Full wwPDB EM Validation Report ⓘ

Aug 8, 2023 – 03:03 pm BST

PDB ID	:	8ASL
EMDB ID	:	EMD-15618
Title	:	RCII/PSI complex, class 2
Authors	:	Zhao, Z.; Vercellino, I.; Knoppova, J.; Sobotka, R.; Murray, J.W.; Nixon, P.J.; Sazanov, L.A.; Komenda, J.
Deposited on	:	2022-08-19
Resolution	:	3.15 Å(reported)
Based on initial models	:	2XBG, 6WJ6, 5OY0

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:

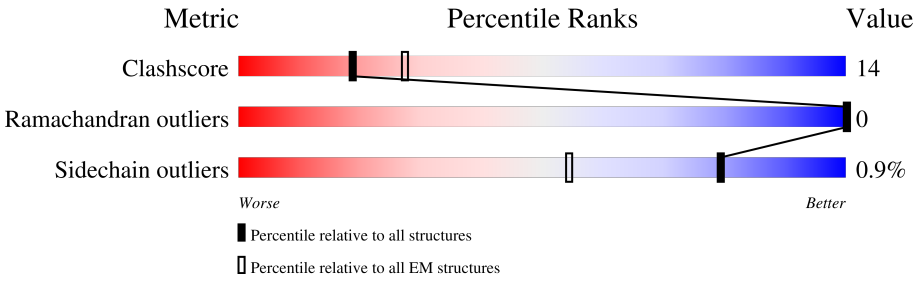
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.15 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	751	98%
2	b	731	99%
3	c	81	96%
4	d	141	99%
5	e	74	93% 7%
6	f	165	5% 86% 14%
7	i	40	5% 100%
8	j	40	5% 100%

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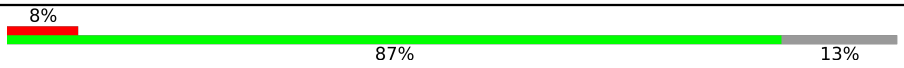
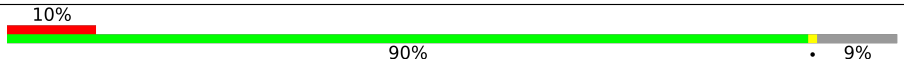
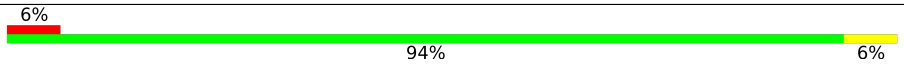
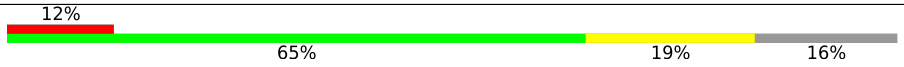
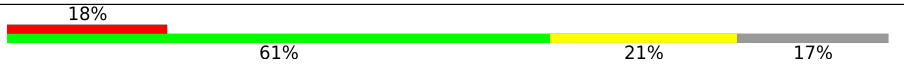
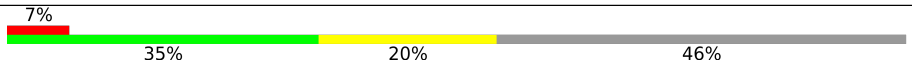
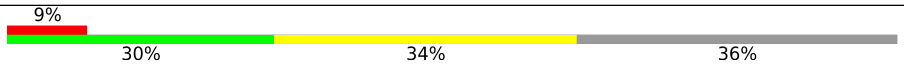
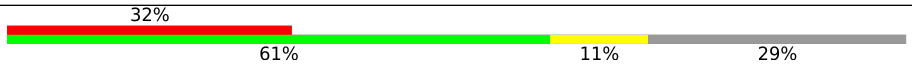
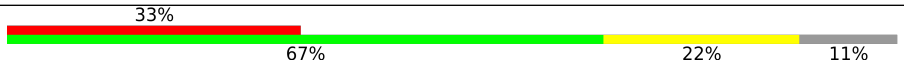
Mol	Chain	Length	Quality of chain
9	k	86	
10	l	157	
11	m	31	
12	A	344	
13	D	336	
14	E	81	
15	F	44	
16	I	38	
17	S	342	

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
18	CL0	a	801	X	-	-	-
19	CLA	A	402	X	-	-	-
19	CLA	A	403	X	-	-	-
19	CLA	A	405	X	-	-	-
19	CLA	D	401	X	-	-	-
19	CLA	D	403	X	-	-	-
19	CLA	D	404	X	-	-	-
19	CLA	a	802	X	-	-	-
19	CLA	a	803	X	-	-	-
19	CLA	a	804	X	-	-	-
19	CLA	a	805	X	-	-	-
19	CLA	a	806	X	-	-	-
19	CLA	a	807	X	-	-	-
19	CLA	a	808	X	-	-	-
19	CLA	a	809	X	-	-	-
19	CLA	a	810	X	-	-	-
19	CLA	a	811	X	-	-	-
19	CLA	a	812	X	-	-	-
19	CLA	a	813	X	-	-	-
19	CLA	a	815	X	-	-	-
19	CLA	a	816	X	-	-	-
19	CLA	a	817	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	a	818	X	-	-	-
19	CLA	a	819	X	-	-	-
19	CLA	a	820	X	-	-	-
19	CLA	a	821	X	-	-	-
19	CLA	a	822	X	-	-	-
19	CLA	a	823	X	-	-	-
19	CLA	a	824	X	-	-	-
19	CLA	a	825	X	-	-	-
19	CLA	a	826	X	-	-	-
19	CLA	a	827	X	-	-	-
19	CLA	a	828	X	-	-	-
19	CLA	a	829	X	-	-	-
19	CLA	a	830	X	-	-	-
19	CLA	a	831	X	-	-	-
19	CLA	a	832	X	-	-	-
19	CLA	a	833	X	-	-	-
19	CLA	a	834	X	-	-	-
19	CLA	a	835	X	-	-	-
19	CLA	a	836	X	-	-	-
19	CLA	a	837	X	-	-	-
19	CLA	a	839	X	-	-	-
19	CLA	a	840	X	-	-	-
19	CLA	a	841	X	-	-	-
19	CLA	a	842	X	-	-	-
19	CLA	a	843	X	-	-	-
19	CLA	a	855	X	-	-	-
19	CLA	a	856	X	-	-	-
19	CLA	a	858	X	-	-	-
19	CLA	b	3002	X	-	-	-
19	CLA	b	3003	X	-	-	-
19	CLA	b	3004	X	-	-	-
19	CLA	b	3005	X	-	-	-
19	CLA	b	3006	X	-	-	-
19	CLA	b	3007	X	-	-	-
19	CLA	b	3008	X	-	-	-
19	CLA	b	3009	X	-	-	-
19	CLA	b	3010	X	-	-	-
19	CLA	b	3011	X	-	-	-
19	CLA	b	3012	X	-	-	-
19	CLA	b	3013	X	-	-	-
19	CLA	b	3014	X	-	-	-
19	CLA	b	3015	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	b	3016	X	-	-	-
19	CLA	b	3017	X	-	-	-
19	CLA	b	3018	X	-	-	-
19	CLA	b	3019	X	-	-	-
19	CLA	b	3020	X	-	-	-
19	CLA	b	3021	X	-	-	-
19	CLA	b	3022	X	-	-	-
19	CLA	b	3023	X	-	-	-
19	CLA	b	3024	X	-	-	-
19	CLA	b	3025	X	-	-	-
19	CLA	b	3026	X	-	-	-
19	CLA	b	3027	X	-	-	-
19	CLA	b	3028	X	-	-	-
19	CLA	b	3029	X	-	-	-
19	CLA	b	3030	X	-	-	-
19	CLA	b	3031	X	-	-	-
19	CLA	b	3032	X	-	-	-
19	CLA	b	3033	X	-	-	-
19	CLA	b	3034	X	-	-	-
19	CLA	b	3035	X	-	-	-
19	CLA	b	3036	X	-	-	-
19	CLA	b	3037	X	-	-	-
19	CLA	b	3038	X	-	-	-
19	CLA	b	3039	X	-	-	-
19	CLA	b	3040	X	-	-	-
19	CLA	b	3041	X	-	-	-
19	CLA	f	201	X	-	-	-
19	CLA	f	203	X	-	-	-
19	CLA	f	204	X	-	-	-
19	CLA	j	102	X	-	-	-
19	CLA	j	103	X	-	-	-
19	CLA	k	4002	X	-	-	-
19	CLA	k	4003	X	-	-	-
19	CLA	l	1501	X	-	-	-
19	CLA	l	1502	X	-	-	-
19	CLA	l	1503	X	-	-	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 32739 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
			Total	C	N	O	S		
1	a	741	5795	3797	984	987	27	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	729	5770	3798	967	990	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	80	600	369	103	117	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	139	1087	688	188	208	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	e	69	538	337	95	106	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	142	1108	715	184	204	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	40	Total	C	N	O	S	0	0
			311	209	44	55	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	j	40	Total	C	N	O	S	0	0
			319	215	47	54	3		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	k	75	Total	C	N	O	S	0	0
			524	343	87	90	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	143	Total	C	N	O	S	0	0
			1069	697	173	197	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	m	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

- Molecule 12 is a protein called Photosystem II protein D1 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	289	Total	C	N	O	S	0	0
			2248	1478	366	389	15		

- Molecule 13 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	278	Total	C	N	O	S	0	0
			2188	1465	351	360	12		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	MET	-	initiating methionine	UNP P09192
D	-4	HIS	-	expression tag	UNP P09192
D	-3	HIS	-	expression tag	UNP P09192
D	-2	HIS	-	expression tag	UNP P09192
D	-1	HIS	-	expression tag	UNP P09192
D	0	HIS	-	expression tag	UNP P09192
D	1	HIS	-	expression tag	UNP P09192

- Molecule 14 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	E	44	Total	C	N	O	S	0	0
			360	245	54	60	1		

- Molecule 15 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	F	28	Total	C	N	O	S	0	0
			222	149	39	33	1		

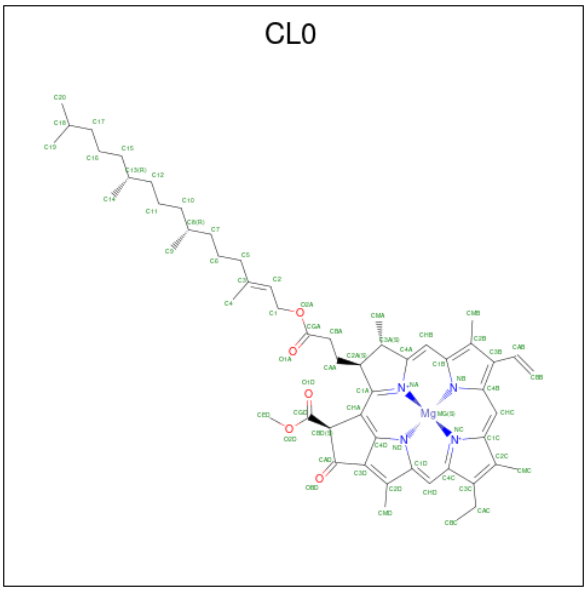
- Molecule 16 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	I	27	Total	C	N	O	0	0
			211	149	28	34		

- Molecule 17 is a protein called Photosystem II assembly lipoprotein Ycf48.

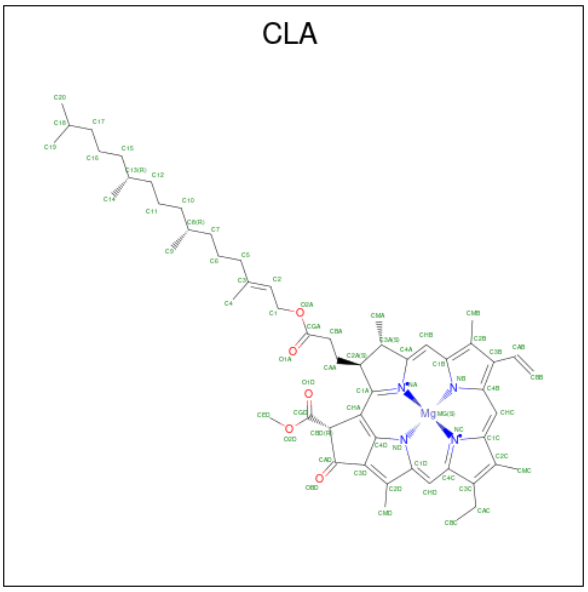
Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	303	Total	C	N	O	S	0	0
			2328	1481	393	451	3		

- Molecule 18 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
18	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 19 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms	AltConf
19	a	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 56 46 1 4 5	0
19	b	1	Total C Mg N O 56 46 1 4 5	0
19	b	1	Total C Mg N O 50 40 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 55 45 1 4 5	0
19	b	1	Total C Mg N O 56 46 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 60 50 1 4 5	0
19	b	1	Total C Mg N O 65 55 1 4 5	0
19	b	1	Total C Mg N O 60 50 1 4 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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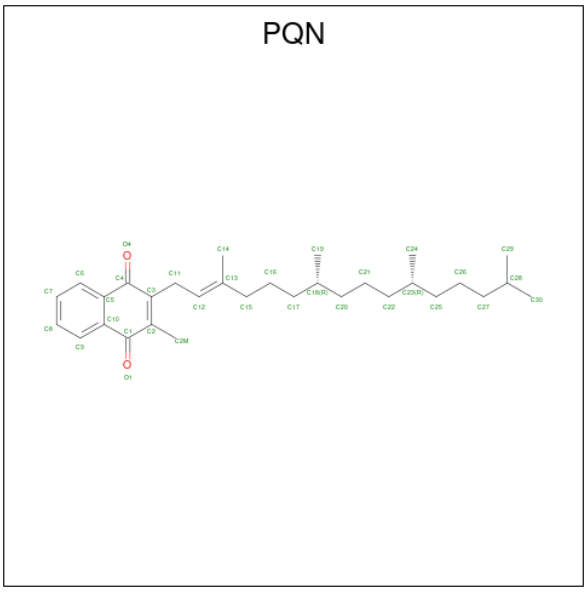
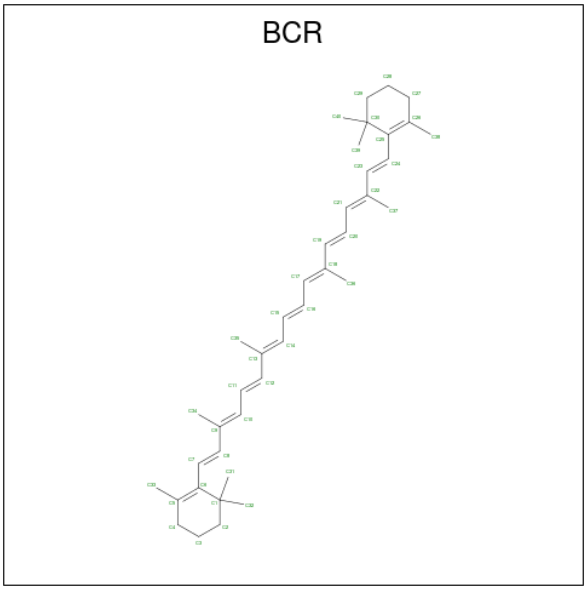
Mol	Chain	Residues	Atoms					AltConf
19	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	j	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	k	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	l	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	D	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	D	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 20 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms	AltConf
20	a	1	Total C O 33 31 2	0
20	b	1	Total C O 33 31 2	0

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
21	a	1	Total C 40 40	0
21	a	1	Total C 40 40	0

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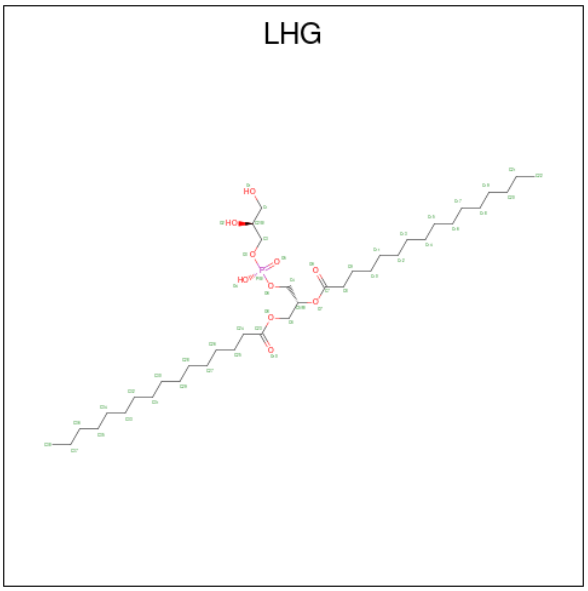
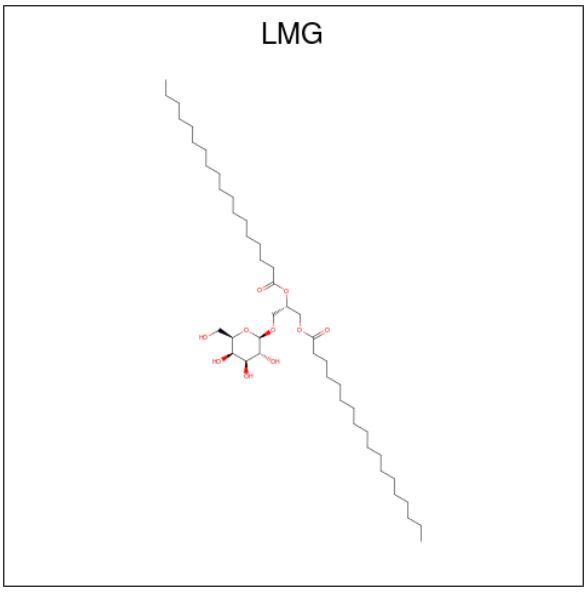
Mol	Chain	Residues	Atoms	AltConf
21	a	1	Total C 40 40	0
21	a	1	Total C 40 40	0
21	a	1	Total C 25 25	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	b	1	Total C 40 40	0
21	f	1	Total C 40 40	0
21	i	1	Total C 40 40	0
21	j	1	Total C 40 40	0
21	j	1	Total C 40 40	0
21	k	1	Total C 40 40	0
21	k	1	Total C 40 40	0
21	l	1	Total C 40 40	0
21	A	1	Total C 40 40	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



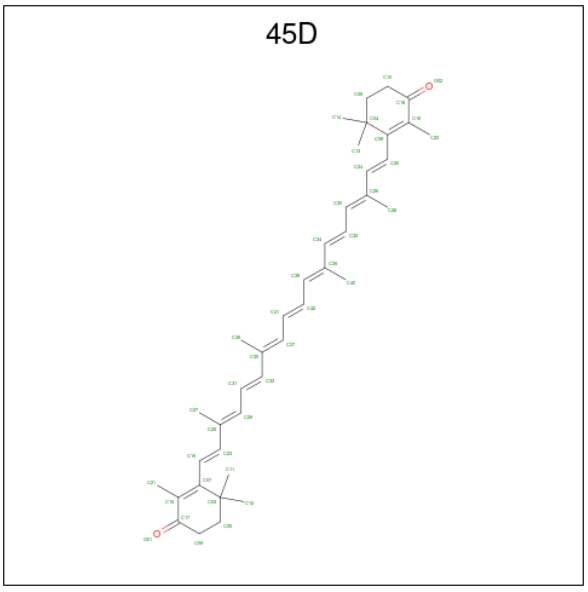
Mol	Chain	Residues	Atoms				AltConf
22	a	1	Total	C	O	P	0
			49	38	10	1	
22	a	1	Total	C	O	P	0
			49	38	10	1	
22	a	1	Total	C	O	P	0
			49	38	10	1	
22	b	1	Total	C	O	P	0
			38	27	10	1	
22	f	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



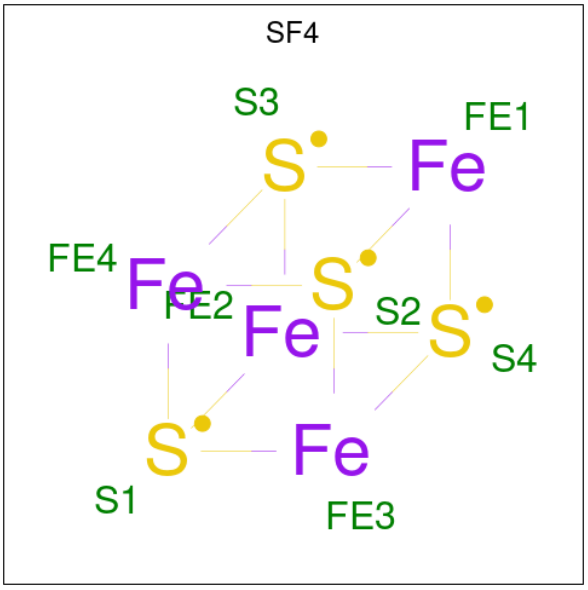
Mol	Chain	Residues	Atoms			AltConf
23	a	1	Total	C	O	0
			50	40	10	
23	a	1	Total	C	O	0
			40	30	10	
23	b	1	Total	C	O	0
			55	45	10	
23	b	1	Total	C	O	0
			55	45	10	

- Molecule 24 is beta,beta-carotene-4,4'-dione (three-letter code: 45D) (formula: $C_{40}H_{52}O_2$).



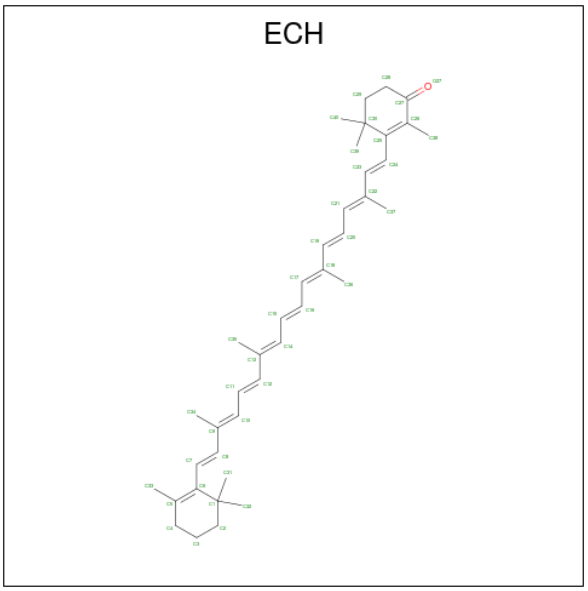
Mol	Chain	Residues	Atoms	AltConf
24	a	1	Total C O 42 40 2	0

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



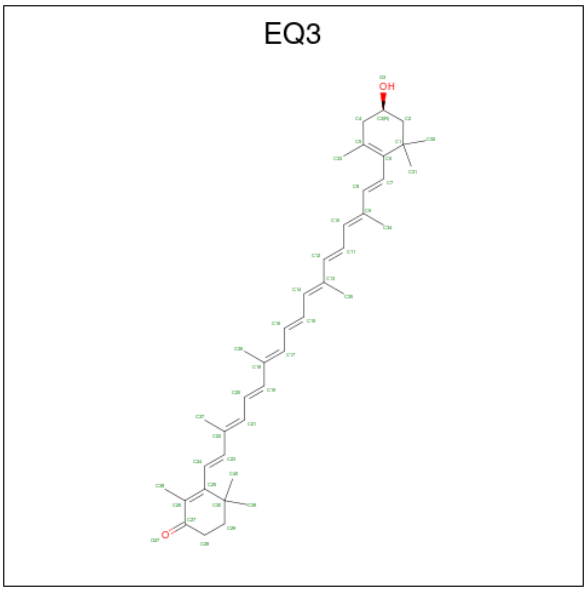
Mol	Chain	Residues	Atoms	AltConf
25	b	1	Total Fe S 8 4 4	0
25	c	1	Total Fe S 8 4 4	0
25	c	1	Total Fe S 8 4 4	0

- Molecule 26 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: $C_{40}H_{54}O$).



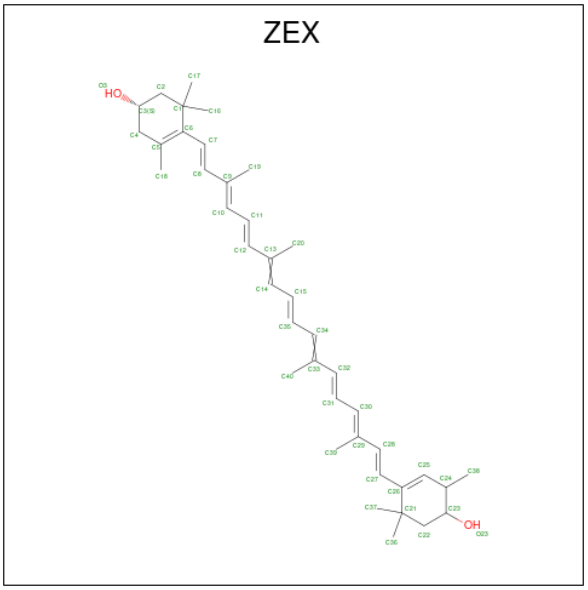
Mol	Chain	Residues	Atoms			AltConf
26	b	1	Total	C	O	0
			41	40	1	
26	m	1	Total	C	O	0
			41	40	1	

- Molecule 27 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (three-letter code: EQ3) (formula: $C_{40}H_{54}O_2$).



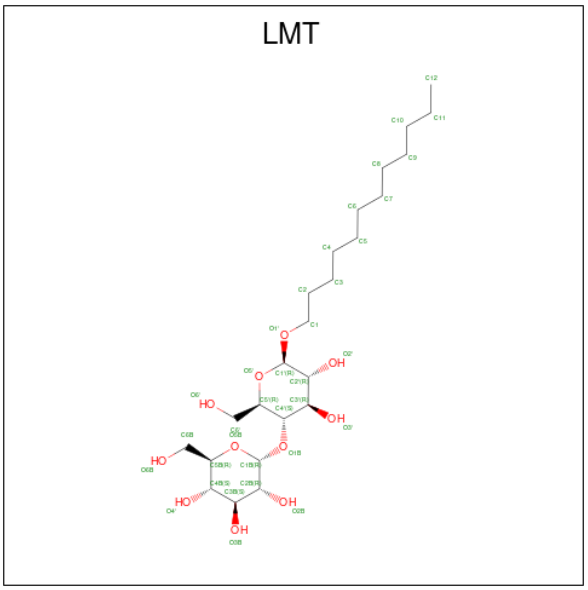
Mol	Chain	Residues	Atoms			AltConf
27	b	1	Total	C	O	0
			42	40	2	

- Molecule 28 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (three-letter code: ZEX) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
28	b	1	42	40	2	0
			Total	C	O	
28	f	1	42	40	2	0

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).

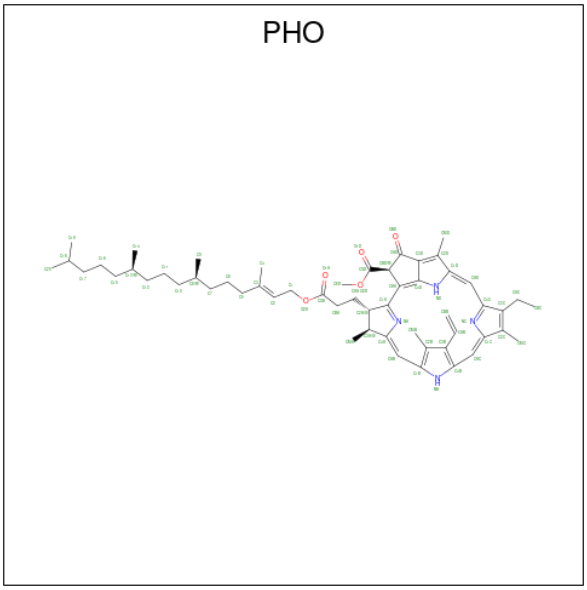


Mol	Chain	Residues	Atoms			AltConf
29	f	1	Total	C	O	0
			35	24	11	

- Molecule 30 is FE (II) ION (three-letter code: FE2) (formula: Fe).

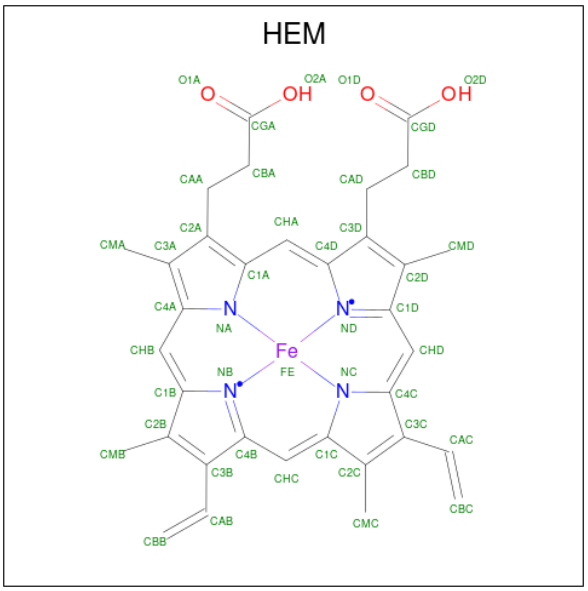
Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total	Fe	0
			1	1	

- Molecule 31 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	N	O	0
			64	55	4	5	
31	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 32 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



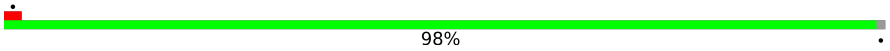
Mol	Chain	Residues	Atoms					AltConf
32	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

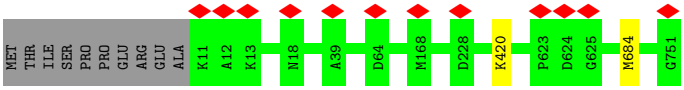
3 Residue-property plots (i)

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

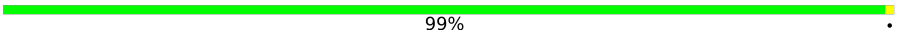
Chain a:





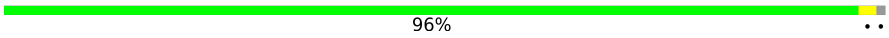
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:



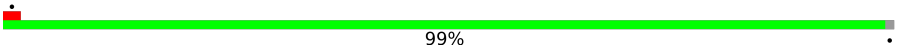
• Molecule 3: Photosystem I iron-sulfur center

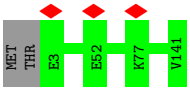
Chain c:



• Molecule 4: Photosystem I reaction center subunit II

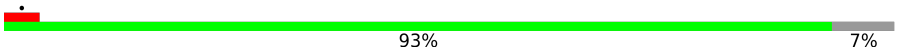
Chain d:

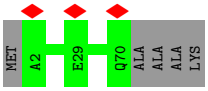




• Molecule 5: Photosystem I reaction center subunit IV

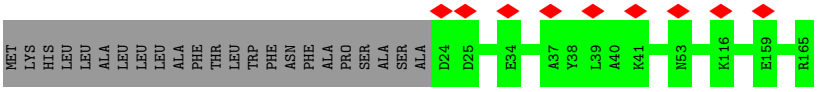
Chain e:





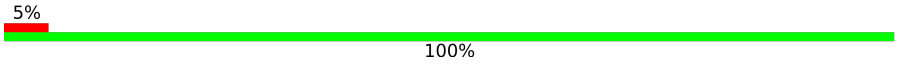
• Molecule 6: Photosystem I reaction center subunit III

Chain f:



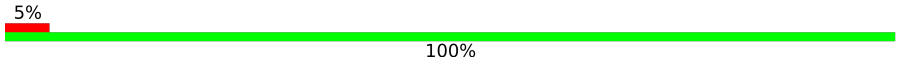
• Molecule 7: Photosystem I reaction center subunit VIII

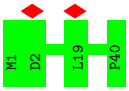
Chain i:



• Molecule 8: Photosystem I reaction center subunit IX

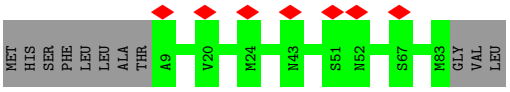
Chain j:





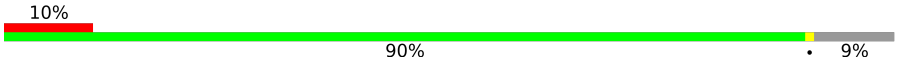
• Molecule 9: Photosystem I reaction center subunit PsaK 1

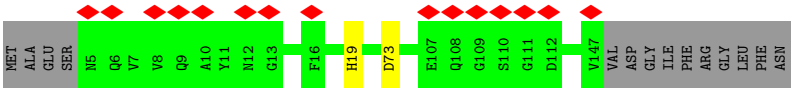
Chain k:



• Molecule 10: Photosystem I reaction center subunit XI

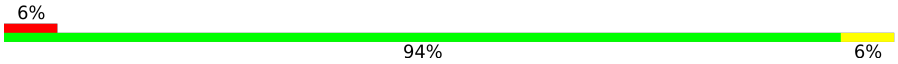
Chain l:

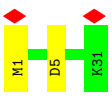




• Molecule 11: Photosystem I reaction center subunit XII

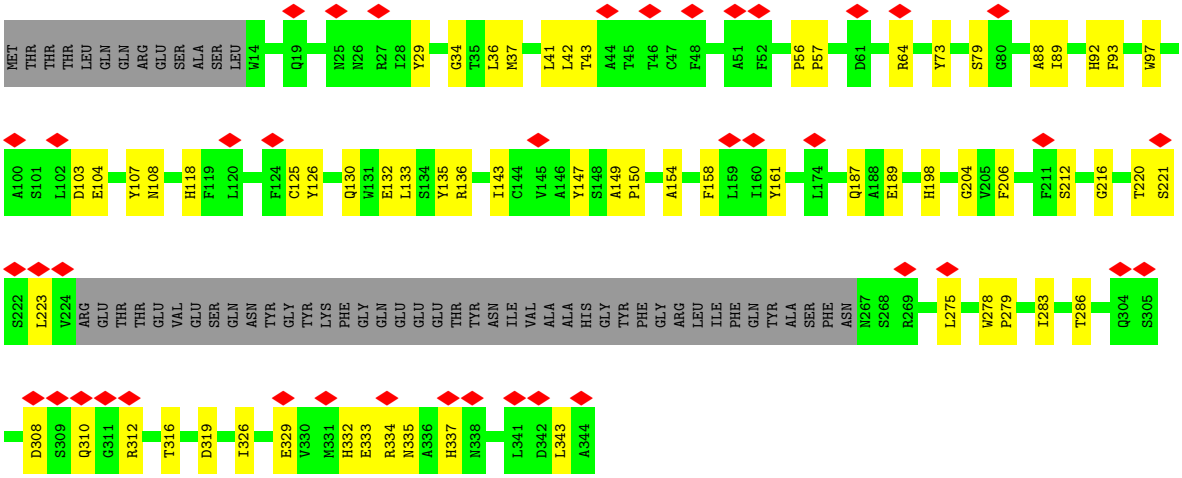
Chain m:





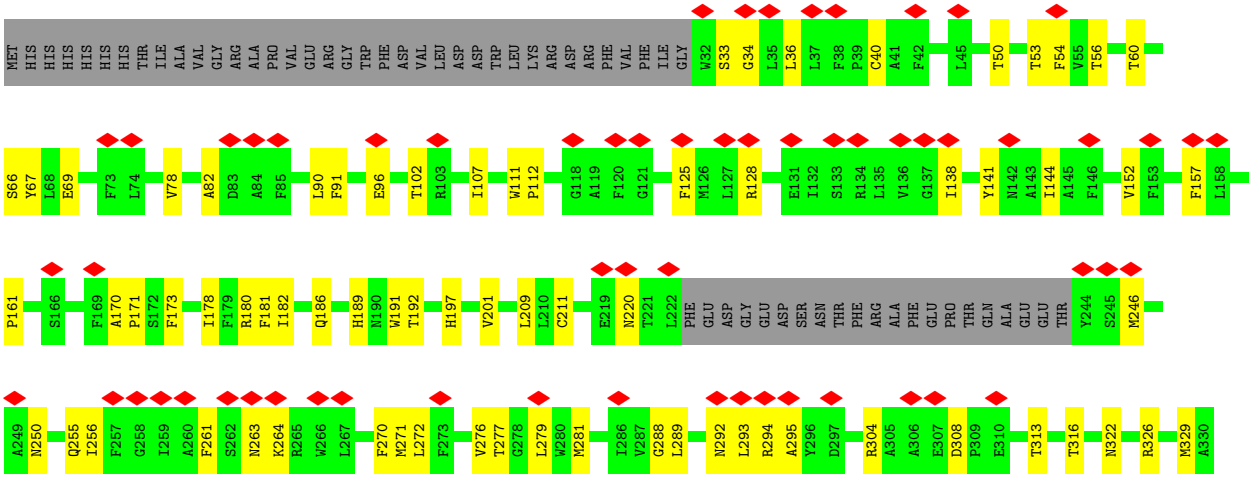
• Molecule 12: Photosystem II protein D1 2

Chain A:



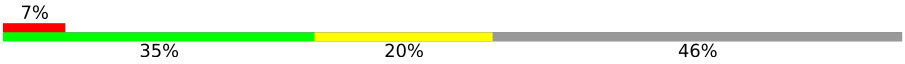
• Molecule 13: Photosystem II D2 protein

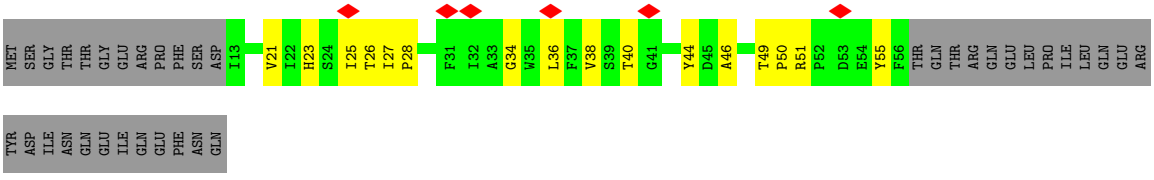
Chain D:



• Molecule 14: Cytochrome b559 subunit alpha

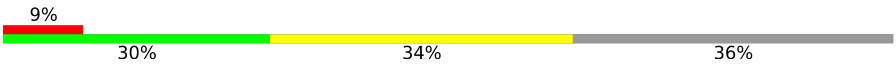
Chain E:

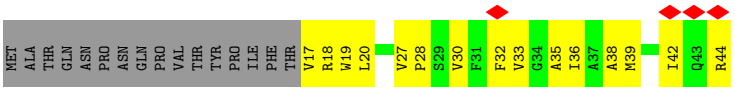




• Molecule 15: Cytochrome b559 subunit beta

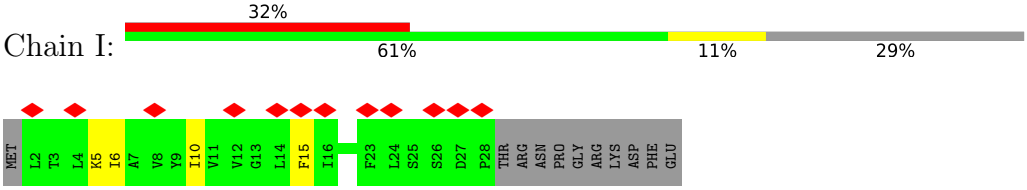
Chain F:





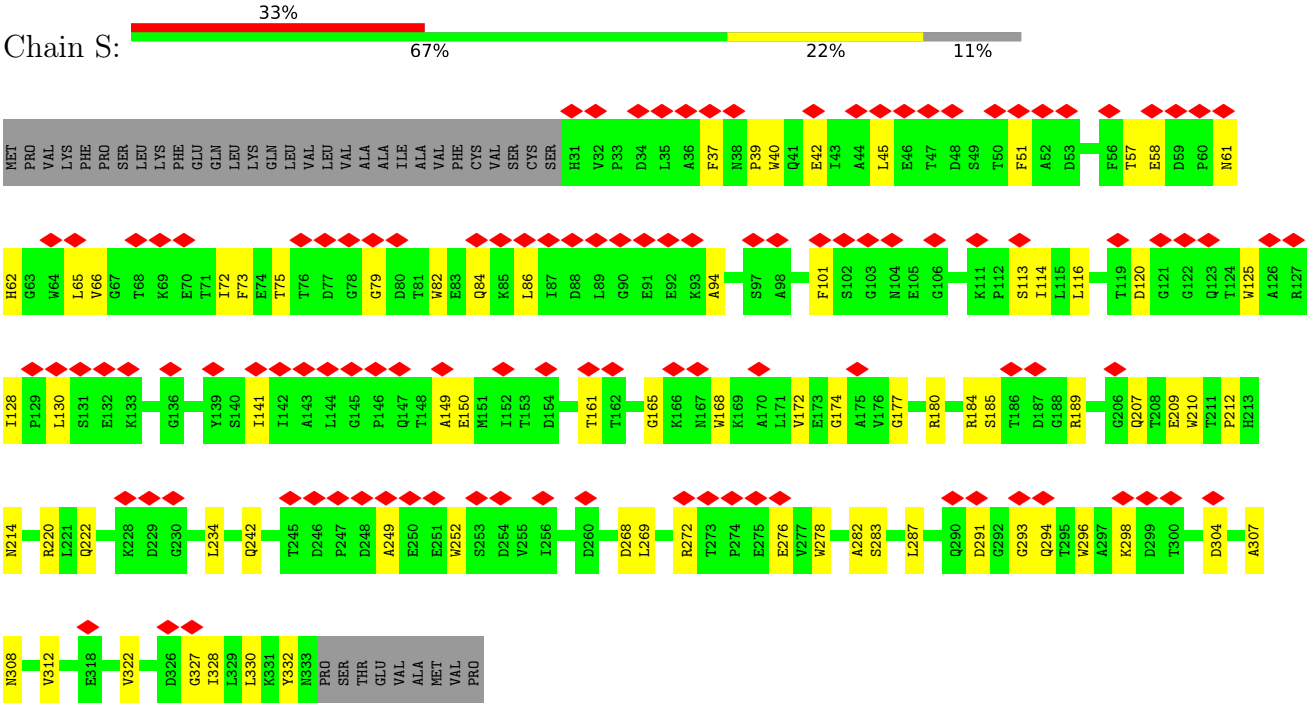
• Molecule 16: Photosystem II reaction center protein I

Chain I:



• Molecule 17: Photosystem II assembly lipoprotein Ycf48

Chain S:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	178513	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	90.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.510	Depositor
Minimum map value	-0.112	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0801	Depositor
Map size (Å)	488.0, 488.0, 488.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZEX, 45D, CLA, CL0, LMG, SF4, ECH, EQ3, PQN, FE2, LMT, HEM, PHO, BCR, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	a	0.29	0/5993	0.44	0/8169
2	b	0.29	0/5981	0.44	0/8178
3	c	0.30	0/610	0.56	0/826
4	d	0.29	0/1111	0.49	0/1497
5	e	0.30	0/547	0.51	0/741
6	f	0.27	0/1138	0.46	0/1546
7	i	0.29	0/322	0.44	0/438
8	j	0.27	0/328	0.43	0/443
9	k	0.26	0/535	0.46	0/726
10	l	0.28	0/1097	0.44	0/1493
11	m	0.27	0/241	0.41	0/326
12	A	0.27	0/2322	0.46	0/3169
13	D	0.27	0/2266	0.44	0/3086
14	E	0.27	0/374	0.46	0/513
15	F	0.29	0/228	0.56	0/309
16	I	0.27	0/216	0.43	0/293
17	S	0.25	0/2390	0.50	0/3258
All	All	0.28	0/25699	0.46	0/35011

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	5795	0	5653	0	0
2	b	5770	0	5547	0	0
3	c	600	0	581	0	0
4	d	1087	0	1082	0	0
5	e	538	0	514	0	0
6	f	1108	0	1100	0	0
7	i	311	0	304	0	0
8	j	319	0	328	0	0
9	k	524	0	547	0	0
10	l	1069	0	1044	0	0
11	m	238	0	260	0	0
12	A	2248	0	2170	48	0
13	D	2188	0	2129	55	0
14	E	360	0	352	12	0
15	F	222	0	230	10	0
16	I	211	0	227	4	0
17	S	2328	0	2227	51	0
18	a	65	0	72	0	0
19	A	161	0	144	11	0
19	D	166	0	154	19	0
19	a	2811	0	2986	0	0
19	b	2410	0	2456	0	0
19	f	165	0	150	0	0
19	j	101	0	82	0	0
19	k	91	0	66	0	0
19	l	167	0	154	0	0
20	a	33	0	46	0	0
20	b	33	0	46	0	0
21	A	40	0	56	2	0
21	a	185	0	257	0	0
21	b	200	0	280	0	0
21	f	40	0	56	0	0
21	i	40	0	56	0	0
21	j	80	0	112	0	0
21	k	80	0	112	0	0
21	l	40	0	56	0	0
22	a	147	0	222	0	0
22	b	38	0	49	0	0
22	f	49	0	74	0	0
23	a	90	0	123	0	0
23	b	110	0	172	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	42	0	52	0	0
25	b	8	0	0	0	0
25	c	16	0	0	0	0
26	b	41	0	54	0	0
26	m	41	0	54	0	0
27	b	42	0	0	0	0
28	b	42	0	56	0	0
28	f	42	0	56	0	0
29	f	35	0	45	0	0
30	A	1	0	0	0	0
31	A	64	0	74	5	0
31	D	64	0	74	4	0
32	F	43	0	30	4	0
All	All	32739	0	32771	173	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 14.

All (173) 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)
13:D:186:GLN:HB2	19:D:403:CLA:HBC1	1.60	0.83
15:F:39:MET:HA	15:F:42:ILE:HG12	1.65	0.77
12:A:133:LEU:HD23	13:D:256:ILE:HG12	1.68	0.76
12:A:143:ILE:HB	13:D:220:ASN:HD21	1.52	0.74
12:A:42:LEU:HB3	21:A:406:BCR:H353	1.69	0.73
13:D:192:THR:HG23	19:D:403:CLA:HBC2	1.72	0.71
17:S:62:HIS:HA	17:S:75:THR:O	1.92	0.70
12:A:29:TYR:HB2	13:D:255:GLN:HB3	1.72	0.70
32:F:101:HEM:HBC2	32:F:101:HEM:HHD	1.75	0.69
17:S:207:GLN:HG2	17:S:209:GLU:H	1.56	0.68
16:I:6:ILE:O	16:I:10:ILE:HG12	1.94	0.68
13:D:197:HIS:HE1	19:D:403:CLA:NC	1.92	0.67
12:A:198:HIS:HE1	19:A:402:CLA:NB	1.92	0.67
12:A:310:GLN:NE2	14:E:55:TYR:O	2.27	0.66
12:A:132:GLU:OE2	12:A:136:ARG:NE	2.27	0.66
13:D:96:GLU:N	13:D:96:GLU:OE1	2.28	0.65
17:S:58:GLU:HB2	17:S:61:ASN:HB3	1.80	0.64
13:D:60:THR:HA	13:D:82:ALA:HB2	1.81	0.63
17:S:322:VAL:HB	17:S:330:LEU:HB2	1.81	0.62
17:S:113:SER:HB3	17:S:130:LEU:HD12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:88:ALA:HB1	17:S:282:ALA:HB2	1.82	0.62
13:D:54:PHE:O	14:E:49:THR:OG1	2.18	0.61
12:A:333:GLU:HB3	12:A:337:HIS:HD2	1.65	0.61
15:F:35:ALA:O	15:F:39:MET:HG3	2.02	0.60
12:A:335:ASN:HA	17:S:174:GLY:HA3	1.84	0.59
13:D:304:ARG:NH1	13:D:308:ASP:OD2	2.36	0.59
12:A:221:SER:HB3	13:D:138:ILE:HD12	1.83	0.58
12:A:161:TYR:OH	12:A:189:GLU:OE2	2.20	0.58
12:A:108:ASN:OD1	17:S:308:ASN:ND2	2.32	0.58
13:D:186:GLN:O	13:D:322:ASN:ND2	2.37	0.58
15:F:17:VAL:HG12	15:F:20:LEU:HD12	1.84	0.57
13:D:141:TYR:HA	13:D:144:ILE:HG12	1.86	0.57
15:F:17:VAL:HG13	15:F:19:TRP:H	1.70	0.57
17:S:185:SER:OG	17:S:189:ARG:N	2.35	0.57
17:S:249:ALA:O	17:S:252:TRP:NE1	2.38	0.57
12:A:41:LEU:HD22	31:A:404:PHO:H91	1.87	0.56
32:F:101:HEM:HBB2	32:F:101:HEM:HMB1	1.87	0.56
19:A:402:CLA:H61	19:D:401:CLA:HAB	1.87	0.56
12:A:332:HIS:HB3	17:S:177:GLY:HA2	1.87	0.56
19:D:401:CLA:HED3	19:D:401:CLA:H2A	1.86	0.56
13:D:277:THR:O	13:D:281:MET:HG2	2.05	0.56
14:E:23:HIS:NE2	32:F:101:HEM:ND	2.53	0.56
17:S:180:ARG:NH1	17:S:222:GLN:O	2.38	0.56
17:S:287:LEU:HD22	17:S:298:LYS:HA	1.87	0.56
17:S:84:GLN:HG2	17:S:86:LEU:HD22	1.87	0.55
12:A:126:TYR:HE2	12:A:130:GLN:HE21	1.55	0.55
12:A:316:THR:N	12:A:319:ASP:OD2	2.38	0.54
12:A:104:GLU:O	12:A:108:ASN:ND2	2.34	0.54
13:D:201:VAL:HG22	19:D:403:CLA:C1B	2.38	0.54
12:A:118:HIS:CD2	19:A:405:CLA:NB	2.74	0.53
13:D:161:PRO:HB3	13:D:170:ALA:HB2	1.91	0.53
12:A:147:TYR:OH	31:A:404:PHO:O1A	2.26	0.53
17:S:268:ASP:OD2	17:S:312:VAL:N	2.32	0.52
13:D:66:SER:OG	13:D:69:GLU:OE1	2.18	0.52
13:D:34:GLY:HA2	13:D:128:ARG:HD2	1.92	0.52
31:A:404:PHO:NC	13:D:209:LEU:HD12	2.24	0.52
14:E:34:GLY:O	14:E:38:VAL:HG22	2.10	0.52
13:D:33:SER:HA	13:D:36:LEU:HD13	1.92	0.52
17:S:45:LEU:HD12	17:S:51:PHE:HZ	1.75	0.52
13:D:56:THR:HG21	14:E:50:PRO:HD3	1.92	0.51
13:D:102:THR:OG1	14:E:46:ALA:O	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:D:288:GLY:O	13:D:292:ASN:N	2.41	0.51
14:E:25:ILE:HG13	14:E:26:THR:HG23	1.92	0.51
12:A:143:ILE:HB	13:D:220:ASN:ND2	2.22	0.51
13:D:111:TRP:HB3	13:D:112:PRO:HD3	1.93	0.51
17:S:150:GLU:OE1	17:S:184:ARG:NH2	2.43	0.51
13:D:191:TRP:CE2	13:D:197:HIS:HB2	2.47	0.50
17:S:57:THR:OG1	17:S:61:ASN:OD1	2.24	0.50
12:A:150:PRO:HB2	19:A:402:CLA:H71	1.93	0.50
13:D:250:ASN:ND2	13:D:261:PHE:O	2.44	0.50
12:A:34:GLY:HA2	12:A:37:MET:HB3	1.93	0.50
12:A:89:ILE:HD11	12:A:108:ASN:HB3	1.93	0.49
12:A:204:GLY:HA2	12:A:278:TRP:CD1	2.47	0.49
13:D:78:VAL:HB	13:D:173:PHE:HB2	1.93	0.49
17:S:65:LEU:HG	17:S:73:PHE:HB2	1.93	0.49
19:A:402:CLA:H122	31:A:404:PHO:H3A	1.95	0.49
12:A:154:ALA:O	12:A:158:PHE:HB2	2.12	0.49
15:F:17:VAL:HG22	15:F:18:ARG:H	1.78	0.49
19:A:403:CLA:HBC3	13:D:178:ILE:HG23	1.93	0.49
12:A:149:ALA:HB1	12:A:283:ILE:HB	1.95	0.49
17:S:161:THR:HB	17:S:168:TRP:CE3	2.47	0.49
17:S:234:LEU:HG	17:S:242:GLN:HB3	1.94	0.48
17:S:66:VAL:HG12	17:S:72:ILE:HG22	1.95	0.48
14:E:21:VAL:O	14:E:25:ILE:HG12	2.14	0.48
13:D:197:HIS:HE1	19:D:403:CLA:C1C	2.26	0.48
12:A:103:ASP:OD1	12:A:103:ASP:N	2.41	0.48
19:A:403:CLA:H3A	19:A:403:CLA:HBA2	1.37	0.47
13:D:292:ASN:O	13:D:294:ARG:HD2	2.13	0.47
12:A:36:LEU:HD22	12:A:125:CYS:SG	2.54	0.47
13:D:171:PRO:HB3	13:D:181:PHE:CG	2.49	0.47
19:D:403:CLA:HMB1	19:D:403:CLA:HBB1	1.96	0.47
19:D:401:CLA:H143	19:D:401:CLA:HMB3	1.96	0.47
17:S:40:TRP:HB3	17:S:330:LEU:HB3	1.95	0.47
17:S:276:GLU:OE2	17:S:278:TRP:NE1	2.37	0.47
15:F:30:VAL:HA	15:F:33:VAL:HG22	1.97	0.47
12:A:283:ILE:HA	12:A:286:THR:HG22	1.95	0.47
12:A:308:ASP:OD1	12:A:312:ARG:N	2.45	0.47
19:A:405:CLA:HAB	16:I:15:PHE:HD2	1.79	0.47
17:S:283:SER:O	17:S:283:SER:OG	2.33	0.47
17:S:116:LEU:HD22	17:S:125:TRP:HB3	1.98	0.46
13:D:263:ASN:OD1	13:D:264:LYS:N	2.48	0.46
17:S:128:ILE:HD13	17:S:165:GLY:HA3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:304:ASP:OD1	17:S:304:ASP:N	2.49	0.46
19:D:403:CLA:H62	19:D:403:CLA:H41	1.72	0.46
17:S:172:VAL:HG21	17:S:210:TRP:CD1	2.50	0.46
13:D:191:TRP:CE3	13:D:289:LEU:HD11	2.51	0.46
13:D:276:VAL:HG12	31:D:402:PHO:HBC1	1.98	0.46
19:D:401:CLA:CHA	19:D:401:CLA:HBA1	2.45	0.46
13:D:125:PHE:HE2	31:D:402:PHO:HBD	1.81	0.46
13:D:152:VAL:HG21	13:D:279:LEU:HD22	1.97	0.46
19:D:404:CLA:H3A	19:D:404:CLA:O1A	2.16	0.46
12:A:275:LEU:HG	13:D:211:CYS:SG	2.55	0.46
17:S:73:PHE:HD2	17:S:82:TRP:HB3	1.81	0.46
13:D:322:ASN:O	13:D:326:ARG:HG2	2.17	0.45
17:S:57:THR:HG22	17:S:101:PHE:CD2	2.51	0.45
12:A:220:THR:HA	12:A:223:LEU:HG	1.98	0.45
15:F:27:VAL:HG12	15:F:28:PRO:HD3	1.98	0.45
15:F:32:PHE:O	15:F:36:ILE:HG13	2.16	0.45
12:A:216:GLY:HA3	13:D:272:LEU:HB2	1.99	0.45
17:S:79:GLY:O	17:S:82:TRP:NE1	2.50	0.45
12:A:57:PRO:HD3	12:A:73:TYR:CZ	2.52	0.45
12:A:212:SER:OG	13:D:211:CYS:HB2	2.17	0.45
15:F:38:ALA:O	15:F:42:ILE:HG23	2.17	0.45
12:A:187:GLN:HB2	19:A:402:CLA:HAC2	1.99	0.44
17:S:272:ARG:HE	17:S:332:TYR:HE2	1.65	0.44
12:A:343:LEU:HB2	17:S:168:TRP:HB2	2.00	0.44
17:S:45:LEU:HD12	17:S:51:PHE:CZ	2.52	0.44
19:A:402:CLA:HMB2	19:D:403:CLA:HMB2	2.00	0.44
17:S:291:ASP:OD1	17:S:291:ASP:N	2.51	0.44
17:S:307:ALA:HB2	17:S:328:ILE:HD12	1.99	0.44
13:D:53:THR:HA	13:D:67:TYR:H	1.82	0.44
12:A:189:GLU:OE1	17:S:220:ARG:NH1	2.51	0.44
12:A:79:SER:HB2	13:D:313:THR:HG21	1.99	0.43
12:A:92:HIS:ND1	12:A:93:PHE:O	2.49	0.43
12:A:326:ILE:O	12:A:329:GLU:HG3	2.18	0.43
13:D:91:PHE:HE1	19:D:404:CLA:HAA1	1.83	0.43
19:D:401:CLA:HMA1	19:D:401:CLA:H142	2.00	0.43
12:A:97:TRP:CG	16:I:5:LYS:HB2	2.53	0.43
13:D:90:LEU:HD22	13:D:107:ILE:HD12	1.99	0.43
13:D:50:THR:HG22	15:F:32:PHE:HZ	1.83	0.43
17:S:149:ALA:HB3	17:S:161:THR:HG22	2.00	0.43
17:S:214:ASN:OD1	17:S:214:ASN:N	2.52	0.43
17:S:45:LEU:HD21	17:S:82:TRP:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:334:ARG:HH22	17:S:212:PRO:HG3	1.84	0.42
13:D:201:VAL:HG22	19:D:403:CLA:C2B	2.48	0.42
17:S:141:ILE:HD11	17:S:149:ALA:HB1	2.00	0.42
13:D:40:CYS:HB2	19:D:404:CLA:HBB1	2.02	0.42
13:D:182:ILE:HA	19:D:403:CLA:HMD2	2.00	0.42
19:D:401:CLA:H2A	19:D:401:CLA:CED	2.49	0.42
17:S:268:ASP:OD1	17:S:269:LEU:N	2.53	0.42
12:A:279:PRO:O	12:A:283:ILE:HG12	2.19	0.42
17:S:293:GLY:HA2	17:S:296:TRP:CE2	2.54	0.42
13:D:157:PHE:CD1	13:D:171:PRO:HG2	2.54	0.42
13:D:279:LEU:HD12	31:D:402:PHO:HBC3	2.02	0.42
14:E:27:ILE:HB	14:E:28:PRO:HD3	2.02	0.42
31:A:404:PHO:H3A	31:A:404:PHO:HBA2	1.70	0.41
17:S:120:ASP:OD1	17:S:120:ASP:N	2.52	0.41
17:S:37:PHE:HE2	17:S:39:PRO:HB3	1.85	0.41
14:E:27:ILE:HG12	32:F:101:HEM:HMC2	2.03	0.41
17:S:42:GLU:HA	17:S:330:LEU:HD23	2.02	0.41
12:A:43:THR:HG23	21:A:406:BCR:H362	2.02	0.41
14:E:44:TYR:CD2	14:E:51:ARG:HG2	2.56	0.41
19:A:405:CLA:HAB	16:I:15:PHE:CD2	2.55	0.41
13:D:189:HIS:ND1	13:D:289:LEU:HD13	2.36	0.41
12:A:206:PHE:CD2	31:D:402:PHO:HBB2	2.56	0.40
13:D:293:LEU:HD21	13:D:295:ALA:HB3	2.02	0.40
17:S:94:ALA:HB1	17:S:114:ILE:HG21	2.03	0.40
17:S:291:ASP:CG	17:S:294:GLN:HB2	2.41	0.40
12:A:56:PRO:HB2	12:A:107:TYR:CE1	2.57	0.40
14:E:36:LEU:O	14:E:40:THR:HG22	2.21	0.40
13:D:69:GLU:OE1	13:D:69:GLU:N	2.44	0.40
13:D:313:THR:HB	13:D:316:THR:HG23	2.04	0.40
17:S:51:PHE:CZ	17:S:327:GLY:HA2	2.56	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	739/751 (98%)	711 (96%)	28 (4%)	0	100	100
2	b	727/731 (100%)	707 (97%)	20 (3%)	0	100	100
3	c	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	d	137/141 (97%)	128 (93%)	9 (7%)	0	100	100
5	e	67/74 (90%)	64 (96%)	3 (4%)	0	100	100
6	f	140/165 (85%)	135 (96%)	5 (4%)	0	100	100
7	i	38/40 (95%)	38 (100%)	0	0	100	100
8	j	38/40 (95%)	38 (100%)	0	0	100	100
9	k	73/86 (85%)	72 (99%)	1 (1%)	0	100	100
10	l	141/157 (90%)	137 (97%)	4 (3%)	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
12	A	285/344 (83%)	273 (96%)	12 (4%)	0	100	100
13	D	274/336 (82%)	268 (98%)	6 (2%)	0	100	100
14	E	42/81 (52%)	42 (100%)	0	0	100	100
15	F	26/44 (59%)	24 (92%)	2 (8%)	0	100	100
16	I	25/38 (66%)	24 (96%)	1 (4%)	0	100	100
17	S	301/342 (88%)	295 (98%)	6 (2%)	0	100	100
All	All	3160/3482 (91%)	3058 (97%)	102 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	593/603 (98%)	591 (100%)	2 (0%)	92	97
2	b	582/583 (100%)	575 (99%)	7 (1%)	71	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	c	68/69 (99%)	66 (97%)	2 (3%)	42 72
4	d	114/116 (98%)	114 (100%)	0	100 100
5	e	57/60 (95%)	57 (100%)	0	100 100
6	f	119/137 (87%)	119 (100%)	0	100 100
7	i	32/32 (100%)	32 (100%)	0	100 100
8	j	35/35 (100%)	35 (100%)	0	100 100
9	k	53/62 (86%)	53 (100%)	0	100 100
10	l	107/118 (91%)	105 (98%)	2 (2%)	57 80
11	m	25/25 (100%)	23 (92%)	2 (8%)	12 39
12	A	235/283 (83%)	233 (99%)	2 (1%)	78 91
13	D	220/271 (81%)	215 (98%)	5 (2%)	50 76
14	E	38/73 (52%)	38 (100%)	0	100 100
15	F	22/37 (60%)	21 (96%)	1 (4%)	27 61
16	I	24/34 (71%)	24 (100%)	0	100 100
17	S	239/279 (86%)	239 (100%)	0	100 100
All	All	2563/2817 (91%)	2540 (99%)	23 (1%)	79 91

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	420	LYS
1	a	684	MET
2	b	44	GLN
2	b	257	PHE
2	b	292	ARG
2	b	350	MET
2	b	408	ARG
2	b	566	ASP
2	b	574	TYR
3	c	32	ASP
3	c	75	ARG
10	l	19	HIS
10	l	73	ASP
11	m	1	MET
11	m	5	ASP
12	A	64	ARG
12	A	135	TYR

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Mol	Chain	Res	Type
13	D	180	ARG
13	D	246	MET
13	D	270	PHE
13	D	271	MET
13	D	329	MET
15	F	44	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	630	ASN
9	k	28	ASN
10	l	105	GLN
12	A	337	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 145 ligands modelled in this entry, 1 is monoatomic - leaving 144 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	a	814	-	65,73,73	1.44	7 (10%)	76,113,113	1.44	8 (10%)
19	CLA	l	1502	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	7 (9%)
21	BCR	j	104	-	41,41,41	1.19	3 (7%)	56,56,56	1.23	7 (12%)
19	CLA	b	3007	-	65,73,73	1.44	7 (10%)	76,113,113	1.39	9 (11%)
19	CLA	k	4003	9	45,53,73	1.79	6 (13%)	52,89,113	1.57	7 (13%)
31	PHO	D	402	-	51,69,69	1.02	4 (7%)	47,99,99	1.21	7 (14%)
19	CLA	a	817	-	46,54,73	1.71	6 (13%)	53,90,113	1.60	6 (11%)
21	BCR	k	4004	-	41,41,41	1.15	2 (4%)	56,56,56	1.25	6 (10%)
23	LMG	b	3051	-	55,55,55	0.76	1 (1%)	63,63,63	1.34	8 (12%)
19	CLA	a	839	-	65,73,73	1.47	7 (10%)	76,113,113	1.35	7 (9%)
19	CLA	b	3035	-	50,58,73	1.69	6 (12%)	58,95,113	1.55	8 (13%)
18	CL0	a	801	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	9 (11%)
19	CLA	b	3031	-	50,58,73	1.63	7 (14%)	58,95,113	1.54	9 (15%)
19	CLA	b	3017	-	65,73,73	1.46	7 (10%)	76,113,113	1.42	9 (11%)
19	CLA	b	3032	-	65,73,73	1.51	7 (10%)	76,113,113	1.34	7 (9%)
19	CLA	b	3034	-	65,73,73	1.46	6 (9%)	76,113,113	1.41	9 (11%)
21	BCR	a	845	-	41,41,41	1.19	2 (4%)	56,56,56	1.22	6 (10%)
21	BCR	f	202	-	41,41,41	1.19	2 (4%)	56,56,56	1.18	5 (8%)
19	CLA	a	826	-	65,73,73	1.45	6 (9%)	76,113,113	1.43	8 (10%)
19	CLA	b	3026	-	65,73,73	1.47	7 (10%)	76,113,113	1.39	7 (9%)
21	BCR	b	3043	-	41,41,41	1.22	2 (4%)	56,56,56	1.25	6 (10%)
19	CLA	a	810	1	51,59,73	1.62	7 (13%)	59,96,113	1.59	8 (13%)
19	CLA	b	3009	2	65,73,73	1.47	7 (10%)	76,113,113	1.38	7 (9%)
19	CLA	b	3022	-	46,54,73	1.75	6 (13%)	53,90,113	1.55	6 (11%)
19	CLA	b	3013	-	65,73,73	1.45	8 (12%)	76,113,113	1.45	9 (11%)
23	LMG	a	853	-	40,40,55	0.81	0	48,48,63	1.32	5 (10%)
19	CLA	a	830	-	65,73,73	1.46	7 (10%)	76,113,113	1.36	8 (10%)
19	CLA	a	837	1	65,73,73	1.47	6 (9%)	76,113,113	1.40	8 (10%)
21	BCR	k	4001	-	41,41,41	1.18	2 (4%)	56,56,56	1.29	7 (12%)
19	CLA	a	807	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	7 (9%)
19	CLA	D	401	-	65,73,73	1.48	5 (7%)	76,113,113	1.36	6 (7%)
21	BCR	b	3047	-	41,41,41	1.20	2 (4%)	56,56,56	1.18	7 (12%)
19	CLA	a	838	-	51,59,73	1.63	7 (13%)	59,96,113	1.58	8 (13%)
21	BCR	a	848	-	41,41,41	1.22	2 (4%)	56,56,56	1.27	7 (12%)
19	CLA	a	811	-	50,58,73	1.64	6 (12%)	58,95,113	1.63	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	a	803	-	65,73,73	1.43	7 (10%)	76,113,113	1.42	7 (9%)
20	PQN	b	3042	-	34,34,34	0.38	0	42,45,45	0.39	0
19	CLA	b	3015	-	55,63,73	1.62	8 (14%)	64,101,113	1.48	8 (12%)
21	BCR	a	847	-	41,41,41	1.19	3 (7%)	56,56,56	1.22	6 (10%)
19	CLA	a	822	-	65,73,73	1.46	7 (10%)	76,113,113	1.40	7 (9%)
19	CLA	b	3012	-	50,58,73	1.68	7 (14%)	58,95,113	1.49	8 (13%)
19	CLA	l	1501	-	50,58,73	1.70	5 (10%)	58,95,113	1.57	8 (13%)
19	CLA	a	819	-	65,73,73	1.48	9 (13%)	76,113,113	1.37	8 (10%)
25	SF4	c	101	3	0,12,12	-	-	-		
19	CLA	a	802	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	8 (10%)
19	CLA	b	3024	-	65,73,73	1.45	6 (9%)	76,113,113	1.40	7 (9%)
19	CLA	b	3039	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	8 (10%)
21	BCR	A	406	-	41,41,41	1.16	2 (4%)	56,56,56	1.22	6 (10%)
20	PQN	a	844	-	34,34,34	0.36	0	42,45,45	0.42	0
19	CLA	b	3008	-	65,73,73	1.46	8 (12%)	76,113,113	1.39	8 (10%)
19	CLA	a	808	-	65,73,73	1.44	7 (10%)	76,113,113	1.43	6 (7%)
27	EQ3	b	3052	-	43,43,43	1.65	9 (20%)	56,60,60	1.57	12 (21%)
21	BCR	j	101	-	41,41,41	1.15	2 (4%)	56,56,56	1.26	7 (12%)
19	CLA	a	805	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	7 (9%)
19	CLA	b	3040	-	65,73,73	1.49	8 (12%)	76,113,113	1.42	6 (7%)
19	CLA	f	201	-	65,73,73	1.47	7 (10%)	76,113,113	1.36	6 (7%)
19	CLA	b	3028	-	65,73,73	1.44	7 (10%)	76,113,113	1.35	7 (9%)
19	CLA	j	102	8	55,63,73	1.61	6 (10%)	64,101,113	1.47	7 (10%)
22	LHG	a	852	19	48,48,48	0.60	1 (2%)	51,54,54	1.28	6 (11%)
19	CLA	a	858	-	65,73,73	1.48	7 (10%)	76,113,113	1.35	7 (9%)
19	CLA	a	833	-	60,68,73	1.51	9 (15%)	70,107,113	1.39	7 (10%)
19	CLA	a	842	-	65,73,73	1.47	7 (10%)	76,113,113	1.41	7 (9%)
19	CLA	b	3029	-	65,73,73	1.47	7 (10%)	76,113,113	1.47	9 (11%)
21	BCR	l	1504	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	8 (14%)
19	CLA	a	804	-	65,73,73	1.46	8 (12%)	76,113,113	1.39	8 (10%)
22	LHG	a	850	-	48,48,48	0.62	1 (2%)	51,54,54	1.27	6 (11%)
22	LHG	a	854	-	48,48,48	0.61	1 (2%)	51,54,54	1.25	6 (11%)
23	LMG	b	3049	-	55,55,55	0.69	0	63,63,63	1.40	8 (12%)
19	CLA	f	204	6	50,58,73	1.69	6 (12%)	58,95,113	1.53	8 (13%)
19	CLA	a	831	-	65,73,73	1.45	6 (9%)	76,113,113	1.50	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	a	820	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	8 (10%)
19	CLA	b	3021	-	60,68,73	1.50	6 (10%)	70,107,113	1.45	7 (10%)
22	LHG	f	206	-	48,48,48	0.57	0	51,54,54	1.26	6 (11%)
19	CLA	b	3003	-	65,73,73	1.46	7 (10%)	76,113,113	1.44	9 (11%)
19	CLA	a	856	-	65,73,73	1.48	8 (12%)	76,113,113	1.36	6 (7%)
19	CLA	A	403	-	46,54,73	1.72	6 (13%)	53,90,113	1.60	6 (11%)
29	LMT	f	207	-	36,36,36	1.19	5 (13%)	47,47,47	1.03	3 (6%)
19	CLA	a	816	-	46,54,73	1.72	6 (13%)	53,90,113	1.59	7 (13%)
19	CLA	f	203	-	50,58,73	1.67	6 (12%)	58,95,113	1.57	8 (13%)
24	45D	a	857	-	43,43,43	1.70	9 (20%)	54,60,60	1.61	10 (18%)
19	CLA	a	813	-	60,68,73	1.55	7 (11%)	70,107,113	1.39	7 (10%)
19	CLA	b	3030	-	51,59,73	1.68	6 (11%)	59,96,113	1.47	7 (11%)
19	CLA	b	3023	-	57,65,73	1.55	6 (10%)	66,103,113	1.43	7 (10%)
28	ZEX	b	3053	-	42,43,43	1.64	8 (19%)	55,60,60	1.60	11 (20%)
26	ECH	b	3045	-	42,42,42	1.70	8 (19%)	55,58,58	2.27	14 (25%)
19	CLA	A	405	-	50,58,73	1.69	6 (12%)	58,95,113	1.54	7 (12%)
19	CLA	a	815	-	65,73,73	1.47	7 (10%)	76,113,113	1.40	8 (10%)
19	CLA	b	3016	-	56,64,73	1.57	7 (12%)	65,102,113	1.46	7 (10%)
19	CLA	a	835	-	65,73,73	1.45	6 (9%)	76,113,113	1.46	8 (10%)
19	CLA	a	829	-	65,73,73	1.44	7 (10%)	76,113,113	1.46	8 (10%)
32	HEM	F	101	15,14	41,50,50	1.50	3 (7%)	45,82,82	1.27	4 (8%)
19	CLA	a	824	-	65,73,73	1.48	7 (10%)	76,113,113	1.41	6 (7%)
19	CLA	b	3025	-	55,63,73	1.57	6 (10%)	64,101,113	1.51	7 (10%)
19	CLA	b	3014	-	65,73,73	1.44	6 (9%)	76,113,113	1.44	7 (9%)
19	CLA	b	3018	-	65,73,73	1.45	6 (9%)	76,113,113	1.41	7 (9%)
19	CLA	A	402	-	65,73,73	1.47	7 (10%)	76,113,113	1.40	6 (7%)
19	CLA	b	3020	-	65,73,73	1.48	7 (10%)	76,113,113	1.35	7 (9%)
19	CLA	a	806	-	65,73,73	1.43	7 (10%)	76,113,113	1.49	8 (10%)
23	LMG	a	851	-	50,50,55	0.76	0	58,58,63	1.33	7 (12%)
19	CLA	a	834	-	65,73,73	1.44	6 (9%)	76,113,113	1.45	8 (10%)
31	PHO	A	404	-	51,69,69	1.02	4 (7%)	47,99,99	1.10	5 (10%)
19	CLA	b	3006	-	65,73,73	1.46	7 (10%)	76,113,113	1.39	8 (10%)
19	CLA	D	404	-	46,54,73	1.72	6 (13%)	53,90,113	1.60	6 (11%)
19	CLA	b	3041	22	46,54,73	1.70	6 (13%)	53,90,113	1.58	7 (13%)
19	CLA	b	3002	-	65,73,73	1.48	7 (10%)	76,113,113	1.34	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	BCR	b	3046	-	41,41,41	1.14	2 (4%)	56,56,56	1.25	7 (12%)
21	BCR	b	3044	-	41,41,41	1.16	2 (4%)	56,56,56	1.20	5 (8%)
19	CLA	a	821	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	7 (9%)
25	SF4	b	3001	2,1	0,12,12	-	-	-		
25	SF4	c	102	3	0,12,12	-	-	-		
19	CLA	j	103	-	46,54,73	1.76	5 (10%)	53,90,113	1.52	6 (11%)
19	CLA	k	4002	-	46,54,73	1.76	6 (13%)	53,90,113	1.53	6 (11%)
19	CLA	a	840	-	65,73,73	1.50	7 (10%)	76,113,113	1.41	7 (9%)
26	ECH	m	101	-	42,42,42	1.78	9 (21%)	55,58,58	1.71	13 (23%)
19	CLA	l	1503	-	52,60,73	1.63	6 (11%)	60,97,113	1.54	6 (10%)
19	CLA	b	3011	-	56,64,73	1.58	7 (12%)	65,102,113	1.48	6 (9%)
21	BCR	a	849	-	25,25,41	1.18	1 (4%)	33,33,56	1.33	5 (15%)
19	CLA	D	403	-	55,63,73	1.57	7 (12%)	64,101,113	1.50	8 (12%)
19	CLA	a	828	-	65,73,73	1.46	7 (10%)	76,113,113	1.39	8 (10%)
19	CLA	a	832	-	56,64,73	1.57	6 (10%)	65,102,113	1.46	6 (9%)
19	CLA	b	3036	-	52,60,73	1.62	7 (13%)	60,97,113	1.55	7 (11%)
21	BCR	a	846	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	6 (10%)
22	LHG	b	3050	19	37,37,48	0.70	1 (2%)	40,43,54	1.22	3 (7%)
19	CLA	a	843	22	56,64,73	1.57	7 (12%)	65,102,113	1.48	8 (12%)
19	CLA	b	3005	-	65,73,73	1.44	7 (10%)	76,113,113	1.45	7 (9%)
19	CLA	a	855	-	65,73,73	1.46	7 (10%)	76,113,113	1.37	6 (7%)
19	CLA	a	818	-	65,73,73	1.42	6 (9%)	76,113,113	1.44	8 (10%)
28	ZEX	f	205	-	42,43,43	1.65	8 (19%)	55,60,60	1.53	10 (18%)
19	CLA	b	3010	-	56,64,73	1.61	7 (12%)	65,102,113	1.42	6 (9%)
19	CLA	b	3019	-	60,68,73	1.53	8 (13%)	70,107,113	1.39	7 (10%)
19	CLA	a	836	-	65,73,73	1.46	8 (12%)	76,113,113	1.38	8 (10%)
19	CLA	a	841	-	65,73,73	1.45	7 (10%)	76,113,113	1.43	8 (10%)
19	CLA	a	827	-	65,73,73	1.46	7 (10%)	76,113,113	1.38	8 (10%)
19	CLA	b	3033	-	65,73,73	1.46	7 (10%)	76,113,113	1.39	8 (10%)
19	CLA	b	3027	-	65,73,73	1.44	7 (10%)	76,113,113	1.41	6 (7%)
19	CLA	a	823	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
19	CLA	b	3038	-	50,58,73	1.71	7 (14%)	58,95,113	1.51	8 (13%)
19	CLA	a	812	-	65,73,73	1.45	6 (9%)	76,113,113	1.38	7 (9%)
21	BCR	b	3048	-	41,41,41	1.13	2 (4%)	56,56,56	1.18	4 (7%)
21	BCR	i	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.21	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	a	809	1	65,73,73	1.46	8 (12%)	76,113,113	1.40	9 (11%)
19	CLA	a	825	-	60,68,73	1.52	7 (11%)	70,107,113	1.45	6 (8%)
19	CLA	b	3004	-	65,73,73	1.48	7 (10%)	76,113,113	1.39	8 (10%)
19	CLA	b	3037	-	65,73,73	1.43	7 (10%)	76,113,113	1.42	8 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	a	814	-	-	16/37/115/115	-
19	CLA	l	1502	-	1/1/15/20	11/37/115/115	-
21	BCR	j	104	-	-	8/29/63/63	0/2/2/2
19	CLA	b	3007	-	1/1/15/20	15/37/115/115	-
19	CLA	k	4003	9	1/1/11/20	4/13/91/115	-
31	PHO	D	402	-	-	10/37/103/103	0/5/6/6
19	CLA	a	817	-	1/1/11/20	8/15/93/115	-
21	BCR	k	4004	-	-	6/29/63/63	0/2/2/2
23	LMG	b	3051	-	-	28/50/70/70	0/1/1/1
19	CLA	a	839	-	1/1/15/20	13/37/115/115	-
19	CLA	b	3035	-	1/1/12/20	8/19/97/115	-
18	CL0	a	801	-	3/3/20/25	10/37/135/135	-
19	CLA	b	3031	-	1/1/12/20	6/19/97/115	-
19	CLA	b	3017	-	1/1/15/20	13/37/115/115	-
19	CLA	b	3032	-	1/1/15/20	11/37/115/115	-
19	CLA	b	3034	-	1/1/15/20	14/37/115/115	-
21	BCR	a	845	-	-	11/29/63/63	0/2/2/2
21	BCR	f	202	-	-	16/29/63/63	0/2/2/2
19	CLA	a	826	-	1/1/15/20	18/37/115/115	-
19	CLA	b	3026	-	1/1/15/20	9/37/115/115	-
21	BCR	b	3043	-	-	10/29/63/63	0/2/2/2
19	CLA	a	810	1	1/1/12/20	3/21/99/115	-
19	CLA	b	3009	2	1/1/15/20	15/37/115/115	-
19	CLA	b	3022	-	1/1/11/20	3/15/93/115	-
19	CLA	b	3013	-	1/1/15/20	21/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LMG	a	853	-	-	15/35/55/70	0/1/1/1
19	CLA	a	830	-	1/1/15/20	16/37/115/115	-
19	CLA	a	837	1	1/1/15/20	13/37/115/115	-
21	BCR	k	4001	-	-	9/29/63/63	0/2/2/2
19	CLA	a	807	-	1/1/15/20	16/37/115/115	-
19	CLA	D	401	-	1/1/15/20	16/37/115/115	-
21	BCR	b	3047	-	-	6/29/63/63	0/2/2/2
19	CLA	a	838	-	-	7/21/99/115	-
21	BCR	a	848	-	-	8/29/63/63	0/2/2/2
19	CLA	a	811	-	1/1/12/20	8/19/97/115	-
19	CLA	a	803	-	1/1/15/20	12/37/115/115	-
20	PQN	b	3042	-	-	0/23/43/43	0/2/2/2
19	CLA	b	3015	-	1/1/13/20	11/25/103/115	-
21	BCR	a	847	-	-	7/29/63/63	0/2/2/2
19	CLA	a	822	-	1/1/15/20	12/37/115/115	-
19	CLA	b	3012	-	1/1/12/20	7/19/97/115	-
19	CLA	l	1501	-	1/1/12/20	8/19/97/115	-
19	CLA	a	819	-	1/1/15/20	22/37/115/115	-
25	SF4	c	101	3	-	-	0/6/5/5
19	CLA	a	802	-	1/1/15/20	15/37/115/115	-
19	CLA	b	3024	-	1/1/15/20	11/37/115/115	-
19	CLA	b	3039	-	1/1/15/20	15/37/115/115	-
21	BCR	A	406	-	-	8/29/63/63	0/2/2/2
20	PQN	a	844	-	-	1/23/43/43	0/2/2/2
19	CLA	b	3008	-	1/1/15/20	10/37/115/115	-
19	CLA	a	808	-	1/1/15/20	14/37/115/115	-
27	EQ3	b	3052	-	-	4/29/68/68	0/2/2/2
21	BCR	j	101	-	-	6/29/63/63	0/2/2/2
19	CLA	a	805	-	1/1/15/20	13/37/115/115	-
19	CLA	b	3040	-	1/1/15/20	9/37/115/115	-
19	CLA	f	201	-	1/1/15/20	19/37/115/115	-
19	CLA	b	3028	-	1/1/15/20	14/37/115/115	-
19	CLA	j	102	8	1/1/13/20	9/25/103/115	-
22	LHG	a	852	19	-	23/53/53/53	-
19	CLA	a	858	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	a	833	-	1/1/14/20	13/31/109/115	-
19	CLA	a	842	-	1/1/15/20	15/37/115/115	-
19	CLA	b	3029	-	1/1/15/20	16/37/115/115	-
21	BCR	l	1504	-	-	10/29/63/63	0/2/2/2
19	CLA	a	804	-	1/1/15/20	6/37/115/115	-
22	LHG	a	850	-	-	27/53/53/53	-
22	LHG	a	854	-	-	23/53/53/53	-
23	LMG	b	3049	-	-	27/50/70/70	0/1/1/1
19	CLA	f	204	6	1/1/12/20	7/19/97/115	-
19	CLA	a	831	-	1/1/15/20	18/37/115/115	-
19	CLA	a	820	-	1/1/15/20	17/37/115/115	-
19	CLA	b	3021	-	1/1/14/20	10/31/109/115	-
22	LHG	f	206	-	-	28/53/53/53	-
19	CLA	b	3003	-	1/1/15/20	20/37/115/115	-
19	CLA	a	856	-	1/1/15/20	17/37/115/115	-
19	CLA	A	403	-	1/1/11/20	8/15/93/115	-
29	LMT	f	207	-	-	15/21/61/61	0/2/2/2
19	CLA	a	816	-	1/1/11/20	9/15/93/115	-
19	CLA	f	203	-	1/1/12/20	5/19/97/115	-
24	45D	a	857	-	-	4/29/69/69	0/2/2/2
19	CLA	a	813	-	1/1/14/20	13/31/109/115	-
19	CLA	b	3030	-	1/1/12/20	7/21/99/115	-
19	CLA	b	3023	-	1/1/13/20	9/28/106/115	-
28	ZEX	b	3053	-	-	5/29/67/67	0/2/2/2
26	ECH	b	3045	-	-	9/29/66/66	0/2/2/2
19	CLA	A	405	-	1/1/12/20	7/19/97/115	-
19	CLA	a	815	-	1/1/15/20	13/37/115/115	-
19	CLA	b	3016	-	1/1/13/20	9/27/105/115	-
19	CLA	a	835	-	1/1/15/20	15/37/115/115	-
19	CLA	a	829	-	1/1/15/20	7/37/115/115	-
32	HEM	F	101	15,14	-	3/12/54/54	-
19	CLA	a	824	-	1/1/15/20	16/37/115/115	-
19	CLA	b	3025	-	1/1/13/20	6/25/103/115	-
19	CLA	b	3014	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	b	3018	-	1/1/15/20	11/37/115/115	-
19	CLA	A	402	-	1/1/15/20	18/37/115/115	-
19	CLA	b	3020	-	1/1/15/20	15/37/115/115	-
19	CLA	a	806	-	1/1/15/20	11/37/115/115	-
23	LMG	a	851	-	-	26/45/65/70	0/1/1/1
19	CLA	a	834	-	1/1/15/20	8/37/115/115	-
31	PHO	A	404	-	-	11/37/103/103	0/5/6/6
19	CLA	b	3006	-	1/1/15/20	12/37/115/115	-
19	CLA	D	404	-	1/1/11/20	5/15/93/115	-
19	CLA	b	3041	22	1/1/11/20	11/15/93/115	-
19	CLA	b	3002	-	1/1/15/20	15/37/115/115	-
21	BCR	b	3046	-	-	6/29/63/63	0/2/2/2
21	BCR	b	3044	-	-	7/29/63/63	0/2/2/2
19	CLA	a	821	-	1/1/15/20	23/37/115/115	-
25	SF4	b	3001	2,1	-	-	0/6/5/5
25	SF4	c	102	3	-	-	0/6/5/5
19	CLA	j	103	-	1/1/11/20	5/15/93/115	-
19	CLA	k	4002	-	1/1/11/20	5/15/93/115	-
19	CLA	a	840	-	1/1/15/20	15/37/115/115	-
26	ECH	m	101	-	-	3/29/66/66	0/2/2/2
19	CLA	l	1503	-	1/1/12/20	9/22/100/115	-
19	CLA	b	3011	-	1/1/13/20	8/27/105/115	-
21	BCR	a	849	-	-	5/18/35/63	0/1/1/2
19	CLA	D	403	-	1/1/13/20	12/25/103/115	-
19	CLA	a	828	-	1/1/15/20	14/37/115/115	-
19	CLA	a	832	-	1/1/13/20	15/27/105/115	-
19	CLA	b	3036	-	1/1/12/20	8/22/100/115	-
21	BCR	a	846	-	-	6/29/63/63	0/2/2/2
22	LHG	b	3050	19	-	21/42/42/53	-
19	CLA	a	843	22	1/1/13/20	9/27/105/115	-
19	CLA	b	3005	-	1/1/15/20	18/37/115/115	-
19	CLA	a	855	-	1/1/15/20	8/37/115/115	-
19	CLA	a	818	-	1/1/15/20	10/37/115/115	-
28	ZEX	f	205	-	-	6/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	b	3010	-	1/1/13/20	9/27/105/115	-
19	CLA	b	3019	-	1/1/14/20	6/31/109/115	-
19	CLA	a	836	-	1/1/15/20	11/37/115/115	-
19	CLA	a	841	-	1/1/15/20	12/37/115/115	-
19	CLA	a	827	-	1/1/15/20	12/37/115/115	-
19	CLA	b	3033	-	1/1/15/20	19/37/115/115	-
19	CLA	b	3027	-	1/1/15/20	13/37/115/115	-
19	CLA	a	823	-	1/1/15/20	14/37/115/115	-
19	CLA	b	3038	-	1/1/12/20	5/19/97/115	-
19	CLA	a	812	-	1/1/15/20	14/37/115/115	-
21	BCR	b	3048	-	-	18/29/63/63	0/2/2/2
21	BCR	i	101	-	-	8/29/63/63	0/2/2/2
19	CLA	a	809	1	1/1/15/20	17/37/115/115	-
19	CLA	a	825	-	1/1/14/20	13/31/109/115	-
19	CLA	b	3004	-	1/1/15/20	17/37/115/115	-
19	CLA	b	3037	-	1/1/15/20	16/37/115/115	-

