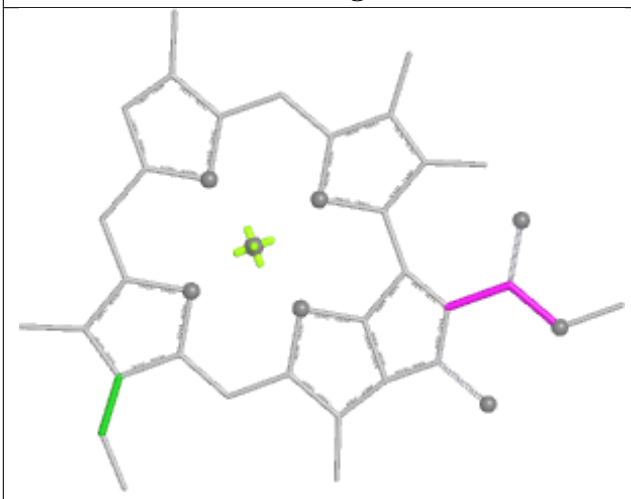
Ligand CLA s 504



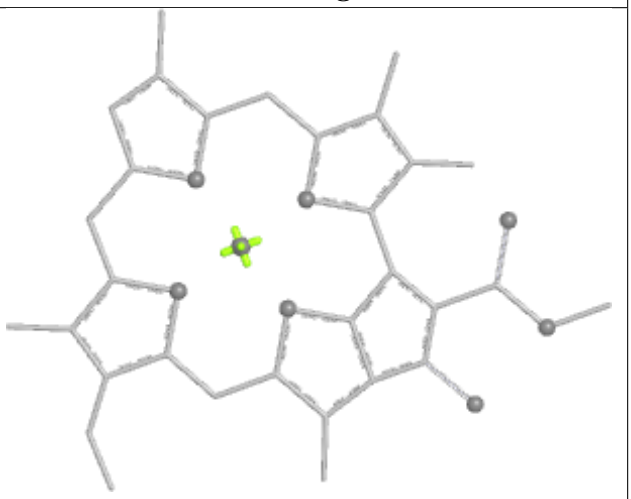
Bond lengths



Bond angles

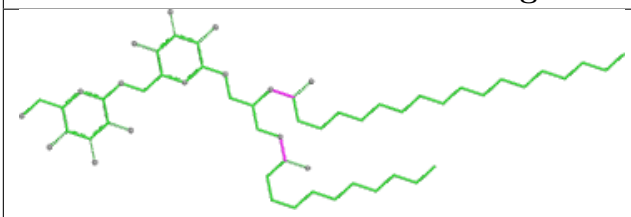


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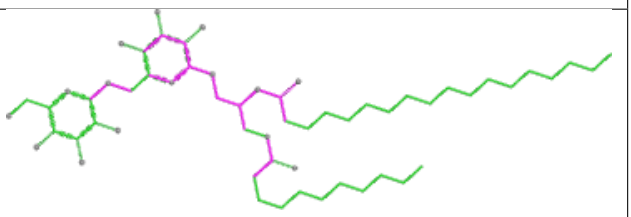


Rings

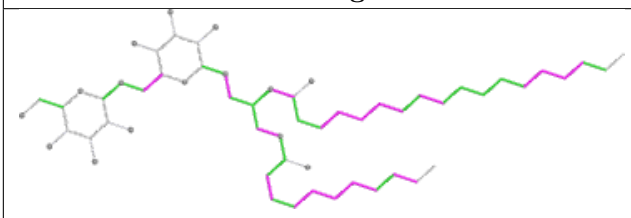
Ligand DGD B 850



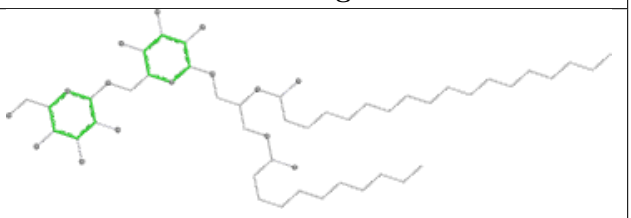
Bond lengths



Bond angles

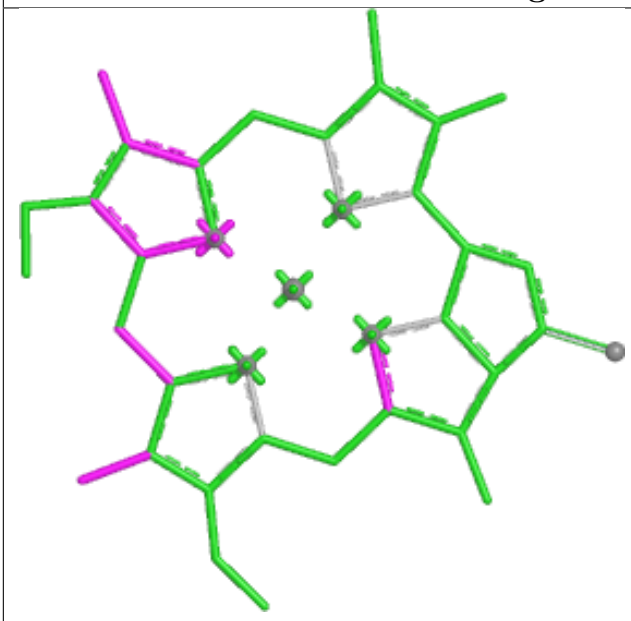


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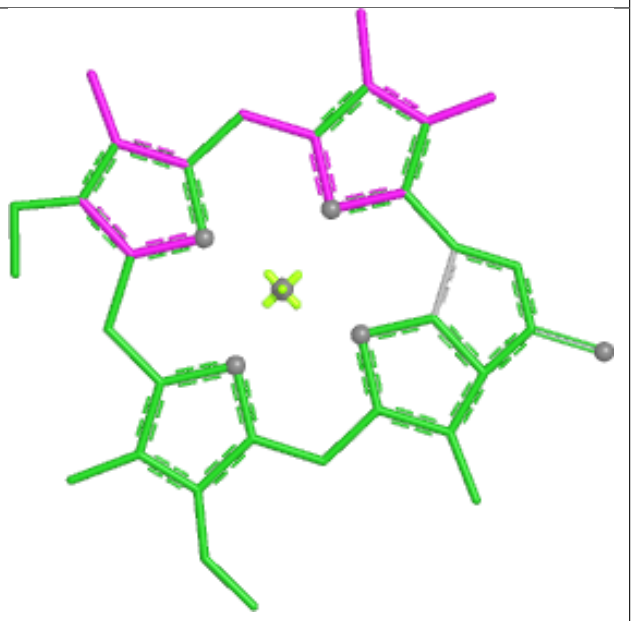


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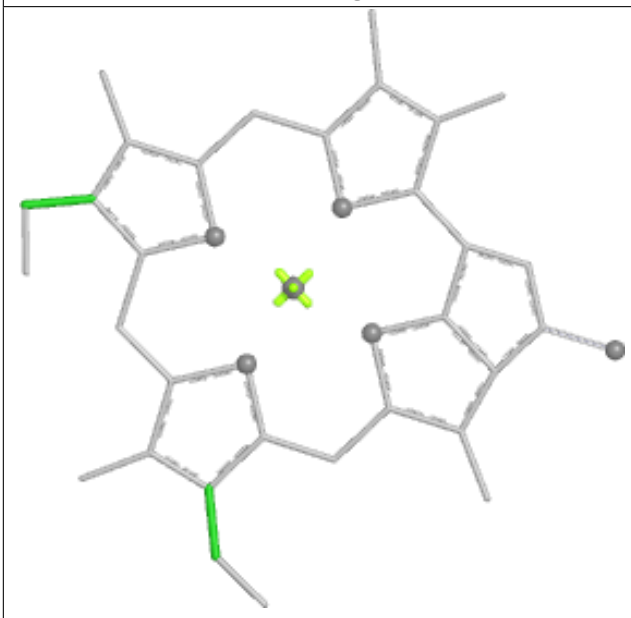
Ligand CLA 3 316



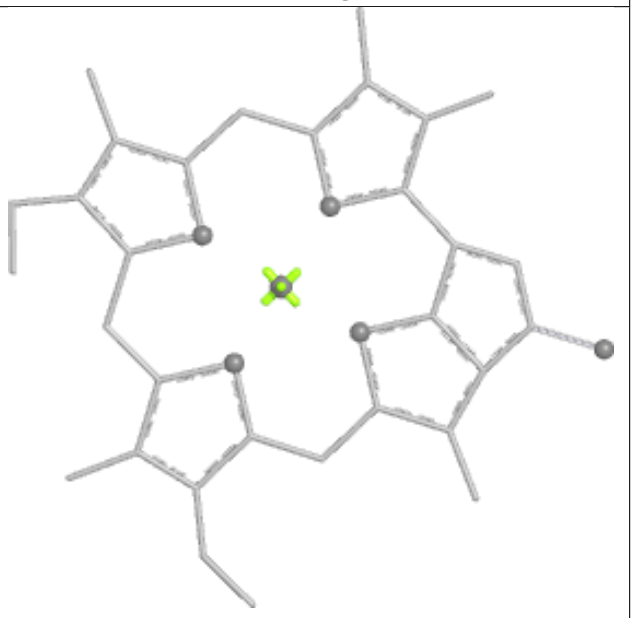
Bond lengths



Bond angles

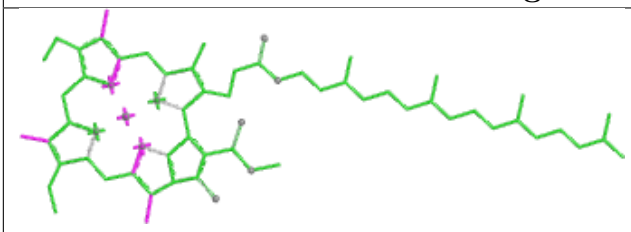


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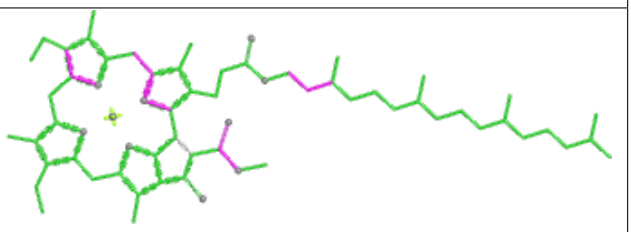


Rings

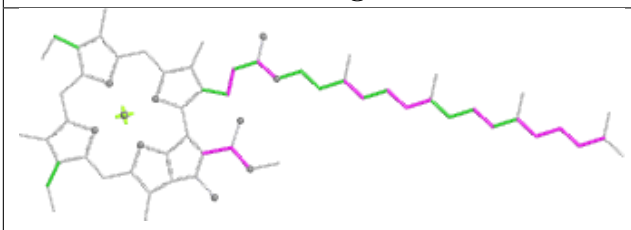
Ligand CLA A 806



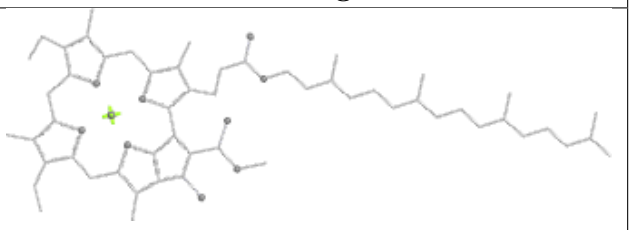
Bond lengths



Bond angles

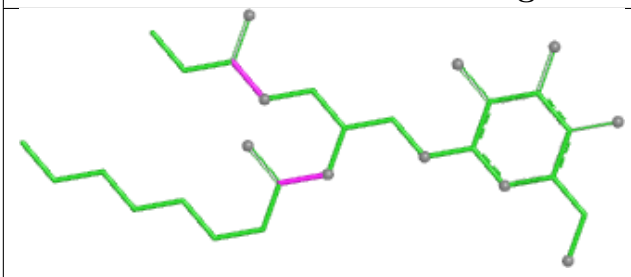


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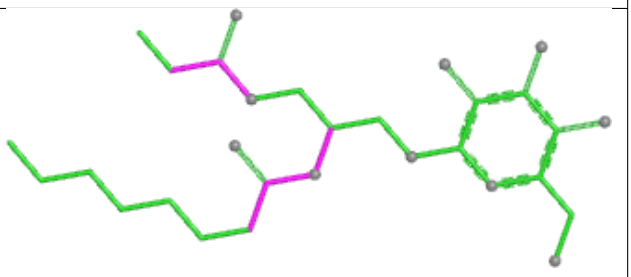


Rings

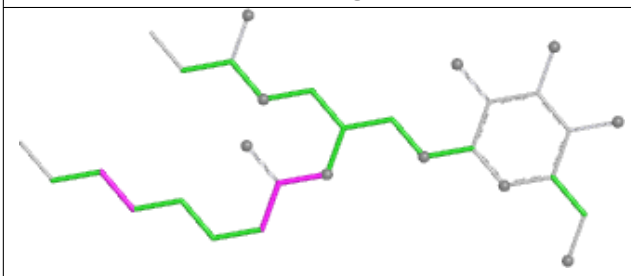
Ligand LMG m 105



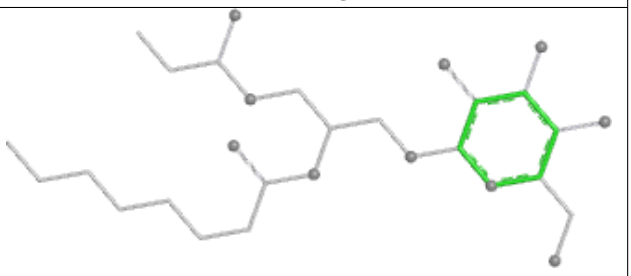
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Bond angles

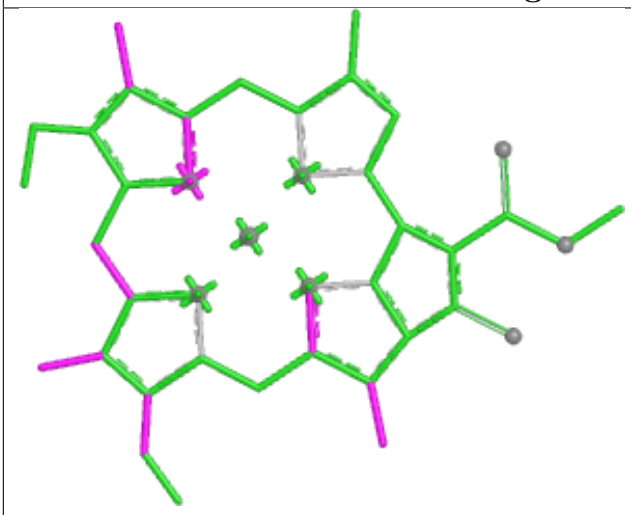


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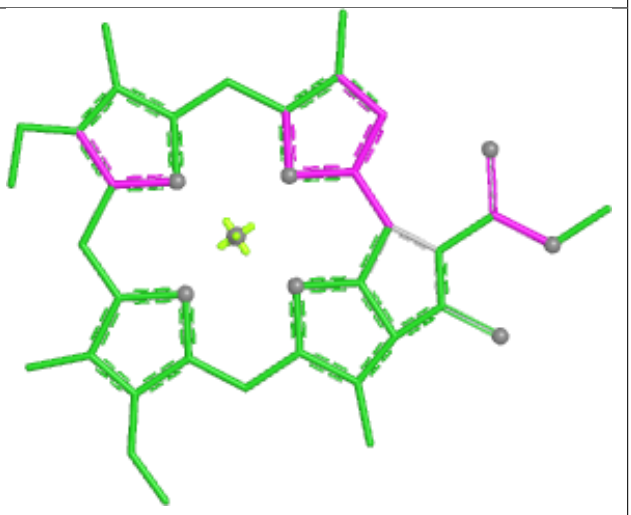


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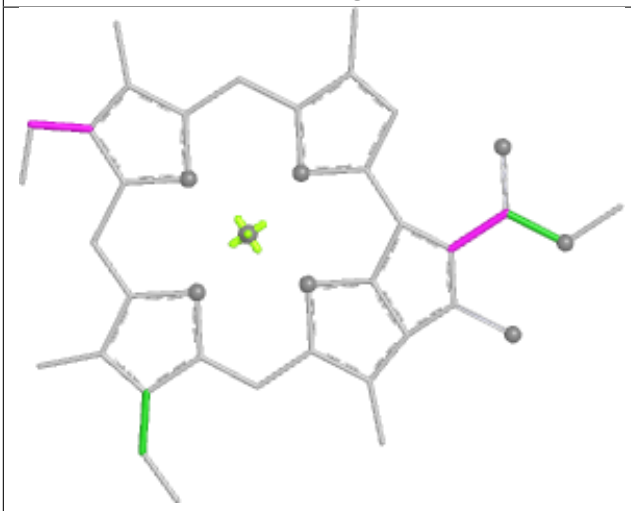
Ligand CLA B 809



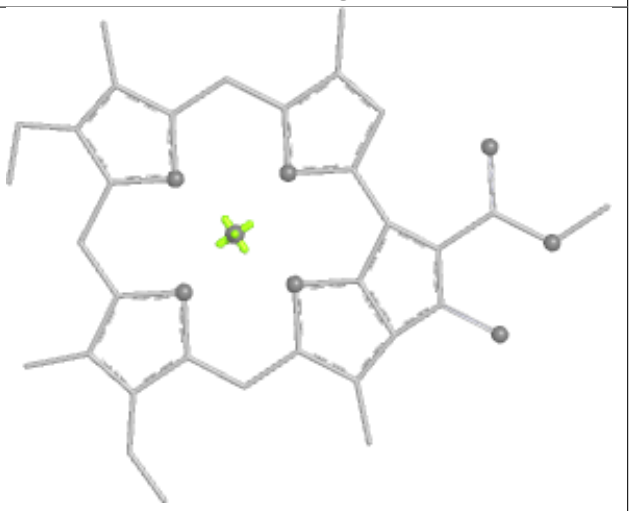
Bond lengths



Bond angles

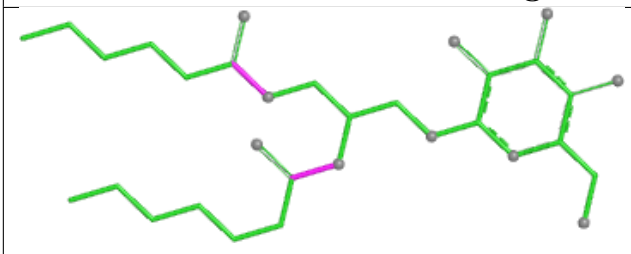


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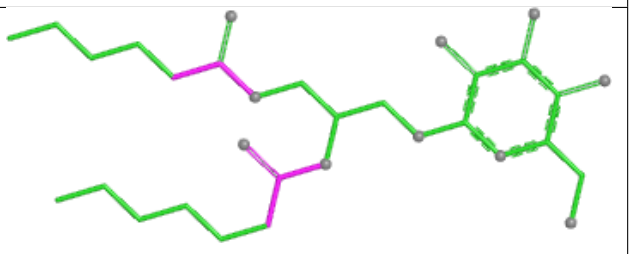


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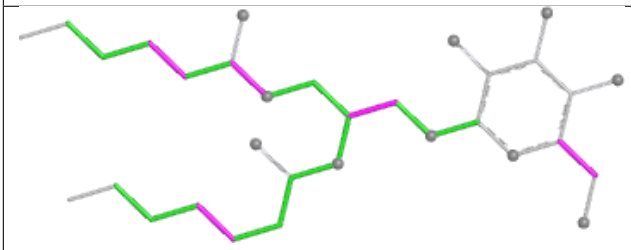
Ligand LMG 5 301



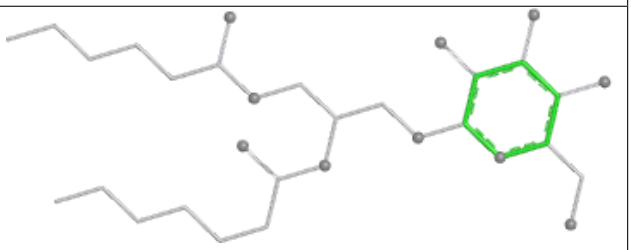
Bond lengths



Bond angles

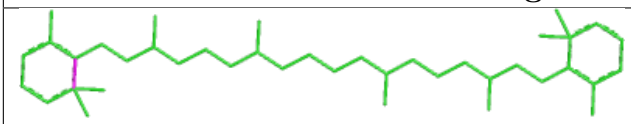


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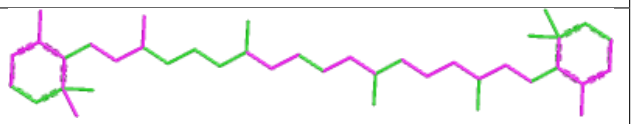


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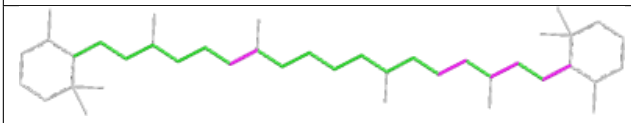
Ligand BCR L 306



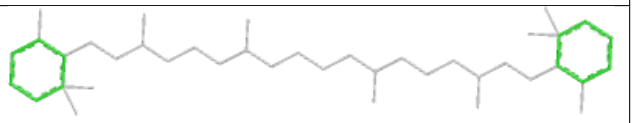
Bond lengths



Bond angles

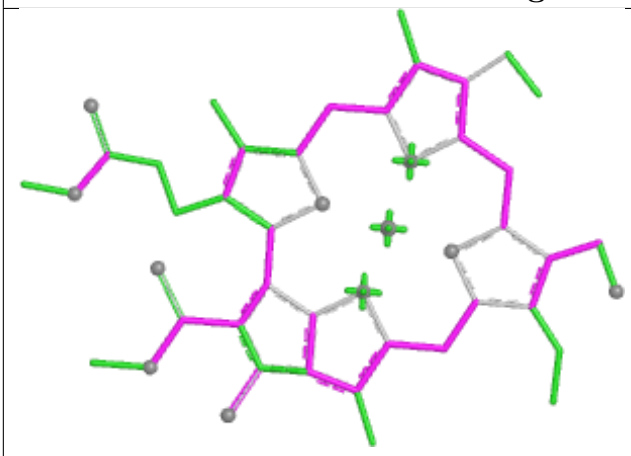


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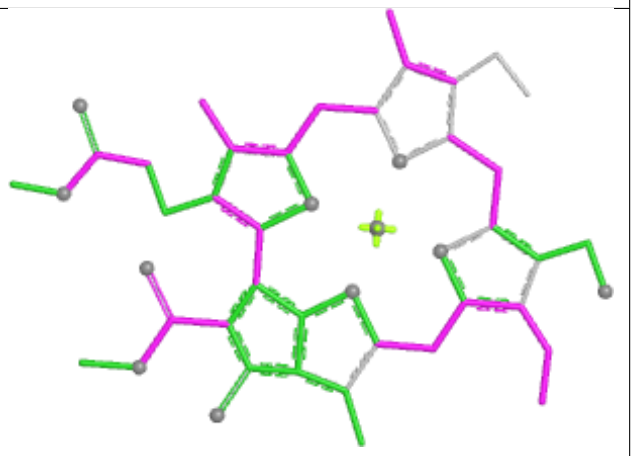


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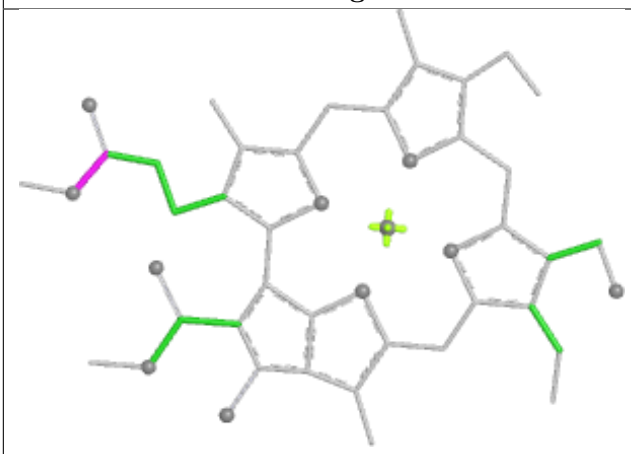
Ligand CHL 3 302



Bond lengths



Bond angles

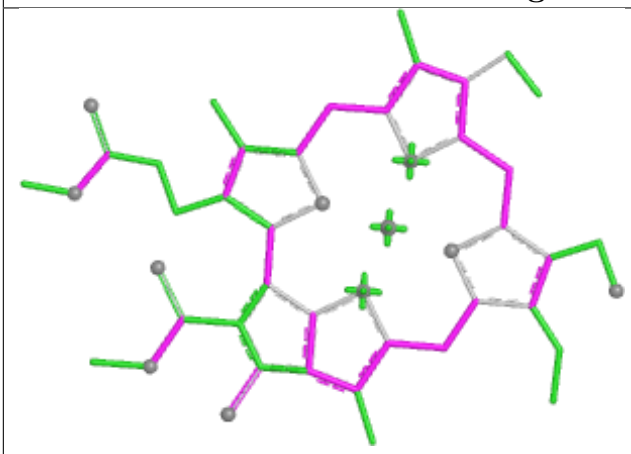


Torsions

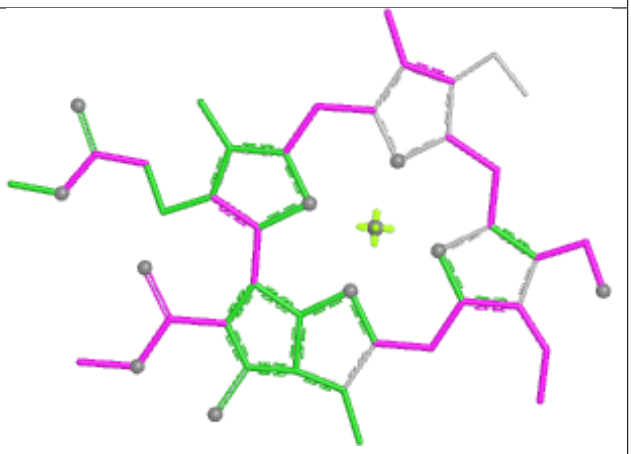


Rings

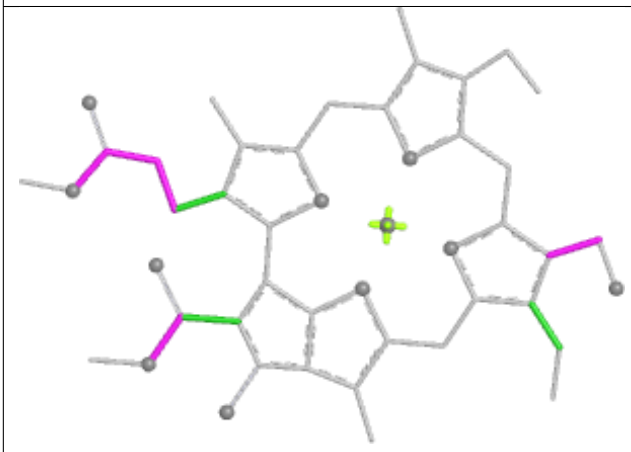
Ligand CHL 1 512



Bond lengths



Bond angles

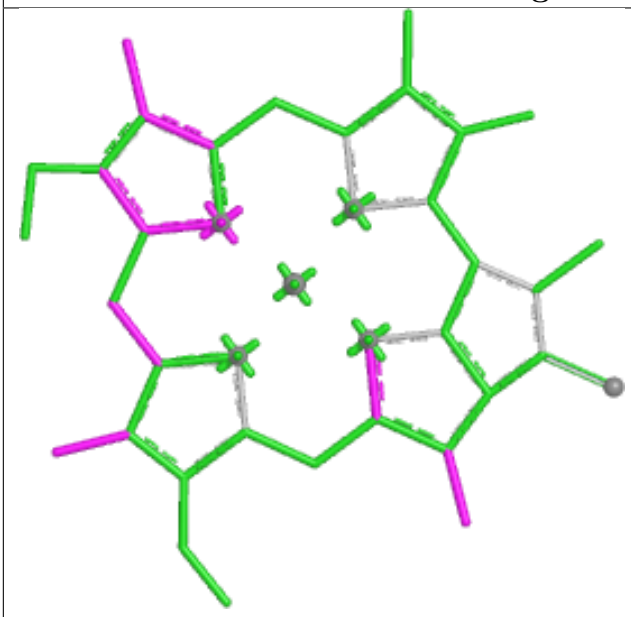


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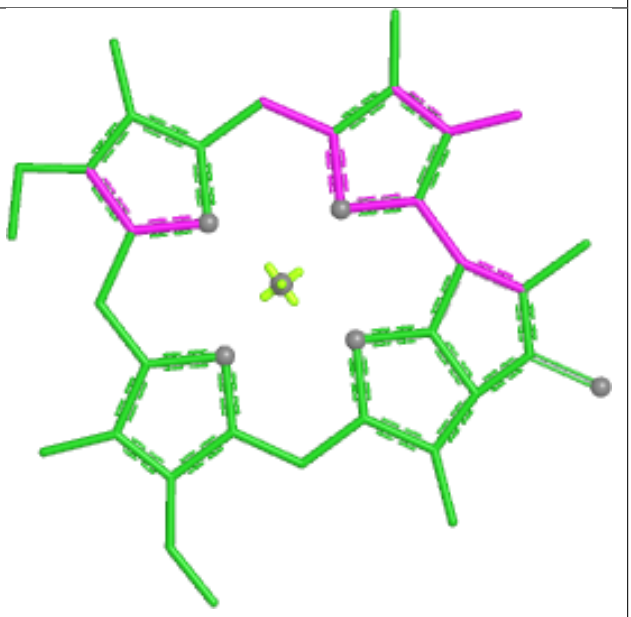


Rings

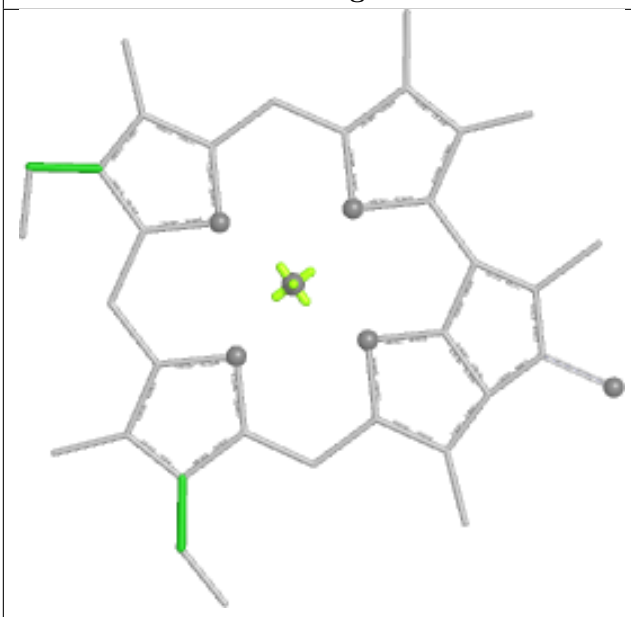
Ligand CLA f 843



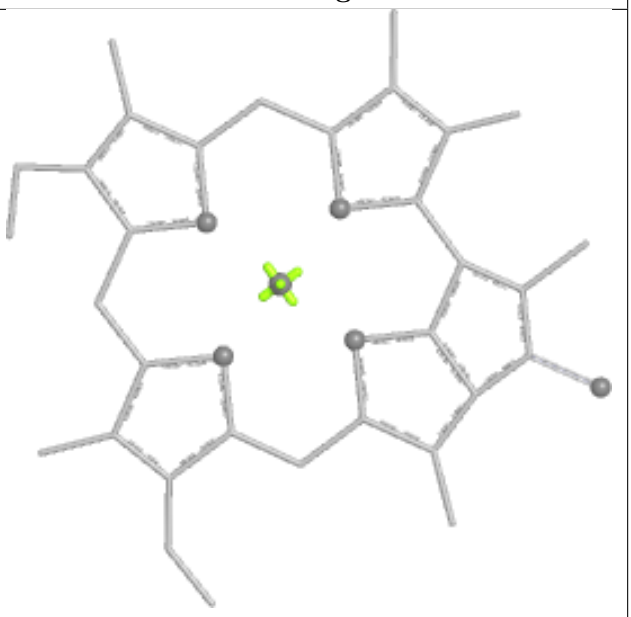
Bond lengths



Bond angles



Torsions

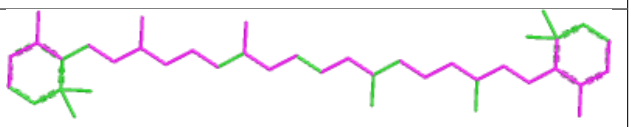


Rings

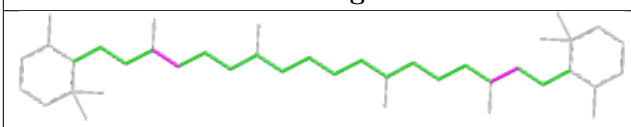
Ligand BCR B 852



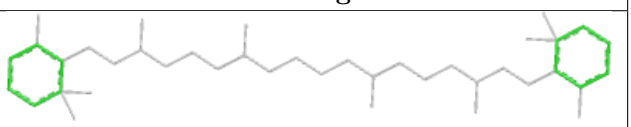
Bond lengths



Bond angles

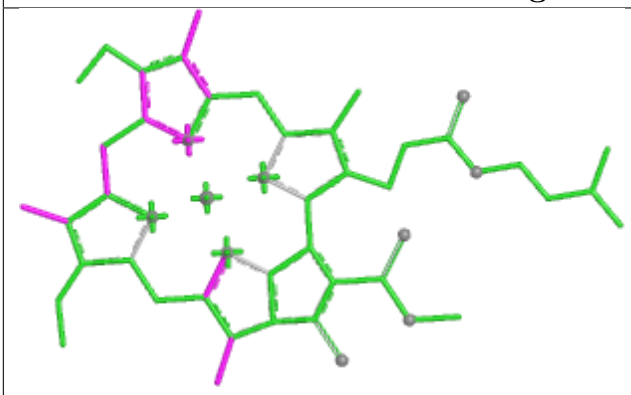


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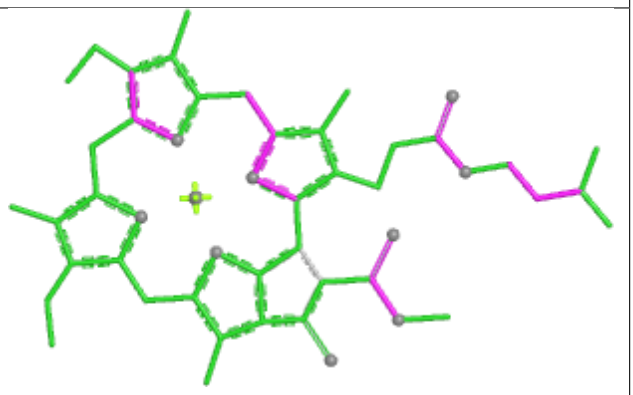


Rings

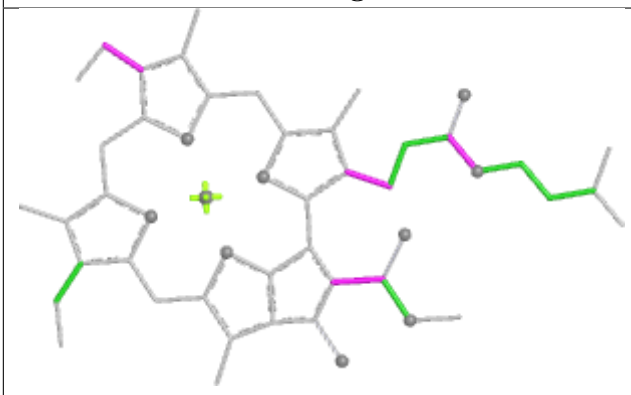
Ligand CLA e 830



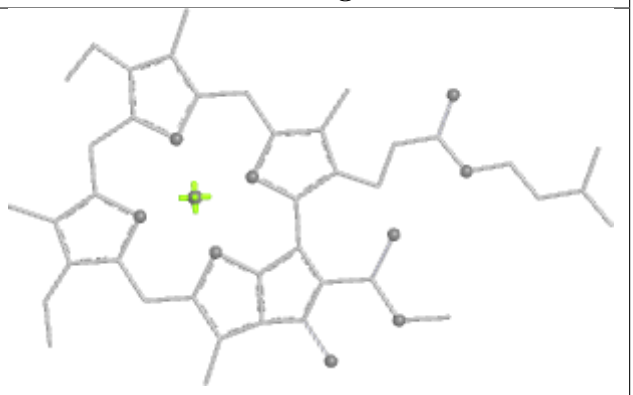
Bond lengths



Bond angles



Torsions

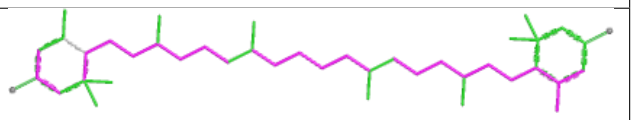


Rings

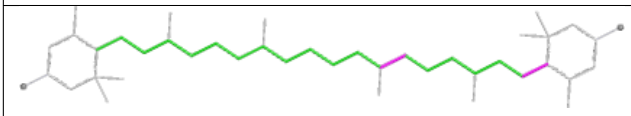
Ligand LUT s 501



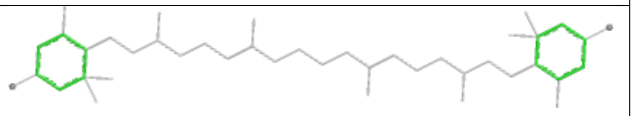
Bond lengths



Bond angles

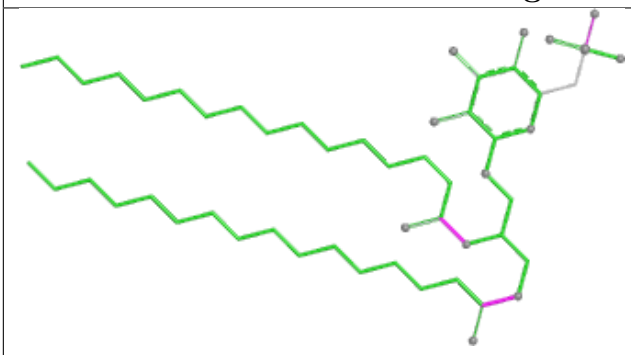


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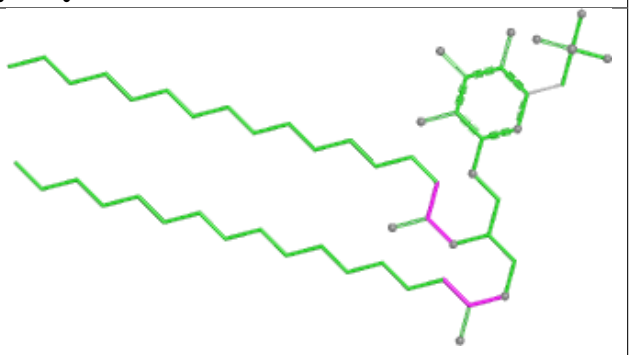


Rings

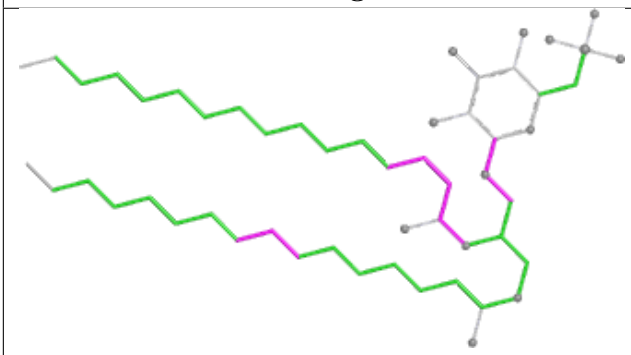
Ligand SQD Q 802



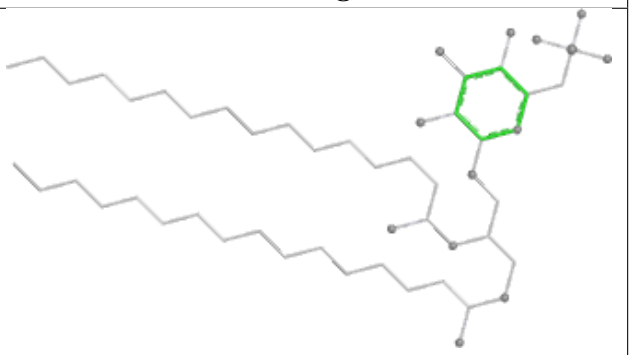
Bond lengths



Bond angles

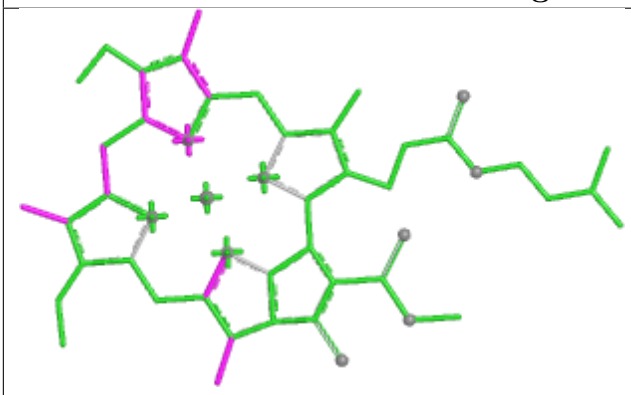


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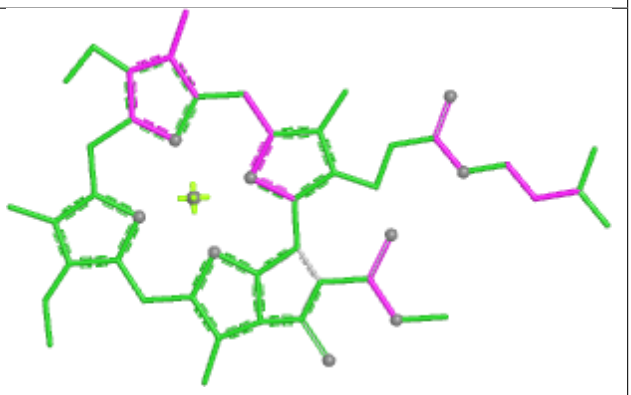


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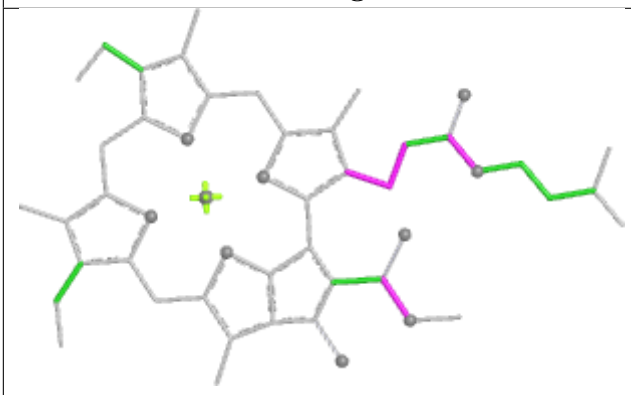
Ligand CLA f 829



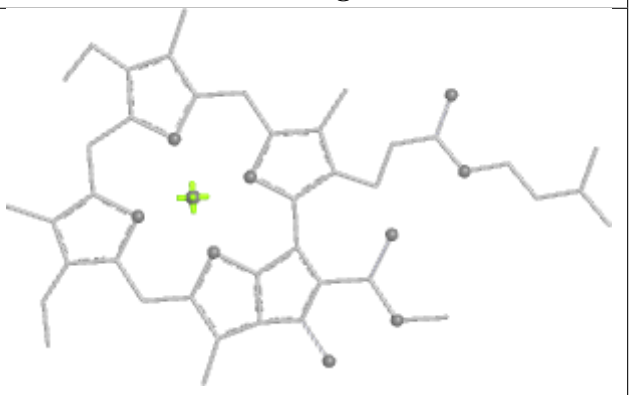
Bond lengths



Bond angles

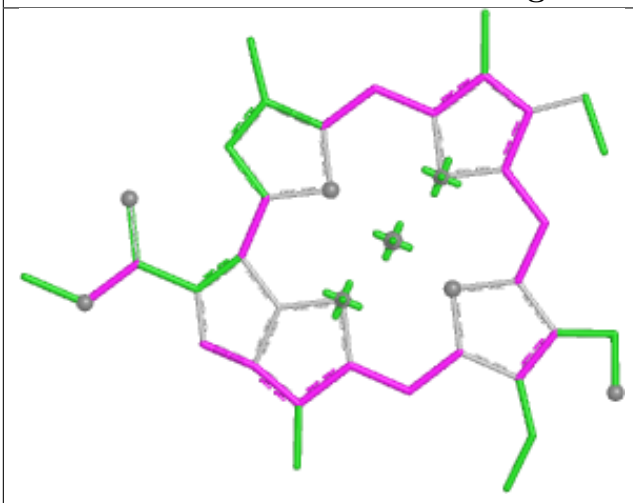


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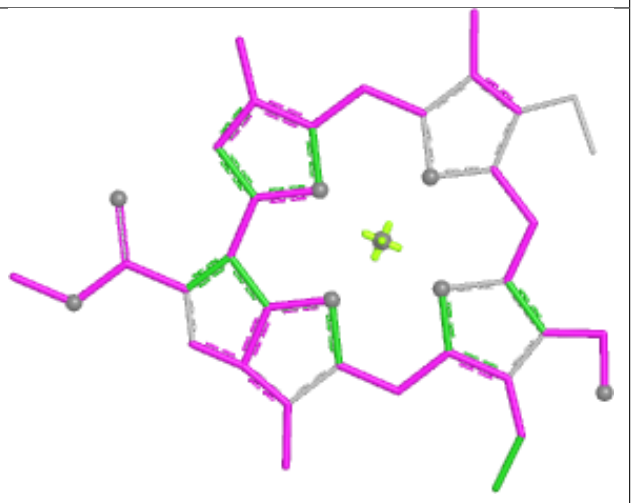


Rings

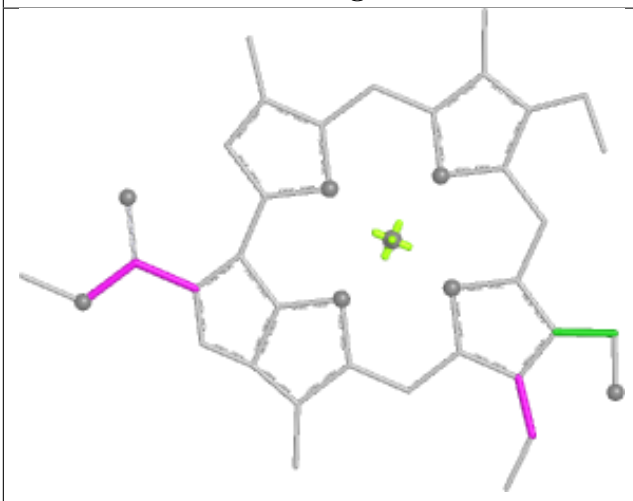
Ligand CHL 2 513



Bond lengths



Bond angles

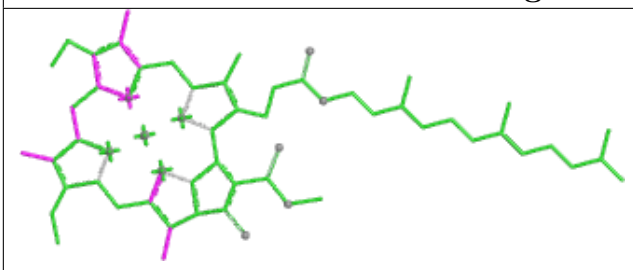


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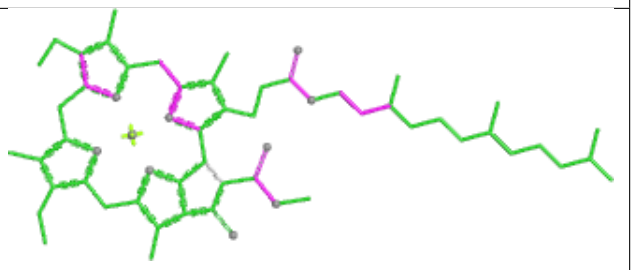


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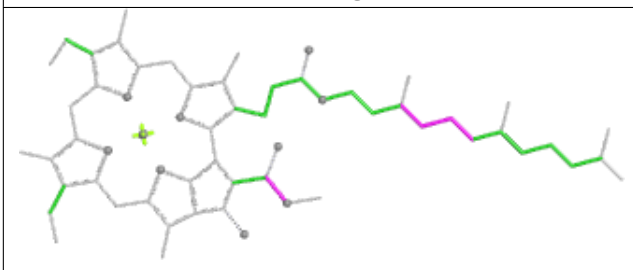
Ligand CLA B 835



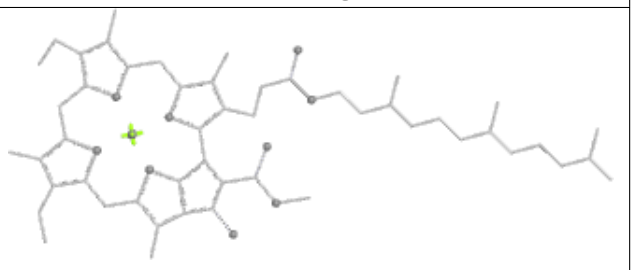
Bond lengths



Bond angles

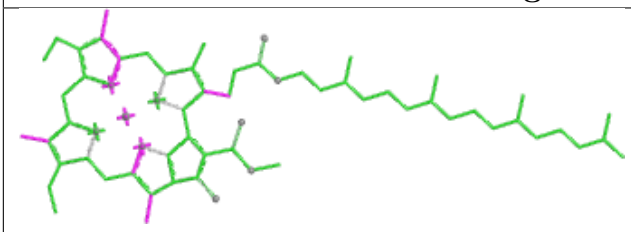


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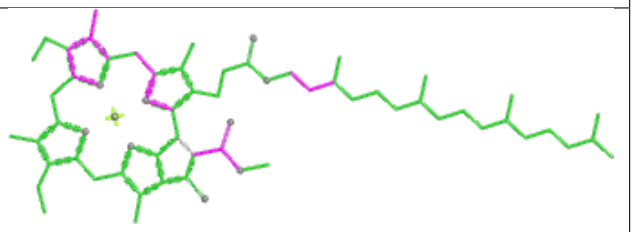


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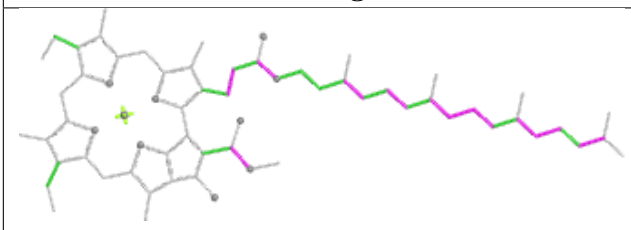
Ligand CLA A 827



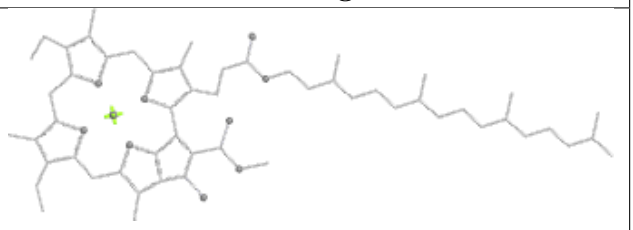
Bond lengths



Bond angles

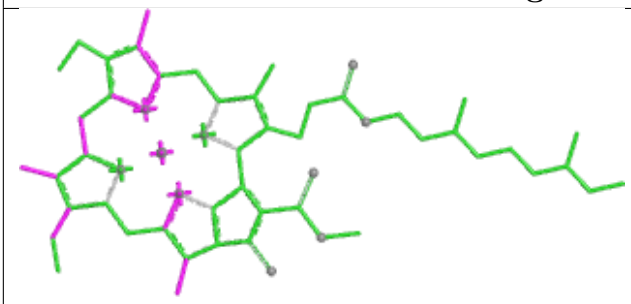


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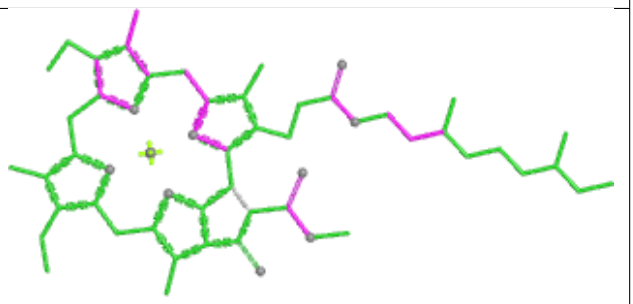


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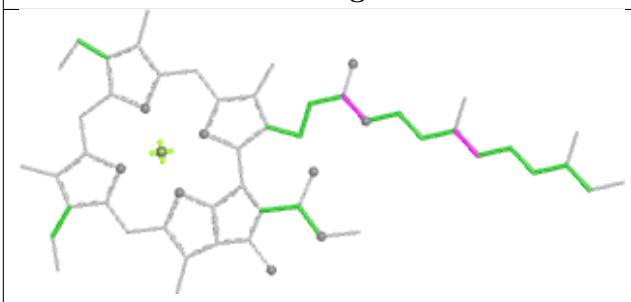
Ligand CLA L 301



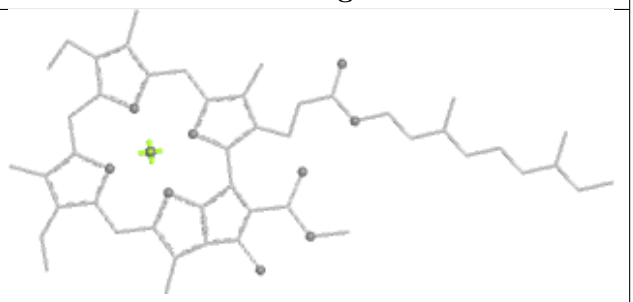
Bond lengths



Bond angles

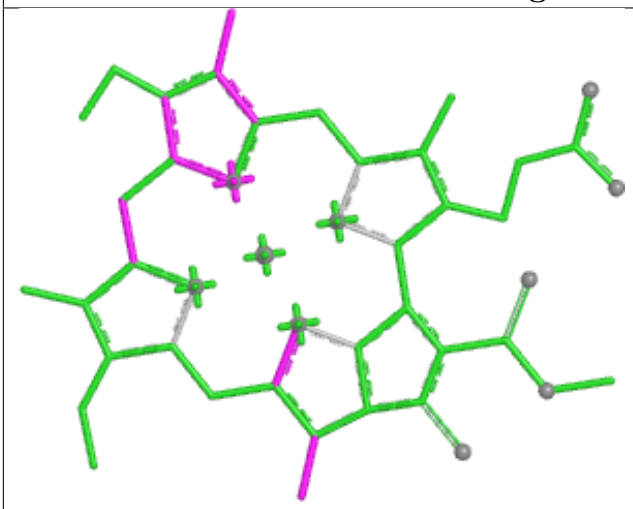


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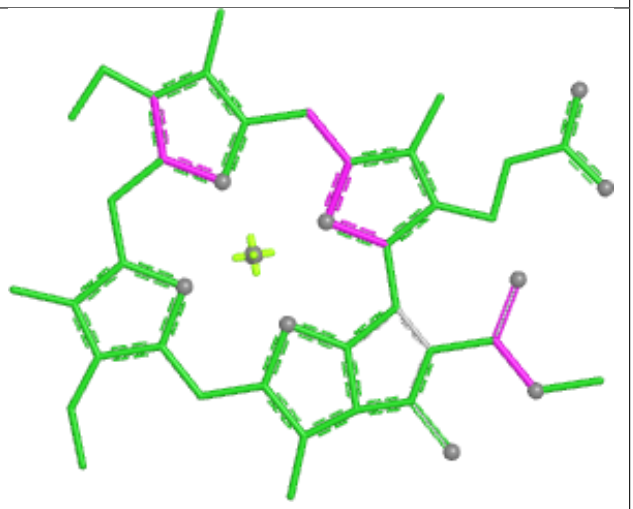


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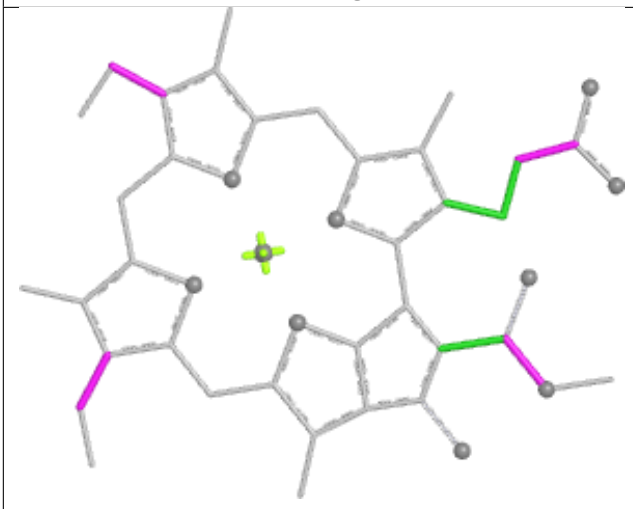
Ligand CLA e 815



Bond lengths



Bond angles

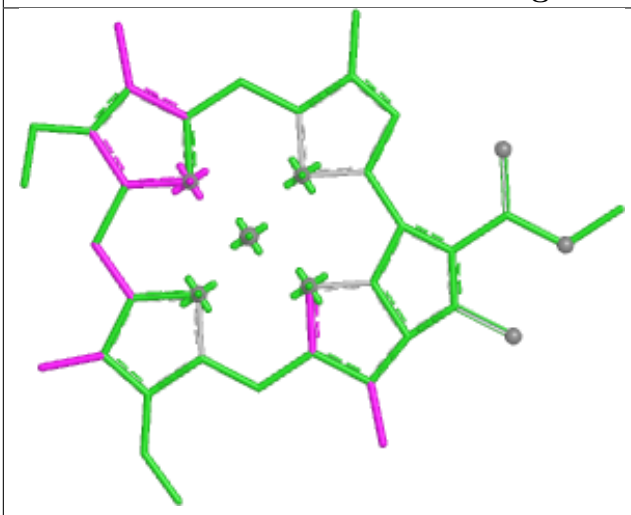


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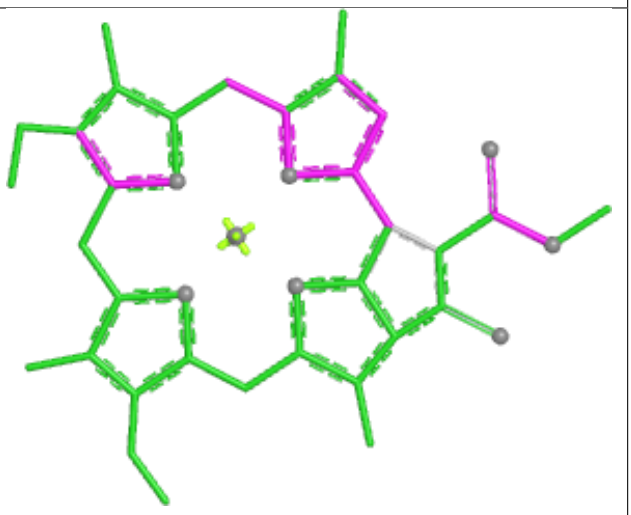


Rings

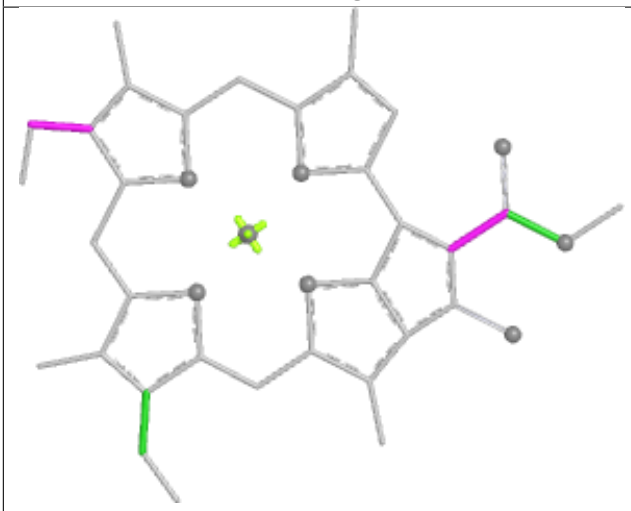
Ligand CLA f 832



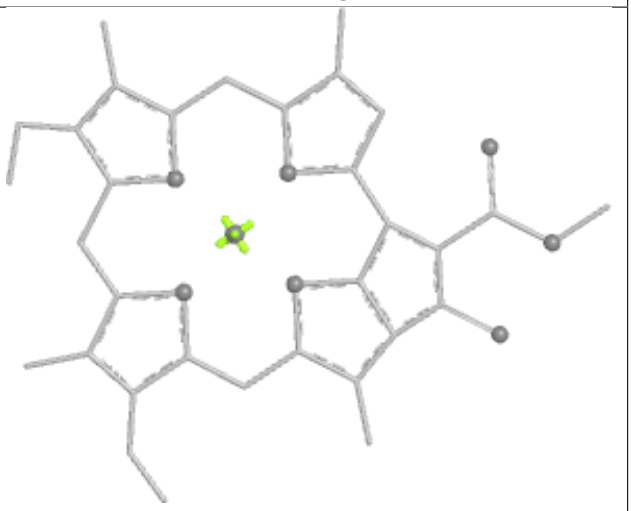
Bond lengths



Bond angles

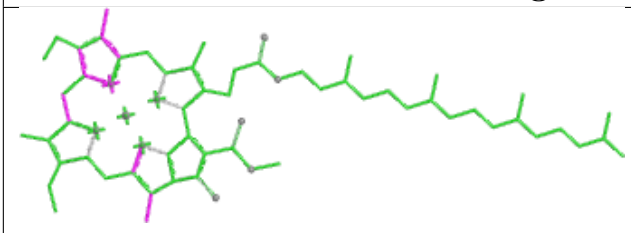


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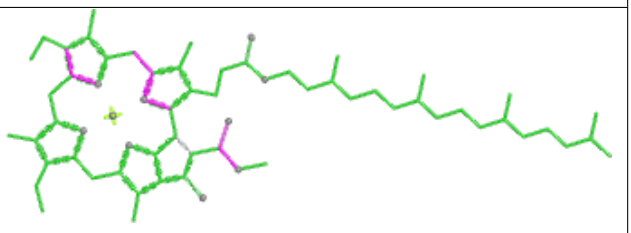


Rings

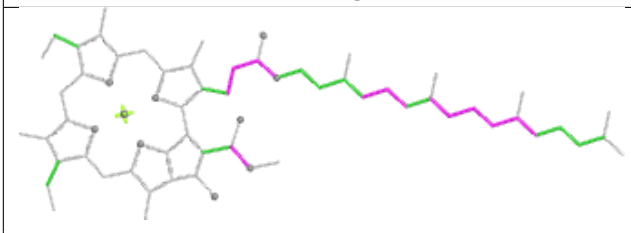
Ligand CLA s 506



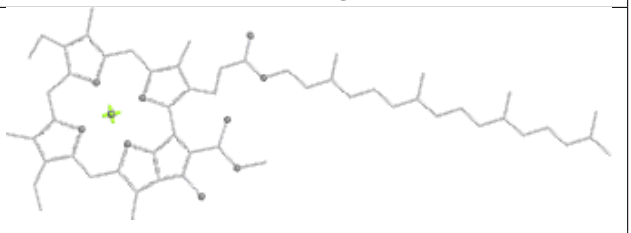
Bond lengths



Bond angles

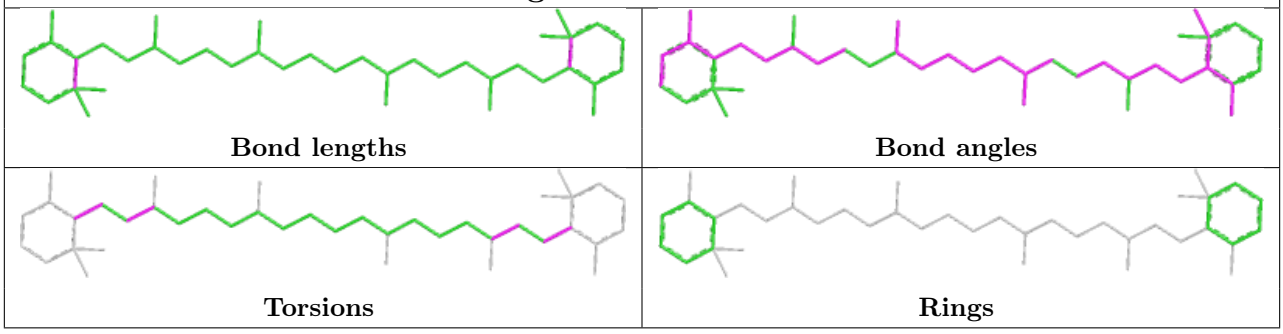


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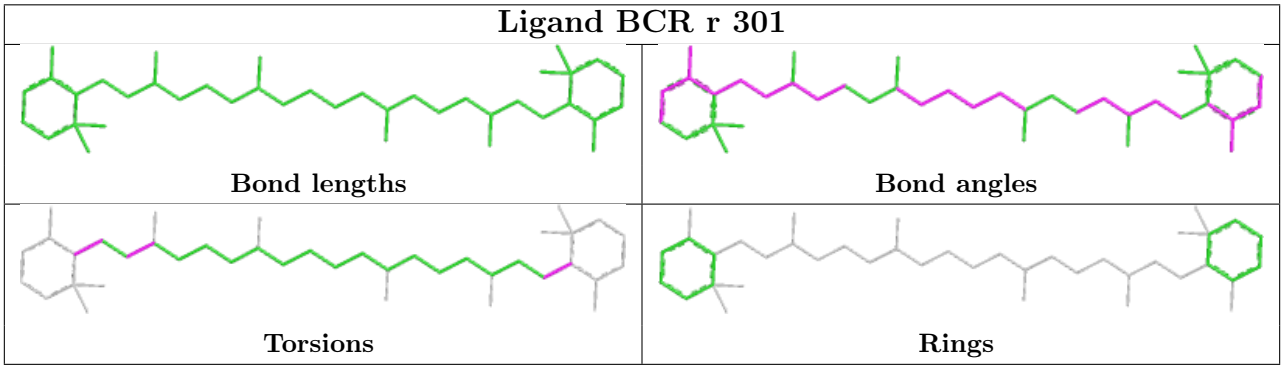