All (793) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	l	1501	CLA	C4B-NB	7.58	1.42	1.35
19	b	3010	CLA	C4B-NB	7.57	1.42	1.35
19	b	3032	CLA	C4B-NB	7.56	1.42	1.35
19	a	805	CLA	C4B-NB	7.56	1.42	1.35
19	a	840	CLA	C4B-NB	7.56	1.42	1.35
19	A	405	CLA	C4B-NB	7.50	1.41	1.35
19	j	103	CLA	C4B-NB	7.48	1.41	1.35
19	b	3038	CLA	C4B-NB	7.46	1.41	1.35
19	k	4003	CLA	C4B-NB	7.44	1.41	1.35
19	b	3022	CLA	C4B-NB	7.44	1.41	1.35
19	b	3015	CLA	C4B-NB	7.41	1.41	1.35
19	k	4002	CLA	C4B-NB	7.40	1.41	1.35
19	b	3030	CLA	C4B-NB	7.39	1.41	1.35
19	a	813	CLA	C4B-NB	7.38	1.41	1.35
19	a	824	CLA	C4B-NB	7.37	1.41	1.35
19	f	204	CLA	C4B-NB	7.36	1.41	1.35
19	b	3040	CLA	C4B-NB	7.36	1.41	1.35
19	b	3012	CLA	C4B-NB	7.32	1.41	1.35
19	a	819	CLA	C4B-NB	7.32	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	3035	CLA	C4B-NB	7.32	1.41	1.35
19	D	401	CLA	C4B-NB	7.31	1.41	1.35
19	b	3004	CLA	C4B-NB	7.28	1.41	1.35
19	a	821	CLA	C4B-NB	7.28	1.41	1.35
19	j	102	CLA	C4B-NB	7.27	1.41	1.35
19	b	3002	CLA	C4B-NB	7.25	1.41	1.35
19	b	3033	CLA	C4B-NB	7.24	1.41	1.35
19	a	858	CLA	C4B-NB	7.24	1.41	1.35
19	a	837	CLA	C4B-NB	7.24	1.41	1.35
19	b	3020	CLA	C4B-NB	7.23	1.41	1.35
19	a	856	CLA	C4B-NB	7.23	1.41	1.35
19	a	815	CLA	C4B-NB	7.22	1.41	1.35
19	f	201	CLA	C4B-NB	7.20	1.41	1.35
19	l	1502	CLA	C4B-NB	7.19	1.41	1.35
19	A	403	CLA	C4B-NB	7.19	1.41	1.35
19	a	842	CLA	C4B-NB	7.19	1.41	1.35
19	b	3009	CLA	C4B-NB	7.19	1.41	1.35
19	b	3029	CLA	C4B-NB	7.17	1.41	1.35
19	a	820	CLA	C4B-NB	7.17	1.41	1.35
19	b	3039	CLA	C4B-NB	7.16	1.41	1.35
19	a	843	CLA	C4B-NB	7.16	1.41	1.35
19	b	3026	CLA	C4B-NB	7.16	1.41	1.35
19	b	3034	CLA	C4B-NB	7.16	1.41	1.35
19	a	823	CLA	C4B-NB	7.16	1.41	1.35
19	l	1503	CLA	C4B-NB	7.16	1.41	1.35
19	a	841	CLA	C4B-NB	7.15	1.41	1.35
19	a	816	CLA	C4B-NB	7.14	1.41	1.35
19	a	839	CLA	C4B-NB	7.14	1.41	1.35
19	f	203	CLA	C4B-NB	7.14	1.41	1.35
19	D	403	CLA	C4B-NB	7.13	1.41	1.35
19	b	3016	CLA	C4B-NB	7.12	1.41	1.35
19	b	3011	CLA	C4B-NB	7.11	1.41	1.35
19	a	827	CLA	C4B-NB	7.11	1.41	1.35
19	b	3023	CLA	C4B-NB	7.11	1.41	1.35
19	a	807	CLA	C4B-NB	7.10	1.41	1.35
19	A	402	CLA	C4B-NB	7.10	1.41	1.35
19	a	804	CLA	C4B-NB	7.09	1.41	1.35
19	b	3041	CLA	C4B-NB	7.08	1.41	1.35
19	b	3003	CLA	C4B-NB	7.08	1.41	1.35
19	a	802	CLA	C4B-NB	7.07	1.41	1.35
19	b	3019	CLA	C4B-NB	7.07	1.41	1.35
19	D	404	CLA	C4B-NB	7.07	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	825	CLA	C4B-NB	7.05	1.41	1.35
19	b	3027	CLA	C4B-NB	7.05	1.41	1.35
19	a	810	CLA	C4B-NB	7.03	1.41	1.35
19	b	3018	CLA	C4B-NB	7.03	1.41	1.35
19	a	855	CLA	C4B-NB	7.02	1.41	1.35
18	a	801	CL0	C4B-NB	7.02	1.41	1.35
19	a	812	CLA	C4B-NB	7.02	1.41	1.35
19	b	3036	CLA	C4B-NB	7.01	1.41	1.35
19	a	817	CLA	C4B-NB	7.00	1.41	1.35
19	a	811	CLA	C4B-NB	7.00	1.41	1.35
19	a	836	CLA	C4B-NB	7.00	1.41	1.35
19	a	830	CLA	C4B-NB	7.00	1.41	1.35
19	a	831	CLA	C4B-NB	7.00	1.41	1.35
19	a	809	CLA	C4B-NB	6.99	1.41	1.35
19	a	838	CLA	C4B-NB	6.98	1.41	1.35
19	a	832	CLA	C4B-NB	6.97	1.41	1.35
19	a	829	CLA	C4B-NB	6.97	1.41	1.35
19	a	835	CLA	C4B-NB	6.96	1.41	1.35
19	a	808	CLA	C4B-NB	6.95	1.41	1.35
19	b	3024	CLA	C4B-NB	6.95	1.41	1.35
19	b	3021	CLA	C4B-NB	6.95	1.41	1.35
19	b	3017	CLA	C4B-NB	6.94	1.41	1.35
19	a	826	CLA	C4B-NB	6.94	1.41	1.35
19	b	3014	CLA	C4B-NB	6.94	1.41	1.35
19	a	822	CLA	C4B-NB	6.93	1.41	1.35
19	b	3025	CLA	C4B-NB	6.93	1.41	1.35
19	b	3008	CLA	C4B-NB	6.92	1.41	1.35
19	b	3007	CLA	C4B-NB	6.90	1.41	1.35
19	b	3005	CLA	C4B-NB	6.89	1.41	1.35
19	b	3031	CLA	C4B-NB	6.89	1.41	1.35
19	a	818	CLA	C4B-NB	6.86	1.41	1.35
19	a	814	CLA	C4B-NB	6.85	1.41	1.35
19	b	3013	CLA	C4B-NB	6.85	1.41	1.35
19	b	3006	CLA	C4B-NB	6.85	1.41	1.35
19	a	834	CLA	C4B-NB	6.83	1.41	1.35
19	b	3028	CLA	C4B-NB	6.79	1.41	1.35
19	b	3037	CLA	C4B-NB	6.79	1.41	1.35
19	a	803	CLA	C4B-NB	6.77	1.41	1.35
19	a	806	CLA	C4B-NB	6.77	1.41	1.35
19	a	828	CLA	C4B-NB	6.73	1.41	1.35
19	a	833	CLA	C4B-NB	6.71	1.41	1.35
32	F	101	HEM	C3C-C2C	-4.81	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	m	101	ECH	C21-C22	4.02	1.41	1.35
26	m	101	ECH	C14-C13	3.95	1.41	1.35
19	j	102	CLA	C1D-ND	3.94	1.42	1.37
19	j	103	CLA	C1D-ND	3.93	1.42	1.37
19	l	1501	CLA	C1D-ND	3.93	1.42	1.37
26	m	101	ECH	C17-C18	3.90	1.41	1.35
26	b	3045	ECH	C21-C22	3.90	1.40	1.35
19	k	4002	CLA	C1D-ND	3.86	1.42	1.37
19	a	826	CLA	C1D-ND	3.86	1.42	1.37
28	f	205	ZEX	C30-C29	3.84	1.40	1.35
21	b	3043	BCR	C1-C6	-3.83	1.48	1.53
19	b	3017	CLA	C1D-ND	3.83	1.42	1.37
26	m	101	ECH	C10-C9	3.81	1.40	1.35
19	f	204	CLA	C1D-ND	3.79	1.42	1.37
19	A	402	CLA	C1D-ND	3.78	1.42	1.37
21	a	848	BCR	C1-C6	-3.77	1.48	1.53
28	f	205	ZEX	C34-C33	3.76	1.40	1.35
19	a	828	CLA	C1D-ND	3.76	1.42	1.37
26	b	3045	ECH	C10-C9	3.76	1.40	1.35
19	a	858	CLA	C1D-ND	3.75	1.42	1.37
24	a	857	45D	C38-C36	3.75	1.40	1.35
19	a	822	CLA	C1D-ND	3.74	1.42	1.37
19	a	842	CLA	C1D-ND	3.73	1.42	1.37
26	b	3045	ECH	C17-C18	3.71	1.40	1.35
19	b	3035	CLA	C1D-ND	3.71	1.42	1.37
19	a	817	CLA	C1D-ND	3.71	1.42	1.37
24	a	857	45D	C37-C35	3.70	1.40	1.35
19	a	824	CLA	C1D-ND	3.70	1.42	1.37
19	A	405	CLA	C1D-ND	3.70	1.42	1.37
19	D	401	CLA	C1D-ND	3.70	1.42	1.37
19	k	4003	CLA	C1D-ND	3.69	1.42	1.37
19	a	814	CLA	C1D-ND	3.69	1.42	1.37
19	a	823	CLA	C1D-ND	3.69	1.42	1.37
19	a	840	CLA	C1D-ND	3.69	1.42	1.37
19	f	203	CLA	C1D-ND	3.69	1.42	1.37
19	b	3038	CLA	C1D-ND	3.69	1.42	1.37
28	b	3053	ZEX	C34-C33	3.68	1.40	1.35
19	a	837	CLA	C1D-ND	3.68	1.42	1.37
19	b	3020	CLA	C1D-ND	3.68	1.42	1.37
19	a	838	CLA	C1D-ND	3.68	1.42	1.37
19	b	3004	CLA	C1D-ND	3.67	1.42	1.37
21	a	847	BCR	C1-C6	-3.67	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	404	CLA	C1D-ND	3.66	1.42	1.37
32	F	101	HEM	C3C-CAC	3.66	1.55	1.47
21	k	4001	BCR	C1-C6	-3.66	1.48	1.53
19	b	3002	CLA	C1D-ND	3.66	1.42	1.37
19	A	403	CLA	C1D-ND	3.66	1.42	1.37
18	a	801	CL0	C1D-ND	3.66	1.42	1.37
21	j	104	BCR	C1-C6	-3.66	1.48	1.53
19	b	3041	CLA	C1D-ND	3.65	1.42	1.37
19	a	815	CLA	C1D-ND	3.65	1.42	1.37
19	a	808	CLA	C1D-ND	3.64	1.42	1.37
19	a	839	CLA	C1D-ND	3.64	1.42	1.37
19	b	3014	CLA	C1D-ND	3.64	1.42	1.37
19	b	3010	CLA	C1D-ND	3.64	1.42	1.37
24	a	857	45D	C30-C26	3.64	1.40	1.35
19	a	856	CLA	C1D-ND	3.63	1.42	1.37
19	b	3021	CLA	C1D-ND	3.63	1.42	1.37
19	b	3022	CLA	C1D-ND	3.63	1.42	1.37
21	f	202	BCR	C1-C6	-3.62	1.48	1.53
19	a	811	CLA	C1D-ND	3.62	1.42	1.37
26	b	3045	ECH	C14-C13	3.62	1.40	1.35
21	a	849	BCR	C1-C6	-3.62	1.48	1.53
19	a	833	CLA	C1D-ND	3.62	1.42	1.37
28	b	3053	ZEX	C14-C13	3.62	1.40	1.35
28	f	205	ZEX	C10-C9	3.61	1.40	1.35
19	b	3029	CLA	C1D-ND	3.61	1.42	1.37
19	b	3039	CLA	C1D-ND	3.61	1.42	1.37
19	a	816	CLA	C1D-ND	3.61	1.42	1.37
19	a	825	CLA	C1D-ND	3.60	1.42	1.37
19	b	3037	CLA	C1D-ND	3.60	1.42	1.37
27	b	3052	EQ3	C21-C22	3.60	1.40	1.35
28	f	205	ZEX	C14-C13	3.60	1.40	1.35
19	l	1503	CLA	C1D-ND	3.59	1.42	1.37
19	a	813	CLA	C1D-ND	3.59	1.42	1.37
19	a	829	CLA	C1D-ND	3.59	1.42	1.37
19	a	841	CLA	C1D-ND	3.59	1.42	1.37
19	a	806	CLA	C1D-ND	3.58	1.42	1.37
19	b	3028	CLA	C1D-ND	3.58	1.42	1.37
19	a	835	CLA	C1D-ND	3.58	1.42	1.37
19	b	3013	CLA	C1D-ND	3.58	1.42	1.37
19	a	812	CLA	C1D-ND	3.58	1.42	1.37
19	b	3026	CLA	C1D-ND	3.58	1.42	1.37
19	b	3006	CLA	C1D-ND	3.58	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	3025	CLA	C1D-ND	3.58	1.42	1.37
19	a	802	CLA	C1D-ND	3.58	1.42	1.37
19	b	3040	CLA	C1D-ND	3.57	1.42	1.37
19	a	821	CLA	C1D-ND	3.57	1.42	1.37
21	b	3047	BCR	C30-C25	-3.57	1.48	1.53
19	b	3016	CLA	C1D-ND	3.57	1.42	1.37
24	a	857	45D	C29-C25	3.57	1.40	1.35
19	b	3018	CLA	C1D-ND	3.56	1.42	1.37
19	b	3034	CLA	C1D-ND	3.56	1.42	1.37
19	b	3030	CLA	C1D-ND	3.56	1.42	1.37
19	b	3036	CLA	C1D-ND	3.56	1.42	1.37
19	b	3031	CLA	C1D-ND	3.56	1.42	1.37
19	a	804	CLA	C1D-ND	3.55	1.42	1.37
19	b	3005	CLA	C1D-ND	3.55	1.42	1.37
19	f	201	CLA	C1D-ND	3.55	1.42	1.37
19	a	809	CLA	C1D-ND	3.55	1.42	1.37
21	a	846	BCR	C1-C6	-3.55	1.48	1.53
19	a	855	CLA	C1D-ND	3.54	1.42	1.37
19	a	831	CLA	C1D-ND	3.54	1.42	1.37
21	a	845	BCR	C1-C6	-3.54	1.48	1.53
19	b	3033	CLA	C1D-ND	3.53	1.42	1.37
19	b	3024	CLA	C1D-ND	3.52	1.42	1.37
28	b	3053	ZEX	C10-C9	3.52	1.40	1.35
19	b	3032	CLA	C1D-ND	3.52	1.42	1.37
19	a	830	CLA	C1D-ND	3.52	1.42	1.37
19	b	3027	CLA	C1D-ND	3.52	1.42	1.37
19	b	3019	CLA	C1D-ND	3.51	1.42	1.37
21	b	3043	BCR	C30-C25	-3.51	1.48	1.53
19	a	819	CLA	C1D-ND	3.50	1.42	1.37
19	a	818	CLA	C1D-ND	3.50	1.42	1.37
19	b	3007	CLA	C1D-ND	3.50	1.42	1.37
19	a	843	CLA	C1D-ND	3.50	1.42	1.37
19	a	803	CLA	C1D-ND	3.49	1.42	1.37
19	b	3015	CLA	C1D-ND	3.49	1.42	1.37
27	b	3052	EQ3	C17-C18	3.49	1.40	1.35
19	D	403	CLA	C1D-ND	3.48	1.42	1.37
21	A	406	BCR	C1-C6	-3.48	1.49	1.53
19	b	3009	CLA	C1D-ND	3.48	1.42	1.37
21	j	101	BCR	C1-C6	-3.47	1.49	1.53
19	a	827	CLA	C1D-ND	3.47	1.42	1.37
19	b	3023	CLA	C1D-ND	3.46	1.42	1.37
19	b	3011	CLA	C1D-ND	3.46	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	a	820	CLA	C1D-ND	3.46	1.42	1.37
19	l	1502	CLA	C1D-ND	3.44	1.42	1.37
19	b	3008	CLA	C1D-ND	3.44	1.42	1.37
19	a	810	CLA	C1D-ND	3.44	1.42	1.37
19	b	3006	CLA	C4D-ND	-3.43	1.33	1.37
19	b	3012	CLA	C1D-ND	3.43	1.42	1.37
26	m	101	ECH	C25-C26	3.42	1.40	1.35
21	b	3048	BCR	C1-C6	-3.42	1.49	1.53
19	a	805	CLA	C1D-ND	3.41	1.42	1.37
19	a	834	CLA	C1D-ND	3.40	1.42	1.37
19	b	3008	CLA	C4D-ND	-3.39	1.33	1.37
21	i	101	BCR	C1-C6	-3.38	1.49	1.53
28	b	3053	ZEX	C30-C29	3.38	1.40	1.35
19	a	807	CLA	C1D-ND	3.38	1.41	1.37
19	a	832	CLA	C1D-ND	3.37	1.41	1.37
21	l	1504	BCR	C1-C6	-3.37	1.49	1.53
19	a	832	CLA	C4D-ND	-3.37	1.33	1.37
21	b	3044	BCR	C1-C6	-3.35	1.49	1.53
21	a	845	BCR	C30-C25	-3.34	1.49	1.53
21	A	406	BCR	C30-C25	-3.32	1.49	1.53
19	a	809	CLA	C4D-ND	-3.32	1.33	1.37
21	j	104	BCR	C30-C25	-3.32	1.49	1.53
19	a	807	CLA	C4D-ND	-3.32	1.33	1.37
21	i	101	BCR	C30-C25	-3.32	1.49	1.53
19	a	828	CLA	C4D-ND	-3.31	1.33	1.37
19	a	836	CLA	C1D-ND	3.31	1.41	1.37
19	b	3005	CLA	C4D-ND	-3.29	1.33	1.37
27	b	3052	EQ3	C14-C13	3.28	1.40	1.35
19	b	3003	CLA	C1D-ND	3.28	1.41	1.37
19	b	3019	CLA	C4D-ND	-3.28	1.33	1.37
19	b	3038	CLA	C4D-ND	-3.27	1.33	1.37
21	b	3047	BCR	C1-C6	-3.27	1.49	1.53
19	b	3030	CLA	C4D-ND	-3.27	1.33	1.37
19	a	855	CLA	C4D-ND	-3.26	1.33	1.37
21	f	202	BCR	C30-C25	-3.26	1.49	1.53
21	k	4004	BCR	C1-C6	-3.25	1.49	1.53
19	b	3036	CLA	C4D-ND	-3.25	1.33	1.37
19	a	806	CLA	C4D-ND	-3.24	1.33	1.37
19	b	3013	CLA	C4D-ND	-3.23	1.33	1.37
21	k	4004	BCR	C30-C25	-3.23	1.49	1.53
19	b	3025	CLA	C4D-ND	-3.22	1.33	1.37
19	a	825	CLA	C4D-ND	-3.22	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	3037	CLA	C4D-ND	-3.22	1.33	1.37
21	a	848	BCR	C30-C25	-3.22	1.49	1.53
19	b	3034	CLA	C4D-ND	-3.22	1.33	1.37
19	a	805	CLA	CHC-C1C	3.22	1.43	1.35
19	b	3039	CLA	C4D-ND	-3.21	1.33	1.37
21	b	3046	BCR	C1-C6	-3.21	1.49	1.53
27	b	3052	EQ3	C10-C9	3.20	1.40	1.35
19	b	3003	CLA	C4D-ND	-3.20	1.33	1.37
19	a	839	CLA	C4D-ND	-3.20	1.33	1.37
19	b	3018	CLA	C4D-ND	-3.20	1.33	1.37
19	j	103	CLA	CHC-C1C	3.19	1.43	1.35
21	k	4001	BCR	C30-C25	-3.19	1.49	1.53
19	a	834	CLA	C4D-ND	-3.19	1.33	1.37
19	a	836	CLA	C4D-ND	-3.18	1.33	1.37
19	a	830	CLA	C4D-ND	-3.18	1.33	1.37
19	b	3028	CLA	C4D-ND	-3.18	1.33	1.37
19	a	813	CLA	C4D-ND	-3.17	1.33	1.37
19	A	402	CLA	C4D-ND	-3.17	1.33	1.37
19	b	3021	CLA	C4D-ND	-3.17	1.33	1.37
19	b	3010	CLA	C4D-ND	-3.17	1.33	1.37
19	f	203	CLA	C4D-ND	-3.17	1.33	1.37
19	a	827	CLA	C4D-ND	-3.17	1.33	1.37
19	a	808	CLA	C4D-ND	-3.16	1.33	1.37
19	b	3026	CLA	C4D-ND	-3.16	1.33	1.37
26	b	3045	ECH	C23-C22	-3.16	1.39	1.45
19	b	3011	CLA	C4D-ND	-3.16	1.33	1.37
19	b	3009	CLA	C4D-ND	-3.16	1.33	1.37
19	a	831	CLA	C4D-ND	-3.16	1.33	1.37
19	a	858	CLA	C4D-ND	-3.16	1.33	1.37
19	b	3012	CLA	C4D-ND	-3.16	1.33	1.37
19	b	3014	CLA	C4D-ND	-3.15	1.33	1.37
19	a	842	CLA	C4D-ND	-3.15	1.33	1.37
19	D	401	CLA	CHC-C1C	3.15	1.43	1.35
19	b	3004	CLA	CHC-C1C	3.15	1.43	1.35
21	a	847	BCR	C30-C25	-3.15	1.49	1.53
19	a	837	CLA	C4D-ND	-3.14	1.33	1.37
19	b	3024	CLA	C4D-ND	-3.14	1.33	1.37
19	b	3023	CLA	C4D-ND	-3.14	1.33	1.37
19	a	814	CLA	C4D-ND	-3.13	1.33	1.37
19	l	1501	CLA	CHC-C1C	3.13	1.43	1.35
19	a	833	CLA	C4D-ND	-3.13	1.33	1.37
19	b	3023	CLA	CHC-C1C	3.13	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	3024	CLA	CHC-C1C	3.13	1.43	1.35
19	b	3004	CLA	C4D-ND	-3.13	1.33	1.37
19	a	810	CLA	C4D-ND	-3.12	1.33	1.37
19	a	816	CLA	C4D-ND	-3.12	1.33	1.37
19	a	823	CLA	C4D-ND	-3.12	1.33	1.37
19	a	821	CLA	C4D-ND	-3.12	1.33	1.37
19	j	102	CLA	CHC-C1C	3.12	1.43	1.35
27	b	3052	EQ3	C8-C9	-3.12	1.39	1.45
19	a	838	CLA	C4D-ND	-3.12	1.33	1.37
19	a	802	CLA	C4D-ND	-3.11	1.33	1.37
19	a	840	CLA	C4D-ND	-3.11	1.33	1.37
19	f	203	CLA	CHC-C1C	3.11	1.42	1.35
28	b	3053	ZEX	C8-C9	-3.11	1.39	1.45
19	a	808	CLA	CHC-C1C	3.11	1.42	1.35
19	b	3003	CLA	CHC-C1C	3.11	1.42	1.35
19	b	3031	CLA	C4D-ND	-3.11	1.33	1.37
19	b	3027	CLA	C4D-ND	-3.11	1.33	1.37
19	l	1503	CLA	C4D-ND	-3.11	1.33	1.37
19	b	3032	CLA	CHC-C1C	3.10	1.42	1.35
19	a	803	CLA	CHC-C1C	3.10	1.42	1.35
24	a	857	45D	C24-C26	-3.10	1.39	1.45
19	b	3040	CLA	C4D-ND	-3.10	1.33	1.37
19	a	827	CLA	CHC-C1C	3.10	1.42	1.35
19	b	3022	CLA	C4D-ND	-3.10	1.33	1.37
19	a	804	CLA	C4D-ND	-3.10	1.33	1.37
19	a	813	CLA	CHC-C1C	3.10	1.42	1.35
19	a	819	CLA	CHC-C1C	3.10	1.42	1.35
19	a	822	CLA	C4D-ND	-3.10	1.33	1.37
19	a	826	CLA	C4D-ND	-3.09	1.33	1.37
19	b	3007	CLA	C4D-ND	-3.09	1.33	1.37
19	b	3026	CLA	CHC-C1C	3.09	1.42	1.35
19	a	837	CLA	CHC-C1C	3.09	1.42	1.35
19	a	824	CLA	C4D-ND	-3.09	1.33	1.37
19	b	3022	CLA	CHC-C1C	3.09	1.42	1.35
19	b	3020	CLA	C4D-ND	-3.09	1.33	1.37
19	a	820	CLA	C4D-ND	-3.08	1.33	1.37
19	k	4003	CLA	CHC-C1C	3.08	1.42	1.35
19	b	3034	CLA	CHC-C1C	3.08	1.42	1.35
19	a	811	CLA	C4D-ND	-3.08	1.33	1.37
19	A	403	CLA	CHC-C1C	3.08	1.42	1.35
19	b	3005	CLA	CHC-C1C	3.08	1.42	1.35
19	a	856	CLA	C4D-ND	-3.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	3020	CLA	CHC-C1C	3.08	1.42	1.35
19	a	815	CLA	C4D-ND	-3.08	1.33	1.37
19	b	3031	CLA	CHC-C1C	3.08	1.42	1.35
19	f	201	CLA	CHC-C1C	3.08	1.42	1.35
19	b	3021	CLA	CHC-C1C	3.08	1.42	1.35
21	b	3048	BCR	C30-C25	-3.08	1.49	1.53
19	a	821	CLA	CHC-C1C	3.08	1.42	1.35
19	a	803	CLA	C4D-ND	-3.07	1.33	1.37
19	a	826	CLA	CHC-C1C	3.07	1.42	1.35
19	b	3041	CLA	CHC-C1C	3.07	1.42	1.35
19	b	3015	CLA	CHC-C1C	3.07	1.42	1.35
19	a	830	CLA	CHC-C1C	3.07	1.42	1.35
19	a	836	CLA	CHC-C1C	3.07	1.42	1.35
19	a	822	CLA	CHC-C1C	3.07	1.42	1.35
19	k	4002	CLA	CHC-C1C	3.07	1.42	1.35
19	D	401	CLA	C4D-ND	-3.07	1.33	1.37
19	a	839	CLA	CHC-C1C	3.07	1.42	1.35
18	a	801	CL0	C4D-ND	-3.07	1.33	1.37
19	l	1502	CLA	C4D-ND	-3.07	1.33	1.37
19	b	3016	CLA	CHC-C1C	3.07	1.42	1.35
19	a	805	CLA	C4D-ND	-3.06	1.33	1.37
19	k	4002	CLA	C4D-ND	-3.06	1.33	1.37
19	b	3002	CLA	CHC-C1C	3.06	1.42	1.35
19	D	403	CLA	C4D-ND	-3.06	1.33	1.37
24	a	857	45D	C23-C25	-3.06	1.39	1.45
19	b	3032	CLA	C4D-ND	-3.06	1.33	1.37
19	b	3002	CLA	C4D-ND	-3.06	1.33	1.37
19	b	3019	CLA	CHC-C1C	3.06	1.42	1.35
19	b	3014	CLA	CHC-C1C	3.06	1.42	1.35
19	f	201	CLA	C4D-ND	-3.06	1.33	1.37
19	a	828	CLA	CHC-C1C	3.05	1.42	1.35
19	b	3036	CLA	CHC-C1C	3.05	1.42	1.35
19	b	3016	CLA	C4D-ND	-3.05	1.33	1.37
21	b	3044	BCR	C30-C25	-3.05	1.49	1.53
19	b	3029	CLA	C4D-ND	-3.05	1.33	1.37
19	a	814	CLA	CHC-C1C	3.05	1.42	1.35
19	f	204	CLA	CHC-C1C	3.05	1.42	1.35
19	a	858	CLA	CHC-C1C	3.05	1.42	1.35
19	a	815	CLA	CHC-C1C	3.05	1.42	1.35
19	b	3012	CLA	CHC-C1C	3.05	1.42	1.35
19	b	3035	CLA	CHC-C1C	3.05	1.42	1.35
19	a	824	CLA	CHC-C1C	3.05	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	3008	CLA	CHC-C1C	3.04	1.42	1.35
19	l	1502	CLA	CHC-C1C	3.04	1.42	1.35
19	b	3017	CLA	C4D-ND	-3.04	1.33	1.37
19	a	843	CLA	CHC-C1C	3.04	1.42	1.35
19	b	3028	CLA	CHC-C1C	3.04	1.42	1.35
19	a	856	CLA	CHC-C1C	3.04	1.42	1.35
19	A	405	CLA	CHC-C1C	3.03	1.42	1.35
19	D	404	CLA	CHC-C1C	3.03	1.42	1.35
19	a	807	CLA	CHC-C1C	3.03	1.42	1.35
19	b	3029	CLA	CHC-C1C	3.03	1.42	1.35
19	a	831	CLA	CHC-C1C	3.03	1.42	1.35
26	m	101	ECH	C23-C22	-3.03	1.39	1.45
19	a	817	CLA	C4D-ND	-3.03	1.33	1.37
19	a	809	CLA	CHC-C1C	3.03	1.42	1.35
19	a	812	CLA	CHC-C1C	3.03	1.42	1.35
19	a	817	CLA	CHC-C1C	3.02	1.42	1.35
19	a	818	CLA	C4D-ND	-3.02	1.33	1.37
19	a	823	CLA	CHC-C1C	3.02	1.42	1.35
21	j	101	BCR	C30-C25	-3.02	1.49	1.53
19	a	802	CLA	CHC-C1C	3.02	1.42	1.35
19	a	829	CLA	CHC-C1C	3.02	1.42	1.35
19	a	843	CLA	C4D-ND	-3.02	1.33	1.37
19	b	3041	CLA	C4D-ND	-3.02	1.33	1.37
19	A	402	CLA	CHC-C1C	3.02	1.42	1.35
19	a	833	CLA	CHC-C1C	3.02	1.42	1.35
19	b	3039	CLA	CHC-C1C	3.02	1.42	1.35
19	b	3033	CLA	CHC-C1C	3.02	1.42	1.35
19	A	403	CLA	C4D-ND	-3.02	1.33	1.37
19	a	816	CLA	CHC-C1C	3.02	1.42	1.35
19	b	3015	CLA	C4D-ND	-3.01	1.33	1.37
19	a	820	CLA	CHC-C1C	3.01	1.42	1.35
21	b	3046	BCR	C30-C25	-3.01	1.49	1.53
19	l	1503	CLA	CHC-C1C	3.01	1.42	1.35
19	a	812	CLA	C4D-ND	-3.01	1.33	1.37
27	b	3052	EQ3	C23-C22	-3.01	1.39	1.45
19	b	3030	CLA	CHC-C1C	3.00	1.42	1.35
19	b	3013	CLA	CHC-C1C	3.00	1.42	1.35
19	a	841	CLA	C4D-ND	-3.00	1.33	1.37
19	a	819	CLA	C4D-ND	-3.00	1.33	1.37
19	a	806	CLA	CHC-C1C	3.00	1.42	1.35
19	b	3037	CLA	CHC-C1C	2.99	1.42	1.35
19	b	3010	CLA	CHC-C1C	2.99	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	403	CLA	CHC-C1C	2.99	1.42	1.35
19	a	835	CLA	C4D-ND	-2.99	1.33	1.37
19	b	3035	CLA	C4D-ND	-2.99	1.33	1.37
19	b	3018	CLA	CHC-C1C	2.99	1.42	1.35
19	a	825	CLA	CHC-C1C	2.99	1.42	1.35
19	b	3038	CLA	CHC-C1C	2.99	1.42	1.35
19	a	835	CLA	CHC-C1C	2.98	1.42	1.35
19	b	3025	CLA	CHC-C1C	2.98	1.42	1.35
32	F	101	HEM	CAB-C3B	2.98	1.55	1.47
19	a	804	CLA	CHC-C1C	2.97	1.42	1.35
19	a	841	CLA	CHC-C1C	2.97	1.42	1.35
19	A	405	CLA	C4D-ND	-2.97	1.33	1.37
19	b	3033	CLA	C4D-ND	-2.97	1.33	1.37
28	f	205	ZEX	C8-C9	-2.97	1.39	1.45
19	D	404	CLA	C4D-ND	-2.97	1.33	1.37
19	a	855	CLA	CHC-C1C	2.97	1.42	1.35
18	a	801	CL0	CHC-C1C	2.97	1.42	1.35
21	a	846	BCR	C30-C25	-2.96	1.49	1.53
19	a	832	CLA	CHC-C1C	2.96	1.42	1.35
19	b	3011	CLA	CHC-C1C	2.96	1.42	1.35
19	a	811	CLA	CHC-C1C	2.96	1.42	1.35
19	b	3009	CLA	CHC-C1C	2.95	1.42	1.35
19	a	842	CLA	CHC-C1C	2.95	1.42	1.35
19	j	102	CLA	C4D-ND	-2.95	1.33	1.37
19	a	834	CLA	CHC-C1C	2.95	1.42	1.35
28	f	205	ZEX	C28-C29	-2.94	1.39	1.45
19	b	3027	CLA	CHC-C1C	2.94	1.42	1.35
19	a	810	CLA	CHC-C1C	2.94	1.42	1.35
19	a	829	CLA	C4D-ND	-2.94	1.33	1.37
19	k	4003	CLA	C4D-ND	-2.94	1.33	1.37
19	b	3040	CLA	CHC-C1C	2.93	1.42	1.35
19	a	838	CLA	CHC-C1C	2.93	1.42	1.35
19	b	3006	CLA	CHC-C1C	2.93	1.42	1.35
26	m	101	ECH	C8-C9	-2.92	1.39	1.45
19	a	818	CLA	CHC-C1C	2.92	1.42	1.35
19	a	840	CLA	CHC-C1C	2.92	1.42	1.35
28	b	3053	ZEX	C28-C29	-2.90	1.39	1.45
19	f	204	CLA	C4D-ND	-2.90	1.33	1.37
19	l	1501	CLA	C4D-ND	-2.87	1.33	1.37
19	j	103	CLA	C4D-ND	-2.87	1.33	1.37
19	b	3007	CLA	CHC-C1C	2.86	1.42	1.35
27	b	3052	EQ3	C25-C26	2.86	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	3017	CLA	CHC-C1C	2.84	1.42	1.35
26	b	3045	ECH	C8-C9	-2.82	1.39	1.45
19	b	3009	CLA	CMB-C2B	-2.80	1.45	1.51
19	b	3040	CLA	CMB-C2B	-2.78	1.45	1.51
21	l	1504	BCR	C30-C25	-2.76	1.50	1.53
31	D	402	PHO	CAC-C3C	-2.75	1.47	1.52
29	f	207	LMT	O3'-C3'	-2.73	1.36	1.43
19	a	822	CLA	CMB-C2B	-2.70	1.46	1.51
19	a	834	CLA	CMB-C2B	-2.69	1.46	1.51
19	a	820	CLA	CMB-C2B	-2.68	1.46	1.51
19	b	3035	CLA	CMB-C2B	-2.67	1.46	1.51
19	a	836	CLA	CMB-C2B	-2.67	1.46	1.51
24	a	857	45D	C08-C16	2.67	1.39	1.35
19	a	856	CLA	CMB-C2B	-2.66	1.46	1.51
31	A	404	PHO	CAC-C3C	-2.66	1.47	1.52
19	b	3029	CLA	CMB-C2B	-2.63	1.46	1.51
28	b	3053	ZEX	C32-C33	-2.63	1.40	1.45
19	a	842	CLA	CMB-C2B	-2.61	1.46	1.51
19	b	3015	CLA	CMB-C2B	-2.61	1.46	1.51
19	b	3002	CLA	CMB-C2B	-2.61	1.46	1.51
19	a	818	CLA	CMB-C2B	-2.61	1.46	1.51
19	b	3011	CLA	CMB-C2B	-2.60	1.46	1.51
19	b	3033	CLA	CMB-C2B	-2.60	1.46	1.51
26	b	3045	ECH	C19-C18	-2.60	1.40	1.45
19	a	804	CLA	CMB-C2B	-2.60	1.46	1.51
18	a	801	CL0	CMB-C2B	-2.59	1.46	1.51
19	b	3032	CLA	CMB-C2B	-2.59	1.46	1.51
19	a	813	CLA	CMB-C2B	-2.58	1.46	1.51
19	a	835	CLA	CMB-C2B	-2.58	1.46	1.51
19	b	3030	CLA	CMB-C2B	-2.58	1.46	1.51
27	b	3052	EQ3	C12-C13	-2.58	1.40	1.45
28	b	3053	ZEX	C12-C13	-2.58	1.40	1.45
19	a	821	CLA	CMB-C2B	-2.58	1.46	1.51
27	b	3052	EQ3	C19-C18	-2.58	1.40	1.45
19	b	3019	CLA	CMB-C2B	-2.57	1.46	1.51
19	a	832	CLA	CMB-C2B	-2.57	1.46	1.51
19	b	3006	CLA	CMB-C2B	-2.57	1.46	1.51
26	b	3045	ECH	C12-C13	-2.57	1.40	1.45
19	a	838	CLA	CMB-C2B	-2.56	1.46	1.51
19	a	831	CLA	CMB-C2B	-2.56	1.46	1.51
29	f	207	LMT	O2'-C2'	-2.56	1.36	1.43
19	b	3010	CLA	CMB-C2B	-2.56	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	857	45D	C33-C35	-2.56	1.40	1.45
19	a	855	CLA	CMB-C2B	-2.56	1.46	1.51
19	f	201	CLA	CMB-C2B	-2.55	1.46	1.51
19	b	3038	CLA	CMB-C2B	-2.55	1.46	1.51
19	a	817	CLA	CMB-C2B	-2.55	1.46	1.51
19	a	824	CLA	CMB-C2B	-2.55	1.46	1.51
19	a	809	CLA	CMB-C2B	-2.55	1.46	1.51
19	b	3013	CLA	CMB-C2B	-2.55	1.46	1.51
19	a	810	CLA	CMB-C2B	-2.54	1.46	1.51
19	a	828	CLA	CMB-C2B	-2.54	1.46	1.51
19	b	3012	CLA	CMB-C2B	-2.54	1.46	1.51
19	b	3037	CLA	CMB-C2B	-2.53	1.46	1.51
19	b	3004	CLA	CMB-C2B	-2.53	1.46	1.51
19	a	827	CLA	CMB-C2B	-2.53	1.46	1.51
19	b	3025	CLA	CMB-C2B	-2.53	1.46	1.51
19	a	826	CLA	CMB-C2B	-2.53	1.46	1.51
19	b	3018	CLA	CMB-C2B	-2.53	1.46	1.51
19	a	811	CLA	CMB-C2B	-2.53	1.46	1.51
19	a	829	CLA	CMB-C2B	-2.53	1.46	1.51
19	a	833	CLA	CMB-C2B	-2.53	1.46	1.51
19	a	819	CLA	CMB-C2B	-2.53	1.46	1.51
19	b	3020	CLA	CMB-C2B	-2.53	1.46	1.51
19	l	1502	CLA	CMB-C2B	-2.53	1.46	1.51
19	b	3023	CLA	CMB-C2B	-2.52	1.46	1.51
19	b	3017	CLA	CMB-C2B	-2.52	1.46	1.51
19	b	3003	CLA	CMB-C2B	-2.52	1.46	1.51
19	b	3026	CLA	CMB-C2B	-2.52	1.46	1.51
19	b	3016	CLA	CMB-C2B	-2.52	1.46	1.51
19	b	3024	CLA	CMB-C2B	-2.52	1.46	1.51
28	f	205	ZEX	C12-C13	-2.52	1.40	1.45
19	b	3005	CLA	CMB-C2B	-2.52	1.46	1.51
19	a	825	CLA	CMB-C2B	-2.51	1.46	1.51
19	b	3039	CLA	CMB-C2B	-2.51	1.46	1.51
19	a	807	CLA	CMB-C2B	-2.51	1.46	1.51
19	b	3008	CLA	CMB-C2B	-2.51	1.46	1.51
19	a	802	CLA	CMB-C2B	-2.50	1.46	1.51
19	a	806	CLA	CMB-C2B	-2.50	1.46	1.51
19	a	840	CLA	CMB-C2B	-2.50	1.46	1.51
19	a	830	CLA	CMB-C2B	-2.50	1.46	1.51
19	a	839	CLA	CMB-C2B	-2.50	1.46	1.51
19	b	3027	CLA	CMB-C2B	-2.49	1.46	1.51
19	f	204	CLA	CMB-C2B	-2.49	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	3022	CLA	CMB-C2B	-2.49	1.46	1.51
19	a	843	CLA	CMB-C2B	-2.49	1.46	1.51
19	a	815	CLA	CMB-C2B	-2.49	1.46	1.51
19	a	805	CLA	CMB-C2B	-2.48	1.46	1.51
19	a	814	CLA	CMB-C2B	-2.48	1.46	1.51
19	b	3007	CLA	CMB-C2B	-2.48	1.46	1.51
19	a	841	CLA	CMB-C2B	-2.48	1.46	1.51
19	b	3034	CLA	CMB-C2B	-2.48	1.46	1.51
19	a	837	CLA	CMB-C2B	-2.48	1.46	1.51
19	D	401	CLA	CMB-C2B	-2.48	1.46	1.51
19	b	3028	CLA	CMB-C2B	-2.47	1.46	1.51
23	b	3051	LMG	O7-C8	-2.47	1.40	1.46
19	b	3031	CLA	CMB-C2B	-2.47	1.46	1.51
19	b	3036	CLA	CMB-C2B	-2.47	1.46	1.51
19	b	3014	CLA	CMB-C2B	-2.46	1.46	1.51
19	b	3003	CLA	CMC-C2C	-2.46	1.45	1.50
19	k	4002	CLA	CMB-C2B	-2.46	1.46	1.51
19	a	803	CLA	CMB-C2B	-2.46	1.46	1.51
19	a	823	CLA	CMB-C2B	-2.45	1.46	1.51
26	m	101	ECH	C12-C13	-2.45	1.40	1.45
19	a	858	CLA	CMB-C2B	-2.45	1.46	1.51
19	j	102	CLA	CMB-C2B	-2.45	1.46	1.51
24	a	857	45D	C34-C36	-2.44	1.40	1.45
19	l	1503	CLA	CMB-C2B	-2.44	1.46	1.51
19	k	4003	CLA	CMB-C2B	-2.43	1.46	1.51
19	a	816	CLA	CMB-C2B	-2.42	1.46	1.51
28	f	205	ZEX	C32-C33	-2.42	1.40	1.45
19	a	812	CLA	CMB-C2B	-2.42	1.46	1.51
19	f	203	CLA	CMB-C2B	-2.41	1.46	1.51
19	D	404	CLA	CMB-C2B	-2.41	1.46	1.51
19	A	403	CLA	CMB-C2B	-2.40	1.46	1.51
19	a	808	CLA	CMB-C2B	-2.40	1.46	1.51
29	f	207	LMT	O2B-C2B	-2.40	1.37	1.43
19	A	402	CLA	CMB-C2B	-2.39	1.46	1.51
19	b	3021	CLA	CMB-C2B	-2.39	1.46	1.51
19	A	405	CLA	CMB-C2B	-2.38	1.46	1.51
19	D	403	CLA	CMB-C2B	-2.37	1.46	1.51
19	l	1501	CLA	CMB-C2B	-2.35	1.46	1.51
19	j	103	CLA	CMB-C2B	-2.32	1.46	1.51
19	b	3041	CLA	CMB-C2B	-2.32	1.46	1.51
22	a	850	LHG	O7-C5	-2.29	1.40	1.46
29	f	207	LMT	O3B-C3B	-2.29	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	m	101	ECH	C19-C18	-2.28	1.41	1.45
19	b	3040	CLA	C3B-C2B	-2.27	1.37	1.40
19	a	810	CLA	CMD-C2D	-2.27	1.46	1.50
19	b	3028	CLA	CMD-C2D	-2.23	1.46	1.50
19	b	3038	CLA	C3B-C2B	-2.23	1.37	1.40
22	b	3050	LHG	O7-C5	-2.23	1.41	1.46
19	b	3029	CLA	CMD-C2D	-2.22	1.46	1.50
19	f	201	CLA	CMD-C2D	-2.22	1.46	1.50
29	f	207	LMT	O4'-C4B	-2.21	1.37	1.43
19	b	3008	CLA	CMD-C2D	-2.20	1.46	1.50
19	b	3026	CLA	CMC-C2C	-2.20	1.46	1.50
19	a	836	CLA	CMD-C2D	-2.20	1.46	1.50
19	a	806	CLA	CMD-C2D	-2.20	1.46	1.50
19	b	3015	CLA	C3B-C2B	-2.20	1.37	1.40
19	a	827	CLA	CMD-C2D	-2.19	1.46	1.50
19	a	828	CLA	CMC-C2C	-2.19	1.46	1.50
18	a	801	CL0	CMD-C2D	-2.19	1.46	1.50
19	a	833	CLA	C3B-CAB	-2.18	1.43	1.47
19	b	3002	CLA	CMD-C2D	-2.17	1.46	1.50
19	b	3013	CLA	CMC-C2C	-2.17	1.46	1.50
19	b	3032	CLA	C3B-C2B	-2.16	1.37	1.40
19	a	803	CLA	CMC-C2C	-2.16	1.46	1.50
19	a	832	CLA	CMD-C2D	-2.16	1.46	1.50
19	b	3024	CLA	CMD-C2D	-2.16	1.46	1.50
19	b	3017	CLA	CMD-C2D	-2.15	1.46	1.50
19	b	3010	CLA	CMD-C2D	-2.15	1.46	1.50
19	b	3025	CLA	CMD-C2D	-2.15	1.46	1.50
19	a	825	CLA	CMC-C2C	-2.15	1.46	1.50
19	a	826	CLA	CMD-C2D	-2.14	1.46	1.50
31	A	404	PHO	CMC-C2C	-2.14	1.46	1.51
19	b	3015	CLA	CMD-C2D	-2.14	1.46	1.50
19	a	830	CLA	CMD-C2D	-2.14	1.46	1.50
19	a	807	CLA	CMD-C2D	-2.14	1.46	1.50
19	a	840	CLA	C3B-C2B	-2.13	1.37	1.40
19	b	3013	CLA	CMD-C2D	-2.13	1.46	1.50
19	b	3039	CLA	CMD-C2D	-2.13	1.46	1.50
19	b	3040	CLA	CMD-C2D	-2.13	1.46	1.50
19	b	3012	CLA	CMD-C2D	-2.13	1.46	1.50
19	a	803	CLA	CMD-C2D	-2.13	1.46	1.50
19	a	829	CLA	CMD-C2D	-2.13	1.46	1.50
19	b	3027	CLA	CMD-C2D	-2.13	1.46	1.50
19	b	3004	CLA	CMC-C2C	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	l	1502	CLA	CMD-C2D	-2.12	1.46	1.50
19	a	831	CLA	CMD-C2D	-2.12	1.46	1.50
19	b	3038	CLA	CMD-C2D	-2.12	1.46	1.50
19	a	839	CLA	CMD-C2D	-2.12	1.46	1.50
19	a	855	CLA	CMD-C2D	-2.12	1.46	1.50
19	a	843	CLA	CMD-C2D	-2.12	1.46	1.50
19	D	403	CLA	CMD-C2D	-2.12	1.46	1.50
19	a	819	CLA	CMC-C2C	-2.12	1.46	1.50
19	b	3007	CLA	CMD-C2D	-2.12	1.46	1.50
19	b	3009	CLA	CMD-C2D	-2.12	1.46	1.50
19	a	856	CLA	CMC-C2C	-2.11	1.46	1.50
19	a	814	CLA	CMD-C2D	-2.11	1.46	1.50
31	D	402	PHO	CMC-C2C	-2.11	1.46	1.51
19	b	3014	CLA	CMD-C2D	-2.11	1.46	1.50
19	b	3011	CLA	C3B-C2B	-2.11	1.37	1.40
19	b	3020	CLA	CMD-C2D	-2.11	1.46	1.50
19	a	806	CLA	CMC-C2C	-2.11	1.46	1.50
19	b	3023	CLA	CMD-C2D	-2.10	1.46	1.50
19	a	819	CLA	C3B-C2B	-2.10	1.37	1.40
19	a	834	CLA	CMD-C2D	-2.10	1.46	1.50
19	a	820	CLA	CMD-C2D	-2.10	1.46	1.50
19	a	813	CLA	CMD-C2D	-2.10	1.46	1.50
19	b	3016	CLA	CMD-C2D	-2.10	1.46	1.50
19	b	3034	CLA	CMD-C2D	-2.10	1.46	1.50
19	a	809	CLA	CMD-C2D	-2.10	1.46	1.50
19	b	3030	CLA	CMD-C2D	-2.09	1.46	1.50
19	a	856	CLA	CMD-C2D	-2.09	1.46	1.50
19	a	837	CLA	CMD-C2D	-2.09	1.46	1.50
19	a	805	CLA	CMD-C2D	-2.09	1.46	1.50
19	a	833	CLA	CMD-C2D	-2.09	1.46	1.50
19	a	819	CLA	CMD-C2D	-2.09	1.46	1.50
19	a	812	CLA	CMD-C2D	-2.09	1.46	1.50
19	a	858	CLA	CMD-C2D	-2.09	1.46	1.50
19	A	405	CLA	CMD-C2D	-2.09	1.46	1.50
19	a	824	CLA	CMD-C2D	-2.09	1.46	1.50
19	b	3019	CLA	CMD-C2D	-2.09	1.46	1.50
19	a	825	CLA	CMD-C2D	-2.08	1.46	1.50
31	D	402	PHO	CMB-C2B	-2.08	1.46	1.51
19	b	3019	CLA	C3B-C2B	-2.08	1.37	1.40
19	a	821	CLA	CMD-C2D	-2.08	1.46	1.50
19	b	3031	CLA	CMD-C2D	-2.08	1.46	1.50
19	a	842	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	402	CLA	CMC-C2C	-2.08	1.46	1.50
31	D	402	PHO	CMD-C2D	-2.08	1.46	1.51
19	a	835	CLA	CMD-C2D	-2.08	1.46	1.50
19	b	3037	CLA	CMD-C2D	-2.08	1.46	1.50
19	a	811	CLA	CMD-C2D	-2.08	1.46	1.50
19	a	822	CLA	CMD-C2D	-2.08	1.46	1.50
19	k	4002	CLA	CMD-C2D	-2.08	1.46	1.50
19	b	3018	CLA	CMD-C2D	-2.08	1.46	1.50
19	b	3026	CLA	CMD-C2D	-2.08	1.46	1.50
19	a	819	CLA	C3B-CAB	-2.08	1.43	1.47
22	a	854	LHG	O7-C5	-2.07	1.41	1.46
31	A	404	PHO	CMD-C2D	-2.07	1.46	1.51
19	a	841	CLA	CMD-C2D	-2.07	1.46	1.50
19	b	3006	CLA	CMC-C2C	-2.07	1.46	1.50
21	j	104	BCR	C33-C5	-2.07	1.47	1.50
19	a	836	CLA	C3B-C2B	-2.07	1.37	1.40
19	a	858	CLA	CMC-C2C	-2.07	1.46	1.50
19	a	816	CLA	CMD-C2D	-2.07	1.46	1.50
19	b	3005	CLA	CMD-C2D	-2.07	1.46	1.50
19	b	3036	CLA	CMD-C2D	-2.07	1.46	1.50
19	a	828	CLA	CMD-C2D	-2.07	1.46	1.50
19	b	3011	CLA	CMD-C2D	-2.07	1.46	1.50
19	a	838	CLA	CMD-C2D	-2.07	1.46	1.50
19	b	3002	CLA	CMC-C2C	-2.07	1.46	1.50
19	b	3003	CLA	CMD-C2D	-2.07	1.46	1.50
19	b	3008	CLA	CMC-C2C	-2.07	1.46	1.50
19	a	840	CLA	CMD-C2D	-2.06	1.46	1.50
19	a	804	CLA	C3B-C2B	-2.06	1.37	1.40
19	a	804	CLA	CMC-C2C	-2.06	1.46	1.50
19	a	818	CLA	CMD-C2D	-2.06	1.46	1.50
19	b	3005	CLA	CMC-C2C	-2.06	1.46	1.50
19	a	802	CLA	CMD-C2D	-2.06	1.46	1.50
19	a	817	CLA	CMD-C2D	-2.06	1.46	1.50
19	a	855	CLA	CMC-C2C	-2.06	1.46	1.50
19	b	3006	CLA	CMD-C2D	-2.06	1.46	1.50
19	b	3015	CLA	CMC-C2C	-2.06	1.46	1.50
19	a	808	CLA	CMD-C2D	-2.06	1.46	1.50
19	a	810	CLA	CMC-C2C	-2.06	1.46	1.50
22	a	852	LHG	O7-C5	-2.06	1.41	1.46
19	b	3031	CLA	CMC-C2C	-2.06	1.46	1.50
19	a	820	CLA	CMC-C2C	-2.05	1.46	1.50
19	b	3033	CLA	CMD-C2D	-2.05	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	404	PHO	CMB-C2B	-2.05	1.46	1.51
19	a	808	CLA	CMC-C2C	-2.05	1.46	1.50
19	b	3021	CLA	CMD-C2D	-2.05	1.46	1.50
19	f	203	CLA	CMD-C2D	-2.05	1.46	1.50
19	a	823	CLA	CMD-C2D	-2.05	1.46	1.50
19	a	815	CLA	CMD-C2D	-2.05	1.46	1.50
19	A	403	CLA	CMD-C2D	-2.05	1.46	1.50
19	a	804	CLA	CMD-C2D	-2.05	1.46	1.50
19	a	838	CLA	CMC-C2C	-2.04	1.46	1.50
19	a	841	CLA	CMC-C2C	-2.04	1.46	1.50
19	b	3032	CLA	CMD-C2D	-2.04	1.46	1.50
19	b	3041	CLA	CMD-C2D	-2.04	1.46	1.50
19	a	802	CLA	CMC-C2C	-2.04	1.46	1.50
19	a	822	CLA	CMC-C2C	-2.04	1.46	1.50
19	b	3004	CLA	CMD-C2D	-2.04	1.46	1.50
19	D	404	CLA	CMD-C2D	-2.04	1.46	1.50
19	b	3027	CLA	CMC-C2C	-2.04	1.46	1.50
19	a	814	CLA	CMC-C2C	-2.03	1.46	1.50
19	f	204	CLA	CMD-C2D	-2.03	1.46	1.50
19	a	833	CLA	CMC-C2C	-2.03	1.46	1.50
19	b	3037	CLA	CMC-C2C	-2.03	1.46	1.50
19	j	102	CLA	CMD-C2D	-2.03	1.46	1.50
21	a	847	BCR	C33-C5	-2.03	1.47	1.50
19	l	1503	CLA	CMD-C2D	-2.03	1.46	1.50
19	a	839	CLA	CMC-C2C	-2.03	1.46	1.50
19	b	3016	CLA	CMC-C2C	-2.03	1.46	1.50
19	a	815	CLA	CMC-C2C	-2.03	1.46	1.50
19	b	3022	CLA	CMD-C2D	-2.03	1.46	1.50
19	a	813	CLA	C3B-C2B	-2.03	1.37	1.40
19	b	3020	CLA	CMC-C2C	-2.03	1.46	1.50
19	b	3035	CLA	CMD-C2D	-2.03	1.46	1.50
19	D	403	CLA	CMC-C2C	-2.03	1.46	1.50
19	b	3019	CLA	C3B-CAB	-2.02	1.43	1.47
19	A	402	CLA	CMD-C2D	-2.02	1.46	1.50
19	a	829	CLA	CMC-C2C	-2.02	1.46	1.50
19	a	836	CLA	CMC-C2C	-2.02	1.46	1.50
19	a	809	CLA	CMC-C2C	-2.02	1.46	1.50
19	l	1502	CLA	CMC-C2C	-2.02	1.46	1.50
19	b	3040	CLA	CMC-C2C	-2.02	1.46	1.50
19	b	3017	CLA	C3B-C2B	-2.02	1.37	1.40
19	b	3033	CLA	CMC-C2C	-2.02	1.46	1.50
19	b	3028	CLA	CMC-C2C	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	k	4003	CLA	CMD-C2D	-2.02	1.46	1.50
19	a	827	CLA	CMC-C2C	-2.01	1.46	1.50
19	b	3012	CLA	CMC-C2C	-2.01	1.46	1.50
19	a	856	CLA	C3B-C2B	-2.01	1.37	1.40
19	a	843	CLA	CMC-C2C	-2.01	1.46	1.50
19	b	3010	CLA	CMC-C2C	-2.01	1.46	1.50
19	f	201	CLA	C3B-C2B	-2.01	1.37	1.40
19	b	3007	CLA	CMC-C2C	-2.01	1.46	1.50
19	a	830	CLA	CMC-C2C	-2.01	1.46	1.50
19	a	824	CLA	CMC-C2C	-2.01	1.46	1.50
19	b	3008	CLA	C3B-CAB	-2.01	1.43	1.47
19	b	3029	CLA	CMC-C2C	-2.00	1.46	1.50
19	a	833	CLA	C3B-C2B	-2.00	1.37	1.40
19	a	842	CLA	CMC-C2C	-2.00	1.46	1.50
19	b	3036	CLA	CMC-C2C	-2.00	1.46	1.50
19	b	3009	CLA	CMC-C2C	-2.00	1.46	1.50
19	a	809	CLA	C3B-CAB	-2.00	1.43	1.47
19	b	3013	CLA	C3B-CAB	-2.00	1.43	1.47