Rings

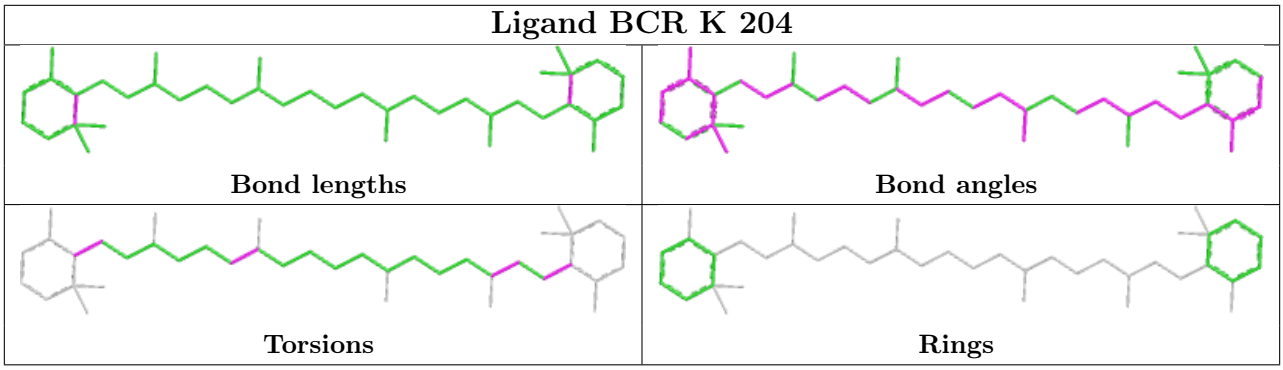
Ligand BCR 3 305



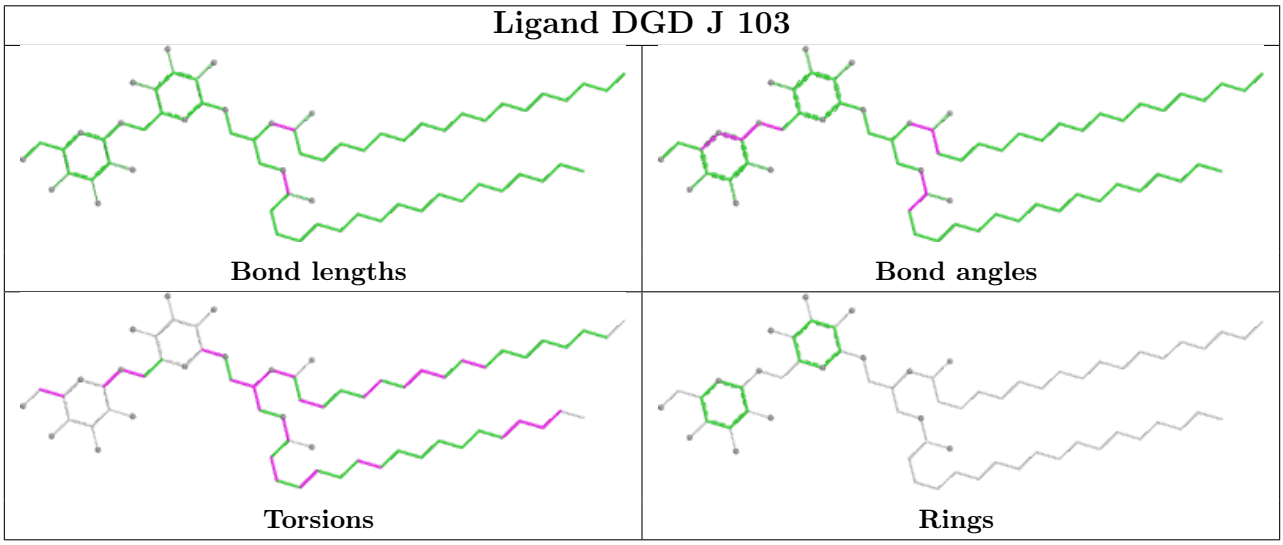
Ligand BCR r 301



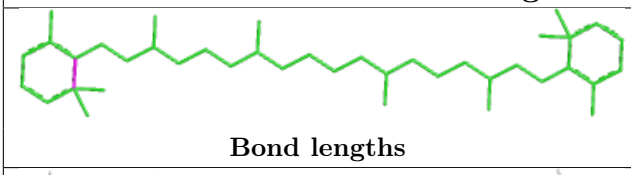
Ligand BCR K 204



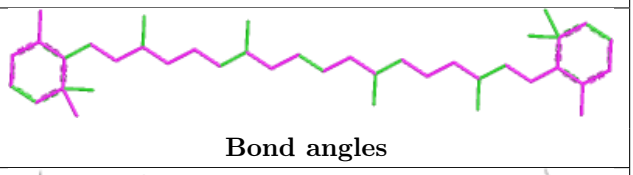
Ligand DGD J 103



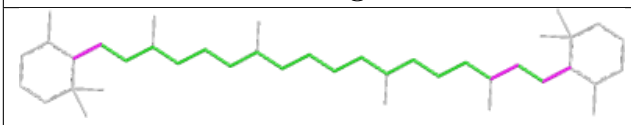
Ligand BCR A 851



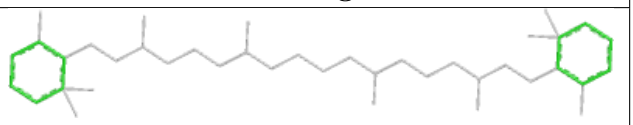
Bond lengths



Bond angles

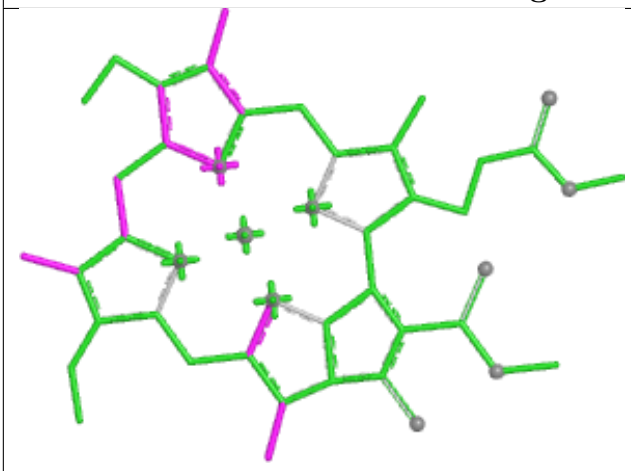


Torsions

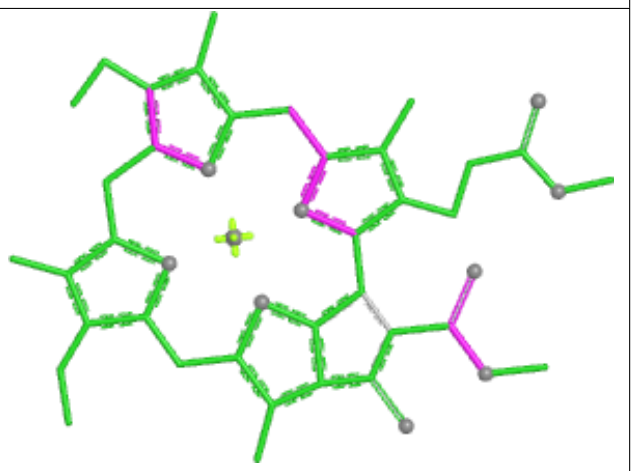


Rings

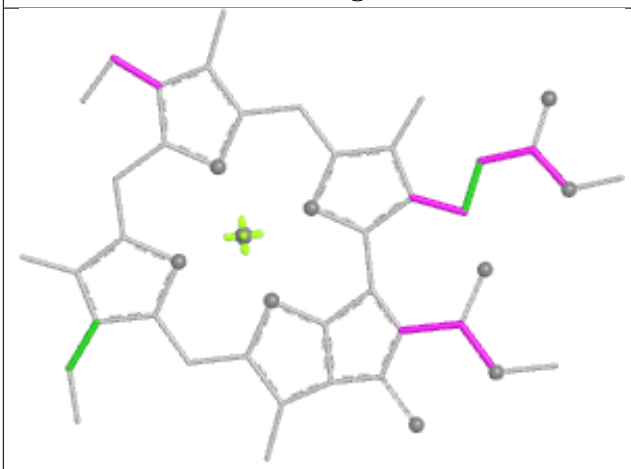
Ligand CLA s 505



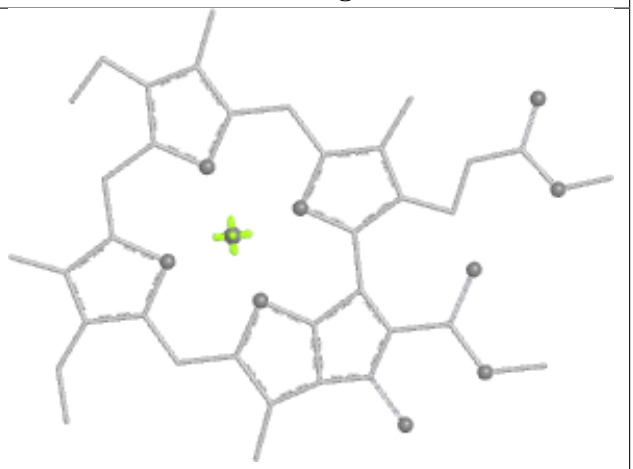
Bond lengths



Bond angles

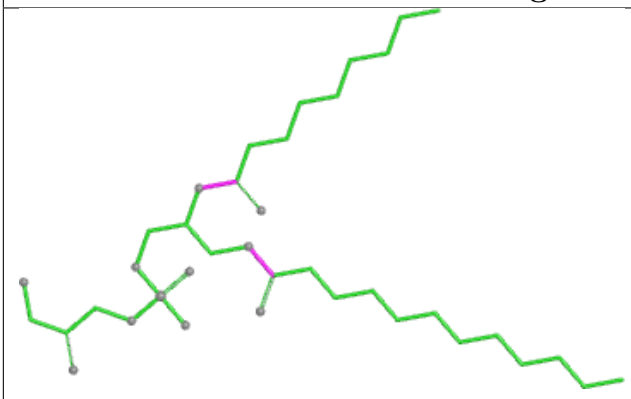


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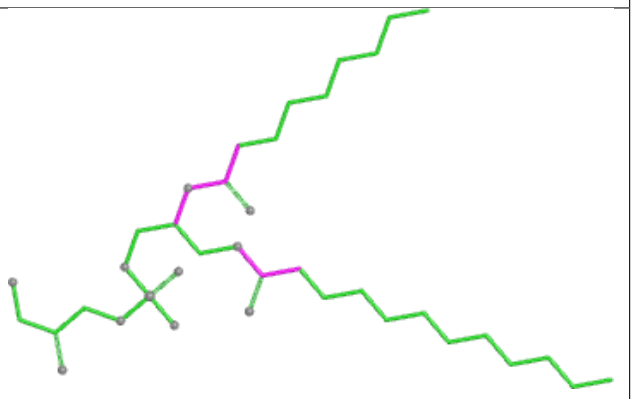


Rings

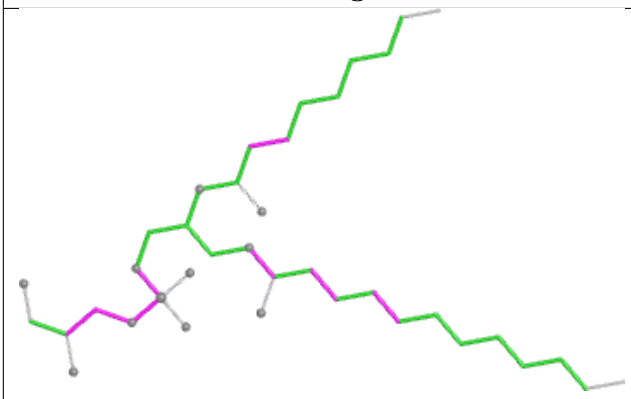
Ligand LHG f 852



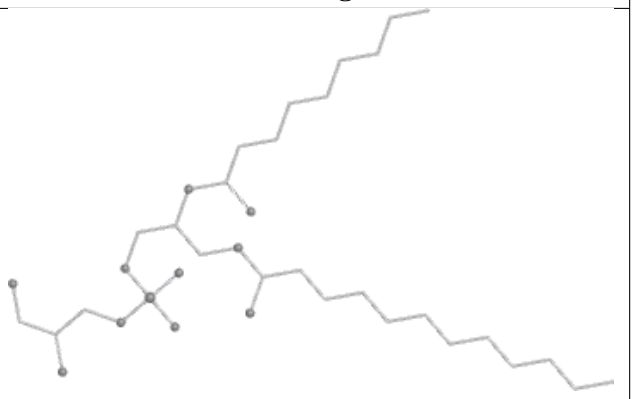
Bond lengths



Bond angles

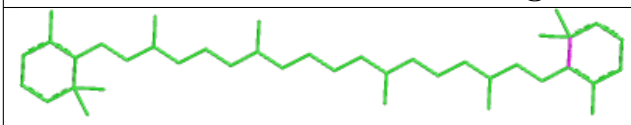


Torsions

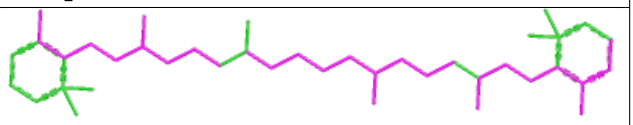


Rings

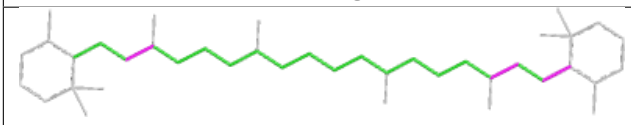
Ligand BCR q 303



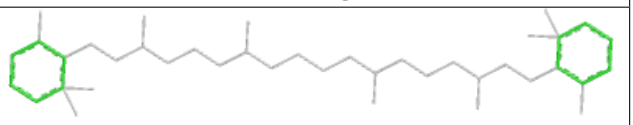
Bond lengths



Bond angles

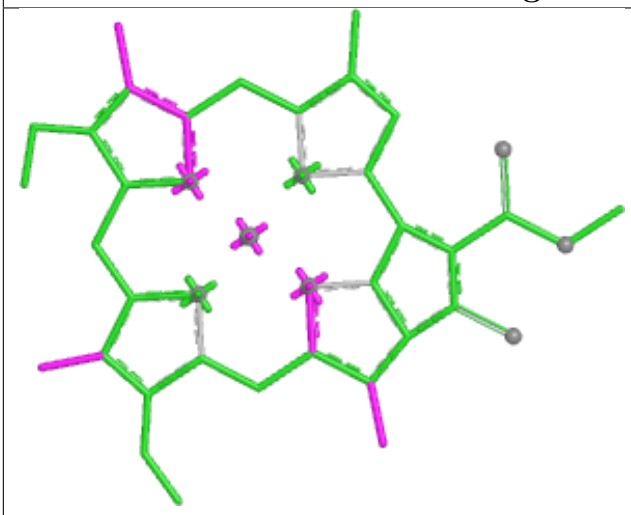


Torsions

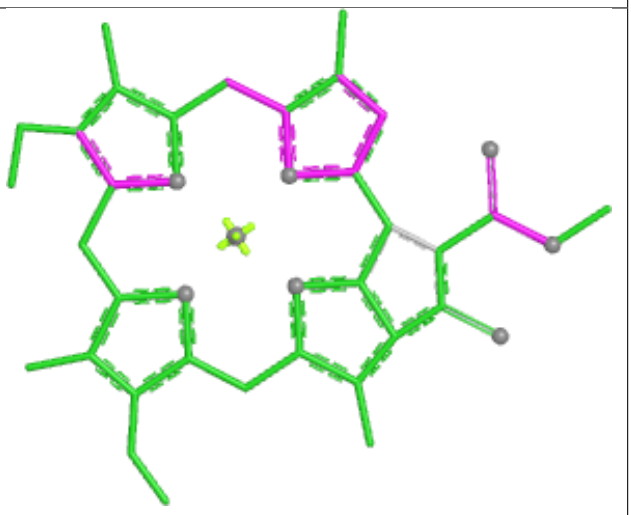


Rings

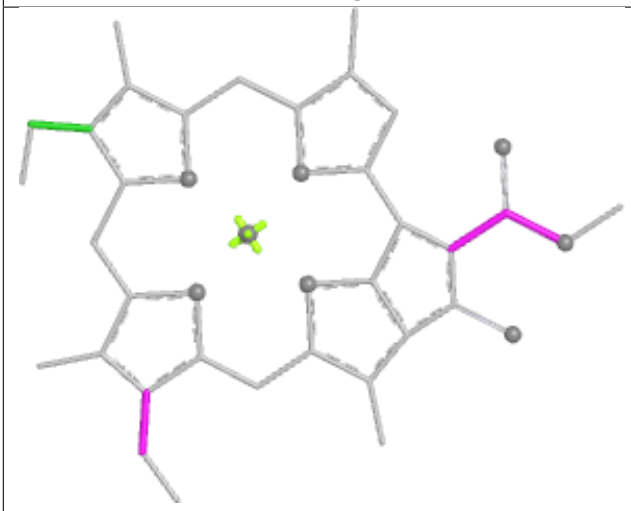
Ligand CLA K 203



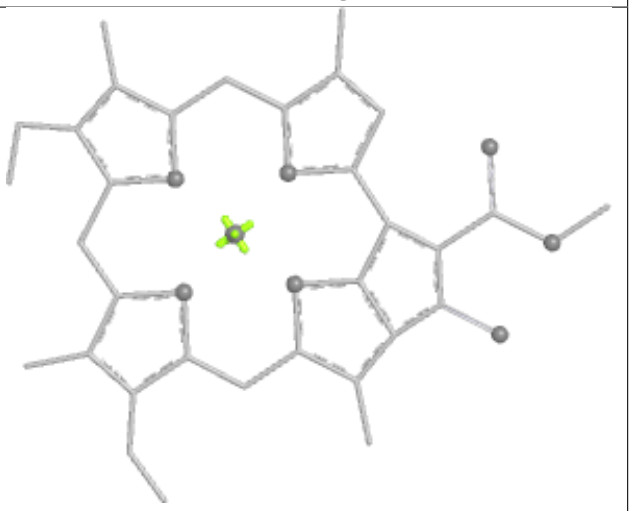
Bond lengths



Bond angles

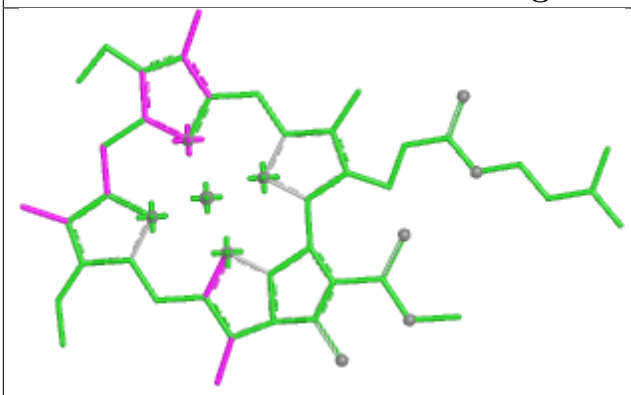


Torsions

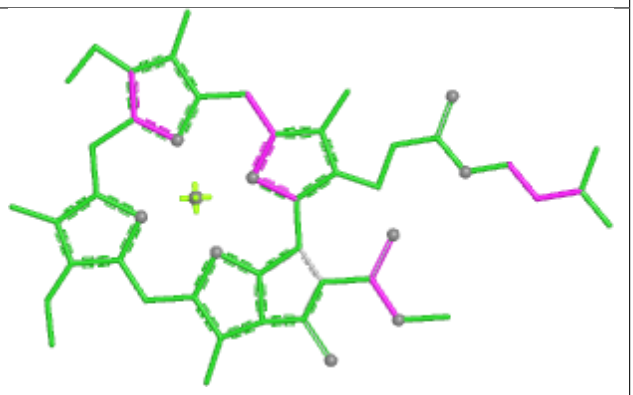


Rings

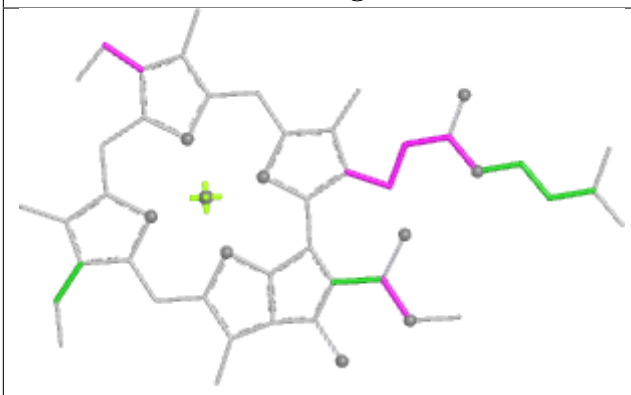
Ligand CLA f 820



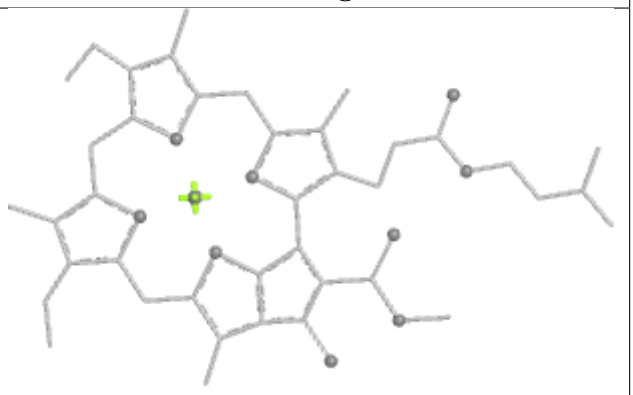
Bond lengths



Bond angles

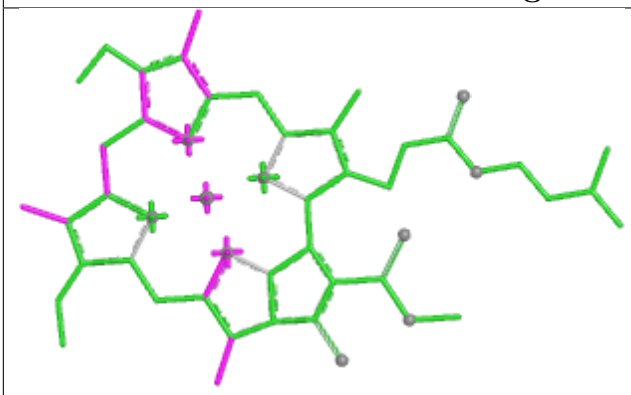


Torsions

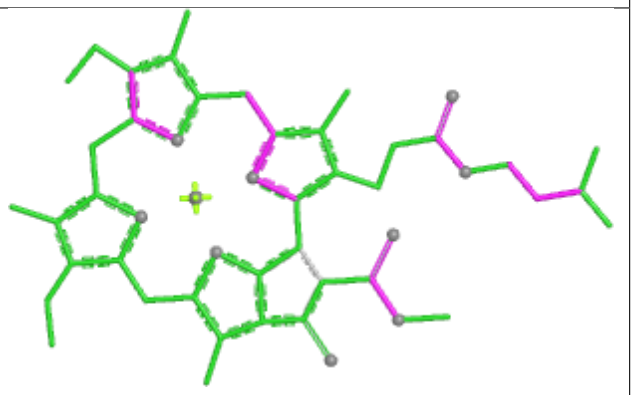


Rings

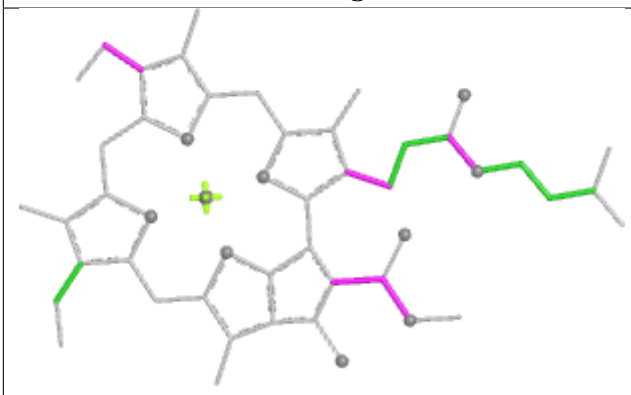
Ligand CLA A 842



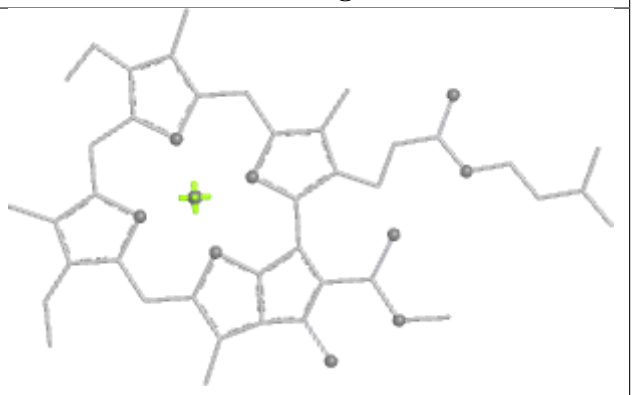
Bond lengths



Bond angles

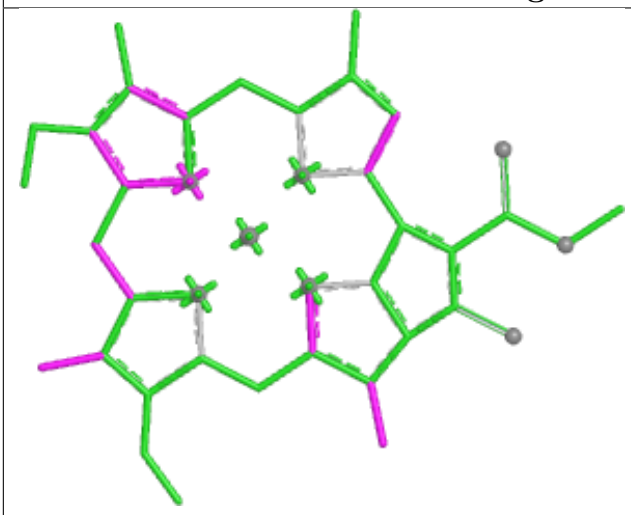


Torsions

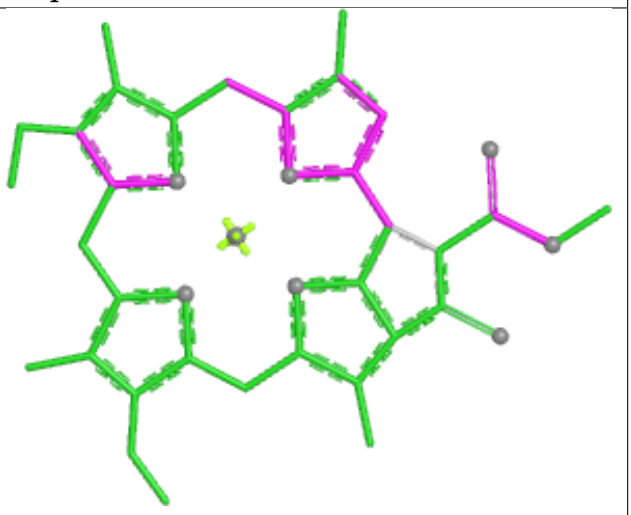


Rings

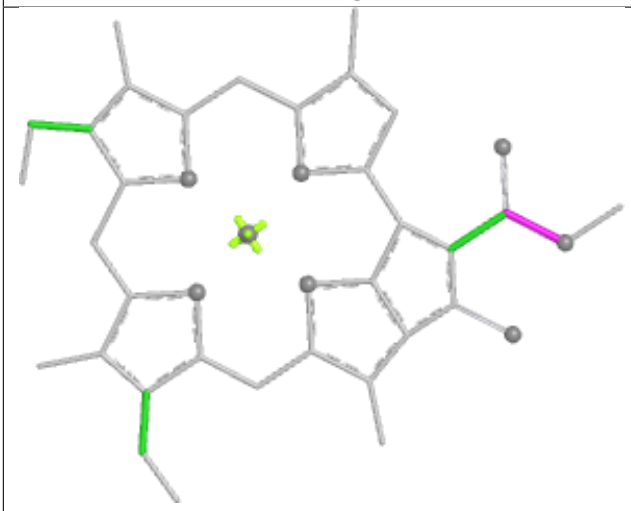
Ligand CLA p 515



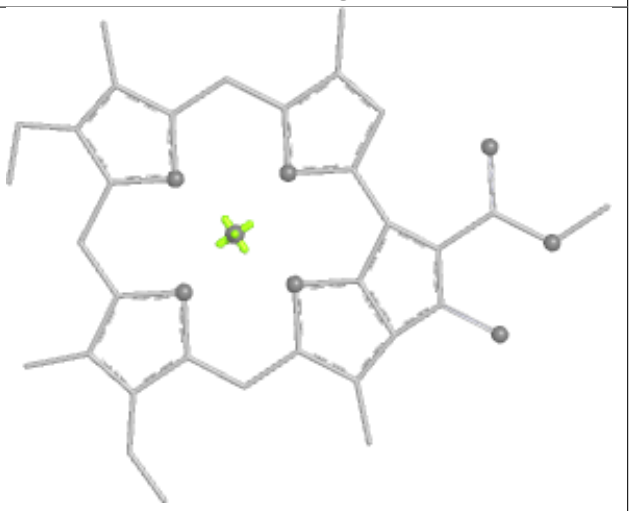
Bond lengths



Bond angles

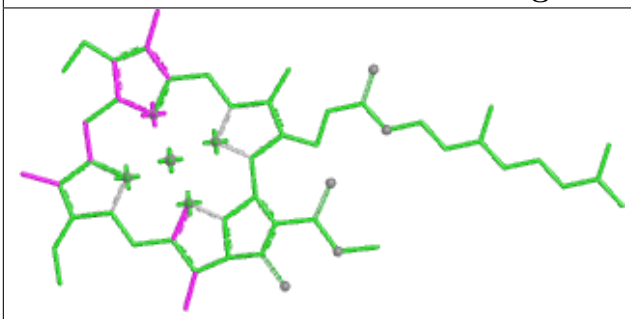


Torsions

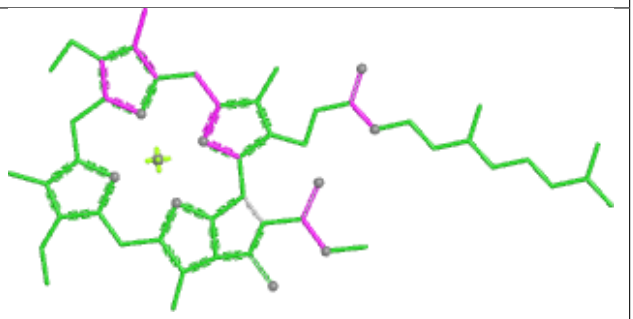


Rings

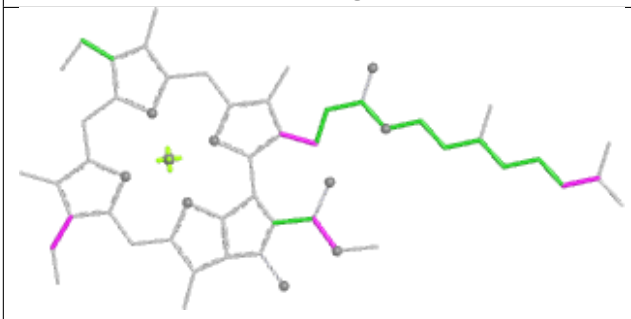
Ligand CLA f 821



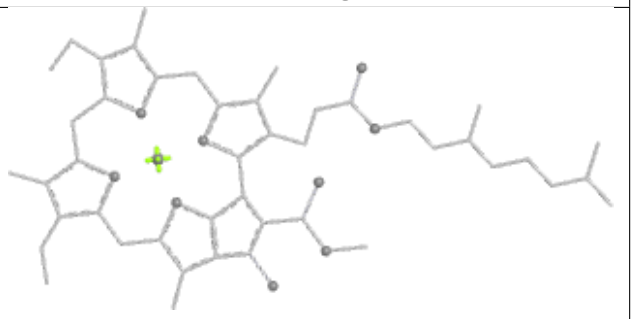
Bond lengths



Bond angles

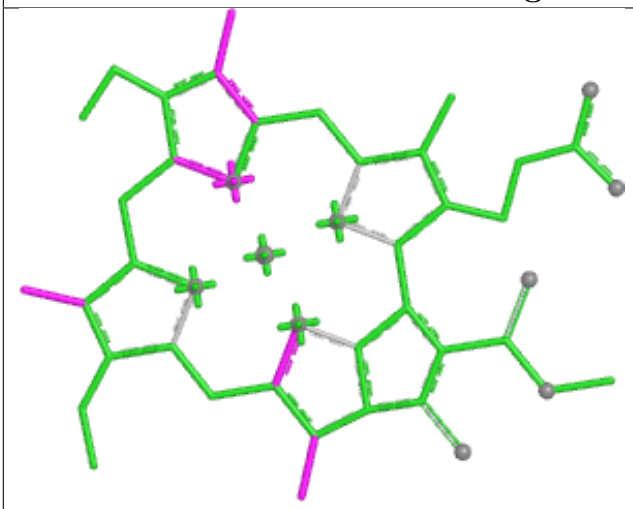


Torsions

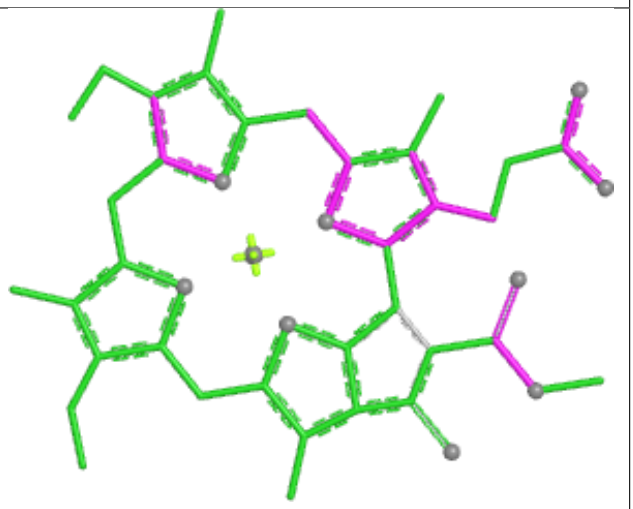


Rings

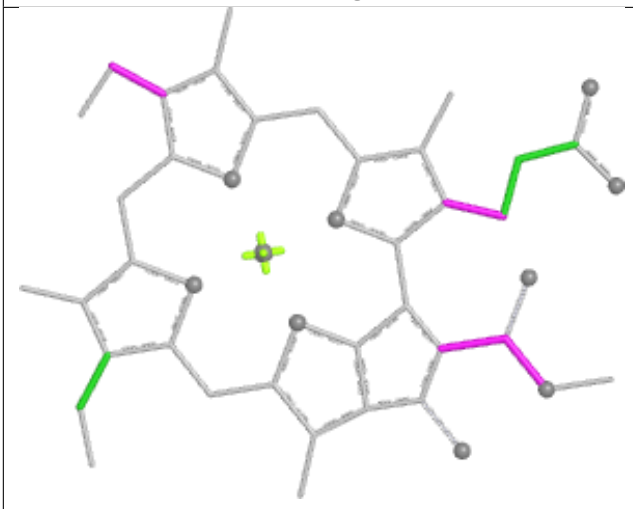
Ligand CLA B 834



Bond lengths



Bond angles

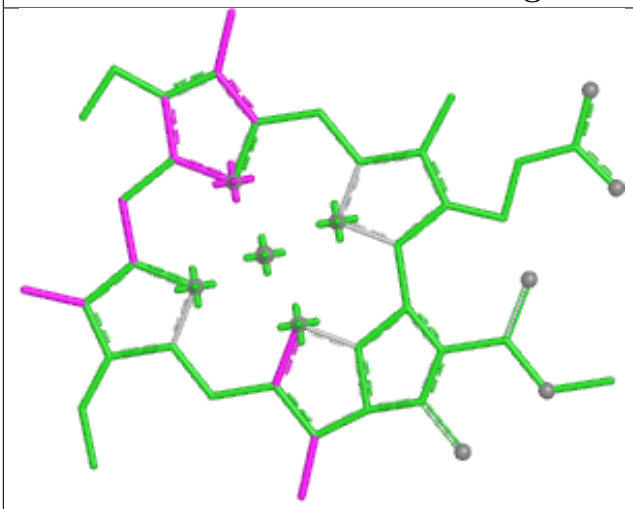


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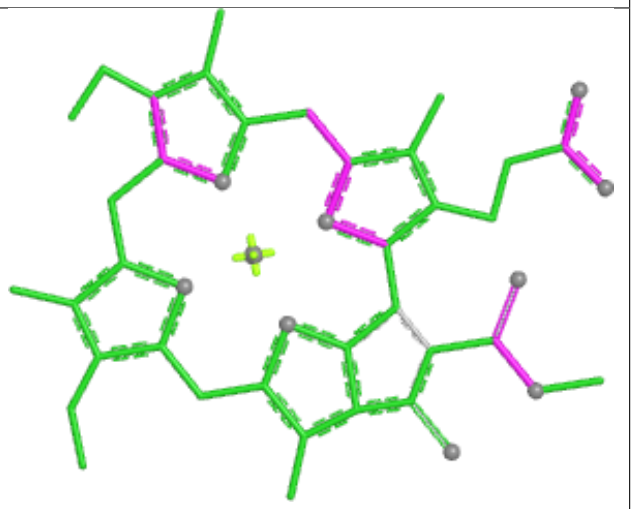


Rings

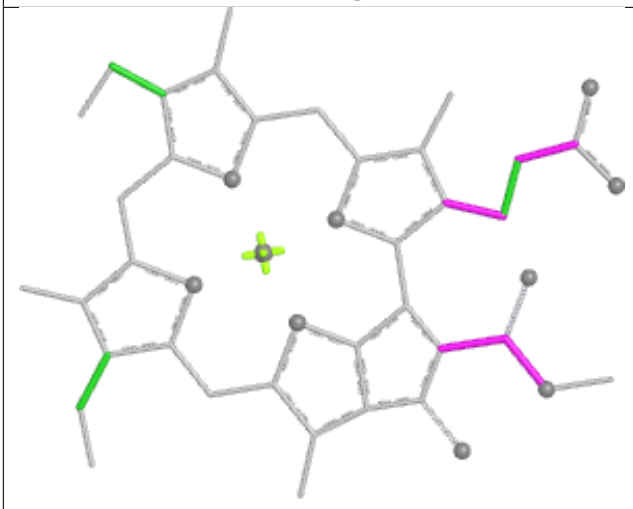
Ligand CLA A 813



Bond lengths



Bond angles

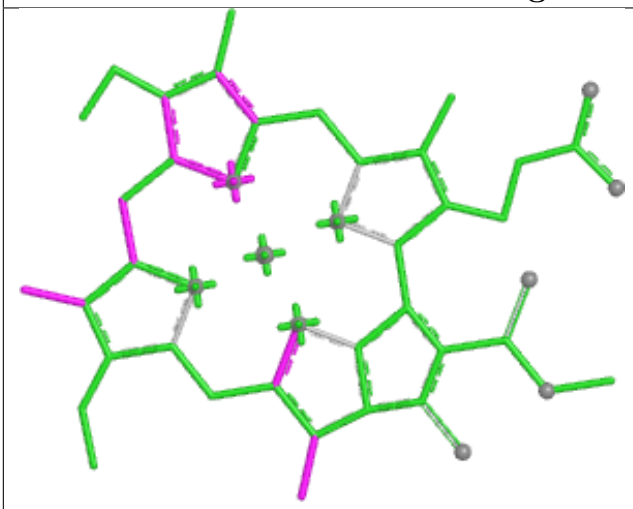


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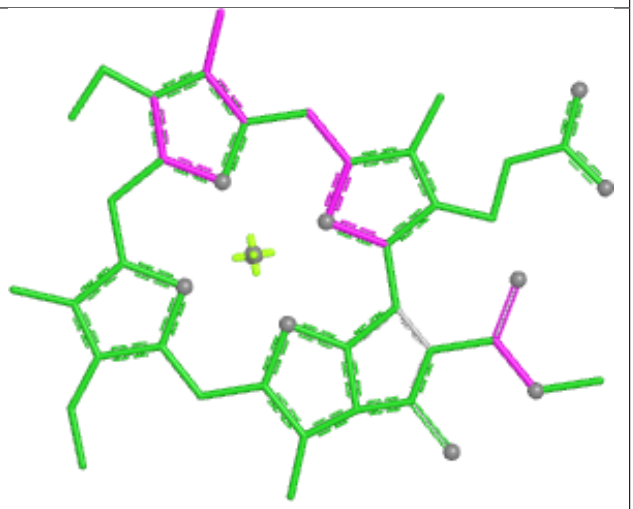


Rings

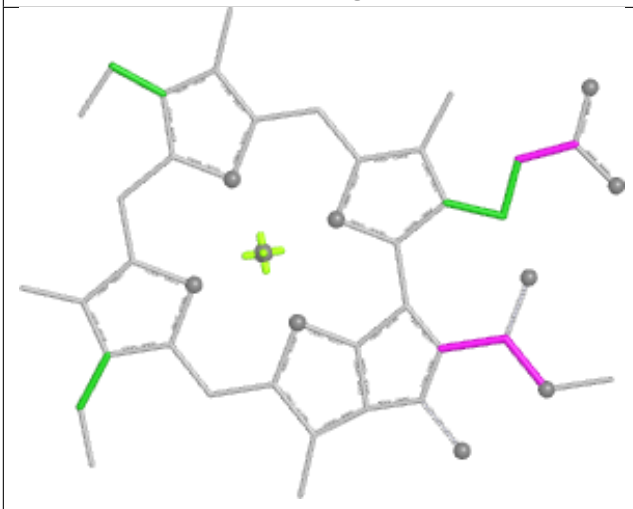
Ligand CLA o 304



Bond lengths



Bond angles

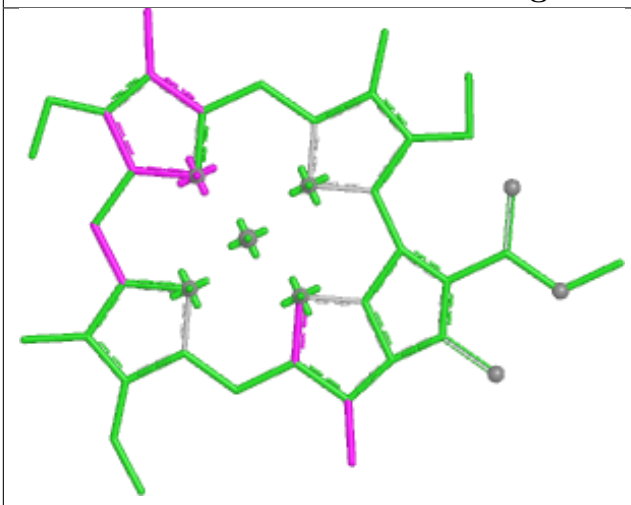


Torsions

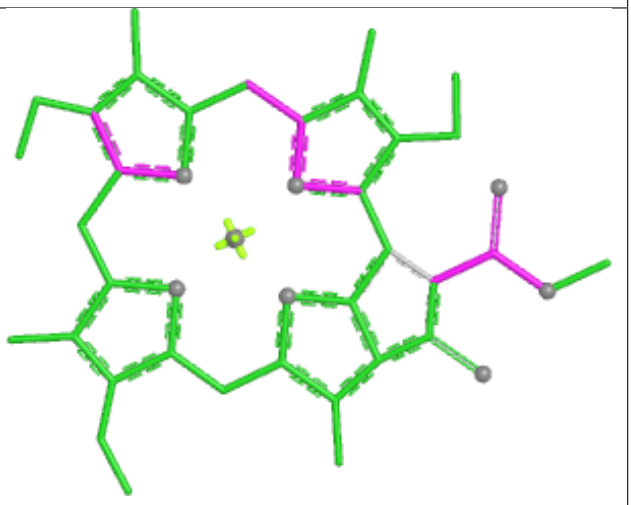


Rings

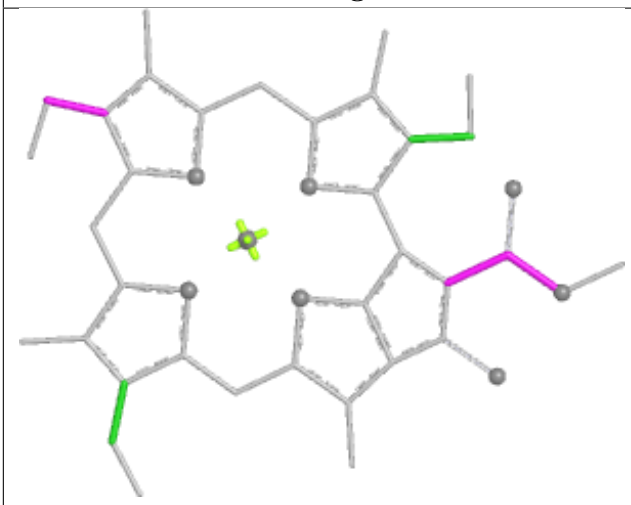
Ligand CLA r 310



Bond lengths



Bond angles

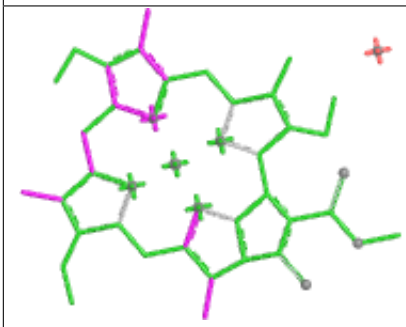


Torsions

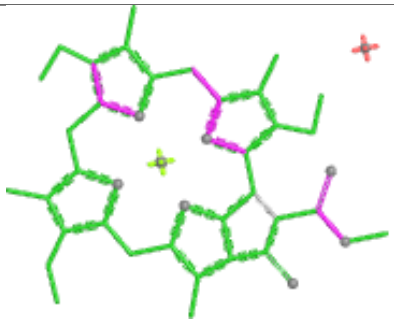


Rings

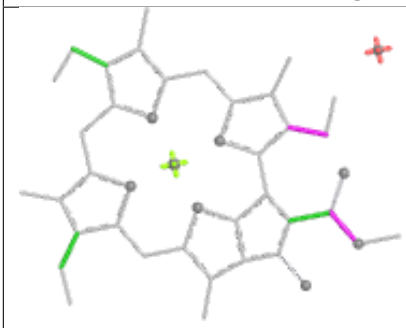
Ligand CLA e 828



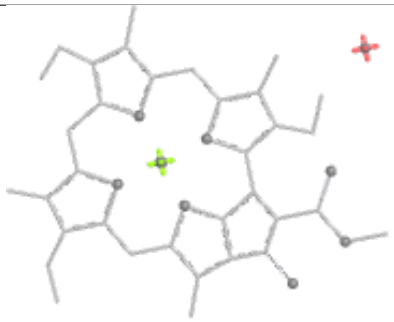
Bond lengths



Bond angles

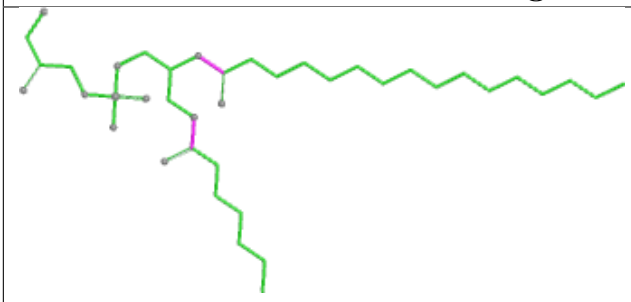


Torsions

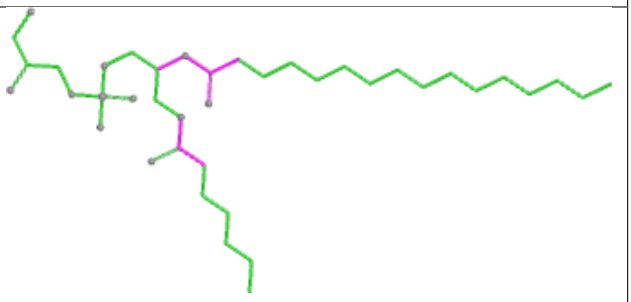


Rings

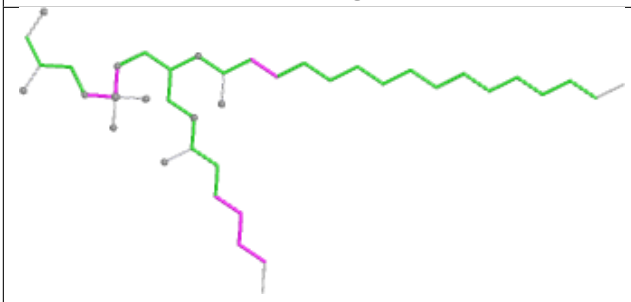
Ligand LHG e 844



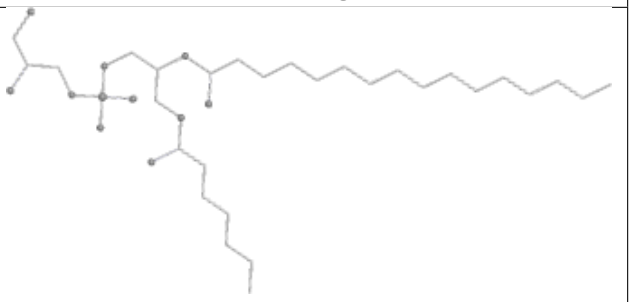
Bond lengths



Bond angles

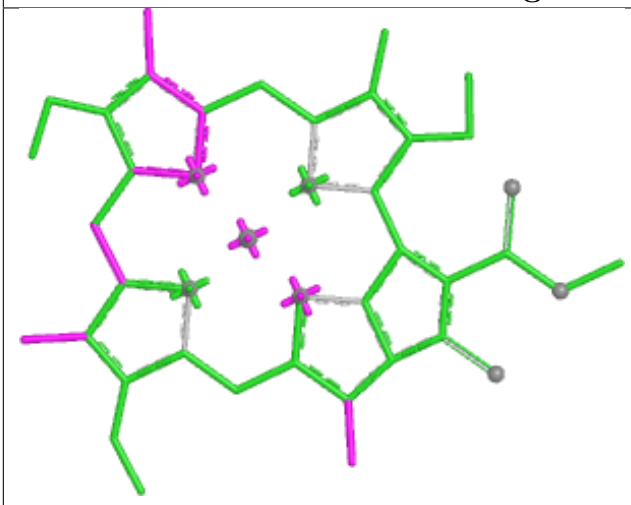


Torsions

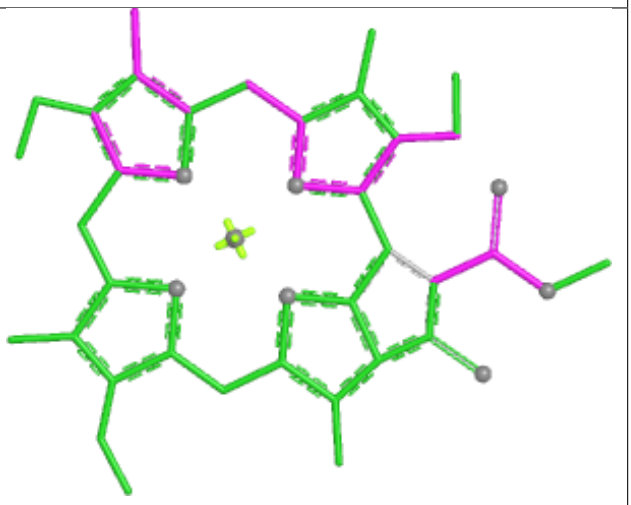


Rings

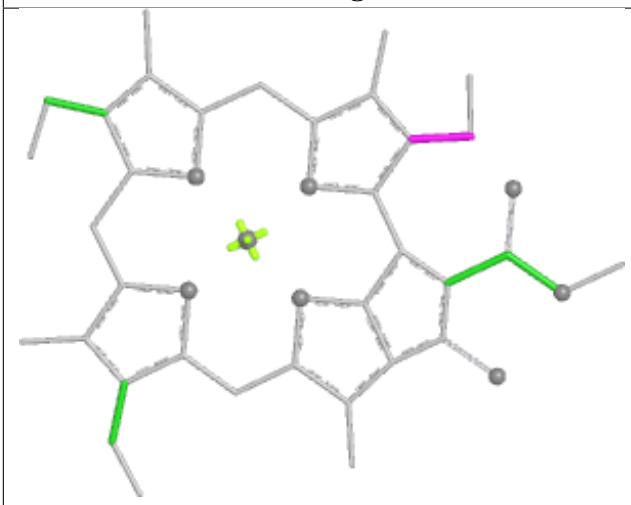
Ligand CLA A 821



Bond lengths



Bond angles

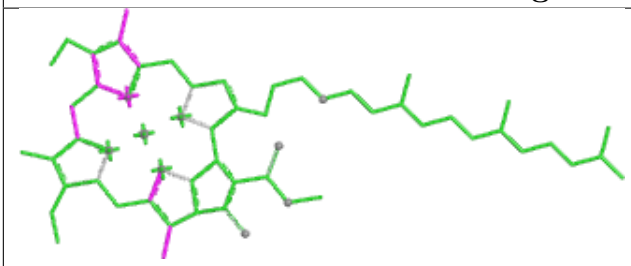


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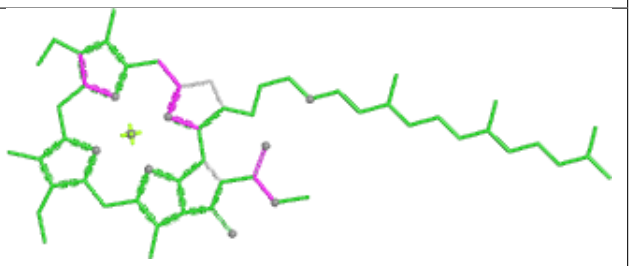


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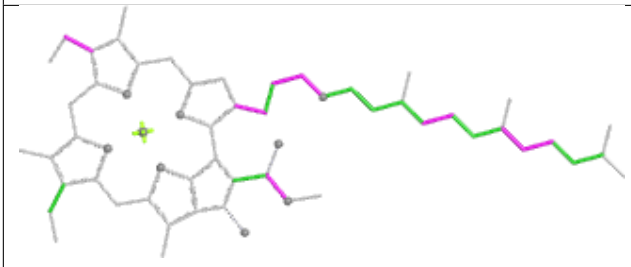
Ligand CLA f 836



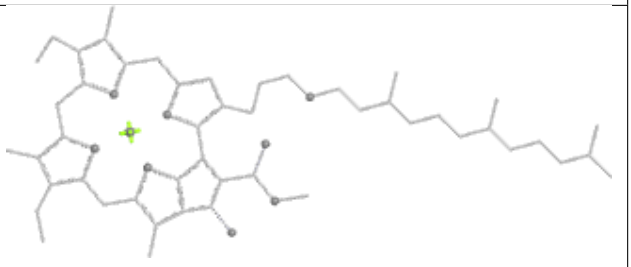
Bond lengths



Bond angles

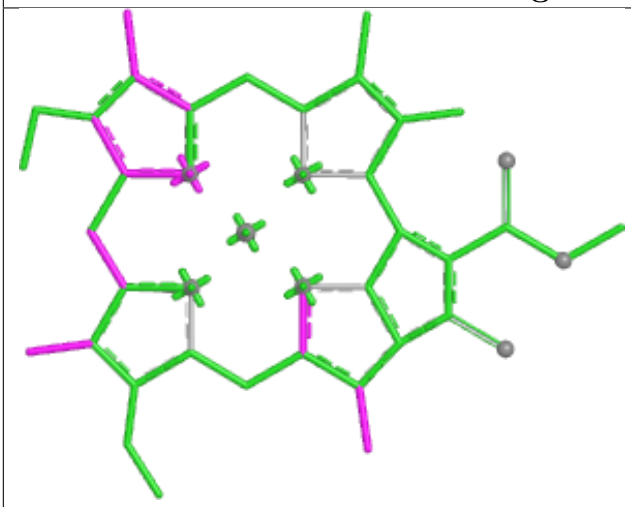


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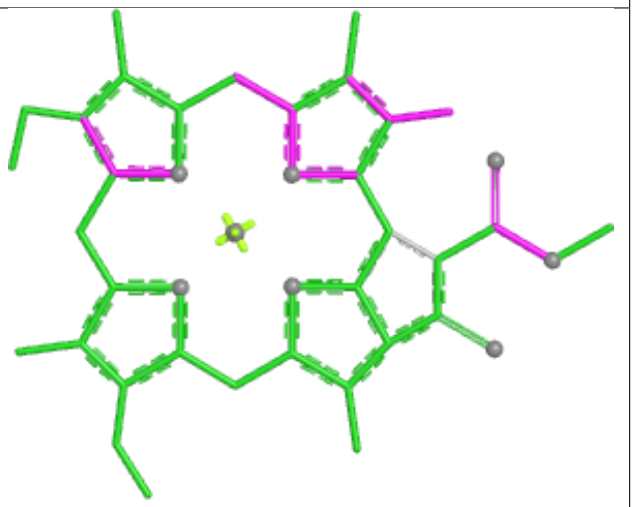


Rings

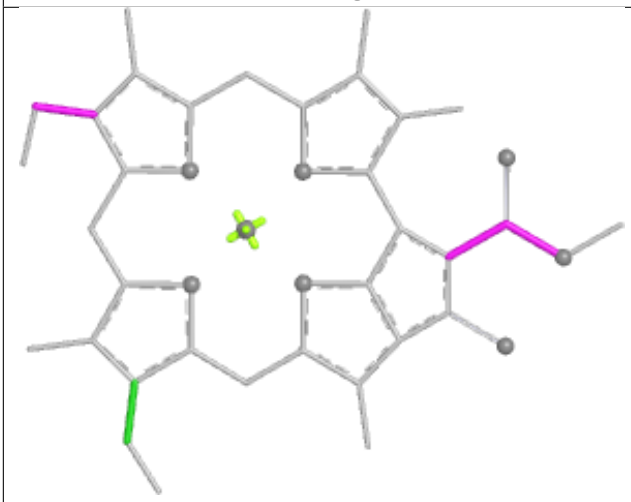
Ligand CLA f 828



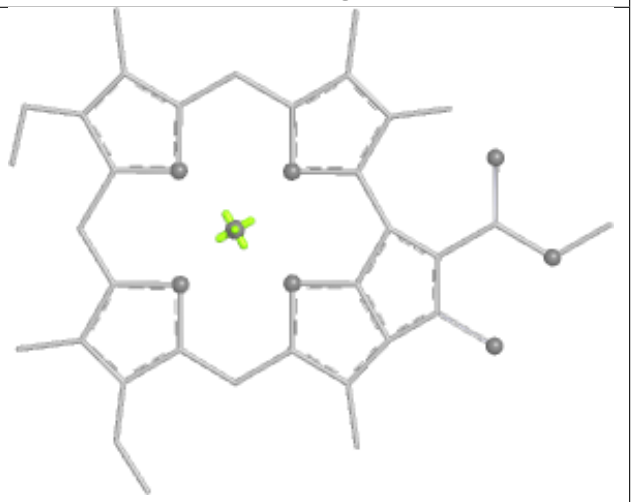
Bond lengths



Bond angles

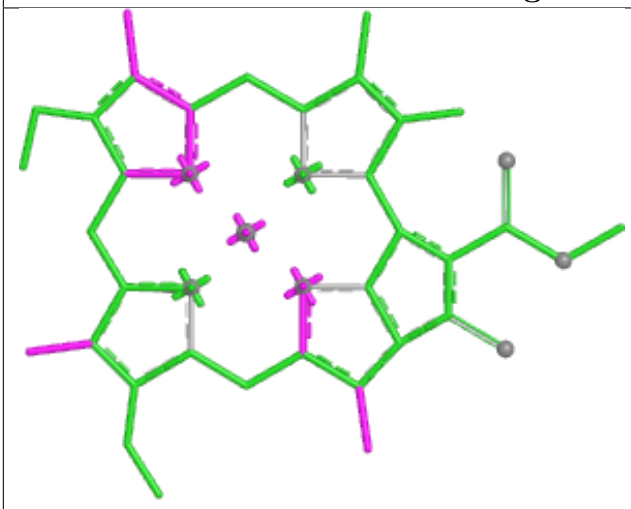


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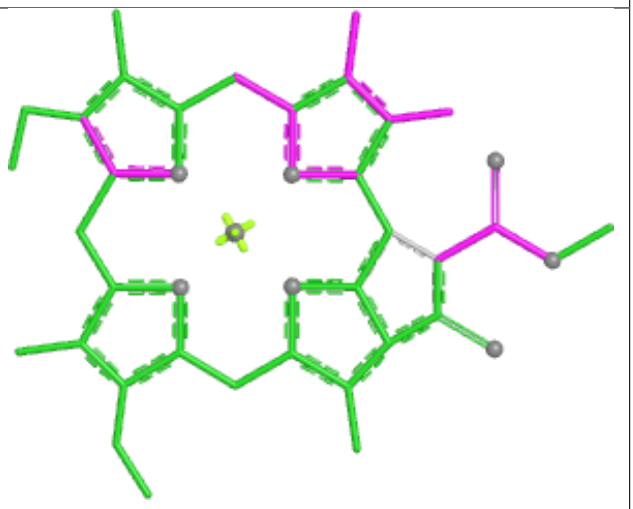


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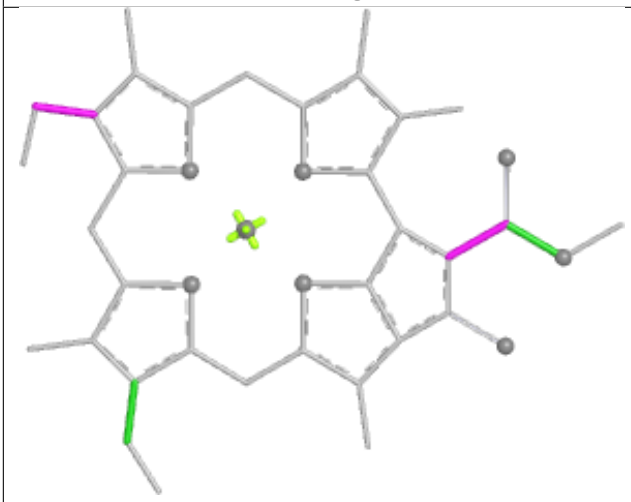
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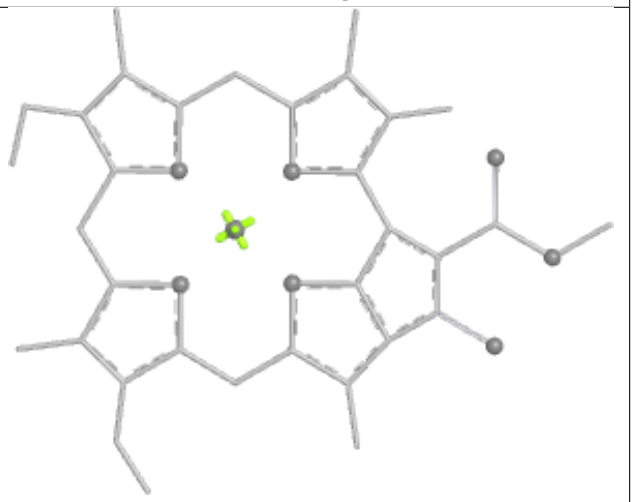
Bond lengths



Bond angles

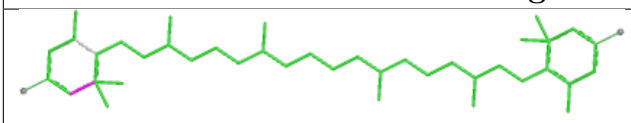


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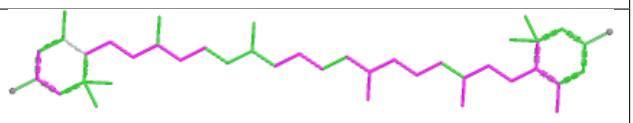


Rings

Ligand LUT 3 303



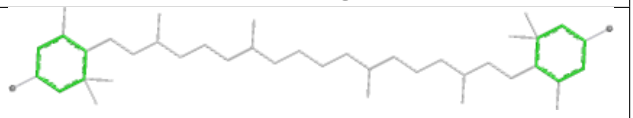
Bond lengths



Bond angles

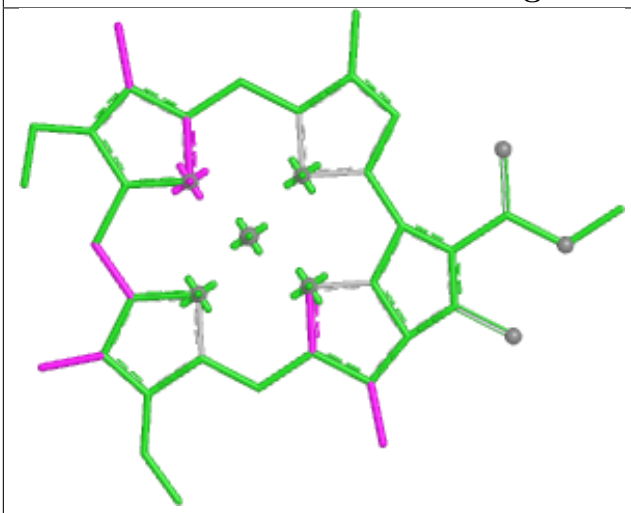


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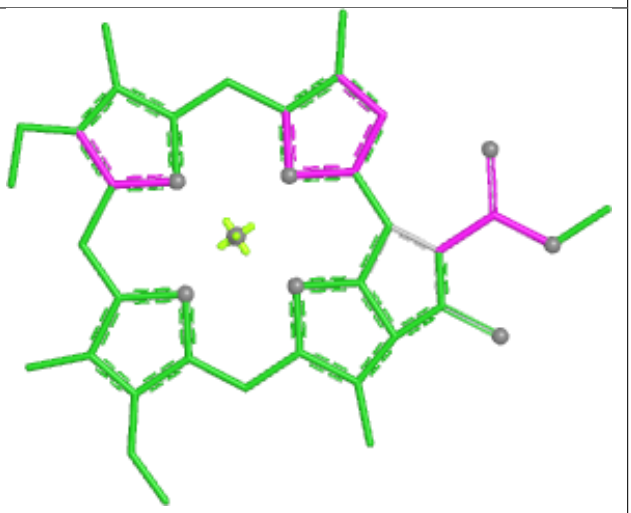


Rings

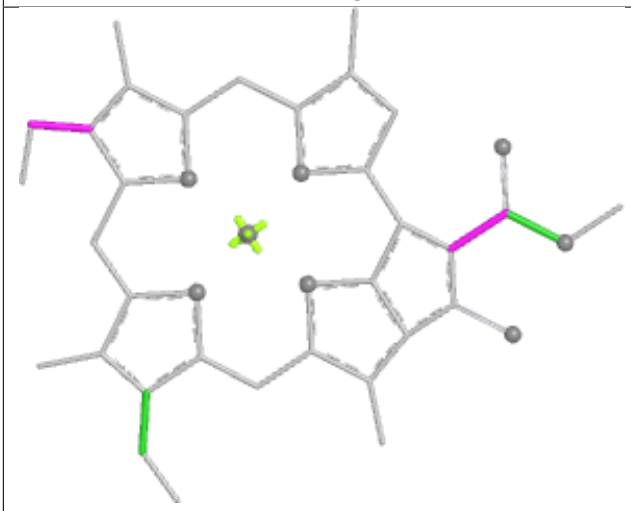
Ligand CLA A 819



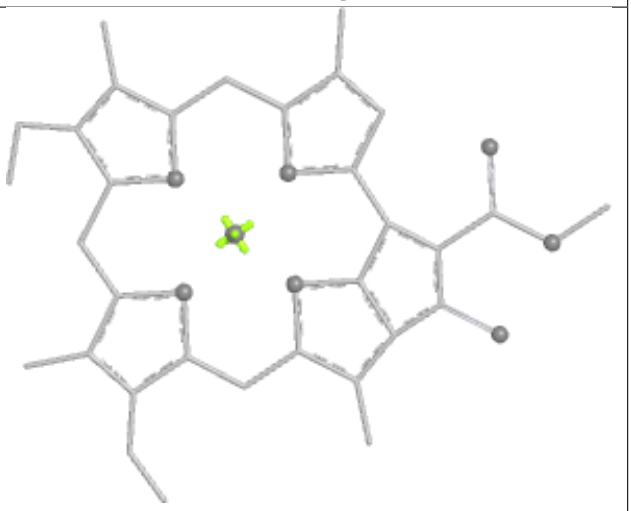
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Bond angles

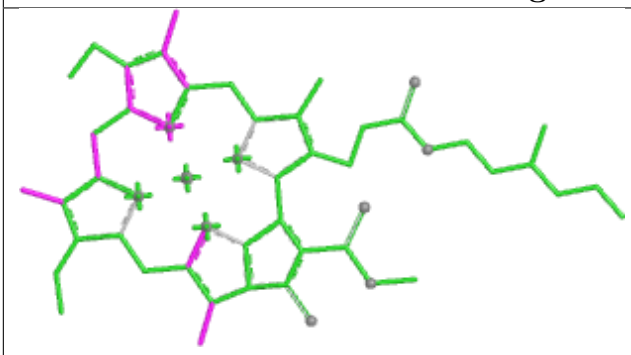


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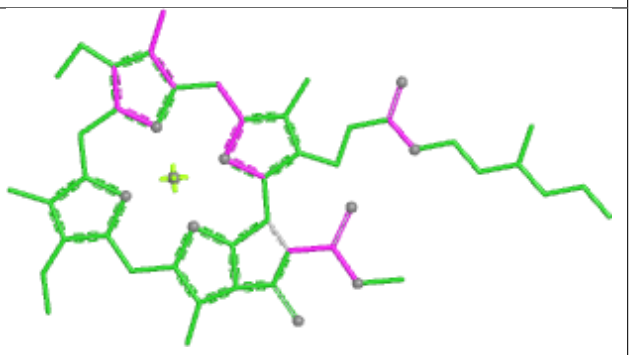


Rings

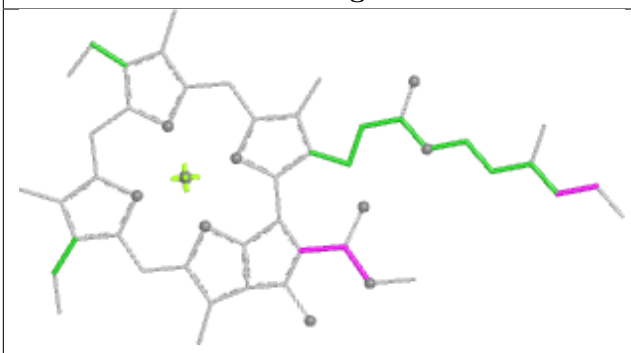
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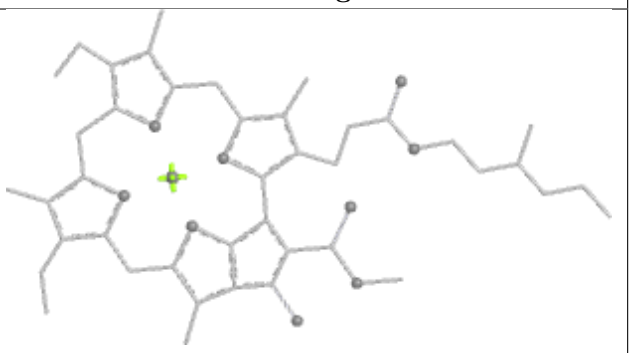
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Bond angles

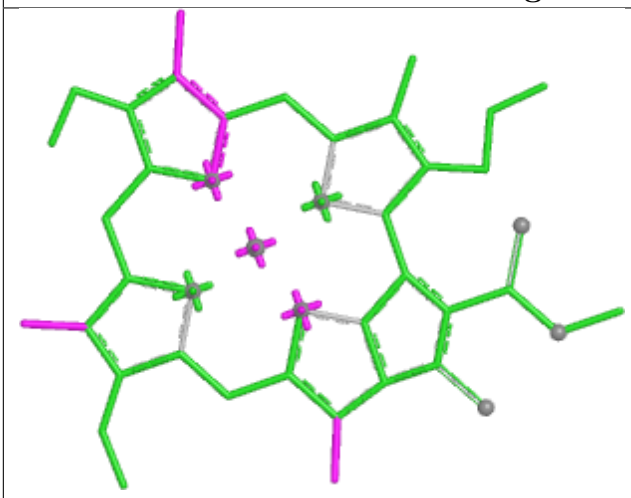


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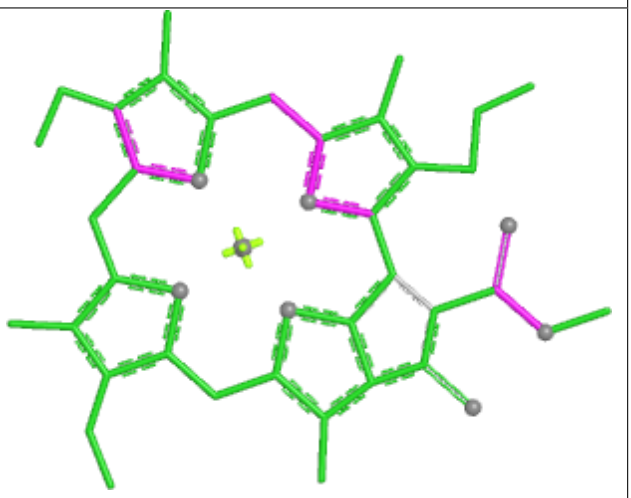


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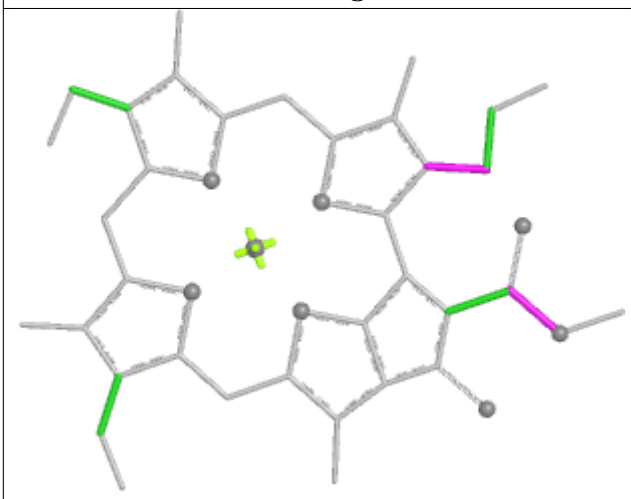
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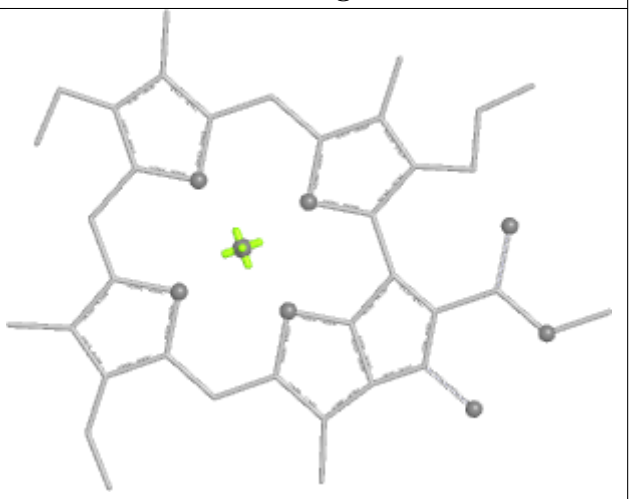
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Bond angles

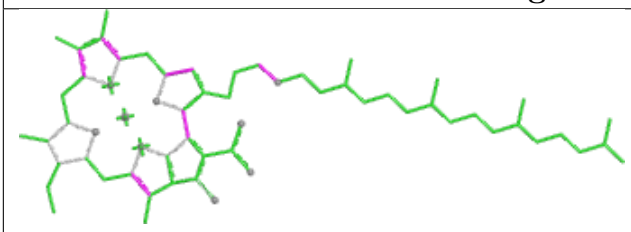


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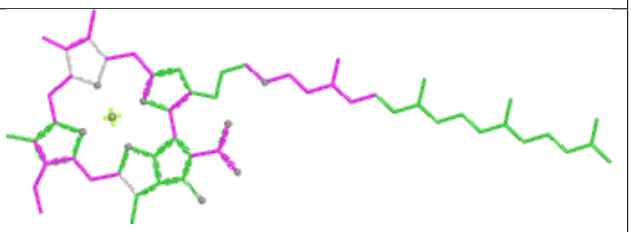


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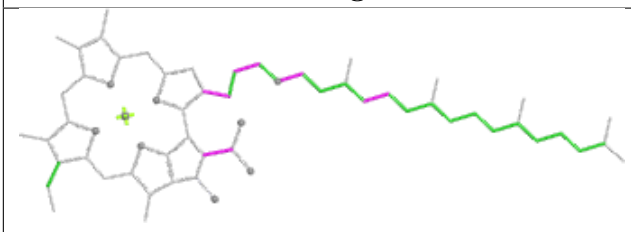
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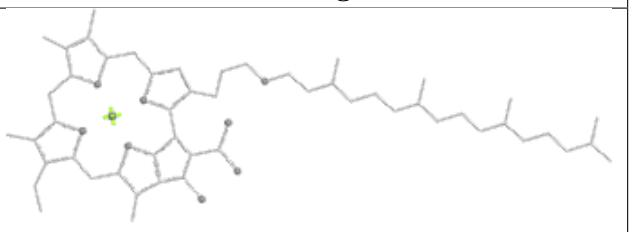
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Bond angles

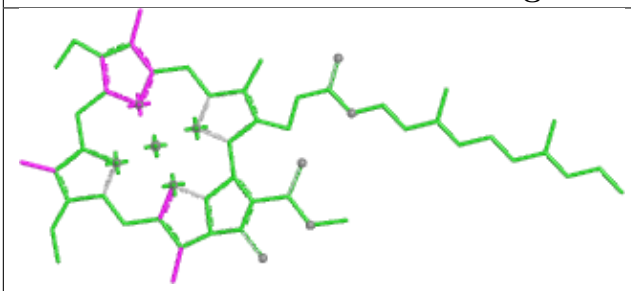


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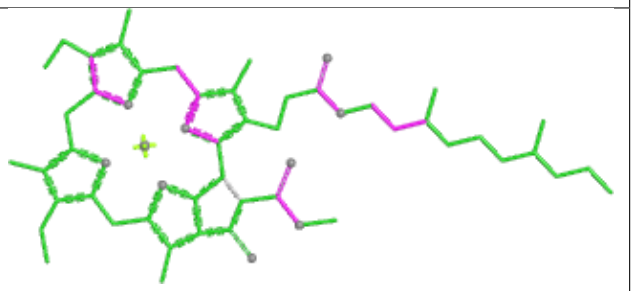


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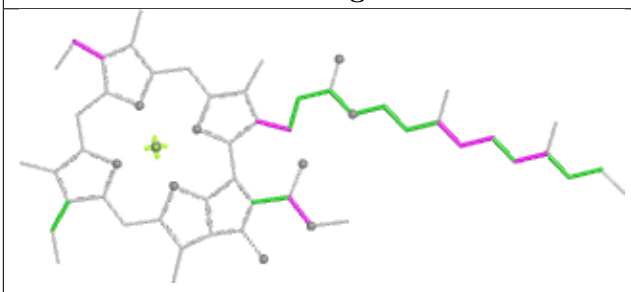
Ligand CLA A 852



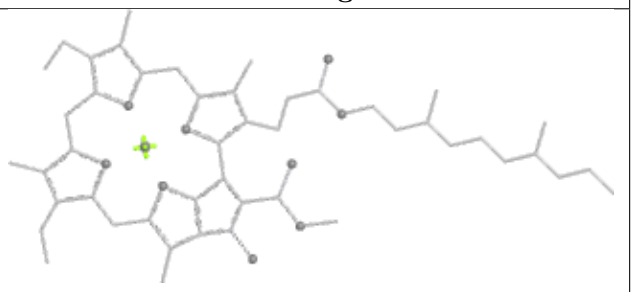
Bond lengths



Bond angles

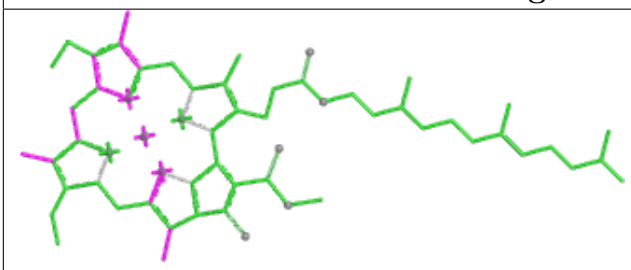


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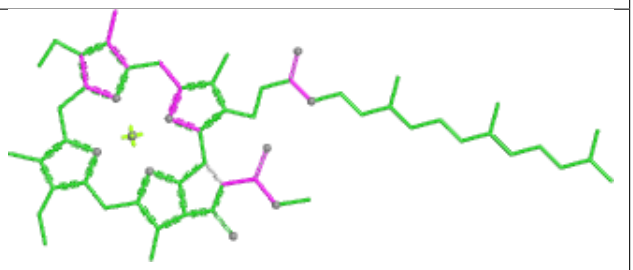


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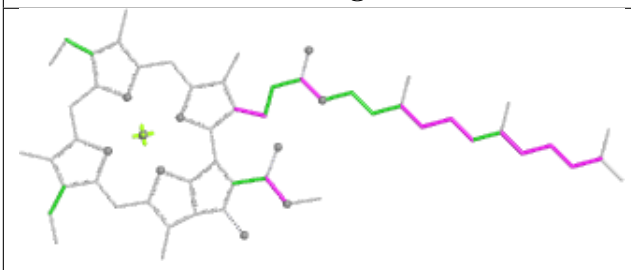
Ligand CLA 2 510



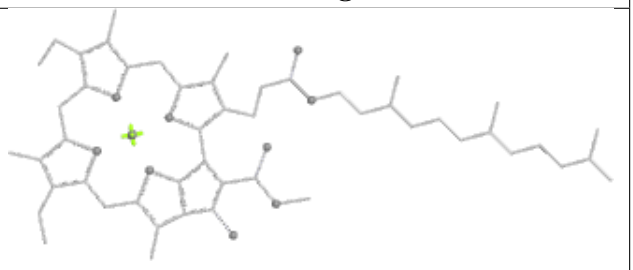
Bond lengths



Bond angles

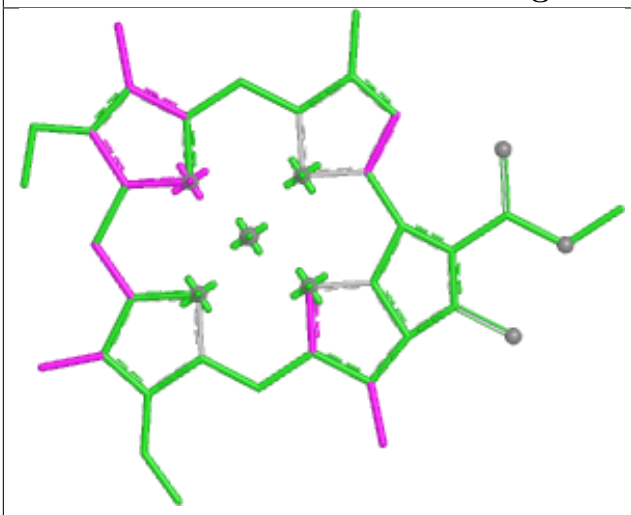


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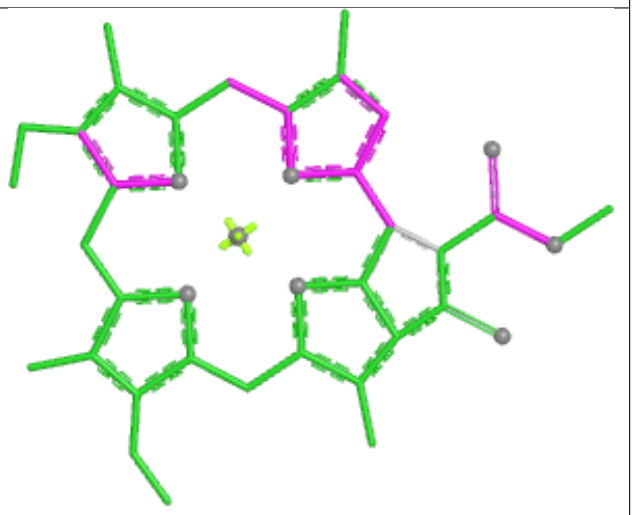


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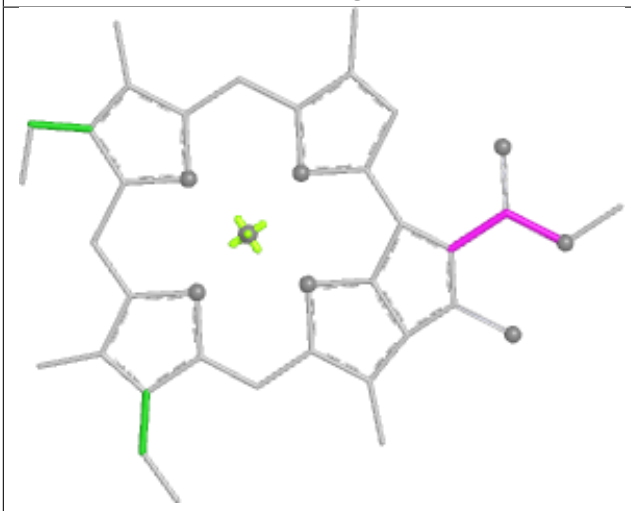
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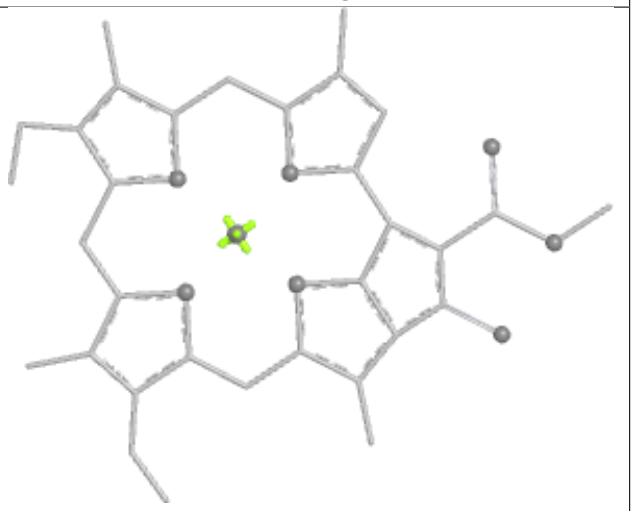
Bond lengths



Bond angles

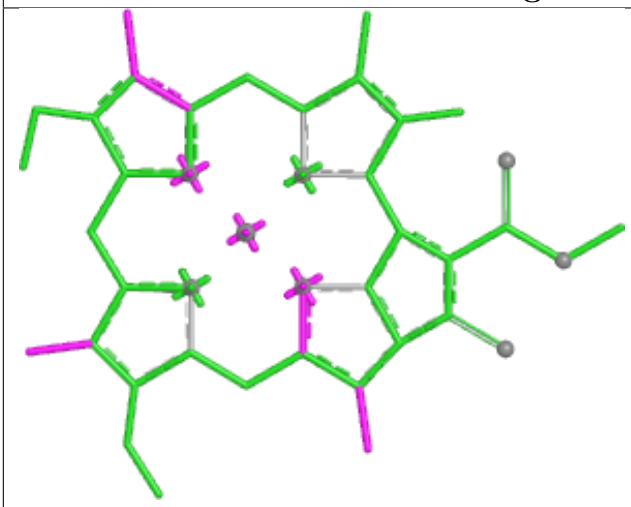


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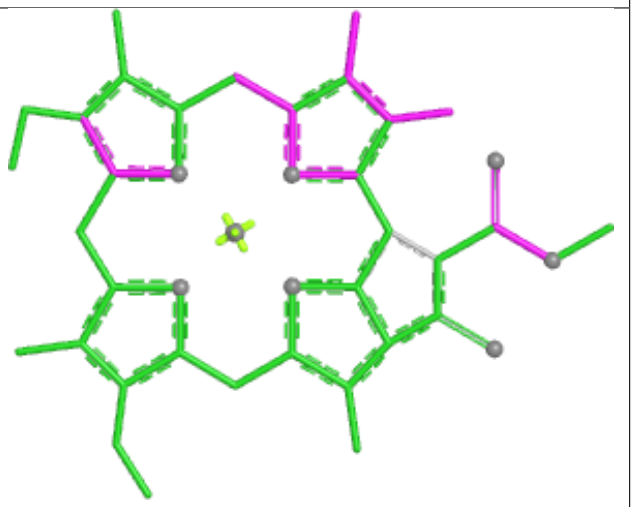


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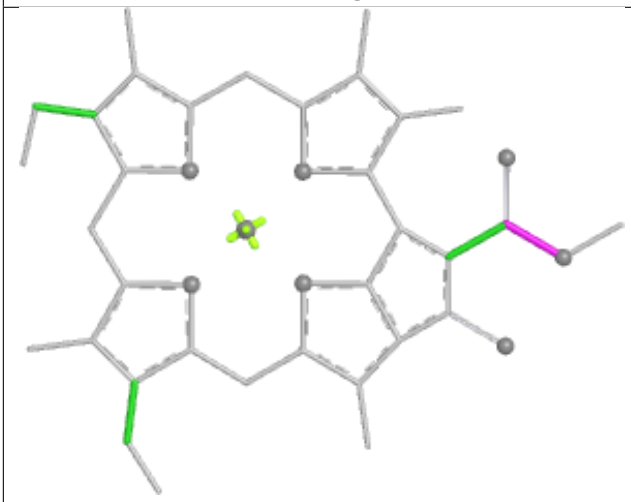
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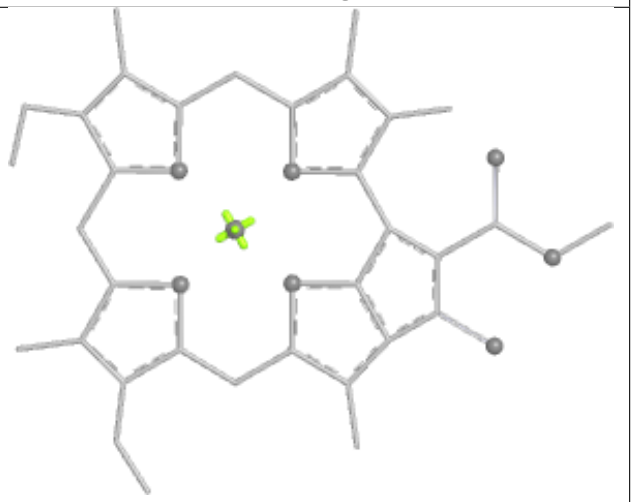
Bond lengths



Bond angles

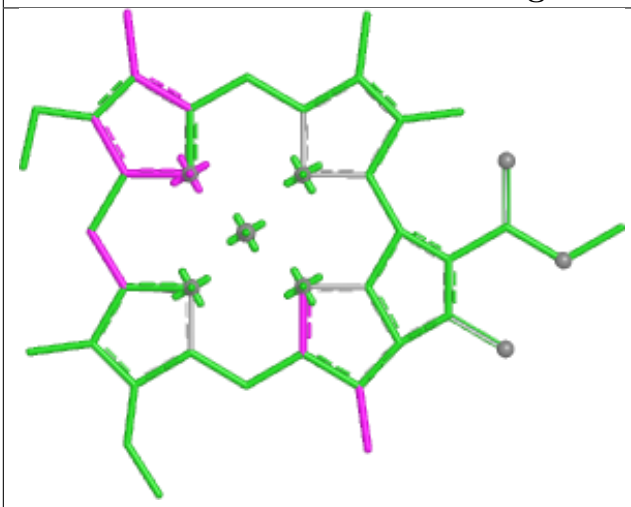


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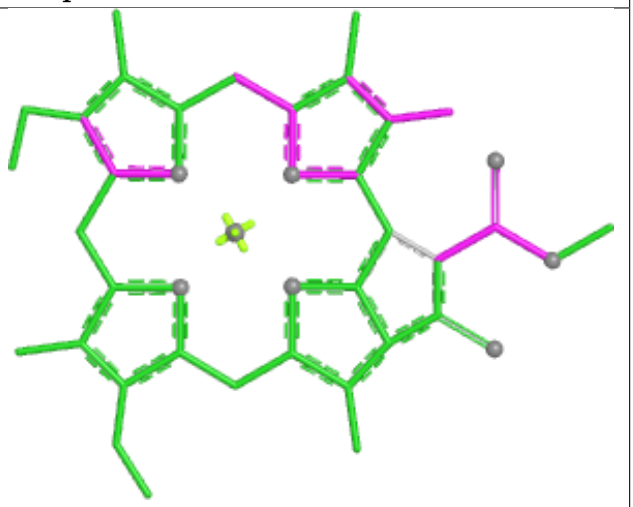


Rings

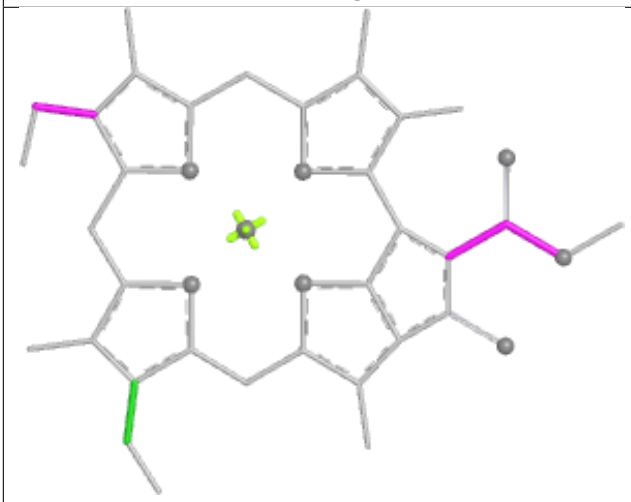
Ligand CLA q 306



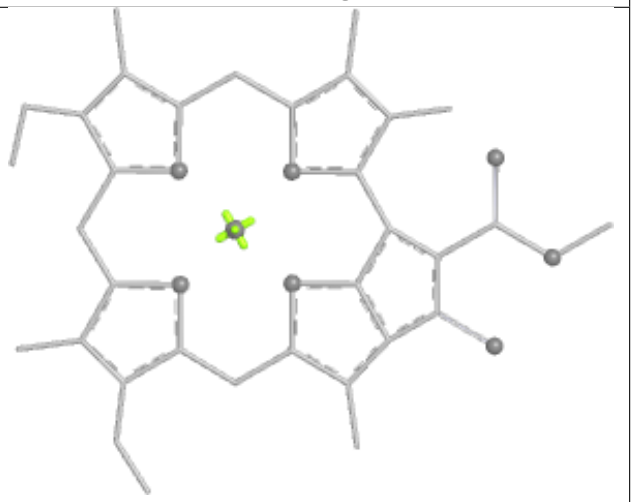
Bond lengths



Bond angles

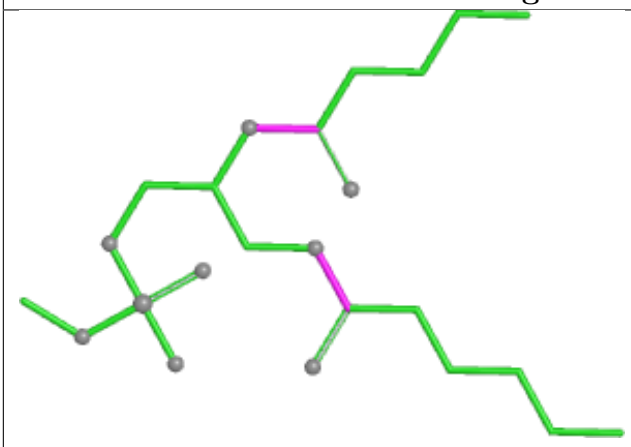


Torsions

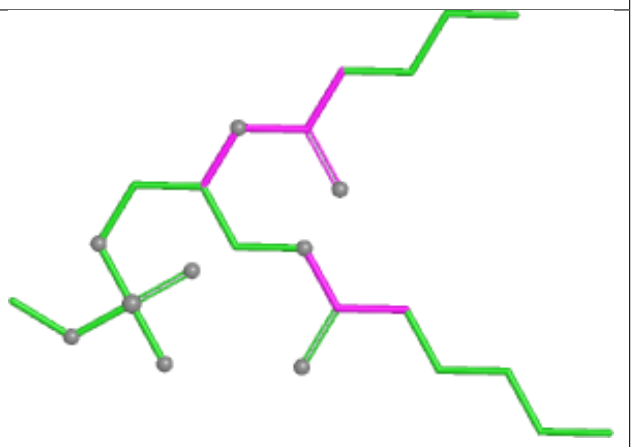


Rings

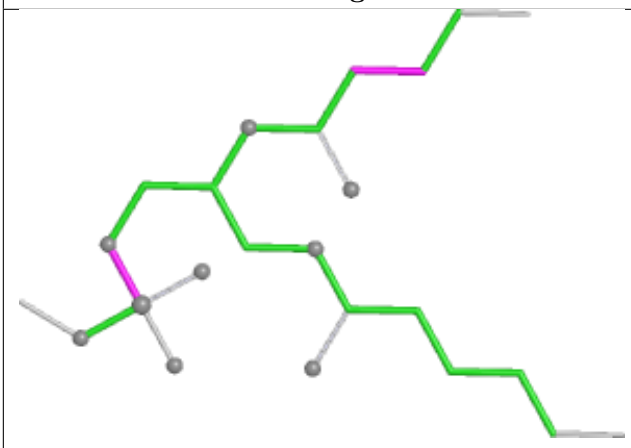
Ligand LHG O 601



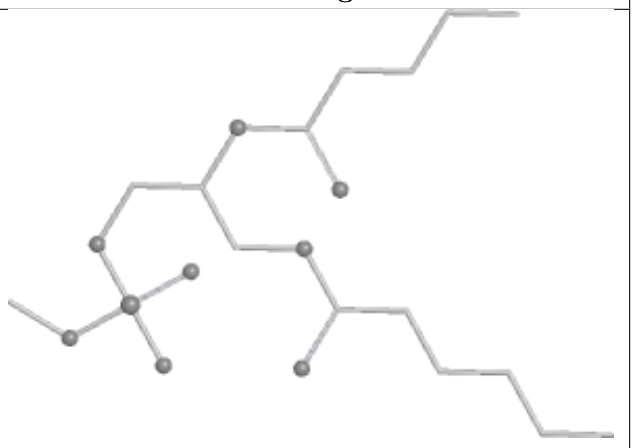
Bond lengths



Bond angles

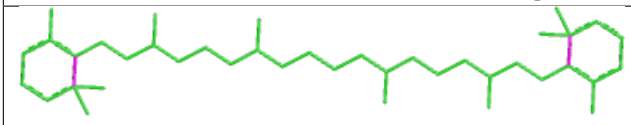


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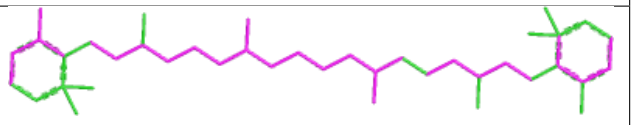


Rings

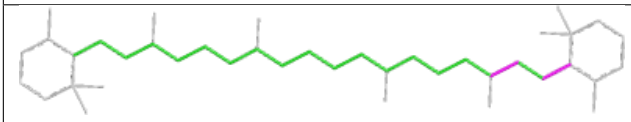
Ligand BCR I 101



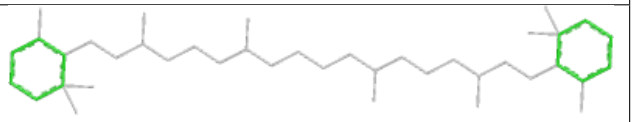
Bond lengths



Bond angles

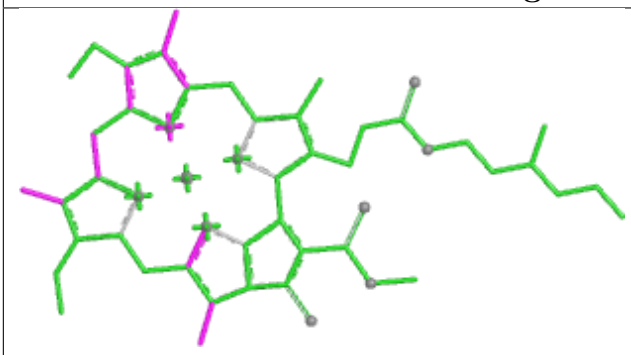


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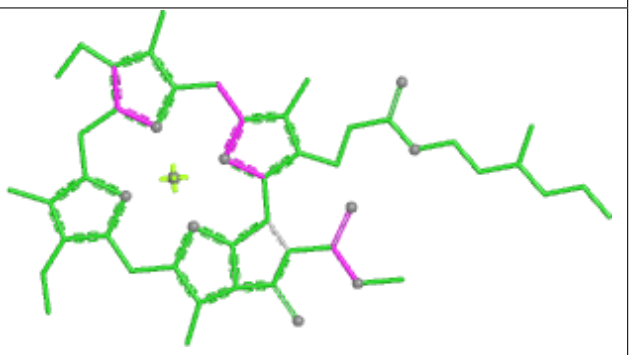


Rings

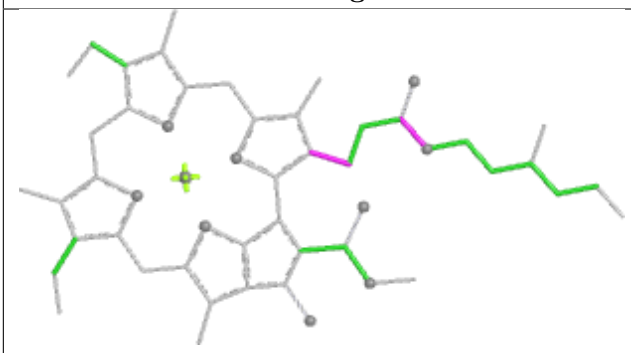
Ligand CLA A 804



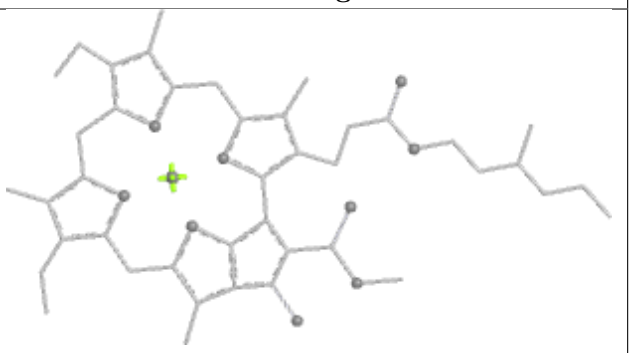
Bond lengths



Bond angles

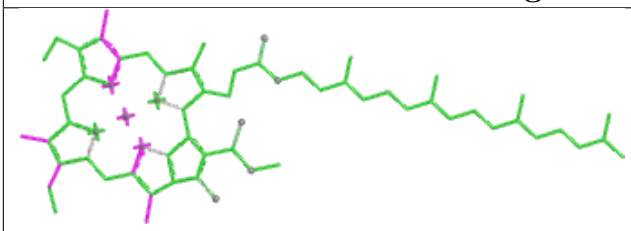


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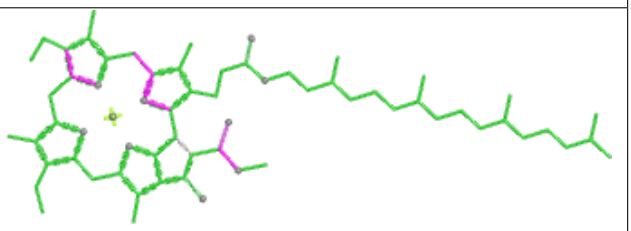


Rings

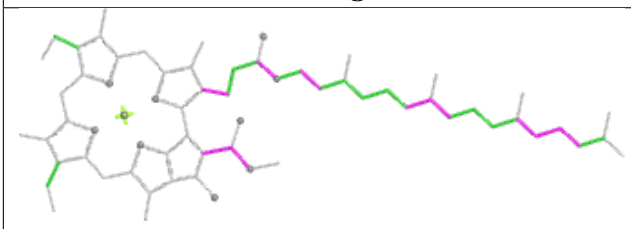
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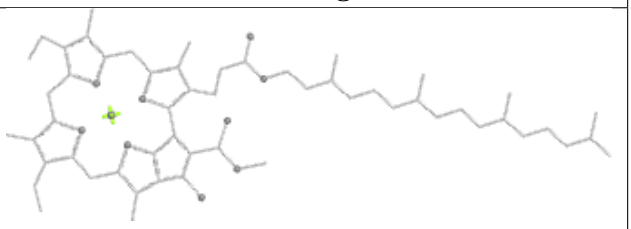
Bond lengths



Bond angles



Torsions



Rings

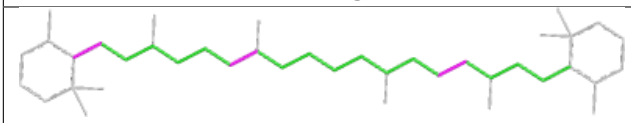
Ligand BCR B 847



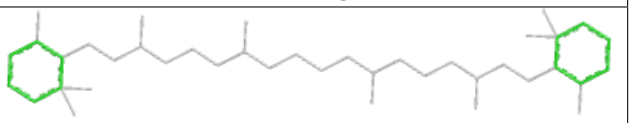
Bond lengths



Bond angles

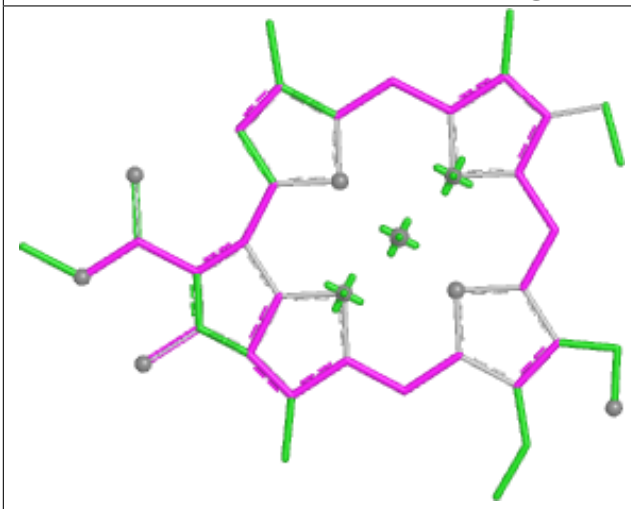


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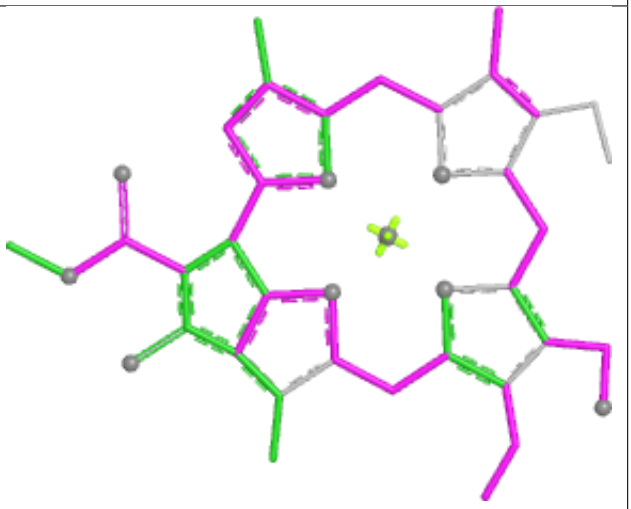


Rings

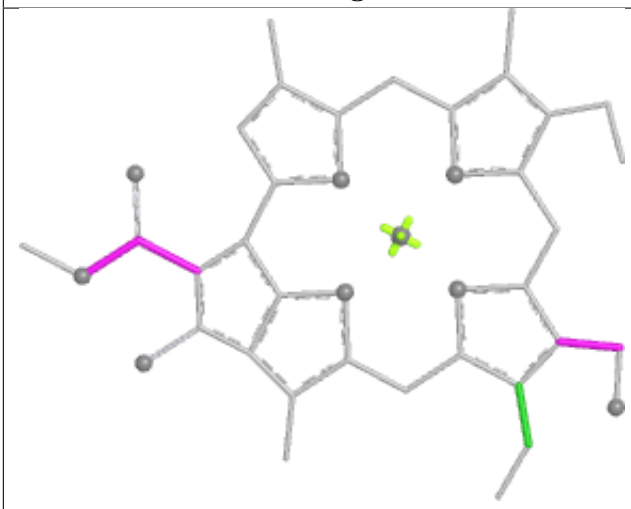
Ligand CHL 1 517



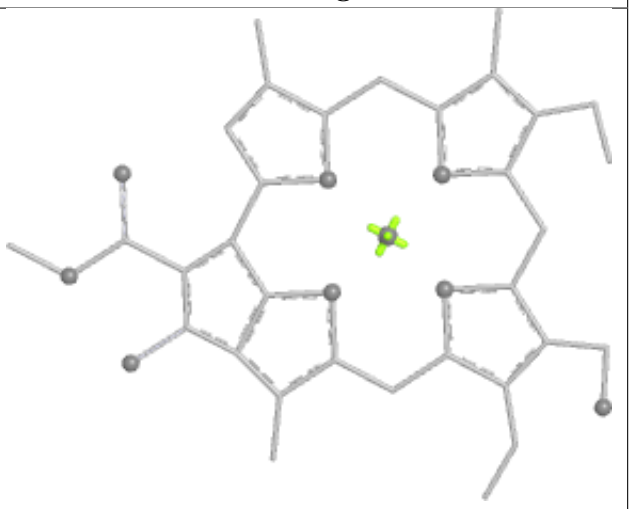
Bond lengths



Bond angles

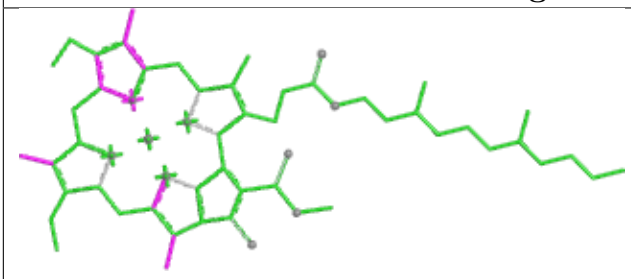


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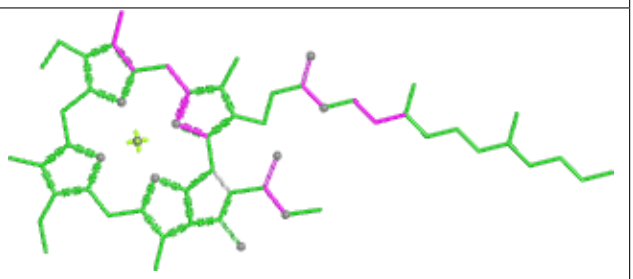


Rings

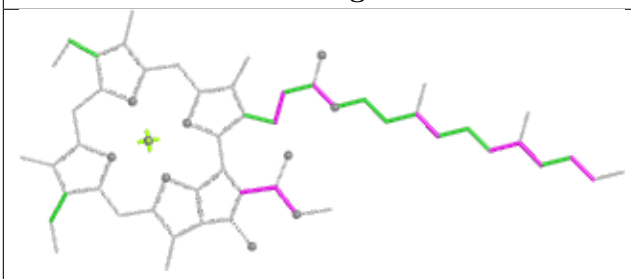
Ligand CLA e 829



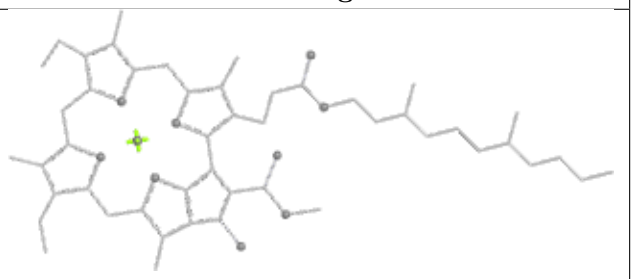
Bond lengths



Bond angles

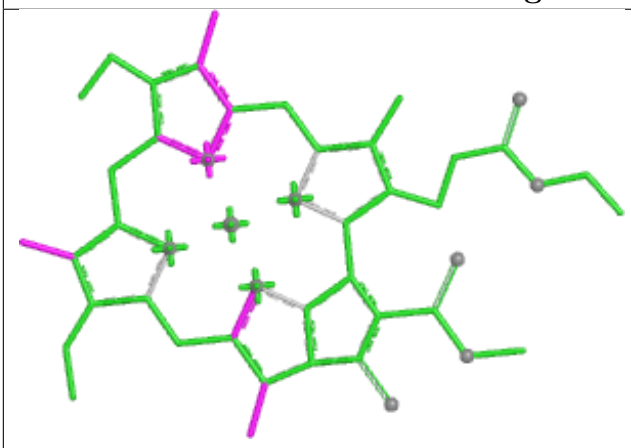


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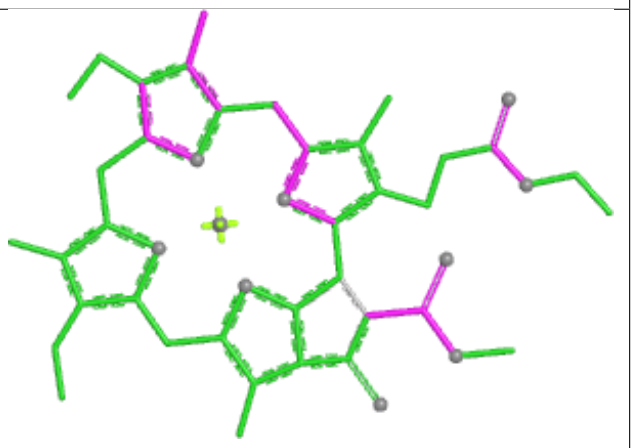


Rings

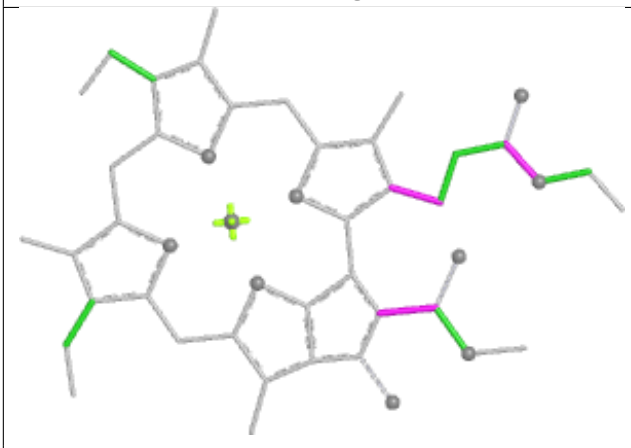
Ligand CLA B 839



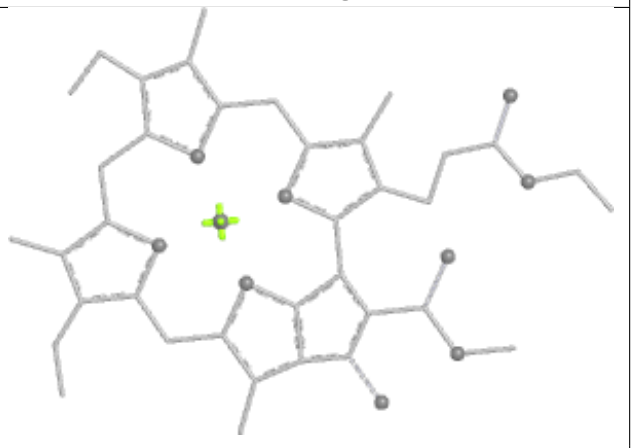
Bond lengths



Bond angles

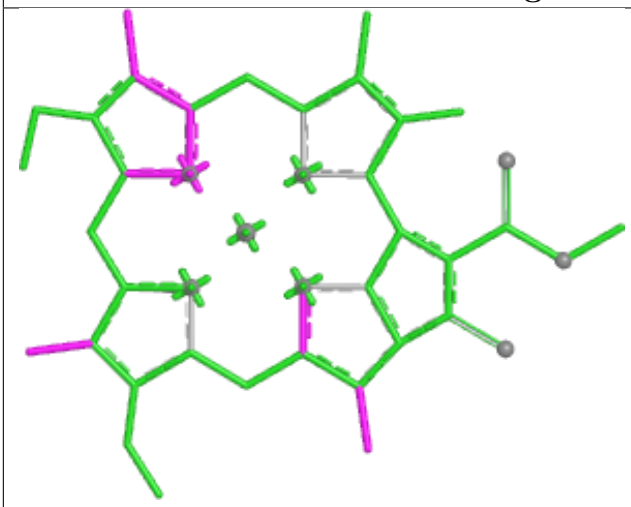


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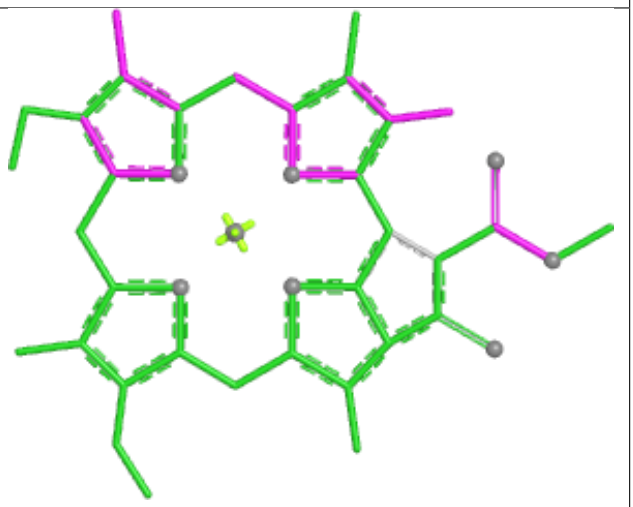


Rings

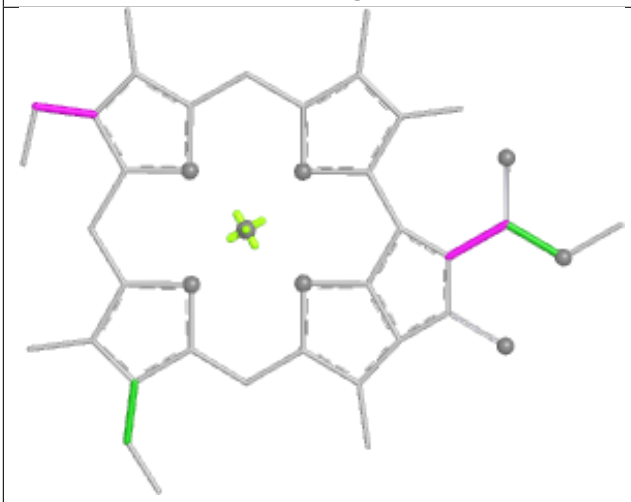
Ligand CLA B 840



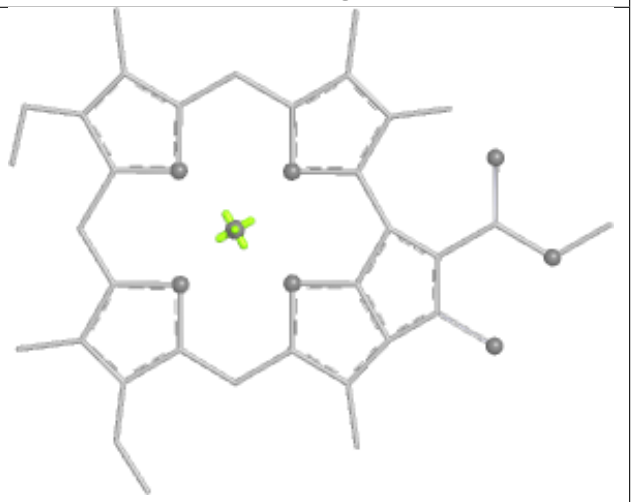
Bond lengths



Bond angles

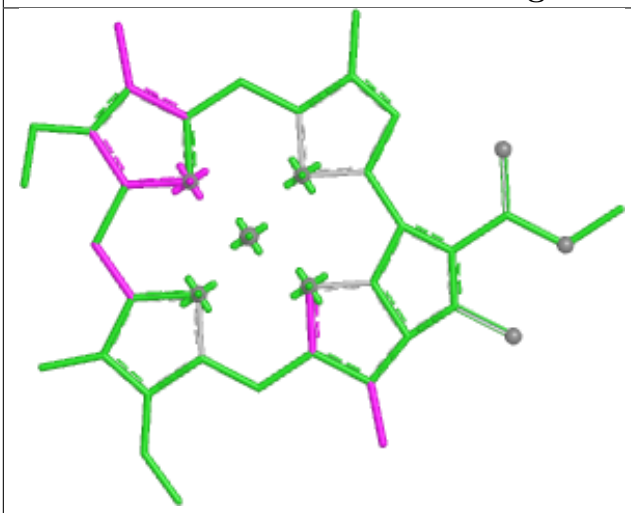


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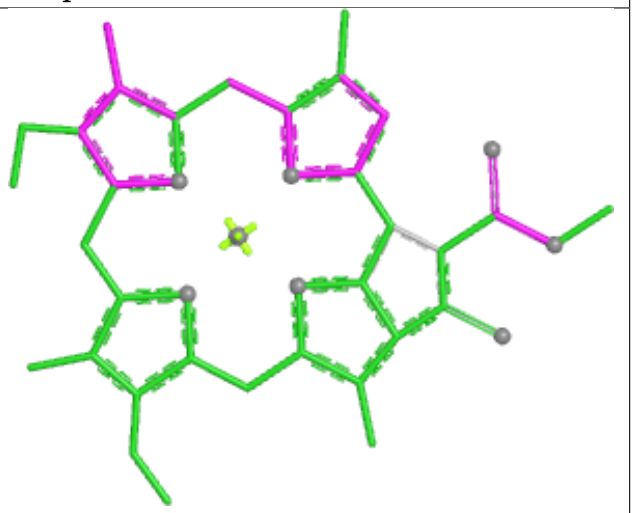


Rings

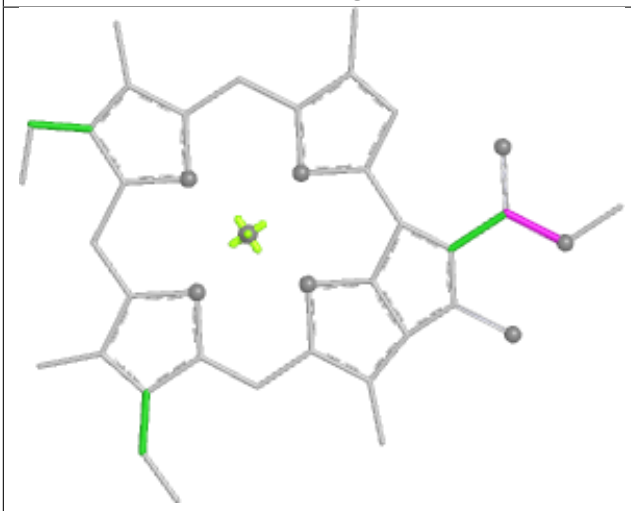
Ligand CLA q 314



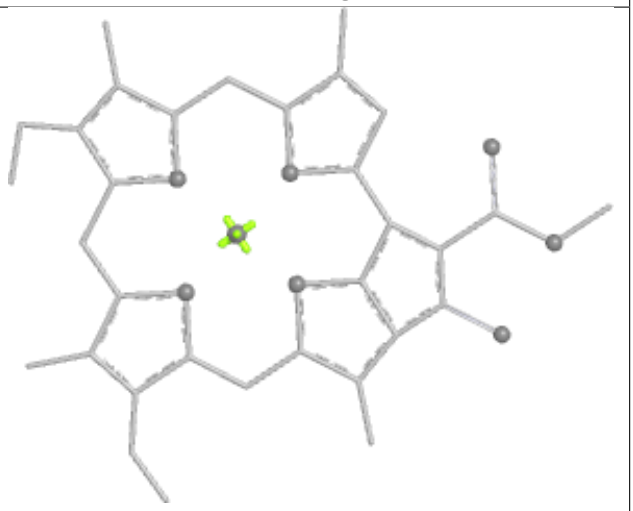
Bond lengths



Bond angles

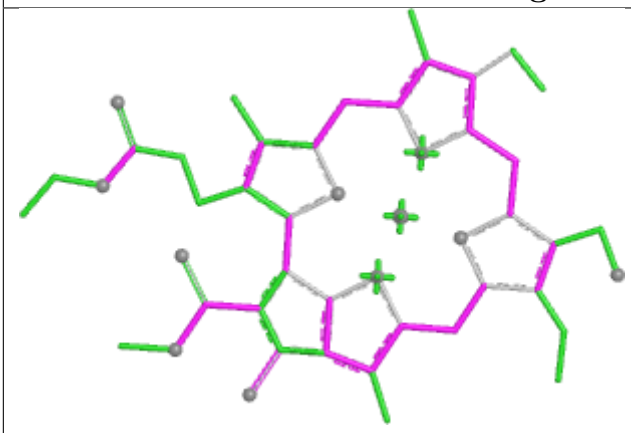


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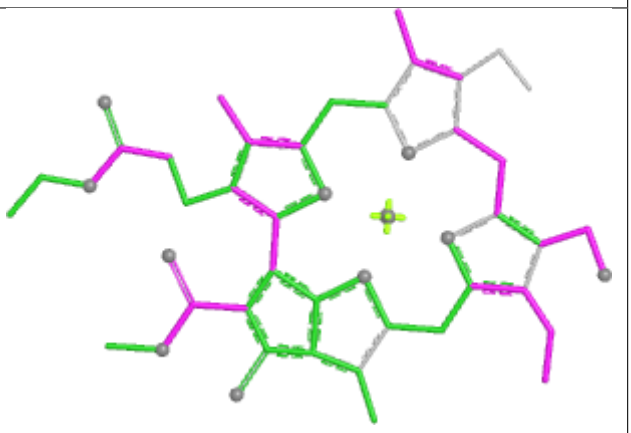


Rings

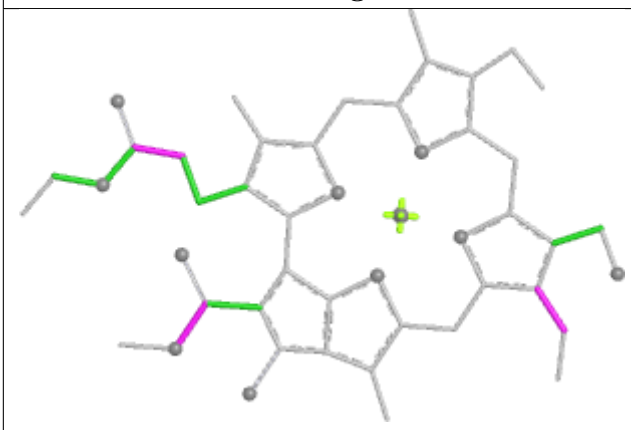
Ligand CHL s 513



Bond lengths



Bond angles

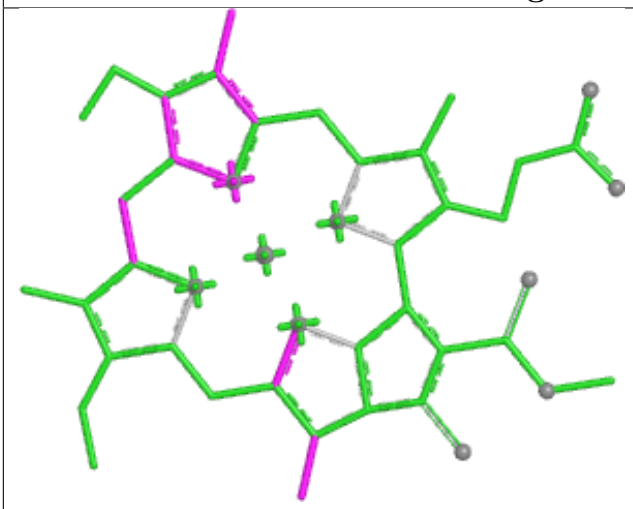


Torsions

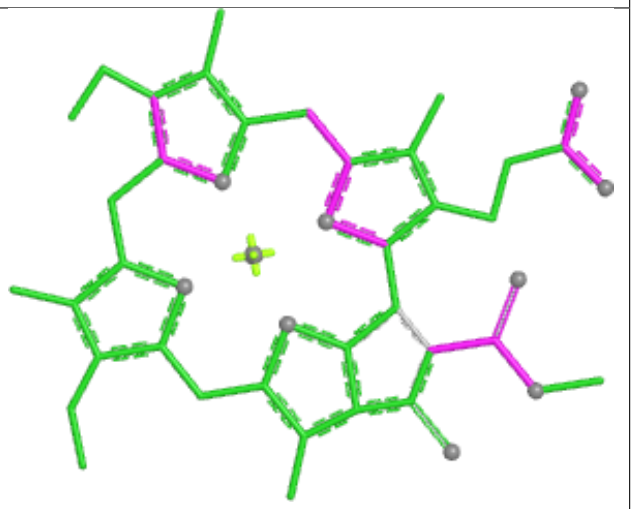


Rings

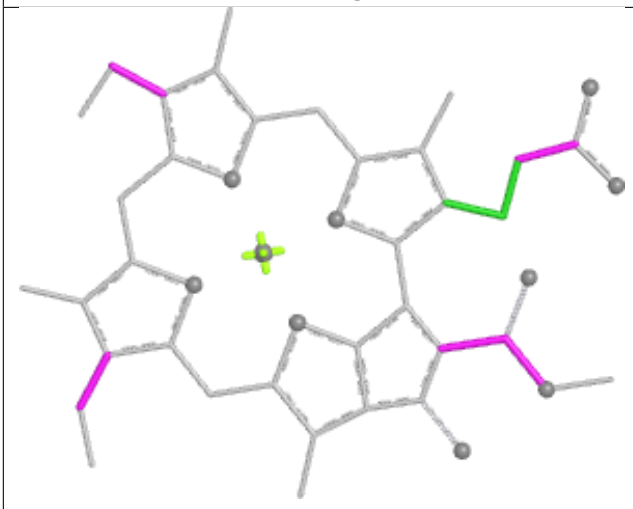
Ligand CLA n 202



Bond lengths



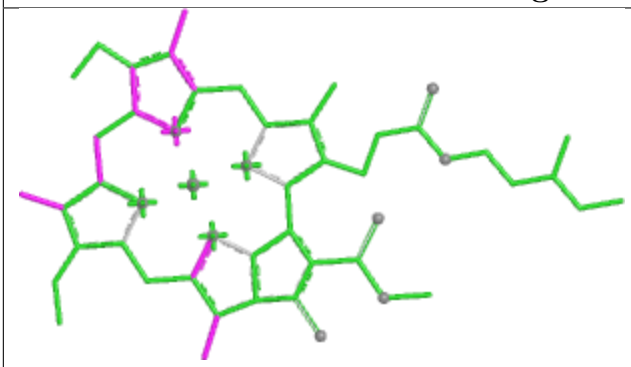
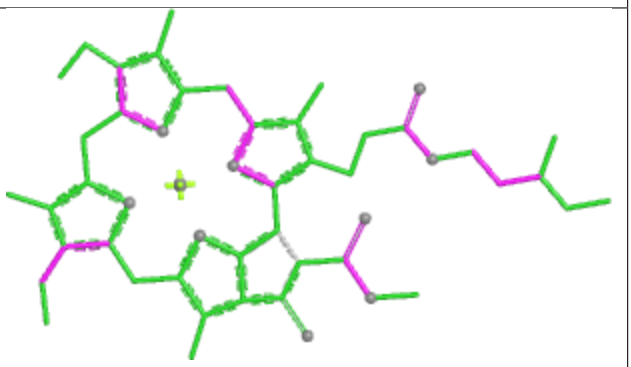
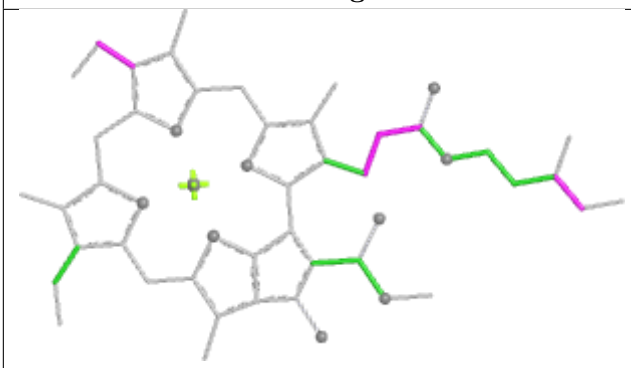
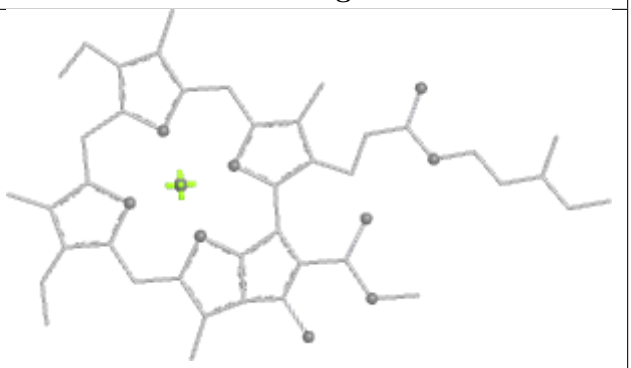
Bond angles

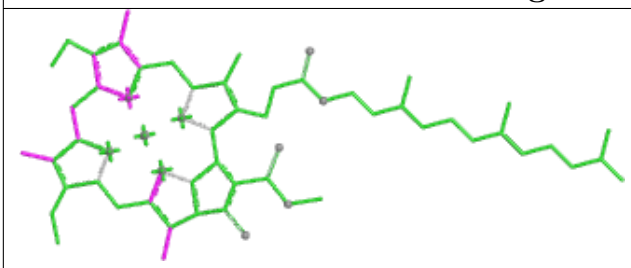
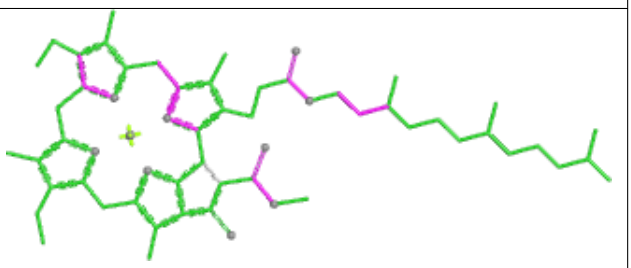
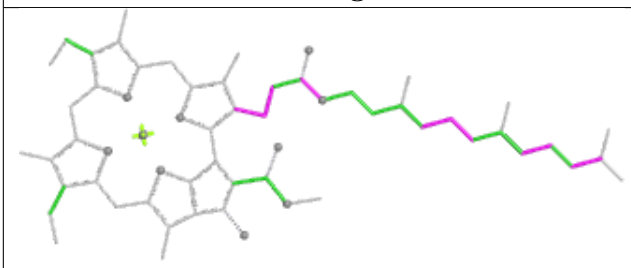
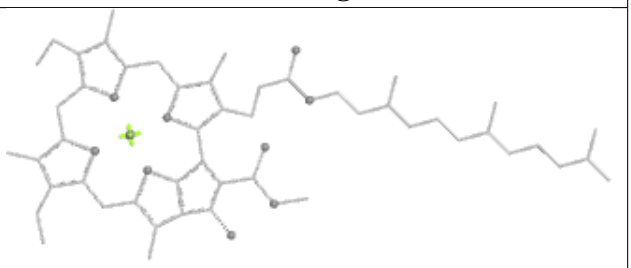


Torsions

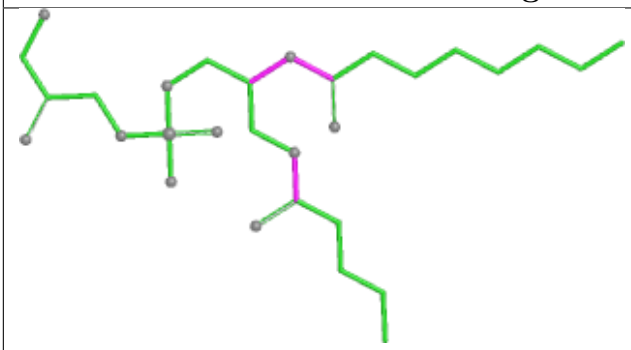


Rings

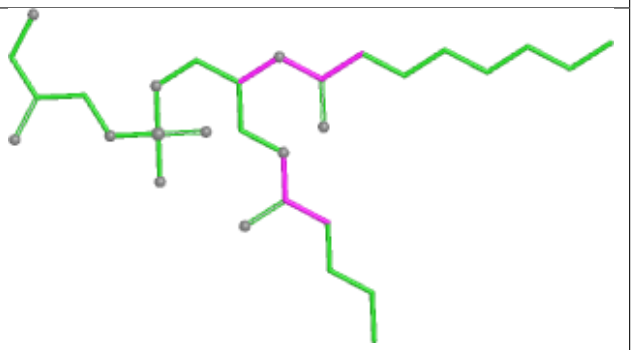
Ligand CLA f 811	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA o 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

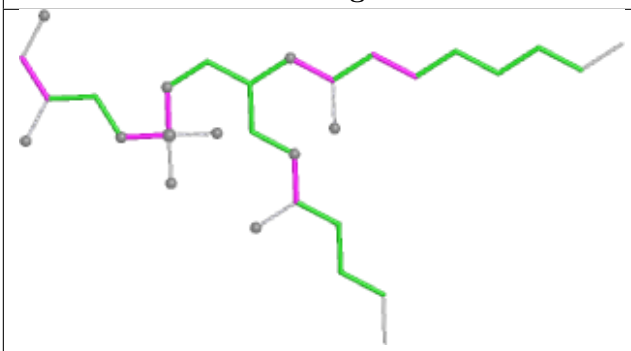
Ligand LHG A 844



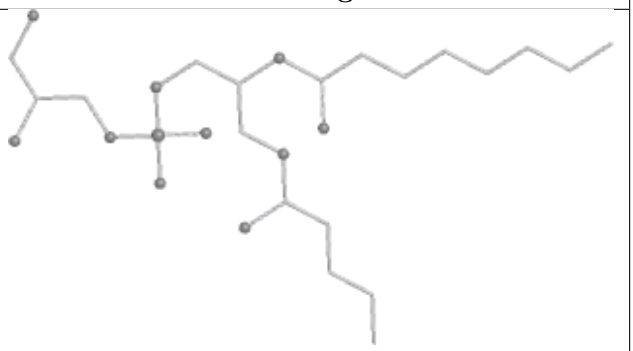
Bond lengths



Bond angles

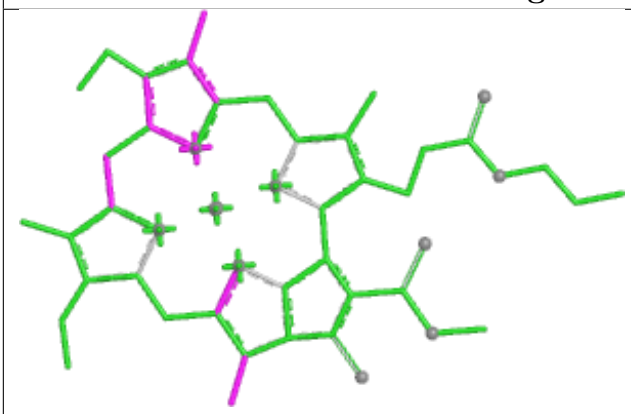


Torsions

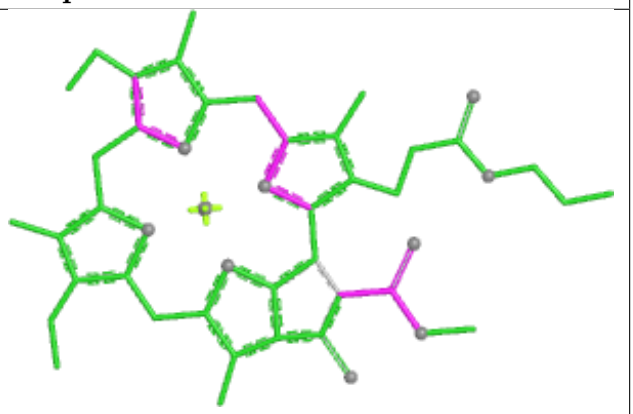


Rings

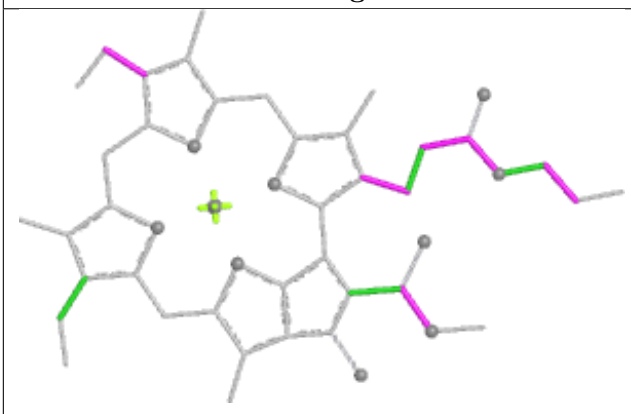
Ligand CLA q 311



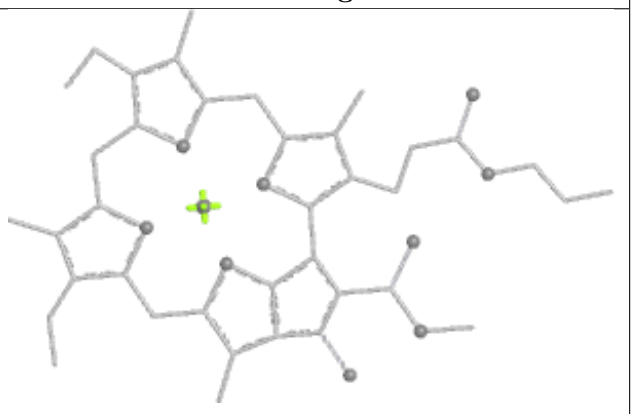
Bond lengths



Bond angles

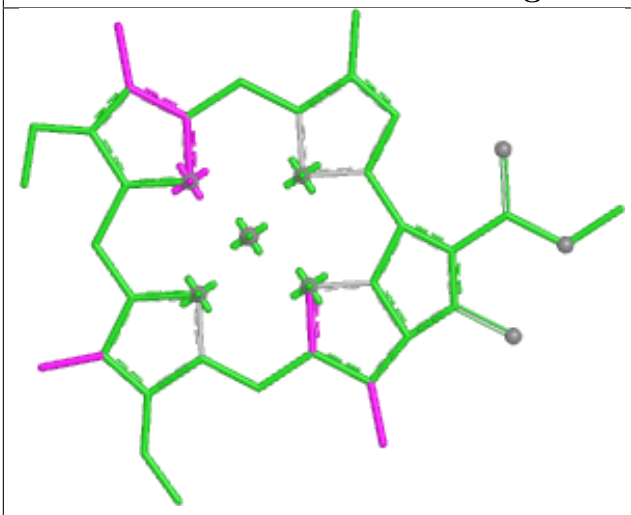


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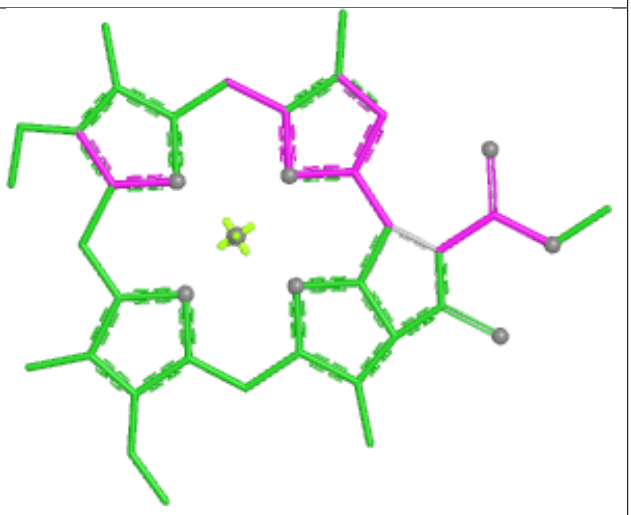