All (1002) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	3045	ECH	C15-C16-C17	8.19	140.25	123.47
19	a	818	CLA	C4A-NA-C1A	7.47	110.07	106.71
19	a	840	CLA	C4A-NA-C1A	7.37	110.02	106.71
19	a	842	CLA	C4A-NA-C1A	7.35	110.01	106.71
19	a	806	CLA	C4A-NA-C1A	7.34	110.00	106.71
19	l	1502	CLA	C4A-NA-C1A	7.28	109.98	106.71
19	b	3040	CLA	C4A-NA-C1A	7.24	109.96	106.71
19	a	841	CLA	C4A-NA-C1A	7.19	109.94	106.71
19	a	810	CLA	C4A-NA-C1A	7.15	109.92	106.71
19	a	811	CLA	C4A-NA-C1A	7.14	109.91	106.71
19	a	835	CLA	C4A-NA-C1A	6.96	109.83	106.71
19	A	403	CLA	C4A-NA-C1A	6.93	109.82	106.71
19	b	3007	CLA	C4A-NA-C1A	6.93	109.82	106.71
19	b	3011	CLA	C4A-NA-C1A	6.92	109.82	106.71
19	b	3033	CLA	C4A-NA-C1A	6.90	109.81	106.71
19	a	824	CLA	C4A-NA-C1A	6.90	109.81	106.71
19	j	102	CLA	C4A-NA-C1A	6.88	109.80	106.71
19	b	3005	CLA	C4A-NA-C1A	6.86	109.79	106.71
19	D	403	CLA	C4A-NA-C1A	6.84	109.78	106.71
19	b	3022	CLA	C4A-NA-C1A	6.79	109.76	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	b	3025	CLA	C4A-NA-C1A	6.77	109.75	106.71
19	a	816	CLA	C4A-NA-C1A	6.76	109.75	106.71
19	a	829	CLA	C4A-NA-C1A	6.75	109.74	106.71
19	a	817	CLA	C4A-NA-C1A	6.75	109.74	106.71
19	b	3017	CLA	C4A-NA-C1A	6.75	109.74	106.71
19	b	3004	CLA	C4A-NA-C1A	6.74	109.74	106.71
19	l	1501	CLA	C4A-NA-C1A	6.73	109.73	106.71
19	A	405	CLA	C4A-NA-C1A	6.72	109.73	106.71
19	a	823	CLA	C4A-NA-C1A	6.72	109.73	106.71
19	b	3035	CLA	C4A-NA-C1A	6.71	109.72	106.71
19	D	404	CLA	C4A-NA-C1A	6.71	109.72	106.71
19	b	3013	CLA	C4A-NA-C1A	6.70	109.72	106.71
18	a	801	CL0	C4A-NA-C1A	6.67	109.71	106.71
19	a	831	CLA	C4A-NA-C1A	6.67	109.70	106.71
19	a	834	CLA	C4A-NA-C1A	6.66	109.70	106.71
19	a	856	CLA	C4A-NA-C1A	6.65	109.70	106.71
19	l	1503	CLA	C4A-NA-C1A	6.65	109.69	106.71
19	a	825	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	b	3037	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	b	3010	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	b	3034	CLA	C4A-NA-C1A	6.62	109.68	106.71
19	a	839	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	a	807	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	b	3016	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	b	3027	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	b	3009	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	a	828	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	b	3039	CLA	C4A-NA-C1A	6.59	109.67	106.71
19	a	821	CLA	C4A-NA-C1A	6.58	109.67	106.71
19	b	3029	CLA	C4A-NA-C1A	6.58	109.67	106.71
19	D	401	CLA	C4A-NA-C1A	6.58	109.66	106.71
19	b	3014	CLA	C4A-NA-C1A	6.58	109.66	106.71
19	a	832	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	b	3008	CLA	C4A-NA-C1A	6.56	109.65	106.71
19	f	201	CLA	C4A-NA-C1A	6.56	109.65	106.71
19	b	3003	CLA	C4A-NA-C1A	6.53	109.64	106.71
19	a	803	CLA	C4A-NA-C1A	6.53	109.64	106.71
19	a	814	CLA	C4A-NA-C1A	6.53	109.64	106.71
19	b	3019	CLA	C4A-NA-C1A	6.53	109.64	106.71
19	A	402	CLA	C4A-NA-C1A	6.53	109.64	106.71
19	a	826	CLA	C4A-NA-C1A	6.49	109.62	106.71
19	a	815	CLA	C4A-NA-C1A	6.49	109.62	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a	808	CLA	C4A-NA-C1A	6.49	109.62	106.71
19	k	4002	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	b	3006	CLA	C4A-NA-C1A	6.47	109.61	106.71
19	a	837	CLA	C4A-NA-C1A	6.47	109.61	106.71
19	a	805	CLA	C4A-NA-C1A	6.46	109.61	106.71
19	b	3038	CLA	C4A-NA-C1A	6.46	109.61	106.71
19	a	813	CLA	C4A-NA-C1A	6.45	109.60	106.71
19	a	804	CLA	C4A-NA-C1A	6.44	109.60	106.71
19	b	3020	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	b	3032	CLA	C4A-NA-C1A	6.40	109.58	106.71
19	b	3030	CLA	C4A-NA-C1A	6.40	109.58	106.71
19	a	827	CLA	C4A-NA-C1A	6.37	109.57	106.71
19	a	836	CLA	C4A-NA-C1A	6.35	109.56	106.71
19	f	204	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	a	833	CLA	C4A-NA-C1A	6.32	109.55	106.71
19	a	819	CLA	C4A-NA-C1A	6.31	109.54	106.71
19	a	858	CLA	C4A-NA-C1A	6.29	109.54	106.71
19	b	3041	CLA	C4A-NA-C1A	6.29	109.53	106.71
19	b	3018	CLA	C4A-NA-C1A	6.27	109.52	106.71
19	f	203	CLA	C4A-NA-C1A	6.25	109.52	106.71
19	a	809	CLA	C4A-NA-C1A	6.22	109.50	106.71
19	b	3002	CLA	C4A-NA-C1A	6.22	109.50	106.71
19	b	3023	CLA	C4A-NA-C1A	6.21	109.50	106.71
19	b	3024	CLA	C4A-NA-C1A	6.21	109.50	106.71
19	k	4003	CLA	C4A-NA-C1A	6.21	109.50	106.71
19	b	3012	CLA	C4A-NA-C1A	6.20	109.49	106.71
19	a	838	CLA	C4A-NA-C1A	6.18	109.49	106.71
19	b	3015	CLA	C4A-NA-C1A	6.18	109.48	106.71
19	b	3026	CLA	C4A-NA-C1A	6.18	109.48	106.71
19	a	802	CLA	C4A-NA-C1A	6.16	109.48	106.71
19	b	3021	CLA	C4A-NA-C1A	6.16	109.47	106.71
19	b	3031	CLA	C4A-NA-C1A	6.15	109.47	106.71
19	a	812	CLA	C4A-NA-C1A	6.11	109.45	106.71
19	a	822	CLA	C4A-NA-C1A	6.05	109.42	106.71
19	a	830	CLA	C4A-NA-C1A	6.01	109.41	106.71
19	a	843	CLA	C4A-NA-C1A	6.01	109.41	106.71
19	b	3028	CLA	C4A-NA-C1A	6.00	109.41	106.71
19	b	3036	CLA	C4A-NA-C1A	5.99	109.40	106.71
19	a	820	CLA	C4A-NA-C1A	5.97	109.39	106.71
19	a	855	CLA	C4A-NA-C1A	5.85	109.34	106.71
19	j	103	CLA	C4A-NA-C1A	5.72	109.28	106.71
24	a	857	45D	C42-C41-C37	5.34	134.41	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	3045	ECH	C19-C18-C17	4.80	126.30	118.94
26	m	101	ECH	C15-C16-C17	4.73	133.16	123.47
26	b	3045	ECH	C12-C13-C14	4.61	126.02	118.94
19	a	808	CLA	CMB-C2B-C1B	-4.50	121.54	128.46
19	a	820	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
19	b	3036	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
28	f	205	ZEX	C35-C15-C14	4.35	132.39	123.47
19	a	834	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
19	b	3021	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
19	a	805	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
19	a	814	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
19	a	802	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
26	b	3045	ECH	C36-C18-C17	-4.30	116.91	122.92
26	b	3045	ECH	C1-C6-C5	-4.29	116.57	122.61
19	b	3014	CLA	CMB-C2B-C1B	-4.29	121.88	128.46
22	a	852	LHG	O4-P-O5	4.28	133.42	112.24
19	a	838	CLA	CMB-C2B-C1B	-4.25	121.94	128.46
19	b	3018	CLA	CMB-C2B-C1B	-4.25	121.94	128.46
19	a	826	CLA	CMB-C2B-C1B	-4.24	121.95	128.46
26	b	3045	ECH	C35-C13-C14	-4.23	117.00	122.92
19	f	203	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
19	b	3005	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
22	a	850	LHG	O4-P-O5	4.22	133.08	112.24
22	b	3050	LHG	O4-P-O5	4.21	133.05	112.24
22	a	854	LHG	O4-P-O5	4.21	133.04	112.24
22	f	206	LHG	O4-P-O5	4.20	133.02	112.24
19	b	3041	CLA	CMB-C2B-C1B	-4.20	122.02	128.46
19	D	403	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
26	m	101	ECH	C37-C22-C21	-4.16	117.10	122.92
19	b	3003	CLA	CMB-C2B-C1B	-4.16	122.08	128.46
19	a	807	CLA	CMB-C2B-C1B	-4.16	122.08	128.46
19	a	822	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
19	a	829	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
19	a	812	CLA	CMB-C2B-C1B	-4.12	122.14	128.46
19	a	831	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
24	a	857	45D	C28-C26-C30	-4.11	117.17	122.92
19	a	806	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
19	b	3026	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
28	b	3053	ZEX	C39-C29-C30	-4.07	117.22	122.92
19	b	3031	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
19	b	3037	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
19	j	103	CLA	CMB-C2B-C1B	-4.06	122.22	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a	855	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
28	f	205	ZEX	C19-C9-C10	-4.05	117.25	122.92
19	b	3034	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
19	b	3024	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
19	a	823	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
19	b	3025	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
24	a	857	45D	C27-C25-C29	-3.98	117.34	122.92
19	A	402	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
28	f	205	ZEX	C39-C29-C30	-3.97	117.37	122.92
19	b	3027	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
28	b	3053	ZEX	C19-C9-C10	-3.95	117.38	122.92
26	m	101	ECH	C34-C9-C10	-3.93	117.42	122.92
19	b	3028	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
19	a	817	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
19	l	1503	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
19	b	3016	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
19	l	1501	CLA	CMB-C2B-C1B	-3.90	122.48	128.46
26	b	3045	ECH	C34-C9-C10	-3.89	117.47	122.92
19	a	810	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
19	a	830	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
19	a	803	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
19	a	816	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
19	a	808	CLA	CMB-C2B-C3B	3.84	131.87	124.68
19	a	825	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
19	b	3009	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
19	b	3036	CLA	CMB-C2B-C3B	3.81	131.80	124.68
26	b	3045	ECH	C24-C23-C22	-3.79	120.50	126.23
19	a	837	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
19	b	3029	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
19	A	403	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
19	A	405	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
27	b	3052	EQ3	C37-C22-C21	-3.75	117.66	122.92
19	a	802	CLA	CMB-C2B-C3B	3.75	131.69	124.68
19	b	3023	CLA	CMB-C2B-C1B	-3.75	122.71	128.46
19	a	841	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
27	b	3052	EQ3	C34-C9-C10	-3.73	117.69	122.92
19	a	835	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
19	b	3013	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
19	b	3021	CLA	CMB-C2B-C3B	3.71	131.63	124.68
19	b	3013	CLA	O2D-CGD-O1D	-3.70	116.60	123.84
26	m	101	ECH	C36-C18-C17	-3.68	117.77	122.92
19	a	820	CLA	CMB-C2B-C3B	3.68	131.56	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a	819	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
19	D	404	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
19	a	829	CLA	CMB-C2B-C3B	3.65	131.51	124.68
19	a	818	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
19	b	3039	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
19	a	815	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
26	b	3045	ECH	C37-C22-C21	-3.64	117.82	122.92
19	a	834	CLA	CMB-C2B-C3B	3.64	131.49	124.68
19	b	3002	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
19	a	843	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
19	a	814	CLA	CMB-C2B-C3B	3.63	131.47	124.68
19	a	856	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
19	b	3004	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
19	b	3018	CLA	CMB-C2B-C3B	3.60	131.41	124.68
19	b	3014	CLA	CMB-C2B-C3B	3.59	131.39	124.68
19	a	828	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
19	a	811	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
19	f	203	CLA	CMB-C2B-C3B	3.57	131.36	124.68
19	a	821	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
19	j	102	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
19	a	809	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
19	a	826	CLA	CMB-C2B-C3B	3.56	131.35	124.68
19	b	3005	CLA	CMB-C2B-C3B	3.55	131.32	124.68
19	a	827	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
19	a	838	CLA	CMB-C2B-C3B	3.54	131.31	124.68
19	a	855	CLA	CMB-C2B-C3B	3.54	131.29	124.68
19	b	3003	CLA	CMB-C2B-C3B	3.54	131.29	124.68
19	b	3041	CLA	CMB-C2B-C3B	3.53	131.29	124.68
28	b	3053	ZEX	C35-C15-C14	3.53	130.71	123.47
19	b	3038	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
19	b	3012	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
19	a	806	CLA	CMB-C2B-C3B	3.51	131.24	124.68
19	b	3026	CLA	CMB-C2B-C3B	3.50	131.24	124.68
19	a	805	CLA	CMB-C2B-C3B	3.50	131.23	124.68
19	D	403	CLA	CMB-C2B-C3B	3.50	131.22	124.68
19	j	103	CLA	CMB-C2B-C3B	3.49	131.20	124.68
19	a	812	CLA	CMB-C2B-C3B	3.47	131.18	124.68
19	b	3022	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
19	k	4003	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
19	a	831	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
19	a	807	CLA	CMB-C2B-C3B	3.47	131.16	124.68
19	a	858	CLA	CMB-C2B-C1B	-3.46	123.14	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a	839	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
26	m	101	ECH	C19-C18-C17	3.46	124.25	118.94
19	a	832	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
19	a	840	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
19	b	3037	CLA	CMB-C2B-C3B	3.45	131.12	124.68
19	a	804	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
19	a	811	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
19	b	3010	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
19	a	815	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
19	b	3007	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
19	b	3027	CLA	CMB-C2B-C3B	3.43	131.10	124.68
27	b	3052	EQ3	C15-C16-C17	3.43	130.50	123.47
19	D	401	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
19	a	831	CLA	CMB-C2B-C3B	3.43	131.09	124.68
19	b	3031	CLA	CMB-C2B-C3B	3.43	131.09	124.68
19	b	3040	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
19	a	838	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
19	a	822	CLA	CMB-C2B-C3B	3.41	131.05	124.68
19	b	3028	CLA	CMB-C2B-C3B	3.41	131.05	124.68
19	A	402	CLA	CMB-C2B-C3B	3.40	131.04	124.68
19	a	823	CLA	CMB-C2B-C3B	3.40	131.04	124.68
19	a	833	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
19	f	204	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
19	b	3029	CLA	CAA-C2A-C3A	-3.39	103.51	112.78
19	k	4002	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
19	b	3029	CLA	O2D-CGD-O1D	-3.38	117.24	123.84
19	b	3020	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
19	b	3035	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
19	b	3034	CLA	CMB-C2B-C3B	3.37	130.99	124.68
19	f	201	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
19	b	3024	CLA	CMB-C2B-C3B	3.37	130.99	124.68
19	a	824	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
28	b	3053	ZEX	C27-C26-C25	-3.34	117.44	122.84
19	b	3033	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
19	b	3006	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
19	a	836	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
19	b	3030	CLA	CMB-C2B-C1B	-3.32	123.35	128.46
19	l	1503	CLA	CMB-C2B-C3B	3.32	130.90	124.68
19	b	3017	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
19	b	3032	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
19	l	1502	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
19	b	3016	CLA	CMB-C2B-C3B	3.31	130.88	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a	814	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
19	b	3025	CLA	CMB-C2B-C3B	3.30	130.85	124.68
19	b	3008	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
27	b	3052	EQ3	C36-C18-C17	-3.29	118.31	122.92
19	a	817	CLA	CMB-C2B-C3B	3.29	130.83	124.68
19	a	813	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
19	a	803	CLA	CMB-C2B-C3B	3.28	130.81	124.68
19	b	3033	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
19	a	842	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
19	a	830	CLA	CMB-C2B-C3B	3.26	130.77	124.68
19	b	3019	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
19	a	805	CLA	O2D-CGD-O1D	-3.25	117.47	123.84
19	b	3015	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
19	a	809	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
26	m	101	ECH	C23-C22-C21	3.22	123.89	118.94
19	a	825	CLA	CMB-C2B-C3B	3.22	130.70	124.68
19	l	1501	CLA	CMB-C2B-C3B	3.22	130.70	124.68
28	f	205	ZEX	C40-C33-C34	-3.22	118.42	122.92
19	a	831	CLA	CAA-C2A-C3A	-3.21	103.99	112.78
19	a	837	CLA	CMB-C2B-C3B	3.20	130.67	124.68
27	b	3052	EQ3	C35-C13-C14	-3.20	118.44	122.92
28	b	3053	ZEX	C39-C29-C28	3.20	123.12	118.08
19	A	405	CLA	CMB-C2B-C3B	3.19	130.65	124.68
19	a	816	CLA	CMB-C2B-C3B	3.19	130.65	124.68
19	a	810	CLA	CMB-C2B-C3B	3.19	130.64	124.68
19	b	3013	CLA	CMB-C2B-C3B	3.18	130.64	124.68
19	a	835	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
27	b	3052	EQ3	C34-C9-C8	3.18	123.08	118.08
19	a	835	CLA	CMB-C2B-C3B	3.17	130.62	124.68
19	A	403	CLA	CMB-C2B-C3B	3.17	130.60	124.68
19	b	3007	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
19	b	3023	CLA	CMB-C2B-C3B	3.15	130.57	124.68
19	a	840	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
19	a	839	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
19	a	841	CLA	CMB-C2B-C3B	3.13	130.54	124.68
19	b	3014	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
19	a	819	CLA	CMB-C2B-C3B	3.13	130.53	124.68
19	a	819	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
19	b	3039	CLA	CMB-C2B-C3B	3.11	130.50	124.68
19	b	3011	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
19	D	404	CLA	CMB-C2B-C3B	3.11	130.49	124.68
19	b	3013	CLA	O2D-CGD-CBD	3.10	116.78	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b	3053	ZEX	C20-C13-C14	-3.10	118.58	122.92
19	a	809	CLA	CMB-C2B-C3B	3.10	130.48	124.68
19	a	843	CLA	CMB-C2B-C3B	3.10	130.48	124.68
19	a	804	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
19	b	3029	CLA	CMB-C2B-C3B	3.08	130.44	124.68
26	b	3045	ECH	C10-C11-C12	3.08	132.83	123.22
19	b	3016	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
19	a	858	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
19	a	826	CLA	O2D-CGD-O1D	-3.08	117.83	123.84
19	a	841	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
19	a	803	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
21	j	101	BCR	C15-C16-C17	-3.06	117.21	123.47
31	D	402	PHO	C4A-C3A-C2A	-3.05	99.93	102.84
19	a	818	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
19	a	832	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
19	b	3037	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
19	a	827	CLA	CMB-C2B-C3B	3.04	130.36	124.68
26	m	101	ECH	C35-C13-C14	-3.04	118.67	122.92
18	a	801	CL0	O2D-CGD-O1D	-3.03	117.91	123.84
19	b	3017	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
19	a	828	CLA	CMB-C2B-C3B	3.03	130.35	124.68
19	b	3003	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
19	a	818	CLA	CMB-C2B-C3B	3.02	130.33	124.68
28	b	3053	ZEX	C27-C28-C29	3.02	130.80	126.23
19	a	828	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
19	b	3002	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
26	b	3045	ECH	C15-C14-C13	3.01	131.61	127.31
19	b	3008	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
19	f	204	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
19	b	3002	CLA	CMB-C2B-C3B	3.01	130.31	124.68
19	a	821	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
19	k	4003	CLA	CMB-C2B-C3B	3.01	130.30	124.68
19	b	3022	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
19	b	3026	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
18	a	801	CL0	CMB-C2B-C1B	-3.00	123.85	128.46
21	k	4004	BCR	C2-C1-C6	3.00	115.11	110.48
19	a	815	CLA	CMB-C2B-C3B	2.99	130.28	124.68
19	a	855	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
19	a	808	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
19	A	403	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
19	b	3025	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
19	a	813	CLA	O2D-CGD-O1D	-2.98	118.01	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	b	3004	CLA	CMB-C2B-C3B	2.98	130.25	124.68
19	l	1502	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
19	a	827	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
19	b	3040	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
28	b	3053	ZEX	C40-C33-C34	-2.97	118.77	122.92
21	k	4001	BCR	C15-C14-C13	-2.96	123.08	127.31
19	a	843	CLA	CAA-C2A-C3A	-2.96	104.67	112.78
19	a	811	CLA	CMB-C2B-C3B	2.96	130.21	124.68
19	b	3005	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
19	b	3007	CLA	CMB-C2B-C3B	2.95	130.20	124.68
19	a	855	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
19	b	3038	CLA	CMB-C2B-C3B	2.95	130.19	124.68
19	a	836	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
28	f	205	ZEX	C20-C13-C14	-2.94	118.80	122.92
19	b	3009	CLA	CMB-C2B-C3B	2.94	130.18	124.68
19	b	3004	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
19	b	3002	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
19	a	810	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
19	b	3011	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
31	A	404	PHO	O1D-CGD-CBD	2.93	129.62	124.74
19	A	405	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
19	a	837	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
19	D	401	CLA	CMB-C2B-C3B	2.92	130.13	124.68
19	a	824	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
19	a	842	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
19	A	402	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
19	a	831	CLA	CHB-C4A-NA	2.90	128.53	124.51
19	a	829	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
21	a	849	BCR	C15-C14-C13	-2.90	123.17	127.31
19	b	3008	CLA	CMB-C2B-C3B	2.90	130.10	124.68
19	j	102	CLA	CMB-C2B-C3B	2.90	130.09	124.68
19	a	833	CLA	CMB-C2B-C3B	2.89	130.09	124.68
24	a	857	45D	C40-C36-C38	-2.89	118.87	122.92
19	a	821	CLA	CMB-C2B-C3B	2.89	130.09	124.68
19	b	3018	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
19	a	820	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
19	D	404	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
19	b	3024	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
19	b	3028	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
19	b	3020	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
19	b	3039	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
19	a	817	CLA	O2D-CGD-O1D	-2.87	118.22	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	b	3012	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
19	a	858	CLA	CMB-C2B-C3B	2.87	130.05	124.68
19	a	835	CLA	CHB-C4A-NA	2.87	128.48	124.51
19	a	856	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
21	b	3043	BCR	C33-C5-C6	-2.87	121.31	124.53
19	b	3030	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
21	a	848	BCR	C15-C16-C17	-2.86	117.61	123.47
28	f	205	ZEX	C15-C35-C34	2.86	129.33	123.47
19	b	3010	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
19	b	3038	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
19	a	832	CLA	CMB-C2B-C3B	2.85	130.01	124.68
19	l	1503	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
19	a	811	CLA	C1-C2-C3	-2.85	122.14	126.75
19	a	822	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
21	a	848	BCR	C33-C5-C6	-2.85	121.33	124.53
19	a	833	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
19	b	3015	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
26	b	3045	ECH	C30-C25-C24	2.84	123.82	115.78
19	k	4002	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	b	3009	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
21	b	3046	BCR	C15-C16-C17	-2.84	117.65	123.47
19	a	834	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
19	b	3029	CLA	CHB-C4A-NA	2.84	128.44	124.51
19	a	830	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
19	f	203	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
19	a	856	CLA	CMB-C2B-C3B	2.83	129.97	124.68
21	j	104	BCR	C15-C16-C17	-2.83	117.68	123.47
19	a	839	CLA	CMB-C2B-C3B	2.83	129.97	124.68
19	D	404	CLA	CHB-C4A-NA	2.83	128.42	124.51
21	a	847	BCR	C15-C16-C17	-2.83	117.68	123.47
21	a	849	BCR	C15-C16-C17	-2.83	117.68	123.47
19	b	3023	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
19	b	3034	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
19	f	204	CLA	CMB-C2B-C3B	2.83	129.97	124.68
19	b	3035	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
19	k	4002	CLA	CMB-C2B-C3B	2.83	129.97	124.68
23	a	853	LMG	O6-C1-O1	-2.82	103.28	109.97
19	a	802	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
19	l	1501	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
19	a	812	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
27	b	3052	EQ3	C16-C15-C14	2.81	129.23	123.47
19	a	804	CLA	CMB-C2B-C3B	2.81	129.93	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a	824	CLA	CHB-C4A-NA	2.81	128.40	124.51
28	f	205	ZEX	C32-C33-C34	2.81	123.25	118.94
28	f	205	ZEX	C27-C26-C25	-2.81	118.30	122.84
19	j	103	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
19	b	3038	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
19	l	1502	CLA	CMB-C2B-C3B	2.80	129.92	124.68
19	a	807	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
19	b	3021	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
19	a	806	CLA	CHB-C4A-NA	2.79	128.37	124.51
19	b	3012	CLA	CMB-C2B-C3B	2.79	129.90	124.68
21	b	3046	BCR	C15-C14-C13	-2.79	123.33	127.31
23	b	3049	LMG	O6-C1-O1	-2.79	103.37	109.97
21	b	3043	BCR	C15-C16-C17	-2.78	117.77	123.47
31	A	404	PHO	CMB-C2B-C3B	2.78	129.88	124.68
19	b	3006	CLA	CMB-C2B-C3B	2.78	129.87	124.68
28	b	3053	ZEX	C15-C35-C34	2.77	129.15	123.47
19	a	825	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
26	b	3045	ECH	C37-C22-C23	2.76	122.43	118.08
19	a	840	CLA	CMB-C2B-C3B	2.76	129.84	124.68
21	b	3047	BCR	C2-C1-C6	2.76	114.73	110.48
19	b	3041	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
29	f	207	LMT	C1'-O5'-C5'	-2.76	108.27	113.69
21	j	101	BCR	C15-C14-C13	-2.76	123.38	127.31
19	a	843	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
19	a	834	CLA	CHB-C4A-NA	2.75	128.32	124.51
19	a	824	CLA	CMB-C2B-C3B	2.75	129.83	124.68
19	b	3017	CLA	CMB-C2B-C3B	2.75	129.82	124.68
19	a	806	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
22	f	206	LHG	O8-C23-C24	2.75	120.52	111.91
19	b	3020	CLA	CMB-C2B-C3B	2.74	129.81	124.68
19	b	3027	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
19	a	816	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
19	b	3019	CLA	CMB-C2B-C3B	2.74	129.80	124.68
22	b	3050	LHG	O8-C23-C24	2.74	120.50	111.91
19	a	811	CLA	CHB-C4A-NA	2.74	128.29	124.51
24	a	857	45D	C39-C35-C37	-2.73	119.09	122.92
21	b	3046	BCR	C2-C1-C6	2.73	114.69	110.48
21	k	4001	BCR	C24-C23-C22	-2.73	122.11	126.23
19	b	3031	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
27	b	3052	EQ3	C37-C22-C23	2.73	122.38	118.08
31	D	402	PHO	O2D-CGD-O1D	-2.72	118.51	123.84
19	b	3032	CLA	O2D-CGD-O1D	-2.72	118.52	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	b	3022	CLA	CMB-C2B-C3B	2.72	129.76	124.68
18	a	801	CL0	CAA-CBA-CGA	-2.72	105.32	113.25
19	a	818	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	b	3039	CLA	C1-C2-C3	-2.71	121.35	126.04
19	b	3017	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	k	4003	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
19	b	3035	CLA	CMB-C2B-C3B	2.71	129.75	124.68
19	a	823	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
19	D	401	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
19	a	836	CLA	CMB-C2B-C3B	2.71	129.74	124.68
21	b	3043	BCR	C24-C23-C22	-2.70	122.15	126.23
19	b	3010	CLA	CMB-C2B-C3B	2.70	129.74	124.68
21	j	104	BCR	C33-C5-C6	-2.70	121.49	124.53
19	a	802	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
23	a	851	LMG	O6-C1-O1	-2.70	103.58	109.97
19	b	3033	CLA	CMB-C2B-C3B	2.70	129.72	124.68
19	f	201	CLA	CMB-C2B-C3B	2.69	129.71	124.68
19	b	3040	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
19	b	3030	CLA	CMB-C2B-C3B	2.69	129.70	124.68
27	b	3052	EQ3	C12-C13-C14	2.68	123.06	118.94
19	j	103	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
19	a	829	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
19	l	1502	CLA	CHB-C4A-NA	2.68	128.21	124.51
24	a	857	45D	C03-C07-C19	2.67	123.34	115.78
19	b	3035	CLA	CHB-C4A-NA	2.67	128.21	124.51
31	A	404	PHO	O2D-CGD-O1D	-2.67	118.62	123.84
19	j	102	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
19	b	3008	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
19	a	820	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
19	b	3019	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
19	b	3019	CLA	CHB-C4A-NA	2.66	128.19	124.51
19	a	843	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
19	b	3015	CLA	CHB-C4A-NA	2.65	128.18	124.51
19	b	3011	CLA	CMB-C2B-C3B	2.65	129.64	124.68
19	D	401	CLA	CHB-C4A-NA	2.65	128.18	124.51
21	j	104	BCR	C24-C23-C22	-2.65	122.24	126.23
19	f	201	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
21	b	3044	BCR	C33-C5-C6	-2.64	121.56	124.53
19	a	836	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	a	842	CLA	CMB-C2B-C3B	2.64	129.62	124.68
19	b	3032	CLA	CMB-C2B-C3B	2.64	129.62	124.68
19	D	403	CLA	O2D-CGD-O1D	-2.64	118.68	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	b	3006	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
19	b	3018	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
19	b	3011	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	A	403	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	b	3036	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
27	b	3052	EQ3	C19-C18-C17	2.63	122.98	118.94
19	k	4003	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
19	a	813	CLA	CMB-C2B-C3B	2.62	129.58	124.68
19	f	203	CLA	C1-C2-C3	-2.62	122.51	126.75
28	b	3053	ZEX	C12-C13-C14	2.62	122.96	118.94
21	k	4001	BCR	C15-C16-C17	-2.62	118.11	123.47
19	j	102	CLA	CHB-C4A-NA	2.62	128.13	124.51
19	b	3028	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
21	a	845	BCR	C24-C23-C22	-2.61	122.29	126.23
19	b	3019	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
19	b	3016	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
19	a	842	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	f	203	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
21	l	1504	BCR	C15-C16-C17	-2.60	118.14	123.47
19	b	3040	CLA	CHB-C4A-NA	2.60	128.11	124.51
21	k	4004	BCR	C24-C23-C22	-2.60	122.30	126.23
21	a	847	BCR	C15-C14-C13	-2.60	123.60	127.31
19	a	826	CLA	CHB-C4A-NA	2.60	128.10	124.51
21	a	849	BCR	C7-C8-C9	-2.59	122.31	126.23
19	f	204	CLA	CHB-C4A-NA	2.59	128.10	124.51
19	a	829	CLA	C1-C2-C3	-2.59	121.56	126.04
19	b	3015	CLA	CMB-C2B-C3B	2.59	129.52	124.68
19	b	3040	CLA	CMB-C2B-C3B	2.59	129.52	124.68
19	k	4002	CLA	CHB-C4A-NA	2.59	128.09	124.51
27	b	3052	EQ3	C24-C23-C22	2.58	130.14	126.23
19	a	843	CLA	CHB-C4A-NA	2.58	128.09	124.51
19	l	1503	CLA	CHB-C4A-NA	2.58	128.08	124.51
19	b	3003	CLA	CAC-C3C-C4C	2.58	128.16	124.81
19	l	1501	CLA	CHB-C4A-NA	2.58	128.08	124.51
19	a	834	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
22	a	850	LHG	O8-C23-C24	2.58	120.00	111.91
21	k	4004	BCR	C15-C16-C17	-2.57	118.20	123.47
19	a	840	CLA	CHB-C4A-NA	2.57	128.07	124.51
19	a	809	CLA	CHB-C4A-NA	2.57	128.07	124.51
19	a	809	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
19	a	802	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
19	l	1501	CLA	C1-C2-C3	-2.56	122.61	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	b	3003	CLA	CHB-C4A-NA	2.56	128.05	124.51
21	b	3043	BCR	C27-C26-C25	2.56	126.44	122.73
19	b	3026	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
18	a	801	CL0	C1B-CHB-C4A	-2.56	125.06	130.12
19	b	3006	CLA	CHB-C4A-NA	2.55	128.04	124.51
19	a	826	CLA	O2D-CGD-CBD	2.55	115.80	111.27
19	b	3034	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
19	a	822	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
19	b	3027	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
19	A	405	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
19	a	821	CLA	CHB-C4A-NA	2.55	128.03	124.51
19	b	3020	CLA	CHB-C4A-NA	2.55	128.03	124.51
19	a	830	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
19	a	803	CLA	CHB-C4A-NA	2.54	128.03	124.51
19	b	3029	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
19	a	810	CLA	CHB-C4A-NA	2.54	128.03	124.51
19	b	3036	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
19	a	824	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
19	a	829	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	a	831	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
19	a	838	CLA	O2D-CGD-CBD	2.54	115.78	111.27
19	a	836	CLA	C1B-CHB-C4A	-2.54	125.10	130.12
21	b	3044	BCR	C15-C16-C17	-2.53	118.28	123.47
19	a	823	CLA	CHB-C4A-NA	2.53	128.01	124.51
18	a	801	CL0	CMB-C2B-C3B	2.53	129.42	124.68
19	a	819	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
22	a	852	LHG	C11-C10-C9	-2.53	101.58	114.42
19	b	3003	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
19	b	3007	CLA	CHB-C4A-NA	2.53	128.01	124.51
27	b	3052	EQ3	C7-C8-C9	2.53	130.06	126.23
19	a	841	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	a	854	LHG	O8-C23-C24	2.53	119.84	111.91
22	a	852	LHG	O8-C23-C24	2.53	119.83	111.91
19	b	3013	CLA	CHB-C4A-NA	2.53	128.00	124.51
19	a	802	CLA	C1-C2-C3	-2.52	121.68	126.04
19	a	803	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
19	b	3007	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
21	j	104	BCR	C15-C14-C13	-2.52	123.71	127.31
23	a	853	LMG	O1-C1-C2	-2.52	104.37	108.30
19	A	402	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
19	b	3035	CLA	C1-C2-C3	-2.52	122.68	126.75
19	b	3004	CLA	CHB-C4A-NA	2.52	127.99	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a	825	CLA	CHB-C4A-NA	2.51	127.99	124.51
21	i	101	BCR	C15-C16-C17	-2.51	118.33	123.47
21	a	846	BCR	C33-C5-C6	-2.51	121.71	124.53
21	j	104	BCR	C27-C26-C25	2.51	126.38	122.73
19	a	804	CLA	CHB-C4A-NA	2.51	127.98	124.51
19	b	3032	CLA	CHB-C4A-NA	2.51	127.98	124.51
21	j	101	BCR	C33-C5-C6	-2.51	121.71	124.53
19	a	805	CLA	CHB-C4A-NA	2.51	127.98	124.51
19	a	814	CLA	CHB-C4A-NA	2.51	127.98	124.51
19	b	3005	CLA	CHB-C4A-NA	2.51	127.98	124.51
19	b	3039	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	a	816	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	a	818	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
19	a	807	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	A	402	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	a	806	CLA	C1-C2-C3	-2.50	121.72	126.04
19	a	823	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
19	a	817	CLA	CHB-C4A-NA	2.50	127.97	124.51
31	D	402	PHO	O1D-CGD-CBD	2.50	128.90	124.74
19	a	819	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	a	853	LMG	O1-C7-C8	-2.49	104.89	110.90
23	a	851	LMG	C38-C37-C36	-2.49	101.78	114.42
19	a	831	CLA	O2D-CGD-CBD	2.49	115.69	111.27
19	b	3008	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
19	a	808	CLA	CHB-C4A-NA	2.49	127.95	124.51
21	a	845	BCR	C15-C16-C17	-2.49	118.38	123.47
22	a	854	LHG	C11-C10-C9	-2.49	101.80	114.42
32	F	101	HEM	C4C-CHD-C1D	2.49	125.84	122.56
26	m	101	ECH	C12-C13-C14	2.48	122.75	118.94
26	m	101	ECH	C16-C15-C14	2.48	128.56	123.47
19	b	3012	CLA	C1-C2-C3	-2.48	122.74	126.75
19	b	3027	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	b	3015	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
19	a	841	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
19	a	858	CLA	CHB-C4A-NA	2.47	127.93	124.51
21	A	406	BCR	C33-C5-C6	-2.47	121.75	124.53
19	a	832	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
19	a	827	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
21	b	3047	BCR	C27-C26-C25	2.47	126.32	122.73
32	F	101	HEM	C4D-ND-C1D	2.47	107.62	105.07
19	a	835	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
23	b	3049	LMG	O1-C7-C8	-2.46	104.95	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	b	3023	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	b	3037	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
19	a	813	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	b	3034	CLA	CHB-C4A-NA	2.46	127.92	124.51
21	b	3048	BCR	C15-C16-C17	-2.46	118.43	123.47
19	a	833	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	b	3022	CLA	CHB-C4A-NA	2.46	127.91	124.51
21	b	3046	BCR	C24-C23-C22	-2.46	122.52	126.23
19	a	828	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
19	k	4002	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
21	a	848	BCR	C15-C14-C13	-2.46	123.80	127.31
19	a	822	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	b	3025	CLA	C1B-CHB-C4A	-2.45	125.25	130.12
21	l	1504	BCR	C15-C14-C13	-2.45	123.81	127.31
19	a	813	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
19	b	3031	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
19	b	3039	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
19	b	3024	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
19	j	102	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
19	a	837	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
19	a	856	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	b	3025	CLA	CHB-C4A-NA	2.44	127.89	124.51
21	i	101	BCR	C27-C26-C25	2.44	126.28	122.73
19	b	3036	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	b	3014	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	b	3005	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
19	b	3026	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	b	3041	CLA	CHB-C4A-NA	2.44	127.88	124.51
21	k	4004	BCR	C15-C14-C13	-2.43	123.83	127.31
19	a	842	CLA	C1-C2-C3	-2.43	121.83	126.04
21	l	1504	BCR	C28-C27-C26	-2.43	109.73	114.08
19	a	828	CLA	CHB-C4A-NA	2.43	127.87	124.51
19	a	811	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
21	k	4001	BCR	C33-C5-C6	-2.43	121.80	124.53
22	f	206	LHG	C11-C10-C9	-2.43	102.09	114.42
21	A	406	BCR	C24-C23-C22	-2.43	122.57	126.23
19	b	3037	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
19	b	3024	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	b	3051	LMG	C40-C39-C38	-2.43	102.11	114.42
19	D	403	CLA	CHB-C4A-NA	2.43	127.87	124.51
21	A	406	BCR	C27-C26-C25	2.42	126.25	122.73
19	b	3008	CLA	CHB-C4A-NA	2.42	127.86	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	850	LHG	C20-C19-C18	-2.42	102.15	114.42
21	b	3048	BCR	C15-C14-C13	-2.42	123.86	127.31
19	a	812	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
19	b	3018	CLA	CHB-C4A-NA	2.42	127.85	124.51
19	a	840	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
21	l	1504	BCR	C11-C10-C9	-2.41	123.87	127.31
28	b	3053	ZEX	C32-C33-C34	2.41	122.64	118.94
21	A	406	BCR	C15-C14-C13	-2.41	123.87	127.31
19	a	837	CLA	CHB-C4A-NA	2.41	127.84	124.51
19	a	827	CLA	CHB-C4A-NA	2.41	127.84	124.51
19	b	3006	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
19	a	814	CLA	O2D-CGD-CBD	2.41	115.55	111.27
19	D	401	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
21	k	4004	BCR	C27-C26-C25	2.41	126.22	122.73
19	b	3011	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
19	b	3035	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
19	b	3016	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	b	3028	CLA	CHB-C4A-NA	2.40	127.83	124.51
21	l	1504	BCR	C2-C1-C6	2.40	114.18	110.48
19	a	825	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
19	a	820	CLA	CHB-C4A-NA	2.40	127.83	124.51
18	a	801	CL0	CHB-C4A-NA	2.39	127.82	124.51
21	a	845	BCR	C27-C26-C25	2.39	126.20	122.73
24	a	857	45D	C24-C26-C30	2.39	122.61	118.94
19	a	839	CLA	CHB-C4A-NA	2.39	127.81	124.51
22	f	206	LHG	C20-C19-C18	-2.39	102.32	114.42
19	a	814	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
19	b	3023	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
21	j	101	BCR	C24-C23-C22	-2.38	122.63	126.23
19	l	1502	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
19	b	3004	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
18	a	801	CL0	C1-C2-C3	-2.38	121.93	126.04
19	b	3031	CLA	CHB-C4A-NA	2.38	127.80	124.51
19	b	3041	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
19	a	804	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
19	b	3017	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
19	a	812	CLA	CHB-C4A-NA	2.37	127.80	124.51
19	a	842	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
19	b	3029	CLA	O2D-CGD-CBD	2.37	115.48	111.27
21	A	406	BCR	C11-C10-C9	-2.37	123.92	127.31
19	a	840	CLA	O2D-CGD-CBD	2.37	115.48	111.27
19	f	201	CLA	CHB-C4A-NA	2.37	127.79	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a	838	CLA	CHB-C4A-NA	2.37	127.79	124.51
19	f	201	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
23	b	3051	LMG	C38-C37-C36	-2.37	102.39	114.42
19	a	808	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
21	a	847	BCR	C27-C26-C25	2.37	126.17	122.73
21	f	202	BCR	C27-C26-C25	2.37	126.17	122.73
19	b	3012	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
19	A	405	CLA	CHB-C4A-NA	2.36	127.78	124.51
19	b	3020	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
19	b	3012	CLA	CHB-C4A-NA	2.36	127.78	124.51
19	b	3032	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
21	l	1504	BCR	C33-C5-C6	-2.36	121.88	124.53
23	b	3049	LMG	C40-C39-C38	-2.36	102.44	114.42
19	b	3030	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
19	a	806	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
19	a	816	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
19	b	3010	CLA	CHB-C4A-NA	2.36	127.77	124.51
19	b	3031	CLA	C1-C2-C3	-2.35	122.94	126.75
19	a	830	CLA	CHB-C4A-NA	2.35	127.77	124.51
19	b	3033	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	b	3033	CLA	O2D-CGD-CBD	2.35	115.44	111.27
19	a	818	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
28	f	205	ZEX	C12-C13-C14	2.35	122.54	118.94
23	a	853	LMG	O2-C2-C1	-2.34	104.35	110.05
22	a	852	LHG	C20-C19-C18	-2.34	102.53	114.42
21	a	848	BCR	C27-C26-C25	2.34	126.13	122.73
19	a	839	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
21	a	845	BCR	C33-C5-C6	-2.34	121.90	124.53
19	f	204	CLA	C1-C2-C3	-2.34	122.97	126.75
19	b	3014	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
19	b	3021	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
19	l	1501	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
21	a	847	BCR	C33-C5-C6	-2.34	121.91	124.53
19	b	3020	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
23	b	3051	LMG	O6-C1-O1	-2.33	104.45	109.97
22	a	850	LHG	C11-C10-C9	-2.33	102.58	114.42
19	D	403	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	b	3021	CLA	CHB-C4A-NA	2.33	127.73	124.51
19	b	3016	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
21	a	846	BCR	C27-C26-C25	2.33	126.11	122.73
19	D	404	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
21	b	3047	BCR	C15-C16-C17	-2.33	118.71	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	f	207	LMT	C3'-C4'-C5'	-2.33	105.59	110.93
23	b	3051	LMG	O3-C3-C2	-2.32	104.98	110.35
19	f	203	CLA	CHB-C4A-NA	2.32	127.72	124.51
31	D	402	PHO	CMB-C2B-C3B	2.32	129.02	124.68
19	a	858	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
19	a	807	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
21	b	3043	BCR	C15-C14-C13	-2.31	124.01	127.31
19	a	855	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
19	a	833	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
19	b	3009	CLA	CHB-C4A-NA	2.31	127.71	124.51
19	k	4003	CLA	CHB-C4A-NA	2.31	127.70	124.51
22	a	854	LHG	C20-C19-C18	-2.31	102.71	114.42
19	a	809	CLA	CHD-C1D-ND	-2.30	122.34	124.45
19	a	832	CLA	CHB-C4A-NA	2.30	127.70	124.51
23	a	851	LMG	O3-C3-C2	-2.30	105.03	110.35
19	l	1503	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	b	3013	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
19	a	815	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
21	b	3048	BCR	C33-C5-C6	-2.30	121.95	124.53
19	a	839	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
23	b	3049	LMG	C38-C37-C36	-2.29	102.78	114.42
19	b	3022	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
19	a	805	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
21	b	3044	BCR	C15-C14-C13	-2.29	124.04	127.31
21	j	101	BCR	C27-C26-C25	2.29	126.06	122.73
19	a	828	CLA	C1-C2-C3	-2.29	122.08	126.04
19	f	204	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
19	a	803	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
21	A	406	BCR	C15-C16-C17	-2.28	118.80	123.47
19	a	856	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
19	a	836	CLA	C1-C2-C3	-2.28	122.11	126.04
19	a	815	CLA	CHB-C4A-NA	2.28	127.66	124.51
19	a	817	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
23	b	3049	LMG	O1-C1-C2	-2.27	104.76	108.30
22	f	206	LHG	C18-C17-C16	-2.27	102.89	114.42
22	b	3050	LHG	C27-C26-C25	-2.27	102.90	114.42
22	a	852	LHG	C27-C26-C25	-2.27	102.90	114.42
21	a	846	BCR	C11-C10-C9	-2.27	124.07	127.31
21	i	101	BCR	C33-C5-C6	-2.27	121.98	124.53
24	a	857	45D	C33-C35-C37	2.27	122.42	118.94
19	b	3006	CLA	C1-C2-C3	-2.27	122.12	126.04
19	b	3009	CLA	C1B-CHB-C4A	-2.27	125.63	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a	837	CLA	C1-C2-C3	-2.26	122.13	126.04
23	b	3051	LMG	C42-C41-C40	-2.26	102.94	114.42
19	a	838	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
19	a	810	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
21	b	3044	BCR	C28-C27-C26	-2.26	110.04	114.08
19	a	823	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
19	b	3038	CLA	C1-C2-C3	-2.26	123.10	126.75
21	a	846	BCR	C7-C8-C9	-2.25	122.83	126.23
21	a	845	BCR	C15-C14-C13	-2.25	124.10	127.31
19	b	3014	CLA	C1-C2-C3	-2.25	122.15	126.04
19	A	403	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
19	b	3030	CLA	CHB-C4A-NA	2.24	127.62	124.51
19	b	3013	CLA	C1-C2-C3	-2.24	122.16	126.04
19	a	826	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
19	b	3010	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
21	a	849	BCR	C11-C10-C9	-2.24	124.12	127.31
23	b	3049	LMG	O3-C3-C2	-2.24	105.18	110.35
19	a	815	CLA	O2D-CGD-CBD	2.23	115.24	111.27
21	f	202	BCR	C24-C23-C22	-2.23	122.86	126.23
19	a	811	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
21	b	3048	BCR	C27-C26-C25	2.23	125.97	122.73
19	b	3037	CLA	CHB-C4A-NA	2.23	127.60	124.51
19	a	815	CLA	CHD-C1D-ND	-2.22	122.41	124.45
19	a	834	CLA	C1-C2-C3	-2.22	122.20	126.04
22	a	854	LHG	C27-C26-C25	-2.22	103.16	114.42
19	b	3039	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
21	b	3046	BCR	C33-C5-C6	-2.22	122.04	124.53
22	a	852	LHG	C18-C17-C16	-2.21	103.18	114.42
22	f	206	LHG	C27-C26-C25	-2.21	103.18	114.42
21	a	849	BCR	C33-C5-C6	-2.21	122.04	124.53
19	b	3034	CLA	CHD-C1D-ND	-2.21	122.42	124.45
23	b	3049	LMG	O2-C2-C1	-2.21	104.67	110.05
21	b	3046	BCR	C27-C26-C25	2.21	125.94	122.73
19	a	841	CLA	CHD-C1D-ND	-2.21	122.42	124.45
31	A	404	PHO	CMC-C2C-C3C	2.21	129.10	124.94
19	a	835	CLA	O2D-CGD-CBD	2.21	115.19	111.27
19	b	3038	CLA	CHB-C4A-NA	2.21	127.56	124.51
21	f	202	BCR	C33-C5-C6	-2.20	122.05	124.53
21	b	3047	BCR	C24-C23-C22	-2.20	122.91	126.23
19	b	3021	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
24	a	857	45D	C34-C36-C38	2.20	122.32	118.94
19	l	1502	CLA	O2A-CGA-O1A	-2.20	118.05	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	a	847	BCR	C24-C23-C22	-2.20	122.92	126.23
19	a	810	CLA	C1-C2-C3	-2.19	122.25	126.04
19	a	830	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
19	a	802	CLA	CHB-C4A-NA	2.19	127.55	124.51
31	D	402	PHO	O2A-CGA-O1A	-2.19	118.06	123.59
21	f	202	BCR	C8-C7-C6	-2.19	121.05	127.20
23	a	851	LMG	C40-C39-C38	-2.19	103.30	114.42
19	a	809	CLA	C1-C2-C3	-2.19	122.25	126.04
31	D	402	PHO	CMC-C2C-C3C	2.19	129.07	124.94
22	a	850	LHG	C27-C26-C25	-2.19	103.32	114.42
19	a	821	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
23	a	853	LMG	O3-C3-C2	-2.18	105.30	110.35
19	b	3004	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
19	a	813	CLA	CHD-C1D-ND	-2.18	122.45	124.45
23	b	3049	LMG	C42-C41-C40	-2.18	103.36	114.42
21	b	3046	BCR	C11-C10-C9	-2.18	124.20	127.31
19	a	837	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
19	b	3031	CLA	CHD-C1D-ND	-2.18	122.45	124.45
21	j	101	BCR	C11-C10-C9	-2.18	124.20	127.31
23	a	851	LMG	O1-C7-C8	-2.18	105.65	110.90
19	b	3007	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
19	j	102	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
21	i	101	BCR	C15-C14-C13	-2.17	124.21	127.31
19	b	3034	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
19	a	826	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
19	b	3032	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	b	3051	LMG	O7-C10-O9	-2.16	118.47	123.70
19	b	3037	CLA	CHD-C1D-ND	-2.16	122.47	124.45
19	a	810	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
21	b	3047	BCR	C15-C14-C13	-2.16	124.23	127.31
19	b	3033	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
31	A	404	PHO	O2A-CGA-O1A	-2.15	118.16	123.59
19	a	809	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
21	a	846	BCR	C15-C16-C17	-2.15	119.07	123.47
22	a	850	LHG	C18-C17-C16	-2.15	103.52	114.42
19	b	3025	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
21	a	846	BCR	C15-C14-C13	-2.15	124.25	127.31
19	b	3036	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
19	j	103	CLA	CHB-C4A-NA	2.15	127.48	124.51
21	k	4001	BCR	C11-C10-C9	-2.15	124.25	127.31
19	A	405	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
19	a	838	CLA	O2A-CGA-O1A	-2.14	118.19	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	l	1504	BCR	C29-C30-C25	2.14	113.78	110.48
19	a	836	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
21	k	4001	BCR	C35-C13-C14	-2.14	119.92	122.92
19	b	3007	CLA	O2D-CGD-CBD	2.14	115.07	111.27
19	a	833	CLA	C1-C2-C3	-2.14	122.35	126.04
19	a	819	CLA	CAA-CBA-CGA	-2.14	107.01	113.25
19	a	806	CLA	CHD-C1D-ND	-2.13	122.49	124.45
19	b	3004	CLA	CHD-C1D-ND	-2.13	122.50	124.45
21	k	4001	BCR	C27-C26-C25	2.13	125.82	122.73
32	F	101	HEM	C1B-NB-C4B	2.13	107.27	105.07
19	a	829	CLA	CHD-C1D-ND	-2.13	122.50	124.45
19	b	3019	CLA	CHD-C1D-ND	-2.12	122.50	124.45
21	b	3043	BCR	C7-C8-C9	-2.12	123.03	126.23
28	f	205	ZEX	C28-C29-C30	2.12	122.19	118.94
19	b	3003	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
19	a	822	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
19	b	3015	CLA	CAC-C3C-C4C	2.11	127.55	124.81
19	a	843	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
19	l	1501	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
21	b	3044	BCR	C2-C1-C6	2.11	113.73	110.48
19	b	3013	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
19	a	827	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
19	b	3017	CLA	CHD-C1D-ND	-2.10	122.52	124.45
19	a	804	CLA	O2D-CGD-CBD	2.10	115.01	111.27
23	a	851	LMG	C42-C41-C40	-2.09	103.79	114.42
19	f	204	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
19	b	3030	CLA	CHD-C1D-ND	-2.09	122.53	124.45
19	a	841	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
19	a	812	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
23	b	3051	LMG	O1-C7-C8	-2.09	105.86	110.90
19	b	3023	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
19	b	3012	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
19	b	3031	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
23	b	3051	LMG	O2-C2-C1	-2.08	104.98	110.05
19	b	3038	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
21	f	202	BCR	C16-C15-C14	-2.08	119.21	123.47
26	m	101	ECH	C29-C30-C25	2.08	113.69	110.48
21	b	3047	BCR	C10-C11-C12	-2.08	116.72	123.22
19	f	203	CLA	CHD-C1D-ND	-2.08	122.54	124.45
19	b	3002	CLA	CHB-C4A-NA	2.08	127.39	124.51
19	a	819	CLA	CHD-C1D-ND	-2.08	122.55	124.45
19	b	3008	CLA	O1D-CGD-CBD	2.07	128.73	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	k	4004	BCR	C7-C8-C9	-2.07	123.10	126.23
19	b	3034	CLA	C1-C2-C3	-2.07	122.46	126.04
19	a	835	CLA	C1-C2-C3	-2.07	122.46	126.04
19	b	3007	CLA	CHD-C1D-ND	-2.07	122.55	124.45
19	a	807	CLA	CHD-C1D-ND	-2.07	122.55	124.45
19	b	3026	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
19	b	3029	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
19	a	805	CLA	CHD-C1D-ND	-2.07	122.56	124.45
24	a	857	45D	C23-C25-C29	2.06	122.11	118.94
22	a	854	LHG	C18-C17-C16	-2.06	103.96	114.42
19	a	814	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
21	l	1504	BCR	C24-C23-C22	-2.06	123.12	126.23
19	b	3018	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
19	b	3003	CLA	CHD-C1D-ND	-2.06	122.56	124.45
19	b	3024	CLA	C1-C2-C3	-2.06	122.49	126.04
29	f	207	LMT	C3B-C4B-C5B	-2.05	106.58	110.24
19	b	3015	CLA	CHD-C1D-ND	-2.05	122.57	124.45
21	i	101	BCR	C8-C7-C6	-2.05	121.44	127.20
19	b	3035	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
19	b	3009	CLA	CAA-CBA-CGA	-2.05	107.26	113.25
19	b	3028	CLA	C2D-C1D-ND	-2.05	108.59	110.10
19	a	830	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	b	3006	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
19	b	3017	CLA	C1-C2-C3	-2.05	122.50	126.04
19	a	804	CLA	CHD-C1D-ND	-2.05	122.57	124.45
32	F	101	HEM	C4B-CHC-C1C	2.05	125.26	122.56
19	D	403	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
19	b	3005	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	a	851	LMG	O2-C2-C1	-2.04	105.09	110.05
21	j	104	BCR	C38-C26-C25	-2.04	122.24	124.53
26	m	101	ECH	C21-C20-C19	2.04	129.58	123.22
18	a	801	CL0	O2A-CGA-O1A	-2.04	118.45	123.59
19	a	834	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
19	k	4003	CLA	CAC-C3C-C4C	2.03	127.45	124.81
19	b	3041	CLA	CHD-C1D-ND	-2.03	122.59	124.45
21	a	848	BCR	C38-C26-C25	-2.03	122.25	124.53
21	a	845	BCR	C11-C10-C9	-2.03	124.42	127.31
21	a	848	BCR	C8-C7-C6	-2.02	121.52	127.20
21	j	104	BCR	C8-C7-C6	-2.02	121.52	127.20
21	a	848	BCR	C35-C13-C14	-2.02	120.09	122.92
26	m	101	ECH	C34-C9-C8	2.02	121.26	118.08
19	a	818	CLA	CHD-C1D-ND	-2.02	122.60	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	b	3033	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
26	m	101	ECH	C1-C6-C5	-2.02	119.77	122.61
21	a	847	BCR	C7-C8-C9	-2.02	123.19	126.23
19	b	3017	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
19	a	827	CLA	CHD-C1D-ND	-2.01	122.60	124.45
19	D	403	CLA	CHD-C1D-ND	-2.01	122.61	124.45
21	b	3047	BCR	C8-C7-C6	-2.01	121.56	127.20
19	a	820	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
19	a	816	CLA	CHD-C1D-ND	-2.01	122.61	124.45
21	j	101	BCR	C8-C7-C6	-2.01	121.56	127.20
26	b	3045	ECH	C34-C9-C8	2.01	121.24	118.08
19	a	820	CLA	CHD-C1D-ND	-2.01	122.61	124.45
19	a	821	CLA	CAA-CBA-CGA	-2.00	107.40	113.25
31	D	402	PHO	C1A-C2A-C3A	-2.00	100.93	102.84
19	a	828	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
19	a	858	CLA	O2A-CGA-O1A	-2.00	118.54	123.59

All (102) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	a	801	CL0	NC
18	a	801	CL0	NA
18	a	801	CL0	ND
19	a	802	CLA	ND
19	a	803	CLA	ND
19	a	804	CLA	ND
19	a	805	CLA	ND
19	a	806	CLA	ND
19	a	807	CLA	ND
19	a	808	CLA	ND
19	a	809	CLA	ND
19	a	810	CLA	ND
19	a	811	CLA	ND
19	a	812	CLA	ND
19	a	813	CLA	ND
19	a	815	CLA	ND
19	a	816	CLA	ND
19	a	817	CLA	ND
19	a	818	CLA	ND
19	a	819	CLA	ND
19	a	820	CLA	ND
19	a	821	CLA	ND

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Mol	Chain	Res	Type	Atom
19	a	822	CLA	ND
19	a	823	CLA	ND
19	a	824	CLA	ND
19	a	825	CLA	ND
19	a	826	CLA	ND
19	a	827	CLA	ND
19	a	828	CLA	ND
19	a	829	CLA	ND
19	a	830	CLA	ND
19	a	831	CLA	ND
19	a	832	CLA	ND
19	a	833	CLA	ND
19	a	834	CLA	ND
19	a	835	CLA	ND
19	a	836	CLA	ND
19	a	837	CLA	ND
19	a	839	CLA	ND
19	a	840	CLA	ND
19	a	841	CLA	ND
19	a	842	CLA	ND
19	a	843	CLA	ND
19	a	855	CLA	ND
19	a	856	CLA	ND
19	a	858	CLA	ND
19	b	3002	CLA	ND
19	b	3003	CLA	ND
19	b	3004	CLA	ND
19	b	3005	CLA	ND
19	b	3006	CLA	ND
19	b	3007	CLA	ND
19	b	3008	CLA	ND
19	b	3009	CLA	ND
19	b	3010	CLA	ND
19	b	3011	CLA	ND
19	b	3012	CLA	ND
19	b	3013	CLA	ND
19	b	3014	CLA	ND
19	b	3015	CLA	ND
19	b	3016	CLA	ND
19	b	3017	CLA	ND
19	b	3018	CLA	ND
19	b	3019	CLA	ND

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Mol	Chain	Res	Type	Atom
19	b	3020	CLA	ND
19	b	3021	CLA	ND
19	b	3022	CLA	ND
19	b	3023	CLA	ND
19	b	3024	CLA	ND
19	b	3025	CLA	ND
19	b	3026	CLA	ND
19	b	3027	CLA	ND
19	b	3028	CLA	ND
19	b	3029	CLA	ND
19	b	3030	CLA	ND
19	b	3031	CLA	ND
19	b	3032	CLA	ND
19	b	3033	CLA	ND
19	b	3034	CLA	ND
19	b	3035	CLA	ND
19	b	3036	CLA	ND
19	b	3037	CLA	ND
19	b	3038	CLA	ND
19	b	3039	CLA	ND
19	b	3040	CLA	ND
19	b	3041	CLA	ND
19	f	201	CLA	ND
19	f	203	CLA	ND
19	f	204	CLA	ND
19	j	102	CLA	ND
19	j	103	CLA	ND
19	k	4002	CLA	ND
19	k	4003	CLA	ND
19	l	1501	CLA	ND
19	l	1502	CLA	ND
19	l	1503	CLA	ND
19	A	402	CLA	ND
19	A	403	CLA	ND
19	A	405	CLA	ND
19	D	401	CLA	ND
19	D	403	CLA	ND
19	D	404	CLA	ND

All (1651) torsion outliers are listed below:

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Mol	Chain	Res	Type	Atoms

Mol	Chain	Res	Type	Atoms
19	a	802	CLA	CBD-CGD-O2D-CED
19	a	802	CLA	C4-C3-C5-C6
19	a	803	CLA	CBA-CGA-O2A-C1
19	a	803	CLA	O1A-CGA-O2A-C1
19	a	803	CLA	CHA-CBD-CGD-O1D
19	a	803	CLA	CHA-CBD-CGD-O2D
19	a	805	CLA	C1A-C2A-CAA-CBA
19	a	805	CLA	C3A-C2A-CAA-CBA
19	a	805	CLA	CHA-CBD-CGD-O1D
19	a	805	CLA	CHA-CBD-CGD-O2D
19	a	806	CLA	C3A-C2A-CAA-CBA
19	a	807	CLA	C2-C3-C5-C6
19	a	807	CLA	C4-C3-C5-C6
19	a	808	CLA	C1A-C2A-CAA-CBA
19	a	808	CLA	C3A-C2A-CAA-CBA
19	a	809	CLA	C3A-C2A-CAA-CBA
19	a	811	CLA	CAD-CBD-CGD-O1D
19	a	813	CLA	C1A-C2A-CAA-CBA
19	a	813	CLA	C3A-C2A-CAA-CBA
19	a	815	CLA	C3A-C2A-CAA-CBA
19	a	815	CLA	CHA-CBD-CGD-O1D
19	a	815	CLA	CHA-CBD-CGD-O2D
19	a	816	CLA	CHA-CBD-CGD-O1D
19	a	816	CLA	CHA-CBD-CGD-O2D
19	a	817	CLA	C1A-C2A-CAA-CBA
19	a	817	CLA	C3A-C2A-CAA-CBA
19	a	817	CLA	CBA-CGA-O2A-C1
19	a	818	CLA	C1A-C2A-CAA-CBA
19	a	819	CLA	C1A-C2A-CAA-CBA
19	a	819	CLA	C3A-C2A-CAA-CBA
19	a	819	CLA	C6-C7-C8-C9
19	a	819	CLA	C11-C10-C8-C9
19	a	820	CLA	C1A-C2A-CAA-CBA
19	a	820	CLA	C3A-C2A-CAA-CBA
19	a	820	CLA	CHA-CBD-CGD-O1D
19	a	820	CLA	CHA-CBD-CGD-O2D
19	a	821	CLA	C1A-C2A-CAA-CBA
19	a	821	CLA	C3A-C2A-CAA-CBA
19	a	821	CLA	C2-C1-O2A-CGA
19	a	821	CLA	CBD-CGD-O2D-CED
19	a	823	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	a	823	CLA	C3A-C2A-CAA-CBA
19	a	823	CLA	CHA-CBD-CGD-O1D
19	a	823	CLA	CBD-CGD-O2D-CED
19	a	824	CLA	C1A-C2A-CAA-CBA
19	a	825	CLA	CHA-CBD-CGD-O1D
19	a	825	CLA	CHA-CBD-CGD-O2D
19	a	827	CLA	C1A-C2A-CAA-CBA
19	a	827	CLA	C3A-C2A-CAA-CBA
19	a	828	CLA	C1A-C2A-CAA-CBA
19	a	828	CLA	C3A-C2A-CAA-CBA
19	a	829	CLA	C1A-C2A-CAA-CBA
19	a	831	CLA	CAD-CBD-CGD-O2D
19	a	832	CLA	C3A-C2A-CAA-CBA
19	a	832	CLA	CHA-CBD-CGD-O1D
19	a	832	CLA	CHA-CBD-CGD-O2D
19	a	833	CLA	C1A-C2A-CAA-CBA
19	a	833	CLA	C3A-C2A-CAA-CBA
19	a	836	CLA	C2-C3-C5-C6
19	a	836	CLA	C4-C3-C5-C6
19	a	837	CLA	CHA-CBD-CGD-O1D
19	a	837	CLA	CHA-CBD-CGD-O2D
19	a	837	CLA	C2-C3-C5-C6
19	a	837	CLA	C4-C3-C5-C6
19	a	838	CLA	C1A-C2A-CAA-CBA
19	a	838	CLA	CHA-CBD-CGD-O1D
19	a	838	CLA	CHA-CBD-CGD-O2D
19	a	839	CLA	C1A-C2A-CAA-CBA
19	a	839	CLA	C3A-C2A-CAA-CBA
19	a	840	CLA	C4-C3-C5-C6
19	a	841	CLA	C1A-C2A-CAA-CBA
19	a	841	CLA	C3A-C2A-CAA-CBA
19	a	842	CLA	C1A-C2A-CAA-CBA
19	a	843	CLA	CHA-CBD-CGD-O1D
19	a	843	CLA	CHA-CBD-CGD-O2D
19	a	856	CLA	C1A-C2A-CAA-CBA
19	a	856	CLA	C3A-C2A-CAA-CBA
19	a	856	CLA	CHA-CBD-CGD-O1D
19	a	856	CLA	CHA-CBD-CGD-O2D
19	b	3002	CLA	CHA-CBD-CGD-O1D
19	b	3002	CLA	CHA-CBD-CGD-O2D
19	b	3002	CLA	CBD-CGD-O2D-CED
19	b	3003	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	b	3003	CLA	CBD-CGD-O2D-CED
19	b	3003	CLA	C2-C3-C5-C6
19	b	3003	CLA	C4-C3-C5-C6
19	b	3004	CLA	C1A-C2A-CAA-CBA
19	b	3005	CLA	O1A-CGA-O2A-C1
19	b	3005	CLA	CHA-CBD-CGD-O1D
19	b	3005	CLA	CHA-CBD-CGD-O2D
19	b	3005	CLA	CAD-CBD-CGD-O1D
19	b	3007	CLA	C1A-C2A-CAA-CBA
19	b	3007	CLA	C3A-C2A-CAA-CBA
19	b	3010	CLA	CHA-CBD-CGD-O1D
19	b	3010	CLA	CHA-CBD-CGD-O2D
19	b	3011	CLA	C1A-C2A-CAA-CBA
19	b	3011	CLA	C3A-C2A-CAA-CBA
19	b	3014	CLA	C4-C3-C5-C6
19	b	3015	CLA	C1A-C2A-CAA-CBA
19	b	3016	CLA	C1A-C2A-CAA-CBA
19	b	3017	CLA	C2-C3-C5-C6
19	b	3017	CLA	C4-C3-C5-C6
19	b	3018	CLA	C1A-C2A-CAA-CBA
19	b	3018	CLA	C3A-C2A-CAA-CBA
19	b	3020	CLA	C1A-C2A-CAA-CBA
19	b	3020	CLA	C3A-C2A-CAA-CBA
19	b	3021	CLA	C1A-C2A-CAA-CBA
19	b	3021	CLA	C3A-C2A-CAA-CBA
19	b	3022	CLA	CBA-CGA-O2A-C1
19	b	3022	CLA	O1A-CGA-O2A-C1
19	b	3024	CLA	C1A-C2A-CAA-CBA
19	b	3024	CLA	C3A-C2A-CAA-CBA
19	b	3025	CLA	C1A-C2A-CAA-CBA
19	b	3025	CLA	C3A-C2A-CAA-CBA
19	b	3026	CLA	C1A-C2A-CAA-CBA
19	b	3026	CLA	C3A-C2A-CAA-CBA
19	b	3026	CLA	C2-C3-C5-C6
19	b	3026	CLA	C4-C3-C5-C6
19	b	3027	CLA	C1A-C2A-CAA-CBA
19	b	3027	CLA	C3A-C2A-CAA-CBA
19	b	3028	CLA	CHA-CBD-CGD-O1D
19	b	3028	CLA	CHA-CBD-CGD-O2D
19	b	3029	CLA	CAD-CBD-CGD-O2D
19	b	3029	CLA	C2-C3-C5-C6
19	b	3029	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	b	3030	CLA	C1A-C2A-CAA-CBA
19	b	3030	CLA	C3A-C2A-CAA-CBA
19	b	3030	CLA	CBD-CGD-O2D-CED
19	b	3033	CLA	C3A-C2A-CAA-CBA
19	b	3033	CLA	CBA-CGA-O2A-C1
19	b	3033	CLA	CHA-CBD-CGD-O1D
19	b	3033	CLA	CHA-CBD-CGD-O2D
19	b	3034	CLA	C1A-C2A-CAA-CBA
19	b	3034	CLA	C3A-C2A-CAA-CBA
19	b	3035	CLA	C1A-C2A-CAA-CBA
19	b	3035	CLA	C3A-C2A-CAA-CBA
19	b	3035	CLA	CBD-CGD-O2D-CED
19	b	3036	CLA	CHA-CBD-CGD-O1D
19	b	3036	CLA	CHA-CBD-CGD-O2D
19	b	3036	CLA	CAD-CBD-CGD-O1D
19	b	3037	CLA	C1A-C2A-CAA-CBA
19	b	3037	CLA	C3A-C2A-CAA-CBA
19	b	3037	CLA	CHA-CBD-CGD-O1D
19	b	3037	CLA	CHA-CBD-CGD-O2D
19	b	3039	CLA	C1A-C2A-CAA-CBA
19	b	3041	CLA	CHA-CBD-CGD-O1D
19	b	3041	CLA	CHA-CBD-CGD-O2D
19	b	3041	CLA	CAD-CBD-CGD-O1D
19	j	102	CLA	C1A-C2A-CAA-CBA
19	j	102	CLA	CBD-CGD-O2D-CED
19	k	4002	CLA	C3A-C2A-CAA-CBA
19	k	4003	CLA	CBD-CGD-O2D-CED
19	l	1501	CLA	C1A-C2A-CAA-CBA
19	l	1501	CLA	C3A-C2A-CAA-CBA
19	l	1501	CLA	C2A-CAA-CBA-CGA
19	l	1503	CLA	CBD-CGD-O2D-CED
19	A	403	CLA	C1A-C2A-CAA-CBA
19	A	403	CLA	C3A-C2A-CAA-CBA
19	A	403	CLA	CBA-CGA-O2A-C1
19	A	405	CLA	C1A-C2A-CAA-CBA
19	D	401	CLA	C1A-C2A-CAA-CBA
19	D	401	CLA	CHA-CBD-CGD-O1D
19	D	401	CLA	CHA-CBD-CGD-O2D
19	D	403	CLA	C3A-C2A-CAA-CBA
19	D	403	CLA	CHA-CBD-CGD-O1D
19	D	403	CLA	CHA-CBD-CGD-O2D
19	D	404	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	D	404	CLA	O1A-CGA-O2A-C1
21	a	845	BCR	C6-C7-C8-C9
21	a	845	BCR	C9-C10-C11-C12
21	a	845	BCR	C21-C22-C23-C24
21	a	846	BCR	C1-C6-C7-C8
21	a	848	BCR	C7-C8-C9-C34
21	a	848	BCR	C14-C15-C16-C17
21	a	848	BCR	C21-C22-C23-C24
21	a	848	BCR	C23-C24-C25-C30
21	a	849	BCR	C6-C7-C8-C9
21	b	3043	BCR	C6-C7-C8-C9
21	b	3043	BCR	C7-C8-C9-C10
21	b	3043	BCR	C7-C8-C9-C34
21	b	3043	BCR	C22-C23-C24-C25
21	b	3044	BCR	C7-C8-C9-C10
21	b	3044	BCR	C7-C8-C9-C34
21	b	3046	BCR	C22-C23-C24-C25
21	b	3047	BCR	C11-C12-C13-C35
21	b	3048	BCR	C6-C7-C8-C9
21	b	3048	BCR	C11-C12-C13-C35
21	b	3048	BCR	C16-C17-C18-C19
21	b	3048	BCR	C16-C17-C18-C36
21	b	3048	BCR	C20-C21-C22-C37
21	b	3048	BCR	C21-C22-C23-C24
21	b	3048	BCR	C37-C22-C23-C24
21	b	3048	BCR	C22-C23-C24-C25
21	f	202	BCR	C7-C8-C9-C34
21	f	202	BCR	C11-C12-C13-C35
21	f	202	BCR	C37-C22-C23-C24
21	i	101	BCR	C10-C11-C12-C13
21	i	101	BCR	C21-C22-C23-C24
21	j	101	BCR	C1-C6-C7-C8
21	j	101	BCR	C21-C22-C23-C24
21	k	4001	BCR	C7-C8-C9-C10
21	k	4001	BCR	C7-C8-C9-C34
21	k	4004	BCR	C17-C18-C19-C20
21	k	4004	BCR	C18-C19-C20-C21
21	k	4004	BCR	C22-C23-C24-C25
21	k	4004	BCR	C23-C24-C25-C30
21	l	1504	BCR	C7-C8-C9-C10
21	l	1504	BCR	C7-C8-C9-C34
21	l	1504	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
21	l	1504	BCR	C37-C22-C23-C24
21	l	1504	BCR	C23-C24-C25-C26
21	A	406	BCR	C1-C6-C7-C8
21	A	406	BCR	C6-C7-C8-C9
21	A	406	BCR	C22-C23-C24-C25
21	A	406	BCR	C23-C24-C25-C30
22	a	850	LHG	O1-C1-C2-C3
22	a	850	LHG	C3-O3-P-O4
22	a	850	LHG	C3-O3-P-O6
22	a	850	LHG	O10-C23-O8-C6
22	a	852	LHG	C3-O3-P-O5
22	a	852	LHG	C3-O3-P-O6
22	a	852	LHG	O7-C5-C6-O8
22	a	854	LHG	C4-O6-P-O5
22	a	854	LHG	O9-C7-O7-C5
22	a	854	LHG	C8-C7-O7-C5
22	b	3050	LHG	C3-O3-P-O4
22	b	3050	LHG	C4-O6-P-O5
22	f	206	LHG	O1-C1-C2-O2
22	f	206	LHG	C3-O3-P-O4
22	f	206	LHG	C4-O6-P-O3
22	f	206	LHG	O6-C4-C5-O7
23	a	851	LMG	C2-C1-O1-C7
23	a	851	LMG	O6-C1-O1-C7
23	a	851	LMG	O9-C10-O7-C8
23	b	3051	LMG	C2-C1-O1-C7
23	b	3051	LMG	O6-C1-O1-C7
26	b	3045	ECH	C5-C6-C7-C8
26	b	3045	ECH	C37-C22-C23-C24
26	b	3045	ECH	C22-C23-C24-C25
26	m	101	ECH	C21-C22-C23-C24
26	m	101	ECH	C37-C22-C23-C24
29	f	207	LMT	O5'-C1'-O1'-C1
31	A	404	PHO	O1A-CGA-O2A-C1
31	A	404	PHO	CBD-CGD-O2D-CED
19	a	811	CLA	O1D-CGD-O2D-CED
19	a	821	CLA	O1D-CGD-O2D-CED
19	b	3015	CLA	O1D-CGD-O2D-CED
19	b	3020	CLA	O1D-CGD-O2D-CED
19	l	1503	CLA	O1D-CGD-O2D-CED
19	a	802	CLA	O1D-CGD-O2D-CED
19	b	3003	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	a	811	CLA	CBD-CGD-O2D-CED
19	a	816	CLA	CBD-CGD-O2D-CED
19	a	841	CLA	CBD-CGD-O2D-CED
19	b	3009	CLA	CBD-CGD-O2D-CED
19	b	3014	CLA	CBD-CGD-O2D-CED
19	b	3015	CLA	CBD-CGD-O2D-CED
19	b	3020	CLA	CBD-CGD-O2D-CED
19	b	3027	CLA	CBD-CGD-O2D-CED
19	b	3034	CLA	CBD-CGD-O2D-CED
19	b	3036	CLA	CBD-CGD-O2D-CED
19	b	3039	CLA	CBD-CGD-O2D-CED
19	f	201	CLA	CBD-CGD-O2D-CED
19	j	103	CLA	CBD-CGD-O2D-CED
19	A	402	CLA	CBD-CGD-O2D-CED
19	a	835	CLA	O1A-CGA-O2A-C1
19	b	3006	CLA	O1A-CGA-O2A-C1
19	b	3011	CLA	O1A-CGA-O2A-C1
19	b	3021	CLA	O1A-CGA-O2A-C1
19	b	3031	CLA	O1A-CGA-O2A-C1
19	b	3033	CLA	O1A-CGA-O2A-C1
19	b	3034	CLA	O1A-CGA-O2A-C1
19	a	817	CLA	O1A-CGA-O2A-C1
19	A	403	CLA	O1A-CGA-O2A-C1
19	b	3030	CLA	O1D-CGD-O2D-CED
19	f	201	CLA	O1D-CGD-O2D-CED
19	k	4003	CLA	O1D-CGD-O2D-CED
19	a	823	CLA	O1D-CGD-O2D-CED
19	b	3002	CLA	O1D-CGD-O2D-CED
19	j	102	CLA	O1D-CGD-O2D-CED
19	a	835	CLA	CBA-CGA-O2A-C1
19	b	3012	CLA	CBA-CGA-O2A-C1
22	a	850	LHG	C24-C23-O8-C6
19	a	807	CLA	CBD-CGD-O2D-CED
19	a	810	CLA	CBD-CGD-O2D-CED
19	a	819	CLA	CBD-CGD-O2D-CED
19	a	855	CLA	CBD-CGD-O2D-CED
19	b	3008	CLA	CBD-CGD-O2D-CED
19	b	3023	CLA	CBD-CGD-O2D-CED
19	b	3028	CLA	CBD-CGD-O2D-CED
19	b	3041	CLA	CBD-CGD-O2D-CED
19	f	203	CLA	CBD-CGD-O2D-CED
19	f	204	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	D	401	CLA	CBD-CGD-O2D-CED
19	D	403	CLA	CBD-CGD-O2D-CED
19	a	802	CLA	O1A-CGA-O2A-C1
19	a	813	CLA	O1A-CGA-O2A-C1
19	a	820	CLA	O1A-CGA-O2A-C1
19	a	821	CLA	O1A-CGA-O2A-C1
19	a	838	CLA	O1A-CGA-O2A-C1
19	b	3003	CLA	O1A-CGA-O2A-C1
19	b	3012	CLA	O1A-CGA-O2A-C1
19	b	3024	CLA	O1A-CGA-O2A-C1
19	b	3038	CLA	O1A-CGA-O2A-C1
19	b	3039	CLA	O1A-CGA-O2A-C1
19	l	1501	CLA	O1A-CGA-O2A-C1
19	l	1502	CLA	O1A-CGA-O2A-C1
19	l	1503	CLA	O1A-CGA-O2A-C1
19	A	405	CLA	O1A-CGA-O2A-C1
22	f	206	LHG	O10-C23-O8-C6
23	a	853	LMG	O10-C28-O8-C9
31	A	404	PHO	O1D-CGD-O2D-CED
19	b	3035	CLA	O1D-CGD-O2D-CED
19	a	824	CLA	CBD-CGD-O2D-CED
19	a	835	CLA	CBD-CGD-O2D-CED
22	f	206	LHG	O9-C7-O7-C5
19	a	855	CLA	O1A-CGA-O2A-C1
19	k	4002	CLA	CBA-CGA-O2A-C1
19	b	3041	CLA	O1A-CGA-O2A-C1
19	k	4002	CLA	O1A-CGA-O2A-C1
19	a	809	CLA	C3-C5-C6-C7
19	a	818	CLA	C3-C5-C6-C7
19	a	824	CLA	C3-C5-C6-C7
19	a	826	CLA	C3-C5-C6-C7
19	a	856	CLA	C3-C5-C6-C7
19	b	3007	CLA	C3-C5-C6-C7
19	b	3013	CLA	C3-C5-C6-C7
19	b	3017	CLA	C3-C5-C6-C7
19	b	3033	CLA	C3-C5-C6-C7
19	b	3039	CLA	C3-C5-C6-C7
19	a	802	CLA	CBA-CGA-O2A-C1
19	a	819	CLA	CBA-CGA-O2A-C1
19	a	820	CLA	CBA-CGA-O2A-C1
19	a	825	CLA	CBA-CGA-O2A-C1
19	a	828	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	a	839	CLA	CBA-CGA-O2A-C1
19	a	856	CLA	CBA-CGA-O2A-C1
19	b	3005	CLA	CBA-CGA-O2A-C1
19	b	3006	CLA	CBA-CGA-O2A-C1
19	b	3011	CLA	CBA-CGA-O2A-C1
19	b	3021	CLA	CBA-CGA-O2A-C1
19	b	3031	CLA	CBA-CGA-O2A-C1
19	b	3034	CLA	CBA-CGA-O2A-C1
19	b	3037	CLA	CBA-CGA-O2A-C1
19	j	102	CLA	CBA-CGA-O2A-C1
19	l	1501	CLA	CBA-CGA-O2A-C1
19	A	402	CLA	CBA-CGA-O2A-C1
19	A	405	CLA	CBA-CGA-O2A-C1
31	A	404	PHO	CBA-CGA-O2A-C1
23	a	851	LMG	C11-C10-O7-C8
19	b	3027	CLA	O1D-CGD-O2D-CED
19	j	103	CLA	O1D-CGD-O2D-CED
19	A	402	CLA	O1D-CGD-O2D-CED
19	a	843	CLA	O1A-CGA-O2A-C1
29	f	207	LMT	O5'-C5'-C6'-O6'
19	b	3041	CLA	CBA-CGA-O2A-C1
19	a	831	CLA	C4-C3-C5-C6
19	b	3007	CLA	C4-C3-C5-C6
19	b	3015	CLA	C4-C3-C5-C6
19	a	802	CLA	C2-C3-C5-C6
19	a	840	CLA	C2-C3-C5-C6
19	b	3014	CLA	C2-C3-C5-C6
19	a	832	CLA	CBD-CGD-O2D-CED
19	b	3040	CLA	CBD-CGD-O2D-CED
19	a	809	CLA	C2A-CAA-CBA-CGA
19	a	815	CLA	C2A-CAA-CBA-CGA
19	a	828	CLA	C2A-CAA-CBA-CGA
19	a	837	CLA	C2A-CAA-CBA-CGA
19	a	842	CLA	C2A-CAA-CBA-CGA
19	a	843	CLA	C2A-CAA-CBA-CGA
19	b	3010	CLA	C2A-CAA-CBA-CGA
19	b	3013	CLA	C2A-CAA-CBA-CGA
19	b	3028	CLA	C2A-CAA-CBA-CGA
19	b	3041	CLA	C2A-CAA-CBA-CGA
19	f	204	CLA	C2A-CAA-CBA-CGA
18	a	801	CL0	O1A-CGA-O2A-C1
19	a	808	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	a	827	CLA	C3-C5-C6-C7
19	a	831	CLA	C3-C5-C6-C7
19	a	833	CLA	C3-C5-C6-C7
19	a	841	CLA	C3-C5-C6-C7
19	a	858	CLA	C3-C5-C6-C7
19	b	3006	CLA	C3-C5-C6-C7
31	D	402	PHO	C3-C5-C6-C7
19	a	804	CLA	CBA-CGA-O2A-C1
19	a	808	CLA	CBA-CGA-O2A-C1
19	a	812	CLA	CBA-CGA-O2A-C1
19	a	813	CLA	CBA-CGA-O2A-C1
19	a	821	CLA	CBA-CGA-O2A-C1
19	a	824	CLA	CBA-CGA-O2A-C1
19	a	830	CLA	CBA-CGA-O2A-C1
19	a	838	CLA	CBA-CGA-O2A-C1
19	a	843	CLA	CBA-CGA-O2A-C1
19	a	855	CLA	CBA-CGA-O2A-C1
19	b	3003	CLA	CBA-CGA-O2A-C1
19	b	3007	CLA	CBA-CGA-O2A-C1
19	b	3016	CLA	CBA-CGA-O2A-C1
19	b	3024	CLA	CBA-CGA-O2A-C1
19	b	3030	CLA	CBA-CGA-O2A-C1
19	b	3038	CLA	CBA-CGA-O2A-C1
19	b	3039	CLA	CBA-CGA-O2A-C1
19	f	201	CLA	CBA-CGA-O2A-C1
19	f	203	CLA	CBA-CGA-O2A-C1
19	f	204	CLA	CBA-CGA-O2A-C1
19	l	1502	CLA	CBA-CGA-O2A-C1
19	l	1503	CLA	CBA-CGA-O2A-C1
22	f	206	LHG	C24-C23-O8-C6
23	a	853	LMG	C29-C28-O8-C9
19	b	3013	CLA	CBD-CGD-O2D-CED
19	l	1501	CLA	CBD-CGD-O2D-CED
19	b	3036	CLA	O1D-CGD-O2D-CED
19	a	804	CLA	O1A-CGA-O2A-C1
19	a	811	CLA	O1A-CGA-O2A-C1
19	a	812	CLA	O1A-CGA-O2A-C1
19	a	819	CLA	O1A-CGA-O2A-C1
19	a	823	CLA	O1A-CGA-O2A-C1
19	a	824	CLA	O1A-CGA-O2A-C1
19	a	825	CLA	O1A-CGA-O2A-C1
19	a	828	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	a	839	CLA	O1A-CGA-O2A-C1
19	a	856	CLA	O1A-CGA-O2A-C1
19	b	3002	CLA	O1A-CGA-O2A-C1
19	b	3017	CLA	O1A-CGA-O2A-C1
19	b	3036	CLA	O1A-CGA-O2A-C1
19	b	3037	CLA	O1A-CGA-O2A-C1
19	f	201	CLA	O1A-CGA-O2A-C1
19	f	203	CLA	O1A-CGA-O2A-C1
19	j	102	CLA	O1A-CGA-O2A-C1
19	A	402	CLA	O1A-CGA-O2A-C1
19	a	816	CLA	O1D-CGD-O2D-CED
19	b	3034	CLA	O1D-CGD-O2D-CED
23	a	851	LMG	O6-C5-C6-O5
19	a	831	CLA	CBD-CGD-O2D-CED
19	D	404	CLA	CBD-CGD-O2D-CED
19	b	3009	CLA	O1D-CGD-O2D-CED
22	a	854	LHG	O2-C2-C3-O3
19	a	819	CLA	C3-C5-C6-C7
19	a	835	CLA	C3-C5-C6-C7
19	b	3004	CLA	C3-C5-C6-C7
19	a	811	CLA	CBA-CGA-O2A-C1
19	a	815	CLA	CBA-CGA-O2A-C1
19	a	822	CLA	CBA-CGA-O2A-C1
19	a	831	CLA	CBA-CGA-O2A-C1
19	a	832	CLA	CBA-CGA-O2A-C1
19	a	837	CLA	CBA-CGA-O2A-C1
19	a	858	CLA	CBA-CGA-O2A-C1
19	b	3027	CLA	CBA-CGA-O2A-C1
19	a	830	CLA	O1A-CGA-O2A-C1
19	b	3007	CLA	O1A-CGA-O2A-C1
19	b	3027	CLA	O1A-CGA-O2A-C1
29	f	207	LMT	C4B-C5B-C6B-O6B
19	b	3014	CLA	O1D-CGD-O2D-CED
19	a	816	CLA	CBA-CGA-O2A-C1
19	a	803	CLA	CBD-CGD-O2D-CED
19	a	814	CLA	CBD-CGD-O2D-CED
19	a	817	CLA	CBD-CGD-O2D-CED
29	f	207	LMT	O5B-C5B-C6B-O6B
22	b	3050	LHG	C32-C33-C34-C35
19	A	403	CLA	CBD-CGD-O2D-CED
19	a	803	CLA	C3-C5-C6-C7
19	b	3037	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	a	801	CL0	CBA-CGA-O2A-C1
19	a	823	CLA	CBA-CGA-O2A-C1
19	b	3002	CLA	CBA-CGA-O2A-C1
19	b	3017	CLA	CBA-CGA-O2A-C1
19	b	3028	CLA	CBA-CGA-O2A-C1
19	b	3036	CLA	CBA-CGA-O2A-C1
19	b	3039	CLA	O1D-CGD-O2D-CED
23	b	3049	LMG	O6-C5-C6-O5
22	a	852	LHG	C29-C30-C31-C32
19	a	815	CLA	O1A-CGA-O2A-C1
19	a	831	CLA	O1A-CGA-O2A-C1
19	b	3016	CLA	O1A-CGA-O2A-C1
19	b	3030	CLA	O1A-CGA-O2A-C1
19	f	204	CLA	O1A-CGA-O2A-C1
19	l	1503	CLA	C3-C5-C6-C7
19	a	856	CLA	C4-C3-C5-C6
19	b	3037	CLA	C4-C3-C5-C6
19	f	201	CLA	C4-C3-C5-C6
19	a	856	CLA	C2-C3-C5-C6
19	b	3037	CLA	C2-C3-C5-C6
19	f	201	CLA	C2-C3-C5-C6
19	b	3033	CLA	CBD-CGD-O2D-CED
19	a	802	CLA	C2A-CAA-CBA-CGA
19	a	811	CLA	C2A-CAA-CBA-CGA
19	a	825	CLA	C2A-CAA-CBA-CGA
19	a	822	CLA	O1A-CGA-O2A-C1
19	a	837	CLA	O1A-CGA-O2A-C1
19	a	858	CLA	O1A-CGA-O2A-C1
19	b	3028	CLA	O1A-CGA-O2A-C1
23	a	851	LMG	O10-C28-O8-C9
29	f	207	LMT	C4'-C5'-C6'-O6'
19	b	3010	CLA	CBA-CGA-O2A-C1
19	b	3029	CLA	CBA-CGA-O2A-C1
19	b	3035	CLA	CBA-CGA-O2A-C1
23	a	851	LMG	C4-C5-C6-O5
19	a	819	CLA	O1D-CGD-O2D-CED
19	a	841	CLA	O1D-CGD-O2D-CED
19	D	403	CLA	O1D-CGD-O2D-CED
19	a	832	CLA	O1A-CGA-O2A-C1
19	a	855	CLA	O1D-CGD-O2D-CED
19	b	3008	CLA	O1D-CGD-O2D-CED
19	a	841	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	b	3029	CLA	O1A-CGA-O2A-C1
19	b	3035	CLA	O1A-CGA-O2A-C1
19	f	201	CLA	C3-C5-C6-C7
19	a	807	CLA	O1D-CGD-O2D-CED
19	a	809	CLA	CBA-CGA-O2A-C1
19	a	826	CLA	CBA-CGA-O2A-C1
19	a	833	CLA	CBA-CGA-O2A-C1
19	a	841	CLA	CBA-CGA-O2A-C1
19	a	842	CLA	CBA-CGA-O2A-C1
19	b	3032	CLA	CBA-CGA-O2A-C1
22	a	852	LHG	C24-C23-O8-C6
23	a	851	LMG	C29-C28-O8-C9
23	b	3051	LMG	C29-C28-O8-C9
19	b	3013	CLA	C5-C6-C7-C8
19	a	837	CLA	C5-C6-C7-C8
19	D	401	CLA	O1D-CGD-O2D-CED
23	b	3049	LMG	C4-C5-C6-O5
19	a	809	CLA	C15-C16-C17-C18
19	a	829	CLA	C10-C11-C12-C13
22	b	3050	LHG	O2-C2-C3-O3
22	a	852	LHG	C7-C8-C9-C10
19	a	831	CLA	C2-C3-C5-C6
19	b	3007	CLA	C2-C3-C5-C6
19	b	3015	CLA	C2-C3-C5-C6
19	a	808	CLA	C6-C7-C8-C9
19	a	818	CLA	C11-C10-C8-C9
19	a	826	CLA	C14-C13-C15-C16
19	a	842	CLA	C11-C12-C13-C14
19	b	3002	CLA	C11-C12-C13-C14
19	b	3003	CLA	C6-C7-C8-C9
19	b	3003	CLA	C11-C12-C13-C14
19	b	3007	CLA	C6-C7-C8-C9
19	b	3029	CLA	C11-C12-C13-C14
19	l	1502	CLA	C6-C7-C8-C9
19	b	3041	CLA	O1D-CGD-O2D-CED
19	f	204	CLA	O1D-CGD-O2D-CED
19	a	816	CLA	C2A-CAA-CBA-CGA
19	l	1503	CLA	C2A-CAA-CBA-CGA
21	a	845	BCR	C7-C8-C9-C34
21	a	845	BCR	C11-C12-C13-C35
21	a	847	BCR	C7-C8-C9-C34
21	a	845	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
26	b	3045	ECH	C21-C22-C23-C24
19	a	832	CLA	C2C-C3C-CAC-CBC
19	a	833	CLA	O1A-CGA-O2A-C1
19	a	843	CLA	C5-C6-C7-C8
19	a	810	CLA	O1D-CGD-O2D-CED
19	b	3023	CLA	O1D-CGD-O2D-CED
19	a	816	CLA	O1A-CGA-O2A-C1
19	b	3028	CLA	O1D-CGD-O2D-CED
19	f	203	CLA	O1D-CGD-O2D-CED
19	a	805	CLA	CBA-CGA-O2A-C1
19	D	401	CLA	CBA-CGA-O2A-C1
32	F	101	HEM	C2A-CAA-CBA-CGA
19	a	809	CLA	C8-C10-C11-C12
19	a	815	CLA	C5-C6-C7-C8
19	b	3013	CLA	C8-C10-C11-C12
19	b	3020	CLA	C10-C11-C12-C13
19	f	201	CLA	C8-C10-C11-C12
19	f	201	CLA	C15-C16-C17-C18
19	l	1502	CLA	C10-C11-C12-C13
19	A	402	CLA	C15-C16-C17-C18
19	a	808	CLA	C8-C10-C11-C12
19	a	812	CLA	C13-C15-C16-C17
19	a	815	CLA	C13-C15-C16-C17
19	a	819	CLA	C13-C15-C16-C17
19	a	822	CLA	C15-C16-C17-C18
19	a	824	CLA	C5-C6-C7-C8
19	a	826	CLA	C5-C6-C7-C8
19	a	828	CLA	C15-C16-C17-C18
19	a	834	CLA	C5-C6-C7-C8
19	a	837	CLA	C8-C10-C11-C12
19	a	839	CLA	C8-C10-C11-C12
19	b	3004	CLA	C10-C11-C12-C13
19	b	3005	CLA	C13-C15-C16-C17
19	b	3005	CLA	C15-C16-C17-C18
19	b	3026	CLA	C8-C10-C11-C12
19	b	3029	CLA	C5-C6-C7-C8
19	A	402	CLA	C13-C15-C16-C17
22	a	852	LHG	C23-C24-C25-C26
22	f	206	LHG	C7-C8-C9-C10
19	a	805	CLA	C5-C6-C7-C8
19	a	822	CLA	C8-C10-C11-C12
19	b	3019	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
20	a	844	PQN	C18-C20-C21-C22
19	a	855	CLA	C2-C1-O2A-CGA
19	b	3006	CLA	C2-C1-O2A-CGA
19	b	3021	CLA	C2-C1-O2A-CGA
19	l	1501	CLA	C2-C1-O2A-CGA
19	a	803	CLA	C10-C11-C12-C13
19	a	815	CLA	C15-C16-C17-C18
19	a	834	CLA	C13-C15-C16-C17
19	b	3039	CLA	C8-C10-C11-C12
22	b	3050	LHG	C23-C24-C25-C26
19	a	830	CLA	CBD-CGD-O2D-CED
19	a	802	CLA	C15-C16-C17-C18
19	a	840	CLA	C5-C6-C7-C8
19	a	840	CLA	C15-C16-C17-C18
19	b	3020	CLA	C15-C16-C17-C18
19	a	805	CLA	C6-C7-C8-C10
19	a	814	CLA	C6-C7-C8-C10
19	a	821	CLA	C6-C7-C8-C10
19	a	822	CLA	C12-C13-C15-C16
19	a	826	CLA	C6-C7-C8-C10
19	a	834	CLA	C6-C7-C8-C10
19	b	3019	CLA	C6-C7-C8-C10
19	b	3024	CLA	C11-C12-C13-C15
19	a	840	CLA	C3-C5-C6-C7
19	a	809	CLA	O1A-CGA-O2A-C1
19	a	842	CLA	O1A-CGA-O2A-C1
19	b	3015	CLA	CBA-CGA-O2A-C1
19	k	4003	CLA	C2A-CAA-CBA-CGA
19	D	404	CLA	C2A-CAA-CBA-CGA
19	a	824	CLA	O1D-CGD-O2D-CED
19	a	835	CLA	O1D-CGD-O2D-CED
19	b	3006	CLA	C15-C16-C17-C18
19	b	3027	CLA	C8-C10-C11-C12
21	a	846	BCR	C6-C7-C8-C9
21	j	101	BCR	C6-C7-C8-C9
19	a	826	CLA	O1A-CGA-O2A-C1
19	b	3032	CLA	O1A-CGA-O2A-C1
19	a	830	CLA	C13-C15-C16-C17
19	a	858	CLA	C10-C11-C12-C13
19	f	201	CLA	C13-C15-C16-C17
21	a	845	BCR	C18-C19-C20-C21
21	b	3048	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	b	3048	BCR	C18-C19-C20-C21
21	f	202	BCR	C10-C11-C12-C13
21	k	4001	BCR	C18-C19-C20-C21
22	a	852	LHG	O2-C2-C3-O3
19	a	802	CLA	C3-C5-C6-C7
19	b	3008	CLA	C10-C11-C12-C13
19	b	3018	CLA	C10-C11-C12-C13
19	a	805	CLA	O1A-CGA-O2A-C1
19	b	3010	CLA	O1A-CGA-O2A-C1
19	a	802	CLA	C5-C6-C7-C8
19	a	824	CLA	C8-C10-C11-C12
19	b	3014	CLA	C5-C6-C7-C8
19	b	3033	CLA	C5-C6-C7-C8
22	f	206	LHG	C8-C7-O7-C5
22	b	3050	LHG	C30-C31-C32-C33
19	a	808	CLA	C5-C6-C7-C8
19	a	809	CLA	C10-C11-C12-C13
19	a	822	CLA	C10-C11-C12-C13
19	a	840	CLA	C8-C10-C11-C12
19	b	3017	CLA	C15-C16-C17-C18
22	a	854	LHG	C4-O6-P-O3
22	b	3050	LHG	C3-O3-P-O6
22	f	206	LHG	C3-O3-P-O6
28	b	3053	ZEX	C25-C26-C27-C28
28	f	205	ZEX	C25-C26-C27-C28
22	a	852	LHG	C1-C2-C3-O3
19	a	825	CLA	C4-C3-C5-C6
19	b	3039	CLA	C10-C11-C12-C13
22	a	854	LHG	C28-C29-C30-C31
19	a	804	CLA	C2A-CAA-CBA-CGA
19	a	814	CLA	C2A-CAA-CBA-CGA
19	a	821	CLA	C2A-CAA-CBA-CGA
19	b	3017	CLA	C2A-CAA-CBA-CGA
19	a	839	CLA	C16-C17-C18-C20
19	b	3023	CLA	CBA-CGA-O2A-C1
21	a	849	BCR	C9-C10-C11-C12
21	b	3044	BCR	C19-C20-C21-C22
22	a	854	LHG	C23-C24-C25-C26
21	a	847	BCR	C16-C17-C18-C36
21	a	848	BCR	C20-C21-C22-C37
21	b	3044	BCR	C16-C17-C18-C36
21	b	3046	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
21	b	3047	BCR	C20-C21-C22-C37
21	i	101	BCR	C20-C21-C22-C37
22	a	850	LHG	C29-C30-C31-C32
22	a	852	LHG	C28-C29-C30-C31
23	a	851	LMG	C18-C19-C20-C21
23	b	3049	LMG	C33-C34-C35-C36
23	b	3049	LMG	C37-C38-C39-C40
23	b	3051	LMG	C15-C16-C17-C18
19	a	802	CLA	C16-C17-C18-C19
19	b	3014	CLA	C16-C17-C18-C20
19	a	814	CLA	CBA-CGA-O2A-C1
22	a	850	LHG	C32-C33-C34-C35
23	a	853	LMG	C12-C13-C14-C15
23	b	3051	LMG	C14-C15-C16-C17
29	f	207	LMT	C3-C4-C5-C6
22	f	206	LHG	C6-C5-O7-C7
19	b	3040	CLA	O1D-CGD-O2D-CED
22	a	850	LHG	C15-C16-C17-C18
22	a	852	LHG	C32-C33-C34-C35
23	b	3051	LMG	C18-C19-C20-C21
19	a	831	CLA	O1D-CGD-O2D-CED
19	l	1501	CLA	O1D-CGD-O2D-CED
22	a	854	LHG	C32-C33-C34-C35
23	a	853	LMG	C32-C33-C34-C35
22	f	206	LHG	C29-C30-C31-C32
18	a	801	CL0	C3-C5-C6-C7
23	a	851	LMG	C28-C29-C30-C31
23	b	3051	LMG	C28-C29-C30-C31
19	a	832	CLA	O1D-CGD-O2D-CED
21	b	3048	BCR	C11-C10-C9-C8
21	b	3048	BCR	C20-C21-C22-C23
21	f	202	BCR	C12-C13-C14-C15
23	b	3051	LMG	C31-C32-C33-C34
19	D	401	CLA	O1A-CGA-O2A-C1
19	a	825	CLA	C11-C12-C13-C14
19	b	3019	CLA	C11-C12-C13-C15
31	D	402	PHO	C16-C17-C18-C19
19	a	827	CLA	C4-C3-C5-C6
22	f	206	LHG	C34-C35-C36-C37
19	a	809	CLA	C11-C12-C13-C14
19	a	814	CLA	C11-C12-C13-C14
19	a	836	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	b	3019	CLA	C6-C7-C8-C9
19	l	1502	CLA	C11-C12-C13-C14
22	a	850	LHG	C28-C29-C30-C31
22	f	206	LHG	C27-C28-C29-C30
23	a	851	LMG	C32-C33-C34-C35
23	b	3051	LMG	C12-C13-C14-C15
19	a	805	CLA	C2A-CAA-CBA-CGA
19	b	3029	CLA	C2A-CAA-CBA-CGA
19	b	3032	CLA	C2A-CAA-CBA-CGA
19	b	3015	CLA	O1A-CGA-O2A-C1
22	a	852	LHG	O1-C1-C2-C3
22	f	206	LHG	O1-C1-C2-C3
19	b	3018	CLA	C3-C5-C6-C7
19	a	858	CLA	C5-C6-C7-C8
22	a	854	LHG	C7-C8-C9-C10
19	b	3013	CLA	O1D-CGD-O2D-CED
22	a	850	LHG	C24-C25-C26-C27
22	a	854	LHG	C11-C10-C9-C8
22	a	854	LHG	C16-C17-C18-C19
23	b	3051	LMG	C41-C42-C43-C44
19	a	805	CLA	C16-C17-C18-C19
19	a	805	CLA	C16-C17-C18-C20
19	a	822	CLA	C16-C17-C18-C19
19	a	822	CLA	C16-C17-C18-C20
19	a	825	CLA	C11-C12-C13-C15
19	a	833	CLA	C11-C12-C13-C15
19	b	3039	CLA	C16-C17-C18-C19
19	b	3040	CLA	C16-C17-C18-C19
18	a	801	CL0	C5-C6-C7-C8
19	b	3017	CLA	C5-C6-C7-C8
23	b	3049	LMG	C32-C33-C34-C35
19	b	3003	CLA	C2C-C3C-CAC-CBC
22	a	854	LHG	C14-C15-C16-C17
23	b	3049	LMG	C34-C35-C36-C37
23	b	3051	LMG	C17-C18-C19-C20
19	b	3013	CLA	C10-C11-C12-C13
19	D	401	CLA	C8-C10-C11-C12
19	b	3023	CLA	O1A-CGA-O2A-C1
22	a	850	LHG	C9-C10-C11-C12
22	b	3050	LHG	C27-C28-C29-C30
23	a	851	LMG	C37-C38-C39-C40
19	D	404	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	a	818	CLA	C3A-C2A-CAA-CBA
19	a	824	CLA	C3A-C2A-CAA-CBA
19	a	829	CLA	C3A-C2A-CAA-CBA
19	a	838	CLA	C3A-C2A-CAA-CBA
19	b	3005	CLA	C3A-C2A-CAA-CBA
19	b	3015	CLA	C3A-C2A-CAA-CBA
19	b	3016	CLA	C3A-C2A-CAA-CBA
19	b	3039	CLA	C3A-C2A-CAA-CBA
19	b	3041	CLA	C3A-C2A-CAA-CBA
19	A	402	CLA	C3A-C2A-CAA-CBA
19	D	401	CLA	C3A-C2A-CAA-CBA
31	D	402	PHO	C3A-C2A-CAA-CBA
19	b	3003	CLA	C10-C11-C12-C13
29	f	207	LMT	C2-C1-O1'-C1'
19	a	833	CLA	C11-C12-C13-C14
19	a	839	CLA	C16-C17-C18-C19
19	b	3014	CLA	C16-C17-C18-C19
19	b	3040	CLA	C16-C17-C18-C20
22	a	852	LHG	C34-C35-C36-C37
19	b	3003	CLA	O2A-C1-C2-C3
19	a	836	CLA	C3-C5-C6-C7
22	a	850	LHG	C23-C24-C25-C26
23	b	3051	LMG	C34-C35-C36-C37
19	b	3032	CLA	C4-C3-C5-C6
19	a	821	CLA	C2-C3-C5-C6
19	a	827	CLA	C2-C3-C5-C6
19	b	3005	CLA	CBD-CGD-O2D-CED
22	a	850	LHG	O1-C1-C2-O2
19	a	832	CLA	C4C-C3C-CAC-CBC
19	a	814	CLA	O1A-CGA-O2A-C1
19	b	3019	CLA	C11-C12-C13-C14
19	b	3039	CLA	C16-C17-C18-C20
19	a	804	CLA	C15-C16-C17-C18
19	a	812	CLA	C8-C10-C11-C12
22	f	206	LHG	C30-C31-C32-C33
18	a	801	CL0	C2-C1-O2A-CGA
19	a	811	CLA	C2-C1-O2A-CGA
19	a	819	CLA	C2-C1-O2A-CGA
19	a	823	CLA	C2-C1-O2A-CGA
19	a	824	CLA	C2-C1-O2A-CGA
19	a	830	CLA	C2-C1-O2A-CGA
19	a	856	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
19	b	3007	CLA	C2-C1-O2A-CGA
19	b	3037	CLA	C2-C1-O2A-CGA
19	b	3038	CLA	C2-C1-O2A-CGA
19	b	3024	CLA	C5-C6-C7-C8
23	b	3049	LMG	C19-C20-C21-C22
23	b	3049	LMG	C23-C24-C25-C26
21	a	846	BCR	C5-C6-C7-C8
21	a	848	BCR	C23-C24-C25-C26
21	b	3043	BCR	C1-C6-C7-C8
21	b	3043	BCR	C5-C6-C7-C8
21	b	3044	BCR	C1-C6-C7-C8
21	b	3044	BCR	C5-C6-C7-C8
21	j	101	BCR	C5-C6-C7-C8
21	j	104	BCR	C1-C6-C7-C8
21	j	104	BCR	C5-C6-C7-C8
21	l	1504	BCR	C23-C24-C25-C30
21	A	406	BCR	C5-C6-C7-C8
21	A	406	BCR	C23-C24-C25-C26
26	b	3045	ECH	C1-C6-C7-C8
27	b	3052	EQ3	C23-C24-C25-C26
23	a	851	LMG	C31-C32-C33-C34
23	b	3049	LMG	C18-C19-C20-C21
19	a	840	CLA	CBA-CGA-O2A-C1
23	b	3051	LMG	C11-C10-O7-C8
23	a	851	LMG	C15-C16-C17-C18
19	b	3004	CLA	CBD-CGD-O2D-CED
23	a	851	LMG	C30-C31-C32-C33
19	a	821	CLA	C10-C11-C12-C13
22	a	850	LHG	C26-C27-C28-C29
19	a	819	CLA	C4-C3-C5-C6
19	a	828	CLA	C4-C3-C5-C6
19	a	803	CLA	O1D-CGD-O2D-CED
18	a	801	CL0	C12-C13-C15-C16
19	a	806	CLA	C11-C12-C13-C15
19	a	813	CLA	C11-C10-C8-C7
19	a	814	CLA	C11-C12-C13-C15
19	a	818	CLA	C11-C10-C8-C7
19	a	824	CLA	C12-C13-C15-C16
19	a	825	CLA	C6-C7-C8-C10
19	a	828	CLA	C2-C3-C5-C6
19	a	830	CLA	C12-C13-C15-C16
19	a	834	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	a	836	CLA	C11-C12-C13-C15
19	b	3003	CLA	C11-C10-C8-C7
19	b	3003	CLA	C11-C12-C13-C15
19	b	3010	CLA	C6-C7-C8-C10
19	b	3013	CLA	C12-C13-C15-C16
19	b	3018	CLA	C11-C10-C8-C7
19	b	3020	CLA	C6-C7-C8-C10
19	b	3029	CLA	C11-C12-C13-C15
19	b	3032	CLA	C2-C3-C5-C6
19	l	1502	CLA	C11-C12-C13-C15
19	A	402	CLA	C6-C7-C8-C10
19	A	402	CLA	C12-C13-C15-C16
19	a	840	CLA	O1A-CGA-O2A-C1
19	a	827	CLA	C5-C6-C7-C8
19	a	842	CLA	C8-C10-C11-C12
19	b	3026	CLA	C5-C6-C7-C8
19	b	3011	CLA	CBD-CGD-O2D-CED
31	D	402	PHO	C16-C17-C18-C20
19	a	814	CLA	O1D-CGD-O2D-CED
19	a	817	CLA	O1D-CGD-O2D-CED
23	a	851	LMG	C10-C11-C12-C13
19	a	803	CLA	C2A-CAA-CBA-CGA
19	a	808	CLA	C2A-CAA-CBA-CGA
19	l	1502	CLA	C2A-CAA-CBA-CGA
19	a	830	CLA	C5-C6-C7-C8
19	b	3033	CLA	O1D-CGD-O2D-CED
22	a	850	LHG	C7-C8-C9-C10
19	A	403	CLA	O1D-CGD-O2D-CED
23	a	853	LMG	C15-C16-C17-C18
23	b	3051	LMG	C30-C31-C32-C33
23	b	3051	LMG	C35-C36-C37-C38
21	b	3047	BCR	C6-C7-C8-C9
19	b	3021	CLA	C11-C12-C13-C14
19	b	3024	CLA	C15-C16-C17-C18
22	b	3050	LHG	C8-C7-O7-C5
23	a	851	LMG	C40-C41-C42-C43
19	b	3028	CLA	C8-C10-C11-C12
19	b	3025	CLA	CBD-CGD-O2D-CED
23	b	3049	LMG	C17-C18-C19-C20
29	f	207	LMT	C2'-C1'-O1'-C1
22	a	850	LHG	O7-C5-C6-O8
23	b	3049	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
19	a	808	CLA	C4-C3-C5-C6
19	a	821	CLA	C4-C3-C5-C6
19	a	823	CLA	C4-C3-C5-C6
19	a	834	CLA	C4-C3-C5-C6
19	a	813	CLA	C2-C3-C5-C6
19	a	802	CLA	C6-C7-C8-C9
19	a	806	CLA	C11-C12-C13-C14
19	a	807	CLA	C14-C13-C15-C16
19	a	808	CLA	C11-C10-C8-C9
19	a	823	CLA	C11-C10-C8-C9
19	a	824	CLA	C14-C13-C15-C16
19	a	825	CLA	C6-C7-C8-C9
19	a	830	CLA	C14-C13-C15-C16
19	a	832	CLA	C6-C7-C8-C9
19	a	837	CLA	C6-C7-C8-C9
19	a	839	CLA	C11-C10-C8-C9
19	a	840	CLA	C11-C10-C8-C9
19	a	842	CLA	C6-C7-C8-C9
19	b	3003	CLA	C11-C10-C8-C9
19	b	3013	CLA	C14-C13-C15-C16
19	A	402	CLA	C6-C7-C8-C9
19	a	813	CLA	C3-C5-C6-C7
19	a	855	CLA	C2A-CAA-CBA-CGA
19	b	3030	CLA	C2A-CAA-CBA-CGA
19	A	405	CLA	C2A-CAA-CBA-CGA
22	f	206	LHG	C15-C16-C17-C18
22	b	3050	LHG	C28-C29-C30-C31
21	f	202	BCR	C11-C12-C13-C14
19	a	806	CLA	C1A-C2A-CAA-CBA
19	a	809	CLA	C1A-C2A-CAA-CBA
19	a	812	CLA	C1A-C2A-CAA-CBA
19	a	815	CLA	C1A-C2A-CAA-CBA
19	a	832	CLA	C1A-C2A-CAA-CBA
19	a	835	CLA	C1A-C2A-CAA-CBA
19	b	3022	CLA	C1A-C2A-CAA-CBA
19	b	3033	CLA	C1A-C2A-CAA-CBA
19	b	3038	CLA	C1A-C2A-CAA-CBA
19	b	3041	CLA	C1A-C2A-CAA-CBA
19	j	103	CLA	C1A-C2A-CAA-CBA
19	k	4002	CLA	C1A-C2A-CAA-CBA
19	A	402	CLA	C1A-C2A-CAA-CBA
19	D	403	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	a	802	CLA	C16-C17-C18-C20
19	a	820	CLA	C16-C17-C18-C20
23	a	851	LMG	C16-C17-C18-C19
21	b	3048	BCR	C13-C14-C15-C16
19	a	828	CLA	C8-C10-C11-C12
23	b	3049	LMG	C28-C29-C30-C31
22	f	206	LHG	C2-C3-O3-P
19	a	856	CLA	C5-C6-C7-C8
19	b	3025	CLA	CBA-CGA-O2A-C1
22	b	3050	LHG	O6-C4-C5-C6
22	f	206	LHG	O6-C4-C5-C6
22	a	852	LHG	C27-C28-C29-C30
23	b	3049	LMG	C16-C17-C18-C19
23	b	3051	LMG	O6-C5-C6-O5
19	D	403	CLA	C4-C3-C5-C6
19	a	809	CLA	C5-C6-C7-C8
22	a	850	LHG	C8-C7-O7-C5
23	b	3051	LMG	C16-C17-C18-C19
18	a	801	CL0	C2A-CAA-CBA-CGA
22	a	852	LHG	C4-C5-C6-O8
22	a	854	LHG	C4-C5-C6-O8
23	a	853	LMG	O1-C7-C8-C9
23	b	3049	LMG	C30-C31-C32-C33
23	a	851	LMG	C19-C20-C21-C22
19	b	3031	CLA	CBD-CGD-O2D-CED
23	a	853	LMG	C16-C17-C18-C19
23	a	853	LMG	C34-C35-C36-C37
31	A	404	PHO	C5-C6-C7-C8
29	f	207	LMT	C5-C6-C7-C8
21	f	202	BCR	C35-C13-C14-C15
19	a	813	CLA	C4-C3-C5-C6
19	b	3004	CLA	C4-C3-C5-C6
19	a	814	CLA	C13-C15-C16-C17
19	a	804	CLA	C5-C6-C7-C8
19	a	814	CLA	C2-C1-O2A-CGA
19	b	3024	CLA	C2-C1-O2A-CGA
19	a	820	CLA	C16-C17-C18-C19
19	b	3021	CLA	C11-C12-C13-C15
19	b	3024	CLA	C10-C11-C12-C13
19	b	3025	CLA	O1A-CGA-O2A-C1
22	a	852	LHG	O10-C23-O8-C6
23	b	3051	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
22	a	852	LHG	C24-C25-C26-C27
23	b	3051	LMG	C21-C22-C23-C24
19	D	401	CLA	C10-C11-C12-C13
23	b	3051	LMG	C19-C20-C21-C22
31	D	402	PHO	CHA-CBD-CGD-O1D
31	D	402	PHO	CHA-CBD-CGD-O2D
23	b	3051	LMG	C32-C33-C34-C35
19	a	802	CLA	C6-C7-C8-C10
19	a	807	CLA	C12-C13-C15-C16
19	a	809	CLA	C6-C7-C8-C10
19	a	812	CLA	C11-C10-C8-C7
19	a	812	CLA	C11-C12-C13-C15
19	a	820	CLA	C11-C10-C8-C7
19	a	820	CLA	C11-C12-C13-C15
19	a	823	CLA	C11-C10-C8-C7
19	a	827	CLA	C11-C10-C8-C7
19	a	831	CLA	C6-C7-C8-C10
19	a	833	CLA	C11-C10-C8-C7
19	a	834	CLA	C11-C12-C13-C15
19	a	837	CLA	C6-C7-C8-C10
19	a	842	CLA	C6-C7-C8-C10
19	b	3002	CLA	C11-C12-C13-C15
19	b	3006	CLA	C12-C13-C15-C16
19	b	3009	CLA	C11-C12-C13-C15
19	b	3033	CLA	C6-C7-C8-C10
19	b	3040	CLA	C11-C12-C13-C15
19	f	201	CLA	C11-C12-C13-C15
19	l	1502	CLA	C6-C7-C8-C10
19	a	805	CLA	C6-C7-C8-C9
19	a	812	CLA	C11-C12-C13-C14
19	a	815	CLA	C6-C7-C8-C9
19	a	820	CLA	C11-C10-C8-C9
19	a	820	CLA	C11-C12-C13-C14
19	a	821	CLA	C11-C12-C13-C14
19	a	822	CLA	C14-C13-C15-C16
19	a	827	CLA	C11-C10-C8-C9
19	a	827	CLA	C14-C13-C15-C16
19	a	831	CLA	C6-C7-C8-C9
19	a	833	CLA	C11-C10-C8-C9
19	a	856	CLA	C6-C7-C8-C9
19	b	3002	CLA	C11-C10-C8-C9
19	b	3006	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	b	3014	CLA	C14-C13-C15-C16
19	b	3018	CLA	C6-C7-C8-C9
19	b	3018	CLA	C11-C10-C8-C9
19	b	3020	CLA	C11-C10-C8-C9
19	b	3023	CLA	C6-C7-C8-C9
19	b	3034	CLA	C11-C10-C8-C9
19	b	3040	CLA	C11-C12-C13-C14
19	f	201	CLA	C11-C12-C13-C14
19	a	836	CLA	CBD-CGD-O2D-CED
19	b	3015	CLA	C2C-C3C-CAC-CBC
23	b	3049	LMG	C39-C40-C41-C42
21	a	846	BCR	C37-C22-C23-C24
28	b	3053	ZEX	C27-C28-C29-C39
28	f	205	ZEX	C27-C28-C29-C39
19	a	836	CLA	C16-C17-C18-C20
21	b	3043	BCR	C21-C22-C23-C24
21	f	202	BCR	C21-C22-C23-C24
22	b	3050	LHG	C1-C2-C3-O3
19	b	3007	CLA	C5-C6-C7-C8
29	f	207	LMT	C4-C5-C6-C7
23	b	3051	LMG	C42-C43-C44-C45
19	a	858	CLA	C13-C15-C16-C17
19	a	819	CLA	C5-C6-C7-C8
19	a	814	CLA	C3-C5-C6-C7
19	b	3013	CLA	C4-C3-C5-C6
19	b	3033	CLA	C4-C3-C5-C6
19	b	3034	CLA	C4-C3-C5-C6
19	b	3004	CLA	C2-C3-C5-C6
19	b	3013	CLA	C2-C3-C5-C6
19	a	828	CLA	C10-C11-C12-C13
23	b	3049	LMG	C38-C39-C40-C41
19	a	842	CLA	C10-C11-C12-C13
19	b	3020	CLA	C5-C6-C7-C8
19	a	830	CLA	O1D-CGD-O2D-CED
19	a	803	CLA	C3A-C2A-CAA-CBA
19	a	812	CLA	C3A-C2A-CAA-CBA
19	a	842	CLA	C3A-C2A-CAA-CBA
19	b	3004	CLA	C3A-C2A-CAA-CBA
19	b	3012	CLA	C3A-C2A-CAA-CBA
19	j	102	CLA	C3A-C2A-CAA-CBA
19	A	405	CLA	C3A-C2A-CAA-CBA
22	a	854	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
19	a	841	CLA	C8-C10-C11-C12
19	a	812	CLA	C15-C16-C17-C18
23	b	3049	LMG	C7-C8-C9-O8
23	b	3051	LMG	C7-C8-C9-O8
19	a	856	CLA	O2A-C1-C2-C3
19	a	826	CLA	C8-C10-C11-C12
31	A	404	PHO	C3-C5-C6-C7
19	a	825	CLA	C2-C3-C5-C6
23	b	3049	LMG	C15-C16-C17-C18
19	b	3040	CLA	C15-C16-C17-C18
22	b	3050	LHG	O6-C4-C5-O7
19	a	836	CLA	C16-C17-C18-C19
19	a	826	CLA	C13-C15-C16-C17
23	b	3051	LMG	O1-C7-C8-O7
22	f	206	LHG	C31-C32-C33-C34
19	b	3026	CLA	C2-C1-O2A-CGA
19	b	3034	CLA	C2-C3-C5-C6
19	b	3002	CLA	C10-C11-C12-C13
19	a	807	CLA	C11-C12-C13-C14
19	a	809	CLA	C11-C10-C8-C9
19	a	822	CLA	C11-C12-C13-C14
19	a	825	CLA	C11-C10-C8-C9
19	a	858	CLA	C6-C7-C8-C9
19	b	3032	CLA	C14-C13-C15-C16
19	b	3037	CLA	C6-C7-C8-C9
23	b	3049	LMG	C31-C32-C33-C34
19	a	821	CLA	C5-C6-C7-C8
19	a	835	CLA	C13-C15-C16-C17
19	b	3034	CLA	C13-C15-C16-C17
28	b	3053	ZEX	C21-C26-C27-C28
28	f	205	ZEX	C21-C26-C27-C28
31	D	402	PHO	C1A-C2A-CAA-CBA
22	a	850	LHG	C18-C19-C20-C21
19	a	817	CLA	C2A-CAA-CBA-CGA
19	a	830	CLA	C16-C17-C18-C20
19	b	3005	CLA	C16-C17-C18-C20
21	a	845	BCR	C1-C6-C7-C8
21	a	845	BCR	C5-C6-C7-C8
21	a	848	BCR	C1-C6-C7-C8
21	b	3043	BCR	C23-C24-C25-C26
21	b	3043	BCR	C23-C24-C25-C30
21	b	3046	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
21	b	3046	BCR	C23-C24-C25-C30
21	f	202	BCR	C1-C6-C7-C8
21	f	202	BCR	C5-C6-C7-C8
21	j	104	BCR	C23-C24-C25-C26
21	j	104	BCR	C23-C24-C25-C30
21	k	4001	BCR	C5-C6-C7-C8
21	k	4001	BCR	C23-C24-C25-C26
21	k	4001	BCR	C23-C24-C25-C30
21	k	4004	BCR	C23-C24-C25-C26
21	l	1504	BCR	C1-C6-C7-C8
21	l	1504	BCR	C5-C6-C7-C8
19	a	805	CLA	C13-C15-C16-C17
19	a	825	CLA	C5-C6-C7-C8
19	b	3005	CLA	O1D-CGD-O2D-CED
19	b	3011	CLA	O1D-CGD-O2D-CED
21	a	849	BCR	C16-C17-C18-C36
21	b	3048	BCR	C17-C18-C19-C20
21	f	202	BCR	C7-C8-C9-C10
19	a	806	CLA	C13-C15-C16-C17
19	a	842	CLA	C13-C15-C16-C17
23	a	851	LMG	C42-C43-C44-C45
19	b	3004	CLA	O1D-CGD-O2D-CED
19	b	3008	CLA	C16-C17-C18-C20
19	b	3028	CLA	C16-C17-C18-C20
19	b	3025	CLA	O1D-CGD-O2D-CED
22	f	206	LHG	C32-C33-C34-C35
29	f	207	LMT	C11-C10-C9-C8
23	a	851	LMG	C34-C35-C36-C37
19	a	807	CLA	C11-C12-C13-C15
19	a	808	CLA	C6-C7-C8-C10
19	a	809	CLA	C11-C12-C13-C15
19	a	815	CLA	C6-C7-C8-C10
19	a	820	CLA	C6-C7-C8-C10
19	a	821	CLA	C11-C12-C13-C15
19	a	822	CLA	C11-C12-C13-C15
19	a	827	CLA	C12-C13-C15-C16
19	a	841	CLA	C6-C7-C8-C10
19	a	856	CLA	C6-C7-C8-C10
19	a	858	CLA	C6-C7-C8-C10
19	a	858	CLA	C12-C13-C15-C16
19	b	3002	CLA	C11-C10-C8-C7
19	b	3008	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	b	3009	CLA	C11-C10-C8-C7
19	b	3014	CLA	C12-C13-C15-C16
19	b	3020	CLA	C11-C10-C8-C7
19	b	3023	CLA	C6-C7-C8-C10
19	b	3034	CLA	C11-C10-C8-C7
19	b	3037	CLA	C6-C7-C8-C10
19	D	401	CLA	C11-C12-C13-C15
19	b	3028	CLA	C16-C17-C18-C19
31	D	402	PHO	CBA-CGA-O2A-C1
19	b	3003	CLA	C2A-CAA-CBA-CGA
19	a	830	CLA	C15-C16-C17-C18
23	a	851	LMG	C29-C30-C31-C32
19	a	833	CLA	C8-C10-C11-C12
19	b	3029	CLA	C13-C15-C16-C17
19	a	808	CLA	CAD-CBD-CGD-O2D
19	a	814	CLA	CAD-CBD-CGD-O2D
19	a	827	CLA	CAD-CBD-CGD-O2D
19	a	835	CLA	CAD-CBD-CGD-O2D
19	a	840	CLA	CAD-CBD-CGD-O2D
19	b	3005	CLA	CAD-CBD-CGD-O2D
19	b	3006	CLA	CAD-CBD-CGD-O2D
19	b	3012	CLA	CAD-CBD-CGD-O2D
19	b	3016	CLA	CAD-CBD-CGD-O2D
19	b	3038	CLA	CAD-CBD-CGD-O2D
19	j	102	CLA	CAD-CBD-CGD-O2D
19	b	3031	CLA	O1D-CGD-O2D-CED
21	f	202	BCR	C6-C7-C8-C9
22	b	3050	LHG	C24-C25-C26-C27
23	a	851	LMG	O1-C7-C8-C9
23	b	3051	LMG	O1-C7-C8-C9
31	D	402	PHO	O1A-CGA-O2A-C1
19	a	820	CLA	C2A-CAA-CBA-CGA
19	a	830	CLA	C16-C17-C18-C19
19	a	806	CLA	CHA-CBD-CGD-O1D
19	a	806	CLA	CHA-CBD-CGD-O2D
19	a	823	CLA	CHA-CBD-CGD-O2D
19	b	3003	CLA	CHA-CBD-CGD-O2D
19	b	3040	CLA	CHA-CBD-CGD-O1D
19	b	3040	CLA	CHA-CBD-CGD-O2D
19	l	1502	CLA	CHA-CBD-CGD-O1D
19	l	1502	CLA	CHA-CBD-CGD-O2D
19	A	403	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	A	403	CLA	CHA-CBD-CGD-O2D
21	a	847	BCR	C16-C17-C18-C19
23	b	3051	LMG	O7-C8-C9-O8
22	b	3050	LHG	C31-C32-C33-C34
19	a	835	CLA	C4-C3-C5-C6
19	a	819	CLA	C2-C3-C5-C6
19	a	819	CLA	C11-C12-C13-C14
19	a	821	CLA	C11-C10-C8-C9
19	a	828	CLA	C11-C10-C8-C9
19	b	3004	CLA	C6-C7-C8-C9
19	b	3007	CLA	C11-C12-C13-C14
19	b	3009	CLA	C11-C10-C8-C9
19	b	3018	CLA	C14-C13-C15-C16
23	b	3049	LMG	C36-C37-C38-C39
19	b	3018	CLA	C5-C6-C7-C8
19	b	3013	CLA	C16-C17-C18-C20
19	j	103	CLA	C2A-CAA-CBA-CGA
19	a	856	CLA	C8-C10-C11-C12
28	f	205	ZEX	C27-C28-C29-C30
19	a	803	CLA	C1A-C2A-CAA-CBA
19	a	810	CLA	C1A-C2A-CAA-CBA
19	a	843	CLA	C1A-C2A-CAA-CBA
19	b	3005	CLA	C1A-C2A-CAA-CBA
19	b	3012	CLA	C1A-C2A-CAA-CBA
19	b	3008	CLA	C16-C17-C18-C19
19	b	3013	CLA	C16-C17-C18-C19
19	a	841	CLA	C2-C1-O2A-CGA
19	b	3003	CLA	C2-C1-O2A-CGA
22	a	854	LHG	C24-C23-O8-C6
21	b	3048	BCR	C15-C16-C17-C18
19	a	836	CLA	O1D-CGD-O2D-CED
19	a	823	CLA	C2-C3-C5-C6
22	b	3050	LHG	C3-O3-P-O5
22	f	206	LHG	C4-O6-P-O4
19	l	1502	CLA	C8-C10-C11-C12
19	b	3005	CLA	C16-C17-C18-C19
19	D	403	CLA	C6-C7-C8-C10
19	a	816	CLA	CAD-CBD-CGD-O1D
19	a	823	CLA	CAD-CBD-CGD-O1D
19	b	3014	CLA	CAD-CBD-CGD-O1D
22	a	854	LHG	C24-C25-C26-C27
19	a	807	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	a	850	LHG	C34-C35-C36-C37
23	b	3049	LMG	C29-C28-O8-C9
22	a	854	LHG	C1-C2-C3-O3
19	a	808	CLA	C2-C3-C5-C6
19	a	814	CLA	C11-C10-C8-C7
19	a	826	CLA	C11-C12-C13-C15
19	a	828	CLA	C11-C10-C8-C7
19	a	828	CLA	C12-C13-C15-C16
19	b	3003	CLA	C6-C7-C8-C10
19	b	3007	CLA	C11-C12-C13-C15
19	b	3013	CLA	C6-C7-C8-C10
19	b	3014	CLA	C6-C7-C8-C10
19	D	401	CLA	C11-C10-C8-C7
22	b	3050	LHG	C7-C8-C9-C10
22	a	852	LHG	C30-C31-C32-C33
19	a	855	CLA	C5-C6-C7-C8
19	a	813	CLA	C2A-CAA-CBA-CGA
19	b	3035	CLA	C2A-CAA-CBA-CGA
19	a	818	CLA	C16-C17-C18-C20
22	a	850	LHG	C4-C5-C6-O8
22	a	854	LHG	O7-C5-C6-O8
19	f	201	CLA	C16-C17-C18-C20
19	b	3008	CLA	C3-C5-C6-C7
19	b	3039	CLA	C4-C3-C5-C6
19	a	832	CLA	C5-C6-C7-C8
19	a	807	CLA	C6-C7-C8-C9
19	a	820	CLA	C6-C7-C8-C9
19	a	821	CLA	C6-C7-C8-C9
19	a	826	CLA	C6-C7-C8-C9
19	a	827	CLA	C6-C7-C8-C9
19	a	829	CLA	C11-C10-C8-C9
19	a	834	CLA	C6-C7-C8-C9
19	a	837	CLA	C11-C10-C8-C9
19	a	841	CLA	C6-C7-C8-C9
19	a	858	CLA	C14-C13-C15-C16
19	D	401	CLA	C11-C12-C13-C14
22	a	850	LHG	C12-C13-C14-C15
21	i	101	BCR	C37-C22-C23-C24
19	b	3009	CLA	C8-C10-C11-C12
19	b	3007	CLA	C16-C17-C18-C20
19	b	3009	CLA	C3-C5-C6-C7
19	a	835	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	a	854	LHG	C6-C5-O7-C7
19	a	831	CLA	C2A-CAA-CBA-CGA
19	a	832	CLA	C2A-CAA-CBA-CGA
19	b	3012	CLA	C2A-CAA-CBA-CGA
19	a	813	CLA	C2-C1-O2A-CGA
19	a	818	CLA	C2-C1-O2A-CGA
19	a	835	CLA	C2-C1-O2A-CGA
19	b	3010	CLA	C2-C1-O2A-CGA
22	a	850	LHG	C11-C10-C9-C8
21	a	846	BCR	C23-C24-C25-C30
21	a	847	BCR	C1-C6-C7-C8
21	a	847	BCR	C5-C6-C7-C8
21	a	848	BCR	C5-C6-C7-C8
21	i	101	BCR	C1-C6-C7-C8
21	i	101	BCR	C5-C6-C7-C8
21	j	101	BCR	C23-C24-C25-C26
21	j	101	BCR	C23-C24-C25-C30
21	k	4001	BCR	C1-C6-C7-C8
19	b	3033	CLA	C2-C3-C5-C6
19	D	403	CLA	C2-C3-C5-C6
19	b	3037	CLA	O1D-CGD-O2D-CED
22	f	206	LHG	C9-C10-C11-C12
19	a	819	CLA	C16-C17-C18-C20
19	D	403	CLA	C6-C7-C8-C9
21	b	3043	BCR	C12-C13-C14-C15
22	f	206	LHG	O7-C5-C6-O8
23	a	853	LMG	O1-C7-C8-O7
19	b	3037	CLA	CBD-CGD-O2D-CED
22	b	3050	LHG	C4-O6-P-O3
31	A	404	PHO	CHA-CBD-CGD-O1D
31	A	404	PHO	CHA-CBD-CGD-O2D
22	f	206	LHG	C4-C5-C6-O8
19	b	3005	CLA	C4-C3-C5-C6
23	b	3051	LMG	C33-C34-C35-C36
19	a	821	CLA	C8-C10-C11-C12
19	a	830	CLA	C8-C10-C11-C12
19	a	840	CLA	C11-C10-C8-C7
19	b	3004	CLA	C6-C7-C8-C10
19	b	3007	CLA	C6-C7-C8-C10
19	b	3009	CLA	C6-C7-C8-C10
19	b	3014	CLA	C11-C10-C8-C7
19	b	3018	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	a	811	CLA	CAA-CBA-CGA-O2A
19	a	807	CLA	C11-C10-C8-C9
19	a	814	CLA	C6-C7-C8-C9
19	a	814	CLA	C11-C10-C8-C9
19	a	828	CLA	C14-C13-C15-C16
19	b	3013	CLA	C6-C7-C8-C9
19	b	3020	CLA	C6-C7-C8-C9
19	b	3026	CLA	C6-C7-C8-C9
19	D	401	CLA	C11-C10-C8-C9
19	b	3003	CLA	C4C-C3C-CAC-CBC
21	b	3044	BCR	C37-C22-C23-C24
21	A	406	BCR	C11-C12-C13-C35
23	a	851	LMG	C38-C39-C40-C41
19	a	826	CLA	C16-C17-C18-C20
19	b	3013	CLA	CBA-CGA-O2A-C1
19	a	841	CLA	C5-C6-C7-C8
21	j	104	BCR	C6-C7-C8-C9
19	D	403	CLA	CBA-CGA-O2A-C1
22	a	850	LHG	C30-C31-C32-C33
19	a	808	CLA	C10-C11-C12-C13
21	f	202	BCR	C18-C19-C20-C21
19	a	806	CLA	C16-C17-C18-C19
19	b	3006	CLA	C4-C3-C5-C6
19	b	3027	CLA	C4-C3-C5-C6
19	a	826	CLA	C2-C1-O2A-CGA
19	b	3016	CLA	C2-C1-O2A-CGA
19	k	4003	CLA	C2C-C3C-CAC-CBC
22	a	852	LHG	C26-C27-C28-C29
19	a	822	CLA	C2A-CAA-CBA-CGA
19	b	3009	CLA	C2A-CAA-CBA-CGA
23	b	3049	LMG	C11-C12-C13-C14
19	a	831	CLA	C3A-C2A-CAA-CBA
19	b	3029	CLA	C3A-C2A-CAA-CBA
19	a	813	CLA	C8-C10-C11-C12
22	b	3050	LHG	C26-C27-C28-C29
19	a	813	CLA	C6-C7-C8-C9
19	a	824	CLA	C11-C10-C8-C9
19	a	836	CLA	C14-C13-C15-C16
19	a	856	CLA	C11-C10-C8-C9
19	b	3024	CLA	C11-C12-C13-C14
19	b	3028	CLA	C14-C13-C15-C16
19	D	401	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	f	201	CLA	C16-C17-C18-C19
19	b	3018	CLA	C8-C10-C11-C12
22	f	206	LHG	C18-C19-C20-C21
19	b	3027	CLA	C13-C15-C16-C17
24	a	857	45D	C28-C26-C30-C32
24	a	857	45D	C39-C35-C37-C41
26	b	3045	ECH	C11-C10-C9-C34
26	b	3045	ECH	C35-C13-C14-C15
27	b	3052	EQ3	C11-C10-C9-C34
28	f	205	ZEX	C20-C13-C14-C15
19	a	819	CLA	C16-C17-C18-C19
19	a	826	CLA	C16-C17-C18-C19
19	b	3007	CLA	C16-C17-C18-C19
19	a	819	CLA	O2A-C1-C2-C3
19	a	824	CLA	O2A-C1-C2-C3
19	A	402	CLA	O2A-C1-C2-C3
21	j	104	BCR	C7-C8-C9-C34
29	f	207	LMT	O5B-C1B-O1B-C4'
19	a	843	CLA	C4-C3-C5-C6
19	a	831	CLA	C1A-C2A-CAA-CBA
19	a	858	CLA	C1A-C2A-CAA-CBA
23	b	3051	LMG	C13-C14-C15-C16
19	a	819	CLA	C11-C12-C13-C15
19	a	826	CLA	C12-C13-C15-C16
19	a	837	CLA	C11-C10-C8-C7
19	b	3026	CLA	C6-C7-C8-C10
19	b	3028	CLA	C11-C12-C13-C15
19	b	3029	CLA	C11-C10-C8-C7
19	f	201	CLA	C6-C7-C8-C10
19	b	3014	CLA	C8-C10-C11-C12
19	b	3019	CLA	C3-C5-C6-C7
21	A	406	BCR	C9-C10-C11-C12
22	a	852	LHG	C4-O6-P-O3
19	b	3033	CLA	C16-C17-C18-C20
19	a	809	CLA	C13-C15-C16-C17
19	a	818	CLA	C10-C11-C12-C13
19	b	3013	CLA	C13-C15-C16-C17
19	a	806	CLA	CAA-CBA-CGA-O2A
19	a	829	CLA	CAA-CBA-CGA-O2A
22	a	854	LHG	C34-C35-C36-C37
19	b	3017	CLA	C16-C17-C18-C20
19	D	403	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	a	820	CLA	C13-C15-C16-C17
19	a	820	CLA	C15-C16-C17-C18
19	b	3005	CLA	C2-C3-C5-C6
19	a	814	CLA	C15-C16-C17-C18
19	a	829	CLA	C5-C6-C7-C8
19	b	3013	CLA	O1A-CGA-O2A-C1
24	a	857	45D	C24-C26-C30-C32
24	a	857	45D	C33-C35-C37-C41
26	b	3045	ECH	C12-C13-C14-C15
27	b	3052	EQ3	C11-C10-C9-C8
28	f	205	ZEX	C12-C13-C14-C15
19	a	839	CLA	C13-C15-C16-C17
23	a	851	LMG	O1-C7-C8-O7
19	a	831	CLA	C13-C15-C16-C17
19	a	842	CLA	O1D-CGD-O2D-CED
19	a	802	CLA	C2-C1-O2A-CGA
19	a	809	CLA	C2-C1-O2A-CGA
31	A	404	PHO	C2-C1-O2A-CGA
19	b	3027	CLA	C2-C3-C5-C6
19	b	3034	CLA	C6-C7-C8-C9
19	b	3004	CLA	C2A-CAA-CBA-CGA
21	a	846	BCR	C23-C24-C25-C26
21	a	847	BCR	C23-C24-C25-C30
21	a	849	BCR	C1-C6-C7-C8
21	b	3046	BCR	C1-C6-C7-C8
21	b	3047	BCR	C23-C24-C25-C30
21	f	202	BCR	C23-C24-C25-C30
21	i	101	BCR	C23-C24-C25-C30
21	k	4004	BCR	C1-C6-C7-C8
21	l	1504	BCR	C15-C16-C17-C18
21	b	3048	BCR	C11-C12-C13-C14
19	b	3032	CLA	C16-C17-C18-C20
23	b	3049	LMG	C22-C23-C24-C25
22	b	3050	LHG	C34-C35-C36-C37
19	b	3002	CLA	C16-C17-C18-C20
19	A	402	CLA	C16-C17-C18-C19
19	b	3004	CLA	C8-C10-C11-C12
19	a	829	CLA	C2A-CAA-CBA-CGA
19	b	3014	CLA	C15-C16-C17-C18
19	b	3020	CLA	C13-C15-C16-C17
19	b	3024	CLA	C3-C5-C6-C7
23	a	853	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
19	a	807	CLA	C11-C10-C8-C7
19	a	843	CLA	C2-C3-C5-C6
23	b	3049	LMG	C14-C15-C16-C17
19	a	840	CLA	CAA-CBA-CGA-O2A
19	b	3023	CLA	CAA-CBA-CGA-O2A
19	b	3020	CLA	CBA-CGA-O2A-C1
21	b	3048	BCR	C11-C10-C9-C34
21	f	202	BCR	C20-C21-C22-C37
21	l	1504	BCR	C20-C21-C22-C37
19	a	831	CLA	CAA-CBA-CGA-O2A
19	b	3039	CLA	C2-C3-C5-C6
18	a	801	CL0	C14-C13-C15-C16
19	a	830	CLA	C11-C10-C8-C9
19	a	839	CLA	C6-C7-C8-C9
19	a	840	CLA	C6-C7-C8-C9
19	a	855	CLA	C14-C13-C15-C16
19	b	3008	CLA	C11-C10-C8-C9
19	b	3010	CLA	C6-C7-C8-C9
19	b	3014	CLA	C6-C7-C8-C9
19	b	3027	CLA	C11-C10-C8-C9
19	b	3028	CLA	C11-C12-C13-C14
19	b	3029	CLA	C11-C10-C8-C9
19	A	402	CLA	C11-C12-C13-C14
19	l	1503	CLA	C3A-C2A-CAA-CBA
19	b	3020	CLA	O1A-CGA-O2A-C1
19	a	812	CLA	CAA-CBA-CGA-O2A
19	a	813	CLA	CAD-CBD-CGD-O2D
19	a	817	CLA	CAD-CBD-CGD-O2D
19	a	819	CLA	CAD-CBD-CGD-O2D
19	a	824	CLA	CAD-CBD-CGD-O2D
19	a	826	CLA	CAD-CBD-CGD-O2D
19	a	834	CLA	CAD-CBD-CGD-O2D
19	a	836	CLA	CAD-CBD-CGD-O2D
19	b	3008	CLA	CAD-CBD-CGD-O2D
19	b	3031	CLA	CAD-CBD-CGD-O2D
19	b	3032	CLA	CAD-CBD-CGD-O2D
19	b	3034	CLA	CAD-CBD-CGD-O2D
19	b	3036	CLA	CAD-CBD-CGD-O2D
19	b	3041	CLA	CAD-CBD-CGD-O2D
19	f	204	CLA	CAD-CBD-CGD-O2D
19	l	1503	CLA	CAD-CBD-CGD-O2D
22	a	854	LHG	C4-C5-O7-C7

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Mol	Chain	Res	Type	Atoms
31	A	404	PHO	C15-C16-C17-C18
19	a	842	CLA	CBD-CGD-O2D-CED
19	b	3004	CLA	C2-C1-O2A-CGA
19	a	807	CLA	CAA-CBA-CGA-O2A
21	f	202	BCR	C22-C23-C24-C25
19	b	3020	CLA	C4-C3-C5-C6
19	b	3023	CLA	C4-C3-C5-C6
19	A	402	CLA	C4-C3-C5-C6
19	a	832	CLA	CAA-CBA-CGA-O2A
21	b	3047	BCR	C11-C12-C13-C14
28	b	3053	ZEX	C27-C28-C29-C30
23	a	853	LMG	C7-C8-C9-O8
29	f	207	LMT	C7-C8-C9-C10
19	b	3037	CLA	C5-C6-C7-C8
19	b	3029	CLA	CAA-CBA-CGA-O2A
19	b	3033	CLA	C16-C17-C18-C19
19	a	803	CLA	O2A-C1-C2-C3
19	a	821	CLA	O2A-C1-C2-C3
19	a	826	CLA	O2A-C1-C2-C3
19	a	839	CLA	O2A-C1-C2-C3
19	b	3016	CLA	O2A-C1-C2-C3
19	b	3037	CLA	O2A-C1-C2-C3
19	A	405	CLA	O2A-C1-C2-C3
19	D	401	CLA	O2A-C1-C2-C3
19	a	812	CLA	C2A-CAA-CBA-CGA
19	a	806	CLA	C10-C11-C12-C13
19	a	821	CLA	C13-C15-C16-C17
19	b	3008	CLA	C5-C6-C7-C8
19	a	821	CLA	CHA-CBD-CGD-O1D
19	a	821	CLA	CHA-CBD-CGD-O2D
19	a	826	CLA	CHA-CBD-CGD-O2D
19	a	839	CLA	CHA-CBD-CGD-O2D
19	b	3009	CLA	CHA-CBD-CGD-O2D
19	b	3013	CLA	CHA-CBD-CGD-O2D
19	b	3017	CLA	CHA-CBD-CGD-O2D
19	b	3027	CLA	CHA-CBD-CGD-O1D
19	b	3027	CLA	CHA-CBD-CGD-O2D
19	f	204	CLA	CHA-CBD-CGD-O1D
19	A	402	CLA	C3-C5-C6-C7
21	i	101	BCR	C20-C21-C22-C23
21	j	104	BCR	C11-C10-C9-C8
26	b	3045	ECH	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
19	a	856	CLA	C10-C11-C12-C13
19	a	830	CLA	CAA-CBA-CGA-O2A
19	b	3011	CLA	CAA-CBA-CGA-O2A
22	f	206	LHG	O7-C7-C8-C9
23	a	853	LMG	O8-C28-C29-C30
19	b	3031	CLA	C2A-CAA-CBA-CGA
19	k	4002	CLA	C2A-CAA-CBA-CGA
22	a	852	LHG	C14-C15-C16-C17
19	b	3004	CLA	CAA-CBA-CGA-O2A
23	a	851	LMG	O8-C28-C29-C30
19	b	3009	CLA	O1A-CGA-O2A-C1
22	a	854	LHG	C17-C18-C19-C20
19	a	842	CLA	C11-C12-C13-C15
19	b	3023	CLA	C2-C3-C5-C6
19	b	3017	CLA	C16-C17-C18-C19
19	a	835	CLA	CAA-CBA-CGA-O2A
19	b	3016	CLA	CAA-CBA-CGA-O2A
23	b	3049	LMG	O7-C10-C11-C12
18	a	801	CL0	C11-C12-C13-C14
19	a	826	CLA	C11-C12-C13-C14
19	b	3005	CLA	C14-C13-C15-C16
19	b	3006	CLA	C6-C7-C8-C9
19	b	3009	CLA	C11-C12-C13-C14
19	b	3032	CLA	C6-C7-C8-C9
19	f	201	CLA	C6-C7-C8-C9
19	A	402	CLA	C11-C10-C8-C9
19	j	102	CLA	CAA-CBA-CGA-O2A
19	a	806	CLA	C16-C17-C18-C20
32	F	101	HEM	CAA-CBA-CGA-O2A
23	b	3049	LMG	O9-C10-C11-C12
21	b	3047	BCR	C7-C8-C9-C34
21	j	104	BCR	C11-C12-C13-C35
22	a	854	LHG	C31-C32-C33-C34
19	a	812	CLA	CAA-CBA-CGA-O1A
19	a	831	CLA	CAA-CBA-CGA-O1A
19	a	840	CLA	CAA-CBA-CGA-O1A
19	b	3029	CLA	CAA-CBA-CGA-O1A
23	a	853	LMG	O10-C28-C29-C30
21	k	4001	BCR	C21-C22-C23-C24
19	a	807	CLA	CBA-CGA-O2A-C1
19	b	3004	CLA	CBA-CGA-O2A-C1
19	a	804	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	b	3002	CLA	C1A-C2A-CAA-CBA
19	b	3010	CLA	C1A-C2A-CAA-CBA
19	b	3013	CLA	C1A-C2A-CAA-CBA
19	b	3017	CLA	C1A-C2A-CAA-CBA
19	b	3028	CLA	C1A-C2A-CAA-CBA
19	f	201	CLA	C1A-C2A-CAA-CBA
19	l	1503	CLA	C1A-C2A-CAA-CBA
22	f	206	LHG	C24-C25-C26-C27
19	a	821	CLA	CAA-CBA-CGA-O2A
19	a	807	CLA	O1A-CGA-O2A-C1
19	b	3034	CLA	C2-C1-O2A-CGA
19	A	405	CLA	C2-C1-O2A-CGA
19	b	3009	CLA	CBA-CGA-O2A-C1
22	a	850	LHG	C10-C11-C12-C13
19	a	818	CLA	C15-C16-C17-C18
19	a	807	CLA	CAA-CBA-CGA-O1A
22	a	850	LHG	C25-C26-C27-C28
19	a	809	CLA	C4-C3-C5-C6
19	a	833	CLA	CAA-CBA-CGA-O2A
19	b	3021	CLA	CAA-CBA-CGA-O2A
19	b	3009	CLA	C5-C6-C7-C8
29	f	207	LMT	C1-C2-C3-C4
22	a	852	LHG	C4-O6-P-O5
19	a	835	CLA	CAA-CBA-CGA-O1A
19	b	3004	CLA	CAA-CBA-CGA-O1A
19	j	102	CLA	CAA-CBA-CGA-O1A
19	b	3004	CLA	O1A-CGA-O2A-C1
29	f	207	LMT	C5'-C4'-O1B-C1B
21	a	845	BCR	C23-C24-C25-C30
21	a	847	BCR	C23-C24-C25-C26
21	a	849	BCR	C5-C6-C7-C8
21	b	3048	BCR	C23-C24-C25-C30
26	m	101	ECH	C23-C24-C25-C30
27	b	3052	EQ3	C23-C24-C25-C30
28	b	3053	ZEX	C1-C6-C7-C8
19	a	830	CLA	CAA-CBA-CGA-O1A
19	b	3039	CLA	CAA-CBA-CGA-O2A
21	a	845	BCR	C10-C11-C12-C13
21	k	4001	BCR	C10-C11-C12-C13
19	a	833	CLA	C2A-CAA-CBA-CGA
19	a	840	CLA	C2A-CAA-CBA-CGA
19	a	832	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
19	a	824	CLA	CAA-CBA-CGA-O2A
23	b	3049	LMG	C29-C30-C31-C32
19	a	818	CLA	CAD-CBD-CGD-O1D
19	a	831	CLA	CAD-CBD-CGD-O1D
19	a	835	CLA	CAD-CBD-CGD-O1D
19	b	3029	CLA	CAD-CBD-CGD-O1D
19	b	3033	CLA	CAD-CBD-CGD-O1D
19	f	203	CLA	CAD-CBD-CGD-O1D
31	D	402	PHO	CAD-CBD-CGD-O1D
19	b	3011	CLA	CAA-CBA-CGA-O1A
19	a	812	CLA	C14-C13-C15-C16
19	b	3013	CLA	C11-C12-C13-C14
19	b	3021	CLA	C6-C7-C8-C9
19	b	3033	CLA	C6-C7-C8-C9
19	b	3033	CLA	C14-C13-C15-C16
19	f	201	CLA	C14-C13-C15-C16
19	a	835	CLA	C4C-C3C-CAC-CBC
22	a	852	LHG	C9-C10-C11-C12
19	a	815	CLA	CAA-CBA-CGA-O2A
19	a	842	CLA	CAA-CBA-CGA-O2A
19	j	103	CLA	CAA-CBA-CGA-O2A
32	F	101	HEM	CAA-CBA-CGA-O1A
18	a	801	CL0	C11-C12-C13-C15
19	a	819	CLA	C6-C7-C8-C10
19	a	819	CLA	C11-C10-C8-C7
19	b	3005	CLA	C12-C13-C15-C16
19	b	3006	CLA	C2-C3-C5-C6
19	b	3006	CLA	C6-C7-C8-C10
19	b	3017	CLA	C3A-C2A-CAA-CBA
19	b	3032	CLA	C6-C7-C8-C10
19	b	3032	CLA	C12-C13-C15-C16
19	f	201	CLA	C12-C13-C15-C16
19	A	402	CLA	C11-C10-C8-C7
22	a	850	LHG	O6-C4-C5-O7
31	A	404	PHO	C11-C10-C8-C7
19	b	3021	CLA	CAA-CBA-CGA-O1A
19	a	838	CLA	CAA-CBA-CGA-O2A
19	b	3015	CLA	CAA-CBA-CGA-O2A
22	a	850	LHG	O8-C23-C24-C25
19	a	831	CLA	C5-C6-C7-C8
21	b	3046	BCR	C21-C22-C23-C24
19	b	3015	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
19	b	3016	CLA	CAA-CBA-CGA-O1A
19	b	3012	CLA	CAA-CBA-CGA-O2A
23	a	853	LMG	C13-C14-C15-C16
23	a	853	LMG	O6-C1-O1-C7
19	b	3002	CLA	C5-C6-C7-C8
19	b	3009	CLA	C13-C15-C16-C17
19	a	833	CLA	CAA-CBA-CGA-O1A
19	b	3039	CLA	CAA-CBA-CGA-O1A
22	b	3050	LHG	C33-C34-C35-C36
19	a	816	CLA	CAA-CBA-CGA-O2A
19	a	839	CLA	CAA-CBA-CGA-O2A
19	b	3002	CLA	C2A-CAA-CBA-CGA
19	b	3033	CLA	C10-C11-C12-C13
19	b	3035	CLA	CAA-CBA-CGA-O2A

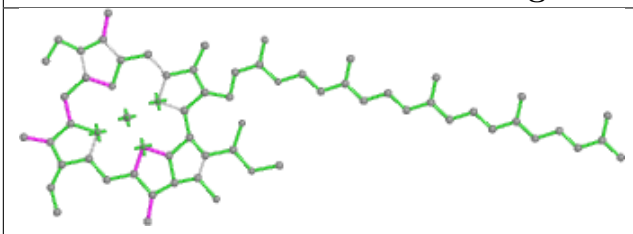
There are no ring outliers.

10 monomers are involved in 42 short contacts:

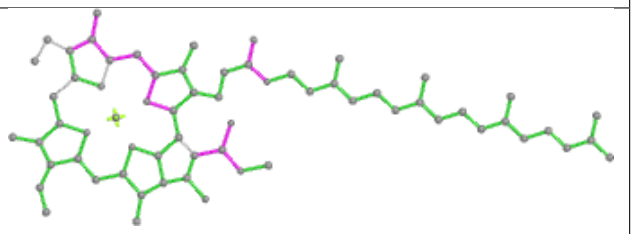
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	D	402	PHO	4	0
19	D	401	CLA	6	0
21	A	406	BCR	2	0
19	A	403	CLA	2	0
19	A	405	CLA	3	0
32	F	101	HEM	4	0
19	A	402	CLA	6	0
31	A	404	PHO	5	0
19	D	404	CLA	3	0
19	D	403	CLA	10	0

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

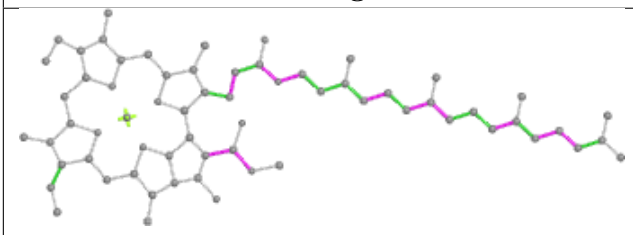
Ligand CLA a 814



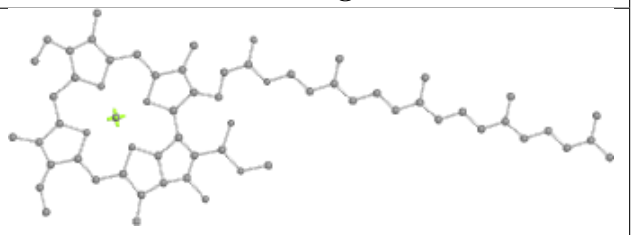
Bond lengths



Bond angles

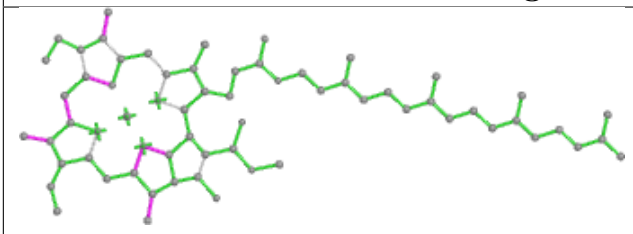


Torsions

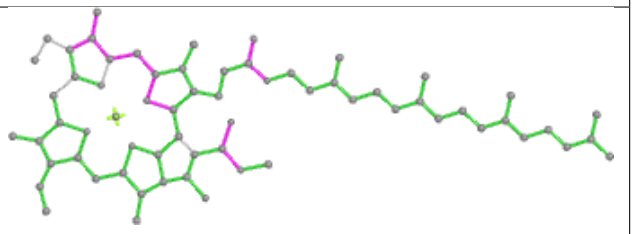


Rings

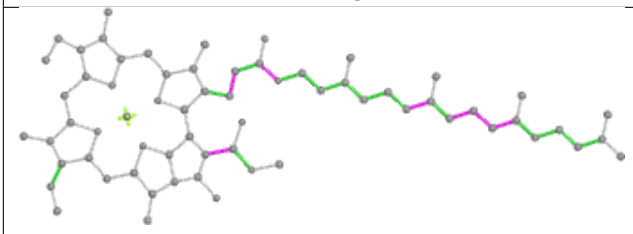
Ligand CLA l 1502



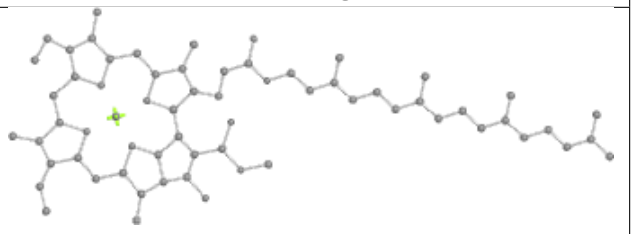
Bond lengths



Bond angles

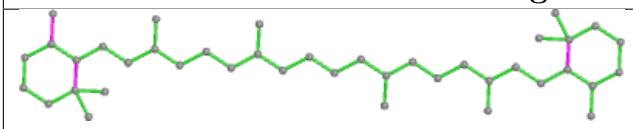


Torsions

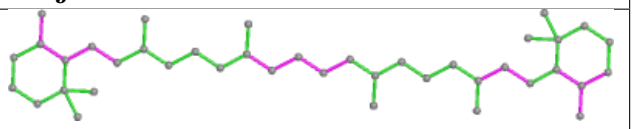


Rings

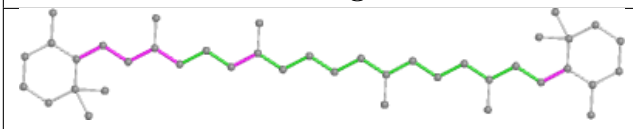
Ligand BCR j 104



Bond lengths



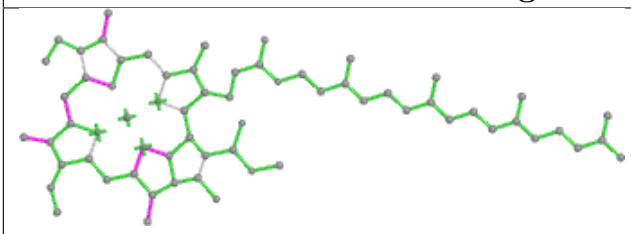
Bond angles



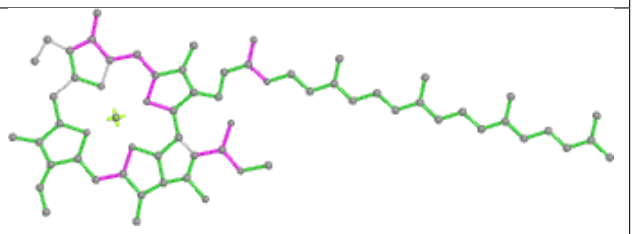
Torsions

Rings

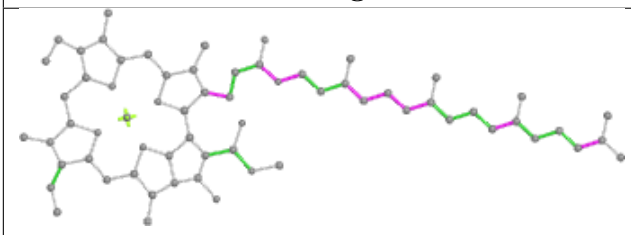
Ligand CLA b 3007



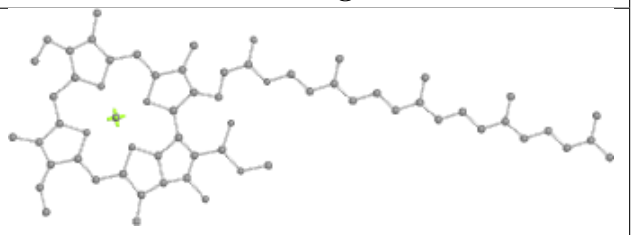
Bond lengths



Bond angles

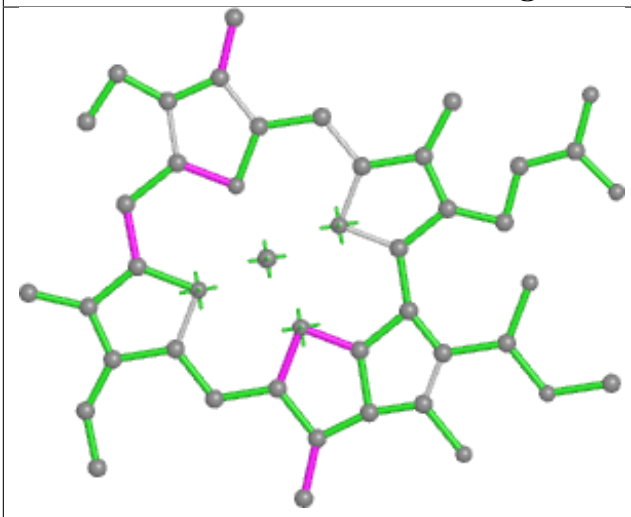


Torsions

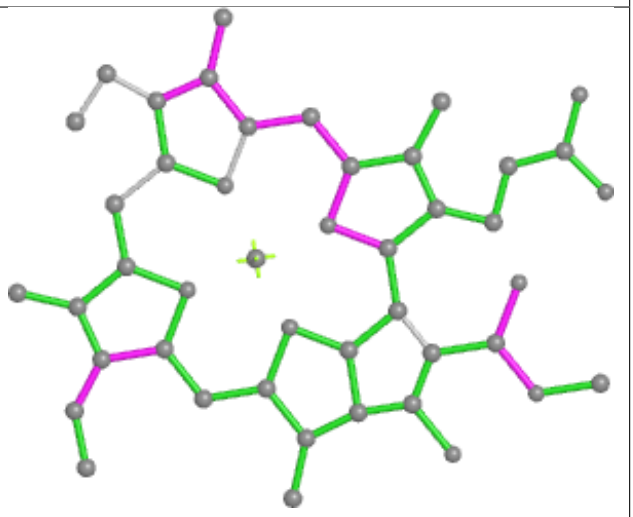


Rings

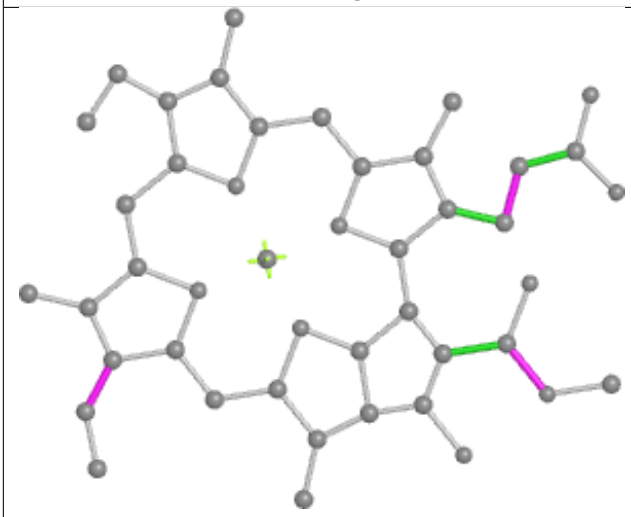
Ligand CLA k 4003



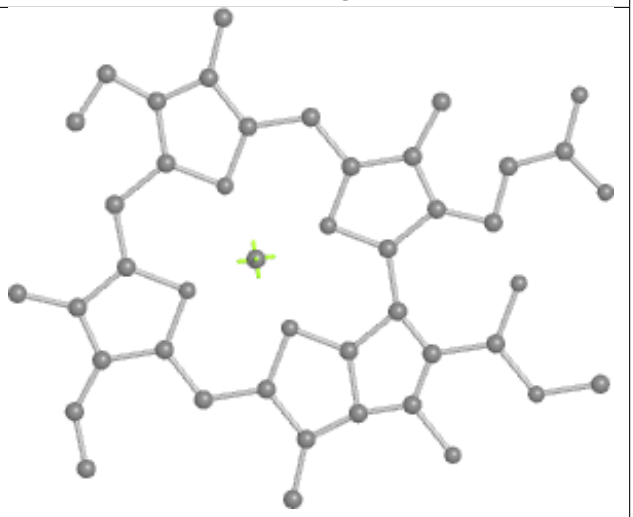
Bond lengths



Bond angles

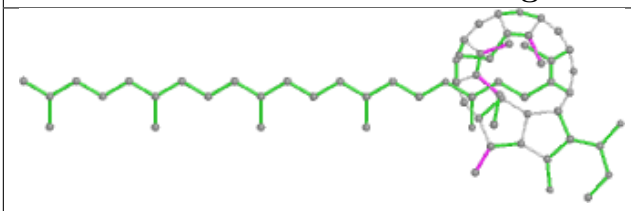


Torsions

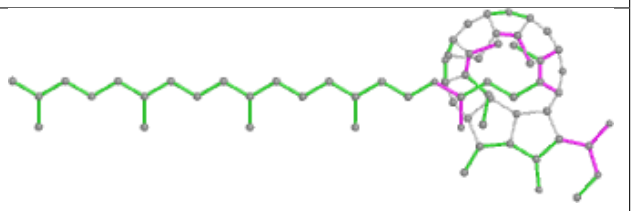


Rings

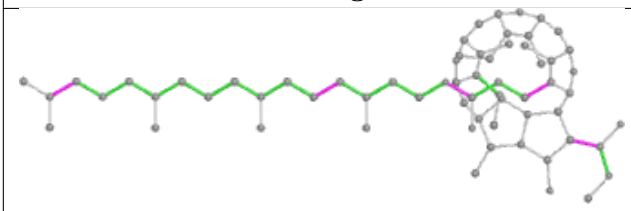
Ligand PHO D 402



Bond lengths



Bond angles



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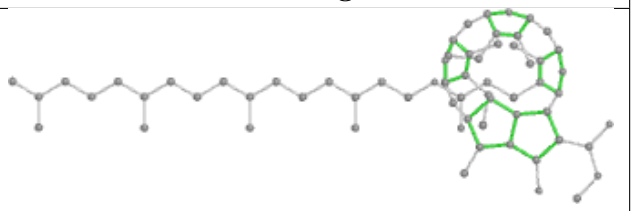
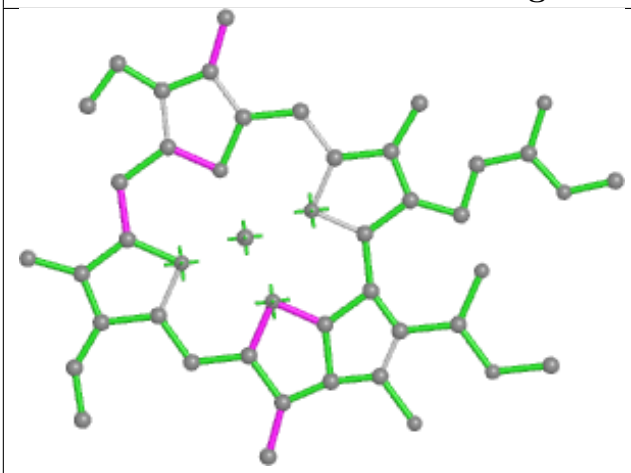
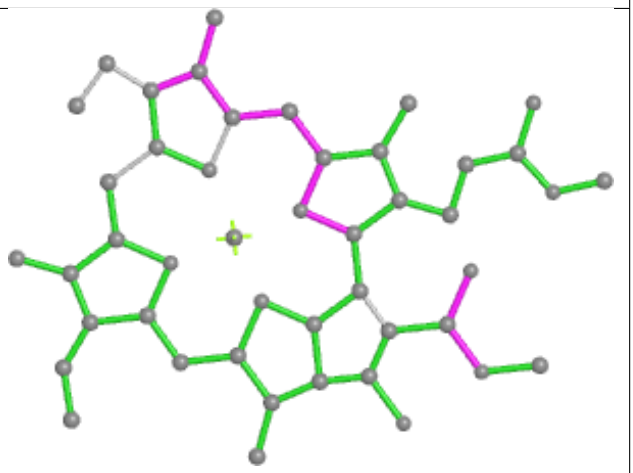