Rings

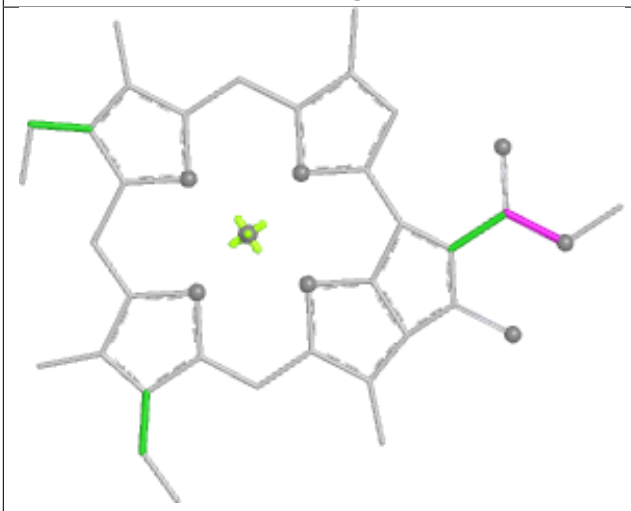
Ligand CLA A 811



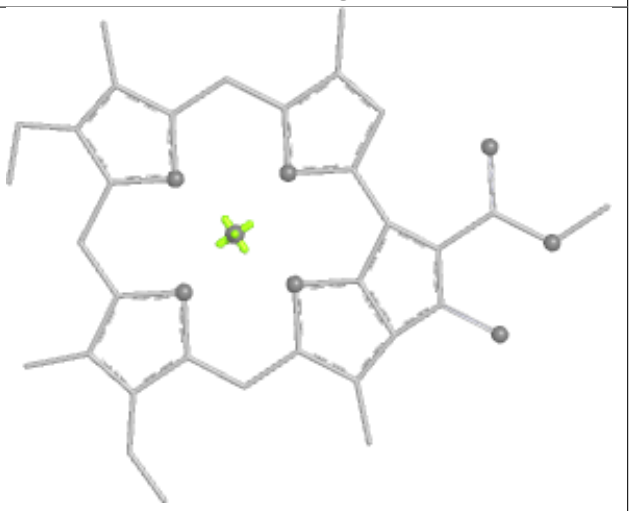
Bond lengths



Bond angles

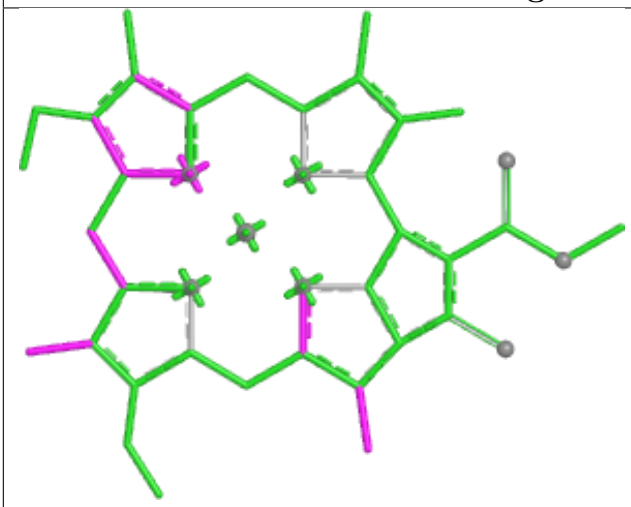


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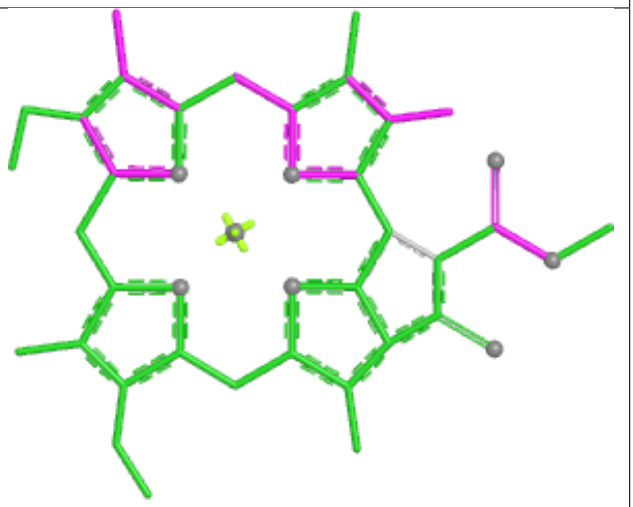


Rings

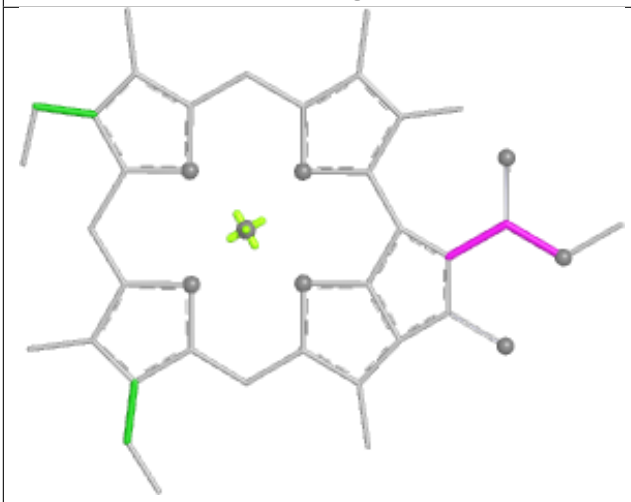
Ligand CLA n 203



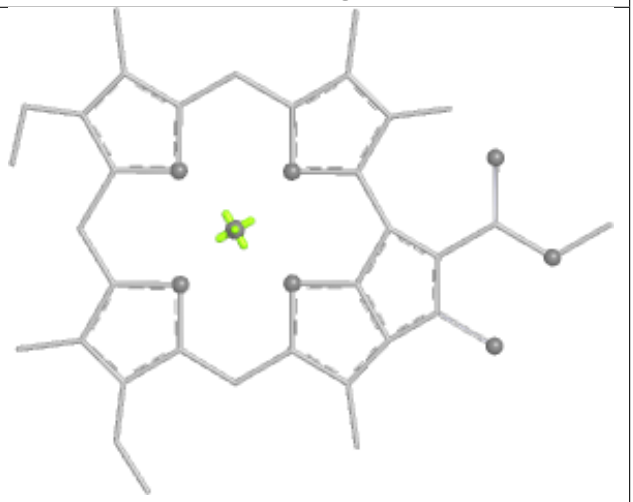
Bond lengths



Bond angles

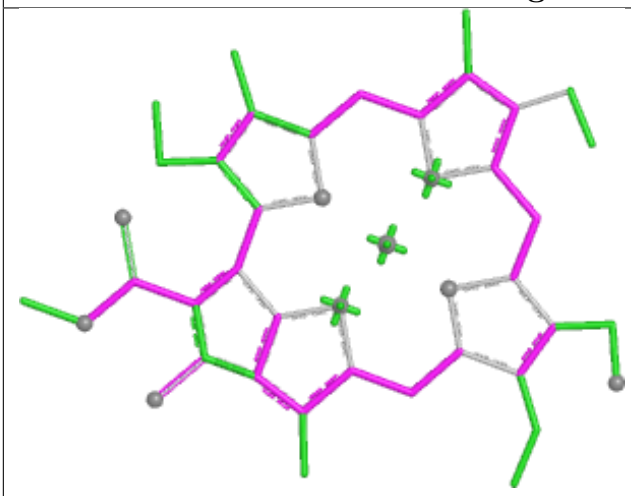


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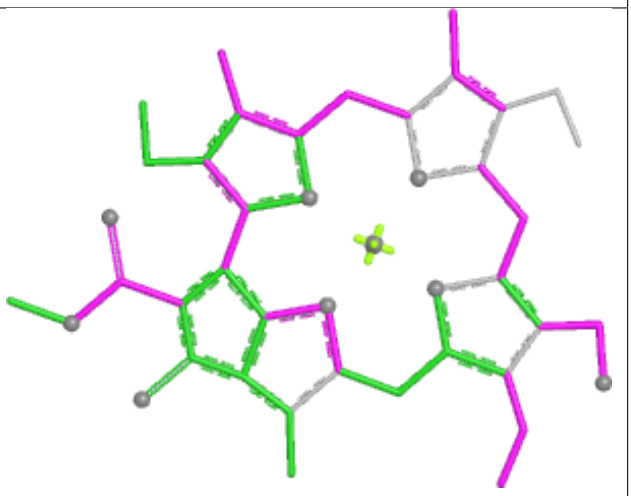


Rings

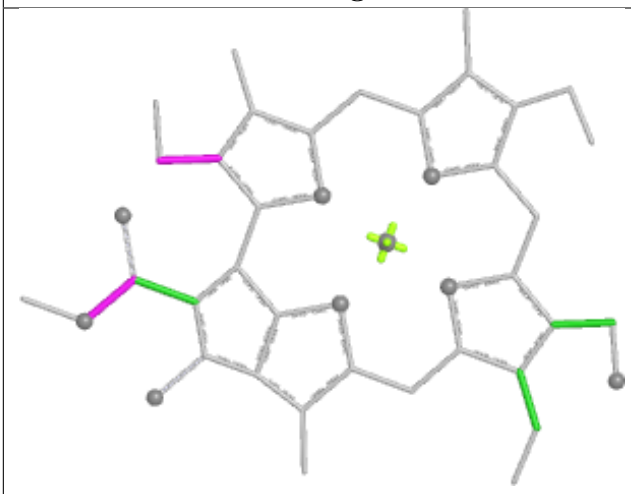
Ligand CHL 3 315



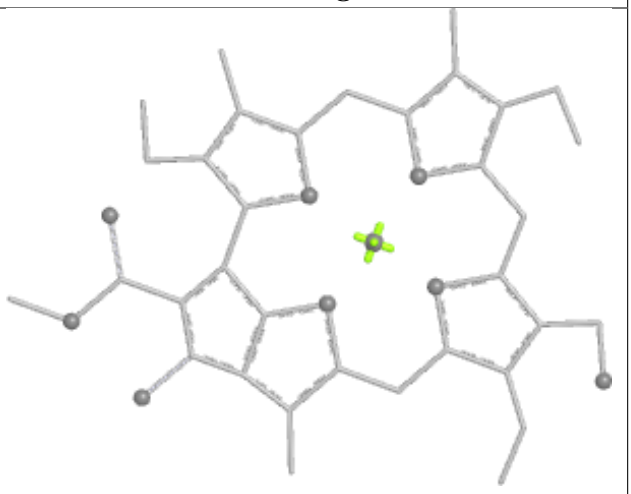
Bond lengths



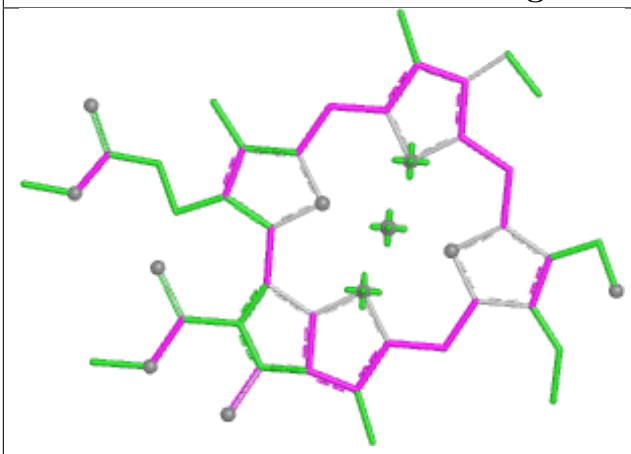
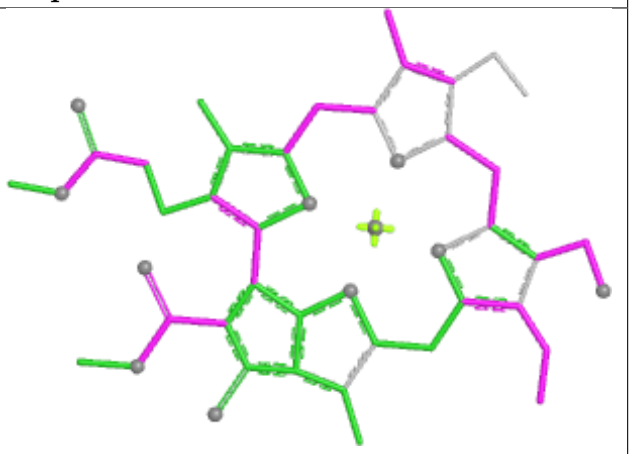
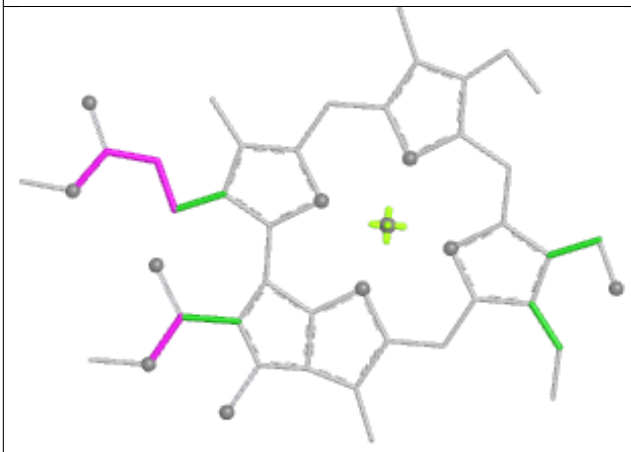
Bond angles

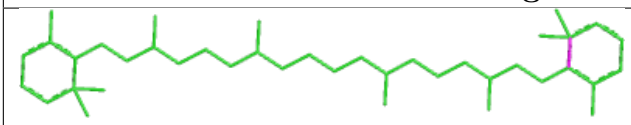
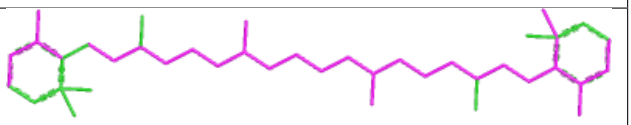
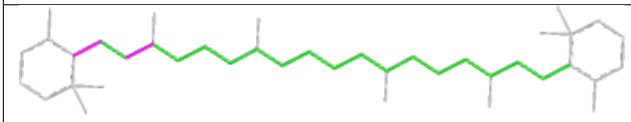
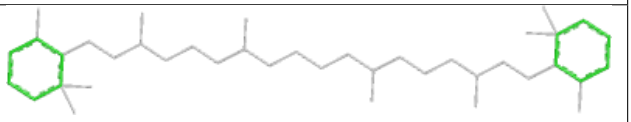


Torsions

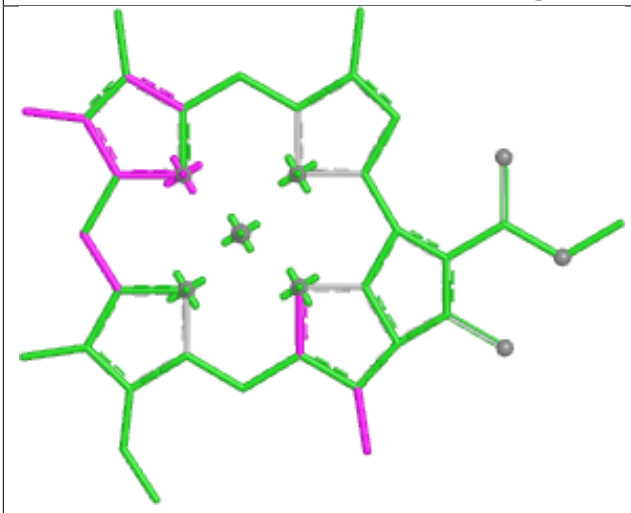


Rings

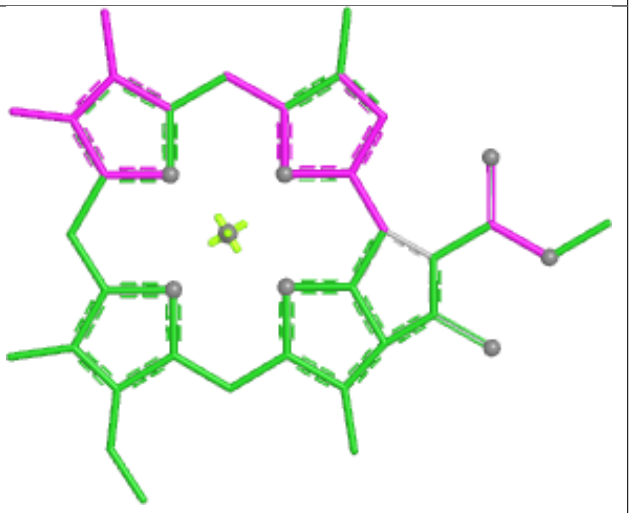
Ligand CHL p 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR B 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

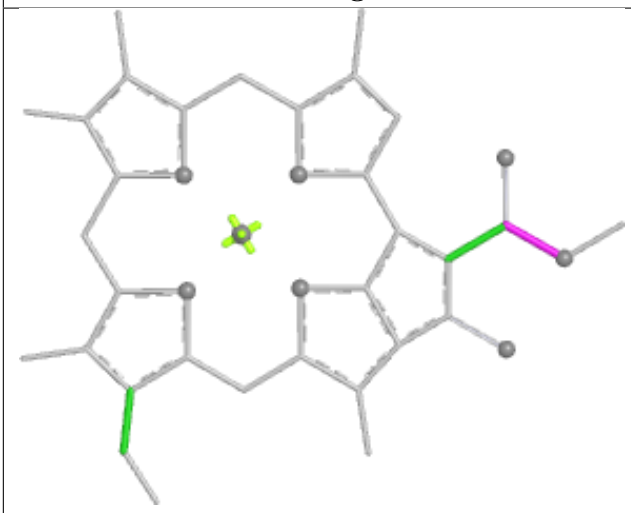
Ligand CLA r 304



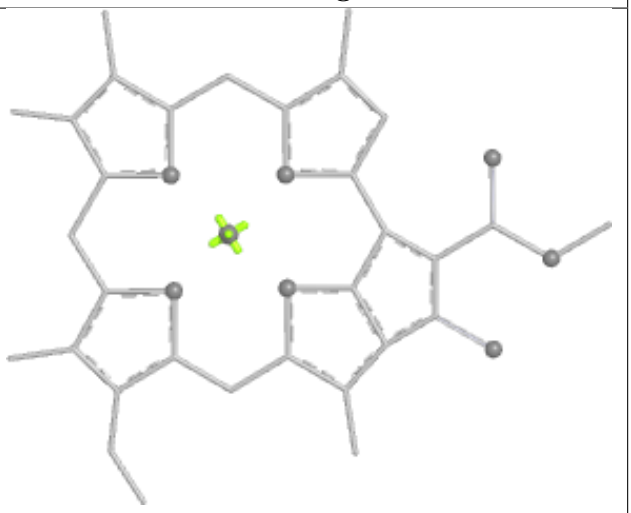
Bond lengths



Bond angles

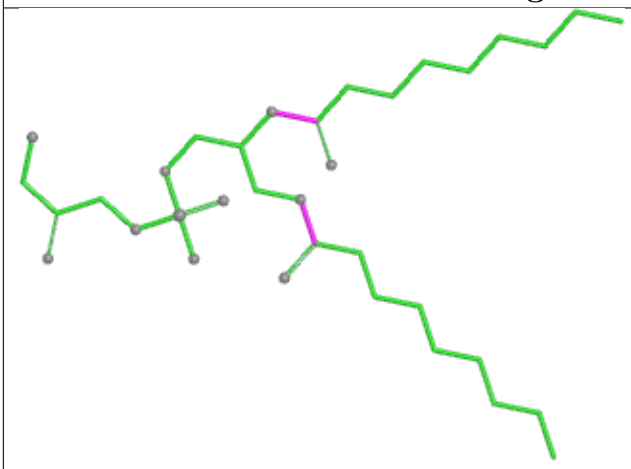


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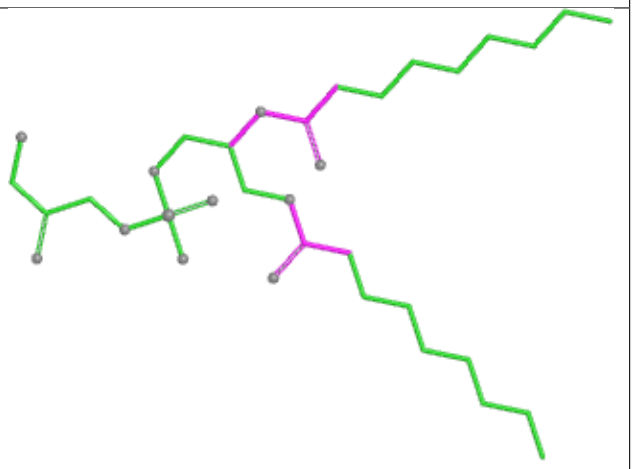


Rings

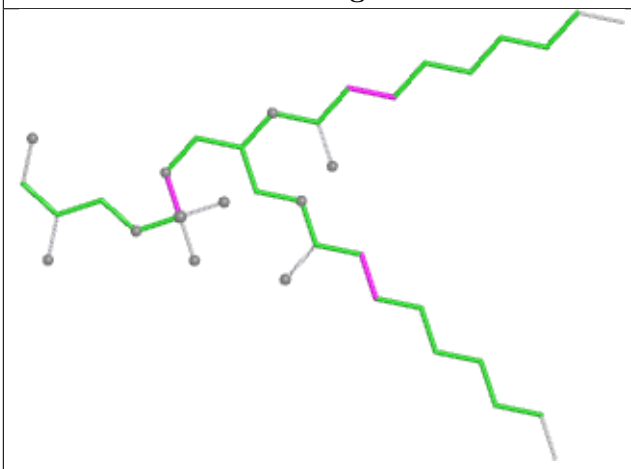
Ligand LHG 2 517



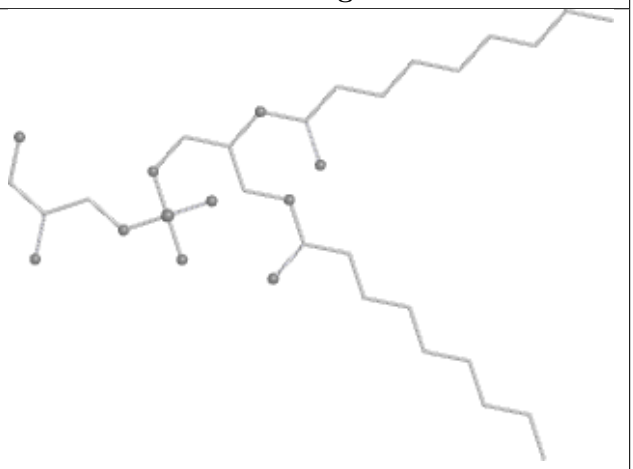
Bond lengths



Bond angles

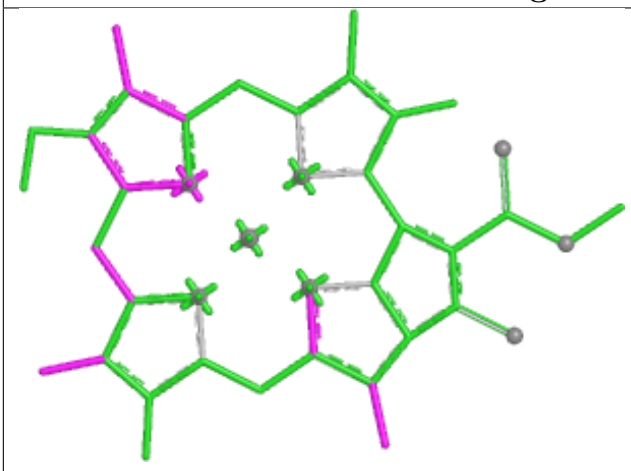


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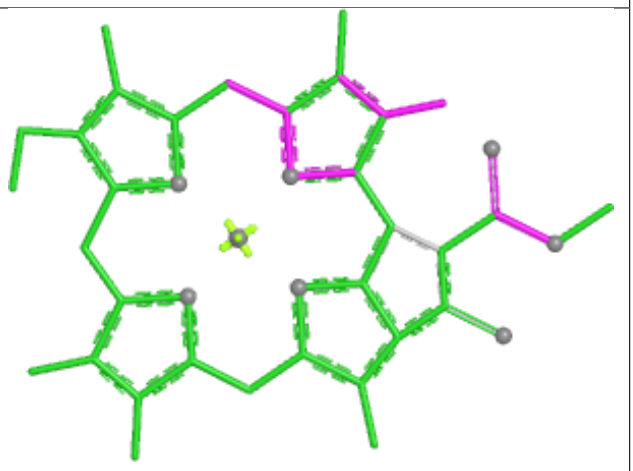


Rings

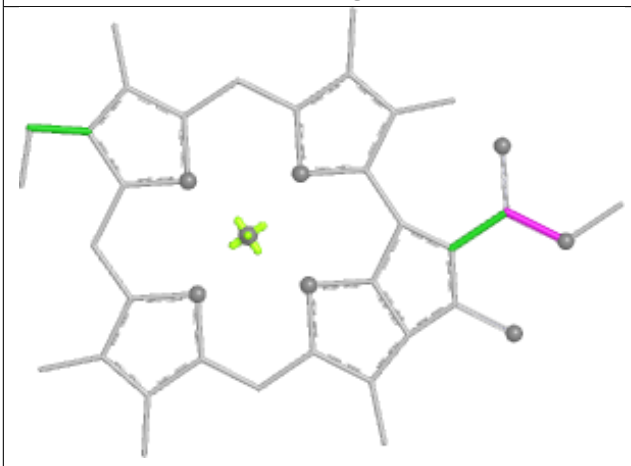
Ligand CLA s 508



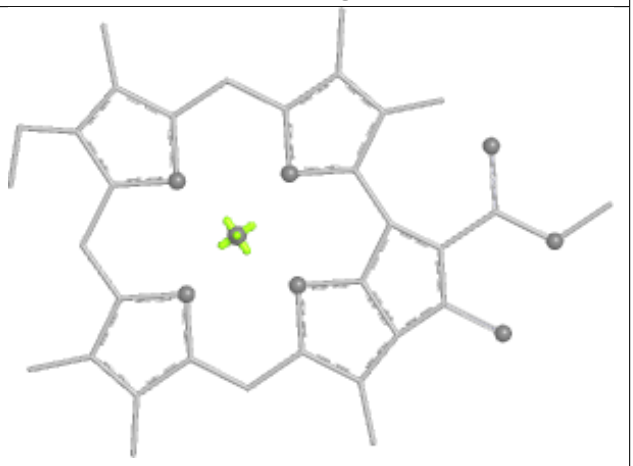
Bond lengths



Bond angles



Torsions

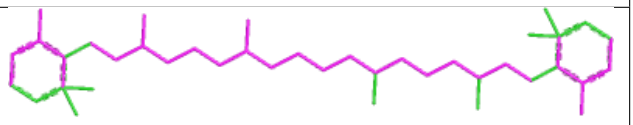


Rings

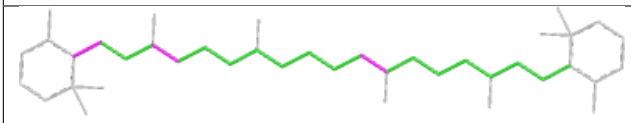
Ligand BCR e 850



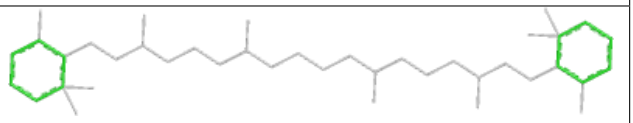
Bond lengths



Bond angles

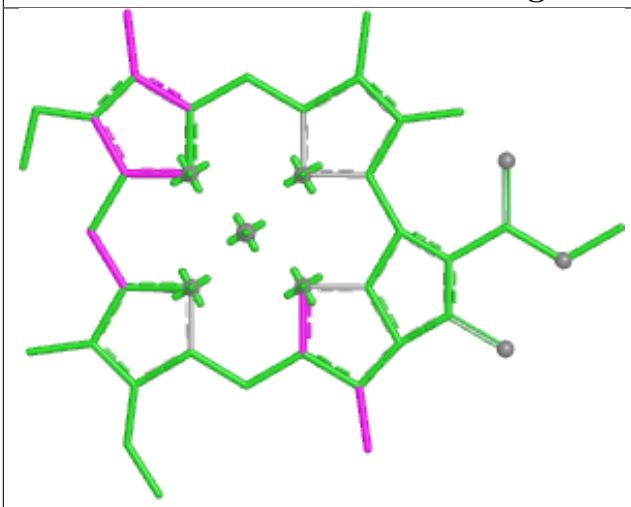


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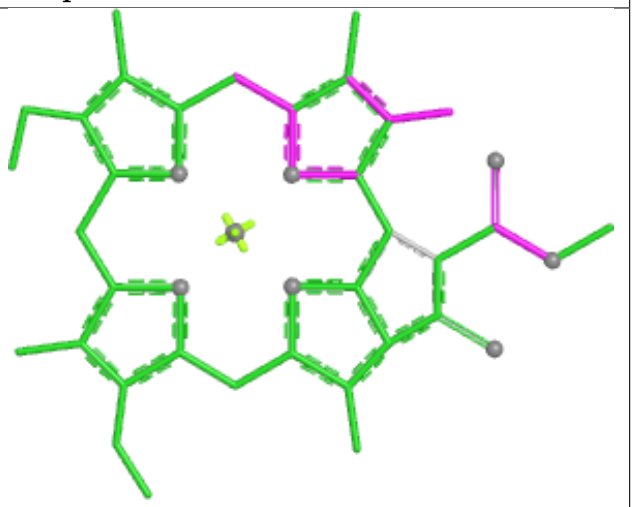


Rings

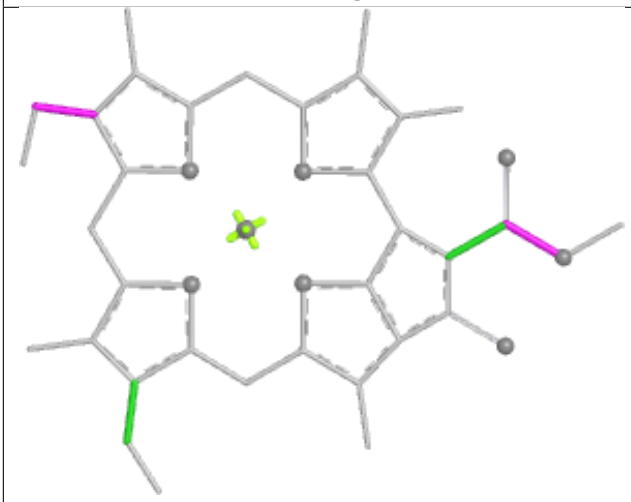
Ligand CLA q 310



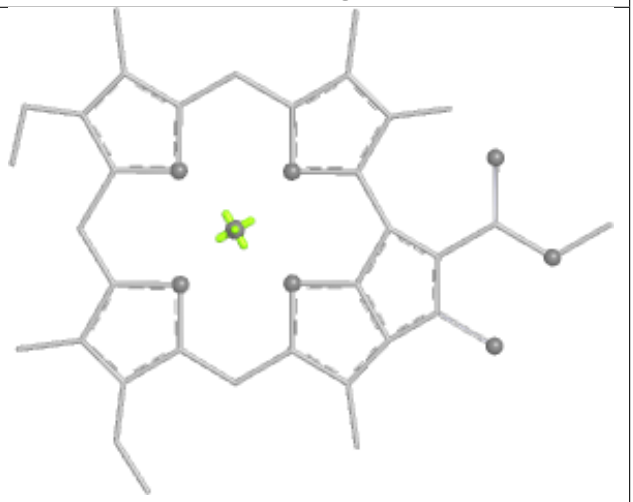
Bond lengths



Bond angles

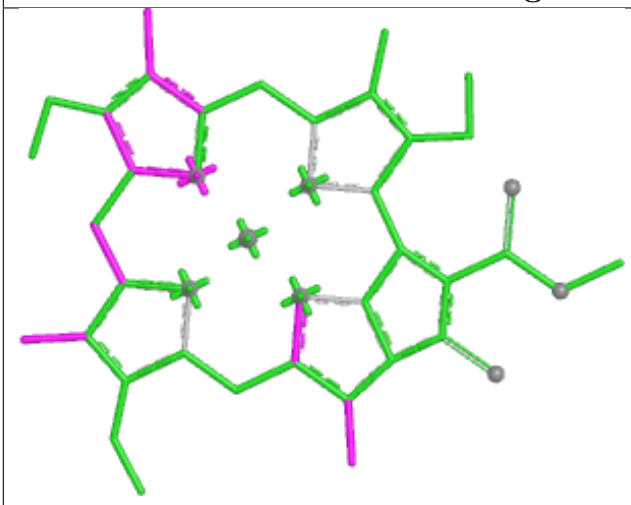


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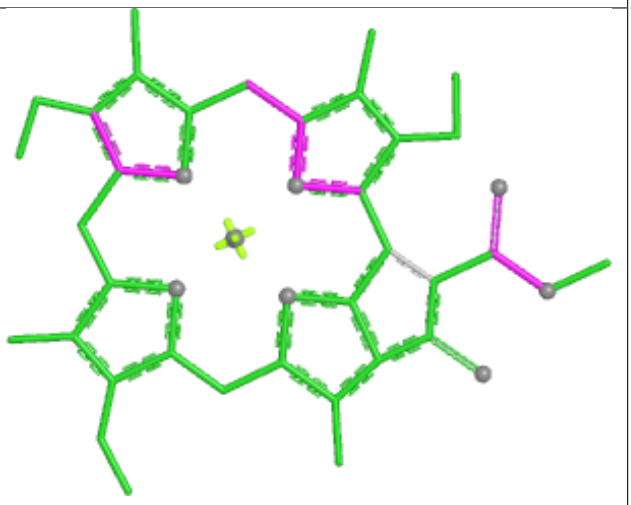


Rings

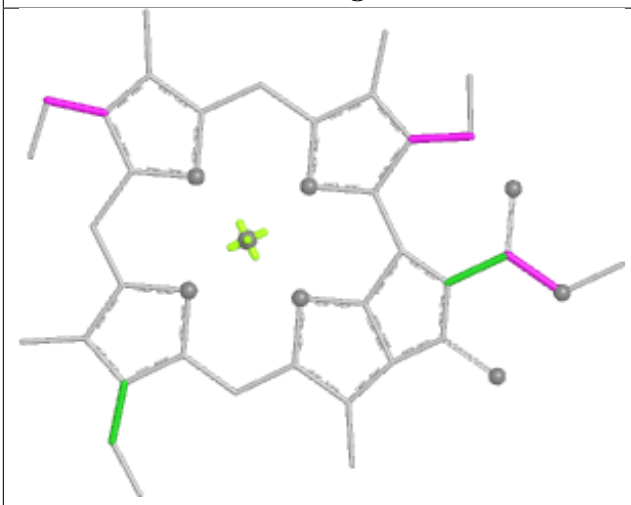
Ligand CLA B 836



Bond lengths



Bond angles

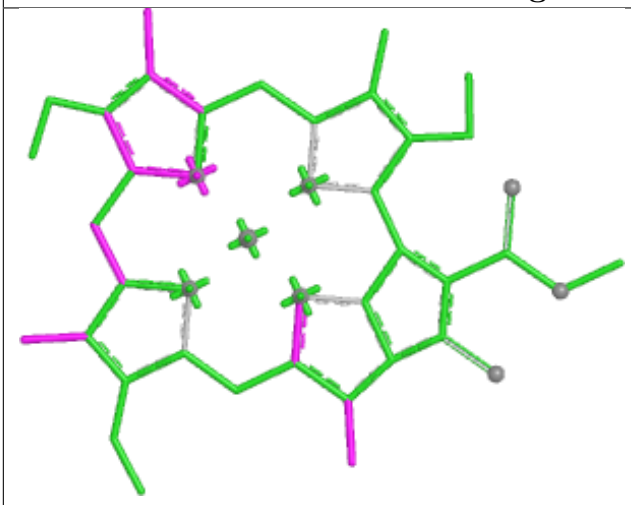


Torsions

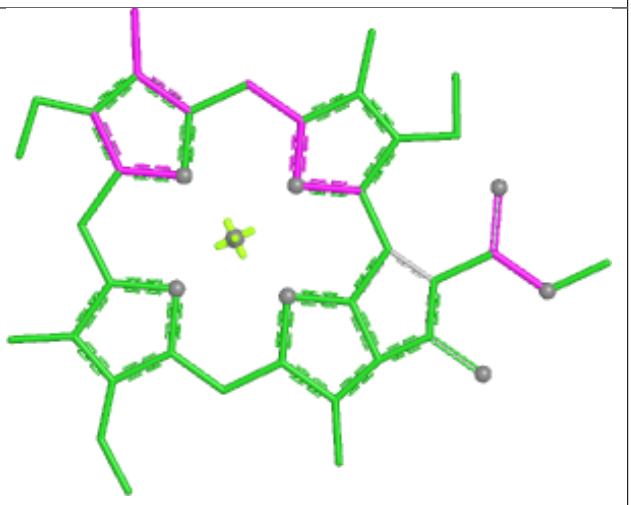


Rings

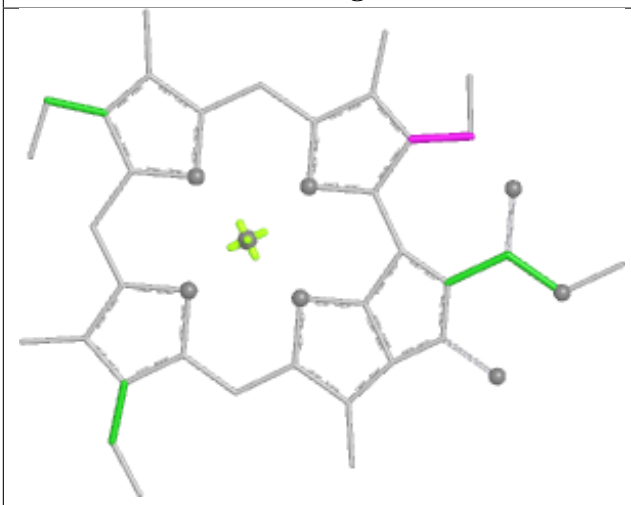
Ligand CLA e 813



Bond lengths



Bond angles

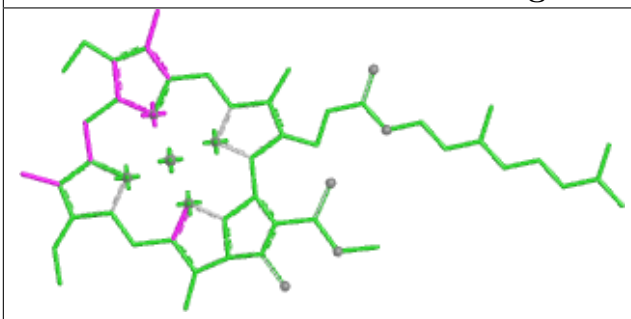


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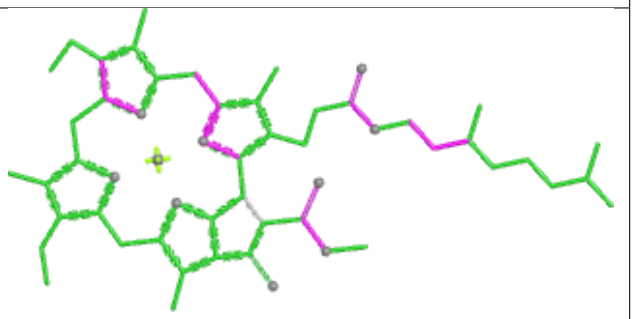


Rings

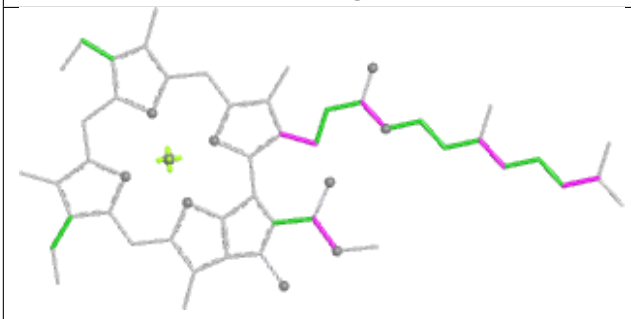
Ligand CLA 1 506



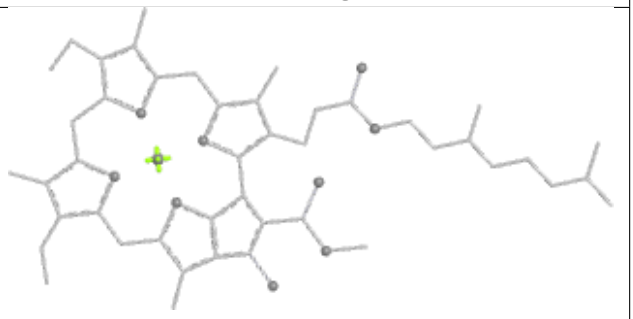
Bond lengths



Bond angles

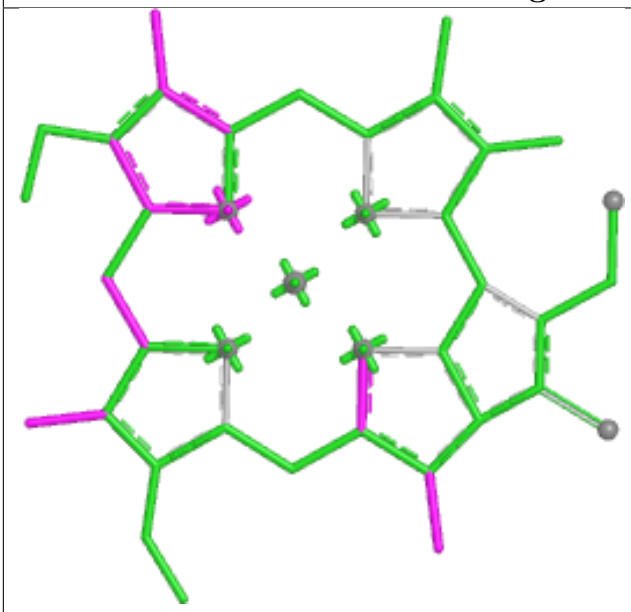


Torsions

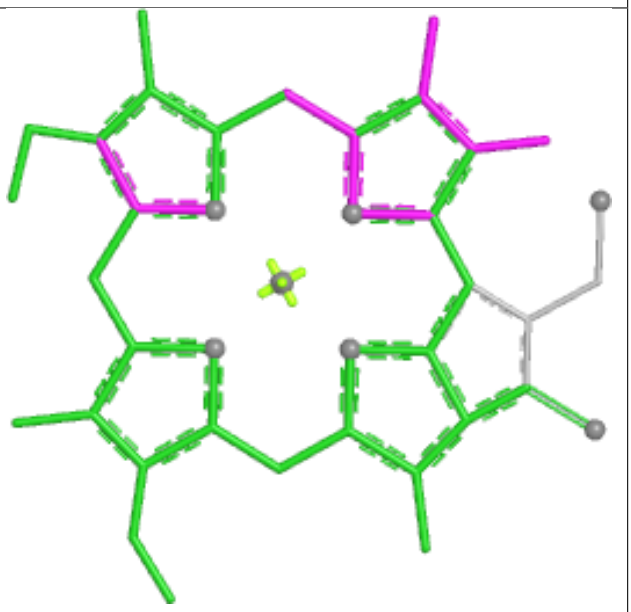


Rings

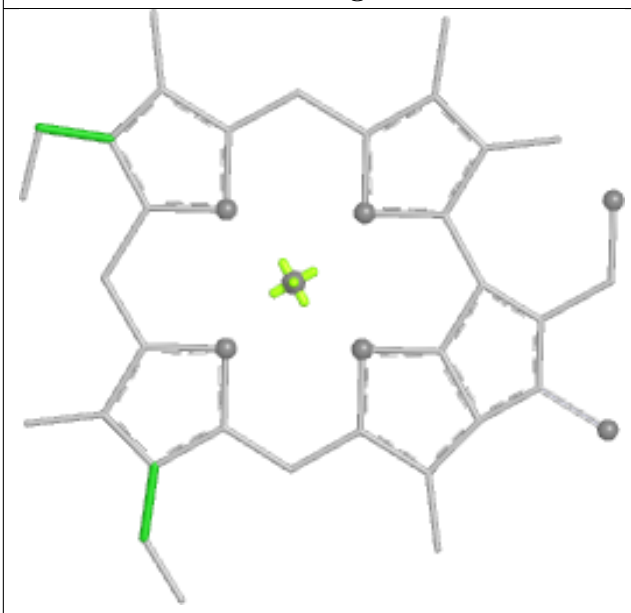
Ligand CLA e 817



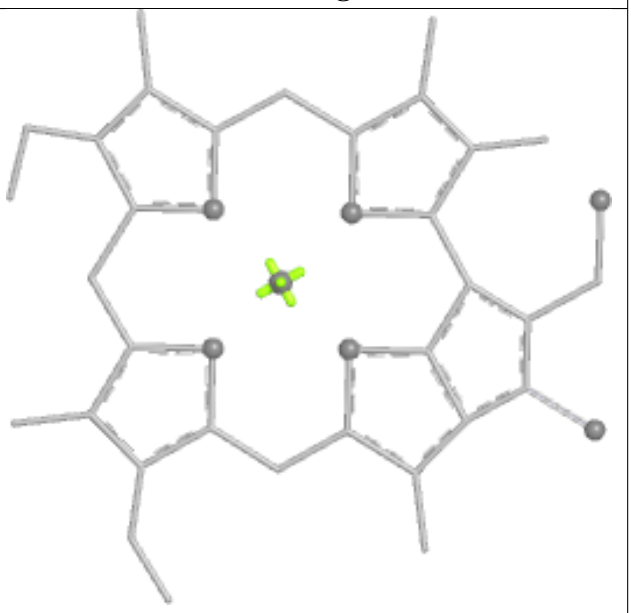
Bond lengths



Bond angles

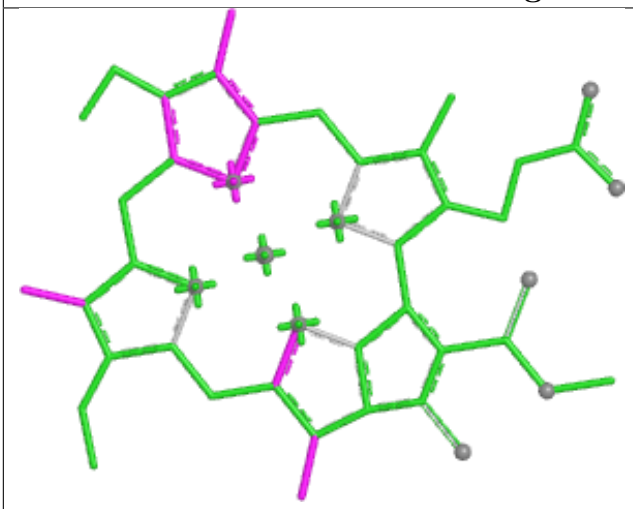


Torsions

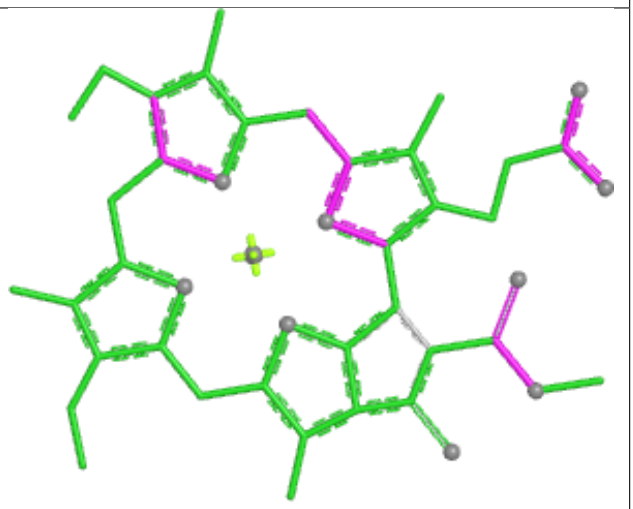


Rings

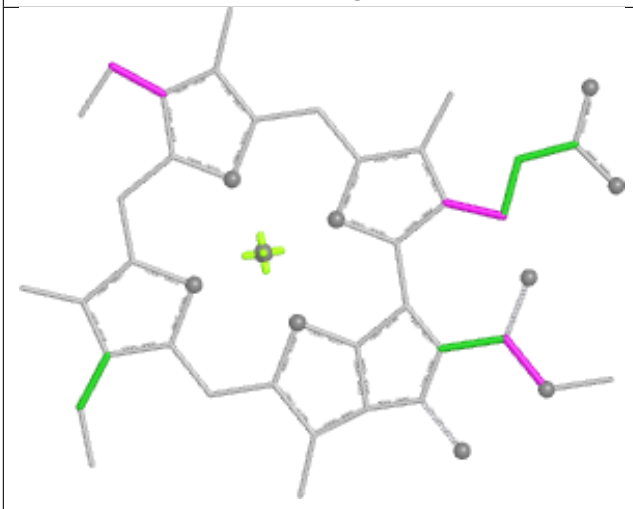
Ligand CLA B 824



Bond lengths



Bond angles

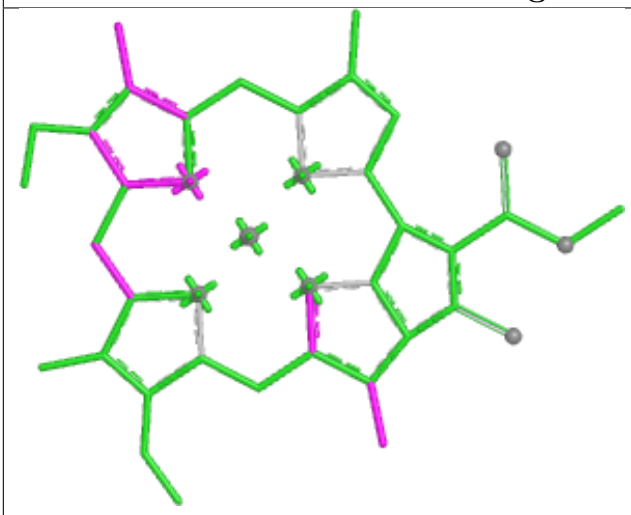


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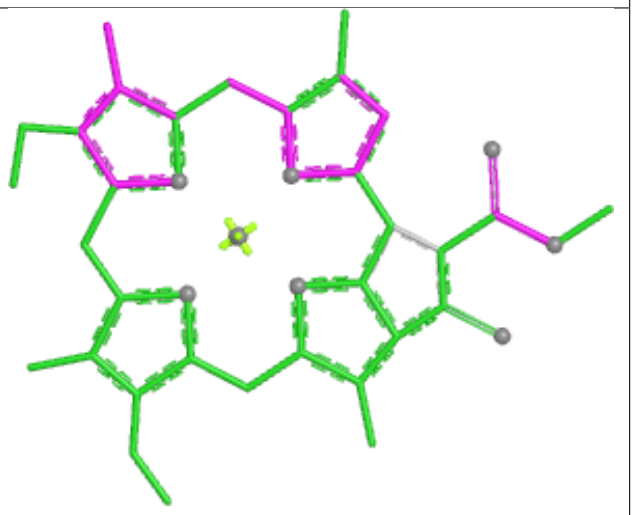


Rings

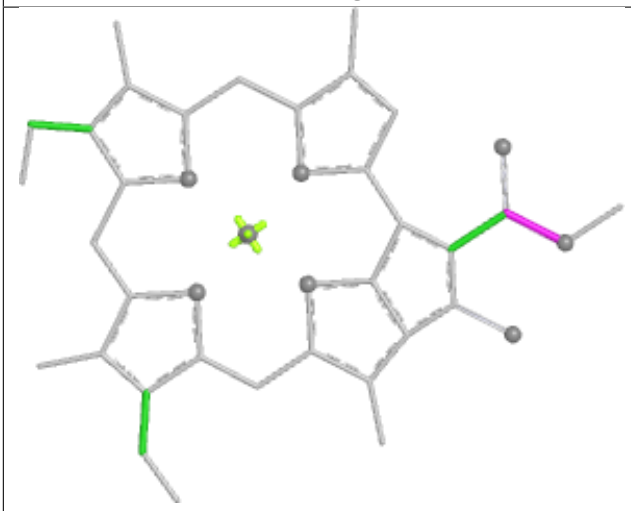
Ligand CLA 1 508



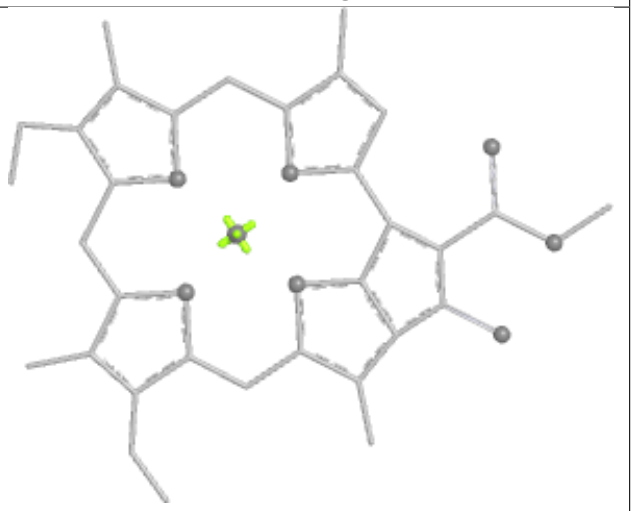
Bond lengths



Bond angles

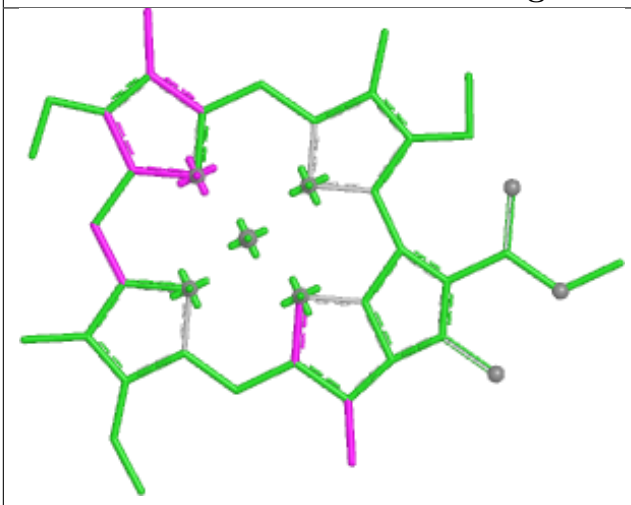


Torsions

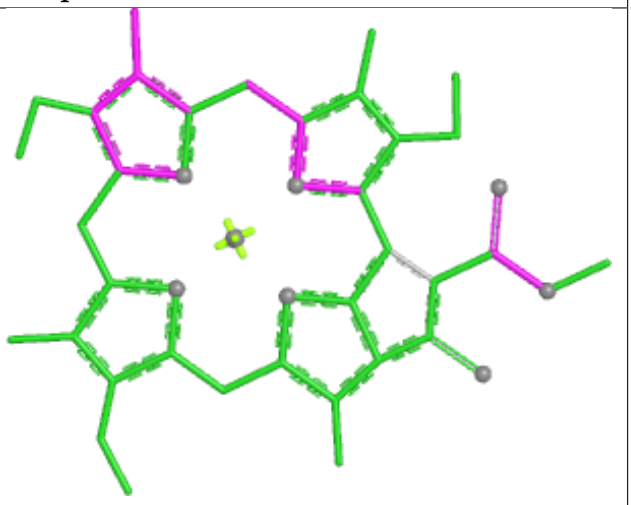


Rings

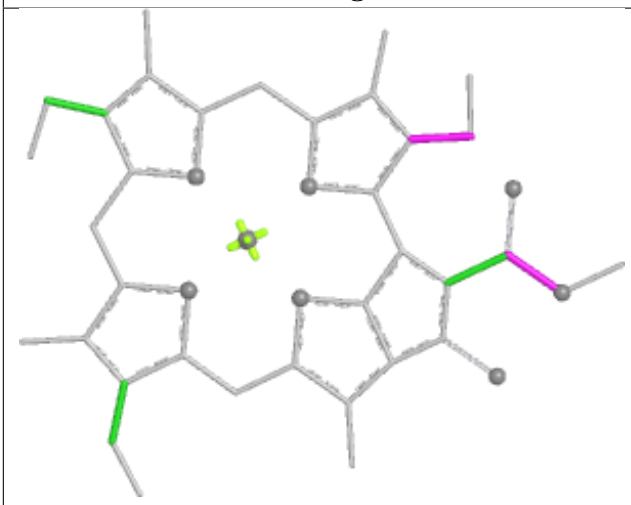
Ligand CLA q 308



Bond lengths



Bond angles



Torsions

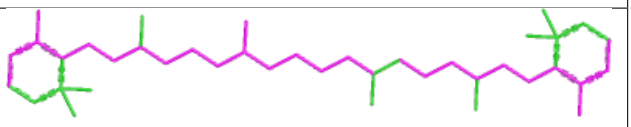


Rings

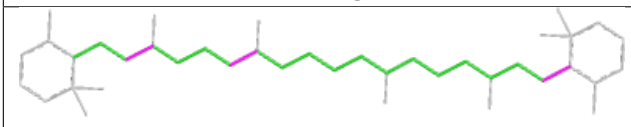
Ligand BCR e 848



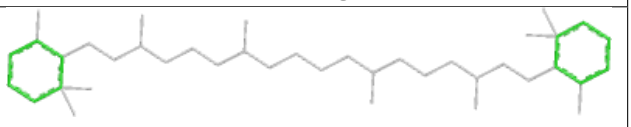
Bond lengths



Bond angles

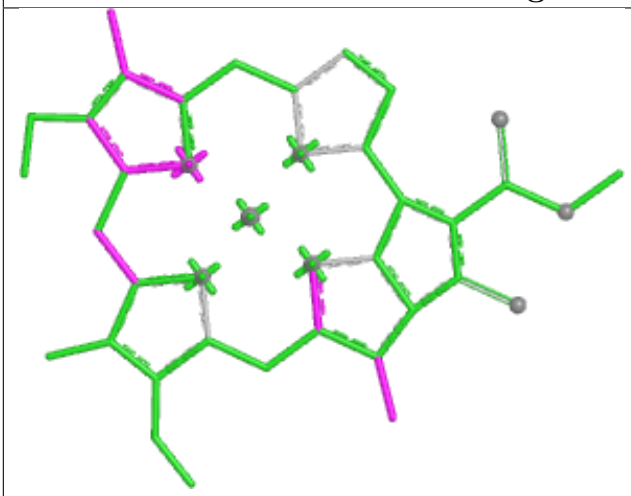


Torsions

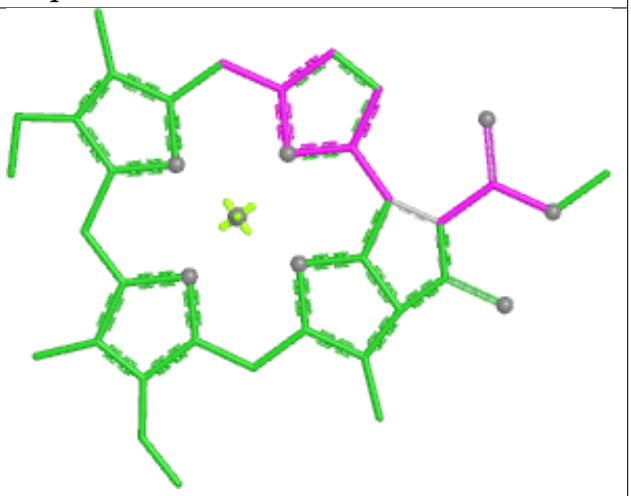


Rings

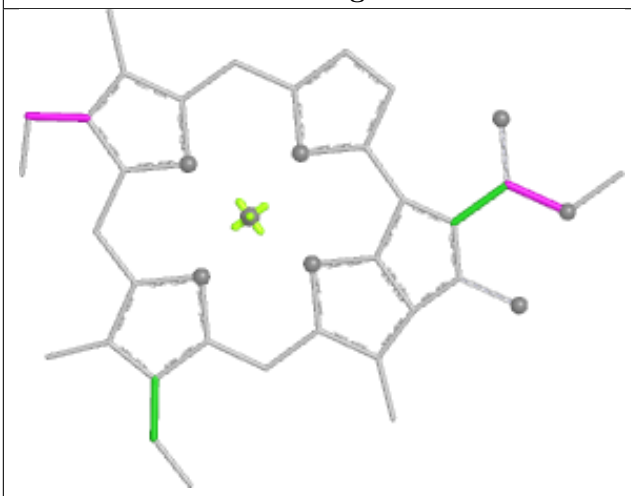
Ligand CLA p 511



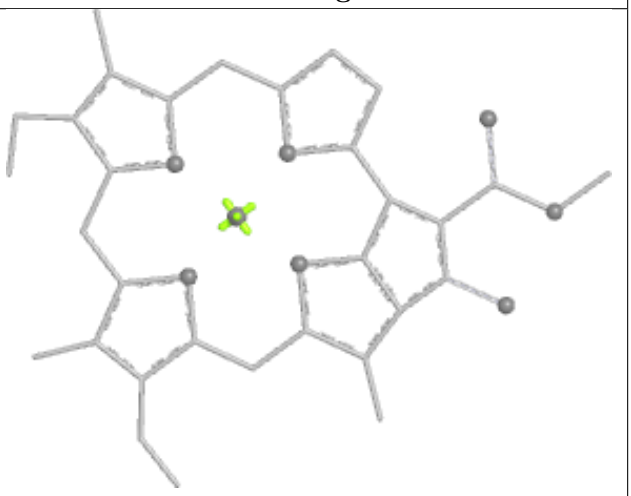
Bond lengths



Bond angles

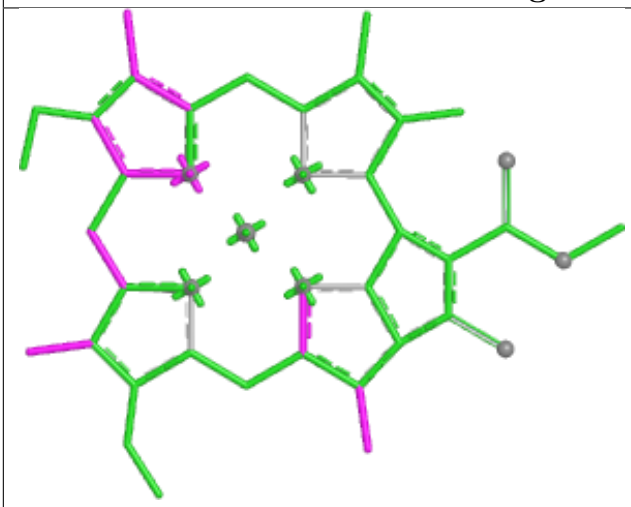


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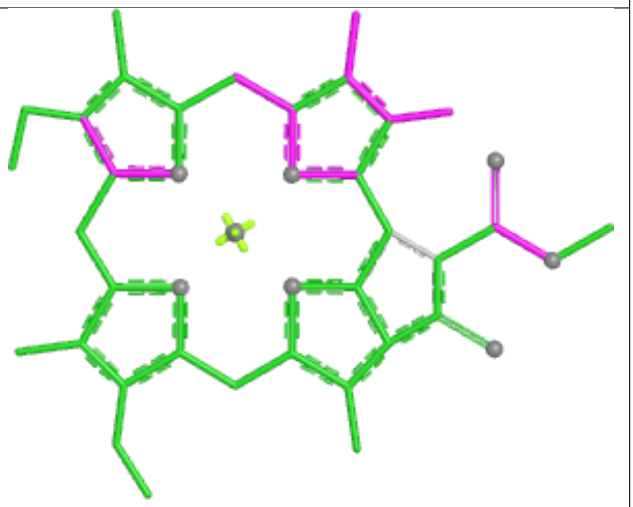


Rings

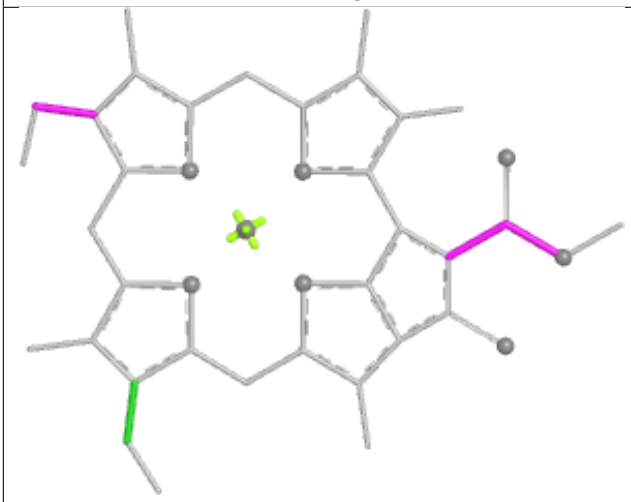
Ligand CLA e 841



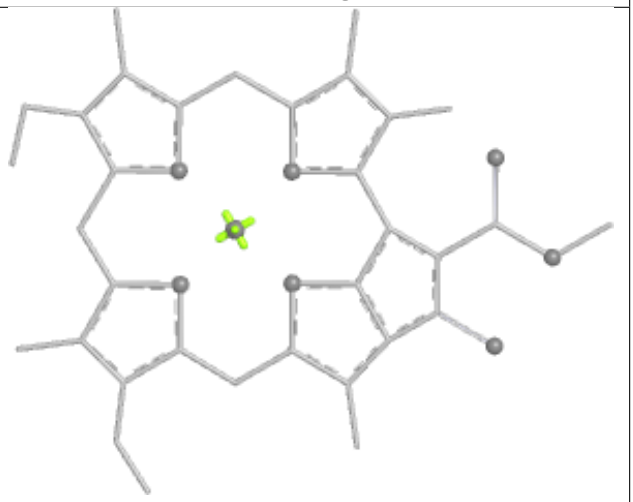
Bond lengths



Bond angles

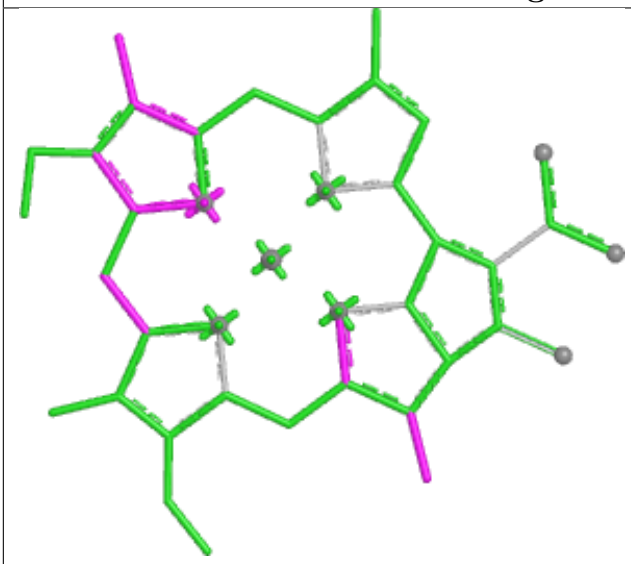


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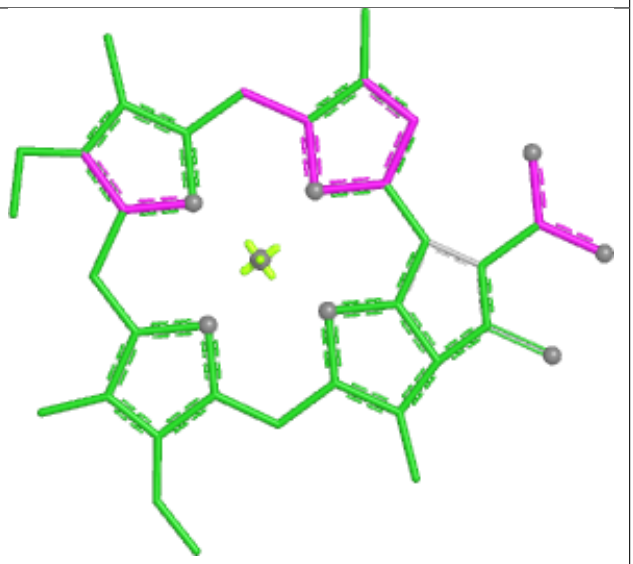


Rings

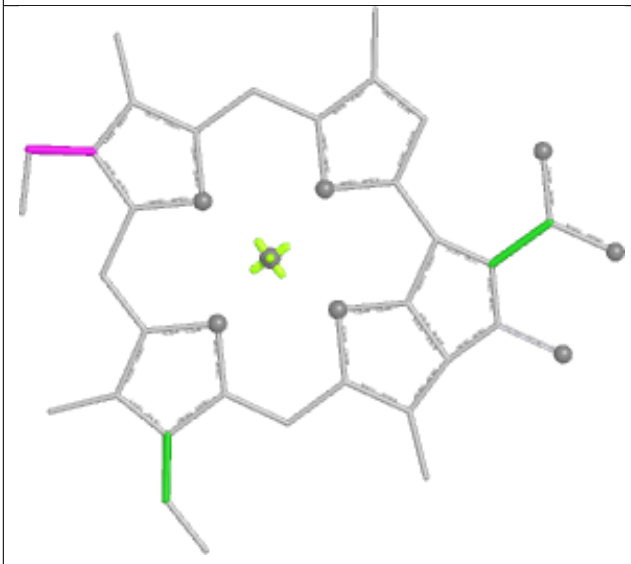
Ligand CLA n 205



Bond lengths



Bond angles

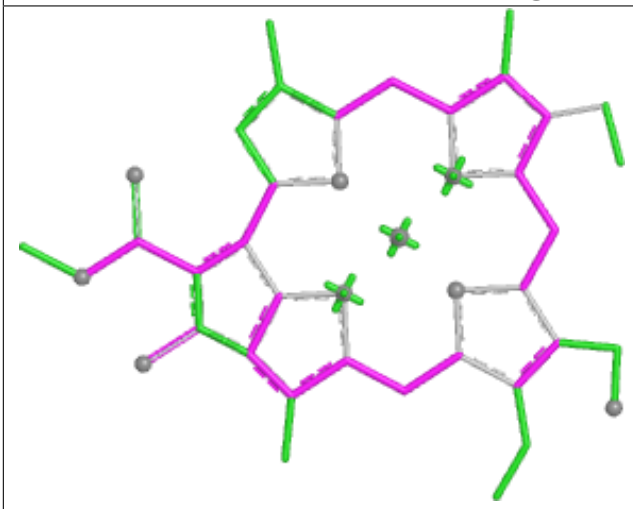


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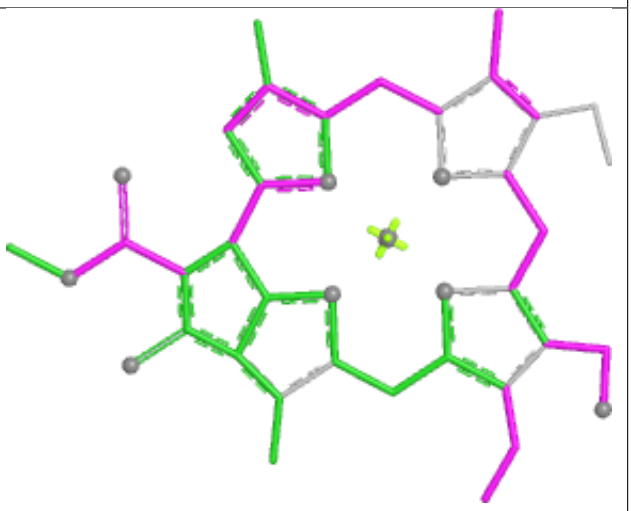