Rings

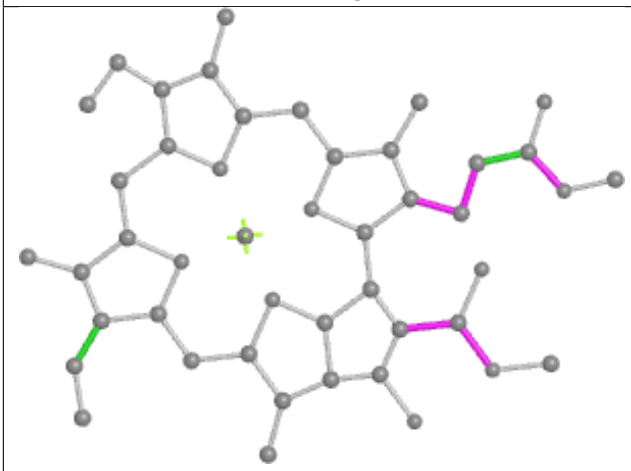
Ligand CLA a 817



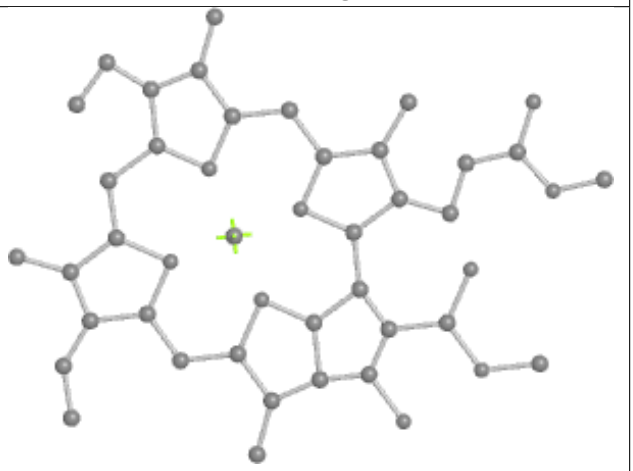
Bond lengths



Bond angles

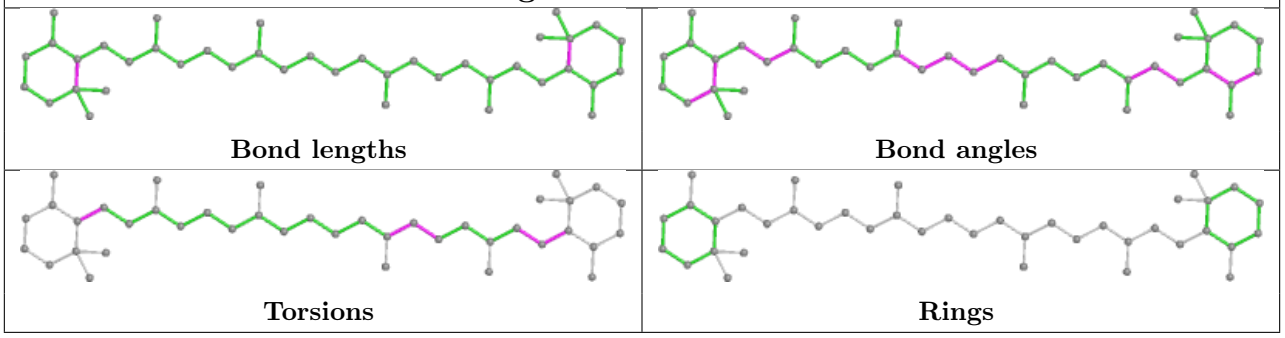


Torsions

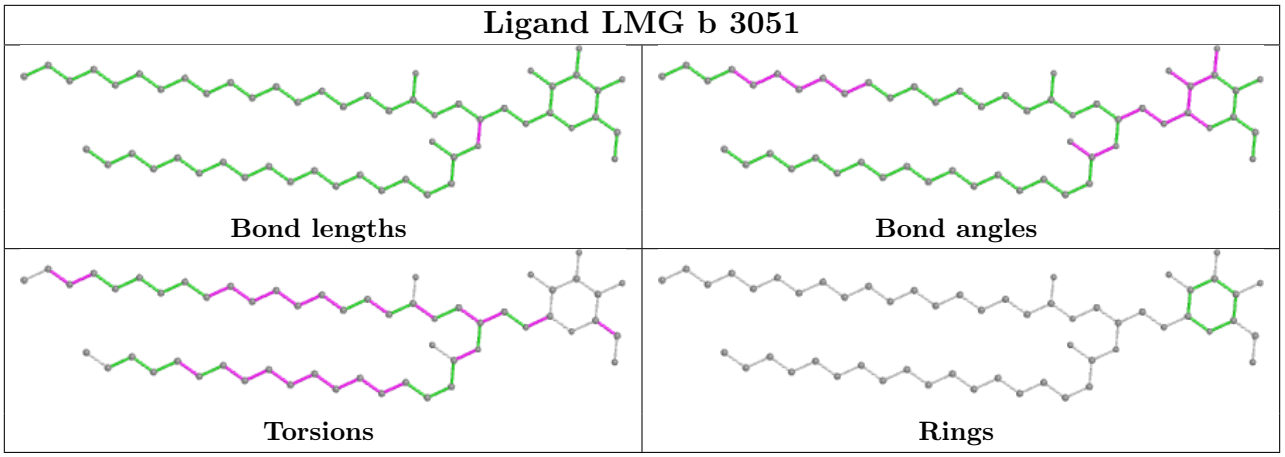


Rings

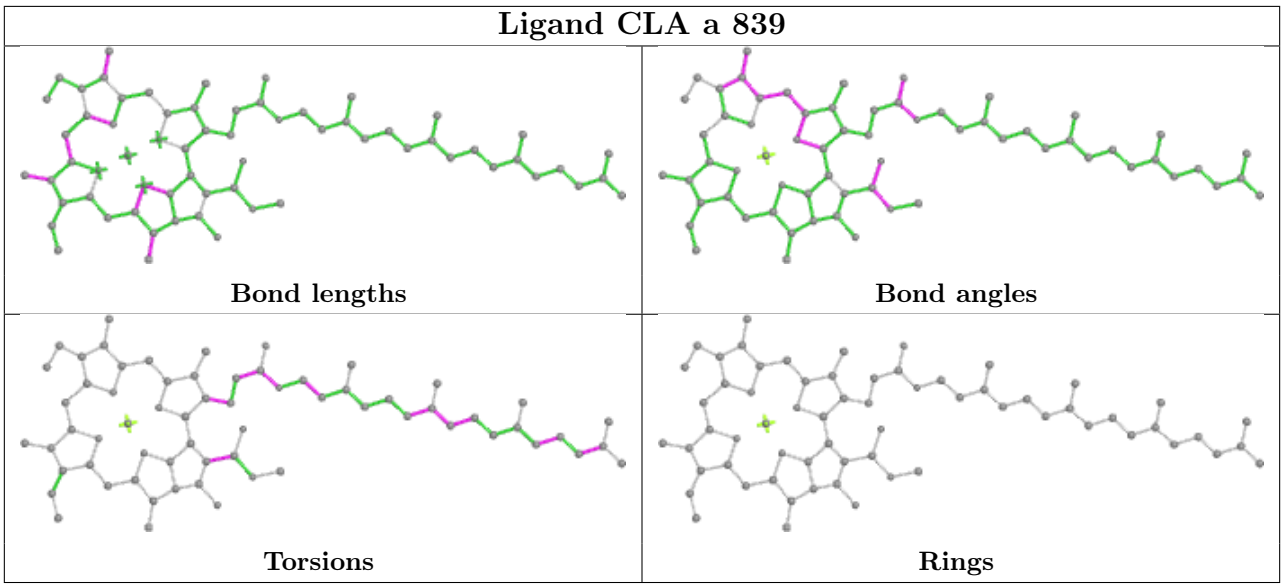
Ligand BCR k 4004



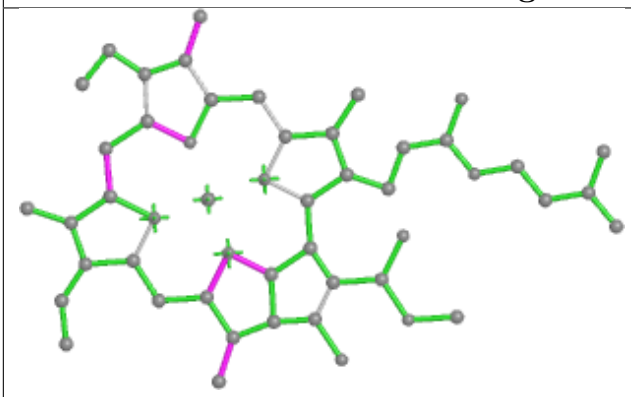
Ligand LMG b 3051



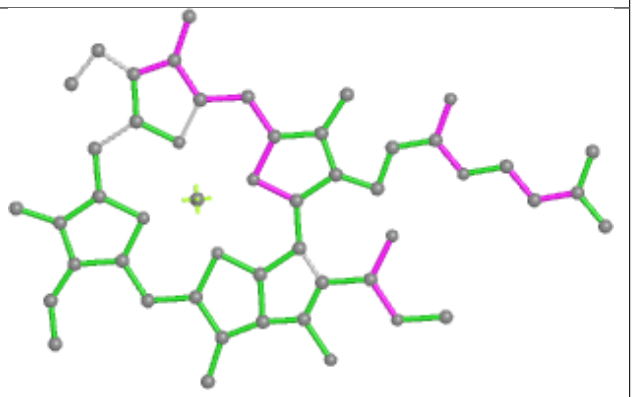
Ligand CLA a 839



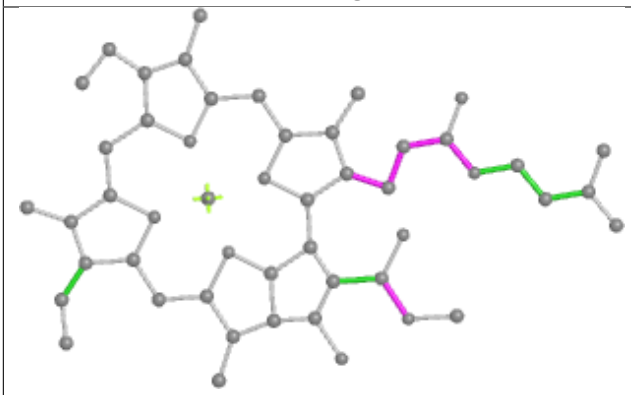
Ligand CLA b 3035



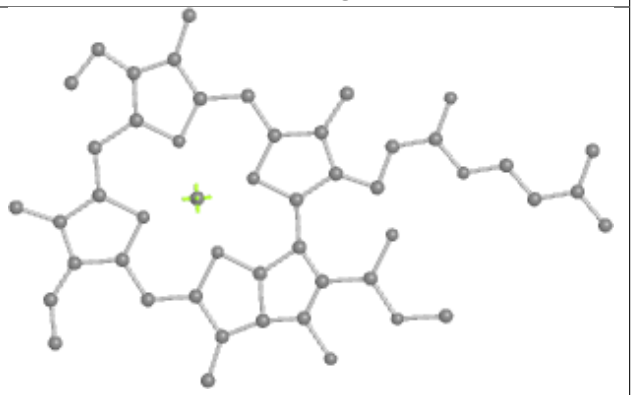
Bond lengths



Bond angles

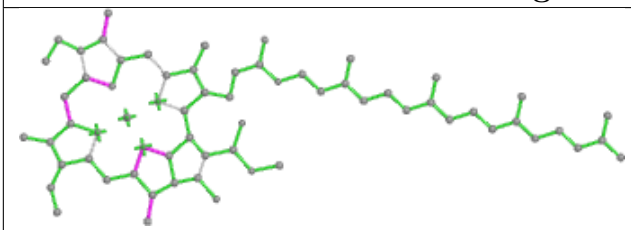


Torsions

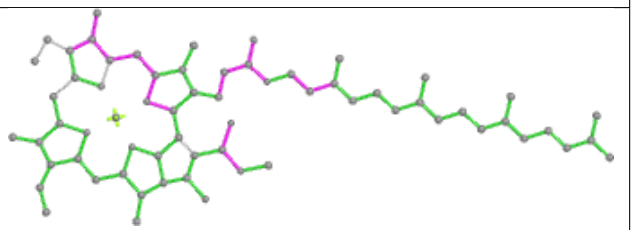


Rings

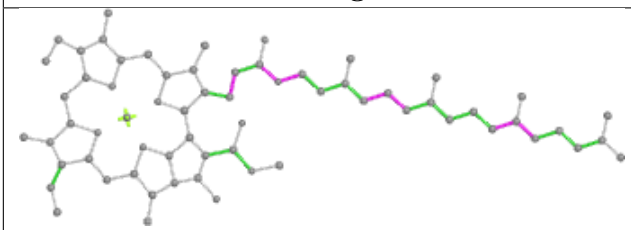
Ligand CL0 a 801



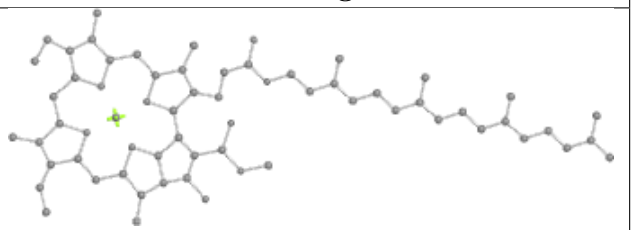
Bond lengths



Bond angles

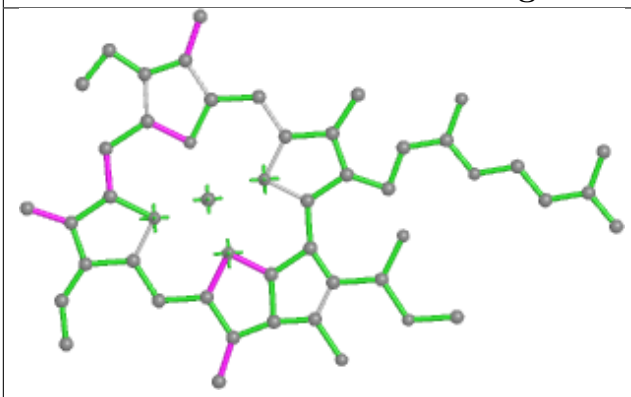


Torsions

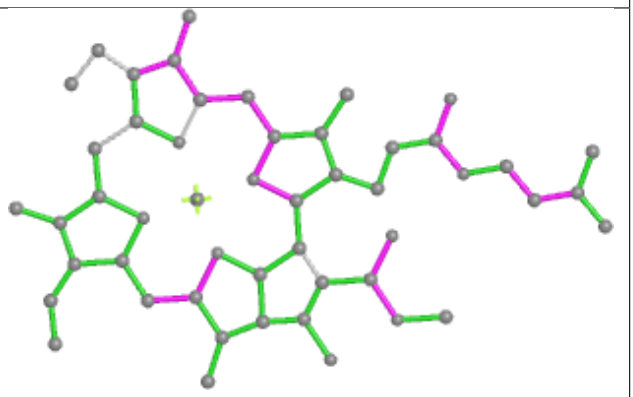


Rings

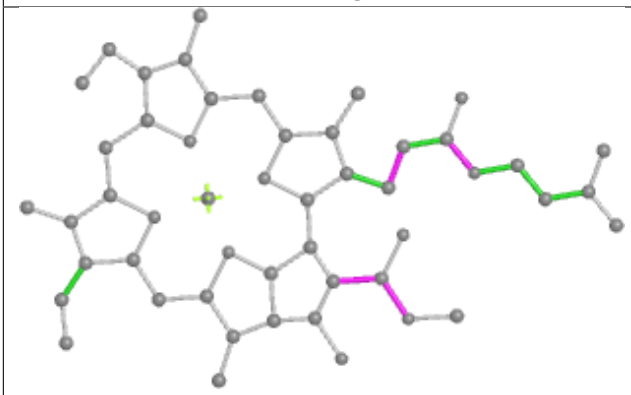
Ligand CLA b 3031



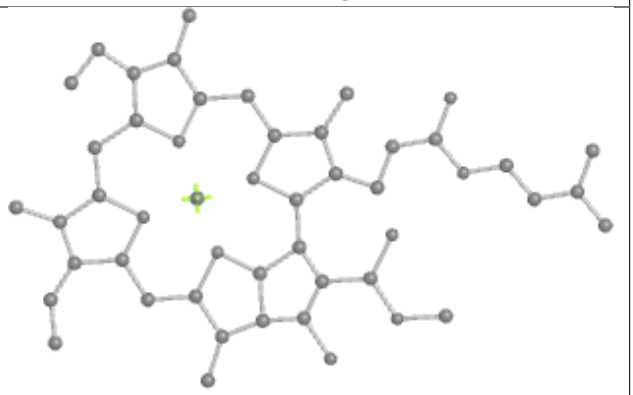
Bond lengths



Bond angles

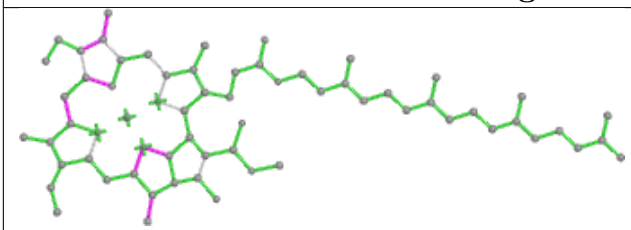


Torsions

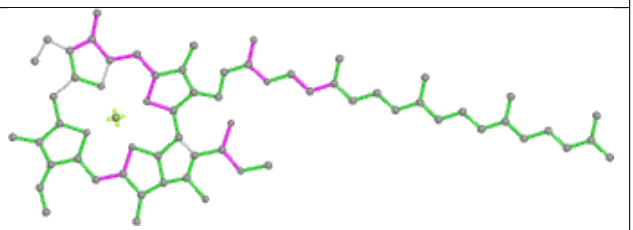


Rings

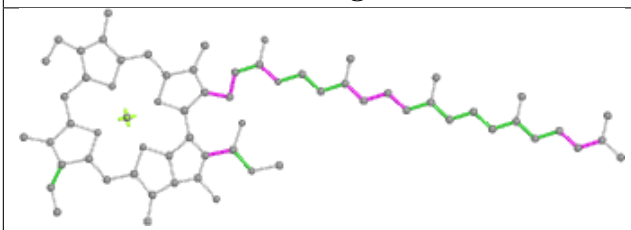
Ligand CLA b 3017



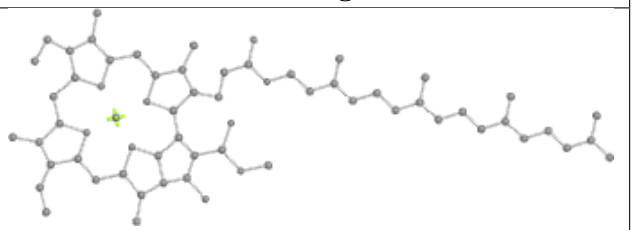
Bond lengths



Bond angles

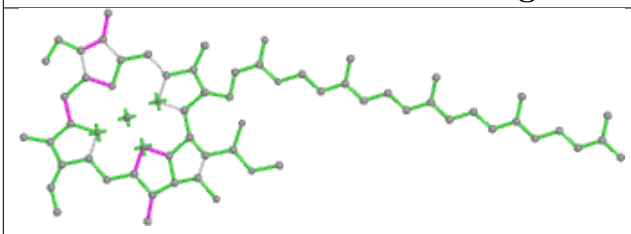


Torsions

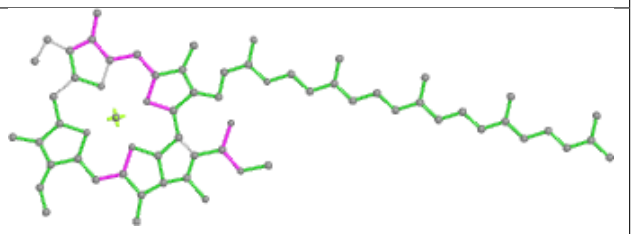


Rings

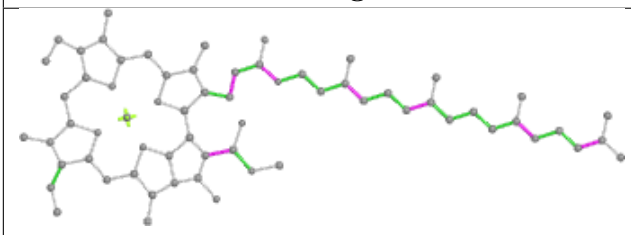
Ligand CLA b 3032



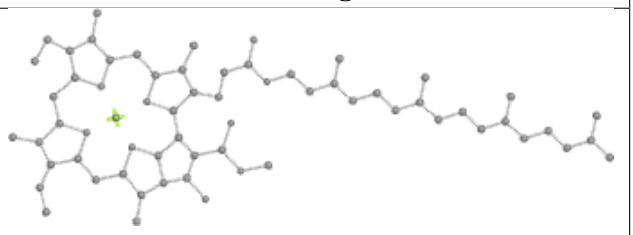
Bond lengths



Bond angles

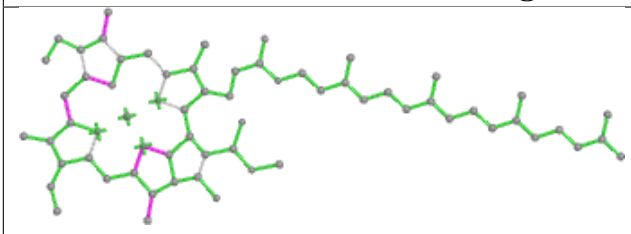


Torsions

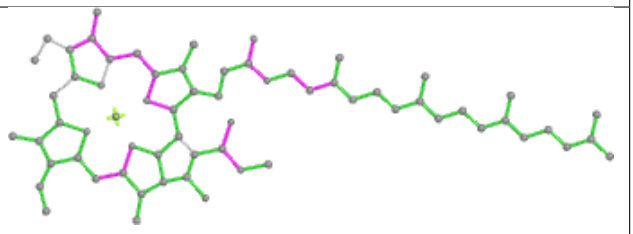


Rings

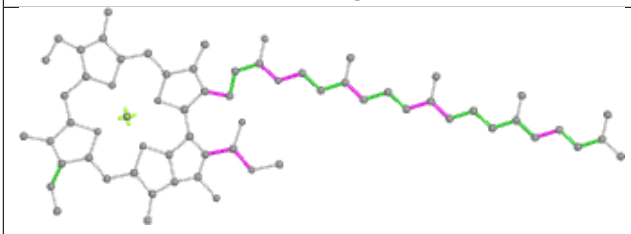
Ligand CLA b 3034



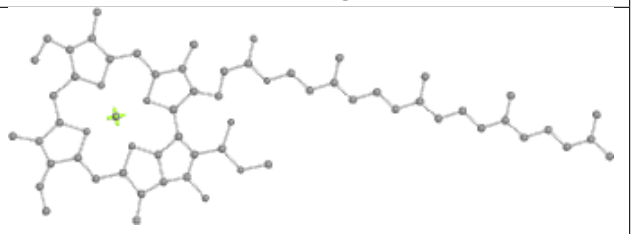
Bond lengths



Bond angles

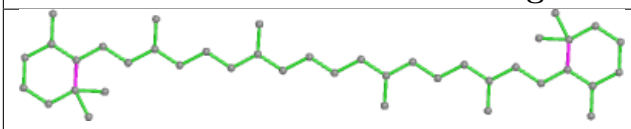


Torsions

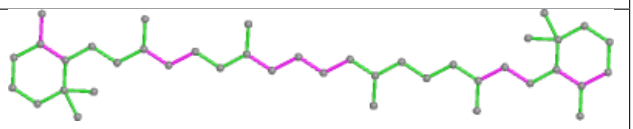


Rings

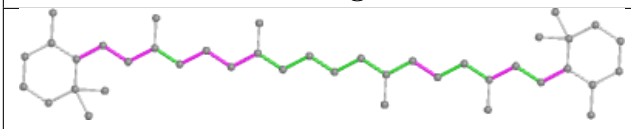
Ligand BCR a 845



Bond lengths



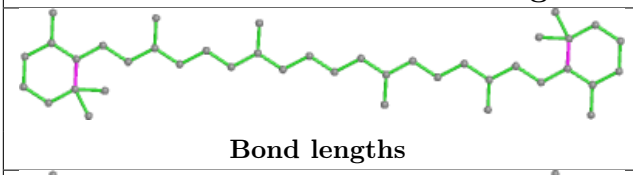
Bond angles



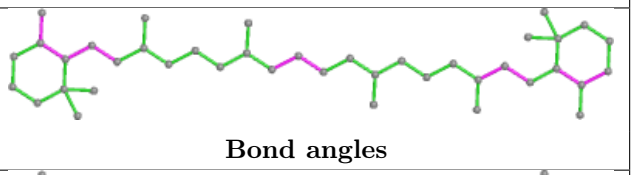
Torsions

Rings

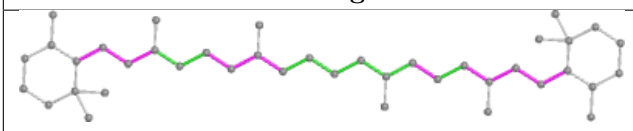
Ligand BCR f 202



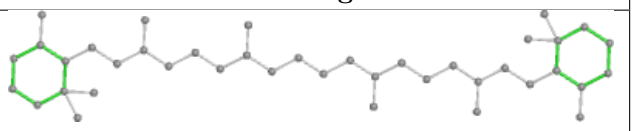
Bond lengths



Bond angles

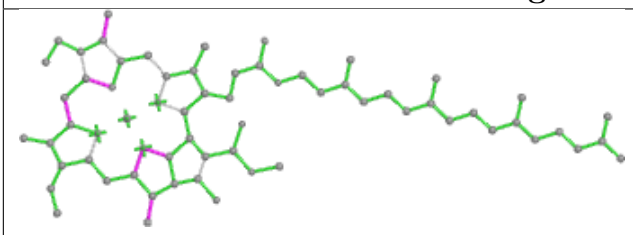


Torsions

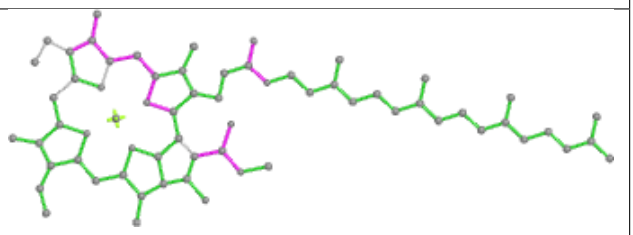


Rings

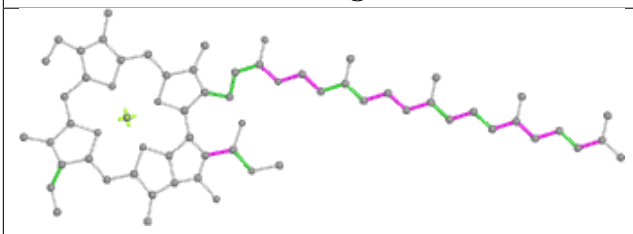
Ligand CLA a 826



Bond lengths



Bond angles



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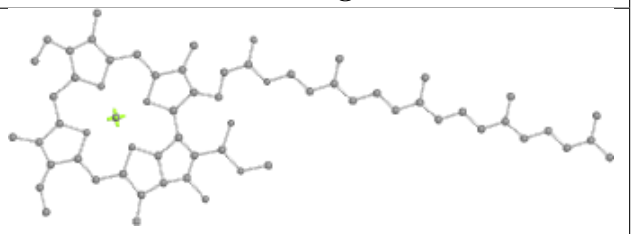
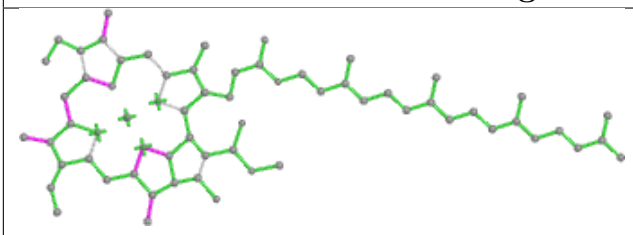
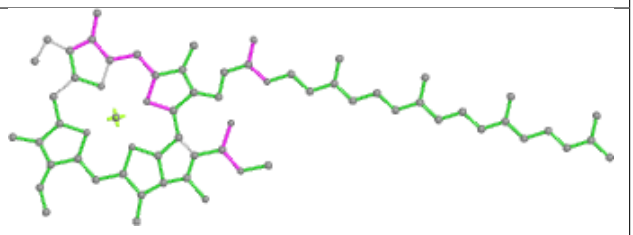


Rings

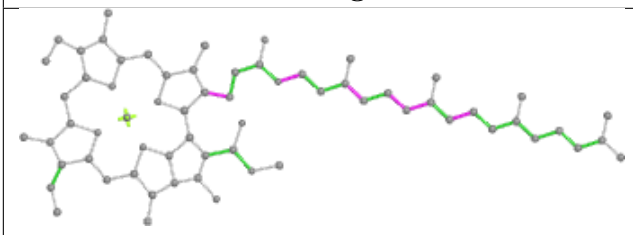
Ligand CLA b 3026



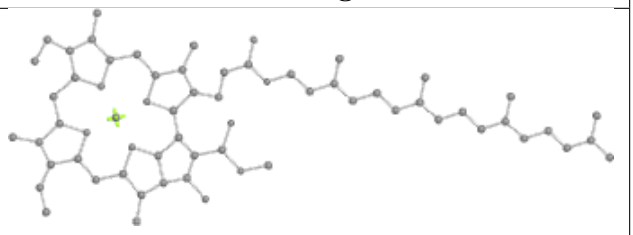
Bond lengths



Bond angles

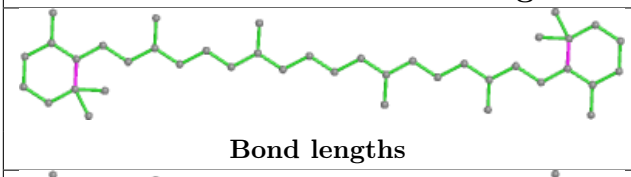


Torsions

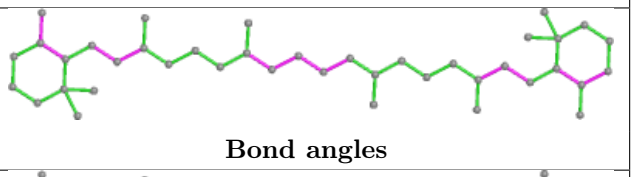


Rings

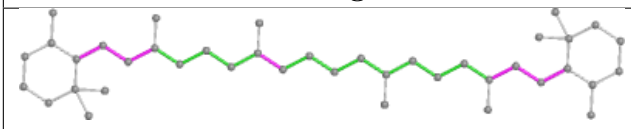
Ligand BCR b 3043



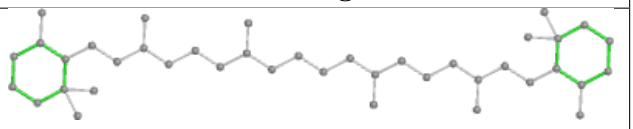
Bond lengths



Bond angles

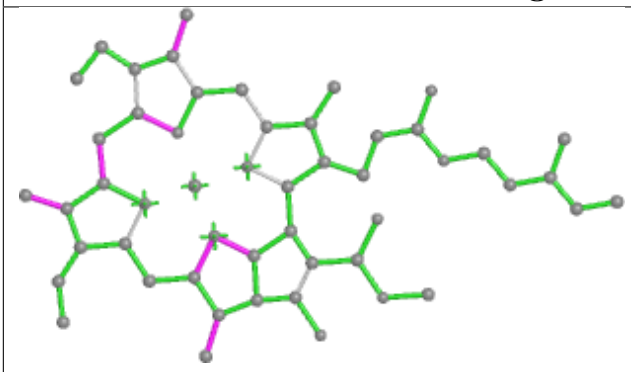


Torsions

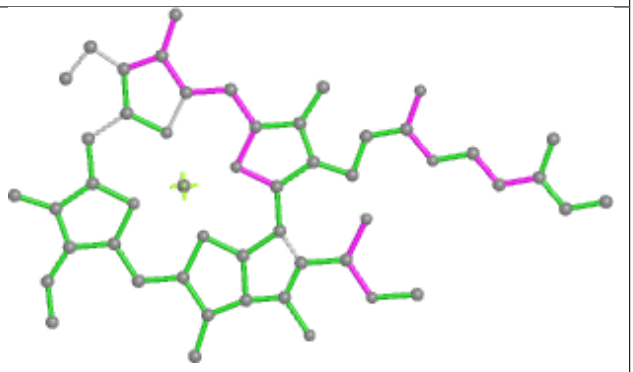


Rings

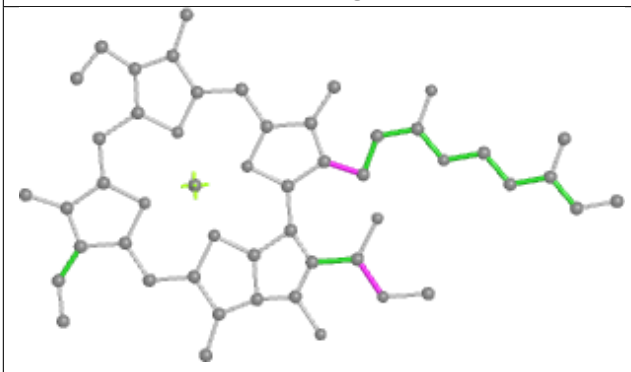
Ligand CLA a 810



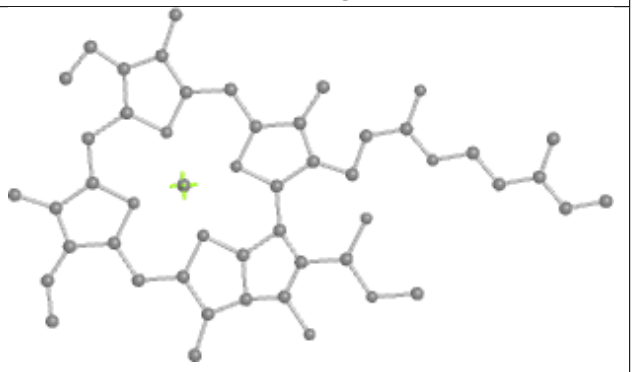
Bond lengths



Bond angles

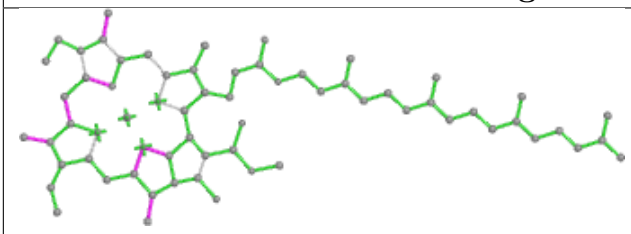


Torsions

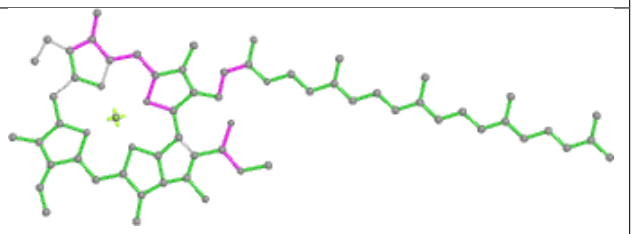


Rings

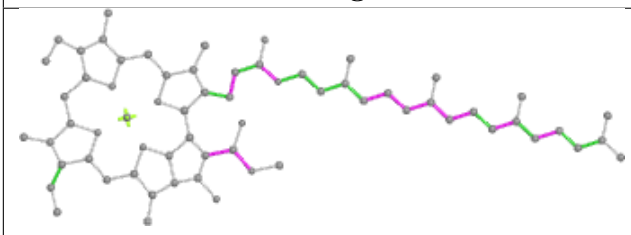
Ligand CLA b 3009



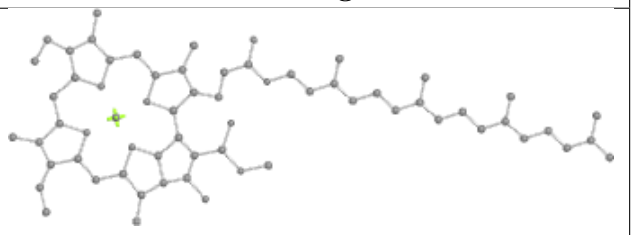
Bond lengths



Bond angles

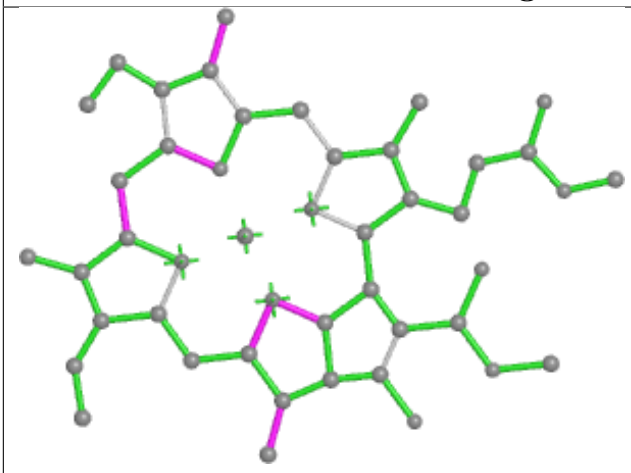


Torsions

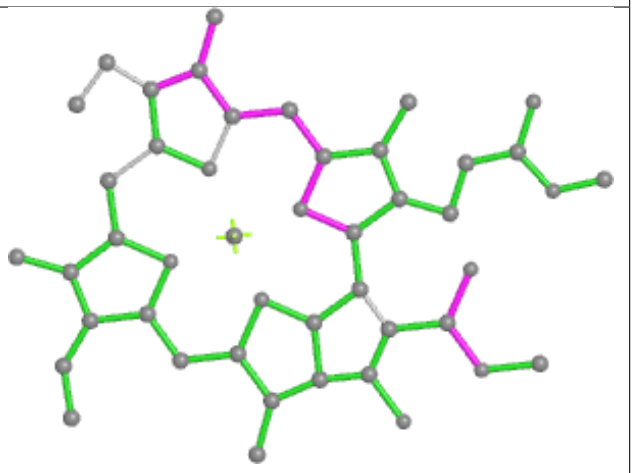


Rings

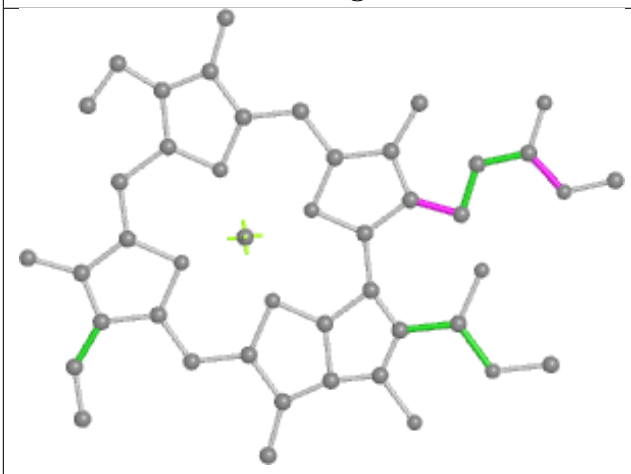
Ligand CLA b 3022



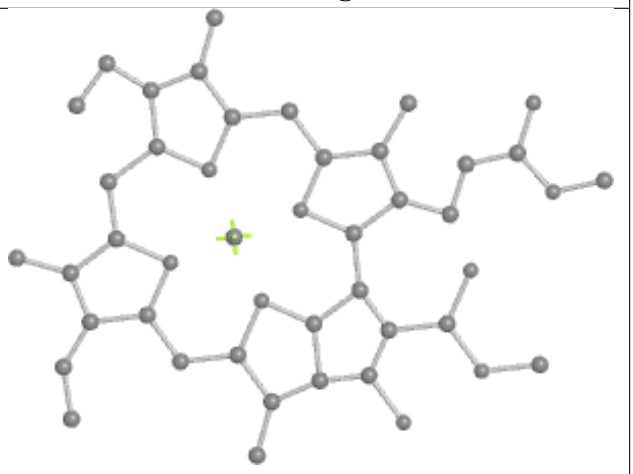
Bond lengths



Bond angles

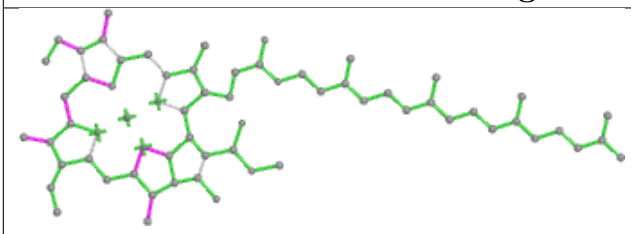


Torsions

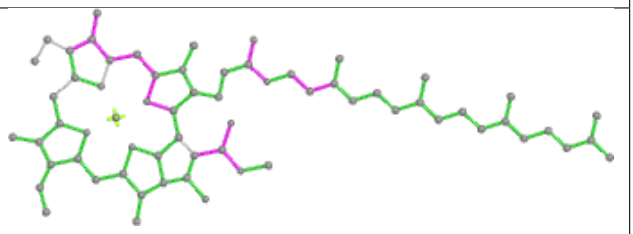


Rings

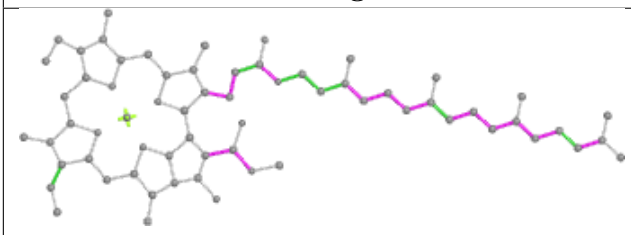
Ligand CLA b 3013



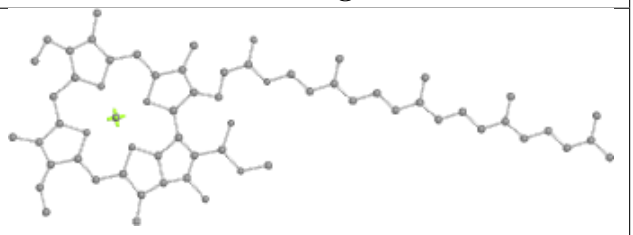
Bond lengths



Bond angles

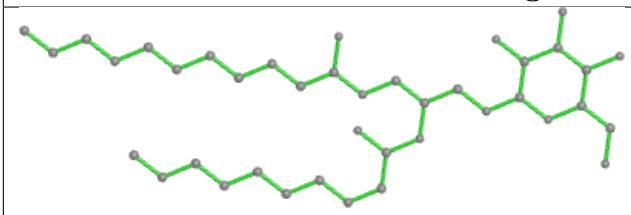


Torsions

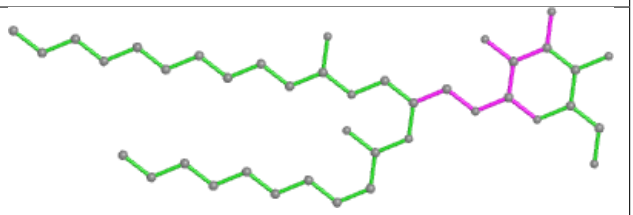


Rings

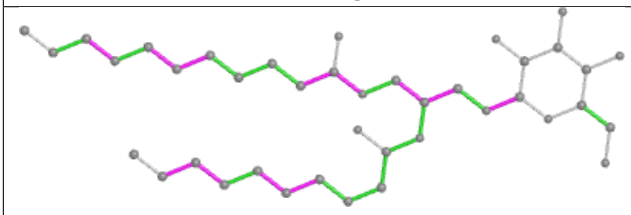
Ligand LMG a 853



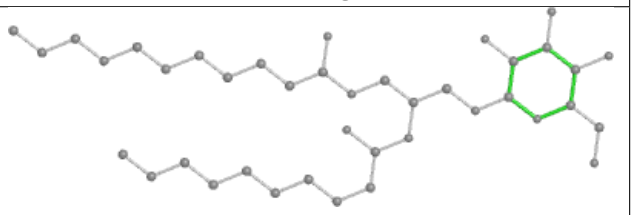
Bond lengths



Bond angles

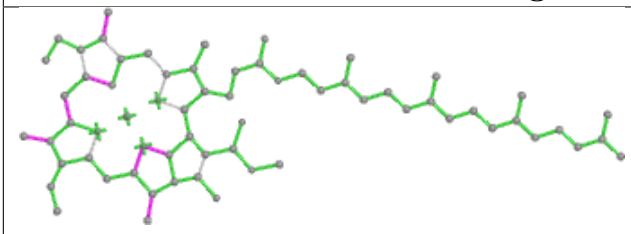


Torsions

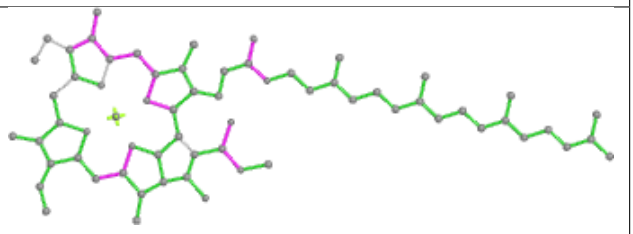


Rings

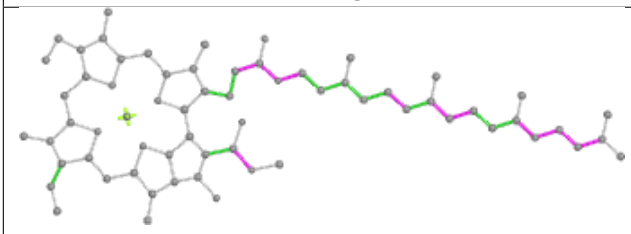
Ligand CLA a 830



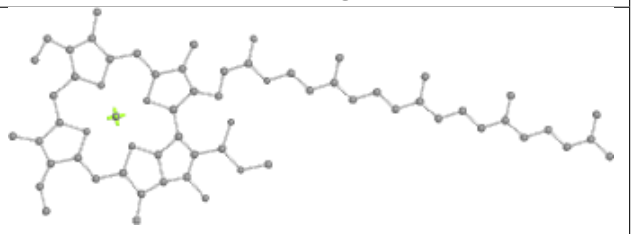
Bond lengths



Bond angles

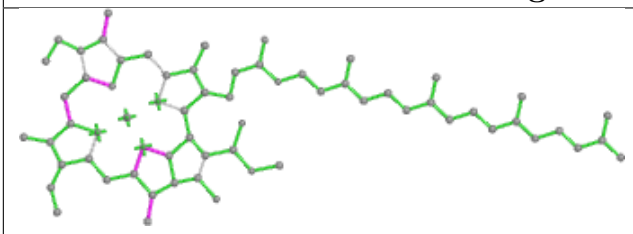


Torsions

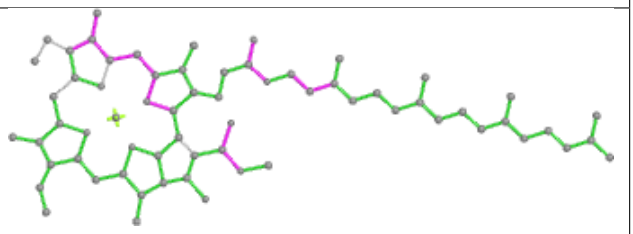


Rings

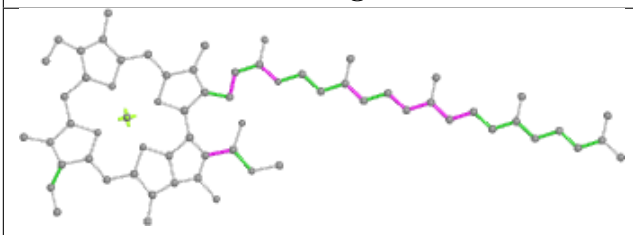
Ligand CLA a 837



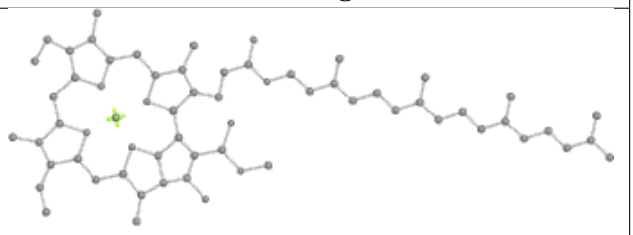
Bond lengths



Bond angles

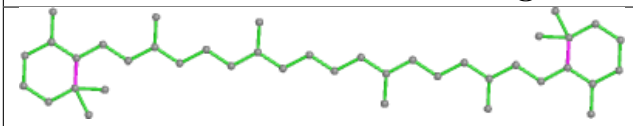


Torsions

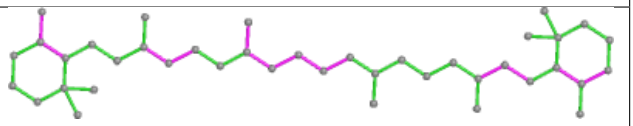


Rings

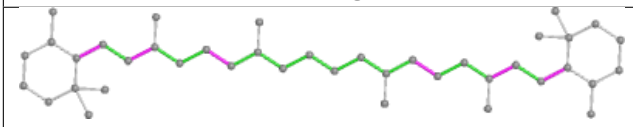
Ligand BCR k 4001



Bond lengths



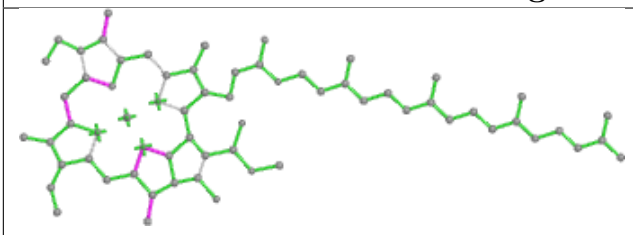
Bond angles



Torsions

Rings

Ligand CLA a 807



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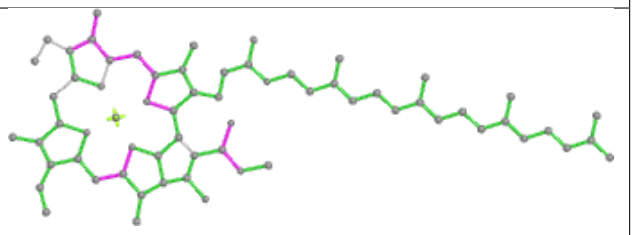
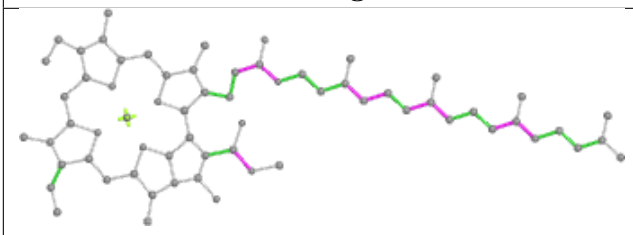
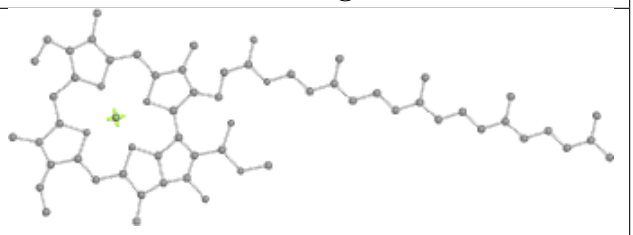


Bond angles

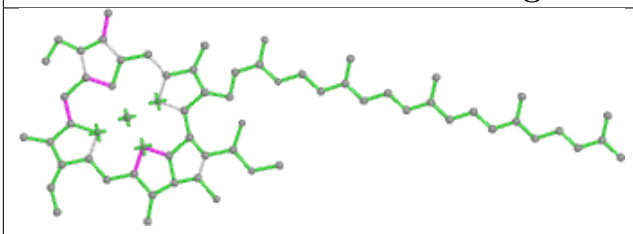


Torsions



Rings

Ligand CLA D 401



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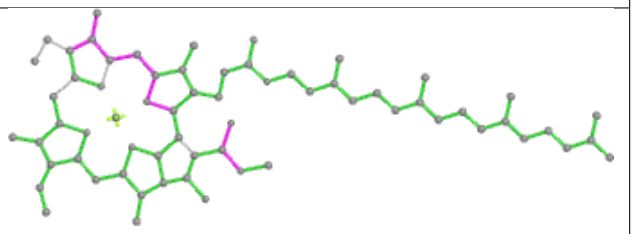
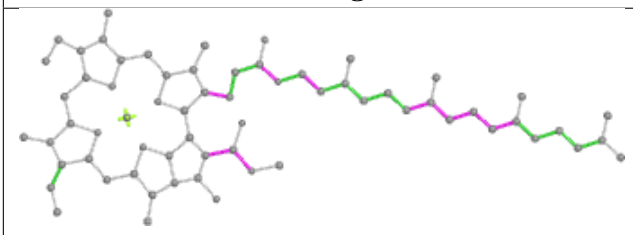
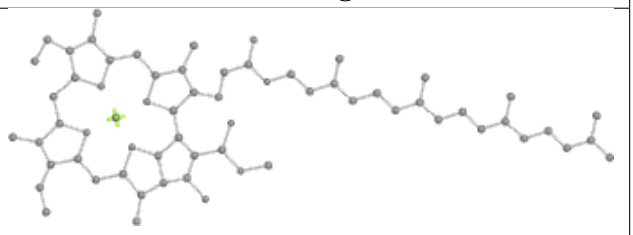


Bond angles

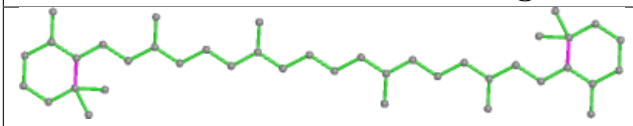


Torsions



Rings

Ligand BCR b 3047



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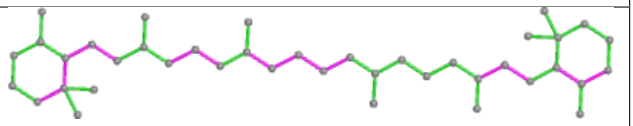
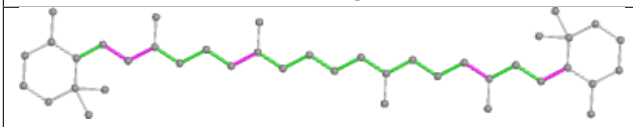


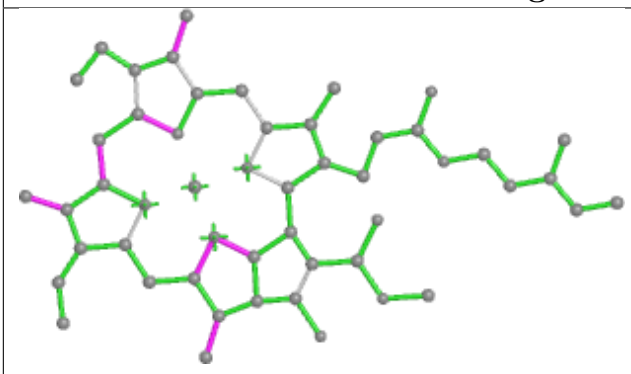
Bond angles



Torsions

Rings

Ligand CLA a 838



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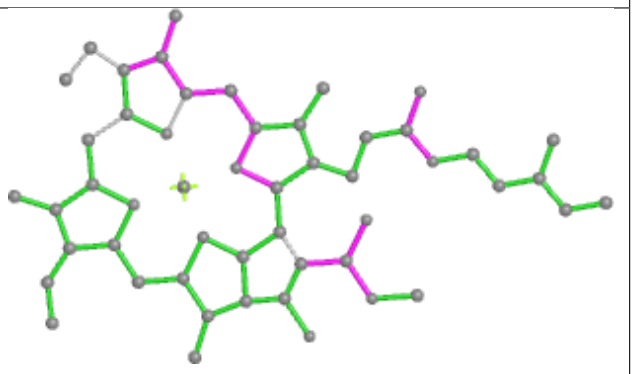

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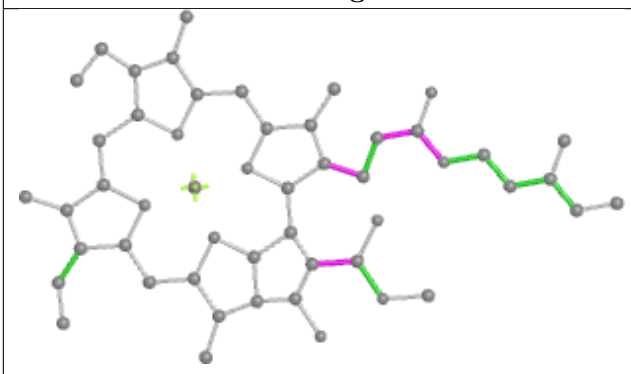
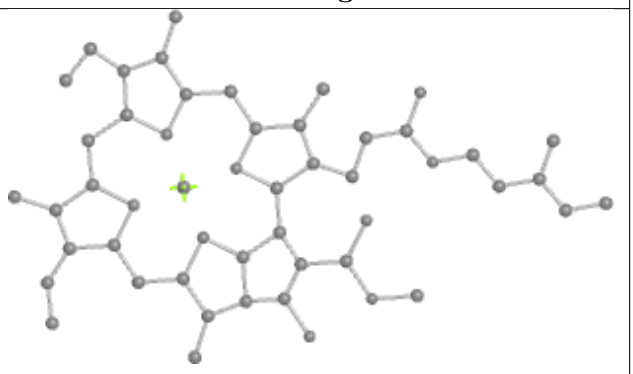
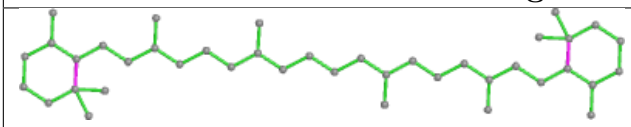


Torsions

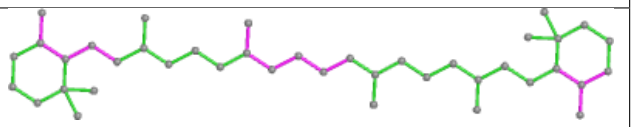


Rings

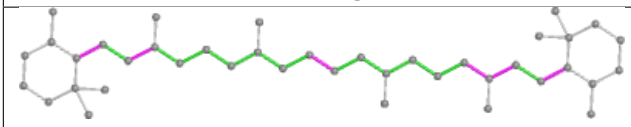
Ligand BCR a 848



Bond lengths

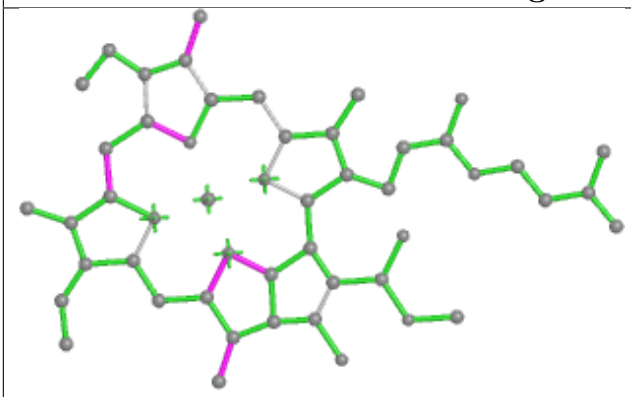
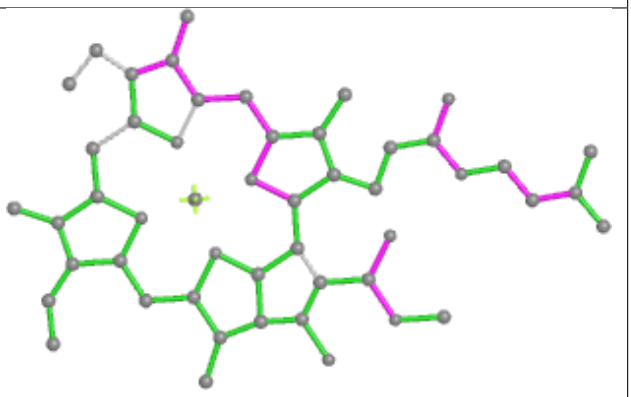
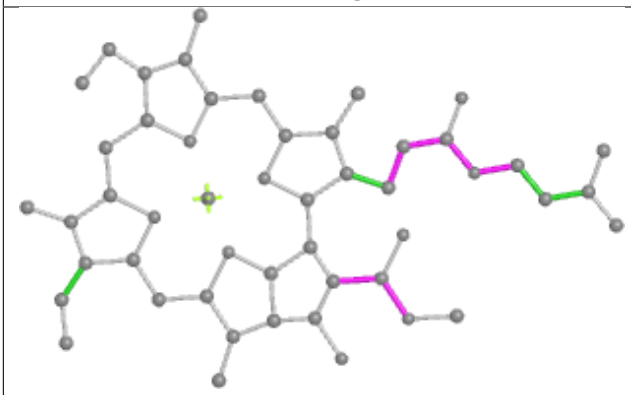
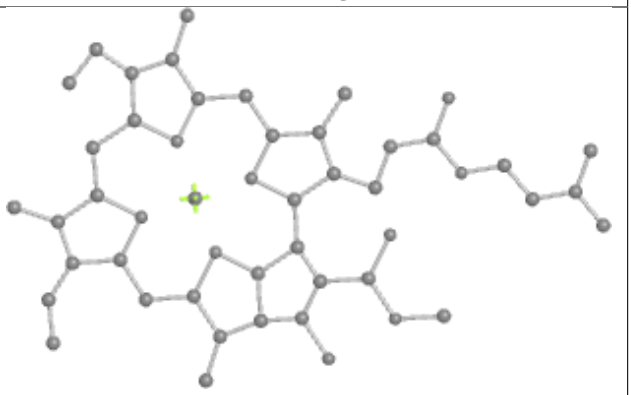


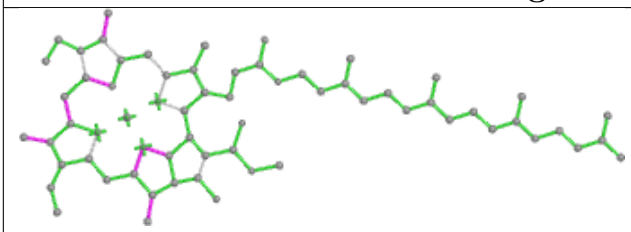
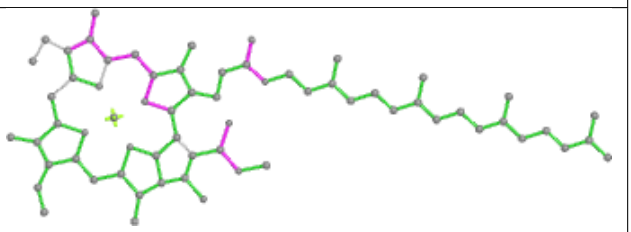
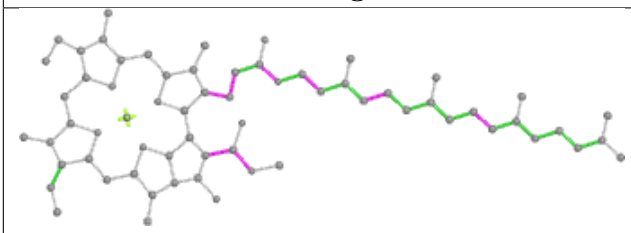
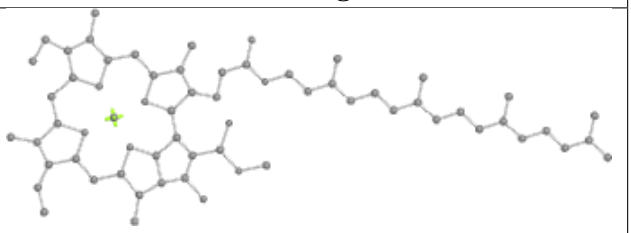
Bond angles



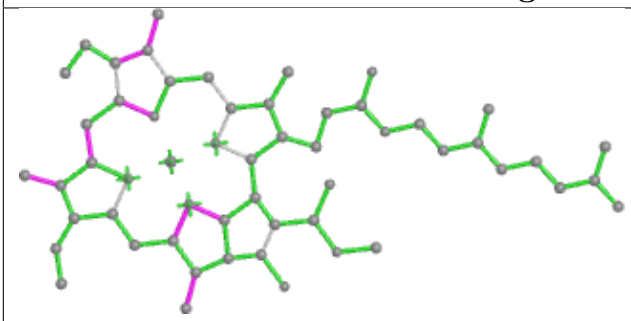
Torsions

Rings

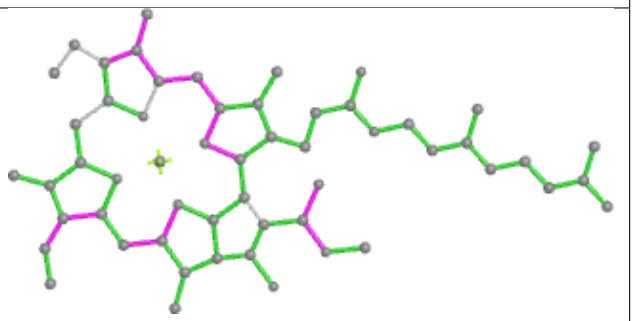
Ligand CLA a 811	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

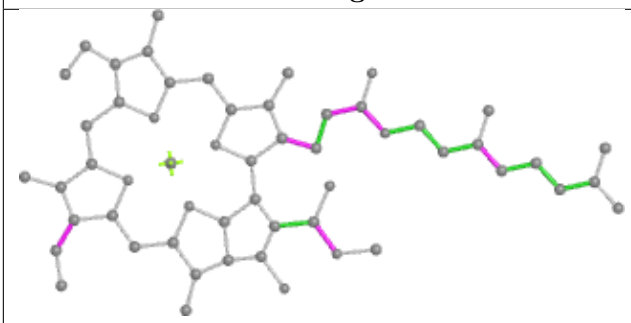
Ligand CLA b 3015



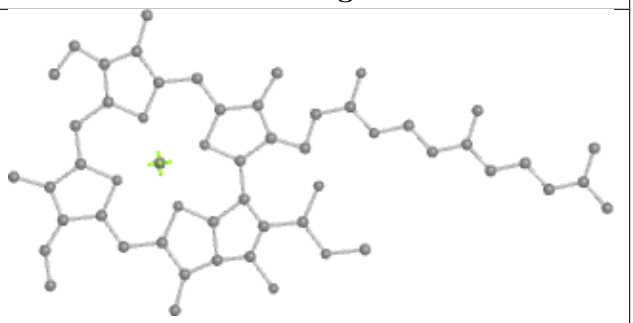
Bond lengths



Bond angles

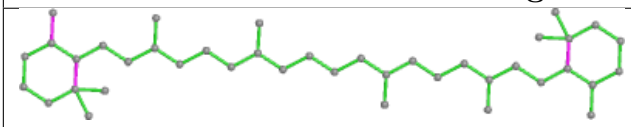


Torsions

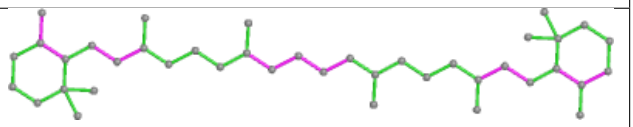


Rings

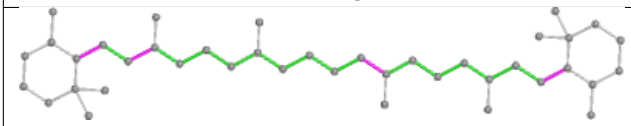
Ligand BCR a 847



Bond lengths



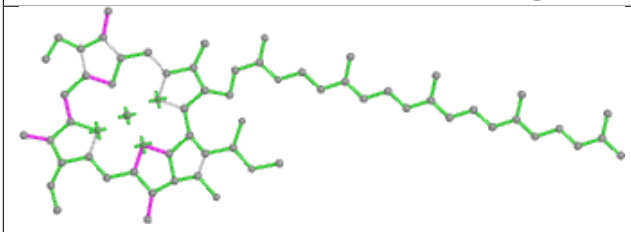
Bond angles



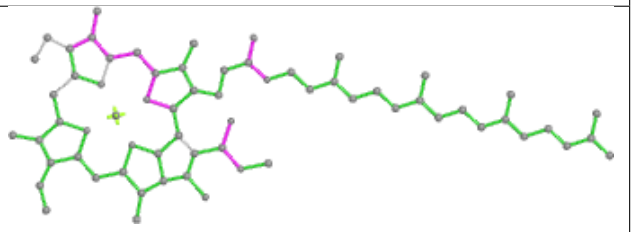
Torsions

Rings

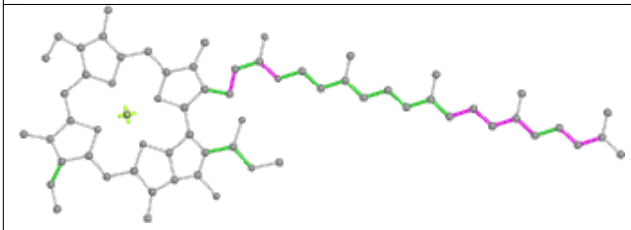
Ligand CLA a 822



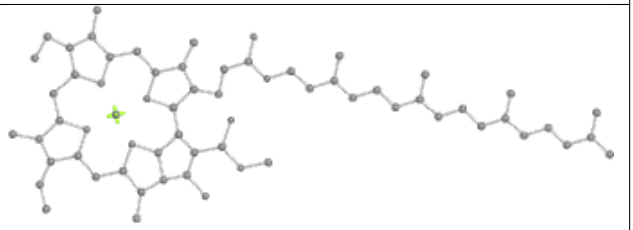
Bond lengths



Bond angles

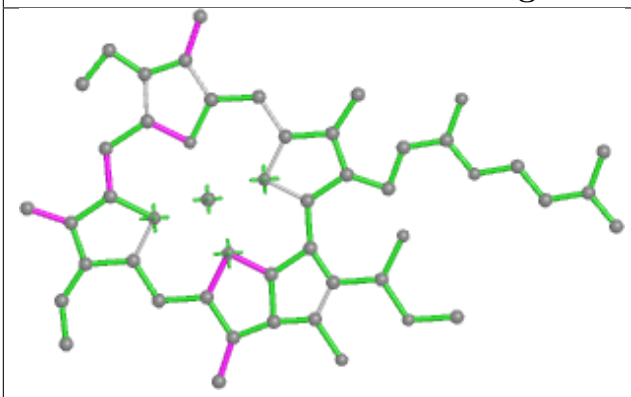


Torsions

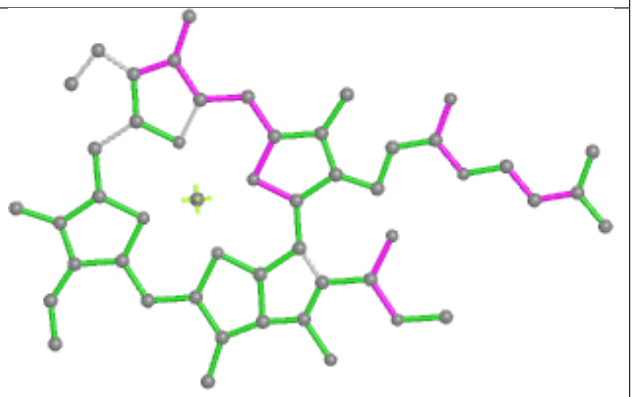


Rings

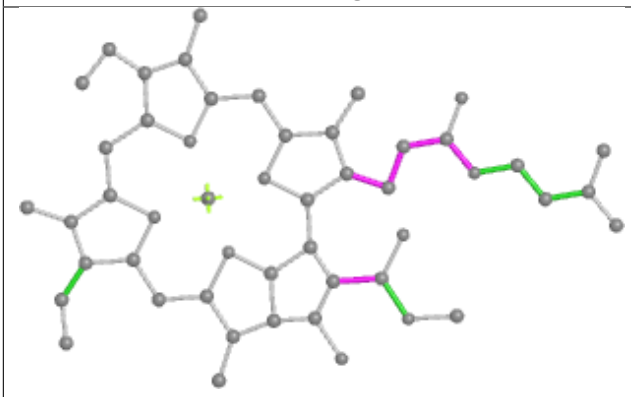
Ligand CLA b 3012



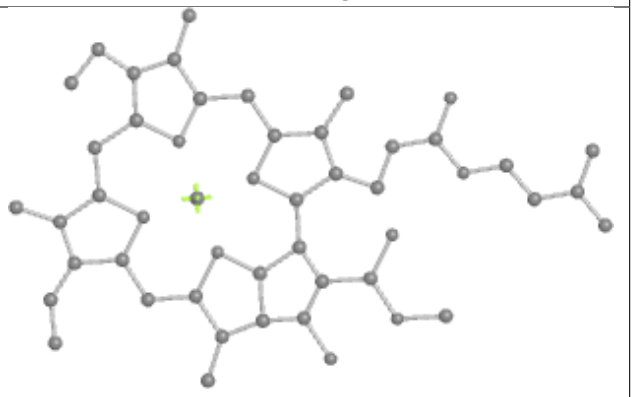
Bond lengths



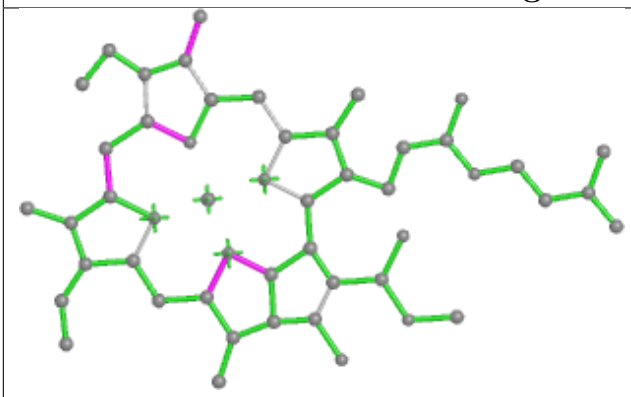
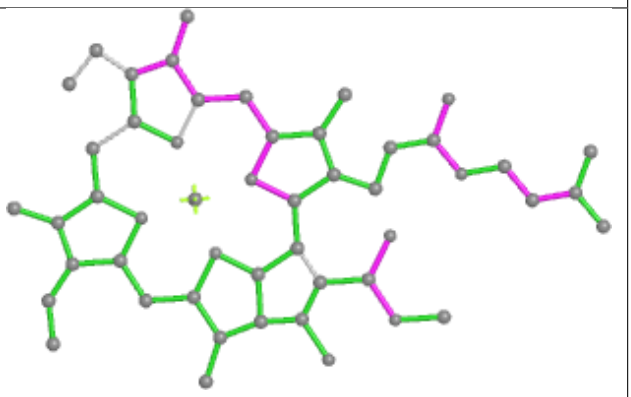
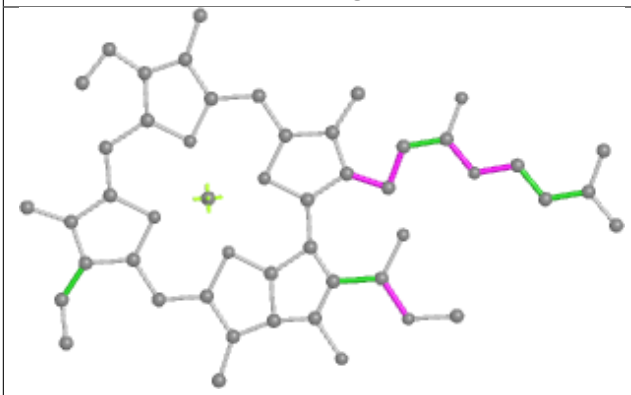
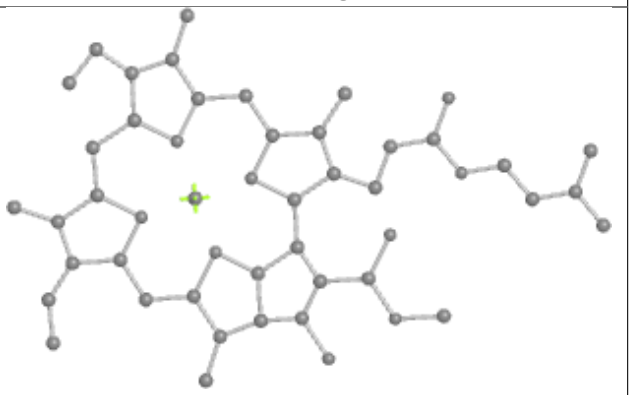
Bond angles

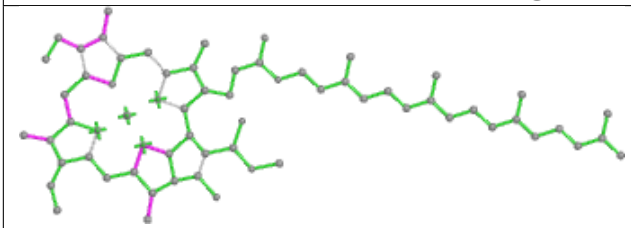
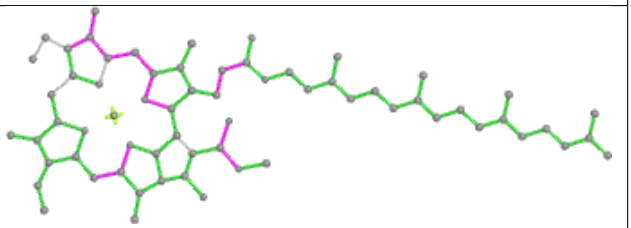
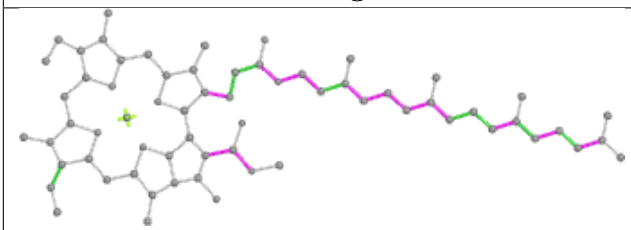
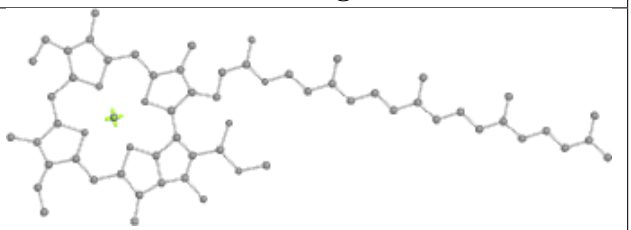


Torsions

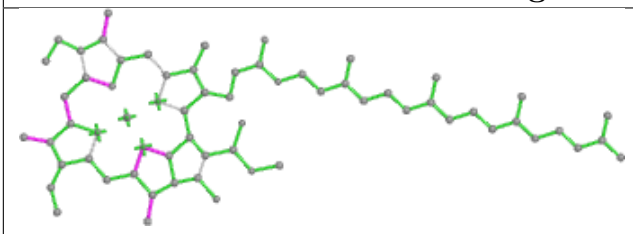


Rings

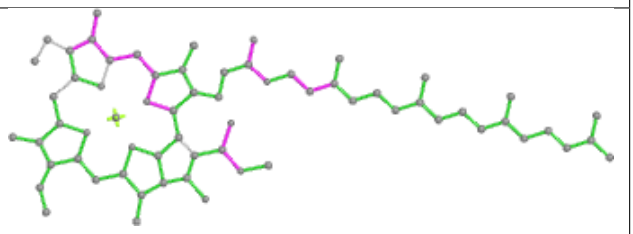
Ligand CLA l 1501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

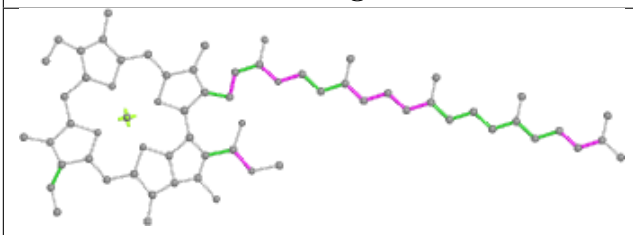
Ligand CLA a 802



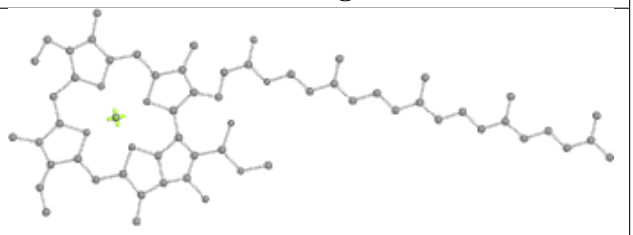
Bond lengths



Bond angles

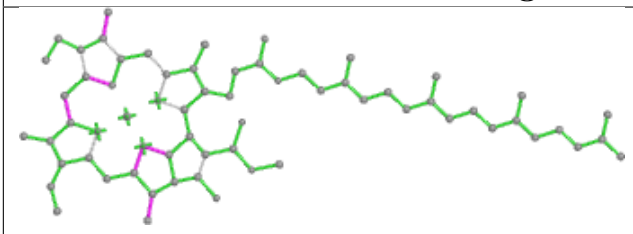


Torsions

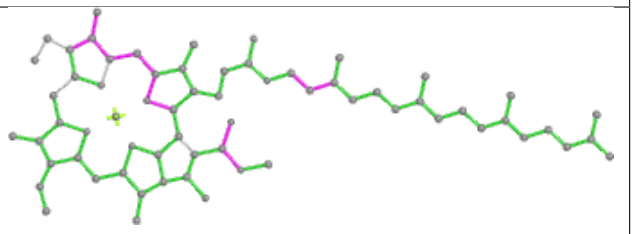


Rings

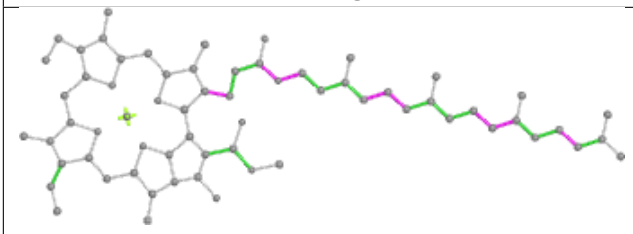
Ligand CLA b 3024



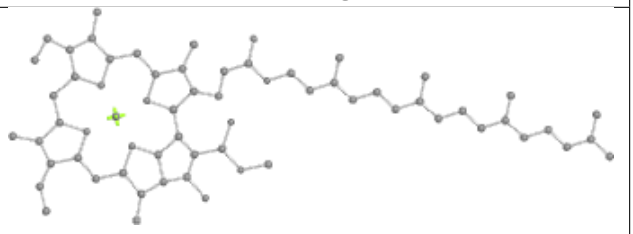
Bond lengths



Bond angles

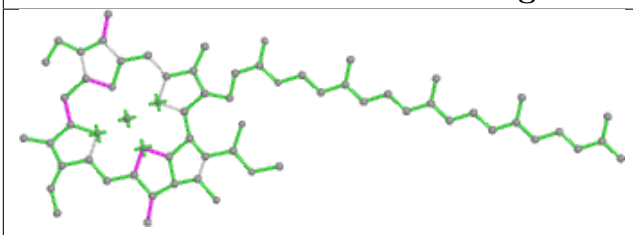


Torsions

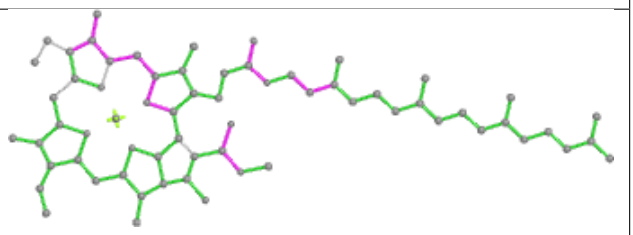


Rings

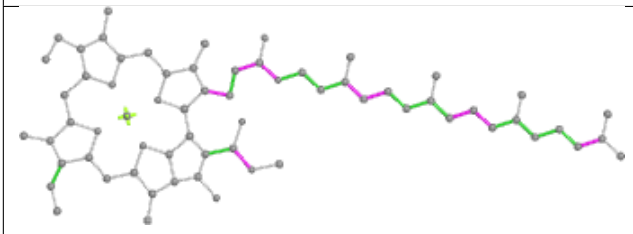
Ligand CLA b 3039



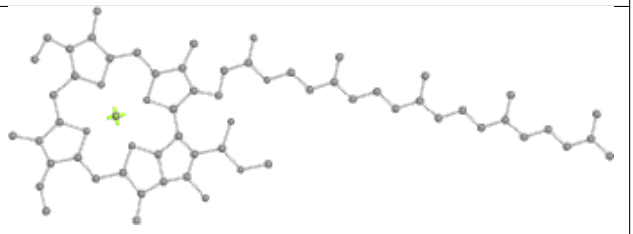
Bond lengths



Bond angles

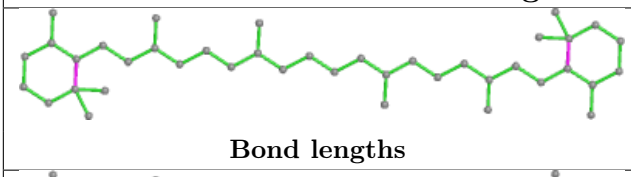


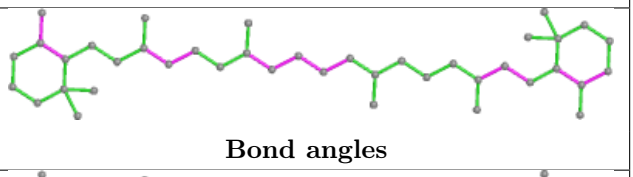
Torsions

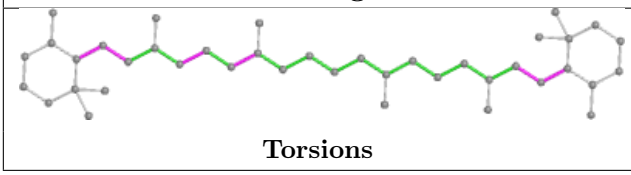


Rings

Ligand BCR A 406


Bond lengths


Bond angles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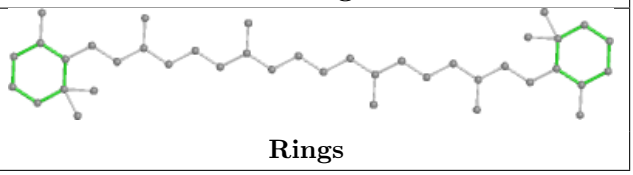
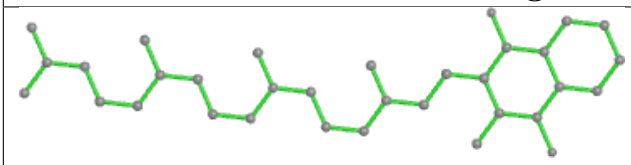
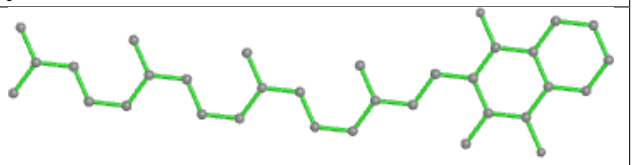
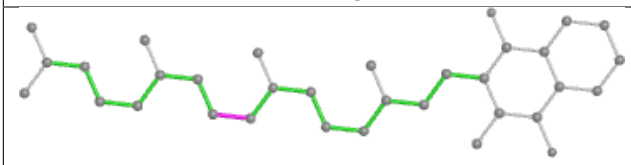
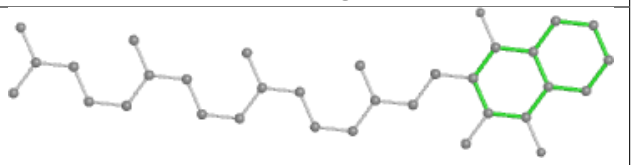

Rings

Ligand PQN a 844

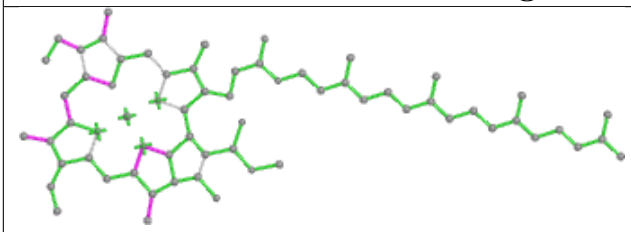

Bond lengths


Bond angles


Torsions


Rings

Ligand CLA b 3008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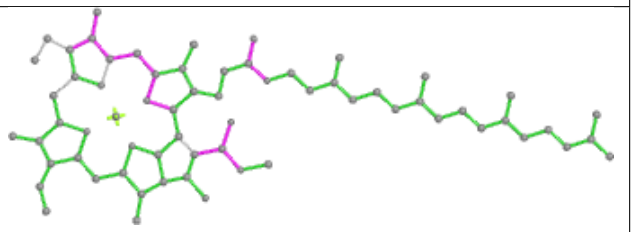
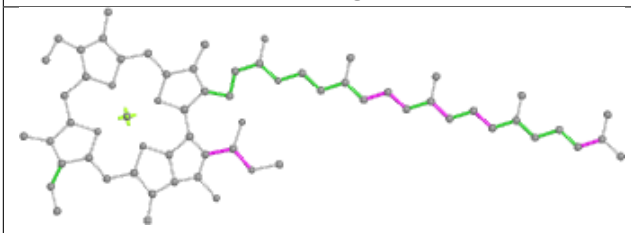

Bond angles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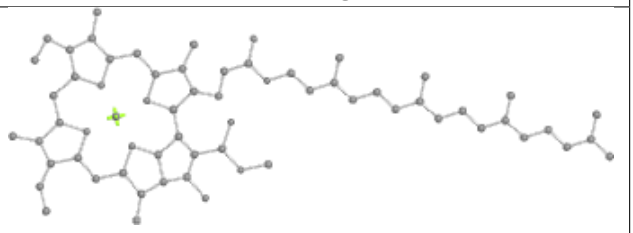
Rings

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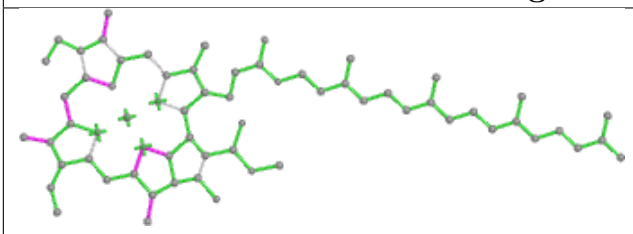
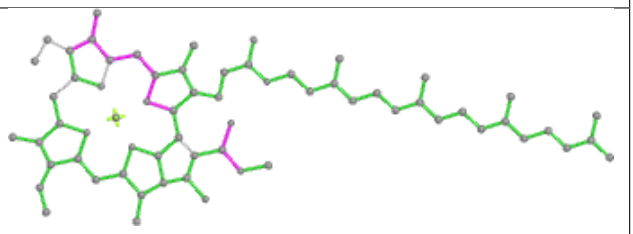
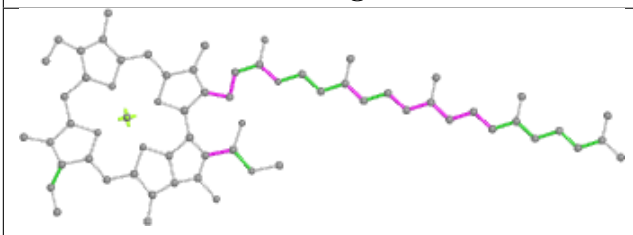


Bond lengths



Bond angles



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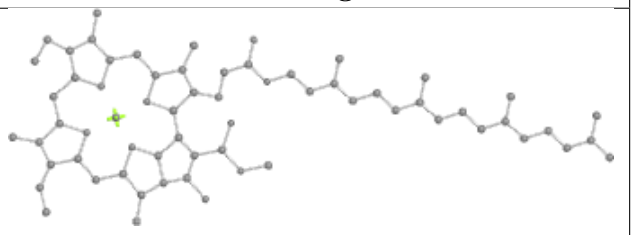
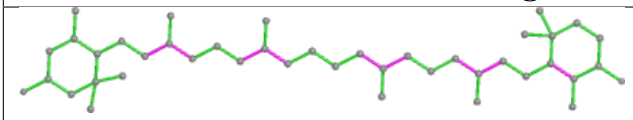


Rings

Ligand EQ3 b 3052



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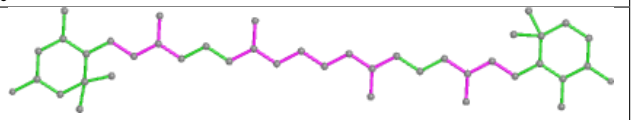
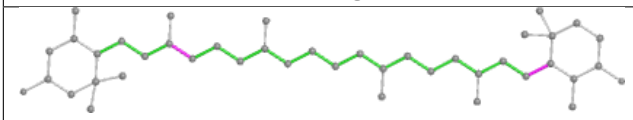


Bond angles



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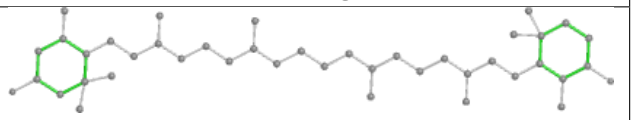
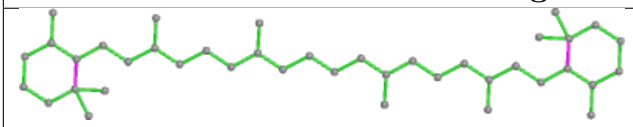


Rings

Ligand BCR j 101



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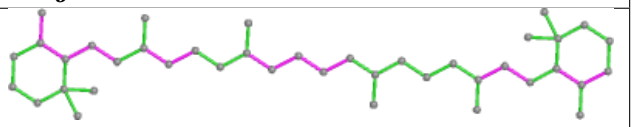
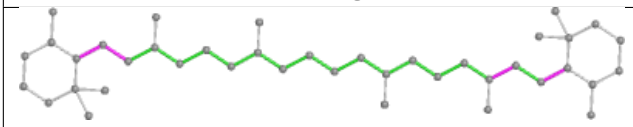


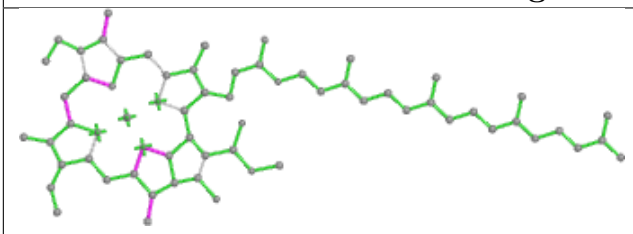
Bond angles



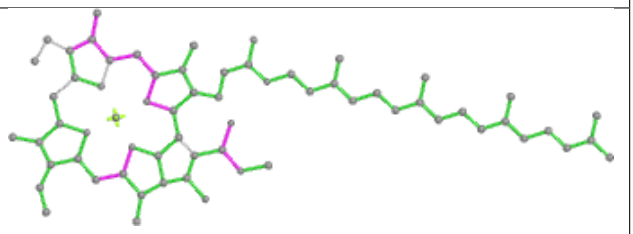
Torsions

Rings

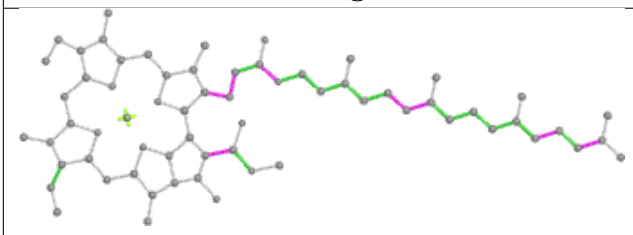
Ligand CLA a 805



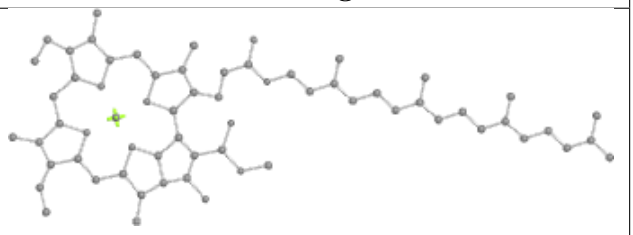
Bond lengths



Bond angles

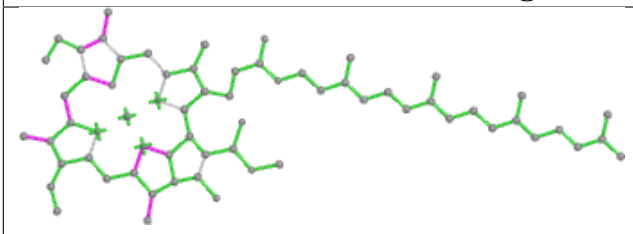


Torsions



Rings

Ligand CLA b 3040



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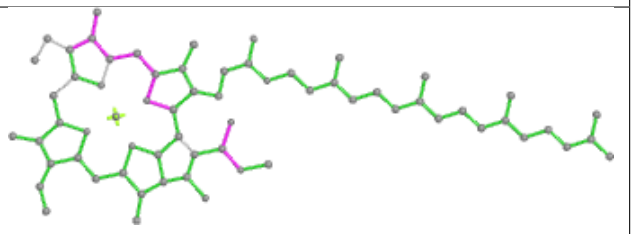
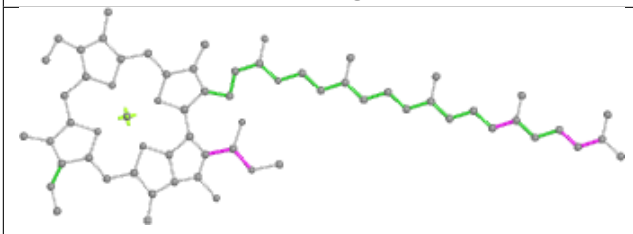
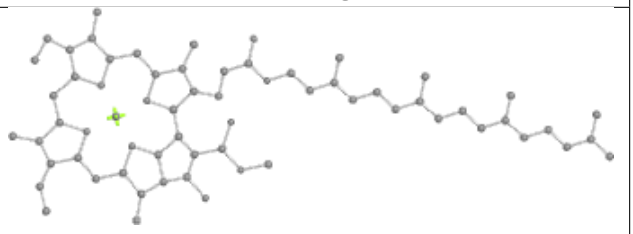


Bond angles

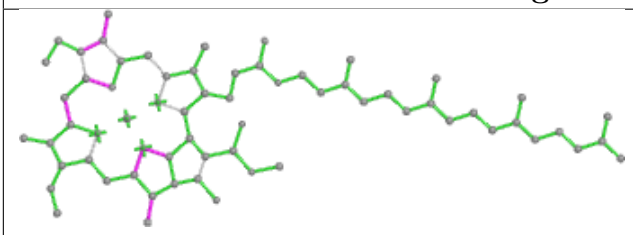


Torsions

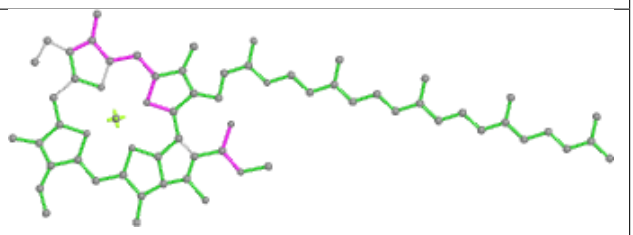


Rings

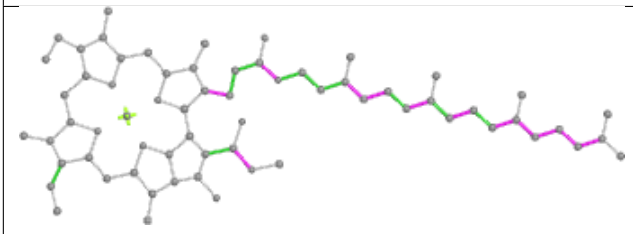
Ligand CLA f 201



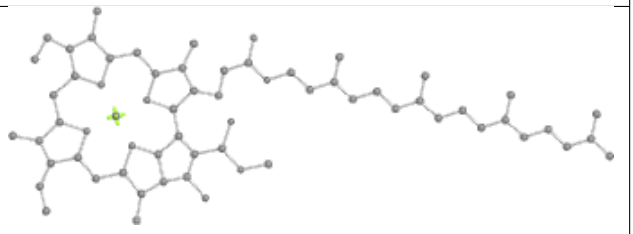
Bond lengths



Bond angles

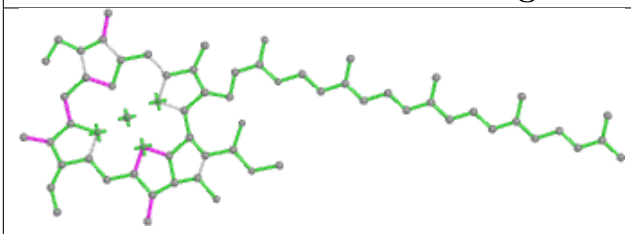


Torsions

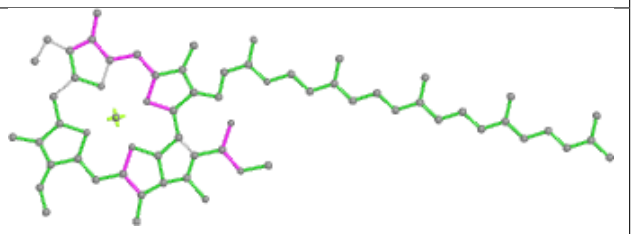


Rings

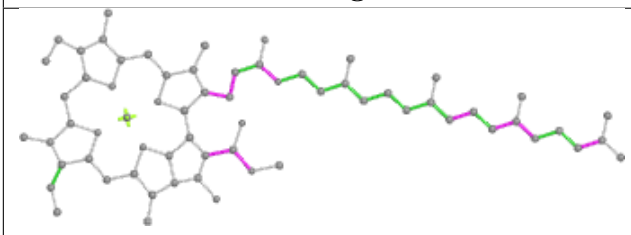
Ligand CLA b 3028



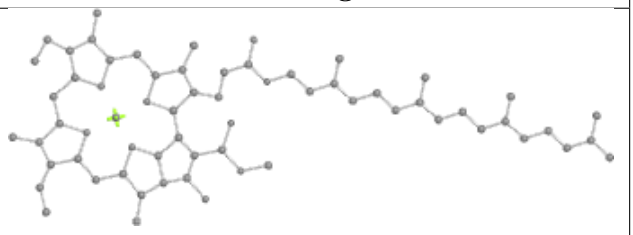
Bond lengths



Bond angles

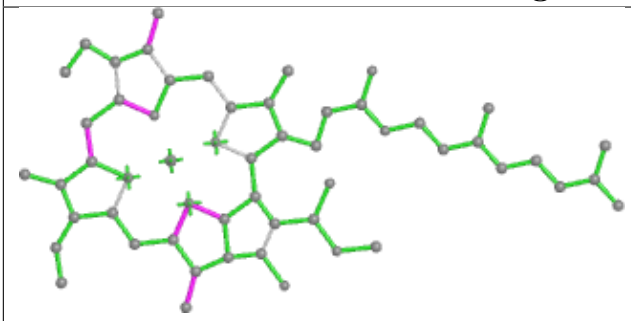


Torsions

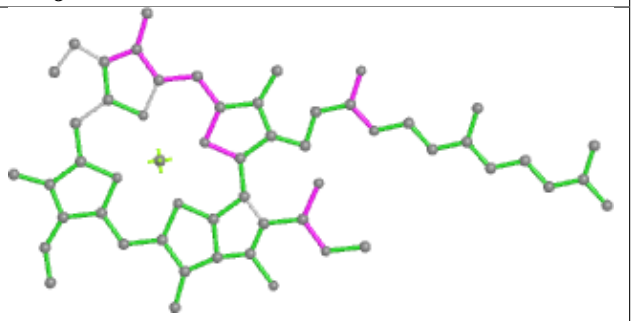


Rings

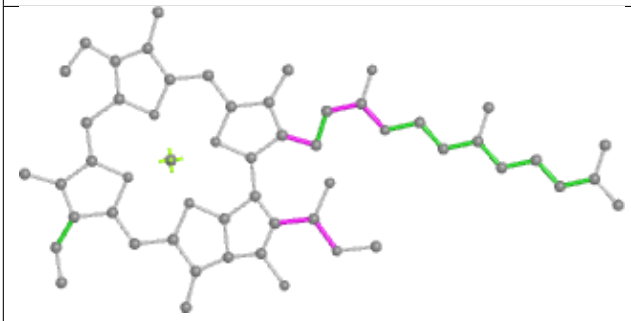
Ligand CLA j 102



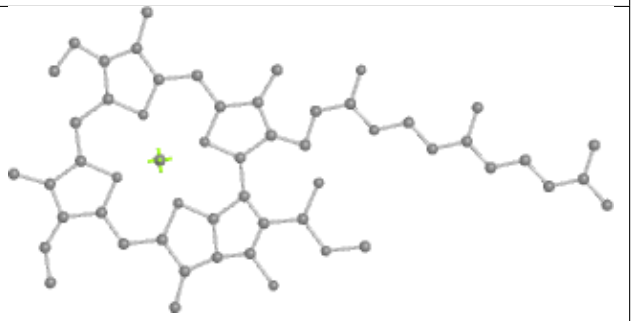
Bond lengths



Bond angles

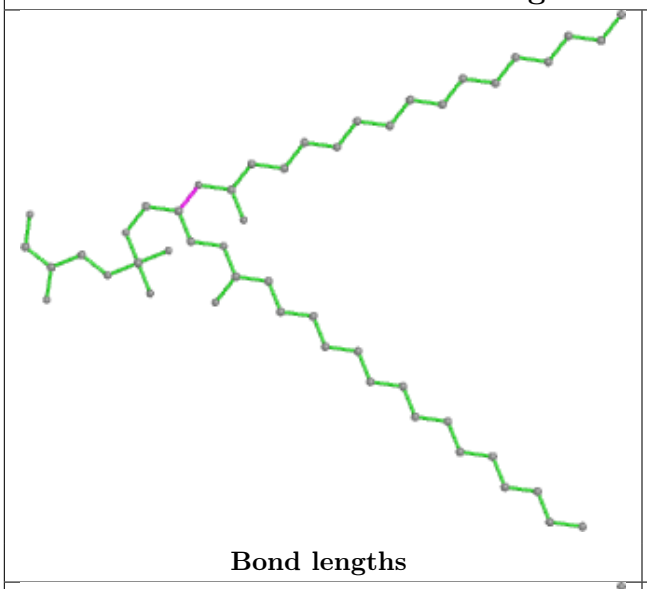


Torsions

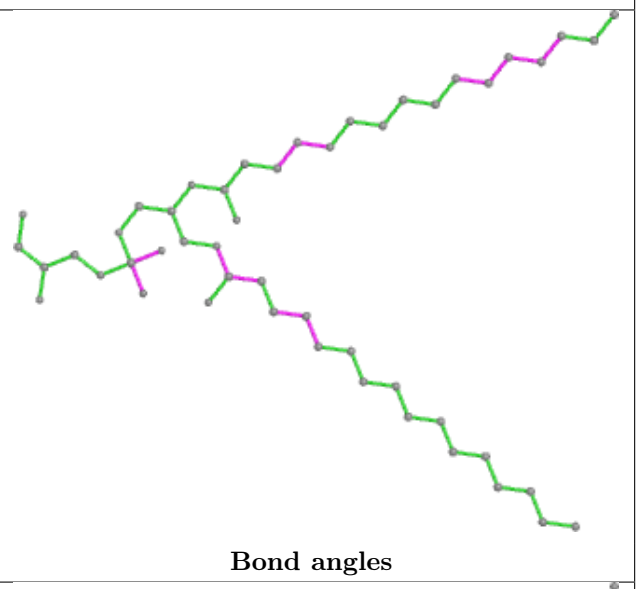


Rings

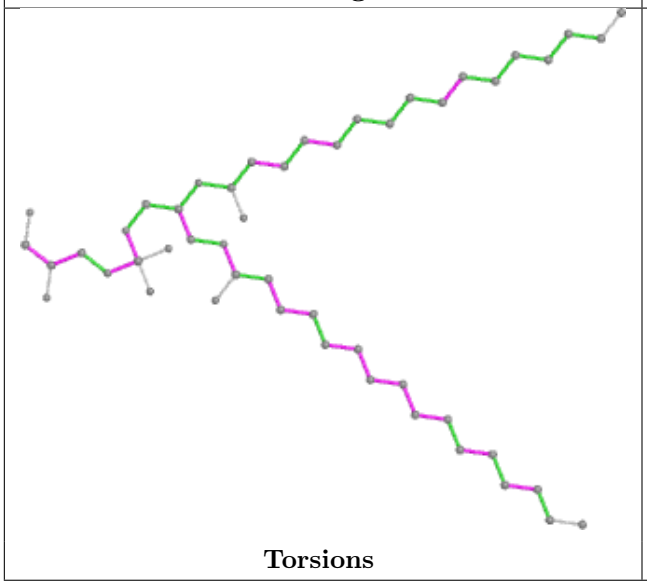
Ligand LHG a 852



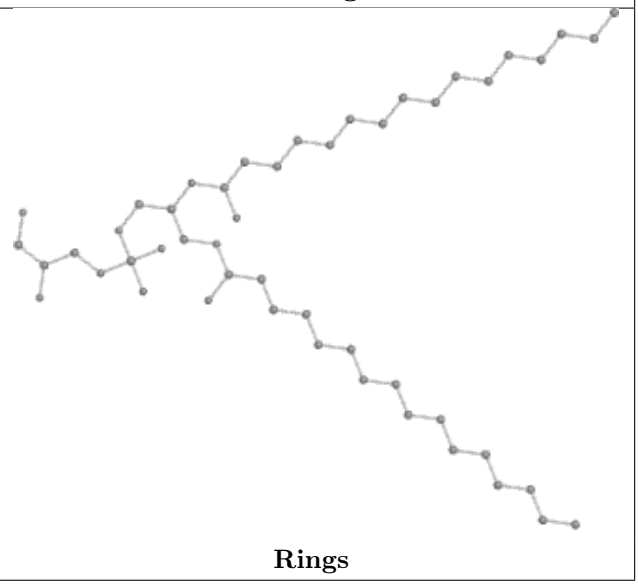
Bond lengths



Bond angles

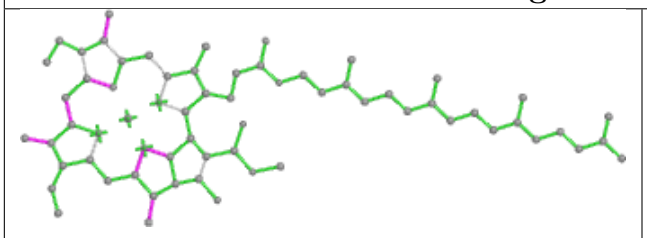


Torsions

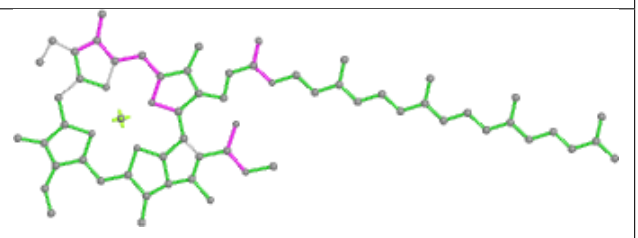


Rings

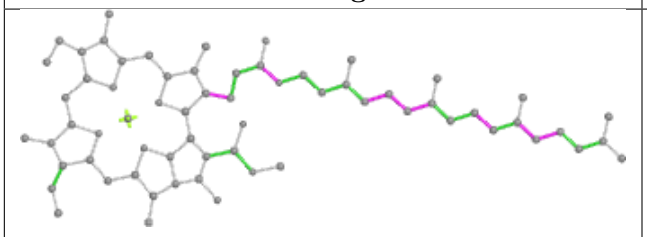
Ligand CLA a 858



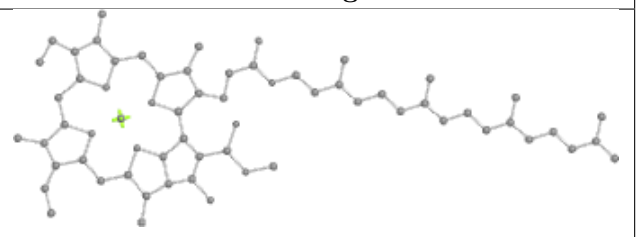
Bond lengths



Bond angles

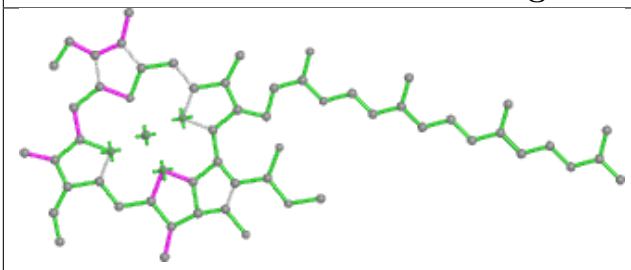


Torsions



Rings

Ligand CLA a 833



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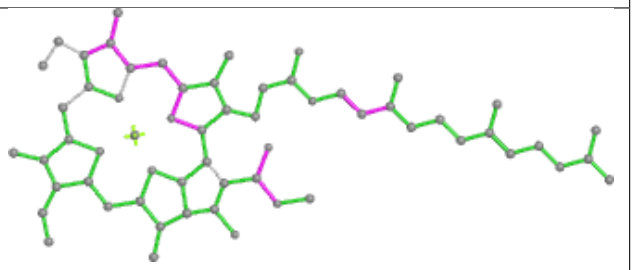
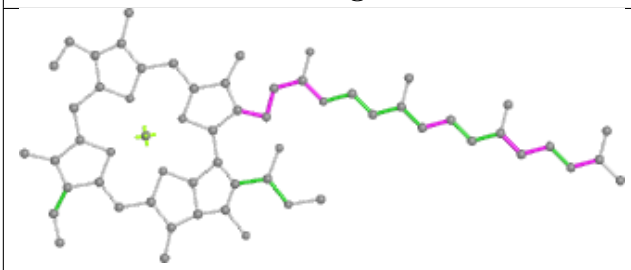
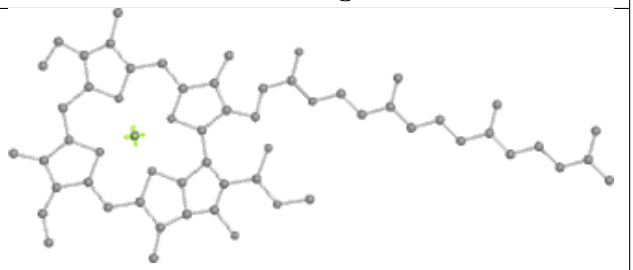


Bond angles

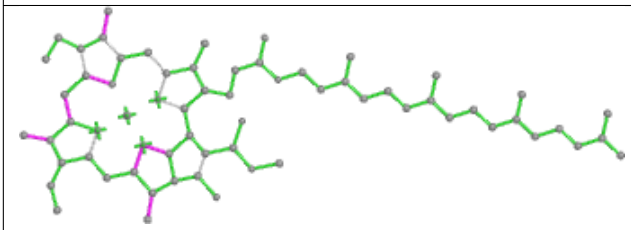


Torsions



Rings

Ligand CLA a 842



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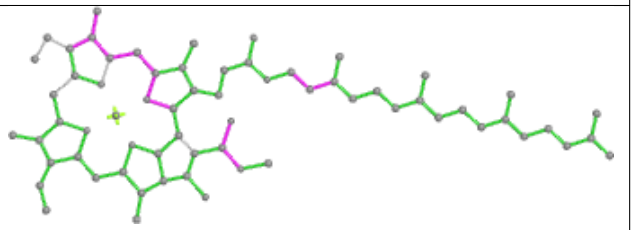
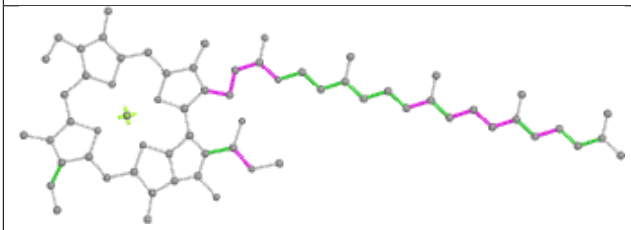
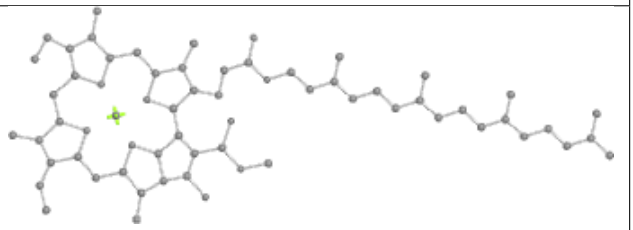


Bond angles

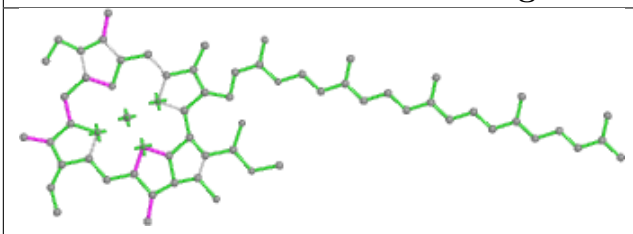


Torsions

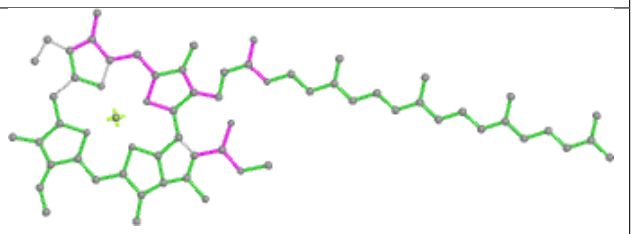


Rings

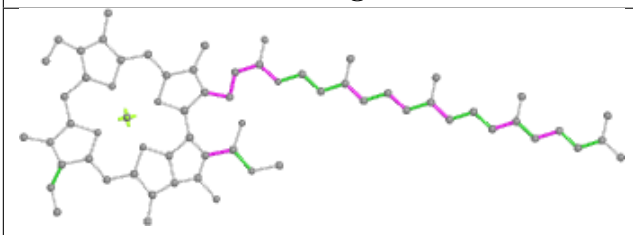
Ligand CLA b 3029



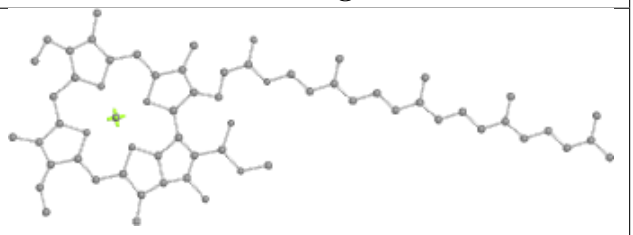
Bond lengths



Bond angles

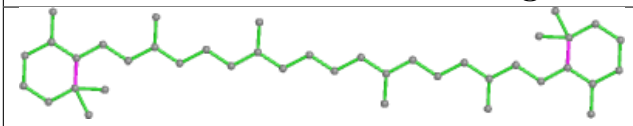


Torsions

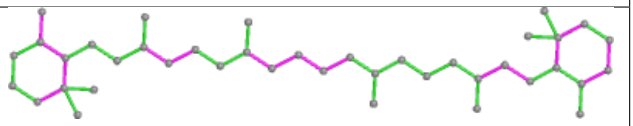


Rings

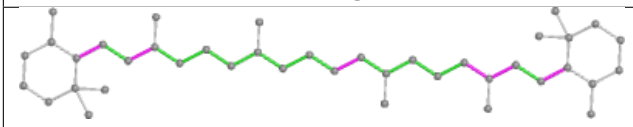
Ligand BCR l 1504



Bond lengths



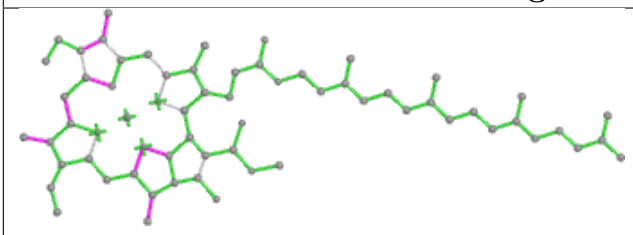
Bond angles



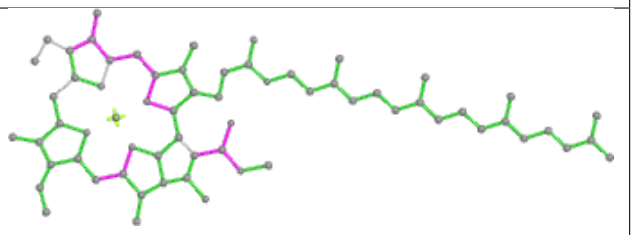
Torsions

Rings

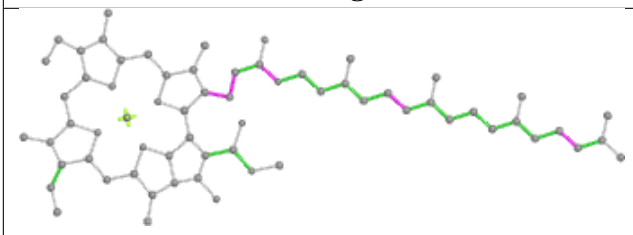
Ligand CLA a 804



Bond lengths



Bond angles



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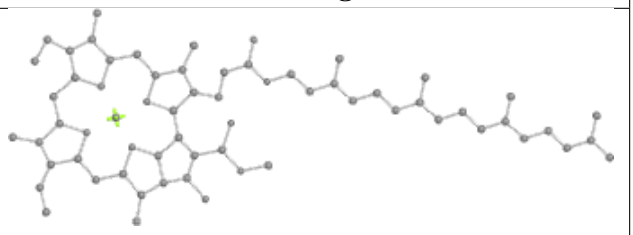
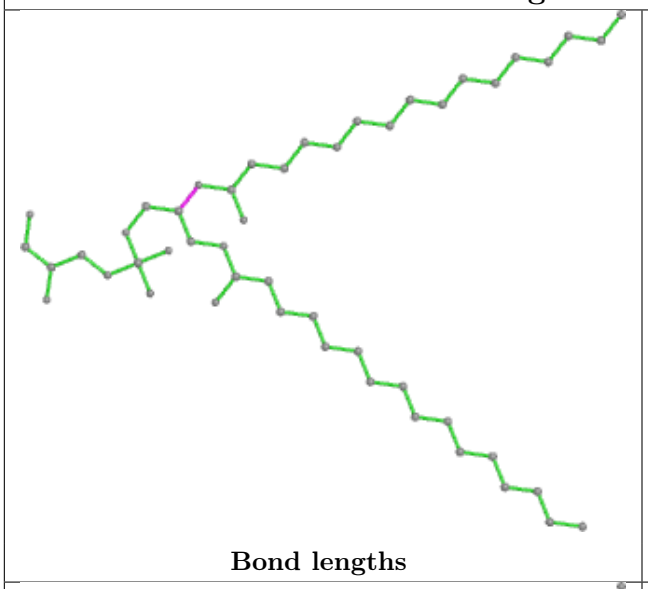
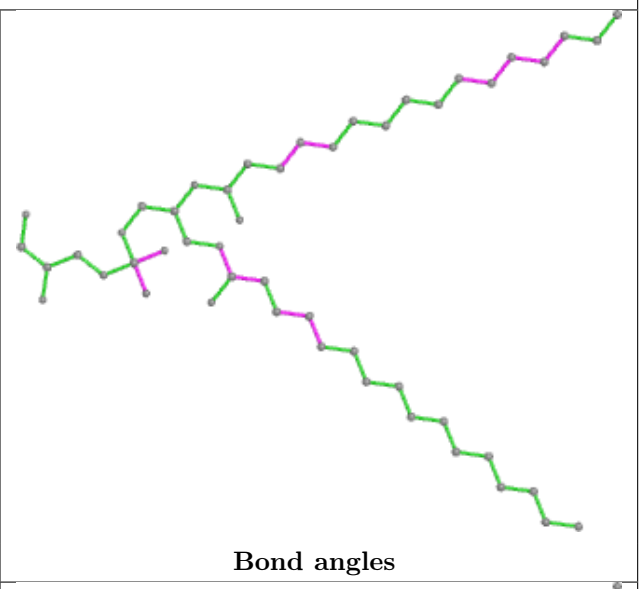


Rings

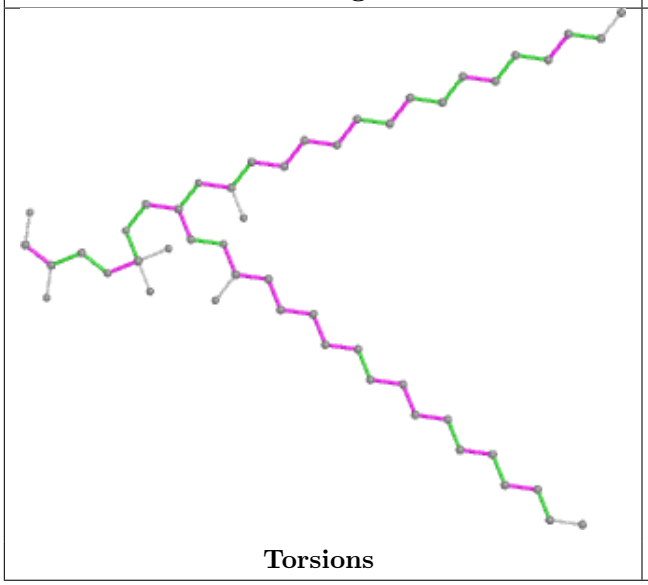
Ligand LHG a 850



Bond lengths



Bond angles



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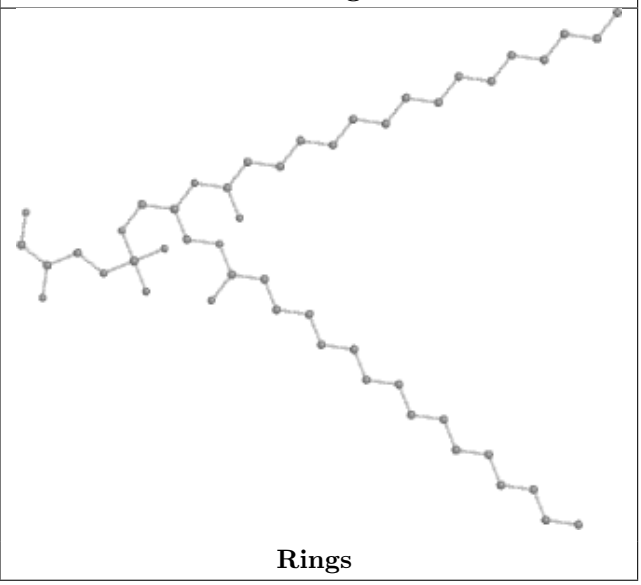
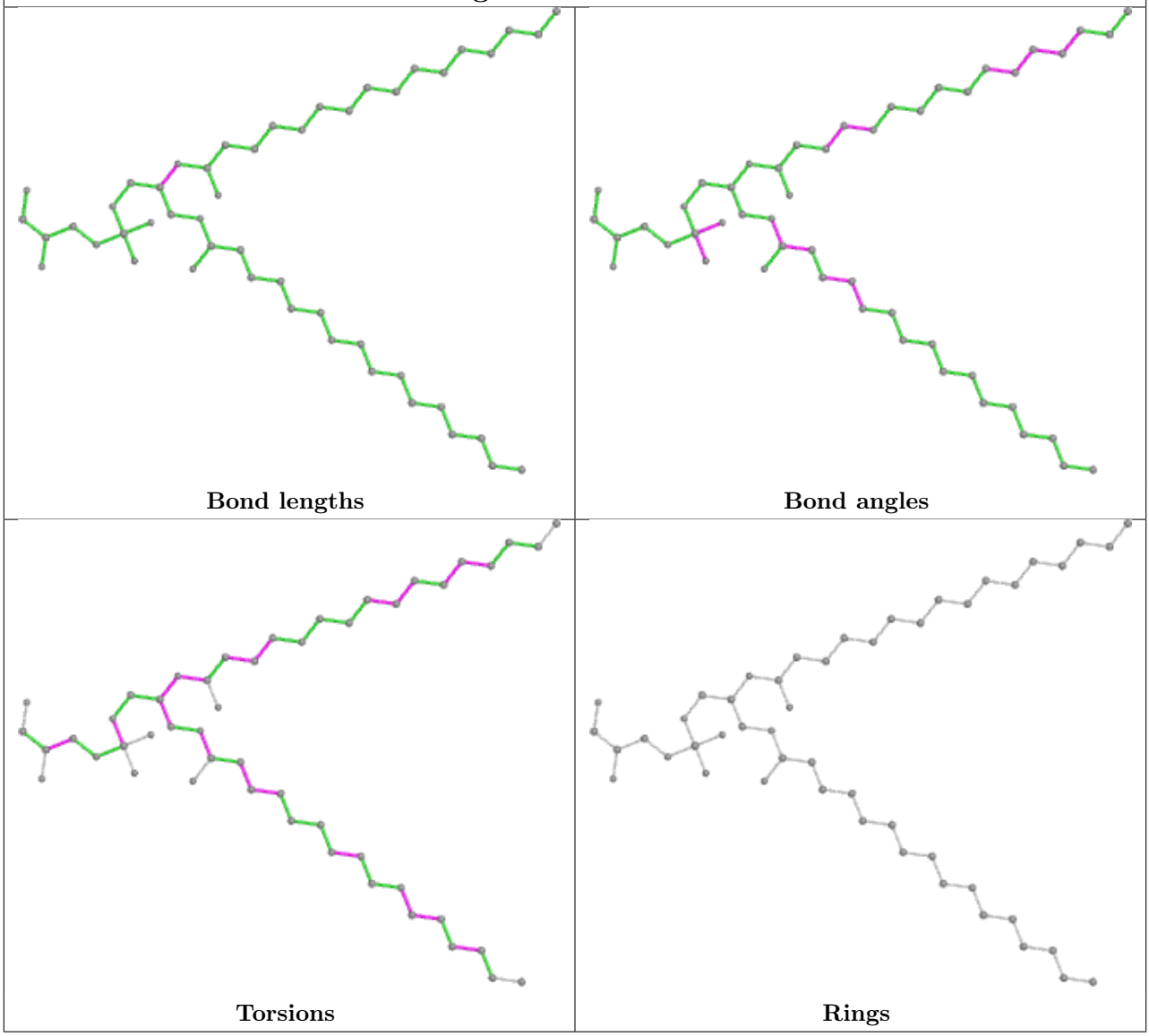
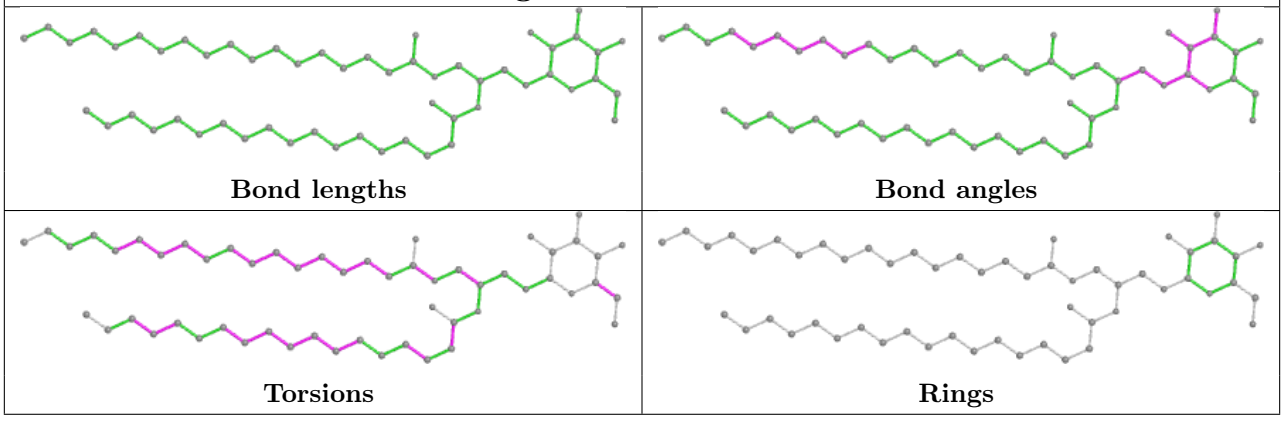


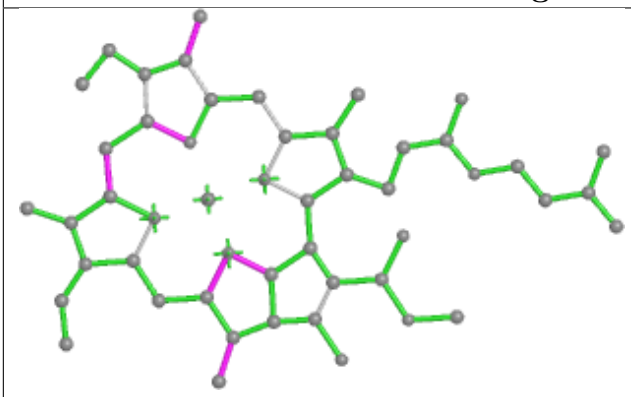
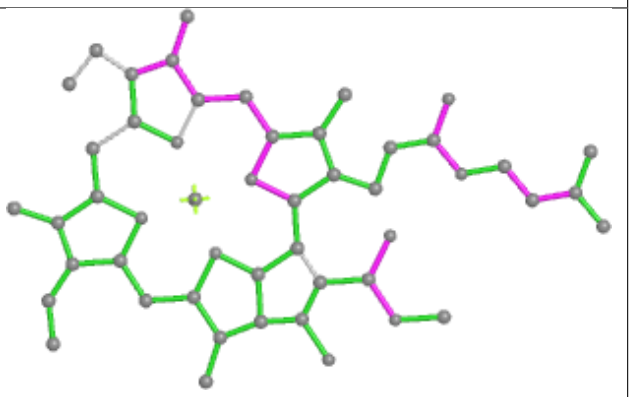
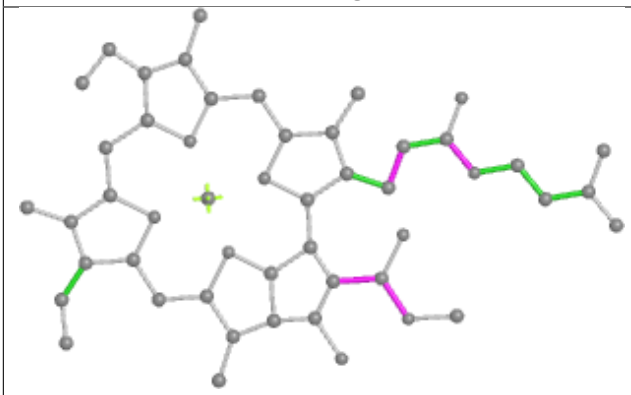
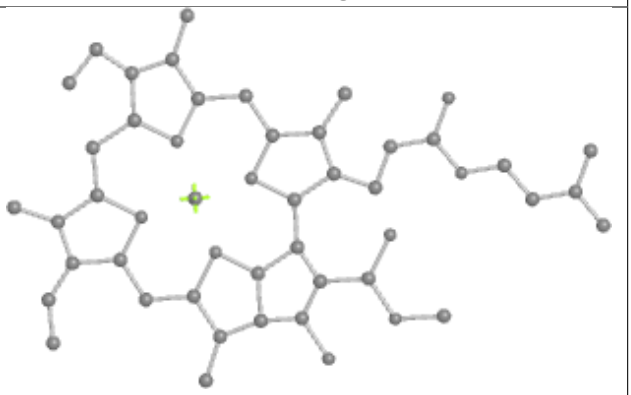
Rings

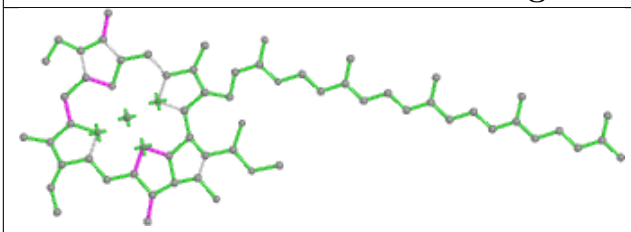
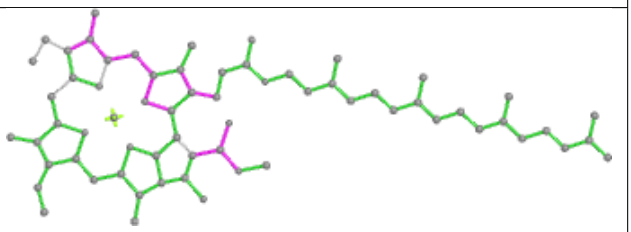
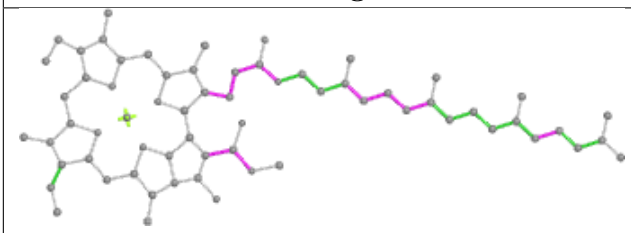
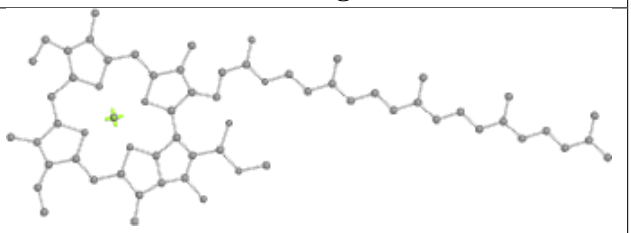
Ligand LHG a 854

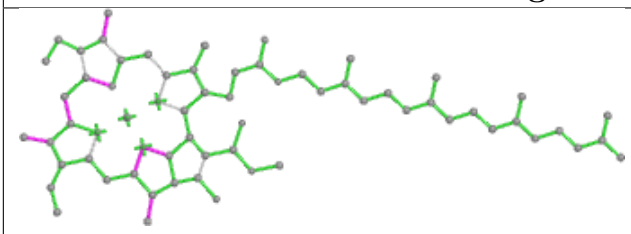
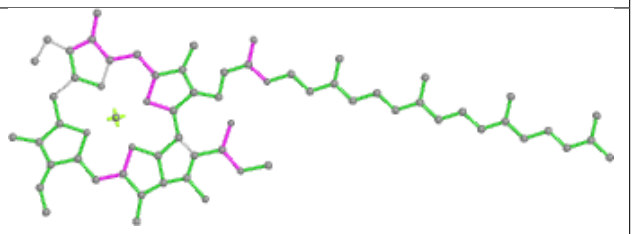
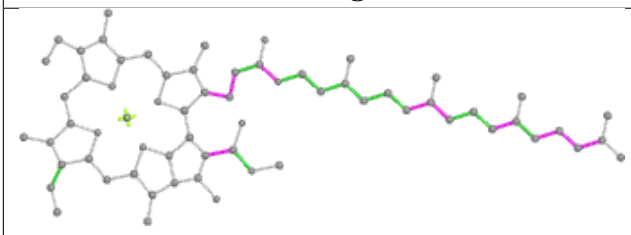
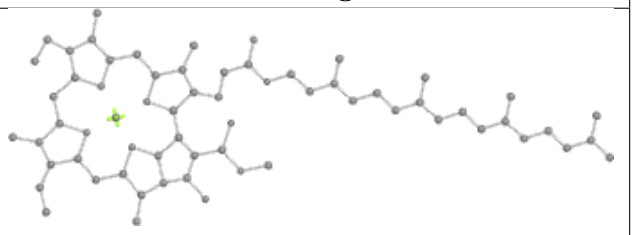


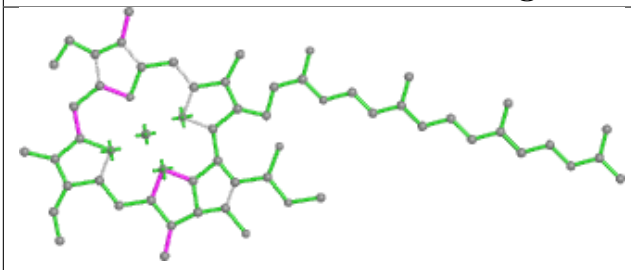
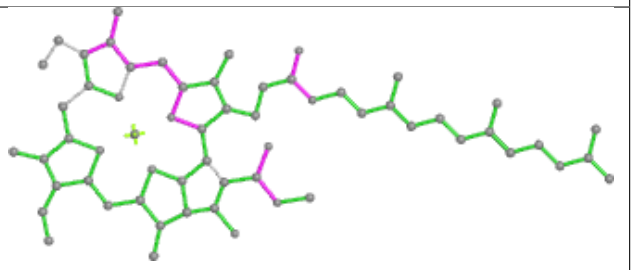
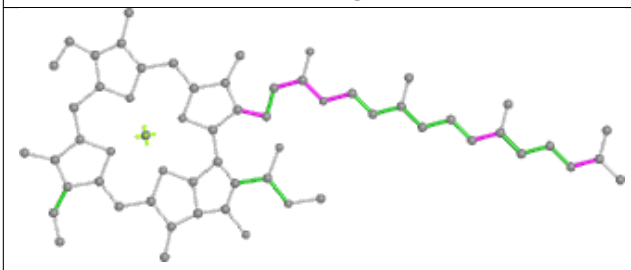
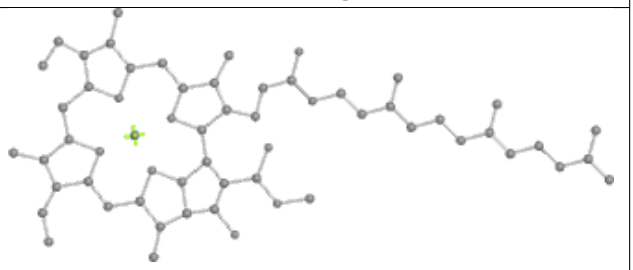
Ligand LMG b 3049



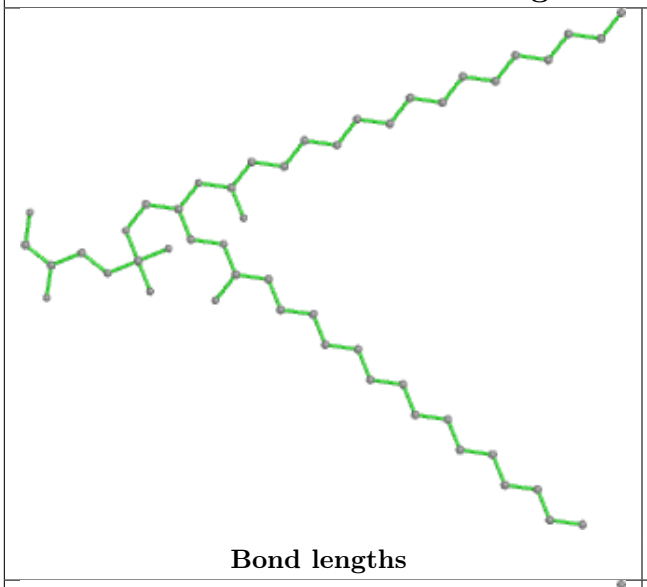
Ligand CLA f 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 831	
 Bond lengths	 Bond angles
 Torsions	 Rings

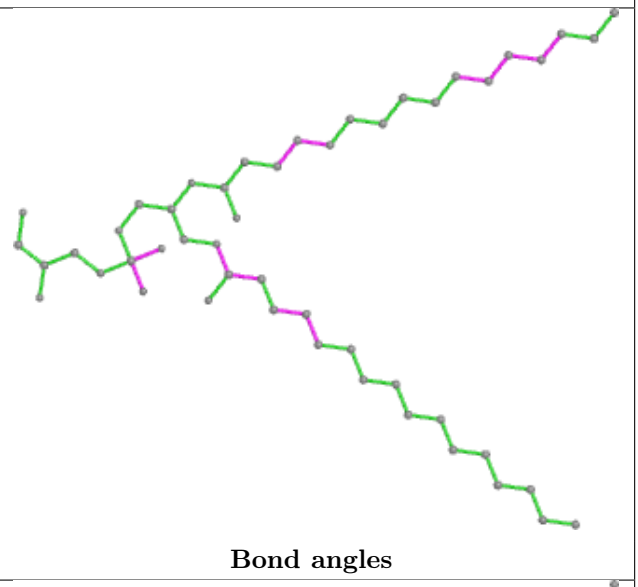
Ligand CLA a 820	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b 3021	
 Bond lengths	 Bond angles
 Torsions	 Rings

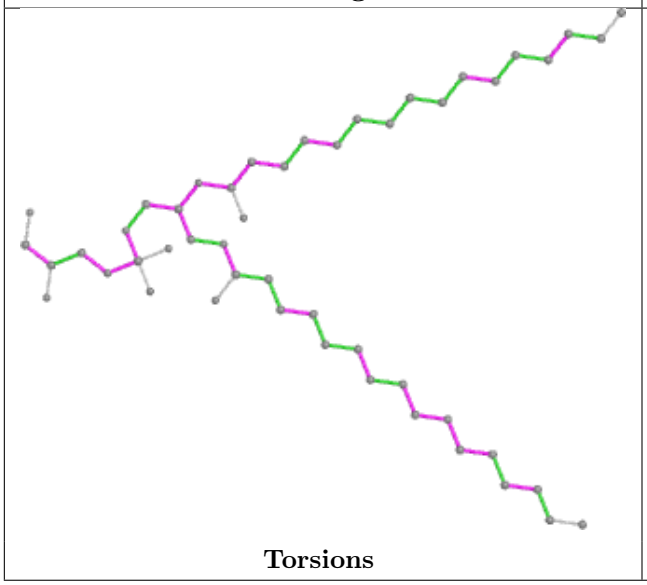
Ligand LHG f 206



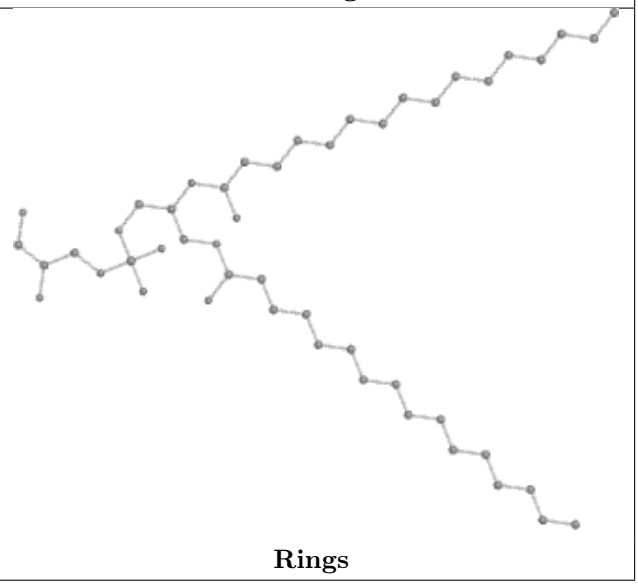
Bond lengths



Bond angles

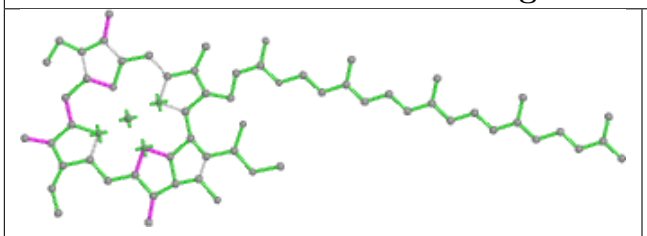


Torsions

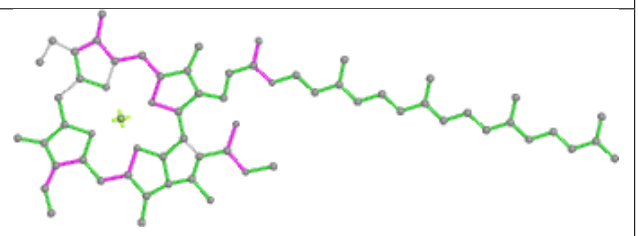


Rings

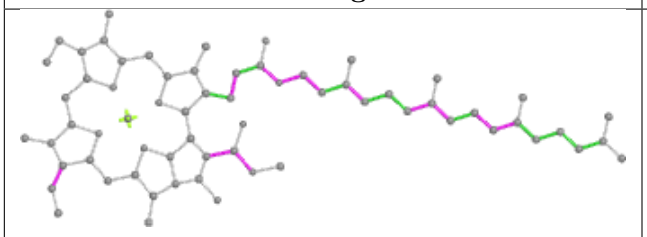
Ligand CLA b 3003



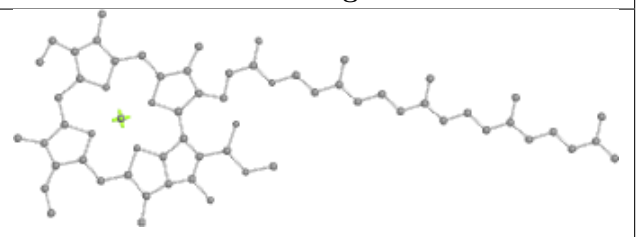
Bond lengths



Bond angles

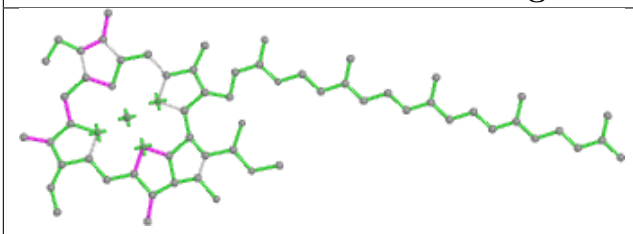


Torsions

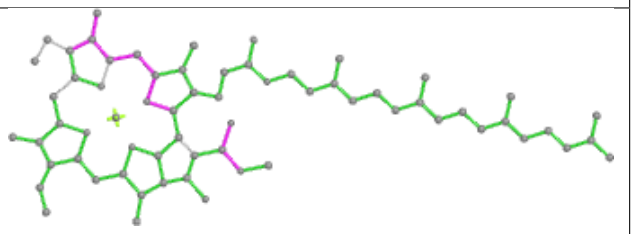


Rings

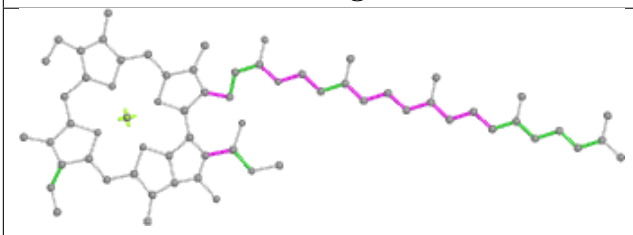
Ligand CLA a 856



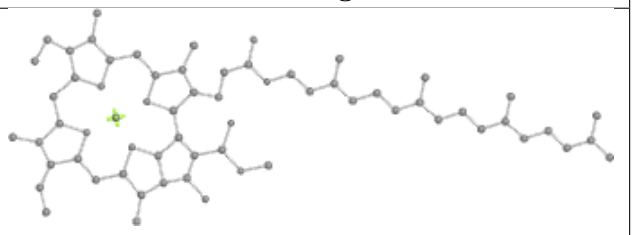
Bond lengths



Bond angles

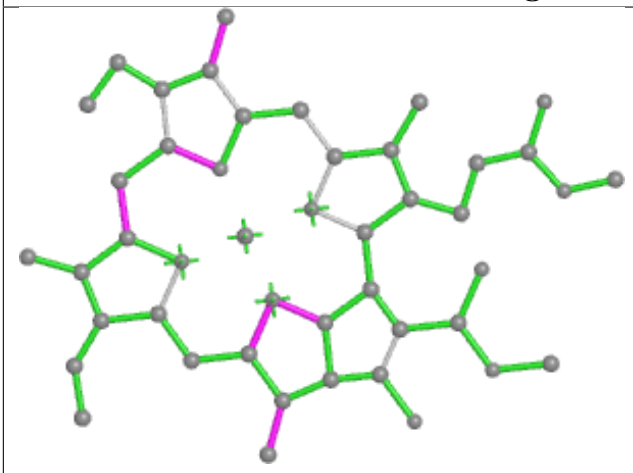


Torsions

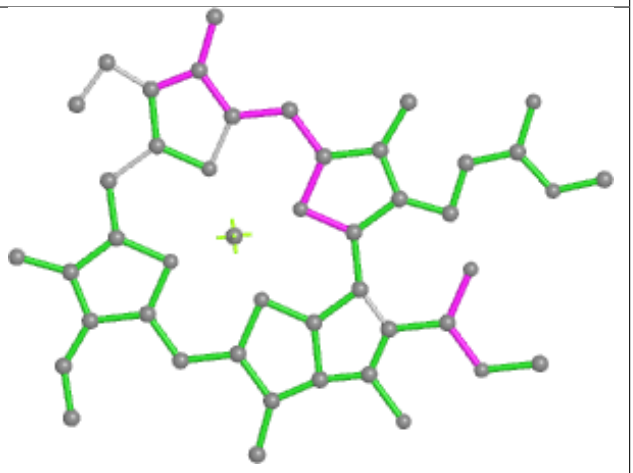


Rings

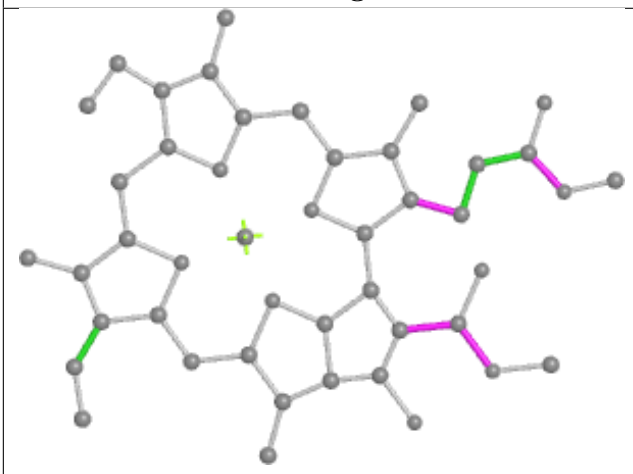
Ligand CLA A 403



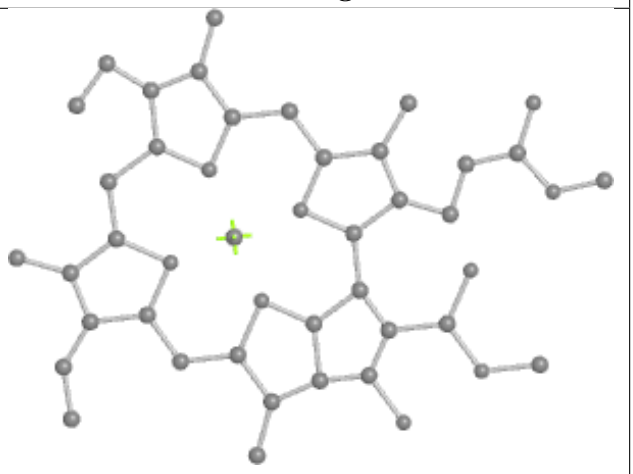
Bond lengths



Bond angles

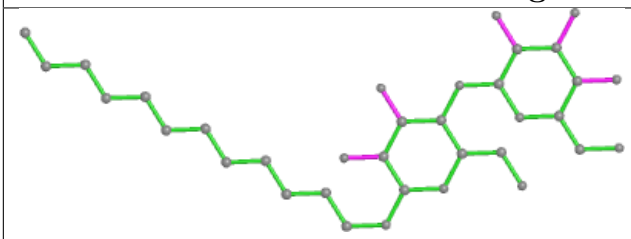


Torsions

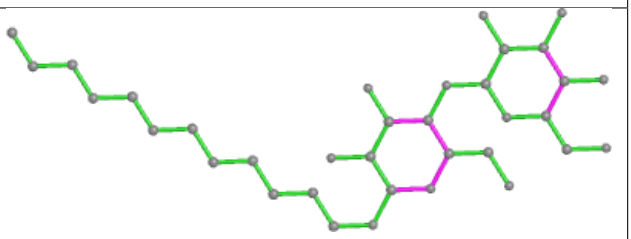


Rings

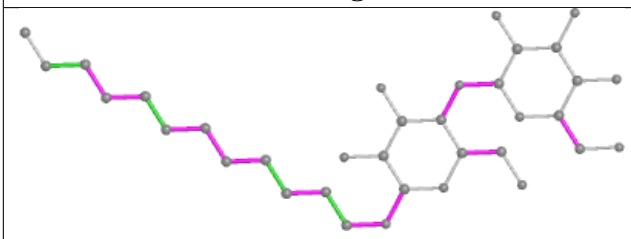
Ligand LMT f 207



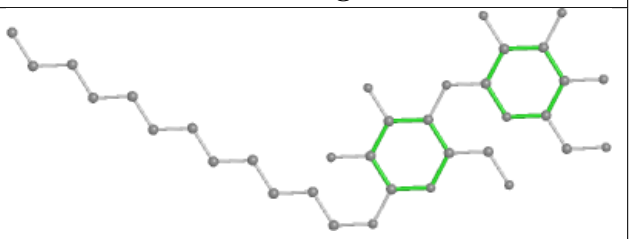
Bond lengths



Bond angles

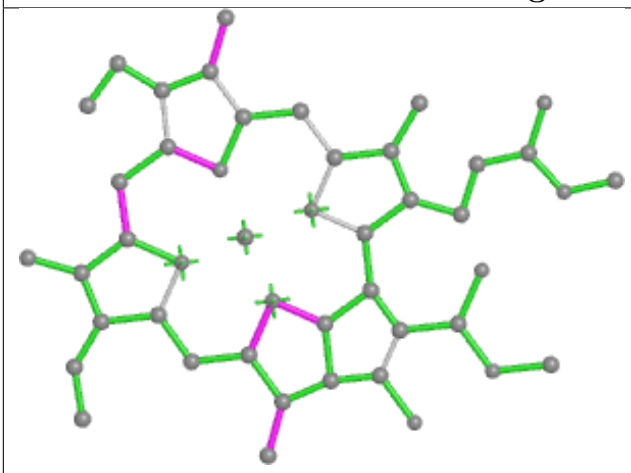


Torsions

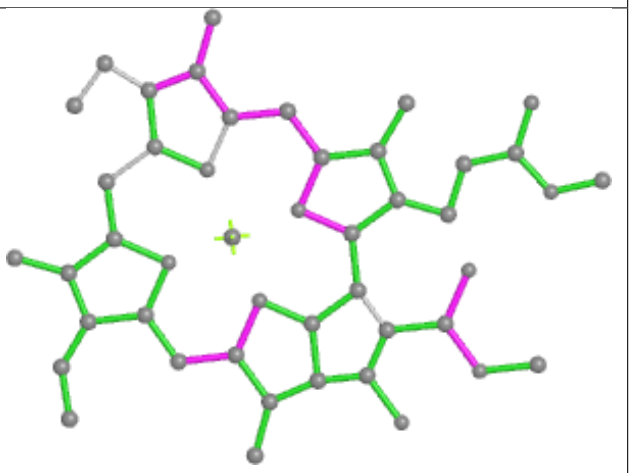


Rings

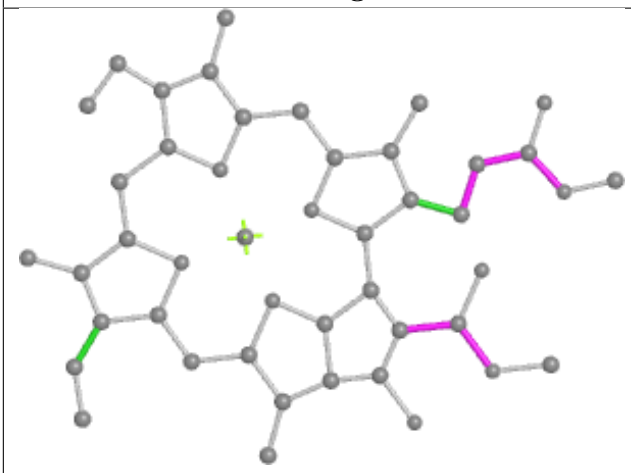
Ligand CLA a 816



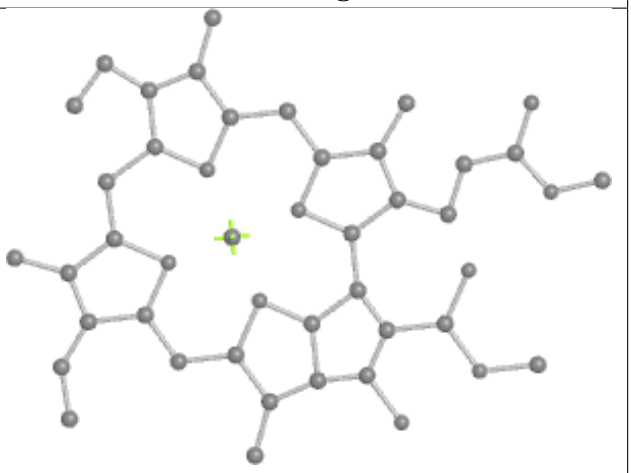
Bond lengths



Bond angles

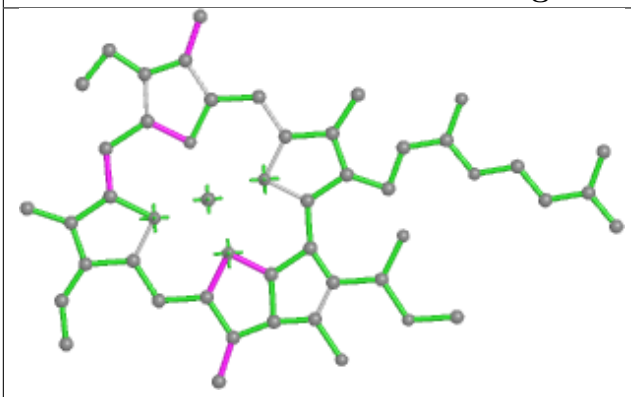


Torsions

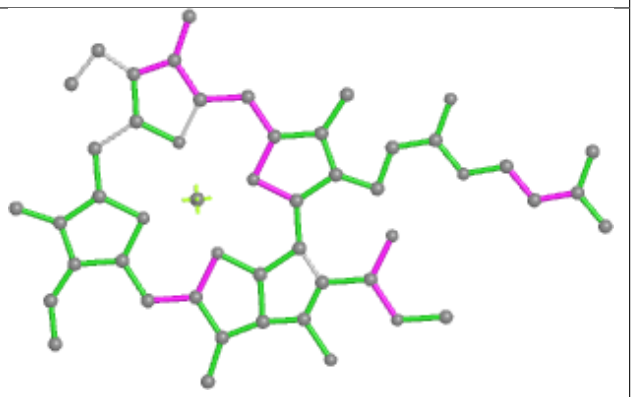


Rings

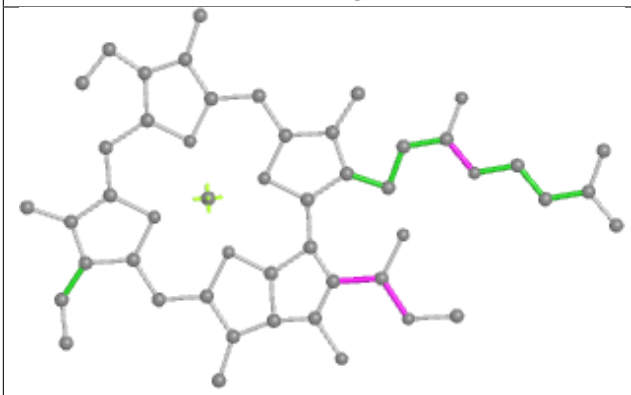
Ligand CLA f 203



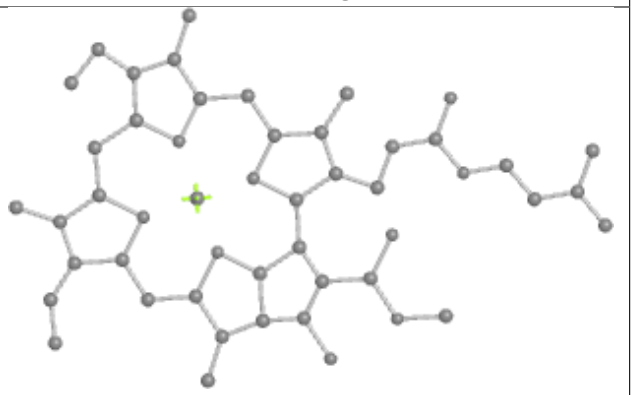
Bond lengths



Bond angles

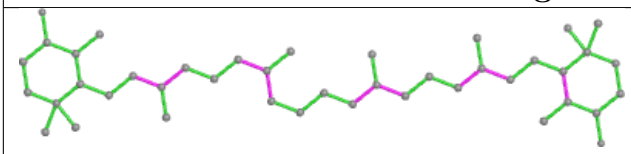


Torsions

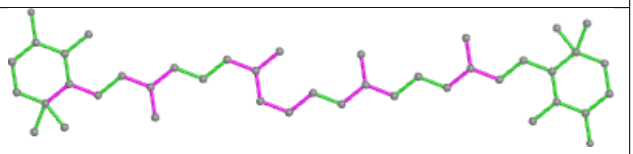


Rings

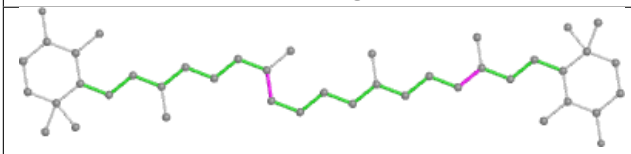
Ligand 45D a 857



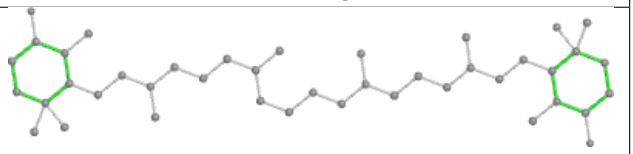
Bond lengths



Bond angles

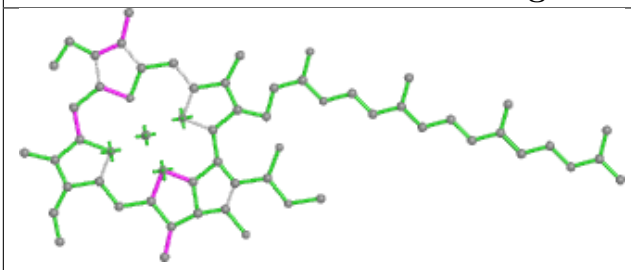


Torsions



Rings

Ligand CLA a 813



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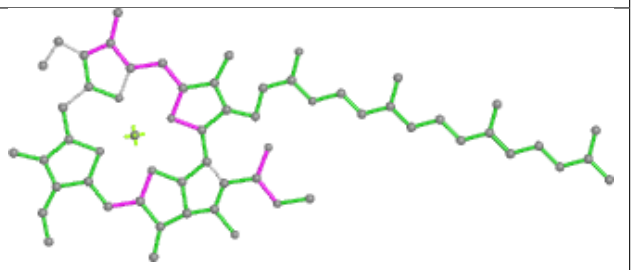
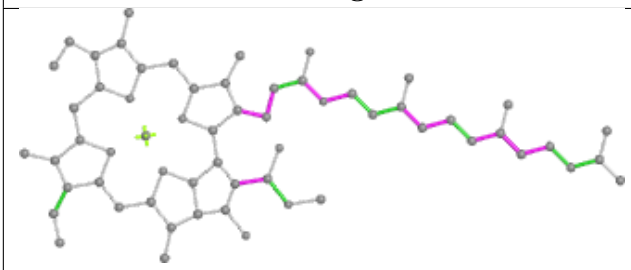
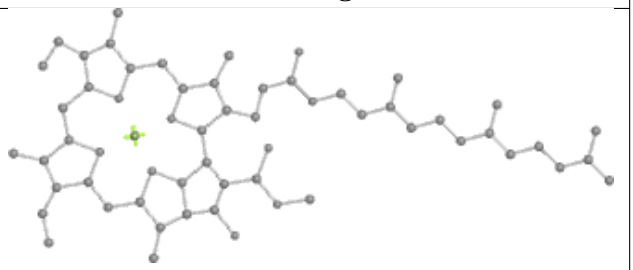


Bond angles

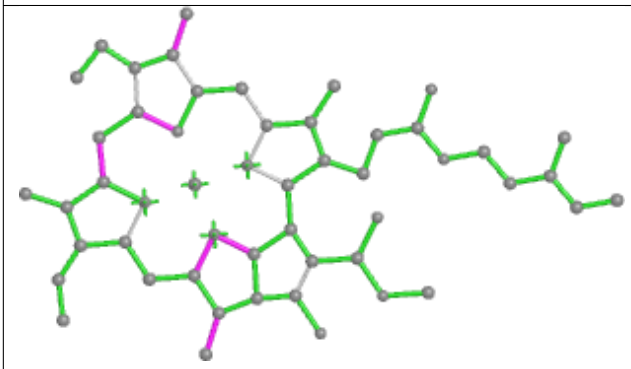


Torsions

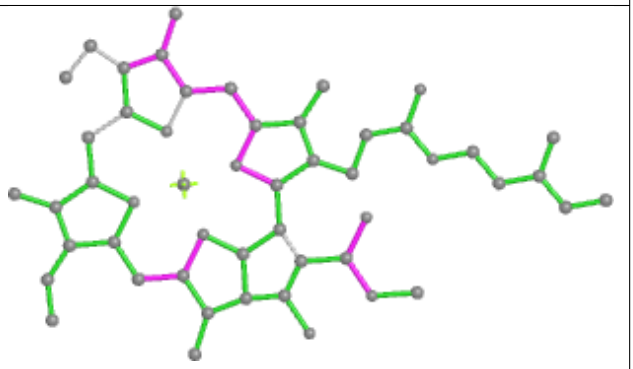


Rings

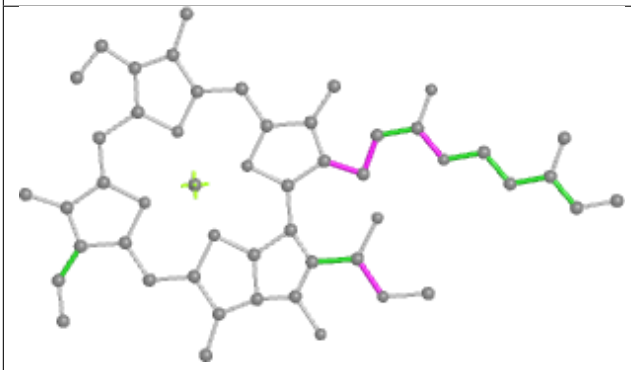
Ligand CLA b 3030



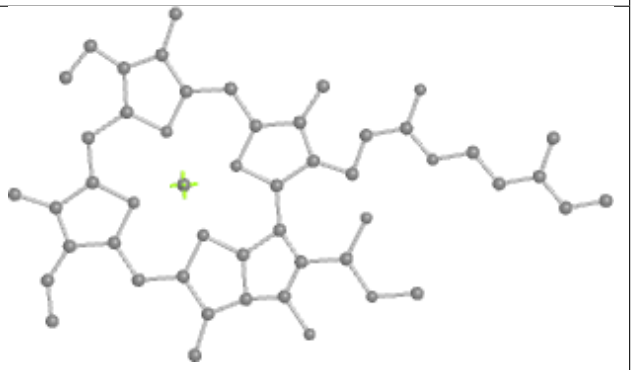
Bond lengths



Bond angles

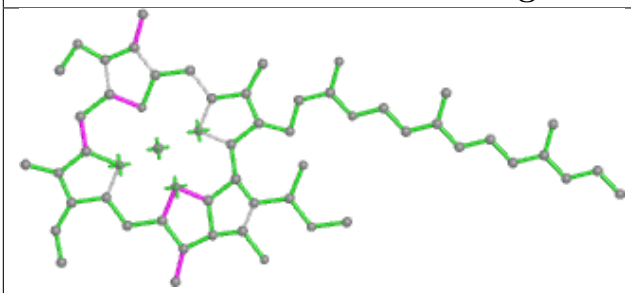


Torsions

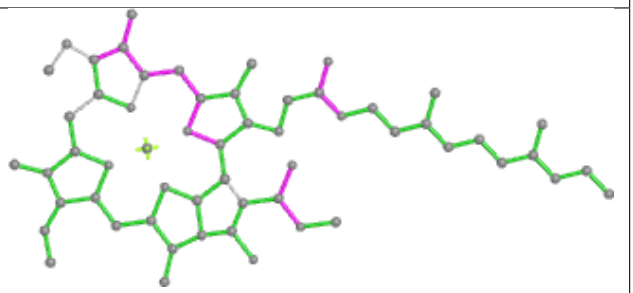


Rings

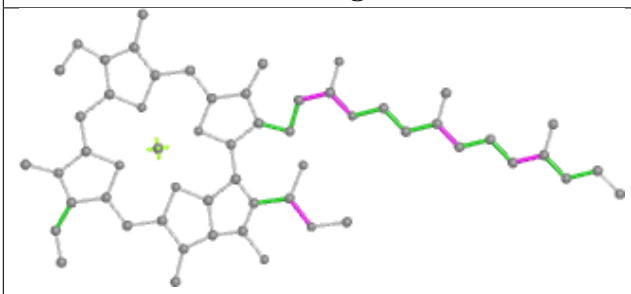
Ligand CLA b 3023



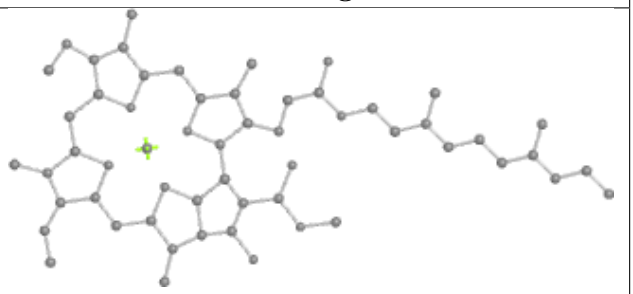
Bond lengths



Bond angles

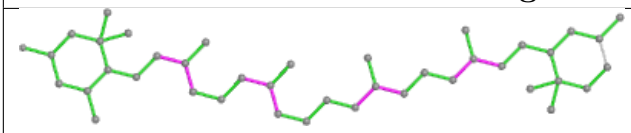


Torsions

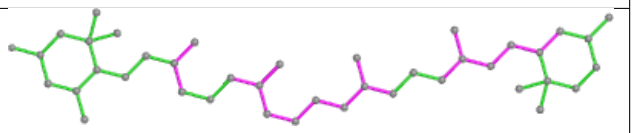


Rings

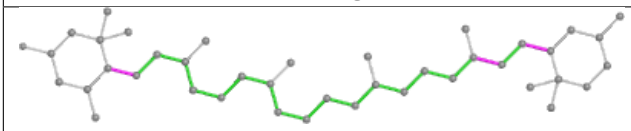
Ligand ZEX b 3053



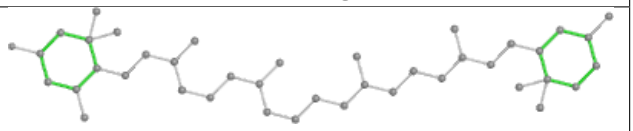
Bond lengths



Bond angles

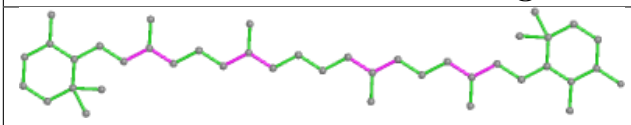


Torsions

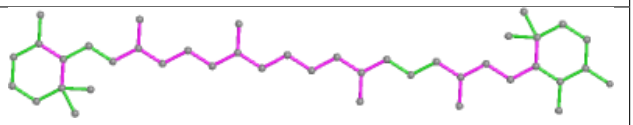


Rings

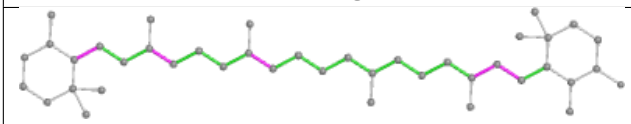
Ligand ECH b 3045



Bond lengths



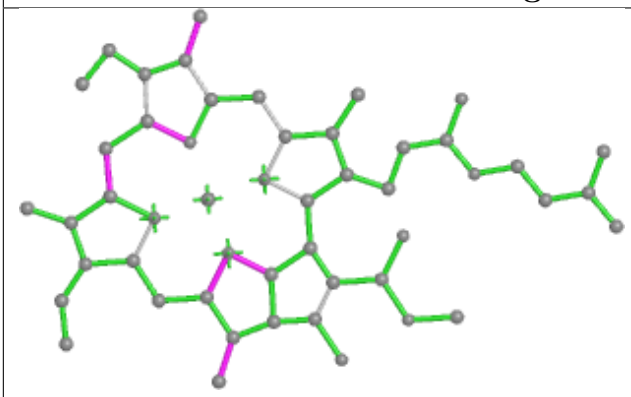
Bond angles



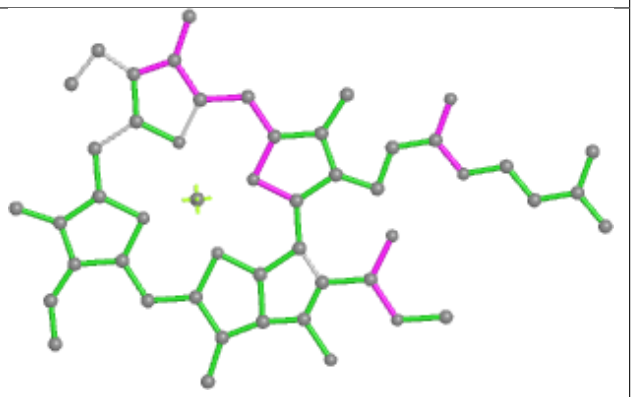
Torsions

Rings

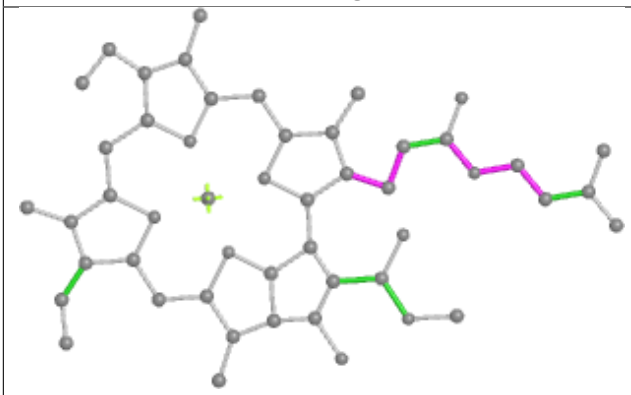
Ligand CLA A 405



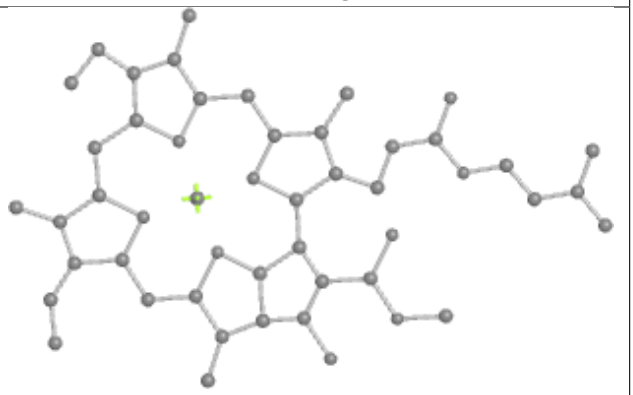
Bond lengths



Bond angles

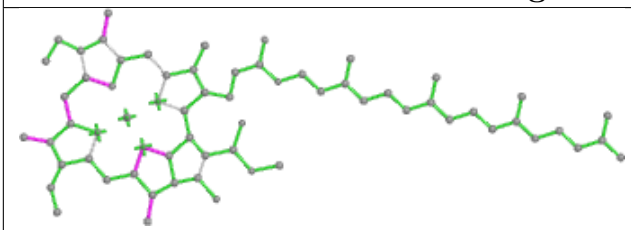


Torsions

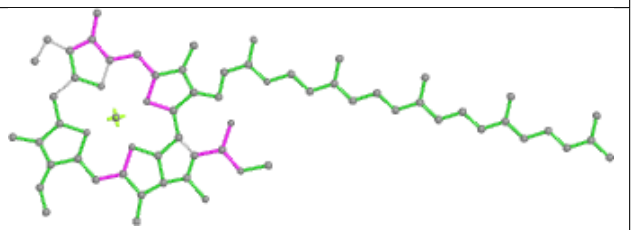


Rings

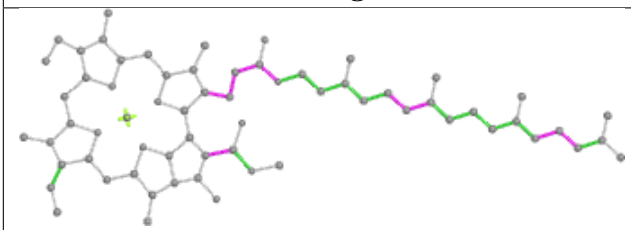
Ligand CLA a 815



Bond lengths



Bond angles



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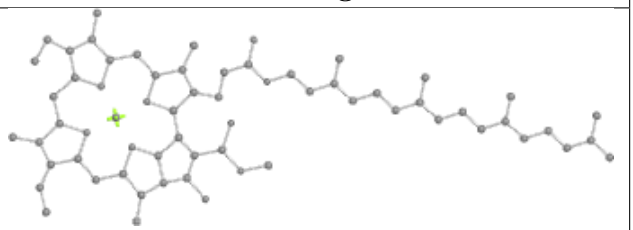
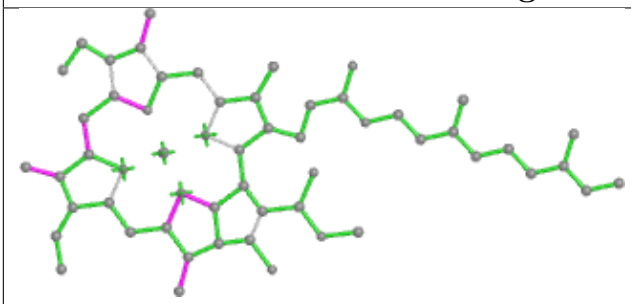