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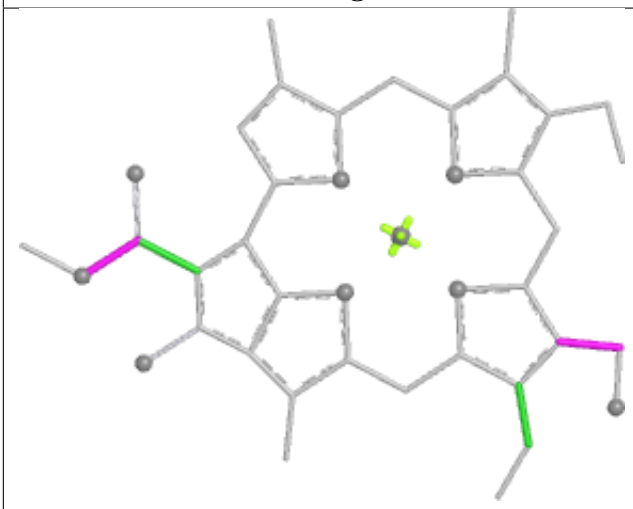
Ligand CHL 1 514



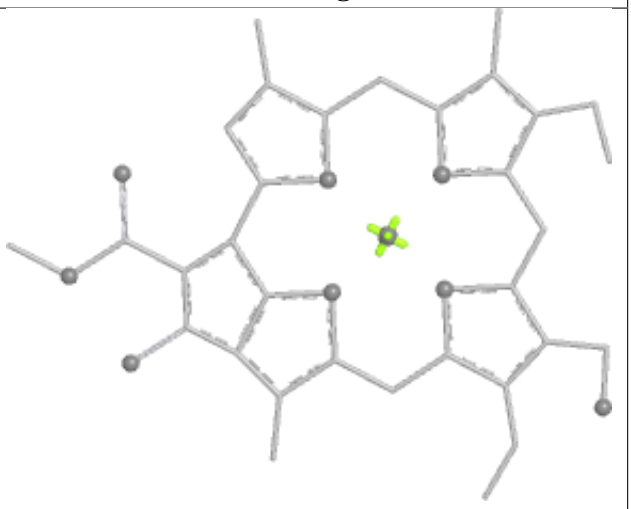
Bond lengths



Bond angles

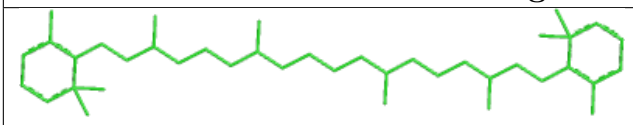


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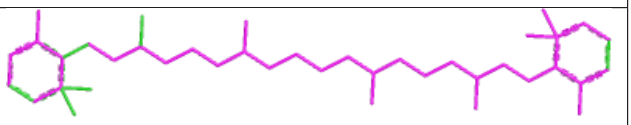


Rings

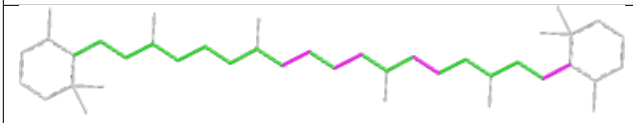
Ligand BCR s 503



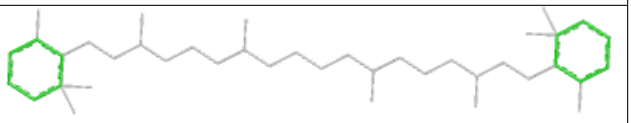
Bond lengths



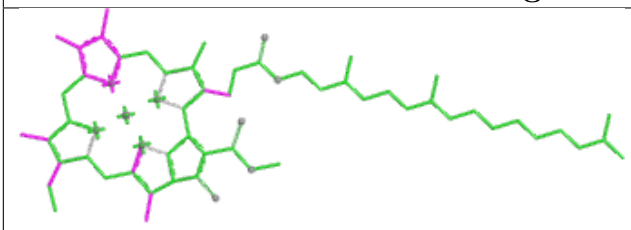
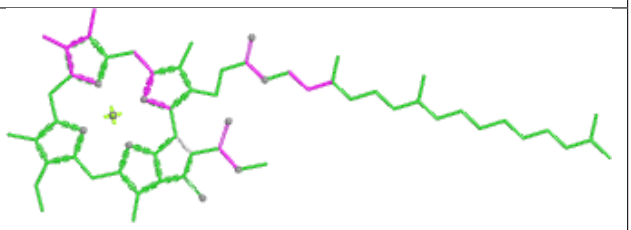
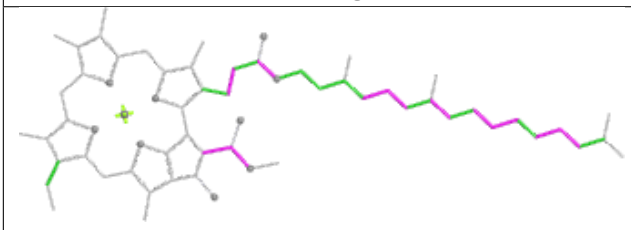
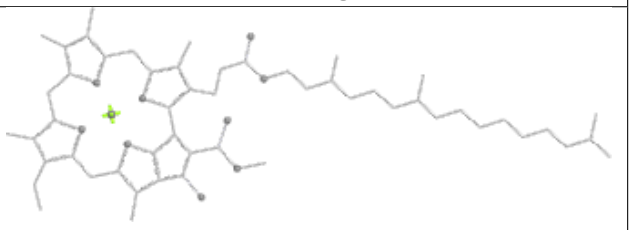
Bond angles

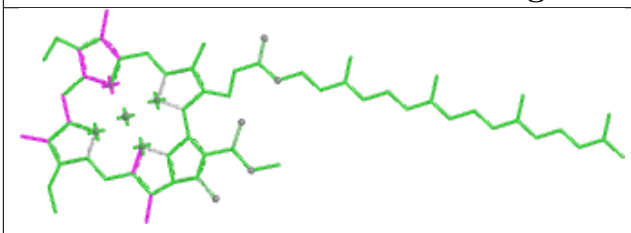
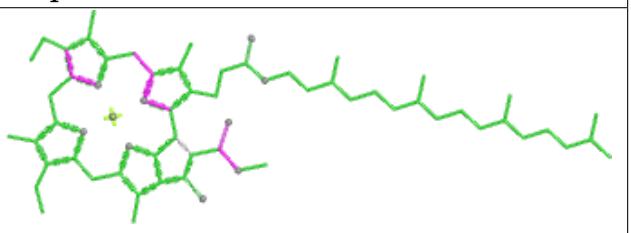
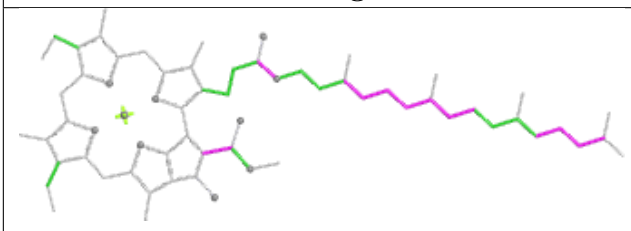
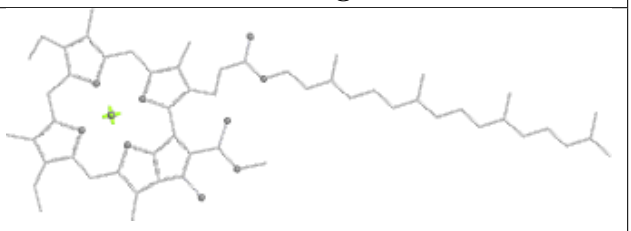


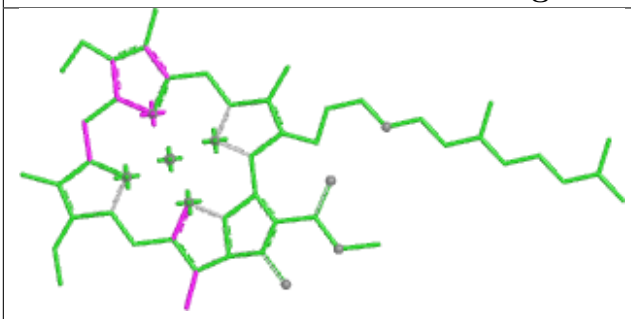
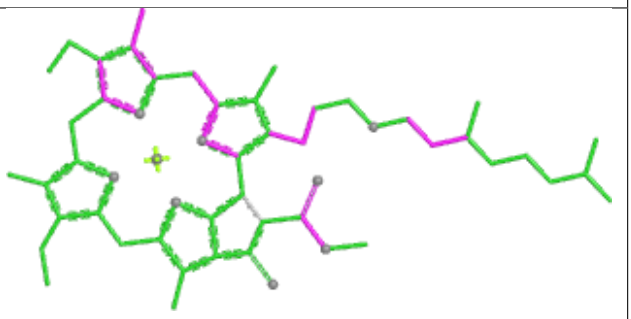
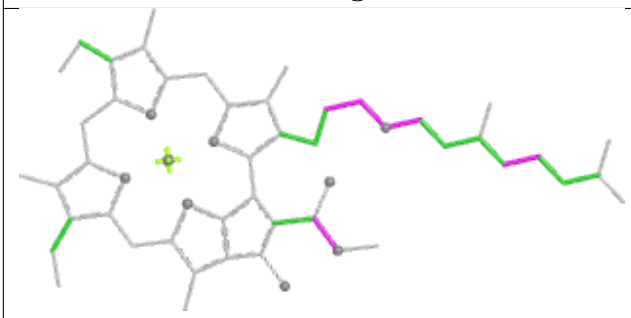
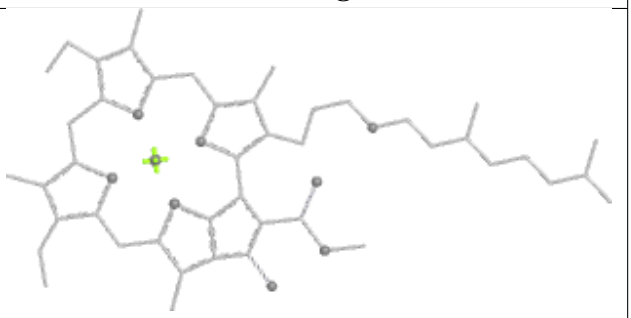
Torsions

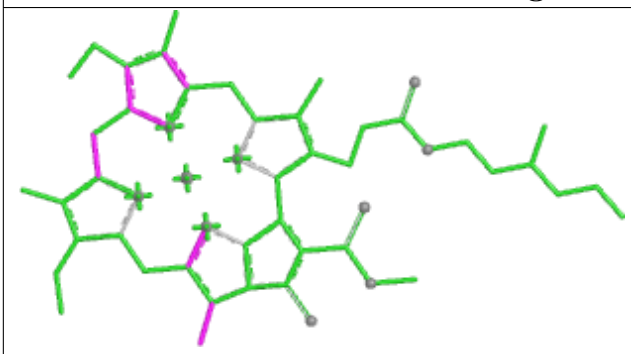
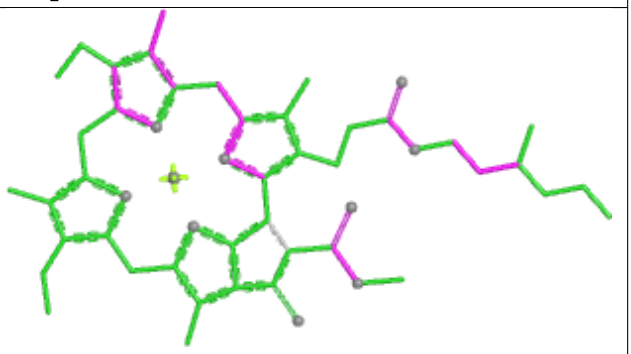
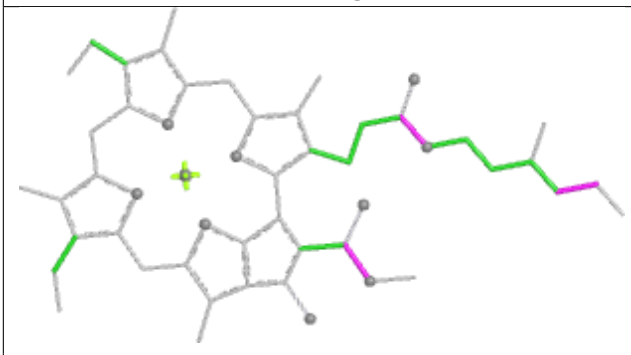
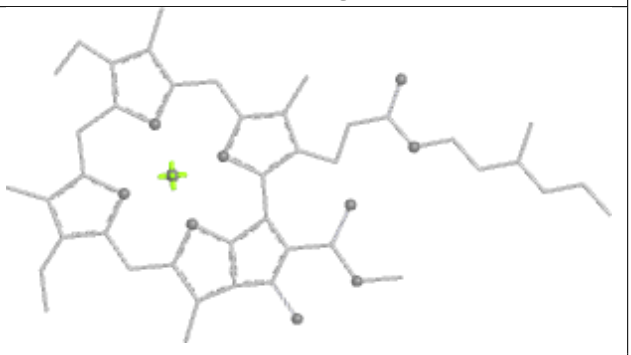


Rings

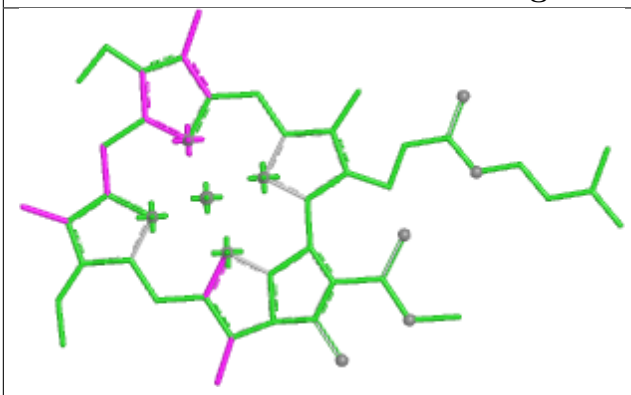
Ligand CLA A 831	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA p 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

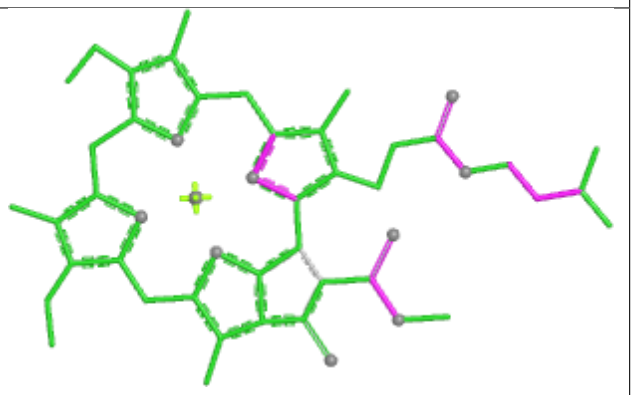
Ligand CLA f 808	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA p 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

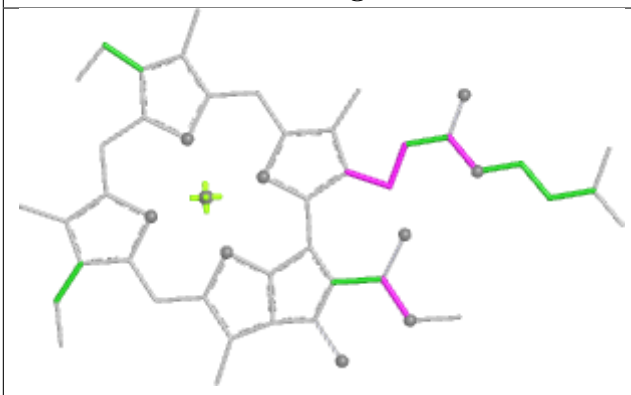
Ligand CLA r 309



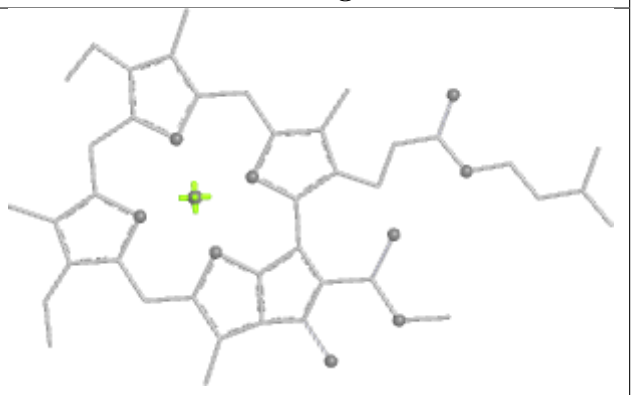
Bond lengths



Bond angles

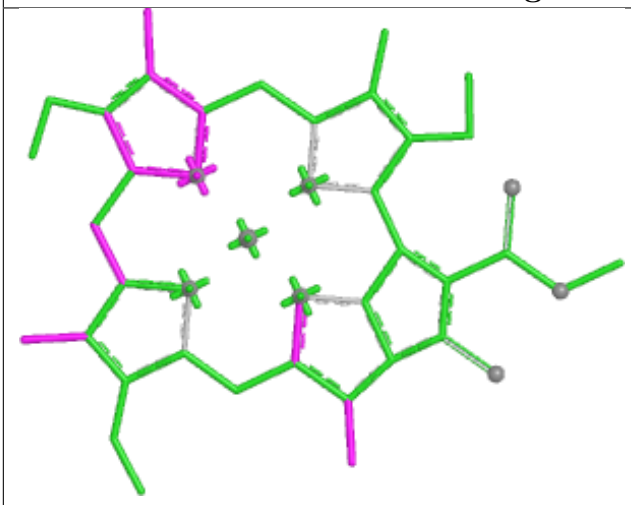


Torsions

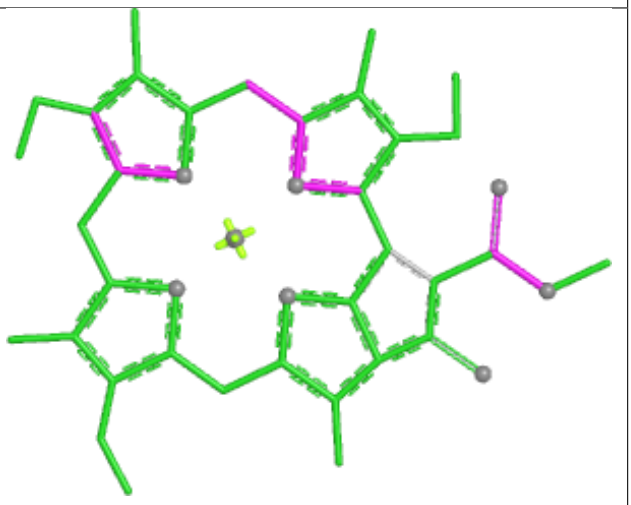


Rings

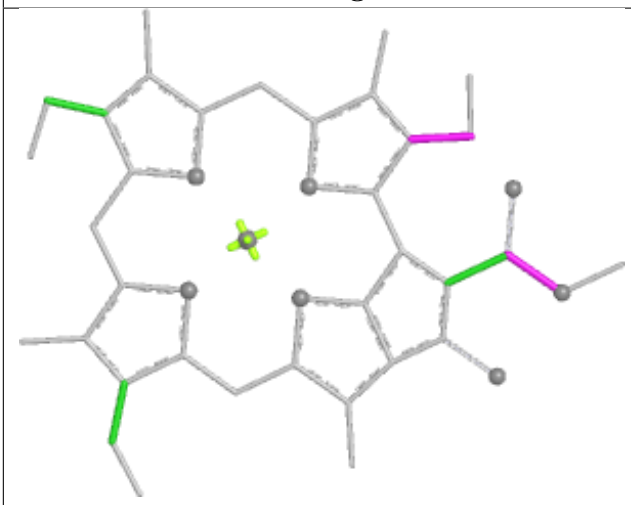
Ligand CLA B 823



Bond lengths



Bond angles

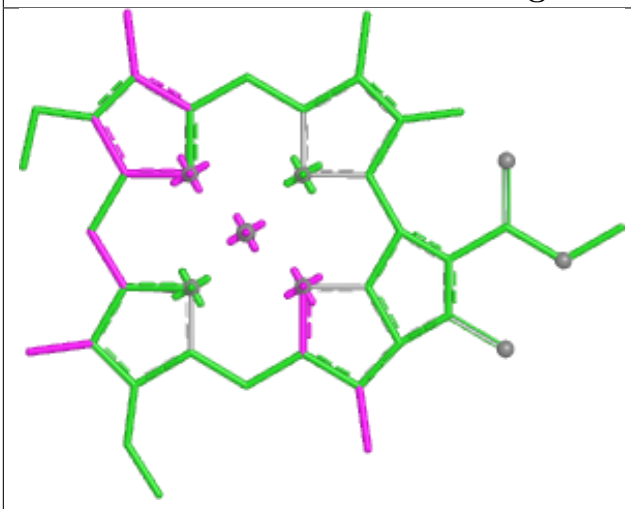


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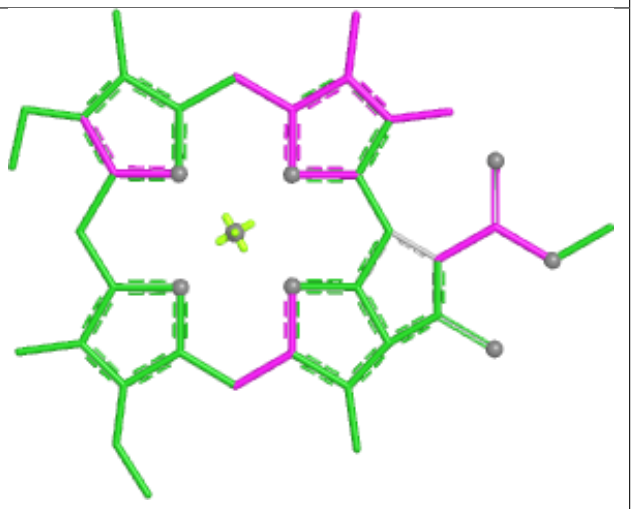


Rings

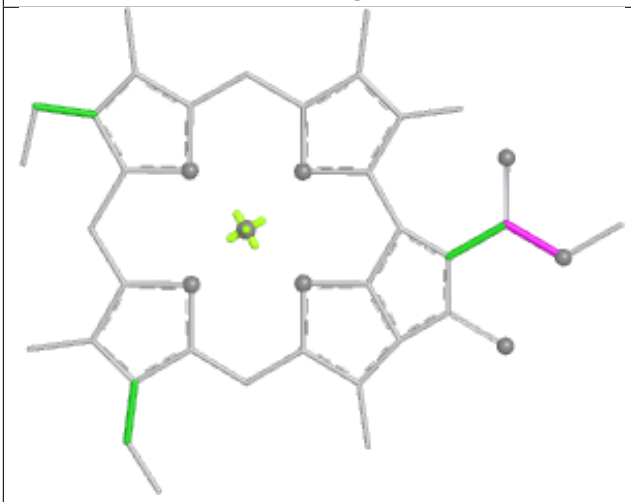
Ligand CLA 3 317



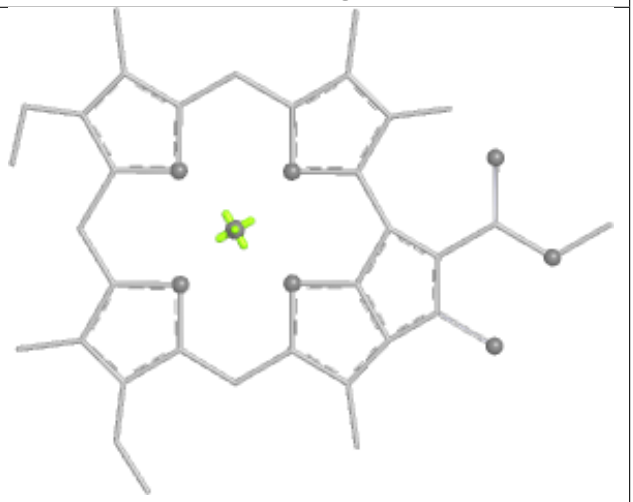
Bond lengths



Bond angles

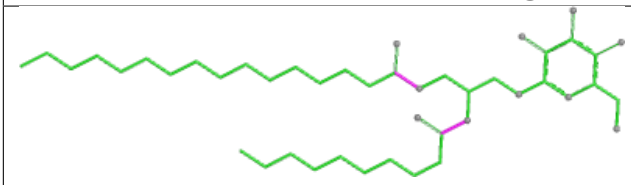


Torsions

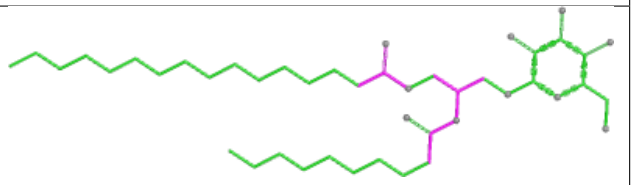


Rings

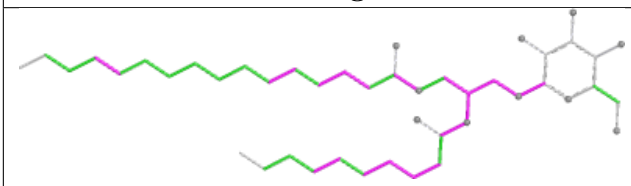
Ligand LMG F 806



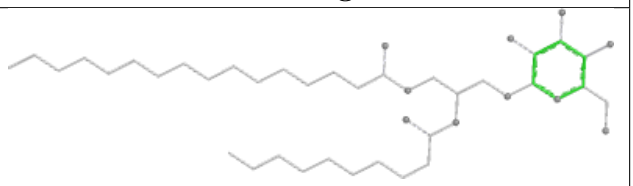
Bond lengths



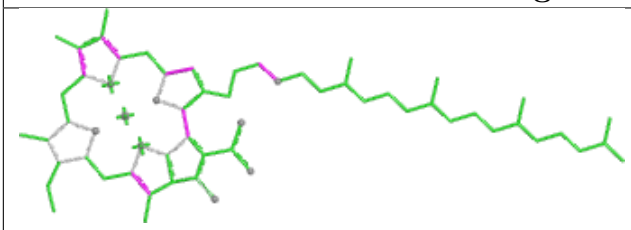
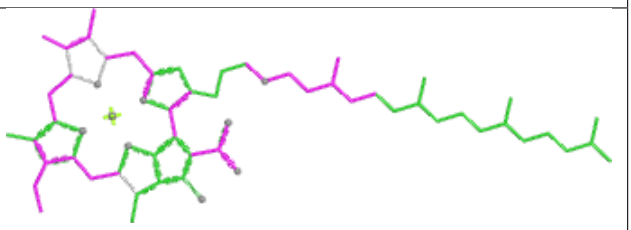
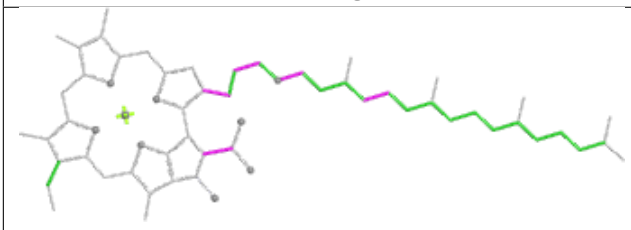
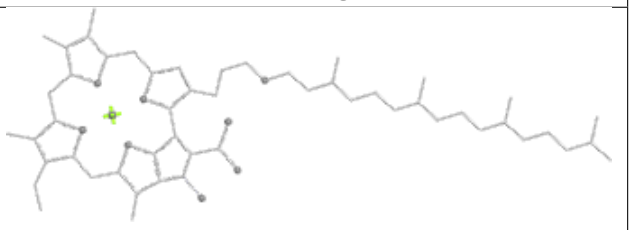
Bond angles

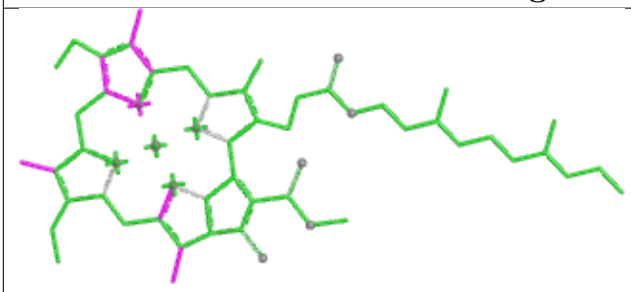
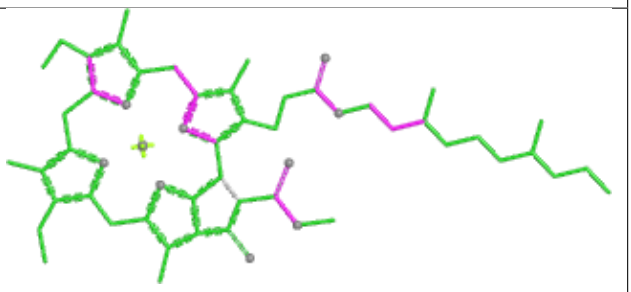
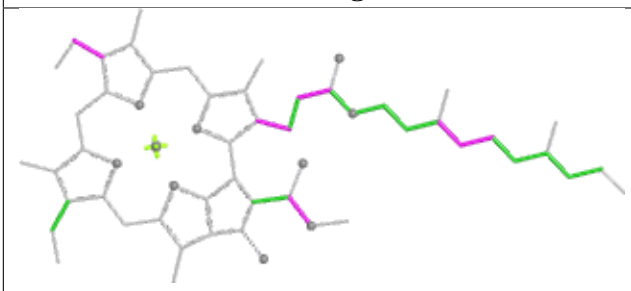
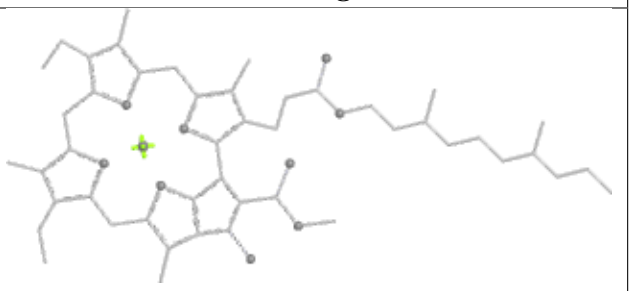


Torsions

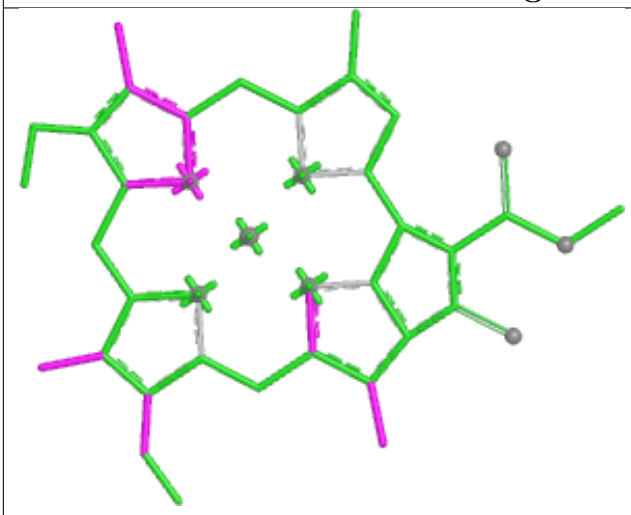


Rings

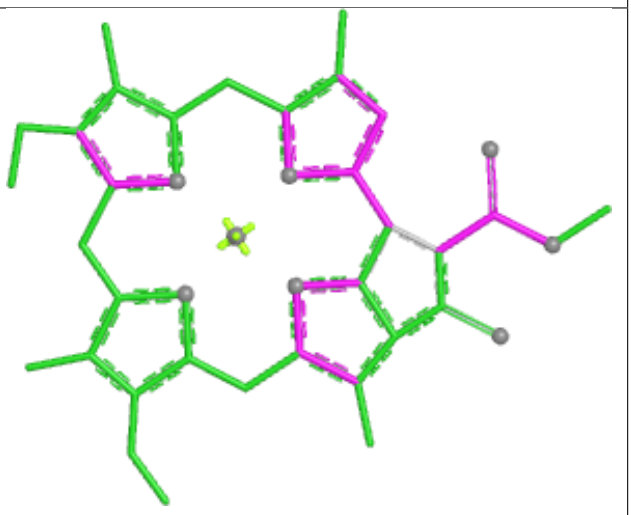
Ligand CL0 e 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA e 852	
	
Bond lengths	Bond angles
	
Torsions	Rings

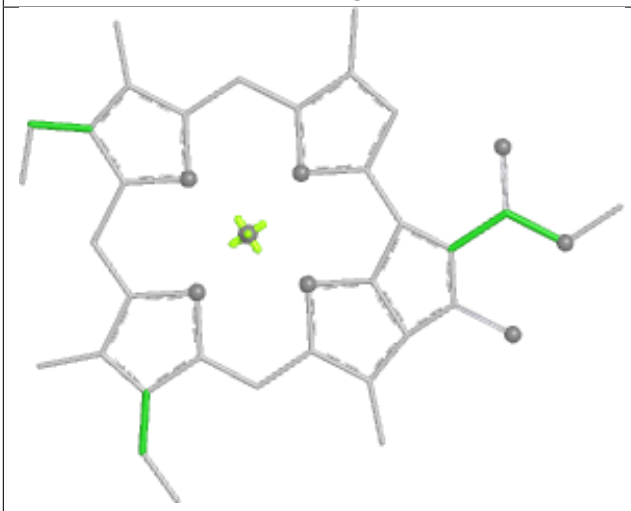
Ligand CLA B 810



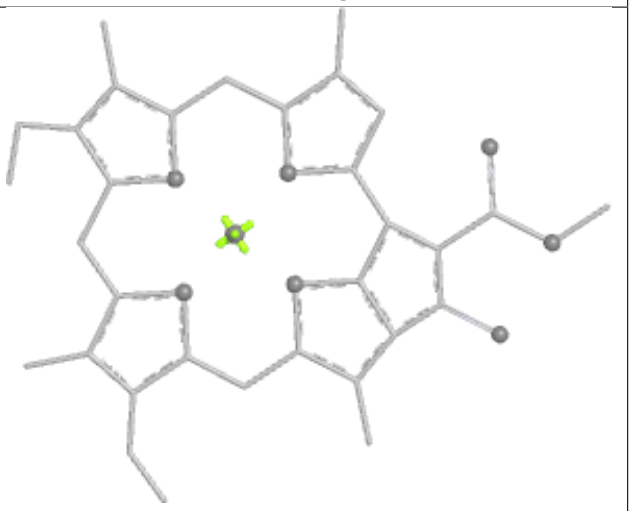
Bond lengths



Bond angles

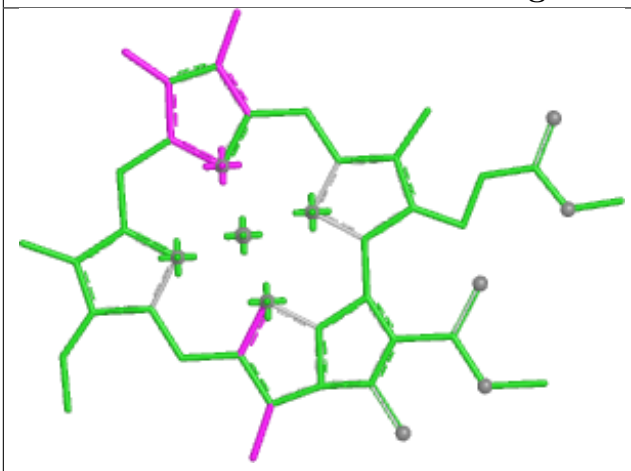


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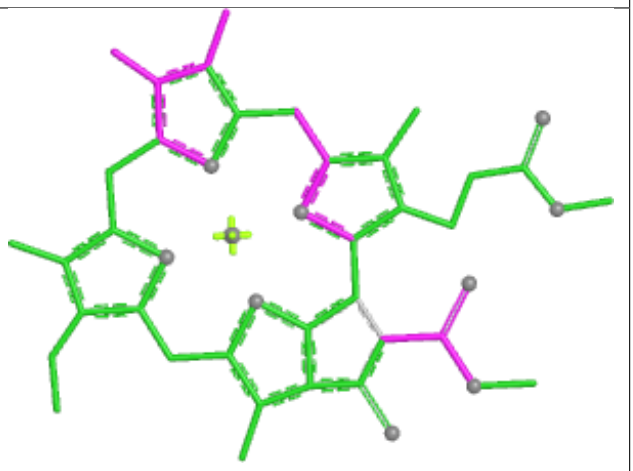


Rings

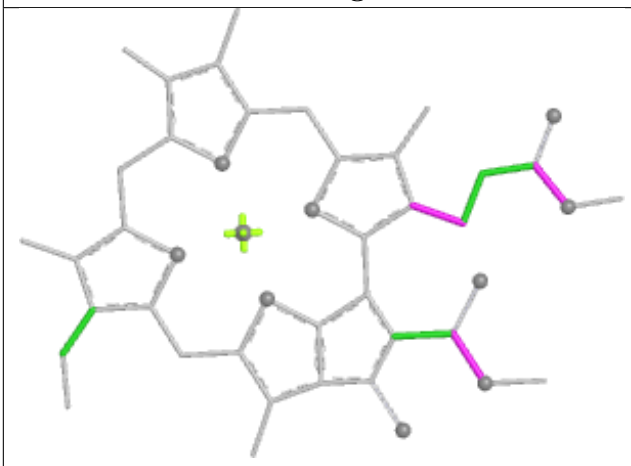
Ligand CLA 3 318



Bond lengths



Bond angles

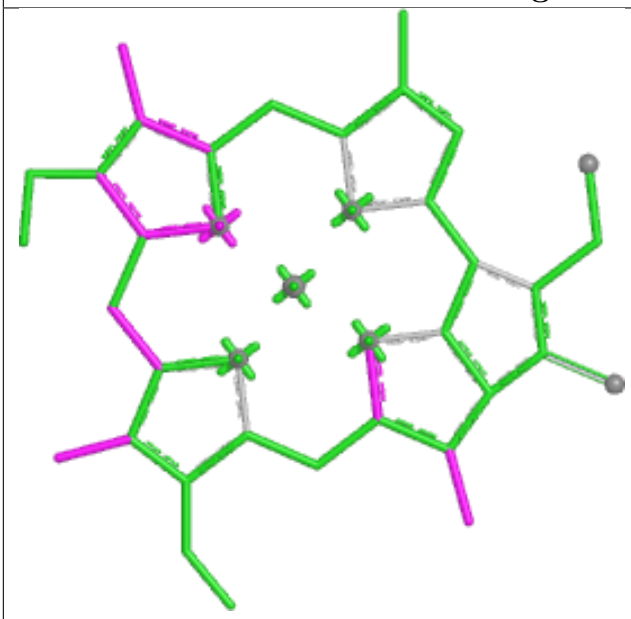


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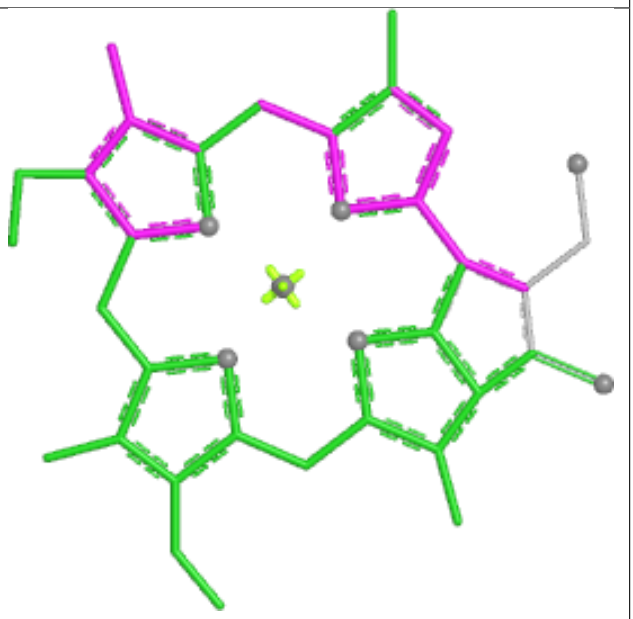


Rings

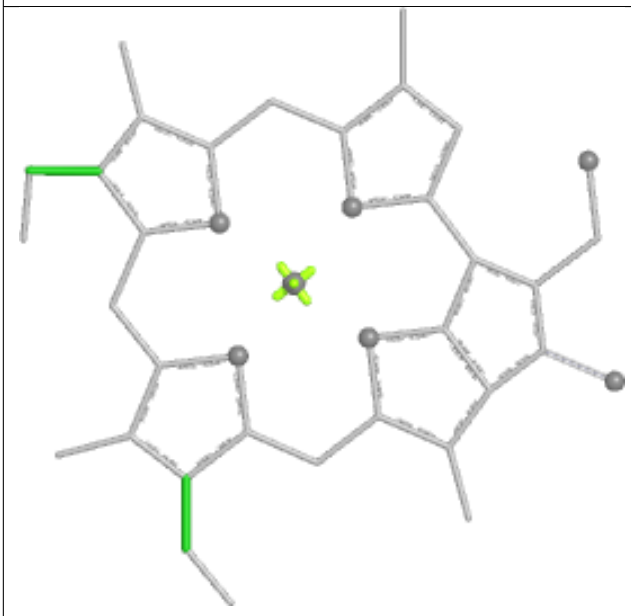
Ligand CLA f 805



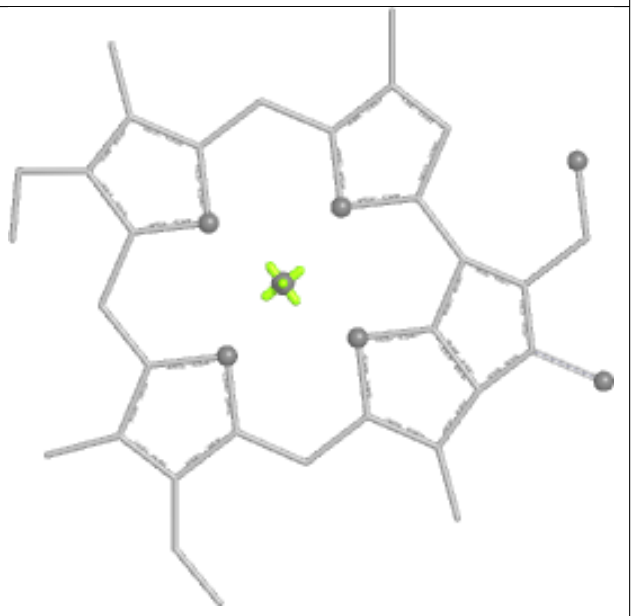
Bond lengths



Bond angles

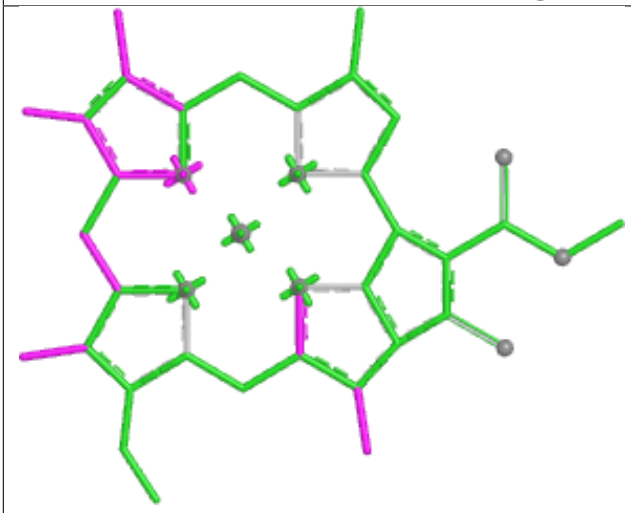


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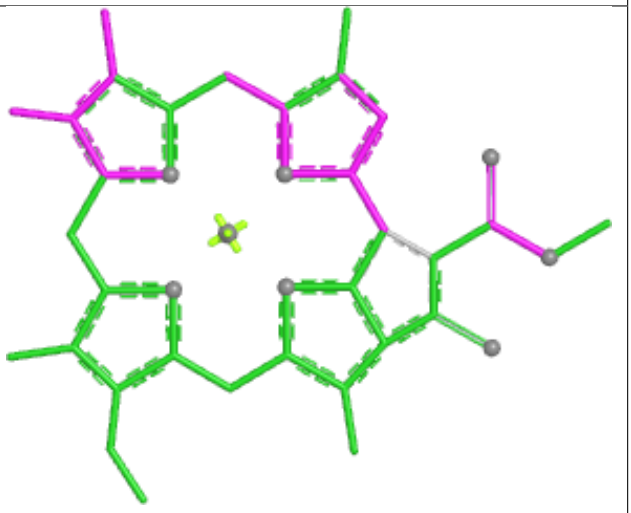


Rings

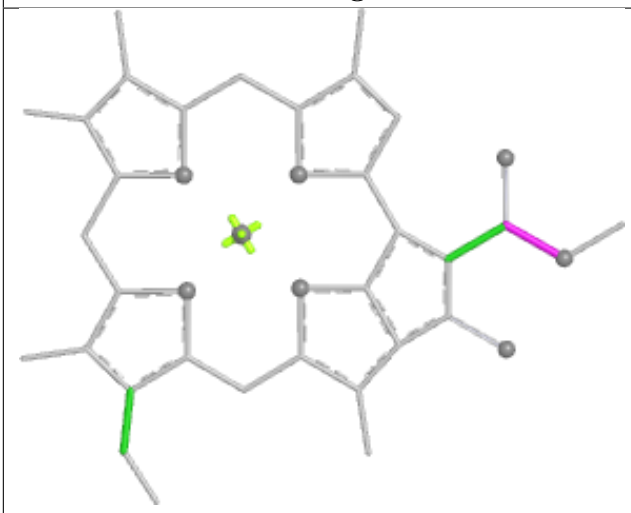
Ligand CLA f 830



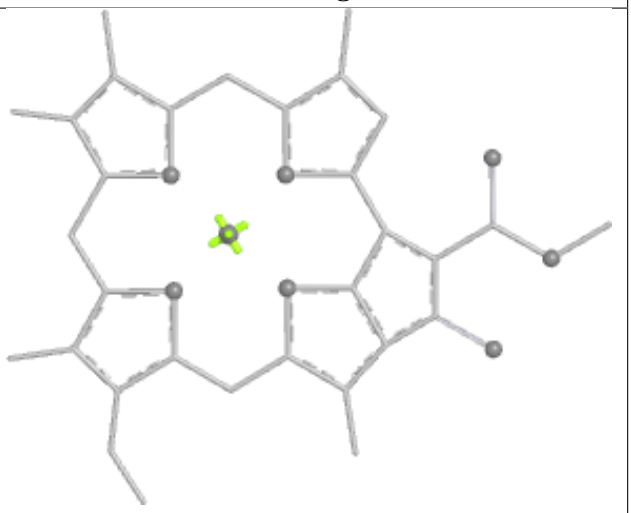
Bond lengths



Bond angles

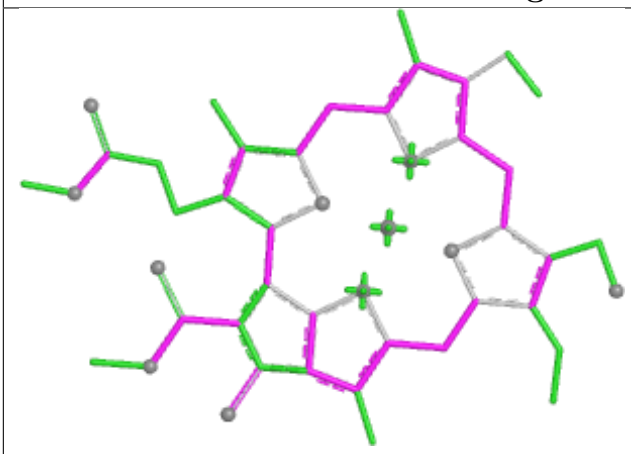


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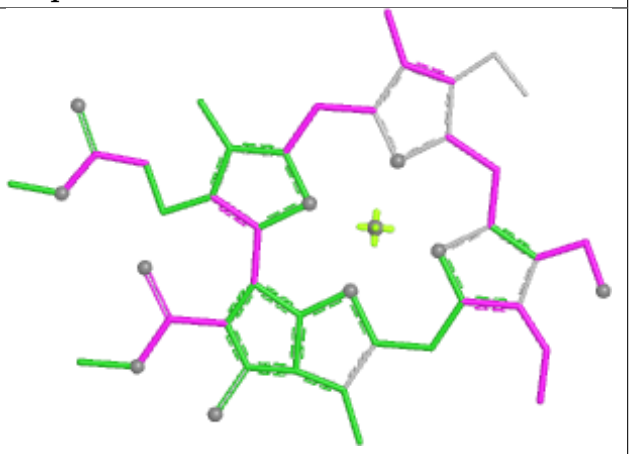


Rings

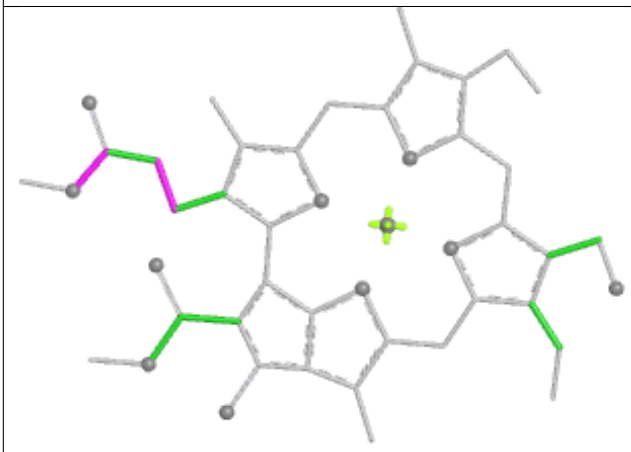
Ligand CHL p 512



Bond lengths



Bond angles

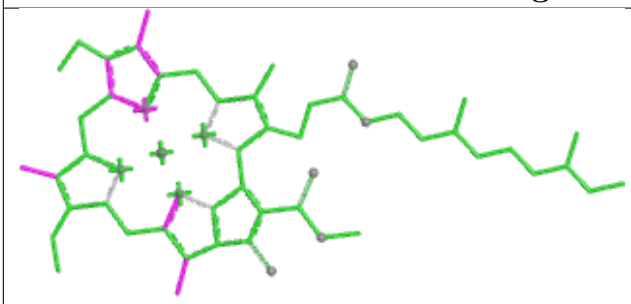


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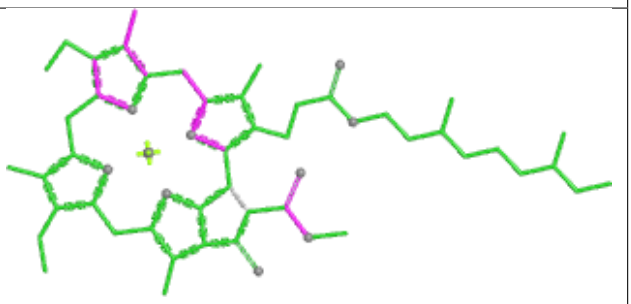


Rings

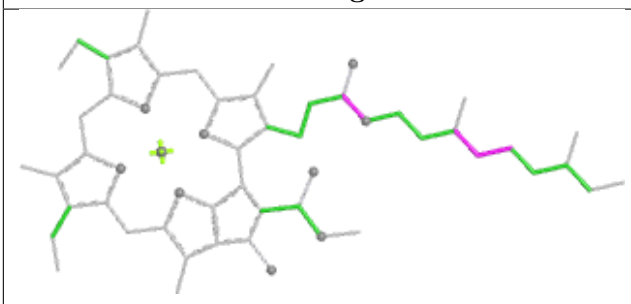
Ligand CLA f 831



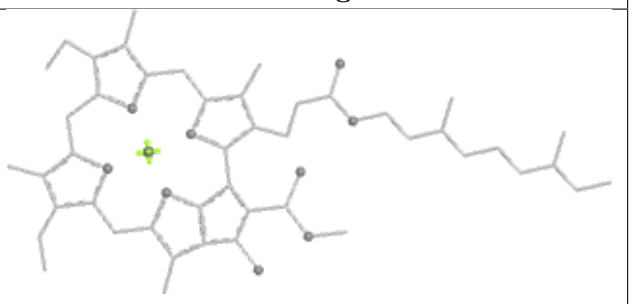
Bond lengths



Bond angles

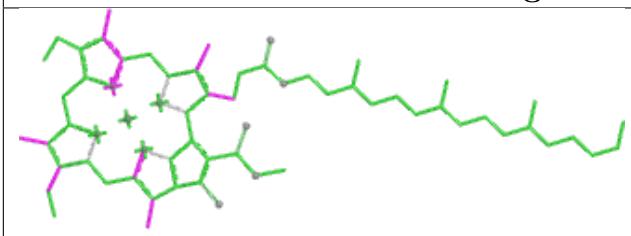


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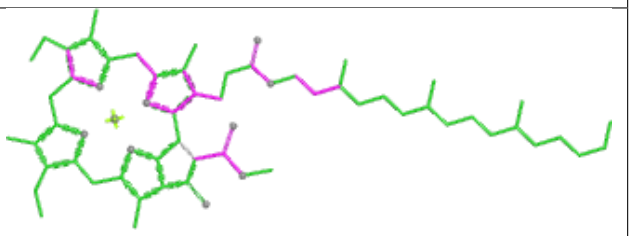


Rings

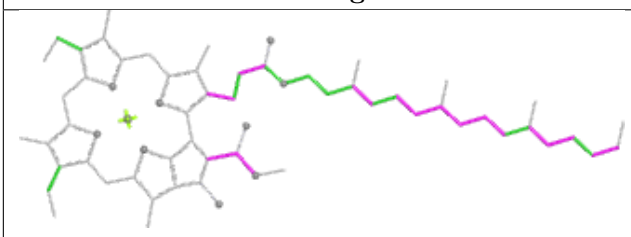
Ligand CLA A 805



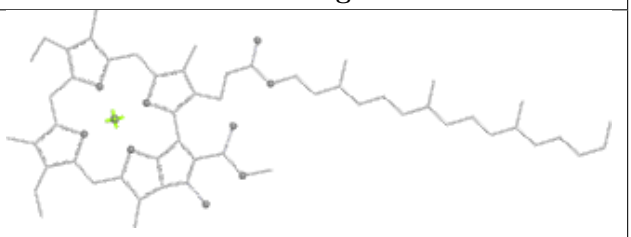
Bond lengths



Bond angles

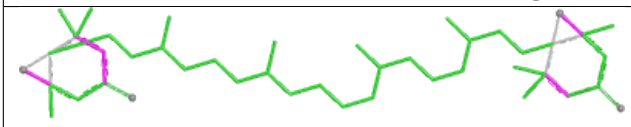


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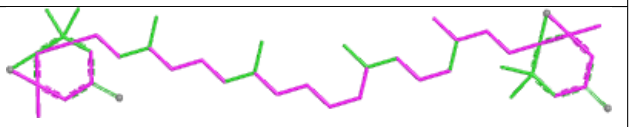


Rings

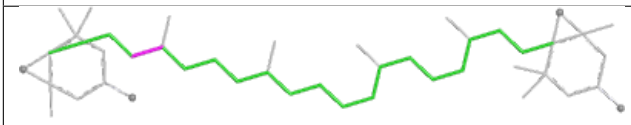
Ligand XAT 5 304



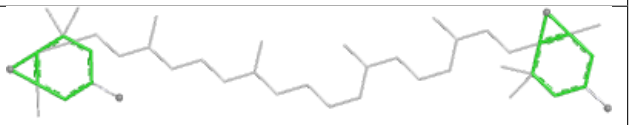
Bond lengths



Bond angles

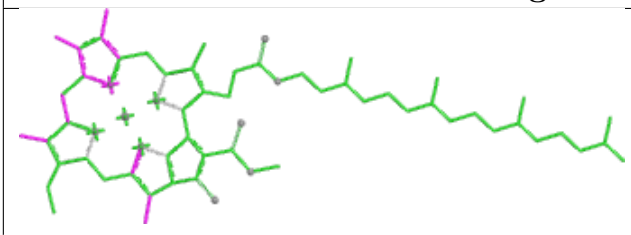


Torsions

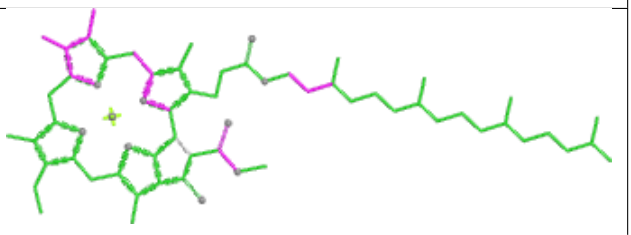


Rings

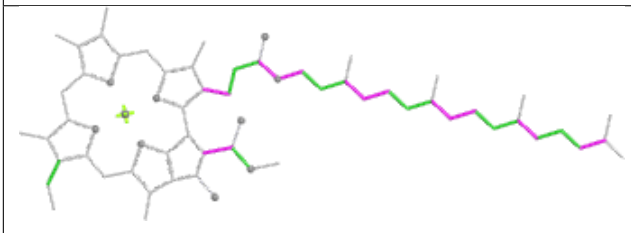
Ligand CLA e 826



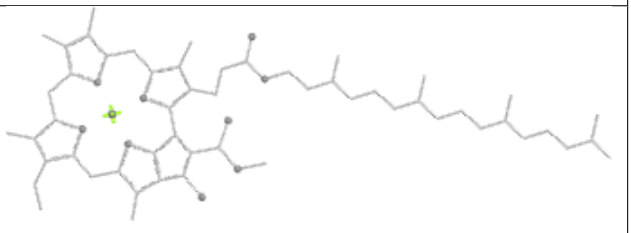
Bond lengths



Bond angles

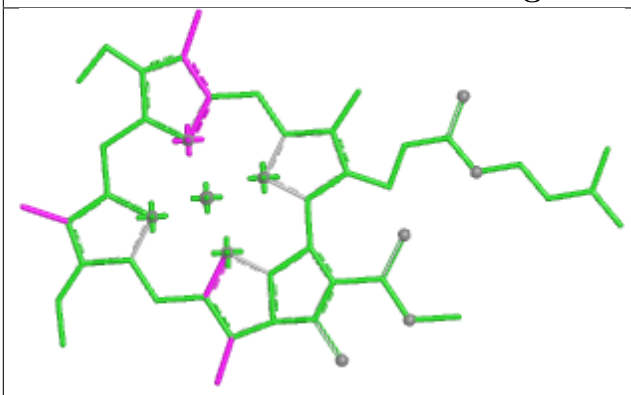


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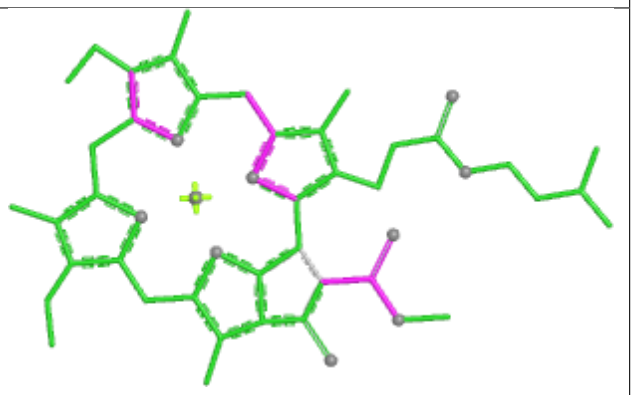


Rings

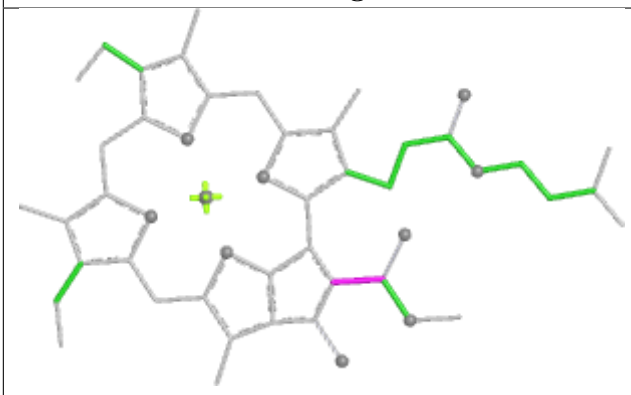
Ligand CLA A 830



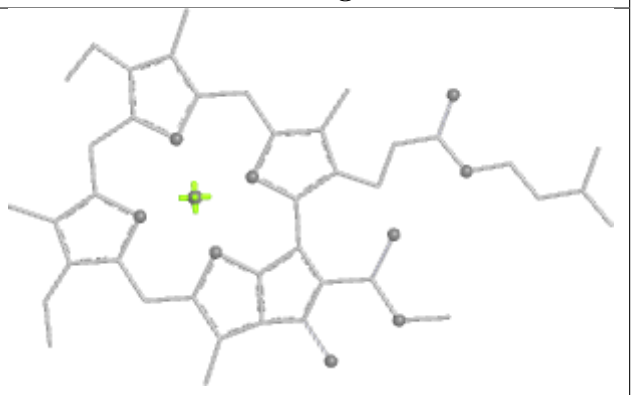
Bond lengths



Bond angles



Torsions

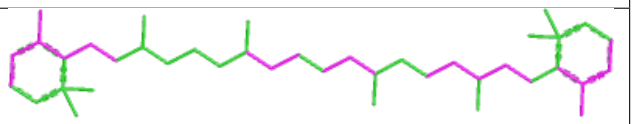


Rings

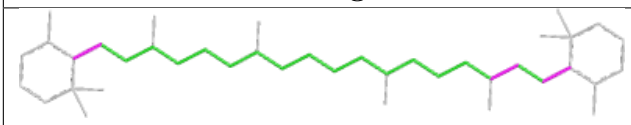
Ligand BCR A 848



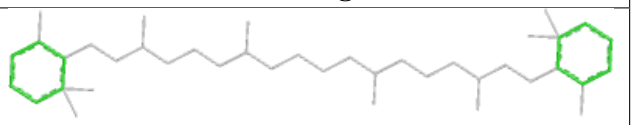
Bond lengths



Bond angles

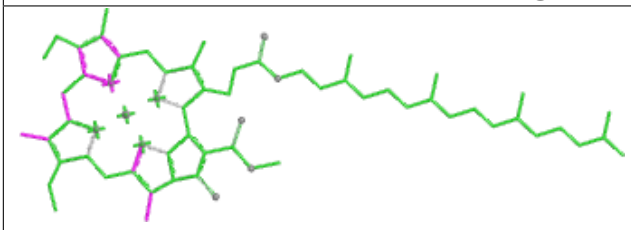


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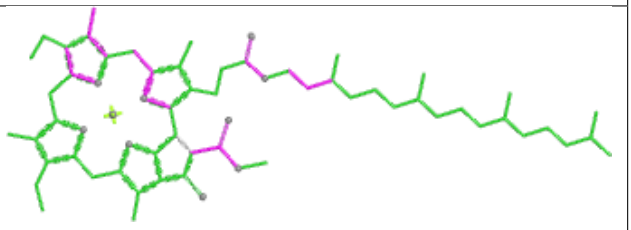


Rings

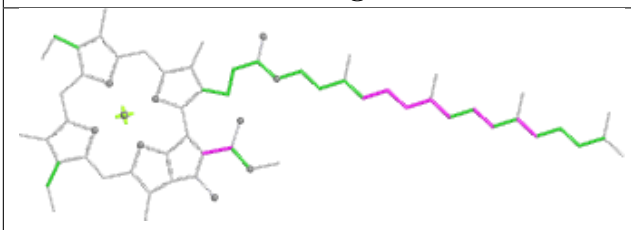
Ligand CLA f 826



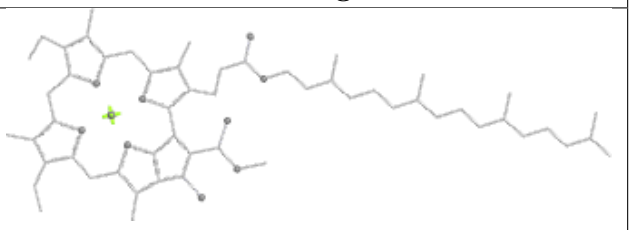
Bond lengths



Bond angles



Torsions

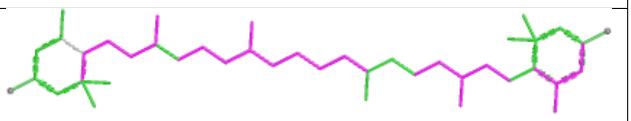


Rings

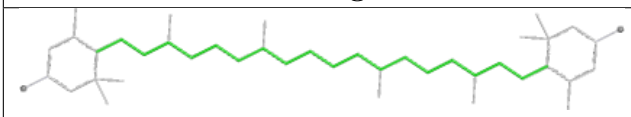
Ligand LUT 2 501



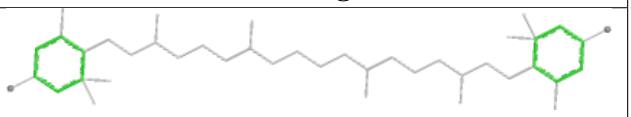
Bond lengths



Bond angles

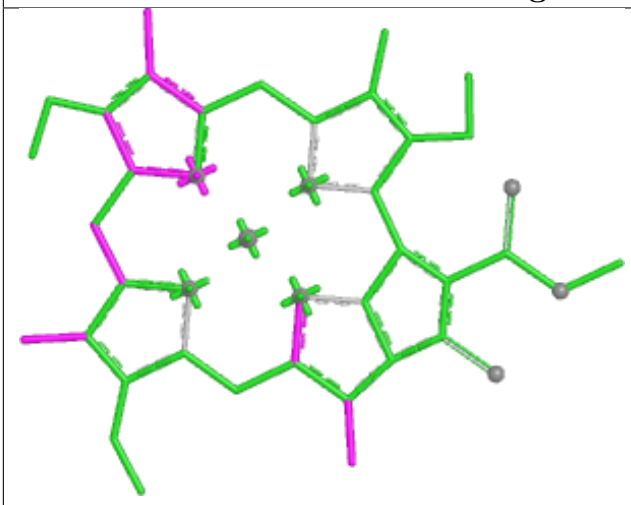


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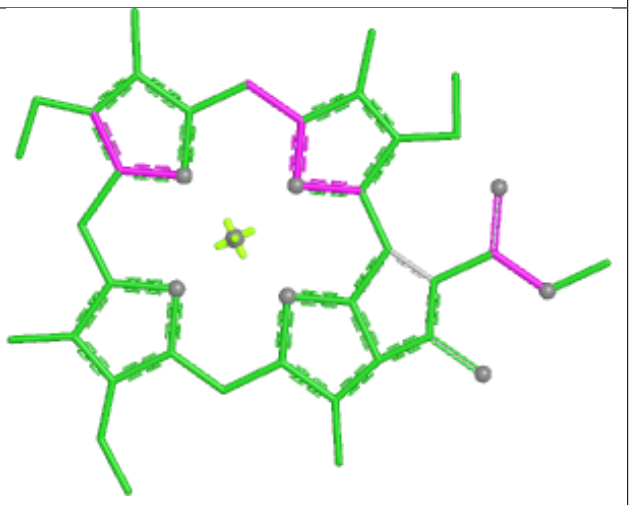


Rings

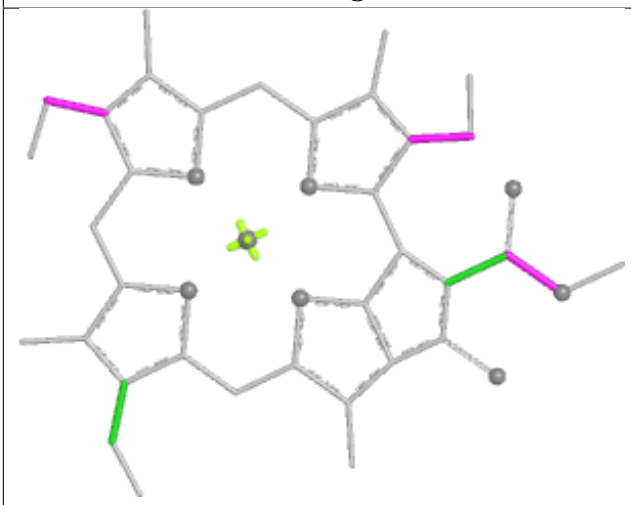
Ligand CLA e 814



Bond lengths



Bond angles

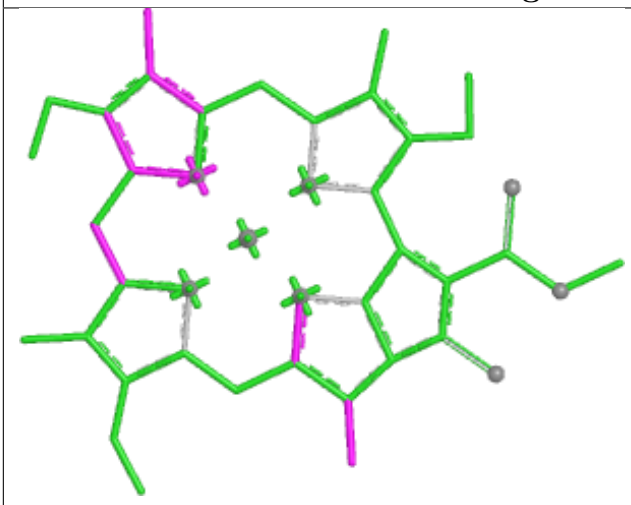


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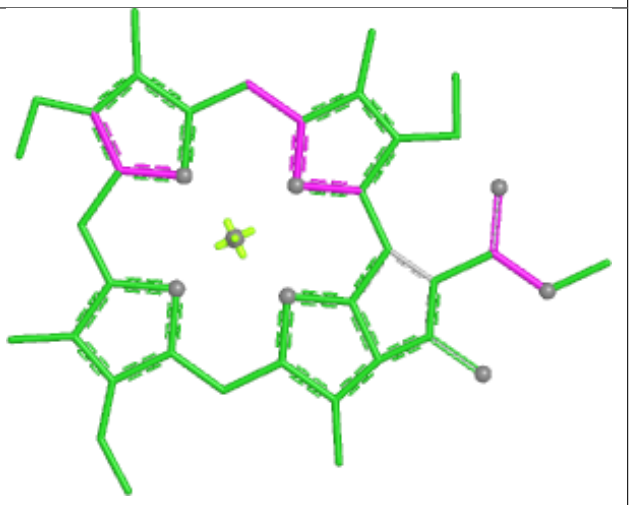


Rings

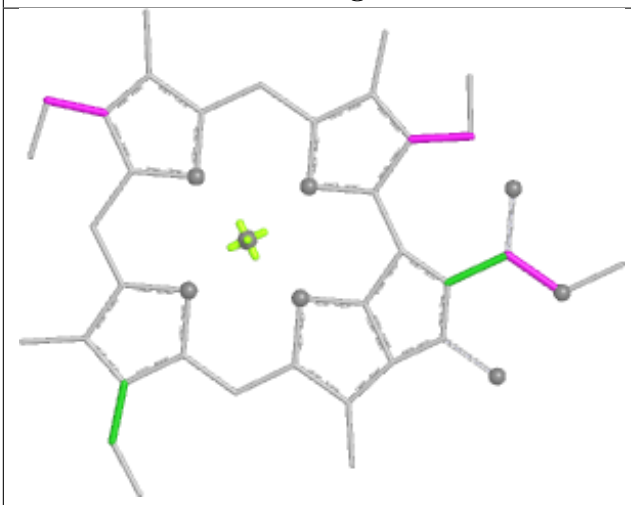
Ligand CLA m 102



Bond lengths



Bond angles



Torsions

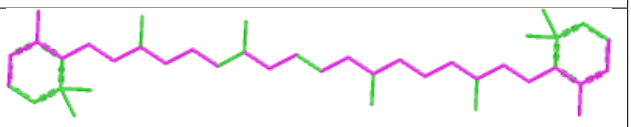


Rings

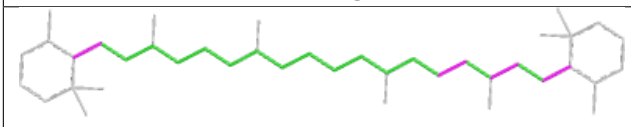
Ligand BCR e 849



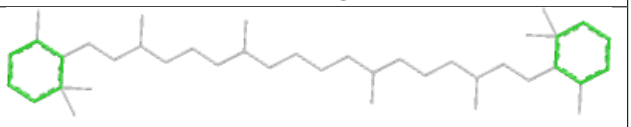
Bond lengths



Bond angles

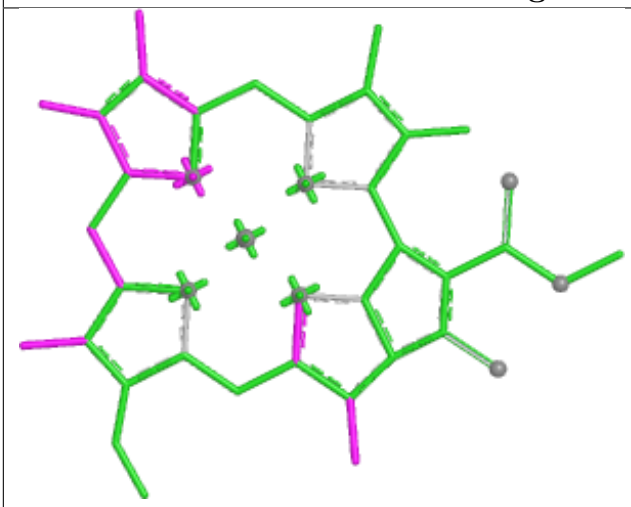


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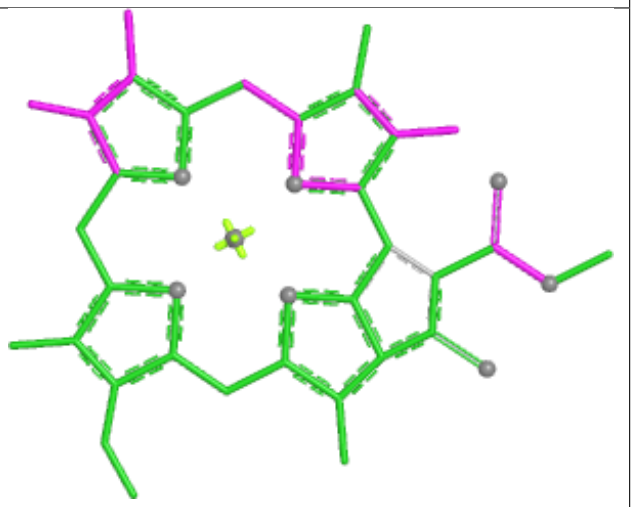


Rings

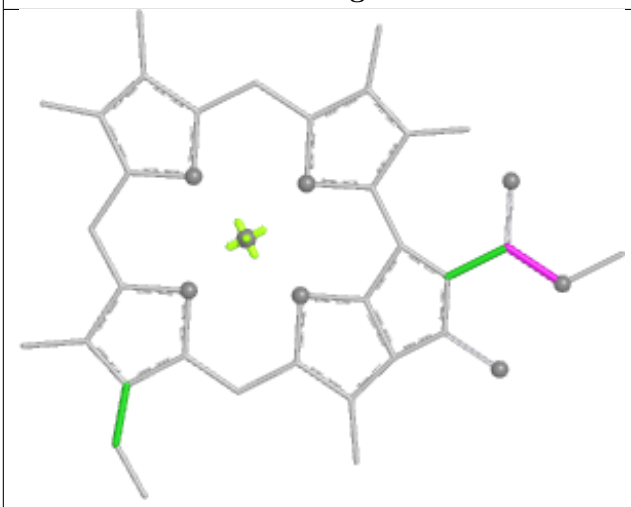
Ligand CLA o 302



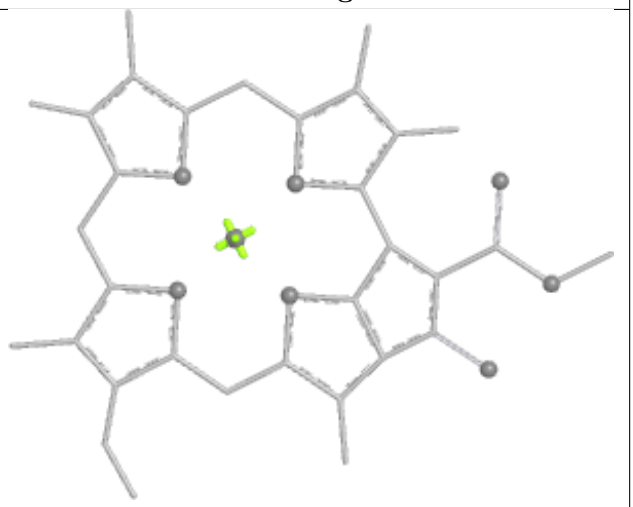
Bond lengths



Bond angles

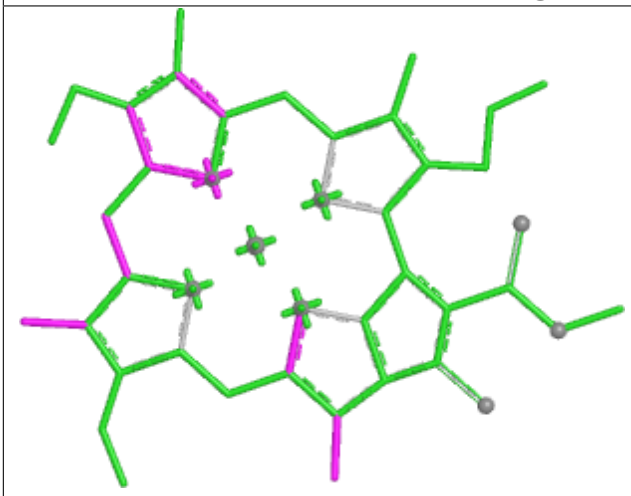


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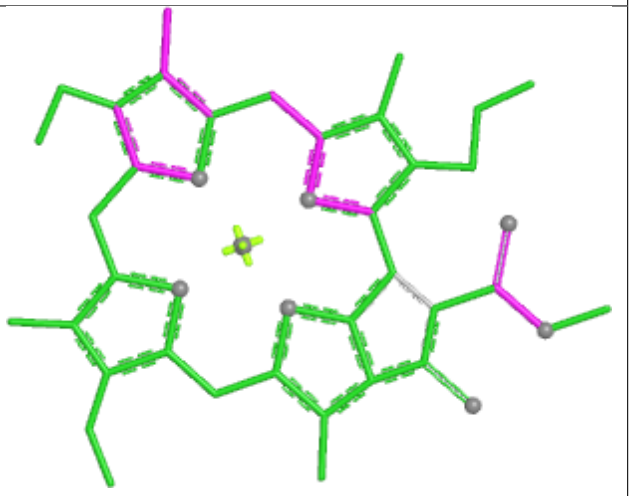


Rings

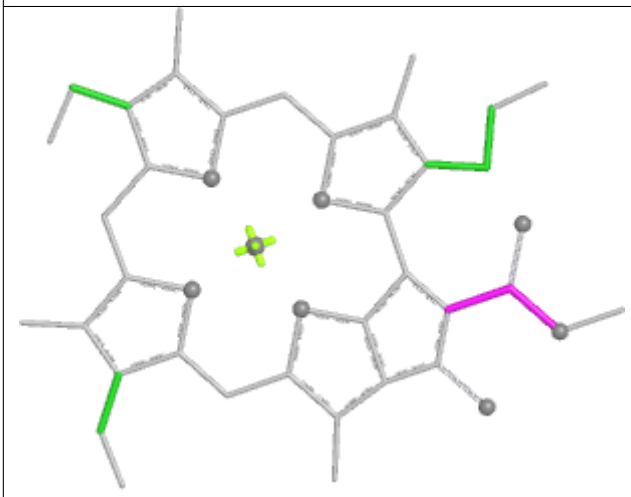
Ligand CLA f 834



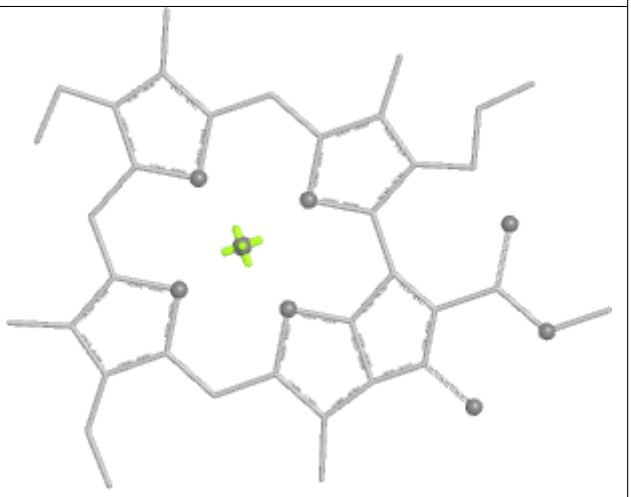
Bond lengths



Bond angles

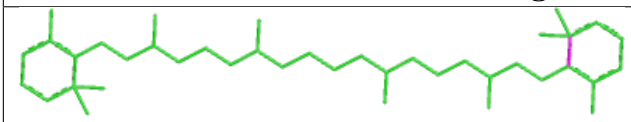


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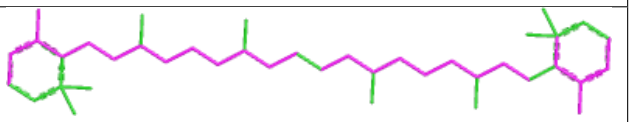


Rings

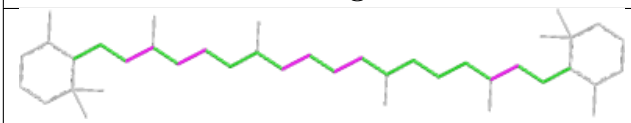
Ligand BCR f 845



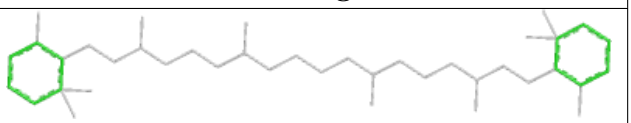
Bond lengths



Bond angles

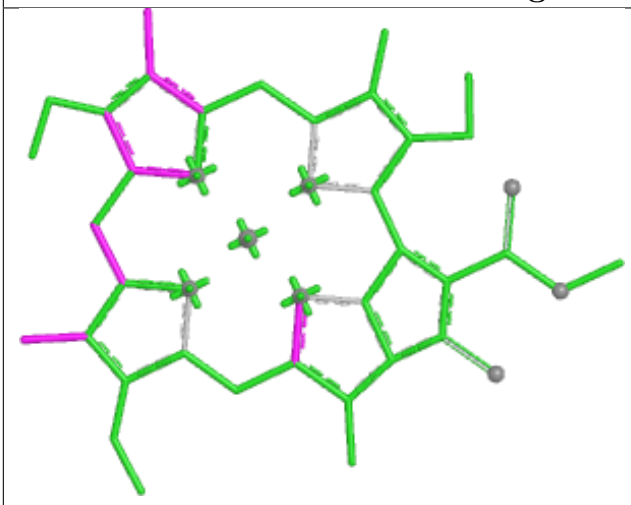


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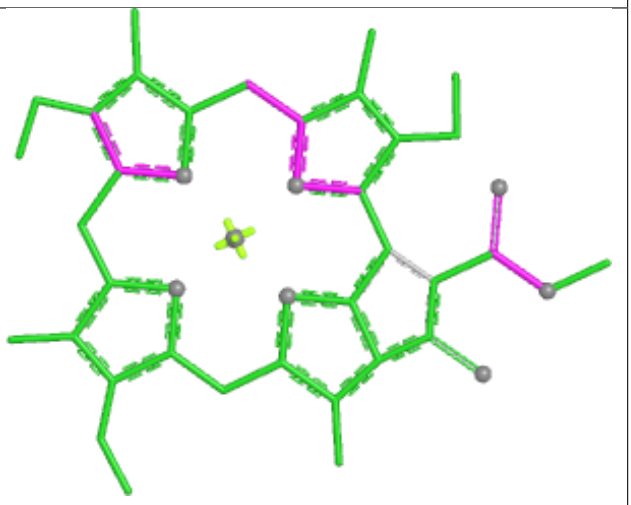


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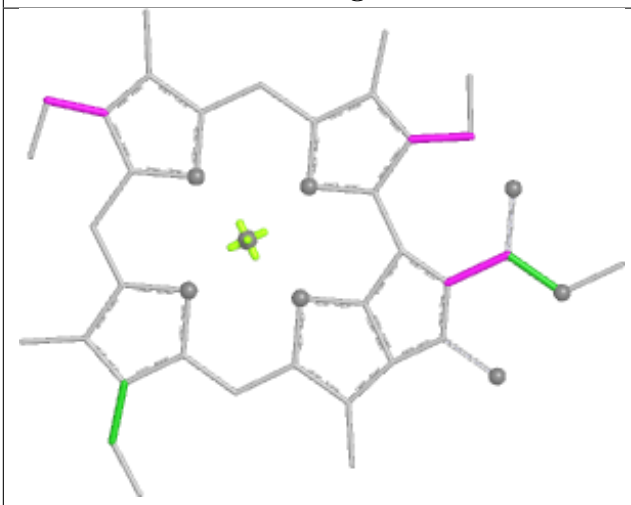
Ligand CLA 1 505



Bond lengths



Bond angles

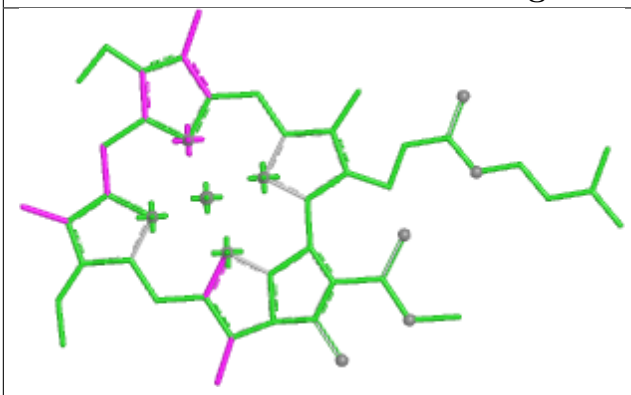


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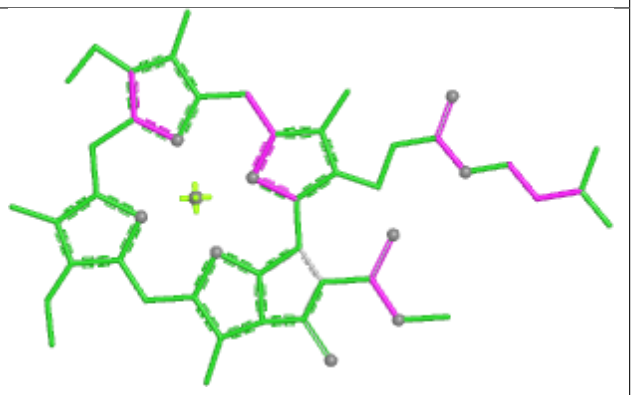


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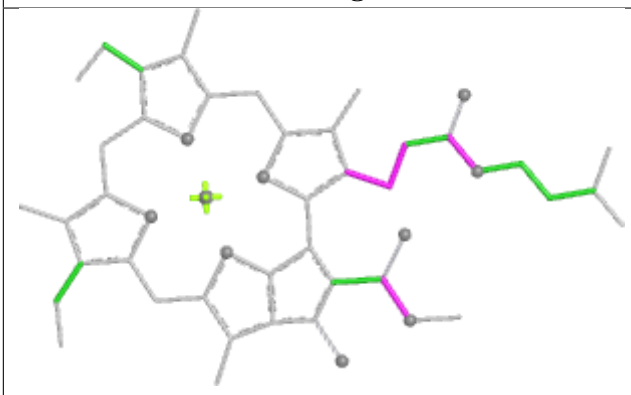
Ligand CLA 2 509



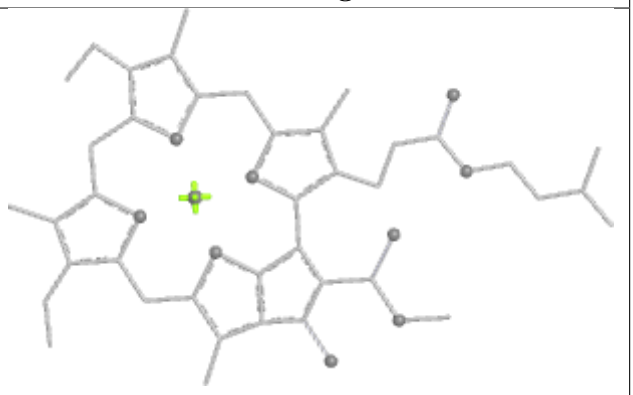
Bond lengths



Bond angles



Torsions

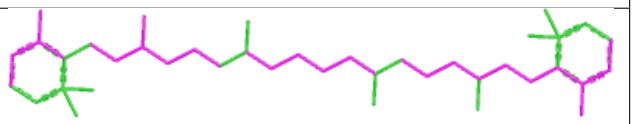


Rings

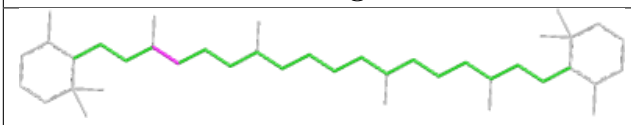
Ligand BCR o 301



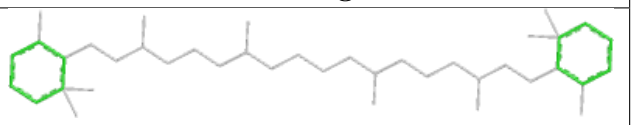
Bond lengths



Bond angles

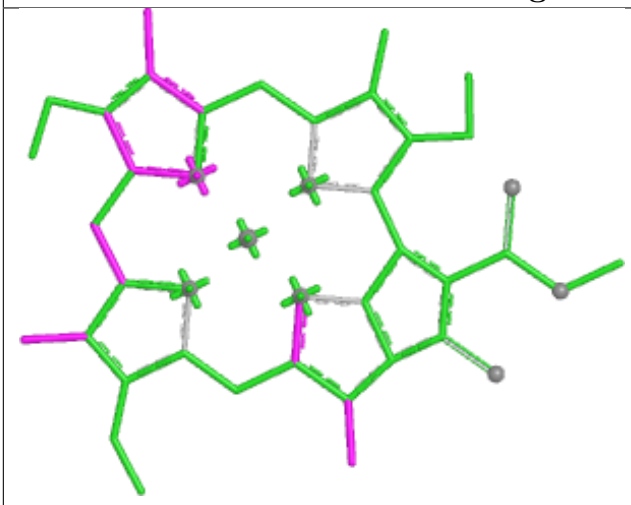


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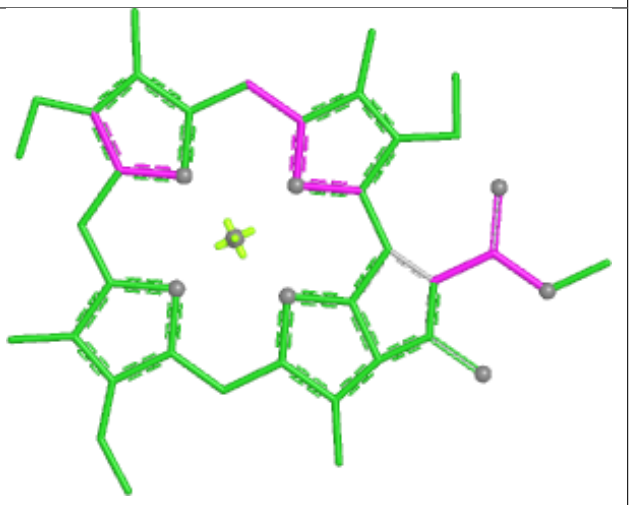


Rings

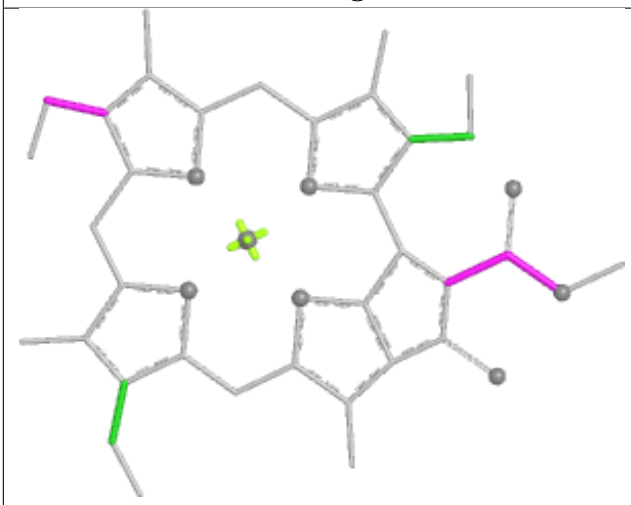
Ligand CLA e 807



Bond lengths



Bond angles

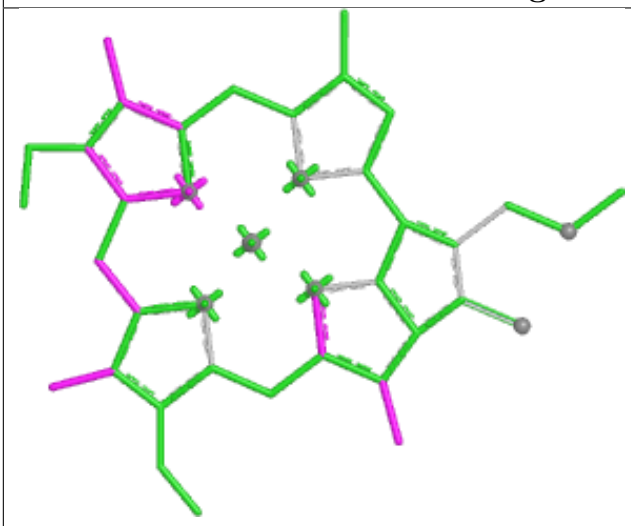


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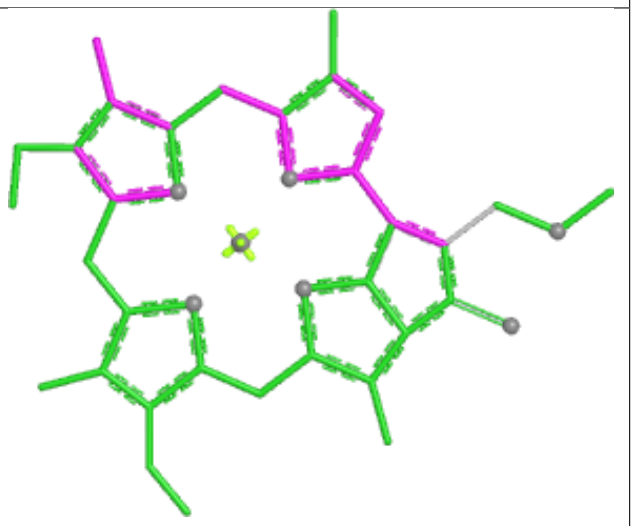


Rings

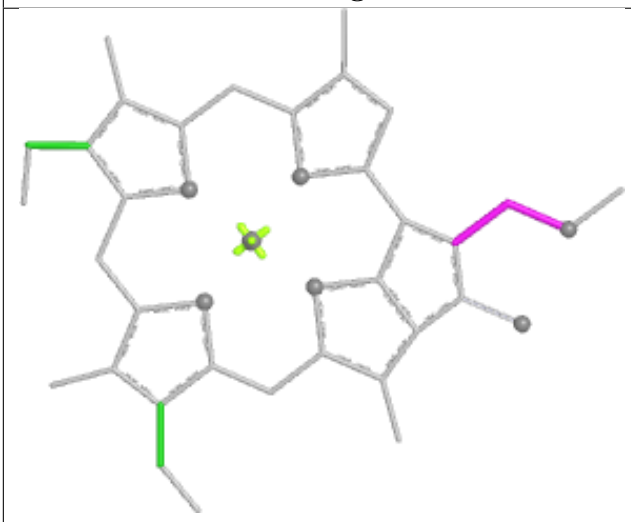
Ligand CLA e 812



Bond lengths



Bond angles

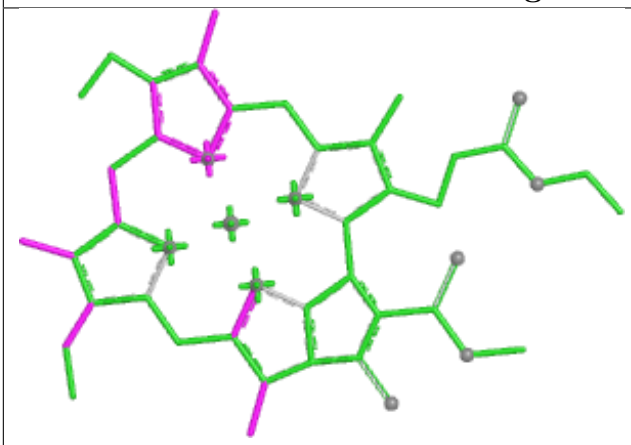


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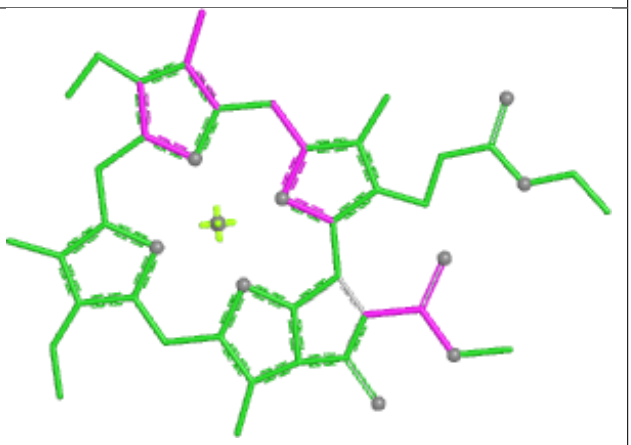


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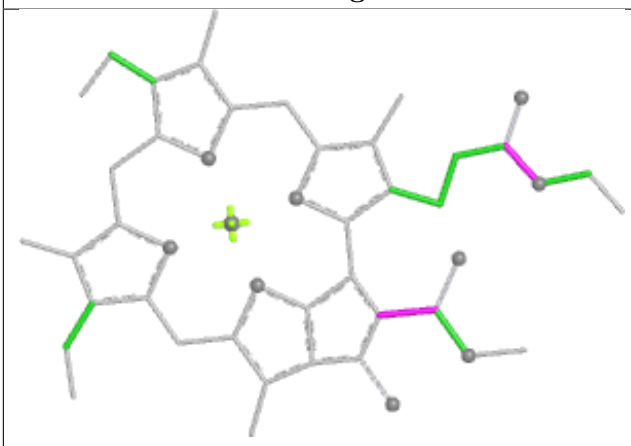
Ligand CLA B 822



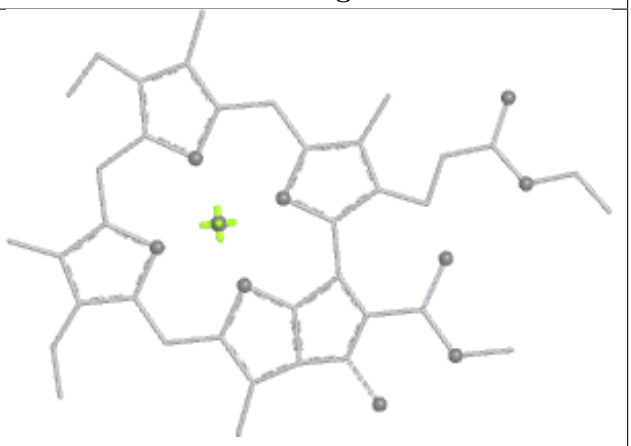
Bond lengths



Bond angles



Torsions

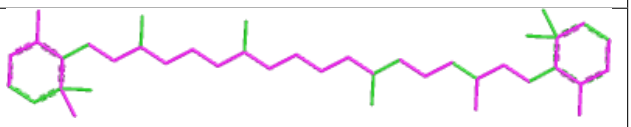


Rings

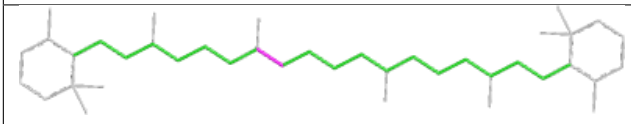
Ligand BCR F 804



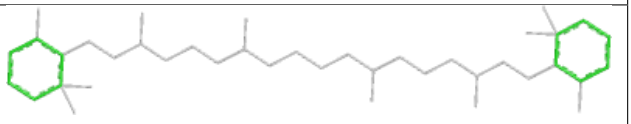
Bond lengths



Bond angles

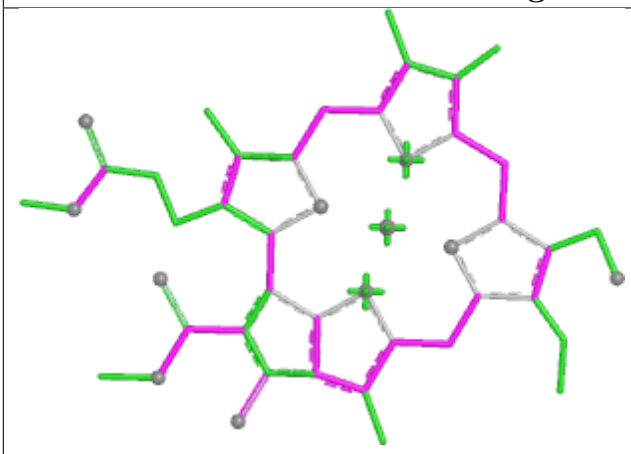


Torsions

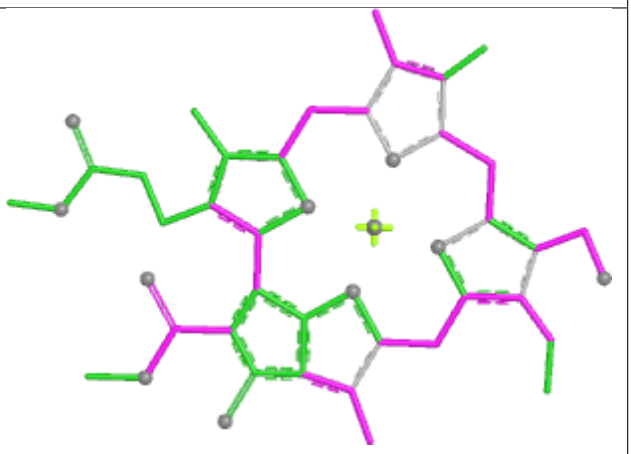


Rings

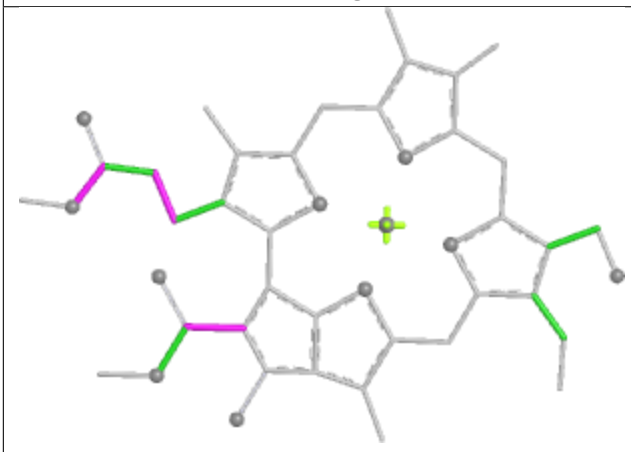
Ligand CHL 2 512



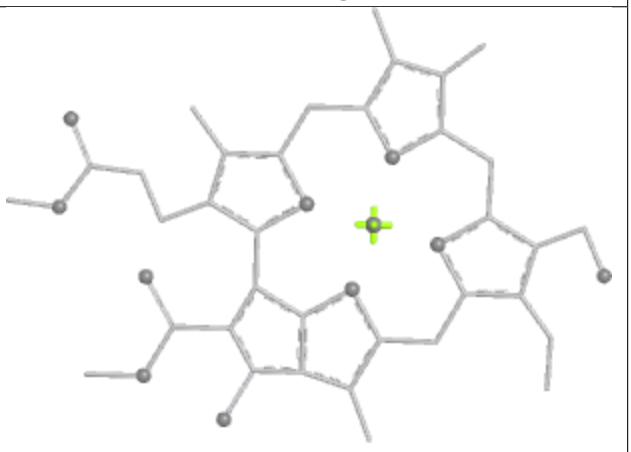
Bond lengths



Bond angles

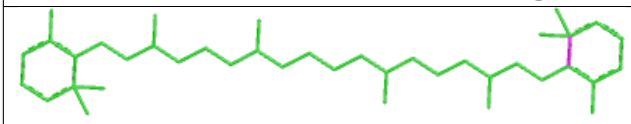


Torsions

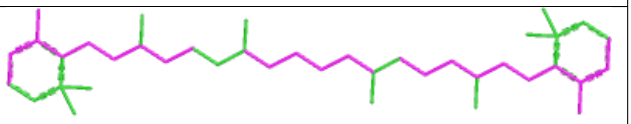


Rings

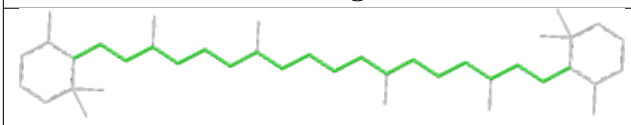
Ligand BCR f 848



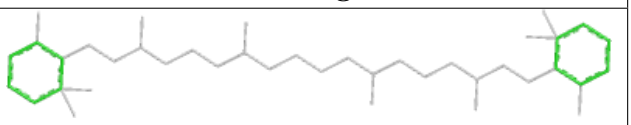
Bond lengths



Bond angles

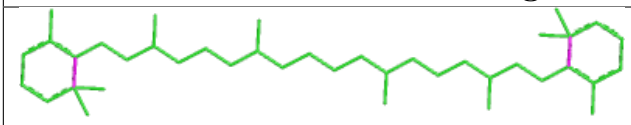


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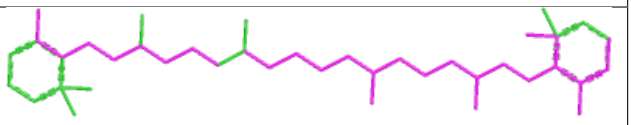


Rings

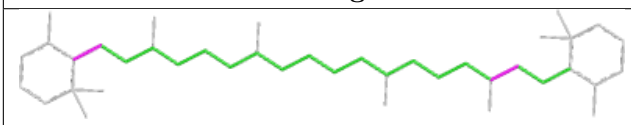
Ligand BCR A 845



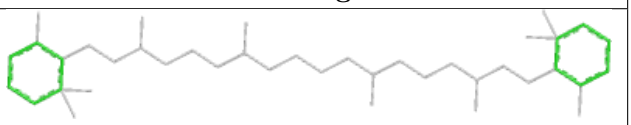
Bond lengths



Bond angles

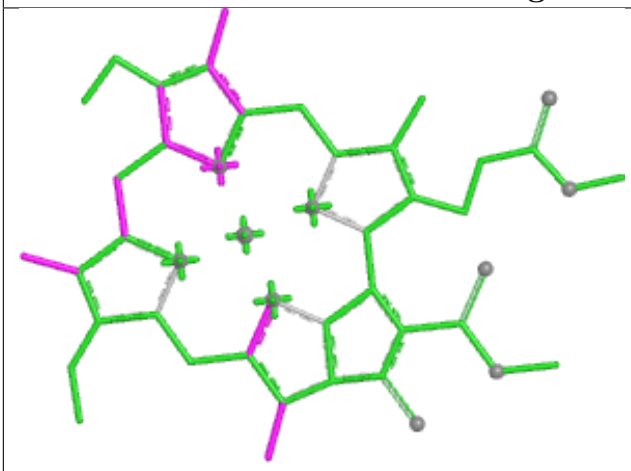


Torsions

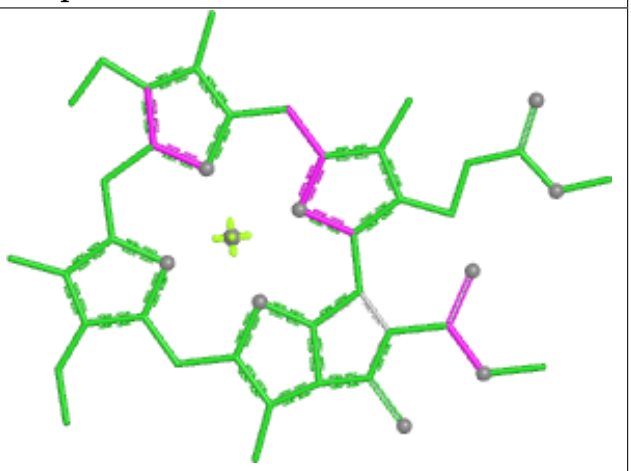


Rings

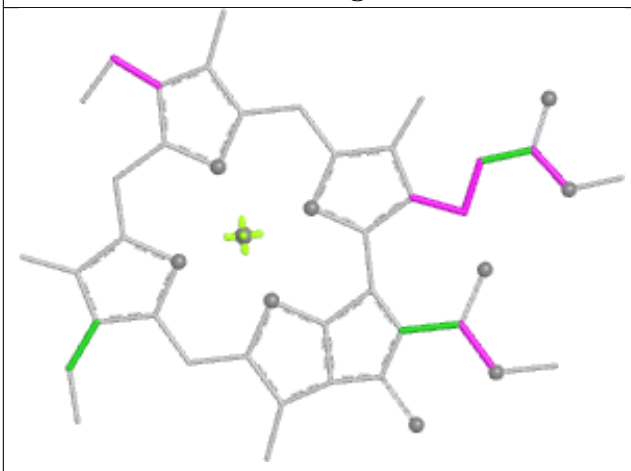
Ligand CLA q 316



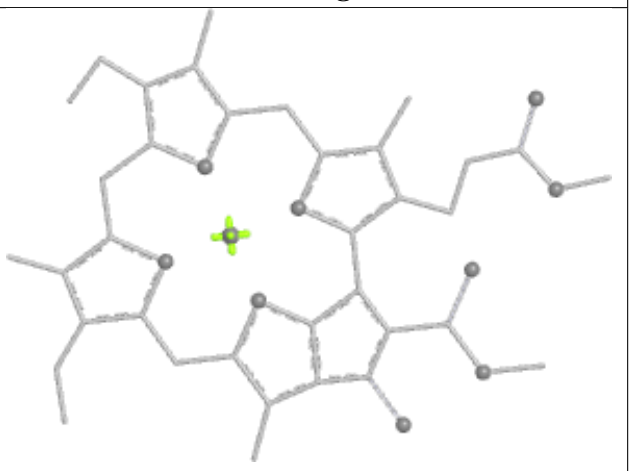
Bond lengths



Bond angles



Torsions

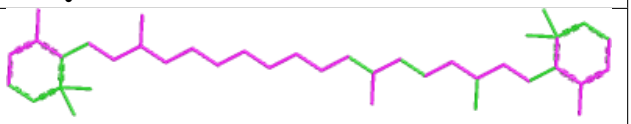


Rings

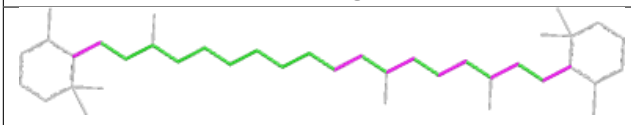
Ligand BCR Q 801



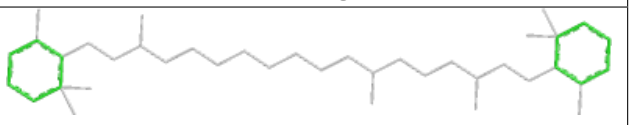
Bond lengths



Bond angles

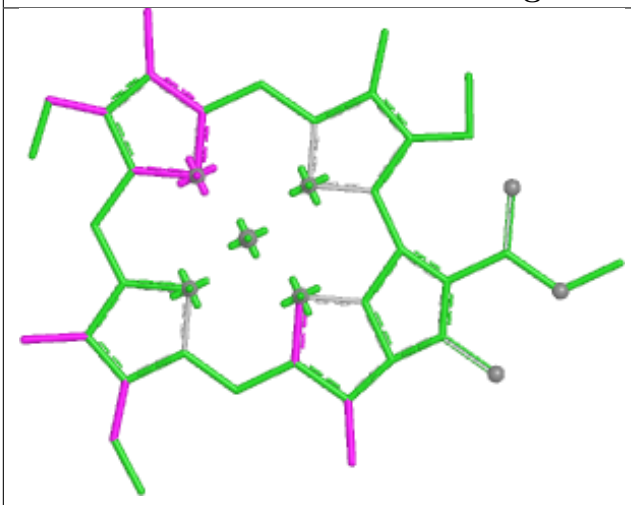


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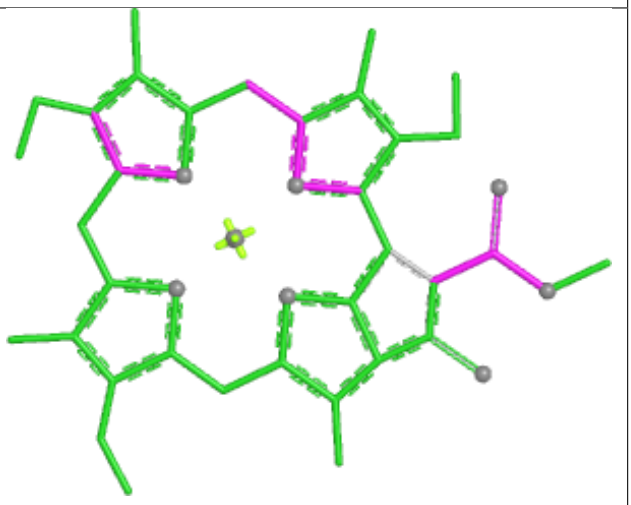


Rings

Ligand CLA A 814



Bond lengths



Bond angles

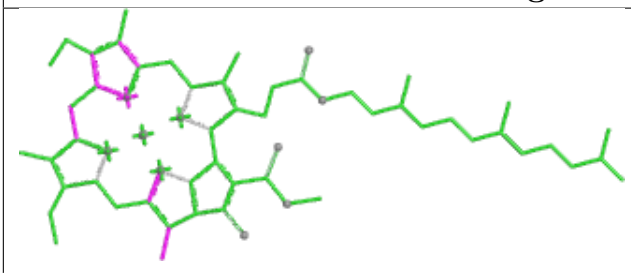


Torsions

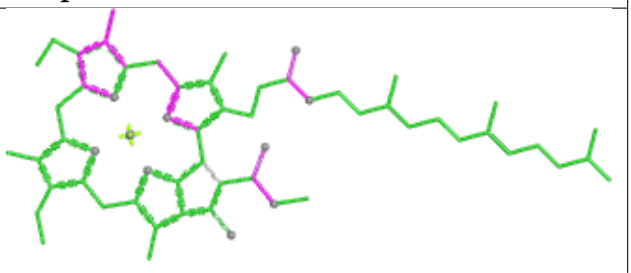


Rings

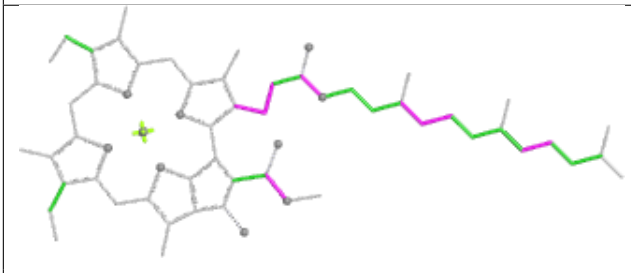
Ligand CLA q 312



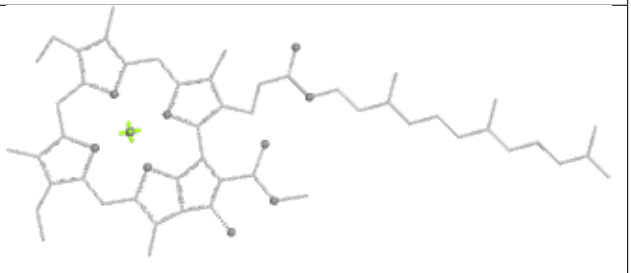
Bond lengths



Bond angles

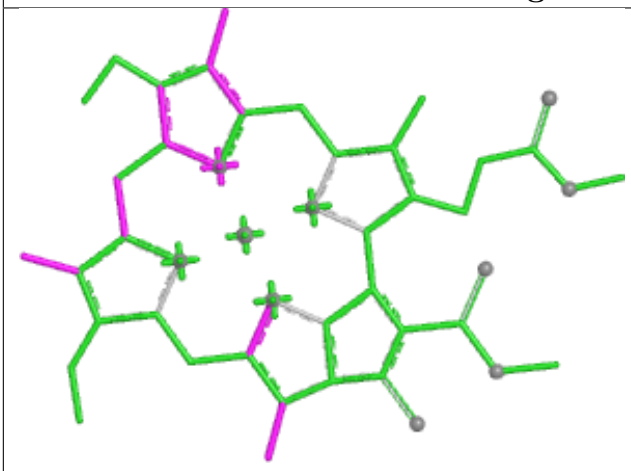


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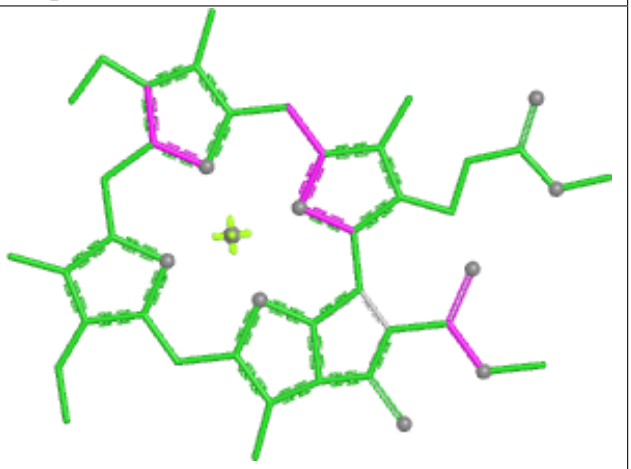


Rings

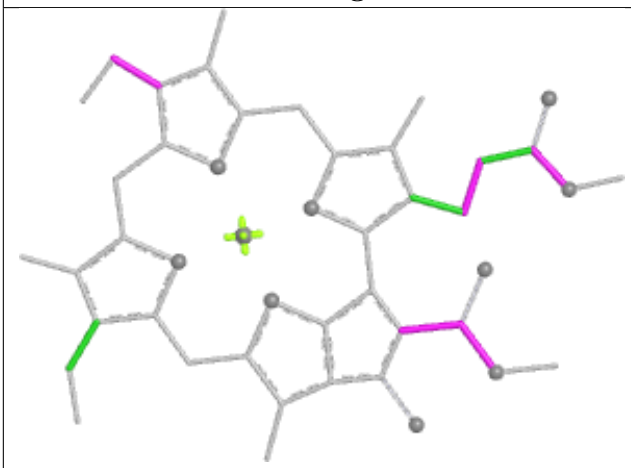
Ligand CLA p 510



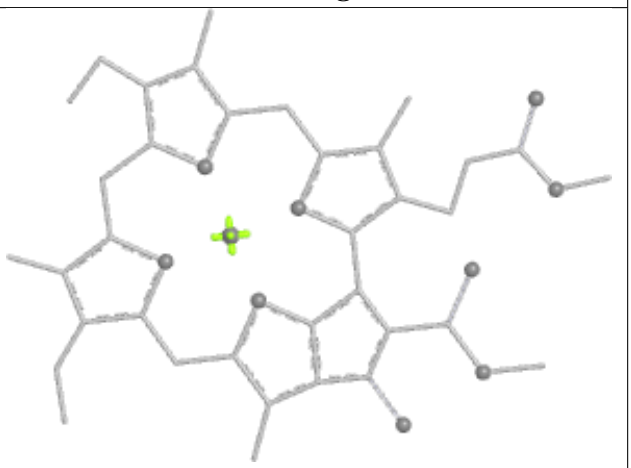
Bond lengths



Bond angles

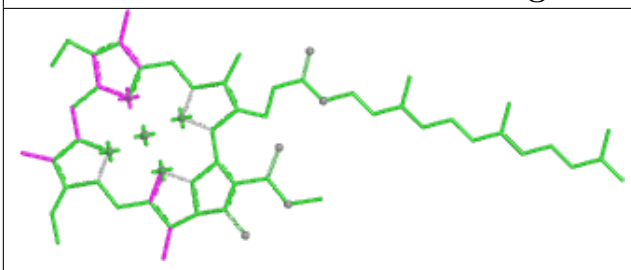


Torsions

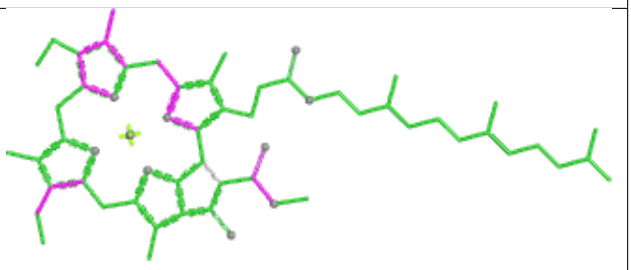


Rings

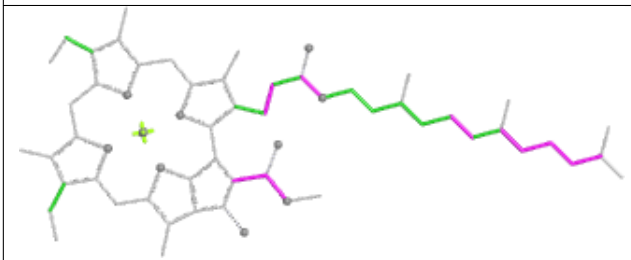
Ligand CLA 5 308



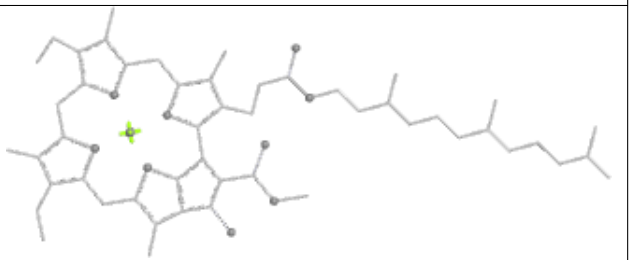
Bond lengths



Bond angles

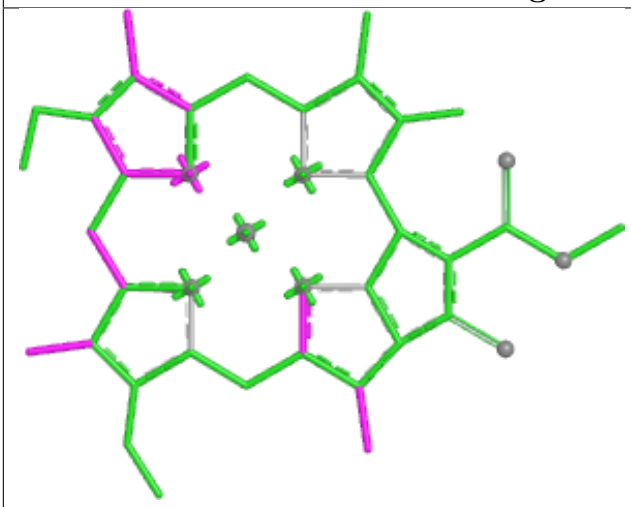


Torsions

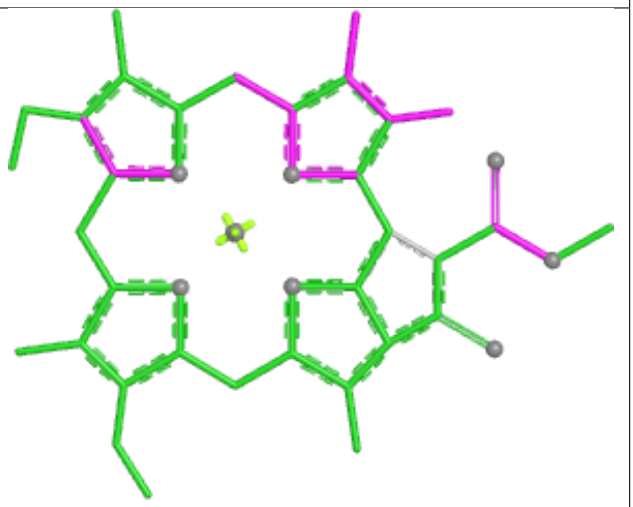


Rings

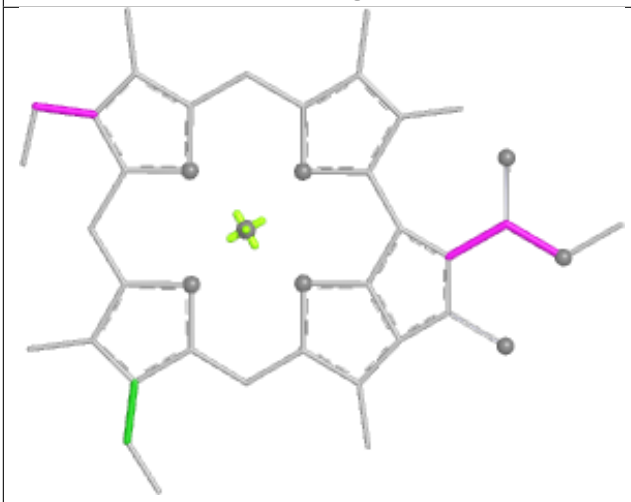
Ligand CLA e 808



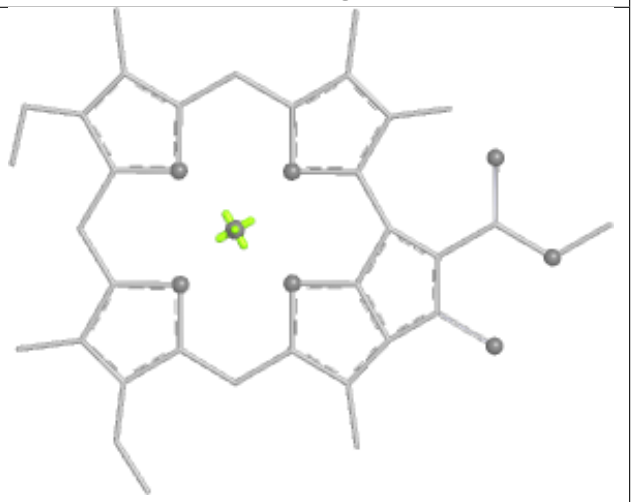
Bond lengths



Bond angles

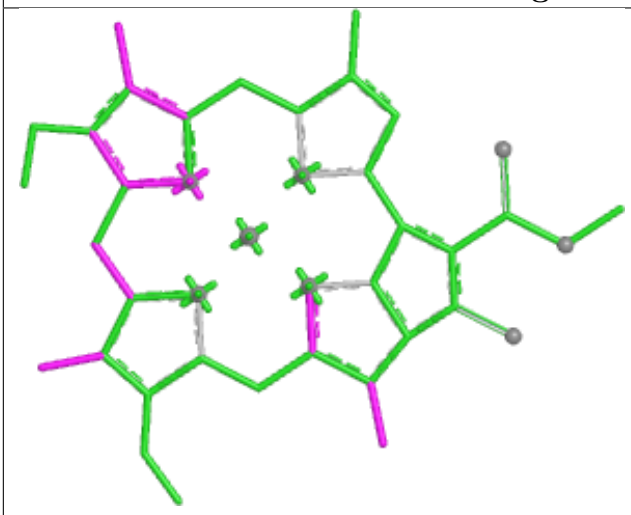


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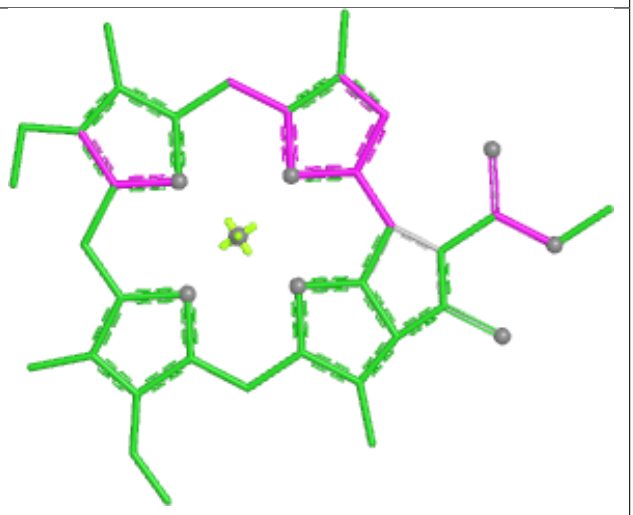


Rings

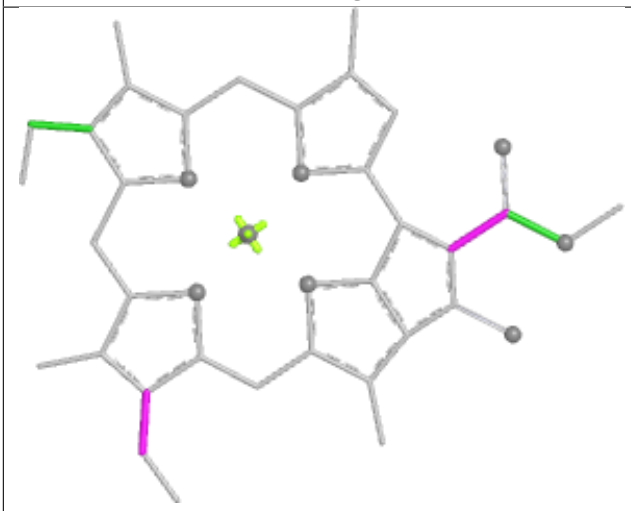
Ligand CLA f 838



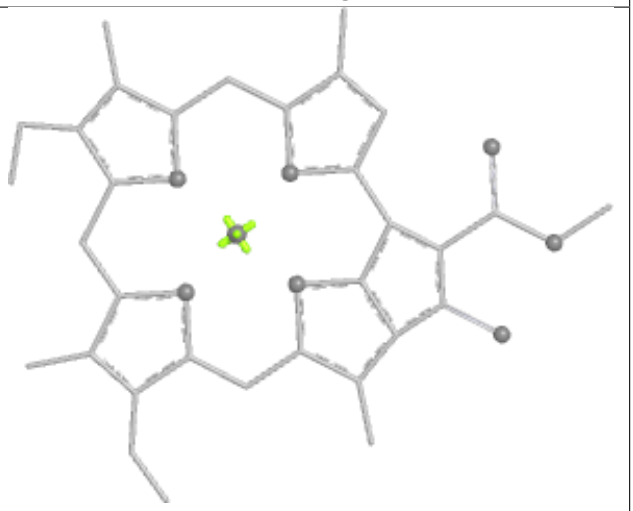
Bond lengths



Bond angles

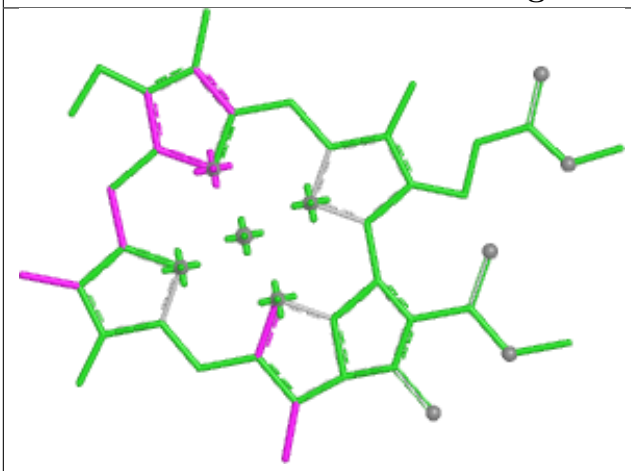


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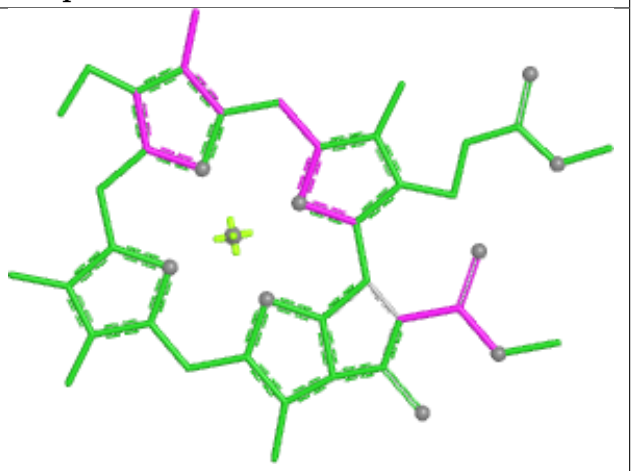


Rings

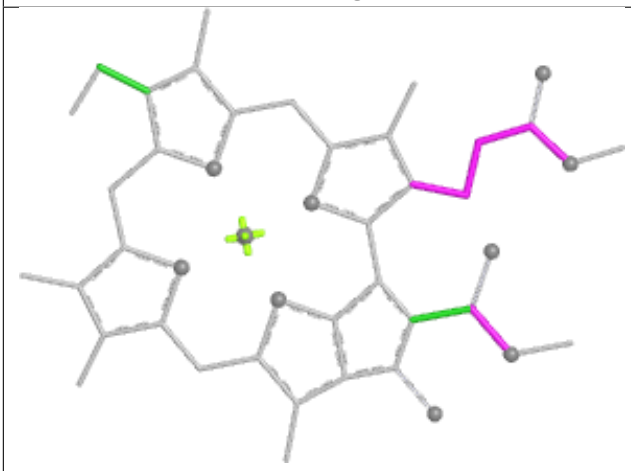
Ligand CLA q 315



Bond lengths



Bond angles

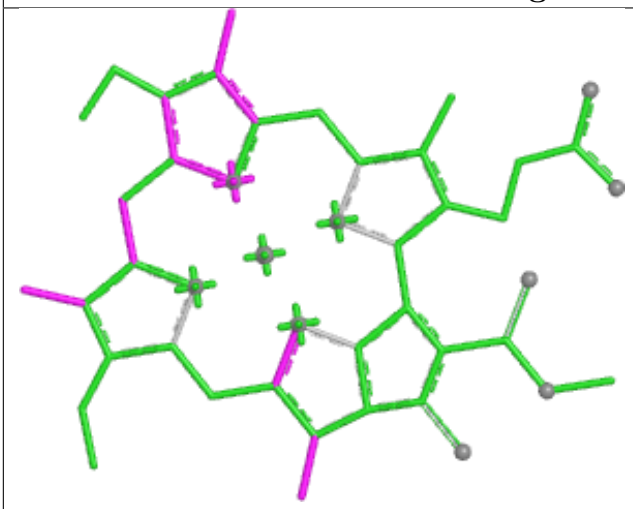


Torsions

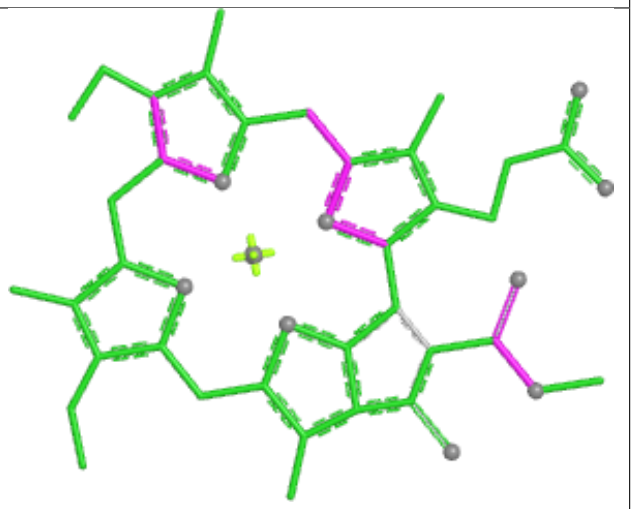


Rings

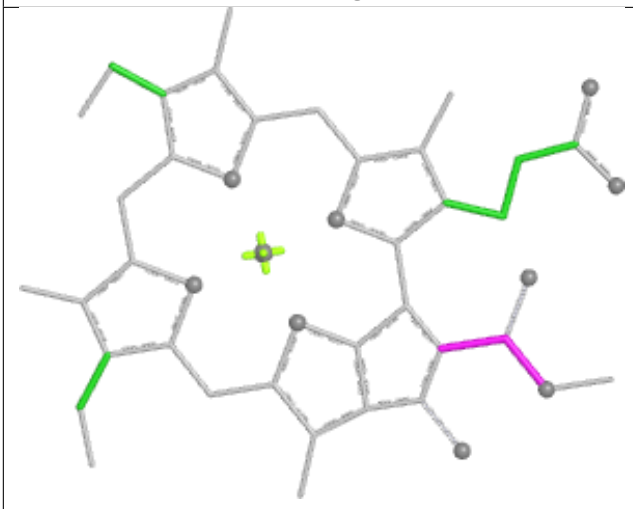
Ligand CLA e 834



Bond lengths



Bond angles

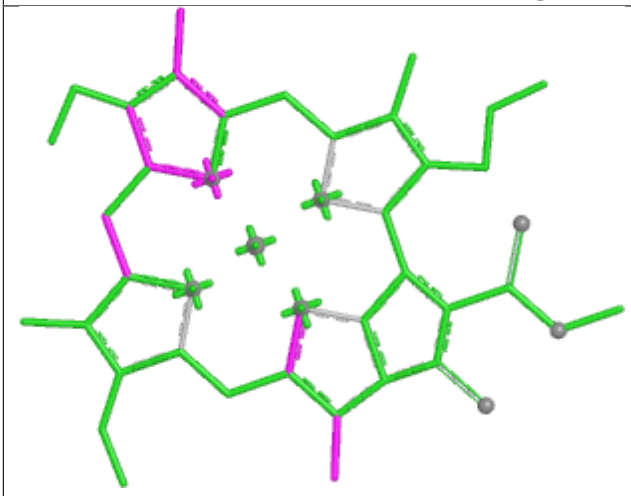


Torsions

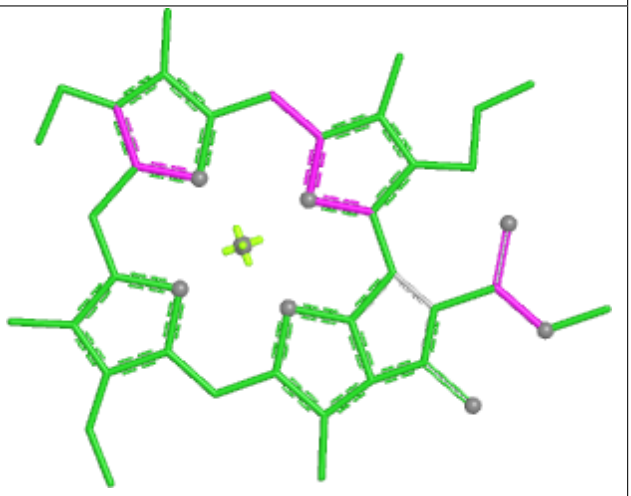


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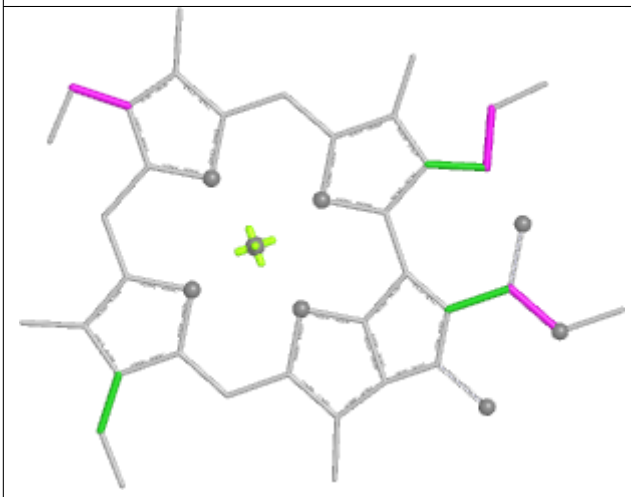
Ligand CLA f 815