Rings

Ligand CLA b 3016



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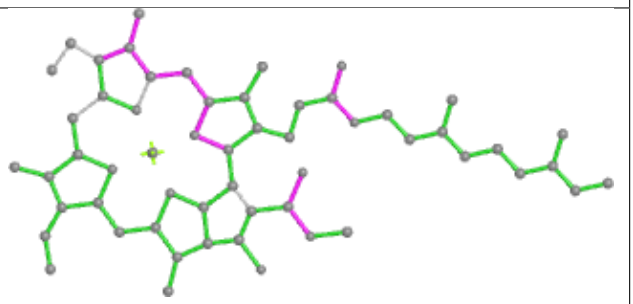
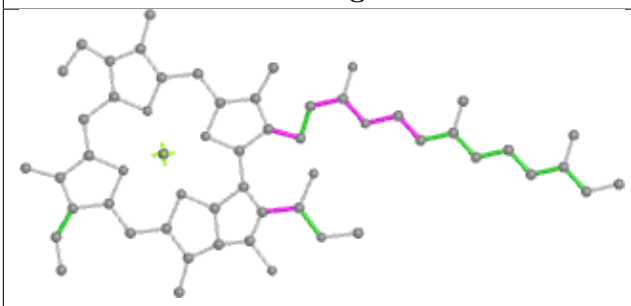
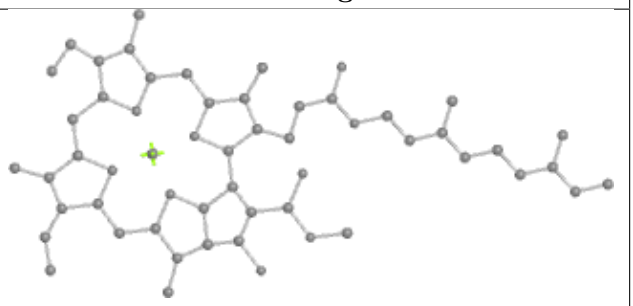


Bond angles

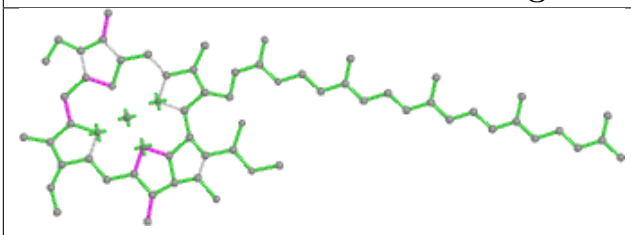


Torsions

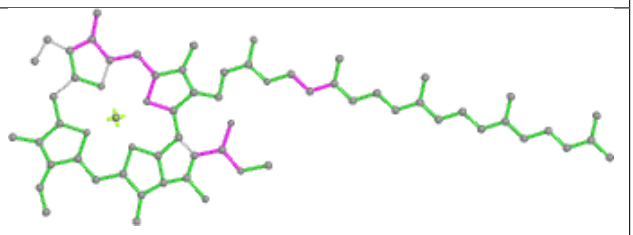


Rings

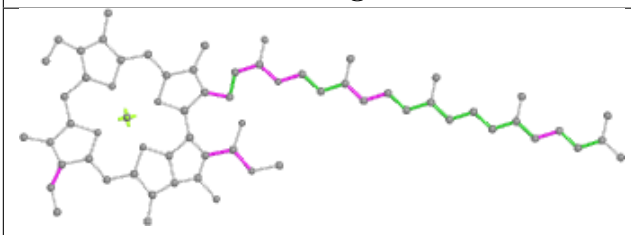
Ligand CLA a 835



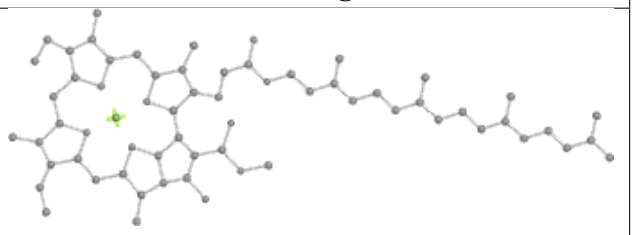
Bond lengths



Bond angles

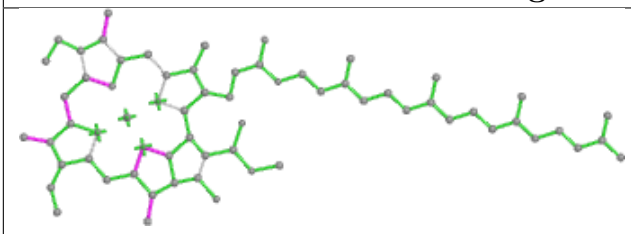


Torsions

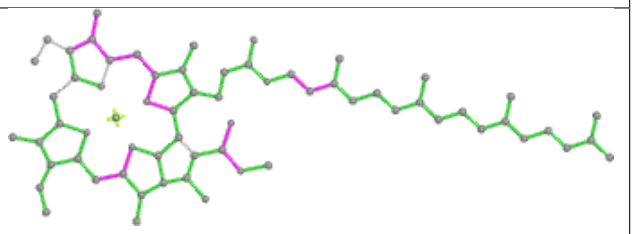


Rings

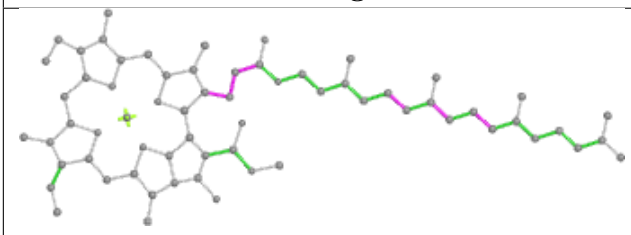
Ligand CLA a 829



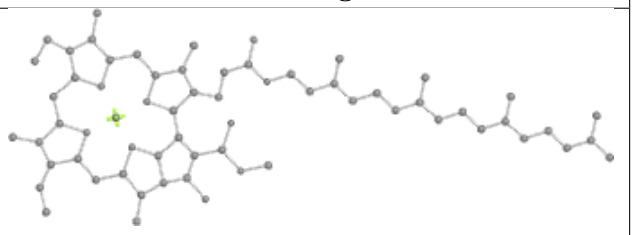
Bond lengths



Bond angles

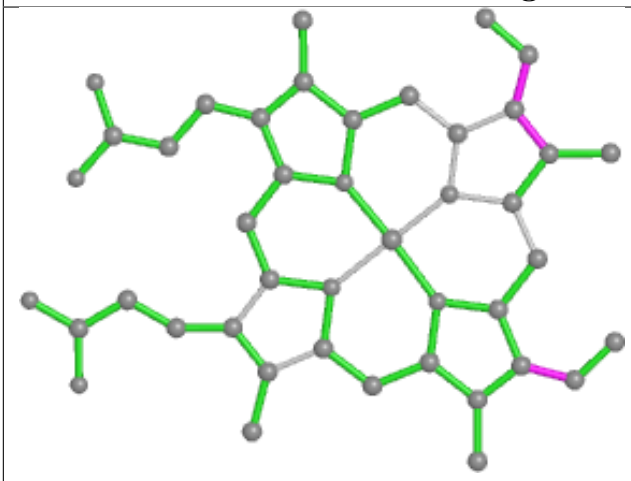


Torsions

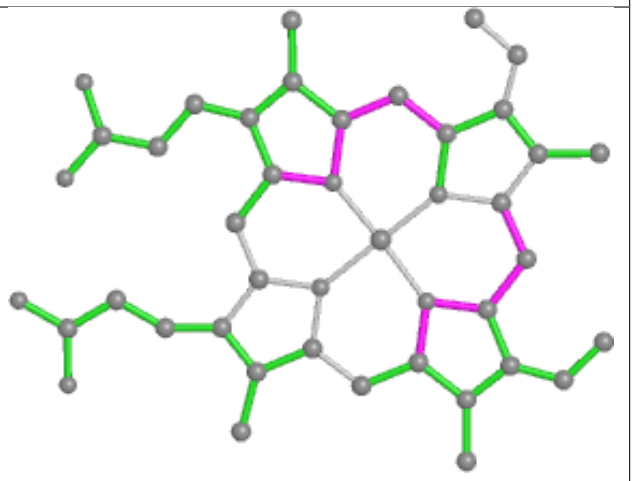


Rings

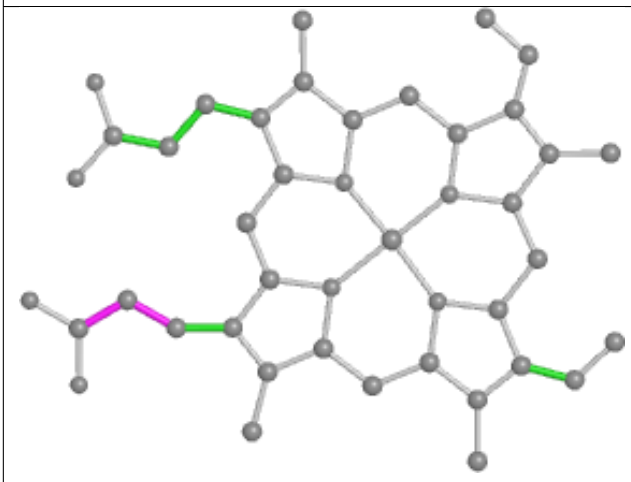
Ligand HEM F 101



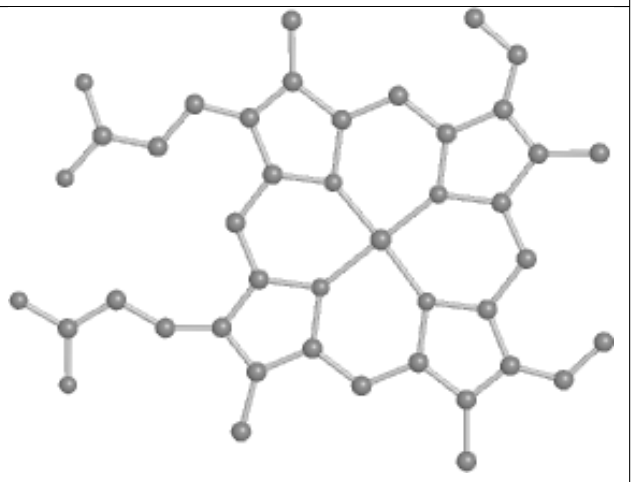
Bond lengths



Bond angles

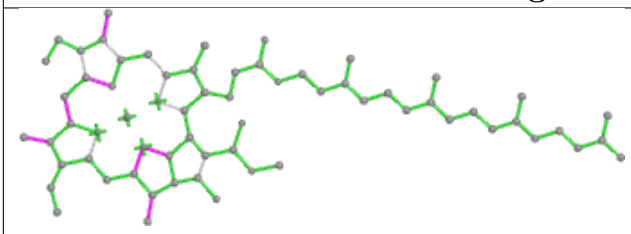


Torsions

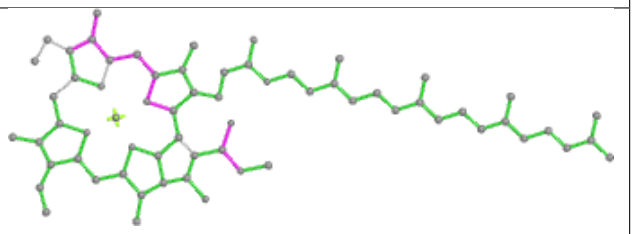


Rings

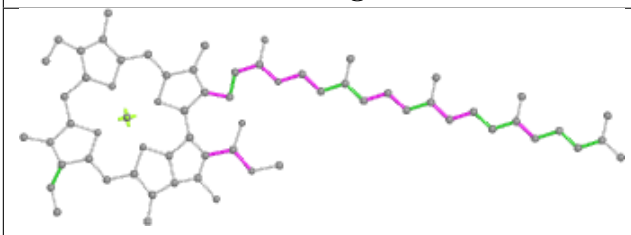
Ligand CLA a 824



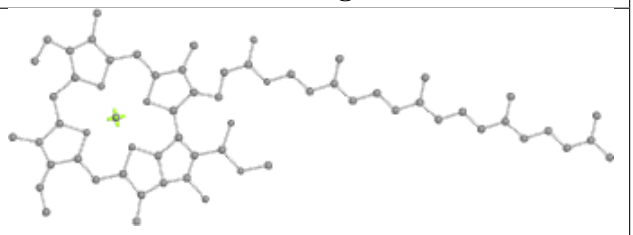
Bond lengths



Bond angles

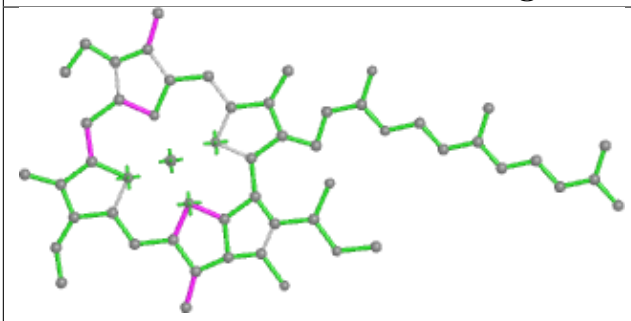


Torsions

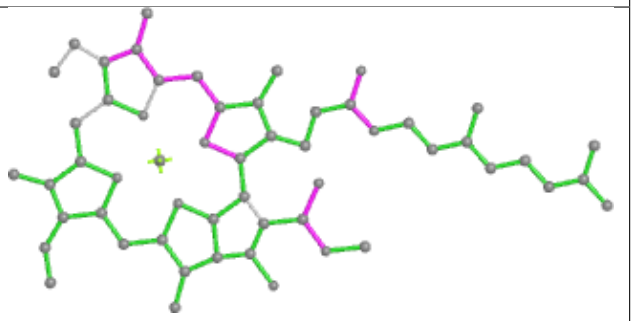


Rings

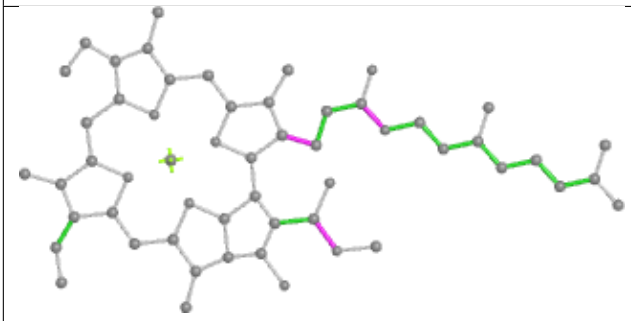
Ligand CLA b 3025



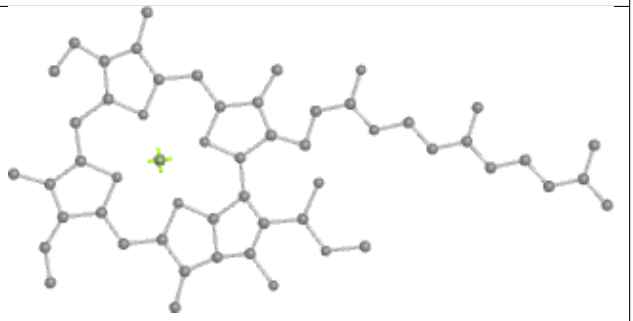
Bond lengths



Bond angles

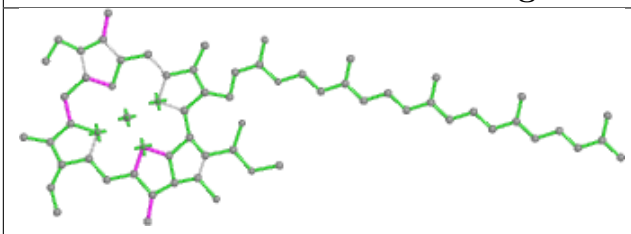


Torsions

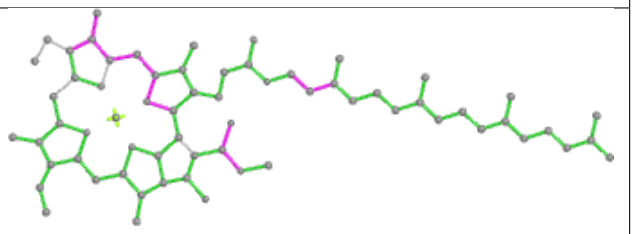


Rings

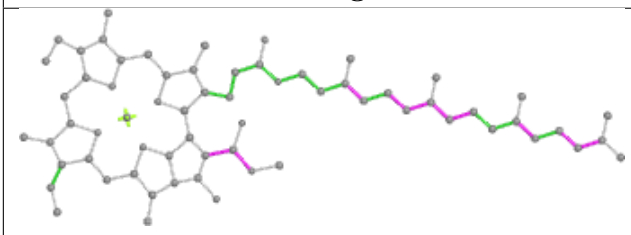
Ligand CLA b 3014



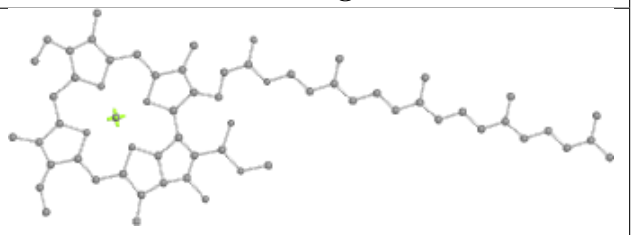
Bond lengths



Bond angles

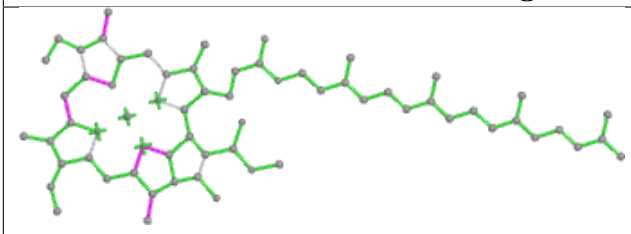


Torsions

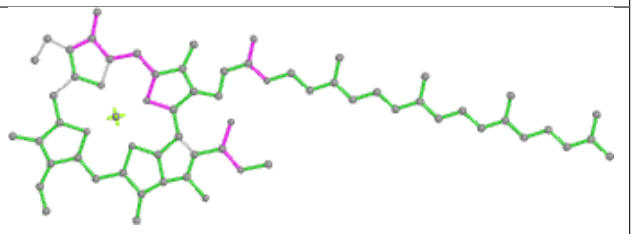


Rings

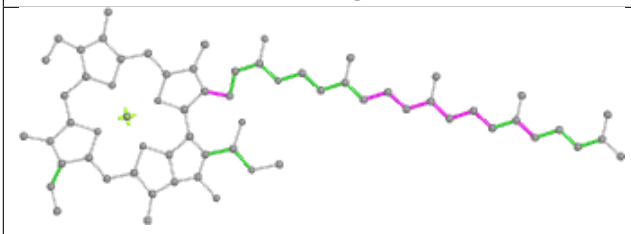
Ligand CLA b 3018



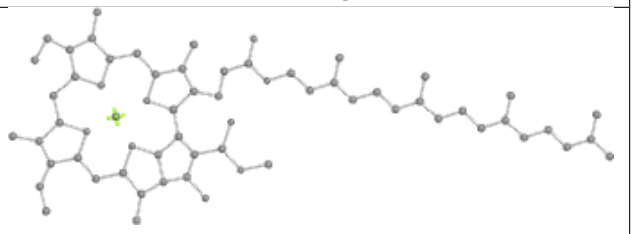
Bond lengths



Bond angles

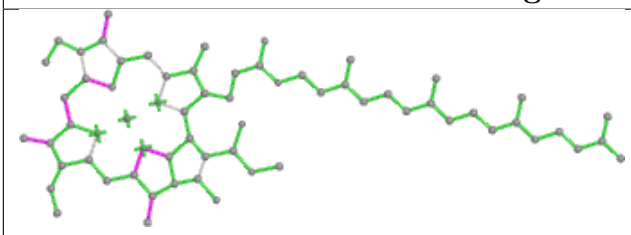


Torsions

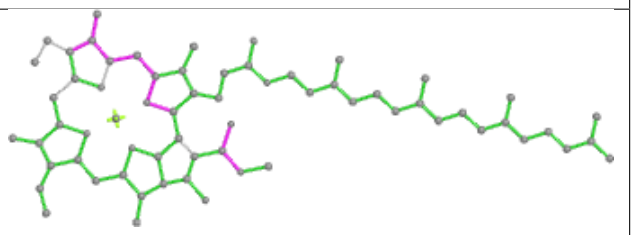


Rings

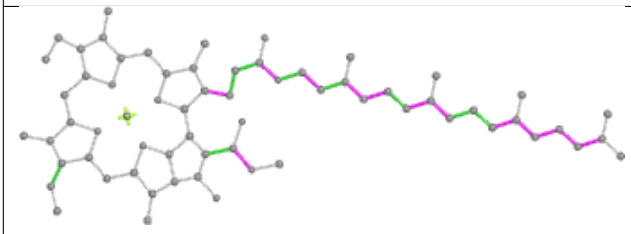
Ligand CLA A 402



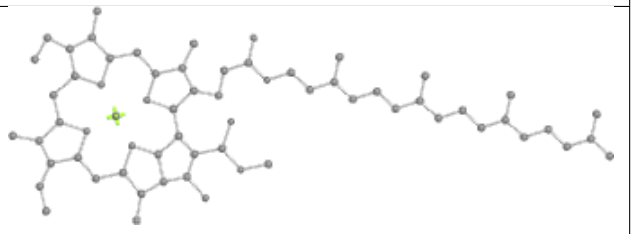
Bond lengths



Bond angles

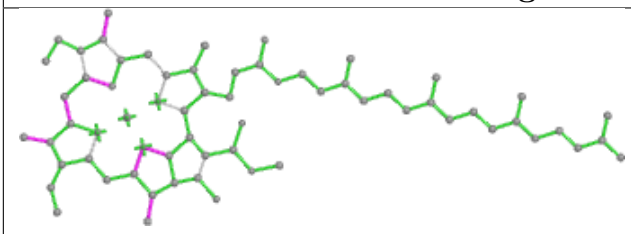


Torsions

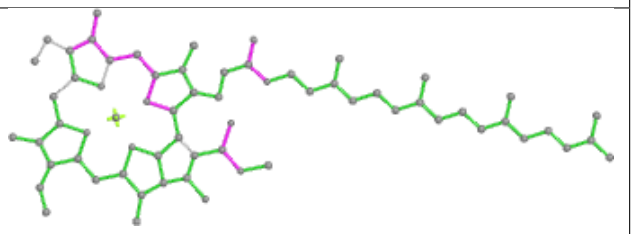


Rings

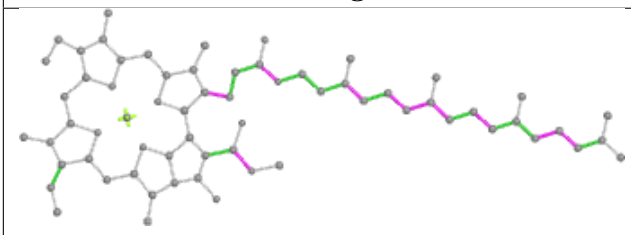
Ligand CLA b 3020



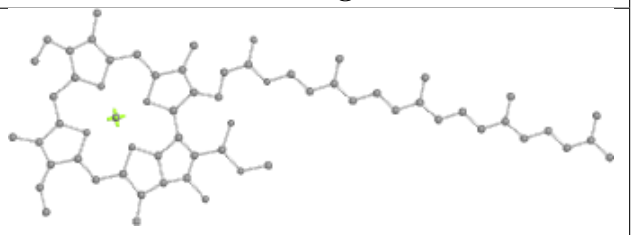
Bond lengths



Bond angles

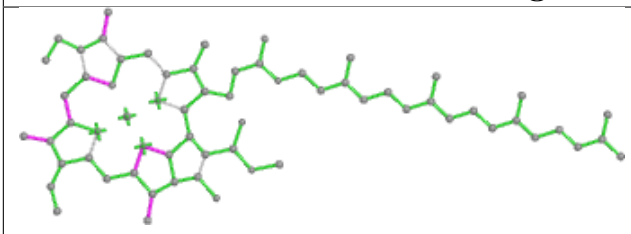


Torsions

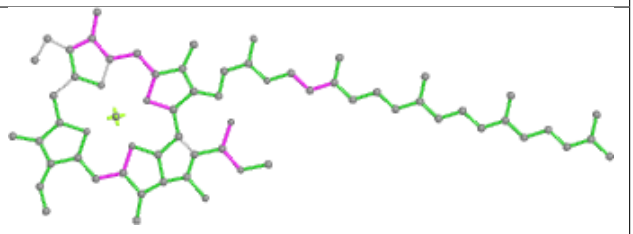


Rings

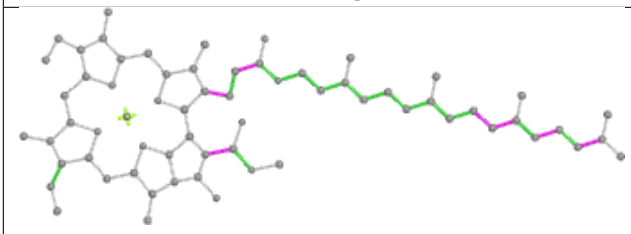
Ligand CLA a 806



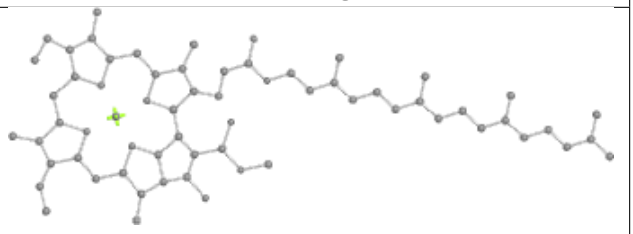
Bond lengths



Bond angles

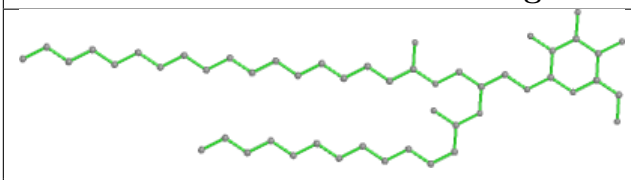


Torsions

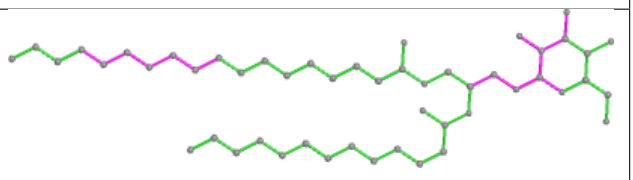


Rings

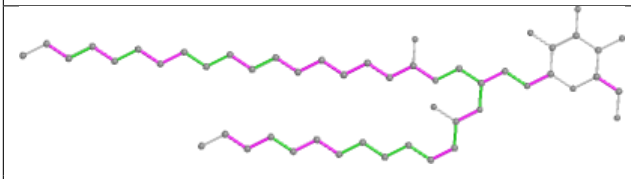
Ligand LMG a 851



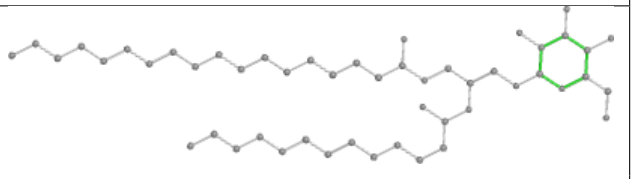
Bond lengths



Bond angles

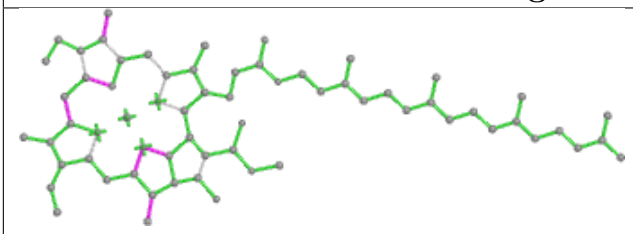


Torsions

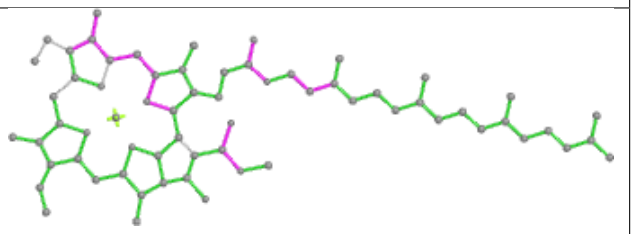


Rings

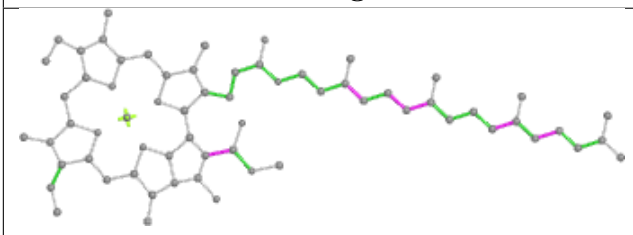
Ligand CLA a 834



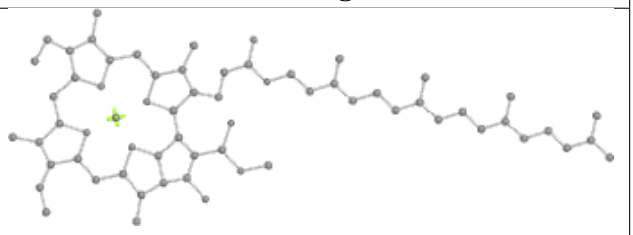
Bond lengths



Bond angles

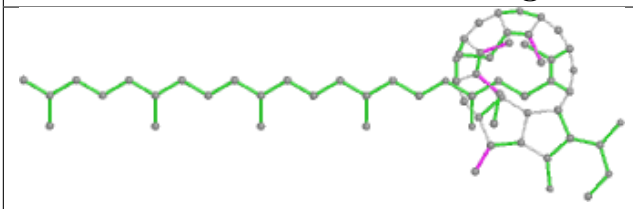


Torsions

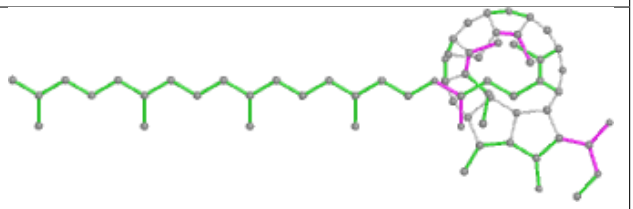


Rings

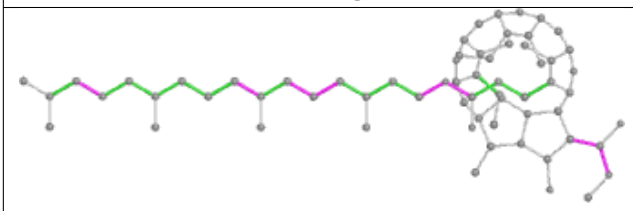
Ligand PHO A 404



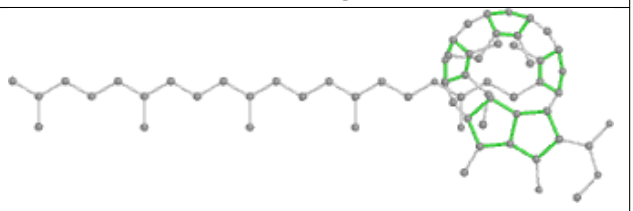
Bond lengths



Bond angles

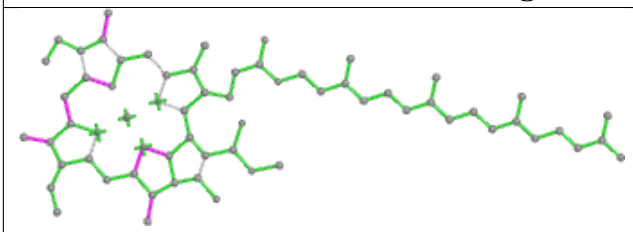


Torsions

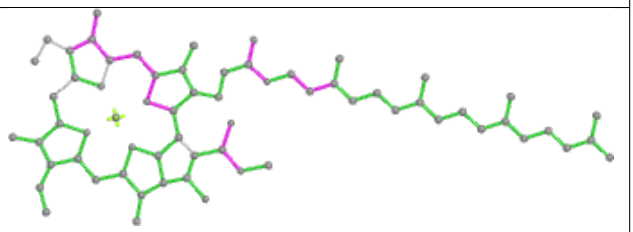


Rings

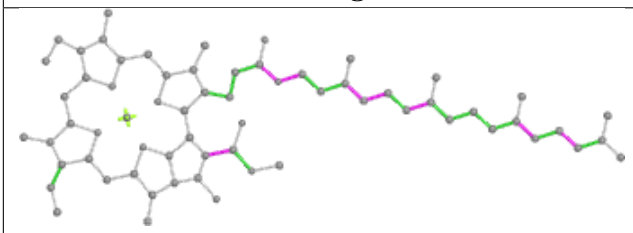
Ligand CLA b 3006



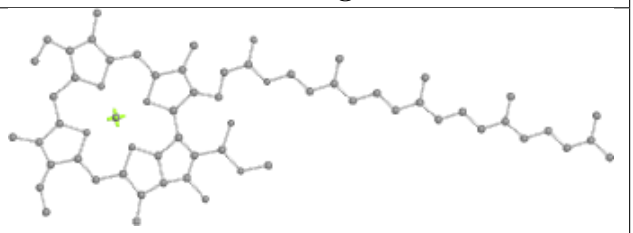
Bond lengths



Bond angles

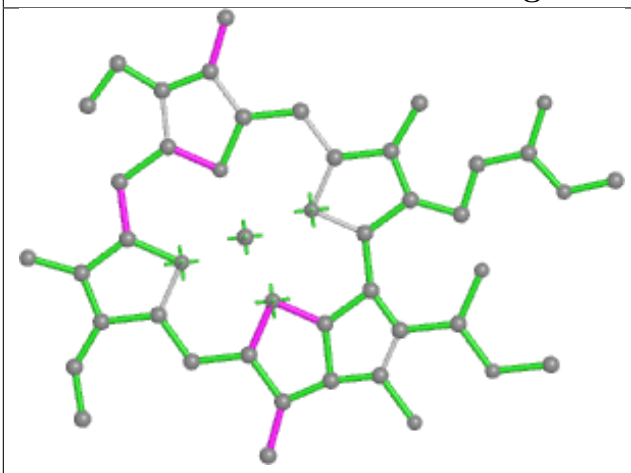


Torsions

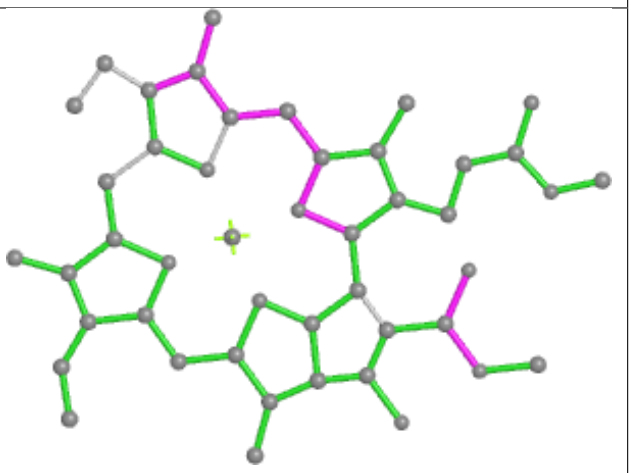


Rings

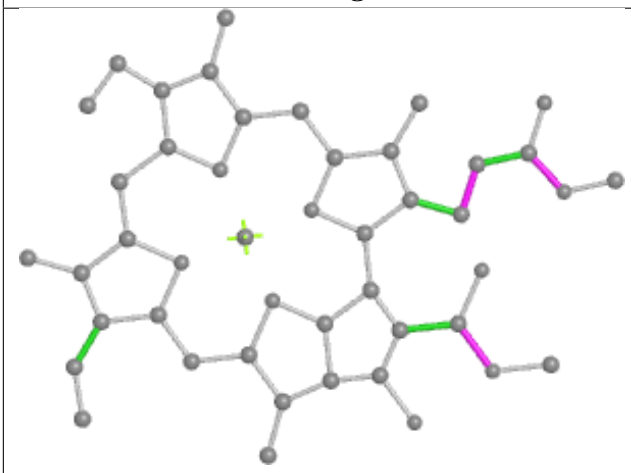
Ligand CLA D 404



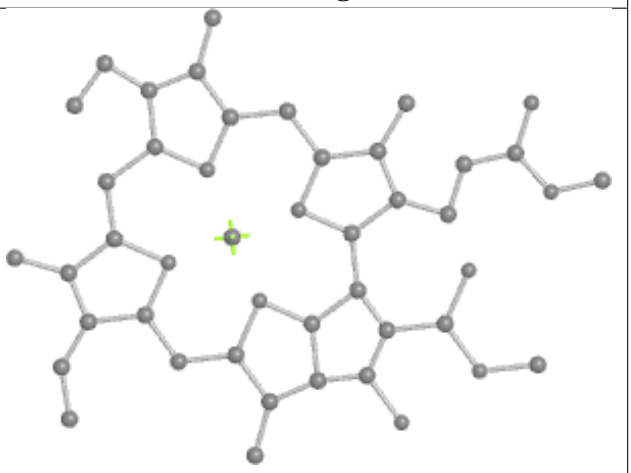
Bond lengths



Bond angles

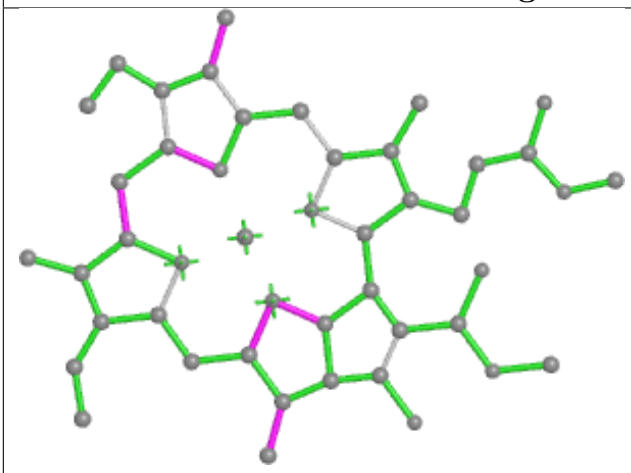


Torsions

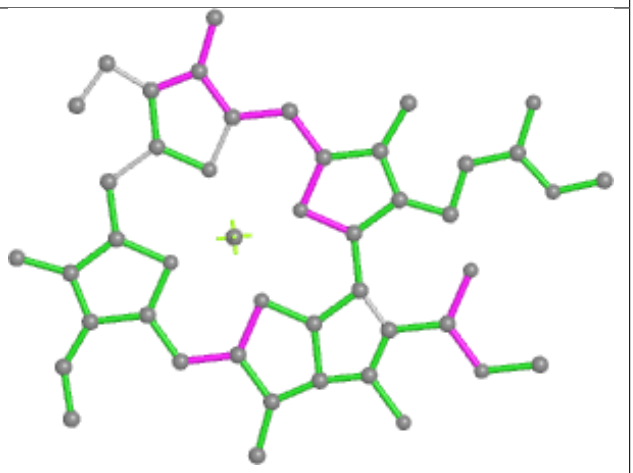


Rings

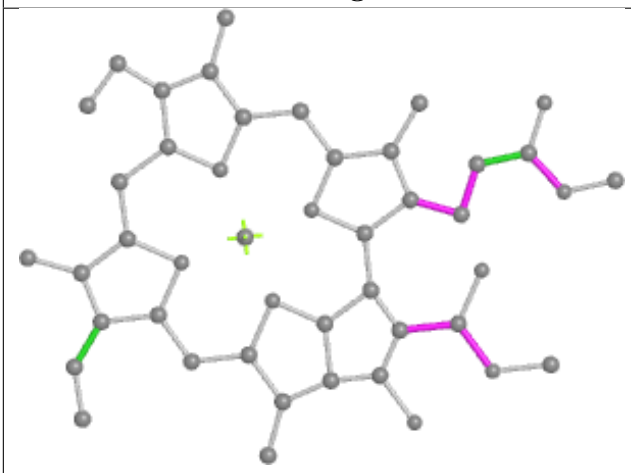
Ligand CLA b 3041



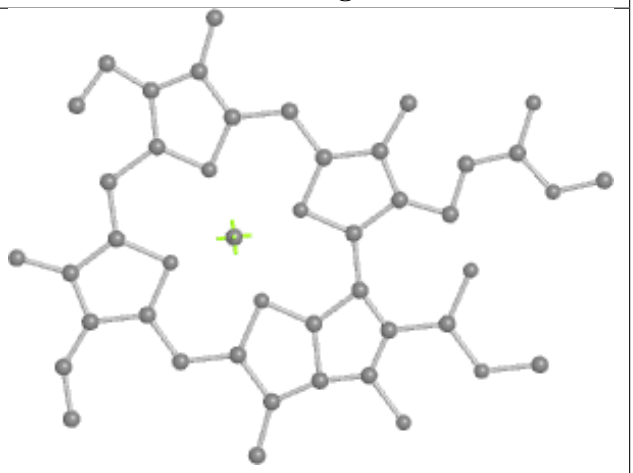
Bond lengths



Bond angles

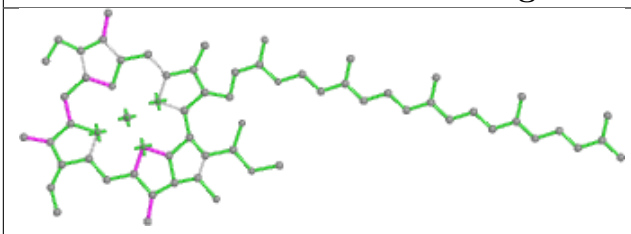


Torsions

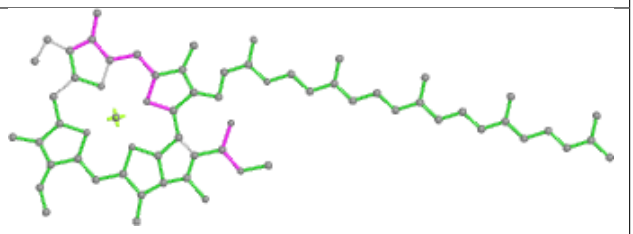


Rings

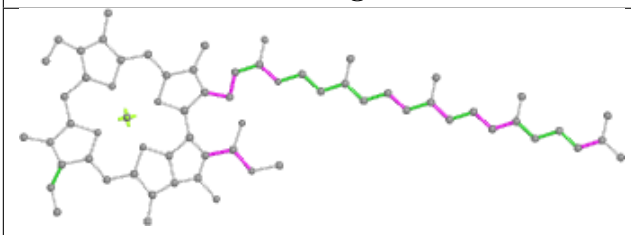
Ligand CLA b 3002



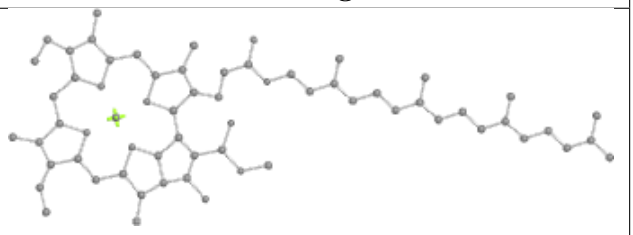
Bond lengths



Bond angles

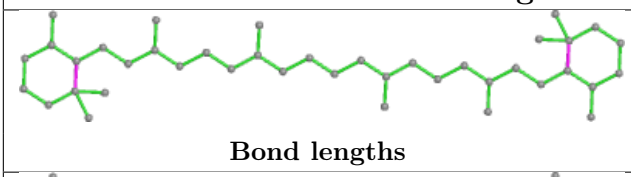


Torsions

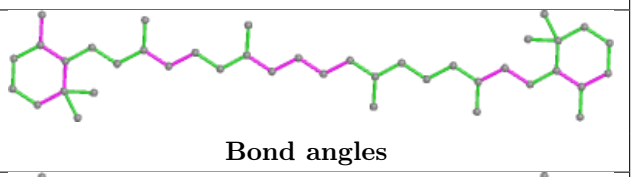


Rings

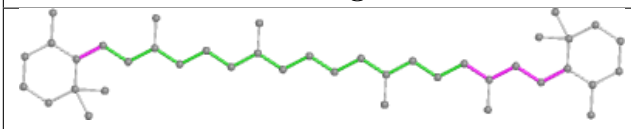
Ligand BCR b 3046



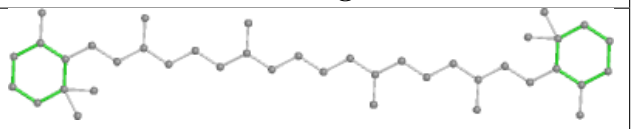
Bond lengths



Bond angles

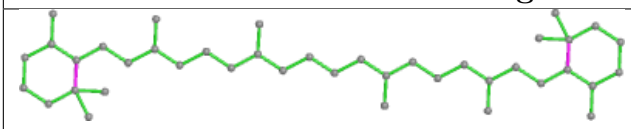


Torsions

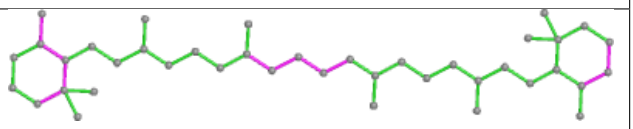


Rings

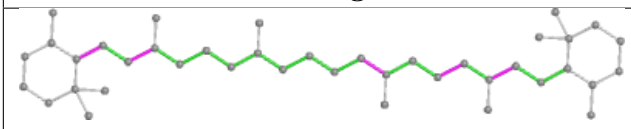
Ligand BCR b 3044



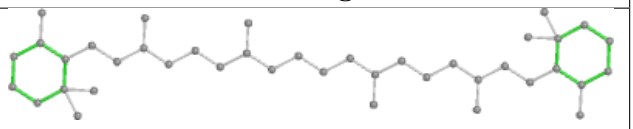
Bond lengths



Bond angles

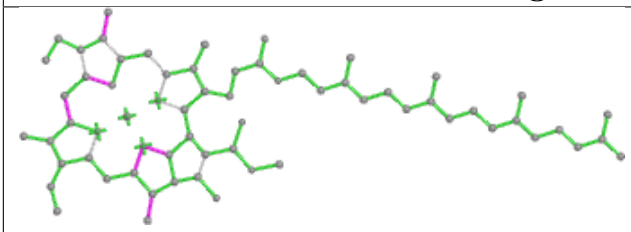


Torsions

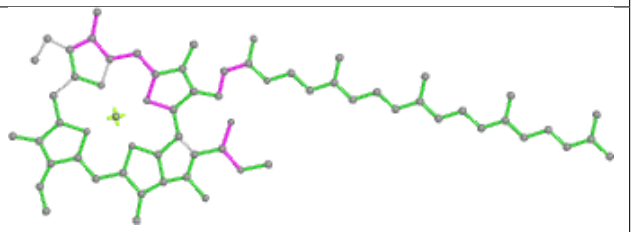


Rings

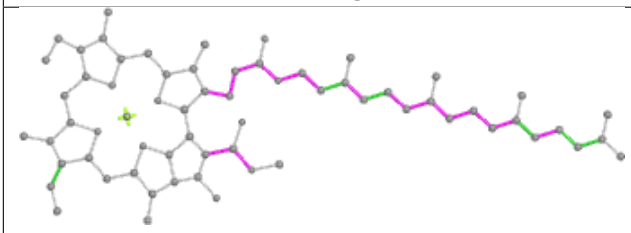
Ligand CLA a 821



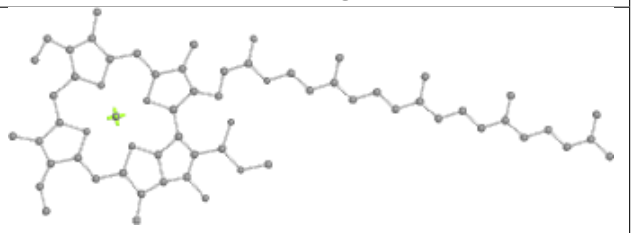
Bond lengths



Bond angles

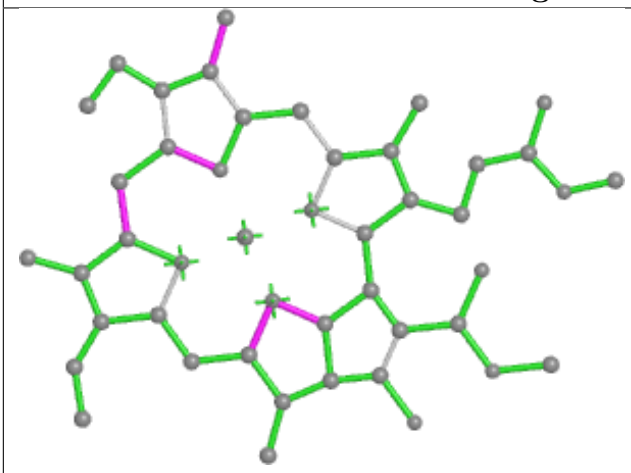


Torsions

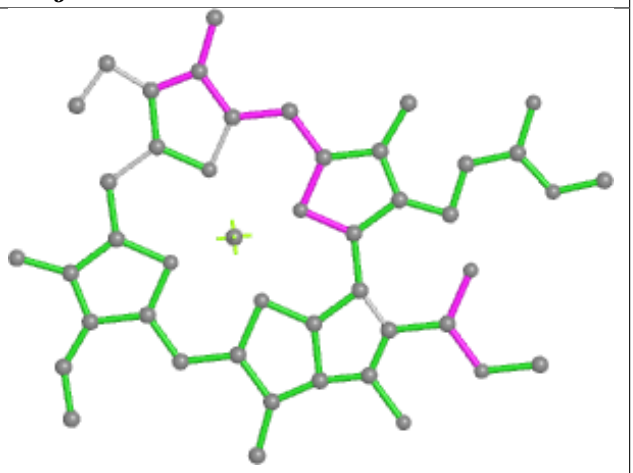


Rings

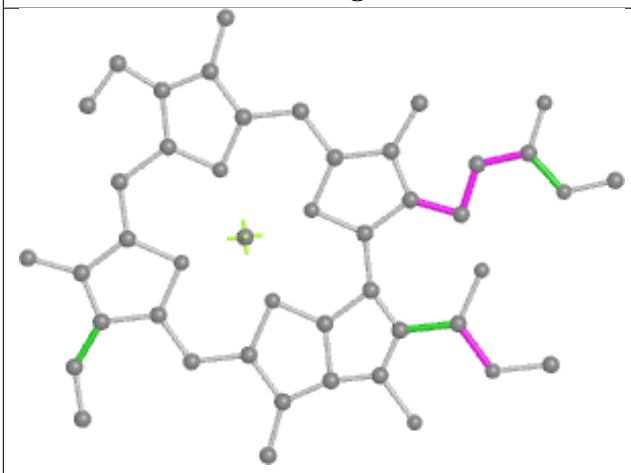
Ligand CLA j 103



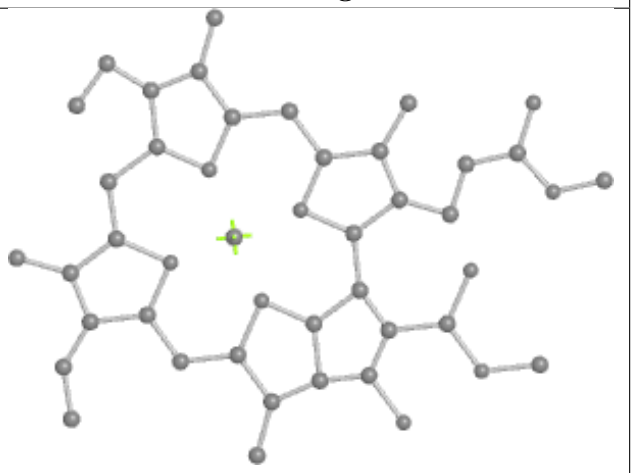
Bond lengths



Bond angles

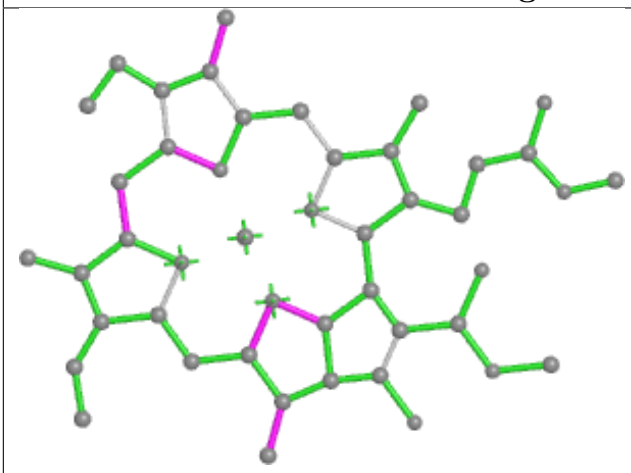


Torsions

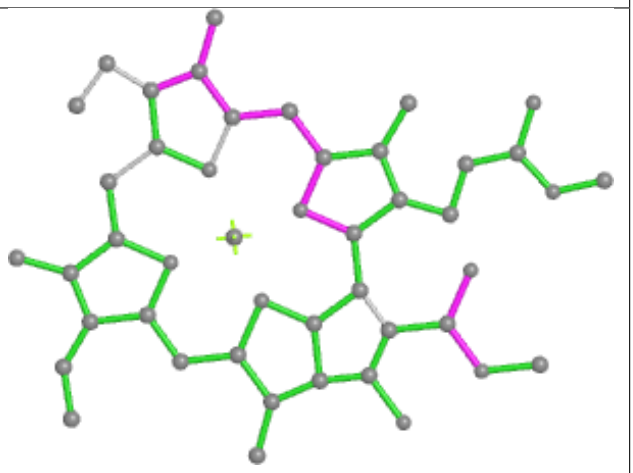


Rings

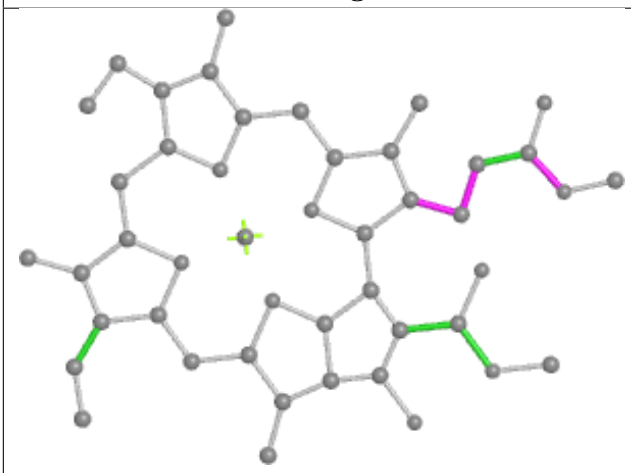
Ligand CLA k 4002



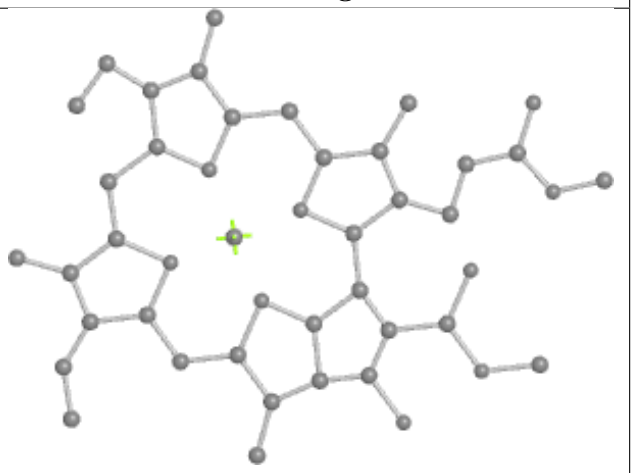
Bond lengths



Bond angles

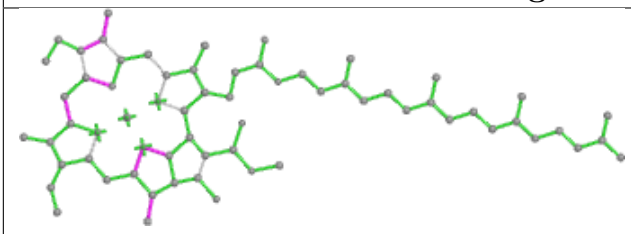


Torsions

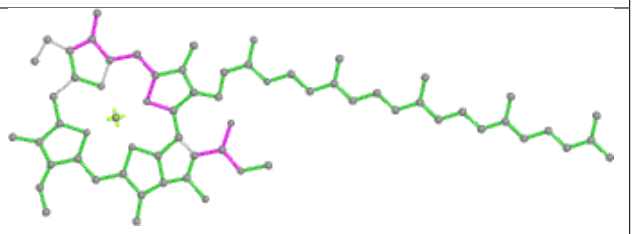


Rings

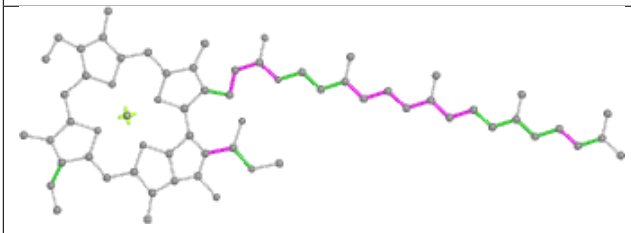
Ligand CLA a 840



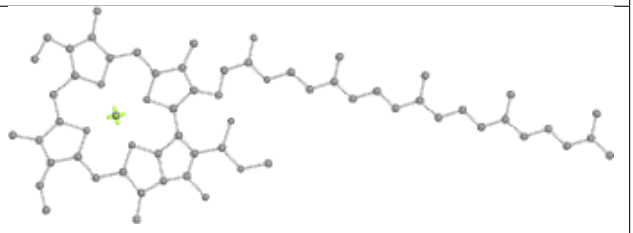
Bond lengths



Bond angles

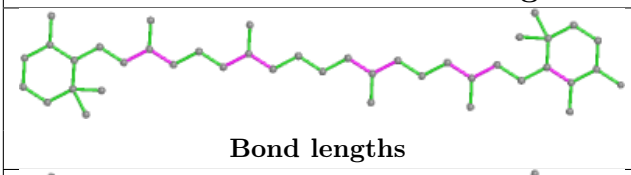


Torsions

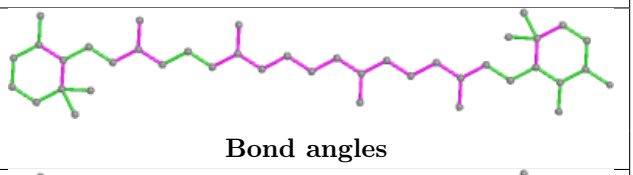


Rings

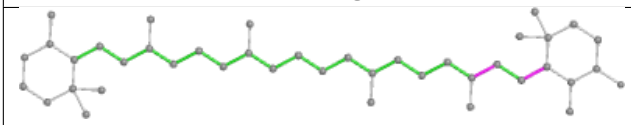
Ligand ECH m 101



Bond lengths



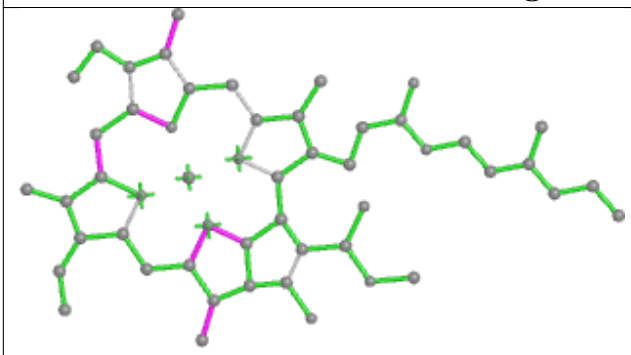
Bond angles



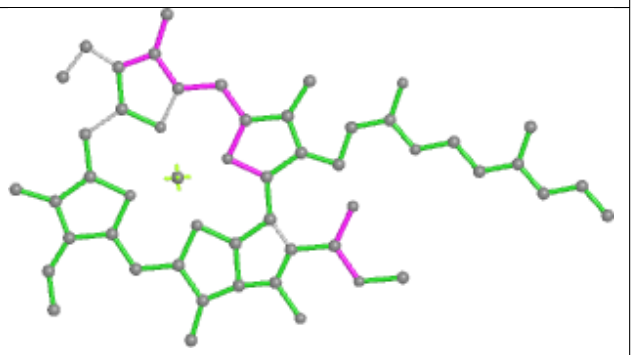
Torsions

Rings

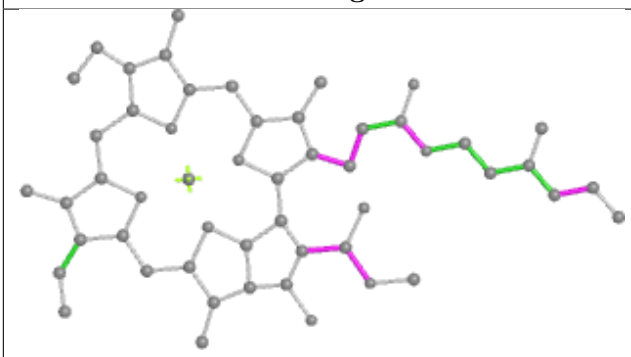
Ligand CLA l 1503



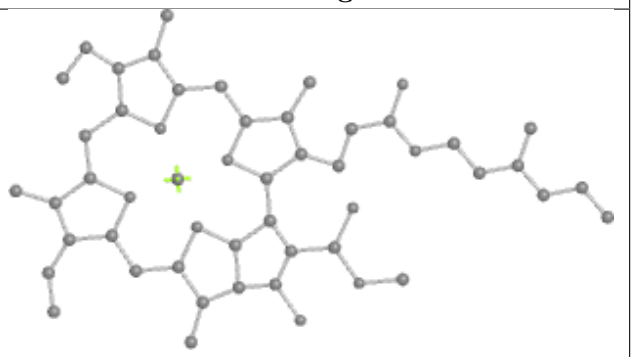
Bond lengths



Bond angles

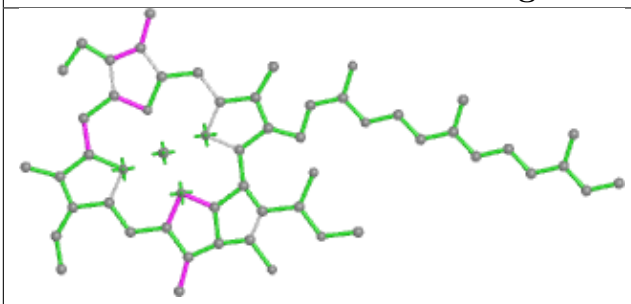


Torsions



Rings

Ligand CLA b 3011



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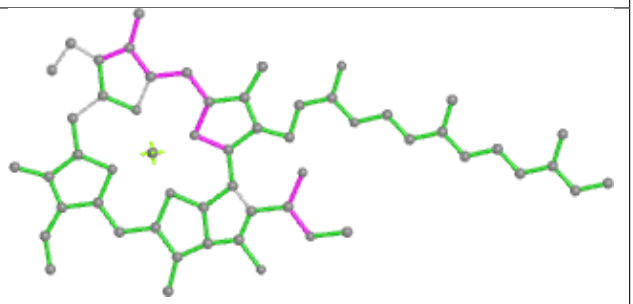
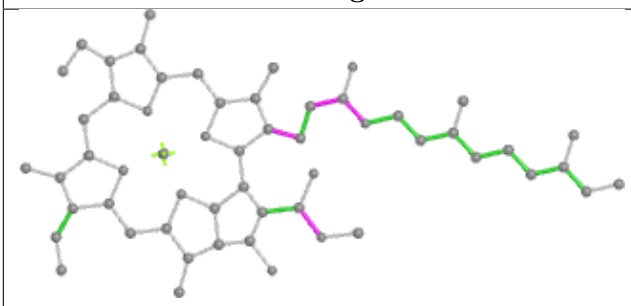
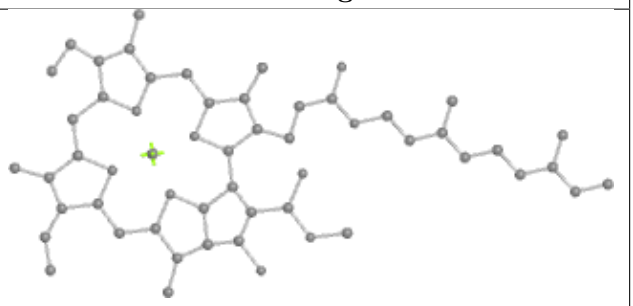


Bond angles

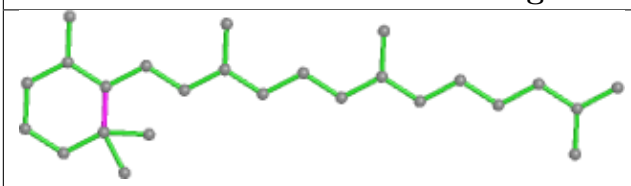


Torsions

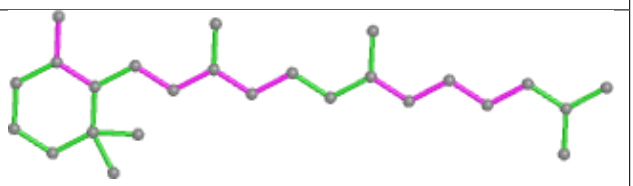


Rings

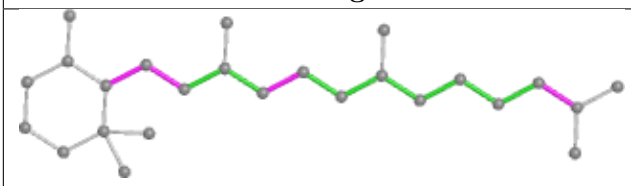
Ligand BCR a 849



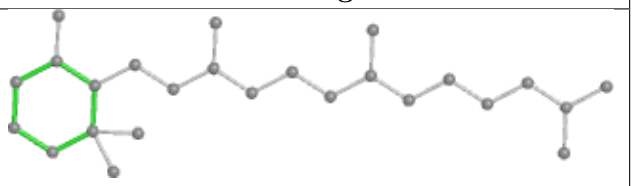
Bond lengths



Bond angles

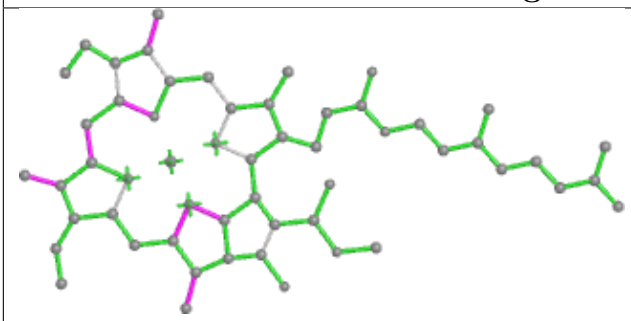


Torsions

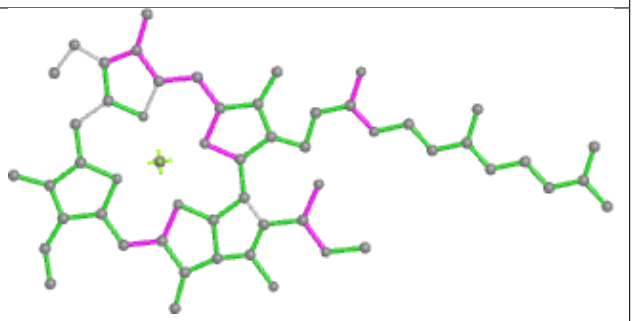


Rings

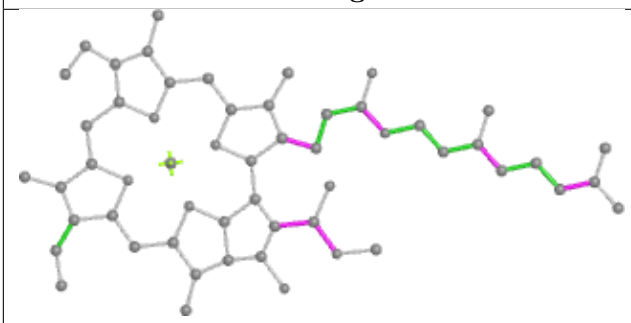
Ligand CLA D 403



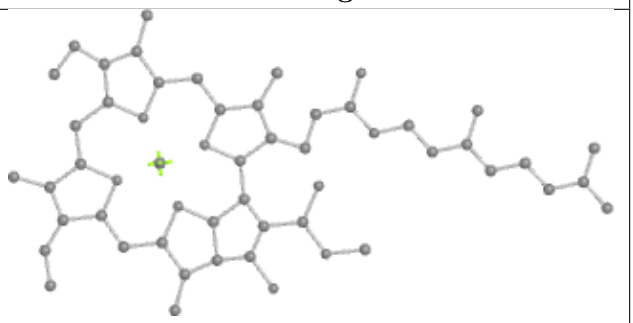
Bond lengths



Bond angles

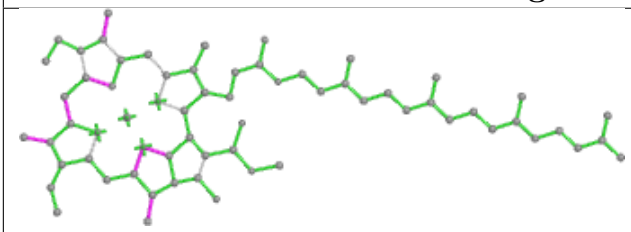


Torsions

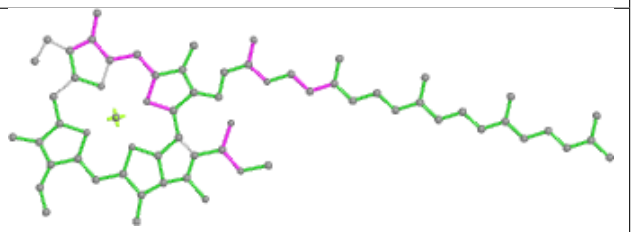


Rings

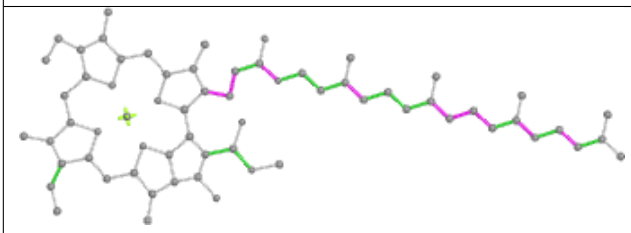
Ligand CLA a 828



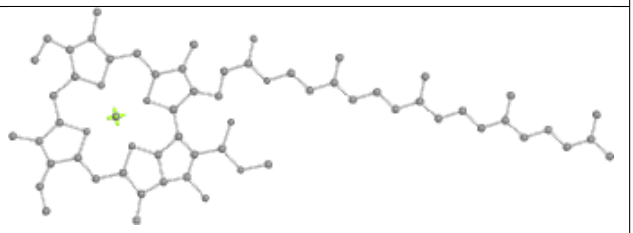
Bond lengths



Bond angles

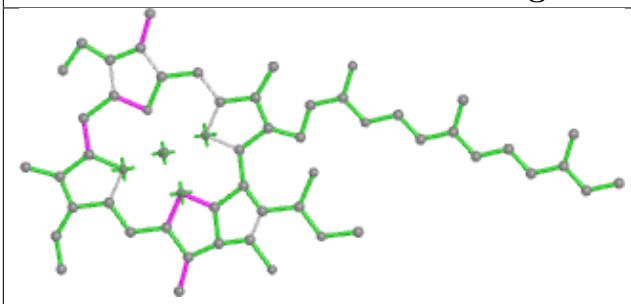


Torsions

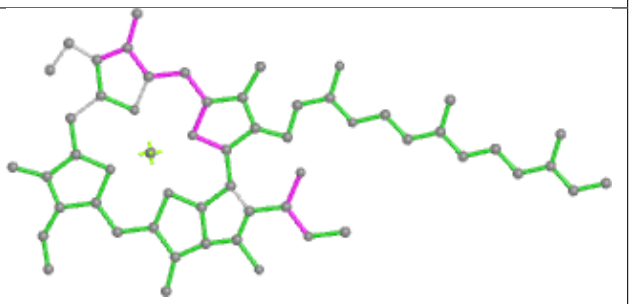


Rings

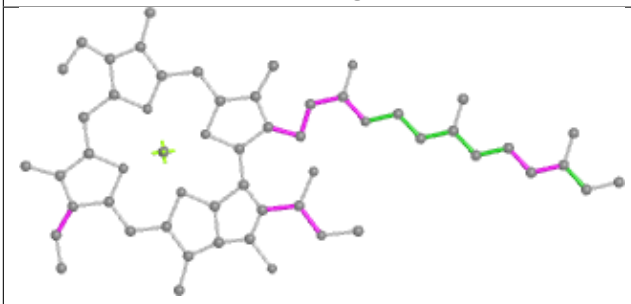
Ligand CLA a 832



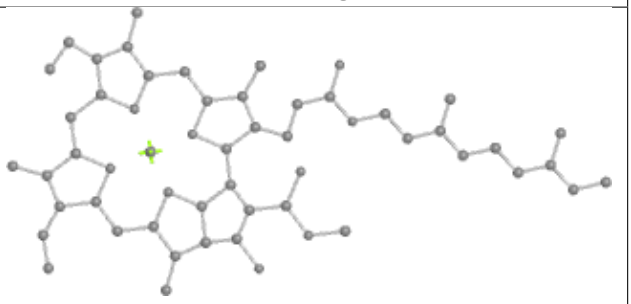
Bond lengths



Bond angles

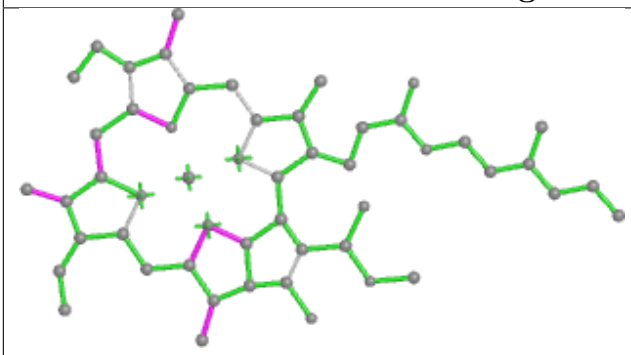


Torsions

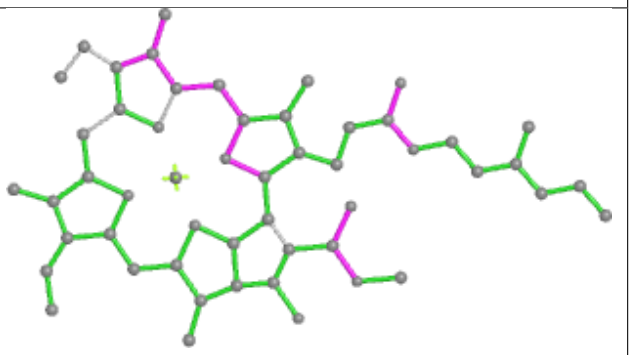


Rings

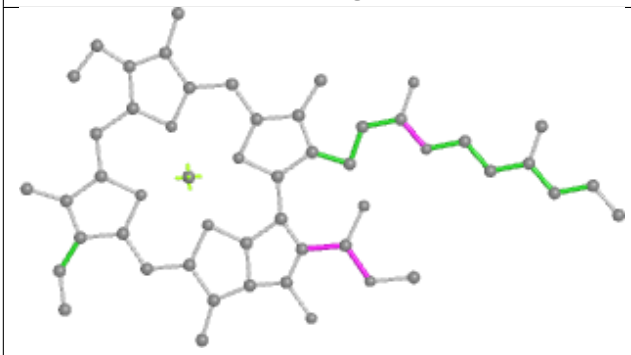
Ligand CLA b 3036



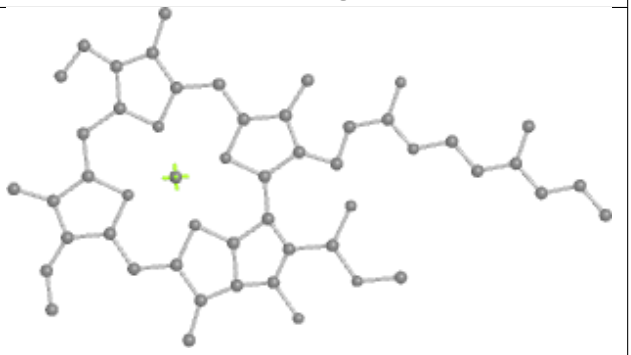
Bond lengths



Bond angles

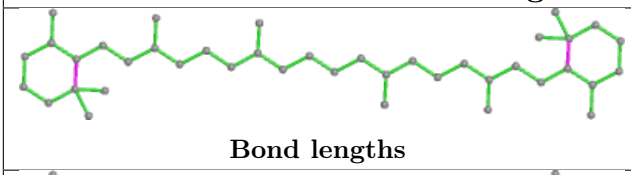


Torsions

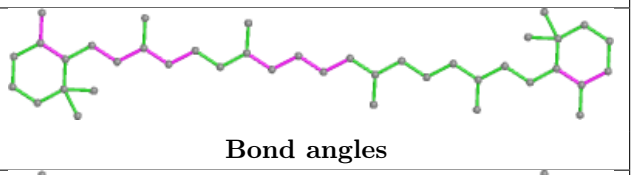


Rings

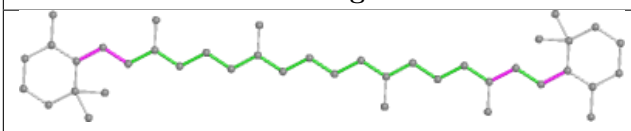
Ligand BCR a 846



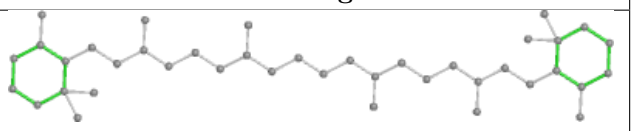
Bond lengths



Bond angles

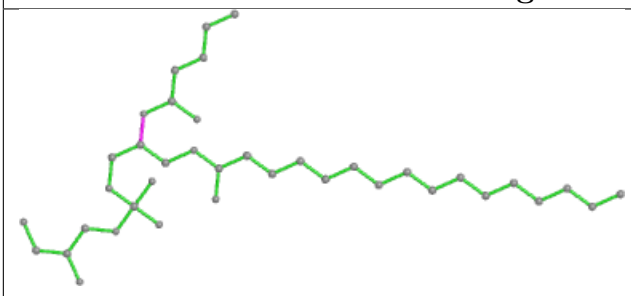


Torsions

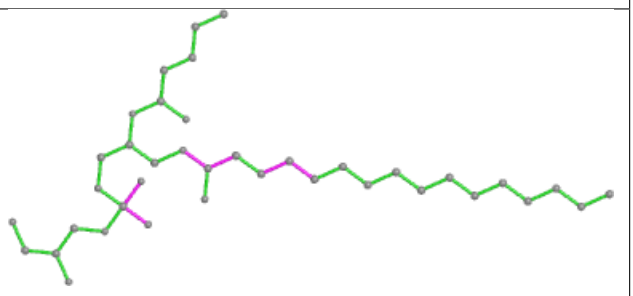


Rings

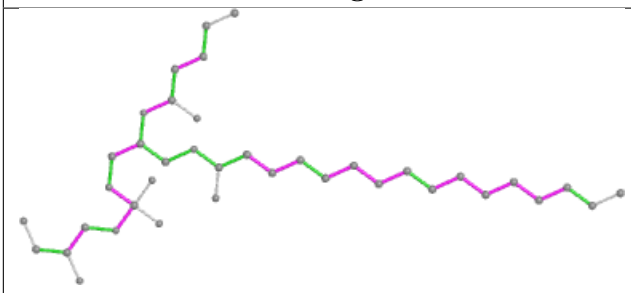
Ligand LHG b 3050



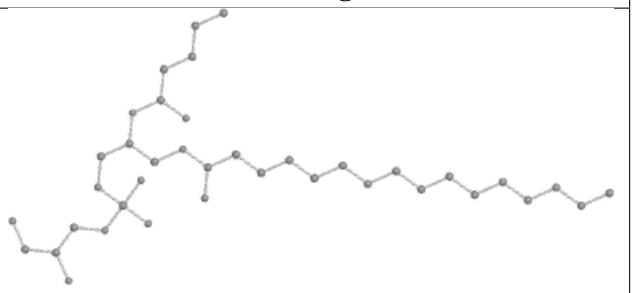
Bond lengths



Bond angles

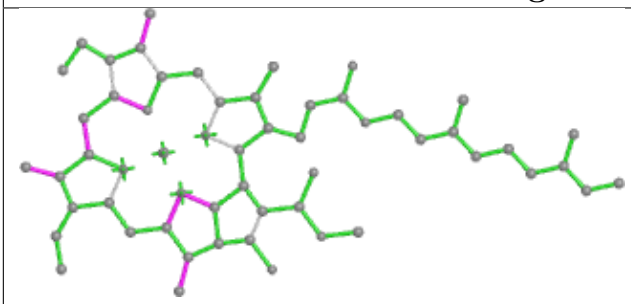


Torsions

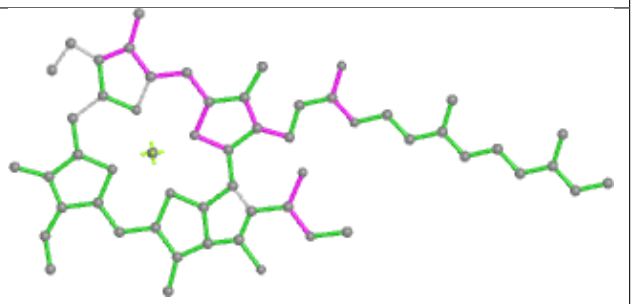


Rings

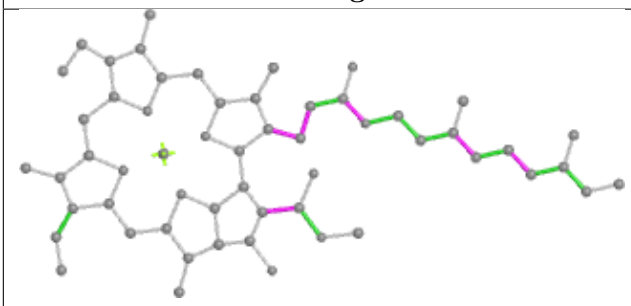
Ligand CLA a 843



Bond lengths



Bond angles



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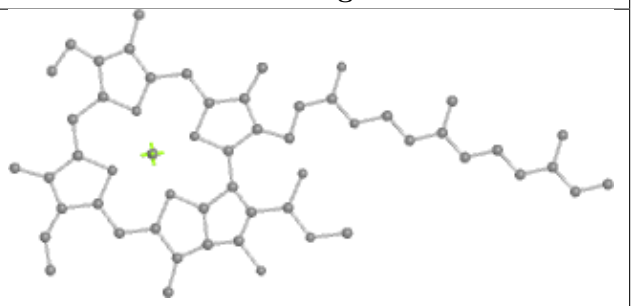
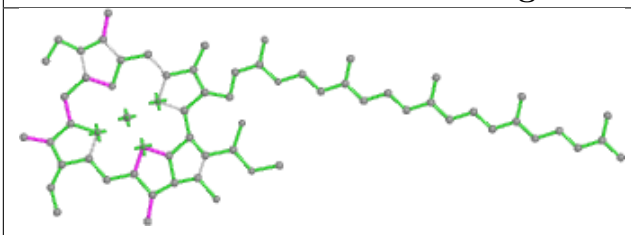
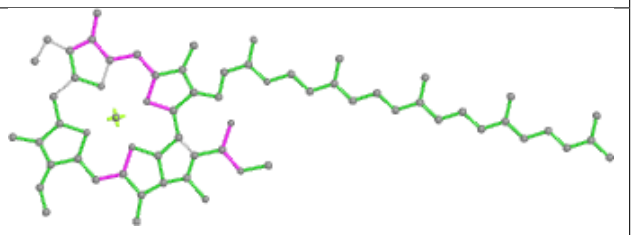