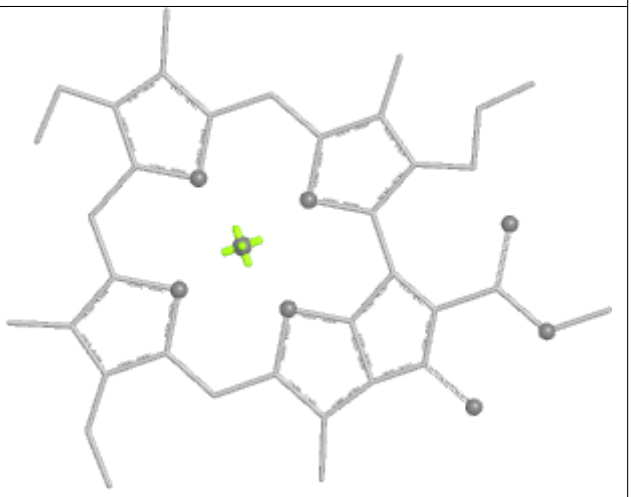
Bond lengths



Bond angles

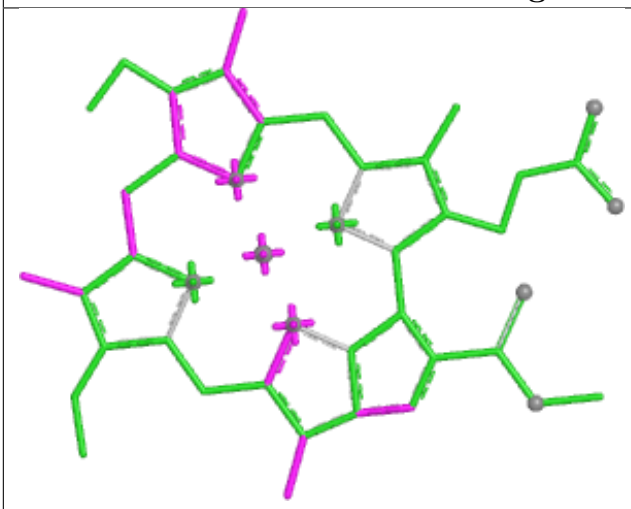


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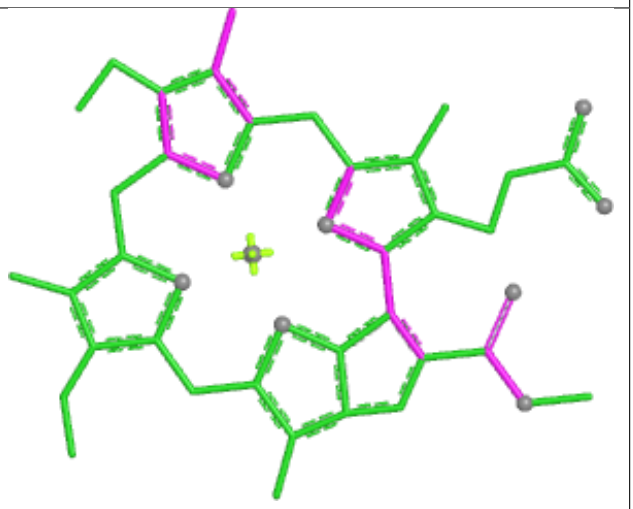


Rings

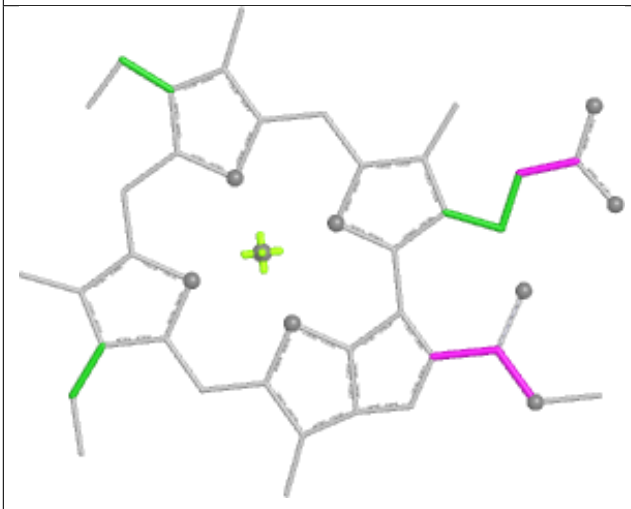
Ligand CLA 1 515



Bond lengths



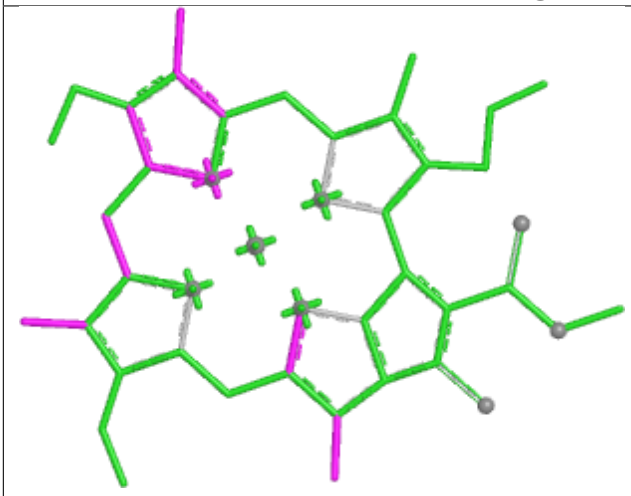
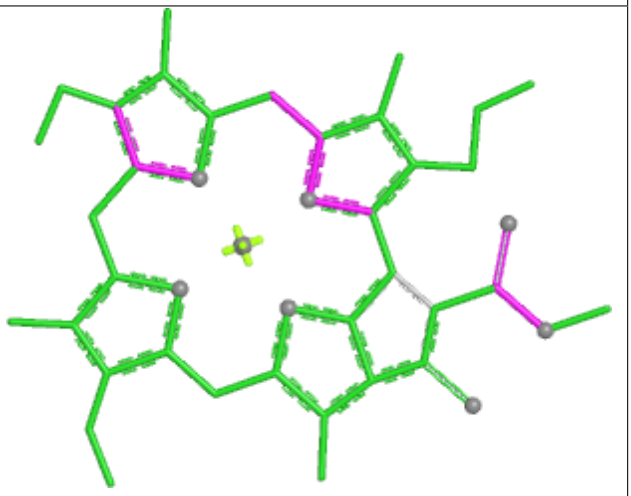
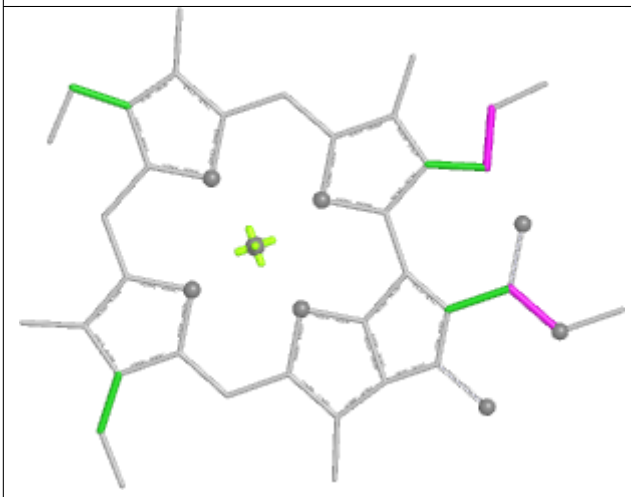
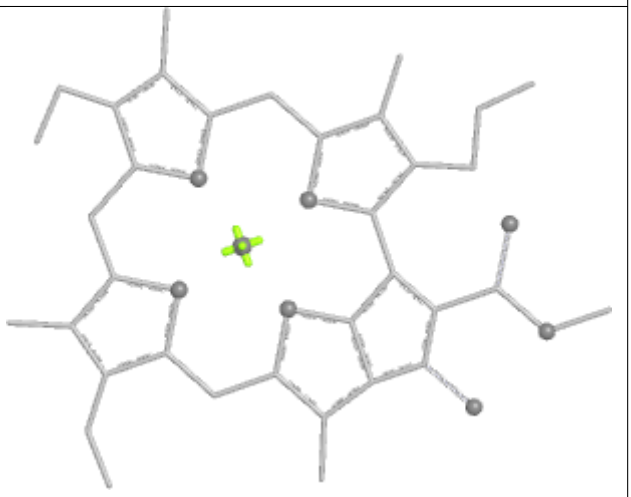
Bond angles

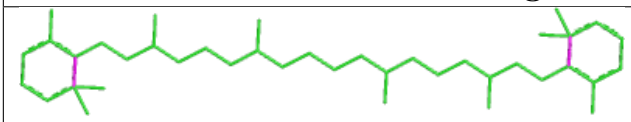
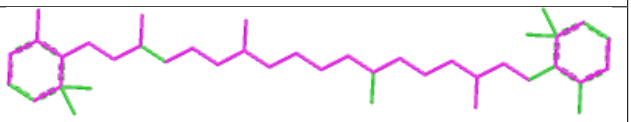
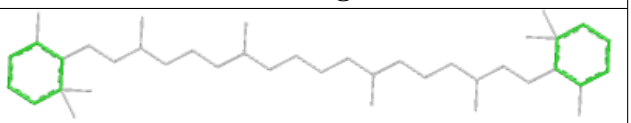


Torsions

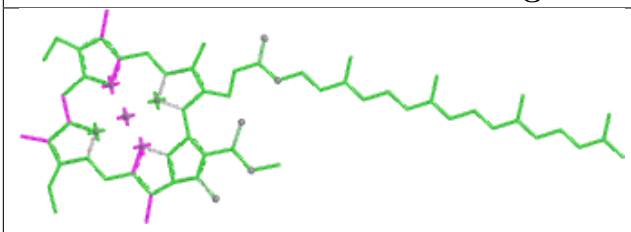


Rings

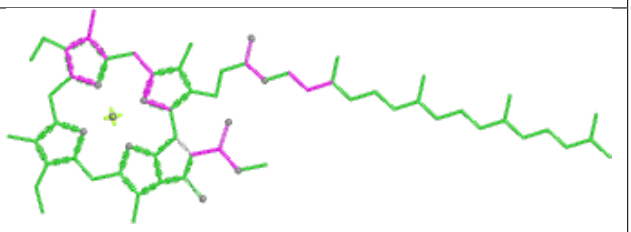
Ligand CLA f 833	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR F 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

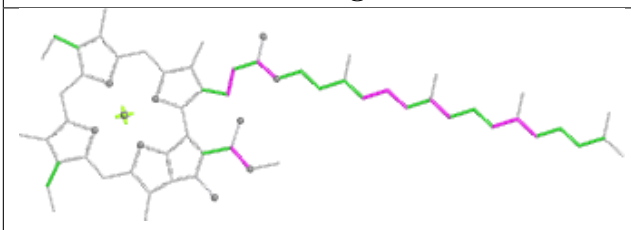
Ligand CLA A 838



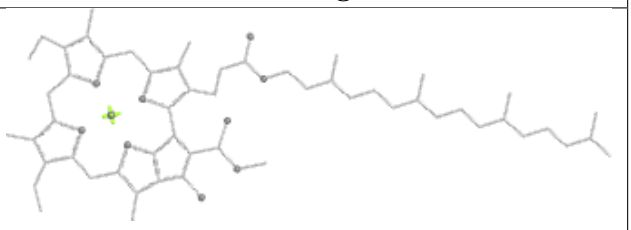
Bond lengths



Bond angles

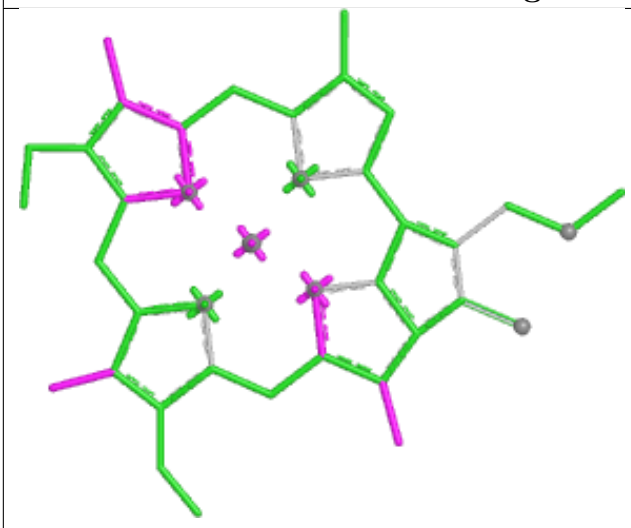


Torsions

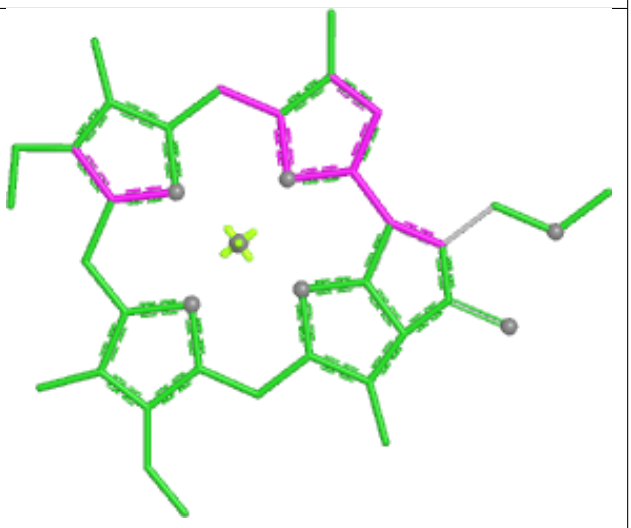


Rings

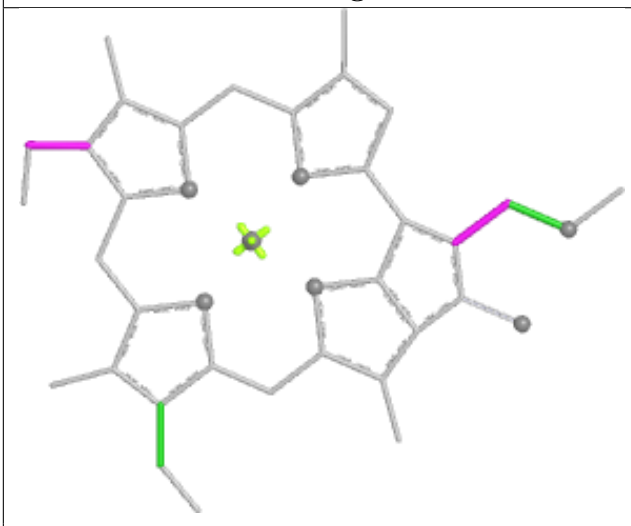
Ligand CLA A 807



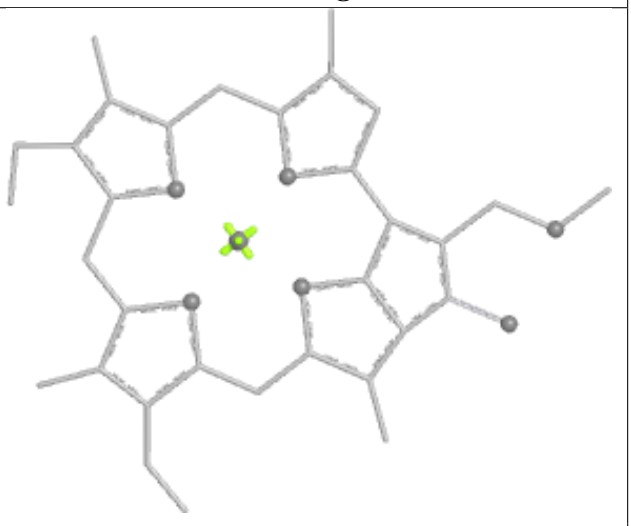
Bond lengths



Bond angles

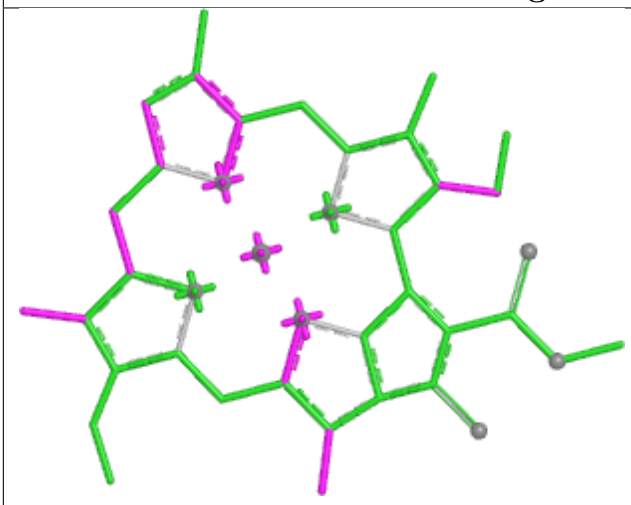


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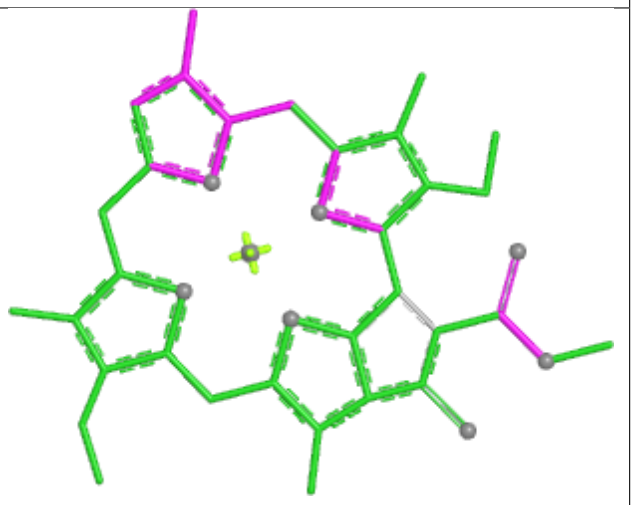


Rings

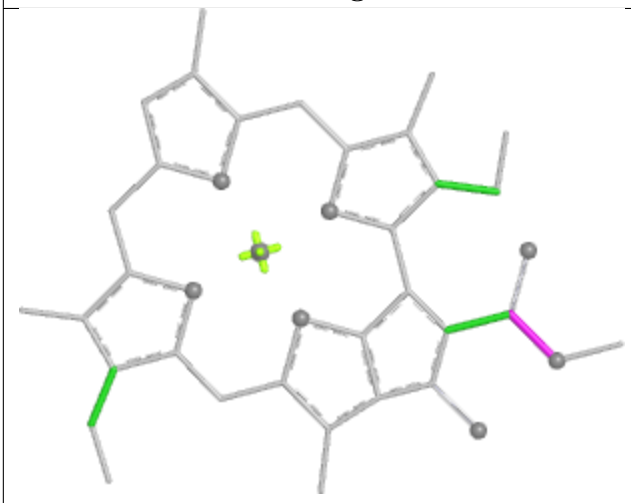
Ligand CLA 3 309



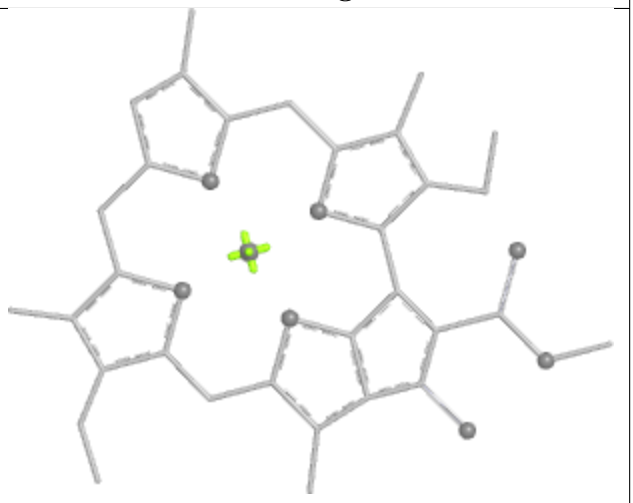
Bond lengths



Bond angles

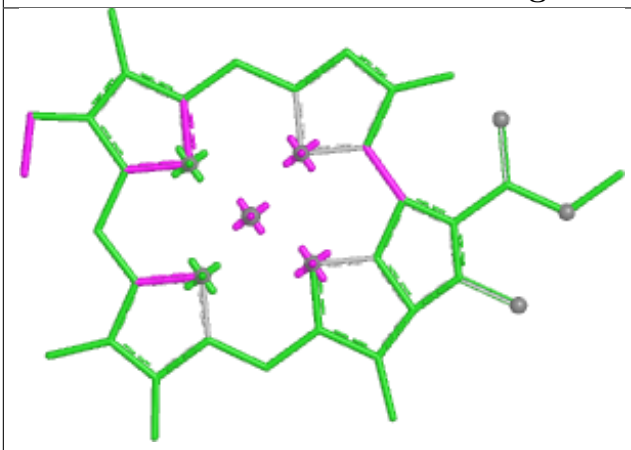


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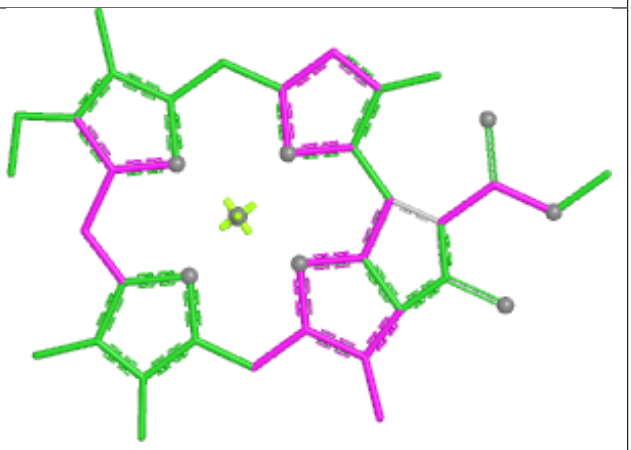


Rings

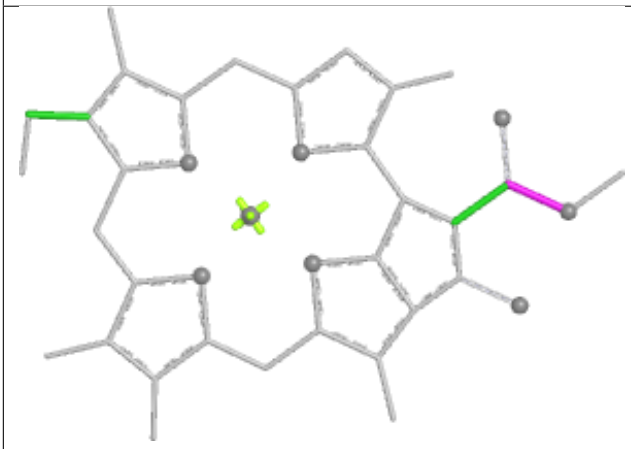
Ligand CLA e 818



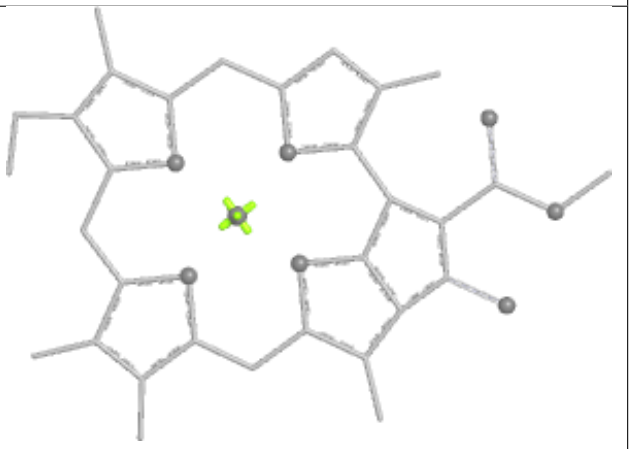
Bond lengths



Bond angles

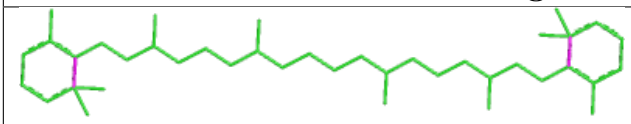


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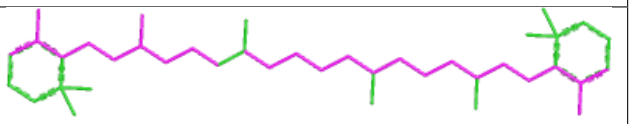


Rings

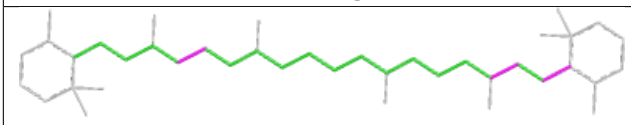
Ligand BCR e 846



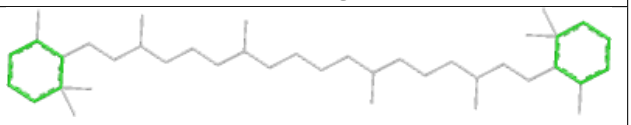
Bond lengths



Bond angles

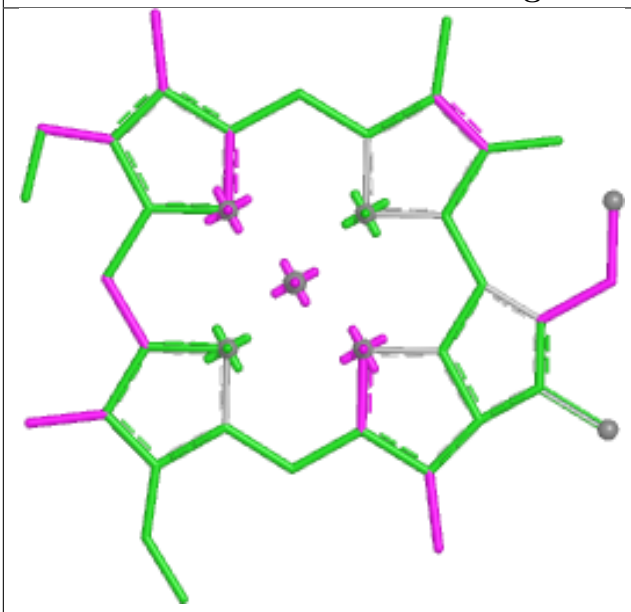


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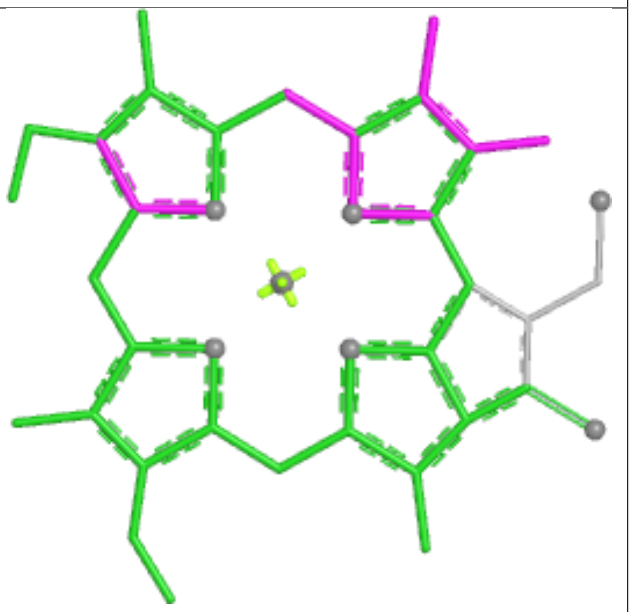


Rings

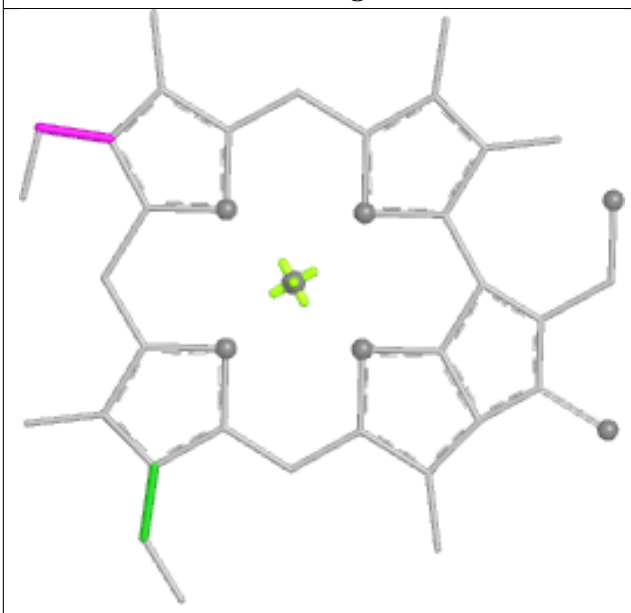
Ligand CLA A 817



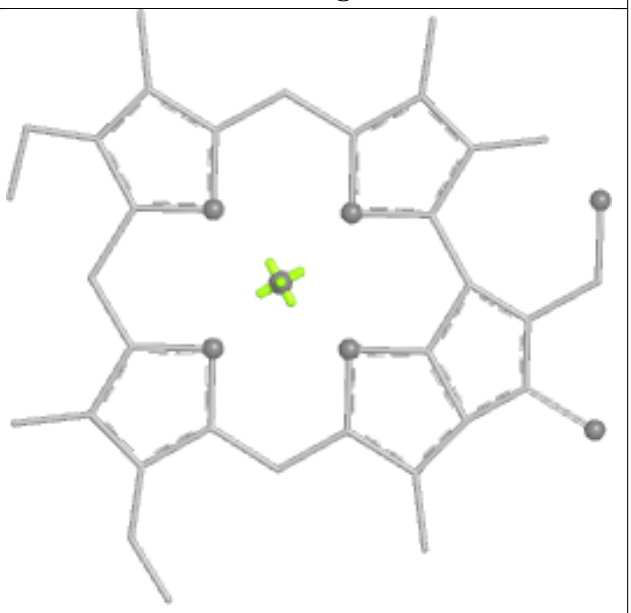
Bond lengths



Bond angles

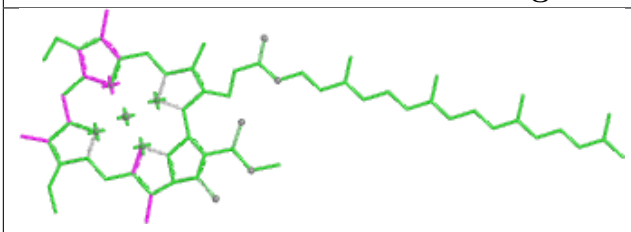


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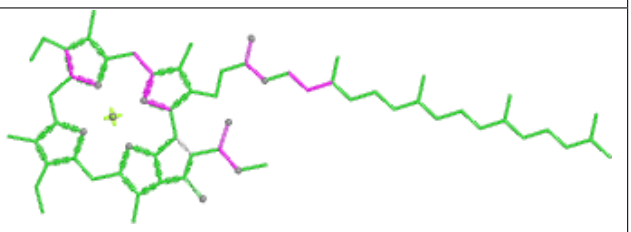


Rings

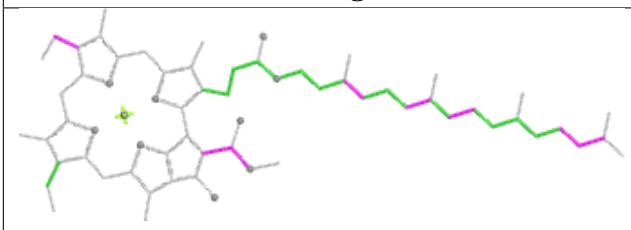
Ligand CLA f 810



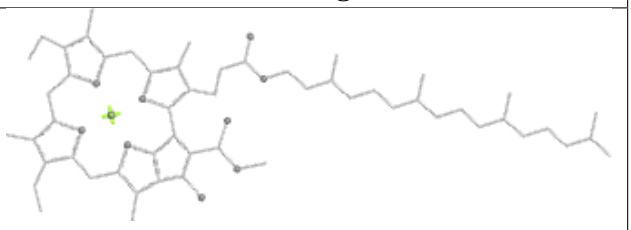
Bond lengths



Bond angles

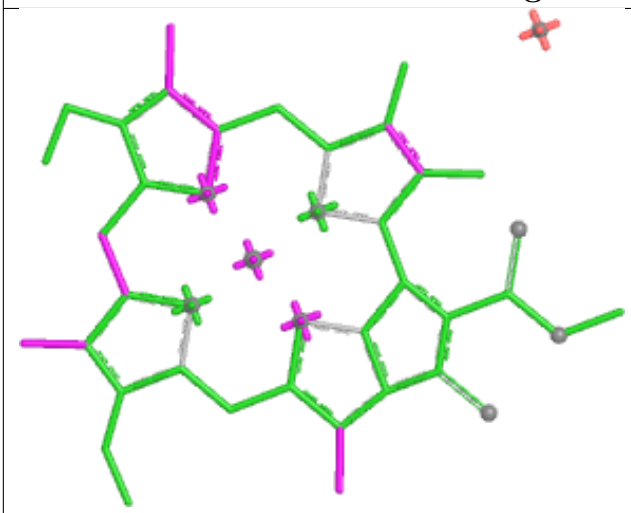


Torsions

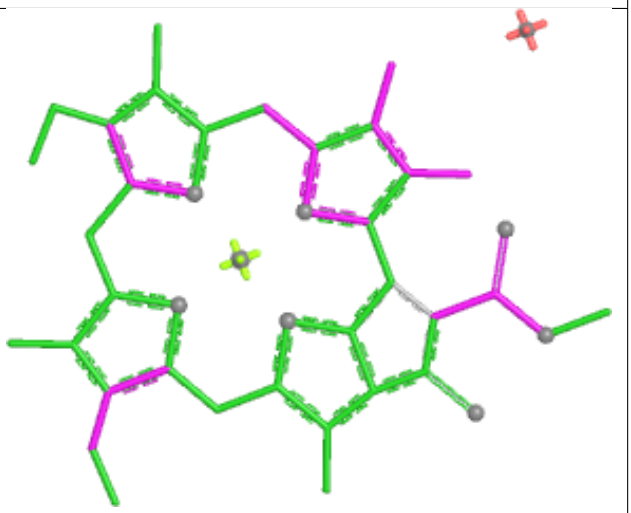


Rings

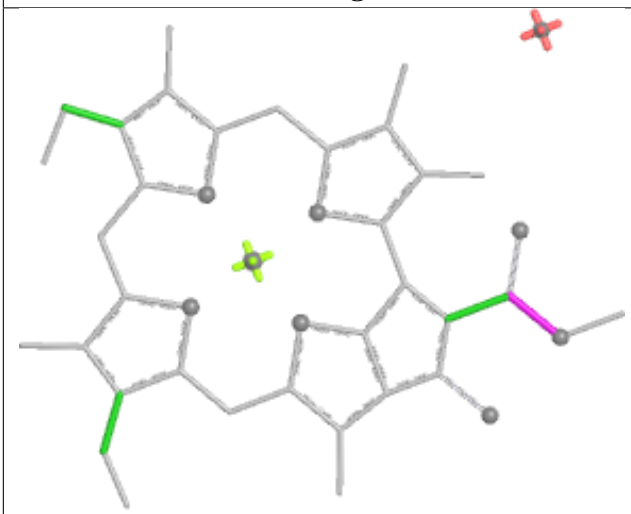
Ligand CLA B 828



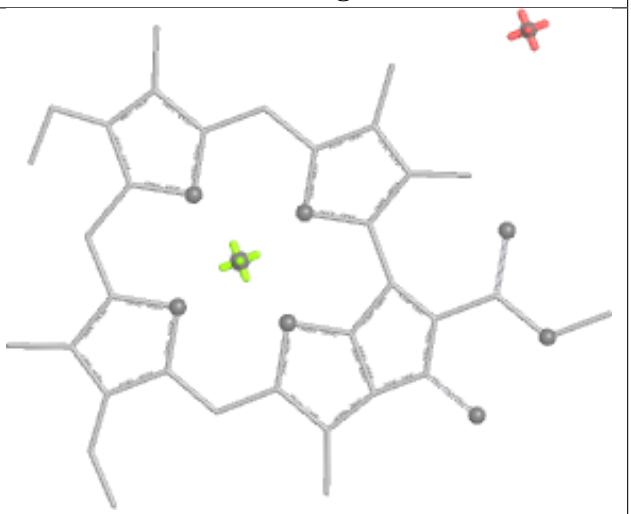
Bond lengths



Bond angles

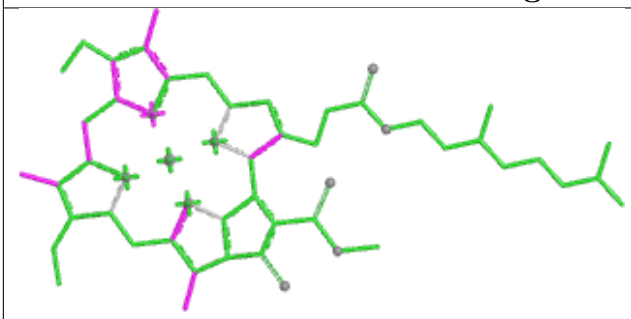


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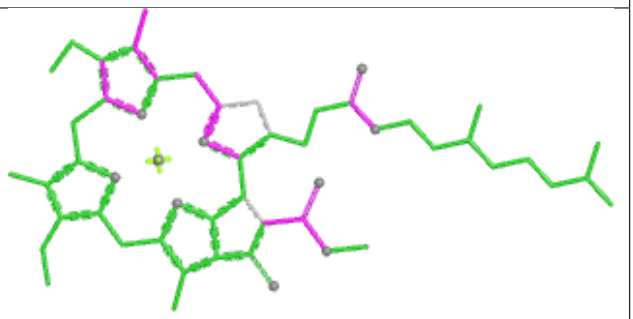


Rings

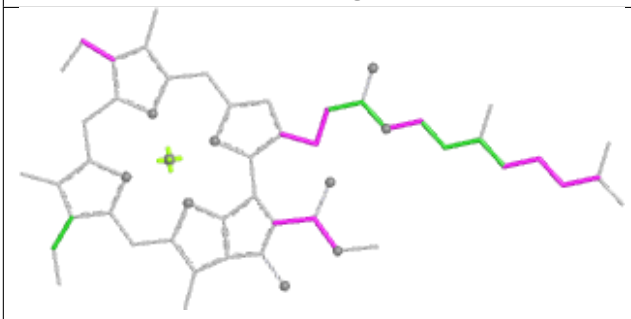
Ligand CLA A 823



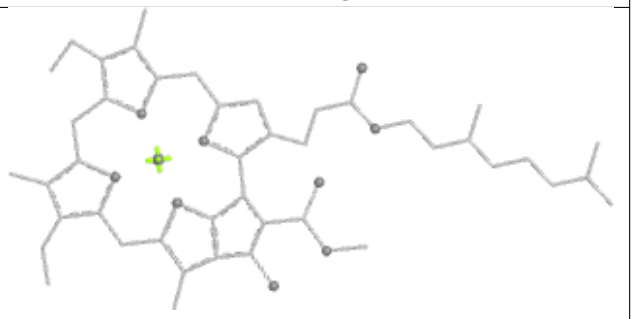
Bond lengths



Bond angles

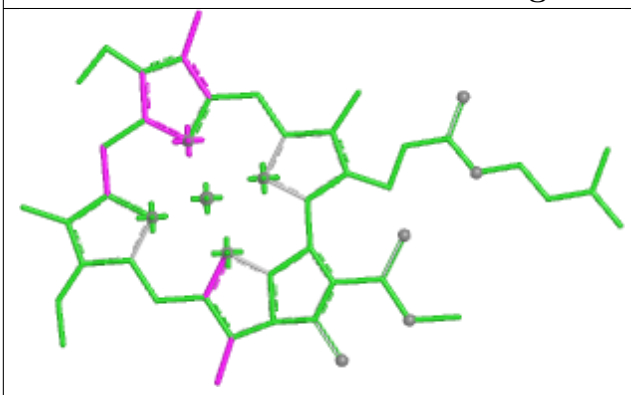


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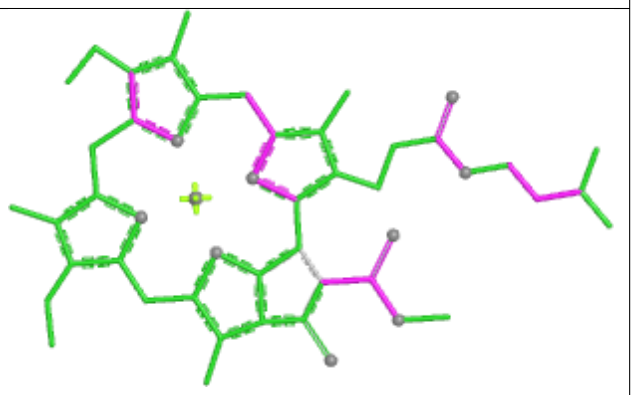


Rings

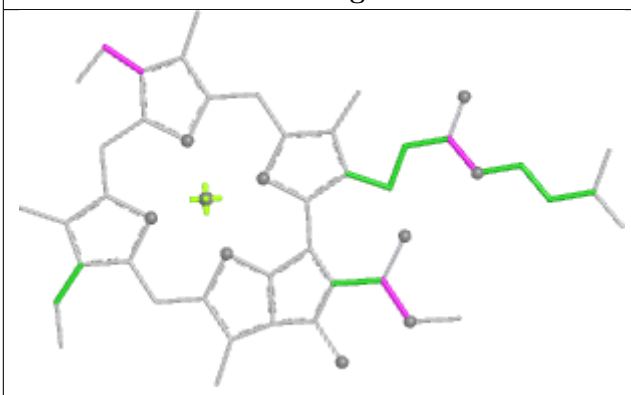
Ligand CLA e 809



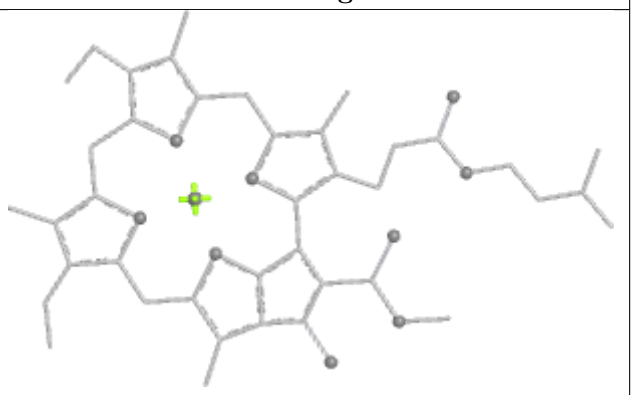
Bond lengths



Bond angles

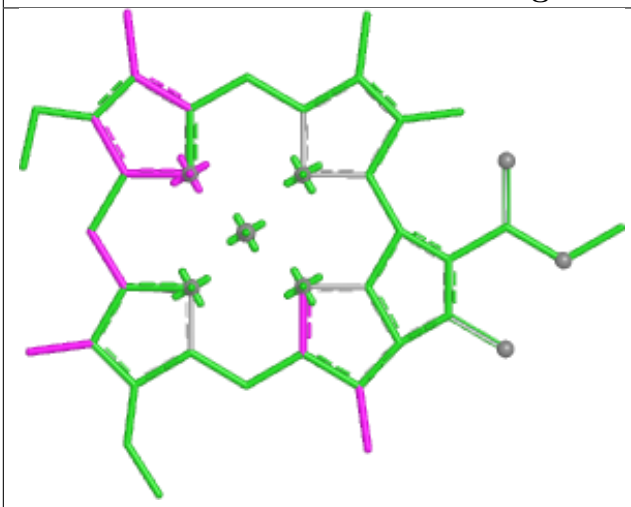


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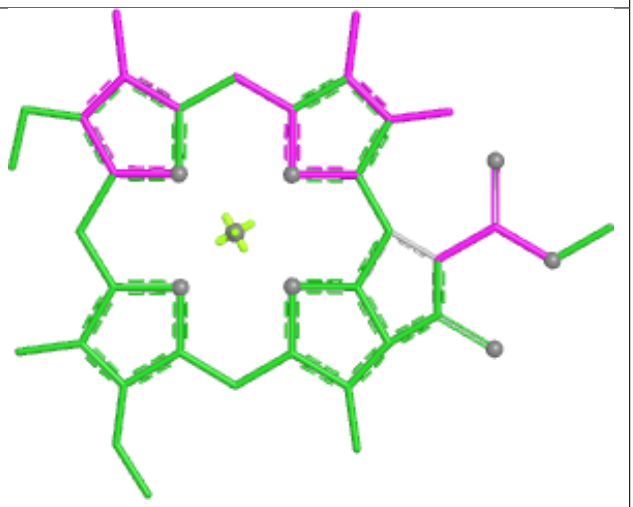


Rings

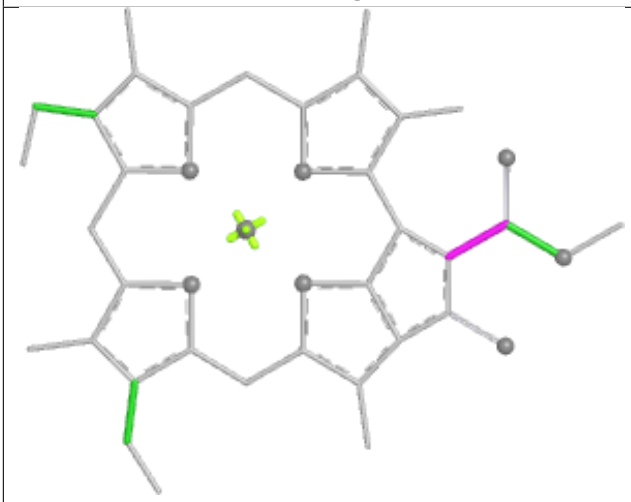
Ligand CLA f 807



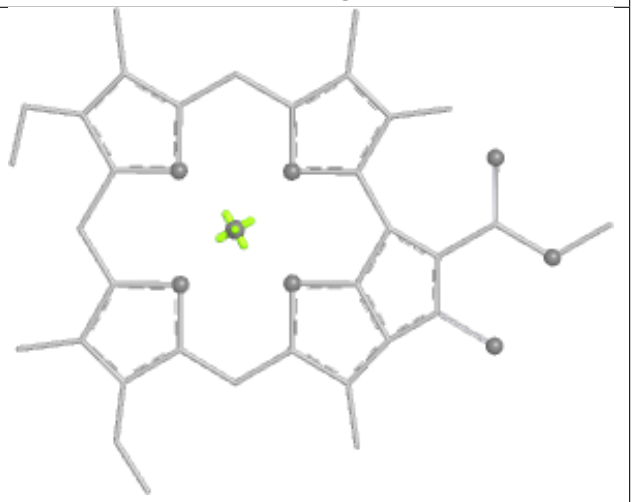
Bond lengths



Bond angles

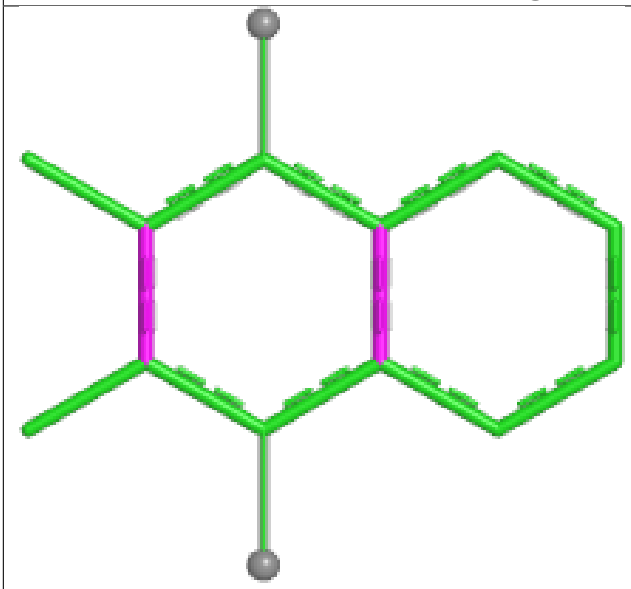


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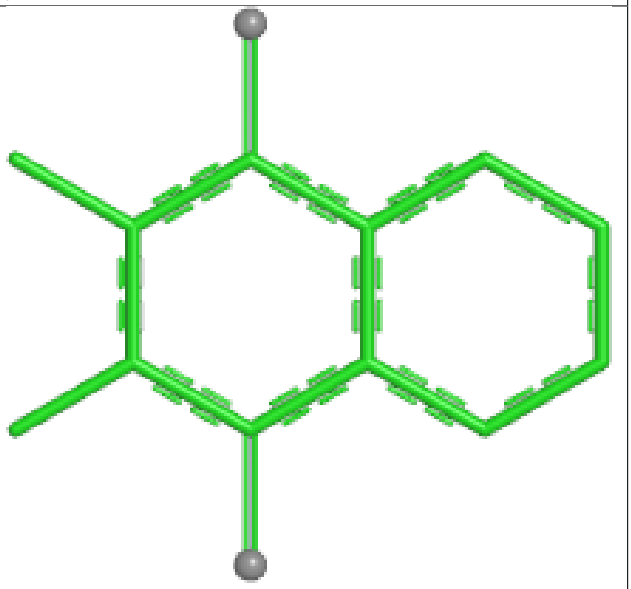


Rings

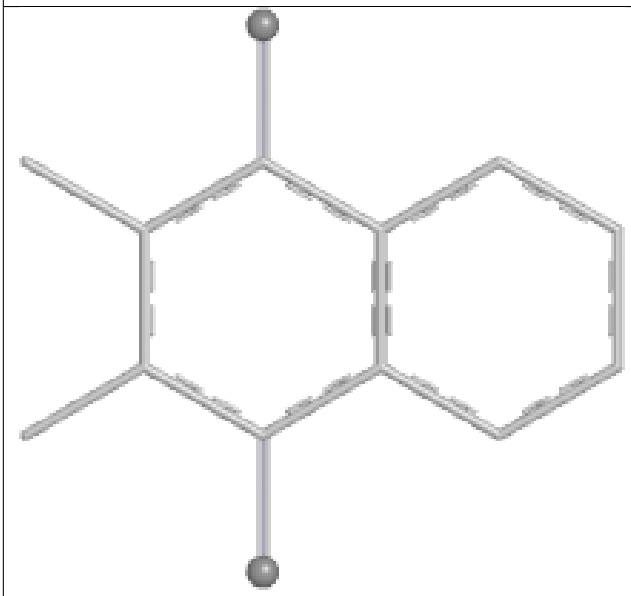
Ligand PQN e 842



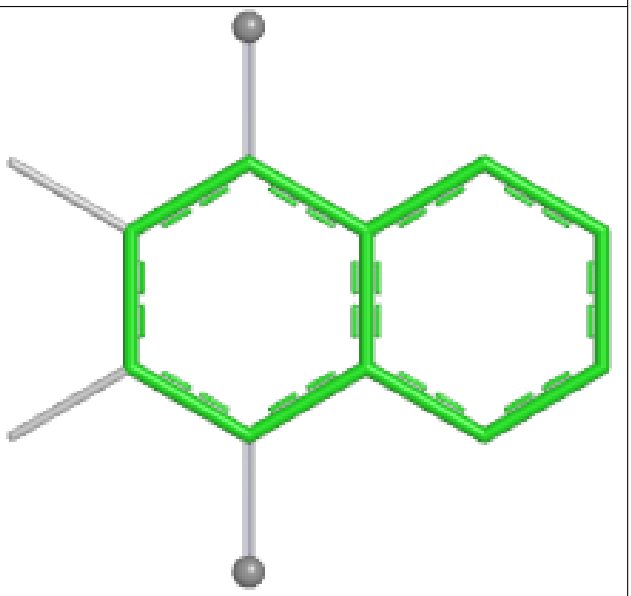
Bond lengths



Bond angles

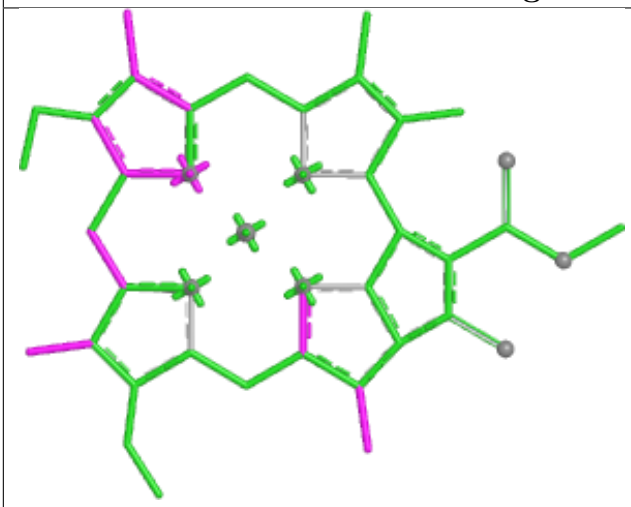


Torsions

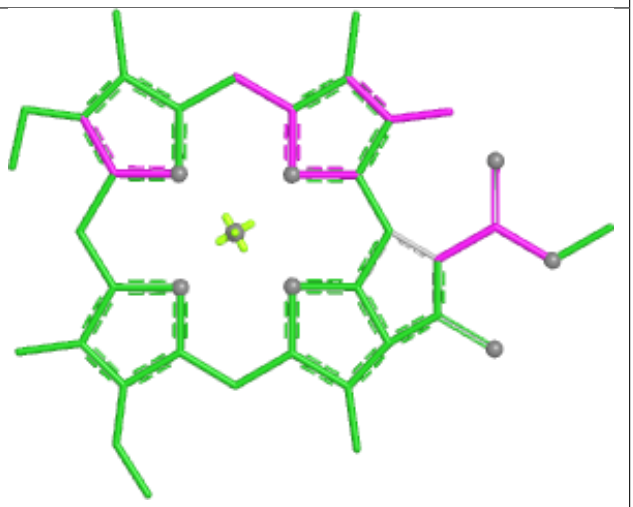


Rings

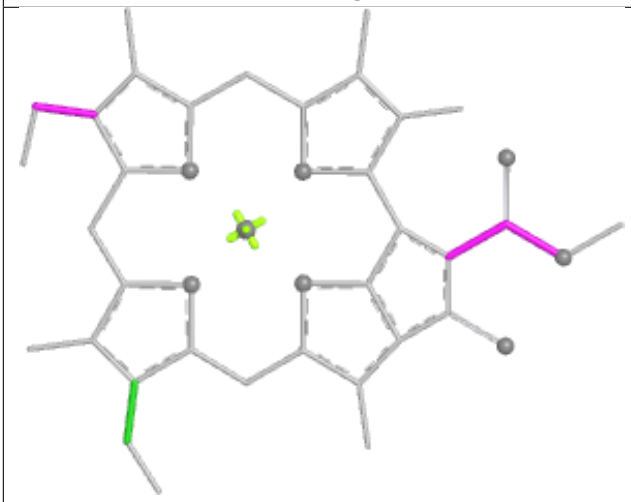
Ligand CLA K 202



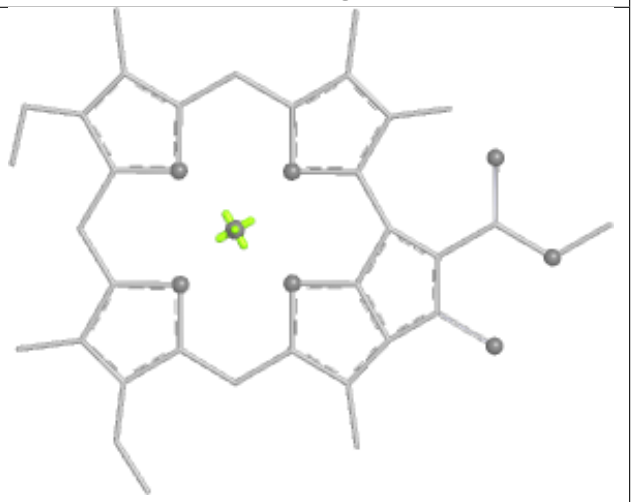
Bond lengths



Bond angles

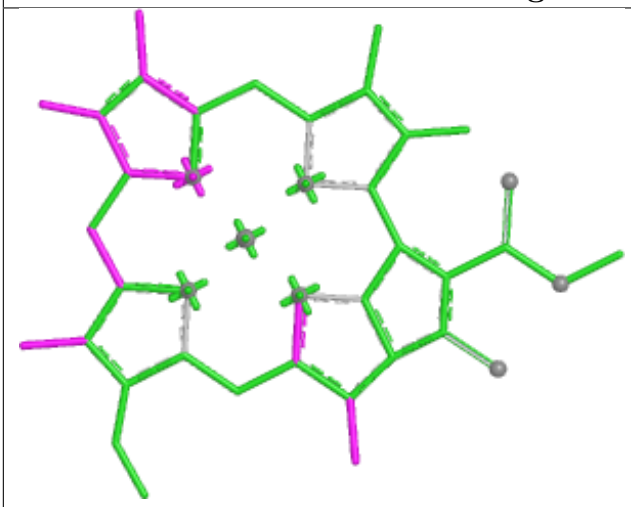


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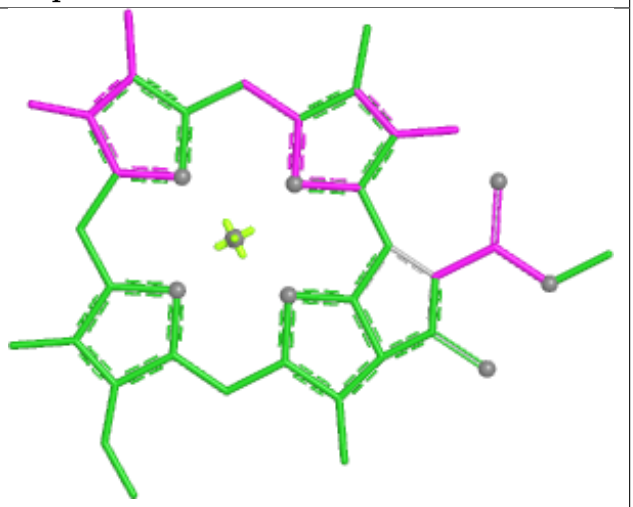


Rings

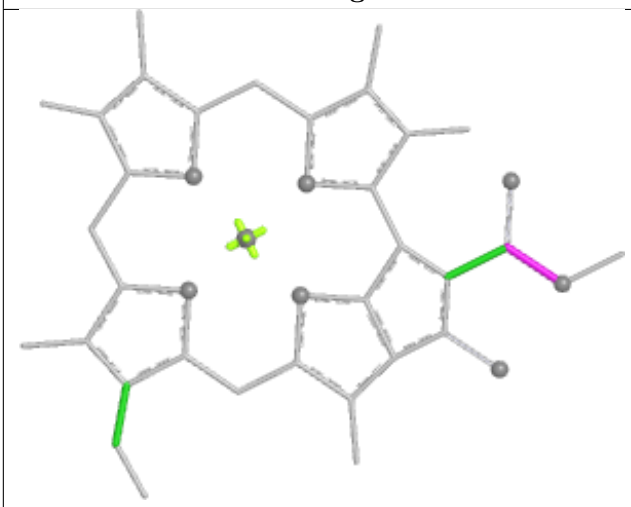
Ligand CLA p 507



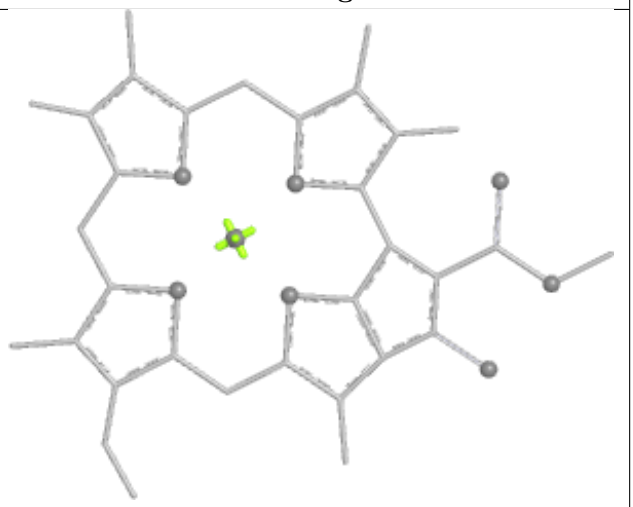
Bond lengths



Bond angles

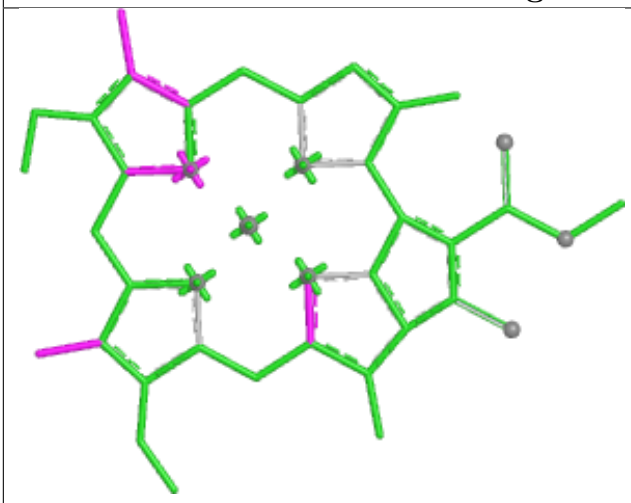


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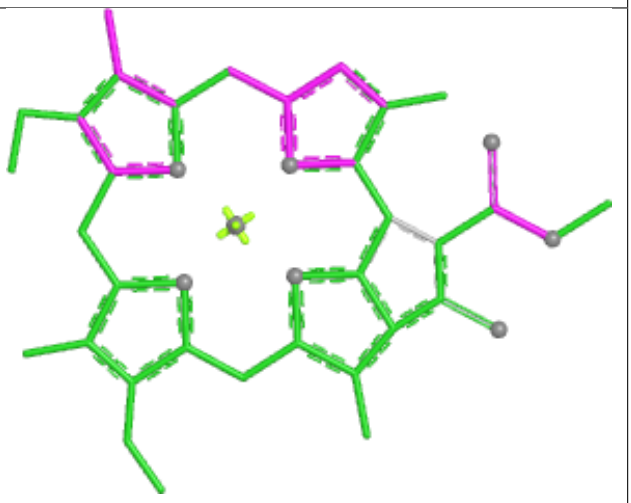


Rings

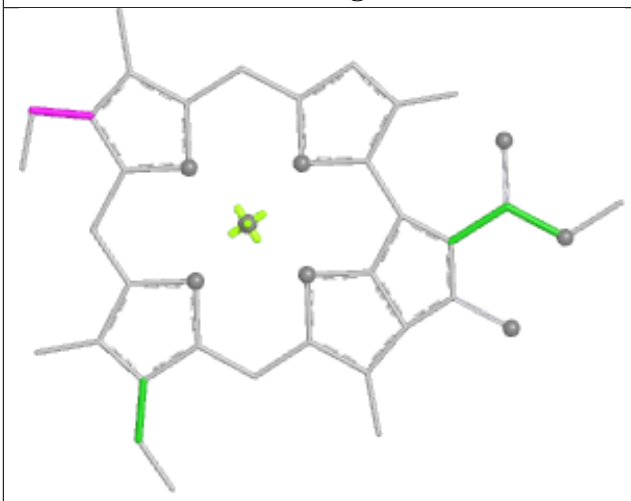
Ligand CLA L 302



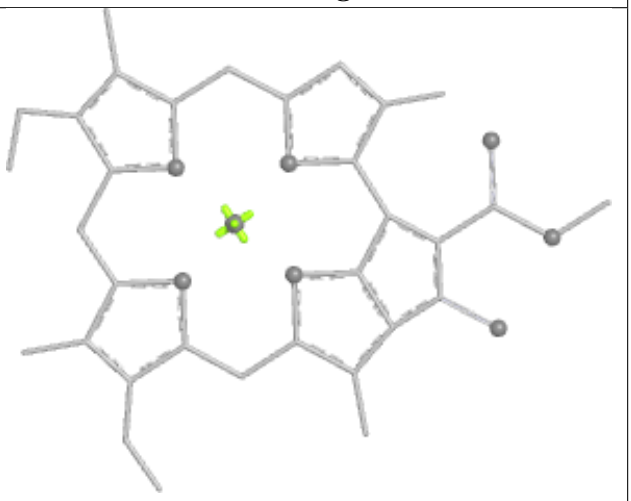
Bond lengths



Bond angles

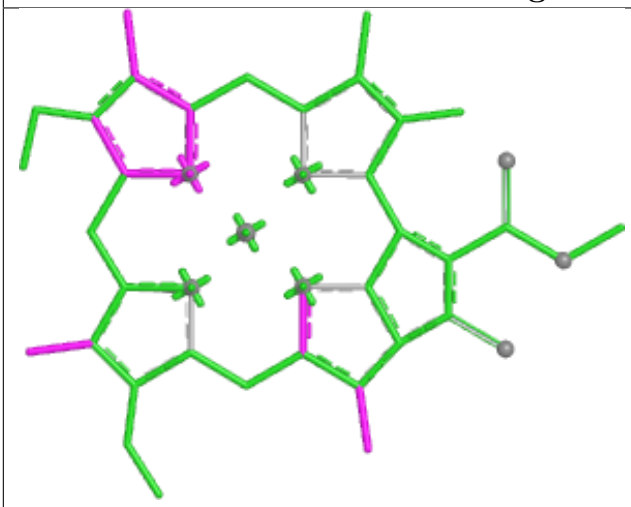


Torsions

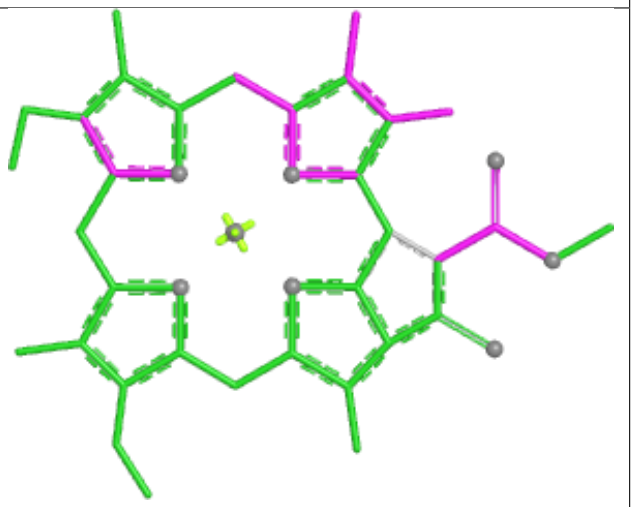


Rings

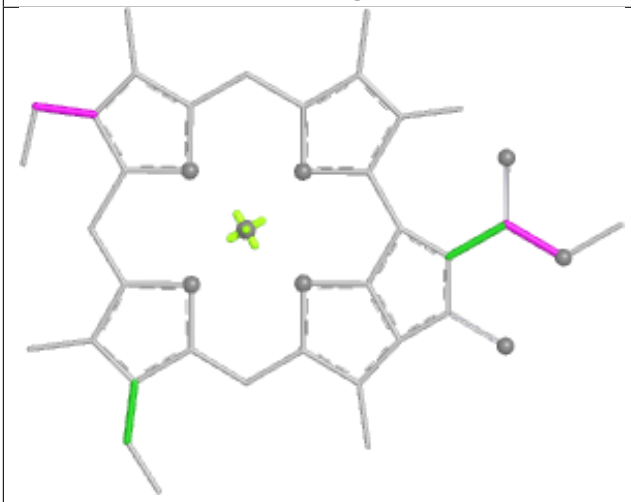
Ligand CLA 3 301



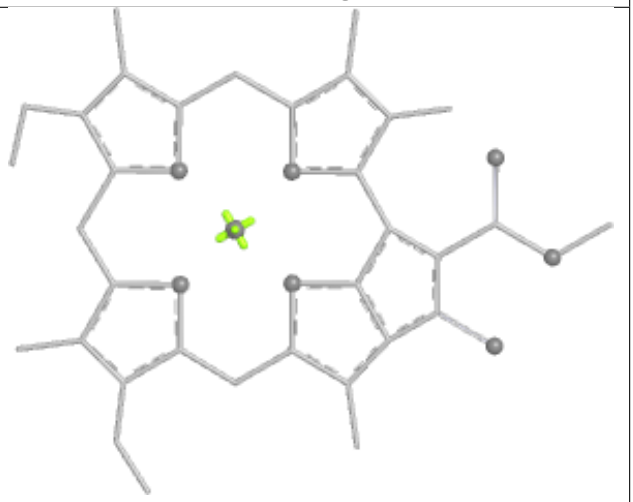
Bond lengths



Bond angles

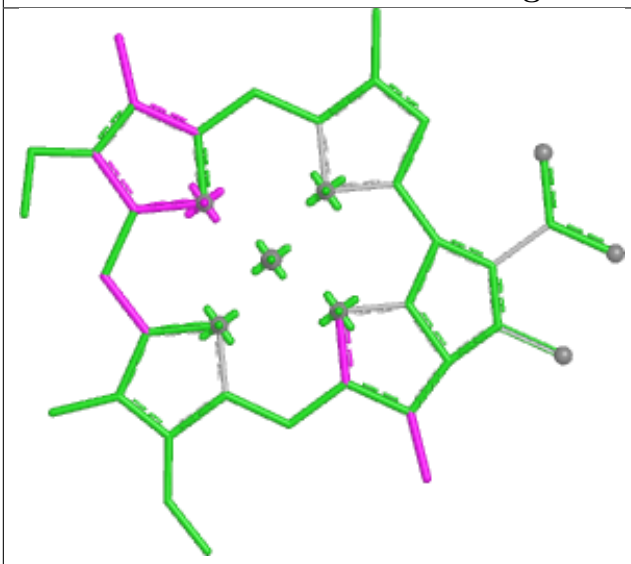


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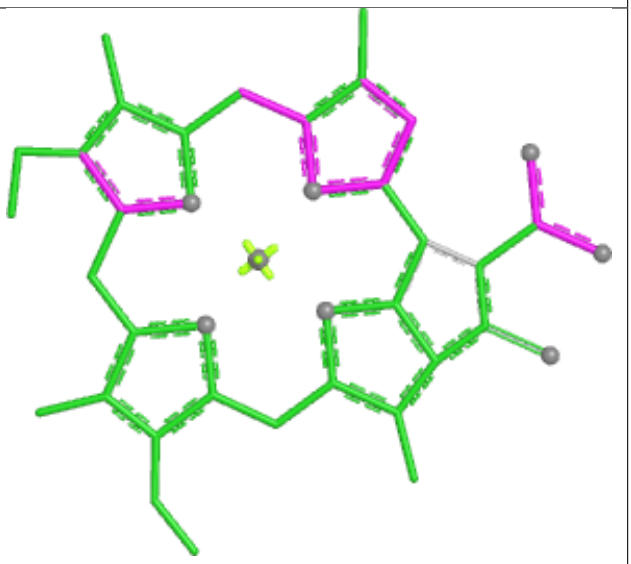


Rings

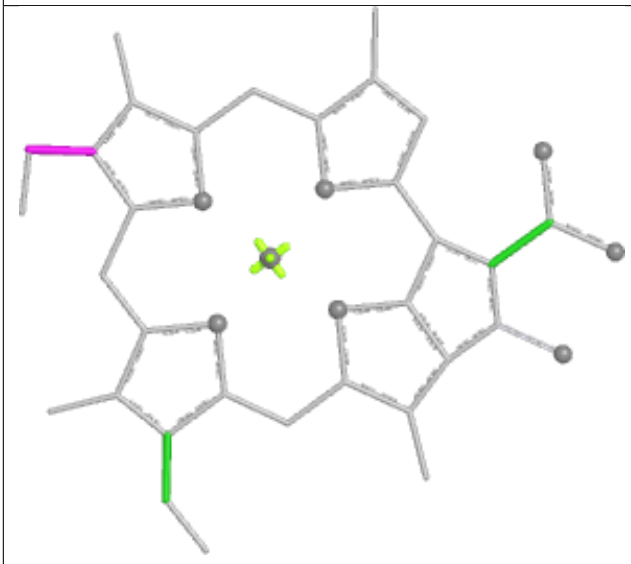
Ligand CLA K 205



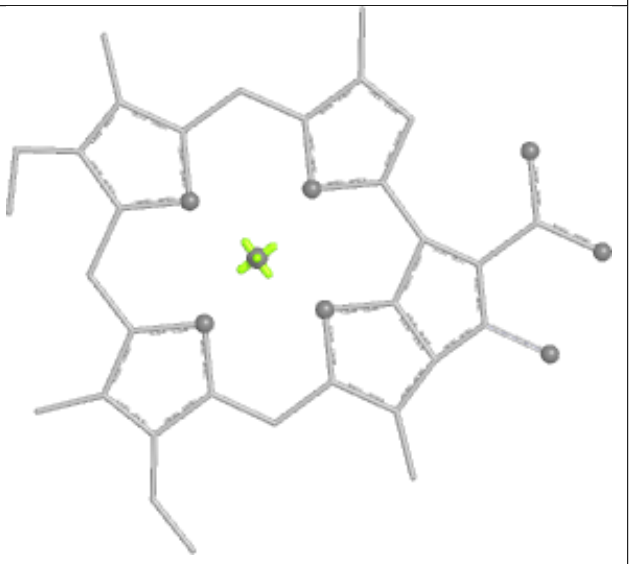
Bond lengths



Bond angles

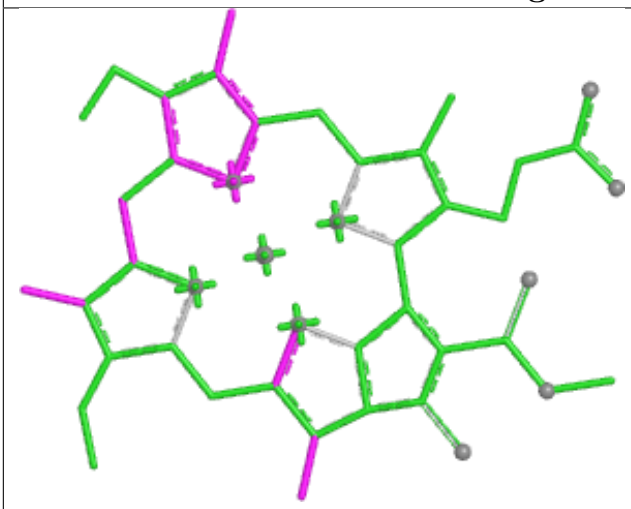


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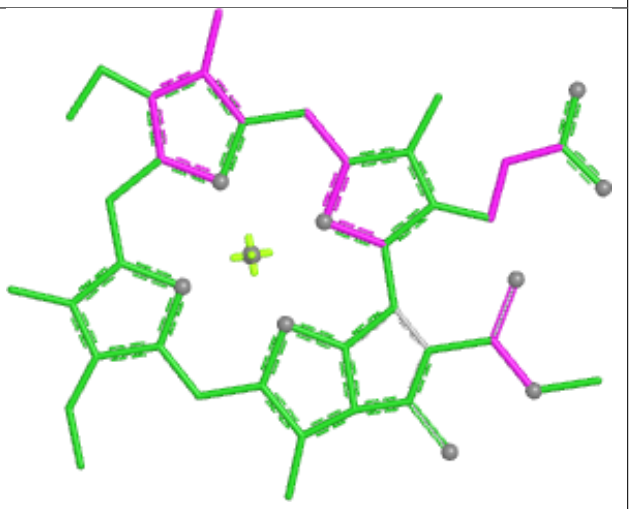


Rings

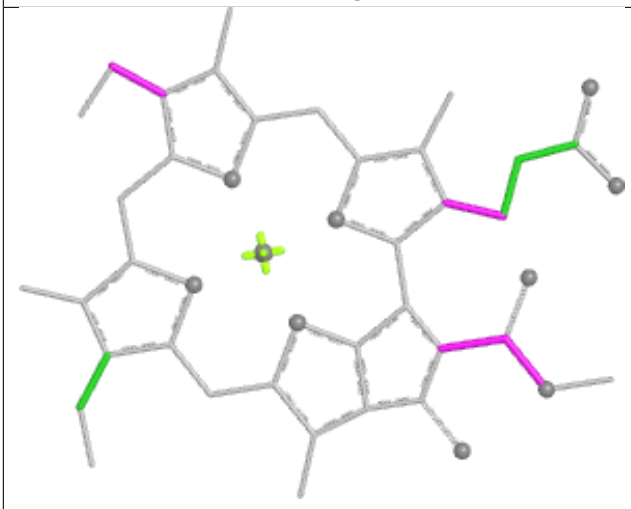
Ligand CLA 5 309



Bond lengths



Bond angles

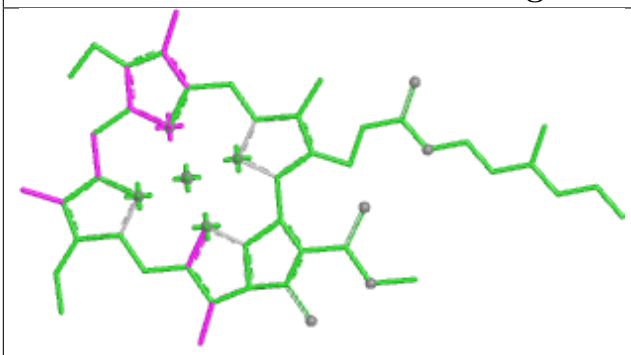


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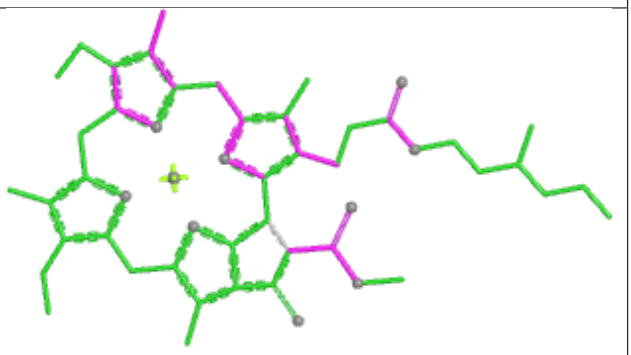


Rings

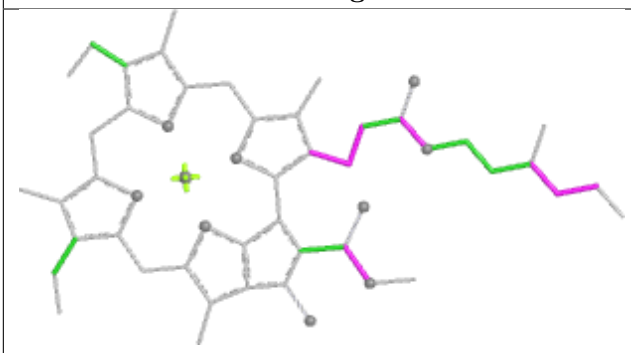
Ligand CLA L 303



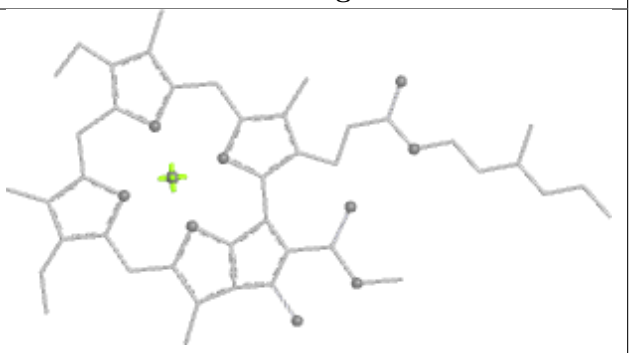
Bond lengths



Bond angles

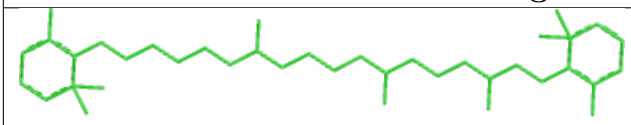


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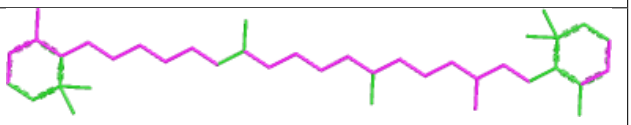


Rings

Ligand BCR f 850



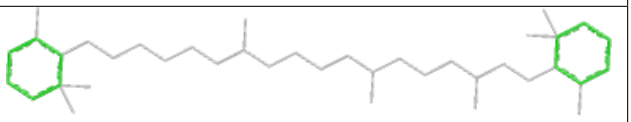
Bond lengths



Bond angles

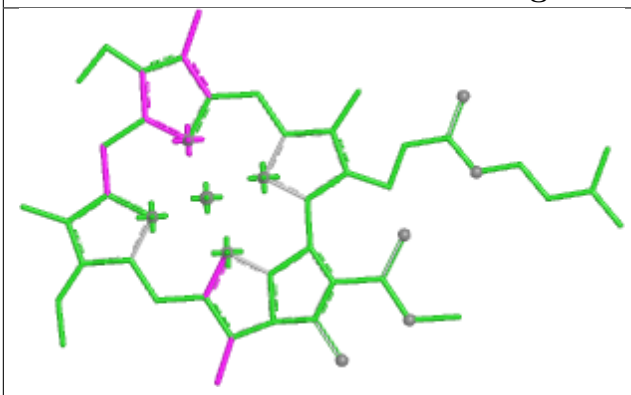


Torsions

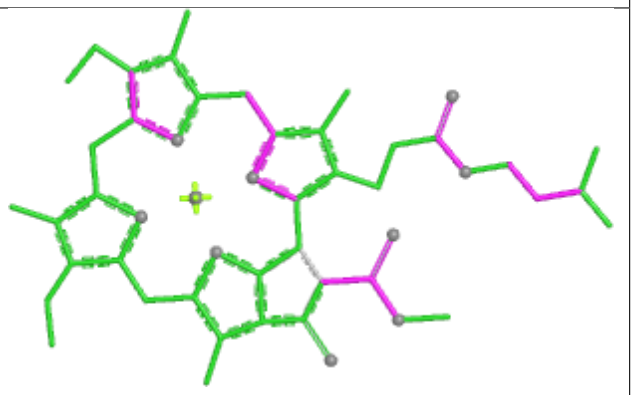


Rings

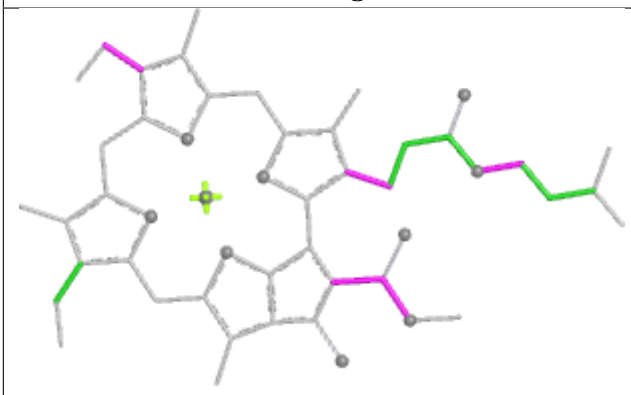
Ligand CLA r 317



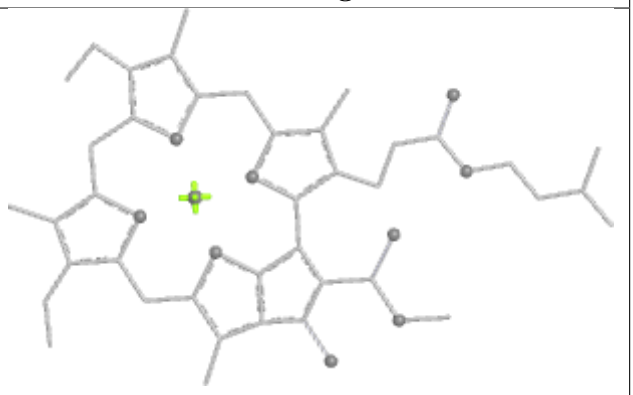
Bond lengths



Bond angles

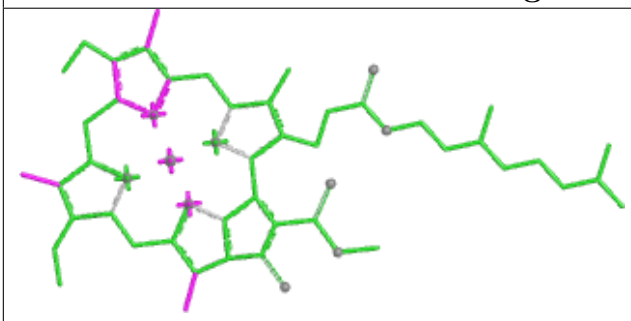


Torsions

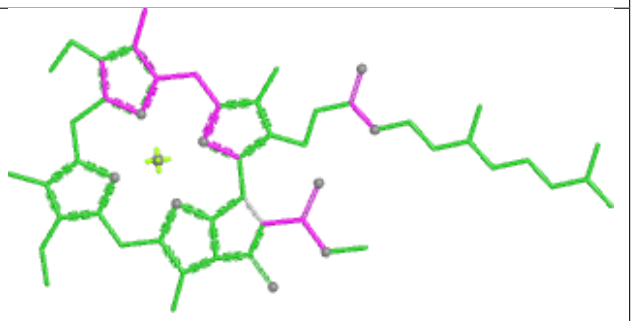


Rings

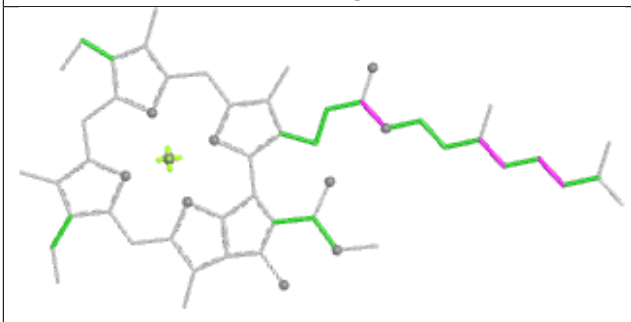
Ligand CLA A 829



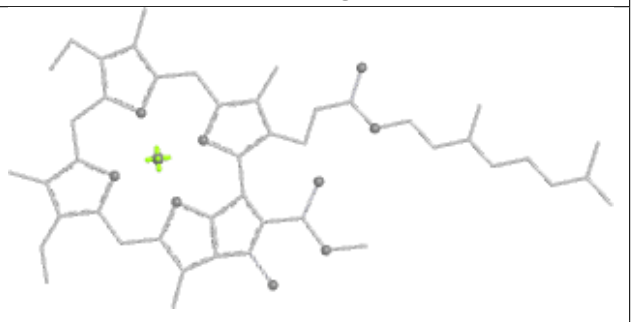
Bond lengths



Bond angles

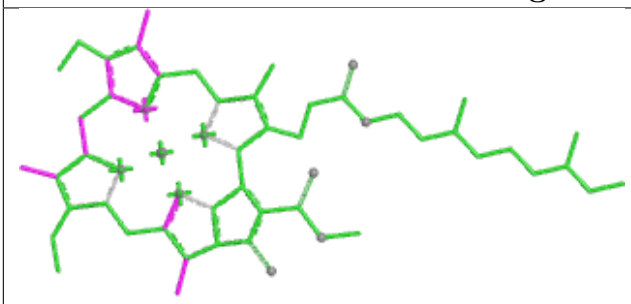


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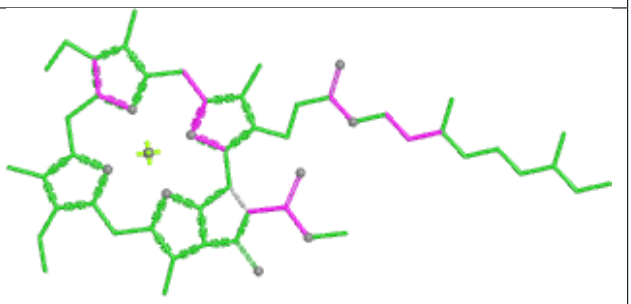


Rings

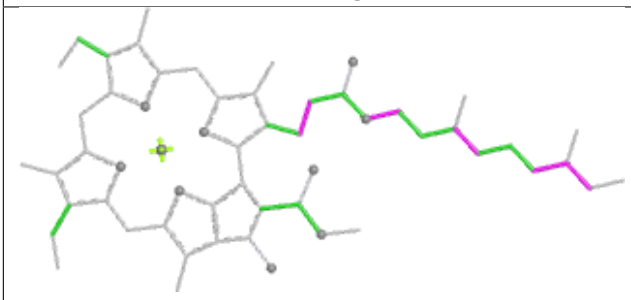
Ligand CLA e 824



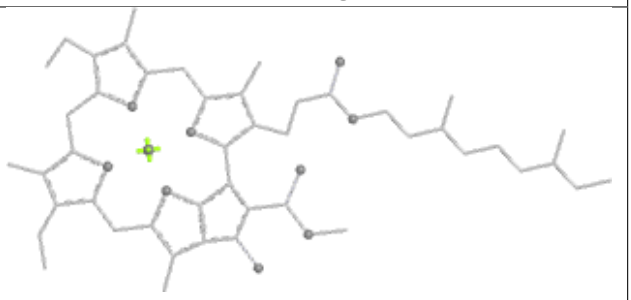
Bond lengths



Bond angles

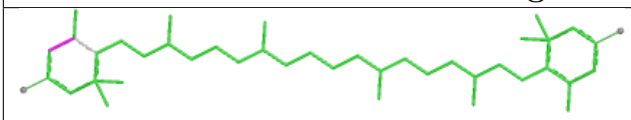


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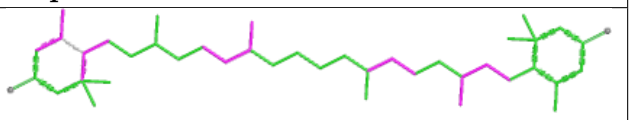


Rings

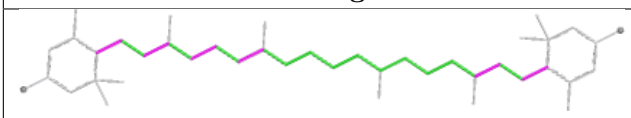
Ligand LUT p 502



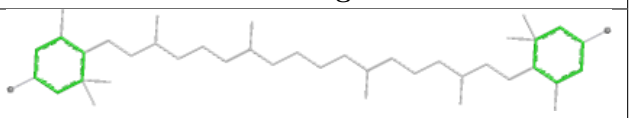
Bond lengths



Bond angles

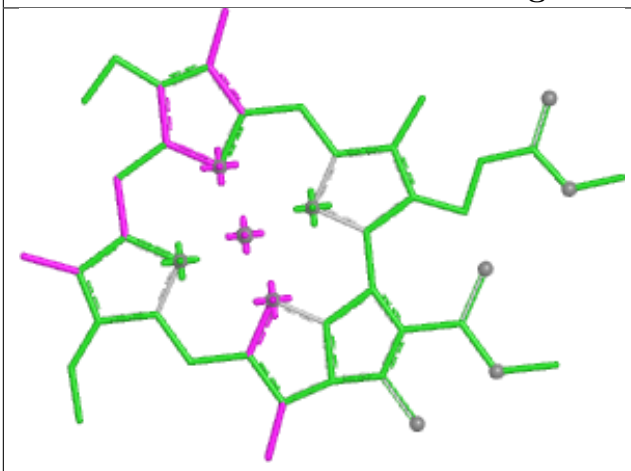


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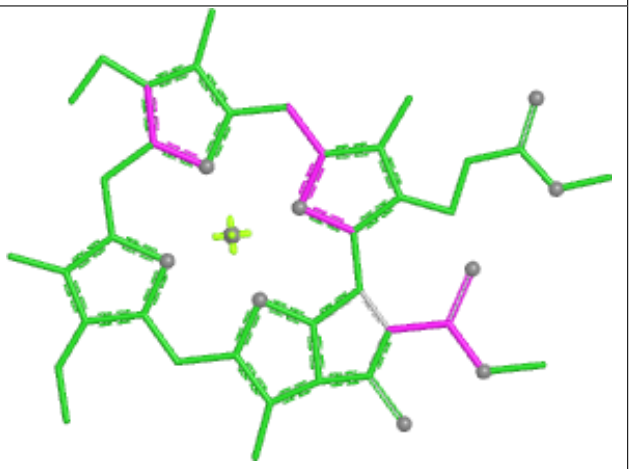


Rings

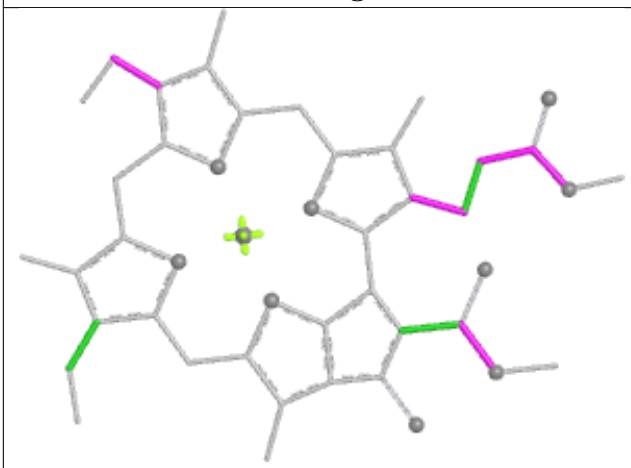
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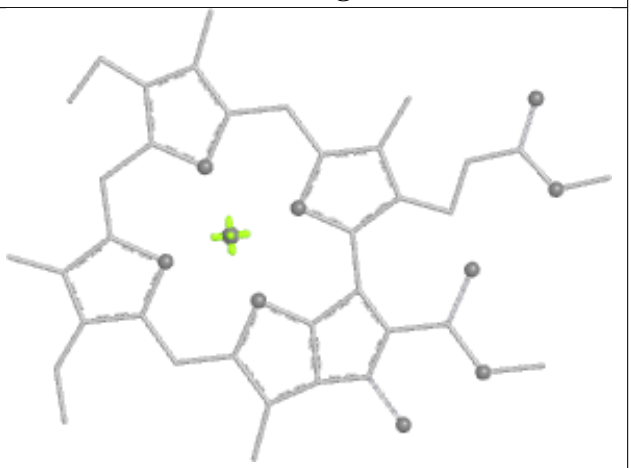
Bond lengths



Bond angles

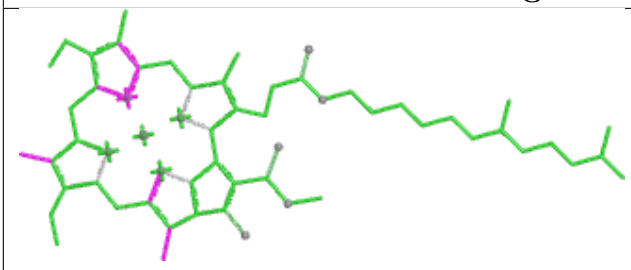


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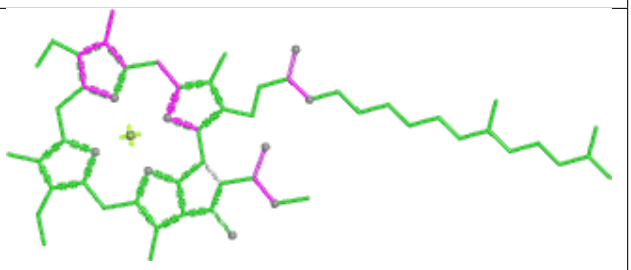


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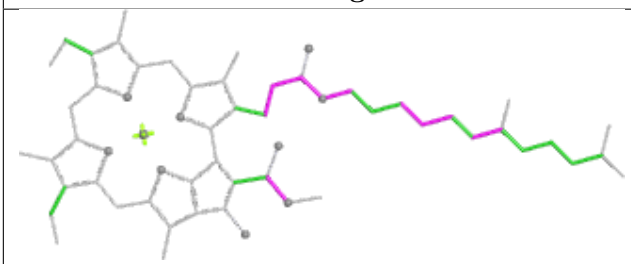
Ligand CLA A 816



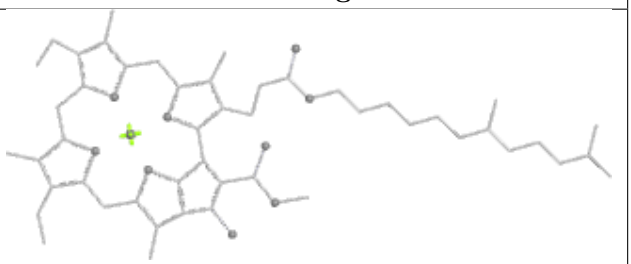
Bond lengths



Bond angles

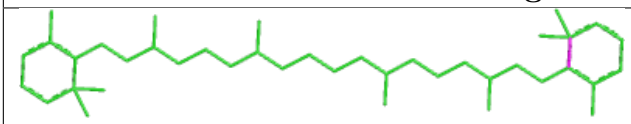


Torsions

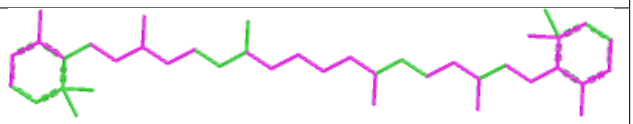


Rings

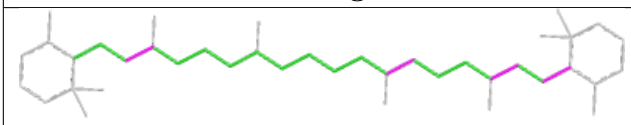
Ligand BCR L 305



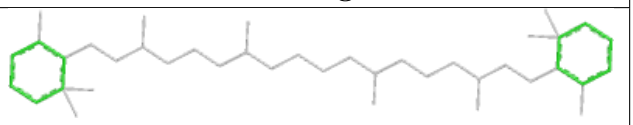
Bond lengths



Bond angles

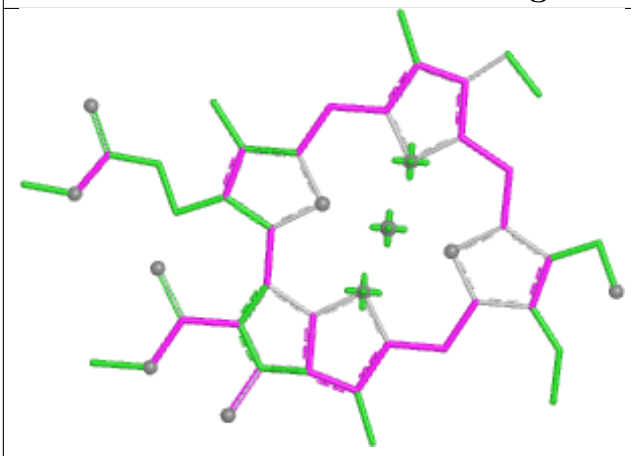


Torsions

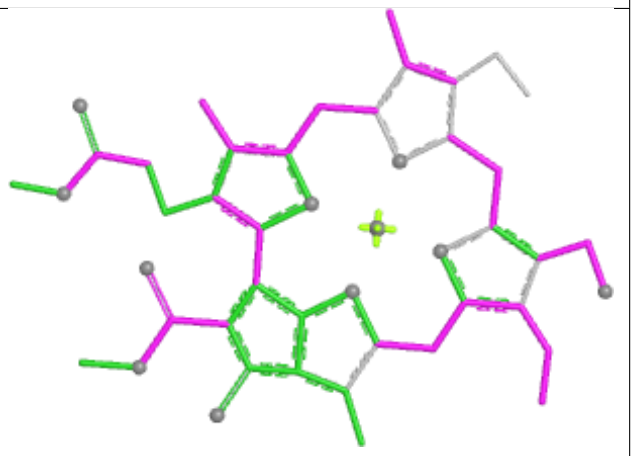


Rings

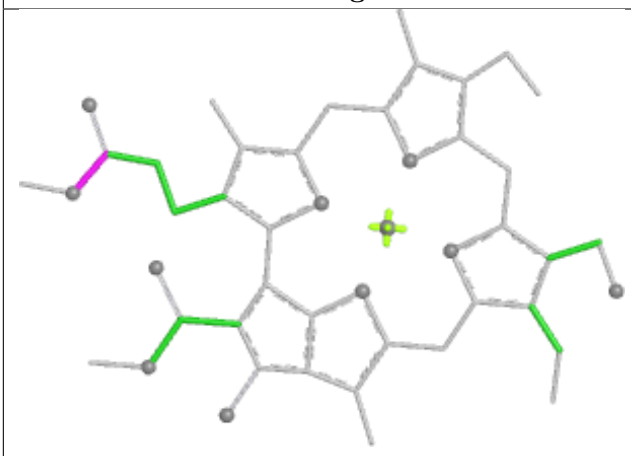
Ligand CHL s 517



Bond lengths



Bond angles

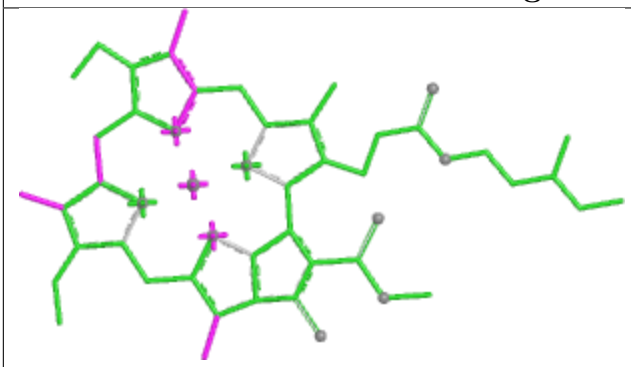


Torsions

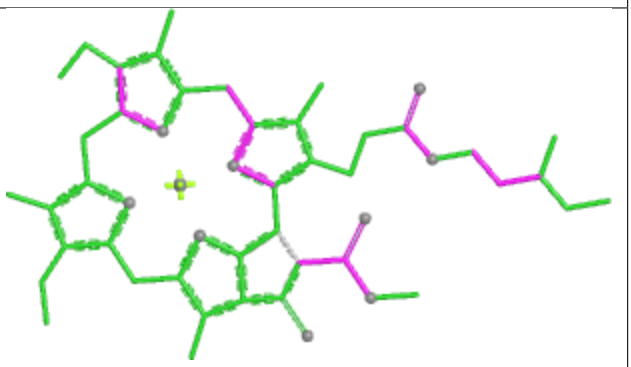


Rings

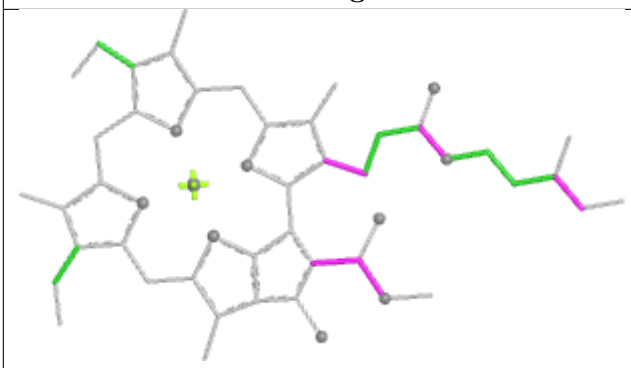
Ligand CLA A 835



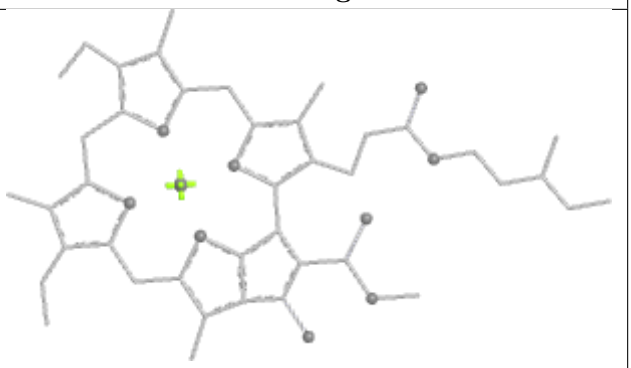
Bond lengths



Bond angles

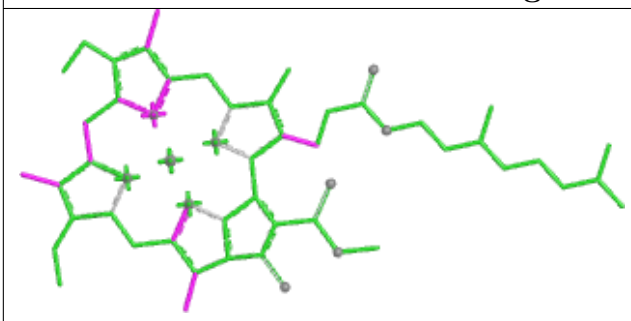


Torsions

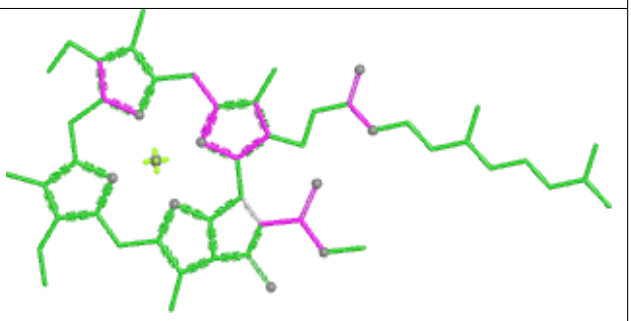


Rings

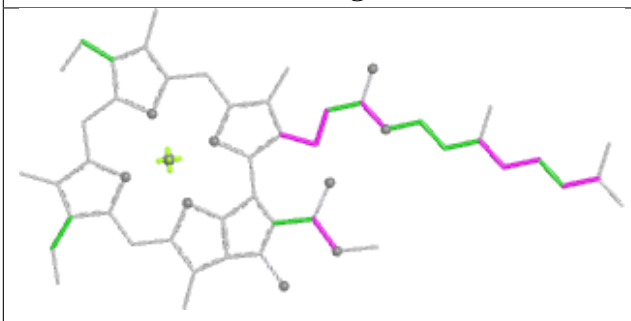
Ligand CLA A 836



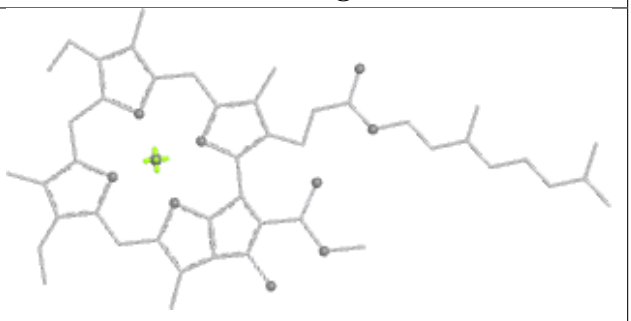
Bond lengths



Bond angles

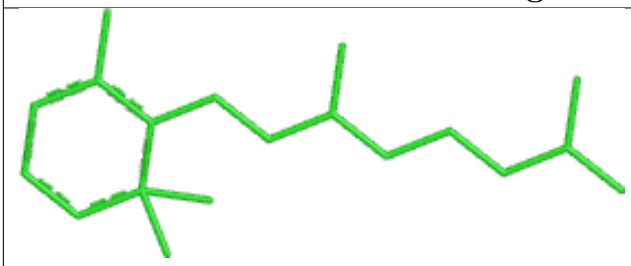


Torsions

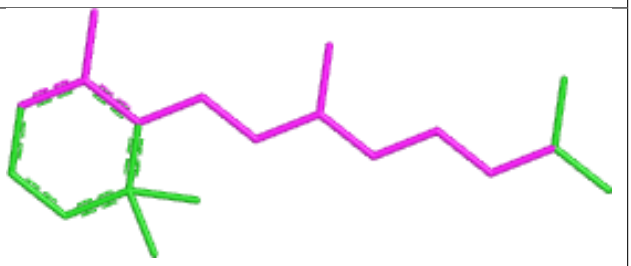


Rings

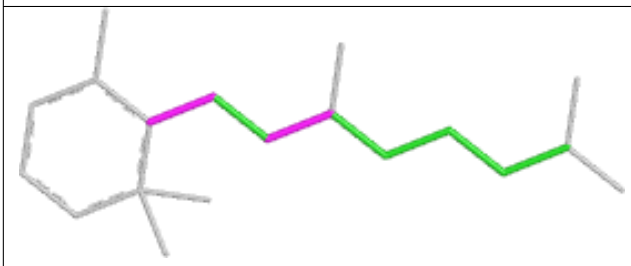
Ligand BCR 1 503



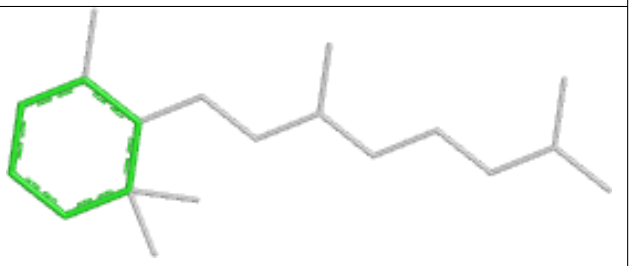
Bond lengths



Bond angles

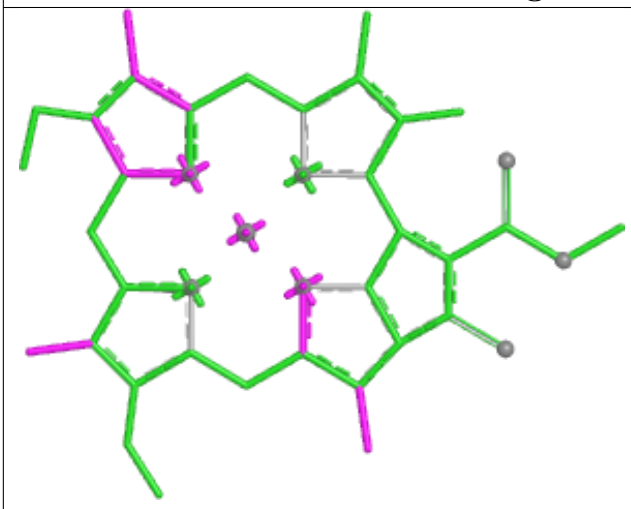


Torsions

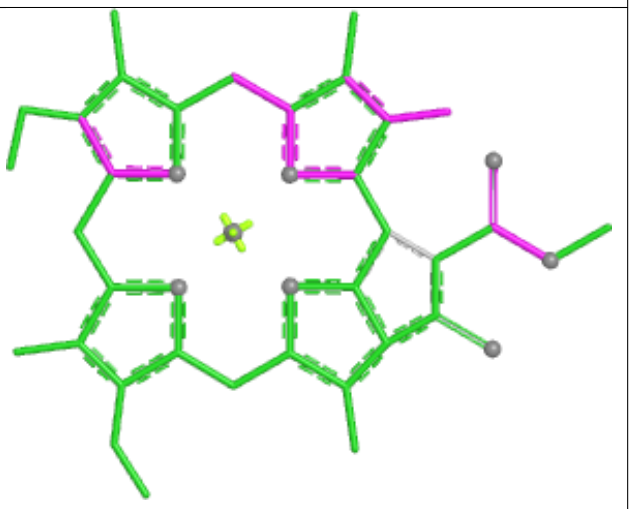


Rings

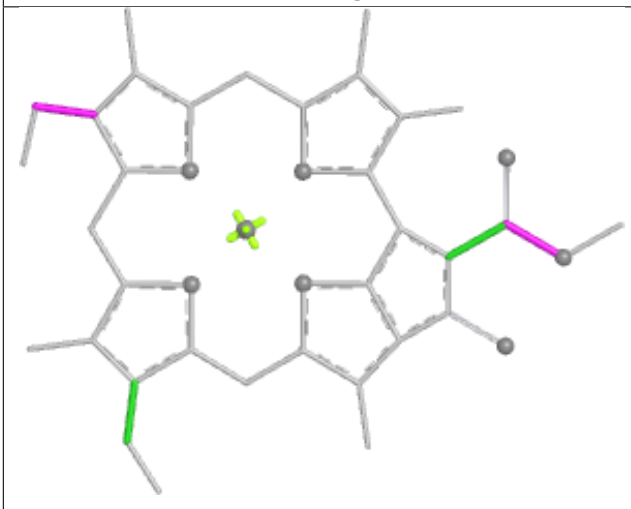
Ligand CLA F 803



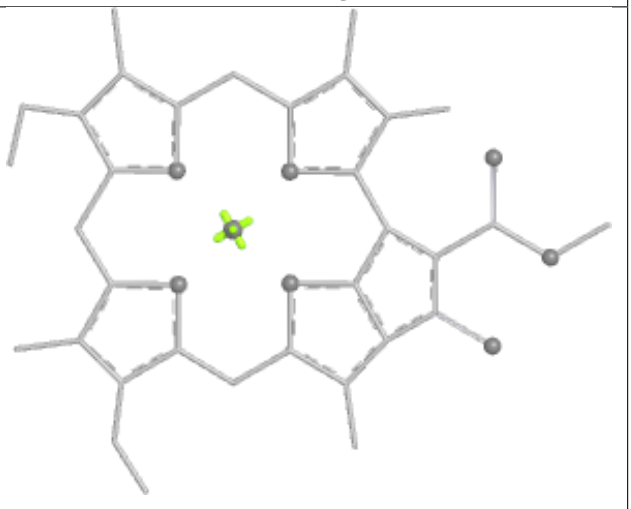
Bond lengths



Bond angles

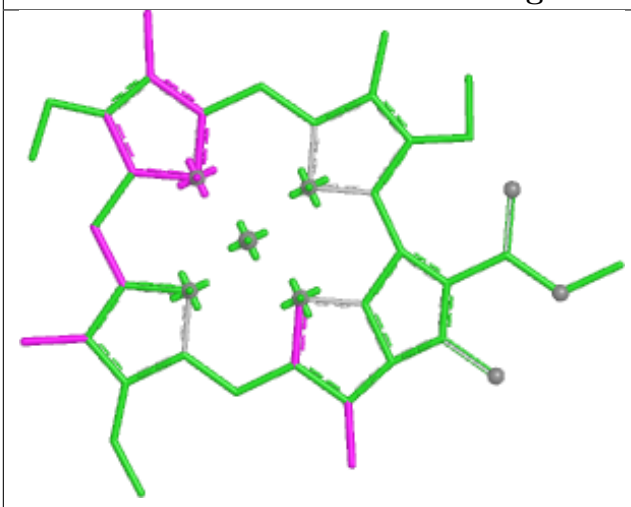


Torsions

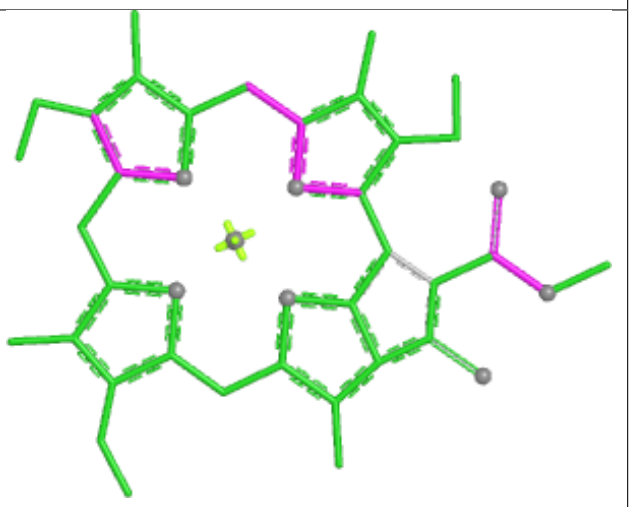


Rings

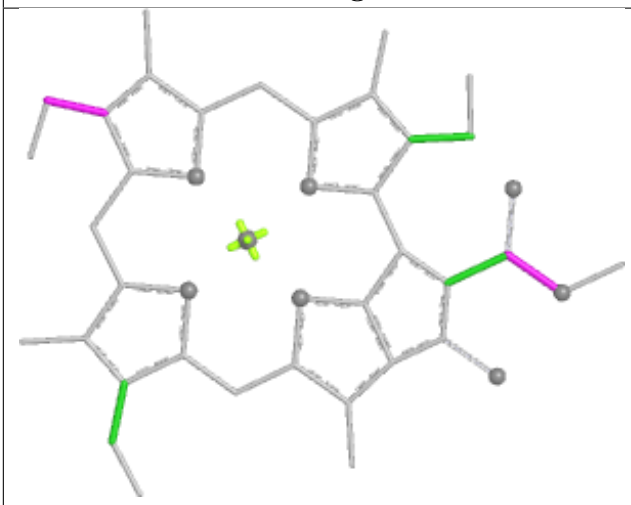
Ligand CLA F 802



Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

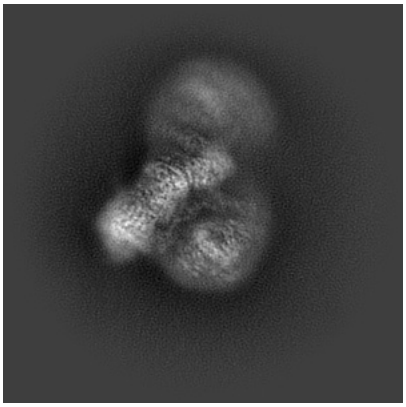
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31498. These allow visual inspection of the internal detail of the map and identification of artifacts.

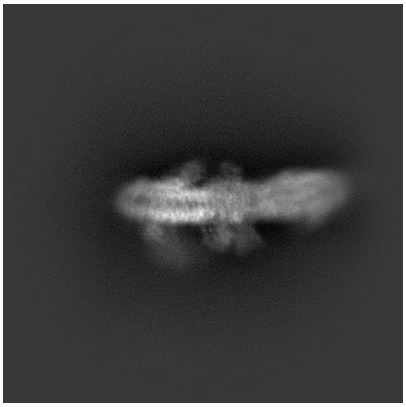
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

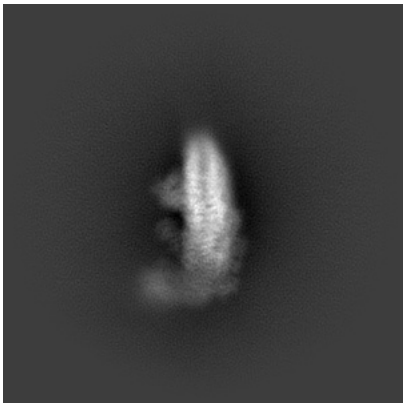
6.1.1 Primary map



X



Y

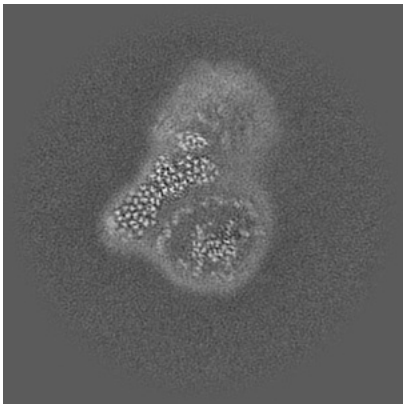


Z

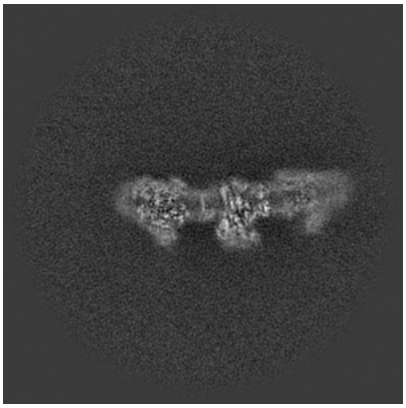
The images above show the map projected in three orthogonal directions.

6.2 Central slices

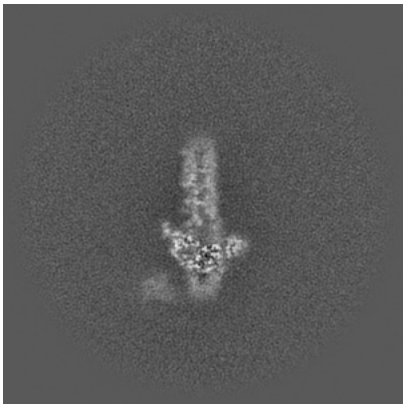
6.2.1 Primary map



X Index: 220



Y Index: 220

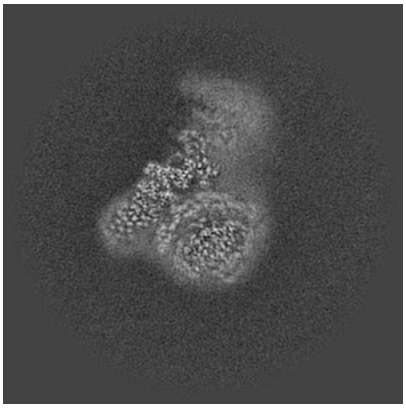


Z Index: 220

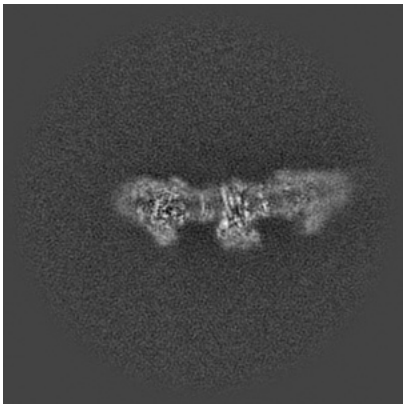
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 209



Y Index: 221

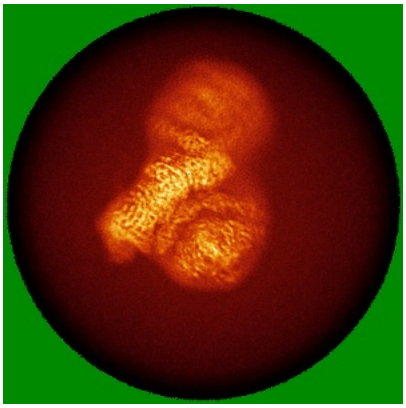


Z Index: 196

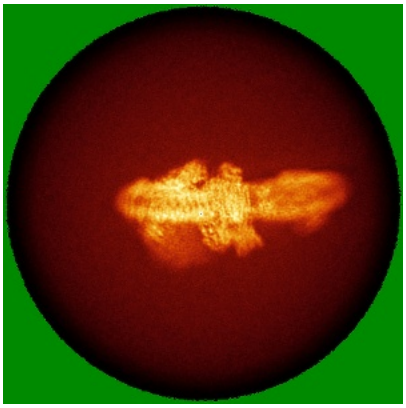
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

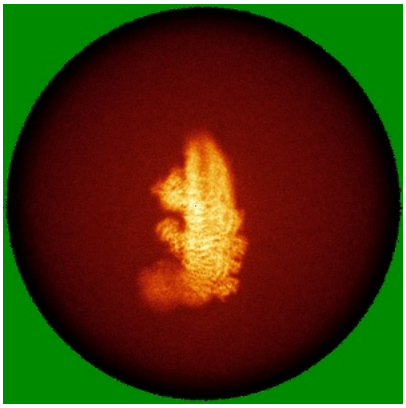
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

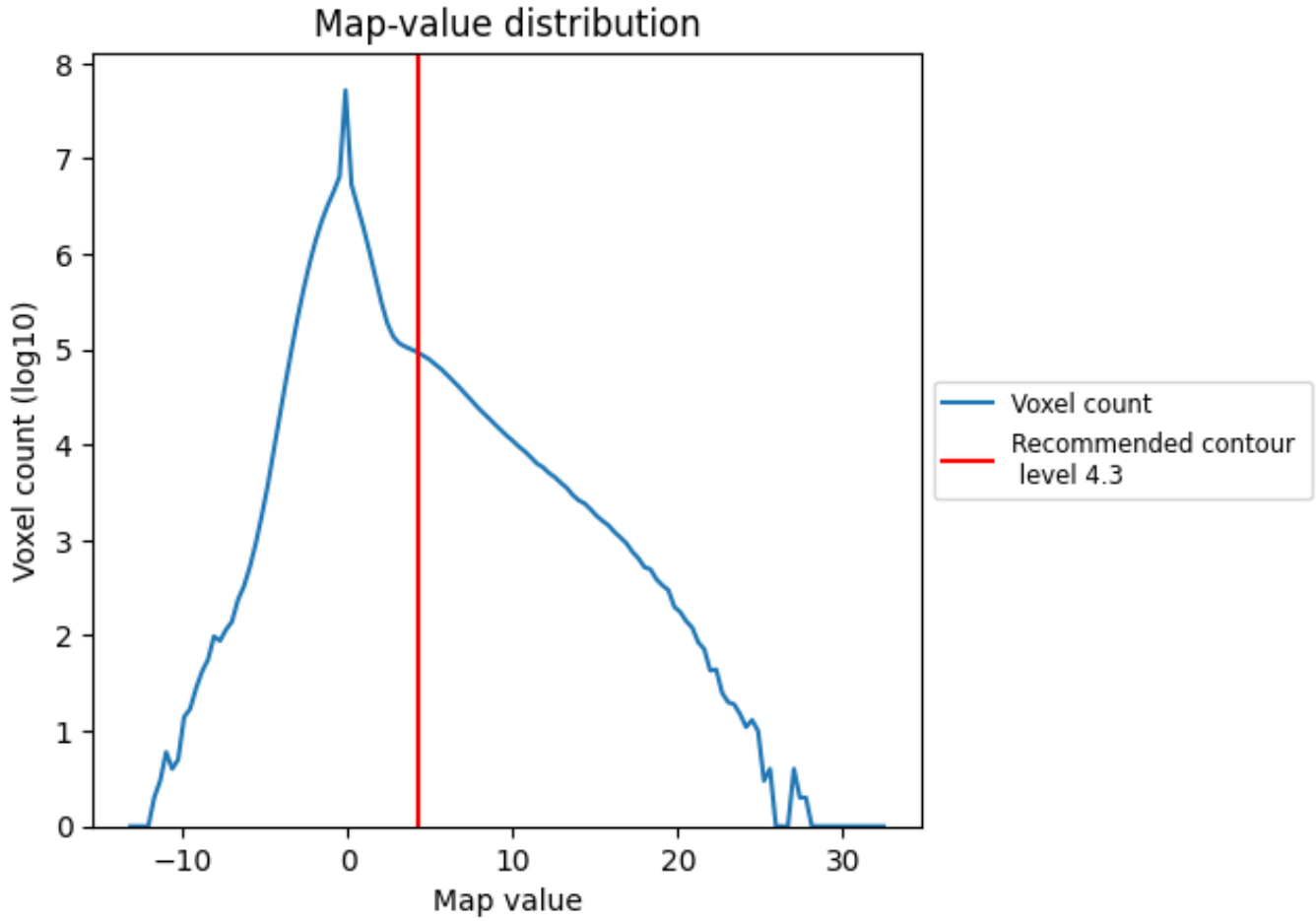
6.6 Mask visualisation (i)

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

7 Map analysis

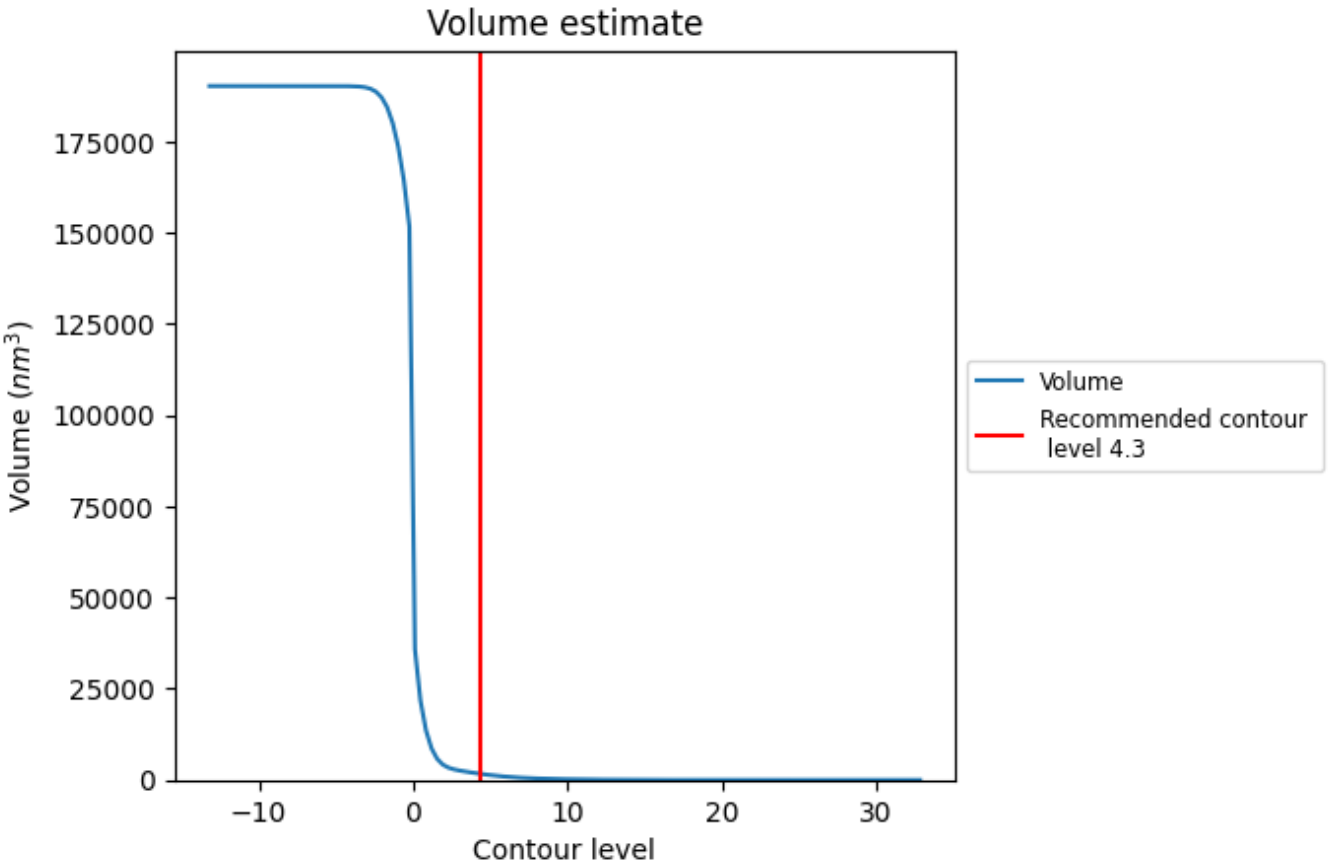
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

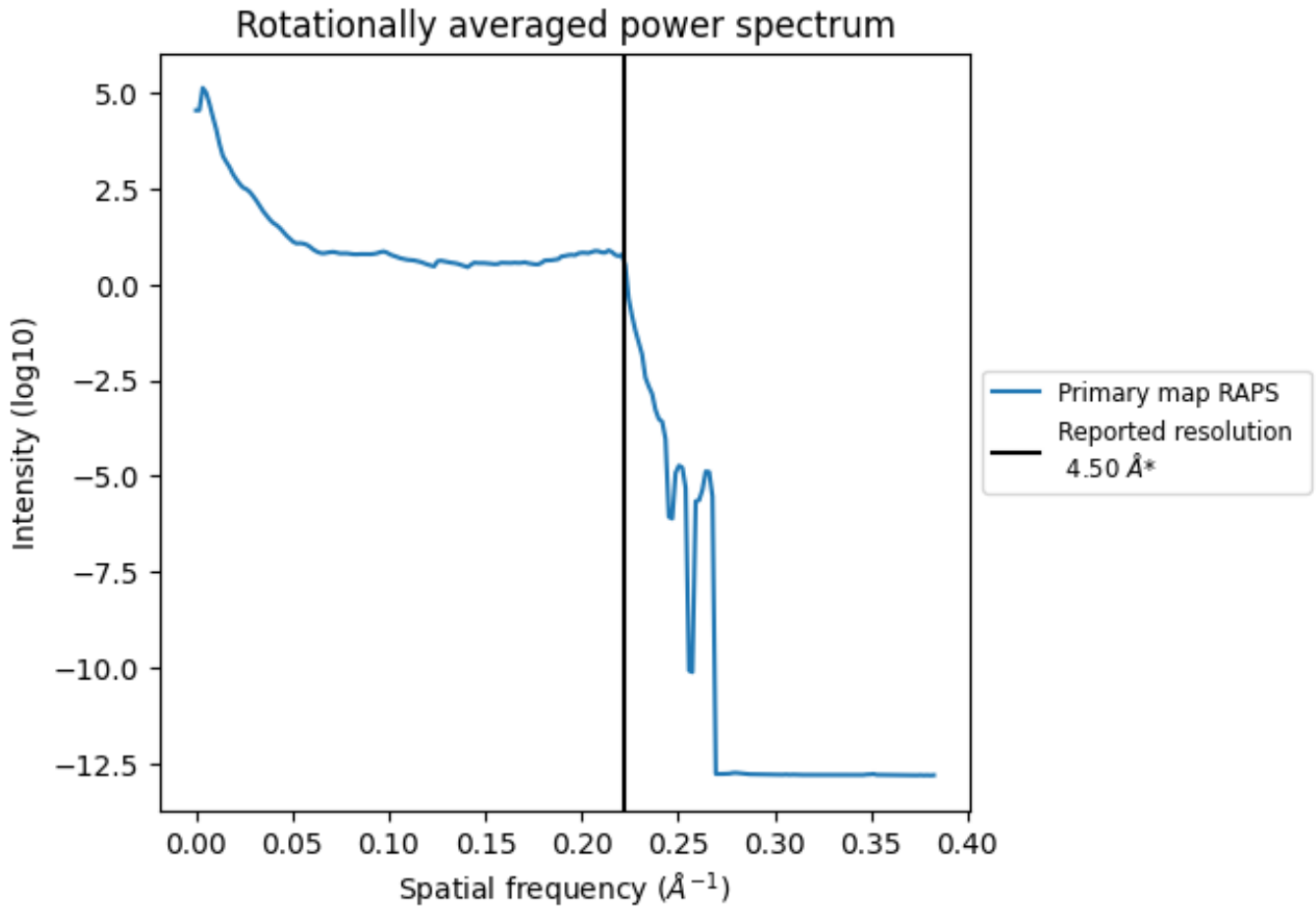
7.2 Volume estimate



The volume at the recommended contour level is 1712 nm^3; this corresponds to an approximate mass of 1547 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

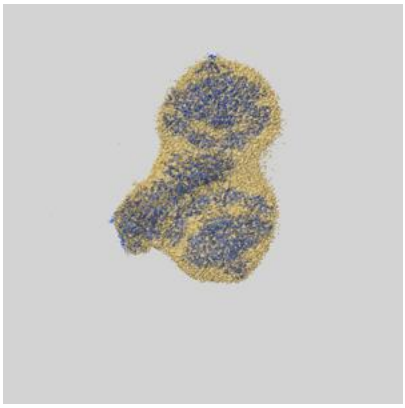
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

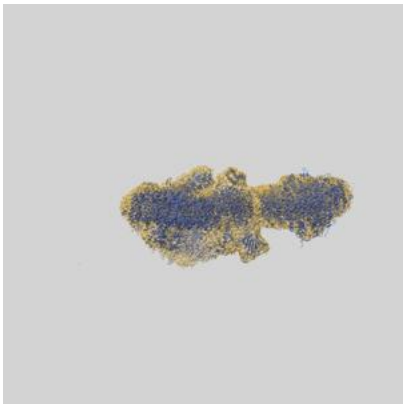
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31498 and PDB model 7F9O. Per-residue inclusion information can be found in section 3 on page 45.

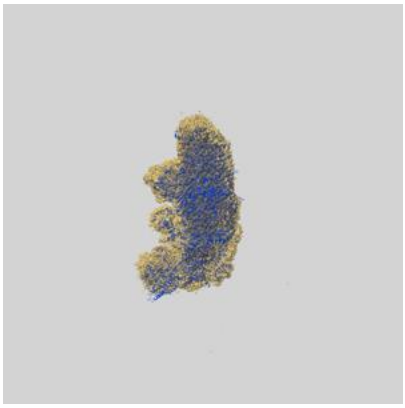
9.1 Map-model overlay



X



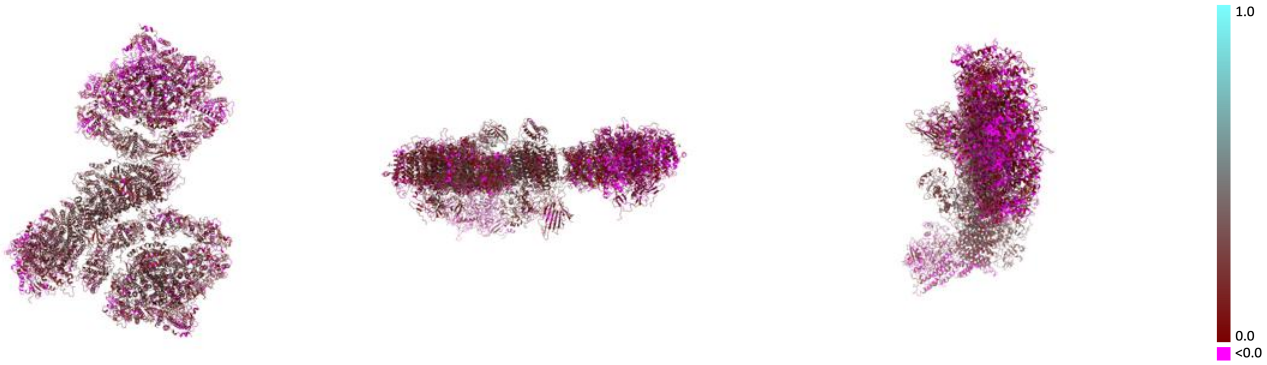
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



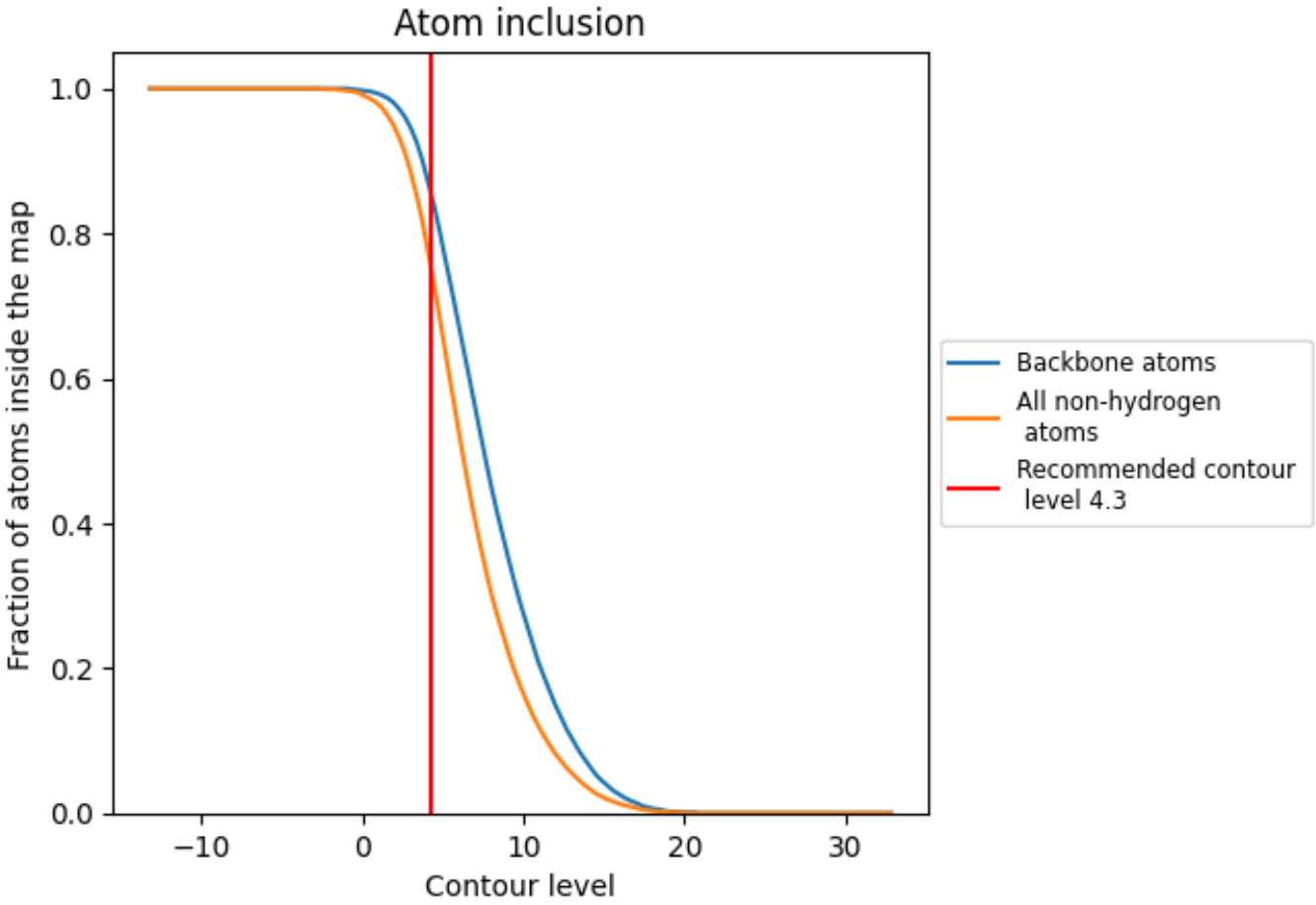
X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7480	0.1530
0	0.9110	0.2790
1	0.8680	0.1670
2	0.8140	0.1560
3	0.7630	0.1310
4	0.9470	0.2970
5	0.8450	0.2040
6	0.9220	0.2590
7	0.9030	0.1660
8	0.9290	0.2190
9	0.9390	0.3030
A	0.7970	0.2100
B	0.8350	0.1920
C	0.9300	0.1900
D	0.8100	0.1390
E	0.8460	0.2510
F	0.7910	0.2080
G	0.7710	0.1410
H	0.6080	0.0710
I	0.7270	0.1620
J	0.7650	0.2130
K	0.5680	0.0740
L	0.6440	0.0840
M	0.8570	0.2760
N	0.8000	0.1930
O	0.8710	0.2910
P	0.8110	0.2610
Q	0.8350	0.2470
R	0.8330	0.2580
S	0.3300	0.0480
T	0.4230	0.0480
U	0.3670	0.0450
V	0.5320	0.0910
W	0.3670	0.0230
X	0.4140	0.0630



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	0.5340	0.0660
Z	0.9210	0.2760
a	0.9320	0.2200
b	0.9430	0.2340
c	0.9380	0.2400
d	0.9200	0.2580
e	0.6790	0.0550
f	0.7370	0.0470
g	0.7540	0.0570
h	0.3020	0.0450
i	0.3880	0.1030
j	0.7210	0.0960
k	0.2970	0.0220
l	0.5890	0.0150
m	0.6500	0.1240
n	0.2750	0.0030
o	0.3410	0.0070
p	0.6930	0.0230
q	0.7070	0.0930
r	0.7970	0.0940
s	0.8690	0.2290