Rings

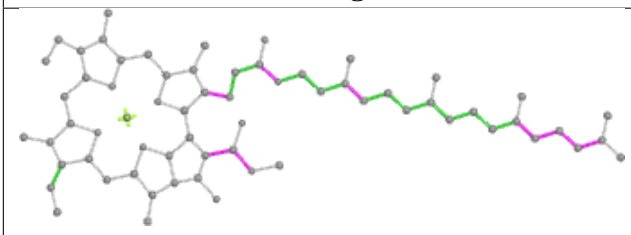
Ligand CLA b 3005



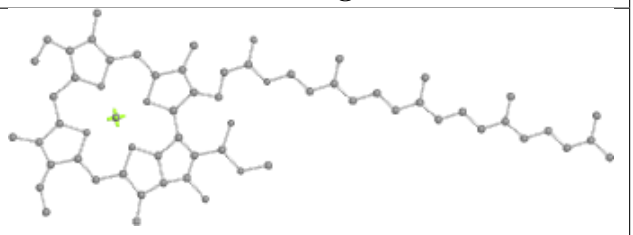
Bond lengths



Bond angles

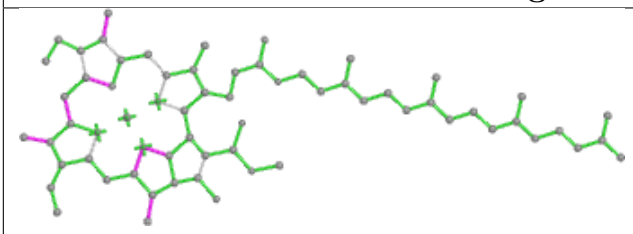


Torsions

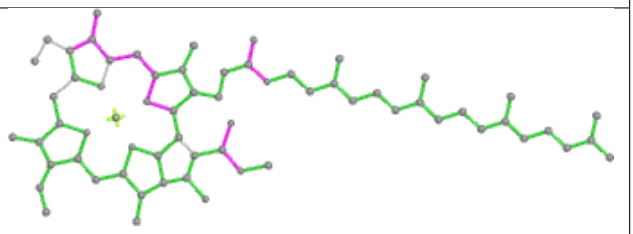


Rings

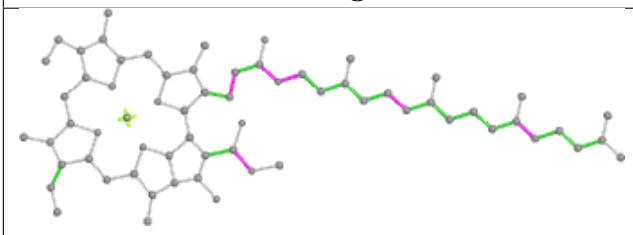
Ligand CLA a 855



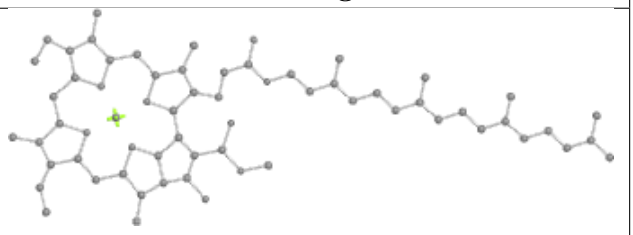
Bond lengths



Bond angles

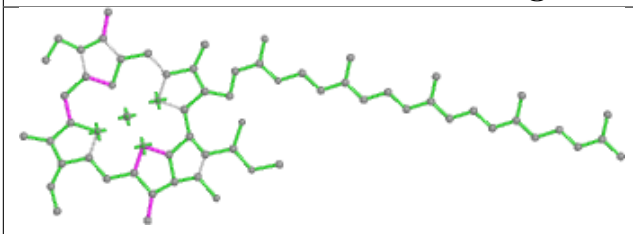


Torsions

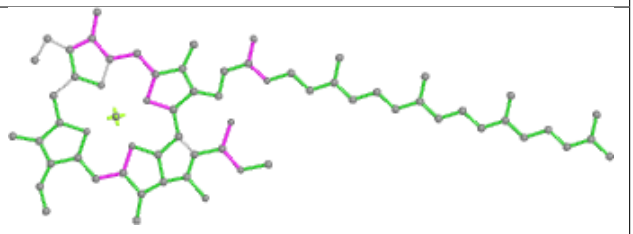


Rings

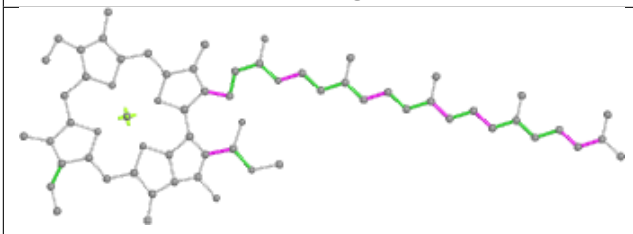
Ligand CLA a 818



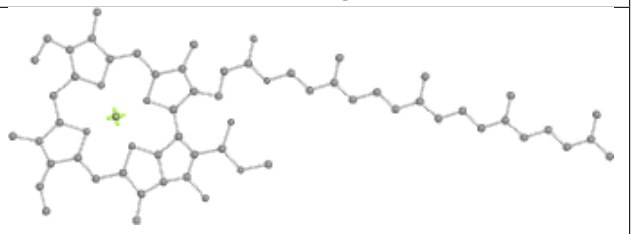
Bond lengths



Bond angles

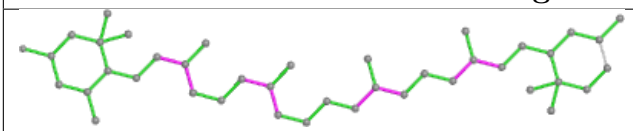


Torsions



Rings

Ligand ZEX f 205



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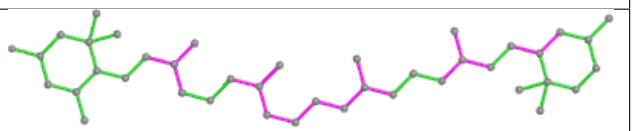
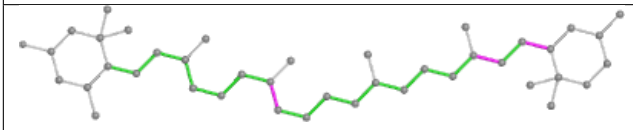


Bond angles



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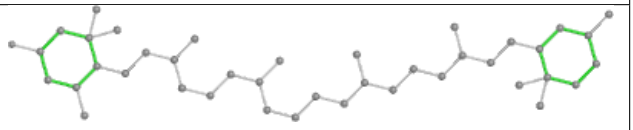
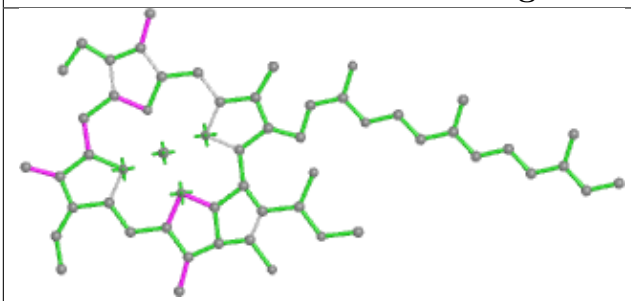


Rings

Ligand CLA b 3010



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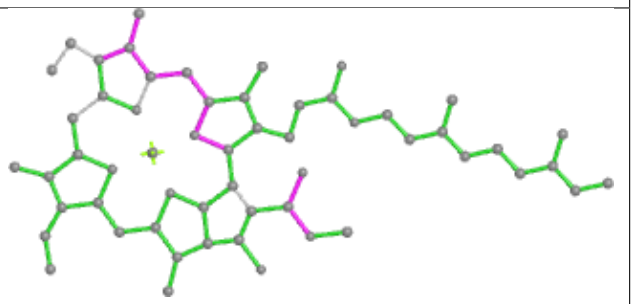
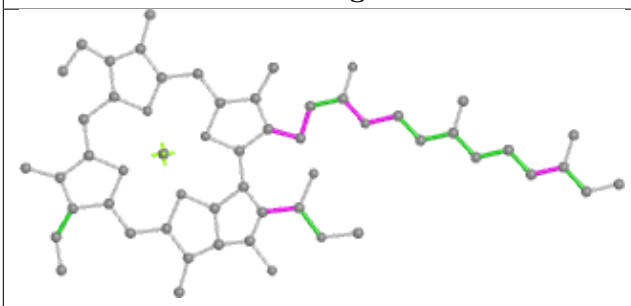


Bond angles



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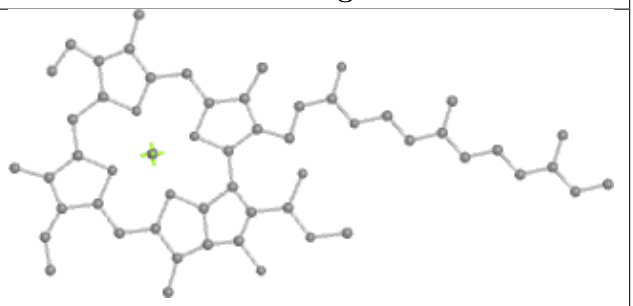
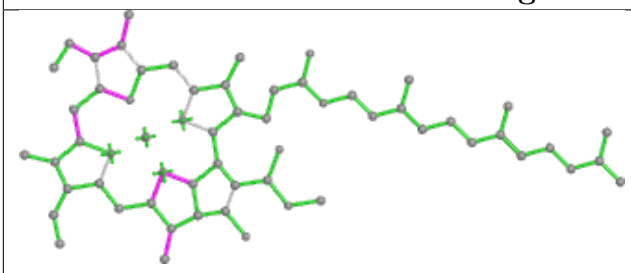
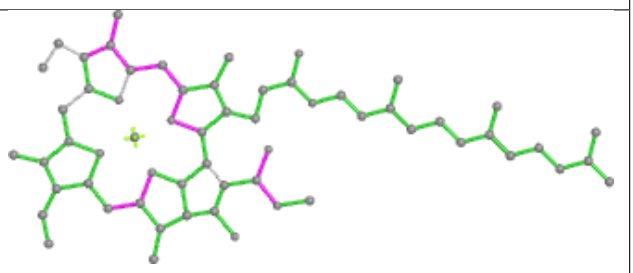


Rings

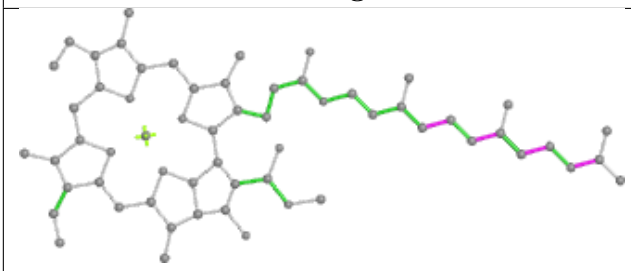
Ligand CLA b 3019



Bond lengths



Bond angles



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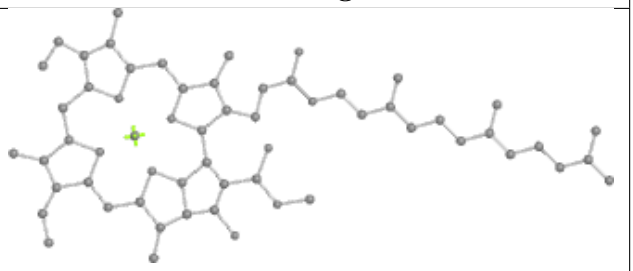
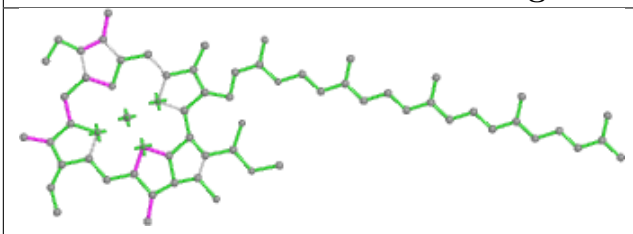


Rings

Ligand CLA a 836



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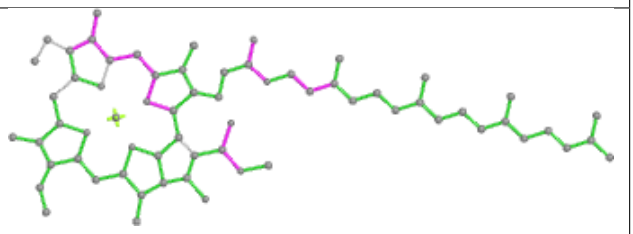
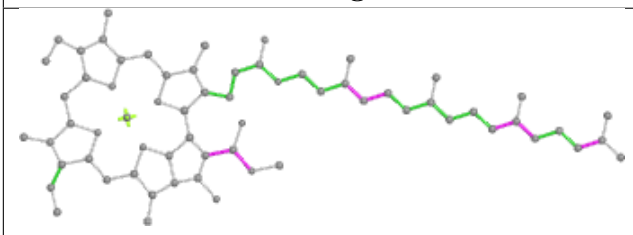
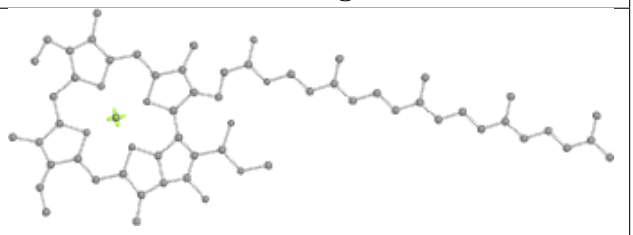


Bond angles

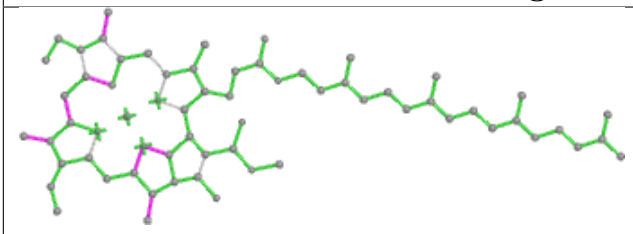


Torsions

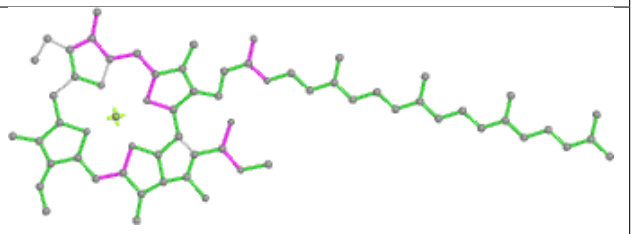


Rings

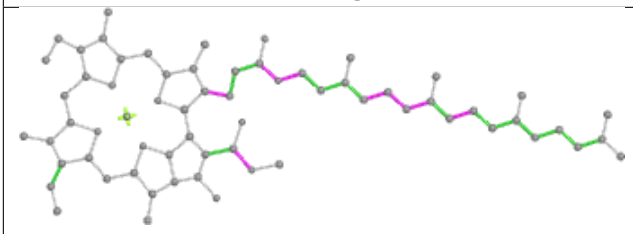
Ligand CLA a 841



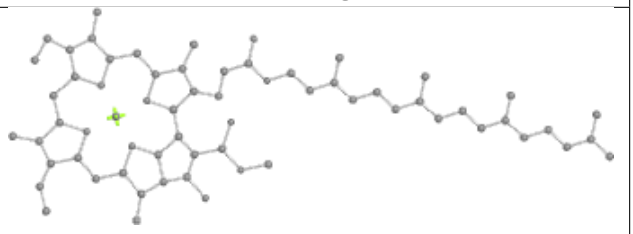
Bond lengths



Bond angles

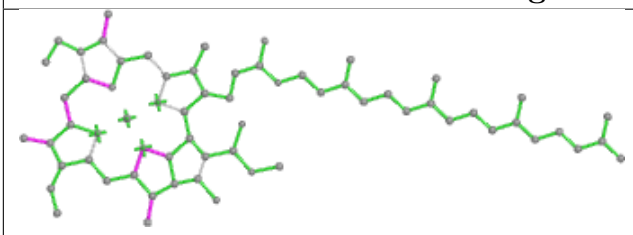


Torsions

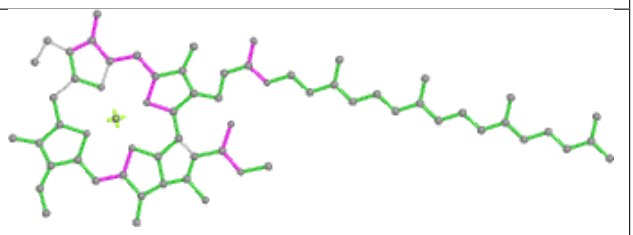


Rings

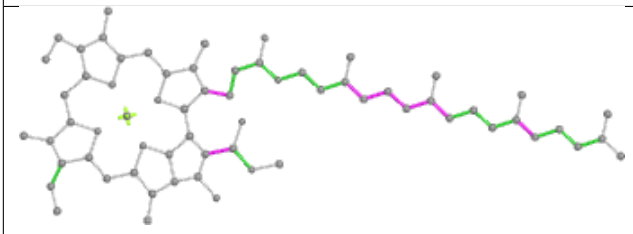
Ligand CLA a 827



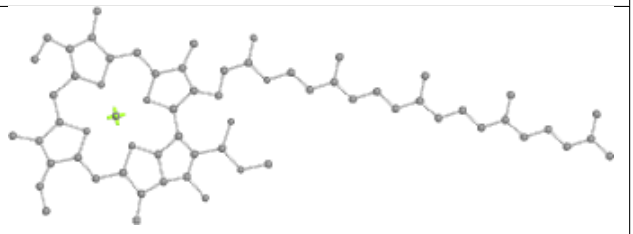
Bond lengths



Bond angles

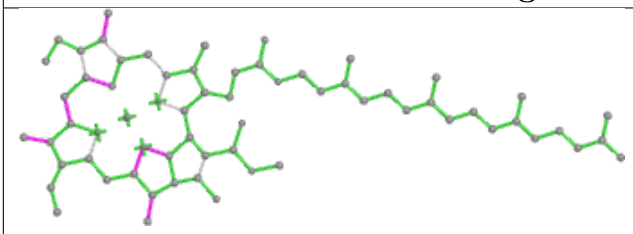


Torsions



Rings

Ligand CLA b 3033



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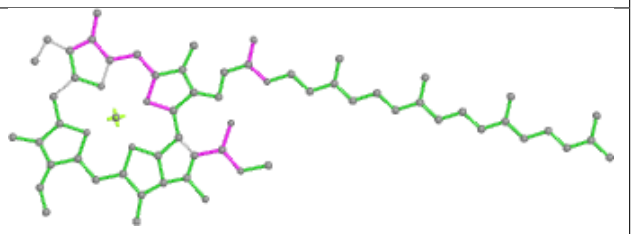
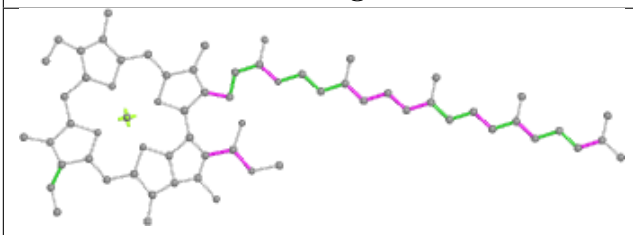


Bond angles



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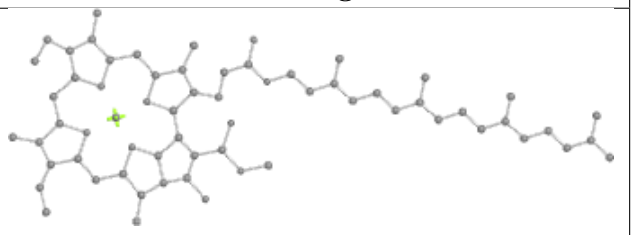
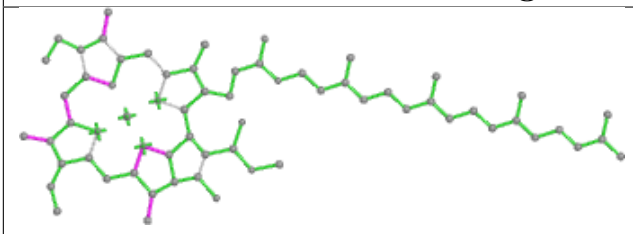
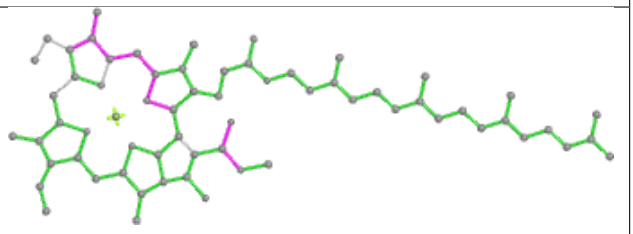


Rings

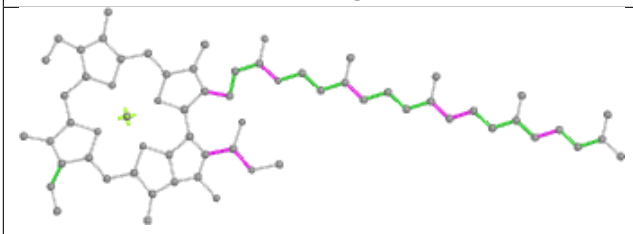
Ligand CLA b 3027



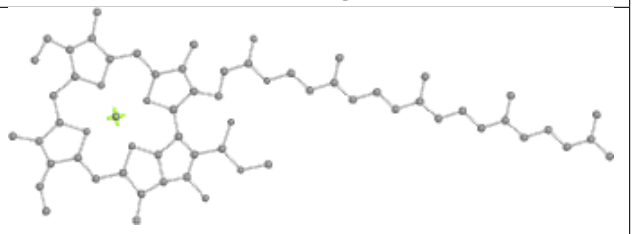
Bond lengths



Bond angles

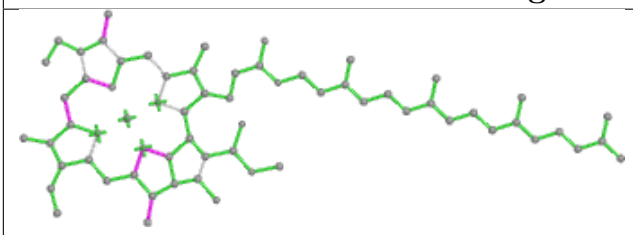


Torsions

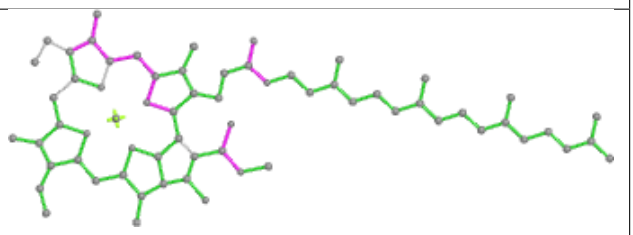


Rings

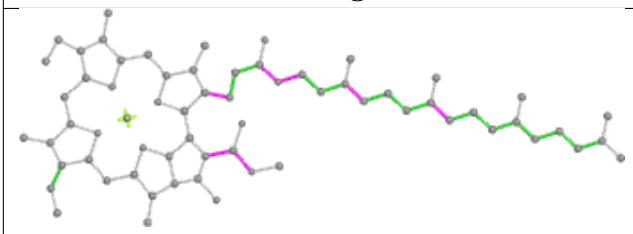
Ligand CLA a 823



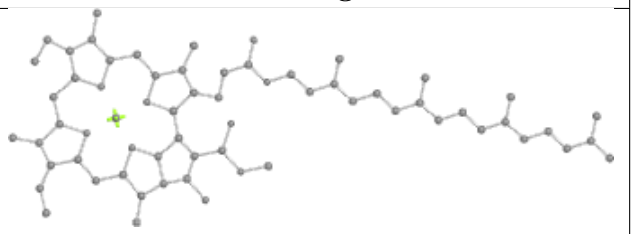
Bond lengths



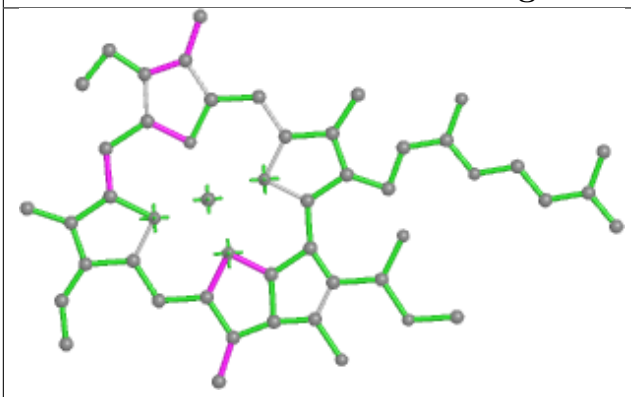
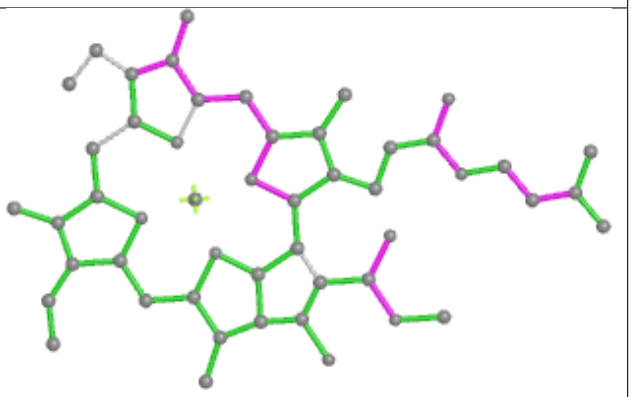
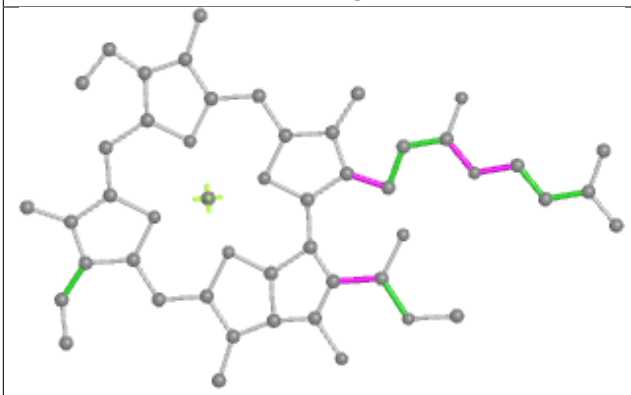
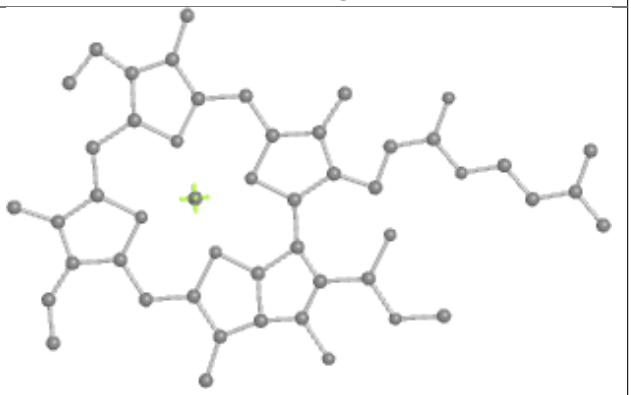
Bond angles

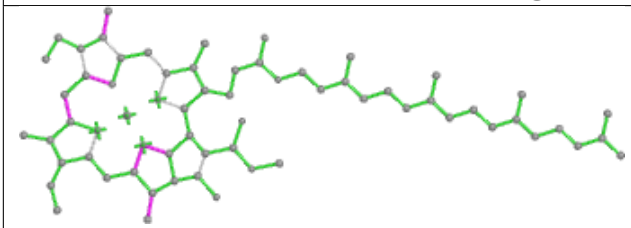
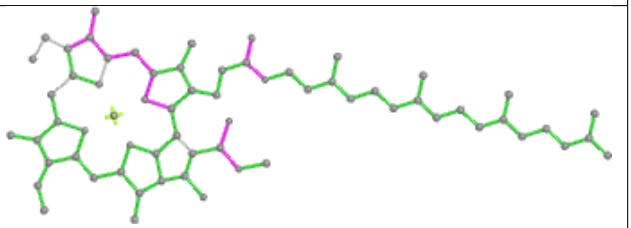
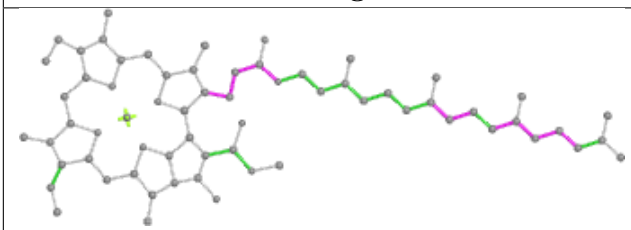
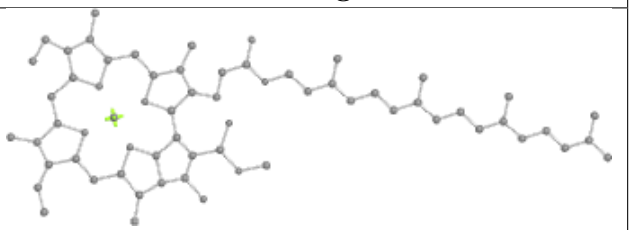


Torsions

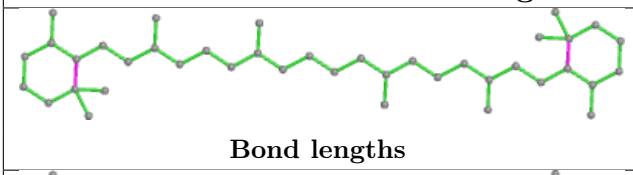


Rings

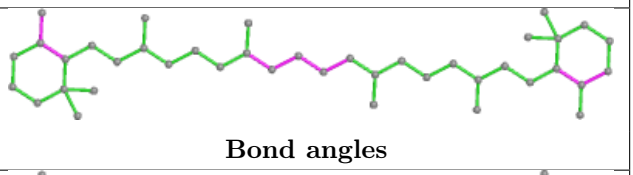
Ligand CLA b 3038	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 812	
 Bond lengths	 Bond angles
 Torsions	 Rings

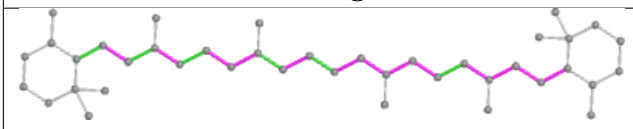
Ligand BCR b 3048



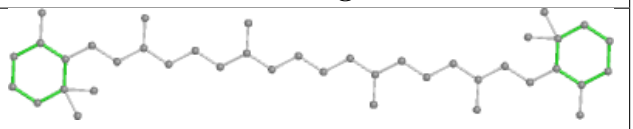
Bond lengths



Bond angles

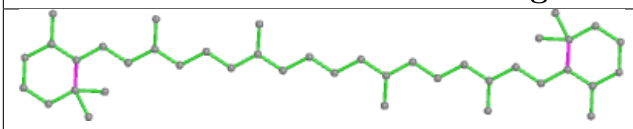


Torsions

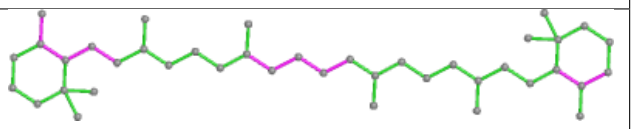


Rings

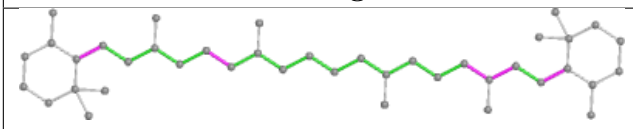
Ligand BCR i 101



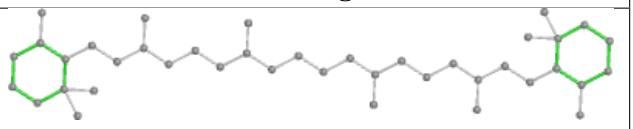
Bond lengths



Bond angles

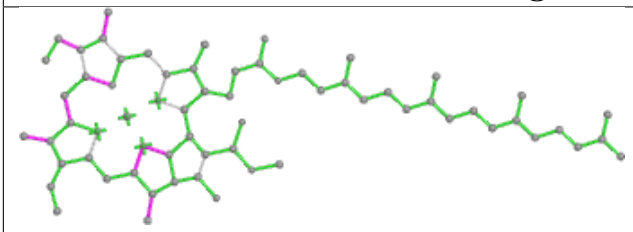


Torsions

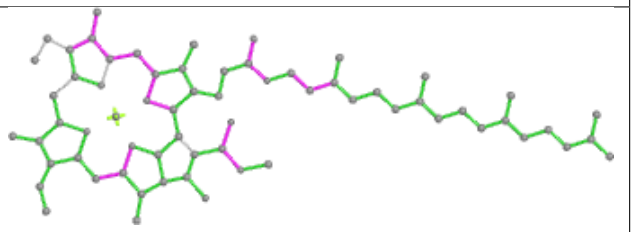


Rings

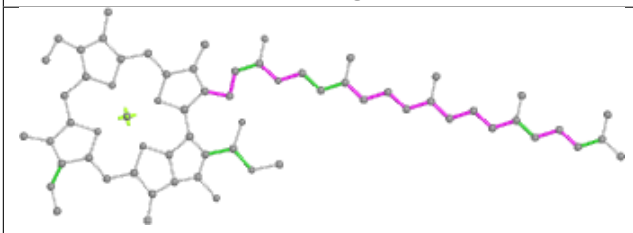
Ligand CLA a 809



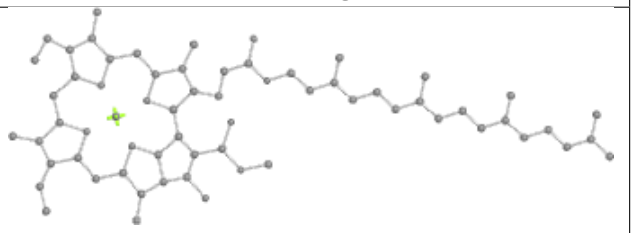
Bond lengths



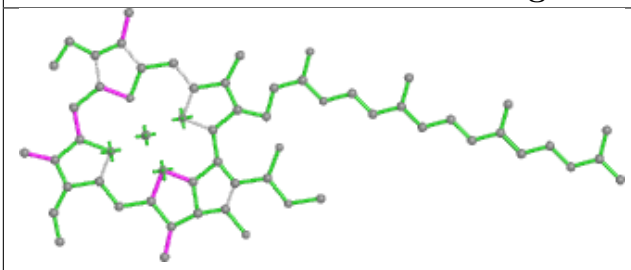
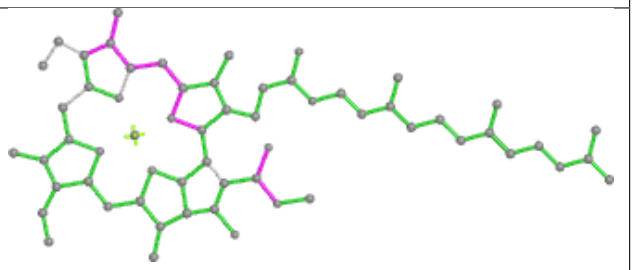
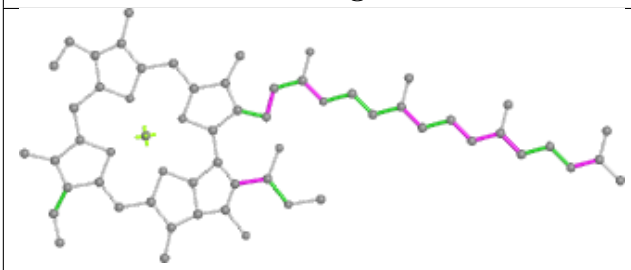
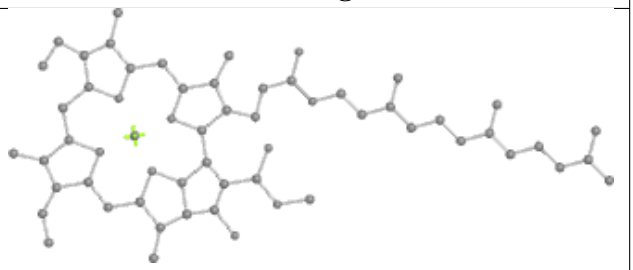
Bond angles

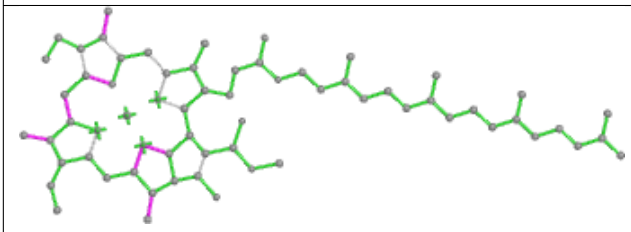
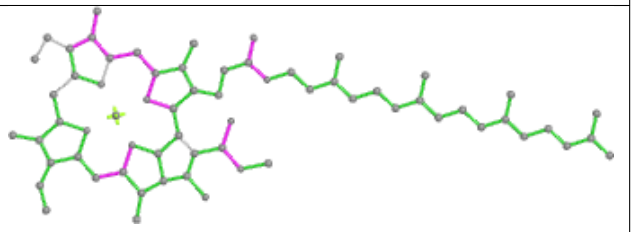
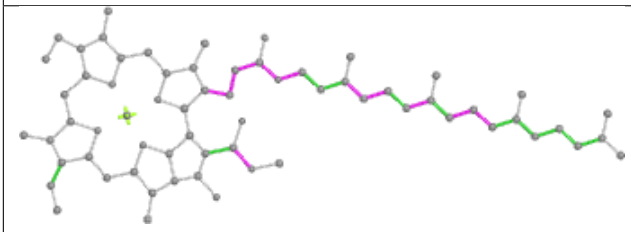
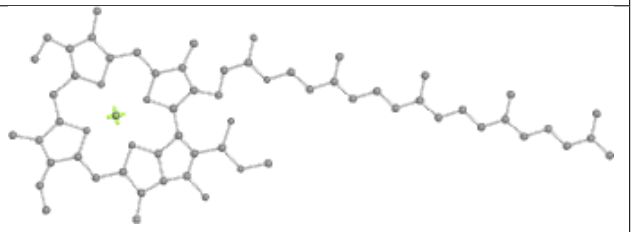


Torsions

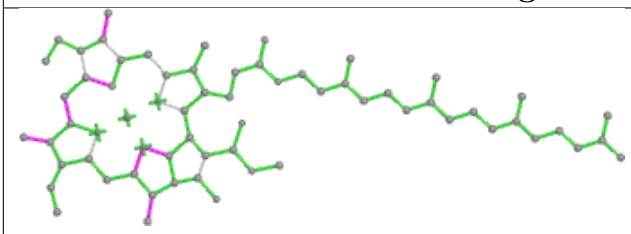


Rings

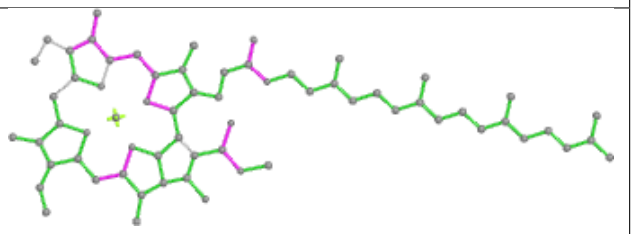
Ligand CLA a 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 3004	
	
Bond lengths	Bond angles
	
Torsions	Rings

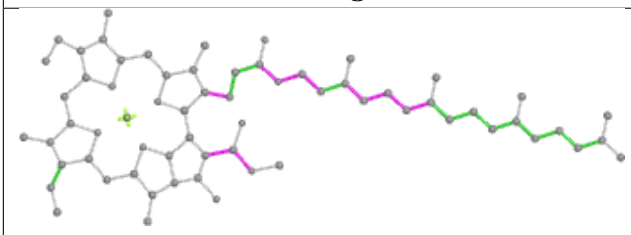
Ligand CLA b 3037



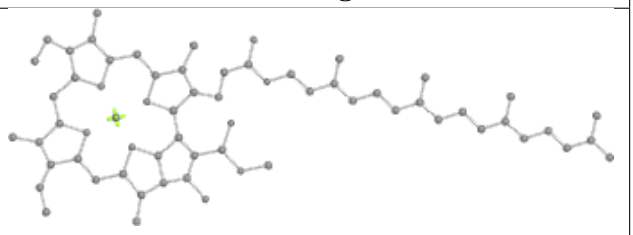
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

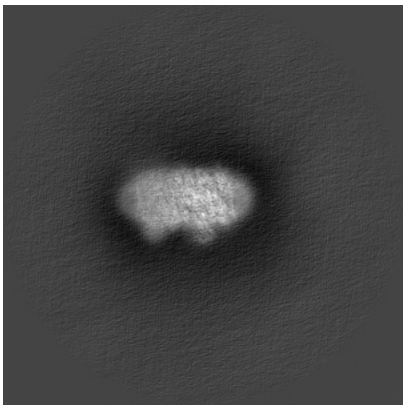
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15618. These allow visual inspection of the internal detail of the map and identification of artifacts.

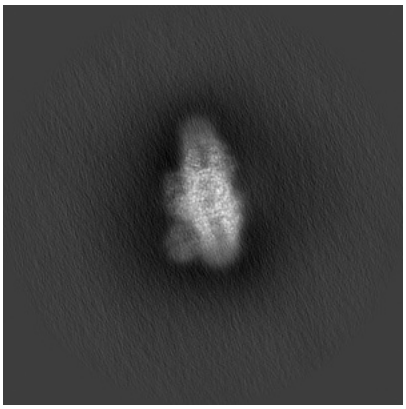
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

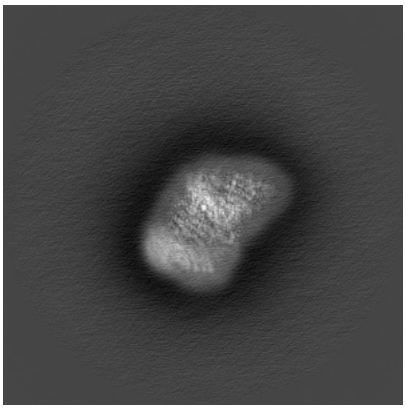
6.1.1 Primary map



X

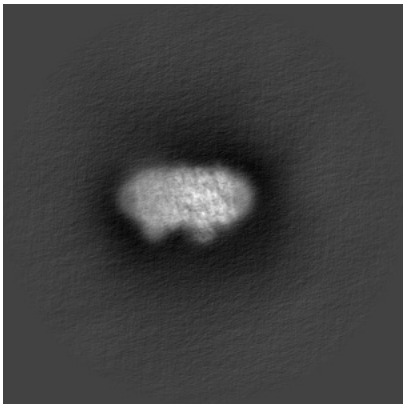


Y

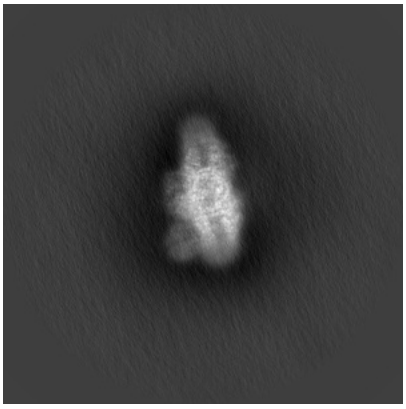


Z

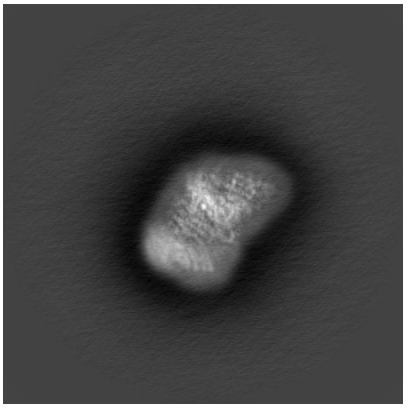
6.1.2 Raw map



X



Y

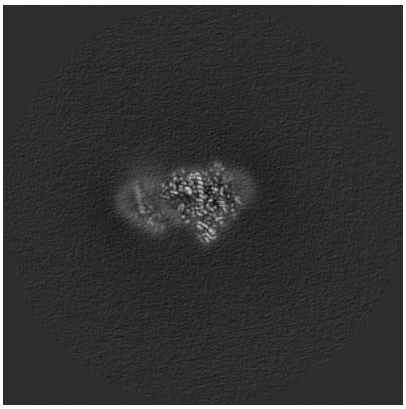


Z

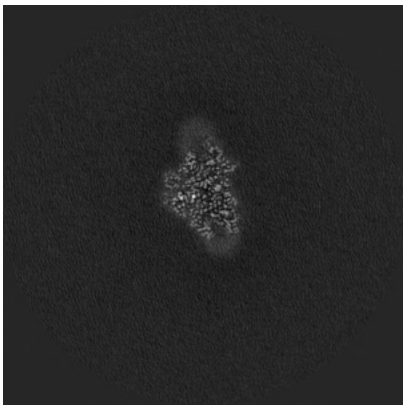
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

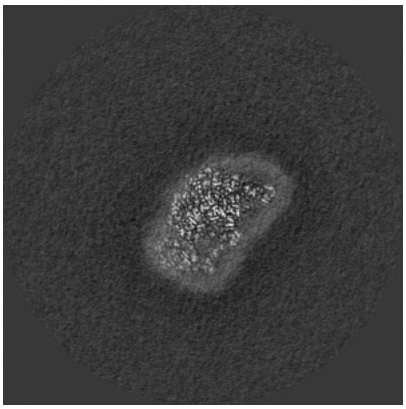
6.2.1 Primary map



X Index: 200

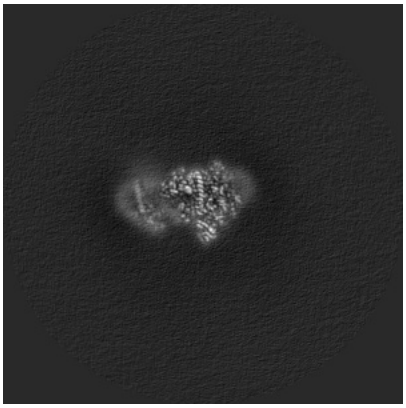


Y Index: 200

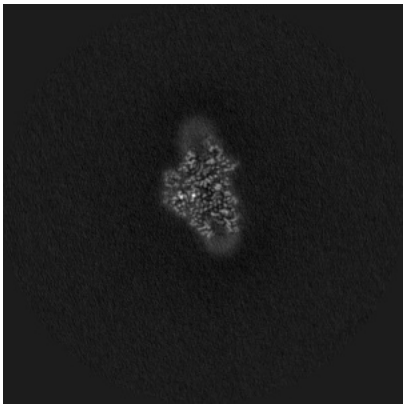


Z Index: 200

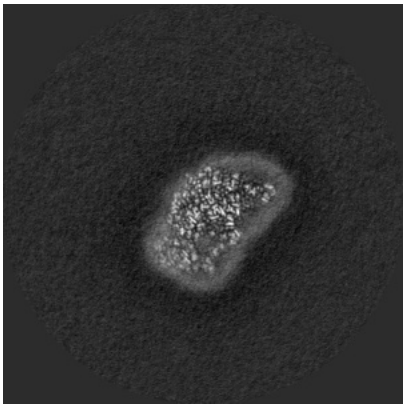
6.2.2 Raw map



X Index: 200



Y Index: 200

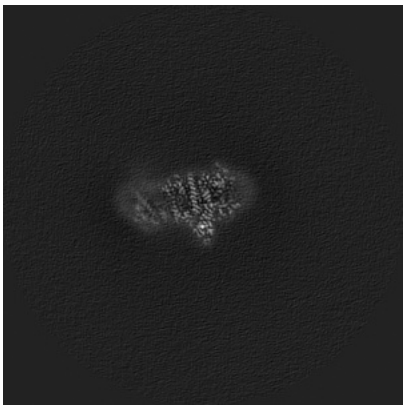


Z Index: 200

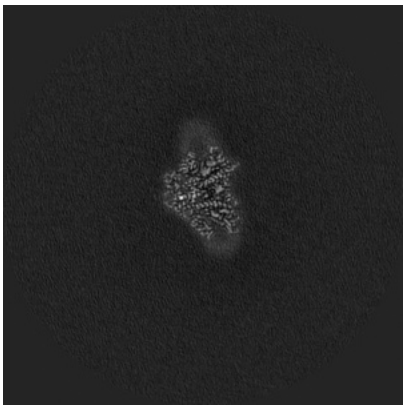
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

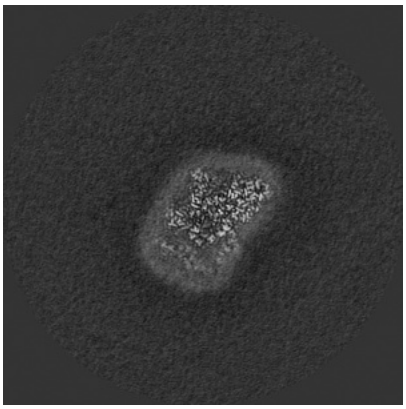
6.3.1 Primary map



X Index: 206

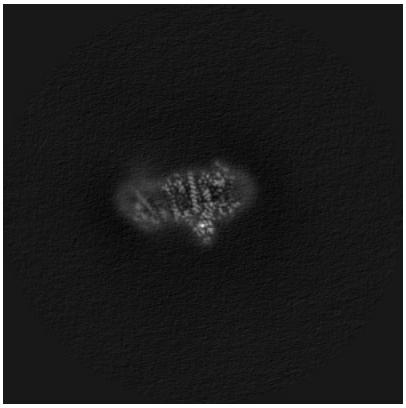


Y Index: 199

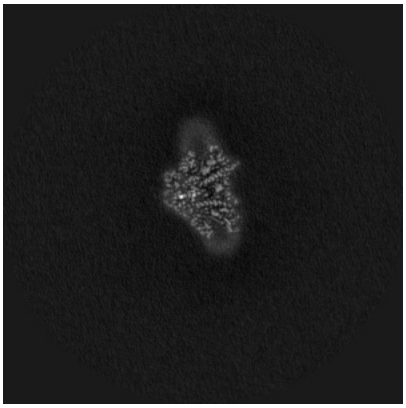


Z Index: 210

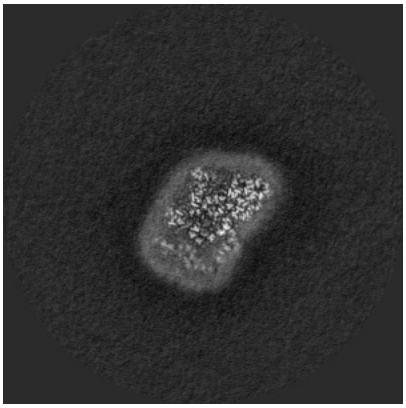
6.3.2 Raw map



X Index: 206



Y Index: 199

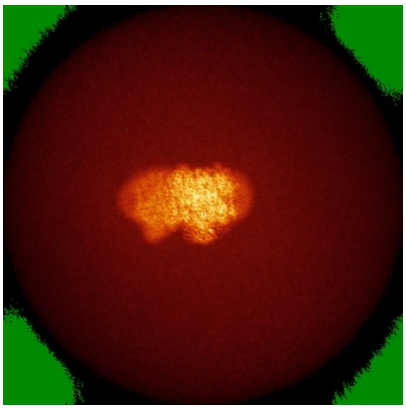


Z Index: 210

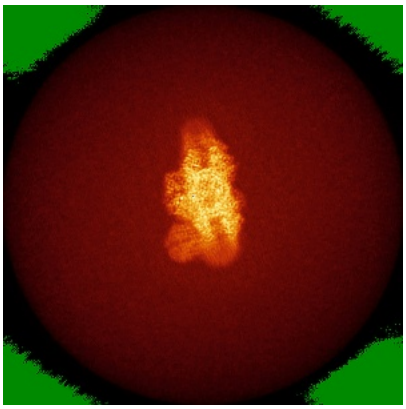
The images above show the largest variance slices of the map in three orthogonal directions.

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

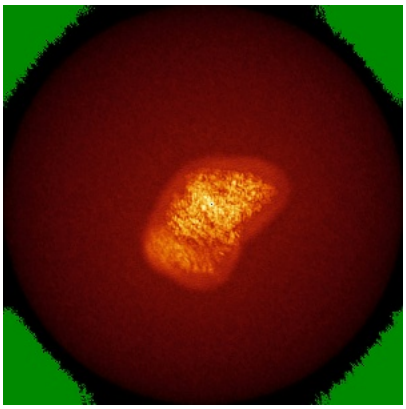
6.4.1 Primary map



X

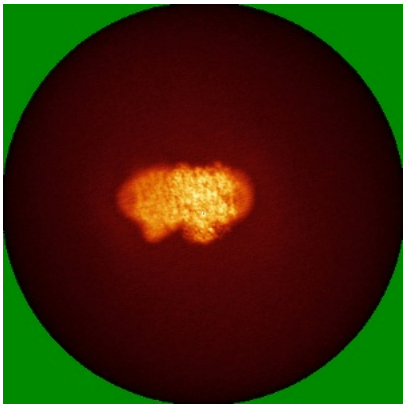


Y

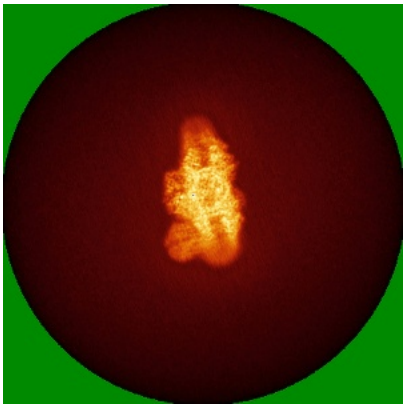


Z

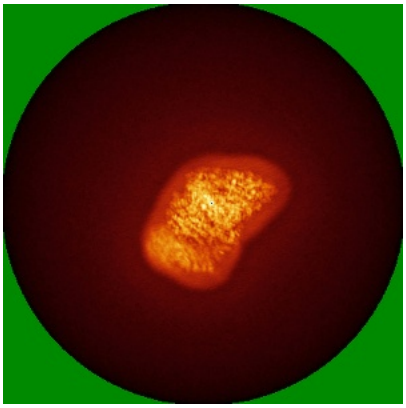
6.4.2 Raw map



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.

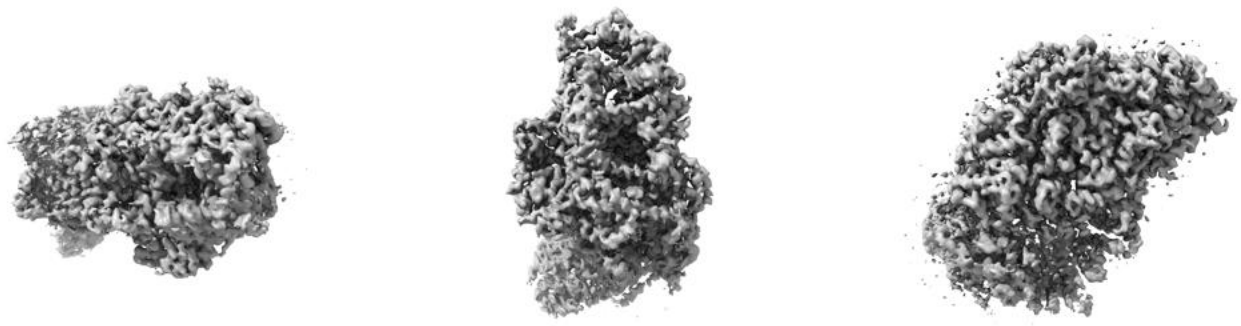
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0801. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

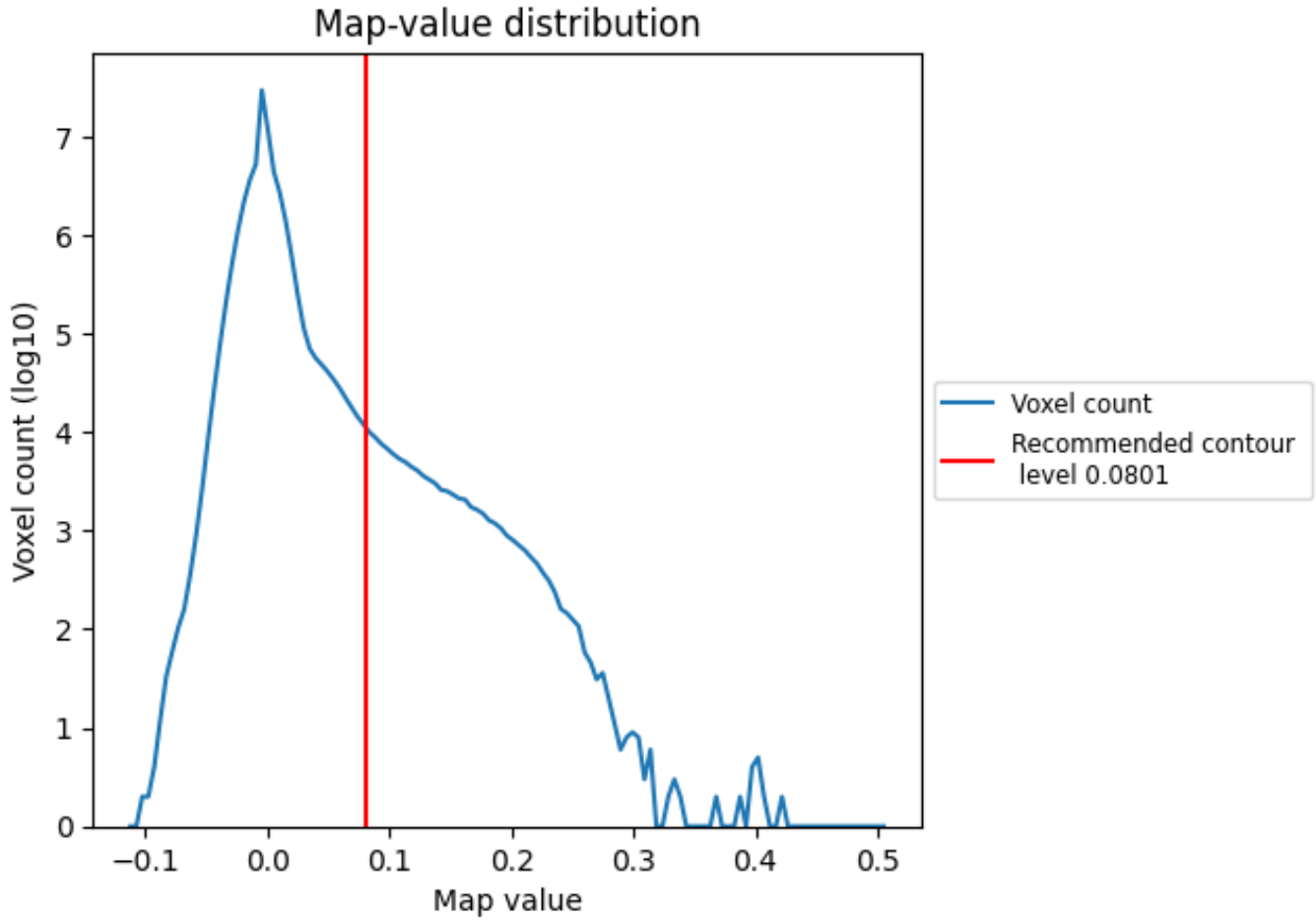
6.6 Mask visualisation (i)

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

7 Map analysis

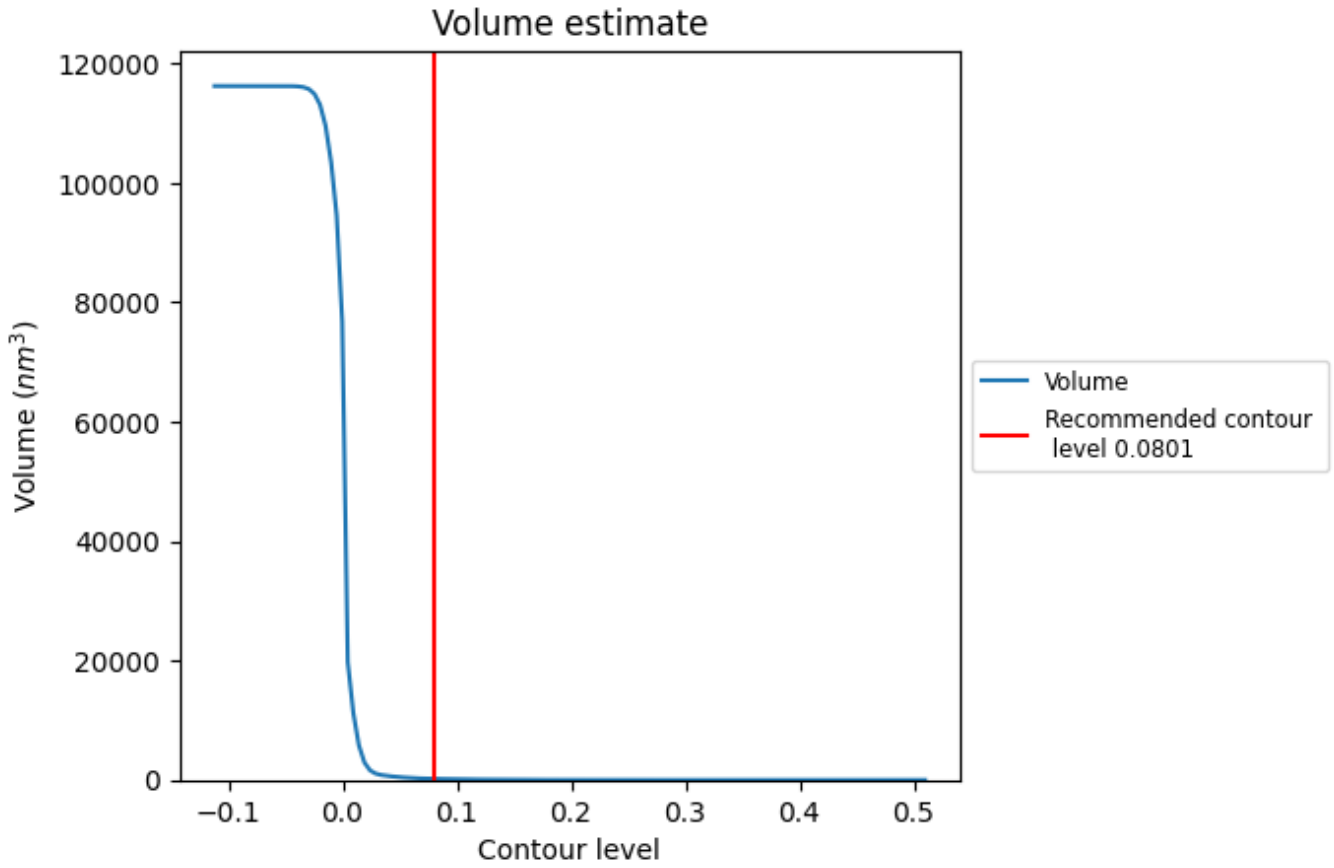
This section contains the results of statistical analysis of the map.

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.

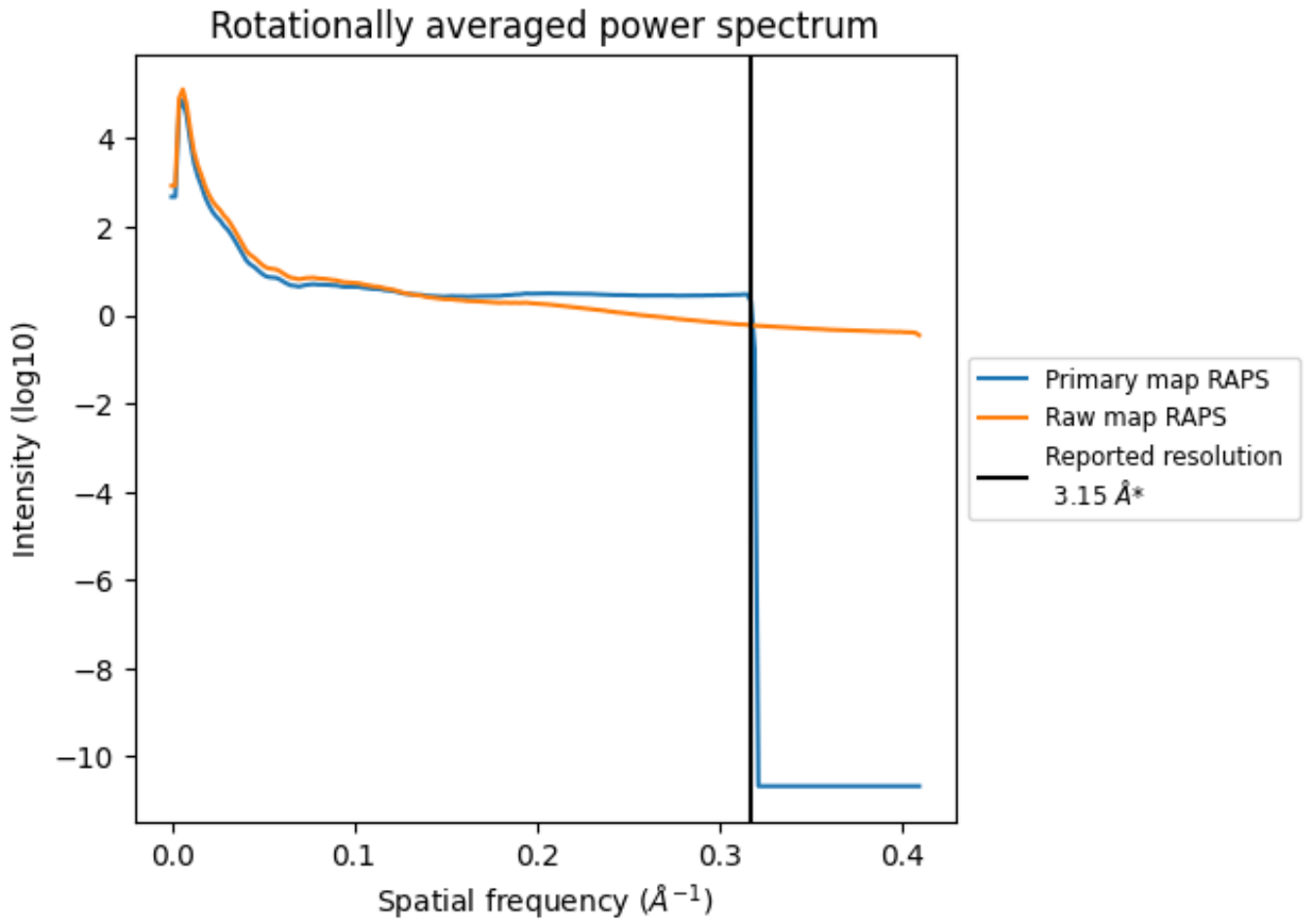
7.2 Volume estimate



The volume at the recommended contour level is 187 nm^3; this corresponds to an approximate mass of 169 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)

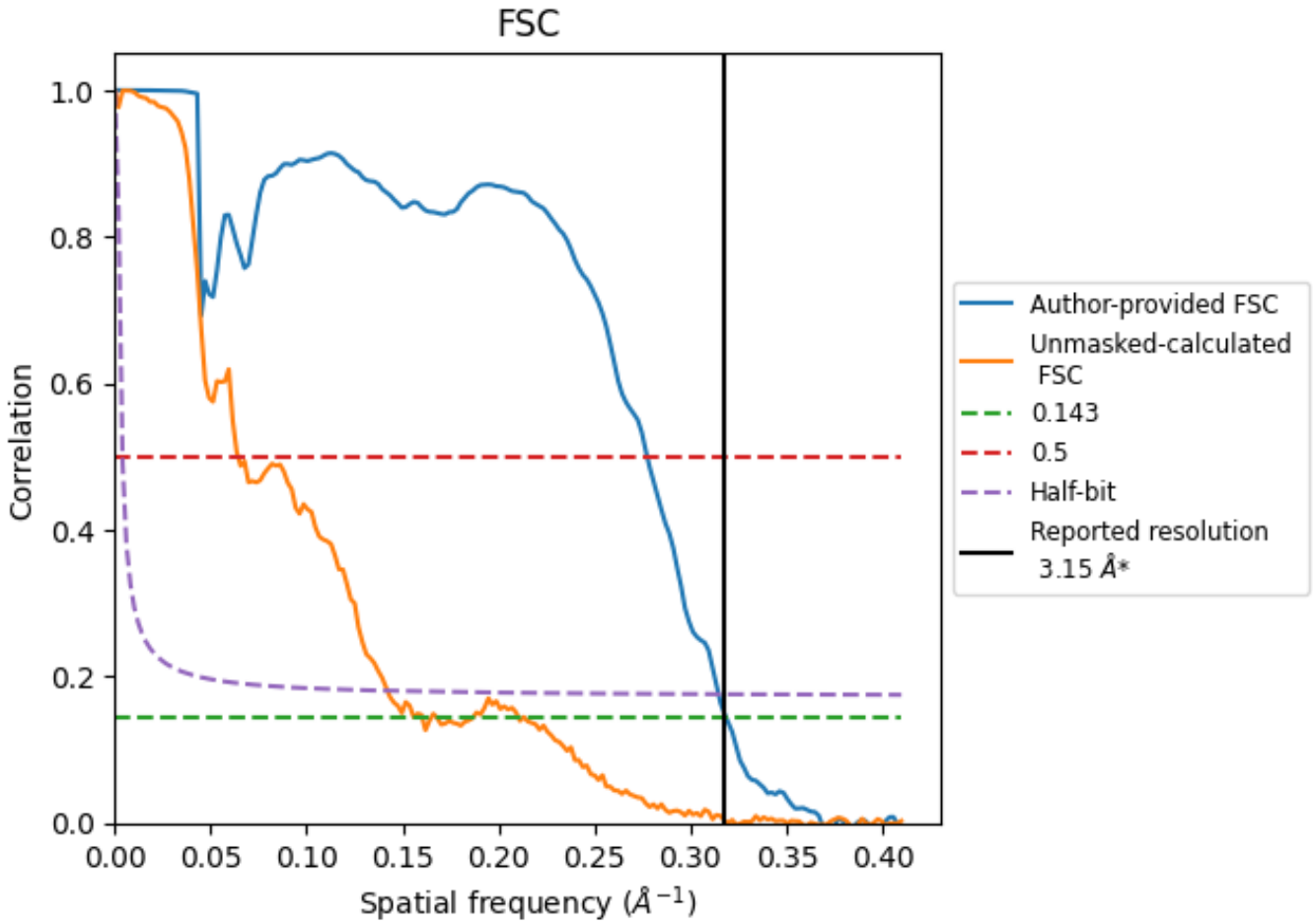


*Reported resolution corresponds to spatial frequency of 0.317 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.317 Å^{-1}

8.2 Resolution estimates (i)

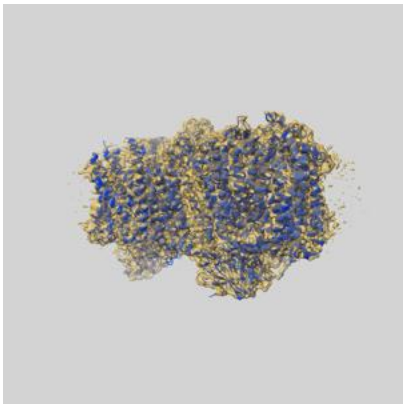
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	3.14	3.60	3.18
Unmasked-calculated*	6.24	15.58	7.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.24 differs from the reported value 3.15 by more than 10 %

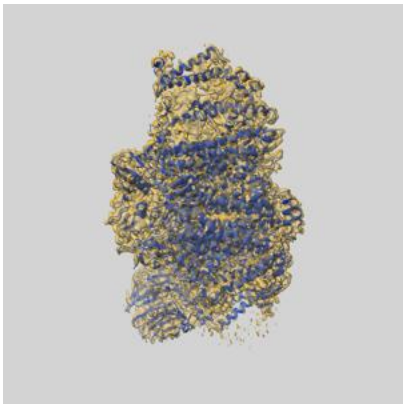
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15618 and PDB model 8ASL. Per-residue inclusion information can be found in section 3 on page 24.

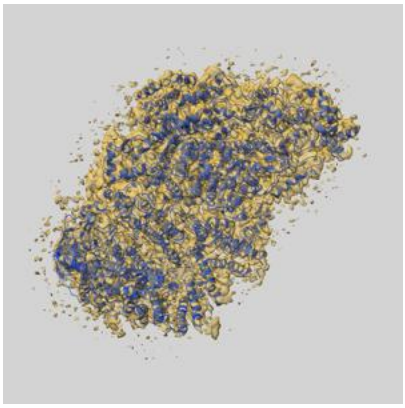
9.1 Map-model overlay



X



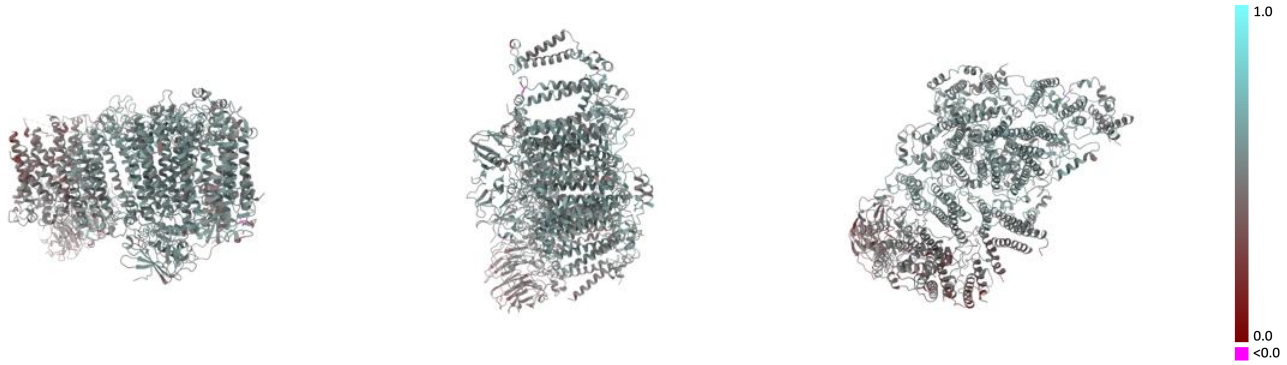
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0801 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.

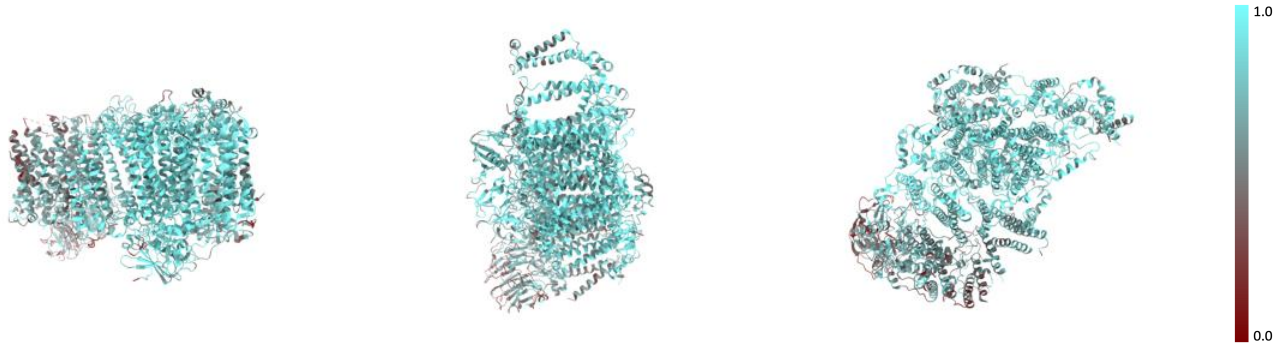
9.2 Q-score mapped to coordinate model (i)



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.

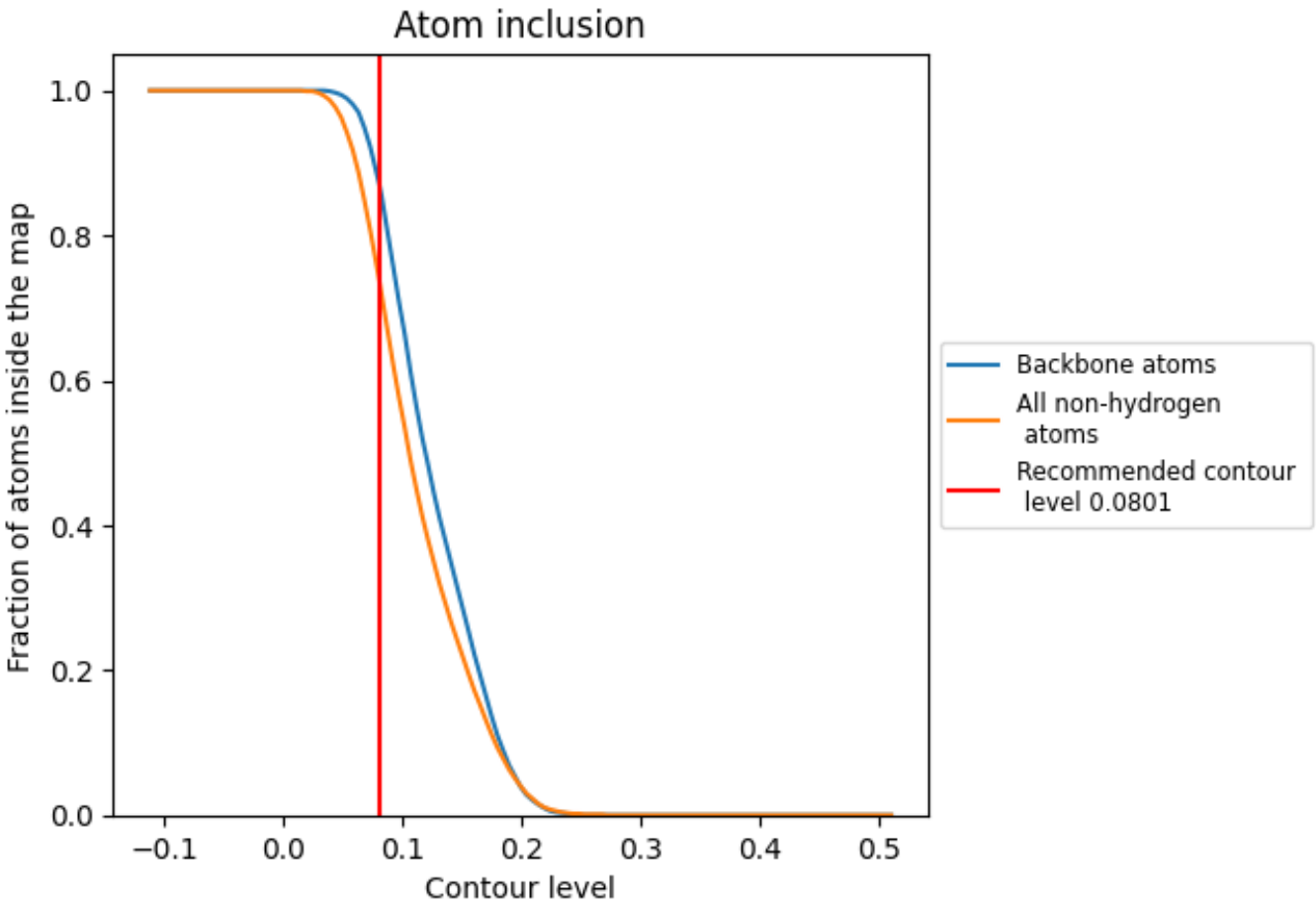
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0801).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 74% 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 (0.0801) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7400	0.5180
A	0.6210	0.4580
D	0.5850	0.4470
E	0.6500	0.4520
F	0.6210	0.4440
I	0.4290	0.3910
S	0.5100	0.3970
a	0.8130	0.5560
b	0.8260	0.5550
c	0.9200	0.5460
d	0.8060	0.5380
e	0.7670	0.5320
f	0.6810	0.5230
i	0.7550	0.5400
j	0.6140	0.4920
k	0.6310	0.5060
l	0.7110	0.4970
m	0.7360	0.5420